Appendix A. Supplementary data

QSAR Modeling for Reaction Rate Constants of e_{aq}^- with Diverse Organic Compounds in Water

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Content

Text A1. Definition of outliers.

Herein, the whisker length is referred to as the upper outer and lower outer fence values.

$$\text{Upper outer fence} = 75\text{th Percentile} + (1.5 \times \text{Interquartile Range}) \quad \text{Eq. (S1)}$$

$$\text{Lower outer fence} = 25\text{th Percentile} - (1.5 \times \text{Interquartile Range}) \quad \text{Eq. (S2)}$$

Data points that lie outside of the fence values are considered to be outliers.

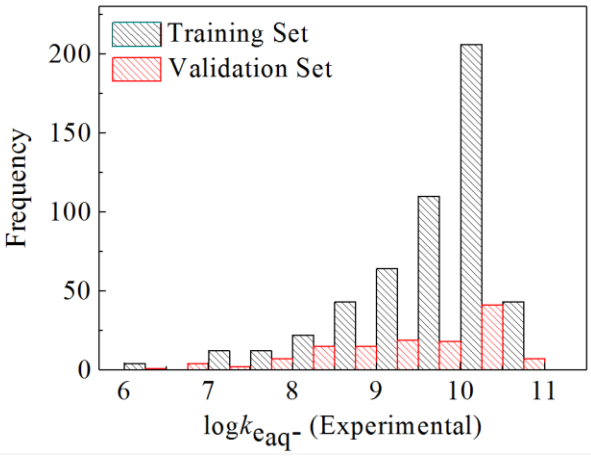

Fig. A1. Distribution of experimental logk_{eaq-} values in the training set and validation set.

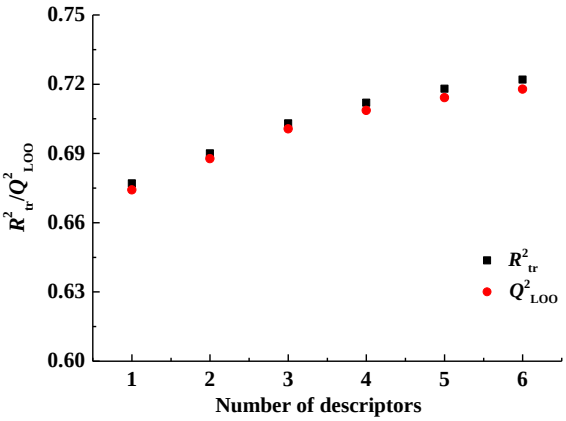

Fig. A2. Progress in R^2_{TR} and Q^2_{LOO} as the number of descriptor increases during the MLR model development.

Table A1. List of compounds in the QSAR modeling

ID	CAS	Name	Charge	pH	$\log k_{e_{aq}^-}$ (Exp.)	$\log k_{e_{aq}^-}$ (MLR)	$\log k_{e_{aq}^-}$ (SVM)	Ref
1	50-18-0	Cyclophosphamide	0	6.8	8.93	8.93	8.82	1
2	50-21-5	2-Hydroxypropionic acid	0	3	8.80	8.87	8.85	1
3	50-21-5	2-Hydroxypropionate	-1	7	7.76	7.62	7.37	1
4	50-32-8	Benzo[a]pyrene	0	7	9.78	10.42	10.32	1
5	50-53-3	Chlorpromazine	0	6.5	10.23	9.75	9.94	1
6	50-59-9	Cephaloridine	0	6	10.45	10.67	10.40	1
7	50-85-1	4-Methyl-salicylate	-1	7	9.64	9.20	9.26	2
8	51-20-7	5-Bromouracil	0	11	10.20	9.90	10.19	1
9	51-21-8	5-Fluorouracil	0	11	10.08	9.93	10.13	1
10	51-35-4	*Hydroxyproline*	-1	7	7.65	7.80	7.48	1
11	51-43-4	*Adrenaline*	0	N.A.	8.40	9.13	9.15	1
12	51-55-8	Atropine	0	9.5	9.62	9.36	9.52	1
13	51-85-4	2,2'-dithiobis(ethylamine)	0	11.1	10.26	9.47	9.72	1
14	54-05-7	*Chloroquine*	0	8.5	10.68	10.12	10.26	1

15	54-25-1	*6-Azauridine*	0	8	9.88	10.26	10.44	1
16	54-47-7	Pyridoxal phosphate	-2	7	10.20	10.51	10.23	1
17	54-85-3	Isoniazid	0	N.A.	10.47	9.96	10.29	3
18	55-18-5	N-Nitrosodiethylamine	0	7	10.21	9.66	9.95	4
19	55-21-0	Benzamide	0	5.7	10.28	9.72	10.07	1
20	55-98-1	Busulfan	0	6.8	7.48	7.90	7.35	1
21	56-23-5	Carbon tetrachloride	0	N.A.	10.11	10.99	10.24	1
22	56-49-5	3-Methylcholanthrene	0	7	9.78	10.20	10.27	1
23	56-75-7	Chloramphenicol	0	N.A.	10.53	10.74	10.51	1
24	56-82-6	DL-glyceraldehyde	0	N.A.	10.40	9.66	10.02	1
25	57-14-7	1,1-Dimethylhydrazine	0	12	7.38	7.73	7.30	1
26	57-63-6	Ethynyl estradiol	0	7	8.16	9.17	9.22	5
27	57-67-0	*Sulfaguanidine*	0	N.A.	9.93	9.56	9.80	1
28	57-68-1	Sulfamethazine	0	5.4-6.0	10.38	9.79	10.07	6
29	58-08-2	Caffeine	0	7	10.08	9.65	9.92	1
30	58-27-5	Menadione	0	7	10.49	11.02	10.44	1
31	58-55-9	Theophylline	0	13	9.00	9.45	9.66	1

32	58-61-7	Adenosine	0	7	10.08	9.55	9.80	1
33	58-63-9	Inosine	0	6.5	9.99	9.68	9.98	1
34	58-96-8	Uridine	0	6	10.15	9.75	10.07	1
35	59-30-3	Folate	-2	12	10.04	10.52	10.30	1
36	59-87-0	Nitrofurazone	0	N.A.	10.45	10.92	10.40	1
37	59-89-2	N-Nitrosomorpholine	0	7	10.34	9.74	10.04	4
38	60-23-1	2-Aminoethanethiol	0	N.A.	9.23	8.60	8.29	1
39	60-34-4	*Methylhydrazine*	0	12	6.81	7.65	7.22	1
40	60-35-5	*Acetamide*	0	5.2	7.65	8.47	8.10	1
41	60-54-8	Tetracycline	0	6.8	10.28	10.40	10.36	1
42	61-32-5	Methicillin	-1	6	9.45	9.40	9.57	1
43	61-33-6	Penicillin G	-1	6	9.45	9.28	9.40	1
44	61-72-3	Cloxacillin	-1	6	9.88	9.76	9.98	1
45	62-56-6	Thiourea	0	6.4	9.46	9.08	9.08	1
46	62-75-9	N-Nitrosodimethylamine	0	7	10.15	9.63	9.91	4
47	63-37-6	Cytidylate	-2	7	9.83	9.77	9.97	1
48	63-74-1	4-Aminobenzenesulfonamide	0	N.A.	9.87	9.51	9.74	1

49	65-23-6	Pyridoxine	0	6.8	10.34	9.54	9.80	1
50	65-46-3	Cytidine	1	7	10.11	10.57	10.50	1
51	65-71-4	Thymine	0	5.5	10.26	9.66	9.97	1
52	65-85-0	Benzoic acid	0	3	9.85	9.92	10.27	1
53	66-22-8	Uracil	0	7	10.18	9.72	10.05	1
54	66-71-7	4,5-Diazaphenanthrene	0	7	10.26	10.08	10.32	1
55	66-72-8	Pyridoxal	0	6.8	9.95	10.44	10.44	7
56	67-20-9	Nitrofurantoin	0	7	10.53	11.01	10.40	1
57	67-52-7	*Barbituric acid*	0	2.6	10.04	9.76	10.15	1
58	67-64-1	2-Propanone	0	N.A.	9.89	9.25	9.42	1
59	67-66-3	Trichloromethane	0	7	10.48	10.31	10.35	1
60	68-12-2	*N,N-Dimethylformamide*	0	N.A.	8.60	8.56	8.22	1
61	68-94-0	6-Hydroxypurine	0	6.5	9.98	9.60	9.87	1
62	69-53-4	Ampicillin	-1	6	9.76	9.31	9.45	1
63	69-65-8	*D-Mannitol*	0	7	6.85	7.90	7.36	1
64	69-89-6	2,6-Dihydroxypurine	0	N.A.	9.59	9.72	10.01	1
65	69-93-2	*Uric acid*	0	5	9.78	9.58	9.82	1

66	71-30-7	Cytosine	0	7	10.11	9.58	9.85	1
67	71-33-0	*5-Azauracil*	0	8	9.45	9.85	10.27	1
68	71-55-6	1,1,1-Trichloroethane	0	N.A.	10.40	10.07	10.27	1
69	72-14-0	Sulfathiazole	0	N.A.	10.08	9.68	9.95	1
70	73-24-5	*Adenine*	0	11	9.04	9.59	9.87	1
71	73-40-5	Guanine	0	7	10.15	9.56	9.80	1
72	74-11-3	4-Chlorobenzoate	-1	10.5-11.5	9.78	9.50	9.59	8
73	74-86-2	Acetylene	0	N.A.	7.30	8.11	7.64	1
74	74-87-3	Methyl chloride	0	N.A.	8.67	8.70	8.85	1
75	74-88-4	Methyl iodide	0	N.A.	10.20	9.78	9.96	1
76	74-95-3	Methylene bromide	0	4	10.30	9.95	10.20	1
77	74-96-4	Ethyl bromide	0	7	9.90	9.57	9.87	1
78	74-98-6	Propane	0	N.A.	6.32	7.15	6.45	1
79	75-00-3	Chloroethane	0	N.A.	8.85	8.64	8.64	1
80	75-01-4	Vinyl chloride	0	6.5	8.40	9.23	9.35	1
81	75-03-6	Iodoethane	0	N.A.	10.18	9.73	9.95	1

82	75-05-8	Acetonitrile	0	N.A.	7.64	8.20	7.85	1
83	75-07-0	Acetaldehyde	0	6.6	9.64	9.40	9.67	1
84	75-11-6	Methylene iodide	0	4	10.53	10.73	10.45	1
85	75-12-7	Formamide	0	N.A.	7.30	8.53	8.22	1
86	75-18-3	Dimethyl sulfide	0	N.A.	7.30	8.38	7.95	1
87	75-25-2	Bromoform	0	7	10.00	10.38	10.13	1
88	75-31-0	Isopropylamine	0	12.3	6.18	7.65	7.19	1
89	75-34-3	1,1-Dichloroethane	0	7	9.95	9.39	9.74	1
90	75-35-4	Vinylidene chloride	0	6.5	10.36	9.66	9.93	1
91	75-45-6	Chlorodifluoromethane	0	N.A.	9.46	9.37	9.59	1
92	75-52-5	*Nitromethane*	0	7	10.34	10.17	10.50	1
93	75-63-8	Bromotrifluoromethane	0	9	10.36	10.27	10.23	1
94	75-66-1	2-Methyl-2-propanethiol	0	7	9.48	8.68	8.41	1
95	75-69-4	*Trichlorofluoromethane*	0	6	10.20	10.76	10.24	1
96	75-71-8	Dichlorodifluoromethane	0	6	10.15	10.37	10.12	1
97	75-72-9	Chlorotrifluoromethane	0	9	9.64	9.74	9.61	1
98	76-06-2	Trichloronitromethane	0	N.A.	10.33	11.16	10.43	9

99	76-13-1	1,1,2-Trichlorotrifluoroethane	0	7	10.15	10.39	10.20	1
100	76-22-2	Camphor	0	9.2	9.49	9.30	9.47	1
101	76-38-0	2,2-Dichloro-1,1-difluoro-1-methoxyethane	0	7	10.15	9.57	9.95	1
102	77-77-0	*Divinyl sulphone*	0	7	10.00	9.90	10.32	1
103	77-81-6	Tabun	0	N.A.	9.57	9.30	9.52	10
104	78-76-2	*2-Bromobutane*	0	7	9.86	9.70	9.94	1
105	78-81-9	*Isobutylamine*	0	11.9	7.04	7.71	7.24	1
106	78-94-4	*Methyl vinyl ketone*	0	5.8	9.40	10.05	10.35	1
107	78-95-5	Chloroacetone	0	N.A.	10.13	9.76	10.01	11
108	79-00-5	1,1,2-Trichloroethane	0	7	9.92	9.68	10.04	1
109	79-01-6	*Trichloroethylene*	0	N.A.	10.28	10.07	10.37	1
110	79-05-0	Propionamide	0	9.2	7.73	8.47	8.10	1
111	79-06-1	Acrylamide	0	N.A.	10.18	9.64	9.99	1
112	79-11-8	Chloroacetic acid	0	1	9.84	9.15	9.31	1
113	79-14-1	Hydroxyacetic acid	0	3	8.63	8.81	8.75	1
114	79-19-6	Thiosemicarbazide	0	7	9.04	9.12	9.15	1

115	79-20-9	*Methyl acetate*	0	N.A.	7.94	8.76	8.64	1
116	79-24-3	Nitroethane	0	N.A.	10.43	10.12	10.48	1
117	79-27-6	*1,1,2,2-Tetrabromoethane*	0	7	10.23	10.18	10.26	1
118	79-39-0	Methacrylamide	0	9.2	10.38	9.49	9.79	1
119	79-41-4	2-Methylpropenoic acid	0	2-3.7	10.28	9.77	10.18	1
120	79-42-5	2-Mercaptopropionic acid	0	1.6-3	9.54	9.09	9.14	1
121	80-08-0	4,4’-Diamino diphenyl sulfone	0	N.A.	9.96	9.73	9.99	12
122	80-15-9	Cumene hydroperoxide	0	N.A.	9.64	9.15	9.23	1
123	80-62-6	Methyl methacrylate	0	9.2	10.11	9.73	10.12	1
124	83-34-1	3-Methylindole	0	8.2	8.41	9.32	9.45	1
125	83-40-9	*3-Methyl-salicylate*	-1	7	9.73	9.24	9.33	2
126	83-42-1	2-Chloro-6-nitrotoluene	0	N.A.	10.52	10.71	10.50	1
127	83-53-4	1,4-Dibromonaphthalene	0	N.A.	10.48	10.27	10.30	1
128	83-67-0	*Theobromine*	0	13	9.34	9.68	9.95	1
129	83-88-5	*Riboflavine*	0	5.9	10.36	10.97	10.39	1
130	84-66-2	*Diethyl phthalate*	0	N.A.	10.00	9.91	10.26	13
131	85-01-8	Phenanthrene	0	12.1	9.60	9.87	10.14	1

