LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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: BF123259.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	12	rVB	416553	495196	9.95%	1.490%
2	5.481	572	577	580	rBV	3105357	2877296	57.84%	8.657%
3	6.492	744	749	764	rVB	2892212	3221361	64.75%	9.692%
4	6.857	807	811	814	rBV	879803	726590	14.61%	2.186%
5	7.416	901	906	909	rBV	2102851	1892567	38.04%	5.694%
6	8.139	1025	1029	1032	rBV	1197363	963255	19.36%	2.898%
7	9.216	1207	1212	1215	rBV	3507172	3183548	63.99%	9.578%
8	9.610	1275	1279	1282	rBV	112925	87166	1.75%	0.262%
9	9.898	1324	1328	1331	rBV	1365102	1113592	22.38%	3.350%
10	10.692	1457	1463	1466	rBV	2165150	2180721	43.84%	6.561%
11	11.386	1577	1581	1584	rBV	1364325	1205778	24.24%	3.628%
12	11.410	1584	1585	1588	rVB	91626	52003	1.05%	0.156%
13	11.921	1668	1672	1684	rBV2	621475	711206	14.30%	2.140%
14	12.457	1751	1763	1773	rBV2	1920972	4974825	100.00%	14.967%
15	12.604	1785	1788	1791	rBV	127982	118725	2.39%	0.357%
16	12.710	1802	1806	1819	rBV	189855	285092	5.73%	0.858%
17	12.833	1823	1827	1829	rBV	147566	165583	3.33%	0.498%
18	12.857	1829	1831	1841	rVB3	128099	207027	4.16%	0.623%
19	12.980	1845	1852	1856	rBV	3828701	3850318	77.40%	11.584%
20	13.463	1926	1934	1939	rBV4	34653	57219	1.15%	0.172%
21	13.757	1978	1984	1991	rBV4	89350	179209	3.60%	0.539%
22	13.898	2002	2008	2025	rBV5	265976	850338	17.09%	2.558%
23	14.039	2027	2032	2035	rBV	1329027	1172111	23.56%	3.526%
24	14.204	2056	2060	2063	rVB	66376	62817	1.26%	0.189%
25	14.357	2079	2086	2093	rBV	83443	158994	3.20%	0.478%
26	14.510	2108	2112	2116	rBV	83689	82200	1.65%	0.247%
27	14.815	2158	2164	2169	rBV2	68885	101382	2.04%	0.305%
28	14.874	2169	2174	2177	rVV	92517	151923	3.05%	0.457%
29	14.915	2177	2181	2187	rVB3	140929	219056	4.40%	0.659%
30	15.157	2218	2222	2226	rVB	70624	73388	1.48%	0.221%
31	15.445	2266	2271	2277	rBV2	88713	129159	2.60%	0.389%
32	15.515	2277	2283	2286	rBV	814657	1066554	21.44%	3.209%
33	15.980	2358	2362	2367	rVB2	51931	72818	1.46%	0.219%
34	16.098	2374	2382	2388	rBV3	72708	218630	4.39%	0.658%
35	16.533	2446	2456	2457	rBV6	63648	136333	2.74%	0.410%
36	17.233	2568	2575	2583	rBV2	77346	193873	3.90%	0.583%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

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

Sum of corrected areas: 33237853

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
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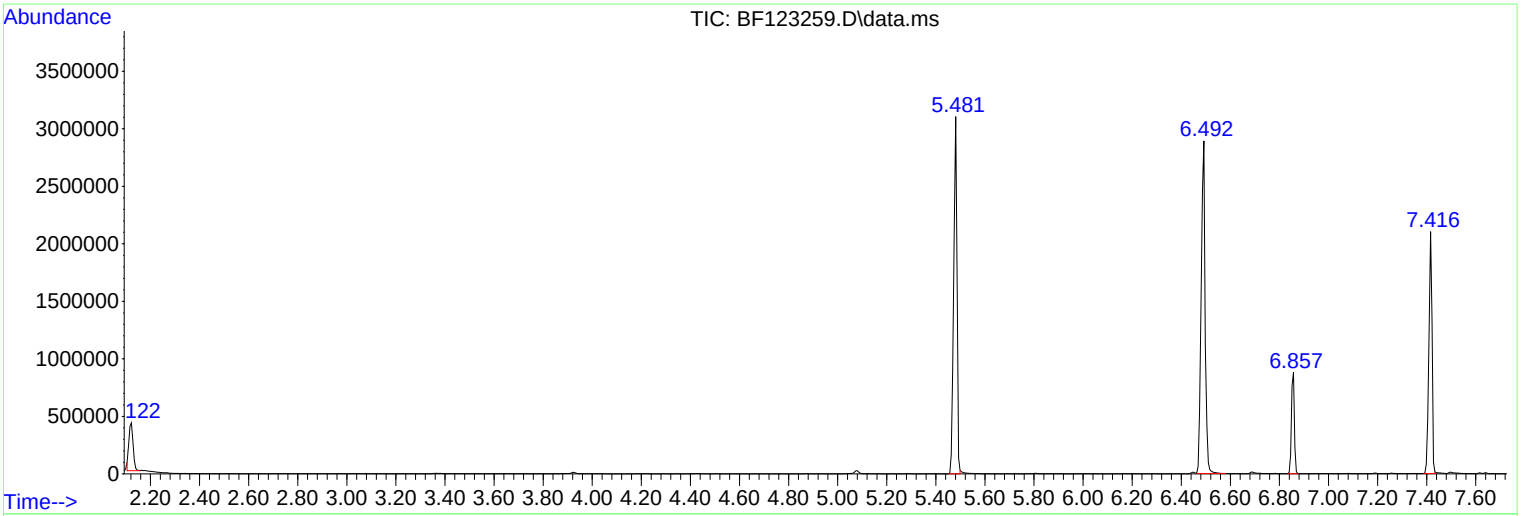
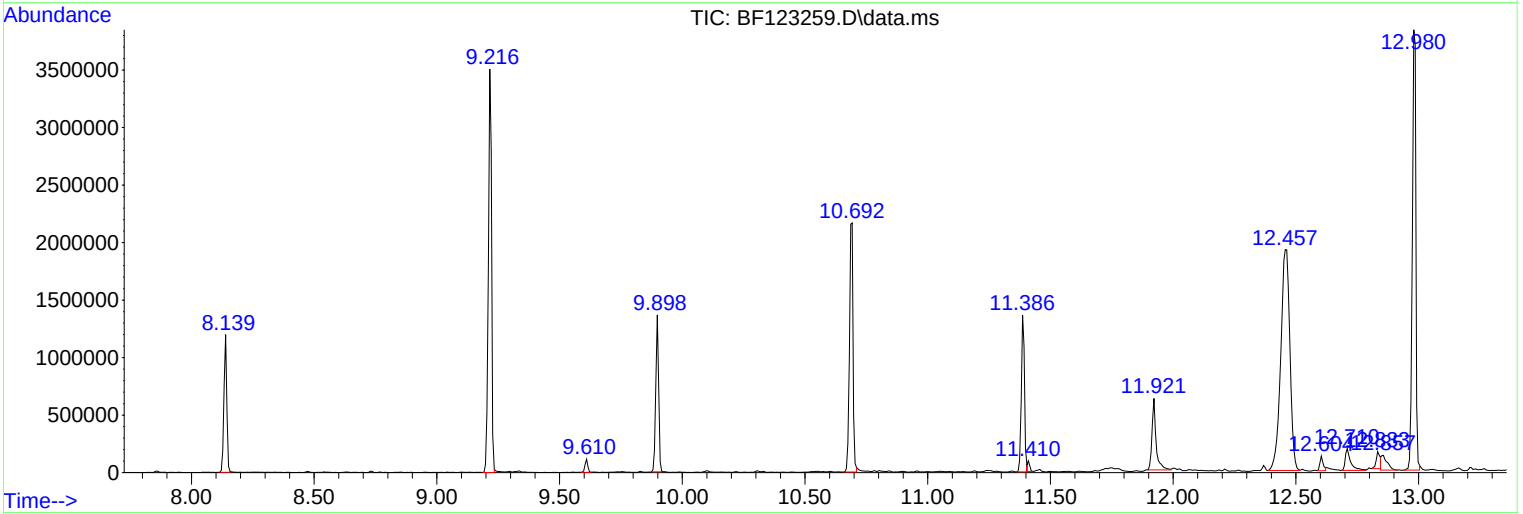
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

