LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098421.D
Acq On : 12 Sep 2017 00:07
Operator : SJ/JU
Sample : I5138-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

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-BF091117.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	3.622	256	261	268	rBV	60792	95922	1.27%	0.155%
2	4.869	469	473	487	rVB	589801	962088	12.78%	1.550%
3	5.287	539	544	547	rBV	6305444	6958522	92.41%	11.213%
4	6.322	715	720	732	rBV	5584744	7529909	100.00%	12.134%
5	6.445	736	741	744	rBV	6592874	6736077	89.46%	10.855%
6	6.669	775	779	788	rBV	1738193	1569140	20.84%	2.529%
7	6.822	801	805	809	rBV	4815270	4805628	63.82%	7.744%
8	7.239	870	876	879	rBV	4411457	4606515	61.18%	7.423%
9	7.951	990	997	1000	rBV	2433790	2135087	28.35%	3.441%
10	8.545	1095	1098	1101	rBV	101302	77543	1.03%	0.125%
11	8.975	1168	1171	1174	rVB	102027	78058	1.04%	0.126%
12	9.028	1174	1180	1183	rBV	6122677	5808613	77.14%	9.360%
13	9.110	1190	1194	1198	rBV2	132517	151378	2.01%	0.244%
14	9.422	1244	1247	1250	rVB	1350554	1086178	14.42%	1.750%
15	9.639	1281	1284	1287	rVB	101644	89450	1.19%	0.144%
16	9.698	1287	1294	1298	rBV	2360030	2153894	28.60%	3.471%
17	10.416	1411	1416	1419	rBV2	89694	112152	1.49%	0.181%
18	10.492	1422	1429	1432	rBV	3524639	3409382	45.28%	5.494%
19	10.604	1444	1448	1450	rBV2	90176	102271	1.36%	0.165%
20	10.757	1472	1474	1477	rVV	155249	138994	1.85%	0.224%
21	10.839	1485	1488	1490	rVB	121382	100155	1.33%	0.161%
22	10.886	1493	1496	1501	rBV	131245	119709	1.59%	0.193%
23	10.957	1501	1508	1517	rVB3	122429	202487	2.69%	0.326%
24	11.069	1521	1527	1532	rBV3	97954	134989	1.79%	0.218%
25	11.180	1541	1546	1549	rBV	2293464	1929275	25.62%	3.109%
26	11.251	1554	1558	1561	rVB2	108628	143609	1.91%	0.231%
27	11.580	1611	1614	1618	rVB2	65014	95193	1.26%	0.153%
28	12.263	1722	1730	1732	rBV	190148	222916	2.96%	0.359%
29	12.280	1732	1733	1738	rVB4	123677	103776	1.38%	0.167%
30	12.380	1746	1750	1754	rBV3	123100	143545	1.91%	0.231%
31	12.663	1793	1798	1803	rBV3	49503	76109	1.01%	0.123%
32	12.763	1811	1815	1819	rBV	3897932	3645774	48.42%	5.875%
33	13.657	1964	1967	1972	rBV	511536	566747	7.53%	0.913%
34	13.810	1989	1993	2001	rVB	1301512	1208263	16.05%	1.947%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098421.D
Acq On : 12 Sep 2017 00:07
Operator : SJ/JU
Sample : I5138-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.198	2056	2059	2065	rBV3	82286	110527	1.47%	0.178%
36	14.286	2071	2074	2078	rBV2	145748	173719	2.31%	0.280%
37	14.563	2118	2121	2127	rBV2	204051	252103	3.35%	0.406%
38	14.886	2173	2176	2179	rBV	514550	535058	7.11%	0.862%
39	14.915	2179	2181	2187	rVB2	335334	337737	4.49%	0.544%
40	15.033	2198	2201	2205	rVB3	106041	110214	1.46%	0.178%
41	15.210	2227	2231	2242	rVB	923904	1164590	15.47%	1.877%
42	15.627	2298	2302	2307	rBV	367608	512887	6.81%	0.826%
43	15.680	2307	2311	2317	rVB	197261	328123	4.36%	0.529%
44	17.056	2539	2545	2548	rBV4	232116	525591	6.98%	0.847%
45	17.774	2661	2667	2673	rBV9	128390	380956	5.06%	0.614%
46	18.915	2855	2861	2871	rVB7	115339	325133	4.32%	0.524%

Sum of corrected areas: 62055986

LSC Report - Integrated Chromatogram

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Operator : SJ/JU
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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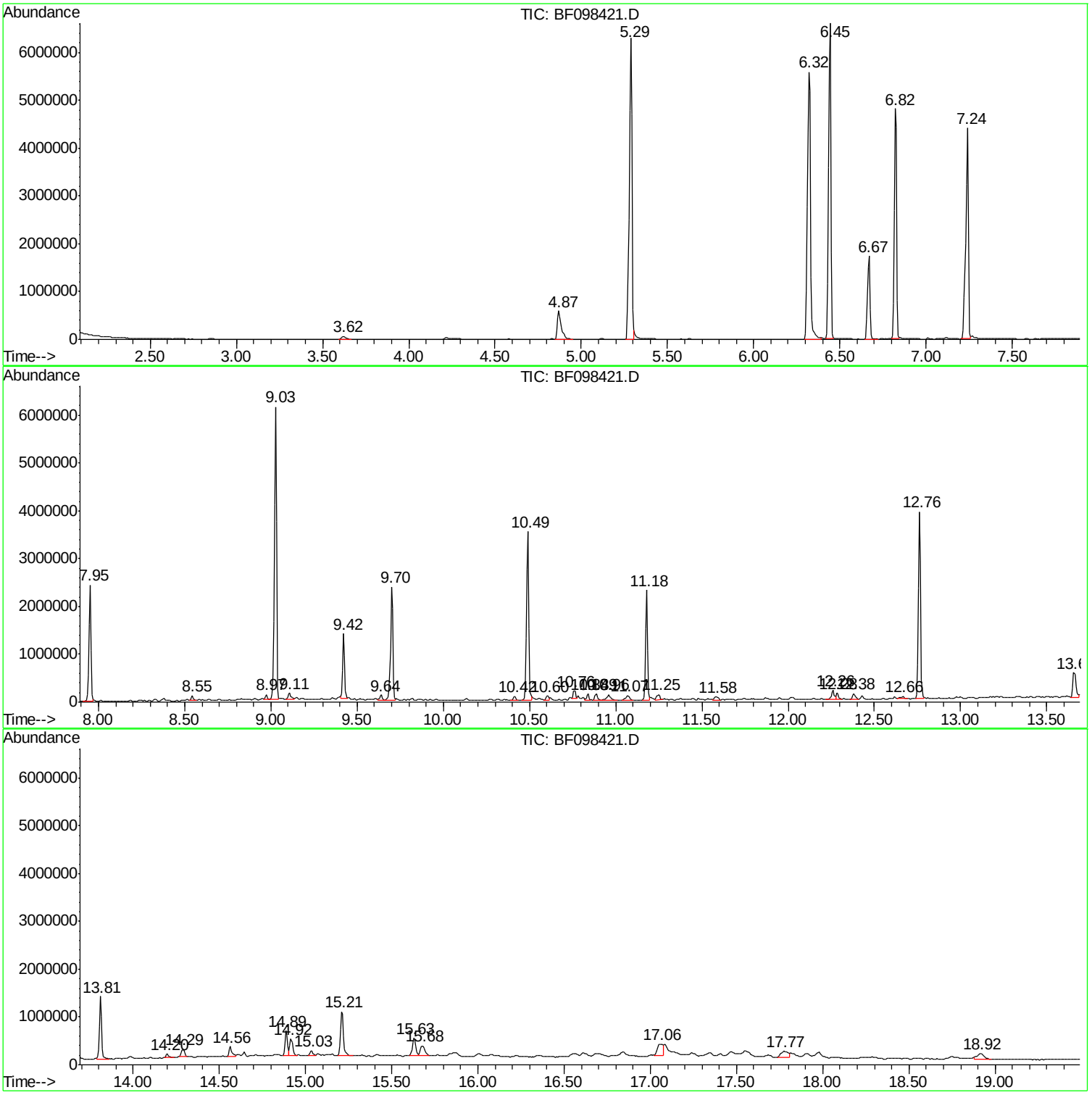
ClientSampleId : EME-UTS-TS004-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098421.D
Acq On : 12 Sep 2017 00:07
Operator : SJ/JU
Sample : I5138-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

