LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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	4.928	479	483	492	rVB	492976	661921	17.76%	1.823%
2	5.351	549	555	558	rBV	3461232	3530783	94.72%	9.725%
3	6.369	723	728	732	rVB	3074727	3727541	100.00%	10.267%
4	6.504	746	751	754	rBV	3521826	3518118	94.38%	9.690%
5	6.581	759	764	770	rVB	119696	114921	3.08%	0.317%
6	6.734	786	790	793	rBV	1353399	1100876	29.53%	3.032%
7	6.892	812	817	820	rVB	2629561	2465076	66.13%	6.790%
8	7.087	847	850	854	rVB2	38247	39135	1.05%	0.108%
9	7.134	854	858	861	rBV2	53296	49153	1.32%	0.135%
10	7.292	879	885	888	rBV	2359915	2320413	62.25%	6.391%
11	7.345	890	894	897	rVB	196014	160335	4.30%	0.442%
12	7.381	897	900	905	rVB2	47667	51862	1.39%	0.143%
13	7.716	952	957	959	rBV2	49959	59137	1.59%	0.163%
14	7.781	965	968	971	rBV	70830	55134	1.48%	0.152%
15	7.822	971	975	978	rBV	55165	50771	1.36%	0.140%
16	8.016	1003	1008	1011	rBV	2057541	1889119	50.68%	5.203%
17	8.092	1019	1021	1024	rVB	118015	78667	2.11%	0.217%
18	8.187	1033	1037	1041	rBV2	31526	40691	1.09%	0.112%
19	8.339	1055	1063	1066	rVV3	114812	244933	6.57%	0.675%
20	8.375	1066	1069	1071	rVB	99830	79871	2.14%	0.220%
21	8.404	1071	1074	1078	rVB	181796	174204	4.67%	0.480%
