LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
Data File : BG016351.D
Acq On : 11 Apr 2015 12:52
Operator : TP/IZ
Sample : G1822-04MSD
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : F5-025MSD

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-BG040615.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	2.794	13	18	27	rVV	130759	218365	11.57%	1.433%
2	2.871	27	31	36	rVV	92716	111614	5.91%	0.732%
3	2.912	36	38	43	rVB2	18316	21460	1.14%	0.141%
4	4.205	254	258	263	rBV	28319	36065	1.91%	0.237%
5	4.804	353	360	369	rVB	119014	171018	9.06%	1.122%
6	5.280	435	441	449	rBV	823775	1142199	60.49%	7.495%
7	6.872	705	712	728	rBV	813408	1260460	66.76%	8.271%
8	7.225	766	772	782	rBV	819370	1263030	66.89%	8.288%
9	7.689	845	851	857	rBV	222441	351189	18.60%	2.304%
10	8.006	899	905	915	rBV	571037	911363	48.27%	5.980%
11	8.846	1041	1048	1061	rBV	466301	761398	40.33%	4.996%
12	10.474	1318	1325	1333	rBV	333741	540991	28.65%	3.550%
13	12.947	1740	1746	1763	rVB	1005149	1488417	78.83%	9.767%
14	13.787	1883	1889	1900	rBV	61296	87765	4.65%	0.576%
15	14.328	1975	1981	1990	rBV2	505929	749812	39.71%	4.920%
16	15.180	2123	2126	2131	rVB	23084	25484	1.35%	0.167%
17	15.820	2226	2235	2246	rBV	728484	1040809	55.12%	6.830%
18	16.044	2268	2273	2276	rBV	24425	32701	1.73%	0.215%
19	17.072	2442	2448	2458	rBV2	637930	872018	46.18%	5.722%
20	17.965	2596	2600	2609	rBV	46265	81382	4.31%	0.534%
21	19.246	2815	2818	2824	rBV4	20191	33566	1.78%	0.220%
22	19.698	2889	2895	2905	rBV	1520320	1888100	100.00%	12.390%
23	20.386	3004	3012	3017	rBV4	14347	25401	1.35%	0.167%
24	20.956	3105	3109	3121	rBV	171690	266354	14.11%	1.748%
25	21.044	3121	3124	3131	rVB7	11743	20312	1.08%	0.133%
26	21.249	3153	3159	3167	rBV	671933	878329	46.52%	5.764%
27	21.396	3181	3184	3189	rBV4	17437	24886	1.32%	0.163%
28	21.825	3254	3257	3263	rBV5	13184	23047	1.22%	0.151%
29	22.283	3333	3335	3341	rVB4	19561	23675	1.25%	0.155%
30	22.413	3354	3357	3362	rVB3	18454	25701	1.36%	0.169%
31	22.795	3419	3422	3426	rVB3	17588	22364	1.18%	0.147%
32	23.488	3533	3540	3553	rVB2	439867	840150	44.50%	5.513%

LSC Area Percent Report

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Data File : BG016351.D
Acq On : 11 Apr 2015 12:52
Operator : TP/IZ
Sample : G1822-04MSD
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5-025MSD

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-BG040615.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

