LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022316\
Data File : BG021050.D
Acq On : 24 Feb 2016 7:11
Operator : UM/SJ
Sample : H1442-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

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-BG022316.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	3.058	32	37	52	rVV	197534	268674	87.66%	12.101%
2	3.199	56	61	68	rBV2	4430	9325	3.04%	0.420%
3	5.291	412	417	425	rBB	19091	28319	9.24%	1.275%
4	5.784	495	501	510	rBB	93177	142473	46.49%	6.417%
5	7.411	770	778	788	rBB	109363	183665	59.93%	8.272%
6	7.752	830	836	844	rBB	104179	177224	57.82%	7.982%
7	8.204	907	913	918	rBB	16237	26936	8.79%	1.213%
8	8.533	962	969	975	rBB	79047	131205	42.81%	5.909%
9	9.385	1107	1114	1122	rBB	68234	120146	39.20%	5.411%
10	11.024	1387	1393	1400	rBB	30524	52087	16.99%	2.346%
11	13.444	1799	1805	1812	rBB	210924	306491	100.00%	13.804%
12	14.273	1940	1946	1951	rBB	19632	27789	9.07%	1.252%
13	14.660	2008	2012	2016	rBB	5409	6284	2.05%	0.283%
14	14.819	2033	2039	2044	rBB2	44196	69989	22.84%	3.152%
15	15.606	2169	2173	2177	rVB	6533	7829	2.55%	0.353%
16	16.305	2285	2292	2298	rBB	138824	194572	63.48%	8.763%
17	16.464	2315	2319	2326	rBB	5363	7979	2.60%	0.359%
18	17.556	2499	2505	2509	rBV	45422	67073	21.88%	3.021%
19	17.592	2509	2511	2516	rVB	5268	6310	2.06%	0.284%
20	18.408	2645	2650	2654	rBV3	2483	3838	1.25%	0.173%
21	19.589	2846	2851	2856	rBV	7556	9881	3.22%	0.445%
22	19.947	2908	2912	2918	rVB2	6722	9124	2.98%	0.411%
23	20.135	2936	2944	2949	rBV	227140	265328	86.57%	11.950%
24	21.404	3156	3160	3164	rBV6	3678	6225	2.03%	0.280%
25	21.821	3224	3231	3236	rBV	27509	46502	15.17%	2.094%
26	23.284	3472	3480	3481	rBV4	5412	9066	2.96%	0.408%
27	25.134	3786	3795	3803	rVB3	13130	35926	11.72%	1.618%

Sum of corrected areas: 2220260

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Operator : UM/SJ
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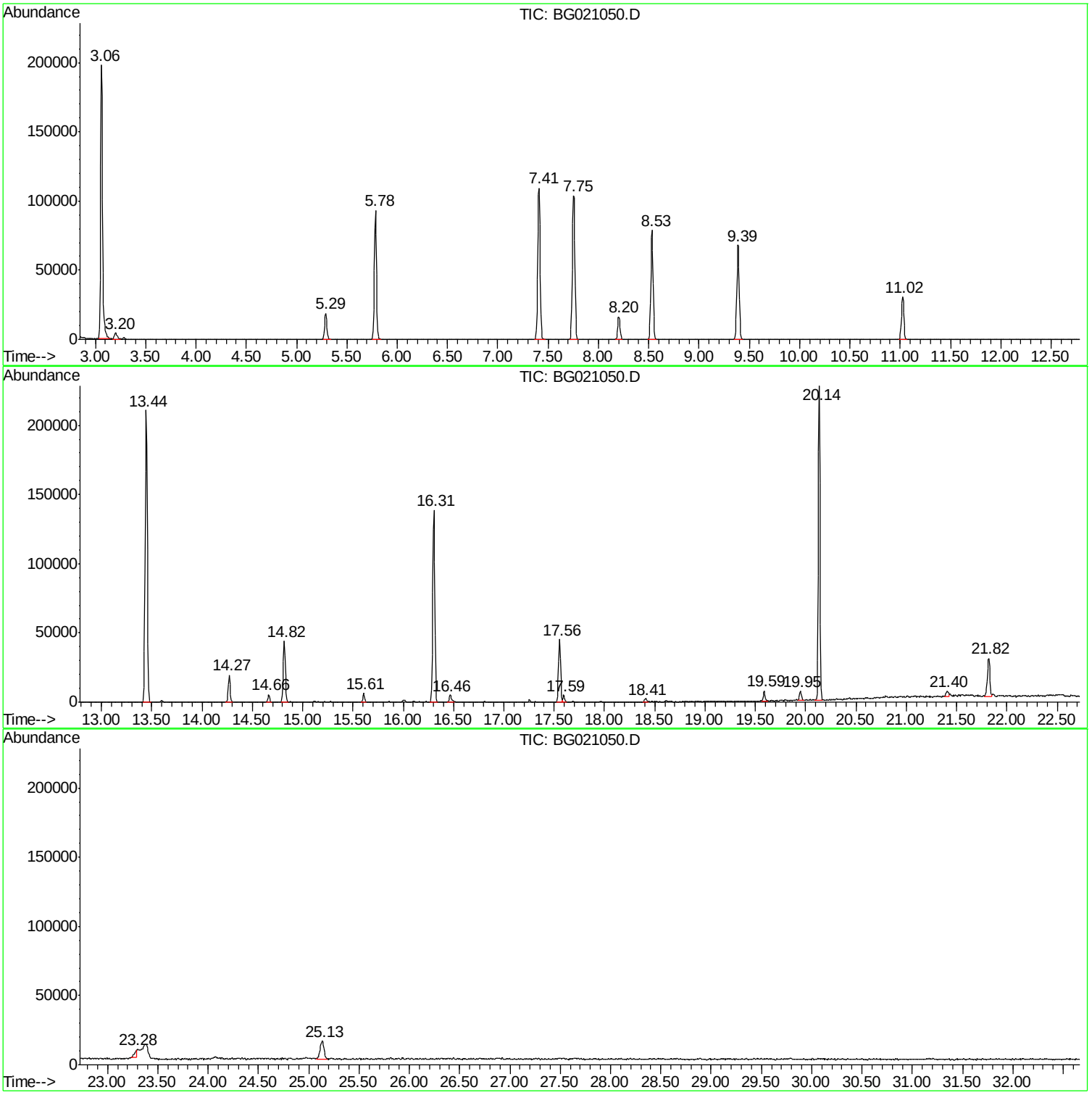
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.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\BG022316\
Data File : BG021050.D
Acq On : 24 Feb 2016 7:11
Operator : UM/SJ
Sample : H1442-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

