LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096362.D
Acq On : 1 Jul 2017 3:20
Operator : SJ/MA
Sample : I3930-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3-6-8.5

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-BF062717.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	2.846	123	129	135	rVB3	20449	43390	1.01%	0.112%
2	3.781	282	288	293	rBV	52968	77058	1.80%	0.198%
3	4.963	484	489	496	rBV	523508	731346	17.10%	1.882%
4	5.345	550	554	555	rBV	79218	72168	1.69%	0.186%
5	5.381	555	560	563	rVB	4111457	4275971	100.00%	11.002%
6	5.604	596	598	604	rVB2	82585	80704	1.89%	0.208%
7	6.216	695	702	705	rBV2	23779	44160	1.03%	0.114%
8	6.298	712	716	722	rVB3	50745	73955	1.73%	0.190%
9	6.398	727	733	736	rVB	3864134	4215818	98.59%	10.847%
10	6.534	750	756	759	rBV	3690875	3993647	93.40%	10.276%
11	6.592	763	766	767	rBV	65441	59431	1.39%	0.153%
12	6.757	791	794	797	rBV	1167036	968935	22.66%	2.493%
13	6.822	802	805	808	rBV2	52642	51511	1.20%	0.133%
14	6.916	817	821	825	rVB	3149644	2921599	68.33%	7.517%
15	7.086	846	850	853	rBV3	33454	48145	1.13%	0.124%
16	7.163	858	863	865	rBV2	44955	48017	1.12%	0.124%
17	7.316	882	889	892	rBV	2364890	2578819	60.31%	6.635%
18	7.369	895	898	901	rVB2	74244	67683	1.58%	0.174%
19	7.410	901	905	909	rBV3	58944	73224	1.71%	0.188%
20	7.539	921	927	931	rBV3	28425	46226	1.08%	0.119%
21	8.039	1008	1012	1015	rBV	1509128	1382931	32.34%	3.558%
22	8.063	1015	1016	1019	rVB	167562	78799	1.84%	0.203%
23	8.480	1082	1087	1090	rBV	64610	65725	1.54%	0.169%
24	8.645	1112	1115	1117	rBV	78197	61215	1.43%	0.158%
25	8.751	1127	1133	1137	rVB	195466	173277	4.05%	0.446%
26	8.851	1146	1150	1153	rVB	154405	121580	2.84%	0.313%
27	9.116	1190	1195	1199	rVB	3149721	3236194	75.68%	8.327%
28	9.210	1208	1211	1214	rVB2	128470	115333	2.70%	0.297%
29	9.375	1233	1239	1244	rBV2	61055	83915	1.96%	0.216%
30	9.451	1250	1252	1255	rBV	84996	77314	1.81%	0.199%
31	9.480	1255	1257	1259	rVV	70956	52956	1.24%	0.136%
32	9.510	1259	1262	1264	rVV	605886	474455	11.10%	1.221%
33	9.651	1281	1286	1289	rVB2	57436	50220	1.17%	0.129%
34	9.739	1298	1301	1304	rVB	152906	122074	2.85%	0.314%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : B3-6-8.5

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-BF062717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.792	1304	1310	1313	rBV	1300507	1154177	26.99%	2.970%
36	9.822	1313	1315	1319	rVB3	44495	47878	1.12%	0.123%
37	9.998	1342	1345	1348	rVB	125206	108832	2.55%	0.280%
38	10.063	1353	1356	1361	rBV4	31886	44444	1.04%	0.114%
39	10.204	1376	1380	1383	rBV3	50763	70503	1.65%	0.181%
40	10.239	1383	1386	1389	rVB	157001	135085	3.16%	0.348%
41	10.333	1399	1402	1405	rBV2	78020	63590	1.49%	0.164%
42	10.457	1419	1423	1426	rBV2	62220	66636	1.56%	0.171%
43	10.498	1427	1430	1435	rVB2	44266	57115	1.34%	0.147%
44	10.580	1439	1444	1447	rBV	1884777	1911138	44.69%	4.917%
45	10.710	1462	1466	1467	rBV	180230	175478	4.10%	0.452%
46	10.886	1487	1496	1497	rBV8	25247	45142	1.06%	0.116%
47	11.074	1525	1528	1532	rVB2	45869	51354	1.20%	0.132%
48	11.127	1532	1537	1539	rVV5	30320	44063	1.03%	0.113%
49	11.157	1539	1542	1545	rVV2	127885	138955	3.25%	0.358%
50	11.186	1545	1547	1551	rVB2	44060	43163	1.01%	0.111%
51	11.274	1558	1562	1564	rBV	1050472	956977	22.38%	2.462%
52	11.298	1564	1566	1568	rVV	314867	249266	5.83%	0.641%
53	11.345	1568	1574	1577	rVB	96271	98194	2.30%	0.253%
54	11.498	1598	1600	1604	rBV2	38463	47821	1.12%	0.123%
55	11.580	1611	1614	1616	rBV	69765	53990	1.26%	0.139%
56	11.733	1636	1640	1644	rBV6	26189	52672	1.23%	0.136%
57	11.774	1644	1647	1649	rVV	81658	80477	1.88%	0.207%
58	11.810	1649	1653	1657	rVV2	442509	471190	11.02%	1.212%
59	11.845	1657	1659	1662	rVV2	57305	63323	1.48%	0.163%
60	11.880	1662	1665	1668	rVV2	114698	137841	3.22%	0.355%
61	11.904	1668	1669	1674	rVB	69752	62871	1.47%	0.162%
62	11.986	1680	1683	1685	rBV	63464	53272	1.25%	0.137%
63	12.068	1694	1697	1699	rBV2	80096	75153	1.76%	0.193%
64	12.321	1737	1740	1743	rBV2	89313	89535	2.09%	0.230%
65	12.374	1747	1749	1752	rVV2	71920	69359	1.62%	0.178%
66	12.404	1752	1754	1758	rVB3	45507	52808	1.23%	0.136%
67	12.480	1764	1767	1771	rBV	361616	299306	7.00%	0.770%
68	12.592	1784	1786	1791	rBV3	78996	87258	2.04%	0.225%
69	12.710	1799	1806	1809	rBV	282286	341994	8.00%	0.880%
70	12.857	1827	1831	1835	rBV	2348576	2244062	52.48%	5.774%
71	13.104	1870	1873	1875	rBV	73594	62994	1.47%	0.162%

LSC Area Percent Report

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Instrument : BNA_F
ClientSampleId : B3-6-8.5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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72	13.339	1910	1913	1920	rVB	377110	382870	8.95%	0.985%
73	13.439	1928	1930	1933	rBV	58607	56358	1.32%	0.145%
74	13.757	1981	1984	1992	rVB2	335887	350500	8.20%	0.902%
75	13.904	2004	2009	2012	rBV	929599	985611	23.05%	2.536%
76	13.927	2012	2013	2015	rVB	133173	70625	1.65%	0.182%
77	14.762	2152	2155	2158	rVB	149655	153109	3.58%	0.394%
78	15.327	2247	2251	2255	rVB	419927	489715	11.45%	1.260%

