LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019123.D
Acq On : 10 Oct 2015 18:43
Operator : UM/NP
Sample : G3929-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

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	3.145	47	52	60	rBV	57864	97737	4.77%	1.167%
2	3.216	60	64	78	rVB	210023	284332	13.89%	3.396%
3	5.137	384	391	398	rBV	51410	75506	3.69%	0.902%
4	5.601	464	470	480	rVB	137064	216991	10.60%	2.592%
5	7.187	734	740	747	rBV	91489	150947	7.37%	1.803%
6	7.564	796	804	812	rBV	287780	480283	23.45%	5.737%
7	8.034	877	884	890	rBV	60013	98106	4.79%	1.172%
8	8.357	931	939	947	rBV	273983	457537	22.34%	5.465%
9	9.191	1074	1081	1089	rBV	259537	446971	21.83%	5.339%
10	10.836	1354	1361	1369	rVB	91407	155510	7.59%	1.858%
11	13.286	1771	1778	1788	rVB	754637	1154909	56.40%	13.795%
12	14.661	2005	2012	2019	rVB2	156493	251708	12.29%	3.007%
13	16.148	2258	2265	2276	rBV	686183	1016181	49.63%	12.138%
14	16.488	2317	2323	2327	rBV	27574	39222	1.92%	0.469%
15	16.541	2327	2332	2339	rVV3	22281	42497	2.08%	0.508%
16	16.606	2339	2343	2347	rVV	24900	36714	1.79%	0.439%
17	16.806	2372	2377	2383	rVB4	19589	35752	1.75%	0.427%
18	16.870	2383	2388	2393	rBV	28139	42448	2.07%	0.507%
19	17.405	2472	2479	2485	rBV	235339	344318	16.81%	4.113%
20	19.714	2867	2872	2877	rBV	19492	20591	1.01%	0.246%
21	20.019	2918	2924	2930	rBV	1611548	2047705	100.00%	24.460%
22	21.676	3199	3206	3213	rBV	277133	442679	21.62%	5.288%
23	24.902	3744	3755	3766	rBV3	143884	411296	20.09%	4.913%
24	29.503	4528	4538	4545	rBV9	6443	21822	1.07%	0.261%

Sum of corrected areas: 8371762

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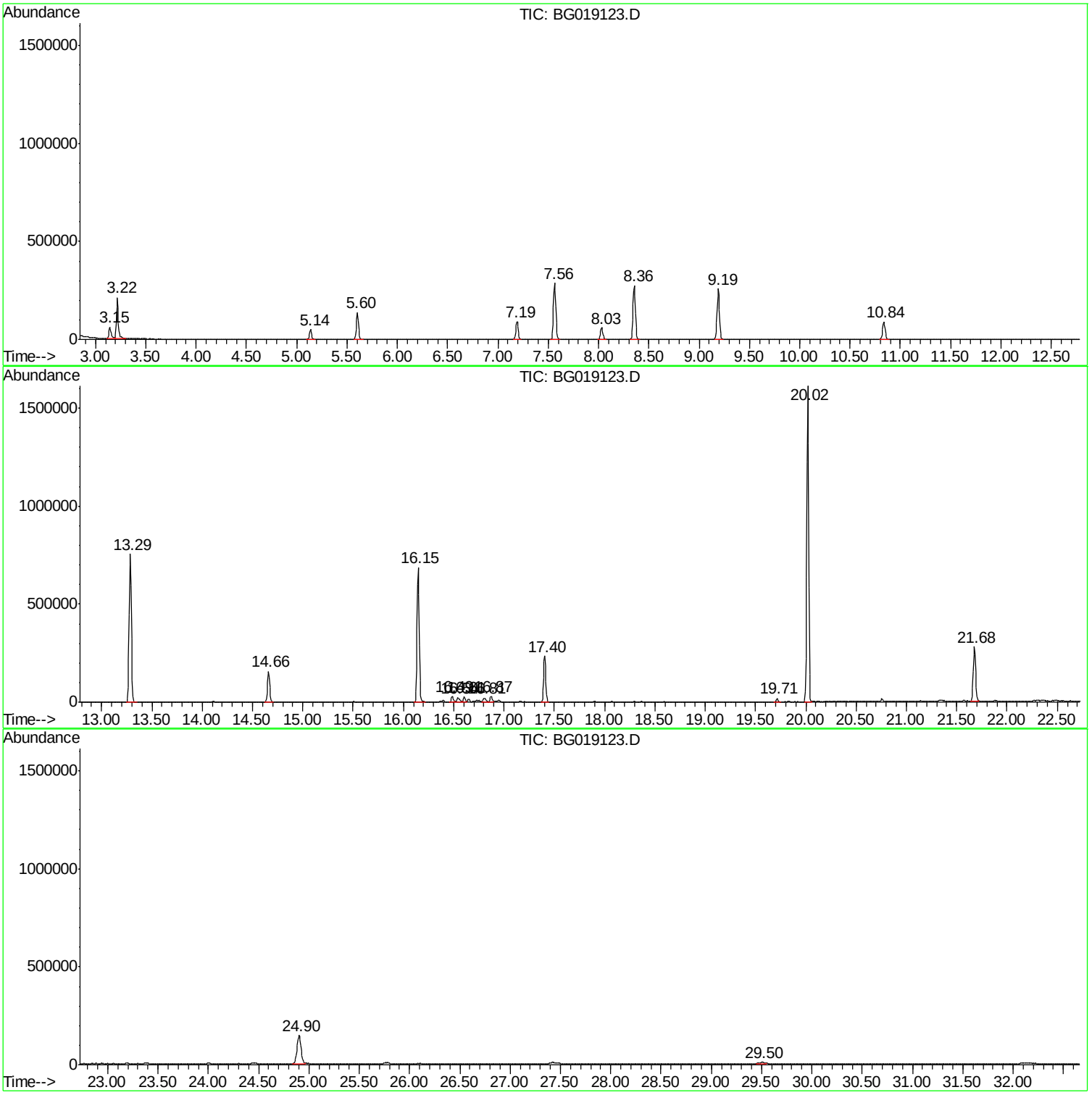
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

