LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019136.D
Acq On : 11 Oct 2015 2:55
Operator : UM/NP
Sample : G3929-11
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-06

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-BG101015.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	3.144	47	52	59	rBV	52926	87360	5.45%	1.060%
2	3.214	59	64	76	rVB	203959	280402	17.48%	3.404%
3	5.136	384	391	401	rBV	70411	105035	6.55%	1.275%
4	5.606	464	471	478	rBV	141013	222104	13.85%	2.696%
5	7.192	733	741	747	rBV	95644	162762	10.15%	1.976%
6	7.562	797	804	812	rVB	285663	480994	29.99%	5.839%
7	8.032	878	884	890	rBV	61043	100546	6.27%	1.221%
8	8.355	932	939	947	rVB	262657	441755	27.54%	5.362%
9	9.190	1074	1081	1089	rBV	256236	445680	27.78%	5.410%
10	10.835	1353	1361	1369	rBV	89888	157124	9.80%	1.907%
11	13.285	1770	1778	1785	rBV	751396	1143970	71.32%	13.886%
12	14.108	1913	1918	1924	rBV	29298	39408	2.46%	0.478%
13	14.660	2006	2012	2020	rVB2	171559	268223	16.72%	3.256%
14	16.146	2258	2265	2283	rVB	693208	1069815	66.69%	12.986%
15	16.487	2316	2323	2327	rBV	21020	31183	1.94%	0.379%
16	16.540	2327	2332	2339	rVV4	26668	47266	2.95%	0.574%
17	16.605	2339	2343	2347	rVV3	20398	28139	1.75%	0.342%
18	16.799	2371	2376	2384	rBV4	26453	55899	3.48%	0.679%
19	16.869	2384	2388	2392	rBV	23403	33582	2.09%	0.408%
20	16.945	2397	2401	2407	rVB4	13068	23683	1.48%	0.287%
21	17.404	2473	2479	2485	rVB2	227203	343907	21.44%	4.175%
22	17.498	2488	2495	2502	rBV2	29781	40540	2.53%	0.492%
23	17.891	2558	2562	2572	rBV2	51156	87449	5.45%	1.062%
24	18.297	2627	2631	2636	rBV3	11873	20898	1.30%	0.254%
25	18.502	2661	2666	2675	rBV3	25822	46384	2.89%	0.563%
26	19.701	2865	2870	2877	rVB	26884	36369	2.27%	0.441%
27	20.018	2918	2924	2930	rBV	1270425	1604085	100.00%	19.472%
28	21.328	3142	3147	3152	rBV7	9994	19497	1.22%	0.237%
29	21.675	3199	3206	3214	rBV	257286	418366	26.08%	5.078%
30	24.901	3745	3755	3770	rVB	137497	395650	24.67%	4.803%

Sum of corrected areas: 8238075

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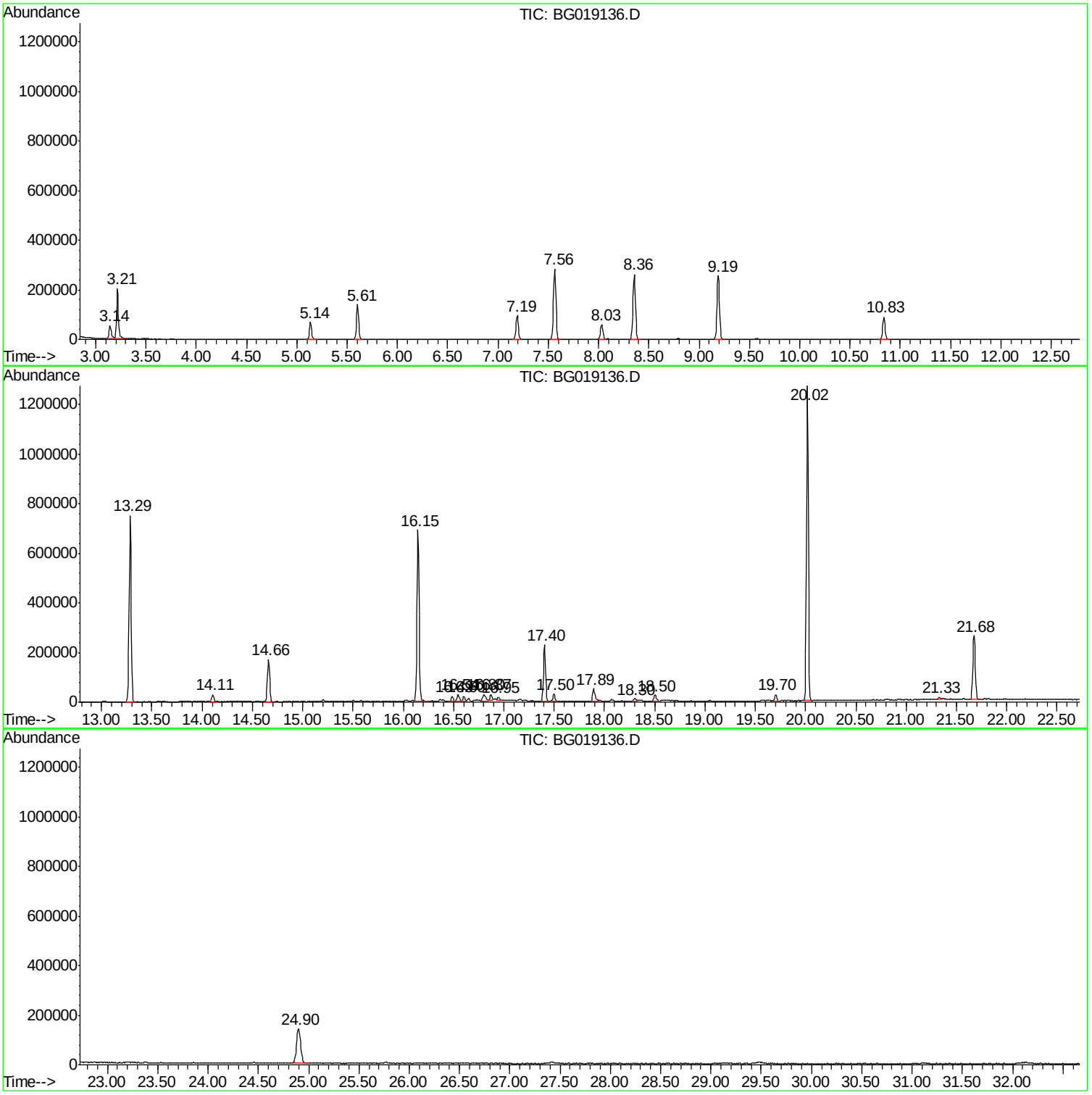
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-06

