Classifying bio-concentration factor with random forest algorithm, influence of the bio-accumulative vs. non-bio-accumulative compound ratio to modelling result, and applicability domain for random forest model

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Supplementary information

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Table S 1. All ID-s for used molecules, their belonging to the training set (T) and to the validation set (V), their CAS numbers and InChI codes, calculated values of descriptors used in modeling, experimental bio-concentration factor (log BCF) values, experimental and calculated classes.

ID	Set ID	CAS no.	InChI	Descriptors					Experimental		Calculated			Comments
				XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	
1	T	50-30-6	InChI=1S/C7H4Cl2O2/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H,10,11)	2.23	144	0.402	37.3	2	-0.22	nB	nB	nB	nB	
2	V	50-32-8	InChI=1S/C20H12/c1-2-7-17-15(4-1)12-16-9-8-13-5-3-6-14-10-11-18(17)20(16)19(13)14/h1-12H	5.97	680	0.355	0	0	2.73	nB	nB	B	B	
3	V	51-28-5	InChI=1S/C6H4N2O5/c9-6-2-1-4(7(10)11)3-5(6)8(12)13/h1-3,9H	1.67	240	-0.147	106.51	0	0.05	nB	nB	nB	nB	
4	V	51-44-5	InChI=1S/C7H4Cl2O2/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3H,(H,10,11)	3.46	152	0.468	37.3	2	-0.17	nB	nB	nB	nB	
5	T	56-23-5	InChI=1S/CCl4/c2-1(3,4)5	2.77	16	0.024	0	0	1.07	nB	nB	nB	nB	
6	#N/A	56-35-9	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.99	B	#N/A	#N/A	#N/A	Tin containing compound
7	T	56-55-3	InChI=1S/C18H12/c1-2-7-15-12-18-16(11-14(15)6-1)10-9-13-5-3-4-8-17(13)18/h1-12H	5.76	553	0.317	0	0	2.54	nB	nB	B	B	
8	V	58-90-2	InChI=1S/C6H2Cl4O/c7-2-1-3(8)6(11)5(10)4(2)9/h1,11H	4.45	140	0.021	20.23	0	2.01	nB	B	B	B	
9	T	59-50-7	InChI=1S/C7H7ClO/c1-5-4-6(9)2-3-7(5)8/h2-4,9H,1H3	3.1	84	0.372	20.23	0	1.02	nB	nB	nB	nB	
10	V	60-29-7	InChI=1S/C4H10O/c1-3-5-4-2/h3-4H2,1-2H3	0.89	20	0.296	9.23	1	0.48	nB	nB	nB	nB	
11	T	60-51-5	InChI=1S/C5H12NO3PS2/c1-6-5(7)4-12-10(11,8-2)9-3/h4H2,1-3H3,(H,6,7)	0.78	218	2.524	114.76	4	0.16	nB	nB	nB	nB	
12	T	62-53-3	InChI=1S/C6H7N/c7-6-4-2-1-3-5-6/h1-5H,7H2	0.9	42	0.401	26.02	1	0.31	nB	nB	nB	nB	
13	V	62-73-7	InChI=1S/C4H7Cl2O4P/c1-8-11(7,9-2)10-3-4(5)6/h3H,1-2H3	1.43	168	1.852	54.57	4	-0.20	nB	nB	nB	nB	
14	T	66-81-9	InChI=1S/C15H23NO4/c1-8-3-9(2)15(20)11(4-8)12(17)5-10-6-13(18)16-14(19)7-10/h8-12,17H,3-7H2,1-2H3,(H,16,18,19)/t8-,9-,11-,12-/m0/s1	0.55	825	1.38	83.47	5	-0.04	nB	nB	nB	nB	
15	V	67-72-1	InChI=1S/C2Cl6/c3-1(4,5)2(6,7)8	4.14	58	0.178	0	0	2.12	nB	nB	B	B	
16	V	70-30-4	InChI=1S/C13H6Cl6O2/c14-6-2-8(16)12(20)4(10(6)18)1-5-11(19)7(15)3-9(17)13(5)21/h2-3,20-21H,1H2	7.54	860	0.247	40.46	0	2.39	nB	nB	B	B	
17	T	71-55-6	InChI=1S/C2H3Cl3/c1-2(3,4)5/h1H3	2.44	16	0.073	0	0	0.48	nB	nB	nB	nB	
18	V	72-55-9	InChI=1S/C14H8Cl4/c15-11-5-1-9(2-6-11)13(14(17)18)10-3-7-12(16)8-4-10/h1-8H	6.51	603	0.159	0	0	4.51	B	B	B	B	
19	T	74-31-7	InChI=1S/C18H16N2/c1-3-7-15(8-4-1)19-17-11-13-18(14-12-17)20-16-9-5-2-6-10-16/h1-14,19-20H	5.04	956	1.839	24.06	2	3.13	B	B	B	B	
20	T	75-25-2	InChI=1S/CHBr3/c2-1(3)4/h1H	2.77	9	0.007	0	0	1.22	nB	nB	nB	nB	
21	V	76-03-9	InChI=1S/C2HCl3O2/c3-2(4,5)1(6)7/h(H,6,7)	1.33	42	0.399	37.3	2	-0.53	nB	nB	nB	nB	
22	V	76-93-7	InChI=1S/C14H12O3/c15-13(16)14(17,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,17H,(H,15,16)	2.3	474	1.052	57.53	3	-0.22	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
23	V	78-40-0	InChI=1S/C6H15O4P/c1-4-8-11(7,9-5-2)10-6-3/h4-6H2,1-3H3	0.8	166	1.848	54.57	4	-0.10	nB	nB	nB	nB	
24	V	78-59-1	InChI=1S/C9H14O/c1-7-4-8(10)6-9(2,3)5-7/h4H,5-6H2,1-3H3	1.7	109	0.474	17.07	1	0.39	nB	nB	nB	nB	
25	T	79-01-6	InChI=1S/C2HCl3/c3-1-2(4)5/h1H	2.42	18	0.082	0	0	1.11	nB	nB	nB	nB	
26	V	79-27-6	InChI=1S/C2H2Br4/c3-1(4)2(5)6/h1-2H	3.59	29	0.073	0	0	0.77	nB	nB	nB	nB	
27	T	79-34-5	InChI=1S/C2H2Cl4/c3-1(4)2(5)6/h1-2H	2.39	29	0.117	0	0	1.03	nB	nB	nB	nB	
28	V	79-92-5	InChI=1S/C10H16/c1-7-8-4-5-9(6-8)10(7,2)3/h8-9H,1,4-6H2,2-3H3	4.22	98	0.163	0	0	2.97	nB	B	B	B	
29	T	80-43-3	InChI=1S/C18H22O2/c1-17(2,15-11-7-5-8-12-15)19-20-18(3,4)16-13-9-6-10-14-16/h5-14H,1-4H3	5.5	848	0.705	18.46	2	2.88	nB	B	B	B	
30	V	81-11-8	InChI=1S/C14H14N2O6S2/c15-11-5-3-9(13(7-11)23(17,18)19)1-2-10-4-6-12(16)8-14(10)24(20,21)22/h1-8H,15-16H2,(H,17,18,19)(H,20,21,22)/b2-1+	-1.7	1350	2.589	177.54	8	0.28	nB	nB	nB	nB	
31	T	81-16-3	InChI=1S/C10H9NO3S/c11-9-6-5-7-3-1-2-4-8(7)10(9)15(12,13)14/h1-6H,11H2,(H,12,13,14)	-1.16	322	1.456	88.77	4	0.28	nB	nB	nB	nB	
32	T	82-05-3	InChI=1S/C17H10O/c18-17-14-8-2-1-7-12(14)13-9-3-5-11-6-4-10-15(17)16(11)13/h1-10H	4.81	503	0.591	17.07	1	2.14	nB	B	B	B	
33	T	82-44-0	InChI=1S/C14H7ClO2/c15-11-7-3-6-10-12(11)14(17)9-5-2-1-4-8(9)13(10)16/h1-7H	4.5	442	0.816	34.14	2	2.42	nB	nB	B	B	
34	T	84-57-1	InChI=1S/C10H8Cl2N2O4S/c1-5-2-10(15)14(13-5)8-3-7(12)9(4-6(8)11)19(16,17)18/h3-4H,2H2,1H3,(H,16,17,18)	1.27	671	1.674	95.42	6	0.80	nB	nB	nB	nB	
35	V	84-74-2	InChI=1S/C16H22O4/c1-3-5-11-19-15(17)13-9-7-8-10-14(13)16(18)20-12-6-4-2/h7-10H,3-6,11-12H2,1-2H3	4.5	912	0.807	52.6	4	2.23	nB	nB	nB	B	
36	T	85-83-6	InChI=1S/C24H20N4O/c1-16-7-3-6-10-21(16)26-25-19-12-13-22(17(2)15-19)27-28-24-20-9-5-4-8-18(20)11-14-23(24)29/h3-15,29H,1-2H3/b26-25+,28-27+	7.1	2598	0.879	69.67	4	0.75	nB	B	B	B	
37	T	87-02-5	InChI=1S/C10H9NO4S/c11-7-1-2-9-6(3-7)4-8(5-10(9)12)16(13,14)15/h1-5,12H,11H2,(H,13,14,15)	-0.86	406	1.686	109	4	-0.16	nB	nB	nB	nB	
38	T	87-61-6	InChI=1S/C6H3Cl3/c7-4-2-1-3-5(8)6(4)9/h1-3H	4.05	82	0.131	0	0	2.96	nB	B	B	B	
39	V	87-83-2	InChI=1S/C7H3Br5/c1-2-3(8)5(10)7(12)6(11)4(2)9/h1H3	5.74	174	-0.085	0	0	2.46	nB	B	B	B	
40	V	88-06-2	InChI=1S/C6H3Cl3O/c7-3-1-4(8)6(10)5(9)2-3/h1-2,10H	3.69	110	0.051	20.23	0	1.89	nB	nB	nB	B	
41	T	88-19-7	InChI=1S/C7H9NO2S/c1-6-4-2-3-5-7(6)11(8,9)10/h2-5H,1H3,(H2,8,9,10)	0.84	144	0.344	68.54	3	0.15	nB	nB	nB	nB	
42	V	88-44-8	InChI=1S/C7H9NO3S/c1-5-2-3-6(8)7(4-5)12(9,10)11/h2-4H,8H2,1H3,(H,9,10,11)	0.9	183	1.392	88.77	4	0.10	nB	nB	nB	nB	
43	T	88-73-3	InChI=1S/C6H4ClNO2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H	2.24	114	-0.045	43.14	0	1.71	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
44	T	88-74-4	InChI=1S/C6H6N2O2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H,7H2	1.85	114	0.126	69.16	1	0.69	nB	nB	nB	nB	
45	T	88-85-7	InChI=1S/C10H12N2O5/c1-3-6(2)8-4-7(11(14)15)5-9(10(8)13)12(16)17/h4-6,13H,3H2,1-2H3	3.56	486	-0.133	106.51	0	0.67	nB	nB	nB	B	
46	T	89-93-0	InChI=1S/C8H11N/c1-7-4-2-3-5-8(7)6-9/h2-5H,6,9H2,1H3	1.33	86	0.603	26.02	1	0.48	nB	nB	nB	nB	
47	T	90-20-0	InChI=1S/C10H9NO7S2/c11-8-3-6(19(13,14)15)1-5-2-7(20(16,17)18)4-9(12)10(5)8/h1-4,12H,11H2,(H,13,14,15)(H,16,17,18)	0.18	745	2.58	171.75	7	0.46	nB	nB	nB	nB	
48	T	90-51-7	InChI=1S/C10H9NO4S/c11-7-2-1-6-3-8(16(13,14)15)5-10(12)9(6)4-7/h1-5,12H,11H2,(H,13,14,15)	-0.86	409	1.663	109	4	0.16	nB	nB	nB	nB	
49	T	90-94-8	InChI=1S/C17H20N2O/c1-18(2)15-9-5-13(6-10-15)17(20)14-7-11-16(12-8-14)19(3)4/h5-12H,1-4H3	3.87	899	1.163	23.55	3	1.59	nB	nB	nB	B	
50	T	91-20-3	InChI=1S/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H	3.3	109	0.197	0	0	2.36	nB	nB	nB	nB	
51	T	91-22-5	InChI=1S/C9H7N/c1-2-6-9-8(4-1)5-3-7-10-9/h1-7H	2.03	109	0.507	12.89	1	0.40	nB	nB	nB	nB	
52	T	91-58-7	InChI=1S/C10H7Cl/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H	3.9	144	0.186	0	0	3.63	B	B	B	B	
53	V	91-94-1	InChI=1S/C12H10Cl2N2/c13-9-5-7(1-3-11(9)15)8-2-4-12(16)10(14)6-8/h1-6H,15-16H2	3.51	440	0.787	52.04	2	2.29	nB	nB	nB	nB	
54	T	91-96-3	InChI=1S/C22H24N2O4/c1-13-9-17(5-7-19(13)23-21(27)11-15(3)25)18-6-8-20(14(2)10-18)24-22(28)12-16(4)26/h5-10H,11-12H2,1-4H3,(H,23,27)(H,24,28)	1.75	2420	1.795	92.34	6	-0.25	nB	nB	nB	nB	
55	T	92-69-3	InChI=1S/C12H10O/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9,13H	3.2	252	0.515	20.23	0	1.68	nB	nB	nB	nB	
56	V	92-84-2	InChI=1S/C12H9NS/c1-3-7-11-9(5-1)13-10-6-2-4-8-12(10)14-11/h1-8,13H	4.15	279	1.219	37.33	1	2.67	nB	nB	nB	B	
57	T	94-52-0	InChI=1S/C7H5N3O2/c11-10(12)5-1-2-6-7(3-5)9-4-8-6/h1-4H,(H,8,9)	1.64	188	1.105	67.86	2	0.23	nB	nB	nB	nB	
58	V	95-49-8	InChI=1S/C7H7Cl/c1-6-4-2-3-5-7(6)8/h2-5H,1H3	3.42	60	0.122	0	0	1.91	nB	nB	nB	nB	
59	V	95-63-6	InChI=1S/C9H12/c1-7-4-5-8(2)9(3)6-7/h4-6H,1-3H3	3.63	84	0.125	0	0	2.26	nB	nB	nB	B	
60	T	95-64-7	InChI=1S/C8H11N/c1-6-3-4-8(9)5-7(6)2/h3-5H,9H2,1-2H3	1.84	84	0.393	26.02	1	0.61	nB	nB	nB	nB	
61	V	95-76-1	InChI=1S/C6H5Cl2N/c7-5-2-1-4(9)3-6(5)8/h1-3H,9H2	2.69	84	0.329	26.02	1	1.15	nB	nB	nB	nB	
62	T	95-78-3	InChI=1S/C8H11N/c1-6-3-4-7(2)8(9)5-6/h3-5H,9H2,1-2H3	1.83	84	0.393	26.02	1	0.49	nB	nB	nB	nB	
63	T	95-95-4	InChI=1S/C6H3Cl3O/c7-3-1-5(9)6(10)2-4(3)8/h1-2,10H	3.72	111	0.17	20.23	0	2.41	nB	nB	nB	B	
64	V	96-18-4	InChI=1S/C3H5Cl3/c4-1-3(6)2-5/h3H,1-2H2	2.27	31	0.108	0	0	1.02	nB	nB	nB	nB	
65	V	96-29-7	InChI=1S/C4H9NO/c1-3-4(2)5-6/h6H,3H2,1-2H3/b5-4+	0.63	31	0.592	32.59	0	0.18	nB	nB	nB	nB	
66	V	96-69-5	InChI=1S/C22H30O2S/c1-13-9-17(23)15(21(3,4)5)11-19(13)25-20-12-16(22(6,7)8)18(24)10-14(20)2/h9-12,23-24H,1-8H3	7.35	1464	0.935	65.76	0	0.82	nB	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
67	T	96-96-8	InChI=1S/C7H8N2O3/c1-12-5-2-3-6(8)7(4-5)9(10)11/h2-4H,8H2,1H3	1.86	193	0.252	78.39	1	0.72	nB	nB	nB	nB	
68	T	98-08-8	InChI=1S/C7H5F3/c8-7(9,10)6-4-2-1-3-5-6/h1-5H	3.01	114	0.013	0	0	1.69	nB	nB	nB	nB	
69	V	98-15-7	InChI=1S/C7H4ClF3/c8-6-3-1-2-5(4-6)7(9,10)11/h1-4H	3.6	148	0.002	0	0	2.32	nB	nB	nB	B	
70	T	98-47-5	InChI=1S/C6H5NO5S/c8-7(9)5-2-1-3-6(4-5)13(10,11)12/h1-4H,(H,10,11,12)	0.01	240	0.864	105.89	3	0.70	nB	nB	nB	nB	
71	T	98-73-7	InChI=1S/C11H14O2/c1-11(2,3)9-6-4-8(5-7-9)10(12)13/h4-7H,1-3H3,(H,12,13)	3.85	252	0.506	37.3	2	0.39	nB	nB	nB	B	
72	T	98-83-9	InChI=1S/C9H10/c1-8(2)9-6-4-3-5-7-9/h3-7H,1H2,2H3	3.48	88	0.152	0	0	1.97	nB	nB	nB	nB	
73	V	98-84-0	InChI=1S/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3	1.16	88	0.625	26.02	1	0.64	nB	nB	nB	nB	
74	V	99-09-2	InChI=1S/C6H6N2O2/c7-5-2-1-3-6(4-5)8(9)10/h1-4H,7H2	1.37	117	0.164	69.16	1	0.52	nB	nB	nB	nB	
75	V	100-02-7	InChI=1S/C6H5NO3/c8-6-3-1-5(2-4-6)7(9)10/h1-4,8H	1.91	120	0.185	63.37	0	0.76	nB	nB	nB	nB	
76	T	101-14-4	InChI=1S/C13H12Cl2N2/c14-10-6-8(1-3-12(10)16)5-9-2-4-13(17)11(15)7-9/h1-4,6-7H,5,16-17H2	3.91	552	0.749	52.04	2	2.41	nB	nB	nB	B	
77	T	101-53-1	InChI=1S/C13H12O/c14-13-8-6-12(7-9-13)10-11-4-2-1-3-5-11/h1-9,14H,10H2	3.47	329	0.477	20.23	0	1.47	nB	nB	nB	nB	
78	T	101-84-8	InChI=1S/C12H10O/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1-10H	4.21	264	0.392	9.23	0	2.64	nB	nB	B	B	
79	V	102-06-7	InChI=1S/C13H13N3/c14-13(15-11-7-3-1-4-8-11)16-12-9-5-2-6-10-12/h1-10H,(H3,14,15,16)	1.66	495	1.211	47.91	3	0.80	nB	nB	nB	nB	
80	T	102-71-6	InChI=1S/C6H15NO3/c8-4-1-7(2-5-9)3-6-10/h8-10H,1-6H2	-1	138	1.645	63.93	4	0.10	nB	nB	nB	nB	
81	V	103-44-6	InChI=1S/C10H20O/c1-4-7-8-10(5-2)9-11-6-3/h6,10H,3-5,7-9H2,1-2H3	4.36	188	0.337	9.23	1	3.09	B	nB	B	B	
82	T	103-50-4	InChI=1S/C14H14O/c1-3-7-13(8-4-1)11-15-12-14-9-5-2-6-10-14/h1-10H,11-12H2	3.31	436	0.392	9.23	1	2.52	nB	nB	nB	nB	
83	T	103-69-5	InChI=1S/C8H11N/c1-2-9-8-6-4-3-5-7-8/h3-7,9H,2H2,1H3	2.16	94	0.548	12.03	1	1.00	nB	nB	nB	nB	
84	T	103-83-3	InChI=1S/C9H13N/c1-10(2)8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3	1.98	126	0.793	3.24	1	0.95	nB	nB	nB	nB	
85	T	105-05-5	InChI=1S/C10H14/c1-3-9-5-7-10(4-2)8-6-9/h5-8H,3-4H2,1-2H3	4.58	125	0.129	0	0	2.73	nB	nB	B	B	
86	T	106-46-7	InChI=1S/C6H4Cl2/c7-5-1-2-6(8)4-3-5/h1-4H	3.44	62	0.069	0	0	2.67	nB	nB	nB	nB	
87	T	106-48-9	InChI=1S/C6H5ClO/c7-5-1-3-6(8)4-2-5/h1-4,8H	2.39	62	0.376	20.23	0	1.21	nB	nB	nB	nB	
88	T	106-93-4	InChI=1S/C2H4Br2/c3-1-2-4/h1-2H2	1.96	10	0.062	0	0	0.67	nB	nB	nB	nB	
89	T	107-39-1	InChI=1S/C8H16/c1-7(2)6-8(3,4)5/h1,6H2,2-5H3	4.55	66	0.155	0	0	2.83	nB	B	B	B	
90	V	108-67-8	InChI=1S/C9H12/c1-7-4-8(2)6-9(3)5-7/h4-6H,1-3H3	3.42	84	0.125	0	0	2.43	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
91	T	108-78-1	InChI=1S/C3H6N6/c4-1-7-2(5)9-3(6)8-1/h(H6,4,5,6,7,8,9)	-1.37	84	1.313	116.73	6	0.08	nB	nB	nB	nB	
92	V	108-86-1	InChI=1S/C6H5Br/c7-6-4-2-1-3-5-6/h1-5H	2.99	42	0.115	0	0	1.43	nB	nB	nB	nB	
93	T	108-87-2	InChI=1S/C7H14/c1-7-5-3-2-4-6-7/h7H,2-6H2,1H3	3.61	42	0.089	0	0	2.37	nB	nB	nB	B	
94	T	109-09-1	InChI=1S/C5H4ClN/c6-5-3-1-2-4-7-5/h1-4H	1.22	42	0.436	12.89	1	0.78	nB	nB	nB	nB	
95	V	109-69-3	InChI=1S/C4H9Cl/c1-2-3-4-5/h2-4H2,1H3	2.64	20	0.078	0	0	1.21	nB	nB	nB	nB	
96	T	110-02-1	InChI=1S/C4H4S/c1-2-4-5-3-1/h1-4H	1.81	15	0.158	28.24	0	0.63	nB	nB	nB	nB	
97	T	110-30-5	InChI=1S/C38H76N2O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-37(41)39-35-36-40-38(42)34-32-30-28-26-24-22-20-18-16-14-12-10-8-6-4-2/h3-36H2,1-2H3,(H,39,41)(H,40,42)	15.68	11559	1.261	58.2	4	0.32	nB	nB	nB	B	
98	V	110-85-0	InChI=1S/C4H10N2/c1-2-6-4-3-5-1/h5-6H,1-4H2	-1.5	27	1.153	24.06	2	0.23	nB	nB	nB	nB	
99	V	110-98-5	InChI=1S/C6H14O3/c1-5(7)3-9-4-6(2)8/h5-8H,3-4H2,1-2H3	-0.42	108	0.932	49.69	3	0.45	nB	nB	nB	nB	
100	V	111-40-0	InChI=1S/C4H13N3/c5-1-3-7-4-2-6/h7H,1-6H2	-2.08	56	1.574	64.07	3	0.34	nB	nB	nB	nB	
101	V	111-44-4	InChI=1S/C4H8Cl2O/c5-1-3-7-4-2-6/h1-4H2	1.29	56	0.282	9.23	1	0.24	nB	nB	nB	nB	
102	T	111-84-2	InChI=1S/C9H20/c1-3-5-7-9-8-6-4-2/h3-9H2,1-2H3	5.65	120	0.085	0	0	3.15	B	B	B	B	
103	T	111-94-4	InChI=1S/C6H9N3/c7-3-1-5-9-6-2-4-8/h9H,1-2,5-6H2	-1.34	120	1.152	59.61	3	-0.27	nB	nB	nB	nB	
104	V	112-41-4	InChI=1S/C12H24/c1-3-5-7-9-11-12-10-8-6-4-2/h3H,1,4-12H2,2H3	6.78	286	0.108	0	0	3.40	B	nB	B	B	
105	T	115-28-6	InChI=1S/C9H4Cl6O4/c10-3-4(11)8(13)2(6(18)19)1(5(16)17)7(3,12)9(8,14)15/h1-2H,(H,16,17)(H,18,19)	2.05	540	0.908	74.6	4	-0.17	nB	nB	nB	nB	
106	T	115-32-2	InChI=1S/C14H9Cl5O/c15-11-5-1-9(2-6-11)13(20,14(17,18)19)10-3-7-12(16)8-4-10/h1-8,20H	5.02	744	0.76	20.23	1	3.81	B	B	B	B	
107	T	115-96-8	InChI=1S/C6H12Cl3O4P/c7-1-4-11-14(10,12-5-2-8)13-6-3-9/h1-6H2	1.44	343	1.827	54.57	4	0.21	nB	nB	nB	nB	
108	T	117-81-7	InChI=1S/C24H38O4/c1-5-9-13-19(7-3)17-27-23(25)21-15-11-12-16-22(21)24(26)28-18-20(8-4)14-10-6-2/h11-12,15-16,19-20H,5-10,13-14,17-18H2,1-4H3	7.45	2388	0.843	52.6	4	1.99	nB	nB	B	B	
109	T	118-44-5	InChI=1S/C12H13N/c1-2-13-12-9-5-7-10-6-3-4-8-11(10)12/h3-9,13H,2H2,1H3	3.45	236	0.608	12.03	1	2.37	nB	nB	nB	nB	
110	T	118-74-1	InChI=1S/C6Cl6/c7-1-2(8)4(10)6(12)5(11)3(1)9	5.73	174	-0.091	0	0	4.21	B	B	B	B	
111	V	119-47-1	InChI=1S/C23H32O2/c1-14-9-16(20(24)18(11-14)22(3,4)5)13-17-10-15(2)12-19(21(17)25)23(6,7)8/h9-12,24-25H,13H2,1-8H3	6.25	1432	0.859	40.46	0	2.60	nB	nB	B	B	
112	V	119-61-9	InChI=1S/C13H10O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H	3.18	307	0.515	17.07	1	0.93	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
113	T	120-52-5	InChI=1S/C20H14N2O4/c23-19(15-7-3-1-4-8-15)25-21-17-11-13-18(14-12-17)22-26-20(24)16-9-5-2-6-10-16/h1-14H/b21-17-,22-18+	4.08	2125	1.303	77.32	2	0.43	nB	nB	nB	B	
114	T	120-54-7	InChI=1S/C12H20N2S6/c15-11(13-7-3-1-4-8-13)17-19-20-18-12(16)14-9-5-2-6-10-14/h1-10H2	2.8	1002	2.191	171.86	2	1.12	nB	nB	nB	nB	
115	T	122-14-5	InChI=1S/C9H12NO5P5/c1-7-6-8(4-5-9(7)10(11)12)15-16(17,13-2)14-3/h4-6H,1-3H3	3.3	540	1.775	112.73	2	1.82	nB	nB	nB	nB	
116	T	122-39-4	InChI=1S/C12H11N/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1-10,13H	3.5	264	1.011	12.03	1	2.30	nB	nB	nB	nB	
117	V	123-48-8	InChI=1S/C12H24/c1-10(8-11(2,3)4)9-12(5,6)7/h8H,9H2,1-7H3/b10-8-	5.22	211	0.205	0	0	3.29	B	B	B	B	
118	V	123-63-7	InChI=1S/C6H12O3/c1-4-7-5(2)9-6(3)8-4/h4-6H,1-3H3	0.67	84	1.118	27.69	3	0.09	nB	nB	nB	nB	
119	T	126-33-0	InChI=1S/C4H8O2S/c5-7(6)3-1-2-4-7/h1-4H2	-0.77	39	0.739	42.52	2	0.38	nB	nB	nB	nB	
120	V	126-72-7	InChI=1S/C9H15Br6O4P/c10-1-7(13)4-17-20(16,18-5-8(14)2-11)19-6-9(15)3-12/h7-9H,1-6H2	4.29	910	1.833	54.57	4	0.38	nB	nB	nB	nB	
121	V	126-73-8	InChI=1S/C12H27O4P/c1-4-7-10-14-17(13,15-11-8-5-2)16-12-9-6-3/h4-12H2,1-3H3	4	616	1.848	54.57	4	1.28	nB	nB	nB	nB	
122	T	127-18-4	InChI=1S/C2Cl4/c3-1(4)2(5)6	3.4	29	0.071	0	0	1.84	nB	nB	nB	nB	
123	T	128-37-0	InChI=1S/C15H24O/c1-10-8-11(14(2,3)4)13(16)12(9-10)15(5,6)7/h8-9,16H,1-7H3	5.1	392	0.523	20.23	0	3.20	B	B	B	B	
124	V	129-43-1	InChI=1S/C14H8O3/c15-11-7-3-6-10-12(11)14(17)9-5-2-1-4-8(9)13(10)16/h1-7,15H	3.52	442	0.736	54.37	2	2.37	nB	nB	nB	nB	
125	V	132-65-0	InChI=1S/C12H8S/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8H	4.38	219	0.278	28.24	0	3.16	B	nB	B	B	
126	V	137-26-8	InChI=1S/C6H12N2S4/c1-7(2)5(9)11-12-6(10)8(3)4/h1-4H3	1.73	226	1.883	121.26	2	0.60	nB	nB	nB	nB	
127	T	198-55-0	InChI=1S/C20H12/c1-5-13-6-2-11-17-18-12-4-8-14-7-3-10-16(20(14)18)15(9-1)19(13)17/h1-12H	6.44	654	0.355	0	0	2.38	nB	B	B	B	
128	T	206-44-0	InChI=1S/C16H10/c1-2-8-13-12(7-1)14-9-3-5-11-6-4-10-15(13)16(11)14/h1-10H	5.16	364	0.295	0	0	3.44	B	B	B	B	
129	T	2497-07-6	InChI=1S/C8H19O3PS3/c1-4-10-12(13,11-5-2)14-7-8-15(9)6-3/h4-8H2,1-3H3	1.73	424	2.718	121.94	3	0.00	nB	nB	nB	nB	
130	V	298-04-4	InChI=1S/C8H19O2PS3/c1-4-9-11(12,10-5-2)14-8-7-13-6-3/h4-8H2,1-3H3	4.02	356	2.104	110.96	2	2.63	nB	nB	B	B	
131	T	226-36-8	InChI=1S/C21H13N/c1-3-7-17-14(5-1)11-12-20-19(17)13-16-10-9-15-6-2-4-8-18(15)21(16)22-20/h1-13H	5.73	971	1.12	12.03	1	2.03	nB	B	B	B	
132	V	2597-03-7	InChI=1S/C12H17O4PS2/c1-4-16-12(13)11(10-8-6-5-7-9-10)19-17(18,14-2)15-3/h5-9,11H,4H2,1-3H3	3.69	694	2.341	111.96	4	1.93	nB	nB	nB	nB	
133	V	294-62-2	InChI=1S/C12H24/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-12H2	4.1	216	0.071	0	0	3.98	B	B	B	B	
134	T	306-52-5	InChI=1S/C2H4Cl3O4P/c3-2(4,5)1-9-10(6,7)8/h1H2,(H2,6,7,8)	0.3	127	2.014	76.57	4	0.08	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
135	T	311-89-7	InChI=1S/C12F27N/c13-1(14,7(25,26)27)4(19,20)10(34,35)40(11(36,37)5(21,22)2(15,16)8(28,29)30)12(38,39)6(23,24)3(17,18)9(31,32)33	9.93	4131	0.484	3.24	1	1.30	nB	nB	nB	B	
136	V	330-54-1	InChI=1S/C9H10Cl2N2O/c1-13(2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H,1-2H3,(H,12,14)	2.68	321	0.82	32.34	3	0.74	nB	nB	nB	nB	
137	V	333-41-5	InChI=1S/C12H21N2O3PS/c1-6-15-18(19,16-7-2)17-11-8-10(5)13-12(14-11)9(3)4/h8-9H,6-7H2,1-5H3	3.81	720	2.559	95.37	4	1.78	nB	nB	nB	nB	
138	T	335-67-1	InChI=1S/C8HF15O2/c9-2(10,1(24)25)3(11,12)4(13,14)5(15,16)6(17,18)7(19,20)8(21,22)23/h(H,24,25)	4.93	1248	0.333	37.3	2	3.12	B	nB	B	B	
139	T	346-10-1	InChI=1S/C30H37F7N2O4/c1-8-22(43-23-14-11-17(26(4,5)9-2)15-19(23)27(6,7)10-3)24(41)38-18-12-13-20(21(40)16-18)39-25(42)28(31,32)29(33,34)30(35,36)37/h11-16,22,40H,8-10H2,1-7H3,(H,38,41)(H,39,42)	9.43	7362	1.442	87.66	4	0.49	nB	nB	nB	B	
140	V	355-46-4	InChI=1S/C6HF13O3S/c7-1(8,3(11,12)5(15,16)17)2(9,10)4(13,14)6(18,19)23(20,21)22/h(H,20,21,22)	3.68	988	0.972	62.75	3	3.60	B	nB	nB	B	
141	T	475-03-6	InChI=1S/C13H18/c1-10-6-7-12-11(9-10)5-4-8-13(12,2)3/h6-7,9H,4-5,8H2,1-3H3	4.54	220	0.162	0	0	3.33	B	B	B	B	
142	T	482-89-3	InChI=1S/C16H10N2O2/c19-15-9-5-1-3-7-11(9)17-13(15)14-16(20)10-6-2-4-8-12(10)18-14/h1-8,17-18H/b14-13-	3.72	752	1.567	58.2	4	0.46	nB	nB	nB	nB	
