LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094784.D
Acq On : 2 May 2017 7:46
Operator : SJ/MA
Sample : I2892-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWS-E(4.5-5)

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-BF041717.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	3.937	336	340	355	rBV	476821	651540	21.09%	2.568%
2	4.331	402	407	424	rBV	2888653	2964844	95.97%	11.686%
3	4.707	467	471	479	rVB	40241	44416	1.44%	0.175%
4	5.401	584	589	605	rBV	2514400	2995502	96.96%	11.807%
5	5.519	605	609	613	rBV	2826508	3050187	98.73%	12.023%
6	5.766	647	651	657	rVB	602298	566523	18.34%	2.233%
7	5.942	676	681	684	rBV	2535079	2316170	74.97%	9.129%
8	6.419	756	762	765	rBV	1790433	1871263	60.57%	7.376%
9	7.254	900	904	913	rBV	840269	765859	24.79%	3.019%
10	8.577	1124	1129	1132	rBV	3176058	3089417	100.00%	12.177%
11	9.083	1211	1215	1222	rBV	481192	479483	15.52%	1.890%
12	9.389	1260	1267	1277	rBV2	662897	694284	22.47%	2.737%
13	9.983	1364	1368	1373	rVB	45746	41312	1.34%	0.163%
14	10.371	1429	1434	1443	rBV	1228299	1449011	46.90%	5.711%
15	10.566	1464	1467	1470	rBV	50878	57390	1.86%	0.226%
16	11.124	1558	1562	1565	rBV	32029	33213	1.08%	0.131%
17	11.213	1573	1577	1581	rBV	615307	608264	19.69%	2.398%
18	11.948	1698	1702	1710	rBV3	55167	77341	2.50%	0.305%
19	12.707	1828	1831	1837	rVB	32181	31711	1.03%	0.125%
20	12.983	1874	1878	1882	rVB	32872	34358	1.11%	0.135%
21	13.195	1908	1914	1917	rBV	2184727	2391137	77.40%	9.425%
22	14.401	2115	2119	2126	rBV4	38089	99690	3.23%	0.393%
23	14.465	2126	2130	2134	rVV	538628	576055	18.65%	2.271%
24	14.624	2154	2157	2162	rBV3	40127	44863	1.45%	0.177%
25	16.095	2403	2407	2416	rVB	385044	436816	14.14%	1.722%

