LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061019\
Data File : BG041167.D
Acq On : 10 Jun 2019 17:38
Operator : HP/JU
Sample : K3214-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5A

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-BG052919.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	3.184	12	16	27	rVB	185516	295859	5.77%	1.483%
2	5.193	348	358	374	rBV	2764384	5125130	100.00%	25.690%
3	5.834	460	467	475	rBV	35047	62813	1.23%	0.315%
4	7.567	755	762	769	rBV	46261	85753	1.67%	0.430%
5	8.108	847	854	865	rVB	176800	305838	5.97%	1.533%
6	8.431	901	909	916	rBV	713412	1224005	23.88%	6.135%
7	9.283	1044	1054	1063	rBV	631168	1165139	22.73%	5.840%
8	10.928	1327	1334	1341	rBV	236125	437480	8.54%	2.193%
9	12.790	1639	1651	1657	rVB4	29702	59805	1.17%	0.300%
10	13.360	1741	1748	1758	rBV	1879909	2842212	55.46%	14.247%
11	14.735	1973	1982	1989	rBV2	406919	672597	13.12%	3.371%
12	17.485	2440	2450	2457	rBV	516141	826958	16.14%	4.145%
13	20.076	2885	2891	2903	rBV	3279003	4312236	84.14%	21.615%
14	21.756	3170	3177	3184	rBV2	502678	919473	17.94%	4.609%
15	24.289	3601	3608	3616	rBV6	39775	103349	2.02%	0.518%
16	25.088	3735	3744	3758	rVB	230187	714204	13.94%	3.580%
17	25.558	3818	3824	3833	rVB5	56198	164019	3.20%	0.822%
18	27.144	4081	4094	4107	rBV6	67634	292546	5.71%	1.466%
19	29.130	4419	4432	4433	rBV5	81048	210209	4.10%	1.054%
20	31.651	4850	4861	4862	rBV4	50991	130430	2.54%	0.654%

Sum of corrected areas: 19950055

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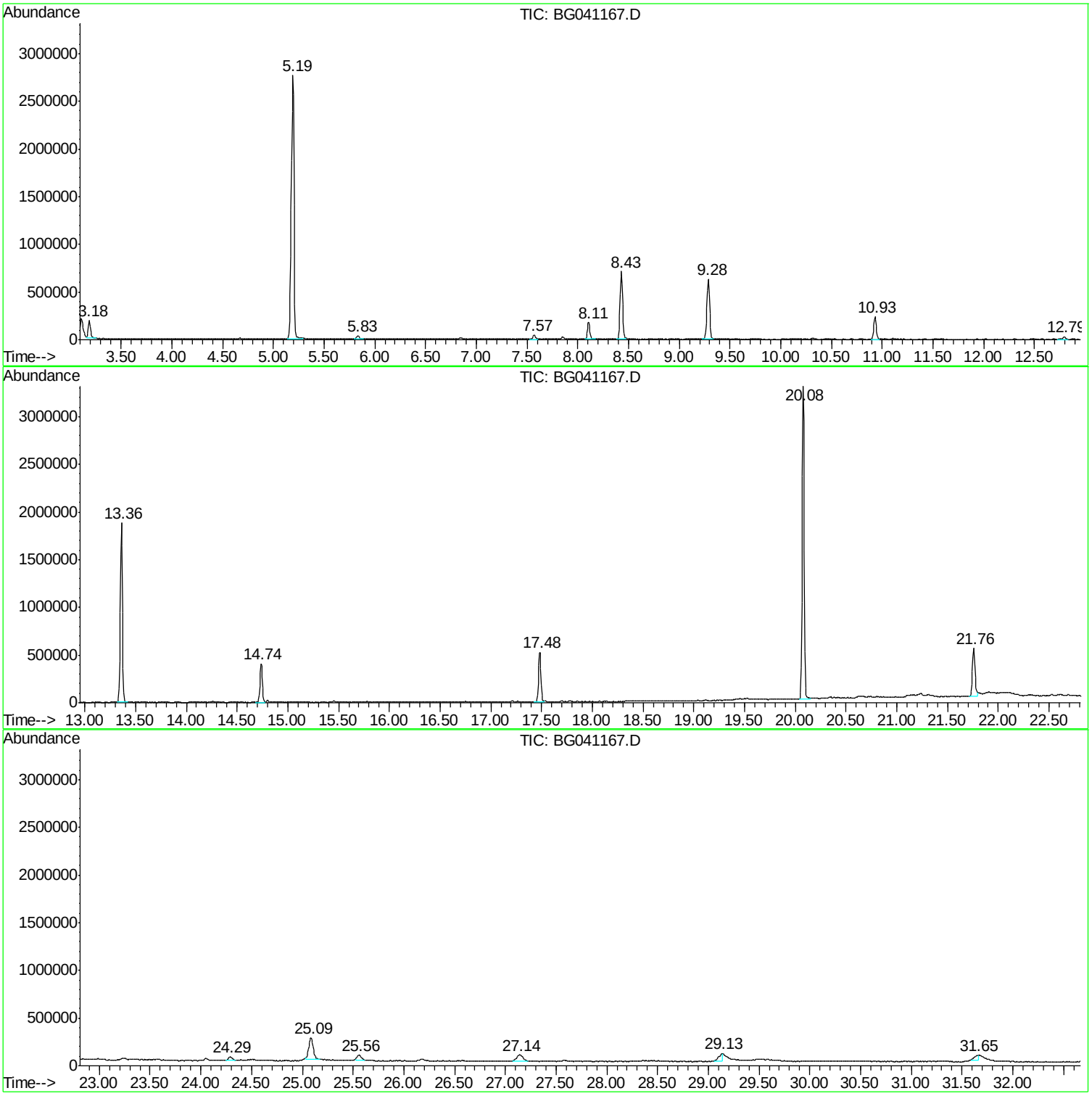
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061019\
Data File : BG041167.D
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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

