LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070117\
Data File : BF096380.D
Acq On : 1 Jul 2017 15:50
Operator : SJ/MA
Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

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-BF070117.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	4.922	476	482	494	rBV	297829	396500	12.46%	0.909%
2	5.345	549	554	568	rBV	2423330	2691719	84.62%	6.169%
3	6.369	723	728	731	rBV	2989651	3181020	100.00%	7.290%
4	6.504	746	751	754	rBV	3134033	3025696	95.12%	6.934%
5	6.734	786	790	793	rBV	2041912	1685363	52.98%	3.863%
6	6.886	812	816	820	rVB	2047850	1947668	61.23%	4.464%
7	7.292	880	885	888	rBV	2036509	1955850	61.48%	4.483%
8	7.422	904	907	910	rVB2	45171	46215	1.45%	0.106%
9	7.757	959	964	969	rBV2	75785	97323	3.06%	0.223%
10	8.016	1003	1008	1011	rBV	2567562	2306570	72.51%	5.286%
11	9.092	1186	1191	1194	rBV	2603145	2436787	76.60%	5.585%
12	9.186	1201	1207	1209	rBV3	38774	46231	1.45%	0.106%
13	9.480	1254	1257	1260	rBV	531923	443906	13.95%	1.017%
14	9.504	1260	1261	1269	rVB5	33761	46493	1.46%	0.107%
15	9.710	1293	1296	1301	rVB	105820	102416	3.22%	0.235%
16	9.769	1301	1306	1309	rVB	2332254	2184229	68.66%	5.006%
17	9.857	1317	1321	1329	rVB10	25232	73514	2.31%	0.168%
18	9.980	1332	1342	1345	rVV3	91389	205075	6.45%	0.470%
19	10.033	1349	1351	1355	rVB3	33449	38819	1.22%	0.089%
20	10.174	1371	1375	1379	rBV2	37320	62150	1.95%	0.142%
21	10.210	1379	1381	1384	rVB	91011	65875	2.07%	0.151%
22	10.433	1414	1419	1421	rBV2	46660	66461	2.09%	0.152%
23	10.551	1434	1439	1442	rBV	1718211	1556618	48.93%	3.568%
24	10.651	1452	1456	1459	rBV	111813	122313	3.85%	0.280%
25	10.680	1459	1461	1470	rVB2	118969	187031	5.88%	0.429%
26	10.886	1493	1496	1501	rBV	130224	161133	5.07%	0.369%
27	11.127	1534	1537	1540	rBV3	55157	54867	1.72%	0.126%
28	11.245	1548	1557	1560	rBV	2153874	2050049	64.45%	4.698%
29	11.269	1560	1561	1564	rVV	152253	75558	2.38%	0.173%
30	11.469	1593	1595	1600	rVB3	28952	35884	1.13%	0.082%
31	11.663	1622	1628	1639	rBV2	590944	1734120	54.51%	3.974%
32	11.786	1643	1649	1658	rVB2	763922	1481771	46.58%	3.396%
33	11.916	1667	1671	1673	rBV2	165143	235434	7.40%	0.540%
34	11.945	1673	1676	1688	rVB	281942	467483	14.70%	1.071%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.298	1732	1736	1741	rBV5	62528	93723	2.95%	0.215%
36	12.368	1745	1748	1751	rVB	65896	67935	2.14%	0.156%
37	12.451	1752	1762	1764	rBV2	291481	552316	17.36%	1.266%
38	12.521	1768	1774	1778	rVV	1243672	2816674	88.55%	6.455%
39	12.563	1778	1781	1792	rVV	1744677	2620371	82.38%	6.006%
40	12.674	1795	1800	1804	rVB2	178863	266822	8.39%	0.612%
41	12.827	1822	1826	1829	rBV	1966023	1758309	55.28%	4.030%
42	13.045	1859	1863	1866	rBV4	37855	73715	2.32%	0.169%
43	13.274	1899	1902	1904	rBV4	36660	53634	1.69%	0.123%
44	13.374	1913	1919	1925	rBV3	169130	273937	8.61%	0.628%
45	13.727	1975	1979	1983	rBV2	223687	250338	7.87%	0.574%
46	13.874	1998	2004	2006	rBV	1313554	1431397	45.00%	3.281%
47	13.892	2006	2007	2012	rVB	67751	52850	1.66%	0.121%
48	14.498	2107	2110	2115	rBV	190902	192413	6.05%	0.441%
49	14.615	2127	2130	2134	rBV	355878	342014	10.75%	0.784%
50	14.874	2172	2174	2177	rBV	50700	60576	1.90%	0.139%
51	15.286	2238	2244	2248	rBV	1080371	1321312	41.54%	3.028%
52	16.104	2379	2383	2389	rVB7	74802	136367	4.29%	0.313%

