LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106471.D
Acq On : 15 Jun 2018 4:37
Operator : JU/SJ
Sample : J3474-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-U-B

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-BF061118.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	492	rBV	91424	89394	2.92%	0.479%
2	5.613	554	557	569	rVB	1026316	1038441	33.95%	5.563%
3	6.607	723	726	734	rBV	768543	754658	24.67%	4.043%
4	6.742	746	749	753	rBV	1804296	1657563	54.20%	8.879%
5	6.966	783	787	790	rBV	786628	614212	20.08%	3.290%
6	7.125	809	814	817	rBV	2583855	2282175	74.62%	12.225%
7	7.531	878	883	886	rBV	1872642	1790727	58.55%	9.593%
8	8.248	1001	1005	1008	rBV	837394	668309	21.85%	3.580%
9	9.325	1183	1188	1191	rBV	2949291	2752258	89.99%	14.743%
10	9.713	1250	1254	1262	rVB	107078	90608	2.96%	0.485%
11	10.007	1297	1304	1312	rVB	722572	638269	20.87%	3.419%
12	10.666	1414	1416	1419	rVB	95185	70514	2.31%	0.378%
13	10.795	1434	1438	1442	rBV	1185156	1092206	35.71%	5.851%
14	10.895	1452	1455	1462	rBV	32043	32009	1.05%	0.171%
15	11.495	1554	1557	1561	rBV	733831	650208	21.26%	3.483%
16	13.083	1823	1827	1831	rBV	3037451	3058511	100.00%	16.384%
17	13.965	1972	1977	1986	rBV2	44634	65500	2.14%	0.351%
18	14.142	2003	2007	2011	rBV	811131	759863	24.84%	4.070%
19	15.001	2149	2153	2156	rBV	46170	48665	1.59%	0.261%
20	15.677	2262	2268	2274	rBV	388819	513630	16.79%	2.751%

