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Testing the JRC TIM Tools to identify emerging chemical risks

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Abstract

Identification of emerging risks in food and feed is a legal obligation for EFSA. Horizon scanning of large data sets can give a useful contribution to this mission. The Joint Research Centre (JRC) has developed two data intelligence tools: Medisys for real-time news analysis of medical and health related topics and TIM Technology for data analytics and knowledge extraction from scientific publications, patents, EU projects, etc. None has been evaluated for its capability to identify emerging chemicals in the food chain in the EU. Both tools were customized and tested in a first phase of two years to test their efficiency and relevancy for this purpose. A screening workflow has been set-up to identify relevant hits. Key words and search strings have been defined, achieving a good compromise between retrieval of useful documents and false positives. Relevant results will be evaluated and validated in collaboration with the EFSA Working Group on emerging chemical risks identification and the Emerging Risks Exchange Network (EREN).

Key words: emerging risks, chemicals, food, feed, environment, hazard

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Summary

Emerging chemical risks may arise from intentional or unintentional contamination of the food chain either by anthropogenic or “natural” chemicals. It is in the EFSA’s remit to identify those risks through systematic processes. Following the REACH regulation for registration, evaluation and authorization of chemicals, a prioritization of substances was done in previous EFSA projects. Substances were assessed and scored for environmental release, biodegradation, bioaccumulation in food/feed and chronic human health hazards. Prioritisation based on the scores assigned and additional data curation steps identified 212 substances that were considered potential emerging risks in the food chain. As a follow-up and in an effort to improve EFSA’s preparedness for future chemical risk assessments new methodologies on horizon scanning are being proposed. JRC has developed the TIM analytics tool[1], specifically “TIM Technology” for extracting knowledge from structured data such as scientific publications (Elsevier-Scopus), patents (European Patent Office- PATSTAT) and EU funded projects (CORDIS) and “TIM News” which analyses media aggregated by the Europe Media Monitor system (EMM)[2], more specifically the news articles collected by a special instance of EMM focusing on health and safety sources, called Medisys[3]. Through a 2-year pilot project, EFSA has screened 60 chemicals through TIM Technology and TIM News. Those 60 chemicals are the top scored ones out of the 212 prioritized substances based on the EFSA REACH projects. EFSA has also used TIM to screen “Newly identified chemicals”. The search strings used to retrieve scientific publications and news articles for all those categories have been developed through several iterations between JRC and EFSA and the criteria for screening have been agreed. Moreover, a customization of the TIM environments has been performed including a marking system for the screening experts, a removal of duplicates, customized visualisations, etc. The screening of the outputs was performed in two phases: EFSA screening first and then experts ‘screening, with the second one using an additional screening tool (Distiller SR[4]). To evaluate the usefulness of TIM to identify emerging chemical risks, the ratio between the number of articles considered relevant in the screening phase and the number of articles retrieved was calculated.

[1] EU, Joint Research Centre, *TIM Analytics*, http://www.timanalytics.eu/
[2]Europe Media Monitor (EMM), https://knowledge4policy.ec.europa.eu/text-mining/topic/europe-media-monitor-emm_en
[3] https://publications.jrc.ec.europa.eu/repository/handle/JRC45523
[4] https://www.distillersr.com/

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1 Introduction

1.1 Background and Terms of Reference as provided by the requestor

The European Food Safety Authority's (EFSA) Founding Regulation (EC) No 178/2002[5], in its Articles 23f and 34, requires EFSA to undertake actions to identify and characterise emerging risks, in the fields within its mission and, to that purpose, to establish monitoring procedures for systematically searching for collecting, collating and analysing information and data.

In the context of emerging chemical risks identification, an 'emerging risk' to human, animal and/or plant health and the environment is understood as:

1) new hazard (new adverse effect in a known chemical or new chemical with an adverse effect) to which significant exposure may occur
2) new or increased exposure (environmental contamination, increased production and/or use) to a known hazard,
3) new driver and
4) new susceptible group.

Emerging chemical risks may arise from intentional or unintentional contamination of the food chain either due to naturally occurring contaminants in the environment or to contaminants artificially introduced by human. It is in the EFSA's remit to identify those risks through systematic processes. Oltmanns at al., (2019) applied a procedure for the identification of potential emerging chemical risks in the food chain associated to substances registered under the REACH Regulation that was previously developed and tested in EFSA-sponsored pilot study (EFSA, 2014). The selection of the substances was limited to those that a) were registered with a full registration, b) met eligibility criteria (e.g. availability of a CAS number and a SMILES notation) and c) were considered to be inside the applicability domain of the models used in this study (excluding e.g. ionisable compounds and metals). By using these criteria, the selection of the substances was reduced from 15000 to 2336. Subsequently, the 2336 substances were assessed in four blocks: environmental releases (based on tonnage and use pattern), biodegradation (using BIOWIN predictions assessed in a battery approach), bioaccumulation in food and feed (using ACC-HUMAN steady modelling) and toxicity (based on classification for carcinogenicity, mutagenicity, reprotoxicity and repeated dose toxicity). After that, a prioritisation of the substances was conducted and 212 potential emerging chemicals were identified that are considered a) to be released to the environment and/or poorly biodegraded, b) bioaccumulate in food/feed and c) to represent a chronic human health hazard (Oltmanns et al., 2019).

The Emerging Chemical Risks Identification Working Group (ECRI WG) has been established to (1) carry out activities to identify emerging chemical risks in food and collect additional data

[5] Regulation (EC) No 178/2002 of the European Parliament and of the Council of 28 January 2002 laying down the general principles and requirements of food law, establishing the European Food Safety Authority and laying down procedures in matters of food safety.

regarding identified emerging chemical issues[6]; and (2) develop, test, and improve current horizon scanning methodologies and approaches. The ECRI WG aims at supporting both activities through two projects:

5) Screening for emerging chemical risks in the food chain (SCREENER project, OC/EFSA/SCER/2020/02),
6) Testing the JRC Tool for Innovation Monitoring (TIM) to identify emerging chemical risks.

In this document, the project on "Testing the JRC Tool for Innovation Monitoring (TIM) to identify emerging chemical risks" is reported.

A multi-source retrospective analysis of historic food safety risks found that public awareness is often preceded by early signals in publications of food safety authorities and the scientific literature (Van De Brug et al., 2014). The detection and recognition of early signals of food safety risks in the scientific literature is challenging, as those signals are hidden in the sheer amount of publications, making manual screening impossible. In addition, traditional literature searches are prone to overlook potentially important information, because they do not capture all the synonyms and language variations. One possible solution to address this challenge is to use computer-based understanding of human language. This allows the scanning of vast amounts of textual data and the extraction of relevant information in an automated, fast, and reproducible manner. In addition, text mining allows to extract not only the relevant terms, but also relationships between terms.

Therefore, horizon scanning, as a systematic process for capturing and monitoring change, possibly with the support of artificial intelligence to scan large data sets, can give a useful contribution to EFSA's mission to identify emerging chemical risks.

Two data intelligence tools developed by JRC have been used in the context of this project: "TIM News", using news articles from the JRC Medical Information system (Medisys) as database of documents and allowing real-time news analysis of medical and health related topics, and "TIM Technology" using scientific publications, patents and EU projects as databases of documents and allowing building data visualisations and extracting knowledge. None has been evaluated for its capability to identify emerging chemicals in the food chain in EU.

1.1.1 TIM Analytics[7]

Through the use of several TIM tools, the JRC supports policy makers with analyzing large and/or complex sets of data. This is done through various means like by developing customized data analytics IT systems, providing online dashboards to explore data, coaching and supporting in interpretation of data visualizations generated by TIM tools, or the delivery of technical reports on specific issues. Text mining and machine learning techniques are used to enrich the datasets injected in TIM e.g., for named entity recognition, geolocation, measurement of semantic similarity or extraction of keywords from raw text content. Various instances of TIM systems have been developed: TIM Technology that includes patents data, Cordis data, and proprietary

[6] Recognising that the available information is often insufficient to conclude whether a risk exists, EFSA subsequently introduced the term 'emerging issue' to describe cases in which 'the information collected is preliminary and too limited to be able to assess whether it is (or it could develop) into an emerging risk'

[7] https://knowledge4policy.ec.europa.eu/text-mining/topic/tim_analytics_en

data on scientific publications from Scopus; TIM Custom used for analytics on user specific datasets, TIM Open access granting free access to data (patents, cordis, semantic scholar, etc).

Another relevant tool is the so-called TIM News for the analysis of newsfeeds provided by the Europe Media Monitor (EMM) [8].

TIM News is based on EMM, whose mission is to deliver independent, relevant information about facts and opinions extracted from on-line media to EU policy makers at all levels.

EMM9 started in 2002 to complement official sources with Internet media monitoring and to send alerts, mainly about political events, to media analysts of the European Commission informing spokespersons and decision makers. It has evolved into a fully automatic software system that gathers an average of 400,000 online news articles per day in up to 80 languages and is now serving several EU bodies and international organisations such as WHO (epidemic intelligence) and African Union (Continental Early Warning System). EMM has extended its scope from socio-political events monitoring to a wider range of domains including natural disasters, public health threats & food safety, conflict early warning, border security, crime, science and innovation.

The EMM-NewsBrief collects related articles, classifies them into thousands of categories, detects stories, extracts information on persons, organisations and locations, produces statistics, performs sentiment and emotion analysis and more. Since the beginning, EMM applications were designed to be as multilingual as possible because language diversity is integral part of the European Union context and because the content found across different languages is complementary.

The system, developed at the JRC in Italy, currently monitors a carefully selected set of about 15,000 web sites.

1.1.2 TIM tools for EFSA

EFSA has explored the potential offered by TIM in the context of the emerging risk activities for the following reasons: (1) not only scientific literature databases are screened, but also EU research project and patent databases. This is particularly interesting to identify new trends in product development, emerging technologies, new food compositions which may be prone to emerging risks; (2) the search strategy functions offers more options than the traditional literature search databases e.g. the tool has also “enrichment” functions whose aim is to reduce the duplication, redundancies and the noise; (3) the tool offers many useful quantitative analysis and visualisation functionalities e.g. time series analysis, cluster effects and the possibility to export data for further analysis.

For the horizon scanning exercise of a selection of 60 prioritized chemicals as well as newly identified chemicals (referred as “Unknown” in the appendices) in media reports and scientific publications, a Service Level Agreement between JRC and EFSA was signed, aiming at collecting and visualising papers and news from TIM Technology and TIM News about the 60 known

[8] https://knowledge4policy.ec.europa.eu/online-resource/europe-media-monitor-emm_en https://emm.newsbrief.eu/
[9] https://emm.newsbrief.eu/overview/180614_EMM_170x240.pdf

emerging chemicals from REACH 2 project[10] and newly identified chemicals. In particular, this consists in the following activities:

- Build and configure the TIM Environment according to EFSA needs. This includes a) the design and test of search strategies for known and newly identified chemicals in TIM Technology and TIM News (cooperation JRC-EFSA) for retrieving relevant papers from peer-reviewed scientific literature (Scopus database) and news articles (from EMM); b) linking TIM to EMM and set up the visualisations related to news articles.
- Collecting peer-reviewed scientific publications (Scopus database) and news articles (through EMM).
- Quality control. JRC and EFSA have jointly set-up criteria for analysing & evaluating the quality of the search strategies both for TIM Technology and for TIM News (EMM), e.g. the relevancy/noise ratio.
- Co-design, test and assess specific indicators and visualisations to identify emerging risks or issues related to known and newly identified chemicals.

2 Data and Methodologies

2.1 Data

As a first step, EFSA provided JRC with a list of 60 chemical substances (see table 1) to focus on for this pilot exercise. Those chemicals are a subset of the 212 prioritized chemicals and specifically the top scored ones based on the REACH2 project (Oltmanns et al., 2019).

Embedded within TIM Technology, the Scopus database of scientific publications from Elsevier (covering 01/1996 to 12/2021) was used for retrieving scientific publications about the 60 chemicals. Scopus is Elsevier's abstract and citation database and covers nearly 36,377 scientific journals from approximately 11,678 publishers, of which 34,346 are peer-reviewed journals in top-level subject fields such as life sciences, social sciences, physical sciences and health sciences.

The news articles have been collected through the JRC software Europe Media Monitor (using the sources in Medisys and linked with TIM News), which monitors a carefully selected set of about 15,000 web sites. Scientific sources have been excluded from the list of websites to focus on the retrieval of news articles (see Appendix A for the list of sources excluded).

Table 1: The 60 substances monitored during this pilot project

1_3-Bis_citraconimidomethylene_benzene	hexabromocyclododecane
1_3-Dimethyl-3_4_5_6-tetrahydro-2_1H_-py	Melamine
1_3-Divinylimidazolidin-2-one	melamine_cyanurate
1-Propanone_2_methyl_1_4_methylthiopheny	Methyl_N-_3-acetylamino_-4-_2-cyano-4-ni

[10] https://www.efsa.europa.eu/en/supporting/pub/en-1597

2_3-dihydro-2_2-dimethyl-1h-pe	n_nprime-di-sec-butyl-p-phenylenediamine
2_4_-Diphenylmethane_diisocyanate	Paracetamol
2_4_hydroxy_benzophenone	paranitronaniline
2_5_diaminotoluene	phenol_2_2_-_1-methyl-1_2-ethanediyl_bis
2_chloroaniline	phenolphtaleine
2_naphtalenamine_etc	Phenylene-1_4-bis-benz-1_3-oxazin-4-one
3_4-Epoxycyclohexylmethyl_3_4-epoxycyclo	phenylnaphtylamine
4_4_-Methylenebis_2_chloroaniline_	Phosphorothioic_acid_OOO-triphenyl_ester
4_4_-Oxybis_benzenesulfonyl_hydrazide	Piperonyl_butoxide
4_4Bis-dimethylamino-4-methylamino_trity	propane_thiol
4_aminophenol	reaction_products_of_phosphorus_oxychlor
4-Chloro-2_5-dimethoxyacetoacetanilide	Retinol
9_10-anthraquinone	retinol_acetate
Antioxydant_2246	Retinol_proprionate
Bis_2_4-dichlorobenzoyl_peroxide	retinyl palmitate
Bis_2_6-diisopropylphenyl_carbodiimide	solvent_blue_35
Bisphenol_A	solvent_blue_4
butylated_hydroxyanisole	solvent_yellow_124
chloral_hydrate	Tegdme
chlorinated_paraffins	Tetrabromobisphenol_A
cyclonite	tetraethylene_glycol_ethyl_methyl_ether
Dicyclohexyl_phthalate	tk11-319
Diphenylmethane_2_2_diisocyanate	triphenylphosphine
diphenylmethane_diisocyanate	Triphenylphosphite
diuron	Tris_1_3-dichloro-2-propyl_phosphate
Glycerol_triglycidyl_ether	Trixylenyl_phosphate

2.2 Methodologies

2.2.1 Search strategies

The Medical Subject Headings (MeSH) entry terms and the Depositor-supplied synonyms that are listed in PubChem have been used to design the first search categories (one per chemical). These categories were refined by successive iterations between JRC and EFSA, with the goal of increasing the percentage of relevant articles and limit the number of false positives. This was achieved by:

- evaluating the proportion of relevant articles over the total number of articles retrieved.
- identifying keywords that were generating false positive results.

- adding host keywords to search string of chemicals retrieving an excessive number of articles (table 2).

Search strategies are detailed in the appendices for both news articles and scientific publications related to known chemicals (see Appendix B and C), as well as newly identified chemicals (see Appendix D and F).

Table 2: Host keywords: The main terms/organisms of interest being used in certain search strings independently of the chemical class.

Host	(algae OR air OR animal% OR aquaculture OR aquatic OR aqueous OR arthropod% OR bioaccumulat% OR bioconcentrat% OR biological+accumulation% OR biological+concentration% OR biological+interaction% OR biota OR bird OR birds OR cattle OR crop% OR dairy OR daphnid% OR ecological OR ecotoxic% OR ecosystem% OR effluent% OR environment% OR estuar% OR fauna OR fish OR fishes OR fishery OR food% OR freshwater% OR groundwater% OR incineration OR influent OR influents OR invertebrate% OR landfill% OR lake% OR leak% OR mammal% OR manure% OR marine% OR meat% OR microalga% OR micropollutant% OR mollusc% OR ocean% OR pollutant% OR pollution OR river% OR seawater% OR sewage OR sludge OR soil OR soils OR vertebrate% OR waste+management OR wastewater% OR water% OR wild+life OR wildlife OR poultry OR pork OR wild+bore OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)

2.2.2 Specific developments

Along the customization of a TIM environment dedicated to the analysis of retrieved scientific publications and news articles, JRC developed, at the request of EFSA, a marking system and a duplicate removal algorithm. The marking system was used to allow EFSA reviewers to mark documents as “seen” and to mark them as “relevant” or “not relevant”. The duplicate removal mechanism, based on text similarity, was requested to eliminate scientific publications and news articles that were describing the same issue, with the view of reducing the number of articles and media reports to revise. Additional buttons were added to the tool, for example those facilitating the export of specific results of interest.

2.2.3 Screening

The screening of the TIM outputs was performed in two phases. As described above, EFSA staff screened the articles retrieved in both TIM Technology and TIM News and marked the relevant hits. Examples of yearly distributions of the retrieved articles are shown in figure 1 and 2 (for TIM Technology) and figure 3 (for TIM News).

Those articles marked as relevant in the first screening were then exported from the TIM tool to the Distiller[11], in order to be screened by the ECRI WG experts in a second phase. The final

[11] https://www.distillersr.com/

selection of articles is intended to be shared with the Emerging Risks Exchange Network (EREN) for further evaluation of the issues by the Member States experts.

Figure 1: example of scientific publications yearly distribution from 2018 up to now for newly identified chemicals (unknown) from TIM Technology

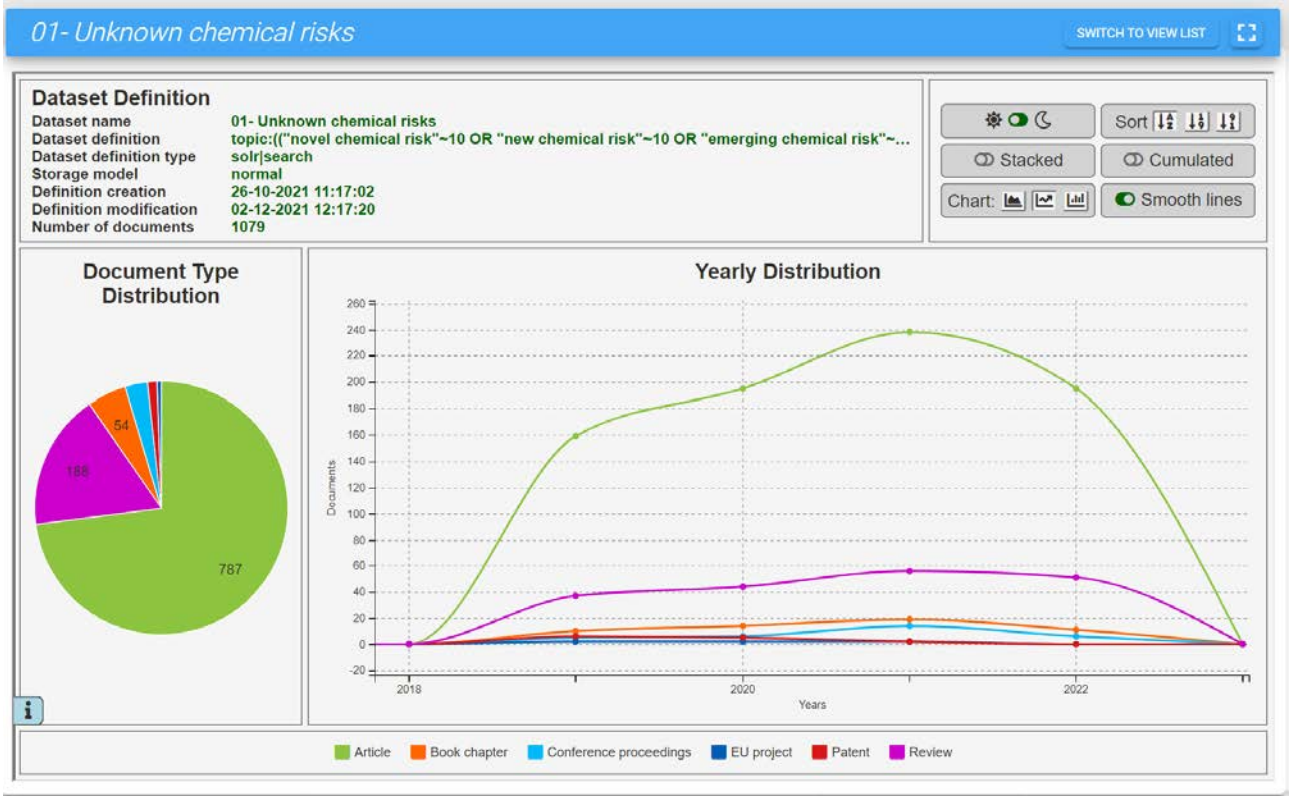
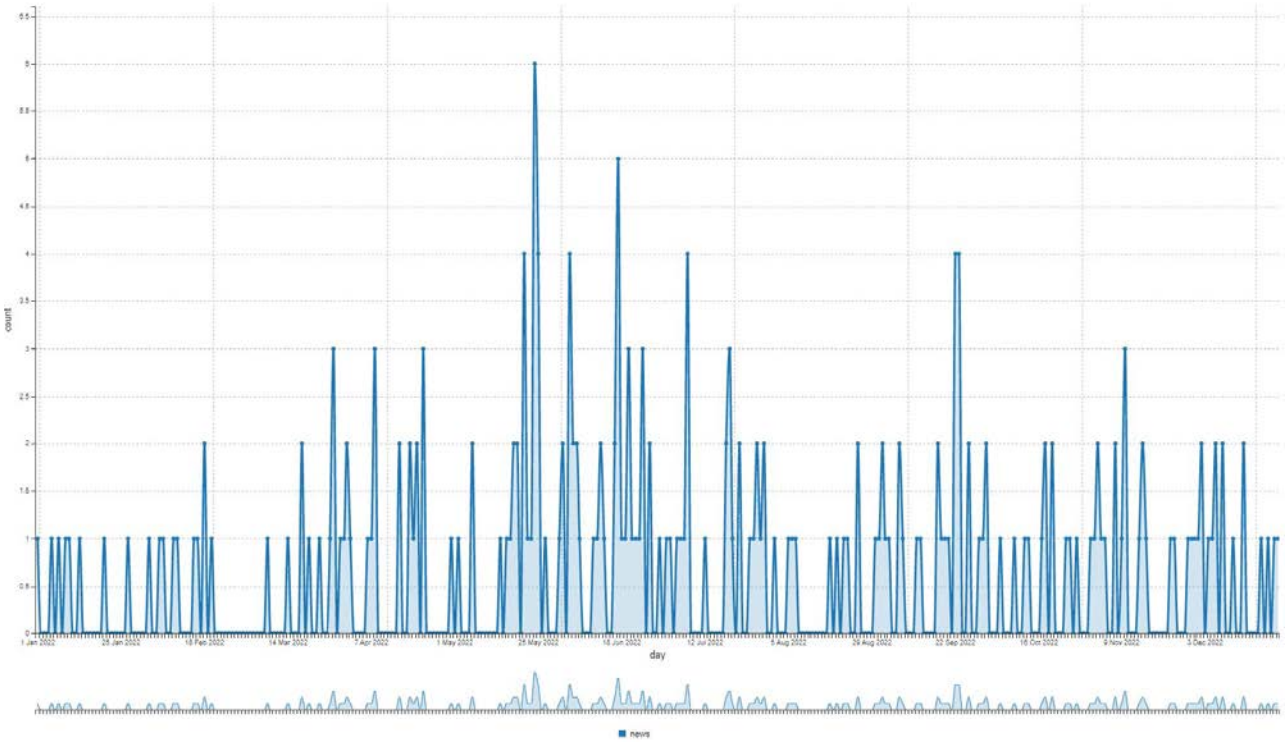


Figure 2: example of scientific yearly distribution in 2020 for one selected known chemical (Bisphenol A) from TIM Technology

Figure 3: example of news daily trend in 2022 for one selected known chemical (Chloral hydrate) from TIM News



3 Assessment

In the 2-year testing phase of this project, key words have been identified, search strings have been developed and criteria for screening have been agreed. It should be noted that few substances that were included in the initial list of the 60 prioritized chemicals have been excluded from the screening as they are by now well studied compounds and therefore do not qualify as emerging. They are Bisphenol A (BPA), tetrabromobisphenol-A (TBBPA), 9,10-anthraquinone, hexabromocyclododecane.

To assess the relevancy of documents collected with TIM technology, two EFSA reviewers performed the first screening by evaluating title and abstract without doing further literature search. The same applied for the review of the three experts (one EFSA expert and two external ones) performing the second screening. The same approach was applied to the news articles collected through Medisys and added to TIM News.

The expertise of the second screening reviewers lies between the disciplines of environmental science, food and analytical chemistry as well as toxicology. The time needed for the screening of outputs corresponded to approximately 3 hours per expert for 150 references. The results received from TIM Technology were about 3000 articles per year for the known chemicals (60 substances) and about 1000 articles per 3 years for the newly identified chemical risks. With respect to TIM News, data used in retrieving news articles was limited to a specific timeframe (427 days). For most of known chemicals very few relevant news articles were retrieved and most of them were referring to well known chemicals such as paracetamol and melamine.

3.1 Screening criteria

The main criteria considered for both screening phases by EFSA as well as by the external experts were the ones that coincide with those used in the context of the EFSA emerging risks Networks. Those criteria are relevant for scientific publications and media reports in both known and newly identified chemicals and are:

- New hazard (new adverse effect in a known chemical or new chemical with an adverse effect),
- Increased exposure (environmental contamination, increased production and/or use),
- New driver
- New susceptible group

Throughout the screening more specific eligibility criteria were developed with the help of the ECRI WG experts. They are detailed below.

3.1.1 Eligibility Criteria for the 1st screening by EFSA

- Inclusion:

  • Outputs from non-EU countries (if the expert judges that they can quickly become relevant for the EU due to global market or EU trends).
  • Chemical accidents if the expert judges that the involved chemicals can reach the food chain.
  • Microplastics: only articles related to occurrence data when information on analytical methods and/or toxicology is also provided.
  • Drinking water.
  • Organophosphate flame retardants (OPFRs)
  • Environmental toxicants acting as endocrine disrupting chemicals.

- Exclusion:

• Effects of known substances when taken as drugs/supplements.
• Removal of contaminants from the environment.
• Combined adverse effects of multiple chemicals.
• The following well known (an EFSA risk assessment has been done) perfluorinated alkylated substances (PFAS): perfluorooctane sulfonate (PFOS), perfluorooctanoic acid (PFOA), perfluorohexanesulfonic acid (PFHxS) and perfluorononanoic acid (PFNA).
• The following already risk assessed phthalates: di-butylphthalate (DBP), butyl-benzyl-phthalate (BBP), bis(2-ethylhexyl)phthalate (DEHP), di-isononylphthalate (DINP, di-isodecylphthalate (DIDP).
• Environmentally persistent free radicals (EPFR).
• Food contact bamboo-melamine plastics (bamboo mixed or coated with melamine) have been assessed and banned in Europe and therefore are not to be considered as an emerging risk.
• Ibogaine (natural product and controlled substance).
• Inhalation and dermal exposure

3.1.2 Eligibility Criteria for the 2nd screening by the WG experts

List of known chemicals

- Inclusion:
  - New evidence about the chemical substance's mode of action.
  - New source of exposure.
  - Increased production/market/use if the ECRI experts consider it as potentially increasing the exposure to levels that might change the outcome of the risk assessment.

- Exclusion:

- data on occurrence levels in the environment
- Reviews of environmental sources, occurrence, temporal/geographical variations
- Risk assessments of known chemicals

- Not relevant but to be collected for future consideration:

  - Novel analytical methods for identification of emerging chemicals
  - New approaches in toxicity testing

List of Newly identified chemicals

- Inclusion:

  - Data on occurrence of chemicals in the environment (if linked to food based on expert judgement)
  - Increased exposure, environmental contamination, increased production/market /use

- Not relevant but to be collected for future consideration:

  - Novel analytical methods for identification of emerging chemicals
  - New approaches in toxicity testing

3.2 Results

3.2.1 Signals from Scientific literature

In order to assess the usefulness of the TIM tools in identifying emerging chemical risks, the number of articles flagged as relevant was evaluated (total number of articles retrieved, number of articles selected in the first screening, number of articles selected in the second screening). This analysis was done for the data on scientific publications, as data inflow is stable (twice a year) i.e. the retrieval of those articles does not depend on the daily scrapping of internet websites.

For the list of known chemicals, the search strings for scientific publications were restricted to the year 2020. Sixteen of those chemicals (randomly selected) were fully evaluated (1st and 2nd screening) and the ratio of relevant articles was calculated (see table 3). The total number of articles retrieved for those 16 chemicals was 1363, from which 148 were selected as potentially relevant in the first screening and 4 out of those were marked as relevant in the 2nd screening (see Appendix G). That corresponds to 0,29% of the initial output.

For the search string of newly identified chemicals, in a restricted period starting from 2019 until November 2021, 831 scientific publications were retrieved. From those, 171 were marked as

relevant in the first screening and 22 of those were selected as relevant in the second screening (see Appendix H). That corresponds to a 2,65% of the initial output.

Table 4: Summary of the output of the screening of selected chemicals for the outputs on scientific publications with restricted search strings for year 2020

TIM ID	Chemical	Ref ID	Total number of articles retrieved in TIM*	Relevant hits **1st screening**	Relevant hits **2nd screening**	**% relevant (for EREN)**
5	Paracetamol	79-124	336	46	0	0
6	Melamine	68 - 78	481	13	0	0
7	Diuron	36 - 67	128	32	1	0.78%
8	4-aminophenol	5 - 9	135	5	0	0%
9	Anti-oxidant 2246	-	10	0	0	0%
11	Butylated hydroxyanisole	125 - 136	131	18	0	0
12	Cyclonite	11 – 24	70	14	2	2.8%
13	Chlorinated paraffins_LC	137 - 148	12	12	0	0
14	Dicyclohexyl_phthalate	25 - 35	15	11	1	6.7%
15	Bis 2,4-dichlorobenzoyl peroxide	10	2	1	0	0%
16	4,4'-Oxybis(benzenesulfonyl h.	-	4	0	0	0%
17	4_4_-Methylenebis_2_chloroaniline	-	9	0	0	0%
18	4-Chloro-2_5-dimethoxyacetoacet.	-	0	0	0	0%
19	2_chloroaniline	4	22	1	0	0
20	2,5-Diaminotoluene	1-3	8	3	0	0%
SUM			1363	148	**4**	**0,29%**

The relevant articles will be further evaluated by the EREN experts through a survey in order to decide on the emerging issue characterization (new hazard, increased exposure of a known hazard, new susceptible group, new driver) as well as the follow up actions (no action, research, monitoring, risk assessment, risk management). Results will be available by the end of April 2023.

Discussion is ongoing on whether the screening should be focused to the category of newly identified chemical risks only, showing a higher percentage of relevant hits indicating potential emerging risks.

3.2.2 Signals from media

First and second screenings were completed for the five chemicals in table 4.

Table 4: Screening summary of selected chemicals for the outputs on news articles

Chemical	Total number of articles retrieved in TIM	Relevant hits 1st screening	% relevant 1st screening	Relevant hits 2nd screening	% relevant 2nd screening
Paracetamol	336	25	7.44%	2	0.60%
Melamine	191	25	13.09%	12	6.28%
melamine_cyanurate	50	3	6.00%	3	6.00%
Butylated hydroxyanisole	246	19	7.72%	6	2.44%
Chlorinated paraffins	58	14	24.14%	0*	-
Articles collected between 1 July 2021 -> 31 August 2022				*not fully reviewed	

The other chemicals were subject to the first screening by efsa experts (see table in Appendix E). This first screening confirmed that the percentage of relevant articles is low for many of the chemicals. In addition, no articles at all were retrieved for 24 of the 60 chemicals investigated. Also, for the newly identified chemicals, after the final optimized search was established, the percentage of relevant articles was around 15% (see Appendix F). The relevancy of articles collected could be improved by further adapting the search strings, but significant efforts were made on this already and the margin for improvement seems tiny.

It has to be pondered whether online media sources is an adequate source of data to collect news articles with the view of detecting emerging risks related to known chemicals. In addition, for the searches that retrieved a significant number of news articles, a regular and resource intensive screening has to be made whose usefulness and impact, considering the low number or relevant articles detected by experts, should be carefully considered.

4 Conclusion

The use of JRC tools (TIM Technology and TIM News) to identify emerging chemical risks has been investigated. Both tools were first customized to address EFSA's purposes. During this 2-year pilot project, a screening workflow has been set-up for scientific publications and for news articles in relation to 60 known chemicals as well as newly identified chemicals in the food chain.

A first screening was conducted by EFSA with the aim of marking relevant hits, while the search strings were adapted to the need of the project to reach a good ratio between relevant articles and noise. Sixteen chemicals out of the sixty chemicals were randomly selected and fully screened (1st and 2nd screening) by the experts of the Emerging Chemical Risks Identification Working Group (ECRI WG). In the 2nd screening 6 articles related to known chemicals were marked as relevant.

The followed procedure and a list of issues associated to emerging chemicals, identified as part of this activity has been shared with the Emerging Risks Exchange Network (EREN) for further evaluation, including the definition of possible follow-up recommendation; results will be available by the end of April 2023. The EREN confirmed the importance of horizon scanning for the identification of emerging chemical risks in the food and feed chain.

The TIM tools offer useful quantitative analysis and visualisation functionalities e.g., time series analysis, cluster effects and the possibility to export data for further analysis. Moreover, user-friendly dashboards have been developed for monitoring trends in publications and news for the different chemicals.

In order to conclude on whether the scanning of scientific publications and news articles through TIM is deemed useful and efficient for the purpose of identifying emerging chemical risks, the resources (number of EFSA staff, number of external experts, time) needed for screening the outputs in relation to the number of relevant hits identified needs to be considered. More specifically, the relevance of the categories (known and newly identified chemicals) and sources (media reports, scientific publications, patents) should be assessed to decide if they should be continually screened.

In this testing phase of the TIM tools a few limitations have been identified. Most importantly, significant resources are necessary to review articles (both from news and from scientific literature) while the resources that have been dedicated for this work were rather limited. More specifically, the number of reviewers in the first and second screening (two and 3 respectively) is insufficient for the number of outputs TIM retrieves monthly. For a proper evaluation of the outputs not only an increase in the number of reviewers is considered necessary, but also the widening of their expertise. The low number of relevant hits both from scientific publications and from news articles also questions the adequateness of this type of data sources for identifying emerging risks related to chemicals. Another consideration, which limits the solidity of the results, is the fact that the criteria for the evaluation where not decided upfront and were instead developed throughout screening ("learning by doing"). Last but not least, the opportunity and feasibility to incorporate artificial intelligence to speed-up the screening has been discussed but discarded, at this stage, as the number of articles is not considered enough to train a machine.

5 Recommendations

Based on the number of relevant results identified and the discussions between the experts of the ECRI Working Group, it is proposed to focus on the screening of the newly identified chemical risks, considering the low number of relevant hits for known chemicals, and specifically on scientific publications rather than evaluating the media reports, as the screening costs is too high compared to the number of relevant hits in the past two years of the testing phase.

External outsourcing of the screening, supported by the implementation of machine learning could enhance the efficiency of the screening. The use of pre-trained models could be explored to make machine learning possible with the amount of papers TIM retrieves.

Finally, the visualization properties of the TIM tools should be explored to improve the efficiency of the screening by considering specific clusters of publications, localization, scientific groups, publication trends etc.

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Abbreviations

ECRI	Emerging Chemical Risk Identification
EFSA	European Food Safety Authority
EMM	Europe Media Monitoring
EREN	Emerging Risks Exchange Network
JRC	Joint Research Centre
MeSH	Medical Subject Headings
TIM	Tools for Innovation Monitoring
WG	Working Group

Appendix A – Sources excluded from EMM for the retrieval of news articles

aas	ecoagri	Jb-asm
abm	eje	jbiolres
academic-aob	ejournals-epublishing	jcm
academic-forestry	ejplantbreeding	JERS
academicjournals	elsevier-es	jhortscib
acta-chimica-slovenica	entomologi	jhr-pensoft
actasciagron	entomologicafennica	jinsectscience
africaninvertebrates	entomology	jjbs
agriculturejournals	esajournals-*	jmir
agrocol	esajournals-ecap	journaldumali
aidsonline	esajournals-ecol	journalnow
annualreviews	esajournals-ecsp	journals-co-za-ento
apc	esajournals-emon	journals-co-za-nzpp
apsjournals-*	esajournals-fron	journals-fcla-flaent
besjournals	eurosurveillance	journals-fcla-mundi
bioone	evodevojournal	journals-fupress
biotrop	flfrevista	journals-nematropica
bmcbiotechnol	foodpoisonjournal	journals-studies-in-mycology
bmcgenomics	frontiersin	journals-tsu
bmcplantbiol	frontiersinzoology	journals-tubitak-botany
bmcresnotes	fruitsci	journals-tubitak-zoology
bmj	fspublishers	jstage
brill-Nematology	graellsia	jstage-Microbes
cambridge-*	horticulturabrasileira	jtropag
castaneajournal	hortsci	jvi
ccarevista	horttech	kjmycology
chembioagro	hrcak	mabjournal
chinaagrisci	hrcak-en	mbio
cmaj	ije	microbiologyresearch-*

cnki-ats	IJER	mycobiota
CSIRO_Publishing_Recent_*	ijidonline	nejm
cnki-ppj	ingentaconnect-mtax	nrcresearchpress-*
cnki-tst	int-res	ojs-openagrar
degruyter-biol	jaids	onehealthjournal
dergipark	jama	openmicrobiologyjournal
dialnet	jamabt	oxforduniversitypress-*

Appendix B – Search strategies for known chemicals in scientific publications

Dataset name	Simplified search	Host	N docs 2020	Difference EMM category	Search string
02. Retinol 2020	(chemical name OR CAS value) AND host NOT skin	YES	405	removed food water, animal from the host string	topic:("retinol" OR "alphalin" OR "axerophthol" OR "afaxin" OR "oleovitamin a" OR "chocola a" OR "alphasterol" OR "apostavit" OR "aquasynth" OR "biosterol" OR "epiteliol" OR "ophthalamin" OR "agiolan" OR "agoncal" OR "anatola" OR "myvpack" OR "prepalin" OR "testavol" OR "veroftal" OR "aoral" OR "apexol" OR "avibon" OR "avitol" OR "axerol" OR "dofsol" OR "vaflol" OR "vitpex" OR "vogan" OR "isatabs tabs" OR "bentavit a" OR "dohyfral a" OR "alcovit a" OR "anatola a" OR "vogan-neu" OR "a-mulsal" OR "plivit a" OR "vi-alpha" OR "a-vitan" OR "atars" OR "vafol" OR "homagenets aoral" OR "hi-a-vita" OR "sehkraft a" OR "a-vi-pel" OR "vi-dom-a" OR "solu-a" OR "nio-a-let" OR "VIOA" OR "antixerophthalmic vitamin" OR "del-vi-a" OR "axerophtholum" OR "thalasphere" OR "wachstumsvitamin" OR "retinolum" OR "antixerophthalmisches vitamin" OR "unii-g2sh0xkk91" OR "ccris 5444" OR "hsdb 815" OR "einecs 200-683-7" OR "chembl986" OR "nsc 122759" OR "brn 0403040" OR "g2sh0xkk91" OR "2e 4e 6e 8e 3,7-dimethyl-9,2,6,6-trimethylcyclohexen-1-yl nona-2,4,6,8-tetraen-1-ol" OR "all-e 3,7-dimethyl-9,2,6,6-trimethyl-1-cyclohexen-1-yl 2,4,6,8-nonatetraen-1-ol" OR "2,4,6,8-nonatetraen-1-ol 3,7-dimethyl-9,2,6,6-trimethyl-1-cyclohexen-1-yl" OR "chebi:17336" OR "3,7-dimethyl-9,2,6,6-trimethyl-1-cyclchexen-1-yl 2,4,6,8-nonatetraen-1-ol" OR "2e 4e 6e 8e 3,7-dimethyl-9,2,6,6-trimethylcyclohex-1-en-1-yl nona-2,4,6,8-tetraen-1-ol" OR "nsc-122759" OR "ncgc00017343-07" OR "cylasphere" OR "retinolo" OR "dsstox_cid_3556" OR "hydrovit a" OR "3,7-dimethyl-9,2,6,6-trimethyl-1-cyclohexen-1-yl 2,4,6,8-nonate-traen-1-ol" OR "alcohol 9 13-dimethyl-7,1,1,5-trimethyl-6-cyclohexen-5-yl 7,9 11 13-nonatetraen-15-ol" OR "dsstox_rid_77080" OR "dsstox_gsid_23556" OR "ro-a-vit" OR "q-201926" OR "w-104683" OR "aquasol a parenteral" OR "rovimix a" OR "2e 4e 6e 8e 3,7-dimethyl-9,2,6,6-trimethylcyclohex-1-enyl nona-2,4,6,8-tetr aen-1-ol" OR "smr000112036" OR "11 12-3h -retinol" OR "9-cis 13-cis-retinol" OR "sr-01000763813" OR "tegosphere vita" OR "alpha.sterol" OR "alpha.lin" OR "retinyl a" OR "trans-retinol acid vitamin a" OR "einecs 234-328-2" OR "mfcd00001552" OR "pubchem18446" OR "spectrum5_000993" OR "spectrum5_001997" OR "ec 200-683-7" OR "schembl3112" OR "all-trans-3,7-dimethyl-9- 2,6,6-trimethyl-1-cyclohexen-1-yl 2,4,6,8-nonatetraen-1-ol" OR "bidd:pxr0102" OR "mls001066379" OR "mls001074751" OR "mls006010008" OR "spectrum1501203" OR "gtpl4053" OR "dtxsid3023556" OR "hms501i08" OR "hms1921b04" OR "hms2092l13" OR "hms2270c05" OR "bcp06593" OR "hy-b1342" OR "zinc3831417" OR "tox21_110818" OR "tox21_202441" OR "tox21_300287" OR "bdbm50092056" OR "bg0050" OR "ccg-38864" OR "lmpr01090001" OR "nsc122759" OR "nsc758150" OR "akos015902578" OR "db00162" OR "nsc-758150" OR "sdccgmls-0066724.p001" OR "idi1_000486" OR "smp2_000102" OR "ncgc00017343-02" OR "ncgc00017343-03" OR "ncgc00017343-04" OR "ncgc00017343-05" OR

					"ncgc00017343-06" OR "ncgc00017343-08" OR "ncgc00017343-09" OR "ncgc00017343-11" OR "ncgc00091784-01" OR "ncgc00091784-02" OR "ncgc00091784-03" OR "ncgc00091784-04" OR "ncgc00091784-05" OR "ncgc00091784-06" OR "ncgc00254024-01" OR "ncgc00259990-01" OR "ac-11701" OR "bs-17906" OR "cc-35617" OR "cc-35618" OR "sc-61936" OR "sc-75819" OR "st057232" OR "sbi-0051690.p002" OR "cs-0013091" OR "ns00003017" OR "33563-ep2272846a1" OR "33563-ep2277869a1" OR "33563-ep2277870a1" OR "33563-ep2281813a1" OR "33563-ep2284174a1" OR "33563-ep2292608a1" OR "33563-ep2301936a1" OR "33563-ep2311820a1" OR "33563-ep2374791a1" OR "ab00052248_05" OR "sr-01000763813-2" OR "sr-01000763813-4" OR "brd-k22429181-001-06-8" OR "brd-k64634304-001-01-5" OR "phenol 2 aminomethyl 5-fluoro hydrochloride" OR "3,6,6-trimethyl-1-cyclohexen-1-yl 2,4,6,8-nonatetraen-1-ol" OR "2,6,8-nonatetraen-1-ol 3,7dimethyl-9,2,6,6-trimethyl-1-cyclohexen-1-yl" OR "3,7-dimethyl-9,2,6,6-trimethyl-1-cyclohexen-1-yl 2,4,6,8-nonatetraen-1-ol" OR "2e 4e 6e 8e 3,7-dimethyl-9,2,6,6-trimethyl-1-cyclohexenyl 1-nona-2,4,6,8-tetraenol" OR "2e 4e 6e 8e 3,7-dimethyl-9- 2,6,6-trimethyl-1-cyclohexenyl nona-2,4,6,8-tetraen-1-ol" OR "2e 4e 6e 8e 3,7-dimethyl-9- 2,6,6-trimethylcyclohex-1-enyl nona-2,4,6,8-tetraen-1-ol" OR "2z 4z 6z 8z 3,7-dimethyl-9- 2,6,6-trimethyl-1-cyclohexen-1-yl 2,4,6,8-nonatetren-1-" OR "cas-68-26-8")
					OR emm_caschemical__value:"68-26-8"
					AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management" OR wastewater OR " waste water" OR "wild life" OR wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
					NOT topic:skin
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
03. Bisphenol A 2020	(chemical name OR CAS value)	YES	1641	added not remediation	topic:(bisfenol OR bisphenol OR BPA) NOT topic:("BPA free"~2)
					OR emm_caschemical__value:"80-05-7"

	AND host NOT remediation				topic:(hormone OR endocrine OR alga OR algae OR air OR animal OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR food OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR waste management OR wastewater OR water OR wild life OR wildlife OR poultry OR pork OR wild bore OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
					NOT topic:(remediation OR "pollutant removal"~3 OR "chemical removal"~2 OR bioremediation)
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
04. Choral hydrate 2020	(chemical name OR CAS value)) AND host	YES	20	-	topic:("1,1,1-trichloro-2,2-dihydroxyethane" OR "1,1,1-trichloro-2,2-ethanediol" OR "1,1-ethanediol 2,2,2-trichloro" OR "1,1-trichloro-2,2-dihydroxyethane" OR "2,2,2-trichloro-1,1-ethanediol" OR "2,2,2-trichloroethane-1,1 diol" OR "2,2,2-trichloroethane-1,1-diol" OR "2,2-trichloro-1,1-ethanediol" OR 418m5916wg OR 6993-ep2269977a2 OR 6993-ep2269992a1 OR 6993-ep2270010a1 OR 6993-ep2272517a1 OR 6993-ep2272813a2 OR 6993-ep2272841a1 OR 6993-ep2272849a1 OR 6993-ep2275395a2 OR 6993-ep2277861a1 OR 6993-ep2277875a2 OR 6993-ep2277876a1 OR 6993-ep2284165a1 OR 6993-ep2292593a2 OR 6993-ep2292602a1 OR 6993-ep2292614a1 OR 6993-ep2292628a2 OR 6993-ep2293650a1 OR 6993-ep2298737a1 OR 6993-ep2298740a1 OR 6993-ep2298744a2 OR 6993-ep2305250a1 OR 6993-ep2305640a2 OR 6993-ep2308852a1 OR 6993-ep2311830a1 OR 6993-ep2311837a1 OR 6993-ep2314558a1 OR 6993-ep2314581a1 OR 6993-ep2316824a1 OR 6993-ep2316832a1 OR 6993-ep2316833a1 OR 6993-ep2316835a1 OR acmc-209hdv OR ai3-00082 OR AI3-00082 OR akos009157238 OR anw-26801 OR aquachloral OR bcp31225 OR "brn 1698497" OR "ccris 4142" OR "chebi 28142" OR chembl455917 OR chloradorm OR "chloral hydrat" OR "chloral hydrate" OR "chloral monohydrate" OR chloraldural OR chloraldurat OR chloralex OR chloralhydrat OR chloralhydrate OR "chlorali hydras" OR chloralvan OR "cloral betaine" OR cohidrate OR ctk1c2451 OR db-047727 OR db01563 OR "dea no 2465" OR dichloralphenazone OR dormal OR dsstox_cid_261 OR dsstox_gsid_20261 OR dsstox_rid_75470 OR dtxsid7020261 OR "einecs 206-117-5 "OR "epa pesticide chemical code 268100" OR "ethanediol 2,2,2-trichloro" OR felsules OR "hydrate de chloral" OR hynos OR kessodrate OR kloralhydrat OR ks-000000z1 OR ksc222i5d OR lorinal OR lycoral OR mcule-8278658791 OR mfcd00044479 OR ncgc00159374-02 OR ncgc00159374-03 OR ncgc00159374-04 OR ncgc00257664-01 OR noctec OR nortec OR novochlorhydrate OR ns00009274 OR "nsc 3210" OR nsc-3210 OR nsc3210 OR nycoton OR nycton OR oradrate OR phaldrone OR rectules OR sc-18707 OR schembl34327 OR "somni sed" OR somnote OR sontec OR stl445706 OR tox21_111614 OR tox21_111614_1 OR tox21_200110 OR trawotox OR trichloracetaldehyd-hydrat OR "trichloro acetaldehyde hydrate" OR "trichloroacetaldehyde hydrate" OR

					"trichloroacetaldehyde hydrated" OR "trichloroacetaldehyde monohydrate" OR "trichloroethanal hydrate" OR unii-418m5916wg OR "wln qyqxggg" OR zinc3872049)
					OR emm_caschemical__value:"302-17-0"
					AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR food OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management OR" wastewater OR "wild life" OR wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
05. Paracetamol 2020	(chem name OR CAS value) AND host AND toxic NOT vaccine NOT remediation	YES	342	added not remediation, "N acetyl para aminophenol"	topic:("acetaminophen" OR "paracetamol" OR "N acetyl para aminophenol")
				removed most paracetamol synonims	OR emm_caschemical__value:"103-90-2"
					AND topic:(toxic OR risk OR hazard OR drug OR analgesic OR tablet OR pill OR prescription) NOT topic:("vaccine" OR "vaccination" OR "covid")
					AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR food OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management OR" wastewater OR "wild life" OR wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
					NOT topic:(remediation OR "pollutant removal"~3 OR "chemical removal"~2 OR bioremediation)
				NOT patents	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR

				"preparation method"	"production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
06. Melamine 2020	(chemical names OR CAS value) AND host NOT remediation NOT "prep method"	YES	477	removed waste, water,animal from the host string	topic:(melamine OR "melamin" OR "1,3,5-triazine-2,4,6-triamine" OR "isomelamine" OR "theoharn" OR "teoharn" OR "triaminotriazine" OR "hicophor pr" OR "s-triazinetriamine" OR "2,4,6-triamino-1,3,5-triazine" OR "yukamelamine" OR "pluragard" OR "cymel" OR "virset 656-4" OR "2,4,6-triamino-s-triazine" OR "spinflam ml 94m" OR "2,4,6-triaminotriazine" OR "pluragard c 133" OR "adk stab zs 27" OR "mark zs 27" OR "dg 002 amine" OR "melamine monomer" OR "nci-c50715" OR "cyanurtriamide" OR "s-triazine 2,4,6-triamino-" OR "1,3,5-triazine-2,4,6,1h 3h 5h -triimine" OR "zs 27" OR "unii-n3gp2ysd88" OR "nsc 2130" OR "dg 002" OR "sym-triaminotriazine" OR "ccris 373" OR "hsdb 2648" OR "einecs 203-615-4" OR "brn 0124341" OR "n3gp2ysd88" OR "ai3-14883" OR "dtxsid6020802" OR "chebi:27915" OR "1,3,5-triazine-2,4,6,1h 3h 5h triimine" OR "sym triaminotriazine" OR "2,6-triaminotriazine" OR "2,4,6-triamino-1,3,5-triazine monomer" OR "dsstox_cid_802" OR "2,6-triamino-s-triazine" OR "melamine-13c3 15n3" OR "ec 203-615-4" OR "s-triazine 4,6-triamino-" OR "dsstox_rid_75795" OR "dsstox_gsid_20802" OR "schembl25853" OR "bidd:er0287" OR "chembl1231106" OR "schembl12192199" OR "ks-00000vsy" OR "melamine metformin impurity d" OR "1,5-triazine-2,4,6-triamine" OR "2,6-triamino-1,3,5-triazine" OR "nsc2130" OR "nsc8152" OR "zinc897751" OR "hy-y1117" OR "nsc-2130" OR "nsc-8152" OR "wln: t6n cn enj bz dz fz" OR "tox21_200503" OR "bbl000010" OR "ls-469" OR "mfcd00006055" OR "sbb000053" OR "stk378738" OR "akos005448714" OR "ccg-266105" OR "mcule-1467355510" OR "ncgc00164014-01" OR "ncgc00164014-02" OR "ncgc00258057-01" OR "cas-108-78-1" OR "st018511" OR "vs-00405" OR "1,3,5-triazine-2,4,6-triamine monomer" OR "cs-0016866" OR "ft-0609833" OR "ft-0670982" OR "ft-0670983" OR "melamine 1,3,5-triazine-2,4,6-triamine" OR "t6897" OR "1,3,5-triazine-2,4,6-triamine melamine" OR "1,5-triazine-2,4,6,1h 3h 5h -triimine" OR "4,6-diamino-1,2-dihydro-2-imino-s-triazine" OR "c08737" OR "78403-ep2270101a1" OR "78403-ep2270113a1" OR "78403-ep2272849a1" OR "78403-ep2272935a1" OR "78403-ep2276751a1" OR "78403-ep2289896a1" OR "78403-ep2298828a1" OR "78403-ep2301924a1" OR "78403-ep2301983a1" OR "78403-ep2308856a1" OR "78403-ep2374895a1" OR "s-triazine 4,6-diamino-1,2-dihydro-2-imino-" OR "q212553" OR "j-002191" OR "cyanuramide" OR "cyanurotriamine" OR "cyanurotriamide" OR "melamine" OR "1,3,5-Triazine-2,4,6-triamine" OR "Isomelamine" OR "Theoharn" OR "Teoharn" OR "Triaminotriazine" OR "Cyanuric triamide" OR "Hicophor PR" OR "s-Triazinetriamine" OR "2,4,6-Triamino-1,3,5-triazine" OR "Yukamelamine" OR "Pluragard" OR "Cymel" OR "Virset 656-4" OR "2,4,6-Triamino-s-triazine" OR "Spinflam ML 94M" OR "2,4,6-Triaminotriazine" OR "Pluragard C 133" OR "ADK Stab ZS 27" OR "Mark ZS 27" OR "DG 002 amine" OR "Melamine Monomer" OR "NCI-C50715" OR "Cyanurtriamide" OR "s-Triazine 2,4,6-triamino-" OR "1,3,5-Triazine-2,4,6,1H 3H 5H -triimine" OR "ZS 27" OR "s-triaminotriazine" OR "UNII-N3GP2YSD88" OR "NSC 2130" OR "DG 002" OR "sym-Triaminotriazine" OR "CCRIS 373" OR "HSDB 2648" OR "EINECS 203-615-4" OR "67297-95-4" OR "BRN 0124341" OR "N3GP2YSD88" OR "2,4,6-triamino sym-triazine" OR "AI3-14883" OR "DTXSID6020802" OR "CHEBI:27915" OR "1,3,5-triazine-2,4,6,1H 3H 5H triimine" OR "melamin" OR "cyan urotriamide" OR "Sym Triaminotriazine" OR "2,6-Triaminotriazine" OR "2,4,6-

					Triamino-1,3,5-triazine Monomer" OR "DSSTox_CID_802" OR "2,6-Triamino-s-triazine" OR "Melamine-13C3 15N3" OR "EC 203-615-4" OR "s-Triazine 4,6-triamino-" OR "DSSTox_RID_75795" OR "DSSTox_GSID_20802" OR "SCHEMBL25853" OR "BIDD:ER0287" OR "CHEMBL1231106" OR "SCHEMBL12192199" OR "KS-00000VSY" OR "Melamine Metformin Impurity D" OR "1,5-Triazine-2,4,6-triamine" OR "2,6-Triamino-1,3,5-triazine" OR "NSC2130" OR "NSC8152" OR "ZINC897751" OR "HY-Y1117" OR "NSC-2130" OR "NSC-8152" OR "WLN: T6N CN ENJ BZ DZ FZ" OR "Tox21_200503" OR "1,3,5-triazinane-2,4,6-triimine" OR "BBL000010" OR "LS-469" OR "MFCD00006055" OR "s9212" OR "SBB000053" OR "STK378738" OR "AKOS005448714" OR "CCG-266105" OR "MCULE-1467355510" OR "NCGC00164014-01" OR "NCGC00164014-02" OR "NCGC00258057-01" OR "1246816-14-7" OR "94977-27-2" OR "CAS-108-78-1" OR "ST018511" OR "VS-00405" OR "1,3,5-Triazine-2,4,6-triamine monomer" OR "CS-0016866" OR "FT-0609833" OR "FT-0670982" OR "FT-0670983" OR "Melamine 1,3,5-Triazine-2,4,6-triamine" OR "T6897" OR "1,3,5-Triazine-2,4,6-triamine Melamine" OR "1,5-Triazine-2,4,6,1H 3H 5H -triimine" OR "4,6-Diamino-1,2-dihydro-2-imino-S-Triazine" OR "C08737" OR "78403-EP2270101A1" OR "78403-EP2270113A1" OR "78403-EP2272849A1" OR "78403-EP2272935A1" OR "78403-EP2276751A1" OR "78403-EP2289896A1" OR "78403-EP2298828A1" OR "78403-EP2301924A1" OR "78403-EP2301983A1" OR "78403-EP2308856A1" OR "78403-EP2374895A1" OR "s-Triazine 4,6-diamino-1,2-dihydro-2-imino-" OR "Q212553" OR "J-002191" OR "cyanuric triamide" OR "Cyanuramide" OR "Cyanurotriamine" OR "Cyanurotriamide")
				added not remediation	OR emm_caschemical__value:"108-78-1"
					AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR food OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management" OR wastewater OR "wild life" OR wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
					NOT topic:(remediation OR "pollutant removal"~3 OR "chemical removal"~2 OR bioremediation)
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

07. Diuron 2020	(chemical names OR CAS value) AND host NOT remediation	YES	124	removed "di-on"	topic:("3,3,4-dichlorophenyl 1,1-dimethylurea" OR "dynex" OR "dichlorfenidim" OR "herbatox" OR "vonduron" OR "dailon" OR "karmex" OR "marmer" OR "cekiuron" OR "crisuron" OR "dirurol" OR "lucenit" OR "unidron" OR "diuron nortox" OR "preventol a 6" OR "urox d" OR "direx 4l" OR "anduron" OR "ansaron" OR "durashield" OR "herburon" OR "seduron" OR "bioron" OR "dcmu 99" OR "diuro 900" OR "hw 920" OR "ditox-800" OR "karamex" OR "aguron" OR "diater" OR "unii-9i3sds92wy" OR "usaf p-7" OR "3,3,4-dichlor-phenyl 1,1-dimethyl" OR "ccris 1012" OR "hsdb 382" OR "direx 80w" OR "chebi:116509" OR "nsc 8950" OR "einecs 206-354-4" OR "af 101" OR "urea 3- 3,4-dichlorophenyl 1,1-dimethyl" OR "epa pesticide chemical code 035505" OR "brn 2215168" OR "9i3sds92wy" OR "ai3-61438" OR "dtxsid0020446" OR "mfcd00018136" OR "3- 3,4-dichlor-phenyl 1,1-dimethyl" OR "ncgc00094525-01" OR "dsstox_cid_446" OR "dsstox_rid_75595" OR "dsstox_gsid_20446" OR "xarmex" OR "desdimethyldiuron" OR "xarmex krovar" OR "m velpar" OR "karmex dl" OR "karmex 80w" OR "spectrum_001823" OR "acmc-1cqjf" OR "specplus_000424" OR "spectrum2_001229" OR "spectrum3_000822" OR "spectrum4_000662" OR "spectrum5_001956" OR "ec 206-354-4" OR "schembl7279" OR "bspbio_002343" OR "kbiogr_001063" OR "kbioss_002328" OR "spectrum330030" OR "mls002207110" OR "divk1c_006520" OR "spbio_001078" OR "chembl278489" OR "ure002" OR "ctk7g2120" OR "kbio1_001464" OR "kbio2_002325" OR "kbio2_004893" OR "kbio2_007461" OR "kbio3_001843" OR "zinc57287" OR "nsc8950" OR "hy-b0860" OR "nsc-8950" OR "tox21_111292" OR "tox21_201438" OR "tox21_301016" OR "anw-27531" OR "bbl003847" OR "bdbm50487027" OR "ccg-39151" OR "stk077954" OR "akos001303464" OR "tox21_111292_1" OR "ls-7325" OR "mcule-1921281405" OR "ks-0000105p" OR "ncgc00094525-02" OR "ncgc00094525-03" OR "ncgc00094525-04" OR "ncgc00094525-05" OR "ncgc00094525-06" OR "ncgc00094525-07" OR "ncgc00094525-08" OR "ncgc00094525-09" OR "ncgc00254918-01" OR "ncgc00258989-01" OR "as-15493" OR "p597" OR "smr000777941" OR "3- 3,4-dichlorophenol 1,1-dimethylurea" OR "db-048327" OR "cs-0012874" OR "d1328" OR "ft-0603378" OR "ft-0667750" OR "n n-dimethyl-n 3,4-dichlorophenyl urea" OR "ns00000265" OR "st50409103" OR "n 3,4-dichlorophenyl n n dimethyl urea" OR "c18428" OR "33329-ep2274983a1" OR "33329-ep2305655a2" OR "33329-ep2305662a1" OR "33329-ep2311815a1" OR "33329-ep2371823a1" OR "n 3,4-dichlorophenyl dimethylamino carboxamide" OR "a821585" OR "q425389" OR "sr-01000195223" OR "j-018992" OR "sr-01000195223-1" OR "brd-k75330923-001-02-6" OR "1,1-dimethyl-3,3,4-dichlorophenyl urea" OR "1,3,4-dichlorophenyl 3,3-dimethylurea" OR "1,3,4-dichlorophenyl 3,3-dimethyluree" OR "3,3,4-dichloor-fenyl 1,1-dimethylureum" OR "3,3,4-dichloro-phenyl 1,1-dimethyl-urea" OR "3,3,4-dichlor-phenyl 1,1-dimethyl-harnstoff" OR "3,3,4-dicloro-fenyl 1,1-dimetil-urea" OR "n 3,4-dichlorophenyl n n-dimethylurea" OR "n 3 n-dimethylurea" OR "n 3,4-dichlorophenyl n n dimethylurea" OR "n 3 n dimethylurea" OR "n n dimethyl-n 3,4-dichlorophenyl urea" OR "urea 4-dichlorophenyl 1,1-dimethyl" OR "urea 4-dichlorophenyl n n-dimethyl" OR "urea n 3,4-dichlorophenyl n n-dimethyl" OR "3,3,4-Dichlorophenyl 1,1-dimethylurea" OR "Dynex" OR "Dichlorfenidim" OR "Herbatox" OR "Vonduron" OR "Dailon" OR "Karmex" OR "Marmer" OR "Cekiuron" OR "Crisuron" OR "Dirurol" OR "Lucenit" OR "Unidron" OR "Diuron Nortox" OR "Preventol A 6" OR "Urox D" OR "Direx 4L" OR "Anduron" OR "Ansaron" OR "Durashield" OR "Herburon" OR

					"Seduron" OR "Bioron" OR "DCMU 99" OR "HW 920" OR "Ditox-800" OR "Karamex" OR "Aguron" OR "Diater" OR "UNII-9I3SDS92WY" OR "USAF P-7" OR "3,3,4-Dichlor-phenyl 1,1-dimethyl" OR "CCRIS 1012" OR "HSDB 382" OR "Direx 80W" OR "CHEBI:116509" OR "NSC 8950" OR "EINECS 206-354-4" OR "AF 101" OR "Urea 3- 3,4-dichlorophenyl 1,1-dimethyl" OR "EPA Pesticide Chemical Code 035505" OR "BRN 2215168" OR "9I3SDS92WY" OR "AI3-61438" OR "DTXSID0020446" OR "MFCD00018136" OR "NCGC00094525-01" OR "DSSTox_CID_446" OR "DSSTox_RID_75595" OR "DSSTox_GSID_20446" OR "Xarmex" OR "Desdimethyldiuron" OR "Xarmex Krovar" OR "M Velpar" OR "Karmex DL" OR "Karmex 80W" OR "Spectrum_001823" OR "1,3,3-dimethylurea" OR "ACMC-1CQJF" OR "SpecPlus_000424" OR "Spectrum2_001229" OR "Spectrum3_000822" OR "Spectrum4_000662" OR "Spectrum5_001956" OR "EC 206-354-4" OR "SCHEMBL7279" OR "3,3,1-dimethyl-harnstoff" OR "BSPBio_002343" OR "KBioGR_001063" OR "KBioSS_002328" OR "SPECTRUM330030" OR "MLS002207110" OR "DivK1c_006520" OR "SPBio_001078" OR "CHEMBL278489" OR "URE002" OR "CTK7G2120" OR "KBio1_001464" OR "KBio2_002325" OR "KBio2_004893" OR "KBio2_007461" OR "KBio3_001843" OR "ZINC57287" OR "NSC8950" OR "HY-B0860" OR "NSC-8950" OR "Tox21_111292" OR "Tox21_201438" OR "Tox21_301016" OR "ANW-27531" OR "BBL003847" OR "BDBM50487027" OR "CCG-39151" OR "STK077954" OR "AKOS001303464" OR "Tox21_111292_1" OR "LS-7325" OR "MCULE-1921281405" OR "KS-0000105P" OR "NCGC00094525-02" OR "NCGC00094525-03" OR "NCGC00094525-04" OR "NCGC00094525-05" OR "NCGC00094525-06" OR "NCGC00094525-07" OR "NCGC00094525-08" OR "NCGC00094525-09" OR "NCGC00254918-01" OR "NCGC00258989-01" OR "AS-15493" OR "P597" OR "SMR000777941" OR "3,3,4-Dichlorophenol 1,1-dimethylurea" OR "DB-048327" OR "CS-0012874" OR "D1328" OR "FT-0603378" OR "FT-0667750" OR "N N-dimethyl-N 3,4-dichlorophenyl urea" OR "NS00000265" OR "ST50409103" OR "N 3,4-dichlorophenyl N N dimethyl urea" OR "C18428" OR "33329-EP2274983A1" OR "33329-EP2305655A2" OR "33329-EP2305662A1" OR "33329-EP2311815A1" OR "33329-EP2371823A1" OR "N 3,4-dichlorophenyl dimethylamino carboxamide" OR "A821585" OR "Q425389" OR "SR-01000195223" OR "J-018992" OR "SR-01000195223-1" OR "BRD-K75330923-001-02-6" OR "1,1-Dimethyl-3,3,4-dichlorophenyl urea" OR "1,3,4-Dichlorophenyl 3,3-dimethylurea" OR "1,3,4-Dichlorophenyl 3,3-dimethyluree" OR "1,4dichlorophenyl urea" OR "3,3,1-dimethylurea" OR "3,3,1-dimethylureum" OR "3,3,1-dimetil-urea" OR "3,3,4-Dichloor-fenyl 1,1-dimethylureum" OR "3,3,4-dichlorophenyl 1,1-dimethyl-urea" OR "3,3,4-Dichloro-phenyl 1,1-dimethyl-urea" OR "3,3,4-Dicloro-fenyl 1,1-dimetil-urea" OR "diuron" OR "N 3,4-Dichlorophenyl N N-dimethylurea" OR "N 3 N-dimethylurea" OR "N 3,4-Dichlorophenyl N N dimethylurea" OR "N 3,4-Dichlorophenyl N N-Dimethylurea" OR "N 3 N dimethylurea" OR "N N Dimethyl-N 3,4-dichlorophenyl urea" OR "Urea 4-dichlorophenyl 1,1-dimethyl" OR "Urea 4-dichlorophenyl N N-dimethyl" OR "Urea N 3,4-dichlorophenyl N N-dimethy")
				added not remediation	OR emm_caschemical__value:"330-54-1"

					AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR food OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management" OR wastewater OR "wild life" OR wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
					NOT topic:(remediation OR "pollutant removal"~3 OR "chemical removal"~2 OR bioremediation)
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
08.4 aminophenol	(chemical names OR CAS value)) AND host NOT "prep method"	YES	124		topic:("CAS 123-30-8" OR "1-amino-4-hydroxybenzene" OR "135807-ep2371803a1" OR "135807-ep2377843a1" OR "4-amino phenol" OR "4-amino-1-hydroxybenzene" OR "4-amino-phenol" OR "4-aminobenzenol" OR "4-aminophenol" OR "4-hydroxy-aniline" OR "4-hydroxyaniline" OR "4-hydroxybenzenamine" OR "4-hydroxyphenylamine" OR "9225-ep2275420a1" OR "9225-ep2280008a2" OR "9225-ep2308872a1" OR "9225-ep2316829a1" OR "a0384" OR "acmc-209aoj" OR "activol" OR "ai3-14872" OR "aj-333 25022099" OR "akos000119829" OR "akos016371265" OR "am86423" OR "aminophenol p" OR "anw-18113" OR "as-54109" OR "as04549" OR "bbl011574" OR "bcp25857" OR "bdbm26195" OR "benzofur p" OR "bmse000462" OR "c i 76550" OR "c02372" OR "ccg-266045" OR "ccris 4146" OR "certinal" OR "chebi 17602" OR "chembl1142" OR "ci 76550" OR "citol" OR "cs-0006652" OR "db14144" OR "dsstox_cid_4499" OR "dsstox_gsid_24499" OR "dsstox_rid_77429" OR "dtxsid3024499" OR "durafur brown rb" OR "ec 204-616-2" OR "einecs 204-616-2" OR "energol" OR "epitope id 117708" OR "f2190-0438" OR "fouramine p" OR "fourrine 84" OR "fourrine p base" OR "ft-0617593" OR "furro p base" OR "hsdb 2640" OR "j-004908" OR "j-514454" OR "kodelon" OR "ks-000000hn" OR "ksc354q5h" OR "l-1224" OR "ls-676" OR "mcule-3319647085" OR "mesalamine impurity a" OR "mfcd00007869" OR "mls001066356" OR "nako brown r" OR "ncgc00090816-01" OR "ncgc00090816-02" OR "ncgc00090816-03" OR "ncgc00090816-04" OR "ncgc00090816-05" OR "ncgc00258583-01" OR "ns00006730" OR "nsc 1545" OR "nsc-1545" OR "nsc1545" OR "p-amino-phenol" OR "p-aminobenzenol" OR "p-aminofenol" OR "p-aminophenol" OR "p-aminophenol phosphate" OR "p-hydroxyphenylamine" OR "para amino phenol" OR "para aminophenol" OR "para-amino-phenol" OR "para-aminophenol" OR "para-hydroxyaniline" OR "paraaminophenol" OR "paramidophenol" OR "paranol" OR "pelagol p base" OR "phenol 4-amino" OR "phenol p-amino" OR "pubchem22199" OR "q2548040" OR "r7p8frp05v" OR "renal ac" OR "sbb059792" OR "sc-19013" OR "schembl15663694" OR "schembl3424" OR "sgcut00256" OR "smr000471841" OR "st088538" OR "stk286017" OR "takatol" OR "tertral p base" OR "tox21_113242" OR "tox21_113477" OR "tox21_113477_1" OR "tox21_201030" OR "to_000006" OR

					"un 2512" OR "unii-r7p8frp05v" OR "ursol p" OR "ursol p base" OR "z57127517" OR "zinc4623758" OR "zoba brown" OR "PAP high sulfite" OR "RODOL P Base" OR "Ursal P")
					OR emm_caschemical__value:"123-30-8"
				added host	AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR food OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management" OR wastewater OR "wild life" OR wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
				added not remediation	NOT topic:(remediation OR "pollutant removal"~3 OR "chemical removal"~2 OR bioremediation)
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

