LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083017\
Data File : BF098175.D
Acq On : 31 Aug 2017 00:18
Operator : SJ/JU
Sample : I5008-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-082817-B

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-BF081517.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	3.681	264	271	278	rBV	113391	170211	15.19%	1.233%
2	4.904	476	479	487	rBV	34883	39801	3.55%	0.288%
3	5.322	546	550	562	rBV	619968	566217	50.54%	4.100%
4	6.357	722	726	737	rBV	625030	622049	55.53%	4.505%
5	6.486	745	748	752	rBV	636908	596017	53.20%	4.316%
6	6.722	785	788	792	rBV	820487	725063	64.72%	5.251%
7	6.881	811	815	821	rBV	509358	461685	41.21%	3.343%
8	7.286	880	884	896	rBV	376269	357908	31.95%	2.592%
9	8.010	1002	1007	1014	rBV	1005572	915096	81.69%	6.627%
10	9.080	1185	1189	1194	rBV	759060	640506	57.18%	4.638%
11	9.169	1200	1204	1208	rBV2	23884	26844	2.40%	0.194%
12	9.351	1233	1235	1240	rVB2	38985	30927	2.76%	0.224%
13	9.480	1253	1257	1260	rBV2	96202	113428	10.13%	0.821%
14	9.510	1260	1262	1265	rVB4	16229	17619	1.57%	0.128%
15	9.622	1278	1281	1285	rBV3	12541	17134	1.53%	0.124%
