

Naphthenic acids aggregation: the salinity role

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Table S1. RESP atomic charges calculated at B3LYP/6-31G(d) level of theory for the following naphthenic acids: c9, c10 aromatic, and c10

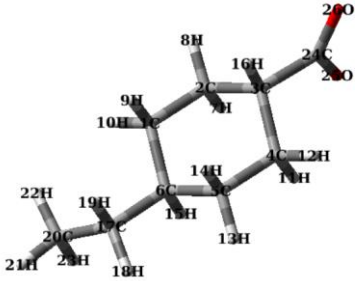
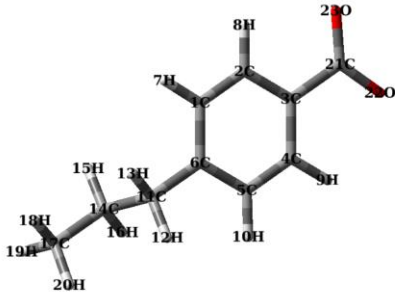
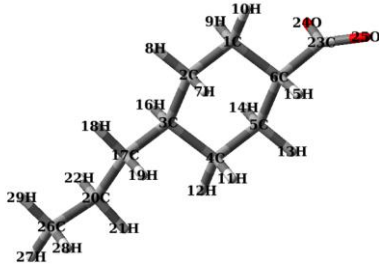
c9			c10 aromatic			c10		
								
Number	Atom	Charge	Number	Atom	Charge	Number	Atom	Charge
1	C	-0.167494	1	C	-0.251181	1	C	-0.001402
2	C	-0.028534	2	C	-0.160937	2	C	-0.162156
3	C	-0.006693	3	C	0.027371	3	C	0.197740
4	C	0.026446	4	C	-0.160941	4	C	-0.208623
5	C	-0.236659	5	C	-0.251168	5	C	-0.012830
6	C	0.231850	6	C	0.112259	6	C	-0.019509
7	H	0.014470	7	H	0.132425	7	H	0.037095
8	H	0.014080	8	H	0.135977	8	H	0.007755
9	H	0.038711	9	H	0.135974	9	H	0.011158
10	H	0.016052	10	H	0.132413	10	H	0.010938
11	H	0.004014	11	C	-0.250655	11	H	0.058774
12	H	0.007674	12	H	0.063027	12	H	0.021905
13	H	0.020276	13	H	0.063018	13	H	0.014693
14	H	0.043758	14	C	0.298821	14	H	0.015791
15	H	0.003880	15	H	-0.046560	15	H	-0.019779
16	H	-0.024756	16	H	-0.046556	16	H	0.019884
17	C	-0.048266	17	C	-0.283672	17	C	-0.315942
18	H	0.006807	18	H	0.053675	18	H	0.064195
19	H	0.008679	19	H	0.045982	19	H	0.062983
20	C	-0.210358	20	H	0.053671	20	C	0.249618
21	H	0.045190	21	C	0.772043	21	H	-0.024245
22	H	0.049637	22	O	-0.787482	22	H	-0.042026
23	H	0.039771	23	O	-0.787506	23	C	0.775160

Table S1. Continuation

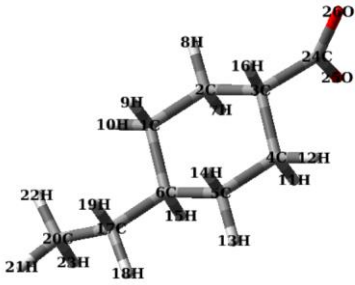
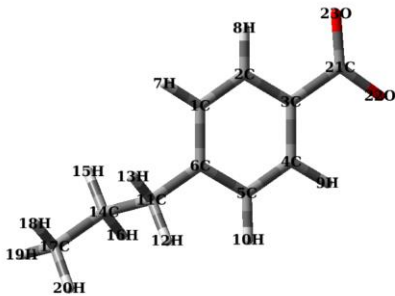
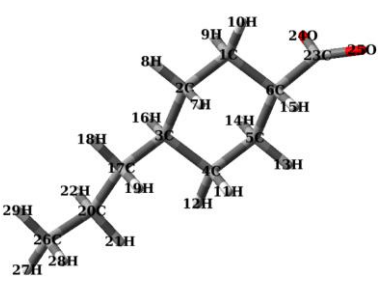
c9			c10 aromatic			c10		
								
Number	Atom	Charge	Number	Atom	Charge	Number	Atom	Charge
24	C	0.773794				24	O	-0.805845
25	O	-0.805989				25	O	-0.814994
26	O	-0.816340				26	C	-0.293774
						27	H	0.047526
						28	H	0.062770
						29	H	0.063139

Table S2. RESP atomic charges calculated at B3LYP/6-31G(d) level of theory for the following naphthenic acids: c11, c12, and c14

