REACH

Oils, vegetable, deodorizer distillates

EC number: 270-700-0 | CAS number: 68476-80-2
Complex combination obtained by steam distillation of mixed vegetable oils followed by condensation of the steam. Contains fatty acids, sterols, aldehydes and ketones.

Environmental fate & pathways

Bioaccumulation: aquatic / sediment

S-01 | Summary

Administrative data

Link to relevant study record(s)

Reference

Reference 1

Endpoint:	bioaccumulation in aquatic species, other
Type of information:	experimental study
Adequacy of study:	weight of evidence
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	study well documented, meets generally accepted scientific principles, acceptable for assessment
Justification for type of information:	The study record represents the experimental result on a substance which represents one chain length of the glyceride and fatty acid constituents of the 'oils, vegetable, deodorizer distillates'.
Principles of method if other than guideline:	Fish, algae and activated sludge were exposed to the test substance for 3 d, 1 d and 5 d respectively and bioaccumulation factors were estimated as a result.
GLP compliance:	no
Test organisms (species):	other: Leuciscus idus melanotus, Chlorella fusca var.vacuolata and activated sludge
Route of exposure:	aqueous
Test type:	static
Water / sediment media type:	natural water: freshwater
Nominal and measured concentrations:	Nominal concentration: 0.05 mg/L
Details on estimation of bioconcentration:	- Bioaccumulation of tristearin and palmitic acid was measured in fish following exposure to the substances for 3 d. The bioconcentration was measured as the concentration of chemical in the fish/average concentration of chemical in water (µg/g). - Bioaccumulation of tristearin and palmitic acid was measured in algae and activated sludge following exposure

	to the substances for 1 d and 5 d respectively. The bioconcentration was measured as the concentration of chemical in algae or sludge/final concentration of chemical in water (µg/g).
	Key result
Conc. / dose:	0.05 mg/L
Type:	BCF
Value:	10 dimensionless
Basis:	whole body w.w.
Remarks on result:	other: Value for tristearin in fish
	Key result
Conc. / dose:	0.05 mg/L
Type:	BCF
Value:	60 dimensionless
Remarks on result:	other: Value for palmitic acid in fish
Details on results:	- The BCF values for tristearin in fish, algae and activated sludge were determined to be <10, 5,840 and 3,600 respectively. - The BCF values for palmitic acid in fish, algae and activated sludge were determined to be 60, 8,400 and 2,800 respectively. The differences observed between fish and algae/activated sludge values respectively suggests a detoxification process in higher developed organisms as fish (metabolism).

Comparing and extrapolating these short term results leads to the following bioaccumulation classification based on long-term tests (carried in accordance with the OECD flow-through-test):

- No or low accumulation: 1,000

- Medium level accumulation: 1,000 -10,000

- High accumulation: 10,000

Based on this, tristearin and palmitic acid both can be considered to have low bioaccumulation potential in fish.

Conclusions:	Under the conditions of the study, both tristearin and palmitic acid can be considered to have a low bioaccumulation potential in fish.
Executive summary:	The bioaccumulation of tristearin and palmitic acid was measured in fish, algae and activated sludge following exposure for 3, 1 and 5 d respectively. The bioconcentration in fish was measured as the concentration of chemical in the fish/average concentration of chemical in water (µg/g) while the bioconcentration in algae and activated sludge was measured as the concentration of chemical in algae or sludge/final concentration of chemical in water (µg/g). The BCF values for tristearin in fish, algae and activated sludge were determined to be <10, 5,840 and 3,600 respectively. The corresponding values for palmitic acid in fish, algae and activated sludge were determined to be 60, 8,400 and 2,800 respectively. The differences observed between fish and algae/activated sludge values respectively suggests a detoxification process in higher developed organisms as fish (metabolism). Comparing and extrapolating the short term results to long term values for both the substances leads to 'no or low' bioaccumulation classification in fish and 'medium' bioaccumulation classification in algae and activated sludge. Under the conditions of the study, both tristearin and palmitic acid can be considered to have a low bioaccumulation potential in fish (Freitag, 1985).

