LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096300.D
Acq On : 29 Jun 2017 19:13
Operator : SJ/MA
Sample : I3932-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-C1-(0-8)

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-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	3.193	185	188	203	rBV2	21127	58748	1.30%	0.155%
2	4.975	486	491	500	rVB	788145	1023528	22.64%	2.695%
3	5.393	556	562	565	rBV	4140889	4489310	99.31%	11.821%
4	6.404	728	734	737	rBV	4169534	4520393	100.00%	11.902%
5	6.540	752	757	760	rBV	4104011	4289106	94.88%	11.293%
6	6.769	792	796	800	rVB	1395796	1140961	25.24%	3.004%
7	6.928	819	823	826	rVB	3323637	3037315	67.19%	7.997%
8	7.328	886	891	894	rBV	2820533	2832231	62.65%	7.457%
9	8.051	1009	1014	1017	rBV	1911503	1591353	35.20%	4.190%
10	9.128	1192	1197	1200	rBV	3810963	3831730	84.77%	10.089%
11	9.516	1259	1263	1266	rBV	613461	532986	11.79%	1.403%
12	9.804	1306	1312	1316	rBV	1795510	1577303	34.89%	4.153%
13	10.245	1385	1387	1390	rVB	66281	55962	1.24%	0.147%
14	10.586	1440	1445	1449	rBV	2233071	2268072	50.17%	5.972%
15	10.722	1464	1468	1469	rBV	69767	63964	1.42%	0.168%
16	11.280	1559	1563	1566	rBV	1412368	1377565	30.47%	3.627%
17	11.816	1650	1654	1658	rBV2	159259	146600	3.24%	0.386%
18	12.492	1766	1769	1772	rBV	107229	93969	2.08%	0.247%
19	12.604	1783	1788	1791	rBV3	46641	64616	1.43%	0.170%
20	12.716	1801	1807	1810	rBV	102248	103953	2.30%	0.274%
21	12.869	1828	1833	1836	rBV	2675367	2529092	55.95%	6.659%
