LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022021\
Data File : BF123246.D
Acq On : 20 Feb 2021 15:40
Operator : JU/CG
Sample : M1430-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H-2

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-BF021921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123246.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	15	rVB	353367	444673	7.02%	0.911%
2	5.081	504	509	514	rVB	52849	64889	1.03%	0.133%
3	5.475	571	576	579	rBV	4231202	3923331	61.98%	8.041%
4	6.481	742	747	759	rBV	3751078	4317926	68.21%	8.850%
5	6.857	807	811	814	rBV	1291659	1079065	17.05%	2.212%
6	7.416	901	906	909	rBV	2883148	2696757	42.60%	5.527%
7	8.139	1024	1029	1032	rBV	1757235	1474270	23.29%	3.022%
8	9.216	1207	1212	1215	rBV	4647341	4280905	67.63%	8.774%
9	9.610	1275	1279	1283	rBV	327640	259600	4.10%	0.532%
10	9.898	1324	1328	1331	rBV	1985058	1627297	25.71%	3.335%
11	10.686	1458	1462	1473	rBV	2094176	1822142	28.78%	3.735%
12	11.339	1569	1573	1577	rBV	119418	124392	1.97%	0.255%
13	11.386	1577	1581	1585	rVV	1982010	1675671	26.47%	3.434%
14	11.692	1627	1633	1642	rBV2	44196	87213	1.38%	0.179%
15	11.774	1642	1647	1651	rBV	52788	66409	1.05%	0.136%
16	11.922	1663	1672	1687	rBV	2129992	3722854	58.81%	7.630%
17	12.186	1711	1717	1723	rVV	272499	340413	5.38%	0.698%
18	12.245	1723	1727	1731	rVB	110258	114649	1.81%	0.235%
19	12.504	1764	1771	1778	rBV2	88115	147857	2.34%	0.303%
20	12.574	1779	1783	1787	rBV	104839	121703	1.92%	0.249%
21	12.639	1787	1794	1800	rBV5	112751	330195	5.22%	0.677%
22	12.716	1801	1807	1818	rBV	2558369	3820163	60.35%	7.830%
23	12.980	1848	1852	1855	rBV	4764387	4376769	69.14%	8.971%
24	13.945	2008	2016	2021	rBV7	182474	612749	9.68%	1.256%
25	14.039	2028	2032	2047	rVB	1632953	1869311	29.53%	3.831%
26	14.892	2172	2177	2186	rBV2	203108	549585	8.68%	1.126%
27	15.204	2211	2230	2254	rVB2	1036526	6330219	100.00%	12.974%
28	15.510	2277	2282	2286	rBV	926177	1132630	17.89%	2.321%
29	15.539	2286	2287	2292	rVB	84110	74035	1.17%	0.152%
30	15.980	2358	2362	2370	rVB2	65183	92975	1.47%	0.191%
31	16.492	2445	2449	2455	rBV3	46091	74429	1.18%	0.153%
32	17.027	2533	2540	2546	rBV4	101483	221804	3.50%	0.455%
33	18.562	2791	2801	2813	rVB3	276949	913407	14.43%	1.872%

Sum of corrected areas: 48790287

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022021\
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Acq On : 20 Feb 2021 15:40
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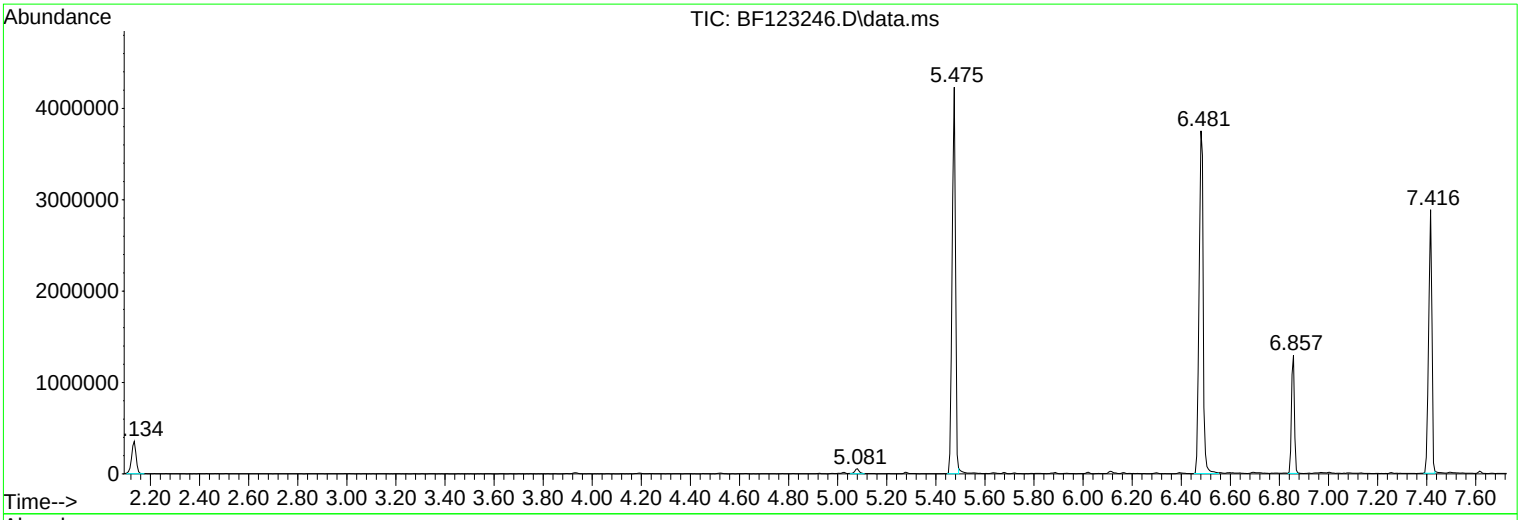
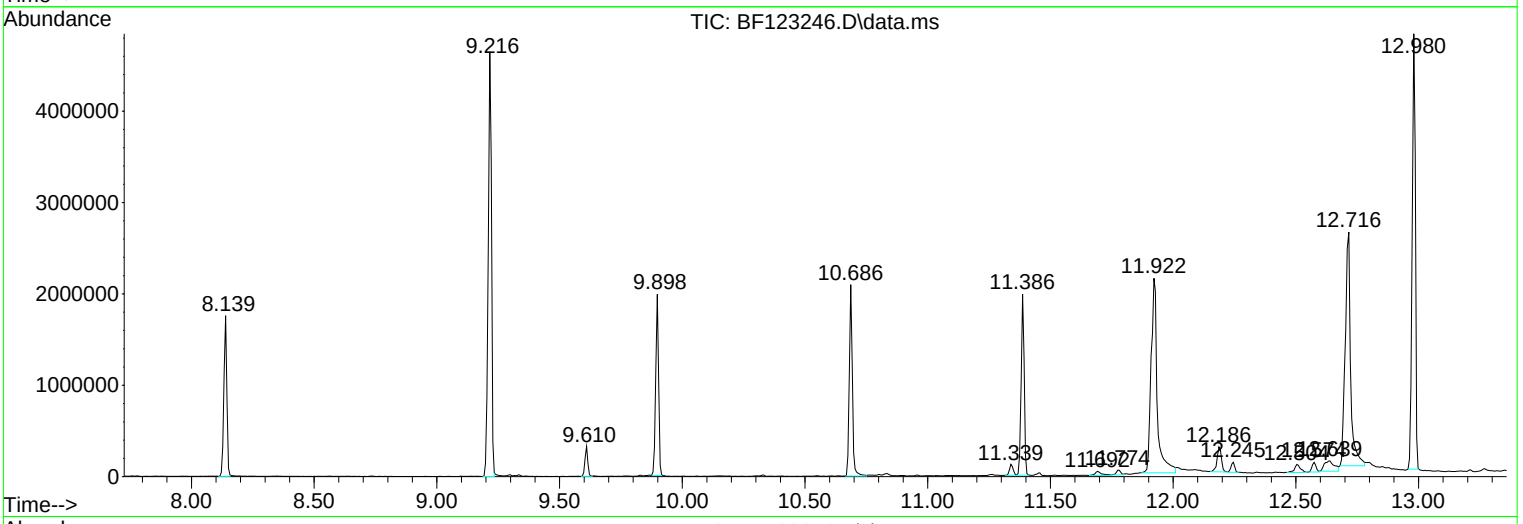
Misc :
ALS Vial : 8 Sample Multiplier: 1