Reference 2

Endpoint:	bioaccumulation in aquatic species, other
Type of information:	(Q)SAR

Adequacy of study:	key study
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	results derived from a valid (Q)SAR model and falling into its applicability domain, with adequate and reliable documentation / justification
Justification for type of information:	See below under 'Overall remarks, attachments' for applicability domain.
Reason / purpose for cross-reference:	reference to other study
Qualifier:	according to guideline
Guideline:	other: REACH guidance on QSARs: Chapter R.6. QSARs and grouping of chemicals
Principles of method if other than guideline:	1. Meylan,WM, Howard,PH, Boethling, RS et al, 1999. Improved method for estimating bioconcentration/bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4):664-672. 2. Zhao C, Boriani E, Chana A, Roncaglioni A and Benfenati E, 2008. A new hybrid system of QSAR models for predicting bioconcentration factors (BCF)", Chemosphere 73:1701–1707. 3. Hamelink, J. L., 1977. Current bioconcentration test methods and theory. In Aquatic Toxicology and Hazard Evaluation, edited by F. L. Mayer and J. L. Hamelink. West Conshohocken, PA ASTM STP.
Details on estimation of bioconcentration:	In absence of experimental data, the bioaccumulation potential (BCF) of the test substance was determined through computational methods (such as BCFBAF v3.01 of EPIWEB v 4.1, BCF (CAESAR) 2.1.14 and T.E.S.T US EPA model v.4.1). Assumption: - The individual BCF values was calculated for the shortest and longest alkyl chain containing representative substances of each class present in the test substance. - These representative substances each should represent at >10 % of the test substance composition. - As the test substance is a UVCB the individual or average estimated Log Kow values for the constituents will be used to represent a range of values for the entire substance. Therefore, the BCF values were determined for the following individual substances, present at >10% : a) Octanoic acid, stearic and oleic acid representing free fatty acids (substance class) The calculation input will be provided in SMILES notation as Octanoic acid: O=C(O)CCCCCCC Stearic acid: O=C(O)CCCCCCCCCCCCCCCCC Oleic acid: O=C(O)CCCCCCCC=CCCCCCCCC b) Triglyceride of Octanoic acid, stearic and oleic acid, representing glycerides of fatty acids (substance class) The calculation input will be provided in SMILES notation as Trioctanoin: CCCCCCCC(=O)OCC(COC(=O)CCCCCCC)OC(=O)CCCCCCC Tristearin: O=C(CCCCCCCCCCCCCCCCC)OC(COC(=O)CCCCCCCCCCCCCCCCC)COC(=O)CCCCCCCCCCCCCCCCC C Triolein: O=C(OC(COC(=O)CCCCCCCC=CCCCCCCCC)COC(=O)CCCCCCCC=CCCCCCCCC)CCCCCCCC=CCCCC CCCC c) alpha-tocopherols, representing tocopherol unsaponifiable matters (substance class) The calculation input will be provided in SMILES notation as Oc1cc2c(c(c1C)C)OC(CCCC(CCCC(CCCC(C)C)C)C)(C)CC2 d) Beta-sitosterol, representing phytosterols unsaponifiable matters (substance class) The calculation input will be provided in SMILES notation as OC(CC(=CCC1C(CC2)C3(C2C(CCC(C(C)C)CC)C)C)C4(C)C1CC3)CC4 - Method details: 1. BCFBAF v3.01 program of EPISuite v 4.1: - For the triglycerides, tocopherols and beta-sitosterols, the BCF values was estimated by using the derived QSAR estimation equation for Log Kow > 7.0 from EPISuite: Log BCF = -0.49 Log Kow + 7.554 + Σ correction factors (n = 35, r2 = 0.634, Q2 = 0.57, std dev = 0.538, avg dev = 0.396) - For the fatty acids, the below equation for ionic compounds was used for the BCF estimation Log BCF = 1.00 (Ionic; Log Kow dependent) 2. CAESAR v.2.1.14: The BCF value via CAESAR is estimated using a combination of 2 Radial Basis Function Neural Network (RBF-NN) models (model A and B) developed with 5 descriptors each, for a total of 8 descriptors (2 are in common between the models). Details about the NN architecture are provided in the supporting information of the paper by Zhao et al., 2008. The estimations are categorised into the following scenarios: - If mean (value given by models A and B) > 2.410: log BCF = 1.052 * [mean (value given by models A and B)] - 0.065 - If 1.355 < mean (value given by models A and B) ≤ 2.410: log BCF = 0.996 * [min (value given by models A and B)] + 0.042 - Otherwise log BCF = 0.936 * [mean (value given by models A and B)] - 0.123 3. T.E.S.T US EPA model v.4.1: This model uses multiple methodologies for prediction of endpoints i.e., - Hierarchical clustering: The toxicity for a given query compound is estimated using the weighted average of the predictions from several different models. The different models are obtained by using Ward's method to divide the training set into a series of structurally similar clusters. A genetic algorithm-based technique is used to generate models for each cluster. The models are generated prior to runtime. - Single model method: Predictions are made using a multilinear regression model that is fit to the

	training set (using molecular descriptors as independent variables) using a genetic algorithm-based approach. The regression model is generated prior to runtime. - Group contribution: Predictions are made using a multilinear regression model that is fit to the training set (using molecular fragment counts as independent variables). The regression model is generated prior to runtime. - FDA method: The prediction for each test chemical is made using a new model that is fit to the chemicals that are most similar to the test compound. Each model is generated at runtime. - Nearest neighbour: The predicted toxicity is estimated by taking an average of the three chemicals in the training set that are most similar to the test chemical. Further details of these methodologies can be found in the publications mentioned in the US EPA website: https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test
	Key result
Type:	other: average BCF for fatty acids
Value:	>= 11 - < 17 L/kg
Basis:	whole body w.w.
Remarks on result:	other: average BCF values estimated using BCFBAF of EPISuite, T.E.S.T. US EPA and CAESAR BCF models
	Key result
Type:	other: Estimated BCF of glycerides
Value:	>= 4 - < 143 L/kg
Basis:	whole body w.w.
Remarks on result:	other: average BCF values estimated using BCFBAF of EPISuite, T.E.S.T. US EPA and CAESAR BCF models
	Key result
Type:	other: Estimated BCF for unsaponifiable matter
Value:	>= 105 - <= 654 L/kg
Basis:	whole body w.w.
Remarks on result:	other: average BCF values estimated using BCFBAF of EPISuite, T.E.S.T. US EPA and CAESAR BCF models
	Key result
Type:	other: Overall estimated BCF for test substance
Value:	>= 4 - < 654 L/kg
Basis:	whole body w.w.
Remarks on result:	other: average BCF values estimated for the individual constituents using BCFBAF of EPISuite, T.E.S.T. US EPA and CAESAR BCF models
Details on results:	Estimation by BCFBAF v3.01 program of EPIWEB v 4.1: (A) Glycerides: SMILES : CCCCCCCC(=O)OCC(COC(=O)CCCCCCC)OC(=O)CCCCCCC CHEM : Trioctanoin MOL FOR: C27 H50 O6 MOL WT : 470.70 ---------- BCFBAF v3.01 ---------- Summary Results: Log BCF (regression-based estimate): 2.45 (BCF = 281 L/kg wet-wt) Biotransformation Half-Life (days) : 0.0857 (normalized to 10 g fish) Log BAF (Arnot-Gobas upper trophic): 0.00 (BAF = 1 L/kg wet-wt) ============================ BCF (Bioconcentration Factor): ============================ Log Kow (estimated) : 9.20 Log Kow (experimental): not available from database Log Kow used by BCF estimates: 9.20 Equation Used to Make BCF estimate: Log BCF = -0.49 log Kow + 7.554 + Correction Correction(s): Value Alkyl chains (8+ -CH2- groups) -0.596 Estimated Log BCF = 2.448 (BCF = 280.6 L/kg wet-wt)