22	8.451	1078	1082	1087	rBV	232512	264854	7.11%	0.730%
23	8.622	1107	1111	1114	rBV	743767	641217	17.20%	1.766%
24	8.716	1124	1127	1130	rVB2	69098	95532	2.56%	0.263%
25	8.822	1142	1145	1149	rVB3	51203	60485	1.62%	0.167%
26	8.904	1156	1159	1160	rBV	89017	74462	2.00%	0.205%
27	8.922	1160	1162	1165	rVV2	76060	82487	2.21%	0.227%
28	8.951	1165	1167	1169	rVB	68301	48536	1.30%	0.134%
29	8.986	1169	1173	1176	rVB	96819	90633	2.43%	0.250%
30	9.022	1176	1179	1182	rBV	78390	73108	1.96%	0.201%
31	9.051	1182	1184	1186	rVB	72929	51524	1.38%	0.142%
32	9.092	1186	1191	1194	rBV	3444458	3058376	82.05%	8.424%
33	9.186	1203	1207	1211	rVB	391400	356812	9.57%	0.983%
34	9.481	1254	1257	1260	rVV	688559	540959	14.51%	1.490%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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	9.710	1293	1296	1299	rVB	153603	122724	3.29%	0.338%
36	9.769	1300	1306	1309	rBV	1514133	1504319	40.36%	4.143%
37	9.969	1338	1340	1344	rVB2	46652	37858	1.02%	0.104%
38	10.175	1367	1375	1378	rBV6	20571	40723	1.09%	0.112%
39	10.210	1378	1381	1384	rVB	165227	132277	3.55%	0.364%
40	10.433	1414	1419	1421	rBV	38732	46464	1.25%	0.128%
41	10.551	1434	1439	1442	rBV	1921901	1796644	48.20%	4.949%
42	10.680	1458	1461	1468	rVB	165935	190915	5.12%	0.526%
