LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099388.D
Acq On : 12 Oct 2017 11:46
Operator : SJ/JU
Sample : I5765-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

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-BF092317.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	2.158	10	12	32	rVB2	100906	253353	8.95%	0.763%
2	5.087	506	510	523	rVB	351387	487285	17.20%	1.468%
3	5.481	573	577	588	rBV	2441208	2680475	94.64%	8.077%
4	6.492	737	749	764	rBV	2372374	2745309	96.93%	8.273%
5	6.628	767	772	775	rBV	2776760	2742854	96.84%	8.265%
6	6.851	806	810	814	rBV	998850	790374	27.91%	2.382%
7	7.010	832	837	840	rBV	2319349	2137287	75.46%	6.440%
8	7.416	901	906	909	rBV	1552514	1725210	60.91%	5.199%
9	7.504	915	921	924	rVB	36210	37256	1.32%	0.112%
10	8.134	1024	1028	1031	rVB	1264237	1058555	37.37%	3.190%
11	9.210	1205	1211	1214	rBV	2872679	2832342	100.00%	8.535%
12	9.469	1251	1255	1260	rBV2	46082	39064	1.38%	0.118%
13	9.598	1273	1277	1280	rBV	598515	468604	16.54%	1.412%
14	9.804	1308	1312	1315	rBV	45174	43360	1.53%	0.131%
15	9.886	1321	1326	1330	rBV	1292974	1119105	39.51%	3.372%
16	10.081	1354	1359	1364	rBV6	27815	37329	1.32%	0.112%
17	10.304	1391	1397	1400	rBV	83800	88270	3.12%	0.266%
18	10.522	1429	1434	1437	rBV	44294	64138	2.26%	0.193%
19	10.680	1456	1461	1464	rBV	1472880	1468444	51.85%	4.425%
20	10.780	1474	1478	1482	rBV	82874	122677	4.33%	0.370%
21	11.222	1550	1553	1556	rBV	60489	59073	2.09%	0.178%
22	11.251	1556	1558	1564	rVB2	40285	45150	1.59%	0.136%
23	11.375	1575	1579	1582	rBV	1143817	971662	34.31%	2.928%
24	11.651	1623	1626	1629	rBV	41412	33295	1.18%	0.100%
25	11.751	1640	1643	1647	rVB	1006422	895469	31.62%	2.698%
26	11.892	1662	1667	1676	rBV	284237	329523	11.63%	0.993%
27	12.057	1691	1695	1702	rVB5	54697	78686	2.78%	0.237%
28	12.198	1717	1719	1728	rVB9	33054	47352	1.67%	0.143%
29	12.445	1756	1761	1762	rBV	2685369	2635123	93.04%	7.941%
30	12.463	1762	1764	1771	rVB2	2548618	2283604	80.63%	6.881%
31	12.545	1774	1778	1782	rVB	643615	508458	17.95%	1.532%
32	12.586	1782	1785	1790	rBV3	48231	85812	3.03%	0.259%
33	12.674	1797	1800	1805	rBV3	46384	48443	1.71%	0.146%
34	12.769	1813	1816	1821	rBV	40932	46889	1.66%	0.141%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5765-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.957	1841	1848	1851	rBV	1914228	1833132	64.72%	5.524%
36	12.980	1851	1852	1861	rVB8	38713	98431	3.48%	0.297%
37	13.192	1886	1888	1894	rVB5	44887	54548	1.93%	0.164%
38	13.269	1898	1901	1903	rVV	57141	49238	1.74%	0.148%
39	13.427	1923	1928	1932	rVB4	31419	47198	1.67%	0.142%
40	13.504	1938	1941	1948	rVB2	33443	52181	1.84%	0.157%
41	13.692	1970	1973	1978	rVB3	50680	68178	2.41%	0.205%
42	13.839	1994	1998	2001	rBV	102167	114517	4.04%	0.345%
43	13.933	2012	2014	2018	rVB	66880	56989	2.01%	0.172%
44	14.010	2023	2027	2031	rBV	679124	691482	24.41%	2.084%
45	14.374	2084	2089	2097	rBV9	59083	146002	5.15%	0.440%
46	14.457	2101	2103	2107	rVV4	30532	30804	1.09%	0.093%
47	15.480	2273	2277	2282	rVB2	529482	678507	23.96%	2.045%
48	15.904	2347	2349	2357	rVB	37991	50468	1.78%	0.152%
49	16.162	2390	2393	2401	rVB3	70049	130165	4.60%	0.392%
50	16.592	2463	2466	2473	rVB4	41641	73467	2.59%	0.221%