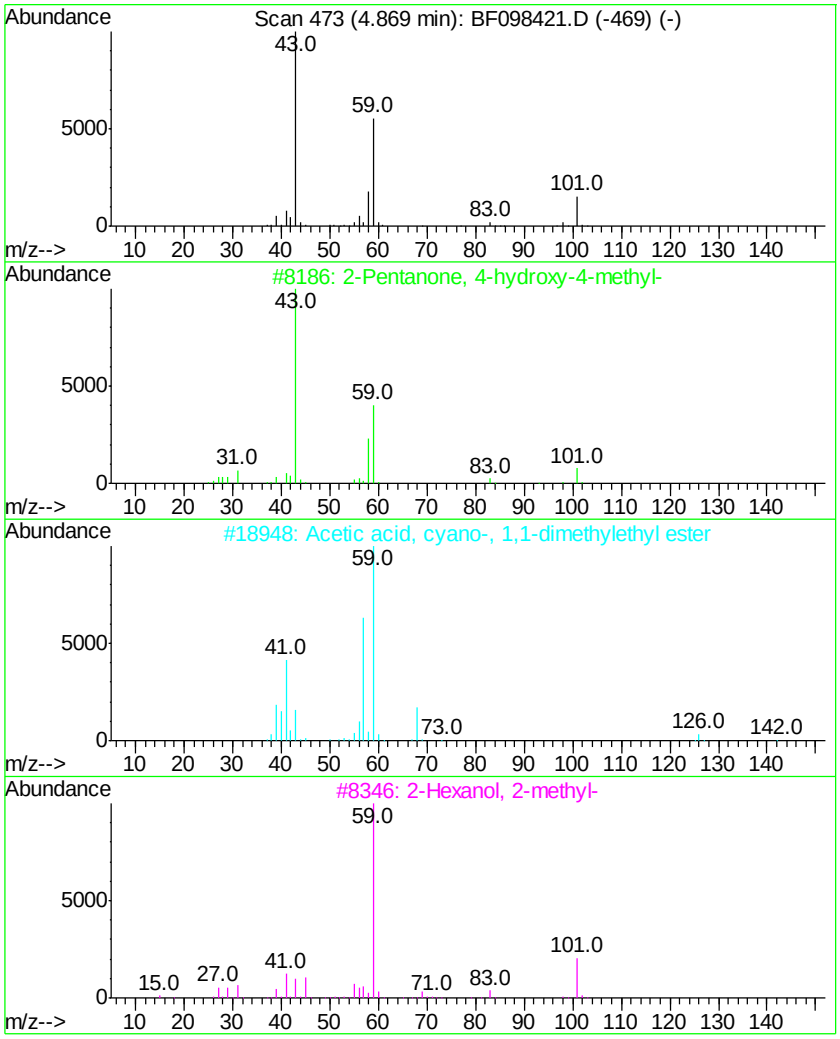
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

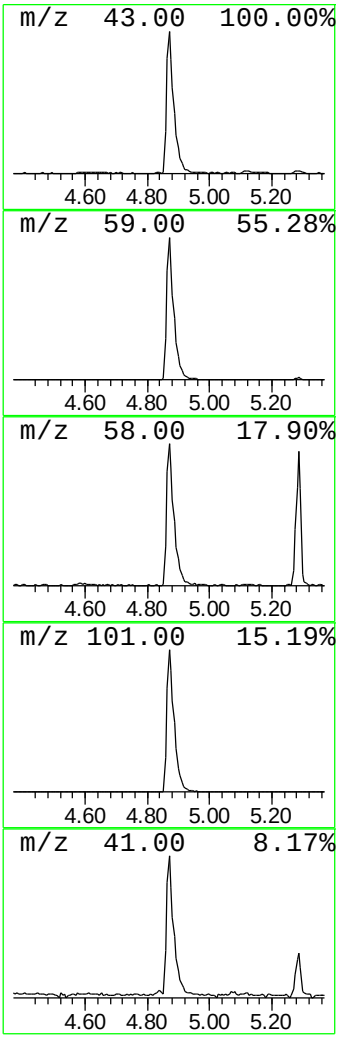
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	12.26 ng	962088	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





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Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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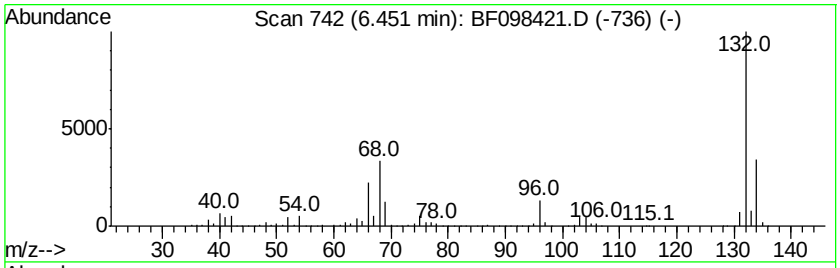
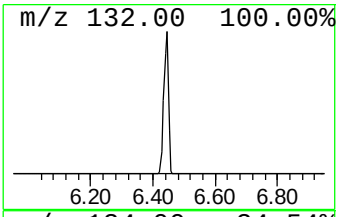
****

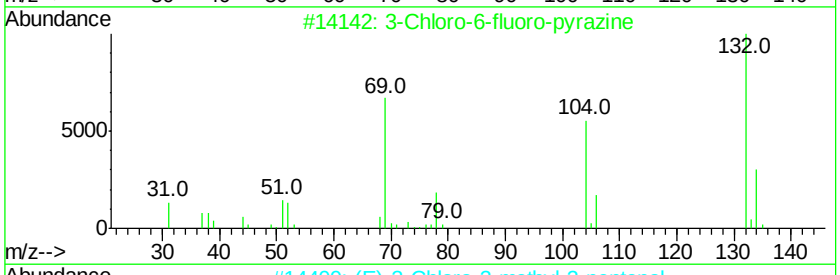
Peak Number 2 unknown6.45 Concentration Rank 1

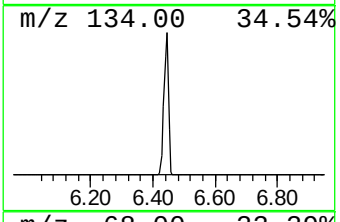
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	85.86 ng	6736080	1,4-Dichlorobenzene-d4	6.67

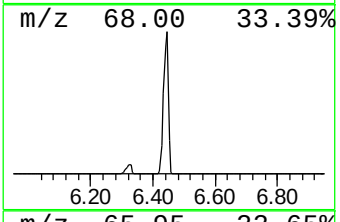
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9

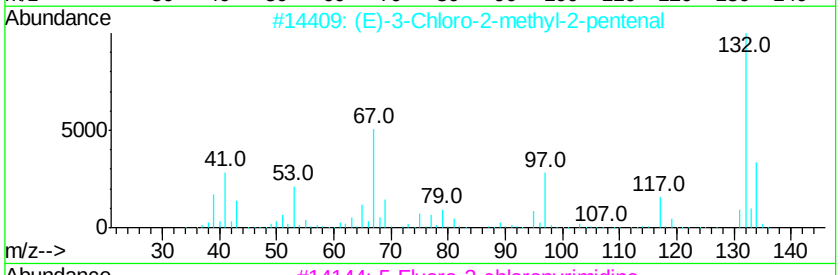


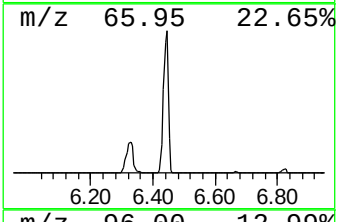


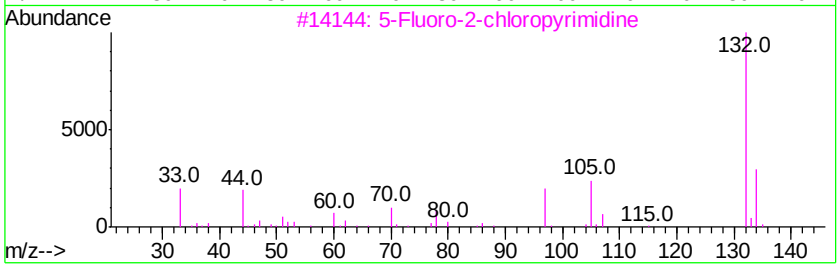


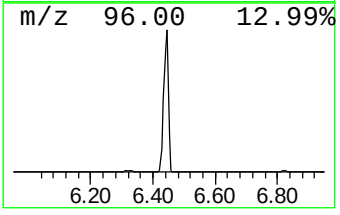












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Misc :
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Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