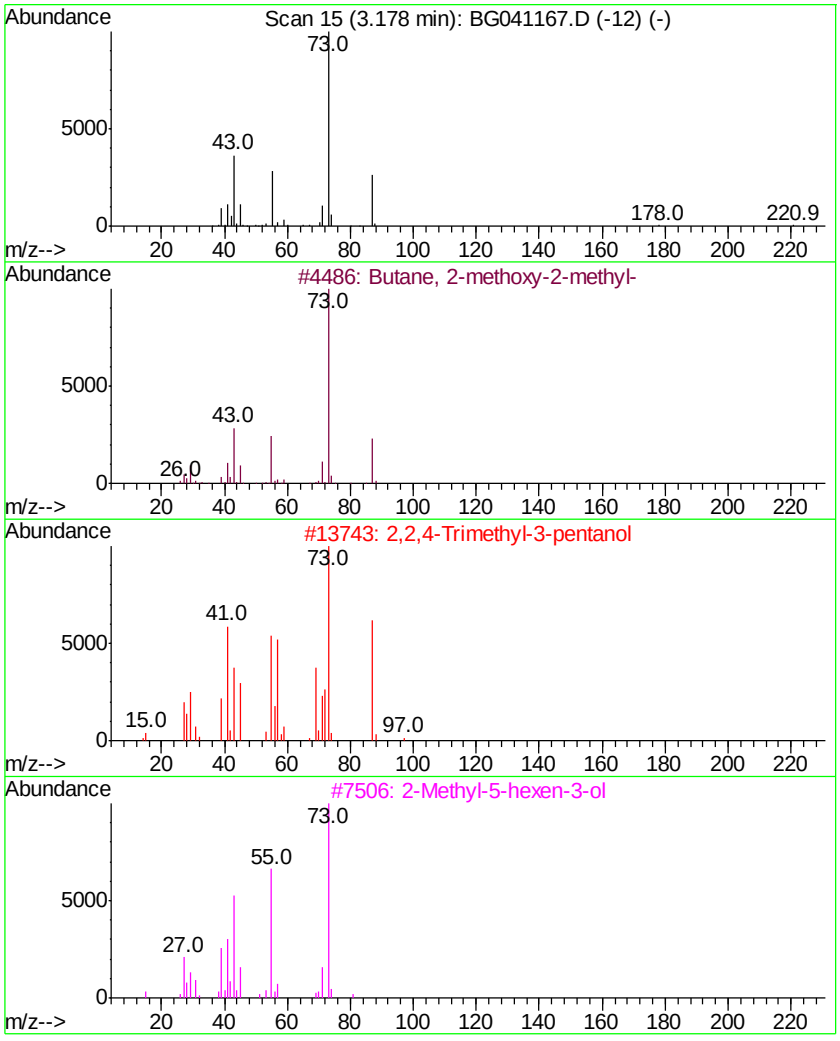
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

