LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101121\
Data File : BM032470.D
Acq On : 12 Oct 2021 22:35
Operator : CG/JU
Sample : M4128-13
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AD0

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: BM032470.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	28	rVB	58425	75619	0.30%	0.057%
2	3.390	90	94	106	rBV	282955	439051	1.76%	0.328%
3	3.643	132	137	147	rVB	31624	57402	0.23%	0.043%
4	3.731	147	152	161	rVV	44314	70462	0.28%	0.053%
5	4.113	212	217	223	rVB	52104	78615	0.31%	0.059%
6	4.696	311	316	324	rVB2	13004	25309	0.10%	0.019%
7	5.690	481	485	494	rVB	19098	32664	0.13%	0.024%
8	6.743	656	664	668	rBV2	22109	43827	0.18%	0.033%
9	6.796	668	673	683	rVB	279457	434419	1.74%	0.325%
10	6.937	688	697	709	rBV	813110	1274744	5.10%	0.953%
11	7.149	723	733	741	rBV	870994	1375635	5.50%	1.029%
12	7.301	755	759	765	rVB3	18204	26958	0.11%	0.020%
13	7.607	804	811	820	rBV	899461	1373780	5.49%	1.027%
14	7.690	820	825	831	rVB	29159	46500	0.19%	0.035%
15	8.337	928	935	948	rBV	829042	1306194	5.22%	0.977%
16	8.713	995	999	1001	rBV	22718	33072	0.13%	0.025%
17	8.760	1001	1007	1019	rVB	1043089	1638246	6.55%	1.225%
18	8.931	1029	1036	1044	rVB	101250	152648	0.61%	0.114%
19	9.237	1080	1088	1094	rVB	42990	67027	0.27%	0.050%
20	9.484	1122	1130	1145	rBV	873210	1406304	5.62%	1.051%
21	10.031	1215	1223	1233	rBV	1354959	2237667	8.95%	1.673%
22	10.178	1241	1248	1260	rBV	867190	1319817	5.28%	0.987%
23	10.313	1265	1271	1276	rVB6	10334	26171	0.10%	0.020%
24	10.395	1276	1285	1292	rBV	1341371	2166272	8.66%	1.620%
25	10.531	1300	1308	1322	rBV	1261069	2035261	8.14%	1.522%
26	11.201	1416	1422	1432	rVB2	22521	41861	0.17%	0.031%
27	11.336	1440	1445	1456	rVB2	32117	54041	0.22%	0.040%
28	11.695	1501	1506	1516	rBV2	136763	288162	1.15%	0.215%
29	11.989	1548	1556	1562	rVB2	26868	45759	0.18%	0.034%
30	12.531	1637	1648	1654	rBV5	16762	42483	0.17%	0.032%
31	12.701	1670	1677	1681	rBV3	26658	39128	0.16%	0.029%
32	12.860	1699	1704	1713	rBV2	20888	35891	0.14%	0.027%
33	13.160	1751	1755	1762	rVV	42820	71790	0.29%	0.054%
34	13.660	1833	1840	1846	rBV	2927610	3826921	15.30%	2.861%
35	13.948	1882	1889	1902	rVB	3099159	4481540	17.92%	3.351%
36	14.254	1935	1941	1951	rBV	2232056	3195018	12.78%	2.389%

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Instrument : BNA_M
ClientSampleId : C0AD0

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	14.336	1951	1955	1960	rVB3	16807	25143	0.10%	0.019%
38	14.460	1971	1976	1988	rBV	291573	455587	1.82%	0.341%
39	14.677	2006	2013	2019	rBV6	17760	32295	0.13%	0.024%
40	14.924	2045	2055	2064	rBV	22851	51907	0.21%	0.039%
41	15.060	2074	2078	2083	rBV3	20359	36062	0.14%	0.027%
42	15.248	2103	2110	2123	rBV	4141032	5889107	23.55%	4.403%
43	15.360	2123	2129	2140	rBV	1371681	1805264	7.22%	1.350%
44	15.483	2145	2150	2154	rBV	52797	74154	0.30%	0.055%
45	15.607	2167	2171	2176	rVB2	19277	27547	0.11%	0.021%
46	15.677	2178	2183	2189	rBV3	18786	30403	0.12%	0.023%
47	15.966	2228	2232	2235	rBV	25123	29569	0.12%	0.022%
48	16.024	2240	2242	2247	rVB5	18794	26670	0.11%	0.020%
49	16.983	2395	2405	2415	rBV	2674561	3700991	14.80%	2.767%
50	17.083	2415	2422	2432	rBV	4779994	6725098	26.89%	5.028%
51	17.177	2434	2438	2444	rVB5	32079	48742	0.19%	0.036%
52	17.648	2513	2518	2526	rBV	799025	991928	3.97%	0.742%
53	17.871	2552	2556	2564	rBV	192366	278860	1.12%	0.208%
54	17.936	2564	2567	2571	rVV	35769	48749	0.19%	0.036%
55	18.060	2584	2588	2595	rVB	199128	248072	0.99%	0.185%
56	18.354	2635	2638	2643	rBV4	22987	29213	0.12%	0.022%
57	18.818	2710	2717	2725	rVB3	93350	140379	0.56%	0.105%
58	18.930	2731	2736	2744	rBV3	65332	115965	0.46%	0.087%
59	19.001	2744	2748	2751	rBV	73866	97851	0.39%	0.073%
60	19.030	2751	2753	2757	rVB2	35557	38716	0.15%	0.029%
61	19.154	2771	2774	2778	rBV	52796	61373	0.25%	0.046%
62	19.307	2793	2800	2804	rBV	15261723	25007606	100.00%	18.697%
63	19.371	2804	2811	2824	rVB	5752570	7881208	31.52%	5.892%
64	19.695	2863	2866	2869	rBV2	22321	27245	0.11%	0.020%
65	19.836	2886	2890	2894	rBV	100368	110662	0.44%	0.083%
66	19.907	2900	2902	2906	rVB2	30219	33703	0.13%	0.025%
67	20.130	2938	2940	2944	rVB3	44945	45085	0.18%	0.034%
68	20.224	2952	2956	2964	rBV	739774	947969	3.79%	0.709%
69	20.342	2970	2976	2980	rBV	13549210	19141724	76.54%	14.311%
70	20.859	3059	3064	3076	rBV2	917065	1366447	5.46%	1.022%
71	20.959	3077	3081	3092	rVV	552943	791250	3.16%	0.592%
72	21.148	3108	3113	3124	rBV	3432656	4172022	16.68%	3.119%
73	21.236	3125	3128	3133	rBV	421106	453888	1.81%	0.339%
74	21.712	3205	3209	3212	rBV	312410	405058	1.62%	0.303%
75	21.759	3212	3217	3228	rVV	6889092	10324901	41.29%	7.719%
76	21.842	3228	3231	3238	rVB2	273541	400188	1.60%	0.299%