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019136.D
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Operator : UM/NP
Sample : G3929-11
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-06

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

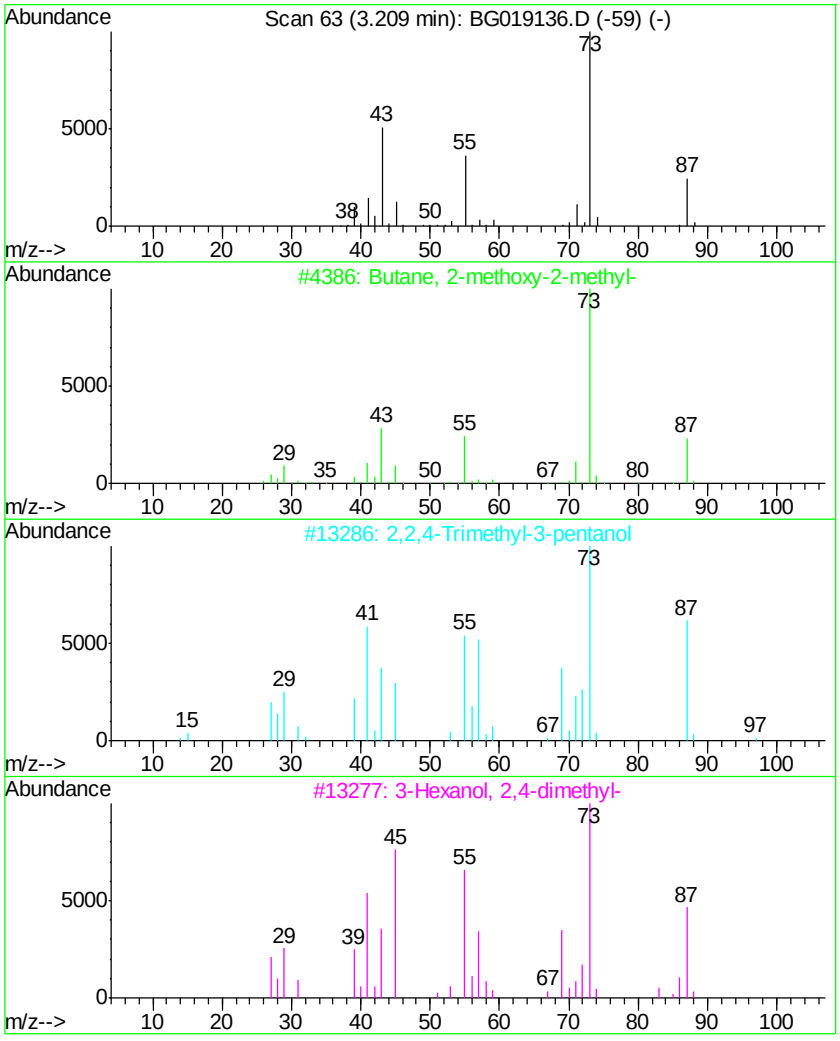
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

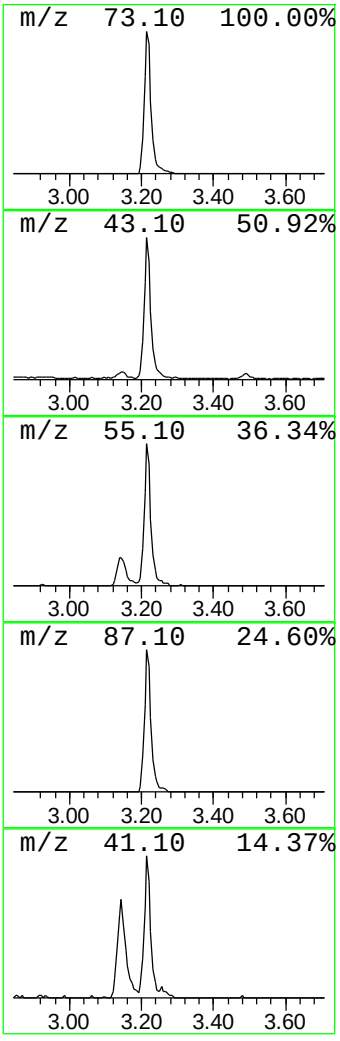
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	55.78 ng	280402	1,4-Dichlorobenzene-d4	8.03