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 : BG019123.D
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Operator : UM/NP
Sample : G3929-01
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

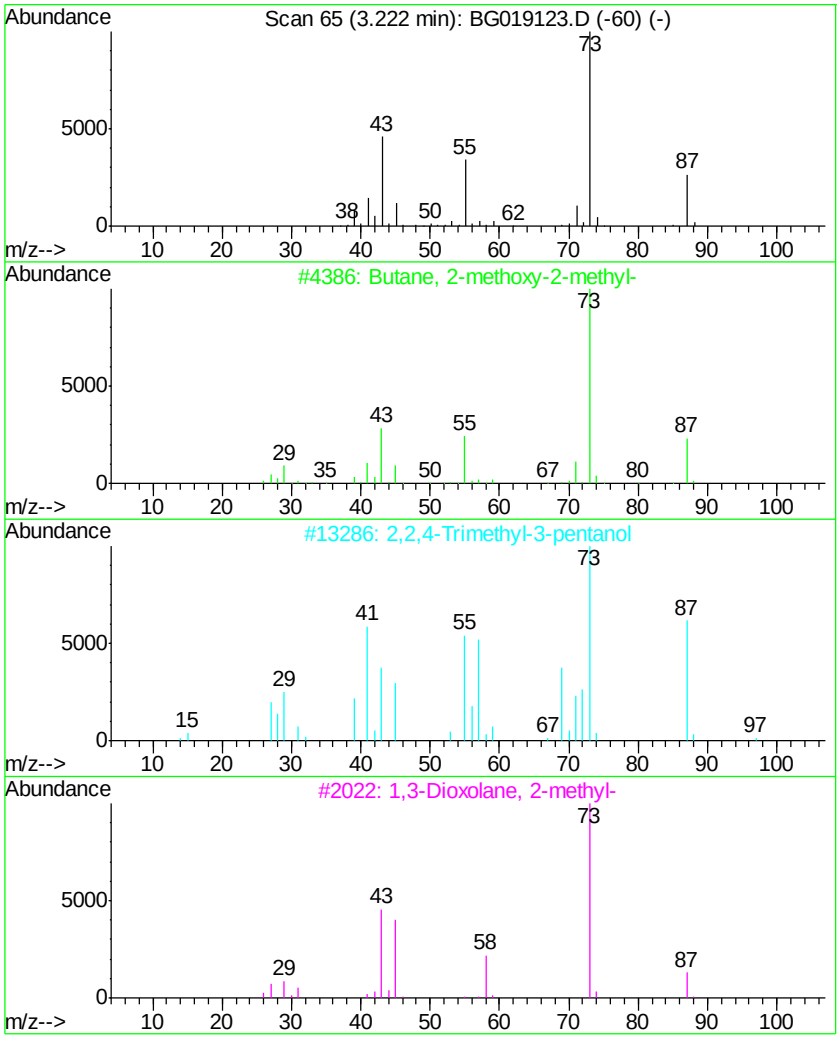
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