10. Antioxidant 2246 2020	chemical names OR CAS value NOT "prep method"	NO	7	deleted "a 22-46" "cao-5" "cao 5" "cao-14" OR "as-13205"	topic:("2 methylenebis 4-methyl-6-tert-butylphenol" OR "2 methylenebis 6-tert-butyl-4-cresol" OR "2,1-dimethylethyl p-cresol" OR "2,2 methylene bis 4-methyl-6-tert butylphenol" OR "2,2 bis 4-methyl-6-tert-butylphenol methane" OR "2,2 bis-6-terc butyl-p-kresylmethan" OR "2,2 methanediylbis 6,1,1-dimethylethyl 4-methylphenol" OR "2,2 methanediylbis 6-tert-butyl-4-methylphenol" OR "2,2 methyl enebis 4-methyl-6-t-butylphenol" OR "2,2 methylene-bis 4-methyl-6-tertiarybutylphenol" OR "2,2 methylene-bis 6-tert-butyl para-cresol" OR "2,2 methylene-bis 6-tert-butyl-4-methylphenol" OR "2,2 methylene-bis 4-methyl-6-t-butylphenol" OR "2,2 methylene-bis 4-methyl-6-tert-butylphenol" OR "2,2 methylene-bis 4-methyl-6-tert butylphenol" OR "2,2 methylenebis 4-methyl-6-t-butylphenol" OR "2,2 methylenebis 4-methyl-6-tert" OR "2,2 methylenebis 4-methyl-6-tert-butylphenol" OR "2,2 methylenebis 6,1,1-dimethylethyl 4-methyl-phenol" OR "2,2 methylenebis 6- 1,1-dimethylethyl p-cresol" OR "2,2 methylenebis 6-t-butyl-4-methylphenol" OR "2,2 methylenebis 6-t-butyl-p-cresol" OR "2,2 methylenebis 6-tert-butyl-4-cresol" OR "2,2 methylenebis 6-tert-butyl-4-methyl-phenol" OR "2,2 methylenebis 6-tert-butyl-4-methylphenol" OR "2,2 methylenebis 6-tert-butyl-p-cresol" OR "2,2 methylenebis 6-tert-4-methylphenol" OR "2,2-methylenebis 4-methyl-6-t-butylphenol" OR "2,2-methylenebis 6-tert-butyl-4-methylphenol" OR "2,2-methylenebis 6-tert-butyl-p-cresol" OR "2 tert-butyl 6,3 tert-butyl 2-hydroxy-5-methylphenyl methyl 4-methylphe nol" OR "2-tert-butyl-6,2-hydroxy-3-tert-butyl-5-methyl-benzyl 4-methyl-phenol" OR "2-tert-butyl-6- 3-tert-butyl-2-hydroxy-5-methylphenyl methyl 4-methylphenol" OR "3,3 di-tert-butyl-2,2 dihydroxy-5,5 dimethyldiphenylmethane" OR "6,6 di-tert-butyl-2,2 methylenedi-p-cresol" OR "6,6 methylenebis 2- tert-butyl 4-methylphenol" OR "6,6 methylenebis 2-tert-butyl-4-methylphenol" OR "6,6-di-tert-butyl-2,2-methylenedi-p-cresol" OR "acmc-1buvj" OR "advastab 405" OR "agidol 2" OR "ai3-18027" OR "ak-28736" OR "akos000447157" OR "alterungsschutzmittel bkf" OR "antage w 400" OR "antioxidant 2246" OR "antioxidant bkf" OR "antioxidant ng-2246" OR "antioxidant omb" OR "antioxydant_2246" OR "anw-17334" OR "ao 1 antioxidant" OR "ax8017725" OR "bbl025607" OR "bidder0324" OR "bis 2-hydroxy-3-tert-butyl-5-methylphenyl methane" OR "bis 2-hydroxy-5-methyl-3-tert-butylphenyl methane" OR "bis 3-tert-butyl-2-hydroxy-5-methylphenyl methane" OR "bis 6-hydroxy-3-methyl-5-tert-butylphenyl methane" OR "bisaklofen bp" OR "bisalkofen bp" OR "brn 2062676" OR "calco 2246" OR "cas-119-47-1" OR "catolin 14" OR "ccg-207916" OR "ccg-208597" OR "chemanox 21" OR "chembl460648" OR "ctk8a9397" OR "cyanox 2246" OR "di 2-hydroxy-5-methyl-3-tert-butylphenyl methane" OR "dsstox_cid_870" OR "dsstox_gsid_20870" OR "dsstox_rid_75838" OR "dtxsid4020870" OR "ec 204-327-1" OR "einecs 204-327-1" OR "fr-0126" OR "ft-0609309" OR "geri-bp002-a" OR "hsdb 5585" OR "ionol 46" OR "ks-00000w13" OR "kvm0x4x57b" OR "lederle 2246" OR "lowinox 22m46" OR "ls-7516" OR "mbmbp" OR "mcule-8897993815" OR "methane 2 -bis 6-tert-butyl-p-cresyl" OR "methane 2,2 -bis 6-t-butyl-p-cresyl" OR "methane 2,2 -bis 6-tert-butyl-p-cresyl" OR "methylene bis methyl butyl phenol" OR "methylene di-t-butyl cresol" OR "methylene di-t-butylcresol" OR "mls-0146298 0001" OR "ncgc00164172-01" OR "ncgc00164172-02" OR "ncgc00256347-01" OR "ncgc00259079-01" OR "ng 2246" OR "nocrac ns 6" OR "nocrack ns 6" OR "ns00010737" OR "nsc 7781" OR "nsc-7781" OR "nsc7781" OR "oprea1_122036" OR "oxy chek 114" OR "p-cresol 2 -methylenebis 6-tert-butyl-" OR "p-cresol 2,2 -methylenebis 6-

					tert- butyl-" OR "p-cresol 2,2 -methylenebis 6-tert-butyl-" OR "phenol 2 methylenebis 6,1,1-dimethylethyl 4-methyl" OR "phenol 2,2 methylenebis 6,1,1-dimethylethyl 4-methyl" OR "plastanox 2246" OR "plastanox 2246 antioxidant" OR "ralox 46" OR "rubber antioxidant 2246" OR "sbb007695" OR "sc-79689" OR "schembl34162" OR "stl377901" OR "sumilizer mdp" OR "synox 5lt" OR "tox21_201529" OR "tox21_302923" OR "unii-kvm0x4x57b" OR "vulkanox bkf" OR "zinc1543799" OR "cas 119-47-1" OR "anti-oxidant 2246" OR ("AO 2246" AND antioxidant) OR "2,2 methylenebis 4-methyl-6-tert-butylphenol")
				added "anti-oxidant 2246" AND ("AO 2246" AND antioxidant) AND "2,2 methylene bis 4-methyl-6-tert-butylpheno l"	OR emm_caschemical__value:"119-47-1"
				NOT patents "preparatio n method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

11. Butylated hydroxyanisole 2020	chemical names OR CAS value NOT "prep method"	NO	131	exclusion criteria for EMM not necessary here	topic:("2,3 t-butyl-4-methoxyphenol" OR "2,3 t-butyl-4-hydroxyanisole" OR "2,3 tert-butyl-4-hydroxyanisole" OR "2,3 tert-butyl-4-methoxyphenol" OR "2,1,1dimethylethyl 4 methyloxy phenol" OR "2,1,1dimethylethyl 4-methoxy-phenol" OR "2,1,1-dimethylethyl 4-methoxyphenol" OR "2 tert-butyl 4-methoxyphenol" OR "2-butyl-4-hydroxyanisole" OR "2-t-butyl-4-methoxyphenol" OR "2-tert-bha" OR "2-tert-butyl-4-methoxphenol" OR "2-tert-butyl-4-methoxy-phenol" OR "2-tert-butyl-4-methoxyphenol" OR "3,1,1-dimethylethyl 4-hydroxyanisole" OR "3-bha" OR "3-t-butyl-4-hydroxyanisole" OR "3-tert-butyl-4-hydroxyanisol" OR "3-tert-butyl-4-hydroxyanisole" OR "3-tert-butyl-p-hydroxyanisole" OR "4-hydroxy-3-tert-butylanisole" OR "4-methoxy-2-tert-butylphenol" OR "4-methoxy-6-tert-butylphenol" OR "amif-72" OR "anisole butylated hydroxy" OR "antioxyne b" OR "antrancine 12" OR "boa antioxidant" OR "butyl methoxyphenol" OR "butylated hydroxyanisole" OR "butylhydroxyanisol" OR "butylhydroxyanisole" OR "butylohydroksyanizol" OR "c11h16o2" OR "ccris 102" OR "chembl4296740" OR "cs-4622" OR "eec no e320" OR "einecs 246-563-8" OR "embanox" OR "fema no 183" OR "hsdb 3913" OR "hy-b1066" OR "ls-1065" OR "nepantiox 1-f" OR "nipantiox 1-f" OR "o-tert-butyl-p-methoxyphenol" OR "o-tert-Butyl-p-methoxyphenol" OR "p-methoxy-o-tert-butylphenol" OR "phenol 1,1-dimethylethyl 4-methoxy" OR "phenol 2,1,1dimethylethyl 4-methoxy" OR "phenol 2-tert-butyl-4-methoxy" OR "phenol tert-butyl-4-methoxy" OR "protex" OR "q409401" OR "rek4960k2u" OR "schembl30330" OR "sustane 1-f" OR "t-butyl hydroxyanisole" OR "tenox bha" OR "tert-butyl-4-methoxyphenol" OR "tert-butylhydroxyanisole" OR "unii-rek4960k2u")
					OR emm_caschemical__value:"25013-16-5"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
12. Cyclonite 2020	(chemical names OR CAS value) AND host NOT "prep method"	YES	64	added RDX "Research Department eXplosive", "Royal Demolition eXplosive", "cyclotrimethylene trinitramine", "hexahydro-1,3,5-trinitro-s-triazine", ("hexogen" AND (RDX OR explosive OR blast OR trinitrotoluene))	topic:("cyclonite" OR "hexolite" OR "1,3,5-trinitro-1,3,5-triazinane" OR "geksogen" OR "cyclotrimethylenetrinitramine" OR "trimethylenetrinitramine" OR "hexogeen" OR "1,3,5-trinitro-1,3,5-triazacyclohexane" OR "trimethyleentrinitramine" OR "cyclotrimethylenenitramine" OR "cyklonit" OR "1,3,5-triazine hexahydro-1,3,5-trinitro-" OR "hexahydro-1,3,5-trinitro-s-triazine" OR "trinitrocyclotrimethylene triamine" OR "trinitrotrimethylenetriamine" OR "sym-trimethylene trinitramine" OR "1,3,5-trinitrohexahydro-s-triazine" OR "cx 84a" OR "cyclonit" OR "1,3,5-triaza-1,3,5-trinitrocyclohexane" OR "1,3,5-trinitrohexahydro-1,3,5-triazine" OR "perhydro-1,3,5-trinitro-1,3,5-triazine" OR "nsc 312447" OR "unii-w91ssv5831" OR "trimethyleentrinitramine dutch" OR "1,3,5-trinitroperhydro-1,3,5-triazine" OR "hsdb 2079" OR "khp 281" OR "einecs 204-500-1" OR "sym-trimethylenetrinitramine" OR "brn 0288466" OR "s-triazine hexahydro-1,3,5-trinitro-" OR "esaidro-1,3,5-trinitro-1,3,5-triazina" OR "hexahydro-1,3,5-trinitro-1,3,5-triazin" OR "dtxsid9024142" OR "w91ssv5831" OR "ccris 9287" OR "trinitrohexahydrotriazine" OR "s-triazine 3,5-trinitro-" OR "schembl19770" OR "chebi:24556" OR "1,5-trinitrohexahydro-s-triazine" OR "hexahydro-1,5-trinitro-s-triazine" OR "nsc312447" OR "stk366162" OR "zinc64622596" OR "akos015914094" OR "1,5-trinitroperhydro-1,3,5-triazine" OR "mcule-5928095574" OR "nsc-312447" OR "1,5-triaza-1,3,5-trinitrocyclohexane" OR "1,5-trinitro-1,3,5-triazacyclohexane" OR "1,5-trinitrohexahydro-1,3,5-triazine"

					OR "esaidro-1,5-trinitro-1,3,5-triazina" OR "1,3,5-trinitro-1,3,5-triazinane #" OR "hexahydro-1,5-trinitro-1,3,5-triazin" OR "hexahydro-1,5-trinitro-1,3,5-triazine" OR "1,3,5-triazacyclohexane 1,3,5-trinitro-" OR "1,5-triazine hexahydro-1,3,5-trinitro-" OR "ls-155436" OR "ns00001970" OR "q190020" OR "CYCLONITE" OR "Hexolite" OR "1,3,5-Trinitro-1,3,5-triazinane" OR "Geksogen" OR "Cyclotrimethylenetrinitramine" OR "Hexahydro-1,3,5-trinitro-1,3,5-triazine" OR "Trimethylenetrinitramine" OR "Hexogeen" OR "1,3,5-Trinitro-1,3,5-triazacyclohexane" OR "Trimethyleentrinitramine" OR "Cyclotrimethylenenitramine" OR "Cyklonit" OR "1,3,5-Triazine hexahydro-1,3,5-trinitro-" OR "Hexahydro-1,3,5-trinitro-s-triazine" OR "Trinitrocyclotrimethylene triamine" OR "Trinitrotrimethylenetriamine" OR "sym-Trimethylene trinitramine" OR "1,3,5-Trinitrohexahydro-s-triazine" OR "CX 84A" OR "Cyclonit" OR "1,3,5-Triaza-1,3,5-trinitrocyclohexane" OR "1,3,5-Trinitrohexahydro-1,3,5-triazine" OR "Perhydro-1,3,5-trinitro-1,3,5-triazine" OR "NSC 312447" OR "UNII-W91SSV5831" OR "Trimethyleentrinitramine Dutch" OR "1,3,5-Trinitroperhydro-1,3,5-triazine" OR "HSDB 2079" OR "KHP 281" OR "EINECS 204-500-1" OR "sym-Trimethylenetrinitramine" OR "BRN 0288466" OR "s-Triazine hexahydro-1,3,5-trinitro-" OR "Esaidro-1,3,5-trinitro-1,3,5-triazina" OR "Hexahydro-1,3,5-trinitro-1,3,5-triazin" OR "DTXSID9024142" OR "W91SSV5831" OR "CCRIS 9287" OR "hexahydro-1" OR "Trinitrohexahydrotriazine" OR "s-Triazine 3,5-trinitro-" OR "cyclo-trimethylenetrinitramine" OR "SCHEMBL19770" OR "CHEBI:24556" OR "1,5-Trinitrohexahydro-s-triazine" OR "Hexahydro-1,5-trinitro-s-triazine" OR "1,3,5-trinitrohexahydro-p-triazine" OR "NSC312447" OR "STK366162" OR "ZINC64622596" OR "AKOS015914094" OR "1,5-Trinitroperhydro-1,3,5-triazine" OR "MCULE-5928095574" OR "NSC-312447" OR "1,5-Triaza-1,3,5-trinitrocyclohexane" OR "1,5-Trinitro-1,3,5-triazacyclohexane" OR "1,5-Trinitrohexahydro-1,3,5-triazine" OR "Esaidro-1,5-trinitro-1,3,5-triazina" OR "1,3,5-Trinitro-1,3,5-triazinane #" OR "Hexahydro-1,5-trinitro-1,3,5-triazin" OR "Hexahydro-1,5-trinitro-1,3,5-triazine" OR "1,3,5-Triazacyclohexane 1,3,5-trinitro-" OR "1,5-Triazine hexahydro-1,3,5-trinitro-" OR "LS-155436" OR "hexahydro-1,3,5-trinitro-1,3,5-triazine" OR "NS00001970" OR "Q190020" OR "CAS 121-82-4" OR "heksogen" OR RDX OR "Research Department eXplosive" OR "Royal Demolition eXplosive" OR "cyclotrimethylene trinitramine" OR "hexahydro-1,3,5-trinitro-s-triazine" OR ("hexogen" AND (RDX OR explosive OR blast OR trinitrotoluene)))
				added host	OR emm_caschemical__value:"121-82-4"
					AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR food OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management" OR wastewater OR "wild life" OR

					wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
13. Chlorinated paraffin 2020	(chemical names OR CAS value) AND host NOT "prep method"	YES	76	added host	topic:("4,8,11,14,17,21-hexachlorotetracosane" OR "chlorinated paraffin" OR "chlorowax 40" OR "ec 264-150-0" OR "schembl2577273" OR "chembl1892619" OR "ncgc00091464-01" OR "ns00014226" OR "Chlorowax 40" OR "cas 63449-39-8")
					OR emm_caschemical__value:"63449-39-8"
					AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR food OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management" OR wastewater OR "wild life" OR wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
14. Dicyclohexyl_phthalate 2020	chemical names OR CAS value NOT "prep method"	NO	13	added (DCHP AND phtalate)	topic:("dicyclohexyl phthalate" OR "ergoplast fdc" OR "unimoll 66" OR "ergoplast.fdc" OR "howflex cp" OR "phthalic acid dicyclohexyl ester" OR "dicyclohexyl benzene-1,2-dicarboxylate" OR "dicyclohexylphthalate" OR "hf 191" OR "kp 201" OR "1,2-benzenedicarboxylic acid dicyclohexyl ester" OR "unii-cgd15m7h2n" OR "nsc 6101" OR "ccris 6190" OR "hsdb 5246" OR "diclohexyl 1,2-benzenedicarboxylate" OR "ai3-00515 usda" OR "einecs 201-545-9" OR "brn 1889288" OR "cgd15m7h2n" OR "ai3-00515" OR "mls000736536" OR "dtxsid5025021" OR "chebi:34693" OR "1,2-benzenedicarboxylic acid 1,2-dicyclohexyl ester" OR "w-104111" OR "morflex 150" OR "unimoll 66 m" OR "uniplex 250" OR "acmc-209pvy" OR "phthalic acid dicyclohexyl" OR "dsstox_cid_5021" OR "ec 201-545-9" OR "dsstox_rid_77631" OR "dsstox_gsid_25021" OR "schembl29302" OR "ksc199e2t" OR "bidd:er0638" OR "chembl3185893" OR "nsc6101" OR "ks-00000g0y" OR "nsc-6101" OR "phthalic acid bis-cyclohexyl ester" OR "zinc1693279" OR "zx-at015572" OR "tox21_303132" OR "anw-37820" OR "mfcd00003849" OR "akos015840876" OR "ls-1835" OR "mcule-6607324429" OR "or61028" OR "cas-84-61-7" OR "ncgc00257008-01" OR "ak307696" OR "cc-26567" OR "ds-11413" OR "smr000528061" OR "db-056812" OR "ft-0624741" OR "ns00004690" OR "p0293" OR "st50319862" OR "c14529" OR "c-30080" OR "q1210373" OR "DICYCLOHEXYL PHTHALATE" OR "Ergoplast FDC" OR "Unimoll 66" OR "Ergoplast.fdc" OR

					"Howflex CP" OR "Phthalic acid dicyclohexyl ester" OR "Dicyclohexyl benzene-1,2-dicarboxylate" OR "Phthalic Acid Dicyclohexyl Ester" OR "Dicyclohexylphthalate" OR "HF 191" OR "KP 201" OR "1,2-Benzenedicarboxylic acid dicyclohexyl ester" OR "UNII-CGD15M7H2N" OR "NSC 6101" OR "CCRIS 6190" OR "HSDB 5246" OR "Diclohexyl 1,2-benzenedicarboxylate" OR "AI3-00515 USDA" OR "EINECS 201-545-9" OR "BRN 1889288" OR "CGD15M7H2N" OR "AI3-00515" OR "MLS000736536" OR "DTXSID5025021" OR "CHEBI:34693" OR "1,2-Benzenedicarboxylic acid 1,2-dicyclohexyl ester" OR "W-104111" OR "Morflex 150" OR "Unimoll 66 M" OR "Uniplex 250" OR "1 dicyclohexyl ester" OR "ACMC-209pvy" OR "Phthalic acid dicyclohexyl" OR "DSSTox_CID_5021" OR "EC 201-545-9" OR "DSSTox_RID_77631" OR "DSSTox_GSID_25021" OR "SCHEMBL29302" OR "KSC199E2T" OR "BIDD:ER0638" OR "CHEMBL3185893" OR "NSC6101" OR "KS-00000G0Y" OR "NSC-6101" OR "Phthalic acid bis-cyclohexyl ester" OR "ZINC1693279" OR "ZX-AT015572" OR "Tox21_303132" OR "ANW-37820" OR "MFCD00003849" OR "AKOS015840876" OR "LS-1835" OR "MCULE-6607324429" OR "OR61028" OR "CAS-84-61-7" OR "NCGC00257008-01" OR "AK307696" OR "CC-26567" OR "DS-11413" OR "SMR000528061" OR "cyclohexyl 2- cyclohexyloxycarbonyl benzoate" OR "DB-056812" OR "FT-0624741" OR "NS00004690" OR "P0293" OR "ST50319862" OR "C14529" OR "C-30080" OR "Q1210373" OR (DCHP AND phtalate))
					OR emm_caschemical__value:"84-61-7"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
15. Bis_2_4-dichlorobenzoyl_peroxide 202	chemical names OR CAS value NOT "prep method"	NO	2	Added "Enox DCBP" OR "NOVIPER DB 50" OR "Perkadox PD"	topic:("2,4-dichlorobenzoyl peroxide" OR "bis 2,4-dichlorobenzoyl peroxide" OR "cadox" OR "siloprene" OR "peroxide bis 2,4-dichlorobenzoyl" OR "unii-0qc93y0l96" OR "einecs 205-094-9" OR "brn 2008711" OR "dtxsid4044539" OR "0qc93y0l96" OR "bis 2,4-dichlorophenyl peroxyanhydride" OR "di- 2,4-dichlorobenzoyl peroxide" OR "perkadox pd" OR "ec 205-094-9" OR "2,4-dichlorobenzoylperoxide" OR "schembl15385" OR "ctk0h7230" OR "zinc1851007" OR "rw1263" OR "akos015849996" OR "cc-07377" OR "db-005856" OR "ls-102454" OR "ft-0631772" OR "ns00009864" OR "133d142" OR "a806566" OR "q27237102" OR "2,4-dichlorobenzoyl 2,4-dichlorobenzenecarboperoxoate" OR "di 2,4-dichlorobenzoyl peroxide" OR "2,4-dichlorobenzoic peroxyanhydride" OR "2,4-dichlorophenyl carbonyl 2,4-bis chloranyl benzenecarboperoxoate" OR "2,4-dichlorobenzenecarboperoxoic acid" OR "2,4-dichlorophenyl oxome" OR "luperco" OR "cas 133-14-2" OR "Enox DCBP" OR "NOVIPER DB 50" OR "Perkadox PD")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
					OR emm_caschemical__value:"133-14-2"

16. 4,4'-Oxybis(benzenesulfonyl h. 2020	chemical names OR CAS value NOT "prep method"	NO	3	-	topic:("4,4 oxybis benzenesulfonyl hydrazide" OR "serogen" OR "genitron" OR "zhenitron" OR "celogen" OR "4,4 oxybis benzenesulfonhydrazide" OR "cellmic" OR "celmike" OR "cenitron" OR "p p oxybis benzenesulfohydrazide" OR "4,4 oxydibenzenesulfonyl hydrazide" OR "diphenyloxide-4,4 disulfohydrazide" OR "4,4 oxydi benzenesulphonohydrazide" OR "diphenyl ether 4,4 disulfohydrazide" OR "p p oxybis benzenesulfonylhydrazine" OR "benzenesulfonic acid 4,4 oxybis dihydrazide" OR "oxybis benzenesulfonylhydrazide" OR "4,4 oxydi benzenesulfonyl dihydrazide" OR "unii-70377ej95z" OR "4,4 oxydibenzenesulfonic acid dihydrazide" OR "hsdb 5237" OR "4,4 oxybis benzenesulfonic acid hydrazide" OR "nsc 5318" OR "p p oxybis benzenesulfonyl hydrazide" OR "einecs 201-286-1" OR "oxybisbenzenesulfonic acid dihydrazide" OR "p p oxybisbenzene disulfonylhydrazide" OR "brn 2954604" OR "4,4 oxydi benzenesulfonic acid hydrazide" OR "dtxsid7026499" OR "4,4 oxybis benzenesulfonic acid dihydrazide" OR "benzenesulfonic acid 4,4 -oxydi dihydrazide" OR "70377ej95z" OR "benzenesulfonic acid 4,4 oxybis 1,1 dihydrazide" OR "w-104230" OR "dsstox_cid_6499" OR "ec 201-286-1" OR "dsstox_rid_78124" OR "dsstox_gsid_26499" OR "oprea1_874031" OR "schembl36774" OR "chembl1882501" OR "ctk5g0707" OR "nsc5318" OR "nsc-5318" OR "p p oxybis benzenesulfonhydrazide" OR "zinc1680846" OR "tox21_301976" OR "mfcd00007587" OR "akos001426105" OR "mcule-2213785759" OR "cas-80-51-3" OR "ncgc00164109-01" OR "ncgc00255179-01" OR "as-14554" OR "ls-32045" OR "sc-18194" OR "benzenesulfonic acid oxybis dihydrazide" OR "p p oxybis-benzenesulfonylhydrazide" OR "benzenesulfonic acid 4 oxybis dihydrazide" OR "benzenesulfonic acid 4 -oxydi dihydrazide" OR "ft-0654030" OR "ns00004831" OR "c-34194" OR "q27265828" OR "4,4 oxybis benzenesulfohydrazide" OR "70377EJ95Z" OR "dihydrazide4,4 oxybis-benzenesulfonic acid" OR "4,4 hydrazinesulfonyl phenoxy benzenesulfonohydrazide" OR "4,4-oxydi benzenesulphonohydrazide" OR "cas 80-51-3")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
					OR emm_caschemical__value:"80-51-3"
17. 4_4_-Methylenebis_2_chloroaniline 20	chemical names OR CAS value NOT "prep method"	NO	9	added "MOCA-HR" OR "Suncure M" OR "Vibracure A 133" OR "Isocross SM-L" OR "Cyanaset" OR "Quodorole" OR "Dacpm" OR "Curalin M" OR "Diamet Kh" OR "MOCA" OR "CUAMINE-	topic:("CAS 101-14-4" OR "CAS 27342-75-2" OR "4,4 amino-3-chlorobenzyl 2-chlorophenyl amine" OR "4,4-Amino-3-chlorobenzyl 2-chlorophenyl amine" OR "2,2 dichloro-4,4 methylendianiline" OR "2,2 methylenebis 4-methyl-6-tert-butylphenol monoacrylate" OR "2,2 Methylenebis 4-Methyl-6-Tert-Butylphenol Monoacrylate" OR "2,2 dichloro-4,4 methylene dianiline" OR "3,3 dichlor-4,4 diaminodiphenylmethan" OR "3,3 dichloro-4,4 diaminodifenilmetano" OR "3,3 dichloro-4,4 diaminodiphenyl methane" OR "3,3 dicloro-4,4 diaminodifenilmetano" OR "3,3 dichloro-4,4 diaminodiphenylmethane" OR "3,4 diaminodifenilmetano" OR "3,4 diaminodiphenylmethan" OR "4,3 dichlorodiphenyl methane" OR "4,4 -bis 2-chloroanilino methane" OR "4,4 diamino-3,3 dichlorodiphenyl methane" OR "4,4 methanediylbis 2chloroaniline" OR "4,4 methylene bis chloroaniline" OR "4,4 methylene bis ochloroaniline" OR "4,4 methylene-bis 2chloroaniline" OR "4,4 methylene-bis 2-chloroaniline" OR "4,4 methylene-bis-2-chloroaniline" OR "4,4 methylenebis 2-chlorobenzenamine" OR "4,4 methylenebis-2-chlorobenzenamine" OR "4,4 diamino3,3 dichlorodiphenylmethane" OR "4,4 methylene bis 2-chloroaniline" OR "4,4 methylenebis 2-chloroaniline" OR "4,4

				M" OR "MBOCA"	methylenebis o-chloroaniline" OR "4,4-methylene bis 2-chloroaniline" OR "4,4-methylenebis 2-chloroaniline" OR "4,4-metilene-bis-o-cloroanilina" OR "4,4-amino-3-chloro-phenyl methyl 2-chloro-aniline" OR "4,4-amino-3-chlorobenzyl 2-chlorophenylamine" OR "4,4-Amino-3-chlorobenzyl 2-chlorophenylamine" OR "4,4-amino-3-chlorophenyl methyl 2-chloroaniline" OR "4,4-amino-3-chlorophenyl methyl 2-chlorophenylamine" OR "acmc-1be7q" OR "akos000120884" OR "albb-010577" OR "aniline 4 methylenebis 2-chloro" OR "aniline 4,4 methylenebis 2-chloro" OR "aniline 4,4 methylenebis 2chloro" OR "anw-14437" OR "ar ar methylenebis 2-chlorobenzenamine" OR "ar ar Methylenebis 2-chlorobenzenamine" OR "benzenamine 4 methylenebis 2-chloro" OR "benzenamine 4,4 methylenebis 2-chloro" OR "benzenamine ar ar methylenebis 2-chloro" OR "bim-0013222 p001" OR "bis 3-chloro-4-aminophenyl methane" OR "bis 4-amino-3-chlorophenyl methane" OR "brn 1882318" OR "c10999" OR "cb03526" OR "cbmicro_013250" OR "ccris 389" OR "chebi 28124" OR "chembl82846" OR "ctk0h5881" OR "cuamine m" OR "cuamine mt" OR "curalin m" OR "curene 442" OR "cyanaset" OR "dacpm" OR "di 4-amino-3-chlorophenyl methane" OR "di 4-amino-3-clorofenil metano" OR "diamet kh" OR "dsstox_cid_865" OR "dsstox_gsid_20865" OR "dsstox_rid_75834" OR "dtxsid5020865" OR "ec 202-918-9" OR "einecs 202-918-9" OR "hms3039n14" OR "hsdb 2629" OR "ks-00000yp6" OR "ksc175q8d" OR "ld 813" OR "mboca" OR "mcule-3758655473" OR "met hylene-bis 2-chloroaniline 4,4" OR "methylene 4,4 bis o-chloroaniline" OR "methylene-4,4 bis o-chloroaniline" OR "methylene-bis 2-chloroaniline 4,4" OR "methylene-bis-orthochloroaniline" OR "methylenebis 2-chloroaniline" OR "methylenebis 3-chloro-4-aminobenzene" OR "methylenebis chloroaniline" OR "mfcd00047829" OR "mls002303002" OR "ncgc00090906-01" OR "ncgc00090906-02" OR "ncgc00258205-01" OR "ns00005883" OR "nsc 52954" OR "nsc-52954" OR "nsc52954" OR "oprea1_093196" OR "p p methylenebis alpha-chloroaniline" OR "p p methylenebis o-chloroaniline" OR "p p methylenebis ortho-chloroaniline" OR "poly bisphenol a-co-4,4 dichlorodiphenyl sulfone" OR "q2257591" OR "quodorole" OR "schembl43509" OR "smr001307314" OR "smsf0004157" OR "sr-01000197737" OR "sr-01000197737-1" OR "st50319834" OR "stk295634" OR "tox21_200651" OR "unii-3l2w5vtt2a" OR "w-108926" OR "w-6359" OR "zinc56414" OR "Suncure M" OR "Vibracure A 133" OR "Isocross SM-L" OR "Cyanaset" OR "Quodorole" OR "Dacpm" OR "Curalin M" OR "Diamet Kh" OR "CUAMINE-M" OR "MBOCA" OR (("MOCA" OR "MOCA-HR" OR "cl-mda") AND (amine OR "chain extender")))
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
				removed OR "bisamine" OR "bisamines" "bisamine" OR "bis-amine a" "cl-mda"	OR emm_caschemical__value:" 101-14-4"

18. 4-Chloro-2_5-dimethoxyacetoacet.	chemical names OR CAS value NOT "prep method"	NO	3	added "AADMC" OR "Acetoacet-4-chloro-2,5-dimethoxyanilide" OR "C.I. Azoic Coupling Component 44" OR "N-Acetoacetyl-4-chloro-2,5-dimethoxyaniline" OR "4-Chloro-2,5-dimethoxy-3-oxobutanamido benzene")	topic:("CAS 4433-79-8" OR "naphthol as-irg" OR "naphtol as-irg" OR "naphtanilide lrg" OR "naphtazol 4j" OR "naphtol as-lgll" OR "naphthol as 13gh" OR "unii-j086qhj1oc" OR "c i 37613" OR "einecs 224-638-6" OR "nsc 50638" OR "j086qhj1oc" OR "dtxsid5029265" OR "dsstox_cid_9265" OR "dsstox_rid_78740" OR "dsstox_gsid_29265" OR "w-106200" OR "cas-4433-79-8" OR "acmc-1akf0" OR "ec 224-638-6" OR "cbdive_007661" OR "schembl1118436" OR "chembl3185016" OR "ctk4i8127" OR "nsc50638" OR "zinc1682065" OR "zx-ah008408" OR "tox21_201666" OR "tox21_303485" OR "anw-30091" OR "bbl003545" OR "nsc-50638" OR "sbb013432" OR "stk520725" OR "akos000165629" OR "acm4433798" OR "mcule-2062409423" OR "aba-9371898" OR "ks-0000127d" OR "ncgc00249094-01" OR "ncgc00257262-01" OR "ncgc00259215-01" OR "ax8020849" OR "ls-167408" OR "st4121989" OR "ft-0654070" OR "ns00008147" OR "y-8542" OR "ab00075319-01" OR "a826549" OR "c-36221" OR "q27280985" OR "4 -chloro-2,5 -dimethoxyacetoacetanilide" OR "n 4-chloro-2,5-dimethoxyphenyl 3-oxobutanamide" OR "butanamide n 4-chloro-2,5-dimethoxyphenyl 3-oxo" OR "2,5-dimethoxy-4-chloroacetoacetanilide" OR "acetoacetyl-2,5-dimethoxy-4-chloroanilide" OR "acetoacetanilide 4 chloro-2,5 -dimethoxy" OR "4-chloro-2,5-dimethoxyacetoacetanilide" OR "acetoacet 2,5 dimethoxy 4 chloroanilide" OR "n 2,5-dimethoxy-4-chlorphenyl acetoacetamid" OR "n 4-chloro-2,5-dimethoxyphenyl acetoacetamide" OR "acetoacetanilide 4 chloro-2,5 dimethoxy 8ci" OR "Naphthol AS-IRG" OR "n 4-chloranyl-2,5-dimethoxy-phenyl 3-oxidanylidene-butanamide" OR "Naphtol AS-IRG" OR "Naphtanilide LRG" OR "Naphtazol 4J" OR "Naphtol AS-LGLL" OR "Naphthol AS 13GH" OR "UNII-J086QHJ1OC" OR "C I 37613" OR "EINECS 224-638-6" OR "NSC 50638" OR "J086QHJ1OC" OR "DTXSID5029265" OR "DSSTox_CID_9265" OR "DSSTox_RID_78740" OR "DSSTox_GSID_29265" OR "W-106200" OR "CAS-4433-79-8" OR "ACMC-1AKF0" OR "EC 224-638-6" OR "CBDivE_007661" OR "SCHEMBL1118436" OR "CHEMBL3185016" OR "CTK4I8127" OR "NSC50638" OR "ZINC1682065" OR "ZX-AH008408" OR "Tox21_201666" OR "Tox21_303485" OR "ANW-30091" OR "BBL003545" OR "NSC-50638" OR "SBB013432" OR "STK520725" OR "AKOS000165629" OR "ACM4433798" OR "MCULE-2062409423" OR "ABA-9371898" OR "KS-0000127D" OR "NCGC00249094-01" OR "NCGC00257262-01" OR "NCGC00259215-01" OR "AX8020849" OR "LS-167408" OR "ST4121989" OR "FT-0654070" OR "NS00008147" OR "Y-8542" OR "AB00075319-01" OR "A826549" OR "C-36221" OR "Q27280985" OR "4 Chloro-2,5 dimethoxyacetoacetanilide" OR "N 4-chloro-2,5-dimethoxyphenyl 3-oxobutanamide" OR "Butanamide N 4-chloro-2,5-dimethoxyphenyl 3-oxo" OR "2,5-Dimethoxy-4-chloroacetoacetanilide" OR "Acetoacetyl-2,5-dimethoxy-4-chloroanilide" OR "Acetoacetanilide 4 chloro-2,5 -dimethoxy" OR "4-Chloro-2,5-dimethoxyacetoacetanilide" OR "Acetoacet 2,5 Dimethoxy 4 Chloroanilide" OR "N 2,5-Dimethoxy-4-chlorphenyl acetoacetamid" OR "N 4-Chloro-2,5-dimethoxyphenyl acetoacetamide" OR "Acetoacetanilide 4 -chloro-2,5 dimethoxy" OR "N 4-chloranyl-2,5-dimethoxy-phenyl 3-oxidanylidene-butanamide" OR "AADMC" OR "Acetoacet-4-chloro-2,5-dimethoxyanilide" OR "C.I. Azoic Coupling Component 44" OR "N-Acetoacetyl-4-chloro-2,5-dimethoxyaniline" OR "4-Chloro-2,5-dimethoxy-3-oxobutanamido benzene")
				NOT patents	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR

				"preparation method"	"production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
					OR emm_caschemical__value:"4433-79-8"
19. 2_chloroaniline 2020	chemical names OR CAS value NOT "prep method"	NO	22	-	topic:("CAS 95-51-2" OR "2-chloroaniline" OR "o-chloroaniline" OR "2-chlorobenzenamine" OR "benzenamine 2-chloro" OR "2-chlorophenylamine" OR "1-amino-2-chlorobenzene" OR "o-aminochlorobenzene" OR "o-chloroaminobenzene" OR "aniline o-chloro" OR "o-chloraniline" OR "benzenamine chloro" OR "nsc 6183" OR "2-chloro aniline" OR "unii-g14i494t2f" OR "ccris 2880" OR "hsdb 2045" OR "2-chloro-aniline" OR "einecs 202-426-4" OR "ai3-16321" OR "g14i494t2f" OR "mfcd00007656" OR "2-chloroanilinium chloride" OR "codeine tms" OR "2-chloro-phenylamine" OR "2-amino-1-chlorobenzene" OR "benzeneamine 2-chloro" OR "dsstox_cid_1810" OR "acmc-209rz5" OR "ec 202-426-4" OR "dsstox_rid_76342" OR "dsstox_gsid_21810" OR "schembl25495" OR "ksc203m7l" OR "mls002454424" OR "bidd:gt0224" OR "chembl389885" OR "dtxsid2021810" OR "ctk1a3675" OR "nsc6183" OR "hms3039d15" OR "zinc164914" OR "ks-000002ly" OR "nsc-6183" OR "str00033" OR "tox21_200802" OR "anw-40527" OR "cc0074" OR "sbb040494" OR "stl168885" OR "akos000119118" OR "am87482" OR "ls-1978" OR "ls11568" OR "mcule-8604040668" OR "ncgc00091121-01" OR "ncgc00091121-02" OR "ncgc00258356-01" OR "sc-22931" OR "smr001372017" OR "db-020908" OR "ds-009850" OR "ft-0611903" OR "ns00010859" OR "st45255279" OR "az0001-0090" OR "79520-ep2305695a2" OR "79520-ep2305696a2" OR "79520-ep2305697a2" OR "79520-ep2305698a2" OR "139415-ep2270008a1" OR "139415-ep2275404a1" OR "139415-ep2280001a1" OR "139415-ep2284157a1" OR "139415-ep2292617a1" OR "j-509009" OR "q2294431" OR "z57127444" OR "f2190-0428" OR "2-CHLOROANILINE" OR "o-Chloroaniline" OR "2-Chlorobenzenamine" OR "Benzenamine 2-chloro" OR "2-Chlorophenylamine" OR "1-Amino-2-chlorobenzene" OR "o-Aminochlorobenzene" OR "o-Chloroaminobenzene" OR "Aniline o-chloro" OR "o-Chloraniline" OR "Benzenamine chloro" OR "NSC 6183" OR "2-Chloro aniline" OR "UNII-G14I494T2F" OR "CCRIS 2880" OR "HSDB 2045" OR "2-CHLORO-ANILINE" OR "EINECS 202-426-4" OR "AI3-16321" OR "G14I494T2F" OR "MFCD00007656" OR "2-Chloroanilinium chloride" OR "6-chloroaniline" OR "o-chloro-aniline" OR "Codeine TMS" OR "2-aminochlorobenzene" OR "2-Chloro-phenylamine" OR "1,2-aminochlorobenzene" OR "2-chlorophenyl amine" OR "2-Amino-1-chlorobenzene" OR "Benzeneamine 2-chloro" OR "DSSTox_CID_1810" OR "ACMC-209rz5" OR "EC 202-426-4" OR "DSSTox_RID_76342" OR "DSSTox_GSID_21810" OR "SCHEMBL25495" OR "KSC203M7L" OR "MLS002454424" OR "BIDD:GT0224" OR "CHEMBL389885" OR "DTXSID2021810" OR "CTK1A3675" OR "NSC6183" OR "HMS3039D15" OR "ZINC164914" OR "KS-000002LY" OR "NSC-6183" OR "STR00033" OR "Tox21_200802" OR "ANW-40527" OR "CC0074" OR "SBB040494" OR "STL168885" OR "AKOS000119118" OR "AM87482" OR "LS-1978" OR "LS11568" OR "MCULE-8604040668" OR "NCGC00091121-01" OR "NCGC00091121-02" OR "NCGC00258356-01" OR "SC-22931" OR "SMR001372017" OR "DB-020908" OR "DS-009850" OR "FT-0611903" OR "NS00010859" OR "ST45255279" OR "AZ0001-0090" OR "79520-EP2305695A2" OR "79520-EP2305696A2" OR "79520-EP2305697A2" OR "79520-EP2305698A2" OR "139415-EP2270008A1" OR "139415-EP2275404A1" OR "139415-EP2280001A1" OR "139415-EP2284157A1" OR

					"139415-EP2292617A1" OR "J-509009" OR "Q2294431" OR "Z57127444" OR "F2190-0428")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
					OR emm_caschemical__value:" 95-51-2"
20. 2,5-Diaminotoluene 2020	chemical names OR CAS value NOT "prep method"	NO	6	added 25TDA, Rodol PTD, ("TD solution" OR PTD) AND ("hair dye" OR hairdresser)	topic:("CAS 95-70-5" OR "1,4-benzenediamine 2-methyl" OR "2-methyl-1,4-benzenediamine" OR "4-amino-2-methylaniline" OR "p-toluylendiamine" OR "p m-tolylenediamine" OR "toluylene-2,5-diamine" OR "para-toluenediamine" OR "para-tolylenediamine" OR "para-toluylenediamine" OR "unii-24jo8z0rju" OR "2-methyl-para-phenylenediamine" OR "ccris 7693" OR "hsdb 6251" OR "einecs 202-442-1" OR "brn 0774521" OR "24jo8z0rju" OR "ci 76042" OR "dtxsid6029123" OR "chebi 53619" OR "epitope id 116061" OR "schembl34217" OR "schembl10580512" OR "ctk3i6913" OR "zinc388337" OR "act07295" OR "ks-000025xa" OR "anw-52954" OR "akos009158791" OR "gs-3190" OR "mcule-8138595213" OR "mp-2047" OR "sb40185" OR "ac-11774" OR "sc-18061" OR "db-057600" OR "ls-154040" OR "d4628" OR "ft-0609940" OR "ft-0610504" OR "ns00014161" OR "c19386" OR "095d705" OR "q2521416" OR "2-hydroxy-n 4-methyl-2-nitro-phenyl 3-nitro-benzamide" OR "2-methylbenzene-1,4-diamine" OR "1,4-Benzenediamine 2-methyl" OR "2-METHYL-1,4-BENZENEDIAMINE" OR "4-Amino-2-methylaniline" OR "2-Methyl-p-phenylenediamine" OR "p-Toluylendiamine" OR "p m-Tolylenediamine" OR "Toluylene-2,5-diamine" OR "para-Toluenediamine" OR "para-Tolylenediamine" OR "para-Toluylenediamine" OR "2-methyl-1,4-phenylenediamine" OR "UNII-24JO8Z0RJU" OR "2-Methyl-para-phenylenediamine" OR "CCRIS 7693" OR "HSDB 6251" OR "EINECS 202-442-1" OR "BRN 0774521" OR "24JO8Z0RJU" OR "CI 76042" OR "1-methyl-2,5-diaminobenzene" OR "2,5-diamino-1-methylbenzene" OR "2-methyl-benzene-1,4-diamine" OR "DTXSID6029123" OR "CHEBI 53619" OR "2,5-diaminotoluene sulphate" OR "p-toluylendiamin" OR "2,5-diamino toluene" OR "Epitope ID 116061" OR "SCHEMBL34217" OR

					"SCHEMBL10580512" OR "CTK3I6913" OR " 4-amino-2-methyl-phenyl amine" OR "ZINC388337" OR "ACT07295" OR "KS-000025XA" OR "ANW-52954" OR "AKOS009158791" OR "GS-3190" OR "MCULE-8138595213" OR "MP-2047" OR "SB40185" OR "AC-11774" OR "SC-18061" OR "2-Methyl-benzene-1,4-diamine" OR "DB-057600" OR "LS-154040" OR "D4628" OR "FT-0609940" OR "FT-0610504" OR "NS00014161" OR "C19386" OR "095D705" OR "Q2521416" OR "2-hydroxy-N 4-methyl-2-nitro-phenyl 3-nitro-benzamide" OR "2,5-diaminotoluene" OR "2,5-toluylenediamine" OR "2-methyl-p-phenylenediamine" OR "p-toluenediamine" OR "toluene-2,5-diamine" OR "toluene-2,5-diamine sulfate" OR "25TDA" OR "Rodol PTD" OR (("TD solution" OR PTD) AND ("hair dye" OR hairdresser)))
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
					OR emm_caschemical__value:"95-70-5"
21. 2,4-dihydroxy benzophenone 2020	chemical names OR CAS value NOT "prep method"	NO	28	added "Speedblock UV-0" , (("2,4-dhb" OR "2,4-DHB" OR "BP 1" OR BP1 OR DHB) AND ("uv filter" OR sunscreen))	topic:("CAS 31-56-6" OR "enzoresorcinol" OR "resbenzophenone" OR "inhibitor dhbp" OR "uvinul 400" OR "advastab 48" OR "uvistat 12" OR "uvinol 400" OR "quinsorb 010" OR "4-benzoyl resorcinol" OR "syntase 100" OR "dastib 263" OR "eastman inhibitor dhpb" OR "4-benzoylresorcinol" OR "nsc 38555" OR "unii-lj54r4z029" OR "hsdb 5617" OR "einecs 205-029-4" OR "brn 1311566" OR "mls000774789" OR "dtxsid8022406" OR "lj54r4z029" OR "mfcd00002277" OR "smr000365551" OR "benzophenone 4-dihydroxy" OR "dsstox_cid_2406" OR "dsstox_rid_76577" OR "dsstox_gsid_22406" OR "methanone 4-dihydroxyphenyl phenyl" OR "cas-131-56-6" OR "enamine_001926" OR "4,6-dihydroxybenzophenone" OR "acmc-209bn8" OR "ec 205-029-4" OR "chembl1392" OR "oprea1_840620" OR "schembl39681" OR "ksc174m3d" OR "bidd er0039" OR "bdbm51223" OR "ctk0h4631" OR "nsc5358" OR "hms1399h12" OR "hms2771p10" OR "zinc225430" OR "bcp25883" OR "ks-00000gu6" OR "nsc-5358" OR "nsc38555" OR "tox21_201285" OR "tox21_302865" OR "anw-19362" OR "bbl013153" OR "nsc-38555" OR "sbb063282" OR "stl163951" OR "akos001019876" OR "mcule-3025914301" OR "ne10164" OR "ncgc00246026-01" OR "ncgc00246026-02" OR "ncgc00256606-01" OR "ncgc00258837-01" OR "ac-11241" OR "ak-57631" OR "ds-15473" OR "ls-38903" OR "d0573" OR "ft-0610114" OR "ns00001568" OR "st50308028" OR "c14215" OR "135d566" OR "ae-641 01968047" OR "q209209" OR "sr-01000388910" OR "q-200188" OR "sr-01000388910-1" OR "92092-63-2" OR "2,4-dihydroxybenzophenone" OR "2,4-dihydroxyphenyl phenyl methanone" OR "benzophenone 2,4-hydroxy" OR "methanone 2,4-dihydroxyphenyl phenyl" OR "4-benzoylbenzene-1,3-diol" OR "2,4-dihydroxyphenyl phenylmethanone" OR "Benzoresorcinol" OR "Resbenzophenone" OR "Inhibitor DHBP" OR "Uvinul 400" OR "Advastab 48" OR "Uvistat 12" OR "Uvinol 400" OR "Quinsorb 010" OR "4-Benzoyl resorcinol" OR "Syntase 100" OR "Dastib 263" OR "Eastman Inhibitor DHPB" OR "Benzophenone 2,4-dihydroxy-" OR "4-Benzoylresorcinol" OR "NSC 38555" OR "UNII-LJ54R4Z029" OR "HSDB 5617" OR "EINECS 205-029-4"

					OR "BRN 1311566" OR "MLS000774789" OR " 2,4-bis oxidanyl phenyl phenyl-methanone" OR "DTXSID8022406" OR "LJ54R4Z029" OR "MFCD00002277" OR "SMR000365551" OR "Benzophenone 4-dihydroxy" OR "DSSTox CID 2406" OR "2,4-dihydroxy-benzophenon"OR "DSSTox RID 76577" OR "DSSTox GSID 22406" OR "2,4-dihydroxyphenyl phenyl ketone" OR "Methanone 4-dihydroxyphenyl phenyl" OR "CAS-131-56-6" OR "benzophenone 1" OR "Enamine_001926" OR "4,6-Dihydroxybenzophenone" OR "ACMC-209bn8" OR "2,4-dihydroxy-benzophenone" OR "EC 205-029-4" OR "cid 8572" OR "CHEMBL1392" OR "2,4-dihydroxybenzo phenone" OR "Oprea1 840620" OR "SCHEMBL39681" OR "hsp90 163" OR "KSC174M3D" OR "BIDD ER0039" OR "BDBM51223" OR "CTK0H4631" OR "NSC5358" OR "HMS1399H12" OR "HMS2771P10" OR "ZINC225430" OR "BCP25883" OR "KS-00000GU6" OR "NSC-5358" OR "NSC38555" OR "Tox21_201285" OR "Tox21_302865" OR "ANW-19362" OR "BBL013153" OR "NSC-38555" OR "SBB063282" OR "STL163951" OR "AKOS001019876" OR "MCULE-3025914301" OR "NE10164" OR "NCGC00246026-01" OR "NCGC00246026-02" OR "NCGC00256606-01" OR "NCGC00258837-01" OR "AC-11241" OR "AK-57631" OR "DS-15473" OR "LS-38903" OR "D0573" OR "FT-0610114" OR "NS00001568" OR "ST50308028" OR "C14215" OR "135D566" OR "AE-641 01968047" OR "Q209209" OR "SR-01000388910" OR "Q-200188" OR "SR-01000388910-1" OR "benzophenone 2,4-dihydroxy" OR "Speedblock UV 0" OR (("2,4-dhb" OR "2,4-DHB" OR "BP 1" OR BP1 OR DHB) AND ("uv filter" OR sunscreen)))
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
					OR emm_caschemical__value:"31-56-6"
22. 1,3-Dimethyl-3,4,5,6-tetr 2020	chemical names OR CAS value NOT "prep method"	NO	9	added "2(1H)-Pyrimidinone, tetrahydro-1,3-dimethyl-" OR "dimethyl propyleneurea" OR "Dimethylpropyleneurea" OR "N,N'-Dimethyltrimethyleneurea" OR "Tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one" OR "cas 7226-23-5" OR (DMPU AND (solvent	topic:("1,3-dimethyl-3,4,5,6-tetrahydro-2,1h -pyrimidinone" OR "1,3-dimethyltetrahydropyrimidin-2,1h -one" OR "dimethylpropyleneurea" OR "2,1h -pyrimidinone tetrahydro-1,3-dimethyl-" OR "n n -dimethylpropyleneurea" OR "n n -dimethyltrimethyleneurea" OR "ccris 4322" OR "n n -dimethylpropylene urea" OR "tetrahydro-1,3-dimethyl-1h-pyrimidin-2-one" OR "einecs 230-625-6" OR "mfcd00006550" OR "brn 0110562" OR "tetrahydro-1,3-dimethyl-2,1h pyrimidine" OR "dtxsid3074575" OR "ak-36216" OR "j-503925" OR "pubchem16903" OR "n n -dimethylproyleneurea" OR "ec 230-625-6" OR "schembl82580" OR "ksc498e3d" OR "chembl12284" OR "ctk3j8231" OR "zinc157131" OR "bcp25854" OR "str03401" OR "zx-at013447" OR "anw-36181" OR "sbb058374" OR "1,3-dimethyl-2-oxohexahydropyrimidine" OR "akos005145503" OR "cm13987" OR "cs-w009128" OR "mcule-5575317893" OR "or13656" OR "1,3-dimethyl-tetrahydro-pyrimidin-2-one" OR "1,3-dimethyltetrahydro-2,1h pyrimidinon" OR "1,3-dimethyltetrahydro-2,1h pyrimidone" OR "cc-03151" OR "1,3-dimethyl-tetrahydro-2,1h pyrimidone" OR "1,3-dimethyl-tetrahydro-2-1h-pyrimidinone" OR "ax8211152" OR "bb0295064" OR "db-011617" OR "ls-136022" OR "1,3-dimethyl tetrahydropyrimidin-2,1h -one" OR "1,3-dimethyltetrahydro-2,1h -pyrimidinone" OR "ft-0606689" OR "ns00005527" OR "st51016259" OR "2-pyrimidone tetrahydro 1,3-dimethyl" OR "en300-82368" OR "ks-00000143" OR "n n -dimethyl-n n -trimethyleneurea" OR "6632-ep1441224a2" OR "tetrahydro-1,3-dimethyl-2,1h pyrimidin-2-onee" OR "113513-ep2281820a2" OR "113513-ep2298754a1" OR

				OR cosolvent)) OR "1,3-dimethyl-3,4,5,6-tetra-hydro-pyrimidin-2(1H)-one"	"a837469" OR "c-34420" OR "dimethyl-3,4,5,6-tetrahydro-2,1h pyrimidinone" OR "n n dimethyl 1,4,5,6-tetrahydro-2-pyrimidone" OR "n n dimethyl-1,4,5,6-tetrahydro-2-pyrimidone" OR "q416637" OR "1,3-dimethyl-3,4,5,6-tetrahydro 2,1h pyrimidone" OR "1,3-dimethyl-3,4,5,6-tetrahydro-2,1h pyrimidone" OR "1,3-dimethyl-3,4,5,6-tetrahydro-2,1h pyrimidinon" OR "1,3-dimethyl-3,4,5,6-tetrahydro-2- 1h pyrimidone" OR "1,3-dimethyl-3,4,5,6-tetrahydro2,1h pyrimidinone" OR "1,3-dimethyl-3,4,5,6tetrahydro-2,1h pyrimidinone" OR "1,3-di-methyl-3,4,5,6-tetrahydro-2,1h pyrimidinone" OR "1,3-dim-ethyl-3,4,5,6-tetrahydro-2,1h pyrimidinone" OR "1,3-dimethyl -3,4,5,6-tetrahydro-2,1h pyrimidinone" OR "1,3-dimethyl-2,4,5,6-tetrahydro-2,1h pyrimidinone" OR "1,3-dimethyl-3,4,5,6-tetrahydro-2,1 h pyrimidinone" OR "1,3-dimethyl-3,4,5,6-tetrahydro-2,1h pyrirnidinone" OR "1,3-dimethyl-3,4,5,6-tetrahydro-2- 1h pyrimidinone" OR "f0001-1844" OR "1,3-di methyl-3,4,5,6-tetrahydro-2,1h pyrimidinone" OR "1,3-dimethyl-3,4,5,6-tetrahydro 2,1h pyrimidinone" OR "1,3-dimethyl-3,4,5,6-tetra-hydro 1h pyrimidin-2-one" OR "1,3-dimethyl-3,4,5,6-tetrahydro 2- 1h pyrimidone" OR "1,3-dimethyl-3,4,5,6-tetrahydro 1h pyrimidin-2-one" OR "1,3-dimethyltetrahydropyrimidin-2,1H one" OR "2(1H)-Pyrimidinone, tetrahydro-1,3-dimethyl-" OR "dimethyl propyleneurea" OR "Dimethylpropyleneurea" OR "N,N'-Dimethyltrimethyleneurea" OR "Tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one" OR "cas 7226-23-5" OR (DMPU AND (solvent OR cosolvent)))
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
					OR emm_caschemical__value:"7226-23-5"
23. 1-propanone, 2-methyl-1-[4-(me	chemical names OR CAS value NOT "prep method"	NO	3	added "genocure pmp" OR "IHT-PI 907" OR "Speedcure 97" OR "UV 907"	topic:("zinc19891833" OR "unii-722clj6h6k" OR "tox21_301664" OR "st50319490" OR "smr000019254" OR "schembl27554" OR "sbb056749" OR "q27266008" OR "ns00003224" OR "ncgc00255462-01" OR "mls000084908" OR "mcule-3119460562" OR "M2028" OR "ksc635c8d" OR "ks-00000c6c" OR "Irgacure 907" OR "hms2360j09" OR "ft-0641373" OR "eu-0035716" OR "dtxsid8038857" OR "dsstox_rid_79410" OR "dsstox_gsid_38857" OR "dsstox_cid_18857" OR "ds-3825" OR "db-055579" OR "ctk5d5181" OR "chembl1411716" OR "CC-11372" OR "cas-71868-10-5" OR "caccure 907" OR "C-17592" OR "brd-k58799690-001-07-3" OR "AX8016092" OR "anw-36110" OR "akos000520617" OR "ak114642" OR "acmc-1bitt" OR "ac-16227" OR "722clj6h6k" OR "2-methyl-4 methylthio-2-morpholinopropiophenone"~2 OR "2-methyl-4 methylthio 2-morpholinopropiophenone"~2 OR "2-methyl-4 methylthio 2-morpholino propiophenone" OR "2-methyl-1 4-methylthiophenyl 2-morpholinopropan-1-one" OR "2-methyl-1 4-methylthiophenyl 2-morpholino-1-propanone" OR "2-methyl-1 4-methylthiophenyl 2-morpholin-4-ylpropan-1-one" OR "2-methyl-1 4-methylsulfanylphenyl 2-morpholino-propan-1-one" OR "2-methyl-1- 4-methylsulfanylphenyl 2-morpholin-4-ylpropan-1-one" OR "2-methyl-1 4 methylthio phenyl 2-morpholinopropan-1-one" OR "2-methyl-1 4 methylthio phenyl 2-morpholino-1-propanone" OR "2-methyl-1 4 methylthio phenyl 2 4-morpholinyl 1-propanone" OR "2-methyl-1 4 methylsulfanyl phenyl 2-morpholin-4-ylpropan-1-one" OR "2-methyl-1 4 methylsulfanyl phenyl 2 morpholin-4-yl propan-1-one" OR "2-methyl-1 4 methylsulfanyl phenyl 2 4-morpholinyl 1-propanone" OR "1-propanone 2-methyl-1 4 methylthio

					phenyl 2 4-morpholinyl" OR "1-propanone 2-methyl-1- 4 methylthio phenyl 2 4-4-morpholinyl" OR "genocure pmp" OR "IHT-PI 907" OR "Speedcure 97" OR "UV 907")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
					OR emm_caschemical__value:"71868-10-5"
24. 3_4-Epoxycyclohexylmethyl_3_4-epoxycyclo	(chemical names OR CAS value)) AND host NOT "prep method"	YES	1	added "CELLOXIDE 2021P" OR "Syna-Epoxy 21" OR "TTA21" OR "Uvi-Cure S105" OR "Uvi-Cure S105E" OR "Uvi-Cure S110LV" OR "UVR-6110")	topic:("3 4-epoxycyclohexyl methyl 3 4-epoxycyclohexylcarboxylate" OR "7-oxabicyclo 4 1 0 heptan-3-ylmethyl 7-oxabicyclo 4 1 0 heptane-3-carboxylate" OR "3 4-epoxycyclohexylmethyl 3 4-epoxycyclohexanecarboxylate" OR "erl-4221" OR "ut-632" OR "chissonox 221 monomer" OR "unii-s224del3p4" OR "3 4-epoxycyclohexylmethyl 3 4-epoxycyclohexane carboxylate" OR "hsdb 5873" OR "einecs 219-207-4" OR "ut 632" OR "3 4-epoxycyclohexylmethyl-3 4-epoxycyclohexanecarboxylate" OR "3 4-epoxycyclohexanecarboxylic acid 3 4-epoxycyclohexylmethyl ester" OR "brn 1381750" OR "7-oxabicyclo 4 1 0 heptane-3-carboxylic acid 7-oxabicyclo 4 1 0 hept-3-ylmethyl ester" OR "s224del3p4" OR "dtxsid2027466" OR "3 4-epoxycyclohexanemethyl 3 4-epoxycyclohexanecarboxylate" OR "ak-78714" OR "dsstox_cid_7466" OR "7-oxabicyclo 4 1 0 hept-3-ylmethyl 7-oxabicyclo 4 1 0 heptane-3-carboxylate" OR "dsstox_rid_78463" OR "dsstox_gsid_27466" OR "w-107371" OR "cas-2386-87-0" OR "ccris 8882" OR "ec 219-207-4" OR "schembl24975" OR "ksc490c3p" OR "chembl2143072" OR "ctk3j0137" OR "bcp32770" OR "cel-2021" OR "tox21_202388" OR "tox21_303312" OR "anw-57541" OR "akos015915254" OR "ks-000001n6" OR "ncgc00164163-01" OR "ncgc00164163-02" OR "ncgc00256981-01" OR "ncgc00259937-01" OR "ls-98670" OR "sc-19925" OR "db-028268" OR "ft-0651573" OR "ns00011515" OR "3 4-epoxycyclohexylmethyl 3 4-epoxycyclohexanecarb" OR "a816945" OR "q19694494" OR "7-oxabicyclo 4 1 0 heptan-3-yl methyl 7-oxabicyclo 4 1 0 heptane-3-carboxylate" OR "7-oxabicyclo 4 1 0 heptan-3-ylmethyl 7-oxabicyclo 4 1 0 heptane" OR "7-Oxabicyclo 4 1 0 heptan-3-ylmethyl 7-oxabicyclo 4 1 0 heptane-3-carboxylate" OR "3 4-Epoxycyclohexylmethyl 3 4-epoxycyclohexanecarboxylate" OR "ERL-4221" OR "UT-632" OR "Chissonox 221 monomer" OR "UNII-S224DEL3P4" OR "3 4-Epoxycyclohexylmethyl 3 4-epoxycyclohexane carboxylate" OR "HSDB 5873" OR "3 4-Epoxycyclohexyl methyl 3 4-epoxycyclohexylcarboxylate" OR "EINECS 219-207-4" OR "UT 632" OR "3 4-Epoxycyclohexanecarboxylic acid 3 4-epoxycyclohexylmethyl ester" OR "BRN 1381750" OR "7-Oxabicyclo 4 1 0 heptane-3-carboxylic acid 7-oxabicyclo 4 1 0 hept-3-ylmethyl ester" OR "S224DEL3P4" OR "DTXSID2027466" OR "7-oxabicyclo 4 1 0 heptan-4-ylmethyl 7-oxabicyclo 4 1 0 heptane-4-carboxylate" OR "3 4-Epoxycyclohexanemethyl 3 4-epoxycyclohexanecarboxylate" OR "AK-78714" OR "DSSTox_CID_7466" OR "7-Oxabicyclo 4 1 0 hept-3-ylmethyl 7-oxabicyclo 4 1 0 heptane-3-carboxylate" OR "DSSTox_RID_78463" OR "DSSTox_GSID_27466" OR "W-107371" OR "7-oxabicyclo 4 1 0 hept-3-ylmethyl7-oxabicyclo 4 1 0 heptane-3-carboxylate" OR "CAS-2386-87-0" OR "CCRIS 8882" OR "EC 219-207-4" OR "3 4-epoxycyclohexylmethyl3 4-epoxycyclo-hexaneca" OR "SCHEMBL24975" OR "KSC490C3P" OR "CHEMBL2143072" OR "CTK3J0137" OR "BCP32770" OR

					"CEL-2021" OR "Tox21_202388" OR "Tox21_303312" OR "ANW-57541" OR "AKOS015915254" OR "KS-000001N6" OR "NCGC00164163-01" OR "NCGC00164163-02" OR "NCGC00256981-01" OR "NCGC00259937-01" OR "LS-98670" OR "SC-19925" OR "DB-028268" OR "FT-0651573" OR "NS00011515" OR "3 4-Epoxycyclohexylmethyl 3 4-epoxycyclohexanecarb" OR "A816945" OR "Q19694494" OR "3 4-epoxycyclohexylmethyl 3 4-epoxy cyclohexanecarboxylate" OR "3 4-epoxycyclohexylmethyl-3 4-epoxycyclohexane carboxylate" OR "7-Oxabicyclo 4 1 0 heptan-3-yl methyl 7-oxabicyclo 4 1 0 heptane-3-carboxylate" OR "7-oxabicyclo 4 1 0 heptane-4-carboxylic acid 7-oxabicyclo 4 1 0 heptan-4-ylmethyl ester" OR "7-Oxabicyclo 4 1 0 heptan-3-ylmethyl 7-oxabicyclo 4 1 0 heptane" OR "CELLOXIDE 2021P" OR "Syna-Epoxy 21" OR "TTA21" OR "Uvi-Cure S105" OR "Uvi-Cure S105E" OR "Uvi-Cure S110LV" OR "UVR-6110")
					OR emm_caschemical__value:"2386-87-0"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
				HOST	AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR food OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management OR" wastewater OR "wild life" OR wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
25.4_4Bis-dimethylamino-4-methylamino tr	(chemical names OR CAS value)) NOT "prep method"	NO	1		topic:("CAS 561-41-1" OR "dtxsid00204642" OR "einecs 209-218-2" OR "c i solvent violet 8" OR "ec 209-218-2" OR "schembl20561184" OR "ctk5a4694" OR "zinc5248289" OR "akos027257545" OR "ns00008275" OR "y1629" OR "benzenemethanol a a-bis 4 dimethylamino phenyl 4 methylamino" OR "alpha alpha-bis 4 dimethylamino phenyl 4 methylamino benzenemethanol" OR "DTXSID00204642" OR "EINECS 209-218-2" OR "C I Solvent Violet 8" OR "EC 209-218-2" OR "SCHEMBL20561184" OR "CTK5A4694" OR "ZINC5248289" OR "AKOS027257545" OR "NS00008275" OR "Y1629" OR "4 4 Bis dimethylamino 4 methylamino trityl alcohol" OR "Benzenemethanol a a-bis 4- dimethylamino phenyl 4 methylamino" OR "bis 4- dimethylamino phenyl 4-

					methylamino phenyl methanol" OR "4 4 bis dimethylamino 4 methylamino trityl alcohol" OR "alpha alpha Bis 4 dimethylamino phenyl 4 methylamino benzenemethanol" OR "alpha alpha-Bis 4 dimethylamino phenyl 4 methylamino benzenemethanol" OR "Solvent Violet 8" OR "Methyl Violet B base")
					OR emm_caschemical__value:"561-41-1"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
26.2,4,-Diphenylmethane diisocyanate	(chemical names OR CAS value)) AND host NOT "prep method"	YES	44		topic:("diphenylmethane diisocyanate" OR "bis 4-isocyanatophenyl methane" OR "isonate" OR "p p diphenylmethane diisocyanate" OR "1 1 methylenebis 4-isocyanatobenzene" OR "methylbisphenyl isocyanate" OR "4 4 methylenediphenyl diisocyanate" OR "4 4 diisocyanatodiphenylmethane" OR "methylene bisphenyl isocyanate" OR "methylene diphenyl diisocyanate" OR "4 4 -methylenebis phenyl isocyanate" OR "bis p-isocyanatophenyl methane" OR "diphenylmethyl diisocyanate" OR "caradate 30" OR "desmodur 44" OR "bis 1 4-isocyanatophenyl methane" OR "nacconate 300" OR "benzene 1 1 methylenebis 4-isocyanato" OR "isonate 125m" OR "methylenebis 4-isocyanatobenzene" OR "methylenebis p-phenyl isocyanate" OR "diphenyl methane diisocyanate" OR "methylenebis 4-phenyl isocyanate" OR "4 4 methylenediphenyl isocyanate" OR "rubinate 44" OR "methylenebis p-phenylene isocyanate" OR "methylenedi-p-phenylene diisocyanate" OR "methylenebis 4-phenylene isocyanate" OR "4 4 methylenedi-p-phenylene diisocyanate" OR "4 4 methylenediphenylene isocyanate" OR "hylene m50" OR "p p methylenebis phenyl isocyanate" OR "bis para-isocyanatophenyl methane" OR "polymeric mdi" OR "methylene di-p-phenylene isocyanate" OR "methylenebis para-phenyl isocyanate" OR "4 4 methylenedi phenyl isocyanate" OR "di 4-isocyanatophenyl methane" OR "difenil-metan-diisocianato" OR "methylenedi-para-phenylene diisocyanate" OR "methylenebis para-phenylene isocyanate" OR "para para diphenylmethane diisocyanate" OR "nci-c50668" OR "methylenediphenyl diisocyanate" OR "para para methylenebis phenyl isocyanate" OR "4 4 methylenediphenylene diisocyanate" OR "unii-b0lo6bbs8c" OR "generic mdi" OR "crude mdi" OR "isocyanic acid methylenedi-p-phenylene ester" OR "methylenebis phenylisocyanate" OR "ccris 2303" OR "4 4 diphenylmethanediisocyante" OR "chebi:53218" OR "isocyanic acid ester with diphenylmethane" OR "diphenylmethane p p diisocyanate" OR "hsdb 2630" OR "diphenylmethane 4 4 diisocyanate" OR "difenylmethaan-dissocyanaat" OR "nsc 9596" OR "einecs 202-966-0" OR "einecs 247-714-0" OR "b0lo6bbs8c" OR "non-isomeric-specific mdi" OR "brn 0797662" OR "diphenylmethan-4 4 diisocyanat" OR "isocyanic acid methylenediphenylene ester" OR "methylenebisphenyl diisocyanate" OR "ai3-15256" OR "dtxsid7025180" OR "methylenedi p-phenyl isocyanate" OR "methylenedi-p-phenyl diisocyanate" OR "4-4 diisocyanate de diphenylmethane" OR "4 4 2 4 2 2 diisocyanatodiphenylmethane" OR "methylenedi p-phenylene isocyanate" OR "4 4 mdi" OR "methylenediphenyl 4 4 diisocyanate" OR "methylenedi p-phenylene diisocyanate" OR "4 4 diisocyanate de diphenylmethane" OR "methylenediphenyl diisocyanate 4 4" OR "4 4 methylenedi phenylene isocyanate" OR "polymeric 4 4-methylenediphenyl diisocyanate" OR

					"dsstox_cid_4196" OR "methylenebis phenylisocyanate diisocyanates" OR "ccris 8160" OR "nocconate 300" OR "un2489" OR "hylene m 50" OR "hylene m-50" OR "difenylmethaan-diisocyanaat" OR "epitope id 113240" OR "ec 202-966-0" OR "dsstox_rid_77697" OR "dsstox_rid_82371" OR "dsstox_gsid_25180" OR "dsstox_gsid_47473" OR "schembl19943" OR "wln ocnr d1r dnco" OR "4-13-00-00396" OR "chembl1488467" OR "4 4 diphenylmethanediisocyanate" OR "ctk5c3260" OR "diphenylmethane 4 4-diisocyanate" OR "4 4-diphenylmethane diisocyanate" OR "nsc9596" OR "polymethylene polyphenyl isocynate" OR "4 4 diphenylmethane diisocyanate" OR "nsc-9596" OR "zinc1700075" OR "tox21_200268" OR "tox21_302585" OR "ls-334" OR "mfcd00036131" OR "sbb060784" OR "akos000119302" OR "methylenebis 4 4 phenyl isocyanate" OR "4 4 methylenedi phenyl diisocyanate" OR "benzene 1 methylenebis 4-isocyanato" OR "isocyanic acid diphenylmethylene ester" OR "mcule-4402925766" OR "ne10917" OR "un 2489" OR "methylenebis 4-phenylisocyanate" OR "ncgc00091061-01" OR "ncgc00091061-02" OR "ncgc00091061-03" OR "ncgc00256765-01" OR "ncgc00257822-01" OR "cas-9016-87-9" OR "ls-166061" OR "d0897" OR "ft-0617061" OR "ft-0625273" OR "st50825935" OR "1-isocyanato-4 4-isocyanatobenzyl benzene" OR "c19453" OR "q417646" OR "w-1089"OR "CAS 5873-54-1")
					OR emm_caschemical__value:"5873-54-1"
					AND topic:(alga OR algae OR air OR aquaculture OR aquatic OR aqueous OR arthropod OR bioaccumulat OR bioconcentrat OR "biological accumulation" OR "biological concentration" OR "biological interaction" OR biota OR bird OR birds OR cattle OR crop OR dairy OR daphnid OR ecological OR ecotoxic OR ecosystem OR effluent OR environment OR estuar OR fauna OR fish OR fishes OR fishery OR freshwater OR groundwater OR incineration OR influent OR influents OR invertebrate OR landfill OR lake OR leak OR mammal OR manure OR marine OR meat OR microalga OR micropollutant OR mollusc OR ocean OR pollutant OR pollution OR river OR seawater OR sewage OR sludge OR soil OR soils OR vertebrate OR "waste management" OR wastewater OR " waste water" OR "wild life" OR wildlife OR poultry OR pork OR "wild bore" OR pollinator OR fruit OR vegetable OR rabbit OR horse OR feed)
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

