LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
Data File : BF123799.D
Acq On : 4 May 2021 1:58
Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-043021

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-BF042721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123799.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	7	12	19	rVB	163699	200726	5.20%	0.523%
2	5.010	494	497	502	rVB	165460	185914	4.81%	0.485%
3	5.428	564	568	579	rVB	4368542	3707950	95.98%	9.664%
4	6.445	737	741	751	rBV	4385721	3863052	100.00%	10.069%
5	6.634	771	773	778	rBV2	37860	43638	1.13%	0.114%
6	6.810	799	803	806	rBV	1947865	1759796	45.55%	4.587%
7	7.369	893	898	901	rBV	2905477	2365515	61.23%	6.165%
8	8.092	1017	1021	1024	rBV	2629428	2129333	55.12%	5.550%
9	9.169	1200	1204	1207	rBV	4297137	3283260	84.99%	8.557%
10	9.286	1220	1224	1228	rBV3	41114	44020	1.14%	0.115%
11	9.563	1267	1271	1275	rBV	135028	117952	3.05%	0.307%
12	9.851	1315	1320	1323	rBV	2268653	1968627	50.96%	5.131%
13	9.875	1323	1324	1328	rVB2	59500	48003	1.24%	0.125%
14	9.969	1337	1340	1344	rBV	60957	56164	1.45%	0.146%
15	10.633	1449	1453	1458	rBV	2131940	1844626	47.75%	4.808%
16	11.333	1568	1572	1575	rBV	2128912	1742408	45.10%	4.541%
17	11.357	1575	1576	1580	rVV2	141107	150802	3.90%	0.393%
18	11.392	1580	1582	1588	rVB3	107797	108808	2.82%	0.284%
19	11.551	1606	1609	1614	rBV5	42198	57512	1.49%	0.150%
20	11.821	1652	1655	1656	rBV	57701	48611	1.26%	0.127%
21	11.869	1660	1663	1674	rVV3	132286	201973	5.23%	0.526%
22	11.951	1674	1677	1683	rVB3	60892	89703	2.32%	0.234%
23	12.033	1688	1691	1694	rVB2	151364	131439	3.40%	0.343%
24	12.280	1727	1733	1736	rBV8	40798	71932	1.86%	0.187%
25	12.386	1747	1751	1753	rBV4	43239	52557	1.36%	0.137%
26	12.433	1756	1759	1763	rVB4	51095	64254	1.66%	0.167%
27	12.545	1775	1778	1781	rBV	326672	264218	6.84%	0.689%
28	12.774	1812	1817	1820	rBV	280747	257770	6.67%	0.672%
29	12.921	1838	1842	1845	rBV	2706572	2228103	57.68%	5.807%
30	13.104	1871	1873	1877	rVB3	47515	44694	1.16%	0.116%
31	13.157	1879	1882	1886	rVB3	70886	100227	2.59%	0.261%
32	13.333	1909	1912	1914	rBV4	49602	69901	1.81%	0.182%
33	13.357	1914	1916	1918	rBV	93158	80981	2.10%	0.211%
34	13.727	1975	1979	1981	rBV3	41108	70964	1.84%	0.185%
35	13.833	1993	1997	2005	rBV2	244986	427407	11.06%	1.114%
36	13.974	2017	2021	2024	rBV	1444648	1405491	36.38%	3.663%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
Data File : BF123799.D
Acq On : 4 May 2021 1:58
Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-043021

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-BF042721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.451	2099	2102	2105	rBV	370906	348790	9.03%	0.909%
38	14.833	2164	2167	2170	rVB	187840	191272	4.95%	0.499%
39	14.898	2176	2178	2186	rVB2	98506	122580	3.17%	0.319%
40	15.010	2195	2197	2200	rBV	93151	101401	2.62%	0.264%
41	15.092	2207	2211	2215	rBV	1411014	1435386	37.16%	3.741%
42	15.433	2265	2269	2273	rBV	837891	990674	25.64%	2.582%
43	15.898	2344	2348	2355	rBV	838663	1244785	32.22%	3.244%
44	17.503	2612	2621	2633	rBV6	686088	2170747	56.19%	5.658%
45	17.945	2689	2696	2704	rBV7	250222	976483	25.28%	2.545%
46	18.021	2706	2709	2721	rVB7	382838	1016427	26.31%	2.649%
47	18.286	2748	2754	2757	rBV8	195959	480314	12.43%	1.252%

Sum of corrected areas: 38367190

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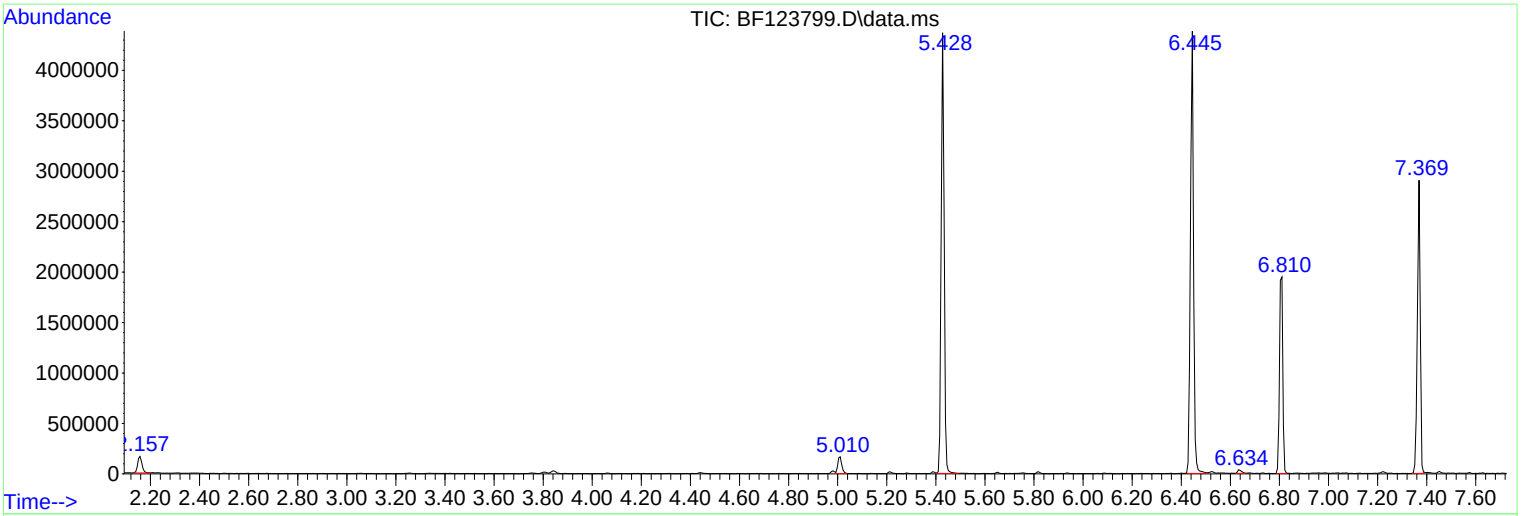
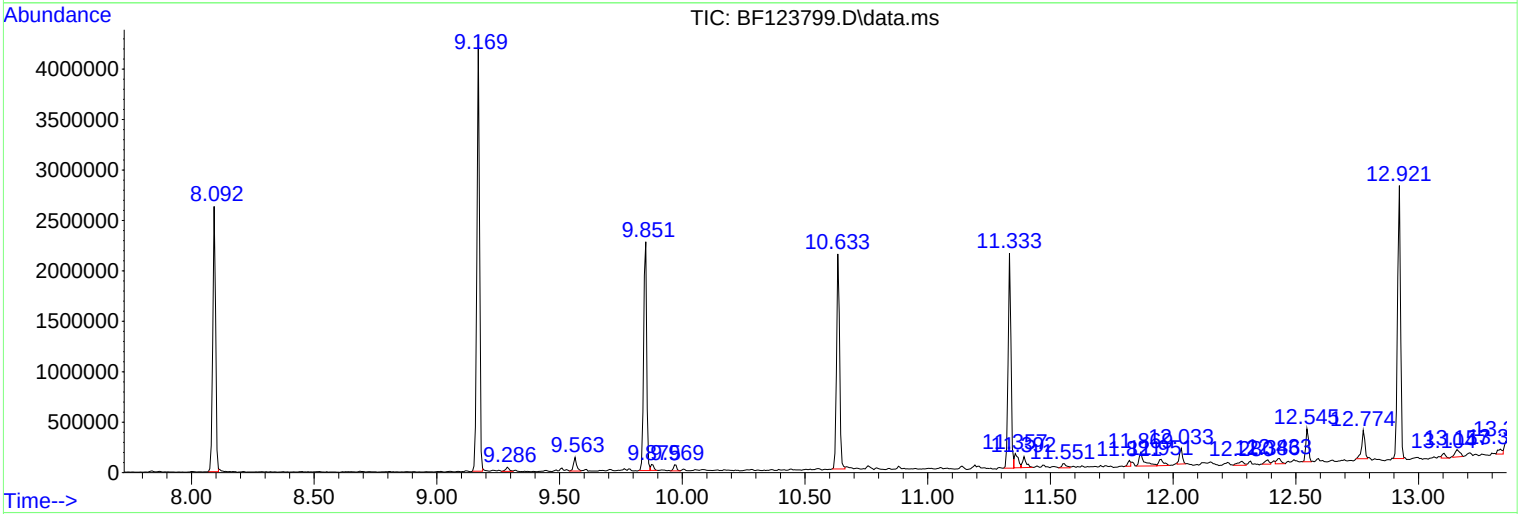
Misc :
ALS Vial : 18 Sample Multiplier: 1