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Whole Body Primary Biotransformation Rate Estimate for Fish:
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------+-----+-----------------------------------------+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag | 3 | Linear C4 terminal chain [CCC-CH3] | 0.0341 | 0.1024
Frag | 3 | Ester [-C(=O)-O-C] | -0.7605 | -2.2816
Frag | 3 | Methyl [-CH3] | 0.2451 | 0.7353
Frag | 20 | -CH2- [linear] | 0.0242 | 0.4837
Frag | 1 | -CH- [linear] | -0.1912 | -0.1912
L Kow| * | Log Kow = 9.20 (KowWin estimate) | 0.3073 | 2.8284
MolWt| * | Molecular Weight Parameter | | -1.2070
Const| * | Equation Constant | | -1.5371
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RESULT | LOG Bio Half-Life (days) | | -1.0671
RESULT | Bio Half-Life (days) | | 0.08569
NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
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Biotransformation Rate Constant:
kM (Rate Constant): 8.089 /day (10 gram fish)
kM (Rate Constant): 4.549 /day (100 gram fish)
kM (Rate Constant): 2.558 /day (1 kg fish)
kM (Rate Constant): 1.438 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = -0.000 (BCF = 0.9996 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 0.001 (BAF = 1.001 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 0.033 (BCF = 1.078 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 0.150 (BAF = 1.412 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 0.042 (BCF = 1.102 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 0.814 (BAF = 6.521 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 2.680 (BCF = 478.2 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 6.374 (BAF = 2.367e+006 L/kg wet-wt)

For C18 chain length i.e. tristerain or glycerol tristearate:
SMILES :
O=C(OC(COC(=O)CCCCCCCCCCCCCCCCC)COC(=O)CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC
C
CHEM : Tristearin
MOL FOR: C57 H110 O6
MOL WT : 891.51
---------- BCFBAF v3.01 ----------
Summary Results:
Log BCF (regression-based estimate): 0.50 (BCF = 3.16 L/kg wet-wt)
Biotransformation Half-Life (days) : 1.28e+003 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): -0.05 (BAF = 0.893 L/kg wet-wt)

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BCF (Bioconcentration Factor):
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Log Kow (estimated) : 23.94
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 23.94

Equation Used to Make BCF estimate:
Log BCF = -0.49 log Kow + 7.554 + Correction

Correction(s): Value
No Applicable Correction Factors
Minimum Log BCF of 0.50 applied when Log Kow > 7

Estimated Log BCF = 0.500 (BCF = 3.162 L/kg wet-wt)

============================================================
Whole Body Primary Biotransformation Rate Estimate for Fish:
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------+-----+-----------------------------------------+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag | 3 | Linear C4 terminal chain [CCC-CH3] | 0.0341 | 0.1024
Frag | 3 | Ester [-C(=O)-O-C] | -0.7605 | -2.2816
Frag | 3 | Methyl [-CH3] | 0.2451 | 0.7353
Frag | 50 | -CH2- [linear] | 0.0242 | 1.2094
Frag | 1 | -CH- [linear] | -0.1912 | -0.1912
L Kow| * | Log Kow = 23.94 (KowWin estimate) | 0.3073 | 7.3565
MolWt| * | Molecular Weight Parameter | | -2.2861
Const| * | Equation Constant | | -1.5371
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RESULT | LOG Bio Half-Life (days) | | 3.1075
RESULT | Bio Half-Life (days) | | 1281
NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
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Biotransformation Rate Constant:
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kM (Rate Constant): 0.0005411 /day (10 gram fish)
kM (Rate Constant): 0.0003043 /day (100 gram fish)
kM (Rate Constant): 0.0001711 /day (1 kg fish)
kM (Rate Constant): 9.623e-005 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = -0.049 (BCF = 0.893 L/kg wet-wt)
Estimated Log BAF (upper trophic) = -0.049 (BAF = 0.893 L/kg wet-wt)
Estimated Log BCF (mid trophic) = -0.031 (BCF = 0.9315 L/kg wet-wt)
Estimated Log BAF (mid trophic) = -0.031 (BAF = 0.9315 L/kg wet-wt)
Estimated Log BCF (lower trophic) = -0.027 (BCF = 0.9402 L/kg wet-wt)
Estimated Log BAF (lower trophic) = -0.027 (BAF = 0.9402 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = -0.049 (BCF = 0.893 L/kg wet-wt)
Estimated Log BAF (upper trophic) = -0.049 (BAF = 0.893 L/kg wet-wt)

SMILES :
O=C(OC(COC(=O)CCCCCCCC=CCCCCCCCC)COC(=O)CCCCCCCC=CCCCCCCCC)CCCCCCCC=CCCCCCCC
CHEM : Triolein
MOL FOR: C57 H104 O6
MOL WT : 885.46
---------- BCFBAF v3.01 ----------
Summary Results:
Log BCF (regression-based estimate): 0.50 (BCF = 3.16 L/kg wet-wt)
Biotransformation Half-Life (days) : 2.36e+003 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): -0.05 (BAF = 0.893 L/kg wet-wt)

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BCF (Bioconcentration Factor):
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Log Kow (estimated) : 23.29
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 23.29

Equation Used to Make BCF estimate:
Log BCF = -0.49 log Kow + 7.554 + Correction

Correction(s): Value
No Applicable Correction Factors
Minimum Log BCF of 0.50 applied when Log Kow > 7

Estimated Log BCF = 0.500 (BCF = 3.162 L/kg wet-wt)

