LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110617\
Data File : BF100273.D
Acq On : 7 Nov 2017 4:34
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

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-BF102317.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	4.992	492	494	507	rBV	21855	58164	4.30%	0.517%
2	5.434	566	569	585	rBV	65715	217199	16.08%	1.930%
3	6.445	739	741	755	rBV2	73220	205663	15.22%	1.827%
4	6.545	755	758	776	rVB	406508	698290	51.68%	6.204%
5	6.763	792	795	807	rBV	426853	495600	36.68%	4.403%
6	6.916	818	821	840	rBV	710161	864944	64.02%	7.684%
7	7.333	890	892	916	rBV	373521	634480	46.96%	5.637%
8	8.045	1010	1013	1027	rBV	597466	770548	57.03%	6.846%
9	8.145	1027	1030	1039	rVB	18707	30329	2.24%	0.269%
10	8.275	1050	1052	1056	rBV2	10591	16581	1.23%	0.147%
11	8.616	1108	1110	1121	rVB	26471	32839	2.43%	0.292%
12	8.704	1121	1125	1128	rBV3	11866	19000	1.41%	0.169%
13	8.769	1134	1136	1144	rBV	33626	36955	2.74%	0.328%
14	8.863	1149	1152	1160	rVB	62870	65626	4.86%	0.583%
15	9.110	1191	1194	1210	rVB	1531820	1351083	100.00%	12.003%
16	9.233	1212	1215	1227	rVB	28801	37637	2.79%	0.334%
17	9.516	1260	1263	1272	rVB	173973	166708	12.34%	1.481%
18	9.598	1272	1277	1281	rVB4	10097	15136	1.12%	0.134%
19	9.792	1307	1310	1314	rBV2	915387	795445	58.87%	7.067%
20	9.827	1314	1316	1327	rVB	225097	229128	16.96%	2.036%
21	9.927	1327	1333	1337	rBV2	13269	18064	1.34%	0.160%
22	10.016	1345	1348	1354	rBV	104921	125299	9.27%	1.113%
23	10.351	1403	1405	1412	rBV	133253	139068	10.29%	1.235%
24	10.510	1429	1432	1437	rBV	137686	115574	8.55%	1.027%
25	10.592	1443	1446	1458	rBV	436908	503994	37.30%	4.477%
26	10.733	1468	1470	1473	rBV	15820	18198	1.35%	0.162%
27	11.092	1529	1531	1533	rBV	30377	27145	2.01%	0.241%
28	11.121	1533	1536	1544	rVB	100822	122744	9.08%	1.090%