Sum of corrected areas: 25370649

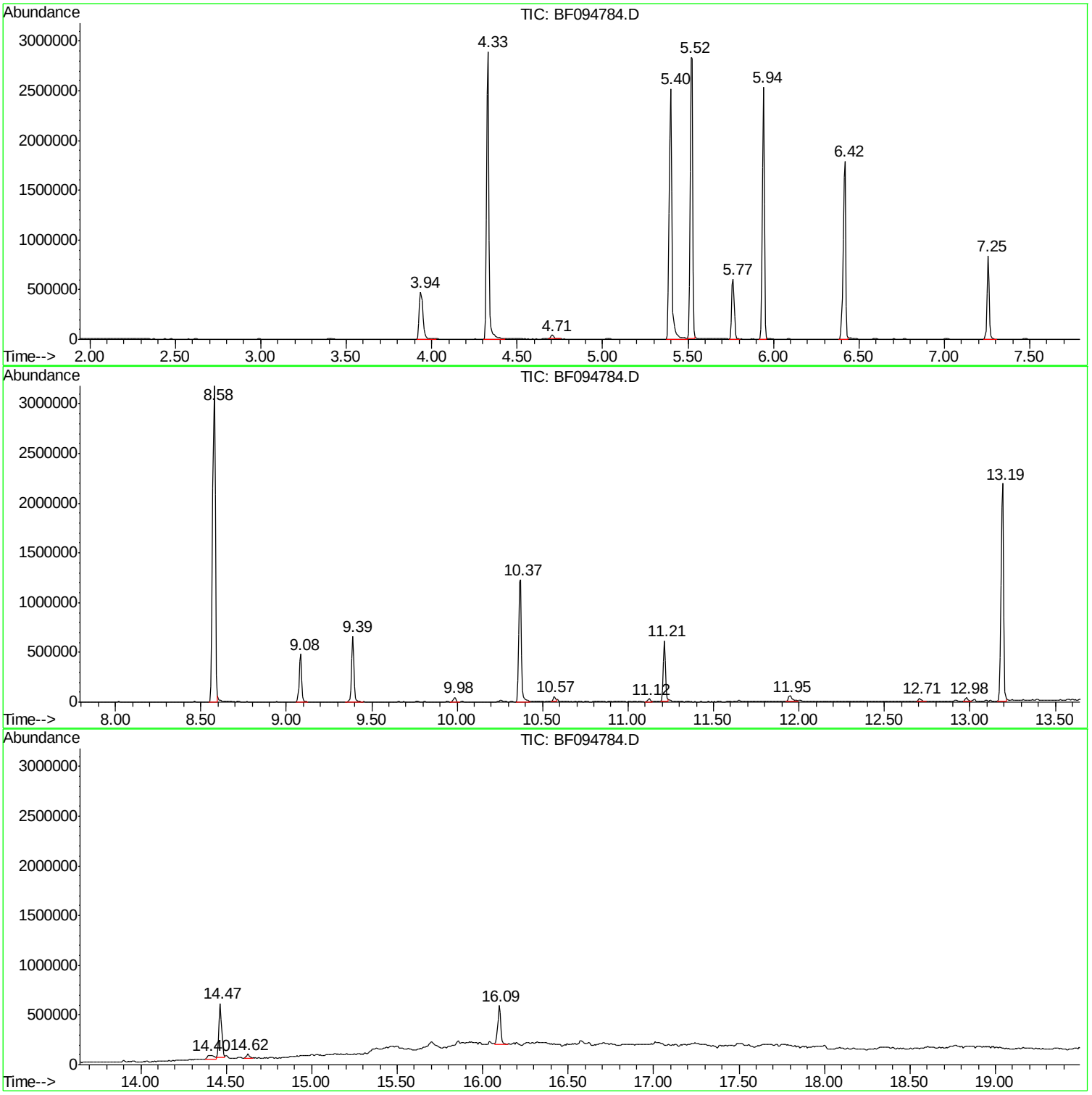
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094784.D
Acq On : 2 May 2017 7:46
Operator : SJ/MA
Sample : I2892-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWS-E(4.5-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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\BF050117\
Data File : BF094784.D
Acq On : 2 May 2017 7:46
Operator : SJ/MA
Sample : I2892-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWS-E(4.5-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

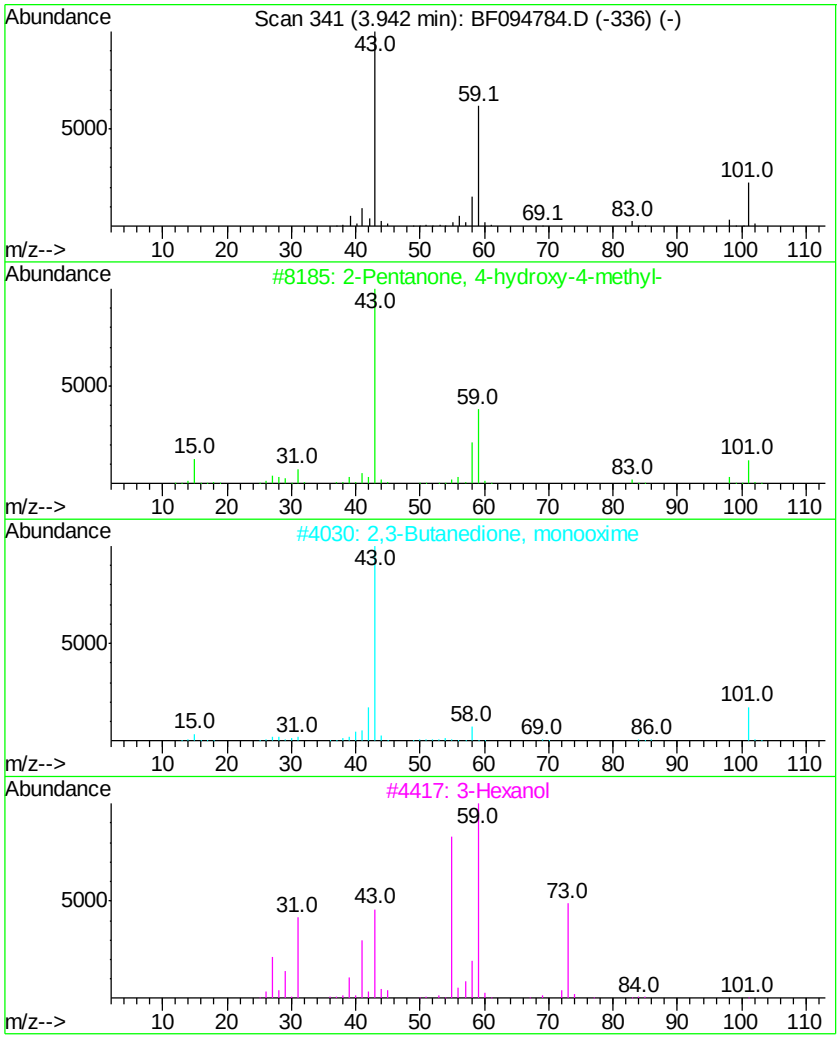
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