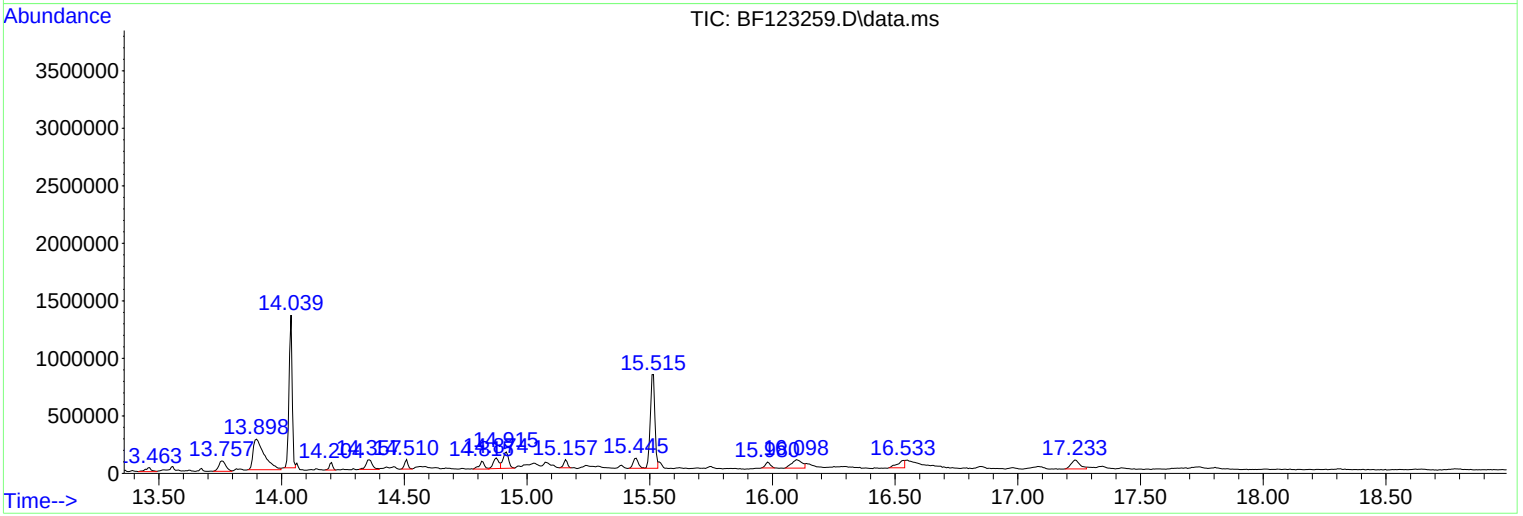
Instrument :
BNA_F
ClientSampleId :
TP-1

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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Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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

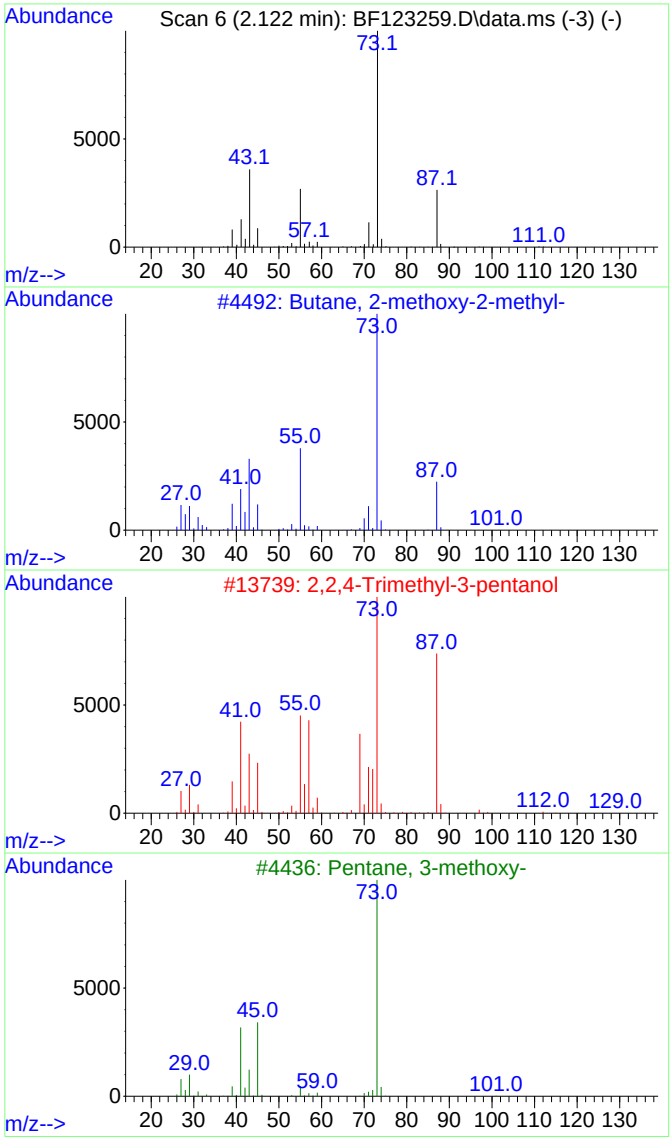
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

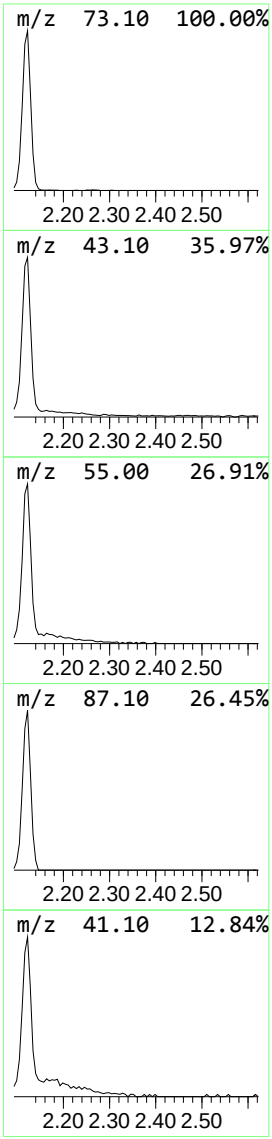
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	13.63 ng	495196	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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10





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Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

