LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106529.D
Acq On : 18 Jun 2018 11:02
Operator : JU/SJ
Sample : J3509-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-061318

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	492	rVB	99495	100579	2.81%	0.402%
2	5.613	553	557	566	rVB	1345223	1395945	39.05%	5.581%
3	6.607	722	726	735	rVB	932277	893214	24.99%	3.571%
4	6.742	745	749	753	rBV	2577249	2441201	68.29%	9.760%
5	6.966	783	787	790	rBV	954651	736857	20.61%	2.946%
6	7.125	809	814	817	rBV	2651555	2411629	67.46%	9.642%
7	7.531	877	883	886	rBV	2093094	2137269	59.79%	8.545%
8	8.248	1001	1005	1008	rBV	1122793	925521	25.89%	3.700%
9	8.801	1094	1099	1102	rBV	135127	108378	3.03%	0.433%
10	9.325	1183	1188	1191	rBV	3529699	3574800	100.00%	14.293%
11	9.713	1250	1254	1258	rBV	272006	229483	6.42%	0.918%
12	10.007	1300	1304	1308	rBV	1229087	1056221	29.55%	4.223%
13	10.378	1363	1367	1371	rBV	172974	135052	3.78%	0.540%
14	10.719	1421	1425	1429	rVB	417433	342476	9.58%	1.369%
15	10.801	1434	1439	1442	rBV	2263995	2286632	63.97%	9.142%
16	11.501	1554	1558	1561	rBV	1267897	1104109	30.89%	4.414%
17	13.089	1823	1828	1831	rBV	3483361	3540987	99.05%	14.157%
18	13.971	1975	1978	1984	rBV	33240	41294	1.16%	0.165%
19	14.154	2005	2009	2013	rBV	922585	884230	24.74%	3.535%
20	15.707	2268	2273	2285	rVB	503833	665617	18.62%	2.661%

Sum of corrected areas: 25011494

LSC Report - Integrated Chromatogram

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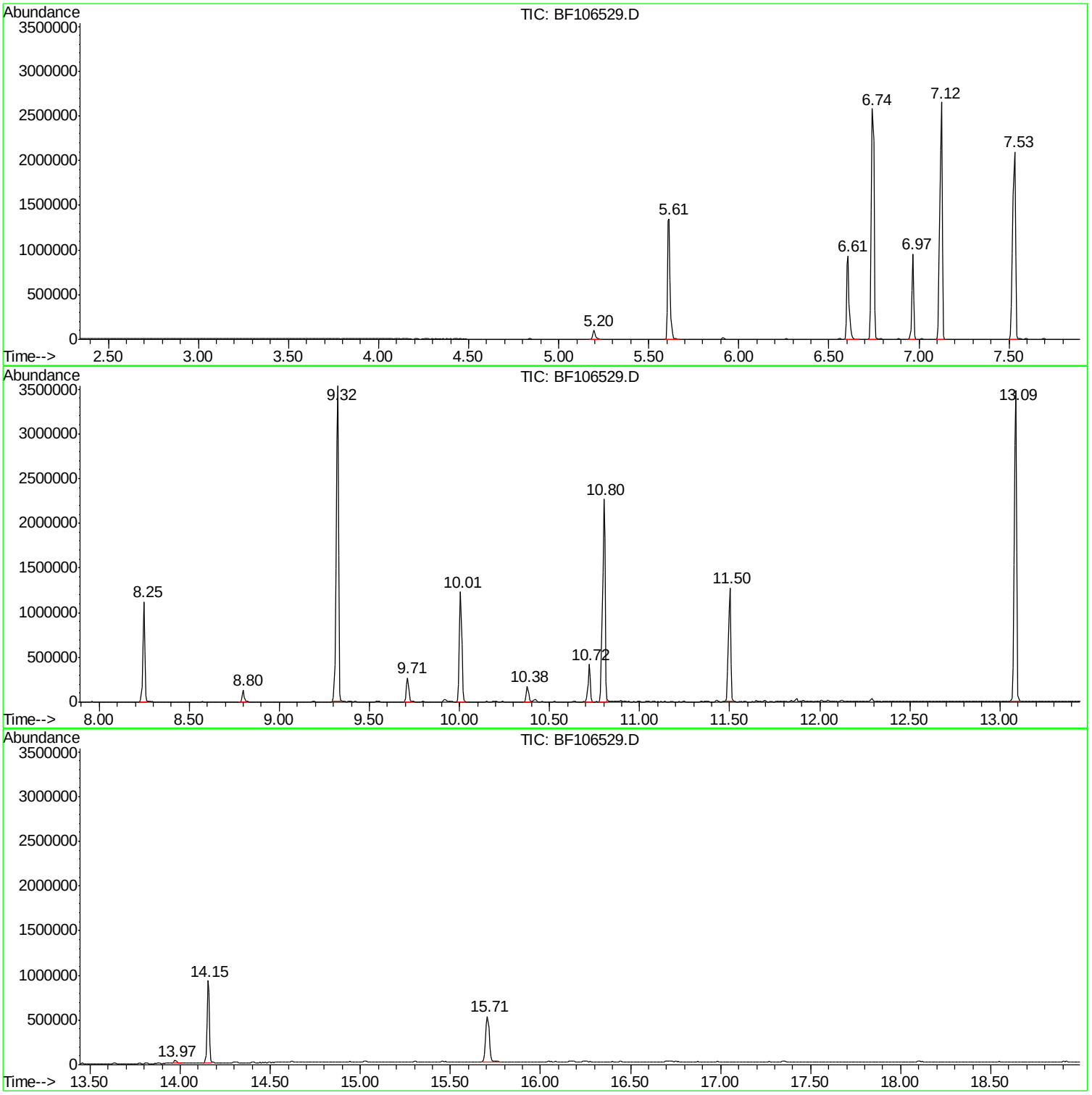
Operator : JU/SJ
Sample : J3509-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-061318

