LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032818\
Data File : BG033396.D
Acq On : 28 Mar 2018 21:29
Operator : SJ/JU
Sample : J2098-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

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-BG031918.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	3.482	26	33	44	rBV	137122	301077	9.09%	1.793%
2	3.576	44	49	60	rVB	85973	148419	4.48%	0.884%
3	5.779	418	424	433	rVB2	43745	75995	2.30%	0.452%
4	6.302	506	513	534	rBV	266711	555174	16.77%	3.305%
5	7.988	792	800	814	rBV	173235	415334	12.55%	2.473%
6	8.382	859	867	886	rBV	566859	1158025	34.98%	6.895%
7	8.864	941	949	959	rBV	139459	285334	8.62%	1.699%
8	9.199	999	1006	1017	rBV	526555	1021198	30.85%	6.080%
9	9.551	1061	1066	1073	rVB3	43350	78619	2.37%	0.468%
10	10.068	1144	1154	1162	rBV	414440	882550	26.66%	5.254%
11	10.139	1162	1166	1173	rVB2	29704	62532	1.89%	0.372%
12	11.137	1328	1336	1346	rBV2	81224	154064	4.65%	0.917%
13	11.748	1429	1440	1451	rBV	221429	447223	13.51%	2.663%
14	14.110	1833	1842	1851	rBV	1475057	2397991	72.43%	14.277%
15	14.904	1972	1977	1983	rBV2	27696	45628	1.38%	0.272%
16	15.485	2070	2076	2083	rBV2	384975	651189	19.67%	3.877%
17	16.249	2203	2206	2210	rVB	31893	37968	1.15%	0.226%
18	16.960	2320	2327	2338	rBV	1056636	1674588	50.58%	9.970%
19	17.101	2347	2351	2355	rBV4	25101	39263	1.19%	0.234%
20	18.211	2534	2540	2547	rBV2	454120	777269	23.48%	4.628%
21	19.016	2672	2677	2681	rBV4	52675	88524	2.67%	0.527%
22	20.250	2883	2887	2893	rBV9	22092	38996	1.18%	0.232%
23	20.432	2914	2918	2923	rBV3	54605	97012	2.93%	0.578%
24	20.544	2933	2937	2941	rBV	72756	103458	3.12%	0.616%
25	20.732	2963	2969	2980	rBV	2377334	3310670	100.00%	19.711%
26	21.419	3083	3086	3092	rVB4	73366	95215	2.88%	0.567%
27	22.559	3273	3280	3290	rBV2	475941	924287	27.92%	5.503%
28	26.331	3913	3922	3937	rVB3	277922	928479	28.05%	5.528%

Sum of corrected areas: 16796081

LSC Report - Integrated Chromatogram

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Data File : BG033396.D
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Misc :
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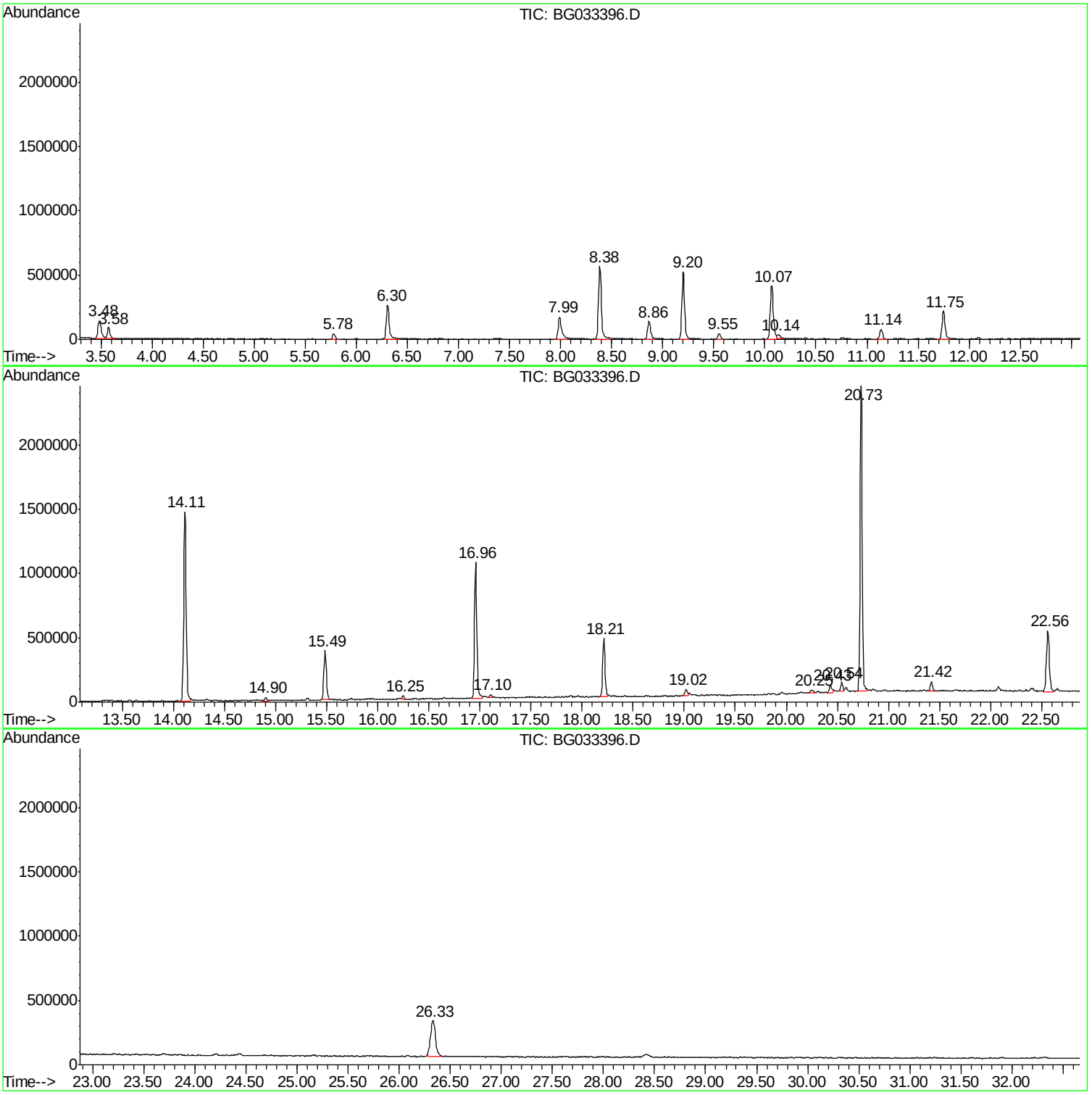
Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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Sample : J2098-01
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ClientSampleId : MW-5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