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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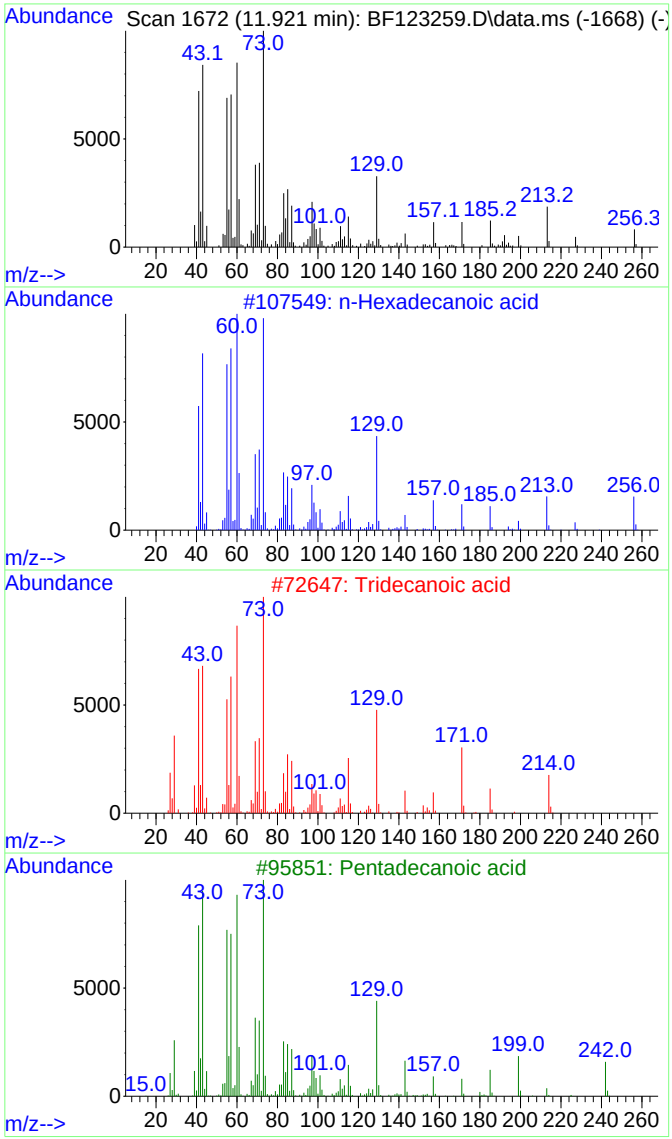
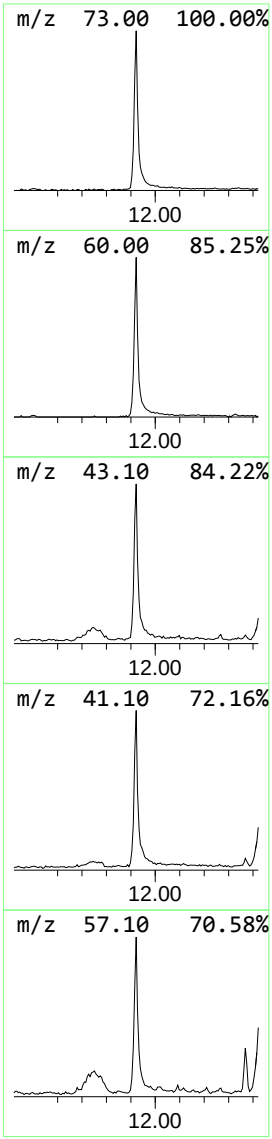
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	11.80 ng	711206	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

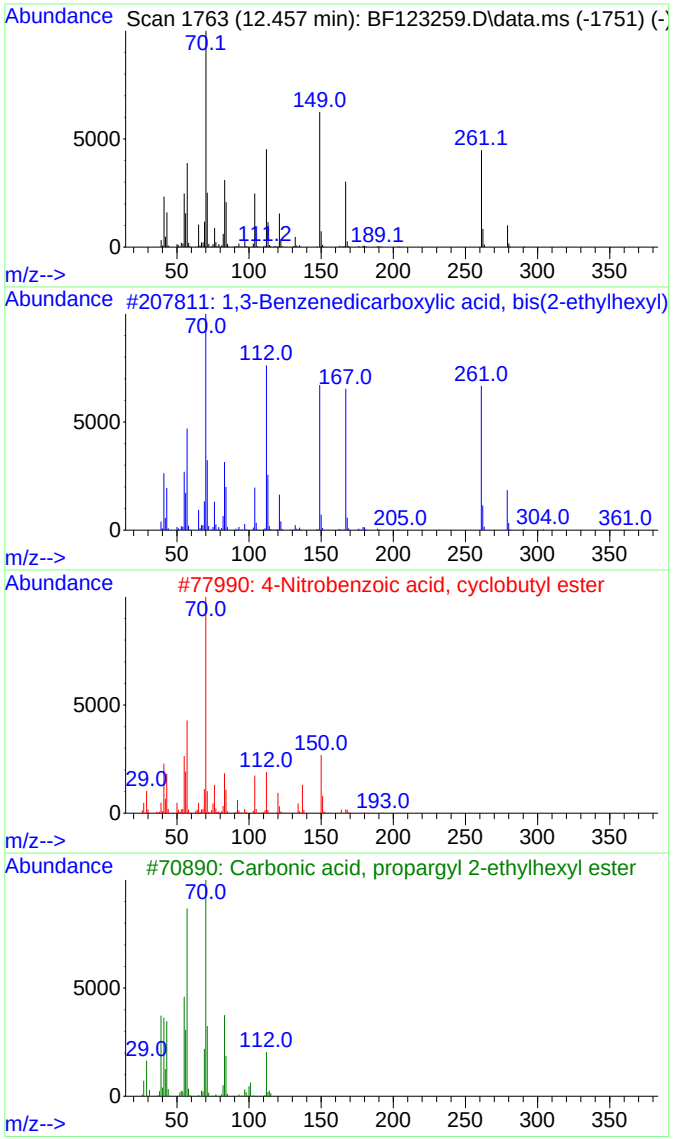
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

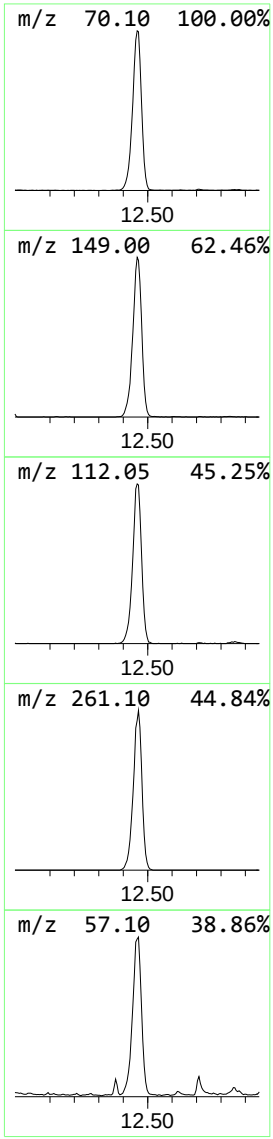
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,3-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	82.52 ng	4974830	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
2	4-Nitrobenzoic acid, cyclobutyl ...	221	C11H11NO4	070335-00-1	35
3	Carbonic acid, propargyl 2-ethyl...	212	C12H20O3	1000357-90-9	22
4	9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	18
5	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
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Sample : M1452-01
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Instrument : BNA_F
ClientSampleId : TP-1