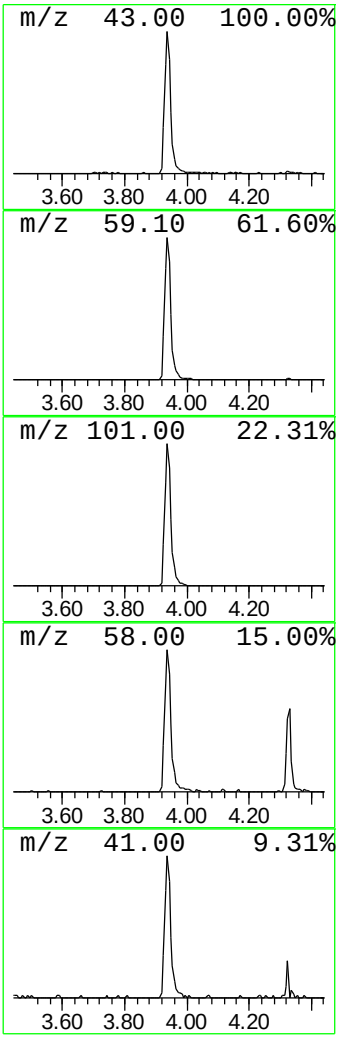
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	23.00 ng	651540	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094784.D
Acq On : 2 May 2017 7:46
Operator : SJ/MA
Sample : I2892-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWS-E(4.5-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

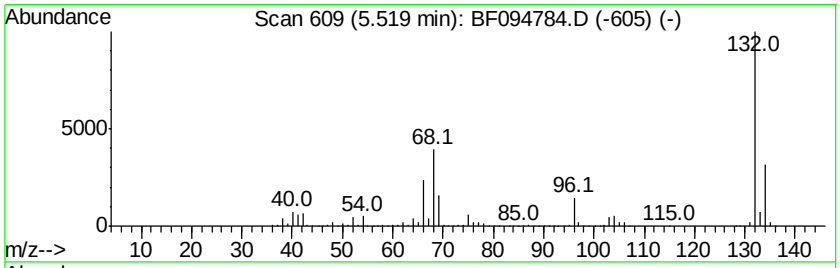
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

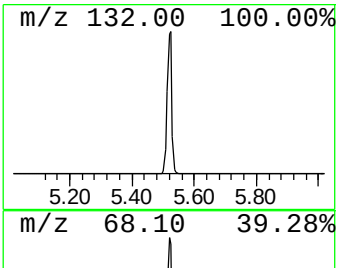
****

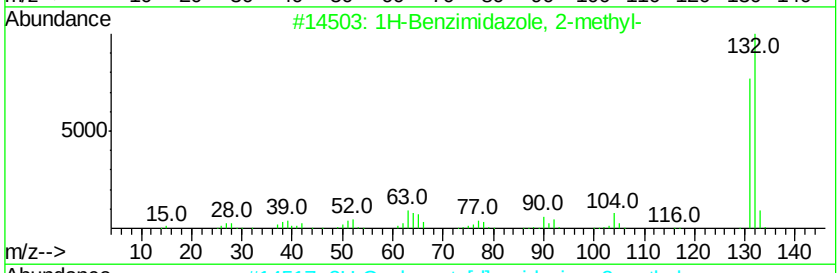
Peak Number 2 unknown5.52 Concentration Rank 1