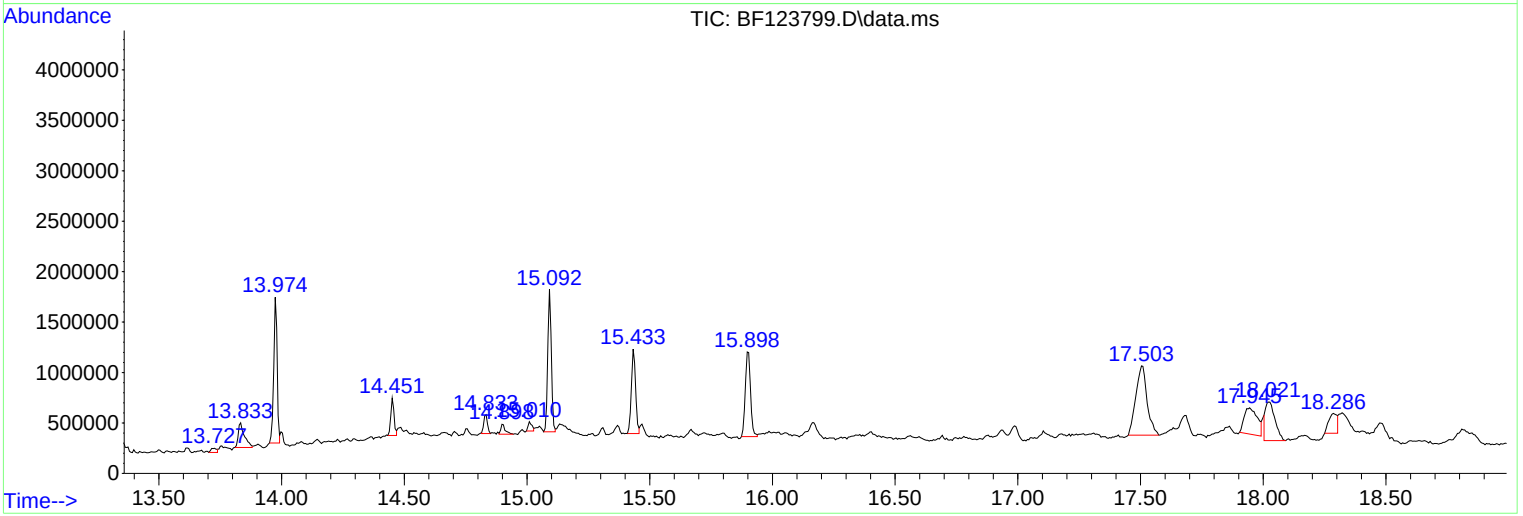
Instrument :
BNA_F
ClientSampleId :
OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

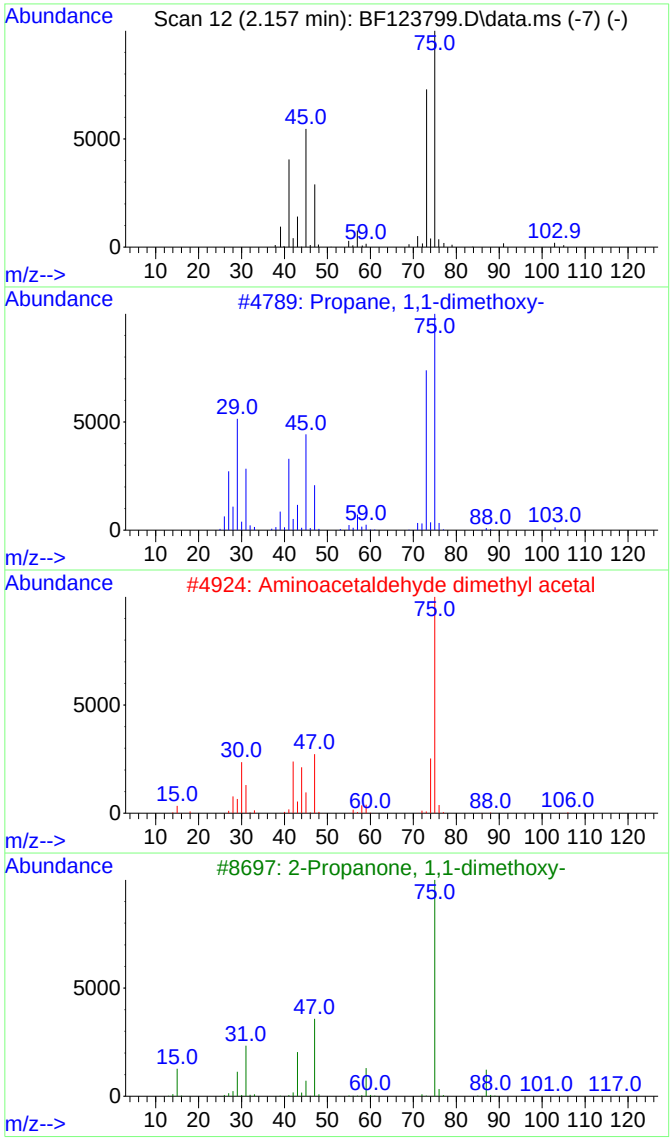
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

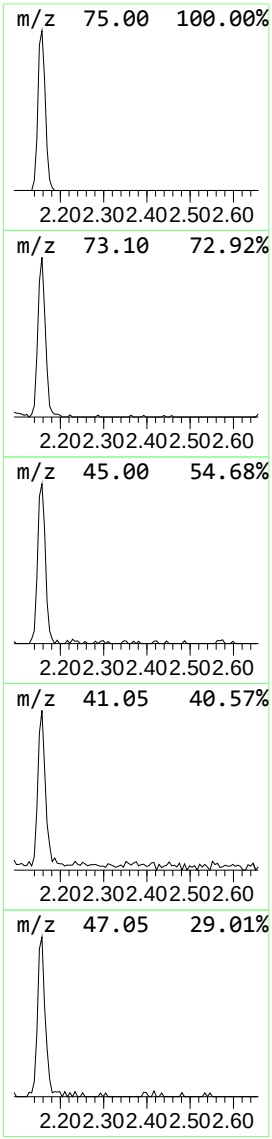
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	2.28 ng	200726	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	36
3	2-Propanone, 1,1-dimethoxy-	118	C5H10O3	006342-56-9	33
4	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	33
5	Methane, trimethoxy-	106	C4H10O3	000149-73-5	28