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Instrument : BNA_M
ClientSampleId : C0AD0

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
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Title : SVOA CALIBRATION

77	22.136	3278	3281	3287	rBV	444170	505114	2.02%	0.378%
78	23.159	3447	3455	3466	rVB2	4047616	7403060	29.60%	5.535%
79	23.295	3472	3478	3487	rVB2	2223013	3858288	15.43%	2.885%

Sum of corrected areas: 133751321

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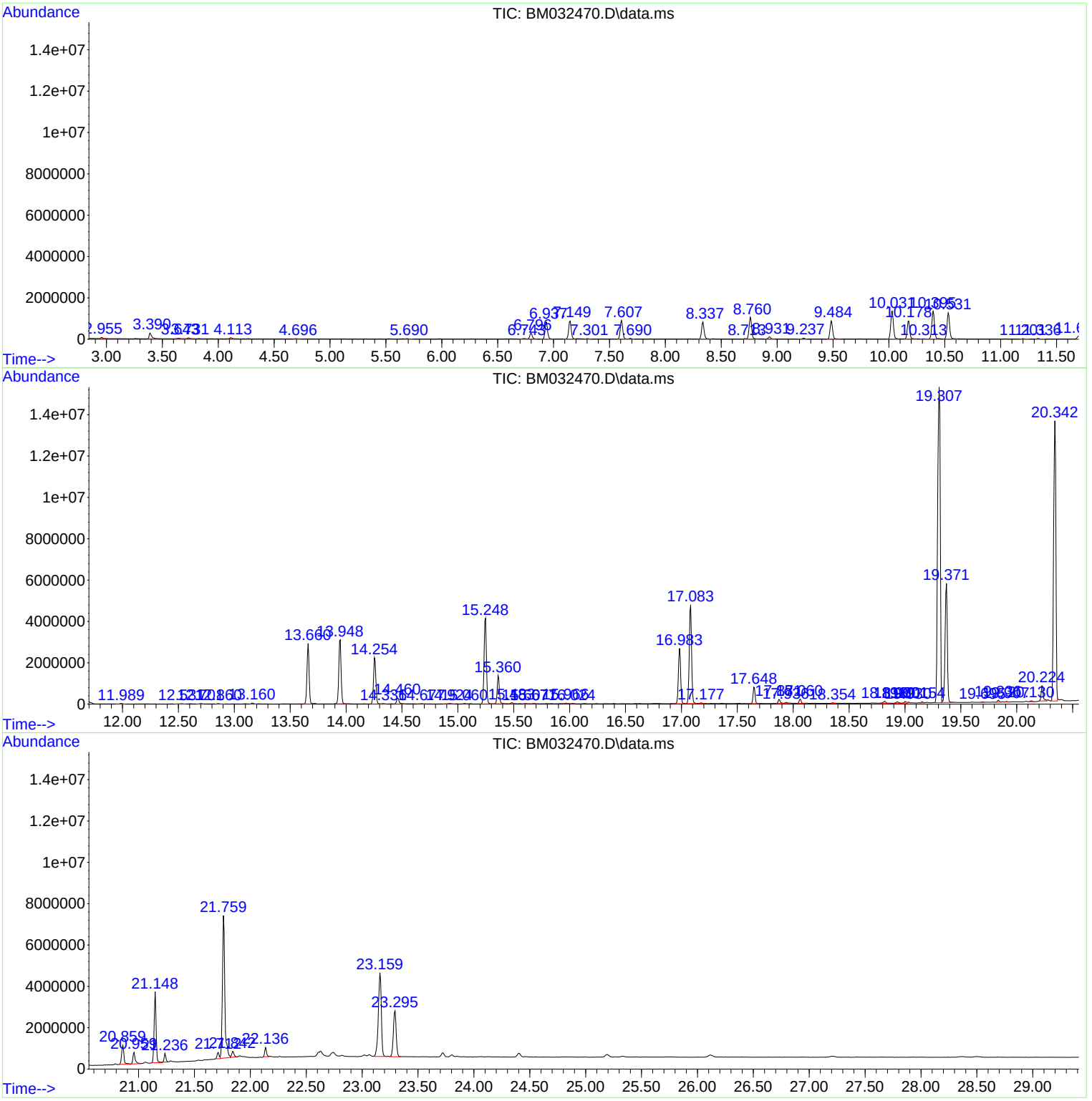
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AD0

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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Data File : BM032470.D
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Instrument : BNA_M
ClientSampleId : C0AD0

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

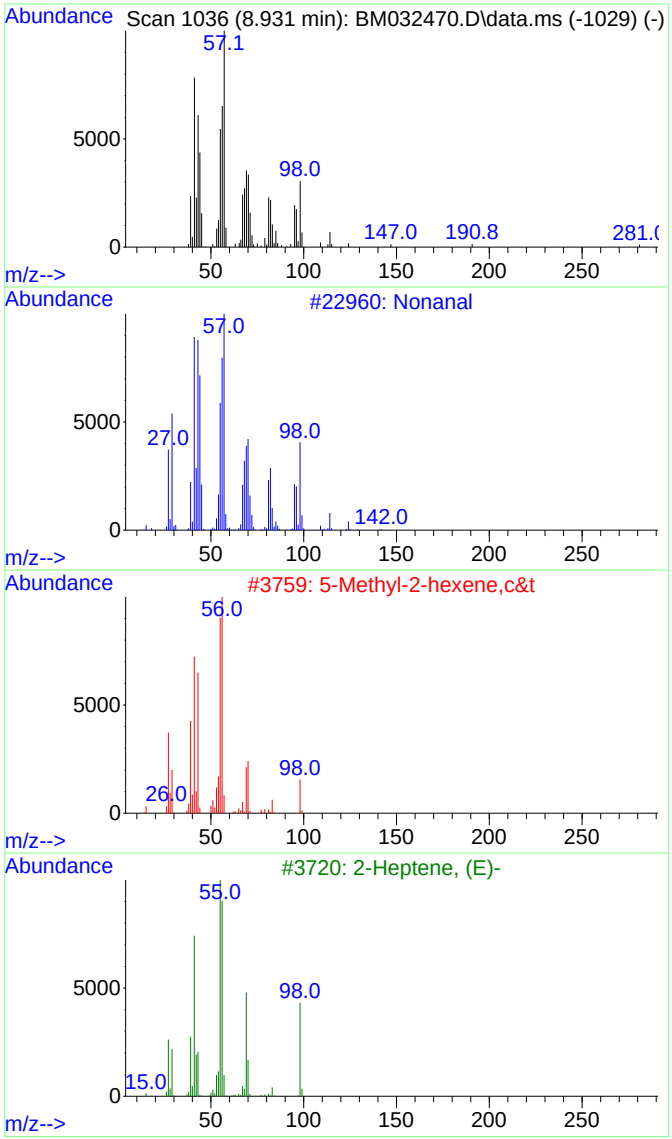
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