43	11.127	1534	1537	1540	rVV2	108243	85332	2.29%	0.235%
44	11.245	1553	1557	1560	rBV	1539087	1309915	35.14%	3.608%
45	11.557	1607	1610	1615	rBV2	57715	62716	1.68%	0.173%
46	11.780	1644	1648	1652	rBV2	186828	201575	5.41%	0.555%
47	11.963	1674	1679	1683	rVB	50766	57990	1.56%	0.160%
48	12.292	1732	1735	1738	rVB3	37398	37314	1.00%	0.103%
49	12.345	1742	1744	1747	rVB	59922	56150	1.51%	0.155%
50	12.451	1759	1762	1766	rBV2	46322	54775	1.47%	0.151%
51	12.563	1778	1781	1788	rBV4	57459	71546	1.92%	0.197%
52	12.722	1805	1808	1810	rBV	47675	44059	1.18%	0.121%
53	12.827	1822	1826	1830	rBV	2045179	1902521	51.04%	5.240%
54	13.074	1865	1868	1870	rBV	62835	53168	1.43%	0.146%
55	13.310	1906	1908	1914	rVB	81499	72786	1.95%	0.200%
56	13.416	1923	1926	1929	rVB	49150	41913	1.12%	0.115%
57	13.727	1976	1979	1989	rBV	316522	367927	9.87%	1.013%
58	13.868	1999	2003	2006	rBV	903479	857475	23.00%	2.362%
59	14.057	2031	2035	2038	rBV	63885	80929	2.17%	0.223%
60	14.363	2084	2087	2092	rBV	53690	69261	1.86%	0.191%
61	14.457	2100	2103	2109	rBV8	28683	61771	1.66%	0.170%
62	14.663	2135	2138	2142	rBV3	46593	64968	1.74%	0.179%
63	14.727	2147	2149	2151	rVB	55488	40676	1.09%	0.112%
64	14.980	2188	2192	2195	rBV3	50110	58969	1.58%	0.162%