Sum of corrected areas: 38864499

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Sample : I3930-11
Misc :
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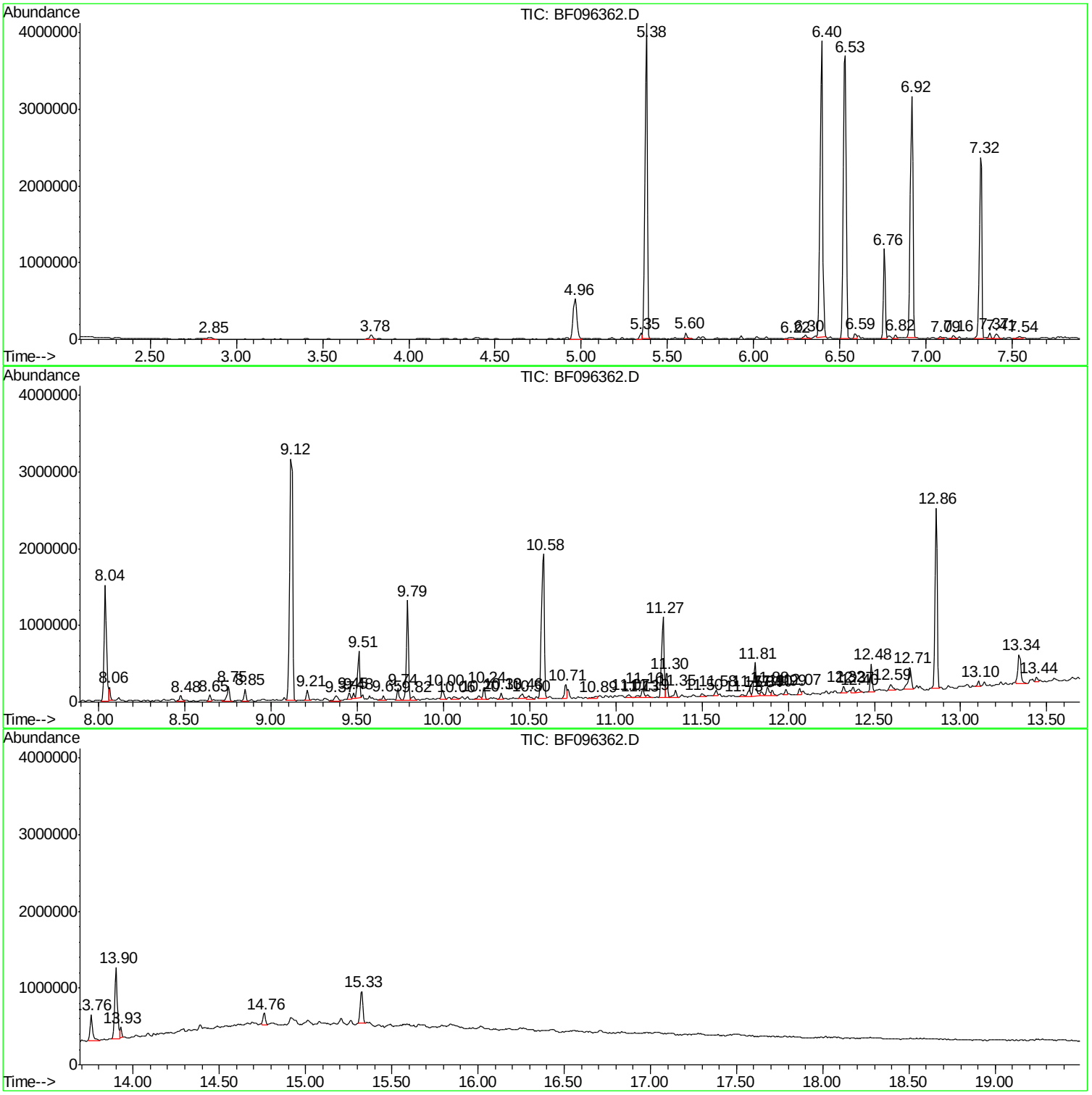
Instrument : BNA_F
ClientSampleId : B3-6-8.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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Acq On : 1 Jul 2017 3:20
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Sample : I3930-11
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

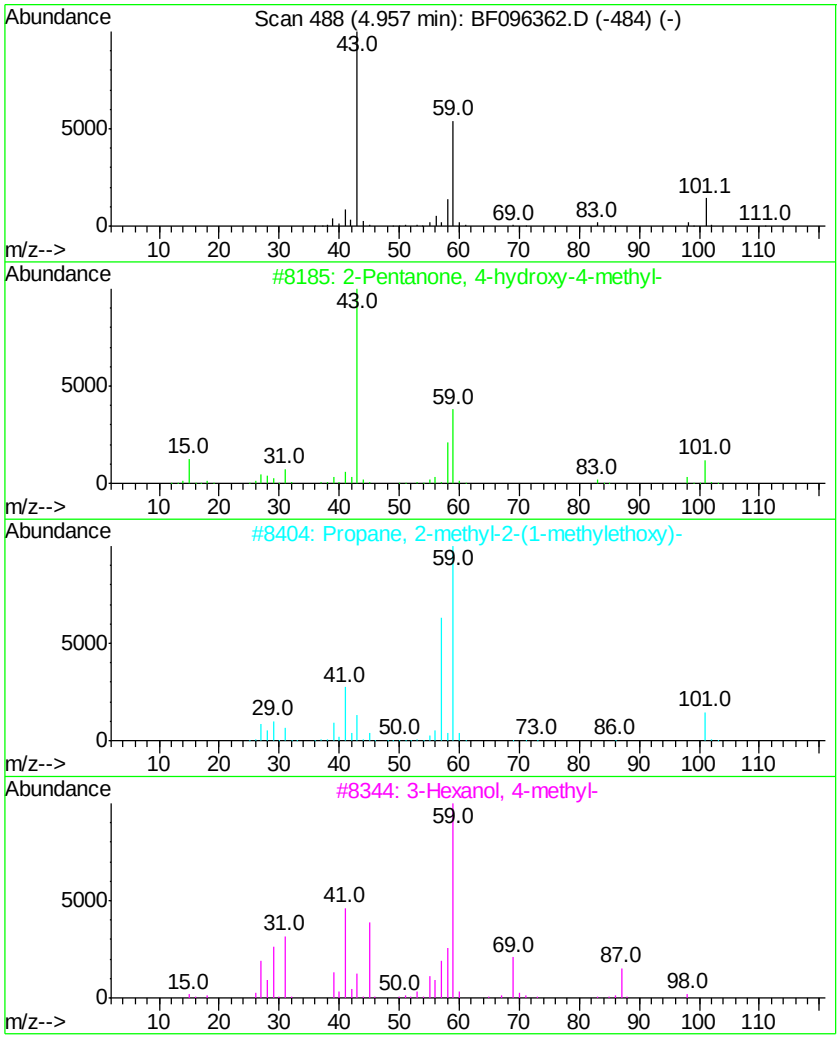
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