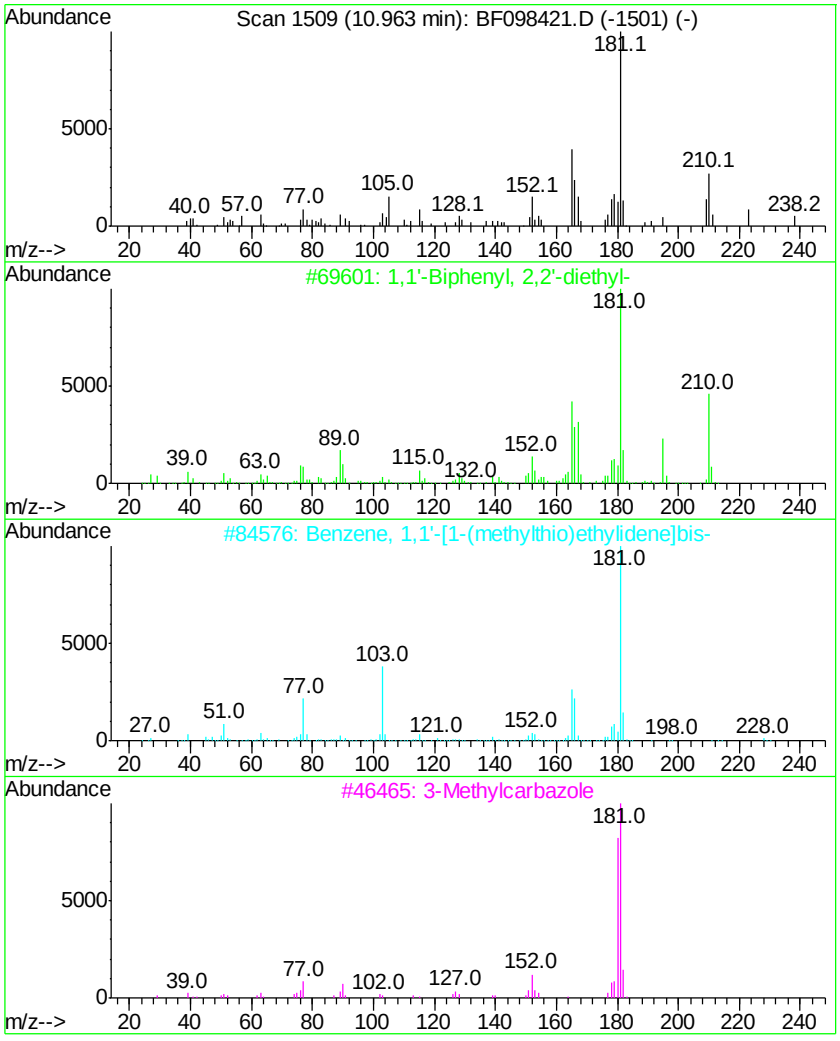
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

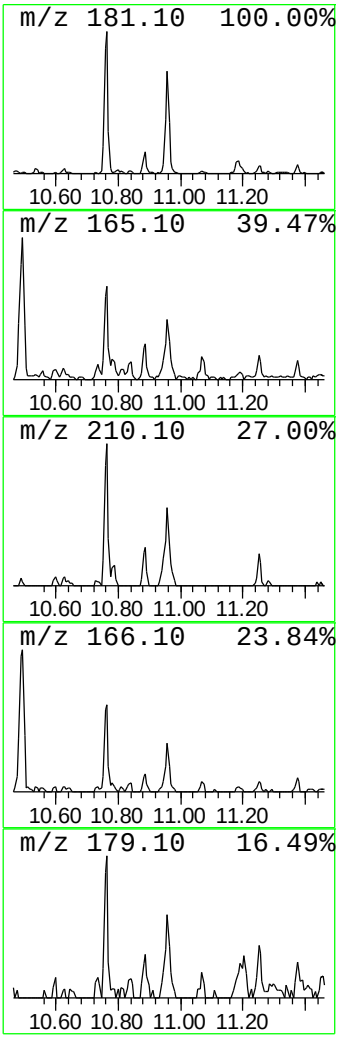
****

Peak Number 4 1,1'-Biphenyl, 2,2'-diethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	2.10 ng	202487	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,2'-diethyl-	210	C16H18	013049-35-9	90
2	Benzene, 1,1'-[1-(methylthio)eth...	228	C15H16S	054851-63-7	72
3	3-Methylcarbazole	181	C13H11N	004630-20-0	60
4	Bifenthrin	422	C23H22ClF3O2	082657-04-3	59
5	4-Methylcarbazole	181	C13H11N	003770-48-7	55





Library Search Compound Report

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Instrument : BNA_F
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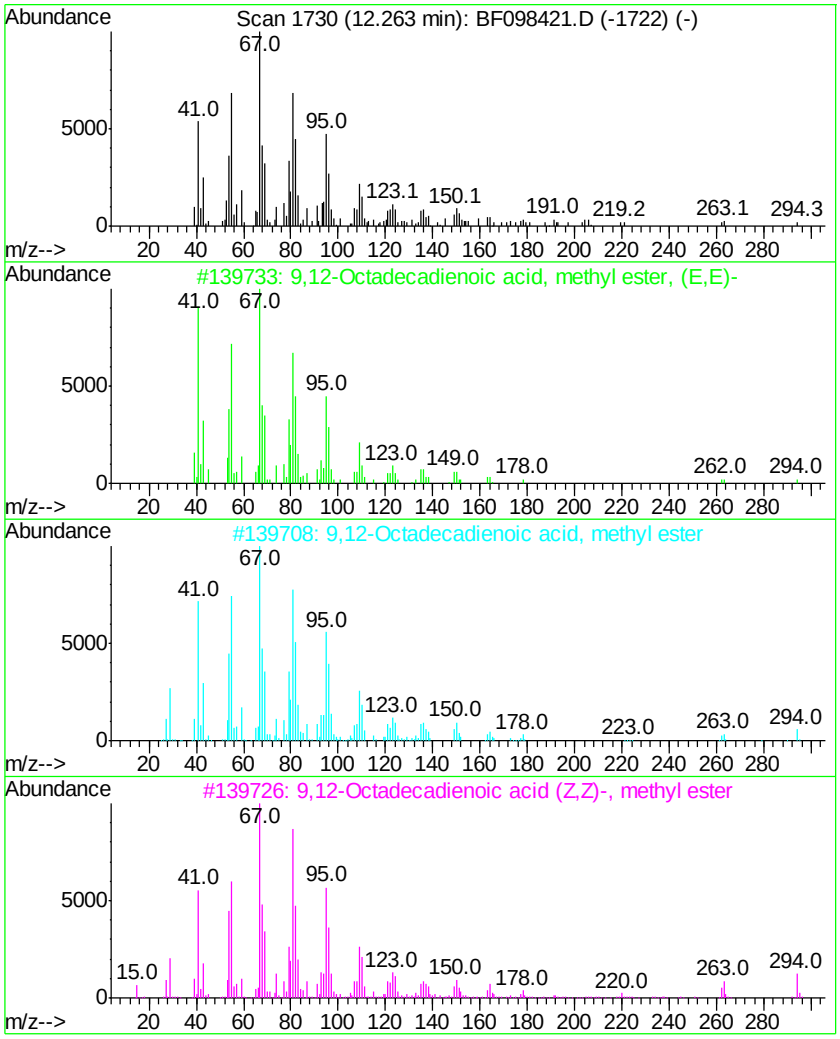
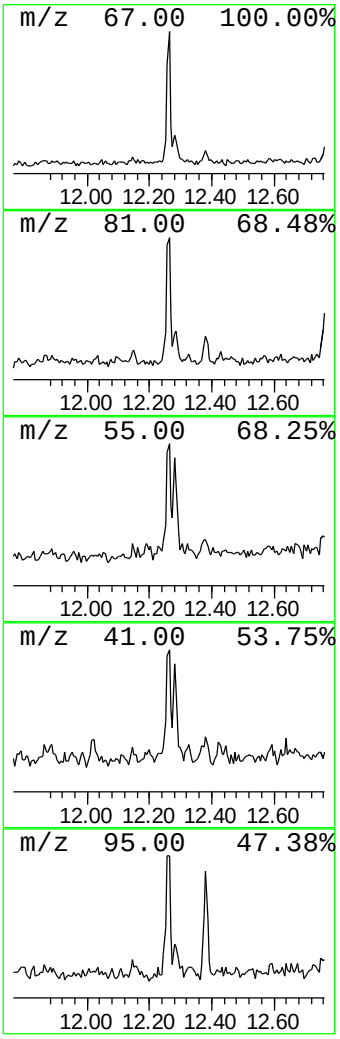
****

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	2.31 ng	222916	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
5	11-Octadecynoic acid, methyl ester	294	C19H34O2	026543-37-3	94





