LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023142.D
Acq On : 16 Jul 2016 11:38
Operator : UM/SJ
Sample : H4015-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-21

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-BG070816.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	2.892	5	9	26	rVB	161750	428621	5.12%	0.833%
2	3.039	29	34	52	rVV	3411666	5049069	60.37%	9.810%
3	3.180	52	58	71	rVB	129621	288047	3.44%	0.560%
4	5.219	399	405	413	rVB	253404	404851	4.84%	0.787%
5	5.695	479	486	494	rBV	1778333	2870235	34.32%	5.576%
6	7.305	751	760	770	rBV	1998514	3524034	42.14%	6.847%
7	7.681	816	824	829	rBV	1791913	3227562	38.59%	6.271%
8	7.722	829	831	836	rVB	234322	288746	3.45%	0.561%
9	8.145	897	903	910	rVB	380314	659235	7.88%	1.281%
10	8.474	952	959	967	rBV	1287392	2218479	26.53%	4.310%
11	9.320	1096	1103	1112	rVB	1212698	2176331	26.02%	4.228%
12	10.977	1376	1385	1397	rVB	581470	1028329	12.30%	1.998%
13	13.415	1791	1800	1808	rBV	3315532	5112516	61.13%	9.933%
14	14.238	1933	1940	1946	rBV	743275	1124907	13.45%	2.186%
15	14.796	2028	2035	2046	rVB2	960829	1599932	19.13%	3.108%
16	16.288	2282	2289	2302	rBV	3256281	5062276	60.53%	9.835%
17	16.476	2317	2321	2333	rVB4	64458	130506	1.56%	0.254%
18	17.275	2452	2457	2460	rBV	74458	97921	1.17%	0.190%
19	17.551	2496	2504	2517	rBV	1373331	2223931	26.59%	4.321%
20	20.154	2940	2947	2954	rBV	5990293	8363343	100.00%	16.249%
21	21.470	3166	3171	3174	rBV7	95007	187055	2.24%	0.363%
22	21.852	3230	3236	3243	rBV	1463593	2517403	30.10%	4.891%
23	23.580	3526	3530	3536	rVB3	95402	162197	1.94%	0.315%
24	25.225	3800	3810	3821	rBV3	771447	2343653	28.02%	4.553%
25	32.169	4982	4992	4994	rBV10	149090	381618	4.56%	0.741%