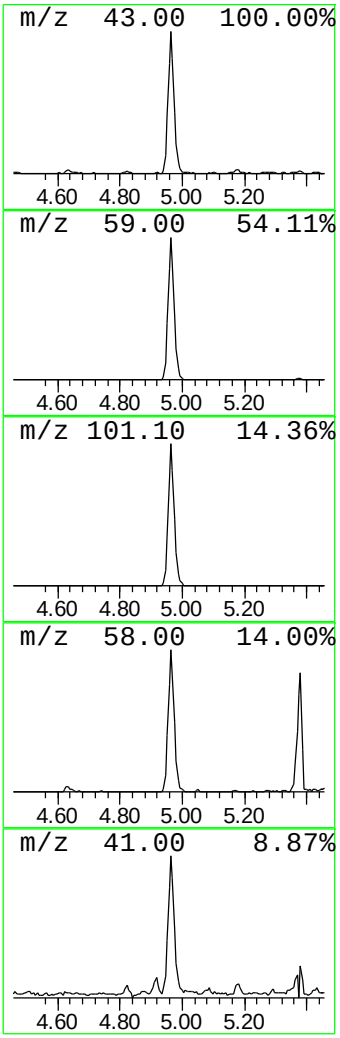
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	15.10 ng	731346	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Operator : SJ/MA
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ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3-6-8.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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TIC Library : C:\DATABASE\NIST11.L
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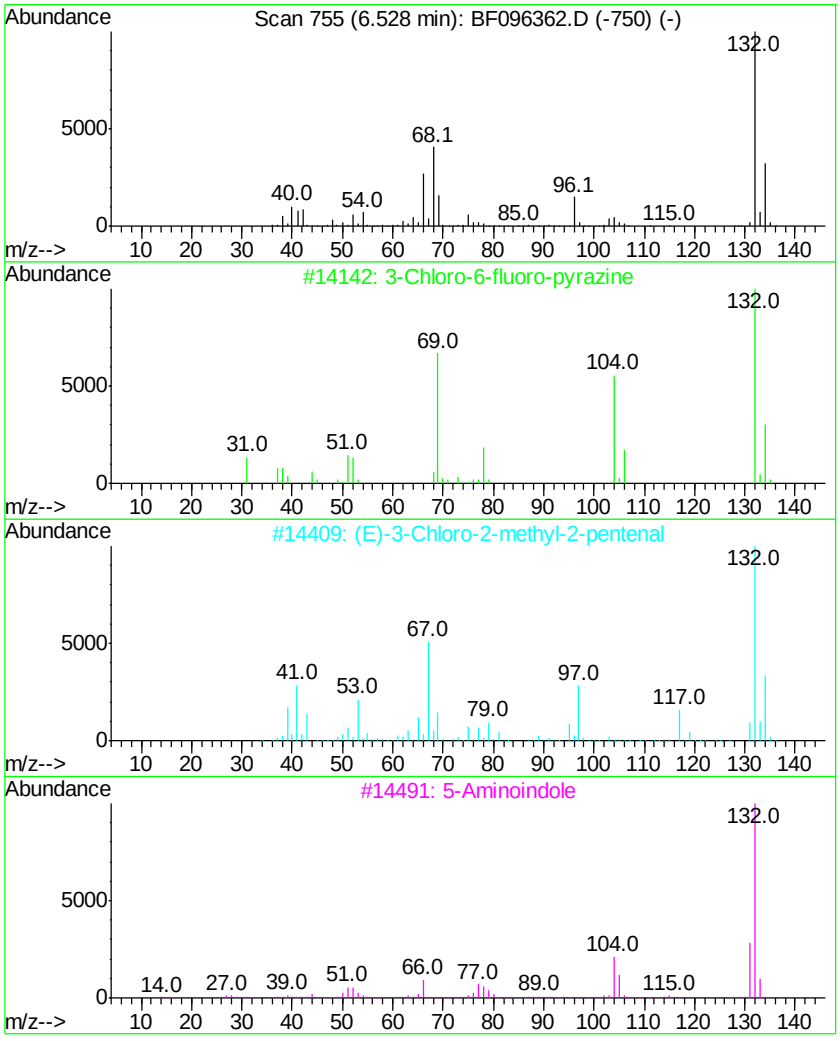
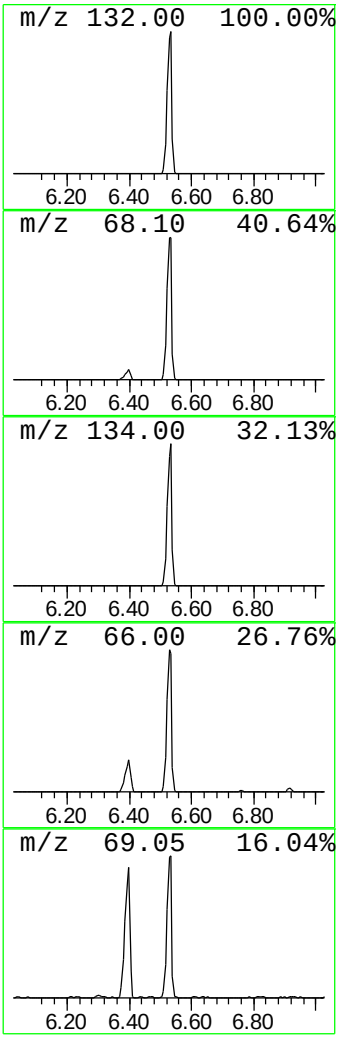
****

Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	82.43 ng	3993650	1,4-Dichlorobenzene-d4	6.76

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	16
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





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Instrument : BNA_F
ClientSampleId : B3-6-8.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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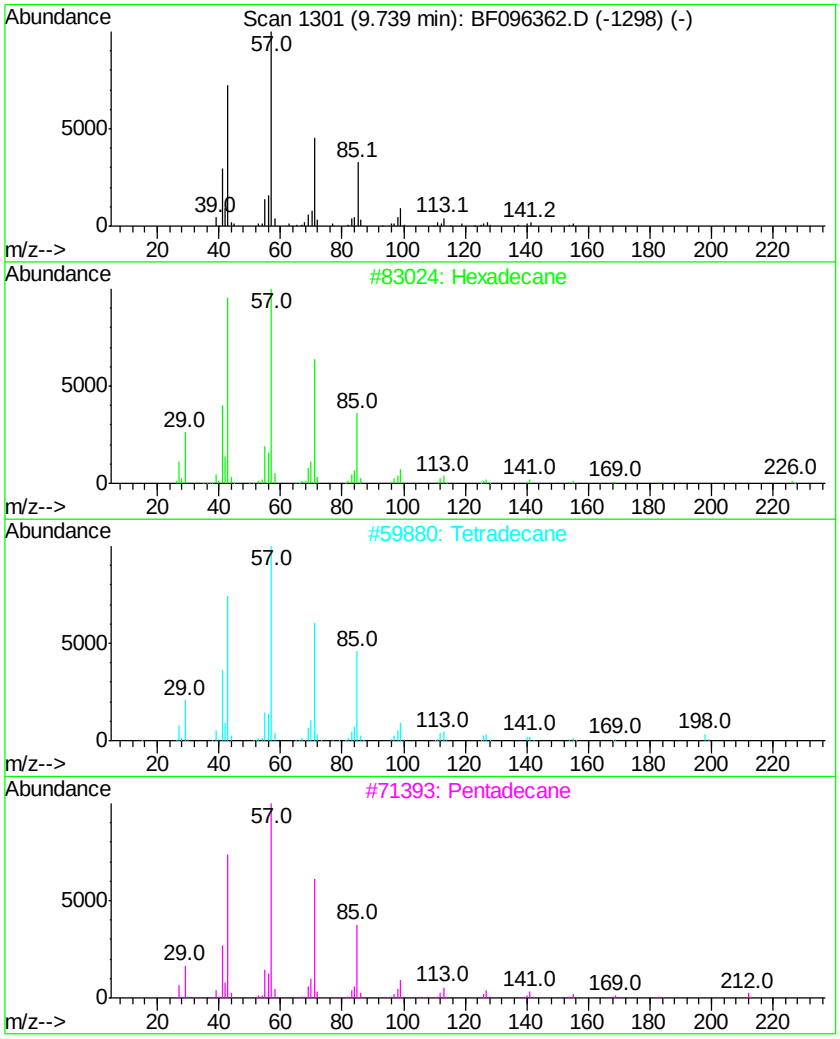
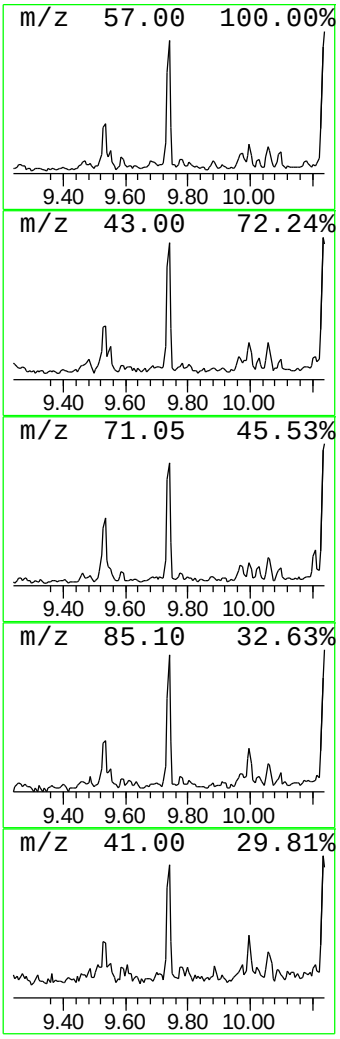
****

