LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107739.D
Acq On : 27 Jul 2018 10:23
Operator : JU/SJ
Sample : J4142-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1B

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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	5.195	483	486	498	rBV	138325	200656	4.32%	0.640%
2	5.595	551	554	577	rBV	886472	1903378	41.00%	6.068%
3	6.548	711	716	721	rVB	44248	49843	1.07%	0.159%
4	6.601	721	725	744	rBV	648188	1530398	32.97%	4.879%
5	6.737	744	748	766	rVV	2530496	3495152	75.29%	11.142%
6	6.966	783	787	806	rBV	451976	877280	18.90%	2.797%
7	7.113	809	812	842	rVB	2698359	3426551	73.81%	10.924%
8	7.525	879	882	903	rBV	1523354	2684598	57.83%	8.558%
9	7.678	905	908	915	rVB	125731	134287	2.89%	0.428%
10	7.813	927	931	938	rVB4	23809	48851	1.05%	0.156%
11	8.242	1001	1004	1021	rBV	800917	1125224	24.24%	3.587%
12	8.725	1083	1086	1090	rVB	47440	50105	1.08%	0.160%
13	8.772	1090	1094	1096	rBV2	40653	52212	1.12%	0.166%
14	9.313	1182	1186	1195	rBV	3816832	4642084	100.00%	14.799%
15	9.383	1195	1198	1202	rVB	170704	200158	4.31%	0.638%
16	9.707	1249	1253	1259	rBV	157455	208164	4.48%	0.664%
17	10.001	1299	1303	1312	rBV	1012471	1108675	23.88%	3.534%
18	10.189	1332	1335	1341	rVB	39030	52887	1.14%	0.169%
19	10.795	1434	1438	1466	rBV	2126582	2761349	59.49%	8.803%
20	11.495	1553	1557	1570	rBV	810548	1058954	22.81%	3.376%
21	12.001	1639	1643	1654	rVB2	91634	137789	2.97%	0.439%
22	13.077	1822	1826	1842	rBV	3267957	3468185	74.71%	11.056%
23	13.954	1972	1975	1980	rBV	65024	68558	1.48%	0.219%
24	14.142	2003	2007	2018	rBV	816664	1019601	21.96%	3.250%
25	15.671	2260	2267	2284	rBV	602387	1063166	22.90%	3.389%