22	13.768	1983	1986	1991	rVB	139767	124333	2.75%	0.327%
23	13.916	2006	2011	2014	rBV	989467	1022323	22.62%	2.692%
24	14.927	2180	2183	2187	rBV2	46808	64373	1.42%	0.169%
25	15.274	2239	2242	2247	rVB	66496	79886	1.77%	0.210%
26	15.339	2248	2253	2257	rBV	829045	991735	21.94%	2.611%
27	16.721	2484	2488	2494	rVB4	33545	67560	1.49%	0.178%

Sum of corrected areas: 37978967

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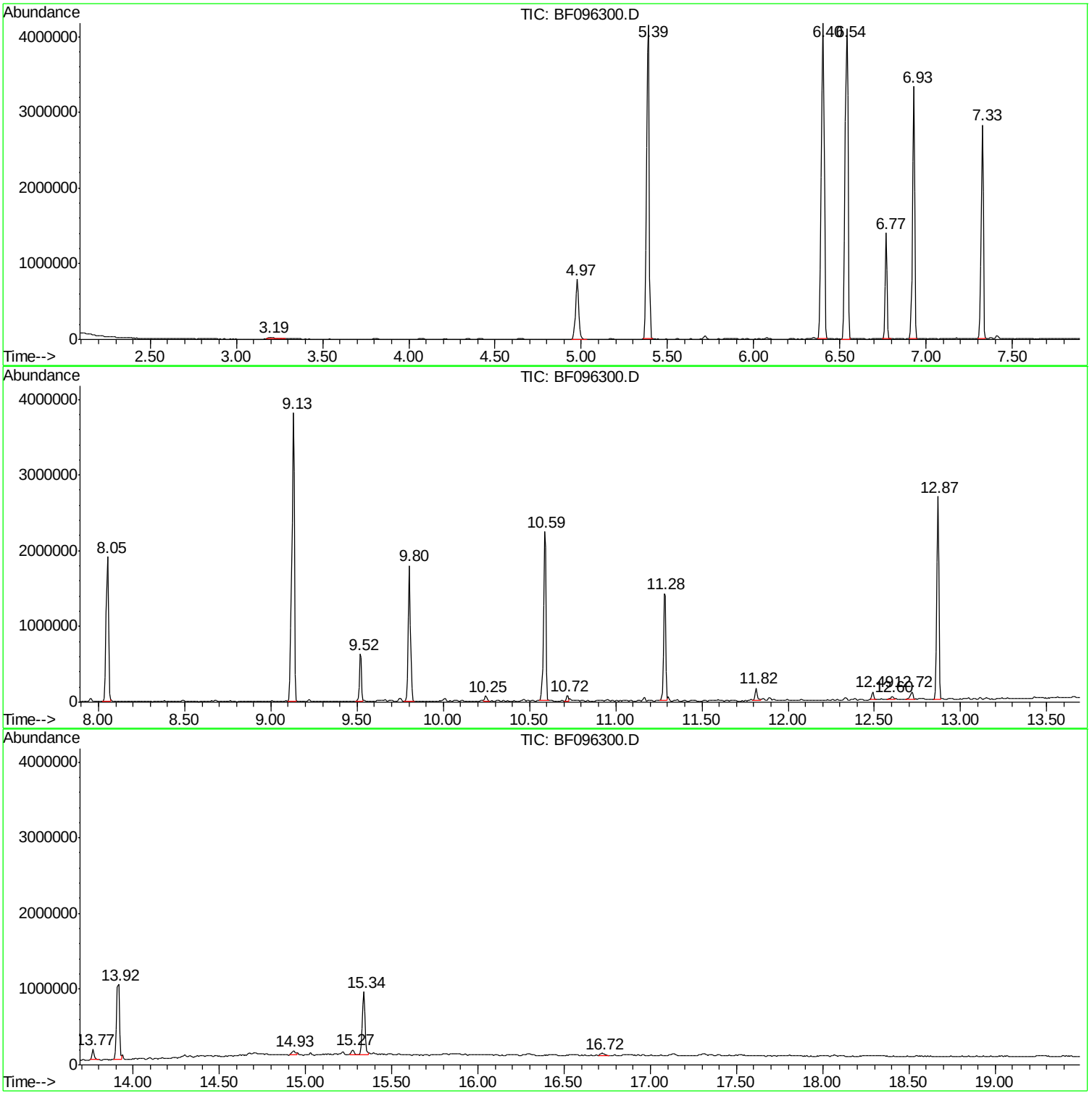
Instrument : BNA_F
ClientSampleId : TP-C1-(0-8)

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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Data File : BF096300.D
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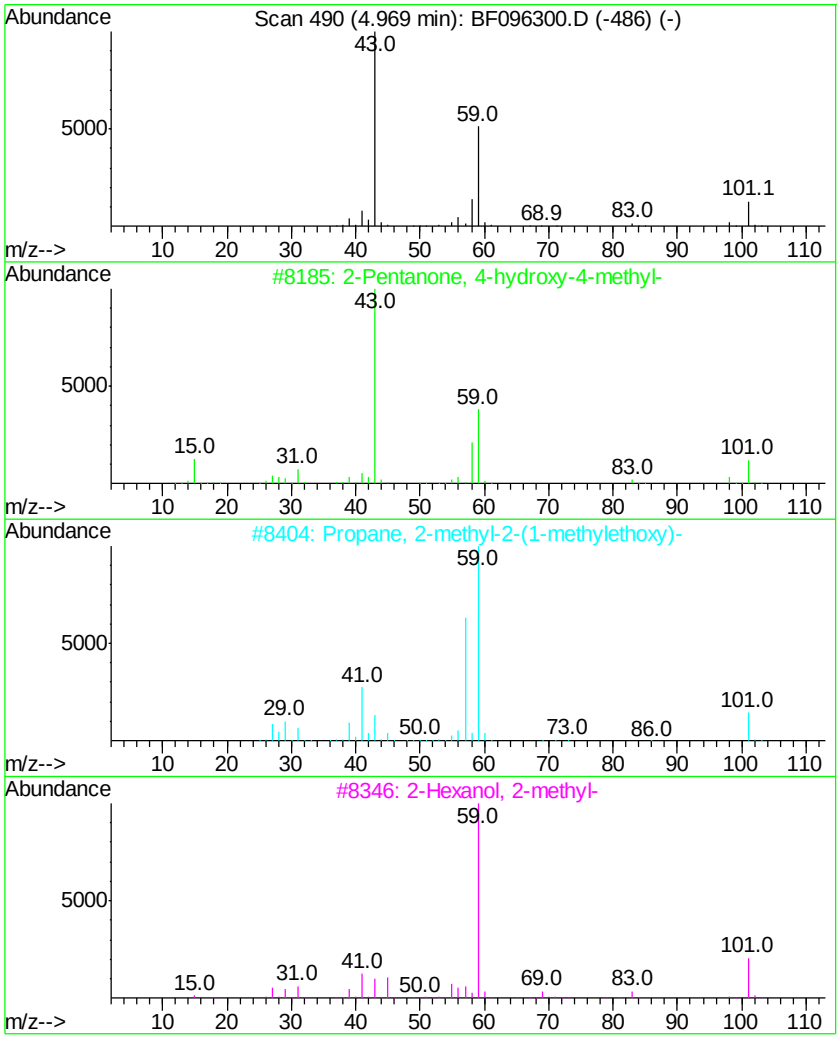
