LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG111117\
Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

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:\HPCHEM1\BNA_G\METHODS\8270-BG111017.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	3.876	94	100	112	rVB	236440	336239	17.87%	2.936%
2	4.287	163	170	178	rVB	28371	45407	2.41%	0.396%
3	5.221	321	329	336	rBV	34979	54498	2.90%	0.476%
4	5.703	404	411	418	rBV	81473	139335	7.40%	1.217%
5	6.114	473	481	491	rBV3	19429	37358	1.99%	0.326%
6	7.307	676	684	699	rVB3	55189	179504	9.54%	1.567%
7	7.460	704	710	718	rBV	37714	66330	3.52%	0.579%
8	7.677	739	747	757	rBV	145081	270511	14.38%	2.362%
9	7.783	760	765	773	rVB2	19997	32034	1.70%	0.280%
10	8.142	813	826	831	rBV	136344	252585	13.42%	2.206%
11	8.471	875	882	895	rVB	231188	452610	24.05%	3.952%
12	9.005	965	973	982	rBV2	14918	33865	1.80%	0.296%
13	9.305	1017	1024	1028	rBV	178805	331265	17.60%	2.893%
14	9.352	1028	1032	1040	rVB	157313	286508	15.23%	2.502%
15	10.815	1274	1281	1294	rVB	271271	499833	26.56%	4.365%
16	10.956	1296	1305	1313	rBV	192045	352958	18.76%	3.082%
17	11.344	1364	1371	1380	rBV	32259	62802	3.34%	0.548%
18	12.254	1521	1526	1533	rBV2	20028	36064	1.92%	0.315%
19	13.382	1711	1718	1729	rBV	634240	1011104	53.73%	8.829%
20	14.205	1852	1858	1867	rBV	245273	379113	20.15%	3.310%
21	14.763	1944	1953	1962	rVB2	367050	620195	32.96%	5.416%
22	16.103	2176	2181	2186	rBV	106594	164255	8.73%	1.434%
23	16.244	2199	2205	2214	rVB	331862	533151	28.33%	4.655%
24	16.449	2233	2240	2248	rVB9	6818	20602	1.09%	0.180%
25	17.231	2363	2373	2378	rBV5	25797	56178	2.99%	0.491%
26	17.284	2378	2382	2394	rVB3	15601	34691	1.84%	0.303%
27	17.501	2413	2419	2432	rVB2	553327	857541	45.57%	7.488%
28	17.766	2459	2464	2474	rBV3	10259	25010	1.33%	0.218%
29	18.371	2561	2567	2574	rBV2	32854	53157	2.82%	0.464%
30	20.092	2854	2860	2869	rVB	1531391	1881704	100.00%	16.431%
31	20.862	2987	2991	2997	rBV8	11441	23105	1.23%	0.202%
32	21.385	3076	3080	3088	rBV2	68356	113358	6.02%	0.990%
33	21.632	3120	3122	3129	rVB2	18950	24441	1.30%	0.213%
34	21.773	3139	3146	3158	rBV	657315	1100612	58.49%	9.611%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG111117\
Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

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:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.954	3341	3347	3355	rVB4	20876	38294	2.04%	0.334%
36	25.080	3698	3709	3721	rBV2	360399	1045870	55.58%	9.133%

Sum of corrected areas: 11452087

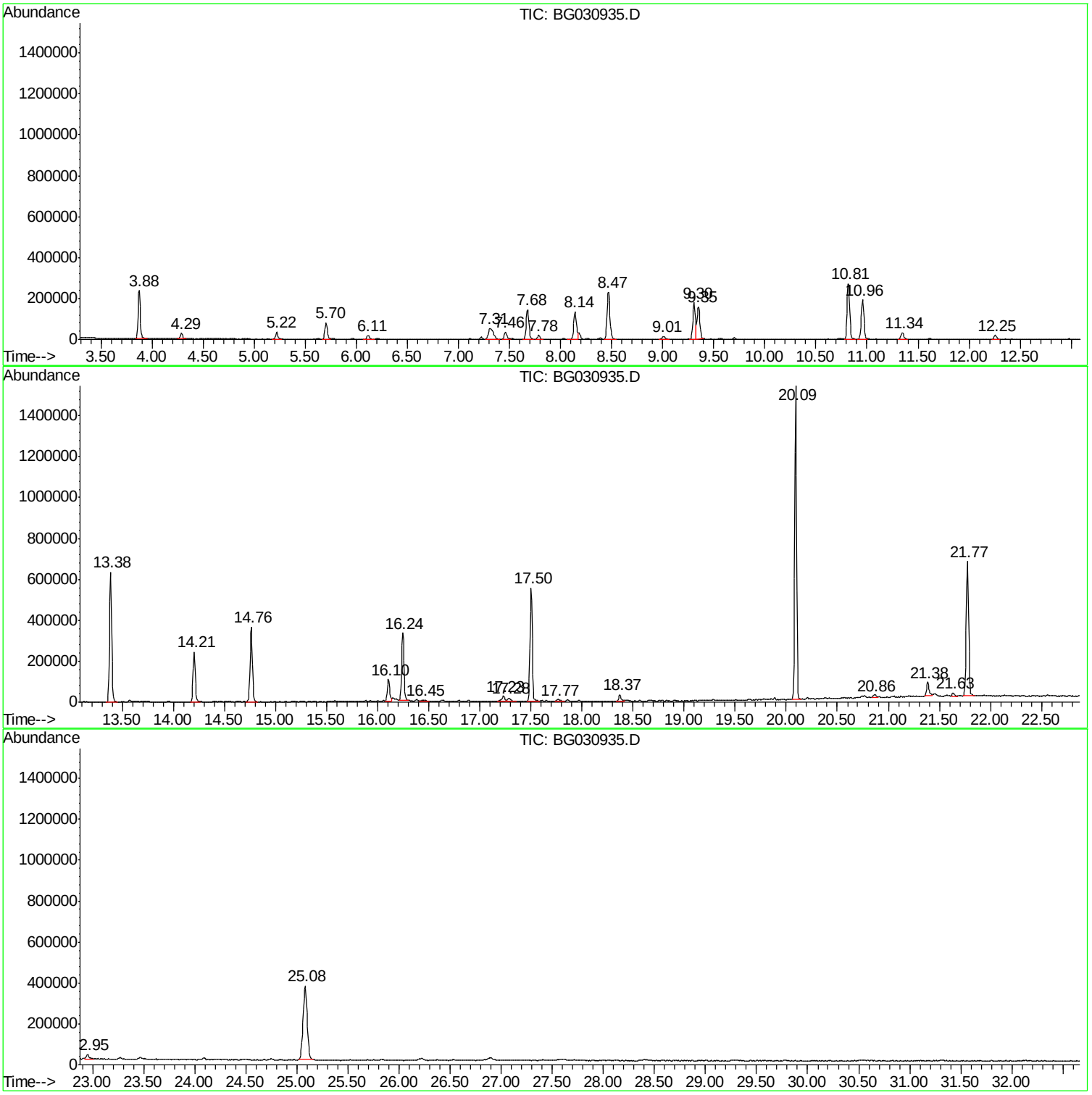
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG111117\
Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.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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Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

