LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038154.D
Acq On : 21 Dec 2022 03:43
Operator : CG/JU
Sample : N6008-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBYB1

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Title : SVOA CALIBRATION

Signal : TIC: BM038154.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	33	36	39	rBV2	9642	10052	0.12%	0.017%
2	3.834	106	110	126	rBV	191918	357739	4.12%	0.611%
3	4.163	163	166	170	rVB3	10193	12739	0.15%	0.022%
4	7.022	647	652	654	rBV6	6520	9446	0.11%	0.016%
5	7.198	676	682	693	rBV	555218	869388	10.02%	1.484%
6	7.369	703	711	719	rBV	274374	429310	4.95%	0.733%
7	7.569	738	745	754	rBV	506430	771015	8.89%	1.316%
8	8.039	818	825	832	rBV	641804	997954	11.50%	1.703%
9	8.751	938	946	957	rBV	599833	930322	10.72%	1.588%
10	9.216	1017	1025	1034	rBV	470713	766120	8.83%	1.308%
11	9.369	1045	1051	1055	rVB8	6376	10687	0.12%	0.018%
12	9.604	1085	1091	1095	rVB8	6082	11796	0.14%	0.020%
13	9.939	1141	1148	1154	rBV	439628	722540	8.33%	1.233%
14	10.157	1180	1185	1187	rBV5	6303	8950	0.10%	0.015%
15	10.475	1232	1239	1253	rBV	885064	1397237	16.11%	2.385%
16	10.857	1297	1304	1312	rBV	943991	1531777	17.66%	2.615%
17	10.998	1320	1328	1342	rBV	520945	894378	10.31%	1.527%
18	11.633	1432	1436	1442	rBV7	6856	13997	0.16%	0.024%
19	12.433	1567	1572	1577	rBV3	11621	18229	0.21%	0.031%
20	13.480	1745	1750	1755	rVB6	7030	11261	0.13%	0.019%
21	13.551	1755	1762	1768	rBV5	16339	33087	0.38%	0.056%
22	13.986	1831	1836	1841	rBV7	10250	14958	0.17%	0.026%
23	14.080	1843	1852	1858	rBV	1586866	2103886	24.25%	3.591%
24	14.368	1893	1901	1910	rVV	1722222	2502951	28.85%	4.272%
25	14.545	1926	1931	1935	rVB5	7960	13517	0.16%	0.023%
26	14.668	1946	1952	1959	rVV	1463750	2059479	23.74%	3.515%
27	14.727	1959	1962	1966	rVV6	10715	16490	0.19%	0.028%
28	14.868	1979	1986	1999	rBV	690727	1036837	11.95%	1.770%
29	15.021	2008	2012	2016	rBV4	14213	22141	0.26%	0.038%
30	15.068	2016	2020	2027	rVV4	20966	32220	0.37%	0.055%
31	15.568	2101	2105	2109	rVB6	12279	12535	0.14%	0.021%
32	15.657	2113	2120	2132	rVB	2395307	3220547	37.12%	5.497%
33	15.774	2134	2140	2148	rBV	651698	848175	9.78%	1.448%
34	15.898	2154	2161	2166	rBV4	12130	23564	0.27%	0.040%
35	15.980	2169	2175	2178	rVV5	10207	16694	0.19%	0.028%
36	16.015	2178	2181	2187	rVB	41965	57395	0.66%	0.098%

LSC Area Percent Report

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Sample : N6008-04
Misc :
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Instrument :
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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Title : SVOA CALIBRATION

37	16.104	2193	2196	2202	rVB8	4410	9237	0.11%	0.016%
38	16.221	2212	2216	2222	rVB8	12175	16359	0.19%	0.028%
39	16.351	2231	2238	2246	rBV6	14969	31237	0.36%	0.053%
40	16.498	2259	2263	2268	rBV5	23403	36831	0.42%	0.063%
41	16.574	2273	2276	2283	rVB7	8754	13212	0.15%	0.023%
42	16.792	2308	2313	2318	rBV3	42333	68862	0.79%	0.118%
43	16.862	2320	2325	2328	rVV6	13076	22374	0.26%	0.038%
44	16.904	2328	2332	2339	rVB7	6233	13309	0.15%	0.023%
45	17.139	2369	2372	2375	rBV5	7952	11849	0.14%	0.020%
46	17.286	2393	2397	2403	rBV	67325	101405	1.17%	0.173%
47	17.351	2404	2408	2411	rVV2	43728	60744	0.70%	0.104%
48	17.409	2411	2418	2426	rVV	1887494	2731138	31.48%	4.662%
49	17.509	2426	2435	2441	rVV	2525455	3629417	41.84%	6.195%
50	17.562	2441	2444	2448	rVV5	29708	44767	0.52%	0.076%
51	17.604	2448	2451	2460	rVB5	34697	56182	0.65%	0.096%
52	17.751	2471	2476	2479	rBV2	63702	80456	0.93%	0.137%
53	17.915	2502	2504	2509	rVB5	11356	15333	0.18%	0.026%
54	18.021	2519	2522	2526	rBV6	16136	23440	0.27%	0.040%
55	18.056	2526	2528	2534	rVB6	15932	19203	0.22%	0.033%
56	18.168	2540	2547	2553	rBV3	63162	123021	1.42%	0.210%
57	18.227	2553	2557	2562	rVV2	81317	112072	1.29%	0.191%
58	18.286	2562	2567	2585	rVV	940889	1338056	15.42%	2.284%
59	18.586	2612	2618	2622	rBV4	39660	74436	0.86%	0.127%
60	18.633	2622	2626	2630	rVV7	17615	25014	0.29%	0.043%
61	18.703	2635	2638	2643	rBV5	15173	22945	0.26%	0.039%
62	18.950	2677	2680	2684	rBV6	11053	11931	0.14%	0.020%
63	19.209	2720	2724	2727	rVB6	12874	18406	0.21%	0.031%
64	19.292	2736	2738	2744	rVB2	22655	29859	0.34%	0.051%
65	19.356	2744	2749	2754	rBV2	41066	67142	0.77%	0.115%
66	19.409	2754	2758	2760	rBV	173195	221694	2.56%	0.378%
67	19.550	2778	2782	2796	rBV	271349	395739	4.56%	0.675%
68	19.792	2817	2823	2835	rBV	3195351	4245668	48.94%	7.247%
69	20.627	2962	2965	2971	rBV5	60914	94264	1.09%	0.161%
70	20.756	2984	2987	2991	rVB2	142510	147284	1.70%	0.251%
71	21.209	3061	3064	3067	rBV	114578	112900	1.30%	0.193%
72	21.262	3068	3073	3081	rBV2	737137	1039930	11.99%	1.775%
73	21.574	3121	3126	3131	rBV	1993839	2516315	29.01%	4.295%
74	22.197	3229	3232	3240	rVB2	189969	286778	3.31%	0.490%
75	23.233	3404	3408	3413	rBV	293311	428791	4.94%	0.732%
76	23.868	3509	3516	3527	rVB	1849930	3625181	41.79%	6.188%