Sum of corrected areas: 43632844

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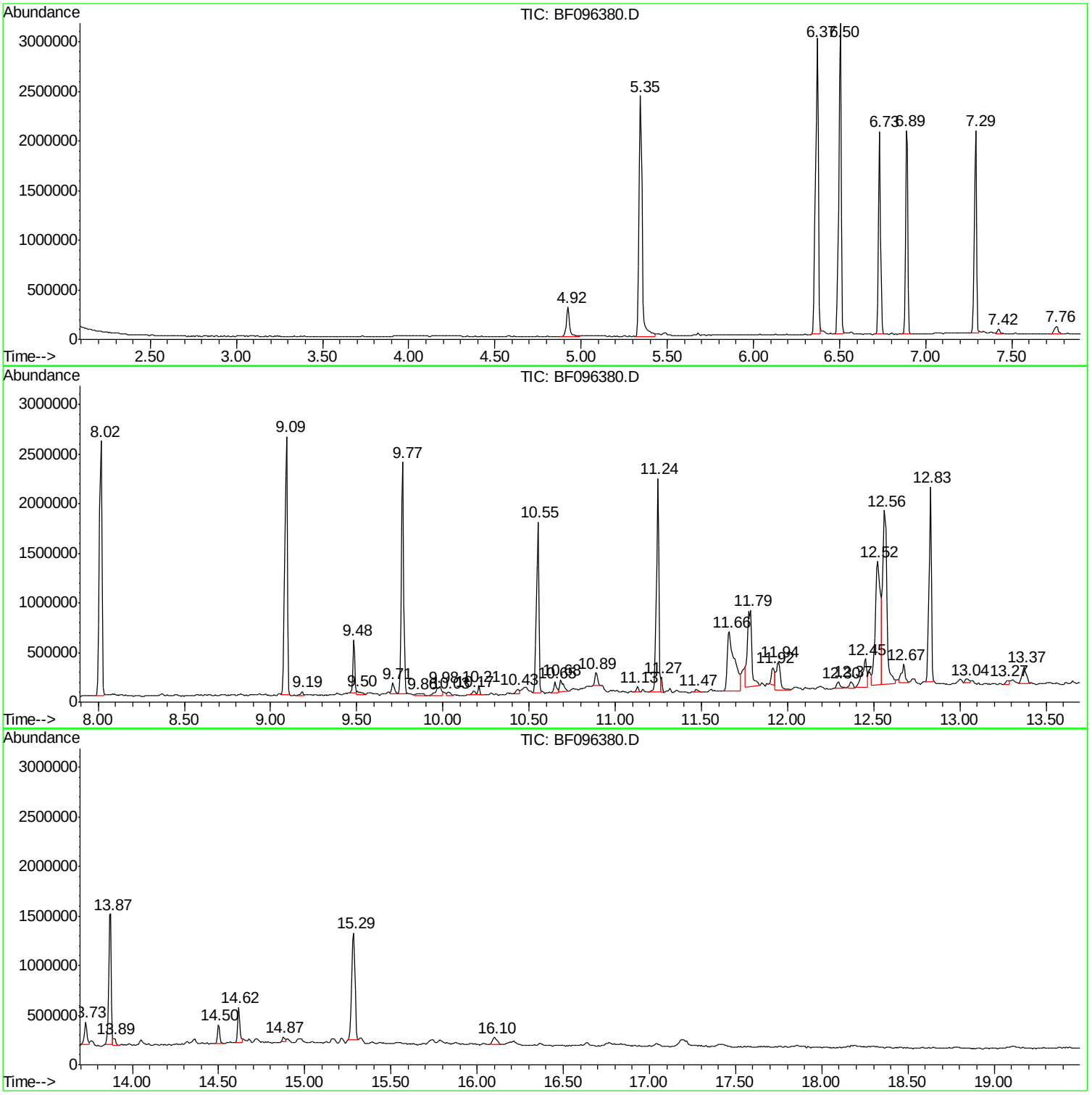
Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF070117\
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Operator : SJ/MA
Sample : I3947-01
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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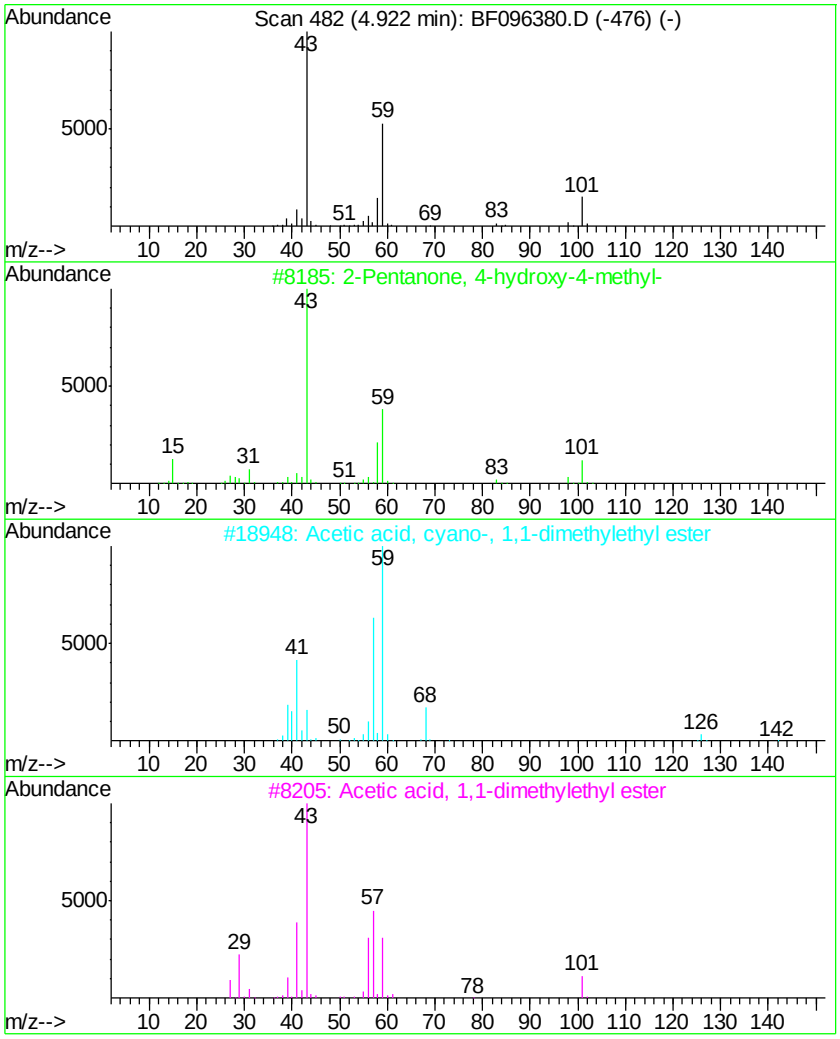
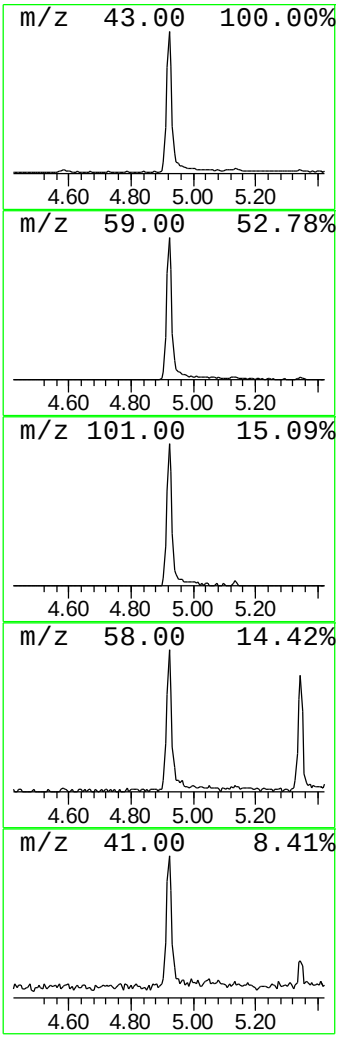
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	4.71 ng	396500	1,4-Dichlorobenzene-d4	6.73

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	25
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Operator : SJ/MA
Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

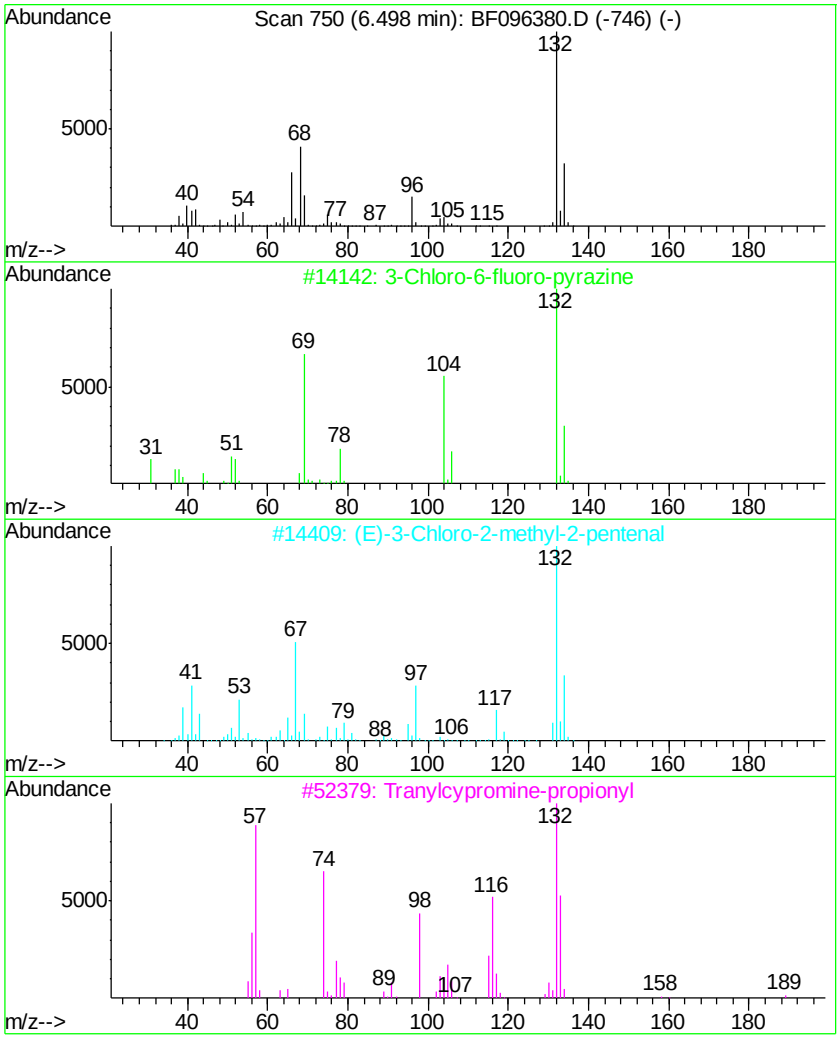
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

