Table 1. List of chemicals used for individual logistic regression model development

CHEMICAL NAME	CHEMICAL CLASS
Ammonia	CONVENT
Sulfide, total (S2)	CONVENT
Antimony	METALS
Arsenic	METALS
Cadmium	METALS
Chromium, total	METALS
Copper	METALS
Lead	METALS
Mercury	METALS
Nickel	METALS
Selenium	METALS
Silver	METALS
Zinc	METALS
Diesel fuel	ORGANIC
Residual Range Organics	ORGANIC
Tributyl Tin (as TBT cation)	ORGMETS
2-Methylnaphthalene	PAH
Acenaphthene	PAH
Acenaphthylene	PAH
Anthracene	PAH
Benzo(a)anthracene	PAH
Benzo(a)pyrene	PAH
Benzo(b)fluoranthene	PAH
Benzo(g,h,i)perylene	PAH
Benzo(k)fluoranthene	PAH
Carbazole	PAH
Chrysene	PAH
Dibenzo(a,h)anthracene	PAH
Dibenzofuran	PAH
Fluoranthene	PAH
Fluorene	PAH
Indeno(1,2,3-c,d)pyrene	PAH
Naphthalene	PAH
PAHs, total	PAH
PAHs, total high molecular weight PAHs	PAH
PAHs, total low molecular weight PAHs	PAH
Phenanthrene	PAH
Pyrene	PAH
Aldrin	PEST-PCB
Chlordane, alpha-	PEST-PCB
Chlordanes, total (calc)	PEST-PCB
DDTs, sum of p,p'-DDD and o,p'-DDD	PEST-PCB
DDTs, sum of p,p'-DDE and o,p'-DDE	PEST-PCB
DDTs, total of 6 isomers	PEST-PCB
Endosulfan-alpha	PEST-PCB
Endrin ketone	PEST-PCB
Hexachlorocyclohexane-alpha	PEST-PCB
Hexachlorocyclohexane-beta	PEST-PCB
Hexachlorocyclohexane-delta	PEST-PCB
Nonachlor, cis-	PEST-PCB
Nonachlor, trans-	PEST-PCB
PCBs, total (calc)	PEST-PCB

o,p'-DDD	PEST-PCB
o,p'-DDE	PEST-PCB
o,p'-DDT	PEST-PCB
p,p'-DDD	PEST-PCB
p,p'-DDE	PEST-PCB
p,p'-DDT	PEST-PCB
4-Methylphenol	SVOL
Benzyl alcohol	SVOL
Bis(2-ethylhexyl) phthalate	SVOL
Di-n-butyl phthalate	SVOL
Phenol	SVOL