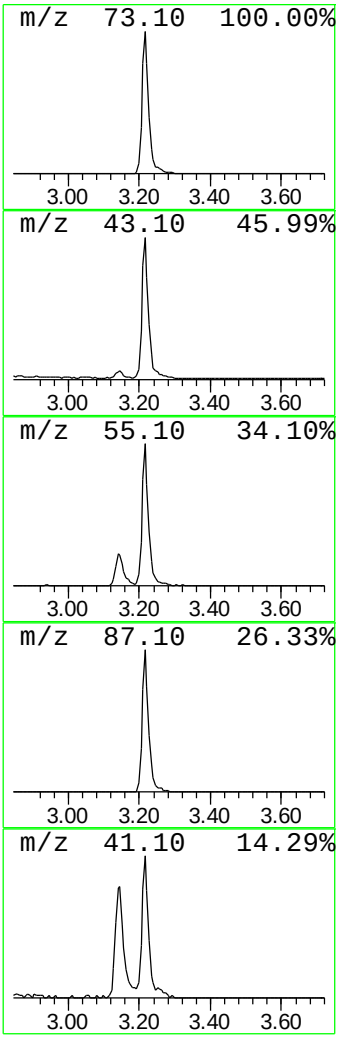
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	57.96 ng	284332	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019123.D
Acq On : 10 Oct 2015 18:43
Operator : UM/NP
Sample : G3929-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

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

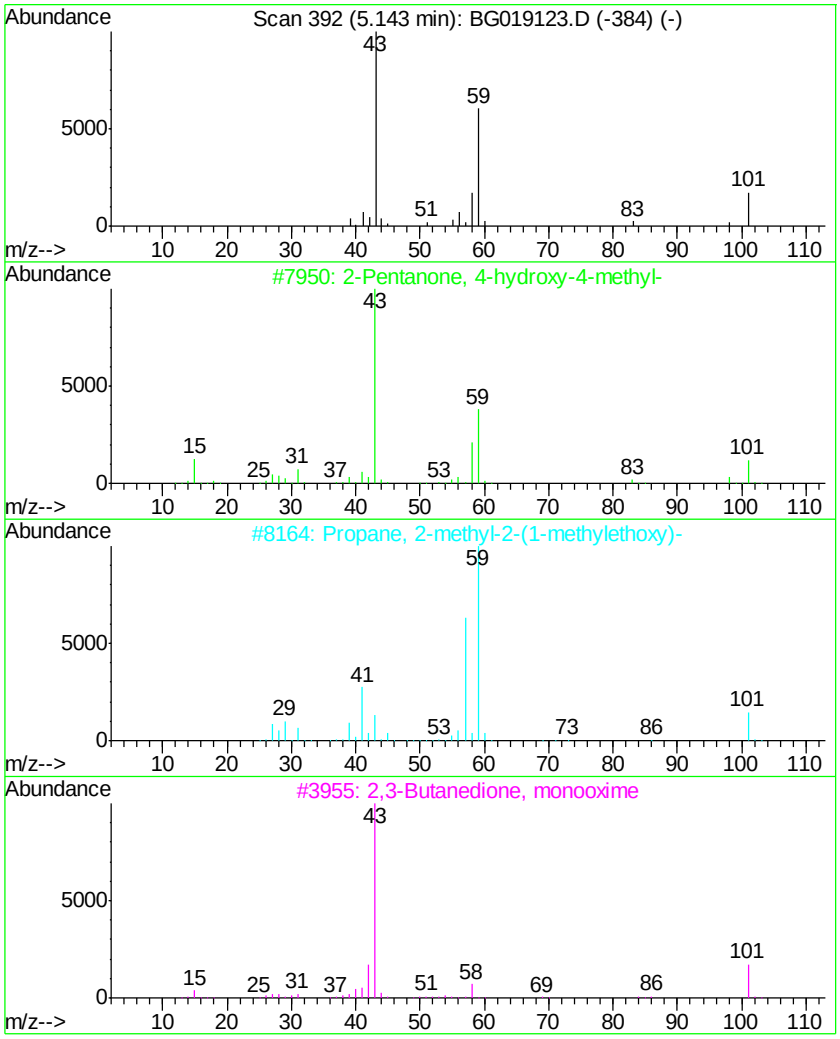
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

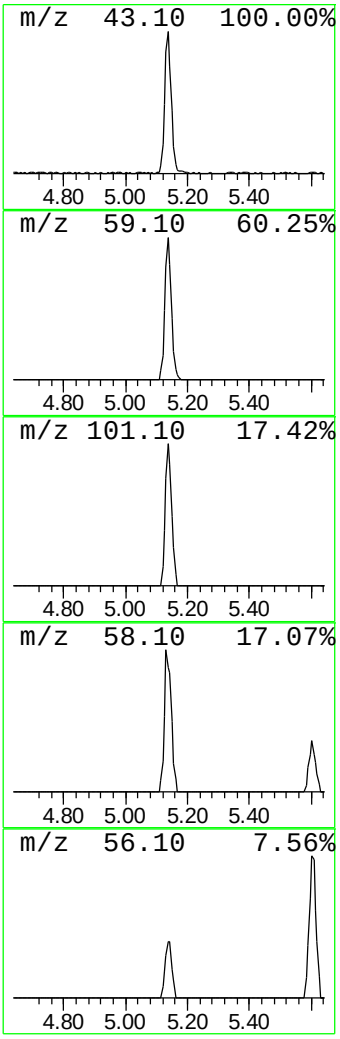
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	15.39 ng	75506	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	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	3-Hexanol	102	C6H14O	000623-37-0	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019123.D
Acq On : 10 Oct 2015 18:43
Operator : UM/NP
Sample : G3929-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