LSC Area Percent Report

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Operator : CG/JU
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Title : SVOA CALIBRATION

77	24.027	3536	3543	3551	rVB	1109563	2150175	24.79%	3.670%
78	24.609	3637	3642	3650	rVB	382722	794085	9.15%	1.355%
79	24.709	3654	3659	3671	rVB2	317831	807577	9.31%	1.378%
80	27.509	4127	4135	4155	rVB4	687230	2446207	28.20%	4.175%
81	28.544	4299	4311	4327	rVB2	2421060	8675001	100.00%	14.807%

Sum of corrected areas: 58585239

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Sample : N6008-04
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Instrument :
BNA_M
ClientSampleId :
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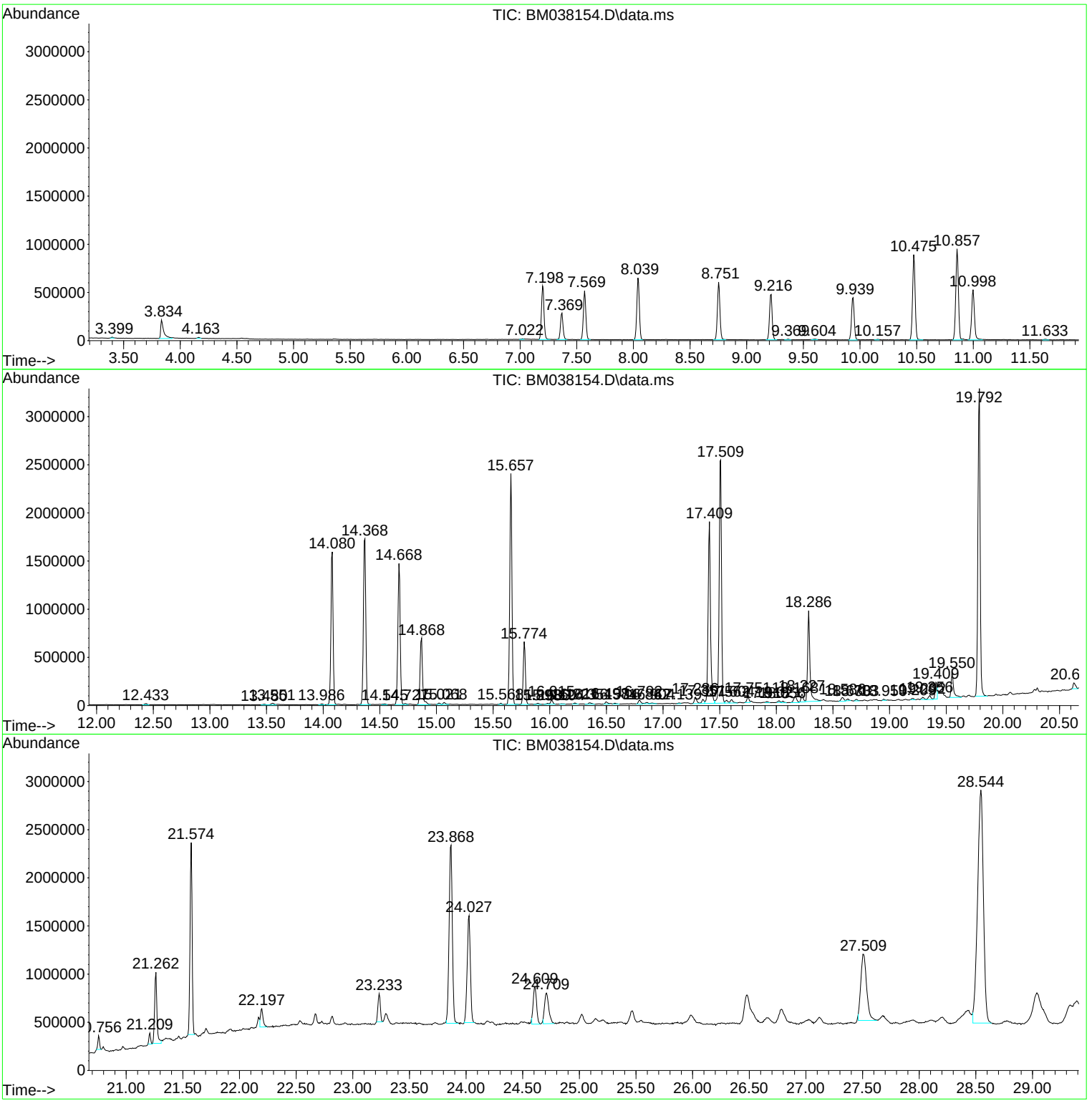
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038154.D
Acq On : 21 Dec 2022 03:43
Operator : CG/JU
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Instrument :
BNA_M
ClientSampleId :
DBYB1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

