LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010719\
Data File : BG038981.D
Acq On : 8 Jan 2019 00:25
Operator : JU/SJ
Sample : K1010-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OK-03-010419

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-BG121218.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	3.194	14	18	27	rVB2	50861	85640	4.21%	0.858%
2	3.488	63	68	75	rVB	42583	55741	2.74%	0.559%
3	4.634	257	263	270	rBV	22646	33565	1.65%	0.336%
4	5.086	334	340	344	rBV	16552	25442	1.25%	0.255%
5	5.133	344	348	356	rVB	47313	75743	3.72%	0.759%
6	5.603	421	428	441	rBV	388389	637464	31.33%	6.390%
7	7.207	694	701	713	rBV	368492	653294	32.11%	6.549%
8	7.577	755	764	772	rBV	417680	742820	36.51%	7.446%
9	8.047	838	844	851	rBV	96518	169697	8.34%	1.701%
10	8.370	891	899	908	rVB	327884	582786	28.65%	5.842%
11	9.222	1036	1044	1055	rBV	264779	492224	24.19%	4.934%
12	10.862	1316	1323	1337	rBV	124191	235116	11.56%	2.357%
13	13.300	1730	1738	1750	rBV	776250	1252794	61.58%	12.558%
14	14.592	1953	1958	1965	rBV2	10578	22192	1.09%	0.222%
15	14.686	1967	1974	1981	rVB3	202744	345010	16.96%	3.458%
16	16.179	2220	2228	2243	rBV2	634880	1054905	51.85%	10.575%
17	17.430	2433	2441	2448	rBV2	279684	440491	21.65%	4.416%
18	20.033	2877	2884	2892	rBV	1540632	2034426	100.00%	20.394%
19	21.708	3162	3169	3179	rBV	283786	495074	24.33%	4.963%
20	23.153	3410	3415	3422	rVB5	12991	25331	1.25%	0.254%
21	23.958	3547	3552	3559	rVB2	16071	32435	1.59%	0.325%
22	24.910	3708	3714	3719	rBV8	12166	27223	1.34%	0.273%
23	24.998	3720	3729	3742	rVB2	154713	456343	22.43%	4.575%