16	9.669	1286	1289	1291	rVV3	18828	22254	1.99%	0.161%
17	9.698	1291	1294	1298	rVV	46434	50044	4.47%	0.362%
18	9.757	1298	1304	1308	rVV	925050	865055	77.22%	6.264%
19	9.816	1312	1314	1320	rVB6	16334	26149	2.33%	0.189%
20	9.927	1330	1333	1335	rBV3	13648	20032	1.79%	0.145%
21	10.016	1344	1348	1351	rBV3	29896	36386	3.25%	0.263%
22	10.192	1375	1378	1381	rBV	84465	63512	5.67%	0.460%
23	10.304	1394	1397	1399	rBV4	17938	23859	2.13%	0.173%
24	10.416	1410	1416	1419	rBV	59829	86340	7.71%	0.625%
25	10.463	1421	1424	1427	rVB3	16252	19342	1.73%	0.140%
26	10.498	1427	1430	1433	rBV4	19189	22565	2.01%	0.163%
27	10.545	1433	1438	1441	rBV	277966	266749	23.81%	1.932%
28	10.669	1455	1459	1467	rVB	117258	179336	16.01%	1.299%
29	10.792	1478	1480	1487	rVB6	14567	23277	2.08%	0.169%
30	11.116	1531	1535	1537	rBV	102267	100958	9.01%	0.731%
31	11.139	1537	1539	1545	rVB	79445	87758	7.83%	0.635%
32	11.239	1552	1556	1559	rBV	855765	742778	66.30%	5.379%
33	11.263	1559	1560	1563	rVV	84254	51794	4.62%	0.375%
34	11.316	1567	1569	1573	rVB	31045	29818	2.66%	0.216%

LSC Area Percent Report

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Acq On : 31 Aug 2017 00:18
