LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023146.D
Acq On : 16 Jul 2016 14:20
Operator : UM/SJ
Sample : H4017-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-13

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	2.894	5	9	27	rVB3	429114	1250828	17.94%	2.390%
2	3.041	28	34	48	rVB	3878511	5980632	85.78%	11.426%
3	3.182	53	58	70	rVB2	213059	474426	6.81%	0.906%
4	5.221	399	405	411	rBV	257085	392159	5.62%	0.749%
5	5.697	478	486	494	rBV	1796549	2882255	41.34%	5.507%
6	7.307	751	760	771	rBV	2013885	3516377	50.44%	6.718%
7	7.677	815	823	832	rBV	1856468	3238888	46.46%	6.188%
8	8.147	897	903	913	rVB	396477	688477	9.88%	1.315%
9	8.476	952	959	967	rVB	1303439	2244949	32.20%	4.289%
10	9.322	1094	1103	1115	rBV	1214791	2250417	32.28%	4.299%
11	9.416	1115	1119	1125	rBV4	40905	72183	1.04%	0.138%
12	10.979	1378	1385	1392	rBV	589480	1081014	15.51%	2.065%
13	13.417	1792	1800	1812	rBV	3119680	4962049	71.17%	9.480%
14	14.240	1932	1940	1945	rBV	793606	1213884	17.41%	2.319%
15	14.798	2025	2035	2043	rBV2	991284	1673185	24.00%	3.197%
16	15.615	2170	2174	2179	rVB3	74161	105167	1.51%	0.201%
17	16.291	2282	2289	2300	rBV	2979880	4642553	66.59%	8.870%
18	16.484	2317	2322	2324	rBV3	73759	115904	1.66%	0.221%
19	17.278	2452	2457	2461	rBV3	86346	126301	1.81%	0.241%
20	17.554	2495	2504	2509	rBV2	1321875	2151600	30.86%	4.111%
21	17.906	2560	2564	2571	rBV3	113786	227207	3.26%	0.434%
22	18.018	2578	2583	2589	rVB2	65197	95553	1.37%	0.183%
23	18.417	2647	2651	2655	rBV4	122480	172535	2.47%	0.330%
24	18.611	2680	2684	2689	rBV6	72132	120943	1.73%	0.231%
25	18.893	2726	2732	2735	rBV8	47598	80606	1.16%	0.154%
26	19.281	2791	2798	2803	rBV8	80620	167003	2.40%	0.319%
27	19.463	2824	2829	2837	rVB8	73072	164881	2.36%	0.315%
28	19.598	2847	2852	2856	rBV	162441	231457	3.32%	0.442%
29	19.675	2860	2865	2871	rBV10	42743	98022	1.41%	0.187%
30	19.963	2910	2914	2918	rVB	127639	175629	2.52%	0.336%
31	20.151	2940	2946	2954	rVB	5357106	6971721	100.00%	13.320%
32	21.461	3165	3169	3174	rBV8	101498	195504	2.80%	0.374%
33	21.855	3228	3236	3242	rBV	1323790	2473239	35.48%	4.725%
34	25.221	3800	3809	3820	rVB4	729855	2103846	30.18%	4.019%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023146.D
Acq On : 16 Jul 2016 14:20
Operator : UM/SJ
Sample : H4017-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C5-13

