

## 多类型表面活性剂临界胶束浓度定量构效关系

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## Quantitative Structure-Property Relationship of the Critical Micelle Concentration of Different Classes of Surfactants

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**Table S1 Experimental and predicted lg(CMC) based on this model, the ADAPT model and the Molconn model, for the set of 175 surfactants**

Surfactants	Experimental	ADAPT model <sup>15</sup>		Molconn model <sup>15</sup>		this work	
	lg(CMC) <sup>11</sup>	pred. lg(CMC)	AD <sup>b</sup>	pred. lg(CMC)	AD	pred. lg(CMC)	AD
Decane-1-sulfonic acid	-1.40	-1.46	0.06	-1.61	0.21	-1.40	0.00
Dodecane-1-sulfonic acid	-1.97	-2.00	0.03	-2.19	0.22	-2.04	0.07
Hexadecyl hydrogen sulfate	-3.26	-3.20	0.06	-3.18	0.08	-3.02	0.24
Hexadecan-4-yl hydrogen sulfate	-2.77	-2.96	0.19	-2.90	0.13	-3.01	0.24
Hexadecan-6-yl hydrogen sulfate	-2.63	-2.81	0.18	-2.78	0.15	-2.82	0.19
Tetradecyl hydrogen sulfate	-2.64	-2.61	0.03	-2.55	0.09	-2.54	0.10
Decyl hydrogen sulfate	-1.48	-1.53	0.05	-1.37	0.11	-1.46	0.02
2-Heptylnonyl hydrogen sulfate	-2.52	-2.65	0.13	-2.44	0.08	-2.42	0.10
Pentadecyl hydrogen sulfate	-2.92	-2.90	0.02	-2.82	0.1	-2.79	0.13
2-Hexyldecyl hydrogen sulfate	-2.64	-2.64	0	-2.72	0.08	-2.51	0.13
Octane-1-sulfonic acid	-0.79	-0.96	0.17	-0.98	0.19	-0.78	0.01
Tetradecane-1-sulfonic acid	-2.60	-2.57	0.03	-2.72	0.12	-2.63 <sup>a</sup>	0.03
Dodecyl hydrogen sulfate	-2.06	-2.05	0.01	-1.93	0.13	-2.01	0.05
Octyl hydrogen sulfate	-0.86	-1.06	0.2	-0.78	0.08	-0.92	0.06
2-Ethyltetradecyl hydrogen sulfate	-3.05	-2.90	0.15	-2.86	0.19	-3.00	0.05
2-Butyldodecyl hydrogen sulfate	-2.82	-2.70	0.12	-2.76	0.06	-2.78	0.04
Tridecyl hydrogen sulfate	-2.37	-2.33	0.04	-2.22	0.15	-2.28	0.09
2-Propyltridecyl hydrogen sulfate	-2.96	-2.72	0.24	-2.80	0.16	-2.90	0.06
2-Methylpentadecyl hydrogen sulfate	-3.10	-2.91	0.19	-2.91	0.19	-3.11	0.01
2-Pentylundecyl hydrogen sulfate	-2.70	-2.79	0.09	-2.74	0.04	-2.66 <sup>a</sup>	0.04
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Pentadecafluorooctanoic acid	-2.01	-0.86	1.15	-2.04	0.03	-2.05	0.04
2-(2-(Dodecyloxy)ethoxy)ethyl hydrogen sulfate	-2.55	-2.50	0.05	-2.51	0.04	-2.72	0.17
Hexane-1-sulfonic acid	-0.50	-0.53	0.03	-0.44	0.06	-0.31	0.19