Sum of corrected areas: 51470797

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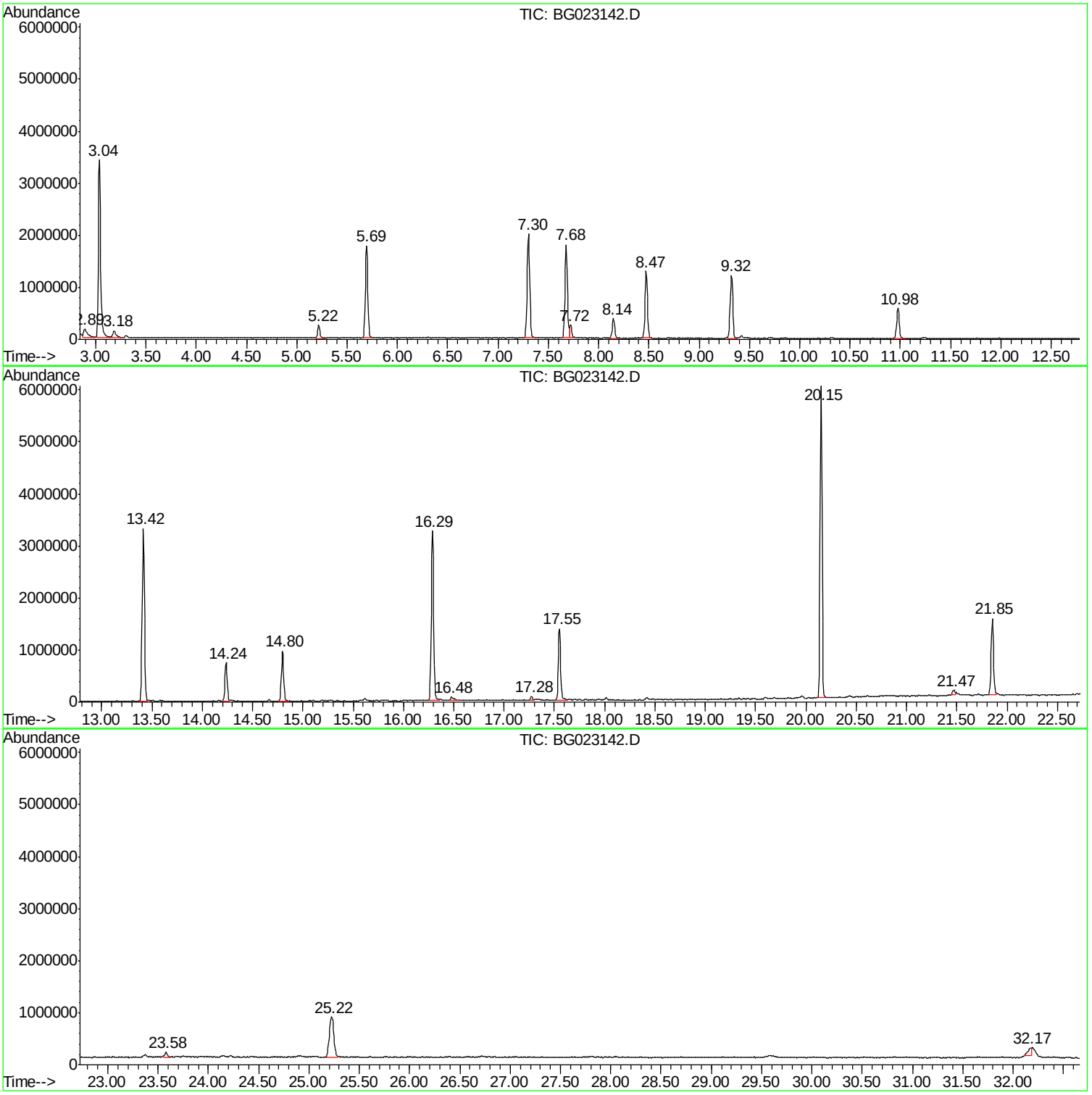
Instrument : BNA_G
ClientSampleId : C5-21

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023142.D
Acq On : 16 Jul 2016 11:38
Operator : UM/SJ
Sample : H4015-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-21