143	V	488-23-3	InChI=1S/C10H14/c1-7-5-6-8(2)10(4)9(7)3/h5-6H,1-4H3	4	109	0.121	0	0	2.82	nB	B	B	B	
144	T	493-02-7	InChI=1S/C10H18/c1-2-6-10-8-4-3-7-9(10)5-1/h9-10H,1-8H2	4.62	109	0.093	0	0	3.52	B	B	B	B	
145	V	504-03-0	InChI=1S/C7H15N/c1-6-4-3-5-7(2)8-6/h6-8H,3-5H2,1-2H3	1.53	61	0.648	12.03	1	0.20	nB	nB	nB	nB	
146	V	504-29-0	InChI=1S/C5H6N2/c6-5-3-1-2-4-7-5/h1-4H,(H2,6,7)	0.49	42	0.669	38.91	2	1.02	nB	nB	nB	nB	
147	V	510-15-6	InChI=1S/C16H14Cl2O3/c1-2-21-15(19)16(20,11-3-7-13(17)8-4-11)12-5-9-14(18)10-6-12/h3-10,20H,2H2,1H3	4.74	876	1.043	46.53	3	2.76	nB	B	B	B	
148	T	512-56-1	InChI=1S/C3H9O4P/c1-5-8(4,6-2)7-3/h1-3H3	-0.65	64	1.848	54.57	4	-0.16	nB	nB	nB	nB	
149	V	526-78-3	InChI=1S/C4H4Br2O4/c5-1(3(7)8)2(6)4(9)10/h1-2H,(H,7,8)(H,9,10)	1	121	0.75	74.6	4	0.43	nB	nB	nB	nB	
150	V	534-52-1	InChI=1S/C7H6N2O5/c1-4-2-5(8(11)12)3-6(7(4)10)9(13)14/h2-3,10H,1H3	2.13	286	-0.151	106.51	0	0.67	nB	nB	nB	nB	
151	V	569-64-2	InChI=1S/C23H25N2/c1-24(2)21-14-10-19(11-15-21)23(18-8-6-5-7-9-18)20-12-16-22(17-13-20)25(3)4/h5-17H,1-4H3/q+1	-0.18	1512	0.563	6.25	1	1.85	nB	nB	nB	nB	
152	T	575-41-7	InChI=1S/C12H12/c1-9-7-10(2)12-6-4-3-5-11(12)8-9/h3-8H,1-2H3	4.42	179	0.189	0	0	3.37	B	nB	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
153	V	591-35-5	InChI=1S/C6H4Cl2O/c7-4-1-5(8)3-6(9)2-4/h1-3,9H	3.62	84	0.306	20.23	0	1.83	nB	nB	nB	B	
154	T	610-39-9	InChI=1S/C7H6N2O4/c1-5-2-3-6(8(10)11)7(4-5)9(12)13/h2-4H,1H3	2.08	234	-0.24	86.28	0	-0.07	nB	nB	nB	nB	
155	V	611-21-2	InChI=1S/C8H11N/c1-7-5-3-4-6-8(7)9-2/h3-6,9H,1-2H3	2.16	86	0.544	12.03	1	0.84	nB	nB	nB	nB	
156	V	612-22-6	InChI=1S/C8H9NO2/c1-2-7-5-3-4-6-8(7)9(10)11/h3-6H,2H2,1H3	2.58	150	-0.069	43.14	0	1.16	nB	nB	nB	nB	
157	T	622-57-1	InChI=1S/C9H13N/c1-3-10-9-6-4-8(2)5-7-9/h4-7,10H,3H2,1-2H3	2.52	127	0.544	12.03	1	0.47	nB	nB	nB	nB	
158	T	626-39-1	InChI=1S/C6H3Br3/c7-4-1-5(8)3-6(9)2-4/h1-3H	4.51	84	-0.034	0	0	3.54	B	B	B	B	
159	T	636-28-2	InChI=1S/C6H2Br4/c7-3-1-4(8)6(10)2-5(3)9/h1-2H	5.13	111	-0.051	0	0	3.80	B	B	B	B	
160	#N/A	639-58-7	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.14	B	#N/A	#N/A	#N/A	Tin containing compound
161	T	680-31-9	InChI=1S/C6H18N3OP/c1-7(2)11(10,8(3)4)9(5)6/h1-6H3	0.28	142	-0.374	36.6	4	-0.80	nB	nB	nB	nB	
162	T	696-44-6	InChI=1S/C8H11N/c1-7-4-3-5-8(6-7)9-2/h3-6,9H,1-2H3	2.19	88	0.544	12.03	1	0.85	nB	nB	nB	nB	
163	T	732-26-3	InChI=1S/C18H30O/c1-16(2,3)12-10-13(17(4,5)6)15(19)14(11-12)18(7,8)9/h10-11,19H,1-9H3	6.06	620	0.574	20.23	0	4.18	B	B	B	B	
164	T	764-13-6	InChI=1S/C8H14/c1-7(2)5-6-8(3)4/h5-6H,1-4H3	3.56	74	0.121	0	0	2.49	nB	nB	nB	nB	
165	T	779-02-2	InChI=1S/C15H12/c1-11-14-8-4-2-6-12(14)10-13-7-3-5-9-15(11)13/h2-10H,1H3	5.07	326	0.253	0	0	2.72	nB	B	B	B	
166	T	782-74-1	InChI=1S/C12H10Cl2N2/c13-9-5-1-3-7-11(9)15-16-12-8-4-2-6-10(12)14/h1-8,15-16H	5.04	472	1.051	24.06	2	3.70	B	B	B	B	
167	T	829-26-5	InChI=1S/C13H14/c1-9-4-5-12-7-10(2)11(3)8-13(12)6-9/h4-8H,1-3H3	4.73	230	0.185	0	0	3.00	B	B	B	B	
168	V	839-90-7	InChI=1S/C9H15N3O6/c13-4-1-10-7(16)11(2-5-14)9(18)12(3-6-15)8(10)17/h13-15H,1-6H2	-2.68	573	1.895	121.62	9	-0.30	nB	nB	nB	nB	
169	T	873-63-2	InChI=1S/C7H7ClO/c8-7-3-1-2-6(4-7)5-9/h1-4,9H,5H2	1.94	88	0.553	20.23	1	1.34	nB	nB	nB	nB	
170	T	883-20-5	InChI=1S/C15H12/c1-11-10-12-6-2-3-8-14(12)15-9-5-4-7-13(11)15/h2-10H,1H3	5.08	322	0.253	0	0	2.56	nB	B	B	B	
171	T	920-66-1	InChI=1S/C3H2F6O/c4-2(5,6)1(10)3(7,8)9/h1,10H	1.66	111	0.227	20.23	1	0.24	nB	nB	nB	nB	
172	T	944-61-6	InChI=1S/C8H6Cl4O2/c1-13-7-5(11)3(9)4(10)6(12)8(7)14-2/h1-2H3	4.86	271	0.129	18.46	0	4.40	B	B	B	B	
173	V	947-04-6	InChI=1S/C12H23NO/c14-12-10-8-6-4-2-1-3-5-7-9-11-13-12/h1-11H2,(H,13,14)	2.92	328	0.715	29.1	2	0.16	nB	nB	nB	nB	
174	T	1014-70-6	InChI=1S/C8H15N5S/c1-4-9-6-11-7(10-5-2)13-8(12-6)14-3/h4-5H2,1-3H3,(H2,9,10,11,12,13)	2.54	318	1.591	88.03	5	0.31	nB	nB	nB	nB	
175	#N/A	1067-97-6	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.92	B	#N/A	#N/A	#N/A	Tin containing compound
176	T	1241-94-7	InChI=1S/C20H27O4P/c1-3-5-12-18(4-2)17-22-25(21,23-19-13-8-6-9-14-19)24-20-15-10-7-11-16-20/h6-11,13-16,18H,3-5,12,17H2,1-2H3	5.73	1596	1.962	54.57	2	2.69	nB	nB	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
177	#N/A	1461-22-9	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.30	B	#N/A	#N/A	#N/A	Tin containing compound
178	T	1502-22-3	InChI=1S/C12H18O/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h6,11H,1-5,7-9H2	3.17	240	0.427	17.07	1	0.59	nB	nB	nB	nB	
179	T	1623-19-4	InChI=1S/C9H15O4P/c1-4-7-11-14(10,12-8-5-2)13-9-6-3/h4-6H,1-3,7-9H2	1.76	343	1.917	54.57	4	-0.09	nB	nB	nB	nB	
180	T	1631-58-9	InChI=1S/C5H11NS2/c1-6(2)5-3-7-8-4-5/h5H,3-4H2,1-2H3	0.79	62	1.085	53.84	1	1.73	nB	nB	nB	nB	
181	T	1678-98-4	InChI=1S/C10H20/c1-9(2)8-10-6-4-3-5-7-10/h9-10H,3-8H2,1-2H3	5.35	126	0.107	0	0	3.30	B	B	B	B	
182	T	1746-01-6	InChI=1S/C12H4Cl4O2/c13-5-1-9-10(2-6(5)14)18-12-4-8(16)7(15)3-11(12)17-9/h1-4H	6.8	571	0.145	18.46	0	4.58	B	B	B	B	
183	V	1805-32-9	InChI=1S/C7H6Cl2O/c8-6-2-1-5(4-10)3-7(6)9/h1-3,10H,4H2	2.74	117	0.573	20.23	1	0.47	nB	nB	nB	nB	
184	V	1806-26-4	InChI=1S/C14H22O/c1-2-3-4-5-6-7-8-13-9-11-14(15)12-10-13/h9-12,15H,2-8H2,1H3	5.22	482	0.429	20.23	0	2.28	nB	B	B	B	
185	V	1825-31-6	InChI=1S/C10H6Cl2/c11-9-5-6-10(12)8-4-2-1-3-7(8)9/h1-6H	4.8	176	0.129	0	0	3.75	B	B	B	B	
186	T	1843-05-6	InChI=1S/C21H26O3/c1-2-3-4-5-6-10-15-24-18-13-14-19(20(22)16-18)21(23)17-11-8-7-9-12-17/h7-9,11-14,16,22H,2-6,10,15H2,1H3	7.21	1697	0.596	46.53	1	2.12	nB	nB	B	B	
187	T	1897-45-6	InChI=1S/C8Cl4N2/c9-5-3(1-13)6(10)8(12)7(11)4(5)2-14	3.05	272	0.244	47.58	2	1.33	nB	nB	nB	nB	
188	T	2216-51-5	InChI=1S/C10H20O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-11H,4-6H2,1-3H3/t8-,9+,10-/m1/s1	3.4	150	0.443	20.23	1	0.89	nB	nB	nB	nB	
189	T	2371-42-8	InChI=1S/C11H20O/c1-9(2)8-5-6-10(9,3)11(4,12)7-8/h8,12H,5-7H2,1-4H3	2.69	154	0.528	20.23	1	1.48	nB	nB	nB	nB	
190	V	2465-27-2	InChI=1S/C17H21N3/c1-19(2)15-9-5-13(6-10-15)17(18)14-7-11-16(12-8-14)20(3)4/h5-12,18H,1-4H3	3.96	899	1.029	30.33	3	1.04	nB	nB	nB	B	
191	T	2498-66-0	InChI=1S/C18H10O2/c19-17-13-7-3-4-8-14(13)18(20)16-12-6-2-1-5-11(12)9-10-15(16)17/h1-10H	4.4	696	0.887	34.14	2	1.57	nB	nB	nB	B	
192	T	2631-40-5	InChI=1S/C11H15NO2/c1-8(2)9-6-4-5-7-10(9)14-11(13)12-3/h4-8H,1-3H3,(H,12,13)	2.31	308	0.488	38.33	2	0.68	nB	nB	nB	nB	
193	T	2668-47-5	InChI=1S/C20H26O/c1-19(2,3)16-12-15(14-10-8-7-9-11-14)13-17(18(16)21)20(4,5)6/h7-13,21H,1-6H3	6.36	844	0.609	20.23	0	3.98	B	nB	B	B	
194	V	2764-72-9	InChI=1S/C12H12N2/c1-3-7-13-9-10-14-8-4-2-6-12(14)11(13)5-1/h1-8H,9-10H2/q+2	1.38	271	0.892	7.76	0	0.38	nB	nB	nB	nB	
195	T	2885-00-9	InChI=1S/C18H38S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h19H,2-18H2,1H3	9.17	1140	0.078	38.8	0	-0.04	nB	nB	nB	B	
196	T	3074-71-3	InChI=1S/C9H20/c1-5-6-7-9(4)8(2)3/h8-9H,5-7H2,1-4H3	4.51	102	0.121	0	0	3.32	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
197	T	3089-11-0	InChI=1S/C15H30N6O6/c1-22-7-19(8-23)13-16-14(20(9-24-3)10-25-4)18-15(17-13)21(11-26-5)12-27-6/h7-12H2,1-6H3	1.04	1818	2.759	103.77	12	0.09	nB	nB	nB	nB	
198	T	3296-90-0	InChI=1S/C5H10Br2O2/c6-1-5(2-7,3-8)4-9/h8-9H,1-4H2	1.06	88	0.7	40.46	2	0.17	nB	nB	nB	nB	
199	T	3319-31-1	InChI=1S/C33H54O6/c1-7-13-16-25(10-4)22-37-31(34)28-19-20-29(32(35)38-23-26(11-5)17-14-8-2)30(21-28)33(36)39-24-27(12-6)18-15-9-3/h19-21,25-27H,7-18,22-24H2,1-6H3	10.43	5730	1.196	78.9	6	0.02	nB	nB	nB	B	
200	T	3380-34-5	InChI=1S/C12H7Cl3O2/c13-7-1-3-11(9(15)5-7)17-12-4-2-8(14)6-10(12)16/h1-6,16H	4.76	536	0.26	29.46	0	1.67	nB	B	B	B	
201	V	3389-71-7	InChI=1S/C7H2Cl6/c8-3-4(9)6(11)2-1-5(3,10)7(6,12)13/h1-2H	3.77	189	0.242	0	0	3.81	B	nB	B	B	
202	T	3520-72-7	InChI=1S/C32H24Cl2N8O2/c1-19-29(31(43)41(39-19)23-9-5-3-6-10-23)37-35-27-15-13-21(17-25(27)33)22-14-16-28(26(34)18-22)36-38-30-20(2)40-42(32(30)44)24-11-7-4-8-12-24/h3-18,29-30H,1-2H3/b37-35+,38-36+	7.59	8694	2.181	114.78	10	0.60	nB	nB	B	B	
203	T	3761-41-9	InChI=1S/C10H15O4PS2/c1-8-7-9(5-6-10(8)17(4)11)14-15(16,12-2)13-3/h5-7H,1-4H3	2.7	540	2.755	105.87	3	0.14	nB	nB	nB	nB	
204	V	3766-81-2	InChI=1S/C12H17NO2/c1-4-9(2)10-7-5-6-8-11(10)15-12(14)13-3/h5-9H,4H2,1-3H3,(H,13,14)	2.78	374	0.488	38.33	2	0.46	nB	nB	nB	nB	
205	V	3811-49-2	InChI=1S/C8H9O3PS/c1-9-12(13)10-6-7-4-2-3-5-8(7)11-12/h2-5H,6H2,1H3	2.67	230	2.249	69.59	2	1.39	nB	nB	nB	nB	
206	T	4162-45-2	InChI=1S/C19H20Br4O4/c1-19(2,11-7-13(20)17(14(21)8-11)26-5-3-24)12-9-15(22)18(16(23)10-12)27-6-4-25/h7-10,24-25H,3-6H2,1-2H3	6.06	1928	1.212	58.92	2	2.26	nB	nB	B	B	
207	T	4175-54-6	InChI=1S/C12H16/c1-9-7-8-10(2)12-6-4-3-5-11(9)12/h3-6,9-10H,7-8H2,1-2H3	3.96	176	0.151	0	0	3.12	B	B	B	B	
208	T	4390-04-9	InChI=1S/C16H34/c1-13(10-14(2,3)4)11-16(8,9)12-15(5,6)7/h13H,10-12H2,1-9H3	7.29	468	0.256	0	0	1.87	nB	B	B	B	
209	V	4821-19-6	InChI=1S/C18H26O/c19-18-16(14-8-3-1-4-9-14)12-7-13-17(18)15-10-5-2-6-11-15/h7,12-15,19H,1-6,8-11H2	6.64	690	0.433	20.23	0	3.12	B	nB	B	B	
210	T	4883-72-1	InChI=1S/C6H12N2O2/c9-7-8(10)6-4-2-1-3-5-6/h6,10H,1-5H2	0.94	121	0.923	52.9	0	0.29	nB	nB	nB	nB	
211	V	4904-61-4	InChI=1S/C12H18/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-2,7-10H,3-6,11-12H2/b2-1-,9-7-,10-8-	5.5	216	0.137	0	0	3.90	B	B	B	B	
212	V	5428-54-6	InChI=1S/C7H7NO3/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4,9H,1H3	2.47	152	0.192	63.37	0	0.89	nB	nB	nB	nB	
213	T	5586-15-2	InChI=1S/C20H14S2/c1-3-7-17-13-19(11-9-15(17)5-1)21-22-20-12-10-16-6-2-4-8-18(16)14-20/h1-14H	6.53	1179	0.637	50.6	0	0.39	nB	B	B	B	
214	T	5707-44-8	InChI=1S/C14H14/c1-2-12-8-10-14(11-9-12)13-6-4-3-5-7-13/h3-11H,2H2,1H3	4.72	319	0.215	0	0	2.82	nB	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
215	V	6358-85-6	InChI=1S/C32H26Cl2N6O4/c1-19(41)29(31(43)35-23-9-5-3-6-10-23)39-37-27-15-13-21(17-25(27)33)22-14-16-28(26(34)18-22)38-40-30(20(2)42)32(44)36-24-11-7-4-8-12-24/h3-18,29-30H,1-2H3,(H,35,43)(H,36,44)/b39-37+,40-38+	8.06	8768	2.375	141.78	10	0.62	nB	nB	B	B	
216	V	6459-94-5	InChI=1S/C37H30N4O10S3/c1-22-4-13-30(14-5-22)54(49,50)51-29-11-9-28(10-12-29)38-39-32-15-6-25(18-23(32)2)26-7-16-33(24(3)19-26)40-41-37-34(42)17-8-27-20-31(52(43,44)45)21-35(36(27)37)53(46,47)48/h4-21,42H,1-3H3,(H,43,44,45)(H,46,47,48)/b39-38+,41-40+	7.68	15558	3.527	246.92	12	1.85	nB	nB	nB	B	Salt - converted into acidic form
217	T	6731-36-8	InChI=1S/C17H34O4/c1-13-10-16(8,9)12-17(11-13,20-18-14(2,3)4)21-19-15(5,6)7/h13H,10-12H2,1-9H3	6.53	894	1.137	36.92	4	4.02	B	nB	B	B	
218	V	7012-37-5	InChI=1S/C12H7Cl3/c13-9-3-1-8(2-4-9)11-6-5-10(14)7-12(11)15/h1-7H	5.62	368	0.151	0	0	4.33	B	B	B	B	
219	T	7267-11-0	InChI=1S/C12H6Cl2O4/c13-7-3-1-5(11(15)16)9-6(12(17)18)2-4-8(14)10(7)9/h1-4H,(H,15,16)(H,17,18)	3.48	525	0.784	74.6	4	-0.20	nB	nB	nB	nB	
220	T	10113-28-7	InChI=1S/C8H11O4P/c1-10-13(9,11-2)12-8-6-4-3-5-7-8/h3-7H,1-2H3	1.22	254	1.896	54.57	3	2.76	nB	nB	nB	nB	
221	T	10315-98-7	InChI=1S/C8H17NO/c1-8(2)7-9-3-5-10-6-4-9/h8H,3-7H2,1-2H3	1.17	126	1.08	12.47	2	0.21	nB	nB	nB	nB	
222	V	10319-14-9	InChI=1S/C18H10BrNO3/c19-14-11-7-3-4-8-12(11)20-15(18(14)23)13-16(21)9-5-1-2-6-10(9)17(13)22/h1-8,13,23H	5.69	1065	1.524	67.26	3	0.97	nB	nB	B	B	
223	T	10496-18-1	InChI=1S/C20H42S2/c1-3-5-7-9-11-13-15-17-19-21-22-20-18-16-14-12-10-8-6-4-2/h3-20H2,1-2H3	9.91	1771	0.421	50.6	0	1.15	nB	nB	nB	B	
224	T	10541-83-0	InChI=1S/C8H9NO2/c1-9-7-4-2-6(3-5-7)8(10)11/h2-5,9H,1H3,(H,10,11)	2.15	162	0.87	49.33	3	-0.25	nB	nB	nB	nB	
225	T	13029-08-8	InChI=1S/C12H8Cl2/c13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14/h1-8H	4.97	287	0.174	0	0	3.53	B	B	B	B	
226	T	13286-32-3	InChI=1S/C11H17O3PS/c1-3-13-15(12,14-4-2)16-10-11-8-6-5-7-9-11/h5-9H,3-4,10H2,1-2H3	3.21	483	2.247	70.64	3	1.51	nB	nB	nB	nB	
227	V	13464-24-9	InChI=1S/C18H20O2/c1-13(14-4-8-16(19)9-5-14)12-18(2,3)15-6-10-17(20)11-7-15/h4-11,19-20H,1,12H2,2-3H3	5.34	860	0.843	40.46	0	1.59	nB	nB	B	B	
228	T	13654-09-6	InChI=1S/C12Br10/c13-3-1(4(14)8(18)11(21)7(3)17)2-5(15)9(19)12(22)10(20)6(2)16	10.46	907	-0.309	0	0	0.67	nB	nB	nB	B	
229	T	14800-24-9	InChI=1S/C10H16N/c1-11(2,3)9-10-7-5-4-6-8-10/h4-8H,9H2,1-3H3/q+1	-2.97	160	0.147	0	0	0.18	nB	nB	nB	nB	
230	V	14816-18-3	InChI=1S/C12H15N2O3PS/c1-3-15-18(19,16-4-2)17-14-12(10-13)11-8-6-5-7-9-11/h5-9H,3-4H2,1-2H3/b14-12+	4.39	760	2.497	105.74	3	2.87	nB	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
231	T	15258-73-8	InChI=1S/C7H6Cl2O/c8-6-2-1-3-7(9)5(6)4-10/h1-3,10H,4H2	2.02	112	0.507	20.23	1	0.39	nB	nB	nB	nB	
232	V	17302-11-3	InChI=1S/C11H24/c1-4-7-8-9-10-11(5-2)6-3/h11H,4-10H2,1-3H3	5.88	196	0.103	0	0	3.32	B	B	B	B	
233	T	19666-30-9	InChI=1S/C15H18Cl2N2O3/c1-8(2)21-12-7-11(9(16)6-10(12)17)19-14(20)22-13(18-19)15(3,4)5/h6-8H,1-5H3	4.8	1031	0.851	51.13	4	2.11	nB	B	B	B	
234	V	20020-02-4	InChI=1S/C10H4Cl4/c11-7-5-3-1-2-4-6(5)8(12)10(14)9(7)13/h1-4H	5.75	263	0.13	0	0	3.33	B	B	B	B	
235	T	25339-17-7	InChI=1S/C10H22O/c1-10(2)8-6-4-3-5-7-9-11/h10-11H,3-9H2,1-2H3	3.79	212	0.403	20.23	1	2.51	nB	nB	B	B	
236	T	26530-20-1	InChI=1S/C11H19NOS/c1-2-3-4-5-6-7-9-12-11(13)8-10-14-12/h8,10H,2-7,9H2,1H3	2.45	390	0.371	45.61	2	2.22	nB	nB	nB	nB	
237	V	26761-40-0	InChI=1S/C28H46O4/c1-23(2)17-11-7-5-9-15-21-31-27(29)25-19-13-14-20-26(25)28(30)32-22-16-10-6-8-12-18-24(3)4/h13-14,19-20,23-24H,5-12,15-18,21-22H2,1-4H3	9.69	4140	0.843	52.6	4	0.86	nB	nB	nB	B	
238	#N/A	26967-76-0	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	1.46	nB	#N/A	#N/A	#N/A	Incompletely defined compound
239	T	27458-92-0	InChI=1S/C13H28O/c1-13(2)11-9-7-5-3-4-6-8-10-12-14/h13-14H,3-12H2,1-2H3	5.38	444	0.403	20.23	1	2.73	nB	B	B	B	
240	T	28680-44-6	InChI=1S/C7H2Cl6/c8-2-3(9)7(13)1-6(2,12)4(10)5(7)11/h1H2	3.66	196	0.145	0	0	3.81	B	nB	nB	B	
241	V	29446-15-9	InChI=1S/C12H6Cl2O2/c13-7-5-11-12(6-8(7)14)16-10-4-2-1-3-9(10)15-11/h1-6H	5.54	408	0.298	18.46	0	2.88	nB	nB	B	B	
242	V	32669-06-0	InChI=1S/C15H15ClO/c16-11-12-17-15(13-7-3-1-4-8-13)14-9-5-2-6-10-14/h1-10,15H,11-12H2	4.38	524	0.403	9.23	1	2.69	nB	nB	nB	B	
243	T	33284-54-7	InChI=1S/C12H6Cl4/c13-8-6-9(14)12(16)10(11(8)15)7-4-2-1-3-5-7/h1-6H	5.86	402	0.075	0	0	4.71	B	B	B	B	
244	T	34883-41-5	InChI=1S/C12H8Cl2/c13-11-6-10(7-12(14)8-11)9-4-2-1-3-5-9/h1-8H	5.41	298	0.162	0	0	3.11	B	B	B	B	
245	T	35693-99-3	InChI=1S/C12H6Cl4/c13-7-1-3-11(15)9(5-7)10-6-8(14)2-4-12(10)16/h1-6H	6.09	412	0.06	0	0	4.64	B	B	B	B	
246	T	36065-30-2	InChI=1S/C10H9Br5O/c1-10(15,4-11)5-16-9-7(13)2-6(12)3-8(9)14/h2-3H,4-5H2,1H3	5.74	454	0.217	9.23	0	4.36	B	B	B	B	
247	V	38444-93-8	InChI=1S/C12H6Cl4/c13-9-5-1-3-7(11(9)15)8-4-2-6-10(14)12(8)16/h1-6H	6.18	408	0.214	0	0	4.17	B	B	B	B	
248	V	40690-89-9	InChI=1S/C24H21N5O4/c25-15-4-16-28(17-18-33-24(30)19-5-2-1-3-6-19)22-11-7-20(8-12-22)26-27-21-9-13-23(14-10-21)29(31)32/h1-3,5-14H,4,16-18H2/b27-26+	4.89	4050	1.061	121.19	6	0.83	nB	B	nB	B	
249	V	41122-70-7	InChI=1S/C19H21N/c1-2-3-4-5-6-16-7-11-18(12-8-16)19-13-9-17(15-20)10-14-19/h7-14H,2-6H2,1H3	6.24	1002	0.335	23.79	1	3.65	B	B	B	B	
250	T	41464-41-9	InChI=1S/C12H6Cl4/c13-7-4-5-9(14)8(6-7)12-10(15)2-1-3-11(12)16/h1-6H	5.62	403	0.048	0	0	4.46	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
251	T	47377-16-2	InChI=1S/C20H34O3S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-15-17-20(18-16-19)24(21,22)23/h15-18H,2-14H2,1H3,(H,21,22,23)	7.84	2011	1.097	62.75	3	0.52	nB	nB	B	B	
252	T	50925-42-3	InChI=1S/C39H34N10O13S4/c1-21-15-23(9-11-31(21)48-46-25-17-29-27(35(19-25)65(57,58)59)5-3-7-33(29)63(51,52)53)41-38-43-37(40-13-14-50)44-39(45-38)42-24-10-12-32(22(2)16-24)49-47-26-18-30-28(36(20-26)66(60,61)62)6-4-8-34(30)64(54,55)56/h3-12,15-20,50H,13-14H2,1-2H3,(H,51,52,53)(H,54,55,56)(H,57,58,59)(H,60,61,62)(H3,40,41,42,43,44,45)/b48-46+,49-47+	5.13	25683	7.182	395.43	23	0.50	nB	nB	nB	B	Salt - converted into acidic form
253	V	57567-84-7	InChI=1S/C9H14O4/c1-5-2-3-6(8(10)11)7(4-5)9(12)13/h5-7H,2-4H2,1H3,(H,10,11)(H,12,13)	1.11	234	0.777	74.6	4	-0.16	nB	nB	nB	nB	
254	T	59039-21-3	InChI=1S/C12H7Cl3O/c13-8-1-4-10(5-2-8)16-12-6-3-9(14)7-11(12)15/h1-7H	5.53	467	0.263	9.23	0	3.79	B	B	B	B	
255	T	59722-76-8	InChI=1S/C20H12BrNO4/c21-10-5-7-11(8-6-10)26-15-9-14(23)16-17(18(15)22)20(25)13-4-2-1-3-12(13)19(16)24/h1-9,23H,22H2	6.07	1581	1.033	89.62	3	1.99	nB	nB	B	B	
256	V	60123-64-0	InChI=1S/C12H5Cl5O/c13-6-1-2-11(9(16)3-6)18-12-5-8(15)7(14)4-10(12)17/h1-5H	6.38	618	0.187	9.23	0	4.21	B	B	B	B	
257	T	60628-17-3	InChI=1S/C25H37O3P/c1-2-3-4-5-6-7-8-9-10-11-18-23-26-29(27-24-19-14-12-15-20-24)28-25-21-16-13-17-22-25/h12-17,19-22H,2-11,18,23H2,1H3	9.83	3082	2.004	41.28	1	1.55	nB	nB	nB	B	
258	T	66735-04-4	InChI=1S/C14H20O2/c1-10(13(15)16)9-11-5-7-12(8-6-11)14(2,3)4/h5-8,10H,9H2,1-4H3,(H,15,16)	3.92	481	0.524	37.3	2	0.24	nB	nB	nB	B	
259	V	74918-40-4	InChI=1S/C12H6Cl2O/c13-7-4-5-8-9-2-1-3-10(14)12(9)15-11(8)6-7/h1-6H	5.44	329	0.26	13.14	0	3.01	B	B	B	B	
260	T	104294-16-8	InChI=1S/C12H5Cl5O/c13-6-1-2-11(8(15)3-6)18-12-9(16)4-7(14)5-10(12)17/h1-5H	6.11	609	0.198	9.23	0	3.95	B	B	B	B	
261	T	123251-96-7	InChI=1S/C12H10Cl2N2O6S2/c13-7-1-5(3-9(11(7)15)23(17,18)19)6-2-8(14)12(16)10(4-6)24(20,21)22/h1-4H,15-16H2,(H,17,18,19)(H,20,21,22)	2.04	1250	2.707	177.54	8	-0.40	nB	nB	nB	nB	
262	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.37	B	#N/A	#N/A	#N/A	CAS N/A
263	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	0.63	nB	#N/A	#N/A	#N/A	CAS N/A
264	T	92-94-4	InChI=1S/C18H14/c1-3-7-15(8-4-1)17-11-13-18(14-12-17)16-9-5-2-6-10-16/h1-14H	6.03	657	0.301	0	0	1.77	nB	B	B	B	
265	T	2814-20-2	InChI=1S/C8H12N2O/c1-5(2)8-9-6(3)4-7(11)10-8/h4-5H,1-3H3,(H,9,10,11)	0.69	150	1.354	41.46	3	-0.04	nB	nB	nB	nB	
266	V	3846-71-7	InChI=1S/C20H25N3O/c1-19(2,3)13-11-14(20(4,5)6)18(24)17(12-13)23-21-15-9-7-8-10-16(15)22-23/h7-12,24H,1-6H3	7.29	1225	0.906	50.42	3	3.54	B	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
267	T	26087-47-8	InChI=1S/C13H21O3PS/c1-11(2)15-17(14,16-12(3)4)18-10-13-8-6-5-7-9-13/h5-9,11-12H,10H2,1-4H3	3.34	651	2.283	70.64	3	1.00	nB	nB	nB	nB	
268	T	1918-02-1	InChI=1S/C6H3Cl3N2O2/c7-1-3(10)2(8)5(9)11-4(1)6(12)13/h(H2,10,11)(H,12,13)	1.9	226	1	76.21	4	0.09	nB	nB	nB	nB	
269	T	2425-06-1	InChI=1S/C10H9Cl4NO2S/c11-9(12)10(13,14)18-15-7(16)5-3-1-2-4-6(5)8(15)17/h1-2,5-6,9H,3-4H2	3.83	567	0.413	62.68	3	1.79	nB	nB	nB	B	
270	T	2439-01-2	InChI=1S/C10H6N2OS2/c1-5-2-3-6-7(4-5)12-9-8(11-6)14-10(13)15-9/h2-4H,1H3	3.78	341	1.314	93.45	3	3.48	B	nB	nB	B	
271	T	3813-05-6	InChI=1S/C9H6ClNO3S/c10-5-2-1-3-6-8(5)11(4-7(12)13)9(14)15-6/h1-3H,4H2,(H,12,13)	1.34	339	1.056	82.91	4	1.56	nB	nB	nB	nB	
272	T	5836-10-2	InChI=1S/C17H16Cl2O3/c1-11(2)22-16(20)17(21,12-3-7-14(18)8-4-12)13-5-9-15(19)10-6-13/h3-11,21H,1-2H3	5.27	993	1.061	46.53	3	3.63	B	nB	B	B	
273	V	10004-44-1	InChI=1S/C4H5NO2/c1-3-2-4(6)5-7-3/h2H,1H3,(H,5,6)	-0.88	41	0.523	38.33	1	-0.31	nB	nB	nB	nB	