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

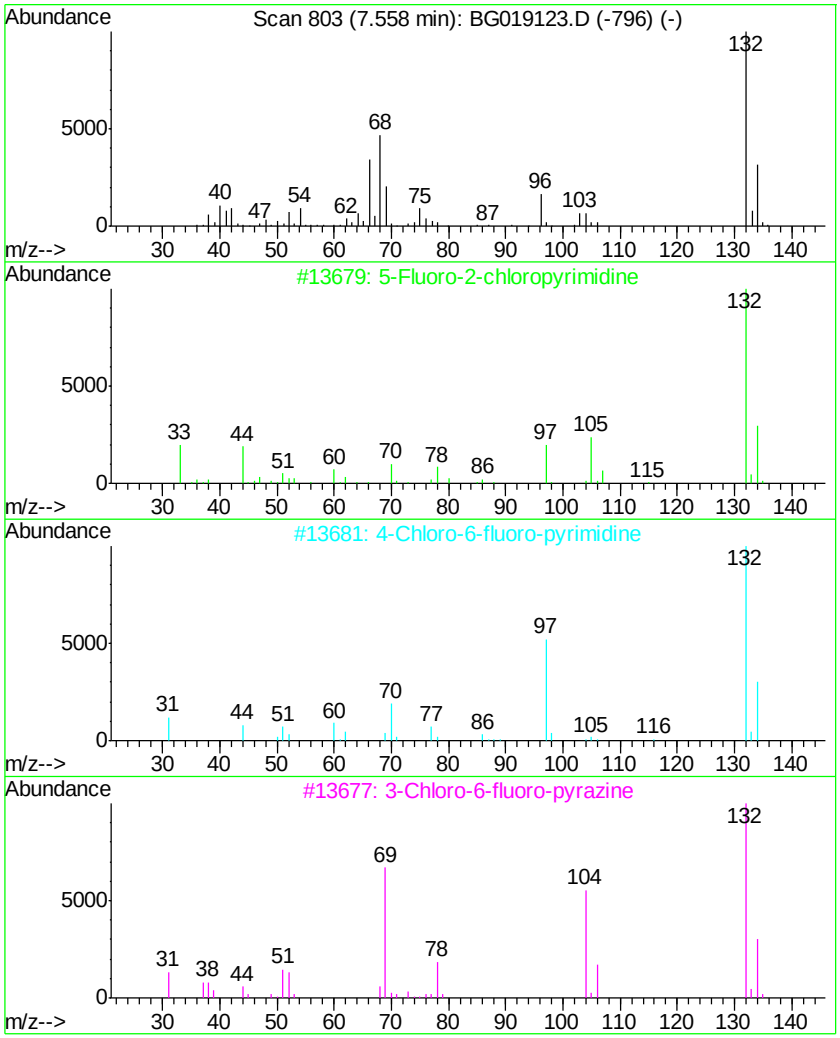
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

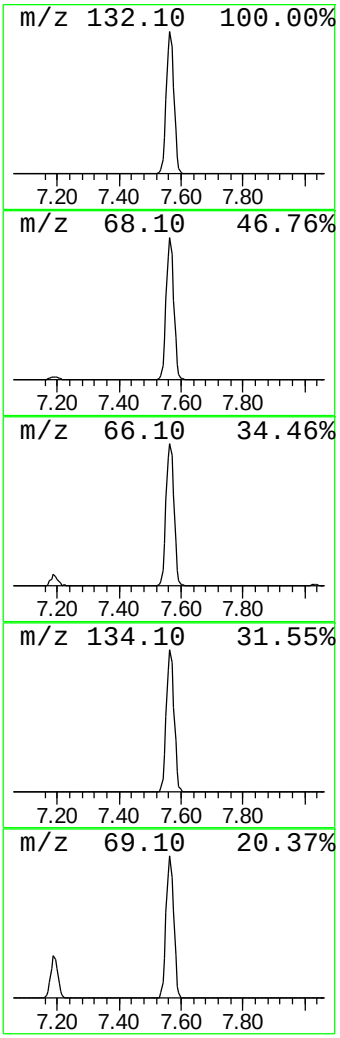
****

Peak Number 4 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	97.91 ng	480283	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22





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Data File : BG019123.D
Acq On : 10 Oct 2015 18:43
Operator : UM/NP
Sample : G3929-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

