LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023059.D
Acq On : 13 Jul 2016 6:48
Operator : UM/SJ
Sample : H3988-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C4.2-4

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	2.893	4	9	25	rVB	844273	1857801	17.68%	2.815%
2	3.039	29	34	52	rVV	3736252	5307831	50.50%	8.044%
3	3.186	53	59	75	rVB	655128	1250209	11.89%	1.895%
4	5.219	399	405	413	rBV	242365	375169	3.57%	0.569%
5	5.695	479	486	497	rBV	2338222	3820502	36.35%	5.790%
6	7.311	751	761	771	rBV	2680739	4833557	45.99%	7.325%
7	7.681	813	824	835	rBV	2514561	4408730	41.95%	6.681%
8	8.151	895	904	911	rBV	399970	675687	6.43%	1.024%
9	8.480	953	960	967	rBV	1718627	3032434	28.85%	4.595%
10	9.326	1092	1104	1112	rBV	1716379	3104185	29.53%	4.704%
11	10.983	1377	1386	1396	rVB	597238	1119232	10.65%	1.696%
12	13.421	1792	1801	1810	rBV	4616129	7508634	71.44%	11.379%
13	14.244	1935	1941	1949	rBV	463559	699258	6.65%	1.060%
14	14.802	2027	2036	2045	rBV2	1081359	1843334	17.54%	2.793%
15	16.300	2283	2291	2301	rBV	4581444	7090962	67.47%	10.746%
16	17.564	2498	2506	2516	rBV	1468553	2307527	21.95%	3.497%
17	18.427	2649	2653	2663	rBV2	259734	393348	3.74%	0.596%
18	19.691	2863	2868	2874	rBV5	68671	114840	1.09%	0.174%
19	20.166	2942	2949	2958	rBV	7762020	10510457	100.00%	15.928%
20	21.483	3167	3173	3181	rBV2	169477	375828	3.58%	0.570%
21	21.870	3232	3239	3246	rBV	1512731	2568629	24.44%	3.893%
22	23.609	3528	3535	3542	rVB	209867	441633	4.20%	0.669%
23	25.255	3805	3815	3829	rBV2	777081	2347473	22.33%	3.557%

Sum of corrected areas: 65987260

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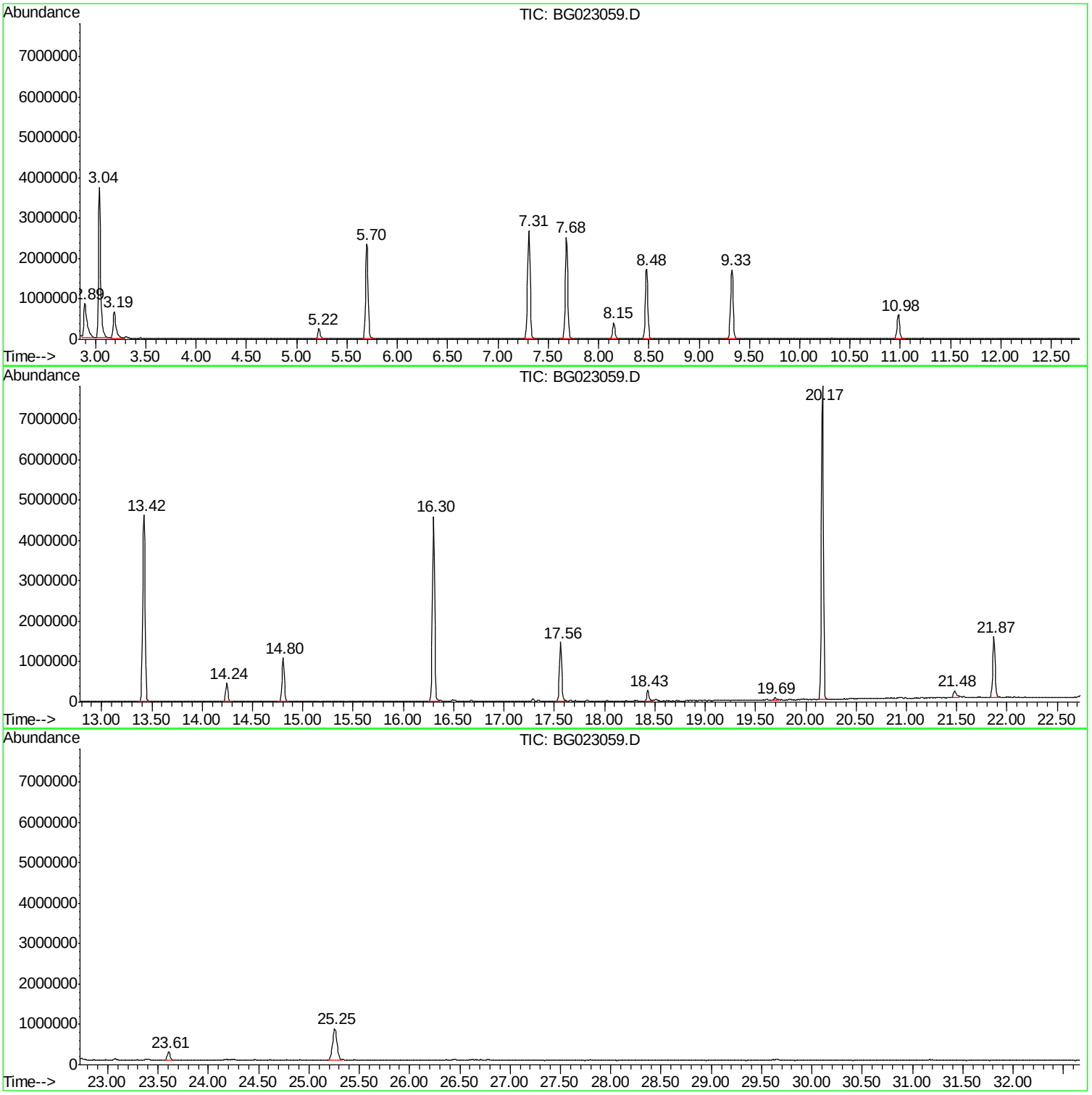
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C4.2-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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\BG071216\
Data File : BG023059.D
Acq On : 13 Jul 2016 6:48
Operator : UM/SJ
Sample : H3988-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C4.2-4