Operator : SJ/JU
Sample : I5008-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-082817-B

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.492	1597	1599	1602	rVB3	22811	20674	1.85%	0.150%
36	11.539	1604	1607	1610	rVB	100253	73319	6.54%	0.531%
37	11.639	1621	1624	1630	rVB	549891	431314	38.50%	3.123%
38	11.768	1644	1646	1649	rVB2	17113	16403	1.46%	0.119%
39	11.851	1658	1660	1664	rVB	24013	21314	1.90%	0.154%
40	11.945	1673	1676	1680	rBV	85833	64172	5.73%	0.465%
41	12.286	1731	1734	1737	rBV2	22122	22860	2.04%	0.166%
42	12.321	1737	1740	1742	rBV	1142020	1104497	98.59%	7.998%
43	12.345	1742	1744	1747	rVB	1474796	1120246	100.00%	8.112%
44	12.427	1755	1758	1760	rBV	285419	255334	22.79%	1.849%
45	12.445	1760	1761	1764	rVB	145908	116812	10.43%	0.846%
46	12.674	1795	1800	1803	rBV	168187	197103	17.59%	1.427%
47	12.704	1803	1805	1808	rVB	64224	53269	4.76%	0.386%
48	12.821	1821	1825	1831	rBV	578937	483442	43.15%	3.501%
49	12.933	1842	1844	1847	rVB2	35262	27734	2.48%	0.201%
50	12.986	1850	1853	1854	rBV3	42238	37316	3.33%	0.270%
51	13.062	1863	1866	1871	rVB2	54414	88589	7.91%	0.642%
