LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106474.D
Acq On : 15 Jun 2018 5:57
Operator : JU/SJ
Sample : J3475-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-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	5.195	482	486	493	rBV	106114	111640	3.73%	0.612%
2	5.613	554	557	567	rBV	1045065	1041798	34.82%	5.715%
3	6.607	723	726	736	rBV	727010	718371	24.01%	3.941%
4	6.742	746	749	753	rBV	1863018	1602730	53.57%	8.792%
5	6.966	783	787	790	rVB	771140	596038	19.92%	3.270%
6	7.125	809	814	817	rBV	2434925	2187881	73.13%	12.002%
7	7.531	877	883	886	rBV	1761026	1702634	56.91%	9.340%
8	8.248	1001	1005	1008	rBV	815550	654561	21.88%	3.591%
9	9.319	1183	1187	1191	rBV	2734687	2612705	87.32%	14.333%
10	9.713	1250	1254	1259	rVB	117560	102443	3.42%	0.562%
11	10.007	1301	1304	1310	rVB	674875	600143	20.06%	3.292%
12	10.666	1413	1416	1419	rVV	139494	102655	3.43%	0.563%
13	10.713	1421	1424	1428	rVB	81914	75177	2.51%	0.412%
14	10.795	1434	1438	1442	rBV	1192939	1055755	35.29%	5.792%
15	11.495	1553	1557	1561	rBV	803321	643263	21.50%	3.529%
16	12.889	1790	1794	1797	rBV	50456	43690	1.46%	0.240%
17	13.083	1822	1827	1830	rBV	3109089	2991944	100.00%	16.413%
18	13.595	1910	1914	1917	rBV	48540	38273	1.28%	0.210%
19	13.965	1973	1977	1983	rBV2	67506	82490	2.76%	0.453%
20	14.142	2003	2007	2011	rBV	795554	738428	24.68%	4.051%
21	15.677	2263	2268	2274	rBV	399505	526209	17.59%	2.887%

Sum of corrected areas: 18228828

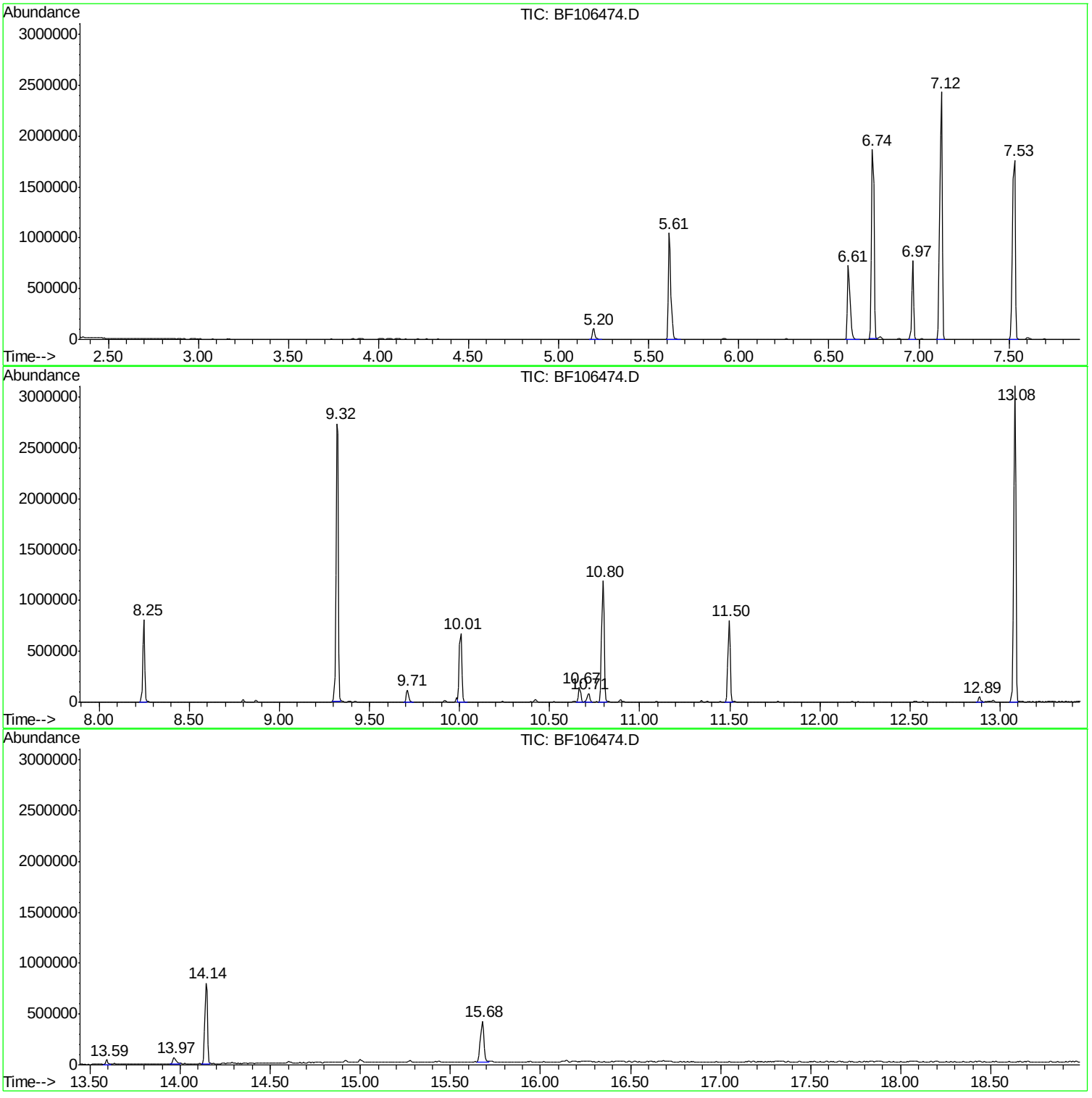
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106474.D
Acq On : 15 Jun 2018 5:57
Operator : JU/SJ
Sample : J3475-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106474.D
Acq On : 15 Jun 2018 5:57
Operator : JU/SJ
Sample : J3475-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-B

