LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
Data File : BF104644.D
Acq On : 19 Apr 2018 22:30
Operator : JU/SJ
Sample : J2457-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	493	497	504	rBV	78546	99364	4.77%	0.468%
2	5.422	562	567	570	rBV	2083051	1991990	95.71%	9.375%
3	6.440	736	740	748	rBV	2023521	2077130	99.80%	9.776%
4	6.575	759	763	766	rBV	2447959	2081375	100.00%	9.796%
5	6.804	798	802	805	rBV	939335	786869	37.81%	3.703%
6	6.957	824	828	832	rBV	1930979	1650113	79.28%	7.766%
7	7.369	893	898	901	rBV	1453246	1267251	60.89%	5.964%
8	7.392	901	902	907	rVB	43292	33725	1.62%	0.159%
9	8.063	1013	1016	1017	rBV	66099	47912	2.30%	0.225%
10	8.087	1017	1020	1023	rVB	1228696	953861	45.83%	4.489%
11	8.498	1087	1090	1093	rBV	30154	27118	1.30%	0.128%
12	8.669	1117	1119	1123	rBV	59710	52441	2.52%	0.247%
13	8.957	1165	1168	1172	rBV3	17243	27527	1.32%	0.130%
14	9.098	1190	1192	1197	rVB	38835	33295	1.60%	0.157%
15	9.163	1199	1203	1206	rBV	2447824	2050609	98.52%	9.651%
16	9.239	1212	1216	1218	rVB	69341	61773	2.97%	0.291%
17	9.557	1264	1270	1272	rBV	305802	285974	13.74%	1.346%
18	9.575	1272	1273	1278	rVB3	30152	25293	1.22%	0.119%
19	9.769	1303	1306	1310	rVB	96657	81382	3.91%	0.383%
20	9.839	1315	1318	1329	rVB	1070930	1062484	51.05%	5.000%
21	10.269	1388	1391	1394	rVB	80204	65718	3.16%	0.309%
22	10.633	1449	1453	1460	rBV	1212270	1110125	53.34%	5.225%
23	10.739	1468	1471	1477	rBV2	100718	108762	5.23%	0.512%
24	10.875	1490	1494	1496	rBV4	20882	25671	1.23%	0.121%
25	10.904	1496	1499	1501	rVV	88229	67824	3.26%	0.319%
26	10.980	1510	1512	1517	rVB3	50319	44830	2.15%	0.211%
27	11.028	1517	1520	1523	rBV	70941	55852	2.68%	0.263%
28	11.098	1528	1532	1542	rVV3	50849	79626	3.83%	0.375%
29	11.186	1545	1547	1549	rBV	39224	31603	1.52%	0.149%
30	11.216	1549	1552	1555	rVB2	57816	52120	2.50%	0.245%
31	11.328	1568	1571	1575	rBV	877452	814310	39.12%	3.832%
32	11.398	1581	1583	1585	rVB	45631	33575	1.61%	0.158%
33	11.851	1657	1660	1665	rBV	56770	52569	2.53%	0.247%
34	12.022	1686	1689	1694	rVB4	22692	23632	1.14%	0.111%

LSC Area Percent Report

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Sample : J2457-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.404	1751	1754	1756	rBV	81613	73151	3.51%	0.344%
36	12.427	1756	1758	1763	rVB4	73389	64804	3.11%	0.305%
37	12.545	1775	1778	1781	rBV	28789	33469	1.61%	0.158%
38	12.580	1781	1784	1788	rVV	198161	164924	7.92%	0.776%
39	12.804	1819	1822	1830	rVB3	25273	43971	2.11%	0.207%
40	12.916	1837	1841	1845	rBV	1538210	1317603	63.30%	6.201%
41	13.345	1911	1914	1919	rBV2	156907	140560	6.75%	0.662%
42	13.810	1989	1993	1996	rBV	89141	97759	4.70%	0.460%
43	13.974	2017	2021	2028	rVB	843659	794886	38.19%	3.741%
44	14.133	2044	2048	2050	rBV5	18899	24667	1.19%	0.116%
45	14.439	2097	2100	2105	rVB2	62462	82046	3.94%	0.386%
46	14.727	2146	2149	2154	rBV4	40880	64629	3.11%	0.304%
47	14.816	2162	2164	2168	rVB	34636	31468	1.51%	0.148%
48	15.074	2205	2208	2213	rBV	133729	135442	6.51%	0.637%
49	15.439	2265	2270	2277	rVB	448277	613730	29.49%	2.888%
50	15.880	2341	2345	2348	rBV	81334	108670	5.22%	0.511%
51	15.933	2350	2354	2363	rVB3	55132	106863	5.13%	0.503%
52	17.439	2607	2610	2615	rBV6	44910	85839	4.12%	0.404%

Sum of corrected areas: 21248184

LSC Report - Integrated Chromatogram

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Operator : JU/SJ
Sample : J2457-04
Misc :
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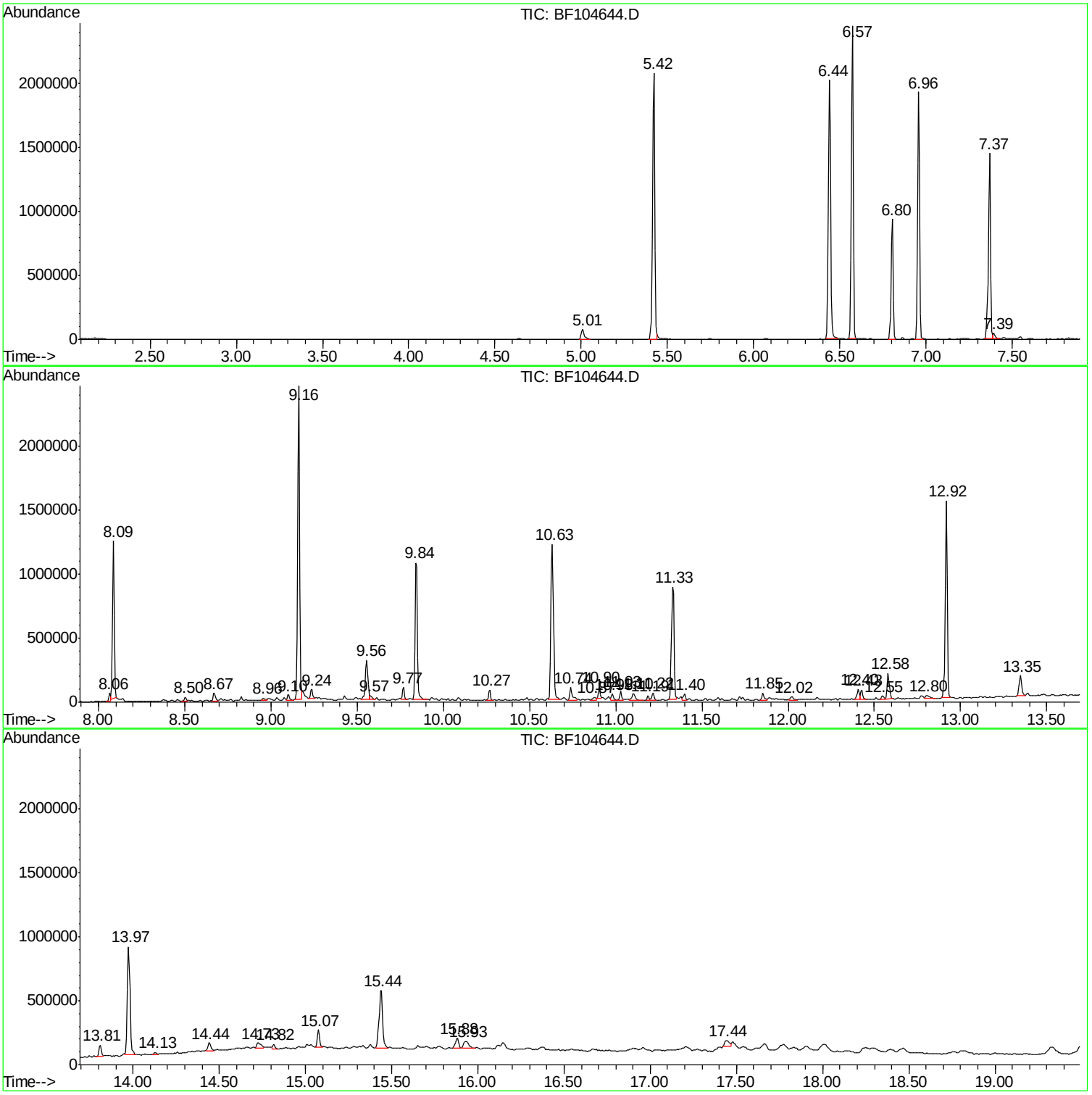
Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
Data File : BF104644.D
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Operator : JU/SJ
Sample : J2457-04
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Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

