LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081516\
Data File : BG023721.D
Acq On : 15 Aug 2016 14:43
Operator : UM/SJ
Sample : H4452-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

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-BG080116.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	2.984	19	25	46	rBV	6550737	11164147	100.00%	16.885%
2	5.169	390	397	407	rBV	767209	1213471	10.87%	1.835%
3	5.651	471	479	488	rBV	2913646	4850928	43.45%	7.337%
4	7.267	745	754	766	rBV	2997568	5348112	47.90%	8.089%
5	7.637	809	817	832	rBV	3030519	5256773	47.09%	7.951%
6	8.107	888	897	905	rBV	509405	886145	7.94%	1.340%
7	8.430	944	952	961	rBV	2089667	3717083	33.29%	5.622%
8	9.287	1089	1098	1108	rBV	1894835	3451394	30.91%	5.220%
9	10.944	1372	1380	1390	rBV	708418	1301482	11.66%	1.968%
10	13.394	1789	1797	1804	rBV	4022845	6463341	57.89%	9.775%
11	14.222	1931	1938	1944	rBV	1222213	1789823	16.03%	2.707%
12	14.780	2026	2033	2042	rBV2	987557	1606077	14.39%	2.429%
13	15.602	2168	2173	2178	rVB	91988	122138	1.09%	0.185%
14	16.284	2282	2289	2306	rBV	2833930	4987892	44.68%	7.544%
15	16.466	2316	2320	2330	rVB	109113	206543	1.85%	0.312%
16	17.547	2496	2504	2509	rBV	1091433	1694945	15.18%	2.564%
17	17.588	2509	2511	2518	rVB	84094	122612	1.10%	0.185%
18	19.609	2848	2855	2860	rBV	221649	323238	2.90%	0.489%
19	19.973	2907	2917	2922	rVB	200928	334635	3.00%	0.506%
20	20.161	2943	2949	2955	rBV	5295026	6971920	62.45%	10.545%
21	21.483	3169	3174	3180	rBV8	85075	182885	1.64%	0.277%