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

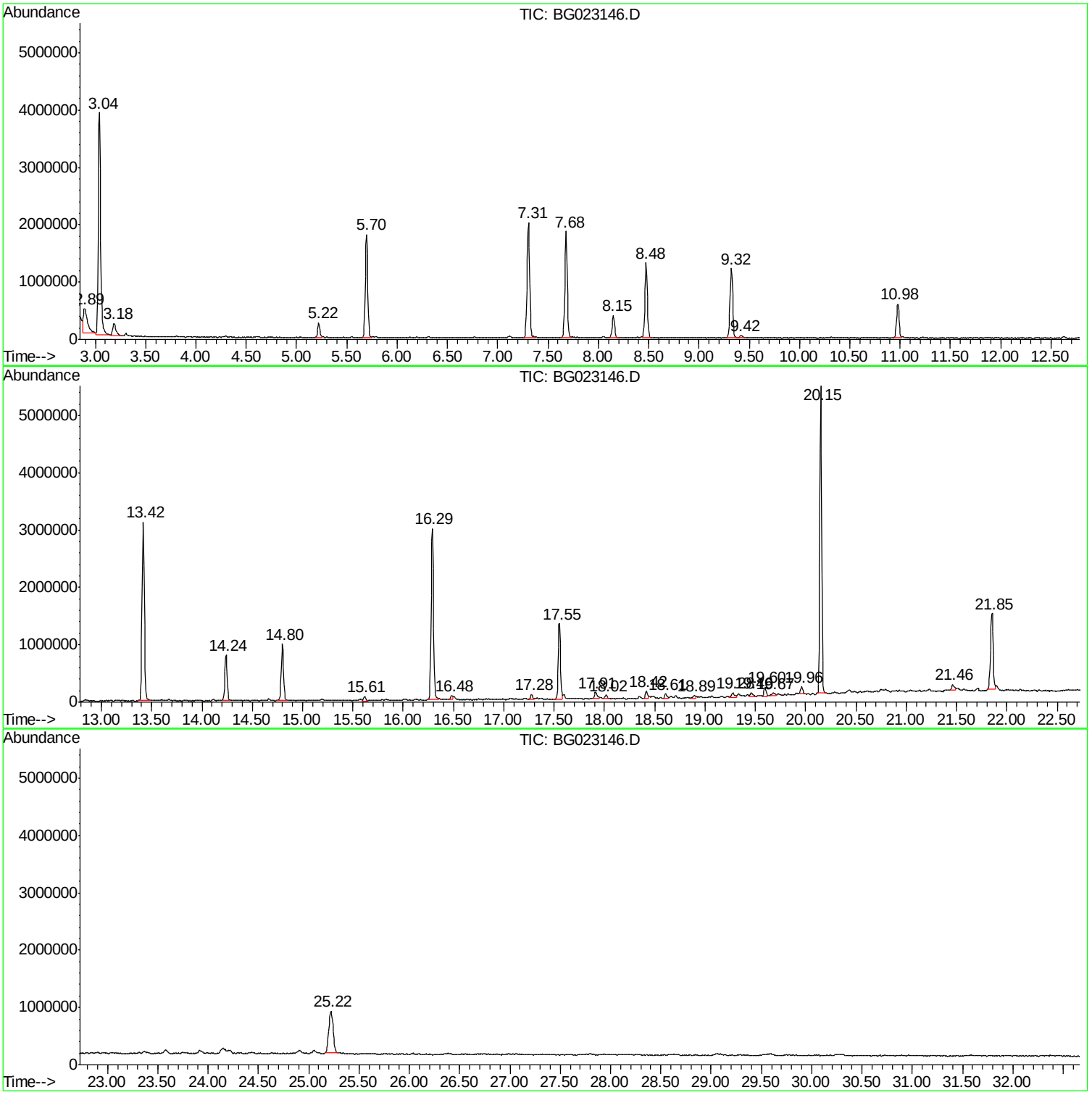
Sum of corrected areas: 52341394

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023146.D
Acq On : 16 Jul 2016 14:20
Operator : UM/SJ
Sample : H4017-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-13

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 : BG023146.D
Acq On : 16 Jul 2016 14:20
Operator : UM/SJ
Sample : H4017-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-13

