LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106468.D
Acq On : 15 Jun 2018 3:18
Operator : JU/SJ
Sample : J3474-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-D-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	5.196	482	486	496	rVB	63846	66656	2.10%	0.369%
2	5.619	554	558	566	rBV	906107	935253	29.53%	5.179%
3	6.613	723	727	735	rBV	636228	669568	21.14%	3.708%
4	6.742	746	749	753	rVB	1720277	1507817	47.61%	8.350%
5	6.966	783	787	790	rBV	749422	583771	18.43%	3.233%
6	7.125	809	814	817	rBV	2409473	2098799	66.27%	11.622%
7	7.531	878	883	886	rBV	1639390	1618161	51.09%	8.961%
8	8.248	1001	1005	1008	rBV	767608	624396	19.71%	3.458%
9	8.801	1096	1099	1104	rBV	62311	52800	1.67%	0.292%
10	9.319	1183	1187	1191	rBV	2564744	2524568	79.71%	13.980%
11	9.713	1250	1254	1258	rBV	177821	150585	4.75%	0.834%
12	10.007	1297	1304	1311	rVB	697953	624197	19.71%	3.457%
13	10.666	1413	1416	1420	rBV	159439	120709	3.81%	0.668%
14	10.719	1421	1425	1428	rVB	200639	168170	5.31%	0.931%
15	10.795	1434	1438	1442	rBV	1207731	1090885	34.44%	6.041%
16	11.495	1554	1557	1561	rBV	757707	683800	21.59%	3.787%
17	13.083	1823	1827	1831	rBV	3108075	3167189	100.00%	17.539%
18	14.148	2004	2008	2011	rBV	813625	790269	24.95%	4.376%
19	15.677	2263	2268	2277	rVB	448329	580544	18.33%	3.215%

Sum of corrected areas: 18058137

LSC Report - Integrated Chromatogram

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Misc :
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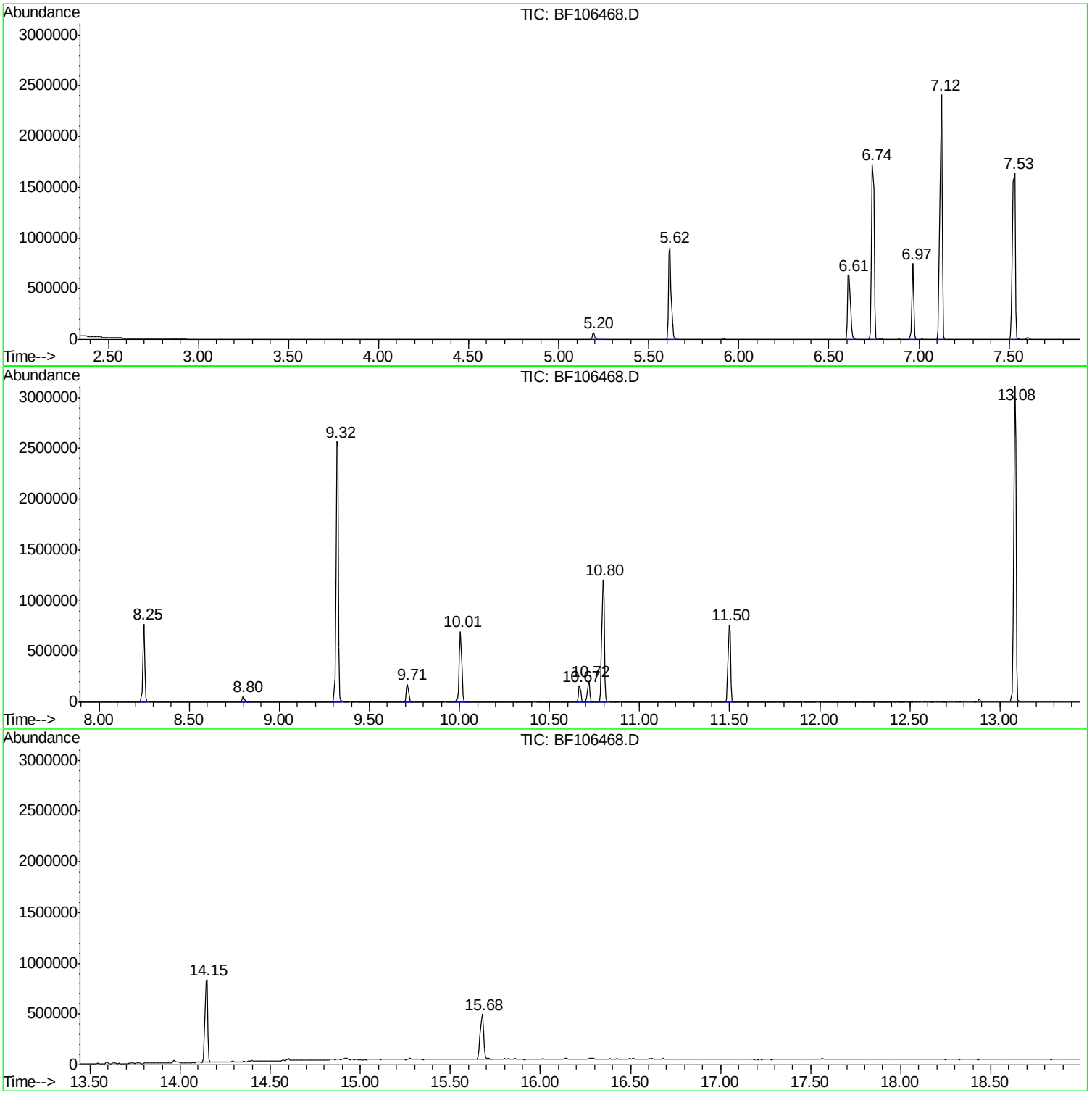
Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-D-B