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\BF061818\
Data File : BF106529.D
Acq On : 18 Jun 2018 11:02
Operator : JU/SJ
Sample : J3509-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-061318

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

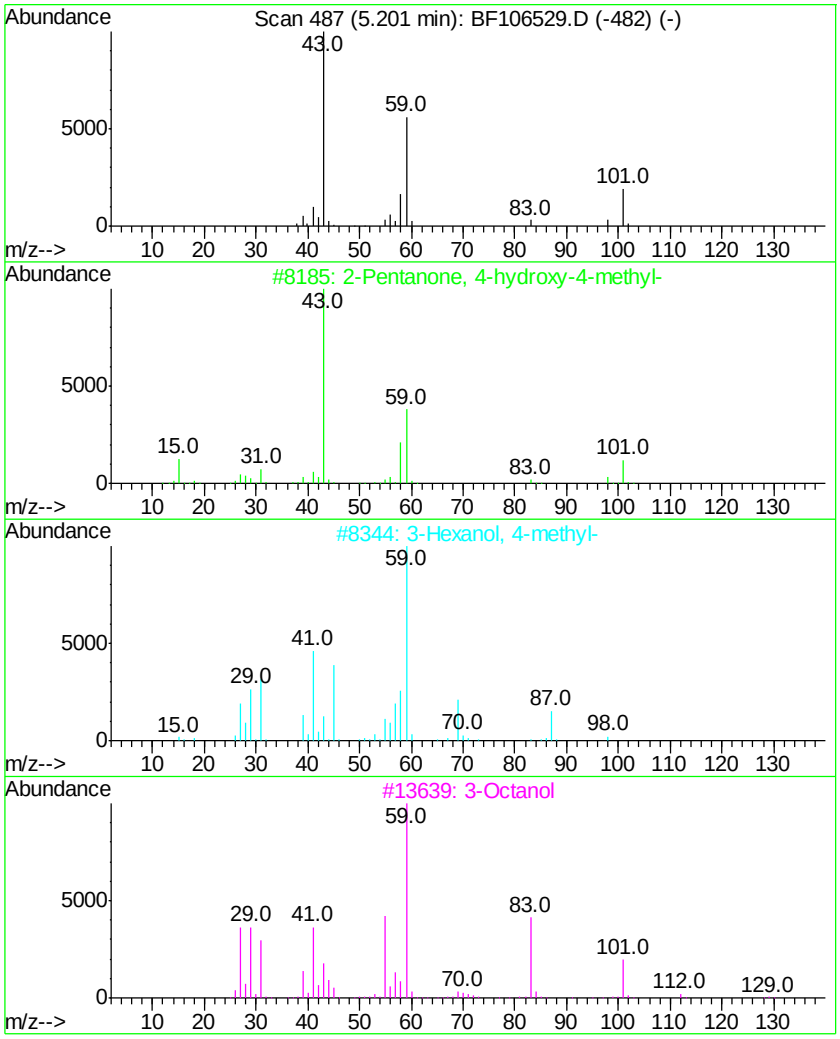
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