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

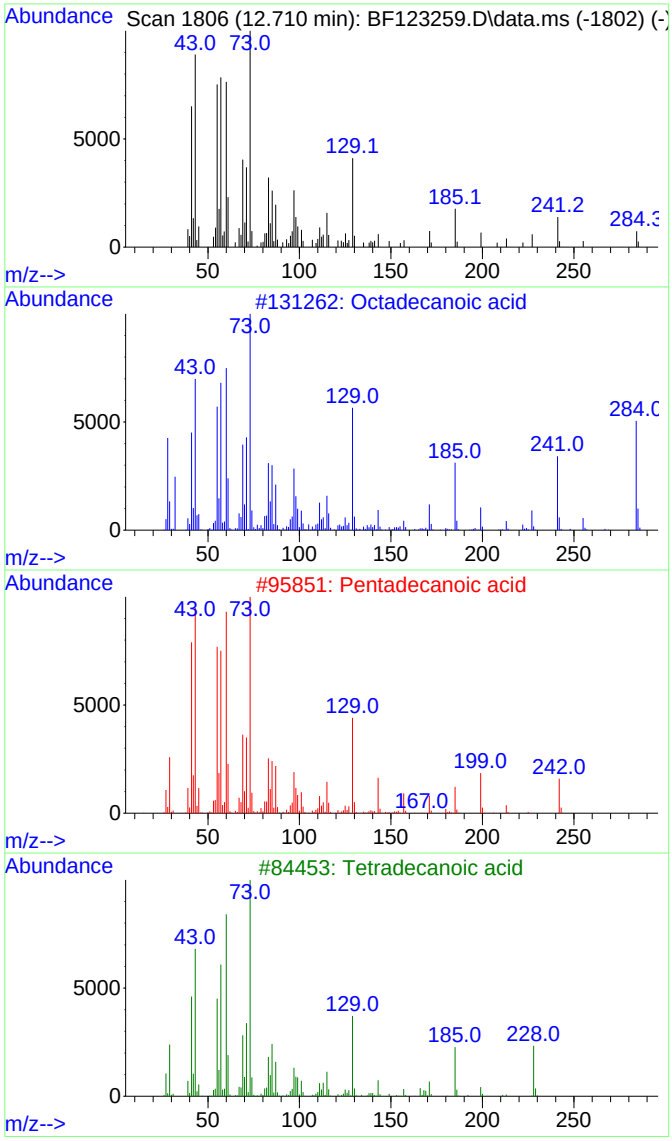
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

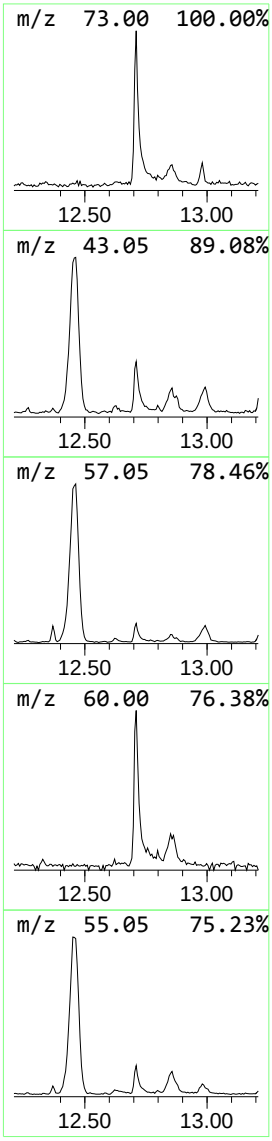
****

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	4.73 ng	285092	Phenanthrene-d10	11.386

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	78
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

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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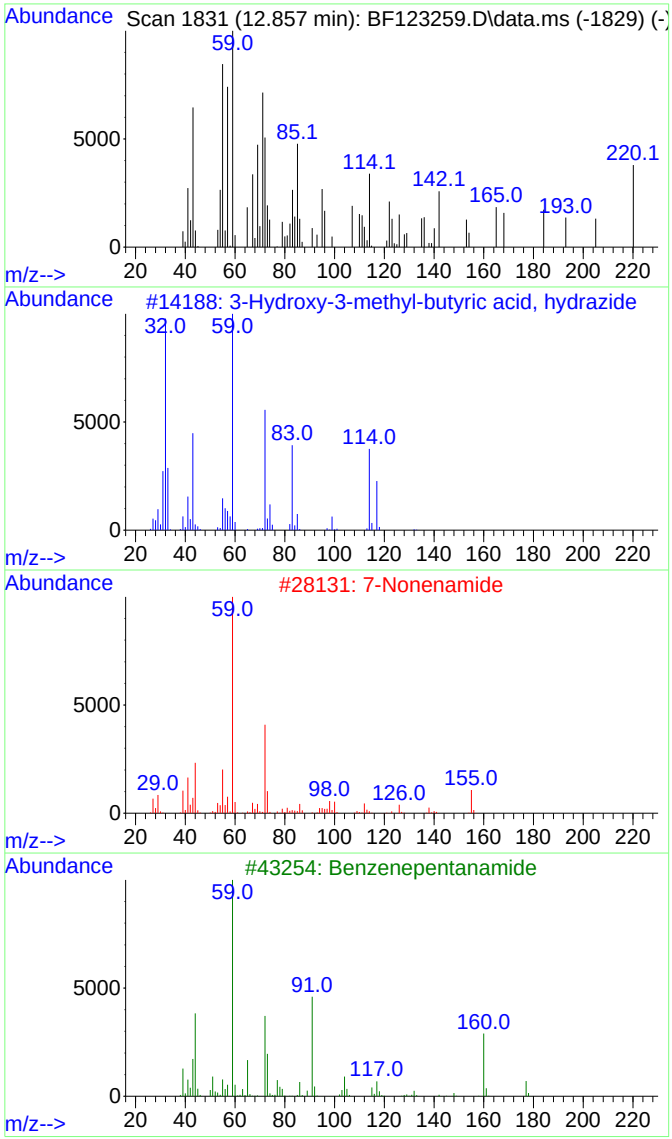
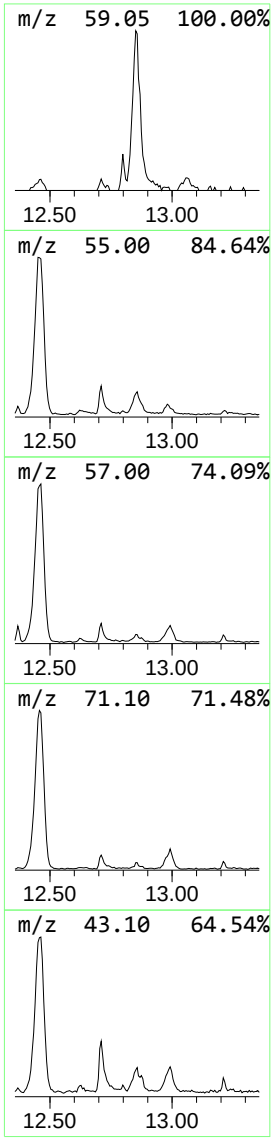
Peak Number 6 unknown12.85 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.857	3.53 ng	207027	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hydroxy-3-methyl-butyric acid,...	132	C5H12N2O2	1000193-80-2	38
2	7-Nonenamide	155	C9H17NO	090949-53-4	27
3	Benzenepentanamide	177	C11H15NO	036603-28-8	16
4	Pentan-2-ol, 4-allyloxy-2-methyl-	158	C9H18O2	102840-52-8	16
5	2-Ethoxyethyl trichloroacetate	234	C6H9Cl3O3	030668-97-4	16