Sum of corrected areas: 33185137

LSC Report - Integrated Chromatogram

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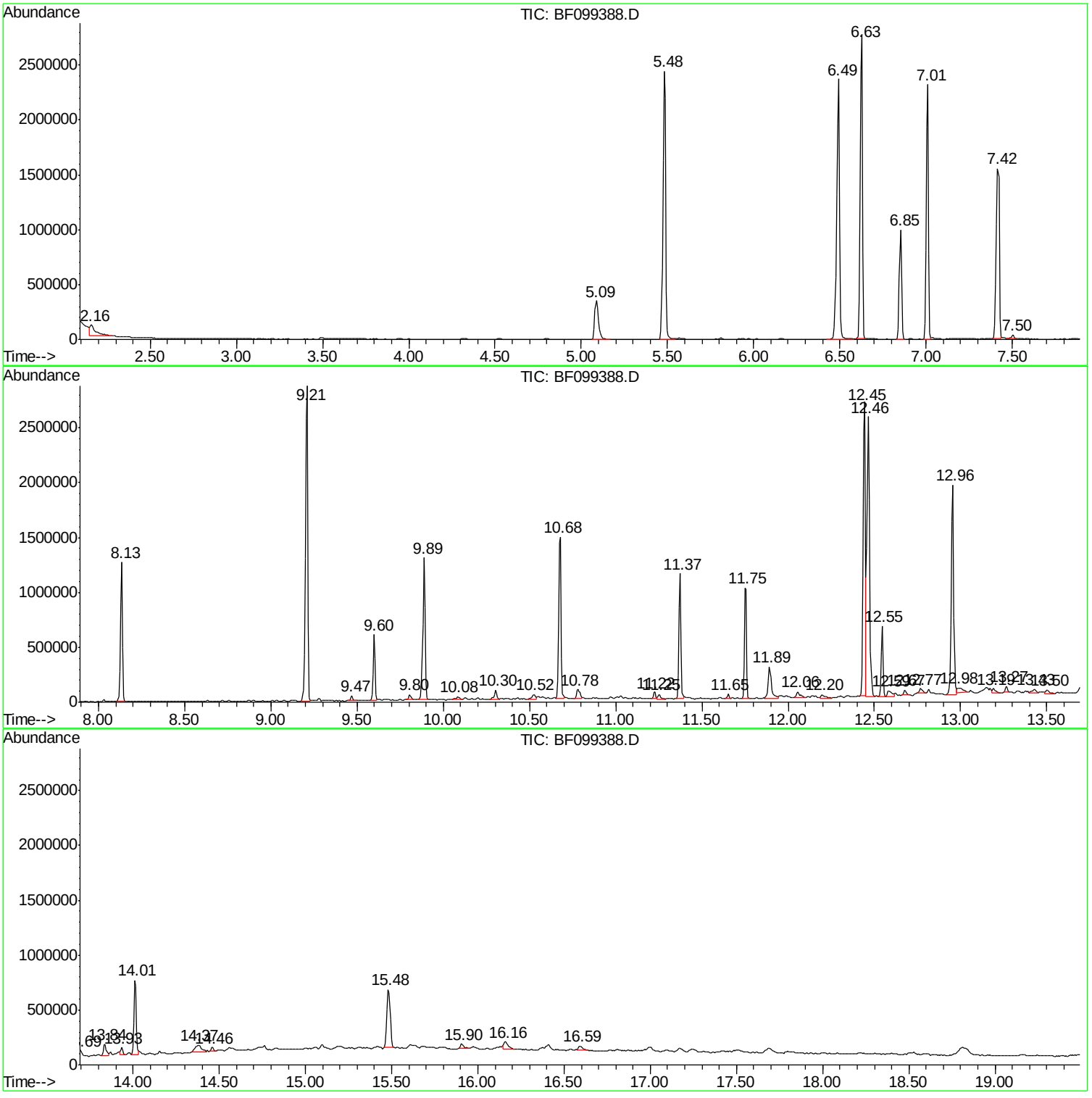
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF099388.D
Acq On : 12 Oct 2017 11:46
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Misc :
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Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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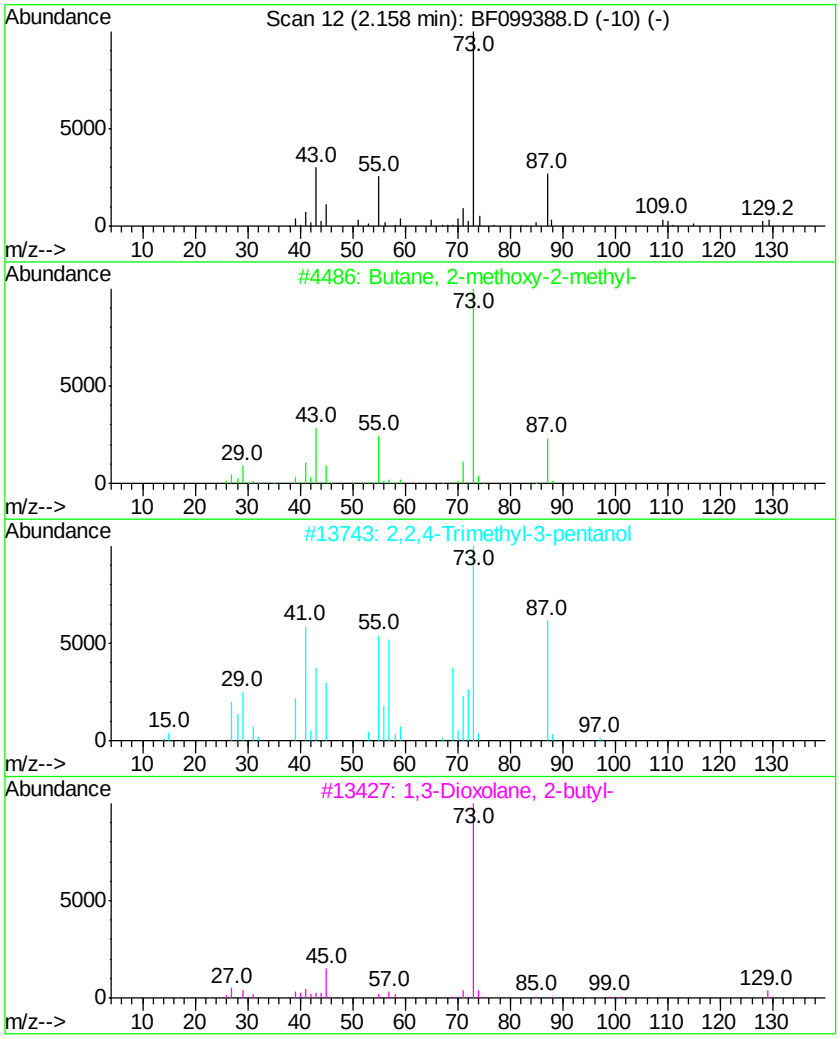
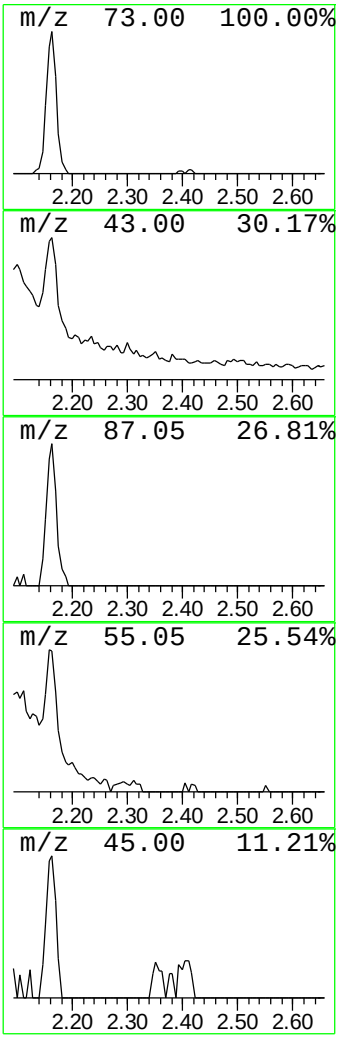
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	6.41 ng	253353	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-butyl-	130	C7H14O2	004360-76-3	17
4	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	12
5	1-Butanamine, 4-methoxy-	103	C5H13NO	034039-36-6	9





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Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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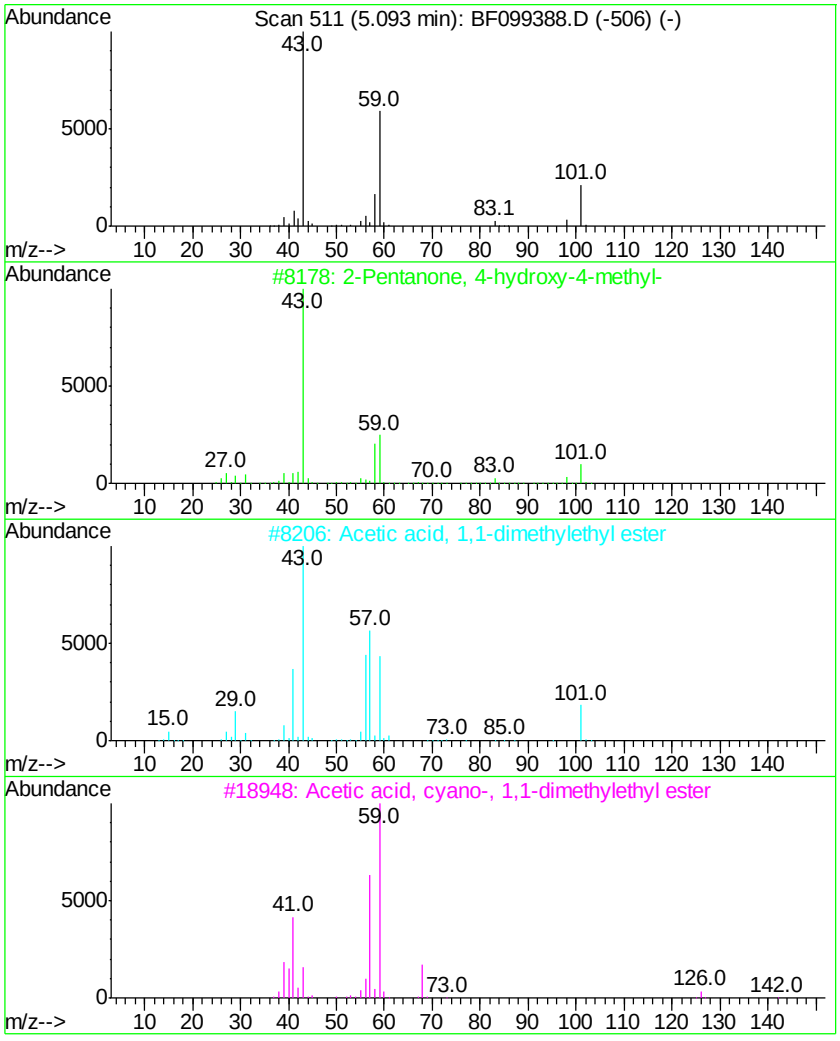
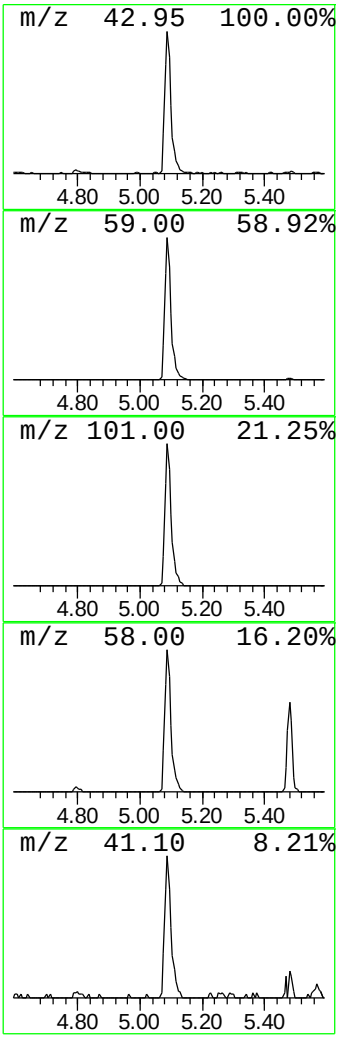
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	12.33 ng	487285	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

