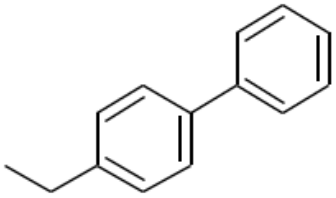
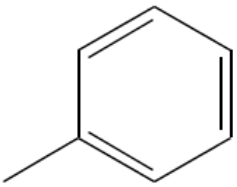
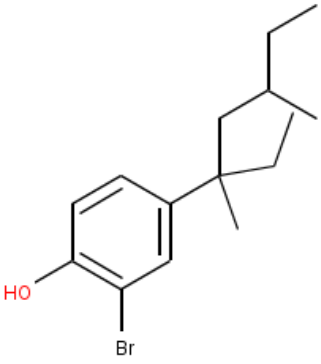
Batch predictions for Consensus method for Bioaccumulation factor

#	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

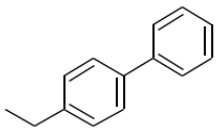
Predicted Bioaccumulation factor for 1 from Consensus method

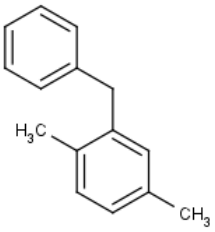
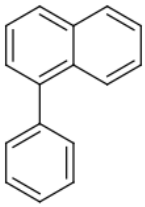
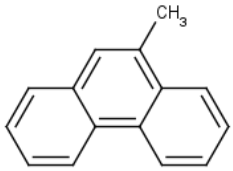
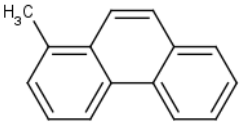
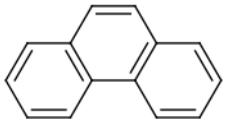
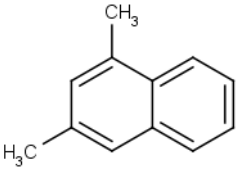
Prediction results		
Endpoint	**Experimental value CAS: 5707-44-8 SAR QSAR Environ Res, 16, p. 531-554 (2005)**	**Predicted value[a]**
Bioaccumulation factor Log10	2,82	2,79
Bioaccumulation factor	667,00	621,70

[a]Note: 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

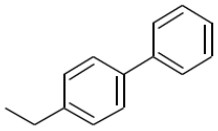
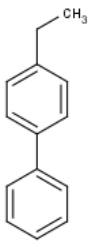
Predicted Bioaccumulation factor for 1 for Nearest neighbor method

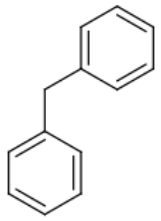
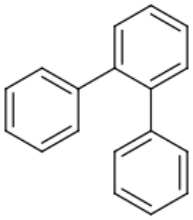
Prediction is determined by averaging the toxicity values of the nearest neighbor chemicals

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

[a]Note: 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		3,00	0,92
84-15-1		3,11	0,87

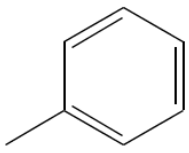
Molecule No.2

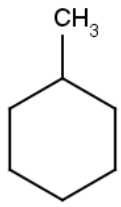
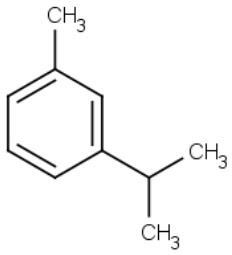
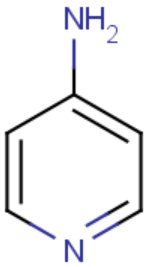
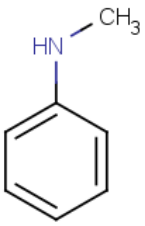
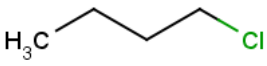
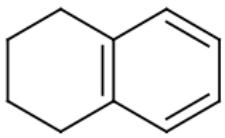
Predicted Bioaccumulation factor for 2 from Consensus method

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

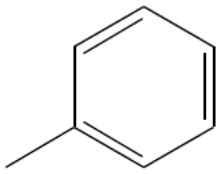
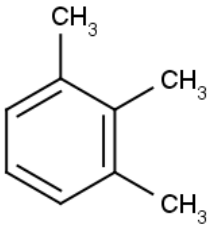
Details of the Nearest neighbor

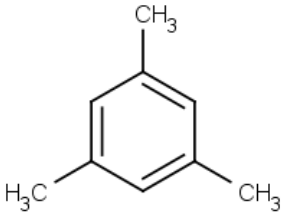
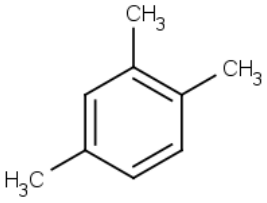
Predicted Bioaccumulation factor for 2 for Nearest neighbor method

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

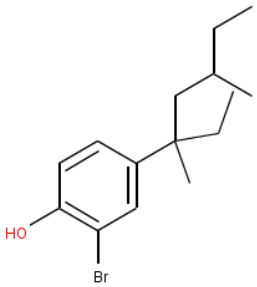
Molecule No.3

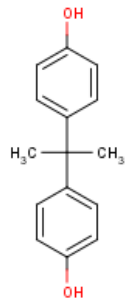
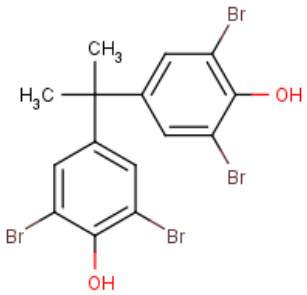
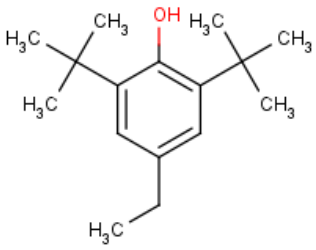
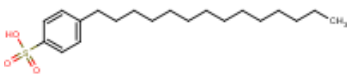
Predicted Bioaccumulation factor for 3 from Consensus method

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		0,77	1,39	1,76
79-94-7		0,64	2,48	2,28
4130-42-1		0,55	3,59	2,98
47377-16-2		0,53	0,52	1,80

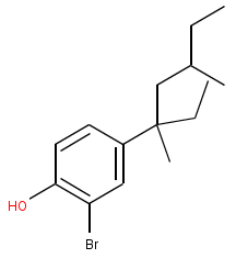
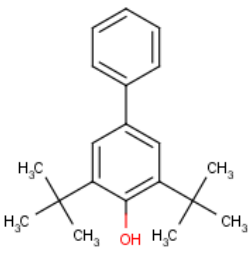
Details of the Nearest neighbor

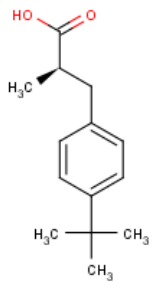
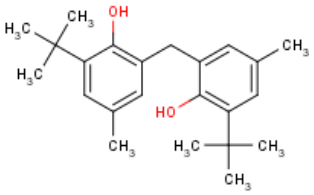
Predicted Bioaccumulation factor for 3 for Nearest neighbor method

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		0,35	0,68
119-47-1		2,60	0,67