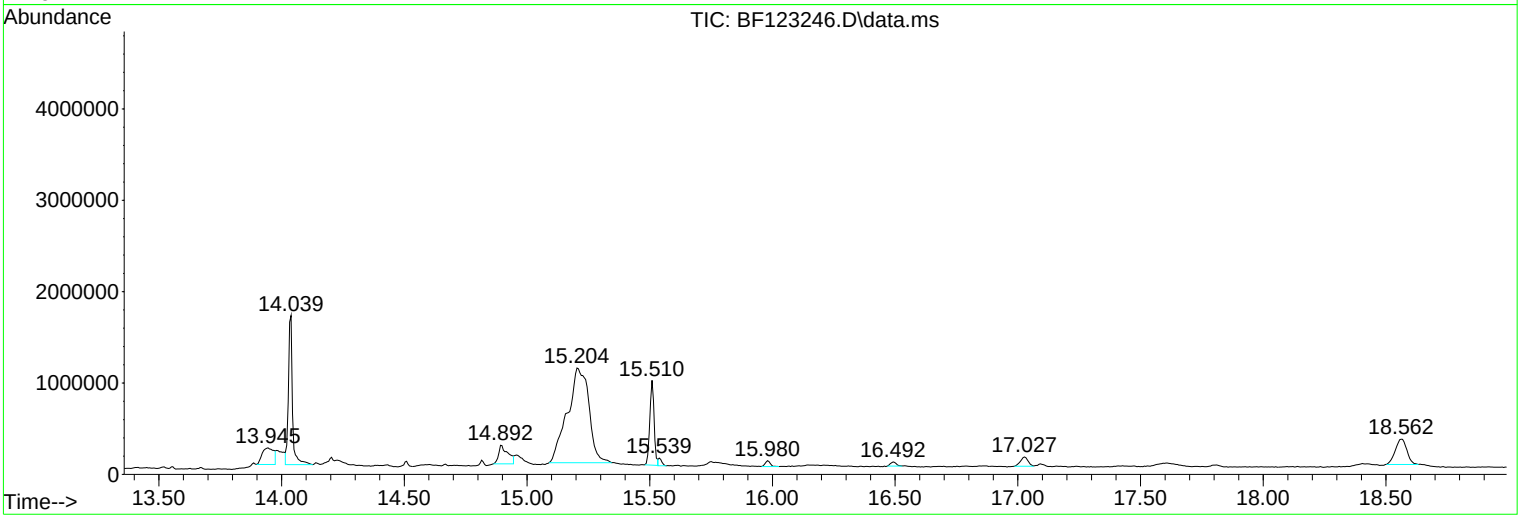
Instrument :
BNA_F
ClientSampleId :
H-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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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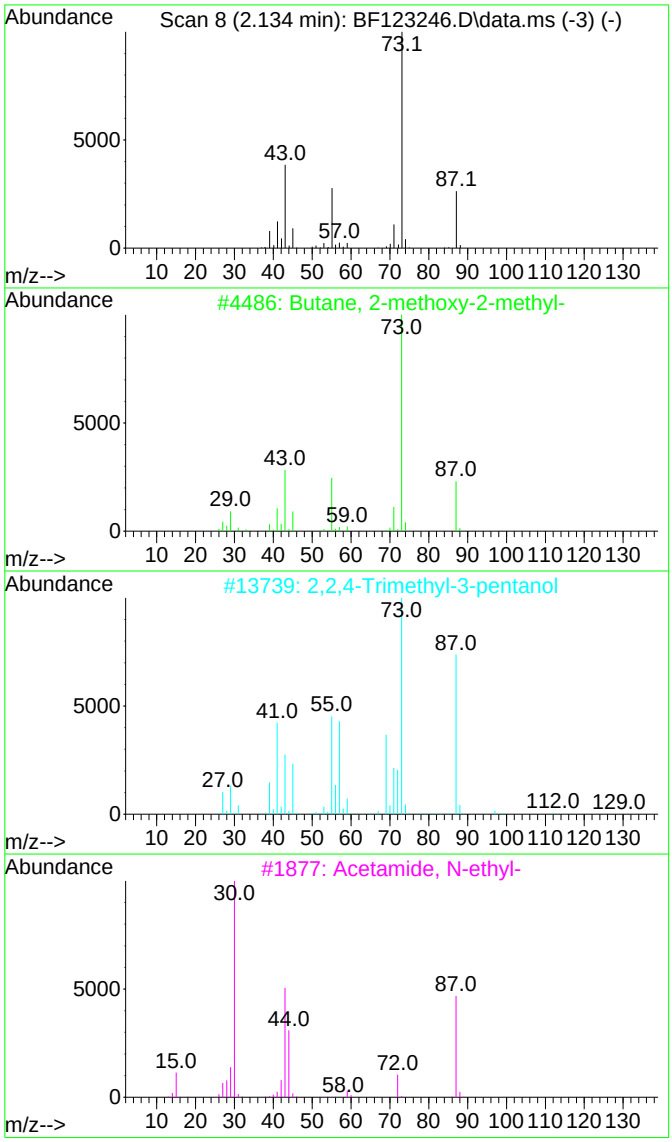
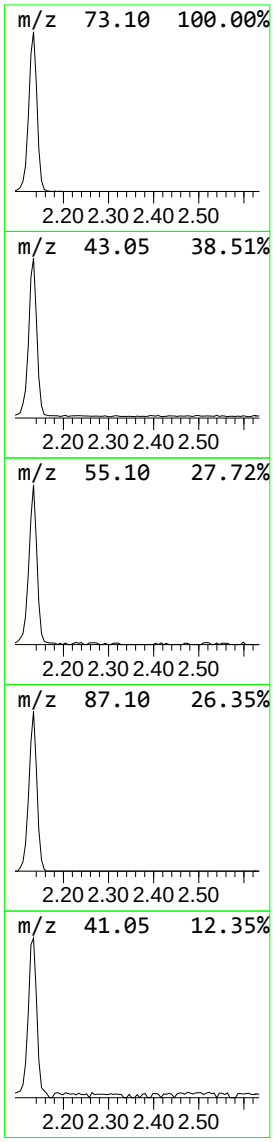
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	8.24 ng	444673	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25





