LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106598.D
Acq On : 19 Jun 2018 22:30
Operator : JU/SJ
Sample : J3498-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-G-S

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-BF061918.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	5.196	482	486	496	rBV	119398	126029	9.31%	0.919%
2	5.607	552	556	563	rBV	1492799	1317274	97.33%	9.602%
3	6.601	721	725	735	rBV	1521100	1311375	96.89%	9.559%
4	6.737	744	748	752	rBV	1534154	1353457	100.00%	9.865%
5	6.960	783	786	790	rBV	715352	574093	42.42%	4.185%
6	7.119	809	813	816	rBV	1244119	1041871	76.98%	7.594%
7	7.525	877	882	885	rBV	891254	823355	60.83%	6.001%
8	8.242	1000	1004	1008	rBV	779261	683218	50.48%	4.980%
9	9.319	1183	1187	1190	rBV	1510947	1297415	95.86%	9.457%
10	9.707	1250	1253	1261	rBV	127246	117995	8.72%	0.860%
11	9.919	1284	1289	1292	rBV	20133	21137	1.56%	0.154%
12	10.007	1300	1304	1307	rBV	679120	643553	47.55%	4.691%
13	10.419	1371	1374	1376	rVB	34556	26578	1.96%	0.194%
14	10.795	1434	1438	1447	rBV	820844	680677	50.29%	4.961%
15	10.889	1452	1454	1460	rVB	29432	29257	2.16%	0.213%
16	11.495	1553	1557	1561	rBV	695881	590924	43.66%	4.307%
17	13.083	1823	1827	1830	rBV	1455910	1287994	95.16%	9.388%
18	13.966	1974	1977	1979	rBV3	37445	39950	2.95%	0.291%
19	14.148	2005	2008	2012	rBV	747454	759029	56.08%	5.533%
20	14.918	2137	2139	2149	rVB4	100297	155159	11.46%	1.131%
21	15.012	2152	2155	2158	rVB	117491	121796	9.00%	0.888%
22	15.695	2266	2271	2281	rVB	445493	717169	52.99%	5.227%