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Whole Body Primary Biotransformation Rate Estimate for Fish:
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------+-----+----------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
------+-----+----------+---------
Frag | 3 | Linear C4 terminal chain [CCC-CH3] | 0.0341 | 0.1024
Frag | 3 | Ester [-C(=O)-O-C] | -0.7605 | -2.2816
Frag | 3 | Methyl [-CH3] | 0.2451 | 0.7353
Frag | 44 | -CH2- [linear] | 0.0242 | 1.0642
Frag | 1 | -CH- [linear] | -0.1912 | -0.1912
Frag | 6 | -C=CH [alkenyl hydrogen] | 0.0988 | 0.5931
Frag | 6 | -C=CH [alkenyl hydrogen] | 0.0000 | 0.0000
L Kow| * | Log Kow = 23.29 (KowWin estimate) | 0.3073 | 7.1582
MolWt| * | Molecular Weight Parameter | | -2.2706
Const| * | Equation Constant | | -1.5371
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RESULT | LOG Bio Half-Life (days) | | 3.3727
RESULT | Bio Half-Life (days) | | 2359
NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
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Biotransformation Rate Constant:
kM (Rate Constant): 0.0002938 /day (10 gram fish)
kM (Rate Constant): 0.0001652 /day (100 gram fish)
kM (Rate Constant): 9.291e-005 /day (1 kg fish)
kM (Rate Constant): 5.225e-005 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = -0.049 (BCF = 0.893 L/kg wet-wt)
Estimated Log BAF (upper trophic) = -0.049 (BAF = 0.893 L/kg wet-wt)
Estimated Log BCF (mid trophic) = -0.031 (BCF = 0.9315 L/kg wet-wt)
Estimated Log BAF (mid trophic) = -0.031 (BAF = 0.9315 L/kg wet-wt)
Estimated Log BCF (lower trophic) = -0.027 (BCF = 0.9402 L/kg wet-wt)
Estimated Log BAF (lower trophic) = -0.027 (BAF = 0.9402 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = -0.049 (BCF = 0.893 L/kg wet-wt)
Estimated Log BAF (upper trophic) = -0.049 (BAF = 0.893 L/kg wet-wt)

(B) Fatty acids:
For C8 chain length i.e. octanoinc acid
SMILES : O=C(O)CCCCCCC
CHEM : Octanoic acid

MOL FOR: C8 H16 O2
MOL WT : 144.22
---------- BCFBAF v3.01 ----------
Summary Results:
Log BCF (regression-based estimate): 0.50 (BCF = 3.16 L/kg wet-wt)
Biotransformation Half-Life (days) : 0.684 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 1.92 (BAF = 83.6 L/kg wet-wt)

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BCF (Bioconcentration Factor):
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Log Kow (estimated) : 3.03
Log Kow (experimental): 3.05
Log Kow used by BCF estimates: 3.05

Equation Used to Make BCF estimate:
Log BCF = 0.50 (Ionic; Log Kow dependent)

Estimated Log BCF = 0.500 (BCF = 3.162 L/kg wet-wt)

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Whole Body Primary Biotransformation Rate Estimate for Fish:
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------+-----+----------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
------+-----+----------+---------
Frag | 1 | Linear C4 terminal chain [CCC-CH3] | 0.0341 | 0.0341
Frag | 1 | Aliphatic acid [-C(=O)-OH] | 0.3803 | 0.3803
Frag | 1 | Methyl [-CH3] | 0.2451 | 0.2451
Frag | 6 | -CH2- [linear] | 0.0242 | 0.1451
L Kow| * | Log Kow = 3.05 (experimental) | 0.3073 | 0.9374
MolWt| * | Molecular Weight Parameter | | -0.3698
Const| * | Equation Constant | | -1.5371
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RESULT | LOG Bio Half-Life (days) | | -0.1648
RESULT | Bio Half-Life (days) | | 0.6842
NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
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Biotransformation Rate Constant:
kM (Rate Constant): 1.013 /day (10 gram fish)
kM (Rate Constant): 0.5697 /day (100 gram fish)
kM (Rate Constant): 0.3204 /day (1 kg fish)
kM (Rate Constant): 0.1802 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 1.922 (BCF = 83.64 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 1.922 (BAF = 83.64 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 1.809 (BCF = 64.46 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 1.810 (BAF = 64.49 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 1.767 (BCF = 58.48 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 1.768 (BAF = 58.65 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 2.081 (BCF = 120.4 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 2.143 (BAF = 139 L/kg wet-wt)

(B) Fatty acids: For C18 chain length i.e. stearic acid:
SMILES : O=C(O)CCCCCCCCCCCCCCCCC
CHEM : Stearic acid
MOL FOR: C18 H36 O2
MOL WT : 284.49
---------- BCFBAF v3.01 ----------
Summary Results:
Log BCF (regression-based estimate): 1.00 (BCF = 10 L/kg wet-wt)
Biotransformation Half-Life (days) : 20.4 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 4.90 (BAF = 7.89e+004 L/kg wet-wt)

==========
BCF (Bioconcentration Factor):
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Log Kow (estimated) : 7.94
Log Kow (experimental): 8.23
Log Kow used by BCF estimates: 8.23

Equation Used to Make BCF estimate:
Log BCF = 1.00 (Ionic; Log Kow dependent)

Estimated Log BCF = 1.000 (BCF = 10 L/kg wet-wt)

==========
Whole Body Primary Biotransformation Rate Estimate for Fish:
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------+-----+----------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
------+-----+----------+---------

Frag | 1 | Linear C4 terminal chain [CCC-CH3] | 0.0341 | 0.0341
Frag | 1 | Aliphatic acid [-C(=O)-OH] | 0.3803 | 0.3803
Frag | 1 | Methyl [-CH3] | 0.2451 | 0.2451
Frag | 16 | -CH2- [linear] | 0.0242 | 0.3870
L Kow| * | Log Kow = 8.23 (experimental) | 0.3073 | 2.5294
MolWt| * | Molecular Weight Parameter | | -0.7295
Const| * | Equation Constant | | -1.5371
------------+---------+---------
RESULT | LOG Bio Half-Life (days) | | 1.3094
RESULT | Bio Half-Life (days) | | 20.39
NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
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Biotransformation Rate Constant:
kM (Rate Constant): 0.034 /day (10 gram fish)
kM (Rate Constant): 0.01912 /day (100 gram fish)
kM (Rate Constant): 0.01075 /day (1 kg fish)
kM (Rate Constant): 0.006046 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 2.331 (BCF = 214.3 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 4.897 (BAF = 7.893e+004 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 2.473 (BCF = 297.4 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 4.985 (BAF = 9.652e+004 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 2.517 (BCF = 328.8 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 5.040 (BAF = 1.097e+005 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 3.411 (BCF = 2577 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 7.025 (BAF = 1.06e+007 L/kg wet-wt)