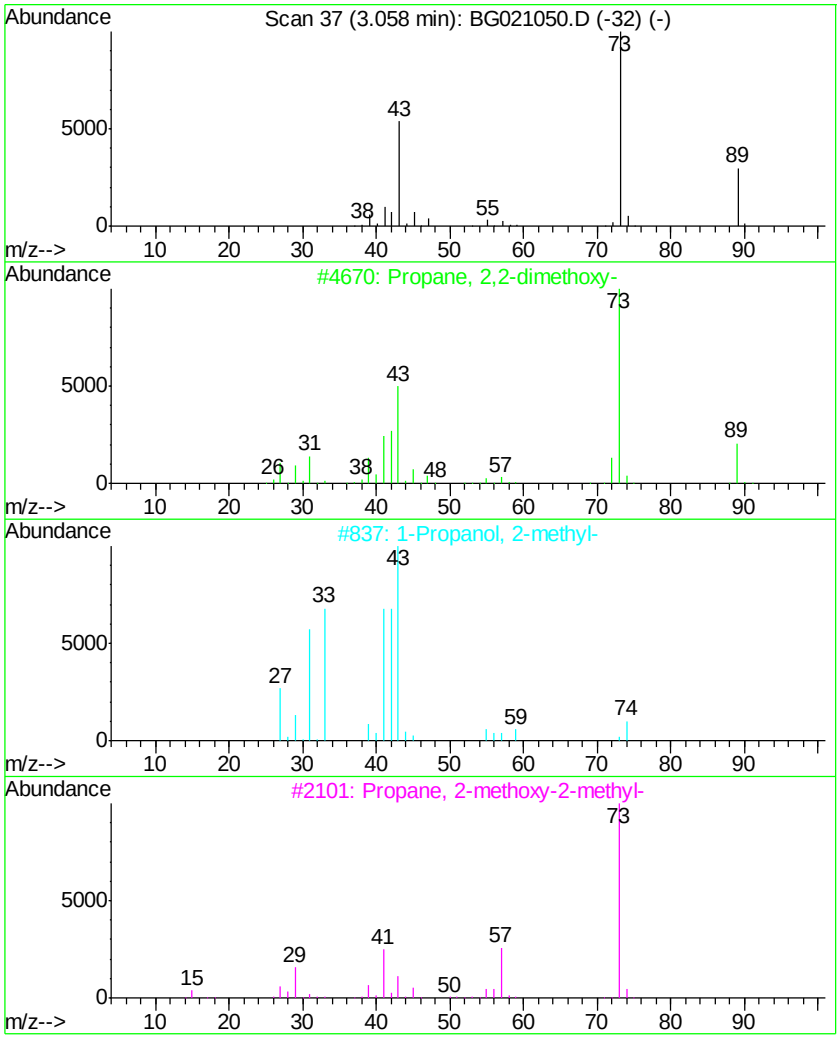
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

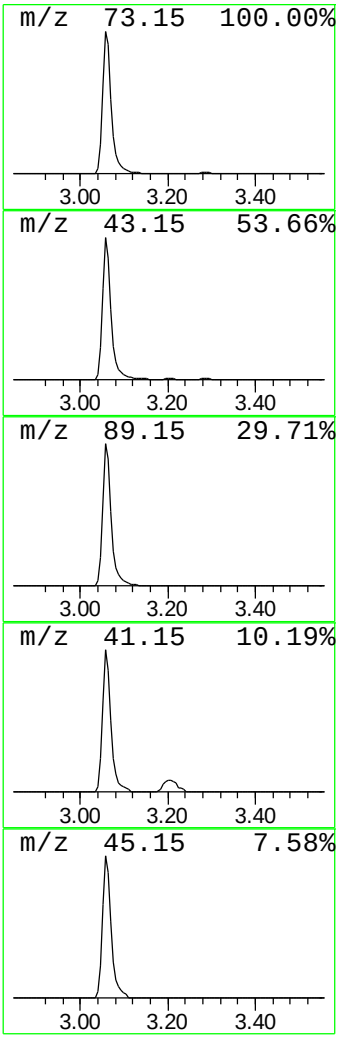
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	199.49 ng	268674	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Data File : BG021050.D
Acq On : 24 Feb 2016 7:11
Operator : UM/SJ
Sample : H1442-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