132	85-32-5	Guanosine monophosphate	0	6	9.49	9.37	9.53	1
133	86-42-0	Amodiaquine	0	7.1	10.59	10.19	10.27	1
134	86-53-3	1-Naphthonitrile	0	11	10.32	10.32	10.40	1
135	86-73-7	*Fluorene*	0	12.1	9.70	9.69	9.96	1
136	87-08-1	Penicillin V	-1	6	9.43	9.23	9.31	1
137	88-67-5	2-Iodobenzoate	-1	10.5-11.5	9.66	9.86	10.06	8
138	88-73-3	1-Chloro-2-nitrobenzene	0	N.A.	10.38	10.75	10.51	1
139	88-75-5	2-Nitrophenolate	-1	10.5-11.5	10.30	10.12	10.21	8
140	89-25-8	Edaravone	0	7	9.38	9.66	9.92	14
141	89-56-5	5-Methyl-salicylate	-1	7	9.67	9.31	9.43	2
142	89-59-8	4-Chloro-2-nitrotoluene	0	N.A.	10.52	10.77	10.50	1
143	89-98-5	2-Chlorobenzaldehyde	0	10	10.34	10.43	10.46	1
144	90-03-9	2-(Chloromercuri)phenol	0	9.4	10.04	9.94	10.13	1
145	90-11-9	1-Bromonaphthalene	0	N.A.	10.26	10.15	10.23	1
146	90-13-1	1-Chloronaphthalene	0	N.A.	10.15	10.06	10.22	1

147	90-15-3	*1-Naphthol*	0	10.5-11.5	8.98	9.78	10.03	8
148	90-34-6	Primaquine	0	7.3	10.23	9.99	10.15	1
149	90-44-8	Anthrone	0	9.2	10.52	10.28	10.43	1
150	90-96-0	*4,4'-Dimethoxybenzophenone*	0	N.A.	10.15	10.13	10.33	1
151	90-99-3	Chlorodiphenylmethane	0	8	8.98	9.80	10.08	1
152	91-00-9	Benzhydrylamine	0	11.2	8.52	9.33	9.51	1
153	91-02-1	2-Benzoylpyridine	0	9	10.40	10.40	10.46	1
154	91-18-9	Pteridine	0	6	10.48	10.80	10.46	1
155	91-19-0	*Quinoxaline*	0	7	10.49	10.38	10.46	1
156	91-20-3	Naphthalene	0	N.A.	9.70	9.84	10.11	1
157	91-22-5	quinoline	0	N.A.	9.85	10.07	10.31	15
158	91-59-8	2-Naphthylamine	0	7	10.26	9.79	10.02	1
159	91-64-5	Coumarin	0	N.A.	10.20	10.29	10.41	1
160	92-52-4	Biphenyl	0	9	10.08	9.65	9.93	1
161	92-55-7	5-Nitro-2-furaldehyde diacetate	0	7	10.48	10.80	10.48	1
162	92-75-1	3-Hydroxy-N-(2',4'-dimethylphenyl)-	0	7	10.38	10.17	10.32	1

		2-naphthamide						
163	92-84-2	Phenothiazine	0	8.7	9.74	9.57	9.79	1
164	92-87-5	Benzidine	0	7	9.32	9.38	9.53	1
165	94-13-3	Propylparaben	0	N.A.	9.99	9.73	10.03	16
166	95-14-7	*Benzotriazole*	0	10.5	9.23	10.05	10.30	1
167	95-49-8	2-Chlorotoluene	0	N.A.	9.04	9.35	9.48	1
168	95-50-1	1,2-Dichlorobenzene	0	11	9.67	9.65	9.81	1
169	95-51-2	*2-Chloroaniline*	0	N.A.	8.73	9.39	9.45	1
170	95-56-7	2-Bromophenol	0	5	9.86	9.60	9.67	1
171	95-57-8	*2-Chlorophenol*	0	5	9.11	9.44	9.55	1
172	95-57-8	2-Chlorophenolate	-1	10.5-11.5	8.38	8.96	8.84	8
173	95-75-0	3,4-Dichlorotoluene	0	N.A.	9.23	9.61	9.76	1
174	96-24-2	*3-Chloro-1,2-propanediol*	0	N.A.	8.83	8.76	8.66	1
175	96-33-3	Methyl acrylate	0	11	9.97	9.81	10.23	1
176	96-35-5	Methyl hydroxyacetate	0	10.6	8.68	8.79	8.71	1
177	97-63-2	Ethyl methacrylate	0	N.A.	9.38	9.71	10.09	1

178	97-77-8	Tetraethylthiuram disulfide	0	9.2	10.04	10.23	10.33	1
179	98-07-7	Benzotrichloride	0	10	9.92	10.09	10.20	1
180	98-08-8	Benzotrifluoride	0	11	9.26	9.68	9.88	1
181	98-10-2	Benzenesulfonamide	0	11	9.99	9.68	10.05	1
182	98-11-3	Benzenesulfonate	-1	10.5-11.5	9.60	9.27	9.39	8
183	98-83-9	1-Methyl-1-phenylethylene	0	5.5	9.48	9.60	9.87	1
184	98-86-2	Acetophenone	0	9.2	10.23	10.06	10.35	1
185	98-92-0	3-Pyridinecarboxamide	0	7.5	10.38	9.89	10.24	1
186	98-95-3	Nitrobenzene	0	N.A.	10.58	10.63	10.51	1
187	99-04-7	3-Methylbenzoate	-1	10.5-11.5	9.41	9.25	9.34	8
188	99-06-9	3-Hydroxybenzoate	-2	10.5-11.5	9.04	8.80	8.77	8
189	99-94-5	4-methylbenzoate	-1	10.5-11.5	9.48	9.21	9.28	8
190	99-96-7	4-Hydroxybenzoate	-2	10.5-11.5	8.60	8.52	8.37	8

191	99-98-9	N,N-Dimethyl-p-phenylenediamine	0	9	8.20	9.18	9.24	1
192	99-99-0	4-Nitrotoluene	0	11	10.28	10.61	10.50	1
193	100-00-5	1-Chloro-4-nitrobenzene	0	N.A.	10.75	10.80	10.51	1
194	100-02-7	*4-Nitrophenol*	0	5.5	10.64	10.58	10.47	1
195	100-02-7	*4-Nitrophenolate*	-1	10.5-11.5	10.40	10.13	10.22	8
196	100-19-6	4-Nitroacetophenone	0	6.8	10.61	10.89	10.46	1
197	100-21-0	Terephthalate	-2	10.5-11.5	9.86	9.29	9.41	8
198	100-42-5	Ethenylbenzene	0	5.5	9.48	9.74	10.03	1
199	100-44-7	*Benzyl chloride*	0	N.A.	9.18	9.67	9.93	1
200	100-46-9	Benzenemethanamine	0	11.2	7.90	9.10	9.13	1
201	100-47-0	Cyanobenzene	0	7.16	10.23	9.92	10.28	1
202	100-51-6	*Benzenemethanol*	0	6.5	8.30	9.11	9.17	1
203	100-52-7	Benzaldehyde	0	7	10.38	10.18	10.43	1
204	100-53-8	Benzyl mercaptan	0	7	9.94	9.35	9.55	1
205	100-65-2	N-Phenylhydroxylamine	0	N.A.	9.26	9.17	9.23	1

206	100-75-4	N-Nitrosopiperidine	0	7	10.24	9.66	9.94	4
207	101-43-9	Cyclohexyl methacrylate	0	7	9.30	9.71	10.10	1
208	102-04-5	1,3-Diphenyl-2-propanone	0	9.2	10.04	9.69	9.99	1
209	103-83-3	N,N-Dimethylbenzylamine	0	11.1	8.18	9.20	9.27	1
210	103-85-5	Phenylthiourea	0	9.2	9.62	9.58	9.83	1
211	103-90-2	Acetaminophen	0	7	8.40	9.29	9.41	1
212	104-15-4	*4-Methylbenzenesulfonate*	-1	10.5-11.5	9.22	9.21	9.31	8
213	104-57-4	Benzyl formate	0	N.A.	9.18	9.36	9.60	1
214	104-88-1	4-Chlorobenzaldehyde	0	10	10.34	10.38	10.44	1
215	105-37-3	*Ethyl propionate*	0	N.A.	7.88	8.71	8.55	1
216	105-55-5	1,3-Diethyl-2-thiourea	0	7	8.70	9.03	8.99	1
217	105-56-6	Ethyl cyanoacetate	0	10.92	8.51	8.98	9.08	1
218	106-39-8	1-Bromo-4-chlorobenzene	0	10	9.62	9.79	9.89	1
219	106-41-2	4-Bromophenol	0	5	9.80	9.73	9.76	1
220	106-41-2	4-Bromophenolate	-1	10.5-11.5	9.46	9.70	9.52	8

221	106-43-4	4-Chlorotoluene	0	11	8.65	9.37	9.49	1
222	106-46-7	1,4-Dichlorobenzene	0	11	9.70	9.69	9.84	1
223	106-47-8	*4-Chloroaniline*	0	N.A.	8.72	9.41	9.48	1
224	106-48-9	4-Chlorophenol	0	5	9.18	9.47	9.59	1
225	106-48-9	4-Chlorophenolate	-1	10.5-11.5	8.81	8.98	8.88	8
226	106-51-4	1,4-Benzoquinone	0	N.A.	10.36	11.24	10.41	1
227	106-94-5	1-Bromopropane	0	7	10.00	9.51	9.82	1
228	106-97-8	Butane	0	7.6-8.5	6.38	7.18	6.50	1
229	106-99-0	Butadiene	0	7	9.90	9.56	9.84	1
230	107-04-0	1-Bromo-2-chloroethane	0	7	9.90	9.78	10.03	1
231	107-06-2	1,2-Dichloroethane	0	N.A.	8.81	9.25	9.58	1
232	107-07-3	2-Chloroethanol	0	N.A.	8.62	8.76	8.72	1
233	107-08-4	1-Iodopropane	0	6.2	10.11	9.69	9.93	1
234	107-13-1	Acrylonitrile	0	N.A.	10.00	9.89	10.31	17
235	107-29-9	Acetaldoxime	0	10.8	7.86	8.93	8.88	1
236	107-96-0	3-Mercaptopropionic acid	0	1.6-3.0	9.73	8.93	8.87	1

237	107-97-1	Sarcosine	-1	7	7.20	7.53	7.33	1
238	108-03-2	1-Nitropropane	0	N.A.	10.43	10.12	10.48	1
239	108-05-4	Vinyl acetate	0	11	9.23	9.25	9.42	1
240	108-13-4	Malonodiamide	0	7	9.04	8.79	8.64	1
241	108-19-0	Biuret	0	10.3	8.40	8.75	8.57	1
242	108-32-7	Propylene carbonate	0	N.A.	7.86	8.28	7.90	1
243	108-36-1	1,3-Dibromobenzene	0	N.A.	10.00	9.74	9.87	18
244	108-37-2	1-Bromo-3-chlorobenzene	0	10	9.71	9.73	9.87	1
245	108-41-8	*1-Chloro-3-methylbenzene*	0	N.A.	8.94	9.36	9.49	1
246	108-42-9	3-Chloroaniline	0	N.A.	8.72	9.39	9.46	1
247	108-43-0	3-Chlorophenol	0	5	9.28	9.45	9.57	1
248	108-43-0	3-Chlorophenolate	-1	10.5-11.5	8.70	8.96	8.83	8
249	108-48-5	2,6-Dimethylpyridine	0	9.5	9.70	9.46	9.73	1
250	108-75-8	2,4,6-Trimethylpyridine	0	9.5	9.64	9.40	9.63	1
251	108-80-5	Cyanuricacid	0	6	9.15	9.14	9.31	19
252	108-86-1	Bromobenzene	0	10	9.58	9.61	9.71	1

253	108-90-7	*Chlorobenzene*	0	11	8.96	9.39	9.53	1
254	108-91-8	*Cyclohexylamine*	0	11.8	6.23	7.52	7.12	1
255	108-99-6	3-Methylpyridine	0	9.5	9.88	9.48	9.77	1
256	109-00-2	3-Hydroxypyridine	0	6.8	10.15	9.54	9.81	1
257	109-12-6	2-Aminopyrimidine	0	5.8	10.08	9.70	9.99	1
258	109-65-9	1-Bromobutane	0	7	9.95	9.49	9.79	1
259	109-69-3	1-Chlorobutane	0	7.6	8.60	8.60	8.50	1
260	110-05-4	*Bis(1,1-dimethylethyl) peroxide*	0	N.A.	8.15	8.50	8.13	1
261	110-14-5	Succinic diamide	0	7.1	8.30	8.61	8.33	1
262	110-15-6	Butanedioic acid	0	3-4	8.57	8.92	8.94	1
263	110-16-7	Maleic acid	0	N.A.	10.46	10.08	10.43	1
264	110-22-5	Diacetyl peroxide	0	N.A.	9.98	9.13	9.34	1
265	110-26-9	N,N'-Methylenebisacrylamide	0	7	10.45	9.76	10.13	1
266	110-44-1	Sorbic acid	0	2-3.7	10.46	10.19	10.38	1
267	110-53-2	1-Bromopentane	0	7	9.90	9.47	9.77	1
268	110-61-2	Succinonitrile	0	3-4	9.23	8.72	8.78	1
269	110-86-1	Pyridine	0	7	9.89	9.48	9.79	1

270	110-88-3	Trioxane	0	11	6.00	7.20	6.69	1
271	115-39-9	*Bromphenol Blue*	0	N.A.	10.04	10.01	10.19	1
272	116-43-8	*Sulfasuccidine*	0	N.A.	10.15	10.01	10.26	1
273	117-39-5	Quercetin	0	7	10.11	10.13	10.28	20
274	117-96-4	Diatrizoate	-1	N.A.	10.33	10.40	10.33	21
275	118-00-3	Guanosine	0	6.7	9.78	9.36	9.52	1
276	118-90-1	o-Toluate	-1	10.5-11.5	9.48	9.23	9.31	8
277	118-91-2	2-Chlorobenzoate	-1	10	9.15	9.38	9.43	22
278	119-53-9	*2-Hydroxy-2-phenylacetophenone*	0	9.2	10.23	10.24	10.40	1
279	119-61-9	Benzophenone	0	N.A.	10.30	10.25	10.43	1
280	119-65-3	*Isoquinoline*	0	N.A.	9.53	10.04	10.29	15
281	120-72-9	*Indole*	0	11	8.41	9.33	9.47	1
282	120-73-0	*Purine*	0	6	10.32	9.90	10.25	1
283	120-83-2	2,4-Dichlorophenol	0	7	8.70	9.72	9.84	1
284	120-92-3	*Cyclopentanone*	0	N.A.	9.87	9.36	9.56	23
285	121-14-2	2,4-Dinitrotoluene	0	N.A.	10.38	10.78	10.51	24