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

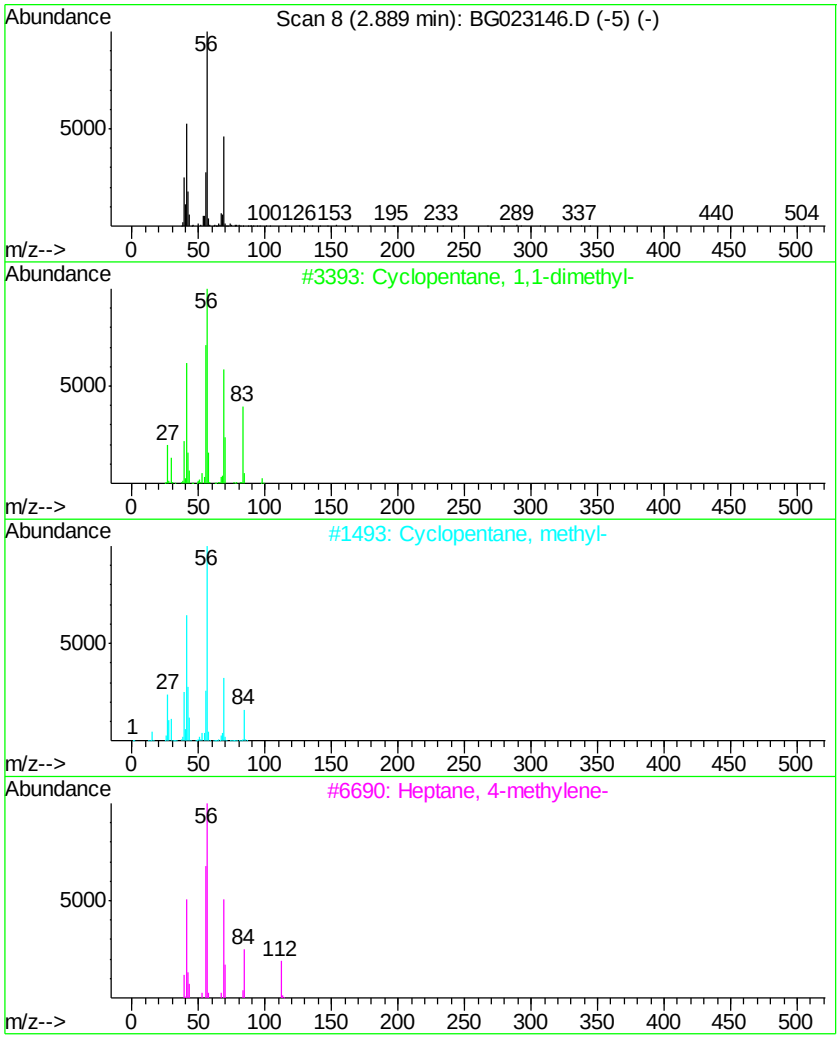
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

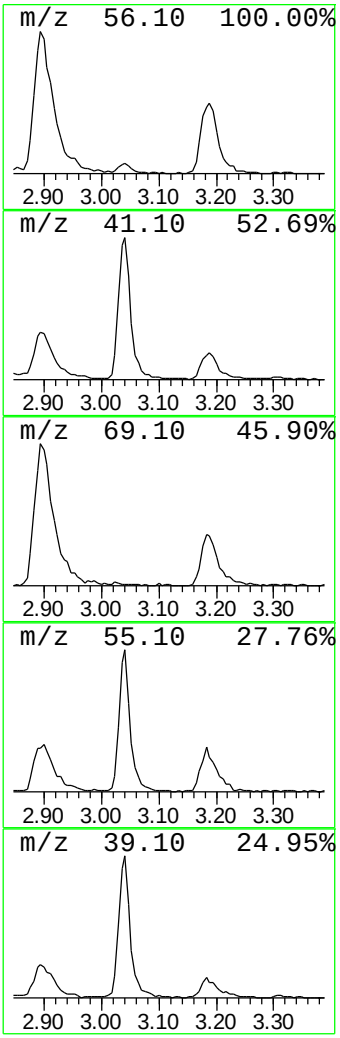
****

Peak Number 1 Cyclopentane, 1,1-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	36.34 ng	1250830	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	64
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	59
3	Heptane, 4-methylene-	112	C8H16	015918-08-8	56
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	38
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	36





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023146.D
Acq On : 16 Jul 2016 14:20
Operator : UM/SJ
Sample : H4017-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-13