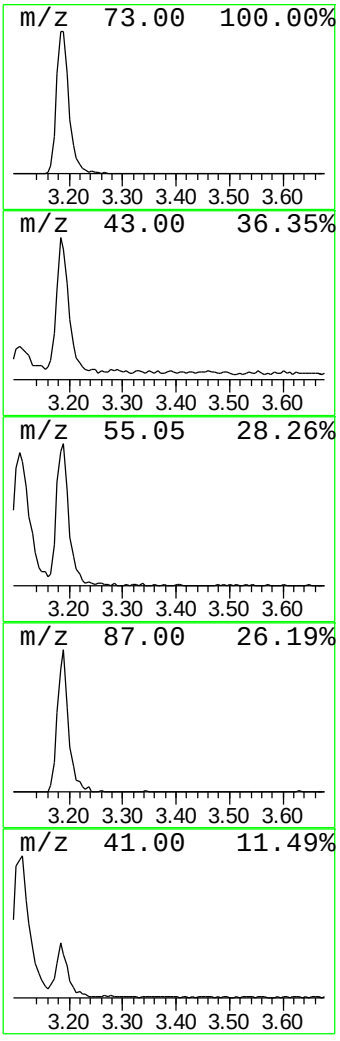
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	19.35 ng	295859	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BG041167.D
Acq On : 10 Jun 2019 17:38
Operator : HP/JU
Sample : K3214-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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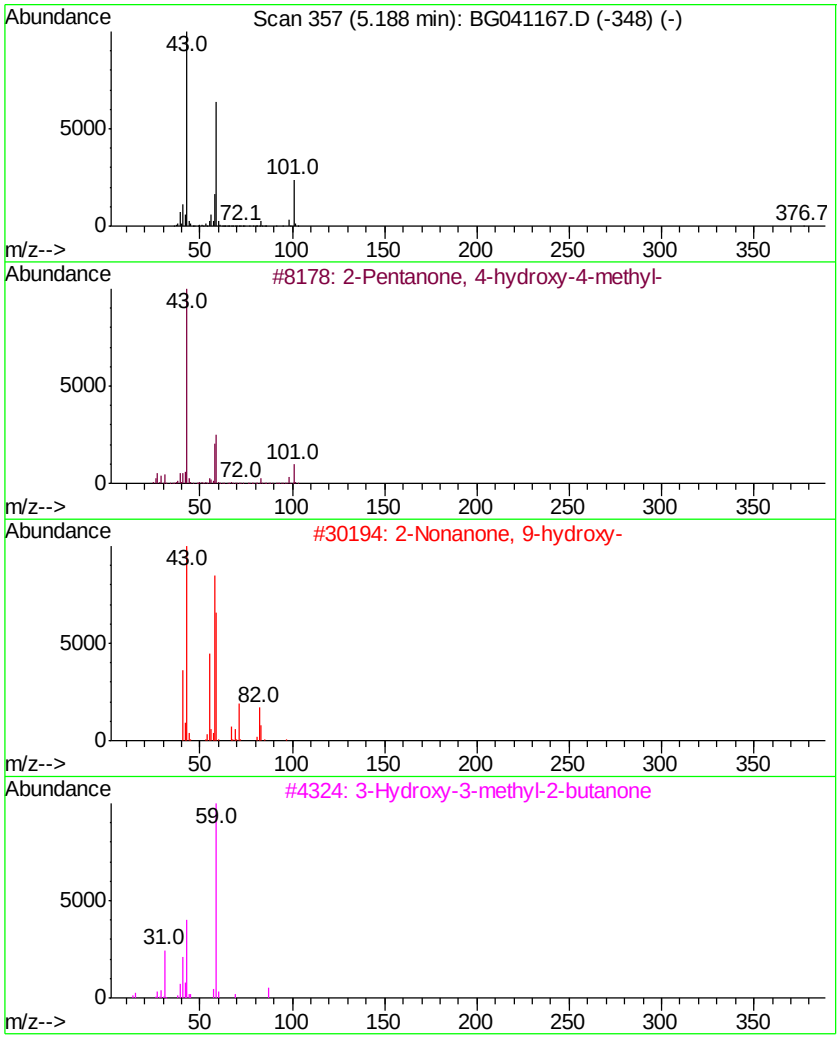
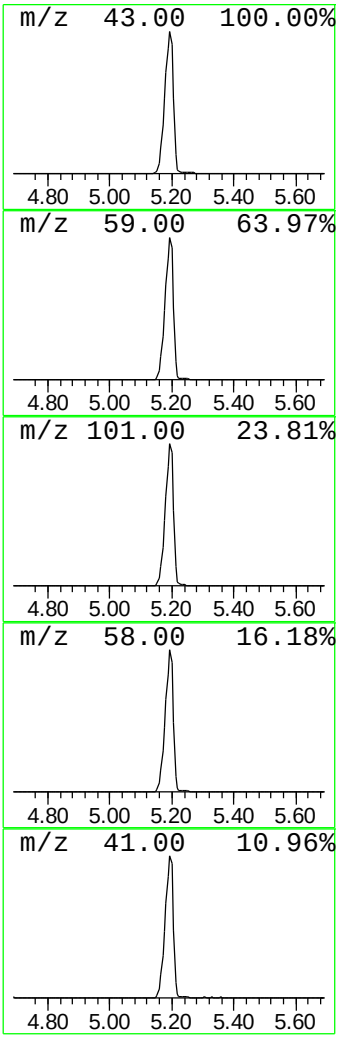
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	335.15 ng	5125130	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061019\
Data File : BG041167.D
Acq On : 10 Jun 2019 17:38
Operator : HP/JU
Sample : K3214-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