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Data File : BF123246.D
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Operator : JU/CG
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Misc :
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Instrument :
BNA_F
ClientSampleId :
H-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
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TIC Integration Parameters: LSCINT.P

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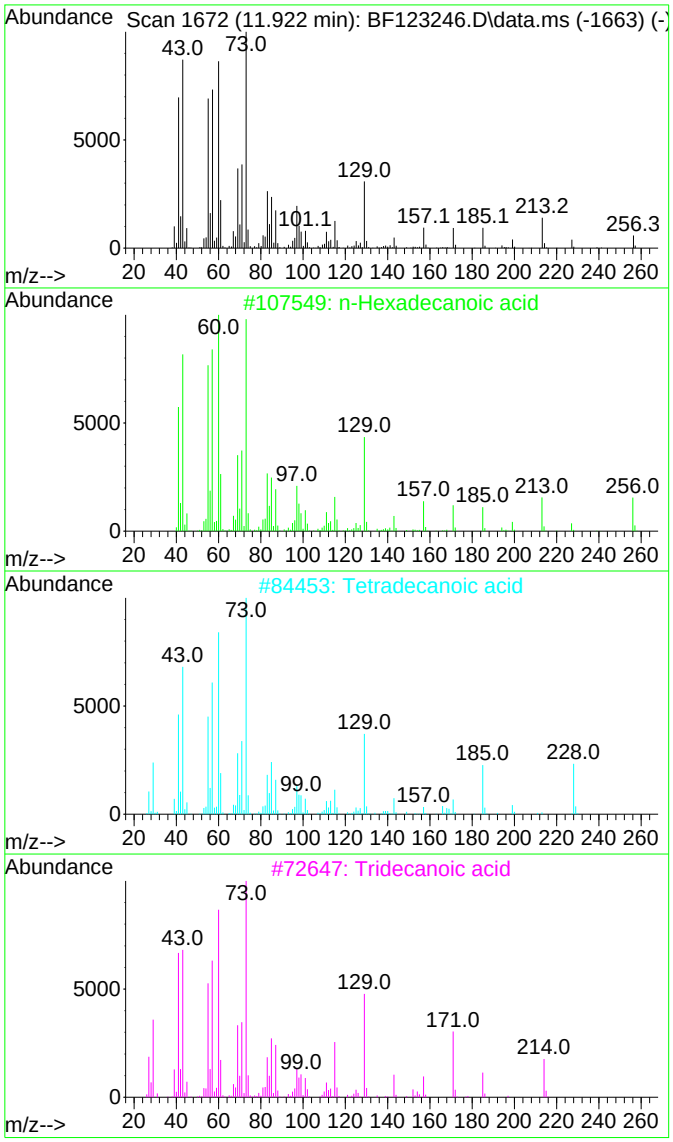
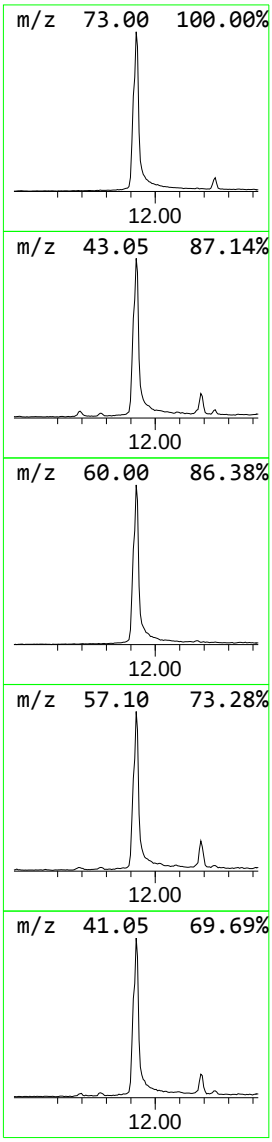
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	44.43 ng	3722850	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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Operator : JU/CG
Sample : M1430-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