Sum of corrected areas: 9975756

LSC Report - Integrated Chromatogram

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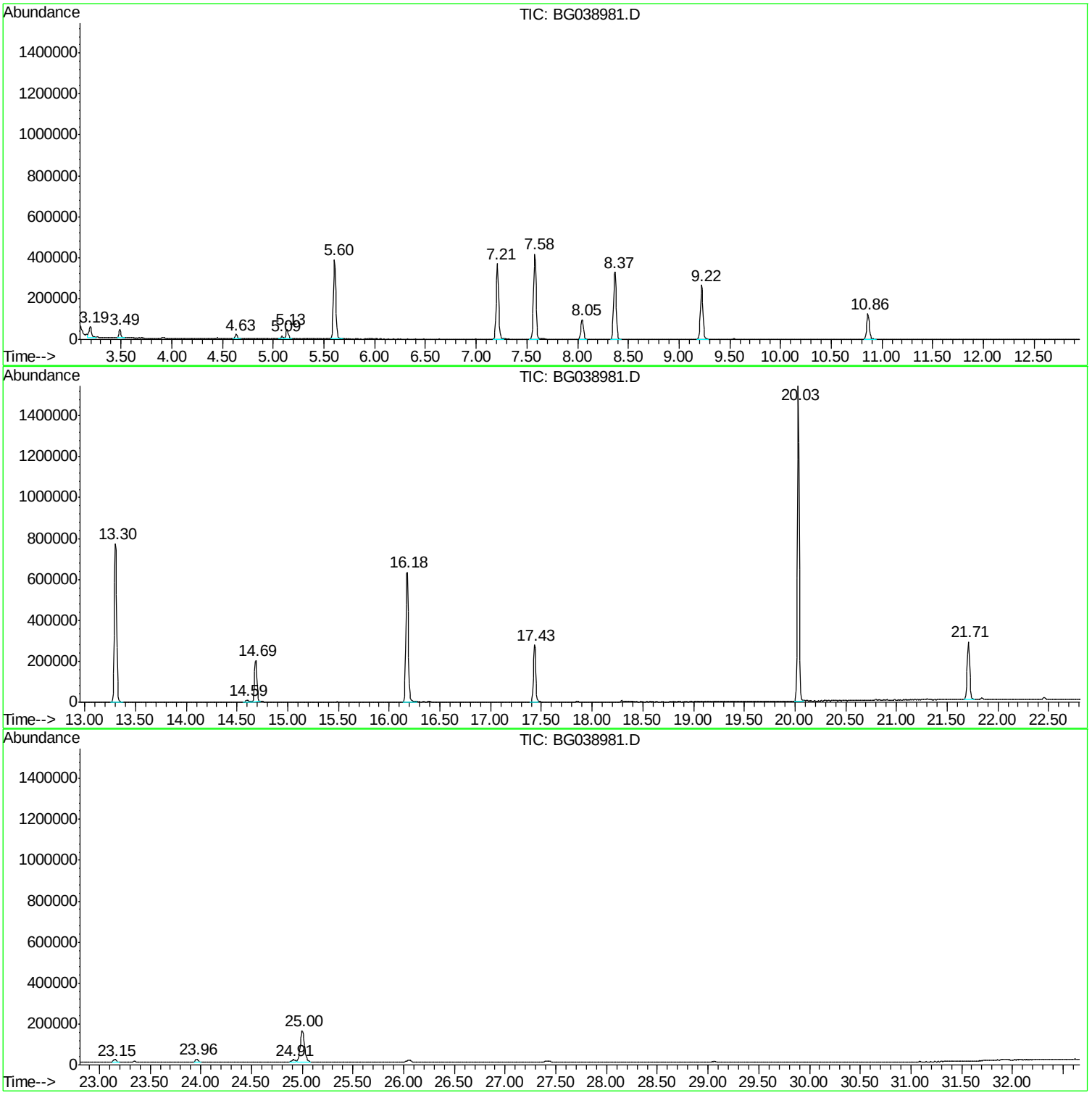
Operator : JU/SJ
Sample : K1010-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OK-03-010419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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\BG010719\
Data File : BG038981.D
Acq On : 8 Jan 2019 00:25
Operator : JU/SJ
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Misc :
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Instrument : BNA_G
ClientSampleId : OK-03-010419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

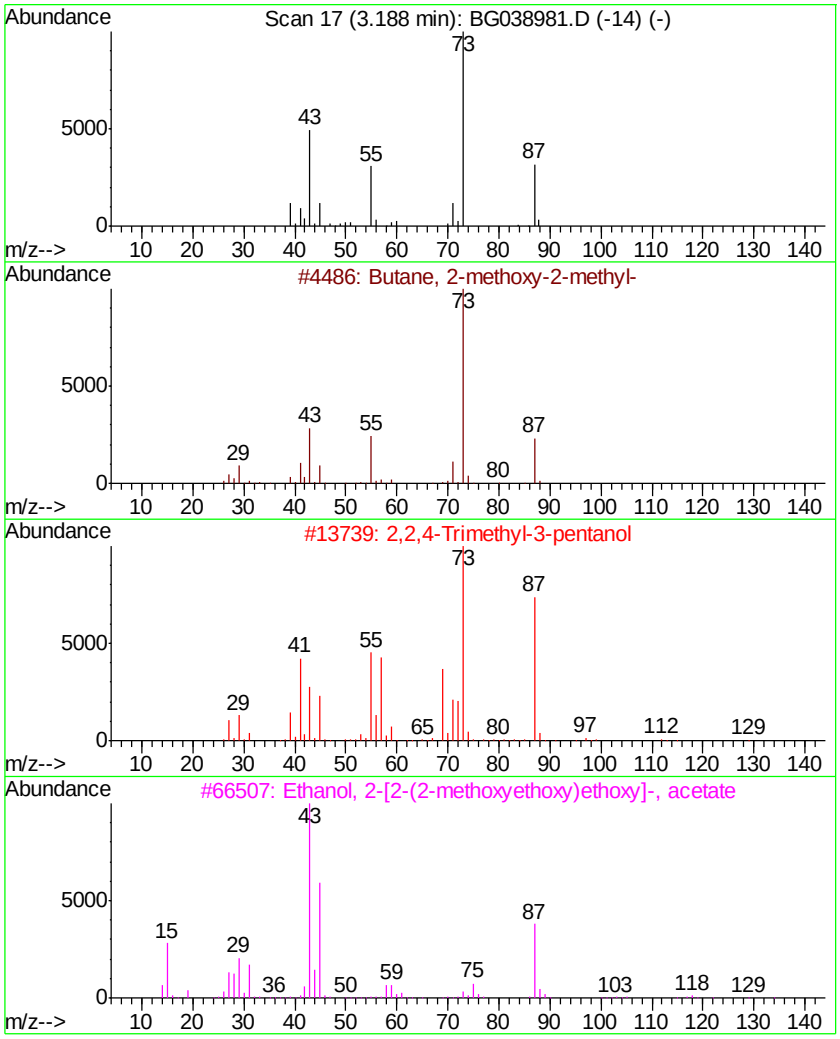
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