286	121-73-3	1-Chloro-3-nitrobenzene	0	N.A.	10.49	10.83	10.51	1
287	122-39-4	Diphenylamine	0	9.2	9.18	9.36	9.51	1
288	123-38-6	Propionaldehyde	0	N.A.	9.53	9.45	9.73	1
289	123-39-7	*N-Methylformamide*	0	9.2	7.85	8.51	8.17	1
290	123-56-8	Succinimide	0	11.4	8.96	9.35	9.60	1
291	123-56-8	*Succinimide*	1	6.5	10.04	10.47	10.58	1
292	123-75-1	*Pyrrolidine*	0	12.08	6.62	7.63	7.23	1
293	127-06-0	Acetone oxime	0	7	8.54	8.82	8.67	1
294	127-07-1	*Hydroxyurea*	0	6.8	8.68	8.26	7.81	1
295	127-18-4	*Tetrachloroethylene*	0	N.A.	10.62	10.46	10.54	1
296	127-19-5	N,N-Dimethylacetamide	0	9.2 N,A,	7.32	8.53	8.17	1
297	127-79-7	Sulfamerazine	0	5.4-6	10.30	9.85	10.12	6
298	128-53-0	N-Ethylmaleimide	0	6	10.58	10.63	10.51	1
299	130-95-0	Quinine	0	8.5	10.23	10.11	10.29	1
300	131-11-3	Dimethyl phthalate	0	7	10.20	9.91	10.27	25
301	131-69-1	4-(2-Acetylsulfamyl)phthalanilic acid	0	N.A.	9.87	10.13	10.36	1

302	134-81-6	Benzil	0	N.A.	10.48	10.58	10.46	1
303	135-19-3	*2-Naphthol*	0	10.5-11.5	9.08	9.82	10.08	8
304	137-18-8	2,5-Dimethyl-1,4-benzoquinone	0	7.2	10.49	11.12	10.42	1
305	138-89-6	*N,N-Dimethyl-4-nitrosoaniline*	0	N.A.	10.53	10.63	10.37	1
306	140-10-3	*trans-Cinnamic acid*	0	2-3.7	10.34	10.32	10.42	1
307	140-11-4	Benzyl acetate	0	N.A.	9.04	9.29	9.48	1
308	140-88-5	Ethyl acrylate	0	11	9.94	9.80	10.22	1
309	141-05-9	Diethyl maleate	0	N.A.	10.34	10.01	10.37	17
310	141-43-5	2-Aminoethanol	0	7.8	7.30	7.58	7.13	1
311	141-78-6	*Ethyl acetate*	0	6.53 N.A.	7.66	8.74	8.60	1
312	141-82-2	Malonic acid	0	N.A.	9.20	8.98	9.06	1
313	142-08-5	2-Pyridone	0	6.8	10.15	9.51	9.78	1
314	144-48-9	Iodoacetamide	0	N.A.	10.70	10.19	10.33	1
315	144-62-7	Oxalic acid	0	1.3	10.40	10.19	10.47	1
316	144-82-1	Sulfamethizole	0	5.4-6	10.30	9.86	10.13	6

317	146-17-8	Flavine mononucleotide	0	6	10.52	11.00	10.39	1
318	153-18-4	Rutin	0	6.9	9.88	10.28	10.35	20
319	253-52-1	Phthalazine	0	7	10.54	10.18	10.39	1
320	260-94-6	Acridine	0	10	10.11	10.53	10.39	1
321	288-47-1	Thiazole	0	8	9.32	9.53	9.84	1
322	289-80-5	Pyridazine	0	7	10.34	9.99	10.28	1
323	289-95-2	Pyrimidine	0	7	10.30	9.79	10.15	1
324	290-37-9	Pyrazine	0	7	10.32	9.99	10.31	1
325	290-87-9	1,3,5-Triazine	0	6	9.72	9.95	10.34	19
326	298-81-7	8-Methoxypsoralen	0	N.A.	10.18	10.28	10.34	1
327	314-50-1	Orotidine	-1	7	9.95	9.66	9.92	1
328	331-39-5	caffeate	-1	7	10.15	9.65	9.87	26
329	343-65-7	Kynurenine	*Z*	7.4	10.36	10.11	10.27	1
330	350-03-8	*3-Acetylpyridine*	0	9.6	10.38	10.21	10.43	1
331	363-72-4	Pentafluorobenzene	0	6.5	10.20	9.87	10.17	1
332	366-18-7	*2,2'-Dipyridyl*	0	8	10.28	10.05	10.31	1
333	366-29-0	N,N,N',N'-Tetramethylbenzidine	0	9	8.23	9.37	9.53	1

334	367-11-3	1,2-Difluorobenzene	0	6.5	9.08	9.46	9.57	1
335	367-12-4	2-Fluorophenolate	-1	10.5-11.5	8.53	8.75	8.57	8
336	371-41-5	*4-Fluorophenolate*	-1	10.5-11.5	8.08	8.95	8.85	8
337	372-20-3	3-Fluorophenolate	-1	10.5-11.5	8.30	8.75	8.57	8
338	392-56-3	*Hexafluorobenzene*	0	N.A.	9.93	9.89	10.29	27
339	430-51-3	*Fluoroacetone*	0	6.7	9.00	9.55	9.76	1
340	431-03-8	2,3-Butanedione	0	N.A.	10.00	10.55	10.46	1
341	431-47-0	Methyl trifluoroacetate	0	10.62	9.28	9.68	10.01	1
342	439-14-5	Diazepam	0	N.A.	10.08	10.20	10.35	1
343	443-48-1	Metronidazole	0	N.A.	10.48	10.62	10.48	1
344	445-29-4	*2-Fluorobenzoate*	-1	10.5-11.5	9.49	9.40	9.45	8
345	446-72-0	Genistein	0	6.9	9.79	9.97	10.19	20
346	455-38-9	3-Fluorobenzoate	-1	10.5-11.5	9.83	9.43	9.50	8

347	456-22-4	4-Fluorobenzoate	-1	10.5-11.5	9.58	9.27	9.27	8
348	460-19-5	*Cyanogen*	0	6	10.32	10.30	10.60	1
349	461-89-2	*6-Azauracil*	0	8	9.66	10.22	10.46	1
350	464-10-8	Tribromonitromethane	0	7	10.36	10.41	10.35	28
351	480-41-1	*Naringenin*	0	6.9	10.08	9.99	10.19	20
352	481-39-0	5-Hydroxy-1,4-naphthoquinone	0	6.4	10.45	11.07	10.40	1
353	481-42-5	5-hydroxy-2-methyl-1,4-naphthoquinone	0	N.A.	10.20	11.00	10.41	29
354	484-78-6	3-Hydroxykynurenine	Z	7.4	10.40	10.09	10.24	1
355	486-25-9	9-Fluorenone	0	N.A.	10.43	10.65	10.43	1
356	487-21-8	Lumazine	0	6.3	10.46	10.52	10.49	1
357	488-82-4	Arabinitol	0	7	7.85	7.94	7.40	1
358	491-67-8	Baicalein	0	7	10.04	10.25	10.34	20
359	491-71-4	Chrysoeriol	0	7	9.72	10.17	10.32	30
360	494-38-2	Acridine Orange	0	6.5	10.48	10.29	10.28	1
361	495-48-7	(Z)-Diphenyldiazene	0	14	10.52	10.41	10.42	1

362	495-54-5	Chrysoidin	0	7	9.86	10.36	10.31	1
363	501-52-0	*Hydrocinnamate*	-1	5.4	8.60	9.15	9.18	1
364	501-98-4	p-Coumarate	-1	7	10.04	9.65	9.88	20
365	503-64-0	(Z)-2-Butenoic acid	0	3	10.26	9.77	10.17	1
366	504-07-4	5,6-Dihydrouracil	0	7	9.65	9.22	9.40	1
367	507-19-7	2-Bromo-2-methylpropane	0	7	9.86	9.95	9.99	1
368	512-85-6	*Ascaridole*	0	N.A.	9.60	9.10	9.11	1
369	513-36-0	1-Chloro-2-methylpropane	0	5.82	8.71	8.54	8.40	1
370	513-86-0	3-Hydroxy-2-butanone	0	N.A.	9.78	9.36	9.58	1
371	513-88-2	1,1-Dichloroacetone	0	N.A.	10.09	10.21	10.30	11
372	527-17-3	2,3,5,6-Tetramethylbenzoquinone	0	7	10.49	10.99	10.43	1
373	527-73-1	2-Nitroimidazole	0	7	10.57	10.74	10.48	1
374	529-59-9	Genistin	0	6.9	9.79	9.98	10.21	20
375	530-48-3	*1,1-Diphenylethylene*	0	5.5	9.11	9.76	10.04	1
376	533-67-5	*Deoxyribose*	0	7	7.00	7.87	7.35	1
377	535-80-8	3-Chlorobenzoate	-1	10.5-11.5	9.74	9.50	9.60	8

378	540-36-3	1,4-Difluorobenzene	0	6.5	9.30	9.60	9.73	1
379	540-51-2	2-Bromoethanol	0	10	9.20	9.46	9.72	1
380	540-54-5	1-Chloropropane	0	7.6	8.79	8.63	8.57	1
381	540-73-8	*1,2-Dimethylhydrazine*	0	12.4	6.79	7.64	7.36	1
382	541-47-9	3,3-Dimethylacrylic acid	0	3	10.18	9.74	10.11	1
383	541-73-1	1,3-Dichlorobenzene	0	7	10.00	9.67	9.84	31
384	542-59-6	2-Hydroxyethyl acetate	0	N.A.	7.41	8.79	8.69	1
385	542-69-8	Butyl iodide	0	7.6	10.08	9.67	9.93	1
386	544-25-2	*Cycloheptatriene*	0	N.A.	9.78	9.72	9.99	1
387	545-06-2	Trichloroacetonitrile	0	7	10.51	10.54	10.39	1
388	551-16-6	6-Aminopenicillanate	-1	6	9.56	8.97	8.88	1
389	551-62-2	1,2,3,4-Tetrafluorobenzene	0	6.5	10.41	9.75	9.97	1
390	553-26-4	4,4'-Dipyridyl	0	8.3	10.40	10.09	10.39	1
391	553-30-0	3,6-Diaminoacridine	0	N.A.	10.53	10.31	10.30	1
392	553-90-2	Dimethyl oxalate	0	N.A.	10.30	10.09	10.41	1
393	554-01-8	5-Methylcytosine	0	7.7	10.00	9.56	9.82	1
394	554-12-1	*Methyl propionate*	0	6.81	7.95	8.73	8.59	1

395	554-84-7	3-Nitrophenolate	-1	10.5-11.5	10.40	10.52	10.25	8
396	555-15-7	Nifuroxime	0	6.8	10.58	10.93	10.43	1
397	556-33-2	Glycylglycylglycine	Z	6.1	9.04	9.29	9.41	1
398	556-50-3	*Glycylglycine*	Z	5.9	8.34	9.22	9.37	1
399	563-70-2	Bromonitromethane	0	7	10.50	10.29	10.50	28
400	567-61-3	6-Methyl-salicylate	-1	7	9.15	9.29	9.41	2
401	578-76-7	7-Methylguanine	0	6	10.20	9.55	9.78	1
402	583-39-1	2-Mercaptobenzimidazole	0	7	9.38	9.45	9.67	1
403	586-76-5	4-Bromobenzoate	-1	10.5-11.5	9.89	9.79	9.76	8
404	587-04-2	3-Chlorobenzaldehyde	0	10	10.34	10.40	10.45	1
405	591-20-8	3-Bromophenolate	-1	10.5-11.5	9.43	9.65	9.51	8
406	591-20-8	*3-Bromophenol*	0	5	9.78	9.64	9.72	1
407	591-22-0	3,5-Dimethylpyridine	0	9.5	9.85	9.49	9.76	1
408	591-50-4	Iodobenzene	0	11	10.08	9.69	9.90	1
409	591-54-8	4-Aminopyrimidine	0	8.2	10.04	9.48	9.74	1

410	592-57-4	*1,3-Cyclohexadiene*	0	11	9.00	9.52	9.75	1
411	598-32-3	3-Buten-2-ol	0	N.A.	7.77	8.80	8.67	1
412	598-41-4	2-Aminoacetamide	0	11.4	8.45	8.46	8.07	1
413	598-42-5	*2-Hydroxyacetamide*	0	8.5	8.46	8.51	8.17	1
414	602-94-8	Pentafluorobenzoate	-1	12	9.98	9.63	9.87	1
415	607-34-1	5-Nitroquinoline	0	7	10.60	10.80	10.46	1
416	607-35-2	8-Nitroquinoline	0	7	10.60	10.64	10.47	1
417	608-31-1	2, 6-Dichloraniline	0	7	10.18	9.63	9.72	32
418	609-40-5	2-Nitrothiophene	0	7	10.48	10.77	10.49	1
419	611-08-5	*5-Nitrouracil*	0	5.9	10.32	10.66	10.51	1
420	611-19-8	2-Chlorobenzyl chloride	0	N.A.	10.00	9.53	9.69	1
421	611-20-1	2-Cyanophenolate	-1	10.5-11.5	9.91	9.44	9.62	8
422	613-46-7	2-Naphthonitrile	0	11	10.32	10.25	10.38	1
423	613-50-3	6-Nitroquinoline	0	7	10.60	10.80	10.46	1
424	613-51-4	7-Nitro-quinoline	0	7	10.60	10.82	10.46	1
425	613-94-5	Benzoic hydrazide	0	N.A.	10.19	9.63	9.95	3