27. Melamine cyanurate	(chemical names OR CAS value)) NOT "prep method"	NO	217		(topic:("melamine cyanurate" OR "melamine isocyanurate" OR "melaminkyanurat" OR "mitec mx 601" OR "einecs 253-575-7" OR "nsc 231587" OR "1 3 5-triazine-2 4 6 1h 3h 5h -trione compound with 1 3 5-triazine-2 4 6-triamine" OR "1 3 5-triazine-2 4 6 1h 3h 5h -trione compound with 1 3 5-triazine-2 4 6-triamine 1:1" OR "s-triazine 2 4 6-triamino- compd. with s-triazine-triol" OR "melaminecyanurate" OR "melamine-cyanuric acid compd." OR "melamine cyanaurate" OR "einecs 240-292-9" OR "ec 253-575-7" OR "schembl34655" OR "c6h9n9o3" OR "dtxsid3068043" OR "ctk0i0670" OR "nsc231587" OR "akos015901107" OR "akos024319632" OR "mcule-6417519120" OR "nsc-231587" OR "as-12328" OR "ls-155567" OR "ft-0639392" OR "640m576" OR "c-24479" OR "q3267336" OR "1 5-triazine-2 4 6 1h 3h 5h -trione compd. with 1 3 5-triazine-2 4 6-triamine 1:1 " OR "Melamine cyanurate" OR "Melamine isocyanurate" OR "Melaminkyanurat" OR "Mitec MX 601" OR "EINECS 253-575-7" OR "NSC 231587" OR "16133-31-6" OR "1 3 5-Triazine-2 4 6 1H 3H 5H -trione compound with 1 3 5-triazine-2 4 6-triamine" OR "1 3 5-Triazine-2 4 6 1H 3H 5H -trione compound with 1 3 5-triazine-2 4 6-triamine 1:1" OR "s-Triazine 2 4 6-triamino- compd. with s-triazine-triol" OR "Melaminecyanurate" OR "1 3 5-triazinane-2 4 6-trione compound with 1 3 5-triazine-2 4 6-triamine 1:1" OR "Melamine-cyanuric acid compd." OR "Melamine cyanaurate" OR "EINECS 240-292-9" OR "melamine cyanuric acid" OR "melamine isocyanuric acid" OR "EC 253-575-7" OR "SCHEMBL34655" OR "C6H9N9O3" OR "DTXSID3068043" OR "CTK0I0670" OR "NSC231587" OR "AKOS015901107" OR "AKOS024319632" OR "MCULE-6417519120" OR "NSC-231587" OR "AS-12328" OR "LS-155567" OR "FT-0639392" OR "640M576" OR "C-24479" OR "Q3267336" OR "1 5-Triazine-2 4 6 1H 3H 5H -trione compd. with 1 3 5-triazine-2 4 6-triamine 1:1 ")
					OR emm_caschemical__value:("16133-31-6" OR "37640-57-6"))
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
28.2-Naphthalenamine, N-(2-ethylhexyl	(chemical names OR CAS value)	NO	0	Solvent Red 19E, N-(2-ethylhexyl)-1-[[2-methyl-4-[(2-methylphenyl)azo]phenyl]azo]naphthalen-1-amine	topic:("CAS 56358-09-9" OR "einecs 260-124-8" OR "ns00008278" OR "ec 260-124-8" OR "EINECS 260-124-8" OR "NS00008278" OR "EC 260-124-8" OR "2-naphthalenamine n-2-ethylhexyl 1 2-methyl-4- 2-methylphenyl azo phenyl azo" OR "n 2-ethylhexyl 1 2-methyl-4 2-methylphenyl azo phenyl azo naphthalen-1-amine" OR "n 2-ethylhexyl 1 2-methyl-4 2-methylphenyl diazenyl phenyl diazenyl 1 2-dihydronaphthalen-1-amine" OR "Solvent Red 19E"
					OR emm_caschemical__value:("56358-09-9")
29. 1,3-Divinylimidazolidin-2-one	(chemical names OR CAS value)	NO	0		topic:("einecs 237-457-2" OR "schembl41850" OR "1 3-divinylimidazolid-2-on" OR "1 3-divinyl-2-imidazolidone" OR "1 3-divinylimidazolidine-2-one" OR "1 3-divinyl-2-imidazolidinone" OR "zinc2526766" OR "akos006292919" OR "ft-0606733" OR "ns00020579" OR "w-110354" OR "q27273319" OR "1 3-Divinylimidazolidin-2-one" OR "2-Imidazolidinone 1 3-diethenyl-" OR "UNII-9WNU043766" OR "DTXSID8074734" OR "1 3-diethenylimidazolidin-2-one" OR "9WNU043766" OR "EINECS 237-457-2" OR "SCHEMBL41850" OR "1 3-Divinylimidazolid-2-on" OR "1 3-Divinyl-2-

					imidazolidone" OR "1 3-Divinylimidazolidine-2-one" OR "1 3-Divinyl-2-imidazolidinone" OR "ZINC2526766" OR "AKOS006292919" OR "FT-0606733" OR "NS00020579" OR "W-110354" OR "Q27273319" OR "CAS 13811-50-2" OR "N,N'-Divinyl-2-imidazolidinone" OR "N,N'-Divinylethyleneurea")
					OR emm_caschemical__value:"13811-50-2"
30.2_3-dihydro-2_2-dimethyl-1h-pe	(chemical names OR CAS value)	NO	0		topic:("CAS 6364-17-6" OR "unii-144c1zsa7u" OR "mls002694859" OR "144c1zsa7u" OR "dtxsid0073370" OR "schembl3171824" OR "chembl1868212" OR "ctk5b9605" OR "hms3085j09" OR "zinc392955" OR "1h-perimidine 2 3-dihydro-2 2-dimethyl-" OR "1h-perimidine 3-dihydro-2 2-dimethyl-" OR "2 2-dimethyl-2 3-dihydro-1h-perimidine" OR "2 3-dihydro-2 2-dimethyl-1h-perimidine" OR "UNII-144C1ZSA7U" OR "MLS002694859" OR "144C1ZSA7U" OR "DTXSID0073370" OR "SCHEMBL3171824" OR "CHEMBL1868212" OR "CTK5B9605" OR "HMS3085J09" OR "ZINC392955" OR "1H-Perimidine 2 3-dihydro-2 2-dimethyl-" OR "1H-Perimidine 3-dihydro-2 2-dimethyl-" OR "2 2-dimethyl-1 3-dihydroperimidine" OR "2 2-dimethyl-2 3-dihydro-1H-perimidine" OR "2 2-dimethyl-2 3-dihydroperimidine" OR "2 3-dihydro-2 2-dimethyl perimidine" OR "2 3-Dihydro-2 2-dimethyl-1H-perimidine")
					OR emm_caschemical__value:"6364-17-6"
31.1_3-Bis_citraconimidomethylene_benzen	(chemical names OR CAS value)) NOT "prep method"	NO	5		topic:("1 3-bis citraconimidomethylene benzene" OR "1 3-bis 3-methyl-2 5-dioxo-1h-pyrrolinylmethyl benzene" OR "dtxsid0073081" OR "bci-mx" OR "ec 412-570-1" OR "acmc-1c2x7" OR "schembl168682" OR "ctk4b1334" OR "zinc21993063" OR "akos015904331" OR "ft-0658961" OR "ns00005991" OR "1 1 1 3-phenylenebis methylene bis 3-methyl-1h-pyrrole-2 5-dione" OR "1h-pyrrole-2 5-dione 1 1 1 3-phenylenebis methylene bis 3-methyl-" OR "alpha alpha bis 3z 2 5-dioxo-3-methyl-3-pyrroline-1-yl m-xylene" OR "1 3-Bis citraconimidomethylene benzene" OR "1 3-bis 3-methyl-2 5-dioxo-1H-pyrrolinylmethyl benzene" OR "1h-pyrrole-2 5-dione 1 1 1 3-phenylenebis methylene bis 3-methyl" OR "3-methyl-1 3 3-methyl-2 5-dioxopyrrol-1-yl methyl phenyl methyl pyrrole-2 5-dione" OR "1 1 1 3-phenylenebis methylene bis 3-methyl-1H-pyrrole-2 5-dione" OR "Chitex AR-7" OR "PERKALINK 900" OR "cas-119462-56-5")
					OR emm_caschemical__value:"119462-56-5"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
32.Tris_1_3-dichloro-2-propyl_phosphate	(chemical names OR CAS value)) NOT "prep method"	NO	167		(topic:("tris 1 3-dichloro-2-propyl phosphate" OR "tris 1 3-dichloroisopropyl phosphate" OR "2-propanol 1 3-dichloro-phosphate 3:1" OR "phosphoric acid tris 1 3-dichloro-2-propyl ester" OR "fyrol fr-2" OR "1 3-dichloro-2-propanol phosphate 3:1" OR "unii-b1prv4g0t0" OR "tris 1-chloromethyl-2-chloroethyl phosphate" OR "tris 2-chloro-1- chloromethyl ethyl phosphate" OR "pf 38/3" OR "ccris 6284" OR "tri beta beta -dichloroisopropyl phosphate" OR "hsdb 4364" OR "einecs 237-159-2" OR "brn 1715458" OR "b1prv4g0t0" OR "fosforan troj-1 3-dwuchloroizopropylowy" OR "dtxsid9026261" OR "2-propanol 1 3-dichloro- 2 2 2 -phosphate" OR "fosforan troj- 1 3-dwuchloroizopropylowy polish" OR "dsstox_cid_6261" OR "dsstox_rid_78078" OR "dsstox_gsid_26261" OR "fyrol fr2" OR "tris- 1 3-dichloro-2-propyl -phosphate" OR "acmc-209c9q" OR "ec 237-159-2" OR "ksc496a6h" OR "schembl333198" OR

					"chembl3182032" OR "ctk3j6063" OR "chebi:143729" OR "tris 1 3-dichlorisopropyl phosphat" OR "ks-00000z7i" OR "zinc2019519" OR "tox21_202166" OR "tox21_300194" OR "anw-20172" OR "ls-798" OR "akos015856734" OR "cs-8011" OR "tris 1.3-dichloro-2-propyl phosphate" OR "tris- 1 3-dichloro-2-propyl phosphate" OR "ncgc00247923-01" OR "ncgc00247923-02" OR "ncgc00254047-01" OR "ncgc00259715-01" OR "ak116066" OR "ax8147868" OR "hy-108712" OR "ft-0654115" OR "ns00010388" OR "tris 1 3-dichlorisopropyl phosphate" OR "tri .beta. .beta. -dichloroisopropyl phosphate" OR "a807122" OR "j-006902" OR "q2454085" OR "Tris 1 3-dichloro-2-propyl phosphate" OR "tris 1 3-dichloropropan-2-yl phosphate" OR "TRIS 1 3-DICHLORO-2-PROPYL PHOSPHATE" OR "Tris 1 3-dichloroisopropyl phosphate" OR "2-Propanol 1 3-dichloro- phosphate 3:1" OR "Phosphoric Acid Tris 1 3-dichloro-2-propyl Ester" OR "Fyrol FR-2" OR "1 3-Dichloro-2-propanol phosphate 3:1" OR "UNII-B1PRV4G0T0" OR "Tris 1-chloromethyl-2-chloroethyl phosphate" OR "Tris 2-chloro-1- chloromethyl ethyl phosphate" OR "PF 38/3" OR "CCRIS 6284" OR "Tri beta beta -dichloroisopropyl phosphate" OR "HSDB 4364" OR "EINECS 237-159-2" OR "BRN 1715458" OR "B1PRV4G0T0" OR "Fosforan troj- 1 3-dwuchloroizopropylowy" OR "DTXSID9026261" OR "2-Propanol 1 3-dichloro- 2 2 2 -phosphate" OR "Fosforan troj- 1 3-dwuchloroizopropylowy Polish" OR "Phosphoric acid tris 1 3-dichloro-2-propyl ester" OR "DSSTox_CID_6261" OR "DSSTox_RID_78078" OR "DSSTox_GSID_26261" OR "Fyrol FR2" OR "Tris- 1 3-dichloro-2-propyl -phosphate" OR "ACMC-209c9q" OR "EC 237-159-2" OR "KSC496A6H" OR "SCHEMBL333198" OR "CHEMBL3182032" OR "CTK3J6063" OR "CHEBI:143729" OR "tri 2 3-dichloropropyl phosphate" OR "Tris 1 3-dichlorisopropyl phosphat" OR "KS-00000Z7I" OR "ZINC2019519" OR "Tox21_202166" OR "Tox21_300194" OR "ANW-20172" OR "LS-798" OR "AKOS015856734" OR "CS-8011" OR "Tris 1.3-dichloro-2-propyl phosphate" OR "Tris- 1 3-dichloro-2-propyl phosphate" OR "NCGC00247923-01" OR "NCGC00247923-02" OR "NCGC00254047-01" OR "NCGC00259715-01" OR "AK116066" OR "AX8147868" OR "HY-108712" OR "FT-0654115" OR "NS00010388" OR "Tris 1 3-dichlorisopropyl phosphate" OR "Tri .beta. .beta. -dichloroisopropyl phosphate" OR "tris 1 3-bis chloranyl propan-2-yl phosphate" OR "A807122" OR "J-006902" OR "Q2454085" OR "phosphoric acid tris 1 3-dichloropropan-2-yl ester" OR "phosphoric acid tris- 2-chloro-1-chloromethyl-ethyl ester"OR ((tdcpp OR TDCP OR TDCIPP) AND phosphate) OR "tris(2-chloro-1-(chloromethyl)ethyl) phosphate" OR "tris (1,3-dichloroisopropyl) phosphate" OR "Fyrol FR-2" OR "Antiblaze 195" OR "13674-87-8
					OR emm_caschemical__value:"13674-87-8"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

33. 1_3-Bis_citraconimidomethylene_benze	(chemical names OR CAS value)) NOT "prep method"	NO	0		1 3-bis citraconimidomethylene benzene OR "1 3-bis 3-methyl-2 5-dioxo-1h-pyrrolinylmethyl benzene" OR "dtxsid0073081" OR "bci-mx" OR "ec 412-570-1" OR "acmc-1c2x7" OR "schembl168682" OR "ctk4b1334" OR "zinc21993063" OR "akos015904331" OR "ft-0658961" OR "ns00005991" OR "1 1 1 3-phenylenebis methylene bis 3-methyl-1h-pyrrole-2 5-dione" OR "1h-pyrrole-2 5-dione 1 1 1 3-phenylenebis methylene bis 3-methyl-" OR "alpha alpha -bis 3z -2 5-dioxo-3-methyl-3-pyrroline-1-yl -m-xylene" OR "1 3-Bis citraconimidomethylene benzene" OR "1 3-bis 3-methyl-2 5-dioxo-1H-pyrrolinylmethyl benzene" OR "DTXSID0073081" OR "1H-Pyrrole-2 5-dione 1 1 1 3-phenylenebis methylene bis 3-methyl-" OR "3-methyl-1 3 3-methyl-2 5-dioxopyrrol-1-yl methyl phenyl methyl pyrrole-2 5-dione" OR "BCI-MX" OR "EC 412-570-1" OR "ACMC-1C2X7" OR "SCHEMBL168682" OR "CTK4B1334" OR "ZINC21993063" OR "1 3-bis citraconimidomethyl benzene" OR "AKOS015904331" OR "FT-0658961" OR "NS00005991" OR "1 1 1 3-Phenylenebis methylene bis 3-methyl-1H-pyrrole-2 5-dione" OR "1H-Pyrrole-2 5-dione 1 1- 1 3-phenylenebis methylene bis 3-methyl-" OR "alpha alpha -Bis 3Z -2 5-dioxo-3-methyl-3-pyrroline-1-yl -m-xylene" OR "alpha alpha bis 3z 2 5-dioxo-3-methyl-3-pyrroline-1-yl m-xylene" OR "1h-pyrrole-2 5-dione 1 1 1 3-phenylenebis methylene bis 3-methyl" OR "1 1 1 3-phenylenebis methylene bis 3-methyl-1H-pyrrole-2 5-dione" OR "CAS 119462-56-5"
					OR emm_caschemical__value:"119462-56-5"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
34. 2_4_-Diphenylmethane_diisocyanate	(chemical names OR CAS value)) NOT "prep method"	NO	0		topic:("o p-isocyanatobenzyl phenyl isocyanate" OR "2 4 diphenylmethane diisocyanate" OR "2 4 diisocyanatodiphenylmethane" OR "unii-yvq6nx5h3y" OR "diphenylmethane-2 4 diisocyanate" OR "benzene 1-isocyanato-2 4-isocyanatophenyl methyl " OR "2 4 diphenylmethanediisocyante" OR "einecs 227-534-9" OR "yvq6nx5h3y" OR "dtxsid9027607" OR "benzene 1-isocyanato-2- 4-isocyanatophenyl methyl " OR "isocyanic acid diester with 2 4 -methylenediphenol" OR "ccris 8159" OR "benzene 1 1 -methylenebis isocyanato polymer and polypropylene glycol" OR "ec 227-534-9" OR "schembl27122" OR "zinc1849831" OR "akos015916627" OR "benzene 1 1 methylenebis isocyanato polymer with alpha-hydro-omega-hydroxypoly oxy methyl-1 2-ethanediyl" OR "poly oxy methyl-1 2-ethanediyl alpha-hydro-omega-hydroxy polymer with 1 1 methylenebis isocyanatobenzene" OR "poly oxy methyl-1 2-ethanediyl alpha-hydro-omega-hydroxy- polymer with 1 1 -methylenebis isocyanatobenzene" OR "ds-021828" OR "ls-168513" OR "ft-0697125" OR "ns00004392" OR "2 4 -methylenebis phenyl isocyanate" OR "q27294734" OR "o p-Isocyanatobenzyl phenyl isocyanate" OR "2 4 Diphenylmethane diisocyanate" OR "2 4 Diisocyanatodiphenylmethane" OR "UNII-YVQ6NX5H3Y" OR "Diphenylmethane-2 4 diisocyanate" OR "Benzene 1-isocyanato-2- 4-isocyanatophenyl methyl" OR "2 4 Diphenylmethanediisocyante" OR "EINECS 227-534-9" OR "YVQ6NX5H3Y" OR "1-isocyanato-2 4-isocyanatobenzyl benzene" OR "DTXSID9027607" OR "Benzene 1-isocyanato-2 4-isocyanatophenyl methyl" OR "Isocyanic acid diester with 2 4 methylenediphenol" OR "CCRIS 8159" OR "Benzene 1 1 methylenebis isocyanato polymer and polypropylene glycol" OR "EC 227-534-9" OR "SCHEMBL27122" OR "diphenylmethan-2 4 diisocyanat" OR "2 4 methylenediphenyl

					diisocyanate" OR "ZINC1849831" OR "AKOS015916627" OR "Benzene 1 1 methylenebis isocyanato polymer" OR "Poly oxy methyl-1 2-ethanediyl alpha-hydro-omega-hydroxy polymer with 1 1 methylenebis isocyanatobenzene" OR "CAS 5873-54-1")
					OR emm_caschemical__value:"5873-54-1"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
35. Bis 2,6-diisopropylphenyl carbodiimi	(chemical names OR CAS value)) NOT "prep method"	NO	5		topic:("bis 2 6-diisopropylphenyl carbodiimide" OR "n n methanediylidenebis 2 6-diisopropylaniline" OR "carbo d" OR "staboxol 1" OR "unii-ypk27z98pl" OR "ypk27z98pl" OR "dtxsid5051862" OR "einecs 218-487-5" OR "n n bis 2 6-bis propan-2-yl phenyl methanediimine" OR "2 2 6 6 tetraisopropyldiphenylcarbodiimide" OR "carbodiimide bis 2 6-diisopropylphenyl" OR "n n methanetetraylbis 2 6-bis 1-methylethyl benzenamine" OR "benzenamine n n -methanetetraylbis 2 6-bis 1-methylethyl" OR "maybridge1_004202" OR "ksc496s8t" OR "schembl134760" OR "ctk3j6989" OR "hms553g24" OR "zinc8637108" OR "anw-24518" OR "mfcd00082211" OR "akos015915473" OR "mcule-5666921352" OR "ak114690" OR "as-10072" OR "ls-28354" OR "sc-28722" OR "sy035749" OR "db-119014" OR "ft-0654584" OR "ns00007917" OR "ec 218-487-5" OR "a815542" OR "w-109755" OR "n n bis 2 6-di propan-2-yl phenyl methanediimine" OR "q27894368" OR "2 6-diisopropylphenyl carbodiimide" OR "n n -bis 2 6-diisopropylphenyl carbodiimide" OR "bis 2 6-di-2-propylphenyl carbodiimide" OR "CAS 2162-74-5")
					OR emm_caschemical__value:"2162-74-5"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
36. Glycerol triglycidyl ether	(chemical names OR CAS value)) NOT "prep method"	NO	18		topic:("glycerol triglycidyl ether" OR "triglycidylglycerol" OR "1 2 3-tris 2 3-epoxypropoxy propane" OR "unii-0kvt2q7z17" OR "oxirane 2 2 2 - 1 2 3-propanetriyltris oxymethylene tris-" OR "0kvt2q7z17" OR "dtxsid00884584" OR "glycerine triglycidyl ether" OR "hsdb 6089" OR "glycerol 1 2 3-triglycidyl ether" OR "einecs 236-211-1" OR "propane 1 2 3-tris 2 3-epoxypropoxy -" OR "oxirane 2 2 2 - 1 2 3-propanetriyltris oxymethylene tris-homopolymer" OR "schembl36444" OR "epon-812" OR "ctk1c3979" OR "2 2 2 - 1 2 3-propanetriyltris oxymethylene trisoxirane" OR "akos015914389" OR "1 2 3-tris- 2 3-epoxypropoxy propane" OR "ns00051314" OR "q27236908" OR "Glycerol triglycidyl ether" OR "TRIGLYCIDYLGLYCEROL" OR "1 2 3-Tris 2 3-epoxypropoxy propane" OR "UNII-0KVT2Q7Z17" OR "Oxirane 2 2 2 - 1 2 3-propanetriyltris oxymethylene tris-" OR "0KVT2Q7Z17" OR "DTXSID00884584" OR "2- 1 3-bis oxiran-2-ylmethoxy propan-2-yloxymethyl oxirane" OR "hloro-2 3-epoxypropane ge 100" OR "Glycerine triglycidyl ether" OR "HSDB 6089" OR "Glycerol 1 2 3-triglycidyl ether" OR "EINECS 236-211-1" OR "Glycerol tris 2 3-epoxypropyl ether" OR "Propane 1 2 3-tris 2 3-epoxypropoxy -" OR "Oxirane 2 2 2 - 1 2 3-propanetriyltris oxymethylene tris-homopolymer" OR "SCHEMBL36444" OR "EPON-812" OR "CTK1C3979" OR "2 2 2 - 1 2 3-Propanetriyltris oxymethylene trisoxirane" OR "glycerol tris 2 3-epoxypropyl ether" OR "AKOS015914389" OR "1 2 3-tris- 2 3-Epoxypropoxy propane" OR "NS00051314" OR "Q27236908" OR "2 2 2 - 1 2 3-

					propanethyltris oxymethylene tris oxirane" OR "2 2 2 -propane-1 2 3-triyltris oxy tris methylene trioxirane" OR "CAS 13236-02-7" OR "CAS 90529-77-4")
					OR emm_caschemical__value:("13236-02-7" OR "90529-77-4")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
36. hexabromocyclododecane	(chemical names OR CAS value)) NOT "prep method"	NO	75		topic:("cyclododecane 1 2 5 6 9 10-hexabromo" OR "1 2 5 6 9 10-hexabromocyclodecane" OR "unii-66oon1wwos" OR "hsdb 6110" OR "einecs 221-695-9" OR "66oon1wwos" OR "dsstox_cid_7527" OR "dsstox_rid_78489" OR "dsstox_gsid_27527" OR "cas-3194-55-6" OR "acmc-1bn89" OR "schembl25669" OR "ksc491m2h" OR "chembl375298" OR "dtxsid4027527" OR "ctk3j1623" OR "chebi:134063" OR "tox21_201402" OR "tox21_303176" OR "anw-27232" OR "akos015836044" OR "1 2 5 6 9 10-hexabromocyclododecan" OR "ks-0000010e" OR "ncgc00164063-01" OR "ncgc00164063-02" OR "ncgc00257050-01" OR "ncgc00258953-01" OR "ak116613" OR "ls-55963" OR "sc-18694" OR "ax8052905" OR "db-068553" OR "ft-0626944" OR "ns00002582" OR "1 2 5 6 9 10-hexabromocyclododecane 95%" OR "1 2 5 6 9 10-hexabromocyclododecane hbcd" OR "q420301" OR "w-106868" OR "Cyclododecane 1 2 5 6 9 10-hexabromo-" OR "1 2 5 6 9 10-Hexabromocyclodecane" OR "UNII-66OON1WWOS" OR "HSDB 6110" OR "EINECS 221-695-9" OR "66OON1WWOS" OR "DSSTox_CID_7527" OR "DSSTox_RID_78489" OR "DSSTox_GSID_27527" OR "CAS-3194-55-6" OR "ACMC-1BN89" OR "SCHEMBL25669" OR "KSC491M2H" OR "CHEMBL375298" OR "DTXSID4027527" OR "CTK3J1623" OR "CHEBI:134063" OR "Tox21_201402" OR "Tox21_303176" OR "ANW-27232" OR "AKOS015836044" OR "1 2 5 6 9 10-Hexabromocyclododecan" OR "KS-0000010E" OR "NCGC00164063-01" OR "NCGC00164063-02" OR "NCGC00257050-01" OR "NCGC00258953-01" OR "AK116613" OR "LS-55963" OR "SC-18694" OR "AX8052905" OR "DB-068553" OR "FT-0626944" OR "NS00002582" OR "1 2 5 6 9 10-Hexabromocyclododecane 95%" OR "1 2 5 6 9 10-Hexabromocyclododecane HBCD" OR "Q420301" OR "W-106868" OR "hexabromocyclododecane" OR "CAS 3194-55-6")
					OR emm_caschemical__value:"3194-55-6"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

38. Methyl_N-_3-acetylamino_-4-_2-cyano-	(chemical names OR CAS value))	NO	0		topic:("dtxsid90889003" OR "methyl n- 3-acetylamino -4- 2-cyano-4-nitrophenylazo phenyl -n- 1-methoxy acetyl glycinate" OR "glycine n- 3- acetylamino -4- 2- 2-cyano-4-nitrophenyl diazenyl phenyl -n- 2-methoxy-2-oxoethyl - methyl ester" OR "acmc-20n5u8" OR "ec 413-040-2" OR "schembl14379275" OR "schembl15886748" OR "ctk4c6396" OR "3- acetylamino -4- 2-cyano-4-nitrophenyl azo phenyl imino diacetic acid dimethyl ester" OR "DTXSID90889003" OR "methyl N- 3-acetylamino -4- 2-cyano-4-nitrophenylazo phenyl -N- 1-methoxy acetyl glycinate" OR "Glycine N- 3-acetylamino -4- 2- 2-cyano-4-nitrophenyl diazenyl phenyl -N-2-methoxy-2-oxoethyl - methyl ester" OR "ACMC-20n5u8" OR "EC 413-040-2" OR "SCHEMBL14379275" OR "SCHEMBL15886748" OR "CTK4C6396" OR "3- Acetylamino -4- 2-cyano-4-nitrophenyl azo phenyl imino diacetic acid dimethyl ester" OR "CAS 149850-30-6")
					OR emm_caschemical__value:"149850-30-6"
39. n_nprime-di-sec-butyl-p-phenylenedia	(chemical names OR CAS value)) NOT "prep method"	NO	9		topic:("antioxidant 22" OR "n1 n4-di-sec-butylbenzene-1 4-diamine" OR "topanol m" OR "kerobit bpd" OR "tenamene 2" OR "santoflex 44" OR "n n -di-sec-butyl-p-phenyldiamine" OR "n n -di-sec-butylparaphenylenediamine" OR "n n -di-sec-butyl-1 4-phenylenediamine" OR "1 4-benzenediamine n n -bis 1-methylpropyl -" OR "nsc 68417" OR "ccris 4603" OR "hsdb 5343" OR "p-phenylenediamine n n -di-sec-butyl-" OR "n n -bis 1-methylpropyl -1 4-benzenediamine" OR "n n -bis 1-methylpropyl -1 4-phenylenediamine" OR "unii-76251wu9i2" OR "n n -di-sek.butyl-p-fenylendiamin" OR "einecs 202-992-2" OR "brn 2805827" OR "dtxsid7024956" OR "1 4-benzenediamine n1 n4-bis 1-methylpropyl -" OR "76251wu9i2" OR "naugalube 403" OR "nn -di-sec-butyl-p-phenylenediamine" OR "n n -1 4-bis sec-butylamino benzene" OR "acmc-1c9jn" OR "dsstox_cid_4956" OR "ec 202-992-2" OR "dsstox_rid_77598" OR "dsstox_gsid_24956" OR "schembl49805" OR "mls002454420" OR "1 4-bis sec-butylamino benzene" OR "chembl1409985" OR "ctk3j0317" OR "1 n n -bis 1-methylpropyl -" OR "kuc107773n" OR "albb-024364" OR "ksc-09-264a" OR "nsc68417" OR "str09249" OR "zx-an022878" OR "tox21_200371" OR "anw-14561" OR "nsc-68417" OR "p-phenylenediamine n -di-sec-butyl-" OR "sbb008194" OR "akos015888191" OR "ks-000016u9" OR "n n -di-sec-butyl-1 4-benzenediamine" OR "n n -di-sec-butyl-benzene-1 4-diamine" OR "ncgc00091814-01" OR "ncgc00091814-02" OR "ncgc00091814-03" OR "ncgc00091814-04" OR "ncgc00257925-01" OR "ak114296" OR "cas-101-96-2" OR "cc-31723" OR "smr001372014" OR "st095686" OR "n n -di butan-2-yl benzene-1 4-diamine" OR "ax8017296" OR "db-080853" OR "ft-0629588" OR "n n -di-sec-butyl-p-phenylenediamine 95%" OR "n1 n4-bis butan-2-yl benzene-1 4-diamine" OR "ns00003277" OR "nn -bis 1-methylpropyl -1 4-phenylenediamine" OR "1 4-benzenediamine n n -bis 1-methylpropyl - dihydrochloride" OR "N N -Di-sec-butyl-p-phenylenediamine" OR "Antioxidant 22" OR "N1 N4-Di-sec-butylbenzene-1 4-diamine" OR "Topanol M" OR "Kerobit BPD" OR "Tenamene 2" OR "Santoflex 44" OR "N N -DI-SEC-BUTYL-P-PHENYLDIAMINE" OR "N N -Di-s-butyl-p-phenylenediamine" OR "N N -Di-sec-butylparaphenylenediamine" OR "N N -Di-sec-butyl-1 4-phenylenediamine" OR "1 4-Benzenediamine N N -bis 1-methylpropyl -" OR "NSC 68417" OR "CCRIS 4603" OR "HSDB 5343" OR "p-Phenylenediamine N N -di-sec-butyl-" OR "N N -Bis 1-methylpropyl -1 4-benzenediamine" OR "N N -Bis 1-methylpropyl -1 4-phenylenediamine" OR "UNII-76251WU9I2"

					OR "N N -Di-sek.butyl-p-fenylendiamin" OR "EINECS 202-992-2" OR "BRN 2805827" OR "DTXSID7024956" OR "1 4-Benzenediamine N1 N4-bis 1-methylpropyl -" OR "76251WU9I2" OR "N N -di-sec-butylbenzene-1 4-diamine" OR "methylpropyl 4- methylpropyl amino phenyl amine" OR "Naugalube 403" OR "NN -Di-sec-butyl-p-phenylenediamine" OR "N N -1 4-Bis sec-butylamino benzene" OR "ACMC-1C9JN" OR "DSSTox_CID_4956" OR "EC 202-992-2" OR "DSSTox_RID_77598" OR "DSSTox_GSID_24956" OR "SCHEMBL49805" OR "MLS002454420" OR "1 4-Bis sec-butylamino benzene" OR "CHEMBL1409985" OR "CTK3J0317" OR "1 N N -bis 1-methylpropyl -" OR "KUC107773N" OR "ALBB-024364" OR "KSC-09-264A" OR "NSC68417" OR "STR09249" OR "ZX-AN022878" OR "Tox21_200371" OR "ANW-14561" OR "NSC-68417" OR "p-Phenylenediamine N -di-sec-butyl-" OR "SBB008194" OR "AKOS015888191" OR "KS-000016U9" OR "n n -di-2-butyl-1 4-phenylenediamine" OR "N N -Di-sec-butyl-1 4-benzenediamine" OR "N N -di-sec-butyl-benzene-1 4-diamine" OR "NCGC00091814-01" OR "NCGC00091814-02" OR "NCGC00091814-03" OR "NCGC00091814-04" OR "NCGC00257925-01" OR "AK114296" OR "CAS-101-96-2" OR "CC-31723" OR "SMR001372014" OR "ST095686" OR "N N -di butan-2-yl benzene-1 4-diamine" OR "AX8017296" OR "DB-080853" OR "FT-0629588" OR "N N -Di-sec-butyl-p-phenylenediamine 95%" OR "N1 N4-bis butan-2-yl benzene-1 4-diamine" OR "NS00003277" OR "NN -Bis 1-methylpropyl -1 4-phenylenediamine" OR "N N -di-sec-butyl-p-phenylenediamine" OR "1 4-benzenediamine N N -bis 1-methylpropyl - dihydrochloride" OR "n n -di-sec-butylbenzene-1 4-diamine" OR "n n -di-sec-butyl-p-phenylene" OR "p-phenylenediamine n n -di-sec-butyl" OR "n n -di(butan-2-yl)benzene-1 4-diamine" OR "1 4-benzenediamine n n -bis(1-methylpropyl)" OR "n n -di-s-butyl-p-phenylenediamine" OR "n n -di-sec-butyl-p-phenylenediamine" OR "CAS 101-96-2")
					OR emm_caschemical__value:"101-96-2"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
40. paranitroaniline	(chemical names OR CAS value)) NOT "prep method"	NO			4-nitroaniline OR "4-nitroaniline monohydrochloride" OR "para-nitroaniline" OR "paranitronaniline" OR "p-nitroaniline" OR "4-nitro-aniline" OR "4-nitro-phenylamine" OR "4-nitrobenzenamine" OR "CAS 100-01-6" OR "4-benzenamine" OR "p-benzenamine" OR "4-nitro benzenamine" OR "4-nitroaniline" OR "p-nitroaniline" OR "4-nitro nitroaniline"
					OR emm_caschemical__value:"100-01-6"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

41. Phenolphtaleine 2020	(chemical names OR CAS value)) NOT "prep method "	NO			"phthalimetten" OR "euchessina" OR "phthalin" OR "espotabs" OR "phenolax" OR "purgophen" OR "koprol" OR "laxogen" OR "trilax" OR "spulmako-lax" OR "chocolax" OR "purgen" OR "correctol" OR "alophen" OR "doxidan" OR "medilax" OR "colax" OR "laxin" OR "femilax" OR "phenophthalein" OR "nci-c55798" OR "unii-6qk969r2if" OR "nsc 10464" OR "ccris 6266" OR "hsdb 4161" OR "einecs 201-004-7" OR "mfcd00005913" OR "brn 0284423" OR "chembl63857" OR "ai3-09081" OR "mls000069592" OR "6qk969r2if" OR "dtxsid0021125" OR "chebi:34914" OR "ncgc00018200-07" OR "smr000059015" OR "dsstox_cid_1125" OR "dsstox_rid_75956" OR "dsstox_gsid_21125" OR "evac-v-lax" OR "1 3h isobenzofuranone 3 3bis 4-hydroxyphenyl " OR "pubchem7084" OR "spectrum_001077" OR "opera_id_1337" OR "spectrum2_001279" OR "spectrum3_000888" OR "spectrum4_000982" OR "spectrum5_001268" OR "ec 201-004-7" OR "schembl27670" OR "bspbio_002518" OR "kbiogr_001383" OR "kbioss_001557" OR "mls001148397" OR "bidd:er0202" OR "divk1c_000929" OR "spectrum1500480" OR "spbio_001278" OR "aronis002962" OR "bcbcmap01_000174" OR "hms502o11" OR "kbio1_000929" OR "kbio2_001557" OR "kbio2_004125" OR "kbio2_006693" OR "kbio3_001776" OR "ks-00000yjd" OR "ninds_000929" OR "hms1920h04" OR "hms2091p06" OR "hms2236i09" OR "hms3374p06" OR "pharmakon1600-01500480" OR "hy-d0211" OR "ks-00003w2p" OR "nsc10464" OR "zinc3831317" OR "tox21_110838" OR "tox21_202219" OR "tox21_300282" OR "bbl002030" OR "bdbm50077844" OR "ccg-39112" OR "nsc-10464" OR "nsc215214" OR "nsc757271" OR "sbb008868" OR "stk029876" OR "akos000493033" OR "tox21_110838_1" OR "mcule-5232154932" OR "nsc-215214" OR "nsc-757271" OR "idi1_000929" OR "smp1_000235" OR "ncgc00018200-01" OR "ncgc00018200-02" OR "ncgc00018200-03" OR "ncgc00018200-04" OR "ncgc00018200-05" OR "ncgc00018200-06" OR "ncgc00018200-08" OR "ncgc00018200-09" OR "ncgc00018200-10" OR "ncgc00018200-12" OR "ncgc00023694-03" OR "ncgc00023694-04" OR "ncgc00023694-05" OR "ncgc00023694-06" OR "ncgc00023694-07" OR "ncgc00254039-01" OR "ncgc00259768-01" OR "ac-14431" OR "ak130019" OR "bp-30100" OR "sc-74728" OR "st072636" OR "sbi-0051481.p003" OR "2 bis 4-hydroxyphenyl methyl benzoic acid" OR "eu-0082600" OR "ft-0659094" OR "ns00008592" OR "en300-92962" OR "alpha alpha di p-hydroxyphenyl phthalide" OR "ab00052070_15" OR "sr-01000000112" OR "sr-01000000112-2" OR "3 3-bis 4-hydroxyphenyl 2-benzofuran-1 3h one " OR "brd-k19227686-001-02-0" OR "brd-k19227686-001-12-9" OR "z57233591" OR "f0921-4309" OR "alpha alpha-di p-hydroxyphenyl phthalide" OR "1 3h isobenzofuranone 3 3-bis 4-hydroxyphenyl " OR "1 3h isobenzofuranone 3-bis 4-hydroxyphenyl " OR "2- bis 4-hydroxyphenyl methyl benzoic acid" OR "3 3-bis p-hydroxyphenyl 1 3h isobenzofuranone" OR "3 3-bis 4-hydroxyphenyl 1 3h isobenzofuranone" OR "3 3-bis 4-hydroxyphenyl 2-benzofuran-1 3h one" OR "3 3-bis 4-hydroxy-phenyl 3h-isobenzofuran-1-one" OR "3 3-bis 4-hydroxyphenyl isobenzofuran-1 3h one" OR "3 3-bis 4-hydroxyphenyl phthalide" OR "3 3-bis p-hydroxyphenyl phthalide" OR "alpha-p-hydroxyphenyl -alpha 4-oxo-2 5-cyclohexadien-1-ylidene o-toluic acid" OR "alpha-di p-hydroxyphenyl phthalide" OR "dihydroxyphthalophenone" OR "fenolftalein" OR "fenolftaleina" OR "phenolphtaleine" OR "phenolphthaleinum"

					OR "phthalide 3 3 bis p-hydroxyphenyl " OR "phthalide 3 -bis p-hydroxyphenyl" OR "CAS 77-09-8"
					OR emm_caschemical__value:"100-01-6"
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
42.phenol, 2,2'-((1-methyl-1,2-ethanediy	(chemical names OR CAS value))	NO	0		topic:("phenol 2 2 - 1-methyl-1 2-ethanediyl bis nitri" OR "phenol 2 2 - 1-methyl-1 2-ethanediyl bis nitrilomethylidyne bis-" OR "propylenedinitrilodi-o-cresol" OR "2 2 - propane-1 2-diylbis nitrilomethylylidene diphenol" OR "α α - propylenedinitrilodi-o-cresol;phenol 2 2 - 1-methyl-1 2-ethanediyl bis nitrilomethylidyne bis-" OR "o-cresol alpha alpha - propylenedinitrilo di-" OR "phenol 2 2 1-methyl-1 2-ethanediyl bis nitrilomethylidyne bis" OR "α α - propylenedinitrilodi-o-cresol" OR "n n -disalicylidene-1 2-diaminopropane alpha alpha - propylenedinitrilo di-o-cresol" OR "CAS 94-91-7")
					OR emm_caschemical__value:"94-91-7"

43. Phenylene-1,4-bis-(benz-1,3-oxazin-4	(chemical names OR CAS value))	NO	0		2 2 - 1 4-phenylene bis-4h-3 1-benzoxazin-4-one OR cyasorb uv-3638 OR "unii-8v348nl4qk OR "8v348nl4qk OR "dtxsid40864845 OR "bas 00298026 OR "ec 418-280-1 OR "oprea1_802650 OR "oprea1_828724 OR "schembl125184 OR "ctk8b9791 OR "ebd2984 OR "bcp12260 OR "zinc2565270 OR "anw-63097 OR "stk296324 OR "akos000640593 OR "mcule-9378837915 OR "uv-3638 OR "acm18600594 OR "ks-000001m3 OR "ak-89768 OR "as-10722 OR "ax8063798 OR "ls-186266 OR "bb 0262678 OR "ft-0654023 OR "ns00003546 OR "st50222003 OR "600p594 OR "a812998 OR "q27271051 OR "2 2- 1 4-phenylene -bis- 4h-3 1-benzoxazin-4-one OR "2 2 - 1 4-phenylene bis 4h-benzo d 1 3 oxazin-4-one OR "4h-3 1-benzoxazin-4-one 2 2 - 1 4-phenylene bis- OR "2/2 - 1 4-phenylene bis-4h-3 1-benzoxazin-4-one OR "2 2 - 1 4-phenylene bis 3 1-benzoxazin-4-one OR "2 2 -benzene-1 4-diylbis 4h-3 1-benzoxazin-4-one OR "2 2- 1 4-phenylene bis 4h-3 1-benzoxazine-4-one OR "phenylene-1 4-bis- benz-1 3-oxazin-4-one OR "2 2- 1 4-phenylene bis-4h-3 1-benzoxazin-4-one OR "2 2 - 1 4-PHENYLENE BIS-4H-3 1-BENZOXAZIN-4-ONE OR "Cyasorb UV-3638 OR "UNII-8V348NL4QK OR "8V348NL4QK OR "DTXSID40864845 OR "2 2 - 1 4-Phenylene bis 4H-3 1-benzoxazin-4-one OR "BAS 00298026 OR "EC 418-280-1 OR "Oprea1_802650 OR "Oprea1_828724 OR "SCHEMBL125184 OR "CTK8B9791 OR "EBD2984 OR "BCP12260 OR "ZINC2565270 OR "ANW-63097 OR "STK296324 OR "AKOS000640593 OR "MCULE-9378837915 OR "UV-3638 OR "ACM18600594 OR "KS-000001M3 OR "AK-89768 OR "AS-10722 OR "AX8063798 OR "LS-186266 OR "BB 0262678 OR "FT-0654023 OR "NS00003546 OR "ST50222003 OR "600P594 OR "A812998 OR "Q27271051 OR "2 2- 1 4-PHENYLENE -BIS- 4H-3 1-BENZOXAZIN-4-ONE OR "2 2 - 1 4-Phenylene bis 4H-benzo d 1 3 oxazin-4-one OR "4H-3 1-Benzoxazin-4-one 2 2 - 1 4-phenylene bis- OR "2/2 - 1 4-PHENYLENE BIS-4H-3 1-BENZOXAZIN-4-ONE OR "2- 4- 4-oxo-3 1-benzoxazin-2-yl phenyl -3 1-benzoxazin-4-one OR "2 2 - 1 4-Phenylene bis 3 1-benzoxazin-4-one OR "2 2 -benzene-1 4-diylbis 4H-3 1-benzoxazin-4-one OR "2 2- 1 4-phenylene bis 4H-3 1-benzoxazine-4-one OR "2 2 - 1 4-phenylene bis 4h-3 1-benzoxazin-4-one OR "2 2 -p-phenylenebis 3 1-benzoxazin-4-one OR "Phenylene-1 4-bis- benz-1 3-oxazin-4-one OR "2 2 -p-phenylenebis 4h-3 1-benzoxazin-4-one OR "2 2- 1 4-Phenylene bis-4H-3 1-benzoxazin-4-one OR "2- 4- 4-oxidanylidene-3 1-benzoxazin-2-yl phenyl -3 1-benzoxazin-4-one OR "2- 4- 4-oxobenzo d 1 3-oxazin-2-yl phenyl benzo d 1 3-oxazin-4-one OR "CAS 18600-59-4"
					OR emm_caschemical__value:"18600-59-4"

44. Phenylnaphthylamine	(chemical names OR CAS value)) NOT "prep method" NOT synthesis	NO	42		"1-phenylethanamine" OR "1-phenylethylamine" OR "alpha-phenylethylamine" OR "dl-alpha-methylbenzylamine" OR "1-phenethylamine" OR "alpha-aminoethylbenzene" OR "1-amino-1-phenylethane" OR "alpha-methylbenzenemethanamine" OR "alpha-phenethylamine" OR "1-phenyl-ethylamine" OR "1-fenylethylamin" OR "benzenemethanamine alpha-methyl" OR "dl-1-phenylethylamine" OR "sumine 2079" OR "ethanamine 1-phenyl" OR "ethylamine 1-phenyl" OR "dl-1-phenethylamine" OR "chebi:670" OR "benzylamine alpha-methyl" OR "chembl278059" OR " -alpha-methylbenzylamine" OR "s -alpha-methylbenzenemethanamine" OR "benzenemethanamine alpha-methyl- s" OR "unii-hz9dm6b2mt" OR "dl-alpha-methylbenzylamine 99%" OR "1-fenylethylamin czech" OR "benzylamine alpha-methyl" OR "s -a-methyl-benzylamine" OR "benzene 1-amino-ethyl" OR "hz9dm6b2mt" OR "benzenemethanamine a-methyl" OR "hsdb 2742" OR "benzenemethanamine alpha-methyl" OR "benzenemethaneamine alpha-methyl" OR "nsc 8391" OR "einecs 202-706-6" OR "einecs 210-545-8" OR "1-phenyl ethylamine" OR "1-phenylethanamine #" OR " 1-aminoethyl benzene" OR "alpha-phenethylamine" OR "pubchem21079" OR "1-phenyl-1-ethanamine" OR "dl-|a-phenylethylamine" OR "alpha-phenylethylamine" OR "dl-|a-methylbenzylamine" OR "ai3-03116" OR "alpha-methylbenzylamine" OR "schembl830" OR "acmc-209j2b" OR "acmc-20aj38" OR "ec 210-545-8" OR "benzenemethanamine alpha-methyl- -" OR " -1-phenylethylamine" OR "rs -alpha-methylbenzylamine" OR " alpha-phenethylamine" OR "wln: 1m1r" OR " -1-phenyl-ethylamine" OR "schembl4701869" OR "l alpha-methylbenzylamine" OR "dtxsid40862301" OR "l -alpha-phenylethylamine" OR "nsc8391" OR "albb-032928" OR "bcp32849" OR "ks-00000g3i" OR "nsc-8391" OR "r -alpha-methylbenzenemethanamine" OR "s -alpha-methylbenzylamine" OR "anw-53664" OR "bbl027673" OR "bdbm50023171" OR "benzenemethaneamine alpha-methyl" OR "mfcd00008069" OR "sbb040514" OR "stk397443" OR "akos000119070" OR "akos016039387" OR "cs-w013564" OR "mcule-6637542099" OR "ps-4601" OR "sc-18396" OR "benzenemethanamine alpha-methyl- r" OR "db-015888" OR "db-054000" OR "am20060838" OR "benzylamine alpha-methyl- " OR "ft-0601072" OR "ft-0604486" OR "ft-0658781" OR "st45255353" OR "c02455" OR "s -1-phenylethanamine; 1s -1-phenylethanamine" OR "83288-ep2270009a1" OR "83288-ep2272822a1" OR "83288-ep2284174a1" OR "83288-ep2298779a1" OR "83288-ep2305655a2" OR "benzenemethanamine alpha-methyl- " OR "benzenemethanamine alpha-methyl- alphar" OR "q3560549" OR "w-105090" OR "f0798-0597" OR "alpha -naphthylphenylamine" OR "alpha -phenylnaphthylamine" OR "1-anilinonaphthalene" OR "1-naphthalenamine n-phenyl" OR "1-naphthyl phenyl amine" OR "1-naphthylamine n-phenyl" OR "alpha natphthylamine" OR "alpha-naphthylphenylamine" OR "fenyl- alpha -naftylamin" OR "fenyl-alpha-naftylamin" OR "n-1-naphthyl aniline" OR "n-1-naphthylaniline" OR "naphthalen-1-yl-phenyl-amine" OR "n-fenyl-1-aminonaftalen" OR "n-phenyl- alpha -naphthylamine" OR "n-phenyl-1-aminonaphthalene" OR "n-phenyl-1-naphthalenamine" OR "n-phenyl-1-naphthylamine" OR "n-phenyl-alpha-naphthylamine" OR "n-phenyl-l-naphthylamine" OR "n-phenyl-n- 1-naphthyl amine" OR "n-phenylnaphthalen-1-amine" OR "n-phenylnaphthylamine" OR "phenyl- alpha -naphthylamine" OR "phenyl-1-naphthylamine" OR "phenyl-alpha-naphthylamine" OR "phenylnaphthylamine" OR "1-Phenylethanamine" OR "1-Phenylethylamine" OR "ALPHA-METHYLBENZYLAMINE" OR

					"alpha-Phenylethylamine" OR "DL-alpha-Methylbenzylamine" OR "1-Phenethylamine" OR "alpha-Aminoethylbenzene" OR "1-Amino-1-phenylethane" OR "1-phenylethan-1-amine" OR "a-methylbenzylamine" OR "alpha-Methylbenzenemethanamine" OR "alpha-Phenethylamine" OR "1-Phenyl-ethylamine" OR "1-Fenylethylamin" OR "Benzenemethanamine alpha-methyl" OR "a-phenylethylamine" OR "DL-1-Phenylethylamine" OR "Sumine 2079" OR "Ethanamine 1-phenyl" OR "Ethylamine 1-phenyl" OR "DL-1-phenethylamine" OR "a-methylbenzenemethanamine" OR "CHEBI:670" OR "Benzylamine alpha-methyl" OR "CHEMBL278059" OR " -alpha-Methylbenzylamine" OR "S -alpha-Methylbenzenemethanamine" OR "Benzenemethanamine alpha-methyl- S" OR "UNII-HZ9DM6B2MT" OR "DL-alpha-Methylbenzylamine 99%" OR "ralpha-phenylethylamine" OR "1-Fenylethylamin Czech" OR "Benzylamine alpha-methyl" OR "S -a-methyl-benzylamine" OR "Benzene 1-amino-ethyl" OR "HZ9DM6B2MT" OR "Benzenemethanamine a-methyl" OR "a-phenethylamine" OR "HSDB 2742" OR "l-phenylethylamine" OR "Benzenemethanamine alpha-methyl" OR "a-aminoethylbenzene" OR "Benzenemethaneamine alpha-methyl" OR "NSC 8391" OR "1-phenylethyl amine" OR "EINECS 202-706-6" OR "EINECS 210-545-8" OR "phenylethan-1-amine" OR "1-Phenyl ethylamine" OR "alpha-methylbezylamine" OR " 1-phenylethyl amine" OR "1-phenyl-ethyl-amine" OR "1-Phenylethanamine #" OR "rac-1-phenylethanamine" OR " 1-Aminoethyl benzene" OR "alpha-Phenethylamine" OR "dl-1-phenylethyl amine" OR "PubChem21079" OR "1-Phenyl-1-ethanamine" OR "alpha-methyl benzylamine" OR "alpha-methyl-benzylamine" OR "alpha-methylbenzyl amine" OR "DL-|A-Phenylethylamine" OR "alpha-Phenylethylamine" OR "DL-|A-Methylbenzylamine" OR "1 r s -phenylethylamine" OR "AI3-03116" OR " -1-phenylethylamine" OR " 1-phenylethylamine" OR "alpha-methyl benzyl amine" OR "alpha-Methylbenzylamine" OR " -alpha-phenylethylamine" OR "SCHEMBL830" OR "ACMC-209j2b" OR "ACMC-20aj38" OR " alpha-phenylethylamine" OR "EC 210-545-8" OR "alpha-methylbenzylamine" OR " -alpha-methylbenzylamine" OR " 1-phenylethan-1-amine" OR " -1-phenylethanamine" OR " alpha-methylbenzylamine" OR "Benzenemethanamine alpha-methyl- " OR " -1-Phenylethylamine" OR "RS -alpha-methylbenzylamine" OR " alpha-Phenethylamine" OR " -alpha-methyl-benzylamine" OR " - alpha-methyl-benzylamine" OR " alpha-methyl-benzylamine" OR "WLN: 1M1R" OR " -1-phenyl-ethanamine" OR " -1-Phenyl-ethylamine" OR "racemic alpha-methylbenzylamine" OR " -alpha-methyl benzyl amine" OR " -1- phenyl ethylamine" OR " - alpha methyl benzyl amine" OR "SCHEMBL4701869" OR "L alpha-Methylbenzylamine" OR "DTXSID40862301" OR "L -alpha-Phenylethylamine" OR "NSC8391" OR " alpha-methylbenzenemethanamine" OR "ALBB-032928" OR "BCP32849" OR "KS-00000G3I" OR "NSC-8391" OR "R -alpha-Methylbenzenemethanamine" OR "S -alpha-Methylbenzylamine" OR "ANW-53664" OR "BBL027673" OR "BDBM50023171" OR "Benzenemethaneamine alpha-methyl" OR "MFCD00008069" OR "SBB040514" OR "STK397443" OR "AKOS000119070" OR "AKOS016039387" OR "CS-W013564" OR "MCULE-6637542099" OR "PS-4601" OR "SC-18396" OR "Benzenemethanamine alpha-methyl- R" OR "DB-015888" OR "DB-054000" OR "AM20060838" OR "Benzylamine alpha-methyl- " OR "FT-0601072" OR "FT-0604486" OR "FT-0658781" OR "ST45255353" OR "C02455" OR "S -1-phenylethanamine; 1S -1-phenylethanamine" OR "83288-EP2270009A1" OR "83288-EP2272822A1" OR "83288-EP2284174A1" OR "83288-EP2298779A1" OR "83288-

					EP2305655A2" OR "Benzenemethanamine alpha-methyl- " OR "Benzenemethanamine alpha-methyl- alphaR" OR "Q3560549" OR "W-105090" OR "F0798-0597" OR " alpha -Naphthylphenylamine" OR "alpha -Phenylnaphthylamine" OR "1- n-phenylamino naphthalene" OR "1-Anilinonaphthalene" OR "1-Naphthalenamine N-phenyl" OR "1-Naphthyl phenyl amine" OR "1-Naphthylamine N-phenyl" OR "1-naphthylphenylamine" OR "1-phenylaminonaphthalene" OR "Alpha Natphthylamine" OR "alpha-Naphthylphenylamine" OR "alpha-naphthyl-phenylamine" OR "Fenyl- alpha -naftylamin" OR "Fenyl-alpha-naftylamin" OR "N- 1-Naphthyl aniline" OR "n-1-naphthyl -n-phenylamine" OR "N-1-Naphthylaniline" OR "Naphthalen-1-yl-phenyl-amine" OR "naphthylphenylamine" OR "N-Fenyl-1-aminonaftalen" OR "N-Phenyl- alpha -naphthylamine" OR "N-Phenyl-1-aminonaphthalene" OR "N-Phenyl-1-naphthalenamine" OR "N-PHENYL-1-NAPHTHYLAMINE" OR "N-Phenyl-alpha-naphthylamine" OR "N-phenyl-l-naphthylamine" OR "N-phenyl-N- 1-naphthyl amine" OR "N-phenylnaphthalen-1-amine" OR "N-Phenylnaphthylamine" OR "n-phenyl-naphthylamine" OR "Phenyl- alpha -naphthylamine" OR "phenyl alpha naphthylamine" OR "Phenyl-1-naphthylamine" OR "Phenyl-alpha-naphthylamine" OR "Phenylnaphthylamine" OR "CAS 618-36-0" OR "CAS 98-84-0" OR "CAS 2627-86-3" OR "CAS 3886-69-9"
					OR emm_caschemical__value:("618-36-0" OR "98-84-0" OR "2627-86-3" OR "3886-69-9")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
				NOT synthesis	NOT topic:synthesis
45.Phosphorothioic_acid_OOO-triphenyl_ester_tert-butyl_derivatives	(chemical names OR CAS value))	NO			topic:("phosphorothioic acid o o o triphenyl esters tert-bu derivs" OR "phosphorothioic acid o o o triphenyl esters tert-bu derivatives" OR "4-tert-butylphenoxy -diphenoxy-sulfanylidene-lambda5-phosphane" OR "4-tert-butylphenoxy -diphenoxy-sulfanylidene 5 -phosphane" OR "Phosphorothioic acid O O O triphenyl esters tert-Bu derivs" OR "Phosphorothioic acid O O O triphenyl esters tert-Bu derivatives" OR "4-Tert-butylphenoxy -diphenoxy-sulfanylidene-lambda5-phosphane" OR "butylated triphenyl phosphorothionate" OR "CAS 192268-65-8")
					OR emm_caschemical__value:("192268-65-8")

46. Piperonyl Butoxide	(chemical names OR CAS value)) NOT "prep method"	NO			"butacide" OR "butocide" OR "ethanol butoxide" OR "pyrenone 606" OR "5- 2- 2-butoxyethoxy ethoxy methyl -6-propylbenzo d 1 3 dioxole" OR "butyl carbitol 6-propylpiperonyl ether" OR "piperonylbutoxide" OR "6-propylpiperonyl butyl diethylene glycol ether" OR "2- 2-butoxyethoxy ethyl 6-propylpiperonyl ether" OR "nci-c02813" OR "fmc 5273" OR "nia 5273" OR "6-propylpiperonyl butylcarbityl ether" OR "1 3-benzodioxole 5-2- 2-butoxyethoxy ethoxy methyl -6-propyl-" OR "unii-lwk91tu9ah" OR "nsc 8401" OR "ccris 522" OR "butylcarbityl 6-propylpiperonyl ether" OR "hsdb 1755" OR "einecs 200-076-7" OR "lwk91tu9ah" OR "3 4-methylenedioxy-6-propylbenzyl n-butyl diethyleneglycol ether" OR "5- 2- 2-butoxyethoxy ethoxymethyl -6-propyl-1 3-benzodioxole" OR "epa pesticide chemical code 067501" OR "brn 0288063" OR "6-propylpiperonyl -butyl carbityl ether" OR "alpha- 2- 2-n-butoxyethoxy -ethoxy -4 5-methylenedioxy-2-propyltoluene" OR "butyl-carbityl 6-propylpiperonyl ether" OR "ai3-14250" OR "dtxsid1021166" OR "3 4-methylendioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether" OR "chebi:32687" OR "5-propyl-4- 2 5 8-trioxa-dodecyl -1 3-benzodioxole" OR "ncgc00090874-02" OR "ncgc00090874-04" OR "ak114177" OR "3 4-methylenedioxy-6-propylbenzyl n-butyldiethyleneglycol ether" OR "5-propyl-4- 2 5 8-trioxa-dodecyl -1 3-benzodioxol german" OR "3 4-methylendioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether german" OR "alpha- 2- 2-butoxyethoxy ethoxy -4 5-methylenedioxy-2-propyltoluene" OR "dsstox_cid_1166" OR "3 4-methylenedioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether german" OR "toluene alpha- 2- 2-butoxyethoxy ethoxy -4 5- methylenedioxy -2-propyl-" OR "dsstox_rid_75988" OR "dsstox_gsid_21166" OR "q-201588" OR "2- 2-butoxyethoxy -1- 6-propyl 2h-benzo d 1 3-dioxolen-5-yl methoxy ethane" OR "pybuthrin" OR "pyrenon" OR "synpren-fish" OR ".alpha. 2- 2-butoxyethoxy ethoxy -4 5-methylenedioxy-2-propyltoluene" OR ".alpha.- 2- 2-n-butoxyethoxy -ethoxy -4 5-methylenedioxy-2-propyltoluene" OR "pubchem15364" OR "ec 200-076-7" OR "schembl5490" OR "5-propyl-4- 2 5 8-trioxa-dodecyl -1 3-benzodioxol" OR "chembl1201131" OR "ks-00000meb" OR "nsc8401" OR "bdbm181115" OR "hms3264a07" OR "3 4-methylenedioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether" OR "acm51036" OR "bcp19227" OR "fac 5273" OR "hy-b1198" OR "nsc-8401" OR "zinc3875342" OR "tox21_111034" OR "tox21_400086" OR "mfcd00005842" OR "akos015951348" OR "toluene 5-methylenedioxy -2-propyl-" OR "tox21_111034_1" OR "ccg-213921" OR "db09350" OR "mcule-7766634514" OR "ncgc00090874-01" OR "ncgc00090874-03" OR "ncgc00090874-05" OR "ncgc00090874-06" OR "st075004" OR "ax8061167" OR "db-051886" OR "propylpiperonyl butyl diethyleneglycol ether" OR "ft-0631218" OR "ns00011484" OR "ab01563216_01" OR "sr-01000944266" OR "5-propyl-4- 2 8-trioxa-dodecyl -1 3-benzodioxol" OR "sr-01000944266-1" OR "4 5-methylenedioxy-2-propylbenzyldiethylene glycol butyl ether" OR "4 5-methylenedioxy-2-propylbenzyldiethyleneglycol butyl ether" OR "benzodioxole 5-2- 2-butoxyethoxy ethoxy methyl -6-propyl-" OR "piperonylbutoxide certified reference material tracecert r" OR " 3 4-methylenedioxy-6-propylbenzyl butyl diethylene glicol ether" OR "3 4-methylenedioxy-6-propylbenzyl n-butyl diethylene glycol ether" OR "5- 2- 2-butoxyethoxy ethoxy methyl -6-propyl-1 3-benzodioxole #" OR "5-{ 2- 2-butoxyethoxy ethoxy methyl}-6-propyl-2h-1 3-benzodioxole" OR "piperonylbutoxide british pharmacopoeia bp reference standard" OR "butylcarbityl 6-propylpiperonyl ether 80% and related compounds 20%" OR "piperonyl butoxide / 2- 2-

					butoxyethoxy ethyl 6-propylpiperonyl ether" OR "toluene .alpha.- 2- 2-butoxyethoxy ethoxy -4 5- methylenedioxy -2-propyl-" OR "2- 2-butoxyethoxy ethyl 6-propylpiperonyl ether 4 5-methylenedioxy-2-propylbenzyldiethyleneglycol butyl ether" OR "piperonyl butoxide" OR "Butacide" OR "Butocide" OR "Ethanol butoxide" OR "Pyrenone 606" OR "5- 2- 2-Butoxyethoxy ethoxy methyl -6-propylbenzo d 1 3 dioxole" OR "Butyl carbitol 6-propylpiperonyl ether" OR "Piperonylbutoxide" OR "6-Propylpiperonyl butyl diethylene glycol ether" OR "2- 2-Butoxyethoxy ethyl 6-propylpiperonyl ether" OR "NCI-C02813" OR "FMC 5273" OR "NIA 5273" OR "6-Propylpiperonyl butylcarbityl ether" OR "1 3-Benzodioxole 5-2- 2-butoxyethoxy ethoxy methyl -6-propyl-" OR "UNII-LWK91TU9AH" OR "NSC 8401" OR "CCRIS 522" OR "Butylcarbityl 6-propylpiperonyl ether" OR "HSDB 1755" OR "EINECS 200-076-7" OR "LWK91TU9AH" OR "3 4-Methylenedioxy-6-propylbenzyl n-butyl diethyleneglycol ether" OR "5- 2- 2-Butoxyethoxy ethoxymethyl -6-propyl-1 3-benzodioxole" OR "EPA Pesticide Chemical Code 067501" OR "BRN 0288063" OR "6- Propylpiperonyl -butyl carbityl ether" OR "alpha- 2- 2-n-Butoxyethoxy -ethoxy -4 5-methylenedioxy-2-propyltoluene" OR "Butyl-carbityl 6-propylpiperonyl ether" OR "AI3-14250" OR "DTXSID1021166" OR "3 4-Methylendioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether" OR "CHEBI:32687" OR "5-Propyl-4- 2 5 8-trioxa-dodecyl -1 3-benzodioxole" OR "NCGC00090874-02" OR "NCGC00090874-04" OR "AK114177" OR "3 4-Methylenedioxy-6-propylbenzyl n-butyldiethyleneglycol ether" OR "5-Propyl-4- 2 5 8-trioxa-dodecyl -1 3-benzodioxol German" OR "5- 2- 2-Butoxyethoxy ethoxy methyl -6-propyl-1 3-benzodioxole" OR "5-{ 2- 2-butoxyethoxy ethoxy methyl}-6-propyl-1 3-benzodioxole" OR " 3 4-Methylenedioxy-6-propylbenzyl butyl diethylene glycol ether" OR "3 4-Methylendioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether German" OR "alpha- 2- 2-Butoxyethoxy ethoxy -4 5-methylenedioxy-2-propyltoluene" OR "DSSTox_CID_1166" OR "3 4-Methylenedioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether German" OR "Toluene alpha- 2- 2-butoxyethoxy ethoxy -4 5- methylenedioxy -2-propyl-" OR "DSSTox_RID_75988" OR "DSSTox_GSID_21166" OR "Q-201588" OR "5-{ 2-{ 2- butyloxy ethyl oxy}ethyl oxy methyl}-6-propyl-1 3-benzodioxole" OR "alpha- 2- 2-butoxyethoxy ethoxy -4 5- methylenedioxy -2-propyltoluene" OR "2- 2-butoxyethoxy -1- 6-propyl 2H-benzo d 1 3-dioxolen-5-yl methoxy ethane" OR "Pybuthrin" OR "Pyrenon" OR "Synpren-fish" OR ".alpha. 2- 2-Butoxyethoxy ethoxy -4 5-methylenedioxy-2-propyltoluene" OR ".alpha.- 2- 2-n-Butoxyethoxy -ethoxy -4 5-methylenedioxy-2-propyltoluene" OR ".alpha.- 2- 2-N-Butoxyethoxy -ethoxy -4 5-methylenedioxy-2-propyltoluene" OR "PubChem15364" OR "EC 200-076-7" OR "SCHEMBL5490" OR "5-Propyl-4- 2 5 8-trioxa-dodecyl -1 3-benzodioxol" OR "CHEMBL1201131" OR "KS-00000MEB" OR "NSC8401" OR "BDBM181115" OR "HMS3264A07" OR "3 4-Methylenedioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether" OR "ACM51036" OR "BCP19227" OR "FAC 5273" OR "HY-B1198" OR "NSC-8401" OR "ZINC3875342" OR "Tox21_111034" OR "Tox21_400086" OR "MFCD00005842" OR "AKOS015951348" OR "Toluene 5-methylenedioxy -2-propyl-" OR "Tox21_111034_1" OR "CCG-213921" OR "DB09350" OR "MCULE-7766634514" OR "NCGC00090874-01" OR "NCGC00090874-03" OR "NCGC00090874-05" OR "NCGC00090874-06" OR "ST075004" OR "AX8061167" OR "DB-051886" OR "Propylpiperonyl butyl diethyleneglycol ether" OR "FT-0631218" OR "NS00011484" OR "AB01563216_01" OR "SR-01000944266" OR "5-Propyl-4-

					2 8-trioxa-dodecyl -1 3-benzodioxol" OR "SR-01000944266-1" OR "1 5- 2- 2-butoxyethoxy ethoxy methyl -6-propyl-" OR "4 5-Methylenedioxy-2-propylbenzyldiethylene glycol butyl ether" OR "4 5-Methylenedioxy-2-propylbenzyldiethyleneglycol butyl ether" OR "Benzodioxole 5- 2- 2-butoxyethoxy ethoxy methyl -6-propyl-" OR "Piperonylbutoxide certified reference material TraceCERT R" OR " 3 4-Methylenedioxy-6-propylbenzyl butyl diethylene glicol ether" OR " 3 4-methylenedioxy-6-propylbenzyl butyl diethylene glycol ether" OR "3 4-Methylenedioxy-6-propylbenzyl n-butyl diethylene glycol ether" OR "5- 2- 2-butoxyethoxy ethoxy methyl -6-propyl-1 3-benzodioxole" OR "5- 2- 2-Butoxyethoxy ethoxy methyl -6-propyl-1 3-benzodioxole #" OR "5-{ 2- 2-butoxyethoxy ethoxy methyl}-6-propyl-2H-1 3-benzodioxole" OR "Piperonylbutoxide British Pharmacopoeia BP Reference Standard" OR "Butylcarbityl 6-propylpiperonyl ether 80% and related compounds 20%" OR "alpha- 2- 2-butoxyethoxy ethoxy -4 5-methylened ioxy-2-propyltoluene" OR "Piperonyl butoxide / 2- 2-butoxyethoxy ethyl 6-propylpiperonyl ether" OR "Toluene .alpha.- 2- 2-butoxyethoxy ethoxy -4 5-methylenedioxy -2-propyl-" OR "2- 2-Butoxyethoxy ethyl 6-propylpiperonyl ether 4 5-Methylenedioxy-2-propylbenzyldiethyleneglycol butyl ether" OR "Piperonyl butoxide" OR "CAS 51-03-6" OR "PBO insecticide"~3
					OR emm_caschemical__value:("51-03-6")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
47. propane_thiol	(chemical names OR CAS value)) NOT "prep method"	NO			1-propanethiol 2 3-bis 2-mercaptoethyl thio - OR "dtxsid20888943" OR "acmc-1c6xi" OR "2 3-bis 2-mercaptoethylthio propane-1-thiol" OR "ec 411-290-7" OR "schembl127070" OR "ctk4b7363" OR "akos028109967" OR "acn-053709" OR "ns00006734" OR "4- mercaptomethyl -3 6-dithia-1 8-octanedithiol" OR "1-propanethiol 2 3-bis[(2-mercaptoethyl)thio]-" OR "2 3-bis(2-mercaptoethylthio)propane-1-thiol" OR "4-(mercaptomethyl)-3 6-dithia-1 8-octanedithiol" OR "2 3-bis 2-mercaptoethyl thio -1-propanethiol" OR "1-Propanethiol 2 3-bis 2-mercaptoethyl thio -" OR "DTXSID20888943" OR "1-propanethiol 2 3-bis 2-mercaptoethyl thio -;2 3-bis 2-mercaptoethyl thio -1-propanethiol;1-propanethiol 2 3-bis 2-mercaptoethyl thio - 2 3-bis 2-mercaptoethyl t"-1" OR propanethiol" OR "ACMC-1C6XI" OR "2 3-Bis 2-mercaptoethylthio propane-1-thiol" OR "EC 411-290-7" OR "SCHEMBL127070" OR "CTK4B7363" OR "AKOS028109967" OR "ACN-053709" OR "NS00006734" OR "1 2-bis 2-mercaptoethylthio -3-mercaptopropane" OR "2 3-bis 2-sulfanylethylsulfanyl propane-1-thiol" OR "2 3-bis 2-sulfanyl

					ethylsulfanyl propane-1-thiol" OR "4- Mercaptomethyl -3 6-dithia-1 8-octanedithiol" OR "2 3-bis((2-mercaptoethyl)thio)-1-propanethiol" OR "1-Propanethiol 2 3-bis[(2-mercaptoethyl)thio]-" OR "2 3-Bis(2-mercaptoethylthio)propane-1-thiol" OR "1 2-bis(2-mercaptoethylthio)-3-mercaptopropane" OR "2 3-bis(2-sulfanylethylsulfanyl)propane-1-thiol" OR "2 3-bis(2-sulfanyl ethylsulfanyl)propane-1-thiol" OR "4-(Mercaptomethyl)-3 6-dithia-1 8-octanedithiol" OR "CAS 131538-00-6"
					OR emm_caschemical__value:("131538-00-6")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
48.reaction_products_of_phosphorus_oxychlor	(chemical names OR CAS value))	NO			tris 4-isopropylphenyl phosphate" OR "tris isopropylphenyl phosphate" OR "tris p-isopropylphenyl phosphate" OR "unii-y3h2fdx0nw" OR "triisopropylated phenyl phosphate" OR "y3h2fdx0nw" OR "phenol isopropylated phosphate 3:1" OR "dtxsid80858783" OR "dsstox_cid_8880" OR "dsstox_rid_78659" OR "dsstox_gsid_28880" OR "c27h33o4p" OR "phenol 4- 1-methylethyl - phosphate 3:1" OR "einecs 219-703-0" OR "isopropylphenylphosphat" OR "tricumol phosphate" OR "phenolisopropylatedphosphate" OR "schembl36617" OR "chembl458602" OR "tri 4-isopropylphenyl phosphate" OR "ctk4f8833" OR "zinc1583667" OR "tox21_202764" OR "tox21_202765" OR "tox21_202766" OR "ethyl 4-methylbenzoyl acetate" OR "ncgc00260311-01" OR "ncgc00260312-01" OR "ncgc00260313-01" OR "ns00003997" OR "phenol 1-methylethyl - phosphate 3:1" OR "phosphoric acid tris 4-isopropylphenyl ester" OR "w-104649" OR "w-107139" OR "q27294219" OR "Tris 4-isopropylphenyl phosphate" OR "Tris isopropylphenyl phosphate" OR "Tris p-isopropylphenyl phosphate" OR "UNII-Y3H2FDX0NW" OR "Triisopropylated phenyl phosphate" OR "Y3H2FDX0NW" OR "Phenol isopropylated phosphate 3:1" OR "DTXSID80858783" OR "DSSTox_CID_8880" OR "DSSTox_RID_78659" OR "DSSTox_GSID_28880" OR "tris 4-propan-2-ylphenyl phosphate" OR "C27H33O4P" OR "Phenol 4- 1-methylethyl - phosphate 3:1" OR "EINECS 219-703-0" OR "Isopropylphenylphosphat" OR "TRICUMOL PHOSPHATE" OR "Phenolisopropylatedphosphate" OR "SCHEMBL36617" OR "CHEMBL458602" OR "Tri 4-isopropylphenyl phosphate" OR "CTK4F8833" OR "ZINC1583667" OR "Tox21_202764" OR "Tox21_202765" OR "Tox21_202766" OR "ETHYL 4-METHYLBENZOYL ACETATE" OR "NCGC00260311-01" OR "NCGC00260312-01" OR "NCGC00260313-01" OR "NS00003997" OR "Phenol 1-methylethyl - phosphate 3:1" OR "Phosphoric acid tris 4-isopropylphenyl ester" OR "W-104649" OR "W-107139" OR "Q27294219" OR "CAS 26967-76-0" OR "CAS 2502-15-0" OR "CAS 68937-41-7"
					OR emm_caschemical__value:("26967-76-0" OR "2502-15-0" OR "68937-41-7")
49. retinol acetate	(chemical names OR CAS value)) NOT "prep method	NO			retinyl acetate OR "vitamin a acetate" OR "retinol acetate" OR "all-trans-retinyl acetate" OR "crystalets" OR "vitamin a1 acetate" OR "all-trans-retinol acetate" OR "vitamin a alcohol acetate" OR "davitan a" OR "vitamin a ester" OR "all-trans-vitamin a acetate" OR "o~15~-acetylretinol" OR "retinol acetate all-trans-" OR "all-trans-retinylacetate" OR "unii-3le3d9d6oy" OR "acetic acid retinyl ester" OR "retinyl acetate all-trans-" OR "nsc 122045" OR "ccris 1907" OR "trans-retinyl