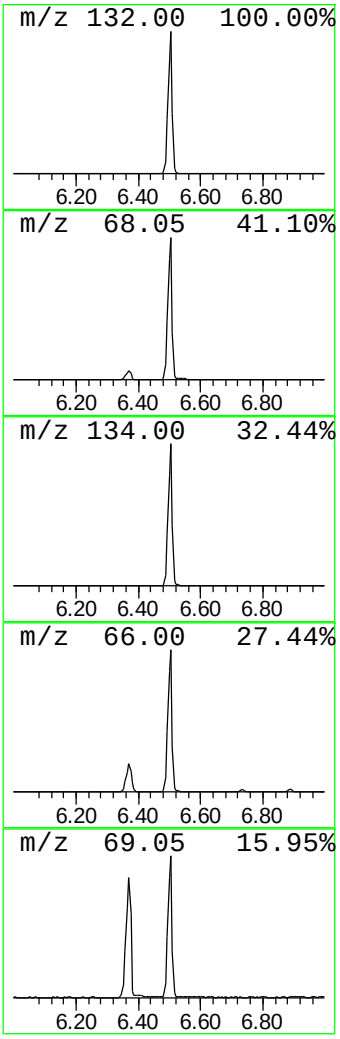
****

Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	35.91 ng	3025700	1,4-Dichlorobenzene-d4	6.73

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070117\
Data File : BF096380.D
Acq On : 1 Jul 2017 15:50
Operator : SJ/MA
Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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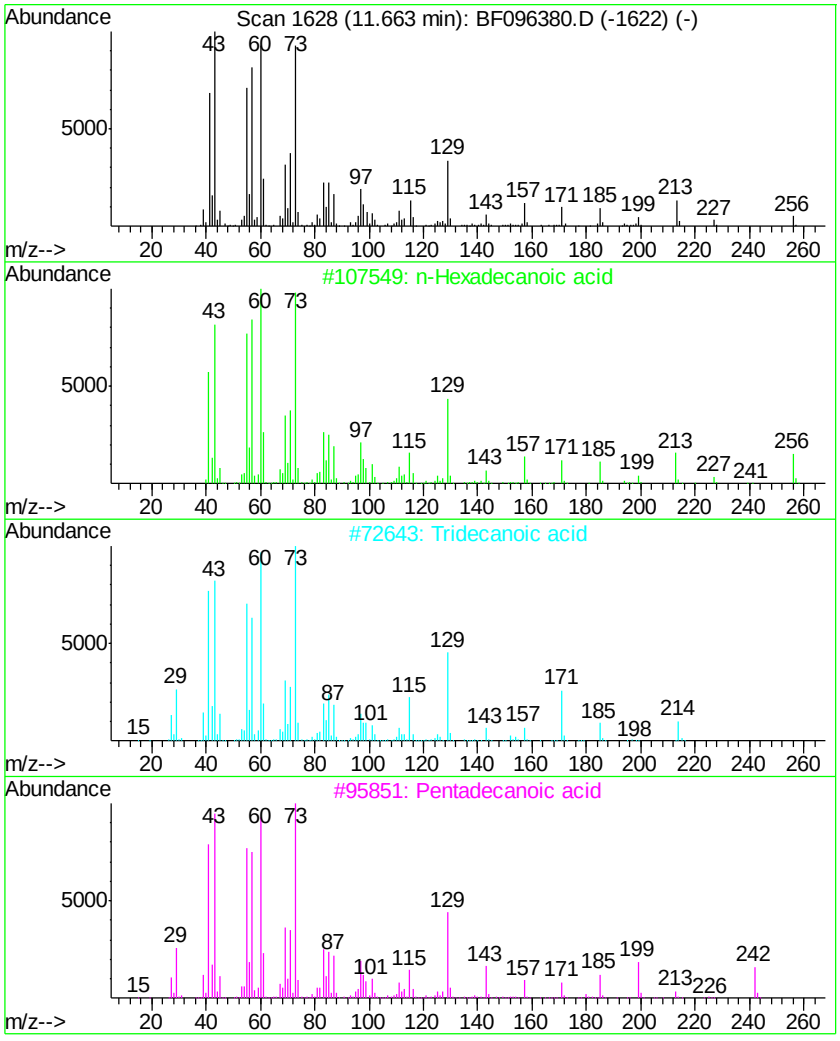
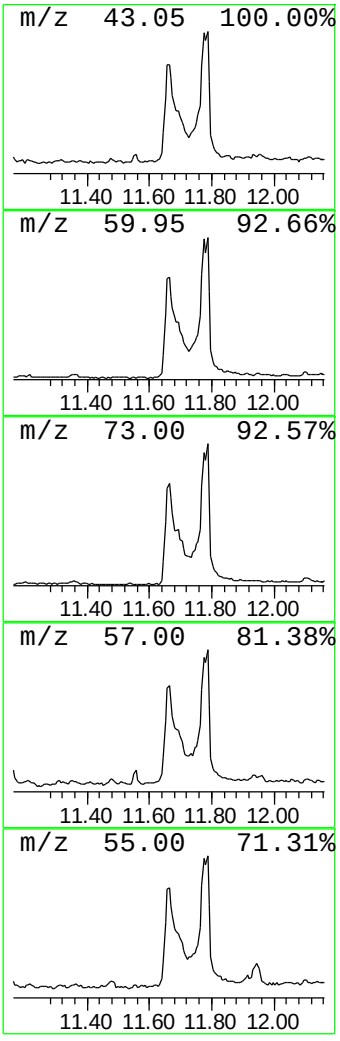
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	16.92 ng	1734120	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





