LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123834.D
Acq On : 5 May 2021 18:39
Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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: BF123834.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.992	491	494	503	rVB	203481	238279	4.25%	0.542%
2	5.410	561	565	569	rBV	5675019	5326929	95.09%	12.117%
3	6.434	735	739	742	rBV	5976812	5601849	100.00%	12.742%
4	6.792	796	800	803	rBV	2022264	1492843	26.65%	3.396%
5	7.357	891	896	899	rBV	4373280	3624468	64.70%	8.245%
6	8.075	1013	1018	1022	rBV	2349965	2013567	35.94%	4.580%
7	9.157	1198	1202	1205	rBV	7043399	5476048	97.75%	12.456%
8	9.239	1213	1216	1219	rBV	77370	67621	1.21%	0.154%
9	9.416	1243	1246	1251	rVB4	47584	70668	1.26%	0.161%
10	9.492	1256	1259	1261	rBV	93996	78808	1.41%	0.179%
11	9.551	1266	1269	1273	rBV	377904	332696	5.94%	0.757%
12	9.833	1311	1317	1320	rBV	2594247	2096819	37.43%	4.770%
13	9.863	1320	1322	1326	rVB	90411	85685	1.53%	0.195%
14	10.380	1407	1410	1415	rBV2	103384	93392	1.67%	0.212%
15	10.621	1447	1451	1455	rBV	3854227	3454520	61.67%	7.858%
16	10.745	1469	1472	1476	rVB2	86943	98650	1.76%	0.224%
17	11.321	1566	1570	1572	rBV	2308446	1854106	33.10%	4.218%
18	11.345	1572	1574	1577	rVV	526899	391897	7.00%	0.891%
19	11.392	1577	1582	1585	rVB	158516	192027	3.43%	0.437%
20	11.821	1650	1655	1658	rBV	153274	149913	2.68%	0.341%
21	11.857	1658	1661	1665	rBV2	256934	270514	4.83%	0.615%
22	11.898	1665	1668	1671	rVB2	70045	75005	1.34%	0.171%
23	11.933	1671	1674	1677	rBV	184216	214166	3.82%	0.487%
24	12.374	1746	1749	1751	rBV2	85702	87029	1.55%	0.198%
25	12.404	1751	1754	1761	rVB5	159552	238293	4.25%	0.542%
26	12.533	1773	1776	1779	rVB	372636	311995	5.57%	0.710%
27	12.763	1810	1815	1818	rBV	476666	447006	7.98%	1.017%
28	12.815	1821	1824	1829	rVB5	53537	76744	1.37%	0.175%
29	12.910	1836	1840	1844	rBV	4373321	3903238	69.68%	8.879%
30	13.092	1869	1871	1874	rVB2	101293	89970	1.61%	0.205%
31	13.162	1877	1883	1886	rBV2	93682	158675	2.83%	0.361%
32	13.198	1886	1889	1892	rVV	77527	71574	1.28%	0.163%
33	13.321	1907	1910	1914	rBV2	75026	69252	1.24%	0.158%
34	13.821	1992	1995	2004	rBV3	320032	651561	11.63%	1.482%
35	13.962	2014	2019	2022	rBV	1447739	1577978	28.17%	3.589%
36	13.992	2022	2024	2026	rVB	191974	146965	2.62%	0.334%

LSC Area Percent Report

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Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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	14.139	2045	2049	2054	rBV2	115301	152877	2.73%	0.348%
38	14.445	2098	2101	2103	rVB	166983	143459	2.56%	0.326%
39	14.745	2149	2152	2156	rBV	146476	148112	2.64%	0.337%
40	14.821	2162	2165	2172	rVB	128497	151257	2.70%	0.344%
41	14.998	2192	2195	2204	rVB	129788	250115	4.46%	0.569%
42	15.080	2206	2209	2212	rBV	172179	163083	2.91%	0.371%
43	15.356	2254	2256	2262	rVB	107832	133434	2.38%	0.304%
44	15.421	2262	2267	2271	rBV2	945671	1163170	20.76%	2.646%
45	15.886	2343	2346	2352	rVB2	126746	161394	2.88%	0.367%
46	17.474	2611	2616	2631	rVB2	154236	364445	6.51%	0.829%

Sum of corrected areas: 43962096

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
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Operator : JU/CG
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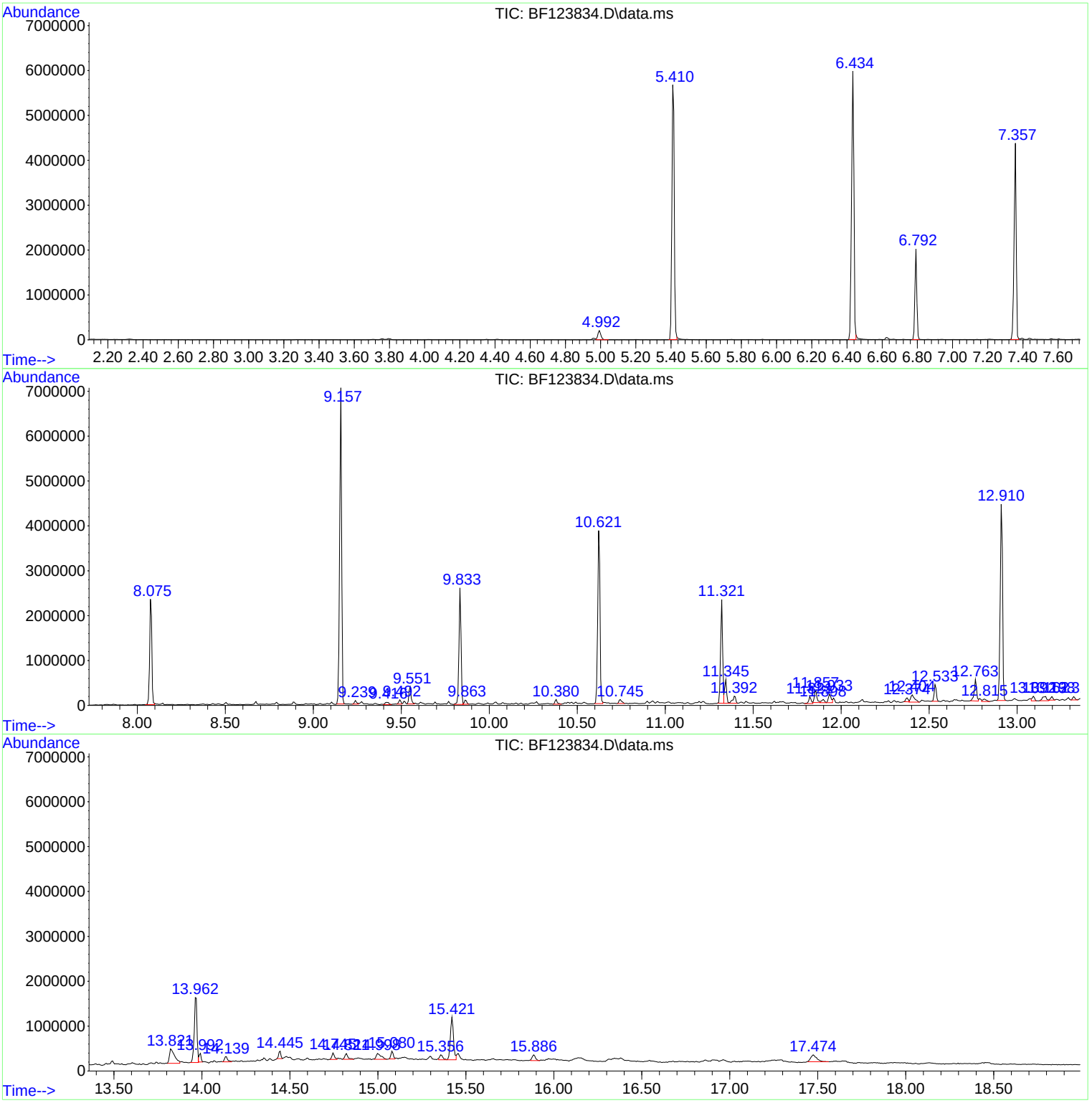
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-16