	" NOT cigarette				acetate" OR "ro 1-5275" OR "trans-vitamin a acetate" OR "einecs 204-844-2" OR "brn 1915439" OR "3le3d9d6oy" OR "chebi:32095" OR "c22h32o2" OR "mfcd00019413" OR "2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethylcyclohexen-1-yl nona-2 4 6 8-tetraenyl acetate" OR "ncgc00090756-09" OR "dsstox_cid_1240" OR "dsstox_rid_76032" OR "dsstox_gsid_21240" OR "w-108382" OR "2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethylcyclohex-1-en-1-yl nona-2 4 6 8-tetraen-1-yl acetate" OR "o 15 -acetylretinol" OR "cas-127-47-9" OR "trans-retinol acetate" OR "sr-05000001431" OR "34356-31-5" OR "vitamin a acetat" OR "acetic acid retinyl" OR "spectrum5_001195" OR "spectrum5_002001" OR "ec 204-844-2" OR "retinol o~15~-acetyl-" OR "bspbio_002833" OR "spectrum1503051" OR "chembl486193" OR "dtxsid6021240" OR "chebi:94695" OR "hms501k04" OR "hms1922a19" OR "hms2089g20" OR "pharmakon1600-01503051" OR "hy-n0679" OR "zinc3874857" OR "tox21_113549" OR "tox21_201423" OR "tox21_302737" OR "bdbm50442911" OR "ccg-39564" OR "gv2742" OR "lmpr01090012" OR "nsc122045" OR "nsc122760" OR "nsc758220" OR "akos015914999" OR "tox21_113549_1" OR "nsc-122045" OR "nsc-122760" OR "nsc-758220" OR "idi1_000522" OR "ncgc00090756-01" OR "ncgc00090756-02" OR "ncgc00090756-03" OR "ncgc00090756-05" OR "ncgc00090756-06" OR "ncgc00090756-07" OR "ncgc00090756-08" OR "ncgc00090756-10" OR "ncgc00090756-11" OR "ncgc00090756-12" OR "ncgc00256509-01" OR "ncgc00258974-01" OR "64536-04-5" OR "ac-19999" OR "ak149484" OR "sc-76802" OR "sbi-0051756.p002" OR "ns00003926" OR "st50307679" OR "3000-ep2305825a1" OR "ab00052305-02" OR "ab00052305_03" OR "q7316808" OR "sr-05000001431-1" OR "sr-05000001431-3" OR "brd-k65331431-001-01-3" OR "CAS 127-47-9
					OR emm_caschemical__value:("127-47-9")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
				NOT cigarette/vaping	NOT (topic:(vaping OR cigarette OR smoke))
50.Retinol_propionate	(chemical names OR CAS value)) NOT "prep method"	NO			topic:("unii-32jk994wmc" OR "32jk994wmc" OR "ec 230-363-2" OR " 2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethylcyclohex-1-en-1-yl nona-2 4 6 8-tetraen-1-yl propionate" OR " 2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethylcyclohexen-1-yl nona-2 4 6 8-tetraenyl propanoate" OR "w-110194" OR "propionic acid retinol ester" OR "einecs 230-363-2" OR "mfcd00129785" OR "zinc16609980" OR "akos024386409" OR "ns00007709" OR "st51037678" OR "q27256177" OR " 2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethylcyclohex-1-enyl nona-2 4 6 8-tetraenyl propanoate" OR " 2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethylcyclohex-1-enyl nona-2 4 6 8-tetraenyl propi" OR "retinyl propionate" OR "retinol propanoate" OR "retinol propionate" OR "vitamin a propionate" OR "UNII-32JK994WMC" OR "32JK994WMC" OR "EC 230-363-2" OR " 2E 4E 6E 8E -3 7-Dimethyl-9- 2 6 6-trimethylcyclohex-1-en-1-yl nona-2 4 6 8-tetraen-1-yl propionate" OR " 2E 4E 6E 8E -3 7-dimethyl-9- 2 6 6-trimethylcyclohexen-1-yl nona-2 4 6 8-tetraenyl propanoate" OR "W-110194" OR "Propionic acid retinol ester" OR "EINECS 230-363-2" OR "MFCD00129785" OR "ZINC16609980" OR "AKOS024386409" OR "NS00007709" OR "ST51037678" OR "Q27256177" OR " 2E 4E 6E 8E -3 7-

					dimethyl-9- 2 6 6-trimethylcyclohex-1-enyl nona-2 4 6 8-tetraenyl propanoate" OR " 2E 4E 6E 8E -3 7-dimethyl-9- 2 6 6-trimethylcyclohex-1-enyl nona-2 4 6 8-tetraenyl propi" OR "Retinyl propionate" OR "Retinol propanoate" OR "Retinol propionate" OR "Vitamin A propionate" OR "CAS 7069-42-3")
					OR emm_caschemical__value:("7069-42-3")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
51.Retinyl_palmitate	(chemical names OR CAS value)) NOT "prep method"	NO			topic:("vitamin a palmitate" OR "retinol palmitate" OR "retinol hexadecanoate" OR "all-trans-retinyl palmitate" OR "arovit" OR "optovit-a" OR "retinyl hexadecanoate" OR "aquapalm" OR "dispatabs tabs" OR "trans-retinyl palmitate" OR "vitazyme a" OR "optovit a" OR "axerophthol palmitate" OR "vitamin a solubilized" OR "trans-retinol palmitate" OR "lutavit a 500 plus" OR "o 15 -hexadecanoylretinol" OR "unii-1d1k0n0vvc" OR "all-trans-retinol palmitate" OR "all-trans-vitamin a palmitate" OR "aquasol a" OR "ccris 3280" OR "retinol palmitate all-trans-" OR "einecs 201-228-5" OR " 2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethylcyclohexen-1-yl nona-2 4 6 8-tetraenyl hexadecanoate" OR "brn 1917366" OR "1d1k0n0vvc" OR "ester found in fish liver oils" OR "retinol all-trans- palmitate" OR "chebi:17616" OR "palmitic acid ester with retinol" OR "ncgc00095056-03" OR "dsstox_cid_1241" OR "dsstox_rid_76033" OR "dsstox_gsid_21241" OR " 2e 4e 6e 8e -hexadecanoic acid 3 7-dimethyl-9- 2 6 6-trimethyl-cyclohex-1-enyl -nona-2 4 6 8 tetraenyl ester" OR "retinyl vitamin a palmitate" OR " 2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethylcyclohex-1-en-1-yl nona-2 4 6 8-tetraen-1-yl hexadecanoate" OR "smr000112463" OR "palmitic acid retinol" OR "retinyl palmitic acid" OR "vitamin- a palmitate" OR "o 15 -palmitoylretinol" OR "retinyl hexadecanoic acid" OR "spectrum5_001201" OR "ec 201-228-5" OR "chembl1675" OR "schembl41649" OR "mls001332437" OR "mls001332438" OR "spectrum1503604" OR "dtxsid1021241" OR "hms500m11" OR "all trans-retinol palmitate" OR "hms1922e10" OR "hms2093g13" OR "hms2268c06" OR "pharmakon1600-01503604" OR "hy-b1384" OR "zinc8214494" OR "tox21_113452" OR "tox21_303008" OR "ccg-39342" OR "lmpr01090013" OR "nsc758478" OR "retinol o 15 - 1-oxohexadecyl -" OR "akos015918435" OR "ls-2307" OR "nsc-758478" OR "idi1_000249" OR "ncgc00095056-01" OR "ncgc00095056-02" OR "ncgc00256427-01" OR "ac-20001" OR "sc-15989" OR "sbi-0051830.p002" OR "cs-0013116" OR "2840-ep2305825a1" OR "c02588" OR "d00164" OR "ab00052360_04" OR "a839762" OR "sr-05000001910" OR "q7316807" OR "sr-05000001910-1" OR "3 7-dimethyl-9- 2 6 6 -trimethyl-1-cyclohexen-1-yl -2 4 6 8-nonatetraen-1-ol palmitate" OR " 2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethyl-cyclohex-en-1-yl -2 4 6 8-nonateetraen-1-yl-palmitate" OR " 2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethylcyclohex-1-enyl nona-2 4 6 8-tetraenyl palmitate" OR "hexadecanoic acid 2e 4e 6e 8e -3 7-dimethyl-9- 2 6 6-trimethyl-1-cyclohexenyl nona-2 4 6 8-tetraenyl ester" OR " 3 7-dimethyl-9- 2 6 6-trimethylcyclohexen-1-yl nona-2 4 6 8-tetraenoyl

					hexadecanoate" OR "retinyl palmitate" OR "VITAMIN A PALMITATE" OR "all-trans-Retinyl palmitate" OR "Arovit" OR "optovit-A" OR "Aquapalm" OR "vitazyme A" OR "optovit A" OR "Lutavit A 500 Plus" OR "O 15 -hexadecanoylretinol" OR "UNII-1D1K0N0VVC" OR "all-trans-Retinol palmitate" OR "all-trans-Vitamin A palmitate" OR "Aquasol A" OR "CCRIS 3280" OR "Retinol palmitate all-trans-" OR "EINECS 201-228-5" OR " 2E 4E 6E 8E -3 7-dimethyl-9- 2 6 6-trimethylcyclohexen-1-yl nona-2 4 6 8-tetraenyl hexadecanoate" OR "BRN 1917366" OR "1D1K0N0VVC" OR "Ester found in fish liver oils" OR "Retinol all-trans- palmitate" OR "CHEBI 17616" OR "Palmitic acid ester with retinol" OR "NCGC00095056-03" OR "DSSTox_CID_1241" OR "DSSTox_RID_76033" OR "DSSTox_GSID_21241" OR "2E 4E 6E 8E -Hexadecanoic acid 3 7-dimethyl-9- 2 6 6-trimethyl-cyclohex-1-enyl -nona-2 4 6 8 tetraenyl ester" OR "Retinyl Vitamin A Palmitate" OR "2E 4E 6E 8E -3 7-dimethyl-9- 2 6 6-trimethylcyclohex-1-en-1-yl nona-2 4 6 8-tetraen-1-yl hexadecanoate" OR "SMR000112463" OR "retinol-palmitate" OR "Palmitic acid retinol" OR "Retinyl palmitic acid" OR "Vitamin- A palmitate" OR "O 15 -palmitoylretinol" OR "Retinyl hexadecanoic acid" OR "Spectrum5_001201" OR "bmse000501" OR "EC 201-228-5" OR "CHEMBL1675" OR "SCHEMBL41649" OR "MLS001332437" OR "MLS001332438" OR "SPECTRUM1503604" OR "all-trans-retinyl hexadecanoate" OR "DTXSID1021241" OR "HMS500M11" OR "ALL TRANS-RETINOL PALMITATE" OR "HMS1922E10" OR "HMS2093G13" OR "HMS2268C06" OR "Pharmakon1600-01503604" OR "HY-B1384" OR "ZINC8214494" OR "Tox21_113452" OR "Tox21_303008" OR "CCG-39342" OR "LMPR01090013" OR "NSC758478" OR "retinol O 15 - 1-oxohexadecyl -" OR "AKOS015918435" OR "LS-2307" OR "NSC-758478" OR "IDI1_000249" OR "NCGC00095056-01" OR "NCGC00095056-02" OR "NCGC00256427-01" OR "AC-20001" OR "SC-15989" OR "SBI-0051830.P002" OR "CS-0013116" OR "2840-EP2305825A1" OR "C02588" OR "D00164" OR "AB00052360_04" OR "A839762" OR "SR-05000001910" OR "Q7316807" OR "SR-05000001910-1" OR "3 7-Dimethyl-9- 2 6 6 -trimethyl-1-cyclohexen-1-yl -2 4 6 8-nonatetraen-1-ol palmitate" OR "2E 4E 6E 8E -3 7-Dimethyl-9- 2 6 6-trimethyl-cyclohex-en-1-yl -2 4 6 8-nonateetraen-1-yl-palmitate" OR "2E 4E 6E 8E -3 7-dimethyl-9- 2 6 6-trimethylcyclohex-1-enyl nona-2 4 6 8-tetraenyl palmitate" OR "110067-62-4" OR "hexadecanoic acid 2E 4E 6E 8E -3 7-dimethyl-9- 2 6 6-trimethyl-1-cyclohexenyl nona-2 4 6 8-tetraenyl ester" OR "3 7-Dimethyl-9- 2 6 6-trimethylcyclohexen-1-yl nona-2 4 6 8-tetraenoyl hexadecanoate" OR "o 15 -hexadecanoylretinoic acid" OR "CAS 79-81-2")
					OR emm_caschemical__value:("79-81-2")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

52.solvent_blue_35	(chemical names OR CAS value)) NOT "prep method"	NO			oil blue 35 OR "dtxsid5044605" OR "w-110453" OR "sudan blue 2" OR "einecs 241-379-4" OR "ci 61554" OR "c.i.solvent blue 35" OR "unii-zvt4q30oqy" OR "zvt4q30oqy" OR "1 4-bis n-butylamino 9 10-anthracenedione" OR "9 10-anthracenedione 1 4-di butylamino " OR "dsstox_cid_24605" OR "dsstox_gsid_44605" OR "schembl156500" OR "chembl3561395" OR "ctk8e7890" OR "solvent blue 35" OR "hy-d0516" OR "ks-00000yd6" OR "zinc4521973" OR "sudan blue ii" OR "tox21_303986" OR "gt5180" OR "mfcd00011714" OR "sbb057328" OR "akos002134522" OR "cs-6262" OR "mcule-1589839876" OR "acm17354142" OR "ncgc00357014-01" OR "ak-60435" OR "as-17198" OR "1 4-di butylamino 9 10-anthracenedione" OR "ax8151705" OR "cas-17354-14-2" OR "eu-0066568" OR "ns00019427" OR "st50997657" OR "q7081287" OR "1 4-bis butylimino 1 4-dihydroanthracene-9 10-diol" OR "1 4-bis butylamino anthracene-9 10-dione" OR "9 10-Anthracenedione 1 4-bis butylamino " OR "1 4-Bis butylamino anthraquinone" OR "OIL BLUE 35" OR "DTXSID5044605" OR "W-110453" OR "9 10-anthracenedione 1 4-bis butylamino " OR "1 4-bis butylamino anthraquinone" OR "solventblue35" OR "anthraquinone 1 4-bis butylamino " OR "Sudan Blue 2" OR "EINECS 241-379-4" OR "CI 61554" OR "C.I.Solvent Blue 35" OR "UNII-ZVT4Q30OQY" OR "ZVT4Q30OQY" OR "1 4-Bis n-butylamino -9 10-anthracenedione" OR "9 10-Anthracenedione 1 4-di butylamino -" OR "DSSTox_CID_24605" OR "DSSTox_GSID_44605" OR "SCHEMBL156500" OR "CHEMBL3561395" OR "CTK8E7890" OR "Solvent blue 35" OR "1 4-di butylamino -anthraquinone" OR "HY-D0516" OR "KS-00000YD6" OR "ZINC4521973" OR "Sudan Blue II" OR "Tox21_303986" OR "GT5180" OR "MFCD00011714" OR "s6101" OR "SBB057328" OR "Anthraquinone 1 4-bis butylamino -" OR "AKOS002134522" OR "CS-6262" OR "MCULE-1589839876" OR "ACM17354142" OR "SOLVENT BLUE 35" OR "NCGC00357014-01" OR "1 4-bis butylamino anthra-9 10-quinone" OR "AK-60435" OR "AS-17198" OR "1 4-Di butylamino -9 10-anthracenedione" OR "AX8151705" OR "CAS-17354-14-2" OR "EU-0066568" OR "NS00019427" OR "ST50997657" OR "Q7081287" OR "1 4-Bis butylimino -1 4-dihydroanthracene-9 10-diol" OR "1 4-Bis butylamino anthracene-9 10-dione" OR "1 4-bis butylamino anthraq" OR "CAS 17354-14-2"
					OR emm_caschemical__value:("17354-14-2")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
53.Solvent_blue_4	(chemical names OR CAS value))	NO			topic:("solvent blue 4" OR "dtxsid4064474" OR "einecs 229-851-8" OR "ec 229-851-8" OR "schembl2390176" OR "zinc31308564" OR "sc-44514" OR "ns00011486" OR "4-anilinonaphthalen-1-yl bis 4 dimethylamino phenyl methanol" OR "alpha alpha-bis 4 dimethylamino phenyl 4 phenylamino 1-naphthalenemethanol" OR "α α-bis 4 dimethylamino phenyl 4 phenylamino naphthalene-1-methanol" OR "Solvent Blue 4" OR "DTXSID4064474" OR "EINECS 229-851-8" OR "EC 229-851-8" OR "SCHEMBL2390176" OR "ZINC31308564" OR "SC-44514" OR "NS00011486" OR "4-anilino-1-naphthyl bis 4 dimethylamino phenyl methanol" OR "4-Anilinonaphthalen-1-yl bis 4- dimethylamino phenyl methanol" OR "1-naphthalenamine 4 bis 4 dimethylamino phenyl methyl n-phenyl " OR "1-naphthalenemethanol alpha alpha-bis 4 dimethylamino phenyl 4 phenylamino " OR "1-naphthalenemethanol α α-bis 4 dimethylamino phenyl 4 phenylamino " OR "a a-bis 4 dimethylamino phenyl 4

					phenylamino naphthalene-1-methanol" OR "alpha alpha-bis 4 Dimethylamino phenyl 4 phenylamino 1-naphthalenemethanol" OR "alpha alpha-bis 4 dimethylamino phenyl 4 phenylamino naphthalene-1-methanol" OR "bis 4 dimethylamino phenyl 4 phenylamino naphthalen-1-yl methanol" OR "bis 4 dimethylamino phenyl 4 phenylamino naphthalene-1-methanol" OR "α α-Bis 4- dimethylamino phenyl -4 phenylamino naphthalene-1-methanol" OR "CAS 6786-83-0")
					OR emm_caschemical__value:("6786-83-0")
54.solvent_yellow_124	(chemical names OR CAS value))	NO			topic:("unii-e880xyt70p" OR "e880xyt70p" OR "w-110846" OR "einecs 252-021-1" OR "c.i. 111155" OR "ec 252-021-1" OR "schembl597248" OR "schembl12492278" OR "ctk8g3173" OR "dtxsid60865718" OR "acm34432923" OR "ns00002855" OR "q60457" OR "n-ethyl-n 2 1 2-methylpropoxy ethoxy ethyl 4 phenylazo aniline" OR "n-ethyl-n 2 1 2-methylpropoxy ethoxy ethyl 4-phenyldiazenylaniline" OR "benzenamine n-ethyl-n 2 1 2-methylpropoxy ethoxy ethyl 4 2-phenyldiazenyl " OR "n-ethyl-n-2-1 2-methylpropoxy ethoxyethyl-4 phenylazo aniline" OR "UNII-E880XYT70P" OR "E880XYT70P" OR "W-110846" OR "EINECS 252-021-1" OR "C.I. 111155" OR "EC 252-021-1" OR "SCHEMBL597248" OR "SCHEMBL12492278" OR "CTK8G3173" OR "DTXSID60865718" OR "ACM34432923" OR "NS00002855" OR "Q60457" OR "solvent yellow 124" OR "N-Ethyl-N- 2- 1- 2-methylpropoxy ethoxy ethyl -4- phenylazo aniline" OR "N-ethyl-N- 2- 1- 2-methylpropoxy ethoxy ethyl -4-phenyldiazenylaniline" OR "Benzenamine N-ethyl-N- 2- 1- 2-methylpropoxy ethoxy ethyl -4- 2-phenyldiazenyl -" OR "N-Ethyl-N-2-1- 2-methylpropoxy ethoxyethyl-4- phenylazo aniline" OR "CAS 34432-92-3")
					OR emm_caschemical__value:("34432-92-3")
54.TEGDME	(chemical names OR CAS value)) NOT "prep method"	NO			topic:("triglyme" OR"glyme+4" OR"ansul+ether+161" OR"glyme-3" OR"tegdime" OR"dimethyl+ether+of+triethylene+glycol" OR"unii-32yxg88kk0" OR"ethane+1+2-bis+2-methoxyethoxy+" OR"nsc+66400" OR"1-methoxy-2+2+2methoxy-ethoxy+ethane" OR"einecs+203-977-3" OR"glycol+triethylene+dimethyl+ether" OR"brn+1700630" OR"ai3-28582" OR"32yxg88kk0" OR"dtxsid8026224" OR"chebi:44842" OR"1+2-bis+2-methoxyethoxy+ethane+reagent" OR"glyme-4" OR"dsstox_cid_6224" OR"2+8+11-tetraoxadodecane" OR"ec+203-977-3" OR"acmc-1c6s6" OR"dsstox_rid_78066" OR"dsstox_gsid_26224" OR"schembl16126" OR"ksc178a6f" OR"1+2-bis+methoxyethoxy+ethane" OR"chembl1235255" OR"ctk0h8062" OR"ethane+2-bis+2-methoxyethoxy+" OR"nsc66400" OR"zinc1693863" OR"tox21_300509" OR"2186aa" OR"anw-16480" OR"mfcd00008504" OR"nsc-66400" OR"sbb060897" OR"akos009158244" OR"db02078" OR"mcule-9670046114" OR"ks-0000006k" OR"ncgc00164017-01" OR"ncgc00164017-02" OR"ncgc00254323-01" OR"cas-112-49-2" OR"cc-35336" OR"db-060211" OR"b0496" OR"ft-0659858" OR"ft-0755020" OR"ns00010633" OR"st50825121" OR"23265-ep2289897a1" OR"23265-ep2314584a1" OR"23265-ep2371797a1" OR"23265-ep2371798a1" OR"23265-ep2371800a1" OR"23265-ep2371804a1" OR"c-34604" OR"q2453066" OR"z1245664652" OR"dimethoxytetraglycol"

					OR"dimethoxytetraethylene+glycol" OR"tegdme" OR"Triglyme" OR"Triethylene+glycol+dimethyl+ether" OR"1+2-Bis+2-methoxyethoxy+ethane" OR"Glyme+4" OR"Ansul+ether+161" OR"Glyme-3" OR"1-methoxy-2+2+2-methoxyethoxy+ethoxy+ethane" OR"TEGDIME" OR"Dimethyl+ether+of+triethylene+glycol" OR"UNII-32YXG88KK0" OR"Ethane+1+2-bis+2-methoxyethoxy+" OR"NSC+66400" OR"triethyleneglycol+dimethyl+ether" OR"1-METHOXY-2-+2-+2-METHOXY-ETHOXY+-ETHANE" OR"EINECS+203-977-3" OR"Glycol+triethylene+dimethyl+ether" OR"BRN+1700630" OR"AI3-28582" OR"32YXG88KK0" OR"DTXSID8026224" OR"CHEBI:44842" OR"1+2-Bis+2-methoxyethoxy+Ethane+Reagent" OR"triethylene+glycoldimethylether+tegdme" OR"Glyme-4" OR"DSSTox_CID_6224" OR"2+8+11-Tetraoxadodecane" OR"EC+203-977-3" OR"ACMC-1C6S6" OR"DSSTox_RID_78066" OR"DSSTox_GSID_26224" OR"SCHEMBL16126" OR"KSC178A6F" OR"1+2-Bis+methoxyethoxy+ethane" OR"triethylene+glycol+dimethylether" OR"CHEMBL1235255" OR"CTK0H8062" OR"Ethane+2-bis+2-methoxyethoxy+" OR"NSC66400" OR"ZINC1693863" OR"Tox21_300509" OR"2186AA" OR"ANW-16480" OR"MFCD00008504" OR"NSC-66400" OR"SBB060897" OR"AKOS009158244" OR"DB02078" OR"MCULE-9670046114" OR"KS-0000006K" OR"triglyme+2+5+8+11-tetraoxadodecane" OR"NCGC00164017-01" OR"NCGC00164017-02" OR"NCGC00254323-01" OR"CAS-112-49-2" OR"CC-35336" OR"DB-060211" OR"B0496" OR"FT-0659858" OR"FT-0755020" OR"NS00010633" OR"ST50825121" OR"23265-EP2289897A1" OR"23265-EP2314584A1" OR"23265-EP2371797A1" OR"23265-EP2371798A1" OR"23265-EP2371800A1" OR"23265-EP2371804A1" OR"C-34604" OR"Q2453066" OR"Z1245664652" OR"2+5+8+11-tetraoxadodecane" OR"1+2-bis+2-methoxyethoxy+ethane" OR"triethylene+glycol+dimethyl+ether" OR"1+2bis+2methoxyethoxy+ethane" OR"triethylene+glycoldimethylether" OR"Dimethoxytetraglycol" OR"Dimethoxytetraethylene+glycol" OR"TEGDME" OR"tetraglyme" OR "CAS 112-49-2")
					OR emm_caschemical__value:("112-49-2")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

55.Tetrabromobisphenol A	(chemical names OR CAS value)) NOT "prep method"	NO			topic:("tetrabromobisphenol+a" OR "3+3+5+5+-tetrabromobisphenol+a" OR "bromdian" OR "2+2-bis+3+5-dibromo-4-hydroxyphenyl+propane" OR "4+4+-isopropylidenebis+2+6-dibromophenol" OR "tetrabromodian" OR "2+2+6+6+-tetrabromobisphenol+a" OR "saytex+rb+100pc" OR "phenol+4+4+-+1-methylethylidene+bis+2+6-dibromo-" OR "tetrabromodiphenylopropane" OR "unii-fqi02rfc3a" OR "3+5+3+5+-tetrabromobisphenol+a" OR "nsc+59775" OR "ccris+6274" OR "hsdb+5232" OR "saytex+rb-100" OR "4+4+-isopropylylidenebis+2+6-dibromophenol" OR "2+2-bis+4-hydroxy-3+5-dibromophenyl+propane" OR "einecs+201-236-9" OR "fqi02rfc3a" OR "2+2+6+6+-tetrabromo-4+4+-isopropylidenediphenol" OR "4+4+-+2+2-propanediyl+bis+2+6-dibromophenol" OR "chembl184450" OR "dtxsid1026081" OR "chebi:33217" OR "phenol+4+4+-isopropylidenebis+2+6-dibromo-" OR "mfcd00013962" OR "dsstox_cid_6081" OR "4+4+-+1-methylethylidene+bis+2+6-dibromophenol+2+2-bis+3+5-dibromo-4-hydroxyphenyl+propane" OR "dsstox_rid_78008" OR "dsstox_gsid_26081" OR "w-104257" OR "tetrabromobisphenola" OR "tetrabromo+bisphenol+a" OR "3+3+5+5+-tetrabromo+bisphenol+a" OR "33+55+-tetrabromobisphenol+a" OR "saytex+rb-100+abs" OR "tetrabromo-4+4+-isopropylidenediphenol" OR "ec+201-236-9" OR "oprea1_822733" OR "schembl18647" OR "mls002152878" OR "bidd:er0631" OR "c15h12br4o2" OR "330396_aldrich" OR "aronis002155" OR "2+6+6+-tetrabromobisphenol+a" OR "ctk4f6165" OR "ks-00003vgg" OR "3+3+5+-tetrabromobisphenol+a" OR "albb-031649" OR "ks-00000wf5" OR "nsc59775" OR "zinc1689786" OR "zx-as004485" OR "tox21_201182" OR "tox21_201981" OR "tox21_300561" OR "bdbm50150793" OR "nsc-59775" OR "sbb080626" OR "stk048486" OR "zinc01689786" OR "akos000491577" OR "3+3\+5+5\+-tetrabromobisphenol+a" OR "mcule-8578472069" OR "ncgc00091463-01" OR "ncgc00091463-02" OR "ncgc00091463-03" OR "ncgc00091463-04" OR "ncgc00091463-05" OR "ncgc00091463-06" OR "ncgc00254356-01" OR "ncgc00258734-01" OR "ncgc00259530-01" OR "ac-11719" OR "ak113742" OR "as-12834" OR "smr001224492" OR "phenol+4+-isopropylidenebis+2+6-dibromo-" OR "3+3+5+5+-tetrabromobisphenol+a+97%" OR "ax8153220" OR "ft-0617111" OR "ft-0682679" OR "phenol+4+-+1-methylethylidene+bis+2+6-dibromo-" OR "sr-01000596914" OR "sr-01000596914-1" OR "2+2+6+6+-tetrabromo-4+4+-isopropylidene+bisphenol" OR "phenol+4+4+-isopropylidenebis+2+6-dibromo-+8ci" OR "3+3+5+5+-tetrabromo-4+4-dihydroxy-2+2-diphenylpropane" OR "3+3+5+5+-tetrabromo-4+4+-dihydroxy-diphenyl-dimethyl-methane" OR "tbbpa" OR "tetrabromobisphenol_a" OR "Tetrabromobisphenol+A" OR "3+3+5+5+-Tetrabromobisphenol+A" OR "Bromdian" OR "4+4+-+propane-2+2-diyl+bis+2+6-dibromophenol" OR "2+2-Bis+3+5-dibromo-4-hydroxyphenyl+propane" OR "4+4+-Isopropylidenebis+2+6-dibromophenol" OR "Tetrabromodian" OR "2+2+6+6+-TETRABROMOBISPHENOL+A" OR "Saytex+RB+100PC" OR "Phenol+4+4+-+1-methylethylidene+bis+2+6-dibromo-" OR "Tetrabromodiphenylopropane" OR "4+4+-propane-2+2-diylbis+2+6-dibromophenol" OR "UNII-FQI02RFC3A" OR "4+4+-+1-Methylethylidene+bis+2+6-dibromophenol" OR "3+5+3+5+-Tetrabromobisphenol+A" OR "NSC+59775" OR "CCRIS+6274" OR "HSDB+5232" OR "Saytex+RB-100" OR "4+4+-Isopropylylidenebis+2+6-dibromophenol" OR "2+2-

					Bis+4-hydroxy-3+5-dibromophenyl+propane" OR "EINECS+201-236-9" OR "FQI02RFC3A" OR "2+2+6+6+-Tetrabromo-4+4+-isopropylidenediphenol" OR "2+6-dibromo-4-+2-+3+5-dibromo-4-hydroxyphenyl+propan-2-yl+phenol" OR "4+4+-+2+2-PROPANEDIYL+BIS+2+6-DIBROMOPHENOL" OR "CHEMBL184450" OR "DTXSID1026081" OR "CHEBI:33217" OR "Phenol+4+4+-isopropylidenebis+2+6-dibromo-" OR "4+4+-+2+2-propanediyl+bis+2+6-dibromo+phenol" OR "MFCD00013962" OR "DSSTox_CID_6081" OR "4+4+-+1-Methylethylidene+bis+2+6-dibromophenol+2+2-bis+3+5-dibromo-4-hydroxyphenyl+propane" OR "DSSTox_RID_78008" OR "DSSTox_GSID_26081" OR "W-104257" OR "2+6-dibromo-4-+1-+3+5-dibromo-4-hydroxyphenyl+-1-methylethyl+phenol" OR "TetrabromobisphenolA" OR "Tetrabromo+bisphenol+A" OR "4+4+-+1-methylethylidene+bis+2+6-dibromophenol" OR "3+3+5+5+-Tetrabromo+bisphenol+A" OR "33+55+-Tetrabromobisphenol+A" OR "4+6-dibromophenol" OR "Saytex+RB-100+ABS" OR "2+5-dibromophenyl+propane" OR "TETRABROMO-4+4+-ISOPROPYLIDENEDIPHENOL" OR "bmse000567" OR "EC+201-236-9" OR "Oprea1_822733" OR "SCHEMBL18647" OR "MLS002152878" OR "BIDD:ER0631" OR "C15H12Br4O2" OR "330396_ALDRICH" OR "ARONIS002155" OR "2+6+6+-Tetrabromobisphenol+A" OR "CTK4F6165" OR "KS-00003VGG" OR "3+3+5+-Tetrabromobisphenol+A" OR "ALBB-031649" OR "KS-00000WF5" OR "NSC59775" OR "ZINC1689786" OR "ZX-AS004485" OR "Tox21_201182" OR "Tox21_201981" OR "Tox21_300561" OR "2+5-dibromo-4-hydroxyphenyl+propane" OR "BDBM50150793" OR "NSC-59775" OR "SBB080626" OR "STK048486" OR "ZINC01689786" OR "2+6-dibromo-4-+1-+3+5-dibromo-4-hydroxy-phenyl+-1-methyl-ethyl+phenol" OR "AKOS000491577" OR "2+2+6+6+-Tetrabromobisphenol+A" OR "3+3+5+5+-tetrabromobisphenol+A" OR "3+3\+5+5\+-tetrabromobisphenol+A" OR "MCULE-8578472069" OR "NCGC00091463-01" OR "NCGC00091463-02" OR "NCGC00091463-03" OR "NCGC00091463-04" OR "NCGC00091463-05" OR "NCGC00091463-06" OR "NCGC00254356-01" OR "NCGC00258734-01" OR "NCGC00259530-01" OR "30496-13-0" OR "AC-11719" OR "AK113742" OR "AS-12834" OR "SMR001224492" OR "Phenol+4+-isopropylidenebis+2+6-dibromo-" OR "3+3+5+5+-Tetrabromobisphenol+A+97%" OR "AX8153220" OR "phenol+4+4+-isopropylidenebis+dibromo-" OR "2+2-bis+3+5dibromo-4-hydroxyphenyl+propane" OR "4+4+-isopropylidene-bis+2+6-dibromophenol" OR "FT-0617111" OR "FT-0682679" OR "2+2-bis+3+5-dibromo-4-hydroxyphenyl+-propane" OR "2+2-bis-+3+5-dibromo-4-hydroxyphenyl+propane" OR "2+2-bis-+3+5-dibromo-4-hydroxyphenyl+-propane" OR "Phenol+4+-+1-methylethylidene+bis+2+6-dibromo-" OR "SR-01000596914" OR "tetrabromodihydroxy+diphenylpropane" OR "SR-01000596914-1" OR "2+2+6+6+-Tetrabromo-4+4+-isopropylidene+bisphenol" OR "2+2-bis-+4+-hydroxy-3+5+-dibromophenyl+-propane" OR "Phenol+4+4+-isopropylidenebis+2+6-dibromo-+8Cl" OR "3+3+5+5+-Tetrabromo-4+4-dihydroxy-2+2-diphenylpropane" OR "3+3+5+5+-Tetrabromo-4+4+-dihydroxy-diphenyl-dimethyl-methane" OR "4-+1-+3+5-dibromo-4-hydroxyphenyl+-isopropyl+-2+6-dibromophenol" OR "TBBPA" OR "tetrabromobisphenol_A" OR "CAS 79-94-7")
					OR emm_caschemical__value:("79-94-7")

				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
56.tetraethylene_glycol_ethyl_methyl_eth	(chemical names OR CAS value))	NO			"schembl316251" OR "ctk2j0661" OR "dtxsid70601664" OR "2 5 8 11 14 pentaoxahexadecane" OR "2 5 8 11 14 Pentaoxahexadecane" OR "1 2 2 2-ethoxyethoxy ethoxy ethoxy 2-methoxyethane" OR "tetraethylene glycol ethyl methyl ether" OR "CAS 89769-11-9"
					OR emm_caschemical__value:("89769-11-9")
57. tk11-39	(chemical names OR CAS value)) NOT "prep method"	NO			topic:("2-benzyl-2 dimethylamino 4 morpholinobutyrophenone" OR "dtxsid5044786" OR "2-benzyl-2 dimethylamino 1 4 morpholin-4-yl phenyl butan-1-one" OR "2-benzyl-2 dimethylamino 1 4 4-morpholinyl phenyl 1-butanone" OR "1-butanone 2 dimethylamino 1 4 4-morpholinyl phenyl 2 phenylmethyl " OR "photocure 3665" OR "pubchem 20904" OR "acmc-20a2em" OR "ec 404-360-3" OR "dsstox_cid_24786" OR "dsstox_rid_80475" OR "dsstox_gsid_44786" OR "schembl35868" OR "chembl3187611" OR "ctk4b1229" OR "tox21_301707" OR "anw-54044" OR "akos015901469" OR "mcule-2935597430" OR "ncgc00256142-01" OR "ds-12208" OR "ls-46712" OR "st058401" OR "ax8071161" OR "cas-119313-12-1" OR "ft-0712767" OR "ns00006098" OR "ks-00001234" OR "q27258386" OR "2-benzyl-2-dimethylamino-1 4-morpholinophenyl butan-1-one" OR "2-benzyl-2 dimethylamino 1 4 morpholino phenyl 1-butanone" OR "2 dimethylamino 1 4 4-morpholinyl phenyl 2 phenylmethyl 1-butanone" OR "2-Benzyl-2-dimethylamino-1 4-morpholinophenyl 1-butanone" OR "2-Benzyl-2 dimethylamino 4 morpholinobutyrophenone" OR "Irgacure 369" OR "2-benzyl-2 dimethylamino 1 4-morpholinophenyl butan-1-one" OR "DTXSID5044786" OR "2-Benzyl-2 dimethylamino 1 4 morpholin-4-yl phenyl butan-1-one" OR "2-Benzyl-2 dimethylamino 1 4 4-morpholinyl phenyl 1-butanone" OR "2-Benzyl-2-dimethylamino-4 morpholinobutyrophenone" OR "1-Butanone 2 dimethylamino 1 4 4-morpholinyl phenyl 2 phenylmethyl " OR "2-benzyl-2 dimethylamino 1 4-morpholin-4-ylphenyl butan-1-one" OR "2-benzyl-2 dimethylamino 4-morpholinobutyrophenone" OR "photoinitiator 369" OR "Photocure 3665" OR "PubChem 20904" OR "ACMC-20a2em" OR "IRGACURE 369" OR "EC 404-360-3" OR "DSSTox_CID_24786" OR "DSSTox_RID_80475" OR "DSSTox_GSID_44786" OR "SCHEMBL35868" OR "CHEMBL3187611" OR "CTK4B1229" OR "Tox21_301707" OR "ANW-54044" OR "AKOS015901469" OR "MCULE-2935597430" OR "NCGC00256142-01" OR "DS-12208" OR "LS-46712" OR "ST058401" OR "AX8071161" OR "CAS-119313-12-1" OR "FT-0712767" OR "NS00006098" OR "KS-00001234" OR "2-benzyl-2-dimethylamino-4-morpholinobutyrophenone" OR "2-benzyl-2- dimethylamino -4 -morpholino-butyroph" OR "Q27258386" OR "2-benzyl-2-dimethylamino-1 - 4morpholinophenyl butan-1-one" OR "2-benzyl-2-dimethylamino-1- 4-morpholinophenyl -butanone-1" OR "2-benzyl-2-dimethylamino-1- 4-morpholinophenyl butan-1-one" OR "2-benzyl-2-dimethylamino-1- 4-morpholinophenyl -1-butanone" OR "2-Benzyl-2-dimethylamino-1- 4-morpholinophenyl -butan-1-one" OR "2- dimethylamino -1- 4-morpholin-4-ylphenyl -2-benzylbutan-1-one" OR "2-Benzyl-2-dimethylamino -1- 4- morpholino phenyl -1-butanone" OR "2-benzyl-2-n n-dimethylamino-1- 4-morpholinophenyl -1-

					butanone" OR "2- Dimethylamino -1- 4- 4-morpholinyl phenyl -2- phenylmethyl -1-butanone" OR "1-butanone 2-(dimethylamino)-1-[4-(4-morpholinyl)phenyl]-2-(phenylmethyl)-" OR "2-benzyl-2-dimethylamino-4 -morpholinobutyrophenone" OR "2-benzyl-2-(dimethylamino)-1-(4-morpholinophenyl)-1-butanone" OR "2-benzyl-2-(dimethylamino)-1-(4-morpholinophenyl)butanone-1" OR "2-benzyl-2-(dimethylamino)-1-[4-(4-morpholinyl)phenyl]-1-butanone" OR "2-benzyl-2-n n-dimethylamino-1-(4-morpholinophenyl)-1-butanone" OR "2-benzyl-2-dimethylamino-1-(4-morpholinophenyl)butanone" OR "cg 25-369" OR "irgacure 369" OR "tk 11-319" OR "CAS 119313-12-1")
					OR emm_caschemical__value:("119313-12-1")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

58.triphenylphosphine	(chemical names OR CAS value)) NOT "prep method" NOT synthesis	NO			topic:("phosphine triphenyl-" OR "triphenylphosphorus" OR "triphenylphosphide" OR "phosphorustriphenyl" OR "triphenyl phosphorous" OR "mfcd00003043" OR "phosphorus triphenyl" OR "nsc 215203" OR "ccris 4889" OR "unii-26d26oa393" OR "hsdb 4266" OR "einecs 210-036-0" OR "brn 0610776" OR "dtxsid5026251" OR "26d26oa393" OR "dsstox_cid_6251" OR "wln: rpr&r" OR "dsstox_rid_78074" OR "dsstox_gsid_26251" OR "q-201896" OR "diphenylphosphino-polystyrene" OR "triphenylphospane" OR "triphenyphosphine" OR "pubchem6417" OR "acmc-1bggs" OR "trisphenylphosphine" OR "c18h14ppol" OR "triphenyl phosphine" OR "schembl101" OR "ec 210-036-0" OR "ph 3p" OR "p ph 3" OR "nsc10" OR "ksc206a0j" OR "nsc-10" OR "schembl1679860" OR "chembl1448331" OR "c6h5 3p" OR "acn-s002163" OR "bcp01148" OR "ebd51172" OR "p c6h5 3" OR "zinc8585891" OR "zx-at007677" OR "tox21_202114" OR "tox21_303294" OR "7817ah" OR "anw-75057" OR "gk1326" OR "nsc215203" OR "or9088" OR "pp-360" OR "rw2519" OR "sbb060439" OR "stl185621" OR "akos009031542" OR "as01621" OR "ls-1438" OR "ls41004" OR "mcule-9122575728" OR "nsc-215203" OR "qc-4207" OR "ks-000002n8" OR "ncgc00091416-01" OR "ncgc00091416-03" OR "ncgc00257211-01" OR "ncgc00259663-01" OR "at-19512" OR "bp-12577" OR "sc-05646" OR "sc-65423" OR "db-050422" OR "bis triphenylphosphine nickel ii dichloride" OR "ft-0604360" OR "ft-0632502" OR "ft-0689298" OR "ft-0698371" OR "ns00002889" OR "st50406239" OR "az0001-0002" OR "c-24254" OR "q115493" OR "f1642-0085" OR "phosphine triphenyl" OR "trifenylfosfin" OR "triphenylphosphane" OR "Phosphine triphenyl-" OR "Triphenylphosphorus" OR "Triphenylphosphide" OR "Triphenylphosphine" OR "Phosphorustriphenyl" OR "39319-11-4" OR "TRIPHENYL PHOSPHOROUS" OR "MFCD00003043" OR "Phosphorus triphenyl" OR "NSC 215203" OR "CCRIS 4889" OR "UNII-26D26OA393" OR "HSDB 4266" OR "EINECS 210-036-0" OR "BRN 0610776" OR "DTXSID5026251" OR "26D26OA393" OR "DSSTox_CID_6251" OR "WLN: RPR&R" OR "DSSTox_RID_78074" OR "DSSTox_GSID_26251" OR "Q-201896" OR "Diphenylphosphino-polystyrene" OR "triphenyphospine" OR "tripenylphosphine" OR "triphenyiphoshine" OR "triphenylphophine" OR "triphenylphospine" OR "tripheylphosphine" OR "Triphenylphospane" OR "Triphenyphosphine" OR "tripbenylphosphine" OR "triphenyiphosphine" OR "tri-phenylphospine" OR "triphenyl phophine" OR "triphenyl phospine" OR "triphenylphosphine" OR "triphenyl phosphorus" OR "triphenyl- phosphine" OR "PubChem6417" OR "ACMC-1BGGS" OR "TRISPHENYLPHOSPHINE" OR "14126-32-0" OR "14264-16-5" OR "C18H14PPol" OR "Triphenyl Phosphine" OR "SCHEMBL101" OR "EC 210-036-0" OR "Ph 3P" OR "P Ph 3" OR "NSC10" OR "KSC206A0J" OR "NSC-10" OR "SCHEMBL1679860" OR "CHEMBL1448331" OR "C6H5 3P" OR "ACN-S002163" OR "BCP01148" OR "EBD51172" OR "P C6H5 3" OR "ZINC8585891" OR "ZX-AT007677" OR "Tox21_202114" OR "Tox21_303294" OR "7817AH" OR "ANW-75057" OR "GK1326" OR "NSC215203" OR "OR9088" OR "PP-360" OR "RW2519" OR "SBB060439" OR "STL185621" OR "AKOS009031542" OR "AS01621" OR "LS-1438" OR "LS41004" OR "MCULE-9122575728" OR "NSC-215203" OR "QC-4207" OR "KS-000002N8" OR "NCGC00091416-01" OR "NCGC00091416-03" OR "NCGC00257211-01" OR "NCGC00259663-01" OR "AT-19512" OR "BP-12577" OR "SC-05646" OR "SC-65423" OR "DB-050422" OR "Bis triphenylphosphine nickel II dichloride" OR "FT-0604360" OR "FT-0632502" OR "FT-0689298" OR "FT-0698371" OR

					"NS00002889" OR "ST50406239" OR "AZ0001-0002" OR "C-24254" OR "Q115493" OR "F1642-0085" OR "Phosphine triphenyl" OR "Trifenylfosfin" OR "triphenyl phosphin" OR "Triphenyl phosphine" OR "triphenylphoshine" OR "Triphenylphosphane" OR "triphenyl-phosphane" OR "triphenylphosphin" OR "TRIPHENYLPHOSPHINE" OR "triphenyl-phosphine" OR "tri-phenylphosphine" OR "tri-phenyl-phosphine" OR "triphenylphosphorane" OR "CAS 603-35-0")
					OR emm_caschemical__value:("603-35-0")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
				NOT synthesis	NOT topic:synthesis
59.Triphenyl_phosphite	(chemical names OR CAS value)) NOT "prep method" NOT synthesis	NO			topic:("triphenyl phosphite" OR "phosphorous acid triphenyl ester" OR "triphenoxyphosphine" OR "phenyl phosphite" OR "stabilizer p 36" OR "trifenoxyfosfin" OR "trifenylfosfit" OR "phosclere t 36" OR "tris phenoxy phosphine" OR "unii-9p45grd24x" OR "nsc 43789" OR "ccris 4890" OR "hsdb 2571" OR "einecs 202-908-4" OR "brn 1079456" OR "advancetpp" OR "ai3-07866" OR "9p45grd24x" OR "dtxsid0026252" OR "dsstox_cid_6252" OR "dsstox_rid_78075" OR "dsstox_gsid_26252" OR "doverphos 10" OR "doverphos 10-hr" OR "pubchem18696" OR "phosphorous acid triphenyl" OR "acmc-2097tu" OR "ec 202-908-4" OR "nciopen2_007800" OR "schembl13289" OR "ksc108a5p" OR "chembl1875503" OR "nsc43789" OR "nsc62219" OR "zinc2504359" OR "tox21_202034" OR "tox21_300002" OR "anw-14416" OR "mfcd00003032" OR "nsc-43789" OR "nsc-62219" OR "akos015902569" OR "ne10254" OR "ncgc00091577-01" OR "ncgc00091577-02" OR "ncgc00091577-03" OR "ncgc00091577-04" OR "ncgc00254028-01" OR "ncgc00259583-01" OR "bp-21353" OR "sc-22578" OR "ft-0689185" OR "ns00009404" OR "ks-00000156" OR "q222290" OR "f0001-0051" OR "TRIPHENYL PHOSPHITE" OR "Phosphorous acid triphenyl ester" OR "Triphenoxyphosphine" OR "Phenyl phosphite" OR "Stabilizer P 36" OR "Trifenoxyfosfin" OR "Trifenylfosfit" OR "Phosclere T 36" OR

					"Phosphorous Acid Triphenyl Ester" OR "Tris phenoxy phosphine" OR "UNII-9P45GRD24X" OR "NSC 43789" OR "CCRIS 4890" OR "HSDB 2571" OR "EINECS 202-908-4" OR "BRN 1079456" OR "Advancetpp" OR "AI3-07866" OR "9P45GRD24X" OR "DTXSID0026252" OR "DSSTox_CID_6252" OR "DSSTox_RID_78075" OR "DSSTox_GSID_26252" OR "triphelyn phosphite" OR "Doverphos 10" OR "Doverphos 10-HR" OR "PubChem18696" OR "Phosphorous acid triphenyl" OR "ACMC-2097tu" OR "EC 202-908-4" OR "Triphenyl Phosphite" OR "NCIOpen2_007800" OR "SCHEMBL13289" OR "KSC108A5P" OR "CHEMBL1875503" OR "NSC43789" OR "NSC62219" OR "ZINC2504359" OR "Tox21_202034" OR "Tox21_300002" OR "ANW-14416" OR "MFCD00003032" OR "NSC-43789" OR "NSC-62219" OR "AKOS015902569" OR "NE10254" OR "NCGC00091577-01" OR "NCGC00091577-02" OR "NCGC00091577-03" OR "NCGC00091577-04" OR "NCGC00254028-01" OR "NCGC00259583-01" OR "BP-21353" OR "SC-22578" OR "FT-0689185" OR "NS00009404" OR "KS-00000156" OR "Q222290" OR "F0001-0051" OR "triphenyl_phosphite" OR "CAS 101-02-0")
					OR emm_caschemical__value:("101-02-0")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
				NOT synthesis	NOT topic:synthesis
60.Tris_1_3-dichloro-2-propyl_phosp	(chemical names OR CAS value)) NOT "prep method"	NO			topic:("tris 1 3-dichloro-2-propyl phosphate" OR "tris 1 3-dichloroisopropyl phosphate" OR "2-propanol 1 3-dichloro- phosphate 3:1" OR "phosphoric acid tris 1 3-dichloro-2-propyl ester" OR "fyrol fr-2" OR "1 3-dichloro-2-propanol phosphate 3:1" OR "unii-b1prv4g0t0" OR "tris 1-chloromethyl-2-chloroethyl phosphate" OR "tris 2-chloro-1- chloromethyl ethyl phosphate" OR "pf 38/3" OR "ccris 6284" OR "tri beta beta -dichloroisopropyl phosphate" OR "hsdb 4364" OR "einecs 237-159-2" OR "brn 1715458" OR "b1prv4g0t0" OR "fosforan troj-1 3-dwuchloroizopropylowy" OR "dtxsid9026261" OR "2-propanol 1 3-dichloro- 2 2 2 -phosphate" OR "fosforan troj- 1 3-dwuchloroizopropylowy polish" OR "dsstox_cid_6261" OR "dsstox_rid_78078" OR "dsstox_gsid_26261" OR "fyrol fr2" OR "tris- 1 3-dichloro-2-propyl -phosphate" OR "acmc-209c9q" OR "ec 237-159-2" OR "ksc496a6h" OR "schembl333198" OR "chembl3182032" OR "ctk3j6063" OR "chebi:143729" OR "tris 1 3-dichlorisopropyl phosphat" OR "ks-00000z7i" OR "zinc2019519" OR "tox21_202166" OR "tox21_300194" OR "anw-20172" OR "ls-798" OR "akos015856734" OR "cs-8011" OR "tris 1.3-dichloro-2-propyl phosphate" OR "tris- 1 3-dichloro-2-propyl phosphate" OR "ncgc00247923-01" OR "ncgc00247923-02" OR "ncgc00254047-01" OR "ncgc00259715-01" OR "ak116066" OR "ax8147868" OR "hy-108712" OR "ft-0654115" OR "ns00010388" OR "tris 1 3-dichlorisopropyl phosphate" OR "tri .beta. .beta. -dichloroisopropyl phosphate" OR "a807122" OR "j-006902" OR "q2454085" OR "Tris 1 3-dichloro-2-propyl phosphate" OR "tris 1 3-dichloropropan-2-yl phosphate" OR "TRIS 1 3-DICHLORO-2-PROPYL PHOSPHATE" OR "Tris 1 3-dichloroisopropyl phosphate" OR "2-Propanol 1 3-dichloro- phosphate 3:1" OR "Phosphoric Acid Tris 1 3-dichloro-2-propyl Ester" OR "Fyrol FR-2" OR "1 3-Dichloro-2-propanol phosphate 3:1" OR "UNII-B1PRV4G0T0" OR "Tris 1-chloromethyl-2-chloroethyl phosphate" OR "Tris 2-chloro-1- chloromethyl ethyl

					phosphate" OR "PF 38/3" OR "CCRIS 6284" OR "Tri beta beta -dichloroisopropyl phosphate" OR "HSDB 4364" OR "EINECS 237-159-2" OR "BRN 1715458" OR "B1PRV4G0T0" OR "Fosforan troj- 1 3-dwuchloroizopropylowy" OR "DTXSID9026261" OR "2-Propanol 1 3-dichloro- 2 2 2 - phosphate" OR "Fosforan troj- 1 3-dwuchloroizopropylowy Polish" OR "Phosphoric acid tris 1 3-dichloro-2-propyl ester" OR "DSSTox_CID_6261" OR "DSSTox_RID_78078" OR "DSSTox_GSID_26261" OR "Fyrol FR2" OR "Tris- 1 3-dichloro-2-propyl -phosphate" OR "ACMC-209c9q" OR "EC 237-159-2" OR "KSC496A6H" OR "SCHEMBL333198" OR "CHEMBL3182032" OR "CTK3J6063" OR "CHEBI:143729" OR "tri 2 3-dichloropropyl phosphate" OR "Tris 1 3-dichlorisopropyl phosphat" OR "KS-00000Z7I" OR "ZINC2019519" OR "Tox21_202166" OR "Tox21_300194" OR "ANW-20172" OR "LS-798" OR "AKOS015856734" OR "CS-8011" OR "Tris 1.3-dichloro-2-propyl phosphate" OR "Tris- 1 3-dichloro-2-propyl phosphate" OR "NCGC00247923-01" OR "NCGC00247923-02" OR "NCGC00254047-01" OR "NCGC00259715-01" OR "AK116066" OR "AX8147868" OR "HY-108712" OR "FT-0654115" OR "NS00010388" OR "Tris 1 3-dichlorisopropyl phosphate" OR "Tri .beta. .beta. -dichloroisopropyl phosphate" OR "tris 1 3-bis chloranyl propan-2-yl phosphate" OR "A807122" OR "J-006902" OR "Q2454085" OR "phosphoric acid tris 1 3-dichloropropan-2-yl ester" OR "phosphoric acid tris- 2-chloro-1-chloromethyl-ethyl ester" OR "CAS 13674-87-8")
					OR emm_caschemical__value:("13674-87-8")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))
61.Trixylenyl_phosphate	(chemical names OR CAS value)) NOT "prep method"	NO			topic:("unii-7m08k25q1j" OR "hsdb 3908" OR "7m08k25q1j" OR "tris 2 4-xylenyl phosphate" OR "nsc 78488" OR "2 4-xylyl phosphate c8h9o 3po" OR "brn 1895059" OR "coalite ntp" OR "ivviol-3" OR "nsc78488" OR "phosflex 179" OR "schembl108984" OR "ccris 4891" OR "hsdb 6094" OR "dtxsid80959466" OR "ebd59818" OR "zinc1718867" OR "einecs 246-677-8" OR "nsc-78488" OR "akos015899549" OR "mcule-4708791677" OR "ls-104534" OR "ec 246-677-8" OR "w-110611" OR "q27268543" OR "2 4-dimethylphenol phosphate 3 1" OR "2 4-xylenol phosphate 3 1" OR "2 4-xylyl phosphate" OR "dimethylphenol phosphate 3 1" OR "phenol 2 4-dimethyl 1 1 1 phosphate" OR "phenol 2 4-dimethyl phosphate 3 1" OR "phenol 4dimethyl phosphate 3 1" OR "phenol dimethyl 1 1 1 phosphate" OR "phosphate trixylyl" OR "phosphoric acid tris 2 4-dimethylphenyl ester" OR "phosphoric acid tris 2 4-xylyl ester" OR "phosphoric acid trixylyl ester" OR "tri 2 4-dimethylphenyl phosphate" OR "tri 2 4-xylenyl phosphate" OR "tri xlylenyl phosphate" OR "tri-2 4-xylyl phosphate" OR "tri-2 4-xylylphosphat" OR "tri-dimethyl phenyl phosphate" OR "trixylenyl phosphate" OR "tri-xylenyl phosphate" OR "xylenol phosphate 3:1" OR "xylyl phosphate" OR "tris 2 4-dimethylphenyl phosphate" OR "CAS 3862-12-2")
					OR emm_caschemical__value:("3862-12-2")
				NOT patents "preparation method"	NOT (class:patent AND topic:("preparation method" OR "material preparation" OR "preparation process" OR "production process" OR "production method" OR "method preparing"~2 OR "method producing"~2))

Appendix C – Search strategies for known chemicals in news articles

Term	Query
Piperonyl_butoxide	(butacide OR butocide OR ethanol+butoxide OR pyrenone+606 OR 5-+2-+2-butoxyethoxy+ethoxy+methyl+-6-propylbenzo+d+1+3+dioxole OR butyl+carbitol+6-propylpiperonyl+ether OR piperonylbutoxide OR 6-propylpiperonyl+butyl+diethylene+glycol+ether OR 2-+2-butoxyethoxy+ethyl+6-propylpiperonyl+ether OR nci-c02813 OR fmc+5273 OR nia+5273 OR 6-+propylpiperonyl+butylcarbityl+ether OR 1+3-benzodioxole+5-+2-+2-butoxyethoxy+ethoxy+methyl+-6-propyl- OR unii-lwk91tu9ah OR nsc+8401 OR ccris+522 OR butylcarbityl+6-propylpiperonyl+ether OR hsdb+1755 OR einecs+200-076-7 OR lwk91tu9ah OR 3+4-methylenedioxy-6-propylbenzyl+n-butyl+diethyleneglycol+ether OR 5-+2-+2-butoxyethoxy+ethoxymethyl+-6-propyl-1+3-benzodioxole OR epa+pesticide+chemical+code+067501 OR brn+0288063 OR 6-+propylpiperonyl+-butyl+carbityl+ether OR alpha-+2-+2-n-butoxyethoxy+-ethoxy+-4+5-methylenedioxy-2-propyltoluene OR butyl-carbityl+6-propylpiperonyl+ether OR ai3-14250 OR dtxsid1021166 OR 3+4-methylendioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether OR chebi:32687 OR 5-propyl-4-+2+5+8-trioxa-dodecyl+-1+3-benzodioxole OR ncgc00090874-02 OR ncgc00090874-04 OR ak114177 OR 3+4-methylenedioxy-6-propylbenzyl+n-butyldiethyleneglycol+ether OR 5-propyl-4-+2+5+8-trioxa-dodecyl+-1+3-benzodioxol+german OR 3+4-methylendioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether+german OR alpha-+2-+2-butoxyethoxy+ethoxy+-4+5-methylenedioxy-2-propyltoluene OR dsstox_cid_1166 OR 3+4-methylenedioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether+german OR toluene+alpha-+2-+2-butoxyethoxy+ethoxy+-4+5-+methylenedioxy+-2-propyl- OR dsstox_rid_75988 OR dsstox_gsid_21166 OR q-201588 OR 2-+2-butoxyethoxy+-1-+6-propyl+2h-benzo+d+1+3-dioxolen-5-yl+methoxy+ethane OR pybuthrin OR pyrenon OR synpren-fish OR .alpha.+2-+2-butoxyethoxy+ethoxy+-4+5-methylenedioxy-2-propyltoluene OR .alpha.-+2-+2-n-butoxyethoxy+-ethoxy+-4+5-methylenedioxy-2-propyltoluene OR pubchem15364 OR ec+200-076-7 OR schembl5490 OR 5-propyl-4-+2+5+8-trioxa-dodecyl+-1+3-benzodioxol OR chembl1201131 OR ks-00000meb OR nsc8401 OR bdbm181115 OR hms3264a07 OR 3+4-methylenedioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether OR acm51036 OR bcp19227 OR fac+5273 OR hy-b1198 OR nsc-8401 OR zinc3875342 OR tox21_111034 OR tox21_400086 OR mfcd00005842 OR akos015951348 OR toluene+5-+methylenedioxy+-2-propyl- OR tox21_111034_1 OR ccg-213921 OR db09350 OR mcule-7766634514 OR ncgc00090874-01 OR ncgc00090874-03 OR ncgc00090874-05 OR ncgc00090874-06 OR st075004 OR ax8061167 OR db-051886 OR propylpiperonyl+butyl+diethyleneglycol+ether OR ft-0631218 OR ns00011484 OR ab01563216_01 OR sr-0 0944266 OR 5-propyl-4-+2+8-trioxa-dodecyl+-1+3-benzodioxol OR sr-0 0944266-1 OR 4+5-methylenedioxy-2-propylbenzyldiethylene+glycol+butyl+ether OR 4+5-methylenedioxy-2-propylbenzyldiethyleneglycol+butyl+ether OR benzodioxole+5-+2-+2-butoxyethoxy+ethoxy+methyl+-6-propyl- OR piperonylbutoxide+certified+reference+material+tracecert+r OR 3+4-methylenedioxy-6-propylbenzyl+butyl+diethylene+glicol+ether OR 3+4-methylenedioxy-6-propylbenzyl+n-butyl+diethylene+glycol+ether OR 5-+2-+2-butoxyethoxy+ethoxy+methyl+-6-propyl-1+3-benzodioxole+# OR 5-{+2-+2-butoxyethoxy+ethoxy+methyl}-6-propyl-2h-1+3-benzodioxole OR piperonylbutoxide+british+pharmacopoeia+bp+reference+standard OR butylcarbityl+6-propylpiperonyl+ether+80%+and+related+compounds+20% OR piperonyl+butoxide+/+2-+2-butoxyethoxy+ethyl+6-propylpiperonyl+ether OR toluene+.alpha.-+2-+2-butoxyethoxy+ethoxy+-4+5-+methylenedioxy+-2-propyl- OR 2-+2-butoxyethoxy+ethyl+6-propylpiperonyl+ether+4+5-methylenedioxy-2-propylbenzyldiethyleneglycol+butyl+ether OR piperonyl+butoxide OR Butacide OR Butocide OR Ethanol+butoxide OR Pyrenone+606 OR 5-+2-+2-Butoxyethoxy+ethoxy+methyl+-6-propylbenzo+d+1+3+dioxole OR Butyl+carbitol+6-propylpiperonyl+ether OR Piperonylbutoxide OR 6-Propylpiperonyl+butyl+diethylene+glycol+ether OR 2-+2-Butoxyethoxy+ethyl+6-propylpiperonyl+ether OR NCI-C02813 OR FMC+5273 OR NIA+5273 OR 6-+Propylpiperonyl+butylcarbityl+ether OR 1+3-Benzodioxole+5-+2-+2-butoxyethoxy+ethoxy+methyl+-6-propyl- OR UNII-LWK91TU9AH OR NSC+8401 OR CCRIS+522 OR Butylcarbityl+6-propylpiperonyl+ether OR HSDB+1755 OR EINECS+200-076-7 OR LWK91TU9AH OR 3+4-Methylenedioxy-6-propylbenzyl+n-butyl+diethyleneglycol+ether OR 5-+2-+2-Butoxyethoxy+ethoxymethyl+-6-propyl-1+3-benzodioxole OR EPA+Pesticide+Chemical+Code+067501 OR BRN+0288063 OR 6-+Propylpiperonyl+-butyl+carbityl+ether OR alpha-+2-+2-n-Butoxyethoxy+-ethoxy+-4+5-methylenedioxy-2-propyltoluene OR Butyl-carbityl+6-propylpiperonyl+ether OR AI3-14250 OR DTXSID1021166 OR 3+4-Methylendioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether OR CHEBI:32687 OR 5-Propyl-4-+2+5+8-trioxa-dodecyl+-1+3-benzodioxole OR NCGC00090874-02 OR NCGC00090874-04 OR AK114177 OR 3+4-Methylenedioxy-6-propylbenzyl+n-butyldiethyleneglycol+ether OR 5-Propyl-4-+2+5+8-trioxa-dodecyl+-1+3-benzodioxol+German OR 5-+2-+2-Butoxyethoxy+ethoxy+methyl+-6-propyl-1+3-benzodioxole OR 5-{+2-+2-butoxyethoxy+ethoxy+methyl}-6-propyl-1+3-benzodioxole OR 3+4-methylenedioxy-6-propylbenzyl+butyl+diethylene+glycol+ether OR 3+4-Methylendioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether+German OR alpha-+2-+2-Butoxyethoxy+ethoxy+-4+5-methylenedioxy-2-propyltoluene OR DSSTox_CID_1166 OR 3+4-Methylenedioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether+German OR Toluene+alpha-+2-+2-butoxyethoxy+ethoxy+-4+5-+methylenedioxy+-2-propyl- OR DSSTox_RID_75988 OR DSSTox_GSID_21166 OR Q-201588 OR 5-{+2-{+2-+butyloxy+ethyl+oxy}ethyl+oxy+methyl}-6-propyl-1+3-benzodioxole OR alpha-+2-+2-butoxyethoxy+ethoxy+-4+5-+methylenedioxy+-2-propyltoluene OR 2-+2-butoxyethoxy+-1-+6-propyl+2H-benzo+d+1+3-dioxolen-5-yl+methoxy+ethane OR Pyrenon OR Synpren-fish OR .alpha.+2-+2-Butoxyethoxy+ethoxy+-4+5-methylenedioxy-2-propyltoluene OR .alpha.-+2-+2-n-Butoxyethoxy+-ethoxy+-4+5-methylenedioxy-2-propyltoluene OR .alpha.-+2-+2-N-Butoxyethoxy+-ethoxy+-4+5-methylenedioxy-2-propyltoluene OR PubChem15364 OR EC+200-076-7 OR SCHEMBL5490 OR 5-Propyl-4-+2+5+8-trioxa-dodecyl+-1+3-benzodioxol OR CHEMBL1201131 OR KS-00000MEB OR NSC8401 OR BDBM181115 OR HMS3264A07 OR 3+4-Methylenedioxy-6-propylbenzyl-n-butyl-diaethylenglykolaether OR ACM51036 OR BCP19227 OR FAC+5273 OR HY-B1198 OR NSC-8401 OR ZINC3875342 OR Tox21_111034 OR Tox21_400086 OR MFCD00005842 OR AKOS015951348 OR Toluene+5-+methylenedioxy+-2-propyl- OR Tox21_111034_1 OR CCG-213921 OR DB09350 OR MCULE-7766634514 OR NCGC00090874-01 OR NCGC00090874-03 OR NCGC00090874-05 OR NCGC00090874-06 OR ST075004 OR AX8061167 OR DB-051886 OR Propylpiperonyl+butyl+diethyleneglycol+ether OR FT-0631218 OR NS00011484 OR AB01563216_01 OR SR-0 0944266 OR 5-Propyl-4-+2+8-trioxa-dodecyl+-1+3-benzodioxol OR