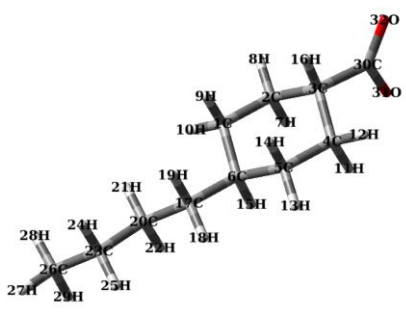
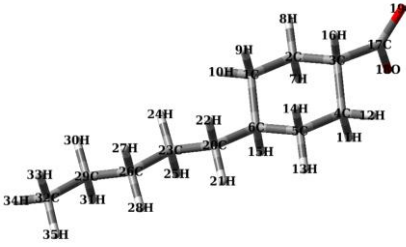
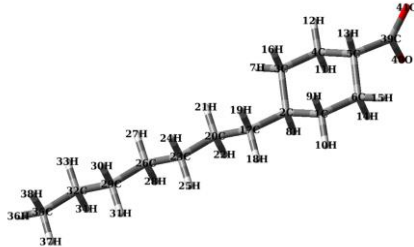
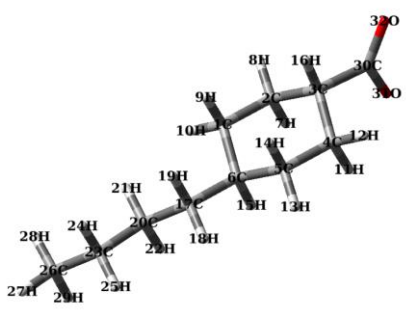
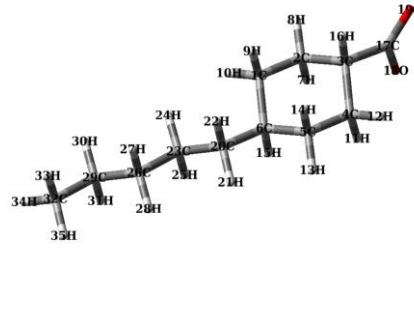
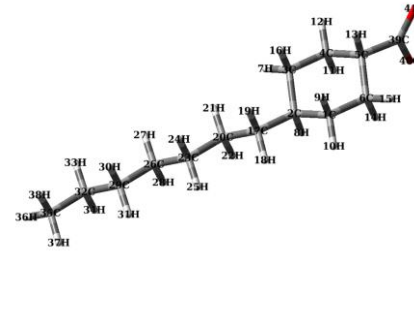
c11			c12			c14		
								
Number	Atom	Charge	Number	Atom	Charge	Number	Atom	Charge
1	C	-0.173376	1	C	-0.160171	1	C	-0.188281
2	C	-0.096153	2	C	-0.092753	2	C	0.388412
3	C	-0.010239	3	C	-0.009983	3	C	-0.208046
4	C	-0.052278	4	C	-0.032837	4	C	-0.064812
5	C	-0.176786	5	C	-0.164015	5	C	-0.009860
6	C	0.399296	6	C	0.315011	6	C	-0.004867
7	H	0.029798	7	H	0.029821	7	H	0.015642
8	H	0.037838	8	H	0.035438	8	H	-0.017991
9	H	0.045842	9	H	0.044460	9	H	0.035834
10	H	0.007865	10	H	0.009024	10	H	0.008794
11	H	0.019624	11	H	0.015114	11	H	0.021971
12	H	0.025131	12	H	0.018775	12	H	0.032498
13	H	0.008737	13	H	0.005420	13	H	-0.024698
14	H	0.035408	14	H	0.030914	14	H	0.006910
15	H	-0.025522	15	H	-0.010804	15	H	0.011561
16	H	-0.018562	16	H	-0.018834	16	H	0.055075
17	C	-0.465341	17	C	0.783065	17	C	-0.477864
18	H	0.075356	18	O	-0.804838	18	H	0.082314
19	H	0.072634	19	O	-0.816805	19	H	0.079556
20	C	0.154635	20	C	-0.323646	20	C	0.178768
21	H	-0.019003	21	H	0.051354	21	H	-0.021685
22	H	-0.030653	22	H	0.051602	22	H	-0.035042

Table S2. Continuation

c11			c12			c14		
								
Number	Atom	Charge	Number	Atom	Charge	Number	Atom	Charge
23	C	0.204863	23	C	0.101622	23	C	0.117354
24	H	-0.033065	24	H	-0.015480	24	H	-0.023614
25	H	-0.036055	25	H	-0.024728	25	H	-0.026453
26	C	-0.373734	26	C	-0.020835	26	C	-0.154355
27	H	0.076604	27	H	0.004461	27	H	0.012614
28	H	0.077091	28	H	0.003104	28	H	0.015285
29	H	0.076527	29	C	0.168439	29	C	0.050606
30	C	0.786244	30	H	-0.032621	30	H	-0.015032
31	O	-0.805046	31	H	-0.033290	31	H	-0.016624
32	O	-0.817673	32	C	-0.262481	32	C	0.229540
			33	H	0.051512	33	H	-0.040343
			34	H	0.054215	34	H	-0.039762
			35	H	0.050771	35	C	-0.347770
						36	H	0.074338
						37	H	0.071032
						38	H	0.071214
						39	C	0.776268
						40	O	-0.803477
						41	O	-0.815010