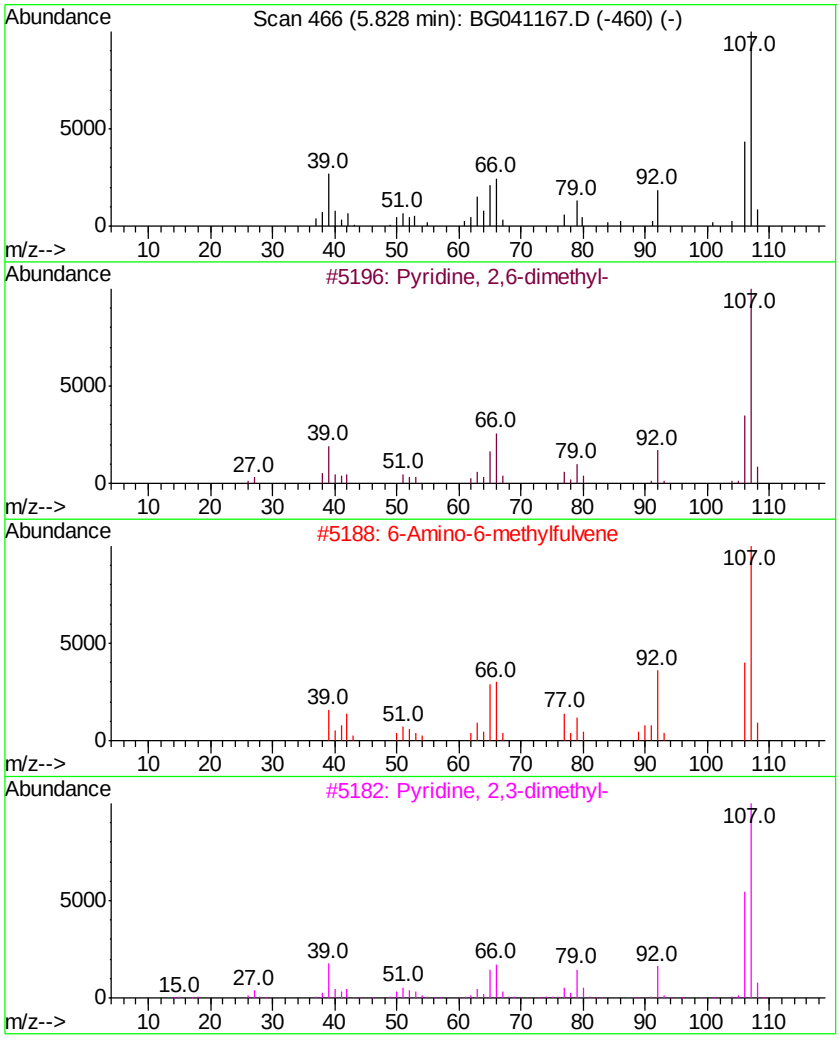
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

