LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109425.D
Acq On : 28 Sep 2018 10:31
Operator : JU/SJ
Sample : J5133-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-SIDI-F-U-M

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-BF092218.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	4.887	473	476	488	rBV	78749	84417	2.56%	0.461%
2	5.310	545	548	567	rBV	844856	837911	25.41%	4.581%
3	6.339	719	723	735	rBV	588938	576834	17.49%	3.153%
4	6.475	742	746	749	rBV	1953465	1620902	49.15%	8.861%
5	6.704	782	785	789	rBV	756489	611824	18.55%	3.345%
6	6.863	808	812	815	rBV	2600993	2316681	70.25%	12.664%
7	7.269	876	881	884	rBV	1973679	1870300	56.71%	10.224%
8	7.986	999	1003	1009	rBV	903504	735175	22.29%	4.019%
9	9.063	1182	1186	1189	rBV	3404088	3297903	100.00%	18.028%
10	9.457	1250	1253	1263	rVB	53739	47706	1.45%	0.261%
11	9.733	1297	1300	1313	rVB	837384	778255	23.60%	4.254%
12	10.522	1430	1434	1445	rBV	1100559	1085054	32.90%	5.932%
13	11.210	1548	1551	1555	rBV	740023	646660	19.61%	3.535%
14	12.792	1816	1820	1824	rBV	2484614	2388847	72.44%	13.059%
15	13.839	1994	1998	2004	rVB	754576	653619	19.82%	3.573%
16	14.686	2138	2142	2147	rVB	139041	121357	3.68%	0.663%
17	14.933	2179	2184	2188	rVB	36680	38104	1.16%	0.208%
18	15.239	2231	2236	2240	rBV	417687	498206	15.11%	2.724%
19	15.280	2240	2243	2250	rVB	34421	45655	1.38%	0.250%
20	15.686	2307	2312	2317	rBV	26594	37353	1.13%	0.204%