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



Library Search Compound Report

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Data File : BF106468.D
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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-D-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

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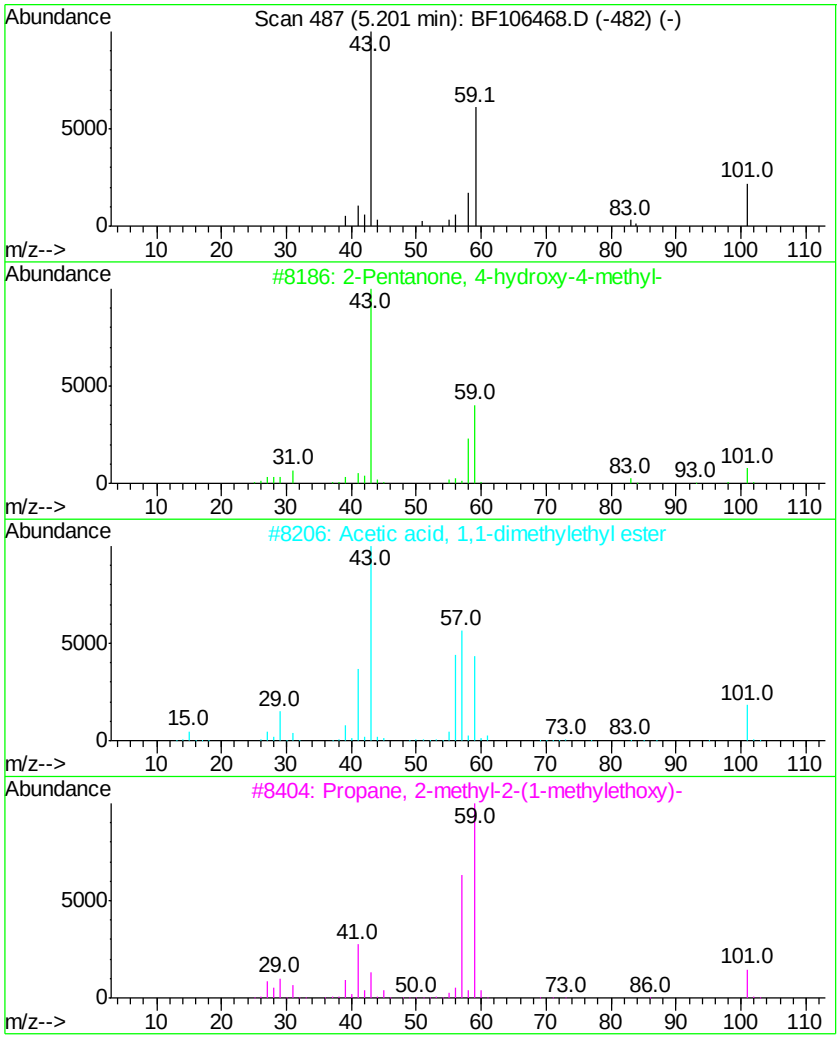
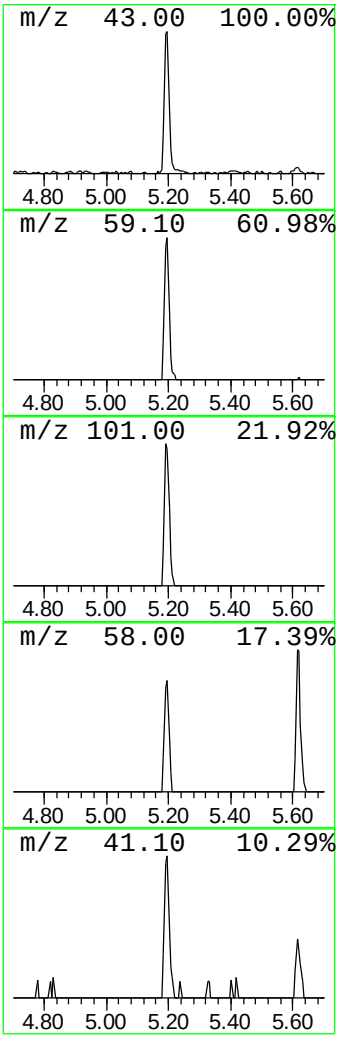
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.28 ng	66656	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : J3474-01
