LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032921\
Data File : BF123501.D
Acq On : 29 Mar 2021 18:11
Operator : JU/CG
Sample : M1813-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L07

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\METHODS\8270-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123501.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	18	26	36	rVB	1118315	1440046	18.74%	2.702%
2	2.346	39	44	51	rVB	192434	233696	3.04%	0.438%
3	3.546	227	248	251	rBV	851831	3790119	49.31%	7.111%
4	5.122	508	516	522	rBV	252011	303767	3.95%	0.570%
5	5.522	579	584	587	rBV	4829080	4426046	57.59%	8.304%
6	6.522	748	754	757	rBV	4477745	4549552	59.20%	8.536%
7	6.898	814	818	821	rBV	2067975	1642811	21.37%	3.082%
8	7.457	908	913	916	rBV	3180402	2927611	38.09%	5.493%
9	8.181	1031	1036	1040	rBV	2384188	2179242	28.35%	4.089%
10	9.263	1214	1220	1223	rBV	4761442	4544224	59.13%	8.526%
11	9.410	1237	1245	1271	rBV	429178	906075	11.79%	1.700%
12	9.651	1282	1286	1290	rBV	132596	104528	1.36%	0.196%
13	9.939	1327	1335	1339	rBV	2657721	2513404	32.70%	4.716%
14	10.728	1464	1469	1473	rBV	3254066	3129279	40.72%	5.871%
15	11.433	1584	1589	1592	rBV	2690997	2427226	31.58%	4.554%
16	11.957	1672	1678	1688	rBV	778508	1016516	13.23%	1.907%
17	12.416	1751	1756	1759	rBV	104946	96182	1.25%	0.180%
18	12.474	1760	1766	1770	rBV3	46962	99391	1.29%	0.186%
19	12.645	1790	1795	1797	rBV	108203	101172	1.32%	0.190%
20	12.745	1807	1812	1823	rBV	248143	344353	4.48%	0.646%
21	13.022	1855	1859	1862	rBV	5059815	4413692	57.43%	8.281%
22	13.504	1932	1941	1944	rBV4	75466	207171	2.70%	0.389%
23	13.563	1948	1951	1956	rVB4	85834	120480	1.57%	0.226%
24	13.951	2012	2017	2032	rVB2	298721	694719	9.04%	1.303%
25	14.068	2032	2037	2042	rBV2	6600274	7685668	100.00%	14.420%
26	14.398	2087	2093	2096	rBV	57894	132963	1.73%	0.249%
27	14.504	2102	2111	2113	rBV5	52519	144208	1.88%	0.271%
28	14.645	2132	2135	2139	rVV	367022	326865	4.25%	0.613%
29	14.716	2143	2147	2151	rVB	905624	814274	10.59%	1.528%
30	15.292	2240	2245	2250	rBV5	51166	122022	1.59%	0.229%
31	15.339	2250	2253	2261	rVB	257555	323035	4.20%	0.606%
32	15.574	2288	2293	2298	rBV	1099816	1381986	17.98%	2.593%
33	15.615	2298	2300	2307	rVB2	56696	77449	1.01%	0.145%
34	16.074	2374	2378	2386	rVB2	53312	78385	1.02%	0.147%