	SR-0 0944266-1 OR 1+5-+2-+2-butoxyethoxy+ethoxy+methyl+-6-propyl- OR 4+5-Methylenedioxy-2-propylbenzyldiethylene+glycol+butyl+ether OR 4+5-Methylenedioxy-2-propylbenzyldiethyleneglycol+butyl+ether OR Benzodioxole+5-+2-+2-butoxyethoxy+ethoxy+methyl+-6-propyl- OR Piperonylbutoxide+certified+reference+material+TraceCERT+R OR 3+4-methylenedioxy-6-propylbenzyl+butyl+diethylene+glicol+ether OR 3+4-methylenedioxy-6-propylbenzyl+butyl+diethylene+glycol+ether OR 3+4-Methylenedioxy-6-propylbenzyl+n-butyl+diethylene+glycol+ether OR 5-+2-+2-butoxyethoxy+ethoxy+methyl+-6-propyl-1+3-benzodioxole OR 5-+2-+2-Butoxyethoxy+ethoxy+methyl+-6-propyl-1+3-benzodioxole+# OR 5-{+2-+2-butoxyethoxy+ethoxy+methyl}-6-propyl-2H-1+3-benzodioxole OR Piperonylbutoxide+British+Pharmacopoeia+BP+Reference+Standard OR Butylcarbityl+6-propylpiperonyl+ether+80%+and+related+compounds+20% OR alpha-+2-+2-butoxyethoxy+ethoxy+-4+5-methylened+ioxy-2-propyltoluene OR Piperonyl+butoxide+/+2-+2-butoxyethoxy+ethyl+6-propylpiperonyl+ether OR Toluene+.alpha.-+2-+2-butoxyethoxy+ethoxy+-4+5-+methylenedioxy+-2-propyl- OR 2-+2-Butoxyethoxy+ethyl+6-propylpiperonyl+ether+4+5-Methylenedioxy-2-propylbenzyldiethyleneglycol+butyl+ether OR Piperonyl+butoxide) OR (proximity 3 AND CAS AND 51-03-6) OR (proximity 10 AND (insecticid% OR insekti% OR insetti%) AND PBO)
hexabromocyclododecane	(cyclododecane+1+2+5+6+9+10-hexabromo- OR 1+2+5+6+9+10-hexabromocyclodecane OR unii-66oon1wwos OR hsdb+6110 OR einecs+221-695-9 OR 66oon1wwos OR dsstox_cid_7527 OR dsstox_rid_78489 OR dsstox_gsid_27527 OR cas-3194-55-6 OR acmc-1bn89 OR schembl25669 OR ksc491m2h OR chembl375298 OR dtxsid4027527 OR ctk3j1623 OR chebi:134063 OR tox21_201402 OR tox21_303176 OR anw-27232 OR akos015836044 OR 1+2+5+6+9+10-hexabromocyclododecan OR ks-0000010e OR ncgc00164063-01 OR ncgc00164063-02 OR ncgc00257050-01 OR ncgc00258953-01 OR ak116613 OR ls-55963 OR sc-18694 OR ax8052905 OR db-068553 OR ft-0626944 OR ns00002582 OR 1+2+5+6+9+10-hexabromocyclododecane+95% OR 1+2+5+6+9+10-hexabromocyclododecane+hbcd OR q420301 OR w-106868 OR Cyclododecane+1+2+5+6+9+10-hexabromo- OR 1+2+5+6+9+10-Hexabromocyclodecane OR UNII-66OON1WWOS OR HSDB+6110 OR EINECS+221-695-9 OR 66OON1WWOS OR DSSTox_CID_7527 OR DSSTox_RID_78489 OR DSSTox_GSID_27527 OR CAS-3194-55-6 OR ACMC-1BN89 OR SCHEMBL25669 OR KSC491M2H OR CHEMBL375298 OR DTXSID4027527 OR CTK3J1623 OR CHEBI:134063 OR Tox21_201402 OR Tox21_303176 OR ANW-27232 OR AKOS015836044 OR 1+2+5+6+9+10-Hexabromocyclododecan OR KS-0000010E OR NCGC00164063-01 OR NCGC00164063-02 OR NCGC00257050-01 OR NCGC00258953-01 OR AK116613 OR LS-55963 OR SC-18694 OR AX8052905 OR DB-068553 OR FT-0626944 OR NS00002582 OR 1+2+5+6+9+10-Hexabromocyclododecane+95% OR 1+2+5+6+9+10-Hexabromocyclododecane+HBCD OR Q420301 OR W-106868 OR hexabromocyclododecane) OR (proximity 3 AND CAS AND 3194-55-6)
Triphenyl_phosphite	(triphenyl+phosphite OR phosphorous+acid+triphenyl+ester OR triphenoxyphosphine OR phenyl+phosphite OR stabilizer+p+36 OR trifenoxyfosfin OR trifenylfosfit OR phosclere+t+36 OR tris+phenoxy+phosphine OR unii-9p45grd24x OR nsc+43789 OR ccris+4890 OR hsdb+2571 OR einecs+202-908-4 OR brn+1079456 OR advancetpp OR ai3-07866 OR 9p45grd24x OR dtxsid0026252 OR dsstox_cid_6252 OR dsstox_rid_78075 OR dsstox_gsid_26252 OR doverphos+10 OR doverphos+10-hr OR pubchem18696 OR phosphorous+acid+triphenyl OR acmc-2097tu OR ec+202-908-4 OR nciopen2_007800 OR schembl13289 OR ksc108a5p OR chembl1875503 OR nsc43789 OR nsc62219 OR zinc2504359 OR tox21_202034 OR tox21_300002 OR anw-14416 OR mfcd00003032 OR nsc-43789 OR nsc-62219 OR akos015902569 OR ne10254 OR ncgc00091577-01 OR ncgc00091577-02 OR ncgc00091577-03 OR ncgc00091577-04 OR ncgc00254028-01 OR ncgc00259583-01 OR bp-21353 OR sc-22578 OR ft-0689185 OR ns00009404 OR ks-00000156 OR q222290 OR f0001-0051 OR TRIPHENYL+PHOSPHITE OR Phosphorous+acid+triphenyl+ester OR Triphenoxyphosphine OR Phenyl+phosphite OR Stabilizer+P+36 OR Trifenoxyfosfin OR Trifenylfosfit OR Phosclere+T+36 OR Phosphorous+Acid+Triphenyl+Ester OR Tris+phenoxy+phosphine OR UNII-9P45GRD24X OR NSC+43789 OR CCRIS+4890 OR HSDB+2571 OR EINECS+202-908-4 OR BRN+1079456 OR Advancetpp OR AI3-07866 OR 9P45GRD24X OR DTXSID0026252 OR DSSTox_CID_6252 OR DSSTox_RID_78075 OR DSSTox_GSID_26252 OR triphelyn+phosphite OR Doverphos+10 OR Doverphos+10-HR OR PubChem18696 OR Phosphorous+acid+triphenyl OR ACMC-2097tu OR EC+202-908-4 OR Triphenyl+Phosphite OR NCIOpen2_007800 OR SCHEMBL13289 OR KSC108A5P OR CHEMBL1875503 OR NSC43789 OR NSC62219 OR ZINC2504359 OR Tox21_202034 OR Tox21_300002 OR ANW-14416 OR MFCD00003032 OR NSC-43789 OR NSC-62219 OR AKOS015902569 OR NE10254 OR NCGC00091577-01 OR NCGC00091577-02 OR NCGC00091577-03 OR NCGC00091577-04 OR NCGC00254028-01 OR NCGC00259583-01 OR BP-21353 OR SC-22578 OR FT-0689185 OR NS00009404 OR KS-00000156 OR Q222290 OR F0001-0051 OR triphenyl_phosphite) OR (proximity 3 AND CAS AND 101-02-0)
Antioxydant_2246	(2+methylenebis+4-methyl-6-tert-butylphenol OR 2+methylenebis+6-tert-butyl-4-cresol OR 2+1-dimethylethyl+p-cresol OR 2+2+methylene+bis+4-methyl-6-tert+butylphenol OR 2+2+bis+4-methyl-6-tert-butylphenol+methane OR 2+2+bis-6-terc+butyl-p-kresylmethan OR 2+2+methanediylbis+6+1+1-dimethylethyl+4-methylphenol OR 2+2+methanediylbis+6-tert-butyl-4-methylphenol OR 2+2+methyl+enebis+4-methyl-6-t-butylphenol OR 2+2+methylene-bis+4-methyl-6-tertiarybutylphenol OR 2+2+methylene-bis+6-tert-butyl+para-cresol OR 2+2+methylene-bis+6-tert-butyl-4-methylphenol OR 2+2+methylene-bis+4-methyl-6-t-butylphenol OR 2+2+methylene-bis+4-methyl-6-tert-butylphenol OR 2+2+methylene-bis+4-methyl-6-tert+butylphenol OR 2+2+methylenebis+4-methyl-6-t-butylphenol OR 2+2+methylenebis+4-methyl-6-tert OR 2+2+methylenebis+4-methyl-6-tert-butylphenol OR 2+2+methylenebis+6+1+1-dimethylethyl+4-methyl-phenol OR 2+2+methylenebis+6-+1+1-dimethylethyl+p-cresol OR 2+2+methylenebis+6-t-butyl-4-methylphenol OR 2+2+methylenebis+6-t-butyl-p-cresol OR 2+2+methylenebis+6-tert-butyl-4-cresol OR 2+2+methylenebis+6-tert-butyl-4-methyl-phenol OR 2+2+methylenebis+6-tert-butyl-4-methylphenol OR 2+2+methylenebis+6-tert-butyl-p-cresol OR 2+2+methylenebis+6-tert-4-methylphenol OR 2+2-methylenebis+4-methyl-6-t-butylphenol OR 2+2-methylenebis+6-tert-butyl-4-methylphenol OR 2+2-methylenebis+6-tert-butyl-p-cresol OR 2+tert-butyl+6+3+tert-butyl+2-hydroxy-5-methylphenyl+methyl+4-methylphe+nol OR 2-tert-butyl-6+2-hydroxy-3-tert-butyl-5-methyl-benzyl+4-methyl-phenol OR 2-tert-butyl-6-+3-tert-butyl-2-hydroxy-5-methylphenyl+methyl+4-methylphenol OR 3+3+di-tert-butyl-2+2+dihydroxy-5+5+dimethyldiphenylmethane OR 6+6+di-tert-butyl-2+2+methylenedi-p-cresol OR 6+6+methylenebis+2-+tert-butyl+4-methylphenol OR 6+6+methylenebis+2-tert-butyl-4-methylphenol OR 6+6-di-tert-butyl-2+2-methylenedi-p-cresol OR a+22-46 OR acmc-1buvj OR advastab+405 OR agidol+2 OR ai3-18027 OR ak-28736 OR akos000447157 OR alterungsschutzmittel+bkf OR antage+w+400 OR antioxidant+2246 OR antioxidant+bkf OR antioxidant+ng-2246 OR antioxidant+omb OR antioxydant_2246 OR anw-17334 OR ao+1+antioxidant OR ao+2246 OR as-13205 OR ax8017725 OR bbl025607

	OR bidd+er0324 OR bis+2-hydroxy-3-tert-butyl-5-methylphenyl+methane OR bis+2-hydroxy-5-methyl-3-tert-butylphenyl+methane OR bis+3-tert-butyl-2-hydroxy-5-methylphenyl+methane OR bis+6-hydroxy-3-methyl-5-tert-butylphenyl+methane OR bisaklofen+bp OR bisalkofen+bp OR brn+2062676 OR calco+2246 OR cao+5 OR cao-14 OR cao-5 OR cas-119-47-1 OR catolin+14 OR ccg-207916 OR ccg-208597 OR chemanox+21 OR chembl460648 OR ctk8a9397 OR cyanox+2246 OR di+2-hydroxy-5-methyl-3-tert-butylphenyl+methane OR dsstox_cid_870 OR dsstox_gsid_20870 OR dsstox_rid_75838 OR dtxsid4020870 OR ec+204-327-1 OR einecs+204-327-1 OR fr-0126 OR ft-0609309 OR geri-bp002-a OR hsdb+5585 OR ionol+46 OR ks-00000w13 OR kvm0x4x57b OR lederle+2246 OR lowinox+22m46 OR ls-7516 OR mbmbp OR mcule-8897993815 OR methane+2+-bis+6-tert-butyl-p-cresyl OR methane+2+2+-bis+6-t-butyl-p-cresyl OR methane+2+2+-bis+6-tert-butyl-p-cresyl OR methylene+bis+methyl+butyl+phenol OR methylene+di-t-butyl+cresol OR methylene+di-t-butylcresol OR mls-0146298+0001 OR ncgc00164172-01 OR ncgc00164172-02 OR ncgc00256347-01 OR ncgc00259079-01 OR ng+2246 OR nocrac+ns+6 OR nocrack+ns+6 OR ns00010737 OR nsc+7781 OR nsc-7781 OR nsc7781 OR oprea1_122036 OR oxy+chek+114 OR p-cresol+2+-methylenebis+6-tert-butyl- OR p-cresol+2+2+-methylenebis+6-tert-+butyl- OR p-cresol+2+2+-methylenebis+6-tert-butyl- OR phenol+2+methylenebis+6+1+1-dimethylethyl+4-methyl OR phenol+2+2+methylenebis+6+1+1-dimethylethyl+4-methyl OR plastanox+2246 OR plastanox+2246+antioxidant OR ralox+46 OR rubber+antioxidant+2246 OR sbb007695 OR sc-79689 OR schembl34162 OR stl377901 OR sumilizer+mdp OR synox+5lt OR tox21_201529 OR tox21_302923 OR unii-kvm0x4x57b OR vulkanox+bkf OR zinc1543799) OR (proximity 3 AND 119-47-1 AND CAS)
paranitronaniline	(4-nitroaniline OR 4-nitroaniline+monohydrochloride OR para-nitroaniline OR paranitronaniline OR p-nitroaniline OR 4-nitro-aniline OR 4-nitro-phenylamine OR 4-nitrobenzenamine) OR (proximity 3 AND CAS AND -01-6) OR ((proximity 3) AND (benzenamine OR nitroaniline) AND (4- OR p- OR 4-nitro))
n_nprime-di-sec-butyl-p-phenylenediamine	(antioxidant+22 OR n1+n4-di-sec-butylbenzene-1+4-diamine OR topanol+m OR kerobit+bpd OR tenamene+2 OR santoflex+44 OR n+n+-di-sec-butyl-p-phenyldiamine OR n+n+-di-sec-butylparaphenylenediamine OR n+n+-di-sec-butyl-1+4-phenylenediamine OR 1+4-benzenediamine+n+n+-bis+1-methylpropyl+- OR nsc+68417 OR ccris+4603 OR hsdb+5343 OR p-phenylenediamine+n+n+-di-sec-butyl- OR n+n+-bis+1-methylpropyl+-1+4-benzenediamine OR n+n+-bis+1-methylpropyl+-1+4-phenylenediamine OR unii-76251wu9i2 OR n+n+-di-sek.butyl-p-fenylendiamin OR einecs+202-992-2 OR brn+2805827 OR dtxsid7024956 OR 1+4-benzenediamine+n1+n4-bis+1-methylpropyl+- OR 76251wu9i2 OR naugalube+403 OR nn+-di-sec-butyl-p-phenylenediamine OR n+n+-1+4-bis+sec-butylamino+benzene OR acmc-1c9jn OR dsstox_cid_4956 OR ec+202-992-2 OR dsstox_rid_77598 OR dsstox_gsid_24956 OR schembl49805 OR mls002454420 OR 1+4-bis+sec-butylamino+benzene OR chembl1409985 OR ctk3j0317 OR 1+n+n+-bis+1-methylpropyl+- OR kuc107773n OR albb-024364 OR ksc-09-264a OR nsc68417 OR str09249 OR zx-an022878 OR tox21_200371 OR anw-14561 OR nsc-68417 OR p-phenylenediamine+n+-di-sec-butyl- OR sbb008194 OR akos015888191 OR ks-000016u9 OR n+n+-di-sec-butyl-1+4-benzenediamine OR n+n+-di-sec-butyl-benzene-1+4-diamine OR ncgc00091814-01 OR ncgc00091814-02 OR ncgc00091814-03 OR ncgc00091814-04 OR ncgc00257925-01 OR ak114296 OR cas-101-96-2 OR cc-31723 OR smr001372014 OR st095686 OR n+n+-di+butan-2-yl+benzene-1+4-diamine OR ax8017296 OR db-080853 OR ft-0629588 OR n+n+-di-sec-butyl-p-phenylenediamine+95% OR n1+n4-bis+butan-2-yl+benzene-1+4-diamine OR ns00003277 OR nn+-bis+1-methylpropyl+-1+4-phenylenediamine OR 1+4-benzenediamine+n+n+-bis+1-methylpropyl+-+dihydrochloride OR N+N+-Di-sec-butyl-p-phenylenediamine OR Antioxidant+22 OR N1+N4-Di-sec-butylbenzene-1+4-diamine OR Topanol+M OR Kerobit+BPD OR Tenamene+2 OR Santoflex+44 OR N+N+-DI-SEC-BUTYL-P-PHENYLDIAMINE OR N+N+-Di-s-butyl-p-phenylenediamine OR N+N+-Di-sec-butylparaphenylenediamine OR N+N+-Di-sec-butyl-1+4-phenylenediamine OR 1+4-Benzenediamine+N+N+-bis+1-methylpropyl+- OR NSC+68417 OR CCRIS+4603 OR HSDB+5343 OR p-Phenylenediamine+N+N+-di-sec-butyl- OR N+N+-Bis+1-methylpropyl+-1+4-benzenediamine OR N+N+-Bis+1-methylpropyl+-1+4-phenylenediamine OR UNII-76251WU9I2 OR N+N+-Di-sek.butyl-p-fenylendiamin OR EINECS+202-992-2 OR BRN+2805827 OR DTXSID7024956 OR 1+4-Benzenediamine+N1+N4-bis+1-methylpropyl+- OR 76251WU9I2 OR N+N+-di-sec-butylbenzene-1+4-diamine OR methylpropyl+4-+methylpropyl+amino+phenyl+amine OR Naugalube+403 OR NN+-Di-sec-butyl-p-phenylenediamine OR N+N+-1+4-Bis+sec-butylamino+benzene OR ACMC-1C9JN OR DSSTox_CID_4956 OR EC+202-992-2 OR DSSTox_RID_77598 OR DSSTox_GSID_24956 OR SCHEMBL49805 OR MLS002454420 OR 1+4-Bis+sec-butylamino+benzene OR CHEMBL1409985 OR CTK3J0317 OR 1+N+N+-bis+1-methylpropyl+- OR KUC107773N OR ALBB-024364 OR KSC-09-264A OR NSC68417 OR STR09249 OR ZX-AN022878 OR Tox21_200371 OR ANW-14561 OR NSC-68417 OR p-Phenylenediamine+N+-di-sec-butyl- OR SBB008194 OR AKOS015888191 OR KS-000016U9 OR n+n+-di-2-butyl-1+4-phenylenediamine OR N+N+-Di-sec-butyl-1+4-benzenediamine OR N+N+-di-sec-butyl-benzene-1+4-diamine OR NCGC00091814-01 OR NCGC00091814-02 OR NCGC00091814-03 OR NCGC00091814-04 OR NCGC00257925-01 OR AK114296 OR CAS-101-96-2 OR CC-31723 OR SMR001372014 OR ST095686 OR N+N+-di+butan-2-yl+benzene-1+4-diamine OR AX8017296 OR DB-080853 OR FT-0629588 OR N+N+-Di-sec-butyl-p-phenylenediamine+95% OR N1+N4-bis+butan-2-yl+benzene-1+4-diamine OR NS00003277 OR NN+-Bis+1-methylpropyl+-1+4-phenylenediamine OR N+N+-di-sec-butyl-p-phenylenediamine OR 1+4-benzenediamine+N+N+-bis+1-methylpropyl+-+dihydrochloride OR n+n+-di-sec-butylbenzene-1+4-diamine OR n+n+-di-sec-butyl-p-phenylene OR p-phenylenediamine+n+n+-di-sec-butyl OR n+n+-di(butan-2-yl)benzene-1+4-diamine OR 1+4-benzenediamine+n+n+-bis(1-methylpropyl) OR n+n+-di-s-butyl-p-phenylenediamine OR n+n+-di-sec-butyl-p-phenylenediamine) OR (proximity 3 AND 101-96-2 AND CAS)

Tegdme	(triglyme OR glyme+4 OR ansul+ether+161 OR glyme-3 OR tegdime OR dimethyl+ether+of+triethylene+glycol OR unii-32yxg88kk0 OR ethane+1+2-bis+2-methoxyethoxy+ OR nsc+66400 OR 1-methoxy-2+2+2methoxy-ethoxy+ethane OR einecs+203-977-3 OR glycol+triethylene+dimethyl+ether OR brn+1700630 OR ai3-28582 OR 32yxg88kk0 OR dtxsid8026224 OR chebi:44842 OR 1+2-bis+2-methoxyethoxy+ethane+reagent OR glyme-4 OR dsstox_cid_6224 OR 2+8+11-tetraoxadodecane OR ec+203-977-3 OR acmc-1c6s6 OR dsstox_rid_78066 OR dsstox_gsid_26224 OR schembl16126 OR ksc178a6f OR 1+2-bis+methoxyethoxy+ethane OR chembl1235255 OR ctk0h8062 OR ethane+2-bis+2-methoxyethoxy+ OR nsc66400 OR zinc1693863 OR tox21_300509 OR 2186aa OR anw-16480 OR mfcd00008504 OR nsc-66400 OR sbb060897 OR akos009158244 OR db02078 OR mcule-9670046114 OR ks-0000006k OR ncgc00164017-01 OR ncgc00164017-02 OR ncgc00254323-01 OR cas-112-49-2 OR cc-35336 OR db-060211 OR b0496 OR ft-0659858 OR ft-0755020 OR ns00010633 OR st50825121 OR 23265-ep2289897a1 OR 23265-ep2314584a1 OR 23265-ep2371797a1 OR 23265-ep2371798a1 OR 23265-ep2371800a1 OR 23265-ep2371804a1 OR c-34604 OR q2453066 OR z1245664652 OR dimethoxytetraglycol OR dimethoxytetraethylene+glycol OR tegdme OR Triglyme OR Triethylene+glycol+dimethyl+ether OR 1+2-Bis+2-methoxyethoxy+ethane OR Glyme+4 OR Ansul+ether+161 OR Glyme-3 OR 1-methoxy-2+2+2-methoxyethoxy+ethoxy+ethane OR TEGDIME OR Dimethyl+ether+of+triethylene+glycol OR UNII-32YXG88KK0 OR Ethane+1+2-bis+2-methoxyethoxy+ OR NSC+66400 OR triethyleneglycol+dimethyl+ether OR 1-METHOXY-2-+2-+2-METHOXY-ETHOXY+-ETHANE OR EINECS+203-977-3 OR Glycol+triethylene+dimethyl+ether OR BRN+1700630 OR AI3-28582 OR 32YXG88KK0 OR DTXSID8026224 OR CHEBI:44842 OR 1+2-Bis+2-methoxyethoxy+Ethane+Reagent OR triethylene+glycoldimethylether+tegdme OR Glyme-4 OR DSSTox_CID_6224 OR 2+8+11-Tetraoxadodecane OR EC+203-977-3 OR ACMC-1C6S6 OR DSSTox_RID_78066 OR DSSTox_GSID_26224 OR SCHEMBL16126 OR KSC178A6F OR 1+2-Bis+methoxyethoxy+ethane OR triethylene+glycol+dimethylether OR CHEMBL1235255 OR CTK0H8062 OR Ethane+2-bis+2-methoxyethoxy+ OR NSC66400 OR ZINC1693863 OR Tox21_300509 OR 2186AA OR ANW-16480 OR MFCD00008504 OR NSC-66400 OR SBB060897 OR AKOS009158244 OR DB02078 OR MCULE-9670046114 OR KS-0000006K OR triglyme+2+5+8+11-tetraoxadodecane OR NCGC00164017-01 OR NCGC00164017-02 OR NCGC00254323-01 OR CAS-112-49-2 OR CC-35336 OR DB-060211 OR B0496 OR FT-0659858 OR FT-0755020 OR NS00010633 OR ST50825121 OR 23265-EP2289897A1 OR 23265-EP2314584A1 OR 23265-EP2371797A1 OR 23265-EP2371798A1 OR 23265-EP2371800A1 OR 23265-EP2371804A1 OR C-34604 OR Q2453066 OR Z1245664652 OR 2+5+8+11-tetraoxadodecane OR 1+2-bis+2-methoxyethoxy+ethane OR triethylene+glycol+dimethyl+ether OR 1+2bis+2methoxyethoxy+ethane OR triethylene+glycoldimethylether OR Dimethoxytetraglycol OR Dimethoxytetraethylene+glycol OR TEGDME OR tetraglyme)OR(proximity 3 AND CAS AND 112-49-2)
tk11-319	(2-benzyl-2+dimethylamino+4+morpholinobutyrophenone OR dtxsid5044786 OR 2-benzyl-2+dimethylamino+1+4+morpholin-4-yl+phenyl+butan-1-one OR 2-benzyl-2+dimethylamino+1+4+4-morpholinyl+phenyl+1-butanone OR 1-butanone+2+dimethylamino+1+4+4-morpholinyl+phenyl+2+phenylmethyl+ OR photocure+3665 OR pubchem+20904 OR acmc-20a2em OR ec+404-360-3 OR dsstox_cid_24786 OR dsstox_rid_80475 OR dsstox_gsid_44786 OR schembl35868 OR chembl3187611 OR ctk4b1229 OR tox21_301707 OR anw-54044 OR akos015901469 OR mcule-2935597430 OR ncgc00256142-01 OR ds-12208 OR ls-46712 OR st058401 OR ax8071161 OR cas-119313-12-1 OR ft-0712767 OR ns00006098 OR ks-00001234 OR q27258386 OR 2-benzyl-2-dimethylamino-1+4-morpholinophenyl+butan-1-one OR 2-benzyl-2+dimethylamino+1+4+morpholino+phenyl+1-butanone OR 2+dimethylamino+1+4+4-morpholinyl+phenyl+2+phenylmethyl+1-butanone OR 2-Benzyl-2-dimethylamino-1+4-morpholinophenyl+1-butanone OR 2-Benzyl-2+dimethylamino+4+morpholinobutyrophenone OR Irgacure+369 OR 2-benzyl-2+dimethylamino+1+4-morpholinophenyl+butan-1-one OR DTXSID5044786 OR 2-Benzyl-2+dimethylamino+1+4+morpholin-4-yl+phenyl+butan-1-one OR 2-Benzyl-2+dimethylamino+1+4+4-morpholinyl+phenyl+1-butanone OR 2-Benzyl-2-dimethylamino-4+morpholinobutyrophenone OR 1-Butanone+2+dimethylamino+1+4+4-morpholinyl+phenyl+2+phenylmethyl+ OR 2-benzyl-2+dimethylamino+1+4-morpholin-4-ylphenyl+butan-1-one OR 2-benzyl-2+dimethylamino+4-morpholinobutyrophenone OR photoinitiator+369 OR Photocure+3665 OR PubChem+20904 OR ACMC-20a2em OR IRGACURE+369 OR EC+404-360-3 OR DSSTox_CID_24786 OR DSSTox_RID_80475 OR DSSTox_GSID_44786 OR SCHEMBL35868 OR CHEMBL3187611 OR CTK4B1229 OR Tox21_301707 OR ANW-54044 OR AKOS015901469 OR MCULE-2935597430 OR NCGC00256142-01 OR DS-12208 OR LS-46712 OR ST058401 OR AX8071161 OR CAS-119313-12-1 OR FT-0712767 OR NS00006098 OR KS-00001234 OR 2-benzyl-2-dimethylamino-4-morpholinobutyrophenone OR 2-benzyl-2-+dimethylamino+-4+-morpholino-butyroph OR Q27258386 OR 2-benzyl-2-dimethylamino-1+-+4morpholinophenyl+butan-1-one OR 2-benzyl-2-dimethylamino-1-+4-morpholinophenyl+-butanone-1 OR 2-benzyl-2-dimethylamino-1-+4-morpholinophenyl+butan-1-one OR 2-benzyl-2-dimethylamino-1-+4-morpholinophenyl+-1-butanone OR 2-Benzyl-2-dimethylamino-1-+4-morpholinophenyl+-butan-1-one OR 2-+dimethylamino+-1-+4-morpholin-4-ylphenyl+-2-benzylbutan-1-one OR 2-Benzyl-2-+dimethylamino+-1-+4-+morpholino+phenyl+-1-butanone OR 2-benzyl-2-n+n-dimethylamino-1-+4-morpholinophenyl+-1-butanone OR 2-+Dimethylamino+-1-+4-+4-morpholinyl+phenyl+-2-+phenylmethyl+-1-butanone OR 1-butanone+2-(dimethylamino)-1-[4-(4-morpholinyl)phenyl]-2-(phenylmethyl)- OR 2-benzyl-2-dimethylamino-4+-morpholinobutyrophenone OR 2-benzyl-2-(dimethylamino)-1-(4-morpholinophenyl)-1-butanone OR 2-benzyl-2-(dimethylamino)-1-(4-morpholinophenyl)butanone-1 OR 2-benzyl-2-(dimethylamino)-1-[4-(4-morpholinyl)phenyl]-1-butanone OR 2-benzyl-2-n+n-dimethylamino-1-(4-morpholinophenyl)-1-butanone OR 2-benzyl-2-dimethylamino-1-(4-morpholinophenyl)butanone OR cg+25-369 OR irgacure+369 OR tk+11-319) OR (proximity 3 AND CAS AND 119313-12-1)
retinol_acetate	(risk% OR adverse OR toxic% OR hazard%) AND (retinyl+acetate OR vitamin+a+acetate OR retinol+acetate OR all-trans-retinyl+acetate OR crystalets OR vitamin+a1+acetate OR all-trans-retinol+acetate OR vitamin+a+alcohol+acetate OR davitan+a OR vitamin+a+ester OR all-trans-vitamin+a+acetate OR o~15~-acetylretinol OR retinol+acetate+all-trans- OR all-trans-retinylacetate OR unii-3le3d9d6oy OR acetic+acid+retinyl+ester OR retinyl+acetate+all-trans- OR nsc+122045 OR ccris+1907 OR trans-retinyl+acetate OR ro+1-5275 OR trans-vitamin+a+acetate OR einecs+204-844-2 OR brn+1915439 OR 3le3d9d6oy OR chebi:32095 OR c22h32o2 OR mfcd00019413 OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethylcyclohexen-1-yl+nona-2+4+6+8-tetraenyl+acetate OR ncgc00090756-09 OR dsstox_cid_1240 OR dsstox_rid_76032 OR dsstox_gsid_21240 OR w-108382 OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-en-1-yl+nona-2+4+6+8-tetraen-1-yl+acetate OR o+15+-acetylretinol OR cas-127-47-9 OR trans-retinol+acetate OR sr-05000001431 OR 34356-31-5 OR vitamin+a+acetat OR acetic+acid+retinyl OR spectrum5_001195 OR spectrum5_002001 OR ec+204-844-2 OR retinol+o~15~-acetyl- OR bspbio_002833 OR spectrum1503051 OR chembl486193 OR dtxsid6021240 OR chebi:94695 OR hms501k04 OR hms1922a19 OR

	hms2089g20 OR pharmakon1600-01503051 OR hy-n0679 OR zinc3874857 OR tox21_113549 OR tox21_201423 OR tox21_302737 OR bdbm50442911 OR ccg-39564 OR gv2742 OR lmpr01090012 OR nsc122045 OR nsc122760 OR nsc758220 OR akos015914999 OR tox21_113549_1 OR nsc-122045 OR nsc-122760 OR nsc-758220 OR idi1_000522 OR ncgc00090756-01 OR ncgc00090756-02 OR ncgc00090756-03 OR ncgc00090756-05 OR ncgc00090756-06 OR ncgc00090756-07 OR ncgc00090756-08 OR ncgc00090756-10 OR ncgc00090756-11 OR ncgc00090756-12 OR ncgc00256509-01 OR ncgc00258974-01 OR 64536-04-5 OR ac-19999 OR ak149484 OR sc-76802 OR sbi-0051756.p002 OR ns00003926 OR st50307679 OR 3000-ep2305825a1 OR ab00052305-02 OR ab00052305_03 OR q7316808 OR sr-05000001431-1 OR sr-05000001431-3 OR brd-k65331431-001-01-3)
propane_thiol	(1-propanethiol+2+3-bis+2-mercaptoethyl+thio+- OR dtxsid20888943 OR acmc-1c6xi OR 2+3-bis+2-mercaptoethylthio+propane-1-thiol OR ec+411-290-7 OR schembl127070 OR ctk4b7363 OR akos028109967 OR acn-053709 OR ns00006734 OR 4-+mercaptomethyl+-3+6-dithia-1+8-octanedithiol OR 1-propanethiol+2+3-bis[(2-mercaptoethyl)thio]- OR 2+3-bis(2-mercaptoethylthio)propane-1-thiol OR 4-(mercaptomethyl)-3+6-dithia-1+8-octanedithiol OR 2+3-bis+2-mercaptoethyl+thio+-1-propanethiol OR 1-Propanethiol+2+3-bis+2-mercaptoethyl+thio+- OR DTXSID20888943 OR 1-propanethiol+2+3-bis+2-mercaptoethyl+thio+-;2+3-bis+2-mercaptoethyl+thio+-1-propanethiol;1-propanethiol+2+3-bis+2-mercaptoethyl+thio+-+2+3-bis+2-mercaptoethyl+thio+-1-propanethiol OR ACMC-1C6XI OR 2+3-Bis+2-mercaptoethylthio+propane-1-thiol OR EC+411-290-7 OR SCHEMBL127070 OR CTK4B7363 OR AKOS028109967 OR ACN-053709 OR NS00006734 OR 1+2-bis+2-mercaptoethylthio+-3-mercaptopropane OR 2+3-bis+2-sulfanylethylsulfanyl+propane-1-thiol OR 2+3-bis+2-sulfanyl+ethylsulfanyl+propane-1-thiol OR 4-+Mercaptomethyl+-3+6-dithia-1+8-octanedithiol OR 2+3-bis((2-mercaptoethyl)thio)-1-propanethiol OR 1-Propanethiol+2+3-bis[(2-mercaptoethyl)thio]- OR 2+3-Bis(2-mercaptoethylthio)propane-1-thiol OR 1+2-bis(2-mercaptoethylthio)-3-mercaptopropane OR 2+3-bis(2-sulfanylethylsulfanyl)propane-1-thiol OR 2+3-bis(2-sulfanyl+ethylsulfanyl)propane-1-thiol OR 4-(Mercaptomethyl)-3+6-dithia-1+8-octanedithiol) OR (proximity 3 AND CAS AND 131538-00-6)
2_4_hydroxy_benzophenone	(enzoresorcinol OR resbenzophenone OR inhibitor+dhbp OR uvinul+400 OR advastab+48 OR uvistat+12 OR uvinol+400 OR quinsorb+010 OR 4-benzoyl+resorcinol OR syntase+ OR dastib+263 OR eastman+inhibitor+dhpb OR 4-benzoylresorcinol OR nsc+38555 OR unii-lj54r4z029 OR hsdb+5617 OR einecs+205-029-4 OR brn+1311566 OR mls000774789 OR dtxsid8022406 OR lj54r4z029 OR mfcd00002277 OR smr000365551 OR benzophenone+4-dihydroxy OR dsstox_cid_2406 OR dsstox_rid_76577 OR dsstox_gsid_22406 OR methanone+4-dihydroxyphenyl+phenyl OR cas-131-56-6 OR 2+4-dhb OR enamine_001926 OR 4+6-dihydroxybenzophenone OR acmc-209bn8 OR ec+205-029-4 OR chembl1392 OR oprea1_840620 OR schembl39681 OR ksc174m3d OR bidd+er0039 OR bdbm51223 OR ctk0h4631 OR nsc5358 OR hms1399h12 OR hms2771p10 OR zinc225430 OR bcp25883 OR ks-00000gu6 OR nsc-5358 OR nsc38555 OR tox21_201285 OR tox21_302865 OR anw-19362 OR bbl013153 OR nsc-38555 OR sbb063282 OR stl163951 OR akos001019876 OR mcule-3025914301 OR ne10164 OR ncgc00246026-01 OR ncgc00246026-02 OR ncgc00256606-01 OR ncgc00258837-01 OR ac-11241 OR ak-57631 OR ds-15473 OR ls-38903 OR d0573 OR ft-0610114 OR ns00001568 OR st50308028 OR c14215 OR 135d566 OR ae-641+01968047 OR q209209 OR sr-0 0388910 OR q-200188 OR sr-0 0388910-1 OR 92092-63-2 OR 2+4-dihydroxybenzophenone OR 2+4-dihydroxyphenyl+phenyl+methanone OR benzophenone+2+4-hydroxy OR methanone+2+4-dihydroxyphenyl+phenyl OR 4-benzoylbenzene-1+3-diol OR 2+4-dihydroxyphenyl+phenylmethanone OR Benzoresorcinol OR Resbenzophenone OR Inhibitor+DHBP OR Uvinul+400 OR Advastab+48 OR Uvistat+12 OR Uvinol+400 OR Quinsorb+010 OR 4-Benzoyl+resorcinol OR Syntase+ OR Dastib+263 OR Eastman+Inhibitor+DHPB OR Benzophenone+2+4-dihydroxy- OR 4-Benzoylresorcinol OR NSC+38555 OR UNII-LJ54R4Z029 OR HSDB+5617 OR EINECS+205-029-4 OR BRN+1311566 OR MLS000774789 OR #NAME? OR DTXSID8022406 OR LJ54R4Z029 OR MFCD00002277 OR SMR000365551 OR Benzophenone+4-dihydroxy OR DSSTox+CID+2406 OR 2+4-dihydroxy-benzophenon OR DSSTox+RID+76577 OR DSSTox+GSID+22406 OR 2+4-dihydroxyphenyl+phenyl+ketone OR Methanone+4-dihydroxyphenyl+phenyl OR CAS-131-56-6 OR benzophenone+1 OR 2+4-DHB OR Enamine_001926 OR 4+6-Dihydroxybenzophenone OR ACMC-209bn8 OR 2+4-dihydroxy-benzophenone OR EC+205-029-4 OR cid+8572 OR CHEMBL1392 OR 2+4-dihydroxybenzo+phenone OR Oprea1+840620 OR SCHEMBL39681 OR hsp90+163 OR KSC174M3D OR BIDD+ER0039 OR BDBM51223 OR CTK0H4631 OR NSC5358 OR HMS1399H12 OR HMS2771P10 OR ZINC225430 OR BCP25883 OR KS-00000GU6 OR NSC-5358 OR NSC38555 OR Tox21_201285 OR Tox21_302865 OR ANW-19362 OR BBL013153 OR NSC-38555 OR SBB063282 OR STL163951 OR AKOS001019876 OR MCULE-3025914301 OR NE10164 OR NCGC00246026-01 OR NCGC00246026-02 OR NCGC00256606-01 OR NCGC00258837-01 OR AC-11241 OR AK-57631 OR DS-15473 OR LS-38903 OR D0573 OR FT-0610114 OR NS00001568 OR ST50308028 OR C14215 OR 135D566 OR AE-641+01968047 OR Q209209 OR SR-0 0388910 OR Q-200188 OR SR-0 0388910-1 OR benzophenone+2+4-dihydroxy) OR (proximity 3 AND CAS AND 131-56-6)
tetraethylene_glycol_ethyl_methylether	(schembl316251 OR ctk2j0661 OR dtxsid70601664 OR 2+5+8+11+14+pentaoxahexadecane OR 2+5+8+11+14+Pentaoxahexadecane OR 1+2+2+2-ethoxyethoxy+ethoxy+ethoxy+2-methoxyethane OR tetraethylene+glycol+ethyl+methyl+ether) OR (proximity 3 AND CAS AND 89769-11-9)
Phenylene-1_4-bis-benz-1_3-oxazin-4-one	(2+2+-+1+4-phenylene+bis-4h-3+1-benzoxazin-4-one OR cyasorb+uv-3638 OR unii-8v348nl4qk OR 8v348nl4qk OR dtxsid40864845 OR bas+00298026 OR ec+418-280-1 OR oprea1_802650 OR oprea1_828724 OR schembl125184 OR ctk8b9791 OR ebd2984 OR bcp12260 OR zinc2565270 OR anw-63097 OR stk296324 OR akos000640593 OR mcule-9378837915 OR uv-3638 OR acm18600594 OR ks-000001m3 OR ak-89768 OR as-10722 OR ax8063798 OR ls-186266 OR bb+0262678 OR ft-0654023 OR ns00003546 OR st50222003 OR 600p594 OR a812998 OR q27271051 OR 2+2-+1+4-phenylene+-bis-+4h-3+1-benzoxazin-4-one OR 2+2+-+1+4-phenylene+bis+4h-benzo+d+1+3+oxazin-4-one OR 4h-3+1-benzoxazin-4-one+2+2+-+1+4-phenylene+bis- OR 2/2+-+1+4-phenylene+bis-4h-3+1-benzoxazin-4-one OR 2+2+-+1+4-phenylene+bis+3+1-benzoxazin-4-one OR 2+2+-benzene-1+4-diylbis+4h-3+1-benzoxazin-4-one OR 2+2-+1+4-phenylene+bis+4h-3+1-benzoxazine-4-one OR phenylene-1+4-bis-+benz-1+3-oxazin-4-one OR 2+2-+1+4-phenylene+bis-4h-3+1-benzoxazin-4-one OR 2+2+-+1+4-PHENYLENE+BIS-4H-3+1-BENZOXAZIN-4-ONE OR Cyasorb+UV-3638 OR UNII-8V348NL4QK OR 8V348NL4QK OR DTXSID40864845 OR 2+2+-+1+4-Phenylene+bis+4H-3+1-benzoxazin-4-one OR BAS+00298026 OR EC+418-280-1 OR Oprea1_802650 OR Oprea1_828724 OR SCHEMBL125184 OR CTK8B9791 OR EBD2984 OR BCP12260 OR ZINC2565270 OR ANW-63097 OR STK296324 OR AKOS000640593 OR MCULE-9378837915 OR UV-3638 OR ACM18600594 OR KS-000001M3 OR AK-89768 OR AS-10722 OR AX8063798 OR LS-186266 OR BB+0262678 OR FT-0654023 OR NS00003546 OR ST50222003 OR 600P594 OR A812998 OR Q27271051 OR 2+2-+1+4-PHENYLENE+-BIS-+4H-3+1-BENZOXAZIN-4-ONE OR 2+2+-+1+4-Phenylene+bis+4H-

	benzo+d+1+3+oxazin-4-one OR 4H-3+1-Benzoxazin-4-one+2+2+-+1+4-phenylene+bis- OR 2/2+-+1+4-PHENYLENE+BIS-4H-3+1-BENZOXAZIN-4-ONE OR 2-+4-+4-oxo-3+1-benzoxazin-2-yl+phenyl+-3+1-benzoxazin-4-one OR 2+2+-+1+4-Phenylene+bis+3+1-benzoxazin-4-one OR 2+2+-benzene-1+4-diylbis+4H-3+1-benzoxazin-4-one OR 2+2-+1+4-phenylene+bis+4H-3+1-benzoxazine-4-one OR 2+2+-+1+4-phenylene+bis+4h-3+1-benzoxazin-4-one OR 2+2+-p-phenylenebis+3+1-benzoxazin-4-one OR Phenylene-1+4-bis-+benz-1+3-oxazin-4-one OR 2+2+-p-phenylenebis+4h-3+1-benzoxazin-4-one OR 2+2-+1+4-Phenylene+bis-4H-3+1-benzoxazin-4-one OR 2-+4-+4-oxidanylidene-3+1-benzoxazin-2-yl+phenyl+-3+1-benzoxazin-4-one OR 2-+4-+4-oxobenzo+d+1+3-oxazin-2-yl+phenyl+benzo+d+1+3-oxazin-4-one) OR (proximity 3 AND CAS AND 18600-59-4)
Phosphorothioic_acid_OO O-triphenyl_ester_tert-butyl_derivatives	(phosphorothioic+acid+o+o+o+triphenyl+esters+tert-bu+derivs OR phosphorothioic+acid+o+o+o+triphenyl+esters+tert-bu+derivatives OR 4-tert-butylphenoxy+-diphenoxy-sulfanylidene-lambda5-phosphane OR 4-tert-butylphenoxy+-diphenoxy-sulfanylidene+5+-phosphane OR Phosphorothioic+acid+O+O+O+triphenyl+esters+tert-Bu+derivs OR Phosphorothioic+acid+O+O+O+triphenyl+esters+tert-Bu+derivatives OR 4-Tert-butylphenoxy+-diphenoxy-sulfanylidene-lambda5-phosphane)
Trixylenyl_phosphate	(unii-7m08k25q1j OR hsdb+3908 OR 7m08k25q1j OR tris+2+4-xylenyl+phosphate OR nsc+78488 OR 2+4-xylyl+phosphate+c8h9o+3po OR brn+1895059 OR coalite+ntp OR ivviol-3 OR nsc78488 OR phosflex+179 OR schembl108984 OR ccris+4891 OR hsdb+6094 OR dtxsid80959466 OR ebd59818 OR zinc1718867 OR einecs+246-677-8 OR nsc-78488 OR akos015899549 OR mcule-4708791677 OR ls-104534 OR ec+246-677-8 OR w-110611 OR q27268543 OR 2+4-dimethylphenol+phosphate+3+1 OR 2+4-xylenol+phosphate+3+1 OR 2+4-xylyl+phosphate OR dimethylphenol+phosphate+3+1 OR phenol+2+4-dimethyl+1+1+1+phosphate OR phenol+2+4-dimethyl+phosphate+3+1 OR phenol+4dimethyl+phosphate+3+1 OR phenol+dimethyl+1+1+1+phosphate OR phosphate+trixylyl OR phosphoric+acid+tris+2+4-dimethylphenyl+ester OR phosphoric+acid+tris+2+4-xylyl+ester OR phosphoric+acid+trixylyl+ester OR tri+2+4-dimethylphenyl+phosphate OR tri+2+4-xylenyl+phosphate OR tri+xlylenyl+phosphate OR tri-2+4-xylyl+phosphate OR tri-2+4-xylylphosphat OR tri-dimethyl+phenyl+phosphate OR trixylenyl+phosphate OR tri-xylenyl+phosphate OR xylenol+phosphate+3:1 OR xylyl+phosphate OR tris+2+4-dimethylphenyl+phosphate) OR (proximity 3 AND CAS AND (25155-23-1 OR 3862-12-2))
solvent_yellow_124	(unii-e880xyt70p OR e880xyt70p OR w-110846 OR einecs+252-021-1 OR c.i.+111155 OR ec+252-021-1 OR schembl597248 OR schembl12492278 OR ctk8g3173 OR dtxsid60865718 OR acm34432923 OR ns00002855 OR q60457 OR n-ethyl-n+2+1+2-methylpropoxy+ethoxy+ethyl+4+phenylazo+aniline OR n-ethyl-n+2+1+2-methylpropoxy+ethoxy+ethyl+4-phenyldiazenylaniline OR benzenamine+n-ethyl-n+2+1+2-methylpropoxy+ethoxy+ethyl+4+2-phenyldiazenyl+ OR n-ethyl-n-2-1+2-methylpropoxy+ethoxyethyl-4+phenylazo+aniline OR UNII-E880XYT70P OR E880XYT70P OR W-110846 OR EINECS+252-021-1 OR C.I.+111155 OR EC+252-021-1 OR SCHEMBL597248 OR SCHEMBL12492278 OR CTK8G3173 OR DTXSID60865718 OR ACM34432923 OR NS00002855 OR Q60457 OR solvent+yellow+124 OR N-Ethyl-N-+2-+1-+2-methylpropoxy+ethoxy+ethyl+-4-+phenylazo+aniline OR N-ethyl-N-+2-+1-+2-methylpropoxy+ethoxy+ethyl+-4-phenyldiazenylaniline OR Benzenamine+N-ethyl-N-+2-+1-+2-methylpropoxy+ethoxy+ethyl+-4-+2-phenyldiazenyl+- OR N-Ethyl-N-2-1-+2-methylpropoxy+ethoxyethyl-4-+phenylazo+aniline) OR (proximity 3 AND 34432-92-3 AND CAS)
4-Chloro-2_5-dimethoxyacetoacetanilide	(naphthol+as-irg OR naphtol+as-irg OR naphtanilide+lrg OR naphtazol+4j OR naphtol+as-lgll OR naphthol+as+13gh OR unii-j086qhj1oc OR c+i+37613 OR einecs+224-638-6 OR nsc+50638 OR j086qhj1oc OR dtxsid5029265 OR dsstox_cid_9265 OR dsstox_rid_78740 OR dsstox_gsid_29265 OR w-106200 OR cas-4433-79-8 OR acmc-1akf0 OR ec+224-638-6 OR cbdive_007661 OR schembl1118436 OR chembl3185016 OR ctk4i8127 OR nsc50638 OR zinc1682065 OR zx-ah008408 OR tox21_201666 OR tox21_303485 OR anw-30091 OR bbl003545 OR nsc-50638 OR sbb013432 OR stk520725 OR akos000165629 OR acm4433798 OR mcule-2062409423 OR aba-9371898 OR ks-0000127d OR ncgc00249094-01 OR ncgc00257262-01 OR ncgc00259215-01 OR ax8020849 OR ls-167408 OR st4121989 OR ft-0654070 OR ns00008147 OR y-8542 OR ab00075319-01 OR a826549 OR c-36221 OR q27280985 OR 4+-chloro-2+5+-dimethoxyacetoacetanilide OR n+4-chloro-2+5-dimethoxyphenyl+3-oxobutanamide OR butanamide+n+4-chloro-2+5-dimethoxyphenyl+3-oxo OR 2+5-dimethoxy-4-chloroacetoacetanilide OR acetoacetyl-2+5-dimethoxy-4-chloroanilide OR acetoacetanilide+4+chloro-2+5+-dimethoxy OR 4-chloro-2+5-dimethoxyacetoacetanilide OR acetoacet+2+5+dimethoxy+4+chloroanilide OR n+2+5-dimethoxy-4-chlorphenyl+acetoacetamid OR n+4-chloro-2+5-dimethoxyphenyl+acetoacetamide OR acetoacetanilide+4+chloro-2+5+dimethoxy+8ci OR Naphthol+AS-IRG OR n+4-chloranyl-2+5-dimethoxy-phenyl+3-oxidanylidene-butanamide OR Naphtol+AS-IRG OR Naphtanilide+LRG OR Naphtazol+4J OR Naphtol+AS-LGLL OR Naphthol+AS+13GH OR UNII-J086QHJ1OC OR C+I+37613 OR EINECS+224-638-6 OR NSC+50638 OR J086QHJ1OC OR DTXSID5029265 OR DSSTox_CID_9265 OR DSSTox_RID_78740 OR DSSTox_GSID_29265 OR W-106200 OR CAS-4433-79-8 OR ACMC-1AKF0 OR EC+224-638-6 OR CBDivE_007661 OR SCHEMBL1118436 OR CHEMBL3185016 OR CTK4I8127 OR NSC50638 OR ZINC1682065 OR ZX-AH008408 OR Tox21_201666 OR Tox21_303485 OR ANW-30091 OR BBL003545 OR NSC-50638 OR SBB013432 OR STK520725 OR AKOS000165629 OR ACM4433798 OR MCULE-2062409423 OR ABA-9371898 OR KS-0000127D OR NCGC00249094-01 OR NCGC00257262-01 OR NCGC00259215-01 OR AX8020849 OR LS-167408 OR ST4121989 OR FT-0654070 OR NS00008147 OR Y-8542 OR AB00075319-01 OR A826549 OR C-36221 OR Q27280985 OR 4+Chloro-2+5+dimethoxyacetoacetanilide OR N+4-chloro-2+5-dimethoxyphenyl+3-oxobutanamide OR Butanamide+N+4-chloro-2+5-dimethoxyphenyl+3-oxo OR 2+5-Dimethoxy-4-chloroacetoacetanilide OR Acetoacetyl-2+5-dimethoxy-4-chloroanilide OR Acetoacetanilide+4+chloro-2+5+-dimethoxy OR 4-Chloro-2+5-dimethoxyacetoacetanilide OR Acetoacet+2+5+Dimethoxy+4+Chloroanilide OR N+2+5-Dimethoxy-4-chlorphenyl+acetoacetamid OR N+4-Chloro-2+5-dimethoxyphenyl+acetoacetamide OR Acetoacetanilide+4+-chloro-2+5+dimethoxy OR N+4-chloranyl-2+5-dimethoxy-phenyl+3-oxidanylidene-butanamide) OR (proximity 3 AND 4433-79-8 AND CAS)

4_4Bis-dimethylamino-4-methylamino_trityl_alcohol	(dtxsid00204642 OR einecs+209-218-2 OR c+i+solvent+violet+8 OR ec+209-218-2 OR schembl20561184 OR ctk5a4694 OR zinc5248289 OR akos027257545 OR ns00008275 OR y1629 OR benzenemethanol+a+a-bis+4+dimethylamino+phenyl+4+methylamino OR alpha+alpha-bis+4+dimethylamino+phenyl+4+methylamino+benzenemethanol OR DTXSID00204642 OR EINECS+209-218-2 OR C+I+Solvent+Violet+8 OR EC+209-218-2 OR SCHEMBL20561184 OR CTK5A4694 OR ZINC5248289 OR AKOS027257545 OR NS00008275 OR Y1629 OR 4+4+Bis+dimethylamino+4+methylamino+trityl+alcohol OR Benzenemethanol+a+a-bis+4-+dimethylamino+phenyl+4+methylamino OR bis+4-+dimethylamino+phenyl+4-+methylamino+phenyl+methanol OR 4+4+bis+dimethylamino+4+methylamino+trityl+alcohol OR alpha+alpha+Bis+4+dimethylamino+phenyl+4+methylamino+benzenemethanol OR alpha+alpha-Bis+4+dimethylamino+phenyl+4+methylamino+benzenemethanol) OR (proximity 3 AND CAS AND 561-41-1)
2_naphtalenamine_etc	(einecs+260-124-8 OR ns00008278 OR ec+260-124-8 OR EINECS+260-124-8 OR NS00008278 OR EC+260-124-8 OR 2-naphthalenamine+n-+2-ethylhexyl+1+2-methyl-4-+2-methylphenyl+azo+phenyl+azo OR n+2-ethylhexyl+1+2-methyl-4+2-methylphenyl+azo+phenyl+azo+naphthalen-1-amine OR n+2-ethylhexyl+1+2-methyl-4+2-methylphenyl+diazenyl+phenyl+diazenyl+1+2-dihydronaphthalen-1-amine) OR (proximity 3 AND CAS AND 56358-09-9)
2_5-diaminotoluene	(1+4-benzenediamine+2-methyl OR 2-methyl-1+4-benzenediamine OR 4-amino-2-methylaniline OR p-toluylendiamine OR p+m-tolylenediamine OR toluylene-2+5-diamine OR para-toluenediamine OR para-tolylenediamine OR para-toluylenediamine OR unii-24jo8z0rju OR 2-methyl-para-phenylenediamine OR ccris+7693 OR hsdb+6251 OR einecs+202-442-1 OR brn+0774521 OR 24jo8z0rju OR ci+76042 OR dtxsid6029123 OR chebi+53619 OR epitope+id+116061 OR schembl34217 OR schembl10580512 OR ctk3i6913 OR zinc388337 OR act07295 OR ks-000025xa OR anw-52954 OR akos009158791 OR gs-3190 OR mcule-8138595213 OR mp-2047 OR sb40185 OR ac-11774 OR sc-18061 OR db-057600 OR ls-154040 OR d4628 OR ft-0609940 OR ft-0610504 OR ns00014161 OR c19386 OR 095d705 OR q2521416 OR 2-hydroxy-n+4-methyl-2-nitro-phenyl+3-nitro-benzamide OR 2-methylbenzene-1+4-diamine OR 1+4-Benzenediamine+2-methyl OR 2-METHYL-1+4-BENZENEDIAMINE OR 4-Amino-2-methylaniline OR 2-Methyl-p-phenylenediamine OR p-Toluylendiamine OR p+m-Tolylenediamine OR Toluylene-2+5-diamine OR para-Toluenediamine OR para-Tolylenediamine OR para-Toluylenediamine OR 2-methyl-1+4-phenylenediamine OR UNII-24JO8Z0RJU OR 2-Methyl-para-phenylenediamine OR CCRIS+7693 OR HSDB+6251 OR EINECS+202-442-1 OR BRN+0774521 OR 24JO8Z0RJU OR CI+76042 OR 1-methyl-2+5-diaminobenzene OR 2+5-diamino-1-methylbenzene OR 2-methyl-benzene-1+4-diamine OR DTXSID6029123 OR CHEBI+53619 OR 2+5-diaminotoluene+sulphate OR p-toluylendiamin OR 2+5-diamino+toluene OR Epitope+ID+116061 OR SCHEMBL34217 OR SCHEMBL10580512 OR CTK3I6913 OR 4-@amino-2-@methyl-@phenyl+@amine OR ZINC388337 OR ACT07295 OR KS-000025XA OR ANW-52954 OR AKOS009158791 OR GS-3190 OR MCULE-8138595213 OR MP-2047 OR SB40185 OR AC-11774 OR SC-18061 OR 2-Methyl-benzene-1+4-diamine OR DB-057600 OR LS-154040 OR D4628 OR FT-0609940 OR FT-0610504 OR NS00014161 OR C19386 OR 095D705 OR Q2521416 OR 2-hydroxy-N+4-methyl-2-nitro-phenyl+3-nitro-benzamide OR 2+5-diaminotoluene OR 2+5-toluylenediamine OR 2-methyl-p-phenylenediamine OR p-toluenediamine OR toluene-2+5-diamine OR toluene-2+5-diamine+sulfate) OR (proximity 3 AND CAS AND 95-70-5)
2_3-dihydro-2_2-dimethyl-1h-perimidine	(unii-144c1zsa7u OR mls002694859 OR 144c1zsa7u OR dtxsid0073370 OR schembl3171824 OR chembl1868212 OR ctk5b9605 OR hms3085j09 OR zinc392955 OR 1h-perimidine+2+3-dihydro-2+2-dimethyl- OR 1h-perimidine+3-dihydro-2+2-dimethyl- OR 2+2-dimethyl-2+3-dihydro-1h-perimidine OR 2+3-dihydro-2+2-dimethyl-1h-perimidine OR UNII-144C1ZSA7U OR MLS002694859 OR 144C1ZSA7U OR DTXSID0073370 OR SCHEMBL3171824 OR CHEMBL1868212 OR CTK5B9605 OR HMS3085J09 OR ZINC392955 OR 1H-Perimidine+2+3-dihydro-2+2-dimethyl- OR 1H-Perimidine+3-dihydro-2+2-dimethyl- OR 2+2-dimethyl-1+3-dihydroperimidine OR 2+2-dimethyl-2+3-dihydro-1H-perimidine OR 2+2-dimethyl-2+3-dihydroperimidine OR 2+3-dihydro-2+2-dimethyl+perimidine OR 2+3-Dihydro-2+2-dimethyl-1H-perimidine) OR (proximity 3 AND CAS AND 6364-17-6)
Retinol_propionate	(unii-32jk994wmc OR 32jk994wmc OR ec+230-363-2 OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-en-1-yl+nona-2+4+6+8-tetraen-1-yl+propionate OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethylcyclohexen-1-yl+nona-2+4+6+8-tetraenyl+propanoate OR w-110194 OR propionic+acid+retinol+ester OR einecs+230-363-2 OR mfcd00129785 OR zinc16609980 OR akos024386409 OR ns00007709 OR st51037678 OR q27256177 OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetr+aenyl+propanoate OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetraenyl+propi OR retinyl+propionate OR retinol+propanoate OR retinol+propionate OR vitamin+a+propionate OR UNII-32JK994WMC OR 32JK994WMC OR EC+230-363-2 OR +2E+4E+6E+8E+-3+7-Dimethyl-9-+2+6+6-trimethylcyclohex-1-en-1-yl+nona-2+4+6+8-tetraen-1-yl+propionate OR +2E+4E+6E+8E+-3+7-dimethyl-9-+2+6+6-trimethylcyclohexen-1-yl+nona-2+4+6+8-tetraenyl+propanoate OR W-110194 OR Propionic+acid+retinol+ester OR EINECS+230-363-2 OR MFCD00129785 OR ZINC16609980 OR AKOS024386409 OR NS00007709 OR ST51037678 OR Q27256177 OR +2E+4E+6E+8E+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetr+aenyl+propanoate OR +2E+4E+6E+8E+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetraenyl+propi OR Retinyl+propionate OR Retinol+propanoate OR Retinol+propionate OR Vitamin+A+propionate) OR (proximity 3 AND CAS AND 7069-42-3)
1-Propanone_2_methyl_1_4_methylthiophenyl_2_4_4_morpholinyl	(zinc19891833 OR unii-722clj6h6k OR tox21_301664 OR st50319490 OR smr000019254 OR schembl27554 OR sbb056749 OR q27266008 OR ns00003224 OR ncgc00255462-01 OR mls000084908 OR mcule-3119460562 OR M2028 OR ksc635c8d OR ks-00000c6c OR Irgacure OR hms2360j09 OR ft-0641373 OR eu-0035716 OR dtxsid8038857 OR dsstox_rid_79410 OR dsstox_gsid_38857 OR dsstox_cid_18857 OR ds-3825 OR db-055579 OR ctk5d5181 OR chembl1411716 OR CC-11372 OR cas-71868-10-5 OR caccure+907 OR C-17592 OR brd-k58799690-001-07-3 OR AX8016092 OR anw-36110 OR akos000520617 OR ak114642 OR acmc-1bitt OR ac-16227 OR 722clj6h6k OR 2-methyl-4+methylthio-2-morpholinopropiophenone OR 2-methyl-4+methylthio+2-morpholinopropiophenone OR 2-methyl-4+methylthio+2-morpholino+propiophenone OR 2-methyl-1+4-methylthiophenyl+2-morpholinopropan-1-one OR 2-methyl-1+4-methylthiophenyl+2-morpholino-1-propanone OR 2-methyl-1+4-methylthiophenyl+2-morpholin-4-ylpropan-1-one OR 2-methyl-1+4-methylsulfanylphenyl+2-morpholino-propan-1-one OR 2-methyl-1-+4-methylsulfanylphenyl+2-morpholin-4-ylpropan-1-one OR 2-methyl-1+4+methylthio+phenyl+2-morpholinopropan-1-one OR 2-methyl-1+4+methylthio+phenyl+2-morpholino-1-propanone OR 2-methyl-1+4+methylthio+phenyl+2+4-morpholinyl+1-propanone OR 2-methyl-1+4+methylsulfanyl+phenyl+2-morpholin-4-ylpropan-1-one OR 2-methyl-1+4+methylsulfanyl+phenyl+2+4-morpholinyl+1-propanone OR 1-propanone+2-methyl-1+4+methylthio+phenyl+2+4-morpholinyl+ OR 1-propanone+2-methyl-1-+4+methylthio+phenyl+2+4-4-morpholinyl+)

phenolphtaleine	(proximity 20) AND (phthalimetten OR euchessina OR phthalin OR espotabs OR phenolax OR purgophen OR koprol OR laxogen OR trilax OR spulmako-lax OR chocolax OR purgen OR correctol OR alophen OR doxidan OR medilax OR colax OR laxin OR femilax OR phenophthalein OR nci-c55798 OR unii-6qk969r2if OR nsc+10464 OR ccris+6266 OR hsdb+4161 OR einecs+201-004-7 OR mfcd00005913 OR brn+0284423 OR chembl63857 OR ai3-09081 OR mls000069592 OR 6qk969r2if OR dtxsid0021125 OR chebi:34914 OR ncgc00018200-07 OR smr000059015 OR dsstox_cid_1125 OR dsstox_rid_75956 OR dsstox_gsid_21125 OR evac-v-lax OR 1+3h+isobenzofuranone+3+3bis+4-hydroxyphenyl+ OR pubchem7084 OR spectrum_001077 OR opera_id_1337 OR spectrum2_001279 OR spectrum3_000888 OR spectrum4_000982 OR spectrum5_001268 OR ec+201-004-7 OR schembl27670 OR bspbio_002518 OR kbiogr_001383 OR kbioss_001557 OR mls001148397 OR bidd:er0202 OR divk1c_000929 OR spectrum1500480 OR spbio_001278 OR aronis002962 OR bcbcmap01_000174 OR hms502o11 OR kbio1_000929 OR kbio2_001557 OR kbio2_004125 OR kbio2_006693 OR kbio3_001776 OR ks-00000yjd OR ninds_000929 OR hms1920h04 OR hms2091p06 OR hms2236i09 OR hms3374p06 OR pharmakon1600-01500480 OR hy-d0211 OR ks-00003w2p OR nsc10464 OR zinc3831317 OR tox21_110838 OR tox21_202219 OR tox21_300282 OR bbl002030 OR bdbm50077844 OR ccg-39112 OR nsc-10464 OR nsc215214 OR nsc757271 OR sbb008868 OR stk029876 OR akos000493033 OR tox21_110838_1 OR mcule-5232154932 OR nsc-215214 OR nsc-757271 OR idi1_000929 OR smp1_000235 OR ncgc00018200-01 OR ncgc00018200-02 OR ncgc00018200-03 OR ncgc00018200-04 OR ncgc00018200-05 OR ncgc00018200-06 OR ncgc00018200-08 OR ncgc00018200-09 OR ncgc00018200-10 OR ncgc00018200-12 OR ncgc00023694-03 OR ncgc00023694-04 OR ncgc00023694-05 OR ncgc00023694-06 OR ncgc00023694-07 OR ncgc00254039-01 OR ncgc00259768-01 OR ac-14431 OR ak130019 OR bp-30 OR sc-74728 OR st072636 OR sbi-0051481.p003 OR 2+bis+4-hydroxyphenyl+methyl+benzoic+acid OR eu-0082600 OR ft-0659094 OR ns00008592 OR en300-92962 OR alpha+alpha+di+p-hydroxyphenyl+phthalide OR ab00052070_15 OR sr-0 0000112 OR sr-0 0000112-2 OR 3+3-bis+4-hydroxyphenyl+2-benzofuran-1+3h+one+ OR brd-k19227686-001-02-0 OR brd-k19227686-001-12-9 OR z57233591 OR f0921-4309 OR alpha+alpha-di+p-hydroxyphenyl+phthalide OR 1+3h+isobenzofuranone+3+3-bis+4-hydroxyphenyl+ OR 1+3h+isobenzofuranone+3-bis+4-hydroxyphenyl+ OR 2-+bis+4-hydroxyphenyl+methyl+benzoic+acid OR 3+3-bis+p-hydroxyphenyl+1+3h+isobenzofuranone OR 3+3-bis+4-hydroxyphenyl+1+3h+isobenzofuranone OR 3+3-bis+4-hydroxyphenyl+2-benzofuran-1+3h+one OR 3+3-bis+4-hydroxy-phenyl+3h-isobenzofuran-1-one OR 3+3-bis+4-hydroxyphenyl+isobenzofuran-1+3h+one OR 3+3-bis+4-hydroxyphenyl+phthalide OR 3+3-bis+p-hydroxyphenyl+phthalide OR alpha-+p-hydroxyphenyl+-alpha+4-oxo-2+5-cyclohexadien-1-ylidene+o-toluic+acid OR alpha-di+p-hydroxyphenyl+phthalide OR dihydroxyphthalophenone OR fenolftalein OR fenolftaleina OR phenolphtaleine OR phenolphthaleinum OR phthalide+3+3+bis+p-hydroxyphenyl+ OR phthalide+3+-bis+p-hydroxyphenyl+) AND (host)
phenylnaphtylamine	(1-phenylethanamine OR 1-phenylethylamine OR alpha-phenylethylamine OR dl-alpha-methylbenzylamine OR 1-phenethylamine OR alpha-aminoethylbenzene OR 1-amino-1-phenylethane OR alpha-methylbenzenemethanamine OR alpha-phenethylamine OR 1-phenyl-ethylamine OR 1-fenylethylamin OR benzenemethanamine+.alpha.-methyl- OR dl-1-phenylethylamine OR sumine+2079 OR ethanamine+1-phenyl- OR ethylamine+1-phenyl- OR dl-1-phenethylamine OR chebi:670 OR benzylamine+.alpha.-methyl- OR chembl278059 OR /-+-alpha-methylbenzylamine OR s+-.alpha.-methylbenzenemethanamine OR benzenemethanamine+.alpha.-methyl-+s+- OR unii-hz9dm6b2mt OR dl-alpha-methylbenzylamine+99% OR 1-fenylethylamin+czech OR benzylamine+alpha-methyl- OR s+-+-+-a-methyl-benzylamine OR benzene+1-amino-ethyl+- OR hz9dm6b2mt OR benzenemethanamine+a-methyl- OR hsdb+2742 OR benzenemethanamine+alpha-methyl- OR benzenemethaneamine+alpha-methyl- OR nsc+8391 OR einecs+202-706-6 OR einecs+210-545-8 OR 1-phenyl+ethylamine OR 1-phenylethanamine+# OR 1-aminoethyl+benzene OR .alpha.-phenethylamine OR pubchem21079 OR 1-phenyl-1-ethanamine OR dl-|a-phenylethylamine OR .alpha.-phenylethylamine OR dl-|a-methylbenzylamine OR ai3-03116 OR .alpha.-methylbenzylamine OR schembl830 OR acmc-209j2b OR acmc-20aj38 OR ec+210-545-8 OR benzenemethanamine+.alpha.-methyl-+.+-.+- OR /-+-1-phenylethylamine OR rs+-alpha-methylbenzylamine OR +-+-.alpha.-phenethylamine OR wln:+1m1r OR /-+-1-phenyl-ethylamine OR schembl4701869 OR l+-+-.alpha.-methylbenzylamine OR dtxsid40862301 OR l-+-+-.alpha.-phenylethylamine OR nsc8391 OR albb-032928 OR bcp32849 OR ks-00000g3i OR nsc-8391 OR r+-.alpha.-methylbenzenemethanamine OR s+-+-+-.alpha.-methylbenzylamine OR anw-53664 OR bbl027673 OR bdbm50023171 OR benzenemethaneamine+.alpha.-methyl- OR mfcd00008069 OR sbb040514 OR stk397443 OR akos000119070 OR akos016039387 OR cs-w013564 OR mcule-6637542099 OR ps-4601 OR sc-18396 OR benzenemethanamine+.alpha.-methyl-+r+- OR db-015888 OR db-054000 OR am20060838 OR benzylamine+.alpha.-methyl-+.+/-.+- OR ft-0601072 OR ft-0604486 OR ft-0658781 OR st45255353 OR c02455 OR s+-1-phenylethanamine;+1s+-1-phenylethanamine OR 83288-ep2270009a1 OR 83288-ep2272822a1 OR 83288-ep2284174a1 OR 83288-ep2298779a1 OR 83288-ep2305655a2 OR benzenemethanamine+.alpha.-methyl-+.+/-.+- OR benzenemethanamine+.alpha.-methyl-+.alpha.r+- OR q3560549 OR w-105090 OR f0798-0597 OR alpha+-naphthylphenylamine OR alpha+-phenylnaphthylamine OR 1-anilinonaphthalene OR 1-naphthalenamine+n-phenyl- OR 1-naphthyl+phenyl+amine OR 1-naphthylamine+n-phenyl- OR alpha+natphthylamine OR alpha-naphthylphenylamine OR fenyl-+alpha+-naftylamin OR fenyl-alpha-naftylamin OR n-+1-naphthyl+aniline OR n-1-naphthylaniline OR naphthalen-1-yl-phenyl-amine OR n-fenyl-1-aminonaftalen OR n-phenyl-+alpha+-naphthylamine OR n-phenyl-1-aminonaphthalene OR n-phenyl-1-naphthalenamine OR n-phenyl-1-naphthylamine OR n-phenyl-alpha-naphthylamine OR n-phenyl-l-naphthylamine OR n-phenyl-n-+1-naphthyl+amine OR n-phenylnaphthalen-1-amine OR n-phenylnaphthylamine OR phenyl-+alpha+-naphthylamine OR phenyl-1-naphthylamine OR phenyl-alpha-naphthylamine OR phenylnaphthylamine OR 1-Phenylethanamine OR 1-Phenylethylamine OR ALPHA-METHYLBENZYLAMINE OR alpha-Phenylethylamine OR DL-alpha-Methylbenzylamine OR 1-Phenethylamine OR alpha-Aminoethylbenzene OR 1-Amino-1-phenylethane OR 1-phenylethan-1-amine OR a-methylbenzylamine OR alpha-Methylbenzenemethanamine OR alpha-Phenethylamine OR 1-Phenyl-ethylamine OR 1-Fenylethylamin OR Benzenemethanamine+.alpha.-methyl- OR a-phenylethylamine OR DL-1-Phenylethylamine OR Sumine+2079 OR Ethanamine+1-phenyl- OR Ethylamine+1-phenyl- OR DL-1-phenethylamine OR a-methylbenzenemethanamine OR CHEBI:670 OR Benzylamine+.alpha.-methyl- OR CHEMBL278059 OR /-+-alpha-