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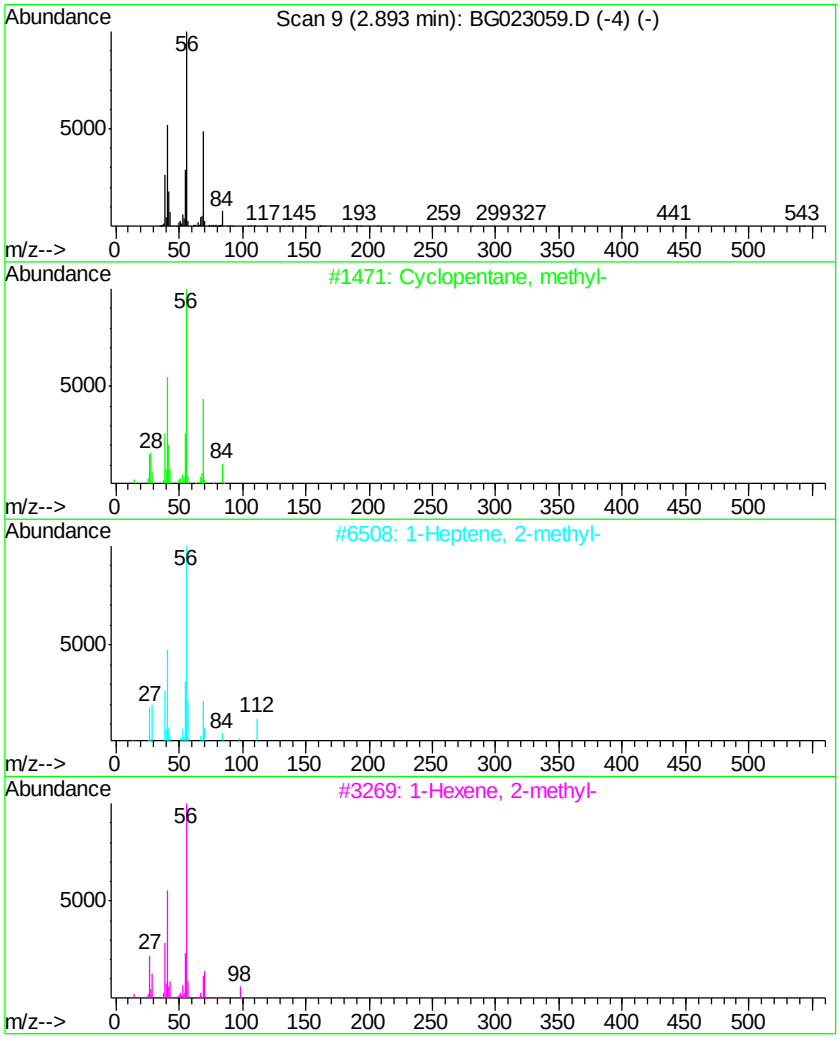
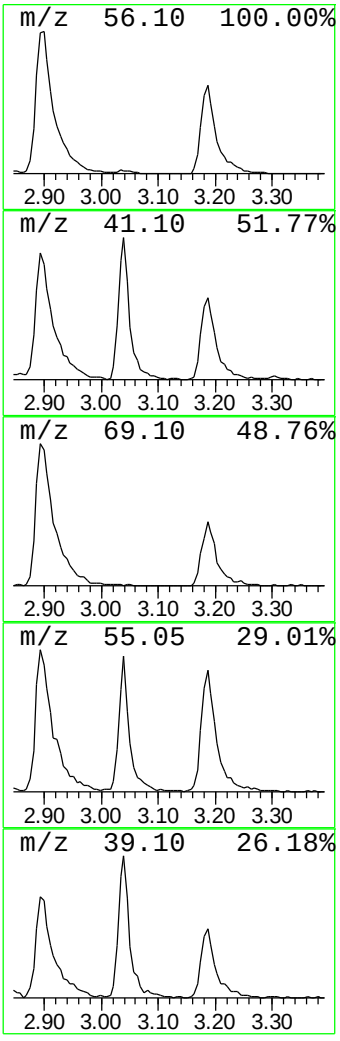
Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	54.99 ng	1857800	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	78
3	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	78
4	Cyclohexane	84	C6H12	000110-82-7	74
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72