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Acq On : 12 Oct 2017 11:46
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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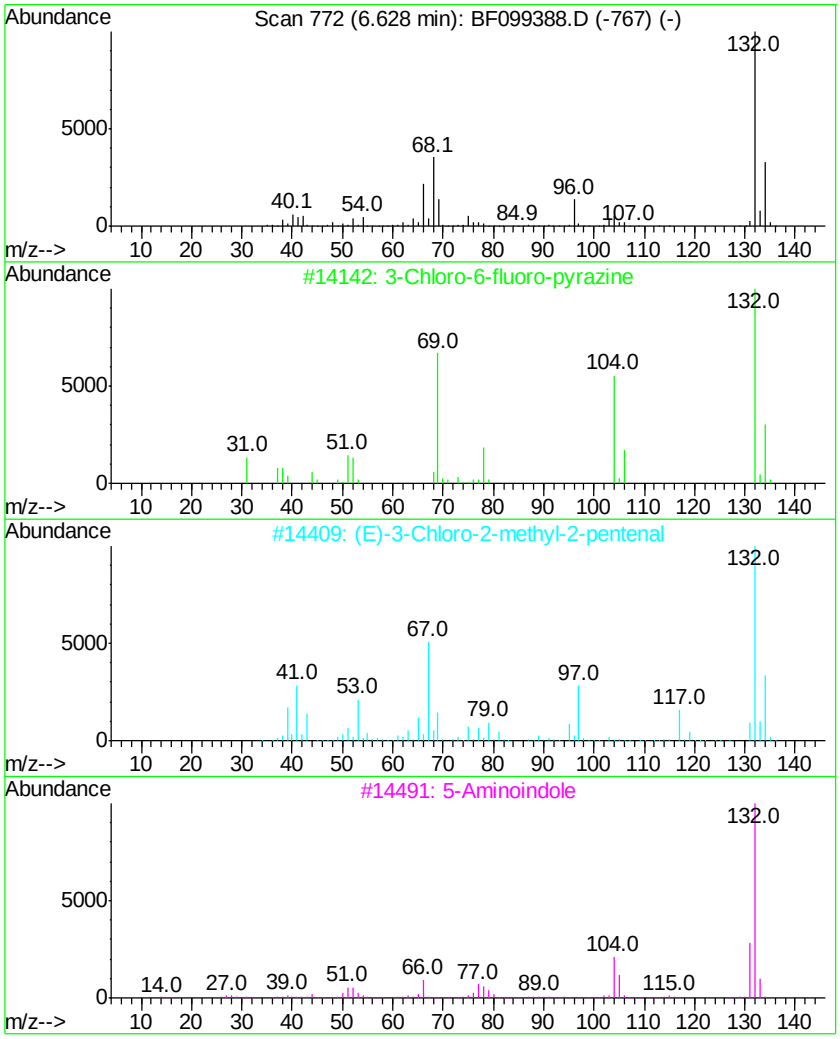
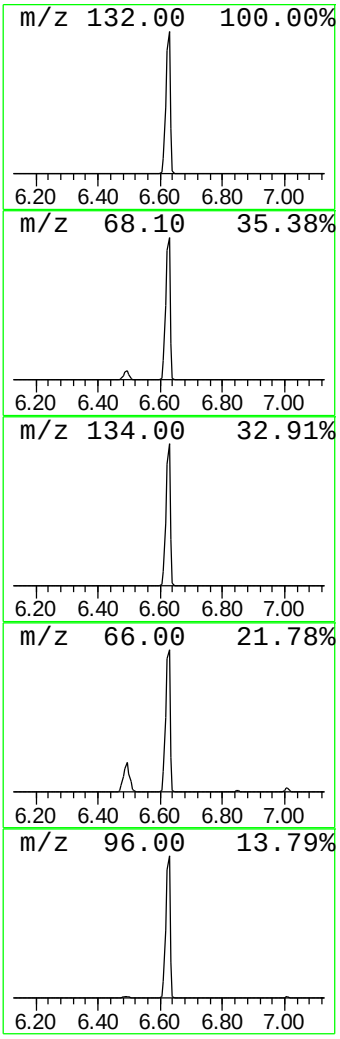
Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	69.41 ng	2742850	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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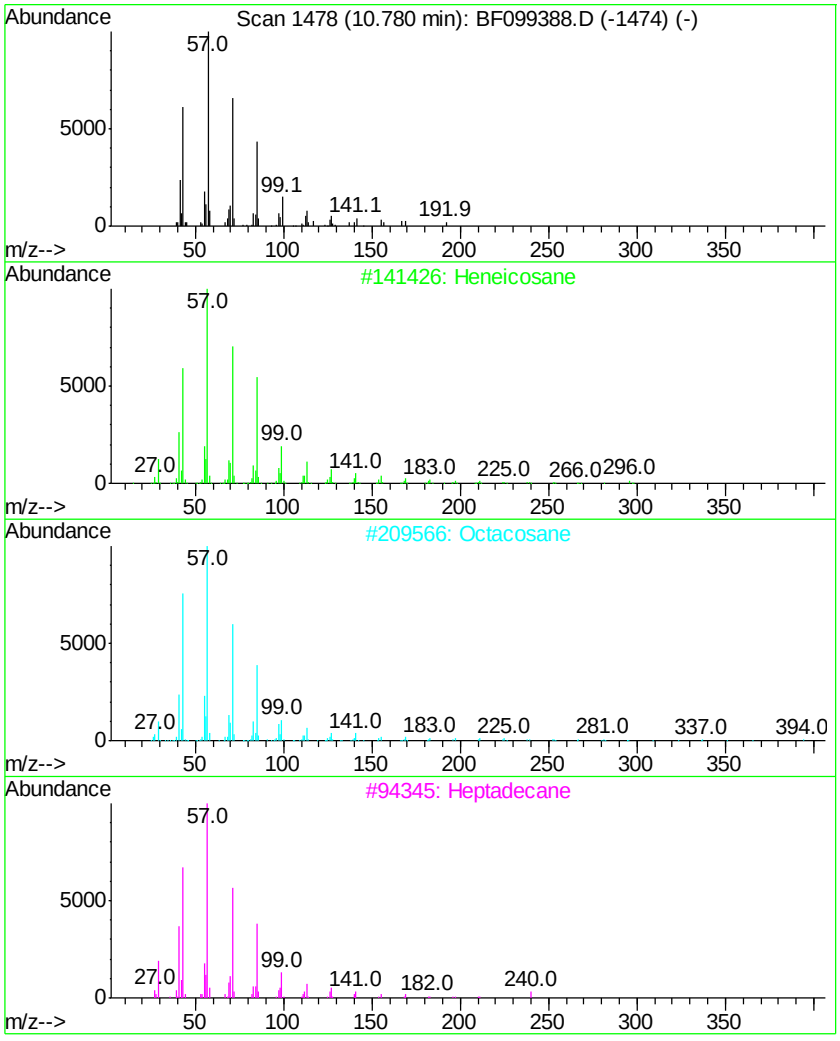
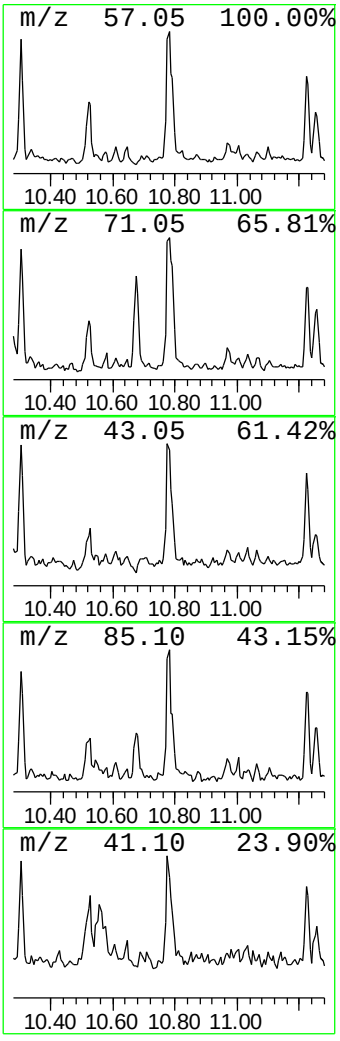
****