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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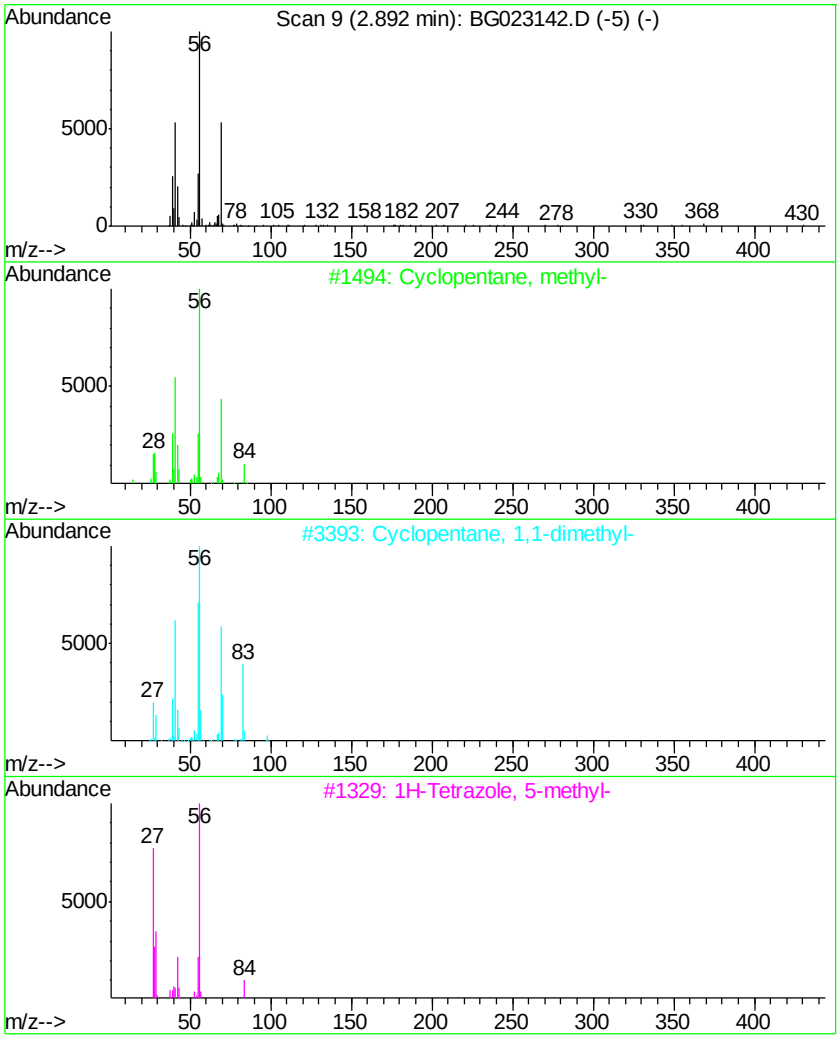
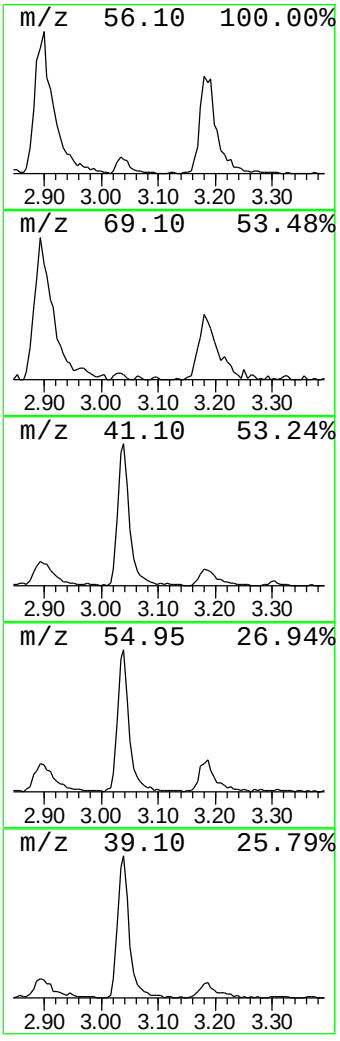
Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	13.00 ng	428621	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
2	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	45
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	42
5	Cyclobutane	56	C4H8	000287-23-0	40





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Operator : UM/SJ
Sample : H4015-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-21