SMILES : O=C(O)CCCCCCCC=CCCCCCCCC
CHEM : Oleic acid
MOL FOR: C18 H34 O2
MOL WT : 282.47
---------- BCFBAF v3.01 ----------
Summary Results:
Log BCF (regression-based estimate): 1.75 (BCF = 56.2 L/kg wet-wt)
Biotransformation Half-Life (days) : 19.2 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 5.18 (BAF = 1.51e+005 L/kg wet-wt)

==========
BCF (Bioconcentration Factor):
==========
Log Kow (estimated) : 7.73
Log Kow (experimental): 7.64
Log Kow used by BCF estimates: 7.64

Equation Used to Make BCF estimate:
Log BCF = 1.75 (Ionic; Log Kow dependent)

Estimated Log BCF = 1.750 (BCF = 56.23 L/kg wet-wt)

==========
Whole Body Primary Biotransformation Rate Estimate for Fish:
==========
------+-----+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
------+-----+---------+---------
Frag | 1 | Linear C4 terminal chain [CCC-CH3] | 0.0341 | 0.0341
Frag | 1 | Aliphatic acid [-C(=O)-OH] | 0.3803 | 0.3803
Frag | 1 | Methyl [-CH3] | 0.2451 | 0.2451
Frag | 14 | -CH2- [linear] | 0.0242 | 0.3386
Frag | 2 | -C=CH [alkenyl hydrogen] | 0.0988 | 0.1977
Frag | 2 | -C=CH [alkenyl hydrogen] | 0.0000 | 0.0000
L Kow| * | Log Kow = 7.64 (experimental) | 0.3073 | 2.3481
MolWt| * | Molecular Weight Parameter | | -0.7243
Const| * | Equation Constant | | -1.5371
------------+---------+---------
RESULT | LOG Bio Half-Life (days) | | 1.2825
RESULT | Bio Half-Life (days) | | 19.17
NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
------------+---------+---------

Biotransformation Rate Constant:
kM (Rate Constant): 0.03617 /day (10 gram fish)
kM (Rate Constant): 0.02034 /day (100 gram fish)
kM (Rate Constant): 0.01144 /day (1 kg fish)
kM (Rate Constant): 0.006431 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 2.839 (BCF = 690.2 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 5.179 (BAF = 1.509e+005 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 2.985 (BCF = 966.1 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 5.288 (BAF = 1.94e+005 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 3.029 (BCF = 1070 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 5.356 (BAF = 2.267e+005 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 3.733 (BCF = 5413 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 7.157 (BAF = 1.436e+007 L/kg wet-wt)

SMILES : OC(CC(=CCC1C(CC2)C3(C2C(CCC(C(C)C)CC)C)C)C4(C)C1CC3)CC4
CHEM : STIGMAST-5-EN-3-OL, (3.BETA.)-
MOL FOR: C29 H50 O1
MOL WT : 414.72
---------- BCFBAF v3.01 ----------
Summary Results:
Log BCF (regression-based estimate): 2.83 (BCF = 671 L/kg wet-wt)
Biotransformation Half-Life (days) : 295 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 5.46 (BAF = 2.87e+005 L/kg wet-wt)

==========
BCF (Bioconcentration Factor):
==========
Log Kow (estimated) : 9.65
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 9.65

Equation Used to Make BCF estimate:
Log BCF = -0.49 log Kow + 7.554 + Correction

Correction(s): Value
No Applicable Correction Factors

Estimated Log BCF = 2.827 (BCF = 671.2 L/kg wet-wt)

==========
Whole Body Primary Biotransformation Rate Estimate for Fish:
==========
------+-----+----------+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
------+-----+----------+---------+---------
Frag | 1 | Aliphatic alcohol [-OH] | -0.0616 | -0.0616
Frag | 2 | Carbon with 4 single bonds & no hydrogens | -0.2984 | -0.5969
Frag | 6 | Methyl [-CH3] | 0.2451 | 1.4706
Frag | 3 | -CH2- [linear] | 0.0242 | 0.0726
Frag | 3 | -CH- [linear] | -0.1912 | -0.5737
Frag | 8 | -CH2- [cyclic] | 0.0963 | 0.7700
Frag | 5 | -CH - [cyclic] | 0.0126 | 0.0630
Frag | 1 | -C=CH [alkenyl hydrogen] | 0.0988 | 0.0988
Frag | 1 | -C=CH [alkenyl hydrogen] | 0.0000 | 0.0000
Frag | 4 | Number of fused acyclic rings | 0.6477 | 2.5907
Frag | 1 | Four or more fused cyclic rings | -1.7279 | -1.7279
Frag | 2 | Polycyclic -CH3 (4 fused rings or more) | 0.0000 | 0.0000
L Kow| * | Log Kow = 9.65 (KowWin estimate) | 0.3073 | 2.9650
MolWt| * | Molecular Weight Parameter | | -1.0635
Const| * | Equation Constant | | -1.5371
============+==========+==========
RESULT | LOG Bio Half-Life (days) | | 2.4702
RESULT | Bio Half-Life (days) | | 295.3
NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
============+==========+==========

Biotransformation Rate Constant:
kM (Rate Constant): 0.002347 /day (10 gram fish)
kM (Rate Constant): 0.00132 /day (100 gram fish)
kM (Rate Constant): 0.0007423 /day (1 kg fish)
kM (Rate Constant): 0.0004174 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 1.891 (BCF = 77.82 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 5.458 (BAF = 2.873e+005 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 2.047 (BCF = 111.4 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 5.126 (BAF = 1.336e+005 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 2.095 (BCF = 124.3 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 4.882 (BAF = 7.614e+004 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 2.266 (BCF = 184.7 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 5.967 (BAF = 9.261e+005 L/kg wet-wt)

