LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG080818\
Data File : BG036226.D
Acq On : 9 Aug 2018 10:27
Operator : JU/SJ
Sample : J4328-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

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_G\METHODS\8270-BG071218.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	5.128	304	313	319	rBV2	27054	49212	1.83%	0.419%
2	5.334	342	348	354	rBV2	17330	30639	1.14%	0.261%
3	5.598	386	393	409	rBV	218428	414268	15.41%	3.527%
4	7.184	654	663	673	rBV	132589	281307	10.46%	2.395%
5	7.267	673	677	687	rVB2	20071	38284	1.42%	0.326%
6	7.543	717	724	739	rVB	443807	806410	29.99%	6.867%
7	8.007	795	803	811	rBV	116480	204744	7.61%	1.743%
8	8.330	849	858	868	rBV	435942	783291	29.13%	6.670%
9	9.170	994	1001	1017	rVB	349158	670352	24.93%	5.708%
10	9.516	1054	1060	1069	rVB	177942	309264	11.50%	2.633%
11	10.809	1272	1280	1291	rBV	138454	268761	9.99%	2.288%
12	10.973	1302	1308	1314	rVB5	21688	43513	1.62%	0.371%
13	13.170	1677	1682	1690	rVB9	13790	30754	1.14%	0.262%
14	13.253	1690	1696	1705	rBV	1011385	1584527	58.92%	13.492%
15	14.633	1925	1931	1938	rBV2	237413	387230	14.40%	3.297%
16	14.692	1938	1941	1947	rVB8	18397	33848	1.26%	0.288%
17	16.125	2178	2185	2199	rBV	839931	1383141	51.43%	11.777%
18	16.648	2270	2274	2279	rVB2	26936	38179	1.42%	0.325%
19	17.376	2392	2398	2404	rBV	341884	516657	19.21%	4.399%
20	19.985	2836	2842	2849	rBV	2055838	2689151	100.00%	22.898%
21	21.641	3117	3124	3131	rBV2	361062	623734	23.19%	5.311%
22	24.825	3657	3666	3677	rBV2	194326	556787	20.70%	4.741%

Sum of corrected areas: 11744053

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG080818\
Data File : BG036226.D
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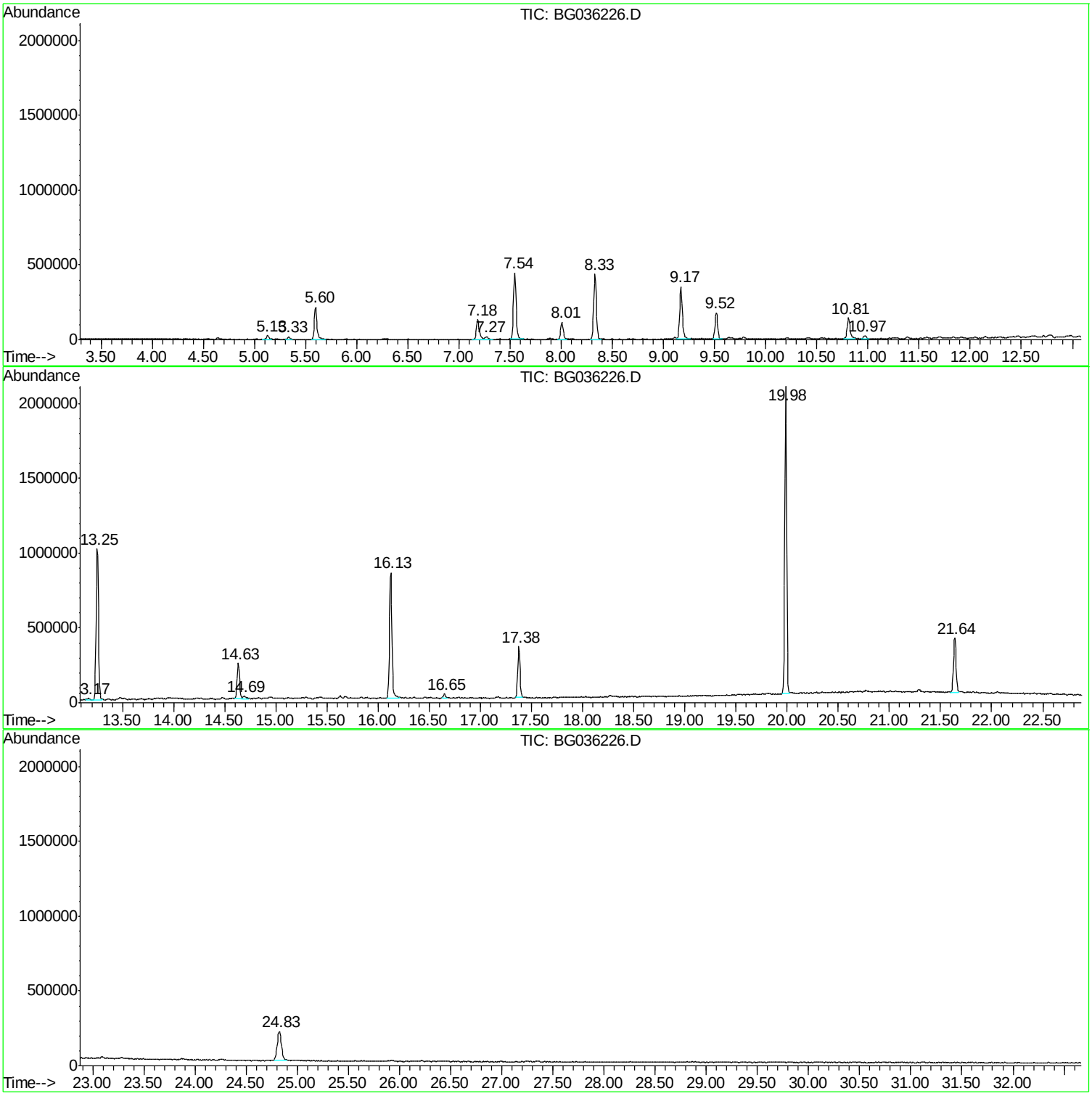
Operator : JU/SJ
Sample : J4328-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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 G\DATA\BG080818\
Data File : BG036226.D
Acq On : 9 Aug 2018 10:27
Operator : JU/SJ
Sample : J4328-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