22	21.876	3233	3241	3247	rBV	1146879	2180400	19.53%	3.298%
23	25.283	3811	3821	3833	rBV3	616529	1942367	17.40%	2.938%

Sum of corrected areas: 66118351

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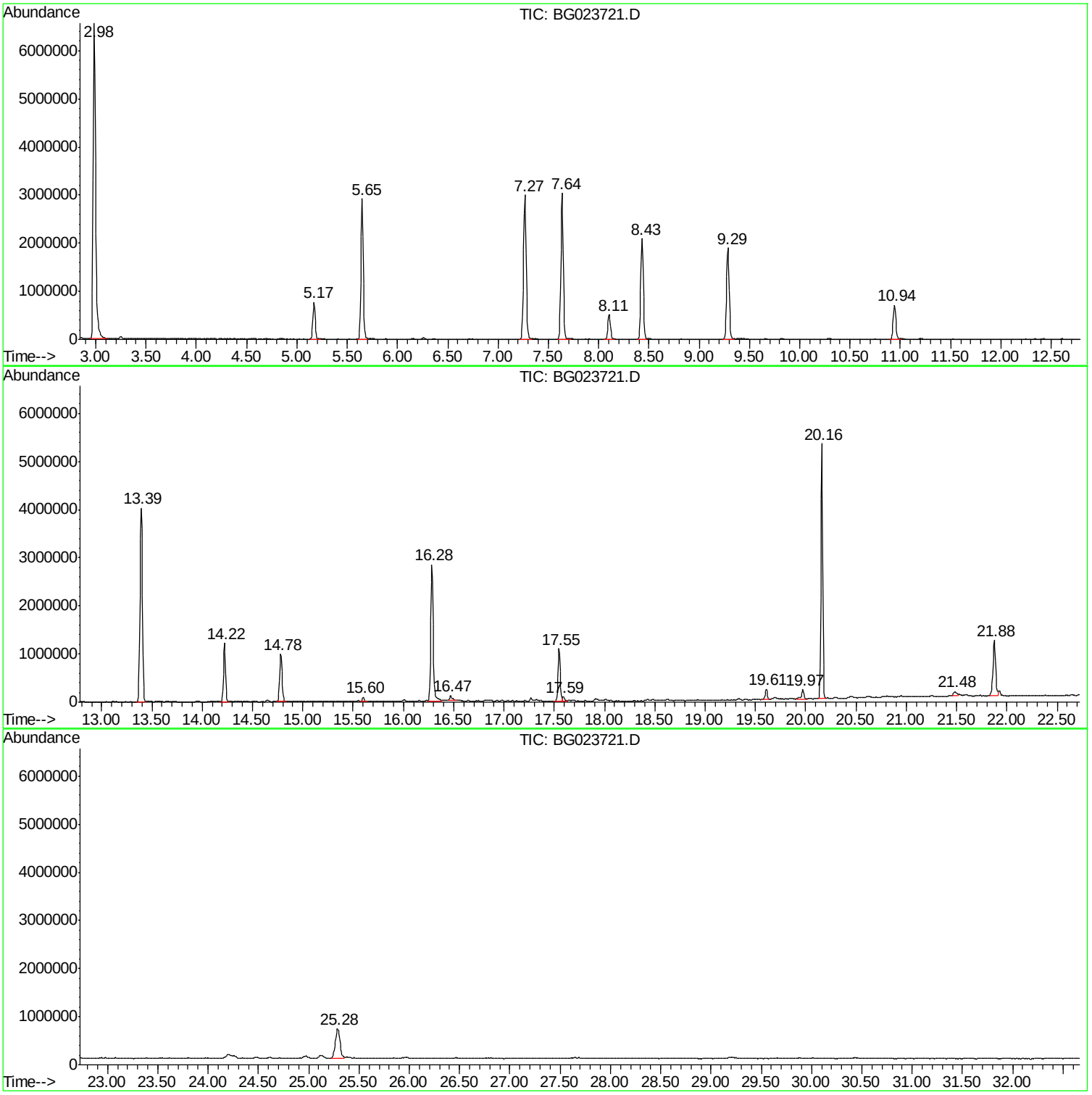
Instrument :
BNA_G
ClientSampleId :
S-2

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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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Data File : BG023721.D
Acq On : 15 Aug 2016 14:43
Operator : UM/SJ
Sample : H4452-03
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
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TIC Integration Parameters: LSCINT.P

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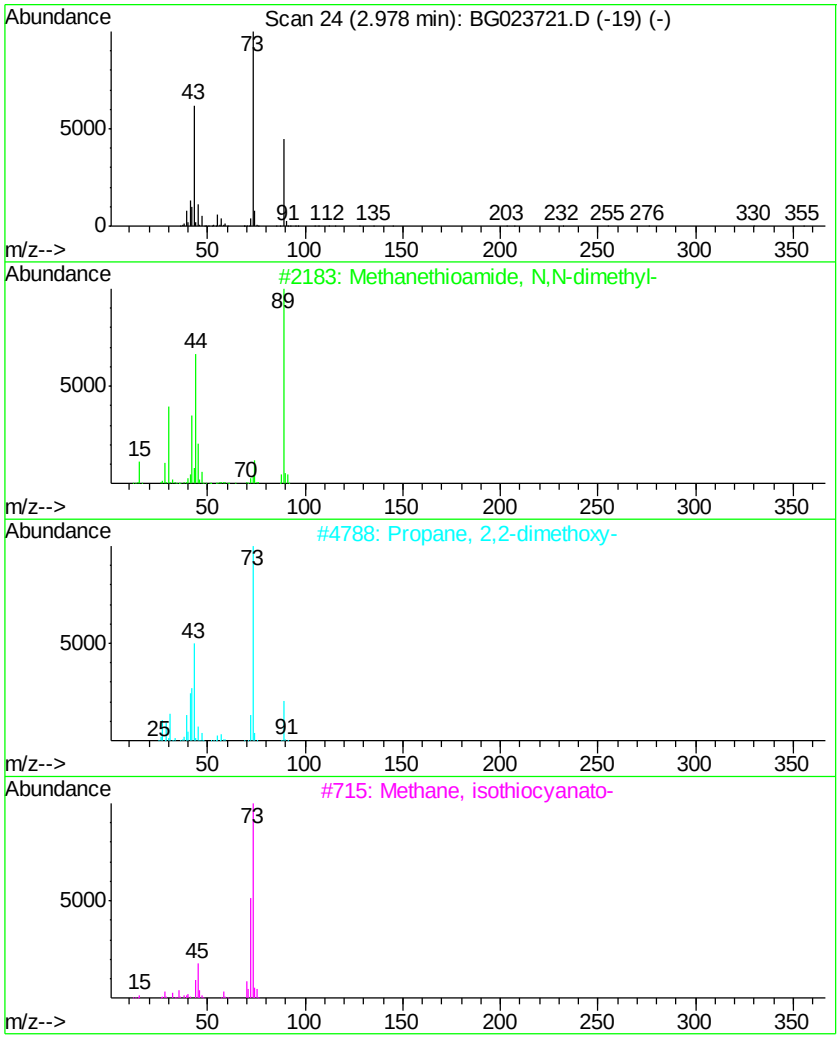