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Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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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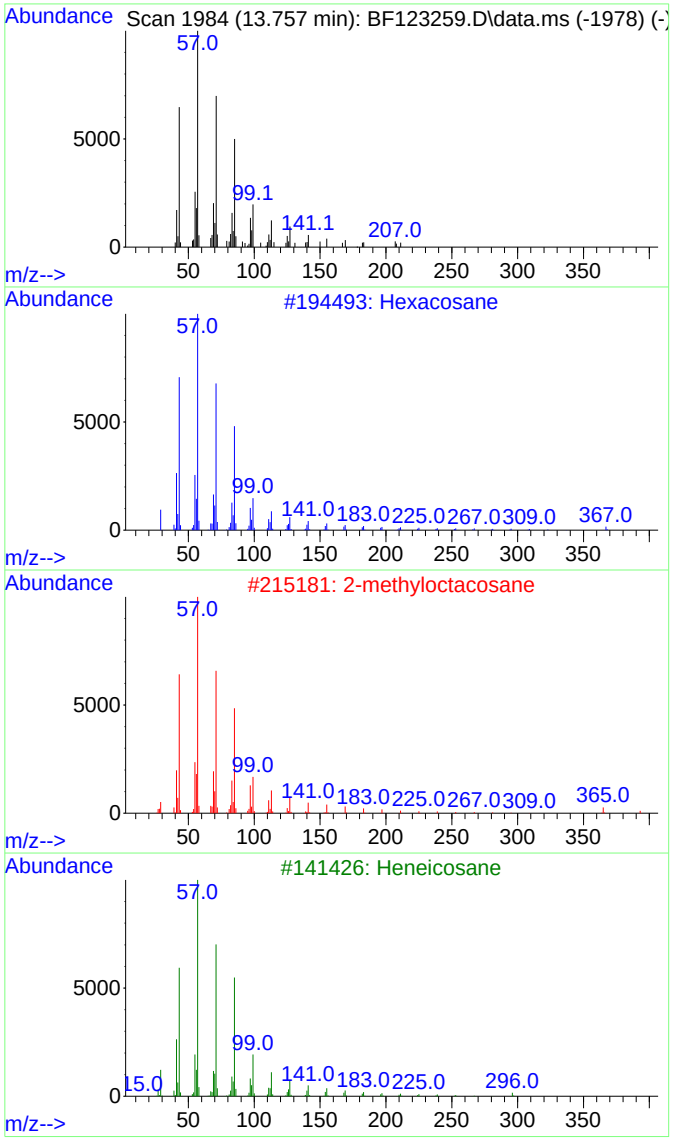
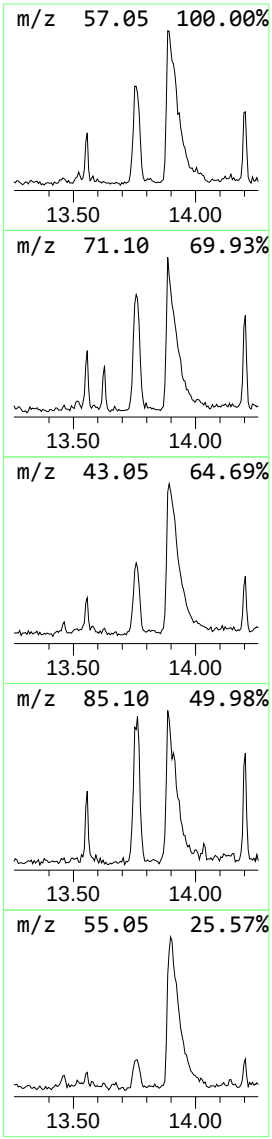
Peak Number 7 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	3.06 ng	179209	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Triacontane	422	C30H62	000638-68-6	91





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Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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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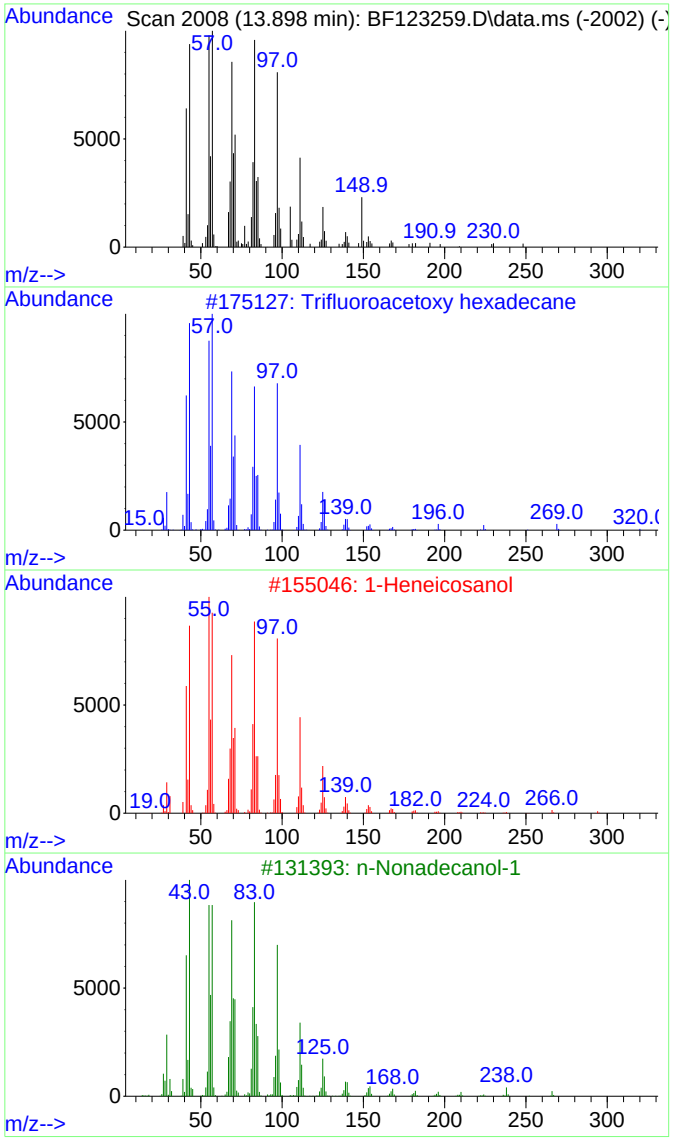
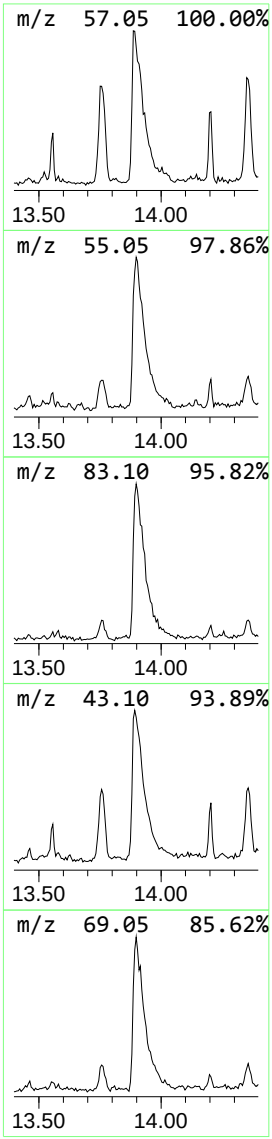
Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	14.51 ng	850338	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





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Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