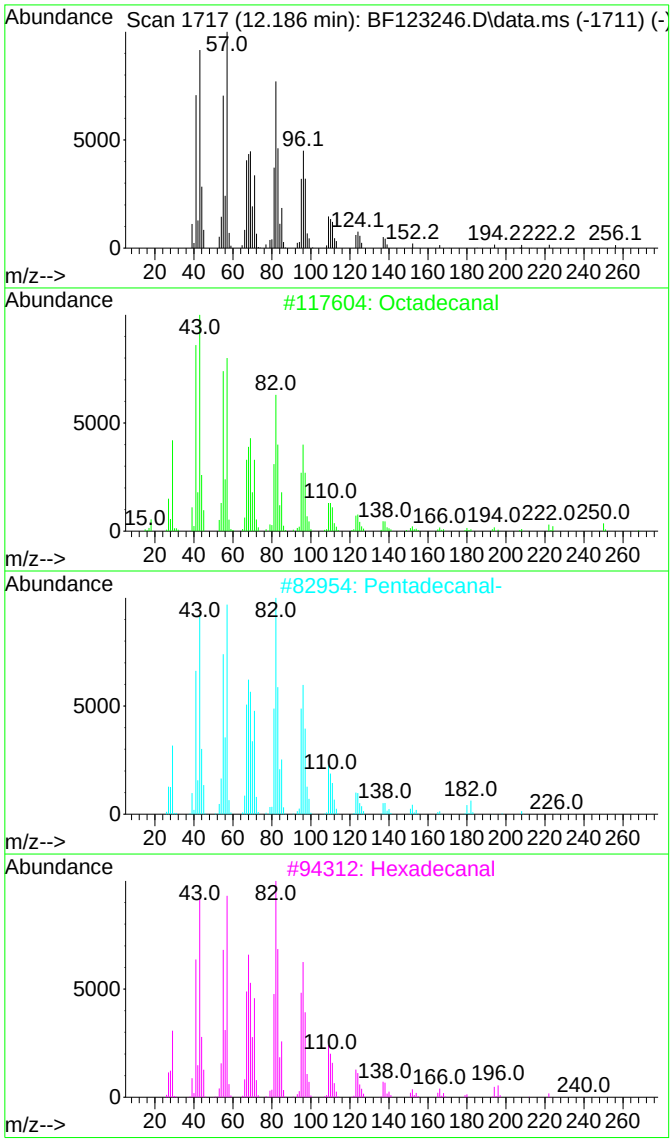
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

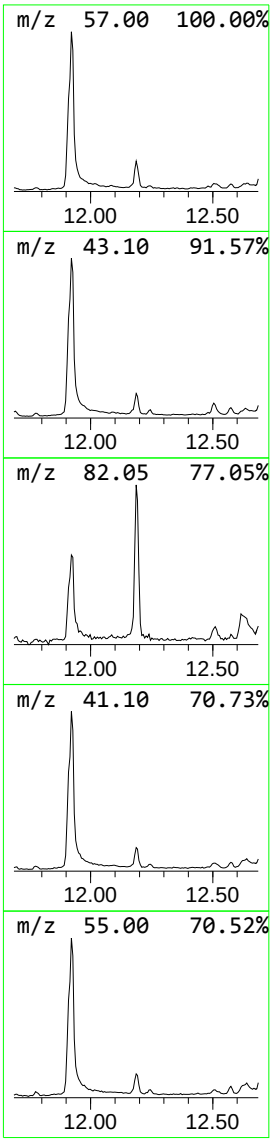
****

Peak Number 3 Octadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.186	4.06 ng	340413	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	95
2	Pentadecanal-	226	C15H30O	002765-11-9	94
3	Hexadecanal	240	C16H32O	000629-80-1	91
4	Oxirane, tridecyl-	226	C15H30O	018633-25-5	91
5	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	91





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Operator : JU/CG
Sample : M1430-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H-2

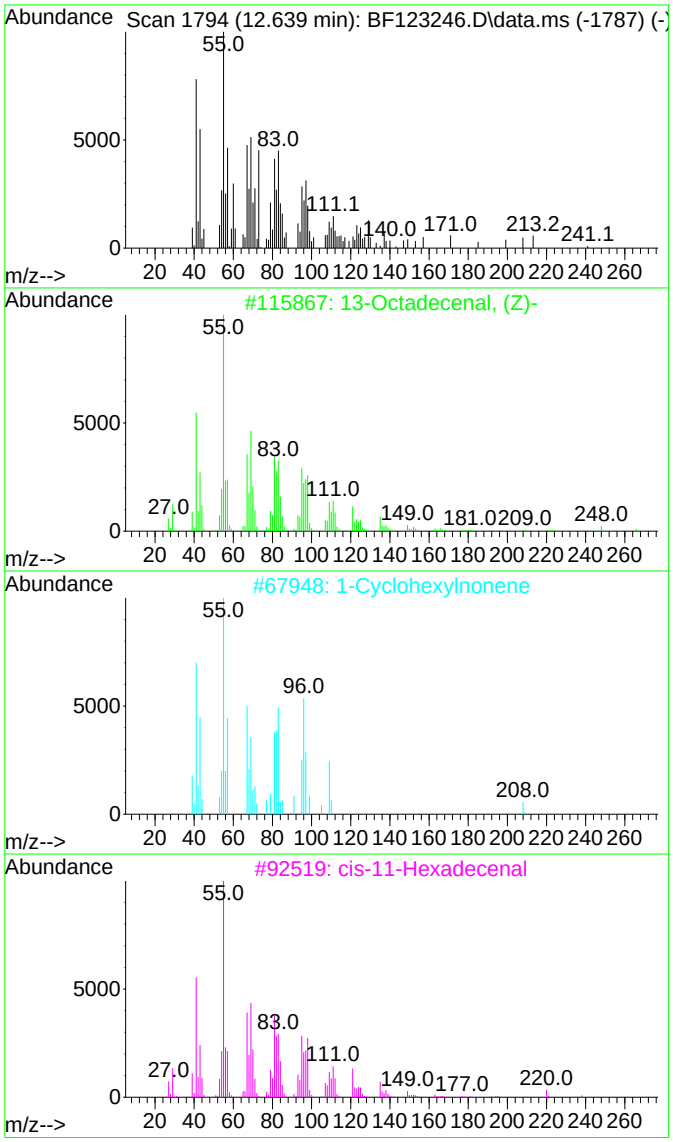
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