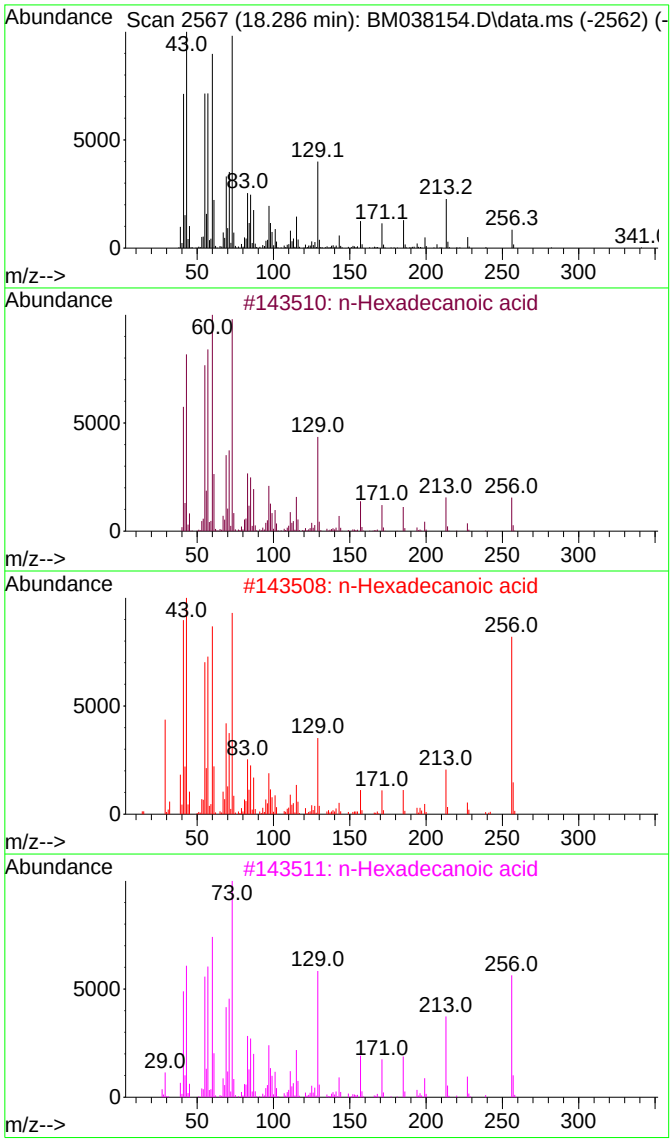
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

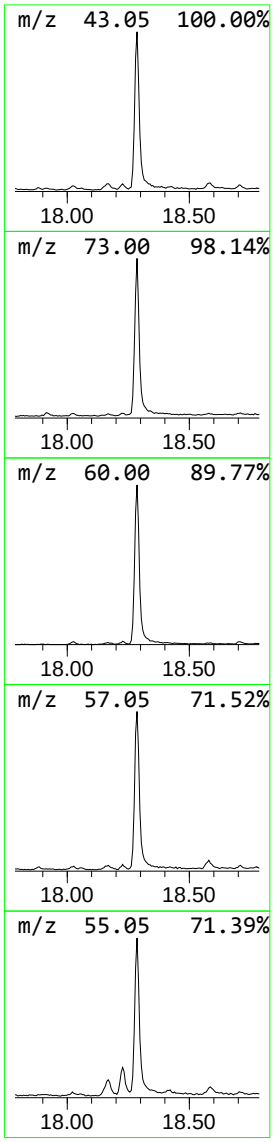
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	9.80 ng/ul	1338060	Phenanthrene-d10	17.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5	Tridecanoic acid	214	C13H26O2	000638-53-9	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038154.D
Acq On : 21 Dec 2022 03:43
Operator : CG/JU
Sample : N6008-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBYB1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

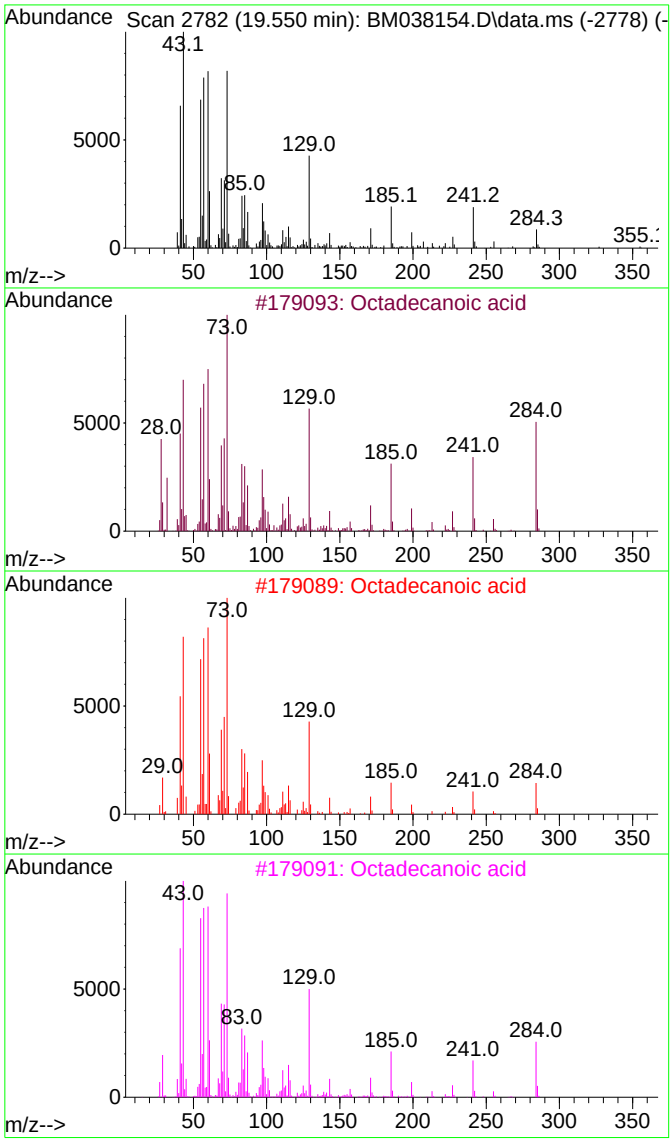
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

