Electronic Supplementary Information

QSARs for Phenols and Phenolates: Oxidation Potential as a Predictor of Reaction Rate Constants with Photochemically Produced Oxidants

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HPLC parameters for the analysis of phenols

Compound	injection volume (μL)	mobile phase composition		flow rate (mL/mi)	column temperature (° C)	detection wavelength (nm)
		% A[a]	% B[b]			
m-cresol	20	10	90	0.50	40	285
p-cresol	20	10	90	0.50	40	285
p-chloro-*m*-cresol	20	20	80	0.50	40	285
2-nitrophenol	20	15	85	0.50	40	285
3-nitrophenol	20	5	95	0.50	40	285
2-chlorophenol	20	15	85	0.50	40	285
3-chlorophenol	20	15	85	0.50	40	285
4-chlorophenol	20	15	85	0.50	40	285
2,3,5-trichlorophenol	20	30	70	0.50	40	250
pentachlorophenol	20	30	70	0.50	40	250
2,4-dimethylphenol	20	20	80	0.50	40	220
2,6-dimethylphenol	20	20	80	0.50	40	220
2,4,6-trimethylphenol	20	30	70	0.50	40	220
2,4,6-tribromophenol	20	40	60	0.50	40	220
BPAP	20	35	65	0.50	40	254
BPAF	20	35	65	0.50	40	254
BPZ	20	35	65	0.50	40	254
BPF	20	15	85	0.50	40	258
BPS	20	10	90	0.50	40	288
sesamol	40	5	95	0.50	40	297
a-tocopherol	40	95	5	0.75	40	285

[a] A = acetonitrile (ACN)

[b] B = 10:90 ACN: pH 5 NH_4OAc (10 mM) buffer

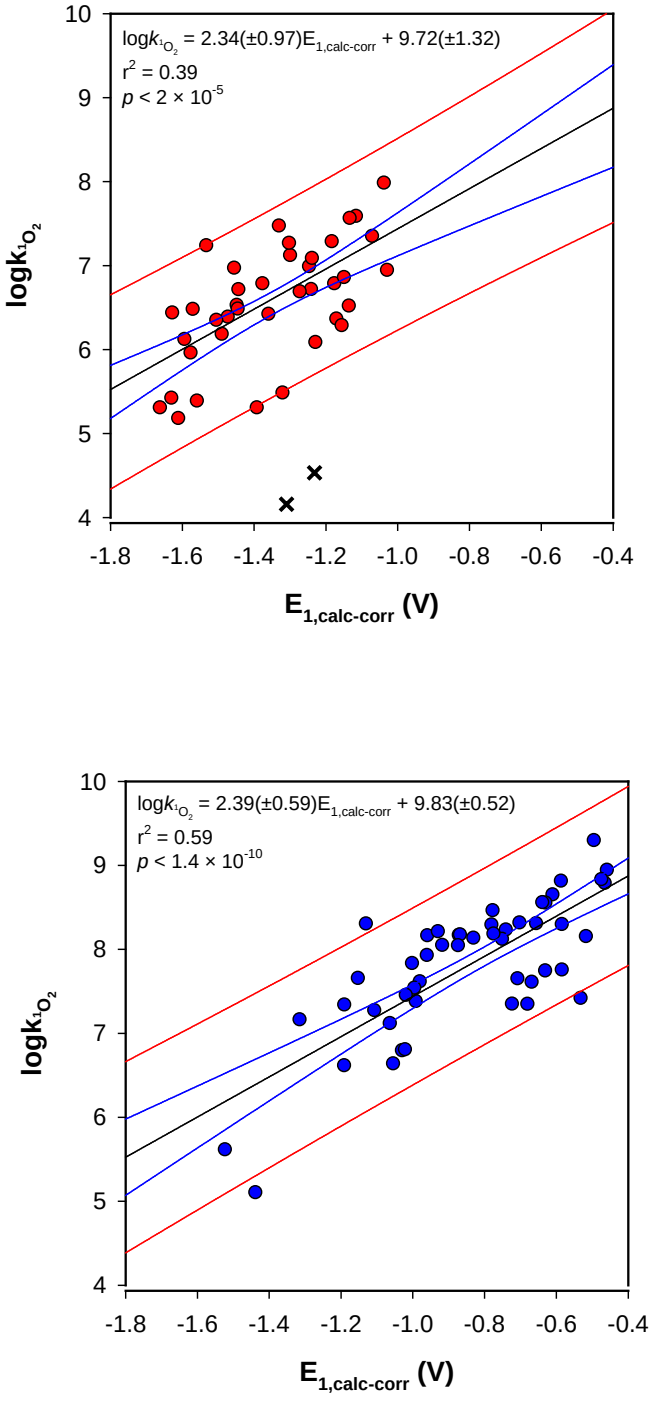
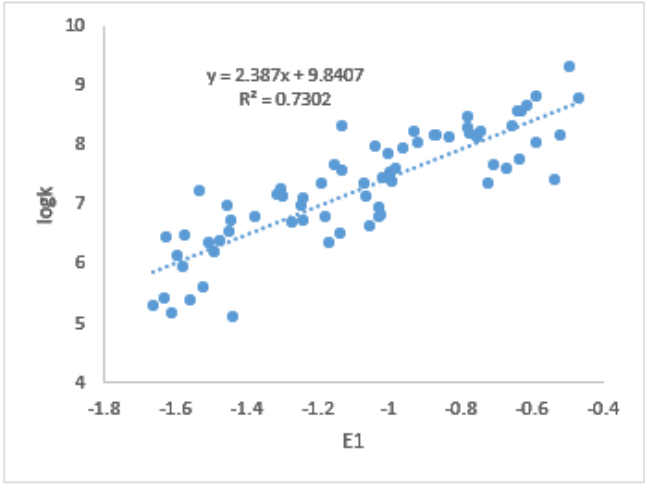


