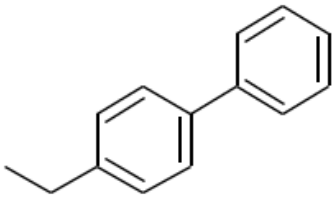
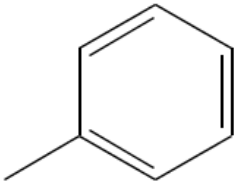
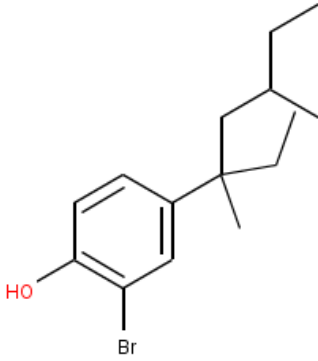


Batch predictions for Consensus method for Bioaccumulation factor

#	ID	Structure	Experimental Value Log10	Predicted Value Log10	Experimental Value	Predicted Value
1	1		2,82	2,79	667,00	621,70
2	2		N/A	1,75	N/A	56,68
3	3		N/A	2,18	N/A	151,34

Molecule No.1

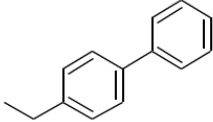
Predicted Bioaccumulation factor for **1** from Consensus method

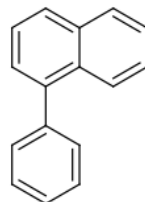
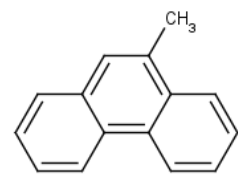
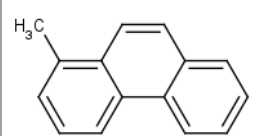
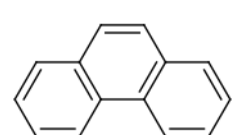
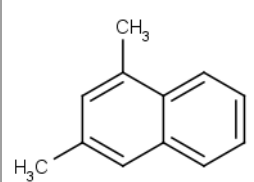
Prediction results		
Endpoint	Experimental value CAS: 5707-44-8 SAR QSAR Environ Res, 16, p. 531-554 (2005)	Predicted value ^a
Bioaccumulation factor Log10	2,82	2,79
Bioaccumulation factor	667,00	621,70

^aNote: the test chemical was present in the training set. The prediction *does not* represent an external prediction.

Individual Predictions	
Method	Predicted value Log10
Hierarchical clustering	2,60
Single model	2,68
Group contribution	2,85
FDA	2,86
Nearest neighbor	2,98

Predictions for the test chemical and for the most similar chemicals in the **external test set**

CAS	Structure	Similarity Coefficient	Experimental value Log10	Predicted value Log10
1 (test chemical)			2,82	2,79

13540-50-6		0,90	3,32	2,69
605-02-7		0,89	3,51	2,74
883-20-5		0,70	2,56	2,77
832-69-9		0,70	3,18	2,73
85-01-8		0,69	3,31	2,72
575-41-7		0,66	3,37	2,75

Details of the Nearest neighbor

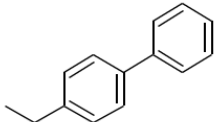
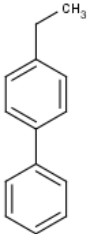
Predicted Bioaccumulation factor for 1 for Nearest neighbor method

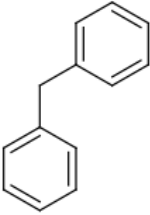
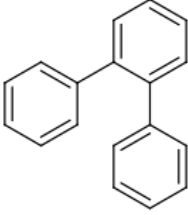
Prediction is determined by averaging the toxicity values of the nearest neighbor chemicals

Prediction results		
Endpoint	Experimental value CAS: 5707-44-8 SAR QSAR Environ Res, 16, p. 531-554 (2005)	Predicted value ^a
Bioaccumulation factor Log10	2,82	2,98
Bioaccumulation factor	667,00	947,09

^aNote: the test chemical was present in the training set. However, the prediction *does* represent an external prediction.