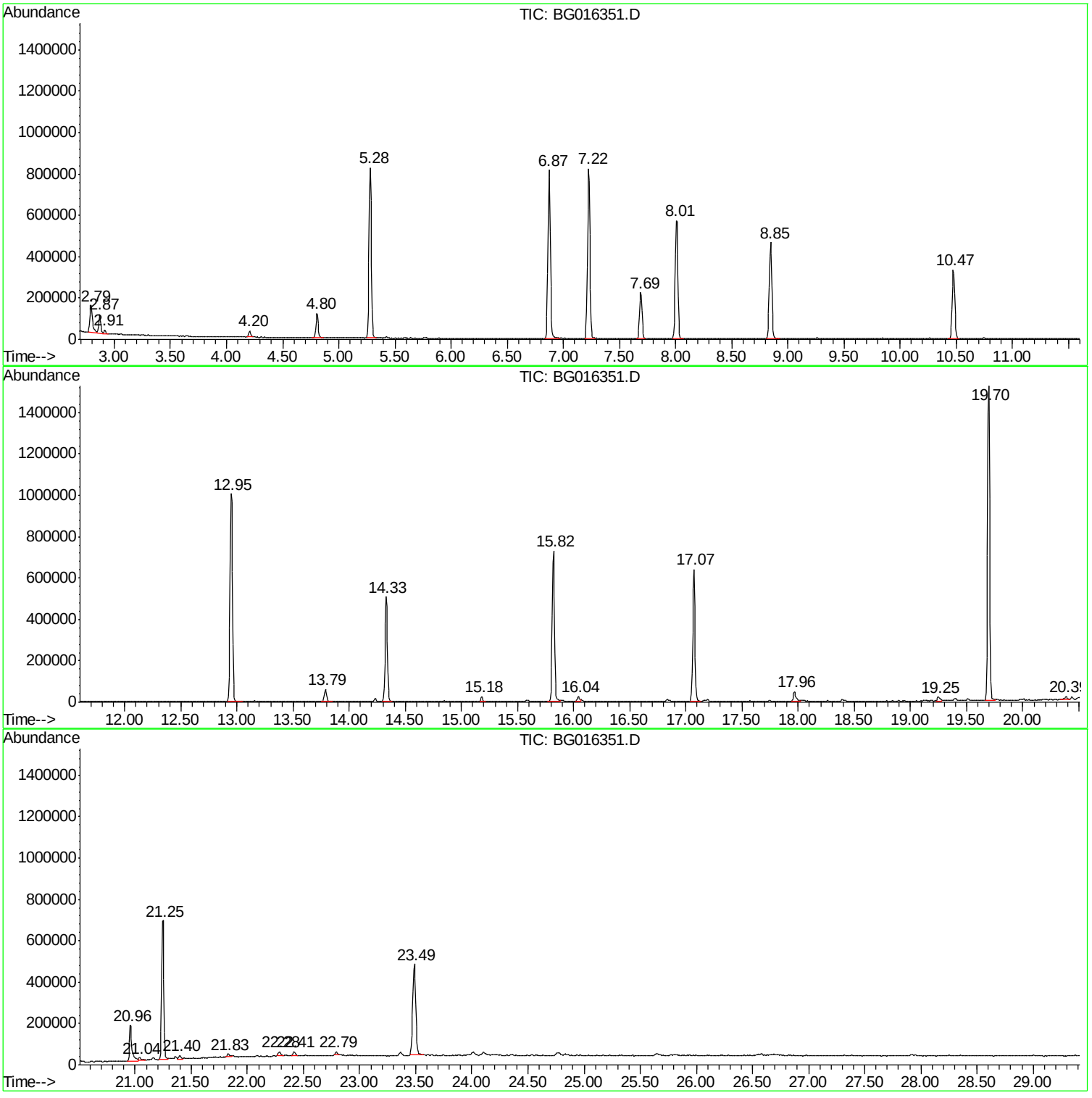
Sum of corrected areas: 15239425

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
Data File : BG016351.D
Acq On : 11 Apr 2015 12:52
Operator : TP/IZ
Sample : G1822-04MSD
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5-025MSD

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
Data File : BG016351.D
Acq On : 11 Apr 2015 12:52
Operator : TP/IZ
Sample : G1822-04MSD
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ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : F5-025MSD