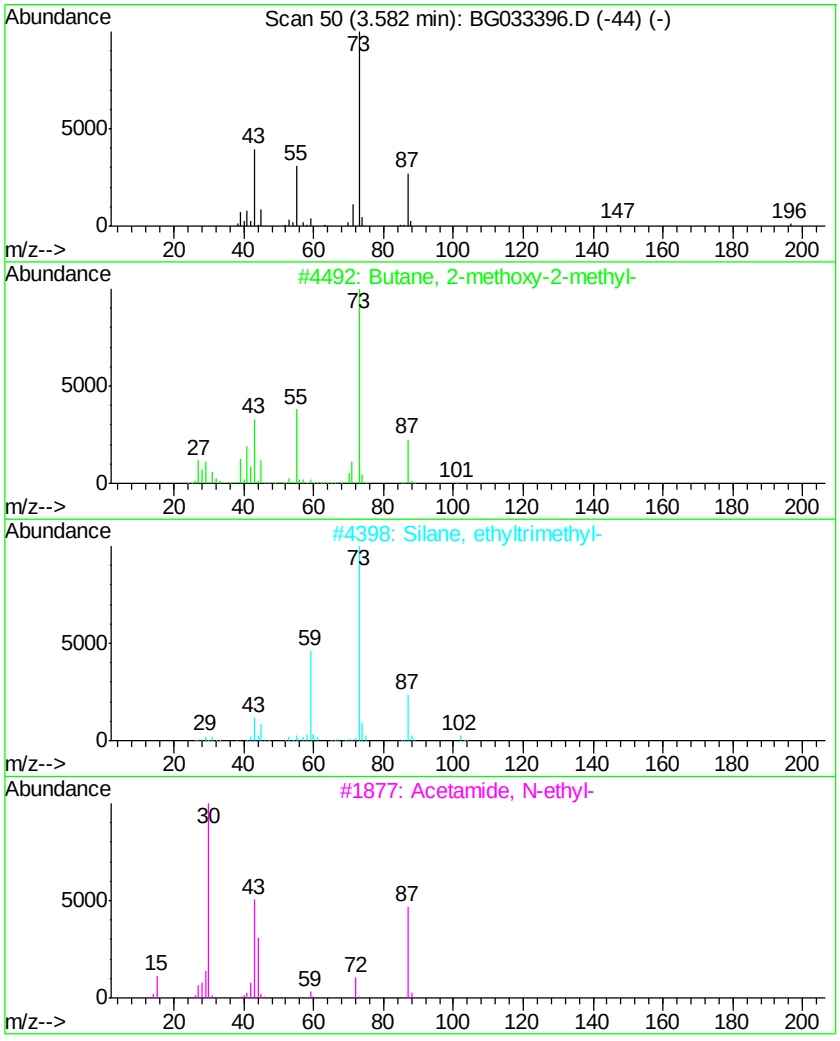
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

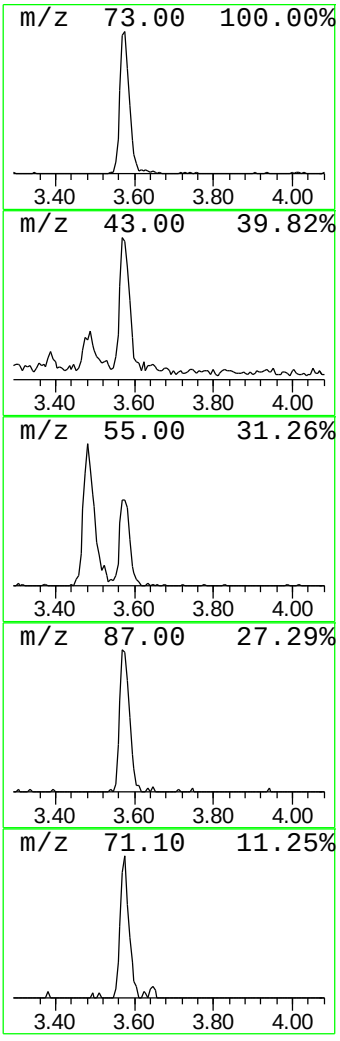
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.58	10.40 ng	148419	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9





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Sample : J2098-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

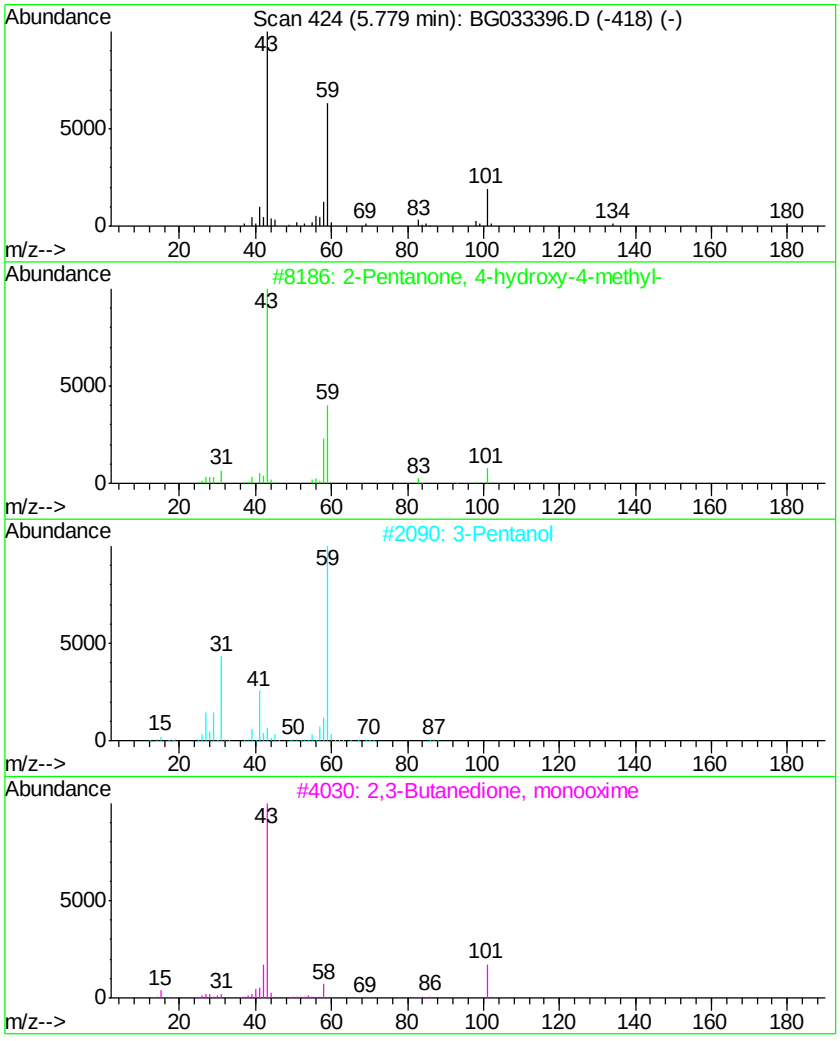
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