Hexadecane-1-sulfonic acid	-3.13	-3.17	0.04	-3.37	0.24	-3.17	0.04
(E)-Dodec-1-ene-1-sulfonic acid	-1.89	-1.85	0.04	-1.91	0.02	-1.72	0.17
(E)-Tetradec-1-ene-1-sulfonic acid	-2.57	-2.41	0.16	-2.50	0.07	-2.31	0.26
(E)-Hexadec-1-ene-1-sulfonic acid	-3.22	-2.99	0.23	-3.10	0.12	-2.85	0.37
(E)-Octadec-1-ene-1-sulfonic acid	-3.75	-3.60	0.15	-3.70	0.05	-3.31	0.44
Dodecane-3-sulfonic acid	-1.73	-1.70	0.03	-1.86	0.13	-1.78	0.05
Dodecane-4-sulfonic acid	-1.64	-1.60	0.04	-1.58	0.06	-1.52	0.12
Dodecane-5-sulfonic acid	-1.55	-1.66	0.11	-1.53	0.02	-1.51	0.04
Dodecane-6-sulfonic acid	-1.44	-1.63	0.19	-1.42	0.02	-1.48	0.04
4-Heptylbenzenesulfonic acid	-1.58	-1.47	0.11	-1.35	0.23	-1.14	0.44
4-Octylbenzenesulfonic acid	-1.91	-1.73	0.18	-1.78	0.13	-1.49	0.42
4-(Nonan-3-yl)benzenesulfonic acid	-1.97	-1.86	0.11	-1.83	0.14	-1.66	0.31
4-(Decan-2-yl)benzenesulfonic acid	-2.30	-2.18	0.12	-2.14	0.16	-2.18 <sup>a</sup>	0.12
4-(Decan-3-yl)benzenesulfonic acid	-2.20	-2.15	0.05	-2.07	0.13	-2.00	0.20
4-(Decan-5-yl)benzenesulfonic acid	-2.05	-1.98	0.07	-2.07	0.02	-1.84	0.21
4-(Undecan-2-yl)benzenesulfonic acid	-2.72	-2.48	0.24	-2.44	0.28	-2.51	0.21
4-(Dodecan-3-yl)benzenesulfonic acid	-2.61	-2.77	0.16	-2.66	0.05	-2.67	0.06
4-(Dodecan-6-yl)benzenesulfonic acid	-2.59	-2.43	0.16	-2.64	0.05	-2.34	0.25
4-(Tridecan-2-yl)benzenesulfonic acid	-3.21	-3.09	0.12	-3.03	0.18	-3.12	0.09
4-(Pentadecan-2-yl)benzenesulfonic acid	-3.58	-3.72	0.14	-3.60	0.02	-3.65	0.07
Octadecyl hydrogen sulfate	-3.79	-3.80	0.01	-3.72	0.07	-3.43	0.36
Tetradecan-3-yl hydrogen sulfate	-2.37	-2.33	0.04	-2.34	0.03	-2.58	0.21
Tetradecan-4-yl hydrogen sulfate	-2.29	-2.31	0.02	-2.28	0.01	-2.32	0.03
Tetradecan-5-yl hydrogen sulfate	-2.17	-2.19	0.02	-2.23	0.06	-2.23	0.06
Tetradecan-7-yl hydrogen sulfate	-2.01	-1.90	0.11	-2.19	0.18	-2.00 <sup>a</sup>	0.01
Pentadecan-3-yl hydrogen sulfate	-2.66	-2.64	0.02	-2.66	0	-2.91	0.25
Hexadecan-8-yl hydrogen sulfate	-2.37	-2.56	0.19	-2.75	0.38	-2.56	0.19
Octadecan-4-yl hydrogen sulfate	-3.35	-3.61	0.26	-3.46	0.11	-3.61 <sup>a</sup>	0.26
Octadecan-6-yl hydrogen sulfate	-3.14	-3.52	0.38	-3.37	0.23	-3.48	0.34