Sum of corrected areas: 18292763

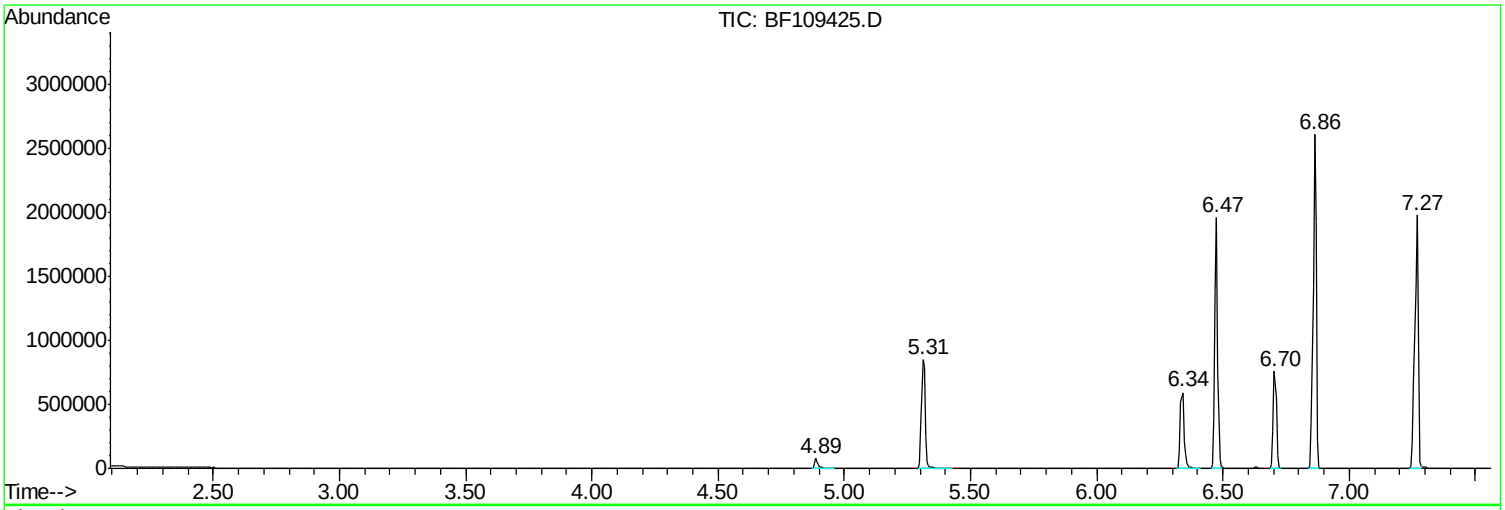
LSC Report - Integrated Chromatogram

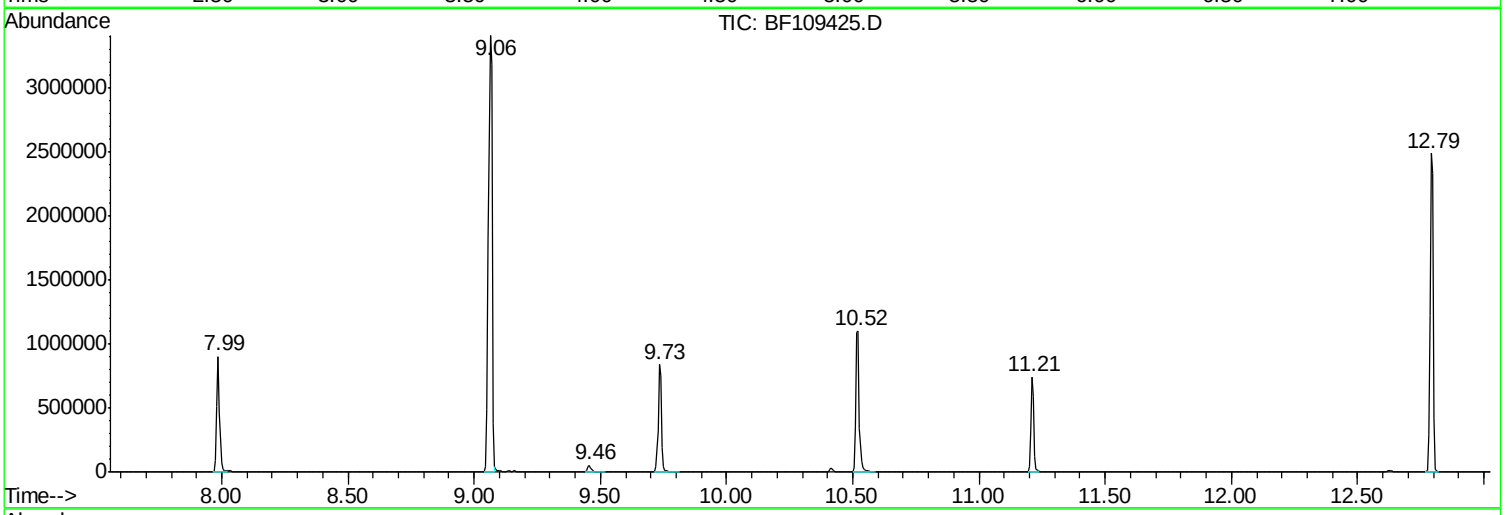
Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109425.D
Acq On : 28 Sep 2018 10:31
Operator : JU/SJ
Sample : J5133-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