	Methylbenzylamine OR S+-.alpha.-Methylbenzenemethanamine OR Benzenemethanamine+.alpha.-methyl-+S+- OR UNII-HZ9DM6B2MT OR DL-alpha-Methylbenzylamine+99% OR r-+-alpha-phenylethylamine OR 1-Fenylethylamin+Czech OR Benzylamine+alpha-methyl- OR S+-+-+-a-methyl-benzylamine OR Benzene+1-amino-ethyl+- OR HZ9DM6B2MT OR Benzenemethanamine+a-methyl- OR a-phenethylamine OR HSDB+2742 OR l-phenylethylamine OR Benzenemethanamine+alpha-methyl- OR a-aminoethylbenzene OR Benzenemethaneamine+alpha-methyl- OR NSC+8391 OR 1-phenylethyl+amine OR EINECS+202-706-6 OR EINECS+210-545-8 OR phenylethan-1-amine OR 1-Phenyl+ethylamine OR alpha-methylbezylamine OR 1-phenylethyl+amine OR 1-phenyl-ethyl-amine OR 1-Phenylethanamine+# OR rac-1-phenylethanamine OR 1-aminoethyl+benzene OR .alpha.-Phenethylamine OR dl-1-phenylethyl+amine OR PubChem21079 OR 1-Phenyl-1-ethanamine OR alpha-methyl+benzylamine OR alpha-methyl-benzylamine OR alpha-methylbenzyl+amine OR DL-|A-Phenylethylamine OR .alpha.-Phenylethylamine OR DL-|A-Methylbenzylamine OR 1+r+s+-phenylethylamine OR AI3-03116 OR +-1-phenylethylamine OR +-+-1-phenylethylamine OR alpha-methyl+benzyl+amine OR .alpha.-Methylbenzylamine OR +-+alpha-phenylethylamine OR SCHEMBL830 OR ACMC-209j2b OR ACMC-20aj38 OR +-+-alpha-phenylethylamine OR EC+210-545-8 OR alpha-methylbenzylamine OR +-alpha-methylbenzylamine OR 1-phenylethan-1-amine OR /-+-1-phenylethanamine OR +-+-alpha-methylbenzylamine OR Benzenemethanamine+.alpha.-methyl-+.+-.+- OR /-+-1-Phenylethylamine OR RS+-alpha-methylbenzylamine OR +-+-.alpha.-Phenethylamine OR +-alpha-methyl-benzylamine OR +-+alpha-methyl-benzylamine OR +-+-alpha-methyl-benzylamine OR WLN:+1M1R OR /-+-1-phenyl-ethanamine OR /-+-1-Phenyl-ethylamine OR racemic+alpha-methylbenzylamine OR +-alpha-methyl+benzyl+amine OR /-+-1-+phenyl+ethylamine OR +-+alpha+methyl+benzyl+amine OR SCHEMBL4701869 OR L+-+-.alpha.-Methylbenzylamine OR DTXSID40862301 OR L-+-+-.alpha.-Phenylethylamine OR NSC8391 OR +-+-alpha-methylbenzenemethanamine OR ALBB-032928 OR BCP32849 OR KS-00000G3I OR NSC-8391 OR R+-.alpha.-Methylbenzenemethanamine OR S+-+-+-.alpha.-Methylbenzylamine OR ANW-53664 OR BBL027673 OR BDBM50023171 OR Benzenemethaneamine+.alpha.-methyl- OR MFCD00008069 OR SBB040514 OR STK397443 OR AKOS000119070 OR AKOS016039387 OR CS-W013564 OR MCULE-6637542099 OR PS-4601 OR SC-18396 OR Benzenemethanamine+.alpha.-methyl-+R+- OR DB-015888 OR DB-054000 OR AM20060838 OR Benzylamine+.alpha.-methyl-+.+/-.+- OR FT-0601072 OR FT-0604486 OR FT-0658781 OR ST45255353 OR C02455 OR S+-1-phenylethanamine;+1S+-1-phenylethanamine OR 83288-EP2270009A1 OR 83288-EP2272822A1 OR 83288-EP2284174A1 OR 83288-EP2298779A1 OR 83288-EP2305655A2 OR Benzenemethanamine+.alpha.-methyl-+.+/-.+- OR Benzenemethanamine+.alpha.-methyl-+.alpha.R+- OR Q3560549 OR W-105090 OR F0798-0597 OR +alpha+-Naphthylphenylamine OR alpha+-Phenylnaphthylamine OR 1-+n-phenylamino+naphthalene OR 1-Anilinonaphthalene OR 1-Naphthalenamine+N-phenyl- OR 1-Naphthyl+phenyl+amine OR 1-Naphthylamine+N-phenyl- OR 1-naphthylphenylamine OR 1-phenylaminonaphthalene OR Alpha+Natphthylamine OR alpha-Naphthylphenylamine OR alpha-naphthyl-phenylamine OR Fenyl-+alpha+-naftylamin OR Fenyl-alpha-naftylamin OR N-+1-Naphthyl+aniline OR n-+1-naphthyl+-n-phenylamine OR N-1-Naphthylaniline OR Naphthalen-1-yl-phenyl-amine OR naphthylphenylamine OR N-Fenyl-1-aminonaftalen OR N-Phenyl-+alpha+-naphthylamine OR N-Phenyl-1-aminonaphthalene OR N-Phenyl-1-naphthalenamine OR N-PHENYL-1-NAPHTHYLAMINE OR N-Phenyl-alpha-naphthylamine OR N-phenyl-l-naphthylamine OR N-phenyl-N-+1-naphthyl+amine OR N-phenylnaphthalen-1-amine OR N-Phenylnaphthylamine OR n-phenyl-naphthylamine OR Phenyl-+alpha+-naphthylamine OR phenyl+alpha+naphthylamine OR Phenyl-1-naphthylamine OR Phenyl-alpha-naphthylamine OR Phenylnaphthylamine) OR ((proximity 3) AND (618-36-0 OR 98-84-0 OR 2627-86-3 OR 3886-69-9) AND CAS)
Glycerol_triglycidyl_ether	(glycerol+triglycidyl+ether OR triglycidylglycerol OR 1+2+3-tris+2+3-epoxypropoxy+propane OR unii-0kvt2q7z17 OR oxirane+2+2+2+-+1+2+3-propanetriyltris+oxymethylene+tris- OR 0kvt2q7z17 OR dtxsid00884584 OR glycerine+triglycidyl+ether OR hsdb+6089 OR glycerol+1+2+3-triglycidyl+ether OR einecs+236-211-1 OR propane+1+2+3-tris+2+3-epoxypropoxy+- OR oxirane+2+2+2+-+1+2+3-propanetriyltris+oxymethylene+tris-+homopolymer OR schembl36444 OR epon-812 OR ctk1c3979 OR 2+2+2+-+1+2+3-propanetriyltris+oxymethylene+trisoxirane OR akos015914389 OR 1+2+3-tris-+2+3-epoxypropoxy+propane OR ns00051314 OR q27236908 OR Glycerol+triglycidyl+ether OR TRIGLYCIDYLGLYCEROL OR 1+2+3-Tris+2+3-epoxypropoxy+propane OR UNII-0KVT2Q7Z17 OR Oxirane+2+2+2+-+1+2+3-propanetriyltris+oxymethylene+tris- OR 0KVT2Q7Z17 OR DTXSID00884584 OR 2-+1+3-bis+oxiran-2-ylmethoxy+propan-2-yloxymethyl+oxirane OR 1+2+3-propanetriol+glycidyl+ethers;glycerol+polymer+with+1-chloro-2+3-epoxypropane;ge+ ;1+2+3-propanetriol+glycidyl+ethers+glycerol+polymer+with+1-chloro-2+3-epoxypropane+ge+ OR Glycerine+triglycidyl+ether OR HSDB+6089 OR Glycerol+1+2+3-triglycidyl+ether OR EINECS+236-211-1 OR Glycerol+tris+2+3-epoxypropyl+ether OR Propane+1+2+3-tris+2+3-epoxypropoxy+- OR Oxirane+2+2+2+-+1+2+3-propanetriyltris+oxymethylene+tris-+homopolymer OR SCHEMBL36444 OR EPON-812 OR CTK1C3979 OR 2+2+2+-+1+2+3-Propanetriyltris+oxymethylene+trisoxirane OR glycerol+tris+2+3-epoxypropyl+ether OR AKOS015914389 OR 1+2+3-tris-+2+3-Epoxypropoxy+propane OR NS00051314 OR Q27236908 OR 2+2+2+-+1+2+3-propanethyltris+oxymethylene+tris+oxirane OR 2+2+2+-+propane-1+2+3-triyltris+oxy+tris+methylene+trioxirane) OR ((proximity 3) AND CAS AND (13236-02-7 OR 90529-77-4))
phenol_2_2_-_1-methyl-1_2-ethanediyl_bis_nitri	(words threshold OR phenol+2+2+-+1-methyl-1+2-ethanediyl+bis+nitri OR phenol+2+2+-+1-methyl-1+2-ethanediyl+bis+nitrilomethylidyne+bis- OR /-+/-+-propylenedinitrilodi-o-cresol OR 2+2+-+propane-1+2-diylbis+nitrilomethylylidene+diphenol OR α+α+-propylenedinitrilodi-o-cresol;phenol+2+2+-+1-methyl-1+2-ethanediyl+bis+nitrilomethylidyne+bis- OR o-cresol+.alpha.+.alpha.+-+propylenedinitrilo+di- OR phenol+2+2+-?+1-methyl-1+2-ethanediyl+bis+nitrilomethylidyne+?bis- OR α+α+-propylenedinitrilodi-o-cresol OR n+n+-disalicylidene-1+2-diaminopropane+.alpha.+.alpha.+-+propylenedinitrilo+di-o-cresol) OR (proximity 3 AND CAS AND 94-91-7)
solvent_blue_35	(oil+blue+35 OR dtxsid5044605 OR w-110453 OR sudan+blue+2 OR einecs+241-379-4 OR ci+61554 OR c.i.solvent+blue+35 OR unii-zvt4q30oqy OR zvt4q30oqy OR 1+4-bis+n-butylamino+9+10-anthracenedione OR 9+10-anthracenedione+1+4-di+butylamino+ OR dsstox_cid_24605 OR dsstox_gsid_44605 OR schembl156500 OR chembl3561395 OR ctk8e7890 OR solvent+blue+35 OR hy-d0516 OR ks-00000yd6 OR zinc4521973 OR sudan+blue+ii OR tox21_303986 OR gt5180 OR mfcd00011714 OR sbb057328 OR akos002134522 OR cs-6262 OR mcule-1589839876 OR acm17354142 OR ncgc00357014-01 OR ak-60435 OR as-17198 OR 1+4-di+butylamino+9+10-anthracenedione OR ax8151705 OR cas-17354-14-2 OR eu-0066568 OR ns00019427 OR st50997657 OR q7081287 OR 1+4-bis+butylimino+1+4-dihydroanthracene-9+10-diol OR 1+4-bis+butylamino+anthracene-9+10-dione OR 9+10-Anthracenedione+1+4-bis+butylamino+ OR 1+4-Bis+butylamino+anthraquinone OR OIL+BLUE+35 OR DTXSID5044605 OR W-110453 OR 9+10-anthracenedione+1+4-bis+butylamino+ OR 1+4-bis+butylamino+anthraquinone OR solventblue35 OR anthraquinone+1+4-bis+butylamino+ OR Sudan+Blue+2 OR EINECS+241-379-4 OR CI+61554 OR C.I.Solvent+Blue+35 OR UNII-ZVT4Q30OQY OR ZVT4Q30OQY OR 1+4-Bis+n-butylamino+-9+10-anthracenedione OR 9+10-Anthracenedione+1+4-di+butylamino+- OR DSSTox_CID_24605 OR DSSTox_GSID_44605 OR

	SCHEMBL156500 OR CHEMBL3561395 OR CTK8E7890 OR Solvent+blue+35 OR 1+4-di+butylamino+-anthraquinone OR HY-D0516 OR KS-00000YD6 OR ZINC4521973 OR Sudan+Blue+II OR Tox21_303986 OR GT5180 OR MFCD00011714 OR s6101 OR SBB057328 OR Anthraquinone+1+4-bis+butylamino+- OR AKOS002134522 OR CS-6262 OR MCULE-1589839876 OR ACM17354142 OR SOLVENT+BLUE+35 OR NCGC00357014-01 OR 1+4-bis+butylamino+anthra-9+10-quinone OR AK-60435 OR AS-17198 OR 1+4-Di+butylamino+-9+10-anthracenedione OR AX8151705 OR CAS-17354-14-2 OR EU-0066568 OR NS00019427 OR ST50997657 OR Q7081287 OR 1+4-Bis+butylimino+-1+4-dihydroanthracene-9+10-diol OR 1+4-Bis+butylamino+anthracene-9+10-dione OR 1+4-bis+butylamino+anthraq) OR (proximity 3 AND CAS AND 17354-14-2)
melamine_cyanurate	(melamine+cyanurate OR melamine+isocyanurate OR melaminkyanurat OR mitec+mx+601 OR einecs+253-575-7 OR nsc+231587 OR 1+3+5-triazine-2+4+6+1h+3h+5h+-trione+compound+with+1+3+5-triazine-2+4+6-triamine OR 1+3+5-triazine-2+4+6+1h+3h+5h+-trione+compound+with+1+3+5-triazine-2+4+6-triamine+1:1 OR s-triazine+2+4+6-triamino-+compd.+with+s-triazine-triol OR melaminecyanurate OR melamine-cyanuric+acid+compd. OR melamine+cyanaurate OR einecs+240-292-9 OR ec+253-575-7 OR schembl34655 OR c6h9n9o3 OR dtxsid3068043 OR ctk0i0670 OR nsc231587 OR akos015901107 OR akos024319632 OR mcule-6417519120 OR nsc-231587 OR as-12328 OR ls-155567 OR ft-0639392 OR 640m576 OR c-24479 OR q3267336 OR 1+5-triazine-2+4+6+1h+3h+5h+-trione+compd.+with+1+3+5-triazine-2+4+6-triamine+1:1+ OR Melamine+cyanurate OR Melamine+isocyanurate OR Melaminkyanurat OR Mitec+MX+601 OR EINECS+253-575-7 OR NSC+231587 OR 16133-31-6 OR 1+3+5-Triazine-2+4+6+1H+3H+5H+-trione+compound+with+1+3+5-triazine-2+4+6-triamine OR 1+3+5-Triazine-2+4+6+1H+3H+5H+-trione+compound+with+1+3+5-triazine-2+4+6-triamine+1:1 OR s-Triazine+2+4+6-triamino-+compd.+with+s-triazine-triol OR Melaminecyanurate OR 1+3+5-triazinane-2+4+6-trione+compound+with+1+3+5-triazine-2+4+6-triamine+1:1 OR Melamine-cyanuric+acid+compd. OR Melamine+cyanaurate OR EINECS+240-292-9 OR melamine+cyanuric+acid OR melamine+isocyanuric+acid OR EC+253-575-7 OR SCHEMBL34655 OR C6H9N9O3 OR DTXSID3068043 OR CTK0I0670 OR NSC231587 OR AKOS015901107 OR AKOS024319632 OR MCULE-6417519120 OR NSC-231587 OR AS-12328 OR LS-155567 OR FT-0639392 OR 640M576 OR C-24479 OR Q3267336 OR 1+5-Triazine-2+4+6+1H+3H+5H+-trione+compd.+with+1+3+5-triazine-2+4+6-triamine+1:1+) OR (proximity 3 AND CAS AND (16133-31-6 OR 37640-57-6))
2_4_-Diphenylmethane_diisocyanate	(o+p-isocyanatobenzyl+phenyl+isocyanate OR 2+4+diphenylmethane+diisocyanate OR 2+4+diisocyanatodiphenylmethane OR unii-yvq6nx5h3y OR diphenylmethane-2+4+diisocyanate OR benzene+1-isocyanato-2+4-isocyanatophenyl+methyl+ OR 2+4+diphenylmethanediisocyante OR einecs+227-534-9 OR yvq6nx5h3y OR dtxsid9027607 OR benzene+1-isocyanato-2-+4-isocyanatophenyl+methyl+ OR isocyanic+acid+diester+with+2+4+-methylenediphenol OR ccris+8159 OR benzene+1+1+-methylenebis+isocyanato+polymer+and+polypropylene+glycol OR ec+227-534-9 OR schembl27122 OR zinc1849831 OR akos015916627 OR benzene+1+1+methylenebis+isocyanato+polymer+with+alpha-hydro-omega-hydroxypoly+oxy+methyl-1+2-ethanediyl OR poly+oxy+methyl-1+2-ethanediyl+alpha-hydro-omega-hydroxy+polymer+with+1+1+methylenebis+isocyanatobenzene OR poly+oxy+methyl-1+2-ethanediyl+alpha-hydro-omega-hydroxy-+polymer+with+1+1+-methylenebis+isocyanatobenzene OR ds-021828 OR ls-168513 OR ft-0697125 OR ns00004392 OR 2+4+-methylenebis+phenyl+isocyanate OR q27294734 OR o+p-Isocyanatobenzyl+phenyl+isocyanate OR 2+4+Diphenylmethane+diisocyanate OR 2+4+Diisocyanatodiphenylmethane OR UNII-YVQ6NX5H3Y OR Diphenylmethane-2+4+diisocyanate OR Benzene+1-isocyanato-2-+4-isocyanatophenyl+methyl OR 2+4+Diphenylmethanediisocyante OR EINECS+227-534-9 OR YVQ6NX5H3Y OR 1-isocyanato-2+4-isocyanatobenzyl+benzene OR DTXSID9027607 OR Benzene+1-isocyanato-2+4-isocyanatophenyl+methyl OR Isocyanic+acid+diester+with+2+4+methylenediphenol OR CCRIS+8159 OR Benzene+1+1+methylenebis+isocyanato+polymer+and+polypropylene+glycol OR EC+227-534-9 OR SCHEMBL27122 OR diphenylmethan-2+4+diisocyanat OR 2+4+methylenediphenyl+diisocyanate OR ZINC1849831 OR AKOS015916627 OR Benzene+1+1+methylenebis+isocyanato+polymer OR Poly+oxy+methyl-1+2-ethanediyl+alpha-hydro-omega-hydroxy+polymer+with+1+1+methylenebis+isocyanatobenzene) OR (proximity 3 AND CAS AND 5873-54-1)
Diphenylmethane_2_2_diisocyanate	(1-isocyanato-2-+2-isocyanatophenyl+methyl+benzene OR diphenylmethane-2+2+-diisocyanate OR 2+2+-methylenediphenyl+diisocyanate OR unii-as00fwt3dm OR as00fwt3dm OR benzene+1+1+-methylenebis+2-isocyanato- OR dtxsid90883107 OR bisphenol+f+diisocyanate OR methylene+diphenyldiisocyanate OR schembl15544 OR methylene-diphenyl+diisocyanate OR einecs+219-799-4 OR akos028110966 OR 1+1+-methylenebis+2-isocyanatobenzene OR as-62089 OR ec+219-799-4 OR q27274092 OR Diphenylmethane-2+2+-diisocyanate OR 2+2+-Methylenediphenyl+diisocyanate OR UNII-AS00FWT3DM OR AS00FWT3DM OR Benzene+1+1+-methylenebis+2-isocyanato- OR DTXSID90883107 OR 2+2+-methylenedi+phenyl+isocyanate OR Bisphenol+F+diisocyanate OR Methylene+diphenyldiisocyanate OR SCHEMBL15544 OR methylene-bis-phenylisocyanate OR bis+2-isocyanatophenyl+methane OR Methylene-diphenyl+diisocyanate OR 2+2-methylenediphenyl+diisocyanate OR EINECS+219-799-4 OR AKOS028110966 OR 1+1+-Methylenebis+2-isocyanatobenzene OR AS-62089 OR EC+219-799-4 OR Q27274092) OR (proximity 3 AND CAS AND 2536-05-2)
2_chloroaniline	(2-chloroaniline OR o-chloroaniline OR 2-chlorobenzenamine OR benzenamine+2-chloro OR 2-chlorophenylamine OR 1-amino-2-chlorobenzene OR o-aminochlorobenzene OR o-chloroaminobenzene OR aniline+o-chloro OR o-chloraniline OR benzenamine+chloro OR nsc+6183 OR 2-chloro+aniline OR unii-g14i494t2f OR ccris+2880 OR hsdb+2045 OR 2-chloro-aniline OR einecs+202-426-4 OR ai3-16321 OR g14i494t2f OR mfcd00007656 OR 2-chloroanilinium+chloride OR codeine+tms OR 2-chloro-phenylamine OR 2-amino-1-chlorobenzene OR benzeneamine+2-chloro OR dsstox_cid_1810 OR acmc-209rz5 OR ec+202-426-4 OR dsstox_rid_76342 OR dsstox_gsid_21810 OR schembl25495 OR ksc203m7l OR mls002454424 OR bidd:gt0224 OR chembl389885 OR dtxsid2021810 OR ctk1a3675 OR nsc6183 OR hms3039d15 OR zinc164914 OR ks-000002ly OR nsc-6183 OR str00033 OR tox21_200802 OR anw-40527 OR cc0074 OR sbb040494 OR stl168885 OR akos000119118 OR am87482 OR ls-1978 OR ls11568 OR mcule-8604040668 OR ncgc00091121-01 OR ncgc00091121-02 OR ncgc00258356-01 OR sc-22931 OR smr001372017 OR db-020908 OR ds-009850 OR ft-0611903 OR ns00010859 OR st45255279 OR az0001-0090 OR 79520-ep2305695a2 OR 79520-ep2305696a2 OR 79520-ep2305697a2 OR 79520-ep2305698a2 OR 139415-ep2270008a1 OR 139415-ep2275404a1 OR 139415-ep2280001a1 OR 139415-ep2284157a1 OR 139415-ep2292617a1 OR j-509009 OR q2294431 OR z57127444 OR f2190-0428 OR 2-CHLOROANILINE OR o-Chloroaniline OR 2-Chlorobenzenamine OR Benzenamine+2-chloro OR 2-Chlorophenylamine OR 1-Amino-2-chlorobenzene OR o-Aminochlorobenzene OR o-Chloroaminobenzene OR Aniline+o-chloro OR o-

	Chloraniline OR Benzenamine+chloro OR NSC+6183 OR 2-Chloro+aniline OR UNII-G14I494T2F OR CCRIS+2880 OR HSDB+2045 OR 2-CHLORO-ANILINE OR EINECS+202-426-4 OR AI3-16321 OR G14I494T2F OR MFCD00007656 OR 2-Chloroanilinium+chloride OR 6-chloroaniline OR o-chloro-aniline OR Codeine+TMS OR 2-aminochlorobenzene OR 2-Chloro-phenylamine OR 1+2-aminochlorobenzene OR 2-chlorophenyl+amine OR 2-Amino-1-chlorobenzene OR Benzeneamine+2-chloro OR DSSTox_CID_1810 OR ACMC-209rz5 OR EC+202-426-4 OR DSSTox_RID_76342 OR DSSTox_GSID_21810 OR SCHEMBL25495 OR KSC203M7L OR MLS002454424 OR BIDD:GT0224 OR CHEMBL389885 OR DTXSID2021810 OR CTK1A3675 OR NSC6183 OR HMS3039D15 OR ZINC164914 OR KS-000002LY OR NSC-6183 OR STR00033 OR Tox21_200802 OR ANW-40527 OR CC0074 OR SBB040494 OR STL168885 OR AKOS000119118 OR AM87482 OR LS-1978 OR LS11568 OR MCULE-8604040668 OR NCGC00091121-01 OR NCGC00091121-02 OR NCGC00258356-01 OR SC-22931 OR SMR001372017 OR DB-020908 OR DS-009850 OR FT-0611903 OR NS00010859 OR ST45255279 OR AZ0001-0090 OR 79520-EP2305695A2 OR 79520-EP2305696A2 OR 79520-EP2305697A2 OR 79520-EP2305698A2 OR 139415-EP2270008A1 OR 139415-EP2275404A1 OR 139415-EP2280001A1 OR 139415-EP2284157A1 OR 139415-EP2292617A1 OR J-509009 OR Q2294431 OR Z57127444 OR F2190-0428) OR (proximity 3 AND CAS AND 95-51-2)
4_4_-Methylenebis_2_chloroaniline_	(4+4+amino-3-chlorobenzyl+2-chlorophenyl+amine OR 4+4-Amino-3-chlorobenzyl+2-chlorophenyl+amine OR 2+2+dichloro-4+4+methylendianiline OR 2+2+methylenebis+4-methyl-6-tert-butylphenol+monoacrylate OR 2+2+Methylenebis+4-Methyl-6-Tert-Butylphenol+Monoacrylate OR 2+2+dichloro-4+4+methylene+dianiline OR 3+3+dichlor-4+4+diaminodiphenylmethan OR 3+3+dichloro-4+4+diaminodifenilmetano OR 3+3+dichloro-4+4+diaminodiphenyl+methane OR 3+3+dicloro-4+4+diaminodifenilmetano OR 3+3+dichloro-4+4+diaminodiphenylmethane OR 3+4+diaminodifenilmetano OR 3+4+diaminodiphenylmethan OR 4+3+dichlorodiphenyl+methane OR 4+4+-bis+2-chloroanilino+methane OR 4+4+diamino-3+3+dichlorodiphenyl+methane OR 4+4+methanediylbis+2chloroaniline OR 4+4+methylene+bis+chloroaniline OR 4+4+methylene+bis+ochloroaniline OR 4+4+methylene-bis+2chloroaniline OR 4+4+methylene-bis+2-chloroaniline OR 4+4+methylene-bis-2-chloroaniline OR 4+4+methylenebis+2-chlorobenzenamine OR 4+4+methylenebis-2-chlorobenzenamine OR 4+4+diamino3+3+dichlorodiphenylmethane OR 4+4+methylene+bis+2-chloroaniline OR 4+4+methylenebis+2-chloroaniline OR 4+4+methylenebis+o-chloroaniline OR 4+4-methylene+bis+2-chloroaniline OR 4+4-methylenebis+2-chloroaniline OR 4+4-metilene-bis-o-cloroanilina OR 4+4-amino-3-chloro-phenyl+methyl+2-chloro-aniline OR 4+4-amino-3-chlorobenzyl+2-chlorophenylamine OR 4+4-Amino-3-chlorobenzyl+2-chlorophenylamine OR 4+4-amino-3-chlorophenyl+methyl+2-chloroaniline OR 4+4-amino-3-chlorophenyl+methyl+2-chlorophenylamine OR acmc-1be7q OR akos000120884 OR albb-010577 OR aniline+4+methylenebis+2-chloro OR aniline+4+4+methylenebis+2-chloro OR aniline+4+4+methylenebis+2chloro OR anw-14437 OR ar+ar+methylenebis+2-chlorobenzenamine OR ar+ar+Methylenebis+2-chlorobenzenamine OR benzenamine+4+methylenebis+2-chloro OR benzenamine+4+4+methylenebis+2-chloro OR benzenamine+ar+ar+methylenebis+2-chloro OR bim-0013222+p001 OR bis+3-chloro-4-aminophenyl+methane OR bis+4-amino-3-chlorophenyl+methane OR bis+amine OR bis-amine+a OR bisamine OR bisamine+s OR brn+1882318 OR c10999 OR cb03526 OR cbmicro_013250 OR ccris+389 OR chebi+28124 OR chembl82846 OR cl-mda OR ctk0h5881 OR cuamine+m OR cuamine+mt OR curalin+m OR curene+442 OR cyanaset OR dacpm OR di+4-amino-3-chlorophenyl+methane OR di+4-amino-3-clorofenil+metano OR diamet+kh OR dsstox_cid_865 OR dsstox_gsid_20865 OR dsstox_rid_75834 OR dtxsid5020865 OR ec+202-918-9 OR einecs+202-918-9 OR hms3039n14 OR hsdb+2629 OR ks-00000yp6 OR ksc175q8d OR ld+813 OR mboca OR mcule-3758655473 OR met+hylene-bis+2-chloroaniline+4+4 OR methylene+4+4+bis+o-chloroaniline OR methylene-4+4+bis+o-chloroaniline OR methylene-bis+2-chloroaniline+4+4 OR methylene-bis-orthochloroaniline OR methylenebis+2-chloroaniline OR methylenebis+3-chloro-4-aminobenzene OR methylenebis+chloroaniline OR mfcd00047829 OR millionate+m OR mls002303002 OR ncgc00090906-01 OR ncgc00090906-02 OR ncgc00258205-01 OR ns00005883 OR nsc+52954 OR nsc-52954 OR nsc52954 OR oprea1_093196 OR p+p+methylenebis+alpha-chloroaniline OR p+p+methylenebis+o-chloroaniline OR p+p+methylenebis+ortho-chloroaniline OR poly+bisphenol+a-co-4+4+dichlorodiphenyl+sulfone OR q2257591 OR quodorole OR schembl43509 OR smr001307314 OR smsf0004157 OR sr-0 0197737 OR sr-0 0197737-1 OR st50319834 OR stk295634 OR tox21_200651 OR unii-3l2w5vtt2a OR w-108926 OR w-6359 OR zinc56414) OR (proximity 3 AND CAS AND (101-14-4 OR 27342-75-2))
cyclonite	(cyclonite OR hexogen OR hexolite OR 1+3+5-trinitro-1+3+5-triazinane OR geksogen OR cyclotrimethylenetrinitramine OR trimethylenetrinitramine OR hexogen+5w OR hexogeen OR 1+3+5-trinitro-1+3+5-triazacyclohexane OR trimethyleentrinitramine OR cyclotrimethylenenitramine OR cyklonit OR 1+3+5-triazine+hexahydro-1+3+5-trinitro- OR hexahydro-1+3+5-trinitro-s-triazine OR trinitrocyclotrimethylene+triamine OR trinitrotrimethylenetriamine OR sym-trimethylene+trinitramine OR 1+3+5-trinitrohexahydro-s-triazine OR cx+84a OR cyclonit OR 1+3+5-triaza-1+3+5-trinitrocyclohexane OR 1+3+5-trinitrohexahydro-1+3+5-triazine OR perhydro-1+3+5-trinitro-1+3+5-triazine OR nsc+312447 OR unii-w91ssv5831 OR trimethyleentrinitramine+dutch OR 1+3+5-trinitroperhydro-1+3+5-triazine OR hsdb+2079 OR khp+281 OR einecs+204-500-1 OR sym-trimethylenetrinitramine OR brn+0288466 OR s-triazine+hexahydro-1+3+5-trinitro- OR esaidro-1+3+5-trinitro-1+3+5-triazina OR hexahydro-1+3+5-trinitro-1+3+5-triazin OR dtxsid9024142 OR w91ssv5831 OR ccris+9287 OR trinitrohexahydrotriazine OR s-triazine+3+5-trinitro- OR schembl19770 OR chebi:24556 OR 1+5-trinitrohexahydro-s-triazine OR hexahydro-1+5-trinitro-s-triazine OR nsc312447 OR stk366162 OR zinc64622596 OR akos015914094 OR 1+5-trinitroperhydro-1+3+5-triazine OR mcule-5928095574 OR nsc-312447 OR 1+5-triaza-1+3+5-trinitrocyclohexane OR 1+5-trinitro-1+3+5-triazacyclohexane OR 1+5-trinitrohexahydro-1+3+5-triazine OR esaidro-1+5-trinitro-1+3+5-triazina OR 1+3+5-trinitro-1+3+5-triazinane+# OR hexahydro-1+5-trinitro-1+3+5-triazin OR hexahydro-1+5-trinitro-1+3+5-triazine OR 1+3+5-triazacyclohexane+1+3+5-trinitro- OR 1+5-triazine+hexahydro-1+3+5-trinitro- OR ls-155436 OR ns00001970 OR q190020 OR CYCLONITE OR Hexogen OR Hexolite OR 1+3+5-Trinitro-1+3+5-triazinane OR Geksogen OR Cyclotrimethylenetrinitramine OR Hexahydro-1+3+5-trinitro-1+3+5-triazine OR Trimethylenetrinitramine OR Hexogen+5W OR Hexogeen OR 1+3+5-Trinitro-1+3+5-triazacyclohexane OR Trimethyleentrinitramine OR Cyclotrimethylenenitramine OR Cyklonit OR 1+3+5-Triazine+hexahydro-1+3+5-trinitro- OR Hexahydro-1+3+5-trinitro-s-triazine OR Trinitrocyclotrimethylene+triamine OR Trinitrotrimethylenetriamine OR sym-Trimethylene+trinitramine OR 1+3+5-Trinitrohexahydro-s-triazine OR CX+84A OR Cyclonit OR 1+3+5-Triaza-1+3+5-trinitrocyclohexane OR 1+3+5-Trinitrohexahydro-1+3+5-triazine OR Perhydro-1+3+5-trinitro-1+3+5-triazine OR NSC+312447 OR UNII-W91SSV5831 OR Trimethyleentrinitramine+Dutch OR 1+3+5-Trinitroperhydro-1+3+5-triazine OR HSDB+2079 OR KHP+281 OR EINECS+204-500-1 OR sym-Trimethylenetrinitramine OR BRN+0288466 OR s-Triazine+hexahydro-

	1+3+5-trinitro- OR Esaidro-1+3+5-trinitro-1+3+5-triazina OR Hexahydro-1+3+5-trinitro-1+3+5-triazin OR DTXSID9024142 OR W91SSV5831 OR CCRIS+9287 OR hexahydro-1 OR Trinitrohexahydrotriazine OR s-Triazine+3+5-trinitro- OR cyclo-trimethylenetrinitramine OR SCHEMBL19770 OR CHEBI:24556 OR 1+5-Trinitrohexahydro-s-triazine OR Hexahydro-1+5-trinitro-s-triazine OR 1+3+5-trinitrohexahydro-p-triazine OR NSC312447 OR STK366162 OR ZINC64622596 OR AKOS015914094 OR 1+5-Trinitroperhydro-1+3+5-triazine OR MCULE-5928095574 OR NSC-312447 OR 1+5-Triaza-1+3+5-trinitrocyclohexane OR 1+5-Trinitro-1+3+5-triazacyclohexane OR 1+5-Trinitrohexahydro-1+3+5-triazine OR Esaidro-1+5-trinitro-1+3+5-triazina OR 1+3+5-Trinitro-1+3+5-triazinane+# OR Hexahydro-1+5-trinitro-1+3+5-triazin OR Hexahydro-1+5-trinitro-1+3+5-triazine OR 1+3+5-Triazacyclohexane+1+3+5-trinitro- OR 1+5-Triazine+hexahydro-1+3+5-trinitro- OR LS-155436 OR hexahydro-1+3+5-trinitro-1+3+5-triazine OR NS00001970 OR Q190020) OR (proximity 20 AND (host) AND heksogen) OR (proximity 3 AND CAS AND 121-82-4)
4_4_-Oxybis_benzenesulfonyl_hydrazide	(4+4+oxybis+benzenesulfonyl+hydrazide OR serogen OR genitron OR zhenitron OR celogen OR 4+4+oxybis+benzenesulfonhydrazide OR cellmic OR celmike OR cenitron OR p+p+oxybis+benzenesulfohydrazide OR 4+4+oxydibenzenesulfonyl+hydrazide OR diphenyloxide-4+4+disulfohydrazide OR 4+4+oxydi+benzenesulphonohydrazide OR diphenyl+ether+4+4+disulfohydrazide OR p+p+oxybis+benzenesulfonylhydrazine OR benzenesulfonic+acid+4+4+oxybis+dihydrazide OR oxybis+benzenesulfonylhydrazide OR 4+4+oxydi+benzenesulfonyl+dihydrazide OR unii-70377ej95z OR 4+4+oxydibenzenesulfonic+acid+dihydrazide OR hsdb+5237 OR 4+4+oxybis+benzenesulfonic+acid+hydrazide OR nsc+5318 OR p+p+oxybis+benzenesulfonyl+hydrazide OR einecs+201-286-1 OR oxybisbenzenesulfonic+acid+dihydrazide OR p+p+oxybisbenzene+disulfonylhydrazide OR brn+2954604 OR 4+4+oxydi+benzenesulfonic+acid+hydrazide OR dtxsid7026499 OR 4+4+oxybis+benzenesulfonic+acid+dihydrazide OR benzenesulfonic+acid+4+4+-oxydi+dihydrazide OR 70377ej95z OR benzenesulfonic+acid+4+4+oxybis+1+1+dihydrazide OR w-104230 OR dsstox_cid_6499 OR ec+201-286-1 OR dsstox_rid_78124 OR dsstox_gsid_26499 OR oprea1_874031 OR schembl36774 OR chembl1882501 OR ctk5g0707 OR nsc5318 OR nsc-5318 OR p+p+oxybis+benzenesulfonhydrazide OR zinc1680846 OR tox21_301976 OR mfcd00007587 OR akos001426105 OR mcule-2213785759 OR cas-80-51-3 OR ncgc00164109-01 OR ncgc00255179-01 OR as-14554 OR ls-32045 OR sc-18194 OR benzenesulfonic+acid+oxybis+dihydrazide OR p+p+oxybis-benzenesulfonylhydrazide OR benzenesulfonic+acid+4+oxybis+dihydrazide OR benzenesulfonic+acid+4+-oxydi+dihydrazide OR ft-0654030 OR ns00004831 OR c-34194 OR q27265828 OR 4+4+oxybis+benzenesulfohydrazide OR 70377EJ95Z OR dihydrazide4+4+oxybis-benzenesulfonic+acid OR 4+4+hydrazinesulfonyl+phenoxy+benzenesulfonohydrazide OR 4+4-oxydi+benzenesulphonohydrazide) OR (proximity 3 AND CAS AND 80-51-3)
Bis_2_4-dichlorobenzoyl_peroxide	(2+4-dichlorobenzoyl+peroxide OR bis+2+4-dichlorobenzoyl+peroxide OR cadox OR siloprene OR peroxide+bis+2+4-dichlorobenzoyl OR unii-0qc93y0l96 OR einecs+205-094-9 OR brn+2008711 OR dtxsid4044539 OR 0qc93y0l96 OR bis+2+4-dichlorophenyl+peroxyanhydride OR di-2+4-dichlorobenzoyl+peroxide OR perkadox+pd OR ec+205-094-9 OR 2+4-dichlorobenzoylperoxide OR schembl15385 OR ctk0h7230 OR zinc185 7 OR rw1263 OR akos015849996 OR cc-07377 OR db-005856 OR ls-102454 OR ft-0631772 OR ns00009864 OR 133d142 OR a806566 OR q27237102 OR 2+4-dichlorobenzoyl+2+4-dichlorobenzenecarboperoxoate OR di+2+4-dichlorobenzoyl+peroxide OR 2+4-dichlorobenzoic+peroxyanhydride OR 2+4-dichlorophenyl+carbonyl+2+4-bis+chloranyl+benzenecarboperoxoate OR 2+4-dichlorobenzenecarboperoxoic+acid OR 2+4-dichlorophenyl+oxome) OR (proximity 20 AND (host) AND luperco) OR (proximity 3 AND CAS AND 133-14-2)
1_3-Divinylimidazolidin-2-one	(1+3-divinylimidazolidin-2-one OR 2-imidazolidinone+1+3-diethenyl- OR unii-9wnu043766 OR dtxsid8074734 OR 9wnu043766 OR einecs+237-457-2 OR schembl41850 OR 1+3-divinylimidazolid-2-on OR 1+3-divinyl-2-imidazolidone OR 1+3-divinylimidazolidine-2-one OR 1+3-divinyl-2-imidazolidinone OR zinc2526766 OR akos006292919 OR ft-0606733 OR ns00020579 OR w-110354 OR q27273319 OR 1+3-Divinylimidazolidin-2-one OR 2-Imidazolidinone+1+3-diethenyl- OR UNII-9WNU043766 OR DTXSID8074734 OR 1+3-diethenylimidazolidin-2-one OR 9WNU043766 OR EINECS+237-457-2 OR SCHEMBL41850 OR 1+3-Divinylimidazolid-2-on OR 1+3-Divinyl-2-imidazolidone OR 1+3-Divinylimidazolidine-2-one OR 1+3-Divinyl-2-imidazolidinone OR ZINC2526766 OR AKOS006292919 OR FT-0606733 OR NS00020579 OR W-110354 OR Q27273319) OR (proximity 3 AND CAS AND 13811-50-2)
1_3-Dimethyl-3_4_5_6-tetrahydro-2_1H_-pyrimidinone	(1+3-dimethyl-3+4+5+6-tetrahydro-2+1h+-pyrimidinone OR 1+3-dimethyltetrahydropyrimidin-2+1h+-one OR dimethylpropyleneurea OR 2+1h+-pyrimidinone+tetrahydro-1+3-dimethyl- OR n+n+-dimethylpropyleneurea OR n+n+-dimethyltrimethyleneurea OR ccris+4322 OR n+n+-dimethylpropylene+urea OR tetrahydro-1+3-dimethyl-1h-pyrimidin-2-one OR einecs+230-625-6 OR mfcd00006550 OR brn+0110562 OR tetrahydro-1+3-dimethyl-2+1h+pyrimidine OR dtxsid3074575 OR ak-36216 OR j-503925 OR pubchem16903 OR n+n+-dimethylproyleneurea OR ec+230-625-6 OR schembl82580 OR ksc498e3d OR chembl12284 OR ctk3j8231 OR zinc157131 OR bcp25854 OR str03401 OR zx-at013447 OR anw-36181 OR sbb058374 OR 1+3-dimethyl-2-oxohexahydropyrimidine OR akos005145503 OR cm13987 OR cs-w009128 OR mcule-5575317893 OR or13656 OR 1+3-dimethyl-tetrahydro-pyrimidin-2-one OR 1+3-dimethyltetrahydro-2+1h+pyrimidinon OR 1+3-dimethyltetrahydro-2+1h+pyrimidone OR cc-03151 OR 1+3-dimethyl-tetrahydro-2+1h+pyrimidone OR 1+3-dimethyl-tetrahydro-2-1h-pyrimidinone OR ax8211152 OR bb0295064 OR db-011617 OR ls-136022 OR 1+3-dimethyl+tetrahydropyrimidin-2+1h+-one OR 1+3-dimethyltetrahydro-2+1h+-pyrimidinone OR ft-0606689 OR ns00005527 OR st51016259 OR 2-pyrimidone+tetrahydro+1+3-dimethyl OR en300-82368 OR ks-00000143 OR n+n+-dimethyl-n+n+-trimethyleneurea OR 6632-ep1441224a2 OR tetrahydro-1+3-dimethyl-2+1h+pyrimidin-2-onee OR 113513-ep2281820a2 OR 113513-ep2298754a1 OR a837469 OR c-34420 OR dimethyl-3+4+5+6-tetrahydro-2+1h+pyrimidinone OR n+n+dimethyl+1+4+5+6-tetrahydro-2-pyrimidone OR n+n+dimethyl-1+4+5+6-tetrahydro-2-pyrimidone OR q416637 OR 1+3-dimethyl-3+4+5+6-tetrahydro+2+1h+pyrimidone OR 1+3-dimethyl-3+4+5+6-tetrahydro-2+1h+pyrimidone OR 1+3-dimethyl-3+4+5+6-tetrahydro-2+1h+pyrimidinon OR 1+3-dimethyl-3+4+5+6-tetrahydro-2-+1h+pyrimidone OR 1+3-dimethyl-3+4+5+6-tetrahydro2+1h+pyrimidinone OR 1+3-dimethyl-3+4+5+6tetrahydro-2+1h+pyrimidinone OR 1+3-di-methyl-3+4+5+6-tetrahydro-2+1h+pyrimidinone OR 1+3-dim-ethyl-3+4+5+6-tetrahydro-2+1h+pyrimidinone OR 1+3-dimethyl+-3+4+5+6-tetrahydro-2+1h+pyrimidinone OR 1+3-dimethyl-2+4+5+6-tetrahydro-2+1h+pyrimidinone OR 1+3-dimethyl-3+4+5+6-tetrahydro-2+1+h+pyrimidinone OR 1+3-dimethyl-3+4+5+6-tetrahydro-2+1h+pyrirnidinone OR 1+3-dimethyl-3+4+5+6-tetrahydro-2-+1h+pyrimidinone OR f0001-1844 OR 1+3-di+methyl-3+4+5+6-tetrahydro-2+1h+pyrimidinone OR 1+3-dimethyl-3+4+5+6-tetrahydro+2+1h+pyrimidinone OR 1+3-dimethyl-3+4+5+6-tetra-hydro+1h+pyrimidin-2-one OR 1+3-dimethyl-3+4+5+6-tetrahydro+2-

	+1h+pyrimidone OR 1+3-dimethyl-3+4+5+6-tetrahydro+1h+pyrimidin-2-one OR 1+3-dimethyltetrahydropyrimidin-2+1H+one)
3_4-Epoxycyclohexylmethyl_3_4-epoxycyclohexanecarboxylate	(proximity 20) AND (3+4-epoxycyclohexyl+methyl+3+4-epoxycyclohexylcarboxylate OR 7-oxabicyclo+4+1+0+heptan-3-ylmethyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR 3+4-epoxycyclohexylmethyl+3+4-epoxycyclohexanecarboxylate OR erl-4221 OR ut-632 OR chissonox+221+monomer OR unii-s224del3p4 OR 3+4-epoxycyclohexylmethyl+3+4-epoxycyclohexane+carboxylate OR hsdb+5873 OR einecs+219-207-4 OR ut+632 OR 3+4-epoxycyclohexylmethyl-3+4-epoxycyclohexanecarboxylate OR 3+4-epoxycyclohexanecarboxylic+acid+3+4-epoxycyclohexylmethyl+ester OR brn+1381750 OR 7-oxabicyclo+4+1+0+heptane-3-carboxylic+acid+7-oxabicyclo+4+1+0+hept-3-ylmethyl+ester OR s224del3p4 OR dtxsid2027466 OR 3+4-epoxycyclohexanemethyl+3+4-epoxycyclohexanecarboxylate OR ak-78714 OR dsstox_cid_7466 OR 7-oxabicyclo+4+1+0+hept-3-ylmethyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR dsstox_rid_78463 OR dsstox_gsid_27466 OR w-107371 OR cas-2386-87-0 OR ccris+8882 OR ec+219-207-4 OR schembl24975 OR ksc490c3p OR chembl2143072 OR ctk3j0137 OR bcp32770 OR cel-2021 OR tox21_202388 OR tox21_303312 OR anw-57541 OR akos015915254 OR ks-000001n6 OR ncgc00164163-01 OR ncgc00164163-02 OR ncgc00256981-01 OR ncgc00259937-01 OR as-17792 OR ls-98670 OR sc-19925 OR db-028268 OR ft-0651573 OR ns00011515 OR 3+4-epoxycyclohexylmethyl+3+4-epoxycyclohexanecarb OR a816945 OR q19694494 OR 7-oxabicyclo+4+1+0+heptan-3-yl+methyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR 7-oxabicyclo+4+1+0+heptan-3-ylmethyl+7-oxabicyclo+4+1+0+heptane OR 7-Oxabicyclo+4+1+0+heptan-3-ylmethyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR 3+4-Epoxycyclohexylmethyl+3+4-epoxycyclohexanecarboxylate OR ERL-4221 OR UT-632 OR Chissonox+221+monomer OR UNII-S224DEL3P4 OR 3+4-Epoxycyclohexylmethyl+3+4-epoxycyclohexane+carboxylate OR HSDB+5873 OR 3+4-Epoxycyclohexyl+methyl+3+4-epoxycyclohexylcarboxylate OR EINECS+219-207-4 OR UT+632 OR 3+4-Epoxycyclohexanecarboxylic+acid+3+4-epoxycyclohexylmethyl+ester OR BRN+1381750 OR 7-Oxabicyclo+4+1+0+heptane-3-carboxylic+acid+7-oxabicyclo+4+1+0+hept-3-ylmethyl+ester OR S224DEL3P4 OR DTXSID2027466 OR 7-oxabicyclo+4+1+0+heptan-4-ylmethyl+7-oxabicyclo+4+1+0+heptane-4-carboxylate OR 3+4-Epoxycyclohexanemethyl+3+4-epoxycyclohexanecarboxylate OR AK-78714 OR DSSTox_CID_7466 OR 7-Oxabicyclo+4+1+0+hept-3-ylmethyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR DSSTox_RID_78463 OR DSSTox_GSID_27466 OR W-107371 OR 7-oxabicyclo+4+1+0+hept-3-ylmethyl7-oxabicyclo+4+1+0+heptane-3-carboxylate OR CAS-2386-87-0 OR CCRIS+8882 OR EC+219-207-4 OR 3+4-epoxycyclohexylmethyl3+4-epoxycyclo-hexaneca OR SCHEMBL24975 OR KSC490C3P OR CHEMBL2143072 OR CTK3J0137 OR BCP32770 OR CEL-2021 OR Tox21_202388 OR Tox21_303312 OR ANW-57541 OR AKOS015915254 OR KS-000001N6 OR NCGC00164163-01 OR NCGC00164163-02 OR NCGC00256981-01 OR NCGC00259937-01 OR AS-17792 OR LS-98670 OR SC-19925 OR DB-028268 OR FT-0651573 OR NS00011515 OR 3+4-Epoxycyclohexylmethyl+3+4-epoxycyclohexanecarb OR A816945 OR Q19694494 OR 3+4-epoxycyclohexylmethyl+3+4-epoxy+cyclohexanecarboxylate OR 3+4-epoxycyclohexylmethyl-3+4-epoxycyclohexane+carboxylate OR 7-Oxabicyclo+4+1+0+heptan-3-yl+methyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR 7-oxabicyclo+4+1+0+heptane-4-carboxylic+acid+7-oxabicyclo+4+1+0+heptan-4-ylmethyl+ester OR 7-Oxabicyclo+4+1+0+heptan-3-ylmethyl+7-oxabicyclo+4+1+0+heptane) AND (host)
Dicyclohexyl_phthalate	(dicyclohexyl+phthalate OR ergoplast+fdc OR unimoll+66 OR ergoplast.fdc OR howflex+cp OR phthalic+acid+dicyclohexyl+ester OR dicyclohexyl+benzene-1+2-dicarboxylate OR dicyclohexylphthalate OR hf+191 OR kp+201 OR 1+2-benzenedicarboxylic+acid+dicyclohexyl+ester OR unii-cgd15m7h2n OR nsc+6101 OR ccris+6190 OR hsdb+5246 OR diclohexyl+1+2-benzenedicarboxylate OR ai3-00515+usda OR einecs+201-545-9 OR brn+1889288 OR cgd15m7h2n OR ai3-00515 OR mls000736536 OR dtxsid5025021 OR chebi:34693 OR 1+2-benzenedicarboxylic+acid+1+2-dicyclohexyl+ester OR w-104111 OR morflex+150 OR unimoll+66+m OR uniplex+250 OR acmc-209pvy OR phthalic+acid+dicyclohexyl OR dsstox_cid_5021 OR ec+201-545-9 OR dsstox_rid_77631 OR dsstox_gsid_25021 OR schembl29302 OR ksc199e2t OR bidd:er0638 OR chembl3185893 OR nsc6101 OR ks-00000g0y OR nsc-6101 OR phthalic+acid+bis-cyclohexyl+ester OR zinc1693279 OR zx-at015572 OR tox21_303132 OR anw-37820 OR mfcd00003849 OR akos015840876 OR ls-1835 OR mcule-6607324429 OR or61028 OR cas-84-61-7 OR ncgc00257008-01 OR ak307696 OR cc-26567 OR ds-11413 OR smr000528061 OR db-056812 OR ft-0624741 OR ns00004690 OR p0293 OR st50319862 OR c14529 OR c-30080 OR q1210373 OR DICYCLOHEXYL+PHTHALATE OR Ergoplast+FDC OR Unimoll+66 OR Ergoplast.fdc OR Howflex+CP OR Phthalic+acid+dicyclohexyl+ester OR Dicyclohexyl+benzene-1+2-dicarboxylate OR Phthalic+Acid+Dicyclohexyl+Ester OR Dicyclohexylphthalate OR HF+191 OR KP+201 OR 1+2-Benzenedicarboxylic+acid+dicyclohexyl+ester OR UNII-CGD15M7H2N OR NSC+6101 OR CCRIS+6190 OR HSDB+5246 OR Diclohexyl+1+2-benzenedicarboxylate OR AI3-00515+USDA OR EINECS+201-545-9 OR BRN+1889288 OR CGD15M7H2N OR AI3-00515 OR MLS000736536 OR DTXSID5025021 OR CHEBI:34693 OR 1+2-Benzenedicarboxylic+acid+1+2-dicyclohexyl+ester OR W-104111 OR Morflex+150 OR Unimoll+66+M OR Uniplex+250 OR 1+dicyclohexyl+ester OR ACMC-209pvy OR Phthalic+acid+dicyclohexyl OR DSSTox_CID_5021 OR EC+201-545-9 OR DSSTox_RID_77631 OR DSSTox_GSID_25021 OR SCHEMBL29302 OR KSC199E2T OR BIDD:ER0638 OR CHEMBL3185893 OR NSC6101 OR KS-00000G0Y OR NSC-6101 OR Phthalic+acid+bis-cyclohexyl+ester OR ZINC1693279 OR ZX-AT015572 OR Tox21_303132 OR ANW-37820 OR MFCD00003849 OR AKOS015840876 OR LS-1835 OR MCULE-6607324429 OR OR61028 OR CAS-84-61-7 OR NCGC00257008-01 OR AK307696 OR CC-26567 OR DS-11413 OR SMR000528061 OR cyclohexyl+2-+cyclohexyloxycarbonyl+benzoate OR DB-056812 OR FT-0624741 OR NS00004690 OR P0293 OR ST50319862 OR C14529 OR C-30080 OR Q1210373) OR (proximity 3 AND CAS AND 84-61-7)
1_3-Bis_citraconimidomethylene_benzene	(1+3-bis+citraconimidomethylene+benzene OR 1+3-bis+3-methyl-2+5-dioxo-1h-pyrrolinylmethyl+benzene OR dtxsid0073081 OR bci-mx OR ec+412-570-1 OR acmc-1c2x7 OR schembl168682 OR ctk4b1334 OR zinc21993063 OR akos015904331 OR ft-0658961 OR ns00005991 OR 1+1+1+3-phenylenebis+methylene+bis+3-methyl-1h-pyrrole-2+5-dione OR 1h-pyrrole-2+5-dione+1+1+1+3-phenylenebis+methylene+bis+3-methyl- OR alpha+alpha+-bis+3z+-2+5-dioxo-3-methyl-3-pyrroline-1-yl+-m-xylene OR 1+3-Bis+citraconimidomethylene+benzene OR 1+3-bis+3-methyl-2+5-dioxo-1H-pyrrolinylmethyl+benzene OR DTXSID0073081 OR 1H-Pyrrole-2+5-dione+1+1+1+3-phenylenebis+methylene+bis+3-methyl- OR 3-methyl-1+3+3-methyl-2+5-dioxopyrrol-1-yl+methyl+phenyl+methyl+pyrrole-2+5-dione OR BCI-MX OR EC+412-570-1 OR ACMC-1C2X7 OR SCHEMBL168682 OR CTK4B1334 OR ZINC21993063 OR 1+3-bis+citraconimidomethyl+benzene OR AKOS015904331 OR FT-0658961 OR NS00005991 OR 1+1+1+3-Phenylenebis+methylene+bis+3-methyl-1H-pyrrole-2+5-dione OR 1H-Pyrrole-2+5-dione+1+1-+1+3-phenylenebis+methylene+bis+3-methyl- OR alpha+alpha+-Bis+3Z+-2+5-dioxo-3-methyl-3-pyrroline-1-yl+-m-

	xylene) OR ((proximity 20) AND (1+3-bis+citraconimidomethylene+benzene OR 1+3-bis+3-methyl-2+5-dioxo-1h-pyrrolinylmethyl+benzene OR dtxsid0073081 OR bci-mx OR ec+412-570-1 OR acmc-1c2x7 OR schembl168682 OR ctk4b1334 OR zinc21993063 OR akos015904331 OR ft-0658961 OR ns00005991 OR 1+1+1+3-phenylenebis+methylene+bis+3-methyl-1h-pyrrole-2+5-dione OR 1h-pyrrole-2+5-dione+1+1+1+3-phenylenebis+methylene+bis+3-methyl- OR alpha+alpha+bis+3z+2+5-dioxo-3-methyl-3-pyrroline-1-yl+m-xylene OR 1+3-Bis+citraconimidomethylene+benzene OR 1+3-bis+3-methyl-2+5-dioxo-1H-pyrrolinylmethyl+benzene OR 1h-pyrrole-2+5-dione+1+1+1+3-phenylenebis+methylene+bis+3-methyl OR 3-methyl-1+3+3-methyl-2+5-dioxopyrrol-1-yl+methyl+phenyl+methyl+pyrrole-2+5-dione OR 1+1+1+3-phenylenebis+methylene+bis+3-methyl-1H-pyrrole-2+5-dione) AND (host))
Tris_1_3-dichloro-2-propyl_phosphate	(tris+1+3-dichloro-2-propyl+phosphate OR tris+1+3-dichloroisopropyl+phosphate OR 2-propanol+1+3-dichloro-+phosphate+3:1 OR phosphoric+acid+tris+1+3-dichloro-2-propyl+ester OR fyrol+fr-2 OR 1+3-dichloro-2-propanol+phosphate+3:1 OR unii-b1prv4g0t0 OR tris+1-chloromethyl-2-chloroethyl+phosphate OR tris+2-chloro-1-+chloromethyl+ethyl+phosphate OR pf+38/3 OR ccris+6284 OR tri+beta+beta+-dichloroisopropyl+phosphate OR hsdb+4364 OR einecs+237-159-2 OR brn+1715458 OR b1prv4g0t0 OR fosforan+troj-+1+3-dwuchloroizopropylowy OR dtxsid9026261 OR 2-propanol+1+3-dichloro-+2+2+2+-phosphate OR fosforan+troj-+1+3-dwuchloroizopropylowy+polish OR dsstox_cid_6261 OR dsstox_rid_78078 OR dsstox_gsid_26261 OR fyrol+fr2 OR tris-+1+3-dichloro-2-propyl+-phosphate OR acmc-209c9q OR ec+237-159-2 OR ksc496a6h OR schembl333198 OR chembl3182032 OR ctk3j6063 OR chebi:143729 OR tris+1+3-dichlorisopropyl+phosphat OR ks-00000z7i OR zinc2019519 OR tox21_202166 OR tox21_300194 OR anw-20172 OR ls-798 OR akos015856734 OR cs-8011 OR tris+1.3-dichloro-2-propyl+phosphate OR tris-+1+3-dichloro-2-propyl+phosphate OR ncgc00247923-01 OR ncgc00247923-02 OR ncgc00254047-01 OR ncgc00259715-01 OR ak116066 OR ax8147868 OR hy-108712 OR ft-0654115 OR ns00010388 OR tris+1+3-dichlorisopropyl+phosphate OR tri+.beta.+.beta.+-dichloroisopropyl+phosphate OR a807122 OR j-006902 OR q2454085 OR Tris+1+3-dichloro-2-propyl+phosphate OR tris+1+3-dichloropropan-2-yl+phosphate OR TRIS+1+3-DICHLORO-2-PROPYL+PHOSPHATE OR Tris+1+3-dichloroisopropyl+phosphate OR 2-Propanol+1+3-dichloro-+phosphate+3:1 OR Phosphoric+Acid+Tris+1+3-dichloro-2-propyl+Ester OR Fyrol+FR-2 OR 1+3-Dichloro-2-propanol+phosphate+3:1 OR UNII-B1PRV4G0T0 OR Tris+1-chloromethyl-2-chloroethyl+phosphate OR Tris+2-chloro-1-+chloromethyl+ethyl+phosphate OR PF+38/3 OR CCRIS+6284 OR Tri+beta+beta+-dichloroisopropyl+phosphate OR HSDB+4364 OR EINECS+237-159-2 OR BRN+1715458 OR B1PRV4G0T0 OR Fosforan+troj-+1+3-dwuchloroizopropylowy OR DTXSID9026261 OR 2-Propanol+1+3-dichloro-+2+2+2+-phosphate OR Fosforan+troj-+1+3-dwuchloroizopropylowy+Polish OR Phosphoric+acid+tris+1+3-dichloro-2-propyl+ester OR DSSTox_CID_6261 OR DSSTox_RID_78078 OR DSSTox_GSID_26261 OR Fyrol+FR2 OR Tris-+1+3-dichloro-2-propyl+-phosphate OR ACMC-209c9q OR EC+237-159-2 OR KSC496A6H OR SCHEMBL333198 OR CHEMBL3182032 OR CTK3J6063 OR CHEBI:143729 OR tri+2+3-dichloropropyl+phosphate OR Tris+1+3-dichlorisopropyl+phosphat OR KS-00000Z7I OR ZINC2019519 OR Tox21_202166 OR Tox21_300194 OR ANW-20172 OR LS-798 OR AKOS015856734 OR CS-8011 OR Tris+1.3-dichloro-2-propyl+phosphate OR Tris-+1+3-dichloro-2-propyl+phosphate OR NCGC00247923-01 OR NCGC00247923-02 OR NCGC00254047-01 OR NCGC00259715-01 OR AK116066 OR AX8147868 OR HY-108712 OR FT-0654115 OR NS00010388 OR Tris+1+3-dichlorisopropyl+phosphate OR Tri+.beta.+.beta.+-dichloroisopropyl+phosphate OR tris+1+3-bis+chloranyl+propan-2-yl+phosphate OR A807122 OR J-006902 OR Q2454085 OR phosphoric+acid+tris+1+3-dichloropropan-2-yl+ester OR phosphoric+acid+tris-+2-chloro-1-chloromethyl-ethyl+ester) OR (proximity 3 AND CAS AND 13674-87-8)
Methyl_N-_3-acetylamino_-4-_2-cyano-4-nitrophenylazo_phenyl_-N-_1-methoxy_acetyl_glycinate	(dtxsid90889003 OR methyl+n-+3-acetylamino+-4-+2-cyano-4-nitrophenylazo+phenyl+-n-+1-methoxy+acetyl+glycinate OR glycine+n-+3-+acetylamino+-4-+2-+2-cyano-4-nitrophenyl+diazenyl+phenyl+-n-+2-methoxy-2-oxoethyl+-+methyl+ester OR acmc-20n5u8 OR ec+413-040-2 OR schembl14379275 OR schembl15886748 OR ctk4c6396 OR 3-+acetylamino+-4-2-cyano-4-nitrophenyl+azo+phenyl+imino+diacetic+acid+dimethyl+ester OR DTXSID90889003 OR methyl+N-+3-acetylamino+-4-+2-cyano-4-nitrophenylazo+phenyl+-N-+1-methoxy+acetyl+glycinate OR Glycine+N-+3-+acetylamino+-4-+2-+2-cyano-4-nitrophenyl+diazenyl+phenyl+-N-+2-methoxy-2-oxoethyl+-+methyl+ester OR ACMC-20n5u8 OR EC+413-040-2 OR SCHEMBL14379275 OR SCHEMBL15886748 OR CTK4C6396 OR 3-+acetylamino+-4-2-cyano-4-nitrophenyl+azo+phenyl+imino+diacetic+acid+dimethyl+ester) OR (proximity 3 AND CAS AND 149850-30-6)
Bis_2_6-diisopropylphenyl_carbodiimide	(bis+2+6-diisopropylphenyl+carbodiimide OR n+n+methanediylidenebis+2+6-diisopropylaniline OR carbo+d OR staboxol+1 OR unii-ypk27z98pl OR ypk27z98pl OR dtxsid5051862 OR einecs+218-487-5 OR n+n+bis+2+6-bis+propan-2-yl+phenyl+methanediimine OR 2+2+6+6+tetraisopropyldiphenylcarbodiimide OR carbodiimide+bis+2+6-diisopropylphenyl OR n+n+methanetetraylbis+2+6-bis+1-methylethyl+benzenamine OR benzenamine+n+n+-methanetetraylbis+2+6-bis+1-methylethyl OR maybridge1_004202 OR ksc496s8t OR schembl134760 OR ctk3j6989 OR hms553g24 OR zinc8637108 OR anw-24518 OR mfcd00082211 OR akos015915473 OR mcule-5666921352 OR ak114690 OR as- 72 OR ls-28354 OR sc-28722 OR sy035749 OR db-119014 OR ft-0654584 OR ns00007917 OR ec+218-487-5 OR a815542 OR w-109755 OR n+n+bis+2+6-di+propan-2-yl+phenyl+methanediimine OR q27894368 OR 2+6-diisopropylphenyl+carbodiimide OR n+n+-bis+2+6-diisopropylphenyl+carbodiimide OR bis+2+6-di-2-propylphenyl+carbodiimide) OR (proximity 3 AND CAS AND 2162-74-5)
Solvent_blue_4	(solvent+blue+4 OR dtxsid4064474 OR einecs+229-851-8 OR ec+229-851-8 OR schembl2390176 OR zinc31308564 OR sc-44514 OR ns00011486 OR 4-anilinonaphthalen-1-yl+bis+4+dimethylamino+phenyl+methanol OR alpha+alpha-bis+4+dimethylamino+phenyl+4+phenylamino+1-naphthalenemethanol OR α+α-bis+4+dimethylamino+phenyl+4+phenylamino+naphthalene-1-methanol OR Solvent+Blue+4 OR DTXSID4064474 OR EINECS+229-851-8 OR EC+229-851-8 OR SCHEMBL2390176 OR ZINC31308564 OR SC-44514 OR NS00011486 OR 4-anilino-1-naphthyl+bis+4+dimethylamino+phenyl+methanol OR 4-Anilinonaphthalen-1-yl+bis+4-+dimethylamino+phenyl+methanol OR 1-naphthalenamine+4+bis+4+dimethylamino+phenyl+methyl+n-phenyl+ OR 1-naphthalenemethanol+alpha+alpha-bis+4+dimethylamino+phenyl+4+phenylamino+ OR 1-naphthalenemethanol+α+α-bis+4+dimethylamino+phenyl+4+phenylamino+ OR a+a-bis+4+dimethylamino+phenyl+4+phenylamino+naphthalene-1-methanol OR alpha+alpha-bis+4+Dimethylamino+phenyl+4+phenylamino+1-naphthalenemethanol OR alpha+alpha-bis+4+dimethylamino+phenyl+4+phenylamino+naphthalene-1-methanol OR bis+4+dimethylamino+phenyl+4+phenylamino+naphthalen-1-yl+methanol OR

	bis+4+dimethylamino+phenyl+4+phenylamino+naphthalene-1-methanol OR α+α-Bis+4-+dimethylamino+phenyl+-4+phenylamino+naphthalene-1-methanol) OR (proximity 3 AND CAS AND 6786-83-0)
Retinyl_palmitate	(vitamin+a+palmitate OR retinol+palmitate OR retinol+hexadecanoate OR all-trans-retinyl+palmitate OR arovit OR optovit-a OR retinyl+hexadecanoate OR aquapalm OR dispatabs+tabs OR trans-retinyl+palmitate OR vitazyme+a OR optovit+a OR axerophthol+palmitate OR vitamin+a+solubilized OR trans-retinol+palmitate OR lutavit+a+500+plus OR o+15+-hexadecanoylretinol OR unii-1d1k0n0vvc OR all-trans-retinol+palmitate OR all-trans-vitamin+a+palmitate OR aquasol+a OR ccris+3280 OR retinol+palmitate+all-trans- OR einecs+201-228-5 OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethylcyclohexen-1-yl+nona-2+4+6+8-tetraenyl+hexadecanoate OR brn+1917366 OR 1d1k0n0vvc OR ester+found+in+fish+liver+oils OR retinol+all-trans-+palmitate OR chebi:17616 OR palmitic+acid+ester+with+retinol OR ncgc00095056-03 OR dsstox_cid_1241 OR dsstox_rid_76033 OR dsstox_gsid_21241 OR +2e+4e+6e+8e+-hexadecanoic+acid+3+7-dimethyl-9-+2+6+6-trimethyl-cyclohex-1-enyl+-nona-2+4+6+8+tetraenyl+ester OR retinyl+vitamin+a+palmitate OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-en-1-yl+nona-2+4+6+8-tetraen-1-yl+hexadecanoate OR smr000112463 OR palmitic+acid+retinol OR retinyl+palmitic+acid OR vitamin-+a+palmitate OR o+15+-palmitoylretinol OR retinyl+hexadecanoic+acid OR spectrum5_001201 OR ec+201-228-5 OR chembl1675 OR schembl41649 OR mls001332437 OR mls001332438 OR spectrum1503604 OR dtxsid1021241 OR hms500m11 OR all+trans-retinol+palmitate OR hms1922e10 OR hms2093g13 OR hms2268c06 OR pharmakon1600-01503604 OR hy-b1384 OR zinc8214494 OR tox21_113452 OR tox21_303008 OR ccg-39342 OR lmpr01090013 OR nsc758478 OR retinol+o+15+-+1-oxohexadecyl+- OR akos015918435 OR ls-2307 OR nsc-758478 OR idi1_000249 OR ncgc00095056-01 OR ncgc00095056-02 OR ncgc00256427-01 OR ac-20001 OR sc-15989 OR sbi-0051830.p002 OR cs-0013116 OR 2840-ep2305825a1 OR c02588 OR d00164 OR ab00052360_04 OR a839762 OR sr-05000001910 OR q7316807 OR sr-05000001910-1 OR 3+7-dimethyl-9-+2+6+6+-trimethyl-1-cyclohexen-1-yl+-2+4+6+8-nonatetraen-1-ol+palmitate OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethyl-cyclohex-en-1-yl+-2+4+6+8-nonateetraen-1-yl-palmitate OR +2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetraenyl+palmitate OR hexadecanoic+acid+2e+4e+6e+8e+-3+7-dimethyl-9-+2+6+6-trimethyl-1-cyclohexenyl+nona-2+4+6+8-tetraenyl+ester OR 3+7-dimethyl-9-2+6+6-trimethylcyclohexen-1-yl+nona-2+4+6+8-tetraenoyl+hexadecanoate OR retinyl+palmitate OR VITAMIN+A+PALMITATE OR all-trans-Retinyl+palmitate OR Arovit OR optovit-A OR Aquapalm OR vitazyme+A OR optovit+A OR Lutavit+A+500+Plus OR O+15+-hexadecanoylretinol OR UNII-1D1K0N0VVC OR all-trans-Retinol+palmitate OR all-trans-Vitamin+A+palmitate OR Aquasol+A OR CCRIS+3280 OR Retinol+palmitate+all-trans- OR EINECS+201-228-5 OR +2E+4E+6E+8E+-3+7-dimethyl-9-+2+6+6-trimethylcyclohexen-1-yl+nona-2+4+6+8-tetraenyl+hexadecanoate OR BRN+1917366 OR 1D1K0N0VVC OR Ester+found+in+fish+liver+oils OR Retinol+all-trans-+palmitate OR CHEBI+17616 OR Palmitic+acid+ester+with+retinol OR NCGC00095056-03 OR DSSTox_CID_1241 OR DSSTox_RID_76033 OR DSSTox_GSID_21241 OR +2E+4E+6E+8E+-Hexadecanoic+acid+3+7-dimethyl-9-+2+6+6-trimethyl-cyclohex-1-enyl+-nona-2+4+6+8+tetraenyl+ester OR Retinyl+Vitamin+A+Palmitate OR +2E+4E+6E+8E+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-en-1-yl+nona-2+4+6+8-tetraen-1-yl+hexadecanoate OR SMR000112463 OR retinol-palmitate OR Palmitic+acid+retinol OR Retinyl+palmitic+acid OR Vitamin-+A+palmitate OR O+15+-palmitoylretinol OR Retinyl+hexadecanoic+acid OR Spectrum5_001201 OR bmse000501 OR EC+201-228-5 OR CHEMBL1675 OR SCHEMBL41649 OR MLS001332437 OR MLS001332438 OR SPECTRUM1503604 OR all-trans-retinyl+hexadecanoate OR DTXSID1021241 OR HMS500M11 OR ALL+TRANS-RETINOL+PALMITATE OR HMS1922E10 OR HMS2093G13 OR HMS2268C06 OR Pharmakon1600-01503604 OR HY-B1384 OR ZINC8214494 OR Tox21_113452 OR Tox21_303008 OR CCG-39342 OR LMPR01090013 OR NSC758478 OR retinol+O+15+-+1-oxohexadecyl+- OR AKOS015918435 OR LS-2307 OR NSC-758478 OR IDI1_000249 OR NCGC00095056-01 OR NCGC00095056-02 OR NCGC00256427-01 OR AC-20001 OR SC-15989 OR SBI-0051830.P002 OR CS-0013116 OR 2840-EP2305825A1 OR C02588 OR D00164 OR AB00052360_04 OR A839762 OR SR-05000001910 OR Q7316807 OR SR-05000001910-1 OR 3+7-Dimethyl-9-+2+6+6+-trimethyl-1-cyclohexen-1-yl+-2+4+6+8-nonatetraen-1-ol+palmitate OR +2E+4E+6E+8E+-3+7-Dimethyl-9-+2+6+6-trimethyl-cyclohex-en-1-yl+-2+4+6+8-nonateetraen-1-yl-palmitate OR +2E+4E+6E+8E+-3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetraenyl+palmitate OR 1 67-62-4 OR hexadecanoic+acid+2E+4E+6E+8E+-3+7-dimethyl-9-+2+6+6-trimethyl-1-cyclohexenyl+nona-2+4+6+8-tetraenyl+ester OR 3+7-dimethyl-9-2+6+6-trimethylcyclohexen-1-yl+nona-2+4+6+8-tetraenoyl+hexadecanoate OR o+15+-hexadecanoylretinoic+acid) OR (proximity 3 AND CAS AND 79-81-2)
Melamine_3	(host) AND (melamine% OR melamin% OR 1+3+5-triazine-2+4+6-triamine OR isomelamine OR theoharn OR teoharn OR triaminotriazine OR hicophor+pr OR s-triazinetriamine OR 2+4+6-triamino-1+3+5-triazine OR yukamelamine OR pluragard OR cymel OR virset+656-4 OR 2+4+6-triamino-s-triazine OR spinflam+ml+94m OR 2+4+6-triaminotriazine OR pluragard+c+133 OR adk+stab+zs+27 OR mark+zs+27 OR dg+002+amine OR melamine+monomer OR nci-c50715 OR cyanurtriamide OR s-triazine+2+4+6-triamino- OR 1+3+5-triazine-2+4+6+1h+3h+5h+-triimine OR zs+27 OR unii-n3gp2ysd88 OR nsc+2130 OR dg+002 OR sym-triaminotriazine OR ccris+373 OR hsdb+2648 OR einecs+203-615-4 OR brn+0124341 OR n3gp2ysd88 OR ai3-14883 OR dtxsid6020802 OR chebi:27915 OR 1+3+5-triazine-2+4+6+1h+3h+5h+triimine OR sym+triaminotriazine OR 2+6-triaminotriazine OR 2+4+6-triamino-1+3+5-triazine+monomer OR dsstox_cid_802 OR 2+6-triamino-s-triazine OR melamine-13c3+15n3 OR ec+203-615-4 OR s-triazine+4+6-triamino- OR dsstox_rid_75795 OR dsstox_gsid_20802 OR schembl25853 OR bidd:er0287 OR chembl1231106 OR schembl12192199 OR ks-00000vsy OR melamine+metformin+impurity+d OR 1+5-triazine-2+4+6-triamine OR 2+6-triamino-1+3+5-triazine OR nsc2130 OR nsc8152 OR zinc897751 OR hy-y1117 OR nsc-2130 OR nsc-8152 OR wln:+t6n+cn+enj+bz+dz+fz OR tox21_200503 OR bbl000010 OR ls-469 OR mfcd00006055 OR sbb000053 OR stk378738 OR akos005448714 OR ccg-266105 OR mcule-1467355510 OR ncgc00164014-01 OR ncgc00164014-02 OR ncgc00258057-01 OR cas-108-78-1 OR st018511 OR vs-00405 OR 1+3+5-triazine-2+4+6-triamine+monomer OR cs-0016866 OR ft-0609833 OR ft-0670982 OR ft-0670983 OR melamine+1+3+5-triazine-2+4+6-triamine OR t6897 OR 1+3+5-triazine-2+4+6-triamine+melamine OR 1+5-triazine-2+4+6+1h+3h+5h+-triimine OR 4+6-diamino-1+2-dihydro-2-imino-s-triazine OR c08737 OR 78403-ep2270101a1 OR 78403-ep2270113a1 OR 78403-ep2272849a1 OR 78403-ep2272935a1 OR 78403-ep2276751a1 OR 78403-ep2289896a1 OR 78403-ep2298828a1 OR 78403-ep2301924a1 OR 78403-ep2301983a1 OR 78403-ep2308856a1 OR 78403-ep2374895a1 OR s-triazine+4+6-diamino-1+2-dihydro-2-imino- OR q212553 OR j-002191 OR cyanuramide OR cyanurotriamine OR cyanurotriamide OR melamine OR 1+3+5-Triazine-2+4+6-triamine OR Isomelamine OR Theoharn OR Teoharn OR Triaminotriazine