Nonadecan-10-yl hydrogen sulfate	-3.03	-3.59	0.56	-3.21	0.18	-3.28	0.25
Nonadecan-5-yl hydrogen sulfate	-3.48	-3.90	0.42	-3.70	0.22	-3.87	0.39
Pentadecane-1-sulfonic acid	-3.14	-2.87	0.27	-3.05	0.09	-2.91	0.23
Heptadecane-1-sulfonic acid	-3.63	-3.47	0.16	-3.65	0.02	-3.41	0.22
Pentadecane-8-sulfonic acid	-2.25	-2.56	0.31	-2.03	0.22	-2.38	0.13
4-(Dodecan-2-yl)benzenesulfonic acid	-2.64	-2.78	0.14	-2.61	0.03	-2.87	0.23
4-(Dodecan-4-yl)benzenesulfonic acid	-2.72	-2.74	0.02	-2.63	0.09	-2.59	0.13
Undecyl hydrogen sulfate	-1.79	-1.78	0.01	-1.66	0.13	-1.73	0.06
2-(Dodecyloxy)ethyl hydrogen sulfate	-2.39	-2.27	0.12	-2.25	0.14	-2.44	0.05
3-Methoxydodecane-1-sulfonic acid	-2.12	-1.99	0.13	-2.05	0.07	-1.99	0.13
3-Ethoxydodecane-1-sulfonic acid	-2.30	-2.12	0.18	-2.21	0.09	-2.18	0.12
3-Propoxydodecane-1-sulfonic acid	-2.42	-2.36	0.06	-2.44	0.02	-2.41	0.01
3-Isopropoxydodecane-1-sulfonic acid	-2.46	-2.21	0.25	-2.32	0.14	-2.41 <sup>a</sup>	0.05
3-Butoxydodecane-1-sulfonic acid	-2.82	-2.55	0.27	-2.65	0.17	-2.67	0.15
3-(Hexyloxy)dodecane-1-sulfonic acid	-3.19	-2.80	0.39	-3.23	0.04	-3.00	0.19
3-(Octyloxy)dodecane-1-sulfonic acid	-3.92	-3.01	0.91	-3.80	0.12	-3.35	0.57
3-(2-Ethylhexyloxy)dodecane-1-sulfonic acid	-3.50	-3.24	0.26	-3.55	0.05	-3.70	0.20
3-Phenoxydodecane-1-sulfonic acid	-2.71	-2.54	0.17	-2.64	0.07	-2.27	0.44
3-Oxododecane-1-sulfonic acid	-1.54	-1.82	0.28	-1.71	0.17	-1.60 <sup>a</sup>	0.06
3-Hydroxydodecane-1-sulfonic acid	-1.61	-1.77	0.16	-1.83	0.22	-1.80	0.19
3-Hydroxytetradecane-1-sulfonic acid	-2.20	-2.32	0.12	-2.42	0.22	-2.48	0.28
3-(2-Hydroxyethyl)tetradecane-1-sulfonic acid	-3.45	-2.75	0.7	-2.83	0.62	-2.81 <sup>a</sup>	0.64
3-(2-(2-Hydroxyethoxy)ethoxy)tetradecane-1-sulfo nic acid	-2.92	-2.54	0.38	-2.74	0.18	-2.83	0.09
3-Phenoxytetradecane-1-sulfonic acid	-3.64	-3.23	0.41	-3.25	0.39	-3.18	0.46
3-(2,4,6-Trichlorophenoxy)tetradecane-1-sulfonic acid	-4.79	-4.29	0.5	-3.04	1.75	-3.93	0.86
3-(Dimethylamino)tetradecane-1-sulfonic acid	-2.97	-2.71	0.26	-3.21	0.24	-3.02	0.05
3-(Propylamino)tetradecane-1-sulfonic acid	-3.20	-3.15	0.05	-3.39	0.19	-3.26 <sup>a</sup>	0.06