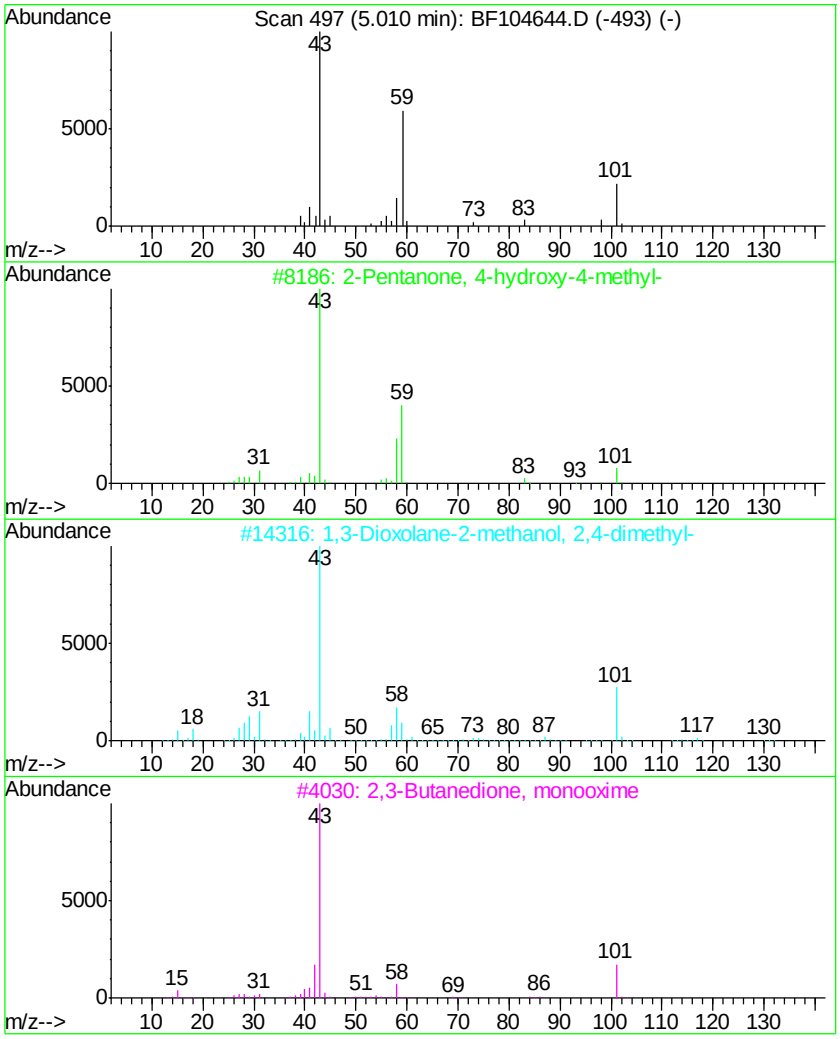
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

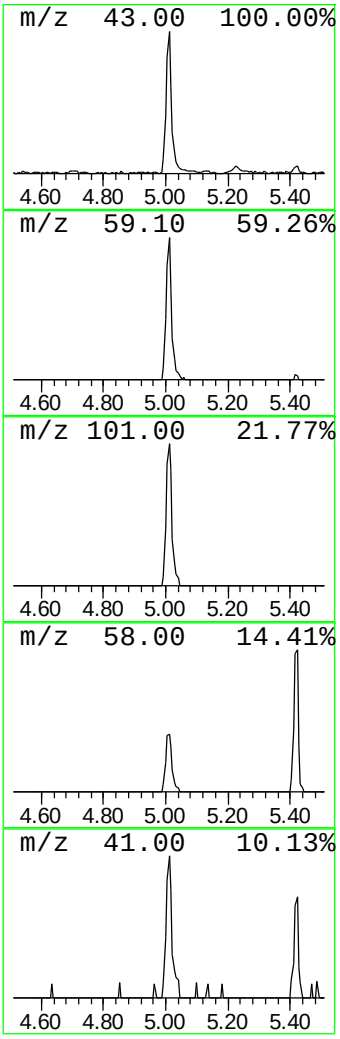
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	2.53 ng	99364	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25





