LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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	4.875	469	474	487	rVB	301128	421577	14.85%	1.673%
2	5.298	541	546	549	rBV	2631157	2643289	93.08%	10.493%
3	6.328	715	721	734	rVB	2388260	2747168	96.74%	10.905%
4	6.451	737	742	746	rBV	2481922	2626441	92.49%	10.426%
5	6.681	777	781	785	rBV	744524	600806	21.16%	2.385%
6	6.839	803	808	811	rBV	2210847	1988872	70.04%	7.895%
7	7.245	871	877	880	rBV	1633317	1683606	59.29%	6.683%
8	7.963	994	999	1002	rBV	961536	826872	29.12%	3.282%
9	9.039	1177	1182	1186	rBV	2638757	2839659	100.00%	11.272%
10	9.433	1245	1249	1252	rBV	238989	191109	6.73%	0.759%
11	9.622	1273	1281	1285	rBV6	19233	37657	1.33%	0.149%
12	9.716	1291	1297	1300	rBV	852719	890453	31.36%	3.535%
13	10.163	1370	1373	1375	rVB	40720	36140	1.27%	0.143%
14	10.380	1403	1410	1412	rBV3	23102	35977	1.27%	0.143%
15	10.498	1425	1430	1434	rBV	1596854	1699759	59.86%	6.747%
16	10.633	1450	1453	1462	rVB	55634	78683	2.77%	0.312%
17	11.192	1544	1548	1551	rBV	1008445	849577	29.92%	3.372%
18	11.263	1555	1560	1563	rBV3	31432	37335	1.31%	0.148%
19	11.433	1585	1589	1594	rBV5	27724	38713	1.36%	0.154%
20	11.733	1637	1640	1642	rBV2	60344	48484	1.71%	0.192%
21	12.245	1724	1727	1730	rVB3	23369	29729	1.05%	0.118%
22	12.398	1750	1753	1756	rBV	106732	82660	2.91%	0.328%
23	12.621	1787	1791	1794	rBV	105641	106095	3.74%	0.421%
24	12.780	1813	1818	1821	rBV	2468184	2564585	90.31%	10.180%
25	13.680	1967	1971	1978	rVB	210059	218390	7.69%	0.867%
26	13.821	1990	1995	1998	rBV	838309	850963	29.97%	3.378%
27	14.310	2075	2078	2083	rBV	79818	86977	3.06%	0.345%
28	14.674	2136	2140	2142	rBV	78052	79090	2.79%	0.314%
29	14.821	2162	2165	2167	rBV	26591	29313	1.03%	0.116%
30	14.915	2178	2181	2189	rVB4	40638	64312	2.26%	0.255%
31	15.215	2227	2232	2238	rBV	474202	561969	19.79%	2.231%
32	15.704	2311	2315	2320	rBV6	23665	35582	1.25%	0.141%
33	16.721	2482	2488	2494	rBV8	24716	60591	2.13%	0.241%
34	17.815	2665	2674	2686	rBV8	28594	99296	3.50%	0.394%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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

Sum of corrected areas: 25191729

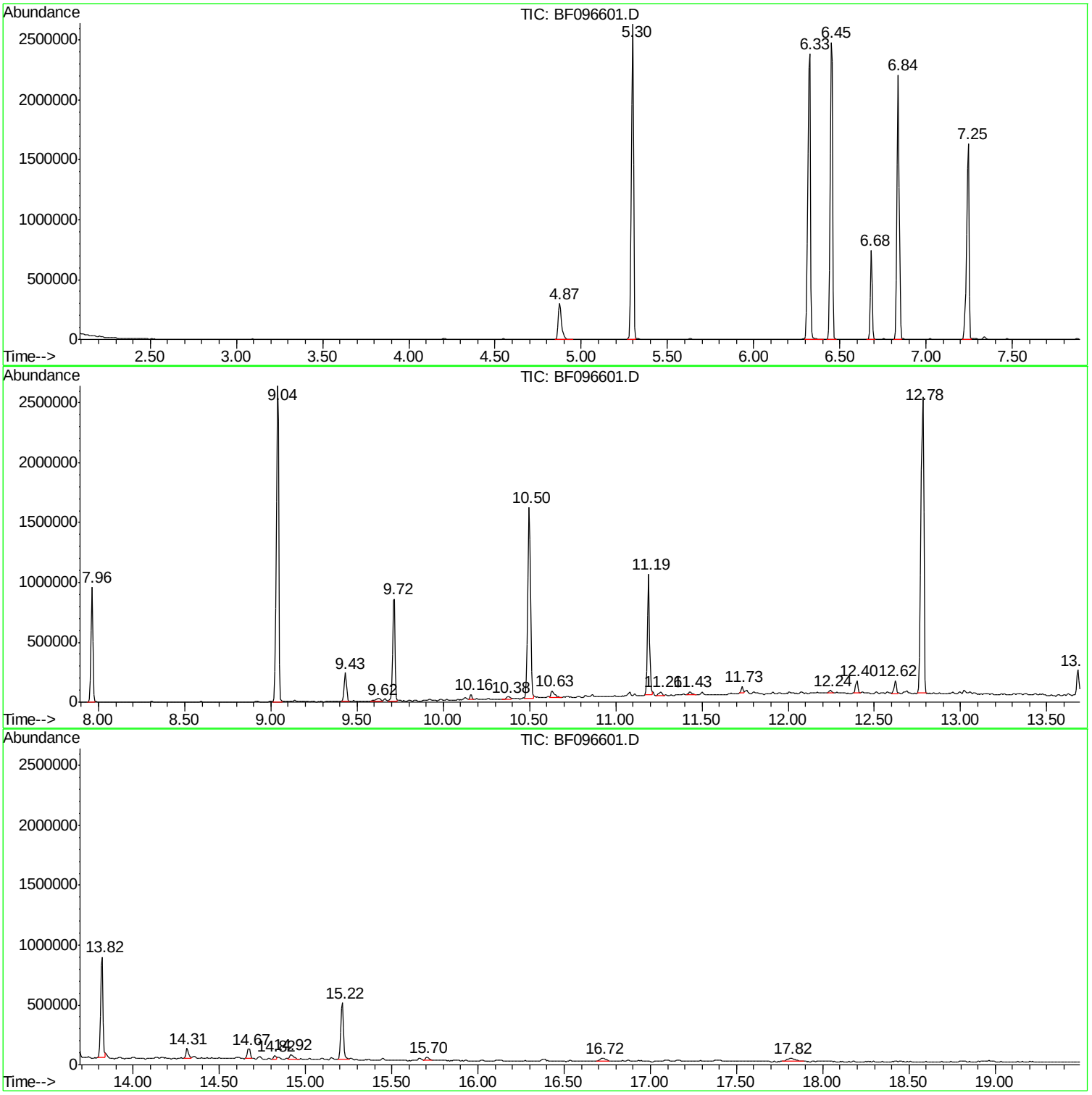
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