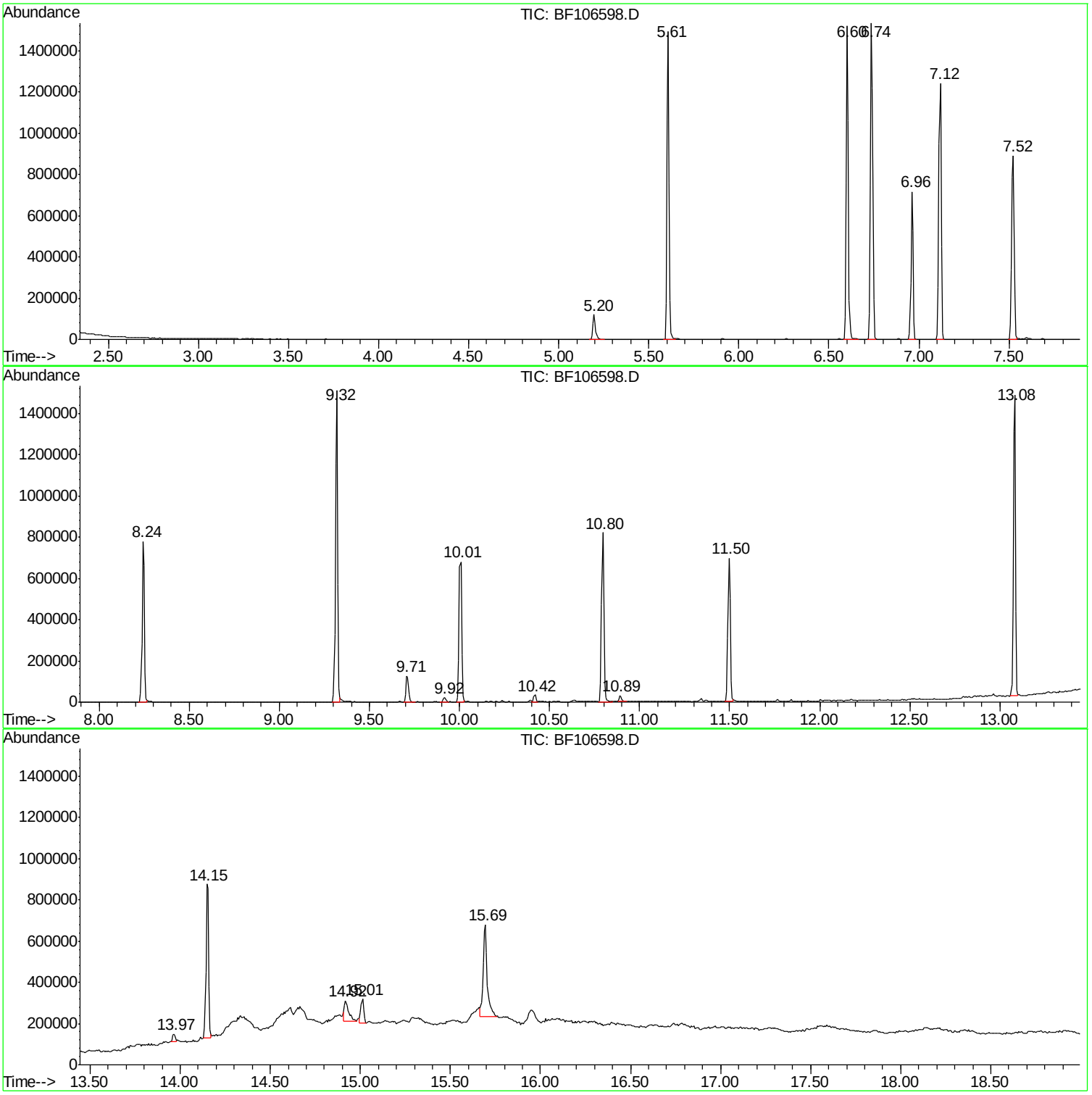
Sum of corrected areas: 13719305

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106598.D
Acq On : 19 Jun 2018 22:30
Operator : JU/SJ
Sample : J3498-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-G-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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\BF061918\
Data File : BF106598.D
Acq On : 19 Jun 2018 22:30
Operator : JU/SJ
Sample : J3498-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-G-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

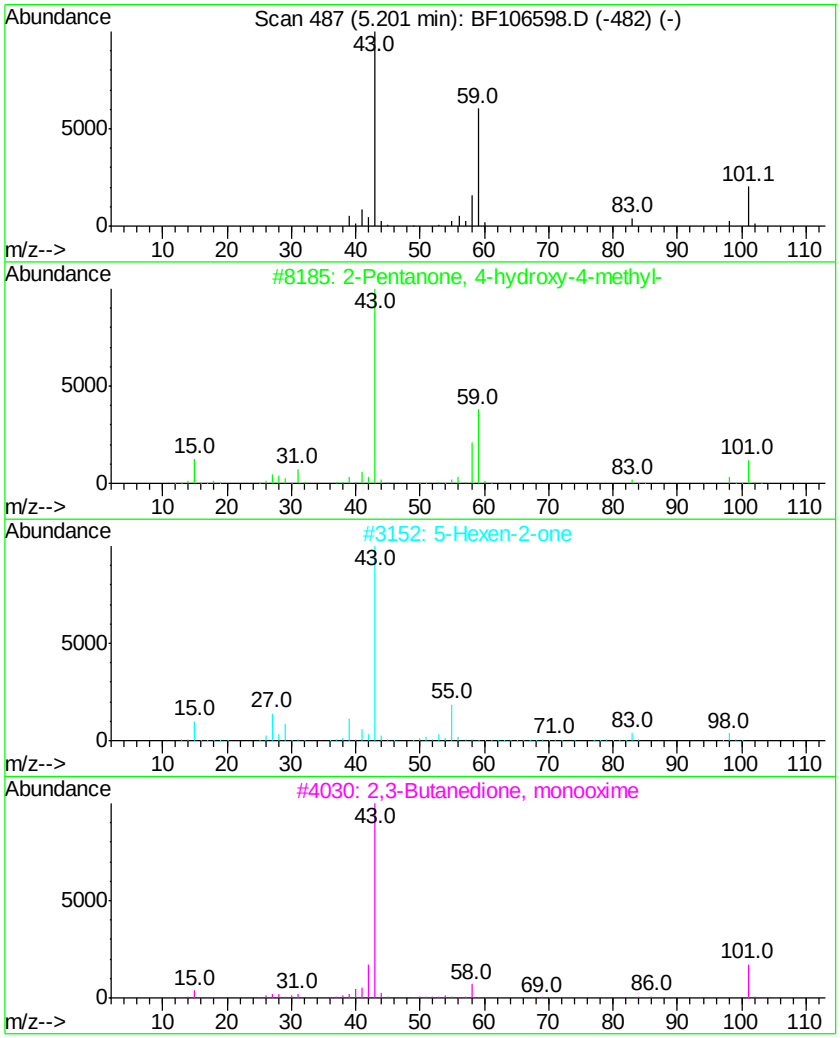
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