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Data File : BG023059.D
Acq On : 13 Jul 2016 6:48
Operator : UM/SJ
Sample : H3988-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C4.2-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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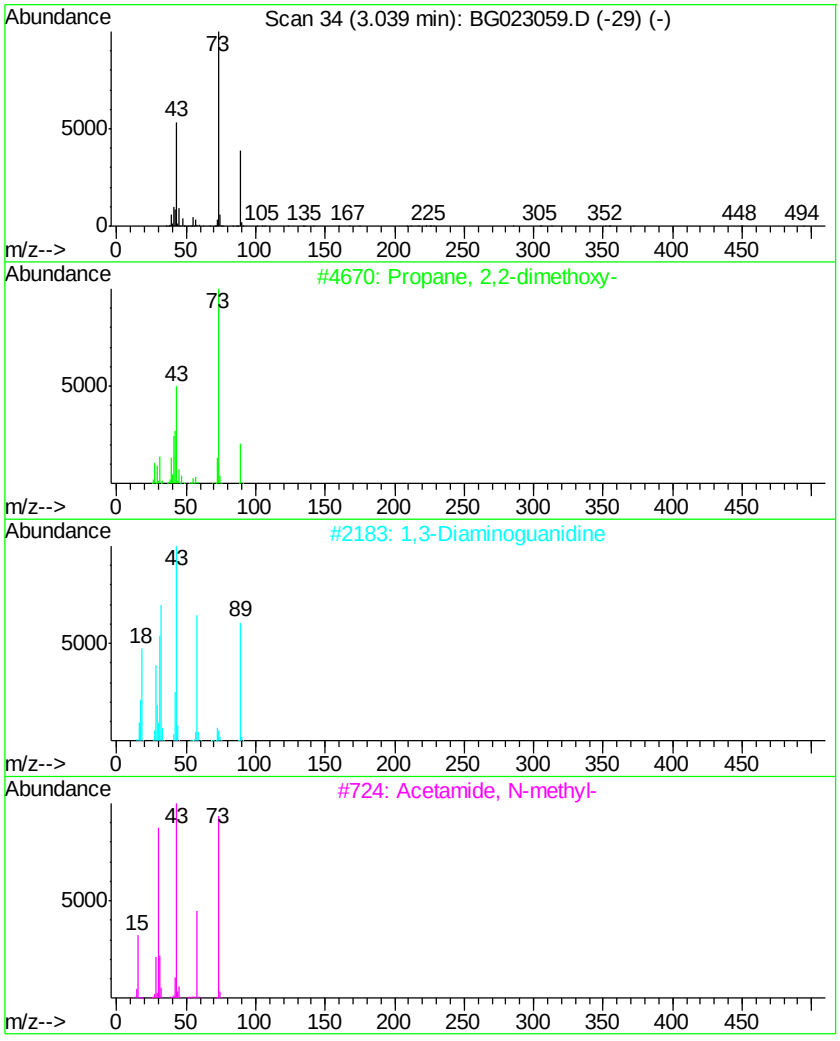
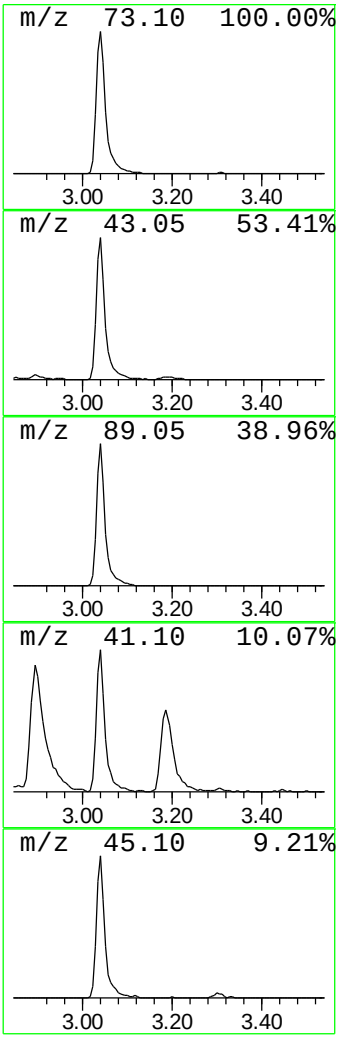
Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	157.11 ng	5307830	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
Data File : BG023059.D
Acq On : 13 Jul 2016 6:48
Operator : UM/SJ
Sample : H3988-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C4.2-4