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Sample : J2457-04
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Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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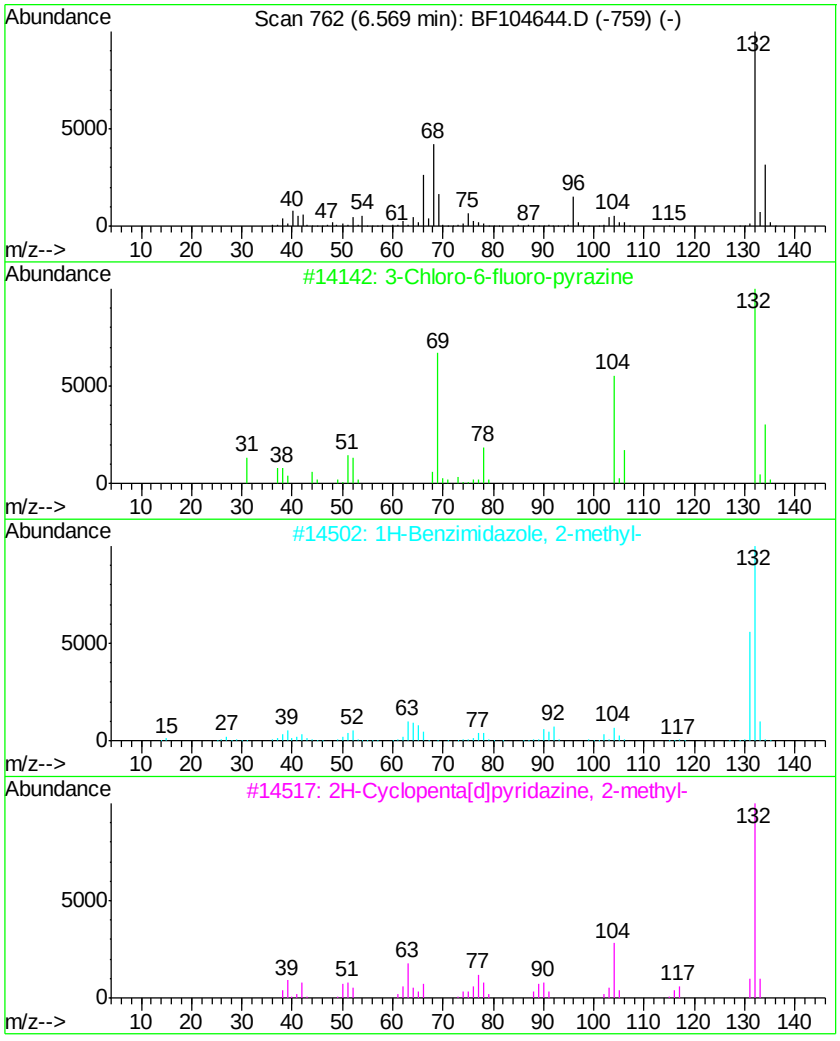
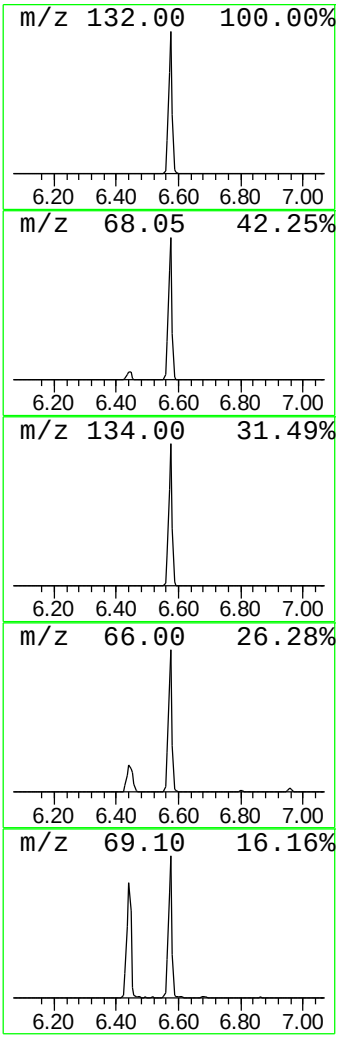
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	52.90 ng	2081380	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Sample : J2457-04
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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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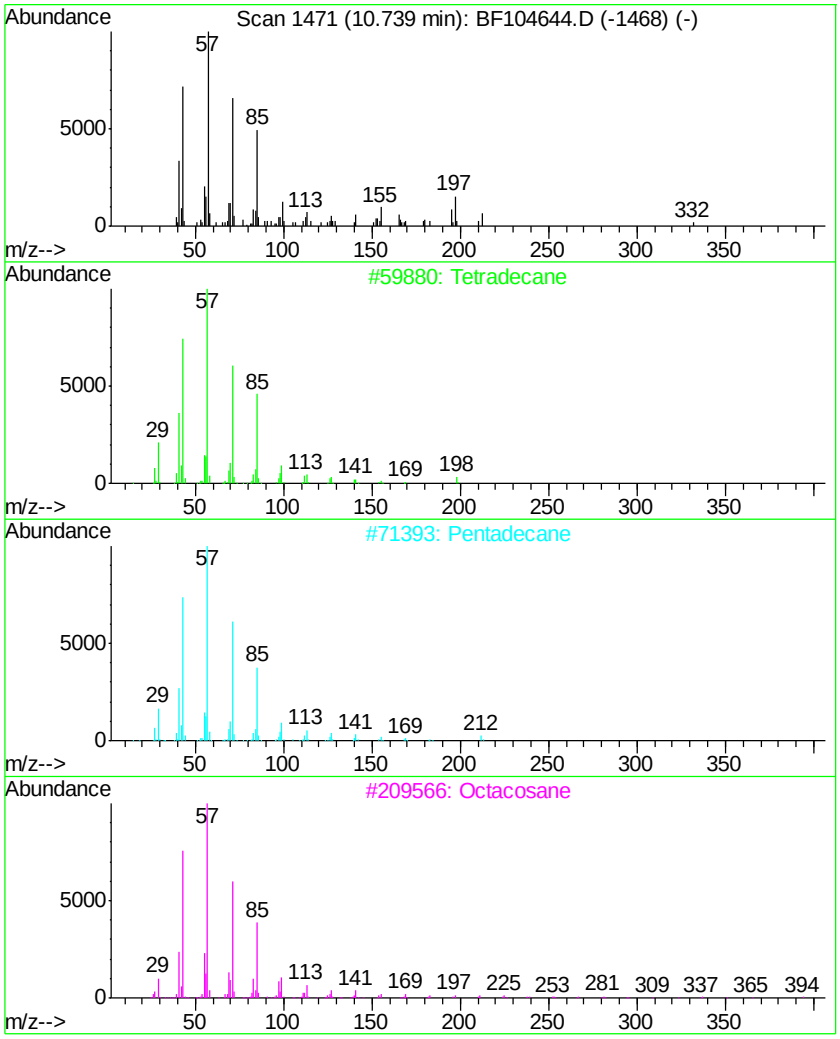
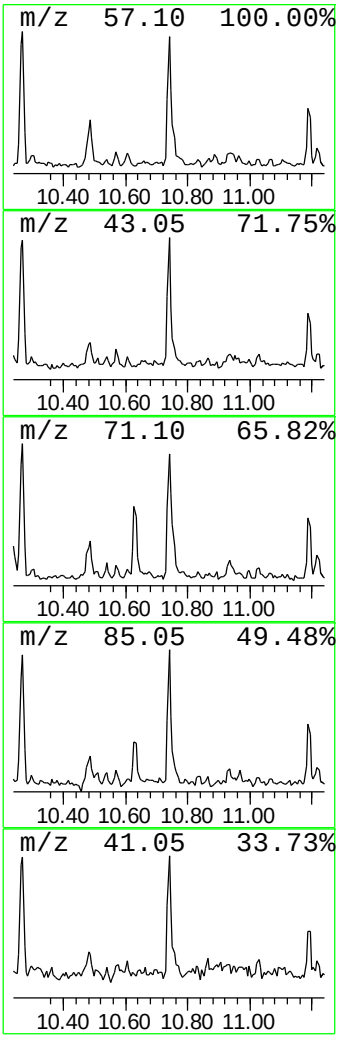
Peak Number 4 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.67 ng	108762	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	96
2	Pentadecane	212	C15H32	000629-62-9	93
3	Octacosane	394	C28H58	000630-02-4	81
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5	Eicosane	282	C20H42	000112-95-8	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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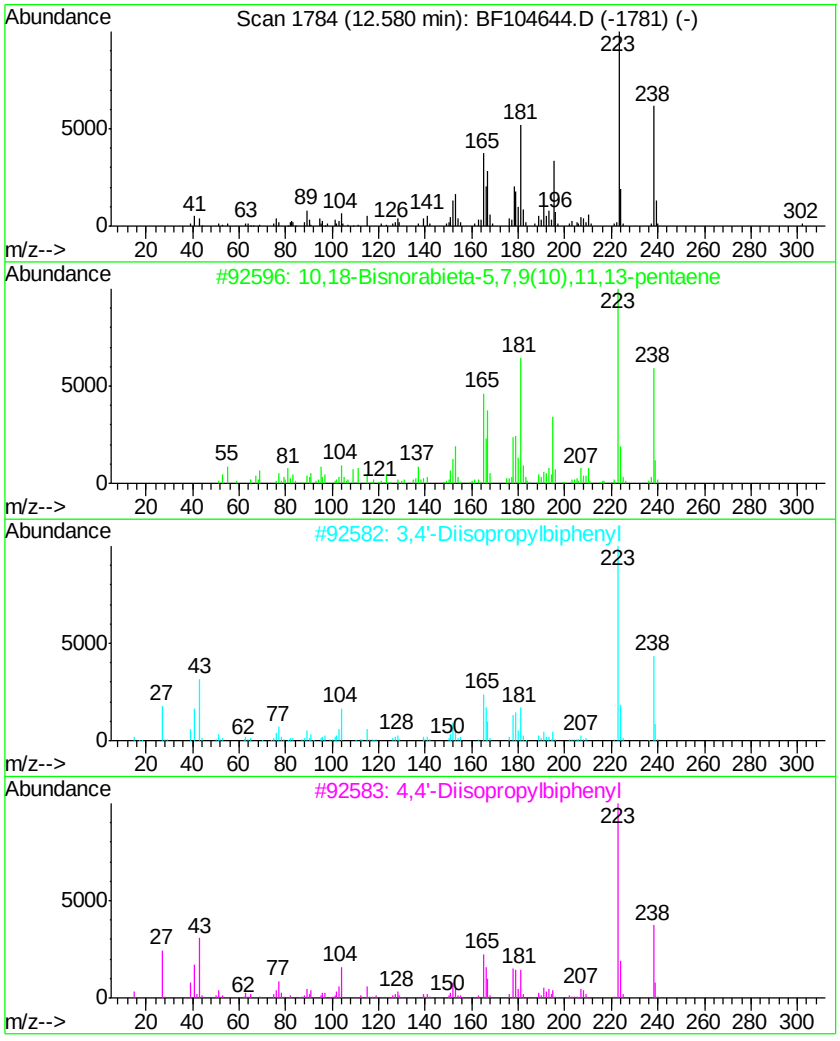
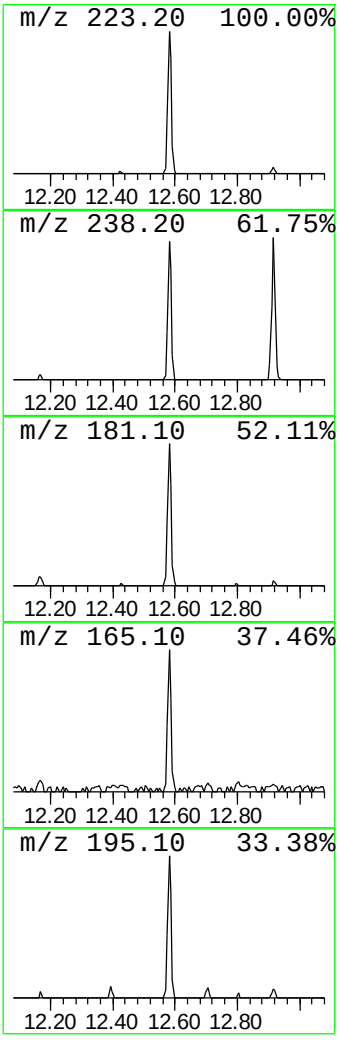
Peak Number 5 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	4.05 ng	164924	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	99
2	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	81
3	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	64
4	Anthracene, 1,4-dimethoxy-	238	C16H14O2	013076-29-4	60
5	Anthracene, 9,10-dimethoxy-	238	C16H14O2	002395-97-3	49