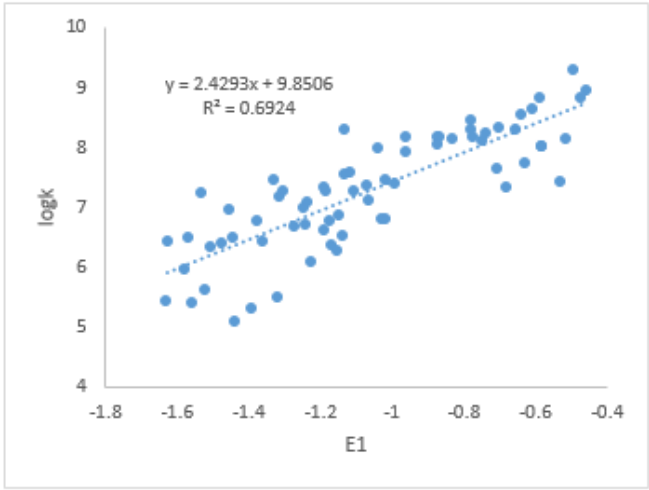
Figure S1. Correlations of singlet oxygen rate constants for phenols (top) and phenolates (bottom) as a function of one electron reduction potential. The data are the same as those in Figure 3 which were analyzed with a single regression.