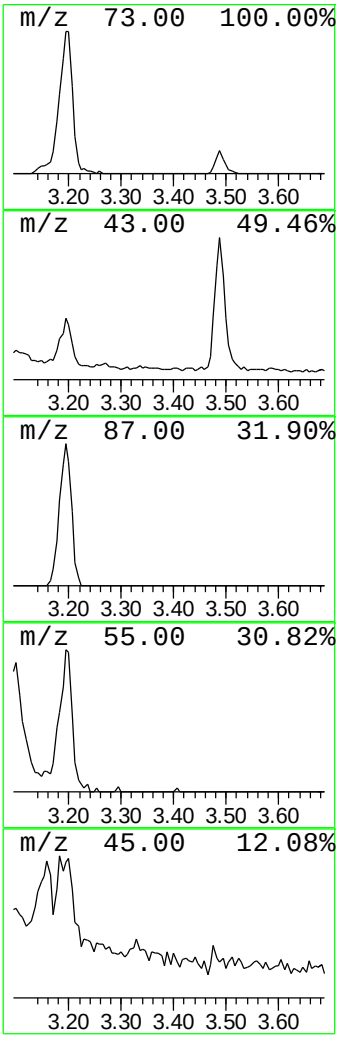
****

Peak Number 1 unknown3.19 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	10.09 ng	85640	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	9
4	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

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Data File : BG038981.D
Acq On : 8 Jan 2019 00:25
Operator : JU/SJ
Sample : K1010-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OK-03-010419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

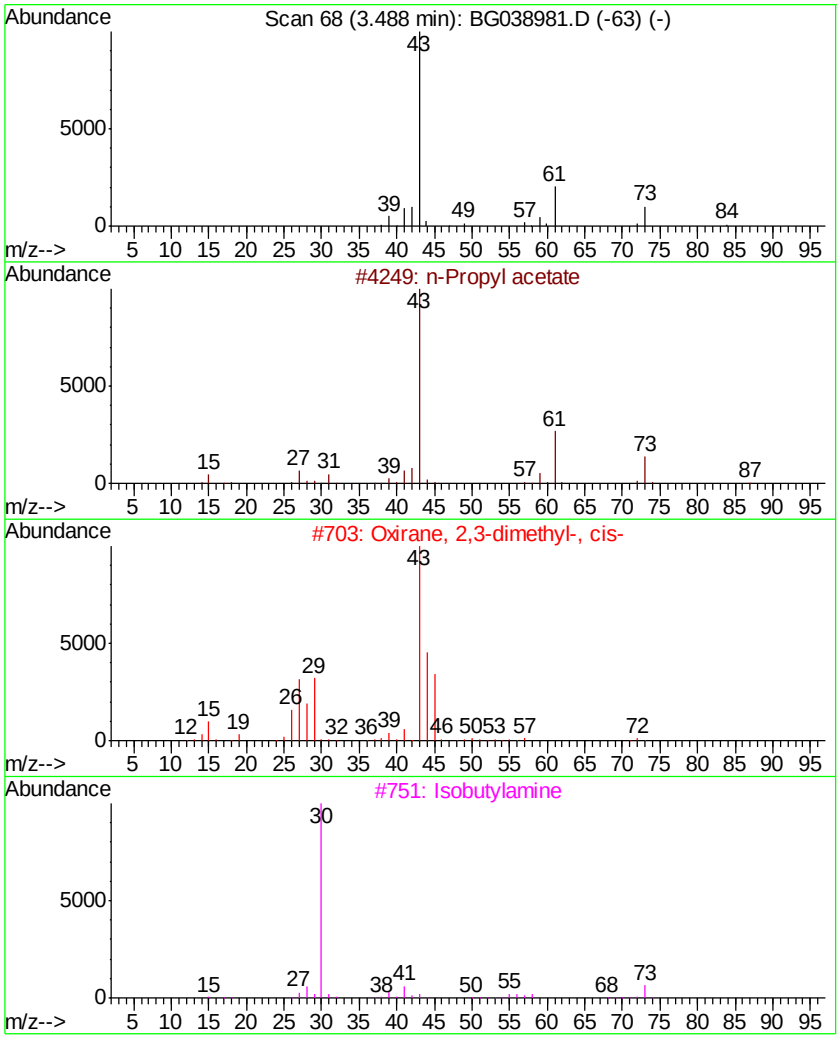
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