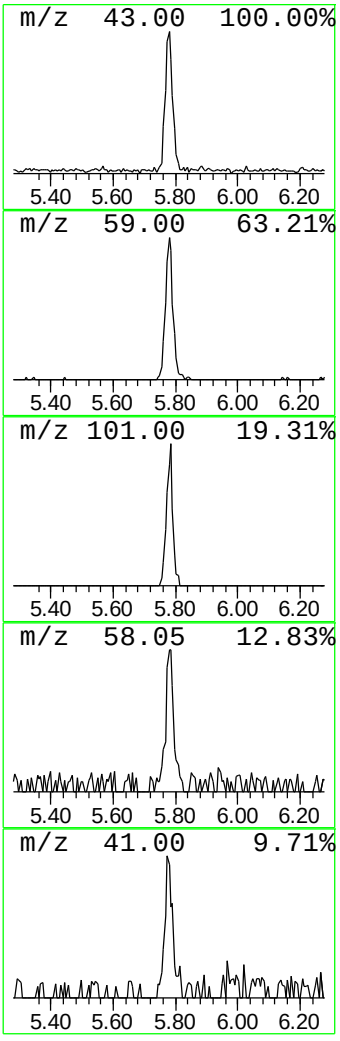
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	5.33 ng	75995	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	3-Pentanol	88	C5H12O	000584-02-1	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
4	3-Hexanol	102	C6H14O	000623-37-0	32
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25





Data Path : Z:\HPCHEM1\BNA G\DATA\BG032818\
Data File : BG033396.D
Acq On : 28 Mar 2018 21:29
Operator : SJ/JU
Sample : J2098-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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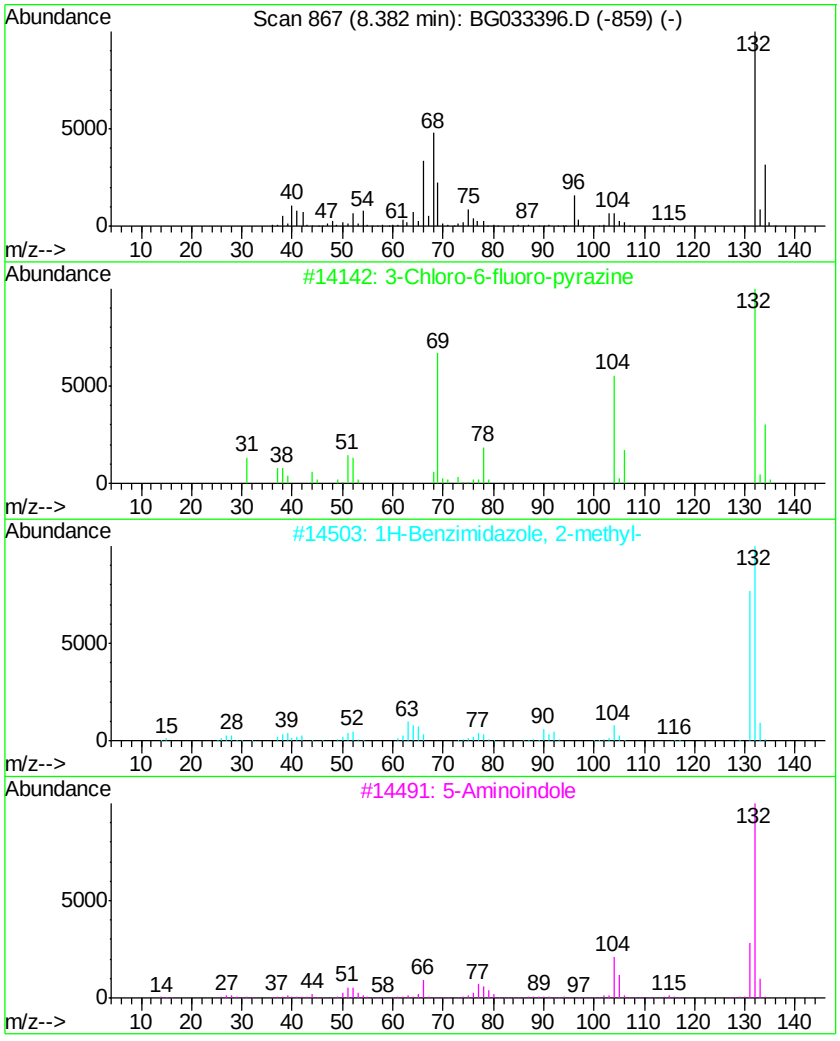
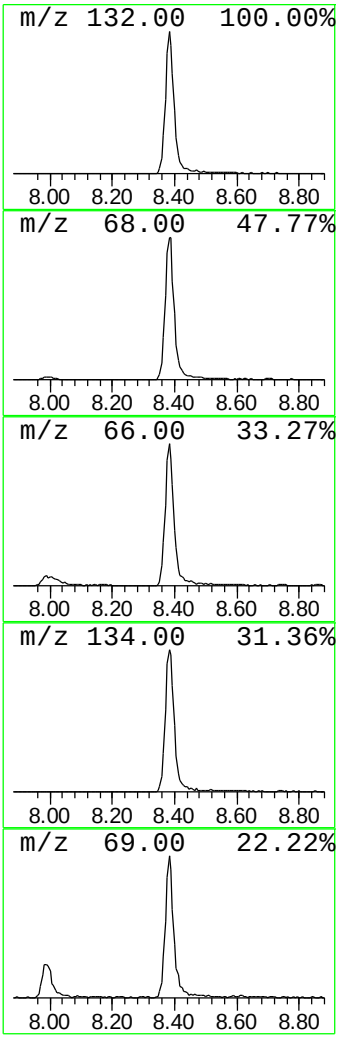
Peak Number 4 unknown8.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	81.17 ng	1158030	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





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Acq On : 28 Mar 2018 21:29
Operator : SJ/JU
Sample : J2098-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