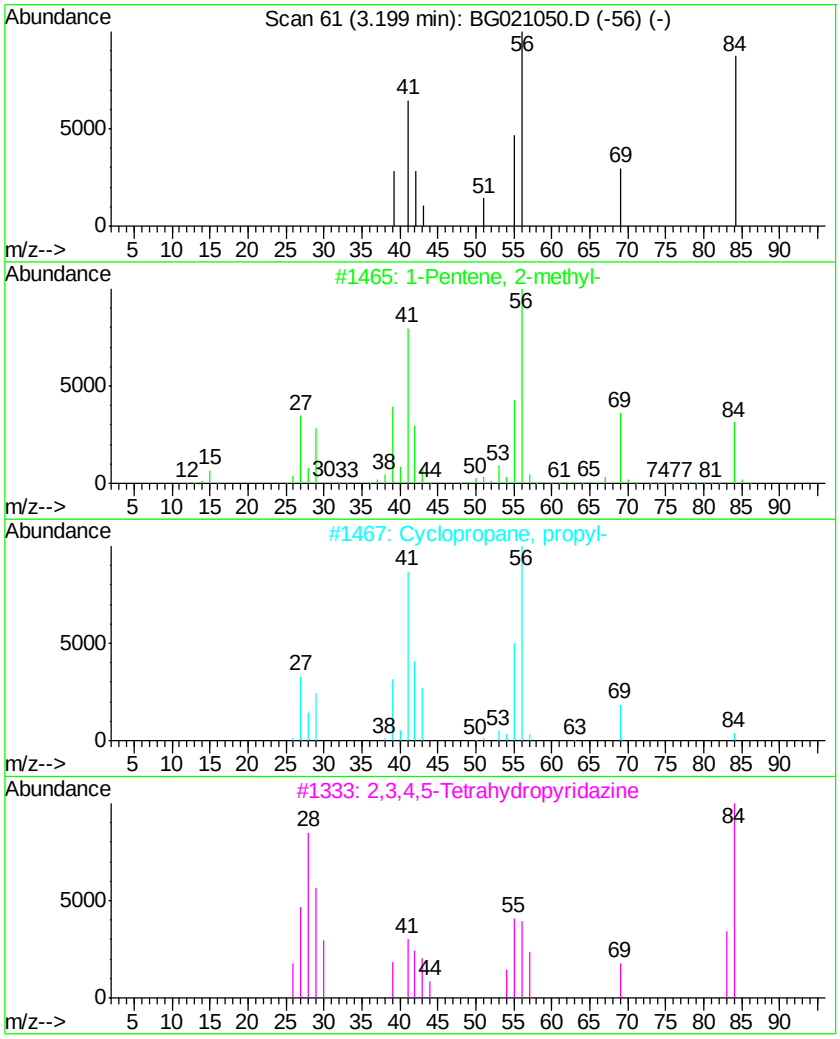
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

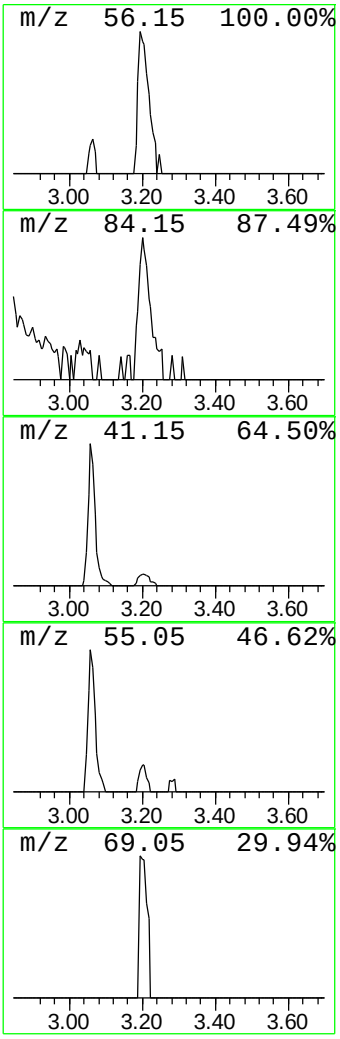
****

Peak Number 2 1-Pentene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	6.92 ng	9325	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	28
3	2,3,4,5-Tetrahydropyridazine	84	C4H8N2	000694-06-4	9
4	1-Hexanol	102	C6H14O	000111-27-3	9
5	Cyclobutane, 1,2-diethyl-	112	C8H16	061141-83-1	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022316\
Data File : BG021050.D
Acq On : 24 Feb 2016 7:11
Operator : UM/SJ
Sample : H1442-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