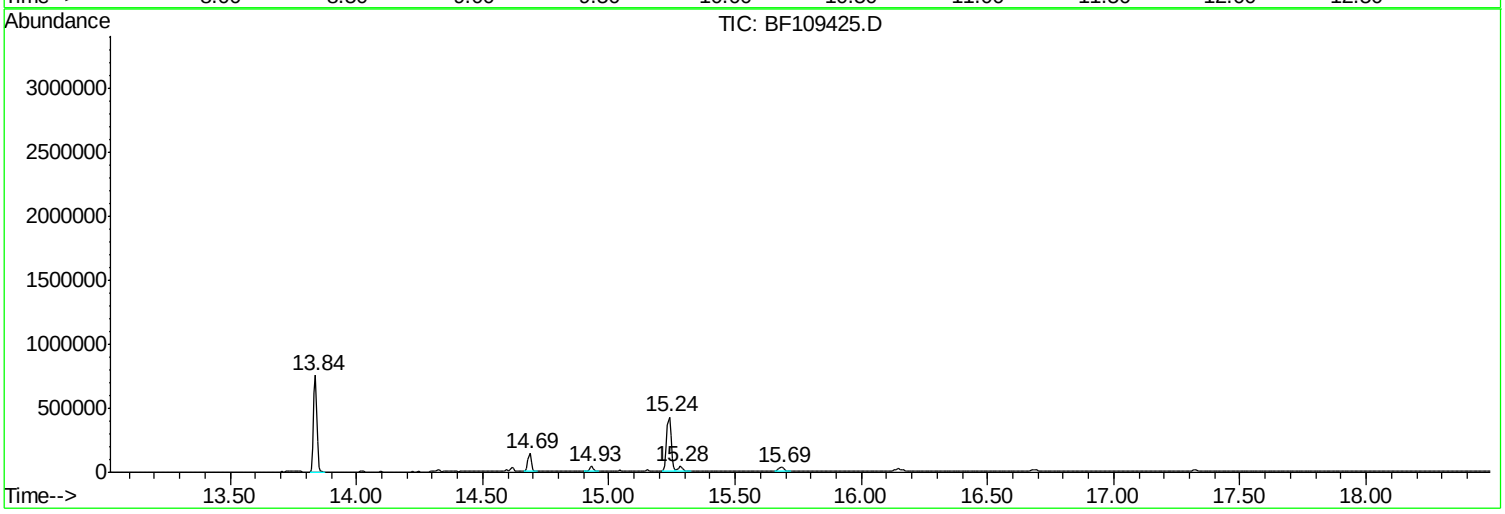
Instrument :
BNA_F
ClientSampleId :
092618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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\BF092718\
Data File : BF109425.D
Acq On : 28 Sep 2018 10:31
Operator : JU/SJ
Sample : J5133-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-SIDI-F-U-M

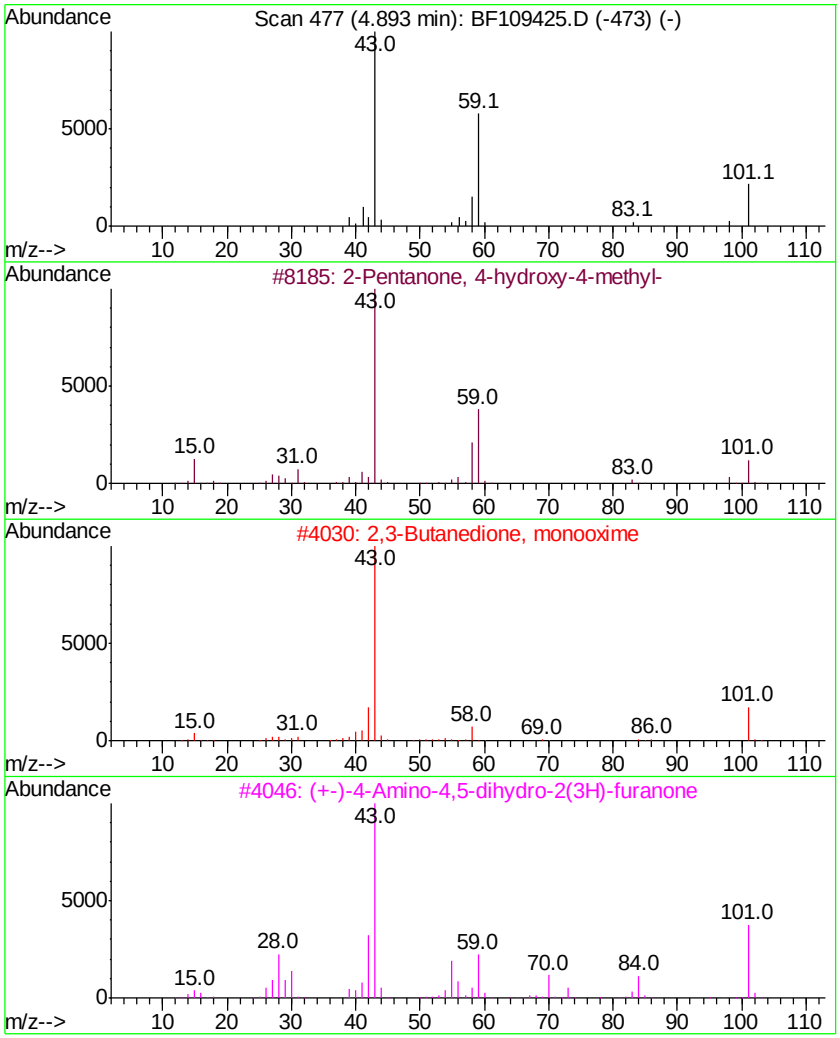
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