Misc :
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Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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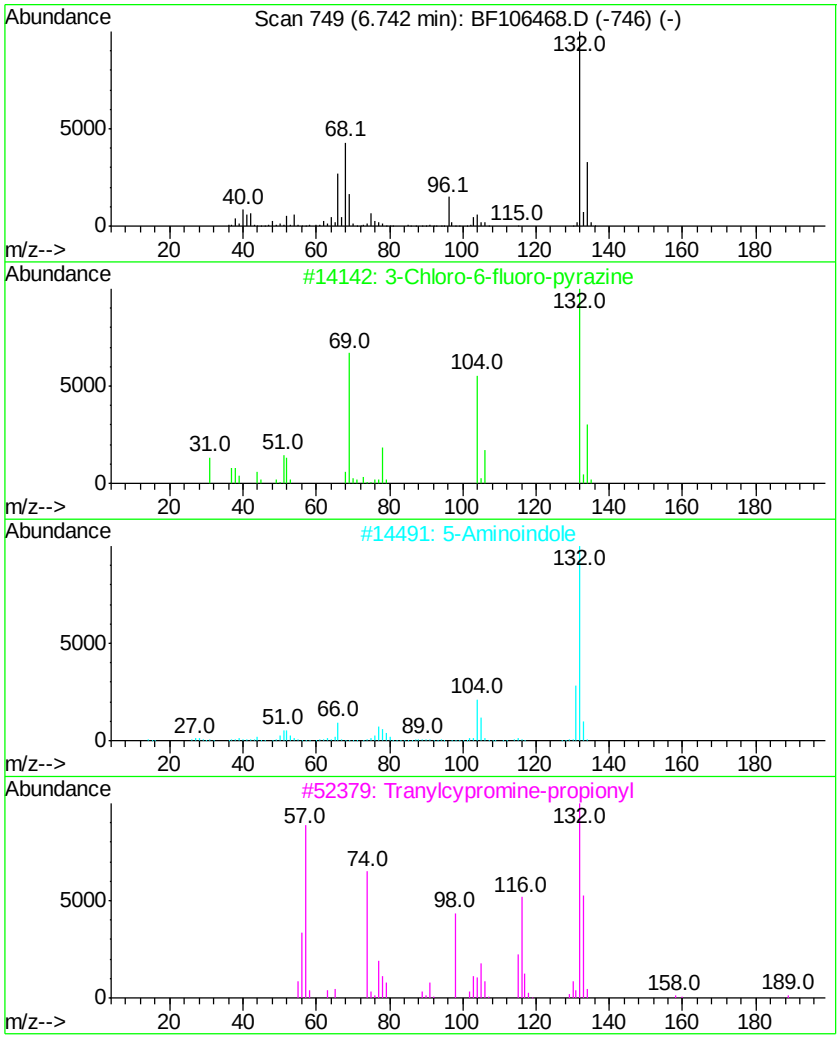
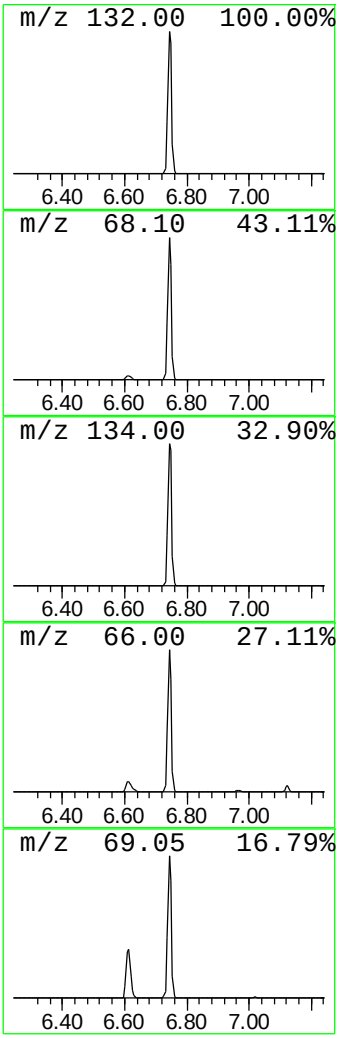
Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	51.66 ng	1507820	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	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-D-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