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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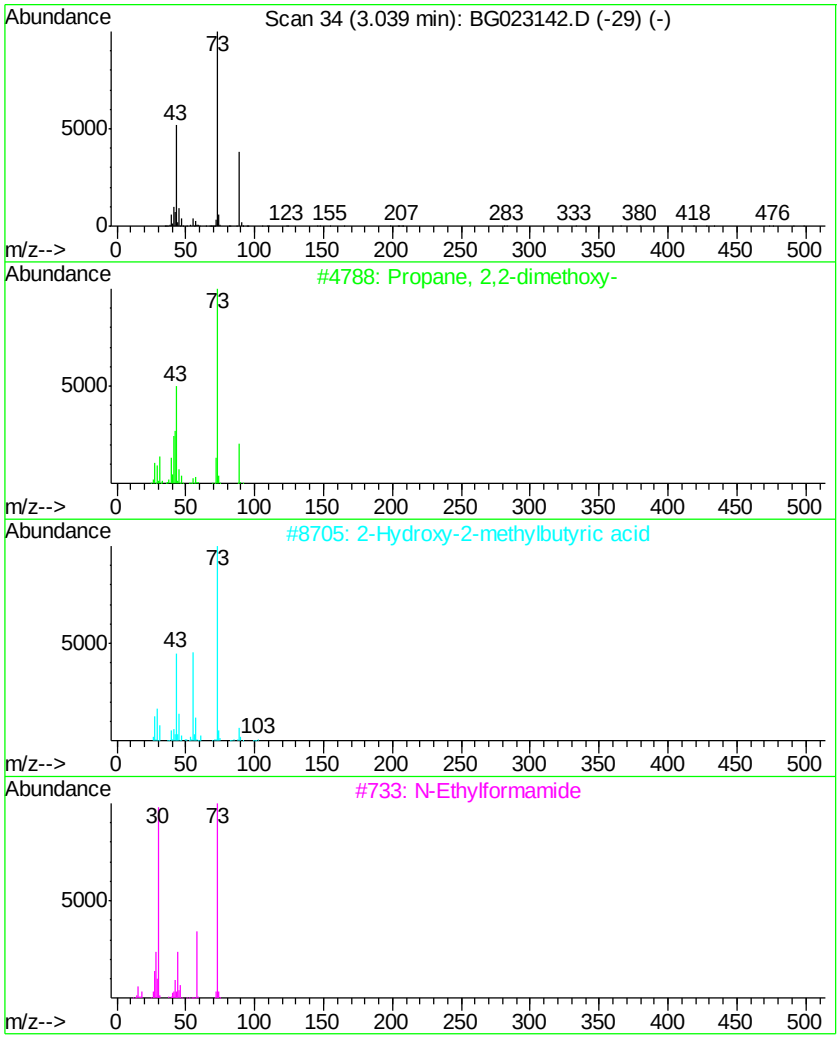
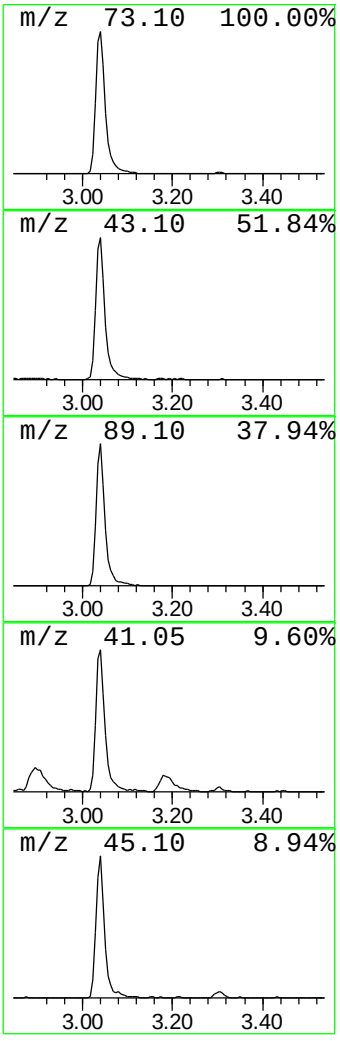
Peak Number 2 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	153.18 ng	5049070	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	33
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9





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Data File : BG023142.D
Acq On : 16 Jul 2016 11:38
Operator : UM/SJ
Sample : H4015-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-21