65	15.163	2220	2223	2228	rBV	37548	46481	1.25%	0.128%
66	15.280	2239	2243	2248	rBV	644878	797138	21.39%	2.196%
67	15.333	2250	2252	2256	rVB3	43828	43347	1.16%	0.119%
68	16.774	2493	2497	2498	rBV4	29593	41895	1.12%	0.115%

Sum of corrected areas: 36306167

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
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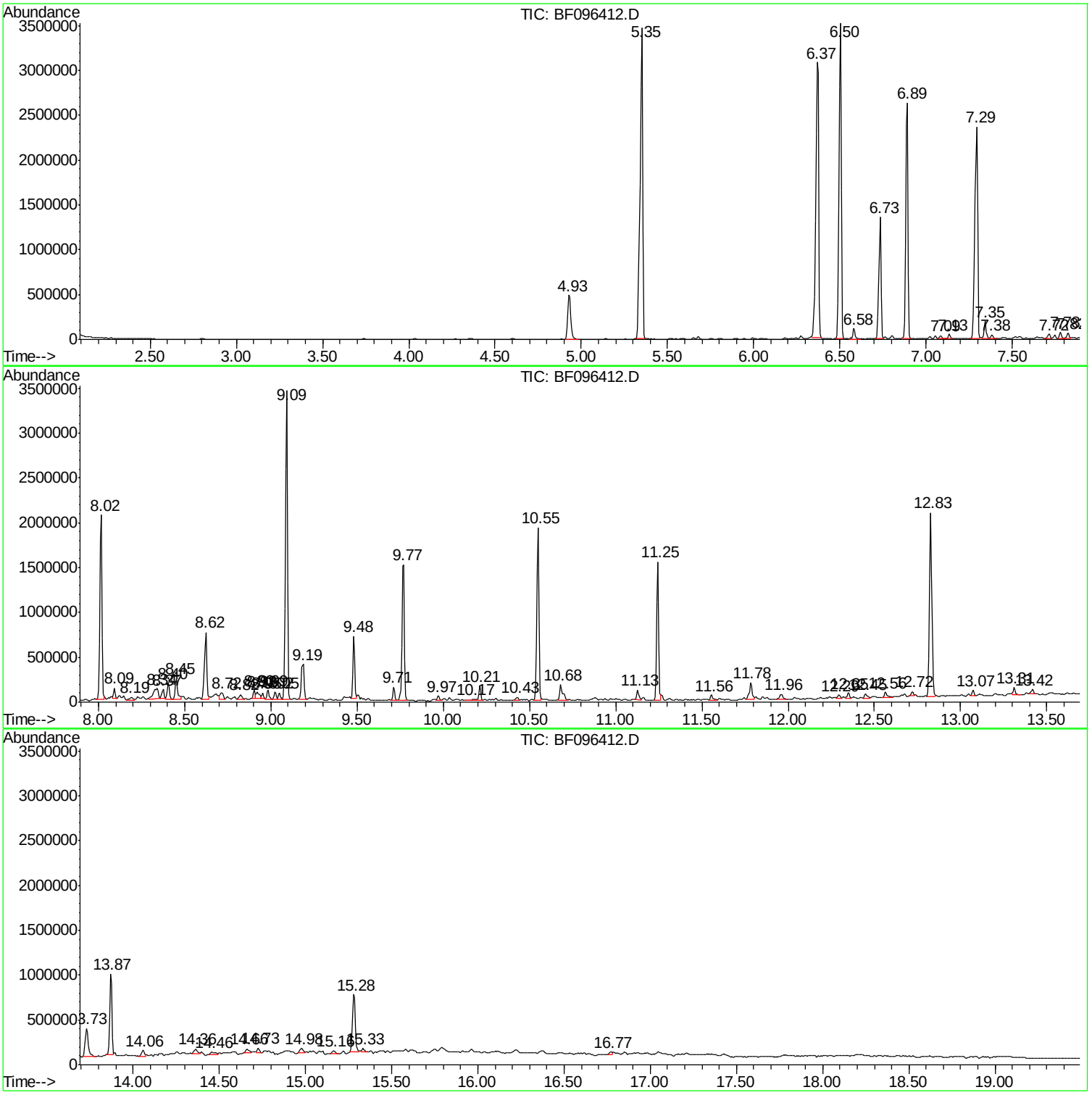
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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\BF070217\
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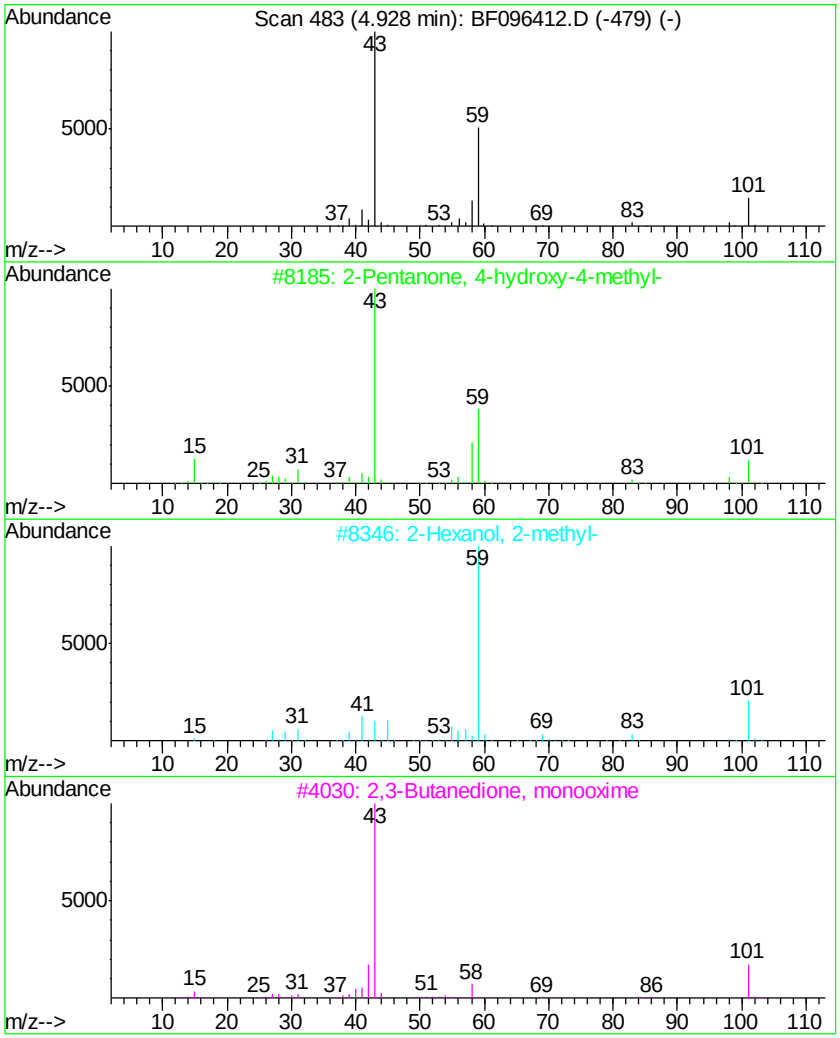
TIC Integration Parameters: LSCINT.P

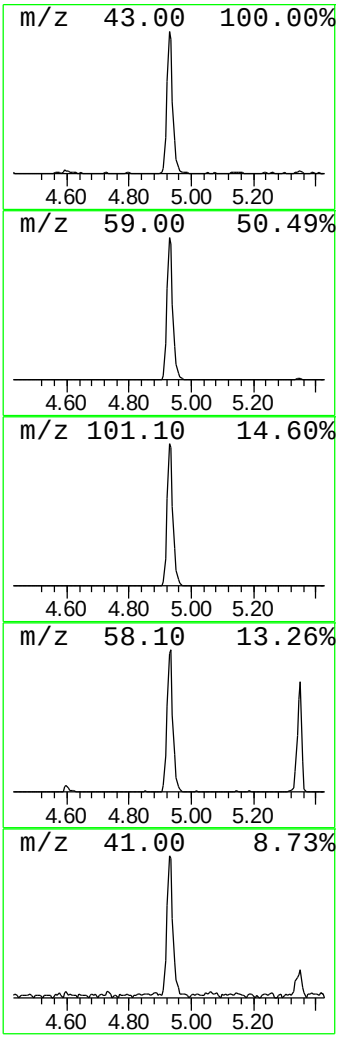
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	12.03 ng	661921	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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

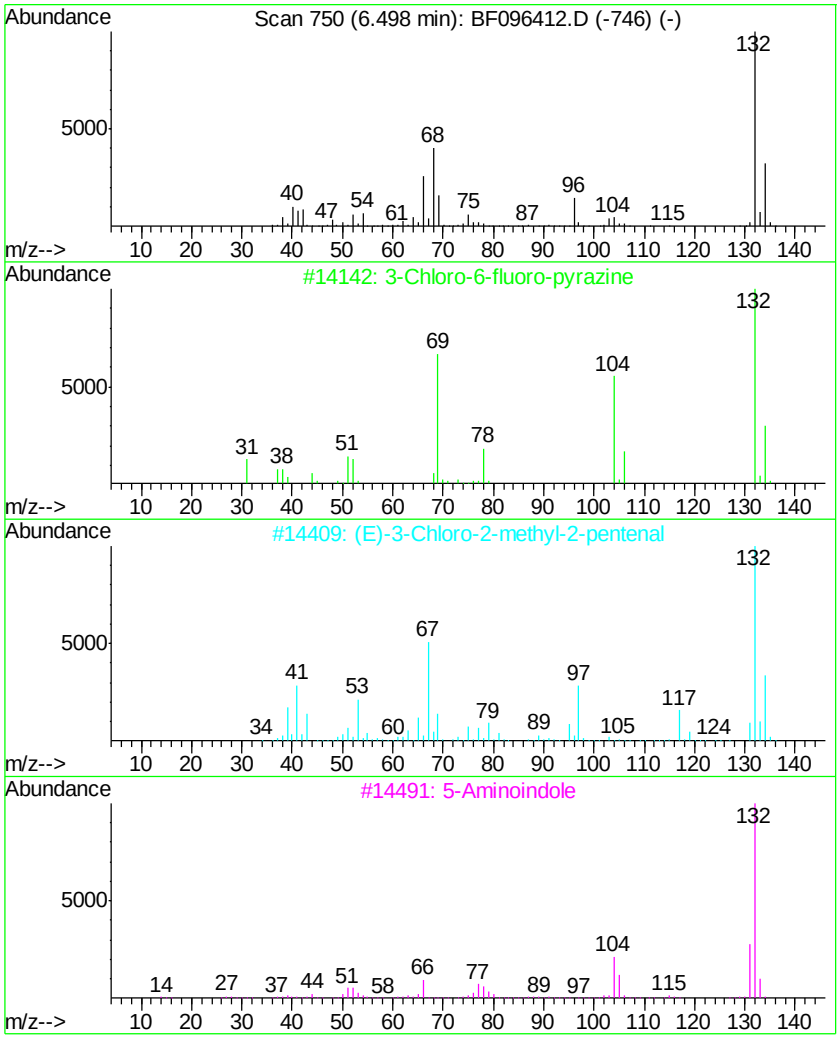
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

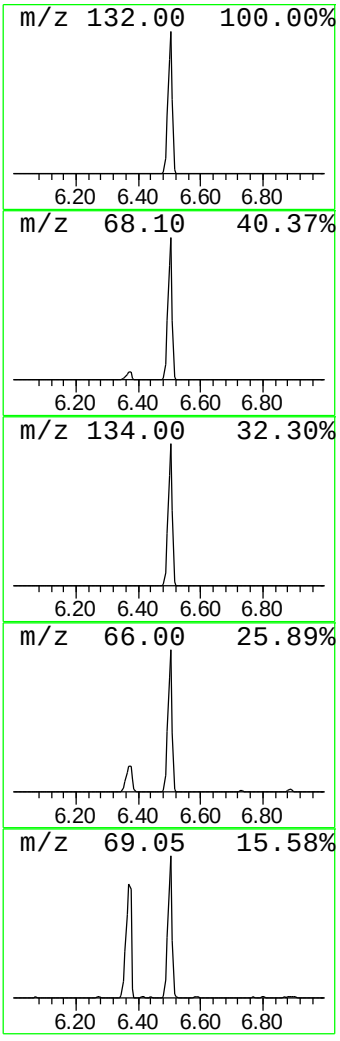
****

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	63.91 ng	3518120	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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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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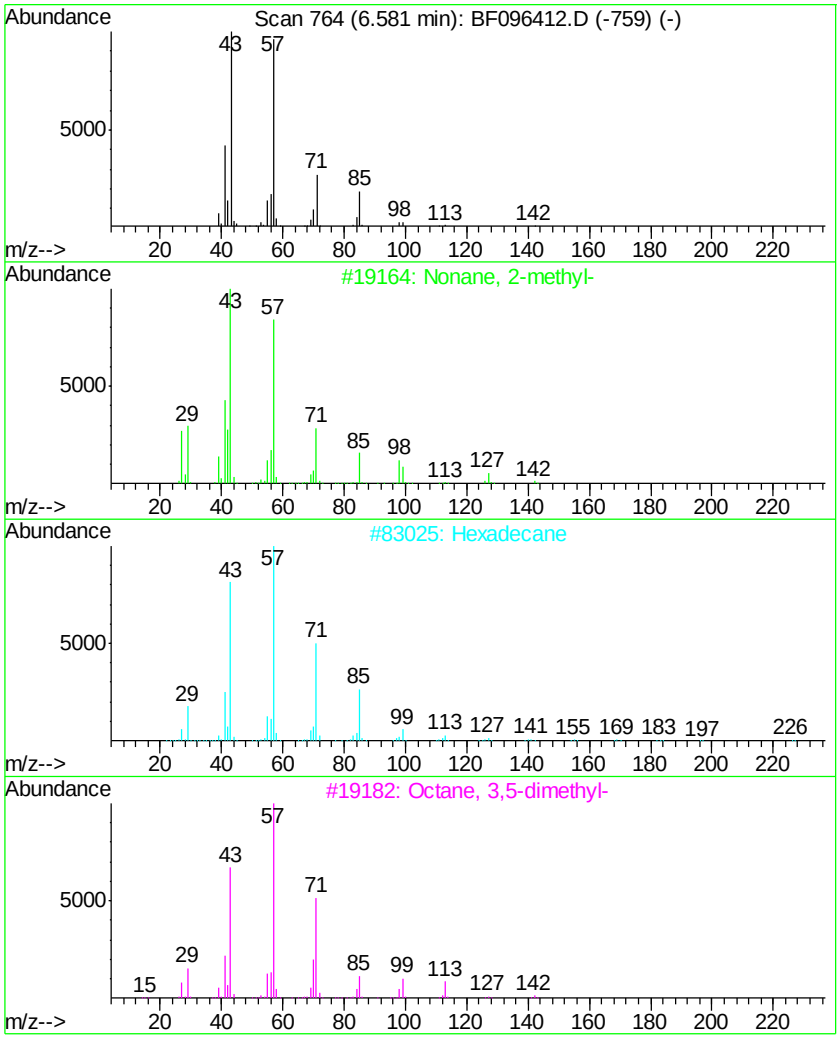