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Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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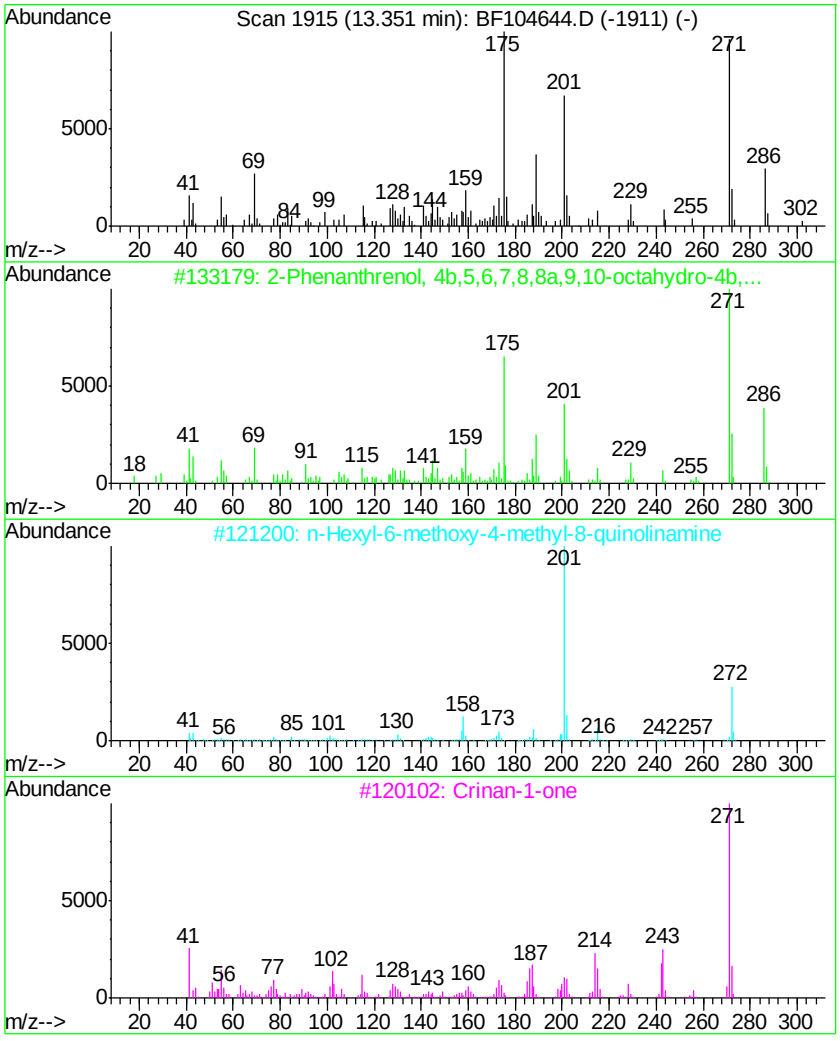
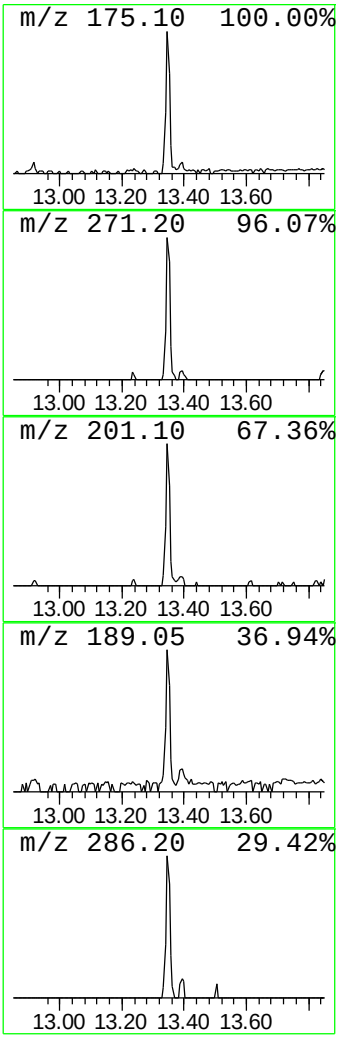
Peak Number 6 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	3.54 ng	140560	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	95
2	n-Hexyl-6-methoxy-4-methyl-8-qui...	272	C17H24N2O	083547-16-4	25
3	Crinan-1-one	271	C16H17NO3	098301-98-5	20
4	Dihydronormorphinone	271	C16H17NO3	014696-23-2	18
5	Oxazole, 2-(1-naphthalenyl)-5-ph...	271	C19H13NO	000846-63-9	18