Peak Number 5 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	2.53 ng	122677	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Pentadecane	212	C15H32	000629-62-9	91
5	Docosane	310	C22H46	000629-97-0	90





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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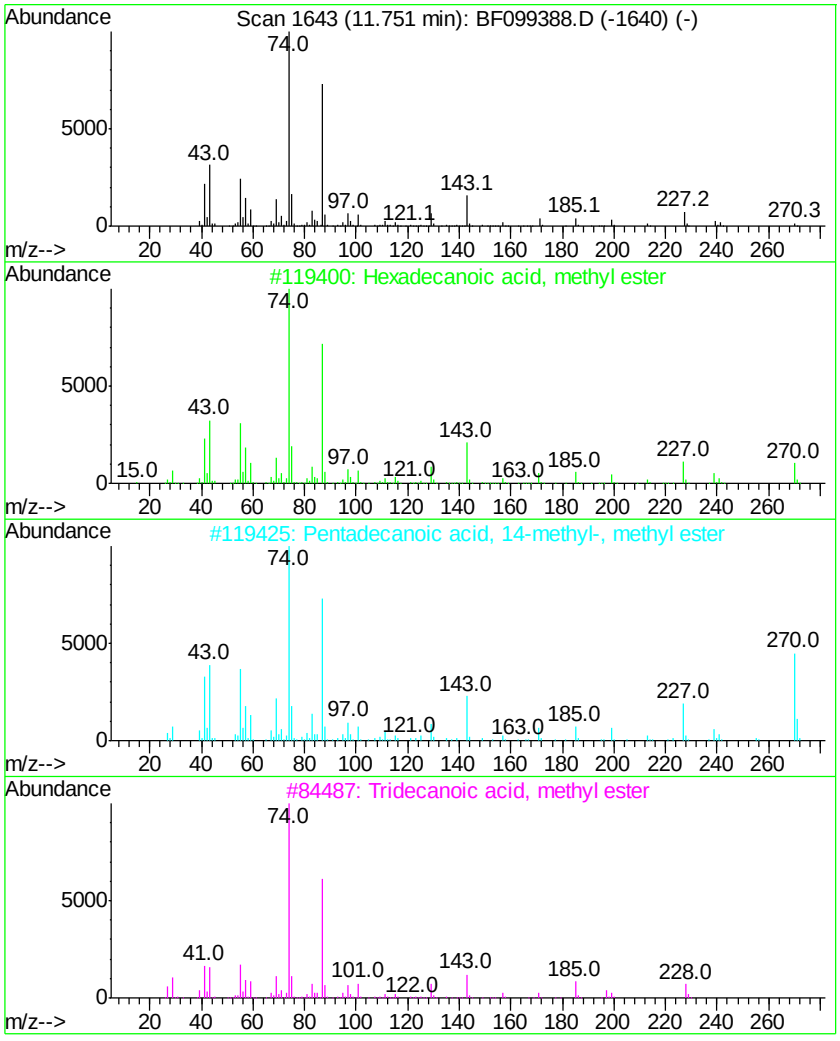
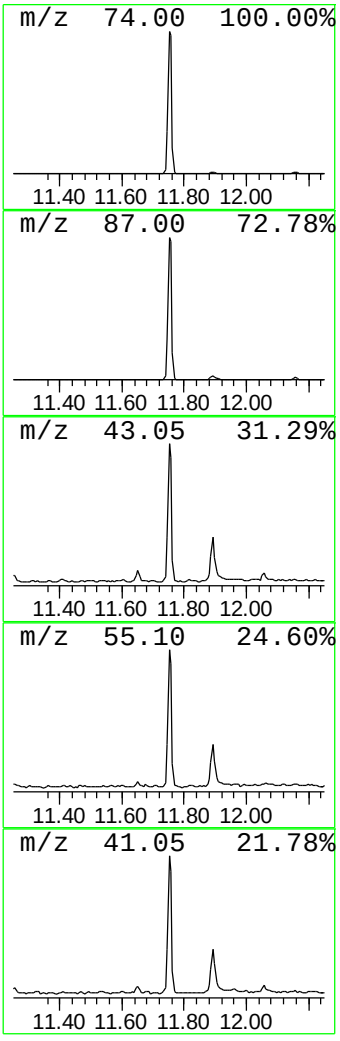
Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	18.43 ng	895469	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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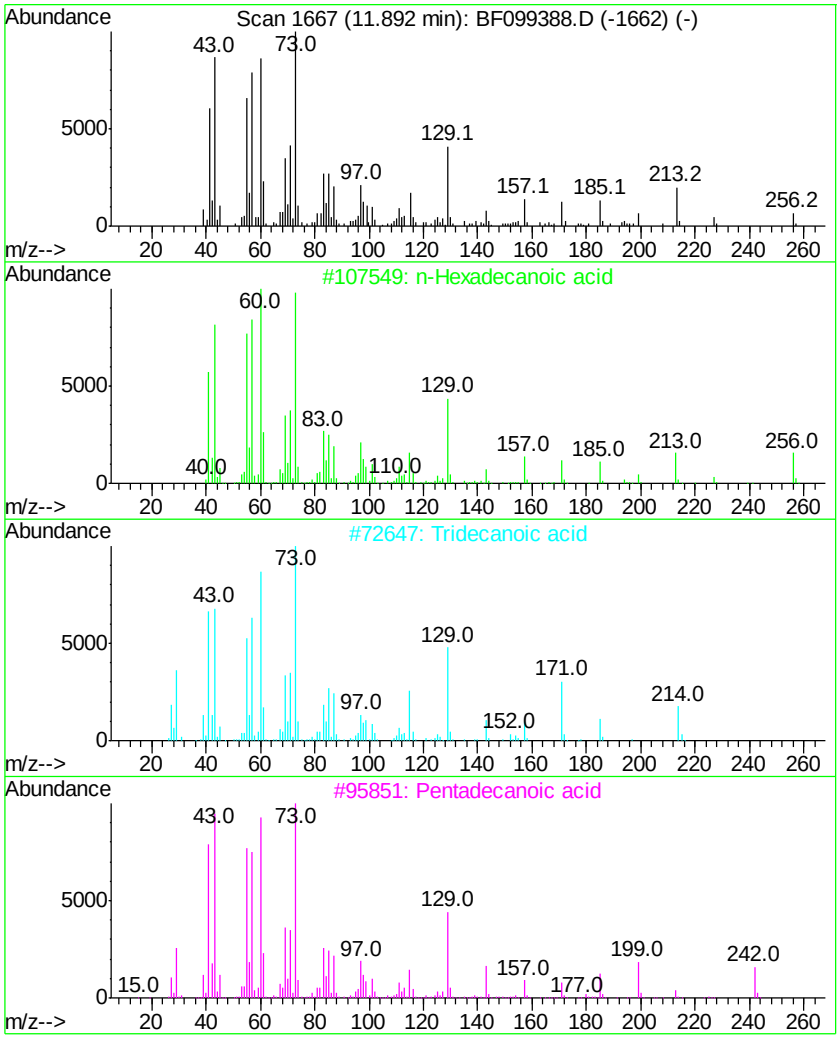
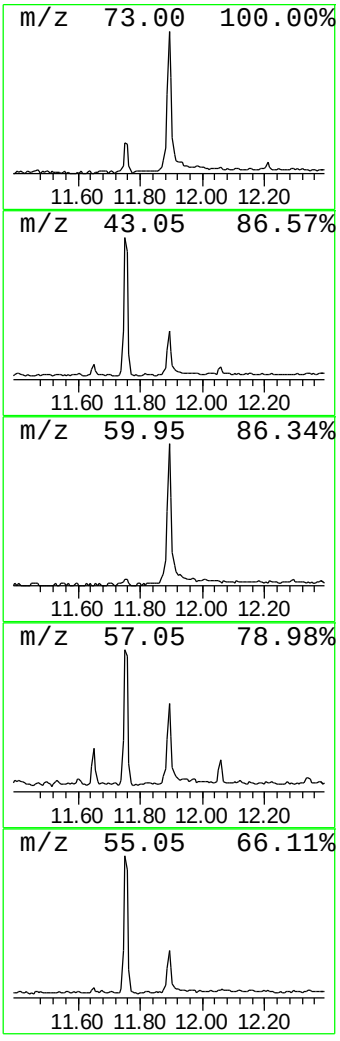
Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	6.78 ng	329523	Phenanthrene-d10	11.37