Training and test sets and validation results for singlet oxygen rate constants

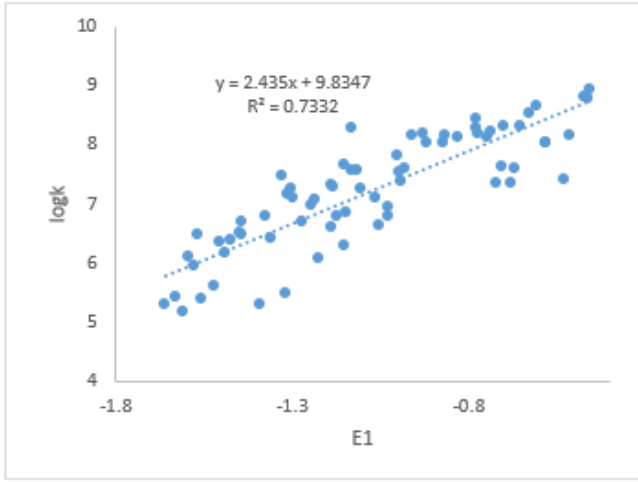
Compound	E1 (V)	logk(exp)	logk(calc)	Unsigned Error
	Set 1			
1,4-dihydroxybenzene	-1.11	7.58	7.18	0.40
benzophenone-3	-1.39	5.30	6.52	1.22
Phenol	-1.36	6.42	6.60	0.18
BPA (phenol)	-1.32	5.48	6.69	1.22
triclosan	-1.44	6.48	6.40	0.08
4 Cl -m - cresol	-1.33	7.47	6.67	0.80
17 B estrdiol.	-1.18	7.28	7.02	0.26
diflunisal	-1.15	6.28	7.09	0.81
tetramethylbisophenol	-1.23	6.08	6.91	0.83
terbutaline	-1.15	6.85	7.10	0.25
2,4,6-trichlorophenolate	-0.96	8.16	7.56	0.60
2,6-dimethoxyphenolate	-0.46	8.94	8.75	0.19
3-methylphenolate	-0.70	8.31	8.17	0.14
4-methoxyphenolate	-0.47	8.82	8.71	0.11
4-nitrophenolate	-1.19	6.61	7.00	0.39
2,6-dimethylphenolate	-0.58	8.02	8.45	0.43
BPAP (anion)	-0.68	7.34	8.22	0.88
BPAF (anion)	-0.87	8.04	7.76	0.28
diadzein (anion)	-1.11	7.26	7.20	0.06
			MUE	**0.48**



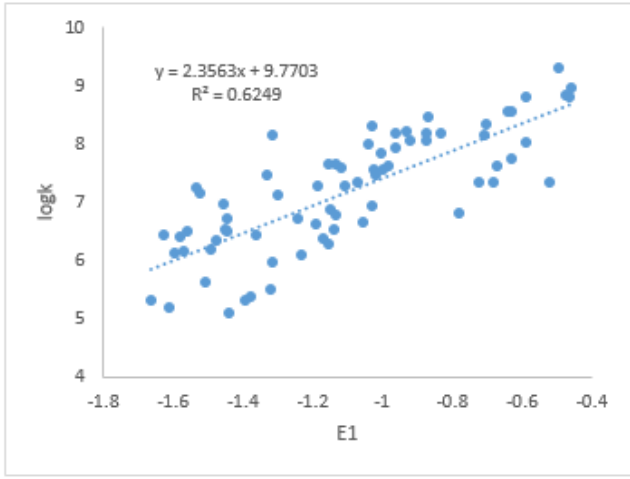
	Set 2			
2,3,5-trichlorophenol	-1.61	5.17	5.94	0.77
2,4-dichlorophenol	-1.44	6.71	6.35	0.36
3-chlorophenol	-1.45	6.52	6.34	0.18
3-methoxyphenol	-1.30	7.11	6.70	0.42
4-acetylphenol	-1.49	6.18	6.24	0.06
pentachlorophenol	-1.66	5.30	5.82	0.52
tyrosine	-1.03	6.94	7.35	0.42
2-nitrophenol	-1.59	6.11	5.98	0.13
2,3,5-trichlorophenolate	-1.05	6.63	7.29	0.66
2,4,6-trimethylphenolate	-0.46	8.78	8.73	0.05
2-nitrophenolate	-1.15	7.65	7.06	0.59
3-nitrophenolate	-0.98	7.61	7.47	0.13
4-methylphenolate	-0.63	8.55	8.32	0.22
triclosan (anion)	-0.92	8.04	7.63	0.42
biochanin A (anion)	-1.00	7.83	7.42	0.40
genestein (anion)	-0.99	7.53	7.44	0.09
equol (anion)	-0.67	7.60	8.23	0.63
methyl salicylate	-0.93	8.20	7.60	0.61
2,2-dihydroxybiphenyl (anion)	-0.72	7.34	8.10	0.76
			MUE	**0.39**