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Sample : J2457-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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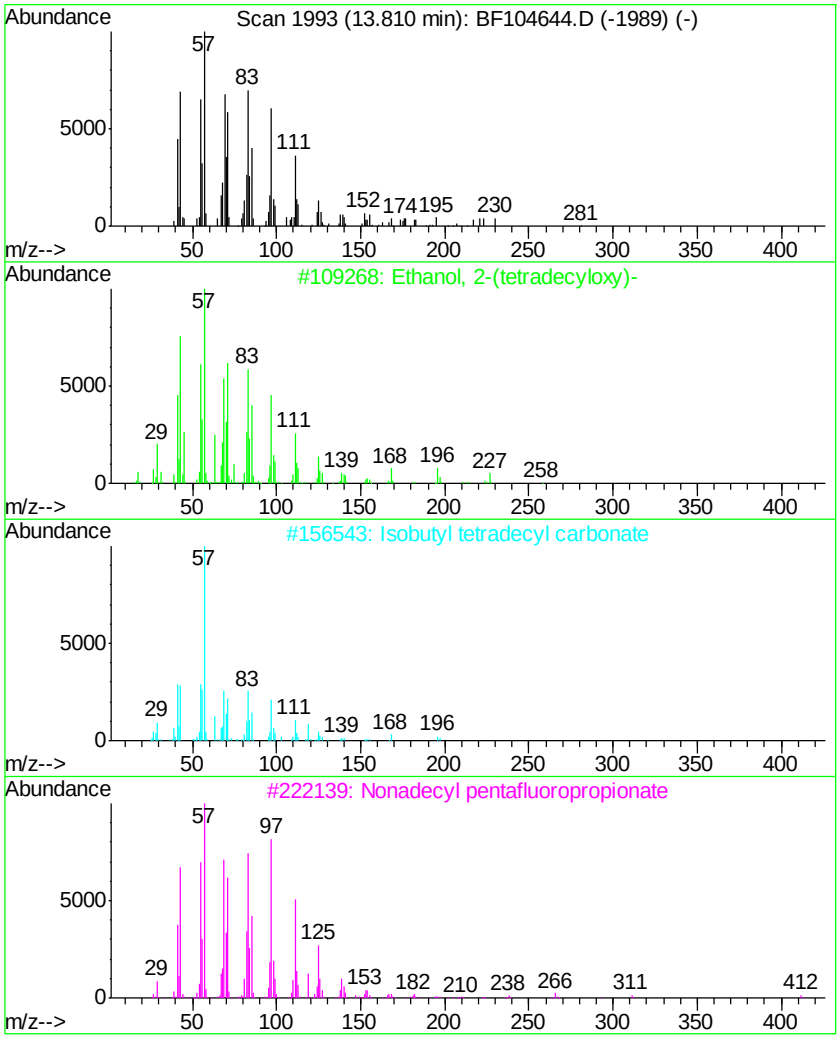
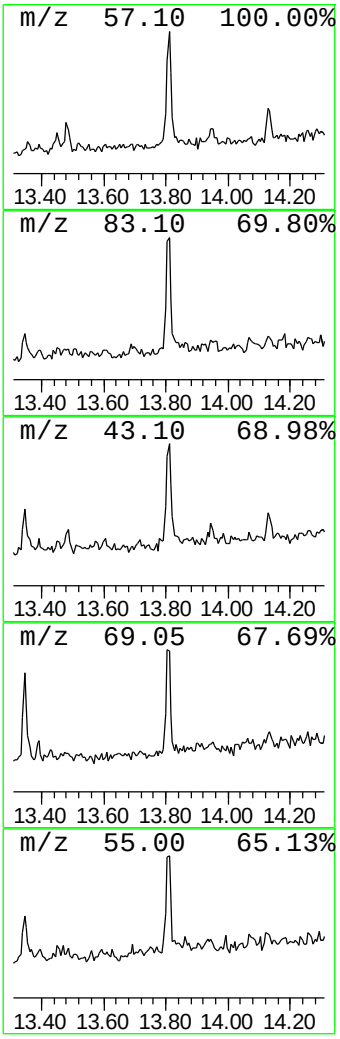
Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	2.46 ng	97759	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
2	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	90
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
4	1-Docosene	308	C22H44	001599-67-3	87
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	87





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Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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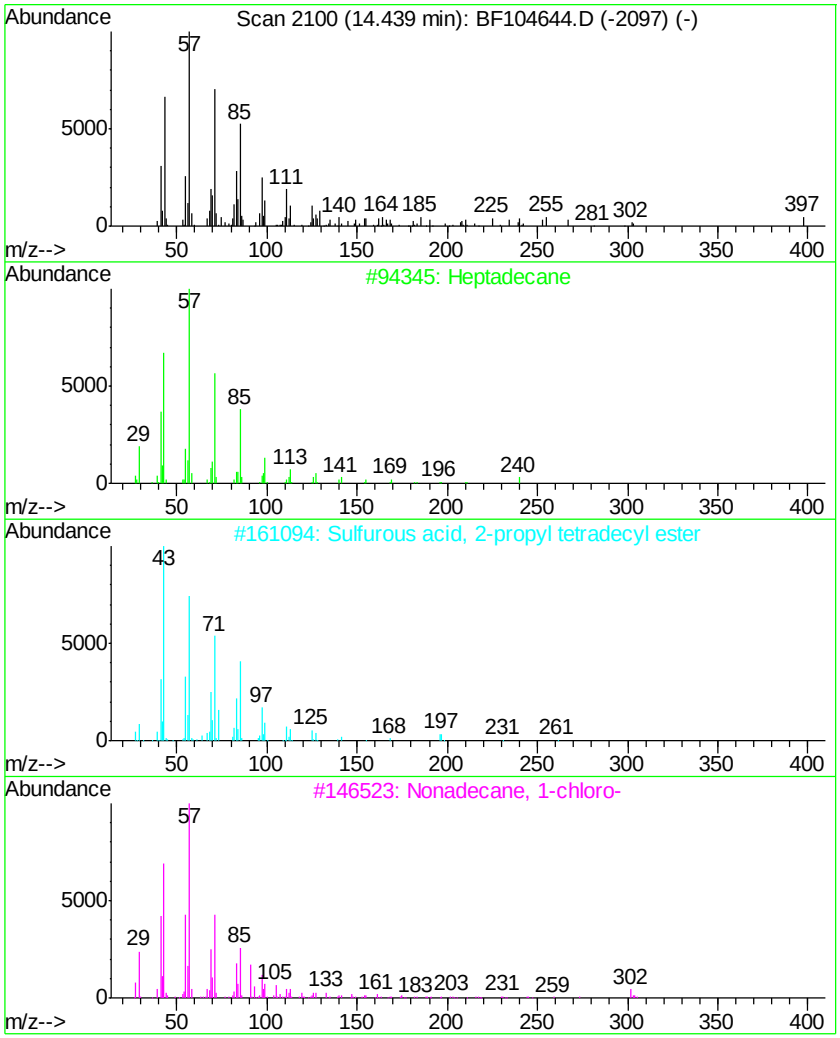
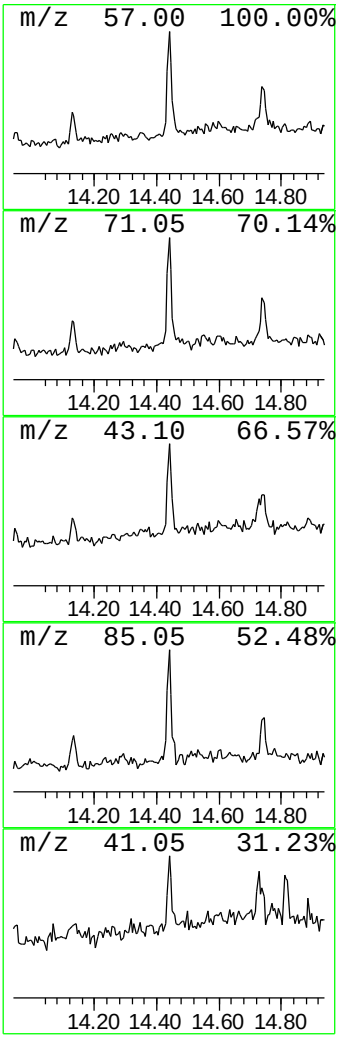
Peak Number 8 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.06 ng	82046	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	92
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	80
3	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	74
4	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	72
5	Hexacosane	366	C26H54	000630-01-3	52