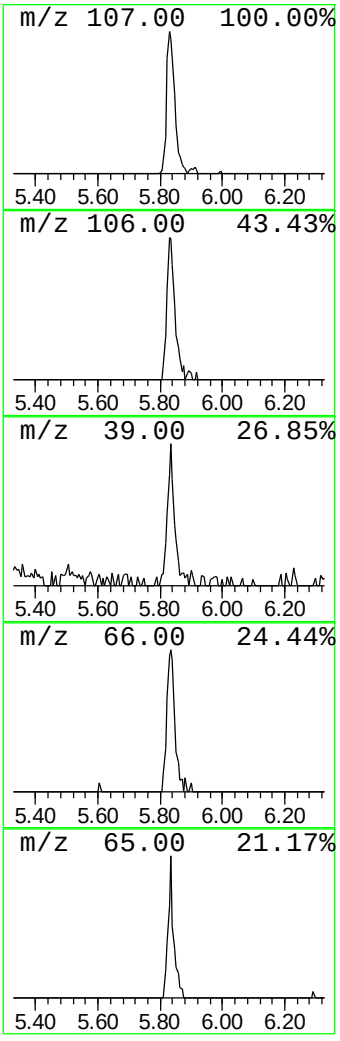
****

Peak Number 3 Pyridine, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.83	4.11 ng	62813	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2,6-dimethyl-	107	C7H9N	000108-48-5	97
2	6-Amino-6-methylfulvene	107	C7H9N	000694-74-6	94
3	Pyridine, 2,3-dimethyl-	107	C7H9N	000583-61-9	90
4	Pyridine, 2,4-dimethyl-	107	C7H9N	000108-47-4	53
5	Pyridine, 3-ethyl-	107	C7H9N	000536-78-7	50





Library Search Compound Report

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Operator : HP/JU
Sample : K3214-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

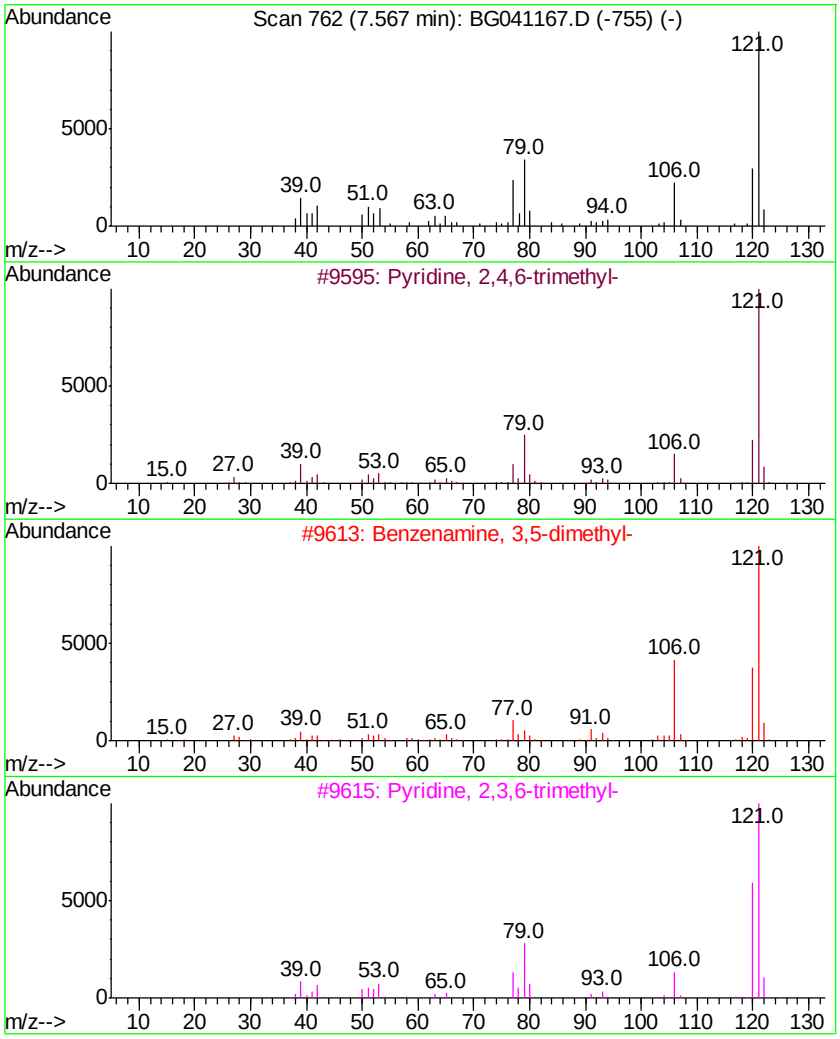
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

