LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
Data File : BG016355.D
Acq On : 11 Apr 2015 15:12
Operator : TP/IZ
Sample : G1791-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LS-SD04C

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	2.790	13	17	27	rVV	132253	209169	11.08%	1.336%
2	2.872	27	31	35	rVV	86980	109604	5.80%	0.700%
3	2.913	35	38	44	rVB2	19205	25330	1.34%	0.162%
4	4.206	254	258	264	rBV	29587	39250	2.08%	0.251%
5	4.805	354	360	370	rVB	124646	172898	9.16%	1.104%
6	5.281	434	441	452	rBV	833082	1178603	62.41%	7.527%
7	6.873	704	712	723	rBV	871093	1321970	70.00%	8.443%
8	7.226	764	772	785	rBV	860602	1322304	70.02%	8.445%
9	7.690	844	851	858	rBV	234536	356574	18.88%	2.277%
10	8.007	898	905	913	rBV	594713	941478	49.85%	6.013%
11	8.847	1040	1048	1057	rBV	487518	776805	41.13%	4.961%
12	10.475	1318	1325	1332	rBV	340490	558921	29.60%	3.570%
13	12.948	1739	1746	1756	rBV	1084492	1555489	82.37%	9.935%
14	13.789	1883	1889	1899	rBV	65043	87900	4.65%	0.561%
15	14.329	1974	1981	1991	rVB2	528624	784630	41.55%	5.011%
16	15.181	2120	2126	2132	rVB	23384	29884	1.58%	0.191%
17	15.816	2228	2234	2244	rBV	753416	1060919	56.18%	6.776%
18	16.039	2268	2272	2281	rBV	24428	39657	2.10%	0.253%
19	17.067	2441	2447	2458	rBV2	626391	890410	47.15%	5.687%
20	17.966	2595	2600	2608	rBV2	50057	85040	4.50%	0.543%
21	19.247	2814	2818	2826	rBV4	19931	36696	1.94%	0.234%
22	19.394	2839	2843	2848	rBV3	17037	19495	1.03%	0.125%
23	19.693	2889	2894	2905	rBV	1499527	1888459	100.00%	12.061%
24	20.387	3007	3012	3018	rBV3	13628	23359	1.24%	0.149%
25	20.957	3105	3109	3120	rBV	190443	269574	14.27%	1.722%
26	21.244	3153	3158	3170	rBV	659726	894528	47.37%	5.713%
27	21.397	3181	3184	3192	rVB4	15751	20913	1.11%	0.134%
28	21.826	3254	3257	3261	rBV3	15826	22668	1.20%	0.145%
29	22.284	3332	3335	3342	rVB5	21320	30432	1.61%	0.194%
30	22.414	3354	3357	3362	rVB2	19265	26012	1.38%	0.166%
31	22.796	3418	3422	3428	rVB4	19850	26733	1.42%	0.171%
32	23.489	3532	3540	3552	rBV2	439019	851681	45.10%	5.439%

LSC Area Percent Report

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Data File : BG016355.D
Acq On : 11 Apr 2015 15:12
Operator : TP/IZ
Sample : G1791-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LS-SD04C