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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TIC Library : C:\DATABASE\NIST11.L
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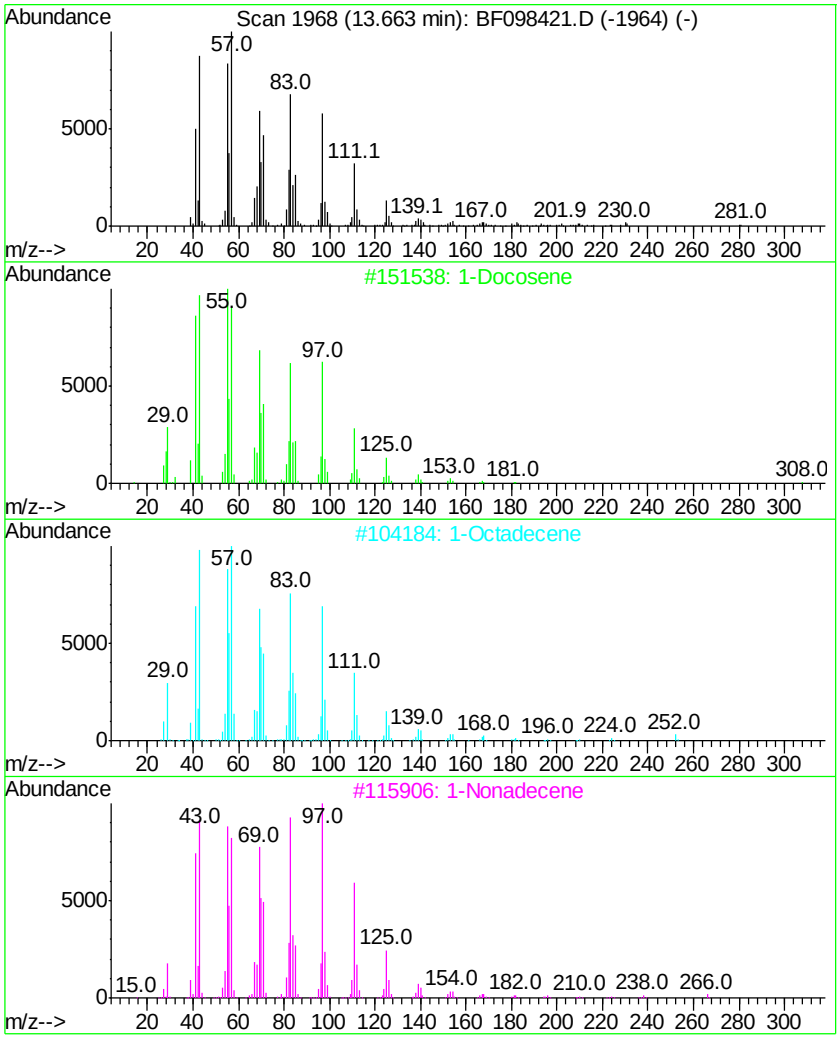
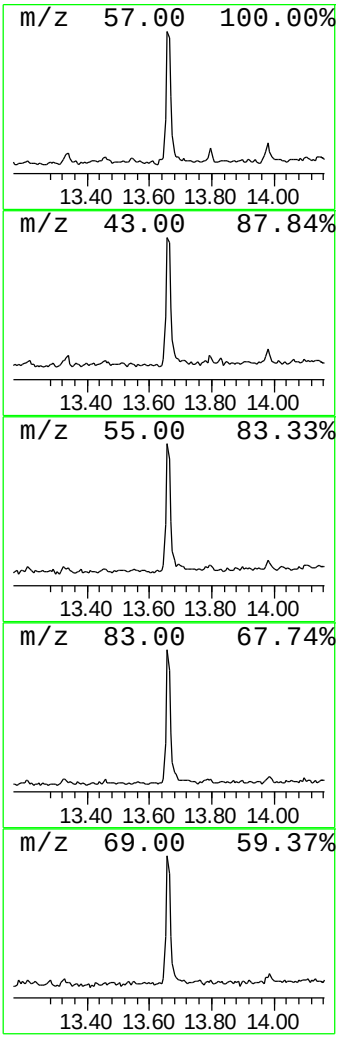
****

Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	9.38 ng	566747	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Octadecene	252	C18H36	000112-88-9	92
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

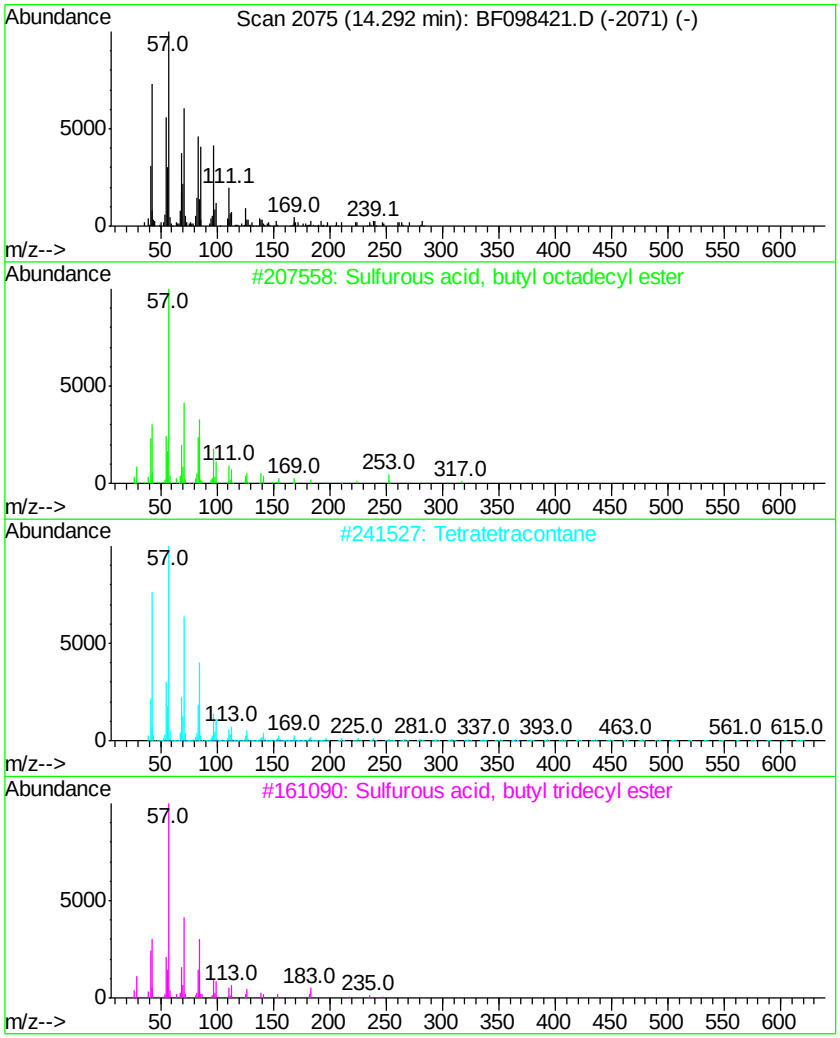
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

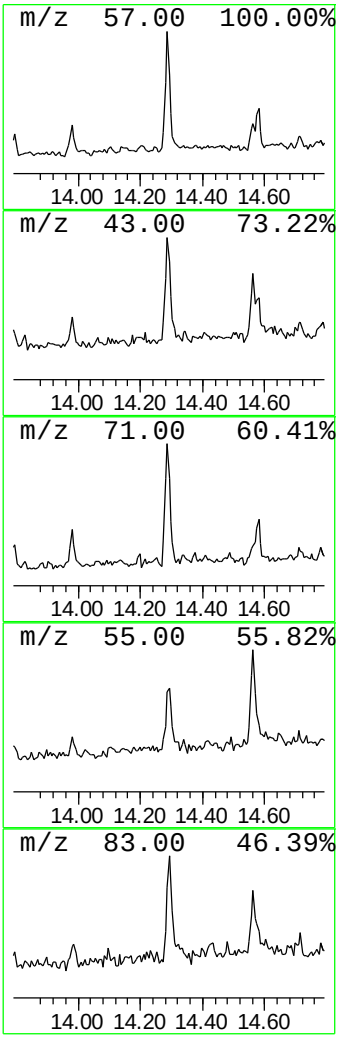
****

Peak Number 7 Sulfurous acid, butyl octad... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.88 ng	173719	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	91
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
5	Tritetracontane	605	C43H88	007098-21-7	91