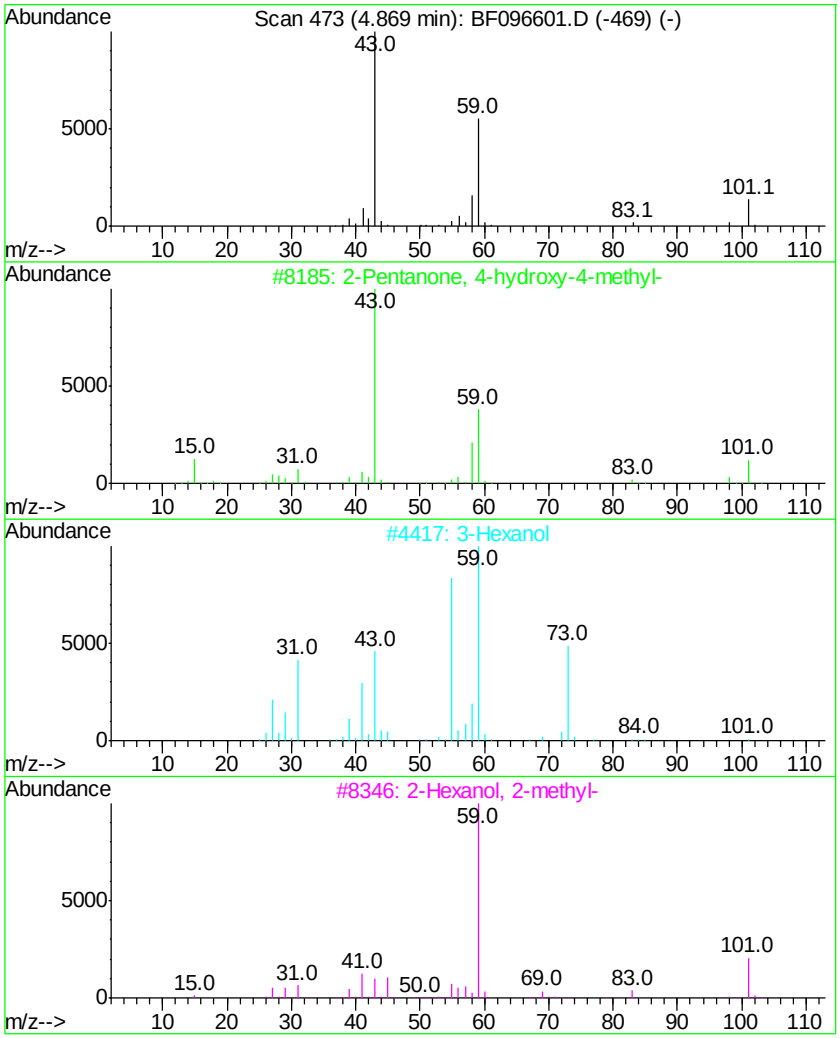
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

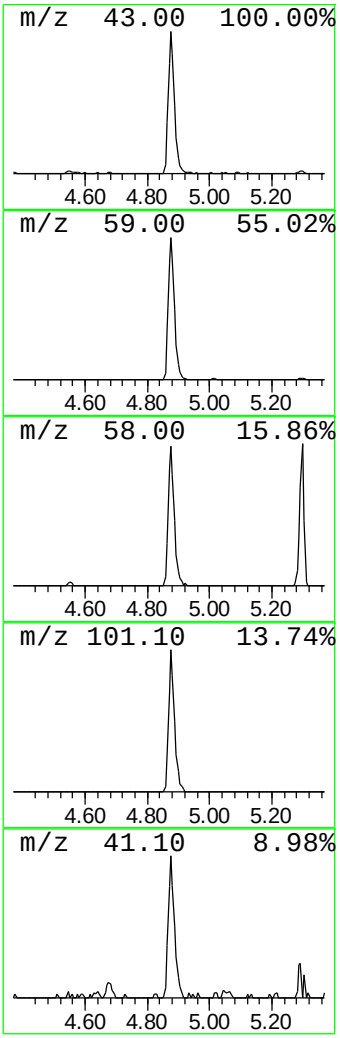
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	14.03 ng	421577	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol	102	C6H14O	000623-37-0	33
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	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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