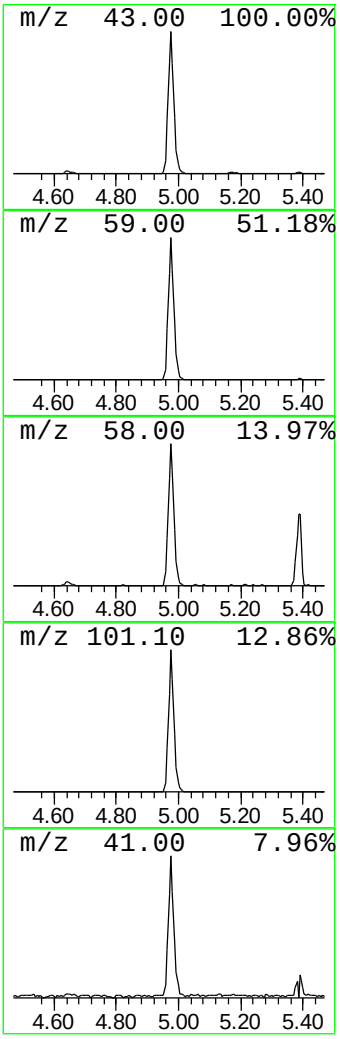
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	17.94 ng	1023530	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





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Sample : I3932-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-C1-(0-8)

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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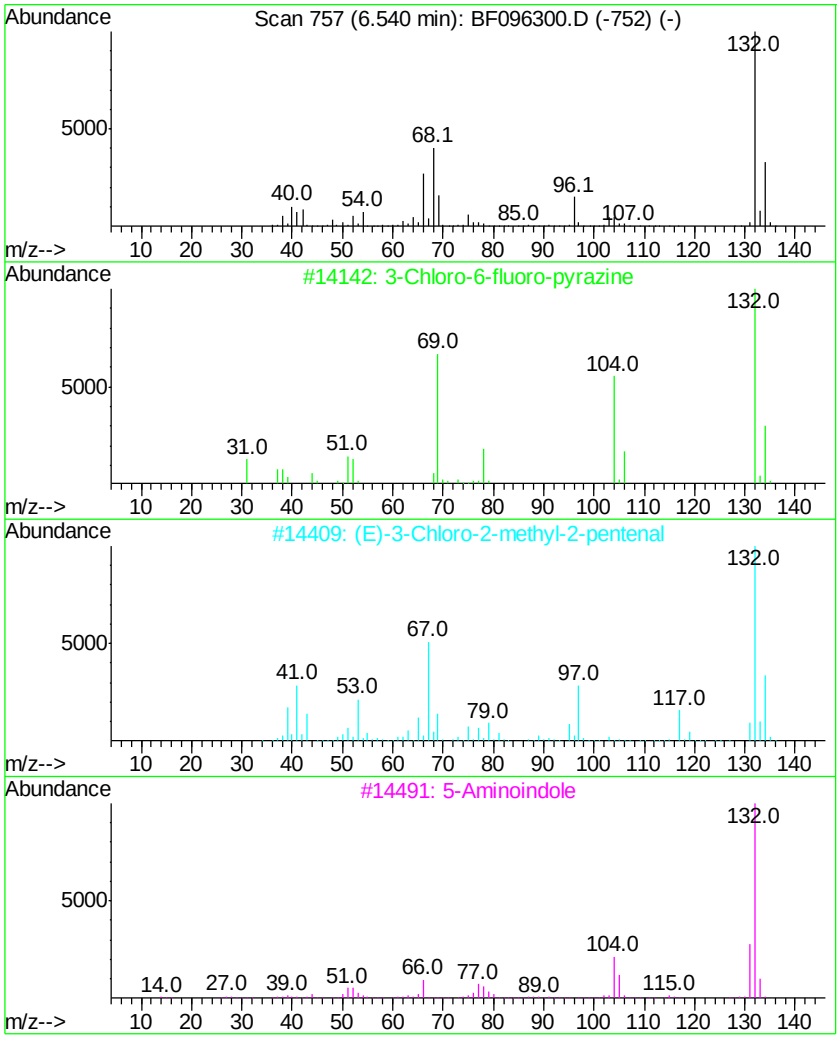
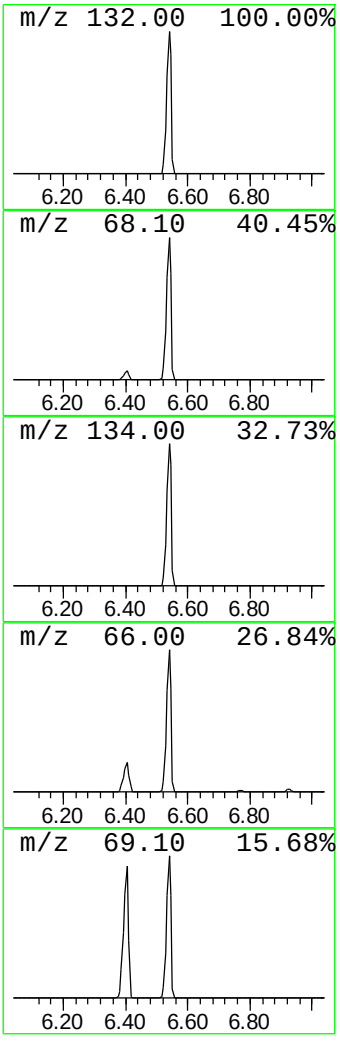
Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	75.18 ng	4289110	1,4-Dichlorobenzene-d4	6.77

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	Amphetaminil	250	C17H18N2	017590-01-1	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Acq On : 29 Jun 2017 19:13
