water

MDPI

Supplementary material

Prediction of Second–Order Rate Constants of Sulfate Radical with Aromatic Contaminants Using Quantitative Structure–Activity Relationship Model

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Table S1. Values of molecular descriptors and $\log k_{SO_4^{\bullet-}}$ for selected aromatic compounds.

No.	Aromatic compound	CAS number	Molecular formula	Electron density	Steric energy	O/C	log*V*	log*P*	$\log k_{SO_4^{\bullet-}}$	References
Training set										
1	1,2,3–Trimethoxybenzene	634–36–6	C9H12O3	5.3097	18.5952	0.3333	2.2060	1.62	9.8451	[1]
2	1,2,4–Trimethoxybenzene	135–77–3	C9H12O3	5.3022	16.7465	0.3333	2.2060	1.64	9.8921	[1]
3	1,2–Dimethoxybenzene	91–16–7	C8H10O2	5.2826	10.8967	0.2500	2.1308	1.61	9.6990	[1]
4	1,3–Dimethoxybenzene	151–10–0	C8H10O2	5.2737	11.6098	0.2500	2.1308	2.03	9.8451	[1]
5	1,4–Dimethoxybenzene	150–78–7	C8H10O2	5.2593	11.4474	0.2500	2.1308	2.05	9.8573	[1]
6	2,3–Dimethoxybenzoate	1521–38–6	C9H9O4	5.2986	18.6652	0.4444	2.2025	–1.74	9.9294	[2]
7	2,4–Dimethoxybenzoate	91–52–1	C9H9O4	5.1884	19.8398	0.4444	2.2025	–1.52	9.5798	[2]
8	2–Bromotoluene	95–46–5	C7H7Br	5.1262	1.6964	0.0000	2.0737	3.15	9.3617	[3]
9	**2–Chlorotoluene***	95–49–8	C7H7Cl	5.1759	1.3082	0.0000	2.0574	3.02	9.2304	[3]
10	2–Hydroxybenzothiazole	934–34–9	C7H5NOS	5.3964	6.2913	0.1111	2.0889	1.82	9.6721	[4]
11	2–Methylthiobenzothiazole	615–22–5	C8H7NS2	5.0370	–0.5450	0.0000	2.1740	3.09	9.1461	[4]
12	3,4,5–trimethoxybenzoate	118–41–2	C10H11O5	5.3323	20.6624	0.5000	2.2670	–1.93	9.6990	[2]
13	3,4–Dichloroaniline	95–76–1	C6H5Cl2N	5.1695	0.0915	0.0000	2.0878	2.30	9.6721	[5]
14	3,4–Dimethoxybenzoate	93–07–2	C9H9O4	5.2955	14.9384	0.4444	2.2025	–1.92	9.6532	[2]
15	3,5–Dimethoxybenzoate	1132–21–4	C9H9O4	5.2516	14.9731	0.4444	2.2025	–1.52	9.6435	[2]
16	**4–(2–Hydroxyethyl)phenol***	501–94–0	C8H10O2	5.2789	0.9682	0.2500	2.1261	1.00	9.2380	[6]
17	**4–Hydroxybenzoate***	456–23–5	C7H5O3	5.3984	1.8176	0.4286	2.0657	–1.43	9.3979	[7]
18	4–Isobutylacetophenone	38861–78–8	C12H16O	5.2500	9.1362	0.0833	2.2703	3.14	9.5211	[8]
19	4–Methoxybenzoate	100–09–4	C8H7O3–	5.3849	9.4362	0.3750	2.1266	–1.50	9.8808	[2]
20	4–Toluate	5118–31–0	C8H7O2–	5.1552	4.3902	0.2500	2.0964	–1.11	9.2553	[7]
21	Acetaminophen	103–90–2	C8H9NO2	5.2475	–7.8295	0.2500	2.1462	0.68	9.6721	[9]
22	Acetanilide	103–84–4	C8H9NO	5.1059	–7.0445	0.1250	2.1205	1.16	9.5563	[7]