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Undecanoic acid	186	C11H22O2	000112-37-8	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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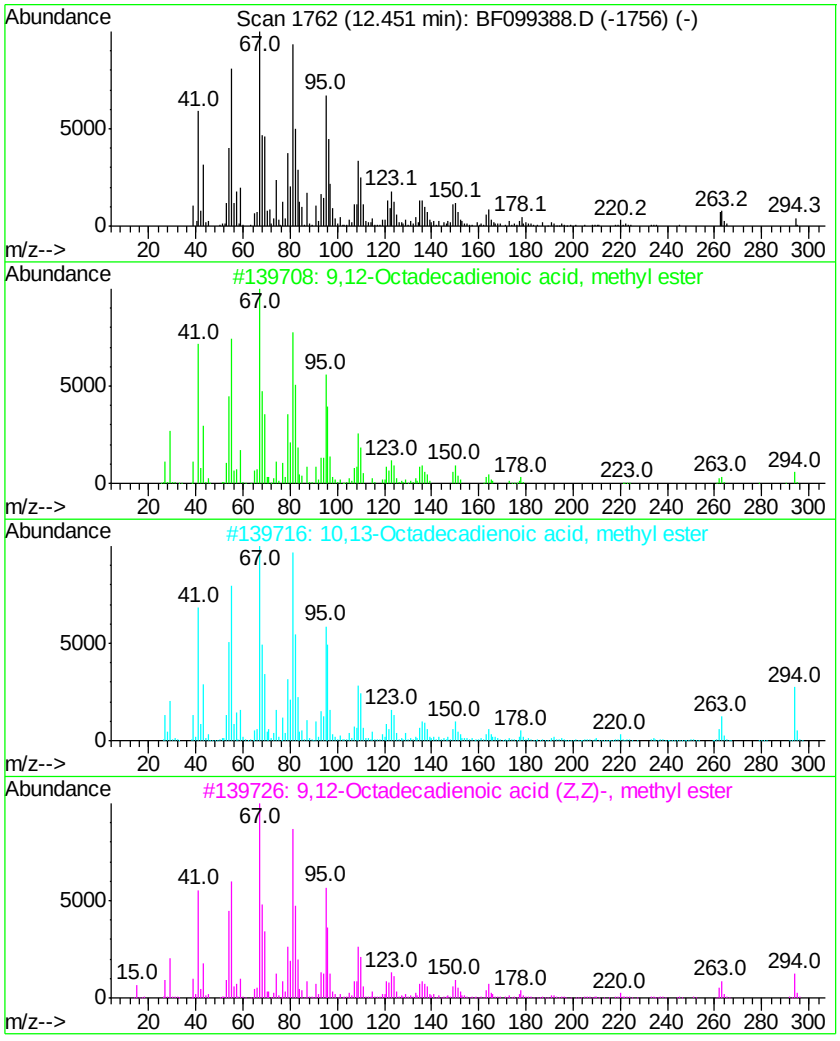
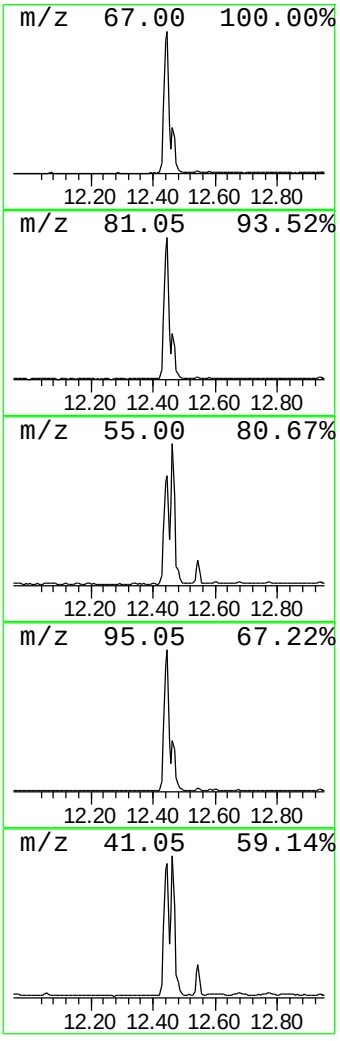
Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	54.24 ng	2635120	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	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	99
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
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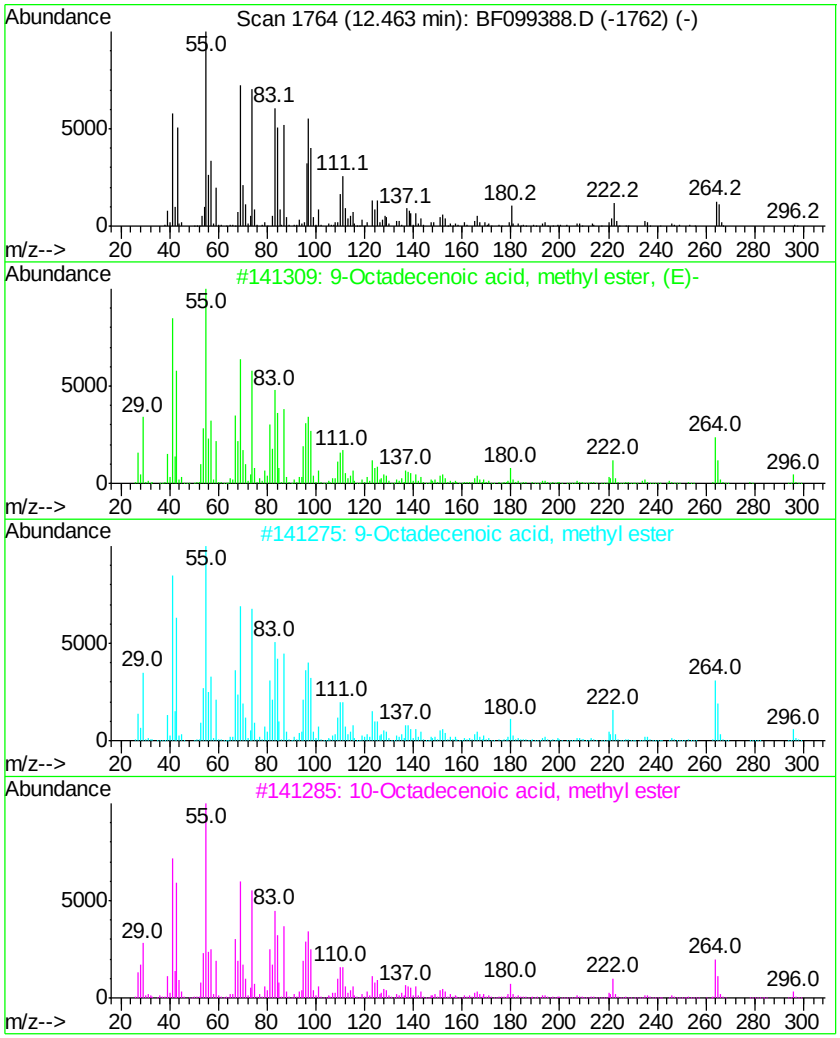
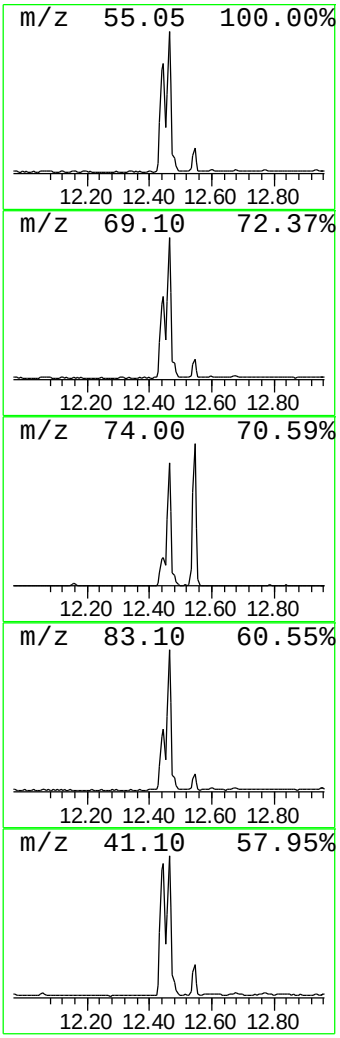
Peak Number 9 9-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	47.00 ng	2283600	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	94
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	94
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	93
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87





