LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020719\
Data File : BG039387.D
Acq On : 7 Feb 2019 18:20
Operator : JU/SJ
Sample : K1389-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M-7

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-BG012919.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	3.230	18	24	32	rBV	211375	408811	8.94%	1.932%
2	3.300	32	36	42	rVB	188820	259696	5.68%	1.228%
3	3.765	110	115	123	rBV	47548	74405	1.63%	0.352%
4	4.840	289	298	307	rVB	32610	51154	1.12%	0.242%
5	5.257	362	369	376	rBV	34594	55934	1.22%	0.264%
6	5.715	439	447	455	rBV	589409	931160	20.36%	4.401%
7	6.032	495	501	508	rBV	52436	85230	1.86%	0.403%
8	7.307	708	718	731	rBV	400631	715412	15.65%	3.382%
9	7.700	777	785	793	rBV	947825	1622376	35.48%	7.669%
10	8.176	859	866	876	rBV	202347	334263	7.31%	1.580%
11	8.499	913	921	930	rVB	786620	1390322	30.41%	6.572%
12	9.351	1057	1066	1077	rBV	697458	1246264	27.25%	5.891%
13	11.002	1338	1347	1354	rVB	266375	483089	10.56%	2.283%
14	13.428	1752	1760	1767	rBV	1828911	2954651	64.62%	13.966%
15	14.797	1986	1993	2004	rVB2	417359	700257	15.31%	3.310%
16	16.283	2239	2246	2259	rBV	1405240	2124555	46.46%	10.042%
17	17.540	2454	2460	2473	rVB2	573727	891518	19.50%	4.214%
18	20.136	2894	2902	2908	rBV	3369239	4572665	100.00%	21.614%
19	21.429	3118	3122	3129	rBV3	33277	52108	1.14%	0.246%
20	21.834	3182	3191	3200	rBV	618913	1059033	23.16%	5.006%
21	23.362	3445	3451	3457	rVB3	24142	46791	1.02%	0.221%
22	24.207	3588	3595	3601	rBV4	24997	56107	1.23%	0.265%
23	25.218	3755	3767	3780	rBV2	342456	1040270	22.75%	4.917%