	OR Cyanuric+triamide OR Hicophor+PR OR s-Triazinetriamine OR 2+4+6-Triamino-1+3+5-triazine OR Yukamelamine OR Pluragard OR Cymel OR Virset+656-4 OR 2+4+6-Triamino-s-triazine OR Spinflam+ML+94M OR 2+4+6-Triaminotriazine OR Pluragard+C+133 OR ADK+Stab+ZS+27 OR Mark+ZS+27 OR DG+002+amine OR Melamine+Monomer OR NCI-C50715 OR Cyanurtriamide OR s-Triazine+2+4+6-triamino- OR 1+3+5-Triazine-2+4+6+1H+3H+5H+-triimine OR ZS+27 OR s-triaminotriazine OR UNII-N3GP2YSD88 OR NSC+2130 OR DG+002 OR sym-Triaminotriazine OR CCRIS+373 OR HSDB+2648 OR EINECS+203-615-4 OR 67297-95-4 OR BRN+0124341 OR N3GP2YSD88 OR 2+4+6-triamino+sym-triazine OR AI3-14883 OR DTXSID6020802 OR CHEBI:27915 OR 1+3+5-triazine-2+4+6+1H+3H+5H+triimine OR melamin OR cyan+urotriamide OR Sym+Triaminotriazine OR 2+6-Triaminotriazine OR 2+4+6-Triamino-1+3+5-triazine+Monomer OR DSSTox_CID_802 OR 2+6-Triamino-s-triazine OR Melamine-13C3+15N3 OR EC+203-615-4 OR s-Triazine+4+6-triamino- OR DSSTox_RID_75795 OR DSSTox_GSID_20802 OR SCHEMBL25853 OR BIDD:ER0287 OR CHEMBL1231106 OR SCHEMBL12192199 OR KS-00000VSY OR Melamine+Metformin+Impurity+D OR 1+5-Triazine-2+4+6-triamine OR 2+6-Triamino-1+3+5-triazine OR NSC2130 OR NSC8152 OR ZINC897751 OR HY-Y1117 OR NSC-2130 OR NSC-8152 OR WLN: +T6N+CN+ENJ+BZ+DZ+FZ OR Tox21_200503 OR 1+3+5-triazinane-2+4+6-triimine OR BBL000010 OR LS-469 OR MFCD00006055 OR s9212 OR SBB000053 OR STK378738 OR AKOS005448714 OR CCG-266105 OR MCULE-1467355510 OR NCGC00164014-01 OR NCGC00164014-02 OR NCGC00258057-01 OR 1246816-14-7 OR 94977-27-2 OR CAS-108-78-1 OR ST018511 OR VS-00405 OR 1+3+5-Triazine-2+4+6-triamine+monomer OR CS-0016866 OR FT-0609833 OR FT-0670982 OR FT-0670983 OR Melamine+1+3+5-Triazine-2+4+6-triamine OR T6897 OR 1+3+5-Triazine-2+4+6-triamine+Melamine OR 1+5-Triazine-2+4+6+1H+3H+5H+-triimine OR 4+6-Diamino-1+2-dihydro-2-imino-S-Triazine OR C08737 OR 78403-EP2270101A1 OR 78403-EP2270113A1 OR 78403-EP2272849A1 OR 78403-EP2272935A1 OR 78403-EP2276751A1 OR 78403-EP2289896A1 OR 78403-EP2298828A1 OR 78403-EP2301924A1 OR 78403-EP2301983A1 OR 78403-EP2308856A1 OR 78403-EP2374895A1 OR s-Triazine+4+6-diamino-1+2-dihydro-2-imino- OR Q212553 OR J-002191 OR cyanuric+triamide OR Cyanuramide OR Cyanurotriamine OR Cyanurotriamide)
Retinol_5	(host) AND (retinol OR vitamin+a OR vitamin+a1 OR alphalin OR axerophthol OR afaxin OR oleovitamin+a OR chocola+a OR alphasterol OR apostavit OR aquasynth OR biosterol OR epiteliol OR ophthalamin OR agiolan OR agoncal OR anatola OR myvpack OR prepalin OR testavol OR veroftal OR aoral OR apexol OR avibon OR avitol OR axerol OR dofsol OR vaflol OR vitpex OR vogan OR isatabs+tabs OR bentavit+a OR dohyfral+a OR alcovit+a OR anatola+a OR vogan-neu OR a-mulsal OR plivit+a OR vi-alpha OR a-vitan OR atars OR vafol OR retrovitamin+a OR homagenets+aoral OR hi-a-vita OR sehkraft+a OR a-vi-pel OR vi-dom-a OR super+a OR solu-a OR nio-a-let OR vio-a OR antixerophthalmic+vitamin OR del-vi-a OR vitavel+a OR axerophtholum OR thalasphere OR wachstumsvitamin OR vitaminum+a OR vitamine+a OR vitavel-a OR retinolum OR antixerophthalmisches+vitamin OR unii-g2sh0xkk91 OR beta.-retinol OR beta-retinol OR ccris+5444 OR hsdb+815 OR einecs+200-683-7 OR chembl986 OR nsc+122759 OR brn+0403040 OR g2sh0xkk91 OR 2e+4e+6e+8e+3+7-dimethyl-9+2+6+6-trimethylcyclohexen-1-yl+nona-2+4+6+8-tetraen-1-ol OR all-e+3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetraen-1-ol OR 2+4+6+8-nonatetraen-1-ol+3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl% OR chebi:17336 OR 3+7-dimethyl-9+2+6+6-trimethyl-1-cyclchexen-1-yl+2+4+6+8-nonatetraen-1-ol OR 2e+4e+6e+8e+3+7-dimethyl-9+2+6+6-trimethylcyclohex-1-en-1-yl+nona-2+4+6+8-tetraen-1-ol OR nsc-122759 OR ncgc00017343-07 OR cylasphere OR retinolo OR dsstox_cid_3556 OR hydrovit+a OR 3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonate-traen-1-ol OR alcohol+9+13-dimethyl-7+1+1+5-trimethyl-6-cyclohexen-5-yl+7+9+11+13-nonatetraen-15-ol OR dsstox_rid_77080 OR dsstox_gsid_23556 OR ro-a-vit OR q-201926 OR w-104683 OR aquasol+a+parenteral OR rovimix+a OR 2e+4e+6e+8e+3+7-dimethyl-9+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetr+aen-1-ol OR smr000112036 OR 11+12-3h+-retinol OR 9-cis+13-cis-retinol OR sr-0 0763813 OR tegosphere+vita OR alpha.sterol OR alpha.lin OR retinyl+a OR trans-retinol+acid+vitamin+a OR einecs+234-328-2 OR mfcd00001552 OR pubchem18446 OR spectrum5_000993 OR spectrum5_001997 OR ec+200-683-7 OR schembl3112 OR all-trans-3+7-dimethyl-9-+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetraen-1-ol OR bidd:pxr0102 OR mls001066379 OR mls001074751 OR mls0060 08 OR spectrum1501203 OR gtpl4053 OR dtxsid3023556 OR hms501i08 OR hms1921b04 OR hms2092l13 OR hms2270c05 OR bcp06593 OR hy-b1342 OR zinc3831417 OR tox21_110818 OR tox21_202441 OR tox21_300287 OR bdbm50092056 OR bg0050 OR ccg-38864 OR lmpr01090001 OR nsc122759 OR nsc758150 OR akos015902578 OR db00162 OR nsc-758150 OR sdccgmls-0066724.p001 OR idi1_000486 OR smp2_000102 OR ncgc00017343-02 OR ncgc00017343-03 OR ncgc00017343-04 OR ncgc00017343-05 OR ncgc00017343-06 OR ncgc00017343-08 OR ncgc00017343-09 OR ncgc00017343-11 OR ncgc00091784-01 OR ncgc00091784-02 OR ncgc00091784-03 OR ncgc00091784-04 OR ncgc00091784-05 OR ncgc00091784-06 OR ncgc00254024-01 OR ncgc00259990-01 OR ac-11701 OR bs-17906 OR cc-35617 OR cc-35618 OR sc-61936 OR sc-75819 OR st057232 OR sbi-0051690.p002 OR cs-0013091 OR ns00003017 OR 33563-ep2272846a1 OR 33563-ep2277869a1 OR 33563-ep2277870a1 OR 33563-ep2281813a1 OR 33563-ep2284174a1 OR 33563-ep2292608a1 OR 33563-ep2301936a1 OR 33563-ep2311820a1 OR 33563-ep2374791a1 OR ab00052248_05 OR sr-0 0763813-2 OR sr-0 0763813-4 OR brd-k22429181-001-06-8 OR brd-k64634304-001-01-5 OR phenol+2+aminomethyl+5-fluoro+hydrochloride% OR 3+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetraen-1-ol OR 2+6+8-nonatetraen-1-ol+3+7dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl% OR 3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetraen-1-ol% OR 2e+4e+6e+8e+3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexenyl+1-nona-2+4+6+8-tetraenol OR 2e+4e+6e+8e+3+7-dimethyl-9-+2+6+6-trimethyl-1-cyclohexenyl+nona-2+4+6+8-tetraen-1-ol OR 2e+4e+6e+8e+3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetraen-1-ol OR 2z+4z+6z+8z+3+7-dimethyl-9-+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetren-1-ol) NOT skin

Paracetamol_6	((proximity 20) AND (acetaminophen OR paracetamol OR 4-acetamidophenol OR n+4-hydroxyphenyl+acetamide OR n-acetyl-p-aminophenol OR p-hydroxyacetanilide OR 4+hydroxyacetanilide OR p-acetamidophenol OR p-acetaminophenol OR p-acetylaminophenol OR acetamide+n+4-hydroxyphenyl OR 4+acetylamino+phenol OR 4-acetaminophenol OR n-acetyl-4-aminophenol OR acetanilide+4+hydroxy OR p-hydroxyphenolacetamide OR 4-hydroxyacetanilide OR acetamide+n+p-hydroxyphenyl OR p+acetylamino+phenol OR acetaminophene OR n+4-hydroxyphenyl+acetanilide OR n-acetyl-4-hydroxyaniline OR 4-acetylaminophenol OR n+4-hydroxyphenyl+ethanamide OR phenol+p-acetamido OR n-acetyl-para-aminophenol OR 4-+n-acetylamino+phenol OR acetaminophen+4 OR hydroxyacetanilide OR hydroxyphenyl+acetamide+tylenol OR 4-acetominophenol OR 4-acetamido+phenol OR 4-acetamido-phenol OR 4-acetamino+phenol OR p-hydroxy-acetanilid OR p-hydroxyacetoanilide OR para-acetylaminophenol OR n-acetyl-4-hydroxyaniline; OR n+4-hydroxyfenyl+ethanamid) AND (host) NOT (vaccine% OR covid% OR vaccination)) OR ((proximity 20) AND (acetaminophen OR paracetamol OR 4-acetamidophenol OR tylenol OR n-+4-hydroxyphenyl+acetamide OR panadol OR acetaminofen OR datril OR n-acetyl-p-aminophenol OR p-hydroxyacetanilide OR 4+-hydroxyacetanilide OR p-acetamidophenol OR algotropyl OR lonarid OR naprinol OR p-acetaminophenol OR acamol OR acenol OR anelix OR multin OR abensanil OR acetagesic OR acetalgin OR clixodyne OR gelocatil OR injectapap OR liquagesic OR pyrinazine OR servigesic OR alvedon OR anaflon OR apamide OR dymadon OR febridol OR febrilix OR febrolin OR finimal OR homoolan OR lestemp OR paracet OR tabalgin OR tralgon OR tussapap OR valadol OR valgesic OR alpiny OR amadil OR anhiba OR calpol OR dirox OR eneril OR fendon OR hedex OR lyteca OR pacemo OR panets OR parmol OR tapar OR tempra OR paracetamolo OR doliprane OR dolprone OR momentum OR ortensan OR paldesic OR banesin OR captin OR disprol OR enelfa OR neopap OR salzone OR exdol OR p-acetylaminophenol OR febro-gesic OR acetamide+n-+4-hydroxyphenyl+- OR biocetamol OR dafalgan OR dolgesic OR elixodyne OR febrectal OR tempanal OR vermidon OR abenol OR apacet OR apadon OR cetadol OR fensum OR janupap OR minoset OR napafen OR neodol OR nobedon OR pacemol OR panodil OR parapan OR pedric OR phendon OR rounox OR suppap OR korum OR pinex OR temlo OR 4-+acetylamino+phenol OR ben-u-ron OR dial-a-gesic OR anacin OR calmanticold OR codoliprane OR demogripal OR dolegrippin OR doloreduct OR dristancito OR duracetamol OR grippostad OR gynospasmine OR medocodene OR paedialgon OR paracetamolum OR paracetanol OR parakapton OR pediapirin OR phenipirin OR phogoglandin OR predualito OR sanicopyrine OR scentalgyl OR sunetheton OR tachiprina OR termalgine OR treuphadol OR abrolet OR acertol OR acetaco OR acetamol OR acetofen OR afebrin OR afebryl OR aferadol OR algesidal OR algomol OR alpinyl OR analter OR antidol OR apitrelal OR atralidon OR babikan OR bacetamol OR cadafen OR calapol OR causalon OR cefalex OR codabrol OR codalgin OR codapane OR codicet OR codisal OR cofamol OR cosutone OR cuponol OR curadon OR custodial OR darocet OR daygrip OR deminofen OR democyl OR desfebre OR dimindol OR dolefin OR dolofugin OR dolorfug OR dolorstop OR dolotec OR dorocoff OR dularin OR durapan OR ecosetol OR excipain OR fanalgic OR farmadol OR febranine OR febrectol OR febricet OR febrinol OR fepanil OR finiweh OR fluparmol OR geluprane OR ildamol OR inalgex OR infadrops OR kataprin OR labamol OR lekadol OR lemgrip OR lupocet OR magnidol OR malidens OR maxadol OR mexalen OR minafen OR miralgin OR nealgyl OR neodolito OR neotrend OR neuridon OR nodolex OR oralgan OR oxycocet OR pacimol OR panacete OR panadeine OR panadiene OR panaleve OR panamax OR panasorbe OR panofen OR pantalgin OR paracemol OR paracenol OR paracetol OR paracin OR paracod OR paracodol OR parador OR paradrops OR paralen OR paralief OR paralink OR paralyoc OR paramol OR paramolan OR paranox OR parasedol OR parasin OR paraspen OR parcetol OR parogal OR pediatrix OR piramin OR pirinasol OR polmofen OR predimol OR prontina OR puernol OR pulmofen OR pyrigesic OR pyromed OR remedol OR rivalgyl OR rubophen OR rupemol OR sanicet OR schmerzex OR sedalito OR semolacin OR seskamol OR setakop OR setamol OR sifenol OR sinaspril OR sinedol OR stanback OR stopain OR supofen OR tazamol OR termacet OR termalgin OR termofren OR titralgan OR tricoton OR upsanol OR utragin OR veralgina OR viruflu OR vivimed OR zatinol OR abrol OR algina OR anapap OR andox OR arfen OR asetam OR asomal OR aspac OR asplin OR benmyo OR curpol OR dhamol OR dolcor OR dolko OR dresan OR dypap OR febrex OR febrin OR lemsip OR malgis OR noral OR oltyl OR paceco OR pacet OR paedol OR painex OR pamol OR panex OR parake OR paroma OR plicet OR prodol OR reliv OR scanol OR setol OR sinmol OR tiffy OR tylex OR tylol OR tymol OR verpol OR volpan OR zolben OR neocitran OR nilnocen OR rubiemol OR supadol+mono OR treupel+mon OR bickie-mol OR fortalidon+p OR gattaphen+t OR gripin+bebe OR influbene+n OR lonarid+mono OR lyteca+syrup OR panadeine+co OR dymadon+co OR toximer+p OR treupel+n OR accu-tap OR 4-acetaminophenol OR helon+n OR malex+n OR spalt+n OR tylex+cd OR n-acetyl-4-aminophenol OR paracetamole OR conacetol OR darvocet OR empracet OR panasorb OR perfalgan OR apamid OR duaneo OR duorol OR ofirmev OR parelan OR prompt OR vicodin OR fevor OR freka-cetamol OR codisal+forte OR dolorol+forte OR dymadon+forte OR junior+disprol OR kinder+finimal OR liquigesic OR mono+praecimed OR percocet-demi OR perdolan+mono OR rockamol+plus OR viclor+richet OR actifed+plus OR kratofin+simplex OR neo-fepramol OR paracetamol+al OR paracetamol+bc OR paracetamol+pb OR acetanilide+4+-hydroxy- OR claradol+codeine OR geralgine-p OR melabon+infantil OR migraleve+yellow OR paracetamol+saar OR pyregesic-c OR anti-algos OR para-suppo OR pasolind+n OR supramol-m OR fever+all OR no-febril OR panado-co OR dol-stop OR anadin+dla+dzieci OR p-hydroxyphenolacetamide OR percocet-5 OR cod-acamol+forte OR contra-schmerz+p OR hy-phen OR medinol+paediatric OR paracetamol+basics OR panado-co+caplets OR paracetamol+von+ct OR paracetamol+fecofar OR paracetamol+harkley OR paracetamol+heumann OR paracetamol+nycomed OR codral+pain+relief OR paracetamol+hanseler OR paracetamol+winthrop OR 4-hydroxyacetanilide OR phenaphen+w/codeine OR capital+with+codeine OR acetominophen OR paracetamol+genericon OR anexsia OR demilets OR endecon OR intensin OR naldegesic OR propacet OR resfenol OR theraflu OR wygesic OR coricidin+sinus OR sudafed+sinus OR coricidin+d OR dafalgan+codeine OR acetamide+n-+p-hydroxyphenyl+- OR aspirin-free+anacin OR nci-c55801 OR tylenol+allergy+sinus OR p-+acetylamino+phenol OR rhinex+d-lay+tablets OR acetaminophene OR midol+regular+strength OR paracetamol+smithkline+beecham OR scherzatabletten+rezeptur+534 OR paracetamolo+italian OR percogesic+with+codeine OR 4-hydroxyanilid+kyseliny+octove OR acenol+pharmaceutical OR bayer+select+head+cold OR n-+4-hydroxyphenyl+acetanilide OR drixoral+sinus OR paracetamol+inn:ban OR ccris+3 OR n-acetyl-4-hydroxyaniline OR bayer+select+allergy-sinus OR bayer+select+headache+pain OR dristan+cold+no+drowsiness OR paracetamolum+inn-latin OR prestwick_13 OR st+joseph+aspirin-free+for+children OR unii-362o9itl9d OR 4-acetylaminophenol OR children+s+acetaminophen+elixir+drops OR children+s+acetaminophen+oral+solution OR midol+pm+night+time+formula OR tavist+allergy/sinus/headache OR triaminic+sore+throat+formula OR n-+4-hydroxyphenyl+ethanamide OR bayer+select+sinus+pain+relief OR drixoral+cold+&+flu OR phenol+p-acetamido-OR sine-off+sinus+medicine+caplets OR chebi:46195 OR hsdb+3001 OR roxicet+5/500 OR tocris-1706 OR n-acetyl-para-aminophenol OR 4-+n-acetylamino+phenol OR acetaminophen+4-hydroxyacetanilide OR bayer+select+menstrual+multi-symptom OR einecs+203-157-5 OR 222+af OR mfcd00002328 OR 4-acetamidophenol+98% OR st.+joseph+cold+tablets+for+children OR chembl112 OR nsc+109028 OR n-+4-hydroxyphenyl+acetamide+tylenol OR 4-hydroxyanilid+kyseliny+octove+czech OR

	children+s+acetaminophen+elixir+solution OR n-+4-hydroxyphenyl+-acetamide OR 362o9itl9d OR anexsia+10/660 OR aminofen OR dtxsid2020006 OR atasol OR component+of+dialog OR component+of+dilone OR nsc-3991 OR component+of+endecon OR component+of+percocet OR nsc-109028 OR component+of+phenaphen OR tyl OR component+of+percogesic OR dsstox_cid_6 OR ncgc00016361-07 OR actamin OR cas-103-90-2 OR pasolind OR redutemp OR robigesic OR valorin OR aceta+elixir OR wln+qr+dmv1 OR dsstox_rid_75318 OR dsstox_gsid_20006 OR component+of+hycomine+compound OR acetavance OR arthralgen OR anuphen OR calonal OR flexsure OR liqiprine OR aceta+tablets OR d+oliprane OR valorin+extra OR panale+ve OR ty+lenol OR snaplets-fr OR oraphen-pd OR phenaphen+caplets OR tylenol+caplet OR tylenol+geltab OR tylenol+8-hour OR smr000112065 OR dapa+x-s OR acetaminophen+usp OR sr-0 0597517 OR acetaminophen+usp:jan OR paracetamol+acetaminophen OR acetaminophenol OR acetominophene OR claratal OR daphalgan OR resprin OR calpol+infant OR daga OR apacet+capsules OR atasol+caplets OR atasol+tablets OR tempra+caplets OR tylenol+caplets OR tylenol+elixir OR tylenol+gelcaps OR tylenol+tablets OR actamin+extra OR actamin+super OR aminofen+max OR apacet+elixir OR atasol+drops OR exdol+strong OR p-acetoaminophen OR tempra+drops OR tempra+syrup OR tylenol+drops OR alpha-per OR citramon+p OR excedrin+caplets OR dial-alpha-gesic OR apo-acetaminophen OR 4-acetominophenol OR genebs+x-tra OR paracetamol;tylenol OR 4-acetamido+phenol OR 4-acetamido-phenol OR tempra+d.s OR 4-acetamino+phenol OR apap+paracetamol OR acetaminophen+650 OR p-hydroxy-acetanilid OR p-hydroxyacetoanilide OR paracetamol+inn OR proxyphene/acetamine OR tylenol+tn OR supac+salt/mix OR tylox+salt/mix OR zydone+salt/mix OR atasol+forte+caplets OR atasol+forte+tablets OR atasol+oral+solution OR para-acetylaminophenol OR anexsia+salt/mix OR endecon+salt/mix OR sinubid+salt/mix OR talacen+salt/mix OR vicodin+salt/mix OR wygesic+salt/mix OR acetaminophen+uniserts OR datril+extra-strength OR tylenol+infants+drops OR demilets+salt/mix OR empracet+salt/mix OR intensin+salt/mix OR propacet+salt/mix OR suppap-120 OR suppap-325 OR suppap-650 OR amodiaquine+impurity+b OR panadol+extra+strength OR theraflu+salt/mix OR coricidin+salt/mix OR liquiprin+salt/mix OR hy-phen+salt/mix OR iv-apap OR phenol+derivative+11 OR pubchem17726 OR spectrum_000016 OR tempra+chewable+tablets OR naldegesic+salt/mix OR actimol+chewable+tablets OR feverall+junior+strength OR darvocet-n+salt/mix OR anacin-3+extra+strength OR liquiprin+infants+drops OR n-acetyl+para+aminophenol OR prestwick0_000868 OR prestwick1_000868 OR prestwick2_000868 OR prestwick3_000868 OR spectrum2_000085 OR spectrum3_000283 OR spectrum4_000140 OR spectrum5_000736 OR coricidin+d+salt/mix OR quiet+world+salt/mix OR genapap+children+s+elixir OR tylenol+children+s+elixir OR actifed+plus+salt/mix OR acetaminophen+paracetamol OR epitope+id:117710 OR genapap+children+s+tablets OR sudafed+sinus+salt/mix OR acetaminophen+paracetemol OR ec+203-157-5 OR actimol+infants+suspension OR drixoral+sinus+salt/mix OR liquiprin+children+s+elixir OR n-acetyl-4-hydroxyaniline; OR schembl3480 OR acetaminophen+jp17/usp OR coricidin+sinus+salt/mix OR n-+4-hydroxyfenyl+ethanamid OR bspbio_000915 OR bspbio_001786 OR dds-06a OR kbiogr_000560 OR kbioss_000356 OR 4-13-00-01091+beilstein+handbook+reference OR actimol+children+s+suspension OR apacet+extra+strength+caplets OR apacet+extra+strength+tablets OR aspirin-free+excedrin+caplets OR genebs+extra+strength+caplets OR ksc492k1n OR mls001146925 OR mls001331684 OR mls002154041 OR bidd:gt0005 OR divk1c_000660 OR spectrum1500101 OR genapap+extra+strength+caplets OR genapap+extra+strength+tablets OR spbio_000010 OR spbio_002836 OR tapanol+extra+strength+caplets OR tapanol+extra+strength+tablets OR tylenol+extra+strength+caplets OR tylenol+extra+strength+gelcaps OR tylenol+extra+strength+tablets OR acmc-20989w OR actimol+junior+strength+caplets OR apacet+regular+strength+tablets OR bpbio1_00 7 OR excedrin+extra+strength+caplets OR genebs+regular+strength+tablets OR gtpl5239 OR panadol+junior+strength+caplets OR sgcut00014 OR tylenol+junior+strength+caplets OR midol+teen+formula+salt/mix OR genapap+regular+strength+tablets OR panadol+maximum+strength+caplets OR panadol+maximum+strength+tablets OR schembl19474893 OR tylenol+regular+strength+caplets OR tylenol+regular+strength+tablets OR aspirin-free+anacin+salt/mix OR bdbm26197 OR ctk3j2516 OR hms502a22 OR kbio1_000660 OR kbio2_000356 OR kbio2_002924 OR kbio2_005492 OR kbio3_001286 OR ebd5728 OR nsc3991 OR tylenol+arthritis+extended+relief OR acetaminophen+analytical+standard OR ninds_000660 OR tylenol+infants+suspension+drops OR bcpp000441 OR drixoral+cold+&+flu+salt/mix OR hms1570n17 OR hms1920a03 OR hms2091g03 OR hms2097n17 OR hms2269g20 OR hms3268a10 OR hms3412d16 OR hms3676d16 OR hms3714n17 OR ls-32 OR pharmakon1600-01500101 OR tylenol+allergy+sinus+salt/mix OR midol+regular+strength+salt/mix OR act06727 OR bcp23431 OR ks-000002nn OR nsc+3991 OR str00901 OR to_000023 OR tylenol+children+s+chewable+tablets OR acetaminophen+bioxtra+>=99.0% OR bayer+select+head+cold+salt/mix OR robitussin+night+relief+salt/mix OR tox21_110397 OR tox21_201930 OR tox21_300 OR anw-14994 OR bbl005229 OR ccg-38901 OR nsc109028 OR nsc755853 OR sbb043758 OR stl140694) AND (toxic% OR risk% OR hazard%) AND (drug OR analgesic OR tablet OR pill OR prescription) AND (host) NOT(vaccine% OR vaccination OR covid%))
Bisphenol_A_4	(host) AND (bısfenol% OR bizfenol% OR bifenol% OR bisfenoli% OR bisphénol% OR bisfenole% OR bisfenol% OR bisfenolo% OR ビスフェノール% OR טנוברקילופב OR 双酚% OR Бисфенол% OR Бисфенолот% OR bisphenol%) NOT (BPA+free OR BPA+%+free OR free+BPA OR free+%+BPA OR free+%+%+BPA)

Melamine_4	(proximity 20) AND (host) AND (melamine% OR melamin% OR 1+3+5-triazine-2+4+6-triamine OR isomelamine OR theoharn OR teoharn OR triaminotriazine OR hicophor+pr OR s-triazinetriamine OR 2+4+6-triamino-1+3+5-triazine OR yukamelamine OR pluragard OR cymel OR virset+656-4 OR 2+4+6-triamino-s-triazine OR spinflam+ml+94m OR 2+4+6-triaminotriazine OR pluragard+c+133 OR adk+stab+zs+27 OR mark+zs+27 OR dg+002+amine OR melamine+monomer OR nci-c50715 OR cyanurtriamide OR s-triazine+2+4+6-triamino- OR 1+3+5-triazine-2+4+6+1h+3h+5h+-triimine OR zs+27 OR unii-n3gp2ysd88 OR nsc+2130 OR dg+002 OR sym-triaminotriazine OR ccris+373 OR hsdb+2648 OR einecs+203-615-4 OR brn+0124341 OR n3gp2ysd88 OR ai3-14883 OR dtxsid6020802 OR chebi:27915 OR 1+3+5-triazine-2+4+6+1h+3h+5h+triimine OR sym+triaminotriazine OR 2+6-triaminotriazine OR 2+4+6-triamino-1+3+5-triazine+monomer OR dsstox_cid_802 OR 2+6-triamino-s-triazine OR melamine-13c3+15n3 OR ec+203-615-4 OR s-triazine+4+6-triamino- OR dsstox_rid_75795 OR dsstox_gsid_20802 OR schembl25853 OR bidd:er0287 OR chembl1231106 OR schembl12192199 OR ks-00000vsy OR melamine+metformin+impurity+d OR 1+5-triazine-2+4+6-triamine OR 2+6-triamino-1+3+5-triazine OR nsc2130 OR nsc8152 OR zinc897751 OR hy-y1117 OR nsc-2130 OR nsc-8152 OR wln:+t6n+cn+enj+bz+dz+fz OR tox21_200503 OR bbl000010 OR ls-469 OR mfcd00006055 OR sbb000053 OR stk378738 OR akos005448714 OR ccg-266105 OR mcule-1467355510 OR ncgc00164014-01 OR ncgc00164014-02 OR ncgc00258057-01 OR cas-108-78-1 OR st018511 OR vs-00405 OR 1+3+5-triazine-2+4+6-triamine+monomer OR cs-0016866 OR ft-0609833 OR ft-0670982 OR ft-0670983 OR melamine+1+3+5-triazine-2+4+6-triamine OR t6897 OR 1+3+5-triazine-2+4+6-triamine+melamine OR 1+5-triazine-2+4+6+1h+3h+5h+-triimine OR 4+6-diamino-1+2-dihydro-2-imino-s-triazine OR c08737 OR 78403-ep2270101a1 OR 78403-ep2270113a1 OR 78403-ep2272849a1 OR 78403-ep2272935a1 OR 78403-ep2276751a1 OR 78403-ep2289896a1 OR 78403-ep2298828a1 OR 78403-ep2301924a1 OR 78403-ep2301983a1 OR 78403-ep2308856a1 OR 78403-ep2374895a1 OR s-triazine+4+6-diamino-1+2-dihydro-2-imino- OR q212553 OR j-002191 OR cyanuramide OR cyanurotriamine OR cyanurotriamide OR melamine OR 1+3+5-Triazine-2+4+6-triamine OR Isomelamine OR Theoharn OR Teoharn OR Triaminotriazine OR Cyanuric+triamide OR Hicophor+PR OR s-Triazinetriamine OR 2+4+6-Triamino-1+3+5-triazine OR Yukamelamine OR Pluragard OR Cymel OR Virset+656-4 OR 2+4+6-Triamino-s-triazine OR Spinflam+ML+94M OR 2+4+6-Triaminotriazine OR Pluragard+C+133 OR ADK+Stab+ZS+27 OR Mark+ZS+27 OR DG+002+amine OR Melamine+Monomer OR NCI-C50715 OR Cyanurtriamide OR s-Triazine+2+4+6-triamino- OR 1+3+5-Triazine-2+4+6+1H+3H+5H+-triimine OR ZS+27 OR s-triaminotriazine OR UNII-N3GP2YSD88 OR NSC+2130 OR DG+002 OR sym-Triaminotriazine OR CCRIS+373 OR HSDB+2648 OR EINECS+203-615-4 OR 67297-95-4 OR BRN+0124341 OR N3GP2YSD88 OR 2+4+6-triamino+sym-triazine OR AI3-14883 OR DTXSID6020802 OR CHEBI:27915 OR 1+3+5-triazine-2+4+6+1H+3H+5H+triimine OR melamin OR cyan+urotriamide OR Sym+Triaminotriazine OR 2+6-Triaminotriazine OR 2+4+6-Triamino-1+3+5-triazine+Monomer OR DSSTox_CID_802 OR 2+6-Triamino-s-triazine OR Melamine-13C3+15N3 OR EC+203-615-4 OR s-Triazine+4+6-triamino- OR DSSTox_RID_75795 OR DSSTox_GSID_20802 OR SCHEMBL25853 OR BIDD:ER0287 OR CHEMBL1231106 OR SCHEMBL12192199 OR KS-00000VSY OR Melamine+Metformin+Impurity+D OR 1+5-Triazine-2+4+6-triamine OR 2+6-Triamino-1+3+5-triazine OR NSC2130 OR NSC8152 OR ZINC897751 OR HY-Y1117 OR NSC-2130 OR NSC-8152 OR WLN:+T6N+CN+ENJ+BZ+DZ+FZ OR Tox21_200503 OR 1+3+5-triazinane-2+4+6-triimine OR BBL000010 OR LS-469 OR MFCD00006055 OR s9212 OR SBB000053 OR STK378738 OR AKOS005448714 OR CCG-266105 OR MCULE-1467355510 OR NCGC00164014-01 OR NCGC00164014-02 OR NCGC00258057-01 OR 1246816-14-7 OR 94977-27-2 OR CAS-108-78-1 OR ST018511 OR VS-00405 OR 1+3+5-Triazine-2+4+6-triamine+monomer OR CS-0016866 OR FT-0609833 OR FT-0670982 OR FT-0670983 OR Melamine+1+3+5-Triazine-2+4+6-triamine OR T6897 OR 1+3+5-Triazine-2+4+6-triamine+Melamine OR 1+5-Triazine-2+4+6+1H+3H+5H+-triimine OR 4+6-Diamino-1+2-dihydro-2-imino-S-Triazine OR C08737 OR 78403-EP2270101A1 OR 78403-EP2270113A1 OR 78403-EP2272849A1 OR 78403-EP2272935A1 OR 78403-EP2276751A1 OR 78403-EP2289896A1 OR 78403-EP2298828A1 OR 78403-EP2301924A1 OR 78403-EP2301983A1 OR 78403-EP2308856A1 OR 78403-EP2374895A1 OR s-Triazine+4+6-diamino-1+2-dihydro-2-imino- OR Q212553 OR J-002191 OR cyanuric+triamide OR Cyanuramide OR Cyanurotriamine OR Cyanurotriamide)
diuron_3	(proximity 20) AND (3+3+4-dichlorophenyl+1+1-dimethylurea OR dynex OR dichlorfenidim OR herbatox OR vonduron OR dailon OR karmex OR di-on OR cekiuron OR crisuron OR dirurol OR lucenit OR unidron OR diuron+nortox OR preventol+a+6 OR urox+d OR diuron+4l OR direx+4l OR anduron OR ansaron OR durashield OR herburon OR seduron OR bioron OR dcmu+99 OR diuron+900 OR hw+920 OR ditox-800 OR karamex OR aguron OR diater OR unii-9i3sds92wy OR usaf+p-7 OR 3+3+4-dichlor-phenyl+1+1-dimethyl% OR ccris+1012 OR hsdb+382 OR direx+80w OR chebi:116509 OR nsc+8950 OR einecs+206-354-4 OR af+101 OR urea+3-+3+4-dichlorophenyl+1+1-dimethyl% OR epa+pesticide+chemical+code+035505 OR brn+2215168 OR 9i3sds92wy OR ai3-61438 OR dtxsid0020446 OR mfcd00018136 OR 3-+3+4-dichlor-phenyl+1+1-dimethyl% OR ncgc00094525-01 OR dsstox_cid_446 OR dsstox_rid_75595 OR dsstox_gsid_20446 OR xarmex OR desdimethyldiuron OR xarmex+krovar OR m+velpar OR karmex+dl OR karmex+80w OR spectrum_001823 OR acmc-1cqjf OR specplus_000424 OR spectrum2_001229 OR spectrum3_000822 OR spectrum4_000662 OR spectrum5_001956 OR ec+206-354-4 OR schembl7279 OR bspbio_002343 OR kbiogr_001063 OR kbioss_002328 OR spectrum330030 OR mls002207110 OR divk1c_006520 OR spbio_001078 OR chembl278489 OR ure002 OR ctk7g2120 OR kbio1_001464 OR kbio2_002325 OR kbio2_004893 OR kbio2_007461 OR kbio3_001843 OR zinc57287 OR nsc8950 OR hy-b0860 OR nsc-8950 OR tox21_111292 OR tox21_201438 OR tox21_301016 OR anw-27531 OR bbl003847 OR bdbm50487027 OR ccg-39151 OR stk077954 OR akos001303464 OR tox21_111292_1 OR ls-7325 OR mcule-1921281405 OR ks-0000105p OR ncgc00094525-02 OR ncgc00094525-03 OR ncgc00094525-04 OR ncgc00094525-05 OR ncgc00094525-06 OR ncgc00094525-07 OR ncgc00094525-08 OR ncgc00094525-09 OR ncgc00254918-01 OR ncgc00258989-01 OR as-15493 OR p597 OR smr000777941 OR 3-+3+4-dichlorophenol+1+1-dimethylurea OR db-048327 OR cs-0012874 OR d1328 OR ft-0603378 OR ft-0667750 OR n+n-dimethyl-n+3+4-dichlorophenyl+urea OR ns00000265 OR st50409103 OR n+3+4-dichlorophenyl+n+n+dimethyl+urea OR c18428 OR 33329-ep2274983a1 OR 33329-ep2305655a2 OR 33329-ep2305662a1 OR 33329-ep2311815a1 OR 33329-ep2371823a1 OR n+3+4-dichlorophenyl+dimethylamino+carboxamide OR a821585 OR q425389 OR sr-0 0195223 OR j-018992 OR sr-0 0195223-1 OR brd-k75330923-001-02-6 OR 1+1-dimethyl-3+3+4-dichlorophenyl+urea OR 1+3+4-dichlorophenyl+3+3-dimethylurea OR 1+3+4-dichlorophenyl+3+3-dimethyluree OR 3+3+4-dichloor-fenyl+1+1-dimethylureum OR 3+3+4-dichloro-phenyl+1+1-dimethyl-urea OR 3+3+4-dichlor-phenyl+1+1-dimethyl-harnstoff OR 3+3+4-dicloro-fenyl+1+1-dimetil-urea OR n+3+4-dichlorophenyl+n+n-dimethylurea OR n+3+n-dimethylurea OR n+3+4-dichlorophenyl+n+n+dimethylurea OR n+3+n+dimethylurea OR n+n+dimethyl-n+3+4-dichlorophenyl+urea OR urea+4-dichlorophenyl+1+1-dimethyl% OR urea+4-dichlorophenyl+n+n-dimethyl% OR urea+n+3+4-dichlorophenyl+n+n-dimethyl% OR 3+3+4-Dichlorophenyl+1+1-dimethylurea OR Dynex OR

	Dichlorfenidim OR Herbatox OR Vonduron OR Dailon OR Karmex OR Marmer OR Di-on OR Cekiuron OR Crisuron OR Dirurol OR Lucenit OR Unidron OR Diuron+Nortox OR Preventol+A+6 OR Urox+D OR Diuron+4L OR Direx+4L OR Anduron OR Ansaron OR Durashield OR Herburon OR Seduron OR Bioron OR DCMU+99 OR Diuron+900 OR HW+920 OR Ditox-800 OR Karamex OR Aguron OR Diater OR UNII-9I3SDS92WY OR USAF+P-7 OR 3+3+4-Dichlor-phenyl+1+1-dimethyl% OR CCRIS+1012 OR HSDB+382 OR Direx+80W OR CHEBI:116509 OR NSC+8950 OR EINECS+206-354-4 OR AF+101 OR Urea+3-+3+4-dichlorophenyl+1+1-dimethyl% OR EPA+Pesticide+Chemical+Code+035505 OR BRN+2215168 OR 9I3SDS92WY OR AI3-61438 OR DTXSID0020446 OR MFCD00018136 OR NCGC00094525-01 OR DSSTox_CID_446 OR DSSTox_RID_75595 OR DSSTox_GSID_20446 OR Xarmex OR Desdimethyldiuron OR Xarmex+Krovar OR M+Velpar OR Karmex+DL OR Karmex+80W OR Spectrum_001823 OR 1+3+3-dimethylurea OR ACMC-1CQJF OR SpecPlus_000424 OR Spectrum2_001229 OR Spectrum3_000822 OR Spectrum4_000662 OR Spectrum5_001956 OR EC+206-354-4 OR SCHEMBL7279 OR 3+3+1-dimethyl-harnstoff OR BSPBio_002343 OR KBioGR_001063 OR KBioSS_002328 OR SPECTRUM330030 OR MLS002207110 OR DivK1c_006520 OR SPBio_001078 OR CHEMBL278489 OR URE002 OR CTK7G2120 OR KBio1_001464 OR KBio2_002325 OR KBio2_004893 OR KBio2_007461 OR KBio3_001843 OR ZINC57287 OR NSC8950 OR HY-B0860 OR NSC-8950 OR Tox21_111292 OR Tox21_201438 OR Tox21_301016 OR ANW-27531 OR BBL003847 OR BDBM50487027 OR CCG-39151 OR STK077954 OR AKOS001303464 OR Tox21_111292_1 OR LS-7325 OR MCULE-1921281405 OR KS-0000105P OR NCGC00094525-02 OR NCGC00094525-03 OR NCGC00094525-04 OR NCGC00094525-05 OR NCGC00094525-06 OR NCGC00094525-07 OR NCGC00094525-08 OR NCGC00094525-09 OR NCGC00254918-01 OR NCGC00258989-01 OR AS-15493 OR P597 OR SMR000777941 OR 3+3+4-Dichlorophenol+1+1-dimethylurea OR DB-048327 OR CS-0012874 OR D1328 OR FT-0603378 OR FT-0667750 OR N+N-dimethyl-N+3+4-dichlorophenyl+urea OR NS00000265 OR ST50409103 OR N+3+4-dichlorophenyl+N+N+dimethyl+urea OR C18428 OR 33329-EP2274983A1 OR 33329-EP2305655A2 OR 33329-EP2305662A1 OR 33329-EP2311815A1 OR 33329-EP2371823A1 OR N+3+4-dichlorophenyl+dimethylamino+carboxamide OR A821585 OR Q425389 OR SR-0 0195223 OR J-018992 OR SR-0 0195223-1 OR BRD-K75330923-001-02-6 OR 1+1-Dimethyl-3+3+4-dichlorophenyl+urea OR 1+3+4-Dichlorophenyl+3+3-dimethylurea OR 1+3+4-Dichlorophenyl+3+3-dimethyluree OR 1+4dichlorophenyl+urea OR 3+3+1-dimethylurea OR 3+3+1-dimethylureum OR 3+3+1-dimetil-urea OR 3+3+4-Dichloor-fenyl+1+1-dimethylureum OR 3+3+4-dichlorophenyl+1+1-dimethyl-urea OR 3+3+4-Dichloro-phenyl+1+1-dimethyl-urea OR 3+3+4-Dicloro-fenyl+1+1-dimetil-urea OR diuron OR N+3+4-Dichlorophenyl+N+N-dimethylurea OR N+3+N-dimethylurea OR N+3+4-Dichlorophenyl+N+N+dimethylurea OR N+3+4-Dichlorophenyl+N+N-Dimethylurea OR N+3+N+dimethylurea OR N+N+Dimethyl-N+3+4-dichlorophenyl+urea OR Urea+4-dichlorophenyl+1+1-dimethyl% OR Urea+4-dichlorophenyl+N+N-dimethyl% OR Urea+N+3+4-dichlorophenyl+N+N-dimethyl%) AND (host)
Retinol_8	(proximity 20) AND (host) AND (retinol OR vitamin+a OR vitamin+a1 OR alphalin OR axerophthol OR afaxin OR oleovitamin+a OR chocola+a OR alphasterol OR apostavit OR aquasynth OR biosterol OR epiteliol OR ophthalamin OR agiolan OR agoncal OR anatola OR myvpack OR prepalin OR testavol OR veroftal OR aoral OR apexol OR avibon OR avitol OR axerol OR dofsol OR vaflol OR vitpex OR vogan OR isatabs+tabs OR bentavit+a OR dohyfral+a OR alcovit+a OR anatola+a OR vogan-neu OR a-mulsal OR plivit+a OR vi-alpha OR a-vitan OR atars OR vafol OR retrovitamin+a OR homagenets+aoral OR hi-a-vita OR sehkraft+a OR a-vi-pel OR vi-dom-a OR solu-a OR nio-a-let OR vio-a OR antixerophthalmic+vitamin OR del-vi-a OR vitavel+a OR axerophtholum OR thalasphere OR wachstumsvitamin OR vitaminum+a OR vitamine+a OR vitavel-a OR retinolum OR antixerophthalmisches+vitamin OR unii-g2sh0xkk91 OR beta.-retinol OR beta-retinol OR ccris+5444 OR hsdb+815 OR einecs+200-683-7 OR chembl986 OR nsc+122759 OR brn+0403040 OR g2sh0xkk91 OR 2e+4e+6e+8e+3+7-dimethyl-9+2+6+6-trimethylcyclohexen-1-yl+nona-2+4+6+8-tetraen-1-ol OR all-e+3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetraen-1-ol OR 2+4+6+8-nonatetraen-1-ol+3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl% OR chebi:17336 OR 3+7-dimethyl-9+2+6+6-trimethyl-1-cyclchexen-1-yl+2+4+6+8-nonatetraen-1-ol OR 2e+4e+6e+8e+3+7-dimethyl-9+2+6+6-trimethylcyclohex-1-en-1-yl+nona-2+4+6+8-tetraen-1-ol OR nsc-122759 OR ncgc00017343-07 OR cylasphere OR retinolo OR dsstox_cid_3556 OR hydrovit+a OR 3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonate-traen-1-ol OR alcohol+9+13-dimethyl-7+1+1+5-trimethyl-6-cyclohexen-5-yl+7+9+11+13-nonatetraen-15-ol OR dsstox_rid_77080 OR dsstox_gsid_23556 OR ro-a-vit OR q-201926 OR w-104683 OR aquasol+a+parenteral OR rovimix+a OR 2e+4e+6e+8e+3+7-dimethyl-9+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetr+aen-1-ol OR smr000112036 OR 11+12-3h+-retinol OR 9-cis+13-cis-retinol OR sr-0 0763813 OR tegosphere+vita OR alpha.sterol OR alpha.lin OR retinyl+a OR trans-retinol+acid+vitamin+a OR einecs+234-328-2 OR mfcd00001552 OR pubchem18446 OR spectrum5_000993 OR spectrum5_001997 OR ec+200-683-7 OR schembl3112 OR all-trans-3+7-dimethyl-9-+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetraen-1-ol OR bidd:pxr0102 OR mls001066379 OR mls001074751 OR mls0060 08 OR spectrum1501203 OR gtpl4053 OR dtxsid3023556 OR hms501i08 OR hms1921b04 OR hms2092l13 OR hms2270c05 OR bcp06593 OR hy-b1342 OR zinc3831417 OR tox21_110818 OR tox21_202441 OR tox21_300287 OR bdbm50092056 OR bg0050 OR ccg-38864 OR lmpr01090001 OR nsc122759 OR nsc758150 OR akos015902578 OR db00162 OR nsc-758150 OR sdccgmls-0066724.p001 OR idi1_000486 OR smp2_000102 OR ncgc00017343-02 OR ncgc00017343-03 OR ncgc00017343-04 OR ncgc00017343-05 OR ncgc00017343-06 OR ncgc00017343-08 OR ncgc00017343-09 OR ncgc00017343-11 OR ncgc00091784-01 OR ncgc00091784-02 OR ncgc00091784-03 OR ncgc00091784-04 OR ncgc00091784-05 OR ncgc00091784-06 OR ncgc00254024-01 OR ncgc00259990-01 OR ac-11701 OR bs-17906 OR cc-35617 OR cc-35618 OR sc-61936 OR sc-75819 OR st057232 OR sbi-0051690.p002 OR cs-0013091 OR ns00003017 OR 33563-ep2272846a1 OR 33563-ep2277869a1 OR 33563-ep2277870a1 OR 33563-ep2281813a1 OR 33563-ep2284174a1 OR 33563-ep2292608a1 OR 33563-ep2301936a1 OR 33563-ep2311820a1 OR 33563-ep2374791a1 OR ab00052248_05 OR sr-0 0763813-2 OR sr-0 0763813-4 OR brd-k22429181-001-06-8 OR brd-k64634304-001-01-5 OR phenol+2+aminomethyl+5-fluoro+hydrochloride% OR 3+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetraen-1-ol OR 2+6+8-nonatetraen-1-ol+3+7dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl% OR 3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetraen-1-ol% OR 2e+4e+6e+8e+3+7-dimethyl-9+2+6+6-trimethyl-1-cyclohexenyl+1-nona-2+4+6+8-tetraenol OR 2e+4e+6e+8e+3+7-dimethyl-9-+2+6+6-trimethyl-1-cyclohexenyl+nona-2+4+6+8-tetraen-1-ol OR 2e+4e+6e+8e+3+7-dimethyl-9-+2+6+6-trimethylcyclohex-1-enyl+nona-2+4+6+8-tetraen-1-ol OR 2z+4z+6z+8z+3+7-dimethyl-9-+2+6+6-trimethyl-1-cyclohexen-1-yl+2+4+6+8-nonatetren-1-ol) AND (risk% OR tox% OR hazard% OR exposure OR adverse) NOT Skin

butylated_hydroxyanisole_2	(proximity 20) AND (host) AND (2+3+t-butyl-4-methoxyphenol OR 2+3+t-butyl-4-hydroxyanisole OR 2+3+tert-butyl-4-hydroxyanisole OR 2+3+tert-butyl-4-methoxyphenol OR 2+1+1dimethylethyl+4+methyloxy+phenol OR 2+1+1dimethylethyl+4-methoxy-phenol OR 2+1+1-dimethylethyl+4-methoxyphenol OR 2+tert-butyl+4-methoxyphenol OR 2-butyl-4-hydroxyanisole OR 2-t-butyl-4-methoxyphenol OR 2-tert-bha OR 2-tert-butyl-4-methoxphenol OR 2-tert-butyl-4-methoxy-phenol OR 2-tert-butyl-4-methoxyphenol OR 3+1+1-dimethylethyl+4-hydroxyanisole OR 3-bha OR 3-t-butyl-4-hydroxyanisole OR 3-tert-butyl-4-hydroxyanisol OR 3-tert-butyl-4-hydroxyanisole OR 3-tert-butyl-p-hydroxyanisole OR 4-hydroxy-3-tert-butylanisole OR 4-methoxy-2-tert-butylphenol OR 4-methoxy-6-tert-butylphenol OR amif-72 OR anisole+butylated+hydroxy OR antioxyne+b OR antrancine+12 OR boa+antioxidant OR butyl+methoxyphenol OR butylated+hydroxyanisole OR butylhydroxyanisol OR butylhydroxyanisole OR butylohydroksyanizol OR c11h16o2 OR ccris+102 OR chembl4296740 OR cs-4622 OR eec+no+e320 OR einecs+246-563-8 OR embanox OR fema+no+183 OR hsdb+3913 OR hy-b1066 OR ls-1065 OR nepantiox+1-f OR nipantiox+1-f OR o-tert-butyl-p-methoxyphenol OR o-tert-Butyl-p-methoxyphenol OR p-methoxy-o-tert-butylphenol OR phenol+1+1-dimethylethyl+4-methoxy OR phenol+2+1+1dimethylethyl+4-methoxy OR phenol+2-tert-butyl-4-methoxy OR phenol+tert-butyl-4-methoxy OR protex OR q409401 OR rek4960k2u OR schembl30330 OR sustane+1-f OR t-butyl+hydroxyanisole OR tenox+bha OR tert-butyl-4-methoxyphenol OR tert-butylhydroxyanisole OR unii-rek4960k2u)
chloral_hydrate_2	(proximity 20) AND (1+1+1-trichloro-2+2-dihydroxyethane OR 1+1+1-trichloro-2+2-ethanediol OR 1+1-ethanediol+2+2+2-trichloro OR 1+1-trichloro-2+2-dihydroxyethane OR 2+2+2-trichloro-1+1-ethanediol OR 2+2+2-trichloroethane-1+1+diol OR 2+2+2-trichloroethane-1+1-diol OR 2+2-trichloro-1+1-ethanediol OR 418m5916wg OR 6993-ep2269977a2 OR 6993-ep2269992a1 OR 6993-ep2270010a1 OR 6993-ep2272517a1 OR 6993-ep2272813a2 OR 6993-ep2272841a1 OR 6993-ep2272849a1 OR 6993-ep2275395a2 OR 6993-ep2277861a1 OR 6993-ep2277875a2 OR 6993-ep2277876a1 OR 6993-ep2284165a1 OR 6993-ep2292593a2 OR 6993-ep2292602a1 OR 6993-ep2292614a1 OR 6993-ep2292628a2 OR 6993-ep2293650a1 OR 6993-ep2298737a1 OR 6993-ep2298740a1 OR 6993-ep2298744a2 OR 6993-ep2305250a1 OR 6993-ep2305640a2 OR 6993-ep2308852a1 OR 6993-ep2311830a1 OR 6993-ep2311837a1 OR 6993-ep2314558a1 OR 6993-ep2314581a1 OR 6993-ep2316824a1 OR 6993-ep2316832a1 OR 6993-ep2316833a1 OR 6993-ep2316835a1 OR acmc-209hdv OR ai3-00082 OR AI3-00082 OR akos009157238 OR anw-26801 OR aquachloral OR bcp31225 OR brn+1698497 OR ccris+4142 OR chebi+28142 OR chembl455917 OR chloradorm OR chloral+hydrat OR chloral+hydrate OR chloral+monohydrate OR chloraldural OR chloraldurat OR chloralex OR chloralhydrat OR chloralhydrate OR chlorali+hydras OR chloralvan OR cloral+betaine OR cohidrate OR ctk1c2451 OR db-047727 OR db01563 OR dea+no+2465 OR dichloralphenazone OR dormal OR dsstox_cid_261 OR dsstox_gsid_20261 OR dsstox_rid_75470 OR dtxsid7020261 OR einecs+206-117-5 OR epa+pesticide+chemical+code+268 OR escre OR ethanediol+2+2+2-trichloro OR felsules OR hsdb+222 OR hydral OR hydrate+de+chloral OR hynos OR kessodrate OR kloralhydrat OR ks-000000z1 OR ksc222i5d OR lorinal OR lycoral OR mcule-8278658791 OR mfcd00044479 OR ncgc00159374-02 OR ncgc00159374-03 OR ncgc00159374-04 OR ncgc00257664-01 OR noctec OR nortec OR novochlorhydrate OR ns00009274 OR nsc+3210 OR nsc-3210 OR nsc3210 OR nycoton OR nycton OR oradrate OR phaldrone OR rectules OR sc-18707 OR schembl34327 OR somni+sed OR somnos OR somnote OR sontec OR stl445706 OR tosyl OR tox21_111614 OR tox21_111614_1 OR tox21_200110 OR trawotox OR trichloracetaldehyd-hydrat OR trichloro+acetaldehyde+hydrate OR trichloroacetaldehyde+hydrate OR trichloroacetaldehyde+hydrated OR trichloroacetaldehyde+monohydrate OR trichloroethanal+hydrate OR unii-418m5916wg OR wln+qyqxggg OR zinc3872049) AND (host)
4_aminophenol_2	(proximity 20) AND (1-amino-4-hydroxybenzene OR 135807-ep2371803a1 OR 135807-ep2377843a1 OR 4-amino+phenol OR 4-amino-1-hydroxybenzene OR 4-amino-phenol OR 4-aminobenzenol OR 4-aminophenol OR 4-hydroxy-aniline OR 4-hydroxyaniline OR 4-hydroxybenzenamine OR 4-hydroxyphenylamine OR 9225-ep2275420a1 OR 9225-ep2280008a2 OR 9225-ep2308872a1 OR 9225-ep2316829a1 OR a0384 OR acmc-209aoj OR activol OR ai3-14872 OR aj-333+25022099 OR akos000119829 OR akos016371265 OR am86423 OR aminophenol+p OR anw-18113 OR as-54109 OR as04549 OR azol OR bbl011574 OR bcp25857 OR bdbm26195 OR benzofur+p OR bmse000462 OR c+i+76550 OR c02372 OR ccg-266045 OR ccris+4146 OR certinal OR chebi+17602 OR chembl1142 OR ci+76550 OR citol OR cs-0006652 OR db14144 OR dsstox_cid_4499 OR dsstox_gsid_24499 OR dsstox_rid_77429 OR dtxsid3024499 OR durafur+brown+rb OR ec+204-616-2 OR einecs+204-616-2 OR energol OR epitope+id+117708 OR f2190-0438 OR fouramine+p OR fourrine+84 OR fourrine+p+base OR ft-0617593 OR furro+p+base OR hsdb+2640 OR j-004908 OR j-514454 OR kodelon OR ks-000000hn OR ksc354q5h OR l-1224 OR ls-676 OR mcule-3319647085 OR mesalamine+impurity+a OR mfcd00007869 OR mls001066356 OR nako+brown+r OR ncgc00090816-01 OR ncgc00090816-02 OR ncgc00090816-03 OR ncgc00090816-04 OR ncgc00090816-05 OR ncgc00258583-01 OR ns00006730 OR nsc+1545 OR nsc-1545 OR nsc1545 OR p-amino-phenol OR p-aminobenzenol OR p-aminofenol OR p-aminophenol OR p-aminophenol+phosphate OR p-hydroxyphenylamine OR para+amino+phenol OR para+aminophenol OR para-amino-phenol OR para-aminophenol OR para-hydroxyaniline OR paraaminophenol OR paramidophenol OR paranol OR pelagol+p+base OR phenol+4-amino OR phenol+p-amino OR pubchem22199 OR q2548040 OR r7p8frp05v OR renal+ac OR rodinal OR sbb059792 OR sc-19013 OR schembl15663694 OR schembl3424 OR sgcut00256 OR smr000471841 OR st088538 OR stk286017 OR takatol OR tertral+p+base OR tox21_113242 OR tox21_113477 OR tox21_113477_1 OR tox21_201030 OR to_000006 OR un+2512 OR unii-r7p8frp05v OR ursol+p OR ursol+p+base OR z57127517 OR zinc4623758 OR zoba+brown) AND (host)
chlorinated_paraffins_2	(proximity 20) AND (4+8+11+14+17+21-hexachlorotetracosane OR chlorinated+paraffin OR chlorinated+paraffins OR chlorowax+40 OR ec+264-150-0 OR schembl2577273 OR chembl1892619 OR ncgc00091464-01 OR ns00014226) AND (host)

diphenylmethane_diisocyanate_2	(proximity 20) AND (diphenylmethane+diisocyanate OR bis+4-isocyanatophenyl+methane OR isonate OR p+p+diphenylmethane+diisocyanate OR 1+1+methylenebis+4-isocyanatobenzene OR methylbisphenyl+isocyanate OR 4+4+methylenediphenyl+diisocyanate OR 4+4+diisocyanatodiphenylmethane OR methylene+bisphenyl+isocyanate OR methylene+diphenyl+diisocyanate OR 4+4+-methylenebis+phenyl+isocyanate OR bis+p-isocyanatophenyl+methane OR diphenylmethyl+diisocyanate OR caradate+30 OR desmodur+44 OR bis+1+4-isocyanatophenyl+methane OR nacconate+300 OR benzene+1+1+methylenebis+4-isocyanato OR isonate+125m OR methylenebis+4-isocyanatobenzene OR methylenebis+p-phenyl+isocyanate OR diphenyl+methane+diisocyanate OR methylenebis+4-phenyl+isocyanate OR 4+4+methylenediphenyl+isocyanate OR rubinate+44 OR methylenebis+p-phenylene+isocyanate OR methylenedi-p-phenylene+diisocyanate OR methylenebis+4-phenylene+isocyanate OR 4+4+methylenedi-p-phenylene+diisocyanate OR 4+4+methylenediphenylene+isocyanate OR hylene+m50 OR p+p+methylenebis+phenyl+isocyanate OR bis+para-isocyanatophenyl+methane OR polymeric+mdi OR methylene+di-p-phenylene+isocyanate OR methylenebis+para-phenyl+isocyanate OR 4+4+methylenedi+phenyl+isocyanate OR di+4-isocyanatophenyl+methane OR difenil-metan-diisocianato OR methylenedi-para-phenylene+diisocyanate OR methylenebis+para-phenylene+isocyanate OR para+para+diphenylmethane+diisocyanate OR nci-c50668 OR methylenediphenyl+diisocyanate OR para+para+methylenebis+phenyl+isocyanate OR 4+4+methylenediphenylene+diisocyanate OR unii-b0lo6bbs8c OR generic+mdi OR crude+mdi OR isocyanic+acid+methylenedi-p-phenylene+ester OR methylenebis+phenylisocyanate OR ccris+2303 OR 4+4+diphenylmethanediisocyante OR chebi:53218 OR isocyanic+acid+ester+with+diphenylmethane OR diphenylmethane+p+p+diisocyanate OR hsdb+2630 OR diphenylmethane+4+4+diisocyanate OR difenylmethaan-dissocyanaat OR nsc+9596 OR einecs+202-966-0 OR einecs+247-714-0 OR b0lo6bbs8c OR non-isomeric-specific+mdi OR brn+0797662 OR diphenylmethan-4+4+diisocyanat OR isocyanic+acid+methylenediphenylene+ester OR methylenebisphenyl+diisocyanate OR ai3-15256 OR dtxsid7025180 OR methylenedi+p-phenyl+isocyanate OR methylenedi-p-phenyl+diisocyanate OR 4-4+diisocyanate+de+diphenylmethane OR 4+4+2+4+2+2+diisocyanatodiphenylmethane OR methylenedi+p-phenylene+isocyanate OR 4+4+mdi OR methylenediphenyl+4+4+diisocyanate OR methylenedi+p-phenylene+diisocyanate OR 4+4+diisocyanate+de+diphenylmethane OR methylenediphenyl+diisocyanate+4+4 OR 4+4+methylenedi+phenylene+isocyanate OR polymeric+4+4-methylenediphenyl+diisocyanate OR dsstox_cid_4196 OR methylenebis+phenylisocyanate+diisocyanates OR ccris+8160 OR nocconate+300 OR un2489 OR hylene+m+50 OR hylene+m-50 OR difenylmethaan-diisocyanaat OR epitope+id+113240 OR ec+202-966-0 OR dsstox_rid_77697 OR dsstox_rid_82371 OR dsstox_gsid_25180 OR dsstox_gsid_47473 OR schembl19943 OR wln+ocnr+d1r+dnco OR 4-13-00-00396 OR chembl1488467 OR 4+4+diphenylmethanediisocyanate OR ctk5c3260 OR diphenylmethane+4+4-diisocyanate OR 4+4-diphenylmethane+diisocyanate OR nsc9596 OR polymethylene+polyphenyl+isocynate OR 4+4+diphenylmethane+diisocyanate OR nsc-9596 OR zinc1700075 OR tox21_200268 OR tox21_302585 OR ls-334 OR mfcd00036131 OR sbb060784 OR akos000119302 OR methylenebis+4+4+phenyl+isocyanate OR 4+4+methylenedi+phenyl+diisocyanate OR benzene+1+methylenebis+4-isocyanato OR isocyanic+acid+diphenylmethylene+ester OR mcule-4402925766 OR ne10917 OR un+2489 OR methylenebis+4-phenylisocyanate OR ncgc00091061-01 OR ncgc00091061-02 OR ncgc00091061-03 OR ncgc00256765-01 OR ncgc00257822-01 OR cas-9016-87-9 OR ls-166061 OR d0897 OR ft-0617061 OR ft-0625273 OR st50825935 OR 1-isocyanato-4+4-isocyanatobenzyl+benzene OR c19453 OR q417646 OR w-108905) AND (host)
9_10-anthraquinone_2	(proximity 20) AND (1+4-bis+2+2-hydroxy-ethylamino+ethylamino+anthraquinone OR 9+10-anthracendion OR 9+10-anthracenedione OR 9+10-anthrachinon OR 9+10-anthraguinone OR 9+10-anthraquinone OR 9+10-dihydro-9+10-dioxoanthracene OR 9+10-dihydroanthracene-9+10-dione OR 9+10-dioxoanthracene OR 9+10-quinone OR ab-131/40003277 OR ac-12719 OR acmc-209pw0 OR ai3-09073 OR ak117080 OR akos000282964 OR anthra-9+10-quinone OR anthracene+10-dihydro-9+10-dioxo OR anthracene+9+10-dihydro-9+10-dioxo OR anthracene-9+10-dione OR anthracene-9+10-quinone OR anthracenequinone OR anthrachinon OR anthrachinone OR anthradione OR anthrapel OR anthraquinone OR anw-37822 OR bbl003001 OR bdbm50094892 OR bis-alkylamino+anthraquinone OR bis-alkylamino_anthraquinone OR brd-k15957397-001-03-4 OR bspbio+003141 OR ccg-39966 OR ccris+649 OR chebi+40448 OR chembl55659 OR corbit OR cs-0008907 OR db-005409 OR divk1c+006741 OR ds-4810 OR dsstox+cid+95 OR dsstox+gsid+20095 OR dsstox+rid+75364 OR dtxsid3020095 OR ec+201-549-0 OR einecs+201-549-0 OR epa+pesticide+chemical+code+122701 OR epitope+id+116191 OR f0001-2133 OR ft-0622417 OR hms1921j14 OR hoelite OR hsdb+2074 OR hy-n0354 OR kbio1+001685 OR kbio2+002007 OR kbio2+004575 OR kbio2+007143 OR kbio3+002641 OR kbiogr+001374 OR kbioss+002007 OR ksc362c5j OR ls-1837 OR mcule-4655011423 OR mfcd00001188 OR morkit OR ncgc00094960-01 OR ncgc00094960-02 OR ncgc00094960-03 OR ncgc00094960-04 OR ncgc00094960-06 OR ns00010810 OR nsc+7957 OR nsc-7957 OR nsc7957 OR q423174 OR s5168 OR sbb060613 OR sc-46775 OR schembl14943 OR spbio+000330 OR specplus+000645 OR spectrum+001527 OR spectrum1502103 OR spectrum2+000405 OR spectrum3+001501 OR spectrum4+000907 OR spectrum5+001897 OR sr-0 0944707 OR st50410412 OR stk398385 OR tox21+111369 OR unii-030ms0jbdo OR zinc3847491) AND (host)
triphenylphosphine_2	(proximity 20) AND host) AND (triphenylphosphorus OR triphenylphosphide OR phosphorustriphenyl OR triphenyl+phosphorous OR mfcd00003043 OR phosphorus+triphenyl OR nsc+215203 OR ccris+4889 OR unii-26d26oa393 OR hsdb+4266 OR einecs+210-036-0 OR brn+0610776 OR dtxsid5026251 OR 26d26oa393 OR dsstox_cid_6251 OR wln:+rpr&r OR dsstox_rid_78074 OR dsstox_gsid_26251 OR q-201896 OR diphenylphosphino-polystyrene OR triphenylphospane OR triphenyphosphine OR pubchem6417 OR acmc-1bggs OR trisphenylphosphine OR c18h14ppol OR triphenyl+phosphine OR schembl101 OR ec+210-036-0 OR ph+3p OR p+ph+3 OR nsc10 OR ksc206a0j OR nsc-10 OR schembl1679860 OR chembl1448331 OR c6h5+3p OR acn-s002163 OR bcp01148 OR ebd51172 OR p+c6h5+3 OR zinc8585891 OR zx-at007677 OR tox21_202114 OR tox21_303294 OR 7817ah OR anw-75057 OR gk1326 OR nsc215203 OR or9088 OR pp-360 OR rw2519 OR sbb060439 OR stl185621 OR akos009031542 OR as01621 OR ls-1438 OR ls4 4 OR mcule-9122575728 OR nsc-215203 OR qc-4207 OR ks-000002n8 OR ncgc00091416-01 OR ncgc00091416-03 OR ncgc00257211-01 OR ncgc00259663-01 OR at-19512 OR bp-12577 OR sc-05646 OR sc-65423 OR db-050422 OR bis+triphenylphosphine+nickel+ii+dichloride OR ft-0604360 OR ft-0632502 OR ft-0689298 OR ft-0698371 OR ns00002889 OR st50406239 OR az0001-0002 OR c-24254 OR q115493 OR f1642-0085 OR phosphine+triphenyl OR trifenylfosfin OR triphenylphosphane OR Phosphine+triphenyl- OR Triphenylphosphorus OR Triphenylphosphide OR Triphenylphosphine OR Phosphorustriphenyl OR 39319-11-4 OR MFCD00003043 OR Phosphorus+triphenyl OR NSC+215203 OR CCRIS+4889 OR UNII-26D26OA393 OR HSDB+4266 OR EINECS+210-036-0 OR BRN+0610776 OR DTXSID5026251 OR 26D26OA393 OR DSSTox_CID_6251 OR WLN:+RPR&R OR DSSTox_RID_78074 OR

	DSSTox_GSID_26251 OR Q-201896 OR Diphenylphosphino-polystyrene OR triphenyphospine OR tripenylphosphine OR triphenyiphoshine OR triphenylphophine OR triphenylphospine OR tripheylphosphine OR Triphenylphospane OR Triphenyphosphine OR tripbenylphosphine OR triphenyiphosphine OR tri-phenylphospine OR triphenyl+phophine OR triphenyl+phospine OR triphenylphosphine OR triphenyl+phosphorus OR triphenyl-+phosphine)
tetrabromobisphenol_A_2	(proximity 20) AND (host) AND (tetrabromobisphenol+a OR 3+3+5+5+-tetrabromobisphenol+a OR bromdian OR 2+2-bis+3+5-dibromo-4-hydroxyphenyl+propane OR 4+4+-isopropylidenebis+2+6-dibromophenol OR tetrabromodian OR 2+2+6+6+-tetrabromobisphenol+a OR saytex+rb+ pc OR phenol+4+4+-+1-methylethylidene+bis+2+6-dibromo- OR tetrabromodiphenylopropane OR unii-fqi02rfc3a OR 3+5+3+5+-tetrabromobisphenol+a OR nsc+59775 OR ccris+6274 OR hsdb+5232 OR saytex+rb- OR 4+4+-isopropylylidenebis+2+6-dibromophenol OR 2+2-bis+4-hydroxy-3+5-dibromophenyl+propane OR einecs+201-236-9 OR fqi02rfc3a OR 2+2+6+6+-tetrabromo-4+4+-isopropylidenediphenol OR 4+4+-+2+2-propanediyl+bis+2+6-dibromophenol OR chembl184450 OR dtxsid1026081 OR chebi:33217 OR phenol+4+4+-isopropylidenebis+2+6-dibromo- OR mfcd00013962 OR dsstox_cid_6081 OR 4+4+-+1-methylethylidene+bis+2+6-dibromophenol+2+2-bis+3+5-dibromo-4-hydroxyphenyl+propane OR dsstox_rid_78008 OR dsstox_gsid_26081 OR w-104257 OR tetrabromobisphenola OR tetrabromo+bisphenol+a OR 3+3+5+5+-tetrabromo+bisphenol+a OR 33+55+-tetrabromobisphenol+a OR saytex+rb- +abs OR tetrabromo-4+4+-isopropylidenediphenol OR ec+201-236-9 OR oprea1_822733 OR schembl18647 OR mls002152878 OR bidd:er0631 OR c15h12br4o2 OR 330396_aldrich OR aronis002155 OR 2+6+6+-tetrabromobisphenol+a OR ctk4f6165 OR ks-00003vgg OR 3+3+5+-tetrabromobisphenol+a OR albb-031649 OR ks-00000wf5 OR nsc59775 OR zinc1689786 OR zx-as004485 OR tox21_201182 OR tox21_201981 OR tox21_300561 OR bdbm50150793 OR nsc-59775 OR sbb080626 OR stk048486 OR zinc01689786 OR akos000491577 OR 3+3\+5+5\+-tetrabromobisphenol+a OR mcule-8578472069 OR ncgc00091463-01 OR ncgc00091463-02 OR ncgc00091463-03 OR ncgc00091463-04 OR ncgc00091463-05 OR ncgc00091463-06 OR ncgc00254356-01 OR ncgc00258734-01 OR ncgc00259530-01 OR ac-11719 OR ak113742 OR as-12834 OR smr001224492 OR phenol+4+-isopropylidenebis+2+6-dibromo- OR 3+3+5+5+-tetrabromobisphenol+a+97% OR ax8153220 OR ft-0617111 OR ft-0682679 OR phenol+4+-+1-methylethylidene+bis+2+6-dibromo- OR sr-0 0596914 OR sr-0 0596914-1 OR 2+2+6+6+-tetrabromo-4+4+-isopropylidene+bisphenol OR phenol+4+4+-isopropylidenebis+2+6-dibromo-+8ci OR 3+3+5+5+-tetrabromo-4+4-dihydroxy-2+2-diphenylpropane OR 3+3+5+5+-tetrabromo-4+4+-dihydroxy-diphenyl-dimethyl-methane OR tbbpa OR tetrabromobisphenol_a OR Tetrabromobisphenol+A OR 3+3+5+5+-Tetrabromobisphenol+A OR Bromdian OR 4+4+-+propane-2+2-diyl+bis+2+6-dibromophenol OR 2+2-Bis+3+5-dibromo-4-hydroxyphenyl+propane OR 4+4+-Isopropylidenebis+2+6-dibromophenol OR Tetrabromodian OR 2+2+6+6+-TETRABROMOBISPHENOL+A OR Saytex+RB+ PC OR Phenol+4+4+-+1-methylethylidene+bis+2+6-dibromo- OR Tetrabromodiphenylopropane OR 4+4+-propane-2+2-diylbis+2+6-dibromophenol OR UNII-FQI02RFC3A OR 4+4+-+1-Methylethylidene+bis+2+6-dibromophenol OR 3+5+3+5+-Tetrabromobisphenol+A OR NSC+59775 OR CCRIS+6274 OR HSDB+5232 OR Saytex+RB- OR 4+4+-Isopropylylidenebis+2+6-dibromophenol OR 2+2-Bis+4-hydroxy-3+5-dibromophenyl+propane OR EINECS+201-236-9 OR FQI02RFC3A OR 2+2+6+6+-Tetrabromo-4+4+-isopropylidenediphenol OR 2+6-dibromo-4-+2-+3+5-dibromo-4-hydroxyphenyl+propan-2-yl+phenol OR 4+4+-+2+2-PROPANEDIYL+BIS+2+6-DIBROMOPHENOL OR CHEMBL184450 OR DTXSID1026081 OR CHEBI:33217 OR Phenol+4+4+-isopropylidenebis+2+6-dibromo- OR 4+4+-+2+2-propanediyl+bis+2+6-dibromo+phenol OR MFCD00013962 OR DSSTox_CID_6081 OR 4+4+-+1-Methylethylidene+bis+2+6-dibromophenol+2+2-bis+3+5-dibromo-4-hydroxyphenyl+propane OR DSSTox_RID_78008 OR DSSTox_GSID_26081 OR W-104257 OR 2+6-dibromo-4-+1-+3+5-dibromo-4-hydroxyphenyl+-1-methylethyl+phenol OR TetrabromobisphenolA OR Tetrabromo+bisphenol+A OR 4+4+-+1-methylethylidene+bis+2+6-dibromophenol OR 3+3+5+5+-Tetrabromo+bisphenol+A OR 33+55+-Tetrabromobisphenol+A OR 4+6-dibromophenol OR Saytex+RB- +ABS OR 2+5-dibromophenyl+propane OR TETRABROMO-4+4+-ISOPROPYLIDENEDIPHENOL OR bmse000567 OR EC+201-236-9 OR Oprea1_822733 OR SCHEMBL18647 OR MLS002152878 OR BIDD:ER0631 OR C15H12Br4O2 OR 330396_ALDRICH OR ARONIS002155 OR 2+6+6+-Tetrabromobisphenol+A OR CTK4F6165 OR KS-00003VGG OR 3+3+5+-Tetrabromobisphenol+A OR ALBB-031649 OR KS-00000WF5 OR NSC59775 OR ZINC1689786 OR ZX-AS004485 OR Tox21_201182 OR Tox21_201981 OR Tox21_300561 OR 2+5-dibromo-4-hydroxyphenyl+propane OR BDBM50150793 OR NSC-59775 OR SBB080626 OR STK048486 OR ZINC01689786 OR 2+6-dibromo-4-+1-+3+5-dibromo-4-hydroxy-phenyl+-1-methyl-ethyl+phenol OR AKOS000491577 OR 2+2+6+6+-Tetrabromobisphenol+A OR 3+3+5+5+-tetrabromobisphenol+A OR 3+3\+5+5\+-tetrabromobisphenol+A OR MCULE-8578472069 OR NCGC00091463-01 OR NCGC00091463-02 OR NCGC00091463-03 OR NCGC00091463-04 OR NCGC00091463-05 OR NCGC00091463-06 OR NCGC00254356-01 OR NCGC00258734-01 OR NCGC00259530-01 OR 30496-13-0 OR AC-11719 OR AK113742 OR AS-12834 OR SMR001224492 OR Phenol+4+-isopropylidenebis+2+6-dibromo- OR 3+3+5+5+-Tetrabromobisphenol+A+97% OR AX8153220 OR phenol+4+4+-isopropylidenebis+dibromo- OR 2+2-bis+3+5dibromo-4-hydroxyphenyl+propane OR 4+4+-isopropylidene-bis+2+6-dibromophenol OR FT-0617111 OR FT-0682679 OR 2+2-bis+3+5-dibromo-4-hydroxyphenyl+-propane OR 2+2-bis-+3+5-dibromo-4-hydroxyphenyl+propane OR 2+2-bis-+3+5-dibromo-4-hydroxyphenyl+-propane OR Phenol+4+-+1-methylethylidene+bis+2+6-dibromo- OR SR-0 0596914 OR tetrabromodihydroxy+diphenylpropane OR SR-0 0596914-1 OR 2+2+6+6+-Tetrabromo-4+4+-isopropylidene+bisphenol OR 2+2-bis-+4+-hydroxy-3+5+-dibromophenyl+-propane OR Phenol+4+4+-isopropylidenebis+2+6-dibromo-+8CI OR 3+3+5+5+-Tetrabromo-4+4-dihydroxy-2+2-diphenylpropane OR 3+3+5+5+-Tetrabromo-4+4+-dihydroxy-diphenyl-dimethyl-methane OR 4-+1-+3+5-dibromo-4-hydroxyphenyl+-isopropyl+-2+6-dibromophenol OR TBBPA OR tetrabromobisphenol_A)

