LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096621.D
Acq On : 11 Jul 2017 00:33
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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	3.010	155	157	169	rBV2	30856	74454	2.65%	0.287%
2	4.869	469	473	487	rVB	415562	587287	20.88%	2.265%
3	5.298	541	546	549	rBV	2791779	2812578	100.00%	10.849%
4	6.328	711	721	724	rBV	2649740	2754340	97.93%	10.624%
5	6.457	738	743	746	rBV	2712121	2709693	96.34%	10.452%
6	6.681	778	781	785	rBV	802741	729900	25.95%	2.815%
7	6.839	804	808	812	rBV	2182046	2053556	73.01%	7.921%
8	7.245	867	877	880	rBV	1664172	1589939	56.53%	6.133%
9	7.357	888	896	898	rBV4	54485	93140	3.31%	0.359%
10	7.492	915	919	924	rVB3	24971	39473	1.40%	0.152%
11	7.610	932	939	944	rVB7	26481	49258	1.75%	0.190%
12	7.875	980	984	987	rVB3	31554	34510	1.23%	0.133%
13	7.963	995	999	1003	rBV	1121829	985998	35.06%	3.803%
14	8.045	1011	1013	1015	rVB	69113	46835	1.67%	0.181%
15	8.180	1033	1036	1040	rVB3	44532	36167	1.29%	0.140%
16	8.269	1046	1051	1053	rBV5	32628	46635	1.66%	0.180%
17	8.404	1070	1074	1078	rBV	97305	107998	3.84%	0.417%
18	8.475	1083	1086	1089	rBV4	36886	34260	1.22%	0.132%
19	8.516	1089	1093	1098	rBV7	37013	48270	1.72%	0.186%
20	8.575	1100	1103	1105	rBV2	44405	45300	1.61%	0.175%
21	8.669	1116	1119	1123	rVB4	42776	47254	1.68%	0.182%
22	8.786	1137	1139	1145	rVB6	26570	34107	1.21%	0.132%
23	8.857	1148	1151	1153	rBV3	28687	30548	1.09%	0.118%
24	9.004	1172	1176	1178	rVB	108273	92660	3.29%	0.357%
25	9.045	1178	1183	1186	rBV	2369643	2315541	82.33%	8.931%
26	9.133	1194	1198	1202	rVB3	69739	83664	2.97%	0.323%
27	9.192	1204	1208	1210	rVB3	21611	29599	1.05%	0.114%
28	9.310	1222	1228	1233	rBV8	32430	68106	2.42%	0.263%
29	9.433	1246	1249	1251	rBV	522820	419673	14.92%	1.619%
30	9.457	1251	1253	1255	rVB	109335	80448	2.86%	0.310%
31	9.633	1281	1283	1286	rVB2	36880	33813	1.20%	0.130%
32	9.663	1286	1288	1292	rBV	81936	66820	2.38%	0.258%
33	9.716	1292	1297	1300	rBV	945773	846586	30.10%	3.265%
34	9.898	1323	1328	1330	rBV5	26476	51697	1.84%	0.199%

LSC Area Percent Report

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Data File : BF096621.D
Acq On : 11 Jul 2017 00:33
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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	9.927	1330	1333	1336	rVV2	48454	60879	2.16%	0.235%
36	9.986	1340	1343	1347	rVV4	54396	55723	1.98%	0.215%
37	10.163	1370	1373	1375	rVB	78520	61253	2.18%	0.236%
38	10.380	1406	1410	1413	rBV	93988	101006	3.59%	0.390%
39	10.498	1426	1430	1434	rVB	1204924	1090358	38.77%	4.206%
40	10.645	1450	1455	1460	rVB2	148562	237426	8.44%	0.916%
41	10.833	1484	1487	1490	rBV3	25568	36170	1.29%	0.140%
42	11.080	1526	1529	1531	rBV	102335	82567	2.94%	0.318%
43	11.110	1531	1534	1539	rVB	96013	97582	3.47%	0.376%
44	11.192	1544	1548	1550	rBV	701640	585772	20.83%	2.259%
45	11.216	1550	1552	1556	rVV	81800	62143	2.21%	0.240%
46	11.263	1557	1560	1564	rVB	45897	48522	1.73%	0.187%
47	11.504	1598	1601	1605	rBV	69490	63134	2.24%	0.244%
48	11.733	1636	1640	1643	rVB3	55552	58409	2.08%	0.225%
49	11.804	1649	1652	1659	rVB3	48577	70933	2.52%	0.274%
50	11.910	1667	1670	1672	rBV	47112	42084	1.50%	0.162%
51	12.245	1723	1727	1730	rBV5	22020	32486	1.16%	0.125%
52	12.298	1734	1736	1739	rVB	36451	38882	1.38%	0.150%
53	12.398	1750	1753	1757	rBV	307210	259799	9.24%	1.002%
54	12.451	1758	1762	1767	rBV6	35966	48468	1.72%	0.187%
55	12.515	1770	1773	1776	rBV5	26866	36222	1.29%	0.140%
56	12.627	1786	1792	1795	rBV	249808	288899	10.27%	1.114%
57	12.774	1813	1817	1821	rBV	1396284	1354842	48.17%	5.226%
58	12.957	1845	1848	1851	rVB	44100	46322	1.65%	0.179%
59	13.021	1856	1859	1862	rVB2	50271	47461	1.69%	0.183%
60	13.057	1862	1865	1868	rBV3	34670	40272	1.43%	0.155%
61	13.227	1891	1894	1897	rVB5	34272	42639	1.52%	0.164%
62	13.680	1968	1971	1982	rVB3	144221	214154	7.61%	0.826%
63	13.821	1990	1995	1998	rBV	769395	827242	29.41%	3.191%
64	13.845	1998	1999	2002	rVB	114431	68268	2.43%	0.263%
65	14.827	2163	2166	2171	rBV	107771	192736	6.85%	0.743%
66	15.221	2229	2233	2236	rBV	499797	552962	19.66%	2.133%