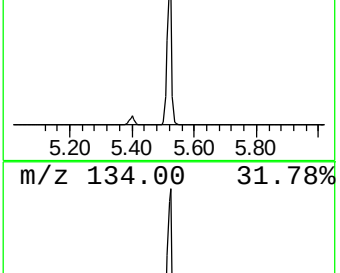
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	107.68 ng	3050190	1,4-Dichlorobenzene-d4	5.77

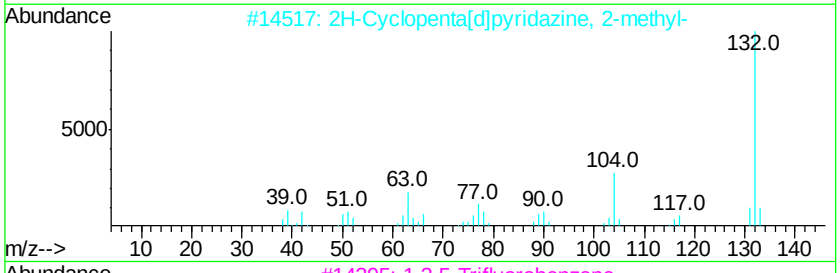
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9

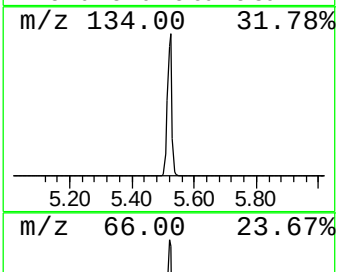


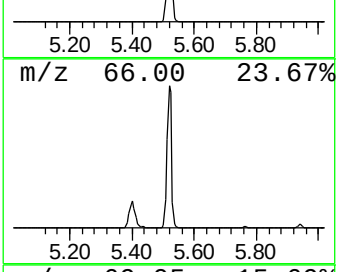


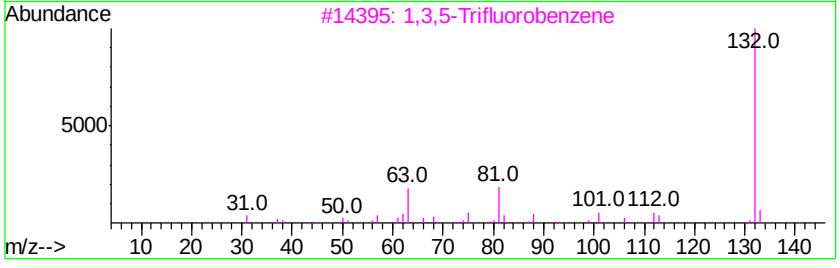


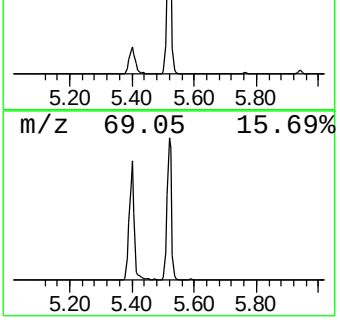












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094784.D
Acq On : 2 May 2017 7:46
Operator : SJ/MA
Sample : I2892-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWS-E(4.5-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