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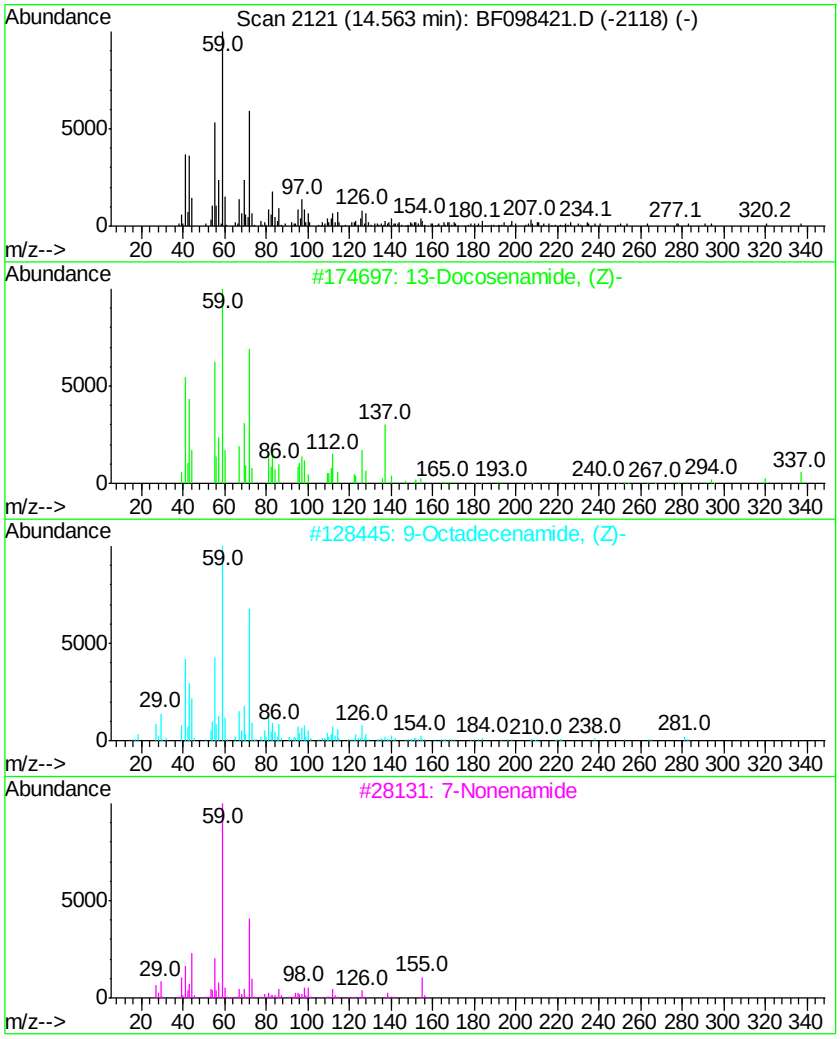
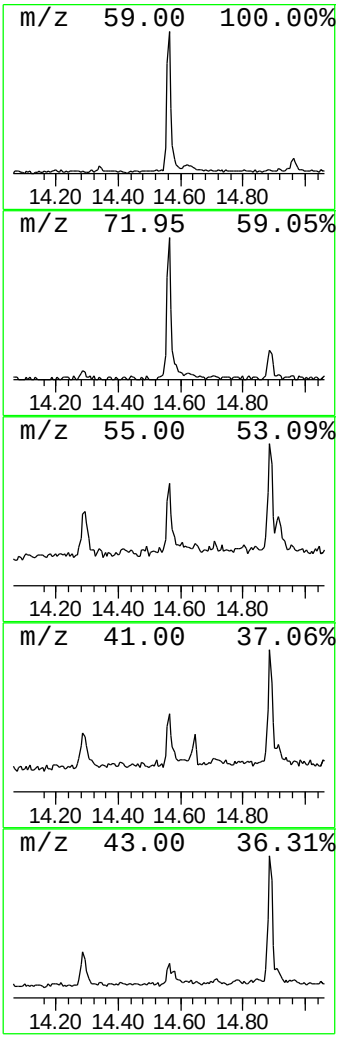
****

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	4.33 ng	252103	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
3	7-Nonenamide	155	C9H17NO	090949-53-4	74
4	Decanamide-	171	C10H21NO	002319-29-1	59
5	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	38





Library Search Compound Report

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Acq On : 12 Sep 2017 00:07
Operator : SJ/JU
Sample : I5138-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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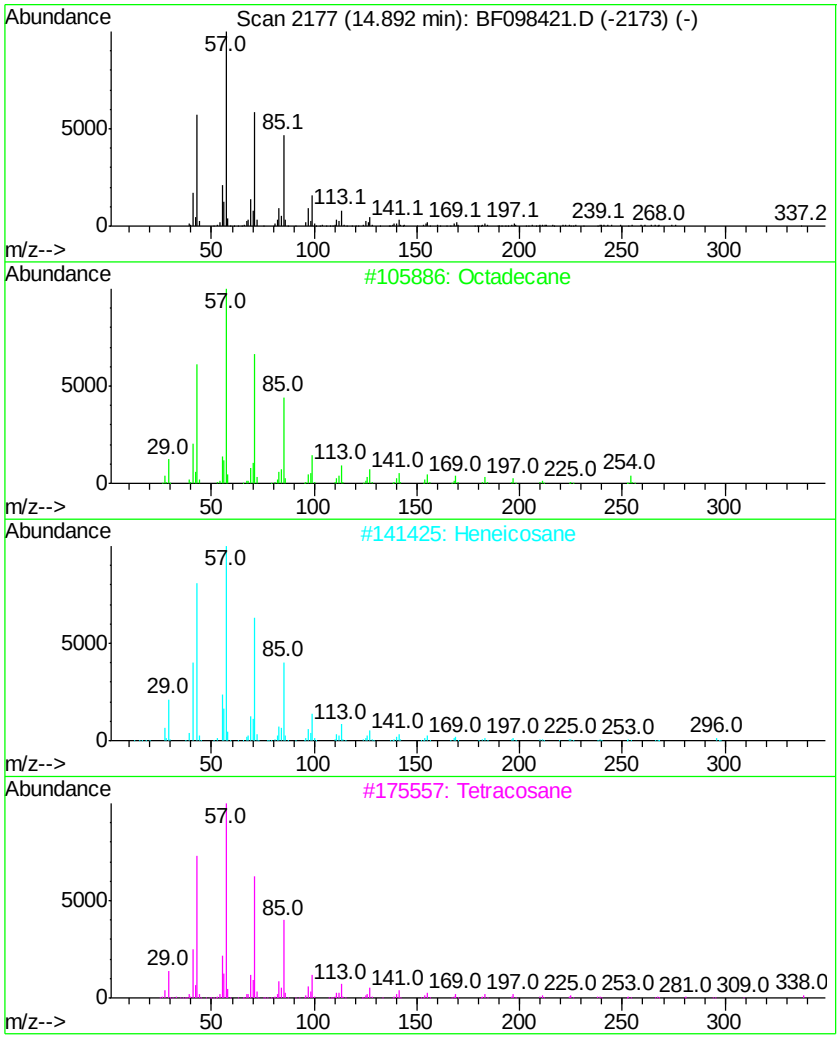
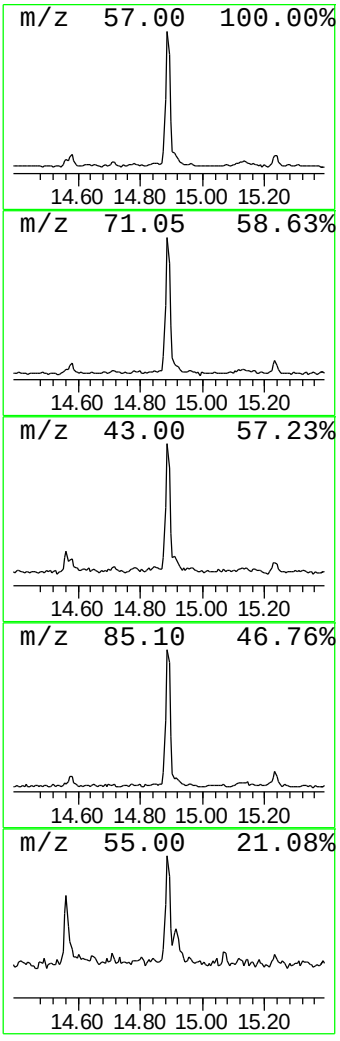
Peak Number 9 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	9.19 ng	535058	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heptacosane	380	C27H56	000593-49-7	91