Sum of corrected areas: 21156071

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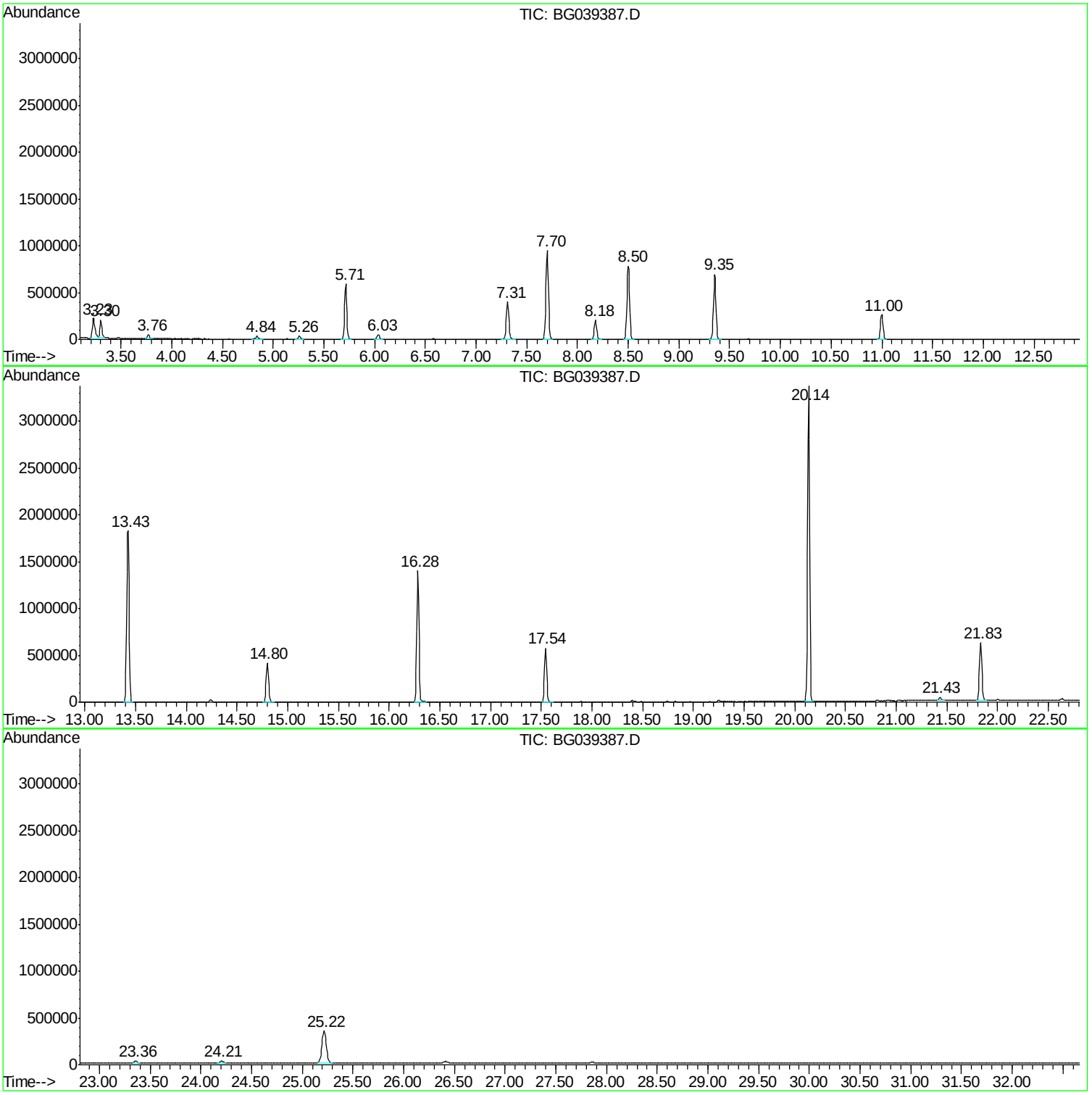
Instrument :
BNA_G
ClientSampleId :
M-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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 : BG039387.D
Acq On : 7 Feb 2019 18:20
Operator : JU/SJ
Sample : K1389-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

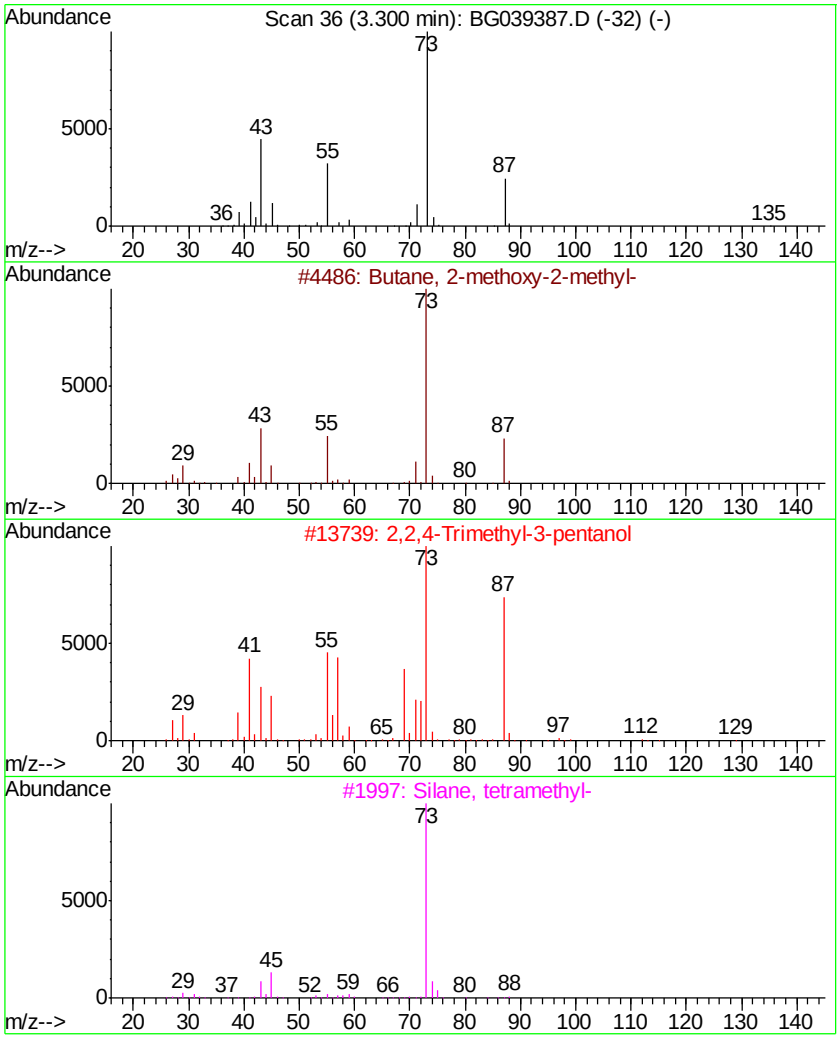
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