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

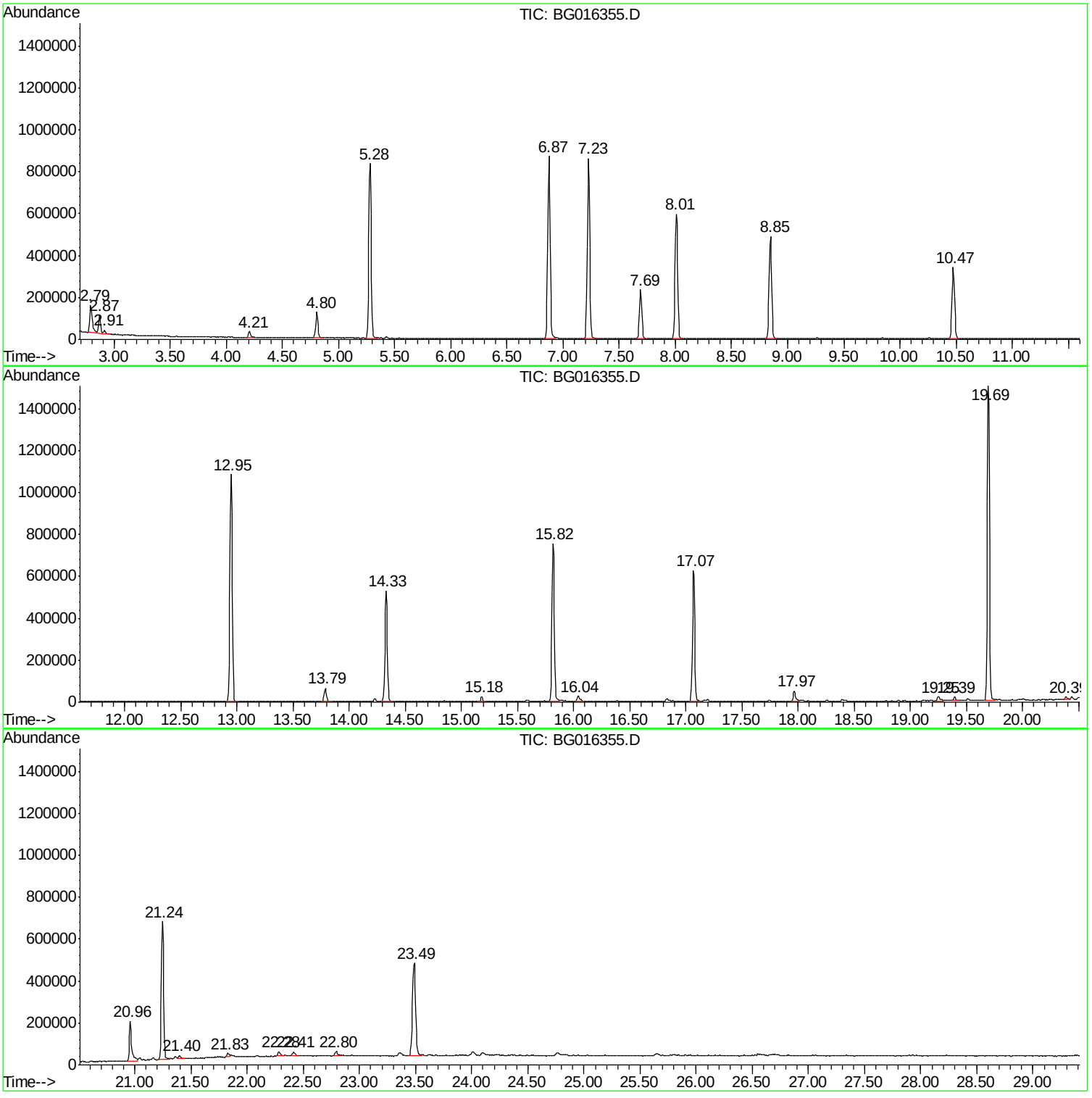
Sum of corrected areas: 15657385

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
Data File : BG016355.D
Acq On : 11 Apr 2015 15:12
Operator : TP/IZ
Sample : G1791-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LS-SD04C

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\
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Acq On : 11 Apr 2015 15:12
Operator : TP/IZ
Sample : G1791-11
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Instrument : BNA_G
ClientSampleId : LS-SD04C