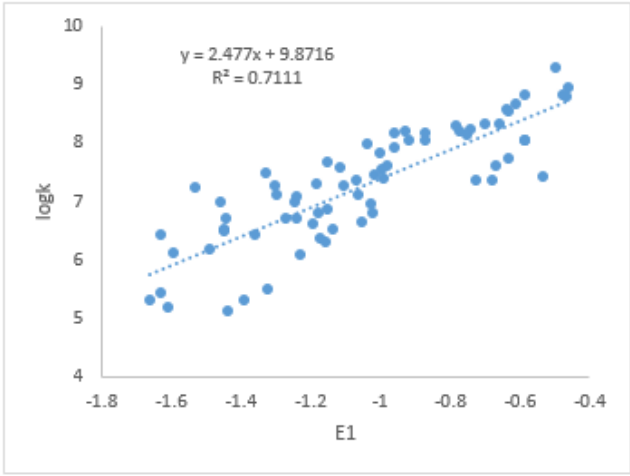
Set 3				
2,4,6-trichlorophenol	-1.53	7.23	6.11	1.12
2,4,6-trimethylphenol	-1.13	6.51	7.07	0.56
2-chlorophenol	-1.45	6.96	6.30	0.67
4-methoxyphenol	-1.07	7.34	7.23	0.11
sesamol	-1.04	7.98	7.31	0.66
2,6-dimethylphenol	-1.24	6.71	6.82	0.11
sesamolate	-0.49	9.29	8.63	0.66
2,4-dimethylphenol	-1.17	6.36	6.99	0.63
2,4,6-tribromophenol	-1.63	6.43	5.88	0.55
2,4-dichlorophenolate	-0.87	8.16	7.72	0.44
4,6-dinitro-2-methylphenolate	-1.44	5.10	6.34	1.24
4-tertbutylphenolate	-0.64	8.55	8.28	0.27
BPZ (anion)	-0.63	7.74	8.30	0.56
2,4,6-tribromophenolate	-0.96	7.92	7.50	0.42
17β estradiol (anion)	-0.59	8.81	8.41	0.40
4-methyl - 2 nitrophenolate	-1.02	7.45	7.36	0.09
benzyl 4-hydroxybenzoate (benzylparaben)	-1.02	6.80	7.35	0.55
			MUE	**0.53**



	Set 4			
2-methoxyphenol	-1.17	6.78	7.21	0.43
4-methylphenol	-1.24	6.98	7.04	0.06
4-nitrophenol	-1.63	5.42	6.14	0.73
4-tertbutylphenol	-1.24	7.08	7.06	0.02
BPZ	-1.27	6.68	6.98	0.30
3-methylphenol	-1.30	7.26	6.91	0.35
2,6-dimethylphenolate	-0.58	8.02	8.60	0.58
2-methoxyphenolate	-0.61	8.64	8.54	0.10
4-acetylphenolate	-0.99	7.37	7.65	0.27
4-chlorophenolate	-0.78	8.29	8.14	0.14
phenolate	-0.74	8.22	8.24	0.01
4-chloro-3-methylphenolate	-0.75	8.11	8.21	0.10
BPS (anion)	-1.06	7.11	7.47	0.36
BPA (anion)	-0.65	8.30	8.44	0.13
2,4-dimethylphenolate	-0.53	7.41	8.73	1.32
tetrabromobisphenolate	-0.77	8.18	8.16	0.02
			MUE	**0.31**