274	T	101007-06-1	InChI=1S/C26H21F6NO5/c1-24(2)18(11-12-20(34)38-23(25(27,28)29)26(30,31)32)21(24)22(35)37-19(14-33)15-7-6-10-17(13-15)36-16-8-4-3-5-9-16/h3-13,18-19,21,23H,1-2H3/b12-11-/t18-,19+,21-/m0/s1	6.75	5454	1.284	85.62	5	3.77	B	B	B	B	
275	T	101200-48-0	InChI=1S/C15H17N5O6S/c1-9-16-13(18-14(17-9)26-4)20(2)15(22)19-27(23,24)11-8-6-5-7-10(11)12(21)25-3/h5-8H,1-4H3,(H,19,22)	1.83	1884	1.505	149.06	10	-1.10	nB	nB	nB	nB	
276	V	101-21-3	InChI=1S/C10H12ClNO2/c1-7(2)14-10(13)12-9-5-3-4-8(11)6-9/h3-7H,1-2H3,(H,12,13)	3.51	335	0.32	38.33	3	2.16	nB	nB	nB	nB	
277	T	101-27-9	InChI=1S/C11H9Cl2NO2/c12-6-1-2-7-16-11(15)14-10-5-3-4-9(13)8-10/h3-5,8H,6-7H2,(H,14,15)	3.23	537	0.323	38.33	3	0.34	nB	nB	nB	nB	
278	T	10265-92-6	InChI=1S/C2H8NO2PS/c1-5-6(3,4)7-2/h1-2H3,(H2,3,4)	-0.8	44	1.313	87.43	3	1.88	nB	nB	nB	nB	
279	V	103055-07-8	InChI=1S/C17H8Cl2F8N2O3/c18-6-5-11(32-17(26,27)14(22)16(23,24)25)7(19)4-10(6)28-15(31)29-13(30)12-8(20)2-1-3-9(12)21/h1-5,14H,(H2,28,29,30,31)	5.12	3276	0.631	67.43	4	3.72	B	B	B	B	
280	V	104653-34-1	InChI=1S/C31H23BrO2S/c32-24-15-13-20(14-16-24)19-9-11-21(12-10-19)23-17-22-5-1-2-6-25(22)27(18-23)29-30(33)26-7-3-4-8-28(26)35-31(29)34/h1-16,23,27,34H,17-18H2	8.3	3758	1.105	62.6	2	4.60	B	B	B	B	
281	T	107-02-8	InChI=1S/C3H4O/c1-2-3-4/h2-3H,1H2	-0.01	10	0.446	17.07	1	2.54	nB	nB	nB	nB	
282	T	108173-90-6	InChI=1S/C18H41N7/c19-17(20)24-15-11-7-3-1-5-9-13-23-14-10-6-2-4-8-12-16-25-18(21)22/h23H,1-16H2,(H4,19,20,24)(H4,21,22,25)	1.73	2556	2.936	140.83	7	-1.40	nB	nB	nB	nB	
283	V	1085-98-9	InChI=1S/C9H11Cl2FN2O2S2/c1-13(2)18(15,16)14(17-9(10,11)12)8-6-4-3-5-7-8/h3-7H,1-2H3	3.7	564	0.489	74.3	4	2.45	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
284	T	110235-47-7	InChI=1S/C14H13N3/c1-3-7-13-10-11(2)15-14(17-13)16-12-8-5-4-6-9-12/h4-6,8-10H,1-2H3,(H,15,16,17)	3.28	554	1.469	37.81	3	2.45	nB	nB	nB	nB	
285	T	1113-02-6	InChI=1S/C5H12NO4PS/c1-6-5(7)4-12-11(8,9-2)10-3/h4H2,1-3H3,(H,6,7)	-0.74	218	2.787	99.74	5	1.88	nB	nB	nB	nB	
286	V	1114-71-2	InChI=1S/C10H21NOS/c1-4-7-8-11(6-3)10(12)13-9-5-2/h4-9H2,1-3H3	3.84	288	0.96	45.61	2	2.56	nB	nB	nB	B	
287	T	112143-82-5	InChI=1S/C13H22N4O3S/c1-7-20-9(18)8-21-11-14-10(13(2,3)4)15-17(11)12(19)16(5)6/h7-8H2,1-6H3	2.69	964	1.576	102.62	7	1.59	nB	nB	nB	nB	
288	V	112281-77-3	InChI=1S/C13H11Cl2F4N3O/c14-9-1-2-10(11(15)3-9)8(4-22-7-20-6-21-22)5-23-13(18,19)12(16)17/h1-3,6-8,12H,4-5H2	3.56	1203	0.555	39.94	4	1.55	nB	nB	nB	nB	
289	T	112-53-8	InChI=1S/C12H26O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h13H,2-12H2,1H3	5.13	364	0.385	20.23	1	3.58	B	B	B	B	
290	V	114-26-1	InChI=1S/C11H15NO3/c1-8(2)14-9-6-4-5-7-10(9)15-11(13)12-3/h4-8H,1-3H3,(H,12,13)	1.52	384	0.514	47.56	2	1.88	nB	nB	nB	nB	
291	T	114369-43-6	InChI=1S/C19H17ClN4/c20-18-8-6-16(7-9-18)10-11-19(12-21,13-24-15-22-14-23-24)17-4-2-1-3-5-17/h1-9,14-15H,10-11,13H2	3.23	1341	0.813	54.5	4	2.20	nB	nB	nB	nB	
292	V	115-29-7	InChI=1S/C9H6Cl6O3S/c10-5-6(11)8(13)4-2-18-19(16)17-1-3(4)7(5,12)9(8,14)15/h3-4H,1-2H2	3.83	552	1.686	54.74	3	3.44	B	nB	nB	B	
293	V	116-06-3	InChI=1S/C7H14N2O2S/c1-7(2,12-4)5-9-11-6(10)8-3/h5H,1-4H3,(H,8,10)/b9-5+	1.13	233	0.856	75.99	2	1.62	nB	nB	nB	nB	
294	T	116714-46-6	InChI=1S/C17H9ClF8N2O4/c18-8-6-7(4-5-11(8)31-16(22,23)14(21)32-17(24,25)26)27-15(30)28-13(29)12-9(19)2-1-3-10(12)20/h1-6,14H,(H2,27,28,29,30)	5.27	3429	0.852	76.66	5	3.32	B	B	B	B	
295	T	117428-22-5	InChI=1S/C18H16F3NO4/c1-24-11-14(17(23)25-2)13-7-4-3-6-12(13)10-26-16-9-5-8-15(22-16)18(19,20)21/h3-9,11H,10H2,1-2H3/b14-11+	3.61	1766	1.142	57.65	4	2.46	nB	nB	nB	nB	
296	V	119738-06-6	InChI=1S/C22H21ClN2O5/c1-14(22(26)28-13-18-3-2-10-27-18)29-16-5-7-17(8-6-16)30-21-12-24-20-11-15(23)4-9-19(20)25-21/h4-9,11-12,14,18H,2-3,10,13H2,1H3	4.32	3100	1.736	79.77	5	2.53	nB	nB	nB	nB	
297	T	120928-09-8	InChI=1S/C20H22N2O/c1-20(2,3)16-10-8-15(9-11-16)12-13-23-19-17-6-4-5-7-18(17)21-14-22-19/h4-11,14H,12-13H2,1-3H3	5.51	1384	1.021	35.01	2	2.70	nB	nB	B	B	
298	T	111-54-6	InChI=1S/C4H8N2S4/c7-3(8)5-1-2-6-4(9)10/h1-2H2,(H2,5,7,8)(H2,6,9,10)	1.22	151	1.295	165.84	2	0.90	nB	nB	nB	nB	
299	T	122-32-7	InChI=1S/C57H104O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-55(58)61-52-54(63-57(60)51-48-45-42-39-36-33-30-27-24-21-18-15-12-9-6-3)53-62-56(59)50-47-44-41-38-35-32-29-26-23-20-17-14-11-8-5-2/h25-30,54H,4-24,31-53H2,1-3H3/b28-25-,29-26-,30-27-	22.39	30600	1.186	78.9	6	2.54	nB	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
300	T	124495-18-7	InChI=1S/C15H8Cl2FNO/c16-9-7-12(17)15-13(8-9)19-6-5-14(15)20-11-3-1-10(18)2-4-11/h1-8H	4.66	809	0.613	22.12	1	3.70	B	nB	B	B	
301	V	126448-41-7	InChI=1S/C7H4N2OS2/c10-7(11)4-2-1-3-5-6(4)12-9-8-5/h1-3H,(H,10,11)	2.83	179	1.204	106.34	3	2.07	nB	nB	nB	nB	
302	V	126833-17-8	InChI=1S/C14H17Cl2NO2/c1-14(7-3-2-4-8-14)13(19)17-9-5-6-10(18)12(16)11(9)15/h5-6,18H,2-4,7-8H2,1H3,(H,17,19)	4.44	706	0.753	49.33	2	2.20	nB	nB	nB	B	
303	T	12771-68-5	InChI=1S/C15H16N2O2/c1-19-14-6-4-12(5-7-14)15(18,11-2-3-11)13-8-16-10-17-9-13/h4-11,18H,2-3H2,1H3	1.91	673	1.527	55.24	3	0.92	nB	nB	nB	nB	
304	T	129630-19-9	InChI=1S/C15H13Cl2F3N2O4/c1-3-24-11(23)6-25-10-4-7(9(18)5-8(10)16)13-12(17)14(22(2)21-13)26-15(19)20/h4-5,15H,3,6H2,1-2H3	4.76	1748	0.978	62.58	4	0.38	nB	B	B	B	
305	T	131341-86-1	InChI=1S/C12H6F2N2O2/c13-12(14)17-10-3-1-2-8(11(10)18-12)9-6-16-5-7(9)4-15/h1-3,5-6,16H	4.12	555	1.039	58.04	2	2.56	nB	nB	nB	B	
306	T	13171-21-6	InChI=1S/C10H19ClNO5P/c1-6-12(7-2)10(13)9(11)8(3)17-18(14,15-4)16-5/h6-7H2,1-5H3/b9-8-	1.32	636	2.562	74.88	6	1.88	nB	nB	nB	nB	
307	V	131-72-6	InChI=1S/C18H24N2O6/c1-4-6-7-8-10-13(3)15-11-14(19(22)23)12-16(20(24)25)18(15)26-17(21)9-5-2/h5,9,11-13H,4,6-8,10H2,1-3H3/b9-5+	5.99	1695	0.054	112.58	1	3.00	B	B	B	B	
308	T	131807-57-3	InChI=1S/C22H18N2O4/c1-22(16-12-14-19(15-13-16)27-18-10-6-3-7-11-18)20(25)24(21(26)28-22)23-17-8-4-2-5-9-17/h2-15,23H,1H3	4.65	2231	0.818	67.87	5	3.48	B	nB	B	B	
309	V	13181-17-4	InChI=1S/C13H7Br2N3O6/c14-9-3-7(4-10(15)13(9)19)6-16-24-12-2-1-8(17(20)21)5-11(12)18(22)23/h1-6,16H	4.16	1498	0.228	124.61	1	2.00	nB	nB	nB	B	
310	V	13194-48-4	InChI=1S/C8H19O2PS2/c1-4-7-12-11(9,10-6-3)13-8-5-2/h4-8H2,1-3H3	3.59	276	2.156	86.71	2	2.35	nB	nB	nB	B	
311	#N/A	13356-08-6	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	2.86	nB	#N/A	#N/A	#N/A	Tin containing compound
312	V	133855-98-8	InChI=1S/C17H13ClFN3O/c18-15-4-2-1-3-14(15)16-17(23-16,9-22-11-20-10-21-22)12-5-7-13(19)8-6-12/h1-8,10-11,16H,9H2/t16-,17-/m1/s1	3.44	1141	0.874	43.24	4	1.85	nB	nB	nB	nB	
313	V	134098-61-6	InChI=1S/C24H27N3O4/c1-17-21(22(27(5)26-17)30-20-9-7-6-8-10-20)15-25-29-16-18-11-13-19(14-12-18)23(28)31-24(2,3)4/h6-15H,16H2,1-5H3/b25-15+	5.01	3340	1.403	74.94	4	3.20	B	nB	B	B	
314	T	13457-18-6	InChI=1S/C14H20N3O5PS/c1-5-19-14(18)11-9-17-12(15-10(11)4)8-13(16-17)22-23(24,20-6-2)21-7-3/h8-9H,5-7H2,1-4H3	3.8	1417	3.17	126.08	7	2.56	nB	nB	nB	nB	
315	V	13684-56-5	InChI=1S/C16H16N2O4/c1-2-21-15(19)18-13-9-6-10-14(11-13)22-16(20)17-12-7-4-3-5-8-12/h3-11H,2H2,1H3,(H,17,20)(H,18,19)	3.39	1241	0.572	76.66	5	2.20	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
316	V	13684-63-4	InChI=1S/C16H16N2O4/c1-11-5-3-6-12(9-11)18-16(20)22-14-8-4-7-13(10-14)17-15(19)21-2/h3-10H,1-2H3,(H,17,19)(H,18,20)	3.59	1221	0.568	76.66	5	2.22	nB	nB	nB	nB	
317	V	137641-05-5	InChI=1S/C19H12F4N2O2/c20-13-7-9-14(10-8-13)24-18(26)16-5-2-6-17(25-16)27-15-4-1-3-12(11-15)19(21,22)23/h1-11H,(H,24,26)	4.87	2094	1.027	51.22	3	2.76	nB	B	B	B	
318	V	140-57-8	InChI=1S/C15H23ClO4S/c1-12(20-21(17)19-10-9-16)11-18-14-7-5-13(6-8-14)15(2,3)4/h5-8,12H,9-11H2,1-4H3	4.56	1158	1.606	63.97	3	3.36	B	nB	nB	B	
319	T	140923-17-7	InChI=1S/C18H28N2O3/c1-11(2)16(20-18(22)23-12(3)4)17(21)19-14(6)15-9-7-13(5)8-10-15/h7-12,14,16H,1-6H3,(H,19,21)(H,20,22)/t14?,16-/m0/s1	3.71	1314	1.13	67.43	5	1.00	nB	nB	nB	nB	
320	T	1420-07-1	InChI=1S/C10H12N2O5/c1-10(2,3)7-4-6(11(14)15)5-8(9(7)13)12(16)17/h4-5,13H,1-3H3	3.44	472	-0.1	106.51	0	2.28	nB	nB	nB	nB	
321	T	142459-58-3	InChI=1S/C14H13F4N3O2S/c1-8(2)21(10-5-3-9(15)4-6-10)11(22)7-23-13-20-19-12(24-13)14(16,17)18/h3-6,8H,7H2,1-2H3	3.2	1473	1.113	83.56	4	1.85	nB	nB	nB	nB	
322	V	143390-89-0	InChI=1S/C18H19NO4/c1-13-8-4-7-11-16(13)23-12-14-9-5-6-10-15(14)17(19-22-3)18(20)21-2/h4-11H,12H2,1-3H3/b19-17+	3.4	1234	1.141	57.12	2	2.34	nB	nB	nB	nB	
323	V	143-50-0	InChI=1S/C10Cl10O/c11-2-1(21)3(12)6(15)4(2,13)8(17)5(2,14)7(3,16)9(6,18)10(8,19)20	5.41	604	0.906	17.07	1	4.78	B	B	B	B	
324	V	148477-71-8	InChI=1S/C21H24Cl2O4/c1-4-20(2,3)19(25)26-17-16(14-9-8-13(22)12-15(14)23)18(24)27-21(17)10-6-5-7-11-21/h8-9,12H,4-7,10-11H2,1-3H3	5.94	1661	0.954	52.6	4	0.15	nB	nB	B	B	
325	V	148-79-8	InChI=1S/C10H7N3S/c1-2-4-8-7(3-1)12-10(13-8)9-5-14-6-11-9/h1-6H,(H,12,13)	2.22	293	0.849	69.81	3	1.99	nB	nB	nB	nB	
326	T	150114-71-9	InChI=1S/C6H4Cl2N2O2/c7-3-1-2(9)4(8)5(10-3)6(11)12/h1H,(H2,9,10)(H,11,12)	1.62	184	0.984	76.21	4	2.00	nB	nB	nB	nB	
327	T	150-68-5	InChI=1S/C9H11ClN2O/c1-12(2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)	1.94	268	0.835	32.34	3	1.88	nB	nB	nB	nB	
328	T	153233-91-1	InChI=1S/C21H23F2NO2/c1-5-25-18-11-13(21(2,3)4)9-10-14(18)17-12-26-20(24-17)19-15(22)7-6-8-16(19)23/h6-11,17H,5,12H2,1-4H3	5.36	1688	1.316	30.82	2	3.46	B	B	B	B	
329	T	156052-68-5	InChI=1S/C14H16Cl3NO2/c1-4-14(3,12(19)7-15)18-13(20)9-5-10(16)8(2)11(17)6-9/h5-6H,4,7H2,1-3H3,(H,18,20)	4.31	816	1.038	46.17	3	2.06	nB	nB	nB	B	
330	T	1563-66-2	InChI=1S/C12H15NO3/c1-12(2)7-8-5-4-6-9(10(8)16-12)15-11(14)13-3/h4-6H,7H2,1-3H3,(H,13,14)	2.32	425	0.649	47.56	2	1.08	nB	nB	nB	nB	
331	T	1610-18-0	InChI=1S/C10H19N5O/c1-6(2)11-8-13-9(12-7(3)4)15-10(14-8)16-5/h6-7H,1-5H3,(H2,11,12,13,14,15)	2.99	458	1.67	71.96	5	1.84	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
332	T	161050-58-4	InChI=1S/C22H28N2O3/c1-14-11-15(2)13-17(12-14)21(26)24(22(4,5)6)23-20(25)18-9-8-10-19(27-7)16(18)3/h8-13H,1-7H3,(H,23,25)	3.7	1818	0.528	58.64	4	1.04	nB	nB	nB	nB	
333	T	1646-88-4	InChI=1S/C7H14N2O4S/c1-7(2,14(4,11)12)5-9-13-6(10)8-3/h5H,1-4H3,(H,8,10)/b9-5+	-0.57	337	1.356	93.21	4	-1.16	nB	nB	nB	nB	
334	V	1698-60-8	InChI=1S/C10H8ClN3O/c11-9-8(12)6-13-14(10(9)15)7-4-2-1-3-5-7/h1-6H,12H2	1.14	352	1.317	58.69	4	1.08	nB	nB	nB	nB	
335	T	1702-17-6	InChI=1S/C6H3Cl2NO2/c7-3-1-2-4(8)9-5(3)6(10)11/h1-2H,(H,10,11)	1.06	148	0.724	50.19	3	0.00	nB	nB	nB	nB	
336	T	173584-44-6	InChI=1S/C22H17ClF3N3O7/c1-33-18(30)21-10-12-9-13(23)3-8-16(12)17(21)27-28(11-35-21)19(31)29(20(32)34-2)14-4-6-15(7-5-14)36-22(24,25)26/h3-9H,10-11H2,1-2H3/t21-/m0/s1	4.76	4014	1.461	106.97	9	2.72	nB	nB	B	B	
337	V	1746-81-2	InChI=1S/C9H11ClN2O2/c1-12(14-2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)	2.3	333	0.393	41.57	2	1.60	nB	nB	nB	nB	
338	#N/A	175217-20-6	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	1.99	nB	#N/A	#N/A	#N/A	Silicon containing compound
339	T	17606-31-4	InChI=1S/C17H21NO4S4/c1-18(2)15(13-23-25(19,20)16-9-5-3-6-10-16)14-24-26(21,22)17-11-7-4-8-12-17/h3-12,15H,13-14H2,1-2H3	3.36	1829	2.531	138.88	5	2.00	nB	nB	nB	nB	
340	T	17804-35-2	InChI=1S/C14H18N4O3/c1-3-4-9-15-13(19)18-11-8-6-5-7-10(11)16-12(18)17-14(20)21-2/h5-8H,3-4,9H2,1-2H3,(H,15,19)(H,16,17,20)	2.12	944	1.317	85.25	7	1.43	nB	nB	nB	nB	
341	#N/A	178928-70-6	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	1.27	nB	#N/A	#N/A	#N/A	Duplicate
342	V	18181-80-1	InChI=1S/C17H16Br2O3/c1-11(2)22-16(20)17(21,12-3-7-14(18)8-4-12)13-5-9-15(19)10-6-13/h3-11,21H,1-2H3	5.4	993	1.039	46.53	3	3.02	B	B	B	B	
343	V	1861-32-1	InChI=1S/C10H6Cl4O4/c1-17-9(15)3-5(11)7(13)4(10(16)18-2)8(14)6(3)12/h1-2H3	4.28	555	0.663	52.6	4	2.94	nB	nB	nB	nB	
344	T	1861-40-1	InChI=1S/C13H16F3N3O4/c1-3-5-6-17(4-2)12-10(18(20)21)7-9(13(14,15)16)8-11(12)19(22)23/h7-8H,3-6H2,1-2H3	5.29	1098	-0.04	89.52	1	3.20	B	B	B	B	
345	V	18691-97-9	InChI=1S/C10H11N3OS/c1-11-9(14)13(2)10-12-7-5-3-4-6-8(7)15-10/h3-6H,1-2H3,(H,11,14)	2.64	365	1.035	73.47	4	1.88	nB	nB	nB	nB	
346	T	189278-12-4	InChI=1S/C14H17IN2O2/c1-3-7-17-13(18)11-9-10(15)5-6-12(11)16-14(17)19-8-4-2/h5-6,9H,3-4,7-8H2,1-2H3	3.72	684	1.635	41.9	4	2.91	nB	nB	nB	nB	
347	V	1918-16-7	InChI=1S/C11H14ClNO/c1-9(2)13(11(14)8-12)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3	2.18	296	0.519	20.31	2	1.57	nB	nB	nB	nB	
348	V	1929-77-7	InChI=1S/C10H21NOS/c1-4-7-11(8-5-2)10(12)13-9-6-3/h4-9H2,1-3H3	3.84	282	0.96	45.61	2	2.56	nB	nB	nB	B	
349	T	1982-49-6	InChI=1S/C14H20N2O/c1-11-7-5-6-10-13(11)16-14(17)15-12-8-3-2-4-9-12/h2-4,8-9,11,13H,5-7,10H2,1H3,(H2,15,16,17)	3.8	572	0.795	41.13	3	1.92	nB	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
350	T	19937-59-8	InChI=1S/C10H13ClN2O2/c1-13(2)10(14)12-7-4-5-9(15-3)8(11)6-7/h4-6H,1-3H3,(H,12,14)	1.64	394	1.038	41.57	3	1.88	nB	nB	nB	nB	
351	T	2104-96-3	InChI=1S/C8H8BrCl2O3PS/c1-12-15(16,13-2)14-8-4-6(10)5(9)3-7(8)11/h3-4H,1-2H3	5.21	434	1.883	69.59	2	0.65	nB	B	B	B	
352	T	210631-68-8	InChI=1S/C16H17N3O5S/c1-9-10(15(20)11-8-17-19(2)16(11)21)4-5-13(25(3,22)23)14(9)12-6-7-24-18-12/h4-5,8,21H,6-7H2,1-3H3	1.57	1385	2.55	119.23	5	-0.52	nB	nB	nB	nB	
353	T	21087-64-9	InChI=1S/C8H14N4OS/c1-8(2,3)5-6(13)12(9)7(14-4)11-10-5/h9H2,1-4H3	1.7	284	1.599	96.35	5	1.00	nB	nB	nB	nB	
354	T	21725-46-2	InChI=1S/C9H13ClN6/c1-4-12-7-13-6(10)14-8(15-7)16-9(2,3)5-11/h4H2,1-3H3,(H2,12,13,14,15,16)	2.22	456	1.73	86.52	6	2.20	nB	nB	nB	nB	
355	V	219714-96-2	InChI=1S/C16H14F5N5O5S/c1-29-10-6-22-15(30-2)26-13(10)23-14(24-26)25-32(27,28)12-8(16(19,20)21)4-3-5-9(12)31-7-11(17)18/h3-6,11H,7H2,1-2H3,(H,24,25)	2.94	2820	2.106	125.32	7	2.00	nB	nB	nB	nB	
356	V	220899-03-6	InChI=1S/C19H21BrO5/c1-10-9-14(23-4)18(24-5)19(25-6)15(10)17(21)16-11(2)12(20)7-8-13(16)22-3/h7-9H,1-6H3	4.57	1350	0.862	53.99	1	2.72	nB	nB	nB	B	
357	T	2275-23-2	InChI=1S/C8H18NO4PS2/c1-7(8(10)9-2)15-5-6-16-14(11,12-3)13-4/h7H,5-6H2,1-4H3,(H,9,10)	0.31	532	2.973	125.04	5	1.88	nB	nB	nB	nB	
358	T	2303-16-4	InChI=1S/C10H17Cl2NOS/c1-7(2)13(8(3)4)10(14)15-6-9(12)5-11/h5,7-8H,6H2,1-4H3/b9-5-	4.49	400	1	45.61	2	2.88	nB	nB	B	B	
359	T	2310-17-0	InChI=1S/C12H15ClNO4PS2/c1-3-16-19(20,17-4-2)21-8-14-10-6-5-9(13)7-11(10)18-12(14)15/h5-7H,3-4,8H2,1-2H3	4.38	959	2.201	115.2	4	2.26	nB	nB	nB	B	
360	T	2312-35-8	InChI=1S/C19H26O4S/c1-5-14-21-24(20)23-18-9-7-6-8-17(18)22-16-12-10-15(11-13-16)19(2,3)4/h1,10-13,17-18H,6-9,14H2,2-4H3	5	1515	1.638	63.97	3	4.15	B	nB	B	B	
361	T	23135-22-0	InChI=1S/C7H13N3O3S/c1-8-7(12)13-9-5(14-4)6(11)10(2)3/h1-4H3,(H,8,12)/b9-5-	-0.47	337	1.508	96.3	4	0.30	nB	nB	nB	nB	
362	T	23184-66-9	InChI=1S/C17H26ClNO2/c1-4-7-11-21-13-19(16(20)12-18)17-14(5-2)9-8-10-15(17)6-3/h8-10H,4-7,11-13H2,1-3H3	4.5	936	0.704	29.54	3	0.38	nB	nB	B	B	
363	V	23950-58-5	InChI=1S/C12H11Cl2NO/c1-4-12(2,3)15-11(16)8-5-9(13)7-10(14)6-8/h1,5-7H,2-3H3,(H,15,16)	3.43	448	0.736	29.1	2	1.69	nB	nB	nB	nB	
364	T	15302-91-7	InChI=1S/C7H16N/c1-8(2)6-4-3-5-7-8/h3-7H2,1-2H3/q+1	-3.62	59	0.085	0	0	0.30	nB	nB	nB	nB	
365	T	25057-89-0	InChI=1S/C10H12N2O3S/c1-7(2)12-10(13)8-5-3-4-6-9(8)11-16(12,14)15/h3-7,11H,1-2H3	2.34	382	0.835	74.86	5	1.32	nB	nB	nB	nB	
366	T	25311-71-1	InChI=1S/C15H24NO4PS/c1-6-18-21(22,16-11(2)3)20-14-10-8-7-9-13(14)15(17)19-12(4)5/h7-12H,6H2,1-5H3,(H,16,22)	4.12	1066	2.187	98.69	4	2.38	nB	nB	nB	nB	
367	V	2540-82-1	InChI=1S/C6H12NO4PS2/c1-7(5-8)6(9)4-14-12(13,10-2)11-3/h5H,4H2,1-3H3	1.48	335	2.546	123.04	5	-1.16	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
368	V	24579-73-5	InChI=1S/C9H20N2O2/c1-4-8-13-9(12)10-6-5-7-11(2)3/h4-8H2,1-3H3,(H,10,12)	1.12	326	1.086	41.57	4	1.73	nB	nB	nB	nB	
369	T	2593-15-9	InChI=1S/C5H5Cl3N2OS/c1-2-11-4-9-3(10-12-4)5(6,7)8/h2H2,1H3	3.37	204	0.871	63.25	2	2.22	nB	nB	nB	nB	
370	T	26225-79-6	InChI=1S/C13H18O5S/c1-5-16-12-13(2,3)10-8-9(18-19(4,14)15)6-7-11(10)17-12/h6-8,12H,5H2,1-4H3	2.7	691	1.367	70.21	3	2.16	nB	nB	nB	nB	
371	V	2631-37-0	InChI=1S/C12H17NO2/c1-8(2)10-5-9(3)6-11(7-10)15-12(14)13-4/h5-8H,1-4H3,(H,13,14)	3.1	380	0.484	38.33	2	1.88	nB	nB	nB	nB	
372	V	26644-46-2	InChI=1S/C10H14Cl6N4O2/c11-9(12,13)7(17-5-21)19-1-2-20(4-3-19)8(18-6-22)10(14,15)16/h5-8H,1-4H2,(H,17,21)(H,18,22)	2.2	1093	2.587	64.68	6	0.00	nB	nB	nB	nB	
373	T	2686-99-9	InChI=1S/C11H15NO2/c1-7-5-10(14-11(13)12-4)6-8(2)9(7)3/h5-6H,1-4H3,(H,12,13)	2.59	312	0.462	38.33	2	1.56	nB	nB	nB	nB	
374	T	27314-13-2	InChI=1S/C12H9ClF3N3O/c1-17-9-6-18-19(11(20)10(9)13)8-4-2-3-7(5-8)12(14,15)16/h2-6,17H,1H3	2.3	797	1.26	44.7	4	1.45	nB	nB	nB	nB	
375	T	27519-02-4	InChI=1S/C23H46/c1-3-5-7-9-11-13-15-17-19-21-23-22-20-18-16-14-12-10-8-6-4-2/h17,19H,3-16,18,20-23H2,1-2H3/b19-17-	11.74	2024	0.107	0	0	1.18	nB	nB	nB	B	
376	T	28772-56-7	InChI=1S/C30H23BrO4/c31-23-16-14-20(15-17-23)19-10-12-22(13-11-19)26(32)18-25(21-6-2-1-3-7-21)28-29(33)24-8-4-5-9-27(24)35-30(28)34/h1-17,25-26,32-33H,18H2	6.06	3860	1.634	66.76	3	2.94	nB	B	B	B	
377	T	29091-05-2	InChI=1S/C11H13F3N4O4/c1-3-16(4-2)9-7(17(19)20)5-6(11(12,13)14)8(15)10(9)18(21)22/h5H,3-4,15H2,1-2H3	4.3	914	0.07	115.54	2	2.37	nB	nB	nB	B	
378	V	29232-93-7	InChI=1S/C11H20N3O3PS/c1-6-14(7-2)11-12-9(3)8-10(13-11)17-18(19,15-4)16-5/h8H,6-7H2,1-5H3	4.2	714	2.785	98.61	5	2.87	nB	nB	nB	nB	
379	T	29973-13-5	InChI=1S/C11H15NO2S/c1-3-15-8-9-6-4-5-7-10(9)14-11(13)12-2/h4-7H,3,8H2,1-2H3,(H,12,13)	2.04	396	0.638	63.63	2	1.88	nB	nB	nB	nB	
380	T	300-76-5	InChI=1S/C4H7Br2Cl2O4P/c1-10-13(9,11-2)12-3(5)4(6,7)8/h3H,1-2H3	1.38	248	1.864	54.57	4	2.78	nB	nB	nB	nB	
381	T	30560-19-1	InChI=1S/C4H10NO3PS/c1-4(6)5-9(7,8-2)10-3/h1-3H3,(H,5,6,7)	-0.85	122	1.367	90.51	4	-1.52	nB	nB	nB	nB	
382	T	31218-83-4	InChI=1S/C10H20NO4PS/c1-6-11-16(17,13-5)15-9(4)7-10(12)14-8(2)3/h7-8H,6H2,1-5H3,(H,11,17)/b9-7+	3.82	586	2.143	98.69	5	2.55	nB	nB	nB	nB	
383	T	314-40-9	InChI=1S/C9H13BrN2O2/c1-4-5(2)12-8(13)7(10)6(3)11-9(12)14/h5H,4H2,1-3H3,(H,11,14)	2.11	280	1.037	49.41	4	0.57	nB	nB	nB	nB	
384	V	32809-16-8	InChI=1S/C13H11Cl2NO2/c1-12-6-13(12,2)11(18)16(10(12)17)9-4-7(14)3-8(15)5-9/h3-5H,6H2,1-2H3	3	542	0.466	37.38	3	1.67	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
385	T	33089-61-1	InChI=1S/C19H23N3/c1-14-6-8-18(16(3)10-14)20-12-22(5)13-21-19-9-7-15(2)11-17(19)4/h6-13H,1-5H3/b20-12+,21-13+	5.5	1261	1.247	27.96	3	3.26	B	nB	B	B	
386	T	33820-53-0	InChI=1S/C15H23N3O4/c1-5-7-16(8-6-2)15-13(17(19)20)9-12(11(3)4)10-14(15)18(21)22/h9-11H,5-8H2,1-4H3	5.58	968	0.098	89.52	1	4.23	B	B	B	B	
387	T	3383-96-8	InChI=1S/C16H20O6P2S3/c1-17-23(25,18-2)21-13-5-9-15(10-6-13)27-16-11-7-14(8-12-16)22-24(26,19-3)20-4/h5-12H,1-4H3	5.96	2272	4.037	164.48	4	3.36	B	nB	nB	B	
388	V	34256-82-1	InChI=1S/C14H20ClNO2/c1-4-12-8-6-7-11(3)14(12)16(10-18-5-2)13(17)9-15/h6-8H,4-5,9-10H2,1-3H3	3.03	585	0.704	29.54	3	1.30	nB	nB	nB	nB	
389	T	35400-43-2	InChI=1S/C12H19O2PS3/c1-4-10-18-15(16,13-5-2)14-11-6-8-12(17-3)9-7-11/h6-9H,4-5,10H2,1-3H3	4.9	666	2.102	110.96	1	3.96	B	B	B	B	