Sum of corrected areas: 31368105

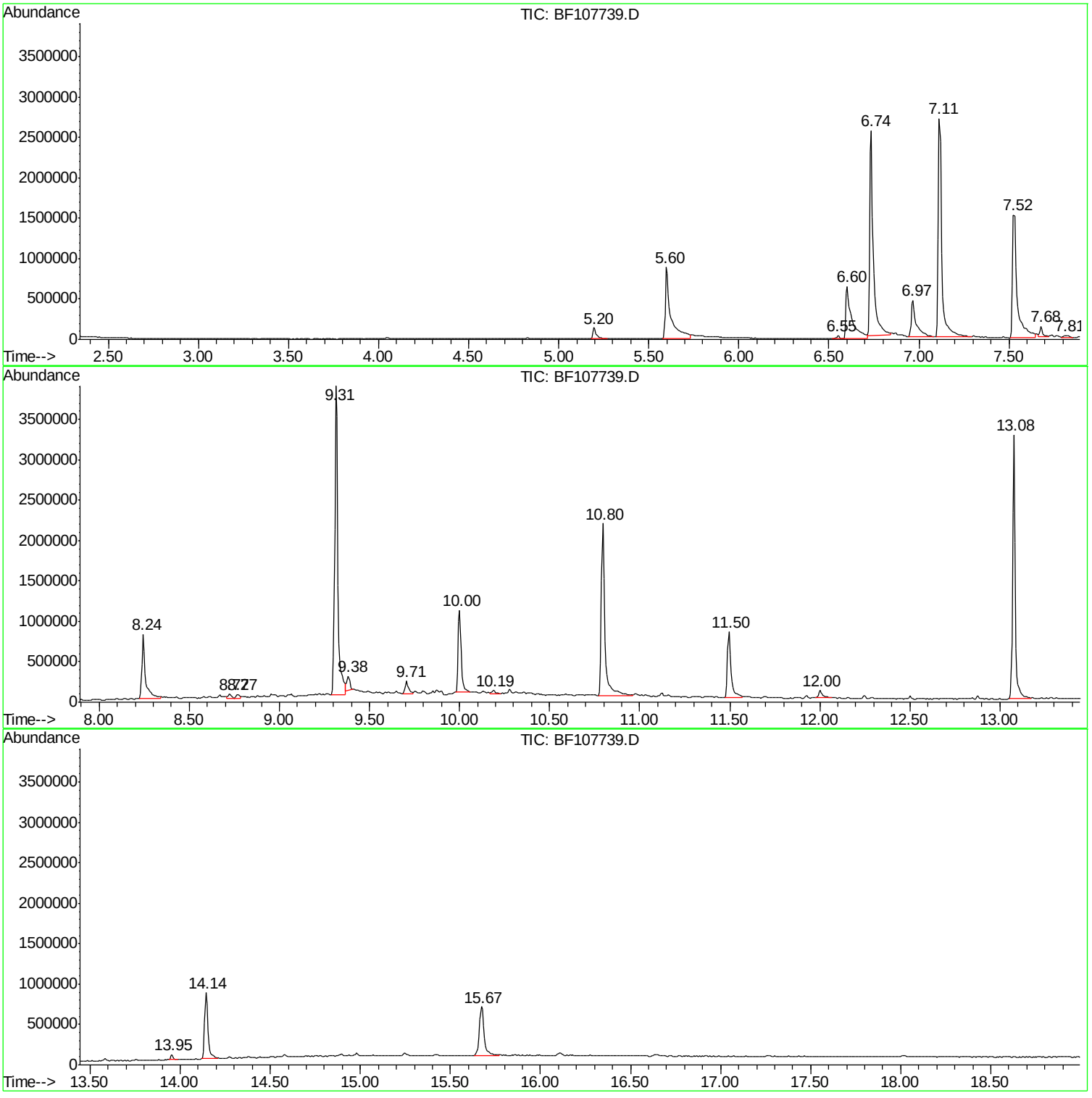
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107739.D
Acq On : 27 Jul 2018 10:23
Operator : JU/SJ
Sample : J4142-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107739.D
Acq On : 27 Jul 2018 10:23
Operator : JU/SJ
Sample : J4142-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

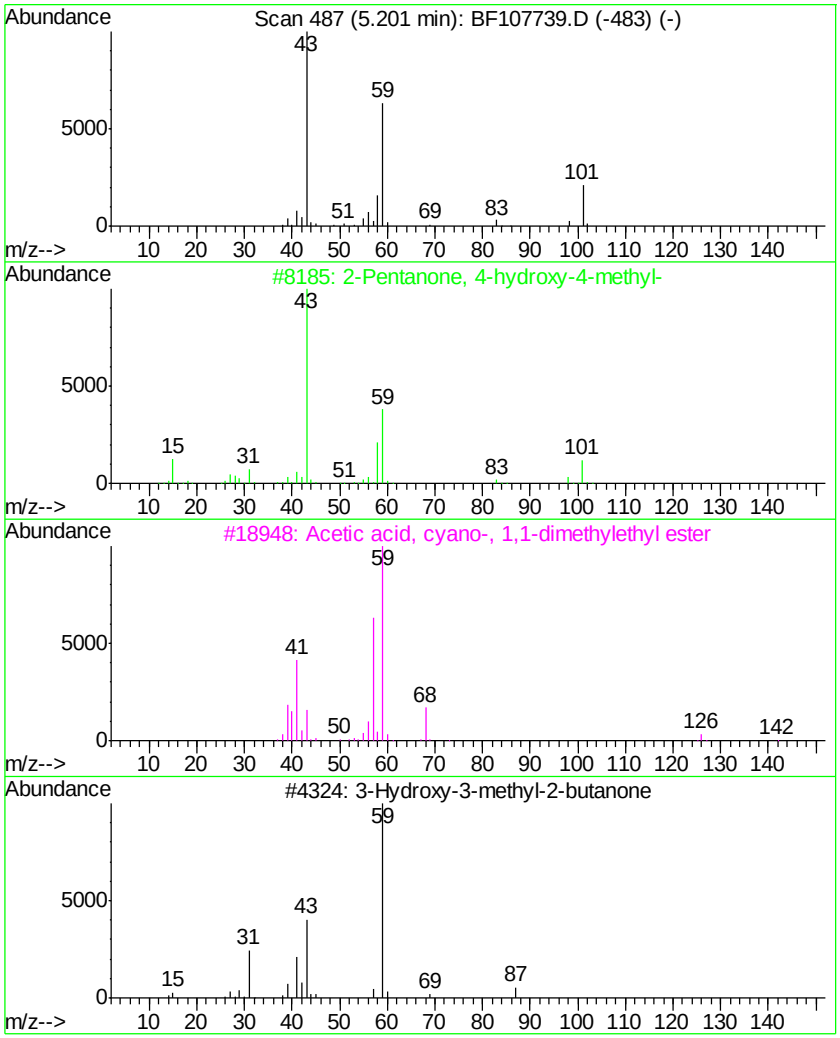
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