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

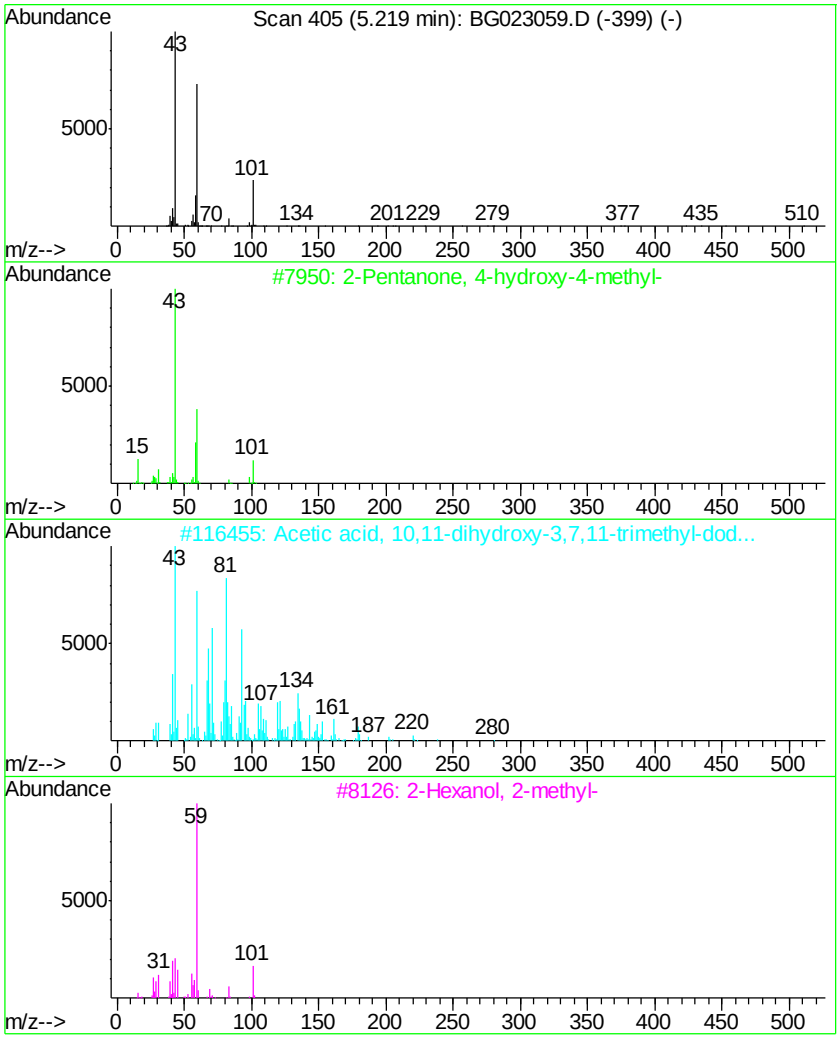
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

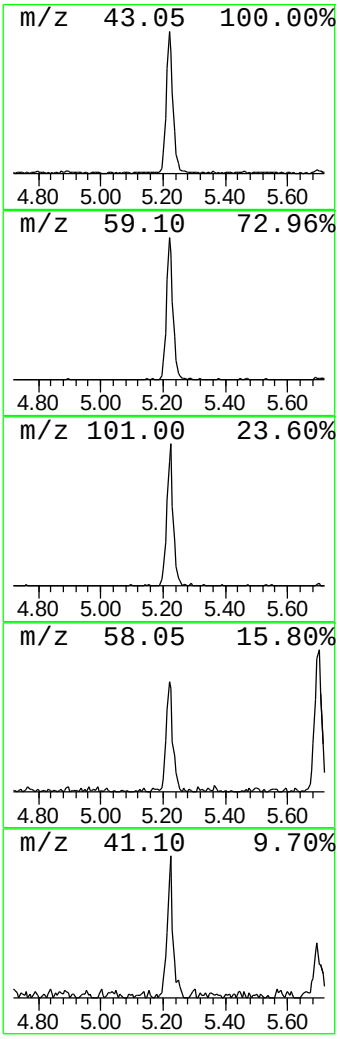
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	11.10 ng	375169	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	37
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17