3-(Butylamino)tetradecane-1-sulfonic acid	-3.71	-3.40	0.31	-3.68	0.03	-3.47	0.24
3-(Morpholino)tetradecane-1-sulfonic acid	-3.11	-2.90	0.21	-3.02	0.09	-3.48 <sup>a</sup>	0.37
3-(Piperidino)tetradecane-1-sulfonic acid	-3.31	-3.60	0.29	-3.56	0.25	-3.76	0.45
3-Oxotetradecane-1-sulfonic acid	-2.17	-2.35	0.18	-2.28	0.11	-2.26	0.09
3-Hydroxyhexadecane-1-sulfonic acid	-2.84	-2.90	0.06	-3.00	0.16	-3.08	0.24
3-Methoxyhexadecane-1-sulfonic acid	-3.47	-3.17	0.3	-3.24	0.23	-3.27	0.20
3-Propoxyhexadecane-1-sulfonic acid	-4.09	-3.64	0.45	-3.62	0.47	-3.72	0.37
3-Butoxyhexadecane-1-sulfonic acid	-4.46	-3.90	0.56	-3.87	0.59	-3.92	0.54
3-Oxohexadecane-1-sulfonic acid	-2.74	-2.93	0.19	-2.86	0.12	-2.84	0.10
3-Hydroxyoctadecane-1-sulfonic acid	-3.42	-3.50	0.08	-3.59	0.17	-3.59	0.17
2-(Decyloxy)ethanesulfonic acid	-1.79	-1.65	0.14	-1.88	0.09	-2.04	0.25
1-Hydroxytetradecane-2-sulfonic acid	-1.79	-2.17	0.38	-2.12	0.33	-2.37	0.58
1-Hydroxyhexadecane-2-sulfonic acid	-2.43	-2.77	0.34	-2.71	0.28	-2.97	0.54
2-(Hexyloxy)-2-oxoethanesulfonic acid	-0.74	-0.69	0.05	-0.64	0.1	-0.68	0.06
2-(Octyloxy)-2-oxoethanesulfonic acid	-1.14	-1.14	0	-1.18	0.04	-1.33	0.19
2-(Decyloxy)-2-oxoethanesulfonic acid	-1.62	-1.64	0.02	-1.74	0.12	-1.99	0.37
3-Oxo-3-(tetradecyloxy)propane-1-sulfonic acid	-3.05	-3.01	0.04	-3.04	0.01	-3.06	0.01
1-Methoxy-1-oxotridecane-2-sulfonic acid	-1.99	-2.02	0.03	-2.20	0.21	-1.93	0.06
1-Methoxy-1-oxopentadecane-2-sulfonic acid	-2.58	-2.63	0.05	-2.78	0.2	-2.59	0.01
1-Methoxy-1-oxoheptadecane-2-sulfonic acid	-3.40	-3.25	0.15	-3.37	0.03	-3.17	0.23
1-Ethoxy-1-oxoheptadecane-2-sulfonic acid	-3.51	-3.45	0.06	-3.44	0.07	-3.46	0.05
1-Oxo-1-propoxyheptadecane-2-sulfonic acid	-3.97	-3.71	0.26	-3.61	0.36	-3.69 <sup>a</sup>	0.28
1-Methoxy-1-oxonadecane-2-sulfonic acid	-4.00	-3.87	0.13	-3.97	0.03	-3.63	0.37
1-Ethoxy-1-oxonadecane-2-sulfonic acid	-4.11	-4.10	0.01	-4.03	0.08	-3.92	0.19
1-Oxo-1-propoxynonadecane-2-sulfonic acid	-4.90	-4.37	0.53	-4.20	0.7	-4.14	0.76
1-Isopropoxy-1-oxonadecane-2-sulfonic acid	-4.57	-4.29	0.28	-4.23	0.34	-4.32 <sup>a</sup>	0.25
1,4-Bis(2-ethylhexyloxy)-1,4-dioxobutane-2-sulfonic acid	-2.57	-2.49	0.08	-2.49	0.08	-2.99	0.42
1,4-Dibutoxy-1,4-dioxobutane-2-sulfonic acid	-0.66	-0.88	0.22	-0.87	0.21	-0.81	0.15