No.	Aromatic compound	CAS number	Molecular formula	Electron density	Steric energy	O/C	log*V*	log*P*	$\log k_{SO_4^{\bullet-}}$	References
23	Amitriptyline HCl	549–18–8	C20H24ClN	5.2880	44.6729	0.0000	2.4551	4.19	9.6812	[10]
24	Amoxicillin	26787–78–0	C16H19N3O5S	5.3046	50.0119	0.3125	2.4870	–1.35	9.5416	[11]
25	Anisole	100–66–3	C7H8O	5.2523	5.5171	0.1429	2.0398	1.99	9.6902	[1]
26	Aspartame	22839–47–0	C14H18N2O5	5.0243	–8.2745	0.3571	2.4241	–0.55	9.3579	[12]
27	Benzene	71–43–2	C6H6	4.9871	–0.5741	0.0000	1.9245	1.94	9.4771	[7]
28	Benzoate	766–76–7	C7H5O2	5.1147	4.0592	0.2857	2.0346	–1.56	9.0792	[7]
29	Benzophenone	119–61–9	C13H10O	5.0665	30.1467	0.0769	2.2416	3.39	9.6021	[13]
30	Benzothiazole	95–16–9	C7H5NS	5.0075	3.6929	0.0000	2.0591	2.37	9.5185	[4]
31	Cefaclor	53994–73–3	C15H14ClN3O4S	5.0678	61.5558	0.2667	2.4627	–1.70	9.2788	[11]
32	Diclofenac	15307–86–5	C14H11Cl2NO2	5.2123	37.6046	0.1429	2.3779	4.57	9.8261	[14]
33	Diuron	330–54–1	C9H10Cl2N2O	5.1128	4.6142	0.1111	2.2751	2.58	9.7160	[5]
34	Fenuron	101–42–8	C9H12N2O	5.0808	–0.0061	0.1111	2.2077	1.30	9.6628	[5]
35	Fluomethuron	2164–17–2	C10H11F3N2O	5.1617	5.9923	0.1000	2.2847	2.17	9.6628	[5]
36	Fluorobenzene	462–06–6	C6H5F	5.0096	–0.6765	0.0000	1.9492	2.10	8.9912	[15]
37	Gallate ion	149–91–7	C7H5O5	5.4847	–13.3754	0.7143	2.1218	–2.01	9.4624	[16]
38	**Gatifloxacin***	112811–59–3	C19H22FN3O4	5.2277	81.6246	0.2105	2.5153	–0.04	9.4771	[17]
39	Ibuprofen	15687–27–1	C13H18O2	5.1125	1.7199	0.1538	2.3247	3.46	9.5798	[18]
40	Isoproturon	34123–59–6	C12H18N2O	5.1328	2.0694	0.0833	2.3249	2.81	9.4624	[5]
41	Linuron	330–55–2	C9H10Cl2N2O2	5.3083	4.2866	0.2222	2.2953	2.93	9.7076	[5]
42	Methyl 2–aminobenzoate	134–20–3	C8H9NO2	5.1238	12.4301	0.2500	2.1457	1.72	9.7482	[19]
43	Metoprolol	51384–51–1	C15H25NO3	5.2594	18.1062	0.2000	2.4361	1.97	9.7084	[20]
44	m–Hydroxybenzaldehyde	100–83–4	C7H6O2	5.2399	4.6039	0.2857	2.0455	1.22	9.6232	[21]
45	Monolinuron	1746–81–2	C9H11ClN2O2	5.1632	1.1854	0.2222	2.2645	2.33	9.7782	[5]
46	N–(p–Amylcinnamoyl)anthranilic acid	110683–10–8	C21H23NO3	5.1129	6.5453	0.1429	2.5119	5.88	9.3997	[11]