52	13.151	1879	1881	1885	rBV	33118	35802	3.20%	0.259%
53	13.262	1898	1900	1904	rBV4	25039	30419	2.72%	0.220%
54	13.310	1906	1908	1912	rVB4	30189	37788	3.37%	0.274%
55	13.404	1921	1924	1926	rBV2	46070	42973	3.84%	0.311%
56	13.580	1950	1954	1957	rVB4	43440	53971	4.82%	0.391%
57	13.727	1976	1979	1984	rBV2	75467	81416	7.27%	0.590%
58	13.821	1992	1995	1997	rBV2	38889	45421	4.05%	0.329%
59	13.874	1999	2004	2006	rVV	751341	774751	69.16%	5.610%
60	13.898	2006	2008	2010	rVB	66202	52548	4.69%	0.381%
61	15.286	2240	2244	2248	rBV	401481	501297	44.75%	3.630%

Sum of corrected areas: 13809295

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083017\
Data File : BF098175.D
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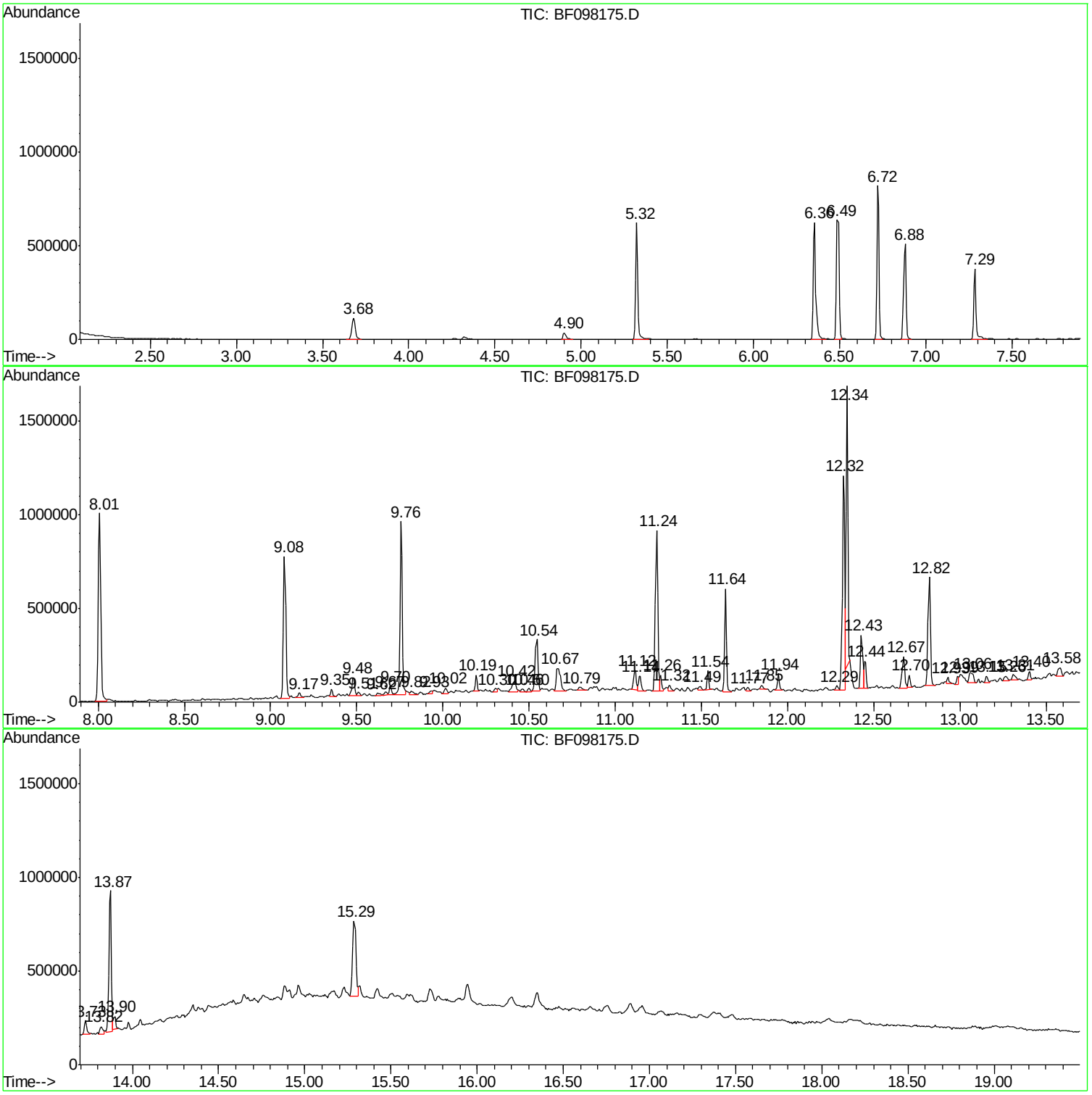
Operator : SJ/JU
Sample : I5008-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-082817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083017\
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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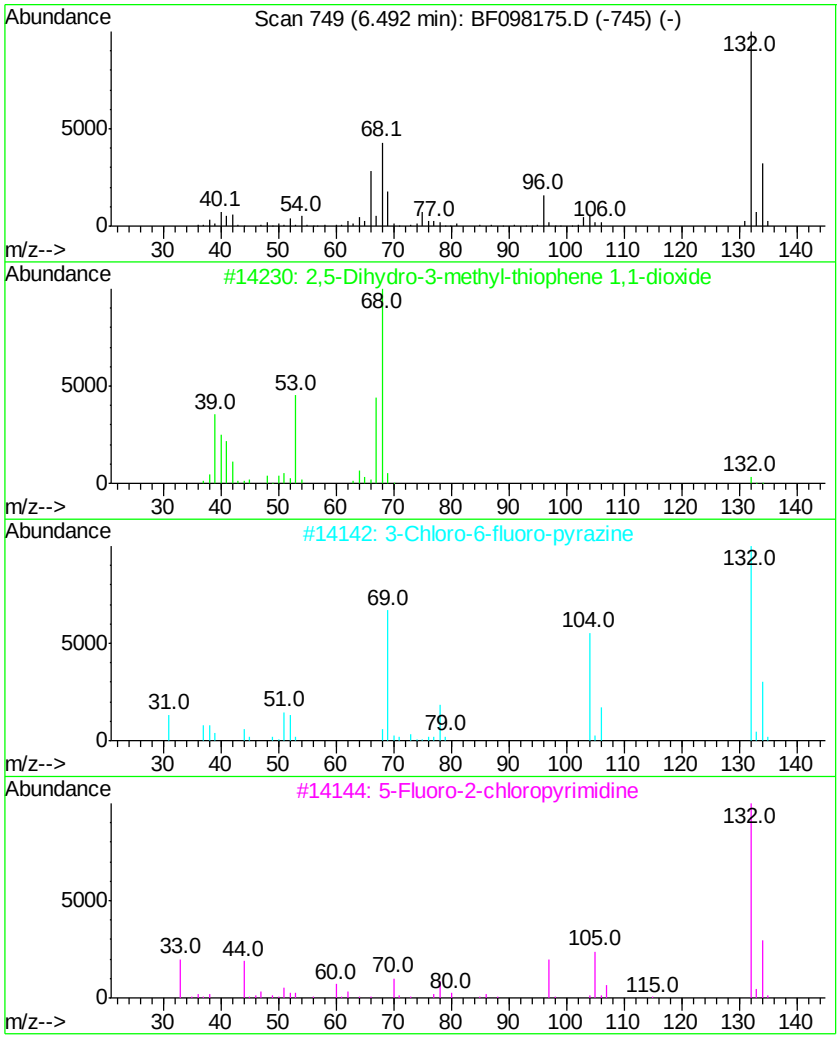
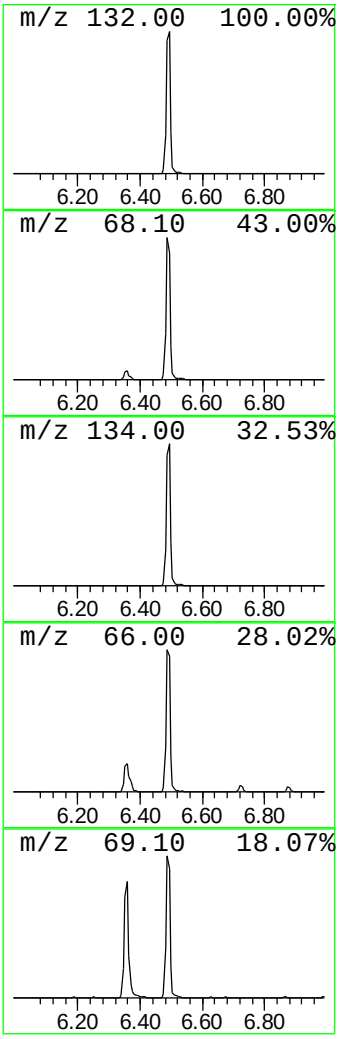