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	43
3	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	33
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Library Search Compound Report

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Data File : BG019136.D
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Operator : UM/NP
Sample : G3929-11
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-06

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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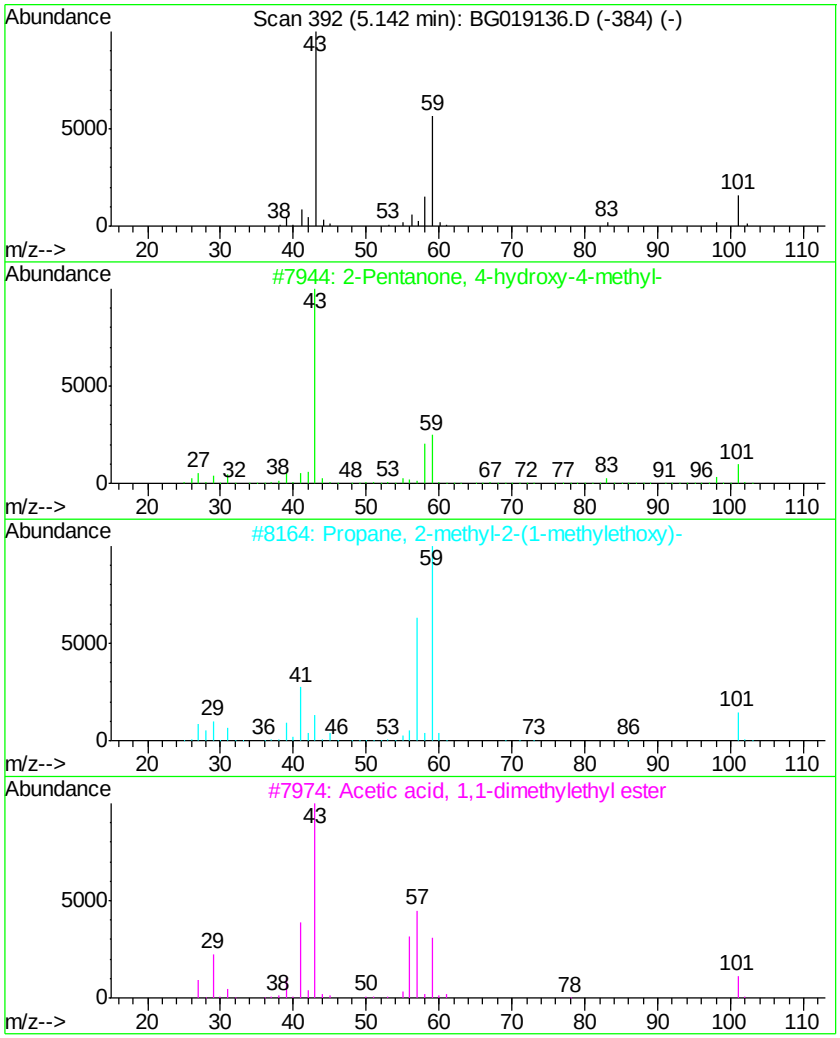
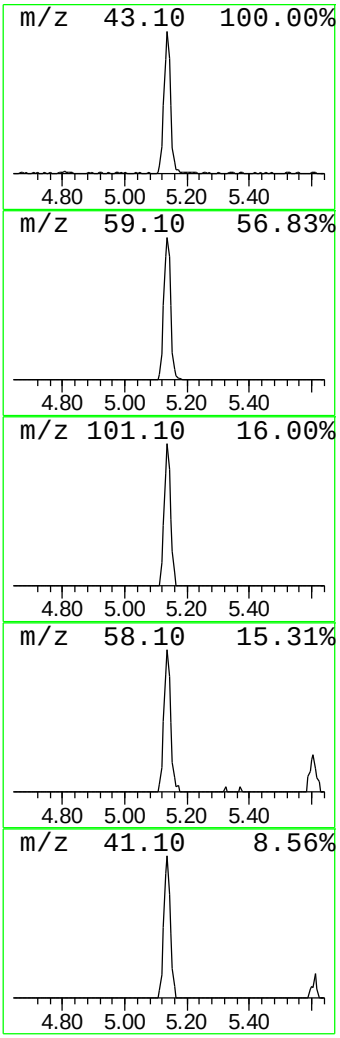
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	20.89 ng	105035	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	3-Heptanol	116	C7H16O	000589-82-2	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019136.D
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Operator : UM/NP
Sample : G3929-11
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-06