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

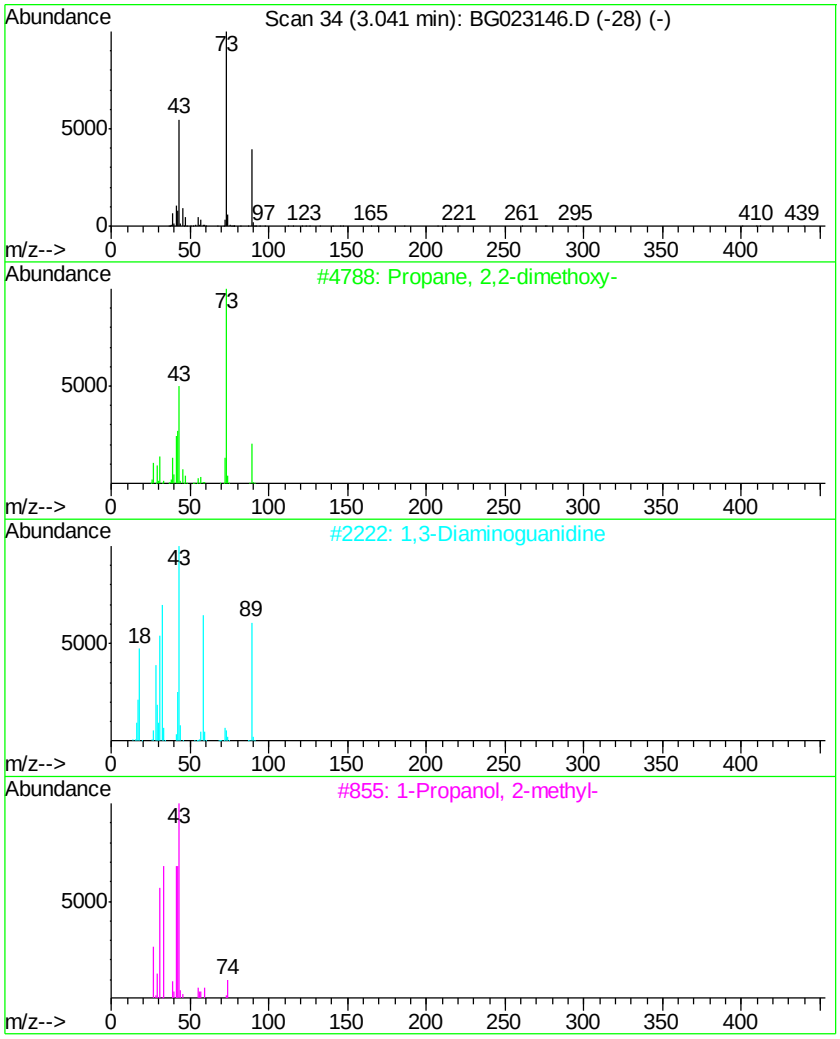
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

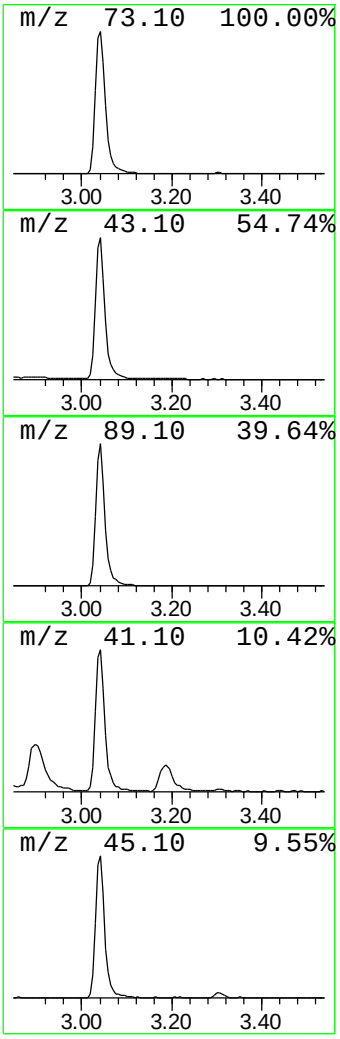
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	173.74 ng	5980630	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	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023146.D
Acq On : 16 Jul 2016 14:20
Operator : UM/SJ
Sample : H4017-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-13