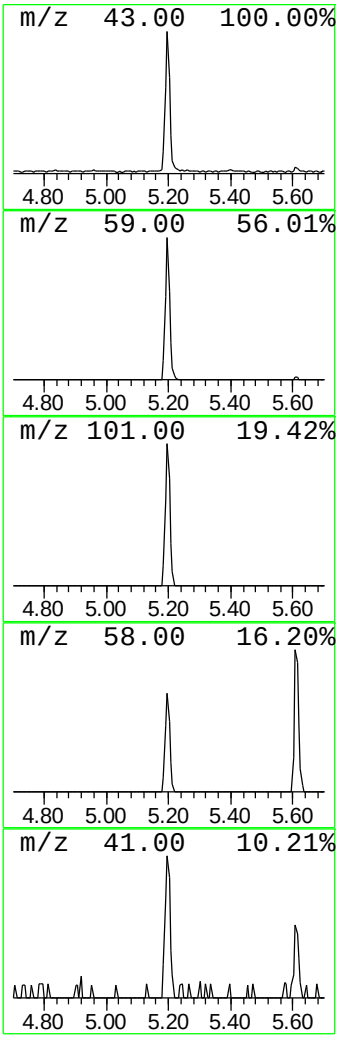
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.73 ng	100579	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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : DUP-061318