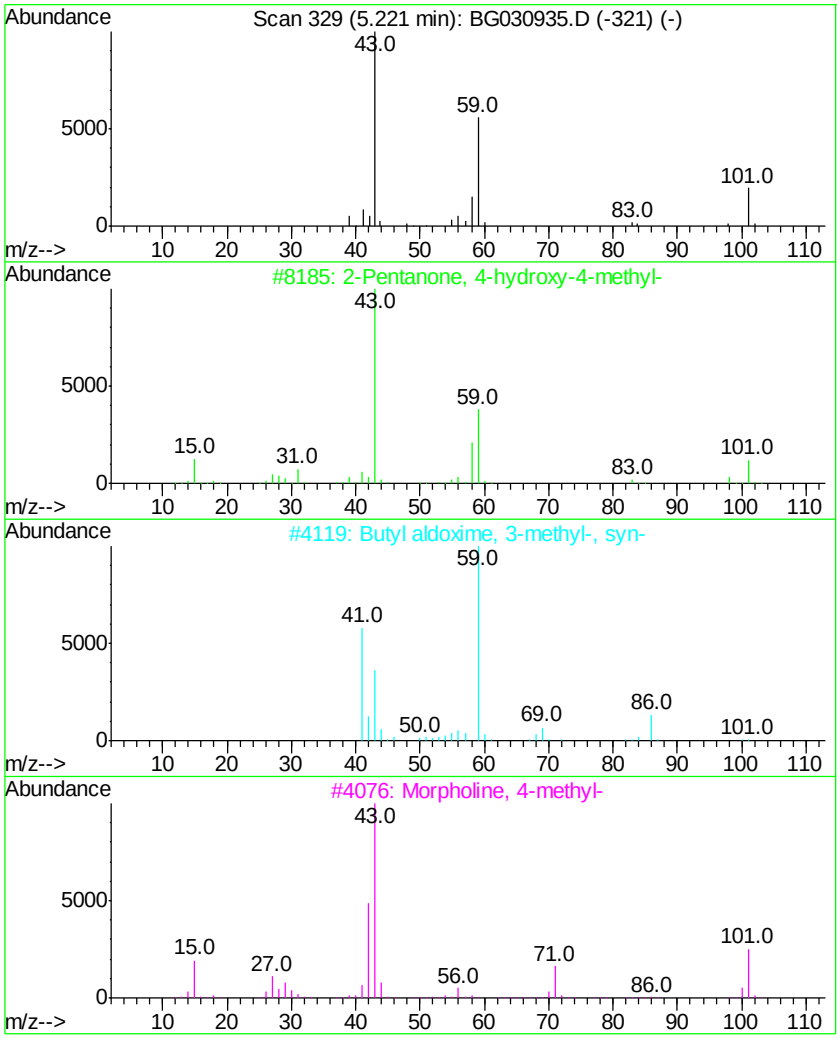
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

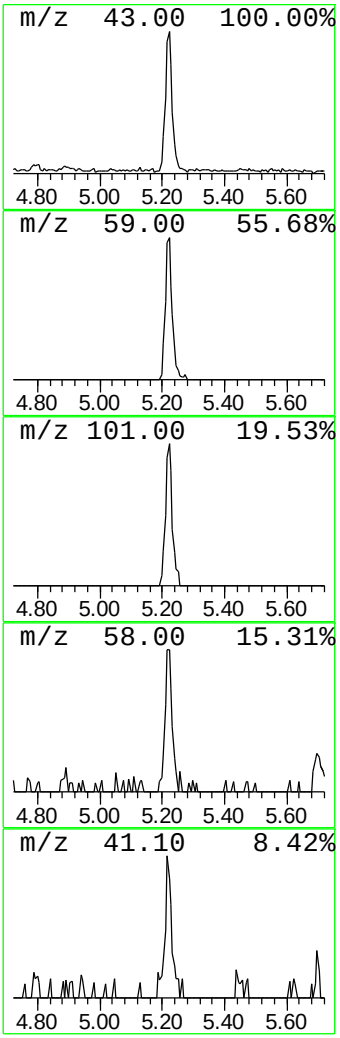
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	4.32 ng	54498	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