Test chemical and chemicals from the training set used to make the prediction

CAS	Structure	Experimental value Log10	Similarity Coefficient
1 (test chemical)		2,82	
5707-44-8		2,82	1,00

101-81-5	 <chem>c1ccccc1Cc2ccccc2</chem>	3,00	0,92
84-15-1	 <chem>c1ccccc1C(c2ccccc2)c3ccccc3</chem>	3,11	0,87

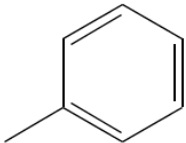
Molecule No.2

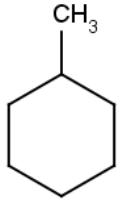
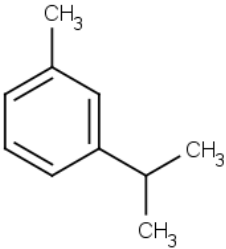
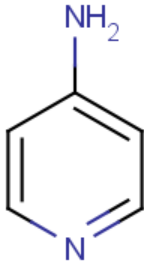
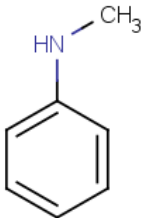
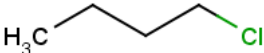
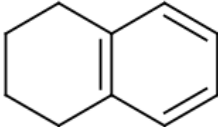
Predicted Bioaccumulation factor for 2 from Consensus method

Prediction results		
Endpoint	Experimental value	Predicted value
Bioaccumulation factor Log10	N/A	1,75
Bioaccumulation factor	N/A	56,68

Individual Predictions	
Method	Predicted value Log10
Hierarchical clustering	1,56
Single model	1,94
Group contribution	1,69
FDA	1,25
Nearest neighbor	2,33

Predictions for the test chemical and for the most similar chemicals in the [external test set](#)

CAS	Structure	Similarity Coefficient	Experimental value Log10	Predicted value Log10
2 (test chemical)			N/A	1,75

108-87-2		0,90	2,37	2,47
535-77-3		0,77	2,77	2,53
504-24-5		0,70	0,22	0,58
100-61-8		0,70	0,66	0,88
109-69-3		0,69	1,21	1,02
119-64-2		0,69	2,47	2,50

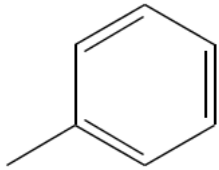
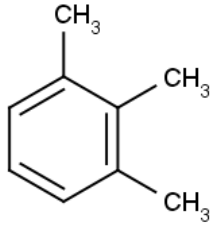
Details of the Nearest neighbor

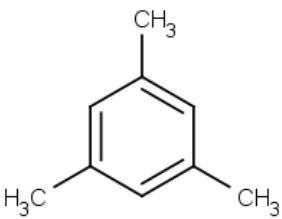
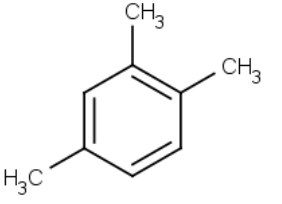
Predicted Bioaccumulation factor for 2 for Nearest neighbor method

Prediction is determined by averaging the toxicity values of the nearest neighbor chemicals

Prediction results		
Endpoint	Experimental value	Predicted value
Bioaccumulation factor Log10	N/A	2,33
Bioaccumulation factor	N/A	215,87

Test chemical and chemicals from the [training set](#) used to make the prediction

CAS	Structure	Experimental value Log10	Similarity Coefficient
2 (test chemical)		N/A	
526-73-8		2,32	0,88

108-67-8		2,43	0,87
95-63-6		2,26	0,86

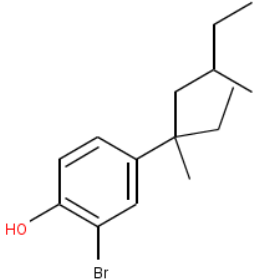
Molecule No.3

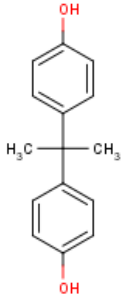
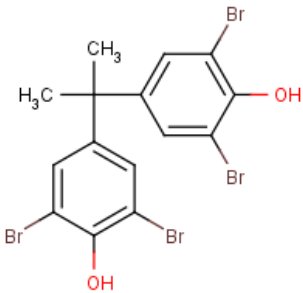
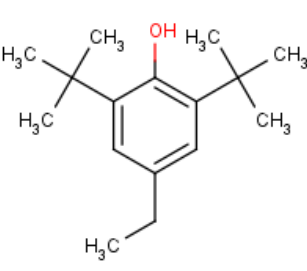
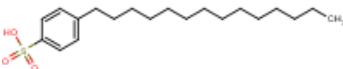
Predicted Bioaccumulation factor for 3 from Consensus method