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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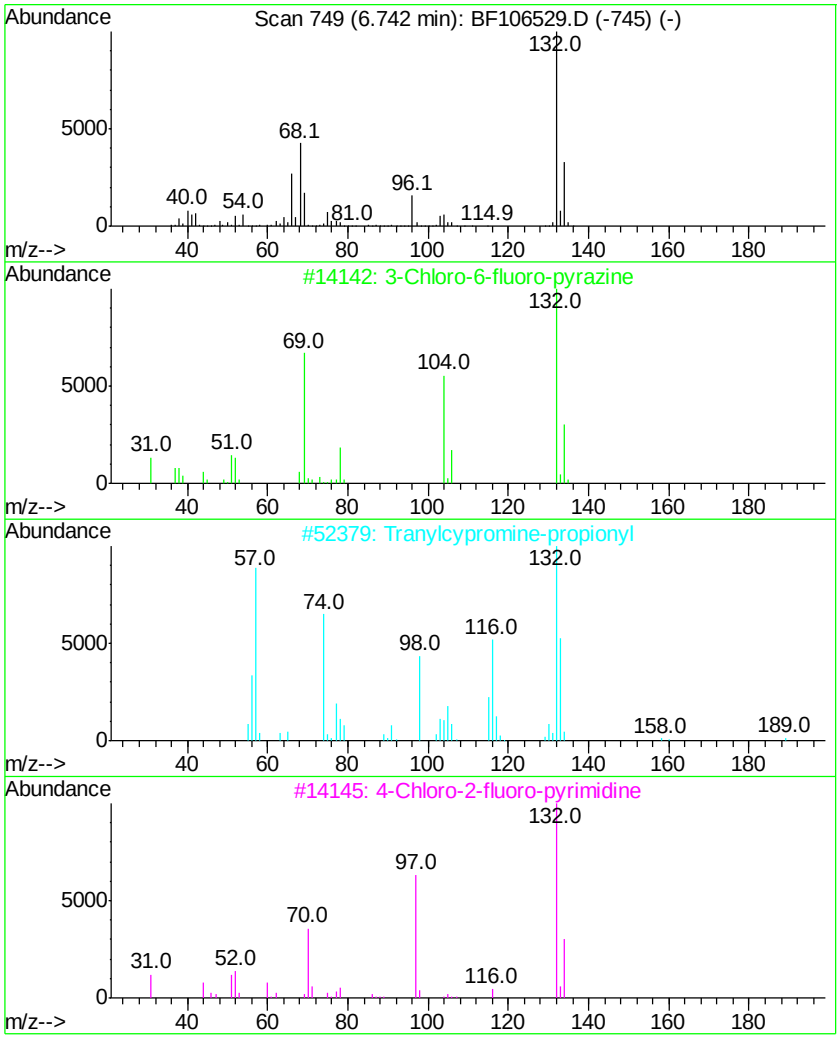
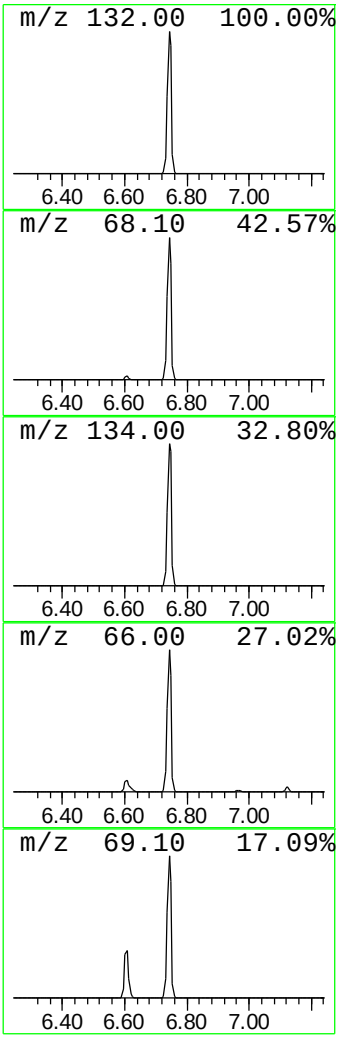
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	66.26 ng	2441200	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Data File : BF106529.D
Acq On : 18 Jun 2018 11:02
Operator : JU/SJ
Sample : J3509-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-061318