426	614-00-6	Methylphenyl nitrosamine	0	7	10.36	9.93	10.21	4
427	616-34-2	Methyl 2-aminoacetate	0	11.2	8.52	8.86	8.73	1
428	616-47-7	1-Methylimidazole	0	10.2	7.52	8.57	8.23	1
429	618-51-9	3-Iodobenzoate	-1	10.5-11.5	10.11	9.69	9.83	8
430	619-58-9	4-Iodobenzoate	-1	10.5-11.5	9.96	9.70	9.84	8
431	619-65-8	*4-Cyanobenzoate*	-1	10.5-11.5	10.00	10.01	10.21	8
432	621-08-9	Dibenzyl sulfoxide	0	4-7	9.54	9.48	9.71	1
433	621-44-3	3-Nitrotyrosine	Z	7.3	10.48	10.62	10.42	33
434	621-64-7	N-Nitrosodipropylamine	0	7	10.18	9.67	9.95	4
435	622-24-2	*Phenethyl chloride*	0	N.A.	8.72	9.34	9.48	1
436	623-26-7	1,4-Dicyanobenzene	0	N.A.	10.45	10.49	10.52	1
437	623-70-1	Ethyl crotonate	0	N.A.	9.91	9.69	10.07	17
438	623-91-6	Diethyl fumarate	0	N.A.	10.34	10.43	10.53	17
439	624-48-6	Dimethyl maleate	0	N.A.	10.52	10.03	10.39	17
440	624-49-7	Dimethyl fumarate	0	N.A.	10.51	10.45	10.54	17

441	625-50-3	N-Ethylacetamide	0	6.7	7.15	8.46	8.08	1
442	625-77-4	Diacetamide	0	6.5	10.04	9.50	9.78	1
443	626-48-2	*6-Methyluracil*	0	12	9.23	9.65	9.96	34
444	626-64-2	4-Pyridinol	0	6.8	9.92	9.25	9.42	1
445	630-10-4	Selenourea	0	6.5	9.60	9.17	9.22	1
446	637-84-3	Glycylglycylglycylglycine	Z	6	9.18	9.10	9.10	1
447	652-29-9	2',3',4',5',6'-Pentafluoroacetophenone	0	7	10.28	10.57	10.39	27
448	652-78-8	*Gossypin*	0	N.A.	10.08	10.17	10.29	20
449	653-34-9	2,3,4,5,6-Pentafluorostyrene	0	14	9.98	10.30	10.27	27
450	653-37-2	Pentafluorobenzaldehyde	0	7	10.38	10.84	10.46	27
451	658-79-7	*GlyTyrOH*	Z	5.7	8.58	9.20	9.27	1
452	683-08-9	Diethyl methylphosphonate	0	N.A.	7.53	7.68	7.09	9
453	687-38-7	Glycylserine	Z	6.2	8.57	8.91	8.78	1
454	694-80-4	1-Bromo-2-chlorobenzene	0	10	9.77	9.58	9.78	1
455	695-96-5	2-Bromo-4-chlorophenol	0	5	9.92	9.74	9.85	1
456	696-07-1	*5-Iodouracil*	0	N.A.	10.23	9.86	10.07	1
457	696-23-1	2-Methyl-4-nitroimidazole	0	7	10.48	10.47	10.47	1

458	698-63-5	5-Nitro-2-furaldehyde	0	7	10.53	11.05	10.45	1
459	704-15-4	Glycylproline	Z	6.2	8.86	9.05	9.01	1
460	723-46-6	*Sulfamethoxazole*	0	5.4-6	10.00	9.65	9.91	6
461	762-75-4	Tert-butyl formate	0	N.A.	8.74	8.90	8.89	35
462	767-00-0	4-Hydroxybenzonitrile	-1	10.5-11.5	9.30	9.16	9.21	8
463	769-78-8	Vinyl benzoate	0	11	9.86	10.06	10.35	1
464	771-60-8	2,3,4,5,6-Pentafluoroaniline	0	7	9.94	9.62	9.87	20
465	771-61-9	Pentafluorophenol	0	4.6	10.38	9.70	10.00	20
466	771-62-0	Pentafluorothiophenolate	-1	7	9.82	9.56	9.94	20
467	773-82-0	pentafluorobenzonitrile	0	7	10.43	10.66	10.43	1
468	818-61-1	2-Hydroxyethyl acrylate	0	11	9.88	9.85	10.25	36
469	822-38-8	*1,3-Dithiolane-2-thione*	0	7	10.48	10.48	10.44	1
470	822-84-4	3-Nitrothiophene	0	7	10.52	10.62	10.50	1
471	827-15-6	*Iodopentafluorobenzene*	0	7	9.75	10.53	10.48	1
472	828-73-9	Pentafluorophenylhydrazine	0	7	9.93	9.63	9.80	27
473	853-34-9	Ketophenylbutazone	0	7.5	9.43	9.70	9.97	1

474	868-77-9	2-Hydroxyethyl methacrylate	0	N.A.	9.40	9.75	10.14	1
475	869-19-2	*Glycylleucine*	Z	5.5	8.43	9.04	9.01	1
476	873-62-1	3-Hydroxybenzonitrile	-1	10.5-11.5	9.68	9.57	9.78	8
477	874-14-6	1,3-Dimethyluracil	0	N.A.	10.00	9.66	9.97	1
478	877-89-4	2,4,6-Trimethoxy-1,3,5-triazine	0	6	9.57	9.28	9.53	19
479	880-78-4	Pentafluoronitrobenzene	0	7	10.64	11.20	10.51	27
480	882-09-7	*Clofibrate*	-1	7	8.82	9.43	9.54	37
481	902-04-5	2'-Deoxyguanosine 5'-monophosphate	0	6	10.26	9.34	9.49	1
482	917-95-3	*2-Methyl-2-nitrosopropane*	0	9.2	9.79	10.53	10.40	1
483	918-00-3	1,1,1-Trichloroacetone	0	N.A.	10.19	10.44	10.38	11
484	918-01-4	Bromodichloronitromethane	0	N.A.	10.43	10.33	10.33	28
485	924-16-3	N-nitrosodibutylamine	0	7	10.19	9.66	9.94	4
486	924-50-5	*Methyl 3-methylcrotonate*	0	N.A.	9.74	9.70	10.06	17
487	926-79-4	*Alanylalanylalanylalanine*	Z	6.1	9.08	9.00	8.99	1
488	930-55-2	*N-Nitrosopyrrolidine*	0	7	10.28	9.66	9.94	4
489	931-07-7	4-Nitroisothiazole	0	7	10.52	10.69	10.53	1

490	931-85-1	*6-Azacytosine*	0	8	9.76	10.08	10.36	1
491	931-86-2	5-Azacytosine	0	8	10.08	9.54	9.85	1
492	932-53-6	6-Azathymine	0	8	9.98	10.12	10.40	1
493	932-83-2	N-Nitrosohexamethyleneimine	0	7	10.19	9.68	9.96	4
494	932-90-1	*Benzaldoxime*	0	N.A.	10.00	9.92	10.20	1
495	935-69-3	7-Methyladenine	0	N.A.	10.11	9.59	9.85	1
496	937-40-6	Methylbenzyl nitrosamine	0	7	10.26	9.71	10.01	4
497	943-39-5	*4-Nitroperoxybenzoic acid*	0	5	10.18	10.83	10.50	1
498	945-51-7	*Diphenyl sulfoxide*	0	7	10.26	9.72	10.03	1
499	983-85-7	Penamecillin	0	6	10.65	9.62	9.93	1
500	1006-94-6	5-Methoxyindole	0	7	8.85	9.34	9.48	1
501	1022-31-7	N-Formylkynurenine	Z	7.6	10.30	10.52	10.44	1
502	1031-07-8	Endosulfan sulfate	0	N.A.	10.53	10.15	10.24	38
503	1086-80-2	Lumichrome	0	6	10.41	10.76	10.43	1
504	1117-77-7	N-Acetylglycine methyl ester	0	8.7	8.52	9.03	9.06	1
505	1121-89-7	Glutarimide	0	N.A.	9.85	9.48	9.79	39
506	1122-47-0	1-Methylcytosine	0	N.A.	10.15	9.56	9.82	1

507	1184-89-0	Dibromochloronitromethane	0	7	10.47	10.42	10.34	28
508	1188-01-8	DL-Alanyl-Glycine	Z	6.22	8.32	9.03	8.98	1
509	1194-02-1	4-Fluorobenzonitrile	0	10	10.20	9.98	10.22	1
510	1445-08-5	2-Methyladenine	0	7	9.92	9.55	9.80	1
511	1453-82-3	4-Pyridinecarboxamide	0	9	10.51	10.03	10.35	1
512	1464-42-2	*Selenomethionine*	Z	N.A.	8.26	8.88	8.74	1
513	1481-93-2	4-Chromanol	0	6.9	8.64	9.23	9.32	20
514	1622-61-3	*Clonazepam*	0	N.A.	10.00	10.79	10.48	1
515	1634-04-4	Methyl tert-butyl ether	0	N.A.	7.24	7.60	7.12	35
516	1794-84-9	Chloronitromethane	0	7	10.48	10.49	10.50	28
517	1820-81-1	5-Chlorouracil	0	11	9.74	10.02	10.21	1
518	1912-24-9	Atrazine	0	6	9.68	9.54	9.77	40
519	1963-21-9	Glycylvaline	Z	5.97	8.41	8.93	8.81	1
520	2004-03-7	6-Methylpurine	0	5.9	10.46	9.81	10.16	1
521	2043-43-8	2-Hydroxypropionamide	0	7	8.28	8.52	8.19	1
522	2140-65-0	1-Methylguanosine	0	9.2	9.89	9.34	9.49	1
523	2210-25-5	N-Isopropylacrylamide	0	7	10.04	9.63	9.95	41

524	2236-60-4	Pterin	0	6.5	10.40	10.38	10.42	1
525	2314-97-8	*Trifluoroiodomethane*	0	N.A.	10.11	11.02	10.34	1
526	2365-48-2	Methyl thioglycolate	-1	10	9.15	8.90	8.80	1
527	2489-13-6	*GlyHis*	Z	7.6	8.79	9.03	8.99	1
528	2577-40-4	*L-Phenylalanyl-L-phenylalanine*	Z	5.7	8.65	9.51	9.74	1
529	2578-57-6	ProGly	-1	6.2	8.98	8.55	8.20	1
530	2620-63-5	N-Acetylglycinamide	0	9.2	8.32	8.73	8.52	1
531	2680-03-7	N,N-Dimethylacrylamide	0	9.2	10.20	9.70	10.01	1
532	2721-32-6	2,3-Diazabicyclo[2.2.1]hept-2-ene	0	N.A.	10.36	9.78	10.09	1
533	2816-24-2	α-Nitrophenyl--D-glucopyranoside	0	N.A.	10.40	10.72	10.47	1
534	2845-89-8	3-Chloroanisole	0	N.A.	8.97	9.43	9.55	1
535	2867-20-1	*Alanylalanine*	Z	6.2	8.43	9.03	8.99	1
536	2935-35-5	L-Phenylglycine	0	N.A.	8.95	9.32	9.53	42
537	3012-37-1	*Benzyl thiocyanate*	0	N.A.	9.30	9.81	10.17	1
538	3034-38-6	4-Nitroimidazole	0	7	10.49	10.49	10.50	1
539	3034-48-8	2-Bromo-5-nitrothiazole	0	7	10.30	10.39	10.43	1
540	3085-42-5	Di(4-chlorophenyl) sulfoxide	0	7	10.00	9.98	10.17	1

541	3270-71-1	Furamazone	0	7	10.52	11.02	10.40	1
542	3321-03-7	Glycylphenylalanine	Z	6.7	8.20	9.17	9.22	1
543	3376-24-7	N-tert-Butyl--phenylnitrone	0	N.A.	10.18	10.04	10.23	1
544	3615-55-2	Ribose-5-phosphate	0	N.A.	8.90	9.74	10.10	1
545	3617-44-5	Phenylalanine	Z	6.9	8.20	9.30	9.45	1
546	3695-73-6	*Glycyl-β-alanine*	Z	6.2	8.46	9.04	9.00	1
547	3964-56-5	4-Bromo-2-chlorophenol	0	5	9.95	9.85	9.89	1
548	4164-28-7	Dimethylnitramine	0	N.A.	10.28	9.65	10.03	43
549	4202-74-8	Glycine anhydride	0	9.2	9.23	9.67	10.00	1
550	4306-24-5	GlyLeuTyr	Z	6.1	8.96	9.17	9.22	1
551	4533-39-5	Nitracrine	0	7	10.65	11.00	10.32	1
552	4549-44-4	N-Nitrosoethylbutylamine	0	7	10.19	9.66	9.95	4
553	4697-36-3	Carbenicillin	-2	6	9.04	9.20	9.27	1
554	5076-82-4	Sarcosine anhydride	0	9.2	9.30	8.74	8.53	1
555	5257-06-7	*N-(2-Acetylphenyl)formamide*	0	7.6	10.26	10.17	10.38	1
556	5327-44-6	3,5-Dinitroanisole	0	N.A.	10.62	10.93	10.44	1
557	5424-19-1	*3-Benzoylpyridine*	0	9	10.48	10.36	10.47	1

558	5502-78-3	9-Methylguanine	0	6	9.88	9.49	9.71	1
559	5625-46-7	*Alanine anhydride*	0	9.2	9.30	8.78	8.61	1
560	5874-90-8	*Alanylalanylalanine*	Z	6	8.69	9.26	9.35	1
561	5875-24-1	3-Chloropropionamide	0	6	9.26	8.81	8.70	1
562	5919-26-6	2-Nitropyrrole	0	7	10.45	10.55	10.46	1
563	5930-94-9	3-Nitropyrrole	0	7	10.52	10.41	10.44	1
564	6290-49-9	Methyl methoxyacetate	0	7	8.64	8.84	8.76	1
565	6359-38-2	Benzoflavine	0	6.5	10.51	10.29	10.29	1
566	6559-91-7	4’-Demethylepipodophyllotoxin	0	N.A.	9.52	9.37	9.53	44
567	6622-92-0	2,4-Dimethyl-6-hydroxypyrimidine	0	6	10.11	9.47	9.77	34
568	6976-37-0	Bistris	0	N.A.	7.48	7.92	7.46	1
569	7004-12-8	Arginine	-1	11.5	7.70	8.06	7.61	1
570	7093-67-6	Glycylglycylglycylglycylglycine	Z	6	9.28	9.24	9.34	1
571	7119-89-3	Dichloronitromethane	0	7	10.51	10.96	10.46	45
572	7119-92-8	Diethylnitramine	0	N.A.	10.25	9.67	10.05	43
573	7298-84-2	LeuAla	Z	6.1	8.23	9.14	9.17	1
574	7314-30-9	Dimethyl-β-propiothietin	0	N.A.	9.60	9.19	9.25	1