Sum of corrected areas: 25925722

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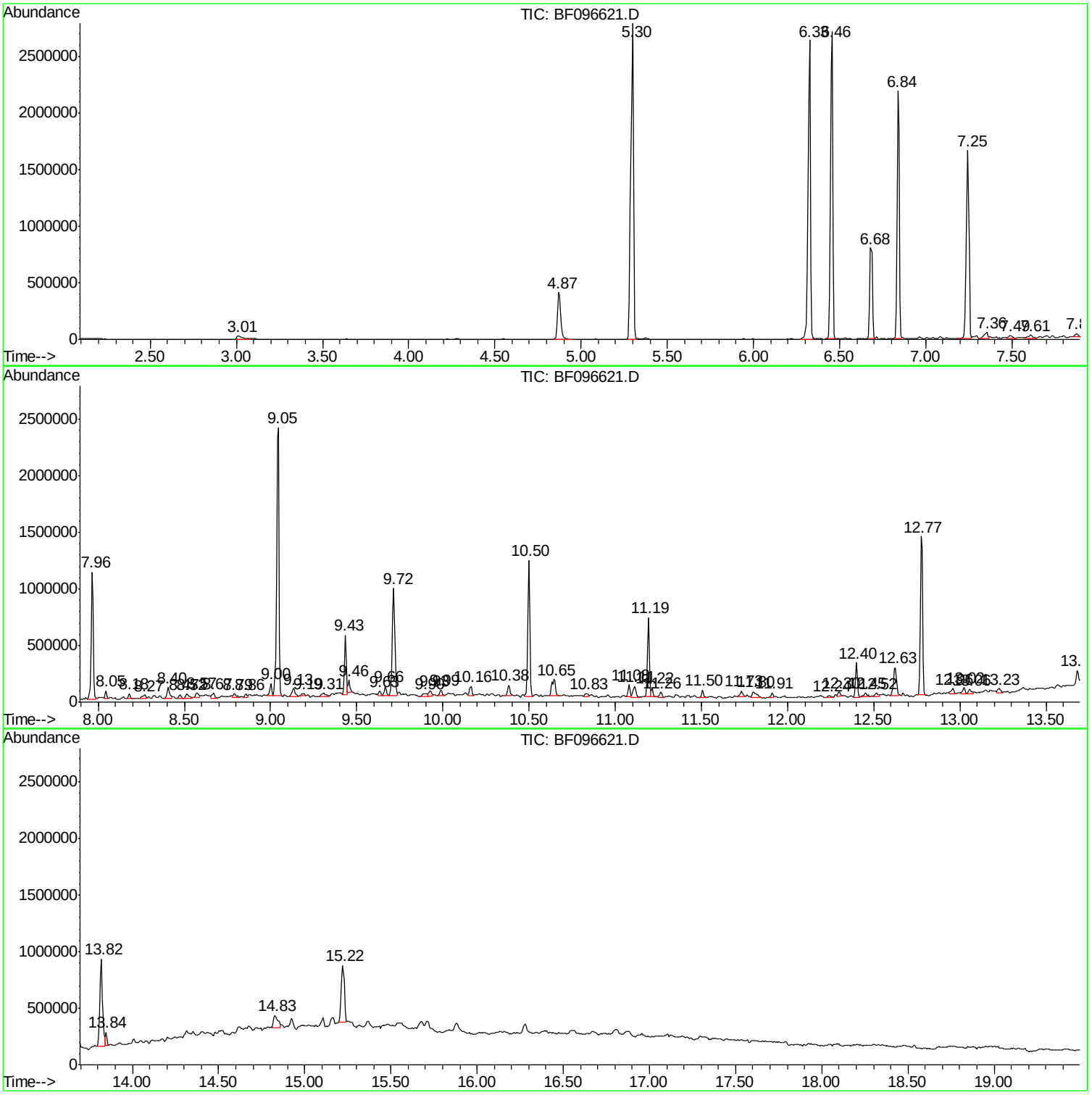
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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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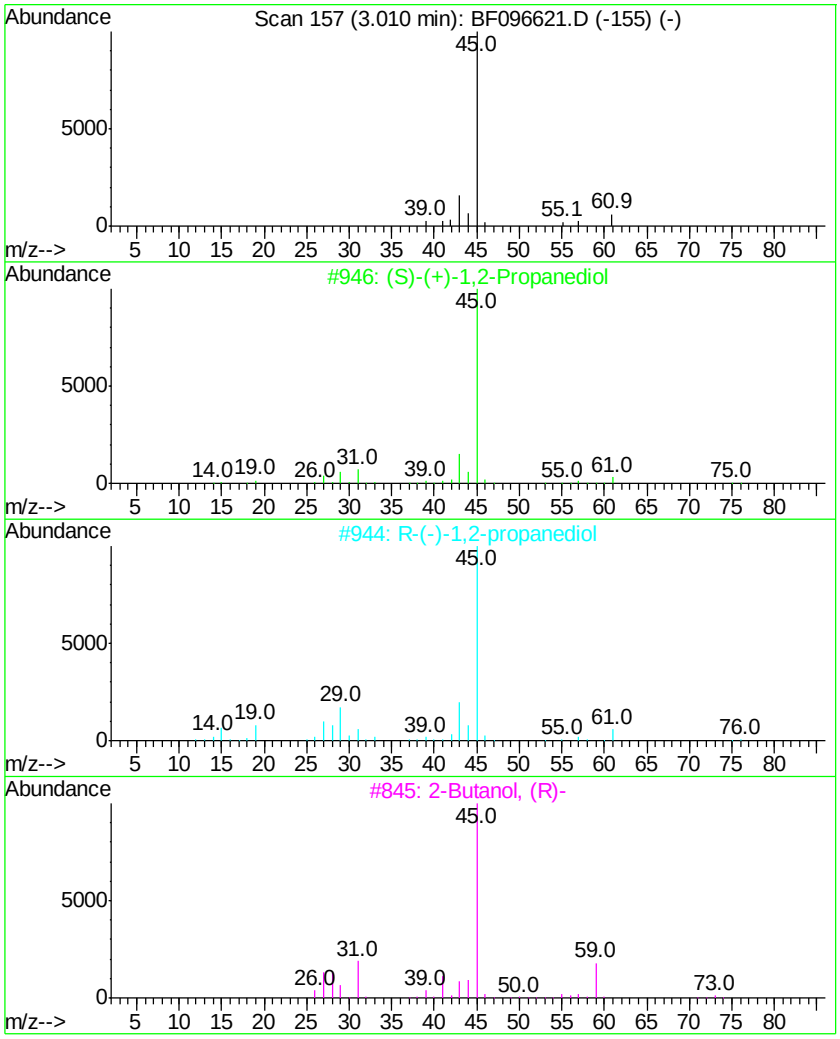
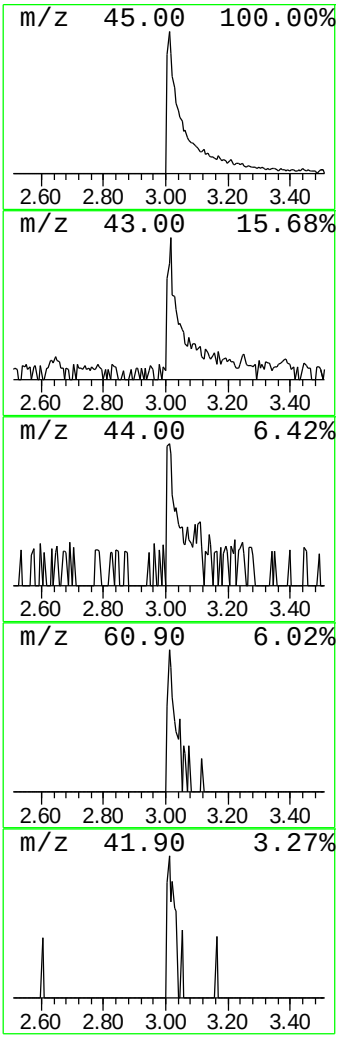
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.01	2.04 ng	74454	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	2-Butanol, (R)-	74	C4H10O	014898-79-4	9
4	2-Butanol	74	C4H10O	000078-92-2	9
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096621.D
Acq On : 11 Jul 2017 00:33
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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