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Sample : J2457-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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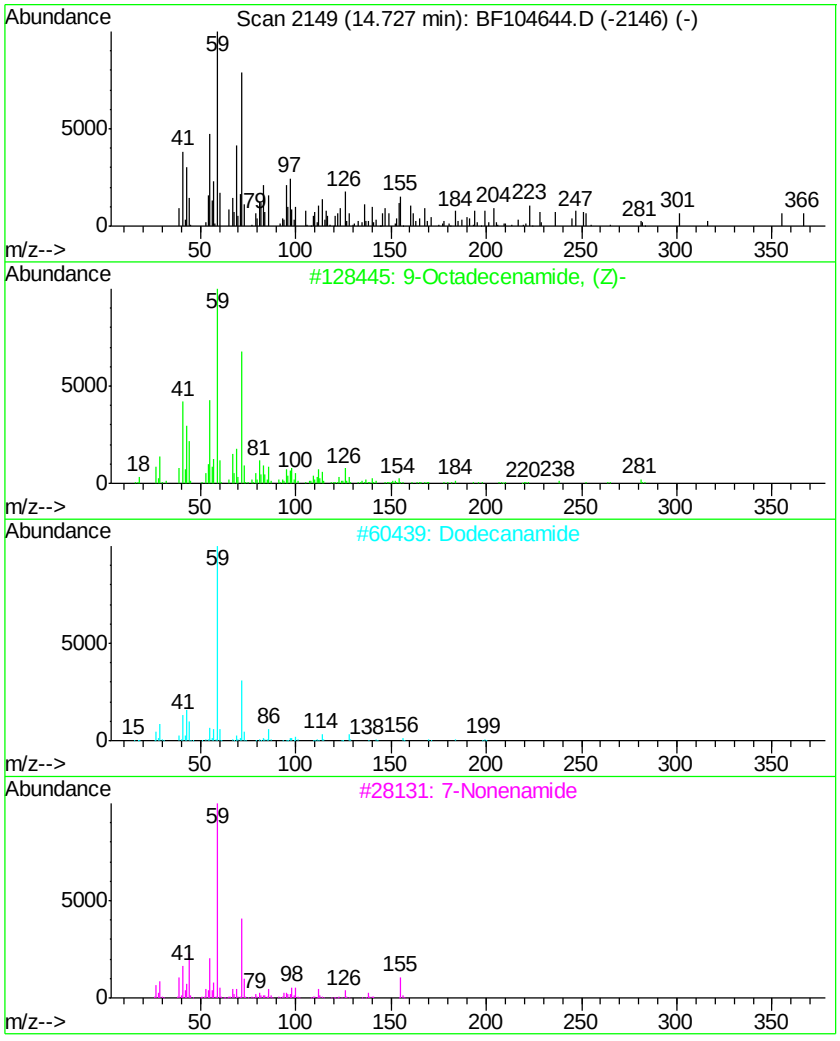
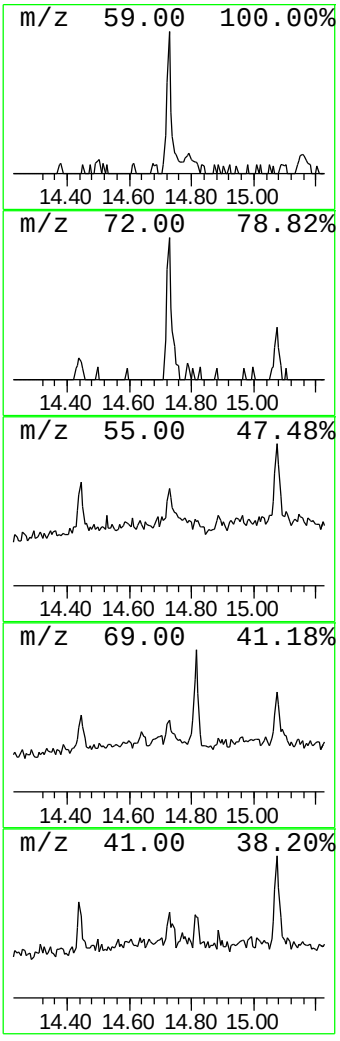
Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.11 ng	64629	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	89
2	Dodecanamide	199	C12H25NO	001120-16-7	53
3	7-Nonenamide	155	C9H17NO	090949-53-4	50
4	Tetradecanamide	227	C14H29NO	000638-58-4	45
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	43





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Data File : BF104644.D
Acq On : 19 Apr 2018 22:30
Operator : JU/SJ
Sample : J2457-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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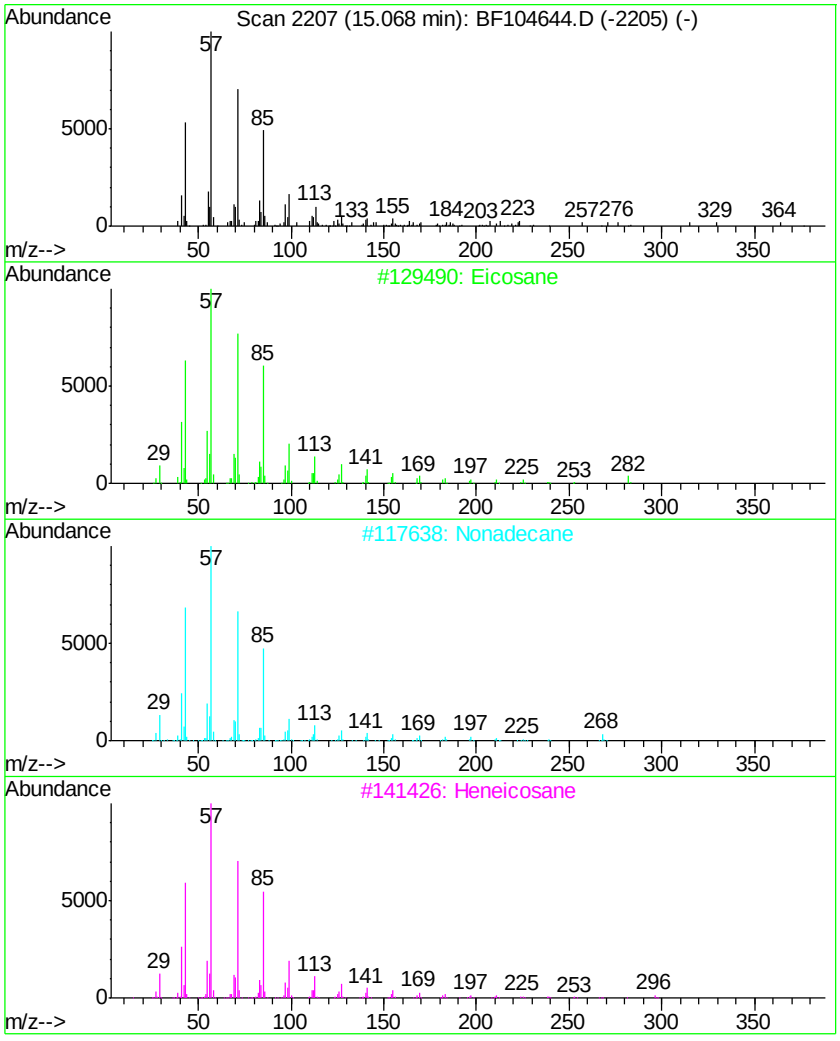
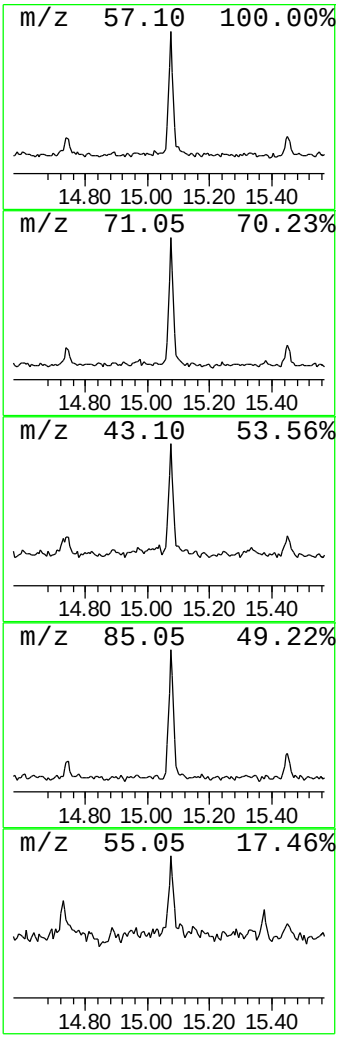
Peak Number 10 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	4.41 ng	135442	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Nonadecane	268	C19H40	000629-92-5	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Tetracosane	338	C24H50	000646-31-1	90