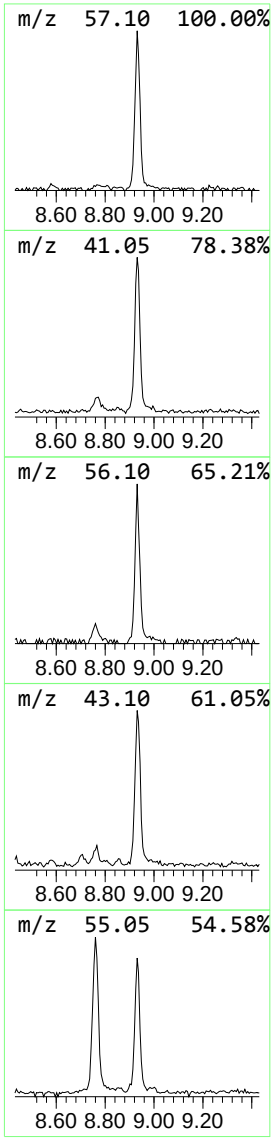
****

Peak Number 1 Nonanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.931	2.22 ng/ul	152648	1,4-Dichlorobenzene-d4	7.607

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	90
2	5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	27
3	2-Heptene, (E)-	98	C7H14	014686-13-6	25
4	2,7-Octadiene, 4-methyl-	124	C9H16	1000061-78-0	25
5	2-Heptene	98	C7H14	000592-77-8	25





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Operator : CG/JU
Sample : M4128-13
Misc :
ALS Vial : 56 Sample Multiplier: 1

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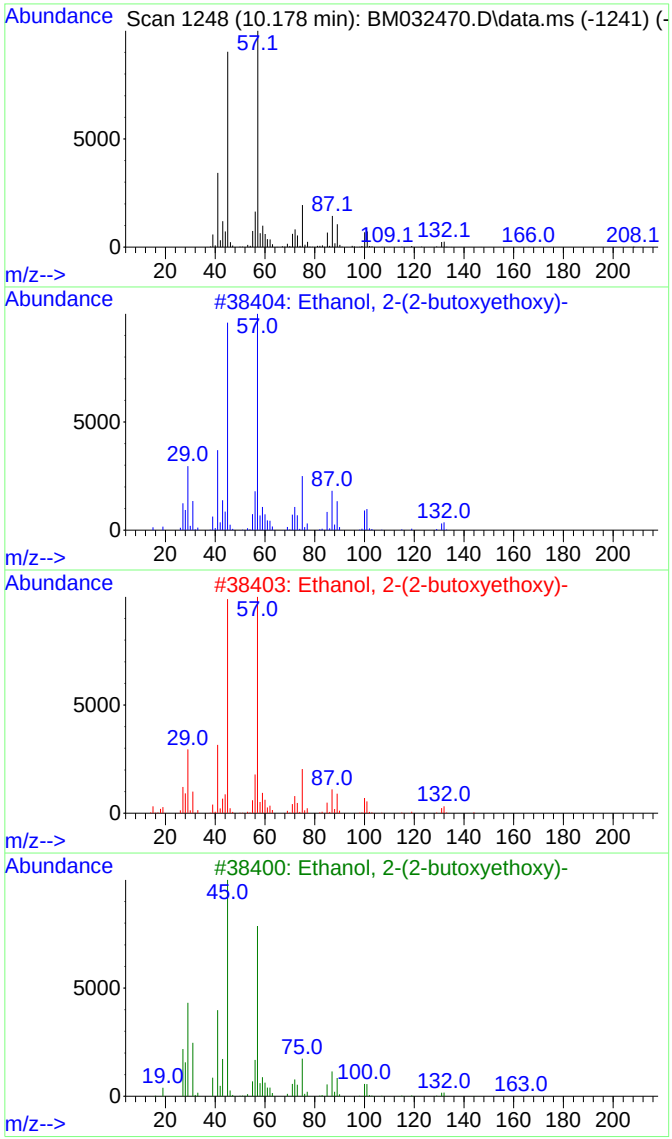
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

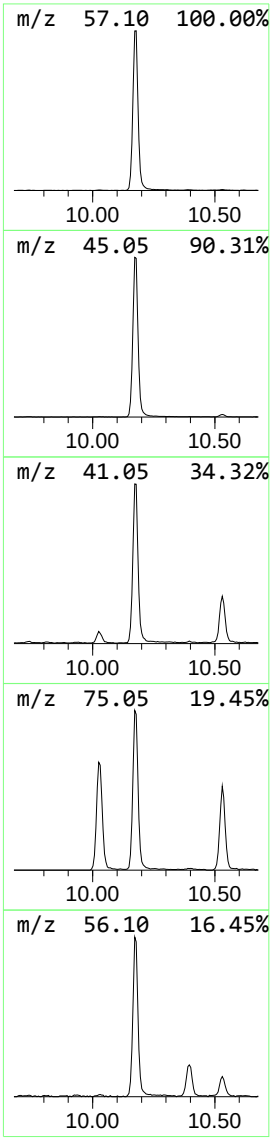
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.178	12.19 ng/ul	1319820	Naphthalene-d8	10.395

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
4	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
5	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72





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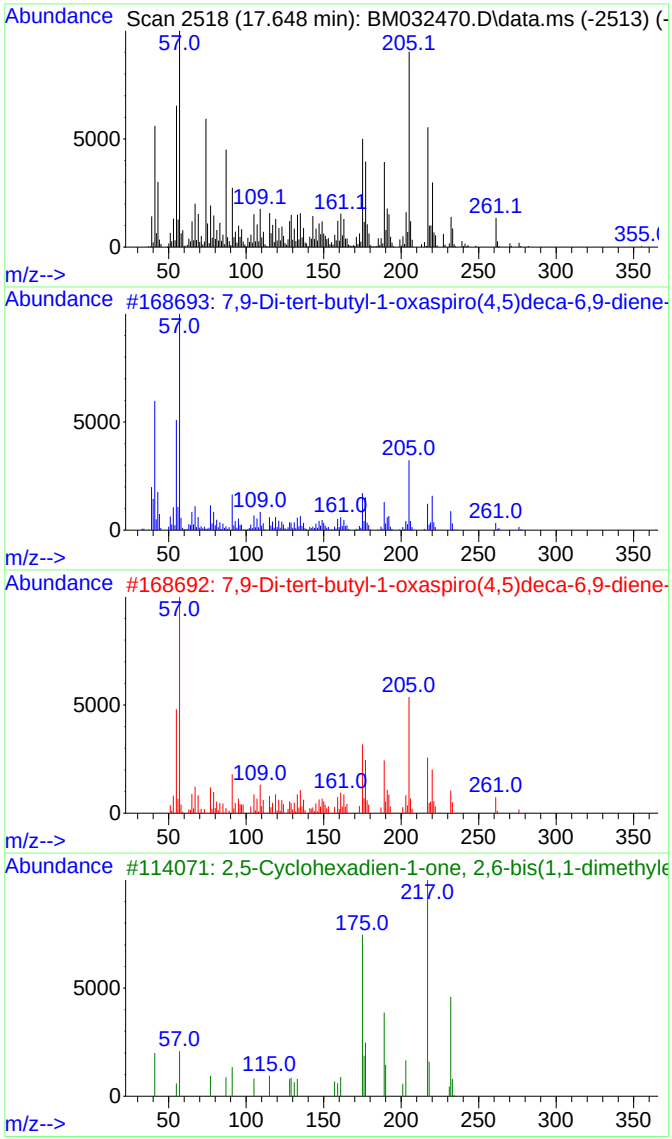
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