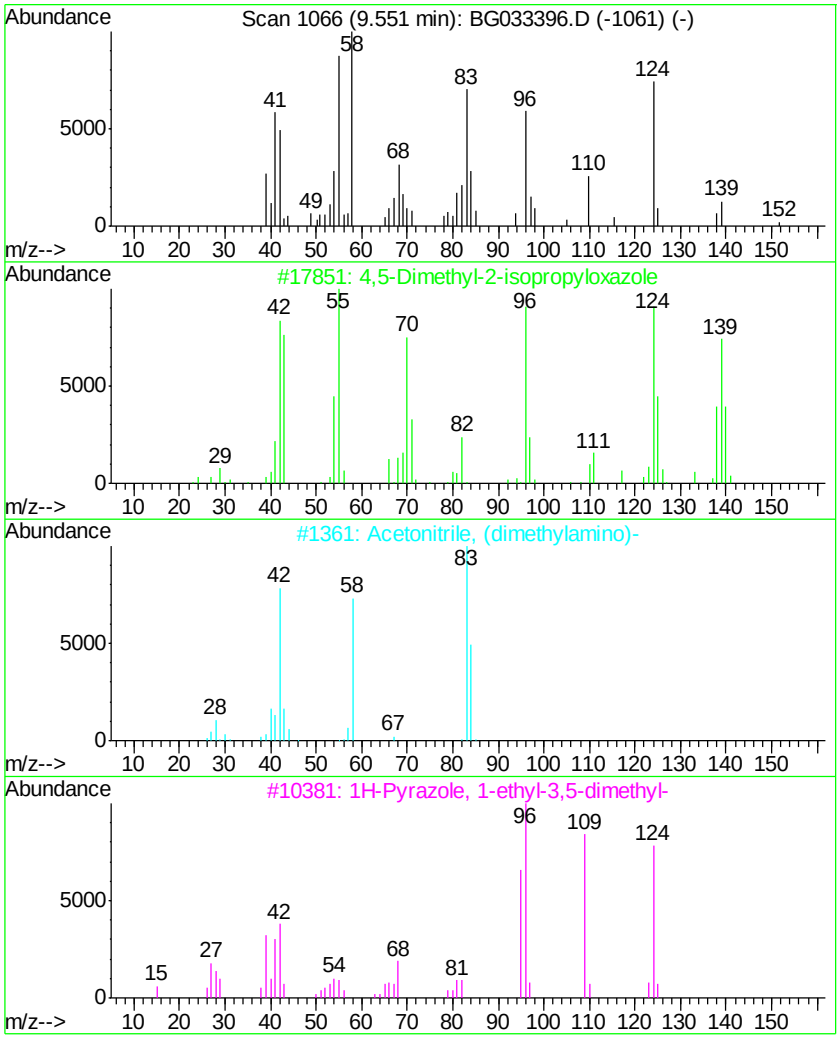
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

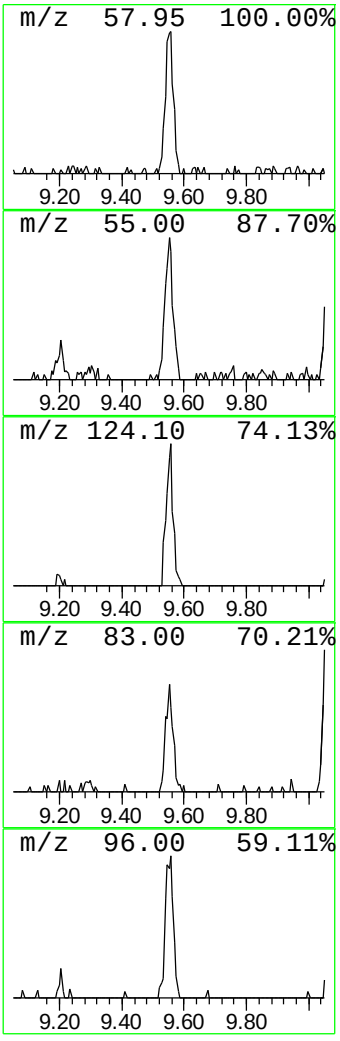
****

Peak Number 6 unknown9.55 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	5.51 ng	78619	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5-Dimethyl-2-isopropyloxazole	139	C8H13NO	019519-45-0	38
2	Acetonitrile, (dimethylamino)-	84	C4H8N2	000926-64-7	38
3	1H-Pyrazole, 1-ethyl-3,5-dimethyl-	124	C7H12N2	017629-26-4	35
4	Piperidine, 1-(2-methyl-1-propen...	139	C9H17N	000673-33-6	30
5	Propyl-2-iden-5-amino-1,2,4-tria...	124	C5H8N4	1000139-49-3	27





Data Path : Z:\HPCHEM1\BNA G\DATA\BG032818\
Data File : BG033396.D
Acq On : 28 Mar 2018 21:29
Operator : SJ/JU
Sample : J2098-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

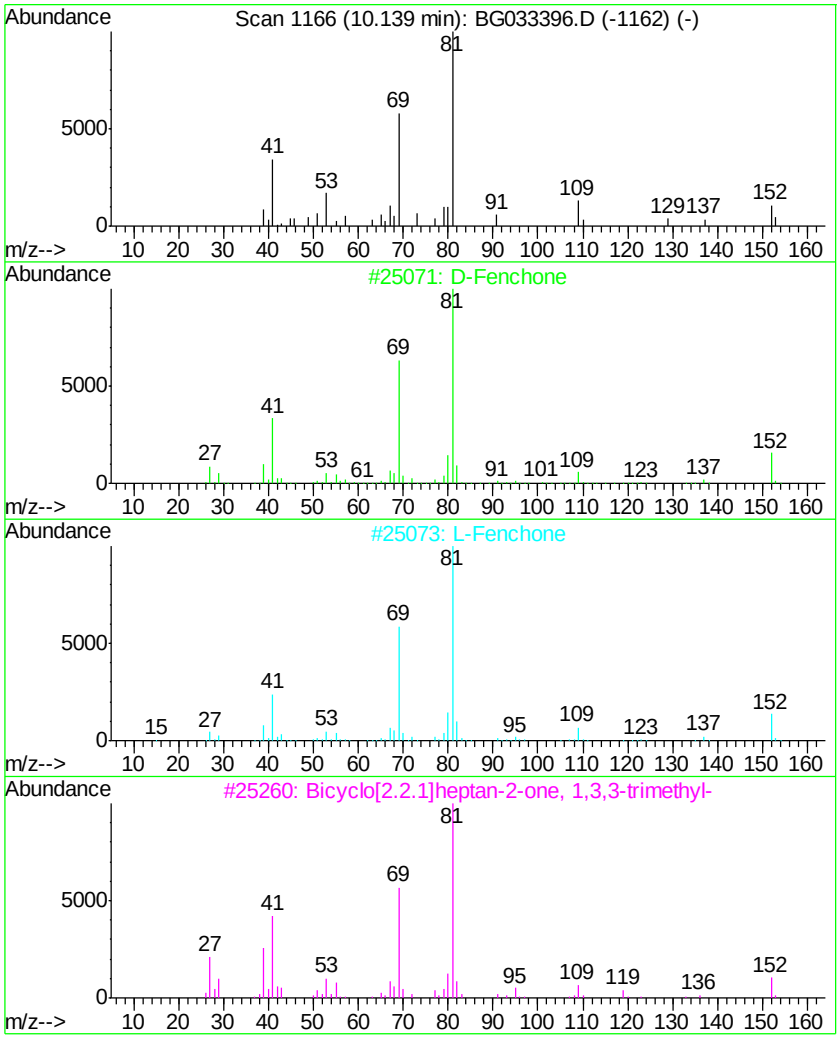
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