Peak Number 4 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	2.12 ng	122074	Acenaphthene-d10	9.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Pentadecane	212	C15H32	000629-62-9	86
4	Tridecane	184	C13H28	000629-50-5	78
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	53





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Instrument : BNA_F
ClientSampleId : B3-6-8.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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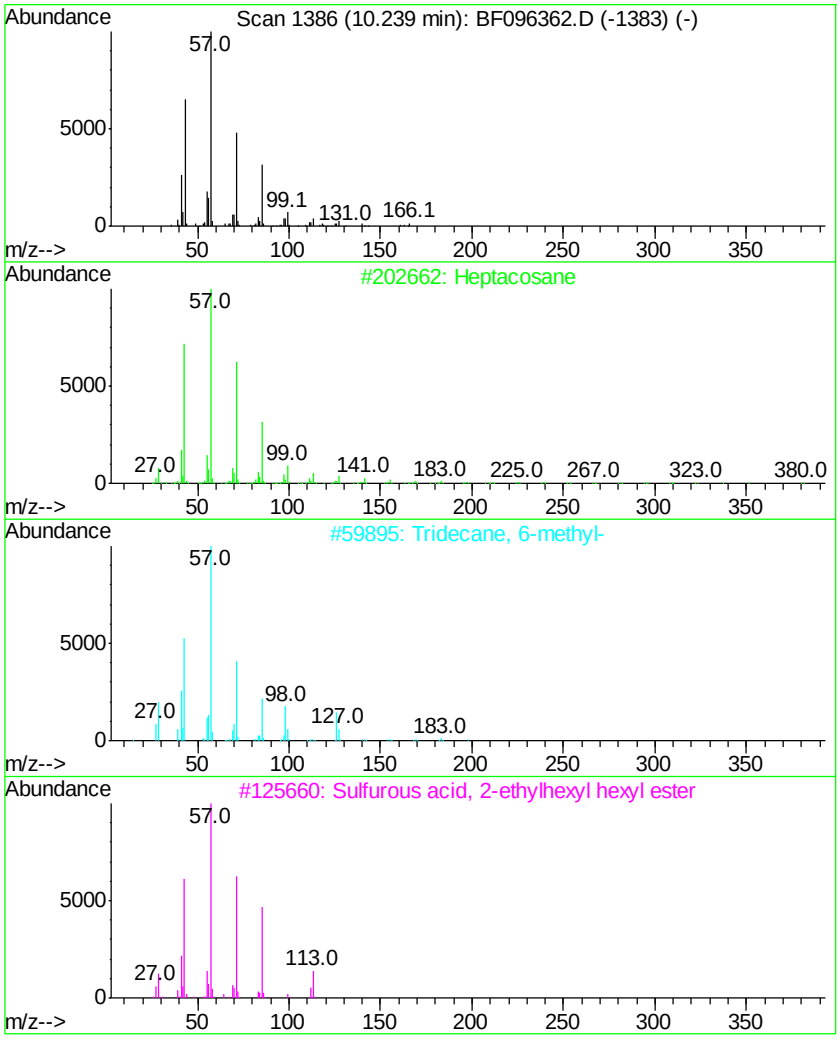
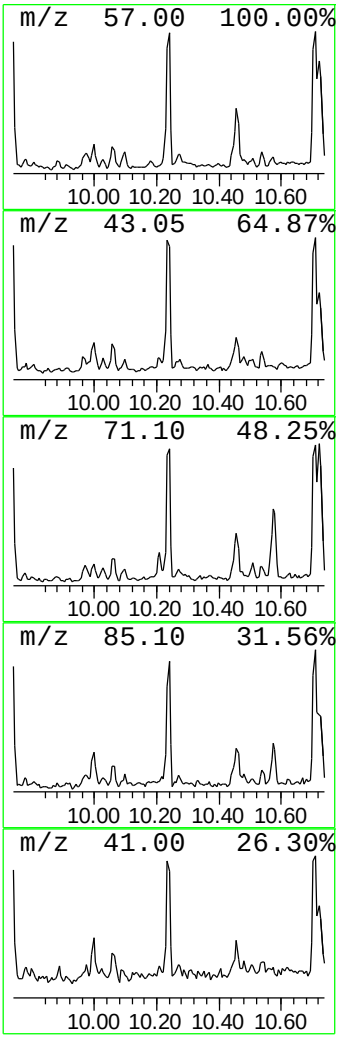
Peak Number 5 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	2.34 ng	135085	Acenaphthene-d10	9.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	83
2	Tridecane, 6-methyl-	198	C14H30	013287-21-3	72
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64
4	Octadecane	254	C18H38	000593-45-3	64
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	59