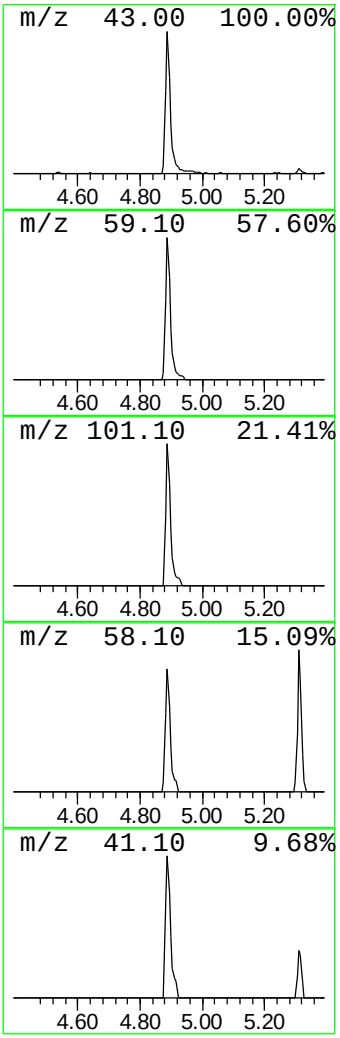
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.76 ng	84417	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109425.D
Acq On : 28 Sep 2018 10:31
Operator : JU/SJ
Sample : J5133-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