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

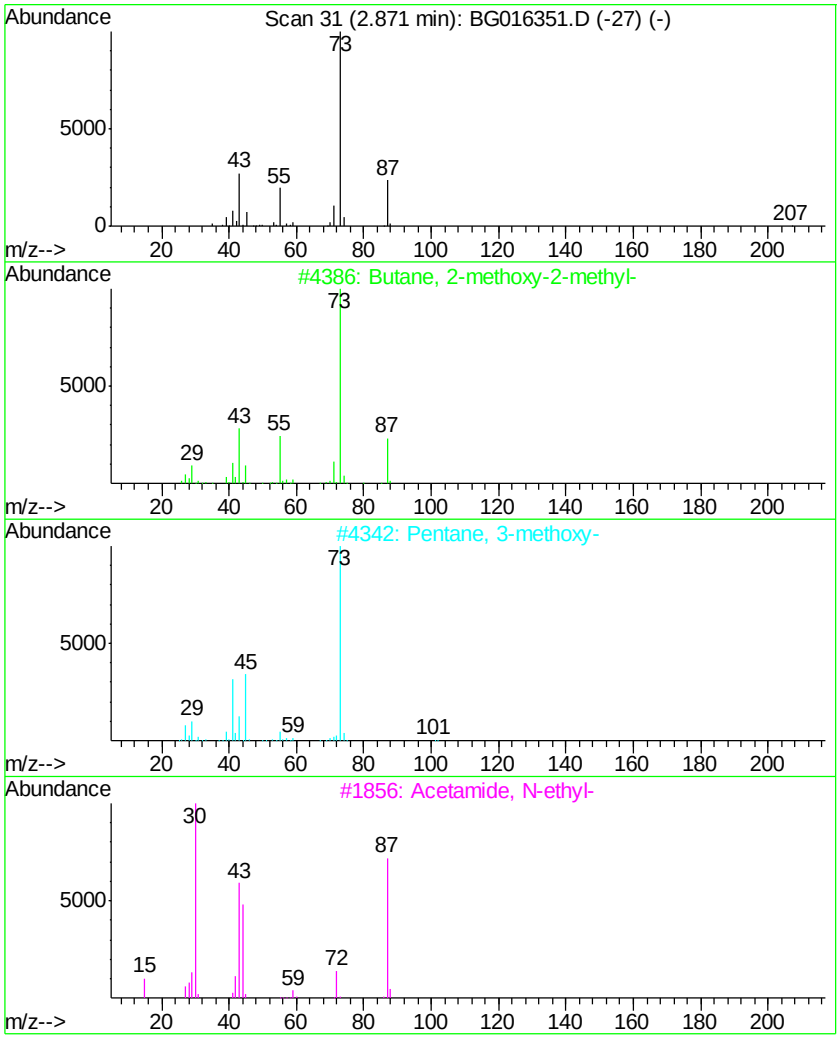
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

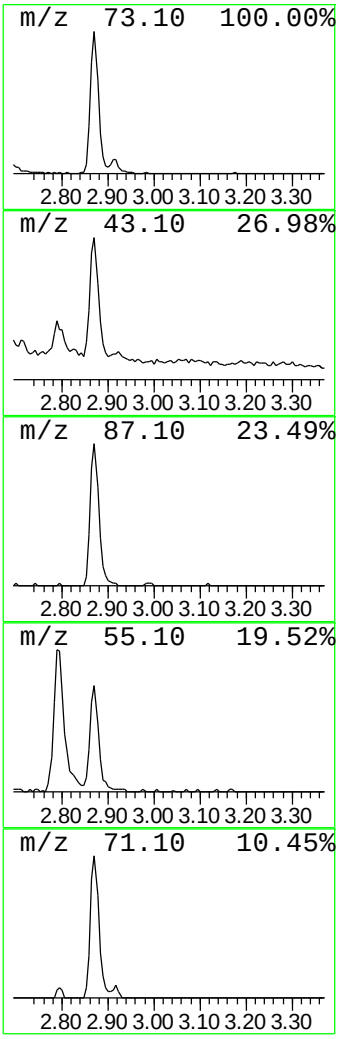
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	6.36 ng	111614	1,4-Dichlorobenzene-d4	7.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
Data File : BG016351.D
Acq On : 11 Apr 2015 12:52
Operator : TP/IZ
Sample : G1822-04MSD
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : F5-025MSD