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Data File : BG023059.D
Acq On : 13 Jul 2016 6:48
Operator : UM/SJ
Sample : H3988-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C4.2-4

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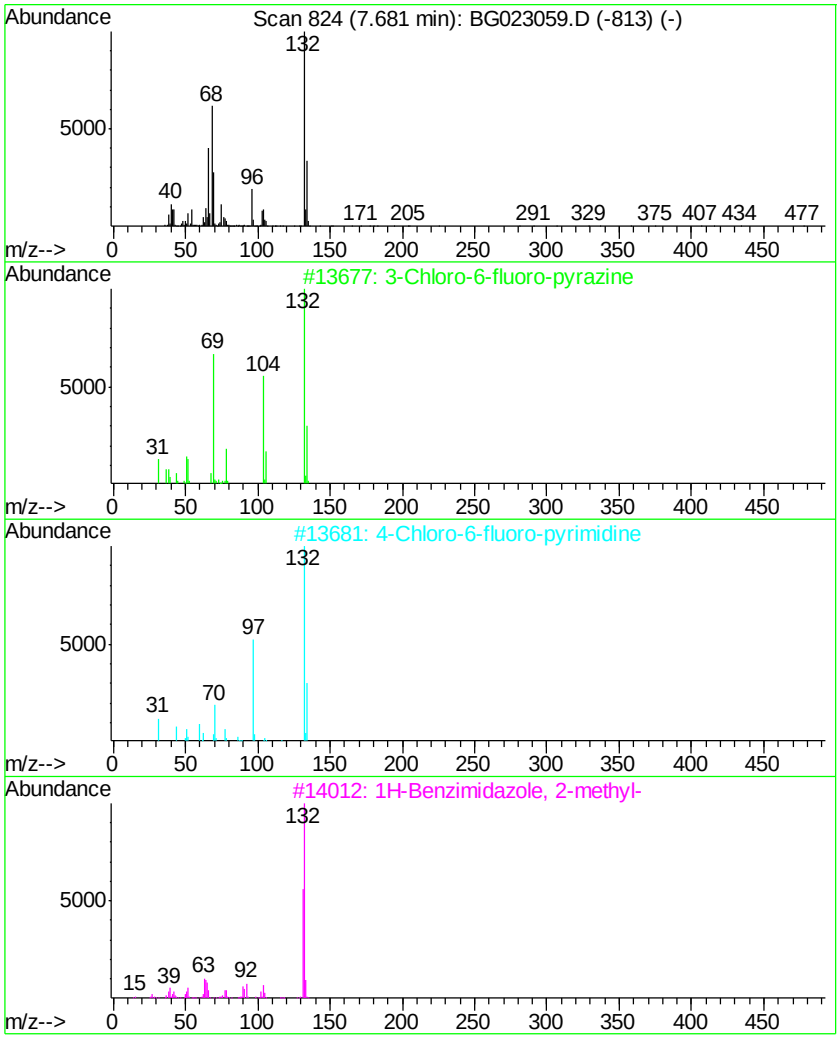
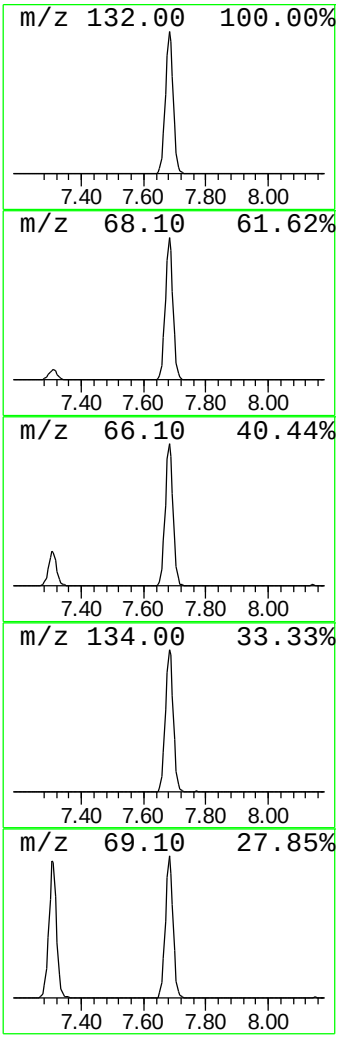
Peak Number 5 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	130.50 ng	4408730	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
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Operator : UM/SJ
Sample : H3988-12
Misc :
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Instrument : BNA_G
ClientSampleId : C4.2-4