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

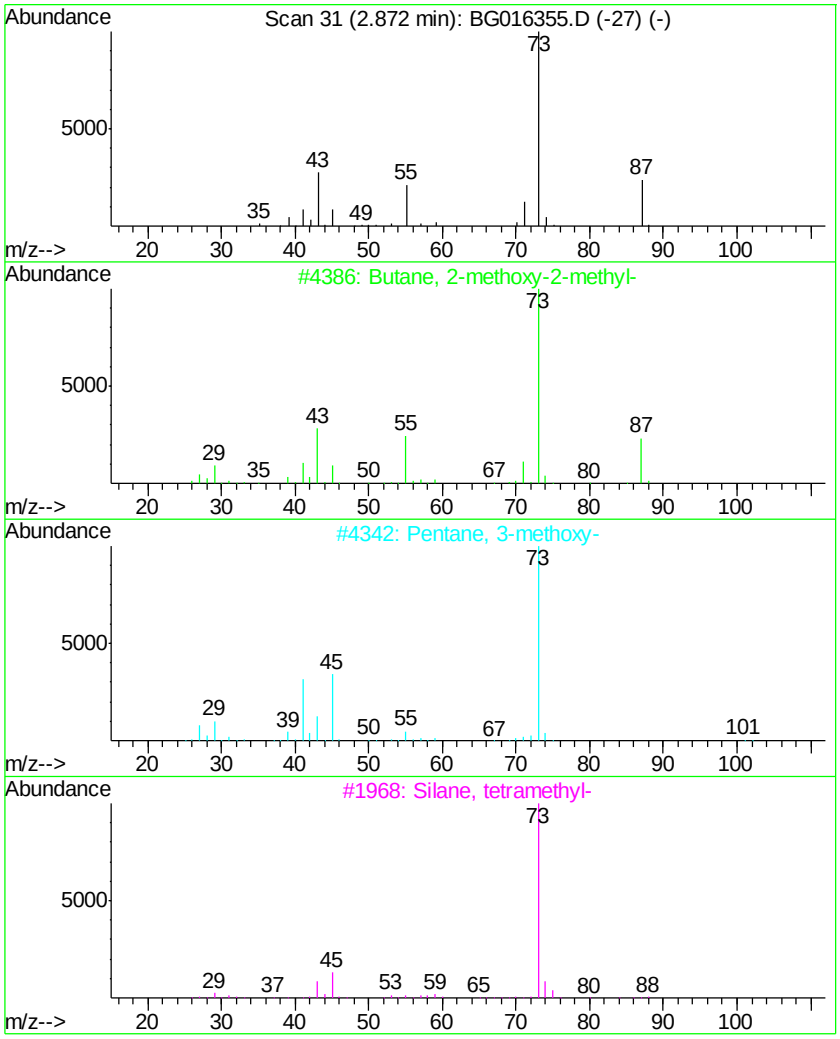
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

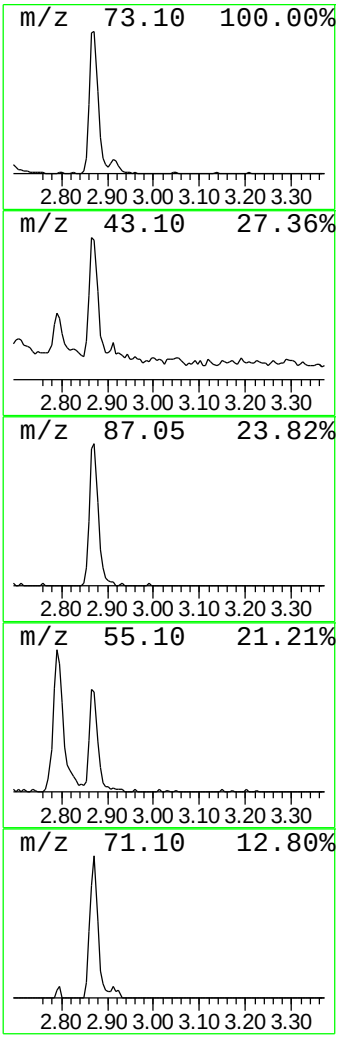
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	6.15 ng	109604	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	17
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
Data File : BG016355.D
Acq On : 11 Apr 2015 15:12
Operator : TP/IZ
Sample : G1791-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LS-SD04C