Chemical Name	Model	Normalization	Species
Ammonia	PH2CHB2_2G_CF	OC_FINES	CH
Sulfide, total (S2)	PH2CHB2_2X_OC	OC	CH
Chromium, total	PH2CHB2_2G_CF	OC_FINES	CH
Copper	PH2CHB1_2X_DW	DW	CH
Lead	PH2CHB2_1X_DW	DW	CH
Mercury	PH2CHB2_1X_CF	OC_FINES	CH
Silver	PH2CHB2_2G_FINES	FINES	CH
Diesel fuel	PH2HYB1_1X_CF	OC_FINES	HY
Tributyl Tin (as TBT cation)	PH2HYB2_1X_DW	DW	HY
2-Methylnaphthalene	PH2CHB2_2X_FINES	FINES	CH
Acenaphthene	PH2HYB3_2G_CF	OC_FINES	HY
Acenaphthylene	PH2HYB2_2X_DW	DW	HY
Anthracene	PH2CHB3_2G_FINES	FINES	CH
Benzo(a)anthracene	PH2HYB2_2X_FINES	FINES	HY
Benzo(a)pyrene	PH2HYB1_2X_FINES	FINES	HY
Benzo(b)fluoranthene	PH2HYB2_1X_CF	OC_FINES	HY
Benzo(g,h,i)perylene	PH2HYB2_1X_FINES	FINES	HY
Benzo(k)fluoranthene	PH2HYB2_1X_CF	OC_FINES	HY
Carbazole	PH2HYB1_1X_DW	DW	HY
Chrysene	PH2HYB1_2X_FINES	FINES	HY
Dibenzo(a,h)anthracene	PH2HYB2_1X_FINES	FINES	HY
Dibenzofuran	PH2HYB1_2X_FINES	FINES	HY
Fluoranthene	PH2HYB3_2G_FINES	FINES	HY
Fluorene	PH2HYB1_2X_FINES	FINES	HY
Indeno(1,2,3-c,d)pyrene	PH2HYB2_1X_FINES	FINES	HY
PAHs, total	PH2CHB3_1X_FINES	FINES	CH
PAHs, total high molecular weight PAHs	PH2HYB2_1X_FINES	FINES	HY
PAHs, total low molecular weight PAHs	PH2HYB3_2G_FINES	FINES	HY
Phenanthrene	PH2HYB3_2G_FINES	FINES	HY
Pyrene	PH2HYB2_1X_FINES	FINES	HY
Chlordane, alpha-	PH2CHB2_1X_FINES	FINES	CH
DDTs, sum of p,p'-DDE and o,p'-DDE	PH2HYB1_2X_OC	OC	HY
Hexachlorocyclohexane-delta	PH2HYB2_1X_FINES	FINES	HY
PCBs, total (calc)	PH2CHB2_1X_FINES	FINES	CH
o,p'-DDD	PH2HYB2_1X_CF	OC_FINES	HY
p,p'-DDD	PH2HYB2_1X_DW	DW	HY
p,p'-DDE	PH2HYB1_2X_CF	OC_FINES	HY
p,p'-DDT	PH2CHB2_1X_CF	OC_FINES	CH
Di-n-butyl phthalate	PH2CHB1_1X_CF	OC_FINES	CH
Phenol	PH2HYB1_2X_OC	OC	HY

Toxicity Category	Screening Approach	Intercept (b0)	Slope (b1)	Normalized Chi-Square	T25	T50
2	2G	-20.1781	5.2134	0.159	4567.74	7420.45
2	2X	-16.7869	4.8893	0.320	1616.96	2712.66
2	2G	-26.1362	7.5439	0.164	2084.10	2914.39
1	2X	-12.3774	4.6753	0.152	258.48	444.02
2	1X	-7.7491	3.3799	0.155	92.82	196.20
2	1X	-4.1198	4.2606	0.187	5.12	9.27
2	2G	1.1650	3.4191	0.179	0.22	0.46
1	1X	-17.1626	4.2802	0.509	5663.60	10227.42
2	1X	-9.0539	2.5952	0.157	1162.48	3081.13
2	2X	-7.6932	3.0341	0.334	149.10	343.23
3	2G	-6.7641	1.2697	0.161	28977.97	212481.64
2	2X	-8.2681	2.4399	0.202	867.83	2447.40
3	2G	-4.7064	1.6242	0.286	166.44	790.08
2	2X	-10.2314	2.4353	0.205	5625.61	15896.06
1	2X	-9.6157	2.5768	0.385	2019.74	5390.68
2	1X	-14.3292	2.5378	0.202	163458.82	442902.19
2	1X	-8.7432	2.1556	0.219	3518.72	11377.32
2	1X	-13.4131	2.6086	0.209	52568.64	138636.27
1	1X	-6.0467	2.2517	0.374	157.58	484.61
1	2X	-9.1793	2.4987	0.380	1713.79	4716.61
2	1X	-7.1066	2.2273	0.209	498.23	1551.24
1	2X	-6.7510	2.5521	0.332	163.98	441.85
3	2G	-6.1951	1.3821	0.157	4869.63	30365.60
1	2X	-7.7422	2.3055	0.351	761.42	2281.10
2	1X	-8.7334	2.1646	0.219	3365.99	10830.50
3	1X	-12.8081	2.7629	0.344	17302.74	43226.00
2	1X	-10.8064	2.0834	0.215	45665.58	153782.18
3	2G	-5.8855	1.2636	0.164	6141.77	45469.90
3	2G	-5.6283	1.2709	0.167	3665.70	26828.35
2	1X	-10.2735	2.1945	0.215	15165.46	48026.00
2	1X	-1.1934	2.8985	0.357	1.08	2.58
1	2X	-11.4096	2.6423	0.154	7985.05	20799.66
2	1X	0.2773	2.4794	0.185	0.28	0.77
2	1X	-6.2647	2.0693	0.168	313.72	1065.24
2	1X	-10.2008	3.0617	0.267	939.55	2146.56
2	1X	-7.1812	2.8207	0.259	143.35	351.47
1	2X	-10.0087	2.6766	0.191	2132.47	5486.98
2	1X	-8.2659	1.8623	0.167	7057.02	27450.09
1	1X	-9.7364	2.6918	0.253	1617.81	4140.56
1	2X	-33.7292	9.6960	0.451	2319.35	3010.73