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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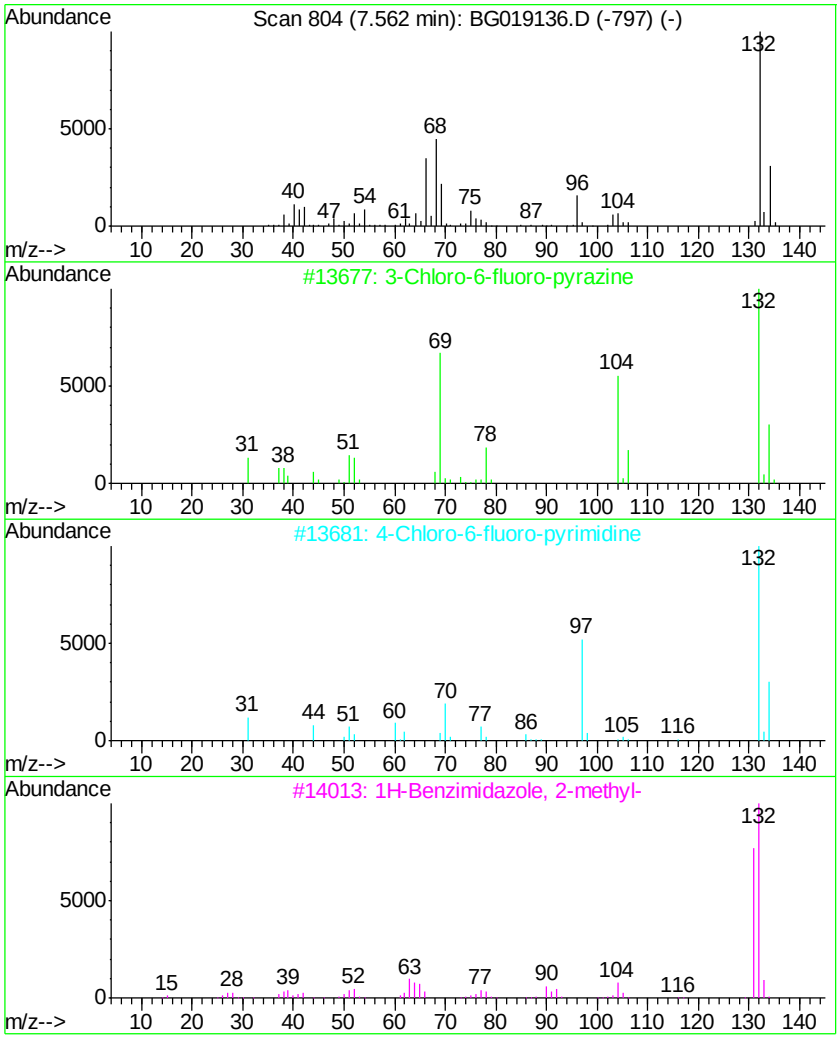
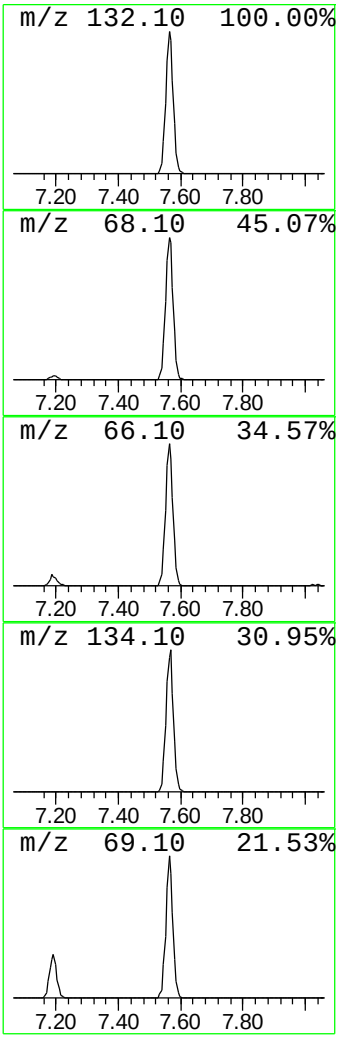
Peak Number 4 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	95.68 ng	480994	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019136.D
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Operator : UM/NP
Sample : G3929-11
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-06

