

Electronic supplementary information

Analysis of naphthenic acids in aqueous solution using HPLC- MS/MS[†]

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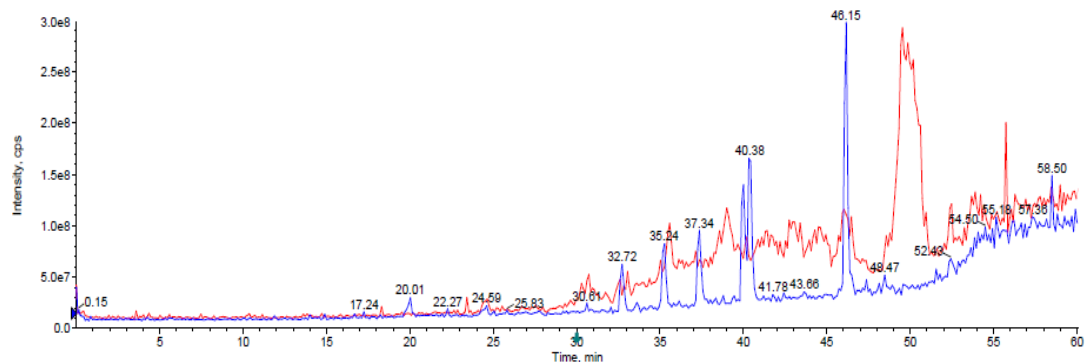


Figure S1– Model NA compounds (blue) and commercial NAs (red) eluted separately from Eclipse Plus C8 column detected by negative-ion-enhanced MS at 20°C

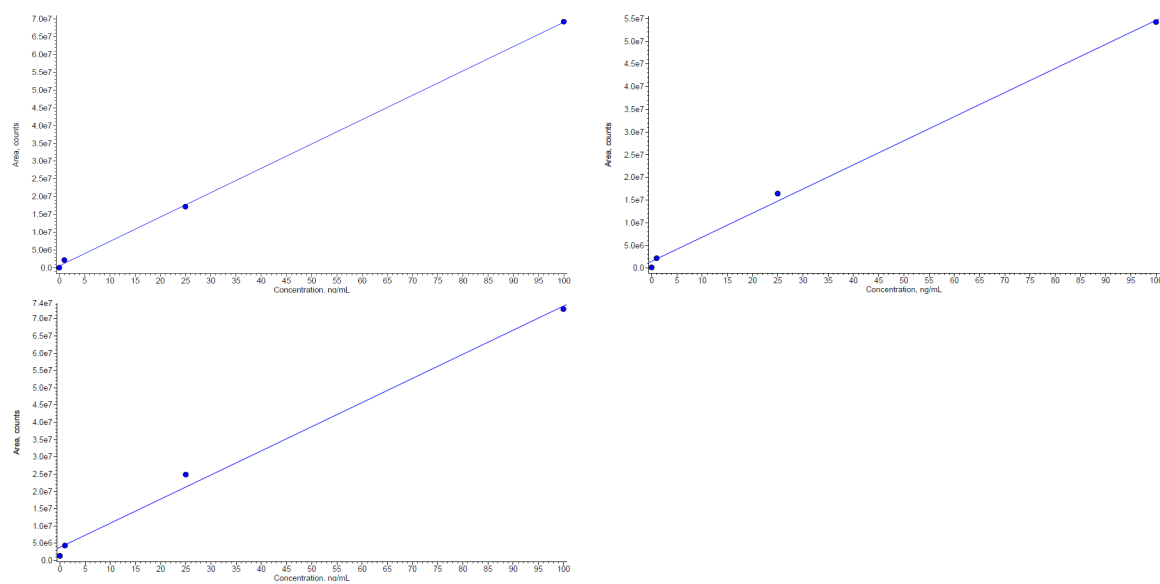


Figure S2 – Calibration curves for 4-tert-butylcyclohexane carboxylic acid (top left, $r = 0.9998$), trans-4-pentylcyclohexane carboxylic acid (top right, $r = 0.9988$) and lauric acid (bottom left, $r = 0.9970$)

Table S1 – Relationship between carbon number, $-Z$, and M_w for NAs

$-Z$ Carbon number	12	10	8	6	4	2	0
5							102.1
6			108	110	112	114.1	116.1
7	118	120	122	124	126.1	128.1	130.1
8	132	134	136	138.1	140.1	142.1	144.1
9	146	148	150.1	152.1	154.1	156.1	158.1
10	160	162.1	164.1	166.1	168.1	170.1	172.1
11	174.1	176.1	178.1	180.1	182.1	184.1	186.2
12	188.1	190.1	192.1	194.1	196.1	198.2	200.2
13	202.1	204.1	206.1	208.1	210.2	212.2	214.2
14	216.1	218.1	220.1	222.2	224.2	226.2	228.2
15	230.1	232.1	234.2	236.2	238.2	240.2	242.2
16	244.1	246.2	248.2	250.2	252.2	254.2	256.2
17	258.2	260.2	262.2	264.2	266.2	268.2	270.2
18	272.2	274.2	276.2	278.2	280.2	282.2	284.3
19	286.2	288.2	290.2	292.2	294.2	296.3	298.2
20	300.2	302.2	304.2	306.2	308.3	310.3	312.3
21	314.2	316.2	318.2	320.3	322.3	324.3	326.3
22	328.2	330.2	332.3	334.3	336.3	338.3	340.3
23	342.2	344.3	346.3	348.3	350.3	352.3	354.3
24	356.3	358.3	360.3	362.3	364.3	366.3	368.4
25	370.3	372.3	374.3	376.3	378.3	380.4	382.4