T75
12054.76
4550.85
4075.46
762.75
414.71
16.78
0.96
18468.81
8166.47
790.07
1558026.54
6901.98
3750.38
44916.85
14387.70
1200071.99
36787.06
365617.54
1490.38
12980.87
4829.78
1190.55
189351.23
6833.79
34848.52
107987.92
517872.73
336631.22
196349.75
152088.79
6.18
54179.50
2.14
3617.09
4904.20
861.74
14118.36
106774.13
10597.23
3908.21

			Proportion Toxic (>= Level 2)				Number of Samples			
CHEMICAL NAME	MODEL	Normalization	PCT25	PCT50	PCT75	PCT100	N25	N50	N75	N100
Ammonia	PH2CH10B2_2G_CF	OC_FINES	0.34	0.43	0.75	1.00	251	37	4	1
Sulfide, total (S2)	PH2CH10B2_2X_OC	OC	0.33	0.58	0.67	0.88	270	12	3	8
Chromium, total	PH2CH10B2_2G_CF	OC_FINES	0.35	0.40	1.00	0.75	278	10	1	4
Copper	PH2CH10B1_2X_DW	DW	0.37	0.13	0.50	1.00	282	8	2	1
Lead	PH2CH10B2_1X_DW	DW	0.36	0.27	1.00	0.75	277	11	1	4
Mercury	PH2CH10B2_1X_CF	OC_FINES	0.33	0.50	0.88	1.00	266	16	8	3
Silver	PH2CH10B2_2G_FINES	FINES	0.33	0.45	0.71	1.00	251	33	7	2
Diesel fuel	PH2HY28B1_1X_CF	OC_FINES	0.32	0.33	0.78	0.88	157	24	9	17
Tributyl Tin (as TBT cation)	PH2HY28B2_1X_DW	DW	0.34	0.00	0.00	1.00	71	2	0	1
2-Methylnaphthalene	PH2CH10B2_2X_FINES	FINES	0.33	0.67	0.67	0.89	275	6	3	9
Acenaphthene	PH2HY28B3_2G_CF	OC_FINES	0.33	0.71	0.67	1.00	271	14	6	2
Acenaphthylene	PH2HY28B2_2X_DW	DW	0.35	0.60	0.67	1.00	280	5	6	2
Anthracene	PH2CH10B3_2G_FINES	FINES	0.32	0.43	0.80	0.82	258	14	10	11
Benzo(a)anthracene	PH2HY28B2_2X_FINES	FINES	0.34	0.71	0.50	1.00	280	7	2	4
Benzo(a)pyrene	PH2HY28B1_2X_FINES	FINES	0.34	0.50	0.67	0.88	271	8	6	8
Benzo(b)fluoranthene	PH2HY28B2_1X_CF	OC_FINES	0.34	0.67	0.67	1.00	277	9	6	1
Benzo(g,h,i)perylene	PH2HY28B2_1X_FINES	FINES	0.34	0.60	0.80	1.00	279	5	5	4
Benzo(k)fluoranthene	PH2HY28B2_1X_CF	OC_FINES	0.34	0.63	0.71	1.00	277	8	7	1
Carbazole	PH2HY28B1_1X_DW	DW	0.34	0.25	0.75	1.00	266	12	8	7
Chrysene	PH2HY28B1_2X_FINES	FINES	0.34	0.50	0.67	0.88	271	8	6	8
Dibenzo(a,h)anthracene	PH2HY28B2_1X_FINES	FINES	0.34	0.57	0.75	1.00	278	7	4	4
Dibenzofuran	PH2HY28B1_2X_FINES	FINES	0.34	0.71	1.00	0.83	277	7	3	6
Fluoranthene	PH2HY28B3_2G_FINES	FINES	0.33	0.70	0.83	1.00	275	10	6	2
Fluorene	PH2HY28B1_2X_FINES	FINES	0.33	0.67	1.00	0.83	275	9	3	6
Indeno(1,2,3-c,d)pyrene	PH2HY28B2_1X_FINES	FINES	0.34	0.60	0.80	1.00	279	5	5	4
PAHs, total	PH2CH10B3_1X_FINES	FINES	0.34	0.33	0.80	0.82	271	6	5	11
PAHs, total high molecular weight PAH	PH2HY28B2_1X_FINES	FINES	0.34	0.71	0.75	1.00	278	7	4	4
PAHs, total low molecular weight PAHs	PH2HY28B3_2G_FINES	FINES	0.33	0.64	0.80	1.00	271	14	5	3
Phenanthrene	PH2HY28B3_2G_FINES	FINES	0.33	0.67	0.80	1.00	273	12	5	3
Pyrene	PH2HY28B2_1X_FINES	FINES	0.34	0.67	0.75	1.00	279	6	4	4