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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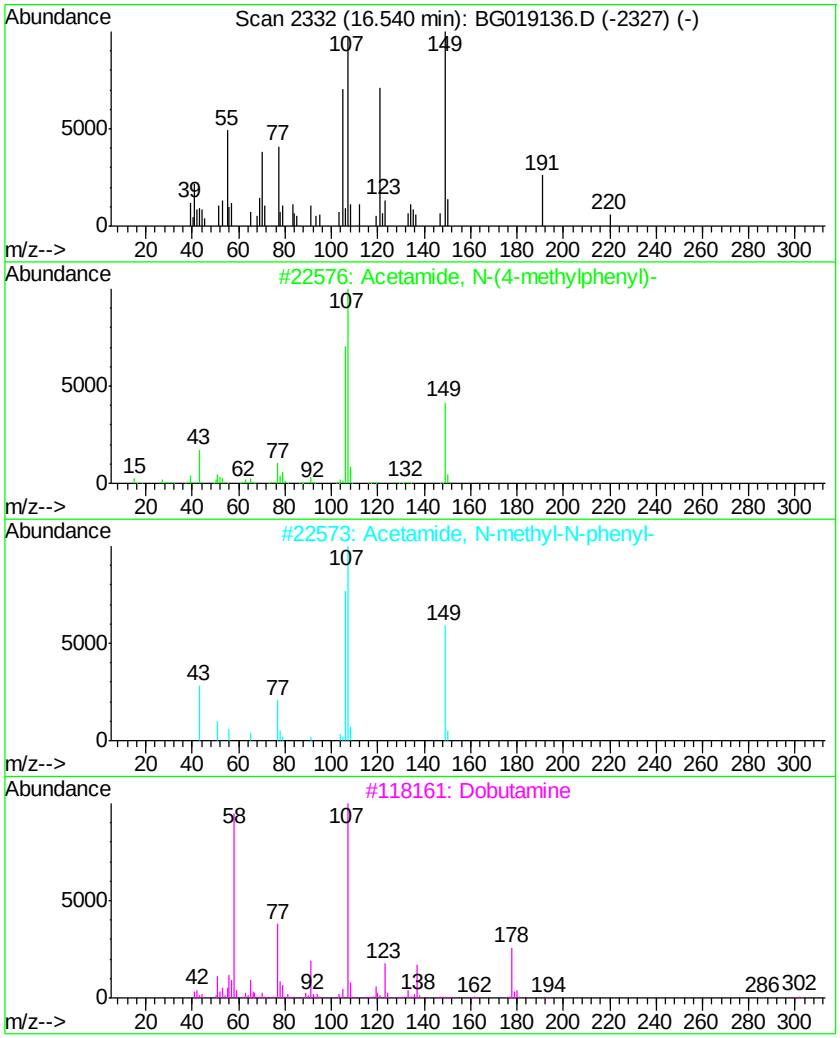
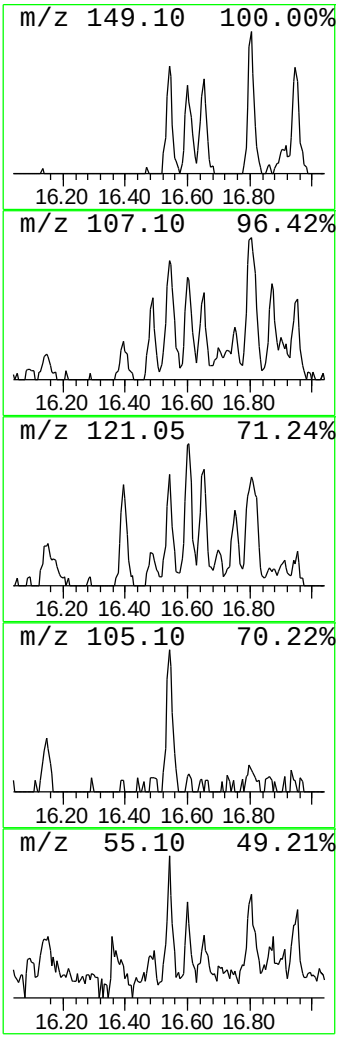
Peak Number 6 unknown16.54 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	2.75 ng	47266	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	47
2	Acetamide, N-methyl-N-phenyl-	149	C9H11NO	000579-10-2	47
3	Dobutamine	301	C18H23NO3	034368-04-2	27
4	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	27
5	3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	27





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019136.D
Acq On : 11 Oct 2015 2:55
Operator : UM/NP
Sample : G3929-11
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-06

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
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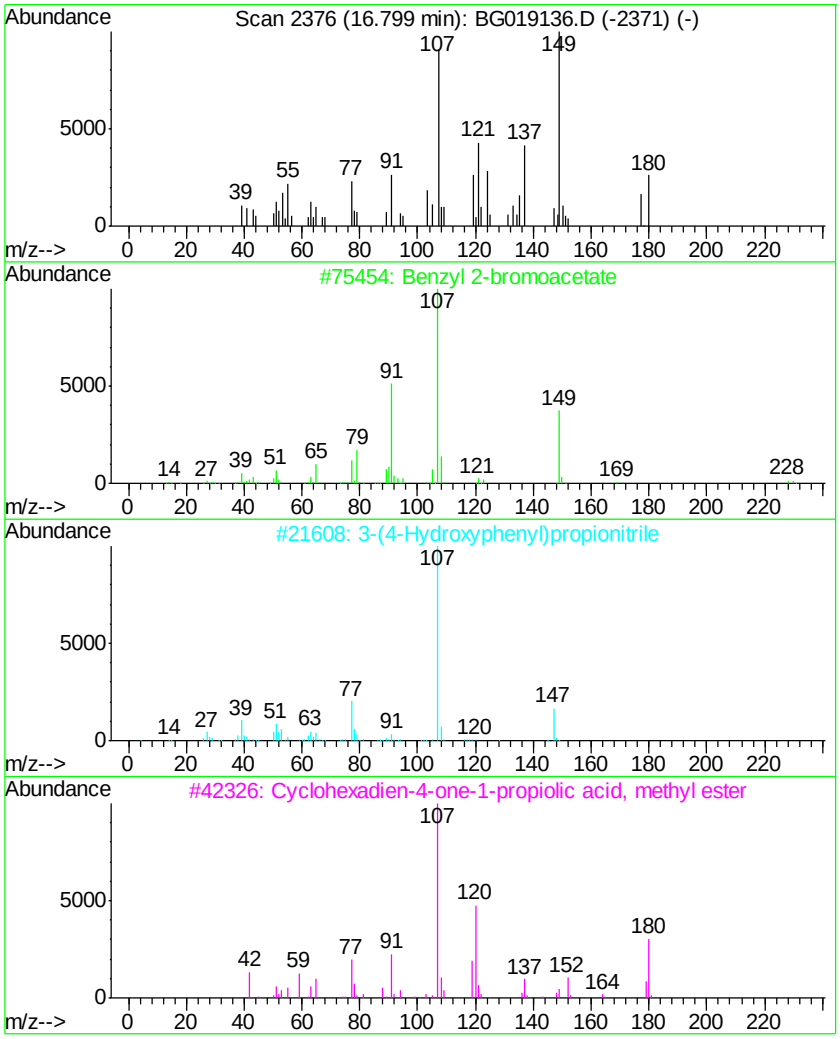
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