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

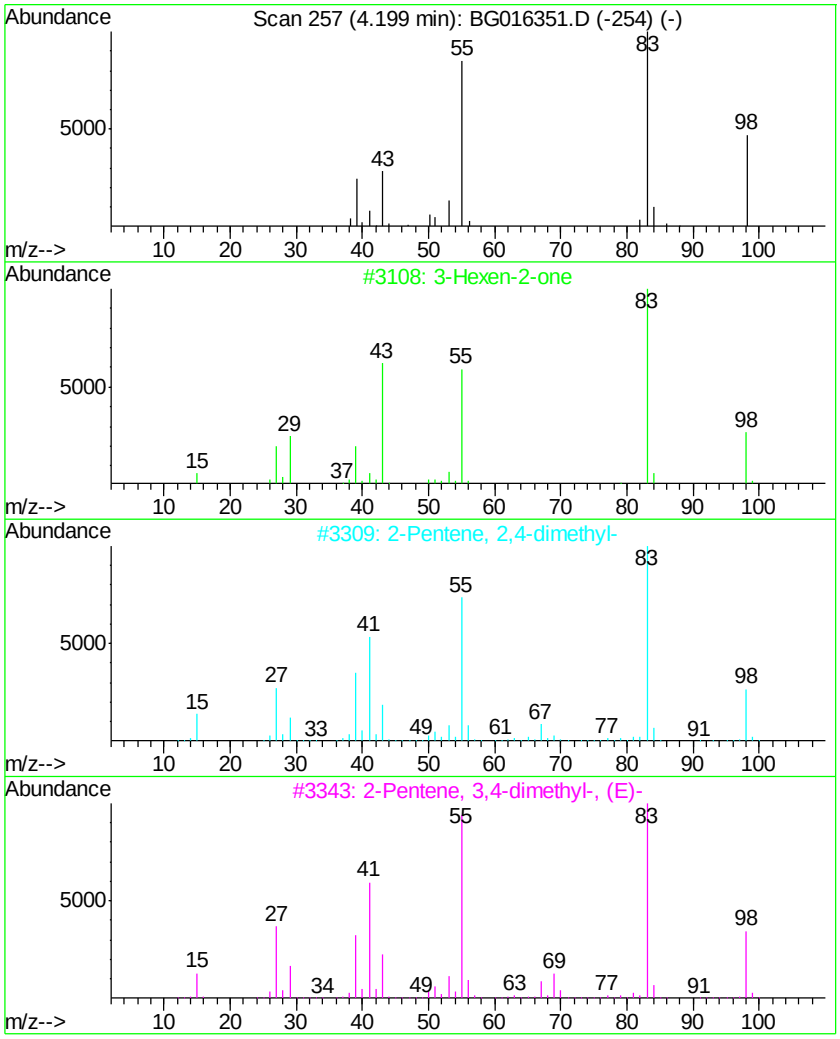
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

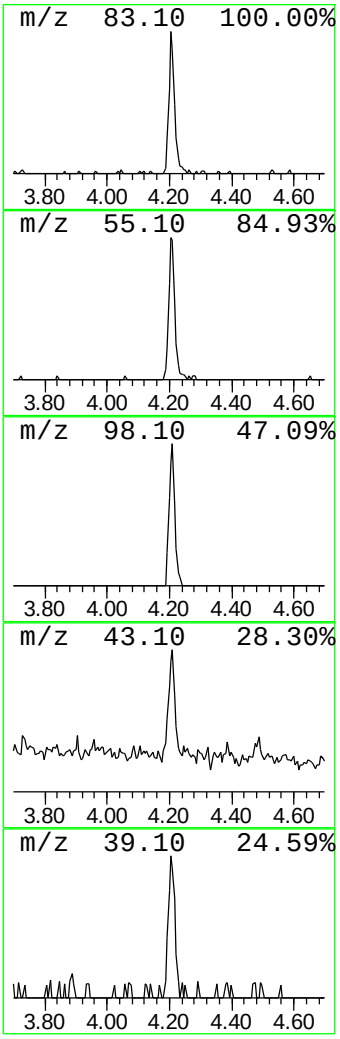
****

Peak Number 3 3-Hexen-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	2.05 ng	36065	1,4-Dichlorobenzene-d4	7.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	90
2	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	83
4	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	83
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
Data File : BG016351.D
Acq On : 11 Apr 2015 12:52
Operator : TP/IZ
Sample : G1822-04MSD
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : F5-025MSD