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

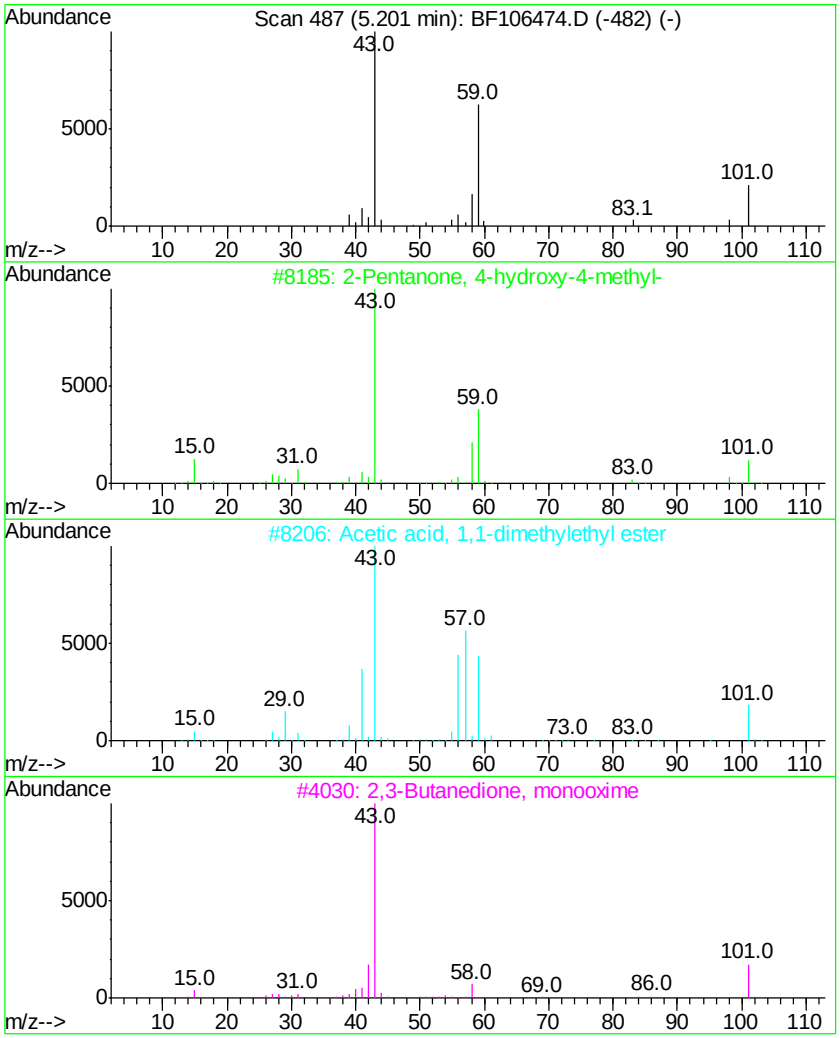
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