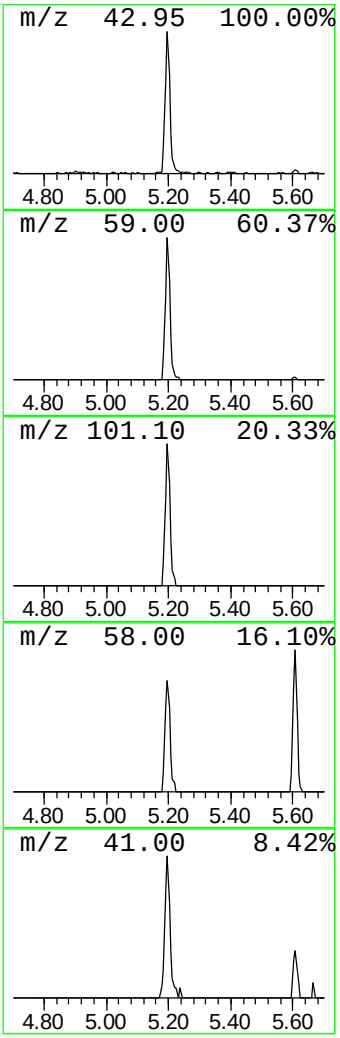
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	4.39 ng	126029	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106598.D
Acq On : 19 Jun 2018 22:30
Operator : JU/SJ
Sample : J3498-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-G-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

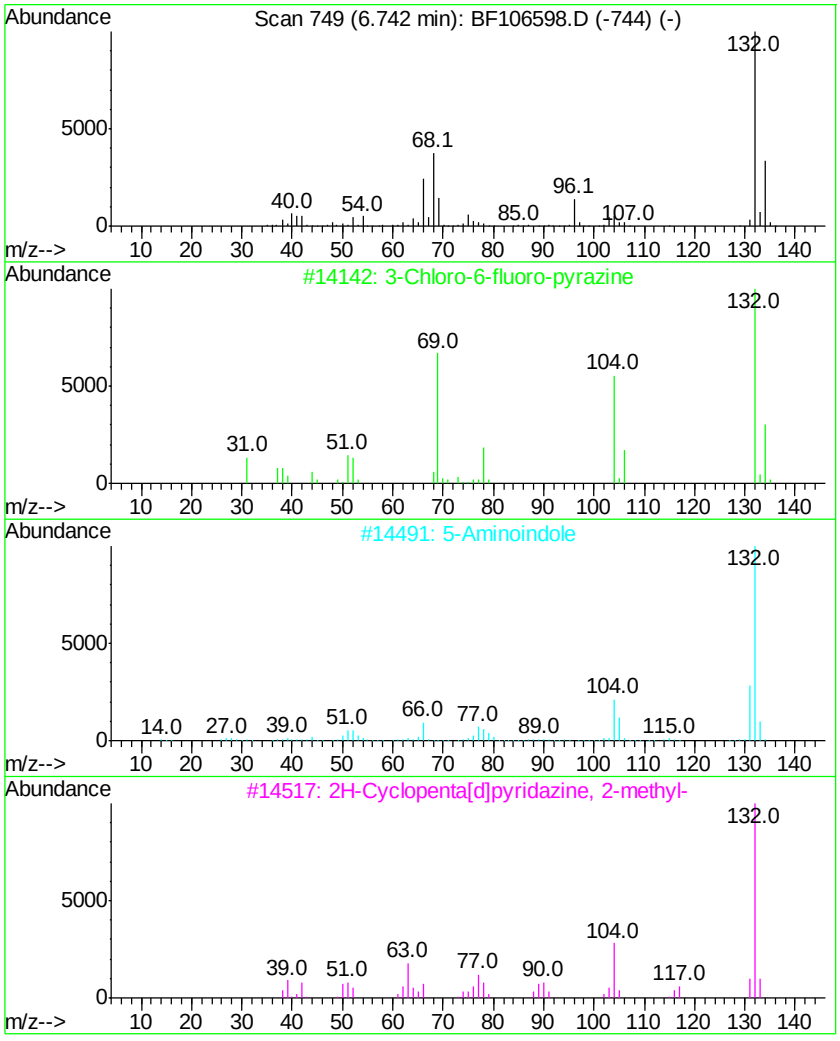
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