Sum of corrected areas: 18667720

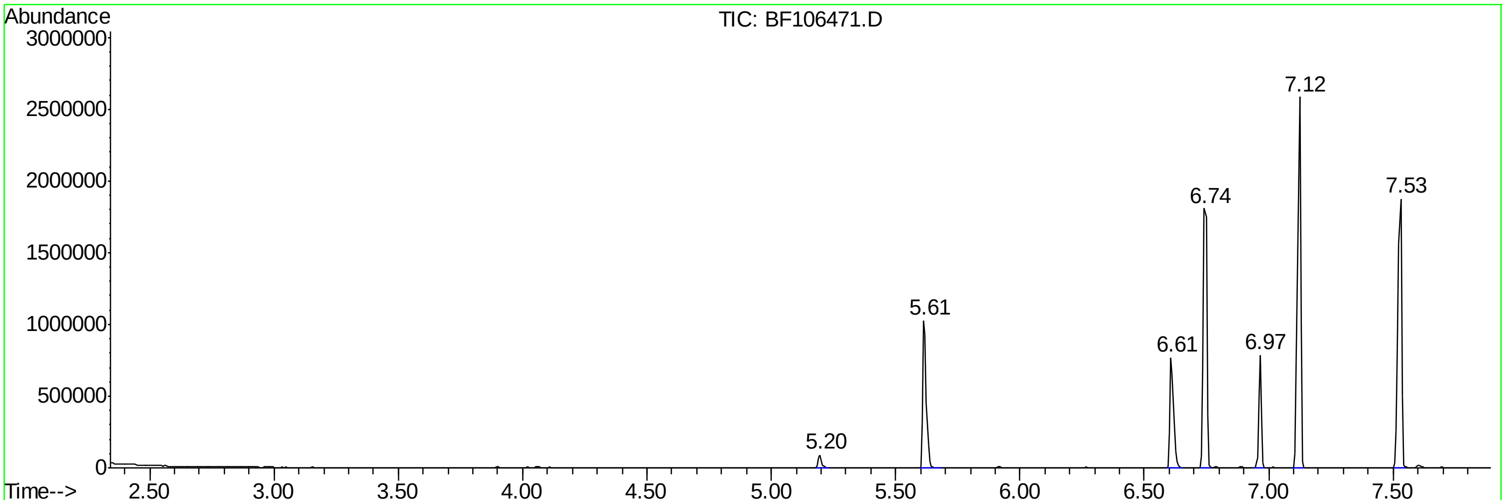
LSC Report - Integrated Chromatogram

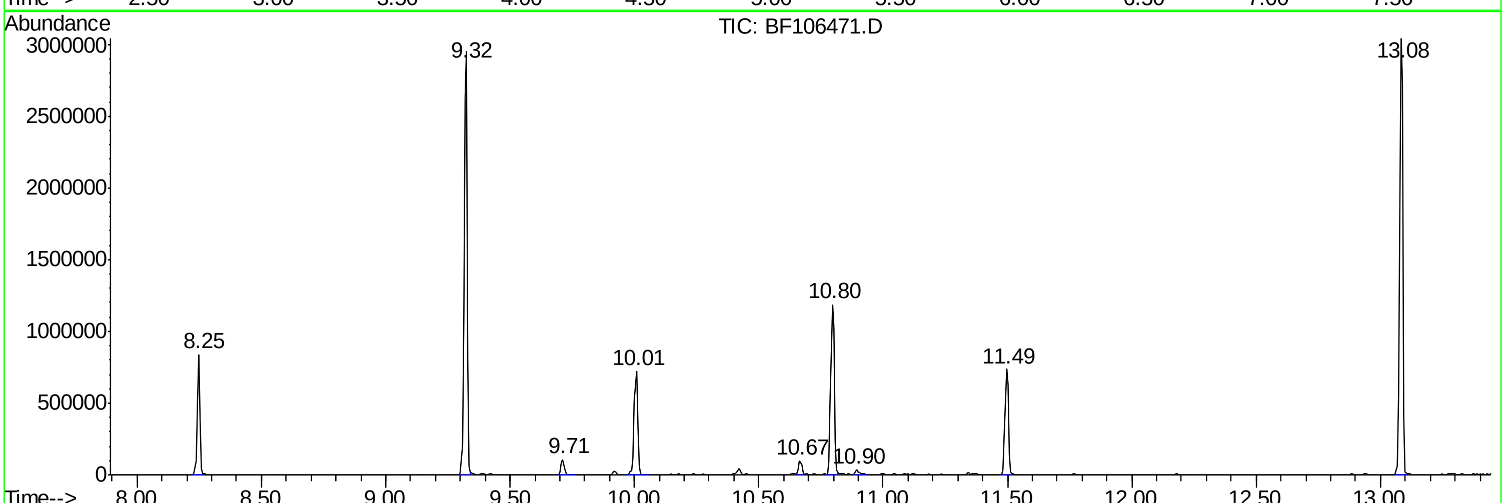
Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106471.D
Acq On : 15 Jun 2018 4:37
Operator : JU/SJ
Sample : J3474-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

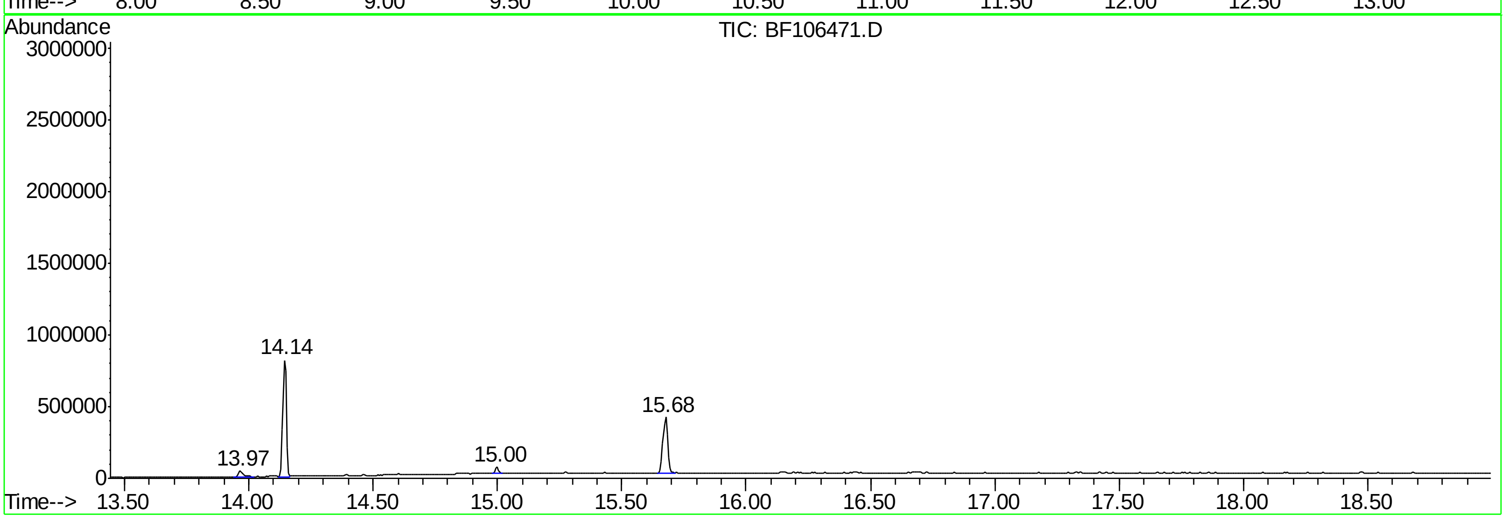
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Instrument :
BNA_F
ClientSampleId :
061118-DBRI-E-U-B







Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106471.D
Acq On : 15 Jun 2018 4:37
Operator : JU/SJ
Sample : J3474-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

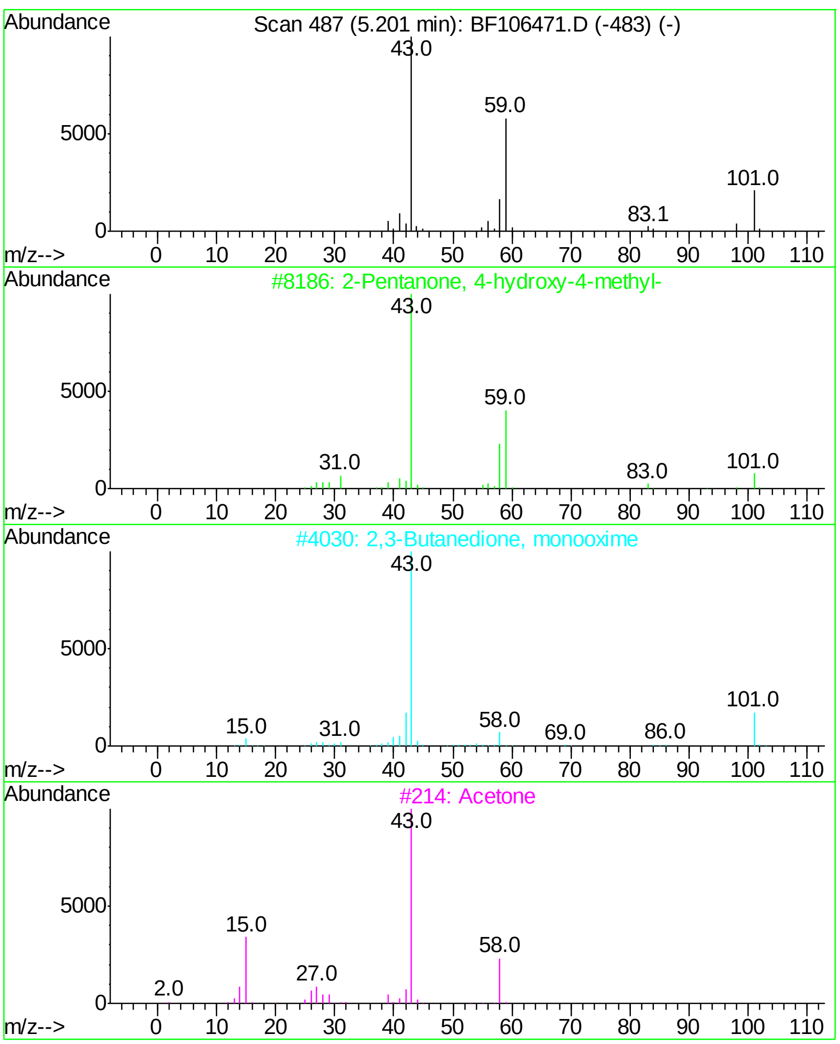
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

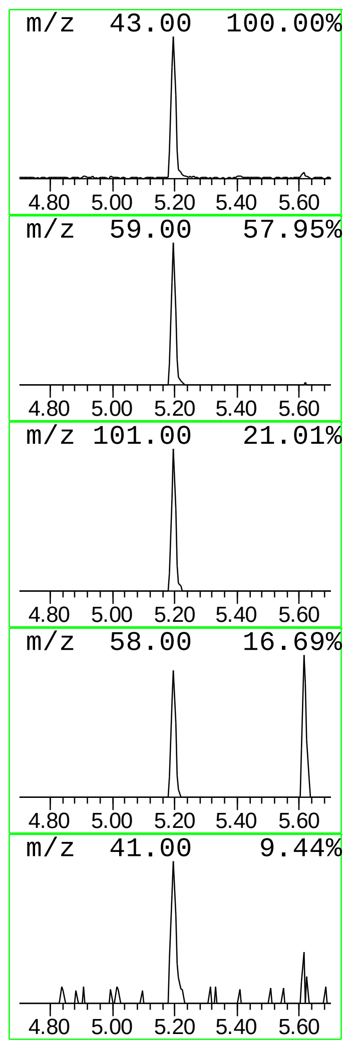
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.91 ng	89394	1,4-Dichlorobenzene-d4	6.97