SMILES : Oc1cc2c(c(c1C)C)OC(CCCC(CCCC(CCCC(C)C)C)C)(C)CC2
CHEM : TOCOPHEROL
MOL FOR: C28 H48 O2
MOL WT : 416.69
---------- BCFBAF v3.01 ----------
Summary Results:
Log BCF (regression-based estimate): 1.26 (BCF = 18.1 L/kg wet-wt)
Biotransformation Half-Life (days) : 28.4 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 1.95 (BAF = 89 L/kg wet-wt)

==========
BCF (Bioconcentration Factor):
==========
Log Kow (estimated) : 11.63

Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 11.63

Equation Used to Make BCF estimate:
Log BCF = -0.49 log Kow + 7.554 + Correction

Correction(s): Value
Alkyl chains (8+ -CH2- groups) -0.596

Estimated Log BCF = 1.258 (BCF = 18.12 L/kg wet-wt)

==========
Whole Body Primary Biotransformation Rate Estimate for Fish:
==========
------+-----+----------+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
------+-----+----------+---------+---------
Frag | 1 | Aromatic alcohol [-OH] | -0.4727 | -0.4727
Frag | 1 | Carbon with 4 single bonds & no hydrogens | -0.2984 | -0.2984
Frag | 1 | Aromatic ether [-O-aromatic carbon] | -0.0694 | -0.0694
Frag | 3 | Alkyl substituent on aromatic ring | 0.1781 | 0.5342
Frag | 2 | Aromatic-CH3 | -0.0872 | -0.1743
Frag | 1 | Aromatic-CH2 | -0.3365 | -0.3365
Frag | 1 | Aromatic-H | 0.2664 | 0.2664
Frag | 5 | Methyl [-CH3] | 0.2451 | 1.2255
Frag | 9 | -CH2- [linear] | 0.0242 | 0.2177
Frag | 3 | -CH- [linear] | -0.1912 | -0.5737
Frag | 1 | -CH2- [cyclic] | 0.0963 | 0.0963
Frag | 1 | Number of fused acyclic rings | 0.6477 | 0.6477
Frag | 1 | Number of fused 6-carbon aromatic rings | -0.5779 | -0.5779
L Kow| * | Log Kow = 11.63 (KowWin estimate) | 0.3073 | 3.5748
MolWt| * | Molecular Weight Parameter | | -1.0685
Const| * | Equation Constant | | -1.5371
============+==========+=========+=========
RESULT | LOG Bio Half-Life (days) | | 1.4540
RESULT | Bio Half-Life (days) | | 28.44
NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
============+==========+=========+=========

Biotransformation Rate Constant:
kM (Rate Constant): 0.02437 /day (10 gram fish)
kM (Rate Constant): 0.0137 /day (100 gram fish)
kM (Rate Constant): 0.007707 /day (1 kg fish)
kM (Rate Constant): 0.004334 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 0.007 (BCF = 1.017 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 1.949 (BAF = 89 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 0.043 (BCF = 1.103 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 1.942 (BAF = 87.51 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 0.053 (BCF = 1.13 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 1.939 (BAF = 86.85 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 0.459 (BCF = 2.881 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 4.004 (BAF = 1.01e+004 L/kg wet-wt)

Estimation by CAESAR v.2.1.14 (Due to space limitations, ony the results for the longest alkyl chain containing fatty acid and glyceride has been presented here; remaining estimations are in the CAESAR BCF report PDF under the "Attached background material") :
(A) Glycerides: For C18 chain length i.e. tristerain or glycerol tristearate:
Compound SMILES:
O=C(OCC(OC(=O)CCCCCCCCCCCCCCCCC)COC(=O)CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC
Experimental value [log(L/kg)]: -
Predicted BCF [log(L/kg)]: -0.07
Predicted BCF [L/kg]: 0.84
Predicted BCF from sub-model 1 (HM) [log(L/kg)]: 0
Predicted BCF from sub-model 2 (GA) [log(L/kg)]: 0.1
Predicted LogP (MLogP): 10.93
Structural alerts: Carbonyl residue (SR 02); >C=O group (PG 09)
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks: none
Compound SMILES:
O=C(OCC(OC(=O)CCCCCCCC=CCCCCCCCC)COC(=O)CCCCCCCC=CCCCCCCCC)CCCCCCCC=CCCCCCCCC
Experimental value [log(L/kg)]: -
Predicted BCF [log(L/kg)]: -0.07
Predicted BCF [L/kg]: 0.85
Predicted BCF from sub-model 1 (HM) [log(L/kg)]: 0
Predicted

(B) Fatty acids:
For C18 chain length i.e. stearic acid:
Compound SMILES: O=C(O)CCCCCCCCCCCCCCCCC
Experimental value [log(L/kg)]: -
Predicted BCF [log(L/kg)]: 1.76
Predicted BCF [L/kg]: 58

Predicted BCF from sub-model 1 (HM) [log(L/kg)]: 1.73
Predicted BCF from sub-model 2 (GA) [log(L/kg)]: 2.47
Predicted LogP (MLogP): 5.69
Structural alerts: Carbonyl residue (SR 02); COOH group (PG 01)
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks: none

(C) Unsaponifiable matters: Beta-sitosterols
Compound SMILES: OC4CC3=CCC1C(CCC2(C)(C(CCC12)C(C)CCC(CC)C(C)C))C3(C)CC4
Experimental value [log(L/kg)]: -Predicted BCF [log(L/kg)]: 1.09
Predicted BCF [L/kg]: 12
Predicted BCF from sub-model 1 (HM) [log(L/kg)]: 1.3
Predicted BCF from sub-model 2 (GA) [log(L/kg)]: 1.3
Predicted LogP (MLogP): 6.79
Structural alerts: OH group (PG 06)
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks: none

(D) Unsaponifiable matters: Tocopherols
Compound SMILES: Oc2cc1c(OC(C)(CC1)CCCC(C)CCCC(C)CCCC(C)C)c(c2C)C
Experimental value [log(L/kg)]: -Predicted BCF [log(L/kg)]: 0.81
Predicted BCF [L/kg]: 6
Predicted BCF from sub-model 1 (HM) [log(L/kg)]: 0.69
Predicted BCF from sub-model 2 (GA) [log(L/kg)]: 1.3
Predicted LogP (MLogP): 6.17
Structural alerts: OH group (PG 06)
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks: none