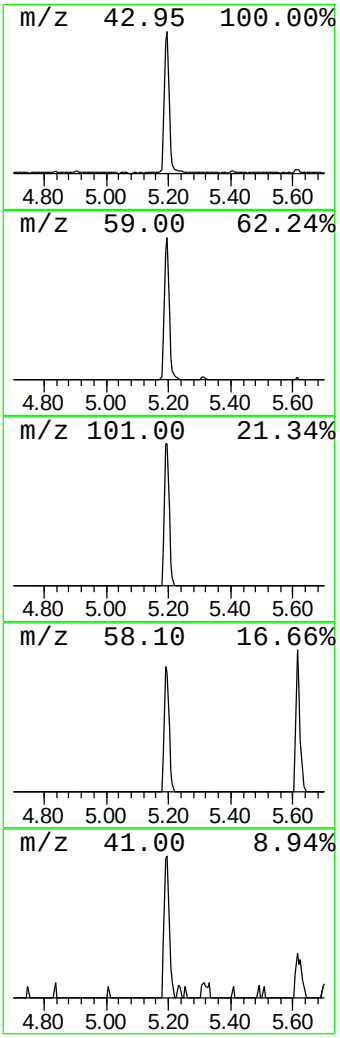
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.75 ng	111640	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	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106474.D
Acq On : 15 Jun 2018 5:57
Operator : JU/SJ
Sample : J3475-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-B

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

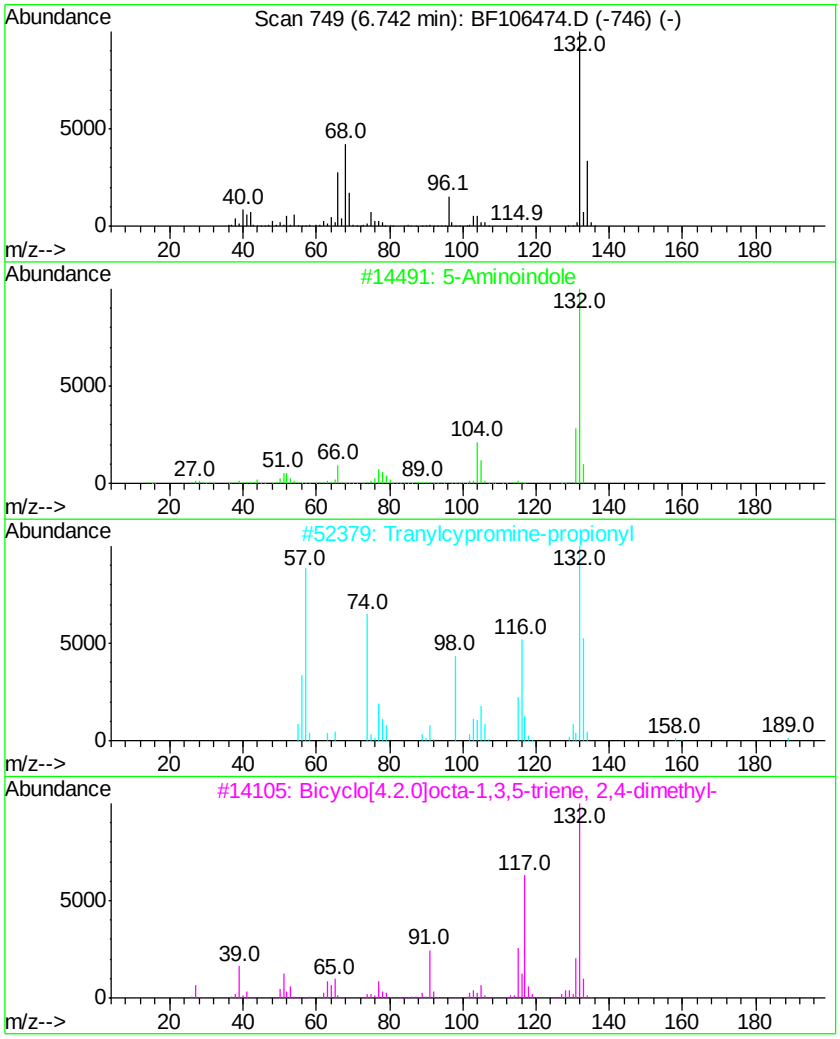
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

