ELECTRONIC SUPPLEMENTARY INFORMATION OF

Aquatic Ecotoxicity of Personal Care Products: QSAR models and ranking for prioritization and safer alternatives' design

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Model graphs and equations for Pseudokirchneriella subcapitata toxicity

- Random splitting

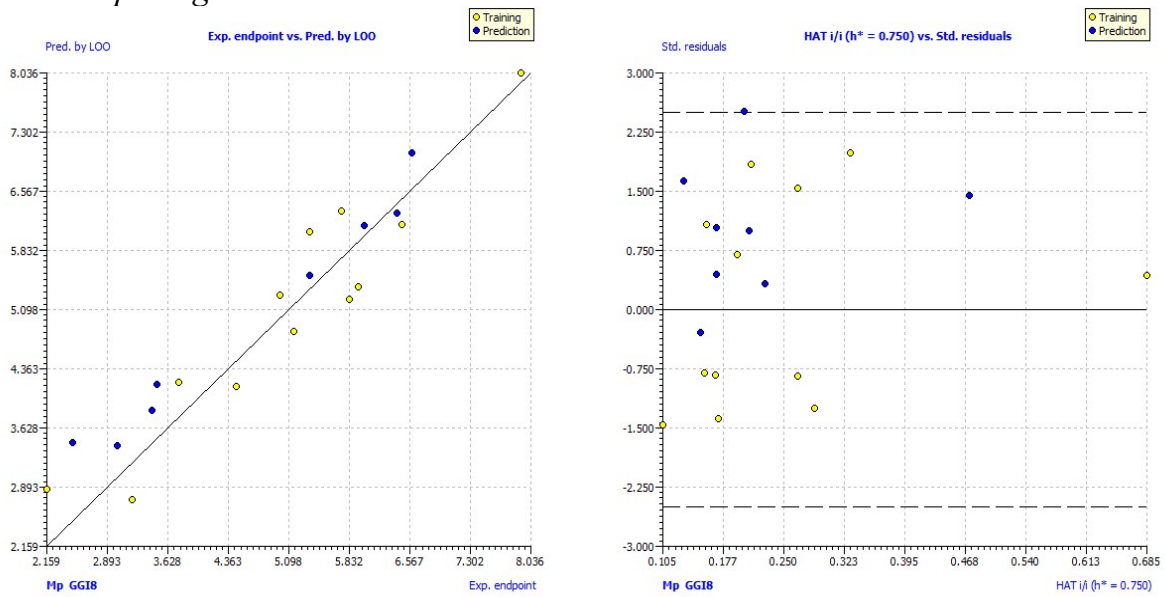


Figure ES1*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.subcapitata PCP split by random model.*

pEC50 ***P.subcapitata*** = -9.50 + 20.55 **Mp** + 12.36 **GGI8**

- Ordered by response splitting

Graphs in the main text

pEC50 ***P.subcapitata*** = -10.60 + 14.05 **GGI8** + 21.83 **Mp**

- Structural similarity splitting

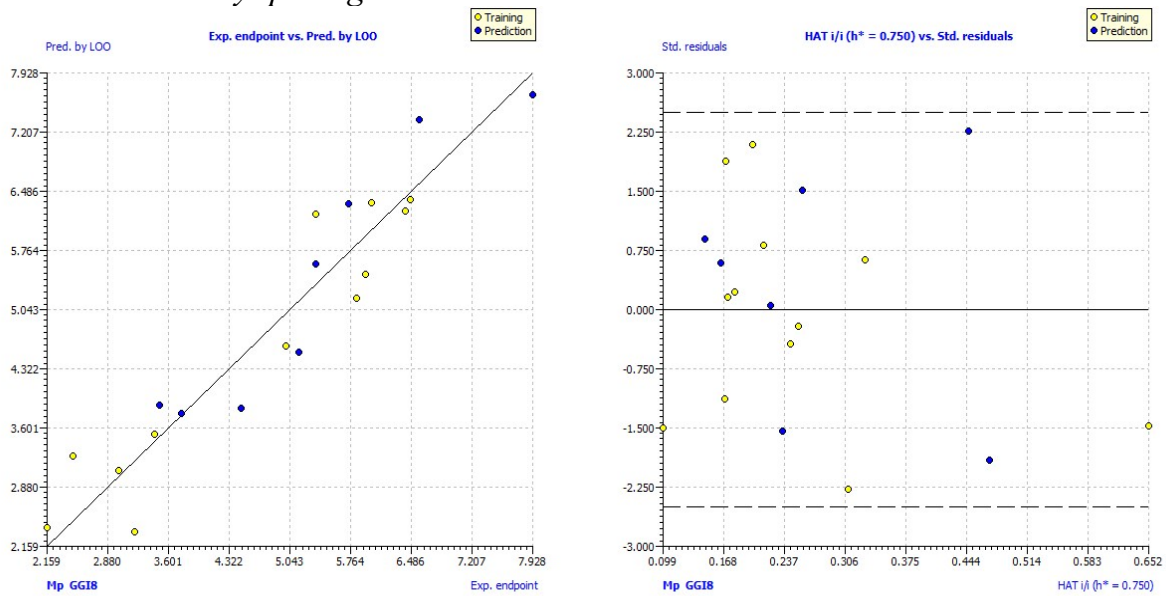


Figure ES2*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.subcapitata PCP split by structural similarity model.*

pEC50 *P.subcapitata* = -9.62 + 14.46 **GGI8** + 20.21 **Mp**

- FULL model

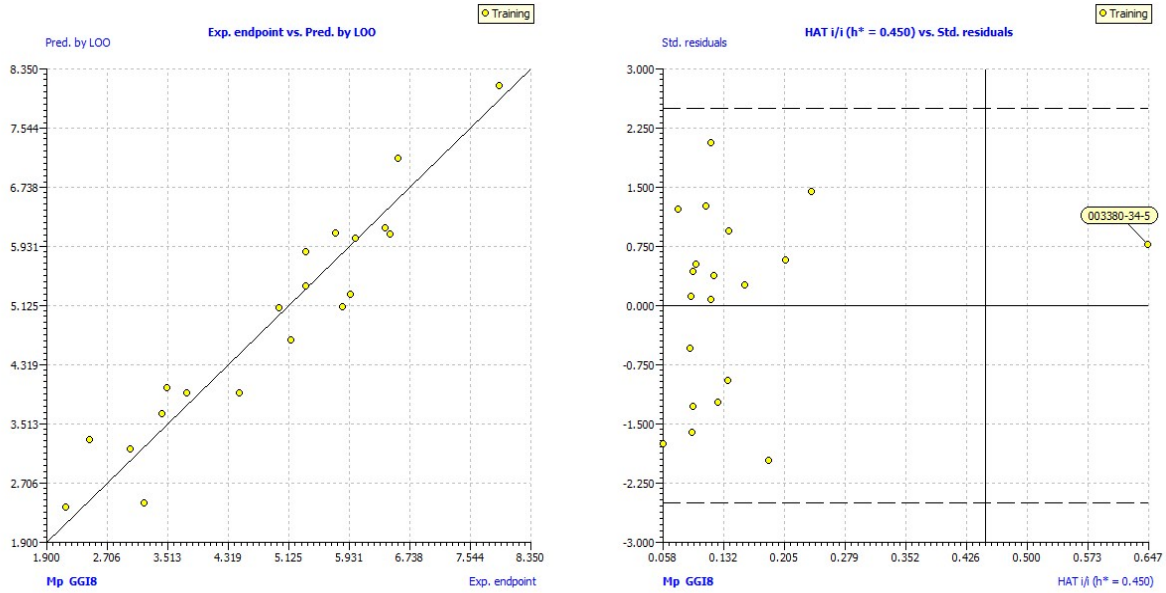
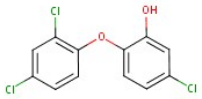


Figure ES3*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.subcapitata PCP full model.*

In the full model, chemical 3380-34-5 (Triclosan, show below) is a structural outlier, influential for the selection of the two modeling variables. No response outliers were detected.



Model graphs for Daphnia magna toxicity

- Random splitting

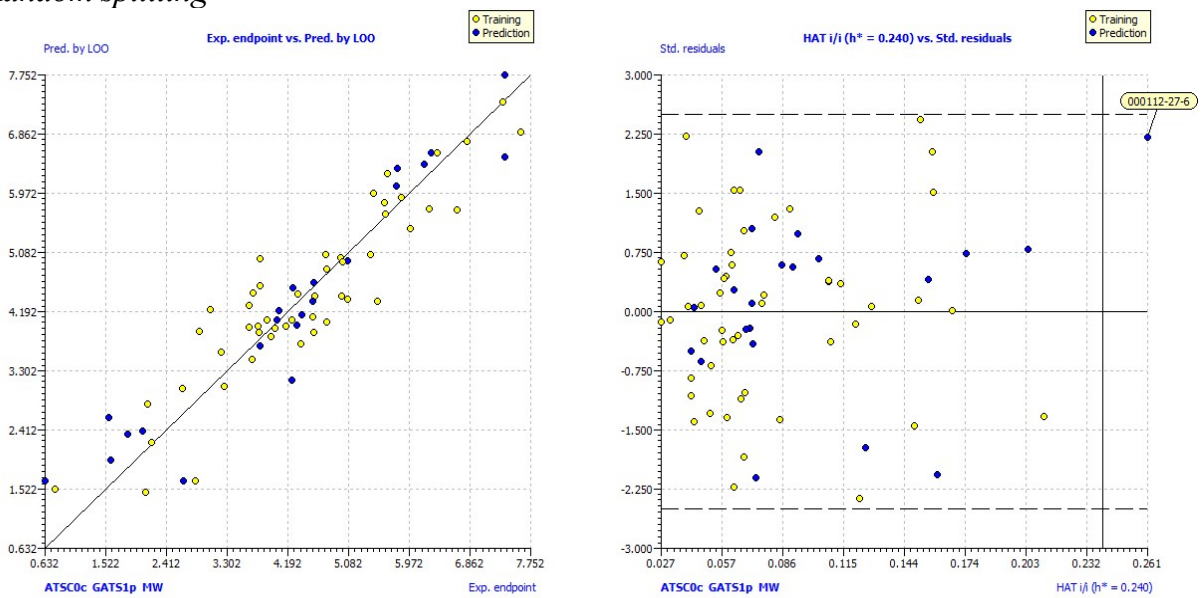
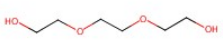


Figure ES4*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the D.magna PCP split by random model.*

Chemical 112-27-6 (Triethylene glycol) is the only outlier for structure, belonging to prediction set.



pEC50 *D.magna* = 4.29 + 0.015 **MW** – 2.94 **ATSC0c** - 1.423 **GATS1p**

- Ordered by response splitting

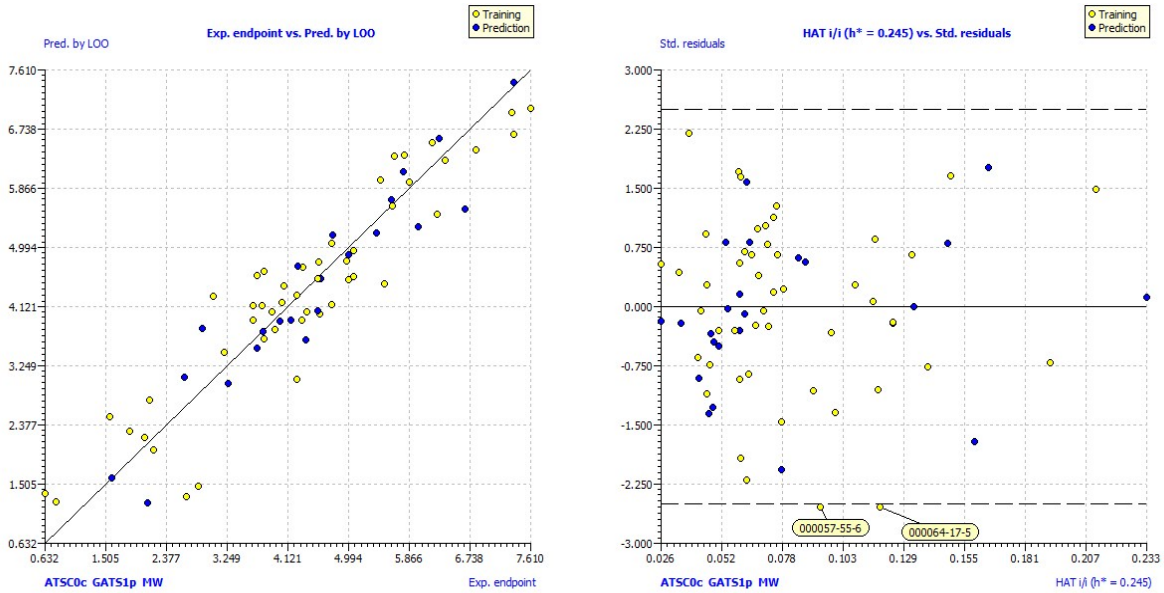


Figure ES5*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the D.magna PCP split by ordered response model.*

pEC50 ***D.magna*** **=** 4.903 + 0.015 **MW** – 3.341 **ATSC0c** - 1.779 **GATS1p**