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Instrument : BNA_F
ClientSampleId : B3-6-8.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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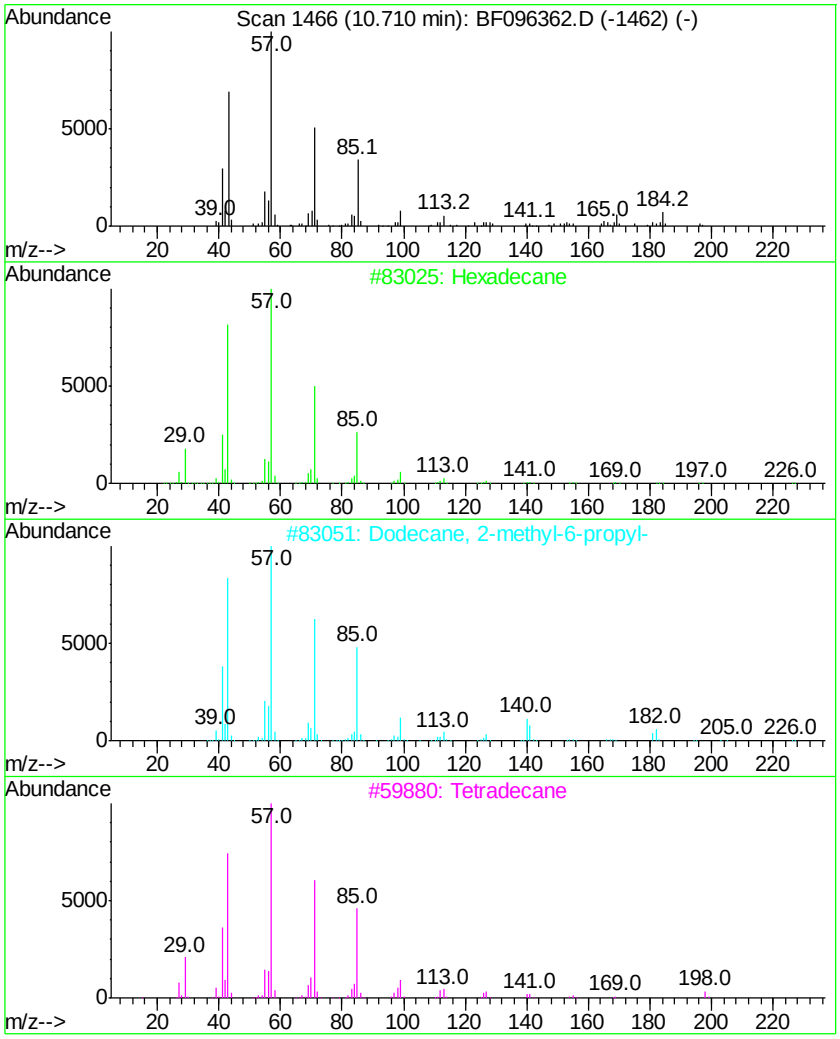
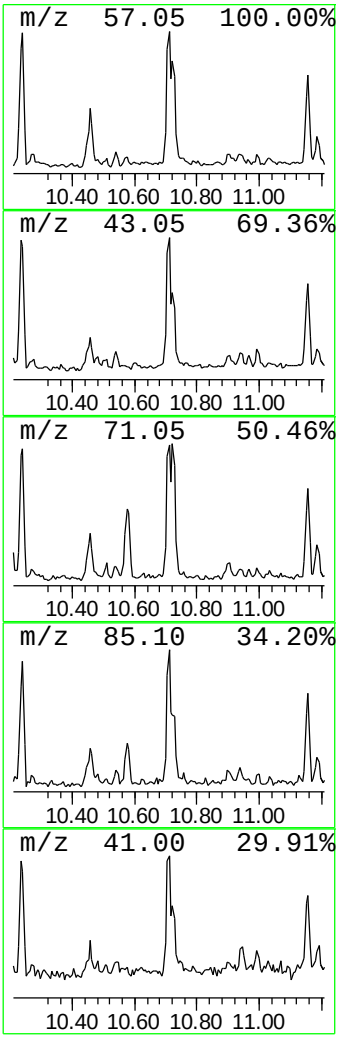
Peak Number 6 Undecane, 5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	3.67 ng	175478	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
3	Tetradecane	198	C14H30	000629-59-4	80
4	Undecane, 2-methyl-	170	C12H26	007045-71-8	80
5	Undecane, 5-methyl-	170	C12H26	001632-70-8	74





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Acq On : 1 Jul 2017 3:20
Operator : SJ/MA
Sample : I3930-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3-6-8.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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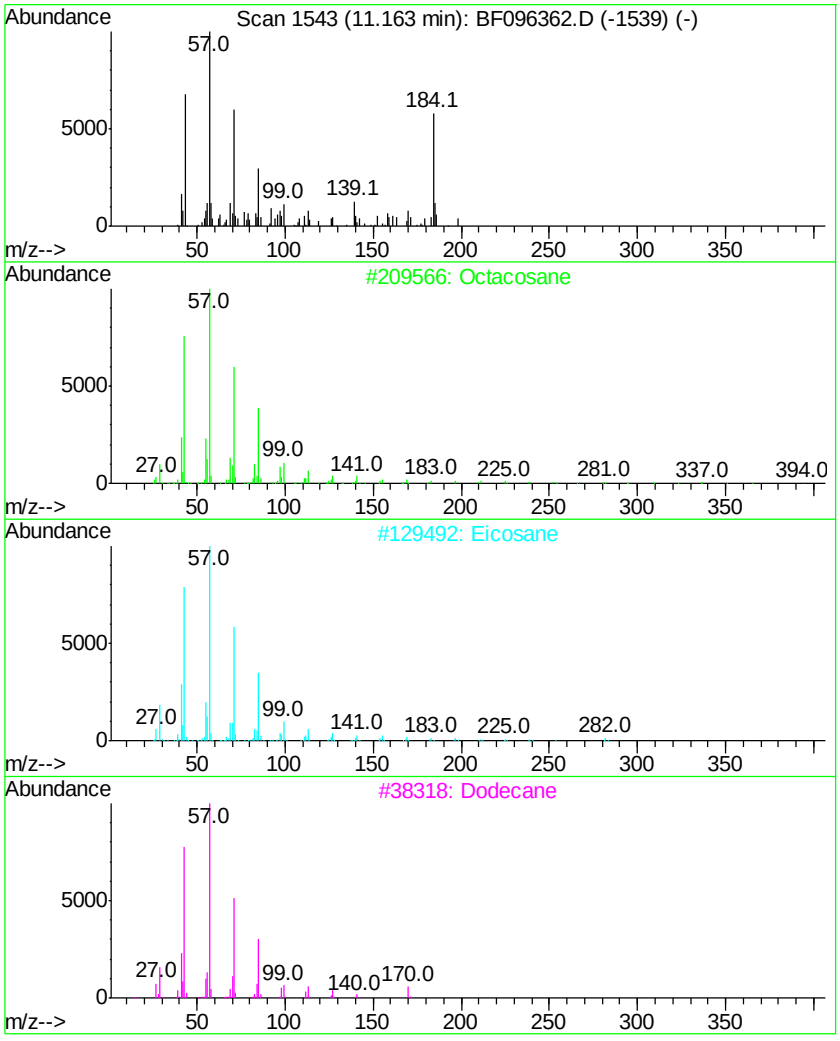
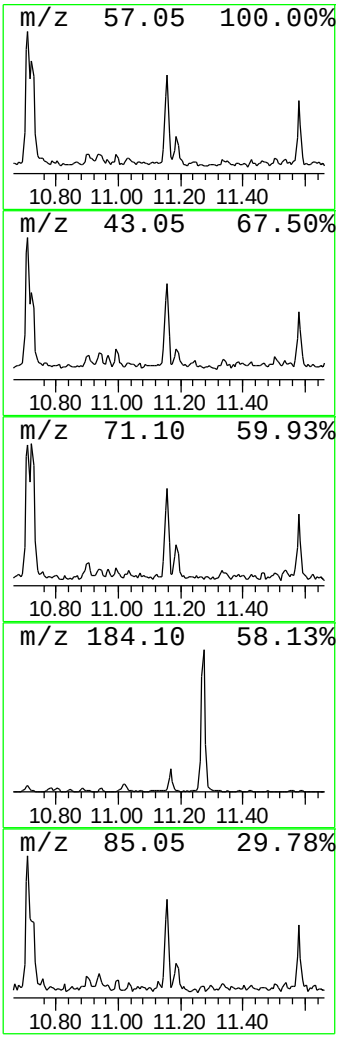
Peak Number 7 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	2.90 ng	138955	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	83
2	Eicosane	282	C20H42	000112-95-8	83
3	Dodecane	170	C12H26	000112-40-3	80
4	Heptacosane	380	C27H56	000593-49-7	80
5	Docosane	310	C22H46	000629-97-0	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096362.D
Acq On : 1 Jul 2017 3:20
Operator : SJ/MA
Sample : I3930-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3-6-8.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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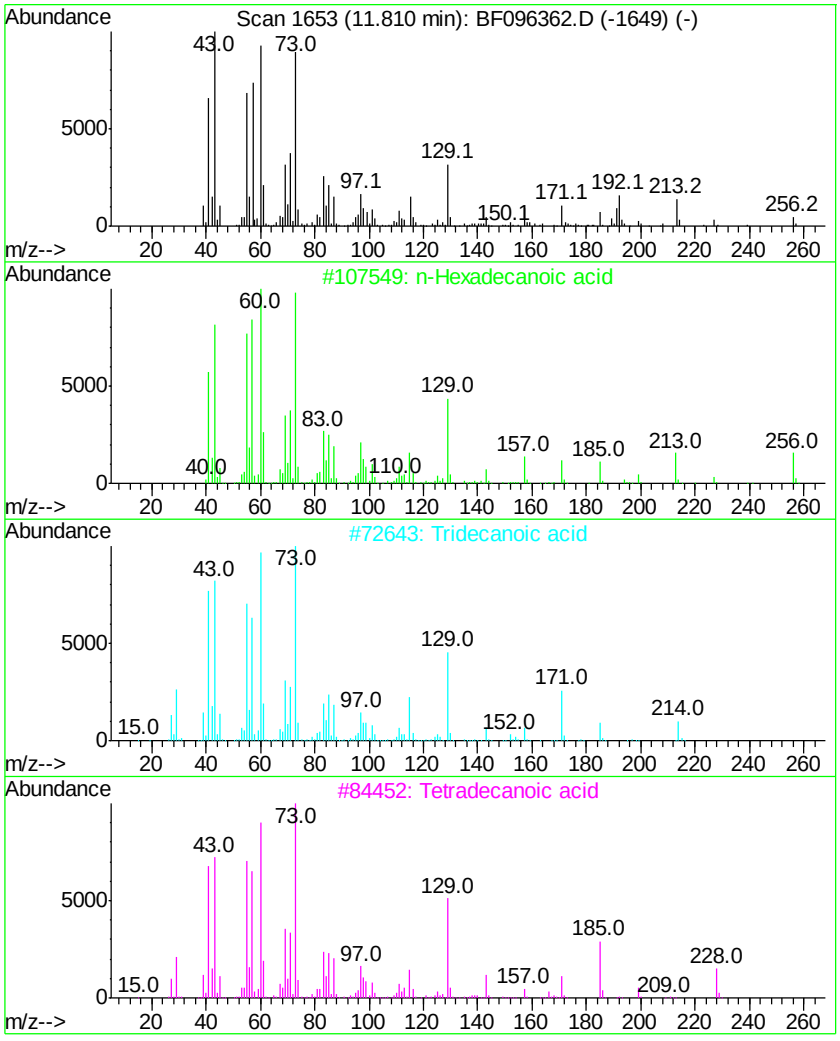
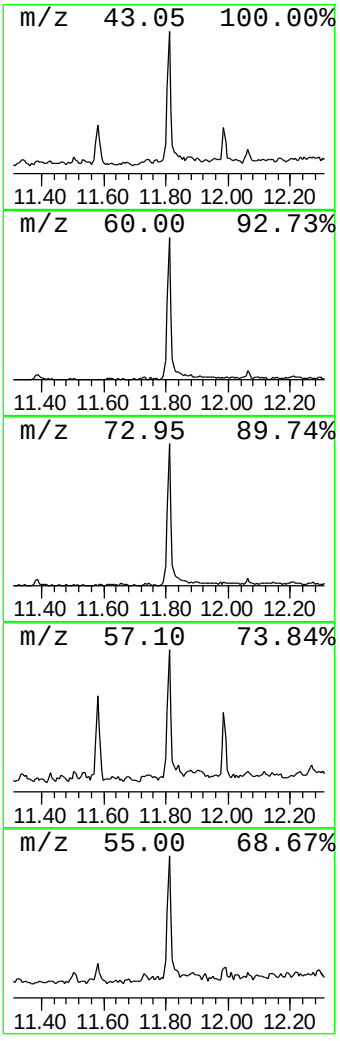
Peak Number 9 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	9.85 ng	471190	Phenanthrene-d10	11.27