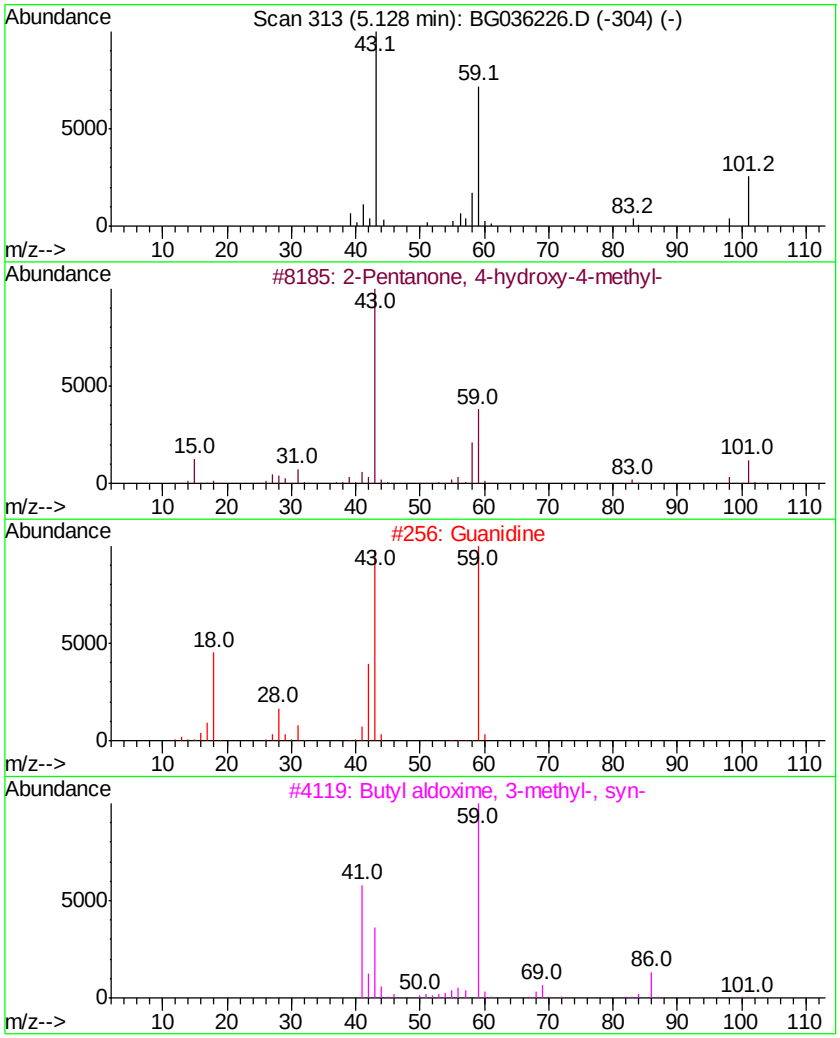
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