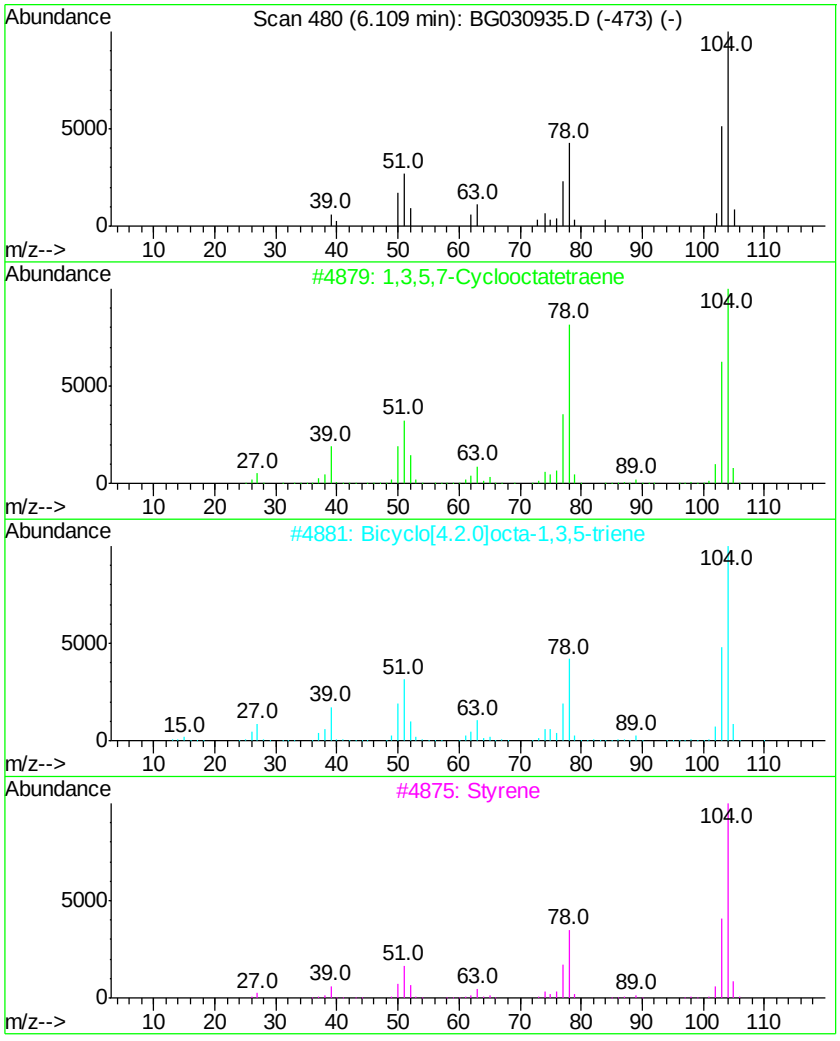
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

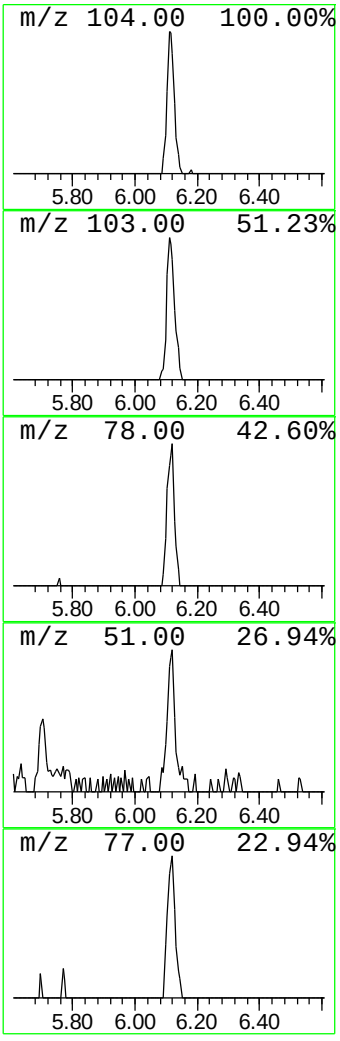
****

Peak Number 4 1,3,5,7-Cyclooctatetraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.11	2.96 ng	37358	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	91
2	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	90
3	Styrene	104	C8H8	000100-42-5	87
4	Butanedioic acid, phenyl-	194	C10H10O4	000635-51-8	59
5	1,3,7-Octatrien-5-yne	104	C8H8	016607-77-5	28





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG111117\
Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

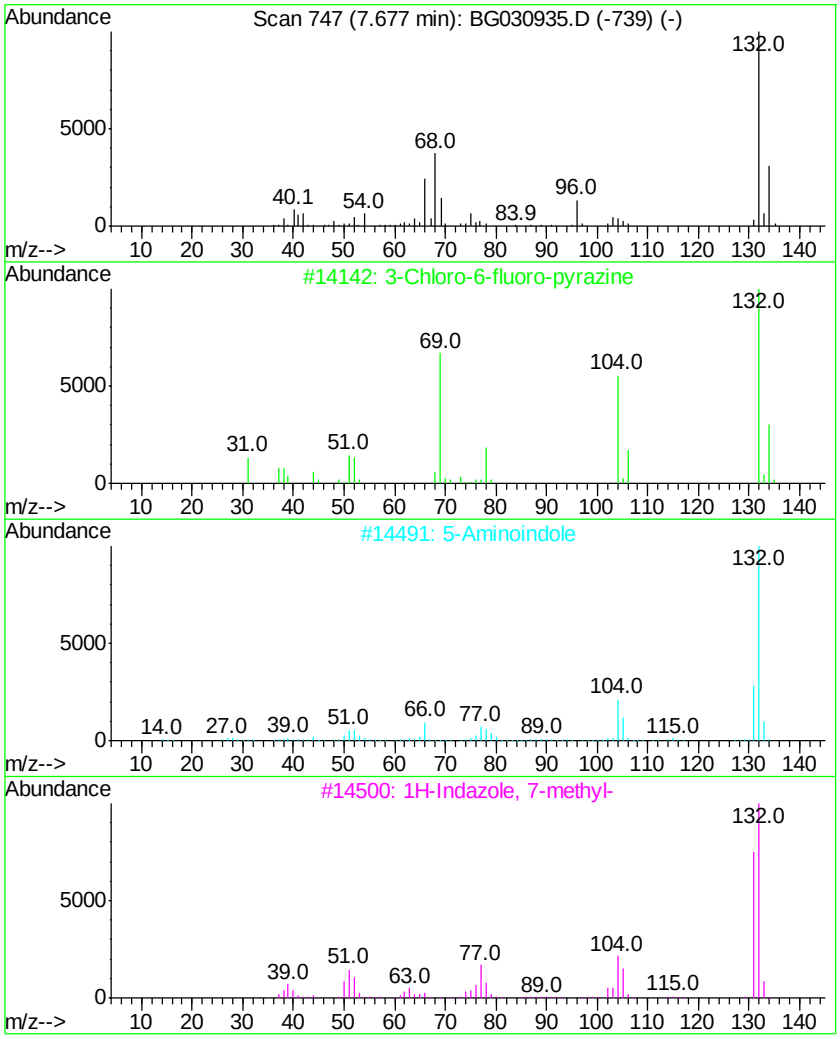
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