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

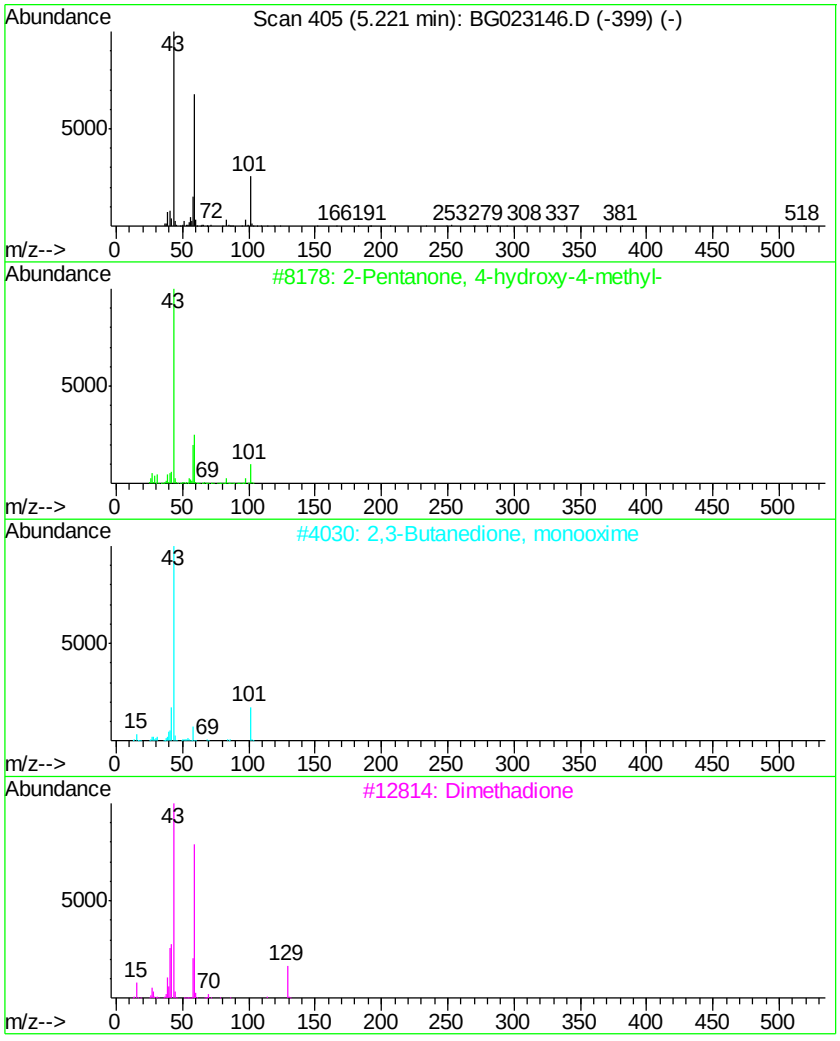
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