- Structural similarity splitting

Graphs in the main text

pEC50 ***D.magna*** **=** 4.403 + 0.015 **MW** – 3.134 **ATSC0c** - 1.492 **GATS1p**

- FULL model

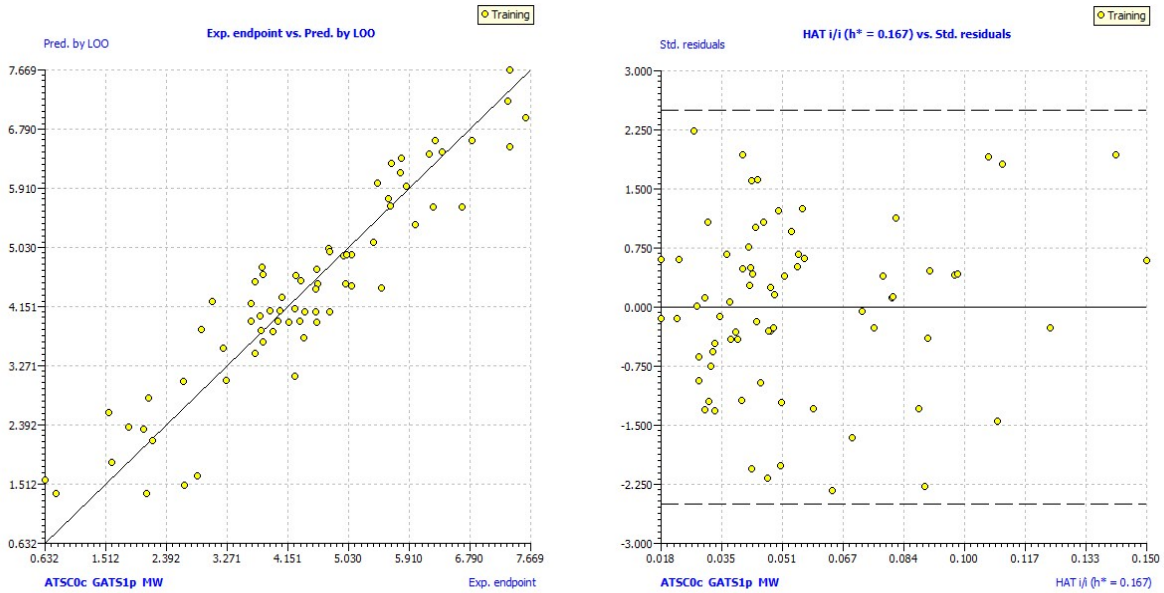


***Figure ES6**: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the D.magna PCP full model.*

Model graphs for Pimephales promelas toxicity

- LogP free model

***Table ES1**: statistical parameters, related to the internal and external validation, of the proposed model for P.promelas toxicity of PCPs, LogPfree. The equation of the full model is also reported.*

LogPfree Model	N_{TR}	N_{PRED}	R^2	Q^2_{LOO}	Q^2_{LMO}	R^2Y_{scr}	CCC_{EXT}	Q^2_{EXT} Fn	RMSEtr	RMSEp	AD 534 PCPs
Split by random	47	20	0.84	0.79	0.77	0.09	0.91	0.79-0.83	0.53	0.62	-
Split by ordered response	46	21	0.85	0.81	0.79	0.09	0.89	0.80-0.87	0.57	0.53	-
Split by structural similarity	46	21	0.87	0.83	0.82	0.09	0.84	0.71-0.85	0.55	0.59	-
pLC50 *P.promelas* = 1.932 + 0.276 **topoDiameter** - 0.873 **SM1_Dzs** + 2.072 **maxHother + 0.681 ATSC2e**	**67**	**-**	**0.84**	**0.81**	**0.80**	**0.06**	**0.90cv**	**-**	**0.55**	**0.60cv**	**93%**

In the Table ES1, the statistical parameters related to the internal and external validation of the split models are reported, regarding the model without LogP ("LogPfree") for *P.promelas* toxicity, together with the full model equation and the coverage of the whole set of 534 PCPs., which is the lower of the entire work presented here (93%). The statistical parameters show that the model is stable and robust, not given by chance correlation, externally predictive on the PCPs included in the three indipendent prediction sets.

The most important descriptor in the model equation is topoDiameter (maximum atom eccentricity), positively correlated with the modeled acute toxicity. The others modeling descriptors are: SM1_Dzs (Spectral moment of order 1 from Barysz matrix, weighted by I-state), negatively correlated with the endpoint, maxHother (maximum E-state for H on aaCH, dCH2 or dsCH) and ATSC2e (Centered broto-moreau autocorrelation lag2, weighted by Sanderson electronegativities), both positively correlated with the pLC_{50} in *P.promelas*.

- Random splitting

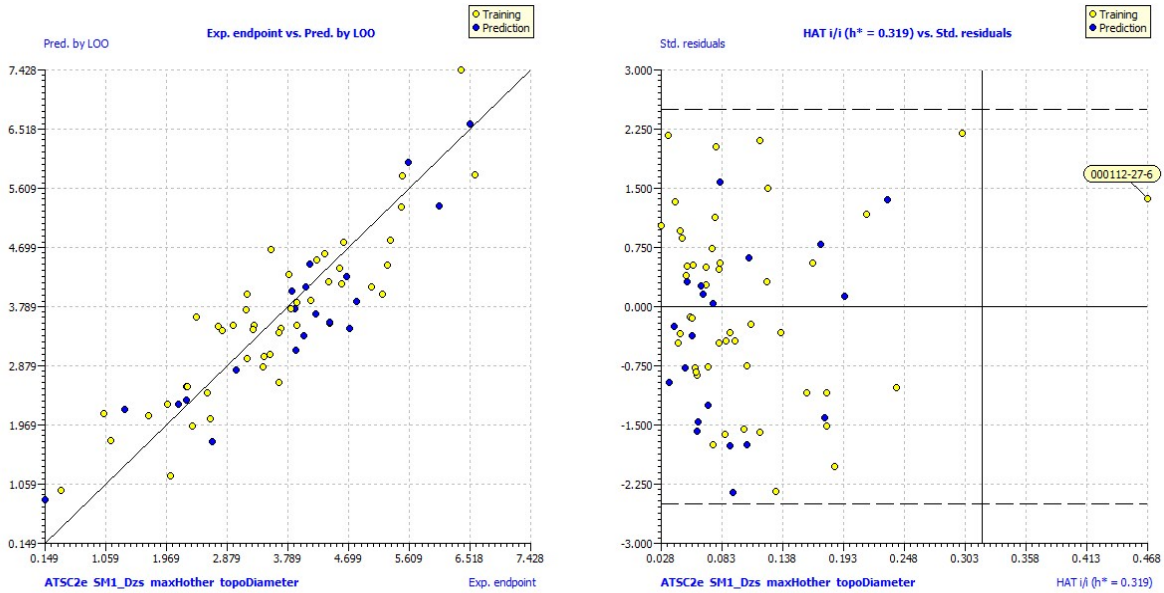


Figure ES7*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.promelas LogPfree PCP split by random model.*

Chemical 112-27-6 (Triethylene glycol) is the only outlier for structure, belonging to training set.

pLC50 *P.promelas* = 1.833 + 0.271 **topoDiameter** - 0.777 **SM1_Dzs** + 1.96 **maxHother** + 0.747 **ATSC2e**

- Ordered by response splitting

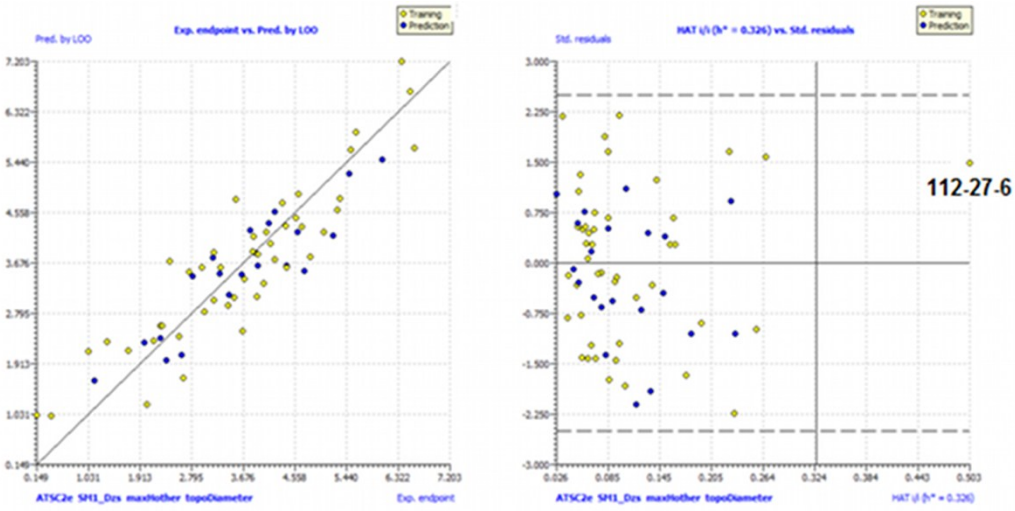


Figure ES8*. Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.promelas LogPfree PCP split ordered by response model.*

pLC50 *P.promelas* = 1.906 + 0.268 **topoDiameter** - 0.842 **SM1_Dzs** + 2.10 **maxHother** + 0.685 **ATSC2e**

- Structural similarity splitting

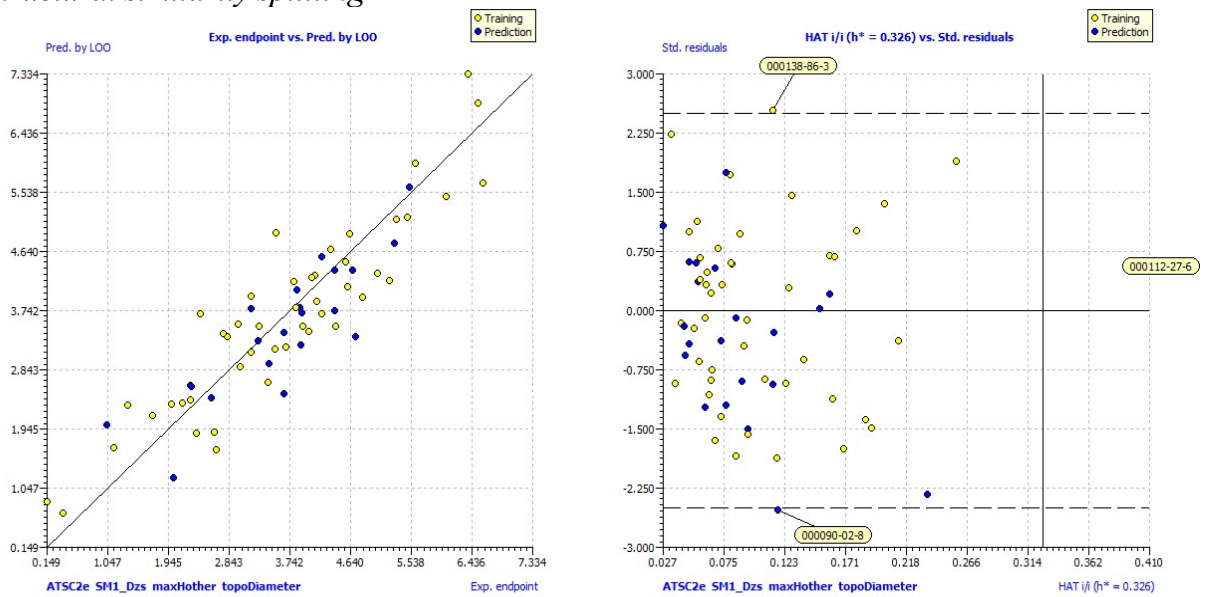


Figure ES9*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.promelas LogPfree PCP split by structural similarity model.*

pLC50 *P.promelas* = 1.911 + 0.289 **topoDiameter** - 0.936 **SM1_Dzs** + 1.878 **maxHother** + 0.724 **ATSC2e**