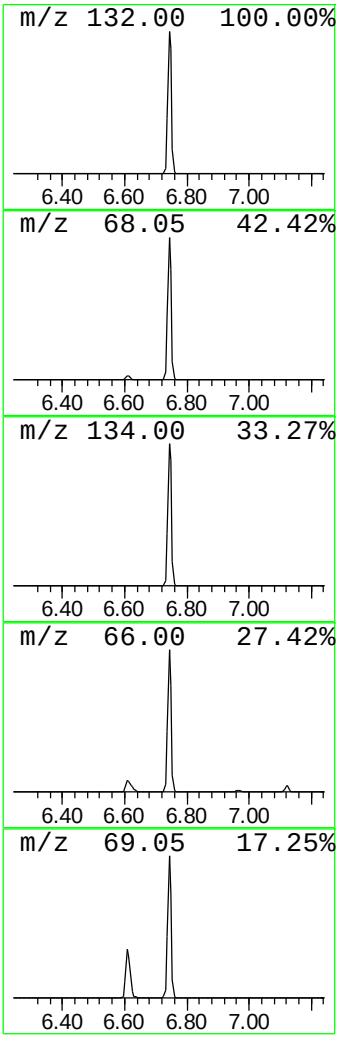
****

Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	53.78 ng	1602730	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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106474.D
Acq On : 15 Jun 2018 5:57
Operator : JU/SJ
Sample : J3475-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-B

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

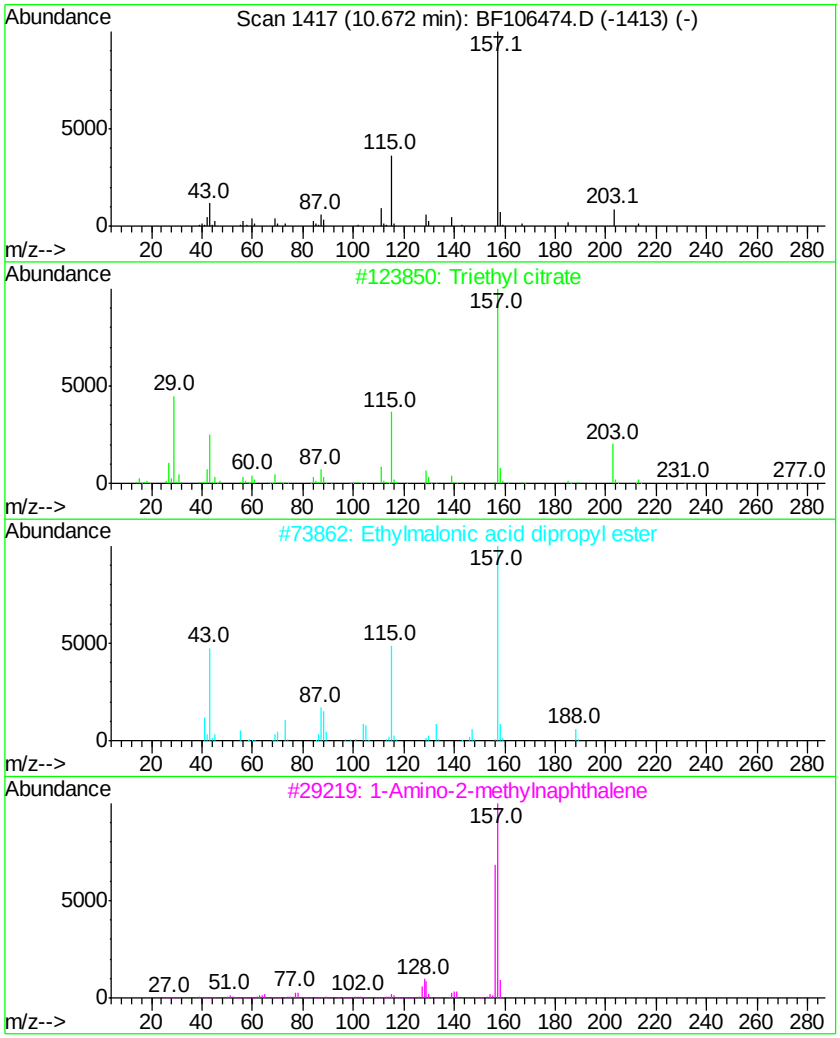
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