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

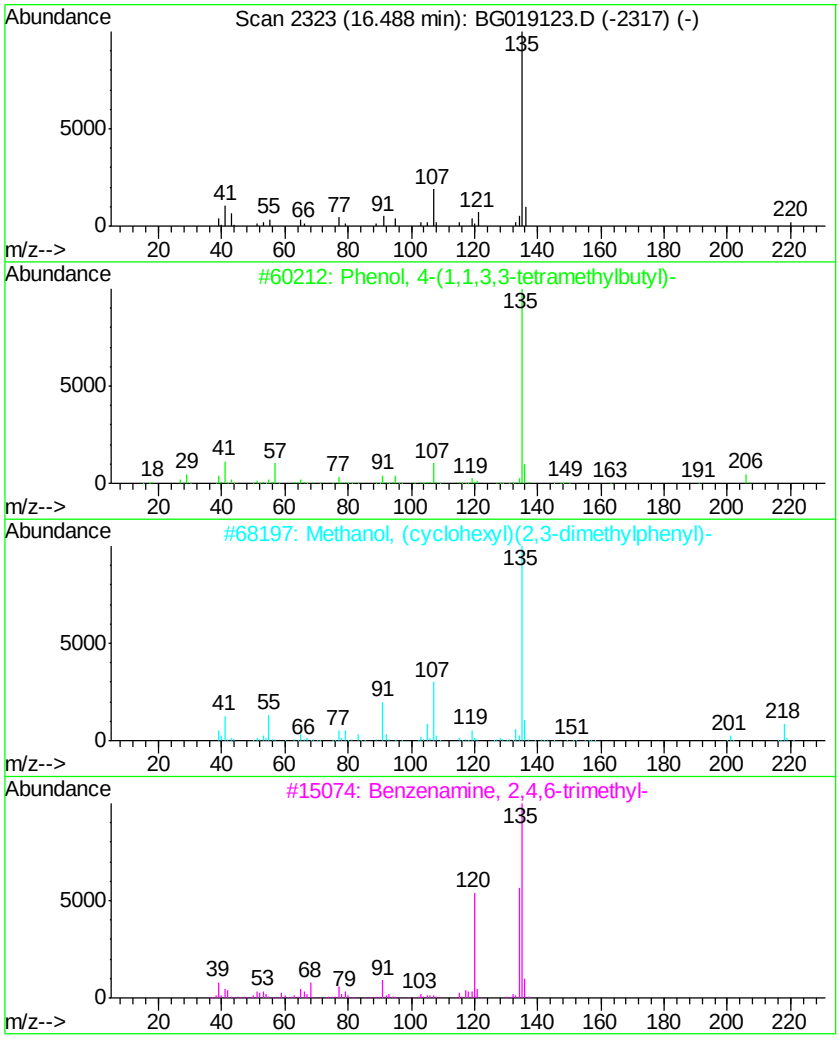
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

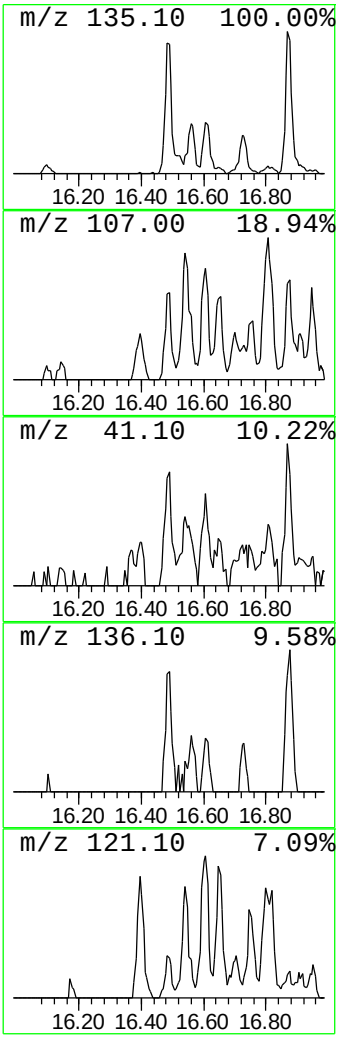
****

Peak Number 6 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.28 ng	39222	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
2	Methanol, (cyclohexyl)(2,3-dimet...	218	C15H22O	349498-47-1	72
3	Benzenamine, 2,4,6-trimethyl-	135	C9H13N	000088-05-1	64
4	1-n-Hexyladamantane	220	C16H28	022458-75-9	59
5	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	56





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019123.D
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Operator : UM/NP
Sample : G3929-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