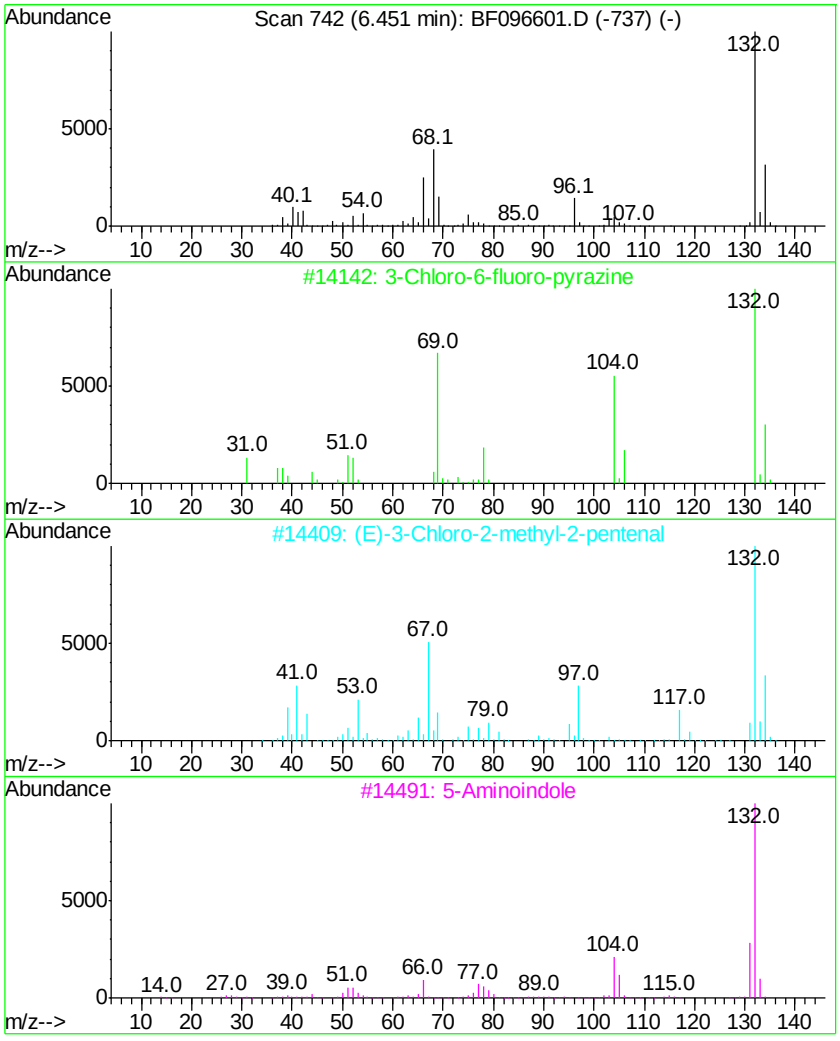
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

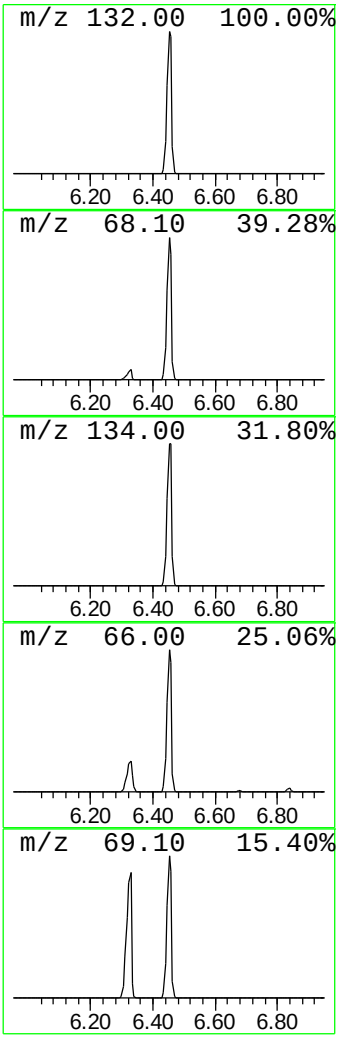
****

Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	87.43 ng	2626440	1,4-Dichlorobenzene-d4	6.68

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-Aminoindan	133	C9H11N	034698-41-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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