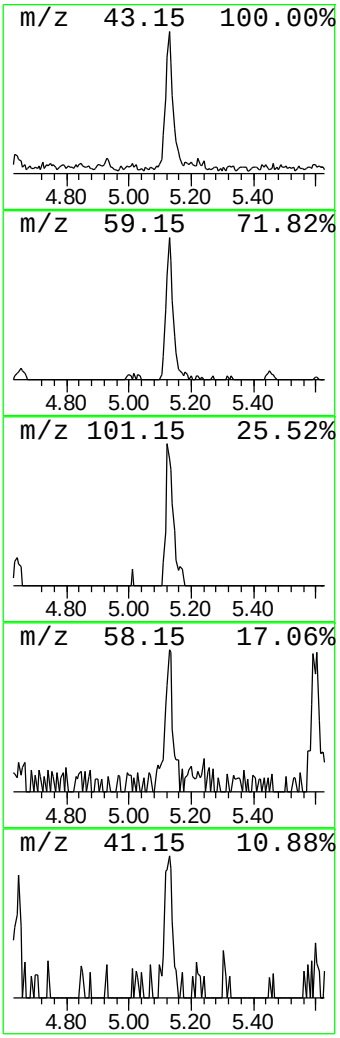
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	4.81 ng	49212	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Guanidine	59	CH5N3	000113-00-8	43
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25





Library Search Compound Report

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Data File : BG036226.D
Acq On : 9 Aug 2018 10:27
Operator : JU/SJ
Sample : J4328-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

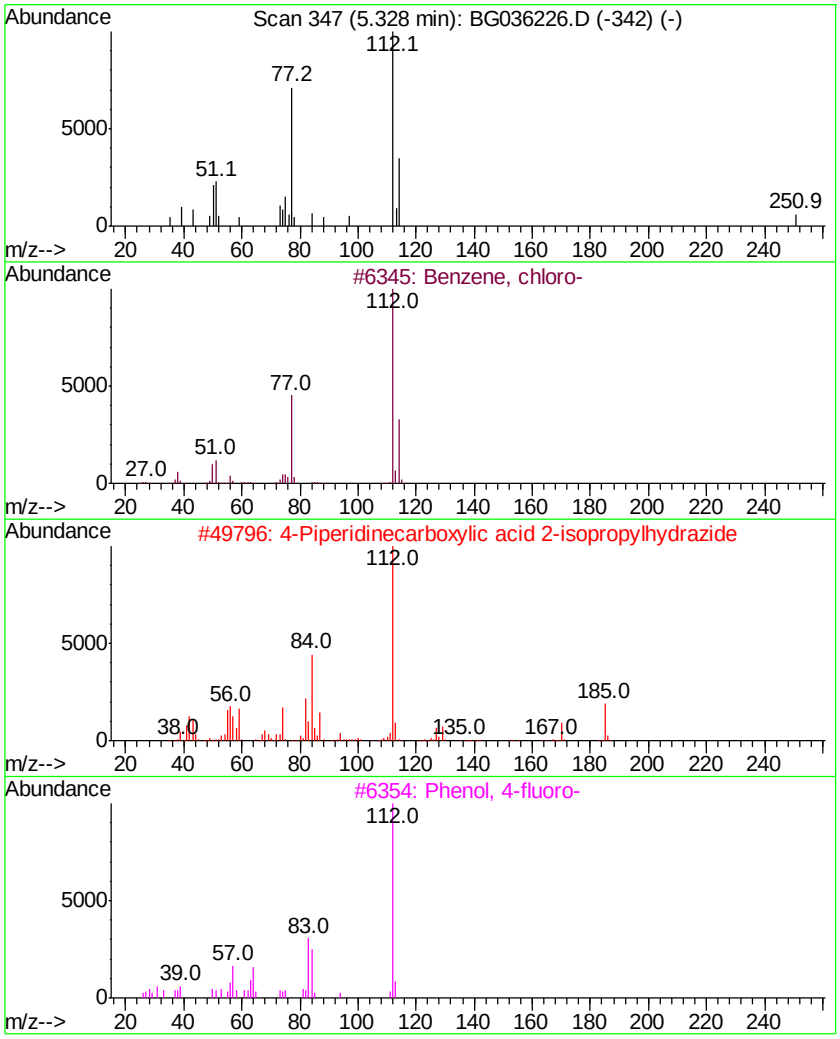
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