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

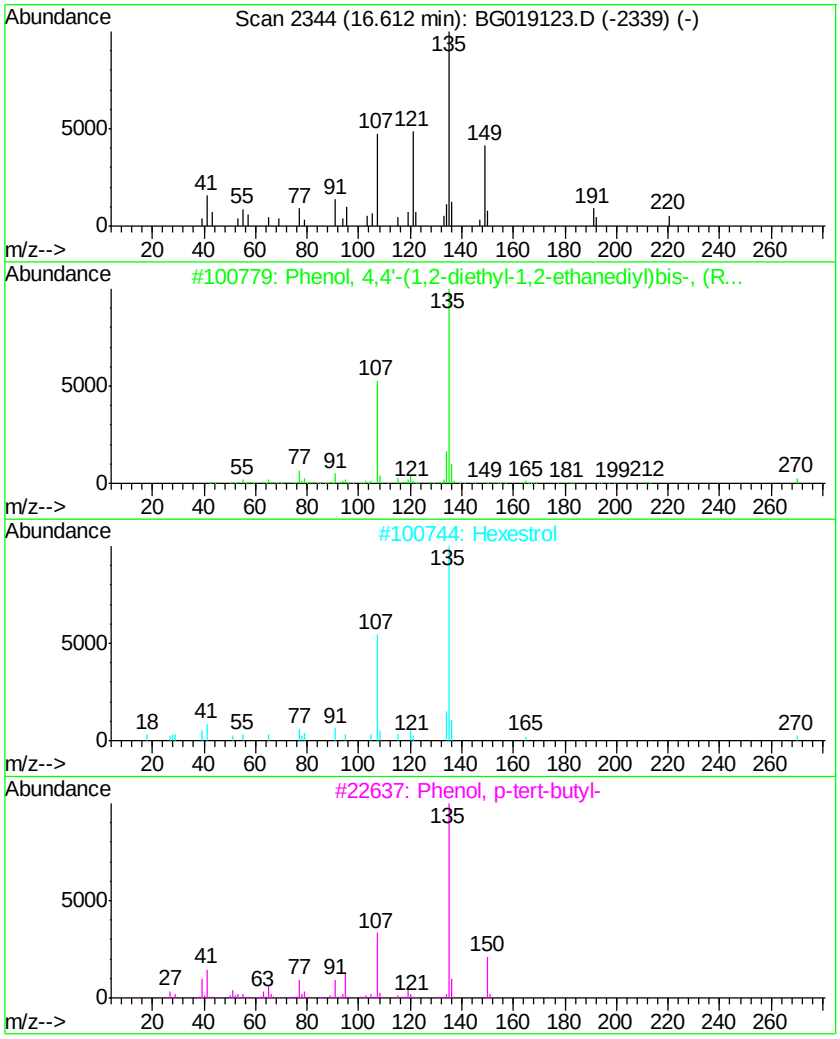
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

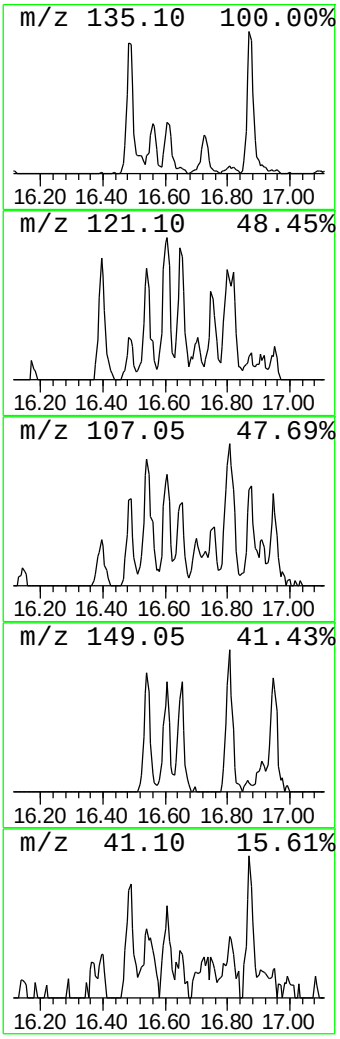
****

Peak Number 8 Phenol, 4,4'-(1,2-diethyl-1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	2.13 ng	36714	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1,2-diethyl-1,2-et...	270	C18H22O2	000084-16-2	50
2	Hexestrol	270	C18H22O2	005635-50-7	50
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	49
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	49
5	4,6-Bis(4-ethoxybenzylthio)-5-ni...	457	C22H23N3O4S2	325957-76-4	47





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Sample : G3929-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-01