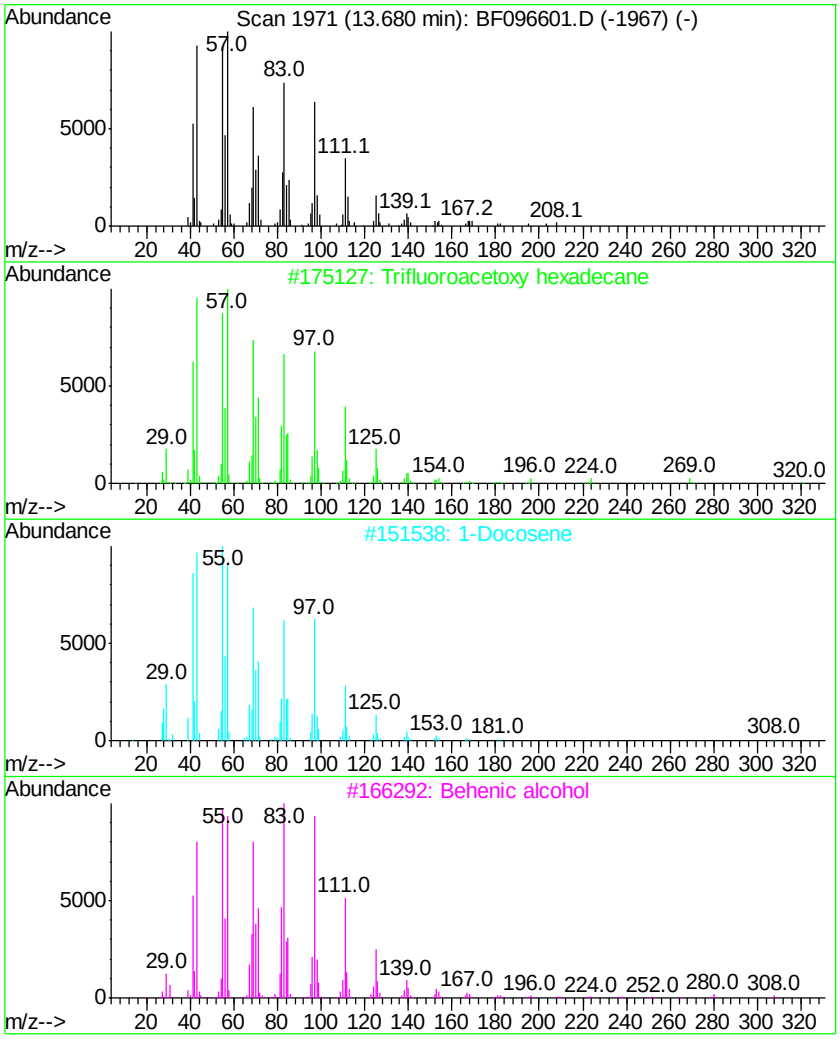
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

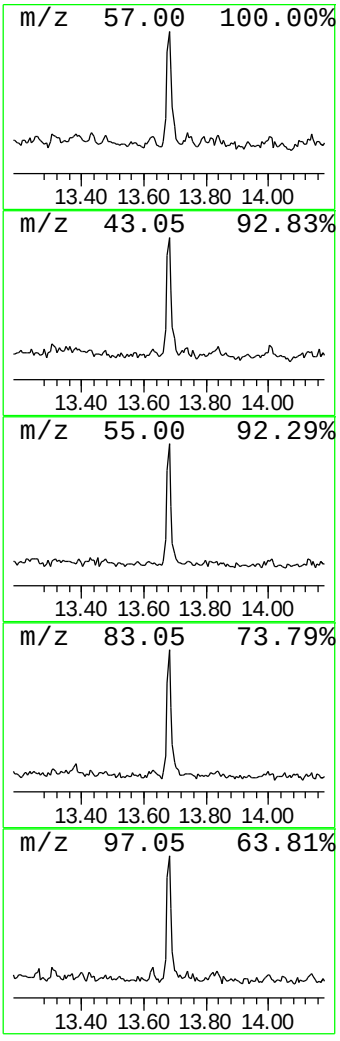
****

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	5.13 ng	218390	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	1-Docosene	308	C22H44	001599-67-3	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Octadecanol	270	C18H38O	000112-92-5	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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

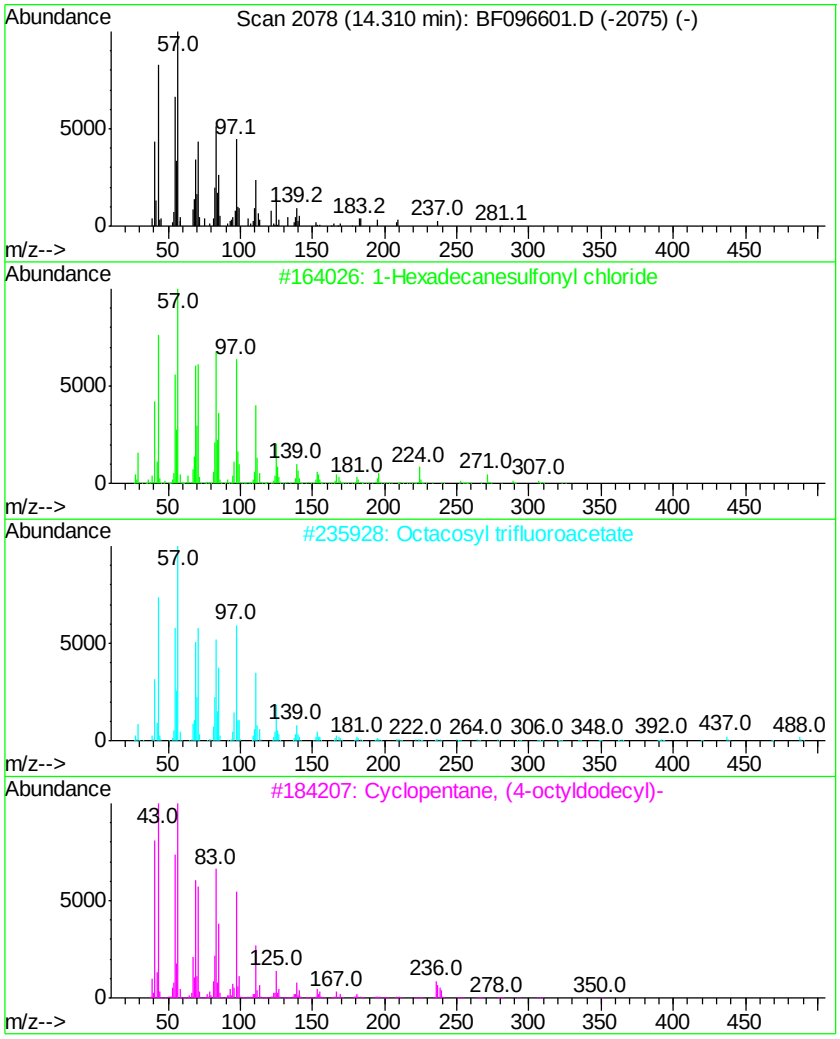
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