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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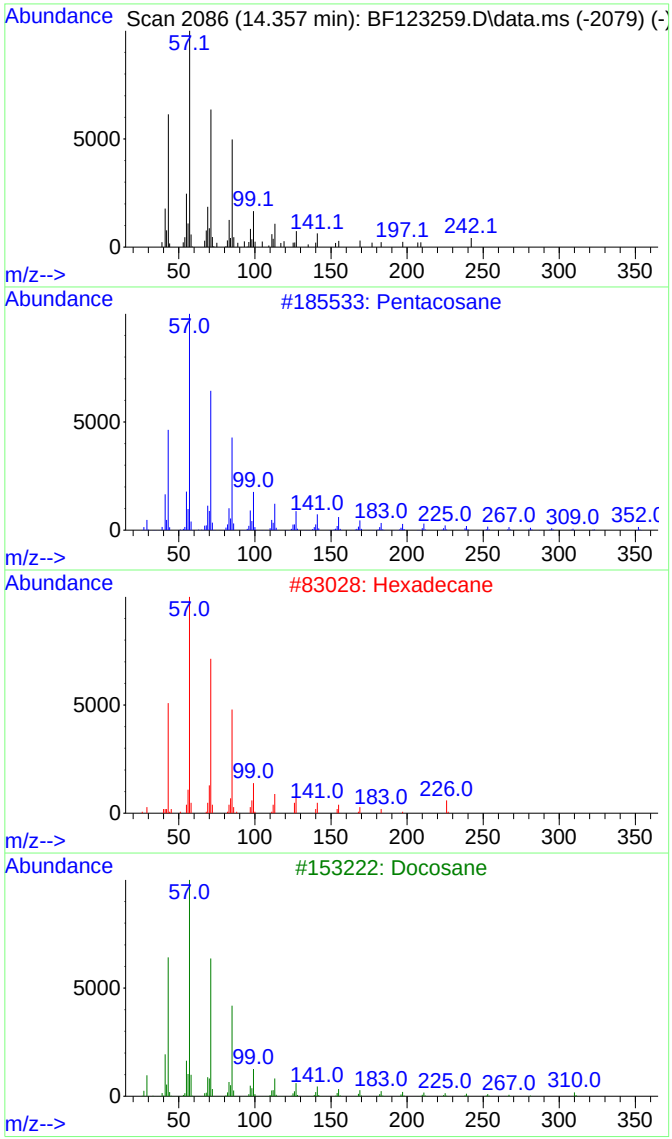
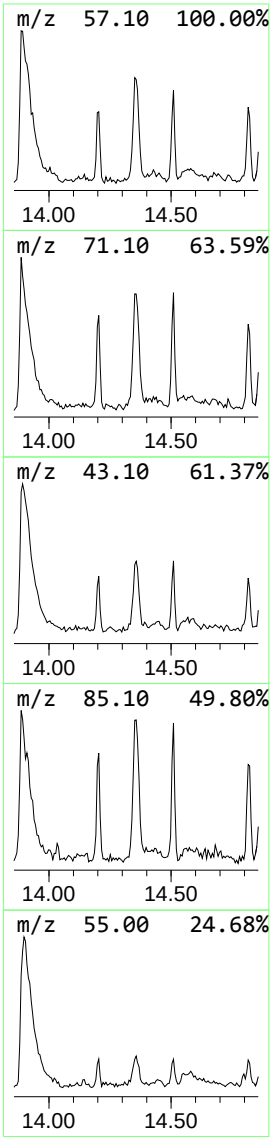
Peak Number 9 Pentacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.357	2.71 ng	158994	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	Hexadecane	226	C16H34	000544-76-3	86
3	Docosane	310	C22H46	000629-97-0	86
4	Triacontane	422	C30H62	000638-68-6	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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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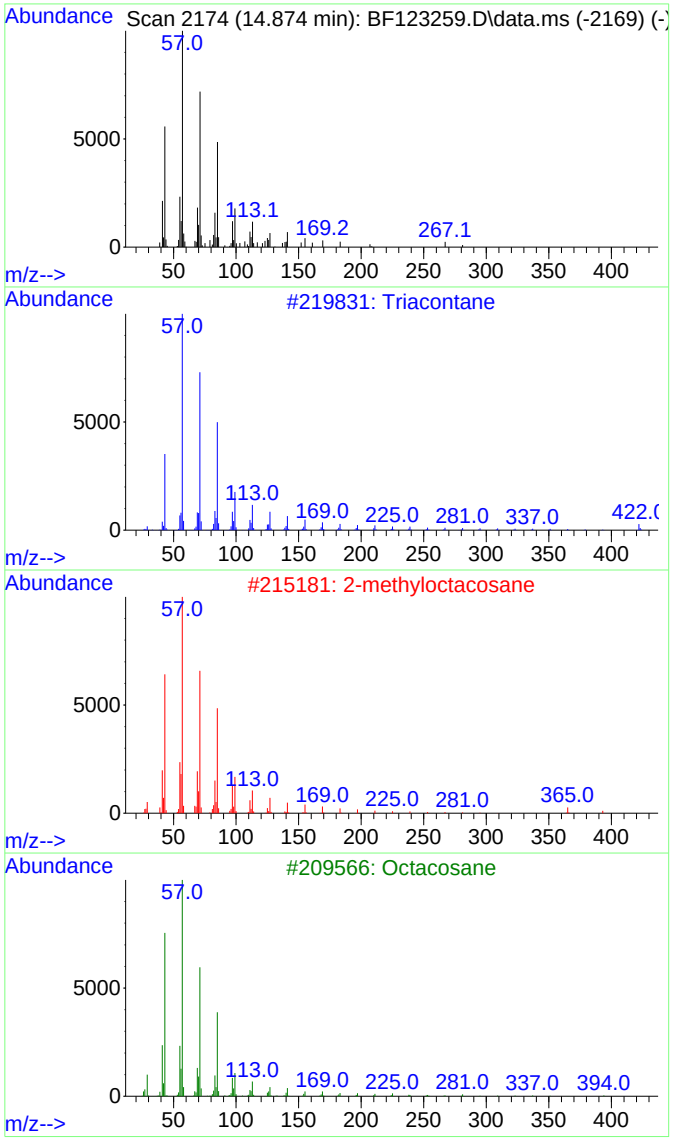
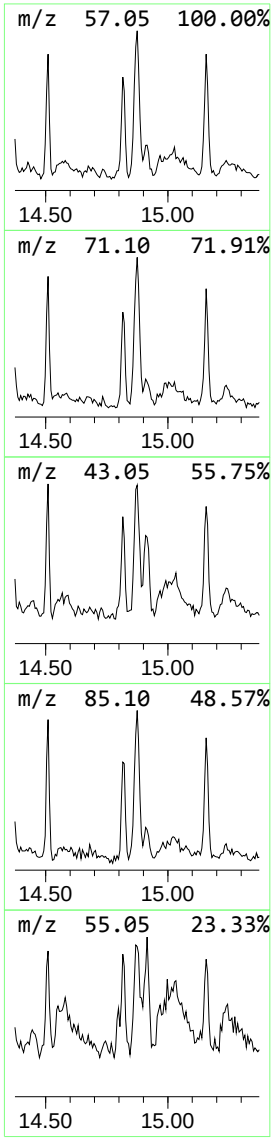
Peak Number 10 Triacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.874	2.85 ng	151923	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90