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123834.D
Acq On : 5 May 2021 18:39
Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-16

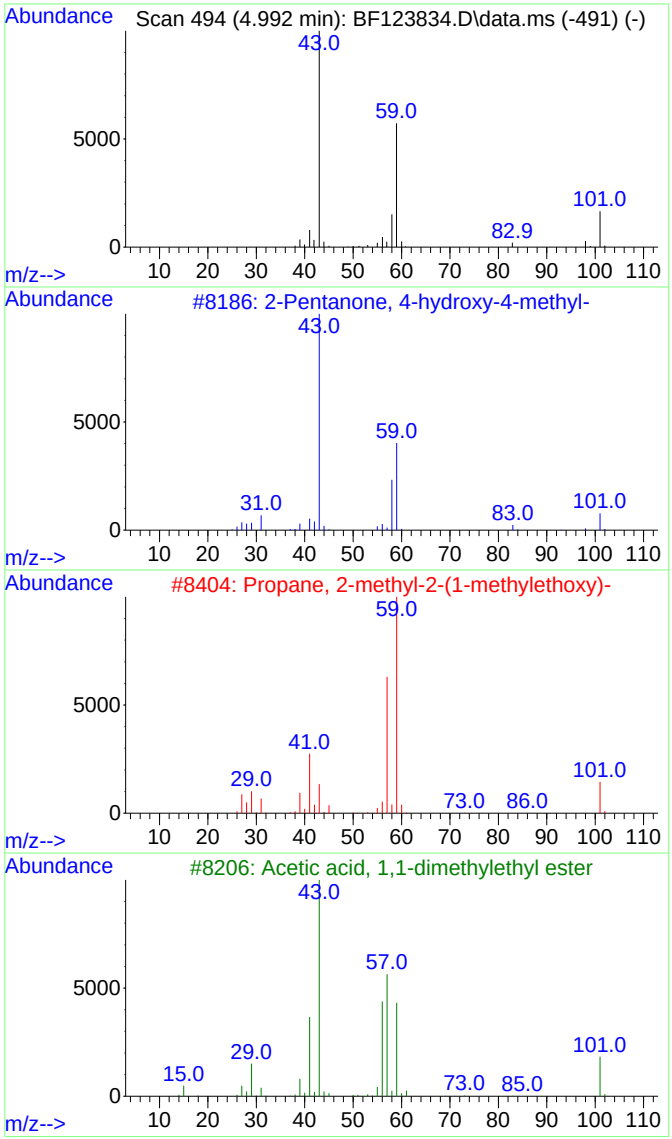
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

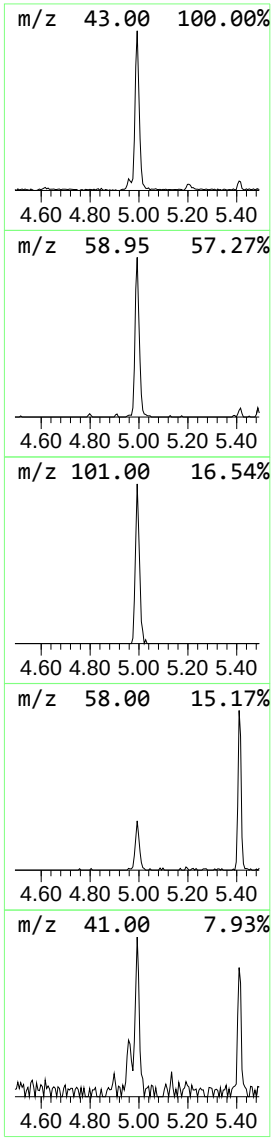
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	3.19 ng	238279	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Octanol	130	C8H18O	000589-98-0	33





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Data File : BF123834.D
Acq On : 5 May 2021 18:39
Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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