575	7412-78-4	Glycyl-L-glutamate	Z	5.7	8.34	9.36	9.51	1
576	7535-48-0	4',5'-Dihydropsoralen	0	N.A.	10.26	10.20	10.33	1
577	10236-47-2	*Naringin*	0	6.9	10.00	9.99	10.23	20
578	10373-78-1	Camphoroquinone	0	7	10.45	10.56	10.43	1
579	10595-95-6	*Methylethylnitrosamine*	0	7	10.22	9.58	9.84	43
580	13551-87-6	Misonidazole	0	N.A.	10.48	10.72	10.48	1
581	13621-50-6	Dehydromethionine	0	5	9.94	9.87	10.16	1
582	13838-16-9	2-Chloro-1,1,2-trifluoro-1-(difluoromethoxy)ethane	0	7	9.43	9.39	9.74	1
583	14548-46-0	4-Benzoylpyridine	0	9	10.45	10.44	10.48	1
584	14684-48-1	1,3-Dimethyllumichrome	0	N.A.	10.46	10.72	10.43	1
585	17576-53-3	3-Nitroquinoline	0	7	10.60	10.86	10.45	1
586	17639-93-9	Methyl 2-chloropropionate	0	N.A.	10.08	9.56	9.88	1
587	19729-30-7	GlyGlyAla	Z	6.1	8.93	9.22	9.30	1
588	20138-79-8	2,1,3-Benzothiadiazole-4,7-dicarbonitrile	0	N.A.	10.26	11.21	10.41	1
589	20461-60-3	2,4-Diethoxypyrimidine	0	7	9.45	9.47	9.72	1

590	20689-96-7	Ethylbenzyl nitrosamine	0	7	10.26	9.77	10.07	4
591	20830-81-3	Daunomycin	0	7	10.20	11.06	10.35	1
592	20902-45-8	D-Penicillamine disulfide	0	7	9.80	9.62	9.91	1
593	21911-69-3	*P-Tolylamino-acetic acid*	0	3.9	9.30	9.23	9.31	1
594	21967-41-9	*Baicalin*	-1	6.9	10.11	10.24	10.31	20
595	23350-58-5	Crotonamide	0	9.2	10.11	9.51	9.81	1
596	23576-42-3	*L-Phenylalanylglycylglycine*	Z	6.6	9.04	9.53	9.76	1
597	24686-78-0	1,2,3,5-Tetramethylisoindole-4,7-dione	0	7	10.38	9.60	9.90	1
598	25005-95-2	2,3-Bis(2-pyridyl)-5,6-dihydropyrazine	0	N.A.	10.38	10.43	10.43	1
599	25005-96-3	2,3-Bis(2-pyridiyl)pyrazine	0	N.A.	10.38	10.13	10.37	1
600	25812-30-0	Gemfibrozil	-1	7	8.80	9.13	9.15	37
601	26305-13-5	5,6-Dimethyluracil	0	12	9.23	9.61	9.90	34
602	26621-44-3	3-Nitropyrazole	0	7	10.54	10.56	10.52	1
603	26638-03-9	Methoxyphenol	0	6.9	9.23	9.05	9.01	1
604	26787-78-0	Amoxicillin	Z	7	9.54	9.52	9.75	46

605	27032-78-6	*2,4-Dioxohexahydro-1,3,5-triazine*	0	6	8.03	8.83	8.73	19
606	27318-90-7	*1,10-Phenanthroline-5,6-dione*	0	N.A.	10.51	11.22	10.40	1
607	27816-36-0	2-Chloropropionamide	0	6	9.76	8.97	8.95	1
608	29816-01-1	Glycylsarcosine	Z	6.4	8.84	9.06	9.03	1
609	33094-66-5	*2-Nitrobenzofuran*	0	7	10.30	10.88	10.44	1
610	33419-42-0	Etoposide	0	7	9.43	9.39	9.56	44
611	33577-16-1	*Methyl methylsulfinylmethyl sulfide*	0	N.A.	8.11	8.73	8.49	1
612	34671-83-5	2,2'-Bipyrimidine	0	7	10.32	10.26	10.42	1
613	34841-39-9	*Bupropion*	0	N.A.	10.44	10.31	10.37	47
614	37350-58-6	*Metoprolol*	0	N.A.	8.24	9.20	9.27	48
615	40024-32-6	5-Hydroxy-2-nitrobenzofuran	0	7	10.30	10.90	10.40	1
616	40497-30-1	4,6-Dihydroxy-2-methylpyrimidine	0	4.5	9.73	9.35	9.58	34
617	40739-73-9	7-Hydroxy-2-nitrobenzofuran	0	7	10.30	10.91	10.40	1
618	42538-53-4	Glycylglycyl-β-alanine	Z	5.5	9.15	9.29	9.40	1
619	42978-66-5	Tri(propylene glycol) diacrylate	0	N.A.	9.46	9.90	10.23	49
620	51209-75-7	S-Nitroso-L-cysteine	Z	7	10.38	10.71	10.44	50

621	54261-98-2	Stachyose	0	7	7.94	8.24	7.77	1
622	55520-40-6	Tyrosine	Z	6.6	8.45	9.33	9.48	1
623	55627-73-1	8-Bromoinosine	0	7	10.23	9.27	10.10	51
624	61276-17-3	Verbascoside	0	N.A.	9.79	10.30	10.35	1
625	61696-29-5	5-Deazalumiflavin	0	7	10.53	10.65	10.41	1
626	63762-74-3	*6-Chloromelatonin*	0	N.A.	9.65	9.52	9.69	52
627	65222-35-7	Pazelliptine	0	7	10.20	10.12	10.24	1
628	66108-95-0	Iohexol	0	N.A.	10.53	10.46	10.45	21
629	70402-14-1	6-Aminophenalenone	0	11	10.38	10.68	10.34	1
630	71628-96-1	*7-O-Methylnogarol*	0	N.A.	10.54	10.77	10.38	1
631	72558-82-8	Ceftazidime	0	N.A.	10.00	10.64	10.39	1
632	73334-07-3	Iopromide	0	N.A.	10.51	10.50	10.46	21
633	79637-11-9	Styrene	0	12.7	10.04	9.74	10.03	23
634	79731-35-4	Glycylaspartate	-1	5.8	8.58	8.87	8.71	1
635	85721-33-1	Ciprofloxacin	0	N.A.	10.42	10.04	10.19	53
636	88191-48-4	Catechin	0	6.9	8.08	9.23	9.31	20
637	88283-41-4	α-(3-Pyridyl 1-oxide)-N-tert-	0	N.A.	10.40	10.01	10.22	1

		butylnitrone						
638	90332-86-8	Guanidine	0	11.9	8.20	8.04	7.53	1
639	93413-69-5	Venlafaxine	0	N.A.	8.66	9.22	9.29	1
640	93839-87-3	*Adenylyl-(2'5')uridine phosphate*	0	9.2	9.30	9.79	10.07	1
641	113617-63-3	Orbifloxacin	0	NA	10.40	10.10	10.22	54
642	116333-41-6	5'-(1,4-Dihydro-1-methyl-3-pyridinylcarbonyl)-3'-azido-2',2'-dideoxythymidine	0	N.A.	10.00	9.93	10.13	1
643	116539-59-4	Duloxetine	0	N.A.	10.33	9.89	10.15	52
644	135531-25-8	*Bromochloronitromethane*	0	7	10.47	10.99	10.47	28
645	152971-80-7	*S-Nitroso-N-acetyl-D,L-penicillamine*	-1	7	10.54	10.63	10.37	51

Note: 1) Compounds names in italics are present in the validation set. 2) N.A.: not available. 3) Z: zwitterion

Table A2. Information for outliers in the SVM-based model.

No.	CAS	Name	δ (SVM)
200	100-46-9	Benzenemethanamine	-3.24
333	366-29-0	N,N,N',N'-Tetramethylbenzidine	-3.43
384	542-59-6	2-Hydroxyethyl acetate	-3.37
544	3615-55-2	Ribose-5-phosphate	-3.16
545	3617-44-5	Phenylalanine	-3.31
575	7412-78-4	L-glutamate	-3.09
636	88191-48-4	Catechin	-3.26

Table A3. Compounds with $h > h^*$ and $|\delta| < 3$ in the MLR- and SVM-based models

No.	CAS	Name	δ (MLR)	δ (SVM)	h
21	56-23-5	Carbon tetrachloride	-1.94	-0.33	0.074
59	67-66-3	Trichloromethane	0.37	0.33	0.040
77	74-96-4	Ethyl bromide	0.74	0.09	0.054
87	75-25-2	Bromoform	-0.85	-0.34	0.058
91	75-45-6	Chlorodifluoromethane	0.21	-0.33	0.042
93	75-63-8	Bromotrifluoromethane	0.21	0.34	0.076
95	75-69-4	Trichlorofluoromethane	-1.03	-0.07	0.073
96	75-71-8	Dichlorodifluoromethane	-0.49	0.07	0.072
97	75-72-9	Chlorotrifluoromethane	-0.21	0.10	0.074
99	76-13-1	1,1,2-Trichlorotrifluoroethane	-0.53	-0.13	0.063
104	78-76-2	2-Bromobutane	0.28	-0.16	0.083

117	79-27-6	1,1,2,2-Tetrabromoethane	0.10	-0.06	0.033
220	106-41-2	4-Bromophenolate	-0.53	-0.16	0.081
227	106-94-5	1-Bromopropane	1.07	0.49	0.048
258	109-65-9	1-Bromobutane	1.03	0.44	0.047
267	110-53-2	1-Bromopentane	0.95	0.35	0.047
295	127-18-4	Tetrachloroethylene	0.30	0.16	0.051
350	464-10-8	Tribromonitromethane	-0.12	0.04	0.119
367	507-19-7	2-Bromo-2-methylpropane	-0.21	-0.35	0.112
379	540-51-2	2-Bromoethanol	-0.57	-1.37	0.030
405	591-20-8	3-Bromophenolate	-0.48	-0.20	0.072
484	918-01-4	Bromodichloronitromethane	0.21	0.26	0.126
507	1184-89-0	Dibromochloronitromethane	0.10	0.34	0.113
525	2314-97-8	Trifluoroiodomethane	-1.66	-0.42	0.075
539	3034-48-8	2-Bromo-5-nitrothiazole	-0.20	-0.34	0.078
623	55627-73-1	8-Bromoinosine	2.13	0.34	0.059

Table A4. List of experimental and predicted logk_{eaq-} by the current MLR model and previous phenyl-based compounds MLR model for some new classes of compounds, as well as deviation (logk_{pre}/ logk_{exp}) between the predicted logk_{eaq-} and experiamental ones.

Name	CAS	logk_{eaq-}			Deviation	
		Experimental	Current model	*Previous phenyl-based compounds model	Current model	*Previous phenyl-based compounds model
Benzo[a]pyrene	50-32-8	9.78	10.42	10.29	1.07	1.05
Cephaloridine	50-59-9	10.45	10.67	11.36	1.02	1.09
6-Azauridine	54-25-1	9.88	10.26	10.13	1.04	1.03
Pyridoxal phosphate	54-47-7	10.20	10.51	11.24	1.03	1.10
Ethynyl estradiol	57-63-6	8.16	9.17	8.82	1.12	1.08
Sulfaguanidine	57-67-0	9.93	9.56	9.66	0.96	0.97
Caffeine	58-08-2	10.08	9.65	9.39	0.96	0.93
Theophylline	58-55-9	9.00	9.45	9.41	1.05	1.05
Adenosine	58-61-7	10.08	9.55	9.35	0.95	0.93
Inosine	58-63-9	9.99	9.68	9.78	0.97	0.98
6-Hydroxypurine	68-94-0	9.98	9.60	9.63	0.96	0.96

2,6-Dihydroxypurine	69-89-6	9.59	9.72	9.72	1.01	1.01
Uric acid	69-93-2	9.78	9.58	9.60	0.98	0.98
5-Azauracil	71-33-0	9.45	9.85	9.90	1.04	1.05
Adenine	73-24-5	9.04	9.59	9.62	1.06	1.06
Guanine	73-40-5	10.15	9.56	9.37	0.94	0.92
Camphor	76-22-2	9.49	9.30	8.63	0.98	0.91
Theobromine	83-67-0	9.34	9.68	9.48	1.04	1.01
Guanosine monophosphate	85-32-5	9.49	9.37	9.63	0.99	1.01
2-(Chloromercuri)phenol	90-03-9	10.04	9.94	9.73	0.99	0.97
Benzotriazole	95-14-7	9.23	10.05	9.64	1.09	1.04
N-Nitrosopiperidine	100-75-4	10.24	9.66	9.03	0.94	0.88
Cyanuricacid	108-80-5	9.15	9.14	9.14	1.00	1.00
Guanosine	118-00-3	9.78	9.36	9.51	0.96	0.97
Purine	120-73-0	10.32	9.90	9.80	0.96	0.95
Quinine	130-95-0	10.23	10.11	9.85	0.99	0.96

Sulfamethizole	144-82-1	10.30	8.98	10.03	0.87	0.97
Phthalazine	253-52-1	10.54	10.18	10.00	0.97	0.95
Pyridazine	289-80-5	10.34	9.99	9.60	0.97	0.93
1,3,5-Triazine	290-87-9	9.72	9.95	9.60	1.02	0.99
6-Azauracil	461-89-2	9.66	10.22	10.07	1.06	1.04
Ascaridole	512-85-6	9.60	9.10	8.48	0.95	0.88
Nifuroxime	555-15-7	10.58	10.93	10.90	1.03	1.03
7-Methylguanine	578-76-7	10.20	9.55	9.26	0.94	0.91
2-Nitrothiophene	609-40-5	10.48	10.77	10.74	1.03	1.02
Benzoic hydrazide	613-94-5	10.19	9.63	9.32	0.95	0.91
3-Nitrothiophene	822-84-4	10.52	10.62	10.56	1.01	1.00
2,4,6-Trimethoxy-1,3,5-triazine	877-89-4	9.57	9.28	9.06	0.97	0.95
4-Nitroisothiazole	931-07-7	10.52	10.69	10.76	1.02	1.02
5-Azacytosine	931-86-2	10.08	9.54	9.40	0.95	0.93
6-Azathymine	932-53-6	9.98	10.12	9.80	1.01	0.98
Benzaldoxime	932-90-1	10.00	9.92	9.37	0.99	0.94

7-Methyladenine	935-69-3	10.11	9.59	9.52	0.95	0.94
Glutarimide	1121-89-7	9.85	9.56	9.02	0.97	0.92
2-Methyladenine	1445-08-5	9.92	9.55	9.46	0.96	0.95
Atrazine	1912-24-9	9.68	9.54	9.27	0.99	0.96
Di(4-chlorophenyl) sulfoxide	3085-42-5	10.00	9.98	9.92	1.00	0.99
9-Methylguanine	5502-78-3	9.88	9.49	9.28	0.96	0.94
Alanine anhydride	5625-46-7	9.30	8.78	8.32	0.94	0.89
3-Nitropyrazole	26621-44-3	10.54	10.56	10.59	1.00	1.00
2,4-Dioxohexahydro-1,3,5-triazine	27032-78-6	8.03	8.83	8.73	1.10	1.09
α-(3-Pyridyl 1-oxide)-N-tert-butylnitrone	88283-41-4	10.40	10.01	9.87	0.96	0.95
Duloxetine	116539-59-4	10.33	9.89	9.63	0.96	0.93

[*] This model is from the research of Li et al. (*Water Res.*, 2019, 151, 468-477).