1,4-Dioxo-1,4-bis(pentyloxy)butane-2-sulfonic acid	-1.24	-1.30	0.06	-1.33	0.09	-1.31	0.07
1,4-Bis(hexyloxy)-1,4-dioxobutane-2-sulfonic acid	-1.82	-1.77	0.05	-1.82	0	-1.78	0.04
1,4-Bis(octyloxy)-1,4-dioxobutane-2-sulfonic acid	-3.13	-2.96	0.17	-2.87	0.26	-2.65	0.48
Tetradecan-2-yl hydrogen sulfate	-2.48	-2.38	0.1	-2.48	0	-2.64	0.16
Pentadecan-2-yl hydrogen sulfate	-2.77	-2.69	0.08	-2.78	0.01	-2.94	0.17
Pentadecan-5-yl hydrogen sulfate	-2.47	-2.59	0.12	-2.52	0.05	-2.59	0.12
Pentadecan-8-yl hydrogen sulfate	-2.18	-2.56	0.38	-2.16	0.02	-2.26	0.08
Heptadecan-2-yl hydrogen sulfate	-3.31	-3.31	0	-3.38	0.07	-3.47	0.16
Heptadecan-9-yl hydrogen sulfate	-2.63	-3.22	0.59	-2.68	0.05	-2.80	0.17
Octanoic acid	-0.43	-0.11	0.32	-0.21	0.22	-0.64	0.21
Octan-2-yl hydrogen sulfate	-0.74	-0.66	0.08	-0.76	0.02	-0.54	0.20
Decan-2-yl hydrogen sulfate	-1.31	-1.22	0.09	-1.32	0.01	-1.26	0.05
Undecan-3-yl hydrogen sulfate	-1.54	-1.34	0.2	-1.50	0.04	-1.48	0.06
Undecan-6-yl hydrogen sulfate	-1.08	-1.28	0.2	-1.16	0.08	-1.08	0.00
Tridecan-2-yl hydrogen sulfate	-2.19	-2.09	0.1	-2.19	0	-2.28 <sup>a</sup>	0.09
Tridecan-7-yl hydrogen sulfate	-1.71	-1.90	0.19	-1.65	0.06	-1.67 <sup>a</sup>	0.04
Dodecane-2-sulfonic acid	-1.83	-1.81	0.02	-1.71	0.12	-1.95	0.12
Heptadecan-2-yl hydrogen sulfate	-3.31	-3.31	0	-3.39	0.08	-3.47	0.16
Octadecan-2-yl hydrogen sulfate	-3.59	-3.62	0.03	-3.68	0.09	-3.71	0.12
Nonacosan-15-yl hydrogen sulfate	-4.10	-7.01	2.91	-5.93	1.83	-4.66	0.56
Hexyl hydrogen sulfate	-0.36	-0.64	0.28	-0.25	0.11	-0.54	0.18
Heptyl hydrogen sulfate	-0.65	-0.84	0.19	-0.51	0.14	-0.44 <sup>a</sup>	0.21
Nonyl hydrogen sulfate	-1.21	-1.28	0.07	-1.07	0.14	-1.20 <sup>a</sup>	0.01
4-Decylbenzenesulfonic acid	-2.51	-2.30	0.21	-2.34	0.17	-2.24	0.27
4-Dodecylbenzenesulfonic acid	-2.92	-2.90	0.02	-2.97	0.05	-2.84	0.08
4-(Undecan-3-yl)benzenesulfonic acid	-2.50	-2.46	0.04	-2.42	0.08	-2.42	0.08
4-(Undecan-4-yl)benzenesulfonic acid	-2.40	-2.41	0.01	-2.37	0.03	-2.29	0.11
4-(Undecan-5-yl)benzenesulfonic acid	-2.30	-2.31	0.01	-2.36	0.06	-2.21	0.09
4-(Undecan-6-yl)benzenesulfonic acid	-2.25	-2.05	0.2	-2.13	0.12	-2.15	0.10