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Data File : BF096380.D
Acq On : 1 Jul 2017 15:50
Operator : SJ/MA
Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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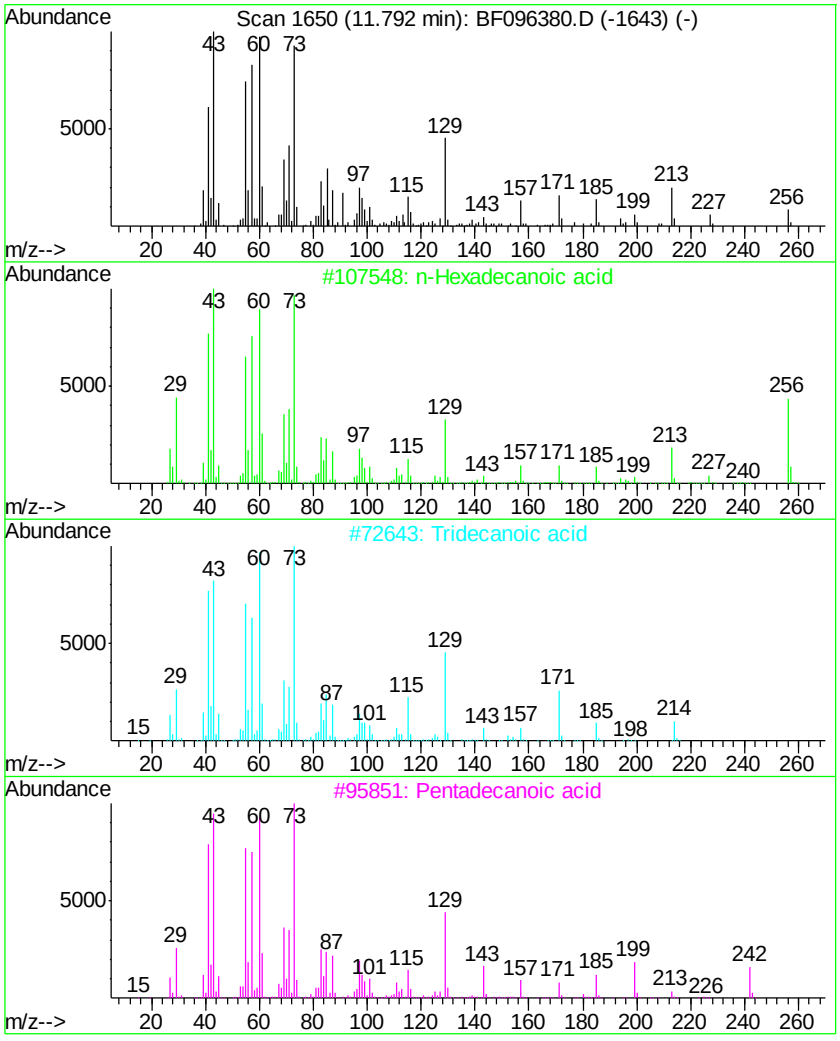
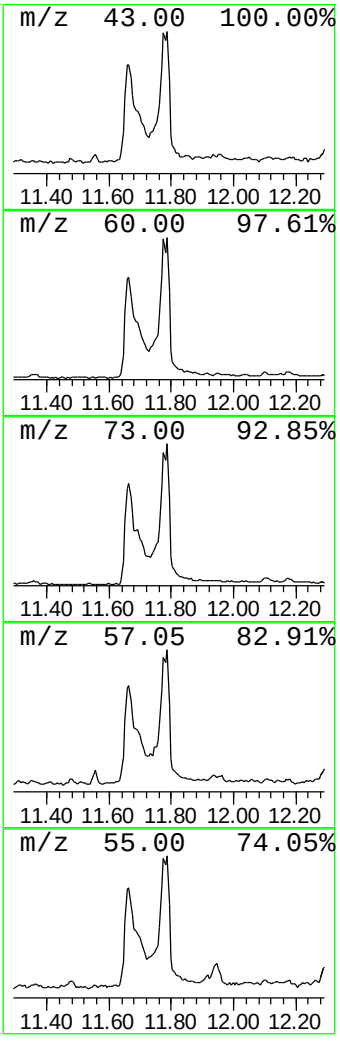
Peak Number 5 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	14.46 ng	1481770	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Sample : I3947-01
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Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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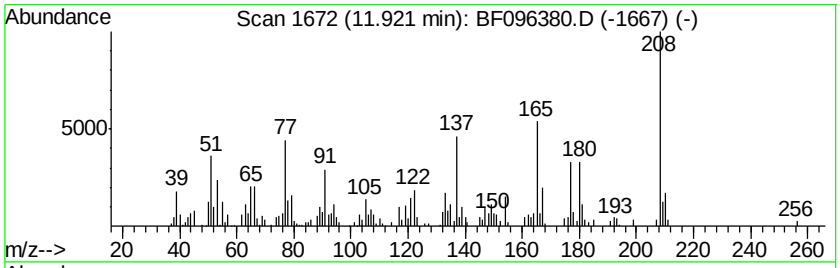
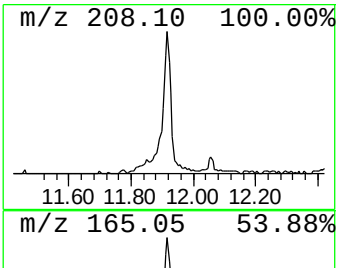
Peak Number 6 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.30 ng	235434	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	91
2	9H-Fluorene, 9-propyl-	208	C16H16	004037-45-0	49
3	Benzene, 1,2,4-trimethoxy-5-(1-p...	208	C12H16O3	000494-40-6	46
4	2-Propenoic acid, 3-(2,3-dimetho...	208	C11H12O4	007345-82-6	46
5	Phenanthrene, 9-methoxy-	208	C15H12O	005085-74-5	43





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Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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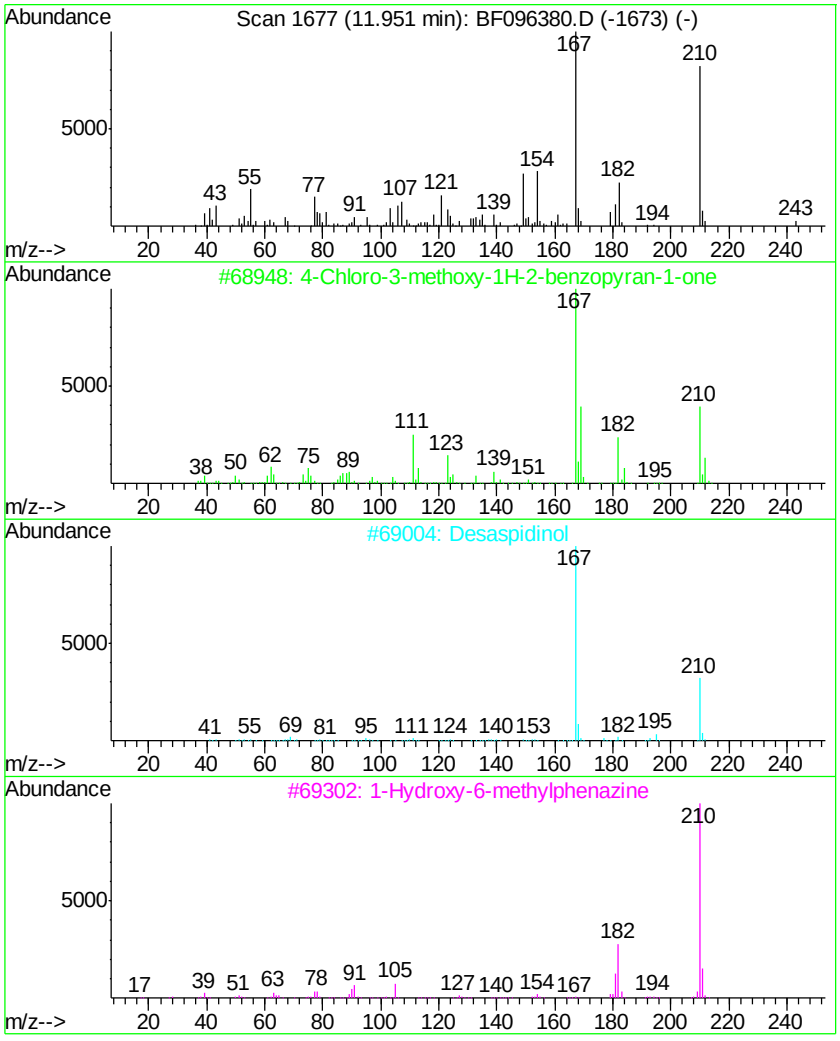
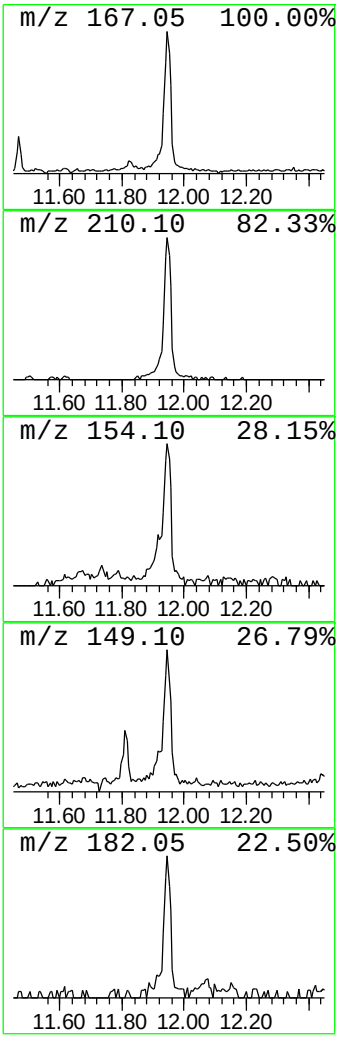
Peak Number 7 4-Chloro-3-methoxy-1H-2-ben... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	4.56 ng	467483	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-3-methoxy-1H-2-benzopyr...	210	C10H7ClO3	024672-89-7	59
2	Desaspidinol	210	C11H14O4	000437-72-9	50
3	1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	38
4	9-Methyl-1-phenazinol	210	C13H10N2O	013860-43-0	38
5	6-Methoxy-4-piperidin-1-yl-1H-[1...	210	C9H14N4O2	1000300-24-3	38