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Acq On : 12 Oct 2017 11:46
Operator : SJ/JU
Sample : I5765-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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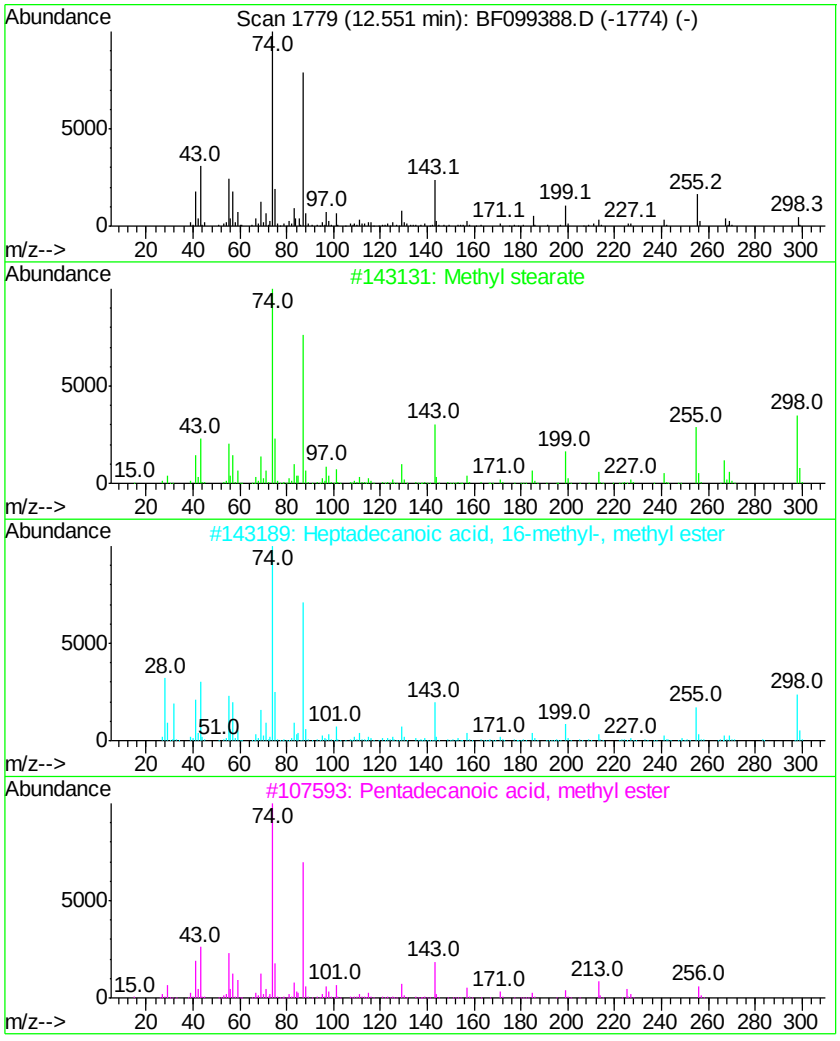
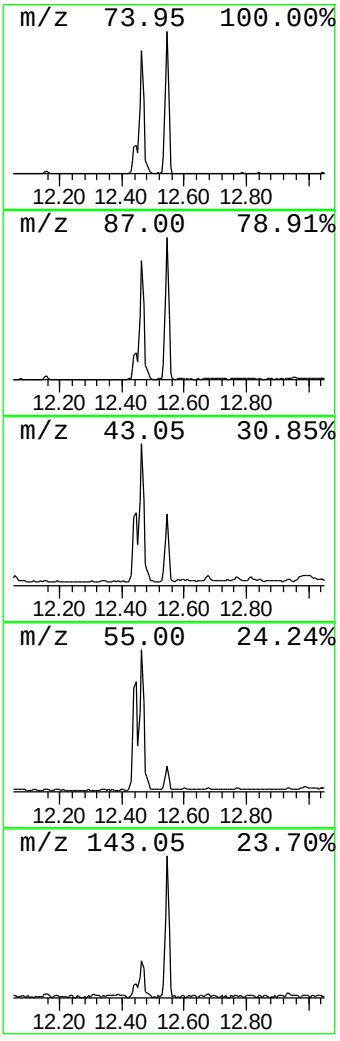
Peak Number 10 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	10.47 ng	508458	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86





Library Search Compound Report

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Sample : I5765-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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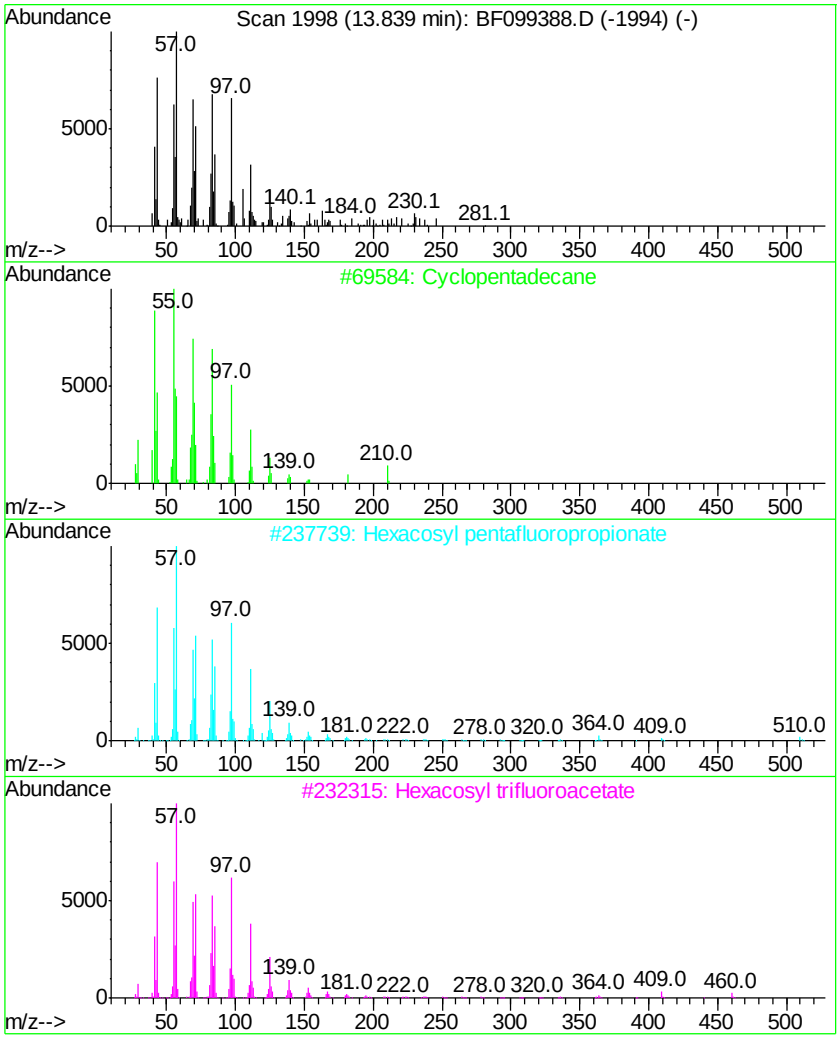
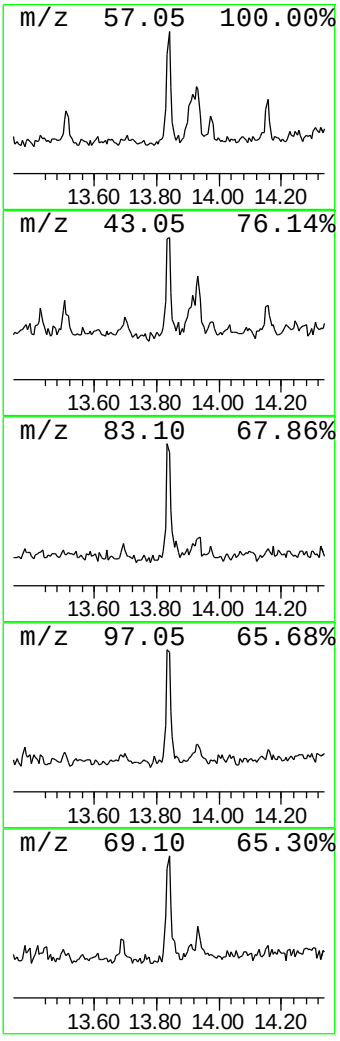
Peak Number 11 Cyclopentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.31 ng	114517	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	90
2	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87
3	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	87
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87
5	17-Pentatriacontene	491	C35H70	006971-40-0	83