TEST US EPA Predictions ((Due to space limitations, ony the results of the longest alkyl chain containing fatty acid and glyceride has been presented here; remaining estimations are in the US EPA TEST results PDF under the "Attached background material"):

A) Predicted Bioaccumulation factor for Tristearin (CAS 555-43-1) from Consensus method

Prediction results:
Bioaccumulation factor Log10: 0.57 (predicted value)
Bioaccumulation factor: 3.70

Individual Predictions:
1. Hierarchical clustering: N/A
2. Single model: N/A
3. Group contribution: N/A
4. FDA: 0.11
5. Nearest neighbor: 1.02

B) Predicted Bioaccumulation factor for Stearic acid (CAS 57-11-4) from Consensus method

Prediction results:
Bioaccumulation factor Log10: 1.08 (predicted value)
Bioaccumulation factor: 12.02

Individual Predictions (Log10):
1. Hierarchical clustering: 0.20
2. Single model: 1.20
3. Group contribution: 1.10
4. FDA: 0.73
5. Nearest neighbor: 2.18

C) Predicted Bioaccumulation factor for beta-sitosterol (CAS 83-46-5) from Consensus method

Prediction results:
Bioaccumulation factor Log10: 2.80 (predicted value)
Bioaccumulation factor: 636.39

Individual Predictions (Log10):
1. Hierarchical clustering: 2.12
2. Single model: 2.23
3. Group contribution: 4.53
4. FDA: 2.44
5. Nearest neighbor: 2.70

(D) Predicted Bioaccumulation factor for tocopherols (CAS 7616-22-0) from Consensus method
Prediction results:
Bioaccumulation factor Log10: 2.02 (predicted value)
Bioaccumulation factor: 105.24

Individual Predictions (Log10):
1. Hierarchical clustering: 2.22
2. Single model: 2.52
3. Group contribution: 3.36
4. FDA: 1.05
5. Nearest neighbor: 0.96

Summary of the BCF estimations using different QSAR models

Substance	EPISuite BCFBAF (BCF L/kg wet-wt)	VEGA CAESAR (BCF L/kg wet-wt)	USEPA Test (BCF L/kg wet-wt)	Average (BCF L/kg wet-wt)	Range of BCF values (L/kg)
C8 fatty acid	3.16	7.00	11.00	11.00	11-17
C18 fatty acid	10.00	58.00	12.02	11.01	
C18-unsatd. fatty acid (oleic acid)	56.2	72.00	16.55	16.55	
C8 triglyceride	281.00	3.00	3.96	142.48	4-143
C18 triglyceride	3.16	0.84	3.70	3.70	
C18-unsatd. Triglyceride (triolein)	3.16	0.85	9.34	9.34	
Tocopherols	18.1	6.00	105.24	105.24	105-654
Beta-sitosterol	671.00	12.00	636.39	653.70	

Refer to the QPRF for reliability discussion on the BCF estimations.

Validity criteria fulfilled:	not applicable
Conclusions:	As per the R.7c guidance, since the Kow value for some of the constituents exceeded 10, the BCF estimations were conducted using more than one QSAR models. Based on these individual BCF estimations for the representative constituents via different QSAR models (i.e. BCFBAF v3.01 of EPIWEB v 4.1, BCF (CAESAR) 2.1.14 and T.E.S.T US EPA model v.4.1.), the overall estimated BCF value for the 'oils, vegetable, deodorizer distillates' was considered to range between 4-654 L/kg.
Executive summary:	The BCF value of 'oils, vegetable, deodorizer distillates' was estimated through the computation methods recommended in Chapter R.7a, in: Guidance on information requirements and chemical safety assessment. Since the Kow values for some of the constituents were >10, the calculations were performed using more than one QSAR programs such as BCFBAF v3.01 of EPIWEB v 4.1, BCF (CAESAR) 2.1.14 and T.E.S.T US EPA model v.4.1 as stated in table R.7.10-3 of the REACH guidance document and/or the ECHA practical guide 5. As the test substance is a UVCB/mixture of different constituents (i.e. glycerides of fatty acids, fatty acids and unsaponifiable matters (UMs)) the BCF values were determined for representative substances of each class present >10% to represent the lower and upperlimit of the test substance. Hence, the BCF estimations were carried out for octanoic acid, stearic acid and oleic acid representing fatty acids and trioctanoin, tristearin and triolein representing glycerides of fatty acids and tocopherols and beta-sitosterols for the UMs. SMILES notations were used as the input parameters for the programs/softwares. The BCF values estimated using BCFBAF v.3.0 for the representative constituents ranged between 3.16 -56.2 L/kg for fatty acids, 3.16 -281 L/kg for the glycerides and 18.1-671 L/kg for the unsaponifiable matters substance class. Except for the Kow value of tristearin, the estimation by this method is more or less accurate as the molecular weight and the Kow range for the different constituents of test substance were determined to be within the molecular weight and Kow range of the training set compounds. Hence, considering this and the fact that all the representative constituent class are hydrophobic with Kow 6, they were additionally modelled using the BCF (CAESAR) 2.1.14 model. This model is based on Dimitrov et al., 2005 experimental database, which is recognised to cover hydrophobic compounds. The BCF values estimated using Caesar BCF model for the representative constituents were estimated to range between 7 -72 L/kg for fatty acids, 0.84 -3 L/kg for glycerides and 6 -12 for unsaponifiable matters. However, these estimations using BCF (CAESAR) were reported to be not very reliable. Therefore, to further, increase the confidence of the predictions, the BCF values were additionally estimated using the BCF interface of the US EPA T.E.S.T QSAR model. This model uses several methodologies (such as hierarchical clustering, single model, group contribution, FDA, nearest neighbour) to predict an overall average BCF value under the name 'consensus method'. The respective average BCF ranges for the representative constituents were estimated to be 11 -16.55 L/kg for fatty acids, 3.7 -9 L/kg for glycerides, 105.24 -636.39 L/kg for unsaponifiable matters. However, the different training set substances used for the BCF estimation for the representative substances via the US EPA TEST program were not very similar and had presence of other functional groups. Overall, considering that the estimated values from the three models lie more or less in the same BCF range, an average estimated BCF value was determined to reduce the overall uncertainty or limitations of each of the models. Therefore, based on the BCF estimations for the representative constituents, the estimated BCF value of the 'oils, vegetable, deodorizer distillates' can be considered to range between 4-654 L/kg (US EPA, 2012b; Zhao et al., 2008). This is in line with the statement stated in chapter R.11 from ECHA i.e., "the aquatic BCF of a substance is probably lower than 2000 if the calculated Log Kow is higher than 10".