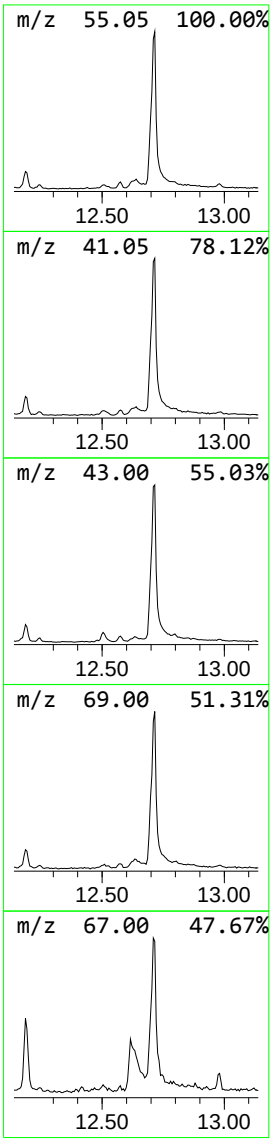
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 13-Octadecenal, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	3.94 ng	330195	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	64
2	1-Cyclohexylnonene	208	C15H28	114614-84-5	60
3	cis-11-Hexadecenal	238	C16H30O	053939-28-9	58
4	Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-92-8	55
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	42





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Operator : JU/CG
Sample : M1430-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
H-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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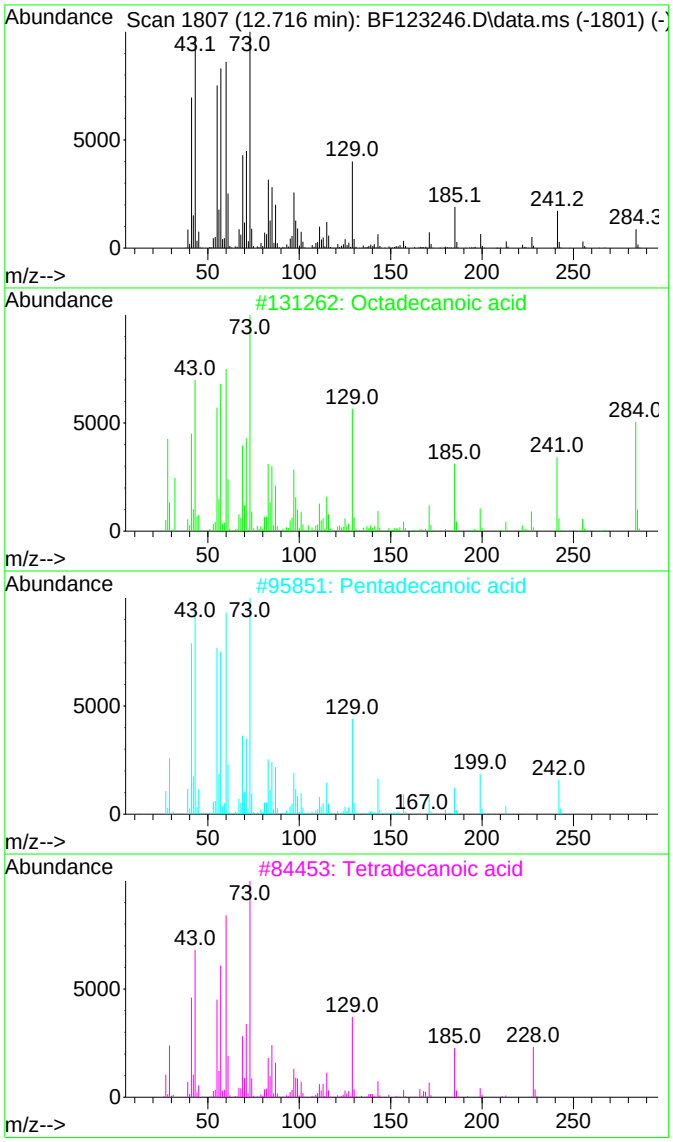
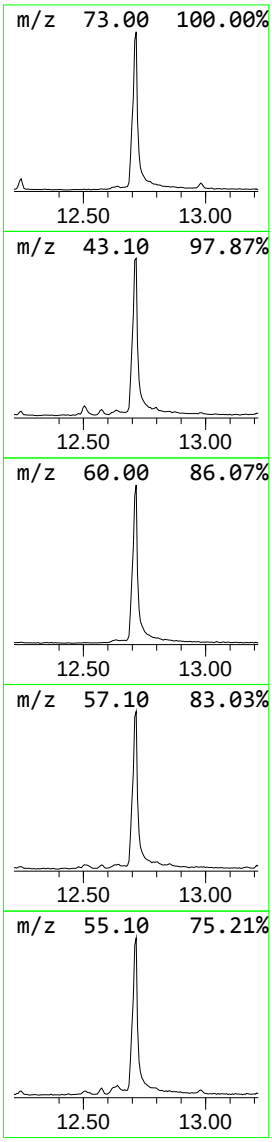
****