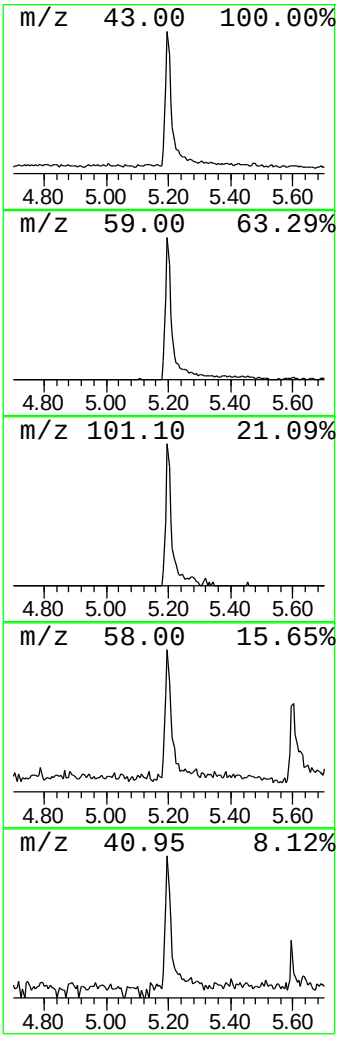
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	4.57 ng	200656	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107739.D
Acq On : 27 Jul 2018 10:23
Operator : JU/SJ
Sample : J4142-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

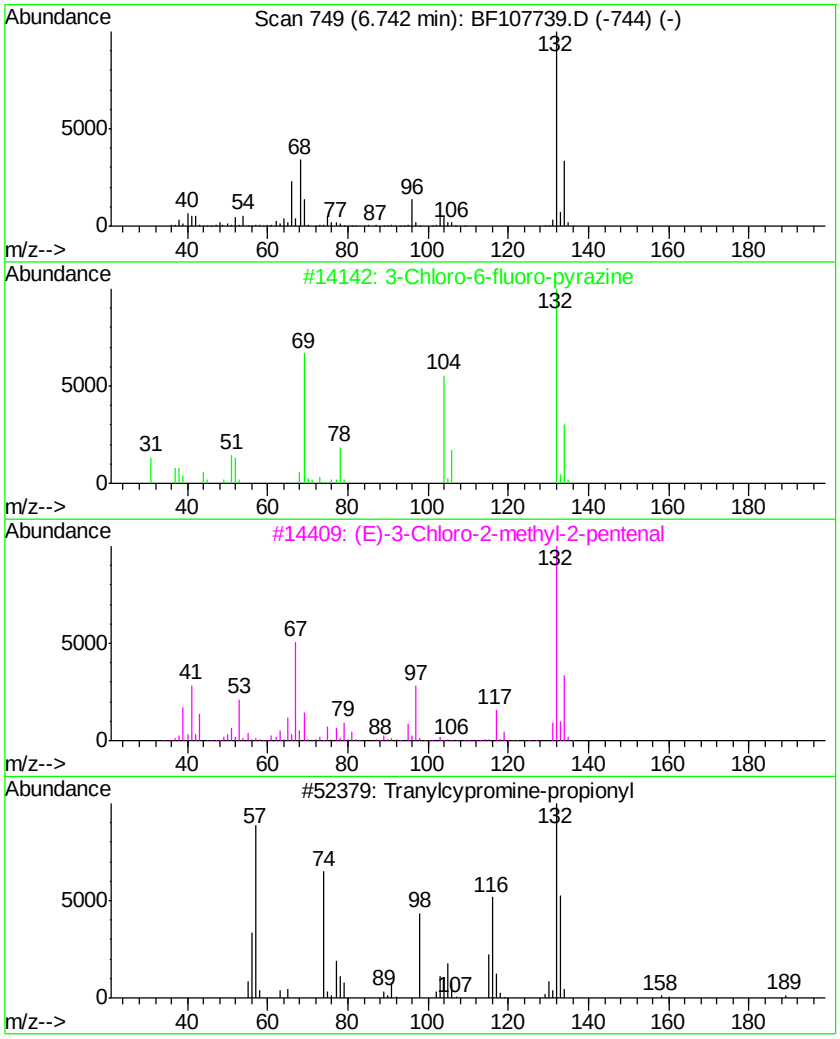
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

