LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101121\
Data File : BM032467.D
Acq On : 12 Oct 2021 20:46
Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

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-BM100521.M
Title : SVOA CALIBRATION

Signal : TIC: BM032467.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.955	17	20	34	rVB	60090	93791	1.17%	0.085%
2	3.260	69	72	76	rBV	11823	15227	0.19%	0.014%
3	3.390	91	94	108	rBV	272601	428135	5.32%	0.386%
4	3.643	131	137	146	rBV	31267	60318	0.75%	0.054%
5	3.737	148	153	163	rVB	46569	76345	0.95%	0.069%
6	3.831	165	169	177	rVB4	13906	23850	0.30%	0.021%
7	4.113	213	217	222	rBV5	8902	14638	0.18%	0.013%
8	4.701	312	317	322	rBV3	9100	14209	0.18%	0.013%
9	5.525	453	457	461	rBV	10485	16240	0.20%	0.015%
10	5.984	530	535	540	rBV	11503	16298	0.20%	0.015%
11	6.637	640	646	652	rBV	24529	40887	0.51%	0.037%
12	6.743	657	664	667	rBV7	5748	16255	0.20%	0.015%
13	6.801	667	674	684	rVB	270332	429790	5.34%	0.387%
14	6.937	690	697	709	rBV	806067	1251454	15.55%	1.128%
15	7.148	726	733	742	rBV	881796	1360987	16.91%	1.227%
16	7.607	804	811	820	rBV	847726	1317501	16.37%	1.187%
17	7.690	820	825	835	rVB	25899	43499	0.54%	0.039%
18	8.337	926	935	944	rBV	810961	1259701	15.65%	1.135%
19	8.713	991	999	1001	rBV	21124	32720	0.41%	0.029%
20	8.760	1001	1007	1022	rVB	1004556	1602234	19.91%	1.444%
21	8.931	1034	1036	1043	rVB7	9136	13894	0.17%	0.013%
22	9.236	1083	1088	1094	rVB3	10435	18982	0.24%	0.017%
23	9.484	1121	1130	1145	rBV	854814	1385338	17.21%	1.249%
24	9.760	1169	1177	1188	rBV	154479	286316	3.56%	0.258%
25	10.031	1215	1223	1238	rBV	1305700	2145329	26.66%	1.934%
26	10.178	1242	1248	1260	rVB	337865	529584	6.58%	0.477%
27	10.395	1278	1285	1293	rBV	1257178	2068005	25.70%	1.864%
28	10.531	1301	1308	1329	rBV	1132365	1930993	23.99%	1.740%
29	10.878	1361	1367	1374	rBV	262772	412534	5.13%	0.372%
30	11.201	1417	1422	1428	rBV2	19387	30033	0.37%	0.027%
31	11.695	1499	1506	1516	rBV2	164647	299087	3.72%	0.270%
32	11.989	1550	1556	1563	rBV	25528	43797	0.54%	0.039%
33	12.554	1643	1652	1657	rBV	233780	377913	4.70%	0.341%
34	12.607	1659	1661	1672	rVB	16778	30290	0.38%	0.027%
35	12.860	1698	1704	1711	rVB	20287	29260	0.36%	0.026%
36	13.101	1740	1745	1749	rBV	11127	16014	0.20%	0.014%

LSC Area Percent Report

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Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

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-BM100521.M
Title : SVOA CALIBRATION

37	13.160	1750	1755	1761	rVV2	35811	59800	0.74%	0.054%
38	13.224	1761	1766	1771	rVB6	7541	14123	0.18%	0.013%
39	13.660	1833	1840	1848	rBV	2985554	4017415	49.92%	3.621%
40	13.724	1848	1851	1855	rVB2	25041	34890	0.43%	0.031%
41	13.948	1878	1889	1900	rBV	3065532	4455391	55.36%	4.016%
42	14.260	1935	1942	1951	rVV	2089746	3098798	38.50%	2.793%
43	14.336	1951	1955	1959	rVB2	19504	27471	0.34%	0.025%
44	14.401	1962	1966	1970	rVB3	10154	14827	0.18%	0.013%
45	14.460	1970	1976	1988	rBV	309394	495380	6.16%	0.446%
46	14.707	2007	2018	2038	rBV	1892930	3067022	38.11%	2.764%
47	14.930	2052	2056	2062	rVB	24834	42525	0.53%	0.038%
48	15.060	2073	2078	2084	rBV4	22565	40902	0.51%	0.037%
49	15.248	2103	2110	2123	rVV	4188684	6007617	74.64%	5.415%
50	15.360	2123	2129	2143	rVV	1457325	2012142	25.00%	1.814%
51	15.483	2146	2150	2156	rVV	59994	90641	1.13%	0.082%
52	15.554	2159	2162	2167	rVV7	10534	17673	0.22%	0.016%
53	15.607	2167	2171	2177	rVB2	22186	33293	0.41%	0.030%
54	15.801	2200	2204	2209	rBV	47313	65203	0.81%	0.059%
55	15.854	2209	2213	2217	rVV	103358	124113	1.54%	0.112%
56	15.924	2221	2225	2229	rVB6	10222	18309	0.23%	0.017%
57	16.030	2239	2243	2247	rVB4	24000	32998	0.41%	0.030%
58	16.142	2255	2262	2268	rBV10	9578	21245	0.26%	0.019%
59	16.242	2275	2279	2286	rBV2	9526	15312	0.19%	0.014%
60	16.401	2301	2306	2315	rBV	257101	346707	4.31%	0.312%
61	16.589	2335	2338	2343	rVB3	16284	21702	0.27%	0.020%
62	16.701	2353	2357	2360	rVV	29102	38446	0.48%	0.035%
63	16.783	2360	2371	2380	rVB2	185703	291961	3.63%	0.263%
64	16.983	2399	2405	2415	rVB	2700397	3618957	44.97%	3.262%
65	17.083	2415	2422	2433	rBV	4983592	6846978	85.07%	6.171%
66	17.171	2433	2437	2448	rVB8	30651	51490	0.64%	0.046%
67	17.265	2448	2453	2457	rBV	3026898	3565041	44.30%	3.213%
68	17.318	2457	2462	2467	rVB	5416584	6452377	80.17%	5.816%
69	17.654	2513	2519	2529	rVV	774060	942929	11.72%	0.850%
70	17.871	2552	2556	2563	rBV	184869	265587	3.30%	0.239%
71	17.936	2564	2567	2571	rVB	36888	51165	0.64%	0.046%
72	18.007	2577	2579	2583	rVB3	13076	13953	0.17%	0.013%
73	18.124	2594	2599	2602	rBV2	32159	45186	0.56%	0.041%
74	18.201	2606	2612	2617	rVB	132465	186578	2.32%	0.168%
75	18.577	2671	2676	2679	rBV	626085	721129	8.96%	0.650%
76	18.618	2679	2683	2691	rVB	1399215	1528951	19.00%	1.378%

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Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Integration Parameters: LSCINT.P
Integrator: RTE
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Sampling : 1 Min Area: 0.1 % of largest Peak
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Title : SVOA CALIBRATION

77	18.930	2732	2736	2743	rBV3	58195	98924	1.23%	0.089%
78	19.006	2744	2749	2756	rVV	69407	109808	1.36%	0.099%
79	19.148	2770	2773	2778	rBV2	48441	65720	0.82%	0.059%
80	19.295	2796	2798	2802	rVB5	16601	15351	0.19%	0.014%
81	19.371	2804	2811	2816	rBV	6024475	8048272	100.00%	7.254%
82	19.418	2816	2819	2826	rVB	139338	179780	2.23%	0.162%
83	19.601	2846	2850	2854	rVB	86657	91258	1.13%	0.082%
84	19.701	2862	2867	2870	rBV	1554718	1774584	22.05%	1.599%
85	19.736	2870	2873	2878	rVB	2692705	2817319	35.01%	2.539%
86	20.500	3001	3003	3008	rBV4	36197	41424	0.51%	0.037%
87	20.665	3027	3031	3033	rBV	1268851	1299602	16.15%	1.171%
88	20.695	3033	3036	3042	rVB	2643919	2732032	33.95%	2.462%
89	20.853	3059	3063	3070	rBV	261867	331566	4.12%	0.299%
90	21.147	3108	3113	3121	rBV	3294890	4006487	49.78%	3.611%
91	21.271	3132	3134	3138	rBV3	71465	106623	1.32%	0.096%
92	21.518	3171	3176	3178	rBV	1316118	1576190	19.58%	1.421%
93	21.547	3178	3181	3188	rVB	2637200	2855346	35.48%	2.574%
94	22.094	3270	3274	3278	rBV	511282	622146	7.73%	0.561%
95	22.136	3278	3281	3285	rVV3	203295	249496	3.10%	0.225%
96	22.177	3286	3288	3292	rVB	167895	190783	2.37%	0.172%
97	22.389	3320	3324	3327	rBV	1397229	1887333	23.45%	1.701%
98	22.424	3327	3330	3342	rVB	2735004	3439206	42.73%	3.100%
99	23.159	3447	3455	3465	rVB2	4295525	7919179	98.40%	7.138%
100	23.289	3471	3477	3486	rVB2	2265389	3964011	49.25%	3.573%