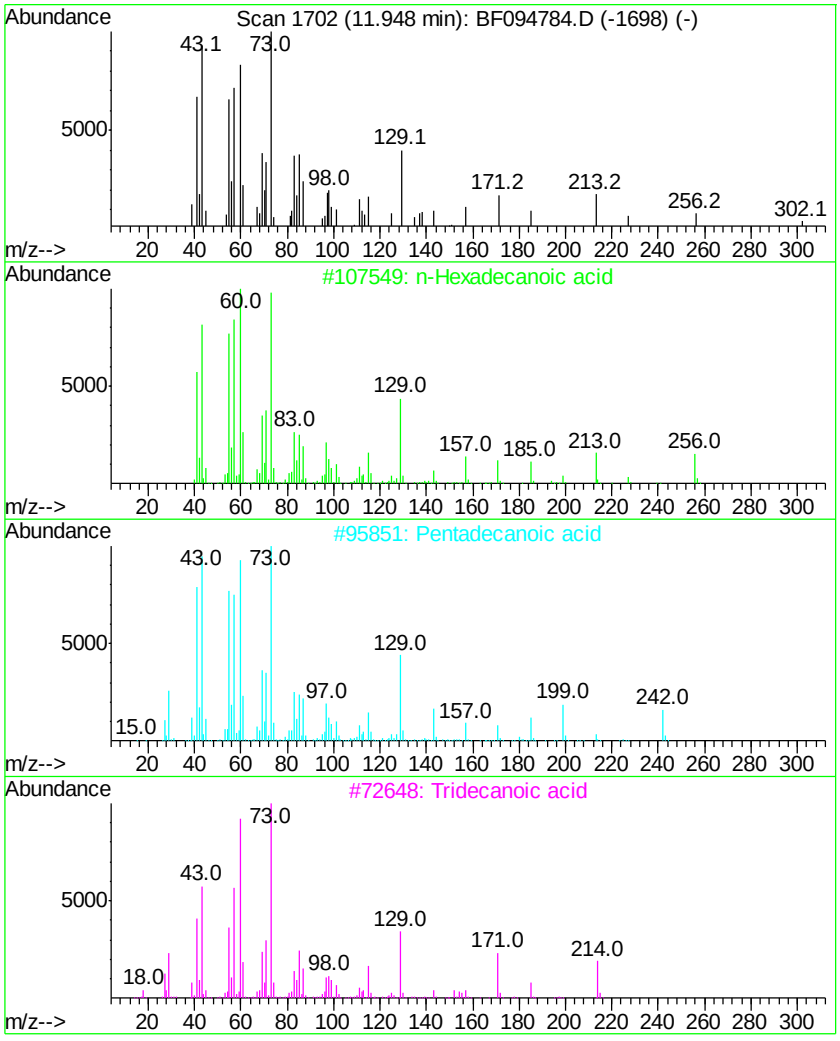
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

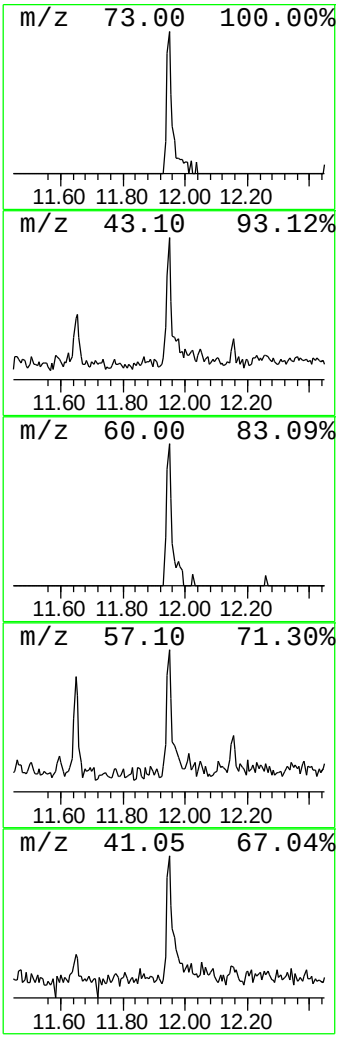
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.54 ng	77341	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	72
5	1-Phenazinecarboxylic acid, 6-[1...	506	C31H42N2O4	120464-92-8	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050117\
Data File : BF094784.D
Acq On : 2 May 2017 7:46
Operator : SJ/MA
Sample : I2892-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWS-E(4.5-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