Sum of corrected areas: 53298157

Instrument :
BNA_F
ClientSampleId :
L07

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032921\
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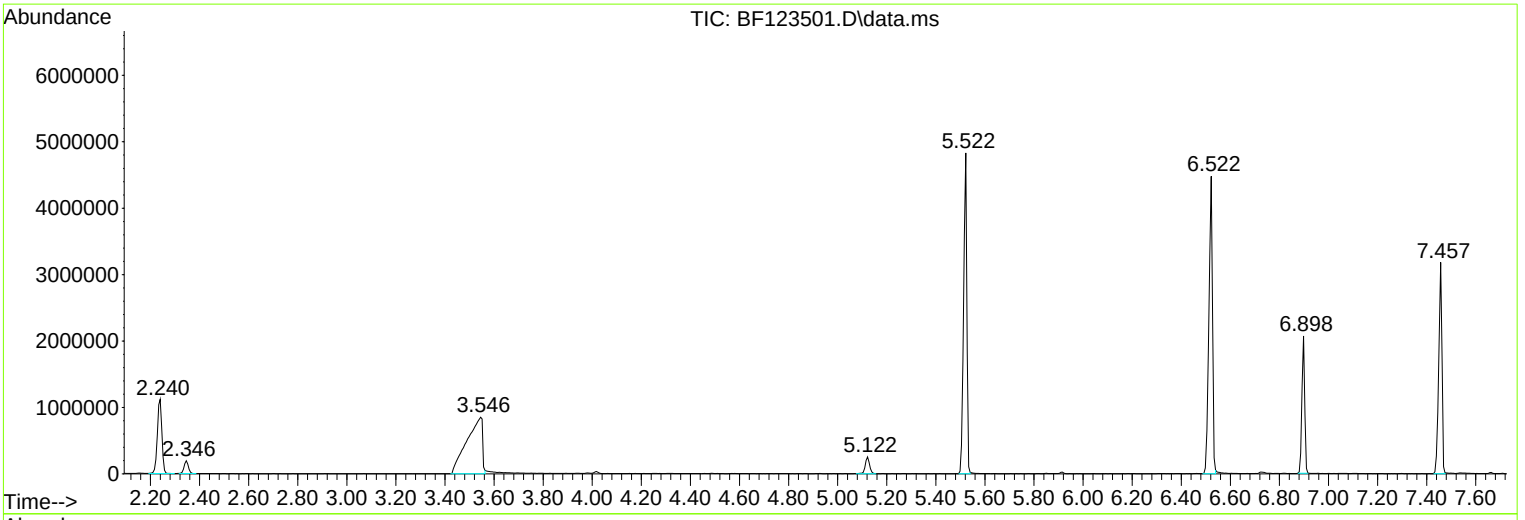
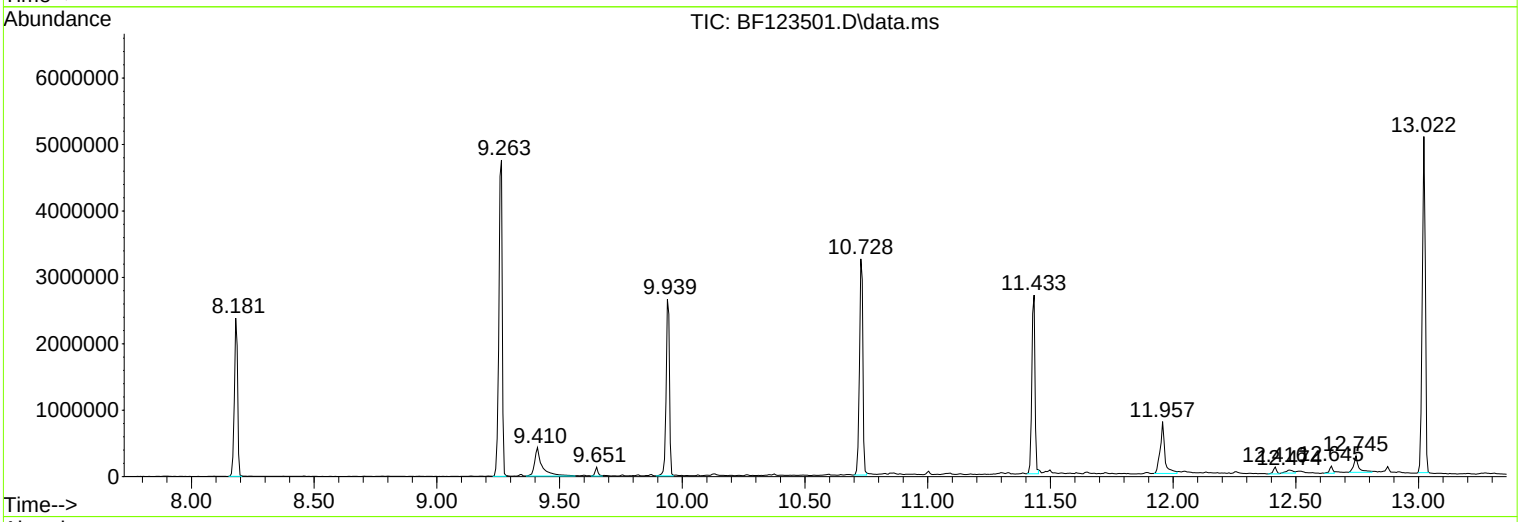
Misc :
ALS Vial : 4 Sample Multiplier: 1