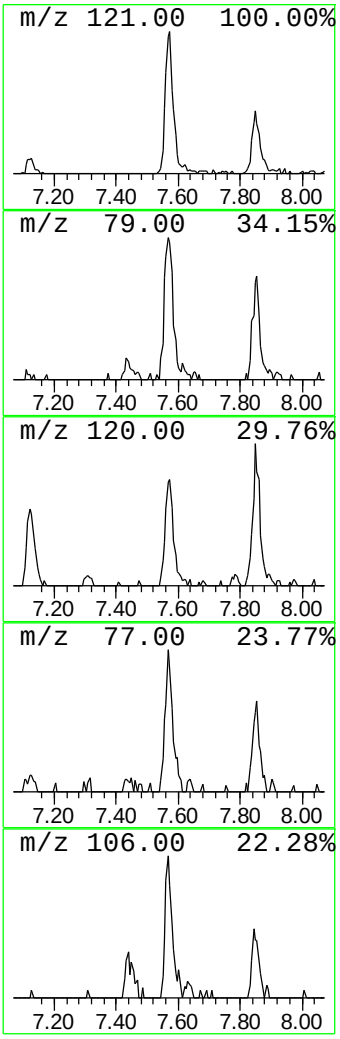
****

Peak Number 4 Pyridine, 2,4,6-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	5.61 ng	85753	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2,4,6-trimethyl-	121	C8H11N	000108-75-8	94
2	Benzenamine, 3,5-dimethyl-	121	C8H11N	000108-69-0	68
3	Pyridine, 2,3,6-trimethyl-	121	C8H11N	001462-84-6	64
4	Benzenamine, 2,4-dimethyl-	121	C8H11N	000095-68-1	52
5	2,6-Xylidine	121	C8H11N	000087-62-7	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061019\
Data File : BG041167.D
Acq On : 10 Jun 2019 17:38
Operator : HP/JU
Sample : K3214-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