Operator : SJ/MA
Sample : I3932-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-C1-(0-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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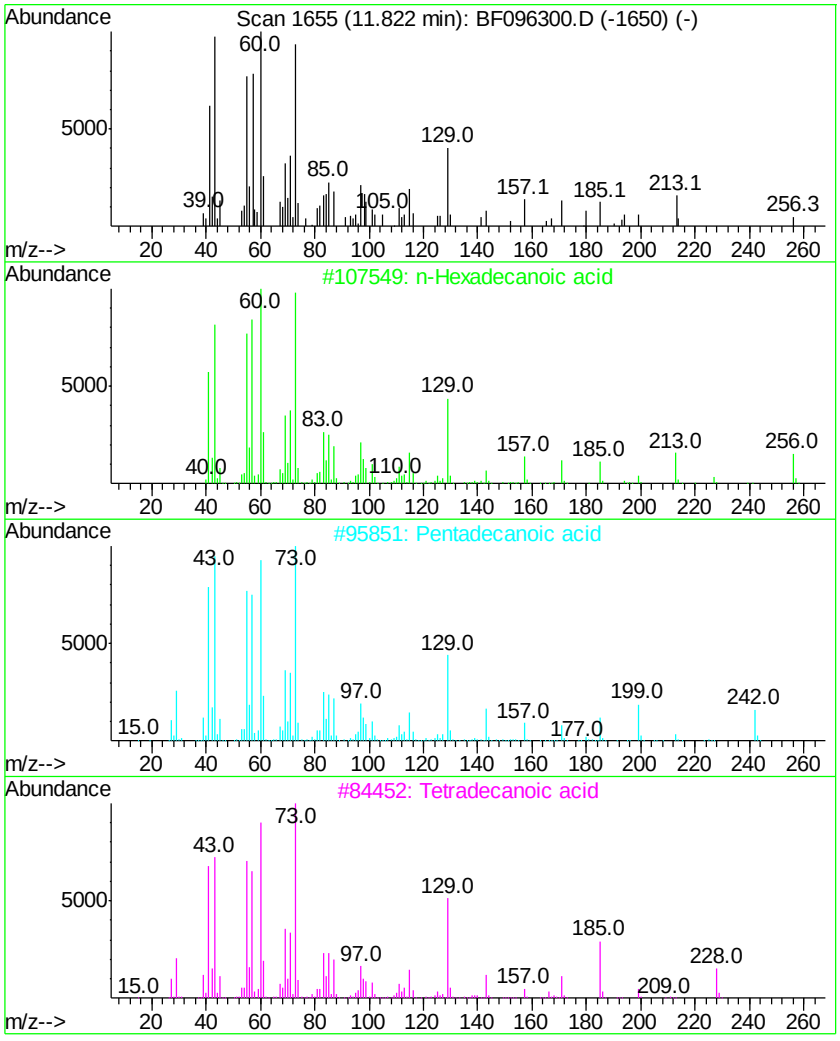
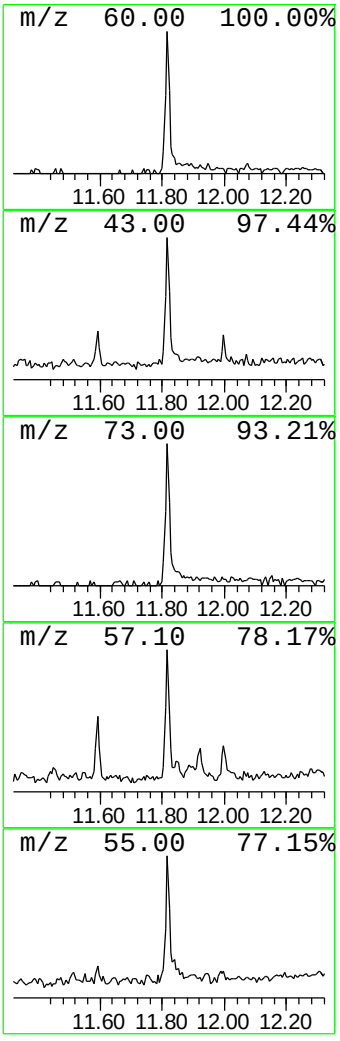
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.13 ng	146600	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096300.D
Acq On : 29 Jun 2017 19:13
Operator : SJ/MA
Sample : I3932-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-C1-(0-8)

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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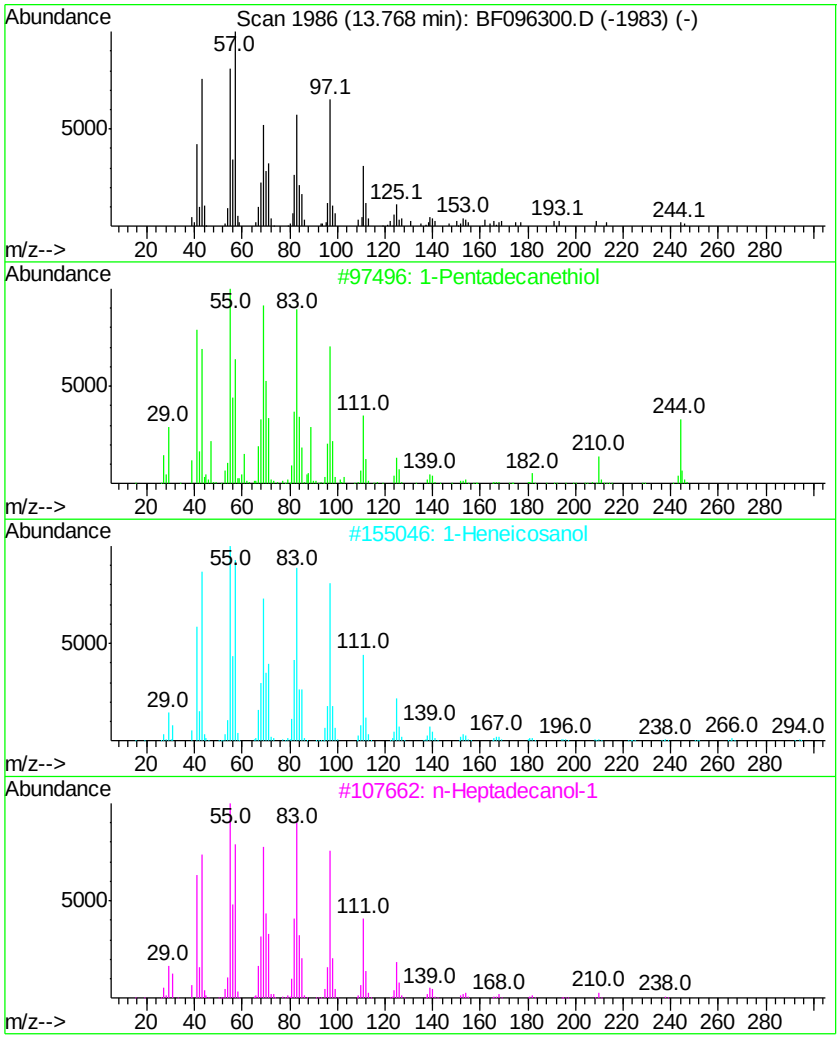