- FULL model

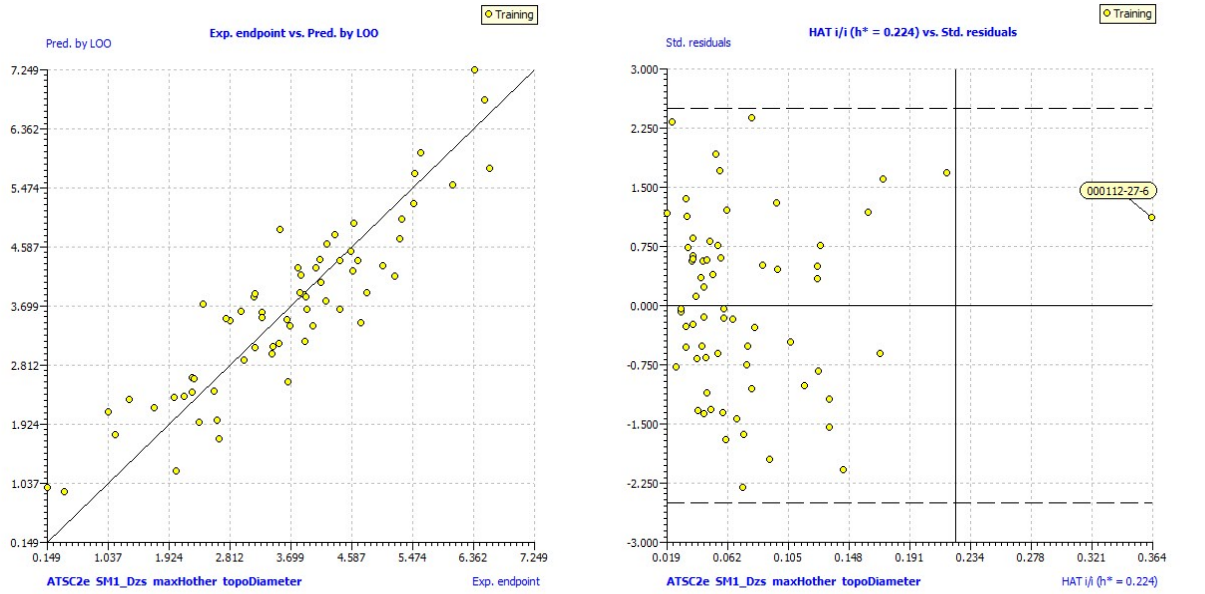


Figure ES10*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.promelas LogPfree PCP full model.*

- LogP model

- Random splitting

Graphs in the main text

pLC50 *P.promelas* = 1.66 + 0.427 **XLogP** + 2.566 m**inHother** + 14.082 **AVP-7**

- Ordered by response splitting

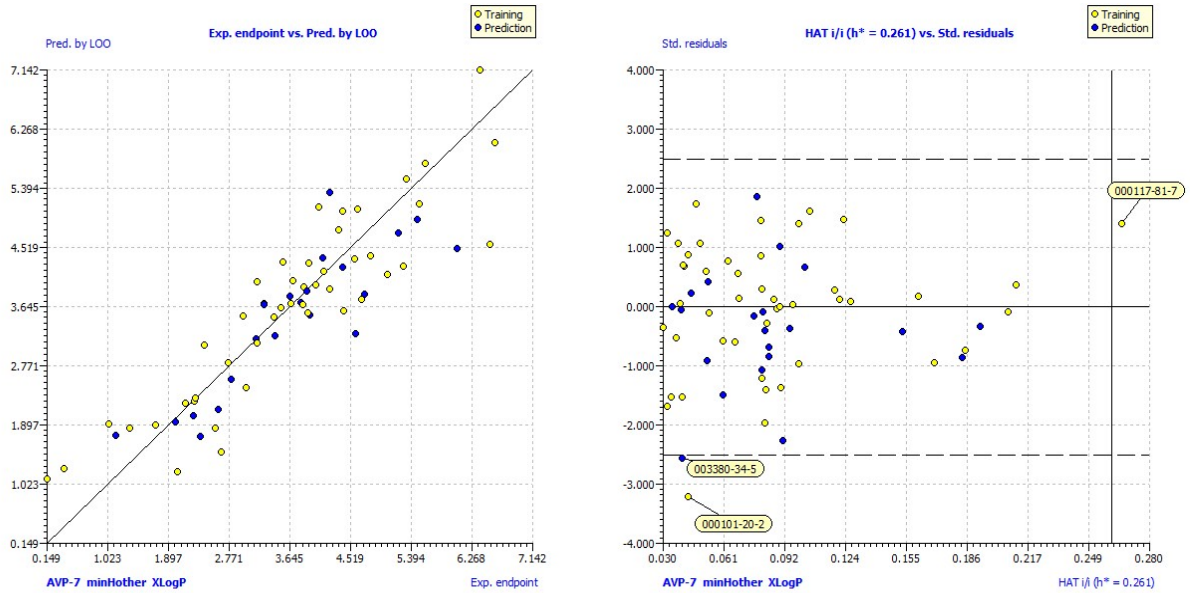
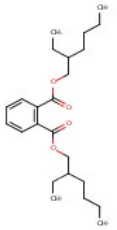


Figure ES11*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.promelas LogP PCP split by ordered response model.*

Bis(2-ethylhexyl)phthalate (CAS 117-81-7) is the only structural outlier, belonging to the training set.



pLC50 *P.promelas* = 1.628 + 0.445 **XLogP** + 2.226 m**inHother** + 15.198 **AVP-7**

- Structural similarity splitting

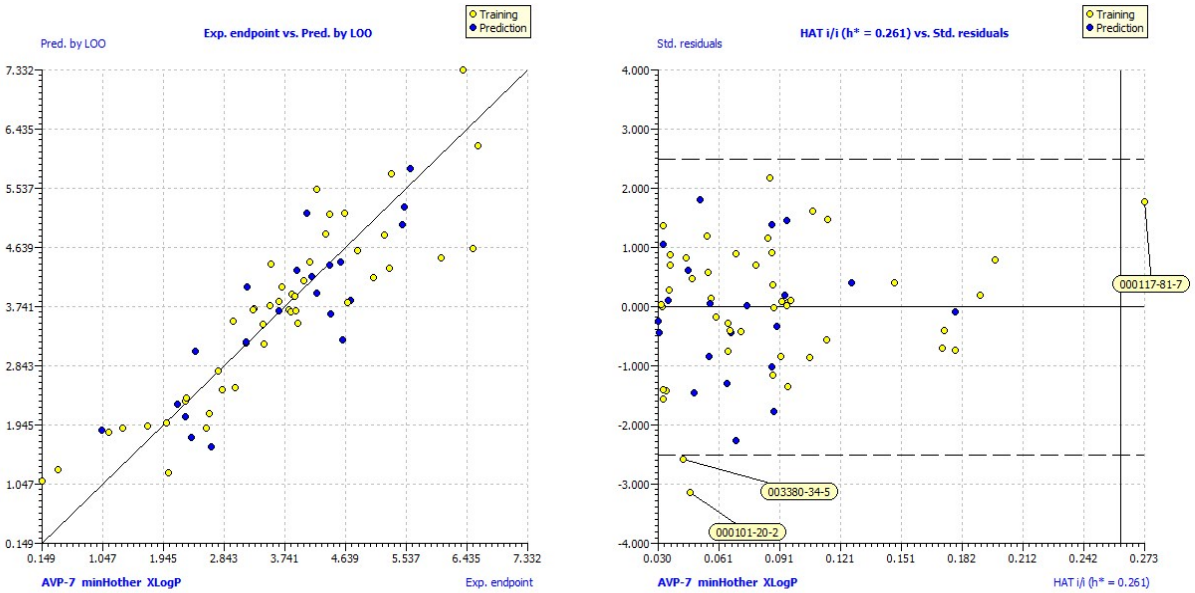


Figure ES12*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.promelas logP PCP split by structural similarity model.*

pLC50 *P.promelas* = 1.652 + 0.463 **XLogP** + 2.115 m**inHother** + 15.973 **AVP-7**

- FULL model

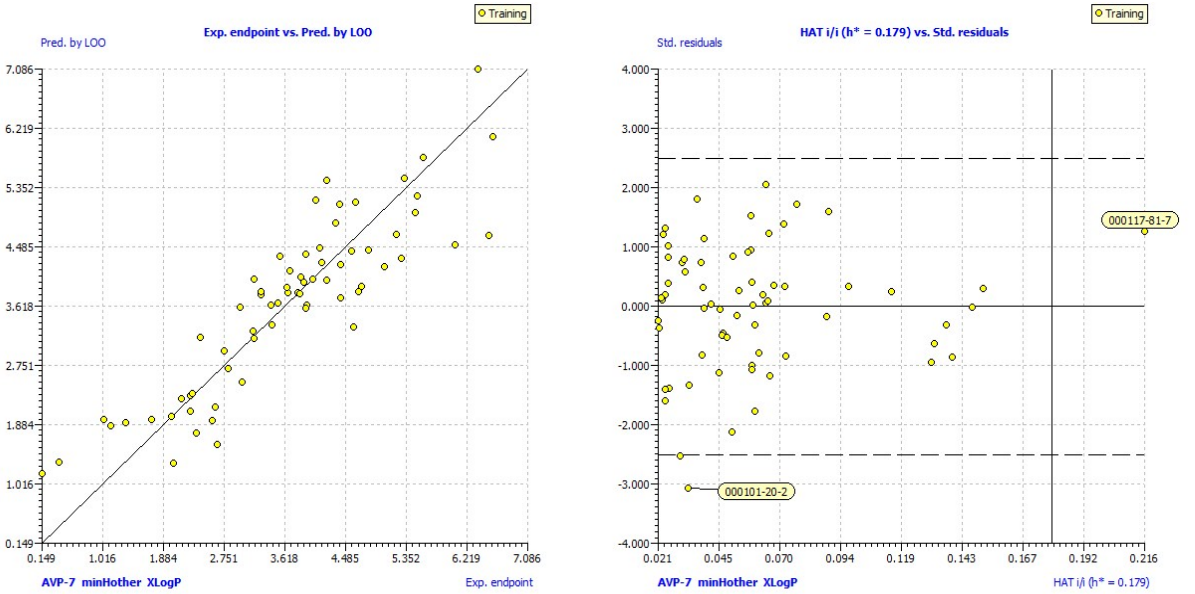


Figure ES13*: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the P.promelas logP PCP full model.*

Comparison with ECOSAR 1.11 tool

Table ES2: *table for ECOSAR comparison with prediction sets*

Endpoint	N PCPs	RMSE UI[a]	RMSE A[b]	RMSE B[c]
P.subcapitata pEC50	**20**	**0.4**	**2.28**	**2.51**
Random prediction set	8	0.5	2.08	2.29
Ord.Resp.prediction set	8	0.5	2.52	2.8
Structural prediction set	8	0.5	2.34	2.63
D.magna pEC50	**72**	**0.52**	**1.36**	**1.2**
Random prediction set	22	0.54	1.43	1.14
Ord.Resp.prediction set	23	0.5	1.27	1.26
Structural prediction set	23	0.57	1.25	1
P.promelas pLC50 **LogP**	**67**	**0.6**	**0.93**	**0.65**
Random prediction set	20	0.56	1.02	0.58
Ord.Resp.prediction set	21	0.63	0.92	0.33
Structural prediction set	21	0.63	0.98	0.55
P.promelas pLC50 **LogP free**	**67**	**0.55**	**0.93**	**0.65**
Random prediction set	20	0.62	0.72	0.49
Ord.Resp.prediction set	21	0.53	0.92	0.33
Structural prediction set	21	0.59	0.71	0.52

[a]: RMSE related to the predictions derived from QSAR models (full) presented in this work; [b]: RMSE related to the predictions derived from ECOSAR Baseline Toxicity equation; [c]: RMSE related to the predictions derived from the ECOSAR worst case scenario, i.e. the lower prediction available for the studied compound.

Table ES3: *table for comparison with ECOSAR Esters class predictions*

Endpoint	N PCPs[a]	RMSE UI[b]	RMSE C[c]
P.subcapitata pEC50	11	0.39	3.05
D.magna pEC50	20	0.40	0.79
P.promelas pLC50 LogP	10	0.42	0.69
P.promelas pLC50 LogP free	10	0.40	0.69

[a]: number of PCPs with an available prediction for the Esters class in ECOSAR; [b]: RMSE related to the predictions derived from QSAR models developed and presented in this work; [c]: RMSE related to the predictions derived from the ECOSAR Esters equation.