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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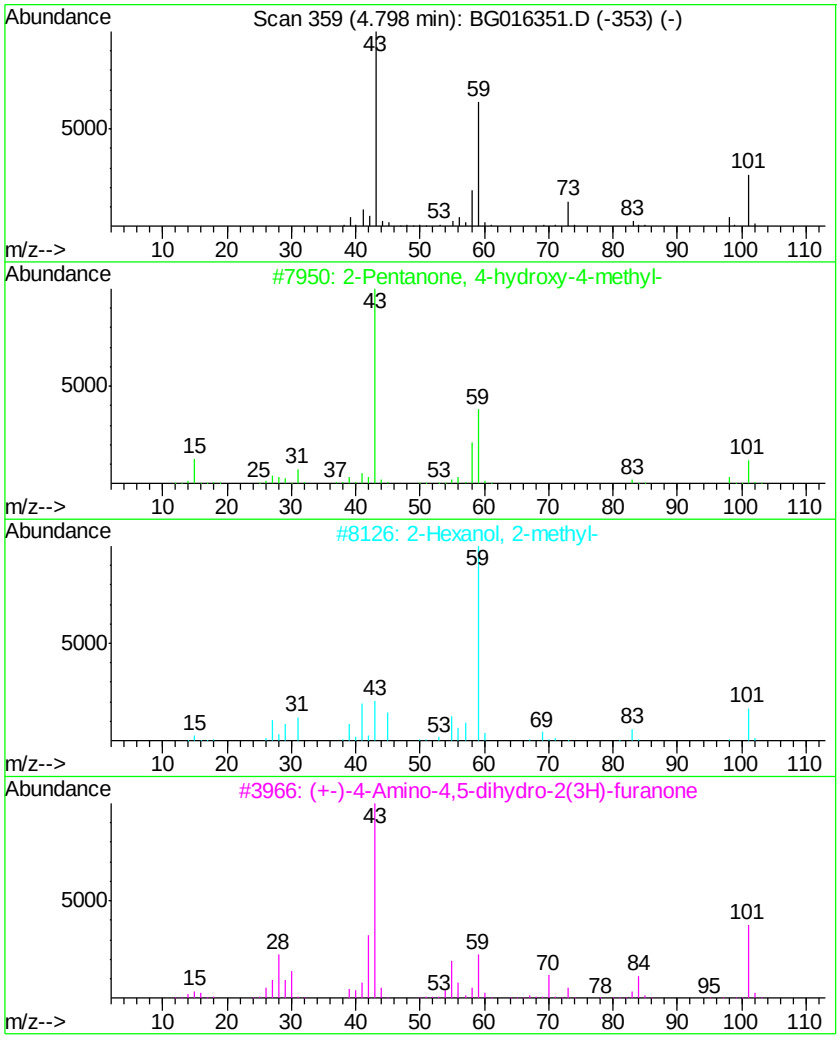
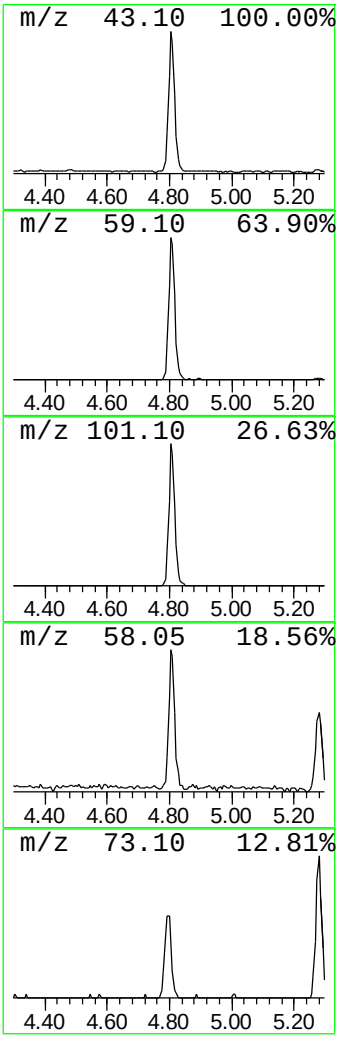
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	9.74 ng	171018	1,4-Dichlorobenzene-d4	7.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	32
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	23
4	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	23
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17





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Acq On : 11 Apr 2015 12:52
Operator : TP/IZ
Sample : G1822-04MSD
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : F5-025MSD