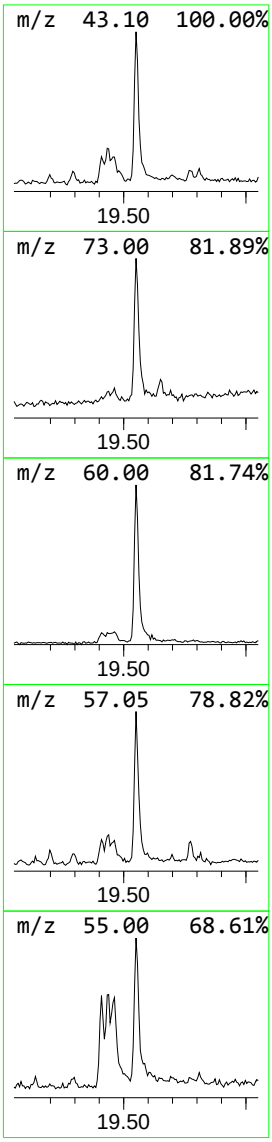
****

Peak Number 2 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	3.15 ng/ul	395739	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	92
3	Octadecanoic acid	284	C18H36O2	000057-11-4	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68





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BNA_M
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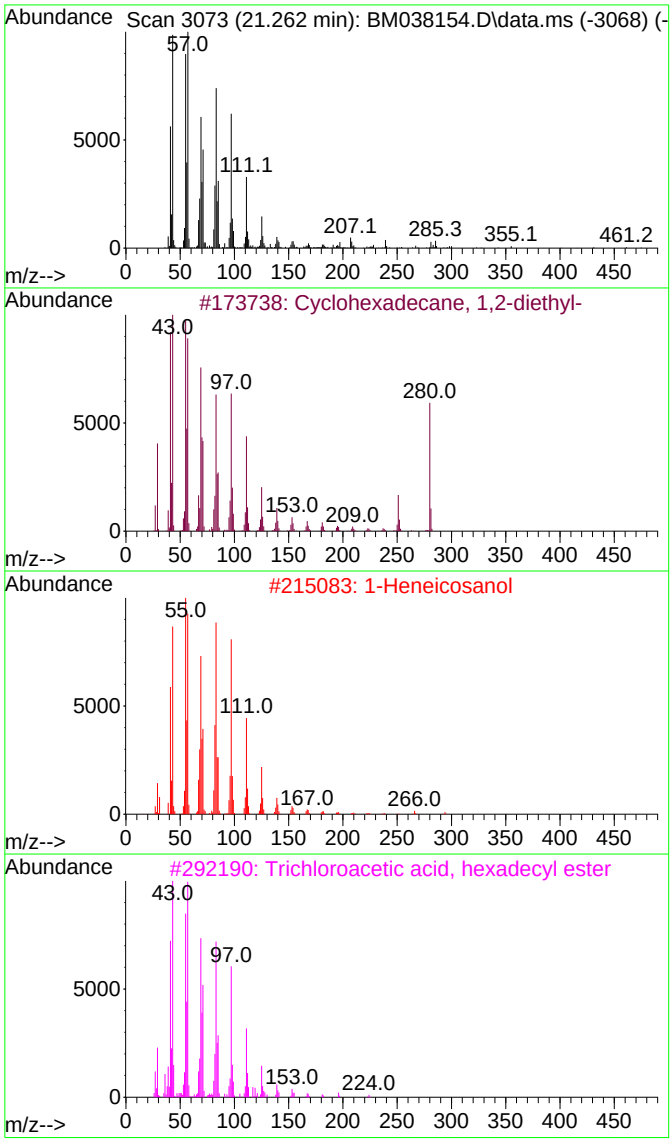
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

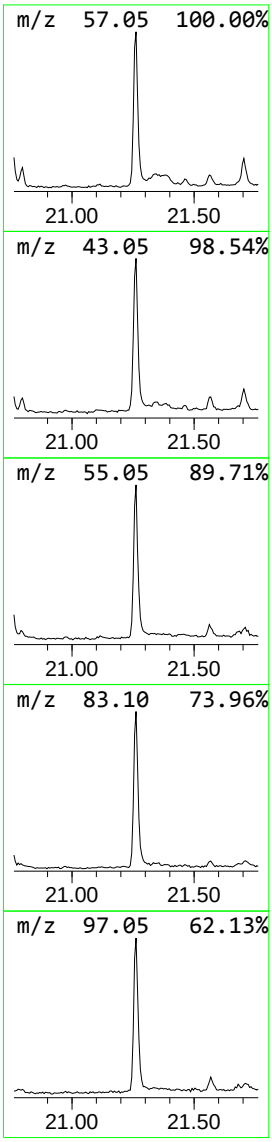
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Cyclic21.262 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.262	8.27 ng/ul	1039930	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	1-Hexacosene	364	C26H52	018835-33-1	91