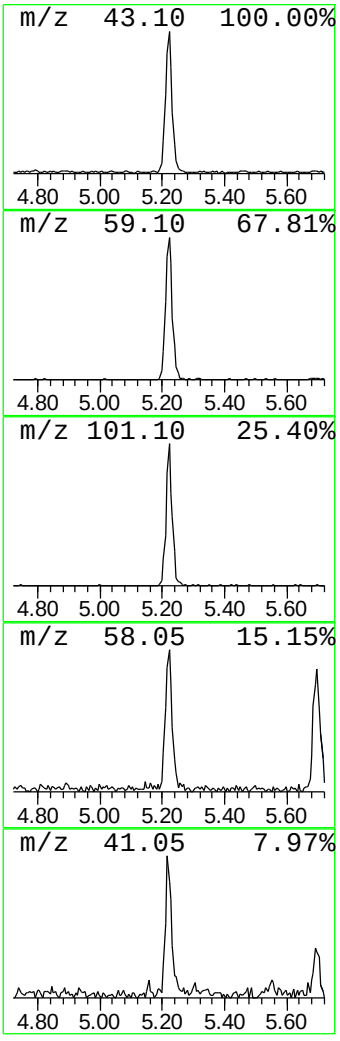
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	11.39 ng	392159	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	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	Dimethadione	129	C5H7NO3	000695-53-4	33
4	1,2-Butanediol	90	C4H10O2	000584-03-2	32
5	Acetic acid, chloro-, 1,1-dimeth...	150	C6H11ClO2	000107-59-5	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023146.D
Acq On : 16 Jul 2016 14:20
Operator : UM/SJ
Sample : H4017-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-13

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

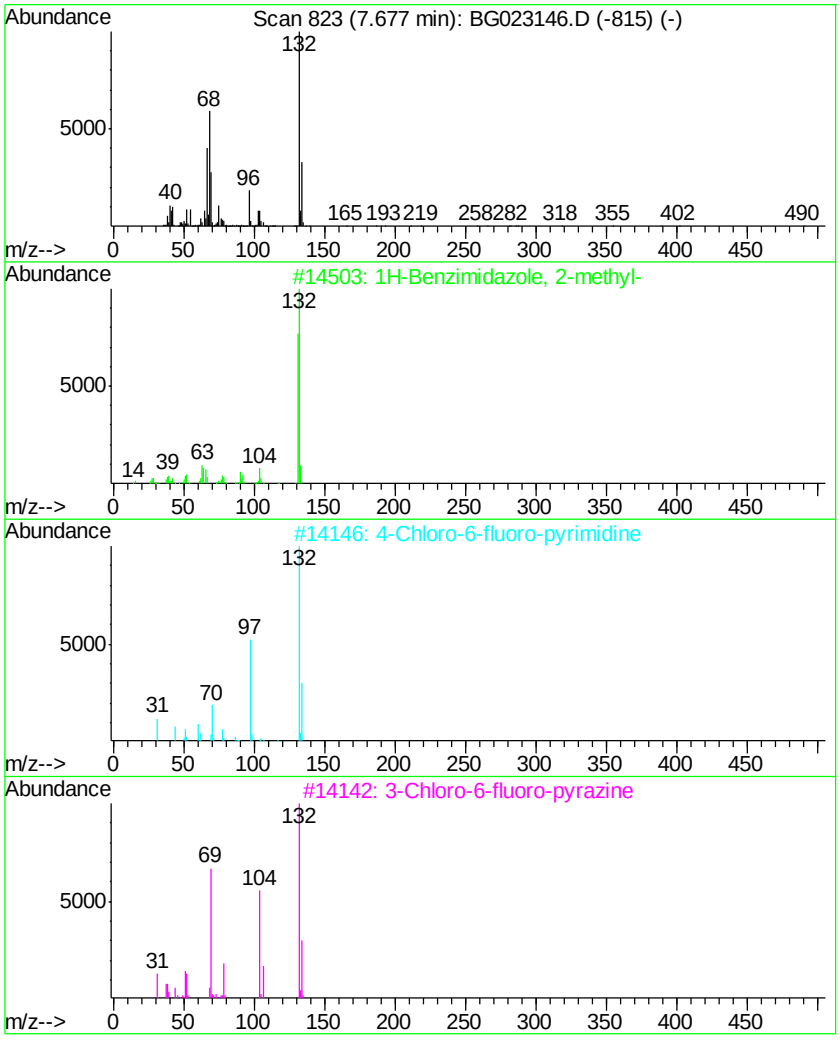
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