390	T	35575-96-3	InChI=1S/C9H10ClN2O5PS/c1-15-18(14,16-2)19-5-12-8-7(17-9(12)13)3-6(10)4-11-8/h3-4H,5H2,1-2H3	1.05	715	2.755	113.07	6	0.19	nB	nB	nB	nB	
391	V	37893-02-0	InChI=1S/C17H10F6N4S/c18-16(19,20)25-13-14(26-17(21,22)23)28-15(24-11-7-3-1-4-8-11)27(13)12-9-5-2-6-10-12/h1-10H/b24-15-,25-13-,26-14-	6.39	1895	1.044	65.62	4	4.00	B	nB	B	B	
392	T	38260-54-7	InChI=1S/C10H17N2O4PS/c1-5-8-11-9(15-6-2)7-10(12-8)16-17(18,13-3)14-4/h7H,5-6H2,1-4H3	3.18	624	2.717	104.6	4	2.53	nB	nB	nB	nB	
393	T	3878-19-1	InChI=1S/C11H8N2O/c1-2-5-9-8(4-1)12-11(13-9)10-6-3-7-14-10/h1-7H,(H,12,13)	2.25	293	0.721	41.82	2	1.57	nB	nB	nB	nB	
394	T	39515-41-8	InChI=1S/C22H23NO3/c1-21(2)19(22(21,3)4)20(24)26-18(14-23)15-9-8-12-17(13-15)25-16-10-6-5-7-11-16/h5-13,18-19H,1-4H3	5.7	1791	1.114	59.32	3	3.04	B	nB	B	B	
395	T	39807-15-3	InChI=1S/C15H14Cl2N2O3/c1-5-6-21-12-8-11(9(16)7-10(12)17)19-14(20)22-13(18-19)15(2,3)4/h1,7-8H,6H2,2-4H3	3.95	1050	0.854	51.13	4	2.82	nB	nB	nB	nB	
396	V	40020-01-7	InChI=1S/C10H7ClN2O/c11-9-6-8(14)10(13-12-9)7-4-2-1-3-5-7/h1-6H,(H,12,14)	2.36	298	1.067	41.46	3	0.30	nB	nB	nB	nB	
397	#N/A	41083-11-8	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.88	B	#N/A	#N/A	#N/A	Tin containing compound
398	T	41198-08-7	InChI=1S/C11H15BrClO3PS/c1-3-7-18-17(14,15-4-2)16-11-6-5-9(12)8-10(11)13/h5-6,8H,3-4,7H2,1-2H3	4.68	633	2.164	70.64	2	3.07	B	B	B	B	
399	T	41394-05-2	InChI=1S/C10H10N4O/c1-7-12-13-9(10(15)14(7)11)8-5-3-2-4-6-8/h2-6H,11H2,1H3	0.83	352	1.428	71.05	5	1.88	nB	nB	nB	nB	
400	T	41814-78-2	InChI=1S/C9H7N3S/c1-6-3-2-4-7-8(6)12-5-10-11-9(12)13-7/h2-5H,1H3	1.7	213	1.712	58.43	3	0.49	nB	nB	nB	nB	
401	V	42509-80-8	InChI=1S/C9H17ClN3O3PS/c1-5-14-17(18,15-6-2)16-9-11-8(10)13(12-9)7(3)4/h7H,5-6H2,1-4H3	3.82	630	2.311	100.3	5	1.88	nB	nB	nB	nB	
402	T	42874-03-3	InChI=1S/C15H11ClF3NO4/c1-2-23-14-8-10(4-5-12(14)20(21)22)24-13-6-3-9(7-11(13)16)15(17,18)19/h3-8H,2H2,1H3	4.73	1442	0.243	61.6	0	3.21	B	nB	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
403	T	43121-43-3	InChI=1S/C14H16ClN3O2/c1-14(2,3)12(19)13(18-9-16-8-17-18)20-11-6-4-10(15)5-7-11/h4-9,13H,1-3H3	2.77	802	1.019	57.01	4	1.81	nB	nB	nB	nB	
404	#N/A	43222-48-6	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	1.30	nB	#N/A	#N/A	#N/A	Structure and CAS did not match
405	T	470-90-6	InChI=1S/C12H14Cl3O4P/c1-3-17-20(16,18-4-2)19-12(8-13)10-6-5-9(14)7-11(10)15/h5-8H,3-4H2,1-2H3/b12-8+	3.1	818	1.85	54.57	4	1.85	nB	nB	nB	nB	
406	T	4824-78-6	InChI=1S/C10H12BrCl2O3PS/c1-3-14-17(18,15-4-2)16-10-6-8(12)7(11)5-9(10)13/h5-6H,3-4H2,1-2H3	6.15	612	1.883	69.59	2	4.00	B	B	B	B	
407	T	50471-44-8	InChI=1S/C12H9Cl2NO3/c1-3-12(2)10(16)15(11(17)18-12)9-5-7(13)4-8(14)6-9/h3-6H,1H2,2H3	3.1	559	0.317	46.61	4	0.81	nB	nB	nB	nB	
408	T	51-03-6	InChI=1S/C19H30O5/c1-3-5-7-20-8-9-21-10-11-22-14-17-13-19-18(23-15-24-19)12-16(17)6-4-2/h12-13H,3-11,14-15H2,1-2H3	4.75	1767	1.217	46.15	3	3.34	B	nB	B	B	
409	V	5234-68-4	InChI=1S/C12H13NO2S/c1-9-11(16-8-7-15-9)12(14)13-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3,(H,13,14)	2.14	459	1.094	63.63	3	1.11	nB	nB	nB	nB	
410	T	52-51-7	InChI=1S/C3H6BrNO4/c4-3(1-6,2-7)5(8)9/h6-7H,1-2H2	-0.63	86	0.555	83.6	2	-0.55	nB	nB	nB	nB	
411	T	52918-63-5	InChI=1S/C22H19Br2NO3/c1-22(2)17(12-19(23)24)20(22)21(26)28-18(13-25)14-7-6-10-16(11-14)27-15-8-4-3-5-9-15/h3-12,17-18,20H,1-2H3/t17-,18+,20-/m0/s1	6.2	2244	1.063	59.32	3	3.15	B	nB	B	B	
412	V	542-75-6	InChI=1S/C3H4Cl2/c4-2-1-3-5/h1-2H,3H2/b2-1+	2.04	20	0.093	0	0	0.66	nB	nB	nB	nB	
413	T	54593-83-8	InChI=1S/C6H11Cl4O3PS/c1-3-11-14(15,12-4-2)13-5(7)6(8,9)10/h5H,3-4H2,1-2H3	4.59	376	2.017	69.59	3	3.40	B	nB	B	B	
414	T	55179-31-2	InChI=1S/C20H23N3O2/c1-20(2,3)18(24)19(23-14-21-13-22-23)25-17-11-9-16(10-12-17)15-7-5-4-6-8-15/h4-14,18-19,24H,1-3H3	4.16	1585	1.142	60.17	4	2.31	nB	nB	nB	nB	
415	V	55283-68-6	InChI=1S/C13H14F3N3O4/c1-4-17(7-8(2)3)12-10(18(20)21)5-9(13(14,15)16)6-11(12)19(22)23/h5-6H,2,4,7H2,1,3H3	5.11	1078	-0.021	89.52	1	3.12	B	B	B	B	
416	T	55335-06-3	InChI=1S/C7H4Cl3NO3/c8-3-1-4(9)7(11-6(3)10)14-2-5(12)13/h1H,2H2,(H,12,13)	2.97	318	0.928	59.42	3	-0.11	nB	nB	nB	nB	
417	T	56073-07-5	InChI=1S/C31H24O3/c32-30-26-12-6-7-13-28(26)34-31(33)29(30)27-19-24(18-23-10-4-5-11-25(23)27)22-16-14-21(15-17-22)20-8-2-1-3-9-20/h1-17,24,27,32H,18-19H2	7.81	3416	1.207	46.53	2	3.96	B	nB	B	B	
418	T	563-12-2	InChI=1S/C9H22O4P2S4/c1-5-10-14(16,11-6-2)18-9-19-15(17,12-7-3)13-8-4/h5-9H2,1-4H3	5.07	792	3.787	171.32	4	2.77	nB	B	B	B	
419	T	56425-91-3	InChI=1S/C15H15F3N2O2/c1-10(2)14(21,12-7-19-9-20-8-12)11-3-5-13(6-4-11)22-15(16,17)18/h3-10,21H,1-2H3	3.34	1064	1.421	55.24	3	1.55	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
420	V	57960-19-7	InChI=1S/C24H32O4/c1-3-4-5-6-7-8-9-10-11-12-17-21-22(26)19-15-13-14-16-20(19)23(27)24(21)28-18(2)25/h13-16H,3-12,17H2,1-2H3	7.63	2463	1.136	60.44	4	2.38	nB	nB	B	B	
421	V	58138-08-2	InChI=1S/C10H7Cl5O/c11-7-1-6(2-8(12)3-7)9(5-16-9)4-10(13,14)15/h1-3H,4-5H2	4.67	422	0.432	12.53	1	3.70	B	nB	B	B	
422	V	5836-29-3	InChI=1S/C19H16O3/c20-18-15-9-3-4-11-16(15)22-19(21)17(18)14-10-5-7-12-6-1-2-8-13(12)14/h1-4,6,8-9,11,14,20H,5,7,10H2	4.98	950	1.059	46.53	2	2.24	nB	B	B	B	
423	T	58667-63-3	InChI=1S/C16H13ClFNO3/c1-10(16(21)22)19(12-7-8-14(18)13(17)9-12)15(20)11-5-3-2-4-6-11/h2-10H,1H3,(H,21,22)	2.9	1001	0.828	57.61	4	1.85	nB	nB	nB	nB	
424	V	5902-51-2	InChI=1S/C9H13ClN2O2/c1-5-6(10)7(13)12(8(14)11-5)9(2,3)4/h1-4H3,(H,11,14)	1.89	269	1.081	49.41	4	0.78	nB	nB	nB	nB	
425	T	5915-41-3	InChI=1S/C9H16ClN5/c1-5-11-7-12-6(10)13-8(14-7)15-9(2,3)4/h5H2,1-4H3,(H2,11,12,13,14,15)	3.06	380	1.467	62.73	5	1.19	nB	nB	nB	nB	
426	T	59756-60-4	InChI=1S/C19H14F3NO/c1-23-11-16(13-6-3-2-4-7-13)18(24)17(12-23)14-8-5-9-15(10-14)19(20,21)22/h2-12H,1H3	3.16	1293	1.073	20.31	2	1.99	nB	nB	nB	nB	
427	T	60207-31-0	InChI=1S/C12H11Cl2N3O2/c13-9-1-2-10(11(14)5-9)12(18-3-4-19-12)6-17-8-15-7-16-17/h1-2,5,7-8H,3-4,6H2	2.32	660	1.104	49.17	5	1.28	nB	nB	nB	nB	
428	V	60207-90-1	InChI=1S/C15H17Cl2N3O2/c1-2-3-12-7-21-15(22-12,8-20-10-18-9-19-20)13-5-4-11(16)6-14(13)17/h4-6,9-10,12H,2-3,7-8H2,1H3	3.5	1000	1.122	49.17	5	2.06	nB	nB	nB	nB	
429	T	60-57-1	InChI=1S/C12H8Cl6O/c13-8-9(14)11(16)5-3-1-2(6-7(3)19-6)4(5)10(8,15)12(11,17)18/h2-7H,1H2	3.67	520	0.617	12.53	1	3.95	B	nB	nB	B	
430	T	63333-35-7	InChI=1S/C14H7Br3F3N3O4/c1-21(13-9(16)2-6(15)3-10(13)17)12-8(14(18,19)20)4-7(22(24)25)5-11(12)23(26)27/h2-5H,1H3	6.22	1630	-0.545	89.52	1	5.08	B	B	B	B	
431	V	63782-90-1	InChI=1S/C19H19ClFNO3/c1-12(2)25-19(24)13(3)22(15-9-10-17(21)16(20)11-15)18(23)14-7-5-4-6-8-14/h4-13H,1-3H3/t13-/m1/s1	3.69	1436	0.859	46.61	4	2.08	nB	nB	nB	nB	
432	T	64628-44-0	InChI=1S/C15H10ClF3N2O3/c16-12-4-2-1-3-11(12)13(22)21-14(23)20-9-5-7-10(8-6-9)24-15(17,18)19/h1-8H,(H2,20,21,22,23)	4.91	1584	0.75	67.43	4	2.79	nB	nB	B	B	
433	T	64902-72-3	InChI=1S/C12H12ClN5O4S/c1-7-14-10(17-12(15-7)22-2)16-11(19)18-23(20,21)9-6-4-3-5-8(9)13/h3-6H,1-2H3,(H2,14,15,16,17,18,19)	2	1268	1.277	131.55	8	1.88	nB	nB	nB	nB	
434	T	67485-29-4	InChI=1S/C25H24F6N4/c1-23(2)15-32-22(33-16-23)35-34-21(13-7-17-3-9-19(10-4-17)24(26,27)28)14-8-18-5-11-20(12-6-18)25(29,30)31/h3-14H,15-16H2,1-2H3,(H2,32,33,35)/b13-7+,14-8+	6.37	4426	1.365	48.78	4	4.54	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
435	T	67-97-0	InChI=1S/C27H44O/c1-19(2)8-6-9-21(4)25-15-16-26-22(10-7-17-27(25,26)5)12-13-23-18-24(28)14-11-20(23)3/h12-13,19,21,24-26,28H,3,6-11,14-18H2,1-2,4-5H3/b22-12+,23-13+/t21-,24+,25-,26+,27-/m1/s1	7.95	2214	0.539	20.23	1	6.00	B	nB	B	B	
436	V	68505-69-1	InChI=1S/C12H16O4S/c1-4-17(13,14)16-9-5-6-11-10(7-9)12(2,3)8-15-11/h5-7H,4,8H2,1-3H3	2.71	507	1.138	60.98	2	1.34	nB	nB	nB	nB	
437	V	69806-50-4	InChI=1S/C19H20F3NO4/c1-3-4-11-25-18(24)13(2)26-15-6-8-16(9-7-15)27-17-10-5-14(12-23-17)19(20,21)22/h5-10,12-13H,3-4,11H2,1-2H3	4.5	2356	1.096	57.65	3	2.82	nB	nB	nB	B	
438	T	709-98-8	InChI=1S/C9H9Cl2NO/c1-2-9(13)12-6-3-4-7(10)8(11)5-6/h3-5H,2H2,1H3,(H,12,13)	3.07	262	0.523	29.1	2	2.05	nB	nB	nB	nB	
439	T	71626-11-4	InChI=1S/C20H23NO3/c1-14-9-8-10-15(2)19(14)21(16(3)20(23)24-4)18(22)13-17-11-6-5-7-12-17/h5-12,16H,13H2,1-4H3	3.4	1272	0.905	46.61	4	1.76	nB	nB	nB	nB	
440	T	72178-02-0	InChI=1S/C15H10ClF3N2O6S/c1-28(25,26)20-14(22)10-7-9(3-4-12(10)21(23)24)27-13-5-2-8(6-11(13)16)15(17,18)19/h2-7H,1H3,(H,20,22)	2.9	2154	0.305	123.99	4	0.78	nB	nB	nB	nB	
441	T	72-43-5	InChI=1S/C16H15Cl3O2/c1-20-13-7-3-11(4-8-13)15(16(17,18)19)12-5-9-14(21-2)10-6-12/h3-10,15H,1-2H3	5.08	932	0.601	18.46	0	3.21	B	B	B	B	
442	V	72619-32-0	InChI=1S/C16H13ClF3NO4/c1-9(15(22)23-2)24-11-3-5-12(6-4-11)25-14-13(17)7-10(8-21-14)16(18,19)20/h3-9H,1-2H3	4.07	1770	1.116	57.65	3	1.23	nB	nB	nB	B	
443	T	7287-36-7	InChI=1S/C13H18ClNO/c1-4-9-13(2,3)12(16)15-11-7-5-10(14)6-8-11/h5-8H,4,9H2,1-3H3,(H,15,16)	3.83	473	0.589	29.1	2	3.07	B	nB	nB	B	
444	V	74051-80-2	InChI=1S/C17H29NO3S/c1-5-8-14(18-21-6-2)17-15(19)10-13(11-16(17)20)9-12(4)22-7-3/h12-13,18H,5-11H2,1-4H3/b17-14-	4.08	1139	1.168	80.7	2	1.35	nB	nB	nB	B	
445	V	74070-46-5	InChI=1S/C12H9ClN2O3/c13-11-10(18-8-4-2-1-3-5-8)7-6-9(12(11)14)15(16)17/h1-7H,14H2	4.04	626	0.316	78.39	1	3.46	B	nB	nB	B	
446	T	741-58-2	InChI=1S/C14H24NO4PS3/c1-12(2)18-20(21,19-13(3)4)22-11-10-15-23(16,17)14-8-6-5-7-9-14/h5-9,12-13,15H,10-11H2,1-4H3	4.2	1358	2.242	140.21	5	2.94	nB	nB	nB	nB	
447	V	74738-17-3	InChI=1S/C11H6Cl2N2/c12-10-3-1-2-8(11(10)13)9-6-15-5-7(9)4-14/h1-3,5-6,15H	4.04	345	0.642	39.58	2	2.54	nB	nB	nB	B	
448	T	74-83-9	InChI=1S/CH3Br/c1-2/h1H3	0.99	1	0.067	0	0	1.88	nB	nB	nB	nB	
449	T	75-08-1	InChI=1S/C2H6S/c1-2-3/h3H,2H2,1H3	0.88	4	0.078	38.8	0	2.00	nB	nB	nB	nB	
450	T	759-94-4	InChI=1S/C9H19NOS/c1-4-7-10(8-5-2)9(11)12-6-3/h4-8H2,1-3H3	3.21	220	0.96	45.61	2	1.78	nB	nB	nB	nB	
451	T	76578-14-8	InChI=1S/C19H17ClN2O4/c1-3-24-19(23)12(2)25-14-5-7-15(8-6-14)26-18-11-21-17-10-13(20)4-9-16(17)22-18/h4-12H,3H2,1-2H3	4.28	2011	1.401	70.54	4	2.76	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
452	V	76738-62-0	InChI=1S/C15H20ClN3O/c1-15(2,3)14(20)13(19-10-17-9-18-19)8-11-4-6-12(16)7-5-11/h4-7,9-10,13-14,20H,8H2,1-3H3	3.2	802	0.838	50.94	4	1.64	nB	nB	nB	nB	
453	T	77732-09-3	InChI=1S/C14H18N2O4/c1-10-5-4-6-11(2)13(10)16(12(17)9-19-3)15-7-8-20-14(15)18/h4-6H,7-9H2,1-3H3	0.8	735	0.351	59.08	6	-0.10	nB	nB	nB	nB	
454	V	78587-05-0	InChI=1S/C17H21ClN2O2S/c1-11-15(12-7-9-13(18)10-8-12)23-17(22)20(11)16(21)19-14-5-3-2-4-6-14/h7-11,14-15H,2-6H2,1H3,(H,19,21)/t11-,15+/m0/s1	4.45	1238	1.443	74.71	4	3.04	B	nB	B	B	
455	T	79-21-0	InChI=1S/C2H4O3/c1-2(3)5-4/h4H,1H3	-0.37	18	0.724	46.53	3	0.00	nB	nB	nB	nB	
456	T	79538-32-2	InChI=1S/C17H14ClF7O2/c1-6-11(19)13(21)7(14(22)12(6)20)5-27-15(26)10-8(16(10,2)3)4-9(18)17(23,24)25/h4,8,10H,5H2,1-3H3/b9-4-	6.5	1966	0.288	26.3	2	3.31	B	nB	B	B	
457	T	79-57-2	InChI=1S/C22H24N2O9/c1-21(32)7-5-4-6-8(25)9(7)15(26)10-12(21)17(28)13-14(24(2)3)16(27)11(20(23)31)19(30)22(13,33)18(10)29/h4-6,12-14,17,25-26,28,30,32-33H,1-3H3,(H2,23,31)/t12-,13-,14+,17+,21-,22+/m1/s1	-0.72	2494	4.128	201.85	10	-0.22	nB	nB	nB	nB	
458	T	79622-59-6	InChI=1S/C13H4Cl2F6N4O4/c14-6-1-4(12(16,17)18)3-22-11(6)23-9-7(24(26)27)2-5(13(19,20)21)8(15)10(9)25(28)29/h1-3H,(H,22,23)	3.56	2126	0.405	111.2	2	3.01	B	nB	nB	nB	
459	T	79983-71-4	InChI=1S/C14H17Cl2N3O/c1-2-3-6-14(20,8-19-10-17-9-18-19)12-5-4-11(15)7-13(12)16/h4-5,7,9-10,20H,2-3,6,8H2,1H3	3.9	790	0.887	50.94	4	2.62	nB	nB	nB	nB	
460	T	24602-86-6	InChI=1S/C19H39NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-20-16-18(2)21-19(3)17-20/h18-19H,4-17H2,1-3H3	6.88	1348	1.098	12.47	2	2.87	nB	nB	B	B	
461	T	82097-50-5	InChI=1S/C14H16ClN5O5S/c1-9-16-12(19-14(17-9)24-2)18-13(21)20-26(22,23)11-6-4-3-5-10(11)25-8-7-15/h3-6H,7-8H2,1-2H3,(H2,16,17,18,19,20,21)	1.1	1797	1.488	140.78	8	0.11	nB	nB	nB	nB	
462	T	82-68-8	InChI=1S/C6Cl5NO2/c7-1-2(8)4(10)6(12(13)14)5(11)3(1)9	4.64	268	-0.282	43.14	0	3.24	B	nB	B	B	
463	T	83121-18-0	InChI=1S/C14H6Cl2F4N2O2/c15-5-4-8(12(20)10(16)11(5)19)21-14(24)22-13(23)9-6(17)2-1-3-7(9)18/h1-4H,(H2,21,22,23,24)	4.56	1412	0.511	58.2	4	2.81	nB	nB	nB	B	
464	T	83130-01-2	InChI=1S/C17H25N3O4S2/c1-5-23-16(21)11-12-20(13-15-9-7-6-8-10-15)26-19(3)17(22)24-18-14(2)25-4/h6-10H,5,11-13H2,1-4H3/b18-14-	3.43	1915	0.829	122.04	5	2.22	nB	nB	nB	nB	
465	T	83164-33-4	InChI=1S/C19H11F5N2O2/c20-12-6-7-16(15(21)10-12)26-17(27)14-5-2-8-25-18(14)28-13-4-1-3-11(9-13)19(22,23)24/h1-10H,(H,26,27)	4.9	2165	1.012	51.22	3	3.11	B	nB	B	B	
466	T	834-12-8	InChI=1S/C9H17N5S/c1-5-10-7-12-8(11-6(2)3)14-9(13-7)15-4/h6H,5H2,1-4H3,(H2,10,11,12,13,14)	2.98	384	1.609	88.03	5	1.52	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
467	T	83-79-4	InChI=1S/C23H22O6/c1-11(2)16-8-14-15(28-16)6-5-12-22(24)21-13-7-18(25-3)19(26-4)9-17(13)27-10-20(21)29-23(12)14/h5-7,9,16,20-21H,1,8,10H2,2-4H3/t16-,20-,21+/m1/s1	4.1	2115	1.636	63.22	1	1.41	nB	nB	nB	B	
468	T	84087-01-4	InChI=1S/C10H5Cl2NO2/c11-6-3-5-1-2-7(12)8(10(14)15)9(5)13-4-6/h1-4H,(H,14,15)	1.04	334	0.807	50.19	3	-0.10	nB	nB	nB	nB	
469	T	84-65-1	InChI=1S/C14H8O2/c15-13-9-5-1-2-6-10(9)14(16)12-8-4-3-7-11(12)13/h1-8H	3.39	378	0.827	34.14	2	2.00	nB	nB	nB	nB	
470	#N/A	85509-19-9	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	2.40	nB	#N/A	#N/A	#N/A	Silicon containing compound
471	T	86479-06-3	InChI=1S/C16H8Cl2F6N2O3/c17-7-4-6(5-8(18)12(7)29-16(23,24)14(21)22)25-15(28)26-13(27)11-9(19)2-1-3-10(11)20/h1-5,14H,(H2,25,26,27,28)	5.68	2502	0.68	67.43	4	3.67	B	nB	B	B	
472	T	86-50-0	InChI=1S/C10H12N3O3PS2/c1-15-17(18,16-2)19-7-13-10(14)8-5-3-4-6-9(8)11-12-13/h3-6H,7H2,1-2H3	2.75	728	2.672	130.69	6	1.60	nB	nB	nB	nB	
473	T	87130-20-9	InChI=1S/C14H21NO4/c1-5-17-12-8-7-11(9-13(12)18-6-2)15-14(16)19-10(3)4/h7-10H,5-6H2,1-4H3,(H,15,16)	2.91	782	0.514	56.79	3	2.52	nB	nB	nB	nB	
474	T	90-43-7	InChI=1S/C12H10O/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9,13H	3.09	240	0.515	20.23	0	1.34	nB	nB	nB	nB	
475	V	94125-34-5	InChI=1S/C15H16F3N5O4S/c1-9-19-12(22-14(20-9)27-2)21-13(24)23-28(25,26)11-6-4-3-5-10(11)7-8-15(16,17)18/h3-6H,7-8H2,1-2H3,(H2,19,20,21,22,23,24)	3.1	2205	1.133	131.55	8	-0.89	nB	nB	nB	nB	
476	T	944-22-9	InChI=1S/C10H15OPS2/c1-3-11-12(13,4-2)14-10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3	3.94	316	1.773	76.43	1	2.48	nB	nB	B	B	
477	T	94-74-6	InChI=1S/C9H9ClO3/c1-6-4-7(10)2-3-8(6)13-5-9(11)12/h2-4H,5H2,1H3,(H,11,12)	3.25	266	0.609	46.53	2	0.00	nB	nB	nB	nB	
478	V	94-75-7	InChI=1S/C8H6Cl2O3/c9-5-1-2-7(6(10)3-5)13-4-8(11)12/h1-3H,4H2,(H,11,12)	2.81	266	0.598	46.53	2	0.25	nB	nB	nB	nB	
479	T	95465-99-9	InChI=1S/C10H23O2PS2/c1-6-9(4)14-13(11,12-8-3)15-10(5)7-2/h9-10H,6-8H2,1-5H3	3.9	386	2.192	86.71	2	2.34	nB	nB	B	B	
480	T	95737-68-1	InChI=1S/C20H19NO3/c1-16(23-20-9-5-6-14-21-20)15-22-17-10-12-19(13-11-17)24-18-7-3-2-4-8-18/h2-14,16H,15H2,1H3	4.79	1693	1.14	40.58	1	3.14	B	nB	B	B	
481	T	96525-23-4	InChI=1S/C18H14F3NO2/c1-22-17-14(12-8-5-9-13(10-12)18(19,20)21)15(23)16(24-17)11-6-3-2-4-7-11/h2-10,16,22H,1H3	3.22	1290	1.281	38.33	3	1.44	nB	nB	nB	nB	
482	V	97-17-6	InChI=1S/C10H13Cl2O3PS/c1-3-13-16(17,14-4-2)15-10-6-5-8(11)7-9(10)12/h5-7H,3-4H2,1-2H3	5.14	532	1.955	69.59	2	3.48	B	B	B	B	
483	T	99129-21-2	InChI=1S/C17H26ClNO3S/c1-4-14(19-22-8-6-7-18)17-15(20)10-13(11-16(17)21)9-12(3)23-5-2/h6-7,12-13,19H,4-5,8-11H2,1-3H3/b7-6+,17-14-	4.28	1350	1.183	80.7	2	0.32	nB	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
484	T	99387-89-0	InChI=1S/C15H15ClF3N3O/c1-2-7-23-9-14(22-6-5-20-10-22)21-13-4-3-11(16)8-12(13)15(17,18)19/h3-6,8,10H,2,7,9H2,1H3/b21-14+	1.4	1203	0.922	39.41	4	2.87	nB	nB	nB	nB	
485	T	7003-89-6	InChI=1S/C5H13ClN/c1-7(2,3)5-4-6/h4-5H2,1-3H3/q+1	-4.6	46	0.092	0	0	-2.00	nB	nB	nB	nB	
486	T	93-76-5	InChI=1S/C8H5Cl3O3/c9-4-1-6(11)7(2-5(4)10)14-3-8(12)13/h1-2H,3H2,(H,12,13)	3.31	318	0.537	46.53	2	1.38	nB	nB	nB	nB	
487	T	2539-17-5	InChI=1S/C7H4Cl4O2/c1-13-7-5(11)3(9)2(8)4(10)6(7)12/h12H,1H3	4.59	220	0.009	29.46	0	2.04	nB	B	B	B	
488	T	57057-83-7	InChI=1S/C7H5Cl3O2/c1-12-7-4(11)2-3(8)5(9)6(7)10/h2,11H,1H3	3.77	181	0.204	29.46	0	2.51	nB	nB	nB	B	
489	T	2668-24-8	InChI=1S/C7H5Cl3O2/c1-12-4-2-3(8)5(9)6(10)7(4)11/h2,11H,1H3	3.72	182	0.074	29.46	0	2.17	nB	nB	nB	B	
490	T	2460-49-3	InChI=1S/C7H6Cl2O2/c1-11-7-3-5(9)4(8)2-6(7)10/h2-3,10H,1H3	3.26	148	0.223	29.46	0	1.92	nB	nB	nB	nB	
491	V	74-11-3	InChI=1S/C7H5ClO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)	2.65	120	0.448	37.3	2	1.00	nB	nB	nB	nB	
492	V	1689-84-5	InChI=1S/C7H3Br2NO/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2,11H	3.16	148	0.276	44.02	1	0.00	nB	nB	nB	nB	
493	#N/A	113136-77-9	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	-0.40	nB	#N/A	#N/A	#N/A	Duplicate
494	T	114311-32-9	InChI=1S/C15H19N3O4/c1-8(2)15(3)14(21)17-12(18-15)11-10(13(19)20)5-9(6-16-11)7-22-4/h5-6,8H,7H2,1-4H3,(H,19,20)(H,17,18,21)	0.86	1028	2.274	100.88	7	-1.00	nB	nB	nB	nB	
495	T	178928-70-6	InChI=1S/C14H15Cl2N3OS/c15-11-4-2-1-3-10(11)7-14(20,13(16)5-6-13)8-19-12(21)17-9-18-19/h1-4,9,20H,5-8H2,(H,17,18,21)	2.74	879	1.715	79.95	4	1.27	nB	nB	nB	nB	
496	V	74051-80-2	InChI=1S/C17H29NO3S/c1-5-8-14(18-21-6-2)17-15(19)10-13(11-16(17)20)9-12(4)22-7-3/h12-13,19H,5-11H2,1-4H3/b18-14+	4.38	1139	1.341	84.19	2	0.51	nB	nB	nB	B	
497	T	93-72-1	InChI=1S/C9H7Cl3O3/c1-4(9(13)14)15-8-3-6(11)5(10)2-7(8)12/h2-4H,1H3,(H,13,14)	3.8	374	0.555	46.53	2	1.76	nB	nB	nB	B	
498	T	22259-30-9	InChI=1S/C11H15N3O2/c1-12-11(15)16-10-6-4-5-9(7-10)13-8-14(2)3/h4-8H,1-3H3,(H,12,15)/b13-8+	1.58	500	1.306	53.93	4	0.00	nB	nB	nB	nB	
499	T	95-16-9	InChI=1S/C7H5NS/c1-2-4-7-6(3-1)8-5-9-7/h1-5H	2.01	79	0.528	41.13	1	0.71	nB	nB	nB	nB	
500	T	361377-29-9	InChI=1S/C21H16ClFN4O5/c1-28-26-18(21-27-30-11-10-29-21)13-6-2-4-8-15(13)31-19-17(23)20(25-12-24-19)32-16-9-5-3-7-14(16)22/h2-9,12H,10-11H2,1H3/b26-18+	5.13	3020	2.87	96.65	3	1.72	nB	nB	B	B	
501	#N/A	892-20-6	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.63	B	#N/A	#N/A	#N/A	Tin containing compound
502	V	535-77-3	InChI=1S/C10H14/c1-8(2)10-6-4-5-9(3)7-10/h4-8H,1-3H3	4.5	117	0.147	0	0	2.77	nB	B	B	B	
503	#N/A	71751-41-2	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	1.84	nB	#N/A	#N/A	#N/A	Mixture

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
504	T	56-38-2	InChI=1S/C10H14NO5PS/c1-3-14-17(18,15-4-2)16-10-7-5-9(6-8-10)11(12)13/h5-8H,3-4H2,1-2H3	3.83	661	1.779	112.73	2	1.95	nB	nB	nB	B	
505	V	61-82-5	InChI=1S/C2H4N4/c3-2-4-1-5-6-2/h1H,(H3,3,4,5,6)	-0.36	26	0.587	67.59	4	0.12	nB	nB	nB	nB	
506	T	62-44-2	InChI=1S/C10H13NO2/c1-3-13-10-6-4-9(5-7-10)11-8(2)12/h4-7H,3H2,1-2H3,(H,11,12)	1.58	280	0.756	38.33	2	0.98	nB	nB	nB	nB	
507	T	67-66-3	InChI=1S/CHCl3/c2-1(3)4/h1H	2.26	9	0.04	0	0	0.80	nB	nB	nB	nB	
508	T	67-68-5	InChI=1S/C2H6OS/c1-4(2)3/h1-2H3	-0.61	9	0.867	36.28	1	0.10	nB	nB	nB	nB	
509	T	68-12-2	InChI=1S/C3H7NO/c1-4(2)3-5/h3H,1-2H3	0.28	18	0.796	20.31	2	-0.11	nB	nB	nB	nB	