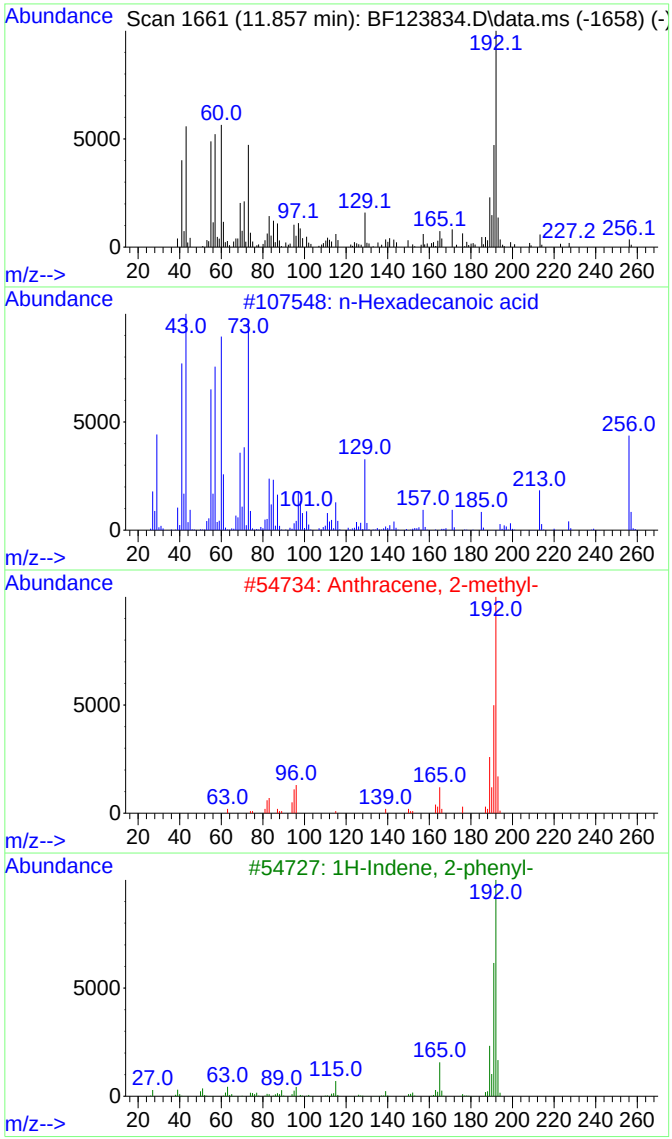
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

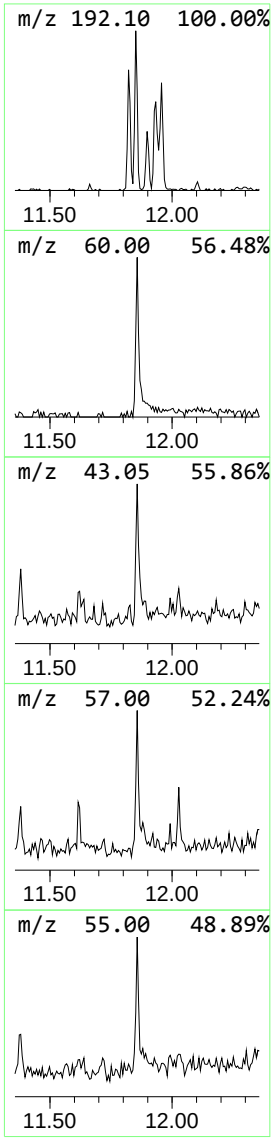
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	2.92 ng	270514	Phenanthrene-d10	11.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	62
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	60
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	53
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123834.D
Acq On : 5 May 2021 18:39
Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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

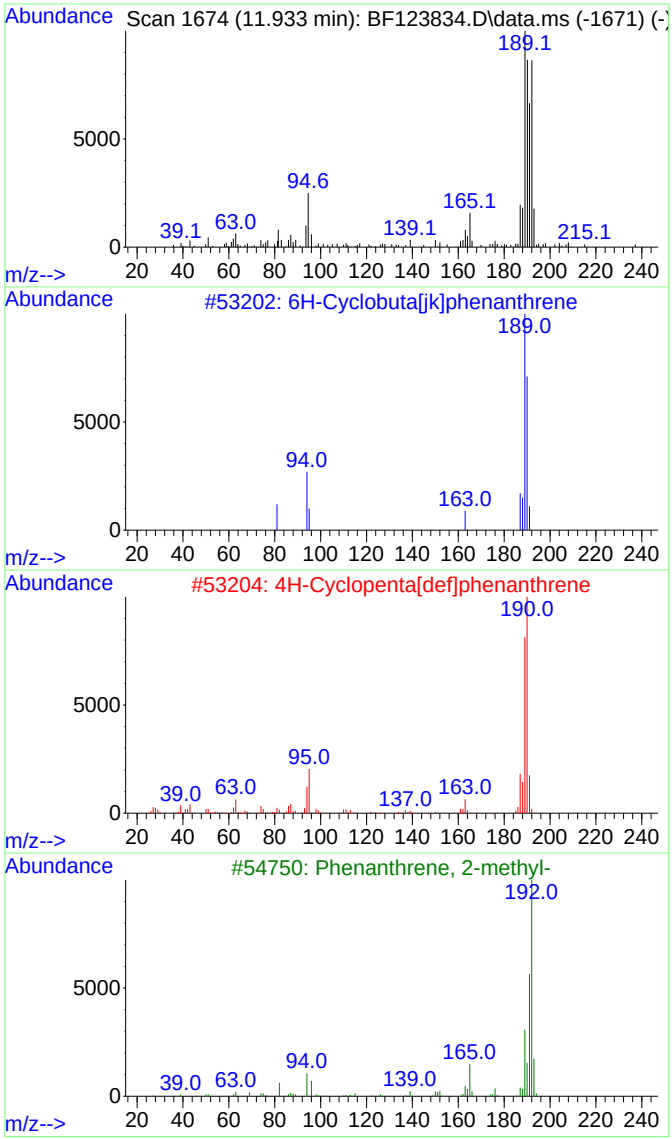
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

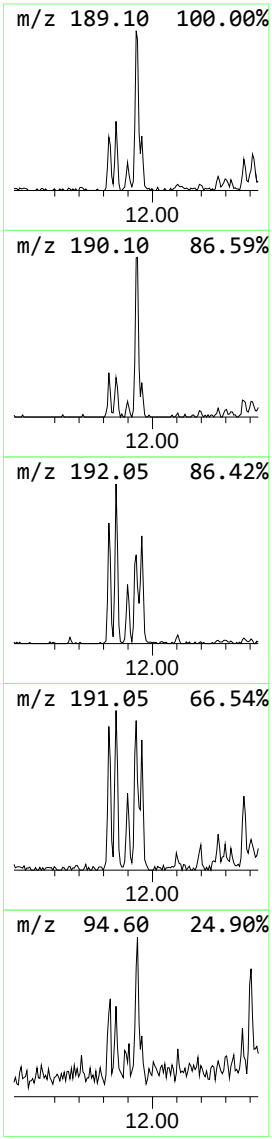
****

Peak Number 3 unknown11.933 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.31 ng	214166	Phenanthrene-d10	11.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	46
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38