29	11.286	1561	1564	1568	rBV	796557	783238	57.97%	6.958%
30	11.392	1577	1582	1587	rVB3	16205	21754	1.61%	0.193%
31	11.492	1596	1599	1607	rBV	32319	34870	2.58%	0.310%
32	11.557	1607	1610	1622	rVB	32200	42970	3.18%	0.382%
33	11.804	1649	1652	1656	rBV	151546	149583	11.07%	1.329%
34	11.833	1656	1657	1667	rVB3	16400	23972	1.77%	0.213%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

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-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.039	1689	1692	1698	rVB2	38297	32553	2.41%	0.289%
36	12.492	1766	1769	1772	rBV5	11287	15245	1.13%	0.135%
37	12.527	1772	1775	1779	rVV	33217	34104	2.52%	0.303%
38	12.586	1782	1785	1793	rBV	55835	72637	5.38%	0.645%
39	12.757	1809	1814	1819	rVB2	18627	28788	2.13%	0.256%
40	12.863	1829	1832	1842	rVB	1106056	1060181	78.47%	9.419%
41	13.739	1976	1981	1989	rBV	117181	128262	9.49%	1.139%
42	13.945	2013	2016	2028	rVB	433781	489451	36.23%	4.348%
43	14.362	2083	2087	2096	rBV4	8104	14786	1.09%	0.131%
44	14.733	2146	2150	2155	rVB	82296	77630	5.75%	0.690%
45	15.409	2261	2265	2282	rVB	259720	434731	32.18%	3.862%

Sum of corrected areas: 11256196

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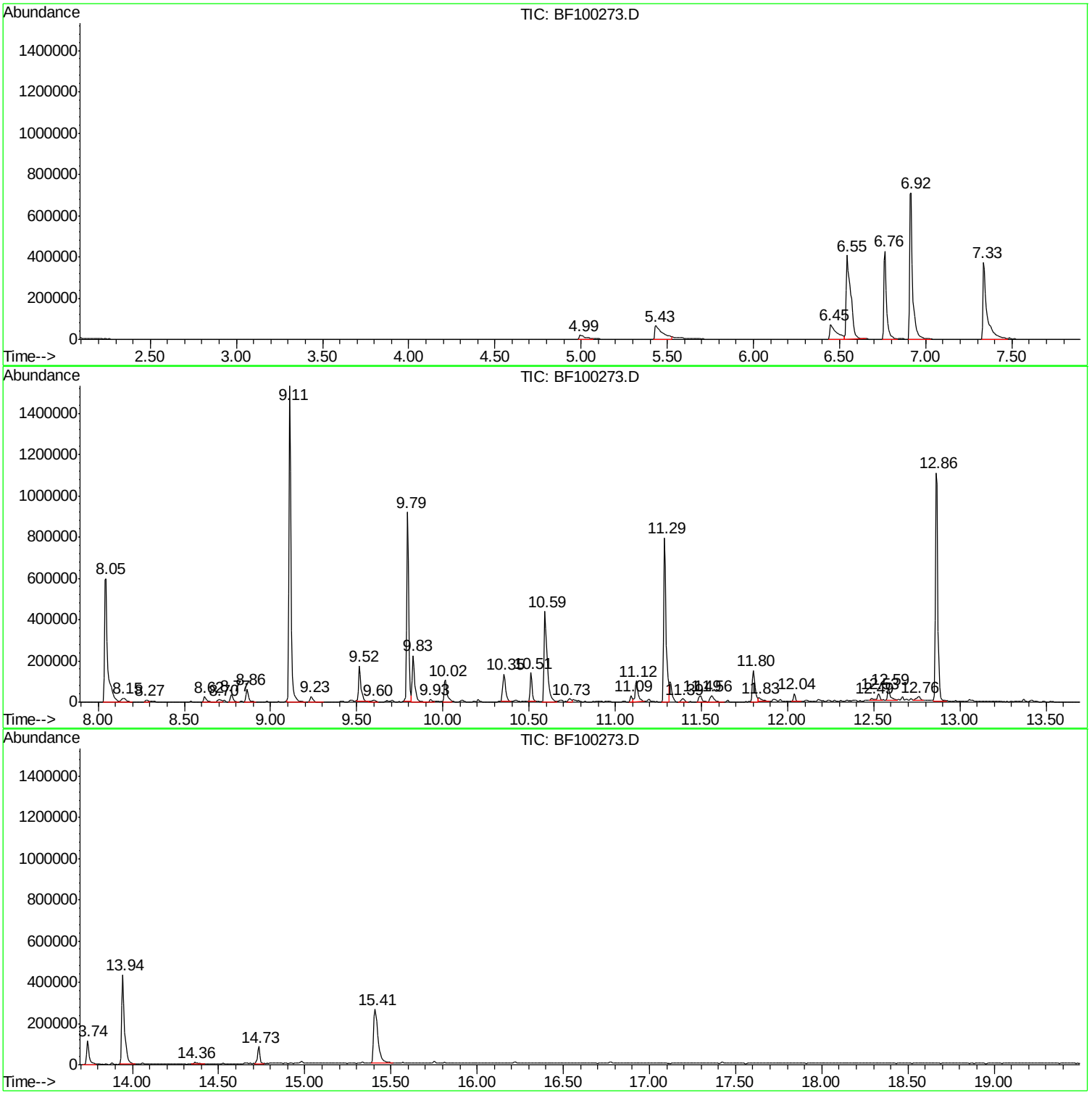
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110617\
Data File : BF100273.D
Acq On : 7 Nov 2017 4:34
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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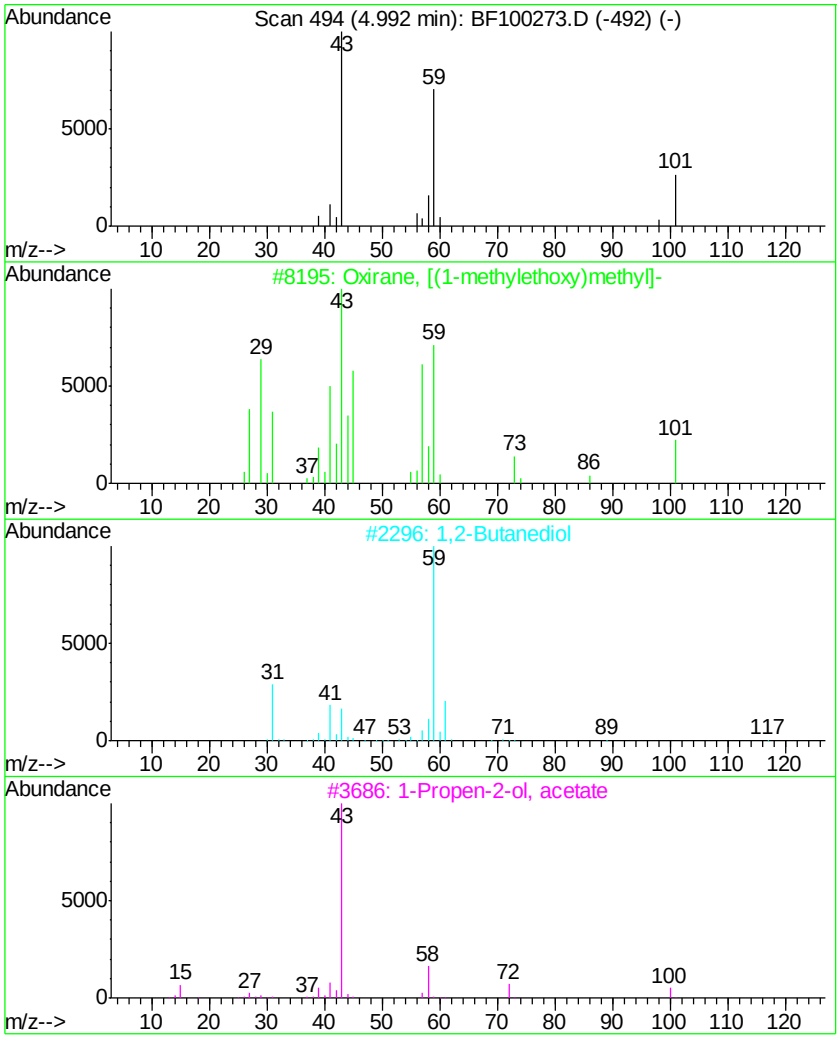
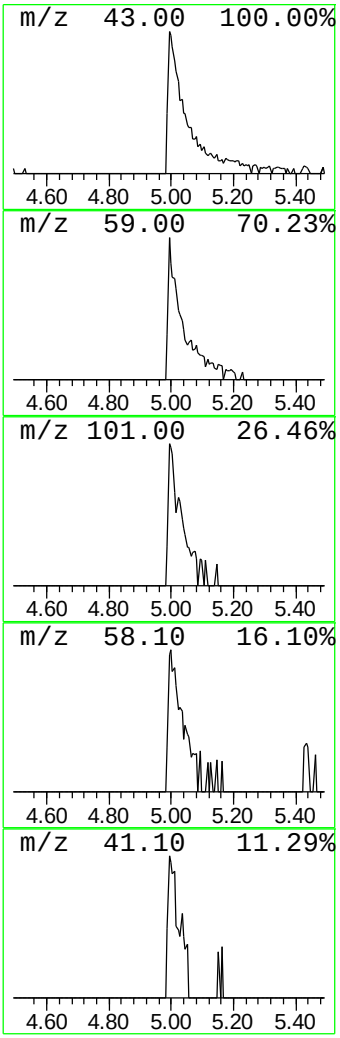
Peak Number 1 unknown4.99 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	2.35 ng	58164	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	43
2	1,2-Butanediol	90	C4H10O2	000584-03-2	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	3-Hexanol	102	C6H14O	000623-37-0	9