510	T	74-97-5	InChI=1S/CH2BrCl/c2-1-3/h1H2	1.67	4	0.046	0	0	0.45	nB	nB	nB	nB	
511	V	75-09-2	InChI=1S/CH2Cl2/c2-1-3/h1H2	1.5	4	0.057	0	0	1.07	nB	nB	nB	nB	
512	T	75-15-0	InChI=1S/CS2/c2-1-3	2.08	4	0.213	64.18	0	1.28	nB	nB	nB	nB	
513	T	75-35-4	InChI=1S/C2H2Cl2/c1-2(3)4/h1H2	2.32	9	0.09	0	0	0.88	nB	nB	nB	nB	
514	T	75-65-0	InChI=1S/C4H10O/c1-4(2,3)5/h5H,1-3H3	0.53	16	0.436	20.23	1	0.37	nB	nB	nB	nB	
515	T	75-98-9	InChI=1S/C5H10O2/c1-5(2,3)4(6)7/h1-3H3,(H,6,7)	1.47	42	0.462	37.3	2	0.10	nB	nB	nB	nB	
516	T	75-99-0	InChI=1S/C3H4Cl2O2/c1-3(4,5)2(6)7/h1H3,(H,6,7)	0.78	42	0.434	37.3	2	0.58	nB	nB	nB	nB	
517	#N/A	76-87-9	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.49	B	#N/A	#N/A	#N/A	Tin containing compound
518	V	78-51-3	InChI=1S/C18H39O7P/c1-4-7-10-20-13-16-23-26(19,24-17-14-21-11-8-5-2)25-18-15-22-12-9-6-3/h4-18H2,1-3H3	3.75	2221	2.481	82.26	7	0.58	nB	nB	nB	nB	
519	T	79-46-9	InChI=1S/C3H7NO2/c1-3(2)4(5)6/h3H,1-2H3	0.93	29	-0.046	43.14	0	0.32	nB	nB	nB	nB	
520	T	81-15-2	InChI=1S/C12H15N3O6/c1-6-9(13(16)17)7(2)11(15(20)21)8(12(3,4)5)10(6)14(18)19/h1-5H3	4.74	774	-0.535	129.42	0	3.65	B	B	B	B	
521	#N/A	81-88-9	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	-0.23	nB	#N/A	#N/A	#N/A	Incompletely defined compound
522	T	82-45-1	InChI=1S/C14H9NO2/c15-11-7-3-6-10-12(11)14(17)9-5-2-1-4-8(9)13(10)16/h1-7H,15H2	3.74	442	1.046	60.16	3	2.08	nB	nB	nB	B	
523	V	82-47-3	InChI=1S/C10H9NO7S2/c11-10-8(20(16,17)18)4-7(19(13,14)15)5-2-1-3-6(12)9(5)10/h1-4,12H,11H2,(H,13,14,15)(H,16,17,18)	0.18	689	2.554	171.75	7	0.90	nB	nB	nB	nB	
524	V	83-32-9	InChI=1S/C12H10/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-6H,7-8H2	3.92	166	0.175	0	0	2.95	nB	B	B	B	
525	V	84-51-5	InChI=1S/C16H12O2/c1-2-10-7-8-13-14(9-10)16(18)12-6-4-3-5-11(12)15(13)17/h3-9H,2H2,1H3	4.37	543	0.823	34.14	2	2.21	nB	nB	nB	B	
526	T	84-87-7	InChI=1S/C10H8O4S/c11-9-5-6-10(15(12,13)14)8-4-2-1-3-7(8)9/h1-6,11H,(H,12,13,14)	-0.44	326	1.411	82.98	3	1.11	nB	nB	nB	nB	
527	T	85-68-7	InChI=1S/C19H20O4/c1-2-3-13-22-18(20)16-11-7-8-12-17(16)19(21)23-14-15-9-5-4-6-10-15/h4-12H,2-3,13-14H2,1H3	4.73	1340	0.855	52.6	4	0.81	nB	nB	B	B	
528	T	86-30-6	InChI=1S/C12H10N2O/c15-13-14(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H	3.13	364	0.715	32.67	1	1.48	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
529	T	86-73-7	InChI=1S/C13H10/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)12/h1-8H,9H2	4.18	219	0.197	0	0	2.81	nB	B	B	B	
530	T	87-68-3	InChI=1S/C4Cl6/c5-1(3(7)8)2(6)4(9)10	4.78	121	0.071	0	0	3.88	B	B	B	B	
531	T	87-86-5	InChI=1S/C6HCl5O/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H	5.12	174	-0.044	20.23	0	2.70	nB	B	B	B	
532	T	88-89-1	InChI=1S/C6H3N3O7/c10-6-4(8(13)14)1-3(7(11)12)2-5(6)9(15)16/h1-2,10H	1.33	408	-0.514	149.65	0	-0.14	nB	nB	nB	nB	
533	T	89-63-4	InChI=1S/C6H5ClN2O2/c7-4-1-2-5(8)6(3-4)9(10)11/h1-3H,8H2	2.72	148	0.034	69.16	1	1.07	nB	nB	nB	nB	
534	V	90-30-2	InChI=1S/C16H13N/c1-2-9-14(10-3-1)17-16-12-6-8-13-7-4-5-11-15(13)16/h1-12,17H	4.2	518	1.071	12.03	1	3.32	B	nB	nB	B	
535	V	90-41-5	InChI=1S/C12H11N/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H,13H2	2.84	240	0.483	26.02	1	1.47	nB	nB	nB	nB	
536	T	92-70-6	InChI=1S/C11H8O3/c12-10-6-8-4-2-1-3-7(8)5-9(10)11(13)14/h1-6,12H,(H,13,14)	3.05	284	0.428	57.53	2	0.32	nB	nB	nB	nB	
537	V	92-77-3	InChI=1S/C17H13NO2/c19-16-11-13-7-5-4-6-12(13)10-15(16)17(20)18-14-8-2-1-3-9-14/h1-11,19H,(H,18,20)	4.52	833	0.612	49.33	2	0.70	nB	nB	nB	B	
538	T	92-86-4	InChI=1S/C12H8Br2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H	5.72	315	0.175	0	0	4.00	B	B	B	B	
539	V	95-48-7	InChI=1S/C7H8O/c1-6-4-2-3-5-7(6)8/h2-5,8H,1H3	1.95	60	0.429	20.23	0	1.03	nB	nB	nB	nB	
540	V	95-50-1	InChI=1S/C6H4Cl2/c7-5-3-1-2-4-6(5)8/h1-4H	3.43	60	0.146	0	0	2.50	nB	nB	nB	nB	
541	V	95-51-2	InChI=1S/C6H6ClN/c7-5-3-1-2-4-6(5)8/h1-4H,8H2	1.9	60	0.421	26.02	1	0.91	nB	nB	nB	nB	
542	T	95-77-2	InChI=1S/C6H4Cl2O/c7-5-2-1-4(9)3-6(5)8/h1-3,9H	3.33	84	0.361	20.23	0	1.81	nB	nB	nB	nB	
543	V	95-80-7	InChI=1S/C7H10N2/c1-5-2-3-6(8)4-7(5)9/h2-4H,8-9H2,1H3	0.14	84	0.626	52.04	2	1.20	nB	nB	nB	nB	
544	T	96-73-1	InChI=1S/C6H4ClNO5S/c7-5-2-1-4(8(9)10)3-6(5)14(11,12)13/h1-3H,(H,11,12,13)	1.13	287	0.838	105.89	3	0.48	nB	nB	nB	nB	
545	V	96-76-4	InChI=1S/C14H22O/c1-13(2,3)10-7-8-12(15)11(9-10)14(4,5)6/h7-9,15H,1-6H3	5.19	342	0.527	20.23	0	2.51	nB	B	B	B	
546	V	98-54-4	InChI=1S/C10H14O/c1-10(2,3)8-4-6-9(11)7-5-8/h4-7,11H,1-3H3	3.31	152	0.48	20.23	0	1.77	nB	nB	nB	nB	
547	T	98-95-3	InChI=1S/C6H5NO2/c8-7(9)6-4-2-1-3-5-6/h1-5H	1.85	88	-0.065	43.14	0	0.64	nB	nB	nB	nB	
548	T	99-99-0	InChI=1S/C7H7NO2/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3	2.37	120	-0.069	43.14	0	0.91	nB	nB	nB	nB	
549	T	100-01-6	InChI=1S/C6H6N2O2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H,7H2	1.39	120	0.153	69.16	1	0.69	nB	nB	nB	nB	
550	T	100-17-4	InChI=1S/C7H7NO3/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3	2.03	162	0.096	52.37	0	0.78	nB	nB	nB	nB	
551	T	100-25-4	InChI=1S/C6H4N2O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1-4H	1.46	206	-0.313	86.28	0	-0.40	nB	nB	nB	nB	
552	T	100-26-5	InChI=1S/C7H5NO4/c9-6(10)4-1-2-5(7(11)12)8-3-4/h1-3H,(H,9,10)(H,11,12)	0.24	206	1.091	87.49	5	0.36	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
553	T	100-40-3	InChI=1S/C8H12/c1-2-8-6-4-3-5-7-8/h2-4,8H,1,5-7H2	3.93	64	0.134	0	0	2.25	nB	nB	B	B	
554	T	100-43-6	InChI=1S/C7H7N/c1-2-7-3-5-8-6-4-7/h2-6H,1H2	1.63	64	0.466	12.89	1	1.94	nB	nB	nB	nB	
555	V	100-61-8	InChI=1S/C7H9N/c1-8-7-5-3-2-4-6-7/h2-6,8H,1H3	1.66	64	0.548	12.03	1	0.65	nB	nB	nB	nB	
556	T	101-77-9	InChI=1S/C13H14N2/c14-12-5-1-10(2-6-12)9-11-3-7-13(15)8-4-11/h1-8H,9,14-15H2	1.59	404	0.709	52.04	2	1.05	nB	nB	nB	nB	
557	V	102-70-5	InChI=1S/C9H15N/c1-4-7-10(8-5-2)9-6-3/h4-6H,1-3,7-9H2	2.59	138	0.814	3.24	1	0.55	nB	nB	nB	nB	
558	V	104-40-5	InChI=1S/C15H24O/c1-2-3-4-5-6-7-8-9-14-10-12-15(16)13-11-14/h10-13,16H,2-9H2,1H3	5.76	594	0.429	20.23	0	2.55	nB	nB	B	B	
559	V	104-88-1	InChI=1S/C7H5ClO/c8-7-3-1-6(5-9)2-4-7/h1-5H	2.1	90	0.46	17.07	1	0.32	nB	nB	nB	nB	
560	T	106-37-6	InChI=1S/C6H4Br2/c7-5-1-2-6(8)4-3-5/h1-4H	3.79	62	0.047	0	0	2.29	nB	nB	nB	B	
561	T	106-43-4	InChI=1S/C7H7Cl/c1-6-2-4-7(8)5-3-6/h2-5H,1H3	3.33	62	0.122	0	0	1.84	nB	nB	nB	nB	
562	T	106-47-8	InChI=1S/C6H6ClN/c7-5-1-3-6(8)4-2-5/h1-4H,8H2	1.88	62	0.344	26.02	1	0.60	nB	nB	nB	nB	
563	T	107-05-1	InChI=1S/C3H5Cl/c1-2-3-4/h2H,1,3H2	1.46	10	0.101	0	0	0.30	nB	nB	nB	nB	
564	T	108-42-9	InChI=1S/C6H6ClN/c7-5-2-1-3-6(8)4-5/h1-4H,8H2	1.88	61	0.355	26.02	1	0.31	nB	nB	nB	nB	
565	V	108-45-2	InChI=1S/C6H8N2/c7-5-2-1-3-6(8)4-5/h1-4H,7-8H2	-0.33	61	0.63	52.04	2	0.80	nB	nB	nB	nB	
566	T	108-60-1	InChI=1S/C6H12Cl2O/c1-5(3-7)9-6(2)4-8/h5-6H,3-4H2,1-2H3	2.48	100	0.318	9.23	1	0.96	nB	nB	nB	nB	
567	T	108-90-7	InChI=1S/C6H5Cl/c7-6-4-2-1-3-5-6/h1-5H	2.84	42	0.126	0	0	1.36	nB	nB	nB	nB	
568	V	110-00-9	InChI=1S/C4H4O/c1-2-4-5-3-1/h1-4H	1.34	15	0.162	13.14	0	0.35	nB	nB	nB	nB	
569	V	111-41-1	InChI=1S/C4H12N2O/c5-1-2-6-3-4-7/h6-7H,1-5H2	-1.69	56	1.4	58.28	3	0.11	nB	nB	nB	nB	
570	T	112-40-3	InChI=1S/C12H26/c1-3-5-7-9-11-12-10-8-6-4-2/h3-12H2,1-2H3	6.1	286	0.085	0	0	2.81	nB	B	B	B	
571	V	115-77-5	InChI=1S/C5H12O4/c6-1-5(2-7,3-8)4-9/h6-9H,1-4H2	-1.69	88	1.336	80.92	4	-0.04	nB	nB	nB	nB	
572	T	117-79-3	InChI=1S/C14H9NO2/c15-8-5-6-11-12(7-8)14(17)10-4-2-1-3-9(10)13(11)16/h1-7H,15H2	3.31	452	1.091	60.16	3	1.59	nB	nB	nB	nB	
573	T	118-32-1	InChI=1S/C10H8O7S2/c11-7-2-1-6-3-8(18(12,13)14)5-10(9(6)4-7)19(15,16)17/h1-5,11H,(H,12,13,14)(H,15,16,17)	-10.93	628	2.363	145.73	6	0.00	nB	nB	nB	nB	
574	V	118-79-6	InChI=1S/C6H3Br3O/c7-3-1-4(8)6(10)5(9)2-3/h1-2,10H	4.13	110	0.018	20.23	0	2.71	nB	B	B	B	
575	T	118-83-2	InChI=1S/C7H3ClF3NO2/c8-4-1-2-6(12(13)14)5(3-4)7(9,10)11/h1-3H	3.2	279	-0.246	43.14	0	2.02	nB	nB	nB	nB	
576	V	118-91-2	InChI=1S/C7H5ClO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H,9,10)	2.05	114	0.448	37.3	2	0.50	nB	nB	nB	nB	
577	T	119-12-0	InChI=1S/C14H17N2O4PS/c1-3-18-21(22,19-4-2)20-13-10-11-14(17)16(15-13)12-8-6-5-7-9-12/h5-11H,3-4H2,1-2H3	3.2	1086	2.748	102.26	6	0.83	nB	nB	nB	nB	
578	T	119-56-2	InChI=1S/C13H11ClO/c14-12-8-6-11(7-9-12)13(15)10-4-2-1-3-5-10/h1-9,13,15H	3.61	378	0.75	20.23	1	1.84	nB	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
579	T	120-12-7	InChI=1S/C14H10/c1-2-6-12-10-14-8-4-3-7-13(14)9-11(12)5-1/h1-10H	4.45	279	0.257	0	0	3.18	B	B	B	B	
580	T	120-82-1	InChI=1S/C6H3Cl3/c7-4-1-2-5(8)6(9)3-4/h1-3H	4.02	84	0.054	0	0	3.04	B	nB	B	B	
581	T	121-44-8	InChI=1S/C6H15N/c1-4-7(5-2)6-3/h4-6H2,1-3H3	1.45	48	0.745	3.24	1	0.20	nB	nB	nB	nB	
582	V	121-75-5	InChI=1S/C10H19O6PS2/c1-5-15-9(11)7-8(10(12)16-6-2)19-17(18,13-3)14-4/h8H,5-7H2,1-4H3	2.36	738	2.632	138.26	6	1.13	nB	nB	nB	nB	
583	T	121-92-6	InChI=1S/C7H5NO4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H,(H,9,10)	1.83	197	0.257	80.44	2	0.35	nB	nB	nB	nB	
584	T	122-20-3	InChI=1S/C9H21NO3/c1-7(11)4-10(5-8(2)12)6-9(3)13/h7-9,11-13H,4-6H2,1-3H3	-0.49	270	1.699	63.93	4	-0.73	nB	nB	nB	nB	
585	T	122-34-9	InChI=1S/C7H12ClN5/c1-3-9-6-11-5(8)12-7(13-6)10-4-2/h3-4H2,1-2H3,(H2,9,10,11,12,13)	2.18	260	1.416	62.73	5	1.32	nB	nB	nB	nB	
586	V	123-91-1	InChI=1S/C4H8O2/c1-2-6-4-3-5-1/h1-4H2	-0.27	27	0.733	18.46	2	-0.27	nB	nB	nB	nB	
587	T	124-11-8	InChI=1S/C9H18/c1-3-5-7-9-8-6-4-2/h3H,1,4-9H2,2H3	5.15	120	0.108	0	0	3.18	B	B	B	B	
588	V	126-30-7	InChI=1S/C5H12O2/c1-5(2,3-6)4-7/h6-7H,3-4H2,1-2H3	0.05	44	0.736	40.46	2	0.16	nB	nB	nB	nB	
589	T	127-90-2	InChI=1S/C6H6Cl8O/c7-3(5(9,10)11)1-15-2-4(8)6(12,13)14/h3-4H,1-2H2	5.09	420	0.372	9.23	1	3.50	B	B	B	B	
590	T	129-00-0	InChI=1S/C16H10/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-10H	4.88	362	0.295	0	0	2.78	nB	B	B	B	
591	T	131-09-9	InChI=1S/C14H7ClO2/c15-8-5-6-11-12(7-8)14(17)10-4-2-1-3-9(10)13(11)16/h1-7H	4.62	452	0.816	34.14	2	2.34	nB	nB	B	B	
592	V	131-57-7	InChI=1S/C14H12O3/c1-17-11-7-8-12(13(15)9-11)14(16)10-5-3-2-4-6-10/h2-9,15H,1H3	3.79	528	0.596	46.53	1	2.09	nB	nB	nB	B	
593	V	132-64-9	InChI=1S/C12H8O/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8H	4.12	219	0.282	13.14	0	3.19	B	nB	B	B	
594	V	134-47-4	InChI=1S/C21H16N2O9S2/c24-19-9-15(33(27,28)29)7-11-5-13(1-3-17(11)19)22-21(26)23-14-2-4-18-12(6-14)8-16(10-20(18)25)34(30,31)32/h1-10,24-25H,(H2,22,23,26)(H,27,28,29)(H,30,31,32)	1.77	3869	3.265	207.09	9	-0.23	nB	nB	nB	nB	
595	T	141-93-5	InChI=1S/C10H14/c1-3-9-6-5-7-10(4-2)8-9/h5-8H,3-4H2,1-2H3	4.57	121	0.129	0	0	2.81	nB	nB	B	B	
596	T	142-96-1	InChI=1S/C8H18O/c1-3-5-7-9-8-6-4-2/h3-8H2,1-2H3	3.21	120	0.296	9.23	1	1.91	nB	nB	nB	nB	
597	T	144-19-4	InChI=1S/C8H18O2/c1-6(2)7(10)8(3,4)5-9/h6-7,9-10H,5H2,1-4H3	1.24	116	0.772	40.46	2	-0.31	nB	nB	nB	nB	
598	T	298-06-6	InChI=1S/C4H11O2PS2/c1-3-5-7(8,9)6-4-2/h3-4H2,1-2H3,(H,8,9)	2.56	96	1.761	99.16	2	0.20	nB	nB	nB	nB	
599	V	328-84-7	InChI=1S/C7H3Cl2F3/c8-5-2-1-4(3-6(5)9)7(10,11)12/h1-3H	4.47	189	0.022	0	0	3.18	B	B	B	B	
600	V	461-58-5	InChI=1S/C2H4N4/c3-1-6-2(4)5/h(H4,4,5,6)	-0.89	32	1.563	85.69	4	-0.02	nB	nB	nB	nB	
601	T	462-08-8	InChI=1S/C5H6N2/c6-5-2-1-3-7-4-5/h1-4H,6H2	0.11	42	0.711	38.91	2	-0.19	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
602	T	479-27-6	InChI=1S/C10H10N2/c11-8-5-1-3-7-4-2-6-9(12)10(7)8/h1-6H,11-12H2	1.78	175	0.69	52.04	2	0.75	nB	nB	nB	nB	
603	V	496-10-6	InChI=1S/C9H16/c1-2-5-9-7-3-6-8(9)4-1/h8-9H,1-7H2	4.08	79	0.093	0	0	2.91	nB	nB	B	B	
604	T	504-24-5	InChI=1S/C5H6N2/c6-5-1-3-7-4-2-5/h1-4H,(H2,6,7)	0.32	42	0.711	38.91	2	0.14	nB	nB	nB	nB	
605	T	526-73-8	InChI=1S/C9H12/c1-7-5-4-6-8(2)9(7)3/h4-6H,1-3H3	3.66	82	0.125	0	0	2.32	nB	nB	B	B	
606	V	538-75-0	InChI=1S/C13H22N2/c1-3-7-12(8-4-1)14-11-15-13-9-5-2-6-10-13/h12-13H,1-10H2	4.67	436	0.493	24.72	2	0.09	nB	nB	B	B	
607	T	541-73-1	InChI=1S/C6H4Cl2/c7-5-2-1-3-6(8)4-5/h1-4H	3.53	61	0.08	0	0	2.54	nB	nB	nB	nB	
608	T	542-18-7	InChI=1S/C6H11Cl/c7-6-4-2-1-3-5-6/h6H,1-5H2	3.03	42	0.082	0	0	2.35	nB	nB	nB	nB	
609	V	544-76-3	InChI=1S/C16H34/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3-16H2,1-2H3	8.28	680	0.085	0	0	1.65	nB	nB	B	B	
610	V	554-00-7	InChI=1S/C6H5Cl2N/c7-4-1-2-6(9)5(8)3-4/h1-3H,9H2	2.91	84	0.329	26.02	1	1.41	nB	nB	nB	nB	
611	V	554-84-7	InChI=1S/C6H5NO3/c8-6-3-1-2-5(4-6)7(9)10/h1-4,8H	2	117	0.196	63.37	0	1.40	nB	nB	nB	nB	
612	V	555-03-3	InChI=1S/C7H7NO3/c1-11-7-4-2-3-6(5-7)8(9)10/h2-5H,1H3	2.16	156	0.107	52.37	0	0.72	nB	nB	nB	nB	
613	#N/A	556-67-2	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	4.09	B	#N/A	#N/A	#N/A	Silicon containing compound
614	T	576-24-9	InChI=1S/C6H4Cl2O/c7-4-2-1-3-5(9)6(4)8/h1-3,9H	2.84	82	0.308	20.23	0	1.40	nB	nB	nB	nB	
615	T	579-10-2	InChI=1S/C9H11NO/c1-8(11)10(2)9-6-4-3-5-7-9/h3-7H,1-2H3	1.12	156	0.508	20.31	2	-0.05	nB	nB	nB	nB	
616	V	583-78-8	InChI=1S/C6H4Cl2O/c7-4-1-2-5(8)6(9)3-4/h1-3,9H	3.06	84	0.231	20.23	0	1.33	nB	nB	nB	nB	
617	V	591-27-5	InChI=1S/C6H7NO/c7-5-2-1-3-6(8)4-5/h1-4,8H,7H2	0.21	61	0.662	46.25	1	1.10	nB	nB	nB	nB	
618	V	605-02-7	InChI=1S/C16H12/c1-2-7-13(8-3-1)16-12-6-10-14-9-4-5-11-15(14)16/h1-12H	5.13	412	0.279	0	0	3.51	B	B	B	B	
619	T	606-20-2	InChI=1S/C7H6N2O4/c1-5-6(8(10)11)3-2-4-7(5)9(12)13/h2-4H,1H3	2.1	234	-0.306	86.28	0	1.34	nB	nB	nB	nB	
620	T	606-28-0	InChI=1S/C15H12O3/c1-18-15(17)13-10-6-5-9-12(13)14(16)11-7-3-2-4-8-11/h2-10H,1H3	2.7	593	0.85	43.37	3	0.87	nB	nB	nB	nB	
621	V	626-67-5	InChI=1S/C6H13N/c1-7-5-3-2-4-6-7/h2-6H2,1H3	1.3	42	0.731	3.24	1	0.31	nB	nB	nB	nB	
622	T	629-62-9	InChI=1S/C15H32/c1-3-5-7-9-11-13-15-14-12-10-8-6-4-2/h3-15H2,1-2H3	7.74	560	0.085	0	0	1.38	nB	B	B	B	
623	V	634-91-3	InChI=1S/C6H4Cl3N/c7-4-1-3(10)2-5(8)6(4)9/h1-2H,10H2	3.32	110	0.279	26.02	1	2.36	nB	nB	nB	nB	
624	T	732-11-6	InChI=1S/C11H12NO4PS2/c1-15-17(18,16-2)19-7-12-10(13)8-5-3-4-6-9(8)11(12)14/h3-6H,7H2,1-2H3	2.78	701	2.684	123.04	5	0.55	nB	nB	nB	nB	
625	T	760-23-6	InChI=1S/C4H6Cl2/c1-2-4(6)3-5/h2,4H,1,3H2	2.09	31	0.125	0	0	0.60	nB	nB	nB	nB	
626	T	767-00-0	InChI=1S/C7H5NO/c8-5-6-1-3-7(9)4-2-6/h1-4,9H	1.6	90	0.553	44.02	1	0.91	nB	nB	nB	nB	
627	#N/A	791-31-1	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	2.85	nB	#N/A	#N/A	#N/A	Silicon containing compound
628	V	872-05-9	InChI=1S/C10H20/c1-3-5-7-9-10-8-6-4-2/h3H,1,4-10H2,2H3	5.7	165	0.108	0	0	3.22	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
629	T	935-95-5	InChI=1S/C6H2Cl4O/c7-2-1-3(8)5(10)6(11)4(2)9/h1,11H	3.88	140	0.021	20.23	0	2.15	nB	B	B	B	
630	T	938-86-3	InChI=1S/C7H4Cl4O/c1-12-4-2-3(8)5(9)7(11)6(4)10/h2H,1H3	4.51	182	0.192	9.23	0	3.35	B	B	B	B	
631	T	947-72-8	InChI=1S/C14H9Cl/c15-14-9-10-5-1-2-6-11(10)12-7-3-4-8-13(12)14/h1-9H	4.87	322	0.246	0	0	3.49	B	nB	B	B	
632	T	961-11-5	InChI=1S/C10H9Cl4O4P/c1-16-19(15,17-2)18-10(5-11)6-3-8(13)9(14)4-7(6)12/h3-5H,1-2H3/b10-5-	3.53	690	1.824	54.57	4	1.65	nB	nB	nB	nB	
633	T	1141-38-4	InChI=1S/C12H8O4/c13-11(14)9-3-1-7-5-10(12(15)16)4-2-8(7)6-9/h1-6H,(H,13,14)(H,15,16)	2.81	442	0.841	74.6	4	0.55	nB	nB	nB	nB	
634	T	1163-19-5	InChI=1S/C12Br10O/c13-1-3(15)7(19)11(8(20)4(1)16)23-12-9(21)5(17)2(14)6(18)10(12)22	10.36	1096	-0.152	9.23	0	1.20	nB	nB	nB	B	
635	T	1212-29-9	InChI=1S/C13H24N2S/c16-13(14-11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h11-12H,1-10H2,(H2,14,15,16)	3.69	495	1.246	56.15	2	0.65	nB	nB	nB	B	
636	#N/A	1461-25-2	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	2.27	nB	#N/A	#N/A	#N/A	Tin containing compound
637	T	1582-09-8	InChI=1S/C13H16F3N3O4/c1-3-5-17(6-4-2)12-10(18(20)21)7-9(13(14,15)16)8-11(12)19(22)23/h7-8H,3-6H2,1-2H3	5.34	1082	-0.04	89.52	1	3.63	B	B	B	B	
638	T	1712-70-5	InChI=1S/C9H9Cl/c1-7(2)8-3-5-9(10)6-4-8/h3-6H,1H2,2H3	4.36	120	0.141	0	0	2.91	nB	B	B	B	
639	T	1763-23-1	InChI=1S/C8HF17O3S/c9-1(10,3(13,14)5(17,18)7(21,22)23)2(11,12)4(15,16)6(19,20)8(24,25)29(26,27)28/h(H,26,27,28)	5.02	1864	0.978	62.75	3	3.73	B	nB	B	B	
640	T	1934-21-0	InChI=1S/C16H12N4O9S2/c21-15-13(18-17-9-1-5-11(6-2-9)30(24,25)26)14(16(22)23)19-20(15)10-3-7-12(8-4-10)31(27,28)29/h1-8,13H,(H,22,23)(H,24,25,26)(H,27,28,29)/b18-17+	0.44	2981	3.26	220.19	13	-0.03	nB	nB	nB	nB	Salt - converted into acidic form
641	V	2027-17-0	InChI=1S/C13H14/c1-10(2)12-8-7-11-5-3-4-6-13(11)9-12/h3-10H,1-2H3	4.62	238	0.211	0	0	4.11	B	B	B	B	
642	V	2050-68-2	InChI=1S/C12H8Cl2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H	5.23	315	0.197	0	0	3.58	B	B	B	B	
643	V	2104-64-5	InChI=1S/C14H14NO4PS/c1-2-18-20(21,14-6-4-3-5-7-14)19-13-10-8-12(9-11-13)15(16)17/h3-11H,2H2,1H3	4.78	966	1.616	103.5	1	2.71	nB	B	B	B	
644	T	2216-69-5	InChI=1S/C11H10O/c1-12-11-8-4-6-9-5-2-3-7-10(9)11/h2-8H,1H3	3.45	182	0.404	9.23	0	2.31	nB	nB	nB	nB	
645	T	2243-62-1	InChI=1S/C10H10N2/c11-9-5-1-3-7-8(9)4-2-6-10(7)12/h1-6H,11-12H2	0.89	176	0.702	52.04	2	0.27	nB	nB	nB	nB	
646	T	2381-21-7	InChI=1S/C17H12/c1-11-5-6-14-8-7-12-3-2-4-13-9-10-15(11)17(14)16(12)13/h2-10H,1H3	5.69	428	0.291	0	0	2.73	nB	nB	B	B	
647	T	2437-79-8	InChI=1S/C12H6Cl4/c13-7-1-3-9(11(15)5-7)10-4-2-8(14)6-12(10)16/h1-6H	6.39	426	0.082	0	0	4.39	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
648	T	2440-02-0	InChI=1S/C7H3Cl7/c8-2-1-5(11)3(9)4(10)6(2,12)7(5,13)14/h2H,1H2	4	231	0.244	0	0	4.05	B	B	B	B	
649	V	2581-34-2	InChI=1S/C7H7NO3/c1-5-4-6(9)2-3-7(5)8(10)11/h2-4,9H,1H3	2.48	150	0.181	63.37	0	1.26	nB	nB	nB	nB	
650	T	2655-14-3	InChI=1S/C10H13NO2/c1-7-4-8(2)6-9(5-7)13-10(12)11-3/h4-6H,1-3H3,(H,11,12)	2.23	258	0.466	38.33	2	0.30	nB	nB	nB	nB	
651	T	3648-21-3	InChI=1S/C22H34O4/c1-3-5-7-9-13-17-25-21(23)19-15-11-12-16-20(19)22(24)26-18-14-10-8-6-4-2/h11-12,15-16H,3-10,13-14,17-18H2,1-2H3	5.8	2141	0.807	52.6	4	0.88	nB	B	B	B	
652	V	3761-42-0	InChI=1S/C10H15O5PS2/c1-8-7-9(15-16(17,13-2)14-3)5-6-10(8)18(4,11)12/h5-7H,1-4H3	2.82	625	2.641	112.11	4	0.48	nB	nB	nB	nB	
653	V	4051-66-5	InChI=1S/C37H76N2O/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-37(40)39-36-34-32-30-28-26-24-22-20-18-16-14-12-10-8-6-4-2/h3-36H2,1-2H3,(H2,38,39,40)	17.04	10299	0.851	41.13	3	1.48	nB	nB	nB	B	
654	T	4130-42-1	InChI=1S/C16H26O/c1-8-11-9-12(15(2,3)4)14(17)13(10-11)16(5,6)7/h9-10,17H,8H2,1-7H3	5.53	466	0.523	20.23	0	3.59	B	nB	B	B	
655	T	4292-75-5	InChI=1S/C12H24/c1-2-3-4-6-9-12-10-7-5-8-11-12/h12H,2-11H2,1H3	6.21	242	0.089	0	0	3.29	B	B	B	B	
656	V	5124-25-4	InChI=1S/C18H15N3O4S/c22-21(23)18-13-16(26(24,25)20-15-9-5-2-6-10-15)11-12-17(18)19-14-7-3-1-4-8-14/h1-13,19-20H	4.6	1747	1.336	109.72	4	1.54	nB	nB	nB	B	
657	T	5409-83-6	InChI=1S/C12H6Cl2O/c13-7-1-3-11-9(5-7)10-6-8(14)2-4-12(10)15-11/h1-6H	5.65	332	0.26	13.14	0	3.66	B	B	B	B	
658	T	5510-99-6	InChI=1S/C14H22O/c1-5-10(3)12-8-7-9-13(14(12)15)11(4)6-2/h7-11,15H,5-6H2,1-4H3	4.36	358	0.461	20.23	0	2.55	nB	nB	B	B	
659	V	6165-51-1	InChI=1S/C16H18/c1-12-9-10-13(2)16(11-12)14(3)15-7-5-4-6-8-15/h4-11,14H,1-3H3	4.9	430	0.191	0	0	2.86	nB	B	B	B	
660	T	10605-21-7	InChI=1S/C9H9N3O2/c1-14-9(13)12-8-10-6-4-2-3-5-7(6)11-8/h2-5H,1H3,(H2,10,11,12,13)	1.17	314	0.741	67.01	5	0.43	nB	nB	nB	nB	