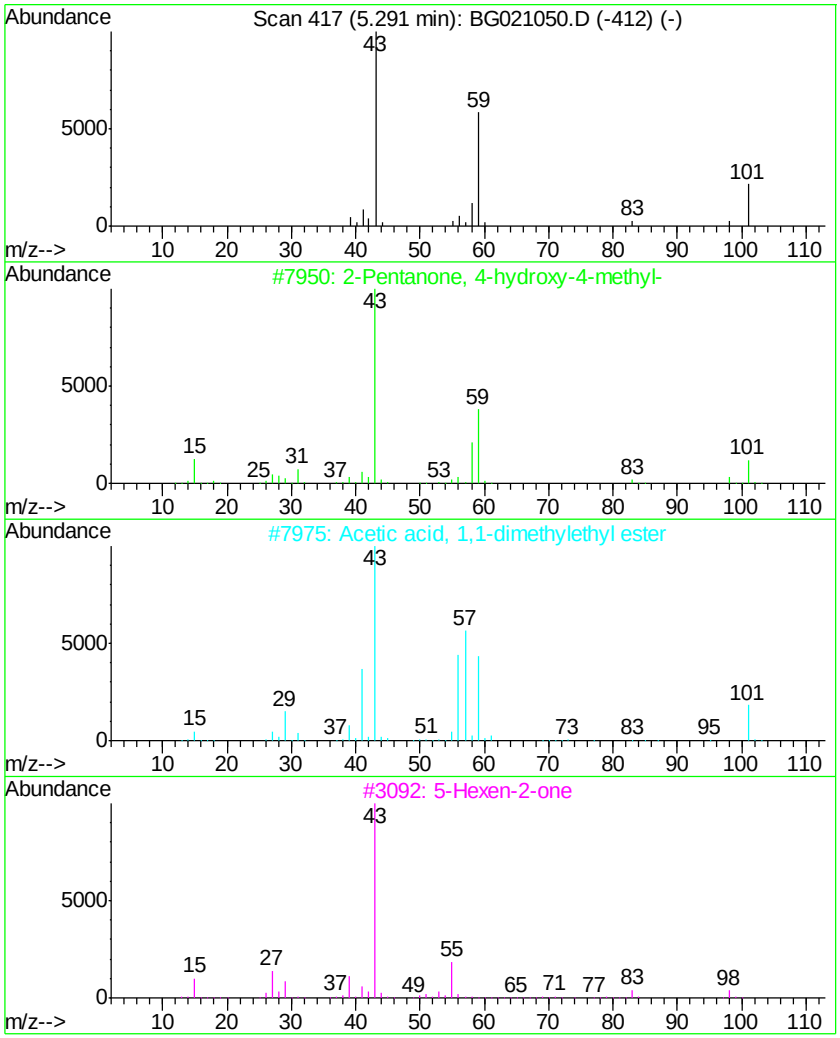
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

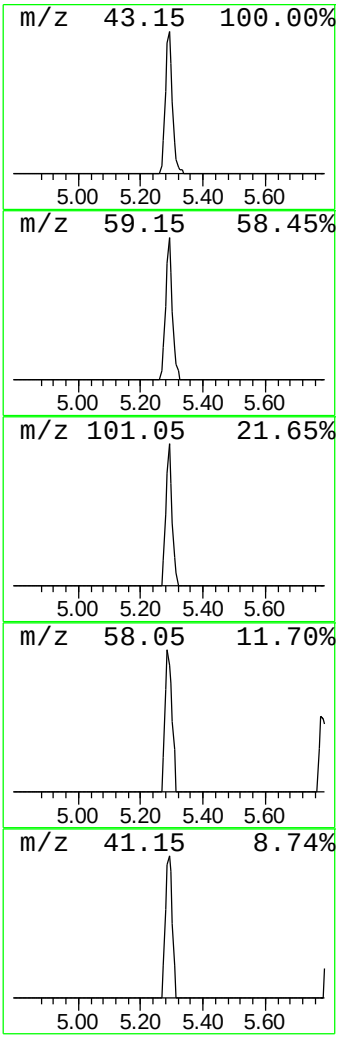
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.29	21.03 ng	28319	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	3-Pentanol	88	C5H12O	000584-02-1	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022316\
Data File : BG021050.D
Acq On : 24 Feb 2016 7:11
Operator : UM/SJ
Sample : H1442-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

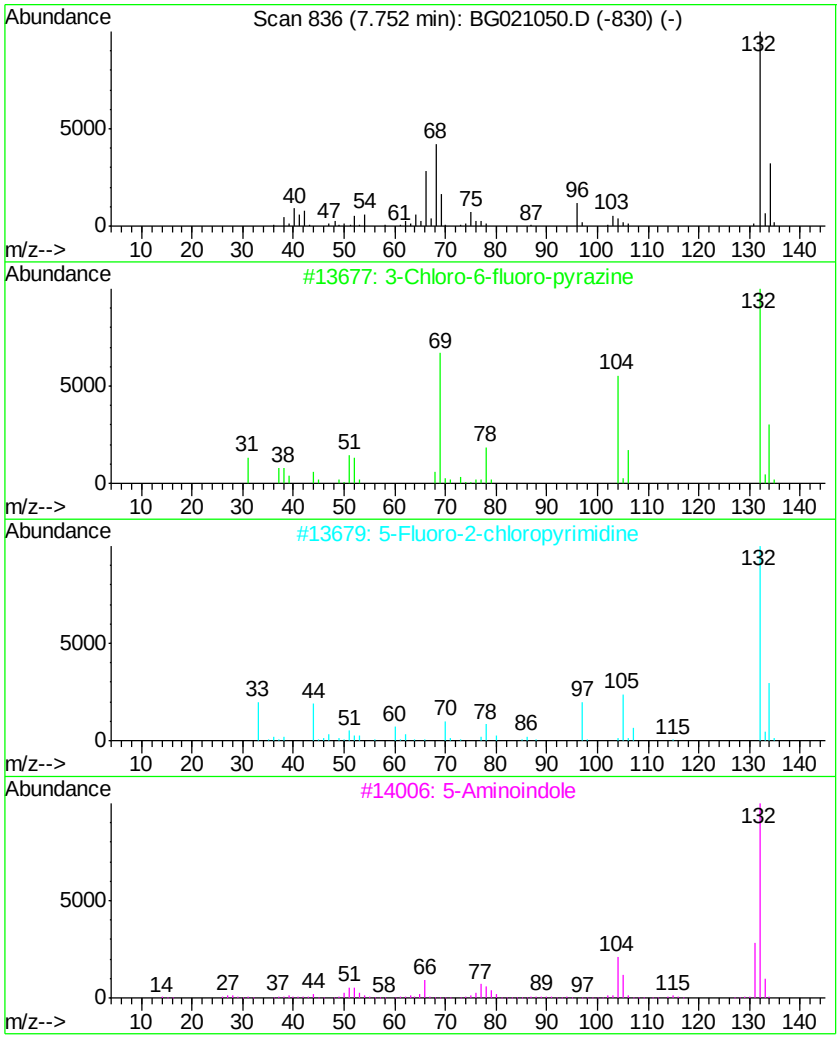
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