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

TIC Library : C:\DATABASE\NIST02.L
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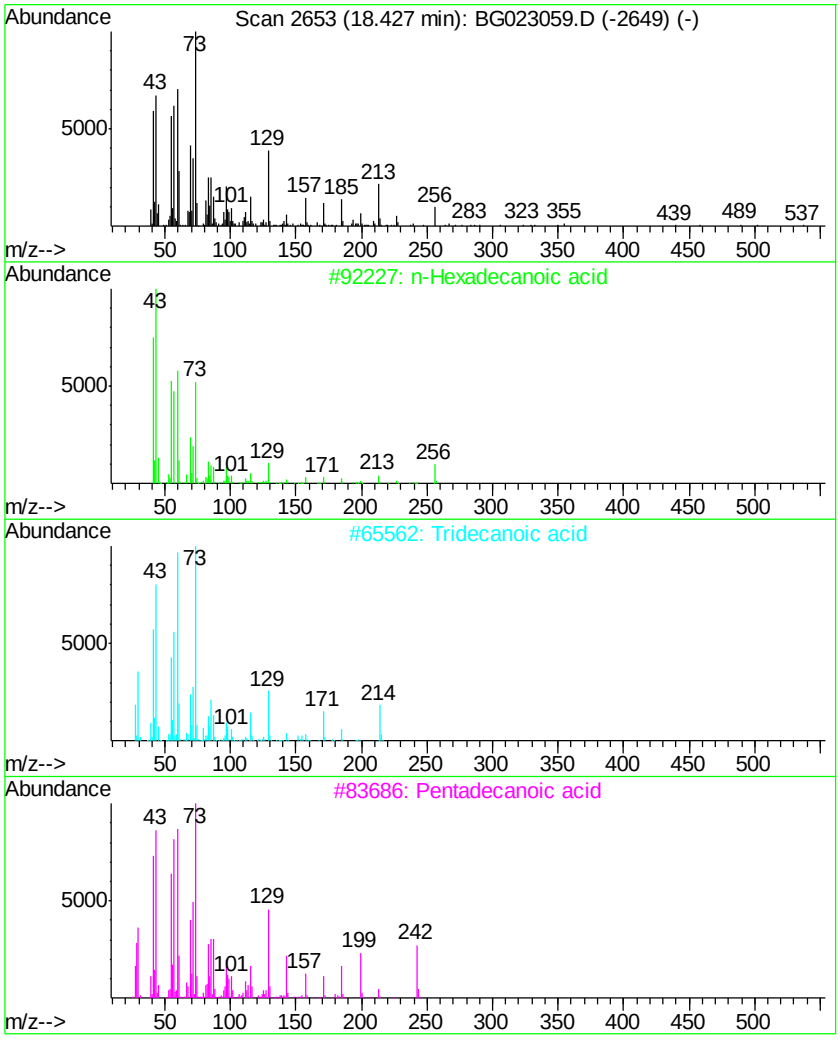
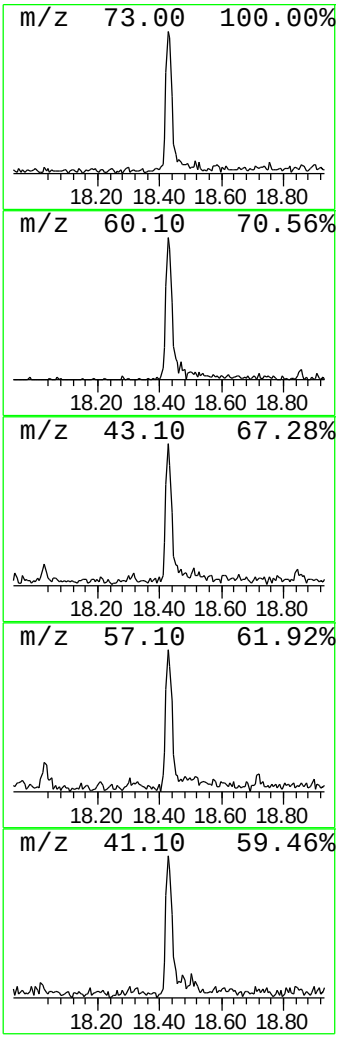
Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	3.41 ng	393348	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	45