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	40.87 ng	3820160	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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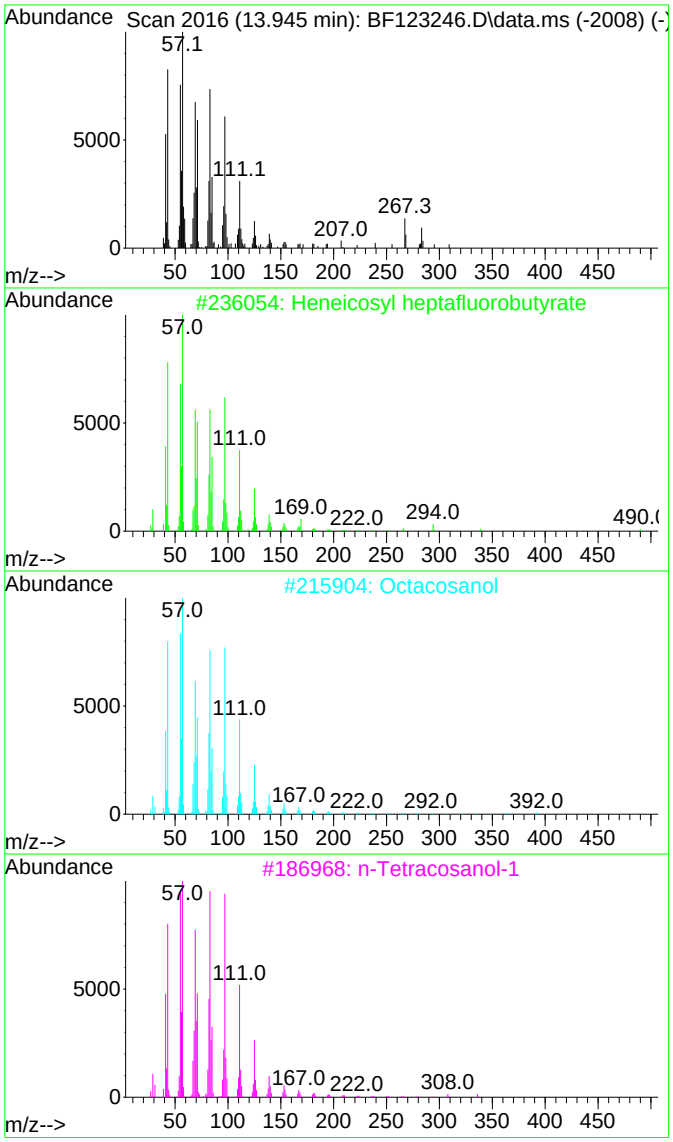
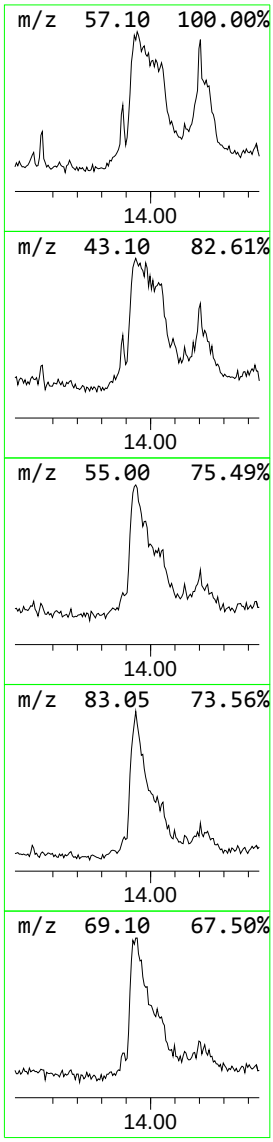
****
Peak Number 6 Heneicosyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	6.56 ng	612749	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	81
2	Octacosanol	410	C28H58O	000557-61-9	81
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	76
4	17-Pentatriacontene	491	C35H70	006971-40-0	74
5	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	74





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Operator : JU/CG
Sample : M1430-10
Misc :
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Instrument :
BNA_F
ClientSampleId :
H-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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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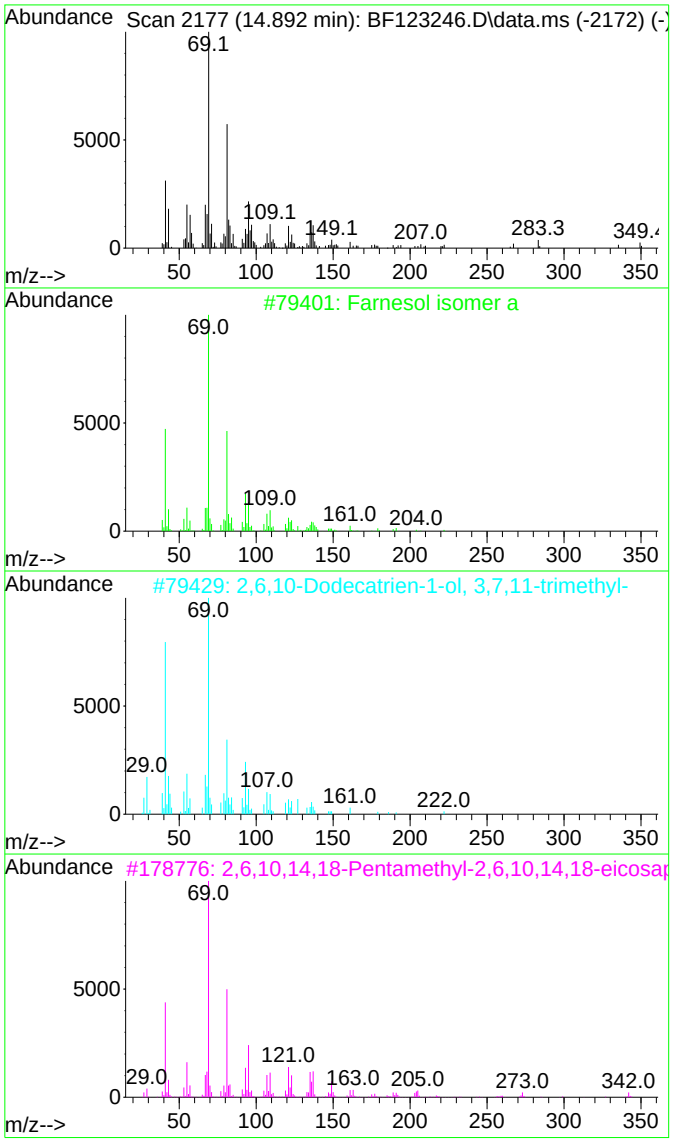
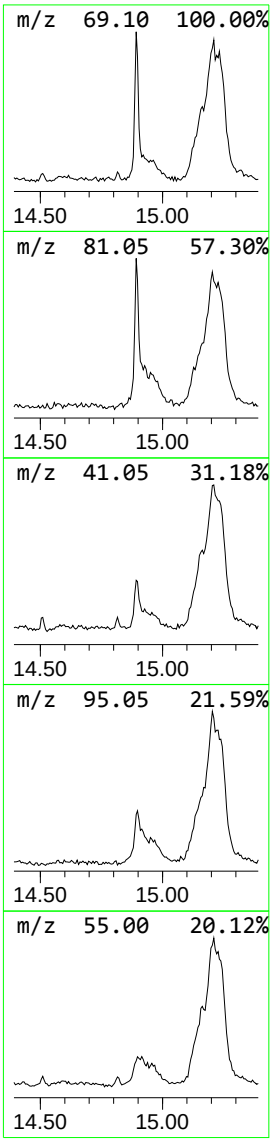
Peak Number 7 Farnesol isomer a Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	9.70 ng	549585	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a	222	C15H26O	1000108-92-4	74
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	74
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	72
4	trans-Farnesol	222	C15H26O	000106-28-5	70
5	Squalene	410	C30H50	000111-02-4	68