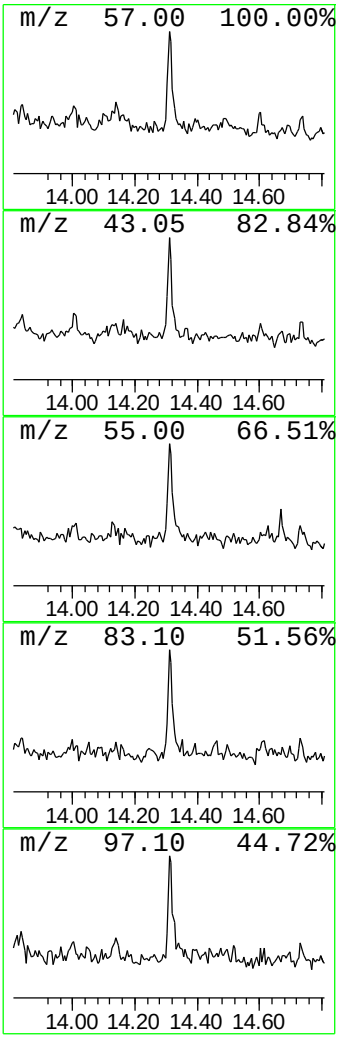
****

Peak Number 6 1-Hexadecanesulfonyl chloride Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	2.04 ng	86977	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
3	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	87
4	Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	83
5	17-Pentatriacontene	491	C35H70	006971-40-0	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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

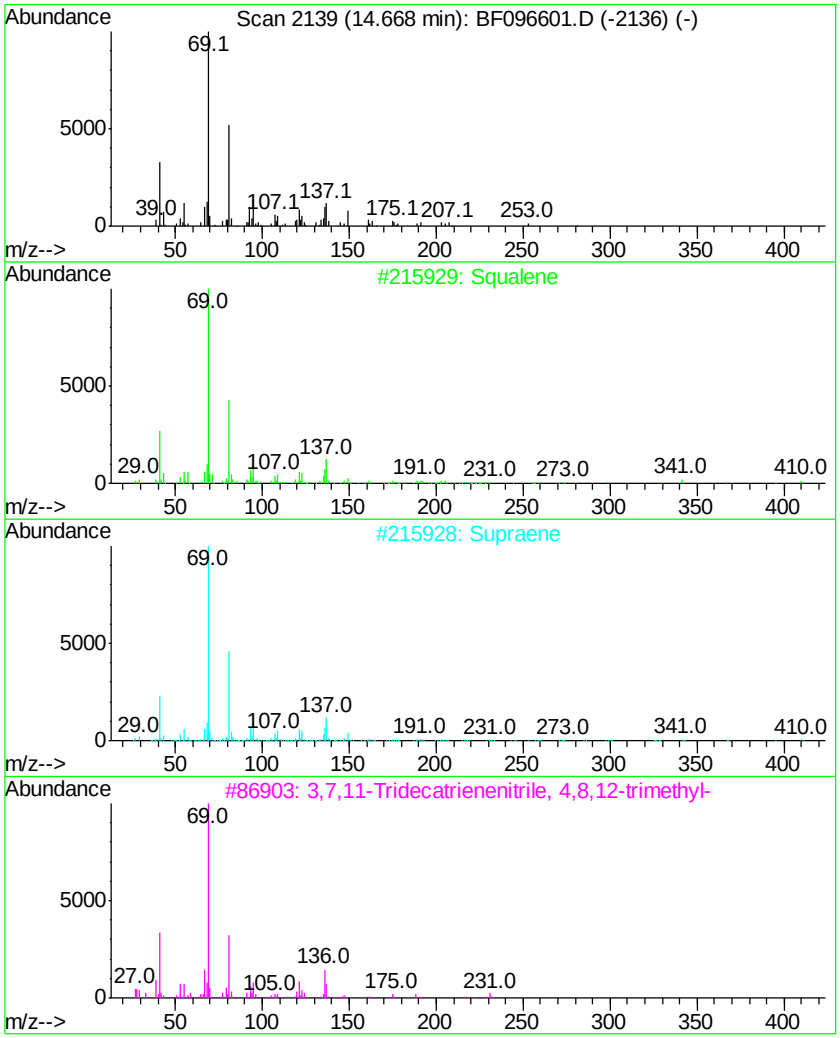
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