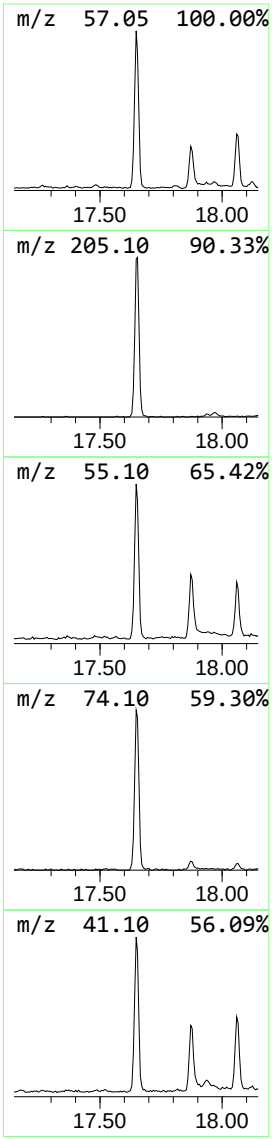
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.648	5.36 ng/ul	991928	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	90
3	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	70
4	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	49
5	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	48





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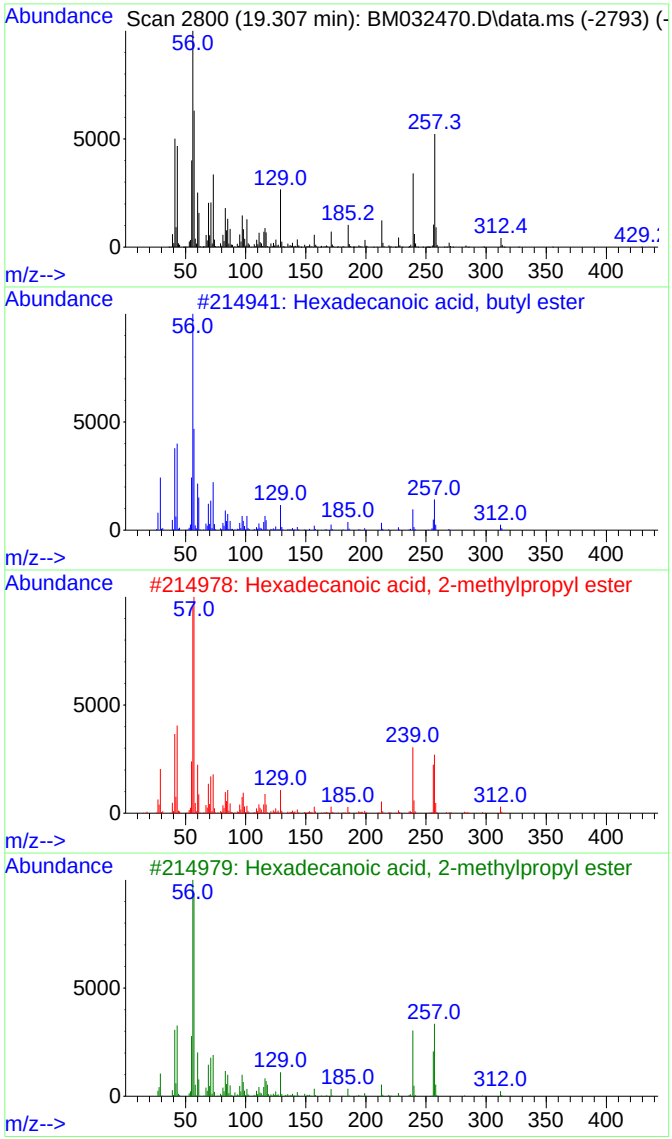
Quant Title : SVOA CALIBRATION

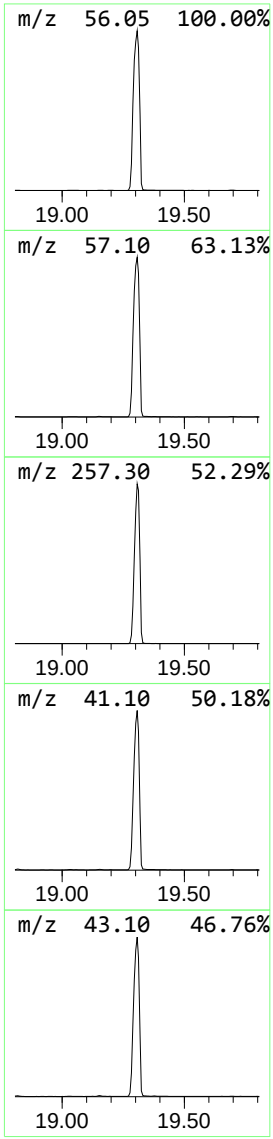
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.307	119.88 ng/ul	25007600	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	92
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	89
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	89
4	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	81
5	Nordextromethorphan	257	C17H23NO	051195-74-5	52