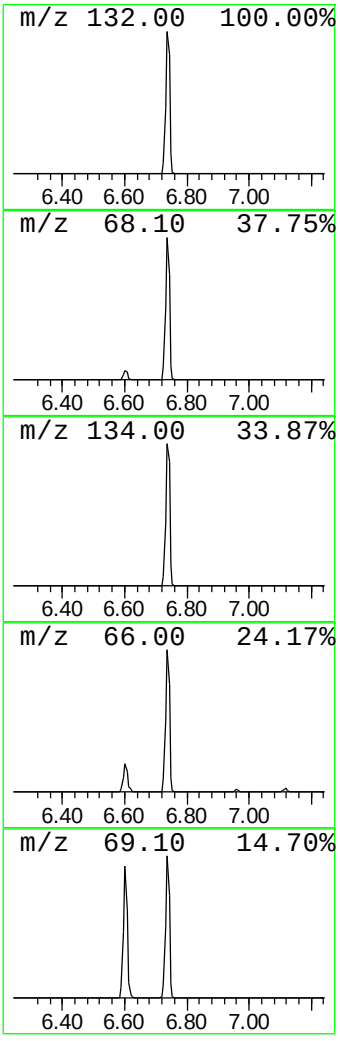
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	47.15 ng	1353460	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106598.D
Acq On : 19 Jun 2018 22:30
Operator : JU/SJ
Sample : J3498-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-G-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