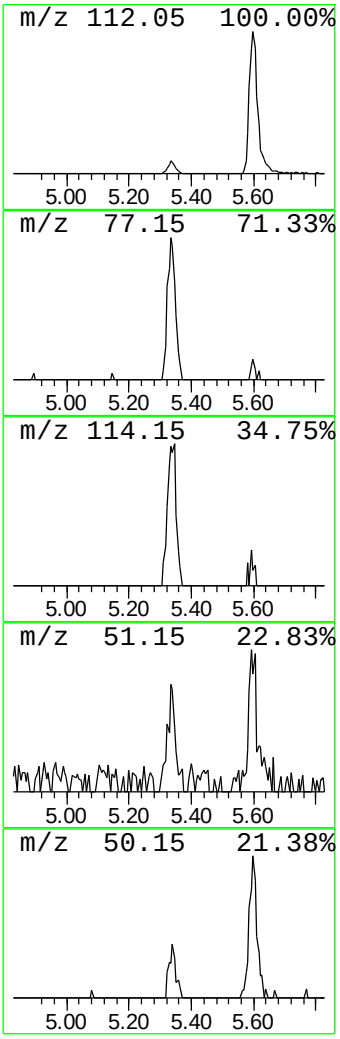
****

Peak Number 2 Benzene, chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	2.99 ng	30639	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, chloro-	112	C6H5Cl	000108-90-7	87
2	4-Piperidinecarboxylic acid 2-is...	185	C9H19N3O	099706-49-7	17
3	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	17
4	2-(2-Hydroxyphenoxy)-1-phenyleth...	230	C14H14O3	328104-89-8	10
5	5-Methylbenzofurazan	134	C7H6N2O	020304-86-3	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG080818\
Data File : BG036226.D
Acq On : 9 Aug 2018 10:27
Operator : JU/SJ
Sample : J4328-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

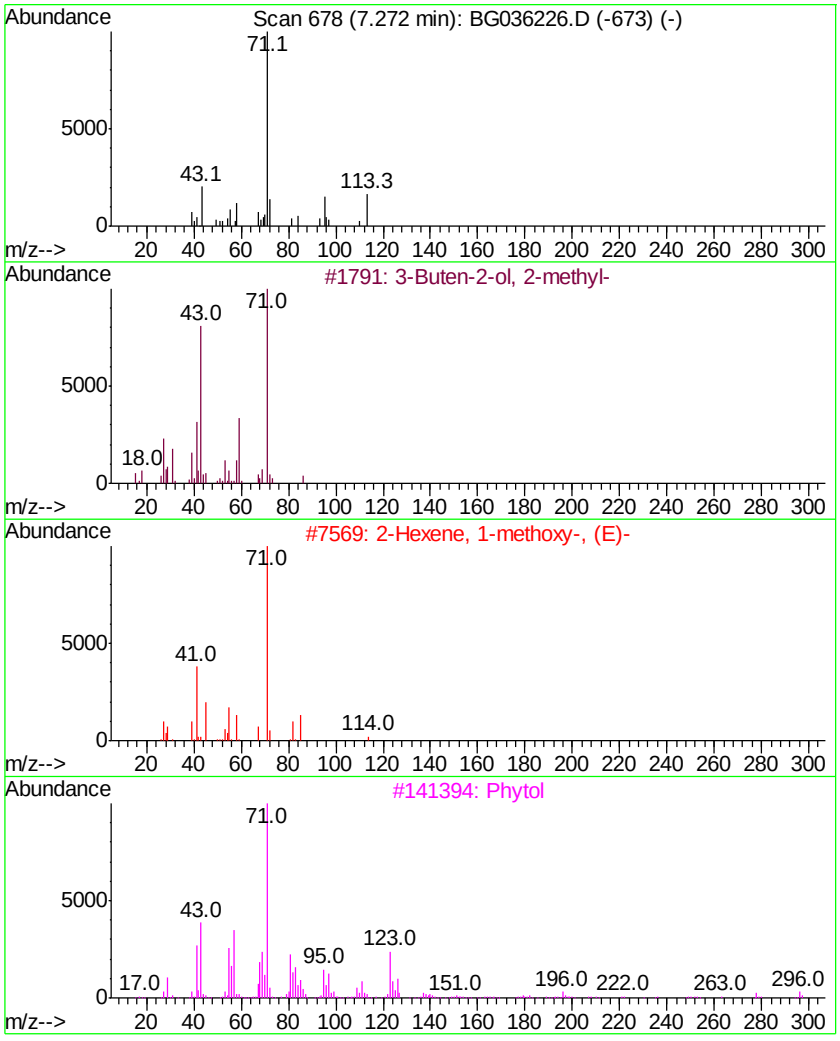
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