Table A5. List of experimental and predicted logk_{eaq-} by the current MLR model and previous aliphatic compounds MLR model for some new classes of compounds, as well as deviation (logk_{pre}/ logk_{exp}) between the predicted logk_{eaq-} and experiamental ones.

Name	CAS	logk_{eaq-}			Deviation	
		Experimental	Current model	*Previous aliphatic compounds model	Current model	*Previous aliphatic compounds model
Cystamine	51-85-4	10.26	9.47	10.40	0.92	1.01
Busulfan	55-98-1	7.48	7.90	9.66	1.06	1.29
Tetraethylthiuram disulfide	97-77-8	10.04	10.23	13.04	1.02	1.30
Cyclohexyl methacrylate	101-43-9	9.30	9.71	9.93	1.04	1.07
1,3-Diethyl-2-thiourea	105-55-5	8.70	9.03	9.31	1.04	1.07
Acetaldoxime	107-29-9	7.86	8.93	8.50	1.14	1.08
Bis(1,1-dimethylethyl) peroxide	110-05-4	8.15	8.50	9.61	1.04	1.18
Diacetyl peroxide	110-22-5	9.98	9.13	10.48	0.91	1.05
Trioxane	110-88-3	6.00	7.20	6.88	1.20	1.15
Cyclopentanone	120-92-3	9.87	9.36	9.18	0.95	0.93
Acetone oxime	127-06-0	8.54	8.82	8.55	1.03	1.00

Cycloheptatriene	544-25-2	9.78	9.72	9.71	0.99	0.99
1,3-Cyclohexadiene	592-57-4	9.00	9.52	9.29	1.06	1.03
Methylphenyl nitrosamine	614-00-6	10.36	9.93	10.40	0.96	1.00
Dibenzyl sulfoxide	621-08-9	9.54	9.48	11.25	0.99	1.18
N-Nitrosodipropylamine	621-64-7	10.18	9.67	9.85	0.95	0.97
Diethyl methylphosphonate	683-08-9	7.53	7.68	8.49	1.02	1.13
2-Methyl-2-nitrosopropane	917-95-3	9.79	10.53	10.11	1.08	1.03
N-nitrosodibutylamine	924-16-3	10.19	9.66	10.17	0.95	1.00
N-Nitrosohexamethyleneimine	932-83-2	10.19	9.68	9.85	0.95	0.97
Endosulfan sulfate	1031-07-8	10.53	10.15	12.14	0.96	1.15
2,3-Diazabicyclo[2.2.1]hept-2-ene	2721-32-6	10.36	9.78	9.74	0.94	0.94
Ribose-5-phosphate	3615-55-2	8.90	9.74	10.59	1.09	1.19
Dimethylnitramine	4164-28-7	10.28	9.65	9.69	0.94	0.94
N-Nitrosoethylbutylamine	4549-44-4	10.19	9.66	9.85	0.95	0.97
Arginine	7004-12-8	7.70	8.06	8.60	1.05	1.12

Diethylnitramine	7119-92-8	10.25	9.67	9.72	0.94	0.95
Methylethylnitrosamine	10595-95-6	10.22	9.58	9.40	0.94	0.92
D-Penicillamine disulfide	20902-45-8	9.80	9.62	11.74	0.98	1.20
Methyl methylthiomethyl sulfoxide	33577-16-1	8.11	8.73	9.21	1.08	1.13
Guanidine	90332-86-8	8.20	8.04	8.16	0.98	0.99

* This model is from the research of Li et al. (*Water Res.*, 2019, 151, 468-477).

Table A6. Comparison of prediction accuracy of different models for some new compounds classes in Table A4 and A5.

Statistics	Phenyl-containing compounds and heterocycles		Aliphatic compounds	
	Current model	*Previous phenyl-based compounds model	Current model	*Previous aliphatic compounds model
MSE	0.210	0.334	0.319	0.676
RMSE	0.458	0.578	0.565	1.075
MAE	0.385	0.495	0.497	0.806

* This model is from the research of Li et al. (*Water Res.*, 2019, 151, 468-477).

Table A7. Classification of organic compounds based on different functional groups.

Group	Compounds
$-COO^-$	2-Hydroxypropionate (50-21-5), 4-Methyl-salicylate (50-85-1), Hydroxyprolin (51-35-4), Pyridoxal phosphate (54-47-7), Folate (59-30-3), Methicillin (61-32-5), Penicillin G (61-33-6), Cloxacillin (61-72-3), Cytidylate (63-37-6), Ampicillin (69-53-4), 4-Chlorobenzoate (74-11-3), 3-Methyl-salicylate (83-40-9), Penicillin V (87-08-1), 2-Iodobenzoate (88-67-5), 2-Nitrophenolate (88-75-5), 5-Methyl-salicylate (89-56-5), 2-Chlorophenolate (95-57-8), Benzenesulfonate (98-11-3), 3-Methylbenzoate (99-04-7), 3-Hydroxybenzoate (99-06-9), 4-methylbenzoate (99-94-5), 4-Hydroxybenzoate (99-96-7), 4-Nitrophenolate (100-02-7), Terephthalate (100-21-0), 4-methylbenzenesulfonate (104-15-4), 4-Bromophenolate (106-41-2), 4-Chlorophenolate (106-48-9),

	Sarcosine (107-97-1), 3-Chlorophenolate (108-43-0), Diatrizoate (117-96-4), o-Toluate (118-90-1), 2-Chlorobenzoate (118-91-2), Orotidine (314-50-1), caffeate (331-39-5), 2-Fluorophenolate (367-12-4), 4-Fluorophenolate (371-41-5), 3-Fluorophenolate (372-20-3), 2-Fluorobenzoate (445-29-4), 3-Fluorobenzoate (455-38-9), 4-Fluorobenzoate (456-22-4), 3-Hydroxykynurenine (484-78-6), Hydrocinnamate (501-52-0), p-Coumarate (501-98-4), 3-Chlorobenzoate (535-80-8), 6-Aminopenicillanate (551-16-6), 3-Nitrophenolate (554-84-7), 6-Methyl-salicylate (567-61-3), 4-Bromobenzoate (586-76-5), 3-Bromophenol (591-20-8), Pentafluorobenzoate (602-94-8), 2-Cyanophenolate (611-20-1), 3-Iodobenzoate (618-51-9), 4-Iodobenzoate (619-58-9), 4-Cyanobenzoate (619-65-8), 3-Nitrotyrosine (621-44-3), Glycylglycylglycylglycine (637-84-3), GlyTyrOH (658-79-7),Glycylserine (687-38-7), Glycylproline (704-15-4), 4-Hydroxybenzonitrile (767-00-0), Pentafluorothiophenolate (771-62-0), Glycylleucine (869-19-2), 3-Hydroxybenzonitrile (873-62-1), Clofibrate (882-09-7), Alanylalanylalanylalanine (26-79-4), N-Formylkynurenine (1022-31-7), DL-Alanyl-Glycine (1188-01-8), Selenomethionine (1464-42-2), Glycylvaline (1963-21-9), Methyl thioglycolate (2365-48-2), ProGly (2578-57-6), Alanylalanine (2867-20-1), Glycylphenylalanine (3321-03-7), Phenylalanine (3617-44-5), Glycyl-β-alanine (3695-73-6), GlyLeuTyr (4306-24-5), Carbenicillin (4697-36-3), Alanylalanylalanine (5874-90-8), Arginine (7004-12-8), Glycylglycylglycylglycylglycine (7093-67-6), LeuAla (7298-84-2), Glycyl-L-glutamate (7412-78-4), GlyGlyAla (19729-30-7), Baicalin (21967-41-9), Gemfibrozil (25812-30-0), Amoxicillin (26787-78-0), Glycylglycyl-β-alanine (42538-53-4), S-Nitroso-L-cysteine (51209-75-7), Tyrosine (55520-40-6), Glycylaspartate (79731-35-4), S-Nitroso-N-acetyl-D,L-penicillamine (152971-80-7)
–OH	2-Hydroxypropionate (50-21-5), 2-Hydroxypropionic acid (50-21-5), Hydroxyproline (51-35-4), Adrenaline (51-43-4), Atropine (51-55-8), 6-Azauridine (54-25-1), Chloramphenicol (56-75-7), DL-glyceraldehyde (56-82-

	6), Ethynyl estradiol (57-63-6), Adenosine (58-61-7), Inosine (58-63-9), Uridine (58-96-8), Tetracycline (60-54-8), Cytidylate (63-37-6), Pyridoxine (65-23-6), Cytidine (65-46-3), Benzoic acid (65-85-0), Pyridoxal (66-72-8), D-Mannitol (69-65-8), Chloroacetic acid (79-11-8), Hydroxyacetic acid (79-14-1), 2-Methylpropenoic acid (79-41-4), 2-Mercaptopropionic acid (79-42-5), Cumene hydroperoxide (80-15-9), Riboflavine (83-88-5), Guanosine monophosphate (85-32-5), 3-Chloro-1,2-propanediol (96-24-2), Methyl hydroxyacetate (96-35-5), Benzenemethanol (100-51-6), N-Phenylhydroxylamine (100-65-2), 2-Chloroethanol (107-07-3), Acetaldoxime (107-29-9), 3-Mercaptopropionic acid (107-96-0), Butanedioic acid (110-15-6), Maleic acid (110-16-7), Sorbic acid (110-44-1), Sulfasuccidine (116-43-8), Quercetin (117-39-5), Guanosine (118-00-3), 2-Hydroxy-2-phenylacetophenone (119-53-9), Acetone oxime (127-06-0), Hydroxyurea (127-07-1), Quinine (130-95-0), 4-(2-Acetylsulfamyl)phthalanilic acid (131-69-1), trans-Cinnamic acid (140-10-3), 2-Aminoethanol (141-43-5), Malonic acid (141-82-2), Oxalic acid (144-62-7), Flavine mononucleotide (146-17-8), Rutin (153-18-4), Orotidine(314-50-1), Metronidazole (443-48-1), Arabinitol (488-82-4), (Z)-2-Butenoic acid (503-64-0), 3-Hydroxy-2-butanone (513-86-0), Genistin (529-59-9), Deoxyribose (533-67-5), 2-Bromoethanol (540-51-2), 3,3-Dimethylacrylic acid (541-47-9), 2-Hydroxyethyl acetate (542-59-6), Nifuroxime (555-15-7), Glycylglycine (556-50-3), 3-Buten-2-ol (598-32-3), 2-Hydroxyacetamide (598-42-5), Gossypin (652-78-8), Glycylserine (687-38-7), 2-Hydroxyethyl acrylate (818-61-1), 2-Hydroxyethyl methacrylate (868-77-9), 2'-Deoxyguanosine 5'-monophosphate (902-04-5), Alanylalanylalanylalanine (926-79-4), Benzaldoxime (932-90-1), 4-Nitroperoxybenzoic acid (943-39-5), 4-Chromanol (1481-93-2), 2-Hydroxypropionamide (2043-43-8), 1-Methylguanosine (2140-65-0), α-Nitrophenyl--D-glucopyranoside (2816-24-2), L-Phenylglycine (2935-35-5), Ribose-5-phosphate (3615-55-2), 4'-Demethylepipodophyllotoxin (006559-91-7), Bistris (6976-37-0), Glycyl-L-glutamate (7412-78-4), Naringin (10236-47-2), Misonidazole (13551-87-6), Daunomycin (20830-81-3), P-Tolylamino-acetic acid (21911-69-3), Baicalin (21967-41-9), Etoposide (33419-42-0), Metoprolol

	(37350-58-6), S-Nitroso-L-cysteine (51209-75-7), Stachyose (54261-98-2), 8-Bromoinosine(55627-73-1), Verbascoside (61276-17-3), Iohexol (66108-95-0), 7-O-Methylnogarol (71628-96-1), Ceftazidime (72558-82-8), Iopromide (73334-07-3), Glycylaspartate (79731-35-4), Ciprofloxacin (85721-33-1), Catechin (88191-48-4), Venlafaxine (93413-69-5), Adenylyl-(2'5')uridine phosphate (93839-87-3), Orbifloxacin (113617-63-3), 5'-(1,4-Dihydro-1-methyl-3-pyridinylcarbonyl)-3'-azido-2',2'-dideoxythymidine (116333-41-6)
–NH_2/–NH–	Hydroxyprolinen (51-35-4), Adrenalinen (51-43-4), 2,2'-dithiobis(ethylamine) (51-85-4), Chloroquine (54-05-7), Sulfaguanidine (57-67-0), Sulfamethazine (57-68-1), Adenosine (58-61-7), Folate (59-30-3), 2-Aminoethanethiol (60-23-1), Cytidylate (63-37-6), 4-Aminobenzenesulfonamide (63-74-1), Ampicillin (69-53-4), Cytosine (71-30-7), Sulfathiazole (72-14-0), Adenine (73-24-5), Guanine (73-40-5), Isopropylamine (75-31-0), Isobutylamine (78-81-9), 4,4'-Diamino diphenyl sulfone (80-08-0), Guanosine monophosphate (85-32-5), Amodiaquine (86-42-0), Primaquine (90-34-6), Benzhydrylamine (91-00-9), 2-Naphthylamine (91-59-8), Phenothiazine (92-84-2), Benzidine (92-87-5), 2-Chloroaniline (95-51-2), N,N-Dimethyl-p-phenylenediamine (99-98-9), Benzenemethanamine (100-46-9), 4-Chloroaniline (106-47-8), Sarcosine (107-97-1), 3-Chloroaniline (108-42-9), Cyclohexylamine (108-91-8), 2-Aminopyrimidine (109-12-6), Guanosine (118-00-3), Diphenylamine (122-39-4), Pyrrolidine (123-75-1), Sulfamerazine (127-79-7), 2-Aminoethanol (141-43-5), Sulfamethizole (144-82-1), Kynurenine (343-65-7), Naringenin (480-41-1 3-Hydroxykynurenine (484-78-6), Chrysoidin(495-54-5), 6-Aminopenicillanate (551-16-6), 3,6-Diaminoacridine (553-30-0), 5-Methylcytosine (554-01-8), Glycylglycine (556-50-3), 7-Methylguanine (578-76-7), 4-Aminopyrimidine (591-54-8), 2-Aminoacetamide (598-41-4), 2, 6-Dichloraniline (608-31-1), Methyl 2-aminoacetate (616-34-2), Selenourea (630-10-4), Sulfamethoxazole (723-46-6), 2,3,4,5,6-Pentafluoroaniline (771-60-8), 2'-Deoxyguanosine 5'-monophosphate (902-04-5), Alanylalanylalanylalanine (926-79-4), 6-Azacytosine (931-85-1), 5-Azacytosine (931-86-2), 7-Methyladenine (935-69-