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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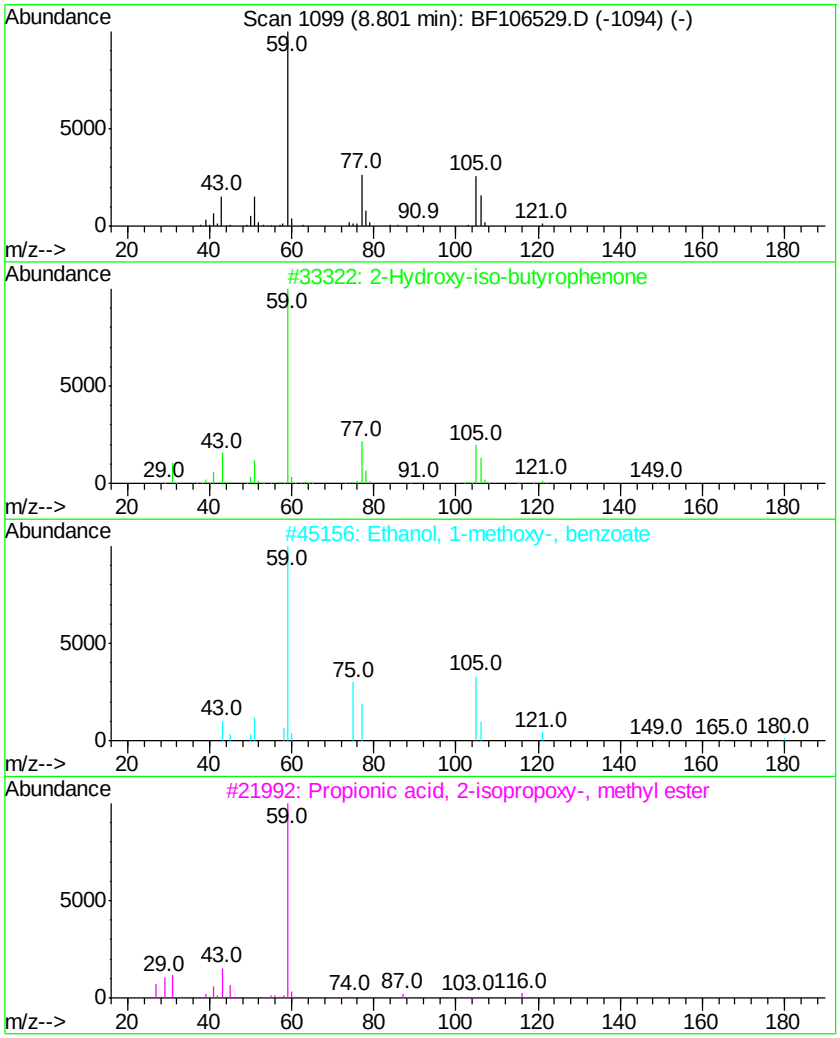
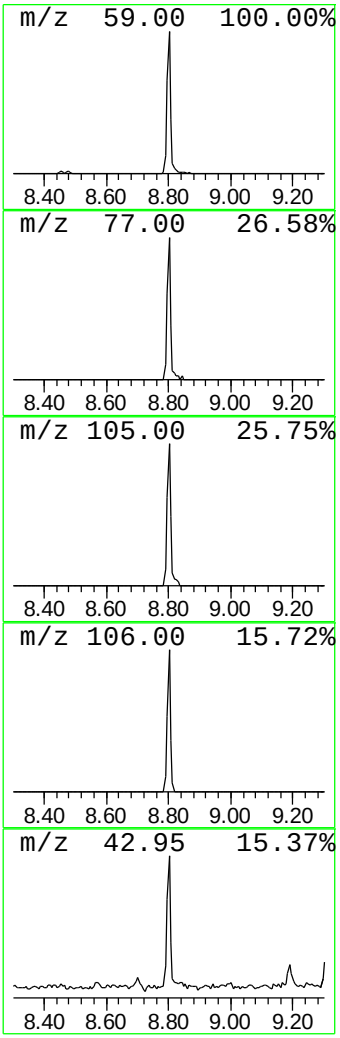
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	2.34 ng	108378	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4	Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	9
5	Guanidine	59	CH5N3	000113-00-8	7





Library Search Compound Report

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Data File : BF106529.D
Acq On : 18 Jun 2018 11:02
Operator : JU/SJ
Sample : J3509-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-061318