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

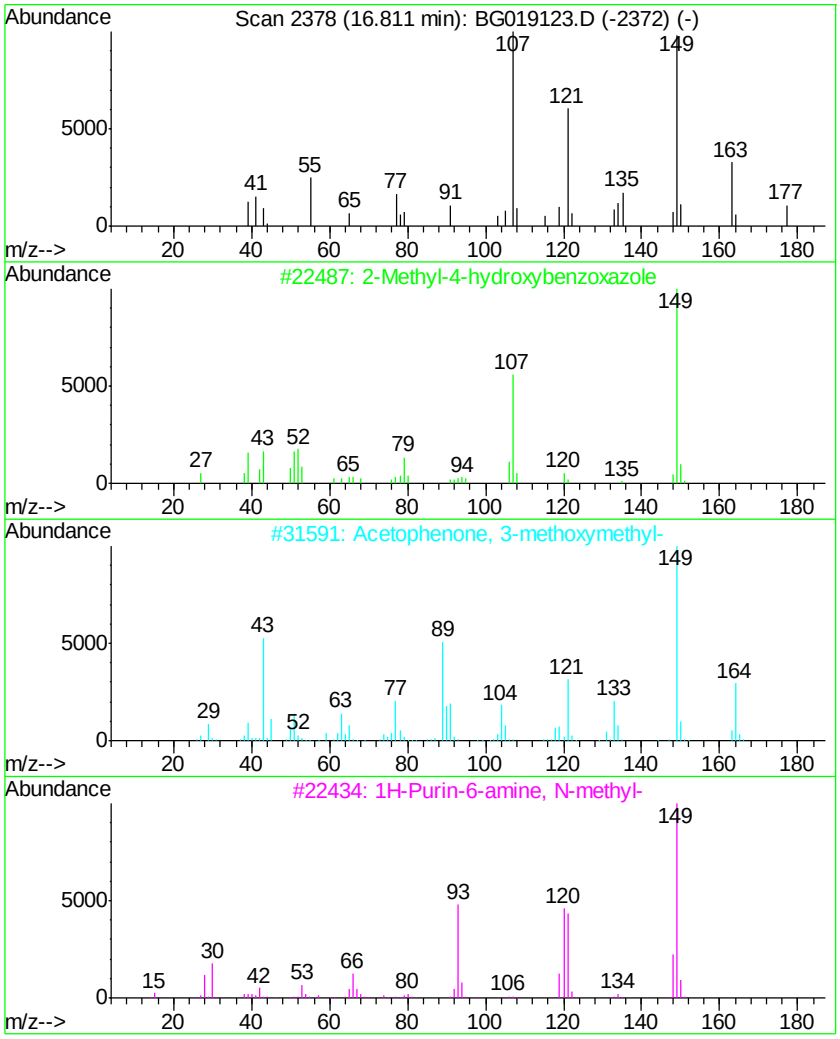
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

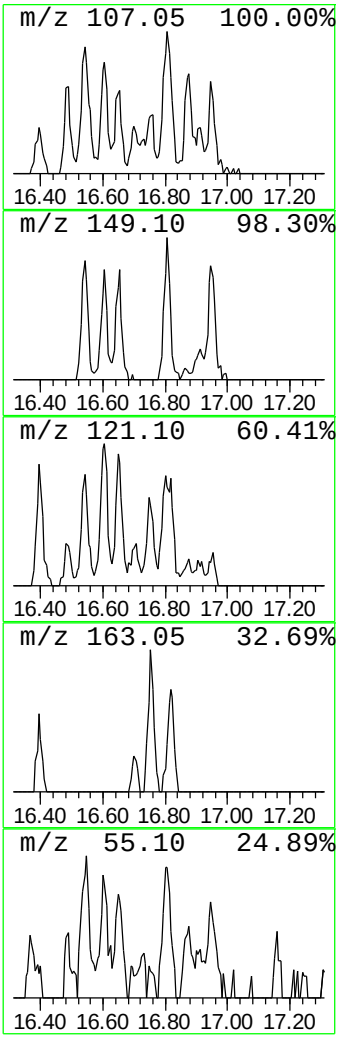
****

Peak Number 9 2-Methyl-4-hydroxybenzoxazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	2.08 ng	35752	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	59
2	Acetophenone, 3-methoxymethyl-	164	C10H12O2	1000159-01-9	37
3	1H-Purin-6-amine, N-methyl-	149	C6H7N5	000443-72-1	35
4	Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	35
5	Benzene, 1-methoxy-4-methyl-2-(1...	164	C11H16O	031574-44-4	35





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Misc :
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Instrument : BNA_G
ClientSampleId : MW-01