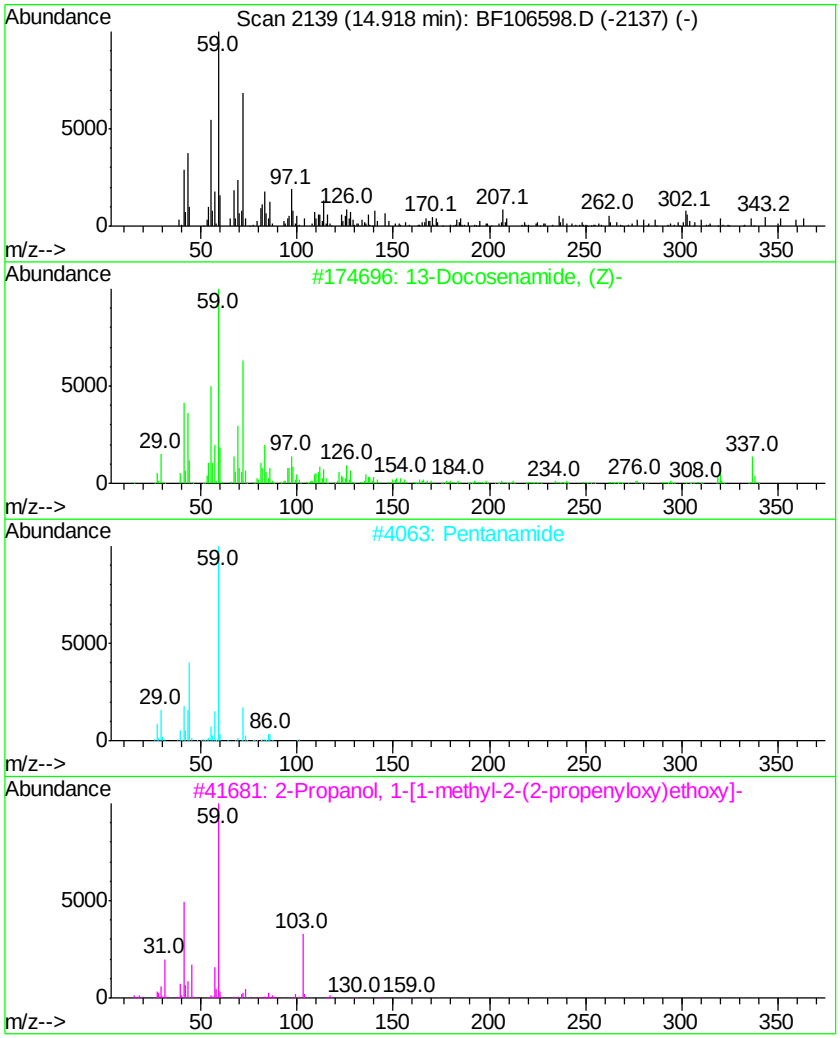
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

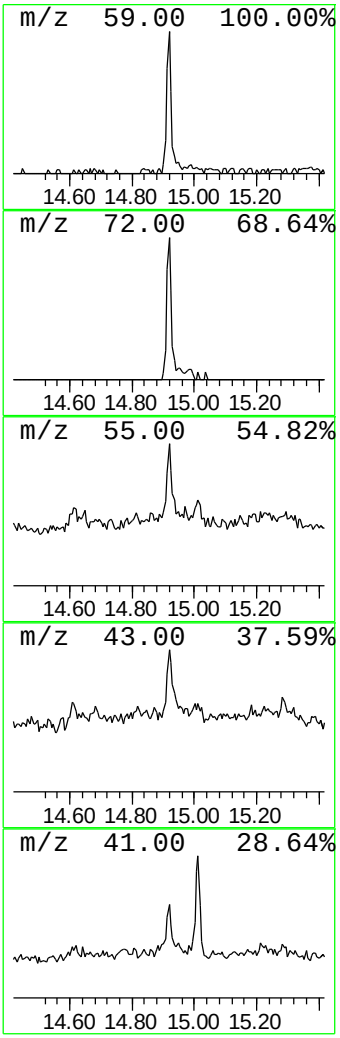
****

Peak Number 4 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.09 ng	155159	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	59
2	Pentanamide	101	C5H11NO	000626-97-1	43
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	38
4	1-Phenyl-9-thioureido-3,6-diazah...	302	C16H22N4S	153464-71-2	38
5	2-Propenoic acid, 3-methoxybutyl...	158	C8H14O3	002768-07-2	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106598.D
Acq On : 19 Jun 2018 22:30
Operator : JU/SJ
Sample : J3498-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-G-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