Sum of corrected areas: 110950115

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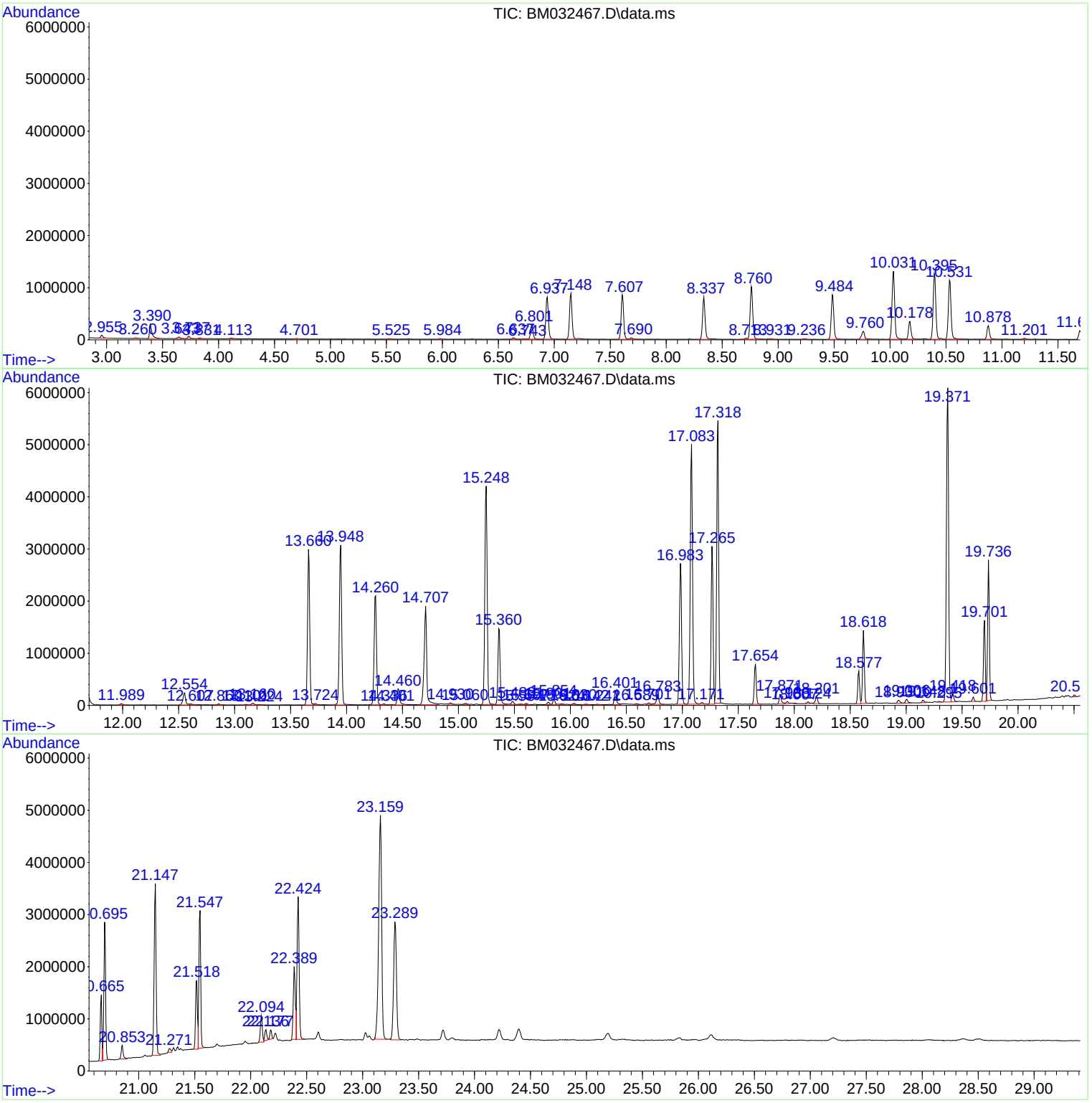
Instrument :
BNA_M
ClientSampleId :
C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

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



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TIC Library : C:\Database\NIST20.L
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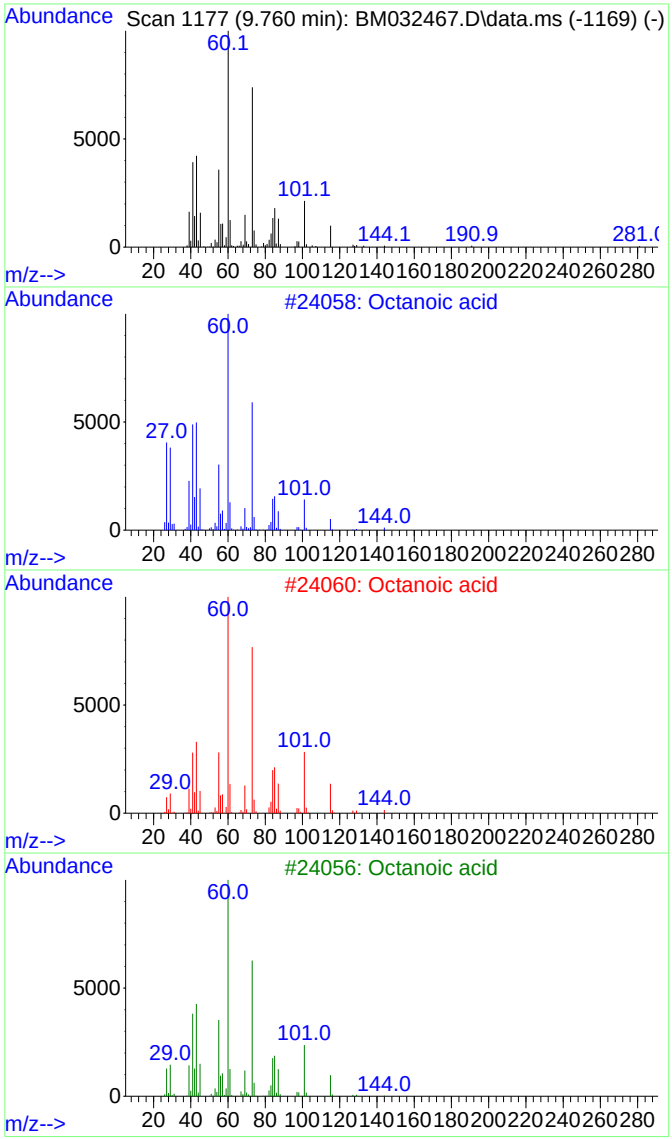
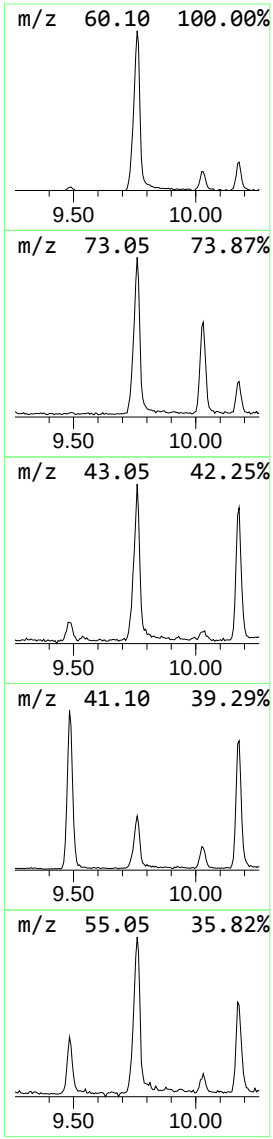
****
Peak Number 1 Octanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.760	2.77 ng/ul	286316	Naphthalene-d8	10.395

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	90
2	Octanoic acid	144	C8H16O2	000124-07-2	90
3	Octanoic acid	144	C8H16O2	000124-07-2	90
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	72
5	Octanoic acid	144	C8H16O2	000124-07-2	64





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Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

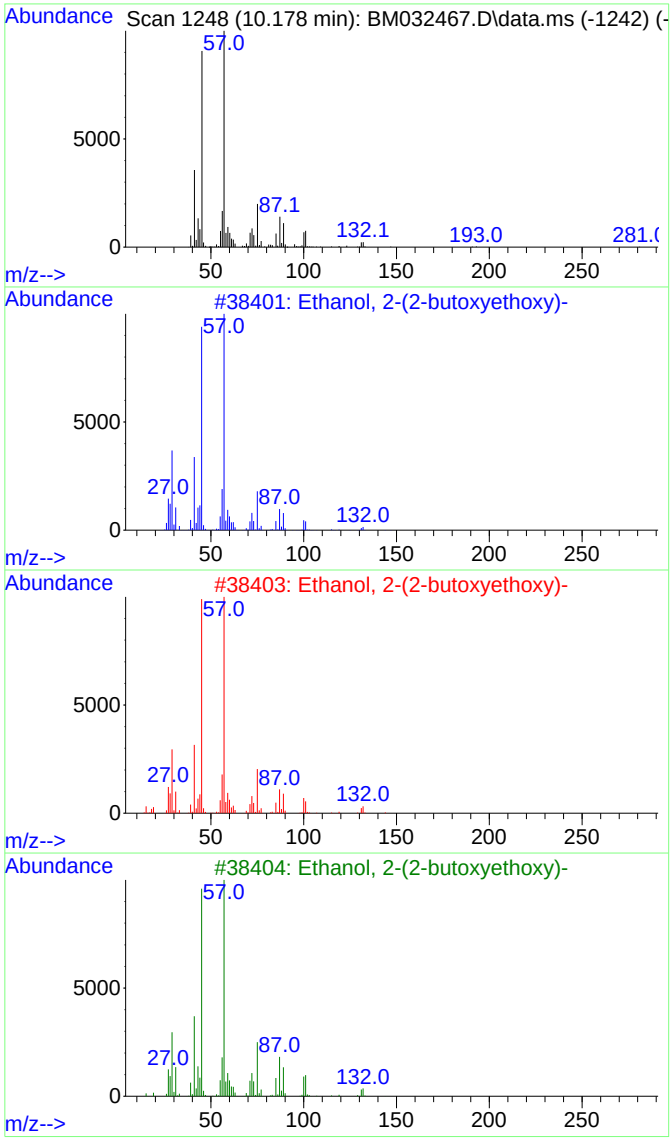
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

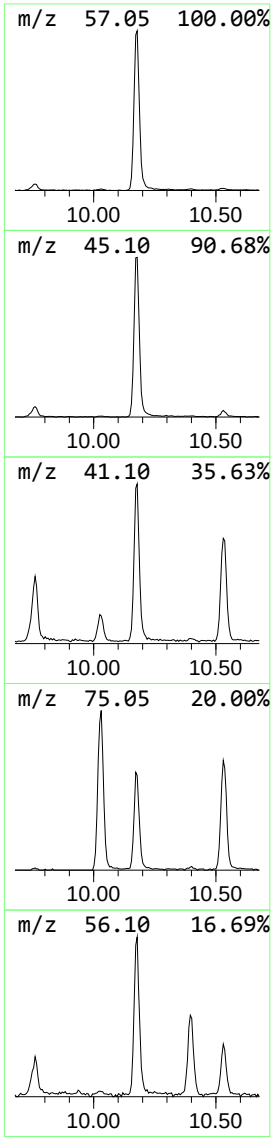
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.178	5.12 ng/ul	529584	Naphthalene-d8	10.395

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
5	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72





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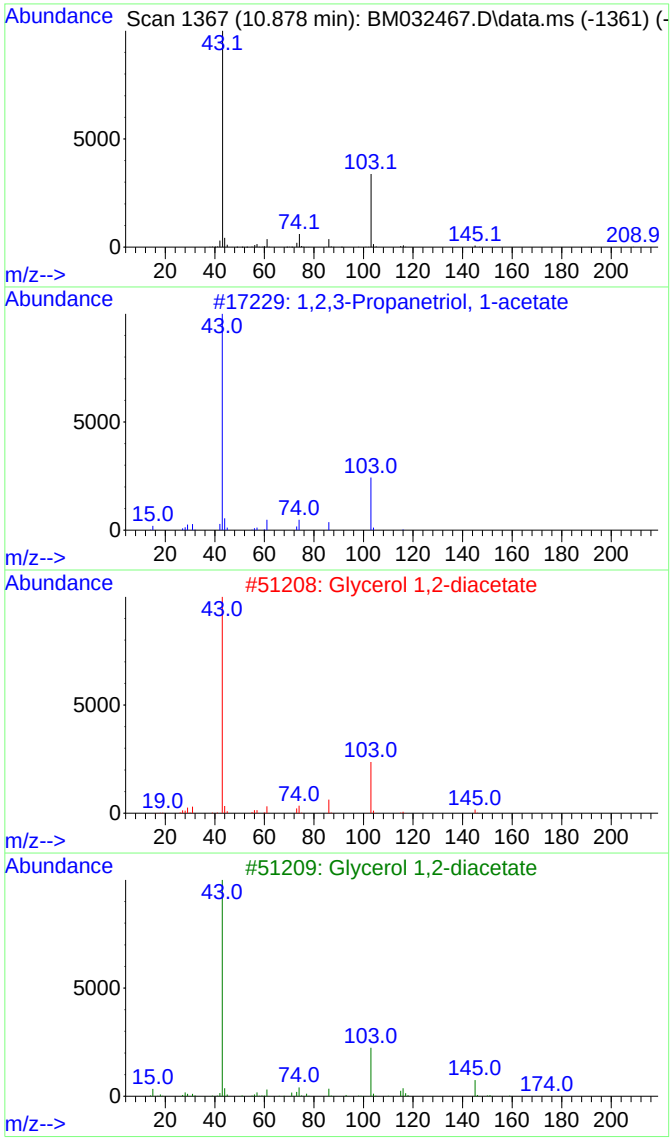
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