4-(Dodecan-5-yl)benzenesulfonic acid	-2.57	-2.66	0.09	-2.65	0.08	-2.52	0.05
4-(Tridecan-3-yl)benzenesulfonic acid	-3.00	-3.08	0.08	-2.99	0.01	-2.94 <sup>a</sup>	0.06
4-(Tridecan-4-yl)benzenesulfonic acid	-2.90	-3.06	0.16	-2.96	0.06	-2.95	0.05
4-(Tridecan-5-yl)benzenesulfonic acid	-2.78	-3.01	0.23	-2.94	0.16	-2.84	0.06
4-(Tridecan-6-yl)benzenesulfonic acid	-2.70	-2.82	0.12	-2.93	0.23	-2.70	0.00
4-(Tridecan-7-yl)benzenesulfonic acid	-2.60	-2.47	0.13	-2.67	0.07	-2.58	0.02
4-(Tetradecan-2-yl)benzenesulfonic acid	-3.39	-3.41	0.02	-3.33	0.06	-3.47	0.08
4-(Tetradecan-3-yl)benzenesulfonic acid	-3.28	-3.40	0.12	-3.25	0.03	-3.37	0.09
4-(Tetradecan-4-yl)benzenesulfonic acid	-3.15	-3.39	0.24	-3.26	0.11	-3.26	0.11
4-(Tetradecan-5-yl)benzenesulfonic acid	-3.05	-3.36	0.31	-3.24	0.19	-3.15	0.10
4-(Tetradecan-6-yl)benzenesulfonic acid	-2.90	-3.21	0.31	-3.23	0.33	-2.99	0.09
4-(Tetradecan-7-yl)benzenesulfonic acid	-2.80	-2.93	0.13	-3.22	0.42	-2.83	0.03
2-(2-(Decyloxy)ethoxy)ethyl hydrogen sulfate	-1.93	-1.92	0.01	-1.91	0.02	-2.36	0.43
3,6,9,12-Tetraoxatetracosyl hydrogen sulfate	-2.79	-2.98	0.19	-2.97	0.18	-2.91	0.12
2-(Tetradecyloxy)ethyl hydrogen sulfate	-2.87	-2.85	0.02	-2.85	0.02	-2.92 <sup>a</sup>	0.05
2-(2-(Tetradecyloxy)ethoxy)ethyl hydrogen sulfate	-3.09	-3.09	0	-3.10	0.01	-3.11	0.02
3,6,9,12-Tetraoxahexacosyl hydrogen sulfate	-3.18	-3.59	0.41	-3.57	0.39	-3.04	0.14
2-(2-(Hexadecyloxy)ethoxy)ethyl hydrogen sulfate	-3.64	-3.70	0.06	-3.71	0.07	-3.38 <sup>a</sup>	0.26
3-(Octyloxy)-3-oxopropane-1-sulfonic acid	-1.31	-1.38	0.07	-1.28	0.03	-1.39	0.08
3-(Decyloxy)-3-oxopropane-1-sulfonic acid	-1.89	-1.89	0	-1.87	0.02	-2.01 <sup>a</sup>	0.12
3-(Dodecyloxy)-3-oxopropane-1-sulfonic acid	-2.52	-2.44	0.08	-2.45	0.07	-2.59 <sup>a</sup>	0.07
7,7,8,8,9,9,10,10,10-Nonafluorodecan-4-yl hydrogen sulfate	-1.70	-1.65	0.05	-1.68	0.02	-1.82	0.12
7,7,8,8,9,9,10,10,11,11,12,12,12-Tridecafluorodode can-4-yl hydrogen sulfate	-2.50	-2.46	0.04	-2.64	0.14	-2.64	0.14
7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-Hepta decafluorotetradecan-4-yl hydrogen sulfate	-3.42	-3.28	0.14	-3.69	0.27	-3.30	0.12
9,9,10,10,11,11,12,12,12-Nonafluorododecan-6-yl hydrogen sulfate	-2.14	-2.14	0	-1.95	0.19	-2.25	0.11