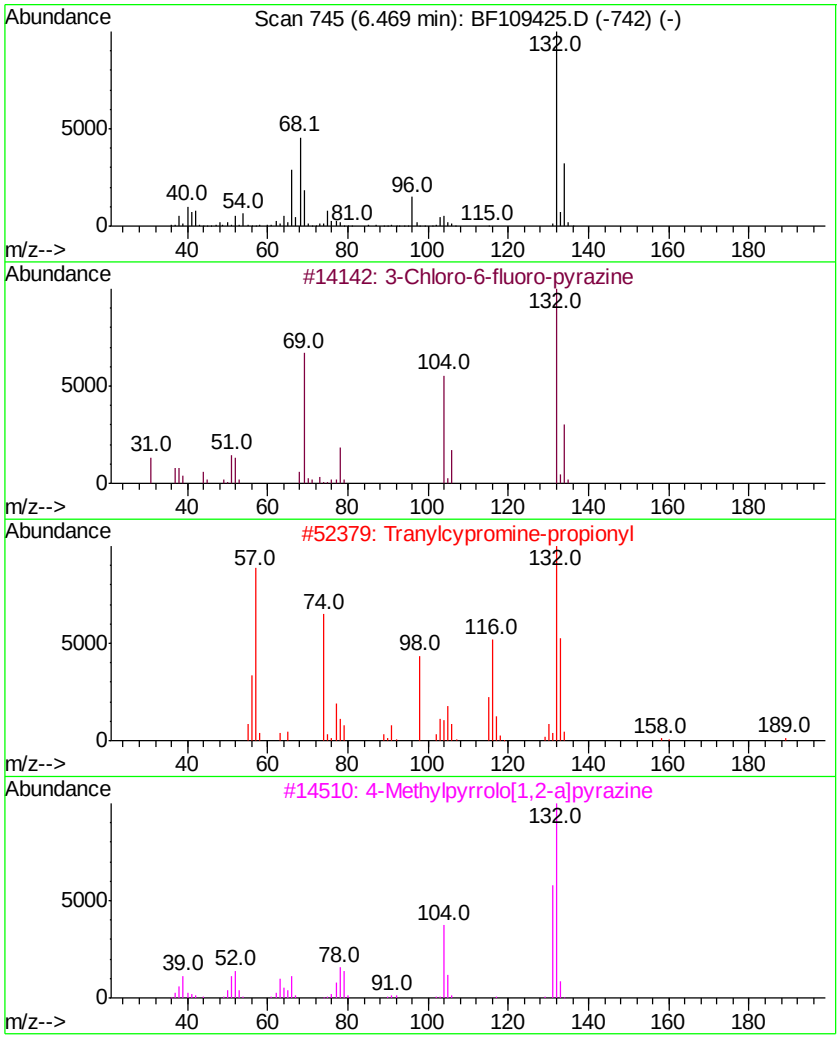
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

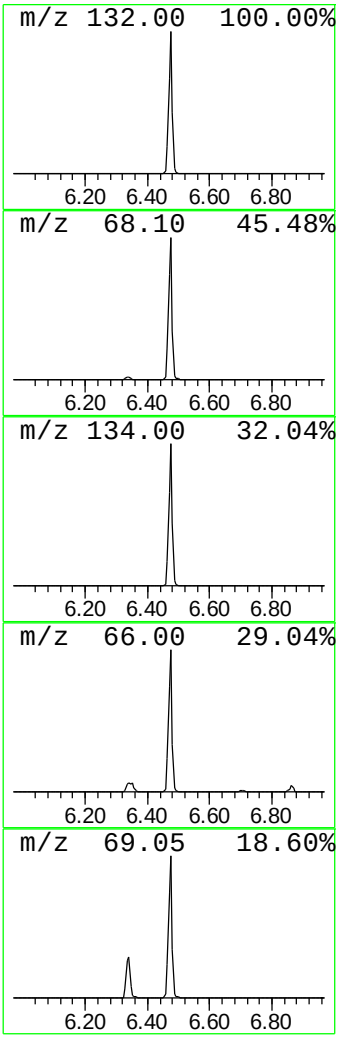
****

Peak Number 2 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	52.99 ng	1620900	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092718\
Data File : BF109425.D
Acq On : 28 Sep 2018 10:31
Operator : JU/SJ
Sample : J5133-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