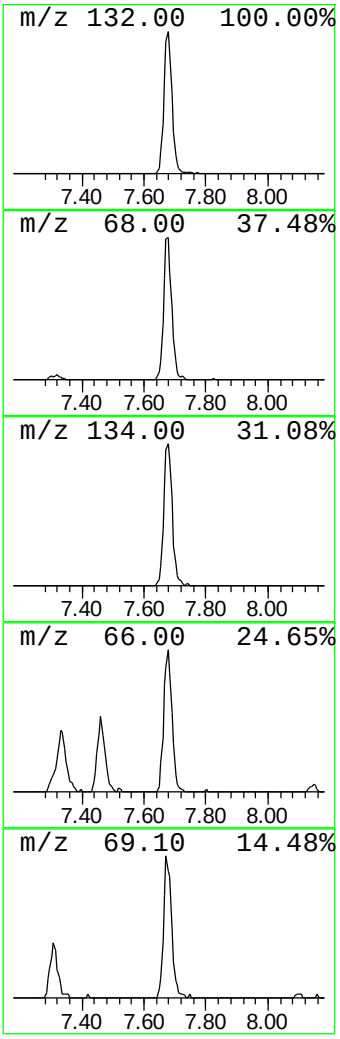
****

Peak Number 5 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	21.42 ng	270511	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG111117\
Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

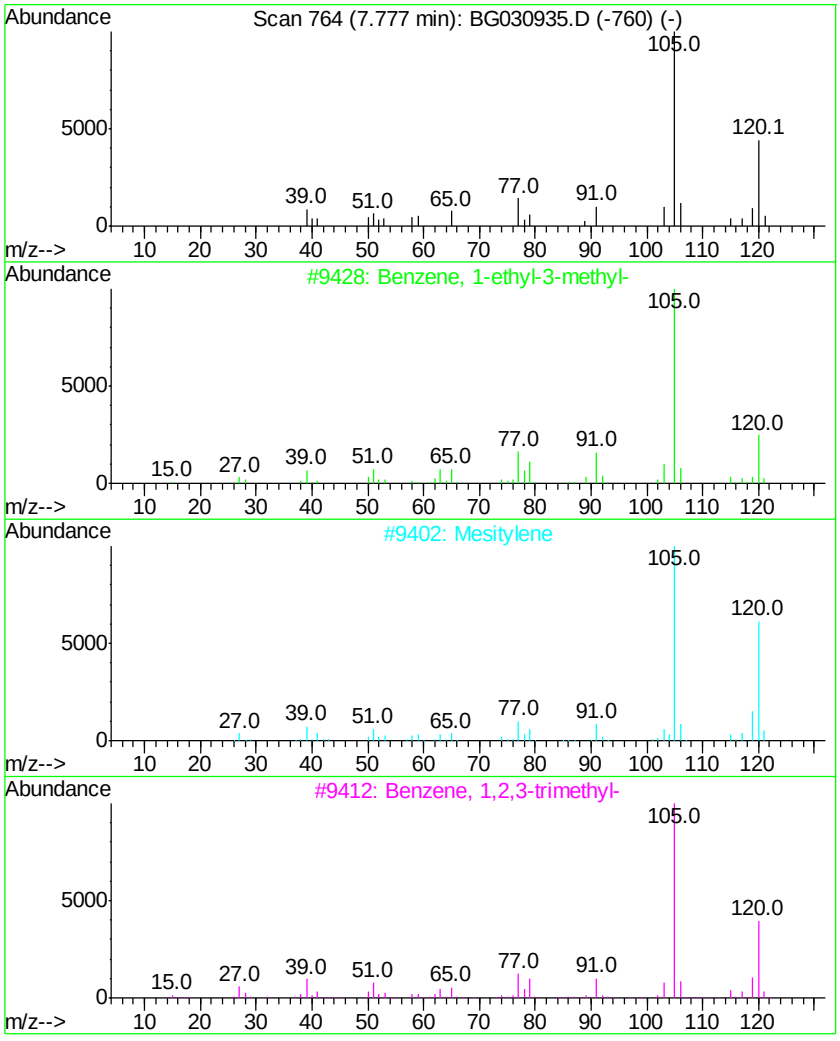
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

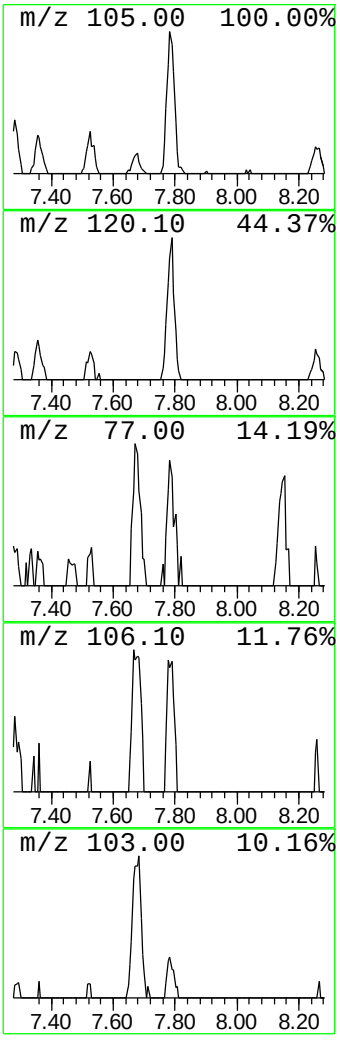
****

Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	2.54 ng	32034	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Mesitylene	120	C9H12	000108-67-8	94
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