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Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-043021

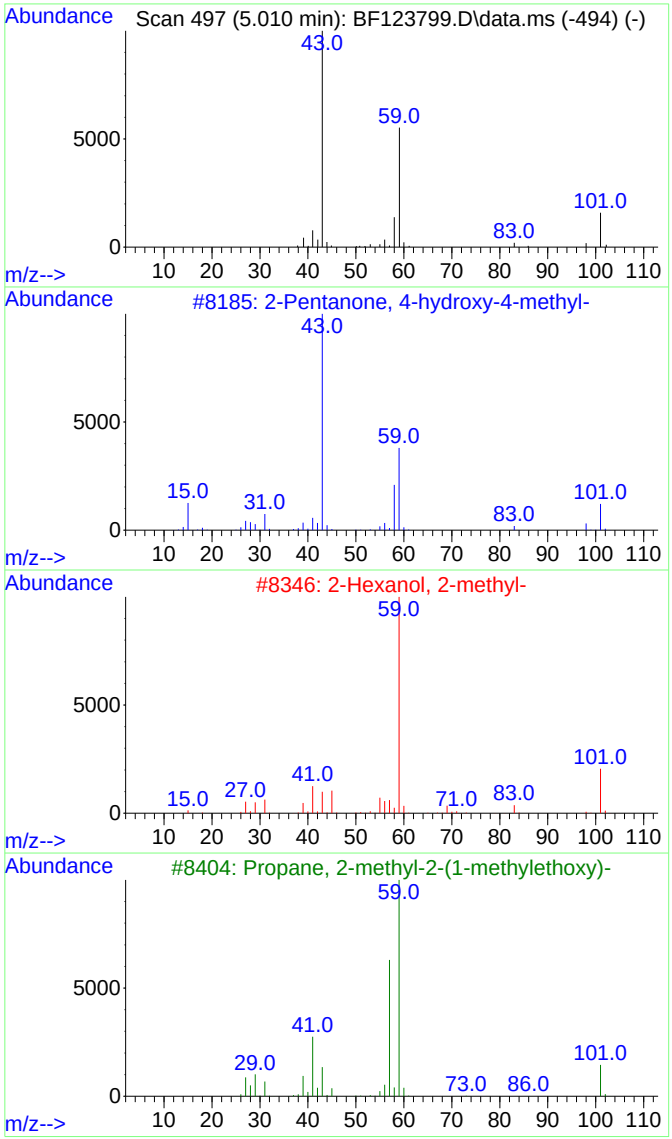
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

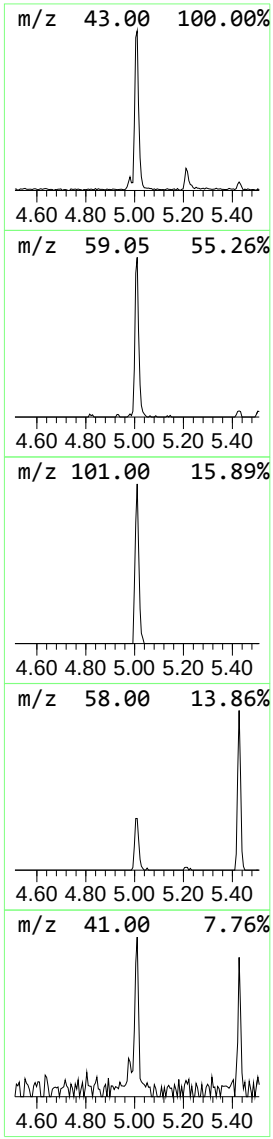
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	2.11 ng	185914	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Octanol	130	C8H18O	000589-98-0	33
5	Guanidine	59	CH5N3	000113-00-8	9





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Data File : BF123799.D
Acq On : 4 May 2021 1:58
Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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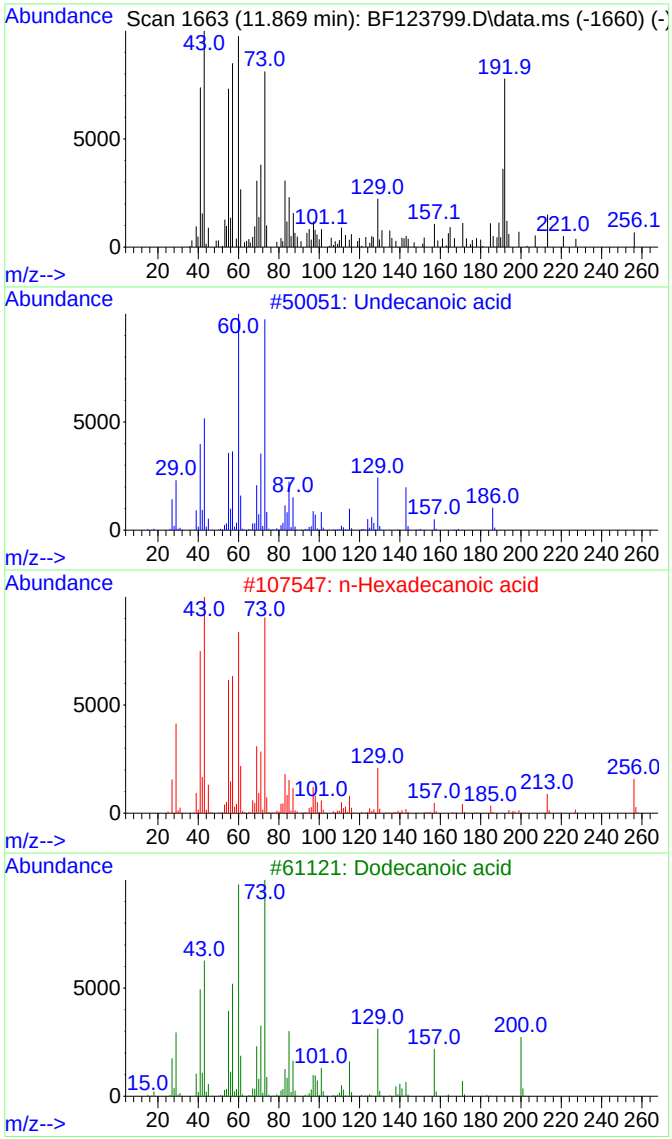
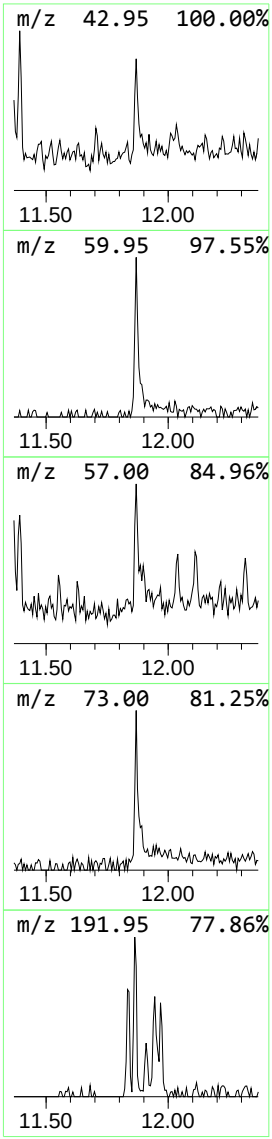
Peak Number 3 Undecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	2.32 ng	201973	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	55
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52
3	Dodecanoic acid	200	C12H24O2	000143-07-7	49
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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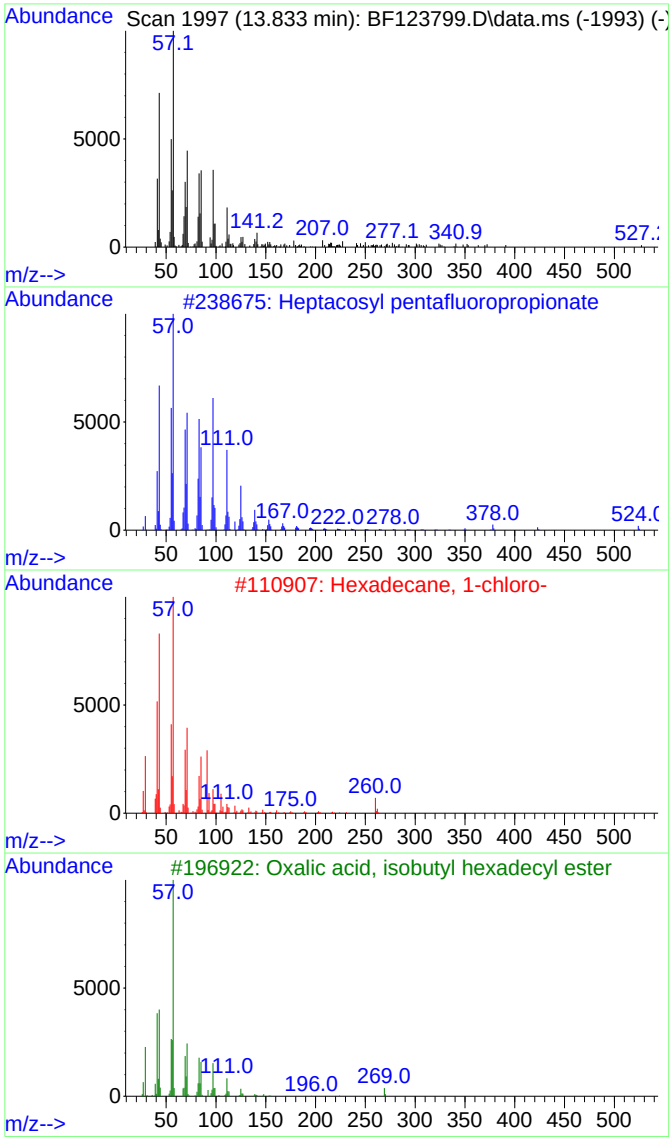
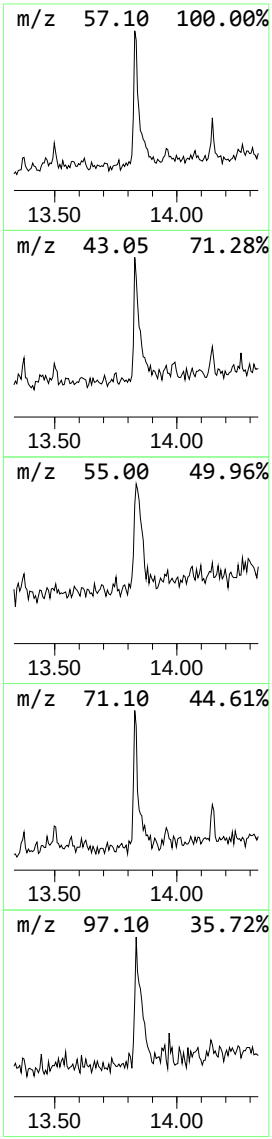
Peak Number 4 Heptacosyl pentafluoropropi... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	6.08 ng	427407	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	90
2	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	86
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	80
4	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	80
5	1-Docosene	308	C22H44	001599-67-3	62