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Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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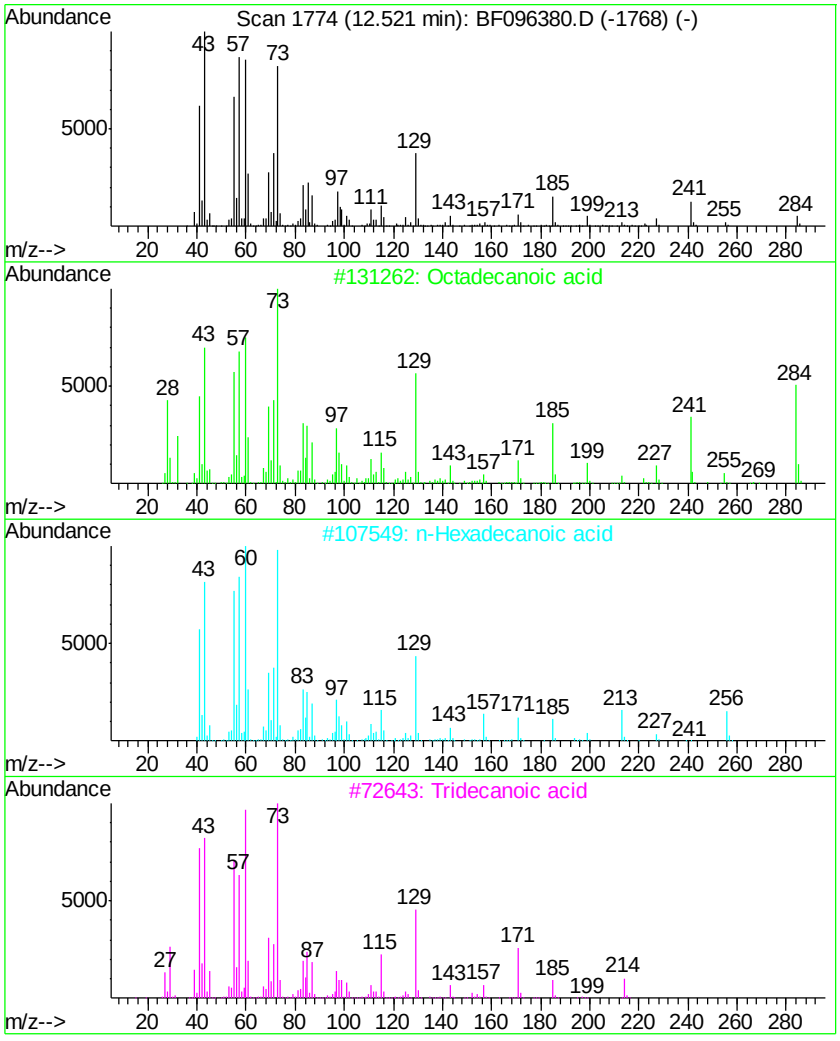
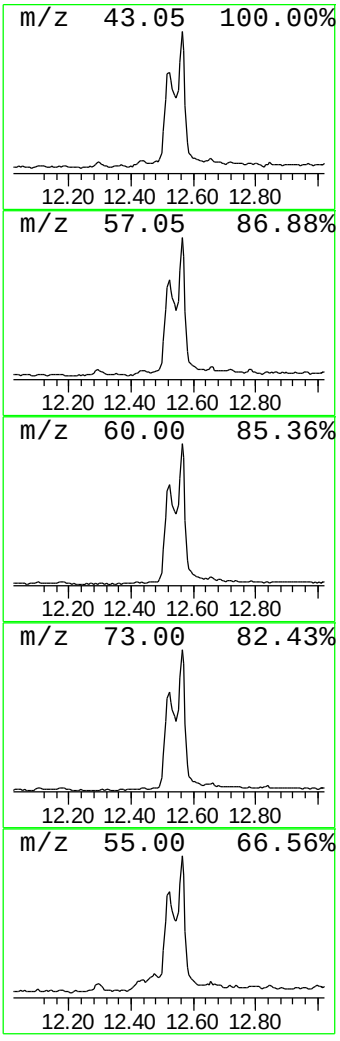
Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	27.48 ng	2816670	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070117\
Data File : BF096380.D
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Operator : SJ/MA
Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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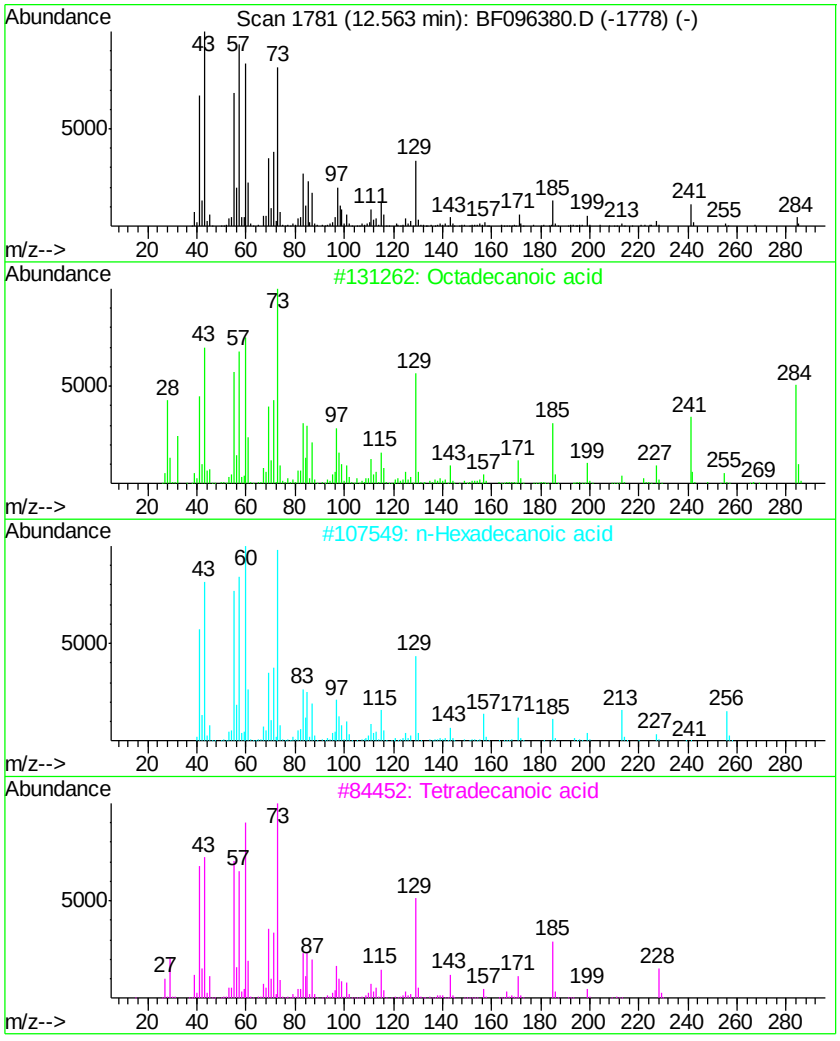
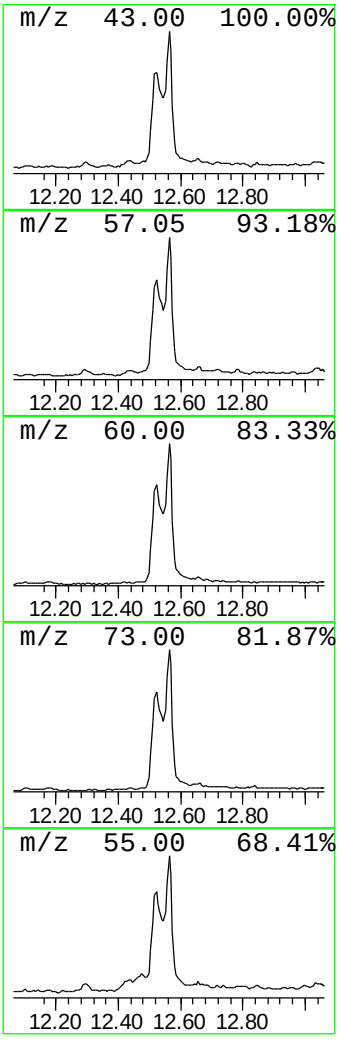
Peak Number 10 Tridecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	36.61 ng	2620370	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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Acq On : 1 Jul 2017 15:50
Operator : SJ/MA
Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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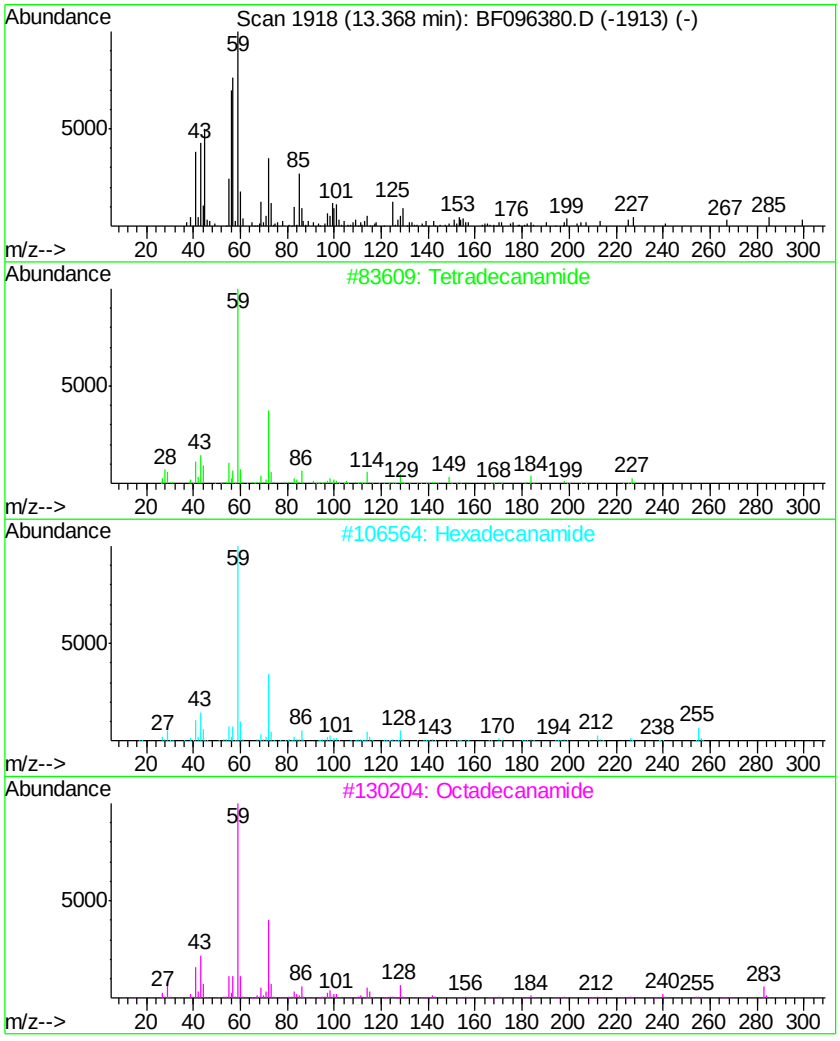
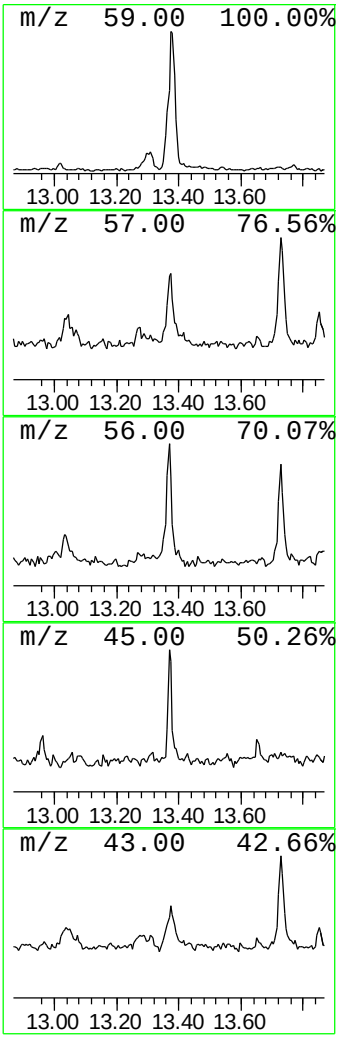
Peak Number 12 Tetradecanamide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	3.83 ng	273937	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	60
2	Hexadecanamide	255	C16H33NO	000629-54-9	60
3	Octadecanamide	283	C18H37NO	000124-26-5	52
4	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	50
5	Nonanamide	157	C9H19NO	001120-07-6	49