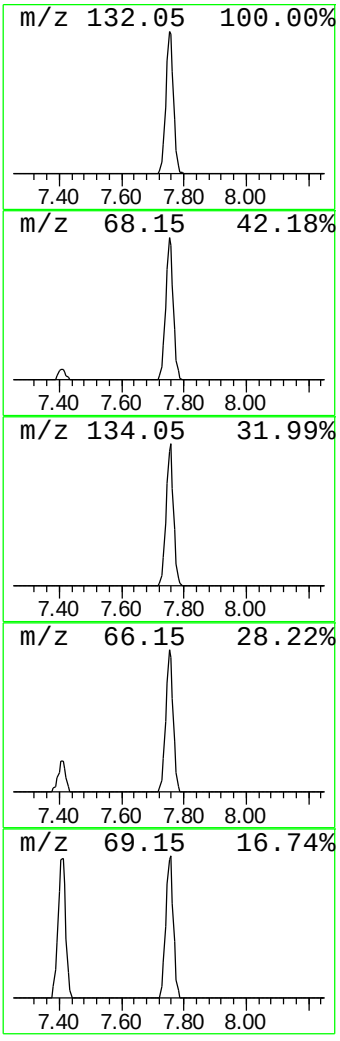
****

Peak Number 4 unknown7.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	131.59 ng	177224	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022316\
Data File : BG021050.D
Acq On : 24 Feb 2016 7:11
Operator : UM/SJ
Sample : H1442-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

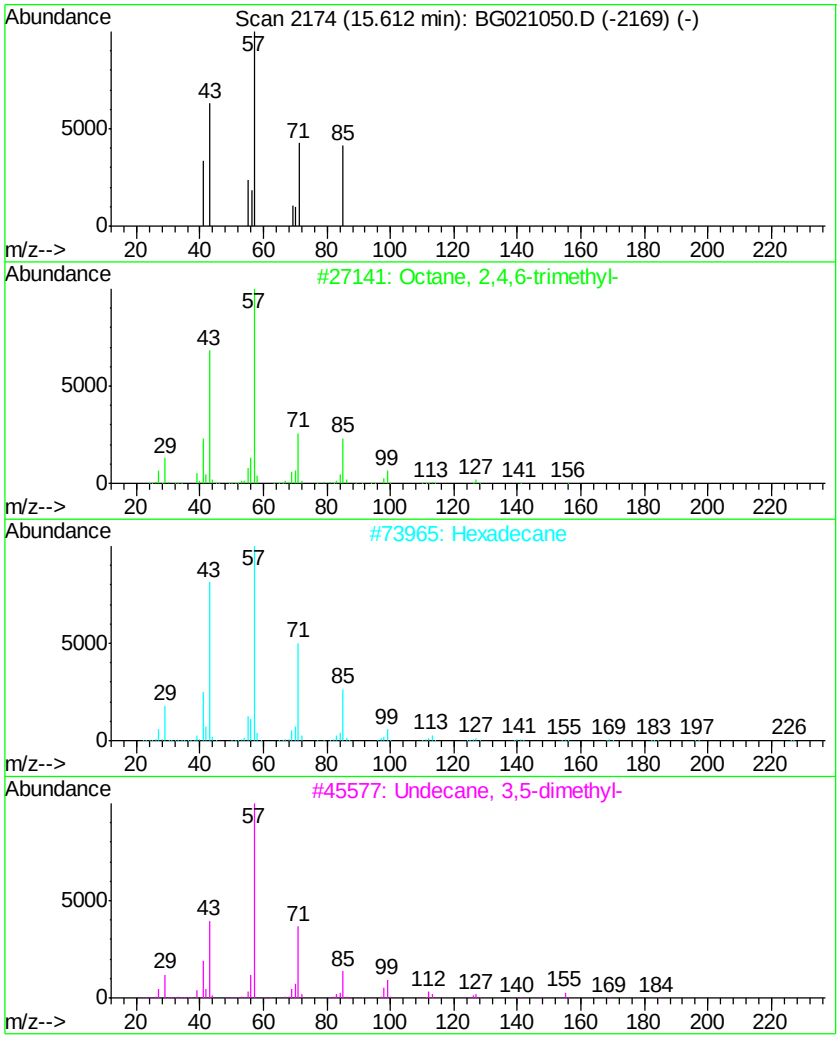
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