No.	Aromatic compound	CAS number	Molecular formula	Electron density	Steric energy	O/C	log*V*	log*P*	$\log k_{SO_4^{\bullet-}}$	References
47	Nortriptylene HCl	894–71–3	C19H21N	5.2812	42.4997	0.0000	2.4206	3.94	10.3010	[22]
48	o–Cresol	95–48–7	C7H8O	5.2732	–2.3763	0.1429	2.0359	2.33	9.8325	[23]
49	o–Hydroxybenzaldehyde	90–02–8	C7H6O2	5.3257	4.7154	0.2857	2.0455	1.67	9.7924	[21]
50	p–Cresol	106–44–5	C7H8O	5.2671	–1.6501	0.1429	2.0359	1.91	9.7634	[23]
51	Penicillin G	61–33–6	C16H18N2O4S	5.0016	60.4921	0.2500	2.4587	1.82	9.1584	[11]
52	**Penicillin V***	87–08–1	C16H18N2O5S	5.2072	61.9168	0.3125	2.4721	1.70	9.3010	[11]
53	Phenanthrene	85–01–8	C14H10	5.0549	–3.5522	0.0000	2.2356	4.30	9.5052	[24]
54	Propranolol	525–66–6	C16H21NO2	5.2752	8.4327	0.1250	2.4113	2.97	9.6803	[20]
55	p–Xylene	106–42–3	C8H10	5.0215	–0.5808	0.0000	2.0688	2.83	9.4314	[25]
56	Sulfacetamide	144–80–9	C8H10N2O3S	5.1557	181.7001	0.3750	2.2423	–0.56	9.7782	[26]
57	Sulfamerazine	127–79–7	C11H12N4O2S	5.3173	185.4982	0.1818	2.3401	0.40	10.6902	[27]
58	Sulfamethazine	57–68–1	C12H14N4O2S	5.4017	184.0830	0.1667	2.3718	0.84	10.5539	[27]
59	Sulfamonomethoxine	1220–83–3	C11H12N4O3S	5.2500	186.1896	0.2727	2.3576	0.38	10.1239	[27]
60	Sulfathiazole	72–14–0	C9H9N3O2S2	5.3000	179.7674	0.2222	2.2948	0.83	10.6730	[27]
61	Sulfisoxazole	127–69–5	C11H13N3O3S	5.6191	189.2402	0.2727	2.3446	0.99	11.2068	[27]
62	Terbutaline	23031–25–6	C12H19NO3	5.1964	2.2294	0.2500	2.3430	1.07	9.6232	[28]
63	Toluene	108–88–3	C7H8	5.0263	–0.5693	0.0000	2.0026	2.39	9.4914	[29]
64	Trimethoprim	738–70–5	C14H18N4O3	5.2699	25.0018	0.2143	2.4202	0.99	9.8871	[30]
65	Venlafaxine	93413–69–5	C17H27NO2	5.2839	26.9026	0.1176	2.4576	3.81	9.5478	[20]
66	α–Terpineol	98–55–5	C10H18O	5.1751	10.4009	0.1000	2.2321	2.60	9.6128	[31]
Validation set										
1	1H–Benzotriazole	95–14–7	C6H5N3	5.0484	8.3711	0.0000	2.0200	1.29	9.0414	[22]
2	2–Methoxybenzoate	579–75–9	C8H7O3–	5.2057	6.6360	0.3750	2.1266	–1.55	9.8451	[2]
3	2–Toluate	118–90–1	C8H7O2–	5.1576	9.7565	0.2500	2.0964	–1.16	9.1461	[7]
4	3–Bromotoluene	591–17–3	C7H7Br	5.2121	–0.1172	0.0000	2.0737	3.17	9.2304	[3]

No.	Aromatic compound	CAS number	Molecular formula	Electron density	Steric energy	O/C	log*V*	log*P*	$\log k_{SO_4^{\bullet-}}$	References
5	3–Methoxybenzoate	586–38–9	C8H7O3–	5.2351	9.8494	0.3750	2.1266	–1.53	9.8808	[2]
6	3–Toluate	99–04–7	C8H7O2–	5.1444	4.4702	0.2500	2.0964	–1.14	9.3010	[7]
7	Acetophenone	98–86–2	C8H8O	5.0543	6.9851	0.1250	2.0777	1.84	9.2553	[13]
8	Ampicillin	69–53–4	C16H19N3O4S	5.0748	55.8551	0.2500	2.4755	–0.87	9.2718	[11]
9	Atenolol	29122–68–7	C14H22N2O3	5.2683	1.1114	0.2143	2.4165	0.72	9.7084	[20]
10	Benzaldehyde	100–52–7	C7H6O	5.0411	5.7158	0.1429	2.0130	1.73	8.8513	[13]
11	Bromobenzene	108–86–1	C6H5Br	5.1604	0.0390	0.0000	2.0083	2.75	9.2553	[29]
12	Carbamazepine	298–46–4	C15H12N2O	5.0417	9.0775	0.0667	2.3326	2.84	9.2833	[32]
13	Chlorobenzene	108–90–7	C6H5Cl	5.1534	–0.1436	0.0000	1.9894	2.62	9.1761	[29]
14	Clofibric acid	882–09–7	C10H11ClO3	5.1938	11.1571	0.3000	2.2629	2.73	9.2380	[33]
15	m–Cresol	108–39–4	C7H8O	5.2734	–1.6118	0.1429	2.0359	1.88	9.8451	[23]
16	Mesitylene	108–67–8	C9H12	5.0792	–0.5166	0.0000	2.1262	3.21	9.1139	[25]
17	Monuron	150–68–5	C9H11ClN2O	5.1618	1.1838	0.1111	2.2427	1.98	9.6990	[5]
18	Naproxen	22204–53–1	C14H14O3	5.2833	6.5893	0.2143	2.3304	3.38	9.7513	[20]
19	Phenol	108–95–2	C6H6O	5.2644	–1.5844	0.1667	1.9641	1.46	9.7924	[23]
20	p–Hydroxybenzaldehyde	123–08–0	C7H6O2	5.3300	4.6324	0.2857	2.0455	1.25	9.7709	[21]
21	Sulfadiazine	68–35–9	C10H10N4O2S	5.3006	186.2394	0.2000	2.3059	–0.04	10.6191	[27]
22	Sulfamethoxazole	723–46–6	C10H11N3O3S	5.3507	187.8270	0.3000	2.3108	0.61	10.2068	[30]