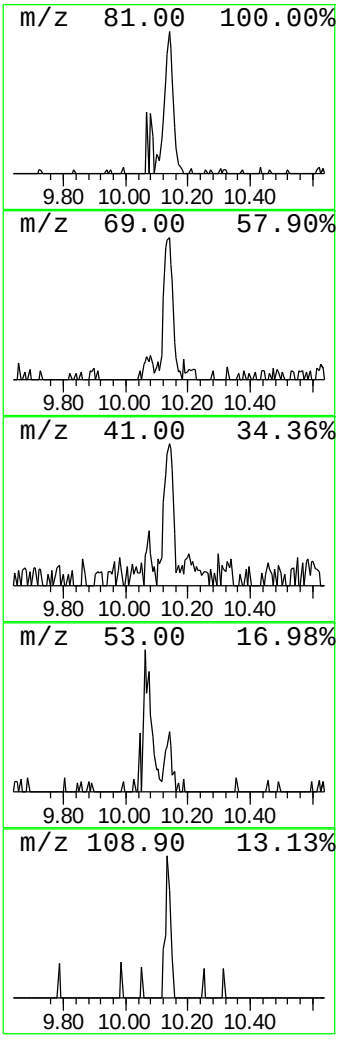
****

Peak Number 7 D-Fenchone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	4.38 ng	62532	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Fenchone	152	C10H16O	004695-62-9	64
2	L-Fenchone	152	C10H16O	007787-20-4	64
3	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	59
4	2-Furanacetaldehyde, .alpha.-pro...	152	C9H12O2	031681-26-2	47
5	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	45





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032818\
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Sample : J2098-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

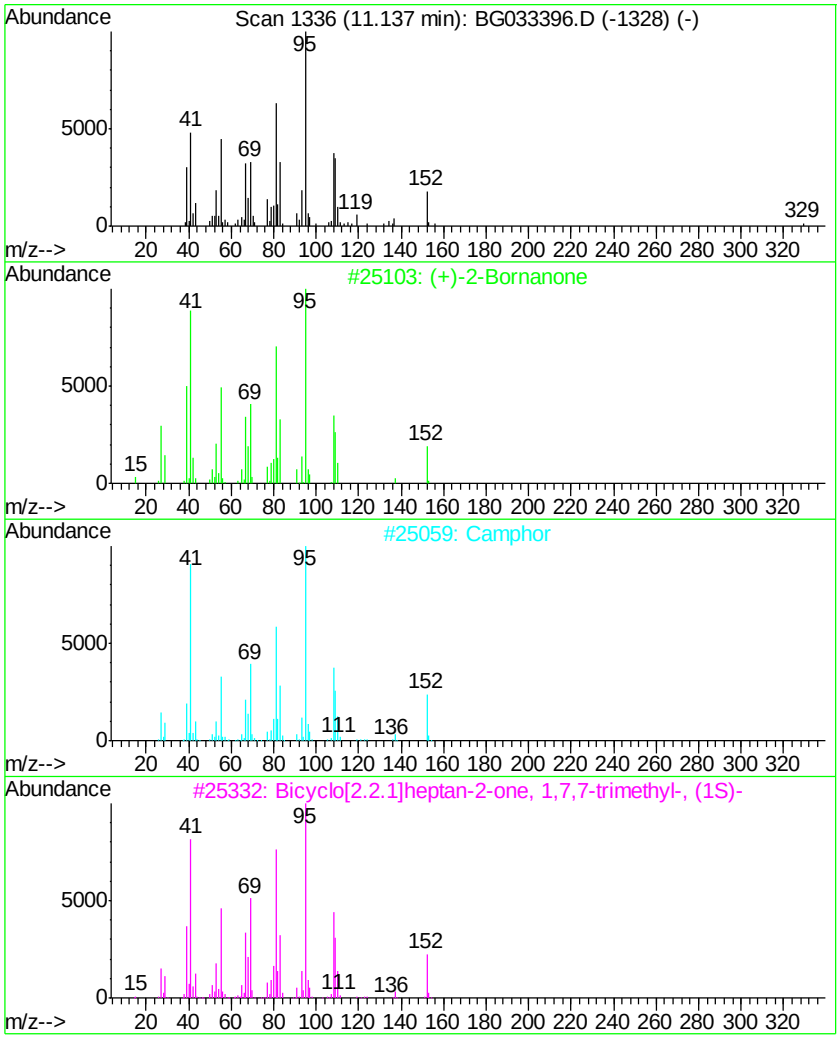
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

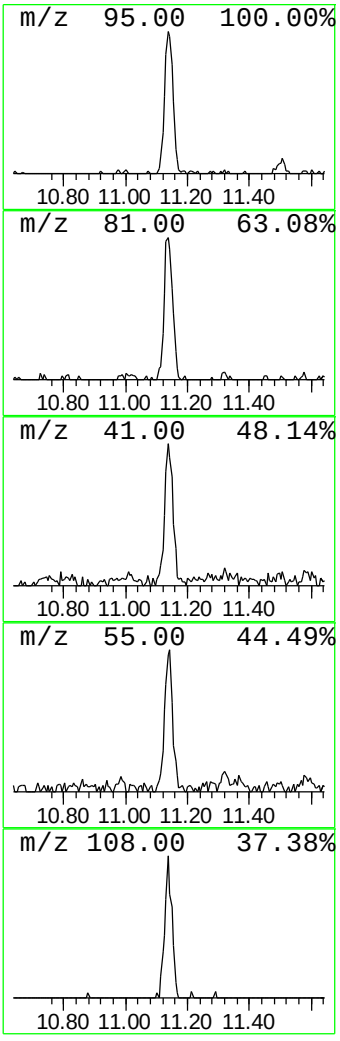
****

Peak Number 8 (+)-2-Bornanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	6.89 ng	154064	Naphthalene-d8	11.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	95
2	Camphor	152	C10H16O	000076-22-2	94
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	76
4	Ketone, 1,5-dimethylbicyclo[2.1....	138	C9H14O	024081-57-0	43
5	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	38