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Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

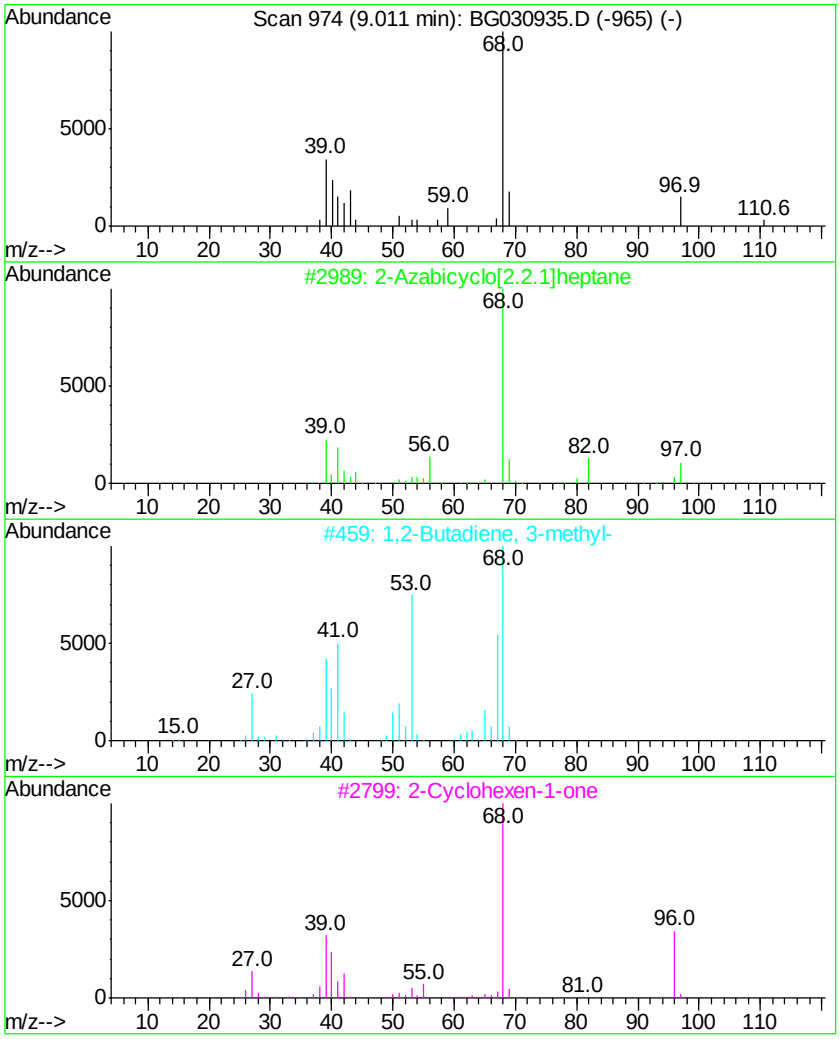
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

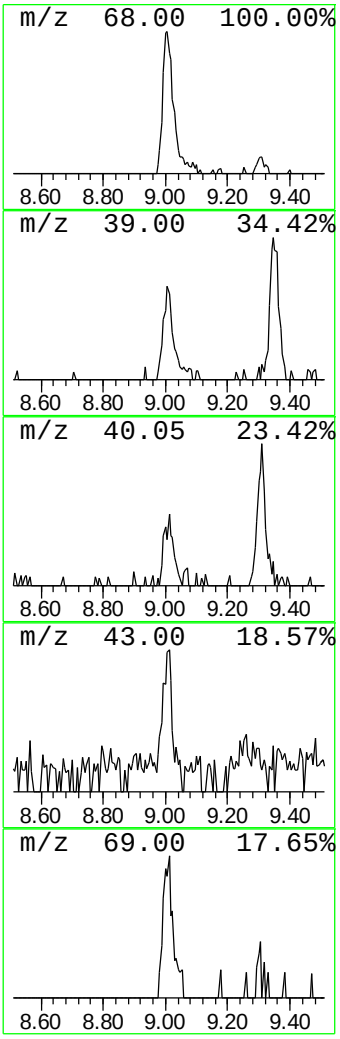
****

Peak Number 7 2-Azabicyclo[2.2.1]heptane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.01	2.68 ng	33865	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Azabicyclo[2.2.1]heptane	97	C6H11N	1000338-38-9	80
2	1,2-Butadiene, 3-methyl-	68	C5H8	000598-25-4	53
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	45
4	2-Pentyne	68	C5H8	000627-21-4	33
5	1H-Pyrazole	68	C3H4N2	000288-13-1	7





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Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