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Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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

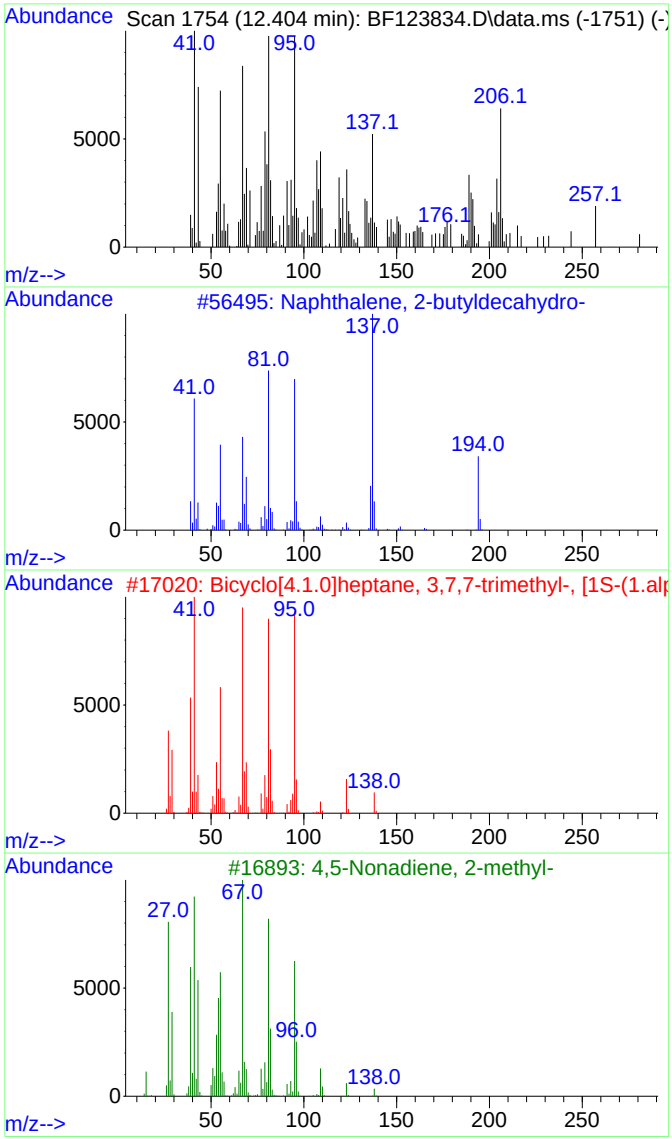
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

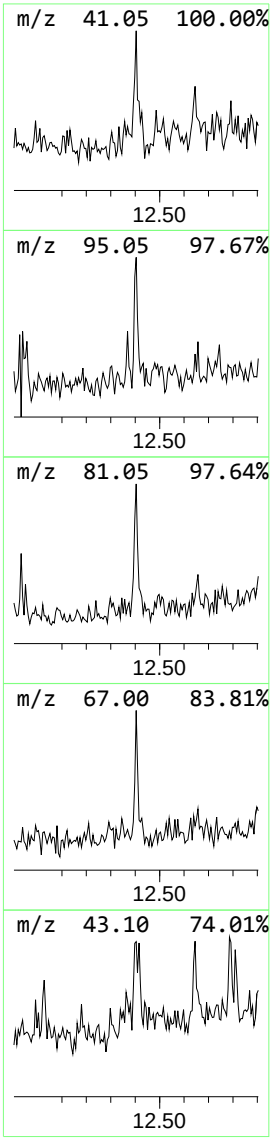
****

Peak Number 4 Naphthalene, 2-butyldecahydro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.404	2.57 ng	238293	Phenanthrene-d10	11.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	60
2	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	006069-97-2	50
3	4,5-Nonadiene, 2-methyl-	138	C10H18	055956-32-6	46
4	1,4-Pentadiene, 3-propyl-	110	C8H14	000996-83-8	43
5	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	38





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Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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
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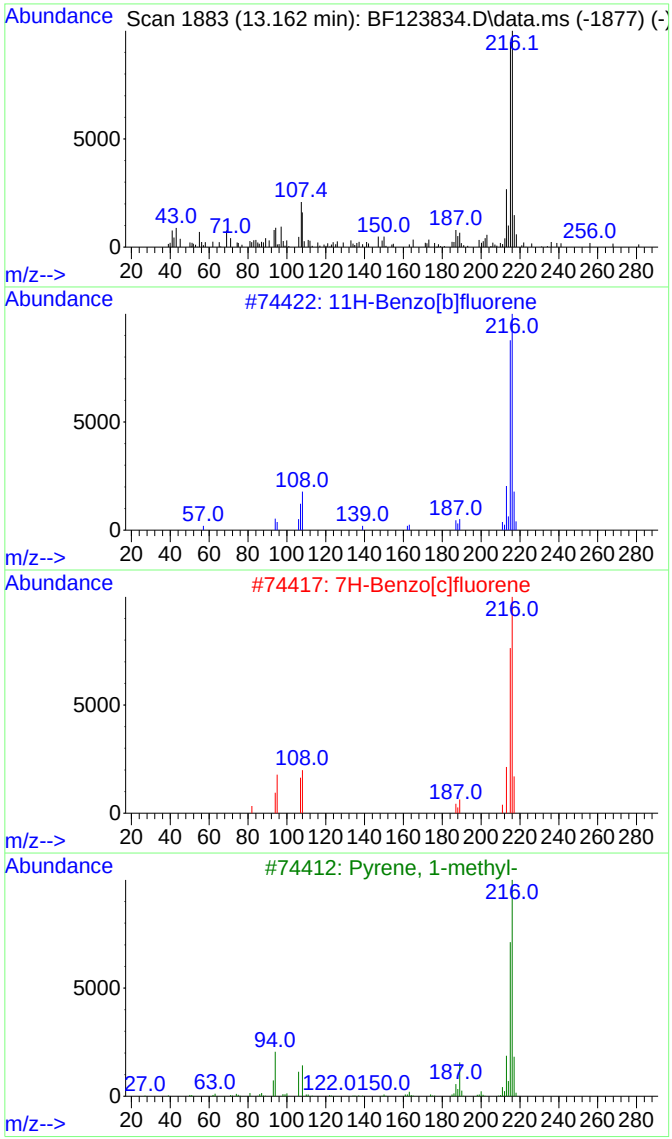
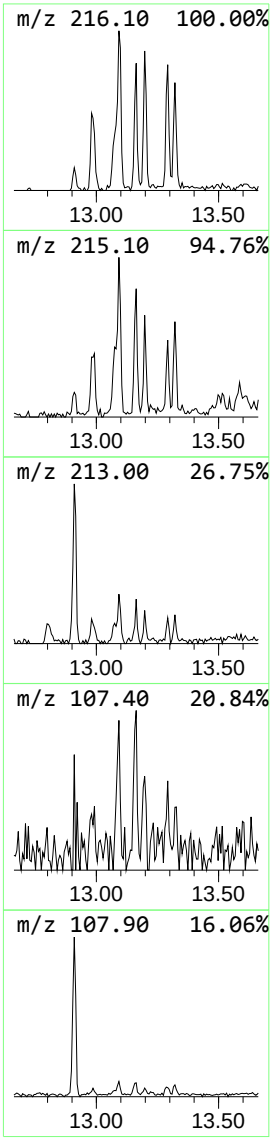
****

Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	2.01 ng	158675	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	68
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	64
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	58
5	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	53





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

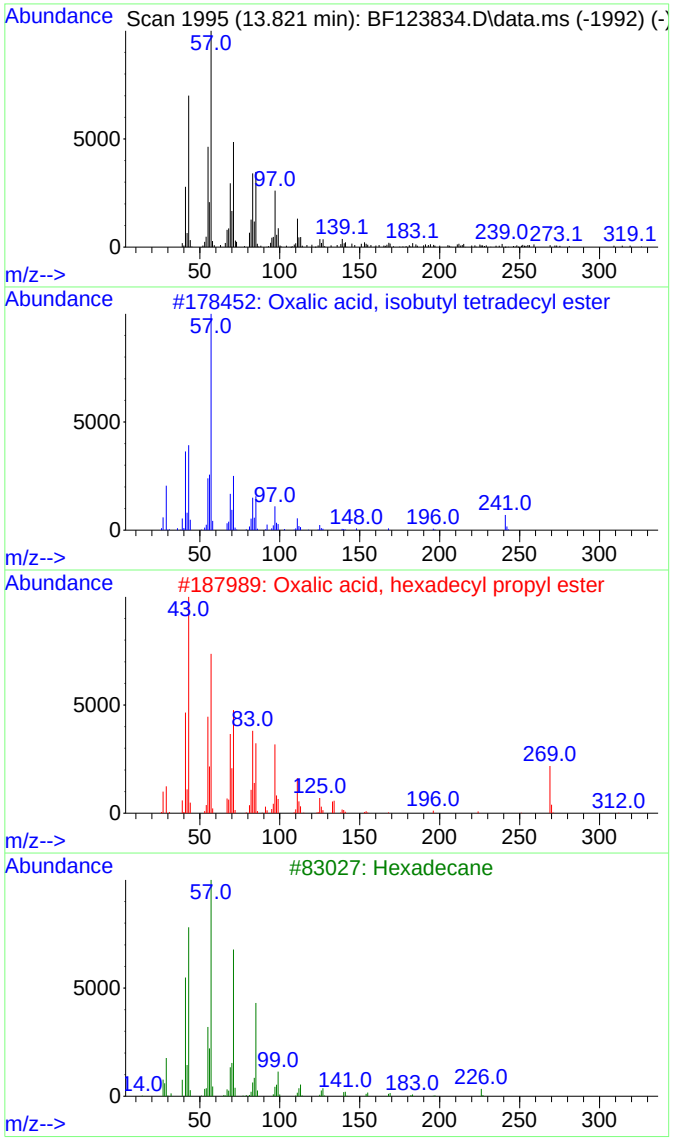
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

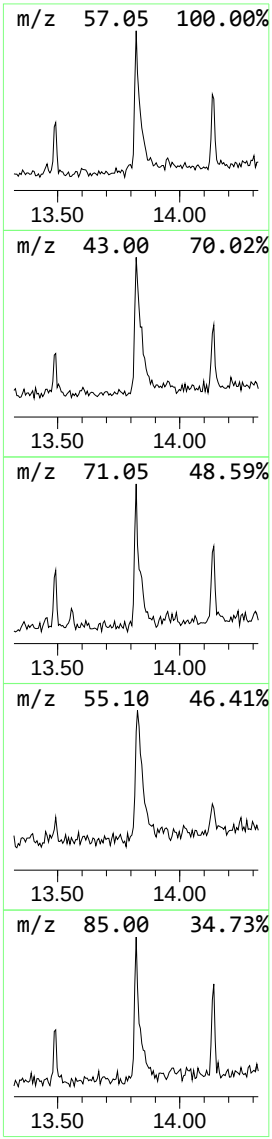
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Oxalic acid, isobutyl tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	8.26 ng	651561	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	90
2	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	86
3	Hexadecane	226	C16H34	000544-76-3	83
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	68
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	62





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Instrument : BNA_F
ClientSampleId : EME-16

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

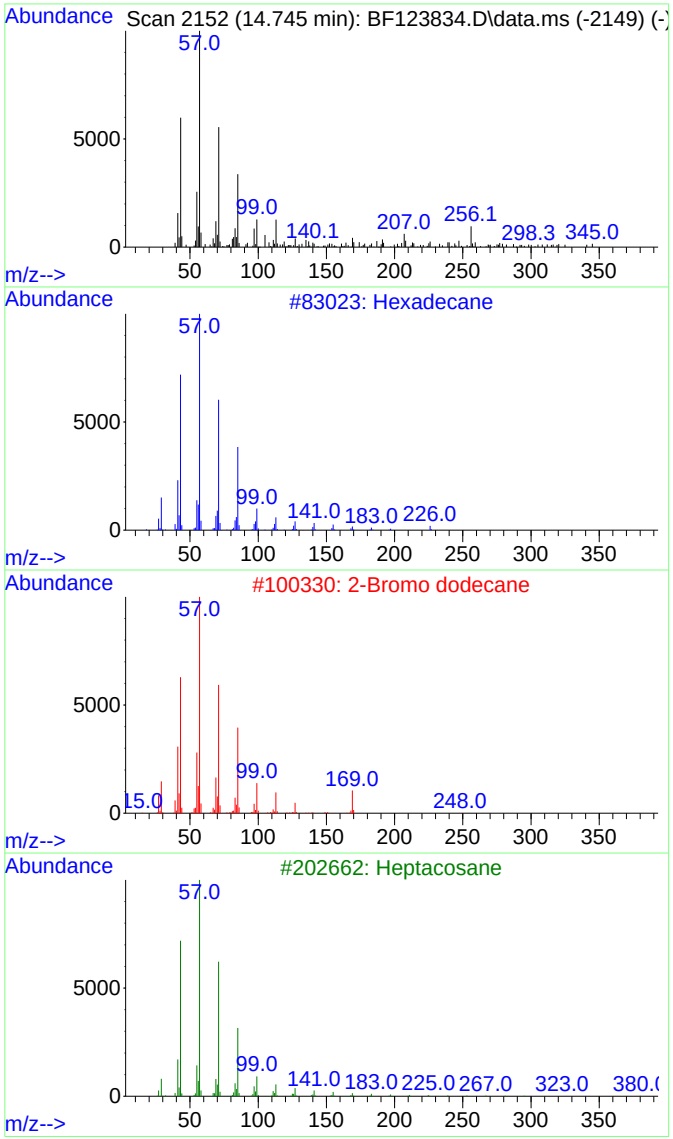
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