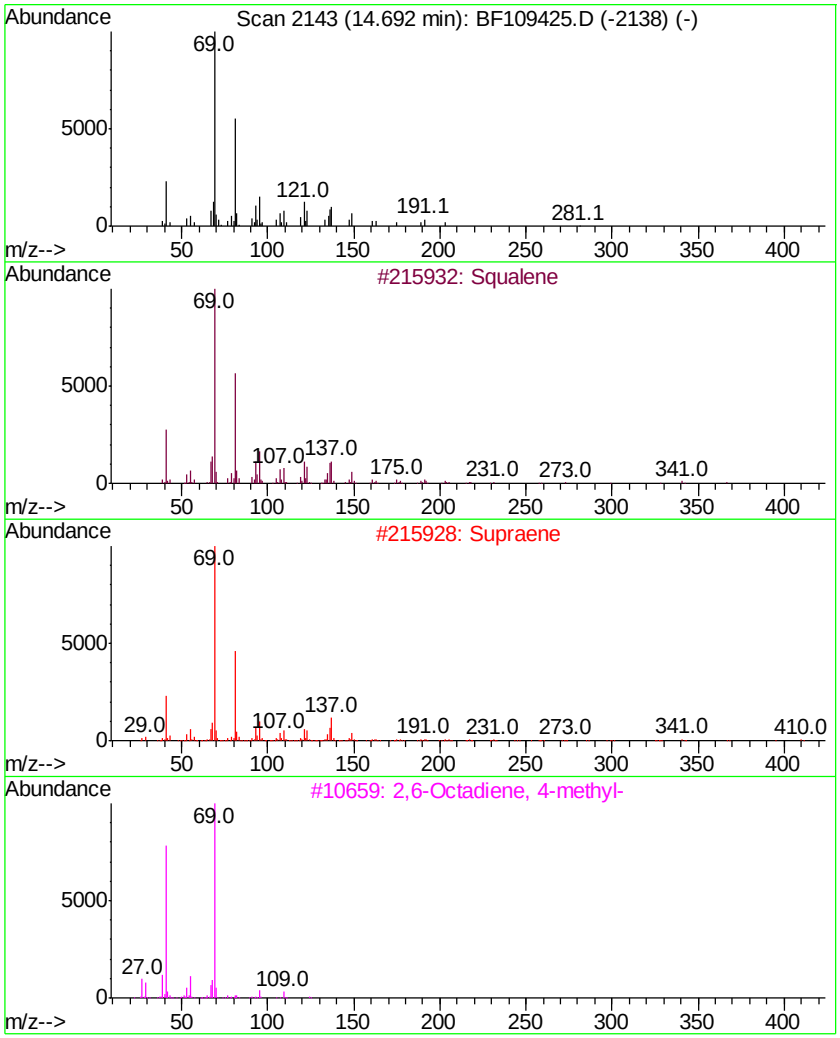
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

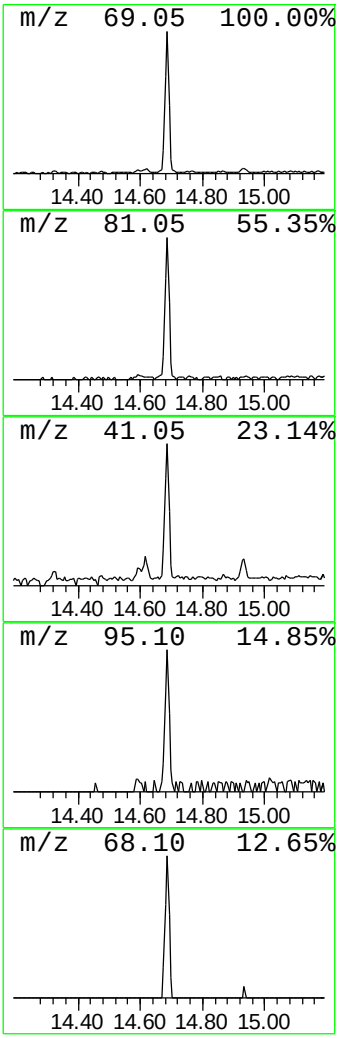
****

Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	4.87 ng	121357	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109425.D
Acq On : 28 Sep 2018 10:31
Operator : JU/SJ
Sample : J5133-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-SIDI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	2.8	ng	84417	1	6.70	611824	20.0
unknown6.47	6.47	53.0	ng	1620900	1	6.70	611824	20.0
Squalene	14.69	4.9	ng	121357	6	15.24	498206	20.0