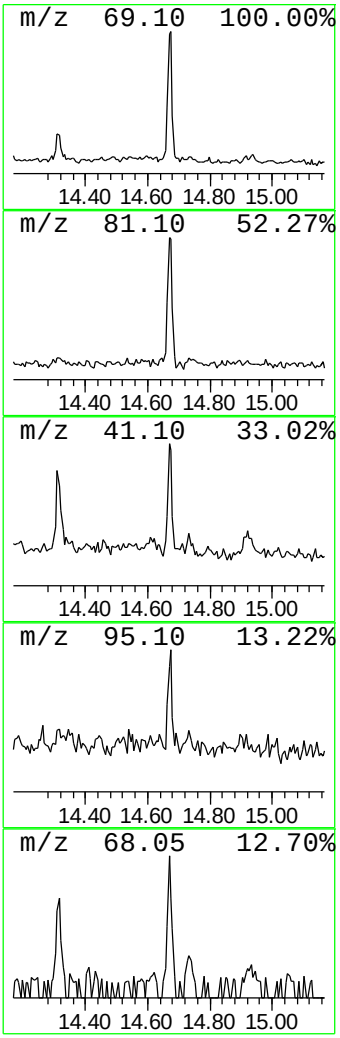
****

Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.81 ng	79090	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	86
2	Supraene	410	C30H50	007683-64-9	80
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
5	trans-Farnesol	222	C15H26O	000106-28-5	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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

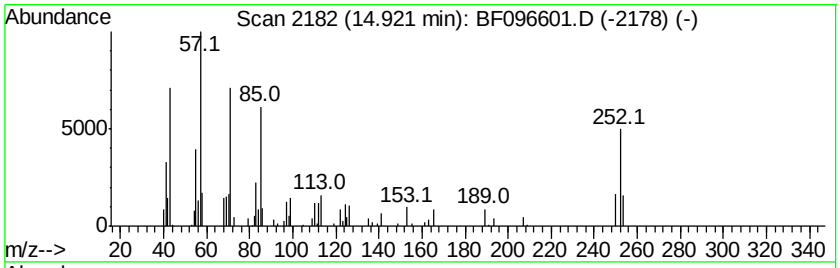
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

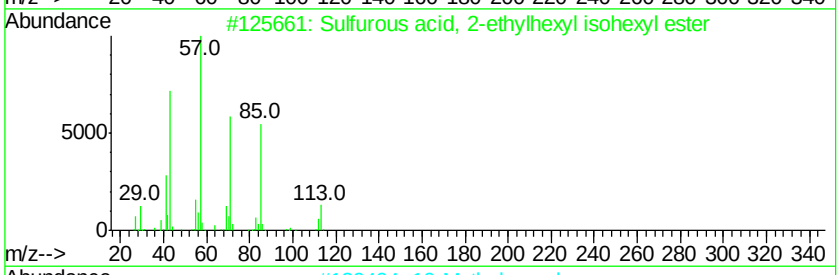
****

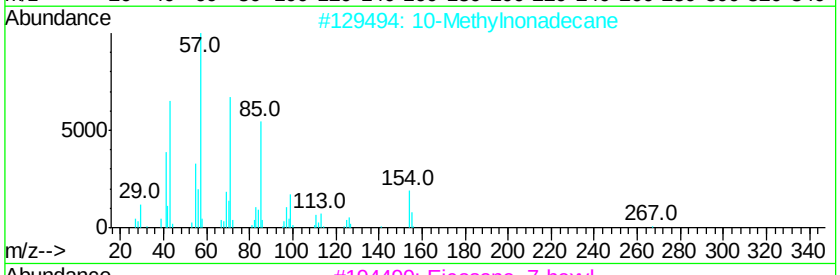
Peak Number 8 unknown14.92 Concentration Rank 8

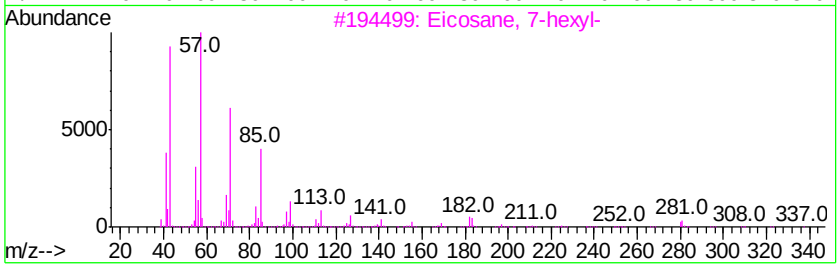
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.29 ng	64312	Perylene-d12	15.22

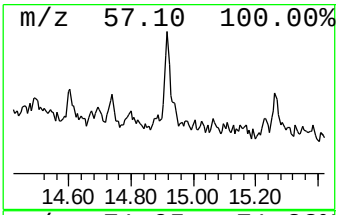
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	49
2	10-Methylnonadecane	282	C20H42	056862-62-5	49
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	47
4	Hentriacontane	437	C31H64	000630-04-6	47
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	47