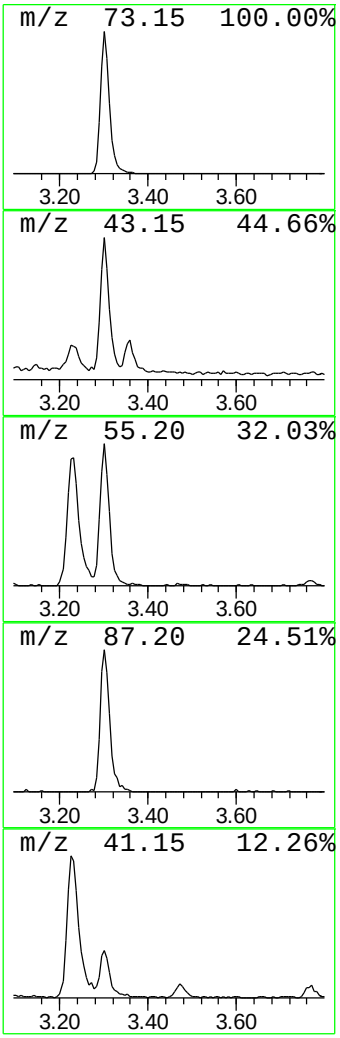
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.30	15.54 ng	259696	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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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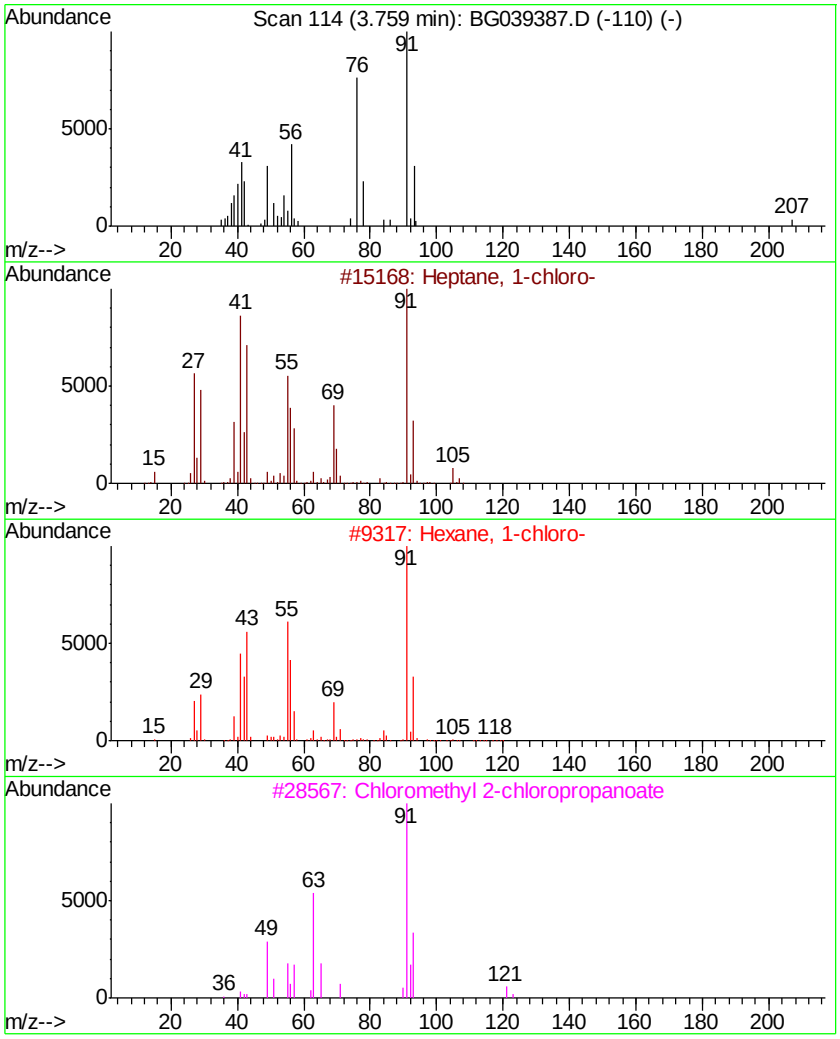
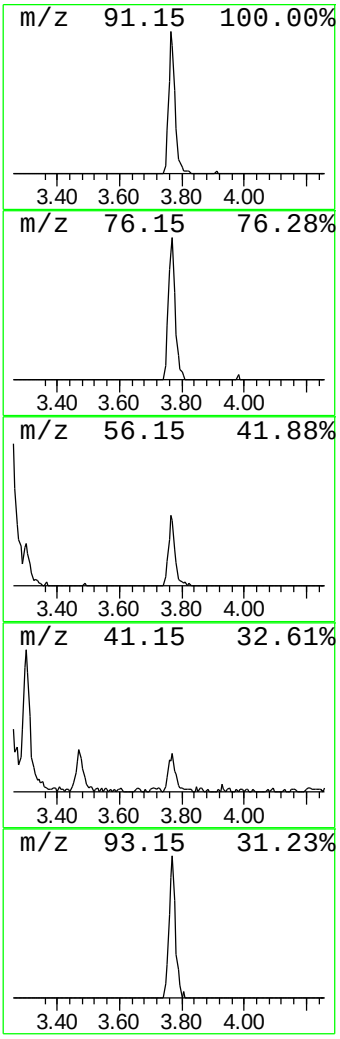
Peak Number 3 unknown3.76 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.76	4.45 ng	74405	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 1-chloro-	134	C7H15Cl	000629-06-1	12
2	Hexane, 1-chloro-	120	C6H13Cl	000544-10-5	12
3	Chloromethyl 2-chloropropanoate	156	C4H6Cl2O2	013398-02-2	9
4	2-Bromo-1-chloro-2-methylpropane	170	C4H8BrCl	002074-80-8	9
5	2-Butanone, 1-chloro-	106	C4H7ClO	000616-27-3	9