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Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

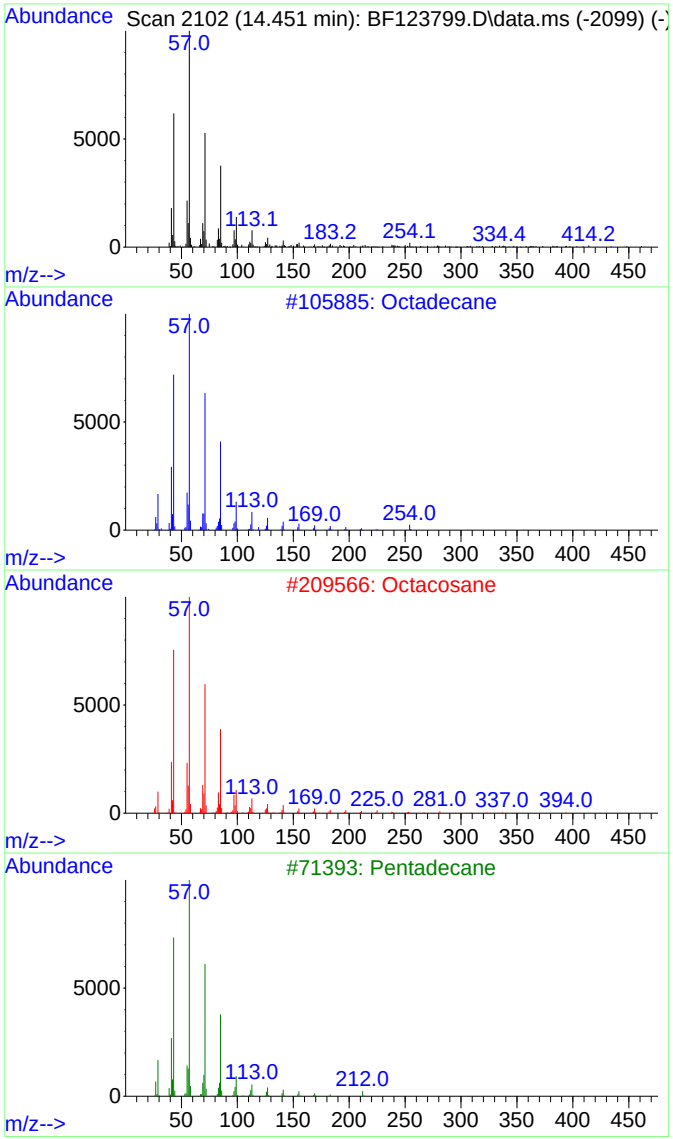
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

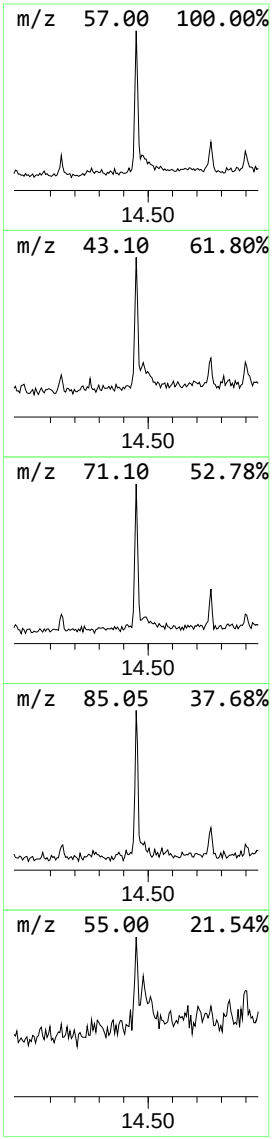
****

Peak Number 5 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	4.96 ng	348790	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Pentadecane	212	C15H32	000629-62-9	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	83