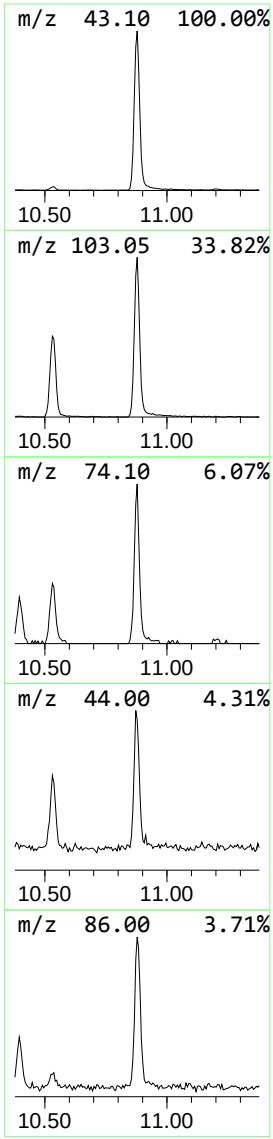
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,2,3-Propanetriol, 1-acetate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.878	3.99 ng/ul	412534	Naphthalene-d8	10.395

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3-Propanetriol, 1-acetate	134	C5H10O4	000106-61-6	59
2	Glycerol 1,2-diacetate	176	C7H12O5	000102-62-5	43
3	Glycerol 1,2-diacetate	176	C7H12O5	000102-62-5	38
4	Glycerol 1,2-diacetate	176	C7H12O5	000102-62-5	38
5	1,2,3-Propanetriol, 1-acetate	134	C5H10O4	000106-61-6	17





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

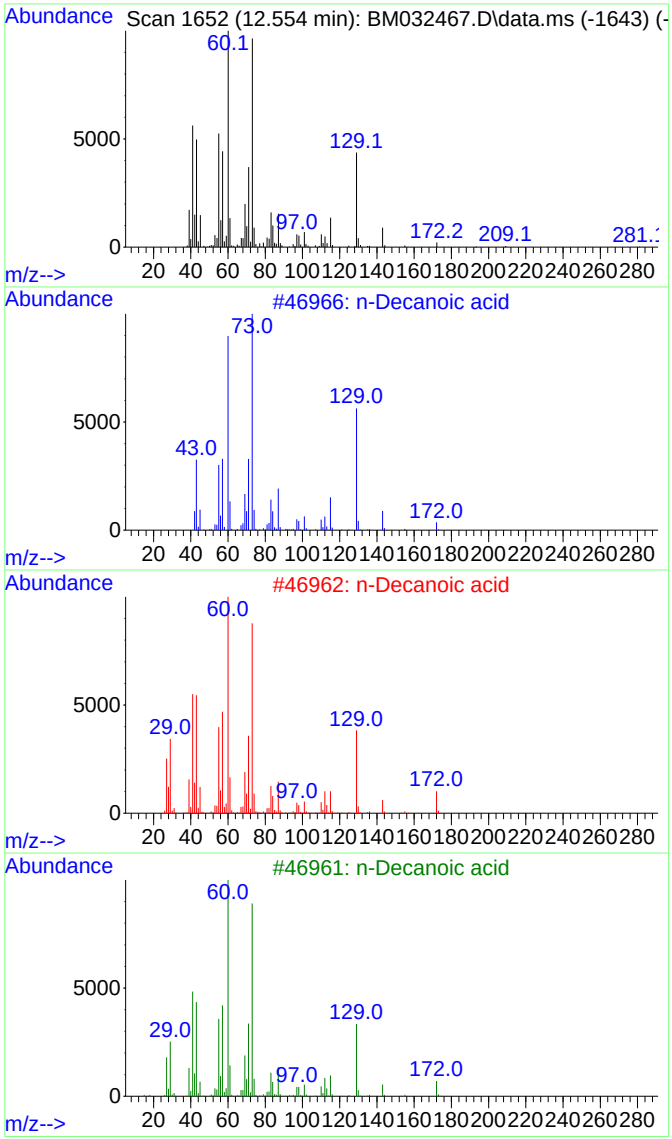
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

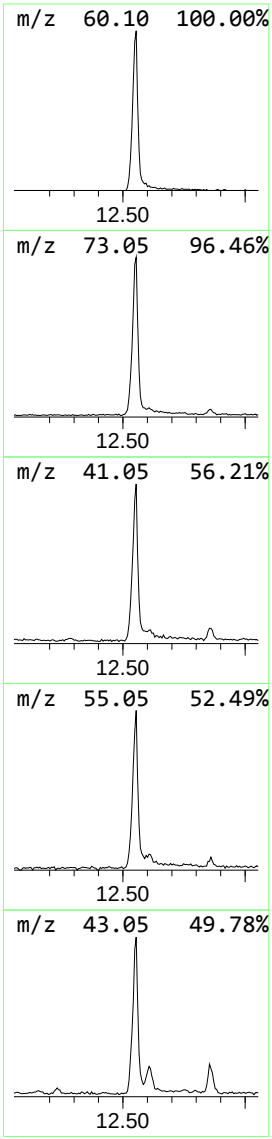
****

Peak Number 4 n-Decanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.554	2.44 ng/ul	377913	Acenaphthene-d10	14.260

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	94
2	n-Decanoic acid	172	C10H20O2	000334-48-5	90
3	n-Decanoic acid	172	C10H20O2	000334-48-5	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	74





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Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

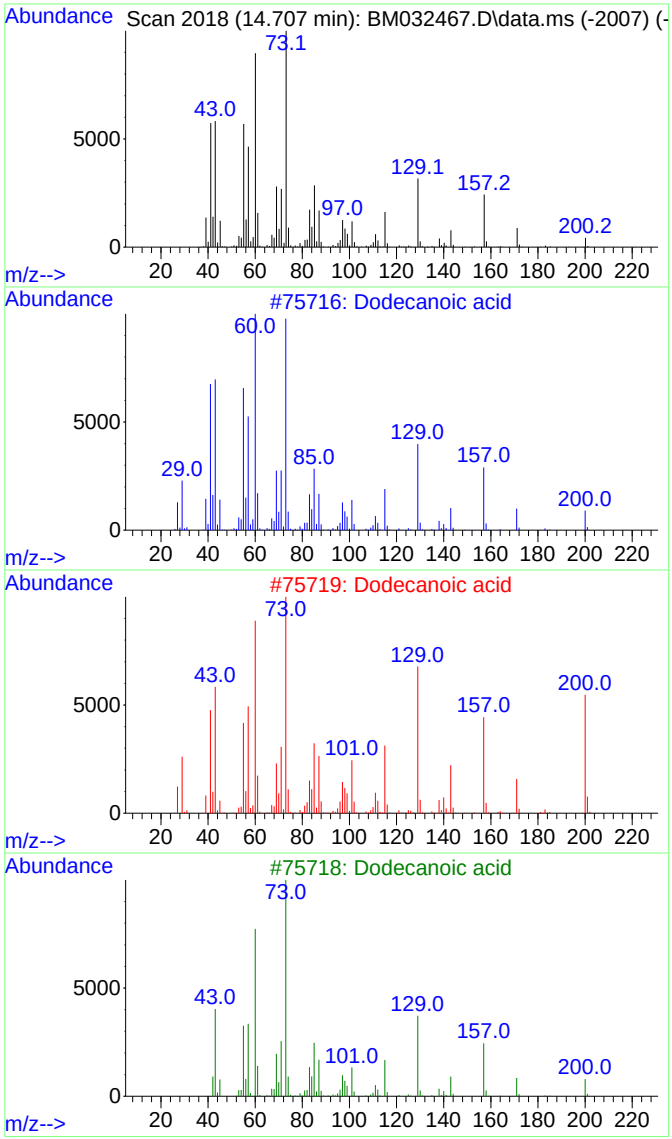
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

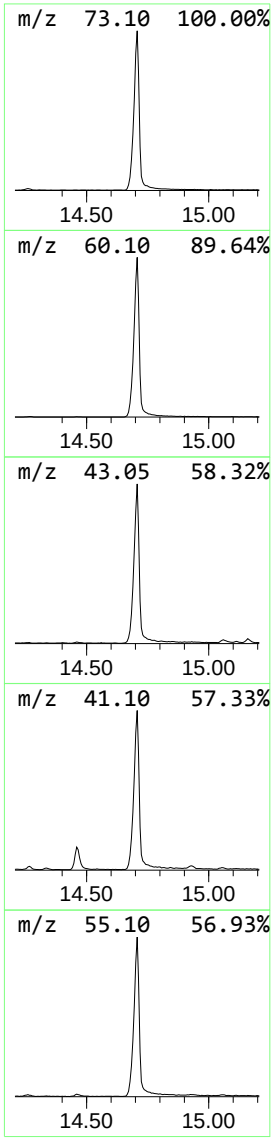
****

Peak Number 5 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.707	19.79 ng/ul	3067020	Acenaphthene-d10	14.260

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	98
2	Dodecanoic acid	200	C12H24O2	000143-07-7	93
3	Dodecanoic acid	200	C12H24O2	000143-07-7	91
4	Dodecanoic acid	200	C12H24O2	000143-07-7	91
5	Dodecanoic acid	200	C12H24O2	000143-07-7	91





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Data File : BM032467.D
Acq On : 12 Oct 2021 20:46
Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