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110617\
Data File : BF100273.D
Acq On : 7 Nov 2017 4:34
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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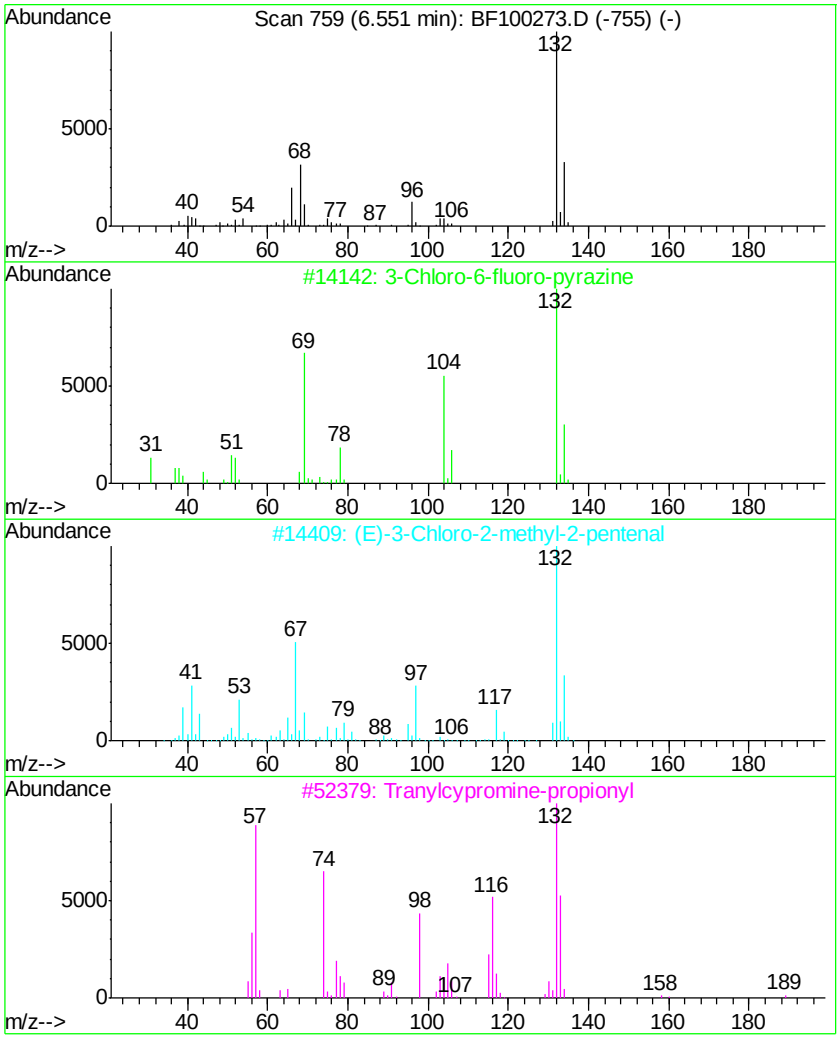
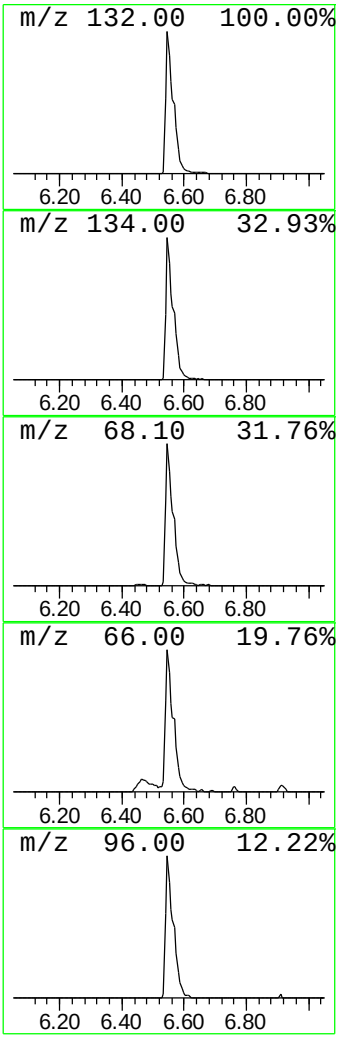
Peak Number 2 unknown6.55 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	28.18 ng	698290	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	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Amphetaminil	250	C17H18N2	017590-01-1	12





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110617\
Data File : BF100273.D
Acq On : 7 Nov 2017 4:34
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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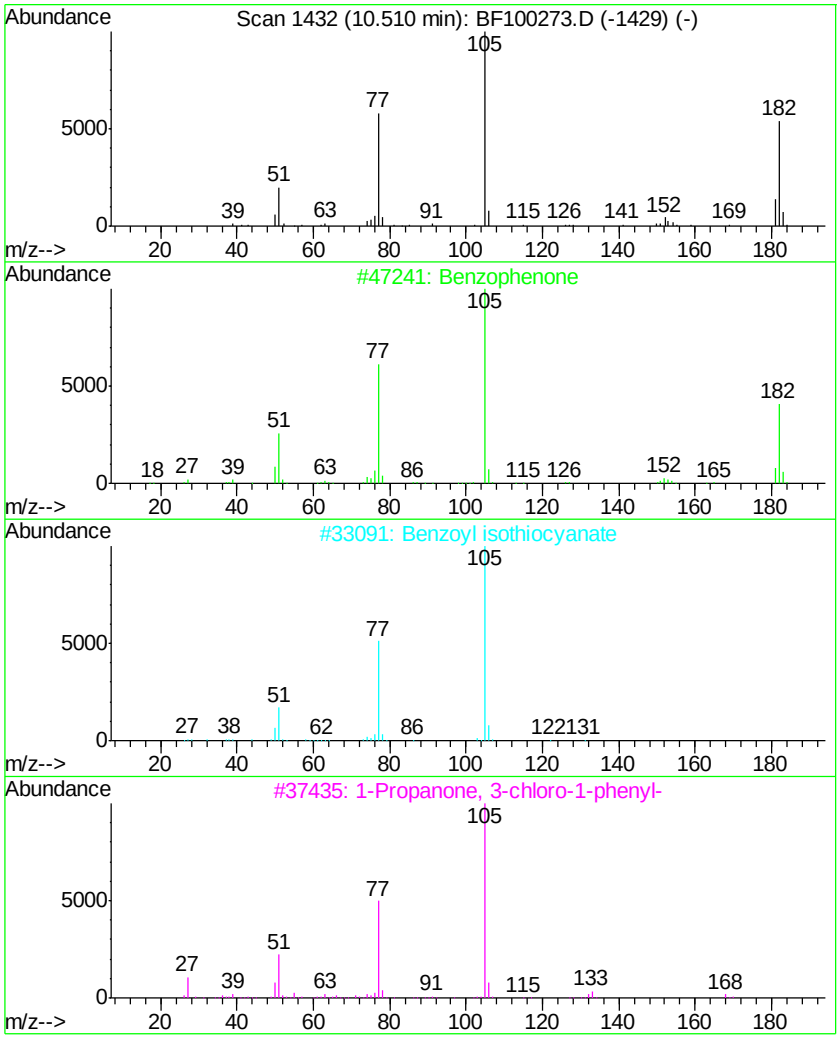
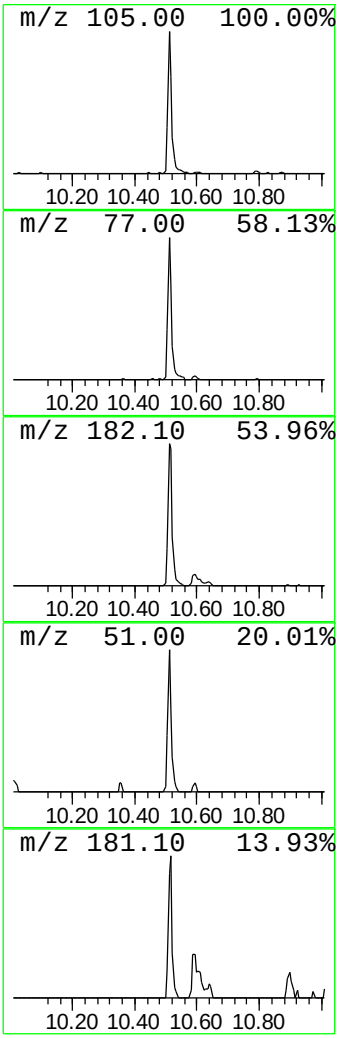
Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	2.91 ng	115574	Acenaphthene-d10	9.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4	Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





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Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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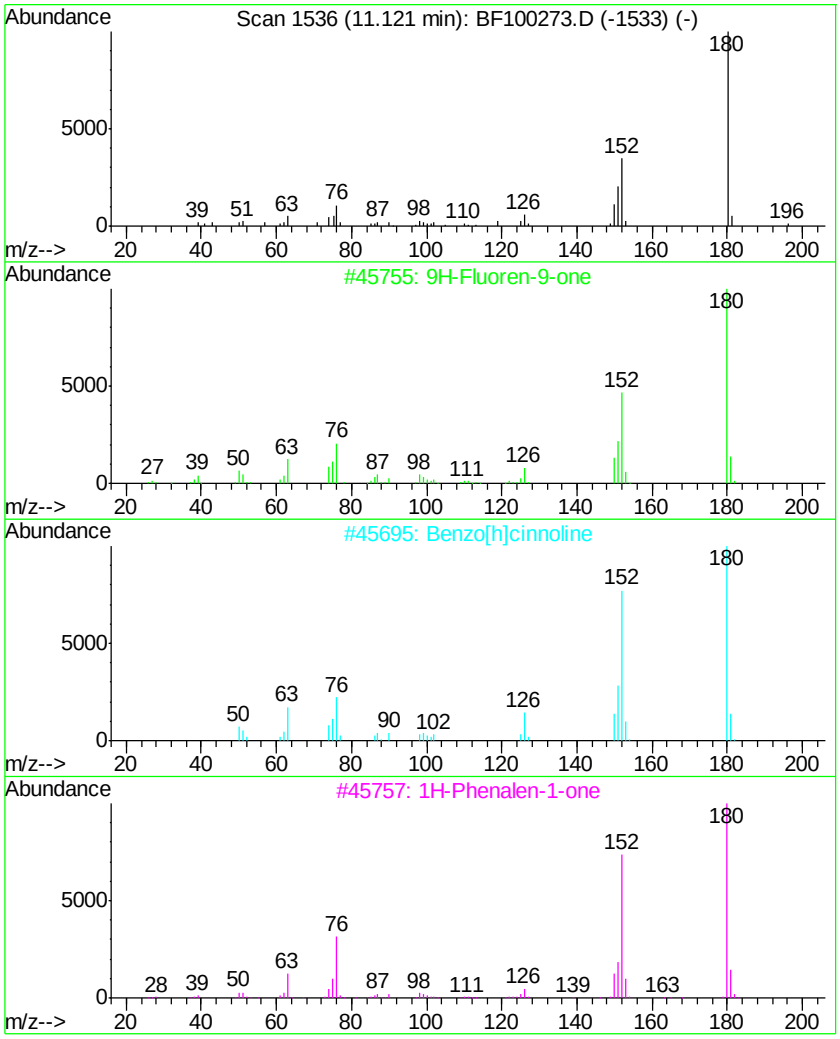
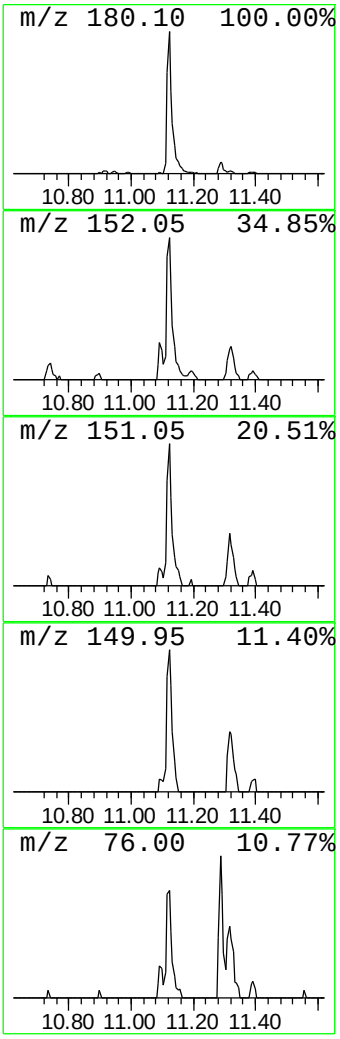
Peak Number 5 9H-Fluoren-9-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.12	3.13 ng	122744	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluoren-9-one	180	C13H8O	000486-25-9	90
2	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	56
3	1H-Phenalen-1-one	180	C13H8O	000548-39-0	53
4	Phenazine	180	C12H8N2	000092-82-0	25
5	Benzeneethanamine, 3,4-dimethoxy-	181	C10H15NO2	000120-20-7	14