Description of key information

Based on the average BCF estimations for the major constituents using QSAR models (i.e., BCFBAF v3.01 of EPIWEB v 4.1, BCF (CAESAR) 2.1.14 and T. E. S. T US EPA model v.4.1), 'Oils, vegetable, deodorizer distillates' can be considered to have a BCF value ranging between 4-654 L/kg. This is further supported by the low BCF results determined in short-term in vitro bioaccumulation studies conducted with tristearin and palmitic acid (Freitag, 1985) as well as the metabolic potential of fish to break down the triglycerides and fatty acids and use as source of energy (Tocher, 2003).

Key value for chemical safety assessment

BCF (aquatic species):	654 L/kg ww

Additional information

The BCF value of 'oils, vegetable, deodorizer distillates' was estimated through the computation methods recommended in Chapter R.7a, in: Guidance on information requirements and chemical safety assessment. Since the Kow values for some of the constituents were >10, the calculations were performed using more than one QSAR programs, such as BCFBAF v3.01 of EPIWEB v 4.1, BCF (CAESAR) 2.1.14 and T.E.S.T US EPA model v.4.1 as stated in table R.7.10-3 of the REACH guidance document. As the test substance is a UVCB/mixture of different constituents (i.e. glycerides of fatty acids, fatty acids and unsaponifiable matters (UMs)), the BCF values were determined for representative substances of each class present at >10% to represent the lower and upper limit. Hence, the BCF estimations were carried out for octanoic acid, stearic acid and oleic acid representing fatty acids and trioctanoin, tristearin and triolein representing glycerides of fatty acids and tocopherols and beta-sitosterols for the UMs. SMILES notations were used as the input parameters for the program/software. The BCF values estimated using BCFBAF v.3.0 for the representative constituents ranged between 3.16 -56.2 L/kg for fatty acids, 3.16 -281 L/kg for the glycerides and 18.1-671 L/kg for the unsaponifiable matters. Except for the Kow value of tristearin, the estimation by this method is more or less accurate as the molecular weight and the Kow range for the different constituents of test substance were determined to be within the molecular weight and Kow range of the training set compounds. Hence, considering this and the fact that all the representative constituents are hydrophobic with log Kow 6, they were additionally modelled using the BCF (CAESAR) 2.1.14 model. This model is based on Dimitrov et al., 2005 experimental database, which is recognised to cover hydrophobic compounds. The BCF values estimated using Caesar BCF model for the representative constituents were estimated to range between 7 -72 L/kg for fatty acids, 0.84 -3 L/kg for glycerides and 6 -12 for unsaponifiable matters. However, these estimations using BCF (CAESAR) were reported not to be very reliable. Therefore, to further increase the confidence of the predictions, the BCF values were additionally estimated using the BCF interface of the US EPA T.E.S.T QSAR model. This model uses several methodologies (such as hierarchical clustering, single model, group contribution, FDA, nearest neighbour etc.) to predict an overall average BCF value under the name 'consensus method'. The respective average BCF ranges for the representative constituents were estimated to be 11 -16.55 L/kg for fatty acids, 3.7 -9 L/kg for glycerides and 105.24 -636.39 L/kg for unsaponifiable matters. However, the different training set substances used for the BCF estimation for the representative substances via the US EPA TEST program were not very similar and had presence of other functional groups. Overall, considering that the estimated values from the three models lie more or less in the same range, an average estimated BCF value was determined to reduce the overall uncertainty or limitations of each of the models. Therefore, based on the BCF estimations for the representative constituents, the estimated BCF value of the 'oils, vegetable, deodorizer distillates' can be considered to range between 4-654 L/kg (US EPA, 2012b; Zhao et al., 2008). This is in line with the statement stated in ECHA guidance R.11 i.e., "the aquatic BCF of a substance is probably lower than 2000 if the calculated Log Kow is higher than 10".

Additional recommended weight of evidence (WoE) in chapter R.11 which supports the overall low bioaccumulation potential of the substance/constituents are:

- Low bioaccumulation based on short term tests with tristearin and palmitic acid: Low bioaccumulation potential has been interpreted based on BCF value of <10 and 60 observed for tristearin and palmitic acid in a short term bioaccumulation study conducted in fish following exposure for 3 d (Freitag et al., 1985).

- Slight water solubility: The water solubility of the test substance may range from 6.4 -40 mg/L at 20 ± 2°C which indicates that there would be relatively low concentration of the substance in the aquatic environment.

- Ready biodegrability of the substance: The ready biodegradation potential of the substance under stringent test conditions indicates that there would be relatively low concentration of the substance in the aquatic environment thereby leading to low bioavailability in aquatic organisms.

- Favourable mammalian toxicokinetic data: This includes low uptake potential of the longer chain glycerides and fatty acids constituents together with the general ability of the mammals to metabolise these constituents and use as source of energy via beta-oxidation.

- Metabolism potential in fish: Similar to the mammals, the triglycerides and their constituent fatty acids are known to be broken down via beta-oxidation to serve as an important source of metabolic energy for growth and reproductionin fish (Tocher, 2003).

Therefore, the above WoE together with the estimated BCF values of the major constituents (ranging from 4-654 L/kg) are both supportive of the fact that the substance will have a low potential for bioaccumulation in aquatic as well as terrestrial organisms.