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Misc :
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Instrument : BNA_G
ClientSampleId : C4.2-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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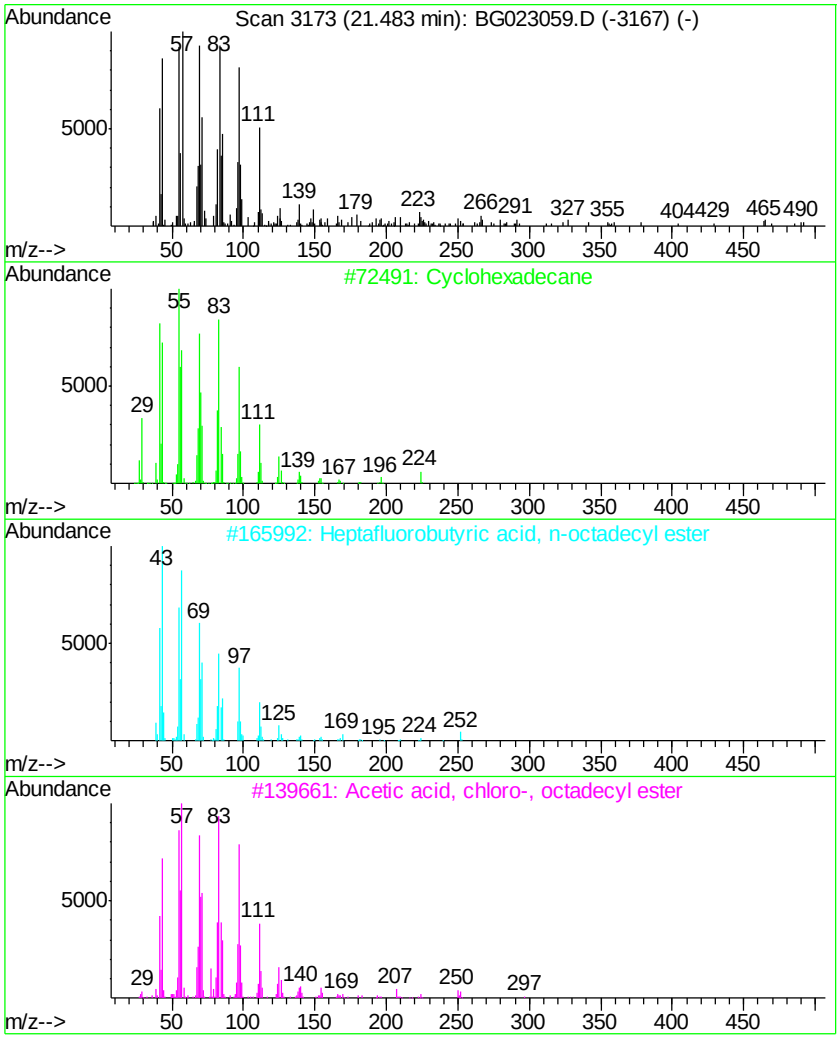
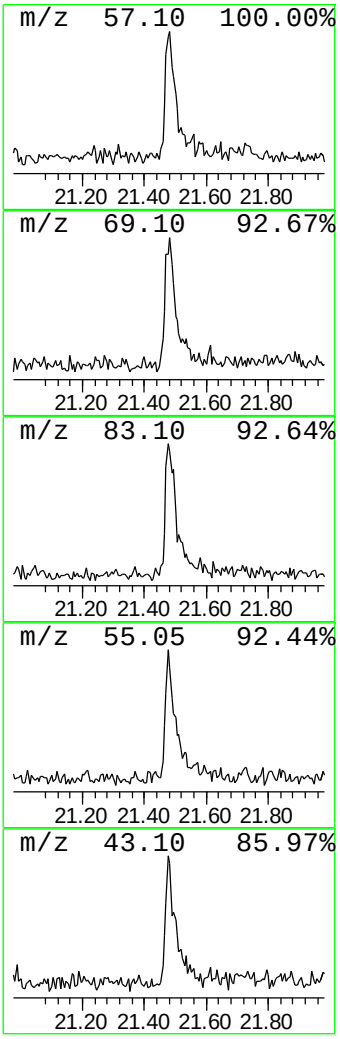
Peak Number 8 Cyclohexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.48	2.93 ng	375828	Chrysene-d12	21.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	91
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91
4	1-Nonadecene	266	C19H38	018435-45-5	90
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	78