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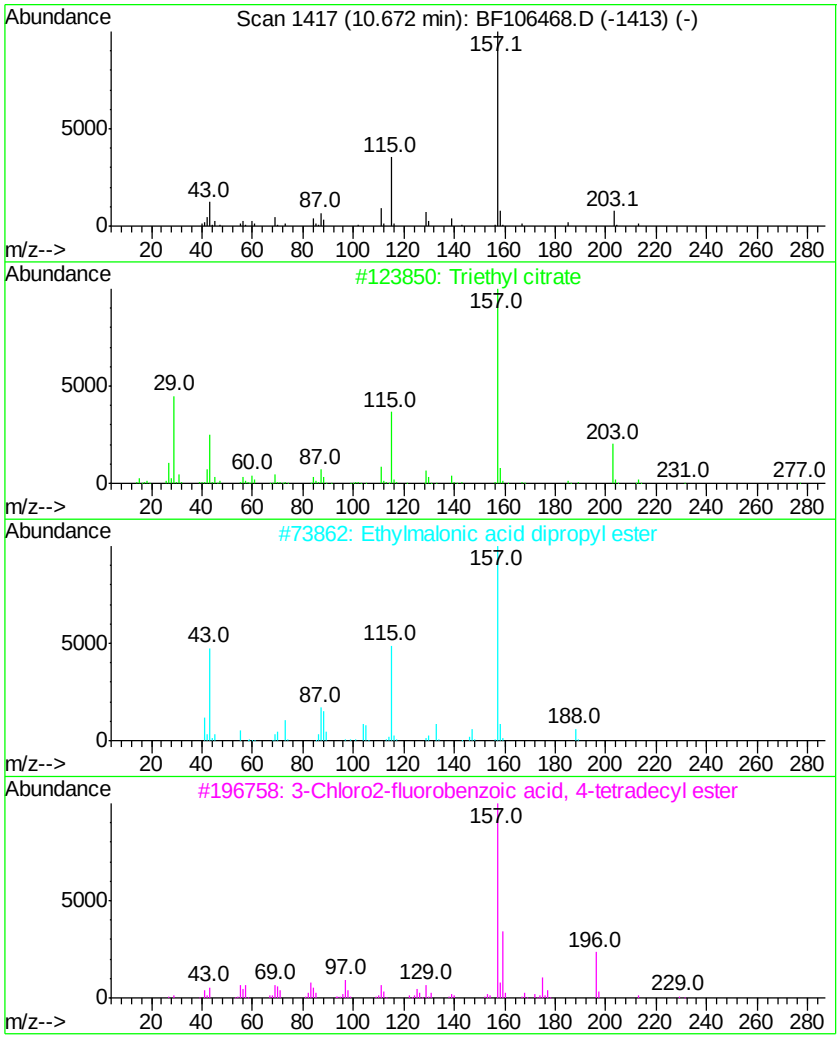
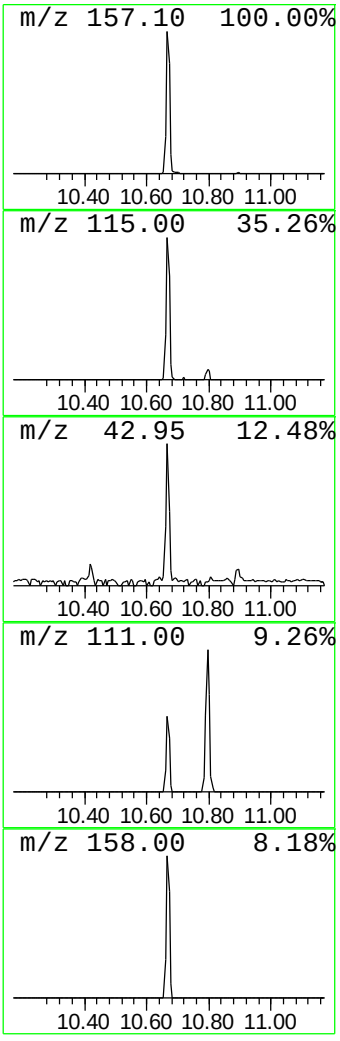
Peak Number 4 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.87 ng	120709	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	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	45
4	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	40
5	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	38