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Sample : I6336-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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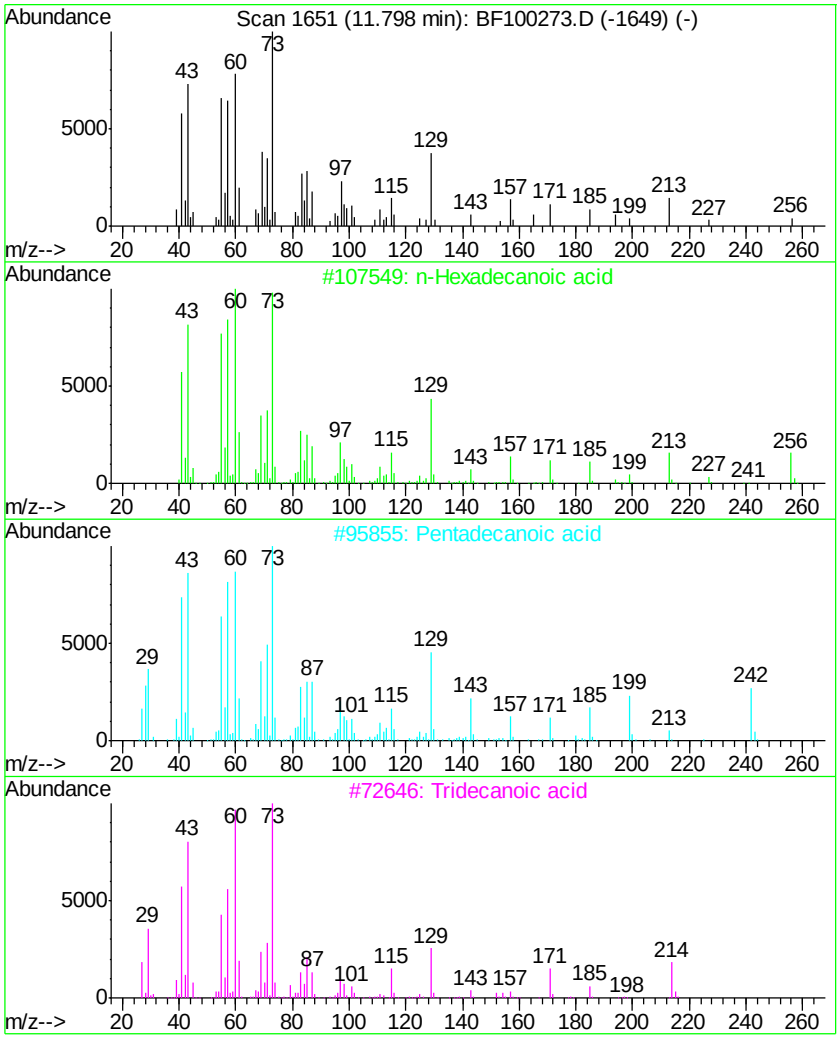
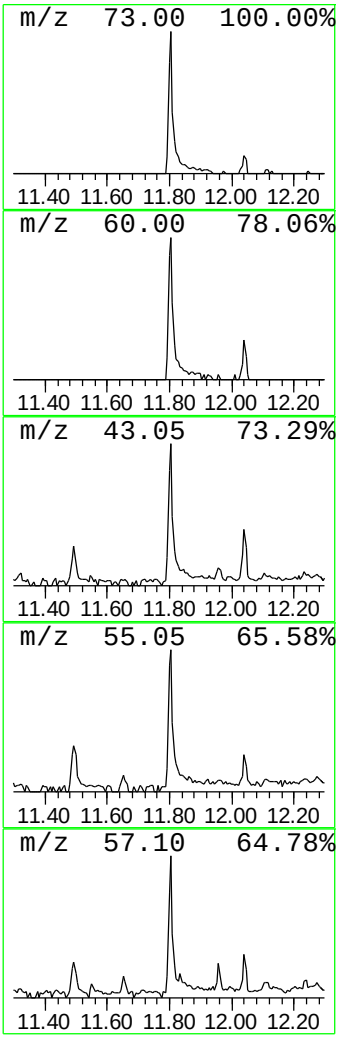
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	3.82 ng	149583	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25
5	Oxalic acid, isobutyl undecyl ester	300	C17H32O4	1000309-37-6	18





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Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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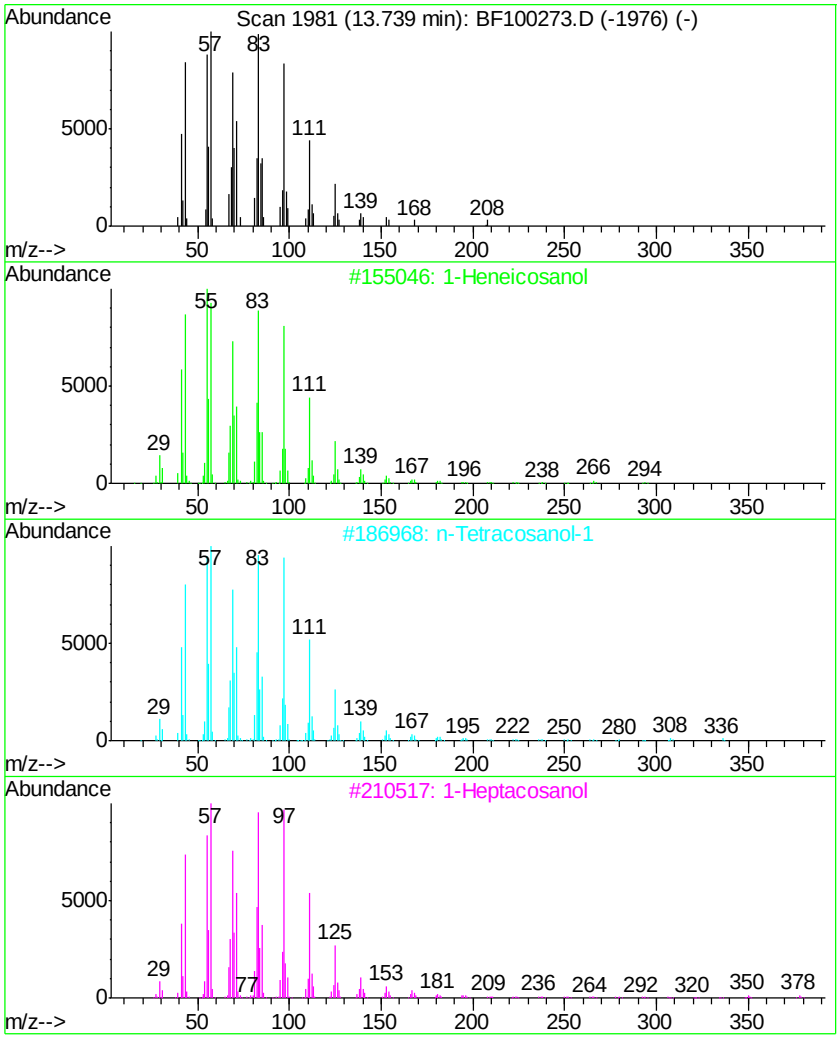
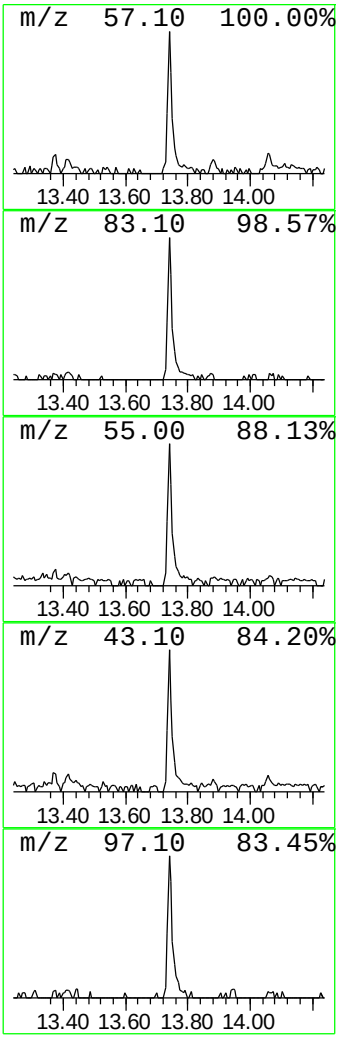
Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	5.24 ng	128262	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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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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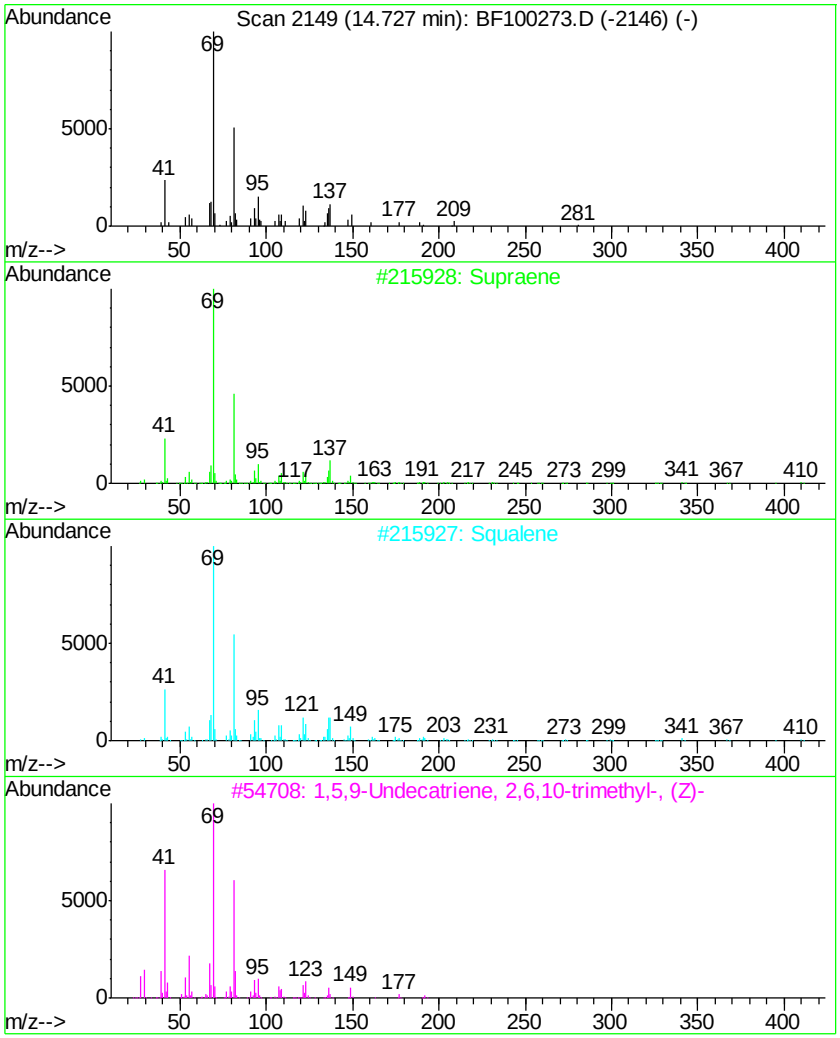