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Instrument : BNA_G
ClientSampleId : C4.2-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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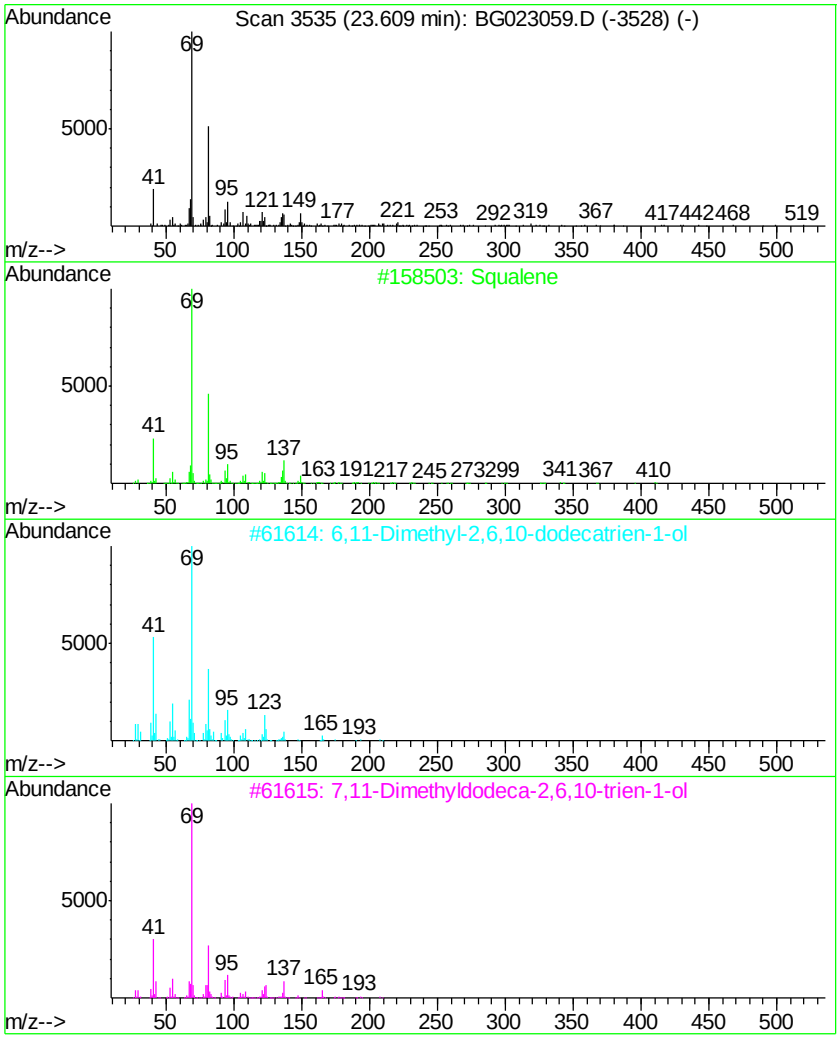
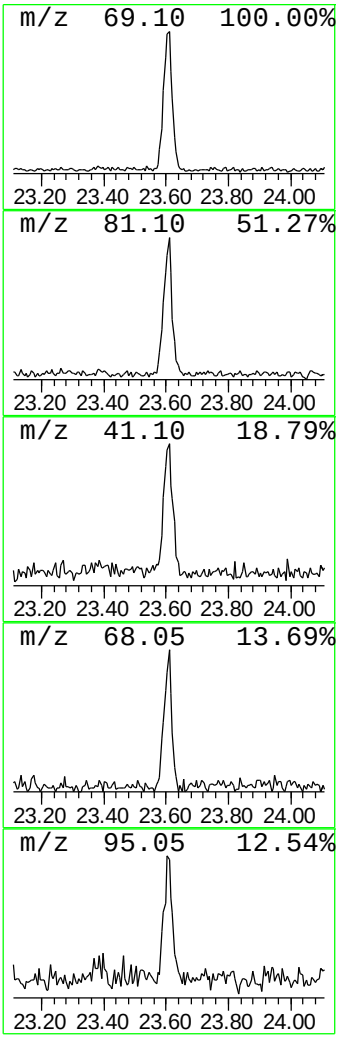
Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.61	3.76 ng	441633	Perylene-d12	25.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	74
2	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	72
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59





Tentatively Identified Compound (LSC) summary

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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
Cyclopentane, met...	2.89	55.0	ng	1857800	1	8.15	675687	20.0
Propane, 2,2-dime...	3.04	157.1	ng	5307830	1	8.15	675687	20.0
2-Pentanone, 4-hy...	5.22	11.1	ng	375169	1	8.15	675687	20.0
unknown7.68	7.68	130.5	ng	4408730	1	8.15	675687	20.0
n-Hexadecanoic acid	18.43	3.4	ng	393348	4	17.56	2307530	20.0
Cyclohexadecane	21.48	2.9	ng	375828	5	21.87	2568630	20.0
Squalene	23.61	3.8	ng	441633	6	25.25	2347470	20.0