661	T	13116-53-5	InChI=1S/C3H4Cl4/c4-1-3(6,7)2-5/h1-2H2	2.72	44	0.146	0	0	1.63	nB	nB	nB	nB	
662	V	13150-81-7	InChI=1S/C12H26/c1-5-6-9-12(4)10-7-8-11(2)3/h11-12H,5-10H2,1-4H3	6.14	253	0.121	0	0	3.18	B	B	B	B	
663	T	13358-11-7	InChI=1S/C22H35NO2/c1-6-8-9-16(7-2)14-23-19(24)17-18(20(23)25)22(15(3)4)12-10-21(17,5)11-13-22/h10,12,15-18H,6-9,11,13-14H2,1-5H3	5.96	1363	0.957	37.38	3	3.16	B	nB	B	B	
664	V	13475-82-6	InChI=1S/C12H26/c1-10(8-11(2,3)4)9-12(5,6)7/h10H,8-9H2,1-7H3	5.55	211	0.205	0	0	3.25	B	B	B	B	
665	T	13674-87-8	InChI=1S/C9H15Cl6O4P/c10-1-7(2-11)17-20(16,18-8(3-12)4-13)19-9(5-14)6-15/h7-9H,1-6H2	3.65	826	1.86	54.57	4	1.28	nB	nB	nB	nB	
666	T	15972-60-8	InChI=1S/C14H20ClNO2/c1-4-11-7-6-8-12(5-2)14(11)16(10-18-3)13(17)9-15/h6-8H,4-5,9-10H2,1-3H3	3.52	569	0.704	29.54	3	1.36	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
667	T	16014-23-6	InChI=1S/C18H14N2O6S/c1-10-6-7-14(15(8-10)27(24,25)26)19-20-16-12-5-3-2-4-11(12)9-13(17(16)21)18(22)23/h2-9,21H,1H3,(H,22,23)(H,24,25,26)/b20-19+	3.78	1796	1.615	145	7	0.84	nB	nB	nB	nB	
668	V	16090-02-1	InChI=1S/C40H40N12O8S2/c53-61(54,55)33-25-31(43-37-45-35(41-29-7-3-1-4-8-29)47-39(49-37)51-17-21-59-22-18-51)15-13-27(33)11-12-28-14-16-32(26-34(28)62(56,57)58)44-38-46-36(42-30-9-5-2-6-10-30)48-40(50-38)52-19-23-60-24-20-52/h1-16,25-26H,17-24H2,(H,53,54,55)(H,56,57,58)(H2,41,43,45,47,49)(H2,42,44,46,48,50)/b12-11+	5.46	20207	7.607	275.9	20	0.96	nB	nB	nB	B	Salt - converted into acidic form
669	T	16219-75-3	InChI=1S/C9H12/c1-2-8-5-7-3-4-9(8)6-7/h2-4,7,9H,5-6H2,1H3/b8-2+	3.82	80	0.133	0	0	2.05	nB	nB	B	B	
670	V	16606-02-3	InChI=1S/C12H7Cl3/c13-9-3-1-8(2-4-9)11-7-10(14)5-6-12(11)15/h1-7H	5.69	362	0.14	0	0	4.05	B	B	B	B	
671	T	17095-24-8	InChI=1S/C26H25N5O19S6/c27-23-22-15(13-20(53(37,38)39)24(23)30-28-16-1-5-18(6-2-16)51(33,34)11-9-49-55(43,44)45)14-21(54(40,41)42)25(26(22)32)31-29-17-3-7-19(8-4-17)52(35,36)12-10-50-56(46,47)48/h1-8,13-14,32H,9-12,27H2,(H,37,38,39)(H,40,41,42)(H,43,44,45)(H,46,47,48)/b30-28+,31-29+	0.08	15535	6.602	450.19	23	0.54	nB	nB	nB	nB	Salt - converted into acidic form
672	V	18708-70-8	InChI=1S/C6H2Cl3NO2/c7-3-1-4(8)6(10(11)12)5(9)2-3/h1-2H	3.69	184	-0.187	43.14	0	2.72	nB	nB	nB	B	
673	T	21564-17-0	InChI=1S/C9H6N2S3/c10-5-12-6-13-9-11-7-3-1-2-4-8(7)14-9/h1-4H,6H2	3.3	334	1.123	115.52	2	1.82	nB	nB	nB	nB	
674	T	22907-72-8	InChI=1S/C12H24/c1-9(2)11-5-7-12(8-6-11)10(3)4/h9-12H,5-8H2,1-4H3	6.35	206	0.143	0	0	3.50	B	B	B	B	
675	T	24019-05-4	InChI=1S/C19H12Cl4N2O5S/c20-10-1-5-16(30-17-6-2-11(21)8-18(17)31(27,28)29)15(7-10)25-19(26)24-12-3-4-13(22)14(23)9-12/h1-9H,(H2,24,25,26)(H,27,28,29)	5.27	2850	1.661	113.11	6	1.92	nB	nB	B	B	
676	V	26306-61-6	InChI=1S/C12H8Cl3NO/c13-7-5-10(14)12(11(15)6-7)17-9-3-1-8(16)2-4-9/h1-6H,16H2	4.61	534	0.488	35.25	1	1.95	nB	nB	nB	B	
677	T	28076-73-5	InChI=1S/C12H6Cl4O/c13-7-1-3-11(9(15)5-7)17-12-4-2-8(14)6-10(12)16/h1-6H	5.95	536	0.248	9.23	0	4.14	B	B	B	B	
678	V	30746-58-8	InChI=1S/C12H4Cl4O2/c13-7-8(14)10(16)12-11(9(7)15)17-5-3-1-2-4-6(5)18-12/h1-4H	6.6	537	0.214	18.46	0	3.50	B	B	B	B	
679	V	32598-10-0	InChI=1S/C12H6Cl4/c13-8-2-3-9(11(15)6-8)7-1-4-10(14)12(16)5-7/h1-6H	6.31	433	0.171	0	0	4.56	B	B	B	B	
680	T	32598-13-3	InChI=1S/C12H6Cl4/c13-9-3-1-7(5-11(9)15)8-2-4-10(14)12(16)6-8/h1-6H	6.63	440	0.237	0	0	4.07	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
681	T	33857-26-0	InChI=1S/C12H6Cl2O2/c13-7-1-3-9-11(5-7)16-10-4-2-8(14)6-12(10)15-9/h1-6H	5.75	414	0.267	18.46	0	2.39	nB	B	B	B	
682	V	34883-39-1	InChI=1S/C12H8Cl2/c13-10-6-7-12(14)11(8-10)9-4-2-1-3-5-9/h1-8H	5.1	293	0.151	0	0	3.86	B	B	B	B	
683	V	35065-27-1	InChI=1S/C12H4Cl6/c13-7-3-11(17)9(15)1-5(7)6-2-10(16)12(18)4-8(6)14/h1-4H	7.12	573	0.03	0	0	5.69	B	B	B	B	
684	V	38380-02-8	InChI=1S/C12H5Cl5/c13-6-1-3-9(14)8(5-6)7-2-4-10(15)12(17)11(7)16/h1-5H	6.85	486	0.122	0	0	4.02	B	B	B	B	
685	T	39569-21-6	InChI=1S/C7H3Br4Cl/c1-2-3(8)4(9)5(10)6(11)7(2)12/h1H3	5.68	174	-0.074	0	0	3.98	B	B	B	B	
686	V	41464-40-8	InChI=1S/C12H6Cl4/c13-7-2-4-11(15)10(5-7)9-3-1-8(14)6-12(9)16/h1-6H	6.22	419	0.071	0	0	4.26	B	B	B	B	
687	V	41464-42-0	InChI=1S/C12H6Cl4/c13-8-1-2-12(16)11(6-8)7-3-9(14)5-10(15)4-7/h1-6H	6.39	419	0.094	0	0	4.85	B	B	B	B	
688	V	42240-73-3	InChI=1S/C13H10Cl4N2/c14-10-6(1-3-8(18)12(10)16)5-7-2-4-9(19)13(17)11(7)15/h1-4H,5,18-19H2	4.99	704	0.719	52.04	2	3.38	B	B	B	B	
689	T	50876-32-9	InChI=1S/C10H20/c1-8-5-9(2)7-10(3,4)6-8/h8-9H,5-7H2,1-4H3	4.4	109	0.158	0	0	3.65	B	nB	B	B	
690	T	51892-26-3	InChI=1S/C12H8Cl2O/c13-9-6-7-12(11(14)8-9)15-10-4-2-1-3-5-10/h1-8H	4.93	384	0.32	9.23	0	3.97	B	nB	B	B	
691	T	52322-80-2	InChI=1S/C12H7Cl3O/c13-9-6-11(15)12(7-10(9)14)16-8-4-2-1-3-5-8/h1-7H	5.44	450	0.259	9.23	0	3.65	B	B	B	B	
692	T	56348-72-2	InChI=1S/C12H6Cl4O/c13-9-3-1-7(5-11(9)15)17-8-2-4-10(14)12(16)6-8/h1-6H	6.36	552	0.248	9.23	0	4.34	B	B	B	B	
693	T	59365-60-5	InChI=1S/C8H9ClO2/c9-7-4-2-1-3-6(7)8(11)5-10/h1-4,8,10-11H,5H2	1.17	152	0.871	40.46	2	0.25	nB	nB	nB	nB	
694	V	60123-65-1	InChI=1S/C12H5Cl5O/c13-7-2-1-6(3-8(7)14)18-12-5-10(16)9(15)4-11(12)17/h1-5H	6.6	627	0.187	9.23	0	4.08	B	B	B	B	
695	#N/A	60782-58-3	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	1.51	nB	#N/A	#N/A	#N/A	Silicon containing compound
696	T	26850-12-4	InChI=1S/C23H26ClN5O7/c1-4-23(32)25-22-14-17(28(9-11-35-15(2)30)10-12-36-16(3)31)5-8-21(22)27-26-20-7-6-18(29(33)34)13-19(20)24/h5-8,13-14H,4,9-12H2,1-3H3,(H,25,32)/b27-26+	3.7	4529	1.469	152.8	9	0.73	nB	nB	nB	nB	
697	V	62615-08-1	InChI=1S/C12H4Cl4O/c13-5-1-2-8-6(3-5)10-9(17-8)4-7(14)11(15)12(10)16/h1-4H	6.23	457	0.265	13.14	0	3.11	B	B	B	B	
698	V	71767-67-4	InChI=1S/C18H14Cl2N6O2/c19-16-11-15(26(27)28)12-17(20)18(16)24-23-13-3-5-14(6-4-13)25(9-1-7-21)10-2-8-22/h3-6,11-12H,1-2,9-10H2/b24-23+	5	2430	0.872	118.68	5	1.58	nB	B	B	B	
699	T	83704-22-7	InChI=1S/C12H4Cl4O/c13-5-1-2-6-8(3-5)17-9-4-7(14)11(15)12(16)10(6)9/h1-4H	6.16	461	0.265	13.14	0	3.41	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
700	T	119168-77-3	InChI=1S/C18H24ClN3O/c1-6-14-15(19)16(22(5)21-14)17(23)20-11-12-7-9-13(10-8-12)18(2,3)4/h7-10H,6,11H2,1-5H3,(H,20,23)	4.61	1343	0.964	46.92	4	2.06	nB	nB	nB	B	
701	T	126690-66-2	InChI=1S/C10H20/c1-8(2)6-10(5)7-9(3)4/h6,8-9H,7H2,1-5H3/b10-6+	4.28	135	0.139	0	0	3.29	B	nB	B	B	
702	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.18	B	#N/A	#N/A	#N/A	CAS N/A
703	T	84-15-1	InChI=1S/C18H14/c1-3-9-15(10-4-1)17-13-7-8-14-18(17)16-11-5-2-6-12-16/h1-14H	6.03	585	0.301	0	0	3.11	B	nB	B	B	
704	T	102-82-9	InChI=1S/C12H27N/c1-4-7-10-13(11-8-5-2)12-9-6-3/h4-12H2,1-3H3	4.02	300	0.745	3.24	1	1.20	nB	nB	B	B	
705	V	117-18-0	InChI=1S/C6HCl4NO2/c7-2-1-3(8)5(10)6(4(2)9)11(12)13/h1H	4.38	222	-0.217	43.14	0	3.27	B	nB	nB	B	
706	V	2439-10-3	InChI=1S/C13H29N3/c1-2-3-4-5-6-7-8-9-10-11-12-16-13(14)15/h2-12H2,1H3,(H4,14,15,16)	4.26	667	1.24	64.4	3	1.20	nB	nB	nB	B	
707	V	101-42-8	InChI=1S/C9H12N2O/c1-11(2)9(12)10-8-6-4-3-5-7-8/h3-7H,1-2H3,(H,10,12)	0.98	212	0.892	32.34	3	0.78	nB	nB	nB	nB	
708	V	1014-69-3	InChI=1S/C8H15N5S/c1-5(2)10-7-11-6(9-3)12-8(13-7)14-4/h5H,1-4H3,(H2,9,10,11,12,13)	2.38	312	1.609	88.03	5	1.32	nB	nB	nB	nB	
709	T	102851-06-9	InChI=1S/C26H22ClF3N2O3/c1-16(2)24(32-22-12-11-18(14-21(22)27)26(28,29)30)25(33)35-23(15-31)17-7-6-10-20(13-17)34-19-8-4-3-5-9-19/h3-14,16,23-24,32H,1-2H3/t23?,24-/m1/s1	7.72	4160	1.403	71.35	4	2.30	nB	B	B	B	
710	V	10453-86-8	InChI=1S/C22H26O3/c1-15(2)10-19-20(22(19,3)4)21(23)25-14-17-12-18(24-13-17)11-16-8-6-5-7-9-16/h5-10,12-13,19-20H,11,14H2,1-4H3	6.14	1786	0.632	39.44	2	2.66	nB	nB	B	B	
711	T	1071-83-6	InChI=1S/C3H8NO5P/c5-3(6)1-4-2-10(7,8)9/h4H,1-2H2,(H,5,6)(H2,7,8,9)	-3.4	139	3.076	116.67	6	-0.30	nB	nB	nB	nB	
712	T	107534-96-3	InChI=1S/C16H22ClN3O/c1-15(2,3)16(21,10-20-12-18-11-19-20)9-8-13-4-6-14(17)7-5-13/h4-7,11-12,21H,8-10H2,1-3H3	3.7	963	0.853	50.94	4	1.95	nB	nB	nB	nB	
713	T	111479-05-1	InChI=1S/C22H22ClN3O5/c1-14(2)26-29-11-10-28-22(27)15(3)30-17-5-7-18(8-6-17)31-21-13-24-20-12-16(23)4-9-19(20)25-21/h4-9,12-13,15H,10-11H2,1-3H3	4.6	3548	1.819	92.13	4	2.77	nB	nB	nB	B	
714	T	112410-23-8	InChI=1S/C22H28N2O2/c1-7-17-8-10-18(11-9-17)20(25)23-24(22(4,5)6)21(26)19-13-15(2)12-16(3)14-19/h8-14H,7H2,1-6H3,(H,23,25)	4.25	1705	0.321	49.41	4	1.85	nB	nB	nB	nB	
715	T	113136-77-9	InChI=1S/C11H9Cl2NO3/c12-6-1-2-8(7(13)5-6)14-9(15)11(3-4-11)10(16)17/h1-2,5H,3-4H2,(H,14,15)(H,16,17)	2.77	527	0.886	66.4	4	-0.40	nB	nB	nB	nB	
716	T	114311-32-9	InChI=1S/C15H19N3O4/c1-8(2)15(3)14(21)17-12(18-15)11-10(13(19)20)5-9(6-16-11)7-22-4/h5-6,8H,7H2,1-4H3,(H,19,20)(H,17,18,21)	0.73	1028	2.274	100.88	7	-0.30	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
717	T	116255-48-2	InChI=1S/C13H12BrCl2N3O/c14-9-4-13(20-5-9,6-19-8-17-7-18-19)11-2-1-10(15)3-12(11)16/h1-3,7-9H,4-6H2	3.24	753	0.773	39.94	4	2.12	nB	nB	nB	nB	
718	T	120116-88-3	InChI=1S/C13H13ClN4O2S/c1-9-4-6-10(7-5-9)12-13(14)16-11(8-15)18(12)21(19,20)17(2)3/h4-7H,1-3H3	2.63	840	1.053	87.37	6	2.46	nB	nB	nB	nB	
719	V	120923-37-7	InChI=1S/C9H15N5O7S2/c1-14(22(4,16)17)23(18,19)13-9(15)12-8-10-6(20-2)5-7(11-8)21-3/h5H,1-4H3,(H2,10,11,12,13,15)	1.63	1270	1.5	173.65	10	0.69	nB	nB	nB	nB	
720	T	121552-61-2	InChI=1S/C14H15N3/c1-10-9-13(11-7-8-11)17-14(15-10)16-12-5-3-2-4-6-12/h2-6,9,11H,7-8H2,1H3,(H,15,16,17)	4	539	1.445	37.81	3	2.59	nB	nB	nB	B	
721	V	122008-85-9	InChI=1S/C20H20FNO4/c1-3-4-11-24-20(23)14(2)25-16-6-8-17(9-7-16)26-19-10-5-15(13-22)12-18(19)21/h5-10,12,14H,3-4,11H2,1-2H3/t14-/m1/s1	4.81	2079	1.05	68.55	3	0.88	nB	B	B	B	
722	T	126535-15-7	InChI=1S/C17H19F3N6O6S/c1-9-6-5-7-10(12(27)31-4)11(9)33(29,30)25-15(28)22-13-21-14(26(2)3)24-16(23-13)32-8-17(18,19)20/h5-7H,8H2,1-4H3,(H2,21,22,23,24,25,28)	2.84	3376	1.712	161.09	11	0.11	nB	nB	nB	nB	
723	V	128639-02-1	InChI=1S/C15H14Cl2F3N3O3/c1-3-26-13(24)10(17)4-8-5-12(11(18)6-9(8)16)23-15(25)22(14(19)20)7(2)21-23/h5-6,10,14H,3-4H2,1-2H3	3.36	1687	1.377	62.21	6	2.25	nB	nB	nB	nB	
724	T	13071-79-9	InChI=1S/C9H21O2PS3/c1-6-10-12(13,11-7-2)15-8-14-9(3,4)5/h6-8H2,1-5H3	4.48	412	2.155	110.96	2	2.46	nB	nB	B	B	
725	#N/A	13121-70-5	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	4.00	B	#N/A	#N/A	#N/A	Tin containing compound
726	#N/A	131983-72-7	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	1.18	nB	#N/A	#N/A	#N/A	Structure and CAS did not match
727	T	132-66-1	InChI=1S/C18H13NO3/c20-17(14-9-3-4-10-15(14)18(21)22)19-16-11-5-7-12-6-1-2-8-13(12)16/h1-11H,(H,19,20)(H,21,22)	3.53	1049	1.025	66.4	4	2.20	nB	nB	nB	nB	
728	V	136426-54-5	InChI=1S/C16H8Cl2FN5O/c17-9-1-4-14(12(18)5-9)24-15(25)11-6-10(19)2-3-13(11)22-16(24)23-8-20-7-21-23/h1-8H	3.24	1333	1.397	63.38	6	1.94	nB	nB	nB	nB	
729	V	144-54-7	InChI=1S/C2H5NS2/c1-3-2(4)5/h1H3,(H2,3,4,5)	0.72	18	0.69	82.92	1	-1.52	nB	nB	nB	nB	
730	T	138261-41-3	InChI=1S/C9H10ClN5O2/c10-8-2-1-7(5-12-8)6-14-4-3-11-9(14)13-15(16)17/h1-2,5H,3-4,6H2,(H,11,13)	0.78	559	1.532	83.66	4	-0.22	nB	nB	nB	nB	
731	T	139-40-2	InChI=1S/C9H16ClN5/c1-5(2)11-8-13-7(10)14-9(15-8)12-6(3)4/h5-6H,1-4H3,(H2,11,12,13,14,15)	2.93	386	1.452	62.73	5	1.79	nB	nB	nB	nB	
732	T	141517-21-7	InChI=1S/C20H19F3N2O4/c1-13(14-8-6-9-16(11-14)20(21,22)23)24-29-12-15-7-4-5-10-17(15)18(25-28-3)19(26)27-2/h4-11H,12H2,1-3H3/b24-13+,25-18-	4.22	2512	1.228	69.48	2	2.63	nB	nB	nB	B	
733	V	141-66-2	InChI=1S/C8H16NO5P/c1-7(6-8(10)9(2)3)14-15(11,12-4)13-5/h6H,1-5H3/b7-6+	0	400	2.573	74.88	6	1.88	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
734	V	142891-20-1	InChI=1S/C19H17Cl2NO4/c1-2-26-19(25)16(21)10-11-9-12(7-8-15(11)20)22-17(23)13-5-3-4-6-14(13)18(22)24/h7-10H,2-6H2,1H3/b16-10-	4.55	1685	0.794	63.68	5	1.38	nB	nB	nB	B	
735	T	145701-23-1	InChI=1S/C12H8F3N5O3S/c1-23-12-16-5-8(15)10-17-11(18-20(10)12)24(21,22)19-9-6(13)3-2-4-7(9)14/h2-5,19H,1H3	1.56	1296	1.945	106.86	7	0.18	nB	nB	nB	nB	
736	T	149961-52-4	InChI=1S/C19H22N2O3/c1-13-9-10-14(2)17(11-13)24-12-15-7-5-6-8-16(15)18(21-23-4)19(22)20-3/h5-11H,12H2,1-4H3,(H,20,22)/b21-18+	3.19	1386	1.386	59.92	2	1.68	nB	nB	nB	nB	
737	V	15299-99-7	InChI=1S/C17H21NO2/c1-4-18(5-2)17(19)13(3)20-16-12-8-10-14-9-6-7-11-15(14)16/h6-13H,4-5H2,1-3H3	3.36	832	1.129	29.54	2	1.99	nB	nB	nB	nB	
738	T	1689-83-4	InChI=1S/C7H3I2NO/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2,11H	3.43	148	0.298	44.02	1	1.87	nB	nB	nB	nB	
739	T	175013-18-0	InChI=1S/C19H18ClN3O4/c1-25-19(24)23(26-2)17-6-4-3-5-14(17)13-27-18-11-12-22(21-18)16-9-7-15(20)8-10-16/h3-12H,13H2,1-2H3	4.13	2067	1.017	65.3	4	2.85	nB	nB	nB	nB	
740	T	180409-60-3	InChI=1S/C20H17F5N2O2/c21-15-9-8-14(20(23,24)25)17(18(15)22)19(27-29-11-13-6-7-13)26-16(28)10-12-4-2-1-3-5-12/h1-5,8-9,13H,6-7,10-11H2,(H,26,27,28)	4.99	2233	1.076	50.69	2	2.72	nB	B	B	B	
741	T	18854-01-8	InChI=1S/C13H16NO4PS/c1-3-15-19(20,16-4-2)18-13-10-12(17-14-13)11-8-6-5-7-9-11/h5-10H,3-4H2,1-2H3	3.73	876	2.287	95.62	2	2.86	nB	nB	nB	B	
742	T	19044-88-3	InChI=1S/C12H18N4O6S/c1-3-5-14(6-4-2)12-10(15(17)18)7-9(23(13,21)22)8-11(12)16(19)20/h7-8H,3-6H2,1-2H3,(H2,13,21,22)	3.73	1082	0.179	158.06	4	1.85	nB	nB	nB	nB	
743	V	1982-47-4	InChI=1S/C15H15ClN2O2/c1-18(2)15(19)17-12-5-9-14(10-6-12)20-13-7-3-11(16)4-8-13/h3-10H,1-2H3,(H,17,19)	3.7	962	1.044	41.57	3	2.02	nB	nB	nB	nB	
744	T	2032-65-7	InChI=1S/C11H15NO2S/c1-7-5-9(14-11(13)12-3)6-8(2)10(7)15-4/h5-6H,1-4H3,(H,12,13)	2.92	380	0.584	63.63	2	1.88	nB	nB	nB	nB	
745	V	2164-17-2	InChI=1S/C10H11F3N2O/c1-15(2)9(16)14-8-5-3-4-7(6-8)10(11,12)13/h3-6H,1-2H3,(H,14,16)	2.42	457	0.768	32.34	3	1.61	nB	nB	nB	nB	
746	T	2212-67-1	InChI=1S/C9H17NOS/c1-2-12-9(11)10-7-5-3-4-6-8-10/h2-8H2,1H3	3.21	206	1.233	45.61	2	1.86	nB	nB	nB	nB	
747	T	2227-17-0	InChI=1S/C10Cl10/c11-1-2(12)6(16)9(19,5(1)15)10(20)7(17)3(13)4(14)8(10)18	6.27	650	0.158	0	0	6.43	B	B	B	B	
748	V	3337-71-1	InChI=1S/C8H10N2O4S/c1-14-8(11)10-15(12,13)7-4-2-6(9)3-5-7/h2-5H,9H2,1H3,(H,10,11)	-0.27	378	0.373	106.87	6	-0.13	nB	nB	nB	nB	
749	T	23505-41-1	InChI=1S/C13H24N3O3PS/c1-6-16(7-2)13-14-11(5)10-12(15-13)19-20(21,17-8-3)18-9-4/h10H,6-9H2,1-5H3	4.85	952	2.785	98.61	5	3.48	B	B	B	B	
750	T	23564-05-8	InChI=1S/C12H14N4O4S2/c1-19-11(17)15-9(21)13-7-5-3-4-6-8(7)14-10(22)16-12(18)20-2/h3-6H,1-2H3,(H2,13,15,17,21)(H2,14,16,18,22)	1.4	1189	1.755	164.9	8	1.88	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
751	T	2385-85-5	InChI=1S/C10Cl12/c11-1-2(12)7(17)4(14)3(13,5(1,15)9(7,19)20)6(1,16)10(21,22)8(2,4)18	6.89	680	0.647	0	0	4.71	B	nB	B	B	
752	V	24017-47-8	InChI=1S/C12H16N3O3PS/c1-3-16-19(20,17-4-2)18-12-13-10-15(14-12)11-8-6-5-7-9-11/h5-10H,3-4H2,1-2H3	3.34	876	2.763	99.78	5	2.48	nB	nB	nB	nB	
753	T	26002-80-2	InChI=1S/C23H26O3/c1-16(2)13-20-21(23(20,3)4)22(24)25-15-17-9-8-12-19(14-17)26-18-10-6-5-7-11-18/h5-14,20-21H,15H2,1-4H3	6.24	1945	0.818	35.53	2	2.86	nB	nB	B	B	
754	T	2675-77-6	InChI=1S/C8H8Cl2O2/c1-11-7-3-6(10)8(12-2)4-5(7)9/h3-4H,1-2H3	3.11	192	0.429	18.46	0	2.22	nB	nB	nB	nB	
755	T	283594-90-1	InChI=1S/C23H30O4/c1-14-11-15(2)18(16(3)12-14)19-20(26-17(24)13-22(4,5)6)23(27-21(19)25)9-7-8-10-23/h11-12H,7-10,13H2,1-6H3	5.14	1679	0.999	52.6	4	2.74	nB	B	B	B	
756	T	298-00-0	InChI=1S/C8H10NO5PS/c1-12-15(16,13-2)14-8-5-3-7(4-6-8)9(10)11/h3-6H,1-2H3	2.86	473	1.779	112.73	2	1.85	nB	nB	nB	nB	
757	T	299-86-5	InChI=1S/C12H19ClNO3P/c1-12(2,3)9-6-7-11(10(13)8-9)17-18(15,14-4)16-5/h6-8H,1-5H3,(H,14,15)	3.42	622	1.478	57.37	3	2.36	nB	nB	nB	nB	
758	V	309-00-2	InChI=1S/C12H8Cl6/c13-8-9(14)11(16)7-5-2-1-4(3-5)6(7)10(8,15)12(11,17)18/h1-2,4-7H,3H2	6.5	448	0.286	0	0	3.78	B	B	B	B	
759	T	3347-22-6	InChI=1S/C14H4N2O2S2/c15-5-9-10(6-16)20-14-12(18)8-4-2-1-3-7(8)11(17)13(14)19-9/h1-4H	2.84	724	1.659	132.32	4	1.43	nB	nB	nB	nB	
760	V	33629-47-9	InChI=1S/C14H21N3O4/c1-6-9(2)15-13-11(16(18)19)7-10(14(3,4)5)8-12(13)17(20)21/h7-9,15H,6H2,1-5H3	4.93	860	0.028	98.31	1	3.29	B	B	B	B	
761	T	35367-38-5	InChI=1S/C14H9ClF2N2O2/c15-8-4-6-9(7-5-8)18-14(21)19-13(20)12-10(16)2-1-3-11(12)17/h1-7H,(H2,18,19,20,21)	3.88	1020	0.606	58.2	4	2.51	nB	nB	nB	nB	
762	V	35554-44-0	InChI=1S/C14H14Cl2N2O/c1-2-7-19-14(9-18-6-5-17-10-18)12-4-3-11(15)8-13(12)16/h2-6,8,10,14H,1,7,9H2	3.82	721	0.88	27.05	3	1.81	nB	nB	nB	B	
763	V	374726-62-2	InChI=1S/C23H22ClNO4/c1-4-14-28-20-11-6-17(16-21(20)27-3)12-13-25-23(26)22(29-15-5-2)18-7-9-19(24)10-8-18/h1-2,6-11,16,22H,12-15H2,3H3,(H,25,26)	3.87	2662	1.258	56.79	3	1.68	nB	nB	nB	B	
764	T	39196-18-4	InChI=1S/C9H18N2O2S/c1-9(2,3)7(6-14-5)11-13-8(12)10-4/h6H2,1-5H3,(H,10,12)/b11-7-	2.75	332	0.852	75.99	2	1.15	nB	nB	nB	nB	
765	T	40487-42-1	InChI=1S/C13H19N3O4/c1-5-10(6-2)14-12-11(15(17)18)7-8(3)9(4)13(12)16(19)20/h7,10,14H,5-6H2,1-4H3	5.18	747	-0.027	98.31	1	3.71	B	B	B	B	
766	T	4151-50-2	InChI=1S/C10H6F17NO2S/c1-2-28-31(29,30)10(26,27)8(21,22)6(17,18)4(13,14)3(11,12)5(15,16)7(19,20)9(23,24)25/h28H,2H2,1H3	5.6	2278	0.232	54.55	3	2.70	nB	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
767	T	42576-02-3	InChI=1S/C14H9Cl2NO5/c1-21-14(18)10-7-9(3-4-12(10)17(19)20)22-13-5-2-8(15)6-11(13)16/h2-7H,1H3	4.48	1089	0.407	78.67	2	3.18	B	nB	nB	B	
768	V	50563-36-5	InChI=1S/C13H18ClNO2/c1-10-5-4-6-11(2)13(10)15(7-8-17-3)12(16)9-14/h4-6H,7-9H2,1-3H3	2.17	504	0.704	29.54	3	1.88	nB	nB	nB	nB	
769	V	51218-45-2	InChI=1S/C15H22ClNO2/c1-5-13-8-6-7-11(2)15(13)17(14(18)9-16)12(3)10-19-4/h6-8,12H,5,9-10H2,1-4H3	3.13	656	0.722	29.54	3	1.84	nB	nB	nB	nB	
770	T	52315-07-8	InChI=1S/C22H19Cl2NO3/c1-22(2)17(12-19(23)24)20(22)21(26)28-18(13-25)14-7-6-10-16(11-14)27-15-8-4-3-5-9-15/h3-12,17-18,20H,1-2H3	6.05	2244	1.085	59.32	3	2.82	nB	nB	B	B	
771	T	5259-88-1	InChI=1S/C12H13NO4S/c1-9-11(18(15,16)8-7-17-9)12(14)13-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3,(H,13,14)	0.77	599	1.594	80.85	5	-0.05	nB	nB	nB	nB	
772	T	52645-53-1	InChI=1S/C21H20Cl2O3/c1-21(2)17(12-18(22)23)19(21)20(24)25-13-14-7-6-10-16(11-14)26-15-8-4-3-5-9-15/h3-12,17,19H,13H2,1-2H3	6.5	1945	0.804	35.53	2	2.48	nB	nB	B	B	
773	V	52888-80-9	InChI=1S/C14H21NOS/c1-3-10-15(11-4-2)14(16)17-12-13-8-6-5-7-9-13/h5-9H,3-4,10-12H2,1-2H3	4.65	596	1.008	45.61	2	2.85	nB	B	B	B	
774	V	533-74-4	InChI=1S/C5H10N2S2/c1-6-3-7(2)5(8)9-4-6/h3-4H2,1-2H3	1.4	84	1.63	63.87	2	0.49	nB	nB	nB	nB	
775	T	55512-33-9	InChI=1S/C19H23ClN2O2S/c1-2-3-4-5-6-10-13-25-19(23)24-16-14-17(20)21-22-18(16)15-11-8-7-9-12-15/h7-9,11-12,14H,2-6,10,13H2,1H3	6.58	1822	1.164	77.38	3	2.06	nB	nB	B	B	
776	T	55634-91-8	InChI=1S/C17H25NO5/c1-6-8-11(18-23-9-7-2)13-12(19)10-17(3,4)14(15(13)20)16(21)22-5/h7,14,18H,2,6,8-10H2,1,3-5H3/b13-11-	3.61	1148	1.395	81.7	4	0.65	nB	nB	nB	nB	
777	T	55814-41-0	InChI=1S/C17H19NO2/c1-12(2)20-15-9-6-8-14(11-15)18-17(19)16-10-5-4-7-13(16)3/h4-12H,1-3H3,(H,18,19)	3.66	880	0.829	38.33	2	2.43	nB	nB	nB	B	
778	T	584-79-2	InChI=1S/C19H26O3/c1-7-8-13-12(4)16(10-15(13)20)22-18(21)17-14(9-11(2)3)19(17,5)6/h7,9,14,16-17H,1,8,10H2,2-6H3	4.78	1112	0.89	43.37	3	3.28	B	nB	B	B	