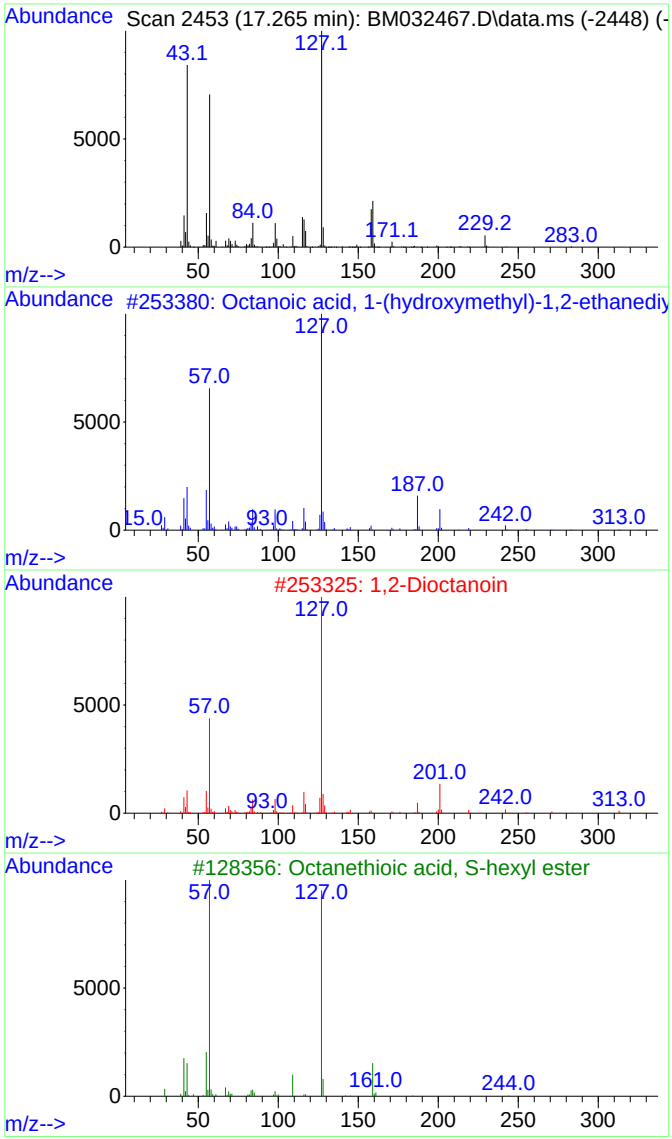
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

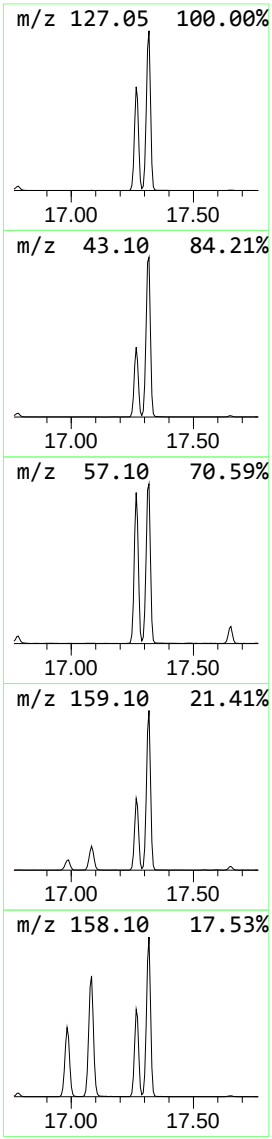
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Octanoic acid, 1-(hydroxyme... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.265	19.70 ng/ul	3565040	Phenanthrene-d10	16.983

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid, 1-(hydroxymethyl)...	344	C19H36O5	060514-48-9	59
2	1,2-Dioctanoin	344	C19H36O5	001069-87-0	53
3	Octanethioic acid, S-hexyl ester	244	C14H28OS	055590-85-7	50
4	Caprylic anhydride	270	C16H30O3	000623-66-5	50
5	1,3,5-Triazin-2(1H)-one, 4,6-dia...	127	C3H5N5O	000645-92-1	43





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Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

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Quant Title : SVOA CALIBRATION

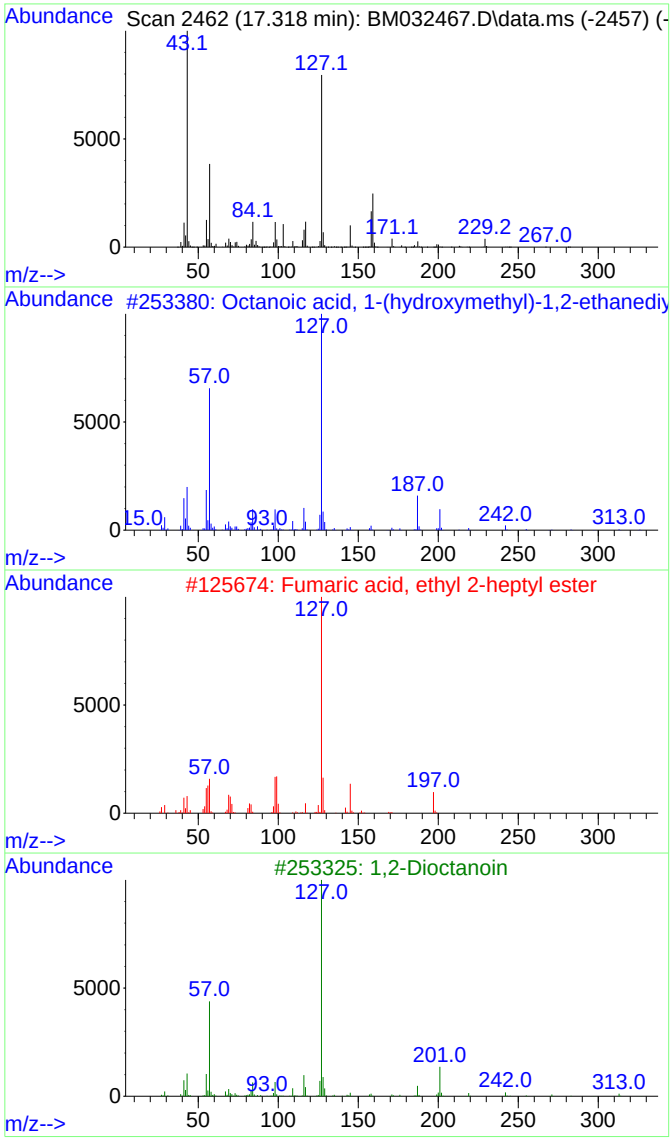
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

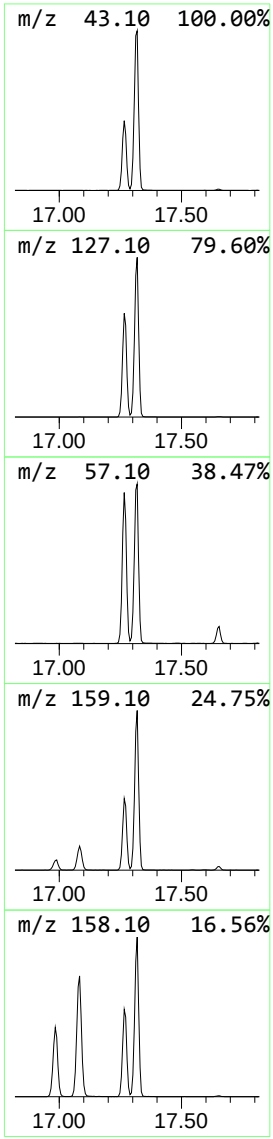
****

Peak Number 7 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.318	35.66 ng/ul	6452380	Phenanthrene-d10	16.983

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid, 1-(hydroxymethyl)...	344	C19H36O5	060514-48-9	38
2	Fumaric acid, ethyl 2-heptyl ester	242	C13H22O4	1000348-62-0	38
3	1,2-Dioctanoin	344	C19H36O5	001069-87-0	37
4	(3,4-Difluorophenyl)methanethiol...	202	C9H8F2OS	873463-82-2	33
5	6-Azathymine	127	C4H5N3O2	000932-53-6	32





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Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AA3

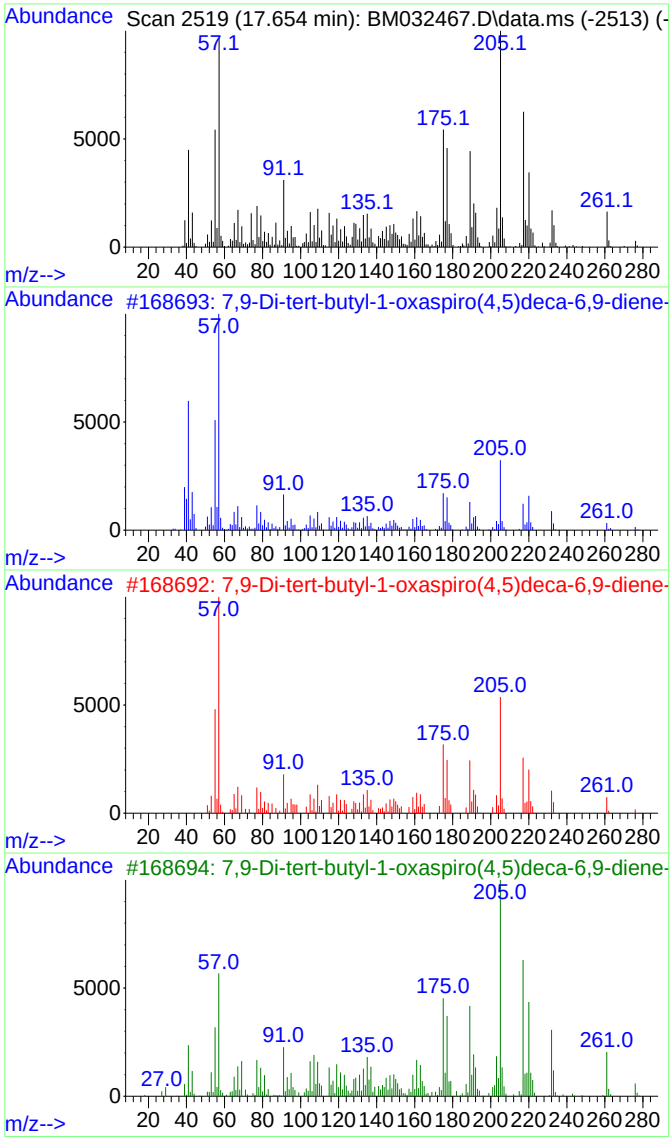
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

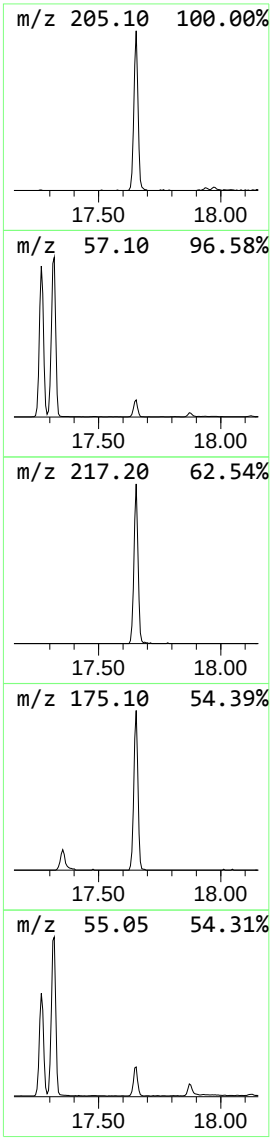
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.654	5.21 ng/ul	942929	Phenanthrene-d10	16.983

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	83
4	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	80
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50





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Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