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Acq On : 12 Oct 2017 11:46
Operator : SJ/JU
Sample : I5765-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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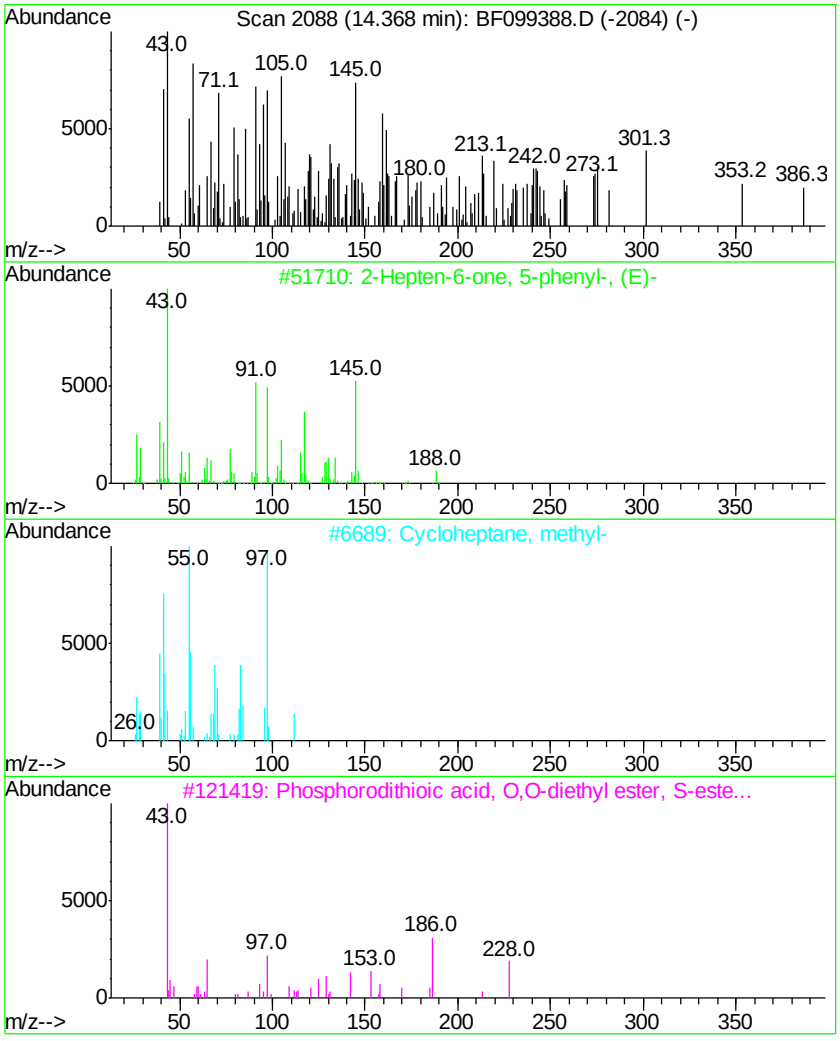
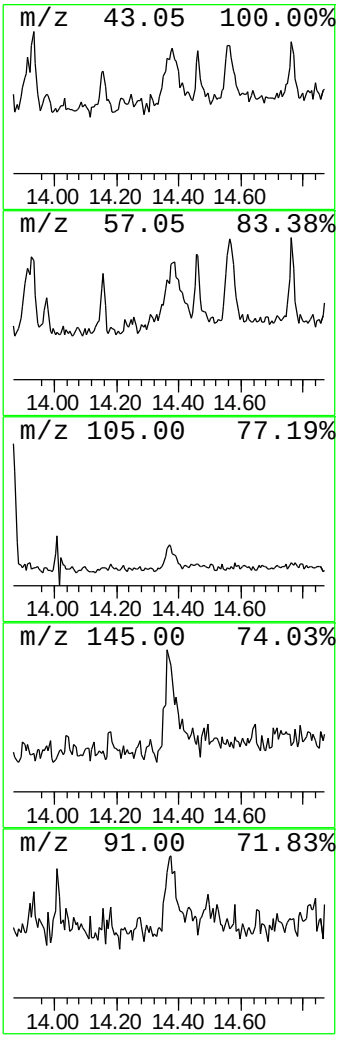
Peak Number 12 unknown14.37 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	4.22 ng	146002	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hepten-6-one, 5-phenyl-, (E)-	188	C13H16O	1000159-12-2	27
2	Cycloheptane, methyl-	112	C8H16	004126-78-7	11
3	Phosphorodithioic acid, O,O-diet...	272	C8H17O4PS2	018327-68-9	10
4	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	10
5	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	10