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

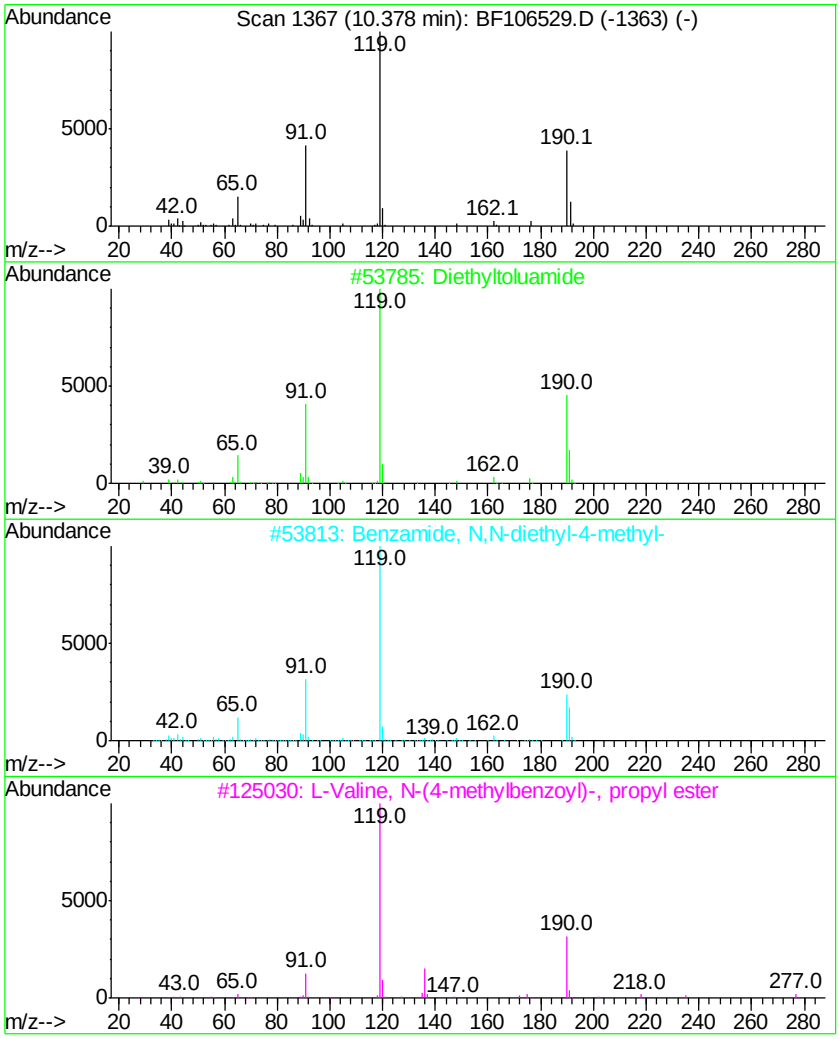
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

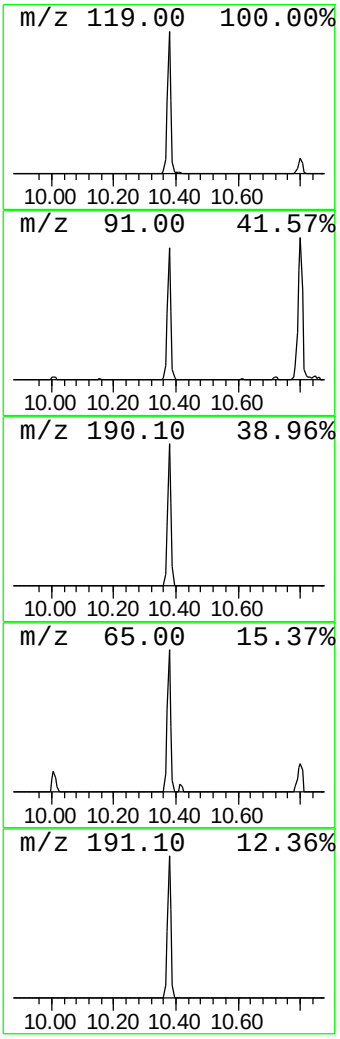
****

Peak Number 5 Diethyltoluamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.56 ng	135052	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	76
3	L-Valine, N-(4-methylbenzoyl)-, ...	277	C16H23NO3	1000346-63-8	72
4	1-Propanone, 2-methyl-1-(4-methy...	162	C11H14O	050390-51-7	58
5	4-Methylbenzoic acid, pentafluor...	302	C14H7F5O2	1000354-15-1	52





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Sample : J3509-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-061318