Hit# of 5

Hit#	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetone	58	C3H6O	000067-64-1	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106471.D
Acq On : 15 Jun 2018 4:37
Operator : JU/SJ
Sample : J3474-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

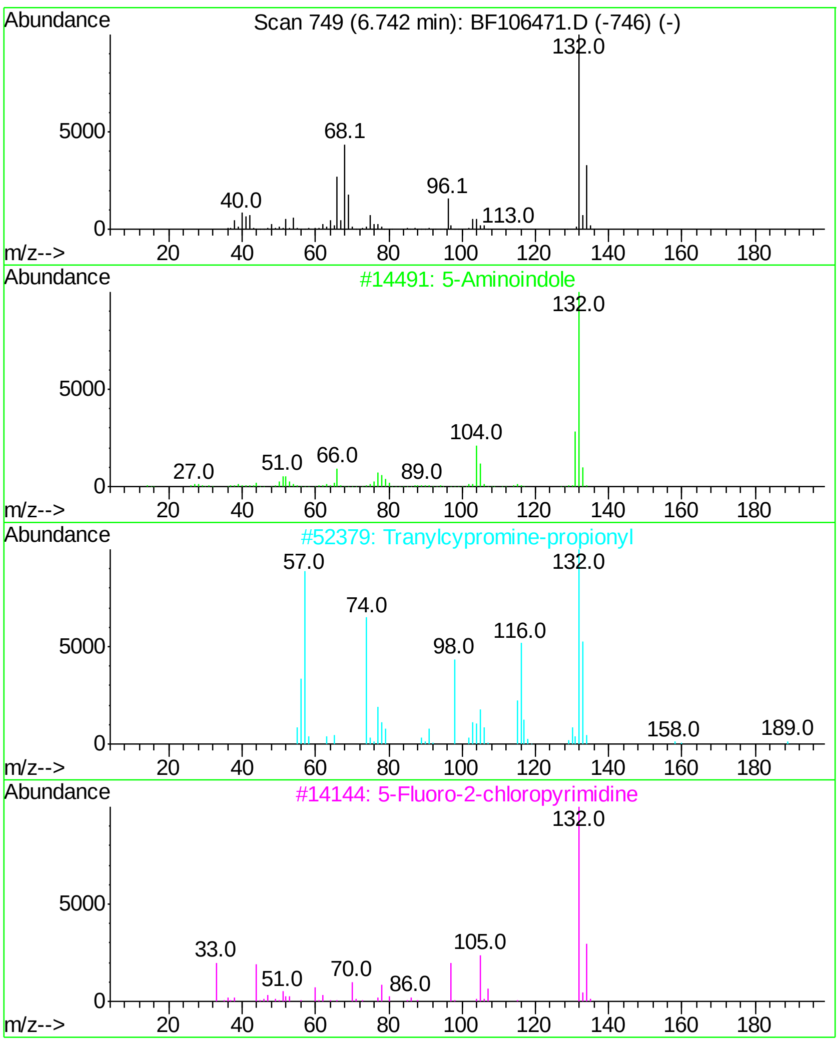
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

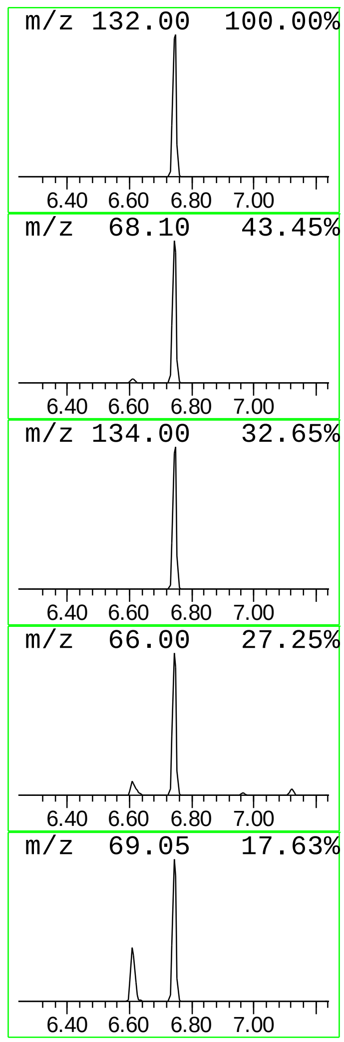
****

Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	53.97 ng	1657560	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106471.D
Acq On : 15 Jun 2018 4:37
Operator : JU/SJ
Sample : J3474-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
061118-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