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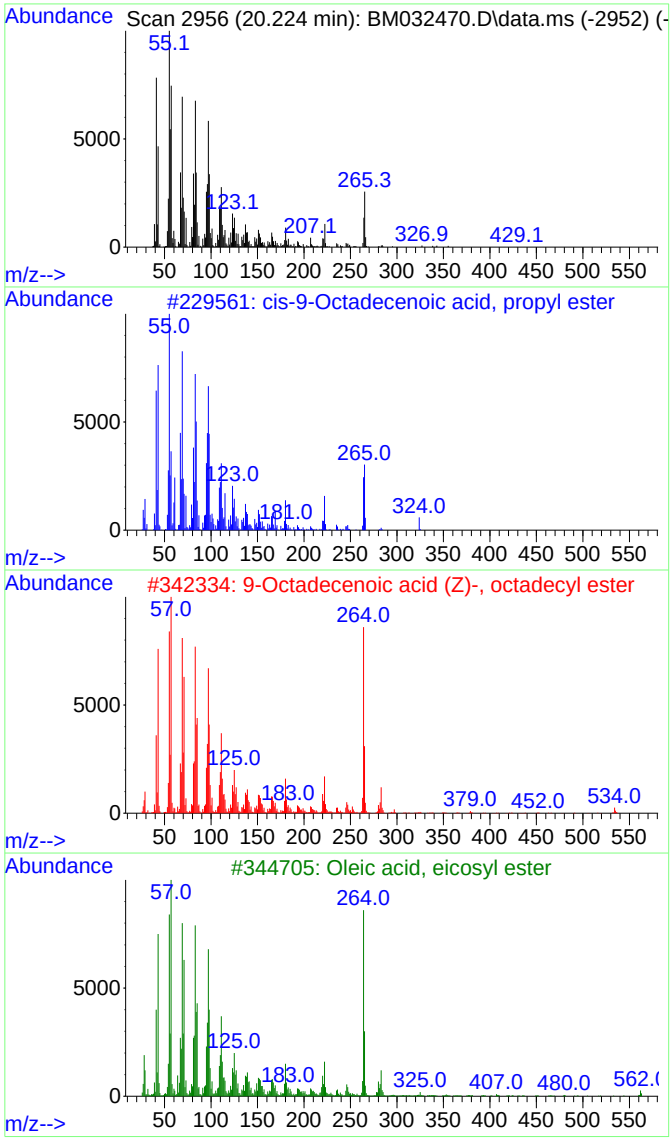
Quant Title : SVOA CALIBRATION

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

****
Peak Number 5 cis-9-Octadecenoic acid, pr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.224	4.54 ng/ul	947969	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-9-Octadecenoic acid, propyl ...	324	C21H40O2	1000405-15-0	91
2	9-Octadecenoic acid (Z)-, octade...	535	C36H70O2	017673-49-3	90
3	Oleic acid, eicosyl ester	563	C38H74O2	022393-88-0	90
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
5	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	87



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Instrument : BNA_M
ClientSampleId : C0AD0

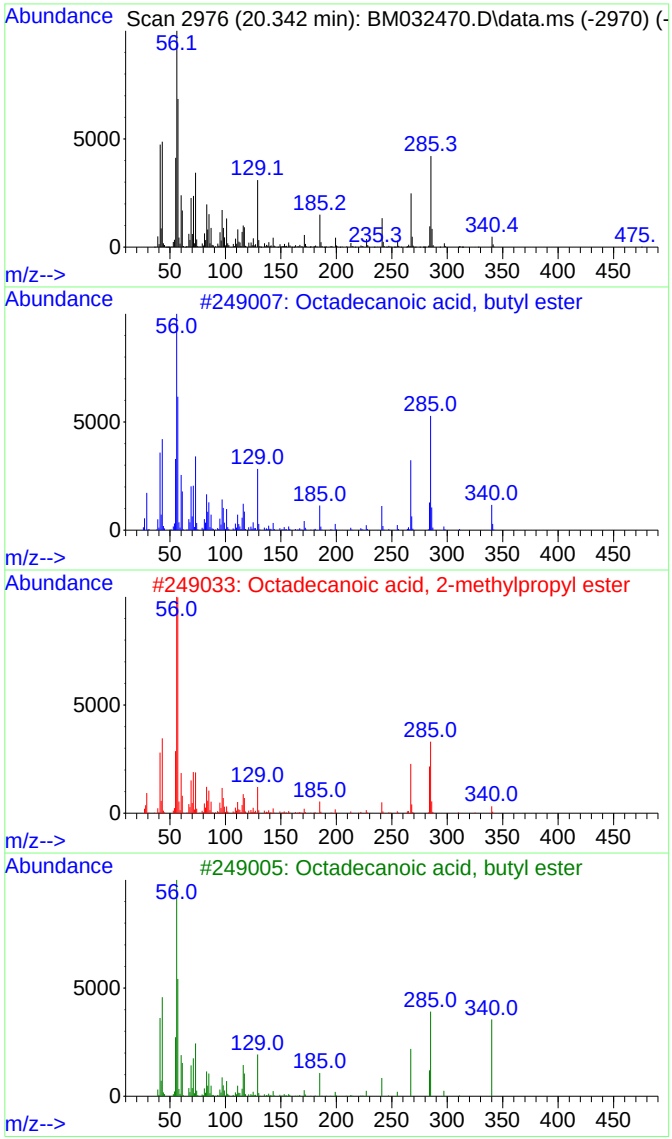
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

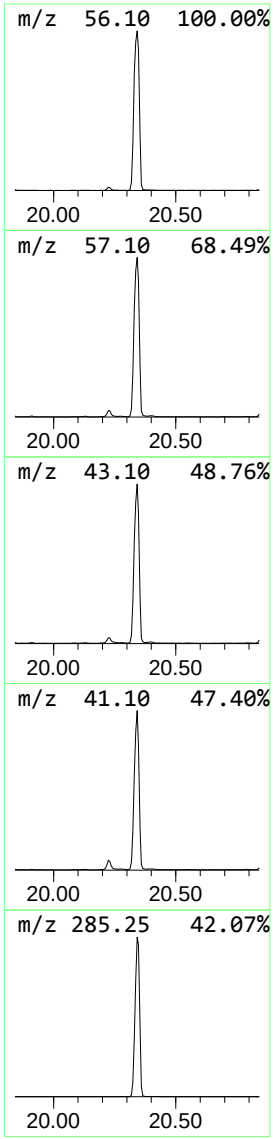
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.342	91.76 ng/ul	19141700	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	99
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	94
3	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
4	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	78





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Instrument : BNA_M
ClientSampleId : C0AD0

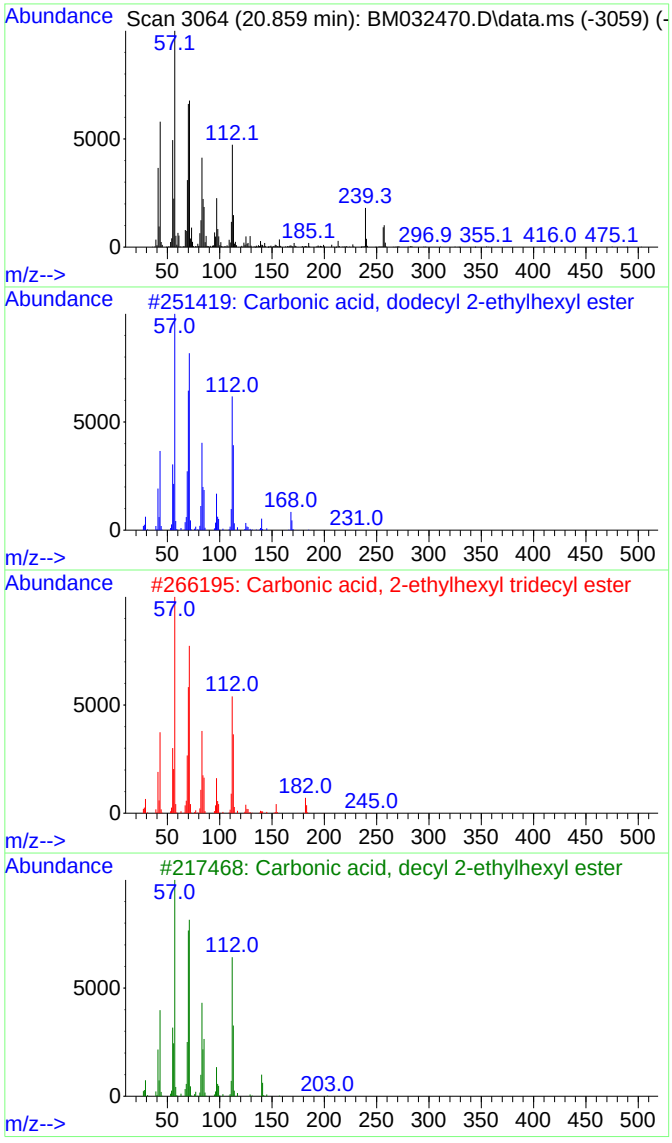
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