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	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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Acq On : 1 Jul 2017 3:20
Operator : SJ/MA
Sample : I3930-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3-6-8.5

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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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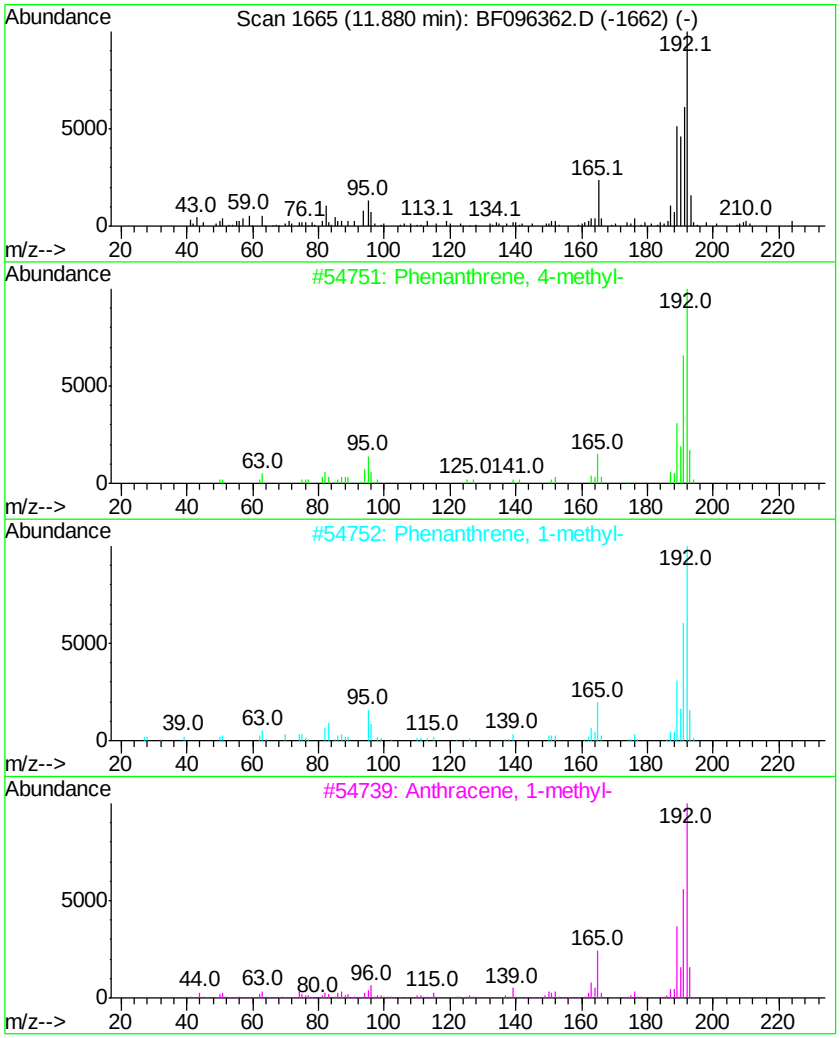
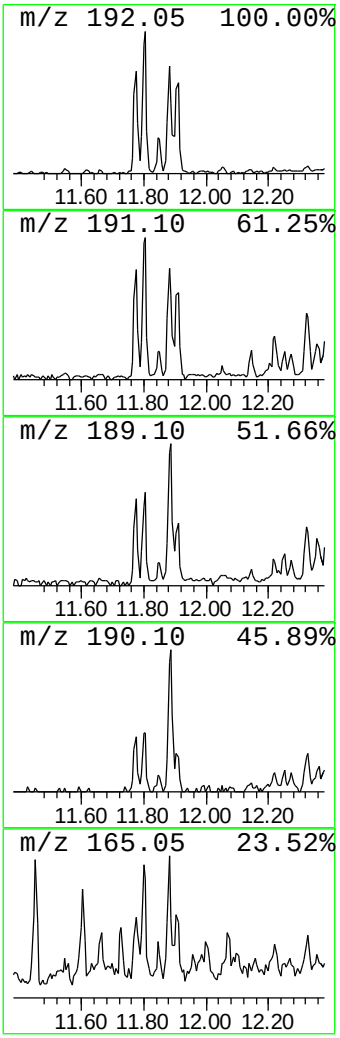
Peak Number 10 Phenanthrene, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	2.88 ng	137841	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	92
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	83
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	64
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	64