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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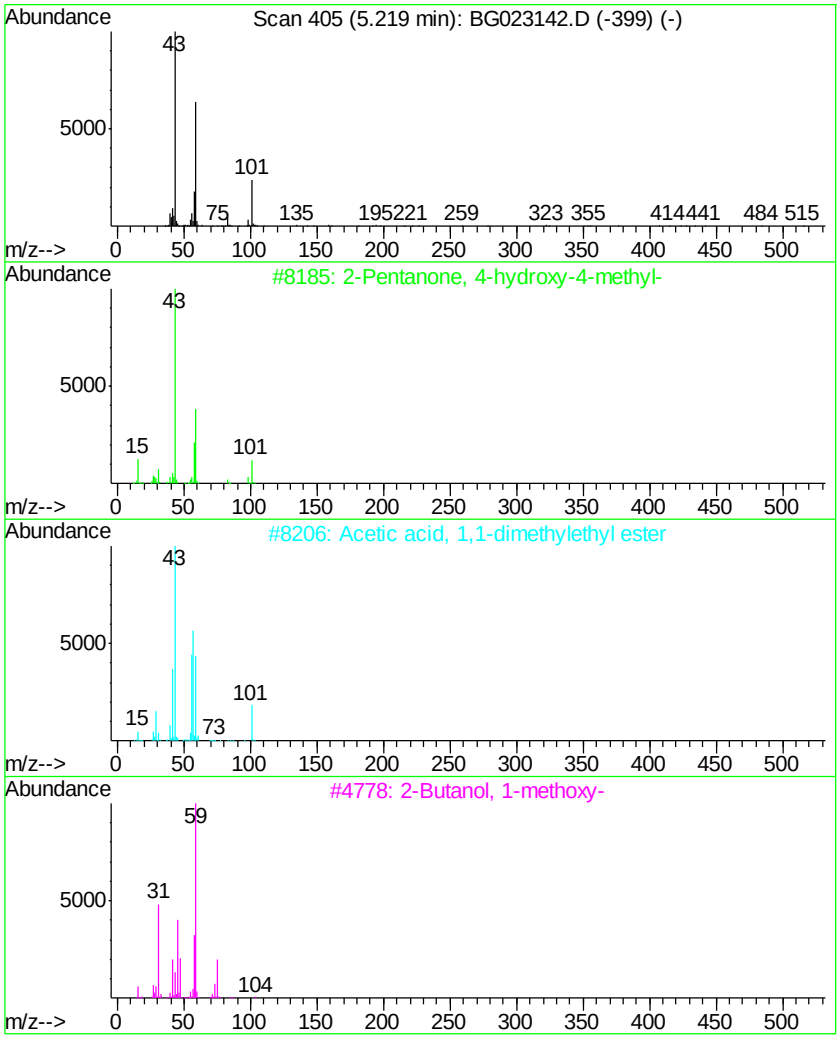
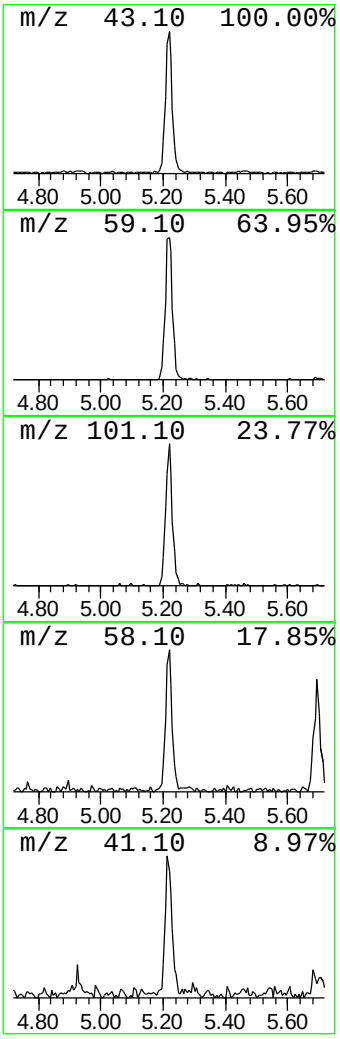
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	12.28 ng	404851	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	35
4	Tetraglyme	222	C10H22O5	000143-24-8	23
5	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	17





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Instrument : BNA_G
ClientSampleId : C5-21