Peak Number 2 unknown6.49 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	16.44 ng	596017	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF083017\
Data File : BF098175.D
Acq On : 31 Aug 2017 00:18
Operator : SJ/JU
Sample : I5008-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-082817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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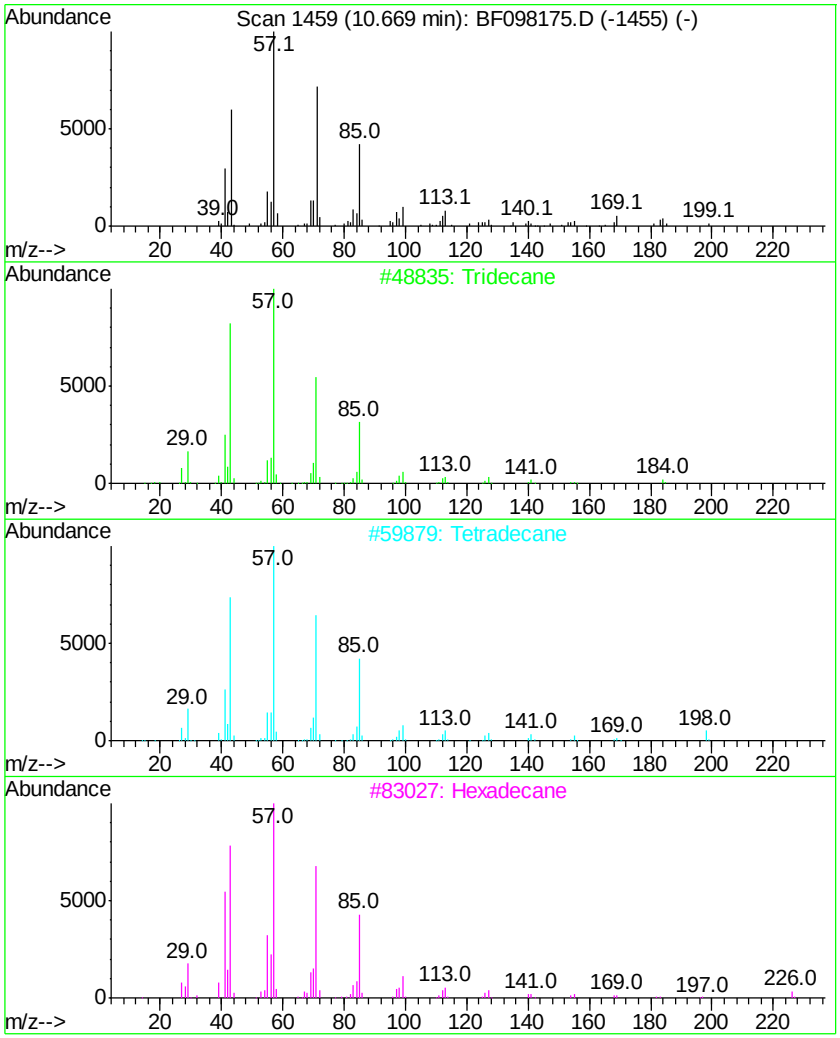
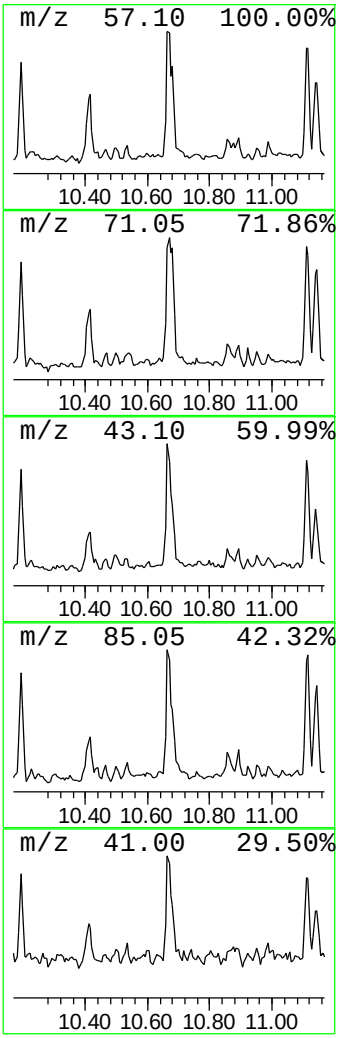
Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	4.83 ng	179336	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
5	Octacosane	394	C28H58	000630-02-4	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF083017\
Data File : BF098175.D
Acq On : 31 Aug 2017 00:18
Operator : SJ/JU
Sample : I5008-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-082817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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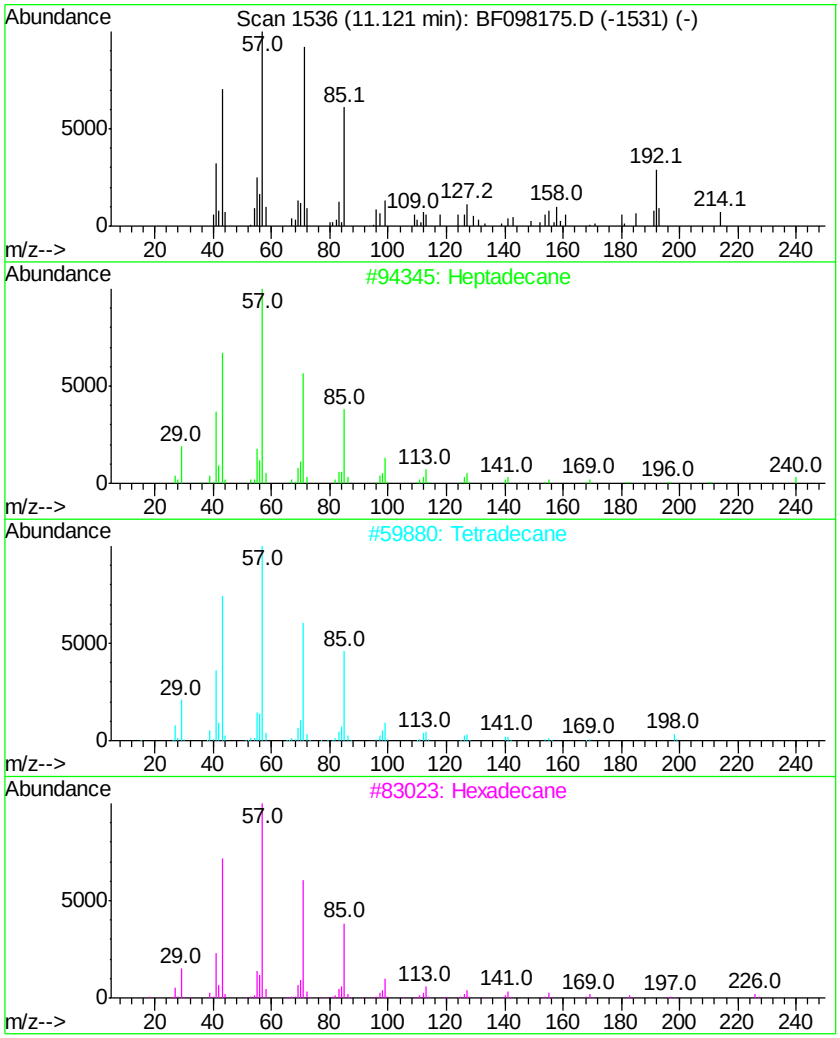
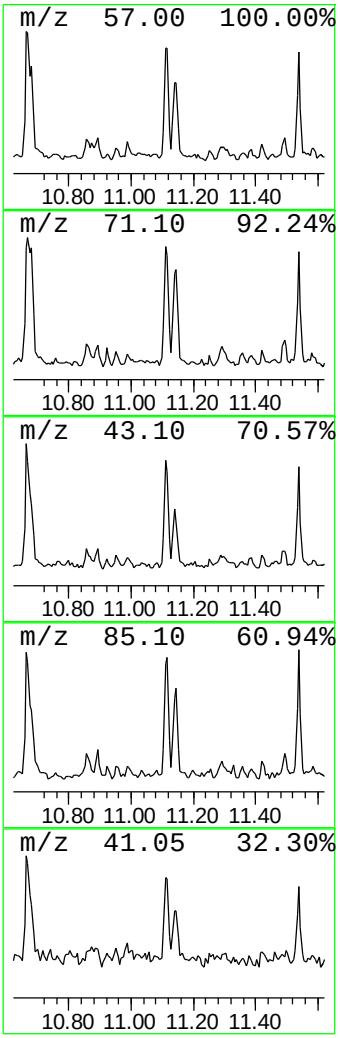
Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.12	2.72 ng	100958	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Heneicosane	296	C21H44	000629-94-7	64