Application of models to 534 PCPs

- Pseudokirchneriella subcapitata model

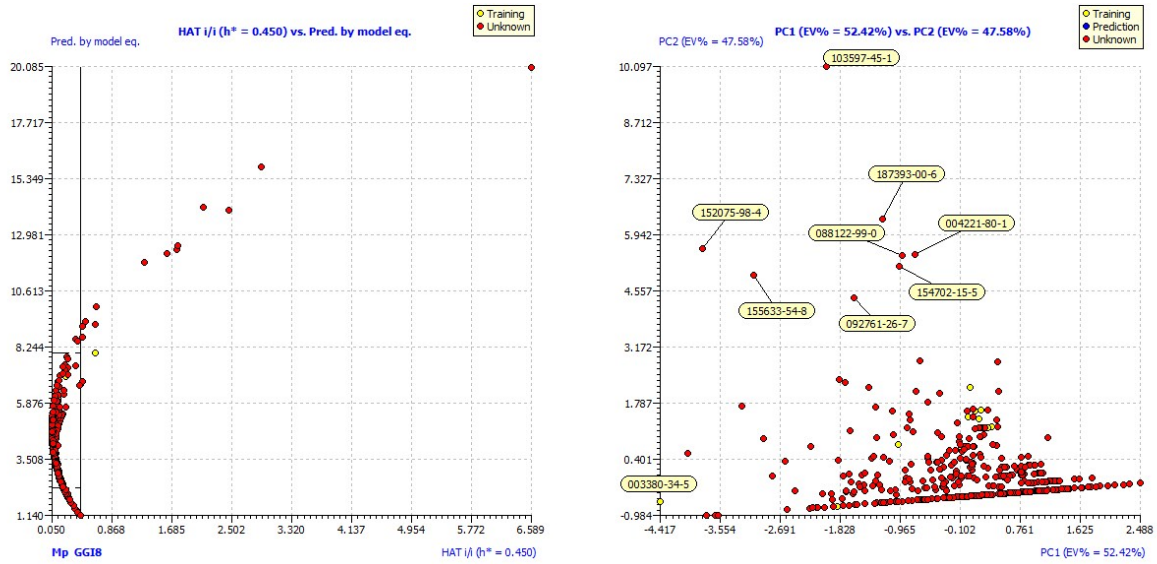


Figure ES14*: Insubria graph (on the left) and PCA of the modeling descriptors (on the right) for the algae model applied to the 534 PCPs without data. Yellow points represent the model training set, while the red points represent the whole set of 534 PCPs. See main text for the magnified Insubria graph.*

- Daphnia magna model

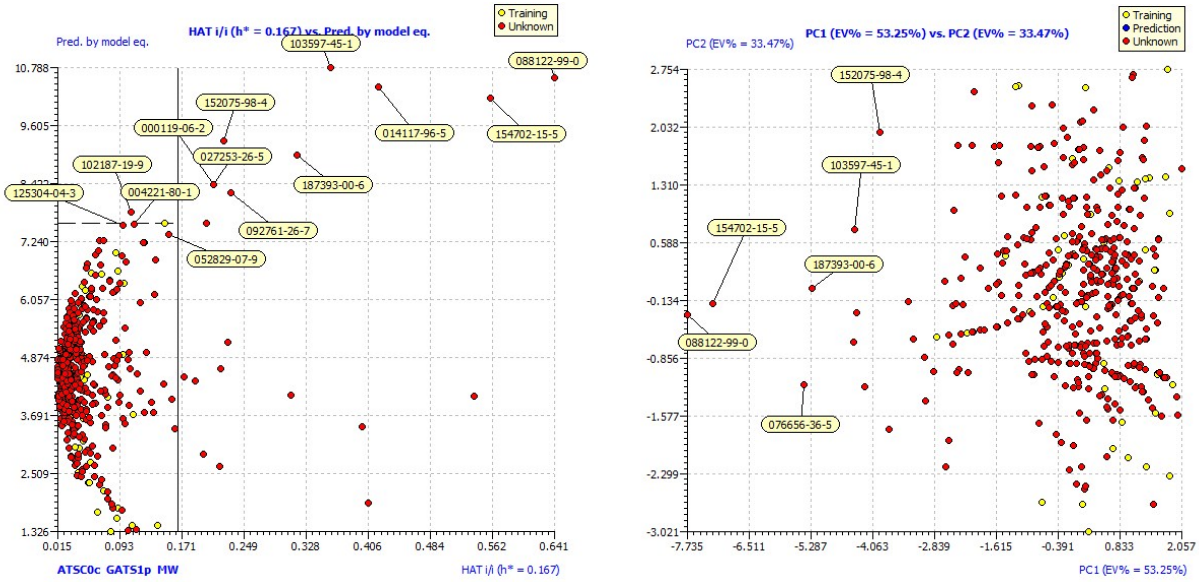


Figure ES15*: Insubria graph (on the left) and PCA of the modeling descriptors (on the right) for the Daphnia model applied to the 534 PCPs without data. Yellow points represent the model training set, while the red points represent the whole set of 534 PCPs.*

- Pimephales promelas LogP model

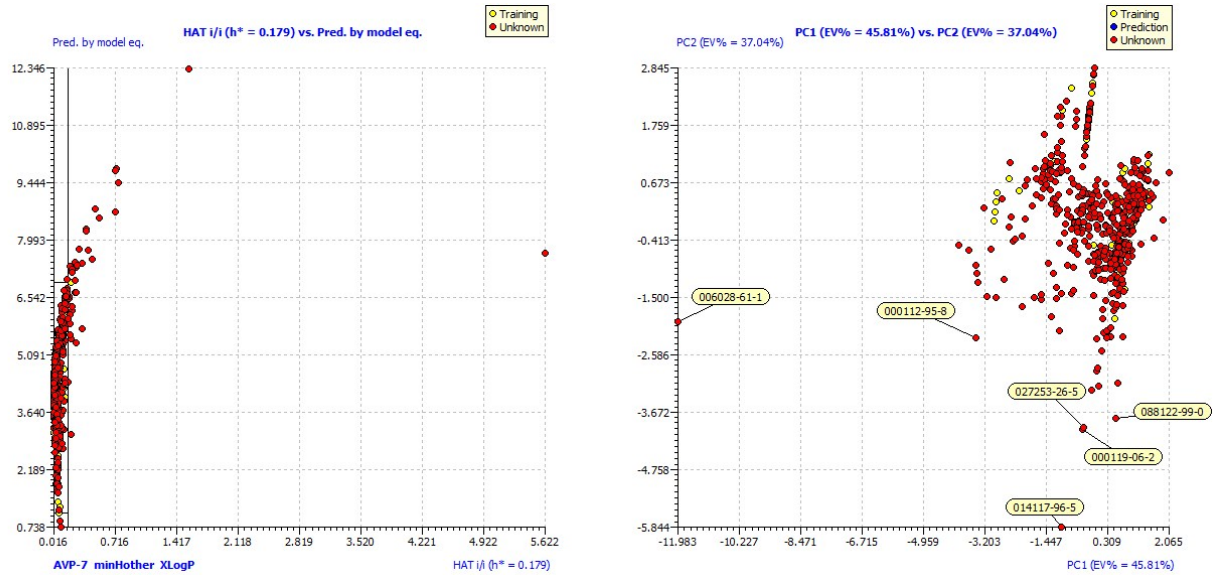


Figure ES16*: Insubria graph (on the left) and PCA of the modeling descriptors (on the right) for the fish logP model applied to the 534 PCPs without data. Yellow points represent the model training set, while the red points represent the whole set of 534 PCPs. See main text for the magnified Insubria graph.*

- Pimephales promelas LogPfree model

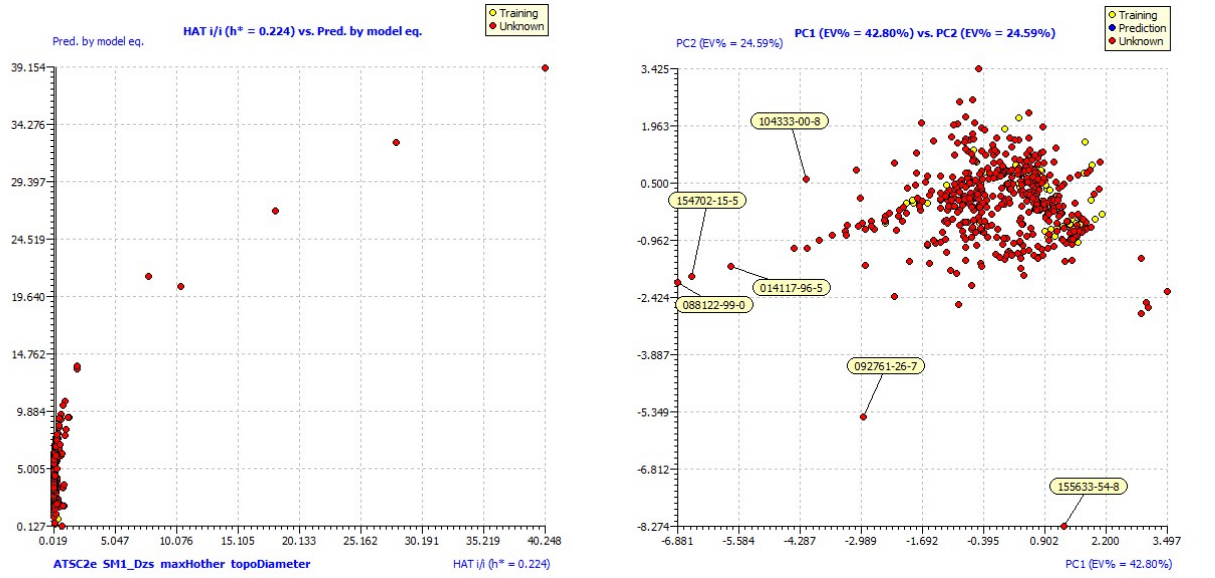


Figure ES17*: Insubria graph (on the left) and PCA of the modeling descriptors (on the right) for the fish logPfree model applied to the 534 PCPs without data. Yellow points represent the model training set, while the red points represent the whole set of 534 PCPs. See main text for the magnified Insubria graph.*