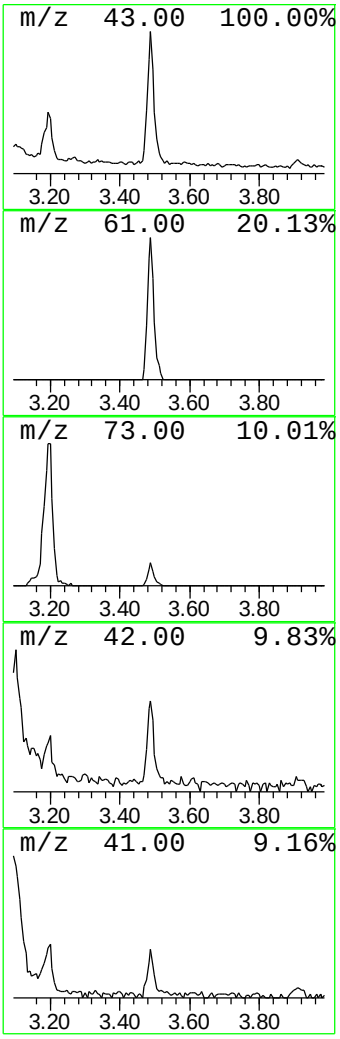
****

Peak Number 2 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.49	6.57 ng	55741	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	72
2	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	1-Butanamine	73	C4H11N	000109-73-9	4
5	Pentane	72	C5H12	000109-66-0	4