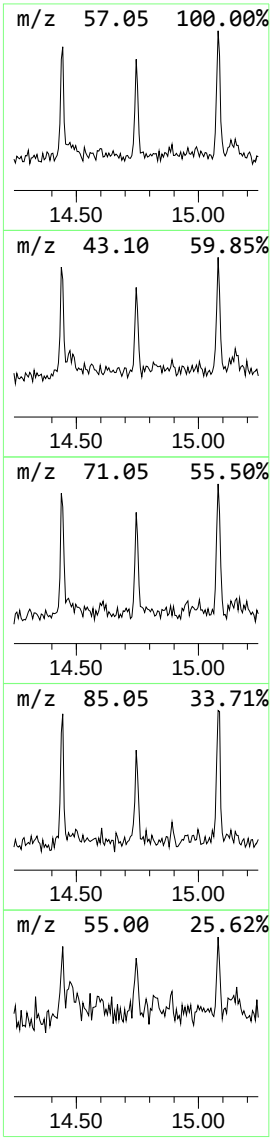
****

Peak Number 7 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	2.55 ng	148112	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	74
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	72
3	Heptacosane	380	C27H56	000593-49-7	72
4	Pentacosane	352	C25H52	000629-99-2	72
5	Heptadecane	240	C17H36	000629-78-7	62





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Data File : BF123834.D
Acq On : 5 May 2021 18:39
Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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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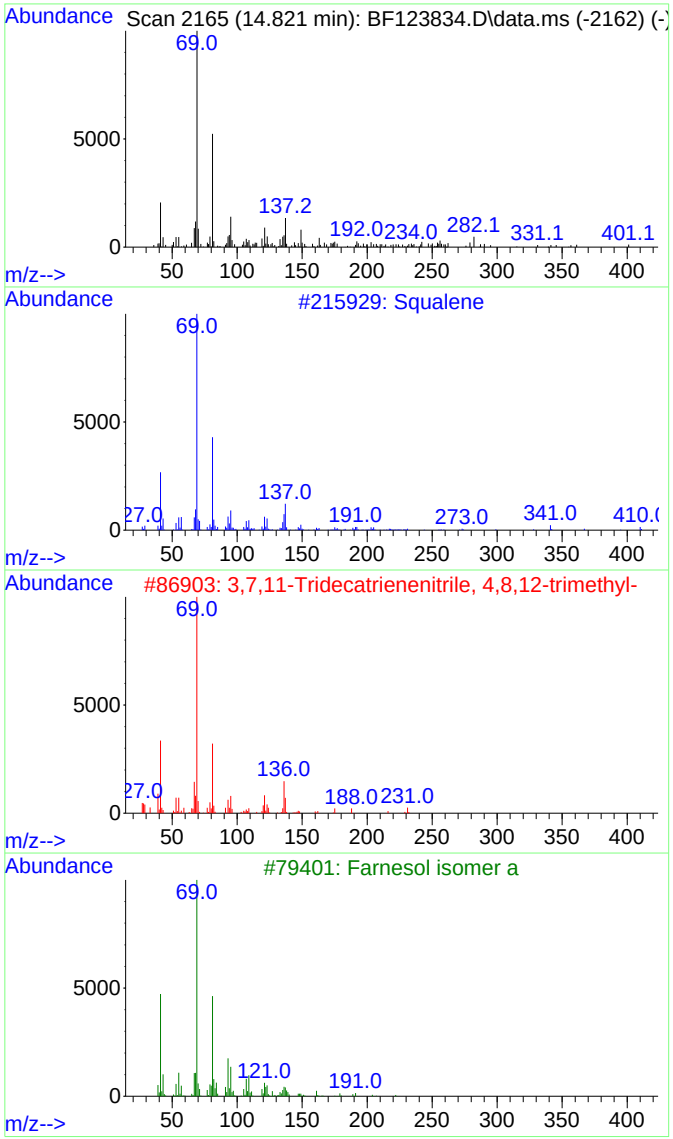
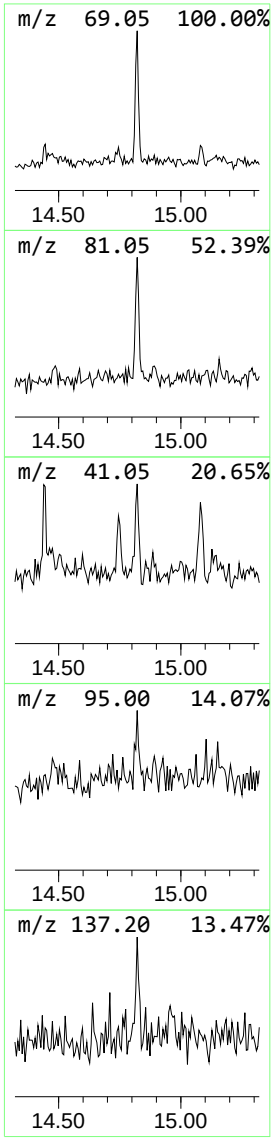
Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.60 ng	151257	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	80