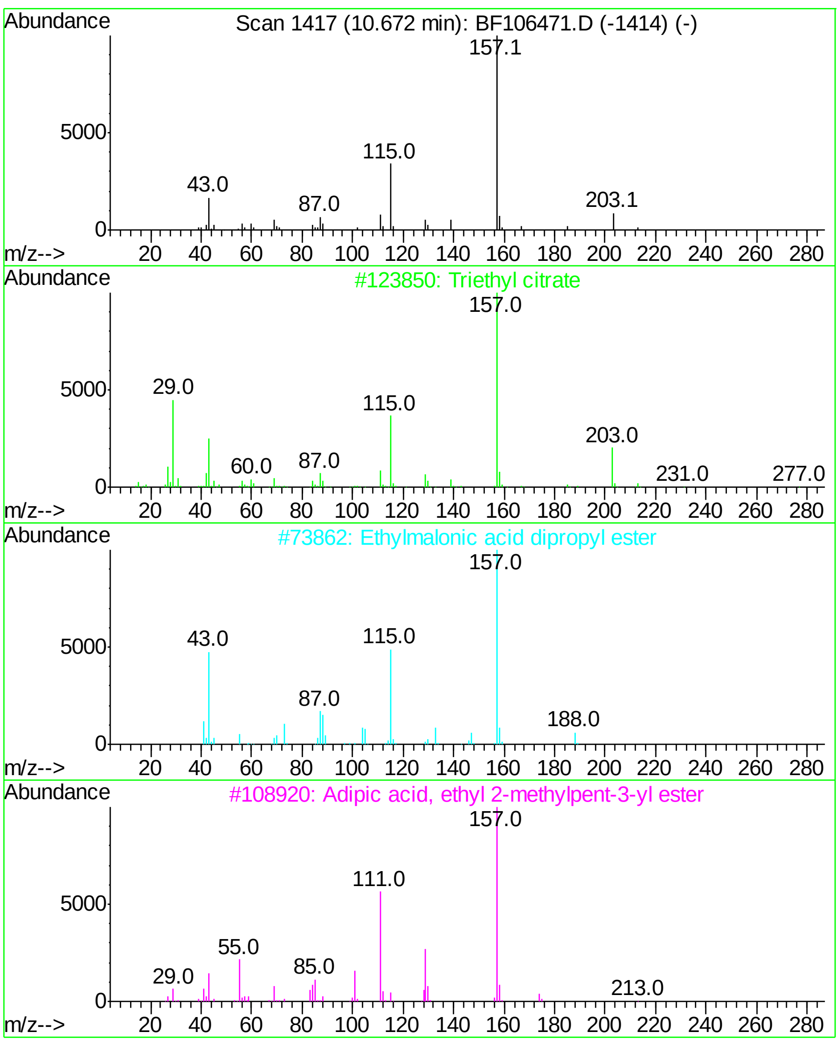
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

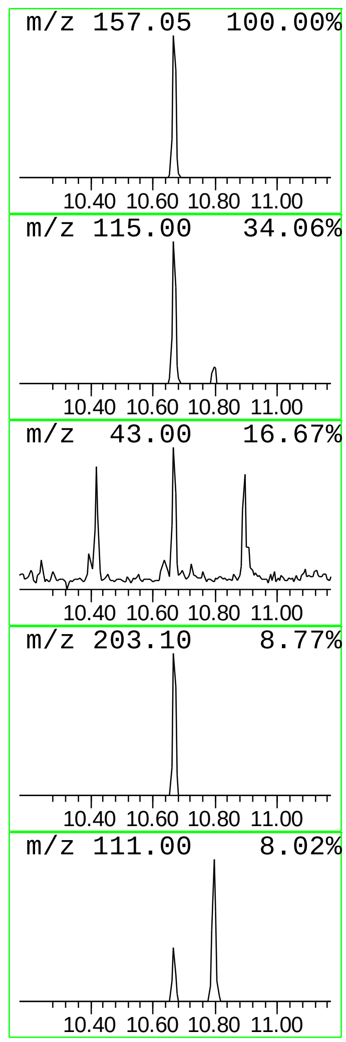
****

Peak Number 4 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.21 ng	70514	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	Adipic acid, ethyl 2-methylpent-...	258	C14H26O4	1000353-55-5	38
4	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	38
5	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	28





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061418\
Data File : BF106471.D
Acq On : 15 Jun 2018 4:37
Operator : JU/SJ
Sample : J3474-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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	2.9	ng	89394	1	6.97	614212	20.0
unknown6.74	6.74	54.0	ng	1657560	1	6.97	614212	20.0
Triethyl citrate	10.67	2.2	ng	70514	3	10.01	638269	20.0