Library Search Compound Report

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Data File : BG039387.D
Acq On : 7 Feb 2019 18:20
Operator : JU/SJ
Sample : K1389-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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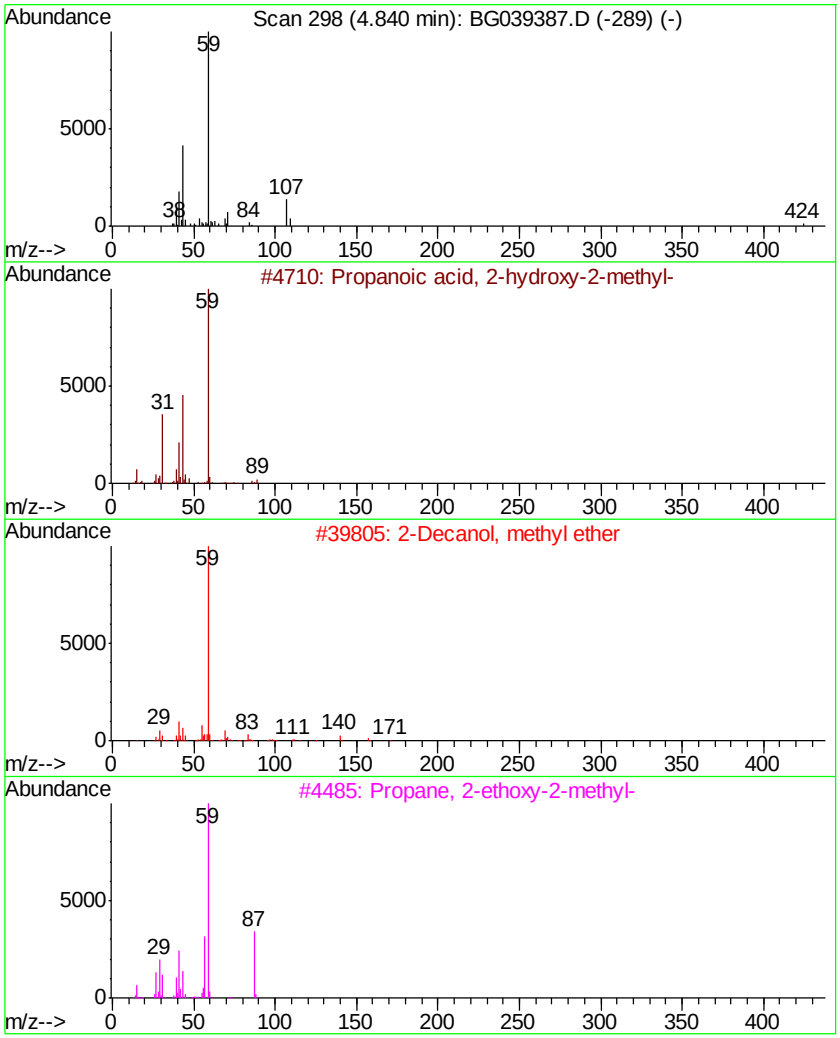
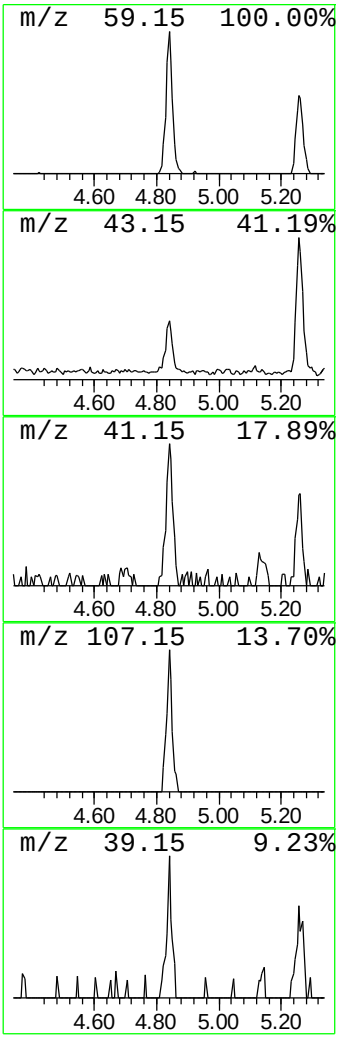
Peak Number 4 unknown4.84 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	3.06 ng	51154	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	42
2	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	38
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	36
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	36
5	Amylene hydrate	88	C5H12O	000075-85-4	36