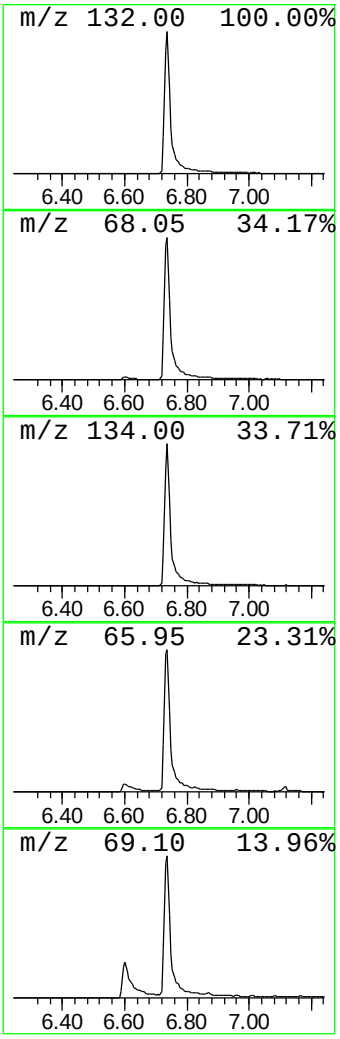
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	79.68 ng	3495150	1,4-Dichlorobenzene-d4	6.97

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	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107739.D
Acq On : 27 Jul 2018 10:23
Operator : JU/SJ
Sample : J4142-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

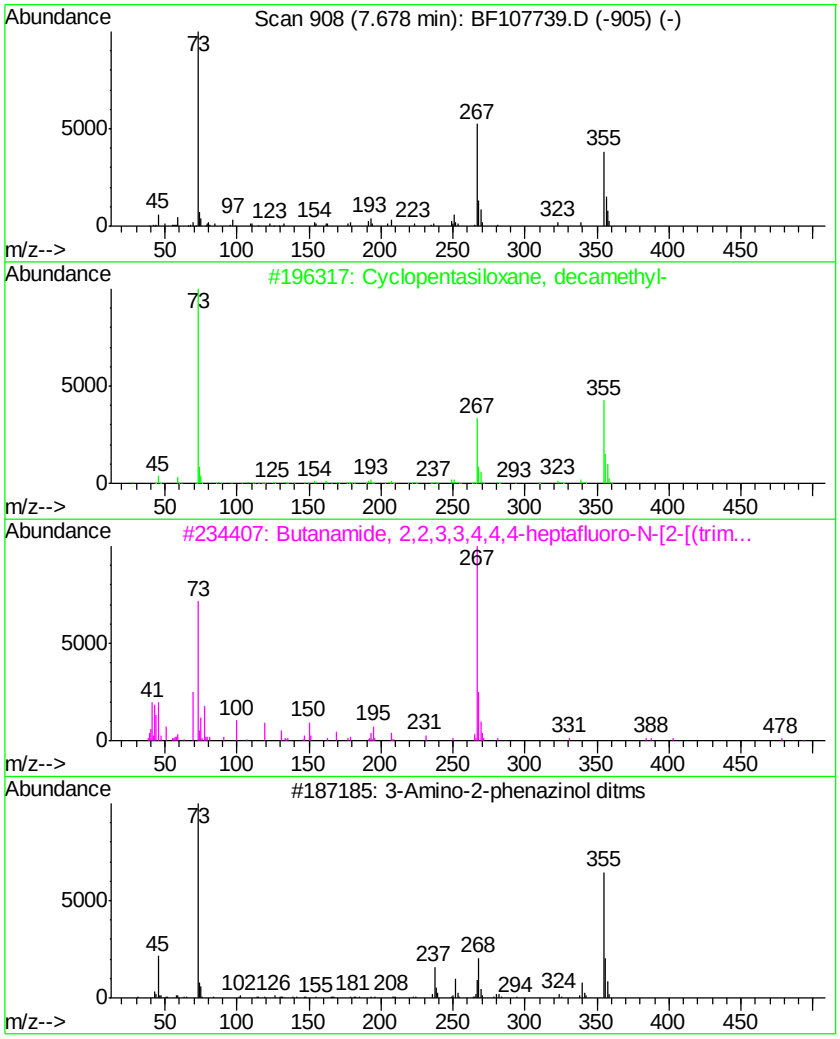
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