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Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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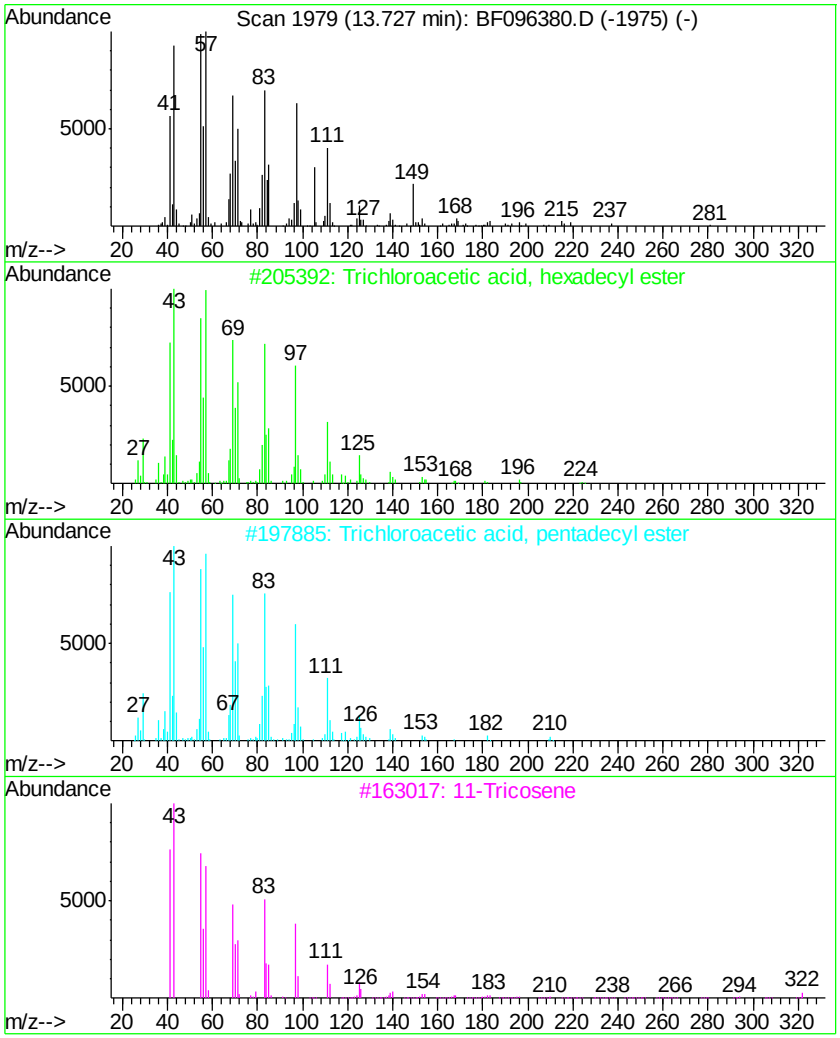
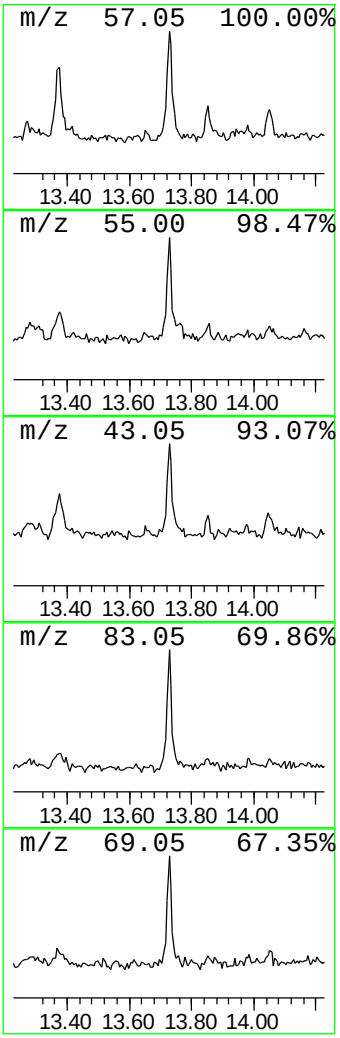
Peak Number 13 Trichloroacetic acid, hexad... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	3.50 ng	250338	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
3	11-Tricosene	322	C23H46	052078-56-5	83
4	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	83
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	83