9,9,10,10,11,11,12,12,13,13,14,14,14-Tridecafluoro tetradecan-6-yl hydrogen sulfate	-3.02	-3.04	0.02	-2.89	0.13	-3.06	0.04
9,9,10,10,11,11,12,12,13,13,14,14,15,15,16,16,16- Heptadecafluorohexadecan-6-yl hydrogen sulfate	-3.90	-3.90	0	-3.89	0.01	-3.67	0.23
1,1,1,2,2,3,3,4,4-Nonafluorotetradecan-7-yl hydrogen sulfate	-2.49	-2.68	0.19	-2.35	0.14	-2.66	0.17
11,11,12,12,13,13,14,14,15,15,16,16,16-Tridecafluoro orohehexadecan-8-yl hydrogen sulfate	-3.40	-3.59	0.19	-3.25	0.15	-3.41	0.01
11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,18,1 8-Heptadecafluorooctadecan-8-yl hydrogen sulfate	-4.25	-4.48	0.23	-4.23	0.02	-4.01	0.24
(5-(Heptylamino)-3,4-dihydroxy-6-methoxytetrahy dro-2H-pyran-2-yl)methyl hydrogen sulfate	-1.60	-1.64	0.04	-1.63	0.03	-2.42	0.82
(3,4-Dihydroxy-6-methoxy-5-(undecylamino)tetrahy dro-2H-pyran-2-yl)methyl hydrogen sulfate	-2.77	-2.76	0.01	-2.76	0.01	-3.39 <sup>a</sup>	0.62
(3,4-Dihydroxy-6-methoxy-5-(pentadecylamino)tetrahy dro-2H-pyran-2-yl)methyl hydrogen sulfate	-3.92	-3.95	0.03	-3.93	0.01	-4.56	0.64
(S)-2-(3-Benzyl-4-oxo-4-(pentyloxy)butanoyl)benzoic sulfonic acid	-1.82	-1.84	0.02	-2.12	0.3	-2.50	0.68
(S)-2-(3-Benzyl-4-(octyloxy)-4-oxobutanoyl)benzoic sulfonic acid	-2.82	-2.76	0.06	-2.91	0.09	-3.04	0.22
(S)-2-(3-Benzyl-4-(decyloxy)-4-oxobutanoyl)benzoic sulfonic acid	-3.45	-3.48	0.03	-3.48	0.03	-3.56	0.11
(S)-2-(3-Benzyl-4-(dodecyloxy)-4-oxobutanoyl)benzoic sulfonic acid	-4.16	-4.19	0.03	-4.06	0.1	-4.05	0.11
(S)-2-(3-Benzyl-4-oxo-4-(tetradecyloxy)butanoyl)benzoic sulfonic acid	-4.76	-4.90	0.14	-4.64	0.12	-4.61	0.15
(S)-2-(4-(Dodecyloxy)-3-methyl-4-oxobutanoyl)benzoic sulfonic acid	-3.35	-3.43	0.08	-3.33	0.02	-3.78	0.43

<sup>a</sup> Computed values for the testing set members

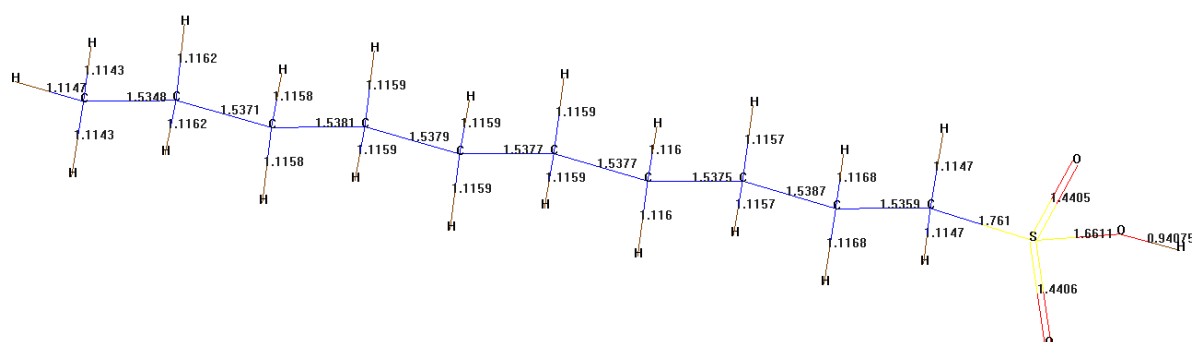


<sup>b</sup> AD: the absolute difference

### Appendix example

Prediction of  $\lg(\text{CMC})$  of Decane-1-sulfonic acid is exemplified as follows. For this compound, the total number of group  $N$  is 36, the number of non-hydrogen group  $N_0$  is 14, and molecular weight  $M$  is 222.347.