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020719\
Data File : BG039387.D
Acq On : 7 Feb 2019 18:20
Operator : JU/SJ
Sample : K1389-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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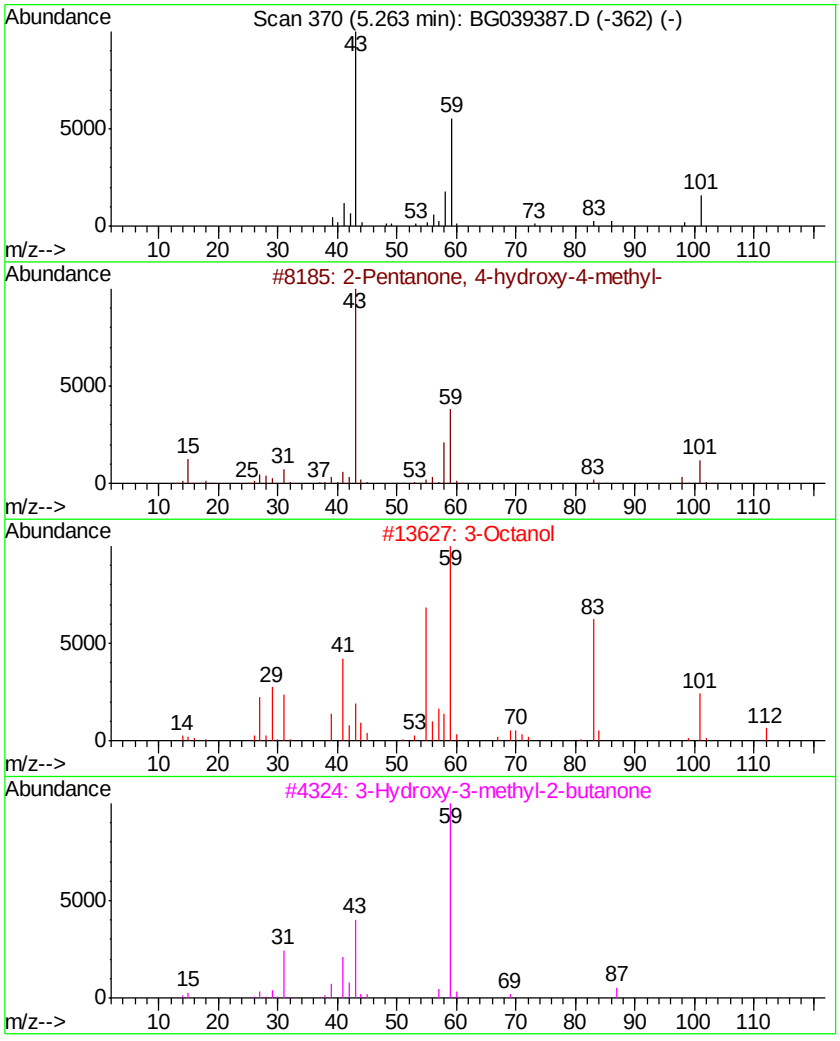
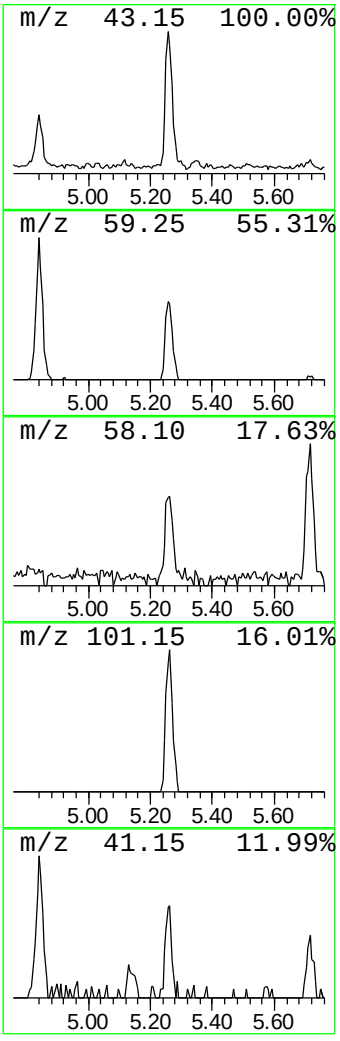
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	3.35 ng	55934	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Octanol	130	C8H18O	000589-98-0	33
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
4	Butane, 2-methoxy-	88	C5H12O	006795-87-5	9
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020719\
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Acq On : 7 Feb 2019 18:20
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Sample : K1389-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : M-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