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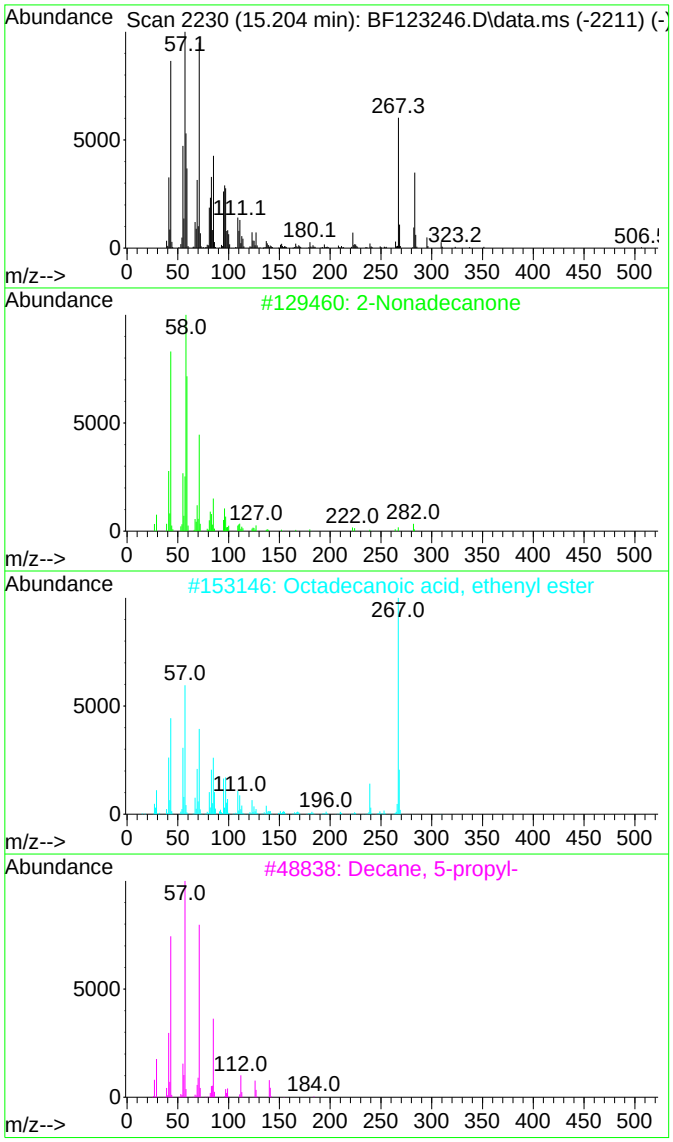
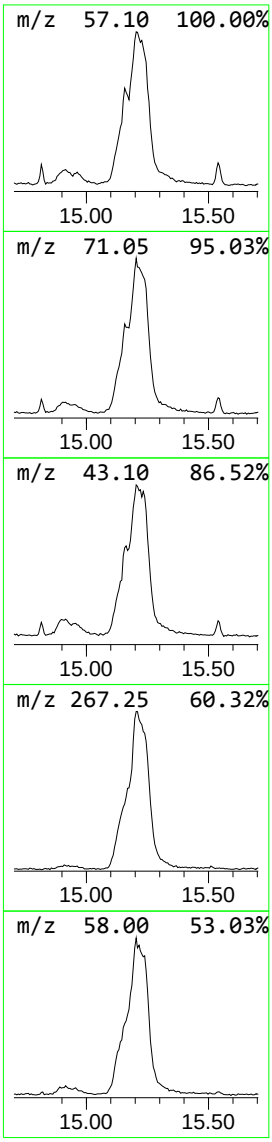
Peak Number 8 2-Nonadecanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	111.78 ng	6330220	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonadecanone	282	C19H38O	000629-66-3	78
2	Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	64
3	Decane, 5-propyl-	184	C13H28	017312-62-8	46
4	Stearic acid hydrazide	298	C18H38N2O	004130-54-5	38
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	38





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
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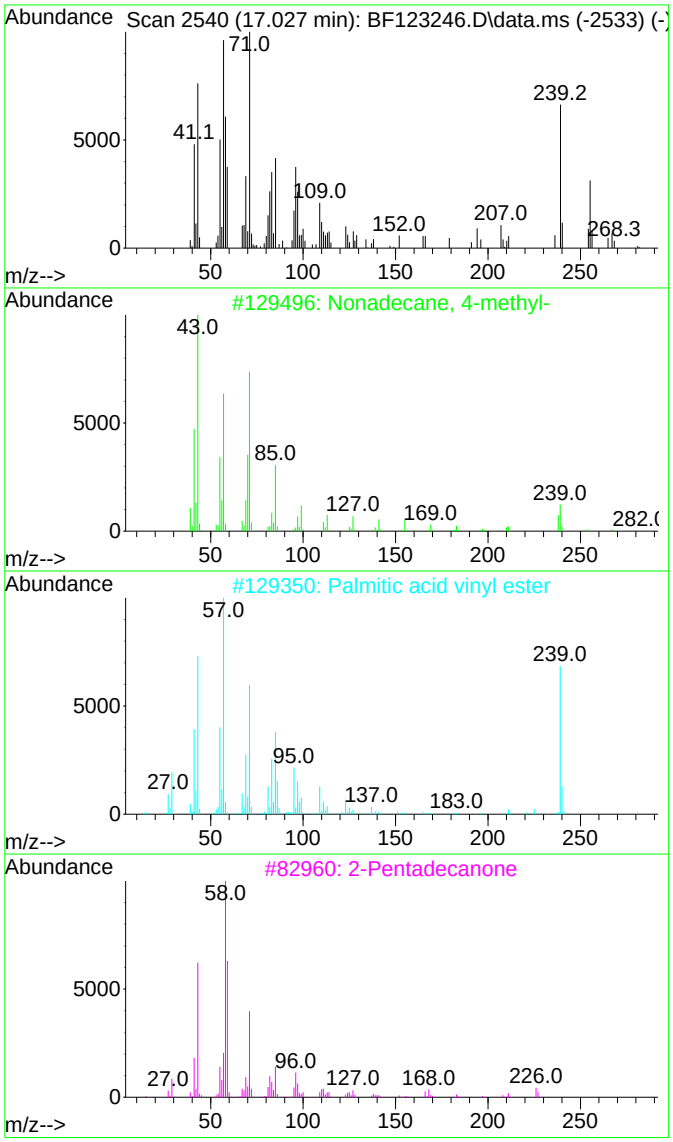
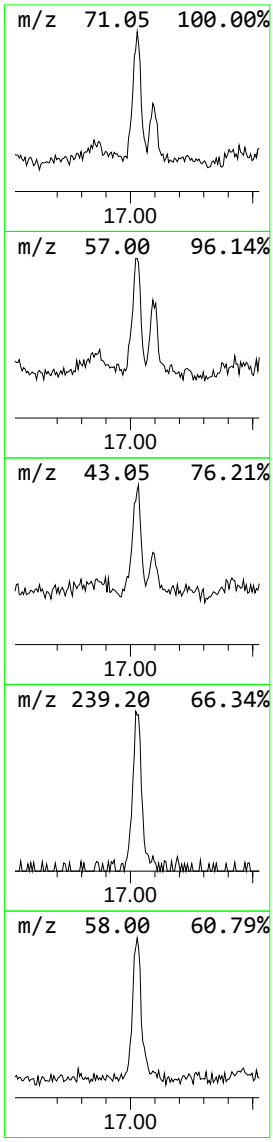
Peak Number 9 unknown17.027 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.027	3.92 ng	221804	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 4-methyl-	282	C20H42	025117-27-5	43
2	Palmitic acid vinyl ester	282	C18H34O2	000693-38-9	43
3	2-Pentadecanone	226	C15H30O	002345-28-0	38
4	1-Nonene, 4,6,8-trimethyl-	168	C12H24	054410-98-9	27
5	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022021\
Data File : BF123246.D
Acq On : 20 Feb 2021 15:40
Operator : JU/CG
Sample : M1430-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
H-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