CHEMICAL NAME	Selected Models	Proportion Toxic with p>=0.50	Positive Likelihood
Ammonia	PH2CH10B2_2G_CF	0.80	7.12
Sulfide, total (S2)	PH2CH10B2_2X_OC	0.82	15.94
Chromium, total	PH2CH10B2_2G_CF	0.80	7.12
Copper	PH2CH10B1_2X_DW	0.67	3.56
Lead	PH2CH10B2_1X_DW	0.80	7.12
Mercury	PH2CH10B2_1X_CF	0.91	17.81
Silver	PH2CH10B2_2G_FINES	0.78	12.22
Diesel fuel	PH2HY28B1_1X_CF	0.85	11.46
Tributyl Tin (as TBT cation)	PH2HY28B2_1X_DW	1.00	-9.00
2-Methylnaphthalene	PH2CH10B2_2X_FINES	0.83	17.71
Acenaphthene	PH2HY28B3_2G_CF	0.75	10.63
Acenaphthylene	PH2HY28B2_2X_DW	0.75	10.63
Anthracene	PH2CH10B3_2G_FINES	0.81	10.04
Benzo(a)anthracene	PH2HY28B2_2X_FINES	0.83	8.77
Benzo(a)pyrene	PH2HY28B1_2X_FINES	0.79	9.60
Benzo(b)fluoranthene	PH2HY28B2_1X_CF	0.71	8.73
Benzo(g,h,i)perylene	PH2HY28B2_1X_FINES	0.89	14.25
Benzo(k)fluoranthene	PH2HY28B2_1X_CF	0.75	10.47
Carbazole	PH2HY28B1_1X_DW	0.87	11.58
Chrysene	PH2HY28B1_2X_FINES	0.79	9.60
Dibenzo(a,h)anthracene	PH2HY28B2_1X_FINES	0.88	12.47
Dibenzofuran	PH2HY28B1_2X_FINES	0.89	12.59
Fluoranthene	PH2HY28B3_2G_FINES	0.88	10.79
Fluorene	PH2HY28B1_2X_FINES	0.89	12.59
Indeno(1,2,3-c,d)pyrene	PH2HY28B2_1X_FINES	0.89	14.25
PAHs, total	PH2CH10B3_1X_FINES	0.81	11.34
PAHs, total high molecular weight PAHs	PH2HY28B2_1X_FINES	0.88	12.47
PAHs, total low molecular weight PAHs	PH2HY28B3_2G_FINES	0.88	12.47
Phenanthrene	PH2HY28B3_2G_FINES	0.88	12.47
Pyrene	PH2HY28B2_1X_FINES	0.88	12.47
Chlordane, alpha-	PH2CH10B2_1X_FINES	0.85	19.28
DDTs, sum of p,p'-DDE and o,p'-DDE	PH2HY28B1_2X_OC	0.75	5.31
Hexachlorocyclohexane-delta	PH2HY28B2_1X_FINES	0.80	8.24
PCBs, total (calc)	PH2CH10B2_1X_FINES	0.67	3.54
o,p'-DDD	PH2HY28B2_1X_CF	0.78	6.29
p,p'-DDD	PH2HY28B2_1X_DW	0.78	6.20
p,p'-DDE	PH2HY28B1_2X_CF	1.00	-9.00
p,p'-DDT	PH2CH10B2_1X_CF	0.60	2.57
Di-n-butyl phthalate	PH2CH10B1_1X_CF	0.75	11.73
Phenol	PH2HY28B1_2X_OC	0.80	7.69