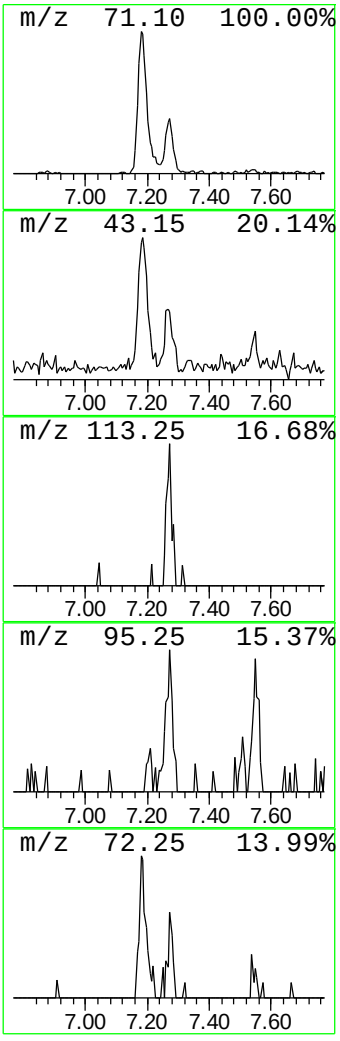
****

Peak Number 3 3-Buten-2-ol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	3.74 ng	38284	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	50
2	2-Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	50
3	Phytol	296	C20H40O	000150-86-7	50
4	Furazan-3-carboxamide, 4-amino-N...	212	C8H12N4O3	309735-27-1	50
5	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG080818\
Data File : BG036226.D
Acq On : 9 Aug 2018 10:27
Operator : JU/SJ
Sample : J4328-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

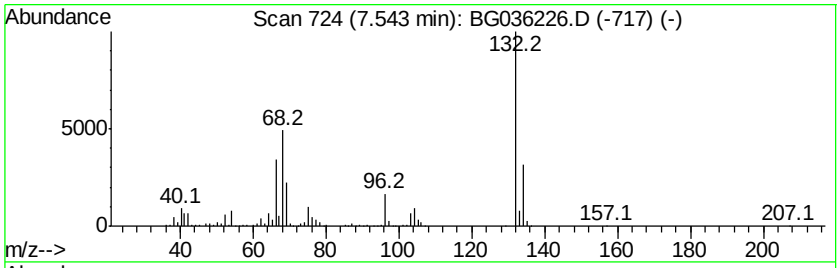
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