5	Eicosane	282	C20H42	000112-95-8	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF083017\
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Sample : I5008-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-082817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

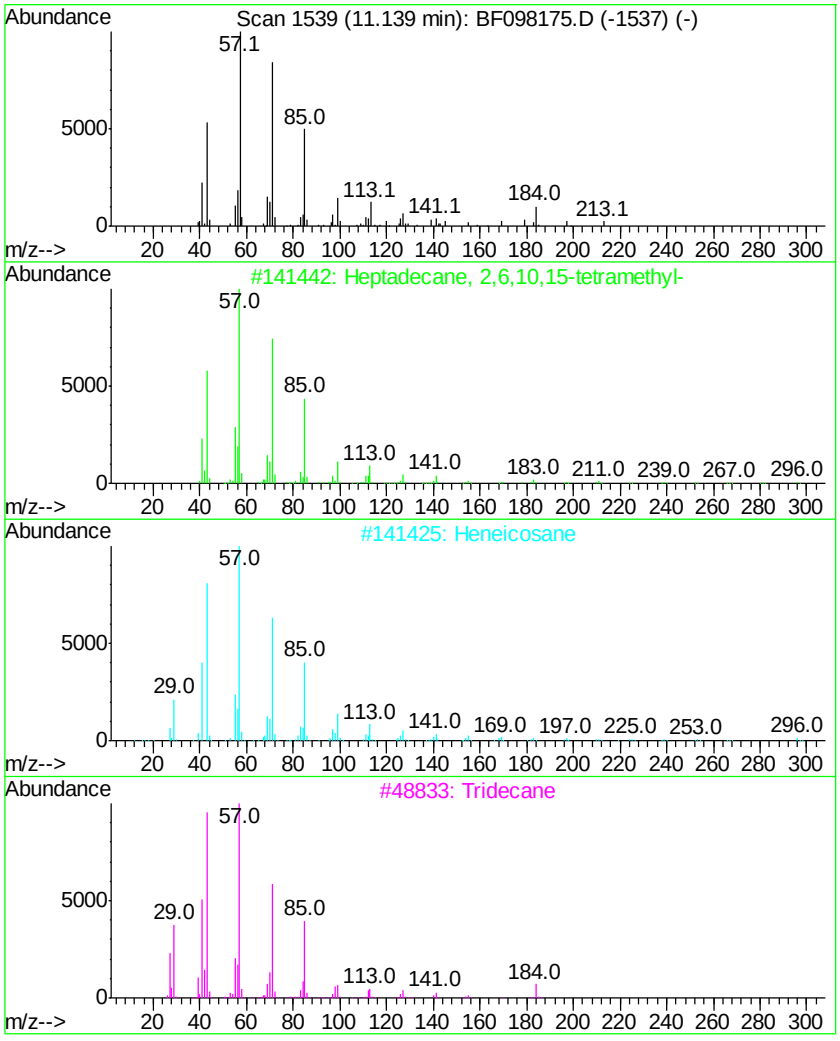
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

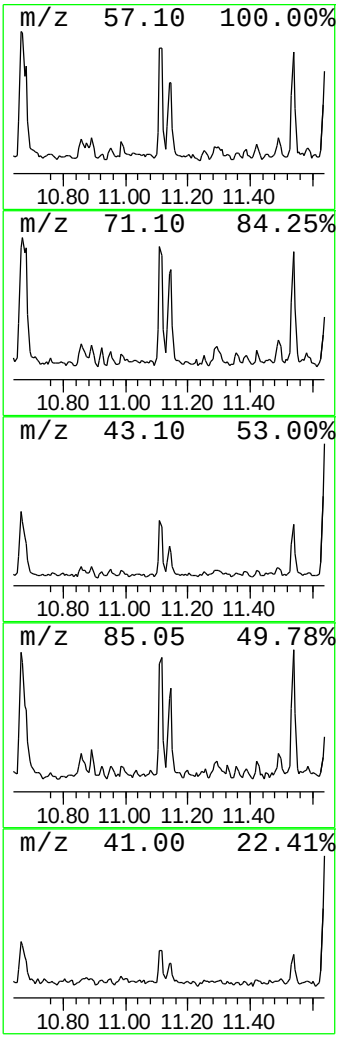
****

Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	2.36 ng	87758	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tridecane	184	C13H28	000629-50-5	87
4	Octacosane	394	C28H58	000630-02-4	86
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





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Misc :
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Instrument : BNA_F
ClientSampleId : NB-08-082817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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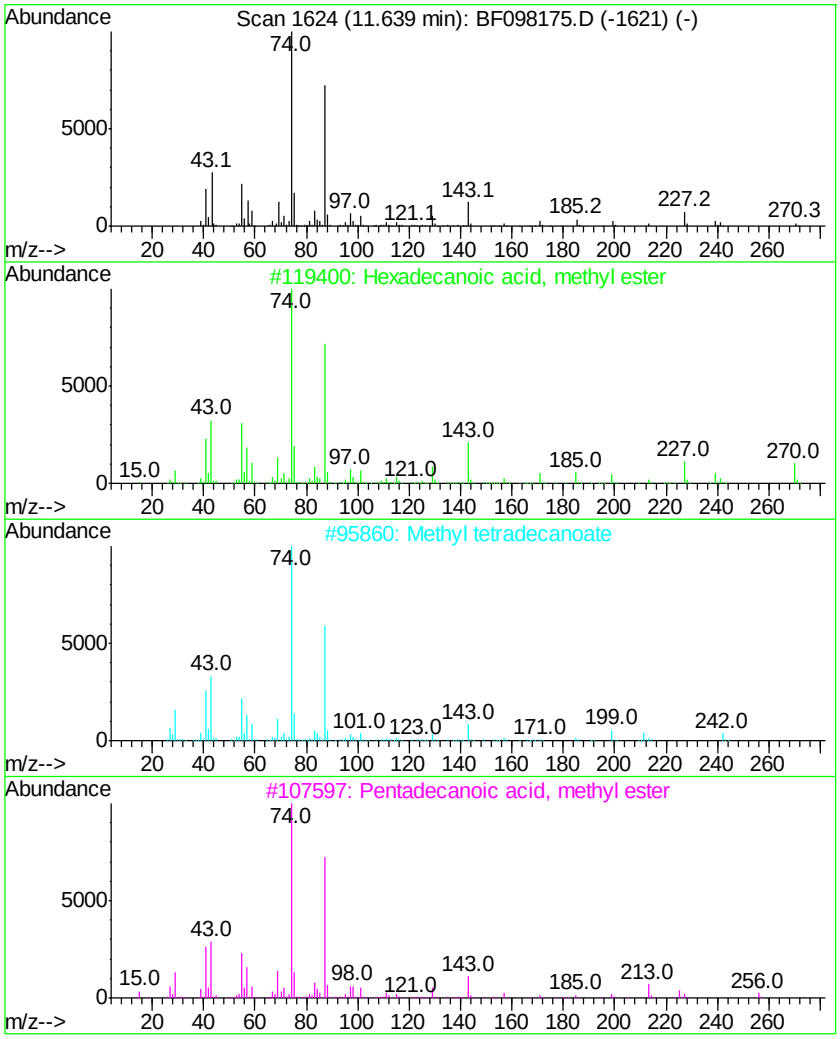
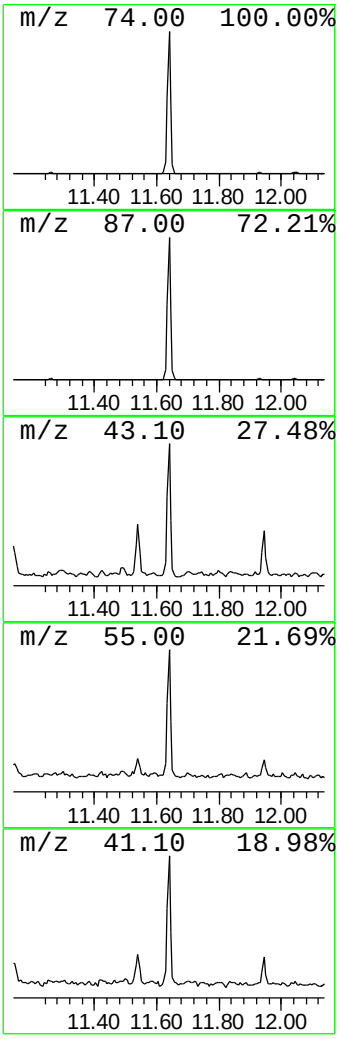
Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.64	11.61 ng	431314	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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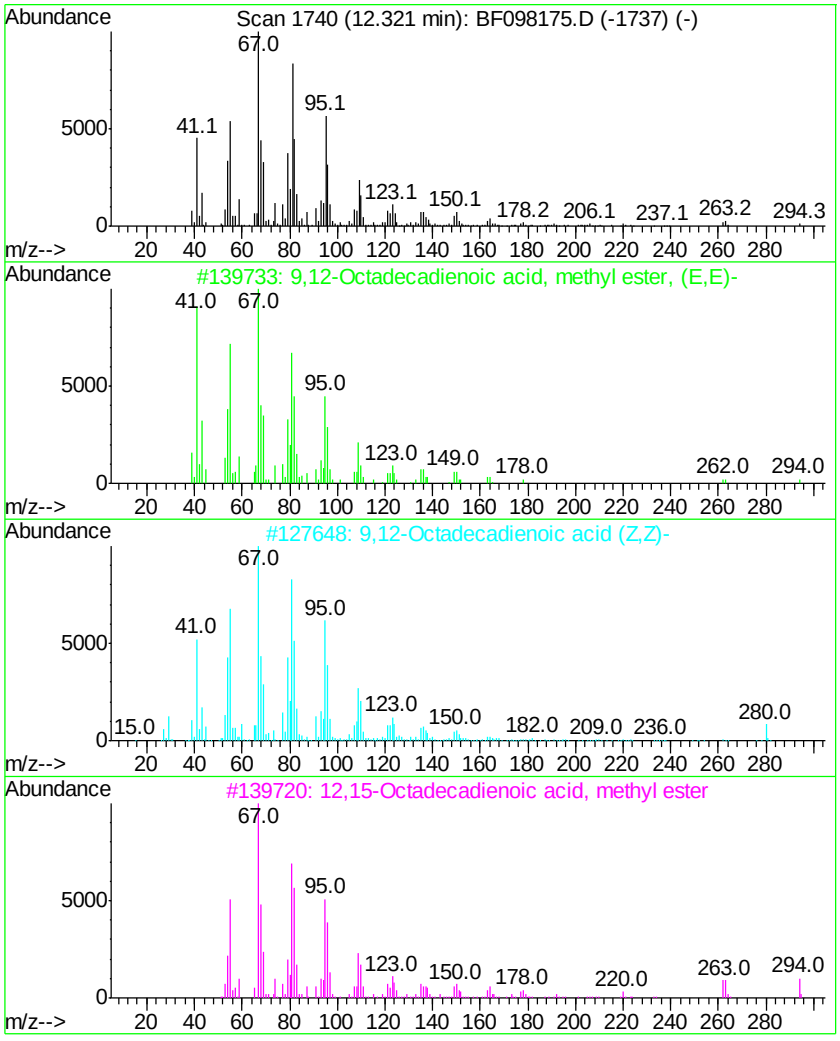
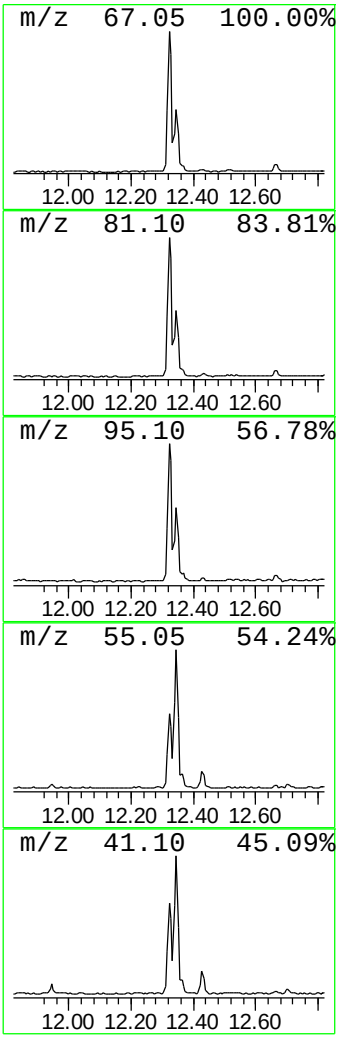
Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	29.74 ng	1104500	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	95
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
3	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	93
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	90
5	7-Hexadecyne	222	C16H30	074685-28-2	80





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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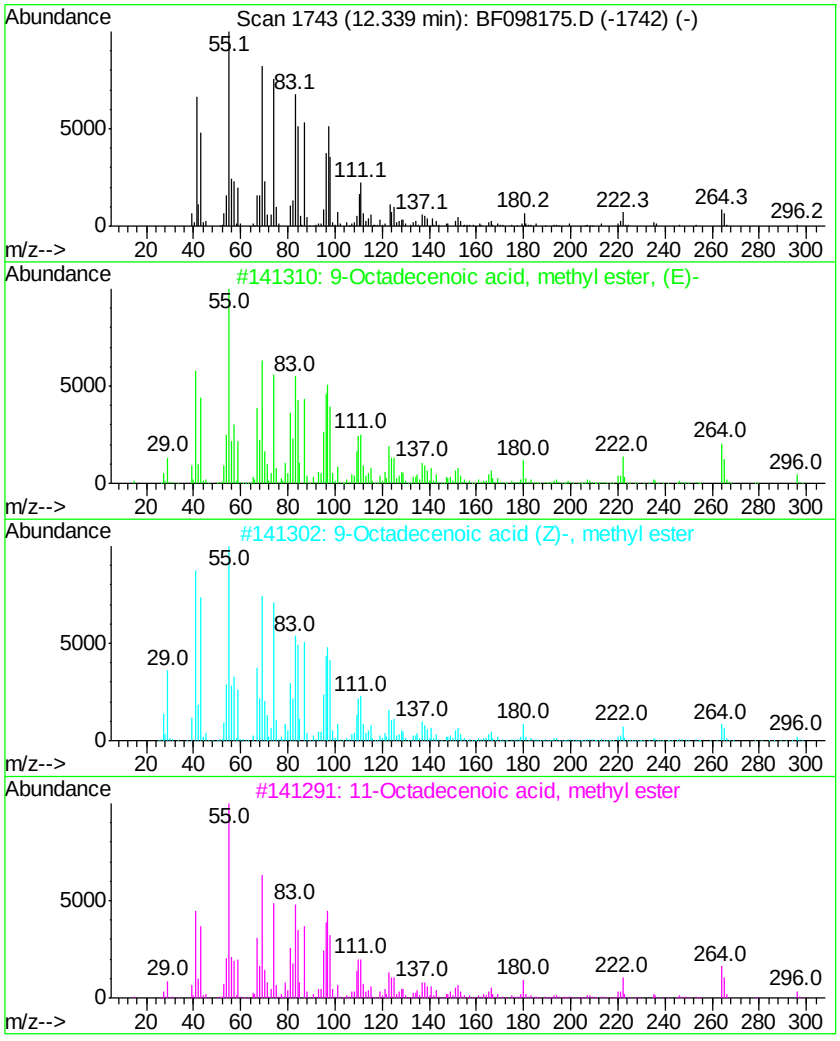
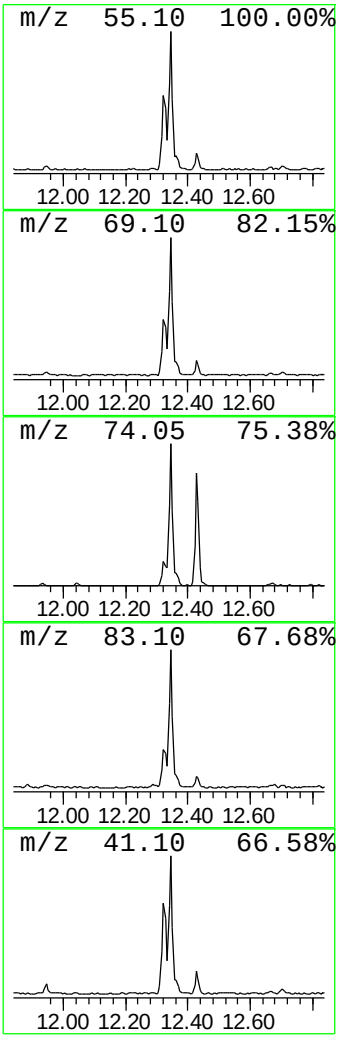
Peak Number 9 9-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	30.16 ng	1120250	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	95
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	89
4	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	86
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	81





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083017\