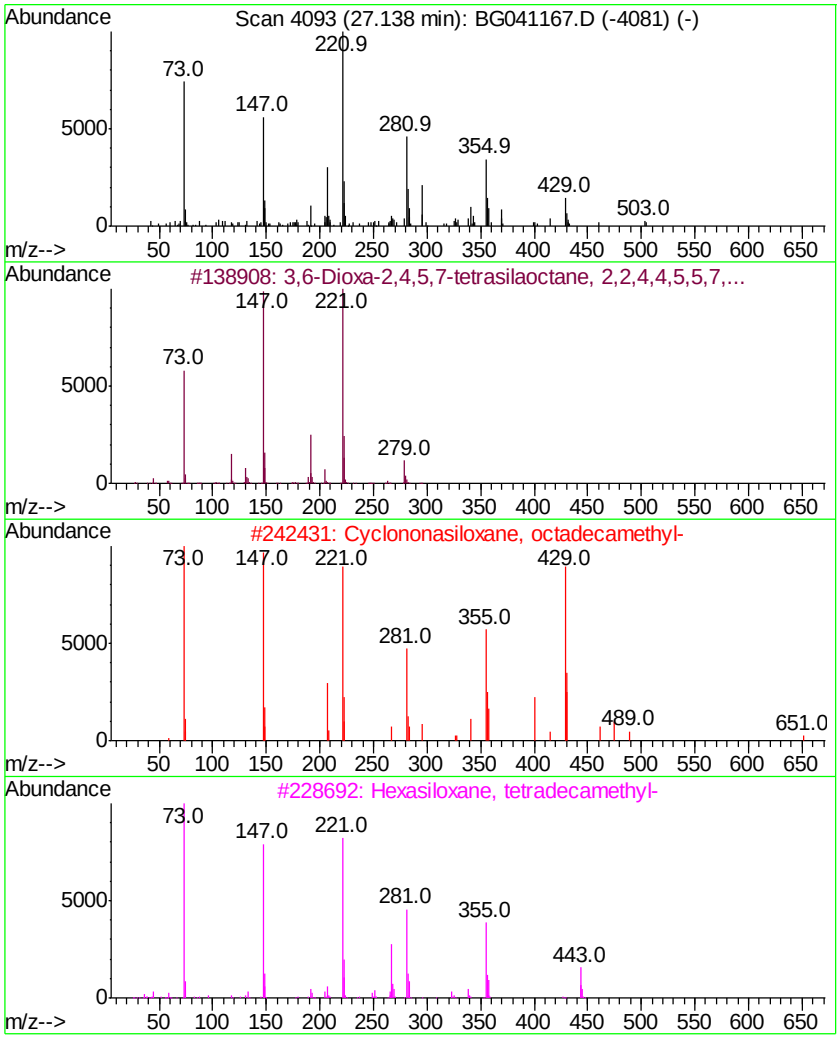
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

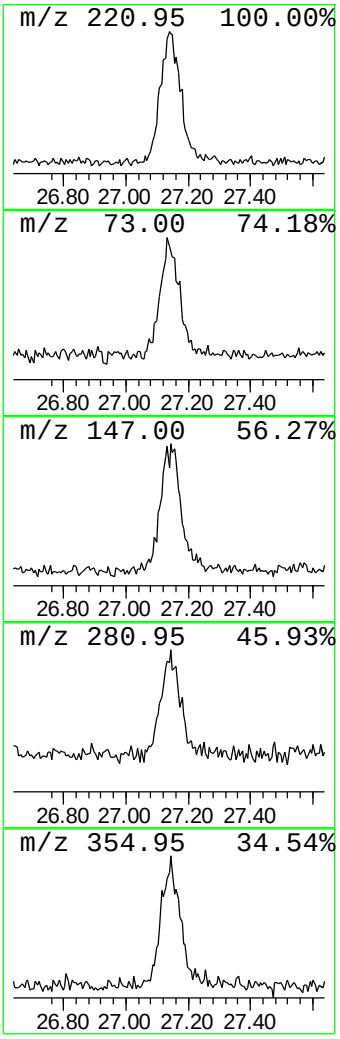
****

Peak Number 9 unknown27.14 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.14	8.19 ng	292546	Perylene-d12	25.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	28
3	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	25
4	9H-Purin-6-amine, N-methyl-9-(tr...	221	C9H15N5Si	032865-83-1	25
5	2-tert-Butyl-6-methylphenol, O-t...	278	C17H30OSi	1000374-86-0	22