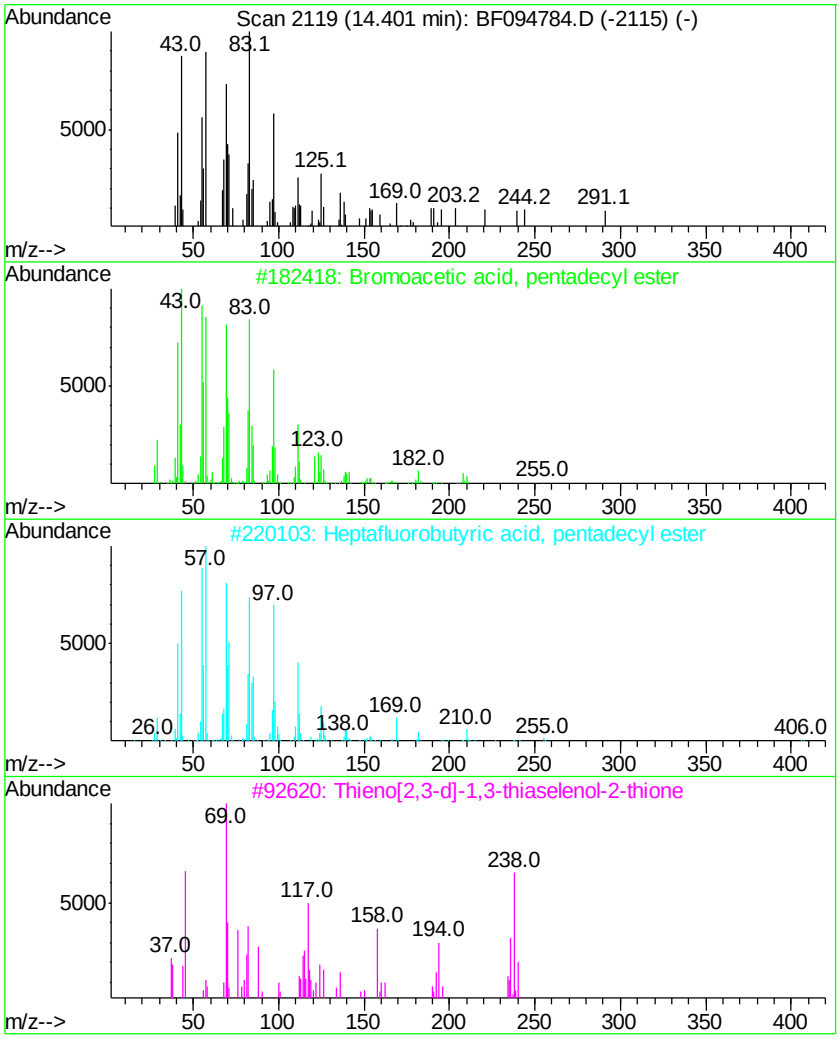
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

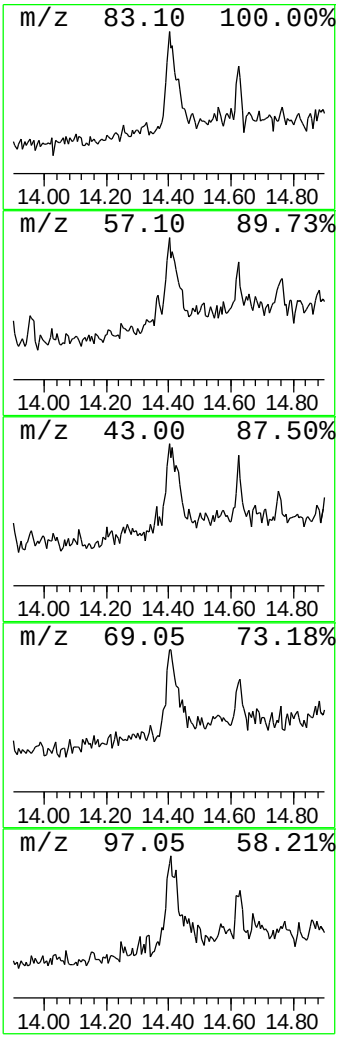
****

Peak Number 5 Bromoacetic acid, pentadecy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	3.46 ng	99690	Chrysene-d12	14.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	80
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	76
3	Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	74
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	68
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050117\
Data File : BF094784.D
Acq On : 2 May 2017 7:46
Operator : SJ/MA
Sample : I2892-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWS-E(4.5-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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...	3.94	23.0	ng	651540	1	5.77	566523	20.0
unknown5.52	5.52	107.7	ng	3050190	1	5.77	566523	20.0
n-Hexadecanoic acid	11.95	2.5	ng	77341	4	11.21	608264	20.0
Bromoacetic acid,...	14.40	3.5	ng	99690	5	14.47	576055	20.0