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

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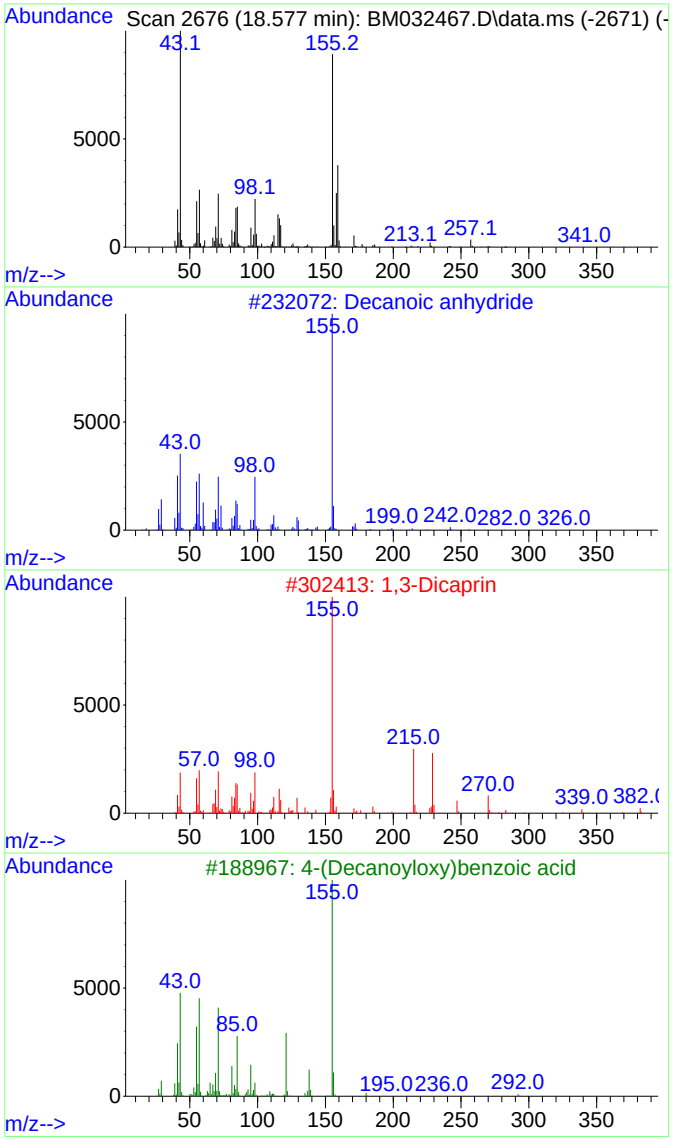
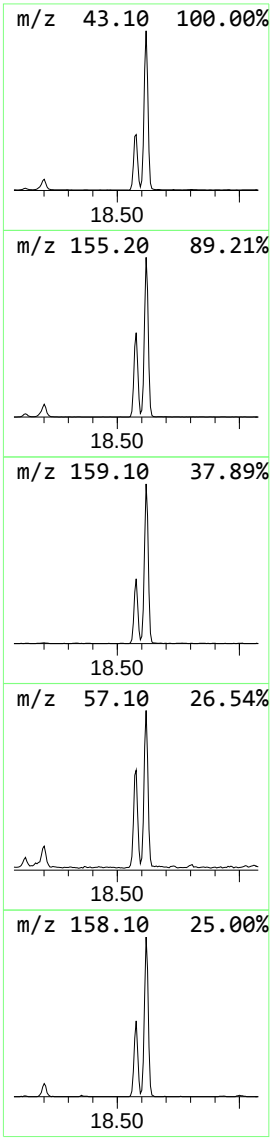
Peak Number 9 Decanoic anhydride Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.577	3.99 ng/ul	721129	Phenanthrene-d10	16.983

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic anhydride	326	C20H38O3	002082-76-0	53
2	1,3-Dicaprin	400	C23H44O5	017598-93-5	50
3	4-(Decanoyloxy)benzoic acid	292	C17H24O4	086960-46-5	43
4	Fumaric acid, butyl 3-hexyl ester	256	C14H24O4	1000348-60-4	43
5	1,2-Dicaprin	400	C23H44O5	017863-69-3	43





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Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

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

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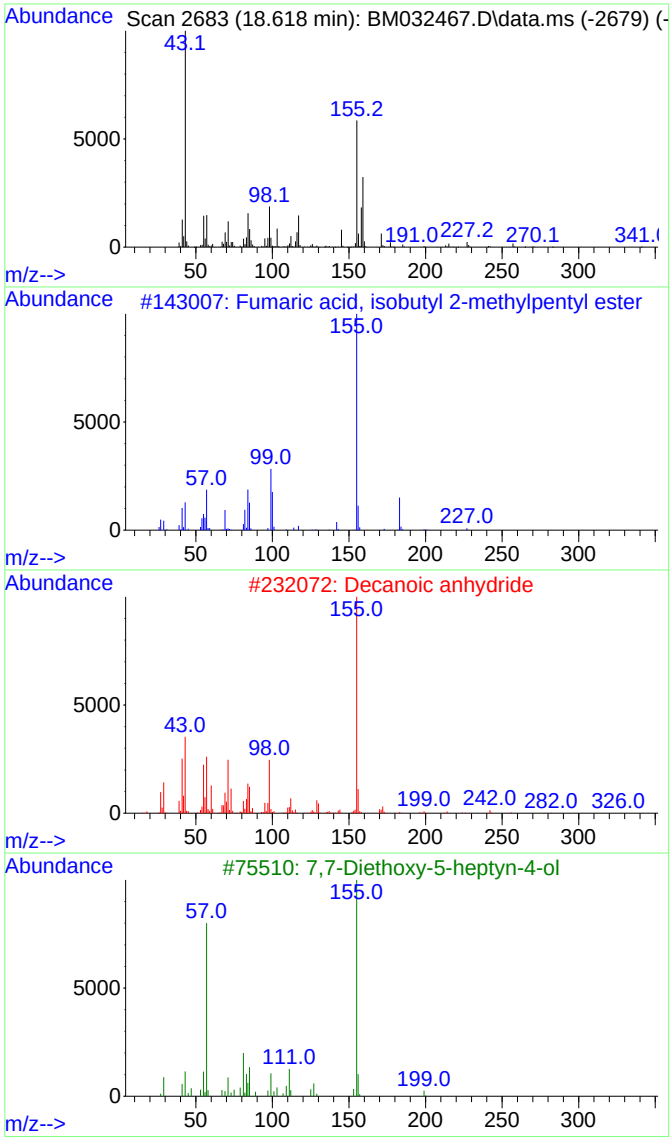
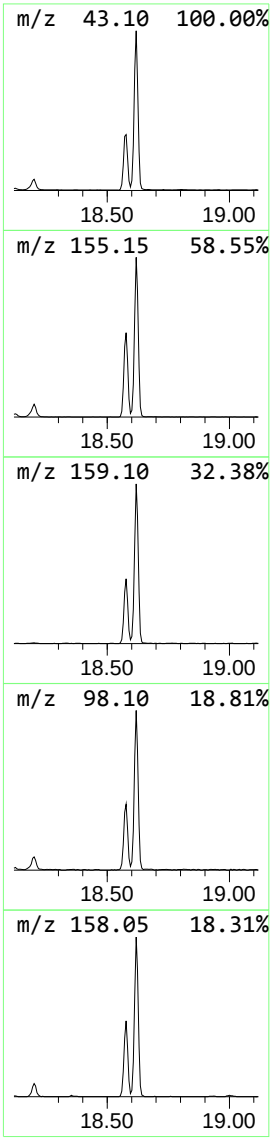
Peak Number 10 unknown-02 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.618	8.45 ng/ul	1528950	Phenanthrene-d10	16.983

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, isobutyl 2-methylp...	256	C14H24O4	1000348-72-1	35
2	Decanoic anhydride	326	C20H38O3	002082-76-0	32
3	7,7-Diethoxy-5-heptyn-4-ol	200	C11H20O3	1000434-41-6	27
4	6-Amino-1,3-dimethyluracil	155	C6H9N3O2	006642-31-5	27
5	Fumaric acid, isobutyl 2-methylp...	256	C14H24O4	1000348-76-0	27





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Operator : CG/JU
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ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

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Quant Title : SVOA CALIBRATION

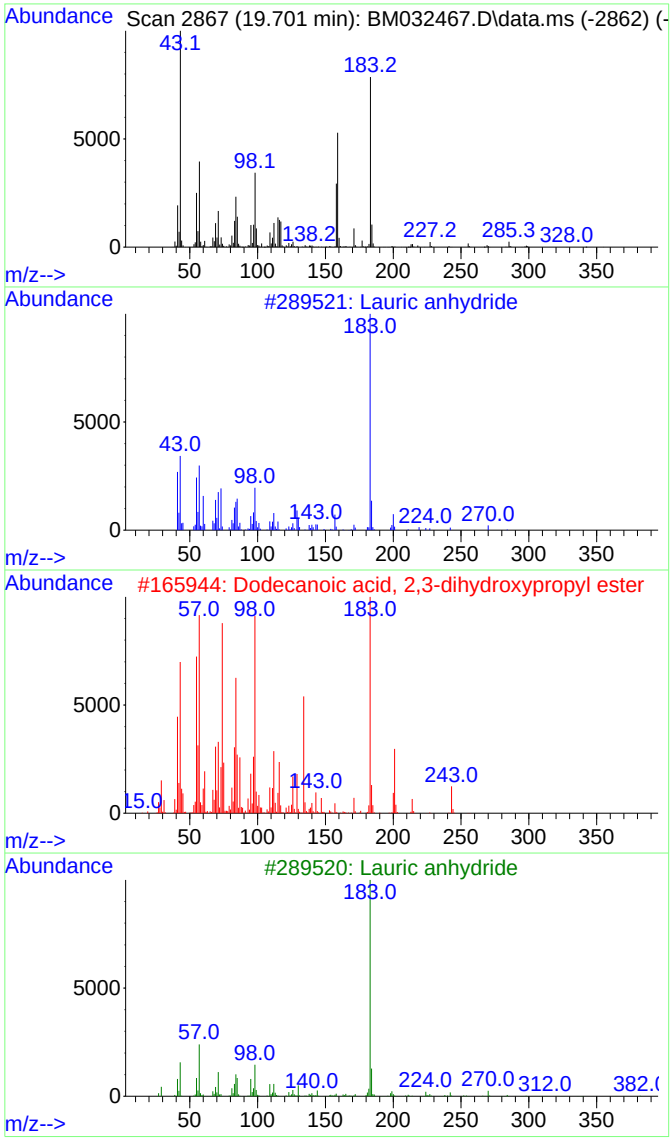
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

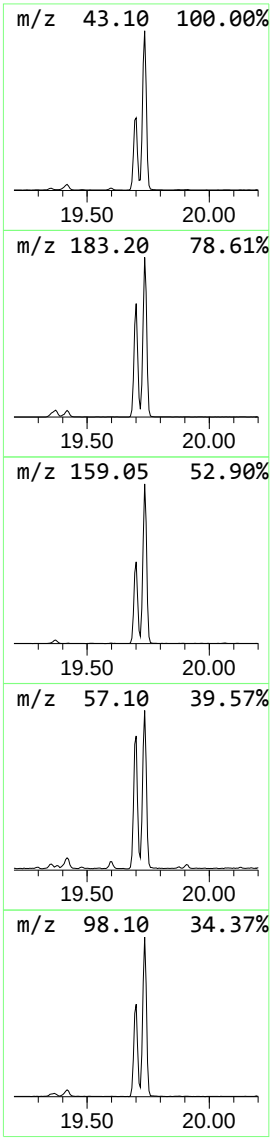
****

Peak Number 11 unknown-03 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.701	8.86 ng/ul	1774580	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lauric anhydride	382	C24H46O3	000645-66-9	43
2	Dodecanoic acid, 2,3-dihydroxypr...	274	C15H30O4	000142-18-7	40
3	Lauric anhydride	382	C24H46O3	000645-66-9	37
4	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	32
5	Fumaric acid, 2-decyl hexyl ester	340	C20H36O4	1000348-58-9	32