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010719\
Data File : BG038981.D
Acq On : 8 Jan 2019 00:25
Operator : JU/SJ
Sample : K1010-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OK-03-010419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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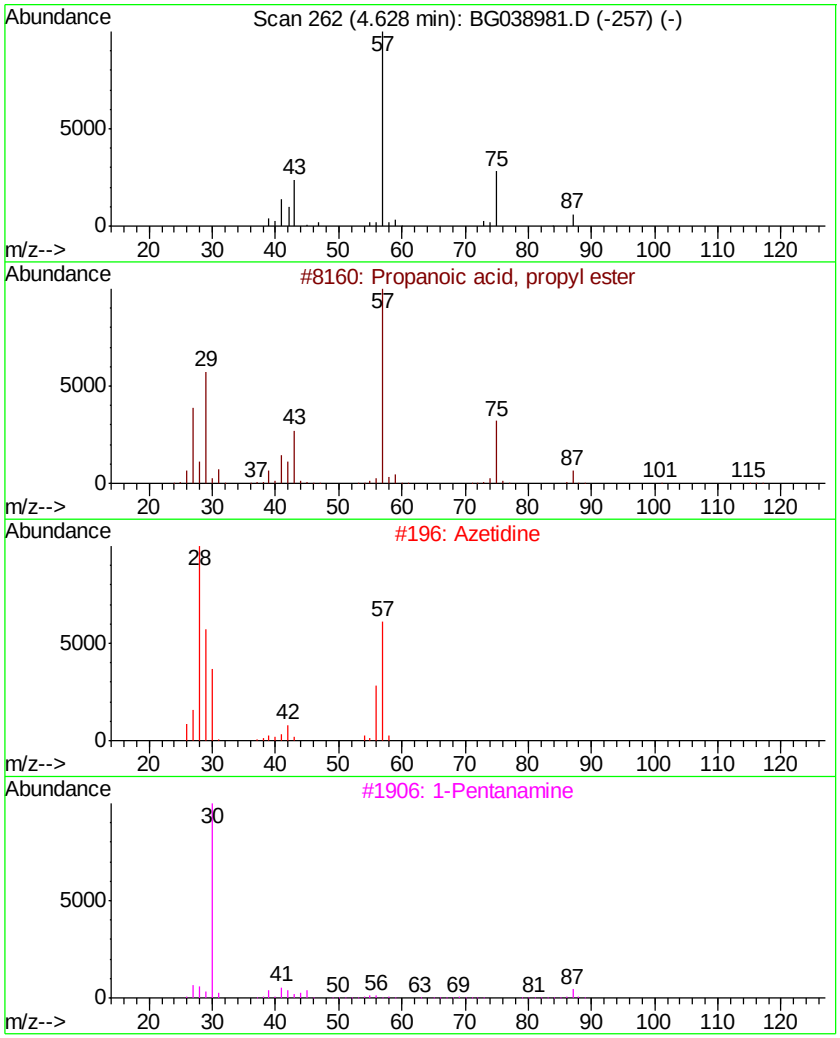
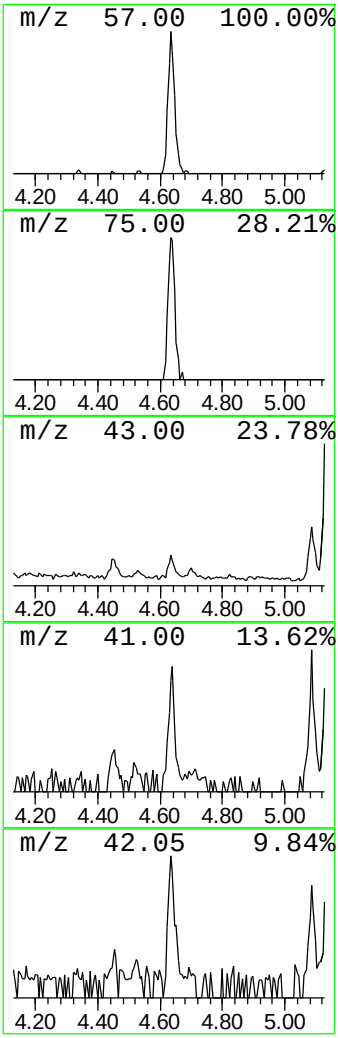
****

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	3.96 ng	33565	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
2	Azetidine	57	C3H7N	000503-29-7	9
3	1-Pentanamine	87	C5H13N	000110-58-7	9
4	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9
5	Formic acid, 2-propenyl ester	86	C4H6O2	001838-59-1	5