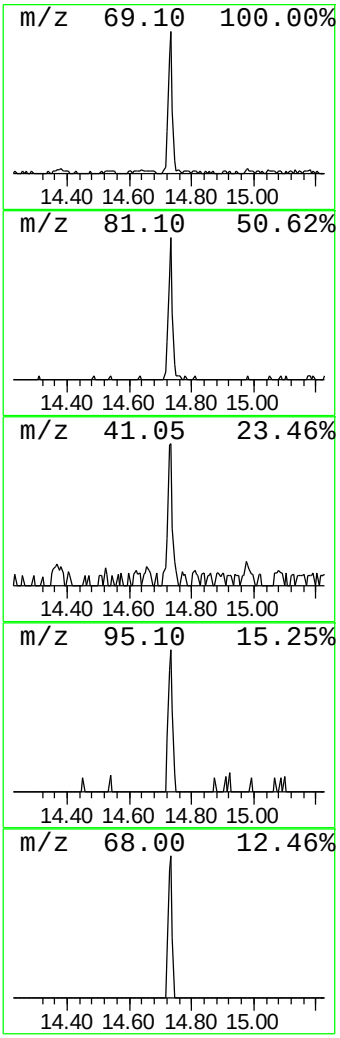
Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	3.57 ng	77630	Perylene-d12	15.41

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	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
5	Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110617\
Data File : BF100273.D
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Operator : SJ/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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
unknown4.99	4.99	2.4	ng	58164	1	6.76	495600	20.0
unknown6.55	6.55	28.2	ng	698290	1	6.76	495600	20.0
Benzophenone	10.51	2.9	ng	115574	3	9.79	795445	20.0
9H-Fluoren-9-one	11.12	3.1	ng	122744	4	11.29	783238	20.0
n-Hexadecanoic acid	11.80	3.8	ng	149583	4	11.29	783238	20.0
1-Heneicosanol	13.74	5.2	ng	128262	5	13.94	489451	20.0
Supraene	14.73	3.6	ng	77630	6	15.41	434731	20.0