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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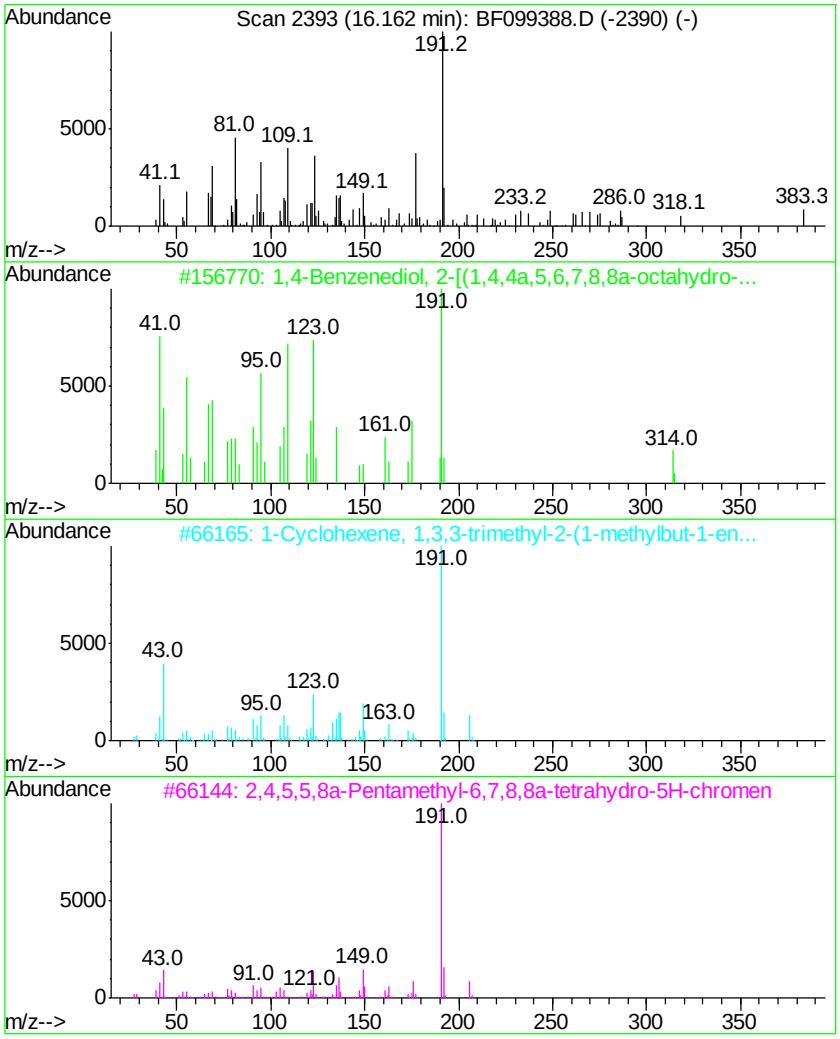
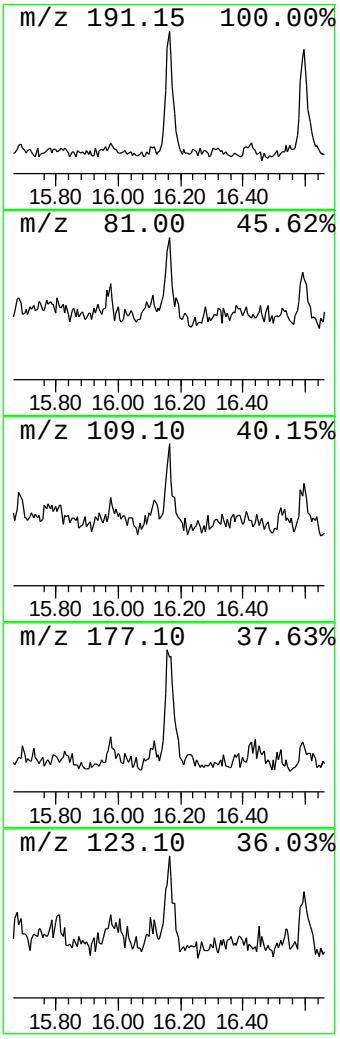
Peak Number 13 unknown16.16 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	3.84 ng	130165	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenediol, 2-[(1,4,4a,5,6,...	314	C21H30O2	039707-55-6	46
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	43
3	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	43
4	4,8a-Dimethyl-6-(2-methyl-oxiran...	234	C15H22O2	1000189-11-4	43
5	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	40





Library Search Compound Report

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Acq On : 12 Oct 2017 11:46
Operator : SJ/JU
Sample : I5765-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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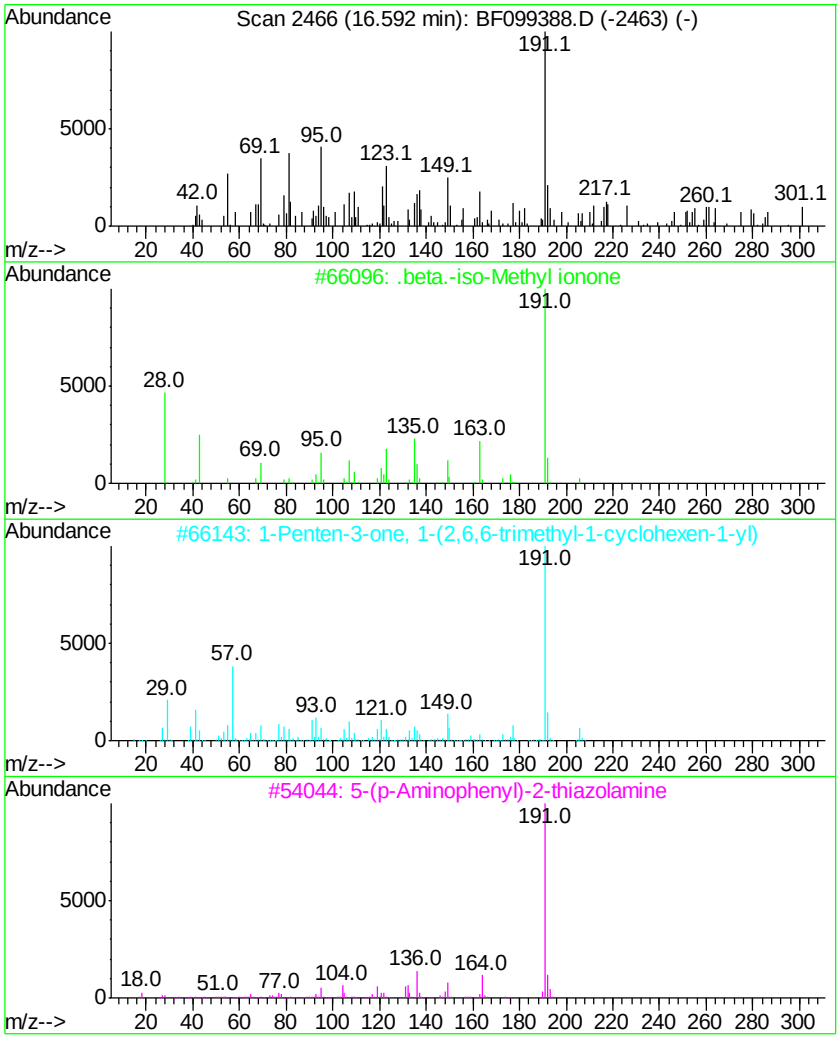
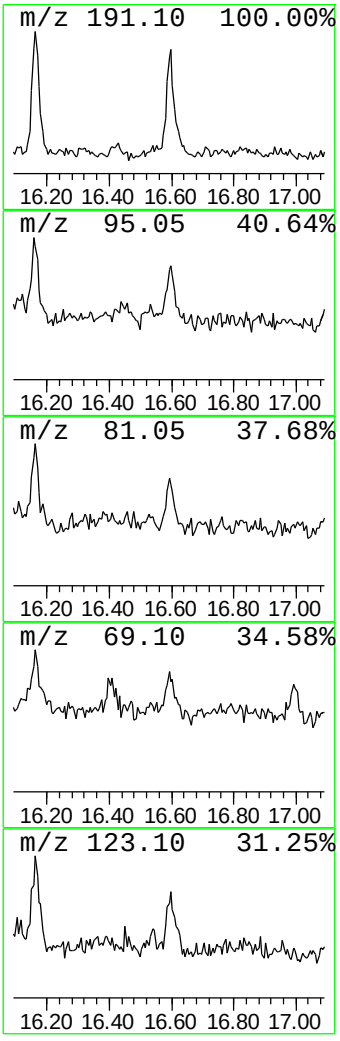
Peak Number 14 unknown16.59 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	2.17 ng	73467	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	47
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
3	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	43
4	Amiphenazole	191	C9H9N3S	000490-55-1	43
5	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38





Tentatively Identified Compound (LSC) summary

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Data File : BF099388.D
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Operator : SJ/JU
Sample : I5765-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-100917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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-methoxy...	2.16	6.4	ng	253353	1	6.85	790374	20.0
2-Pentanone, 4-hy...	5.09	12.3	ng	487285	1	6.85	790374	20.0
unknown6.63	6.63	69.4	ng	2742850	1	6.85	790374	20.0
Heneicosane	10.78	2.5	ng	122677	4	11.37	971662	20.0
Hexadecanoic acid...	11.75	18.4	ng	895469	4	11.37	971662	20.0
n-Hexadecanoic acid	11.89	6.8	ng	329523	4	11.37	971662	20.0
9,12-Octadecadien...	12.45	54.2	ng	2635120	4	11.37	971662	20.0
9-Octadecenoic ac...	12.46	47.0	ng	2283600	4	11.37	971662	20.0
Methyl stearate	12.55	10.5	ng	508458	4	11.37	971662	20.0
Cyclopentadecane	13.84	3.3	ng	114517	5	14.01	691482	20.0
unknown14.37	14.37	4.2	ng	146002	5	14.01	691482	20.0
unknown16.16	16.16	3.8	ng	130165	6	15.48	678507	20.0
unknown16.59	16.59	2.2	ng	73467	6	15.48	678507	20.0