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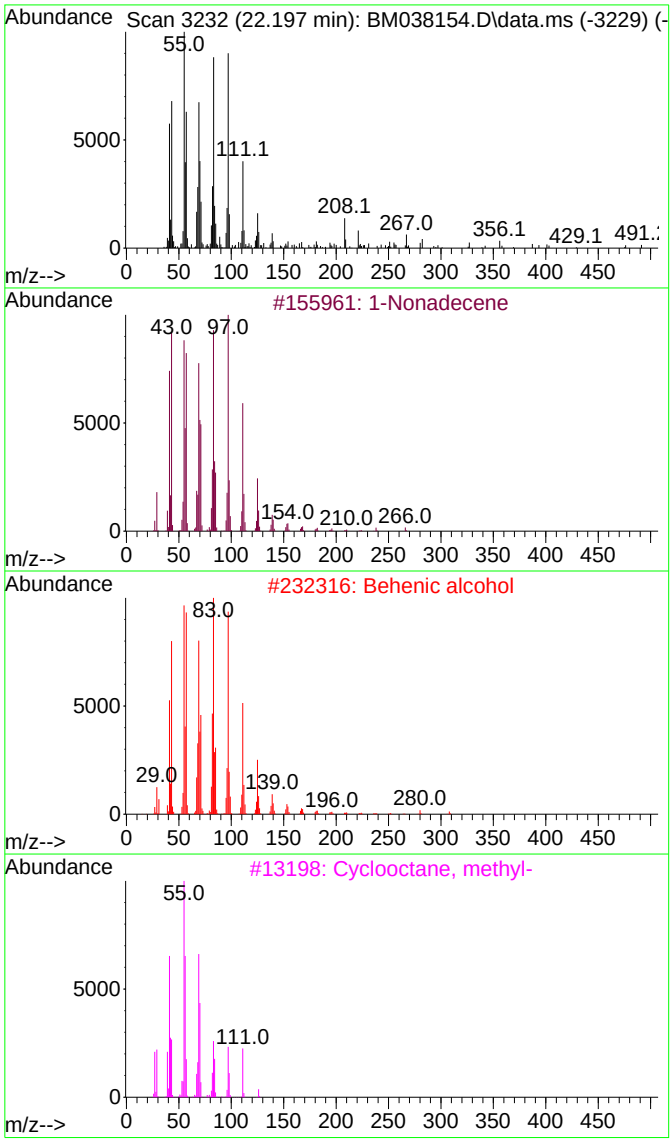
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

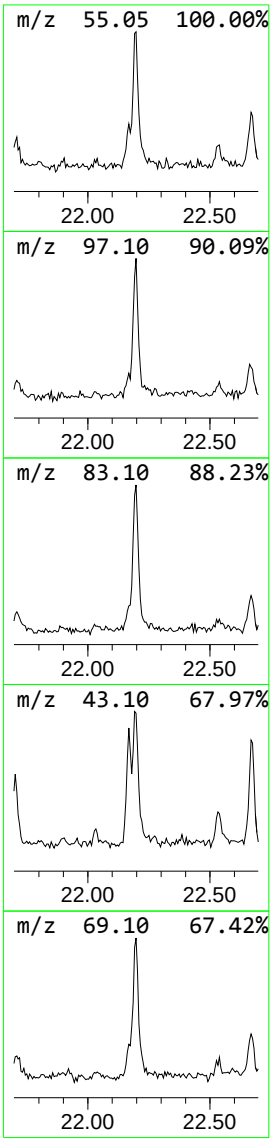
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.197	2.28 ng/ul	286778	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	87
2	Behenic alcohol	326	C22H46O	000661-19-8	62
3	Cyclooctane, methyl-	126	C9H18	001502-38-1	55
4	1-Hexadecanol	242	C16H34O	036653-82-4	53
5	trans-1,3-Diethylcyclopentane	126	C9H18	1000113-87-1	53





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Operator : CG/JU
Sample : N6008-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBYB1

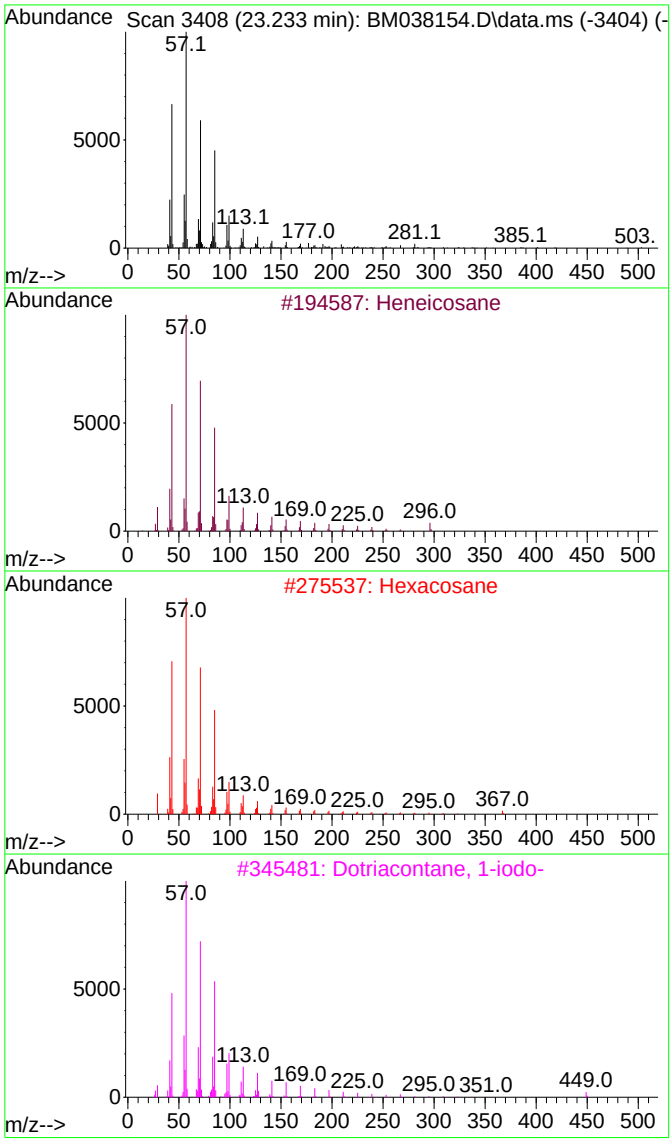
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