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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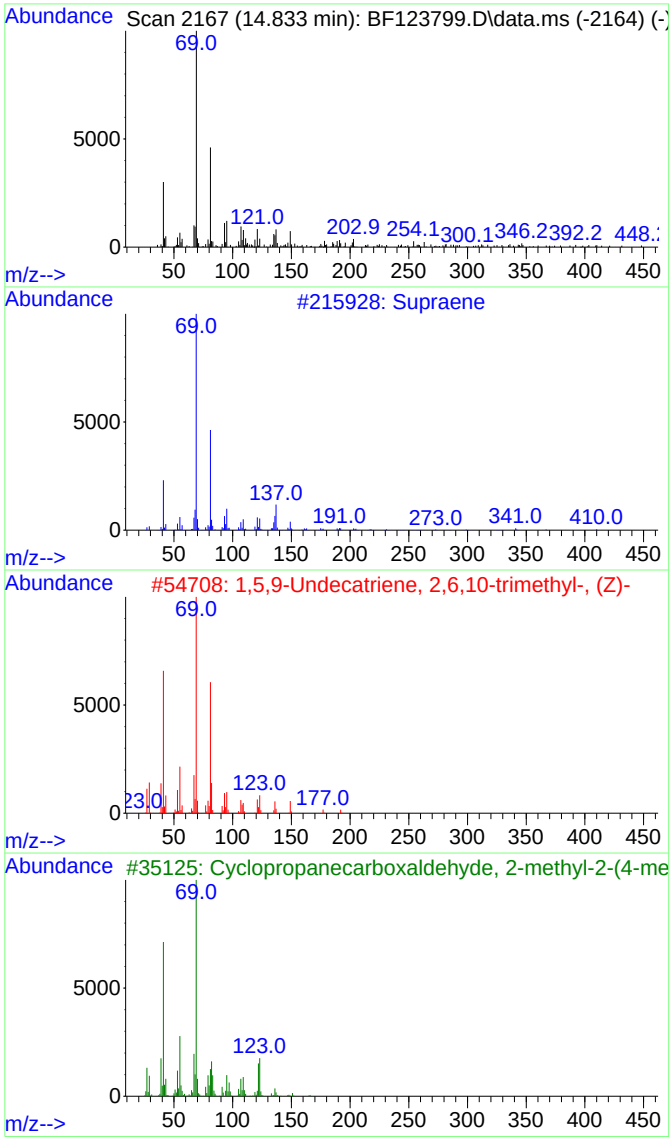
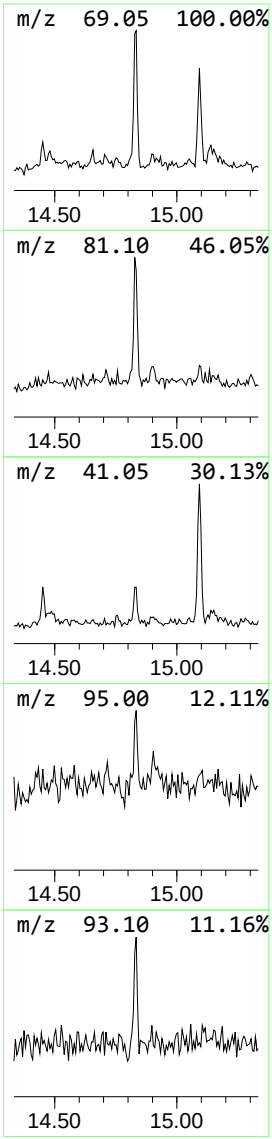
Peak Number 6 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	3.86 ng	191272	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
3	Cyclopropanecarboxaldehyde, 2-me...	166	C11H18O	097231-35-1	72
4	trans-Farnesol	222	C15H26O	000106-28-5	72
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	64





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BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

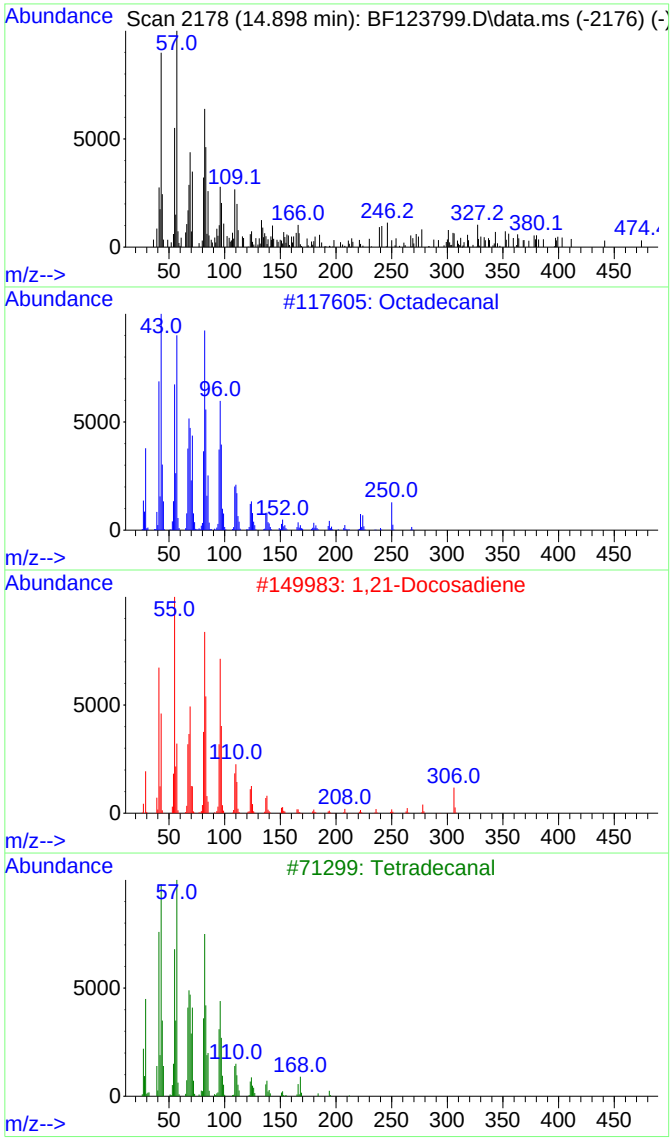
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