Aquatic Toxicity Index (ATI) model for PCPs

- Random split model

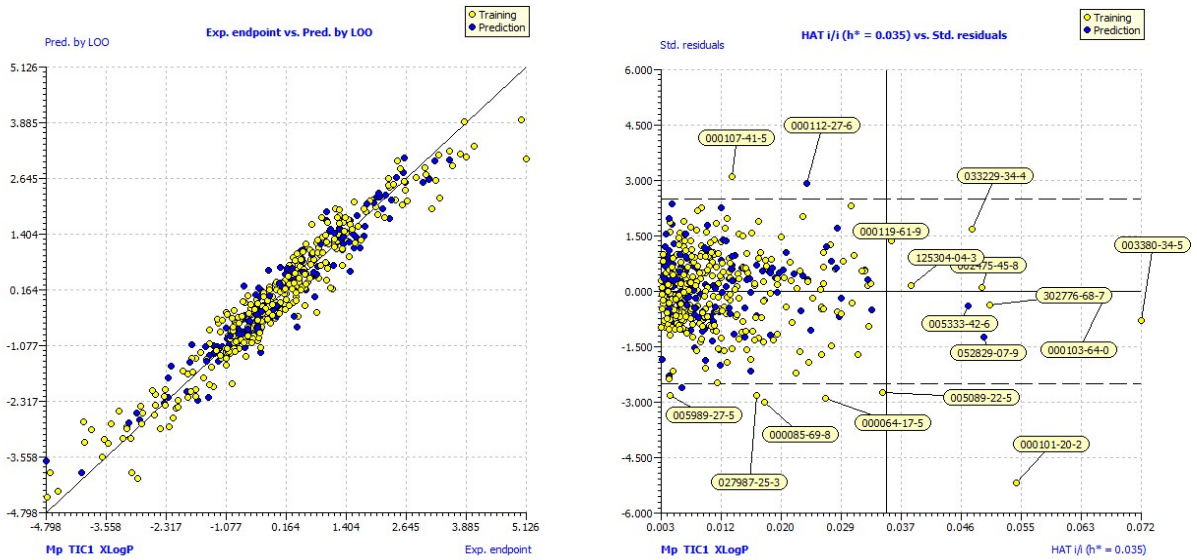


***Figure ES18**: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the ATI split by random model.*

- Ordered by response split model

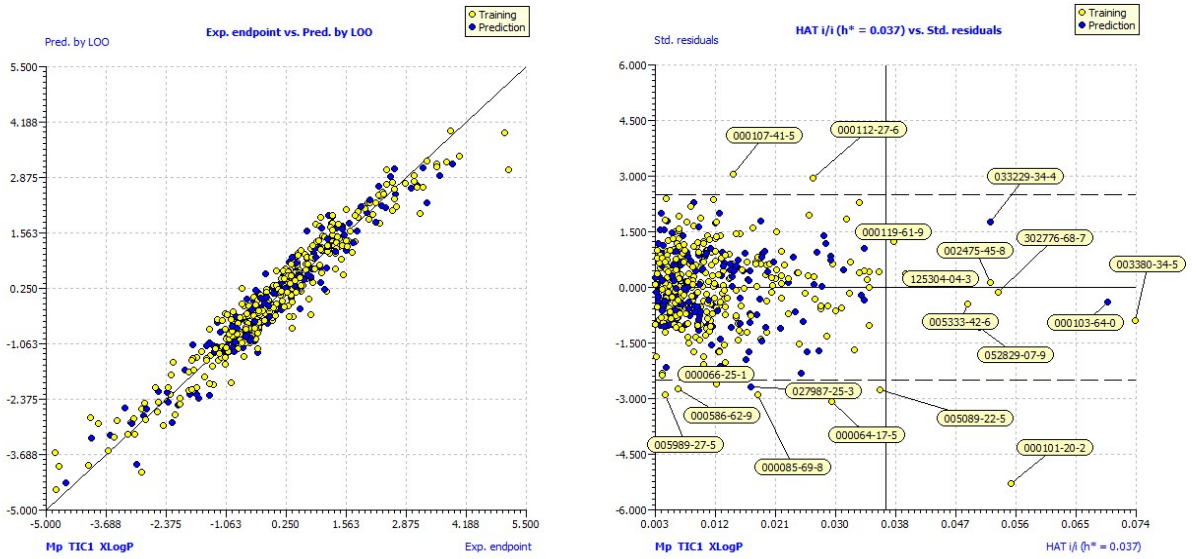


***Figure ES19**: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the ATI split by ordered response model.*

- Structural similarity split model

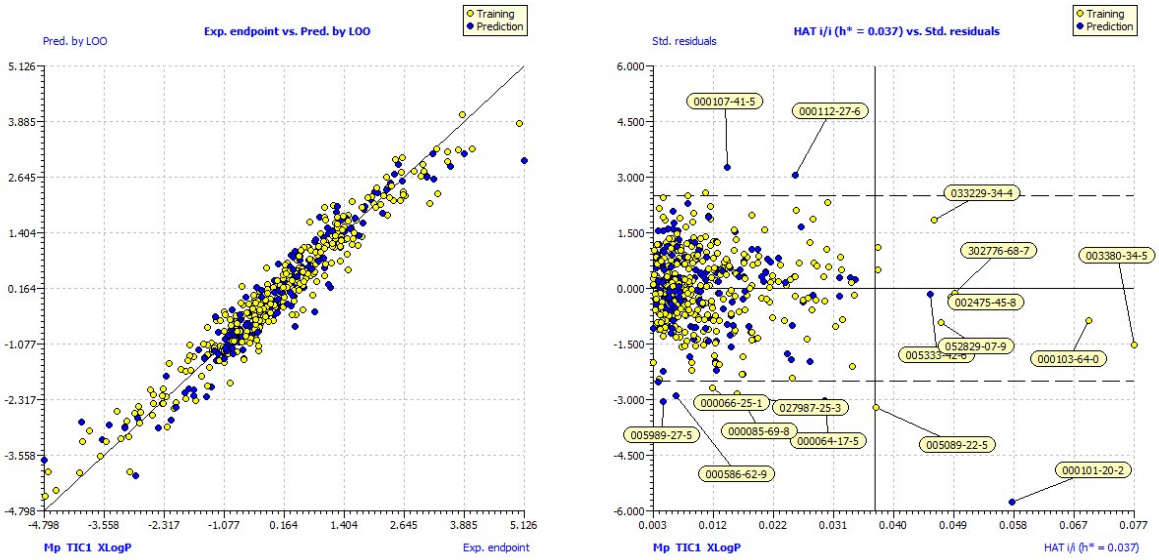


***Figure ES20**: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the ATI split by structural similarity model.*

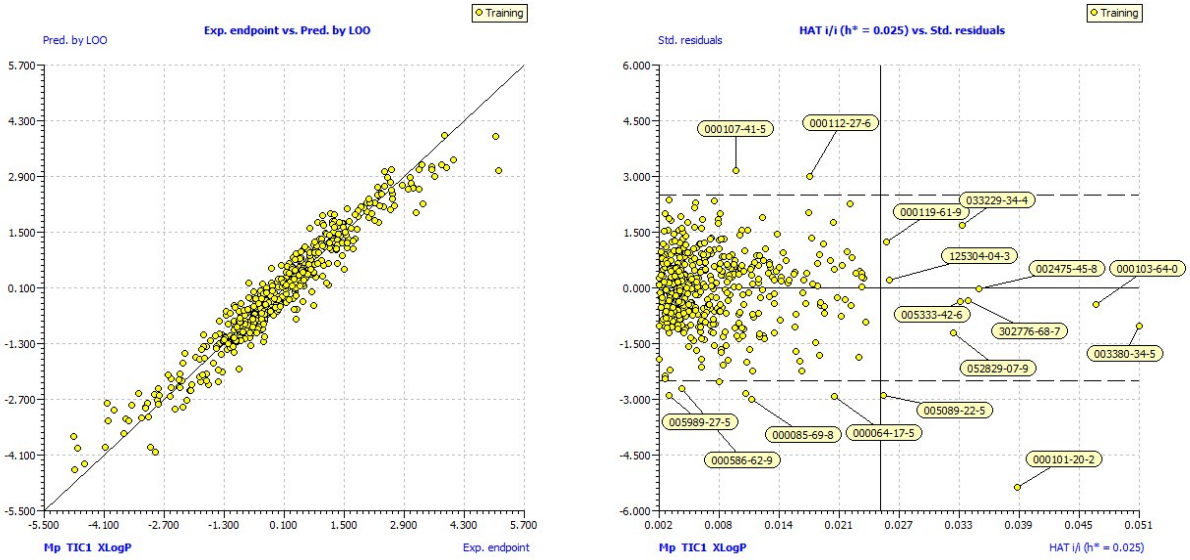
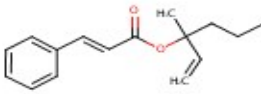
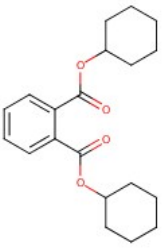
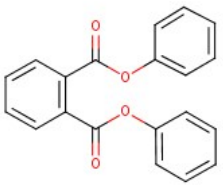
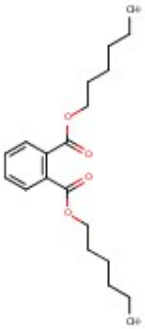
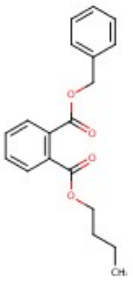
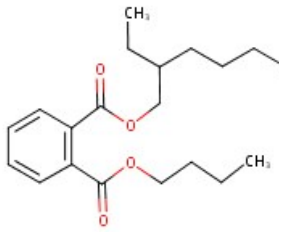
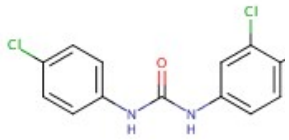
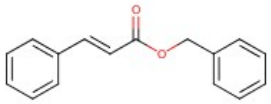
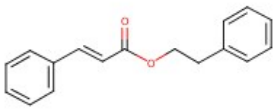
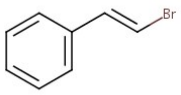


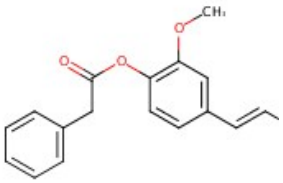
***Figure ES21**: Graph of experimental vs. predicted values (on the left) and Williams Plot (on the right) for the ATI full model.*

Table ES4: *CAS, name, SMILES and structure for the 40 prioritized PCPs listed in Table 6 of the main text.*

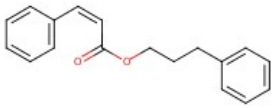
CAS	Name	SMILES	Structure
000078-37-5	3,7-Dimethyl-1,6-octadien-3-yl cinnamtae	c1ccccc1/C=C/C(=O)O[C@@](C=C)(C)CCC=C(C)C	
000084-61-7	Dicyclohexyl phthalate	c1(ccccc1C(=O)OC1CCCCC1)C(=O)OC1CCCCC1	
000084-62-8	Diphenyl phthalate	c1ccc(cc1)OC(=O)c1ccccc1C(=O)Oc1ccccc1	
000084-75-3	Dihexyl phthalate	CCCCCCOC(=O)c1ccccc1C(=O)OCCCCCC	
000085-68-7	Butyl benzyl phthalate	CCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1	

000085-69-8	2-Ethylhexyl butyl phthalate	CCCCOC(=O)c1cccc(c1)C(=O)OC[C@@H](CC)CCCC	
000101-20-2	Triclocarban	c1(c(ccc(c1)NC(=O)Nc1ccc(cc1)Cl)Cl)Cl	
000103-41-3	Benzyl cinnamate	c1ccccc1/C=C/C(=O)OCc1ccccc1	
000103-53-7	Phenethyl cinnamate	c1ccccc1/C=C\C(=O)OCCc1ccccc1	
000103-64-0	beta-Bromostyrene	c1ccc(cc1)/C=C/Br	
000117-81-7	Bis(2-ethylhexyl)phthalate	CCCC[C@H](CC)COC(=O)c1ccccc1C(=O)OC[C@@H](CC)CCCC	

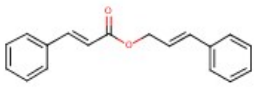
000120-24-1	Isoeugenyl alpha-toluate	C/C=C/c1cc(c(cc1)OC(=O)Cc1ccccc1)OC



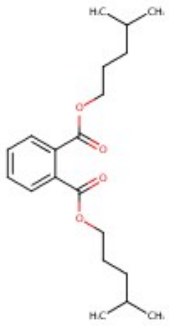
000122-68-9	3-Phenylpropyl cinnamate	c1ccccc1/C=C/C(=O)OCCCc1ccccc1



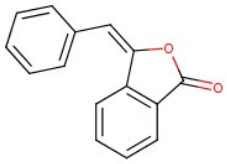
000122-69-0	Cinnamyl cinnamate	c1ccccc1/C=C/C(=O)OC/C=C\c1ccccc1



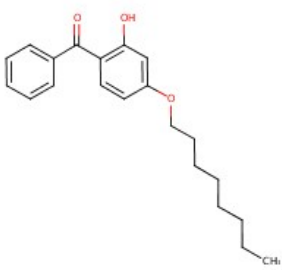
000146-50-9	Diisohexyl phthalate	CC(C)CCCOC(=O)c1ccccc1C(=O)OCCCC(C)C

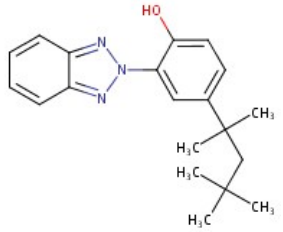
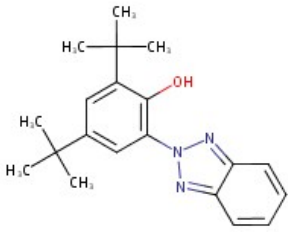
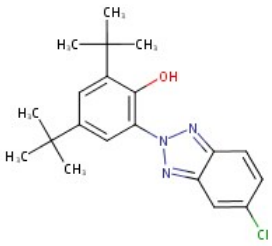
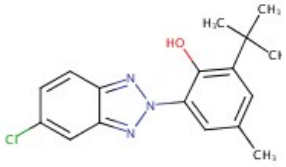
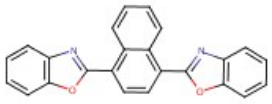


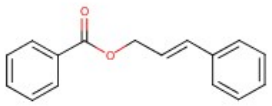
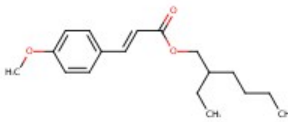
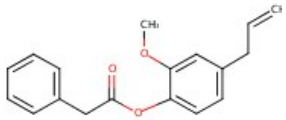
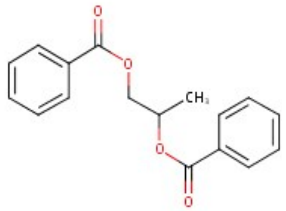
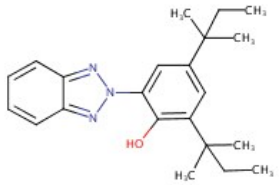
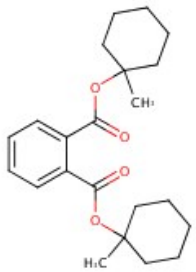
000575-61-1	Benzalphthalide	c1ccc2c(c1)/C(=C/c1ccccc1)/OC2=O



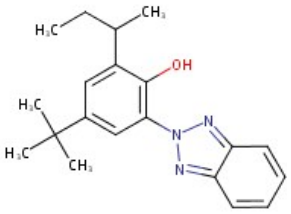
001843-05-6	Octabenzone	CCCCCCCCOc1cc(c(cc1)C(=O)c1ccccc1)O