Prediction results		
Endpoint	Experimental value	Predicted value
Bioaccumulation factor Log10	N/A	2,18
Bioaccumulation factor	N/A	151,34

Individual Predictions	
Method	Predicted value Log10
Hierarchical clustering	2,77
Single model	2,26
Group contribution	2,82
FDA	0,75
Nearest neighbor	2,31

Predictions for the test chemical and for the most similar chemicals in the [external test set](#)

CAS	Structure	Similarity Coefficient	Experimental value Log10	Predicted value Log10
3 (test chemical)			N/A	2,18

80-05-7	 <p>Chemical structure of 4,4'-bis(2-hydroxyphenyl)propane, showing two phenolic rings connected by a central carbon atom bonded to two methyl groups. Each phenolic ring has a hydroxyl group (OH) at the ortho position relative to the central carbon.</p>	0,77	1,39	1,76
79-94-7	 <p>Chemical structure of 2,2-bis[4-bromo-3,5-dihydroxyphenyl]propane, showing a central carbon atom bonded to two methyl groups and two phenolic rings. Each phenolic ring has a hydroxyl group (OH) at the 3-position and a bromine atom (Br) at the 4-position relative to the central carbon.</p>	0,64	2,48	2,28
4130-42-1	 <p>Chemical structure of 2,2-bis[4-(2-methylpropyl)-5-hydroxyphenyl]propane, showing a central carbon atom bonded to two methyl groups and two phenolic rings. Each phenolic ring has a hydroxyl group (OH) at the 5-position and a 2-methylpropyl group at the 4-position relative to the central carbon.</p>	0,55	3,59	2,98
47377-16-2	 <p>Chemical structure of 4-(4-sulfophenyl)decane, showing a decane chain (10 carbons) attached to a phenolic ring at the 4-position. The phenolic ring has a sulfonic acid group (SO₃H) at the para position relative to the decane chain.</p>	0,53	0,52	1,80

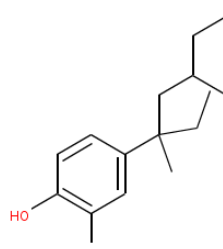
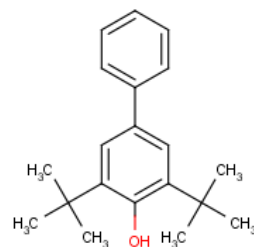
Details of the Nearest neighbor

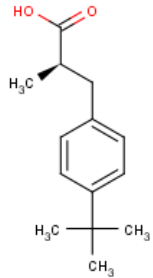
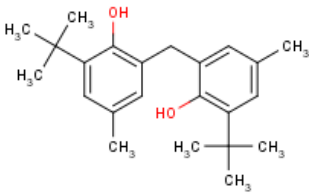
Predicted Bioaccumulation factor for 3 for Nearest neighbor method

Prediction is determined by averaging the toxicity values of the nearest neighbor chemicals

Prediction results		
Endpoint	Experimental value	Predicted value
Bioaccumulation factor Log10	N/A	2,31
Bioaccumulation factor	N/A	202,80

Test chemical and chemicals from the [training set](#) used to make the prediction

CAS	Structure	Experimental value Log10	Similarity Coefficient
3 (test chemical)		N/A	
2668-47-5		3,98	0,70

66735-04-4	 <p>The structure shows a central carbon atom bonded to three methyl groups (CH₃) and a propyl chain. The propyl chain is substituted with a carboxylic acid group (HO-C=O) at the 3-position and a methyl group (H₃C) at the 2-position. The propyl chain is attached to a para-substituted phenyl ring.</p>	0,35	0,68
119-47-1	 <p>The structure shows two phenyl rings connected by a central ethane bridge. Each phenyl ring is substituted with a methyl group (CH₃) at the 3-position and a hydroxyl group (OH) at the 1-position. The ethane bridge is substituted with two methyl groups (CH₃) at each of the two carbon atoms.</p>	2,60	0,67