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Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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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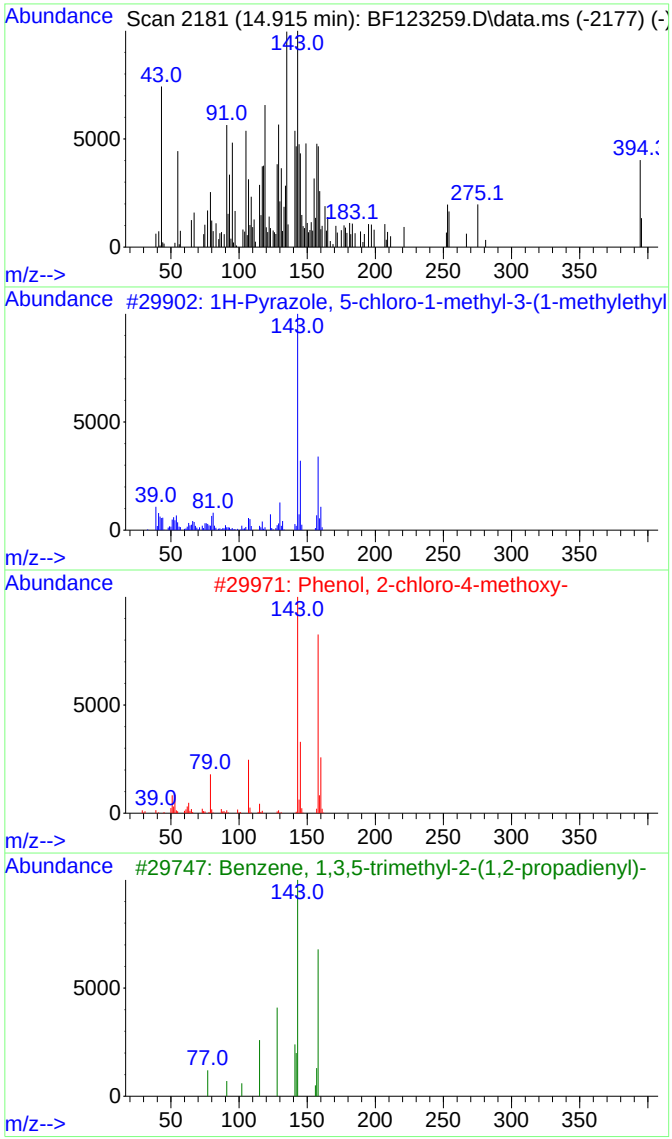
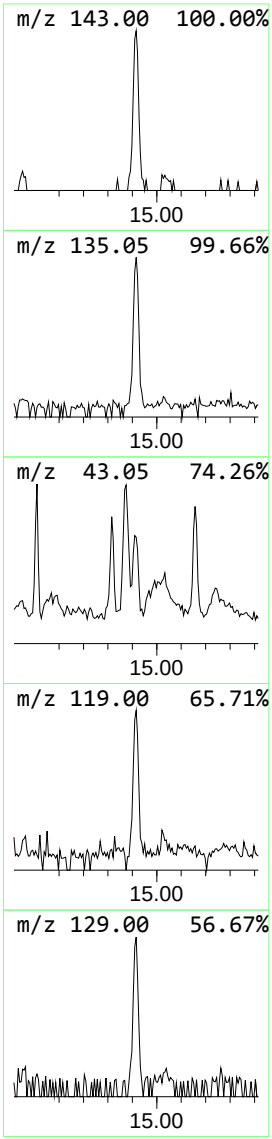
Peak Number 11 unknown14.91 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.915	4.11 ng	219056	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 5-chloro-1-methyl-3...	158	C7H11ClN2	1000319-90-4	25
2	Phenol, 2-chloro-4-methoxy-	158	C7H7ClO2	018113-03-6	14
3	Benzene, 1,3,5-trimethyl-2-(1,2-...	158	C12H14	029555-07-5	14
4	4-Fluorobenzal chloride	178	C7H5Cl2F	000456-19-9	10
5	Quinoline, 4-methyl-	143	C10H9N	000491-35-0	10





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Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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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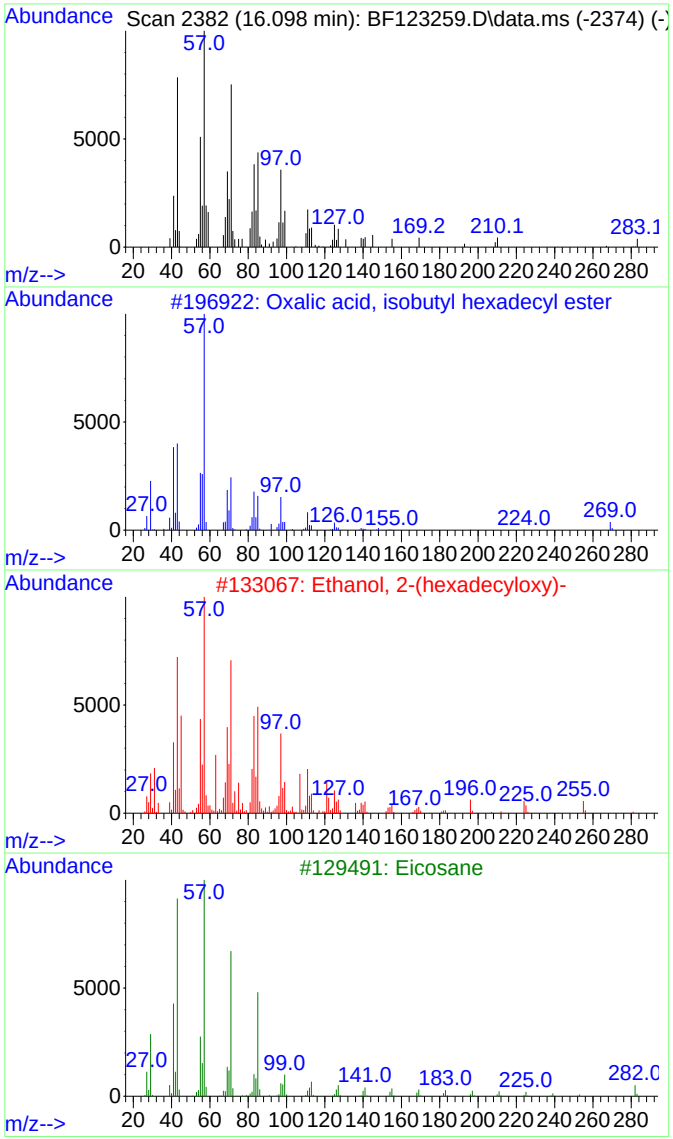
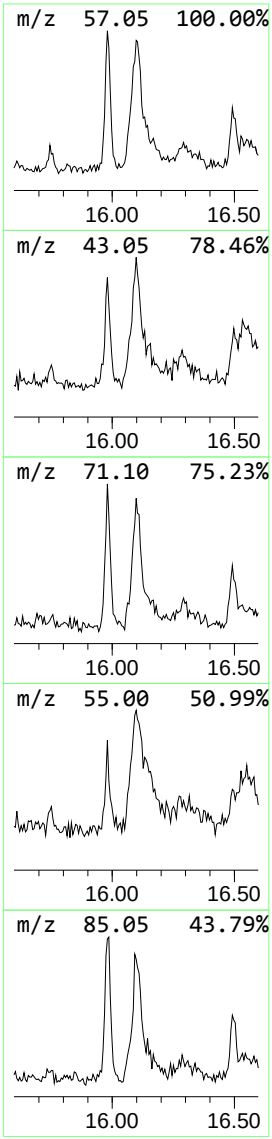
Peak Number 13 Oxalic acid, isobutyl hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.098	4.10 ng	218630	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87
3	Eicosane	282	C20H42	000112-95-8	70
4	Cyclopentadecane	210	C15H30	000295-48-7	56
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	50