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Acq On : 12 Oct 2021 20:46
Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

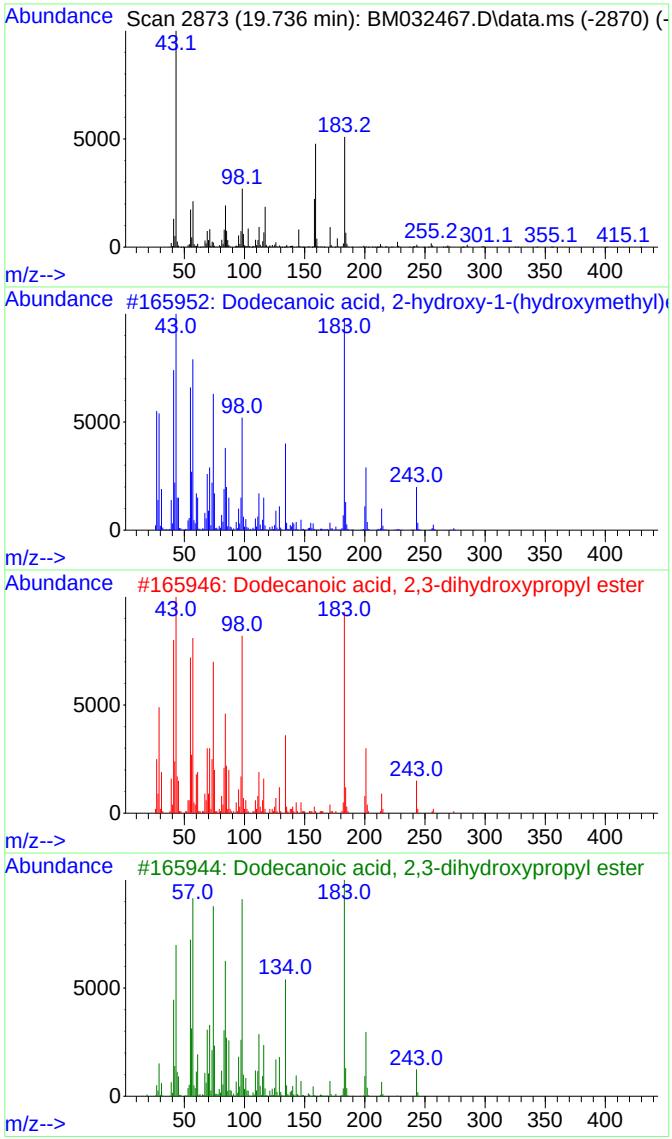
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

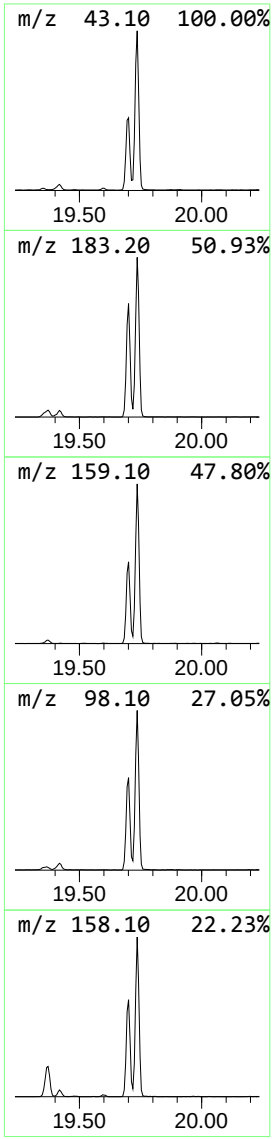
****

Peak Number 12 unknown-04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.736	14.06 ng/ul	2817320	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	38
2	Dodecanoic acid, 2,3-dihydroxypr...	274	C15H30O4	000142-18-7	27
3	Dodecanoic acid, 2,3-dihydroxypr...	274	C15H30O4	000142-18-7	25
4	Dodecanoyl chloride	218	C12H23ClO	000112-16-3	16
5	Fumaric acid, hexyl 2-hexyl ester	284	C16H28O4	1000348-74-5	16





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Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

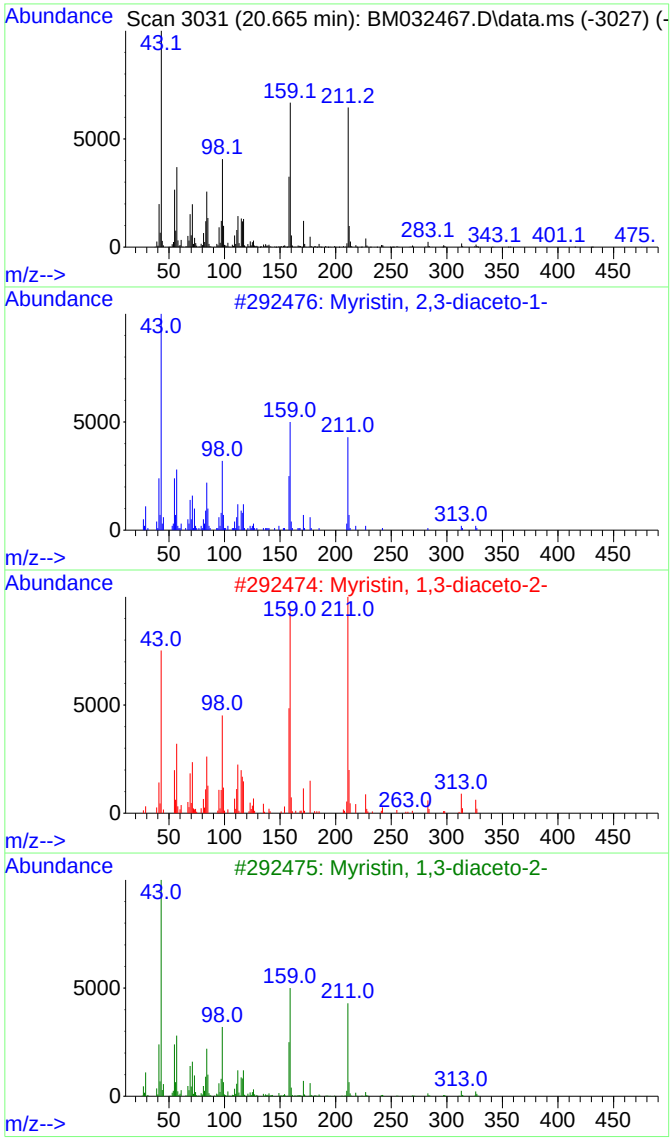
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

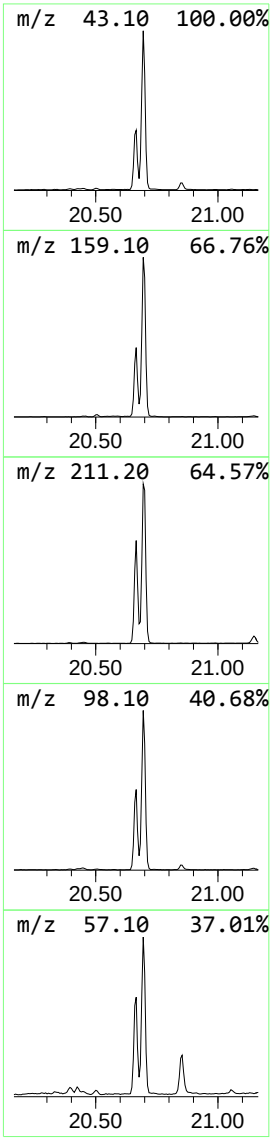
****

Peak Number 13 Myristin, 2,3-diaceto-1- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.665	6.49 ng/ul	1299600	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	91
2	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	91
3	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	91
4	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	53
5	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	38





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Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

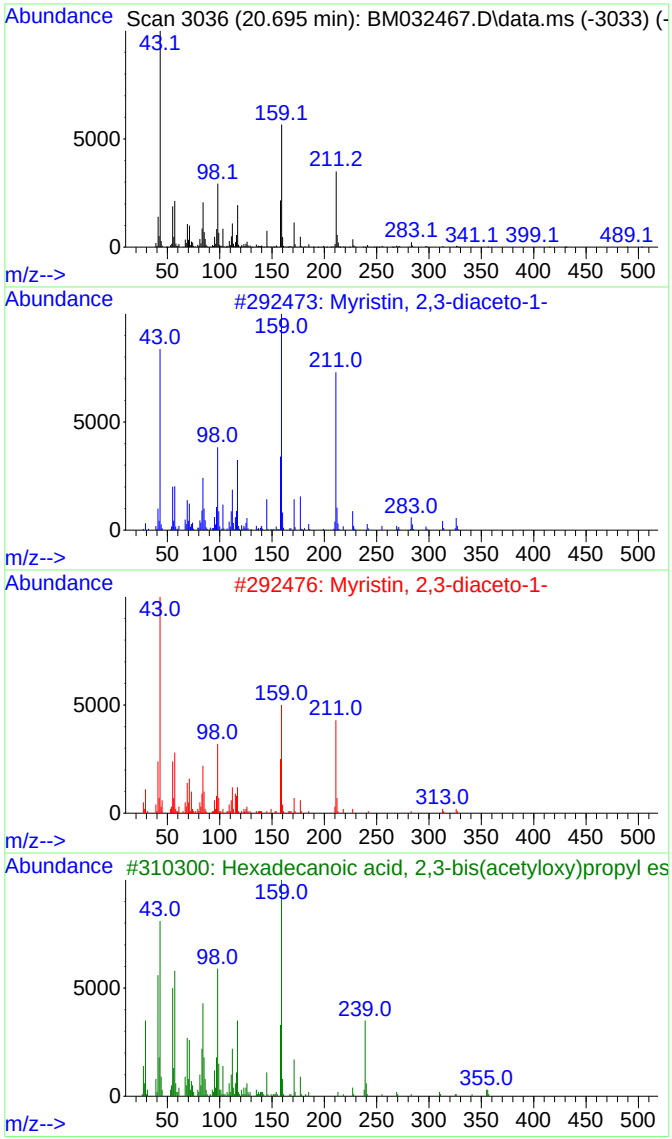
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

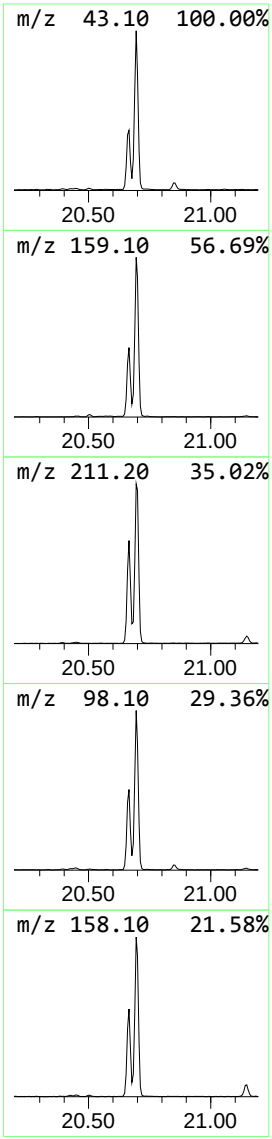
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Hexadecanoic acid, 2,3-bis(... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.695	13.64 ng/ul	2732030	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	83
2	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	78
3	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	68
4	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	58
5	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	45