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Sample : I3930-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3-6-8.5

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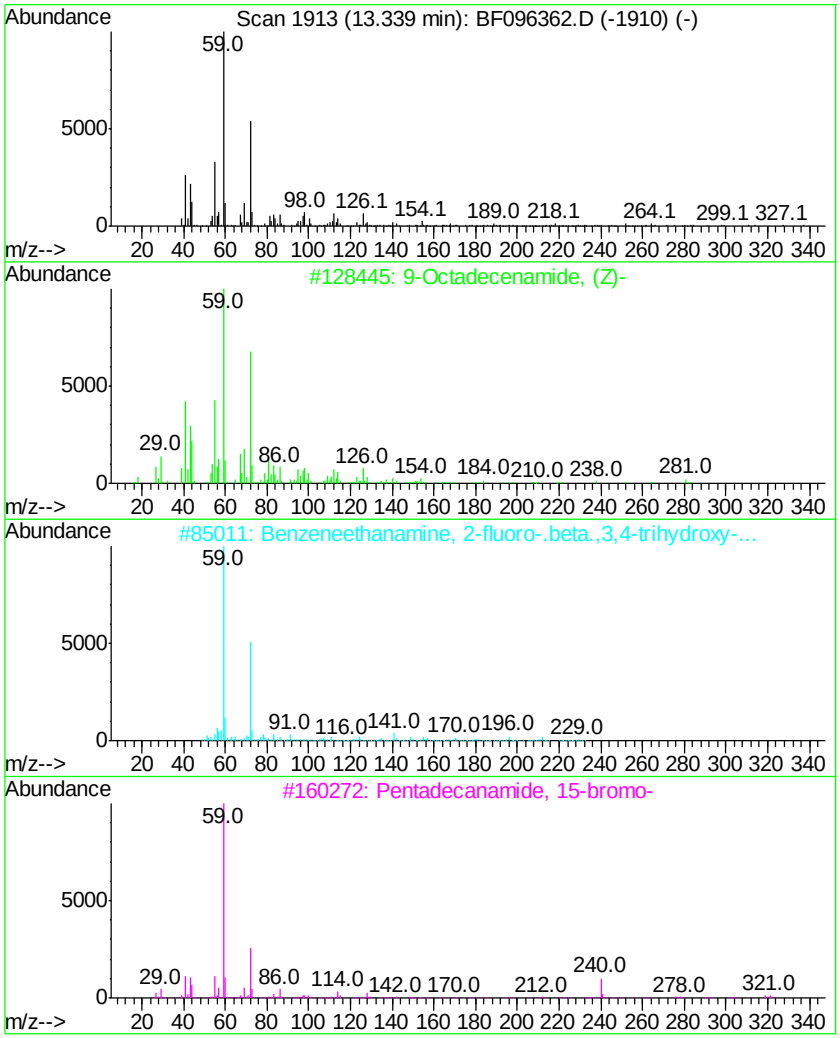
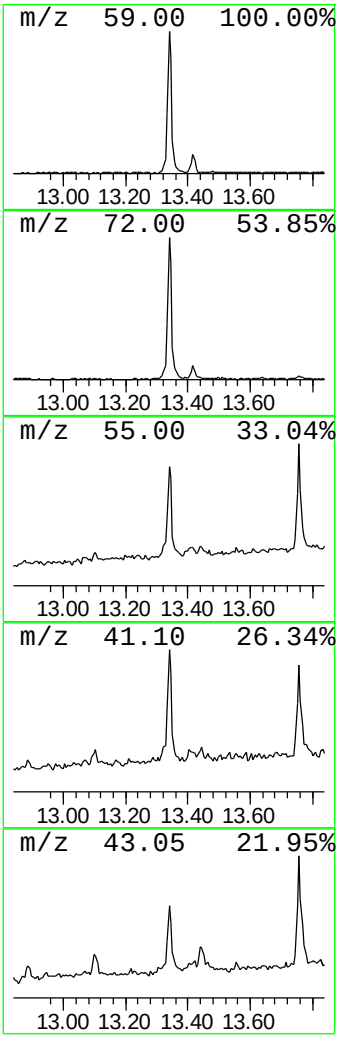
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	7.77 ng	382870	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
3	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
4	Dodecanamide	199	C12H25NO	001120-16-7	56
5	Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	53