Phenolphtalein_nohost	(phthalimetten OR euchessina OR phthalin OR espotabs OR phenolax OR purgophen OR koprol OR laxogen OR trilax OR spulmako-lax OR chocolax OR purgen OR correctol OR alophen OR doxidan OR medilax OR colax OR laxin OR femilax OR phenophthalein OR nci-c55798 OR unii-6qk969r2if OR nsc+10464 OR ccris+6266 OR hsdb+4161 OR einecs+201-004-7 OR mfcd00005913 OR brn+0284423 OR chembl63857 OR ai3-09081 OR mls000069592 OR 6qk969r2if OR dtxsid0021125 OR chebi:34914 OR ncgc00018200-07 OR smr000059015 OR dsstox_cid_1125 OR dsstox_rid_75956 OR dsstox_gsid_21125 OR evac-v-lax OR 1+3h+isobenzofuranone+3+3bis+4-hydroxyphenyl+ OR pubchem7084 OR spectrum_001077 OR opera_id_1337 OR spectrum2_001279 OR spectrum3_000888 OR spectrum4_000982 OR spectrum5_001268 OR ec+201-004-7 OR schembl27670 OR bspbio_002518 OR kbiogr_001383 OR kbioss_001557 OR mls001148397 OR bidd:er0202 OR divk1c_000929 OR spectrum1500480 OR spbio_001278 OR aronis002962 OR bcbcmap01_000174 OR hms502o11 OR kbio1_000929 OR kbio2_001557 OR kbio2_004125 OR kbio2_006693 OR kbio3_001776 OR ks-00000yjd OR ninds_000929 OR hms1920h04 OR hms2091p06 OR hms2236i09 OR hms3374p06 OR pharmakon1600-01500480 OR hy-d0211 OR ks-00003w2p OR nsc10464 OR zinc3831317 OR tox21_110838 OR tox21_202219 OR tox21_300282 OR bbl002030 OR bdbm50077844 OR ccg-39112 OR nsc-10464 OR nsc215214 OR nsc757271 OR sbb008868 OR stk029876 OR akos000493033 OR tox21_110838_1 OR mcule-5232154932 OR nsc-215214 OR nsc-757271 OR idi1_000929 OR smp1_000235 OR ncgc00018200-01 OR ncgc00018200-02 OR ncgc00018200-03 OR ncgc00018200-04 OR ncgc00018200-05 OR ncgc00018200-06 OR ncgc00018200-08 OR ncgc00018200-09 OR ncgc00018200-10 OR ncgc00018200-12 OR ncgc00023694-03 OR ncgc00023694-04 OR ncgc00023694-05 OR ncgc00023694-06 OR ncgc00023694-07 OR ncgc00254039-01 OR ncgc00259768-01 OR ac-14431 OR ak130019 OR bp-30 OR sc-74728 OR st072636 OR sbi-0051481.p003 OR 2+bis+4-hydroxyphenyl+methyl+benzoic+acid OR eu-0082600 OR ft-0659094 OR ns00008592 OR en300-92962 OR alpha+alpha+di+p-hydroxyphenyl+phthalide OR ab00052070_15 OR sr-0 0000112 OR sr-0 0000112-2 OR 3+3-bis+4-hydroxyphenyl+2-benzofuran-1+3h+one+ OR brd-k19227686-001-02-0 OR brd-k19227686-001-12-9 OR z57233591 OR f0921-4309 OR alpha+alpha-di+p-hydroxyphenyl+phthalide OR 1+3h+isobenzofuranone+3+3-bis+4-hydroxyphenyl+ OR 1+3h+isobenzofuranone+3-bis+4-hydroxyphenyl+ OR 2-+bis+4-hydroxyphenyl+methyl+benzoic+acid OR 3+3-bis+p-hydroxyphenyl+1+3h+isobenzofuranone OR 3+3-bis+4-hydroxyphenyl+1+3h+isobenzofuranone OR 3+3-bis+4-hydroxyphenyl+2-benzofuran-1+3h+one OR 3+3-bis+4-hydroxy-phenyl+3h-isobenzofuran-1-one OR 3+3-bis+4-hydroxyphenyl+isobenzofuran-1+3h+one OR 3+3-bis+4-hydroxyphenyl+phthalide OR 3+3-bis+p-hydroxyphenyl+phthalide OR alpha-+p-hydroxyphenyl+-alpha+4-oxo-2+5-cyclohexadien-1-ylidene+o-toluic+acid OR alpha-di+p-hydroxyphenyl+phthalide OR dihydroxyphthalophenone OR fenolftalein OR fenolftaleina OR phenolphtaleine OR phenolphthaleinum OR phthalide+3+3+bis+p-hydroxyphenyl+ OR phthalide+3+-bis+p-hydroxyphenyl+)
3_4-Epoxycyclohexylmethyl_3_4-epoxycyclohexanecarboxylate_nohost	(3+4-epoxycyclohexyl+methyl+3+4-epoxycyclohexylcarboxylate OR 7-oxabicyclo+4+1+0+heptan-3-ylmethyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR 3+4-epoxycyclohexylmethyl+3+4-epoxycyclohexanecarboxylate OR erl-4221 OR ut-632 OR chissonox+221+monomer OR unii-s224del3p4 OR 3+4-epoxycyclohexylmethyl+3+4-epoxycyclohexane+carboxylate OR hsdb+5873 OR einecs+219-207-4 OR ut+632 OR 3+4-epoxycyclohexylmethyl-3+4-epoxycyclohexanecarboxylate OR 3+4-epoxycyclohexanecarboxylic+acid+3+4-epoxycyclohexylmethyl+ester OR brn+1381750 OR 7-oxabicyclo+4+1+0+heptane-3-carboxylic+acid+7-oxabicyclo+4+1+0+hept-3-ylmethyl+ester OR s224del3p4 OR dtxsid2027466 OR 3+4-epoxycyclohexanemethyl+3+4-epoxycyclohexanecarboxylate OR ak-78714 OR dsstox_cid_7466 OR 7-oxabicyclo+4+1+0+hept-3-ylmethyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR dsstox_rid_78463 OR dsstox_gsid_27466 OR w-107371 OR cas-2386-87-0 OR ccris+8882 OR ec+219-207-4 OR schembl24975 OR ksc490c3p OR chembl2143072 OR ctk3j0137 OR bcp32770 OR cel-2021 OR tox21_202388 OR tox21_303312 OR anw-57541 OR akos015915254 OR ks-000001n6 OR ncgc00164163-01 OR ncgc00164163-02 OR ncgc00256981-01 OR ncgc00259937-01 OR as-17792 OR ls-98670 OR sc-19925 OR db-028268 OR ft-0651573 OR ns00011515 OR 3+4-epoxycyclohexylmethyl+3+4-epoxycyclohexanecarb OR a816945 OR q19694494 OR 7-oxabicyclo+4+1+0+heptan-3-yl+methyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR 7-oxabicyclo+4+1+0+heptan-3-ylmethyl+7-oxabicyclo+4+1+0+heptane OR 7-Oxabicyclo+4+1+0+heptan-3-ylmethyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR 3+4-Epoxycyclohexylmethyl+3+4-epoxycyclohexanecarboxylate OR ERL-4221 OR UT-632 OR Chissonox+221+monomer OR UNII-S224DEL3P4 OR 3+4-Epoxycyclohexylmethyl+3+4-epoxycyclohexane+carboxylate OR HSDB+5873 OR 3+4-Epoxycyclohexyl+methyl+3+4-epoxycyclohexylcarboxylate OR EINECS+219-207-4 OR UT+632 OR 3+4-Epoxycyclohexanecarboxylic+acid+3+4-epoxycyclohexylmethyl+ester OR BRN+1381750 OR 7-Oxabicyclo+4+1+0+heptane-3-carboxylic+acid+7-oxabicyclo+4+1+0+hept-3-ylmethyl+ester OR S224DEL3P4 OR DTXSID2027466 OR 7-oxabicyclo+4+1+0+heptan-4-ylmethyl+7-oxabicyclo+4+1+0+heptane-4-carboxylate OR 3+4-Epoxycyclohexanemethyl+3+4-epoxycyclohexanecarboxylate OR AK-78714 OR DSSTox_CID_7466 OR 7-Oxabicyclo+4+1+0+hept-3-ylmethyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR DSSTox_RID_78463 OR DSSTox_GSID_27466 OR W-107371 OR 7-oxabicyclo+4+1+0+hept-3-ylmethyl7-oxabicyclo+4+1+0+heptane-3-carboxylate OR CAS-2386-87-0 OR CCRIS+8882 OR EC+219-207-4 OR 3+4-epoxycyclohexylmethyl3+4-epoxycyclo-hexaneca OR SCHEMBL24975 OR KSC490C3P OR CHEMBL2143072 OR CTK3J0137 OR BCP32770 OR CEL-2021 OR Tox21_202388 OR Tox21_303312 OR ANW-57541 OR AKOS015915254 OR KS-000001N6 OR NCGC00164163-01 OR NCGC00164163-02 OR NCGC00256981-01 OR NCGC00259937-01 OR AS-17792 OR LS-98670 OR SC-19925 OR DB-028268 OR FT-0651573 OR NS00011515 OR 3+4-Epoxycyclohexylmethyl+3+4-epoxycyclohexanecarb OR A816945 OR Q19694494 OR 3+4-epoxycyclohexylmethyl+3+4-epoxy+cyclohexanecarboxylate OR 3+4-epoxycyclohexylmethyl-3+4-epoxycyclohexane+carboxylate OR 7-Oxabicyclo+4+1+0+heptan-3-yl+methyl+7-oxabicyclo+4+1+0+heptane-3-carboxylate OR 7-oxabicyclo+4+1+0+heptane-4-carboxylic+acid+7-oxabicyclo+4+1+0+heptan-4-ylmethyl+ester OR 7-Oxabicyclo+4+1+0+heptan-3-ylmethyl+7-oxabicyclo+4+1+0+heptane)
reaction_products_of_phosphorus_oxychloride_or_phenol_or_isopropylated_phenol	(tris+4-isopropylphenyl+phosphate OR tris+isopropylphenyl+phosphate OR tris+p-isopropylphenyl+phosphate OR unii-y3h2fdx0nw OR triisopropylated+phenyl+phosphate OR y3h2fdx0nw OR phenol+isopropylated+phosphate+3:1 OR dtxsid80858783 OR dsstox_cid_8880 OR dsstox_rid_78659 OR dsstox_gsid_28880 OR c27h33o4p OR phenol+4-+1-methylethyl+-+phosphate+3:1 OR einecs+219-703-0 OR isopropylphenylphosphat OR tricumol+phosphate OR phenolisopropylatedphosphate OR schembl36617 OR chembl458602 OR tri+4-isopropylphenyl+phosphate OR ctk4f8833 OR zinc1583667 OR tox21_202764 OR tox21_202765 OR tox21_202766 OR ethyl+4-methylbenzoyl+acetate OR ncgc00260311-01 OR ncgc00260312-01 OR ncgc00260313-01 OR ns00003997 OR phenol+1-methylethyl+-+phosphate+3:1 OR phosphoric+acid+tris+4-isopropylphenyl+ester OR w-104649 OR w-107139 OR q27294219 OR Tris+4-isopropylphenyl+phosphate OR Tris+isopropylphenyl+phosphate OR Tris+p-isopropylphenyl+phosphate OR UNII-Y3H2FDX0NW OR

	Triisopropylated+phenyl+phosphate OR Y3H2FDX0NW OR Phenol+isopropylated+phosphate+3:1 OR DTXSID80858783 OR DSSTox_CID_8880 OR DSSTox_RID_78659 OR DSSTox_GSID_28880 OR tris+4-propan-2-ylphenyl+phosphate OR C27H33O4P OR Phenol+4-+1-methylethyl+-+phosphate+3:1 OR EINECS+219-703-0 OR Isopropylphenylphosphat OR TRICUMOL+PHOSPHATE OR Phenolisopropylatedphosphate OR SCHEMBL36617 OR CHEMBL458602 OR Tri+4-isopropylphenyl+phosphate OR CTK4F8833 OR ZINC1583667 OR Tox21_202764 OR Tox21_202765 OR Tox21_202766 OR ETHYL+4-METHYLBENZOYL+ACETATE OR NCGC00260311-01 OR NCGC00260312-01 OR NCGC00260313-01 OR NS00003997 OR Phenol+1-methylethyl+-+phosphate+3:1 OR Phosphoric+acid+tris+4-isopropylphenyl+ester OR W-104649 OR W-107139 OR Q27294219) OR ((proximity 3) AND CAS AND (26967-76-0 OR 2502-15-0 OR 68937-41-7))

Appendix D – Search strategies for newly identified chemicals ("Unknown") in news articles

Period	Search	Detail	#articles collected	% relevant articles	Observation	Decision
28-29 September 2020	Unknown chemicals Large	[(novelORnewORunknownORemerging) AND(risk%Orhazard%ORadverseORtoxic)AND(compound%ORsubstance%ORproduct%ORchemical%)]	246	1%	too many non relevant articles	Decision to create a more stringent search using proximity between keywords -> Unknown Chemical WP20
08-14 October 2020	Unknown chemicals Large		9076	2%	Only 16 October was reviewed for relevant articles (641 articles)	
	Unknown Chemical WP20	Word proximity 20 on [(novelORnewORunknownORemerging) AND(risk%ORhazard%ORadverseORtoxic)AND(chemical%)]	27	44%	Introduction of a word proximity between the various semantic concepts and removal of substance, product and compound from the keywords. 4 searches were built on the basis of unknown chemicals WP20.	4 searches are built on unknown_chemical_WP20 to assess the impact of the word product and the impact of extending the semantic block describing "novelty" Unknown Chem_Large_WP20 Unknown Chem_large(noproduct)_WP20 Unknown Chem_su

						perlarge_WP20 UnknownChem_superlarge(noproduct)_WP20
14-16 October 2021	Unknown chemicals Large		5515		Not revised	
	Unknown Chemical WP20		15	32%	High relevancy	
	UnknownChem_Large_WP20	Word proximity 20 on [(novelORnewORunknownORemerging) AND(risk%ORhazard%ORadverseORtoxic)AND(compound%ORsubstance%ORproduct%ORchemical%)]	98	4%	keywords compound/product/substance are added. This generates a drop in relevancy.	
	UnknownChem_large(noproduct)_WP20	Word proximity 20 on [(novelORnewORunknownORemerging) AND(risk%ORhazard%ORadverseORtoxic)AND(compound%Orsubstance%ORchemical%)]	19	25%	The keyword "product" is removed. Relevancy is much better than UnknownChem_Large_WP20	
	UnknownChem_superlarge_WP20	Word proximity 20 on [(novelORnewORunknownORemergingORabnormalORatypicalORfirstORmysteriousORrareORnewlyORunusualORincreasedexposureORincreasedoccurenceORincreasesusceptibilityORincreaseinexposureORincreaseinoccurenceORincreaseinsusceptibilityORascendingtrendORupwardtrendORuptrend)AND(risk%ORhazard%ORadverseORtoxic)AND(compound%Orsubstance%ORchemical%ORproduct%)]	135	6%	Additional keywords added to unknownchem_large_WP20 to extend the semantic block about "novelty". Relevancy is low.	

	UnknownChem_superlarge(noproduct)_WP20	Word proximity 20 on [(novelORnewORunknownORemergingORabnormalORatypicalORfirstORmysteriousORrareORnewlyORunusualORincreasedexposureORincreasedoccurenceORincreasesusceptibilityORincreaseinexposureORincreaseinoccurenceORincreaseinsusceptibilityORascendingtrendORupwardtrendORuptrend)AND(risk%ORhazard%ORadverseORtoxic)AND(compound%Orsubstance%ORchemical%)]	38	16%	Same as UnknownChem_superlarge_WP20 without the keyword product. Relevancy increases back.	Decision to - exclude "product" from the search on unknown risks. - stop looking at the largest category unknown_chemical_large. - enlarge the detection of unknown risks by adding a semantic block on "new regulations" - test a lower word proximity (10).
23-28 October 2021	Unknown Chemical WP20		14	31%		
	UnknownChem_large(noproduct)_WP20		32	35%		
	UnknownChem_superlarge(noprod)_WP20		42	42%		
	UnknownChem_superlarge(noprod)_WP10	Word proximity 10 on [(novelORnewORunknownORemergingORabnormalORatypicalORfirstORmysteriousORrareORnewlyORunusualORincreasedexposureORincreasedoccurenceORincreasesusceptibilityORincreaseinexposureORincreaseinoccurenceORincreaseinsusceptibilityORascendingtrendORupwardtrendORuptrend)AND(risk%ORhazard%ORadverseORtoxic)AND(compound%Orsubstance%ORchemical%)]	14	36%	Relevancy drops a little bit compared to same search with WP at 20, for three times less articles.	

	UnknownChem_megalarge(noprod)_WP20	Word proximity 20 on [("amendment%+regulation%"~5OR"amendment%+legislation%"~5OR"amendment%+law%"~5OR"amendment%+directive%"~5OR"change%+regulation%"~5OR"change%+legislation%"~5OR"change%+law%"~5OR"change%+directive%"~5OR"modification%+regulation%"~5OR"modification%+legislation%"~5OR"modification%+law%"~5OR"modification%+directive%"~5OR"update%+regulation%"~5OR"update%+legislation%~5OR"update%+law%"~5OR"update%+directive%"~5ORnovelORnewORunknownORemergingORabnormalORatypicalORfirstORmysteriousORrareORnewlyORunusualORincreasedexposureORincreasedoccurenceORincreasesusceptibilityORincreaseinexposureORincreaseinoccurenceORincreaseinsusceptibilityORascendingtrendORupwardtrendORuptrend)AND(risk%ORhazard%ORadverseORtoxic)AND(compound%Orsubstance%ORchemical%)]	44	39%	category including the new block on "new regulations". 2 more articles (non relevant) compared to unknownChem_superlarge(noprod)_WP20	
	UnknownChem_megalarge(noprod)_WP10	Word proximity 10 on [("amendment%+regulation%"~5OR"amendment%+legislation%"~5OR"amendment%+law%"~5OR"amendment%+directive%"~5OR"change%+regulation%"~5OR"change%+legislation%"~5OR"change%+law%"~5OR"change%+directive%"~5OR"modification%+regulation%"~5OR"modification%+legislation%"~5OR"modification%+law%"~5OR"modification%+directive%"~5OR"up	13	42%	Less articles but very small gain in relevancy comlpared to same search with WP=20	Decision to - keep WP20 - continue monitor superlarge and megalarge

		date%+regulation%"~5OR"update%+legislation%~5OR"update%+law%"~5OR"update%+directive%"~5ORnovelORnewORunknownORemergingORabnormalORatypicalORfirstORmysteriousORrareORnewlyORunusualORincreasedexposureORincreasedoccurenceORincreasesusceptibilityORincreaseinexposureORincreaseinoccurenceORincreaseinsusceptibilityORascendingtrendORupwardtrendORuptrend)AND(risk%ORhazard%ORadverseORtoxic)AND(compound%Orsubstance%ORchemical%)]				
						17 November 2020: Decision to exclude kw: toxic%, perfume, fragrance, scent
31october-29november 2021	UnknownChem_superlarge(noprod)_WP20		194	20%		
	UnknownChem_megalarge(noprod)_WP20		201	20%	almost no differences between UnknownChem_superlarge(noprod)_WP20 and UnknownChem_megalarge(noprod)_WP20.	Decision to look only from now on at UnknownChem_megalarge(noprod)_WP20
16december2020-14January2021	UnknownChem_megalarge(noprod)_WP20		280	11%	significant drop in relevancy. No explanation. NOT keywords will be explored.	Decision to find NOT KW to add
						31 January 2021: Decision to add a NOT KW (stock

						market) and to divide the search in two parts (WP10 for novel block, WP20 for regulatio n block)
31Jan-15Feb 2021	UnknownChe m_megalarge(noprod)_WP20		158	12%		
	megalargeplus plus_2partsno prodNOTword _WP20	Word proximity 10 on [(novelORnewORun knownORemerging ORabnormalORatyp icalORfirstORmyster iousORrareORnewly ORunusualORincrea sedexposureORincr easedoccurenceORi ncreasesusceptibilit yORincreaseinexpos ureORincreaseinocc urenceORincreasein susceptibilityORasc endingtrendORupw ardtrendORuptrend)AND(risk%ORhaza rd%ORadverseORto xic)AND(compound %Orsubstance%OR chemical%)NOT(sto ckmarket)] OR Word proximity 20 on [(“amendment%+r egulation%”~5OR“ amendment%+legi slation%”~5OR“am endment%+law%” ~5OR“amendment %+directive%”~5O R“change%+regula tion%”~5OR“chang e%+legislation%”~ 5OR“change%+law %”~5OR“change% +directive%”~5OR“ modification%+reg ulation%”~5OR“mo dification%+legislat ion%”~5OR“modific ation%+law%”~5O R“modification%+di rective%”~5OR“up date%+regulation %”~5OR“update% +legislation%~5OR “update%+law%”~ 5OR“update%+dire ctive%”~5OR)AND(	72	15%	Decrease of number of articles by 2 and increase of relevancy of the articles collected.	

		risk%ORhazard%ORadverseORtoxic)AND(compound%ORsubstance%ORchemical%)NOT(stockmarket)]				
	Final optimised search:	Word proximity 10 on [(novelORnewORunknownORemergingORabnormalORatypicalORfirstORmysteriousORrareORnewlyORunusualORincreasedexposureORincreasedoccurenceORincreasesusceptibilityORincreaseinexposureORincreaseinoccurenceORincreaseinsusceptibilityORascendingtrendORupwardtrendORuptrend)AND(risk%ORhazard%ORadverseORtoxic)AND(compound%Orsubstance%ORchemical%)NOT(stockmarketORkamala_harrisORbidenORnavalnyORvaccination)] OR Word proximity 20 on [(“amendment%+regulation%”~5OR“amendment%+legislation%”~5OR“amendment%+law%”~5OR“amendment%+directive%”~5OR“change%+regulation%”~5OR“change%+legislation%”~5OR“change%+law%”~5OR“change%+directive%”~5OR“				22 February 2021: Decision to improve megalargeplusplus_2partsnoprodNOTword_WP20 with NOT KW (Joe biden, president Biden, Kamala Harris, Vice president harris, navalny, vaccination) This search is considered as the optimised search for unknown chemicals

		modification%+regulation%"~5OR"modification%+legislation%"~5OR"modification%+law%"~5OR"modification%+directive%"~5OR"update%+regulation%"~5OR"update%+legislation%~5OR"update%+law%"~5OR"update%+directive%"~5OR)AND(risk%ORhazard%ORadverseORtoxic)AND(compound%Orsubstance%ORchemical%) NOT(stockmarketORkamala_harrisORbidenORnavalnyORvaccination)]				

Appendix E – Results of first screening for known chemicals in news (period 1st July 2021 ->31st August 2022)

Chemical	Collected articles	relevant articles	% relevant
1_3-Bis_citraconimidomethylene_benzene	0	0	-
1_3-Dimethyl-3_4_5_6-tetrahydro-2_1H_-py	1	0	0.00%
1_3-Divinylimidazolidin-2-one	0	0	-
1-Propanone_2_methyl_1_4_methylthiopheny	6	0	0.00%
2_3-dihydro-2_2-dimethyl-1h-perimidine	0	0	-
2_4_-Diphenylmethane_diisocyanate	0	0	-
2_4_hydroxy_benzophenone	3	0	0.00%
2_5-diaminotoluene	4	1	25.00%
2_chloroaniline	4	0	0.00%
2_naphtalenamine	0	0	-
3 4-Epoxycyclohexylmethyl	0	0	-
4_4_-Methylenebis_2_chloroaniline_	5	0	0.00%
4_4_-Oxybis_benzenesulfonyl_hydrazide	3	0	0.00%
4_4Bis-dimethylamino-4-methylamino_trity	0	0	-
4-aminophenol	0	0	-
4-Chloro-2_5-dimethoxyacetoacetanilide	1	0	0.00%
Antioxydant_2246	89	1	1.12%
Bis_2_4-dichlorobenzoyl_peroxide	3	0	0.00%
Bis_2_6-diisopropylphenyl_carbodiimide	0	0	-
Chloral hydrate	0	0	-
cyclonite	16	0	0.00%
Dicyclohexyl_phthalate	3	0	0.00%
Diphenylmethane diisocyanate	0	0	-
Diphenylmethane_2_2_diisocyanate	1	0	0.00%
Diuron	4	1	25.00%
Glycerol_triglycidyl_ether	0	0	-
Methyl_N-_3-acetylamino_-4-_2-cyano-4-ni	0	0	-
n_nprime-di-sec-butyl-p-phenylenediamine	0	0	-
paranitronaniline	4	0	0.00%
phenol_2_2_-_1-methyl-1_2-ethanediyl_bis	0	0	-
Phenolphtaleine	1	0	0.00%
Phenylene-1_4-bis-benz-1_3-oxazin-4-one	0	0	-
phenylnaphtylamine	6	0	0.00%
Phosphorothioic_acid_OOO-triphenyl_ester	0	0	-
Piperonyl_butoxide	28	0	0.00%
propane_thiol	0	0	-

reaction_products_of_phosphorus_oxychlor	0	0	-
Retinol	1	0	0.00%
retinol_acetate	4	0	0.00%
Retinol_proprionate	2	0	0.00%
Retinyl_palmitate	32	0	0.00%
solvent_blue_35	0	0	-
Solvent_blue_4	0	0	-
solvent_yellow_124	3	0	0.00%
Tegdme	6	0	0.00%
tetraethylene_glycol_ethyl_methyl_ether	0	0	-
tk11-319	1	0	0.00%
Triphenyl_phosphite	1	0	0.00%
Triphenylphosphine	0	0	-
Tris_1_3-dichloro-2-propyl_phosphate	11	1	9.09%
Trixylenyl_phosphate	0	0	-
Articles collexcted between 1 july 2021 and 31 August 2022			
BPA, Tetrabromobisphenol-A, hexabromocyclododecane, 9,10-anthraquinone: not evaluated			

Appendix F – Search strategies for newly identified chemicals ("Unknown") in scientific publications

Dataset name	Simplified search	N docs 2020	Search strings
01. Unknown	[Chemical risks OR chemical hazards OR substance risks OR substance hazards OR substance adverse OR compound risk OR compound hazard OR compound adverse OR contaminant risk OR contaminant hazard OR contaminant adverse OR chemical toxic] AND [2019 TO *] NOT (emergency preparedness; emergency management; substance use; psychoactive; psychotropic; abuse)	266	topic:(("novel chemical risk"~10 OR "new chemical risk"~10 OR "emerging chemical risk"~10 OR "unknown chemical risk"~10 OR "rare chemical risk"~10 OR "newly chemical risk"~10 OR "unusual chemical risk"~10) OR ("novel chemical hazard"~10 OR "new chemical hazard"~10 OR "emerging chemical hazard"~10 OR "unknown chemical hazard"~10 OR "abnormal chemical hazard"~10 OR "atypical chemical hazard"~10 OR "first chemical hazard"~10 OR "mysterious chemical hazard"~10 OR "rare chemical hazard"~10 OR "newly chemical hazard"~10 OR "unusual chemical hazard"~10) OR ("novel chemical adverse"~10 OR "new chemical adverse"~10 OR "emerging chemical adverse"~10 OR "unknown chemical adverse"~10 OR "abnormal chemical adverse"~10 OR "atypical chemical adverse"~10 OR "first chemical adverse"~10 OR "mysterious chemical adverse"~10 OR "rare chemical adverse"~10 OR "newly chemical adverse"~10 OR "unusual chemical adverse"~10) OR ("novel substance risk"~10 OR "new substance risk"~10 OR "emerging substance risk"~10 OR "unknown substance risk"~10 OR "rare substance risk"~10 OR "newly substance risk"~10 OR "unusual substance risk"~10) OR ("novel substance hazard"~10 OR "new substance hazard"~10 OR "emerging substance hazard"~10 OR "unknown substance hazard"~10 OR "abnormal substance hazard"~10 OR "atypical substance hazard"~10 OR "first substance hazard"~10 OR "mysterious substance hazard"~10 OR "rare substance hazard"~10 OR "newly substance hazard"~10 OR "unusual substance hazard"~10) OR ("novel substance adverse"~10 OR "new substance adverse"~10 OR "emerging substance adverse"~10 OR "unknown substance adverse"~10 OR "abnormal substance adverse"~10 OR "atypical substance adverse"~10 OR "first substance adverse"~10 OR "mysterious substance adverse"~10 OR "rare substance adverse"~10 OR "newly substance adverse"~10 OR "unusual substance adverse"~10) OR ("novel compound risk"~10 OR "new compound risk"~10 OR "emerging compound risk"~10 OR "unknown compound risk"~10 OR "rare compound risk"~10 OR "newly compound risk"~10 OR "unusual compound risk"~10) OR ("novel compound hazard"~10 OR "new compound hazard"~10 OR "emerging compound hazard"~10 OR "unknown compound hazard"~10 OR "abnormal compound hazard"~10 OR "atypical compound hazard"~10 OR "first compound hazard"~10 OR "mysterious compound hazard"~10 OR "rare compound hazard"~10 OR "newly compound hazard"~10 OR "unusual compound hazard"~10) OR

			("novel compound adverse"~10 OR "new compound adverse"~10 OR "emerging compound adverse"~10 OR "unknown compound adverse"~10 OR "abnormal compound adverse"~10 OR "atypical compound adverse"~10 OR "first compound adverse"~10 OR "mysterious compound adverse"~10 OR "rare compound adverse"~10 OR "newly compound adverse"~10 OR "unusual compound adverse"~10) OR ("novel contaminant risk"~10 OR "new contaminant risk"~10 OR "emerging contaminant risk"~10 OR "unknown contaminant risk"~10 OR "rare contaminant risk"~10 OR "newly contaminant risk"~10 OR "unusual contaminant risk"~10) OR ("novel contaminant hazard"~10 OR "new contaminant hazard"~10 OR "emerging contaminant hazard"~10 OR "unknown contaminant hazard"~10 OR "abnormal contaminant hazard"~10 OR "atypical contaminant hazard"~10 OR "first contaminant hazard"~10 OR "mysterious contaminant hazard"~10 OR "rare contaminant hazard"~10 OR "newly contaminant hazard"~10 OR "unusual contaminant hazard"~10) OR ("novel contaminant adverse"~10 OR "new contaminant adverse"~10 OR "emerging contaminant adverse"~10 OR "unknown contaminant adverse"~10 OR "abnormal contaminant adverse"~10 OR "atypical contaminant adverse"~10 OR "first contaminant adverse"~10 OR "mysterious contaminant adverse"~10 OR "rare contaminant adverse"~10 OR "newly contaminant adverse"~10 OR "unusual contaminant adverse"~10) OR ("novel chemical toxic"~10 OR "new chemical toxic"~10 OR "emerging chemical toxic"~10 OR "unknown chemical toxic"~10 OR "rare chemical toxic"~10 OR "newly chemical toxic"~10 OR "unusual chemical toxic"~10)OR "unintended chemical"~3) AND emm_year:[2019 TO *] NOT (topic:("emergency preparedness"~10 OR "emergency management"~3 OR "substance use") OR ti:(psychoactive OR psychotropic OR abuse))

Appendix G – Relevant articles from TIM Technology for known chemicals

Analysis of samples of explosives excavated from the Baltic Sea floor[12]

Chemical: cyclonite

Abstract: After World War II, conventional and chemical ammunition containing mainly secondary and primary explosives was dumped in the sea. Explosives have medium toxicity to aquatic organisms, earthworms and indigenous soil microorganisms. Therefore, environmental monitoring is required, especially for dumped munitions. The main aspect of this work was to analyse the samples of lumps and sediments taken from the Baltic seabed. These samples were potentially explosives. The main goal of the study was to identify the type and composition of studied materials. In order to determine the chemical composition of samples of explosives, we used as follows: GC–MS/MS, LC-HRMS and NMR. Additionally, to determine the energetic properties we performed microcalorimetric-thermogravimetric analysis. Based on the obtained results, the composition of this explosive was TNT (41%), RDX (53%), aluminium powder (5%), and degradation products (below 1%). The resulting composition indicates that the analysed material can be classified in the "torpex" family, widely used during World War II. Regarding the results of the microcalorimetric analysis, we can conclude that excavated fragments of explosives are in very good condition and they still can detonate after being initiated. Therefore, there is a threat that they could be used for criminal or terrorist purposes.

First evidence of explosives and their degradation products in dab (Limanda limanda L.) from a munition dumpsite in the Baltic Sea[13]

Chemical: cyclonite

Abstract: Corrosion and disintegration of munition shells from the World Wars increase the risk that explosives are released into the marine environment, exposing a variety of organisms. Only few studies investigated contamination of fish with explosives in the field under environmental conditions. Here we present a comprehensive study on the contamination status of dab (Limanda limanda) from a munition dumpsite and from reference sites in the Baltic Sea. Bile of 236 dab from four different study sites, including a dumpsite for conventional munitions, was investigated and explosive compounds were detected by high performance liquid chromatography-mass spectrometry. Five explosive compounds were identified, including 2,4,6-trinitrotoluene, 4-amino-2,6-dinitrolouene, and hexahydro-1,3,5-trinitro-1,3,5-triazine. 48% of the samples from the dumpsite contained at least one explosive compound. The results prove that toxic explosive compounds from a dumpsite in the Baltic Sea are accumulated by flatfish and may therefore pose a risk to fish health and human food safety.

Non-occupational exposure to phthalates in Finland[14]

Chemical: Dicyclohexyl_phthalate

Abstract:

The aim of this study was to assess phthalate exposure of non-occupationally exposed working aged population in Finland.

[12] Link: http://doi.org/10.1016/j.scitotenv.2019.135198
[13] Link: http://doi.org/10.1016/j.marpolbul.2020.111131
[14] Link: http://doi.org/10.1016/j.toxlet.2020.06.021

Metabolites of DEP, DnBP and DiBP were detected in all the first morning void urine samples of the non-occupationally exposed volunteers (n = 60; 42 women and 18 men; aged 25–63). Metabolite of BBP and secondary metabolites of DEHP and DiNP were detected in >90% of the samples. The phthalate metabolite levels were mostly comparable to the published levels in adult population in Europe and the US. One notable difference was the observed higher exposure of the Finnish study population to DnBP in comparison to the German, Austrian, Norwegian and US populations. In most cases, higher exposure to phthalates was seen in females in comparison to males, which is in accordance with other studies. The urinary levels were compared to the biomonitoring equivalents (BEs), which were calculated on the basis of published DNELs (derived no-effect levels). The P95 levels of individual phthalates remained below the respective Bes. Using the P95 levels, combined exposure to DnBP, DiBP, DEHP and BBP resulted in risk characterization ratio exceeding 1. This suggests a need to limit the exposure to these phthalates.

Suspect and Nontarget Screening for Contaminants of Emerging Concern in an Urban Estuary[15]

Chemical: Diuron

Abstract:

This study used suspect and nontarget screening with high-resolution mass spectrometry to characterize the occurrence of contaminants of emerging concern (CECs) in the nearshore marine environment of Puget Sound (WA). In total, 87 non-polymeric CECs were identified; those confirmed with reference standards (45) included pharmaceuticals, herbicides, vehicle-related compounds, plasticizers, and flame retardants. Eight polyfluoroalkyl substances were detected; perfluorooctanesulfonic acid (PFOS) concentrations were as high as 72–140 ng/L at one location. Low levels of methamphetamine were detected in 41% of the samples. Transformation products of pesticides were tentatively identified, including two novel transformation products of tebuthiuron. While a hydrodynamic simulation, analytical results, and dilution calculations demonstrated the prevalence of wastewater effluent to nearshore marine environments, the identity and abundance of selected CECs revealed the additional contributions from stormwater and localized urban and industrial sources. For the confirmed CECs, risk quotients were calculated based on concentrations and predicted toxicities, and eight CECs had risk quotients >1. Dilution in the marine estuarine environment lowered the risks of most wastewater-derived CECs, but dilution alone is insufficient to mitigate risks of localized inputs. These findings highlighted the necessity of suspect and nontarget screening and revealed the importance of localized contamination sources in urban marine environments.

[15] Link: http://doi.org/10.1021/acs.est.9b06126

Appendix H – Relevant articles from TIM Technology for newly identified chemicals

A Review of Environmental Occurrence, Fate, and Toxicity of Novel Brominated Flame Retardants[16]

Use of legacy brominated flame retardants (BFRs), including polybrominated diphenyl ethers (PBDEs) and hexabromocyclododecane (HBCD), has been reduced due to adverse effects of these chemicals. Several novel brominated flame retardants (NBFRs), such decabromodiphenyl ethane (DBDPE) and bis(2,4,6-tribromophenoxy) ethane (BTBPE), have been developed as replacements for PBDEs. NBFRs are used in various industrial and consumer products, which leads to their ubiquitous occurrence in the environment. This article reviews occurrence and fate of a select group of NBFRs in the environment, as well as their human exposure and toxicity. Occurrence of NBFRs in both abiotic, including air, water, dust, soil, sediment and sludge, and biotic matrices, including bird, fish, and human serum, have been documented. Evidence regarding the degradation, including photodegradation, thermal degradation and biodegradation, and bioaccumulation and biomagnification of NBFRs is summarized. The toxicity data of NBFRs show that several NBFRs can cause adverse effects through different modes of action, such as hormone disruption, endocrine disruption, genotoxicity, and behavioral modification. The primary ecological risk assessment shows that most NBFRs exert no significant environmental risk, but it is worth noting that the result should be carefully used owing to the limited toxicity data.

Measured concentrations of consumer product chemicals in California house dust: Implications for sources, exposure, and toxicity potential[17]

Indoor dust is a reservoir for commercial consumer product chemicals, including many compounds with known or suspected health effects. However, most dust exposure studies measure few chemicals in small samples. We systematically searched the U.S. indoor dust literature on phthalates, replacement flame retardants (RFRs), perfluoroalkyl substances (PFASs), synthetic fragrances, and environmental phenols and estimated pooled geometric means (GMs) and 95% confidence intervals for 45 chemicals measured in ≥3 data sets. In order to rank and contextualize these results, we used the pooled GMs to calculate residential intake from dust ingestion, inhalation, and dermal uptake from air, and then identified hazard traits from the Safer Consumer Products Candidate Chemical List. Our results indicate that U.S. indoor dust consistently contains chemicals from multiple classes. Phthalates occurred in the highest concentrations, followed by phenols, RFRs, fragrance, and PFASs. Several phthalates and RFRs had the highest residential intakes. We also found that many chemicals in dust share hazard traits such as reproductive and endocrine toxicity. We offer recommendations to maximize comparability of studies and advance indoor exposure science. This information is critical in

[16] Link: https://doi.org/10.1021/acs.est.9b03159
[17] Link: https://doi.org/10.1111/ina.12607

shaping future exposure and health studies, especially related to cumulative exposures, and in providing evidence for intervention development and public policy.

Benchmarking the in Vitro Toxicity and Chemical Composition of Plastic Consumer Products[18]

Plastics are known sources of chemical exposure and few, prominent plastic-associated chemicals, such as bisphenol A and phthalates, have been thoroughly studied. However, a comprehensive characterization of the complex chemical mixtures present in plastics is missing. In this study, we benchmark plastic consumer products, covering eight major polymer types, according to their toxicological and chemical signatures using in vitro bioassays and nontarget high-resolution mass spectrometry. Most (74%) of the 34 plastic extracts contained chemicals triggering at least one end point, including baseline toxicity (62%), oxidative stress (41%), cytotoxicity (32%), estrogenicity (12%), and antiandrogenicity (27%). In total, we detected 1411 features, tentatively identified 260, including monomers, additives, and nonintentionally added substances, and prioritized 27 chemicals. Extracts of polyvinyl chloride (PVC) and polyurethane (PUR) induced the highest toxicity, whereas polyethylene terephthalate (PET) and high-density polyethylene (HDPE) caused no or low toxicity. High baseline toxicity was detected in all "bioplastics" made of polylactic acid (PLA). The toxicities of low-density polyethylene (LDPE), polystyrene (PS), and polypropylene (PP) varied. Our study demonstrates that consumer plastics contain compounds that are toxic in vitro but remain largely unidentified. Since the risk of unknown compounds cannot be assessed, this poses a challenge to manufacturers, public health authorities, and researchers alike. However, we also demonstrate that products not inducing toxicity are already on the market.

Insights from TSCA Reform: a Case for Identifying New Emerging Contaminants[19]

Federal and state environmental agencies regulate chemicals under a variety of environmental laws. The Lautenberg Chemical Safety for the 21st Century Act (LCSA) amended the Toxic Substances Control Act (TSCA) in 2016, and this update provides a mechanism by which the U.S. Environmental Protection Agency (USEPA) can regulate chemicals used by industry in order to prevent or limit exposures to chemicals. In particular, TSCA requires USEPA to assess the risk of injury to human health or the environment from exposure to chemicals identified as active. USEPA is currently assessing 10 chemicals and recently identified another 20 high priority and 20 low priority chemicals for evaluation. These risk evaluations, which may reflect new toxicological data, may identify new dose-response factors that change our understanding of the toxicity of many chemicals. This could result in either restrictions to chemical use, new cleanup standards, or more stringent cleanup standards. In this article, the authors review the process for identifying high priority chemicals and make predictions for the next set of emerging chemicals. Regulation of these chemicals could lead to a requirement for process changes as well as identify additional chemicals for evaluation at hazardous waste sites.

[18] Link: https://pubs.acs.org/doi/10.1021/acs.est.9b02293
[19] Link: https://doi.org/10.1007/s40726-019-00117-4

First nationwide investigation and environmental risk assessment of 72 pharmaceuticals and personal care products from Sri Lankan surface waterways[20]

Pharmaceuticals and personal care products (PPCPs) are known as an emerging class of water contaminants due to their potential adverse effects on aquatic ecosystems. In this study, we conducted the first nationwide survey to understand the distribution and environmental risk of 72 PPCPs in surface waterways of Sri Lanka. Forty-one out of 72 targeted compounds were detected with total concentrations ranging between 5.49 and 993 ng/L in surface waterways in Sri Lanka. The highest level of PPCP contamination was detected in an ornamental fish farm. Sulfamethoxazole was found with the highest concentration (934 ng/L) followed by N,N-diethyl-meta-toluamide (202 ng/L) and clarithromycin (119 ng/L). Diclofenac, mefenamic acid, ibuprofen, trimethoprim, and erythromycin were detected ubiquitously throughout the country. Our data revealed that hospital and domestic wastewater, and aquaculture activities potentially contribute to the presence of PPCPs in Sri Lankan waterways. The calculated risk quotients indicated that several locations face medium to high ecological risk to aquatic organisms from ibuprofen, sulfamethoxazole, diclofenac, mefenamic acid, tramadol, clarithromycin, ciprofloxacin, triclocarban, and triclosan. The aforementioned compounds could affect aquatic organisms from different trophic levels like algae, crustacean and fish, and also influence the emergence of antibiotic resistant bacteria. These findings emphasize that a wide variety of pharmaceuticals have become pervasive environmental contaminants in the country. This data will serve to expand the inventory of global PPCP pollution. Further monitoring of PPCPs is needed in Sri Lanka in order to identify PPCP point sources and to implement strategies for contaminant reduction in wastewater to protect the aquatic ecosystem, wildlife, and human health.

Environmental risks associated with contaminants of legacy and emerging concern at European aquaculture areas[21]

The contamination of marine ecosystems by contaminants of emerging concern such as personal care products or per- and polyfluoroalkyl substances is of increasing concern. This work assessed the concentrations of selected contaminants of emerging concern in water and sediment of European aquaculture areas, to evaluate their co-variation with legacy contaminants (polycyclic aromatic hydrocarbons) and faecal biomarkers, and estimate the risks associated with their occurrence. The 9 study sites were selected in 7 European countries to be representative of the aquaculture activities of their region: 4 sites in the Atlantic Ocean and 5 in the Mediterranean Sea. Musks, UV filters, preservatives, per- and polyfluoroalkyl substances and polycyclic aromatic hydrocarbons were detected in at least one of the sites with regional differences. While personal care products appear to be the main component of the water contamination, polycyclic aromatic hydrocarbons were mostly found in sediments. As expected, generally higher levels of personal care products were found in sewage impacted sites, urbanised coasts and estuaries. The risk assessment for water and sediment revealed a potential risk for the local aquatic environment from contaminants of both legacy and emerging concern, with a significant contribution of the UV filter octocrylene. Despite marginal contributions of per- and polyfluoroalkyl substances to the total concentrations, PFOS (perfluorooctane sulfonate) aqueous

[20] Link: https://doi.org/10.1016/j.scitotenv.2019.07.042
[21] Link: https://doi.org/10.1016/j.envpol.2019.05.133

concentrations combined to its low ecotoxicity thresholds produced significant hazard quotients indicating a potential risk to the ecosystems.

Phytotoxins eliminated by milk: A review[22]

Milk is a complex emulsion of lipids suspended in aqueous protein solution that can be a carrier of various contaminants, but generally it is not an important route of toxic excretion. The main problem is chronic repetitive exposure, as it occurs with ingestion of toxic plants and its potential danger to animals that consume the milk. Previously reported hazardous phytotoxins eliminated by milk include: indolizidine alkaloids, causing oligosaccharide storage disease; piperidine alkaloids, causing acute poisoning or malformations; pyrrolizidine alkaloids, which cause hepatic lesions; quinolizidine alkaloids, as a cause of skeletal defects; glucosinolates, which cause changes in the thyroid; tremetol (or tremetone), which causes a disease characterized by tremors in animals and milk sickness in humans; sodium monofluoracetate, which causes the death of kids after ingestion of colostrum from goats that have ingested Amorimia septentrionalis during gestation; ptaquiloside, which induces carcinogenesis in animals that ingest milk or derivatives produced by animals that have ingested Pteridium spp. Ipomoea asarifolia, which contains indole diterpenes causing tremors in suckling pups. Chrysocoma ciliata causes alopecia in suckling pups, but its toxic compound is still unknown. Knowledge about the risk of exposure to these substances via milk and its dissemination are important for veterinary and human health. (New hazard, New/increased exposure).

The occurrence, potential toxicity, and toxicity mechanism of bisphenol S, a substitute of bisphenol A: A critical review of recent progress[23]

Bisphenol S (BPS) has been introduced into the industry as a safer alternative to bisphenol A (BPA). The distribution of BPS has recently become an important issue worldwide, but investigations on the toxicity and mechanisms of BPS remain limited. A review of the literature reveals that BPS has widespread presence in environmental media, such as indoor dust, surface water, sediments, and sewage sludge. It has been detected in plants, paper products, some food items, and even in the human body. In addition, compared to BPA, BPS has a lower acute toxicity, similar or less endocrine disruption, similar neurotoxicity and immunotoxicity, and lower reproductive and developmental toxicity. The mechanisms underlying BPS toxicity may be related to the chemical properties of BPS in the human body, including interactions with estrogen receptors, and binding to DNA and some proteins, subsequently including exerting oxidative stress. However, further investigation on the potential risks of BPS to humans and its mechanisms of toxicity should be conducted to better understand and control the risks of such novel chemicals.

[22] Link: https://doi.org/10.1590/1678-5150-PVB-6058
[23] Link: https://doi.org/10.1016/j.ecoenv.2019.01.114

Uptake and accumulation of emerging contaminants in soil and plant treated with wastewater under real-world environmental conditions in the Al Hayer area (Saudi Arabia)[24]

In arid and semi-arid areas the use of treated wastewater for crop irrigation and other agricultural practices, such as the use of pesticides, increase the number of emerging contaminants (ECs) in crops. Hazards of these practices to human being are largely unknown since there are few studies yet covering a short range of compounds and most of them under non-realistic conditions. This study aims at assessing this problem that will become global soon in an area of Saudi Arabia heavily affected by the reuse of treated wastewater and pesticide in order to ascertain its scale. The novelty of the study relays in the large number of ECs covered and the variety of crops (cabbage, barley, green beans, eggplants, chili, tomato and zucchini) analysed. Extraction procedure developed provided an appropriate extraction yield (up to 50% of the compounds were recovered within a 70–120% range), with good repeatability (relative standard deviations below 20% in most cases) and sensitivity (LOQ < 25 ng g−1) for the model compounds. Determination by liquid chromatography quadrupole time-of-flight (LC-QqTOF-MS) is able to identify >2000 contaminants. Sixty-four ECs were identified in wastewater but of the sixty-four compounds, six pharmaceuticals (atenolol, caffeine, carbamazepine and its metabolites 10,11-epoxycarbamazepine, gemfibrozil, and naproxen) and seven pesticides (acetamiprid, atrazine deethyl, azoxystrobin, bupirimate, diazinon, malathion, pirimicarb and some of their metabolites) were detected in plants. Furhermore, one metabolite of the ibuprofen (not detected in water or soil), the ibuprofen hexoside was also found in plants. Up to our knowledge, this study demonstrate for the first time the accumulation of ECs in crops irrigated with treated wastewater under real non-controlled environmental conditions.

A review of a class of emerging contaminants: The classification, distribution, intensity of consumption, synthesis routes, environmental effects and expectation of pollution abatement to organophosphate flame retardants (opfrs)[25]

Organophosphate flame retardants (OPFRs) have been detected in various environmental matrices and have been identified as emerging contaminants (EC). Given the adverse influence of OPFRs, many researchers have focused on the absorption, bioaccumulation, metabolism, and internal exposure processes of OPFRs in animals and humans. This paper first reviews the evolution of various types of flame retardants (FRs) and the environmental pollution of OPFRs, the different absorption pathways of OPFRs by animals and humans (such as inhalation, ingestion, skin absorption and absorption), and then summarizes the environmental impacts of OPFRs, including their biological toxicity, bioaccumulation, persistence, migration, endocrine disruption and carcinogenicity. Based on limited available data and results, this study also summarizes the bioaccumulation and biomagnification potential of OPFRs in different types of biological and food nets. In addition, a new governance idea for the replacement of existing OPFRs from the source is proposed, seeking environmentally friendly alternatives to OPFRs in order to provide new ideas and theoretical guidance for the removal of OPFRs.

[24] Link: https://doi.org/10.1016/j.scitotenv.2018.10.224
[25] Link: https://doi.org/10.3390/ijms20122874

Realistic low-doses of two emerging contaminants change size distribution of an annual flowering plant population[26]

HHCB [1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylcyclopenta(g)-2-benzopyran] and 4-tert-octylphenol [4-(1,1,3,3-tetramethylbutyl)phenol] are widely used emerging contaminants that have the potential to cause adverse effects in the environment. The purpose of this study was to observe if and how environmentally realistic concentrations of these contaminants alter growth in plant populations. It was hypothesized that within an exposed Gypsophila elegans Bieb (annual baby's breath) population especially fast-growing seedlings are impaired even when the population mean is unaffected, and small doses can cause hormesis and, thus, an increase in shoot or root length. In a dose-response experiment, an experimental population of G. elegans was established (total 15.600 seeds, 50 seeds per replicate, 24 replicates per concentration, 5.2 seedlings/cm2) and exposed to 12 doses of HHCB or 4-tert-octylphenol. After five days, shoot and root length values were measured and population averages, as well as slow- and fast-growing subpopulations, were compared with unexposed controls. Growth responses were predominantly monophasic. HHCB seemed to selectively inhibit both root and shoot elongation among slow- and fast-growing individuals, while 4-tert-octylphenol selectively inhibited both root and shoot elongation of mainly fast-growing seedlings. The ED50 values (dose causing 50% inhibition) revealed that the slow-growing seedlings were more sensitive and fast-growing seedlings less sensitive than the average of all individuals. Although there was toxicant specific variation between the effects, selective toxicity was consistently found among both slow- and fast-growing plants starting already at concentrations of 0.0067 µM, that are usually considered to be harmless. This study indicates that these contaminants can change size distribution of a plant population at low concentrations in the nM/µM range.

Fingerprinting Plastic-Associated Inorganic and Organic Matter on Plastic Aged in the Marine Environment for a Decade [27]

The long-term aging of plastic leads to weathering and biofouling that can influence the behavior and fate of plastic in the marine environment. This is the first study to fingerprint the contaminant profiles and bacterial communities present in plastic-associated inorganic and organic matter (PIOM) isolated from 10 year-aged plastic. Plastic sleeves were sampled from an oyster aquaculture farm and the PIOM was isolated from the intertidal, subtidal, and sediment-buried segments to investigate the levels of metal(loid)s, polyaromatic hydrocarbons (PAHs), per-fluoroalkyl substances (PFAS) and explore the microbial community composition. Results indicated that the PIOM present on long-term aged high-density polyethylene plastic harbored high concentrations of metal(loid)s, PAHs, and PFAS. Metagenomic analysis revealed that the bacterial composition in the PIOM differed by habitat type, which consisted of potentially pathogenic taxa including Vibrio, Shewanella, and Psychrobacter. This study provides new insights into PIOM as a potential sink for hazardous environmental contaminants and its role in enhancing the vector potential of plastic. Therefore, we recommend the inclusion of PIOM analysis in current biomonitoring regimes and that plastics be used with caution in aquaculture

[26]Link: https://doi.org/10.1007/s10646-019-02069-3
[27]Link: https://doi.org/10.1021/acs.est.1c00262

settings to safeguard valuable food resources, particularly in areas of point-source contamination.

Identification of chemicals of emerging concern in urine of Flemish adolescents using a new suspect screening workflow for LC-QTOF-MS.[28]

An essential step in human biomonitoring or molecular epidemiology programs is to estimate human exposure to environmental chemicals. Despite significant progress in the capabilities of analytical methods, the number of pollutants and their metabolites keeps increasing continuously. Some of these relatively unknown chemicals of emerging concern (CECs) may pose significant health risks to humans and biota, but remain virtually undetected in traditional HBM-studies. Non-target and suspect screening techniques based on high-resolution mass spectrometry (HRMS) perform the detection and identification of compounds without any a priori compound selection or chemical information and provide a more holistic overview of human exposure. In this study, 50 urine samples (25 female and 25 male) from a larger cohort of the Flemish Environment and Health Study (FLEHS IV, 2016–2020) have been submitted to suspect screening analysis, with the aim of detecting and identifying new CECs. For this purpose, an analytical method has been developed, optimised and evaluated in terms of analytical performance. Satisfactory results were obtained in terms of reproducibility, sensitivity and quality control. Data-mining was performed through the combination of two different workflows. The use of two complementary workflows enhanced the number of identified compounds. As a result, 45 CECs have been identified with a level of confidence ranged between 3 and 1. Most of the identified compounds were metabolisation products, many of which were currently not included in the targeted measurements of FLEHS IV. The identified chemicals and metabolites could be used as candidate biomarkers of exposure in future studies. Overall, the newly developed suspect screening workflow of this pilot study provided complementary and promising results for future HBM-programs.

Airborne Microplastics: A Review on the Occurrence, Migration and Risks to Humans:[29]

As emerging environmental contaminants, microplastics may cause potential hazard to global ecosphere (including water, soil and air) and human health. To date, the occurance and ecological effects of microplastics in water and soil were systematically summarized. However, there are few reviews of microplastics in air (i.e. airborne microplastics). Recently, microplastics have been observed in atmospheric fallout collected from some areas. Although the studies are limited, most of the research showed that synthetic textiles are the main source of airborne microplastics, and fibers are the dominant shape. Airborne microplastics are contributors to microplastic pollution in aquatic and soil environments. In addition, airborne microplastics can be directly inhaled and posed health risks to humans. Therefore, this review summarized the current knowledge and provide insights into further research to better understand airborne microplastics and their risks to human.

[28] Link: https://doi.org/10.1016/j.chemosphere.2021.130683
[29] Link: https://doi.org/10.1007/s00128-021-03180-0

Occurrence and distribution of uv filters in beach sediments of the southern baltic seacoast:[30]

The interest in UV filters' occurrence in the environment has increased since they were recognized as "emerging contaminants" having potentially adverse impacts on many ecosystems and organisms. Increased worldwide demand for sunscreens is associated with temperature anomalies, high irradiance, and changes in the tourist market. Recently, it has been demonstrated that personal care products, including sunscreens, appear in various ecosystems and geographic locations causing an ecotoxicological threat. Our goal was to determine for the first time the presence of selected organic UV filters at four beaches in the central Pomeranian region in northern Poland and to assess their horizontal and vertical distribution as well as temporal variation at different locations according to the touristic pressure. In this pioneering study, the concentration of five UV filters was measured in core sediments dredged from four exposed beaches (Darłowo, Ustka, Rowy, and Czołpino). UV filters were detected in 89.6% of collected cores at detection frequencies of 0–22.2%, 75–100%, 0–16.7%, and 2.8–25% for benzophenone-1 (BP-1), benzophenone-2 (BP-2), benzophenone-3 (BP-3), and enzacamene (4-MBC), respectively. In terms of seasonality, the concentration of UV filters generally increased in the following order: summer > autumn > spring. No detectable levels of 3-BC (also known as 3-benzylidene camphor) were recorded. No differences were found in the concentration of UV filters according to the depth of the sediment core. During the summer and autumn seasons, all UV filters were detected in higher concentrations in the bathing area or close to the waterline than halfway or further up the beach. Results presented in this study demonstrate that the Baltic Sea coast is not free from UV filters. Even if actual concentrations can be quantified as ng·kg−1 causing limited environmental threat, much higher future levels are expected due to the Earth's principal climatic zones shifting northward.

Non-target screening of organic pollutants and target analysis of halogenated polycyclic aromatic hydrocarbons in the atmosphere around metallurgical plants by high-resolution GC/Q-TOF-MS:[31]

Background: The 16 priority polycyclic aromatic hydrocarbons (PAHs) issued by US Environmental protection agency are a major focus in atmosphere in previous studies. Many more PAH congeners or their substitutes could be produced during combustion or thermal industrial processes and released into the atmosphere. However, a full screening of various organic pollutants in air surrounding important industrial sources has not been conducted. Identifying and characterizing organic pollutants in air is essential for accurate risk assessment. This study conducted non-target screening of organic pollutants and simultaneous target analysis of emerging contaminants including 8 polychlorinated naphthalenes and 30 higher cyclic halogenated PAHs by high-resolution gas chromatography quadrupole time-of-flight mass spectrometry (GC/Q-TOF-MS) and applied to the air samples collected surrounding metallurgical plants. Emerging organic chemicals of high toxicity in air were identified. Results: We identified and characterized 187 organic chemicals categorized as PAHs, alkylated polycyclic aromatic compounds (PACs), heterocyclic PACs, and aliphatic hydrocarbons in atmosphere around industrial sources. Some of these identified chemicals, such as phthalic acid esters, dimethylbenz[a]anthracene, and hydroquinone with alkane substituents are of potential high

[30] Link: https://doi.org/10.3390/w12113024
[31] Link: https://doi.org/10.1186/s12302-020-00376-9

toxicities and have not been the focus of previous studies of airborne contaminants. Moreover, hydroquinone with alkane substituents may be critical intermediates and precursors of an emerging contaminant—environmentally persistent free radicals. Thus, the presence of those identified highly toxic chemicals in the air merits attention. Moreover, 38 chlorinated and brominated PAHs as target compounds were accurately quantitated by using isotopic dilution method by application of GC/Q-TOF-MS, and the findings were similar to those of high-resolution magnetic mass spectrometry. Conclusion: In this study, both non-target screening of organic pollutants and target analysis of halogenated PAHs in air were achieved by GC/Q-TOF-MS. The method could be of significance for simultaneous analysis of those trace pollutants containing multiple congeners. Specific pollutants of potential high toxicity in atmosphere around industrial sources were identified. Those knowledge could be helpful for comprehensively recognizing the organic contaminants in air surrounding metallurgical plants and better understanding their potential health risks.

Exposure to organophosphate esters, phthalates, and alternative plasticizers in association with uterine fibroids:[32]

Exposure to endocrine disrupting chemicals is suggested to be responsible for the development or progression of uterine fibroids. However, little is known about risks related to emerging chemicals, such as organophosphate esters (OPEs) and alternative plasticizers (APs). A case-control study was conducted to investigate whether exposures to OPEs, APs, and phthalates, were associated with uterine fibroids in women of reproductive age. For this purpose, the cases (n = 32) and the matching controls (n = 79) were chosen based on the results of gynecologic ultrasonography among premenopausal adult women in Korea and measured for metabolites of several OPEs, APs, and major phthalates. Logistic regression models were employed to assess the associations between chemical exposure and disease status. Factor analysis was conducted for multiple chemical exposure assessments as a secondary analysis. Among OPE metabolites, diphenyl phosphate (DPHP), 2-ethylhexyl phenyl phosphate (EHPHP), and 1-hydroxy-2-propyl bis(1-chloro-2-propyl) phosphate (BCIPHIPP) were detected in >80% of the subjects. Among APs, metabolites of di-isononyl phthalate (DINP) and di(2-propylheptyl) phthalate (DPrHpP) were detected in >75% of the urine samples. The odds ratios (ORs) of uterine fibroids were significantly higher among the women with higher exposures to tris(1,3-dichloro-2-propyl) phosphate (TDCIPP) and tris(2-butoxyethyl) phosphate (TBOEP), di(2-ethylhexyl) terephthalate (DEHTP), DPrHpP, and di-(iso-nonyl)-cyclohexane-1,2-dicarboxylate (DINCH). In addition, urinary concentrations of mono(2-ethyl-5-oxohexyl) phthalate (MEOHP), a sum of five di(2-ethylhexyl) phthalate metabolites (∑5DEHP), and mono(4-methyl-7-hydroxyoctyl) phthalate (OH-MINP) were significantly higher in the cases. In factor analysis, a factor heavily loaded with DPrHpP and DEHP was significantly associated with uterine fibroids, supporting the observation from the single chemical regression model. We found for the first time that several metabolites of OPEs and APs are associated with increased risks of uterine fibroids among pre-menopausal women. Further epidemiological and mechanistic studies are warranted to validate the associations observed in the present study.

[32] Link: https://doi.org/10.1016/j.envres.2020.109874

Retrospective screening of high-resolution mass spectrometry archived digital samples can improve environmental risk assessment of emerging contaminants: A case study on antifungal azoles[33]

Environmental risk assessment associated with aquatic and terrestrial contamination is mostly based on predicted or measured environmental concentrations of a limited list of chemicals in a restricted number of environmental compartments. High resolution mass spectrometry (HRMS) can provide a more comprehensive picture of exposure to harmful chemicals, particularly through the retrospective analysis of digitally stored HRMS data. Using this methodology, our study characterized the contamination of various environmental compartments including 154 surface water, 46 urban effluent, 67 sediment, 15 soil, 34 groundwater, 24 biofilm, 41 gammarid and 49 fish samples at 95 sites widely distributed over the Swiss Plateau. As a proof-of-concept, we focused our investigation on antifungal azoles, a class of chemicals of emerging concern due to their endocrine disrupting effects on aquatic organisms and humans. Our results demonstrated the occurrence of antifungal azoles and some of their (bio)transformation products in all the analyzed compartments (0.1–100 ng/L or ng/g d.w.). Comparison of actual and predicted concentrations showed the partial suitability of level 1 fugacity modelling in predicting the exposure to azoles. Risk quotient calculations additionally revealed risk of exposure especially if some of the investigated rivers and streams are used for drinking water production. The case study clearly shows that the retrospective analysis of HRMS/MS data can improve the current knowledge on exposure and the related risks to chemicals of emerging concern and can be effectively employed in the future for such purposes.

Unexpected culprit of increased estrogenic effects: Oligomers in the photodegradation of preservative ethylparaben in water:[34]

Widespread occurrence of emerging organic contaminants (EOCs) in water have been explicitly associated with adverse effects on human health, therefore representing a major risk to public health. Especially the increased toxicity is frequently observed during the photodegradation of EOCs in natural water, and even wastewater treatment plants. However, the culprit of increased toxicity and formation mechanism has yet to be recognized regarding the estrogenic activity. In this study, by combining laboratory experiments with quantum chemical calculations, the induction of human estrogenic activity was investigated using the yeast two-hybrid reporter assay during the photodegradation of preservatives ethylparaben (EP), along with identification of toxic products and formation mechanisms. Results showed that the increase in estrogenic effect was induced by photochemically generated oligomers, rather than the expected OH-adduct. The maximum estrogenic activity corresponded to the major formation of oligomers, while OH-adducts were less than 12%. Two photochemically generated oligomers were found to contribute to estrogenic activity, produced from the cleavage of excited triplet state molecules and subsequent radical-radical reactions. Computational toxicology results showed that the increased estrogenic activity was attributed to oligomer [4-Hydroxy-isophthalic acid 1-ethyl ester 3-(4-hydroxy-phenyl)] and its EC50 was lower than that of the parent EP. In contrast, OH-adducts exhibited higher EC50 values than the parent EP, while still possessing estrogenic

[33] Link: https://doi.org/10.1016/j.envint.2020.105708
[34] Link: https://doi.org/10.1016/j.watres.2020.115745

activity. Therefore, more attention should be paid to these photodegradation products of EOCs, including OH-adducts.

Visualized Metabolic Disorder and Its Chemical Inducer in Wild Crucian Carp from Taihu Lake, China:[35]

A variety of anthropogenic chemicals can disrupt the equilibrium of intrinsic biological metabolites in organisms, leading to metabolic disorders and an increased risk of metabolic syndromes. However, exposure to pollutants that induce metabolic disorders in wildlife as a cause of adverse effects is unknown. In this study, approximately 3108 compounds, including 11 groups of metabolites and 388 pollutants, were simultaneously identified in the blood of wild crucian carp (Carassius auratus) captured in three bays of Taihu Lake, China. A visualized network linking thousands of co-regulated metabolites was automatically produced for the screened signals. This comprehensive view of the differences in blood metabolite profiles in carp from the north and south bays showed that triglycerides (TGs) were the intrinsic molecules most affected by differing environmental pollution in each bay. The regional differences in metabolite profiles were linked to exposure to screened perfluorinated compounds that displayed corresponding regional differences in concentrations and effects on TGs in in vivo exposure tests. Perfluoroundecanoic acid (PFUnDA) was the key pollutant responsible for the variation in blood TGs in wild crucian carp, and exposure to PFUnDA resulted in extremely high biological activity on lipid deposition in the liver tissues of crucian carp at environmental levels.

Potential emerging chemical risks in the food chain associated with substances registered under REACH[36]

A screening procedure for the identification of potential emerging chemical risks in the food and feed chain developed in a previous EFSA-sponsored pilot study was applied to 15021 substances registered under the REACH Regulation at the time of evaluation. Eligible substances were selected from this dataset by excluding (a) intermediates handled under strictly controlled conditions, (b) substances lacking crucial input data and (c) compounds considered to be outside the applicability domain of the models used. Selection of eligible substances resulted in a considerable reduction to 2336 substances. These substances were assessed and scored for environmental release (tonnage and use information from REACH registration dossiers), biodegradation (predictions from BIOWIN models 3, 5 and 6 evaluated in a battery approach), bioaccumulation in food/feed (ACC-HUMANsteady modelling) and chronic human health hazards (classification according to the CLP Regulation for carcinogenicity, mutagenicity, reproductive toxicity and repeated dose toxicity as well as IARC classification for carcinogenicity). Prioritisation based on the scores assigned and additional data curation steps identified 212 substances that are considered potential emerging risks in the food chain. Overall, 53% of these substances were prioritised due to chronic hazards identified in REACH registrations dossiers only (i.e. hazards not identified in classifications from other sources). Bioaccumulation in food and feed predicted on the basis of ACC-HUMANsteady modelling identified many substances that are not considered bioaccumulative in aquatic or terrestrial organisms based on screening criteria of the relevant ECHA guidance documents. Furthermore, 52% of the priority substances

[35] Link: https://doi.org/10.1021/acs.est.0c00099
[36] Link: https://doi.org/10.1039/C9EM00369J

have not yet been assessed for their presence in food/feed by EU regulatory agencies. This finding and illustrative examples suggest that the screening procedure identified substances that have the potential to be emerging chemical risks in the food chain. Future research should investigate whether they actually represent emerging chemical risks as defined in EFSA's mandate.

Experimental Study of OH-Initiated Heterogeneous Oxidation of Organophosphate Flame Retardants: Kinetics, Mechanism, and Toxicity[37]

The environmental risks and health impacts associated with particulate organophosphate flame retardants (OPFRs), which are ubiquitous in the global atmosphere, have not been adequately assessed due to the lack of data on the reaction kinetics, products, and toxicity associated with their atmospheric transformations. Here, the importance of such transformations for OPFRs are explored by investigating the reaction kinetics, degradation chemical mechanisms, and toxicological evolution of two OPFRs (2-ethylhexyl diphenyl phosphate (EHDP) and diphenyl phosphate (DPhP)) coated on (NH4)2SO4 particles upon heterogeneous OH oxidation. The derived reaction rate constants for the heterogeneous loss of EHDP and DPhP are (1.12 ± 0.22) × 10-12 and (2.33 ± 0.14) × 10-12 cm3 molecules-1 s-1, respectively. Using recently developed real-time particle chemical composition measurements, particulate products from heterogeneous photooxidation and the associated degradation mechanisms for particulate OPFRs are reported for the first time. Subsequent cytotoxicity analysis of the unreacted and oxidized OPFR particles indicated that the overall particle cytotoxicity was reduced by up to 94% with heterogeneous photooxidation, likely due to a significantly lower cytotoxicity associated with the oxidized OPFR products relative to the parent OPFRs. The present work not only provides guidance for future field sampling for the detection of transformation products of OPFRs, but also strongly supports the ongoing risk assessment of these emerging chemicals and most critically, their products.

[37] Link: https://doi.org/10.1021/acs.est.9b05327