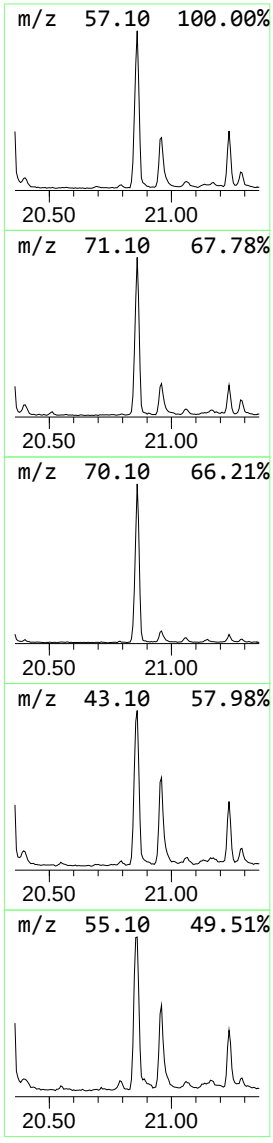
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Carbonic acid, dodecyl 2-et... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.859	6.55 ng/ul	1366450	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, dodecyl 2-ethylhe...	342	C21H42O3	1000383-13-9	74
2	Carbonic acid, 2-ethylhexyl trid...	356	C22H44O3	1000383-14-0	74
3	Carbonic acid, decyl 2-ethylhexy...	314	C19H38O3	1000383-13-7	74
4	Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	72
5	Carbonic acid, 2-ethylhexyl hept...	412	C26H52O3	1000383-14-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101121\
Data File : BM032470.D
Acq On : 12 Oct 2021 22:35
Operator : CG/JU
Sample : M4128-13
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AD0

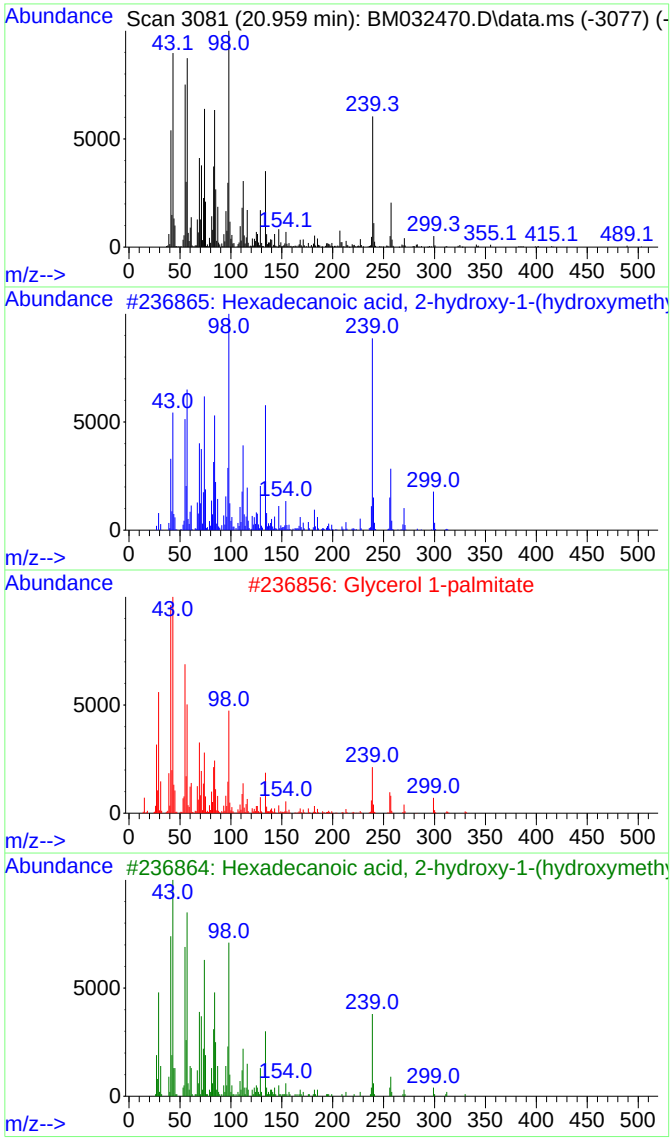
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

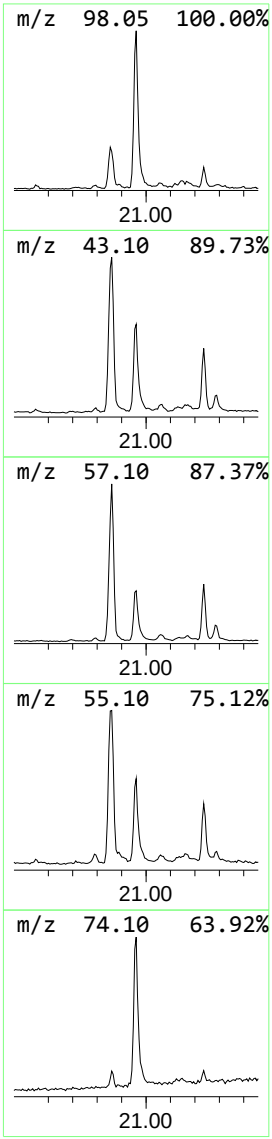
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexadecanoic acid, 2-hydrox... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.959	3.79 ng/ul	791250	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2-hydroxy-1-(...	330	C19H38O4	023470-00-0	80
2	Glycerol 1-palmitate	330	C19H38O4	000542-44-9	80
3	Hexadecanoic acid, 2-hydroxy-1-(...	330	C19H38O4	023470-00-0	76
4	Acetonitrile, isothiocyanato-	98	C3H2N2S	032772-75-1	35
5	Dodecanedioic acid	230	C12H22O4	000693-23-2	35