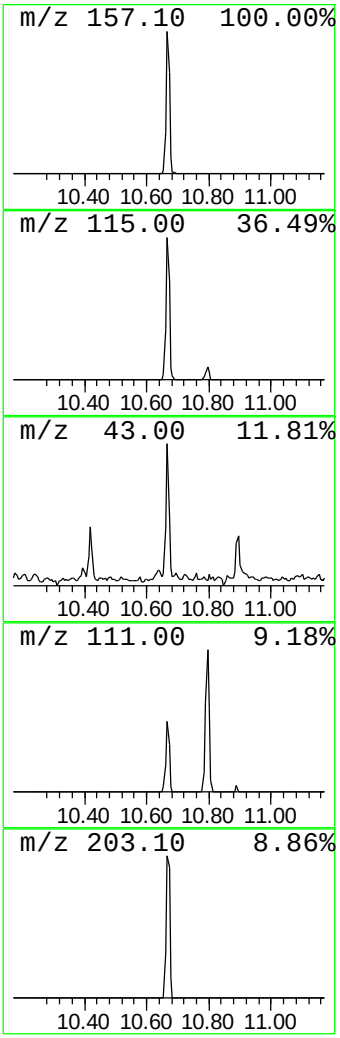
****

Peak Number 4 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.42 ng	102655	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	90
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	45
3	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	40
4	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	40
5	Adipic acid, ethyl pent-4-en-2-y...	242	C13H22O4	1000354-11-7	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106474.D
Acq On : 15 Jun 2018 5:57
Operator : JU/SJ
Sample : J3475-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-B