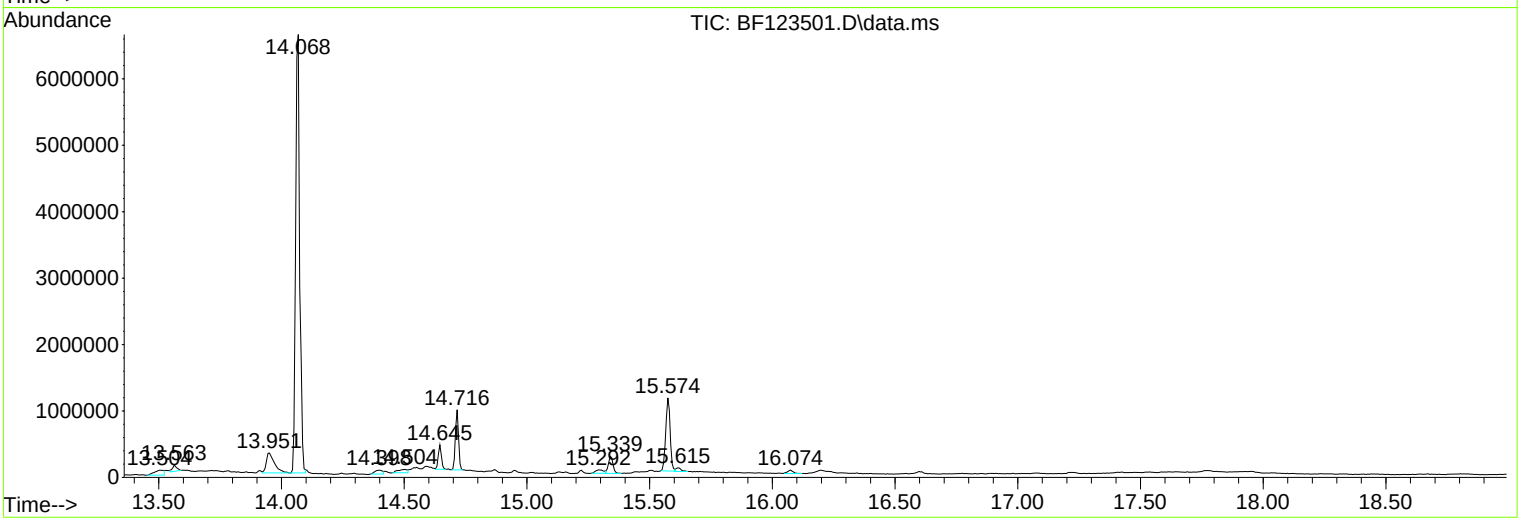
Instrument :
BNA_F
ClientSampleId :
L07

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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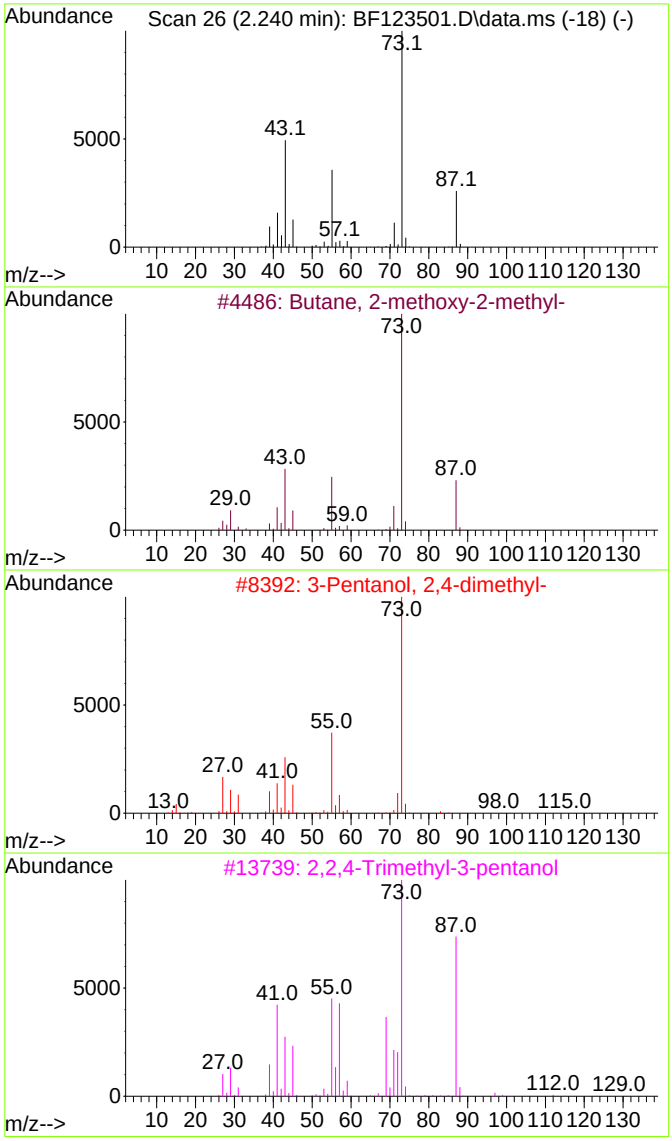
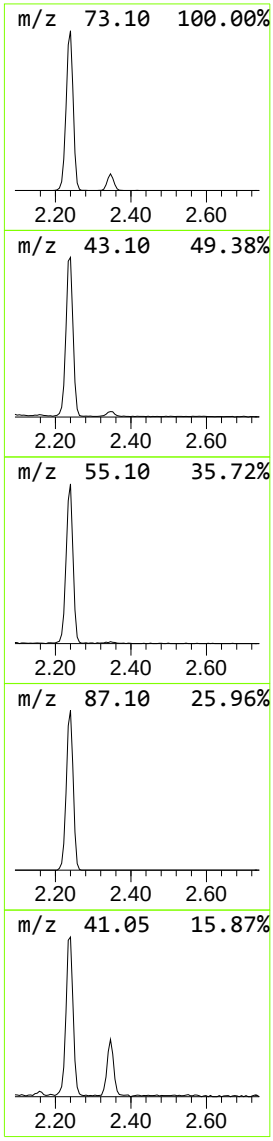
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	17.53 ng	1440050	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Instrument : BNA_F
ClientSampleId : L07

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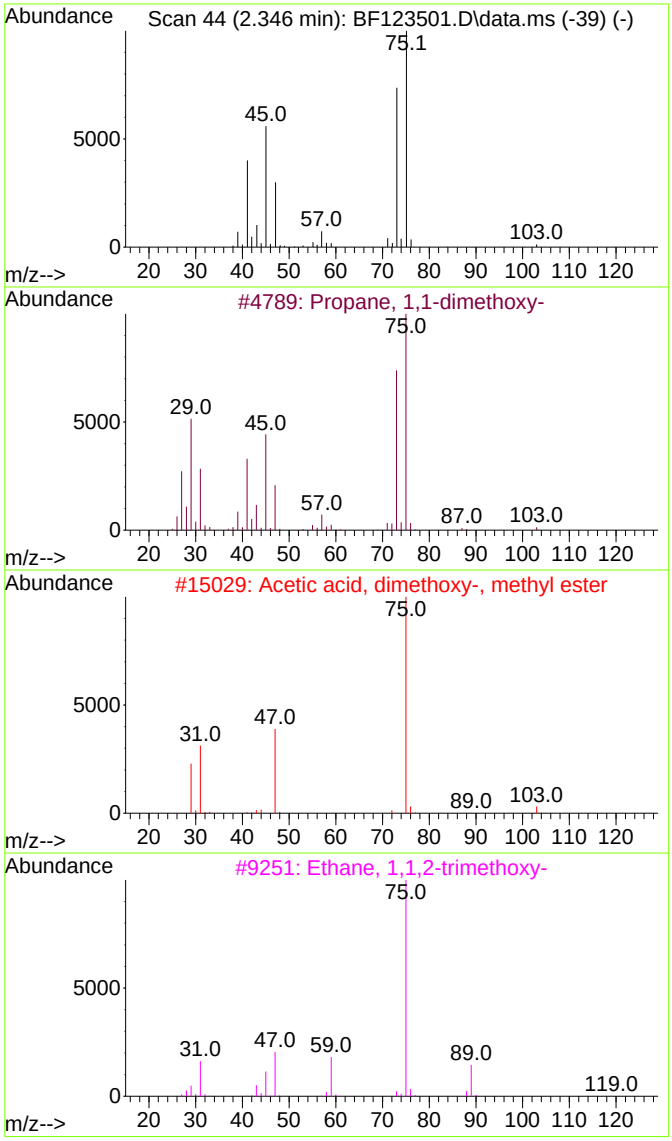
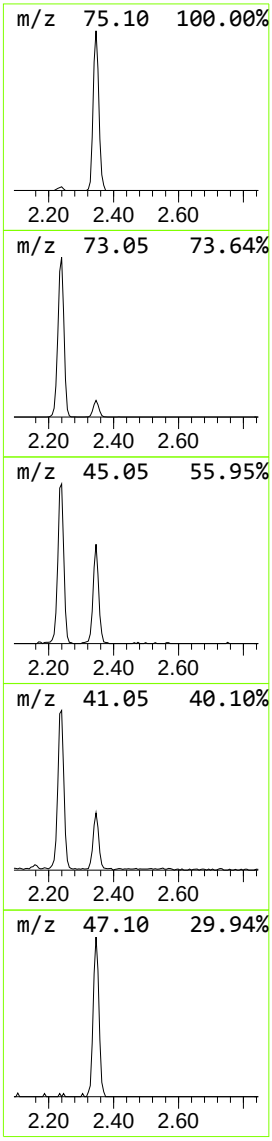
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.346	2.85 ng	233696	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	38
3	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	33
4	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
5	2-Propanone, 1,1-dimethoxy-	118	C5H10O3	006342-56-9	28