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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TIC Library : C:\DATABASE\NIST02.L
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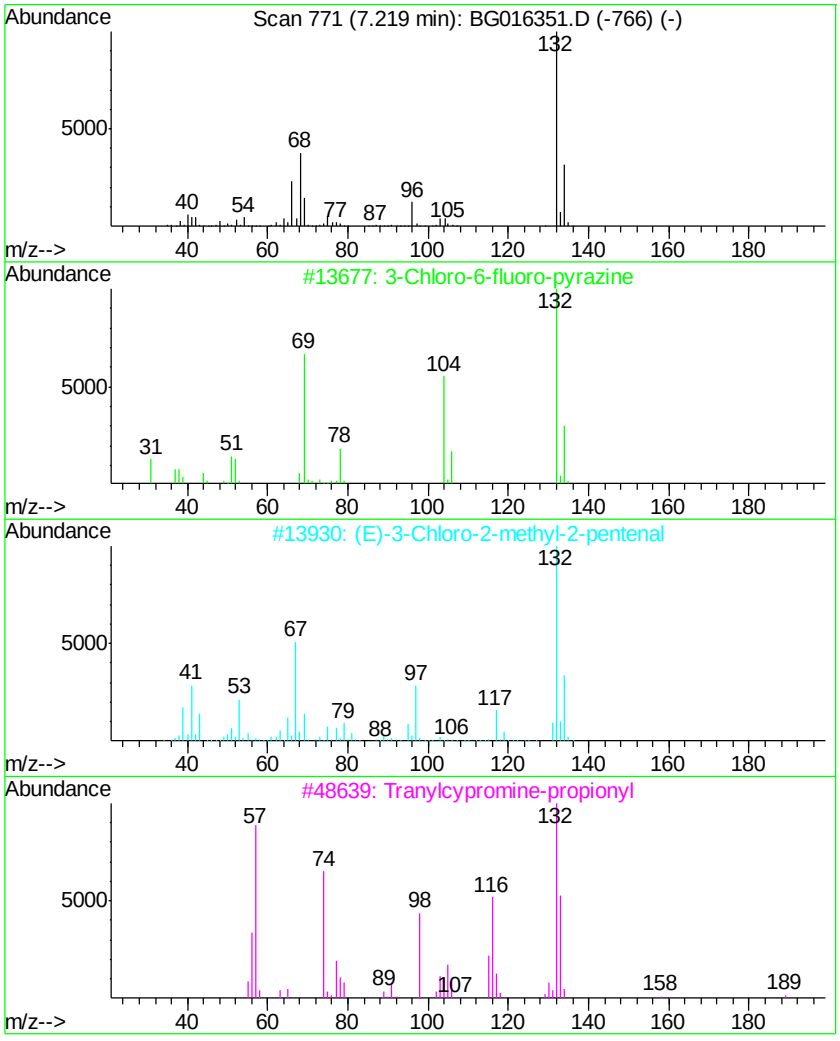
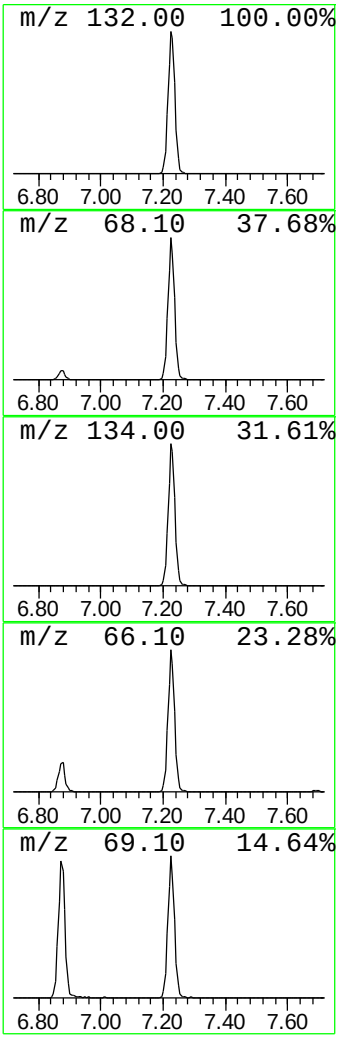
****

Peak Number 5 unknown7.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	71.93 ng	1263030	1,4-Dichlorobenzene-d4	7.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Misc :
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Instrument : BNA_G
ClientSampleId : F5-025MSD