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Misc :
ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId : EME-UTS-TS004-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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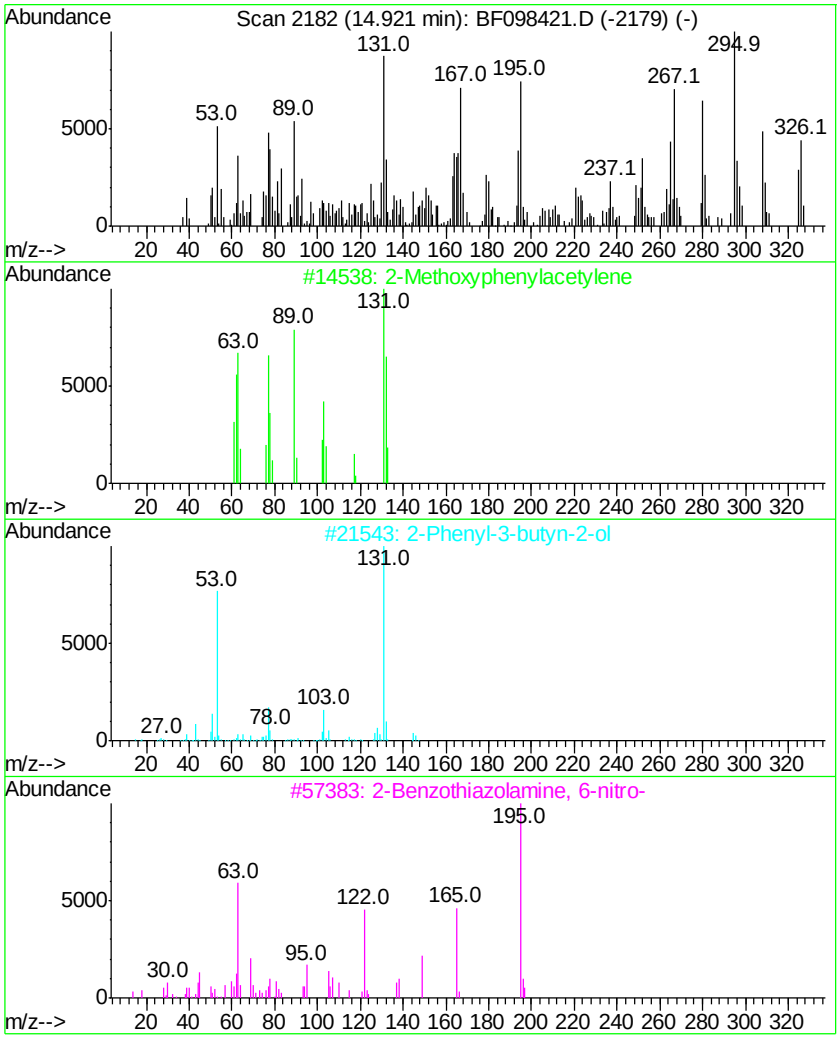
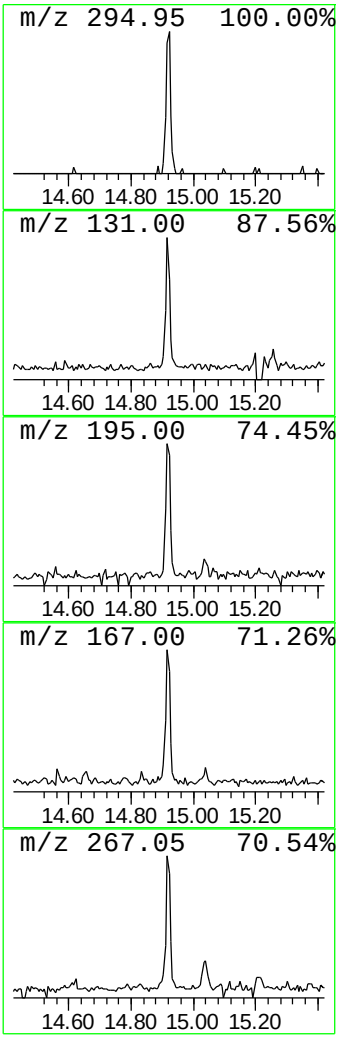
Peak Number 10 unknown14.92 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	5.80 ng	337737	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methoxyphenylacetylene	132	C9H8O	000767-91-9	38
2	2-Phenyl-3-butyn-2-ol	146	C10H10O	000127-66-2	27
3	2-Benzothiazolamine, 6-nitro-	195	C7H5N3O2S	006285-57-0	25
4	Phenol, 2,6-dinitro-4-(trifluoro...	252	C7H3F3N2O5	000393-77-1	18
5	1,3-Cyclopentadiene, 2-bromo-3-(...	182	C8H7Br	1000142-00-7	15





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Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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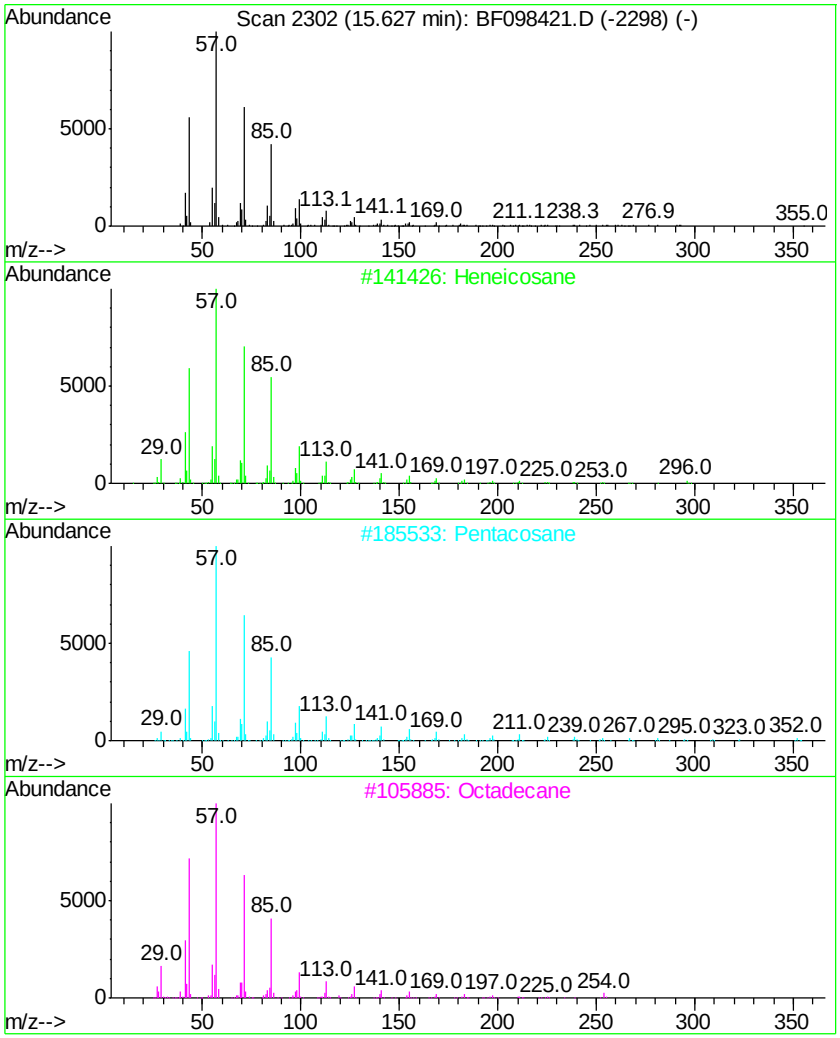
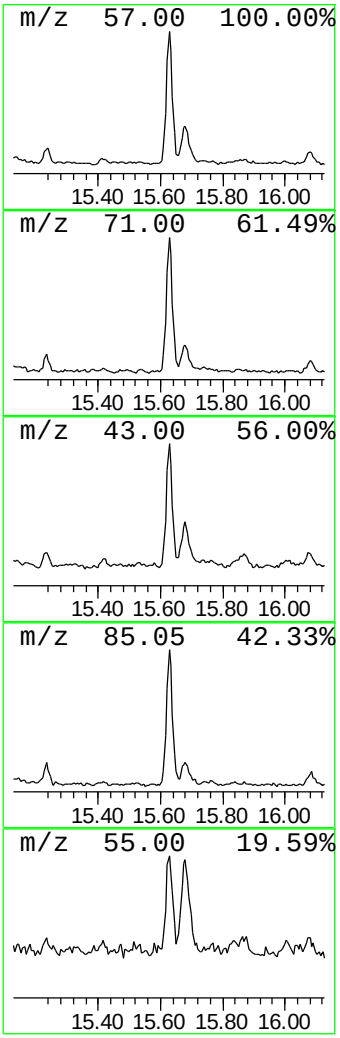
Peak Number 11 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	8.81 ng	512887	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	Octadecane	254	C18H38	000593-45-3	86
4	Nonadecane	268	C19H40	000629-92-5	86
5	Tetradecane	198	C14H30	000629-59-4	83