Library Search Compound Report

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Data File : BG038981.D
Acq On : 8 Jan 2019 00:25
Operator : JU/SJ
Sample : K1010-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OK-03-010419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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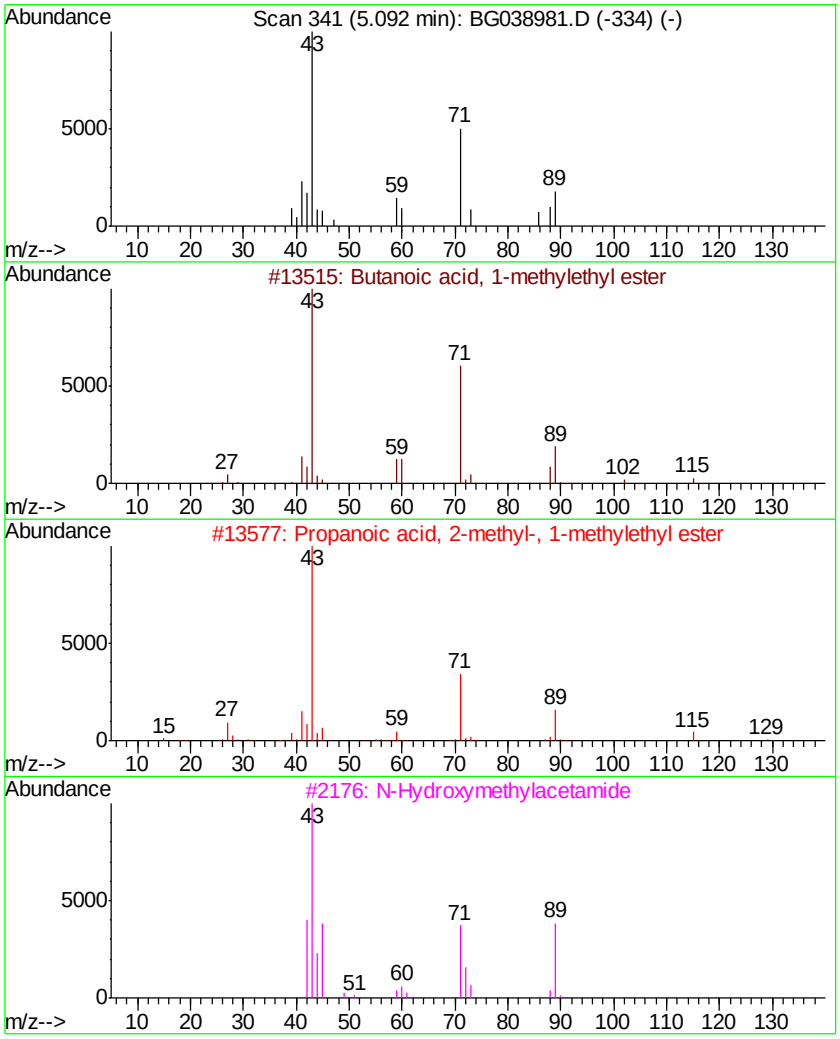
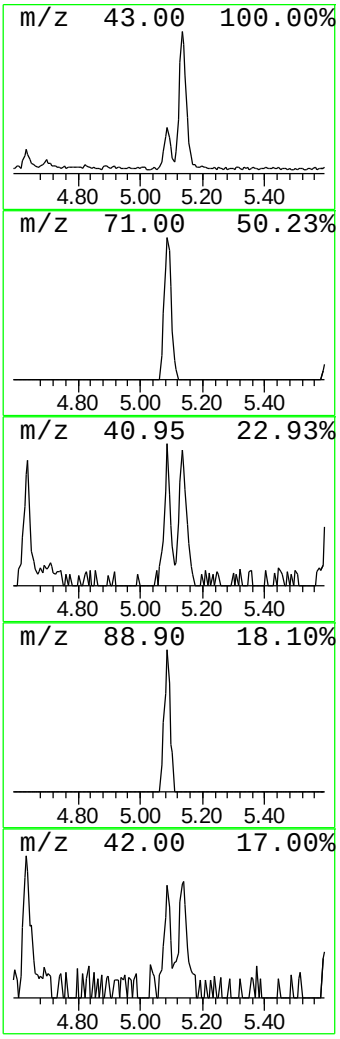
****

Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	3.00 ng	25442	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	36
4	Propyl nitrite	89	C3H7NO2	000543-67-9	12
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010719\
Data File : BG038981.D
Acq On : 8 Jan 2019 00:25
Operator : JU/SJ
Sample : K1010-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : OK-03-010419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