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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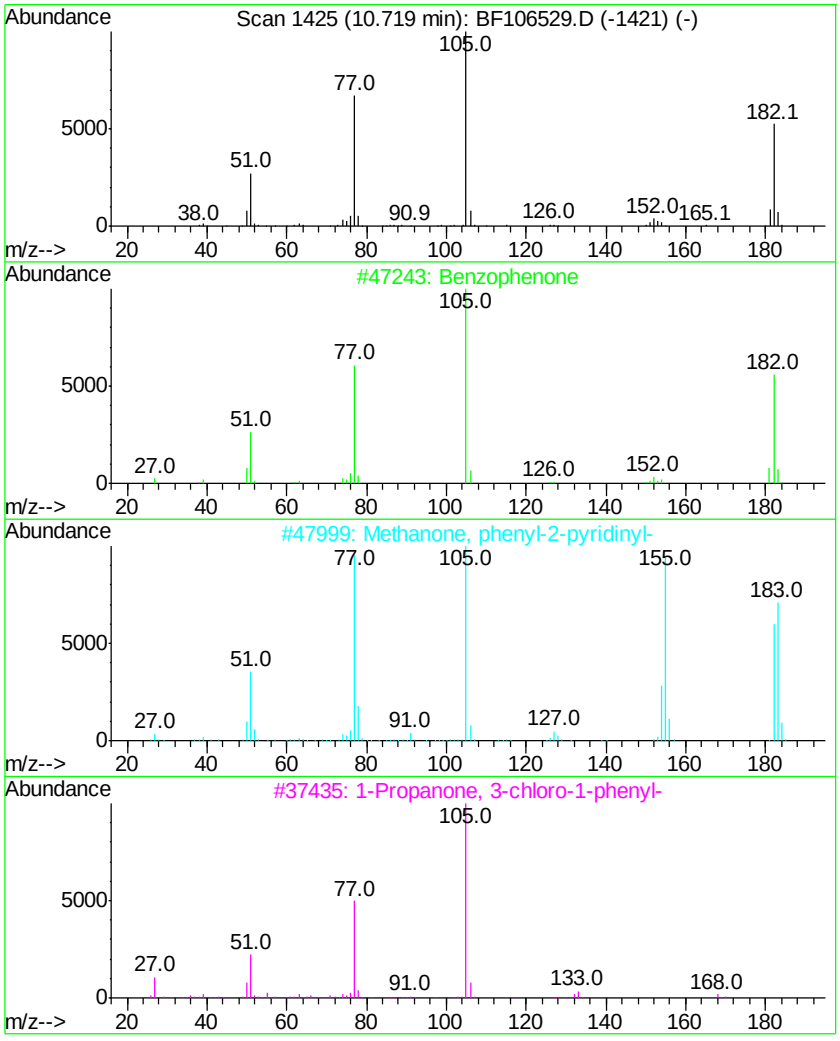
TIC Integration Parameters: LSCINT.P

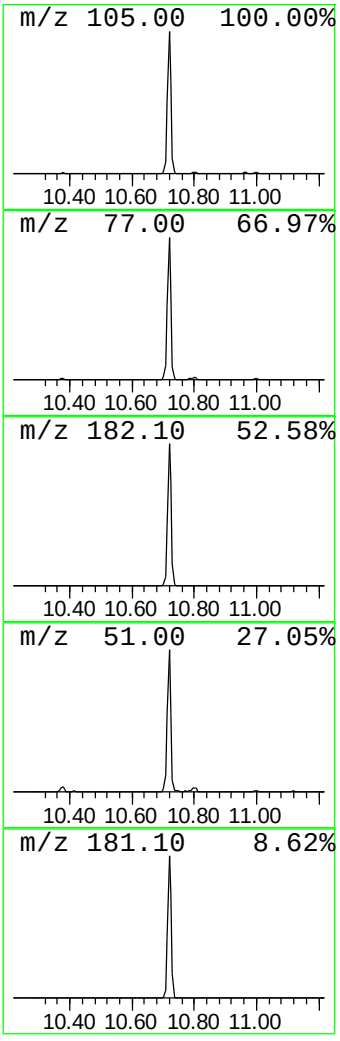
****

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	6.48 ng	342476	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	72
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_F
ClientSampleId : DUP-061318

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	2.7	ng	100579	1	6.97	736857	20.0
unknown6.74	6.74	66.3	ng	2441200	1	6.97	736857	20.0
2-Hydroxy-iso-but...	8.80	2.3	ng	108378	2	8.25	925521	20.0
Diethyltoluamide	10.38	2.6	ng	135052	3	10.01	1056220	20.0
Benzophenone	10.72	6.5	ng	342476	3	10.01	1056220	20.0