	3), 1-Methylcytosine (1122-47-0), 2-Methyladenine (1445-08-5), Atrazine (1912-24-9), 1-Methylguanosine (2140-65-0), Pterin (2236-60-4), ProGly (2578-57-6), L-Phenylglycine (2935-35-5), Glycine anhydride (4202-74-8), Nitracrine (4533-39-5), 9-Methylguanine (5502-78-3), Benzoflavine (6359-38-2), Arginine (7004-12-8), Daunomycin (20830-81-3), P-Tolylamino-acetic acid (21911-69-3), Bupropion (34841-39-9), Metoprolol (37350-58-6), S-Nitroso-L-cysteine (51209-75-7), Pazelliptine (65222-35-7), 6-Aminophenalenone (70402-14-1), Ceftazidime (72558-82-8), Glycylaspartate (79731-35-4), Ciprofloxacin (85721-33-1), Guanidine (90332-86-8), Adenylyl-(2'5')uridine phosphate (93839-87-3), Orbifloxacin (113617-63-3), Duloxetine (116539-59-4)
–COOH	2-Hydroxypropionic acid (50-21-5), Benzoic acid (65-85-0), Chloroacetic acid (79-11-8), Hydroxyacetic acid (79-14-1), 2-Methylpropenoic acid (79-41-4), 2-Mercaptopropionic acid (79-42-5), 3-Mercaptopropionic acid (107-96-0), Sorbic acid (110-44-1), Sulfasuccidine (116-43-8), 4-(2-Acetylsulfamyl)phthalanilic acid (131-69-1), trans-Cinnamic acid (140-10-3), (Z)-2-Butenoic acid (503-64-0), 3,3-Dimethylacrylic acid (541-47-9), Glycylglycine (556-50-3), P-Tolylamino-acetic acid (21911-69-3), Ceftazidime (72558-82-8), Glycylaspartate (79731-35-4), Butanedioic acid (110-15-6), Maleic acid (110-16-7), Malonic acid (141-82-2), Oxalic acid (144-62-7), L-Phenylglycine (2935-35-5), S-Nitroso-L-cysteine (51209-75-7), Ciprofloxacin (85721-33-1), Orbifloxacin (113617-63-3)
–X	Cyclophosphamide (50-18-0), Chlorpromazine (50-53-3), 5-Bromouracil (51-20-7), 5-Fluorouracil (51-21-8), Chloroquine (54-05-7), Carbon tetrachloride (56-23-5), Chloramphenicol (56-75-7), Cloxacillin (61-72-3), Trichloromethane (67-66-3), 1,1,1-Trichloroethane (71-55-6), 4-Chlorobenzoate (74-11-3), Methyl chloride (74-87-3), Methyl iodide (74-88-4), Methylene bromide (74-95-3), Ethyl bromide (74-96-4), Chloroethane (75-00-3), Vinyl chloride (75-01-4), Iodoethane (75-03-6), Methylene iodide (75-11-6), Bromoform (75-25-2), 1,1-Dichloroethane (75-34-3), Vinylidene chloride (75-35-4), Chlorodifluoromethane (75-45-6), Bromotrifluoromethane (75-63-8),

	Trichlorofluoromethane (75-69-4), Dichlorodifluoromethane (75-71-8), Chlorotrifluoromethane (75-72-9), Trichloronitromethane (76-06-2), 1,1,2-Trichlorotrifluoroethane (76-13-1), 2,2-Dichloro-1,1-difluoro-1-methoxyethane (76-38-0), 2-Bromobutane (78-76-2), Chloroacetone (78-95-5), 1,1,2-Trichloroethane (79-00-5), Trichloroethylene (79-01-6), Chloroacetic acid (79-11-8), 1,1,2,2-Tetrabromoethane (79-27-6), 2-Chloro-6-nitrotoluene (83-42-1), 1,4-Dibromonaphthalene (83-53-4) Amodiaquine (86-42-0), 2-Iodobenzoate (88-67-5), 1-Chloro-2-nitrobenzene (88-73-3), 4-Chloro-2-nitrotoluene (89-59-8), 2-Chlorobenzaldehyde (89-98-5), 2-(Chloromercuri)phenol (90-03-9), 1-Bromonaphthalene (90-11-9), 1-Chloronaphthalene (90-13-1), Chlorodiphenylmethane (90-99-3), 2-Chlorotoluene (95-49-8), 1,2-Dichlorobenzene (95-50-1), 2-Chloroaniline (95-51-2), 2-Bromophenol (95-56-7), 2-Chlorophenol (95-57-8), 2-Chlorophenolate (95-57-8), 3,4-Dichlorotoluene (95-75-0), 3-Chloro-1,2-propanediol (96-24-2), Benzotrichloride (98-07-7), Benzotrifluoride (98-08-8), 1-Chloro-4-nitrobenzene (100-00-5), Benzyl chloride (100-44-7), 4-Chlorobenzaldehyde (104-88-1), 1-Bromo-4-chlorobenzene (106-39-8), 4-Bromophenol (106-41-2), 4-Bromophenolate (106-41-2), 4-Chlorotoluene (106-43-4), 1,4-Dichlorobenzene (106-46-7), 4-Chloroaniline (106-47-8), 4-Chlorophenol (106-48-9), 4-Chlorophenolate (106-48-9), 1-Bromopropane (106-94-5), 1-Bromo-2-chloroethane (107-04-0), 1,2-Dichloroethane (107-06-2), 2-Chloroethanol (107-07-3), 1-Iodopropane (107-08-4), 1,3-Dibromobenzene (108-36-1), 1-Bromo-3-chlorobenzene (108-37-2), 1-Chloro-3-methylbenzene (108-41-8), 3-Chloroaniline (108-42-9), 3-Chlorophenol (108-43-0), 3-Chlorophenolate (108-43-0), Bromobenzene (108-86-1), Chlorobenzene (108-90-7), 1-Bromobutane(109-65-9), 1-Chlorobutane (109-69-3), 1-Bromopentane(110-53-2), Bromphenol Blue (115-39-9), Diatrizoate (117-96-4), 2-Chlorobenzoate (118-91-2), 2,4-Dichlorophenol (120-83-2), 1-Chloro-3-nitrobenzene (121-73-3), Tetrachloroethylene (127-18-4), Iodoacetamide (144-48-9), Pentafluorobenzene (363-72-4), 1,2-Difluorobenzene (367-11-3), 2-Fluorophenolate (367-12-4), 4-Fluorophenolate (371-41-5), 3-Fluorophenolate

	(372-20-3), Hexafluorobenzene (392-56-3), Fluoroacetone (430-51-3), Methyl trifluoroacetate (431-47-0), Diazepam (439-14-5), 2-Fluorobenzoate (445-29-4), 3-Fluorobenzoate (455-38-9), 4-Fluorobenzoate (456-22-4), Tribromonitromethane (464-10-8), 2-Bromo-2-methylpropane (507-19-7), 1-Chloro-2-methylpropane (513-36-0), 1,1-Dichloroacetone (513-88-2), 3-Chlorobenzoate (535-80-8), 1,4-Difluorobenzene (540-36-3), 2-Bromoethanol (540-51-2), 1-Chloropropane (540-54-5), 1,3-Dichlorobenzene (541-73-1), Butyl iodide (542-69-8), Trichloroacetonitrile (545-06-2), 1,2,3,4-Tetrafluorobenzene (551-62-2), Bromonitromethane (563-70-2), 4-Bromobenzoate (586-76-5), 3-Chlorobenzaldehyde (587-04-2), 3-Bromophenolate (591-20-8), 3-Bromophenol (591-20-8), Iodobenzene (591-50-4), Pentafluorobenzoate (602-94-8), 2, 6-Dichloraniline (608-31-1), 2-Chlorobenzyl chloride (611-19-8), 3-Iodobenzoate (618-51-9), 4-Iodobenzoate (619-58-9), Phenethyl chloride (622-24-2), 2',3',4',5',6'-Pentafluoroacetophenone (652-29-9), 2,3,4,5,6-Pentafluorostyrene (653-34-9), Pentafluorobenzaldehyde (653-37-2), 1-Bromo-2-chlorobenzene (694-80-4), 2-Bromo-4-chlorophenol (695-96-5), 5-Iodouracil (696-07-1), 2,3,4,5,6-Pentafluoroaniline (771-60-8), Pentafluorophenol (771-61-9), Pentafluorothiophenolate (771-62-0), pentafluorobenzonitrile (773-82-0), Iodopentafluorobenzene (827-15-6), Pentafluorophenylhydrazine (828-73-9), Pentafluoronitrobenzene (880-78-4), Clofibrate (882-09-7), 1,1,1-Trichloroacetone (918-00-3), Bromodichloronitromethane (918-01-4), Endosulfan sulphate (1031-07-8), Dibromochloronitromethane (1184-89-0), 4-Fluorobenzonitrile (1194-02-1), Clonazepam (1622-61-3), Chloronitromethane (1794-84-9), 5-Chlorouracil (1820-81-1), Atrazine (1912-24-9), Trifluoroiodomethane (2314-97-8), 3-Chloroanisole (2845-89-8), 2-Bromo-5-nitrothiazole (3034-48-8), Di (4-chlorophenyl) sulfoxide (3085-42-5), 4-Bromo-2-chlorophenol (3964-56-5), 3-Chloropropionamide (5875-24-1), Dichloronitromethane (7119-89-3), 2-Chloro-1,1,2-trifluoro-1-(difluoromethoxy)ethane (13838-16-9), Methyl 2-chloropropionate (17639-93-9), 2-Chloropropionamide (27816-36-0), Bupropion (34841-39-9), 8-Bromoinosine (55627-73-1), 6-Chloromelatonin

	(63762-74-3), Iohexol (66108-95-0), Iopromide (73334-07-3), Ciprofloxacin (85721-33-1), α-(3-Pyridyl 1-oxide)-N-tert-butylnitrone (88283-41-4), Orbifloxacin (113617-63-3), Bromochloronitromethane (135531-25-8)
–Ph	Chlorpromazine (50-53-3), 4-Methyl-salicylate (50-85-1), Adrenaline (51-43-4), Chloroquine (54-05-7), Pyridoxal phosphate (54-47-7), Benzamide (55-21-0), Chloramphenicol (56-75-7), Ethynyl estradiol (57-63-6), Sulfaguanidine (57-67-0), Sulfamethazine (57-68-1), Menadione (58-27-5), Adenosine (58-61-7), Inosine (58-63-9), Folate (59-30-3), Nitrofurazone (59-87-0), Tetracycline (60-54-8), Methicillin (61-32-5), Cloxacillin (61-72-3), 4-Aminobenzenesulfonamide (63-74-1), Pyridoxine (65-23-6), Benzoic acid (65-85-0), Pyridoxal (66-72-8), Nitrofurantoin (67-20-9), 6-Hydroxypurine (68-94-0), Sulfathiazole(72-14-0), Adenine (73-24-5), Guanine (73-40-5), 4-Chlorobenzoate (74-11-3), 4,4'-Diamino diphenyl sulfone (80-08-0), 3-Methyl-salicylate (83-40-9),2-Chloro-6-nitrotoluene (83-42-1),1,4-Dibromonaphthalene (83-53-4), Riboflavine (83-88-5), Diethyl phthalate (84-66-2), Guanosine monophosphate (85-32-5), Amodiaquine (86-42-0), 1-Naphthonitrile (86-53-3), Penicillin V (87-08-1), 2-Iodobenzoate (88-67-5), 1-Chloro-2-nitrobenzene (88-73-3), 5-Methyl-salicylate (89-56-5), 4-Chloro-2-nitrotoluene (89-59-8), 2-Chlorobenzaldehyde (89-98-5), 2-(Chloromercuri)phenol (90-03-9), 1-Bromonaphthalene (90-11-9), 1-Chloronaphthalene (90-13-1), 1-naphthol (90-15-3), Primaquine(90-34-6), Anthrone (90-44-8), 4,4'-Dimethoxybenzophenone (90-96-0), 2-Benzoylpyridine (91-02-1), 2-Naphthylamine (91-59-8), 5-Nitro-2-furaldehyde diacetate (92-55-7), 3-Hydroxy-N-(2',4'-dimethylphenyl)-2-naphthamide (92-75-1), Phenothiazine (92-84-2), Benzidine (92-87-5), Propylparaben (94-13-3), Chlorotoluene (95-49-8), 1,2-Dichlorobenzene (95-50-1), 2-Chloroaniline (95-51-2), 2-Bromophenol (95-56-7), 2-Chlorophenol (95-57-8), 3,4-Dichlorotoluene (95-75-0), Acetophenone (98-86-2), 3 Pyridinecarboxamide(98-92-0), Nitrobenzene (98-95-3), N,N-Dimethyl-p-phenylenediamine (99-98-9), 4-Nitrotoluene (99-99-0), 1-Chloro-4-nitrobenzene (100-00-5), 4-Nitrophenol (100-02-7), 4-Nitroacetophenone (100-19-6),