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Sample : M1813-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L07

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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TIC Library : C:\DATABASE\NIST11.L
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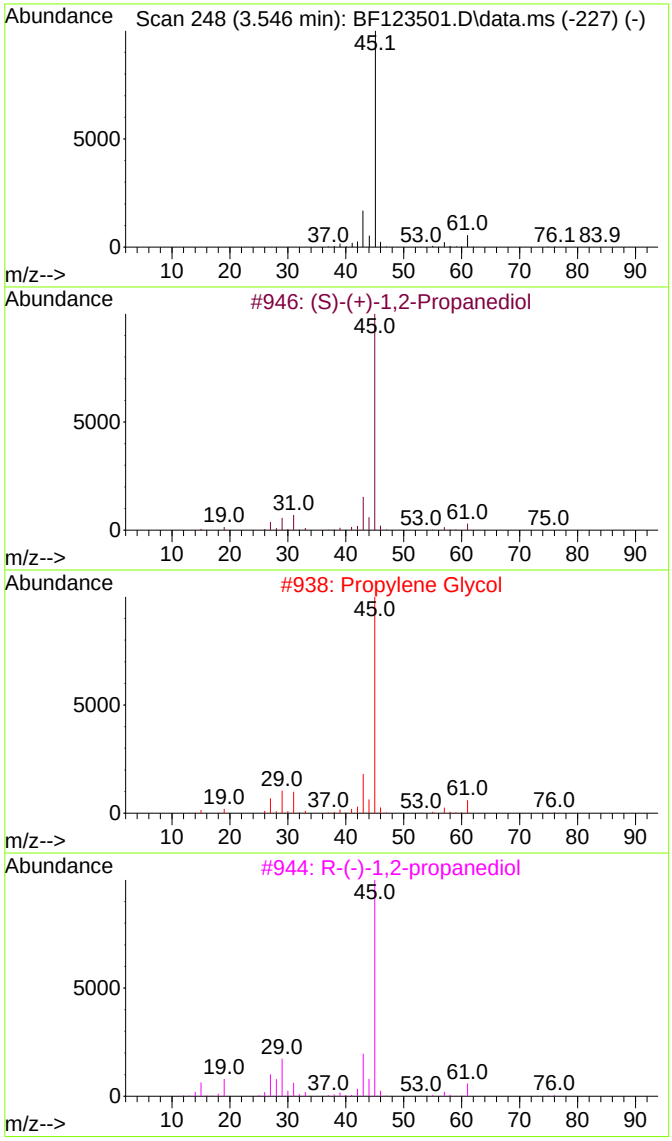
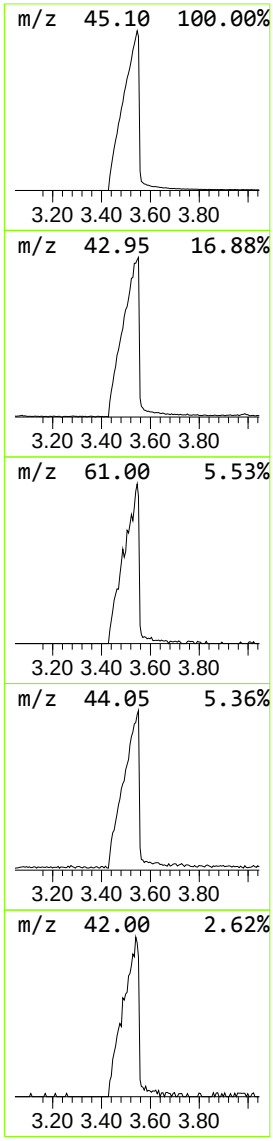
****

Peak Number 3 (S)-(+)-1,2-Propanediol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.546	46.14 ng	3790120	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	47
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	7