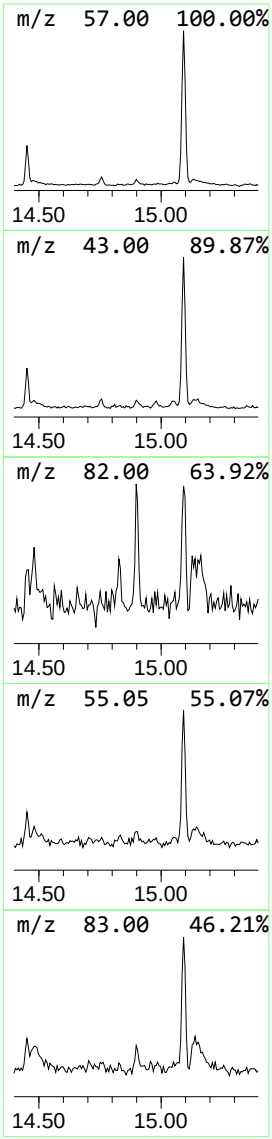
****

Peak Number 7 Octadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.47 ng	122580	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	15
2	1,21-Docosadiene	306	C22H42	053057-53-7	14
3	Tetradecanal	212	C14H28O	000124-25-4	14
4	Decane, 2-cyclohexyl-	224	C16H32	013151-73-0	11
5	Undecane, 2-cyclohexyl-	238	C17H34	013151-77-4	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
Data File : BF123799.D
Acq On : 4 May 2021 1:58
Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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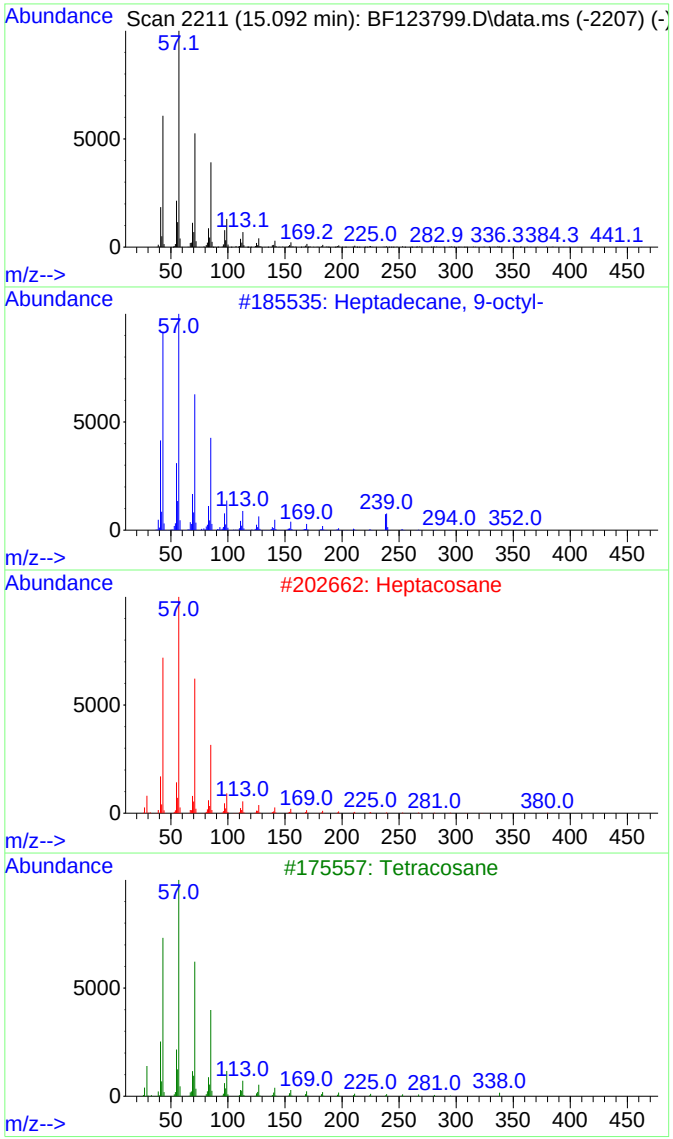
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

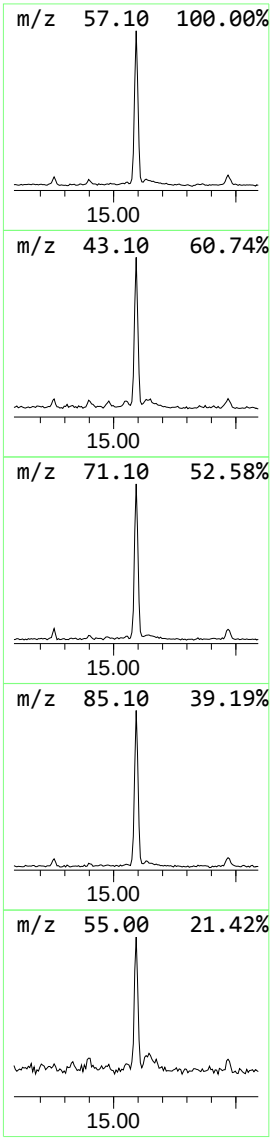
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	28.98 ng	1435390	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Pentacosane	352	C25H52	000629-99-2	90





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Acq On : 4 May 2021 1:58
Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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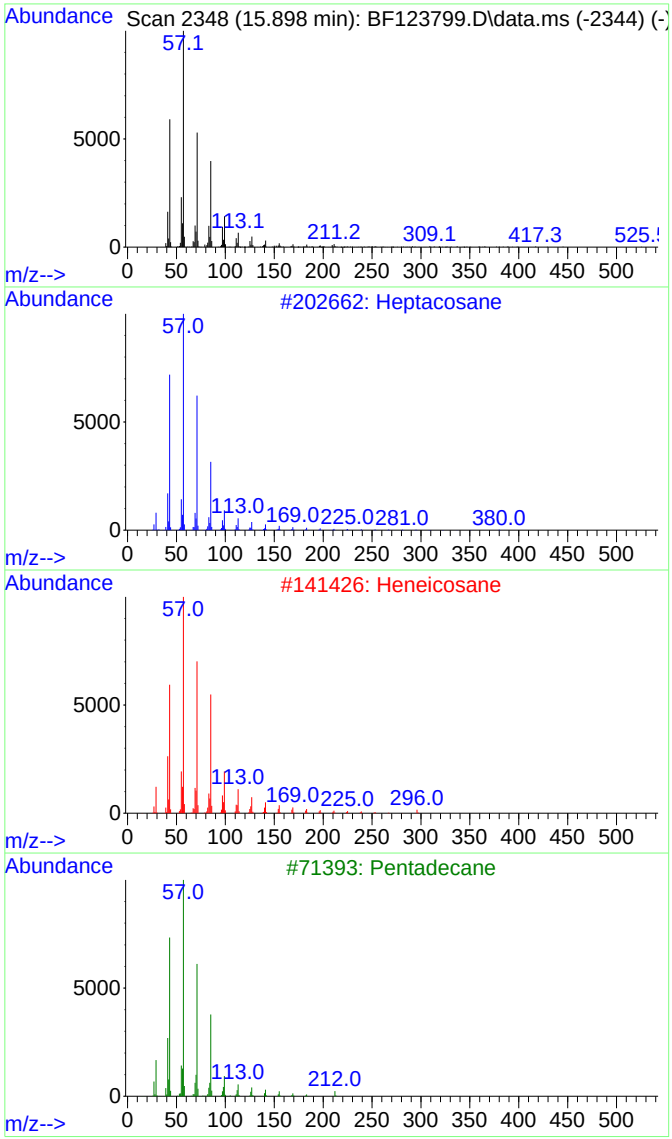
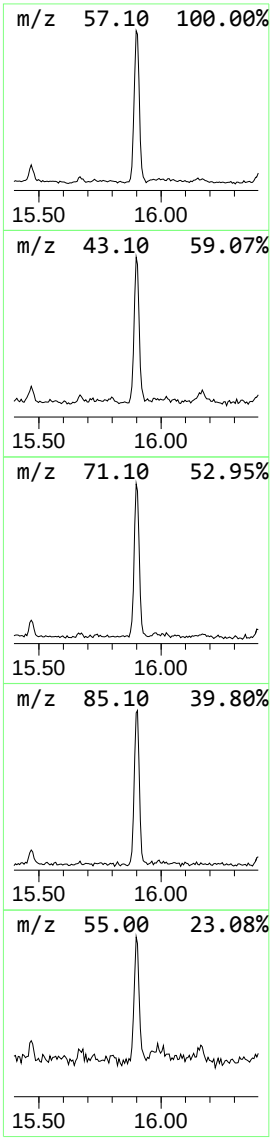
Peak Number 9 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	25.13 ng	1244790	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	98
2	Heneicosane	296	C21H44	000629-94-7	97
3	Pentadecane	212	C15H32	000629-62-9	94
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
5	Tetracosane	338	C24H50	000646-31-1	91