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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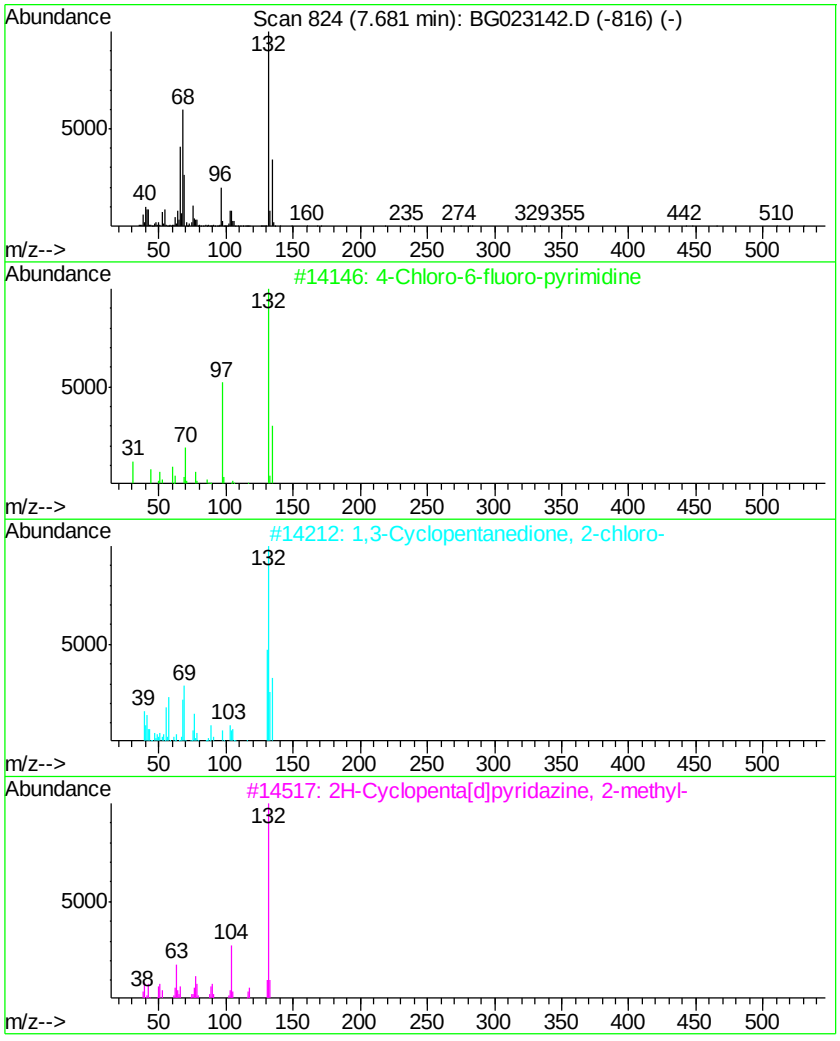
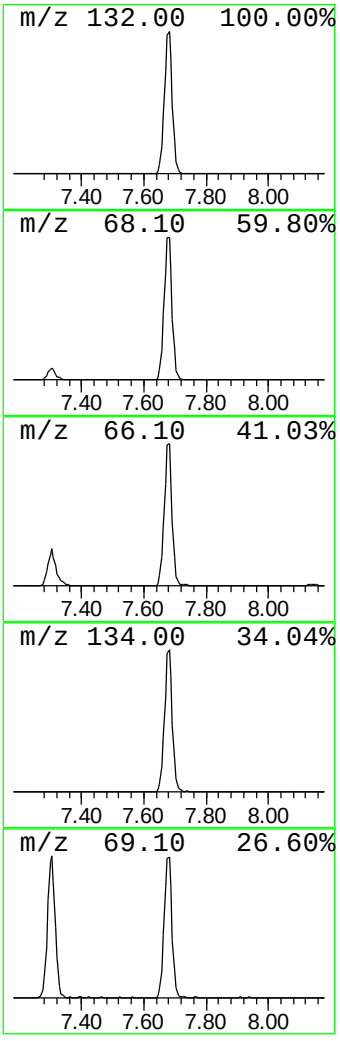
Peak Number 5 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	97.92 ng	3227560	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





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Operator : UM/SJ
Sample : H4015-16
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-21