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Instrument : BNA_F
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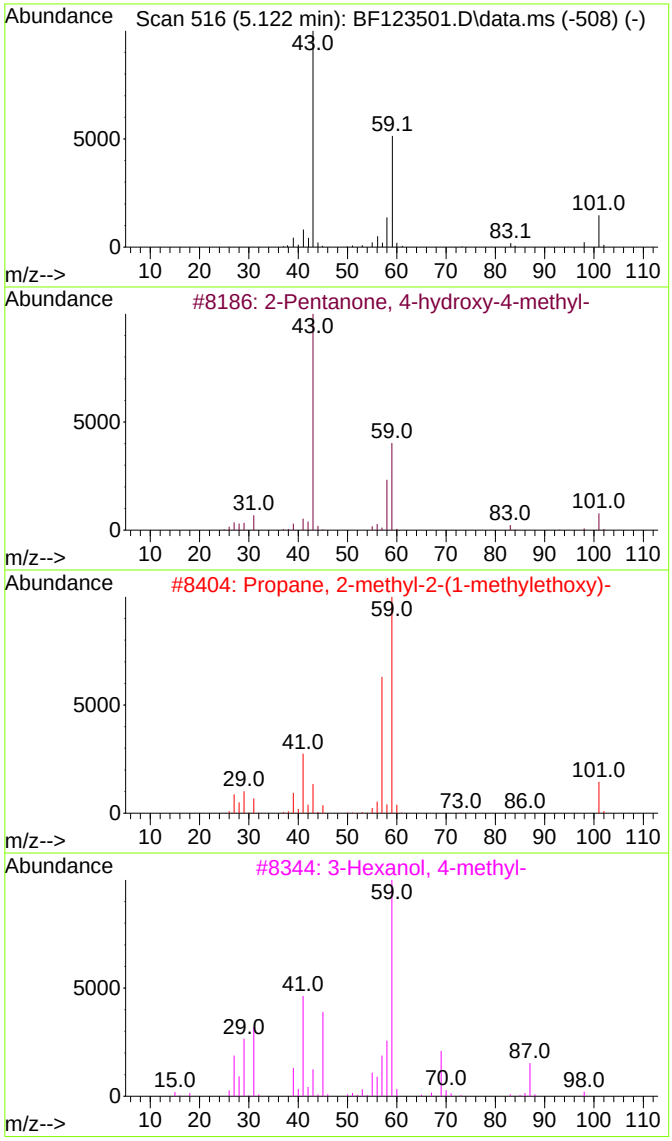
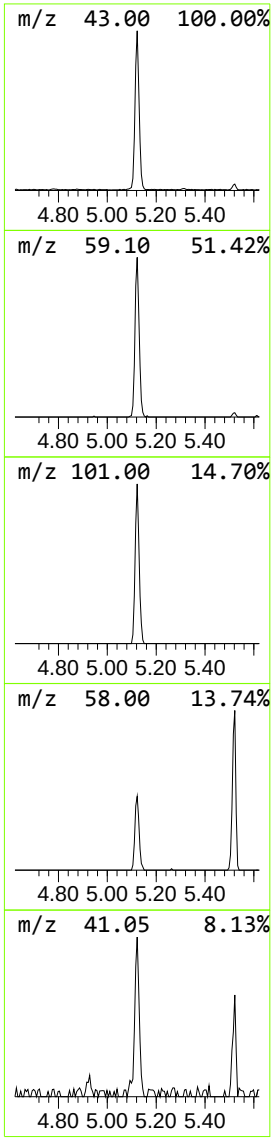
****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	3.70 ng	303767	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Instrument : BNA_F
ClientSampleId : L07

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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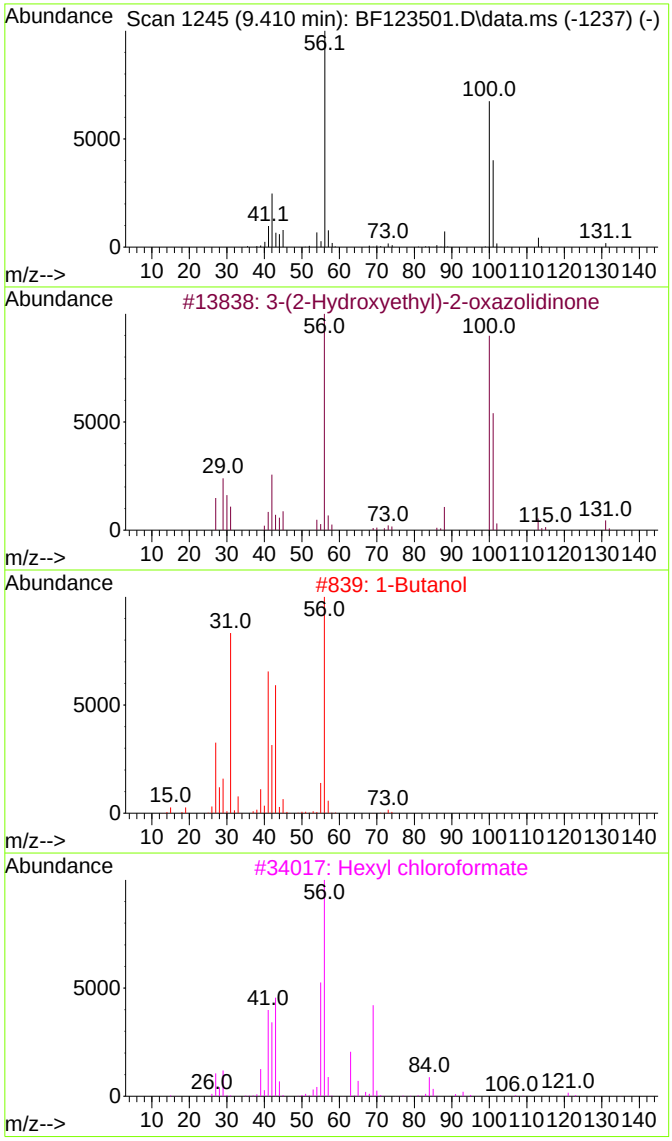
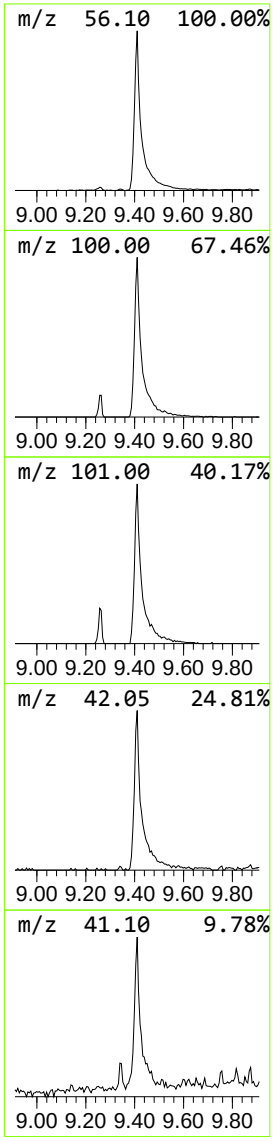
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.410	7.21 ng	906075	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	83
2	1-Butanol	74	C4H10O	000071-36-3	38
3	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	23
4	4-Morpholineethanol	131	C6H13NO2	000622-40-2	22
5	2H-1,4-Oxazine-4-propanoic acid,...	173	C8H15NO3	1000362-52-8	10