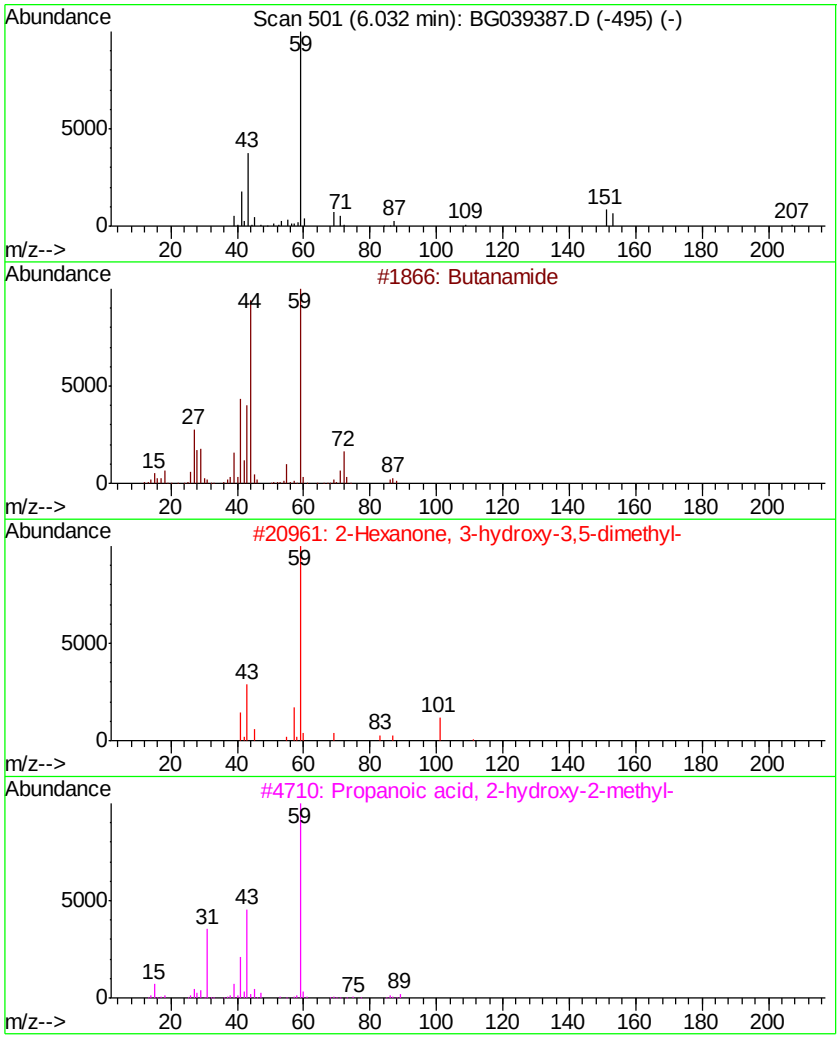
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

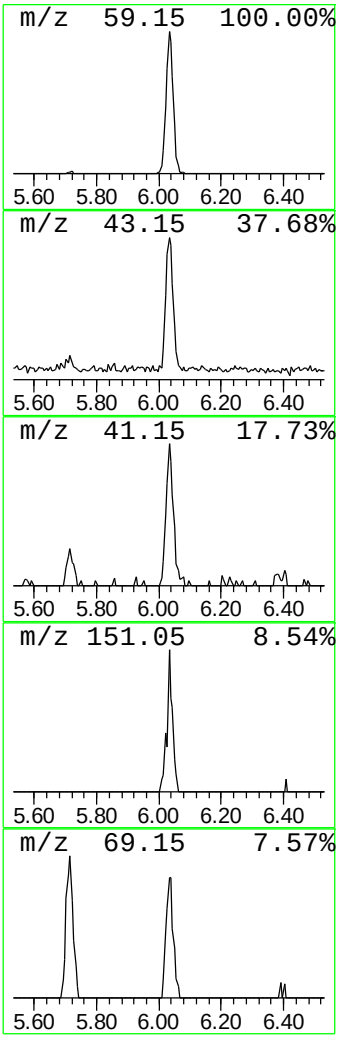
****

Peak Number 6 Butanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.03	5.10 ng	85230	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanamide	87	C4H9NO	000541-35-5	64
2	2-Hexanone, 3-hydroxy-3,5-dimethyl-	144	C8H16O2	006321-14-8	59
3	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	59
4	Acetic acid, 3-methoxy-2-butyl e...	146	C7H14O3	1000151-29-7	50
5	4-Methyl-2-pentanol, methyl ether	116	C7H16O	1000333-93-5	50





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Instrument : BNA_G
ClientSampleId : M-7