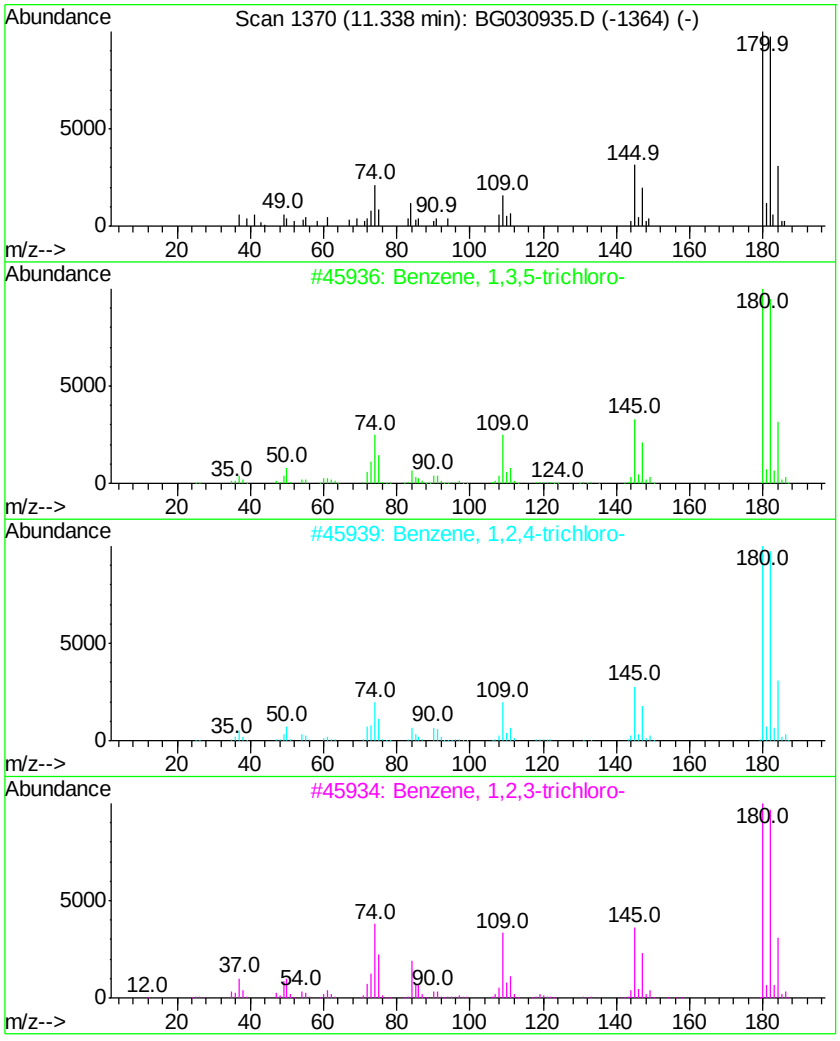
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

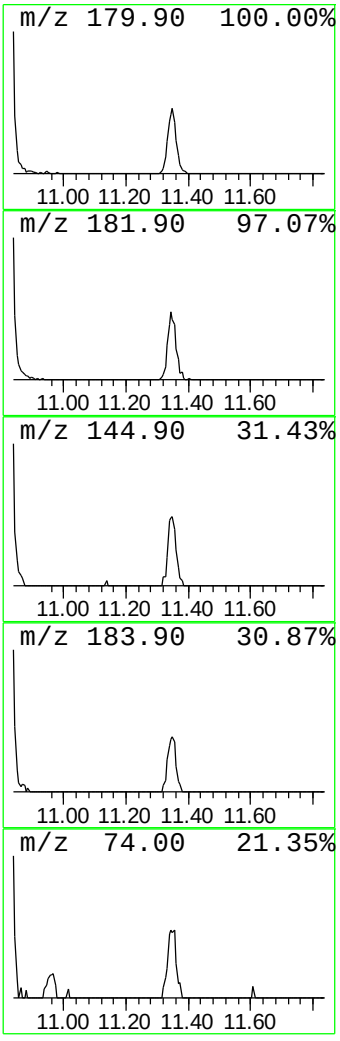
****

Peak Number 8 Benzene, 1,3,5-trichloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.34	3.56 ng	62802	Naphthalene-d8	10.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
2	Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	98
3	Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	97
4	Benzene, (bromoethynyl)-	180	C8H5Br	000932-87-6	52
5	Benzene, 1-chloro-4-(trifluorome...	180	C7H4ClF3	000098-56-6	38





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Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

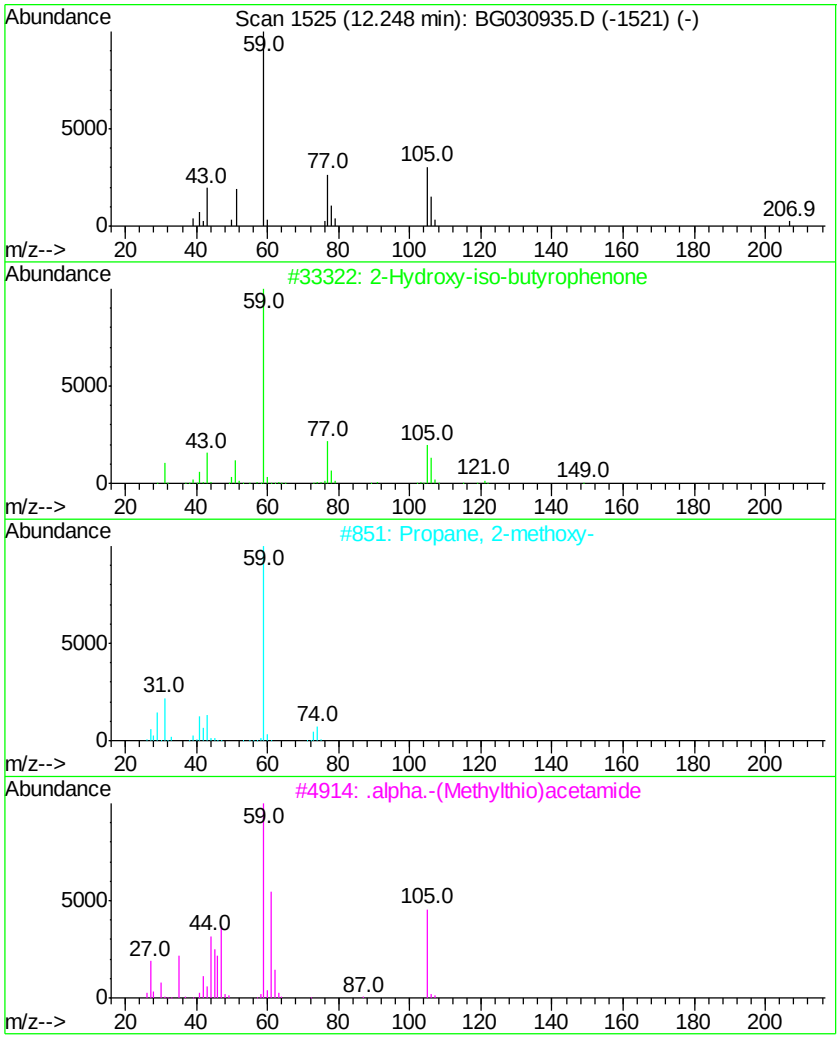
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