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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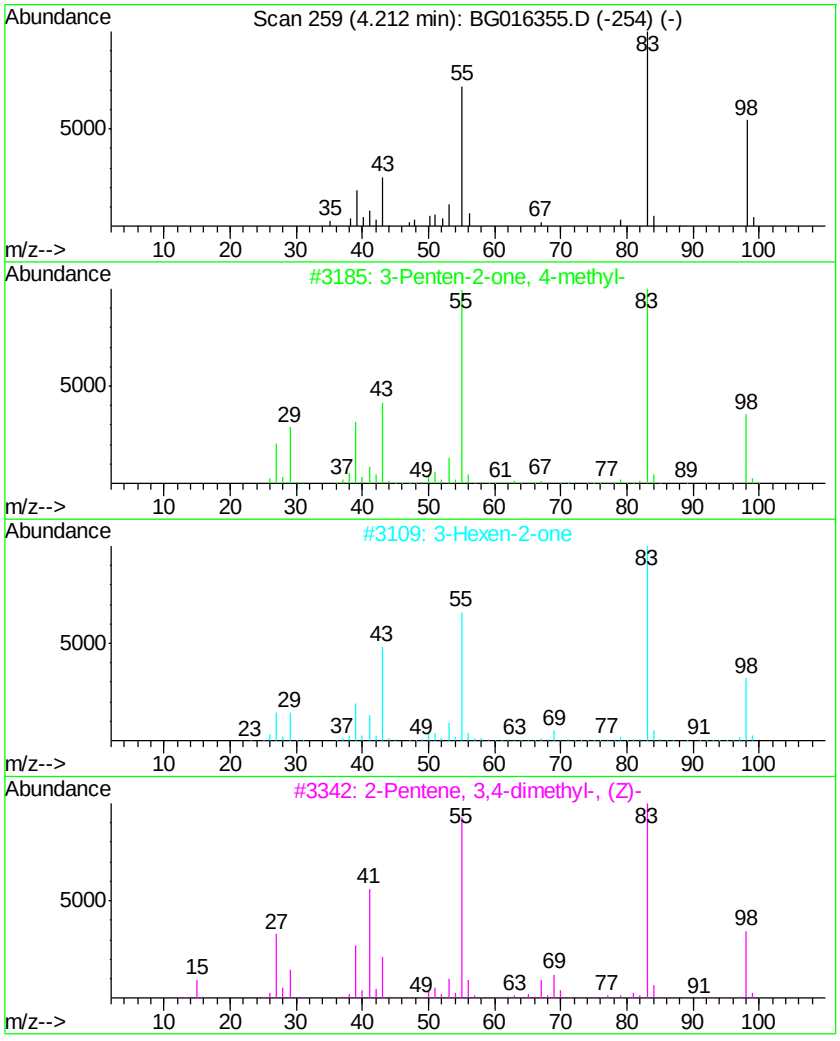
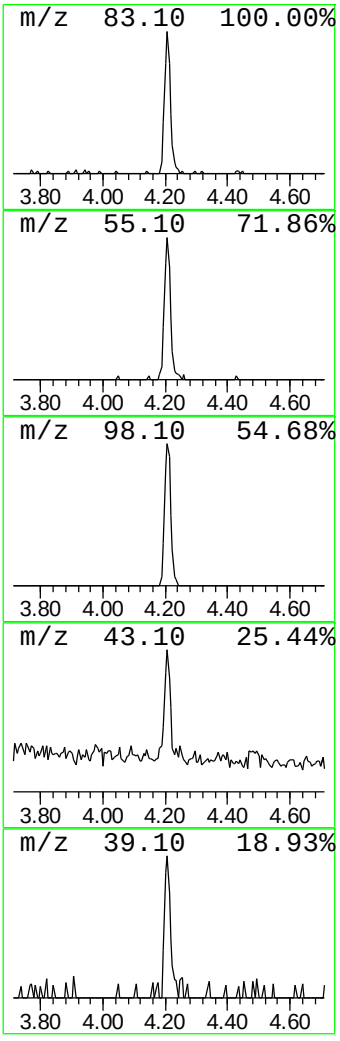
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.21	2.20 ng	39250	1,4-Dichlorobenzene-d4	7.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	83
2	3-Hexen-2-one	98	C6H10O	000763-93-9	83
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5	Furan, 2,5-dihydro-2,5-dimethyl-	98	C6H10O	059242-27-2	72





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
Data File : BG016355.D
Acq On : 11 Apr 2015 15:12
Operator : TP/IZ
Sample : G1791-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LS-SD04C