	Cyanobenzene (100-47-0), Benzaldehyde (100-52-7), N-Phenylhydroxylamine (100-65-2), Acetaminophen (103-90-2), 4-Chlorobenzaldehyde (104-88-1), 1-Bromo-4-chlorobenzene (106-39-8), 4-Bromophenol (106-41-2), 4-Chlorotoluene (106-43-4), 1,4-Dichlorobenzene (106-46-7), 4-Chloroaniline (106-47-8), 4-Chlorophenol (106-48-9), 1,3-Dibromobenzene (108-36-1), 1-Bromo-3-chlorobenzene (108-37-2), 1-Chloro-3-methylbenzene (108-41-8), 3 Chloroaniline (108-42-9), 3-Chlorophenol (108-43-0), Bromobenzene (108-86-1), Chlorobenzene (108-90-7), 3 Hydroxypyridine (109-00-2), 2-Aminopyrimidine (109-12-6), Bromphenol Blue (115-39-9), Quercetin (117-39-5), Diatrizoae (117-96-4), Guanosine (118-00-3), 2-Chlorobenzoate (118-91-2), 2-Hydroxy-2-phenylacetophenone (119-53-9) Benzophenone (119-61-9), 2,4-Dichlorophenol (120-83-2), 2,4 Dinitrotoluene (121-14-2), 1-Chloro-3-nitrobenzene (121-73-3), Diphenylamine (122-39-4), Sulfamerazine (127-79-7), Quinine (130-95-0), Dimethyl phthalate (131-11-3), 4-(2-Acetylsulfamyl)phthalanilic acid (131-69-1), Benzil (134-81-6), 2-Naphthol (135-19-3), N,N-Dimethyl-4-nitrosoaniline (138-89-6), 2-Pyridone (142-08-5), Sulfamethizole (144-82-1), Flavinemononucleotide (146-17-8), Rutin (153-18-4), 8-Methoxypsoralen (298-81-7), caffeate (331-39-5), Kynurenine (343-65-7), 3-Acetylpyridine (350-03-8), Pentafluorobenzene (363-72-4), N,N,N',N'-Tetramethylbenzidine (366-29-0), 1,2-Difluorobenzene (367-11-3), Hexafluorobenzene (392-56-3), Diazepam(439-14-5), Metronidazole (443-48-1), 2-Fluorobenzoate (445-29-4), Genistein (446-72-0), 3-Fluorobenzoate (455-38-9), 4-Fluorobenzoate (456-22-4), Naringenin (480-41-1), 5-Hydroxy-1,4-naphthoquinone (481-39-0), 5-hydroxy-2-methyl-1,4-naphthoquinone (481-42-5), 3-Hydroxykynurenine (484-78-6), 9-Fluorenone (486-25-9), Baicalein (491-67-8), Chrysoeriol (491-71-4), Acridine Orange(494-38-2), Chrysoidin (495-54-5), p-Coumarate (501-98-4), 2-Nitroimidazole (527-73-1), Genistin (529-59-9), 3-Chlorobenzoate (535-80-8), 1,4-Difluorobenzene (540-36-3), 1,3-Dichlorobenzene (541-73-1), 1,2,3,4-Tetrafluorobenzene (551-62-2), 3,6-Diaminoacridine (553-30-0), Nifuroxime (555-15-7), 6-Methyl-salicylate (567-61-3), 7-Methylguanine (578-76-7), 4-Bromobenzoate (586-76-5), 3-

	Chlorobenzaldehyde (587-04-2), 3-Bromophenolate (591-20-8), Iodobenzene (591-50-4), 4-Aminopyrimidine (591-54-8), Pentafluorobenzoate(602-94-8), 5-Nitroquinoline (607-34-1), 8-Nitroquinoline (607-35-2), 2, 6-Dichloraniline (608-31-1), 2-Nitrothiophene (609-40-5), 2-Chlorobenzyl chloride(611-19-8), 2-Naphthonitrile (613-46-7), 6-Nitroquinoline (613-50-3), 7-Nitro-quinoline (613-51-4), Methylphenyl nitrosamine (614-00-6), 3-Iodobenzoate (618-51-9), 4-Iodobenzoate (619-58-9), 4-Cyanobenzoate (619-65-8), 3-Nitrotyrosine (621-44-3), 1,4-Dicyanobenzene (623-26-7), 4-Pyridinol (626-64-2), 2',3',4',5',6'-Pentafluoroacetophenone (652-29-9), Gossypin (652-78-8), 2,3,4,5,6-Pentafluorostyrene (653-34-9), Pentafluorobenzaldehyde (653-37-2), GlyTyrOH(658-79-7), 1-Bromo-2-chlorobenzene (694-80-4),2-Bromo-4-chlorophenol (695-96-5), 5-Iodouracil (696-07-1), 2-Methyl-4-nitroimidazole (696-23-1), 5-Nitro-2-furaldehyde (698-63-5), Sulfamethoxazole (723-46-6), Vinyl benzoate (769-78-8), 2,3,4,5,6-Pentafluoroaniline (771-60-8), Pentafluorophenol (771-61-9), Pentafluorothiophenolate (771-62-0), pentafluorobenzonitrile (773-82-0), 3-Nitrothiophene (822-84-4), Iodopentafluorobenzene (827-15-6), Pentafluorophenylhydrazine (828-73-9), 2,4,6-Trimethoxy-1,3,5-triazine (877-89-4), Pentafluoronitrobenzene (880-78-4), Clofibrate (882-09-7), 2'-Deoxyguanosine 5'-monophosphate (902-04-5), 4-Nitroisothiazole (931-07-7), 5-Azacytosine (931-86-2), Benzaldoxime (932-90-1), 7-Methyladenine (935-69-3), 4-Nitroperoxybenzoic acid (943-39-5), 5-Methoxyindole (1006-94-6), N-Formylkynurenine (1022-31-7), 4-Fluorobenzonitrile (1194-02-1), 2-Methyladenine (1445-08-5), 4-Pyridinecarboxamide (1453-82-3), 4-Chromanol (1481-93-2), Clonazepam (1622-61-3), Atrazine (1912-24-9), 1-Methylguanosine (2140-65-0), Pterin (2236-60-4), α-Nitrophenyl-D-glucopyranoside (2816-24-2), 3-Chloroanisole (2845-89-8), 4-Nitroimidazole (3034-38-6), 2-Bromo-5-nitrothiazole (3034-48-8), Di (4-chlorophenyl) sulfoxide (3085-42-5), Furamazone (3270-71-1), 4-Bromo-2-chlorophenol (3964-56-5), GlyLeuTyr (4306-24-5), Nitracrine (4533-39-5), N-(2-Acetylphenyl)formamide (5257-06-7), 3,5-Dinitroanisole (5327-44-6), 3-Benzoylpyridine (5424-19-1), 9-Methylguanine (5502-78-3), 2-

	Nitropyrrole (5919-26-6), 3-Nitropyrrole(5930-94-9), Benzoflavine (6359-38-2), 4’-Demethylepipodophyllotoxin (6559-91-7), 2,4-Dimethyl-6-hydroxypyrimidine (6622-92-0), 4',5'-Dihydropsoralen (7535-48-0), Naringin (10236-47-2), Misonidazole (13551-87-6), 4-Benzoylpyridine (14548-46-0), 3-Nitroquinoline (17576-53-3), 2,1,3-Benzothiadiazole-4,7-dicarbonitrile (20138-79-8), 2,4-Diethoxypyrimidine (20461-60-3), Daunomycin (20830-81-3), P-Tolylamino-acetic acid (21911-69-3), Baicalin (21967-41-9), 1,2,3,5-Tetramethylisoindole-4,7-dione (24686-78-0), 2,3-Bis(2-pyridyl)-5,6-dihydropyrazine (25005-95-2), Gemfibrozil (25812-30-0),3-Nitropyrazole (26621-44-3), Methoxyphenol (26638-03-9), Amoxicillin (26787-78-0), 1,10-Phenanthroline-5,6-dione (27318-90-7), 2-Nitrobenzofuran (33094-66-5), Etoposide (33419-42-0), Bupropion (34841-39-9), Metoprolol (37350-58-6), 5-Hydroxy-2-nitrobenzofuran (40024-32-6), 4,6-Dihydroxy-2-methylpyrimidine (40497-30-1), 7-Hydroxy-2-nitrobenzofuran (40739-73-9), Tyrosine (55520-40-6), 8-Bromoinosine (55627-73-1), Verbascoside (61276-17-3), 5-Deazalumiflavin (61696-29-5), 6-Chloromelatonin (63762-74-3), Pazelliptine (65222-35-7), Iohexol (66108-95-0), 6-Aminophenalenone (70402-14-1), 7-O-Methylnogarol (71628-96-1), Ceftazidime (72558-82-8), Iopromide (73334-07-3), Ciprofloxacin (85721-33-1), Catechin (88191-48-4), α-(3-Pyridyl 1-oxide)-N-tert-butylnitrone (88283-41-4), Venlafaxine (93413-69-5), Adenylyl-(2'5')uridine phosphate (93839-87-3), Orbifloxacin (113617-63-3), Duloxetine (116539-59-4)
–CO–R	Menadione (58-27-5), Tetracycline (60-54-8), 2-Propanone (67-64-1), Camphor (76-22-2), Methyl vinyl ketone (78-94-4), Chloroacetone (78-95-5), 2-Nitrophenolate (88-75-5), Anthrone (90-44-8), 4,4'-Dimethoxybenzophenone (90-96-0), 2-Benzoylpyridine (91-02-1), 2-Chlorophenolate (95-57-8), Acetophenone (98-86-2), 3-Hydroxybenzoate (99-06-9), 4-Hydroxybenzoate (99-96-7), 4-Nitrophenolate (100-02-7), 4-Nitroacetophenone (100-19-6), 1,3-Diphenyl-2-propanone (102-04-5), 4-Bromophenolate (106-41-2), 4-Chlorophenolate (106-48-9), 1,4-Benzoquinone (106-51-4), 3-Chlorophenolate

	(108-43-0), Quercetin (117-39-5), 2-Hydroxy-2-phenylacetophenone (119-53-9), Benzophenone (119-61-9), Cyclopentanone (120-92-3), Benzil(134-81-6), 2,5-Dimethyl-1,4-benzoquinone (137-18-8), Rutin (153-18-4), Kynurenine (343-65-7), 3-Acetylpyridine (350-03-8), 2-Fluorophenolate (367-12-4), 4-Fluorophenolate (371-41-5), 3-Fluorophenolate (372-20-3), Fluoroacetone (430-51-3), 2,3-Butanedione (431-03-8), Genistein (446-72-0), 5-Hydroxy-1,4-naphthoquinone (481-39-0), 5-hydroxy-2-methyl-1,4-naphthoquinone (481-42-5), 3-Hydroxykynurenine (484-78-6), 9-Fluorenone (486-25-9), Baicalein (491-67-8), Chrysoeriol (491-71-4), 3-Hydroxy-2-butanone (513-86-0), 1,1-Dichloroacetone (513-88-2), 2,3,5,6-Tetramethylbenzoquinone (527-17-3), Genistin (529-59-9), 3-Nitrophenolate (554-84-7), 3-Bromophenol (591-20-8), 2-Cyanophenolate (611-20-1), 2',3',4',5',6' Pentafluoroacetophenone (652-29-9), Gossypin (652-78-8), 4-Hydroxybenzonitrile (767-00-0), Ketophenylbutazone (853-34-9), 3-Hydroxybenzonitrile (873-62-1), 1,1,1-Trichloroacetone (918-00-3), N-Formylkynurenine (1022-31-7), N-(2-Acetylphenyl)formamide (5257-06-7), 3-Benzoylpyridine (5424-19-1), Naringin (10236-47-2), Camphoroquinone (10373-78-1), 4-Benzoylpyridine (14548-46-0), Daunomycin (20830-81-3), Baicalin (21967-41-9), 1,2,3,5-Tetramethylisoindole-4,7-dione (24686-78-0), 1,10-Phenanthroline-5,6-dione (27318-90-7), Bupropion (34841-39-9), 6-Aminophenalenone (70402-14-1),7-O-Methylnogarol (71628-96-1), Ciprofloxacin (85721-33-1), Orbifloxacin (113617-63-3), 5'-(1,4-Dihydro-1-methyl-3-pyridinylcarbonyl)-3'-azido-2',2'-dideoxythymidine (116333-41-6)
–CHO	Pyridoxal phosphate (54-47-7), DL-glyceraldehyde (56-82-6), Pyridoxal(66-72-8), Acetaldehyde (75-07-0), 2 Chlorobenzaldehyde (89-98-5), Benzaldehyde (100-52-7), 4-Chlorobenzaldehyde (104-88-1), Propionaldehyde (123-38-6), 3-Chlorobenzaldehyde (587-04-2), Pentafluorobenzaldehyde (653-37-2), 5-Nitro-2-furaldehyde (698-63-5), Ribose-5-phosphate (3615-55-2)
$–NO_2$	Chloramphenicol (56-75-7), Nitrofurazone (59-87-0), Nitrofurantoin (67-20-9), Nitromethane (75-52-5), Trichloronitromethane (76-06-2), Nitroethane (79-24-3), 2-Chloro-6-nitrotoluene(83-42-1), 1-Chloro-2-nitrobenzene (88-73-3), 2-

	Nitrophenolate (88-75-5), 4-Chloro-2-nitrotoluene (89-59-8), 5-Nitro-2-furaldehyde diacetate (92-55-7), Nitrobenzene (98-95-3), 4-Nitrotoluene (99-99-0), 1-Chloro-4-nitrobenzene (100-00-5), 4-Nitrophenol (100-02-7), 4-Nitrophenolate (100-02-7), 4-Nitroacetophenone (100-19-6), 1-Nitropropane (108-03-2), 2,4-Dinitrotoluene (121-14-2), 1-Chloro-3-nitrobenzene (121-73-3), Metronidazole (443-48-1), Tribromonitromethane (464-10-8), 2-Nitroimidazole (527-73-1), 3-Nitrophenolate (554-84-7), Nifuroxime (555-15-7), Bromonitromethane (563-70-2), 5-Nitroquinoline (607-34-1), 8-Nitroquinoline (607-35-2), 2-Nitrothiophene (609-40-5), 5-Nitrouracil (611-08-5), 6-Nitroquinoline (613-50-3), 7-Nitro-quinoline (613-51-4), 3-Nitrotyrosine (621-44-3), 2-Methyl-4-nitroimidazole (696-23-1), 5-Nitro-2-furaldehyde (698-63-5), 3-Nitrothiophene (822-84-4), Pentafluoronitrobenzene (880-78-4),Bromodichloronitromethane (918-01-4), 4-Nitroisothiazole (931-07-7), 4-Nitroperoxybenzoic acid (943-39-5), Dibromochloronitromethane (1184-89-0), Clonazepam (1622-61-3), Chloronitromethane (1794-84-9), α-Nitrophenyl--D-glucopyranoside (2816-24-2), 4-Nitroimidazole (3034-38-6), 2-Bromo-5-nitrothiazole (3034-48-8), Furamazone (3270-71-1), Nitracrine (4533-39-5), 3,5-Dinitroanisole (5327-44-6), 2-Nitropyrrole (5919-26-6), 3-Nitropyrrole (5930-94-9), Dichloronitromethane (7119-89-3), Misonidazole (13551-87-6), 3-Nitroquinoline (17576-53-3), 3-Nitropyrazole (26621-44-3), 2-Nitrobenzofuran (33094-66-5), 5-Hydroxy-2-nitrobenzofuran (40024-32-6), 7-Hydroxy-2-nitrobenzofuran (40739-73-9), Bromochloronitromethane (135531-25-8)

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