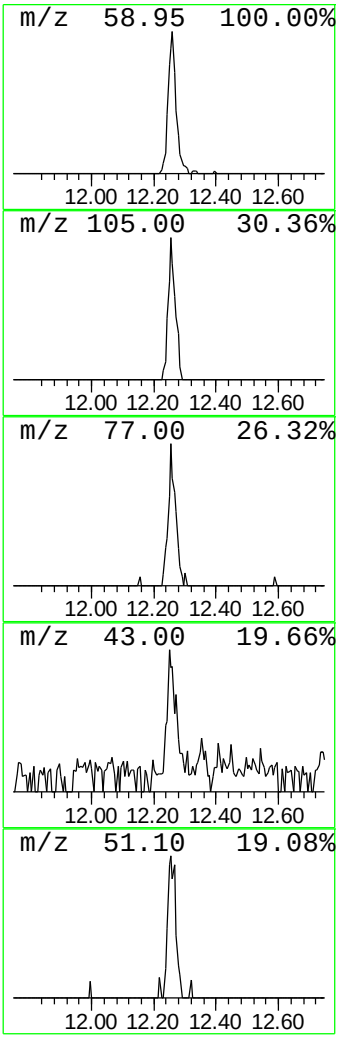
****

Peak Number 9 2-Hydroxy-iso-butyrophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	2.04 ng	36064	Naphthalene-d8	10.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	74
2	Propane, 2-methoxy-	74	C4H10O	000598-53-8	9
3	.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7
4	Guanidine	59	CH5N3	000113-00-8	7
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG111117\
Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.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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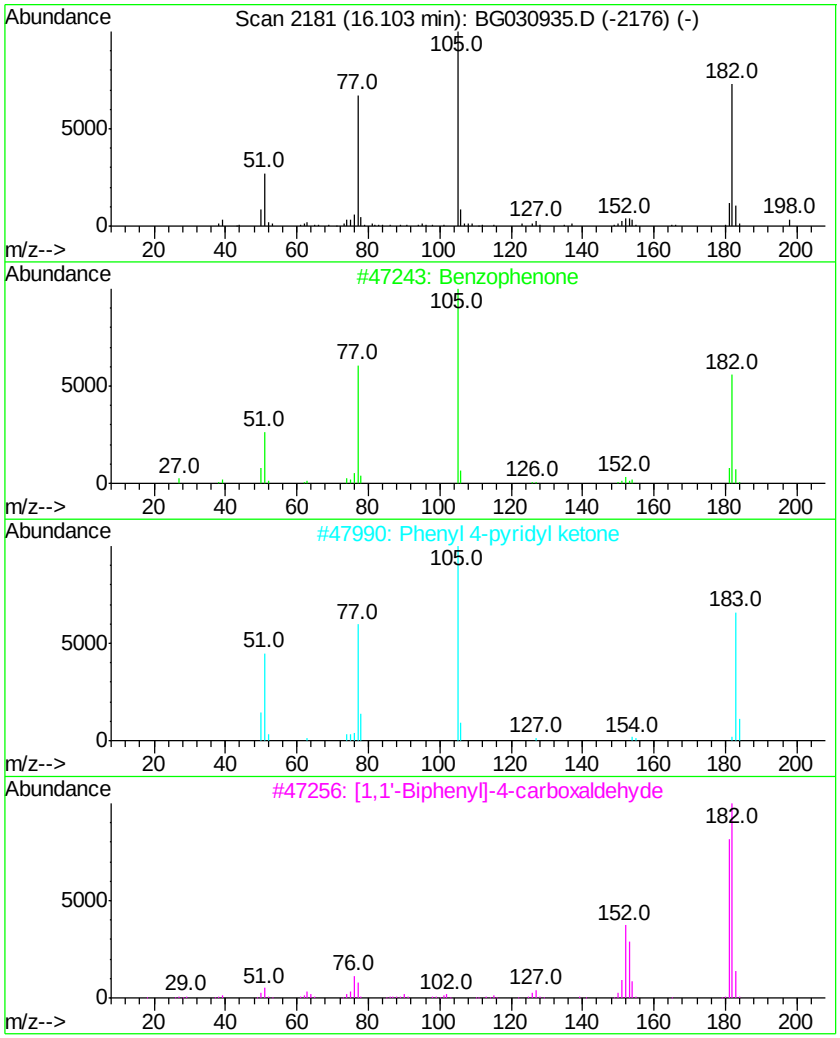
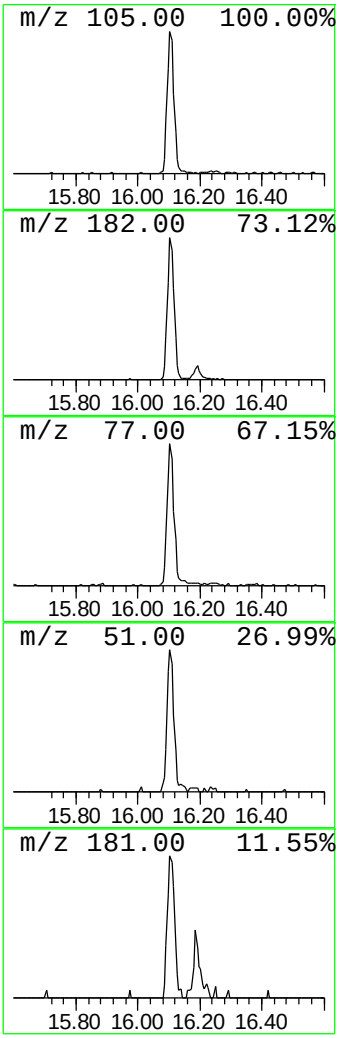
Peak Number 10 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	5.30 ng	164255	Acenaphthene-d10	14.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	46
3	[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	46
4	Benzoylformic acid	150	C8H6O3	000611-73-4	38
5	Glyoxylohydroximoyl chloride, 2-...	183	C8H6ClNO2	004937-87-5	35