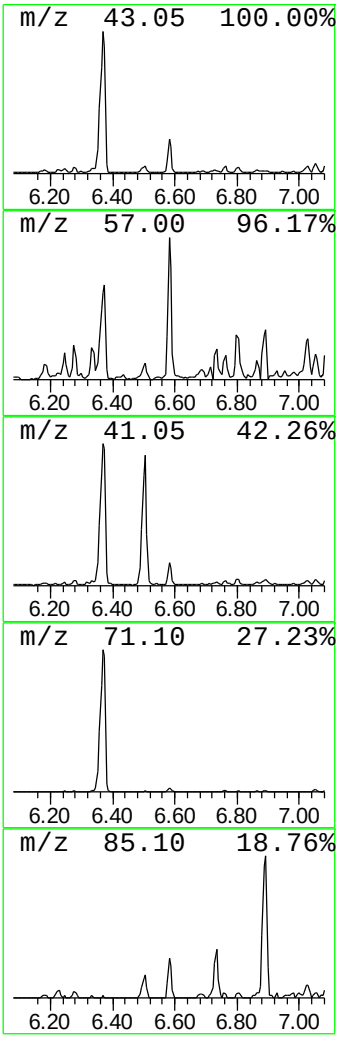
Peak Number 3 Nonane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	2.09 ng	114921	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 2-methyl-	142	C10H22	000871-83-0	80
2	Hexadecane	226	C16H34	000544-76-3	72
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	64
4	Decane	142	C10H22	000124-18-5	59
5	Nonane, 4-methyl-	142	C10H22	017301-94-9	58





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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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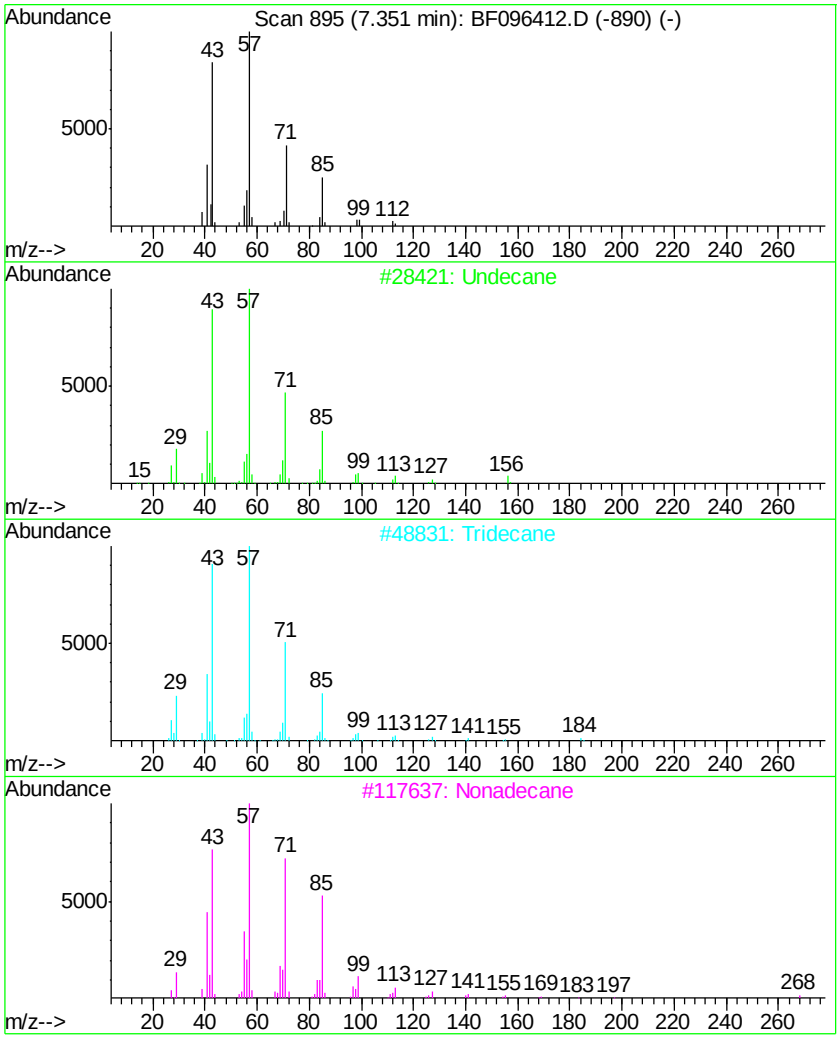
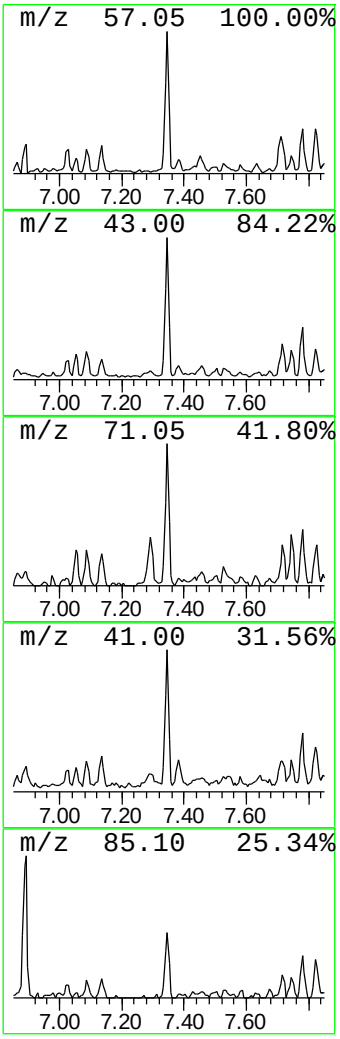
Peak Number 5 Undecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.35	2.91 ng	160335	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	83
2	Tridecane	184	C13H28	000629-50-5	83
3	Nonadecane	268	C19H40	000629-92-5	78
4	Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64
5	Tetradecane	198	C14H30	000629-59-4	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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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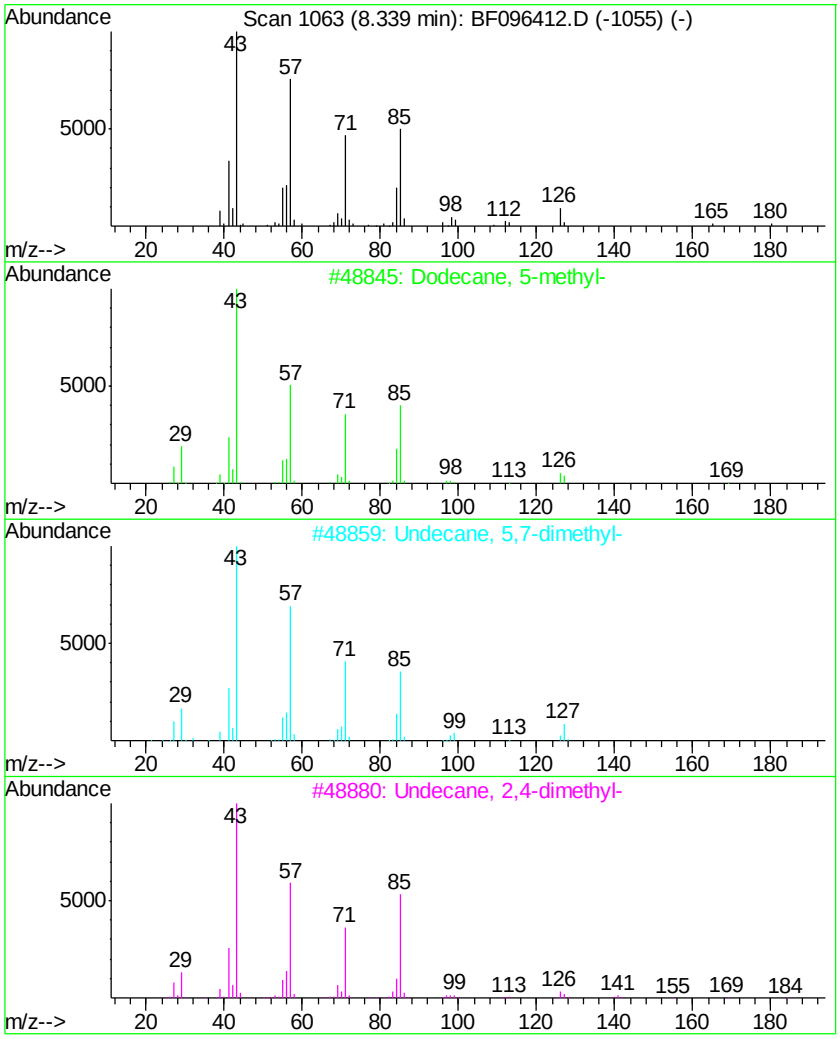