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Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

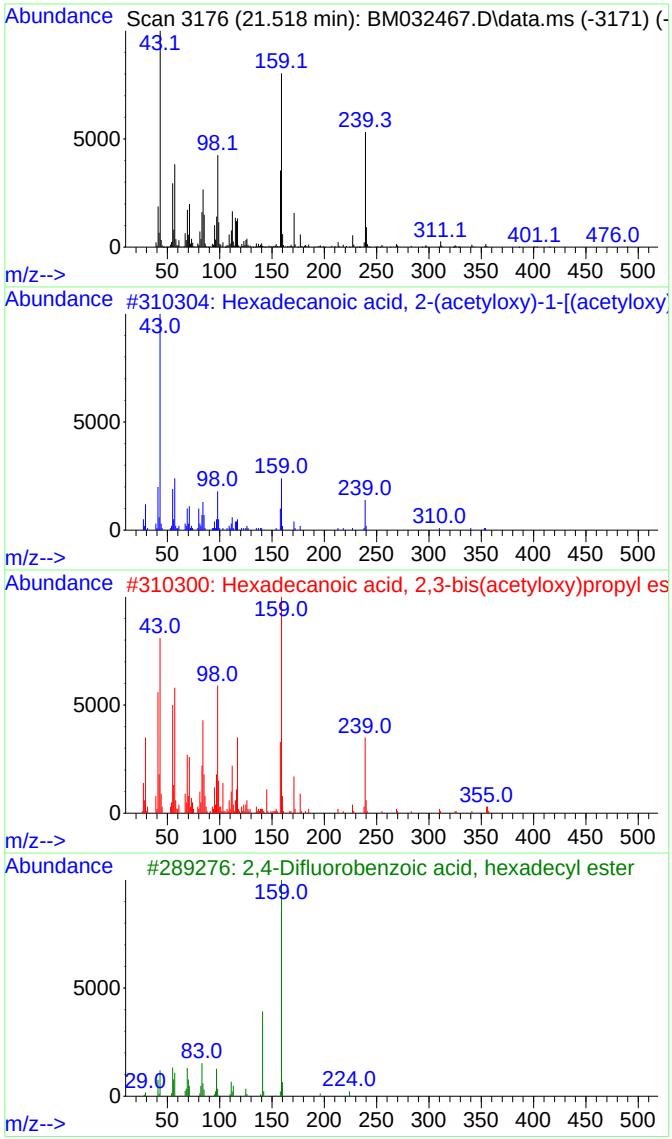
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

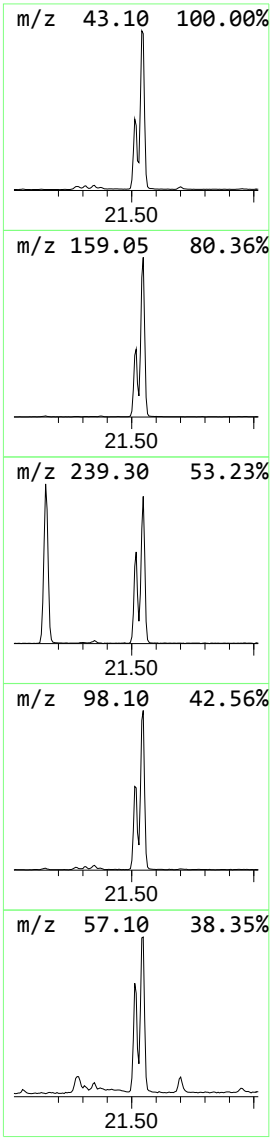
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Hexadecanoic acid, 2-(acety... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.518	7.87 ng/ul	1576190	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	91
2	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	87
3	2,4-Difluorobenzoic acid, hexade...	382	C23H36F2O2	1000338-79-4	22
4	2,4-Difluorobenzoic acid, heptad...	396	C24H38F2O2	1000338-79-5	22
5	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	22





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Instrument : BNA_M
ClientSampleId : C0AA3

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Quant Title : SVOA CALIBRATION

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

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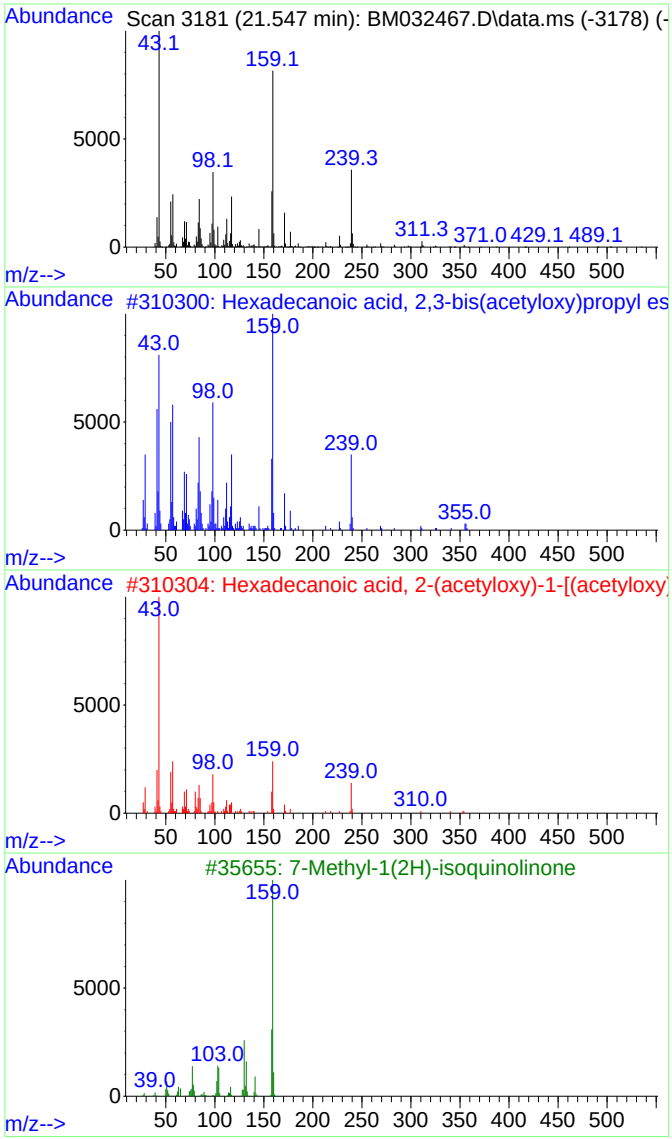
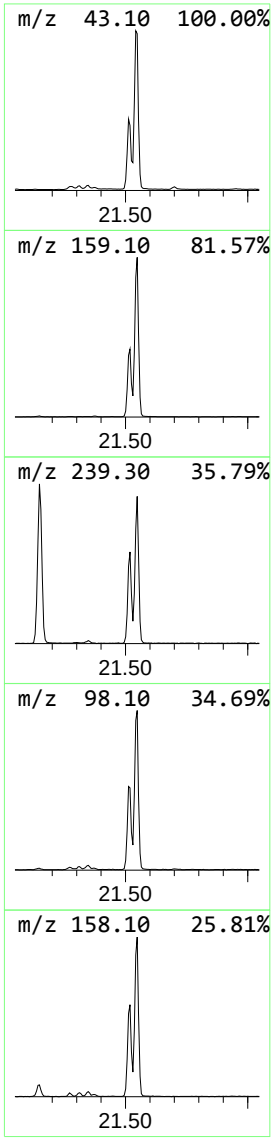
Peak Number 16 unknown-05 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.547	14.25 ng/ul	2855350	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	62
2	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	62
3	7-Methyl-1(2H)-isoquinolinone	159	C10H9NO	026829-47-0	38
4	Pyridine, 1,2,3,6-tetrahydro-4-p...	159	C11H13N	010338-69-9	35
5	2,3-Dihydroxypropyl 12-methyltri...	386	C21H38O6	1000488-66-8	35





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Sample : M4128-12
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ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

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Quant Title : SVOA CALIBRATION

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

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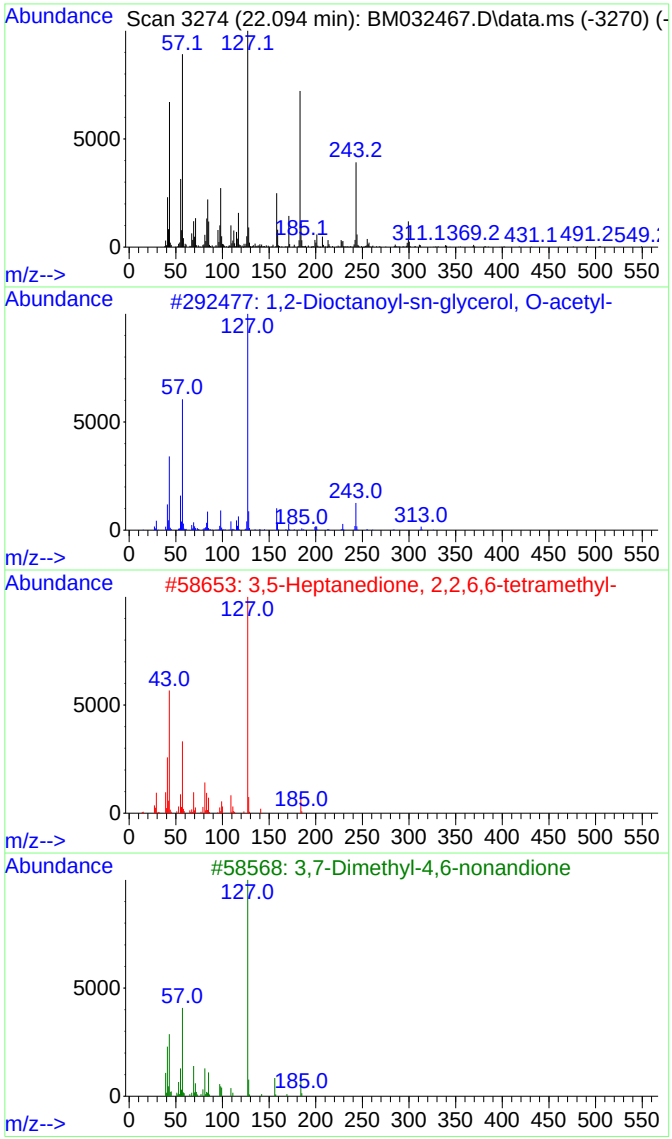
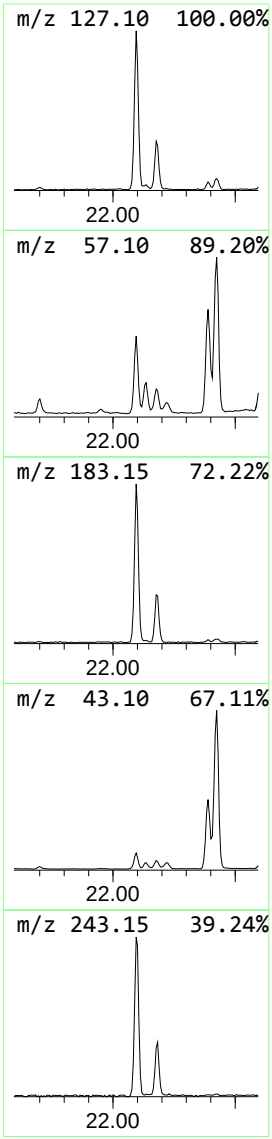
Peak Number 17 unknown-06 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.095	3.11 ng/ul	622146	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dioctanoyl-sn-glycerol, O-ac...	386	C21H38O6	1000452-09-1	35
2	3,5-Heptanedione, 2,2,6,6-tetram...	184	C11H20O2	001118-71-4	30
3	3,7-Dimethyl-4,6-nonandione	184	C11H20O2	1000374-12-6	30
4	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	30
5	3,5-Heptanedione, 2,2,6,6-tetram...	184	C11H20O2	001118-71-4	30