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Data File : BF104644.D
Acq On : 19 Apr 2018 22:30
Operator : JU/SJ
Sample : J2457-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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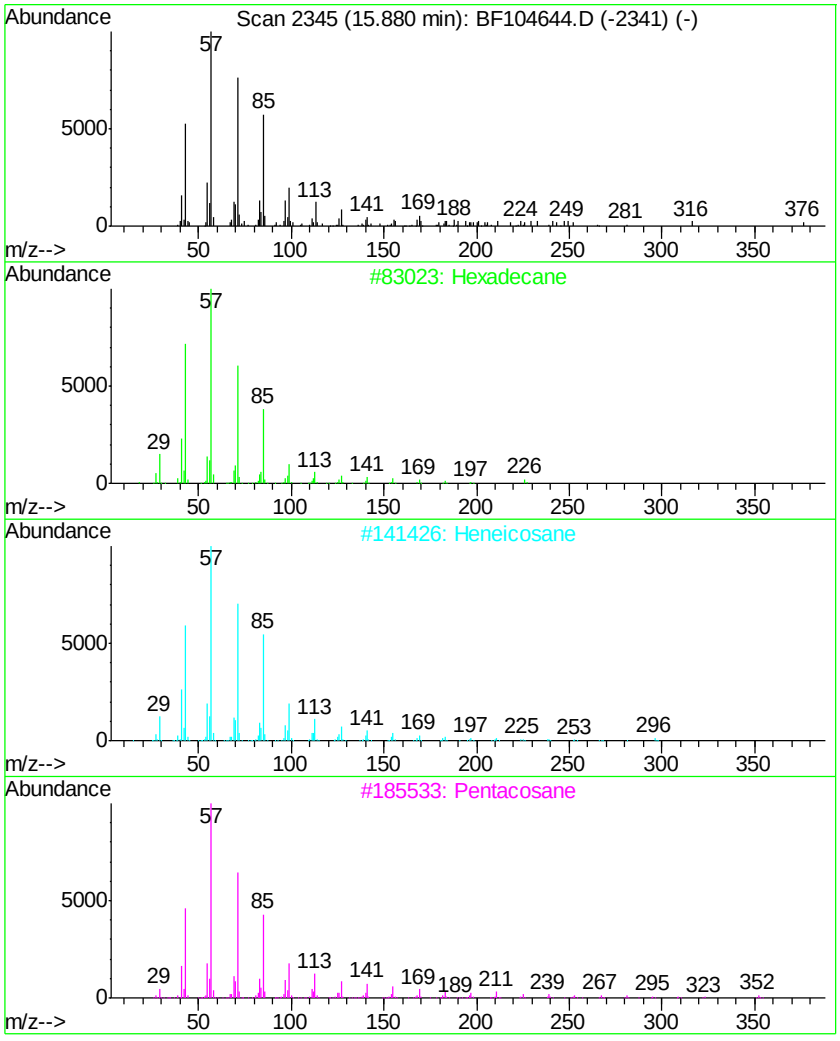
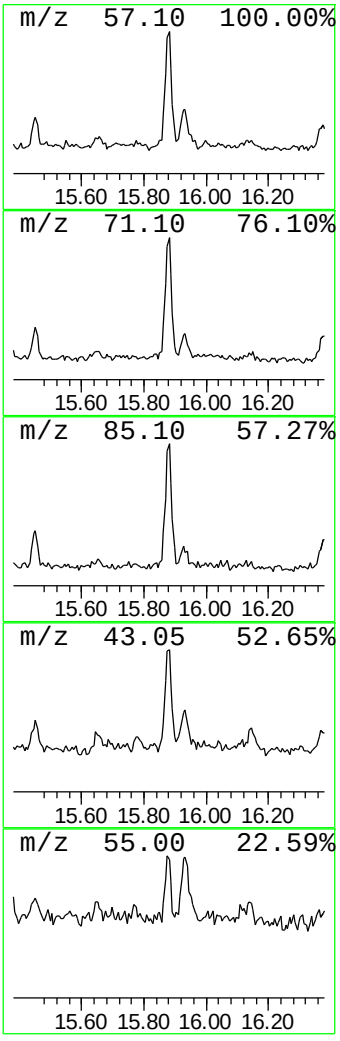
Peak Number 11 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	3.54 ng	108670	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
5	Heptadecane	240	C17H36	000629-78-7	87