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Data File : BM032470.D
Acq On : 12 Oct 2021 22:35
Operator : CG/JU
Sample : M4128-13
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AD0

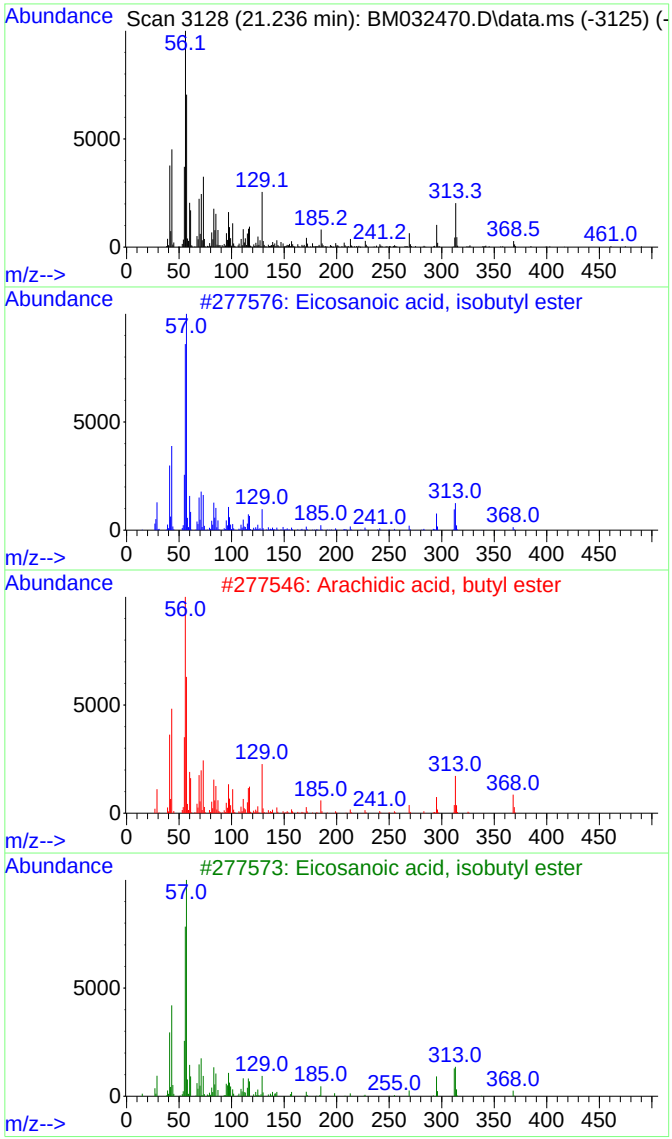
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM100521.M
Quant Title : SVOA CALIBRATION

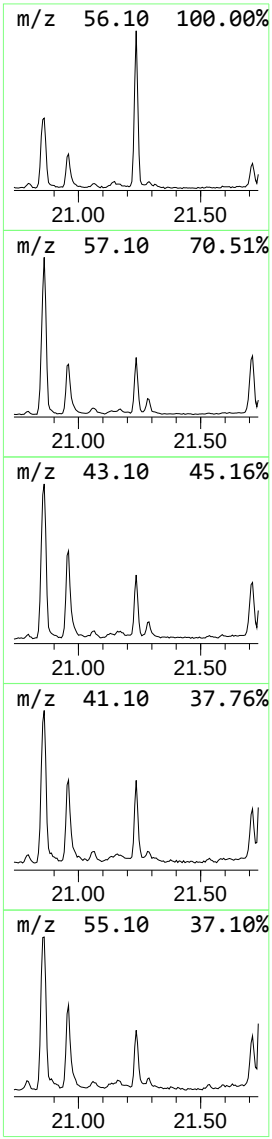
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Eicosanoic acid, isobutyl e... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.236	2.18 ng/ul	453888	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, isobutyl ester	368	C24H48O2	1000451-98-5	95
2	Arachidic acid, butyl ester	368	C24H48O2	026718-91-2	94
3	Eicosanoic acid, isobutyl ester	368	C24H48O2	1000451-98-5	93
4	Arachidic acid, butyl ester	368	C24H48O2	026718-91-2	83
5	Tetracosanoic acid, butyl ester	424	C28H56O2	042233-42-1	76





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Data File : BM032470.D
Acq On : 12 Oct 2021 22:35
Operator : CG/JU
Sample : M4128-13
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0AD0

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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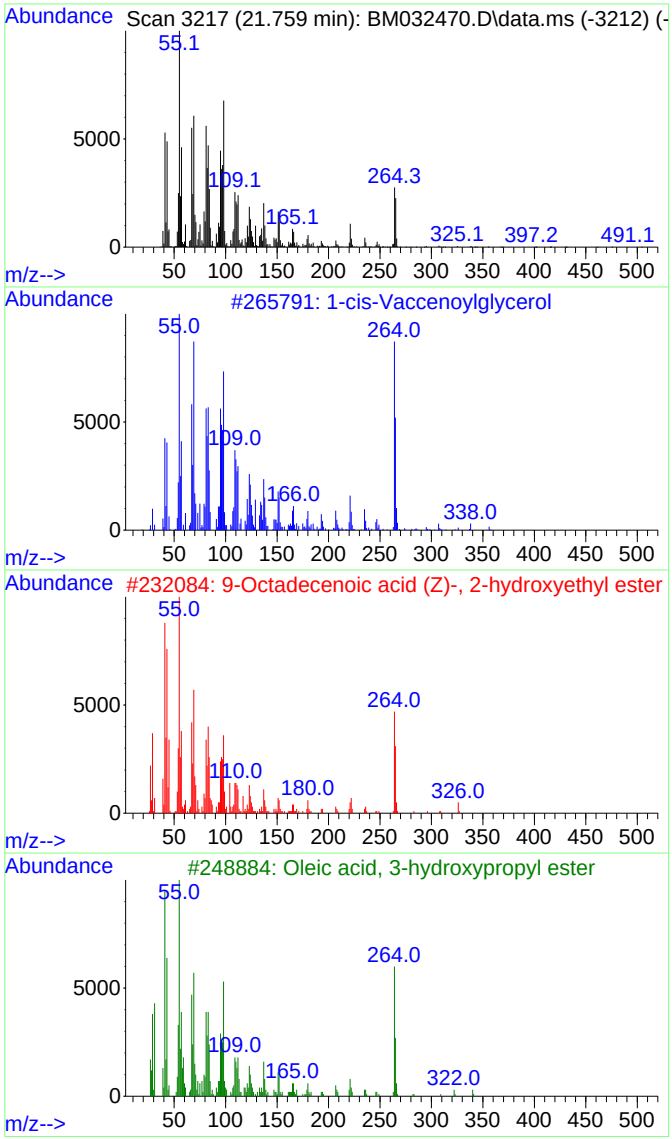
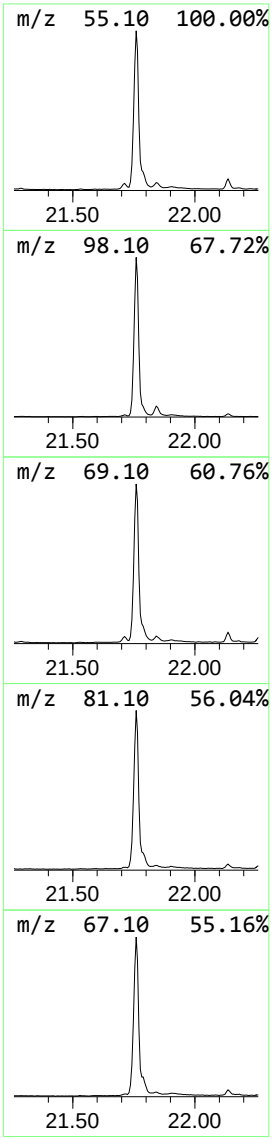
Peak Number 10 1-cis-Vaccenoylglycerol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.759	49.50 ng/ul	10324900	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-cis-Vaccenoylglycerol	356	C21H40O4	020379-67-3	90
2	9-Octadecenoic acid (Z)-, 2-hydr...	326	C20H38O3	004500-01-0	90
3	Oleic acid, 3-hydroxypropyl ester	340	C21H40O3	000821-17-0	87
4	9-Octadecenoic acid (Z)-, 2,3-di...	356	C21H40O4	000111-03-5	83
5	9-Octadecenoic acid (Z)-, 2-hydr...	356	C21H40O4	003443-84-3	81