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Acq On : 1 Jul 2017 15:50
Operator : SJ/MA
Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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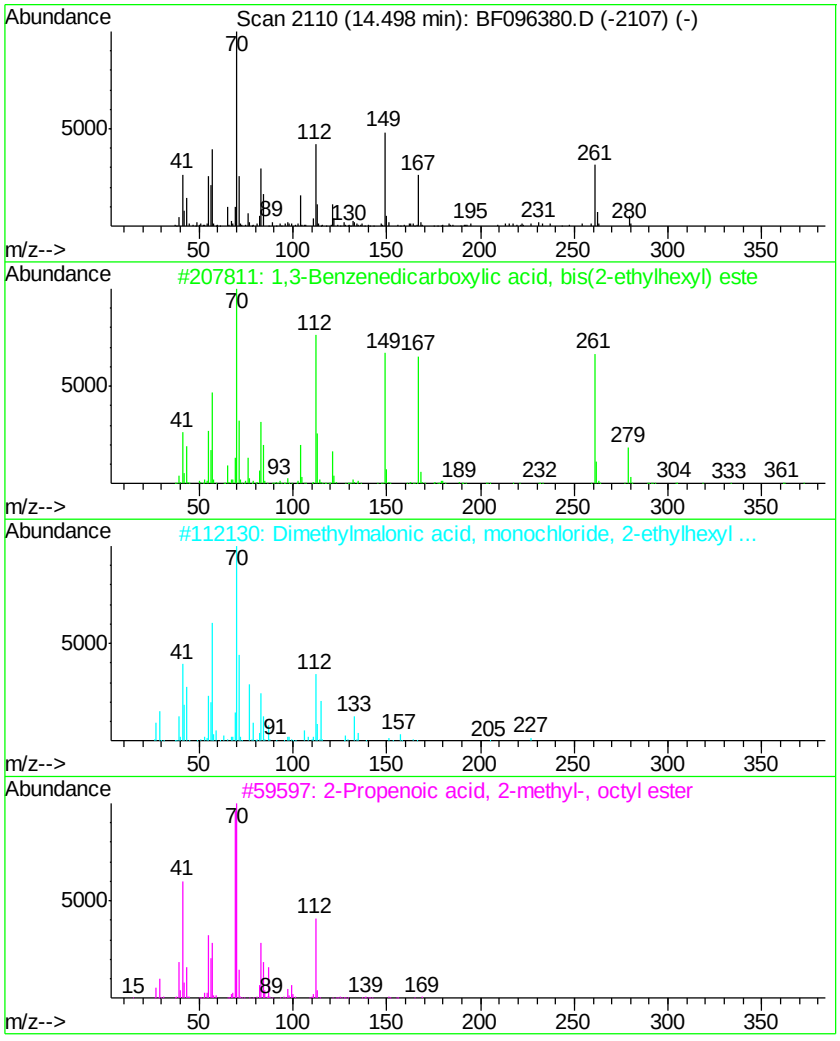
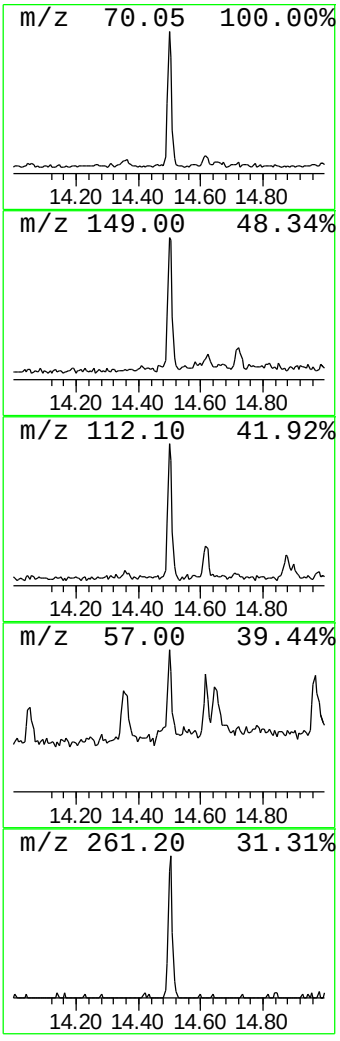
Peak Number 14 unknown14.50 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.69 ng	192413	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	43
2	Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	37
3	2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	32
4	Fumaric acid, ethyl 2-ethylhexyl...	256	C14H24O4	1000339-13-5	32
5	1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	25





Library Search Compound Report

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Acq On : 1 Jul 2017 15:50
Operator : SJ/MA
Sample : I3947-01
Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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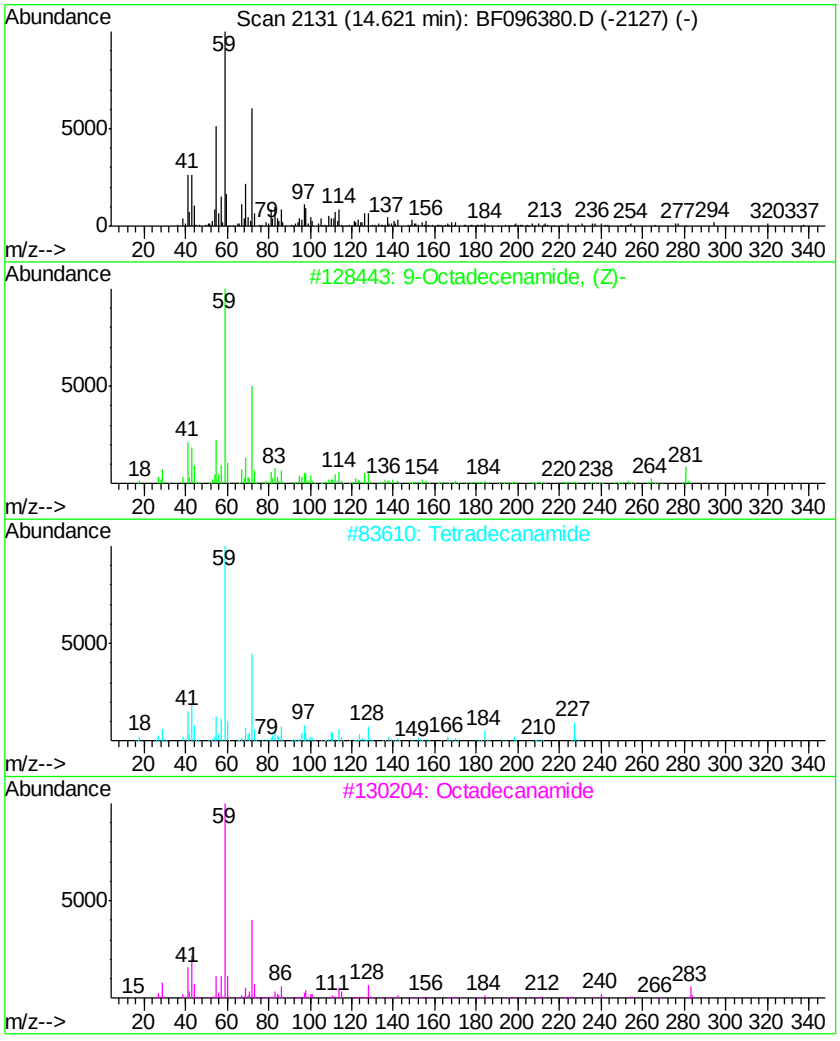
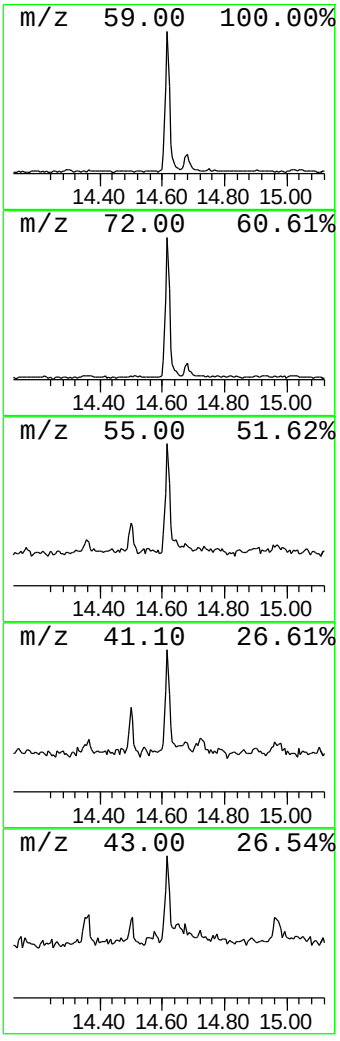
Peak Number 15 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	5.18 ng	342014	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Tetradecanamide	227	C14H29NO	000638-58-4	90
3	Octadecanamide	283	C18H37NO	000124-26-5	78
4	7-Nonenamide	155	C9H17NO	090949-53-4	64
5	Nonanamide	157	C9H19NO	001120-07-6	53