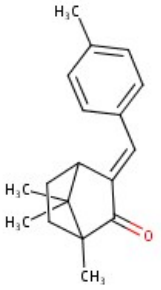
003147-75-9	Octrizole	c1(c(cc(cc1)C(C)(CC(C)(C)C)C)n1nc2c(n1)cccc2)O	
003380-34-5	Triclosan	c1(cc(ccc1Oc1ccc(cc1Cl)Cl)Cl)O	
003846-71-7	2-(2'-Hydroxy-3',5'-di-tert-butylphenyl)benzotriazole	c1(c(cc(cc1C(C)(C)C)C(C)(C)C)n1nc2c(n1)cccc2)O	
003864-99-1	2,4-Di-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)phenol	c1(c(cc(cc1n1nc2c(n1)cc(cc2)Cl)C(C)(C)C)C(C)(C)C)O	
003896-11-5	Bumetrizole	c1(c(cc(cc1n1nc2c(n1)cc(cc2)Cl)C)C(C)(C)C)O	
005089-22-5	Fluorescent brightener 367	c1cccc2c(c3nc4c(cccc4)o3)ccc(c12)c1oc2c(n1)cccc2	

005320-75-2	2-Propen-1-ol, 3-phenyl-, 1-benzoate	c1ccccc1/C=C\COC(=O)c1ccccc1	
005466-77-3	Octinoxate	COc1ccc(cc1)/C=C/C(=O)OC[C@@H](CC)CCCC	
010402-33-2	Eugenyl phenylacetate	C=CCc1cc(c(cc1)OC(=O)Cc1ccccc1)O	
019224-26-1	Propylene glycol dibenzoate	c1ccccc1C(=O)O[C@@H](C)COC(=O)c1ccccc1	
025973-55-1	2-(2H-Benzotriazol-2-yl)-4,6-di-tert-pentylphenol	n1(c2c(c(cc(c2)C(CC)(C)C)C(CC)(C)C)O)nc2ccccc2n1	
027987-25-3	Bis(methylcyclohexyl) phthalate	C1CC(CCC1)(C)OC(=O)c1c(C(=O)OC2(CCCCC2)C)cccc1	

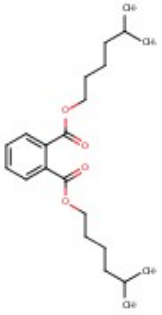
036437-37-3	4-tert-Butyl-6-sec-butyl-2-(2H-benzotriazol-2-yl)phenol	c1ccc2c(c1)nn(n2)c1cc(cc(c1O)[C@@H](C)CC)C(C)(C)C



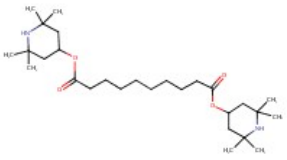
036861-47-9	Enzacamene	C1([C@@]2(C(=O)/C(=C\c3ccc(C)cc3)/[C@H]1CC2)C)(C)C



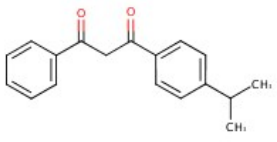
041451-28-9	Di-(5-methylhexyl)phthalate	CC(C)CCCCOC(=O)c1ccccc1C(=O)OCCCCC(C)C



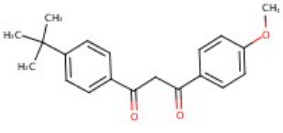
052829-07-9	Bis(2,2,6,6-tetramethyl-4-piperidinyl) sebacate	CC1(NC(C)(C)CC(C1)OC(=O)CCCCCCCCC(=O)OC1CC(CC(C1)(C)C)(C)C)C

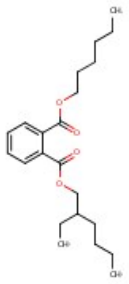
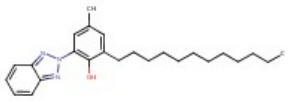
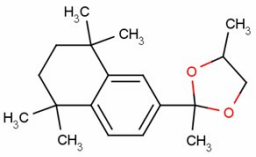
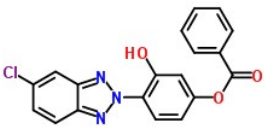
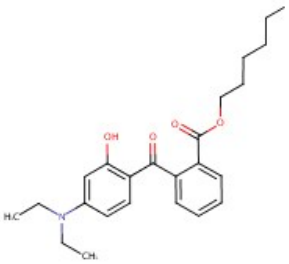


063250-25-9	Isopropyl dibenzoylmethane	c1c(cccc1)C(=O)CC(=O)c1ccc(cc1)C(C)C



070356-09-1	Avobenzone	COc1ccc(cc1)C(=O)CC(=O)c1ccc(cc1)C(C)(C)C



075673-16-4	1,2-Benzenedicarboxylic acid, 2-ethylhexyl hexyl ester	CCCCCCOC(=O)c1ccccc1C(=O)OC[C@@H](CC)CCCC	
125304-04-3	Benzotriazolyl dodecyl p-cresol	c1(c(cc(cc1CCCCCCCCCCCC)C)n1nc2c(n1)cccc2)O	
131812-52-7	Ambroxan	C1CC(c2c(C1(C)C)cc(cc2)[C@@H]1O[C@H](O[C@H]1C)C)(C)C	
169198-72-5	1,3-Benzenediol, 4-(5-chloro-2H-benzotriazol-2-yl)-, 1-benzoate	c1(ccc2c(c1)nn(n2)c1c(cc(cc1)OC(=O)c1ccccc1)O)Cl	
302776-68-7	Diethylamino hydroxybenzoyl hexyl benzoate	CCN(CC)c1cc(c(cc1)C(=O)c1ccccc1C(=O)OCCCCCC)O	

ATI model predictions

Table ES5: *ATI predictions (and "experimental" values, i.e. PC1 scores, when available) for the whole set of 534 PCPs, together with the AD belonging. The first 484 chemicals belonging to the ATI training set. Molecules in red are those that should be included in the priority list, in addition to the 40 compounds listed in Table 6 of the main text.*

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
1	000034-74-2	0.3134	0.4418	interpol.
2	000056-81-5	-4.5517	-4.3151	interpol.
3	000057-55-6	-3.0121	-3.8725	interpol.
4	000060-12-8	-0.3337	-0.2846	interpol.
5	000060-33-3	1.4907	1.7256	interpol.
6	000064-17-5	-2.8925	-4.0025	interpol.
7	000066-25-1	-0.9416	-1.9209	interpol.
8	000071-41-0	-2.8506	-2.7176	interpol.
9	000075-91-2	-3.0446	-3.1338	interpol.
10	000076-22-2	-1.0012	-1.0708	interpol.
11	000077-53-2	-0.1788	0.2446	interpol.
12	000077-92-9	-3.8557	-2.981	interpol.
13	000077-93-0	-2.2124	-1.5356	interpol.
14	000078-35-3	0.5781	0.1703	interpol.
15	000078-36-4	0.3922	0.2414	interpol.
16	000078-37-5	2.4508	2.6754	interpol.
17	000078-59-1	-1.7781	-1.0574	interpol.
18	000078-70-6	-0.9277	-0.8373	interpol.
19	000078-83-1	-3.5911	-3.1755	interpol.
20	000078-93-3	-3.4406	-2.8333	interpol.
21	000079-06-1	-2.1671	-2.696	interpol.
22	000079-20-9	-3.2116	-3.1511	interpol.
23	000079-41-4	-1.8505	-2.2316	interpol.
24	000079-46-9	-2.4293	-2.9202	interpol.
25	000079-69-6	0.0258	0.2392	interpol.
26	000079-70-9	0.2791	0.3356	interpol.
27	000079-77-6	0.1829	0.08	interpol.
28	000079-92-5	-0.9072	-0.2908	interpol.
29	000080-27-3	0.0436	-0.2624	interpol.
30	000080-54-6	1.2337	1.2378	interpol.
31	000081-14-1	1.1408	0.718	interpol.
32	000081-15-2	1.5	0.5723	interpol.
33	000083-66-9	0.307	0.5278	interpol.
34	000083-72-7	0.2988	0.6487	interpol.
35	000084-61-7	2.3061	1.7654	interpol.
36	000084-62-8	3.6177	2.9219	interpol.
37	000084-66-2	-0.7055	0.2308	interpol.
38	000084-69-5	1.4654	0.916	interpol.
39	000084-74-2	1.7088	1.0985	interpol.
40	000084-75-3	2.5817	2.081	interpol.
41	000085-68-7	2.3618	2.496	interpol.
42	000085-69-8	3.1772	2.0177	interpol.
43	000087-20-7	0.2181	0.6608	interpol.
44	000087-22-9	1.5776	2.1075	interpol.
45	000087-44-5	0.6838	1.0451	interpol.

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
46	000088-29-9	1.1963	1.9775	interpol.
47	000089-25-8	0.4354	0.3513	interpol.
48	000089-79-2	-0.9156	-1.0535	interpol.
49	000089-81-6	-0.4875	-0.8588	interpol.
50	000089-83-8	-0.2156	-0.0649	interpol.
51	000090-02-8	0.5571	-0.2127	interpol.
52	000090-05-1	-0.8809	-0.9417	interpol.
53	000090-72-2	-0.8007	-0.9206	interpol.
54	000091-16-7	-1.029	-0.8825	interpol.
55	000091-87-2	1.067	1.4894	interpol.
56	000093-15-2	-0.3319	0.0297	interpol.
57	000093-16-3	-0.3432	0.1266	interpol.
58	000093-51-6	-0.9631	-0.7677	interpol.
59	000094-09-7	-0.5401	-0.4076	interpol.
60	000094-13-3	-0.0121	-0.2222	interpol.
61	000094-18-8	1.2546	1.3847	interpol.
62	000094-26-8	0.3712	0.0042	interpol.
63	000095-14-7	0.3625	0.0959	interpol.
64	000095-70-5	-0.6806	-1.1389	interpol.
65	000095-87-4	-0.4183	-0.4849	interpol.
66	000096-17-3	-1.658	-2.3019	interpol.
67	000096-26-4	-4.059	-3.9006	interpol.
68	000096-91-3	-0.3074	-0.5742	interpol.
69	000097-53-0	-0.4401	-0.0646	interpol.
70	000097-54-1	-0.4494	0.0431	interpol.
71	000097-86-9	-1.2193	-1.4229	interpol.
72	000097-99-4	-3.1284	-2.8953	interpol.
73	000098-51-1	0.448	0.7918	interpol.
74	000098-55-5	-0.9035	-1.0065	interpol.
75	000099-48-9	-0.7091	-0.8876	interpol.
76	000099-57-0	-0.4633	-0.8742	interpol.
77	000099-76-3	-0.5974	-0.5546	interpol.
78	000099-85-4	-0.1433	-0.3699	interpol.
79	000099-87-6	0.1954	0.5888	interpol.
80	000099-96-7	-1.0646	-0.7163	interpol.
81	000100-41-4	0.2082	0.3243	interpol.
82	000100-42-5	0.5413	0.7203	interpol.
83	000100-51-6	-0.4378	-0.5387	interpol.
84	000100-52-7	0.1282	0.1574	interpol.
85	000101-20-2	5.1256	3.1306	extrapol.
86	000101-72-4	1.7723	1.3419	interpol.
87	000101-80-4	0.8447	0.3918	interpol.
88	000101-84-8	1.1833	1.1934	interpol.
89	000101-85-9	0.804	1.201	interpol.
90	000101-86-0	1.4549	1.7272	interpol.
91	000102-22-7	2.031	2.0251	interpol.
92	000103-09-3	-1.3399	-1.0637	interpol.
93	000103-26-4	0.4699	0.6629	interpol.
94	000103-36-6	0.6853	0.8236	interpol.
95	000103-38-8	0.5808	0.5344	interpol.
96	000103-41-3	2.3109	2.4267	interpol.
97	000103-53-7	2.5845	2.7592	interpol.
98	000103-54-8	0.74	0.8244	interpol.
99	000103-56-0	0.8577	0.9537	interpol.
100	000103-59-3	1.2134	1.0818	interpol.