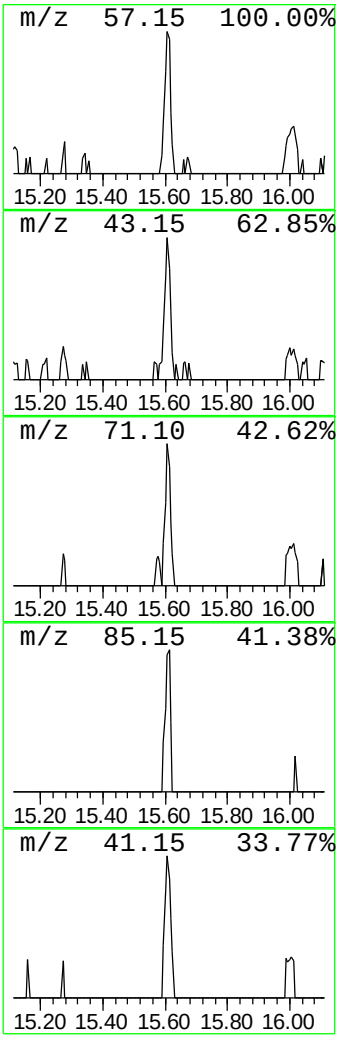
****

Peak Number 6 Octane, 2,4,6-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	2.24 ng	7829	Acenaphthene-d10	14.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	83
2	Hexadecane	226	C16H34	000544-76-3	74
3	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	64
4	Nonane, 2,5-dimethyl-	156	C11H24	017302-27-1	59
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59





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Sample : H1442-05
Misc :
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Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

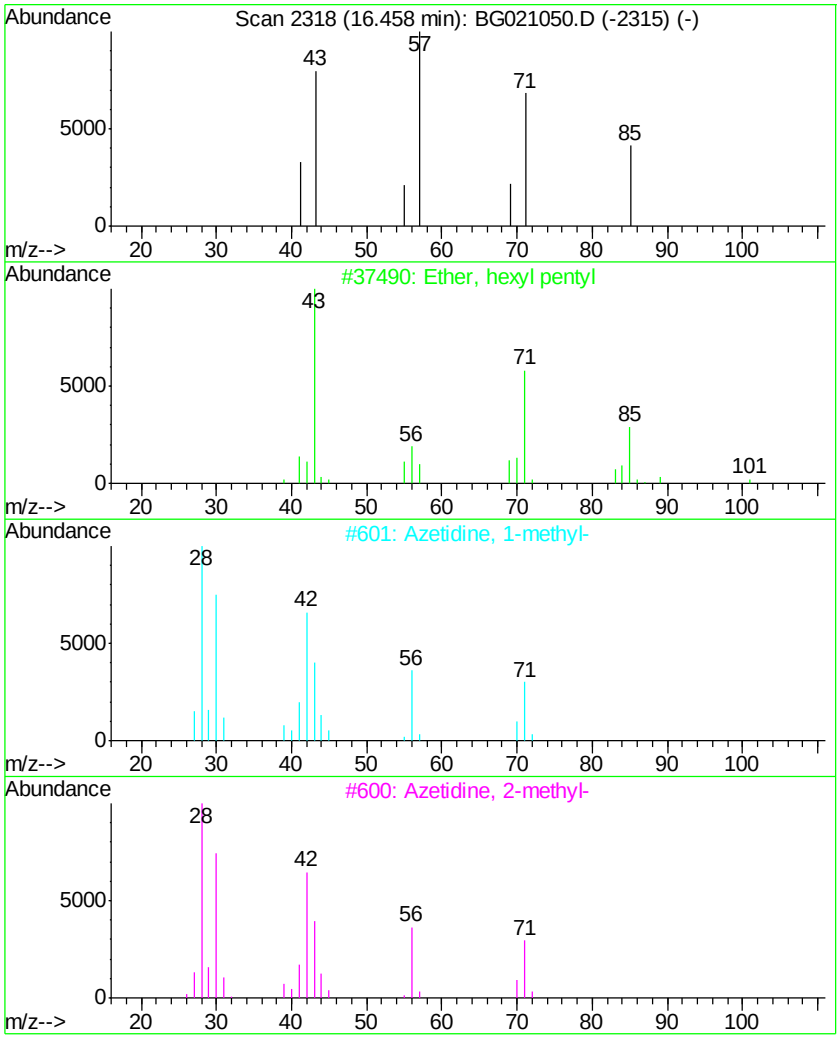
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

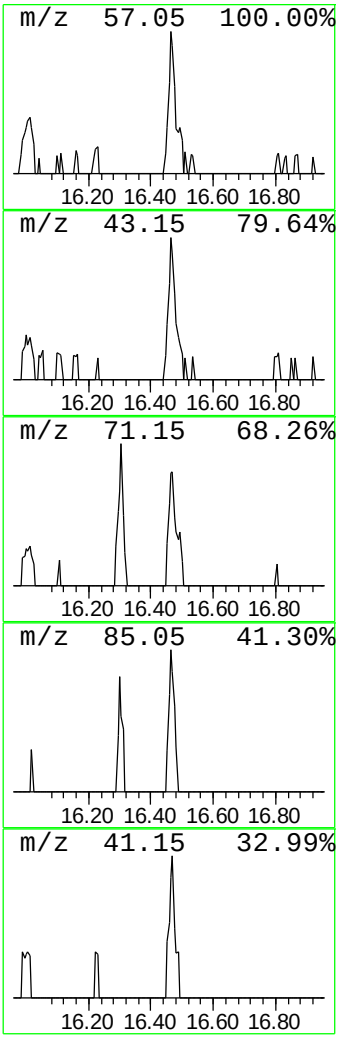
****

Peak Number 7 unknown16.46 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.38 ng	7979	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ether, hexyl pentyl	172	C11H24O	032357-83-8	43
2	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	9
3	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	9
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	9
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	9