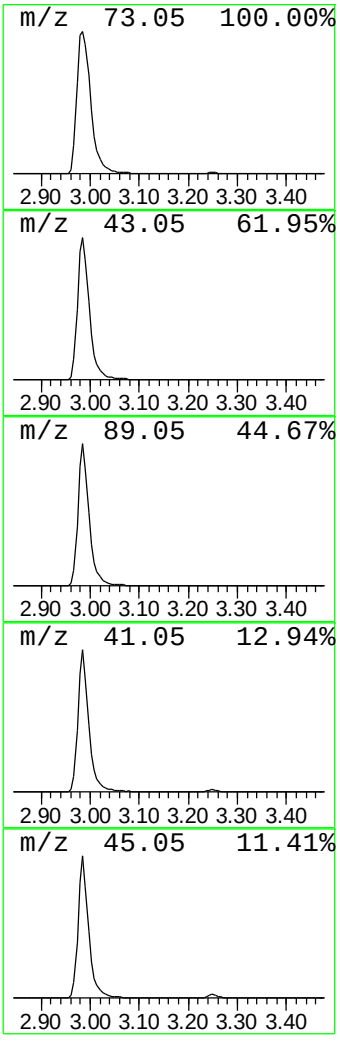
Peak Number 1 unknown2.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	251.97 ng	11164100	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	47
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	12
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Data File : BG023721.D
Acq On : 15 Aug 2016 14:43
Operator : UM/SJ
Sample : H4452-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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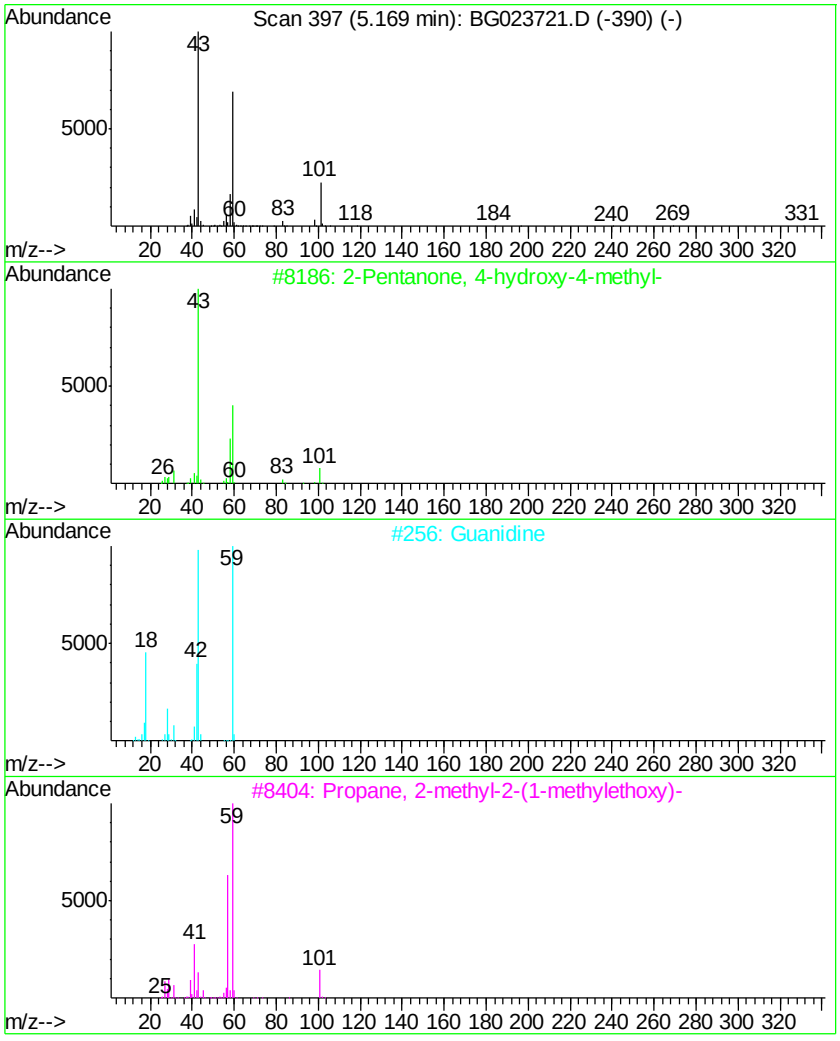
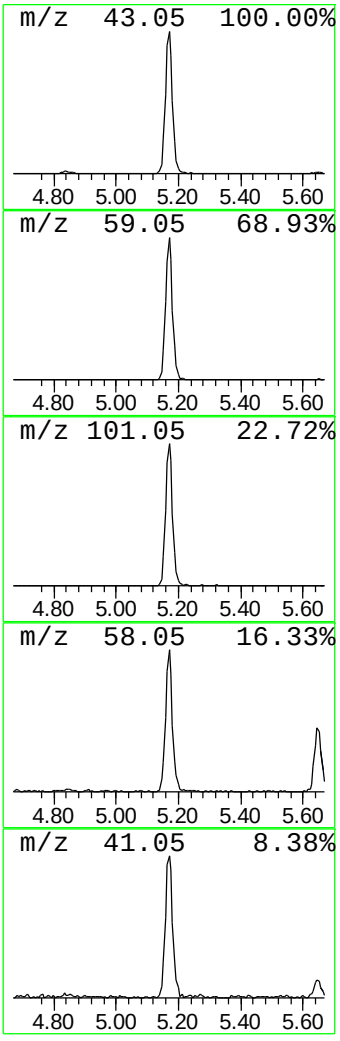
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	27.39 ng	1213470	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081516\
Data File : BG023721.D