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

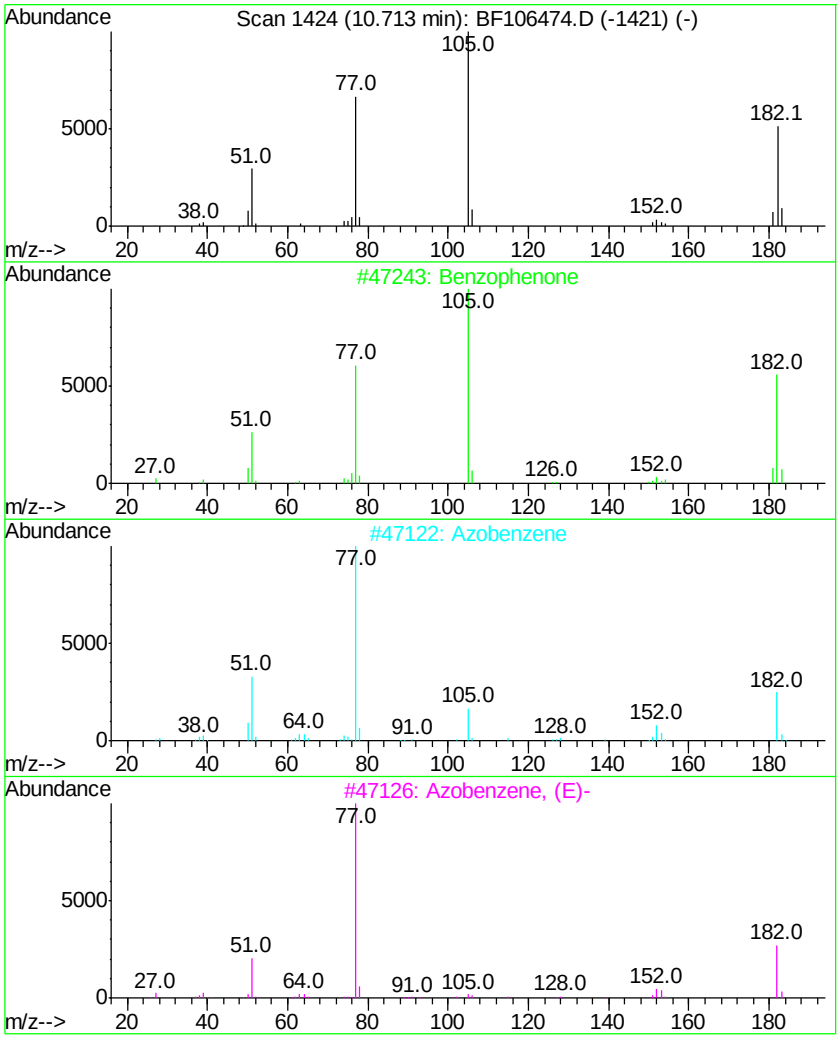
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

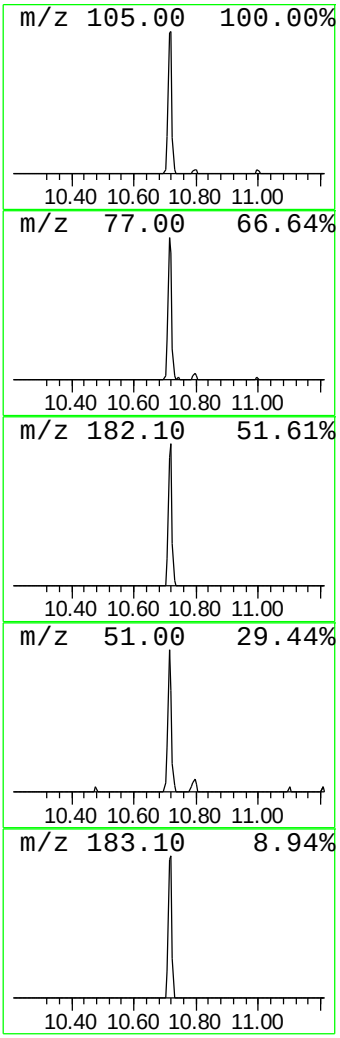
****

Peak Number 5 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	2.51 ng	75177	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Azobenzene, (E)-	182	C12H10N2	017082-12-1	53
4	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
5	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106474.D
Acq On : 15 Jun 2018 5:57
Operator : JU/SJ
Sample : J3475-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-B

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

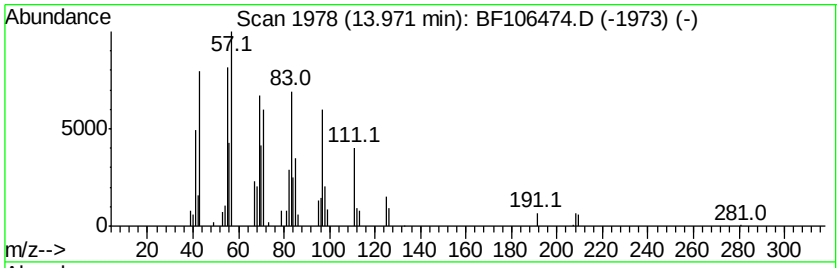
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