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Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

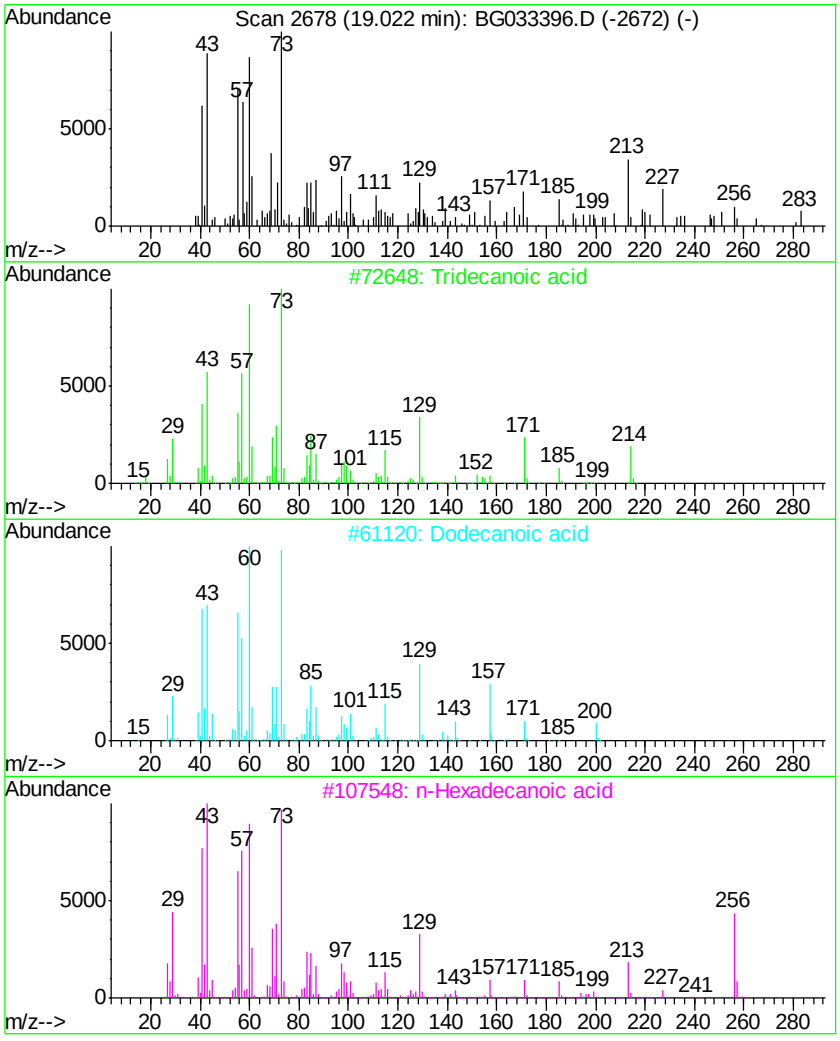
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

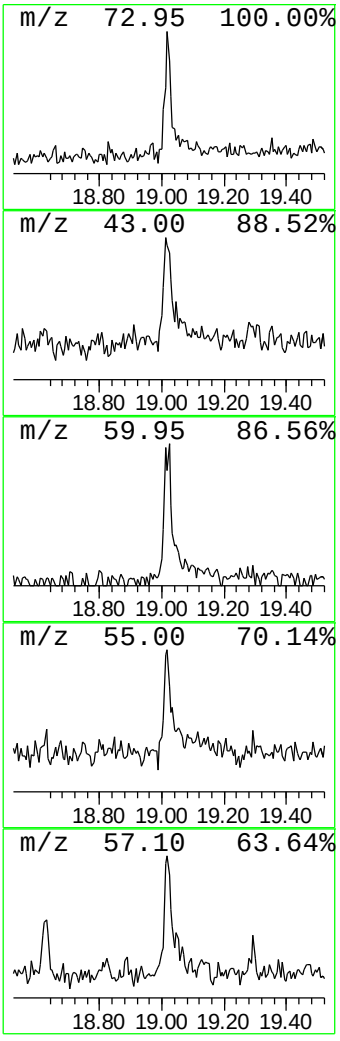
****

Peak Number 9 unknown19.02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	2.28 ng	88524	Phenanthrene-d10	18.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	46
2	Dodecanoic acid	200	C12H24O2	000143-07-7	41
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	35
4	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35
5	Octanoic acid	144	C8H16O2	000124-07-2	30