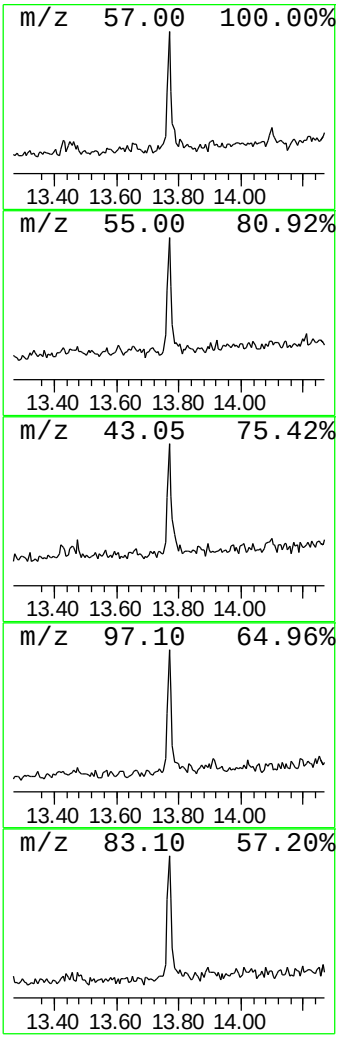
Peak Number 6 1-Pentadecanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.43 ng	124333	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol	244	C15H32S	025276-70-4	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062917\
Data File : BF096300.D
Acq On : 29 Jun 2017 19:13
Operator : SJ/MA
Sample : I3932-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-C1-(0-8)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	17.9	ng	1023530	1	6.77	1140960	20.0
unknown6.54	6.54	75.2	ng	4289110	1	6.77	1140960	20.0
n-Hexadecanoic acid	11.82	2.1	ng	146600	4	11.28	1377570	20.0
1-Pentadecanethiol	13.77	2.4	ng	124333	5	13.92	1022320	20.0