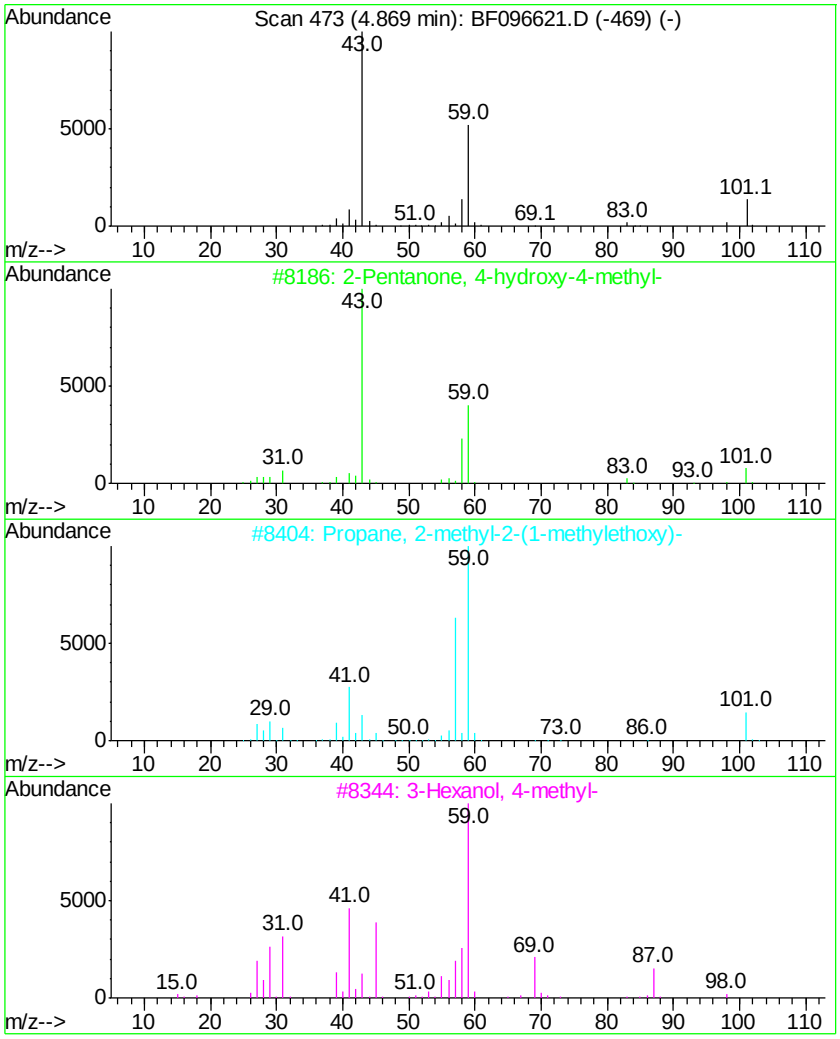
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

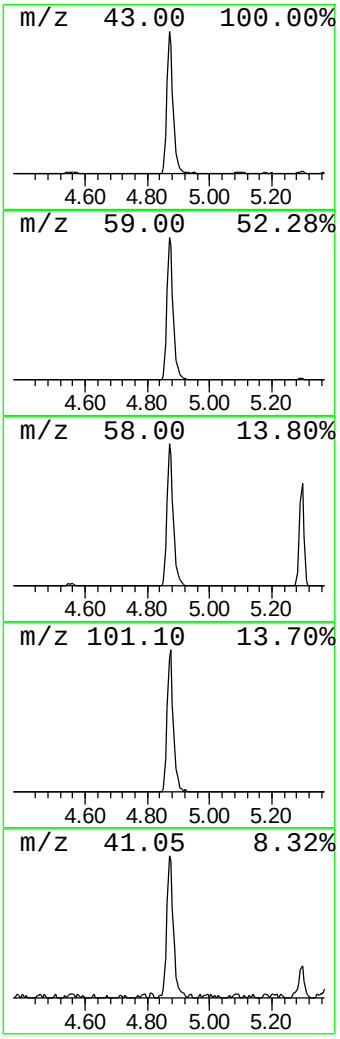
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	16.09 ng	587287	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096621.D
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Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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

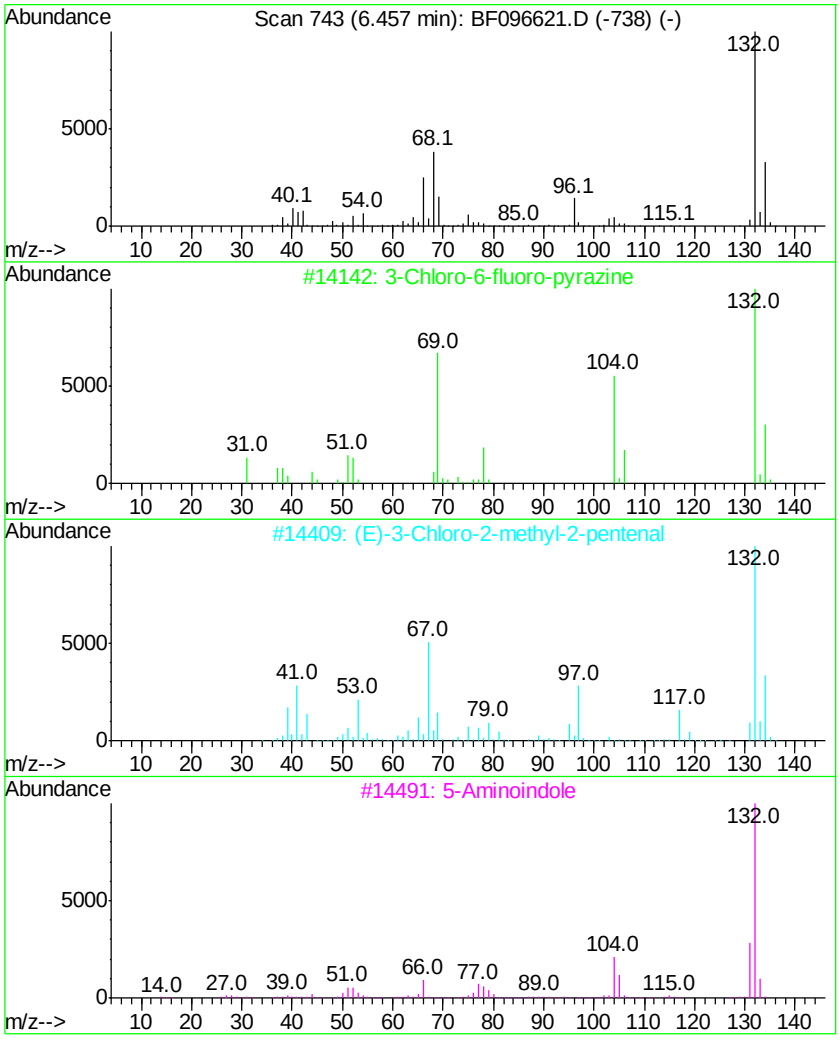
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

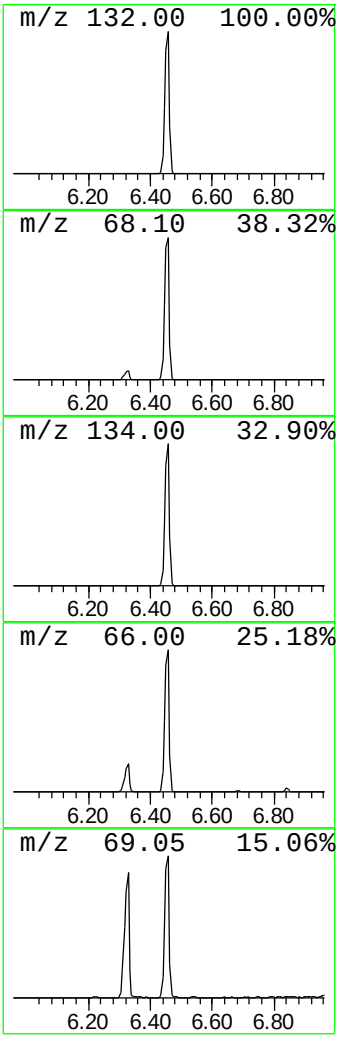
****

Peak Number 3 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	74.25 ng	2709690	1,4-Dichlorobenzene-d4	6.69