Acq On : 15 Aug 2016 14:43
Operator : UM/SJ
Sample : H4452-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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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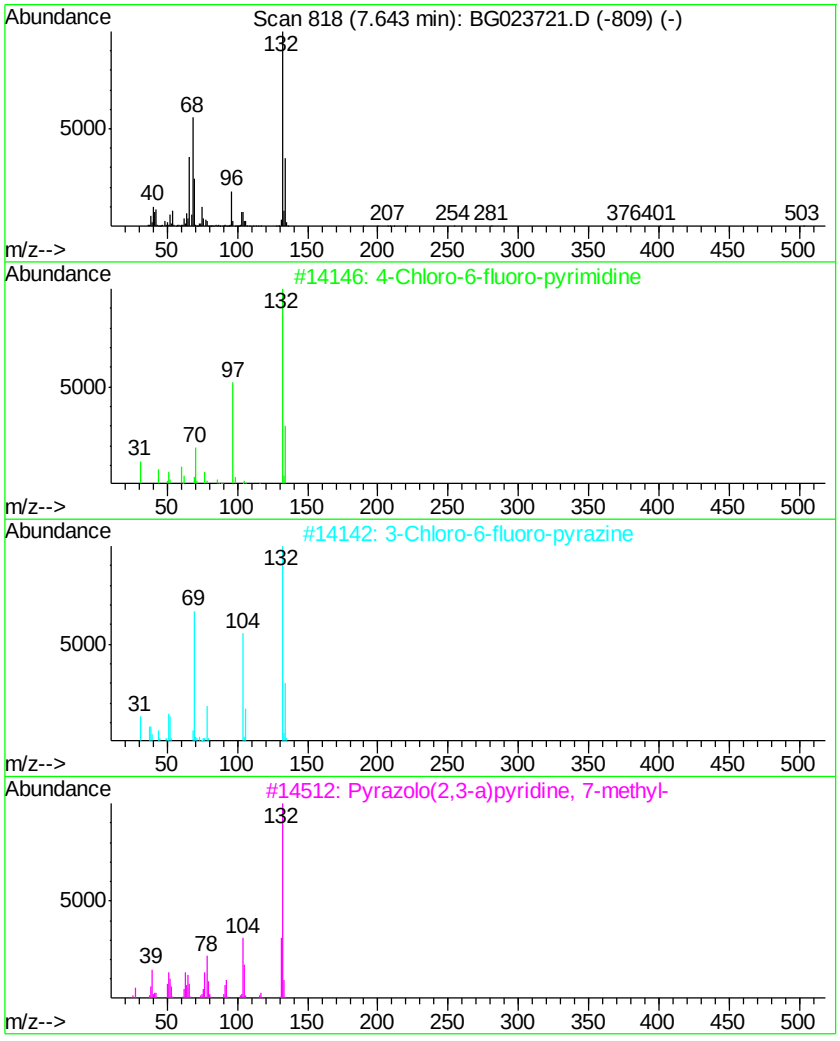
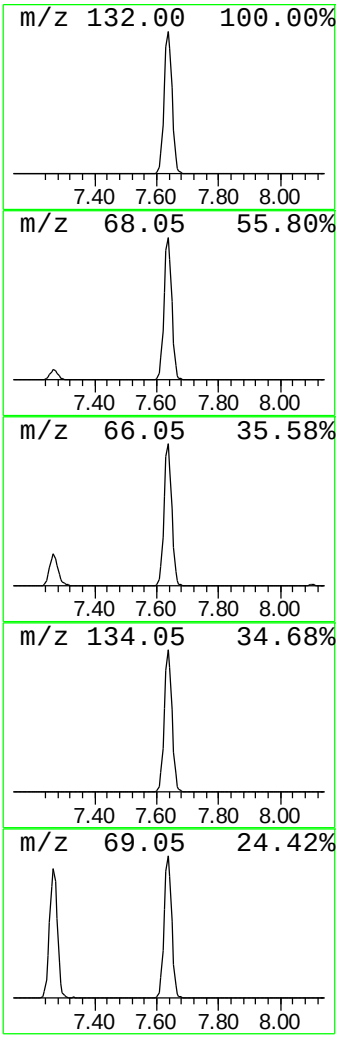
Peak Number 3 unknown7.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	118.64 ng	5256770	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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Operator : UM/SJ
Sample : H4452-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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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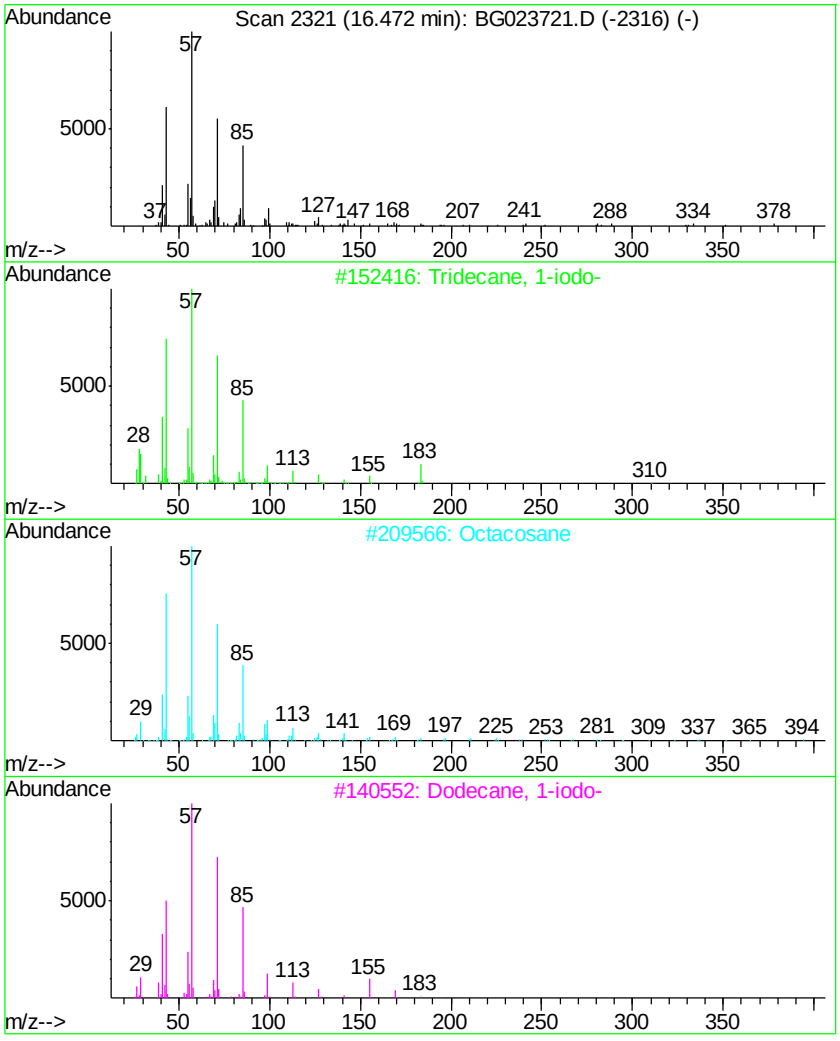