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

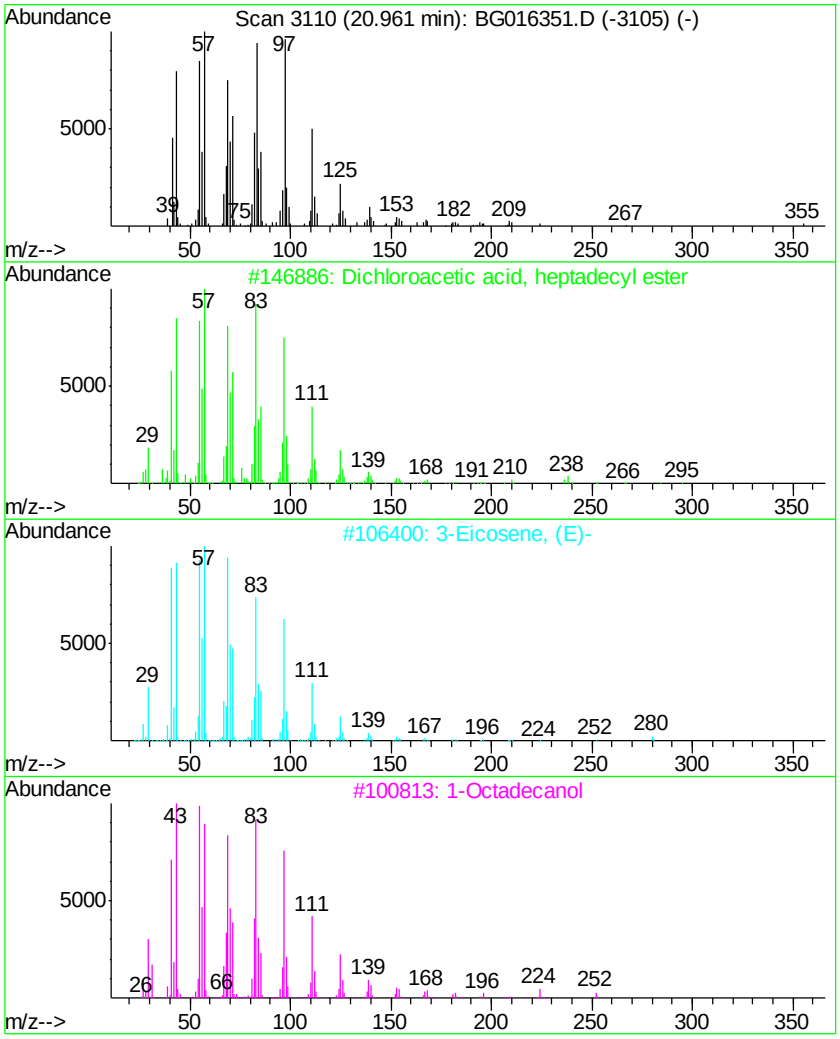
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

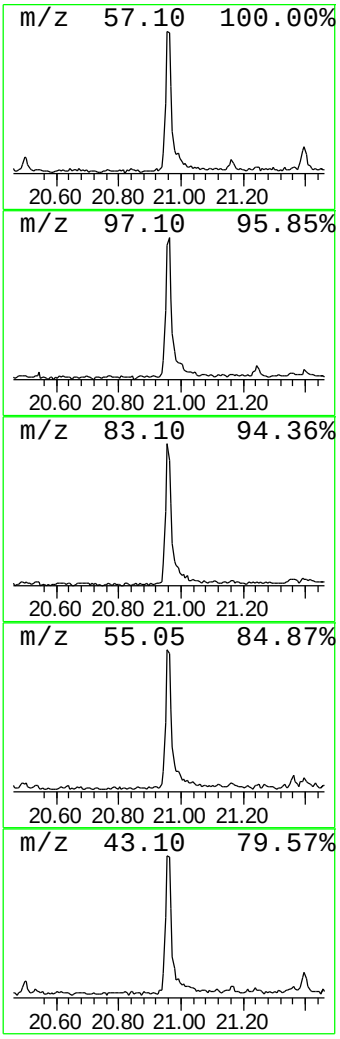
****

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.96	6.07 ng	266354	Chrysene-d12	21.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Octadecanol	270	C18H38O	000112-92-5	90
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
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Acq On : 11 Apr 2015 12:52
Operator : TP/IZ
Sample : G1822-04MSD
Misc :
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Instrument : BNA_G
ClientSampleId : F5-025MSD

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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...	2.87	6.4	ng	111614	1	7.69	351189	20.0
3-Hexen-2-one	4.20	2.0	ng	36065	1	7.69	351189	20.0
2-Pentanone, 4-hy...	4.80	9.7	ng	171018	1	7.69	351189	20.0
unknown7.22	7.22	71.9	ng	1263030	1	7.69	351189	20.0
Dichloroacetic ac...	20.96	6.1	ng	266354	5	21.25	878329	20.0