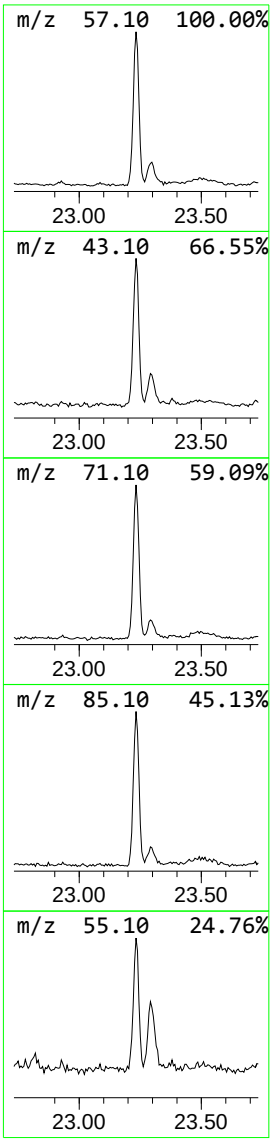
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.233	3.99 ng/ul	428791	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	92
2	Hexacosane	366	C26H54	000630-01-3	87
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5	Octadecane	254	C18H38	000593-45-3	83





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Data File : BM038154.D
Acq On : 21 Dec 2022 03:43
Operator : CG/JU
Sample : N6008-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBYB1

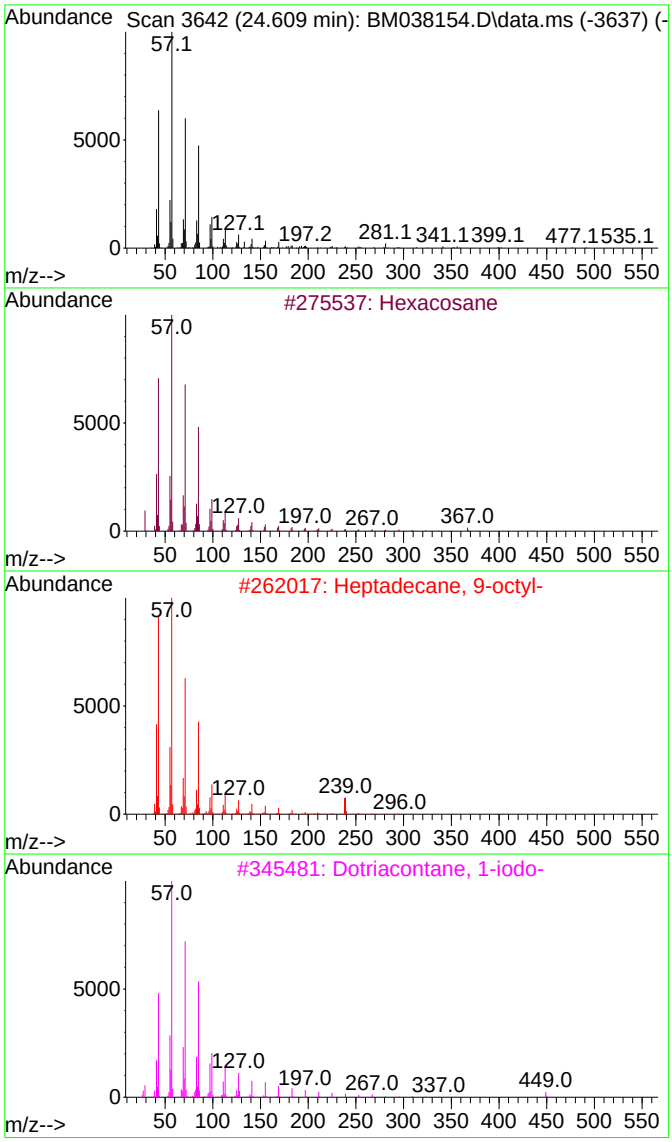
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

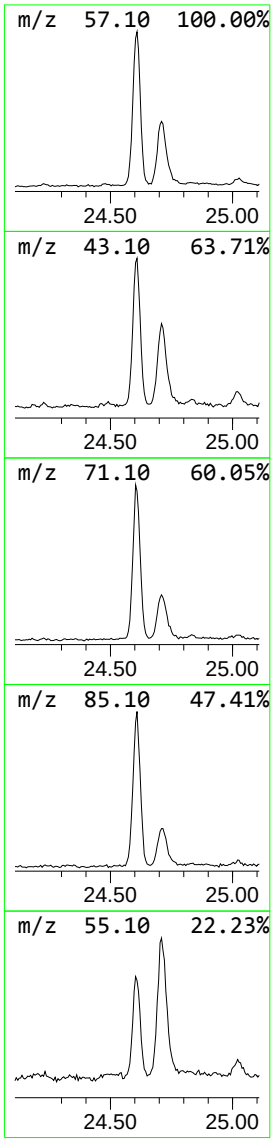
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.609	7.39 ng/ul	794085	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Heneicosane	296	C21H44	000629-94-7	87





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Data File : BM038154.D
Acq On : 21 Dec 2022 03:43
Operator : CG/JU
Sample : N6008-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBYB1