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





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Sample : I4108-01
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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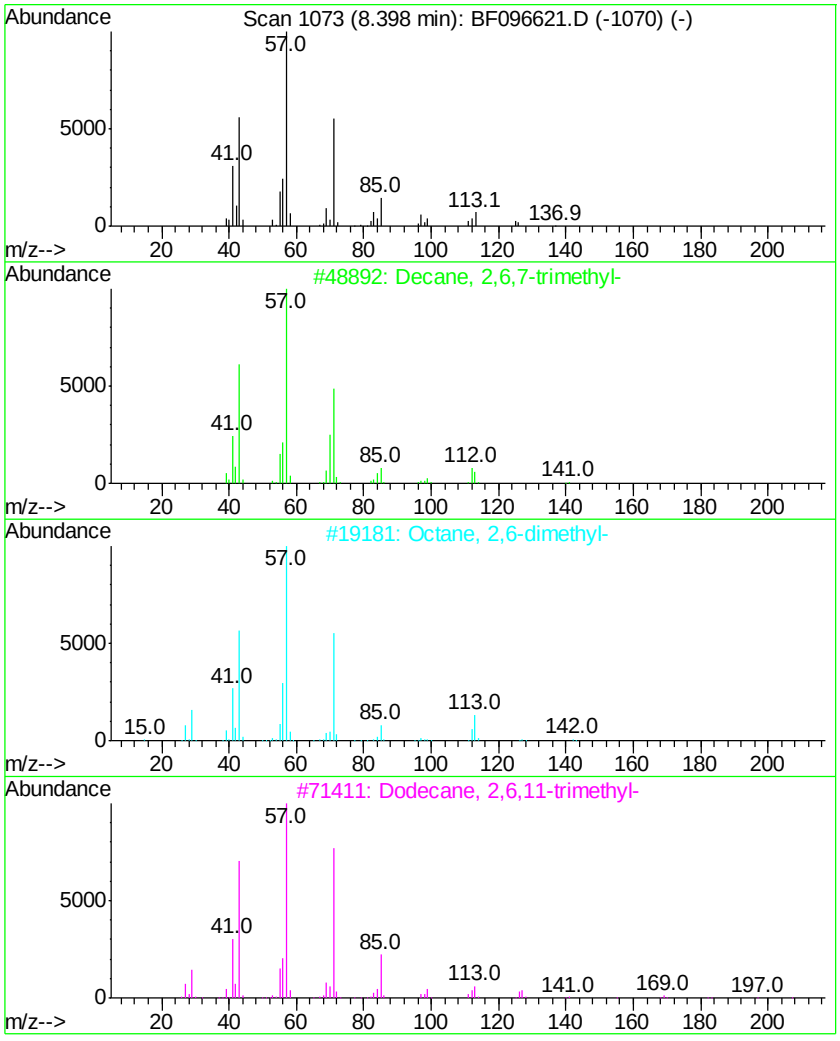
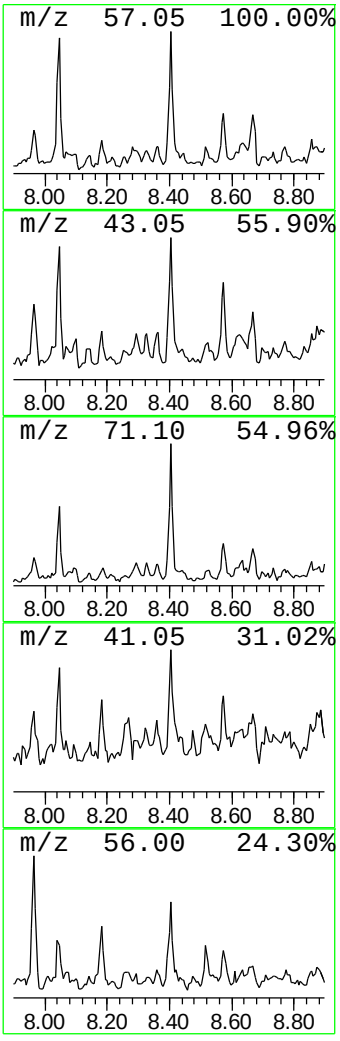
****

Peak Number 5 Decane, 2,6,7-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	2.19 ng	107998	Naphthalene-d8	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	83
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
3	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
4	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	64
5	Nonane, 3-methyl-	142	C10H22	005911-04-6	64





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Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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

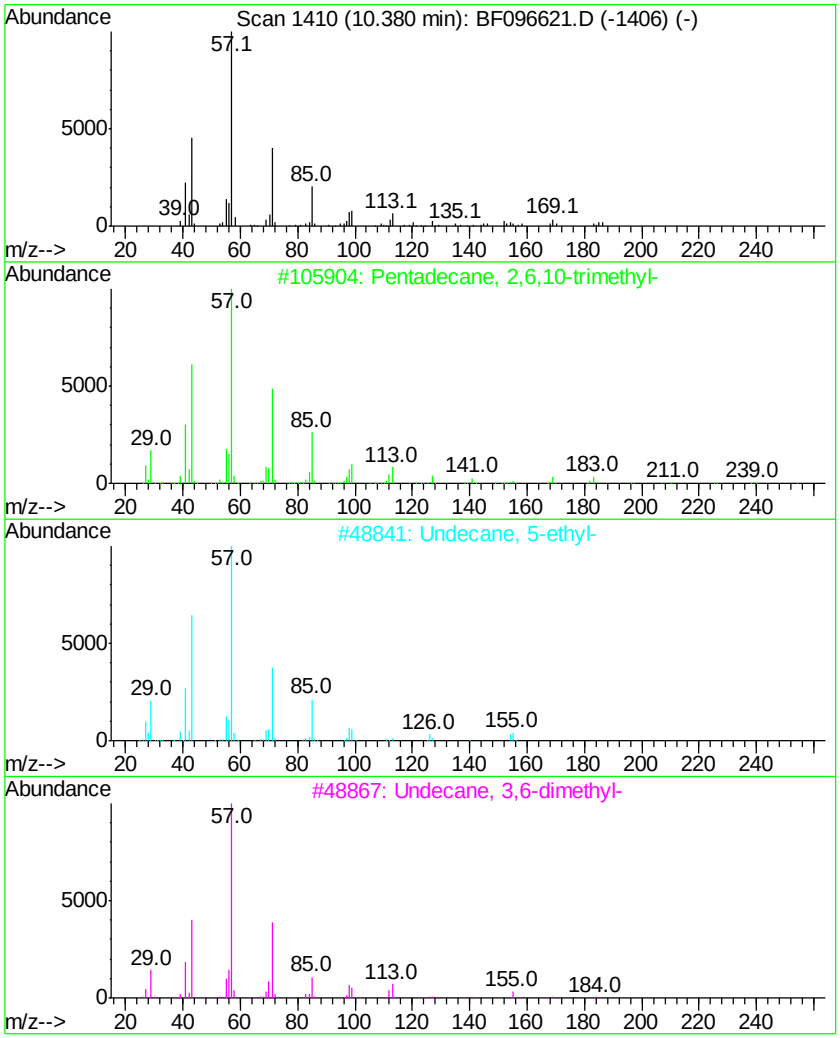
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