2	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
3	Farnesol isomer a	222	C15H26O	1000108-92-4	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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Data File : BF123834.D
Acq On : 5 May 2021 18:39
Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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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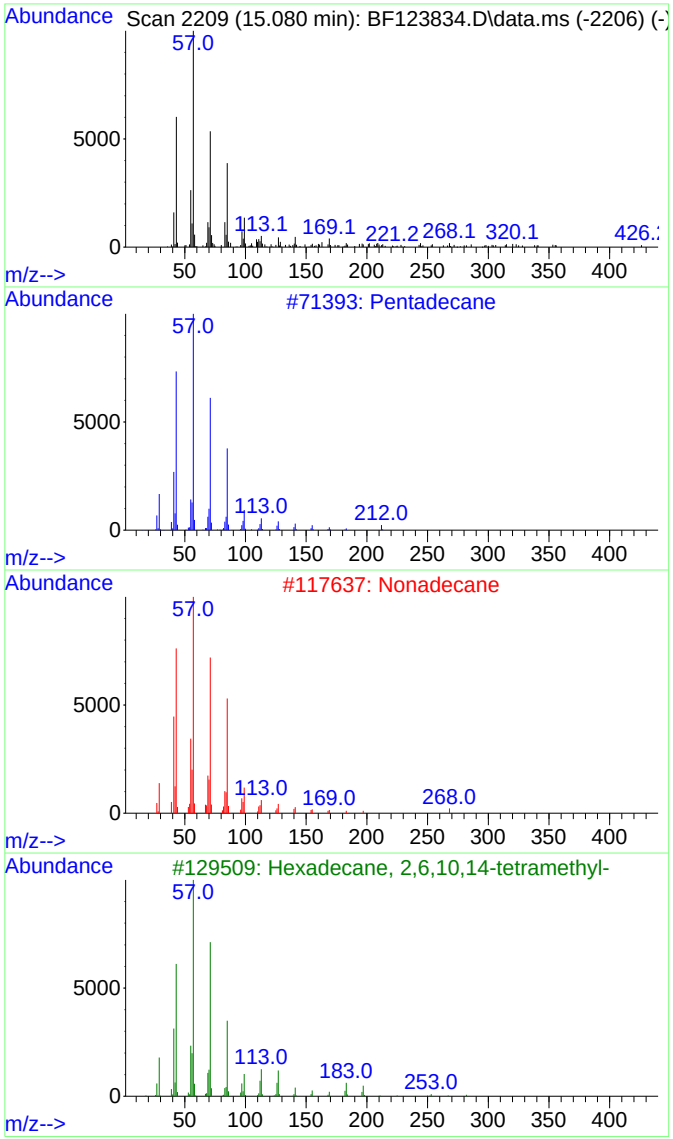
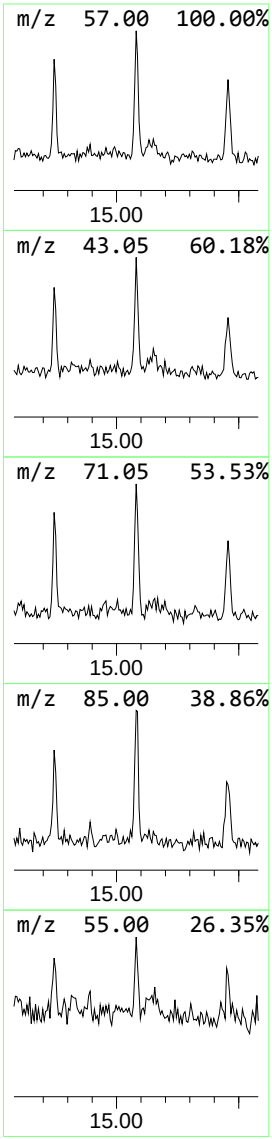
Peak Number 9 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	2.80 ng	163083	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	94
2	Nonadecane	268	C19H40	000629-92-5	93
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
4	1-Iodoundecane	282	C11H23I	004282-44-4	87
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87