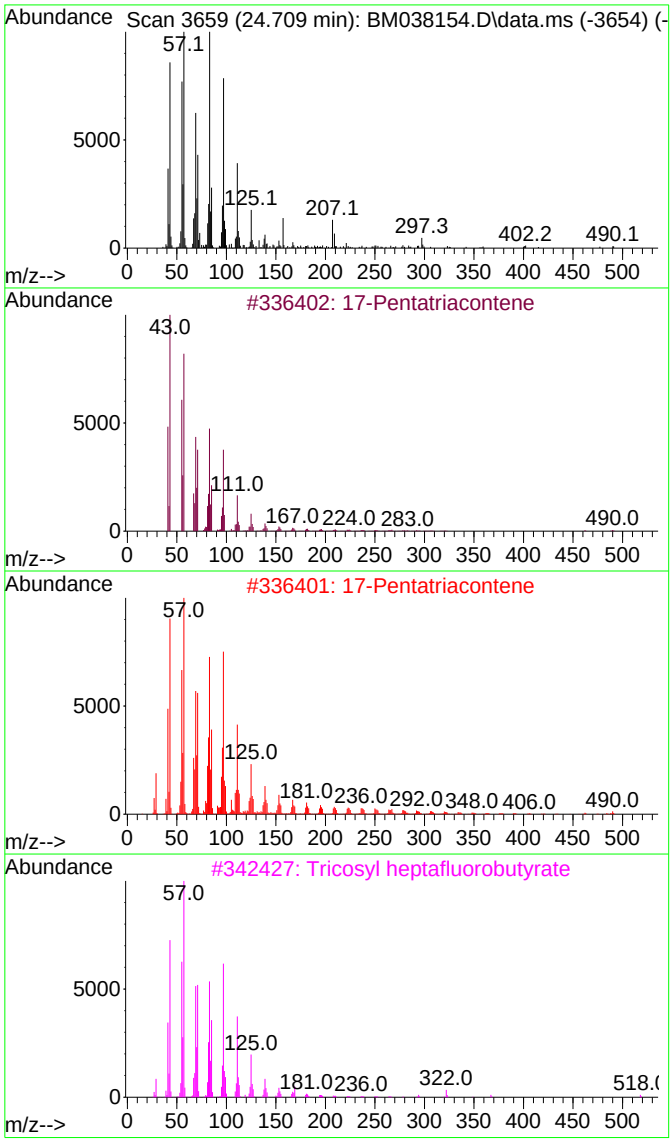
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

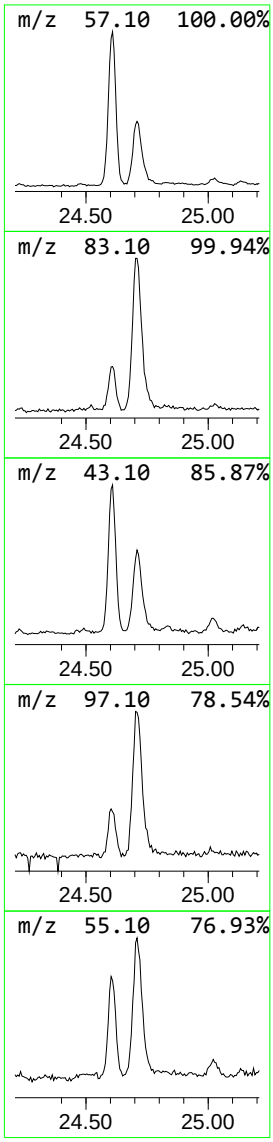
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.709	7.51 ng/ul	807577	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	86
2	17-Pentatriacontene	491	C35H70	006971-40-0	60
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	60
4	Cyclohexane, 1,1'-(2-propyl-1,3-...	250	C18H34	055030-21-2	58
5	Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	53





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Data File : BM038154.D
Acq On : 21 Dec 2022 03:43
Operator : CG/JU
Sample : N6008-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBYB1

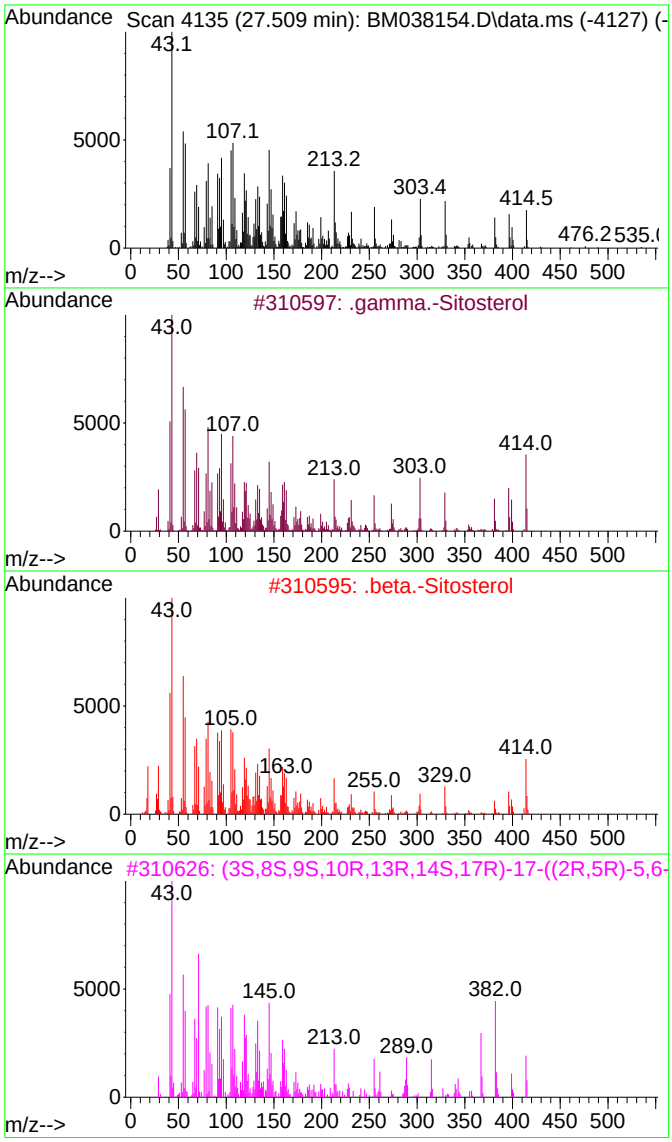
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