Library Search Compound Report

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Operator : SJ/MA
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Misc :
ALS Vial : 3 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : TP1-TP2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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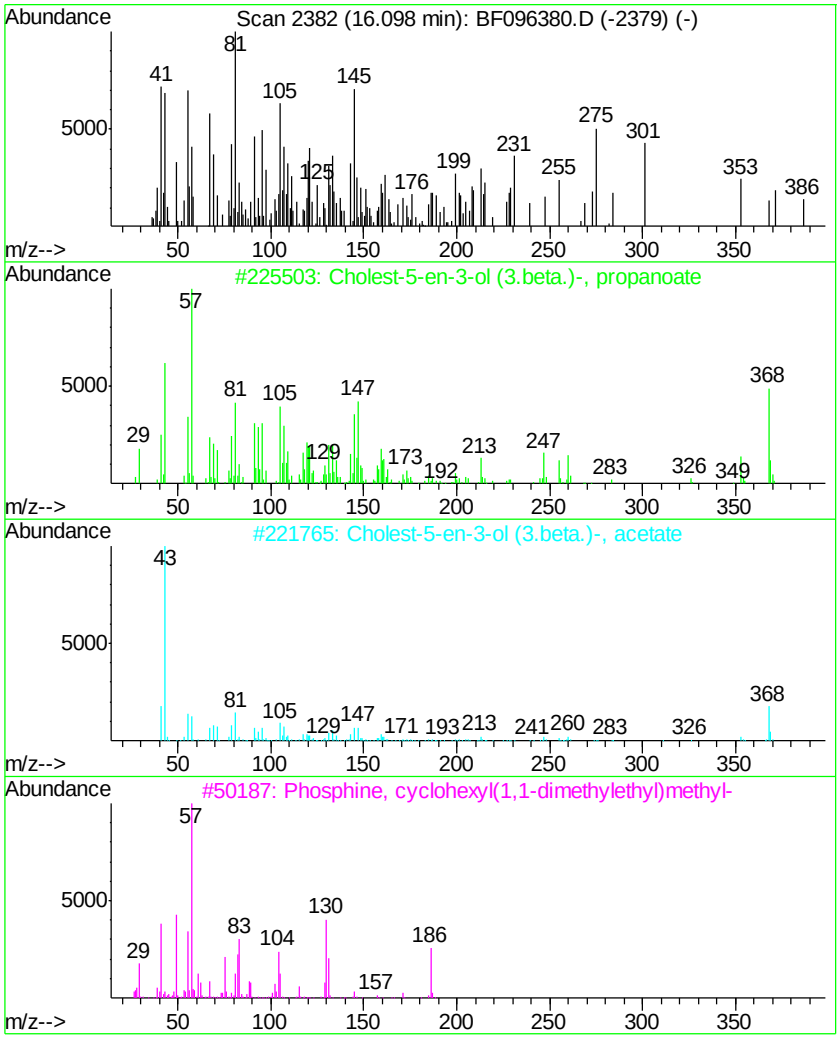
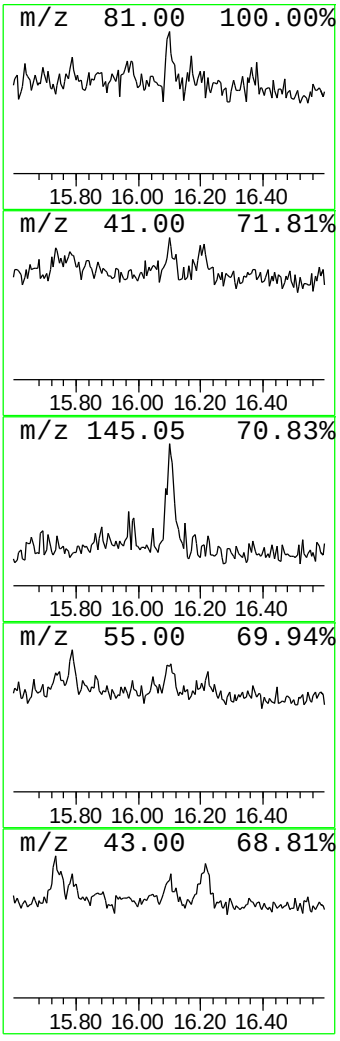
Peak Number 16 unknown16.10 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.06 ng	136367	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-en-3-ol (3.beta.)-, pr...	442	C30H50O2	000633-31-8	10
2	Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	10
3	Phosphine, cyclohexyl(1,1-dimeth...	186	C11H23P	074685-81-7	10
4	Chloromethyl 3-chlorobutanoate	170	C5H8Cl2O2	080418-48-0	10
5	trans-2-Chlorovinylacetate	120	C4H5ClO2	1000288-27-5	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070117\
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Operator : SJ/MA
Sample : I3947-01
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.92	4.7	ng	396500	1	6.73	1685360	20.0
unknown6.50	6.50	35.9	ng	3025700	1	6.73	1685360	20.0
n-Hexadecanoic acid	11.66	16.9	ng	1734120	4	11.24	2050050	20.0
Undecanoic acid	11.79	14.5	ng	1481770	4	11.24	2050050	20.0
3,5-Dimethoxy-4-h...	11.92	2.3	ng	235434	4	11.24	2050050	20.0
4-Chloro-3-methox...	11.95	4.6	ng	467483	4	11.24	2050050	20.0
Octadecanoic acid	12.52	27.5	ng	2816670	4	11.24	2050050	20.0
Tridecanoic acid	12.56	36.6	ng	2620370	5	13.87	1431400	20.0
Tetradecanamide	13.37	3.8	ng	273937	5	13.87	1431400	20.0
Trichloroacetic a...	13.73	3.5	ng	250338	5	13.87	1431400	20.0
unknown14.50	14.50	2.7	ng	192413	5	13.87	1431400	20.0
9-Octadecenamide,...	14.62	5.2	ng	342014	6	15.29	1321310	20.0
unknown16.10	16.10	2.1	ng	136367	6	15.29	1321310	20.0