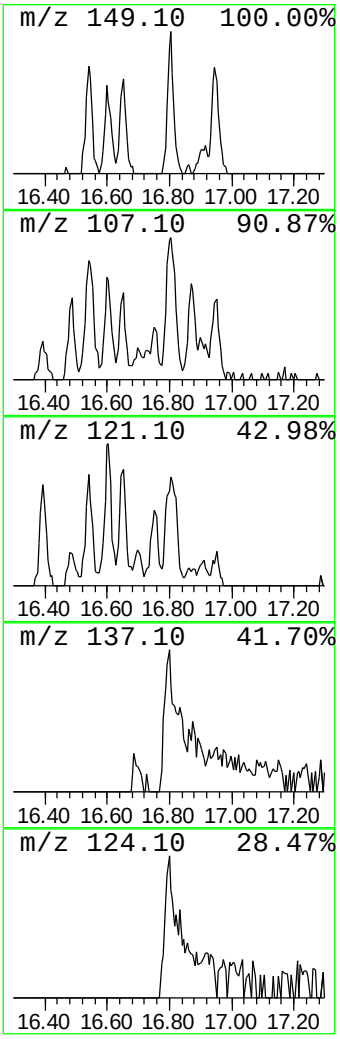
****

Peak Number 7 unknown16.80 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	3.25 ng	55899	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzyl 2-bromoacetate	228	C9H9BrO2	005437-45-6	43
2	3-(4-Hydroxyphenyl)propionitrile	147	C9H9NO	017362-17-3	35
3	Cyclohexadien-4-one-1-propiolic ...	180	C10H12O3	1000124-47-3	27
4	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	27
5	Benzeneacetic acid, 4-ethoxy-	180	C10H12O3	004919-33-9	25





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
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Instrument : BNA_G
ClientSampleId : MW-06

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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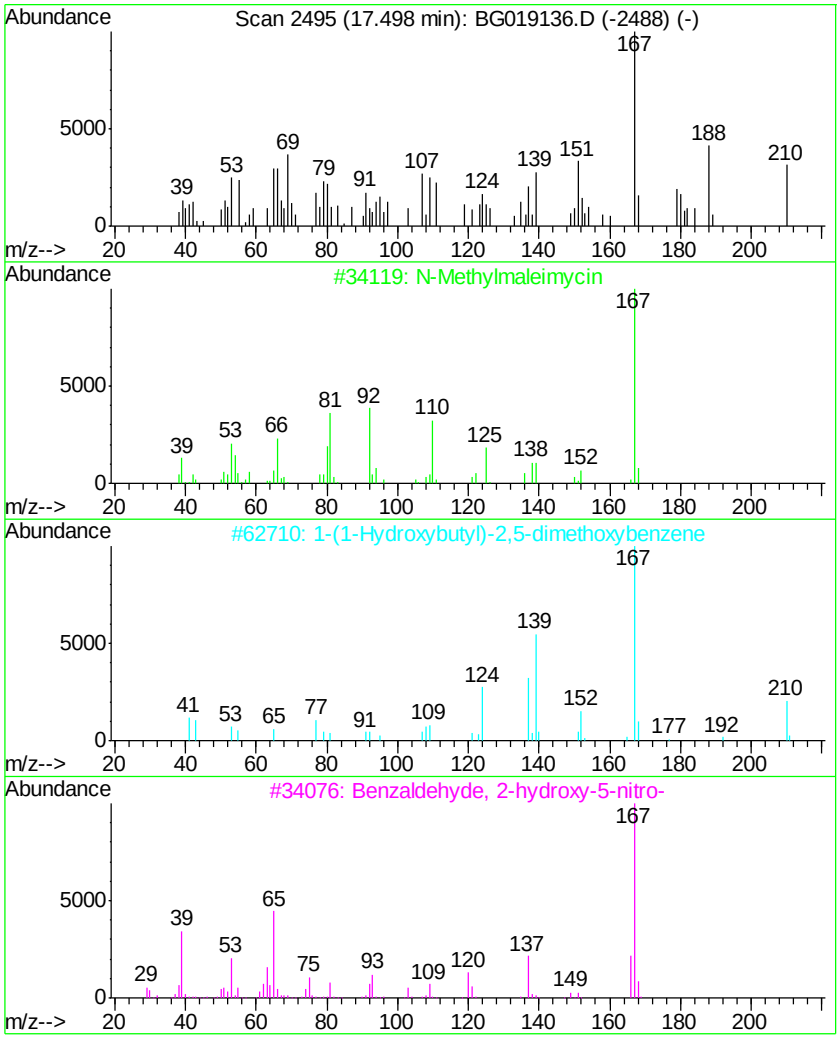
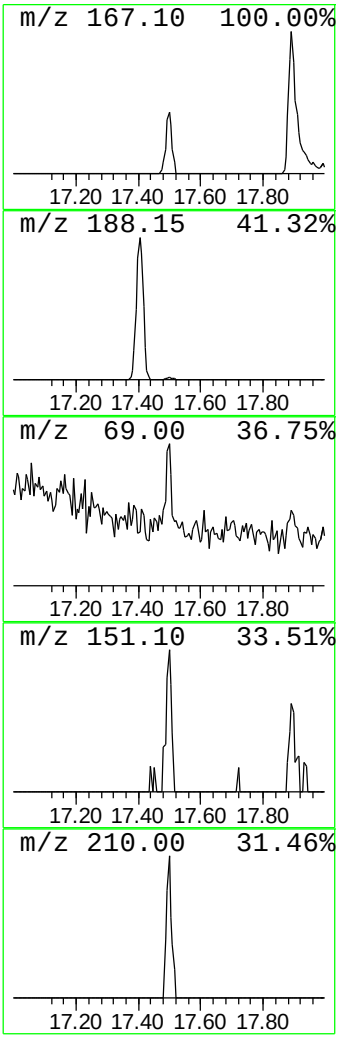
Peak Number 8 unknown17.50 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.50	2.36 ng	40540	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Methylmaleimycin	167	C8H9NO3	078776-95-1	43
2	1-(1-Hydroxybutyl)-2,5-dimethoxy...	210	C12H18O3	149083-03-4	27
3	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	18
4	Silane, dimethoxymethylphenyl-	182	C9H14O2Si	003027-21-2	14
5	Benzene, 1-ethoxy-4-nitro-	167	C8H9NO3	000100-29-8	14