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Data File : BF123834.D
Acq On : 5 May 2021 18:39
Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-16

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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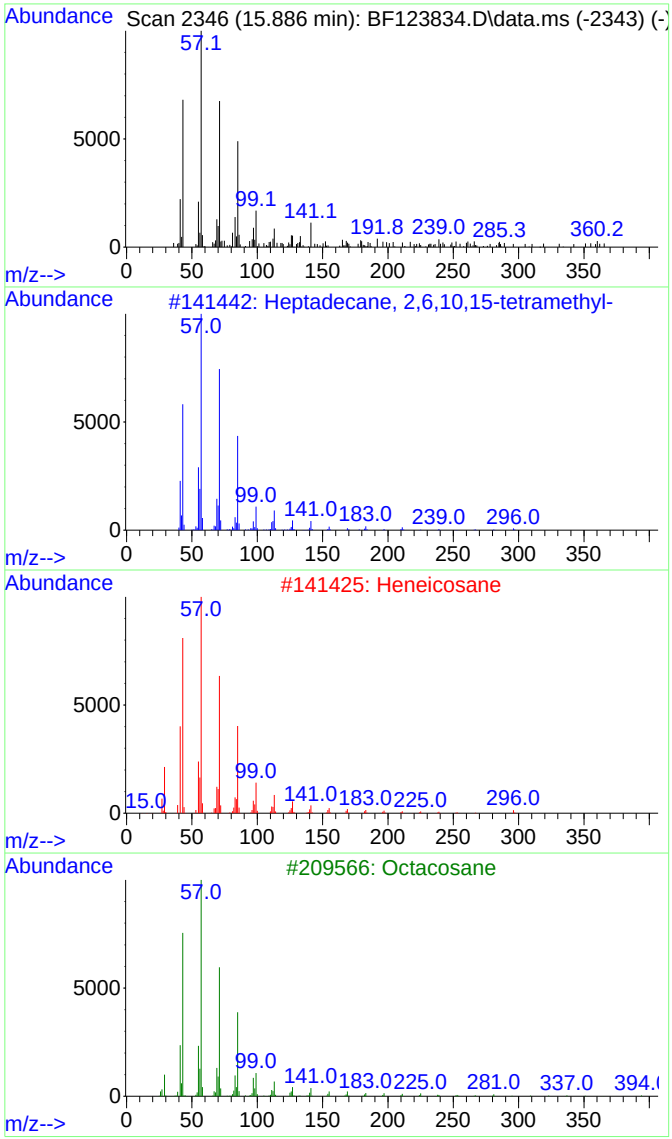
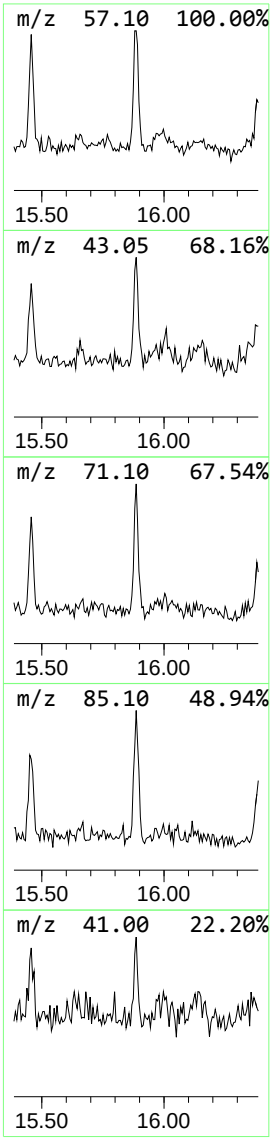
Peak Number 10 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	2.78 ng	161394	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
2	Heneicosane	296	C21H44	000629-94-7	83
3	Octacosane	394	C28H58	000630-02-4	80
4	Tetracosane	338	C24H50	000646-31-1	80
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123834.D
Acq On : 5 May 2021 18:39
Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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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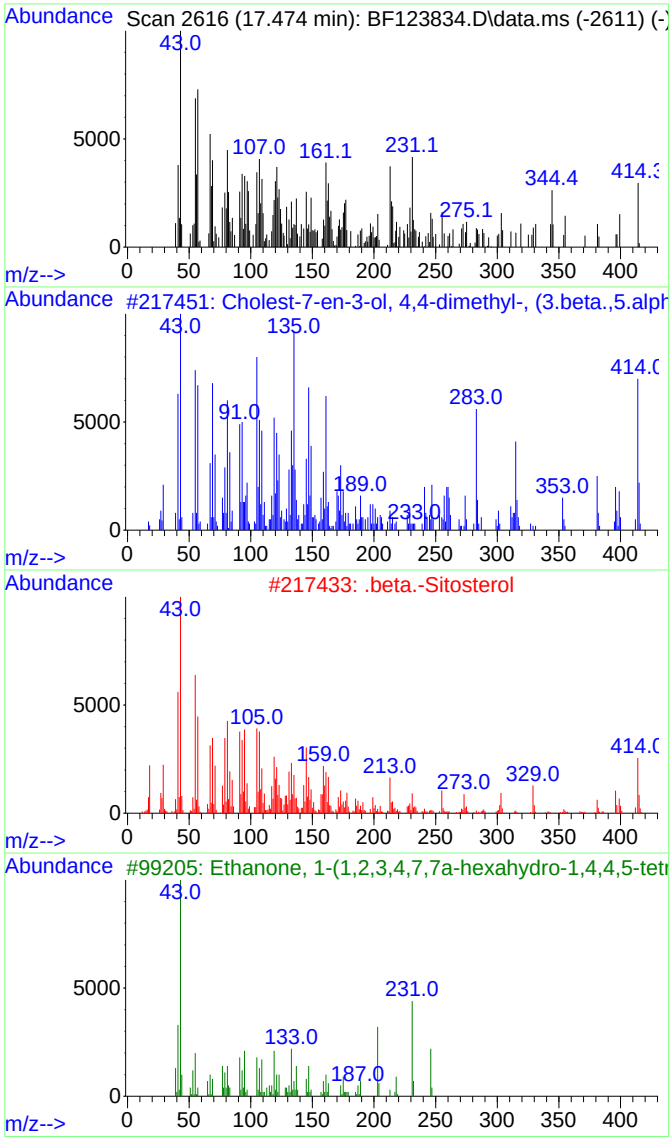
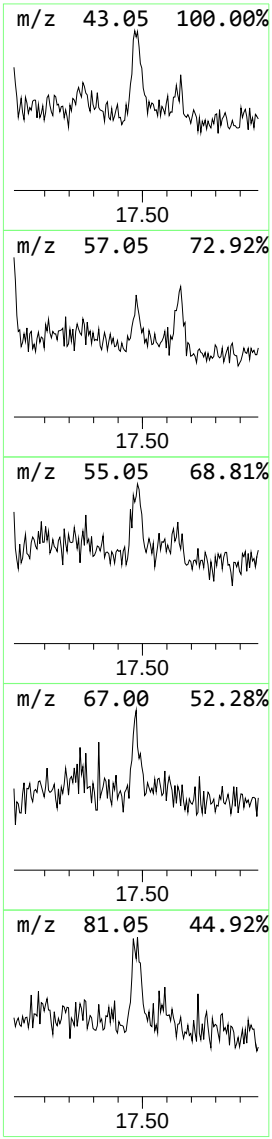
Peak Number 11 unknown17.474 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.474	6.27 ng	364445	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-7-en-3-ol, 4,4-dimethyl-...	414	C29H50O	006384-28-7	25
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	25
3	Ethanone, 1-(1,2,3,4,7,7a-hexahy...	246	C17H26O	032388-58-2	25
4	Cholic acid, triacetate	534	C30H46O8	052840-09-2	12
5	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123834.D
Acq On : 5 May 2021 18:39
Operator : JU/CG
Sample : M2279-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-16

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
2-Pentanone, 4-...	4.992	3.2	ng	238279	1	6.792	1492840	20.0
n-Hexadecanoic ...	11.857	2.9	ng	270514	4	11.321	1854110	20.0
unknown11.933	11.933	2.3	ng	214166	4	11.321	1854110	20.0
Naphthalene, 2-...	12.404	2.6	ng	238293	4	11.321	1854110	20.0
11H-Benzo[b]flu...	13.163	2.0	ng	158675	5	13.968	1577980	20.0
Oxalic acid, is...	13.821	8.3	ng	651561	5	13.968	1577980	20.0
Hexadecane	14.745	2.5	ng	148112	6	15.421	1163170	20.0
Squalene	14.821	2.6	ng	151257	6	15.421	1163170	20.0
Pentadecane	15.080	2.8	ng	163083	6	15.421	1163170	20.0
Heptadecane, 2,...	15.886	2.8	ng	161394	6	15.421	1163170	20.0
unknown17.474	17.474	6.3	ng	364445	6	15.421	1163170	20.0