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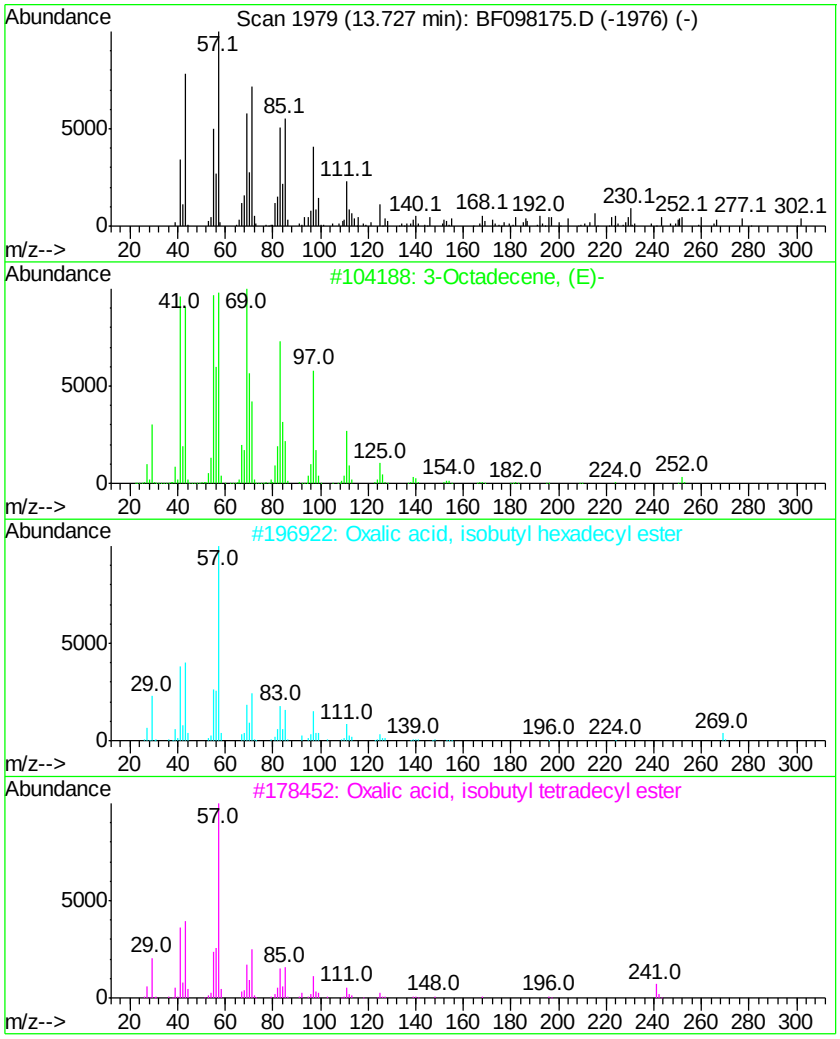
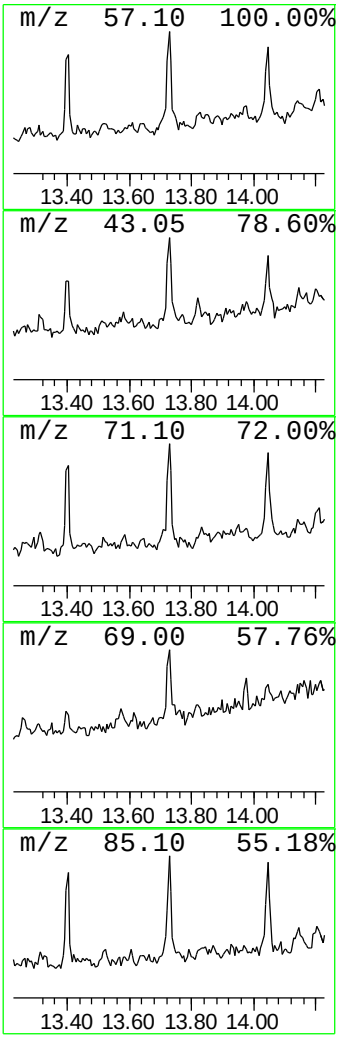
Peak Number 11 3-Octadecene, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.10 ng	81416	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	90
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	83
3	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	83
4	Cyclohexadecane	224	C16H32	000295-65-8	80
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF083017\
Data File : BF098175.D
Acq On : 31 Aug 2017 00:18
Operator : SJ/JU
Sample : I5008-04 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-082817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
unknown6.49	6.49	16.4	ng	596017	1	6.72	725063	20.0
Tridecane	10.67	4.8	ng	179336	4	11.24	742778	20.0
Heptadecane	11.12	2.7	ng	100958	4	11.24	742778	20.0
Heptadecane, 2,6,...	11.14	2.4	ng	87758	4	11.24	742778	20.0
Hexadecanoic acid...	11.64	11.6	ng	431314	4	11.24	742778	20.0
9,12-Octadecadien...	12.32	29.7	ng	1104500	4	11.24	742778	20.0
9-Octadecenoic ac...	12.34	30.2	ng	1120250	4	11.24	742778	20.0
3-Octadecene, (E)-	13.73	2.1	ng	81416	5	13.87	774751	20.0