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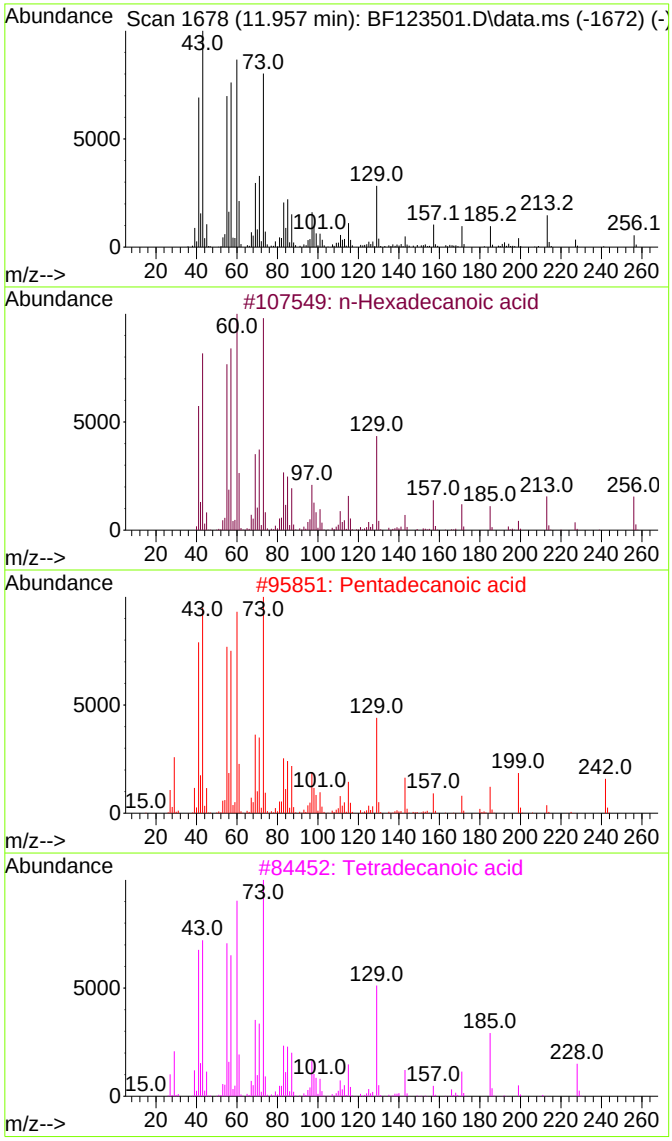
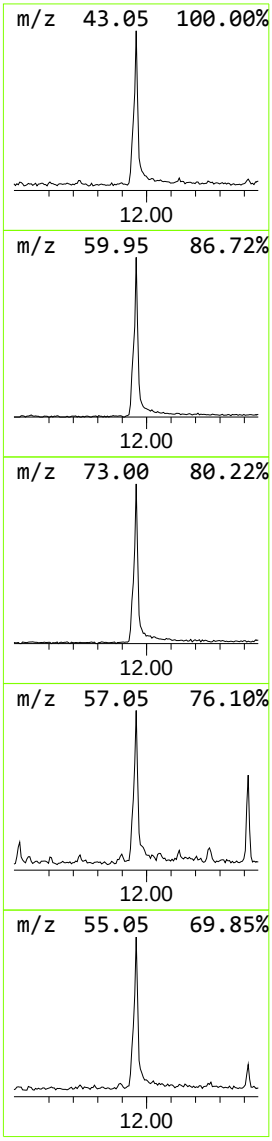
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	8.38 ng	1016520	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	78
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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TIC Library : C:\DATABASE\NIST11.L
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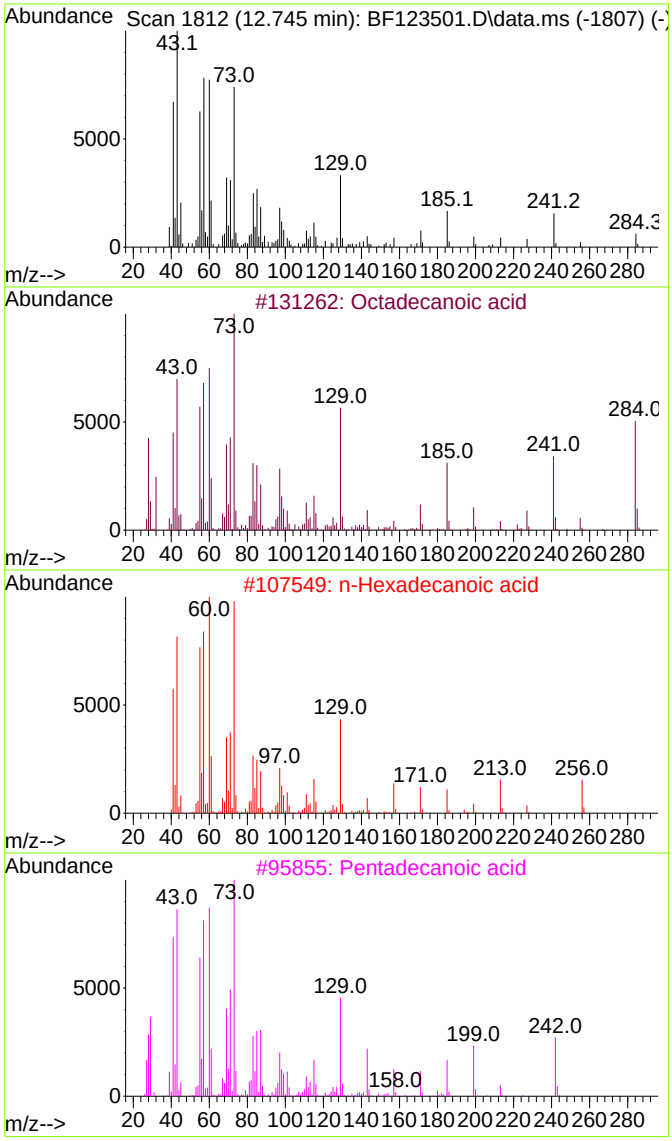
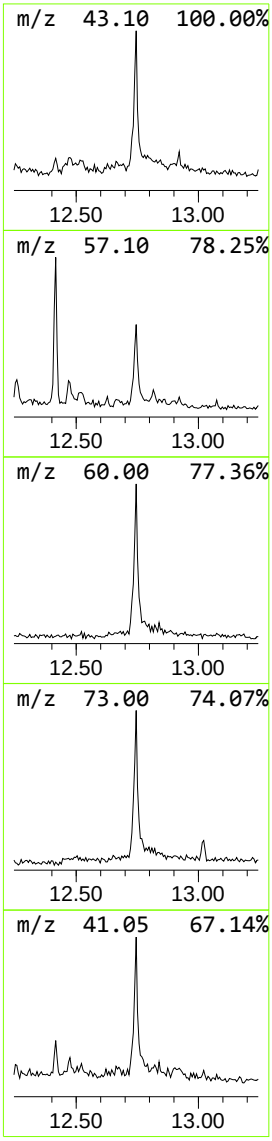
****