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
101	000103-61-7	1.0271	1.2088	interpol.
102	000103-64-0	2.6417	2.4827	extrapol.
103	000103-93-5	0.1483	0.2314	interpol.
104	000104-09-6	0.2815	0.2991	interpol.
105	000104-28-9	0.0921	0.2727	interpol.
106	000104-54-1	0.0916	0.2953	interpol.
107	000104-55-2	0.4644	0.6319	interpol.
108	000104-65-4	0.6831	0.6991	interpol.
109	000104-87-0	0.2385	0.2559	interpol.
110	000104-93-8	-0.3692	-0.3912	interpol.
111	000105-45-3	-2.8341	-2.4319	interpol.
112	000105-67-9	-0.0427	-0.4849	interpol.
113	000105-87-3	-0.0341	-0.4276	interpol.
114	000105-90-8	0.1574	-0.2138	interpol.
115	000105-91-9	0.1574	-0.2138	interpol.
116	000105-95-3	-0.4529	-0.1866	interpol.
117	000106-02-5	-0.3004	-0.18	interpol.
118	000106-22-9	-0.9769	-0.9139	interpol.
119	000106-24-1	-0.5392	-1.0122	interpol.
120	000106-25-2	-0.8421	-1.0122	interpol.
121	000106-29-6	0.3764	0.1022	interpol.
122	000106-33-2	-0.1878	-0.3093	interpol.
123	000106-50-3	-0.6633	-1.331	interpol.
124	000106-65-0	-2.9105	-2.578	interpol.
125	000107-21-1	-4.7717	-4.4533	interpol.
126	000107-41-5	-4.0236	-2.7913	interpol.
127	000107-75-5	-0.9888	-1.2326	interpol.
128	000108-10-1	-2.273	-2.2203	interpol.
129	000108-11-2	-2.5332	-2.3869	interpol.
130	000108-22-5	-1.6933	-2.0512	interpol.
131	000108-39-4	-0.8106	-0.476	interpol.
132	000108-45-2	-0.6613	-1.331	interpol.
133	000108-46-3	-0.7998	-1.1634	interpol.
134	000108-59-8	-3.2757	-2.5509	interpol.
135	000108-93-0	-2.3459	-2.3627	interpol.
136	000108-94-1	-1.8721	-2.1162	interpol.
137	000110-62-3	-1.7029	-2.2093	interpol.
138	000110-93-0	-1.3626	-1.5613	interpol.
139	000111-03-5	1.2457	1.7674	interpol.
140	000111-12-6	-0.9328	-0.7242	interpol.
141	000111-27-3	-2.3193	-2.3857	interpol.
142	000111-46-6	-4.7108	-3.9247	interpol.
143	000111-70-6	-1.8043	-2.0756	interpol.
144	000111-76-2	-3.0742	-2.7861	interpol.
145	000111-77-3	-3.6237	-3.5459	interpol.
146	000111-81-9	0.162	-0.1478	interpol.
147	000111-82-0	-0.098	-0.2643	interpol.
148	000111-87-5	-1.5312	-1.7801	interpol.
149	000111-90-0	-3.9914	-3.2472	interpol.
150	000112-05-0	-1.5999	-1.2124	interpol.
151	000112-27-6	-4.7981	-3.6369	interpol.
152	000112-30-1	-0.3596	-1.2176	interpol.
153	000112-34-5	-2.7947	-2.5819	interpol.
154	000112-42-5	-0.4177	-0.9459	interpol.
155	000112-53-8	0.0185	-0.1544	interpol.

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
156	000112-62-9	1.6671	1.6174	interpol.
157	000112-72-1	-0.0082	-0.1544	interpol.
158	000112-80-1	1.4155	1.4726	interpol.
159	000115-95-7	-0.2977	-0.2346	interpol.
160	000115-99-1	-0.3159	-0.36	interpol.
161	000116-02-9	-1.6949	-1.3593	interpol.
162	000116-66-5	1.24	1.2626	interpol.
163	000117-81-7	3.2518	3.0761	interpol.
164	000117-82-8	-0.1716	-0.0704	interpol.
165	000117-83-9	1.6141	1.3522	interpol.
166	000117-99-7	1.0964	1.4676	interpol.
167	000118-56-9	1.3474	1.6618	interpol.
168	000118-58-1	1.2807	1.7853	interpol.
169	000118-60-5	0.9284	1.3424	interpol.
170	000118-61-6	-0.6101	0.009	interpol.
171	000119-34-6	-0.3484	-0.7302	interpol.
172	000119-36-8	-0.6748	-0.1539	interpol.
173	000119-53-9	1.2802	1.4925	interpol.
174	000119-61-9	1.2268	1.7008	extrapol.
175	000120-11-6	1.964	2.1524	interpol.
176	000120-14-9	-0.8906	-0.5918	interpol.
177	000120-24-1	2.2936	2.6316	interpol.
178	000120-47-8	-0.4406	-0.3916	interpol.
179	000120-51-4	1.6282	1.7903	interpol.
180	000120-72-9	0.3138	-0.1531	interpol.
181	000120-92-3	-2.057	-2.3159	interpol.
182	000121-32-4	-0.9541	-0.488	interpol.
183	000121-33-5	-0.8845	-0.6509	interpol.
184	000121-88-0	-0.468	-0.8742	interpol.
185	000122-03-2	0.1649	0.5124	interpol.
186	000122-40-7	1.27	1.5123	interpol.
187	000122-48-5	-0.7296	-0.5025	interpol.
188	000122-67-8	1.1739	1.1175	interpol.
189	000122-68-9	2.4631	3.027	interpol.
190	000122-69-0	2.6201	3.0768	interpol.
191	000122-91-8	-0.3759	-0.4808	interpol.
192	000123-35-3	-0.0195	-0.1156	interpol.
193	000123-38-6	-2.2411	-2.8757	interpol.
194	000124-19-6	-0.3551	-1.1103	interpol.
195	000125-12-2	-0.7623	-0.4757	interpol.
196	000126-64-7	1.8226	1.9098	interpol.
197	000126-91-0	-0.7462	-0.8373	interpol.
198	000127-41-3	0.1151	0.3149	interpol.
199	000127-51-5	0.1527	0.3779	interpol.
200	000127-91-3	-0.1039	-0.1769	interpol.
201	000128-37-0	0.3261	0.8795	interpol.
202	000128-39-2	0.2335	0.7124	interpol.
203	000128-95-0	0.7093	0.9104	interpol.
204	000131-11-3	-0.7169	-0.1252	interpol.
205	000131-16-8	0.537	0.6085	interpol.
206	000131-17-9	0.8675	0.9382	interpol.
207	000131-18-0	1.7995	1.5889	interpol.
208	000131-53-3	0.5225	1.0374	interpol.
209	000131-55-5	-0.0396	0.2545	interpol.
210	000131-56-6	0.8545	1.0671	interpol.

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
211	000131-57-7	0.9812	1.3461	interpol.
212	000134-09-8	1.4886	1.6313	interpol.
213	000136-44-7	-0.8208	-0.9138	interpol.
214	000136-85-6	0.2878	0.155	interpol.
215	000138-86-3	-1.0699	-0.3347	interpol.
216	000140-10-3	0.3813	0.5651	interpol.
217	000140-11-4	-0.1173	-0.0185	interpol.
218	000140-27-2	1.42	1.4245	interpol.
219	000140-88-5	-1.331	-1.9884	interpol.
220	000141-14-0	0.0548	-0.1001	interpol.
221	000141-78-6	-2.8219	-2.8093	interpol.
222	000141-79-7	-1.4206	-1.9541	interpol.
223	000141-97-9	-2.536	-2.1686	interpol.
224	000142-19-8	-0.3695	-0.6917	interpol.
225	000142-90-5	1.3394	0.7418	interpol.
226	000142-91-6	1.1666	1.2731	interpol.
227	000143-08-8	-1.0685	-1.495	interpol.
228	000143-28-2	1.2336	1.2806	interpol.
229	000144-39-8	0.164	-0.0452	interpol.
230	000145-39-1	-0.1837	0.6087	interpol.
231	000146-50-9	2.6796	2.1778	interpol.
232	000150-13-0	-0.511	-0.7152	interpol.
233	000150-78-7	-0.8436	-0.8825	interpol.
234	000432-25-7	-0.3873	-0.7838	interpol.
235	000469-61-4	0.662	1.0619	interpol.
236	000470-67-7	-1.0722	-1.3061	interpol.
237	000470-82-6	-1.1588	-1.3061	interpol.
238	000470-99-5	-1.1799	-1.1274	interpol.
239	000475-20-7	0.7197	0.9948	interpol.
240	000505-32-8	2.0741	1.8879	interpol.
241	000507-70-0	-1.2586	-1.1077	interpol.
242	000538-65-8	0.9863	1.2088	interpol.
243	000541-91-3	0.4391	0.3454	interpol.
244	000544-35-4	1.976	2.1225	interpol.
245	000546-79-2	-1.1452	-1.1003	interpol.
246	000556-82-1	-2.0957	-2.4746	interpol.
247	000562-74-3	-0.913	-1.1481	interpol.
248	000563-80-4	-2.554	-2.6235	interpol.
249	000575-61-1	2.2853	2.4436	interpol.
250	000576-26-1	-0.5759	-0.5557	interpol.
251	000586-62-9	0.3934	-0.6637	interpol.
252	000590-86-3	-1.4267	-2.2297	interpol.
253	000605-54-9	0.3467	0.329	interpol.
254	000611-99-4	1.0163	0.7107	interpol.
255	000615-05-4	-1.162	-1.3775	interpol.
256	000620-17-7	-0.3332	-0.3073	interpol.
257	000626-82-4	-1.0771	-1.1407	interpol.
258	000639-99-6	0.1871	0.655	interpol.
259	000646-01-5	-0.9775	-1.2195	interpol.
260	000693-23-2	-0.7491	-0.7593	interpol.
261	000713-95-1	-0.3475	-0.6248	interpol.
262	000763-32-6	-2.0728	-2.4517	interpol.
263	000835-11-0	0.5873	1.1402	interpol.
264	000868-77-9	-2.3471	-2.206	interpol.
265	000873-94-9	-1.4047	-1.2971	interpol.

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
266	000928-96-1	-2.3229	-2.0539	interpol.
267	001074-95-9	-1.0508	-1.1347	interpol.
268	001085-12-7	0.824	0.7006	interpol.
269	001118-27-0	0.5473	0.5608	interpol.
270	001120-36-1	1.0262	0.6805	interpol.
271	001137-42-4	1.3122	1.2528	interpol.
272	001139-30-6	0.3009	0.5236	interpol.
273	001143-72-2	0.4763	0.9933	interpol.
274	001191-41-9	2.0408	2.2545	interpol.
275	001195-79-5	-1.0745	-1.3607	interpol.
276	001220-94-6	0.8758	1.1599	interpol.
277	001222-05-5	0.7096	1.613	interpol.
278	001335-66-6	-0.5024	-0.6461	interpol.
279	001423-46-7	-0.5024	-0.6461	interpol.
280	001470-79-7	0.4477	0.4929	interpol.
281	001490-04-6	-1.3052	-1.2131	interpol.
282	001502-22-3	-0.1758	-0.531	interpol.
283	001504-55-8	0.1623	0.4978	interpol.
284	001504-74-1	-0.027	0.1415	interpol.
285	001506-02-1	1.2715	1.957	interpol.
286	001843-05-6	2.5325	2.8734	interpol.
287	001866-31-5	1.0443	1.1532	interpol.
288	001885-38-7	1.0114	1.1653	interpol.
289	001948-33-0	-0.6727	-0.4066	interpol.
290	002050-08-0	0.2972	0.6338	interpol.
291	002102-59-2	-0.7091	-0.8876	interpol.
292	002146-71-6	1.0095	0.4099	interpol.
293	002173-57-1	1.3584	1.3522	interpol.
294	002198-61-0	-0.7424	-0.8088	interpol.
295	002216-51-5	-1.0652	-1.2131	interpol.
296	002226-11-1	0.7231	0.4641	interpol.
297	002244-16-8	-0.3433	-0.6703	interpol.
298	002311-46-8	-1.4804	-1.3739	interpol.
299	002349-07-7	-1.0301	-1.2186	interpol.
300	002351-90-8	-0.4097	-0.6265	interpol.
301	002396-84-1	-0.8246	-0.9852	interpol.
302	002409-55-4	-0.1627	0.1576	interpol.
303	002416-94-6	-0.2738	-0.5116	interpol.
304	002436-90-0	-0.2171	-0.2094	interpol.
305	002440-22-4	1.355	1.3071	interpol.
306	002475-45-8	-0.144	-0.1468	extrapol.
307	002563-07-7	-0.7963	-0.5817	interpol.
308	002778-42-9	0.9025	1.7573	interpol.
309	002784-94-3	-0.8301	-0.4549	interpol.
310	002835-99-6	-0.7594	-0.9715	interpol.
311	002871-01-4	-0.8171	-0.7168	interpol.
312	003147-75-9	3.0472	2.89	interpol.
313	003198-29-6	-0.5512	-0.295	interpol.
314	003209-13-0	-0.9107	-0.7677	interpol.
315	003380-34-5	3.5564	3.1861	extrapol.
316	003387-41-5	-0.0278	-0.1769	interpol.
317	003452-97-9	-1.7734	-1.3574	interpol.
318	003487-99-8	1.1713	1.432	interpol.
319	003613-30-7	-0.6146	-1.0066	interpol.
320	003846-71-7	3.1169	2.6473	interpol.