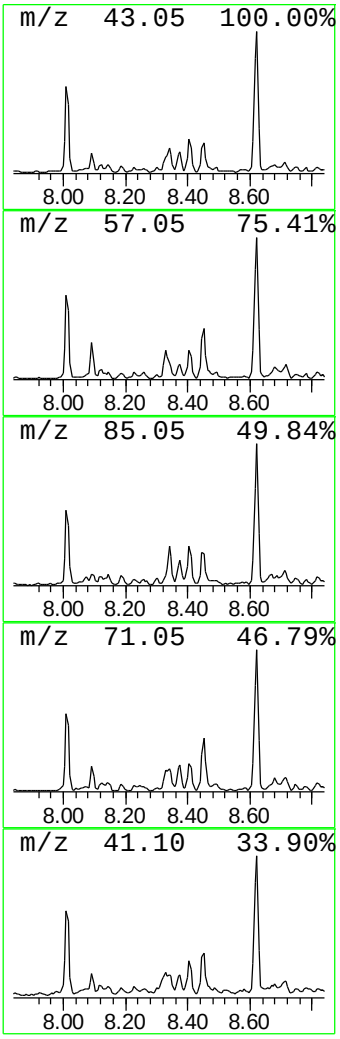
Peak Number 6 Dodecane, 5-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	2.59 ng	244933	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 5-methyl-	184	C13H28	017453-93-9	78
2	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	78
3	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	72
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5	Undecane, 5-methyl-	170	C12H26	001632-70-8	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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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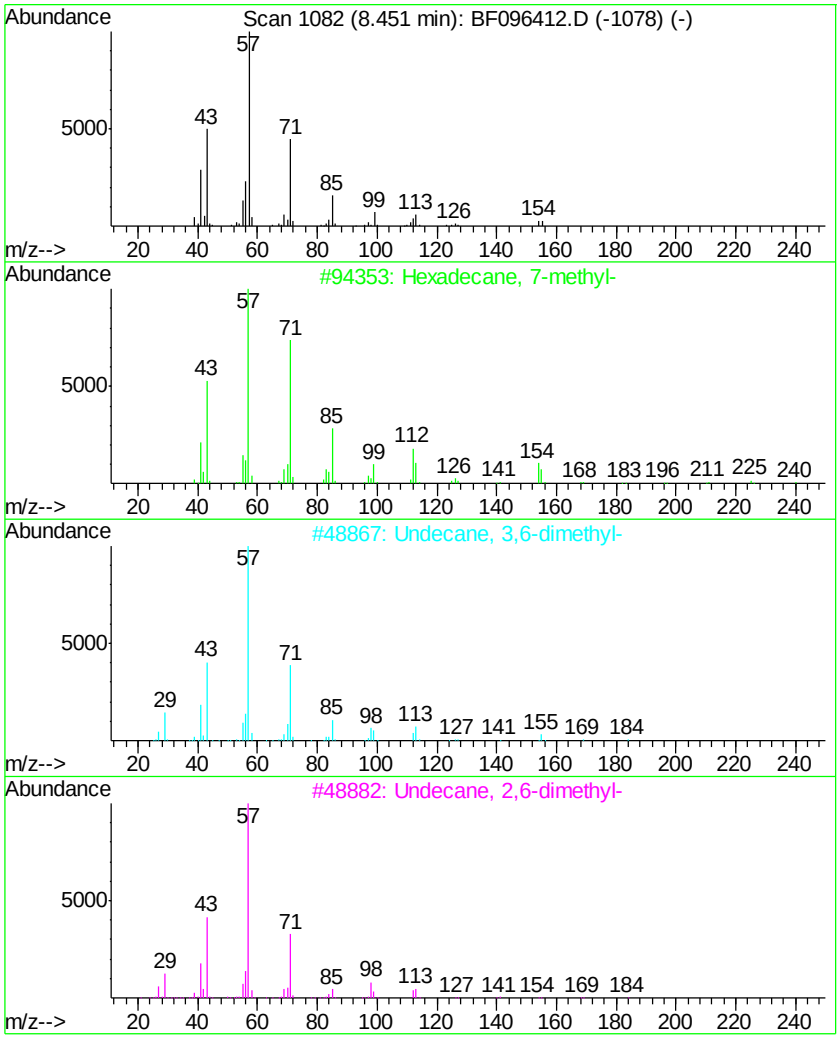
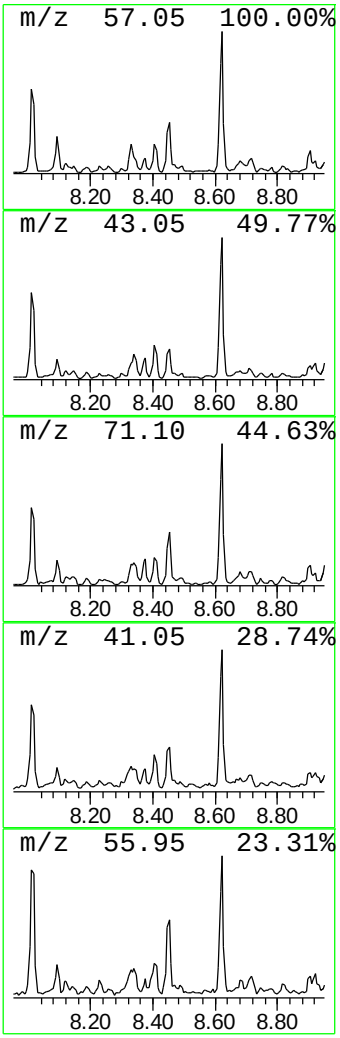
Peak Number 7 Hexadecane, 7-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	2.80 ng	264854	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	72
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
3	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	64
4	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
5	Nonane, 3-methyl-	142	C10H22	005911-04-6	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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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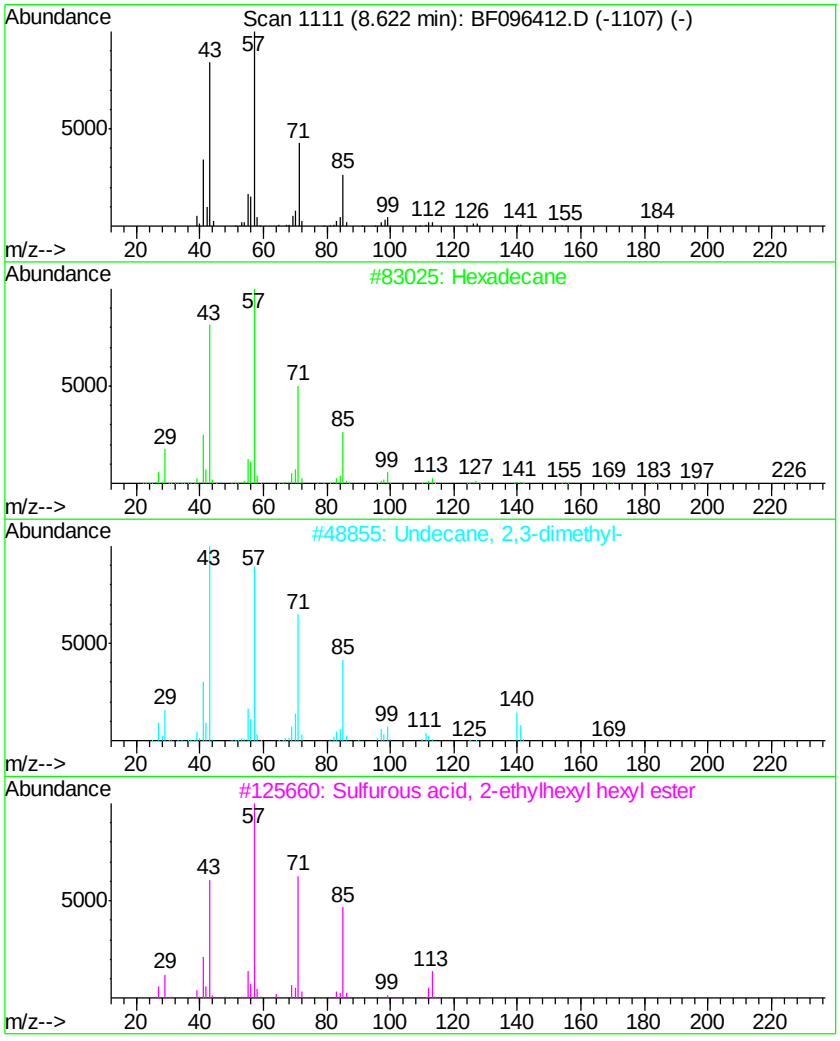