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Data File : BF104644.D
Acq On : 19 Apr 2018 22:30
Operator : JU/SJ
Sample : J2457-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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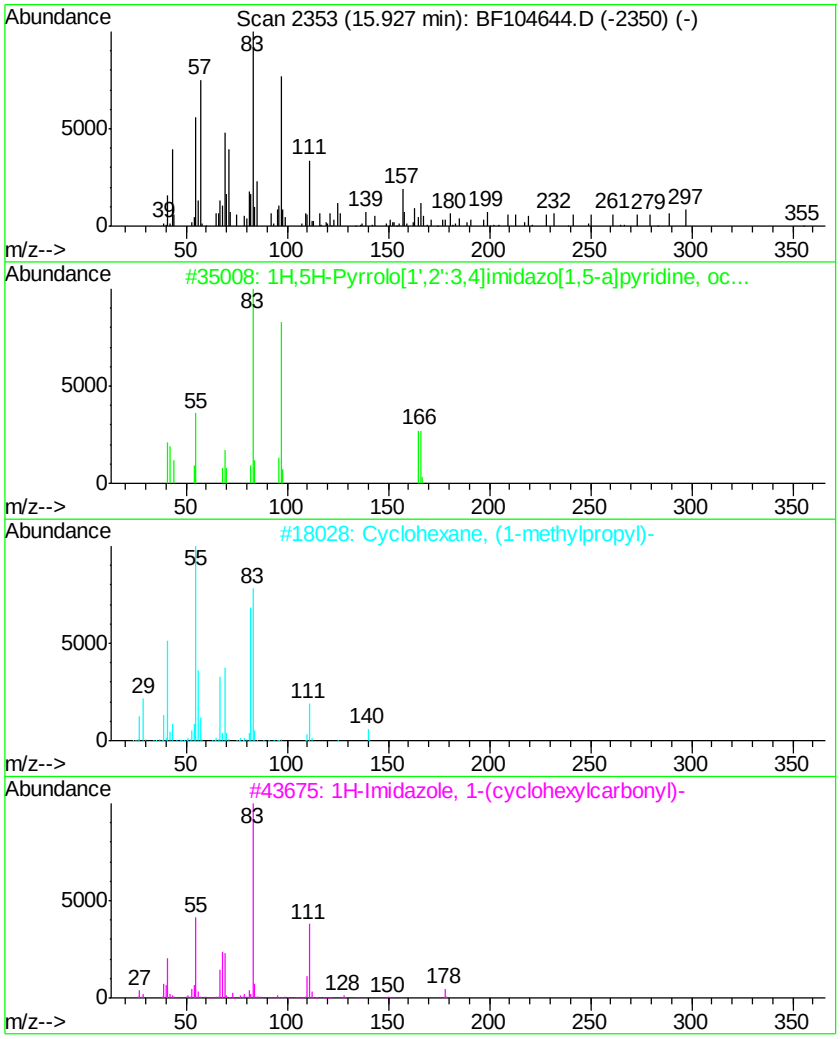
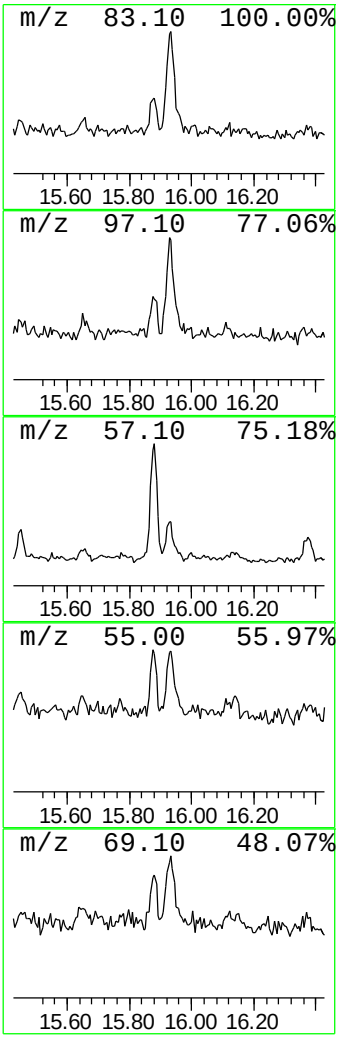
Peak Number 12 unknown15.93 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	3.48 ng	106863	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H,5H-Pyrrolo[1',2':3,4]imidazo[...	166	C10H18N2	054966-11-9	43
2	Cyclohexane, (1-methylpropyl)-	140	C10H20	007058-01-7	38
3	1H-Imidazole, 1-(cyclohexylcarbo...	178	C10H14N2O	060718-45-8	35
4	Cyclohexanecarboxylic acid, 3,5-...	240	C13H14F2O2	1000293-69-2	35
5	Cyclohexanecarboxylic acid, (1H-...	195	C8H13N5O	1000310-78-1	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
Data File : BF104644.D
Acq On : 19 Apr 2018 22:30
Operator : JU/SJ
Sample : J2457-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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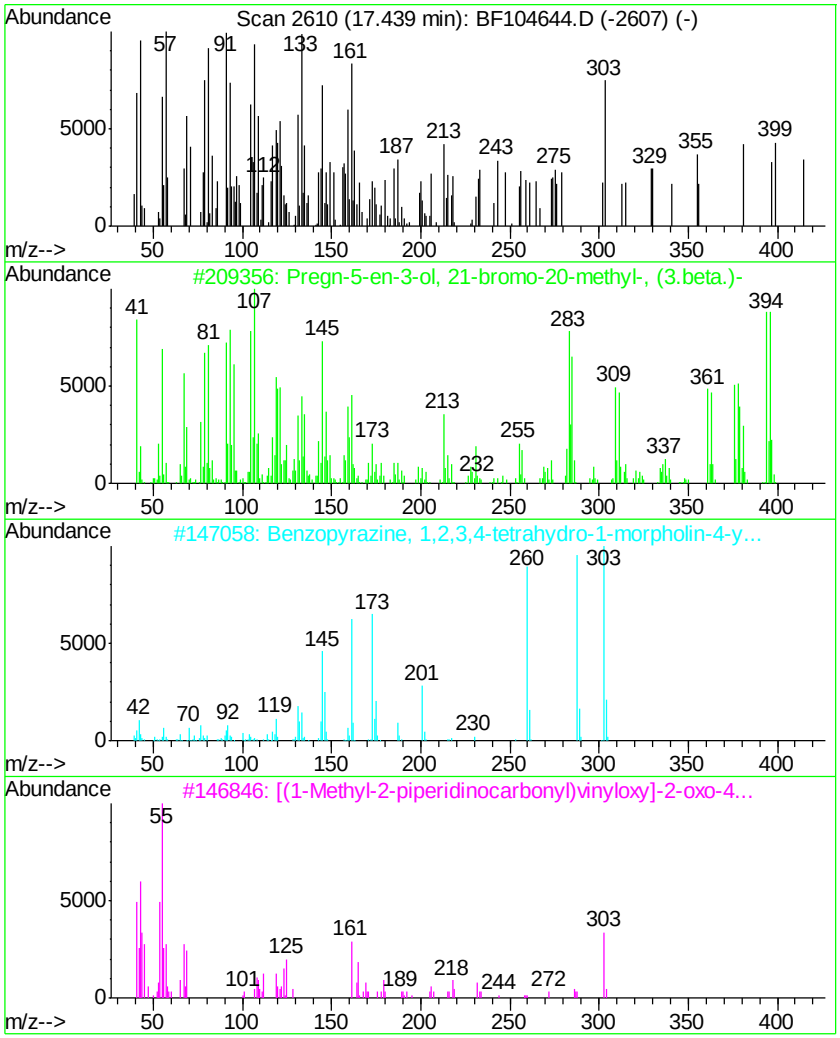
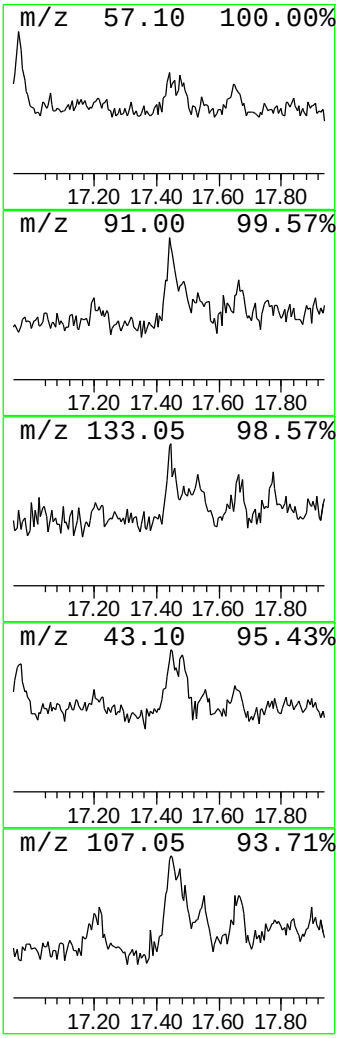
Peak Number 13 unknown17.44 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	2.80 ng	85839	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	10
2	Benzopyrazine, 1,2,3,4-tetrahydr...	303	C16H21N3O3	342390-29-8	9
3	[(1-Methyl-2-piperidinocarbonyl)...	303	C13H22NO5P	1000140-89-0	9
4	Acetamide, N-[4-(chlorodifluorom...	381	C17H14ClF2N3O3	1000302-92-1	9
5	1-Phenanthrenecarboxylic acid, 7...	318	C20H30O3	057397-38-3	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041918\
Data File : BF104644.D
Acq On : 19 Apr 2018 22:30
Operator : JU/SJ
Sample : J2457-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-FW-TS001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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-hy...	5.01	2.5	ng	99364	1	6.80	786869	20.0
unknown6.57	6.57	52.9	ng	2081380	1	6.80	786869	20.0
Tetradecane	10.74	2.7	ng	108762	4	11.33	814310	20.0
10,18-Bisnorabiet...	12.58	4.0	ng	164924	4	11.33	814310	20.0
2-Phenanthrenol, ...	13.35	3.5	ng	140560	5	13.97	794886	20.0
Ethanol, 2-(tetra...	13.81	2.5	ng	97759	5	13.97	794886	20.0
Heptadecane	14.44	2.1	ng	82046	5	13.97	794886	20.0
9-Octadecenamide,...	14.73	2.1	ng	64629	6	15.44	613730	20.0
Eicosane	15.07	4.4	ng	135442	6	15.44	613730	20.0
Hexadecane	15.88	3.5	ng	108670	6	15.44	613730	20.0
unknown15.93	15.93	3.5	ng	106863	6	15.44	613730	20.0
unknown17.44	17.44	2.8	ng	85839	6	15.44	613730	20.0