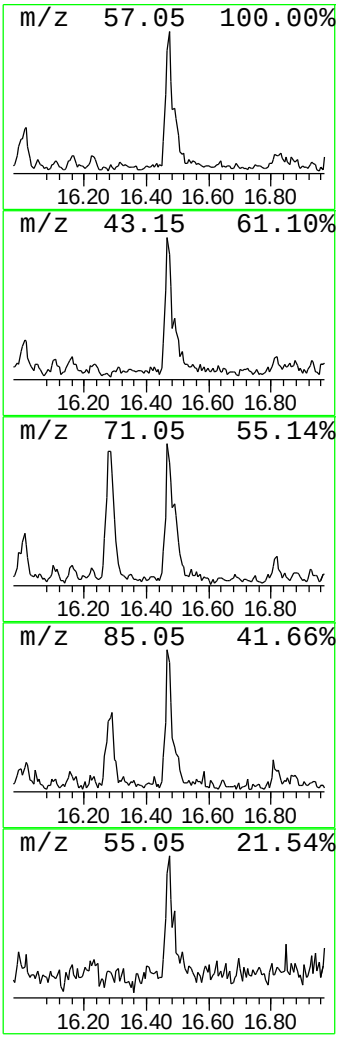
Peak Number 4 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	2.44 ng	206543	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
2	Octacosane	394	C28H58	000630-02-4	86
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
5	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081516\
Data File : BG023721.D
Acq On : 15 Aug 2016 14:43
Operator : UM/SJ
Sample : H4452-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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
unknown2.98	2.98	252.0	ng	11164100	1	8.11	886145	20.0
2-Pentanone, 4-hy...	5.17	27.4	ng	1213470	1	8.11	886145	20.0
unknown7.64	7.64	118.6	ng	5256770	1	8.11	886145	20.0
Tridecane, 1-iodo-	16.47	2.4	ng	206543	4	17.55	1694950	20.0