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

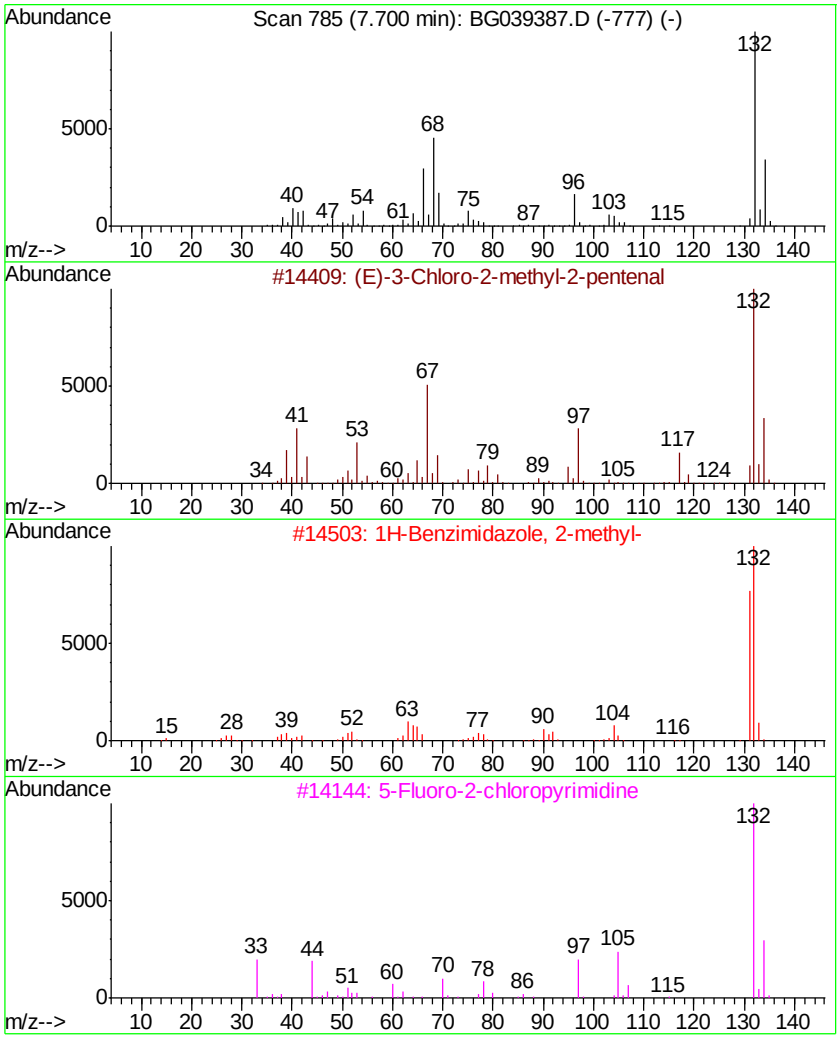
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

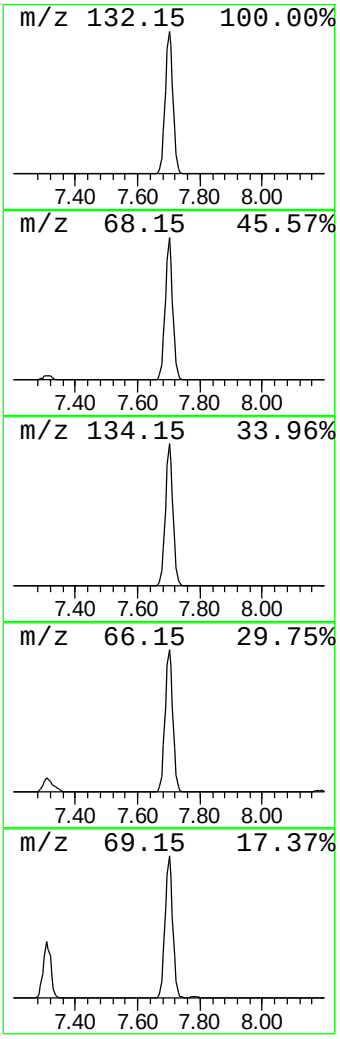
****

Peak Number 7 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	97.07 ng	1622380	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	30
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	5-Aminoindole	132	C8H8N2	005192-03-0	10





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
Butane, 2-methoxy...	3.30	15.5	ng	259696	1	8.18	334263	20.0
unknown3.76	3.76	4.5	ng	74405	1	8.18	334263	20.0
unknown4.84	4.84	3.1	ng	51154	1	8.18	334263	20.0
2-Pentanone, 4-hy...	5.26	3.4	ng	55934	1	8.18	334263	20.0
Butanamide	6.03	5.1	ng	85230	1	8.18	334263	20.0
unknown7.70	7.70	97.1	ng	1622380	1	8.18	334263	20.0