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Operator : UM/SJ
Sample : H1442-05
Misc :
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Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

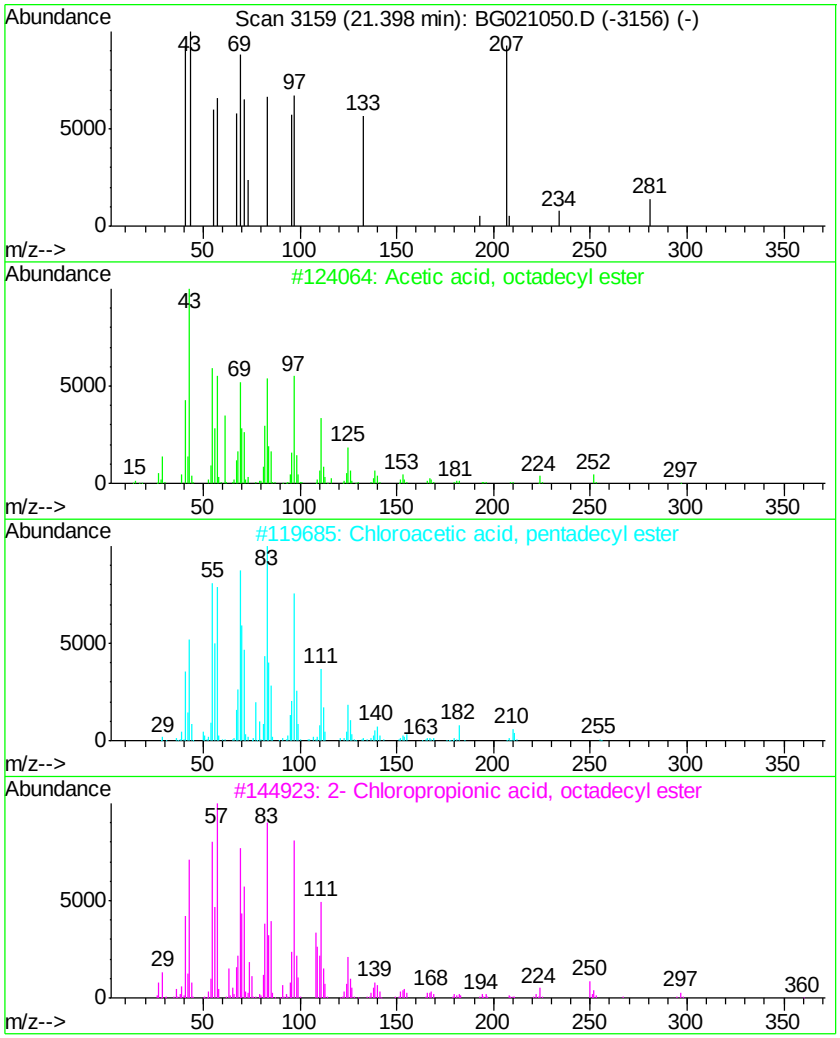
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

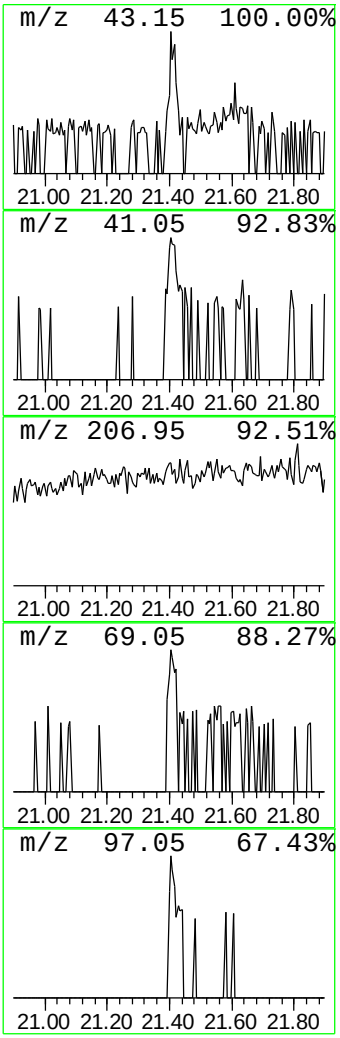
****

Peak Number 8 unknown21.40 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	2.68 ng	6225	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	47
2	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	43
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	43
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	43
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	43





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Operator : UM/SJ
Sample : H1442-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