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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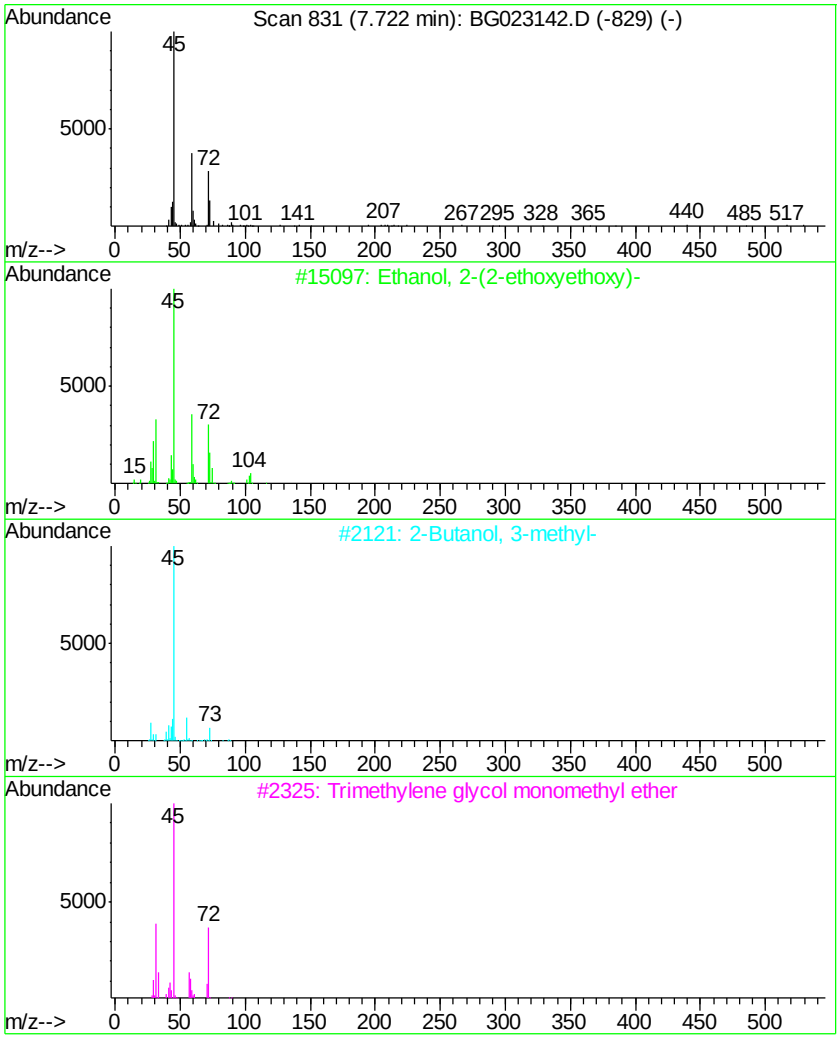
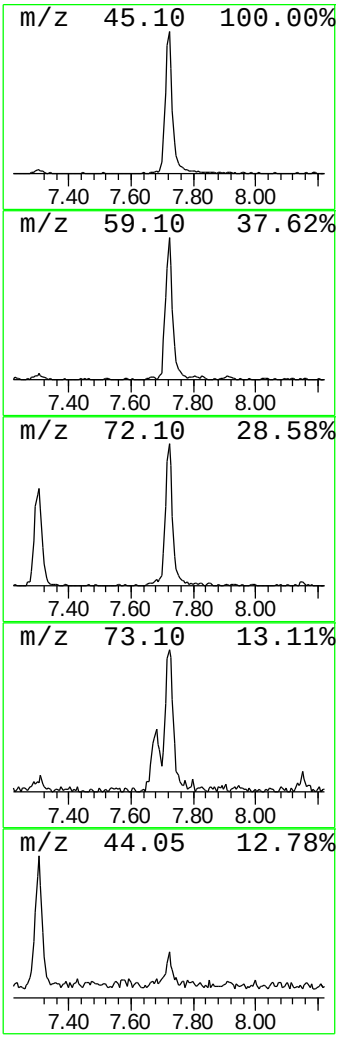
Peak Number 6 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	8.76 ng	288746	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	78
2	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	49
3	Trimethylene glycol monomethyl e...	90	C4H10O2	001589-49-7	42
4	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	38
5	2-Butanol, 3-methyl-, (S)-	88	C5H12O	001517-66-4	38





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Misc :
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Instrument : BNA_G
ClientSampleId : C5-21