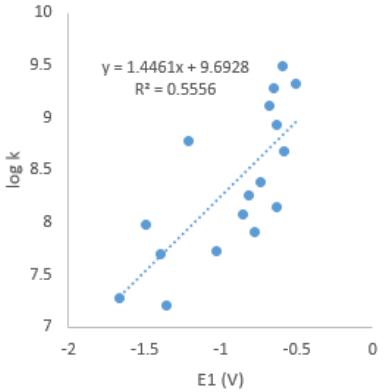


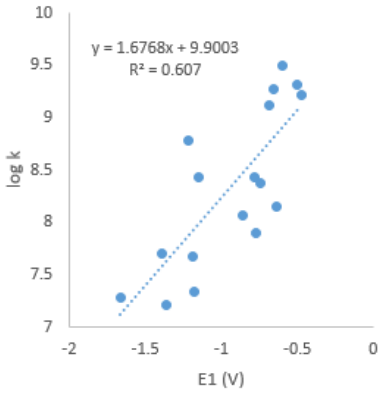
Set 5				
2,6-dimethoxyphenol	-1.13	7.56	7.07	0.49
4-chlorophenol	-1.37	6.78	6.47	0.31
4-cyanophenol	-1.56	5.38	6.01	0.63
3-nitrophenol	-1.57	6.47	5.99	0.49
tetrabromobisphenol	-1.57	5.95	5.97	0.02
n-butyl paraben	-1.47	6.38	6.23	0.15
benzyl 4-hydroxybenzoate (benzylparaben)	-1.50	6.34	6.15	0.19
2,4-dinitrophenolate	-1.52	5.61	6.10	0.50
2,6-dinitro-4-methylphenolate	-1.31	7.16	6.62	0.54
2-chlorophenolate	-0.83	8.13	7.82	0.31
3-chlorophenolate	-0.87	8.17	7.73	0.44
3-methoxyphenolate	-0.78	8.45	7.95	0.50
4-cyanophenolate	-1.03	6.79	7.33	0.54
pentachlorophenolate	-1.13	8.30	7.08	1.22
2-hydroxybiphenylate	-0.71	7.64	8.12	0.48
tetramethylbisophenolate	-0.52	8.15	8.59	0.45
2-nitro-4- chlorophenolate	-1.19	7.33	6.93	0.40
			MUE	**0.45**

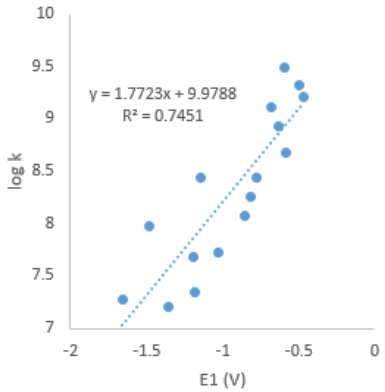


Training and test sets and validation results for carbonate radical rate constants

Compound name	E_1 (V)	log*k*(exp)	log*k*	Unsigned error
	Set 1			
4-chlorophenolate	-0.78	8.43	8.57	0.14
4-methoxyphenolate	-0.47	9.21	9.01	0.21
4-nitrophenolate	-1.19	7.68	7.97	0.29
paracetamol	-1.14	8.44	8.04	0.40
17b-estradiol	-1.18	7.34	7.99	0.64
			MUE	**0.34**
	Set 2			
4-bromophenolate	-0.81	8.26	8.54	0.28
4-methylphenolate	-0.63	8.92	8.85	0.08
4-cyanophenolate	-1.03	7.72	8.18	0.46
17b-estradiol (anion)	-0.59	8.68	8.92	0.24
4-carboxyphenol	-1.49	7.97	7.41	0.57
			MUE	**0.32**
	Set 3			
4-carboxyphenolate	-0.77	7.90	8.61	0.70
paracetamol anion	-0.65	9.28	8.83	0.45
phenolate	-0.74	8.38	8.67	0.29
tyrosine (anion)	-0.63	8.15	8.86	0.71
4-hydroxyphenylacetate	-1.21	8.78	7.83	0.95
benzophenone-3	-1.39	7.70	7.52	0.18
			MUE	**0.55**







	Set 4			
1,4-dihydroxylphenolate	-0.50	9.32	8.78	0.54
1-naptholate	-0.60	9.49	8.67	0.82
2-naptholate	-0.68	9.11	8.58	0.54
vanillinate	-0.86	8.07	8.37	0.30
pentachlorophenol	-1.66	7.28	7.45	0.18
phenol	-1.36	7.21	7.80	0.59
			MUE	**0.49**