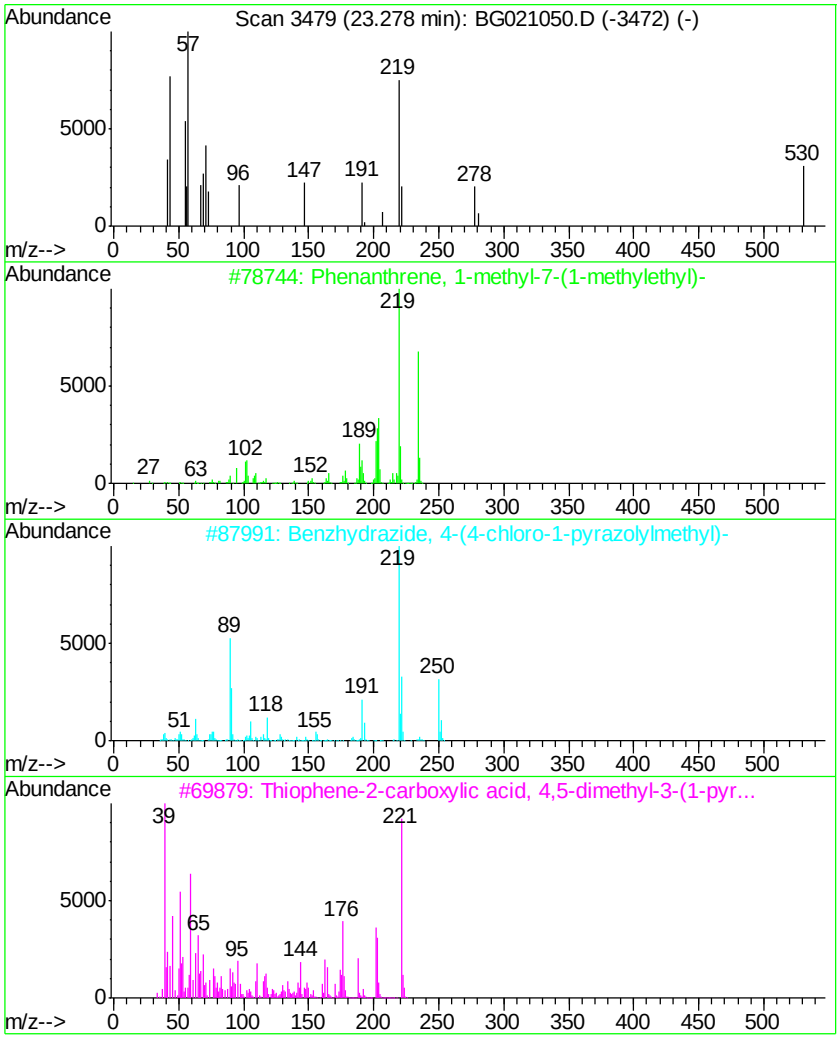
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

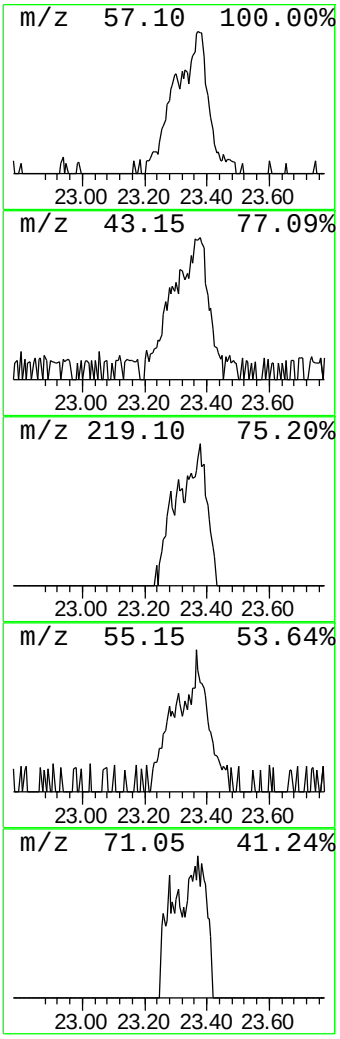
****

Peak Number 9 unknown23.28 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	3.90 ng	9066	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-7-(1-meth...	234	C18H18	000483-65-8	23
2	Benzhydrazide, 4-(4-chloro-1-pyr...	250	C11H11ClN4O	1000273-85-4	12
3	Thiophene-2-carboxylic acid, 4,5...	221	C11H11NO2S	1000263-99-4	10
4	2-Methyl-3-carbethoxy-5-hydroxyi...	219	C12H13NO3	007598-91-6	9
5	s-Triazine, 2,4,6-tris(methylthio)-	219	C6H9N3S3	005759-58-0	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022316\
Data File : BG021050.D
Acq On : 24 Feb 2016 7:11
Operator : UM/SJ
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Instrument : BNA_G
ClientSampleId : POST-EX-14-20160211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022316.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
Propane, 2,2-dime...	3.06	199.5	ng	268674	1	8.20	26936	20.0
1-Pentene, 2-methyl-	3.20	6.9	ng	9325	1	8.20	26936	20.0
2-Pentanone, 4-hy...	5.29	21.0	ng	28319	1	8.20	26936	20.0
unknown7.75	7.75	131.6	ng	177224	1	8.20	26936	20.0
Octane, 2,4,6-tri...	15.61	2.2	ng	7829	3	14.82	69989	20.0
unknown16.46	16.46	2.4	ng	7979	4	17.55	67073	20.0
unknown21.40	21.40	2.7	ng	6225	5	21.82	46502	20.0
unknown23.28	23.28	3.9	ng	9066	5	21.82	46502	20.0