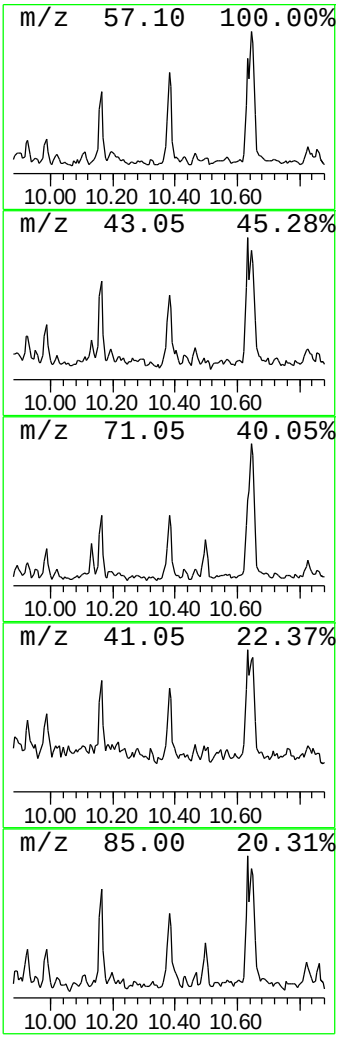
****

Peak Number 6 Pentadecane, 2,6,10-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.39 ng	101006	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
2	Undecane, 5-ethyl-	184	C13H28	017453-94-0	78
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	76
4	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	70
5	Octacosane	394	C28H58	000630-02-4	64





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Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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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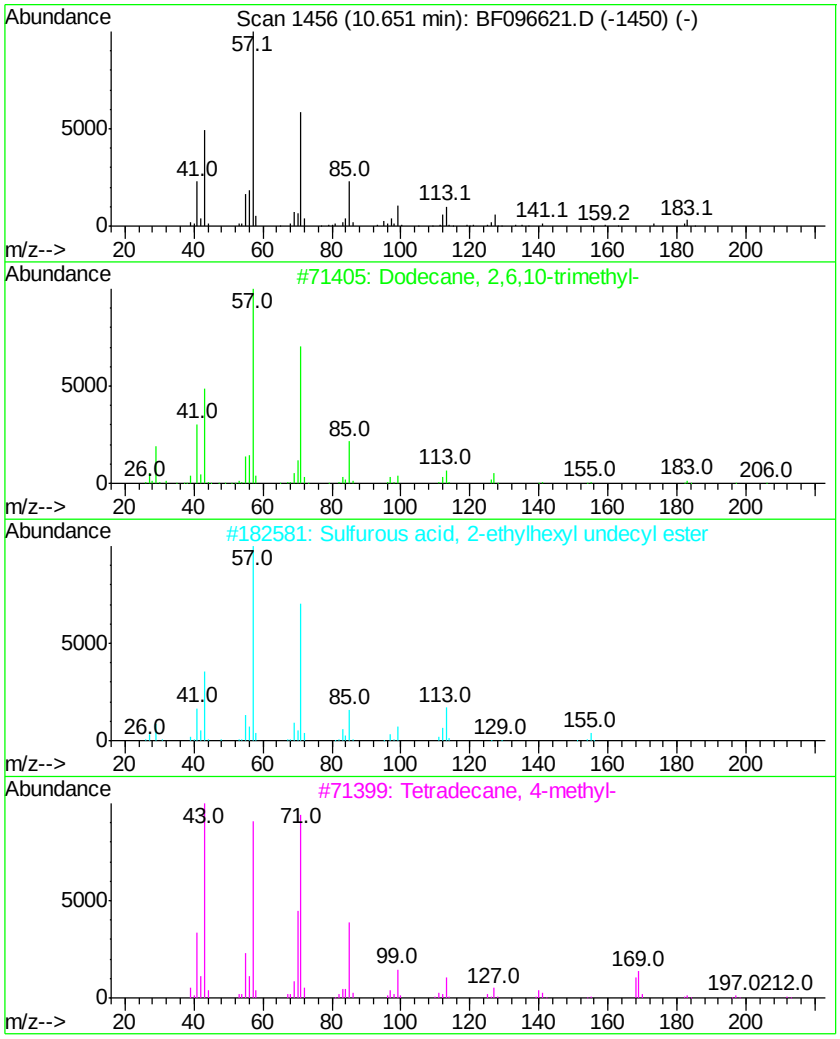
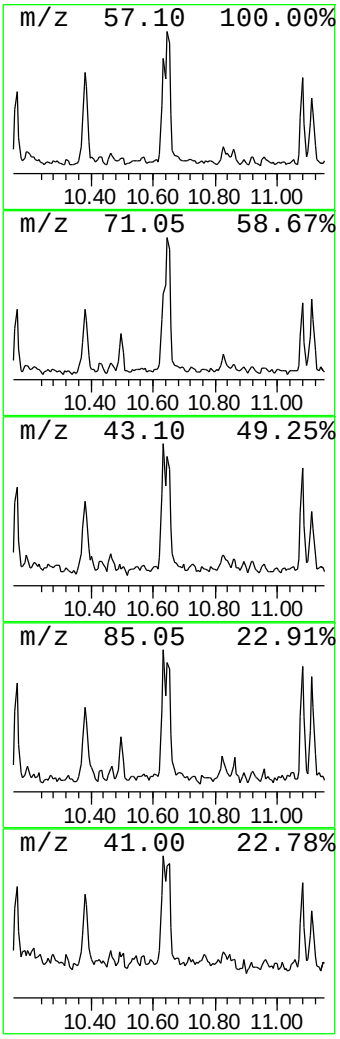
Peak Number 7 Dodecane, 2,6,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	8.11 ng	237426	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	78
2	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	64
3	Tetradecane, 4-methyl-	212	C15H32	025117-24-2	59
4	Tridecane, 6-methyl-	198	C14H30	013287-21-3	53
5	Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096621.D
Acq On : 11 Jul 2017 00:33
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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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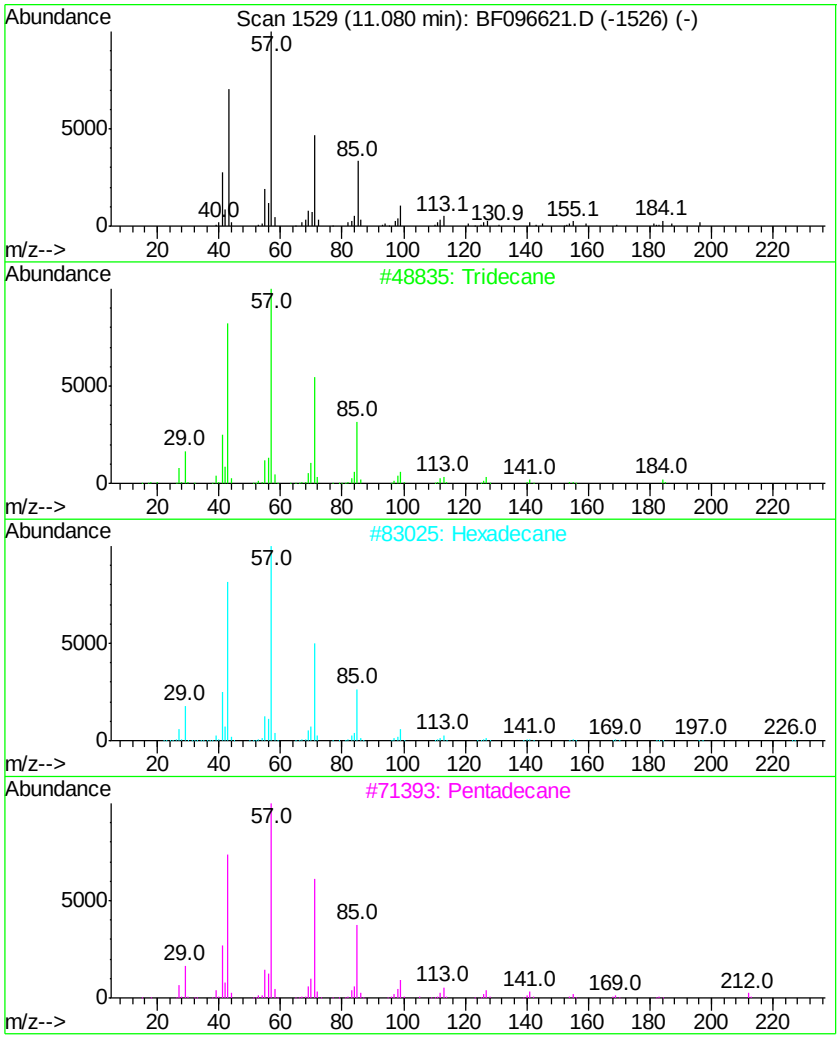
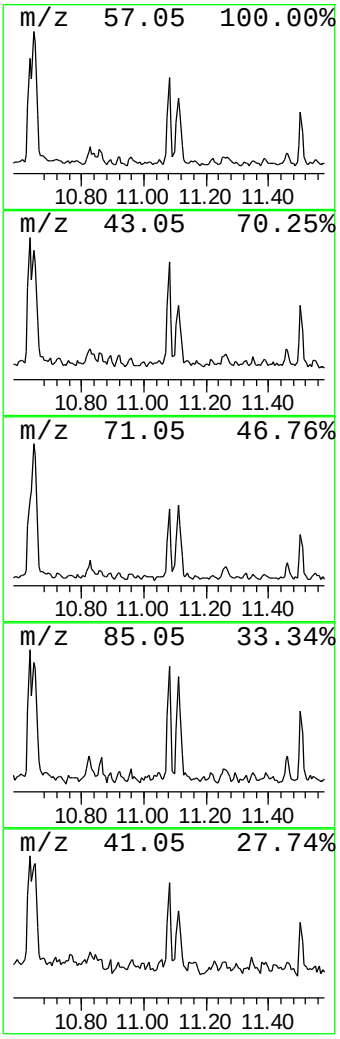
Peak Number 8 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	2.82 ng	82567	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tetradecane	198	C14H30	000629-59-4	86
5	Tetracosane	338	C24H50	000646-31-1	83