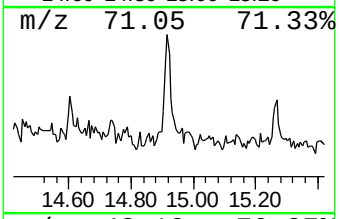


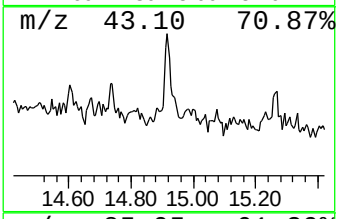


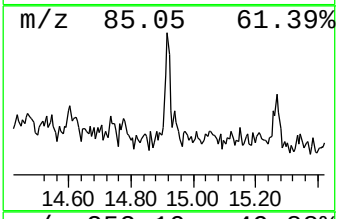


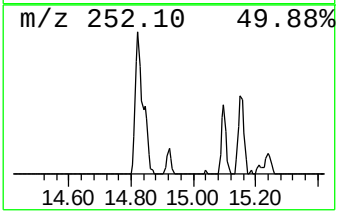












Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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

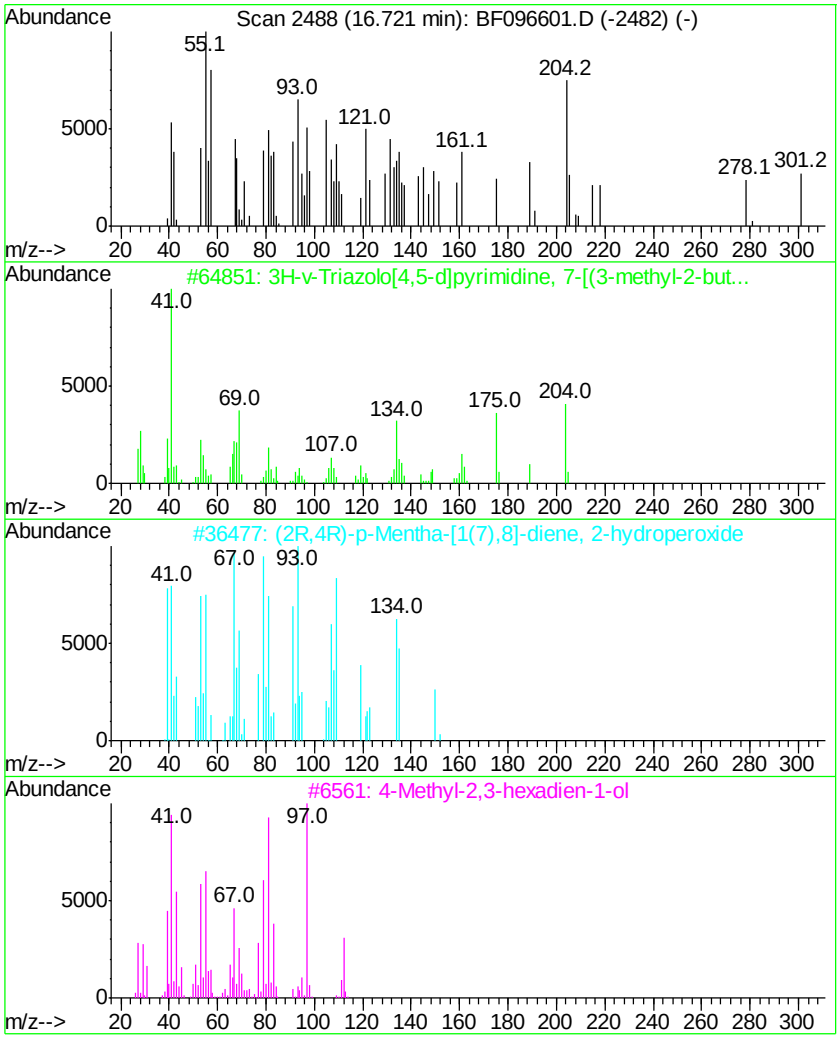
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

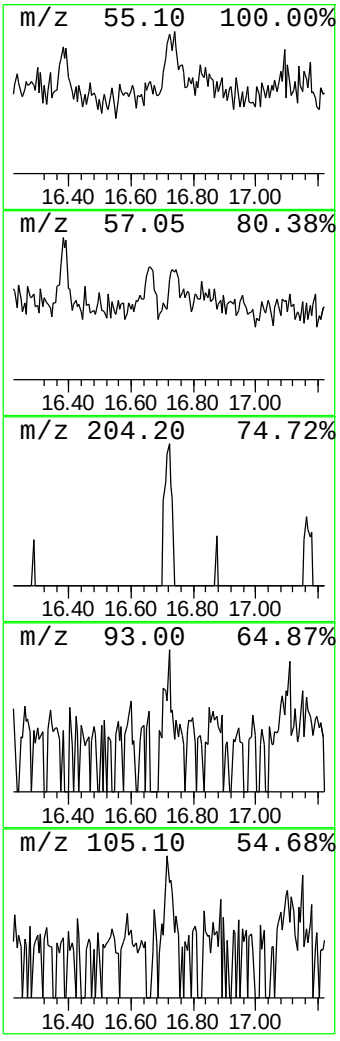
****

Peak Number 9 unknown16.72 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.16 ng	60591	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-v-Triazolo[4,5-d]pyrimidine, ...	204	C9H12N6	034257-66-4	43
2	(2R,4R)-p-Mentha-[1(7),8]-diene,...	168	C10H16O2	1000292-74-1	27
3	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	27
4	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	25
5	Cyclopropane, 1,1-dichloro-3-(1,...	194	C9H16Cl2	017171-92-5	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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