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Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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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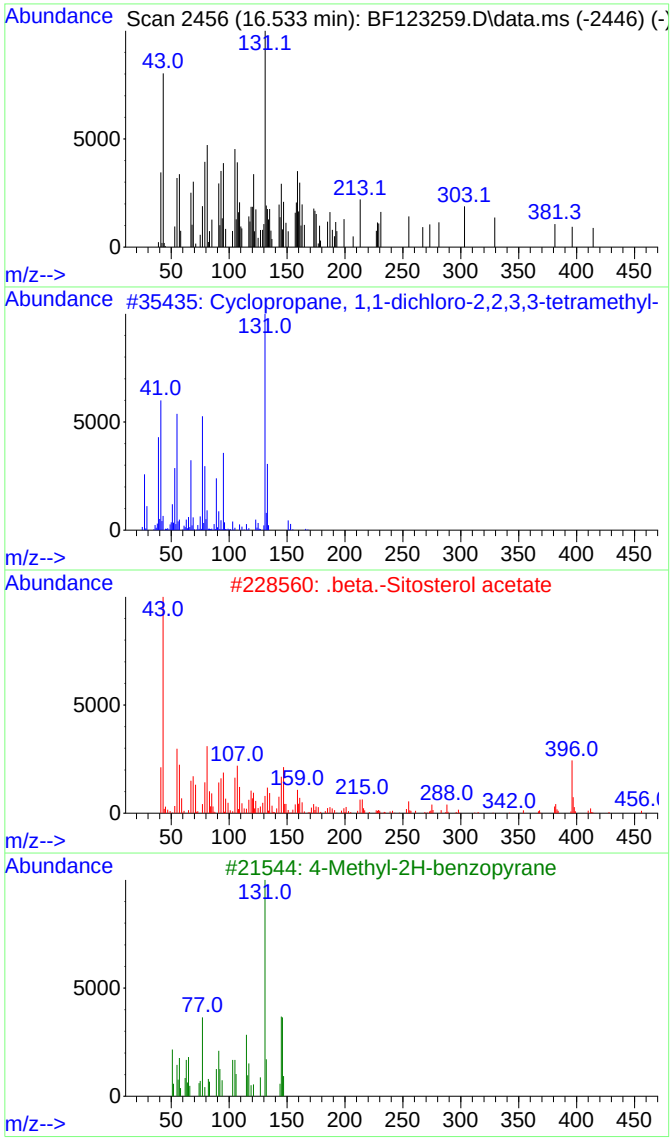
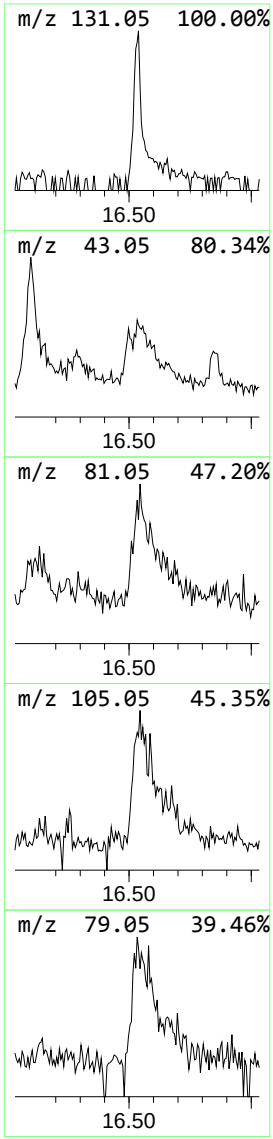
Peak Number 14 unknown16.53 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.533	2.56 ng	136333	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dichloro-2,2,3...	166	C7H12Cl2	003141-45-5	23
2	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	22
3	4-Methyl-2H-benzopyrane	146	C10H10O	021776-94-3	22
4	Difluoro(methylamino)phosphine s...	131	CH4F2NPS	1000306-16-8	22
5	4,5-Diphenylocta-1,7-diene(dl)	262	C20H22	1000215-92-8	22





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Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

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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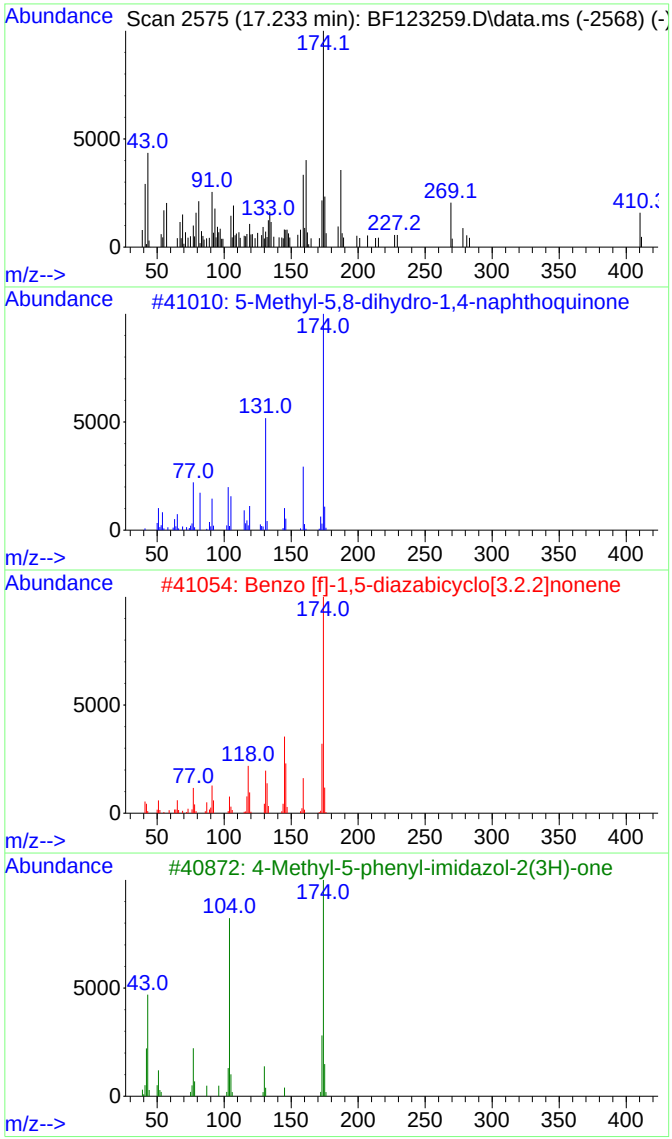
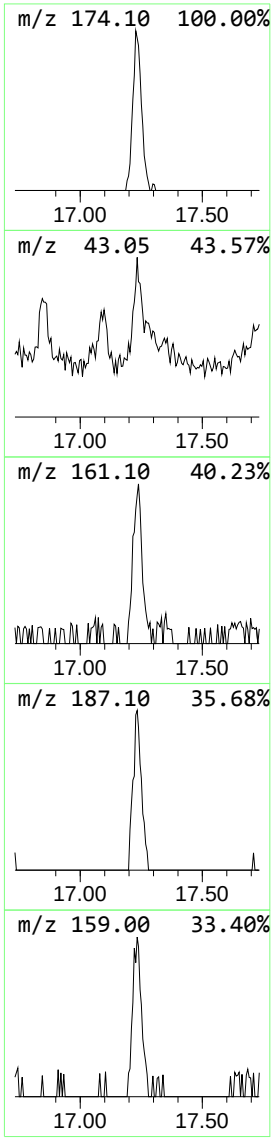
Peak Number 15 unknown17.23 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.233	3.64 ng	193873	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	38
2	Benzo [f]-1,5-diazabicyclo[3.2.2...	174	C11H14N2	007092-76-4	35
3	4-Methyl-5-phenyl-imidazol-2(3H)...	174	C10H10N2O	1000147-06-1	27
4	N-Benzyl-2-cyano-acetamide	174	C10H10N2O	1000300-42-1	27
5	4-Fluoro-6-phenylpyrimidine	174	C10H7FN2	041270-94-4	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123259.D
Acq On : 22 Feb 2021 15:23
Operator : JU/CG
Sample : M1452-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-1

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...	2.122	13.6	ng	495196	1	6.857	726590	20.0
n-Hexadecanoic ...	11.922	11.8	ng	711206	4	11.386	1205780	20.0
1,3-Benzenedica...	12.457	82.5	ng	4974830	4	11.386	1205780	20.0
Octadecanoic acid	12.710	4.7	ng	285092	4	11.386	1205780	20.0
unknown12.85	12.857	3.5	ng	207027	5	14.039	1172110	20.0
Hexacosane	13.757	3.1	ng	179209	5	14.039	1172110	20.0
Trifluoroacetox...	13.898	14.5	ng	850338	5	14.039	1172110	20.0
Pentacosane	14.357	2.7	ng	158994	5	14.039	1172110	20.0
Triacontane	14.874	2.9	ng	151923	6	15.515	1066550	20.0
unknown14.91	14.915	4.1	ng	219056	6	15.515	1066550	20.0
Oxalic acid, is...	16.098	4.1	ng	218630	6	15.515	1066550	20.0
unknown16.53	16.533	2.6	ng	136333	6	15.515	1066550	20.0
unknown17.23	17.233	3.6	ng	193873	6	15.515	1066550	20.0