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Data File : BM032467.D
Acq On : 12 Oct 2021 20:46
Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AA3

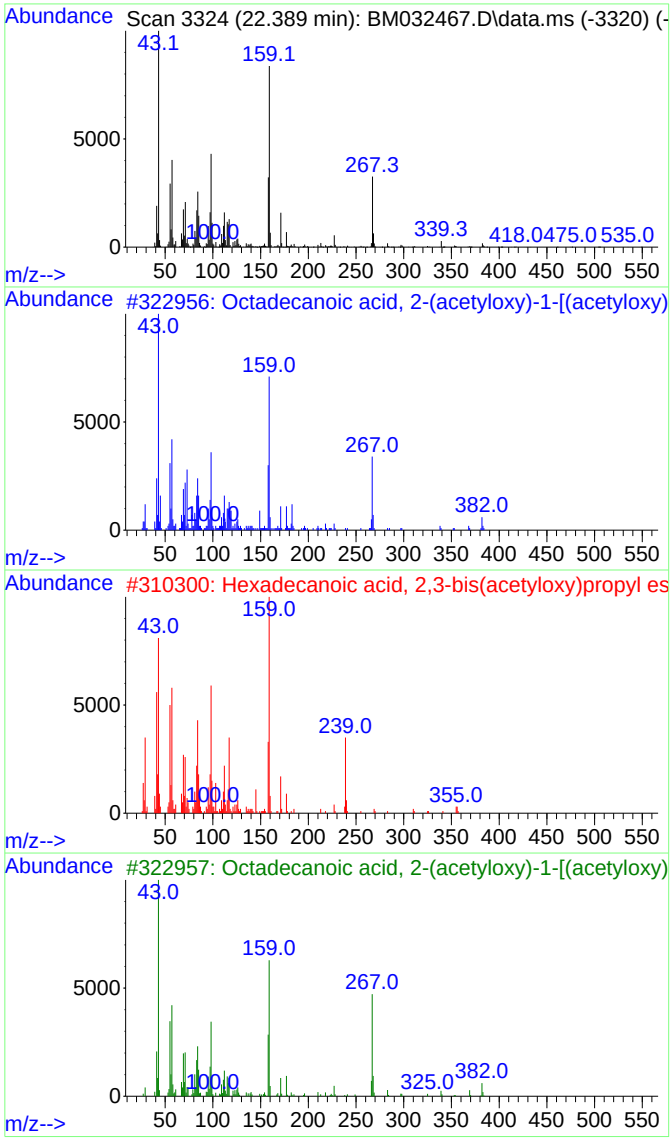
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

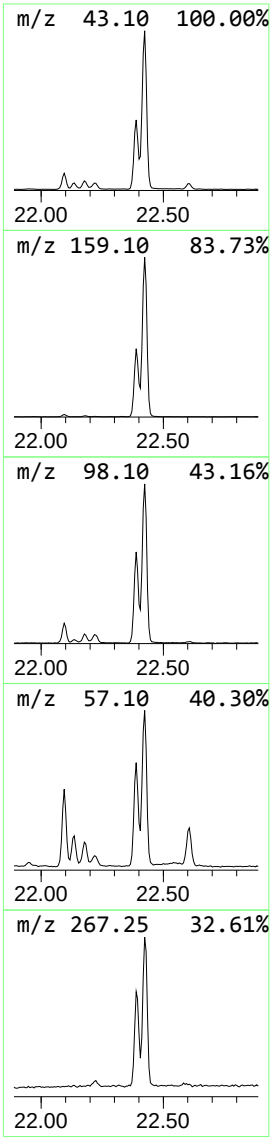
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Octadecanoic acid, 2-(acety... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.389	9.52 ng/ul	1887330	Perylene-d12	23.288

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	90
2	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	83
3	Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	80
4	Octadecanoic acid, 2,3-bis(acety...	442	C25H46O6	033599-07-4	64
5	2,3-Dihydroxypropyl 12-methyltri...	386	C21H38O6	1000488-66-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101121\
Data File : BM032467.D
Acq On : 12 Oct 2021 20:46
Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

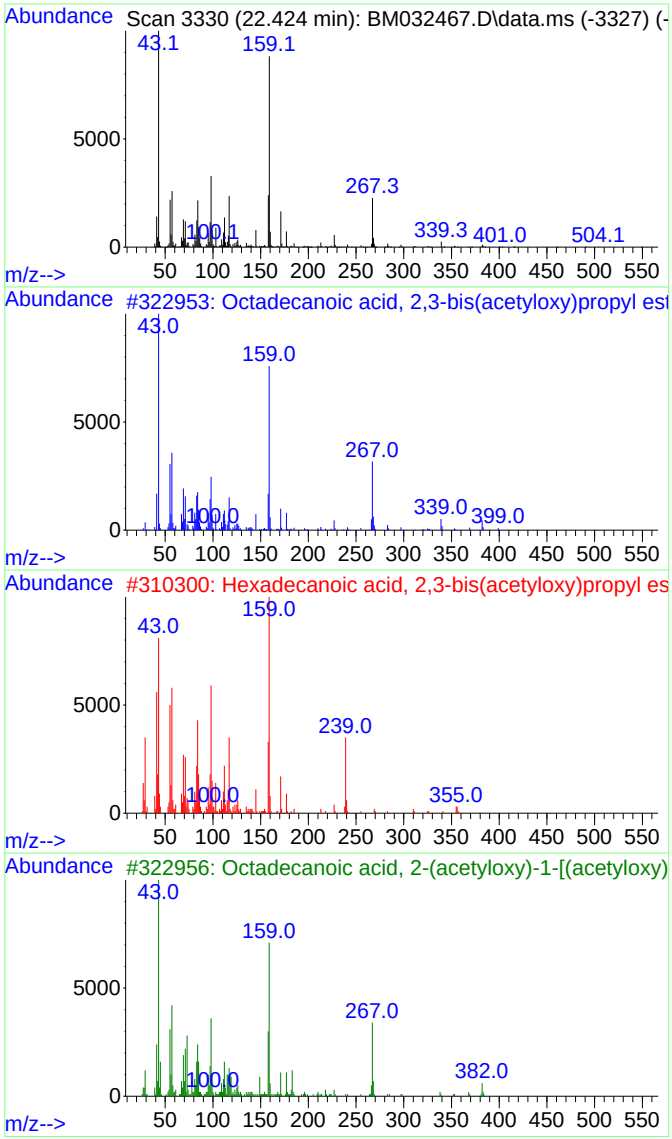
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

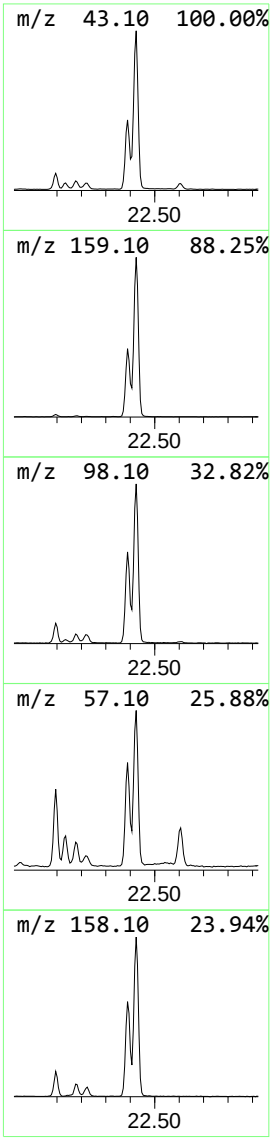
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Octadecanoic acid, 2,3-bis(... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.424	17.35 ng/ul	3439210	Perylene-d12	23.288

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2,3-bis(acety...	442	C25H46O6	033599-07-4	64
2	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	58
3	Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	50
4	2,3-Dihydroxypropyl 12-methyltri...	386	C21H38O6	1000488-66-8	47
5	2,3,4-Trifluorobenzoic acid, 6-e...	316	C17H23F3O2	1000282-58-3	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101121\
Data File : BM032467.D
Acq On : 12 Oct 2021 20:46
Operator : CG/JU
Sample : M4128-12
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AA3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.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
Octanoic acid	9.760	2.8	ng/ul	286316	2	10.395	2068010	20.0
Ethanol, 2-(2-b...	10.178	5.1	ng/ul	529584	2	10.395	2068010	20.0
1,2,3-Propanetr...	10.878	4.0	ng/ul	412534	2	10.395	2068010	20.0
n-Decanoic acid	12.554	2.4	ng/ul	377913	3	14.260	3098800	20.0
Dodecanoic acid	14.707	19.8	ng/ul	3067020	3	14.260	3098800	20.0
Octanoic acid, ...	17.265	19.7	ng/ul	3565040	4	16.983	3618960	20.0
unknown-01	17.318	35.7	ng/ul	6452380	4	16.983	3618960	20.0
7,9-Di-tert-but...	17.654	5.2	ng/ul	942929	4	16.983	3618960	20.0
Decanoic anhydride	18.577	4.0	ng/ul	721129	4	16.983	3618960	20.0
unknown-02	18.618	8.4	ng/ul	1528950	4	16.983	3618960	20.0
unknown-03	19.701	8.9	ng/ul	1774580	5	21.148	4006490	20.0
unknown-04	19.736	14.1	ng/ul	2817320	5	21.148	4006490	20.0
Myristin, 2,3-d...	20.665	6.5	ng/ul	1299600	5	21.148	4006490	20.0
Hexadecanoic ac...	20.695	13.6	ng/ul	2732030	5	21.148	4006490	20.0
Hexadecanoic ac...	21.518	7.9	ng/ul	1576190	5	21.148	4006490	20.0
unknown-05	21.547	14.3	ng/ul	2855350	5	21.148	4006490	20.0
unknown-06	22.095	3.1	ng/ul	622146	5	21.148	4006490	20.0
Octadecanoic ac...	22.389	9.5	ng/ul	1887330	6	23.288	3964010	20.0
Octadecanoic ac...	22.424	17.4	ng/ul	3439210	6	23.288	3964010	20.0