*Outliers.

Text S1. Python code for the y–randomisation test.

```
import numpy as np
from sklearn.linear_model import LinearRegression
from sklearn.metrics import r2_score
import pandas as pd
import matplotlib.pyplot as plt

df = pd.read_excel("training_dataset.xlsx")
Y = df['logK'].to_numpy()
X = df[['E', 'S', 'O/C']].to_numpy()
shuffled_r2 = []

for i in range(100):
    np.random.shuffle(Y)
    reg = LinearRegression()
    reg.fit(X, Y)
    ypred = reg.predict(X)
    shuffled_r2.append(r2_score(Y, ypred))

ypoints = np.array(shuffled_r2)
xpoints = np.arange(1, 101, 1)

plt.plot(xpoints, ypoints)
plt.xlabel("Shuffled times")
plt.ylabel('R\u00b2')
plt.savefig("FigureS1.jpg", dpi=600)
```

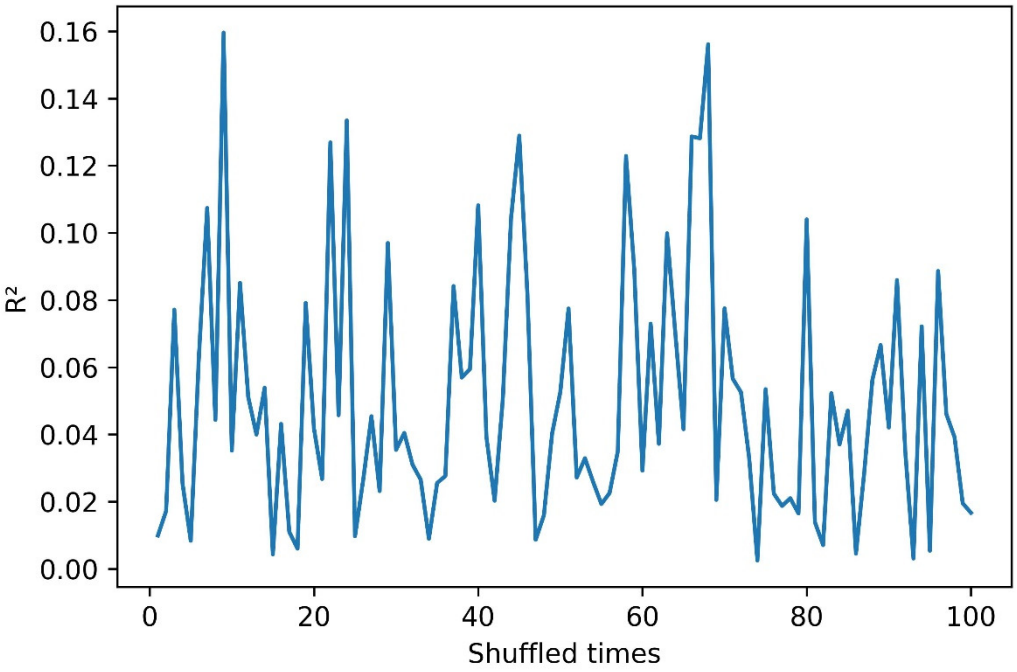

Figure S1. The R^2 of shuffled $\log k_{SO_4^{\bullet-}}$ regressed against fixed *E*, *S* and O/C.

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