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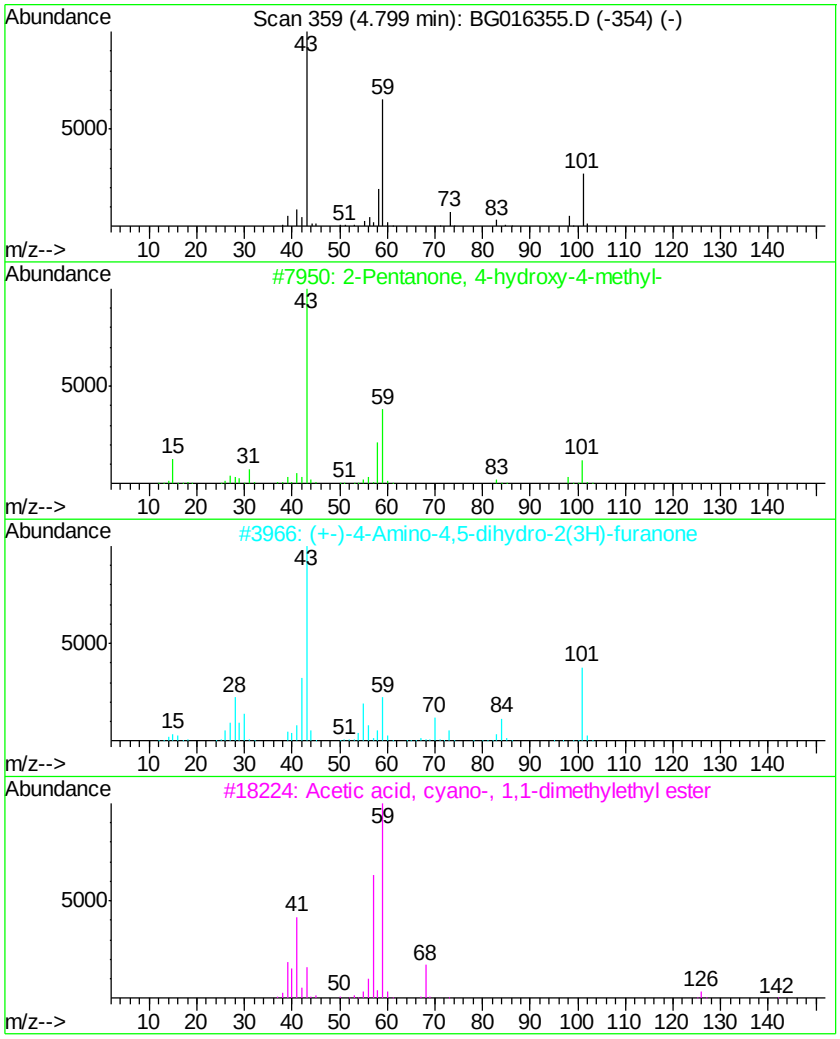
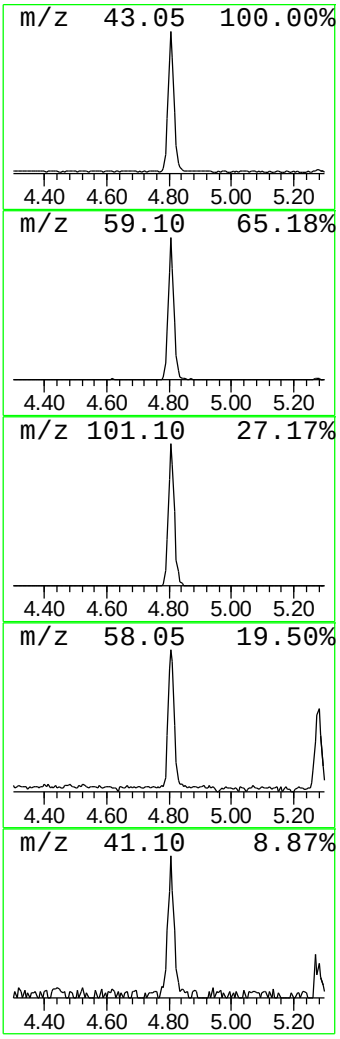
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	9.70 ng	172898	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	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	32
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 11 Apr 2015 15:12
Operator : TP/IZ
Sample : G1791-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LS-SD04C