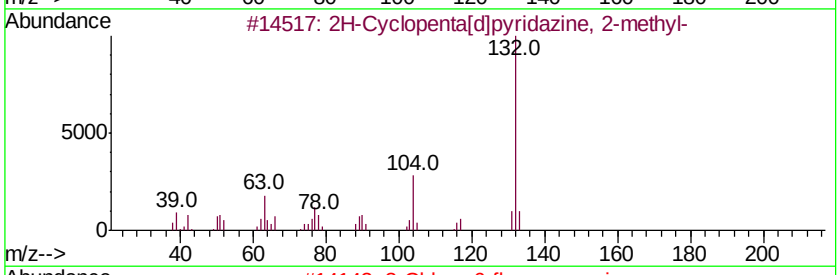
****

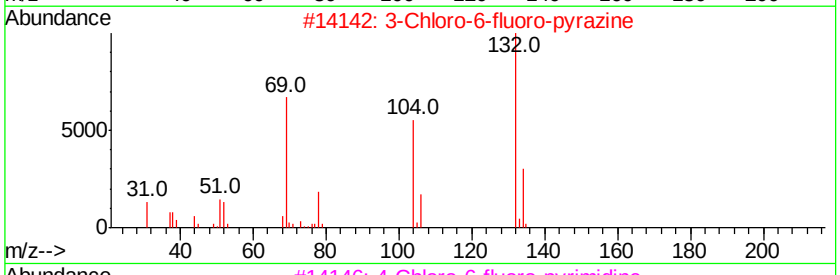
Peak Number 4 unknown7.54 Concentration Rank 1

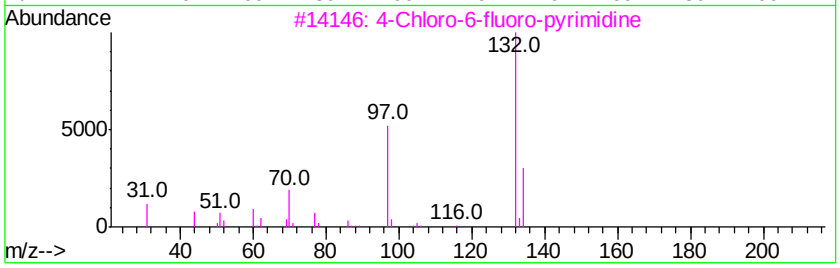
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	78.77 ng	806410	1,4-Dichlorobenzene-d4	8.01

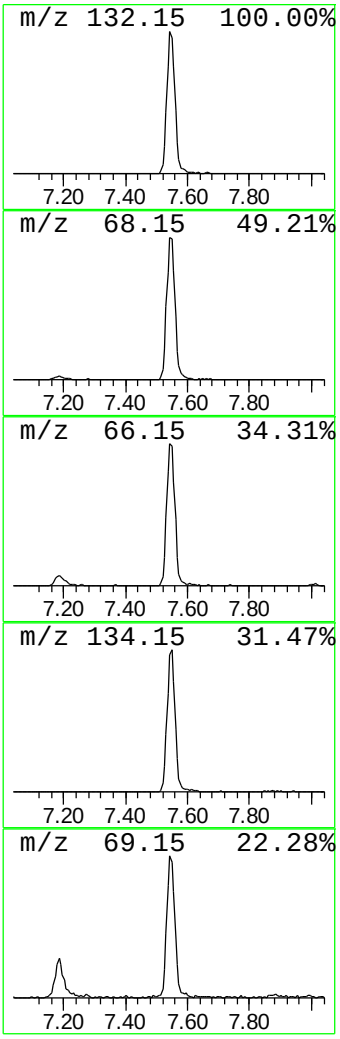
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	30
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12











Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG080818\
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Sample : J4328-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

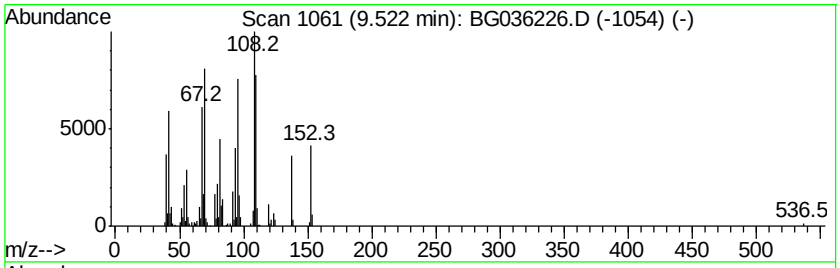
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

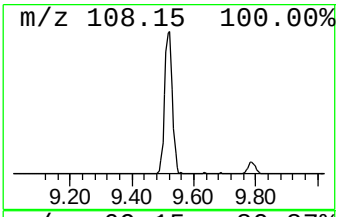
****

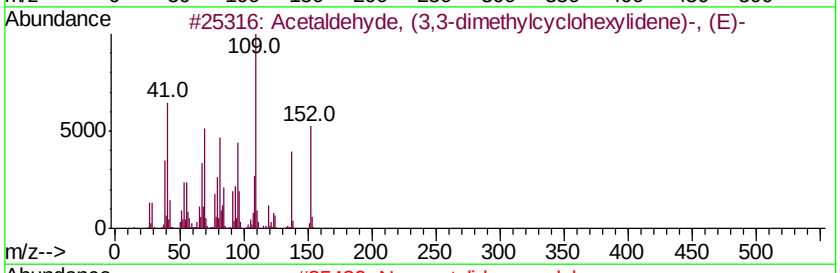
Peak Number 6 Acetaldehyde, (3,3-dimethyl... Concentration Rank 3