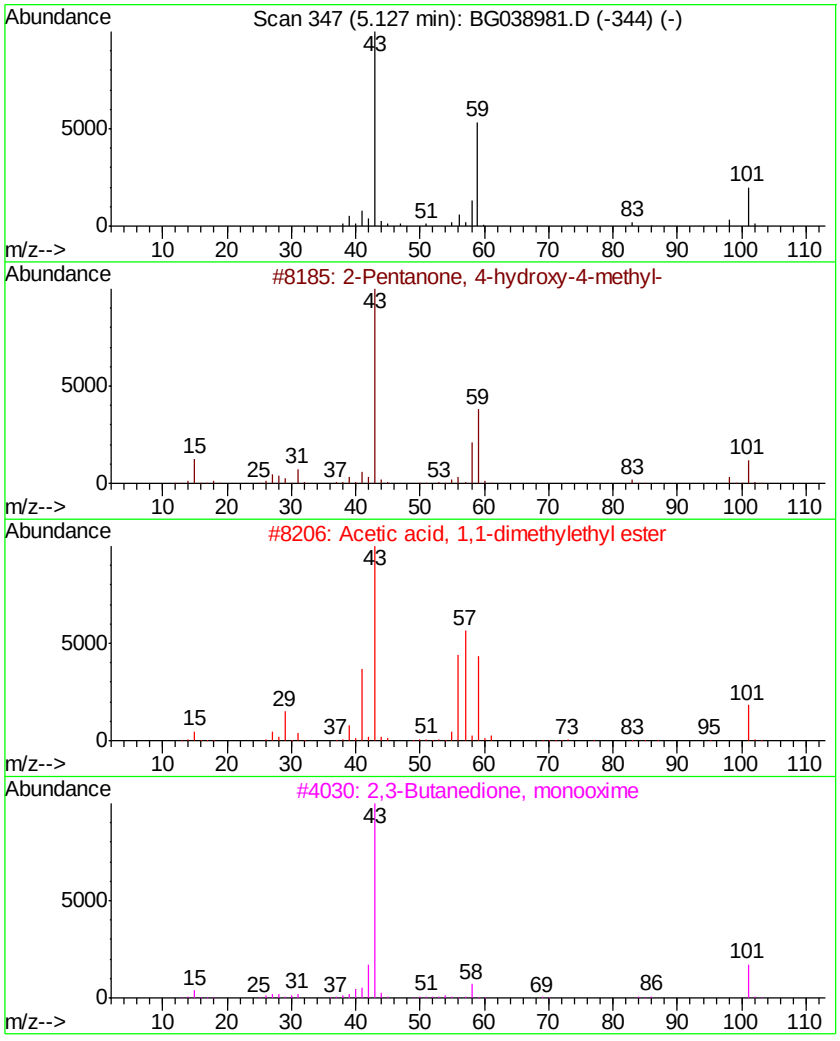
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

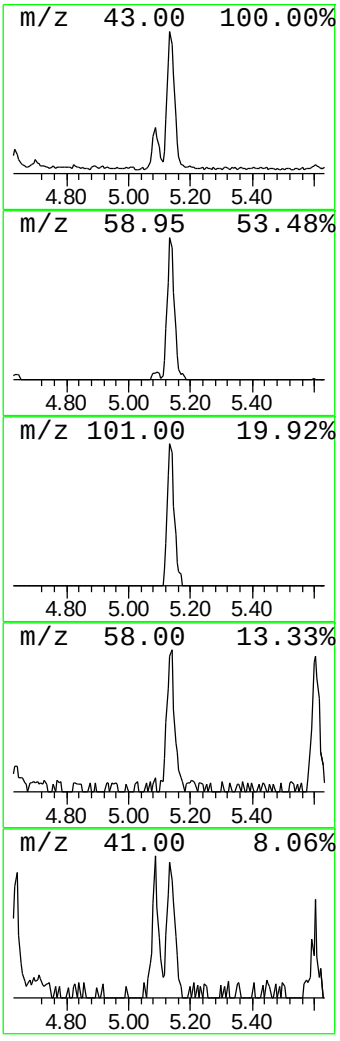
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	8.93 ng	75743	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9





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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