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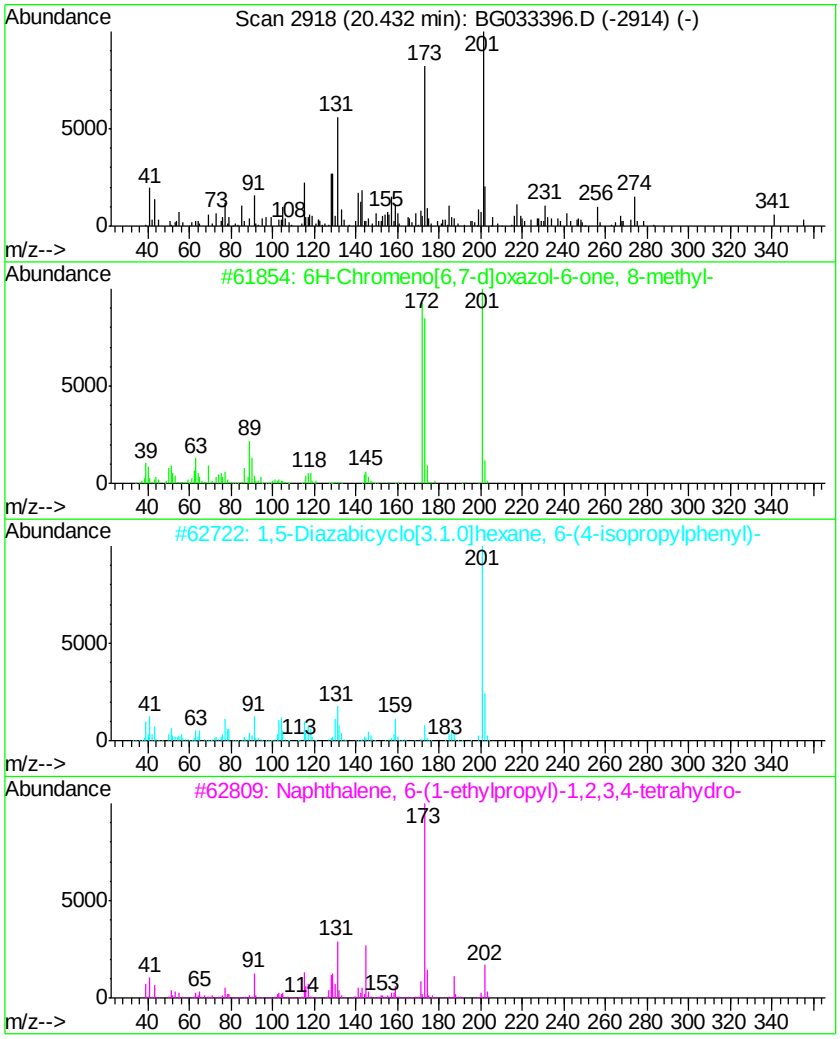
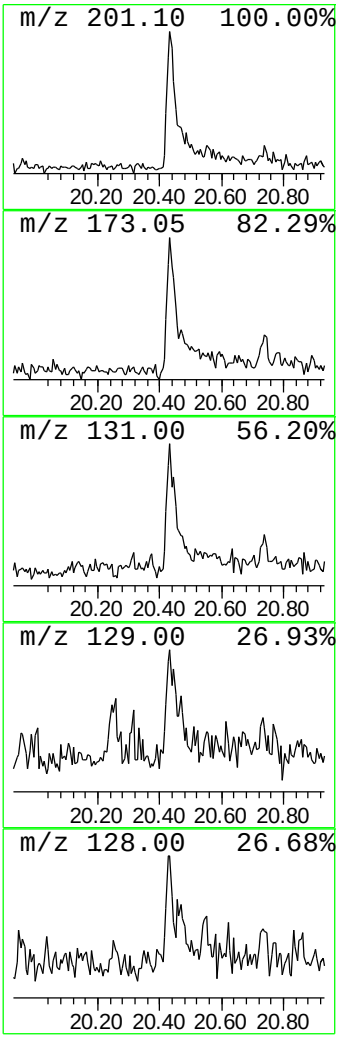
****

Peak Number 10 unknown20.43 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	2.10 ng	97012	Chrysene-d12	22.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Chromeno[6,7-d]oxazol-6-one, ...	201	C11H7NO3	1000272-31-8	38
2	1,5-Diazabicyclo[3.1.0]hexane, 6...	202	C13H18N2	1000277-07-5	30
3	Naphthalene, 6-(1-ethylpropyl)-1...	202	C15H22	054889-56-4	25
4	4-(1-Methylpropylamino)pyrido[3,...	202	C11H14N4	1000326-90-2	25
5	Glycine, N-(2-trifluoromethylben...	275	C12H12F3NO3	1000314-45-3	22





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

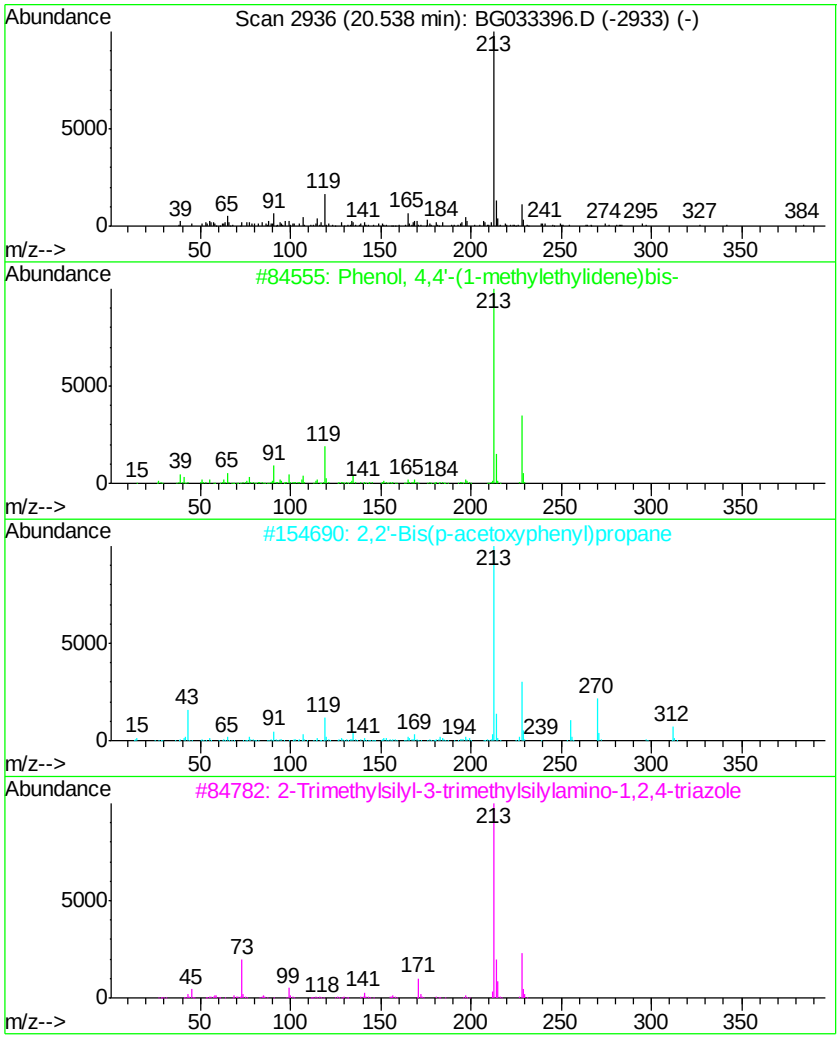
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

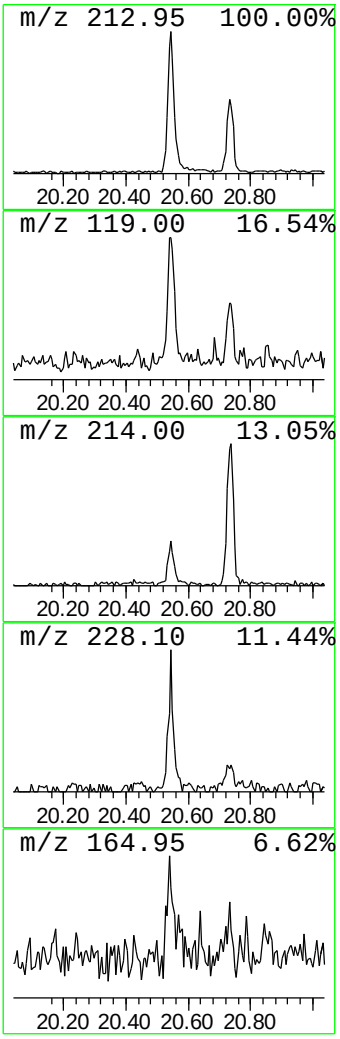
****

Peak Number 11 Phenol, 4,4'-(1-methylethyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.54	2.24 ng	103458	Chrysene-d12	22.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	86
2	2,2'-Bis(p-acetoxyphenyl)propane	312	C19H20O4	010192-62-8	78
3	2-Trimethylsilyl-3-trimethylsily...	228	C8H20N4Si2	1000373-05-5	72
4	Sebacic acid, ethyl neopentyl ester	300	C17H32O4	1000354-46-3	53
5	5-Acetyl-4-(2-furyl)-4,5,6,7-tet...	274	C15H18N2O3	1000224-56-0	52