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.745	2.84 ng	344353	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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TIC Library : C:\DATABASE\NIST11.L
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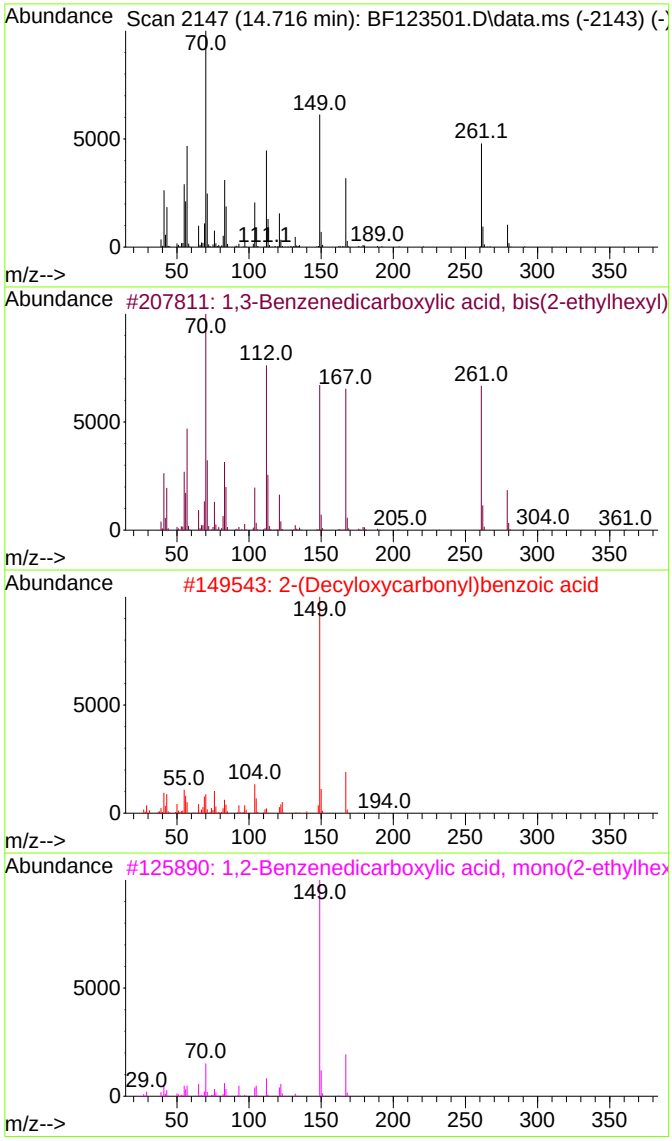
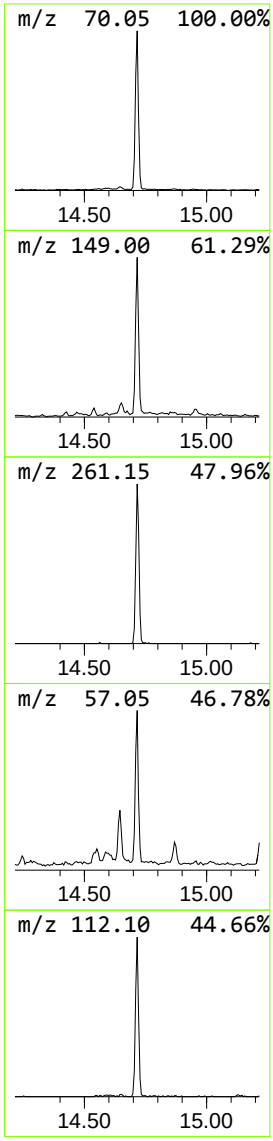
****
Peak Number 8 1,3-Benzenedicarboxylic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.716	2.12 ng	814274	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	68
2	2-(Decyloxycarbonyl)benzoic acid	306	C18H26O4	1000373-53-2	35
3	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	32
4	Cyclohexaneamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	25
5	9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	25