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Misc :
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Instrument : BNA_G
ClientSampleId : MW-06

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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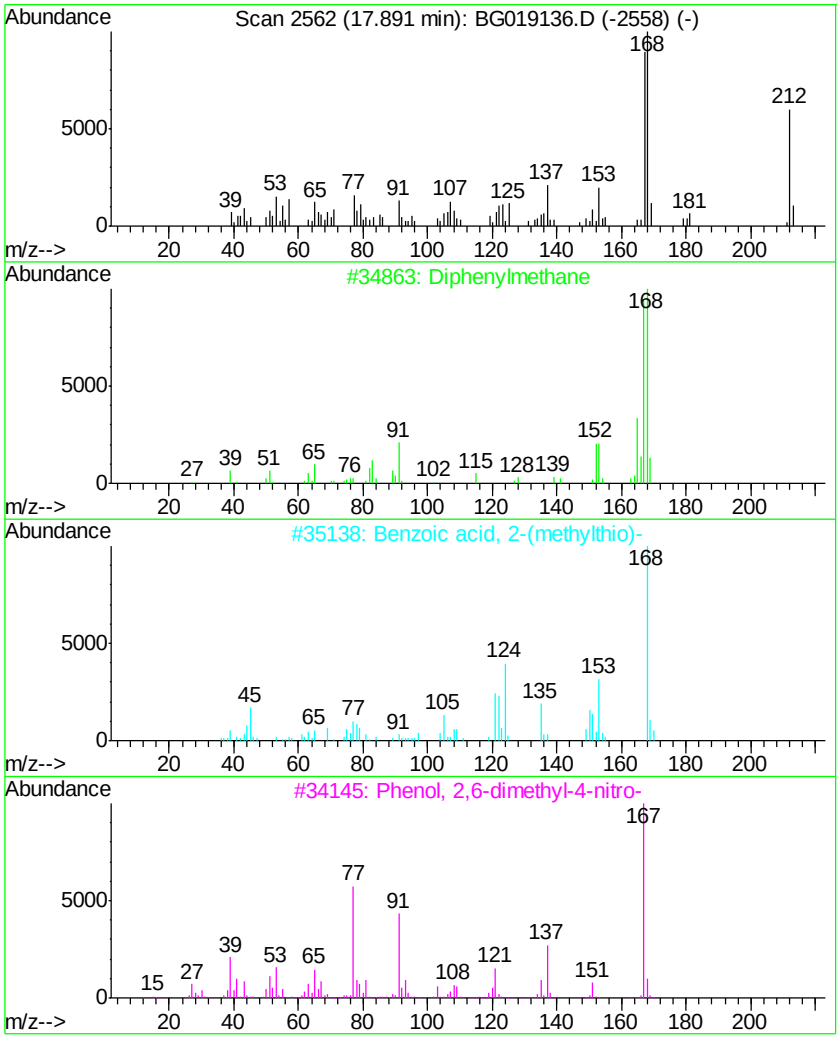
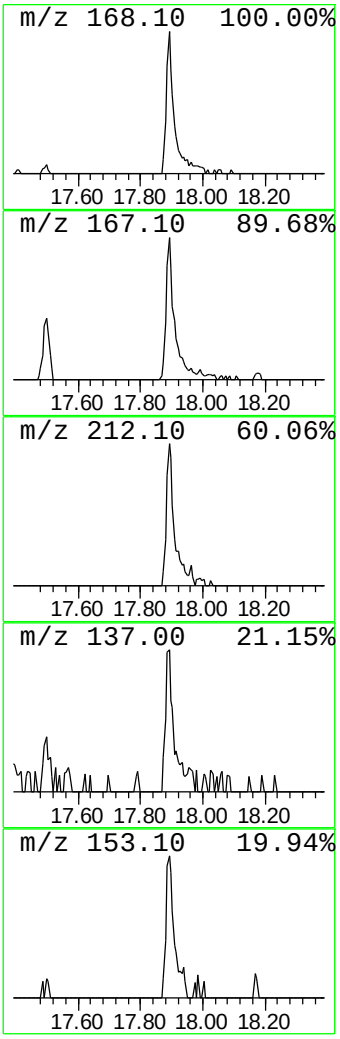
Peak Number 9 Diphenylmethane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	5.09 ng	87449	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diphenylmethane	168	C13H12	000101-81-5	50
2	Benzoic acid, 2-(methylthio)-	168	C8H8O2S	003724-10-5	38
3	Phenol, 2,6-dimethyl-4-nitro-	167	C8H9NO3	002423-71-4	38
4	Benzenemethanol, 3,4-dimethoxy-	168	C9H12O3	000093-03-8	38
5	Benzoic acid, 2,4,5-trimethoxy-	212	C10H12O5	000490-64-2	35