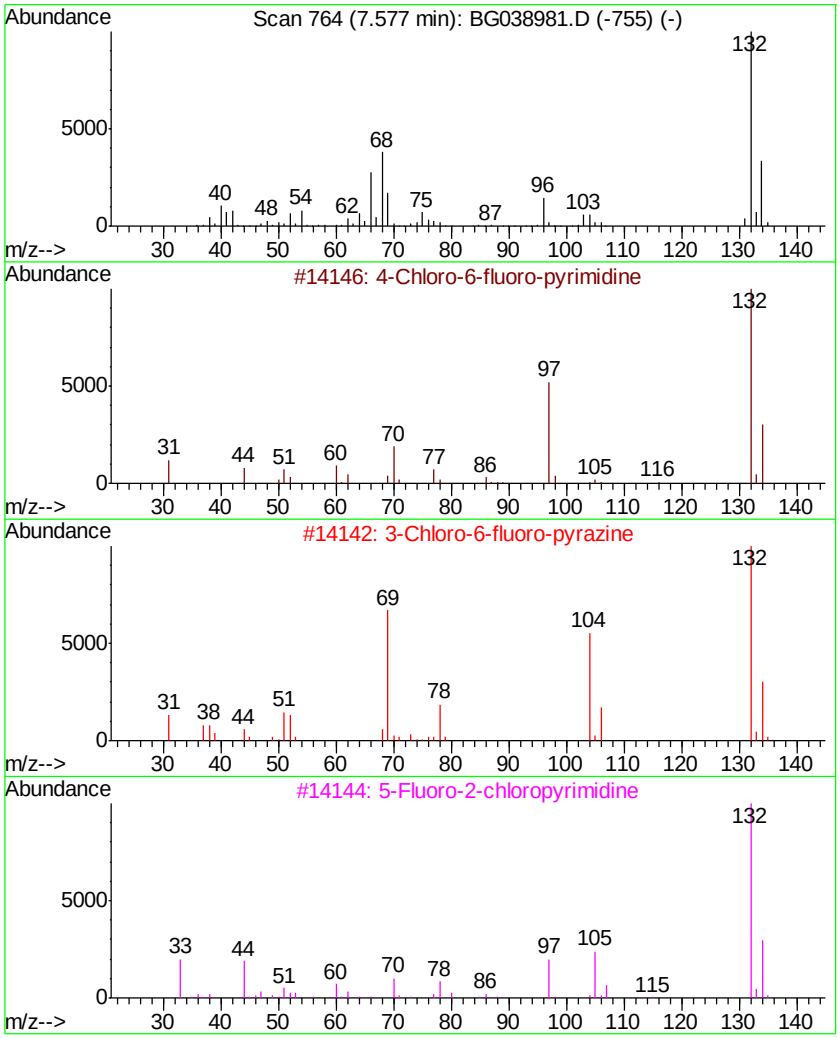
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

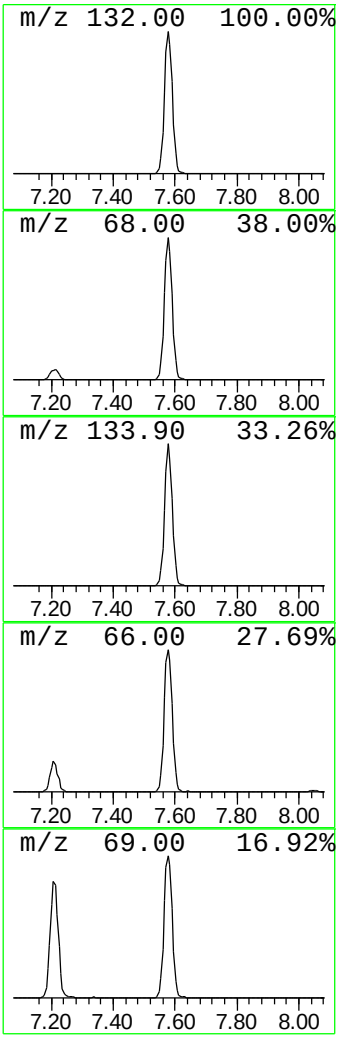
****

Peak Number 6 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	87.55 ng	742820	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	16
5	5-Aminoindole	132	C8H8N2	005192-03-0	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG010719\
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.19	3.19	10.1	ng	85640	1	8.05	169697	20.0
n-Propyl acetate	3.49	6.6	ng	55741	1	8.05	169697	20.0
Propanoic acid, p...	4.63	4.0	ng	33565	1	8.05	169697	20.0
Butanoic acid, 1-...	5.09	3.0	ng	25442	1	8.05	169697	20.0
2-Pentanone, 4-hy...	5.13	8.9	ng	75743	1	8.05	169697	20.0
unknown7.58	7.58	87.5	ng	742820	1	8.05	169697	20.0