779	V	58-89-9	InChI=1S/C6H6Cl6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-6H	3.72	174	0.215	0	0	2.70	nB	nB	B	B	
780	T	59669-26-0	InChI=1S/C10H18N4O4S3/c1-7(19-5)11-17-9(15)13(3)21-14(4)10(16)18-12-8(2)20-6/h1-6H3/b11-7+,12-8+	1.7	1140	0.617	159.7	4	0.80	nB	nB	nB	nB	
781	T	59682-52-9	InChI=1S/C3H8NO4P/c1-2-8-9(6,7)3(4)5/h2H2,1H3,(H2,4,5)(H,6,7)	-1.49	90	2.641	99.43	5	1.08	nB	nB	nB	nB	
782	V	60168-88-9	InChI=1S/C17H12Cl2N2O/c18-14-7-5-12(6-8-14)17(22,13-9-20-11-21-10-13)15-3-1-2-4-16(15)19/h1-11,22H	3.6	942	1.473	46.01	3	2.05	nB	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
783	T	61213-25-0	InChI=1S/C12H10Cl2F3NO/c13-5-7-6-18(11(19)10(7)14)9-3-1-2-8(4-9)12(15,16)17/h1-4,7,10H,5-6H2	3.36	684	0.448	20.31	2	2.47	nB	nB	nB	nB	
784	T	63-25-2	InChI=1S/C12H11NO2/c1-13-12(14)15-11-8-4-6-9-5-2-3-7-10(9)11/h2-8H,1H3,(H,13,14)	2.36	362	0.534	38.33	2	1.64	nB	nB	nB	nB	
785	T	640-15-3	InChI=1S/C6H15O2PS3/c1-4-11-5-6-12-9(10,7-2)8-3/h4-6H2,1-3H3	3.15	234	2.104	110.96	2	2.24	nB	nB	nB	nB	
786	T	64-19-7	InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)	-0.21	9	0.411	37.3	2	0.51	nB	nB	nB	nB	
787	T	65733-16-6	InChI=1S/C19H34O3/c1-15(2)22-18(20)14-17(4)11-8-10-16(3)12-9-13-19(5,6)21-7/h8,11,14-16H,9-10,12-13H2,1-7H3/b11-8+,17-14+	5.5	1414	0.762	35.53	3	2.66	nB	nB	B	B	
788	T	66063-05-6	InChI=1S/C19H21ClN2O/c20-16-12-10-15(11-13-16)14-22(18-8-4-5-9-18)19(23)21-17-6-2-1-3-7-17/h1-3,6-7,10-13,18H,4-5,8-9,14H2,(H,21,23)	4.82	1237	0.933	32.34	3	2.35	nB	nB	B	B	
789	T	66246-88-6	InChI=1S/C13H15Cl2N3/c1-2-3-10(7-18-9-16-8-17-18)12-5-4-11(14)6-13(12)15/h4-6,8-10H,2-3,7H2,1H3	3.52	615	0.423	30.71	3	2.24	nB	nB	nB	nB	
790	T	66441-23-4	InChI=1S/C18H16ClNO5/c1-3-22-17(21)11(2)23-13-5-7-14(8-6-13)24-18-20-15-9-4-12(19)10-16(15)25-18/h4-11H,3H2,1-2H3	4.12	1795	1.124	70.79	3	1.61	nB	nB	nB	B	
791	V	66841-25-6	InChI=1S/C22H19Br4NO3/c1-21(2)17(19(23)22(24,25)26)18(21)20(28)30-16(12-27)13-7-6-10-15(11-13)29-14-8-4-3-5-9-14/h3-11,16-19H,1-2H3/t16-,17-,18+,19+/m1/s1	7.95	2661	1.075	59.32	3	3.08	B	B	B	B	
792	T	62-49-7	InChI=1S/C5H14NO/c1-6(2,3)4-5-7/h7H,4-5H2,1-3H3/q+1	-0.4	46	0.399	20.23	1	-0.23	nB	nB	nB	nB	
793	T	67564-91-4	InChI=1S/C20H33NO/c1-15(12-21-13-16(2)22-17(3)14-21)11-18-7-9-19(10-8-18)20(4,5)6/h7-10,15-17H,11-14H2,1-6H3/t15?,16-,17+	4.93	1212	1.211	12.47	2	2.83	nB	B	B	B	
794	T	67747-09-5	InChI=1S/C15H16Cl3N3O2/c1-2-4-20(15(22)21-5-3-19-10-21)6-7-23-14-12(17)8-11(16)9-13(14)18/h3,5,8-10H,2,4,6-7H2,1H3	4.6	1313	1.386	47.36	4	2.58	nB	nB	nB	B	
795	T	68085-85-8	InChI=1S/C23H19ClF3NO3/c1-22(2)17(12-19(24)23(25,26)27)20(22)21(29)31-18(13-28)14-7-6-10-16(11-14)30-15-8-4-3-5-9-15/h3-12,17-18,20H,1-2H3/b19-12-	6.8	2982	0.972	59.32	3	3.29	B	B	B	B	
796	T	68359-37-5	InChI=1S/C22H18Cl2FNO3/c1-22(2)15(11-19(23)24)20(22)21(27)29-18(12-26)13-8-9-16(25)17(10-13)28-14-6-4-3-5-7-14/h3-11,15,18,20H,1-2H3	5.95	2425	1.105	59.32	3	2.70	nB	B	B	B	
797	V	69377-81-7	InChI=1S/C7H5Cl2FN2O3/c8-3-5(11)4(9)7(12-6(3)10)15-1-2(13)14/h1H2,(H2,11,12)(H,13,14)	0.9	372	1.184	85.44	4	1.79	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
798	T	70124-77-5	InChI=1S/C26H23F2NO4/c1-17(2)24(18-11-13-21(14-12-18)32-26(27)28)25(30)33-23(16-29)19-7-6-10-22(15-19)31-20-8-4-3-5-9-20/h3-15,17,23-24,26H,1-2H3	6.2	3560	1.217	68.55	3	4.07	B	B	B	B	
799	T	7085-19-0	InChI=1S/C10H11ClO3/c1-6-5-8(11)3-4-9(6)14-7(2)10(12)13/h3-5,7H,1-2H3,(H,12,13)	3.13	316	0.627	46.53	2	0.48	nB	nB	nB	nB	
800	V	731-27-1	InChI=1S/C10H13Cl2FN2O2S2/c1-8-4-6-9(7-5-8)15(18-10(11,12)13)19(16,17)14(2)3/h4-7H,1-3H3	3.9	664	0.485	74.3	4	1.87	nB	nB	nB	nB	
801	T	74115-24-5	InChI=1S/C14H8Cl2N4/c15-11-7-3-1-5-9(11)13-17-19-14(20-18-13)10-6-2-4-8-12(10)16/h1-8H	3.1	852	1.059	51.56	4	2.39	nB	nB	nB	nB	
802	V	74223-64-6	InChI=1S/C14H15N5O6S/c1-8-15-12(18-14(16-8)25-3)17-13(21)19-26(22,23)10-7-5-4-6-9(10)11(20)24-2/h4-7H,1-3H3,(H2,15,16,17,18,19,21)	2.2	1753	1.592	157.85	10	0.00	nB	nB	nB	nB	
803	T	77-73-6	InChI=1S/C10H12/c1-2-9-7-4-5-8(6-7)10(9)3-1/h1-2,4-5,7-10H,3,6H2	2.48	98	0.159	0	0	2.40	nB	nB	nB	nB	
804	T	78-48-8	InChI=1S/C12H27OPS3/c1-4-7-10-15-14(13,16-11-8-5-2)17-12-9-6-3/h4-12H2,1-3H3	5.7	616	2.113	102.78	1	3.48	B	B	B	B	
805	T	786-19-6	InChI=1S/C11H16ClO2PS3/c1-3-13-15(16,14-4-2)18-9-17-11-7-5-10(12)6-8-11/h5-8H,3-4,9H2,1-2H3	5.33	708	2.095	110.96	2	3.00	B	B	B	B	
806	T	79127-80-3	InChI=1S/C17H19NO4/c1-2-20-17(19)18-12-13-21-14-8-10-16(11-9-14)22-15-6-4-3-5-7-15/h3-11H,2,12-13H2,1H3,(H,18,19)	4.3	1386	0.894	56.79	3	2.33	nB	nB	nB	B	
807	V	79277-27-3	InChI=1S/C12H13N5O6S2/c1-6-13-10(16-12(14-6)23-3)15-11(19)17-25(20,21)7-4-5-24-8(7)9(18)22-2/h4-5H,1-3H3,(H2,13,14,15,16,17,19)	1.56	1591	1.613	186.09	10	-0.10	nB	nB	nB	nB	
808	#N/A	8001-35-2	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	4.04	B	#N/A	#N/A	#N/A	Mixture
809	T	80-33-1	InChI=1S/C12H8Cl2O3S/c13-9-1-5-11(6-2-9)17-18(15,16)12-7-3-10(14)4-8-12/h1-8H	4.32	638	0.758	51.75	2	2.48	nB	nB	nB	B	
810	V	81335-37-7	InChI=1S/C17H17N3O3/c1-9(2)17(3)16(23)19-14(20-17)13-11(15(21)22)8-10-6-4-5-7-12(10)18-13/h4-9H,1-3H3,(H,21,22)(H,19,20,23)	1.86	1103	2.127	91.65	6	-0.41	nB	nB	nB	nB	
811	T	81777-89-1	InChI=1S/C12H14ClNO2/c1-12(2)8-16-14(11(12)15)7-9-5-3-4-6-10(9)13/h3-6H,7-8H2,1-2H3	2.5	436	0.6	29.54	1	1.60	nB	nB	nB	nB	
812	T	82558-50-7	InChI=1S/C18H24N2O4/c1-6-18(3,7-2)14-11-15(24-20-14)19-17(21)16-12(22-4)9-8-10-13(16)23-5/h8-11H,6-7H2,1-5H3,(H,19,21)	3.94	1387	1.247	73.59	2	1.85	nB	nB	nB	B	
813	T	82560-54-1	InChI=1S/C20H30N2O5S/c1-7-25-17(23)11-12-22(14(2)3)28-21(6)19(24)26-16-10-8-9-15-13-20(4,5)27-18(15)16/h8-10,14H,7,11-13H2,1-6H3	4.3	2276	0.647	93.61	5	1.95	nB	nB	nB	nB	
814	T	82657-04-3	InChI=1S/C23H22ClF3O2/c1-14-16(10-7-11-17(14)15-8-5-4-6-9-15)13-29-21(28)20-18(22(20,2)3)12-19(24)23(25,26)27/h4-12,18,20H,13H2,1-3H3/b19-12-	6	2490	0.514	26.3	2	3.23	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
815	V	886-50-0	InChI=1S/C10H19N5S/c1-6-11-7-12-8(15-10(2,3)4)14-9(13-7)16-5/h6H2,1-5H3,(H2,11,12,13,14,15)	3.74	452	1.642	88.03	5	1.86	nB	nB	nB	nB	
816	T	90035-08-8	InChI=1S/C33H25F3O4/c34-33(35,36)24-13-9-20(10-14-24)19-39-25-15-11-21(12-16-25)23-17-22-5-1-2-6-26(22)28(18-23)30-31(37)27-7-3-4-8-29(27)40-32(30)38/h1-16,23,28,37H,17-19H2	8.53	6000	1.256	55.76	2	3.30	B	nB	nB	B	
817	#N/A	900-95-8	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	3.40	B	#N/A	#N/A	#N/A	Tin containing compound
818	T	92-52-4	InChI=1S/C12H10/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-10H	3.98	198	0.219	0	0	3.43	B	nB	B	B	
819	V	94361-06-5	InChI=1S/C15H18ClN3O/c1-11(12-2-3-12)15(20,8-19-10-17-9-18-19)13-4-6-14(16)7-5-13/h4-7,9-12,20H,2-3,8H2,1H3	2.9	767	0.955	50.94	4	1.45	nB	nB	nB	nB	
820	T	98886-44-3	InChI=1S/C9H18NO3PS2/c1-4-8(3)16-14(12,13-5-2)10-6-7-15-9(10)11/h8H,4-7H2,1-3H3	1.68	424	1.602	107.02	4	0.51	nB	nB	nB	nB	
821	T	99-30-9	InChI=1S/C6H4Cl2N2O2/c7-4-1-3(10(11)12)2-5(8)6(4)9/h1-2H,9H2	2.8	188	0.088	69.16	1	1.88	nB	nB	nB	nB	
822	T	108-39-4	InChI=1S/C7H8O/c1-6-3-2-4-7(8)5-6/h2-5,8H,1H3	1.96	61	0.429	20.23	0	1.03	nB	nB	nB	nB	
823	T	1779-48-2	InChI=1S/C6H7O2P/c7-9(8)6-4-2-1-3-5-6/h1-5,9H,(H,7,8)	0.9	88	1.95	60.77	2	-0.59	nB	nB	nB	nB	
824	#N/A	25155-30-0	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	2.02	nB	#N/A	#N/A	#N/A	Incompletely defined compound
825	T	119446-68-3	InChI=1S/C19H17Cl2N3O3/c1-13-9-25-19(27-13,10-24-12-22-11-23-24)17-7-6-16(8-18(17)21)26-15-4-2-14(20)3-5-15/h2-8,11-13H,9-10H2,1H3	4.3	1930	1.331	58.4	5	2.51	nB	nB	nB	nB	
826	T	50-29-3	InChI=1S/C14H9Cl5/c15-11-5-1-9(2-6-11)13(14(17,18)19)10-3-7-12(16)8-4-10/h1-8,13H	6.91	678	0.165	0	0	3.60	B	B	B	B	
827	T	55-38-9	InChI=1S/C10H15O3PS2/c1-8-7-9(5-6-10(8)16-4)13-14(15,11-2)12-3/h5-7H,1-4H3	4.09	457	2.141	94.89	2	2.26	nB	nB	B	B	
828	T	57-15-8	InChI=1S/C4H7Cl3O/c1-3(2,8)4(5,6)7/h8H,1-2H3	2.03	58	0.424	20.23	1	0.30	nB	nB	nB	nB	
829	T	62-56-6	InChI=1S/CH4N2S/c2-1(3)4/h(H4,2,3,4)	-0.83	9	1.104	84.13	2	-0.20	nB	nB	nB	nB	
830	T	75-71-8	InChI=1S/CCl2F2/c2-1(3,4)5	2.27	16	-0.048	0	0	0.88	nB	nB	nB	nB	
831	V	76-83-5	InChI=1S/C19H15Cl/c20-19(16-10-4-1-5-11-16,17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15H	5.25	730	0.273	0	0	2.62	nB	B	B	B	
832	T	77-47-4	InChI=1S/C5Cl6/cc6-1-2(7)4(9)5(10,11)3(1)8	5.04	132	0.094	0	0	1.18	nB	B	B	B	
833	T	78-42-2	InChI=1S/C24H51O4P/c1-7-13-16-22(10-4)19-26-29(25,27-20-23(11-5)17-14-8-2)28-21-24(12-6)18-15-9-3/h22-24H,7-21H2,1-6H3	8.9	2560	1.902	54.57	4	1.01	nB	nB	B	B	
834	T	78-79-5	InChI=1S/C5H8/c1-4-5(2)3/h4H,1-2H2,3H3	2.42	18	0.127	0	0	1.13	nB	nB	nB	nB	
835	T	79-94-7	InChI=1S/C15H12Br4O2/c1-15(2,7-3-9(16)13(20)10(17)4-7)8-5-11(18)14(21)12(19)6-8/h3-6,20-21H,1-2H3	6.77	876	0.27	40.46	0	2.48	nB	B	B	B	
836	T	80-05-7	InChI=1S/C15H16O2/c1-15(2,11-3-7-13(16)8-4-11)12-5-9-14(17)10-6-12/h3-10,16-17H,1-2H3	3.32	516	0.824	40.46	0	1.39	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
837	T	84-86-6	InChI=1S/C10H9NO3S/c11-9-5-6-10(15(12,13)14)8-4-2-1-3-7(8)9/h1-6H,11H2,(H,12,13,14)	-0.77	326	1.379	88.77	4	0.78	nB	nB	nB	nB	
838	T	86-87-3	InChI=1S/C12H10O2/c13-12(14)8-10-6-3-5-9-4-1-2-7-11(9)10/h1-7H,8H2,(H,13,14)	2.24	292	0.519	37.3	2	0.11	nB	nB	nB	nB	
839	V	87-84-3	InChI=1S/C6H6Br5Cl/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-6H	4.72	174	0.16	0	0	2.45	nB	B	B	B	
840	V	91-23-6	InChI=1S/C7H7NO3/c1-11-7-5-3-2-4-6(7)8(9)10/h2-5H,1H3	1.73	150	0.173	52.37	0	0.49	nB	nB	nB	nB	
841	T	91-57-6	InChI=1S/C11H10/c1-9-6-7-10-4-2-3-5-11(10)8-9/h2-8H,1H3	3.86	144	0.193	0	0	3.11	B	nB	B	B	
842	T	91-66-7	InChI=1S/C10H15N/c1-3-11(4-2)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3	3.31	158	0.461	3.24	1	2.07	nB	nB	nB	nB	
843	T	95-57-8	InChI=1S/C6H5ClO/c7-5-3-1-2-4-6(5)8/h1-4,8H	2.15	60	0.323	20.23	0	1.06	nB	nB	nB	nB	
844	T	95-69-2	InChI=1S/C7H8ClN/c1-5-4-6(8)2-3-7(5)9/h2-4H,9H2,1H3	1.89	84	0.34	26.02	1	1.21	nB	nB	nB	nB	
845	T	95-82-9	InChI=1S/C6H5Cl2N/c7-4-1-2-5(8)6(9)3-4/h1-3H,9H2	2.92	84	0.329	26.02	1	1.29	nB	nB	nB	nB	
846	T	96-45-7	InChI=1S/C3H6N2S/c6-3-4-1-2-5-3/h1-2H2,(H2,4,5,6)	-0.66	26	1.224	56.15	2	-0.29	nB	nB	nB	nB	
847	V	98-10-2	InChI=1S/C6H7NO2S/c7-10(8,9)6-4-2-1-3-5-6/h1-5H,(H2,7,8,9)	0.31	114	0.348	68.54	3	0.36	nB	nB	nB	nB	
848	T	99-65-0	InChI=1S/C6H4N2O4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H	1.49	197	-0.302	86.28	0	0.77	nB	nB	nB	nB	
849	T	99-71-8	InChI=1S/C10H14O/c1-3-8(2)9-4-6-10(11)7-5-9/h4-8,11H,3H2,1-2H3	3.08	160	0.447	20.23	0	1.39	nB	nB	nB	nB	
850	T	100-00-5	InChI=1S/C6H4ClNO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H	2.39	120	-0.122	43.14	0	1.62	nB	nB	nB	nB	
851	T	101-02-0	InChI=1S/C18H15O3P/c1-4-10-16(11-5-1)19-22(20-17-12-6-2-7-13-17)21-18-14-8-3-9-15-18/h1-15H	5.52	1116	2.052	41.28	0	2.39	nB	nB	B	B	
852	T	106-41-2	InChI=1S/C6H5BrO/c7-5-1-3-6(8)4-2-5/h1-4,8H	2.59	62	0.365	20.23	0	1.24	nB	nB	nB	nB	
853	V	108-36-1	InChI=1S/C6H4Br2/c7-5-2-1-3-6(8)4-5/h1-4H	3.75	61	0.058	0	0	2.78	nB	nB	nB	B	
854	V	108-43-0	InChI=1S/C6H5ClO/c7-5-2-1-3-6(8)4-5/h1-4,8H	2.5	61	0.387	20.23	0	1.07	nB	nB	nB	nB	
855	V	110-82-7	InChI=1S/C6H12/c1-2-4-6-5-3-1/h1-6H2	3.44	27	0.071	0	0	1.97	nB	nB	nB	nB	
856	V	119-64-2	InChI=1S/C10H12/c1-2-6-10-8-4-3-7-9(10)5-1/h1-2,5-6H,3-4,7-8H2	3.49	109	0.115	0	0	2.47	nB	nB	nB	nB	
857	T	119-93-7	InChI=1S/C14H16N2/c1-9-7-11(3-5-13(9)15)12-4-6-14(16)10(2)8-12/h3-8H,15-16H2,1-2H3	2.34	440	0.739	52.04	2	1.60	nB	nB	nB	nB	
858	T	120-71-8	InChI=1S/C8H11NO/c1-6-3-4-8(10-2)7(9)5-6/h3-5H,9H2,1-2H3	1.74	116	0.576	35.25	1	0.82	nB	nB	nB	nB	
859	T	120-78-5	InChI=1S/C14H8N2S4/c1-3-7-11-9(5-1)15-13(17-11)19-20-14-16-10-6-2-4-8-12(10)18-14/h1-8H	5.61	896	1.299	132.86	2	1.15	nB	B	B	B	
860	V	128-86-9	InChI=1S/C14H10N2O10S2/c15-3-1-5(27(21,22)23)11(17)9-7(3)13(19)10-8(14(9)20)4(16)2-6(12(10)18)28(24,25)26/h1-2,17-18H,15-16H2,(H,21,22,23)(H,24,25,26)	-0.06	1744	2.911	252.14	10	0.31	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
861	T	135-88-6	InChI=1S/C16H13N/c1-2-8-15(9-3-1)17-16-11-10-13-6-4-5-7-14(13)12-16/h1-12,17H	4.38	546	1.071	12.03	1	2.39	nB	nB	nB	B	
862	T	156-43-4	InChI=1S/C8H11NO/c1-2-10-8-5-3-7(9)4-6-8/h3-6H,2,9H2,1H3	1.24	127	0.562	35.25	1	0.52	nB	nB	nB	nB	
863	V	208-96-8	InChI=1S/C12H8/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-8H	3.94	166	0.197	0	0	2.52	nB	B	B	B	
864	T	330-55-2	InChI=1S/C9H10Cl2N2O2/c1-13(15-2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H,1-2H3,(H,12,14)	3.2	394	0.378	41.57	2	1.37	nB	nB	nB	nB	
865	T	527-60-6	InChI=1S/C9H12O/c1-6-4-7(2)9(10)8(3)5-6/h4-5,10H,1-3H3	2.73	110	0.421	20.23	0	0.89	nB	nB	nB	nB	
866	T	581-40-8	InChI=1S/C12H12/c1-9-7-11-5-3-4-6-12(11)8-10(9)2/h3-8H,1-2H3	4.4	182	0.189	0	0	2.71	nB	B	B	B	
867	V	603-11-2	InChI=1S/C8H5NO6/c10-7(11)4-2-1-3-5(9(14)15)6(4)8(12)13/h1-3H,(H,10,11)(H,12,13)	0.75	336	0.579	117.74	4	0.18	nB	nB	nB	nB	
868	T	608-93-5	InChI=1S/C6HCl5/c7-2-1-3(8)5(10)6(11)4(2)9/h1H	5.17	140	-0.026	0	0	3.93	B	B	B	B	
869	T	610-09-3	InChI=1S/C8H12O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h5-6H,1-4H2,(H,9,10)(H,11,12)	0.86	188	0.759	74.6	4	-0.20	nB	nB	nB	nB	
870	T	613-12-7	InChI=1S/C15H12/c1-11-6-7-14-9-12-4-2-3-5-13(12)10-15(14)8-11/h2-10H,1H3	5	342	0.253	0	0	2.41	nB	nB	B	B	
871	V	615-74-7	InChI=1S/C7H7ClO/c1-5-2-3-6(8)7(9)4-5/h2-4,9H,1H3	2.9	84	0.319	20.23	0	0.56	nB	nB	nB	nB	
872	T	623-26-7	InChI=1S/C8H4N2/c9-5-7-1-2-8(6-10)4-3-7/h1-4H	0.93	125	0.377	47.58	2	0.16	nB	nB	nB	nB	
873	V	634-66-2	InChI=1S/C6H2Cl4/c7-3-1-2-4(8)6(10)5(3)9/h1-2H	4.6	109	0.07	0	0	3.66	B	B	B	B	
874	T	933-12-0	InChI=1S/C9H16/c1-8-5-4-6-9(2,3)7-8/h4-5,8H,6-7H2,1-3H3	3.44	82	0.162	0	0	2.87	nB	nB	nB	nB	
875	V	1460-02-2	InChI=1S/C18H30/c1-16(2,3)13-10-14(17(4,5)6)12-15(11-13)18(7,8)9/h10-12H,1-9H3	6.94	552	0.278	0	0	4.39	B	nB	B	B	
876	V	1477-55-0	InChI=1S/C8H12N2/c9-5-7-2-1-3-8(4-7)6-10/h1-4H,5-6,9-10H2	-0.34	121	1.077	52.04	2	-0.05	nB	nB	nB	nB	
877	T	1570-64-5	InChI=1S/C7H7ClO/c1-5-4-6(8)2-3-7(5)9/h2-4,9H,1H3	2.78	84	0.372	20.23	0	1.22	nB	nB	nB	nB	
878	V	1836-77-7	InChI=1S/C12H6Cl3NO3/c13-7-5-10(14)12(11(15)6-7)19-9-3-1-8(2-4-9)16(17)18/h1-6H	4.97	752	0.022	52.37	0	3.31	B	B	B	B	
879	T	2050-67-1	InChI=1S/C12H8Cl2/c13-11-5-1-3-9(7-11)10-4-2-6-12(14)8-10/h1-8H	5.27	301	0.197	0	0	2.63	nB	B	B	B	
880	T	2050-76-2	InChI=1S/C10H6Cl2O/c11-8-5-9(12)10(13)7-4-2-1-3-6(7)8/h1-5,13H	4.23	218	0.291	20.23	0	1.02	nB	nB	B	B	
881	T	2173-57-1	InChI=1S/C14H16O/c1-11(2)10-15-14-8-7-12-5-3-4-6-13(12)9-14/h3-9,11H,10H2,1-2H3	4.8	392	0.422	9.23	0	2.93	nB	B	B	B	
882	V	3229-00-3	InChI=1S/C5H8Br4/c6-1-5(2-7,3-8)4-9/h1-4H2	3.99	88	0.064	0	0	2.40	nB	B	B	B	
883	T	4101-68-2	InChI=1S/C10H20Br2/c11-9-7-5-3-1-2-4-6-8-10-12/h1-10H2	5.83	286	0.049	0	0	2.08	nB	B	B	B	
884	T	4685-14-7	InChI=1S/C12H14N2/c1-13-7-3-11(4-8-13)12-5-9-14(2)10-6-12/h3-10H,1-2H3/q+2	-5.82	315	0.995	7.76	0	0.28	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
885	T	13540-50-6	InChI=1S/C15H16/c1-12-8-9-13(2)15(10-12)11-14-6-4-3-5-7-14/h3-10H,11H2,1-2H3	5.65	378	0.173	0	0	3.32	B	B	B	B	
886	T	13936-21-5	InChI=1S/C19H18O2/c1-2-3-4-7-13-10-11-16-17(12-13)19(21)15-9-6-5-8-14(15)18(16)20/h5-6,8-12H,2-4,7H2,1H3	5.99	928	0.823	34.14	2	3.09	B	nB	B	B	
887	V	15862-07-4	InChI=1S/C12H7Cl3/c13-10-7-12(15)11(14)6-9(10)8-4-2-1-3-5-8/h1-7H	5.81	354	0.136	0	0	3.97	B	B	B	B	
888	T	15958-19-7	InChI=1S/C17H13ClN2O4S/c1-10-8-14(16(9-13)(10)18)25(22,23)24)19-20-17-12-5-3-2-4-11(12)6-7-15(17)21/h2-9,21H,1H3,(H,22,23,24)/b20-19+	4.33	1472	1.588	107.7	5	1.07	nB	nB	nB	nB	
889	T	16766-29-3	InChI=1S/C8H7Cl3O2/c1-12-5-3-4(9)6(10)7(11)8(5)13-2/h3H,1-2H3	4.01	228	0.194	18.46	0	3.50	B	B	B	B	
890	T	19780-74-6	InChI=1S/C11H22/c1-4-7-9-11(6-3)10-8-5-2/h4,11H,1,5-10H2,2-3H3	5.37	188	0.126	0	0	3.43	B	B	B	B	
891	T	25747-06-2	InChI=1S/C16H11ClN2O6S/c17-8-6-12(16(22)14(7-8)26(23,24)25)19-18-11-5-4-9-10(15(11)21)2-1-3-13(9)20/h1-7,20-22H,(H,23,24,25)/b19-18+	3.81	1718	2.043	148.16	5	0.58	nB	nB	nB	nB	
892	V	28249-77-6	InChI=1S/C12H16ClNOS/c1-3-14(4-2)12(15)16-9-10-5-7-11(13)8-6-10/h5-8H,3-4,9H2,1-2H3	3.4	505	0.997	45.61	2	2.30	nB	nB	nB	nB	
893	V	31508-00-6	InChI=1S/C12H5Cl5/c13-8-2-1-6(3-10(8)15)7-4-11(16)12(17)5-9(7)14/h1-5H	7.12	504	0.145	0	0	4.38	B	B	B	B	
894	T	36559-22-5	InChI=1S/C12H6Cl4/c13-7-4-5-8(11(15)6-7)9-2-1-3-10(14)12(9)16/h1-6H	5.98	417	0.148	0	0	4.53	B	B	B	B	
895	T	39227-58-2	InChI=1S/C12H5Cl3O2/c13-6-5-7(14)11-12(10(6)15)17-9-4-2-1-3-8(9)16-11/h1-5H	6.35	464	0.279	18.46	0	2.82	nB	B	B	B	
896	T	50375-10-5	InChI=1S/C7H5Cl3O/c1-11-7-5(9)3-2-4(8)6(7)10/h2-3H,1H3	3.64	144	0.288	9.23	0	2.53	nB	nB	B	B	
897	T	60145-21-3	InChI=1S/C12H5Cl5/c13-6-1-2-9(15)8(3-6)12-10(16)4-7(14)5-11(12)17/h1-5H	6.5	480	-0.033	0	0	4.58	B	B	B	B	
898	T	61328-45-8	InChI=1S/C12H6Cl4O/c13-7-1-3-8(4-2-7)17-12-6-10(15)9(14)5-11(12)16/h1-6H	5.99	542	0.202	9.23	0	4.11	B	B	B	B	
899	T	61328-46-9	InChI=1S/C12H6Cl4O/c13-7-1-4-12(11(16)5-7)17-8-2-3-9(14)10(15)6-8/h1-6H	6.13	544	0.248	9.23	0	4.24	B	B	B	B	
900	T	62338-09-4	InChI=1S/C13H28/c1-6-7-8-9-10-11-12(2)13(3,4)5/h12H,6-11H2,1-5H3	6.53	308	0.154	0	0	3.34	B	B	B	B	
901	T	66230-04-4	InChI=1S/C25H22ClNO3/c1-17(2)24(18-11-13-20(26)14-12-18)25(28)30-23(16-27)19-7-6-10-22(15-19)29-21-8-4-3-5-9-21/h3-15,17,23-24H,1-2H3	6.2	2659	1.081	59.32	3	3.30	B	B	B	B	
902	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	2.03	nB	#N/A	#N/A	#N/A	CAS N/A
903	V	86-74-8	InChI=1S/C12H9N/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8,13H	3.39	219	0.551	15.79	1	2.13	nB	nB	nB	nB	
904	T	99-62-7	InChI=1S/C12H18/c1-9(2)11-6-5-7-12(8-11)10(3)4/h5-10H,1-4H3	5.26	197	0.165	0	0	3.16	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
905	T	115-86-6	InChI=1S/C18H15O4P/c19-23(20-16-10-4-1-5-11-16,21-17-12-6-2-7-13-17)22-18-14-8-3-9-15-18/h1-15H	4.59	1204	1.992	54.57	1	2.48	nB	nB	nB	B	
906	T	1634-04-4	InChI=1S/C5H12O/c1-5(2,3)6-4/h1-4H3	0.94	28	0.347	9.23	1	0.18	nB	nB	nB	nB	
907	T	101-05-3	InChI=1S/C9H5Cl3N4/c10-5-3-1-2-4-6(5)13-9-15-7(11)14-8(12)16-9/h1-4H,(H,13,14,15,16)	3	449	1.561	50.7	4	2.32	nB	nB	nB	nB	
908	T	115-26-4	InChI=1S/C4H12FN2OP/c1-6(2)9(5,8)7(3)4/h1-4H3	-0.13	84	0.244	33.36	3	-0.52	nB	nB	nB	nB	
909	T	116-29-0	InChI=1S/C12H6Cl4O2S/c13-7-1-3-8(4-2-7)19(17,18)12-6-10(15)9(14)5-11(12)16/h1-6H	4.61	672	0.659	42.52	2	2.28	nB	nB	B	B	
910	T	118134-30-8	InChI=1S/C18H35NO2/c1-6-12-19(7-2)13-16-14-20-18(21-16)10-8-15(9-11-18)17(3,4)5/h15-16H,6-14H2,1-5H3	4.24	1017	1.517	21.7	3	1.90	nB	nB	nB	B	
911	T	1194-65-6	InChI=1S/C7H3Cl2N/c8-6-2-1-3-7(9)5(6)4-10/h1-3H	2.74	112	0.2	23.79	1	1.80	nB	nB	nB	nB	
912	T	125116-23-6	InChI=1S/C17H22ClN3O/c1-16(2)8-7-14(9-13-3-5-15(18)6-4-13)17(16,22)10-21-12-19-11-20-21/h3-6,11-12,14,22H,7-10H2,1-2H3	3.85	1034	0.857	50.94	4	2.11	nB	nB	nB	nB	
913	V	22224-92-6	InChI=1S/C13H22NO3PS/c1-6-16-18(15,14-10(2)3)17-12-7-8-13(19-5)11(4)9-12/h7-10H,6H2,1-5H3,(H,14,15)	3.23	738	1.543	82.67	3	2.04	nB	nB	nB	nB	