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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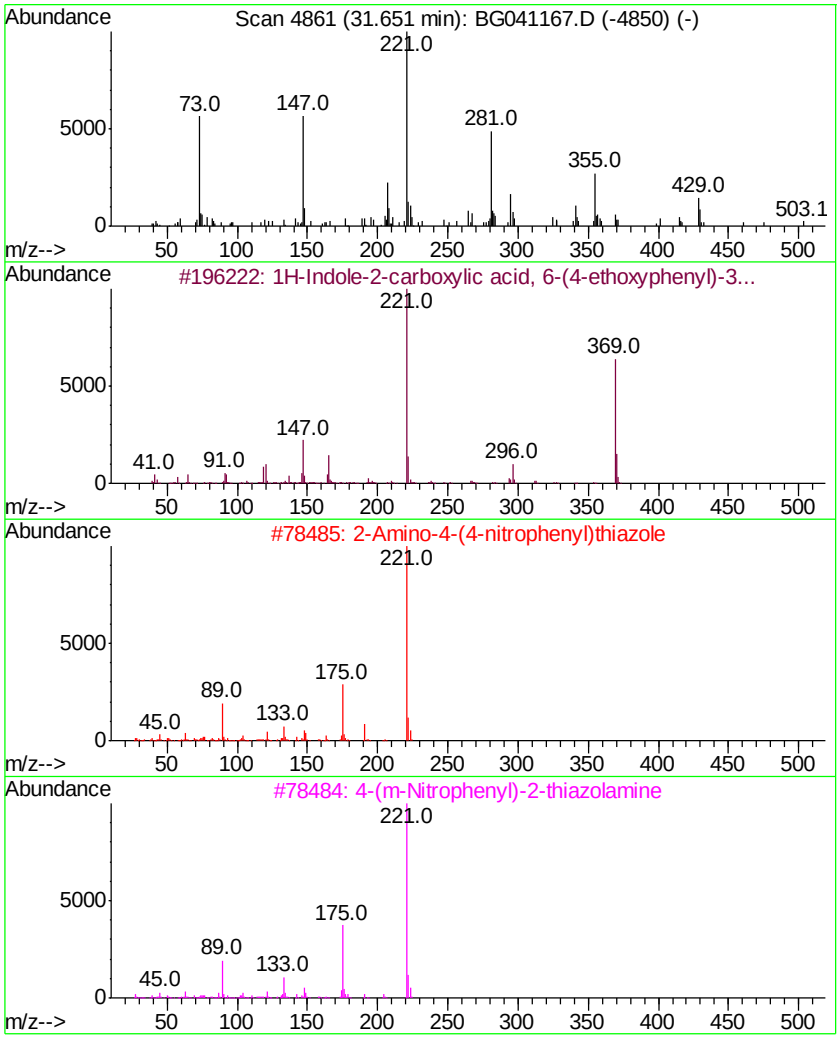
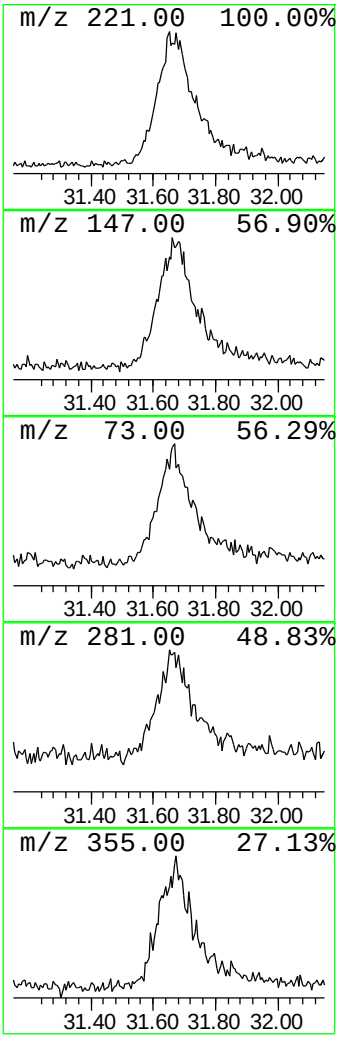
****

Peak Number 11 unknown31.65 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.65	3.65 ng	130430	Perylene-d12	25.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole-2-carboxylic acid, 6-(...	369	C22H27NO4	1000316-17-3	35
2	2-Amino-4-(4-nitrophenyl)thiazole	221	C9H7N3O2S	002104-09-8	22
3	4-(m-Nitrophenyl)-2-thiazolamine	221	C9H7N3O2S	057493-24-0	22
4	Pyrimidine-2,4,6(1H,3H,5H)-trion...	356	C13H13BrN2O3S	346612-47-3	22
5	4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	16





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methoxy...	3.18	19.4	ng	295859	1	8.11	305838	20.0
2-Pentanone, 4-hy...	5.19	335.1	ng	5125130	1	8.11	305838	20.0
Pyridine, 2,6-dim...	5.83	4.1	ng	62813	1	8.11	305838	20.0
Pyridine, 2,4,6-t...	7.57	5.6	ng	85753	1	8.11	305838	20.0
unknown27.14	27.14	8.2	ng	292546	6	25.09	714204	20.0
unknown31.65	31.65	3.6	ng	130430	6	25.09	714204	20.0