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
321	003864-99-1	3.8965	3.1462	interpol.
322	003896-11-5	3.2595	2.6085	interpol.
323	004191-73-5	-0.1924	-0.2224	interpol.
324	004247-02-3	0.3802	-0.087	interpol.
325	004407-36-7	0.0916	0.2953	interpol.
326	004455-13-4	-0.8891	-1.2197	interpol.
327	004602-84-0	0.5501	0.2086	interpol.
328	004707-47-5	-1.0372	-0.3928	interpol.
329	005089-22-5	5.0361	3.9443	extrapol.
330	005307-14-2	-0.4012	-0.9202	interpol.
331	005320-75-2	2.3918	2.4807	interpol.
332	005333-42-6	1.5666	1.4356	extrapol.
333	005392-40-5	-0.39	-0.7208	interpol.
334	005466-77-3	2.2151	1.7992	interpol.
335	005533-03-9	-1.4069	-1.052	interpol.
336	005595-79-9	-1.191	-0.7888	interpol.
337	005638-85-7	-0.3661	-0.0306	interpol.
338	005988-91-0	-0.4292	-0.7506	interpol.
339	005989-27-5	0.8011	-0.3347	interpol.
340	006091-50-5	-0.4875	-0.8588	interpol.
341	006259-76-3	0.4926	0.8661	interpol.
342	006290-17-1	-2.2623	-1.7846	interpol.
343	006413-10-1	-2.5996	-2.0817	interpol.
344	006658-48-6	1.4313	1.2468	interpol.
345	006931-54-0	-1.0516	-0.9324	interpol.
346	007143-69-3	1.9046	2.1572	interpol.
347	007370-44-7	0.6232	0.3571	interpol.
348	007370-92-5	-0.1027	-0.3789	interpol.
349	007392-19-0	-0.7025	-1.0164	interpol.
350	007420-86-2	1.8376	2.0522	interpol.
351	007540-51-4	-0.9769	-0.9139	interpol.
352	007540-53-6	0.6575	0.4554	interpol.
353	007764-50-3	-0.5177	-0.9223	interpol.
354	007778-83-8	0.8157	0.988	interpol.
355	007779-23-9	0.9864	0.7901	interpol.
356	007779-65-9	1.3803	1.4589	interpol.
357	007779-81-9	-1.0089	-1.213	interpol.
358	007779-94-4	-0.4199	-0.6743	interpol.
359	007780-06-5	0.9166	0.9878	interpol.
360	007787-20-4	-1.0745	-1.3607	interpol.
361	008000-41-7	-0.2033	-0.0781	interpol.
362	008003-22-3	2.6342	2.3451	interpol.
363	010031-71-7	1.3496	1.1997	interpol.
364	010031-87-5	-1.9549	-1.6375	interpol.
365	010032-05-0	-1.8652	-1.6865	interpol.
366	010058-43-2	0.4419	0.5064	interpol.
367	010233-13-3	0.505	0.246	interpol.
368	010361-39-4	0.5237	0.5548	interpol.
369	010402-33-2	2.2272	2.2533	interpol.
370	010444-50-5	0.148	-0.2592	interpol.
371	010461-98-0	1.2717	1.627	interpol.
372	010486-14-3	2.0985	2.2499	interpol.
373	010580-25-3	0.8949	0.7255	interpol.
374	013020-57-0	1.1651	1.2528	interpol.
375	013171-00-1	1.0015	1.7245	interpol.

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
376	013477-62-8	-1.3052	-1.2388	interpol.
377	014073-97-3	-1.0508	-1.1347	interpol.
378	014779-78-3	0.7911	0.4922	interpol.
379	014901-07-6	0.139	0.08	interpol.
380	015087-24-8	1.7737	1.9603	interpol.
381	015323-35-0	1.0323	1.6696	interpol.
382	015356-60-2	-1.3052	-1.2131	interpol.
383	016409-43-1	-0.8575	-0.9912	interpol.
384	017851-53-5	1.3329	1.0631	interpol.
385	018368-91-7	-0.9165	-0.8573	interpol.
386	018479-58-8	-0.8118	-0.804	interpol.
387	018871-14-2	-0.9021	-0.7519	interpol.
388	019224-26-1	2.4319	2.147	interpol.
389	020053-88-7	-0.5499	-0.6925	interpol.
390	020770-40-5	0.7756	0.5318	interpol.
391	021145-77-7	1.2715	1.957	interpol.
392	021245-01-2	0.8026	0.5191	interpol.
393	021245-02-3	1.4765	1.239	interpol.
394	023787-90-8	-0.0248	0.3307	interpol.
395	023911-56-0	0.2662	0.5293	interpol.
396	023985-25-3	-0.3436	-0.5438	interpol.
397	024237-00-1	-0.5912	-0.7794	interpol.
398	024717-85-9	0.7373	0.5717	interpol.
399	024851-98-7	-0.6159	-0.6544	interpol.
400	025013-16-5	-0.5509	-0.1605	interpol.
401	025265-71-8	-3.5142	-3.2423	interpol.
402	025340-17-4	0.3043	0.5748	interpol.
403	025485-88-5	0.4983	0.7982	interpol.
404	025966-79-4	0.0353	0.3307	interpol.
405	025973-55-1	3.7746	3.2132	interpol.
406	026896-48-0	-1.2731	-1.1414	interpol.
407	027458-94-2	-1.4731	-1.4115	interpol.
408	027987-25-3	3.3456	2.2469	interpol.
409	028219-61-6	-0.175	0.0378	interpol.
410	030772-79-3	0.0259	-0.3572	interpol.
411	030960-39-5	0.4456	0.4216	interpol.
412	031906-04-4	0.4112	-0.4197	interpol.
413	032210-23-4	-0.7458	-0.4245	interpol.
414	032214-91-8	1.5782	1.1187	interpol.
415	032388-55-9	0.3964	0.9739	interpol.
416	033229-34-4	-1.2359	-0.6019	extrapol.
417	033704-61-9	-0.3079	-0.2005	interpol.
418	034590-94-8	-3.1234	-2.9208	interpol.
419	034902-57-3	0.5568	0.5158	interpol.
420	036437-37-3	3.0651	2.7365	interpol.
421	036861-47-9	2.3454	2.1749	interpol.
422	037677-14-8	0.7632	0.0134	interpol.
423	038462-22-5	-0.2454	-0.2658	interpol.
424	039067-39-5	-0.1182	-0.1602	interpol.
425	039067-80-6	0.4793	0.1626	interpol.
426	041451-28-9	2.8573	2.7007	interpol.
427	041678-36-8	-0.6277	-0.6846	interpol.
428	051414-25-6	0.3309	-0.4197	interpol.
429	051566-62-2	-0.4238	-0.5224	interpol.
430	052475-86-2	1.1345	0.1817	interpol.

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
431	052829-07-9	3.5587	3.111	extrapol.
432	054464-57-2	0.0554	0.1271	interpol.
433	054982-83-1	-0.578	-0.38	interpol.
434	056172-46-4	0.5759	0.3089	interpol.
435	056932-44-6	-0.5401	-1.0047	interpol.
436	057345-19-4	0.4837	0.8558	interpol.
437	057378-68-4	0.0901	0.2284	interpol.
438	058817-05-3	1.5902	1.2354	interpol.
439	059259-38-0	-1.2486	-0.4847	interpol.
440	059820-43-8	-0.9888	-0.8684	interpol.
441	060770-00-5	-0.4028	0.2035	interpol.
442	061792-12-9	1.532	1.5053	interpol.
443	062406-73-9	-0.9247	-0.746	interpol.
444	063187-91-7	-1.4105	-0.7161	interpol.
445	063250-25-9	2.6227	2.5737	interpol.
446	063500-71-0	-1.8155	-1.4362	interpol.
447	065405-77-8	0.5123	1.0122	interpol.
448	065405-84-7	0.3635	0.5478	interpol.
449	066327-54-6	1.0912	0.2315	interpol.
450	066408-78-4	-0.151	-0.5684	interpol.
451	067633-96-9	-1.1979	-1.2794	interpol.
452	067845-30-1	0.1343	0.1654	interpol.
453	068039-49-6	-0.6222	-0.8642	interpol.
454	068133-75-5	1.3916	1.7656	interpol.
455	068140-48-7	1.0096	1.9241	interpol.
456	068527-74-2	-1.1407	-0.5359	interpol.
457	068527-76-4	-0.6066	-0.3678	interpol.
458	068738-94-3	0.832	1.2605	interpol.
459	068738-96-5	0.151	0.1849	interpol.
460	068991-97-9	0.2254	-0.1754	interpol.
461	069929-16-4	-0.2139	-0.4801	interpol.
462	070356-09-1	3.1228	2.6238	interpol.
463	071617-10-2	1.3262	1.0931	interpol.
464	071735-79-0	0.2173	0.4801	interpol.
465	075673-16-4	2.9945	2.5946	interpol.
466	082654-98-6	-0.3313	-0.3044	interpol.
467	083763-47-7	-1.2797	-1.1945	interpol.
468	084041-77-0	-0.9175	-0.6643	interpol.
469	086803-90-9	-0.3682	-0.7954	interpol.
470	092952-81-3	-0.4861	-0.2824	interpol.
471	100418-33-5	-0.4082	-0.154	interpol.
472	121251-67-0	-0.2983	0.1022	interpol.
473	121251-68-1	-0.2983	0.1022	interpol.
474	122021-01-6	1.7162	1.3	interpol.
475	125304-04-3	3.8502	3.9337	extrapol.
476	128489-04-3	-0.2985	-0.0116	interpol.
477	131766-73-9	-1.4845	-1.0856	interpol.
478	131812-52-7	2.1591	1.986	interpol.
479	154171-77-4	0.0465	0.6763	interpol.
480	166301-22-0	-1.7526	-1.656	interpol.
481	169198-72-5	4.0573	3.3528	interpol.
482	190085-41-7	2.092	2.3376	interpol.
483	211299-54-6	0.3652	0.8227	interpol.
484	302776-68-7	3.3295	3.2058	extrapol.
485	000067-71-0	-	-2.0672	interpol.

ATI ID	CAS	ATI (PC1 score "exp")	ATI Predicted	AD ATI
486	000075-18-3	-	-1.1298	interpol.
487	000077-90-7	-	0.5168	interpol.
488	000078-69-3	-	-1.2587	interpol.
489	000084-76-4	-	3.5638	extrapol.
490	000084-77-5	-	4.0588	extrapol.
491	000085-70-1	-	1.4033	interpol.
492	000111-84-2	-	-1.0815	extrapol.
493	000112-40-3	-	-0.2915	extrapol.
494	000112-95-8	-	1.7161	extrapol.
495	000117-84-0	-	3.0689	interpol.
496	000119-06-2	-	5.5431	extrapol.
497	000124-18-5	-	-0.8139	extrapol.
498	000124-28-7	-	1.2224	extrapol.
499	000137-26-8	-	1.6619	extrapol.
500	000142-22-3	-	-0.6343	interpol.
501	000624-92-0	-	0.8985	extrapol.
502	000629-50-5	-	-0.0349	extrapol.
503	000629-59-4	-	0.2194	extrapol.
504	002985-59-3	-	3.829	interpol.
505	003648-20-2	-	4.5538	extrapol.
506	003648-21-3	-	2.5745	interpol.
507	004065-45-6	-	1.4803	interpol.
508	004221-80-1	-	4.5172	extrapol.
509	006028-61-1	-	0.9495	interpol.
510	006197-30-4	-	4.4194	interpol.
511	006422-86-2	-	2.6545	interpol.
512	006628-37-1	-	1.4803	interpol.
513	010236-16-5	-	2.484	interpol.
514	014117-96-5	-	8.0102	extrapol.
515	016883-83-3	-	3.8473	extrapol.
516	024295-03-2	-	0.6724	extrapol.
517	025724-58-7	-	3.0689	interpol.
518	026761-40-0	-	4.2413	extrapol.
519	027253-26-5	-	5.7612	extrapol.
520	027503-81-7	-	1.8589	interpol.
521	027554-26-3	-	3.2177	interpol.
522	028553-12-0	-	3.4747	extrapol.
523	056039-58-8	-	1.7818	extrapol.
524	076656-36-5	-	0.883	extrapol.
525	088122-99-0	-	9.1915	extrapol.
526	092761-26-7	-	4.0958	extrapol.
527	102187-19-9	-	4.4028	extrapol.
528	103597-45-1	-	7.9528	extrapol.
529	104333-00-8	-	0.1696	interpol.
530	116242-27-4	-	-0.5062	extrapol.
531	152075-98-4	-	4.5401	extrapol.
532	154702-15-5	-	8.4515	extrapol.
533	155633-54-8	-	5.7532	extrapol.
534	187393-00-6	-	6.5905	extrapol.