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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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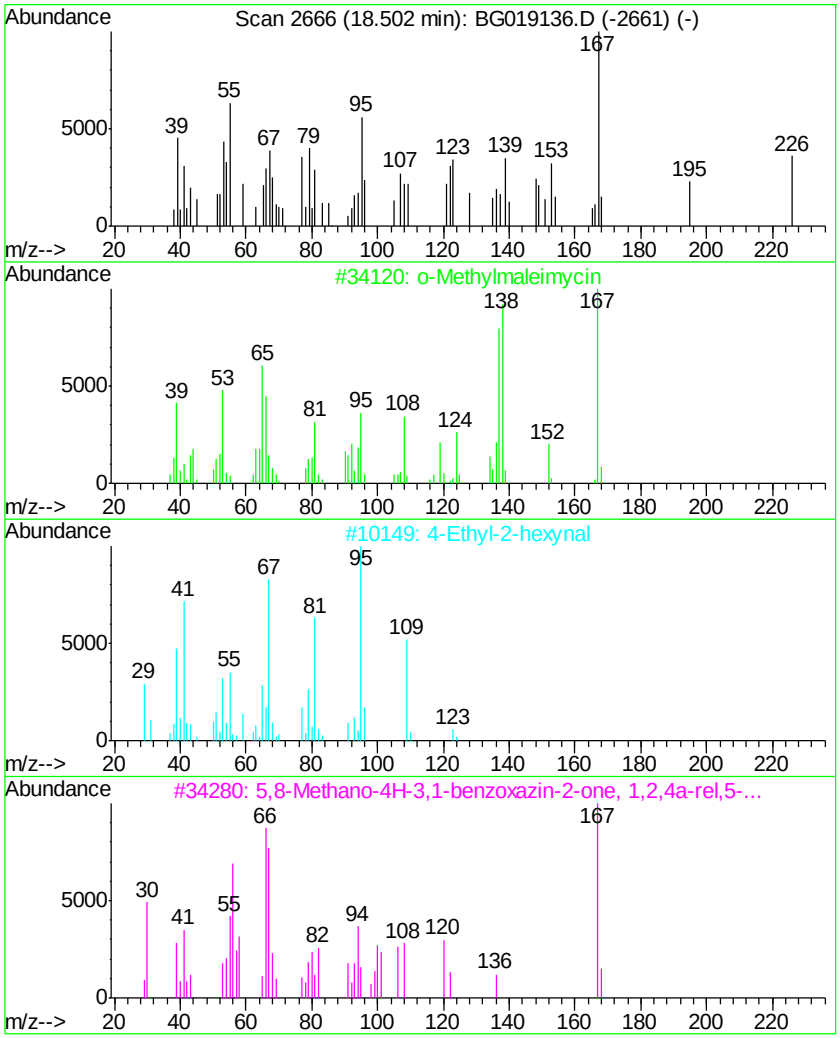
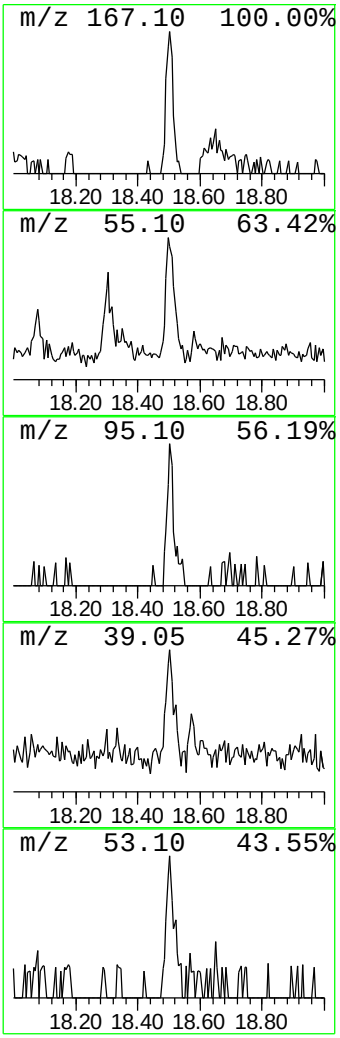
Peak Number 10 unknown18.50 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	2.70 ng	46384	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Methylmaleimycin	167	C8H9NO3	078776-98-4	38
2	4-Ethyl-2-hexynal	124	C8H12O	071932-97-3	32
3	5,8-Methano-4H-3,1-benzoxazin-2-...	167	C9H13NO2	1000146-94-4	14
4	5,8-Methano-4H-3,1-benzoxazin-2-...	167	C9H13NO2	1000142-76-3	14
5	2,8-Bornanediol, stereoisomer	170	C10H18O2	013429-50-0	14





Tentatively Identified Compound (LSC) summary

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Data File : BG019136.D
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Operator : UM/NP
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.21	55.8	ng	280402	1	8.03	100546	20.0
2-Pentanone, 4-hy...	5.14	20.9	ng	105035	1	8.03	100546	20.0
unknown7.56	7.56	95.7	ng	480994	1	8.03	100546	20.0
unknown16.54	16.54	2.8	ng	47266	4	17.40	343907	20.0
unknown16.80	16.80	3.3	ng	55899	4	17.40	343907	20.0
unknown17.50	17.50	2.4	ng	40540	4	17.40	343907	20.0
Diphenylmethane	17.89	5.1	ng	87449	4	17.40	343907	20.0
unknown18.50	18.50	2.7	ng	46384	4	17.40	343907	20.0