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
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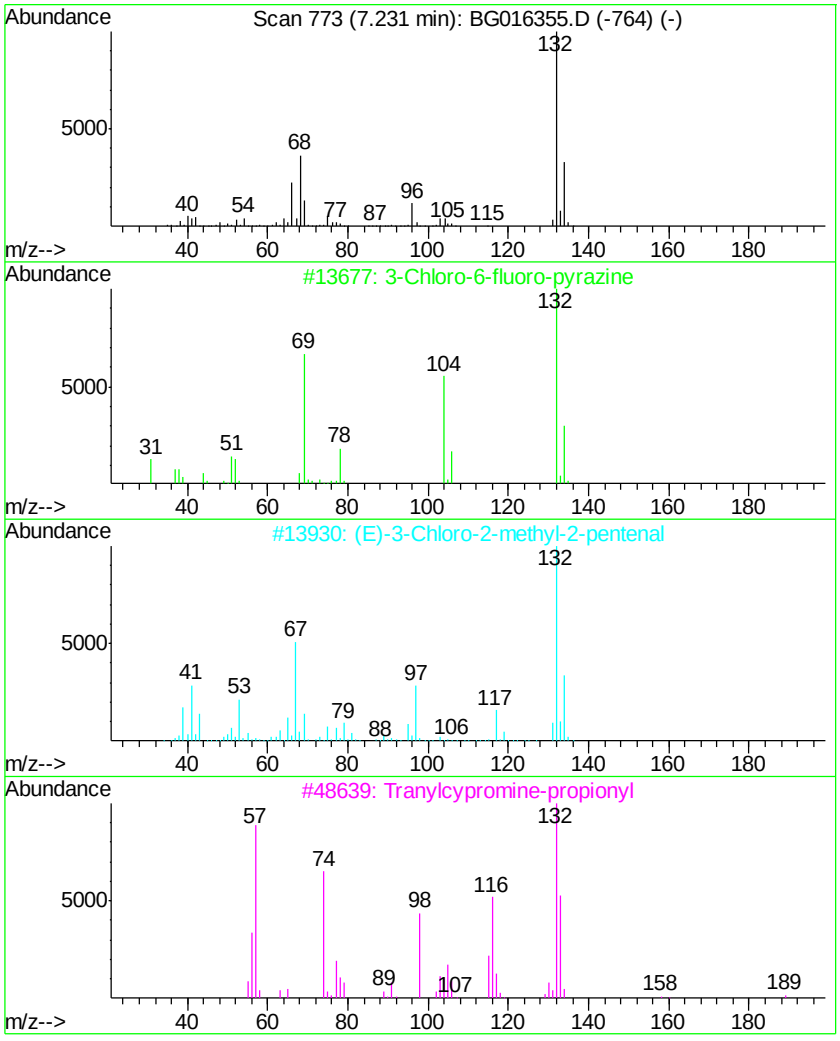
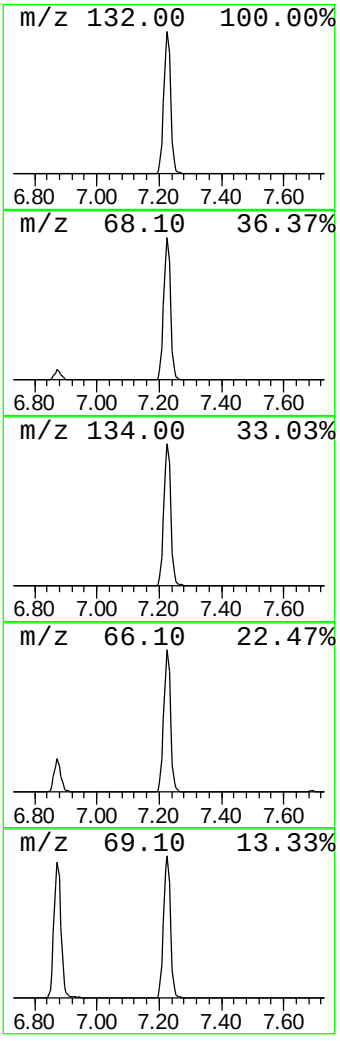
****

Peak Number 5 unknown7.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	74.17 ng	1322300	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	38
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-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : G1791-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LS-SD04C