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Data File : BM032470.D
Acq On : 12 Oct 2021 22:35
Operator : CG/JU
Sample : M4128-13
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AD0

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

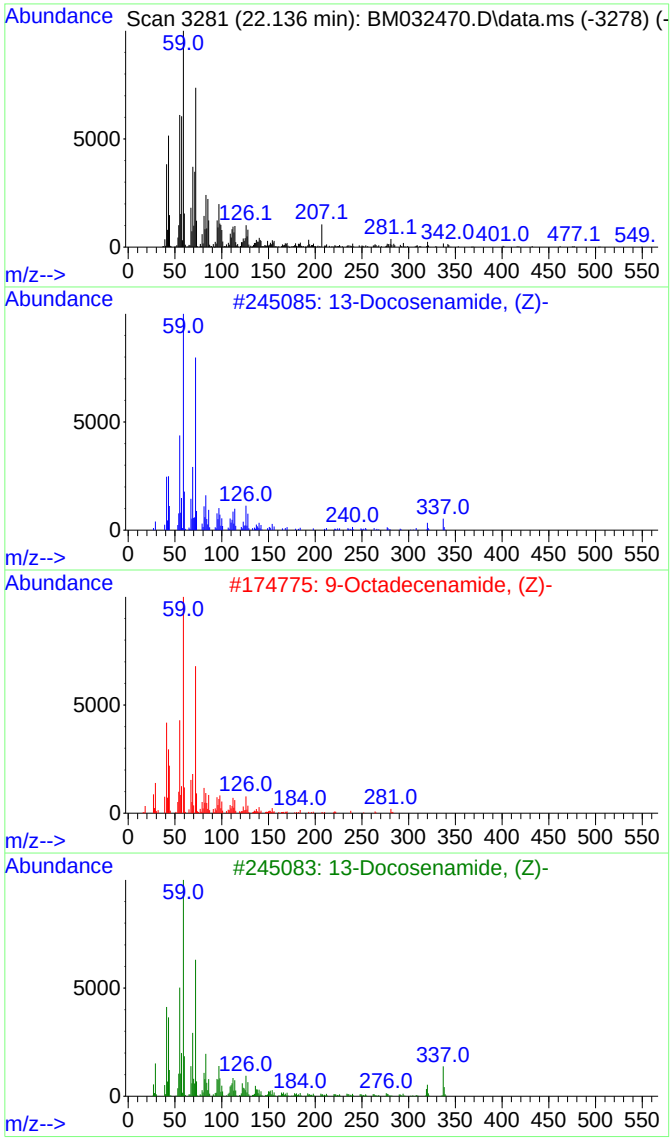
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

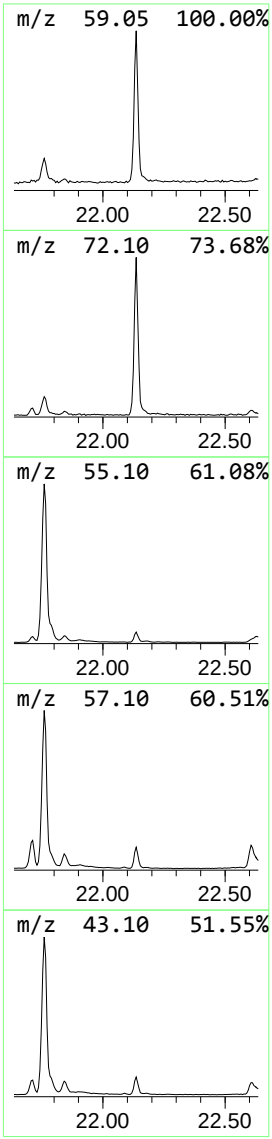
****

Peak Number 11 13-Docosenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.136	2.42 ng/ul	505114	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	95
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	89
4	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	70
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68





Tentatively Identified Compound (LSC) summary

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Data File : BM032470.D
Acq On : 12 Oct 2021 22:35
Operator : CG/JU
Sample : M4128-13
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Instrument :
BNA_M
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C0AD0

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
Nonanal	8.931	2.2	ng/ul	152648	1	7.607	1373780	20.0
Ethanol, 2-(2-b...	10.178	12.2	ng/ul	1319820	2	10.395	2166270	20.0
7,9-Di-tert-but...	17.648	5.4	ng/ul	991928	4	16.983	3700990	20.0
Hexadecanoic ac...	19.307	119.9	ng/ul	25007600	5	21.148	4172020	20.0
cis-9-Octadecen...	20.224	4.5	ng/ul	947969	5	21.148	4172020	20.0
Octadecanoic ac...	20.342	91.8	ng/ul	19141700	5	21.148	4172020	20.0
Carbonic acid, ...	20.859	6.5	ng/ul	1366450	5	21.148	4172020	20.0
Hexadecanoic ac...	20.959	3.8	ng/ul	791250	5	21.148	4172020	20.0
Eicosanoic acid...	21.236	2.2	ng/ul	453888	5	21.148	4172020	20.0
1-cis-Vaccenoyl...	21.759	49.5	ng/ul	10324900	5	21.148	4172020	20.0
13-Docosenamide...	22.136	2.4	ng/ul	505114	5	21.148	4172020	20.0