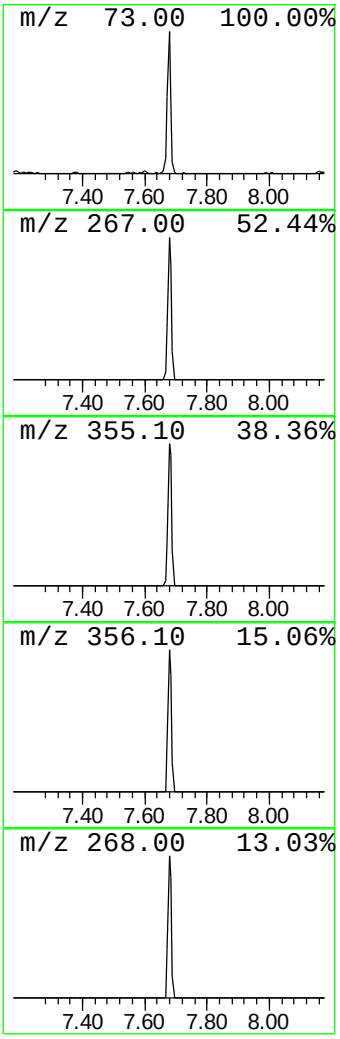
****

Peak Number 4 Cyclopentasiloxane, decamet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	2.39 ng	134287	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	74
2	Butanamide, 2,2,3,3,4,4,4-heptaf...	493	C18H26F7NO3Si2	055471-01-7	38
3	3-Amino-2-phenazinol ditms	355	C18H25N3OSi2	1000332-15-5	38
4	N-(Trifluoroacetyl)-O,O',O''-tri...	481	C19H34F3NO4Si3	1000072-26-3	38
5	Benzeneethanamine, N-butyl-.beta...	353	C18H35NO2Si2	040629-66-1	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107739.D
Acq On : 27 Jul 2018 10:23
Operator : JU/SJ
Sample : J4142-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