Number of Toxic Samples with p>=0.5	Number of Samples with p>=0.5	Rank: Proportion Toxic	Rank: Positive Likelihood
4	5	1	1
9	11	14	1
4	5	1	1
2	3	2	1
4	5	1	1
10	11	1	1
7	9	2	1
22	26	35	25
1	1	1	1
10	12	11	1
6	8	19	1
6	8	6	1
17	21	11	2
5	6	3	1
11	14	9	1
5	7	20	1
8	9	5	1
6	8	7	1
13	15	18	4
11	14	6	1
7	8	3	1
7	9	1	1
6	8	1	1
7	9	1	1
8	9	4	1
13	16	12	1
7	8	1	1
7	8	1	1
7	8	1	1
7	8	1	1
11	13	1	1
3	4	1	2
4	5	5	1
4	6	1	6
7	9	1	3
7	9	1	4
4	4	1	31
3	5	1	1
6	8	15	1
4	5	5	1

Table 5. The number and proportion of toxic samples for PMax >0.5 by chemical with the highest probability for an individual sample

Chemical Name	Number of Toxic Samples for p>0.50	Number of Samples for p>0.50	Proportion Toxic for p>0.50
Ammonia	0	0	
Sulfide, total (S2)	6	8	0.75
Chromium, total	4	4	1.00
Copper	2	3	0.67
Lead	2	3	0.67
Mercury	5	6	0.83
Silver	2	3	0.67
Diesel fuel	10	14	0.71
Tributyl Tin (as TBT cation)	1	1	1.00
2-Methylnaphthalene	3	4	0.75
Acenaphthene	0	0	
Acenaphthylene	0	0	
Anthracene	1	1	1.00
Benzo(a)anthracene	0	0	
Benzo(a)pyrene	0	0	
Benzo(b)fluoranthene	0	0	
Benzo(g,h,i)perylene	0	0	
Benzo(k)fluoranthene	0	0	
Carbazole	1	1	1.00
Chrysene	0	0	
Dibenzo(a,h)anthracene	0	0	
Dibenzofuran	1	1	1.00
Fluoranthene	0	0	
Fluorene	0	0	
Indeno(1,2,3-c,d)pyrene	0	0	
PAHs, total	1	2	0.50
PAHs, total high molecular weight PAHs	0	0	
PAHs, total low molecular weight PAHs	0	0	
Phenanthrene	0	0	
Pyrene	0	0	
Chlordane, alpha-	3	5	0.60
DDTs, sum of p,p'-DDE and o,p'-DDE	0	0	
Hexachlorocyclohexane-delta	2	2	1.00
PCBs, total (calc)	1	3	0.33
o,p'-DDD	1	1	1.00
p,p'-DDD	0	0	
p,p'-DDE	1	1	1.00
p,p'-DDT	0	0	
Di-n-butyl phthalate	3	5	0.60
Phenol	3	4	0.75