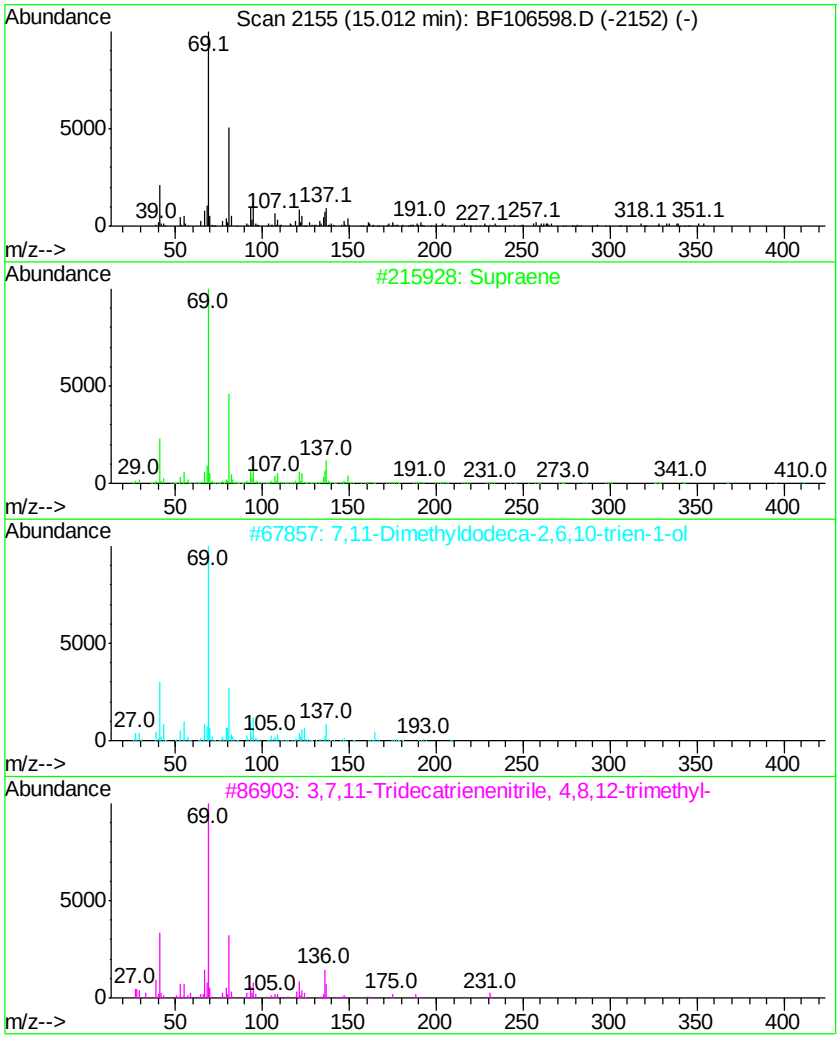
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

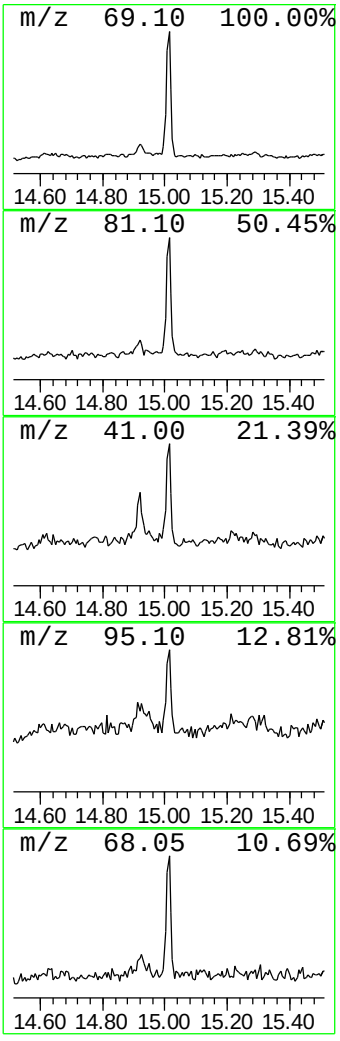
****

Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	3.40 ng	121796	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	80
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061918\
Data File : BF106598.D
Acq On : 19 Jun 2018 22:30
Operator : JU/SJ
Sample : J3498-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-G-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	4.4	ng	126029	1	6.96	574093	20.0
unknown6.74	6.74	47.1	ng	1353460	1	6.96	574093	20.0
13-Docosenamide, ...	14.92	4.1	ng	155159	5	14.15	759029	20.0
Supraene	15.01	3.4	ng	121796	6	15.69	717169	20.0