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Sample : I5138-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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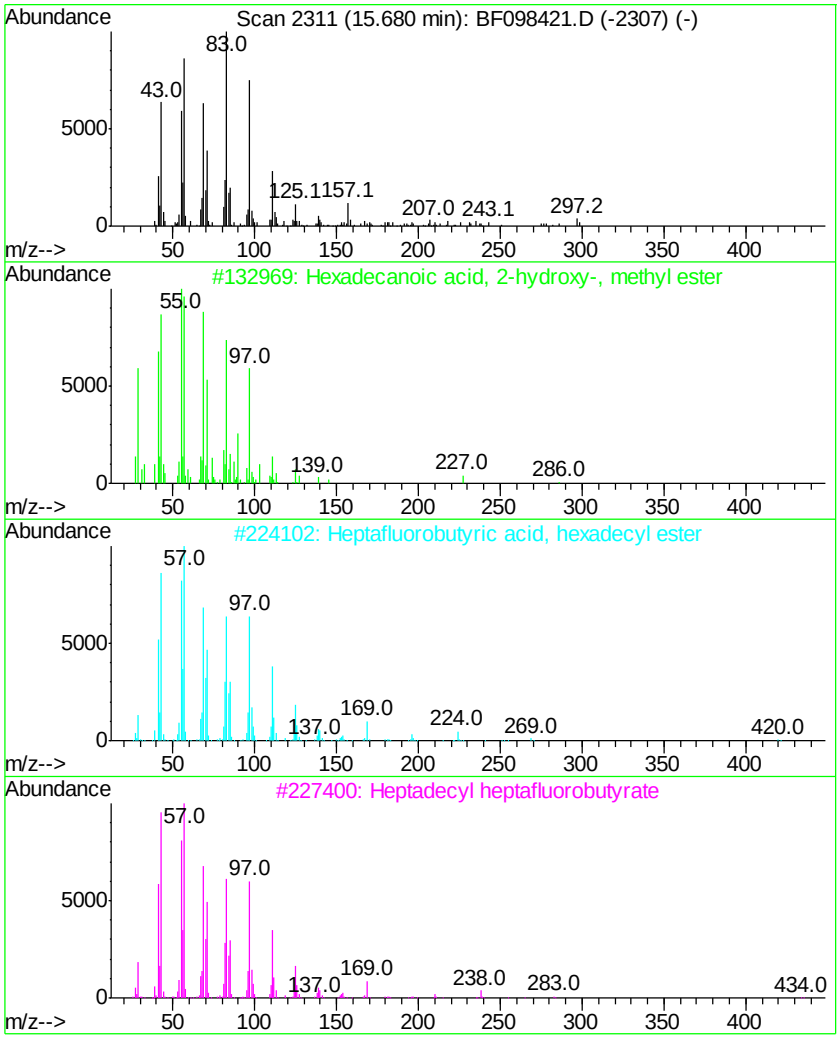
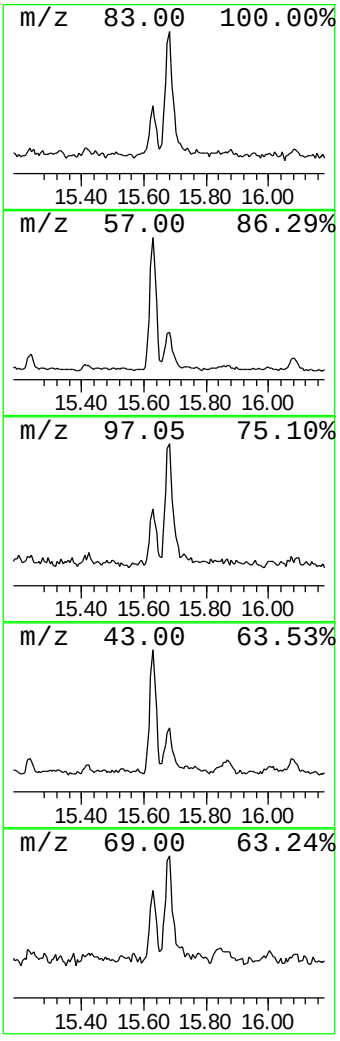
Peak Number 12 Hexadecanoic acid, 2-hydrox... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	5.64 ng	328123	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	58
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	55
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	49
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	38
5	17-Pentatriacontene	491	C35H70	006971-40-0	38





Library Search Compound Report

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Acq On : 12 Sep 2017 00:07
Operator : SJ/JU
Sample : I5138-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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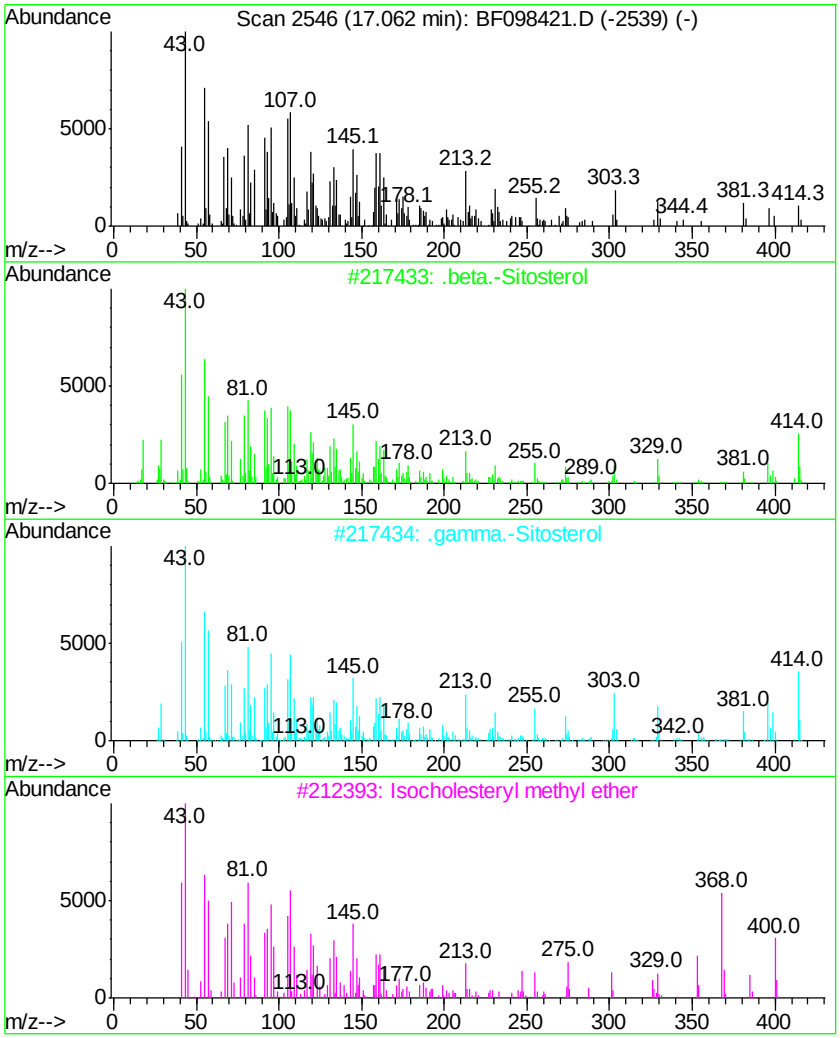
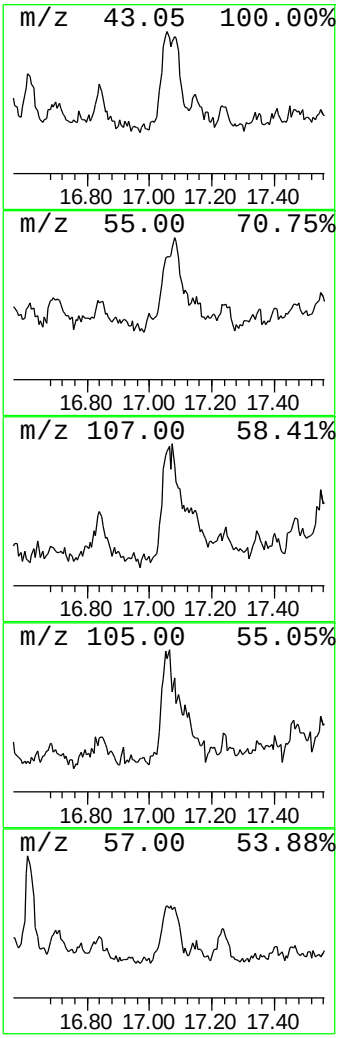
Peak Number 13 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.06	9.03 ng	525591	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	95
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	91
3	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	70
4	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	68
5	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	46