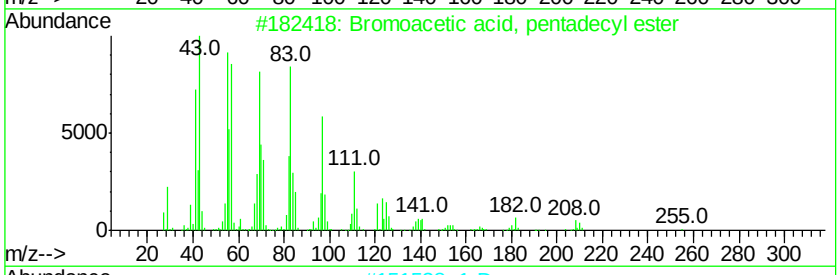
****

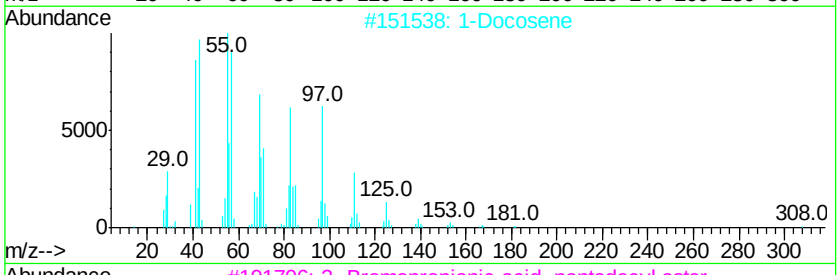
Peak Number 6 Bromoacetic acid, pentadecy... Concentration Rank 6

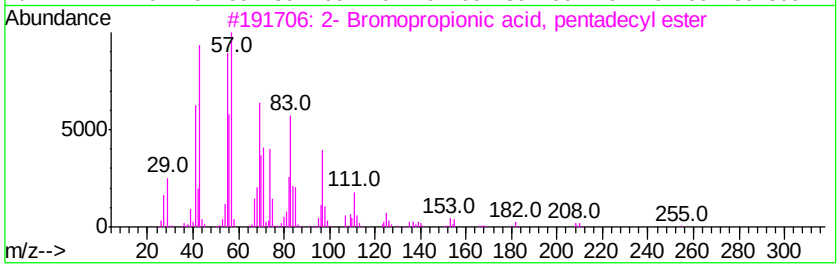
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.23 ng	82490	Chrysene-d12	14.14

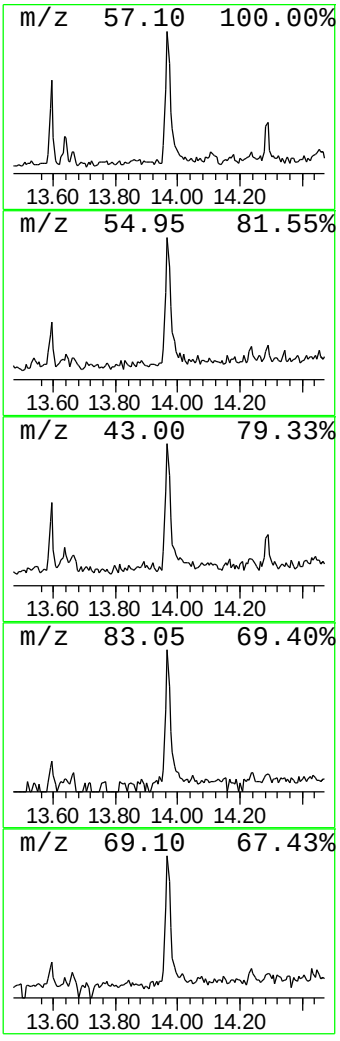
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	93
2	1-Docosene	308	C22H44	001599-67-3	91
3	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061418\
Data File : BF106474.D
Acq On : 15 Jun 2018 5:57
Operator : JU/SJ
Sample : J3475-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	3.8	ng	111640	1	6.97	596038	20.0
unknown6.74	6.74	53.8	ng	1602730	1	6.97	596038	20.0
Triethyl citrate	10.67	3.4	ng	102655	3	10.01	600143	20.0
Benzophenone	10.71	2.5	ng	75177	3	10.01	600143	20.0
Bromoacetic acid,...	13.97	2.2	ng	82490	5	14.14	738428	20.0