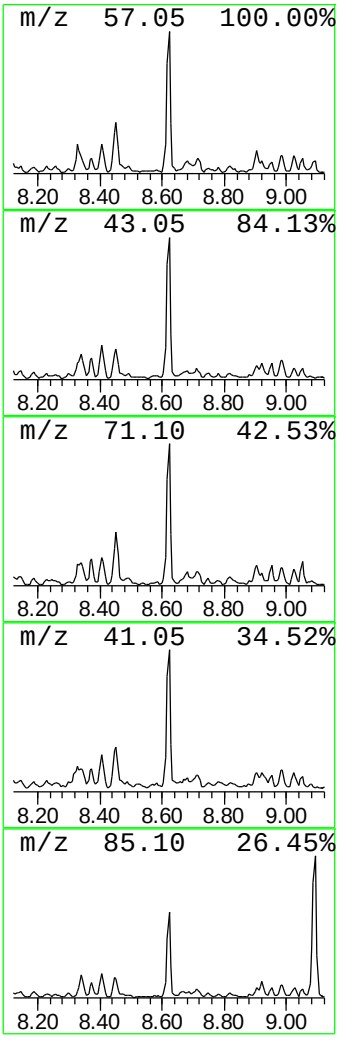
Peak Number 8 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	6.79 ng	641217	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	72
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
4	Dodecane, 3-methyl-	184	C13H28	017312-57-1	59
5	Undecane	156	C11H24	001120-21-4	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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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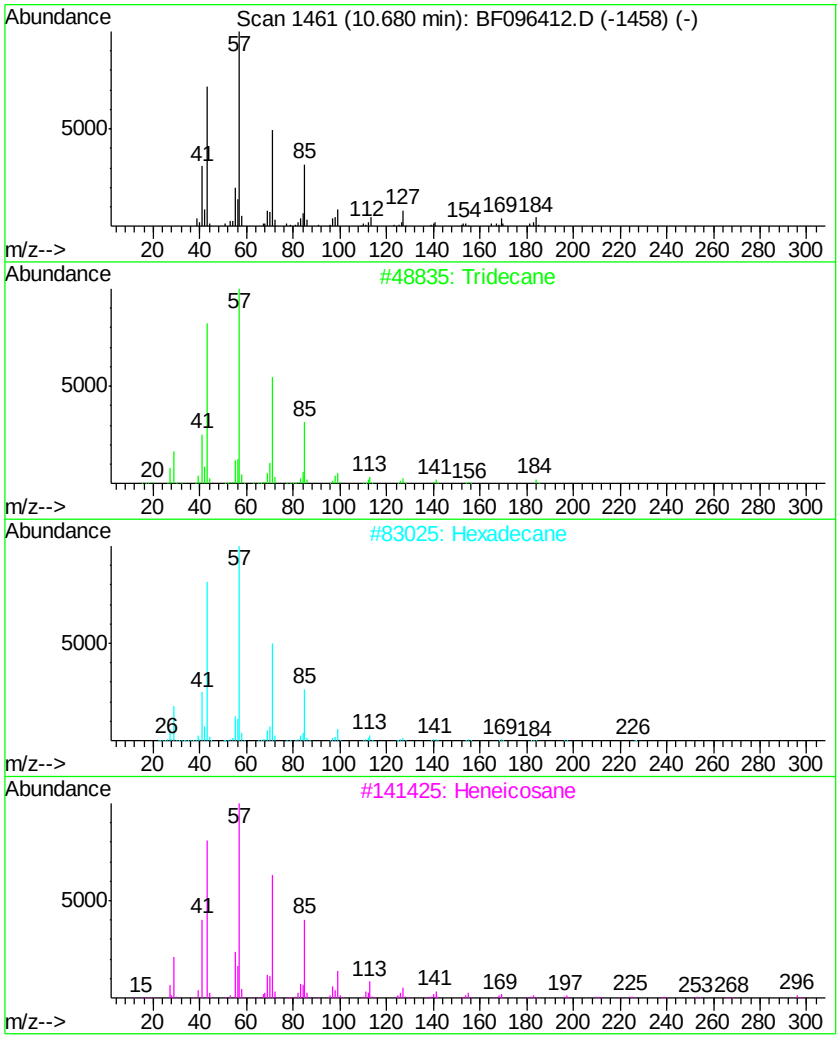
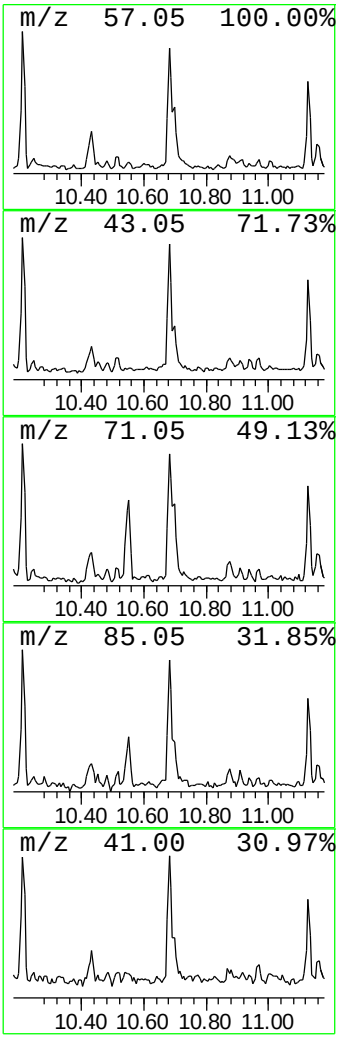
Peak Number 10 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.91 ng	190915	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Hexadecane	226	C16H34	000544-76-3	80
3	Heneicosane	296	C21H44	000629-94-7	80
4	Eicosane	282	C20H42	000112-95-8	80
5	Heptadecane	240	C17H36	000629-78-7	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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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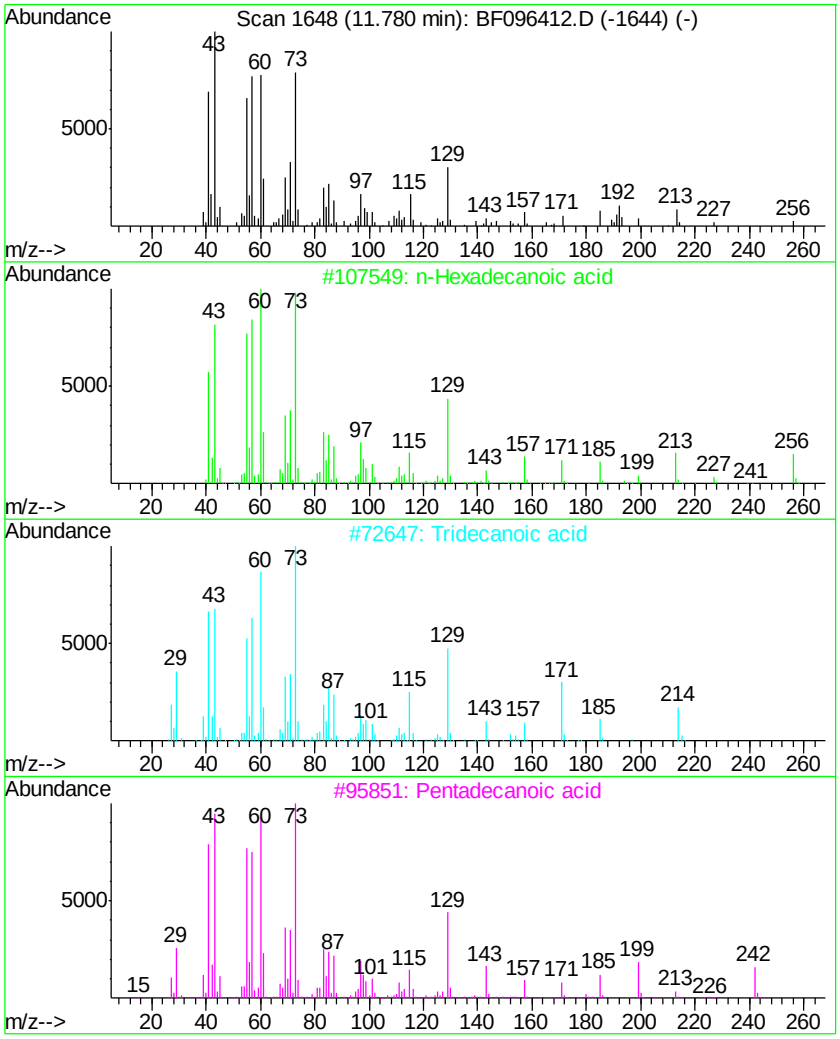
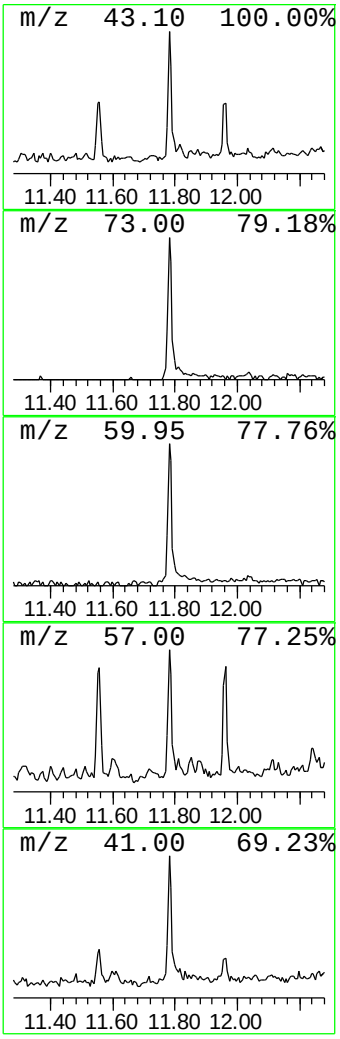