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Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
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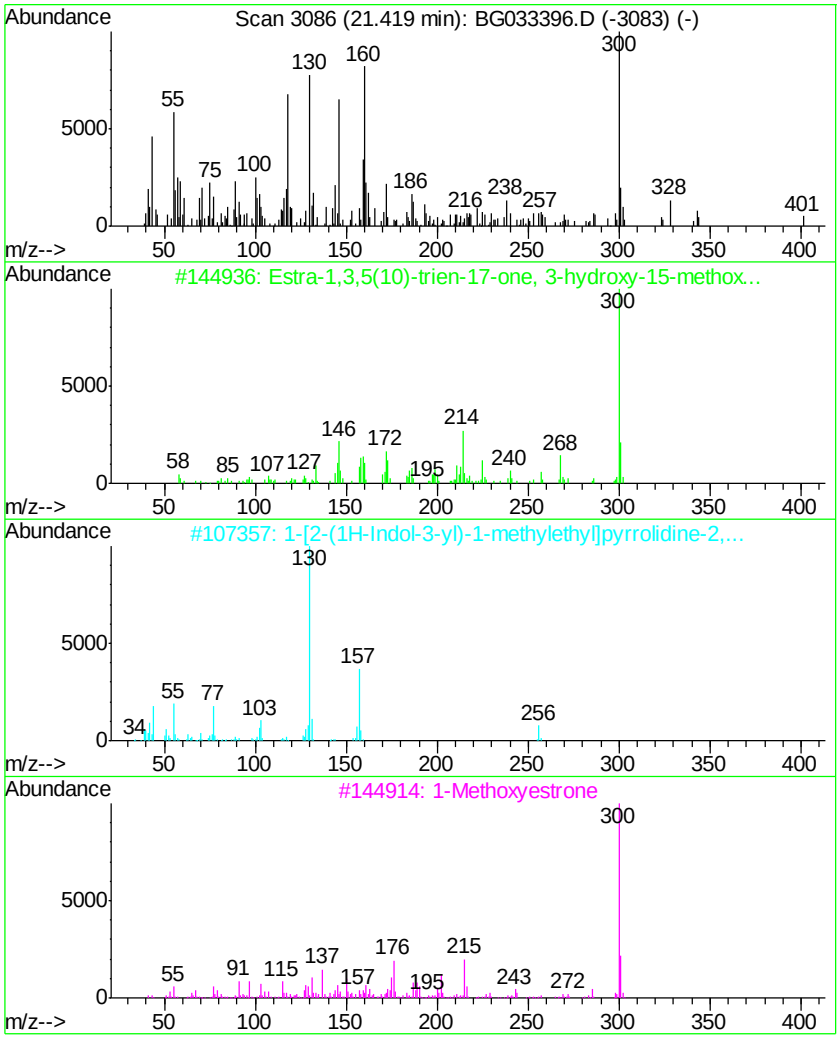
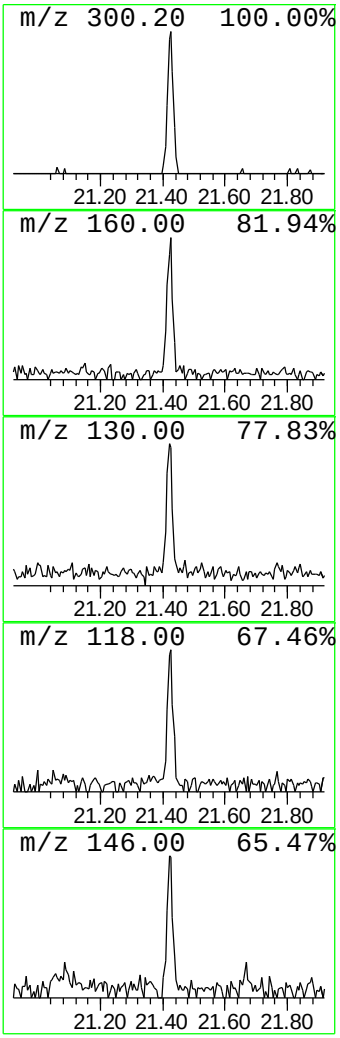
Peak Number 12 unknown21.42 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	2.06 ng	95215	Chrysene-d12	22.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Estra-1,3,5(10)-trien-17-one, 3-...	300	C19H24O3	074299-15-3	41
2	1-[2-(1H-Indol-3-yl)-1-methyleth...	256	C15H16N2O2	1000260-40-6	25
3	1-Methoxyestrone	300	C19H24O3	119831-01-5	25
4	Diboroxide, trimethylphenyl-	160	C9H14B2O	1000162-60-0	20
5	Pyrazolo[3,4-b]thiopyrano[4,3-d]...	300	C15H16N4OS	1000276-74-3	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032818\
Data File : BG033396.D
Acq On : 28 Mar 2018 21:29
Operator : SJ/JU
Sample : J2098-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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
Butane, 2-methoxy...	3.58	10.4	ng	148419	1	8.87	285334	20.0
2-Pentanone, 4-hy...	5.78	5.3	ng	75995	1	8.87	285334	20.0
unknown8.38	8.38	81.2	ng	1158030	1	8.87	285334	20.0
unknown9.55	9.55	5.5	ng	78619	1	8.87	285334	20.0
D-Fenchone	10.14	4.4	ng	62532	1	8.87	285334	20.0
(+)-2-Bornanone	11.14	6.9	ng	154064	2	11.75	447223	20.0
unknown19.02	19.02	2.3	ng	88524	4	18.21	777269	20.0
unknown20.43	20.43	2.1	ng	97012	5	22.56	924287	20.0
Phenol, 4,4'-(1-m...	20.54	2.2	ng	103458	5	22.56	924287	20.0
unknown21.42	21.42	2.1	ng	95215	5	22.56	924287	20.0