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Sample : I3930-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3-6-8.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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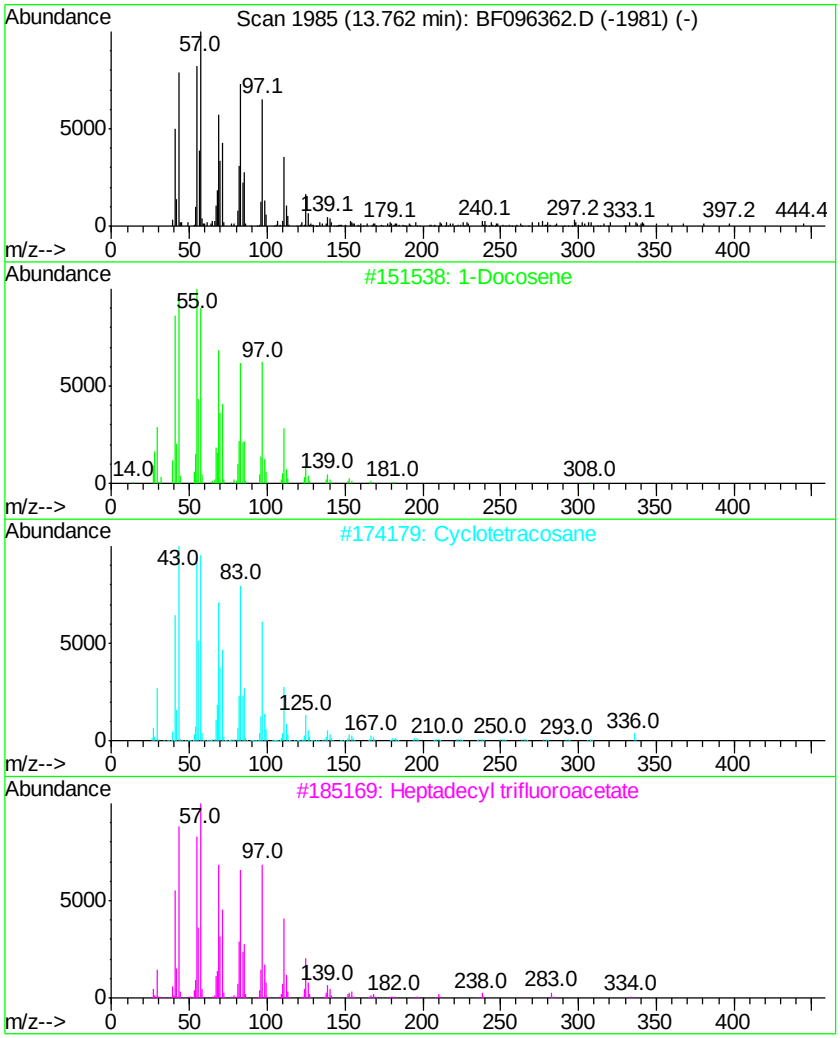
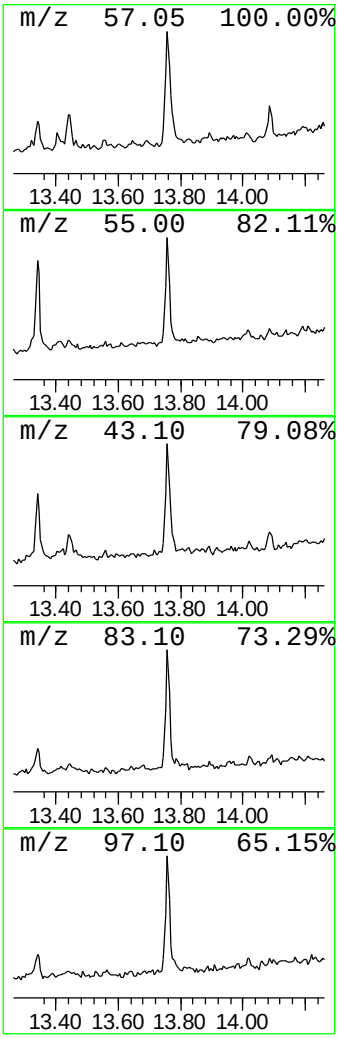
Peak Number 12 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	7.11 ng	350500	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	96
2	Cyclotetracosane	336	C24H48	000297-03-0	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5	1-Tricosene	322	C23H46	018835-32-0	91





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Sample : I3930-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B3-6-8.5

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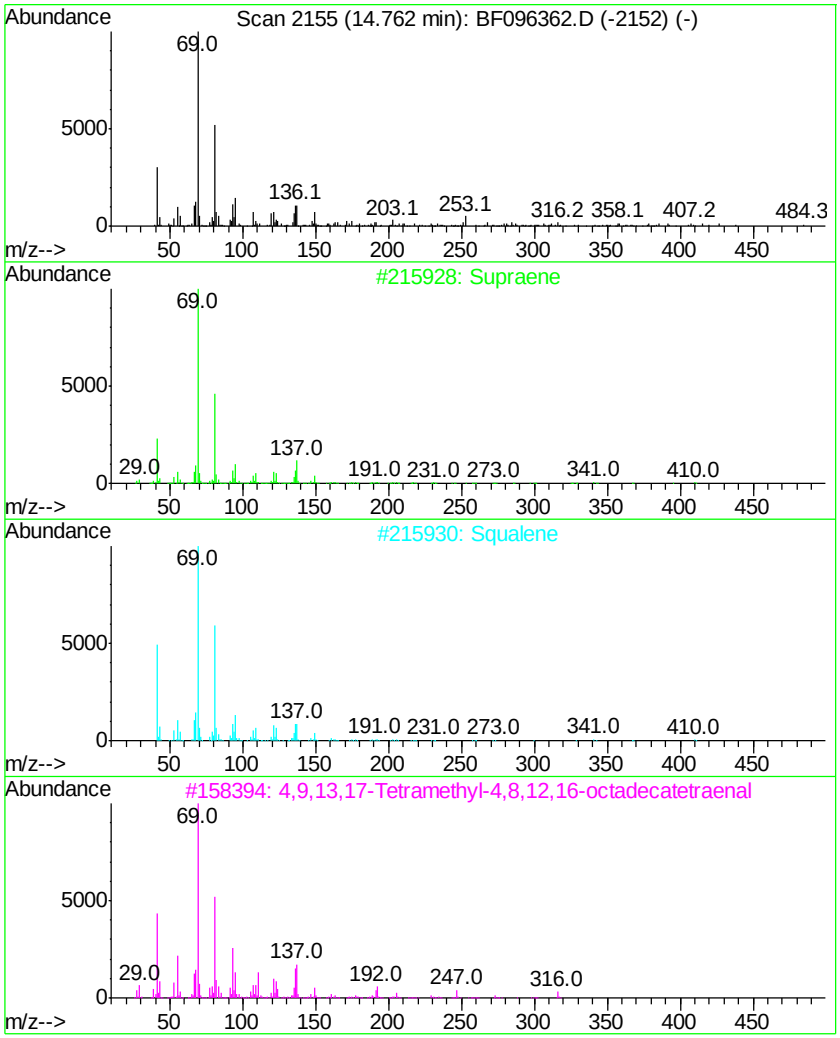
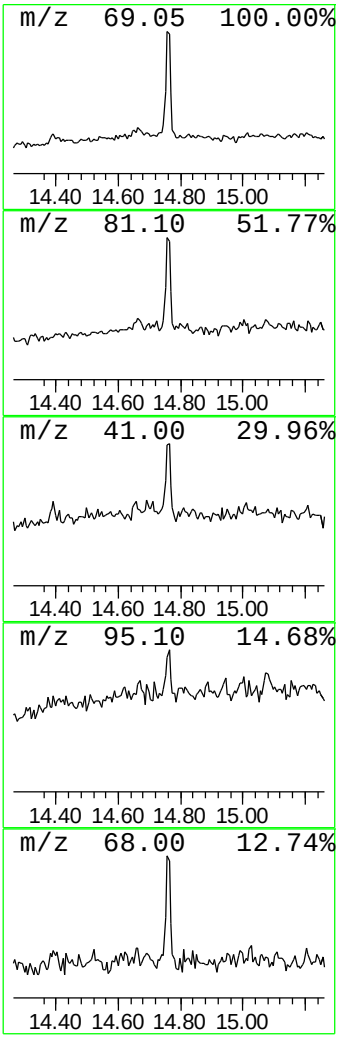
Peak Number 13 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	6.25 ng	153109	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	trans-Farnesol	222	C15H26O	000106-28-5	64





Tentatively Identified Compound (LSC) summary

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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...	4.96	15.1	ng	731346	1	6.76	968935	20.0
unknown6.53	6.53	82.4	ng	3993650	1	6.76	968935	20.0
Hexadecane	9.74	2.1	ng	122074	3	9.79	1154180	20.0
Heptacosane	10.24	2.3	ng	135085	3	9.79	1154180	20.0
Undecane, 5-methyl-	10.71	3.7	ng	175478	4	11.27	956977	20.0
Octacosane	11.16	2.9	ng	138955	4	11.27	956977	20.0
n-Hexadecanoic acid	11.81	9.8	ng	471190	4	11.27	956977	20.0
Phenanthrene, 4-m...	11.88	2.9	ng	137841	4	11.27	956977	20.0
9-Octadecenamide,...	13.34	7.8	ng	382870	5	13.90	985611	20.0
1-Docosene	13.76	7.1	ng	350500	5	13.90	985611	20.0
Supraene	14.76	6.3	ng	153109	6	15.33	489715	20.0