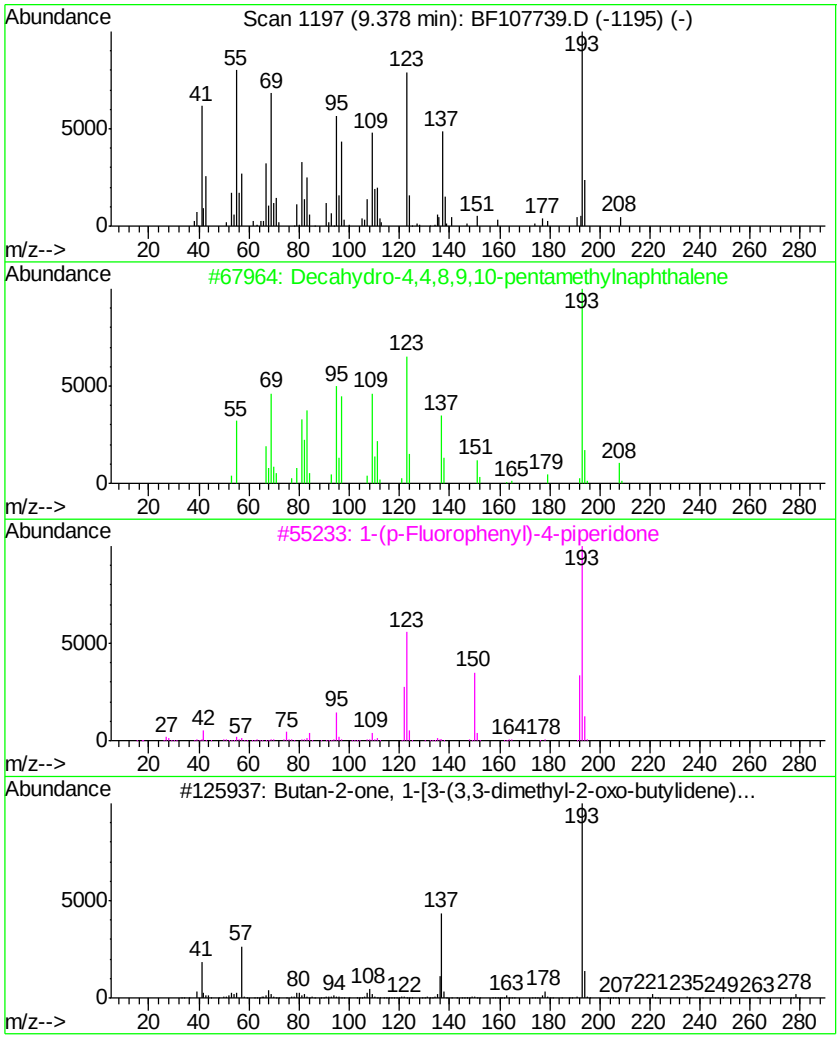
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

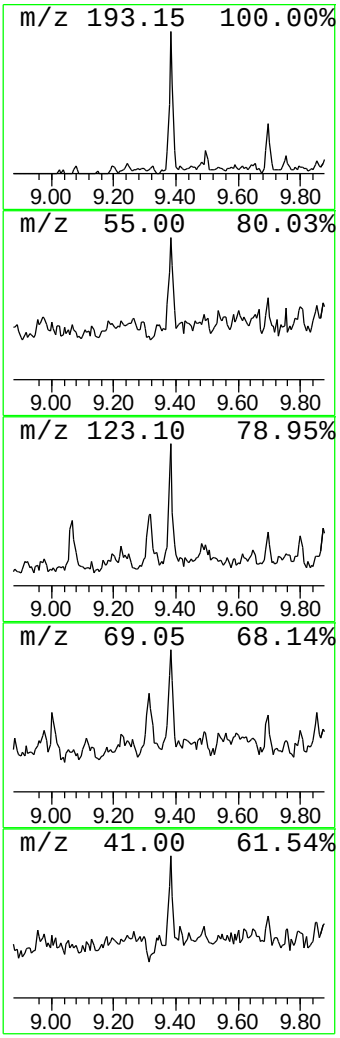
****

Peak Number 5 Decahydro-4,4,8,9,10-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.38	3.61 ng	200158	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	91
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	43
3	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	30
4	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	25
5	2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	054699-31-9	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107739.D
Acq On : 27 Jul 2018 10:23
Operator : JU/SJ
Sample : J4142-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