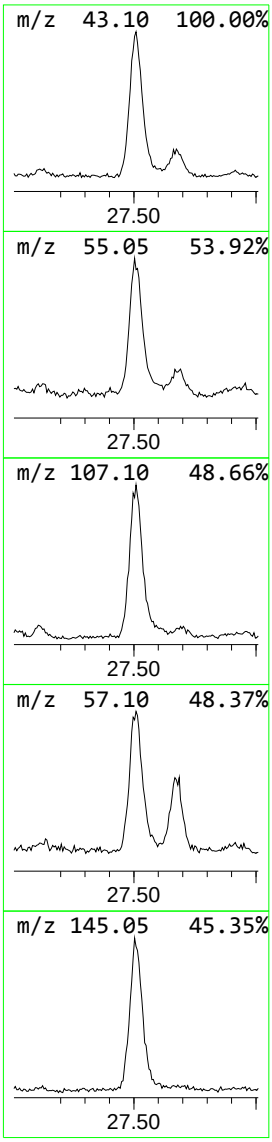
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.509	22.75 ng/ul	2446210	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	97
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	94
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	84
4	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	49
5	Campesterol	400	C28H48O	000474-62-4	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038154.D
Acq On : 21 Dec 2022 03:43
Operator : CG/JU
Sample : N6008-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBYB1

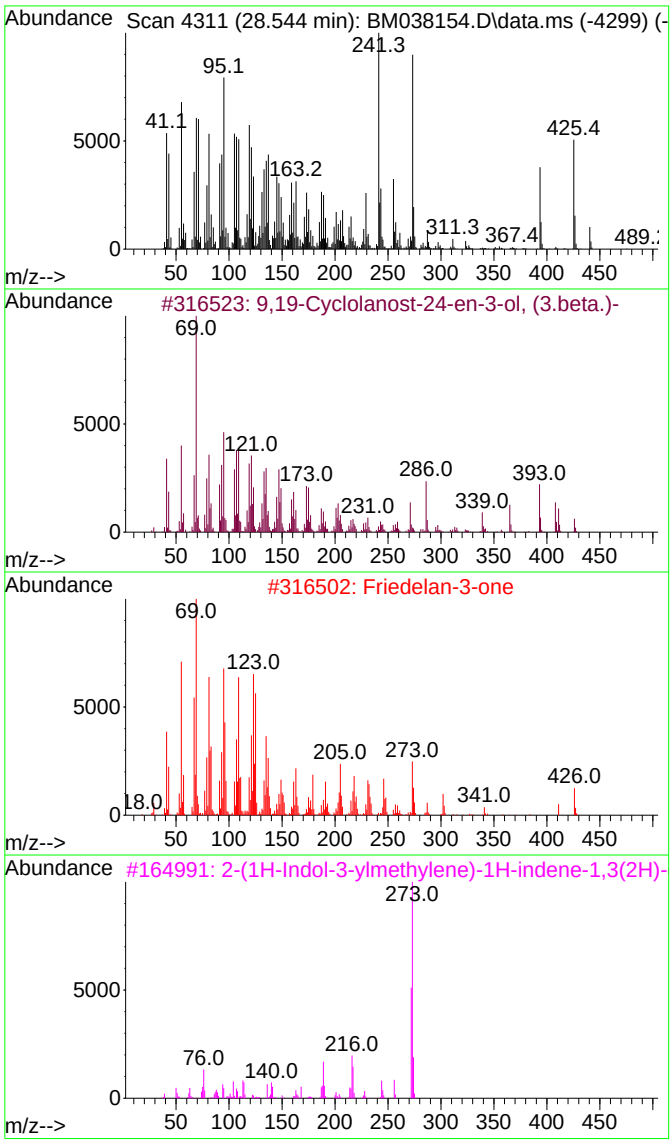
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

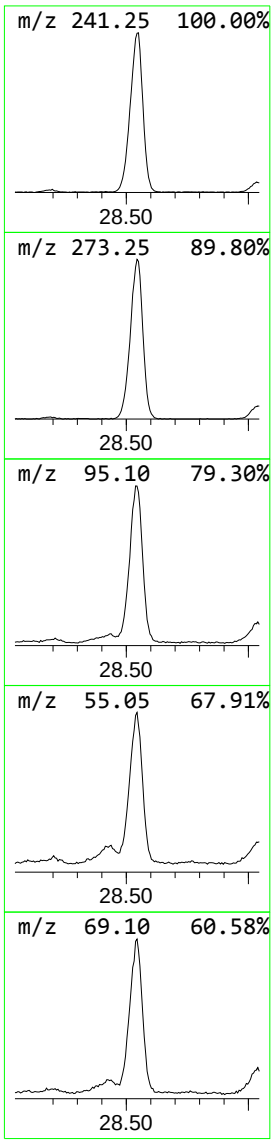
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 9,19-Cyclolanost-24-en-3-ol... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.544	80.69 ng/ul	8675000	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,19-Cyclolanost-24-en-3-ol, (3....	426	C30H50O	000469-38-5	51
2	Friedelan-3-one	426	C30H50O	000559-74-0	45
3	2-(1H-Indol-3-ylmethylene)-1H-in...	273	C18H11NO2	031060-64-7	25
4	Friedelan-3-one	426	C30H50O	000559-74-0	18
5	2-{[(4-Methyl-2-pyridinyl)amino]...	256	C13H16N4Si	1010494-07-4	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038154.D
Acq On : 21 Dec 2022 03:43
Operator : CG/JU
Sample : N6008-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBYB1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.286	9.8	ng/ul	1338060	4	17.409	2731140	20.0
Octadecanoic acid	19.551	3.1	ng/ul	395739	5	21.574	2516320	20.0
(DEL) Alkane: C...	21.262	8.3	ng/ul	1039930	5	21.574	2516320	20.0
(DEL) Alkane: S...	22.197	2.3	ng/ul	286778	5	21.574	2516320	20.0
(DEL) Alkane: S...	23.233	4.0	ng/ul	428791	6	24.027	2150180	20.0
(DEL) Alkane: S...	24.609	7.4	ng/ul	794085	6	24.027	2150180	20.0
(DEL) Alkane: S...	24.709	7.5	ng/ul	807577	6	24.027	2150180	20.0
.gamma.-Sitosterol	27.509	22.8	ng/ul	2446210	6	24.027	2150180	20.0
9,19-Cyclolanos...	28.544	80.7	ng/ul	8675000	6	24.027	2150180	20.0