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

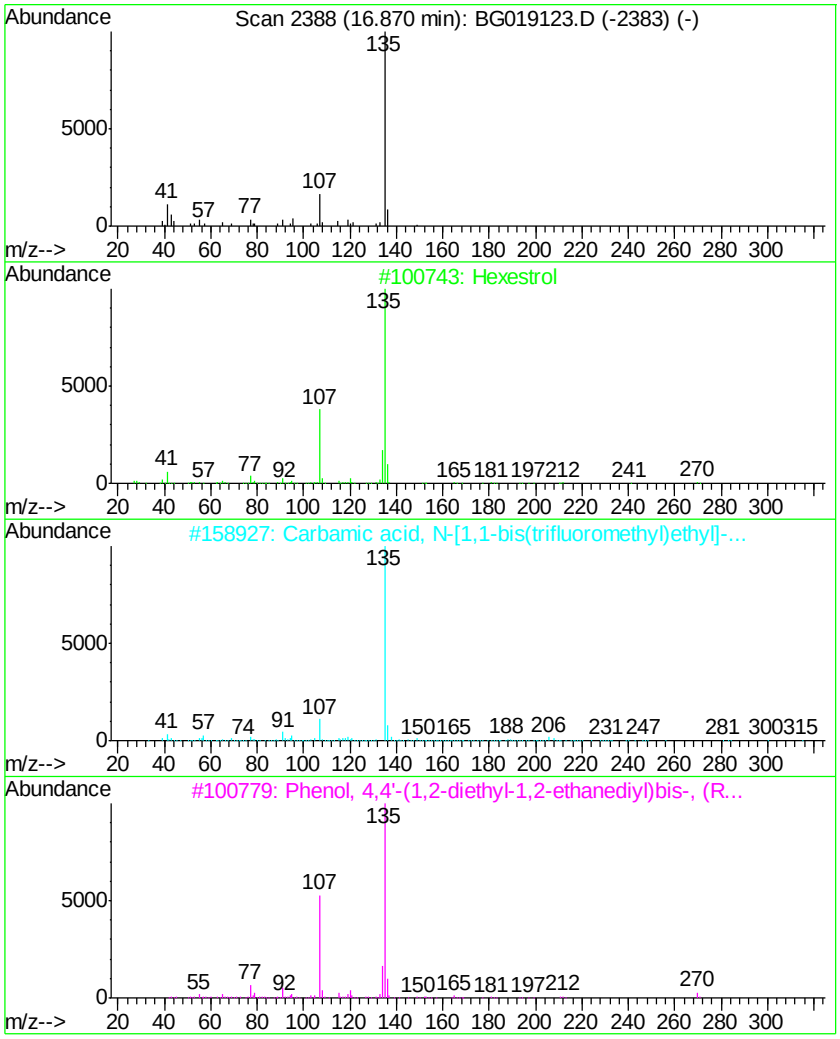
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

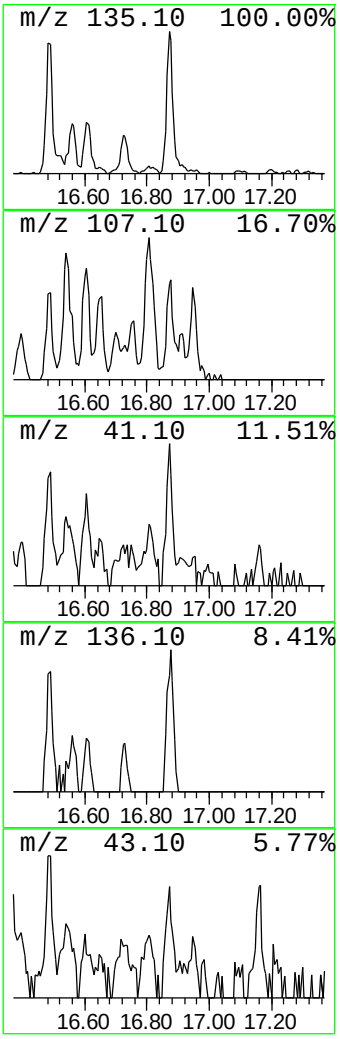
****

Peak Number 10 Hexestrol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.87	2.47 ng	42448	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexestrol	270	C18H22O2	005635-50-7	78
2	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	78
3	Phenol, 4,4'-(1,2-diethyl-1,2-et...	270	C18H22O2	000084-16-2	50
4	1-Adamantanecarboxylic acid, 2-i...	314	C20H26O3	1000293-75-6	45
5	1-Adamantanemethanol	166	C11H18O	000770-71-8	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101015\
Data File : BG019123.D
Acq On : 10 Oct 2015 18:43
Operator : UM/NP
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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...	3.22	58.0	ng	284332	1	8.03	98106	20.0
2-Pentanone, 4-hy...	5.14	15.4	ng	75506	1	8.03	98106	20.0
unknown7.56	7.56	97.9	ng	480283	1	8.03	98106	20.0
Phenol, 4-(1,1,3,...	16.49	2.3	ng	39222	4	17.40	344318	20.0
Phenol, 4,4'-(1,2...	16.61	2.1	ng	36714	4	17.40	344318	20.0
2-Methyl-4-hydrox...	16.81	2.1	ng	35752	4	17.40	344318	20.0
Hexestrol	16.87	2.5	ng	42448	4	17.40	344318	20.0