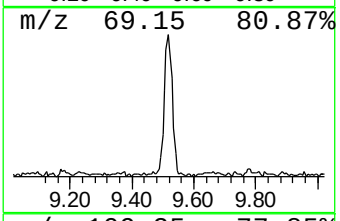
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.52	23.01 ng	309264	Naphthalene-d8	10.81

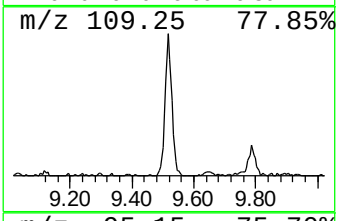
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	86
2	Neopentylidenecyclohexane	152	C11H20	039546-80-0	43
3	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	27
4	2-Acetyl-4,4-dimethyl-cyclopent-...	152	C9H12O2	081979-96-6	27
5	Phenacetin	179	C10H13NO2	000062-44-2	27

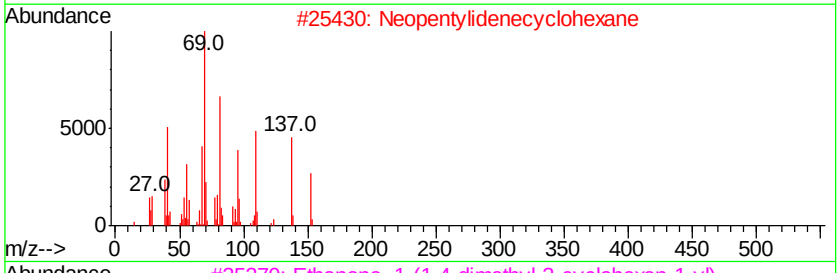


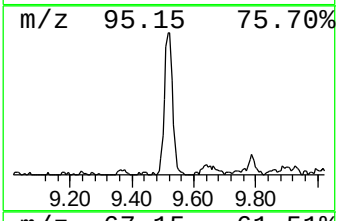


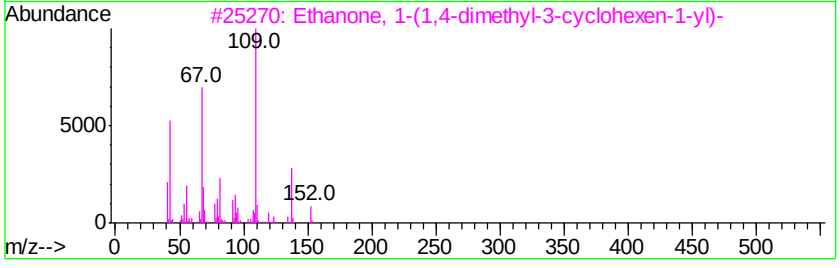


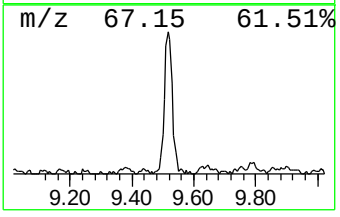












Library Search Compound Report

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

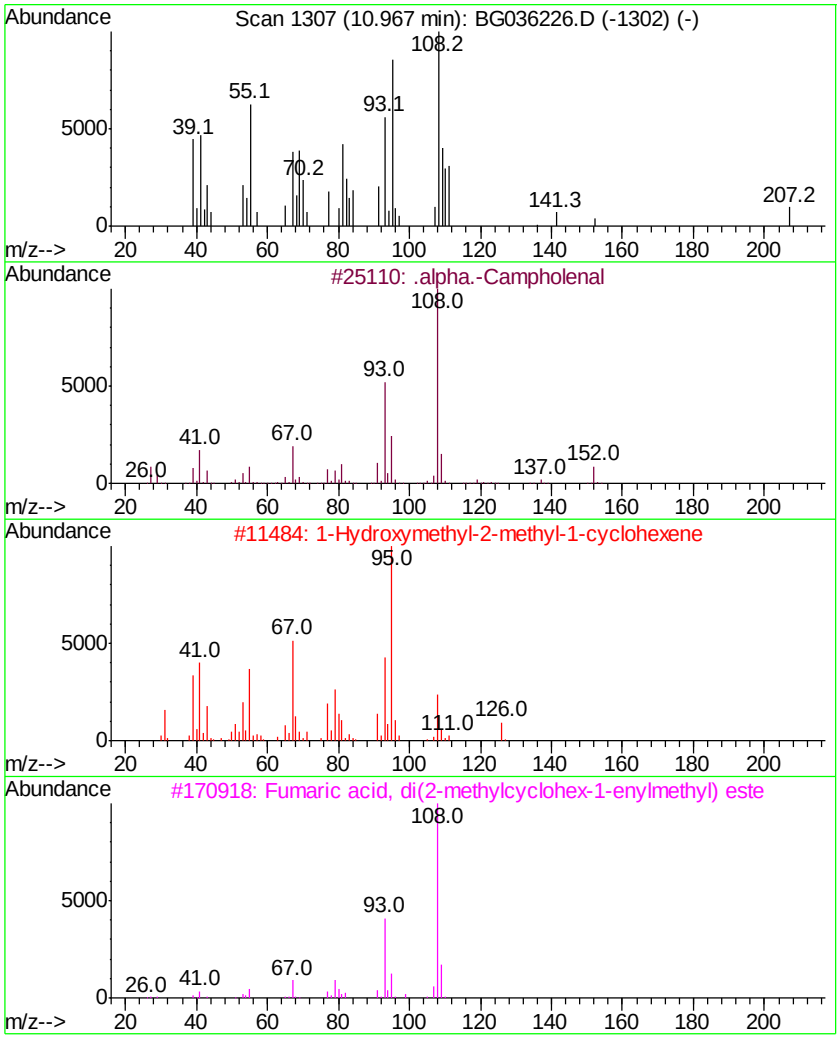
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

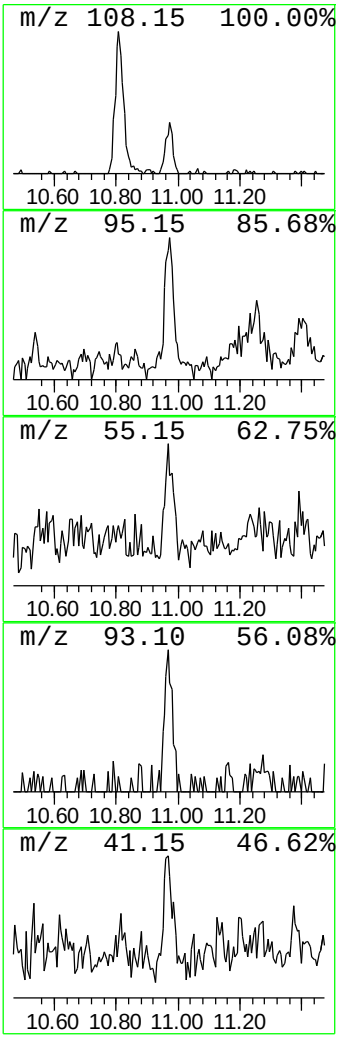
****

Peak Number 7 unknown10.97 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	3.24 ng	43513	Naphthalene-d8	10.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Campholenal	152	C10H16O	004501-58-0	43
2	1-Hydroxymethyl-2-methyl-1-cyclo...	126	C8H14O	029474-11-1	40
3	Fumaric acid, di(2-methylcyclohe...	332	C20H28O4	1000345-16-5	38
4	5-Methyl-5-hexen-3-yn-2-ol	110	C7H10O	068017-33-4	35
5	5-Octen-2-yn-4-ol	124	C8H12O	1000196-87-1	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG080818\
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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...	5.13	4.8	ng	49212	1	8.01	204744	20.0
Benzene, chloro-	5.33	3.0	ng	30639	1	8.01	204744	20.0
3-Buten-2-ol, 2-m...	7.27	3.7	ng	38284	1	8.01	204744	20.0
unknown7.54	7.54	78.8	ng	806410	1	8.01	204744	20.0
Acetaldehyde, (3,...	9.52	23.0	ng	309264	2	10.81	268761	20.0
unknown10.97	10.97	3.2	ng	43513	2	10.81	268761	20.0