Peak Number 11 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	3.08 ng	201575	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Nonanoic acid	158	C9H18O2	000112-05-0	58





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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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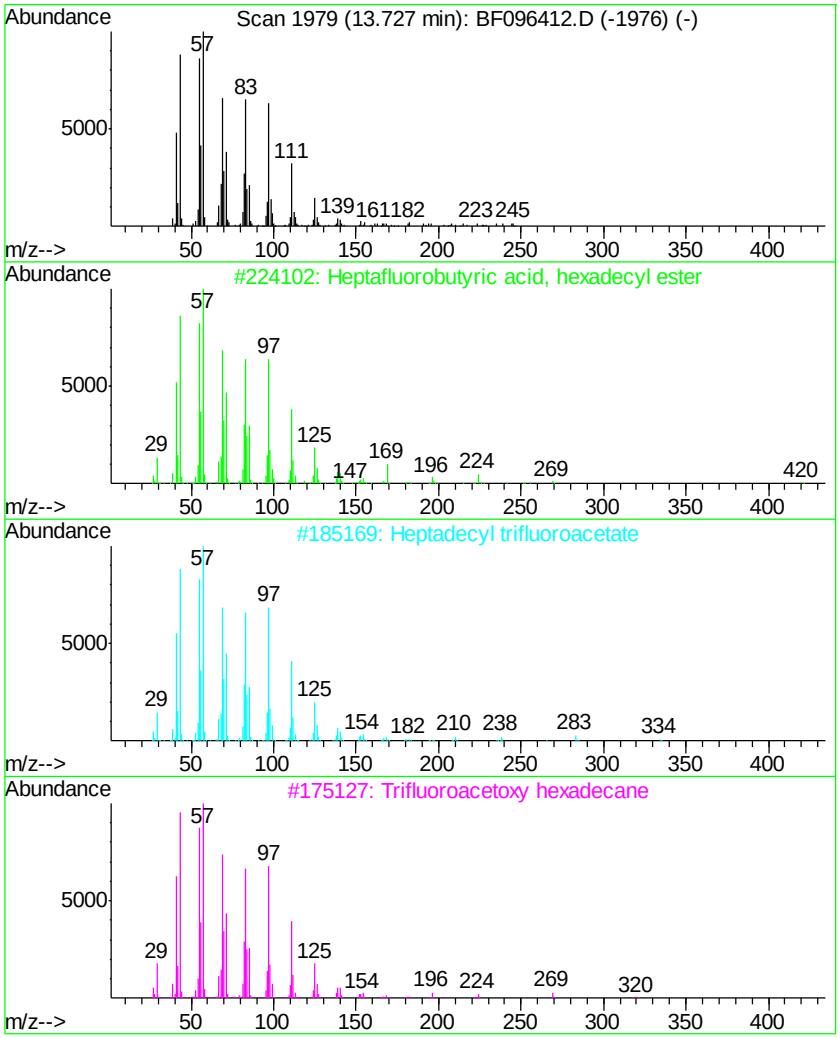
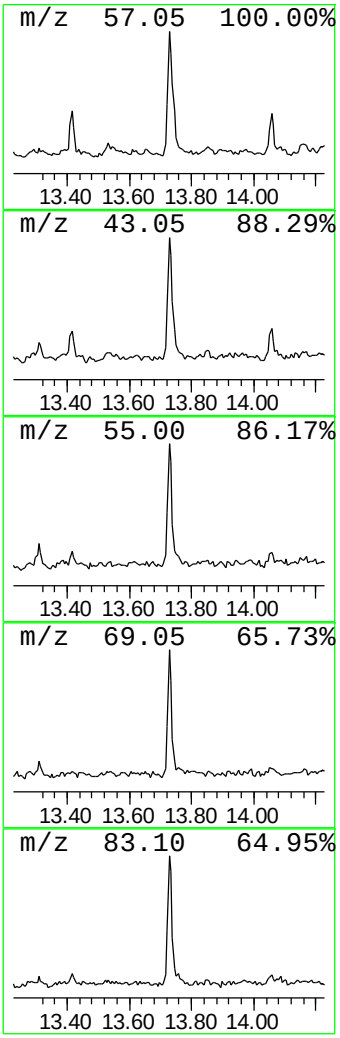
Peak Number 12 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	8.58 ng	367927	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096412.D
Acq On : 2 Jul 2017 13:25
Operator : SJ/MA
Sample : I3950-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B4-6-8

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...	4.93	12.0	ng	661921	1	6.73	1100880	20.0
unknown6.50	6.50	63.9	ng	3518120	1	6.73	1100880	20.0
Nonane, 2-methyl-	6.58	2.1	ng	114921	1	6.73	1100880	20.0
Undecane	7.35	2.9	ng	160335	1	6.73	1100880	20.0
Dodecane, 5-methyl-	8.34	2.6	ng	244933	2	8.02	1889120	20.0
Hexadecane, 7-met...	8.45	2.8	ng	264854	2	8.02	1889120	20.0
Hexadecane	8.62	6.8	ng	641217	2	8.02	1889120	20.0
Tridecane	10.68	2.9	ng	190915	4	11.25	1309920	20.0
n-Hexadecanoic acid	11.78	3.1	ng	201575	4	11.25	1309920	20.0
Heptafluorobutyri...	13.73	8.6	ng	367927	5	13.87	857475	20.0