Firstly, the structure for the Decane-1-sulfonic acid is drawn and optimized by using the software of heperchem.7.0.



Secondly, the distant matrix  $Md$ , and the extended matrix  $Me$  is described as below.

$$Md = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 11 & 11 \\ 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 10 & 10 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 9 & 9 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 8 & 8 \\ 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 7 & 7 \\ 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 6 & 6 \\ 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 5 & 5 \\ 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 4 & 4 \\ 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 3 & 3 \\ 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 2 & 2 \\ 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 1 & 1 \\ 11 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 2 & 2 \\ 11 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 2 & 0 & 2 \\ 11 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 2 & 2 & 0 \end{bmatrix}$$

$$Me = \begin{bmatrix} \frac{2.55}{38.4} & \frac{2.55}{38.4} & \frac{2.55}{38.4} & \frac{2.55}{38.4} & \frac{2.55}{38.4} & \frac{2.55}{38.4} & \frac{2.55}{38.4} & \frac{2.55}{38.4} & \frac{2.55}{38.4} & \frac{2.55}{38.4} & \frac{2.58}{38.4} & \frac{3.44}{38.4} & \frac{3.44}{38.4} & \frac{3.44}{38.4} \\ 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 1.85 & 1.42 & 1.42 & 1.42 \\ 1.5348 & 1.5348 & 1.5371 & 1.5379 & 1.5377 & 1.5377 & 1.5375 & 1.5375 & 1.5359 & 1.5359 & 1.4405 & 1.6611 & 1.4405 & 1.4406 \\ 1 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 4 & 1 & 1 & 1 \\ 3 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 0 & 1 & 0 & 0 \end{bmatrix}$$

The norm values of the extended matrix are calculated in this work and shown as in Table S2.

Table S2 The *norm* values of extended matrix

extended matrix	<i>norm</i> ( <i>M</i> , 1)	<i>norm</i> ( <i>M</i> , 2)	<i>norm</i> ( <i>M</i> , <i>fro</i> )
$M_D$	95.60121	63.97285	75.2605
$M_A$	11.35769	13.21865	14.49631
$M_B$	11.60231	13.23459	14.63362
$M_C$	11.60231	13.18057	14.35768

Lastly, from parameters in Table 2, the lg(CMC) of the Decane-1-sulfonic acid is predicted by Eq. (1):

$$\begin{aligned} \lg(\text{CMC}) &= -0.0154 \times 95.6012 + 0.1448 \times 63.9729 - 0.0898 \times 75.2605 \\ &\quad + 3.1042 \times \tanh(95.6012 / 222.347) + 56.1018 \times \tanh(63.9729 / 222.347) \\ &\quad - 45.0189 \times \tanh(75.2605 / 222.347) + 0.4424 \times 11.35769 - 11.794 \times 13.21865 \\ &\quad - 0.9161 \times 14.49631 - 0.1067 \times 11.60231 + 26.4656 \times 13.2346 \\ &\quad - 3.0314 \times 14.63362 + 0.2030 \times 11.60231 - 16.1246 \times 13.18057 + 3.4070 \times 14.35768 \\ &\quad - 64.109 \times \exp(1/14) - 168.934 \times \exp(1/36) + 746.772 \times \exp(1/222.347) - 491.547 \\ &= -1.3959 \end{aligned}$$

The calculated lg(CMC) result is -1.3959 while the experimental lg(CMC) is -1.40.