Library Search Compound Report

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Operator : JU/SJ
Sample : J3474-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

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

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

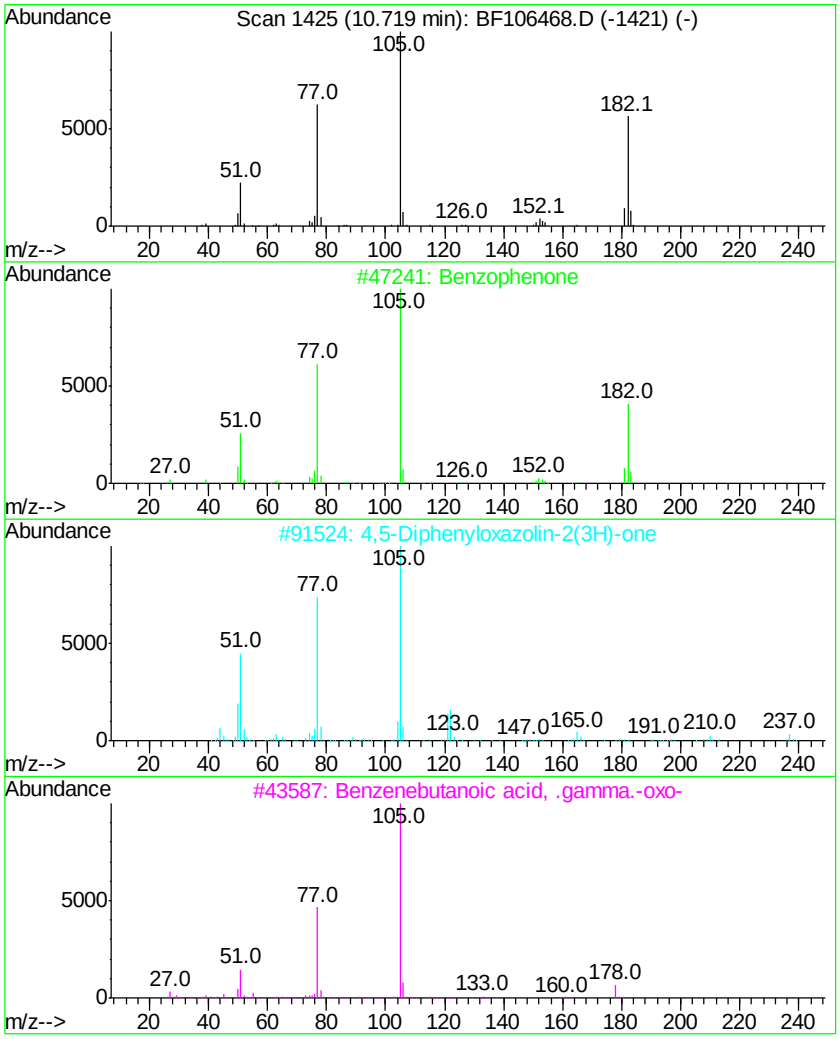
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

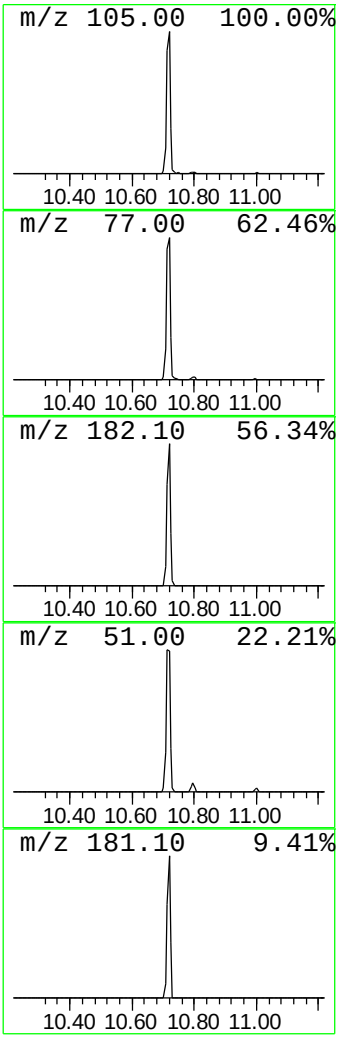
****

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	5.39 ng	168170	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	4,5-Diphenyloxazolin-2(3H)-one	237	C15H11NO2	005014-83-5	47
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47





Tentatively Identified Compound (LSC) summary

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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	2.3	ng	66656	1	6.97	583771	20.0
unknown6.74	6.74	51.7	ng	1507820	1	6.97	583771	20.0
Triethyl citrate	10.67	3.9	ng	120709	3	10.01	624197	20.0
Benzophenone	10.72	5.4	ng	168170	3	10.01	624197	20.0