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Data File : BF096621.D
Acq On : 11 Jul 2017 00:33
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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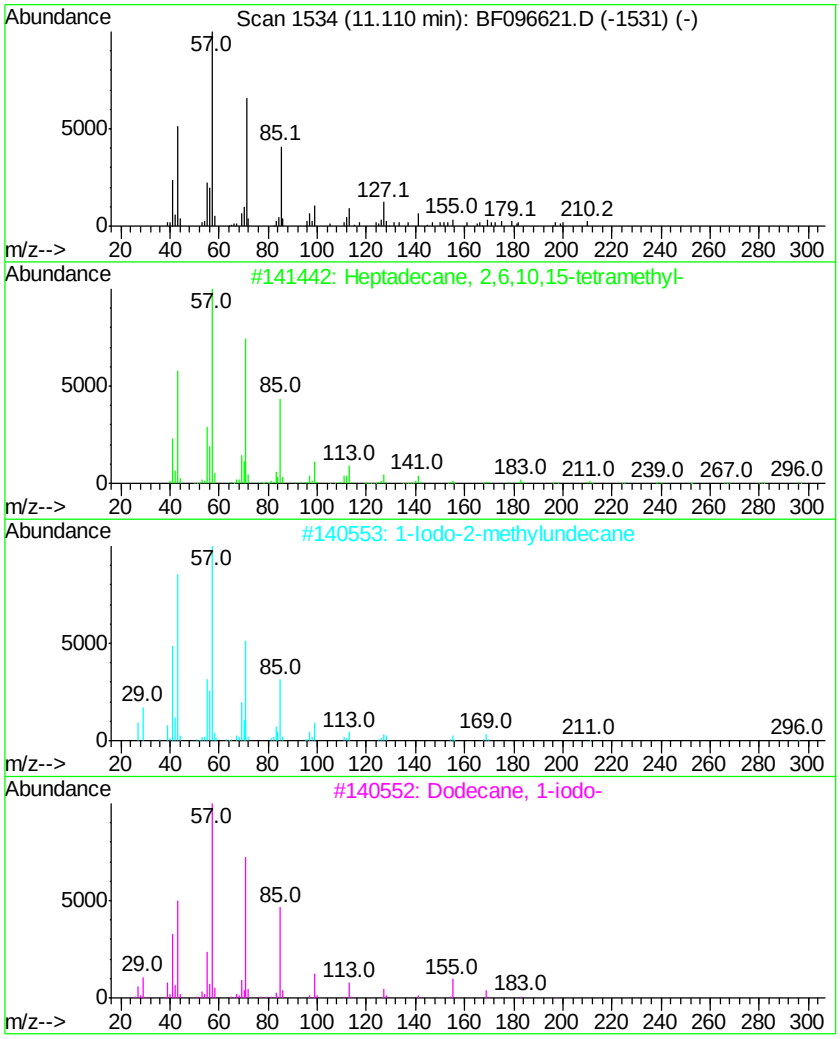
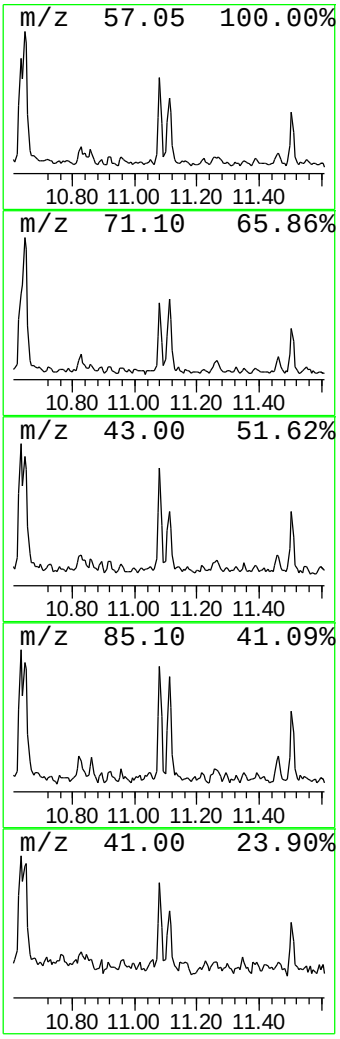
Peak Number 9 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.11	3.33 ng	97582	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	72
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
4	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096621.D
Acq On : 11 Jul 2017 00:33
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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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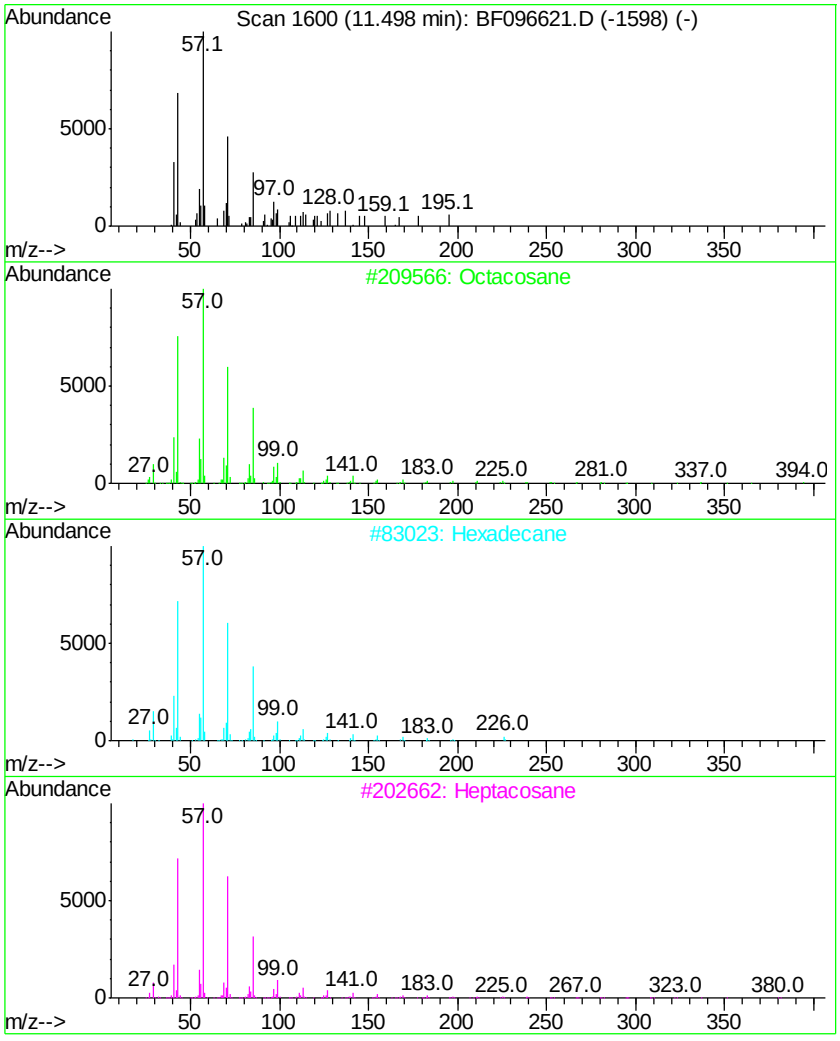
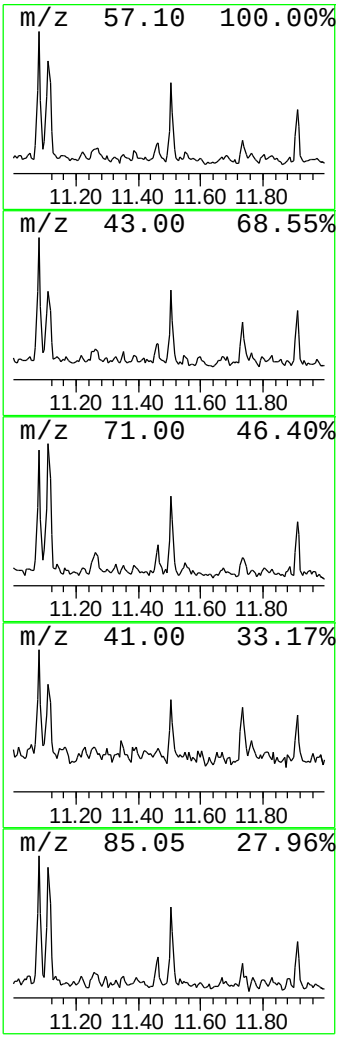