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Acq On : 12 Sep 2017 00:07
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Sample : I5138-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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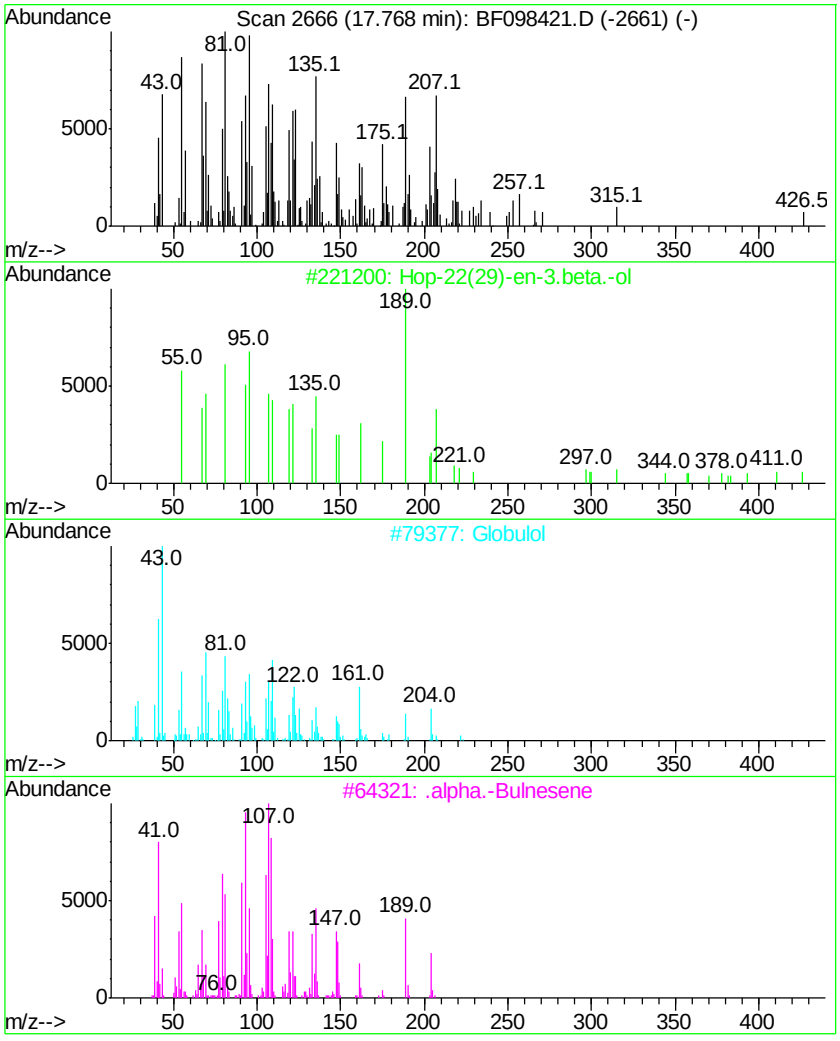
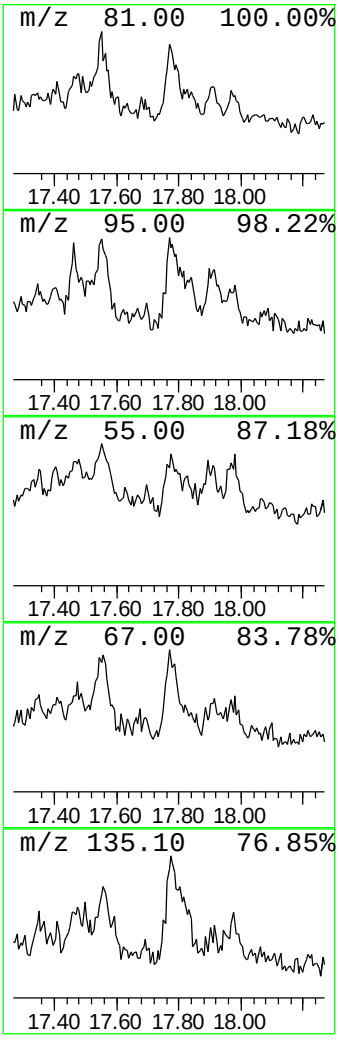
Peak Number 14 Hop-22(29)-en-3.beta.-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.77	6.54 ng	380956	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	70
2	Globulol	222	C15H26O	051371-47-2	64
3	.alpha.-Bulnesene	204	C15H24	1000374-19-9	35
4	Caparratriene	206	C15H26	1000374-08-7	30
5	Longifolenaldehyde	220	C15H24O	019890-84-7	30





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Sample : I5138-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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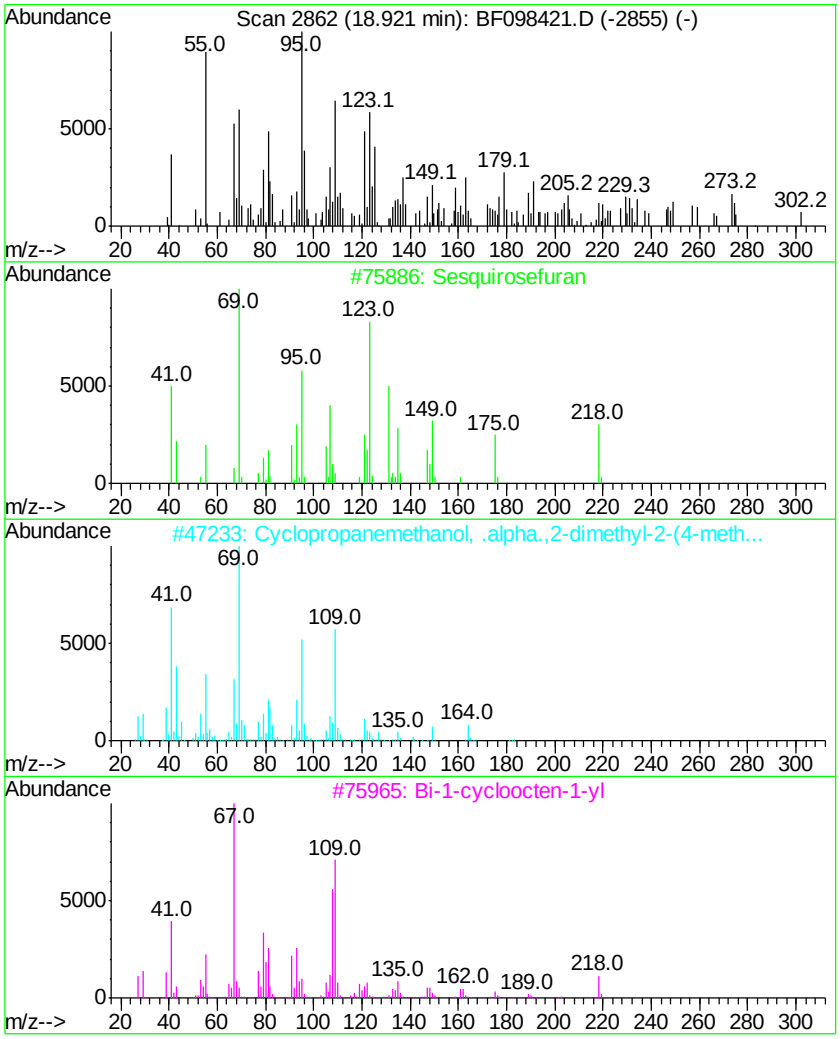
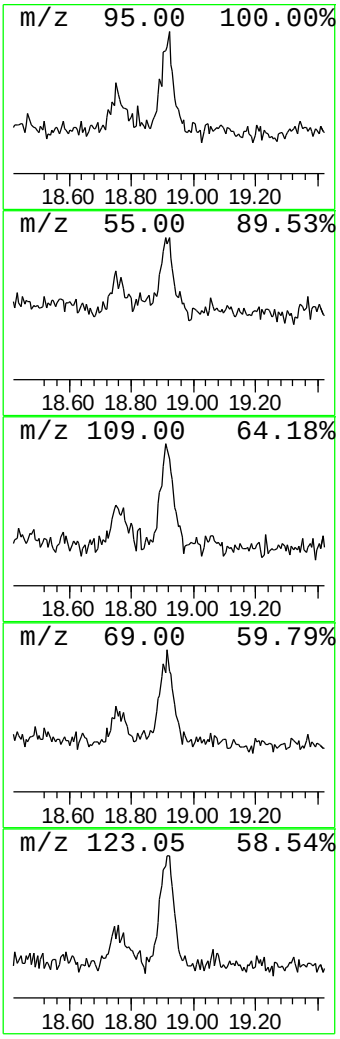
Peak Number 15 unknown18.92 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.92	5.58 ng	325133	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sesquirosefuran	218	C15H22O	039007-93-7	42
2	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	35
3	Bi-1-cycloocten-1-yl	218	C16H26	061468-42-6	25
4	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	22
5	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	20





Tentatively Identified Compound (LSC) summary

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Acq On : 12 Sep 2017 00:07
Operator : SJ/JU
Sample : I5138-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EME-UTS-TS004-01

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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...	4.87	12.3	ng	962088	1	6.67	1569140	20.0
unknown6.45	6.45	85.9	ng	6736080	1	6.67	1569140	20.0
1,1'-Biphenyl, 2,...	10.96	2.1	ng	202487	4	11.18	1929280	20.0
9,12-Octadecadien...	12.26	2.3	ng	222916	4	11.18	1929280	20.0
1-Docosene	13.66	9.4	ng	566747	5	13.81	1208260	20.0
Sulfurous acid, b...	14.29	2.9	ng	173719	5	13.81	1208260	20.0
13-Docosenamide, ...	14.56	4.3	ng	252103	6	15.21	1164590	20.0
Octadecane	14.89	9.2	ng	535058	6	15.21	1164590	20.0
unknown14.92	14.92	5.8	ng	337737	6	15.21	1164590	20.0
Heneicosane	15.63	8.8	ng	512887	6	15.21	1164590	20.0
Hexadecanoic acid...	15.68	5.6	ng	328123	6	15.21	1164590	20.0
.beta.-Sitosterol	17.06	9.0	ng	525591	6	15.21	1164590	20.0
Hop-22(29)-en-3.b...	17.77	6.5	ng	380956	6	15.21	1164590	20.0
unknown18.92	18.92	5.6	ng	325133	6	15.21	1164590	20.0