914	T	23103-98-2	InChI=1S/C11H18N4O2/c1-7-8(2)12-10(14(3)4)13-9(7)17-11(16)15(5)6/h1-6H3	1.7	518	1.347	58.56	5	1.38	nB	nB	nB	nB	
915	T	335-77-3	InChI=1S/C10HF21O3S/c11-1(12,3(15,16)5(19,20)7(23,24)9(27,28)29)2(13,14)4(17,18)6(21,22)8(25,26)10(30,31)35(32,33)34/h(H,32,33,34)	6.36	3136	0.984	62.75	3	3.41	B	B	B	B	
916	T	298-02-2	InChI=1S/C7H17O2PS3/c1-4-8-10(11,9-5-2)13-7-12-6-3/h4-7H2,1-3H3	3.56	280	2.104	110.96	2	2.68	nB	nB	nB	B	
917	V	51707-55-2	InChI=1S/C9H8N4OS/c14-9(12-8-6-10-13-15-8)11-7-4-2-1-3-5-7/h1-6H,(H2,11,12,14)	1.77	411	1.204	95.15	5	0.79	nB	nB	nB	nB	
918	T	55219-65-3	InChI=1S/C14H18ClN3O2/c1-14(2,3)12(19)13(18-9-16-8-17-18)20-11-6-4-10(15)5-7-11/h4-9,12-13,19H,1-3H3	3.08	802	1.003	60.17	4	1.32	nB	nB	nB	nB	
919	T	55285-14-8	InChI=1S/C20H32N2O3S/c1-6-8-13-22(14-9-7-2)26-21(5)19(23)24-17-12-10-11-16-15-20(3,4)25-18(16)17/h10-12H,6-9,13-15H2,1-5H3	5.81	1838	0.29	67.31	3	3.00	B	B	B	B	
920	T	55290-64-7	InChI=1S/C6H10O4S2/c1-5-6(2)12(9,10)4-3-11(5,7)8/h3-4H2,1-2H3	-0.17	172	1.421	85.04	4	0.63	nB	nB	nB	nB	
921	T	5598-13-0	InChI=1S/C7H7Cl3NO3PS/c1-12-15(16,13-2)14-7-5(9)3-4(8)6(10)11-7/h3H,1-2H3	4.31	434	2.285	82.48	3	3.26	B	nB	nB	B	
922	V	57018-04-9	InChI=1S/C9H11Cl2O3PS/c1-6-4-7(10)9(8(11)5-6)14-15(16,12-2)13-3/h4-5H,1-3H3	4.56	427	2.028	69.59	2	2.83	nB	nB	B	B	
923	T	57-74-9	InChI=1S/C10H6Cl8/c11-3-1-2-4(5(3)12)9(16)7(14)6(13)8(2,15)10(9,17)18/h2-5H,1H2	6.16	459	0.277	0	0	4.29	B	nB	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
924	V	57837-19-1	InChI=1S/C15H21NO4/c1-10-7-6-8-11(2)14(10)16(13(17)9-19-4)12(3)15(18)20-5/h6-8,12H,9H2,1-5H3	1.65	754	1.068	55.84	5	1.01	nB	nB	nB	nB	
925	V	66332-96-5	InChI=1S/C17H16F3NO2/c1-11(2)23-13-7-5-6-12(10-13)21-16(22)14-8-3-4-9-15(14)17(18,19)20/h3-11H,1-2H3,(H,21,22)	3.7	1252	0.709	38.33	2	2.00	nB	nB	nB	B	
926	T	94-82-6	InChI=1S/C10H10Cl2O3/c11-7-3-4-9(8(12)6-7)15-5-1-2-10(13)14/h3-4,6H,1-2,5H2,(H,13,14)	3.53	434	0.598	46.53	2	2.24	nB	nB	nB	nB	
927	T	95977-29-0	InChI=1S/C15H11ClF3NO4/c1-8(14(21)22)23-10-2-4-11(5-3-10)24-13-12(16)6-9(7-20-13)15(17,18)19/h2-8H,1H3,(H,21,22)	3.74	1565	1.103	68.65	3	1.09	nB	nB	nB	nB	
928	T	96489-71-3	InChI=1S/C19H25ClN2OS/c1-18(2,3)14-9-7-13(8-10-14)12-24-15-11-21-22(19(4,5)6)17(23)16(15)20/h7-11H,12H2,1-6H3	6.37	1510	1.109	57.97	3	1.68	nB	nB	B	B	
929	T	65-85-0	InChI=1S/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)	1.87	88	0.459	37.3	2	1.00	nB	nB	nB	nB	
930	T	260-94-6	InChI=1S/C13H9N/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)14-12/h1-9H	3.4	279	0.567	12.89	1	2.40	nB	nB	nB	nB	
931	T	50-31-7	InChI=1S/C7H3Cl3O2/c8-3-1-2-4(9)6(10)5(3)7(11)12/h1-2H,(H,11,12)	2.86	181	0.376	37.3	2	0.58	nB	nB	nB	nB	
932	V	53-70-3	InChI=1S/C22H14/c1-3-7-19-15(5-1)9-11-17-14-22-18(13-21(17)19)12-10-16-6-2-4-8-20(16)22/h1-14H	6.75	971	0.377	0	0	2.80	nB	nB	B	B	
933	T	76-12-0	InChI=1S/C2Cl4F2/c3-1(4,7)2(5,6)8	3.41	58	0.106	0	0	1.90	nB	nB	nB	nB	
934	T	76-13-1	InChI=1S/C2Cl3F3/c3-1(4,6)2(5,7)8	3.16	58	0.07	0	0	1.62	nB	nB	nB	nB	
935	T	79-00-5	InChI=1S/C2H3Cl3/c3-1-2(4)5/h2H,1H2	1.89	18	0.094	0	0	0.53	nB	nB	nB	nB	
936	T	85-01-8	InChI=1S/C14H10/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-10H	4.46	271	0.257	0	0	3.31	B	B	B	B	
937	V	87-40-1	InChI=1S/C7H5Cl3O/c1-11-7-5(9)2-4(8)3-6(7)10/h2-3H,1H3	4.11	146	0.222	9.23	0	2.81	nB	B	B	B	
938	T	87-65-0	InChI=1S/C6H4Cl2O/c7-4-2-1-3-5(8)6(4)9/h1-3,9H	2.75	82	0.178	20.23	0	1.26	nB	nB	nB	nB	
939	T	88-72-2	InChI=1S/C7H7NO2/c1-6-4-2-3-5-7(6)8(9)10/h2-5H,1H3	2.3	114	-0.069	43.14	0	1.34	nB	nB	nB	nB	
940	V	88-75-5	InChI=1S/C6H5NO3/c8-6-4-2-1-3-5(6)7(9)10/h1-4,8H	1.79	114	0.136	63.37	0	1.00	nB	nB	nB	nB	
941	V	88-98-2	InChI=1S/C8H10O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h1-2,5-6H,3-4H2,(H,9,10)(H,11,12)	0.44	188	0.781	74.6	4	-0.20	nB	nB	nB	nB	
942	T	91-15-6	InChI=1S/C8H4N2/c9-5-7-3-1-2-4-8(7)6-10/h1-4H	0.99	117	0.377	47.58	2	0.40	nB	nB	nB	nB	
943	V	95-56-7	InChI=1S/C6H5BrO/c7-5-3-1-2-4-6(5)8/h1-4,8H	2.35	60	0.312	20.23	0	1.51	nB	nB	nB	nB	
944	T	95-94-3	InChI=1S/C6H2Cl4/c7-3-1-4(8)6(10)2-5(3)9/h1-2H	4.64	111	-0.007	0	0	3.74	B	B	B	B	
945	T	96-12-8	InChI=1S/C3H5Br2Cl/c4-1-3(5)2-6/h3H,1-2H2	2.96	31	0.086	0	0	1.13	nB	nB	nB	nB	
946	T	97-23-4	InChI=1S/C13H10Cl2O2/c14-10-1-3-12(16)8(6-10)5-9-7-11(15)2-4-13(9)17/h1-4,6-7,16-17H,5H2	4.26	520	0.659	40.46	0	2.01	nB	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
947	T	99-08-1	InChI=1S/C7H7NO2/c1-6-3-2-4-7(5-6)8(9)10/h2-5H,1H3	2.45	117	-0.069	43.14	0	0.95	nB	nB	nB	nB	
948	V	99-54-7	InChI=1S/C6H3Cl2NO2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H	3.12	152	-0.137	43.14	0	1.92	nB	nB	nB	nB	
949	T	101-81-5	InChI=1S/C13H12/c1-3-7-12(8-4-1)11-13-9-5-2-6-10-13/h1-10H,11H2	4.14	264	0.181	0	0	3.00	B	nB	B	B	
950	T	108-70-3	InChI=1S/C6H3Cl3/c7-4-1-5(8)3-6(9)2-4/h1-3H	4.19	84	-0.001	0	0	3.29	B	nB	B	B	
951	V	108-80-5	InChI=1S/C3H3N3O3/c7-1-4-2(8)6-3(9)5-1/h(H3,4,5,6,7,8,9)	-0.09	84	1.661	99.36	3	-0.65	nB	nB	nB	nB	
952	T	108-95-2	InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H	1.46	42	0.433	20.23	0	0.76	nB	nB	nB	nB	
953	V	110-91-8	InChI=1S/C4H9NO/c1-3-6-4-2-5-1/h5H,1-4H2	-0.86	27	0.943	21.26	2	-0.06	nB	nB	nB	nB	
954	T	119-33-5	InChI=1S/C7H7NO3/c1-5-2-3-7(9)6(4-5)8(10)11/h2-4,9H,1H3	2.37	148	0.132	63.37	0	0.96	nB	nB	nB	nB	
955	T	120-83-2	InChI=1S/C6H4Cl2O/c7-4-1-2-6(9)5(8)3-4/h1-3,9H	3.06	84	0.231	20.23	0	1.66	nB	nB	nB	nB	
956	T	121-14-2	InChI=1S/C7H6N2O4/c1-5-2-3-6(8(10)11)4-7(5)9(12)13/h2-4H,1H3	1.98	240	-0.306	86.28	0	0.83	nB	nB	nB	nB	
957	T	121-69-7	InChI=1S/C8H11N/c1-9(2)8-6-4-3-5-7-8/h3-7H,1-2H3	2.31	88	0.461	3.24	1	1.02	nB	nB	nB	nB	
958	T	134-32-7	InChI=1S/C10H9N/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,11H2	2.25	140	0.461	26.02	1	1.47	nB	nB	nB	nB	
959	V	134-62-3	InChI=1S/C12H17NO/c1-4-13(5-2)12(14)11-8-6-7-10(3)9-11/h6-9H,4-5H2,1-3H3	2.02	307	0.836	20.31	2	0.29	nB	nB	nB	nB	
960	V	148-75-4	InChI=1S/C10H8O7S2/c11-9-4-6-1-2-8(18(12,13)14)3-7(6)5-10(9)19(15,16)17/h1-5,11H,(H,12,13,14)(H,15,16,17)	0.86	668	2.452	145.73	6	0.30	nB	nB	nB	nB	
961	V	217-59-4	InChI=1S/C18H12/c1-2-8-14-13(7-1)15-9-3-4-11-17(15)18-12-6-5-10-16(14)18/h1-12H	5.89	513	0.317	0	0	2.41	nB	nB	B	B	
962	T	218-01-9	InChI=1S/C18H12/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h1-12H	5.81	545	0.317	0	0	2.24	nB	nB	B	B	
963	T	2497-06-5	InChI=1S/C8H19O4PS3/c1-4-11-13(14,12-5-2)15-7-8-16(9,10)6-3/h4-8H2,1-3H3	1.87	494	2.604	128.18	4	0.34	nB	nB	nB	nB	
964	V	298-07-7	InChI=1S/C16H35O4P/c1-5-9-11-15(7-3)13-19-21(17,18)20-14-16(8-4)12-10-6-2/h15-16H,5-14H2,1-4H3,(H,17,18)	5.24	1136	1.973	65.57	4	0.60	nB	nB	B	B	
965	V	544-01-4	InChI=1S/C10H22O/c1-9(2)5-7-11-8-6-10(3)4/h9-10H,5-8H2,1-4H3	4.25	204	0.332	9.23	1	2.37	nB	nB	B	B	
966	T	577-11-7	InChI=1S/C20H38O7S/c1-5-9-11-16(7-3)14-26-19(21)13-18(28(23,24)25)20(22)27-15-17(8-4)12-10-6-2/h16-18H,5-15H2,1-4H3,(H,23,24,25)	5.15	2411	1.785	115.35	7	0.46	nB	nB	B	B	Salt - converted into acidic form
967	T	591-20-8	InChI=1S/C6H5BrO/c7-5-2-1-3-6(8)4-5/h1-4,8H	2.63	61	0.376	20.23	0	1.02	nB	nB	nB	nB	
968	V	609-89-2	InChI=1S/C6H3Cl2NO3/c7-3-1-4(8)6(10)5(2-3)9(11)12/h1-2,10H	3.49	184	-0.136	63.37	0	1.37	nB	nB	nB	nB	
969	V	615-54-3	InChI=1S/C6H3Br3/c7-4-1-2-5(8)6(9)3-4/h1-3H	4.27	84	0.021	0	0	3.41	B	B	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
970	V	626-17-5	InChI=1S/C8H4N2/c9-5-7-2-1-3-8(4-7)6-10/h1-4H	0.8	121	0.377	47.58	2	0.40	nB	nB	nB	nB	
971	T	634-67-3	InChI=1S/C6H4Cl3N/c7-3-1-2-4(10)6(9)5(3)8/h1-2H,10H2	3.68	109	0.345	26.02	1	2.00	nB	nB	nB	B	
972	T	634-93-5	InChI=1S/C6H4Cl3N/c7-3-1-4(8)6(10)5(9)2-3/h1-2H,10H2	3.69	110	0.279	26.02	1	2.08	nB	nB	nB	B	
973	V	636-30-6	InChI=1S/C6H4Cl3N/c7-3-1-5(9)6(10)2-4(3)8/h1-2H,10H2	3.69	111	0.268	26.02	1	2.33	nB	nB	nB	B	
974	T	832-69-9	InChI=1S/C15H12/c1-11-5-4-8-15-13(11)10-9-12-6-2-3-7-14(12)15/h2-10H,1H3	5.08	326	0.253	0	0	3.18	B	nB	B	B	
975	T	950-37-8	InChI=1S/C6H11N2O4PS3/c1-10-5-7-8(6(9)16-5)4-15-13(14,11-2)12-3/h4H2,1-3H3	2.2	471	3.014	152.86	6	0.76	nB	nB	nB	nB	
976	T	1116-76-3	InChI=1S/C24H51N/c1-4-7-10-13-16-19-22-25(23-20-17-14-11-8-5-2)24-21-18-15-12-9-6-3/h4-24H2,1-3H3	10.52	2088	0.745	3.24	1	1.97	nB	nB	nB	B	
977	V	1839-63-0	InChI=1S/C9H18/c1-7-4-8(2)6-9(3)5-7/h7-9H,4-6H2,1-3H3	4.01	84	0.125	0	0	3.34	B	B	B	B	
978	T	1912-24-9	InChI=1S/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H,4H2,1-3H3,(H2,10,11,12,13,14)	2.61	319	1.434	62.73	5	0.57	nB	nB	nB	nB	
979	T	2042-14-0	InChI=1S/C7H7NO3/c1-5-2-3-6(9)4-7(5)8(10)11/h2-4,9H,1H3	2.18	148	0.192	63.37	0	1.03	nB	nB	nB	nB	
980	T	2921-88-2	InChI=1S/C9H11Cl3NO3PS/c1-3-14-17(18,15-4-2)16-9-7(11)5-6(10)8(12)13-9/h5H,3-4H2,1-2H3	4.96	612	2.285	82.48	3	3.01	B	B	B	B	
981	V	3010-80-8	InChI=1S/C19H13Cl3O/c20-16-7-1-13(2-8-16)19(23,14-3-9-17(21)10-4-14)15-5-11-18(22)12-6-15/h1-12,23H	6.1	1108	0.94	20.23	1	3.95	B	B	B	B	
982	T	3674-75-7	InChI=1S/C16H14/c1-2-12-11-13-7-3-4-9-15(13)16-10-6-5-8-14(12)16/h3-11H,2H2,1H3	5.22	388	0.253	0	0	2.71	nB	B	B	B	
983	T	6130-75-2	InChI=1S/C7H5Cl3O/c1-11-7-3-5(9)4(8)2-6(7)10/h2-3H,1H3	3.85	148	0.211	9.23	0	2.78	nB	B	B	B	
984	V	6639-30-1	InChI=1S/C7H5Cl3/c1-4-2-6(9)7(10)3-5(4)8/h2-3H,1H3	4.56	111	0.05	0	0	3.68	B	B	B	B	
985	T	13674-84-5	InChI=1S/C9H18Cl3O4P/c1-7(4-10)14-17(13,15-8(2)5-11)16-9(3)6-12/h7-9H,4-6H2,1-3H3	2.59	538	1.881	54.57	4	0.47	nB	nB	nB	nB	
986	T	15087-24-8	InChI=1S/C17H20O/c1-16(2)14-9-10-17(16,3)15(18)13(14)11-12-7-5-4-6-8-12/h4-8,11,14H,9-10H2,1-3H3/b13-11+	4.15	561	0.577	17.07	1	2.44	nB	nB	nB	B	
987	T	16605-91-7	InChI=1S/C12H8Cl2/c13-11-8-4-7-10(12(11)14)9-5-2-1-3-6-9/h1-8H	5.02	291	0.228	0	0	3.72	B	nB	B	B	
988	T	18259-05-7	InChI=1S/C12H5Cl5/c13-8-7(6-4-2-1-3-5-6)9(14)11(16)12(17)10(8)15/h1-5H	6.75	470	0.056	0	0	4.85	B	B	B	B	
989	V	26787-65-5	InChI=1S/C30H60O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-30(32)33-29-28-31/h31H,2-29H2,1H3	13.32	5876	0.724	46.53	3	1.27	nB	nB	nB	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
990	T	29761-21-5	InChI=1S/C22H31O4P/c1-20(2)14-8-4-3-5-13-19-24-27(23,25-21-15-9-6-10-16-21)26-22-17-11-7-12-18-22/h6-7,9-12,15-18,20H,3-5,8,13-14,19H2,1-2H3	5.44	2242	1.962	54.57	2	2.63	nB	nB	B	B	
991	T	32598-14-4	InChI=1S/C12H5Cl5/c13-8-3-1-6(5-10(8)15)7-2-4-9(14)12(17)11(7)16/h1-5H	6.79	502	0.222	0	0	4.28	B	B	B	B	
992	T	33284-53-6	InChI=1S/C12H6Cl4/c13-9-6-8(7-4-2-1-3-5-7)10(14)12(16)11(9)15/h1-6H	6.41	412	0.152	0	0	4.39	B	B	B	B	
993	T	37680-73-2	InChI=1S/C12H5Cl5/c13-6-1-2-9(14)7(3-6)8-4-11(16)12(17)5-10(8)15/h1-5H	6.97	488	0.045	0	0	4.63	B	B	B	B	
994	T	51207-31-9	InChI=1S/C12H4Cl4O/c13-7-1-5-6-2-8(14)10(16)4-12(6)17-11(5)3-9(7)15/h1-4H	6.53	472	0.3	13.14	0	3.77	B	nB	B	B	
995	T	54135-80-7	InChI=1S/C7H5Cl3O/c1-11-5-3-2-4(8)6(9)7(5)10/h2-3H,1H3	3.74	146	0.288	9.23	0	2.96	nB	nB	nB	B	
996	T	54135-81-8	InChI=1S/C7H5Cl3O/c8-5-1-4(3-11)7(10)6(9)2-5/h1-2,11H,3H2	3.93	146	0.481	20.23	1	3.09	B	nB	B	B	
997	T	56558-16-8	InChI=1S/C12H5Cl5/c13-6-4-9(16)12(10(17)5-6)11-7(14)2-1-3-8(11)15/h1-5H	5.81	470	-0.068	0	0	4.81	B	B	B	B	
998	T	56558-17-9	InChI=1S/C12H5Cl5/c13-7-4-10(16)12(11(17)5-7)6-1-2-8(14)9(15)3-6/h1-5H	6.62	496	0.09	0	0	4.81	B	B	B	B	
999	V	57465-28-8	InChI=1S/C12H5Cl5/c13-8-2-1-6(3-9(8)14)7-4-10(15)12(17)11(16)5-7/h1-5H	7.26	510	0.222	0	0	4.68	B	B	B	B	
1000	T	67028-18-6	InChI=1S/C12H4Cl4O2/c13-5-1-2-7-8(3-5)17-9-4-6(14)10(15)11(16)12(9)18-7/h1-4H	6.9	558	0.187	18.46	0	3.35	B	B	B	B	
1001	T	2164-08-1	InChI=1S/C13H18N2O2/c16-12-10-7-4-8-11(10)14-13(17)15(12)9-5-2-1-3-6-9/h9H,1-8H2,(H,14,17)	1.69	474	1.027	49.41	4	1.26	nB	nB	nB	nB	
1002	T	105512-06-9	InChI=1S/C17H13ClFNO4/c1-3-8-22-17(21)11(2)23-13-4-6-14(7-5-13)24-16-15(19)9-12(18)10-20-16/h1,4-7,9-11H,8H2,2H3/t11-/m1/s1	3.9	1623	1.192	57.65	3	1.53	nB	nB	nB	B	
1003	T	108-62-3	InChI=1S/C8H16O4/c1-5-9-6(2)11-8(4)12-7(3)10-5/h5-8H,1-4H3	0.12	188	1.467	36.92	4	1.04	nB	nB	nB	nB	
1004	V	120068-37-3	InChI=1S/C12H4Cl2F6N4OS/c13-5-1-4(11(15,16)17)2-6(14)8(5)24-10(22)9(7(3-21)23-24)26(25)12(18,19)20/h1-2H,22H2	4	1575	1.609	103.39	5	2.51	nB	nB	nB	nB	
1005	T	120-36-5	InChI=1S/C9H8Cl2O3/c1-5(9(12)13)14-8-3-2-6(10)4-7(8)11/h2-5H,1H3,(H,12,13)	3.43	316	0.616	46.53	2	0.78	nB	nB	nB	nB	
1006	V	133-07-3	InChI=1S/C9H4Cl3NO2S/c10-9(11,12)16-13-7(14)5-3-1-2-4-6(5)8(13)15/h1-4H	2.85	405	0.336	62.68	3	1.75	nB	nB	nB	nB	
1007	V	141112-29-0	InChI=1S/C15H12F3NO4S/c1-24(21,22)12-6-9(15(16,17)18)4-5-10(12)13(20)11-7-19-23-14(11)8-2-3-8/h4-8H,2-3H2,1H3	2.32	1255	1.233	85.62	3	1.04	nB	nB	nB	nB	
1008	T	14214-32-5	InChI=1S/C16H18N2O3/c1-18(2)16(19)17-12-4-6-14(7-5-12)21-15-10-8-13(20-3)9-11-15/h4-11H,1-3H3,(H,17,19)	2.54	1118	1.262	50.8	3	1.46	nB	nB	nB	nB	
1009	V	145-73-3	InChI=1S/C8H10O5/c9-7(10)5-3-1-2-4(13-3)6(5)8(11)12/h3-6H,1-2H2,(H,9,10)(H,11,12)	1.91	219	0.992	83.83	5	-0.40	nB	nB	nB	nB	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
1010	T	1918-00-9	InChI=1S/C8H6Cl2O3/c1-13-7-5(10)3-2-4(9)6(7)8(11)12/h2-3H,1H3,(H,11,12)	2.21	226	0.594	46.53	2	1.18	nB	nB	nB	nB	
1011	T	2008-41-5	InChI=1S/C11H23NOS/c1-6-14-11(13)12(7-9(2)3)8-10(4)5/h9-10H,6-8H2,1-5H3	4.15	326	0.996	45.61	2	2.61	nB	nB	nB	B	
1012	T	20354-26-1	InChI=1S/C9H6Cl2N2O3/c1-12-8(14)13(16-9(12)15)5-2-3-6(10)7(11)4-5/h2-4H,1H3	2.7	422	0.33	49.85	3	1.51	nB	nB	nB	nB	
1013	T	22781-23-3	InChI=1S/C11H13NO4/c1-11(2)15-8-6-4-5-7(9(8)16-11)14-10(13)12-3/h4-6H,1-3H3,(H,12,13)	1.7	425	0.76	56.79	2	1.81	nB	nB	nB	nB	
1014	T	239110-15-7	InChI=1S/C14H8Cl3F3N2O/c15-8-2-1-3-9(16)12(8)13(23)22-6-11-10(17)4-7(5-21-11)14(18,19)20/h1-5H,6H2,(H,22,23)	4.43	1300	0.887	41.99	3	2.08	nB	nB	nB	B	
1015	T	25366-23-8	InChI=1S/C6H7F3N4OS/c1-10-4(14)13(2)5-12-11-3(15-5)6(7,8)9/h1-2H3,(H,10,14)	1.85	375	1.029	86.36	5	0.79	nB	nB	nB	nB	
1016	T	2595-54-2	InChI=1S/C10H20NO5PS2/c1-5-14-10(13)11(4)9(12)8-19-17(18,15-6-2)16-7-3/h5-8H2,1-4H3	2.45	794	2.295	132.27	6	1.88	nB	nB	nB	nB	
1017	T	2642-71-9	InChI=1S/C12H16N3O3PS2/c1-3-17-19(20,18-4-2)21-9-15-12(16)10-7-5-6-8-11(10)13-14-15/h5-8H,3-4,9H2,1-2H3	3.4	976	2.672	130.69	6	2.00	nB	nB	nB	nB	
1018	V	272451-65-7	InChI=1S/C23H22F7IN2O4S/c1-12-10-13(21(24,22(25,26)27)23(28,29)30)8-9-16(12)32-18(34)14-6-5-7-15(31)17(14)19(35)33-20(2,3)11-38(4,36)37/h5-10H,11H2,1-4H3,(H,32,34)(H,33,35)	5.27	4892	1.809	100.72	6	1.82	nB	nB	B	B	
1019	T	34014-18-1	InChI=1S/C9H16N4OS/c1-9(2,3)6-11-12-8(15-6)13(5)7(14)10-4/h1-5H3,(H,10,14)	1.79	375	1.2	86.36	5	0.42	nB	nB	nB	nB	
1020	V	36734-19-7	InChI=1S/C13H13Cl2N3O3/c1-7(2)16-12(20)17-6-11(19)18(13(17)21)10-4-8(14)3-9(15)5-10/h3-5,7H,6H2,1-2H3,(H,16,20)	3	915	1.113	69.72	6	1.85	nB	nB	nB	nB	
1021	V	41483-43-6	InChI=1S/C13H24N4O3S/c1-6-8-9-11-10(3)15-13(14-7-2)16-12(11)20-21(18,19)17(4)5/h6-9H2,1-5H3,(H,14,15,16)	2.7	926	1.672	92.8	6	2.27	nB	nB	nB	nB	
1022	T	51235-04-2	InChI=1S/C12H20N4O2/c1-14(2)10-13-11(17)16(12(18)15(10)3)9-7-5-4-6-8-9/h9H,4-8H2,1-3H3	1.85	571	2.102	56.22	6	0.85	nB	nB	nB	nB	
1023	T	50594-66-6	InChI=1S/C14H7ClF3NO5/c15-10-5-7(14(16,17)18)1-4-12(10)24-8-2-3-11(19(22)23)9(6-8)13(20)21/h1-6H,(H,20,21)	3.7	1421	0.362	89.67	2	2.45	nB	nB	nB	B	
1024	T	65907-30-4	InChI=1S/C18H26N2O5S/c1-6-7-11-23-16(21)19(4)26-20(5)17(22)24-14-10-8-9-13-12-18(2,3)25-15(13)14/h8-10H,6-7,11-12H2,1-5H3	4.7	1896	0.09	93.61	5	1.96	nB	B	B	B	
1025	T	66215-27-8	InChI=1S/C6H10N6/c7-4-10-5(8)12-6(11-4)9-3-1-2-3/h3H,1-2H2,(H5,7,8,9,10,11,12)	-0.21	201	1.464	102.74	6	0.00	nB	nB	nB	nB	
1026	T	67306-00-7	InChI=1S/C19H31N/c1-16(15-20-12-6-5-7-13-20)14-17-8-10-18(11-9-17)19(2,3)4/h8-11,16H,5-7,12-15H2,1-4H3	5.53	940	0.844	3.24	1	2.21	nB	nB	B	B	

ID	Set ID	CAS no.	InChI	XLogP3	WPATH	MLFER_BH	TopoPSA	nHBAcc	log BCF	class	M1	M2	M3	Comments
1027	T	69327-76-0	InChI=1S/C16H23N3OS/c1-12(2)19-14(17-16(3,4)5)21-11-18(15(19)20)13-9-7-6-8-10-13/h6-10,12H,11H2,1-5H3/b17-14-	4.3	896	1.347	61.21	4	2.71	nB	nB	nB	nB	
1028	T	7287-19-6	InChI=1S/C10H19N5S/c1-6(2)11-8-13-9(12-7(3)4)15-10(14-8)16-5/h6-7H,1-5H3,(H2,11,12,13,14,15)	3.51	458	1.627	88.03	5	1.93	nB	nB	nB	nB	
1029	V	76-44-8	InChI=1S/C10H5Cl7/c11-4-2-1-3-5(4)9(15)7(13)6(12)8(3,14)10(9,16)17/h1-5H	4.35	388	0.275	0	0	3.94	B	nB	B	B	
1030	V	78-87-5	InChI=1S/C3H6Cl2/c1-3(5)2-4/h3H,2H2,1H3	1.98	18	0.102	0	0	0.57	nB	nB	nB	nB	
1031	T	81335-77-5	InChI=1S/C15H19N3O3/c1-5-9-6-10(13(19)20)11(16-7-9)12-17-14(21)15(4,18-12)8(2)3/h6-8H,5H2,1-4H3,(H,19,20)(H,17,18,21)	2.9	885	2.063	91.65	6	0.20	nB	nB	nB	nB	
1032	V	83055-99-6	InChI=1S/C16H18N4O7S/c1-25-12-8-13(26-2)18-15(17-12)19-16(22)20-28(23,24)9-10-6-4-5-7-11(10)14(21)27-3/h4-8H,9H2,1-3H3,(H2,17,18,19,20,22)	2.18	2240	1.654	154.19	9	0.20	nB	nB	nB	nB	
1033	V	87820-88-0	InChI=1S/C20H27NO3/c1-6-16(21-24-7-2)20-17(22)10-15(11-18(20)23)19-13(4)8-12(3)9-14(19)5/h8-9,15,21H,6-7,10-11H2,1-5H3/b20-16-	4.5	1346	1.018	55.4	2	1.51	nB	nB	nB	B	
1034	T	957-51-7	InChI=1S/C16H17NO/c1-17(2)16(18)15(13-9-5-3-6-10-13)14-11-7-4-8-12-14/h3-12,15H,1-2H3	3.02	575	0.906	20.31	2	1.73	nB	nB	nB	nB	
1035	V	973-21-7	InChI=1S/C14H18N2O7/c1-5-9(4)11-6-10(15(18)19)7-12(16(20)21)13(11)23-14(17)22-8(2)3/h6-9H,5H2,1-4H3	4.32	1144	-0.212	121.81	2	2.48	nB	nB	nB	B	
1036	V	105-67-9	InChI=1S/C8H10O/c1-6-3-4-8(9)7(2)5-6/h3-5,9H,1-2H3	2.3	84	0.425	20.23	0	1.18	nB	nB	nB	nB	

Table S 2. Most frequent descriptors in the preliminary models and descriptors (bold) selected to the final model.

Model 1

<i>Descriptor ID</i>	<i>Description</i>
XLogP3	Octanol-Water Partition Coefficient
SaasC	Sum of atom-type E-State: :C:-
MLFER_BH	Overall or summation solute hydrogen bond basicity
minaaCH	Minimum atom-type E-State: :CH:
maxaasC	Maximum atom-type E-State: :C:-
minwHBa	Minimum E-States for weak Hydrogen Bond acceptors
BCUTw-1h	nlow highest atom weighted BCUTS
WPATH	Wiener index
maxwHBa	Maximum E-States for weak Hydrogen Bond acceptors
TopoPSA	Topological polar surface area
ATSp4	ATS autocorrelation descriptor, weighted by polarizability
minsCl	Minimum atom-type E-State: -Cl

Model 2

<i>Descriptor ID</i>	<i>Description</i>
XLogP3	Octanol-Water Partition Coefficient
MLFER_BH	Overall or summation solute hydrogen bond basicity
nHBAcc	Number of hydrogen bond acceptors
minaaCH	Minimum atom-type E-State: :CH:
WPATH	Wiener index
ATSp4	ATS autocorrelation descriptor, weighted by polarizability
SaasC	Sum of atom-type E-State: :C:-
maxwHBa	Maximum E-States for weak Hydrogen Bond acceptors
minwHBa	Minimum E-States for weak Hydrogen Bond acceptors
VP-7	Valence path, order 7
fragC	Complexity of a system
TopoPSA	Topological polar surface area

Model 3

<i>Descriptor ID</i>	<i>Description</i>
XLogP3	Octanol-Water Partition Coefficient
minsssN	Minimum atom-type E-State: >N-
nHBAcc	Number of hydrogen bond acceptors
WPATH	Wiener index
MDEO-12	Molecular distance edge between all primary and secondary oxygens