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Acq On : 4 May 2021 1:58
Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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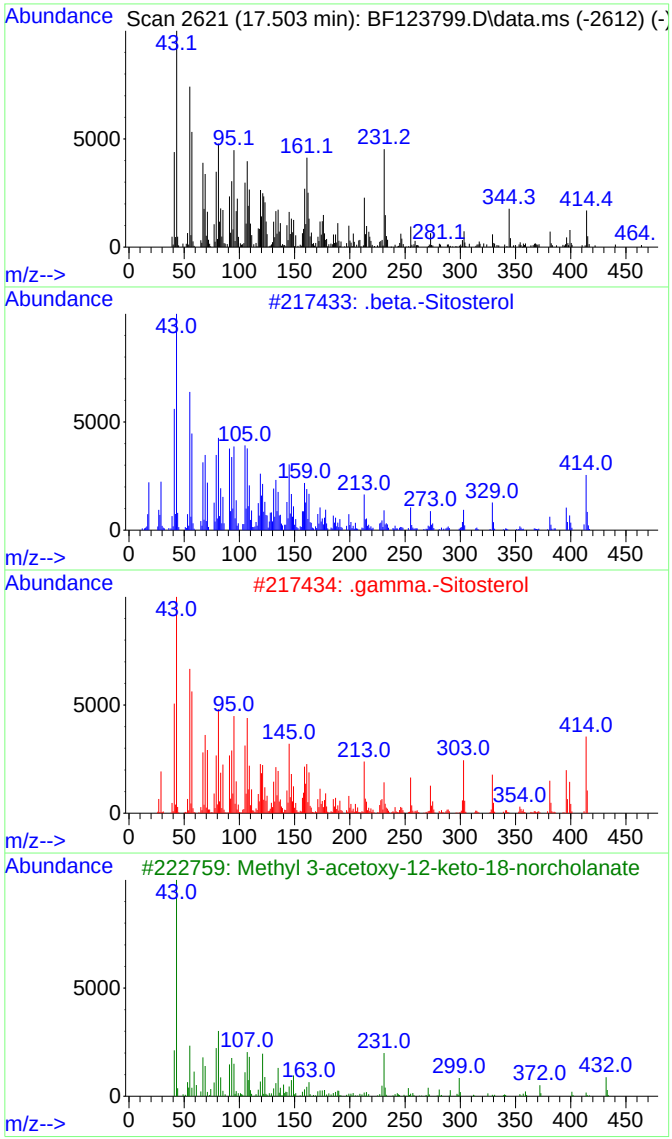
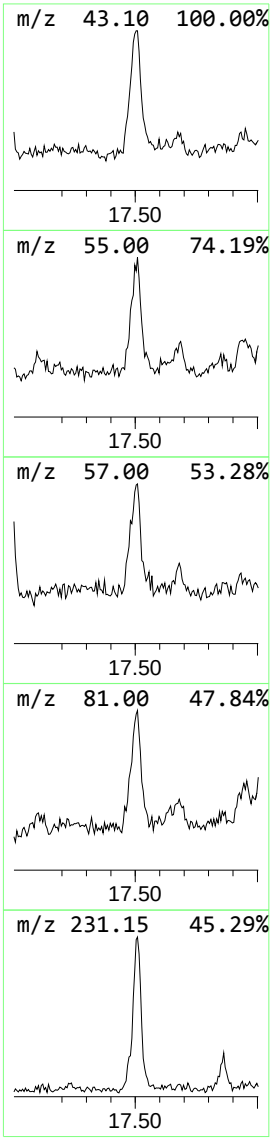
Peak Number 10 unknown17.503 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.503	43.82 ng	2170750	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	38
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	35
3	Methyl 3-acetoxy-12-keto-18-norc...	432	C26H40O5	1000251-87-8	25
4	Stigmastan-7-one	414	C29H50O	055331-88-9	25
5	5.beta.-Cholan-24-oic acid, 3-oxo-	374	C24H38O3	001553-56-6	25





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Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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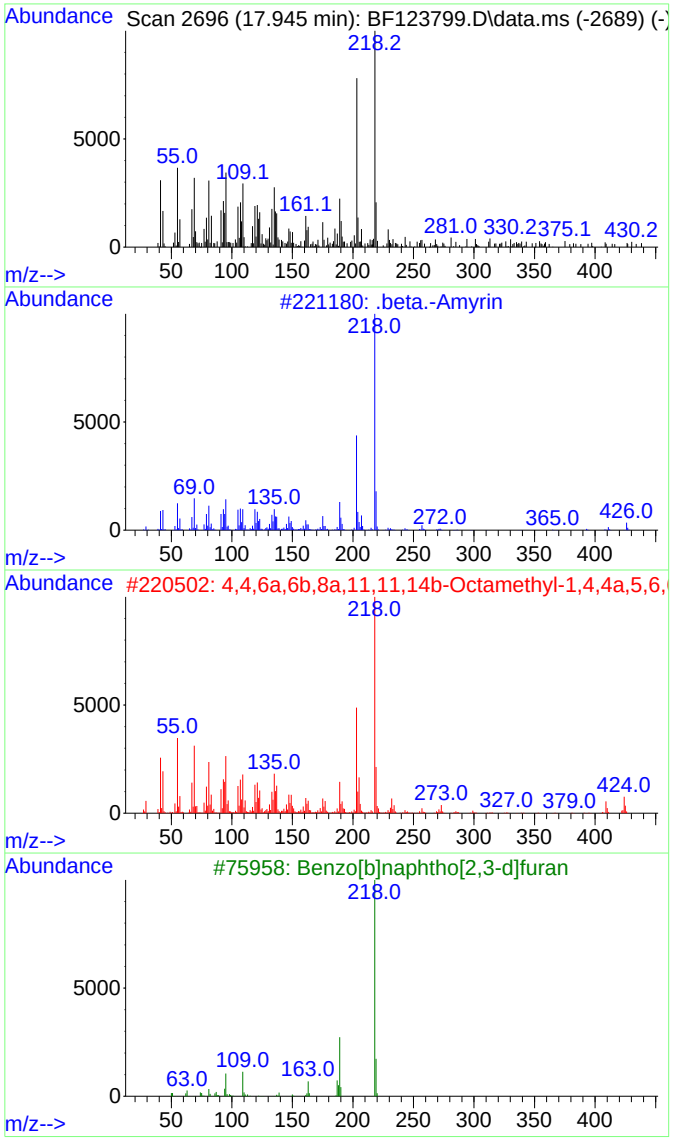
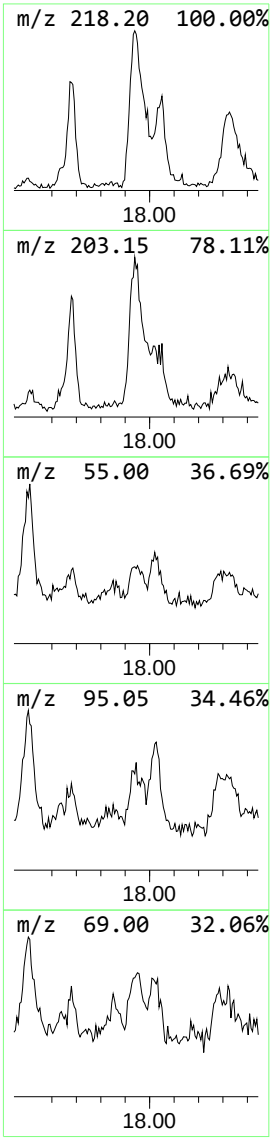
Peak Number 11 .beta.-Amyrin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.945	19.71 ng	976483	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Amyrin	426	C30H50O	000559-70-6	64
2	4,4,6a,6b,8a,11,11,14b-Octamethy...	424	C30H48O	1000194-62-4	58
3	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	45
4	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	45
5	Pyrido[1,2-a]perimidine	218	C15H10N2	000200-42-0	27