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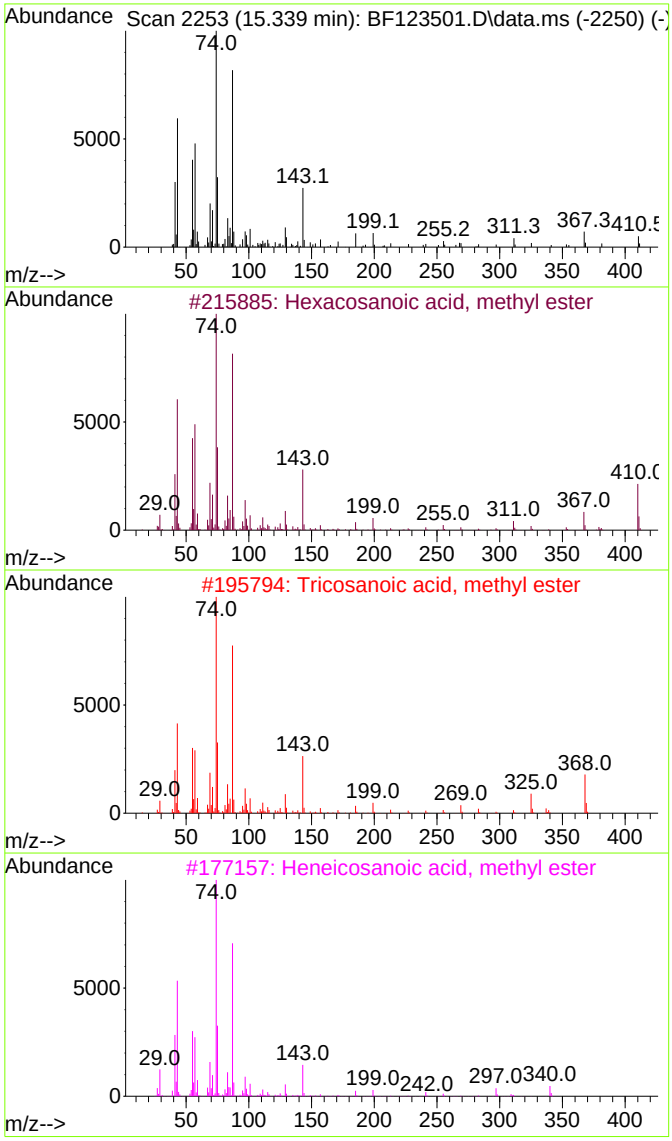
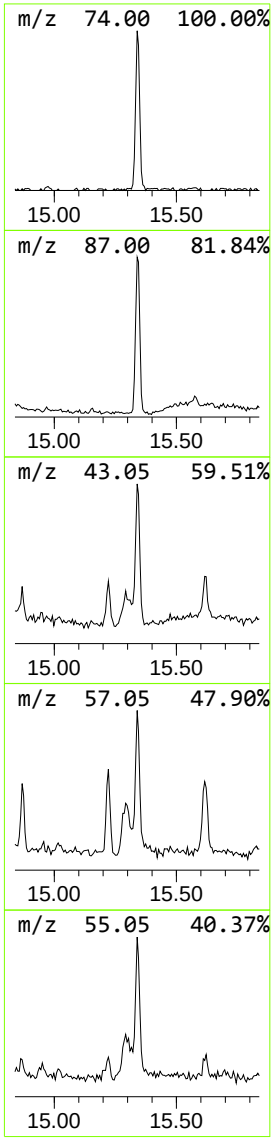
****
Peak Number 9 Hexacosanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	4.67 ng	323035	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosanoic acid, methyl ester	410	C27H54O2	005802-82-4	95
2	Tricosanoic acid, methyl ester	368	C24H48O2	002433-97-8	90
3	Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	86
4	Methyl stearate	298	C19H38O2	000112-61-8	86
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032921\
Data File : BF123501.D
Acq On : 29 Mar 2021 18:11
Operator : JU/CG
Sample : M1813-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L07

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.240	17.5	ng	1440050	1	6.898	1642810	20.0
Propane, 1,1-di...	2.346	2.9	ng	233696	1	6.898	1642810	20.0
(S)-(+)-1,2-Pro...	3.546	46.1	ng	3790120	1	6.898	1642810	20.0
2-Pentanone, 4-...	5.122	3.7	ng	303767	1	6.898	1642810	20.0
3-(2-Hydroxyeth...	9.410	7.2	ng	906075	3	9.939	2513400	20.0
n-Hexadecanoic ...	11.957	8.4	ng	1016520	4	11.433	2427230	20.0
Octadecanoic acid	12.745	2.8	ng	344353	4	11.433	2427230	20.0
1,3-Benzenedica...	14.716	2.1	ng	814274	5	14.080	7685670	20.0
Hexacosanoic ac...	15.339	4.7	ng	323035	6	15.574	1381990	20.0