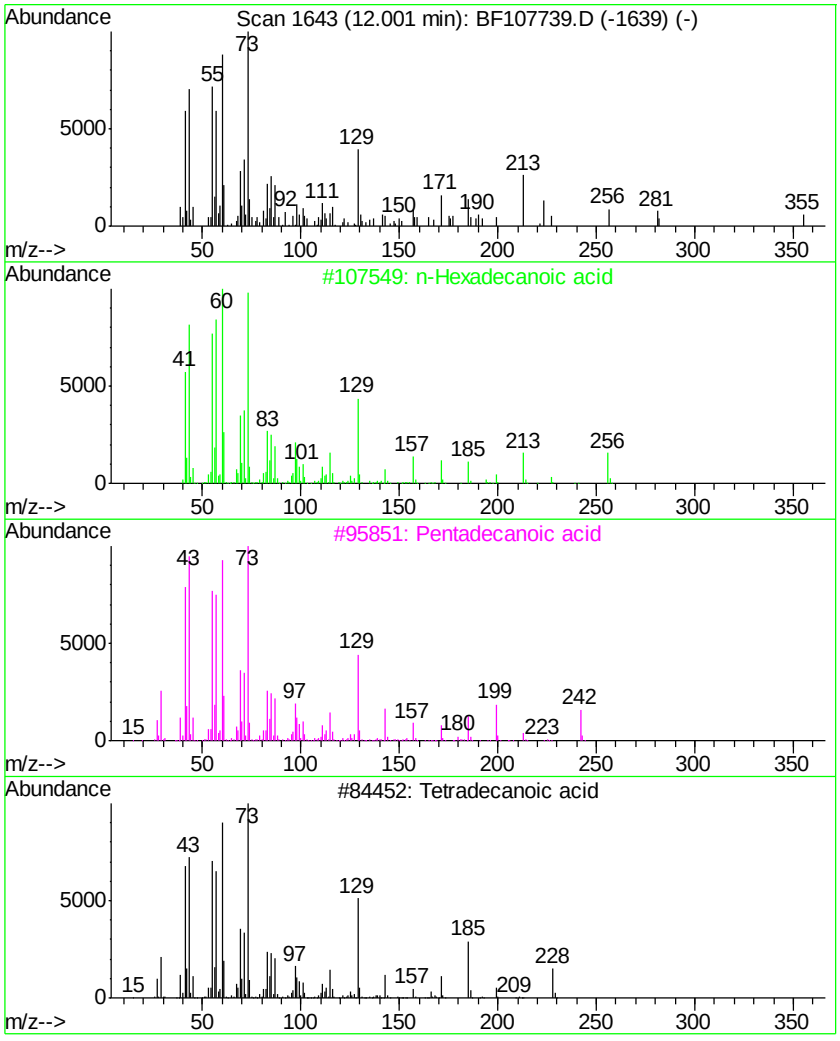
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

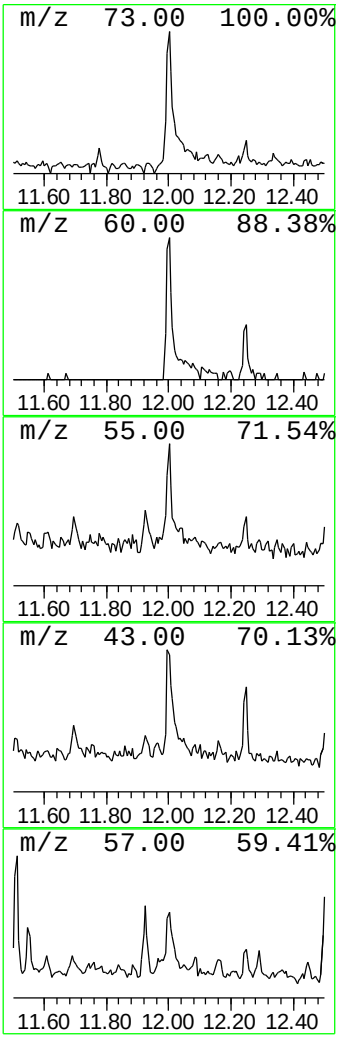
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	2.60 ng	137789	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107739.D
Acq On : 27 Jul 2018 10:23
Operator : JU/SJ
Sample : J4142-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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...	5.20	4.6	ng	200656	1	6.97	877280	20.0
unknown6.74	6.74	79.7	ng	3495150	1	6.97	877280	20.0
Cyclopentasiloxan...	7.68	2.4	ng	134287	2	8.24	1125220	20.0
Decahydro-4,4,8,9...	9.38	3.6	ng	200158	3	10.00	1108680	20.0
n-Hexadecanoic acid	12.00	2.6	ng	137789	4	11.50	1058950	20.0