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Data File : BF123799.D
Acq On : 4 May 2021 1:58
Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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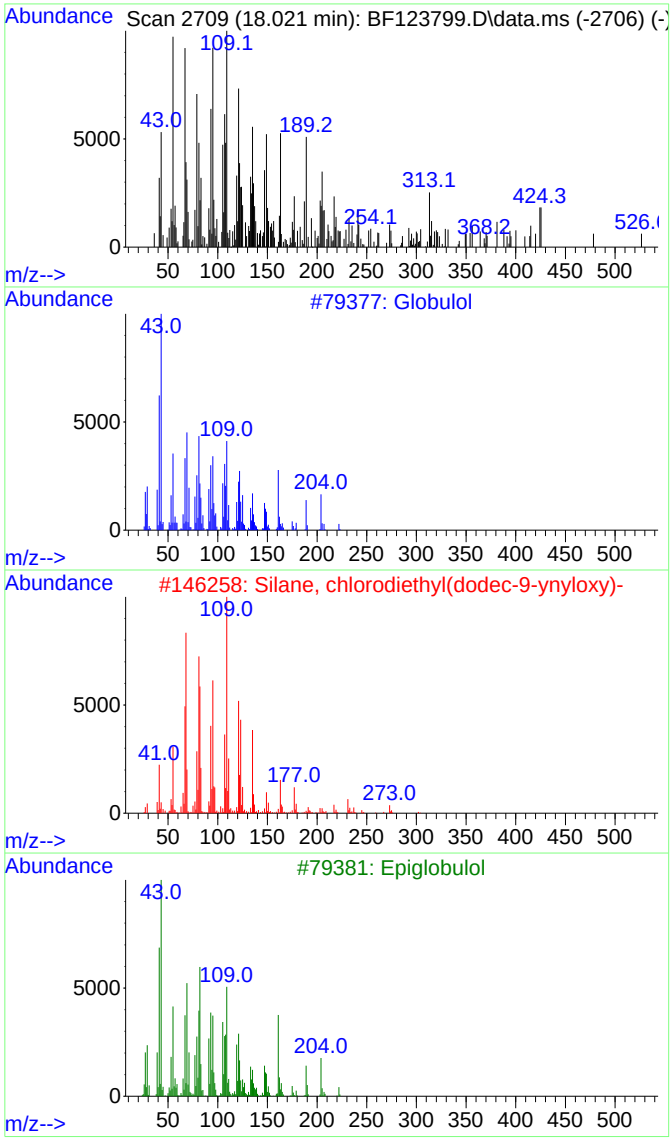
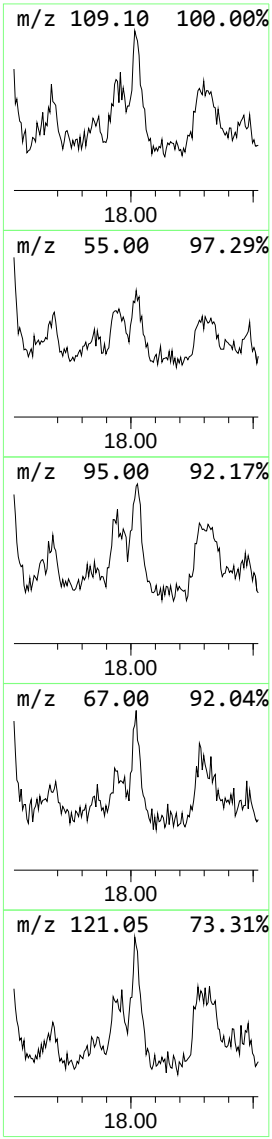
Peak Number 12 unknown18.021 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.021	20.52 ng	1016430	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Globulol	222	C15H26O	051371-47-2	46
2	Silane, chlorodiethyl(dodec-9-yn...	302	C16H31ClOSi	1000363-59-2	38
3	Epiglobulol	222	C15H26O	1000150-05-1	25
4	cis-13,16-Docasadienoic acid, me...	350	C23H42O2	1000333-60-3	20
5	Thiocyanic acid, 4-oxotricyclo[3...	207	C11H13NOS	056781-89-6	18





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Data File : BF123799.D
Acq On : 4 May 2021 1:58
Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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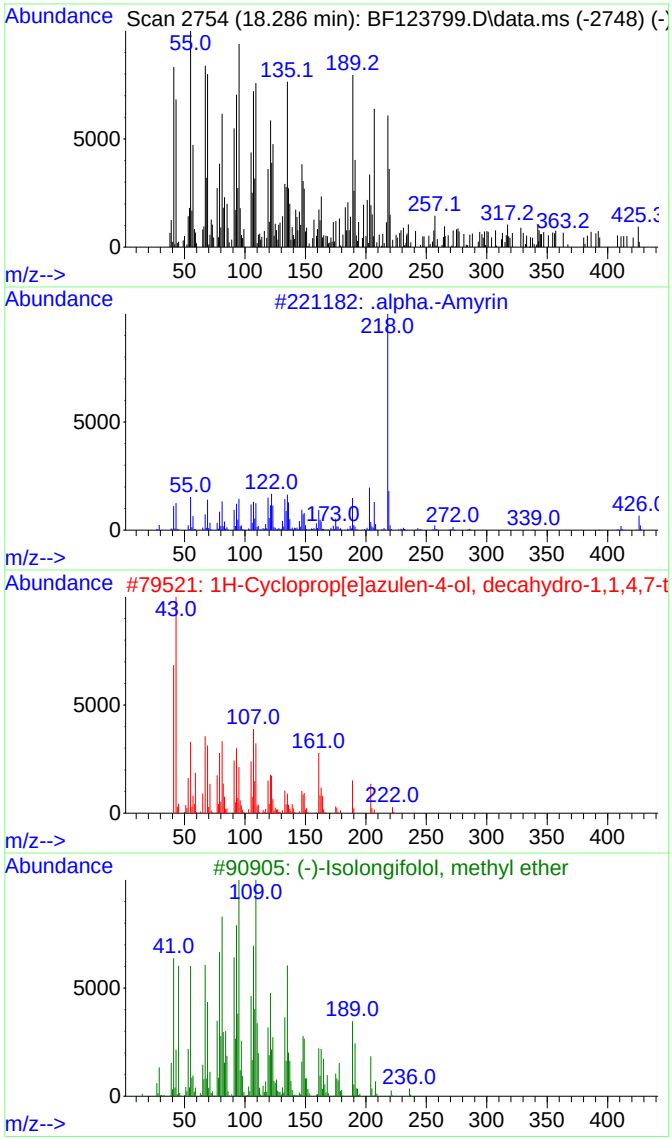
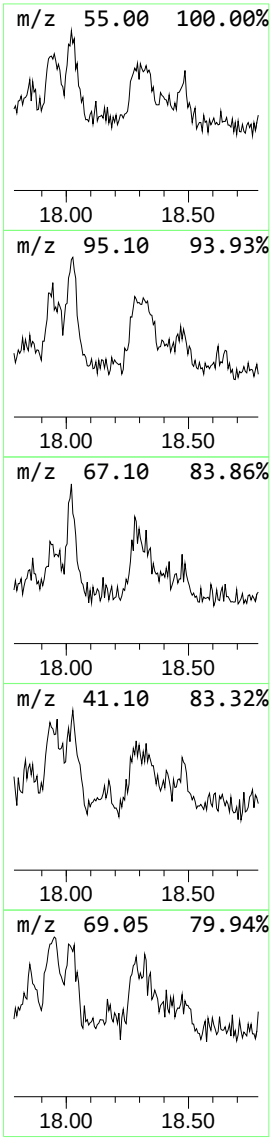
Peak Number 13 unknown18.286 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	9.70 ng	480314	Perylene-d12	15.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Amyrin	426	C30H50O	000638-95-9	47
2	1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	46
3	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	41
4	2,4,4-Trimethyl-3-hydroxymethyl-...	222	C15H26O	1000144-10-5	38
5	Tricyclo[4.3.0.0(7,9)]nonane, 2,...	206	C15H26	054832-82-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
Data File : BF123799.D
Acq On : 4 May 2021 1:58
Operator : JU/CG
Sample : M2235-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-043021

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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
Propane, 1,1-di...	2.157	2.3	ng	200726	1	6.810	1759800	20.0
2-Pentanone, 4-...	5.010	2.1	ng	185914	1	6.810	1759800	20.0
Undecanoic acid	11.869	2.3	ng	201973	4	11.333	1742410	20.0
Heptacosyl pent...	13.833	6.1	ng	427407	5	13.974	1405490	20.0
Octadecane	14.451	5.0	ng	348790	5	13.974	1405490	20.0
Supraene	14.833	3.9	ng	191272	6	15.433	990674	20.0
Octadecanal	14.898	2.5	ng	122580	6	15.433	990674	20.0
Heptadecane, 9-...	15.092	29.0	ng	1435390	6	15.433	990674	20.0
Heptacosane	15.898	25.1	ng	1244790	6	15.433	990674	20.0
unknown17.503	17.503	43.8	ng	2170750	6	15.433	990674	20.0
.beta.-Amyrin	17.945	19.7	ng	976483	6	15.433	990674	20.0
unknown18.021	18.021	20.5	ng	1016430	6	15.433	990674	20.0
unknown18.286	18.286	9.7	ng	480314	6	15.433	990674	20.0