Peak Number 10 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	2.16 ng	63134	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Heptacosane	380	C27H56	000593-49-7	80
4	Tetradecane	198	C14H30	000629-59-4	78
5	Octadecane	254	C18H38	000593-45-3	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096621.D
Acq On : 11 Jul 2017 00:33
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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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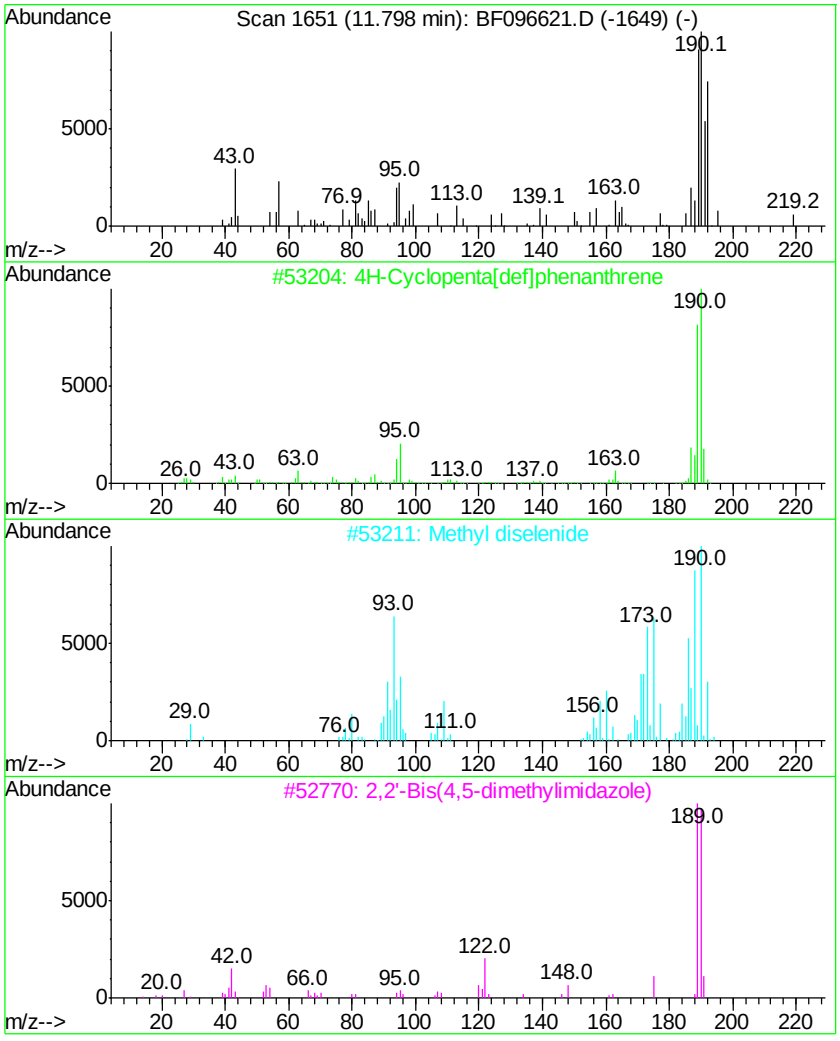
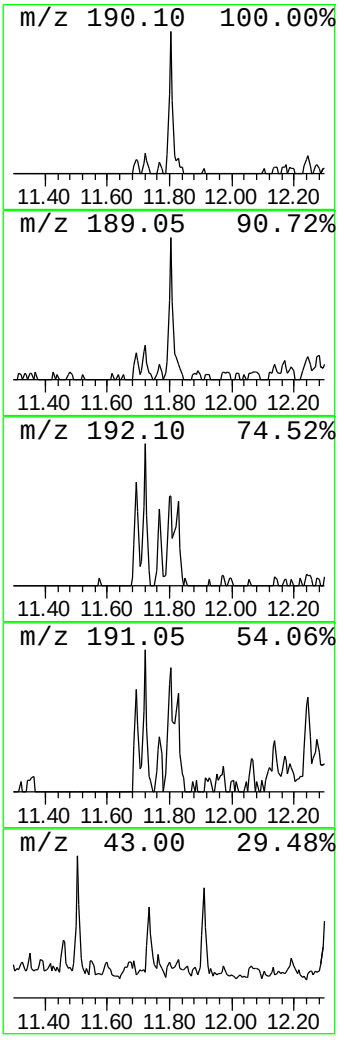
Peak Number 11 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.42 ng	70933	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Methyl diselenide	190	C2H6Se2	007101-31-7	53
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43
4	1-Methyl-2-phenylpiperidin-4-one	189	C12H15NO	091640-05-0	38
5	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	37