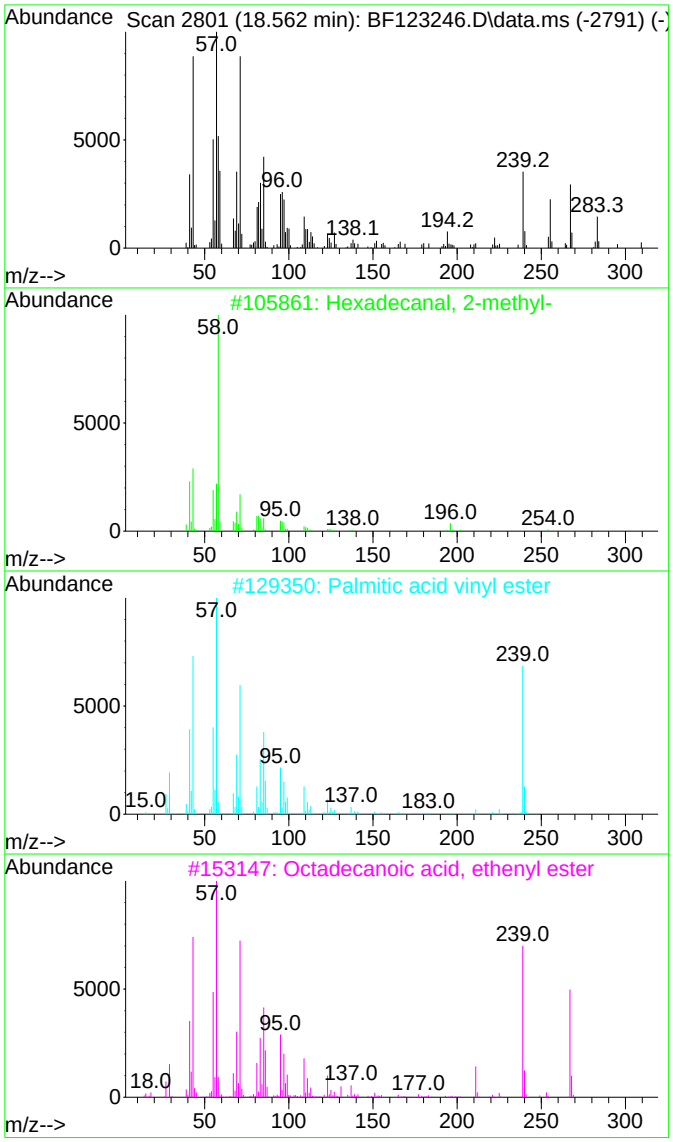
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

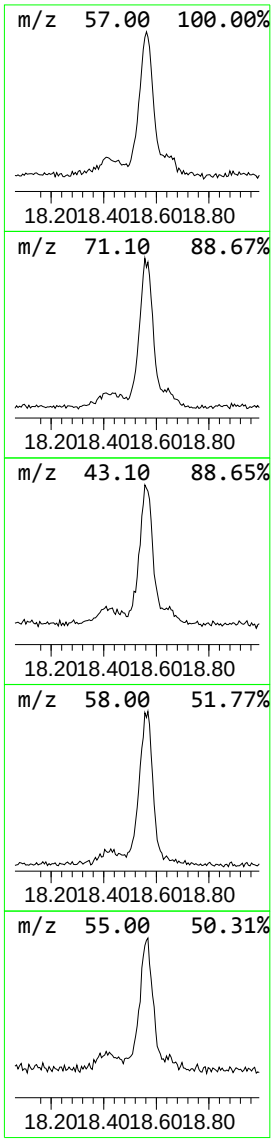
****

Peak Number 10 Hexadecanal, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.562	16.13 ng	913407	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal, 2-methyl-	254	C17H34O	055019-46-0	60
2	Palmitic acid vinyl ester	282	C18H34O2	000693-38-9	53
3	Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	52
4	Stearic acid hydrazide	298	C18H38N2O	004130-54-5	43
5	4-Octanone	128	C8H16O	000589-63-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022021\
Data File : BF123246.D
Acq On : 20 Feb 2021 15:40
Operator : JU/CG
Sample : M1430-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : H-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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...	2.134	8.2	ng	444673	1	6.857	1079070	20.0
n-Hexadecanoic ...	11.922	44.4	ng	3722850	4	11.386	1675670	20.0
Octadecanal	12.186	4.1	ng	340413	4	11.386	1675670	20.0
13-Octadecenal,...	12.639	3.9	ng	330195	4	11.386	1675670	20.0
Octadecanoic acid	12.716	40.9	ng	3820160	5	14.039	1869310	20.0
Heneicosyl hept...	13.945	6.6	ng	612749	5	14.039	1869310	20.0
Farnesol isomer a	14.892	9.7	ng	549585	6	15.509	1132630	20.0
2-Nonadecanone	15.204	111.8	ng	6330220	6	15.509	1132630	20.0
unknown17.027	17.027	3.9	ng	221804	6	15.509	1132630	20.0
Hexadecanal, 2-...	18.562	16.1	ng	913407	6	15.509	1132630	20.0