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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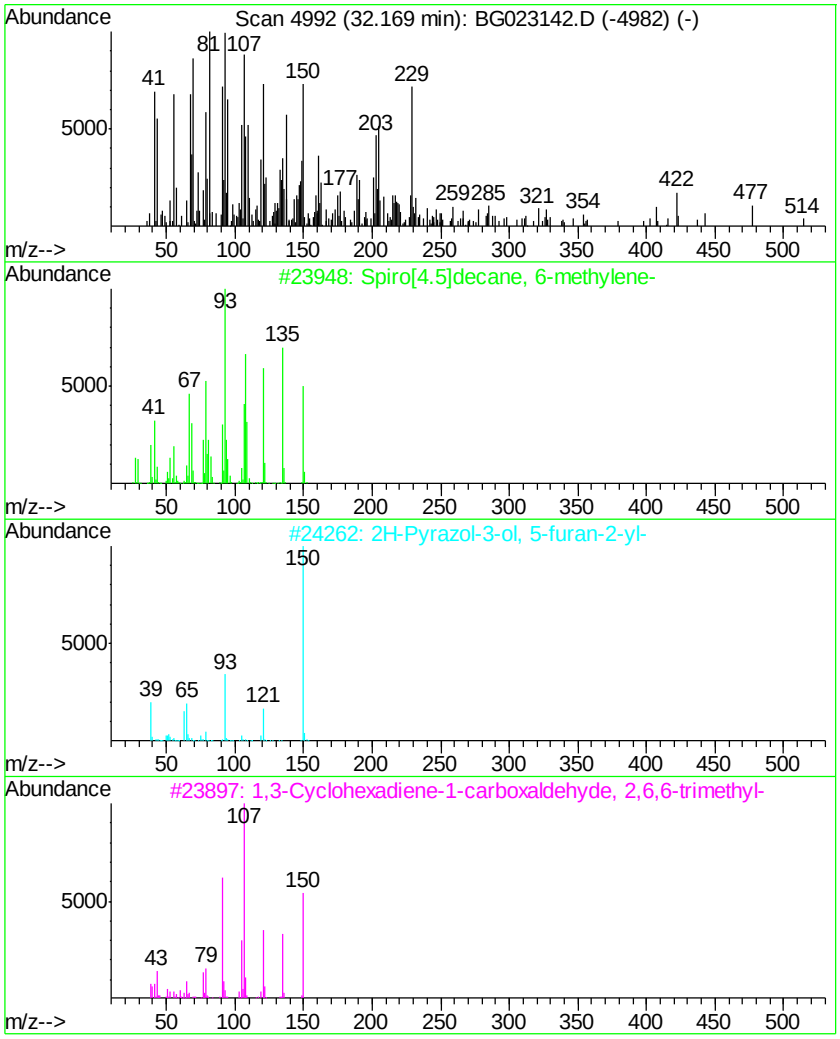
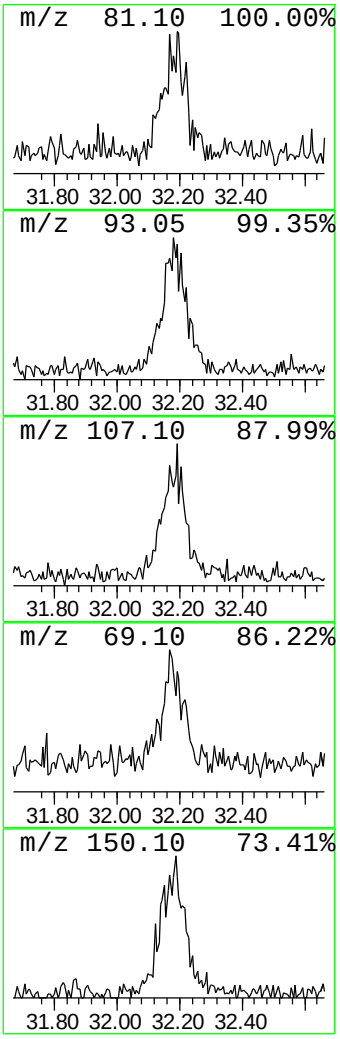
Peak Number 8 unknown32.17 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
32.17	3.26 ng	381618	Perylene-d12	25.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[4.5]decane, 6-methylene-	150	C11H18	019144-01-5	38
2	2H-Pyrazol-3-ol, 5-furan-2-yl-	150	C7H6N2O2	1000310-25-9	30
3	1,3-Cyclohexadiene-1-carboxaldeh...	150	C10H14O	000116-26-7	27
4	Bicyclo[3.1.1]hept-3-en-2-one, 4...	150	C10H14O	000080-57-9	27
5	Bicyclo[3.1.1]hept-2-en-6-one, 2...	150	C10H14O	000473-06-3	27





Tentatively Identified Compound (LSC) summary

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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
Cyclopentane, met...	2.89	13.0	ng	428621	1	8.14	659235	20.0
unknown3.04	3.04	153.2	ng	5049070	1	8.14	659235	20.0
2-Pentanone, 4-hy...	5.22	12.3	ng	404851	1	8.14	659235	20.0
unknown7.68	7.68	97.9	ng	3227560	1	8.14	659235	20.0
Ethanol, 2-(2-eth...	7.72	8.8	ng	288746	1	8.14	659235	20.0
unknown32.17	32.17	3.3	ng	381618	6	25.22	2343650	20.0