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096621.D
Acq On : 11 Jul 2017 00:33
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-01-070617-A

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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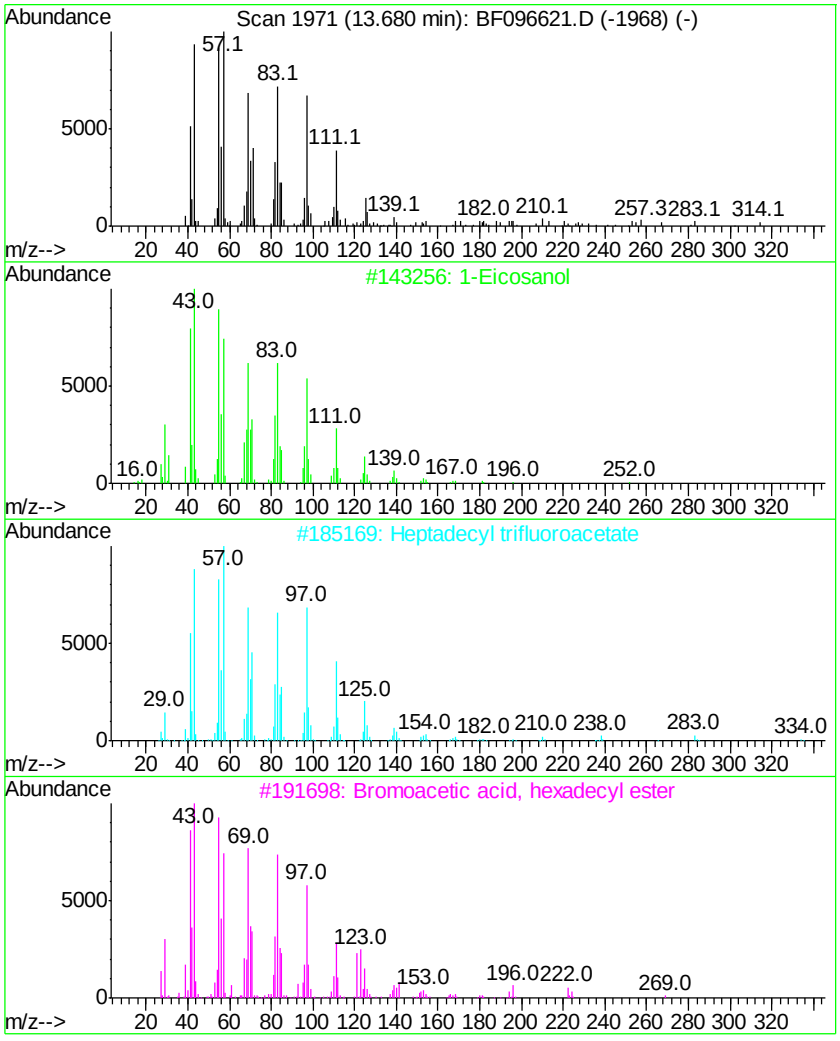
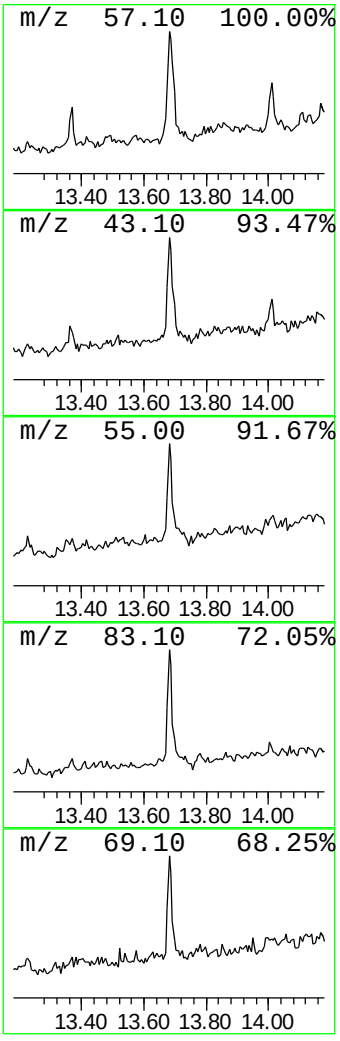
Peak Number 12 1-Eicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	5.18 ng	214154	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	91
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
4	1-Docosene	308	C22H44	001599-67-3	87
5	Octacosanol	410	C28H58O	000557-61-9	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
Data File : BF096621.D
Acq On : 11 Jul 2017 00:33
Operator : SJ/JU
Sample : I4108-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-01-070617-A

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
(S)-(+)-1,2-Propa...	3.01	2.0	ng	74454	1	6.69	729900	20.0
2-Pentanone, 4-hy...	4.87	16.1	ng	587287	1	6.69	729900	20.0
unknown6.46	6.46	74.3	ng	2709690	1	6.69	729900	20.0
Decane, 2,6,7-tri...	8.40	2.2	ng	107998	2	7.96	985998	20.0
Pentadecane, 2,6,...	10.38	2.4	ng	101006	3	9.72	846586	20.0
Dodecane, 2,6,10-...	10.65	8.1	ng	237426	4	11.19	585772	20.0
Tridecane	11.08	2.8	ng	82567	4	11.19	585772	20.0
Heptadecane, 2,6,...	11.11	3.3	ng	97582	4	11.19	585772	20.0
Octacosane	11.50	2.2	ng	63134	4	11.19	585772	20.0
4H-Cyclopenta[def...	11.80	2.4	ng	70933	4	11.19	585772	20.0
1-Eicosanol	13.68	5.2	ng	214154	5	13.82	827242	20.0