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

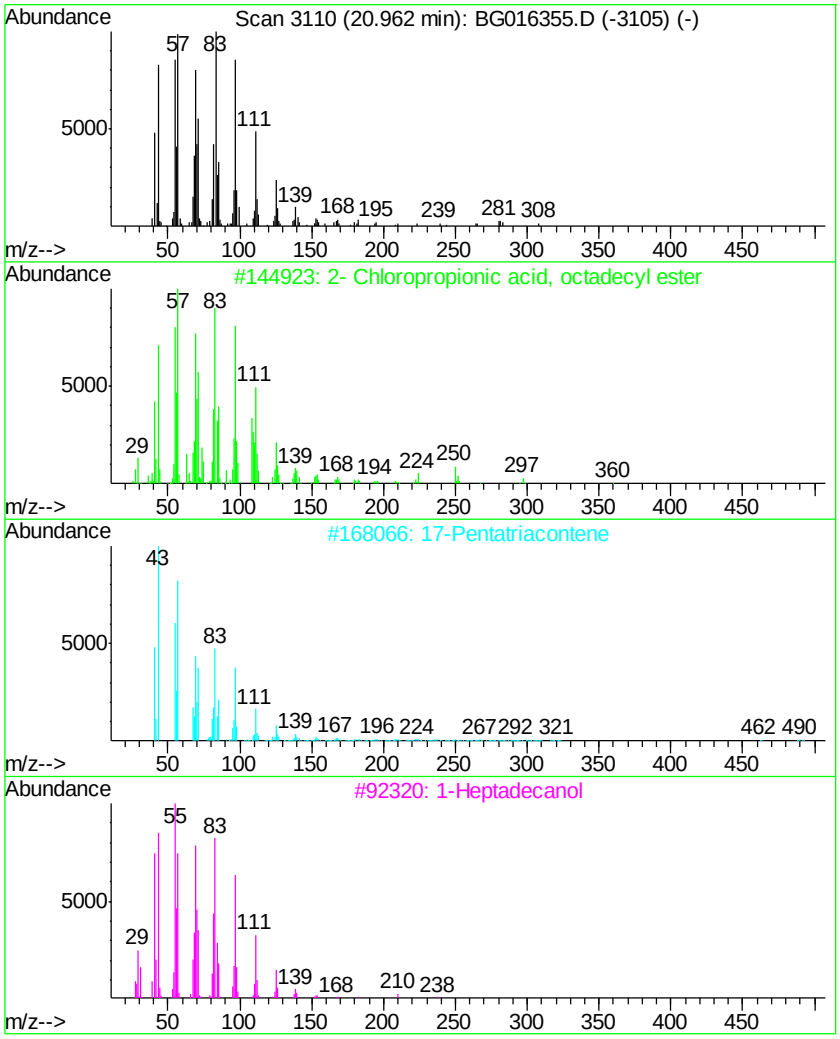
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

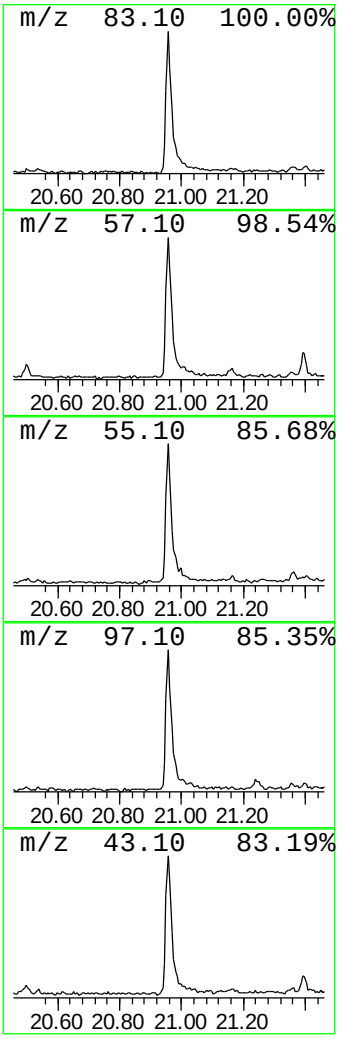
****

Peak Number 7 2- Chloropropionic acid, oc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.96	6.03 ng	269574	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	1-Heptadecanol	256	C17H36O	001454-85-9	91
4	1-Octadecanol	270	C18H38O	000112-92-5	87
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041015\
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Instrument : BNA_G
ClientSampleId : LS-SD04C

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	6.2	ng	109604	1	7.69	356574	20.0
3-Penten-2-one, 4...	4.21	2.2	ng	39250	1	7.69	356574	20.0
2-Pentanone, 4-hy...	4.80	9.7	ng	172898	1	7.69	356574	20.0
unknown7.23	7.23	74.2	ng	1322300	1	7.69	356574	20.0
2- Chloropropioni...	20.96	6.0	ng	269574	5	21.24	894528	20.0