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG111117\
Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

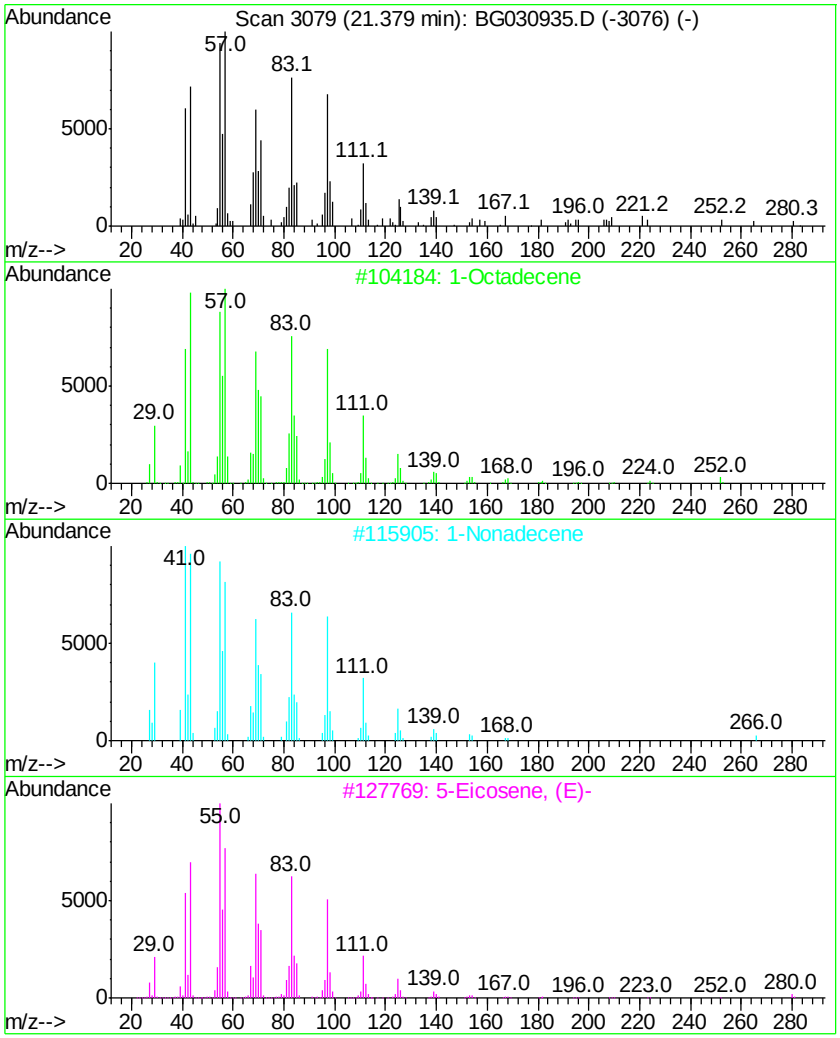
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

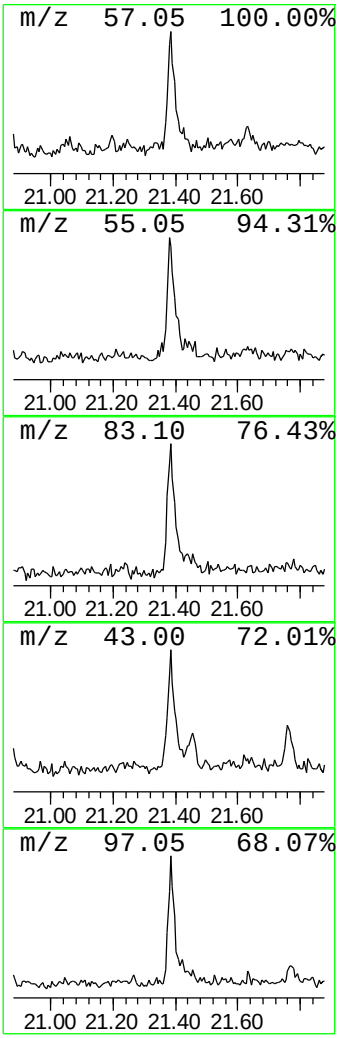
****

Peak Number 11 1-Octadecene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	2.06 ng	113358	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	97
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG111117\
Data File : BG030935.D
Acq On : 11 Nov 2017 9:37
Operator : SJ/JU
Sample : I6413-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FM728

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.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...	5.22	4.3	ng	54498	1	8.14	252585	20.0
1,3,5,7-Cycloocta...	6.11	3.0	ng	37358	1	8.14	252585	20.0
unknown7.68	7.68	21.4	ng	270511	1	8.14	252585	20.0
Benzene, 1-ethyl-...	7.78	2.5	ng	32034	1	8.14	252585	20.0
2-Azabicyclo[2.2....	9.01	2.7	ng	33865	1	8.14	252585	20.0
Benzene, 1,3,5-tr...	11.34	3.6	ng	62802	2	10.96	352958	20.0
2-Hydroxy-iso-but...	12.25	2.0	ng	36064	2	10.96	352958	20.0
Benzophenone	16.10	5.3	ng	164255	3	14.76	620195	20.0
1-Octadecene	21.38	2.1	ng	113358	5	21.77	1100610	20.0