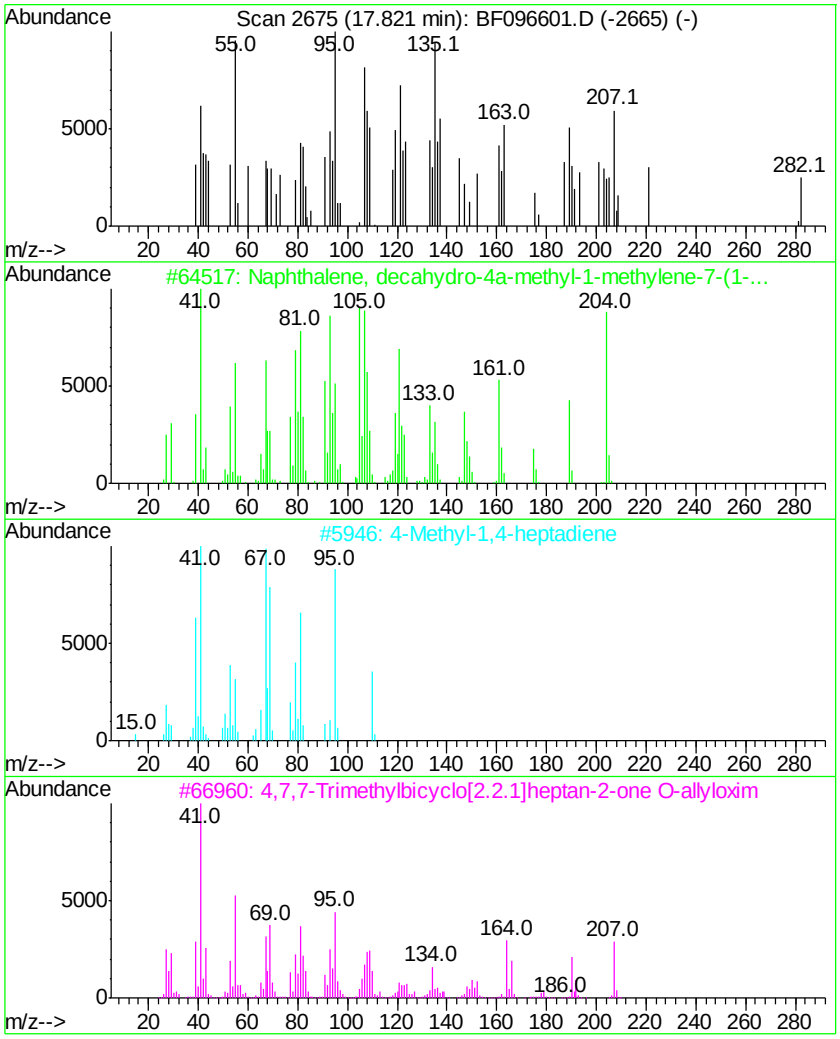
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

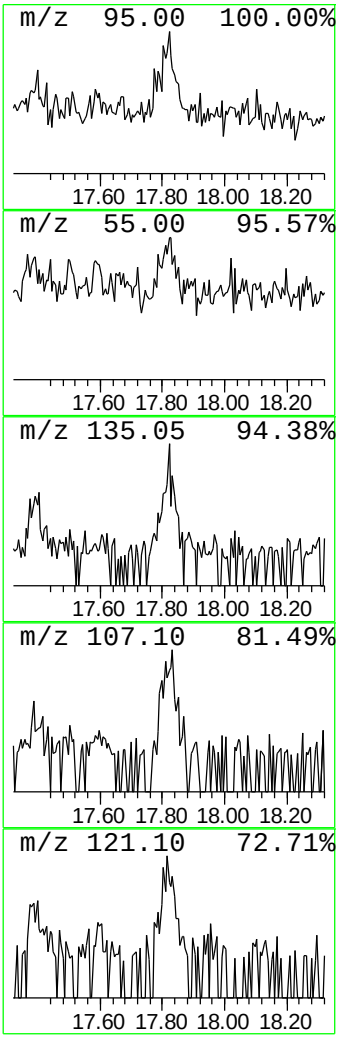
****

Peak Number 10 unknown17.82 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	3.53 ng	99296	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	46
2	4-Methyl-1,4-heptadiene	110	C8H14	013857-55-1	38
3	4,7,7-Trimethylbicyclo[2.2.1]hep...	207	C13H21NO	1000210-89-8	30
4	1,6-Cyclodecadiene	136	C10H16	007049-13-0	25
5	.alpha.-Bulnesene	204	C15H24	1000374-19-9	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
Data File : BF096601.D
Acq On : 10 Jul 2017 15:18
Operator : SJ/JU
Sample : I4061-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-D

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...	4.87	14.0	ng	421577	1	6.68	600806	20.0
unknown6.45	6.45	87.4	ng	2626440	1	6.68	600806	20.0
Trifluoroacetoxy ...	13.68	5.1	ng	218390	5	13.82	850963	20.0
1-Hexadecanesulfo...	14.31	2.0	ng	86977	5	13.82	850963	20.0
Squalene	14.67	2.8	ng	79090	6	15.22	561969	20.0
unknown14.92	14.92	2.3	ng	64312	6	15.22	561969	20.0
unknown16.72	16.72	2.2	ng	60591	6	15.22	561969	20.0
unknown17.82	17.82	3.5	ng	99296	6	15.22	561969	20.0