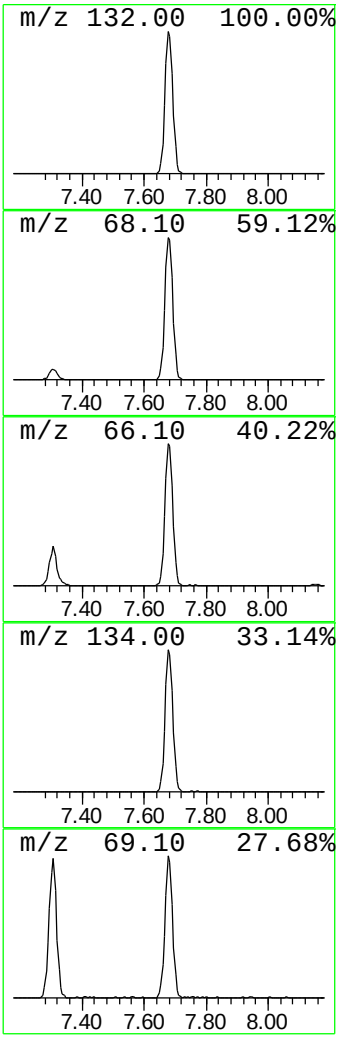
****

Peak Number 5 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	94.09 ng	3238890	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10





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Sample : H4017-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-13

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

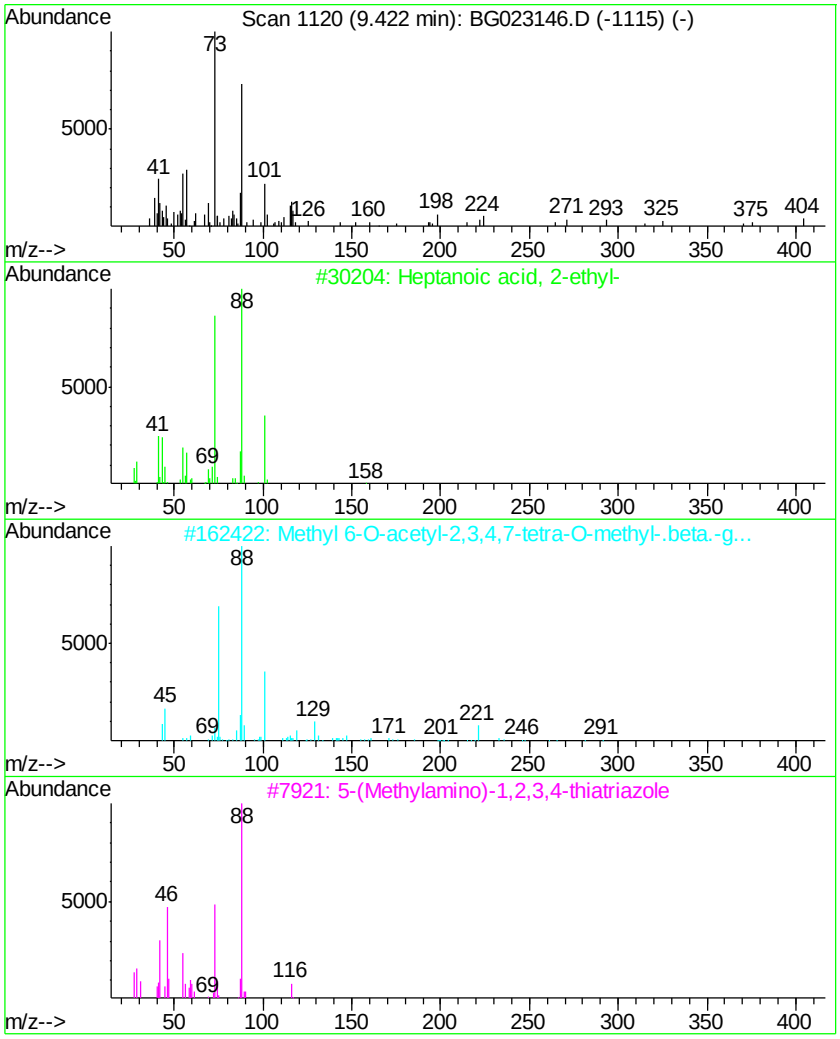
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

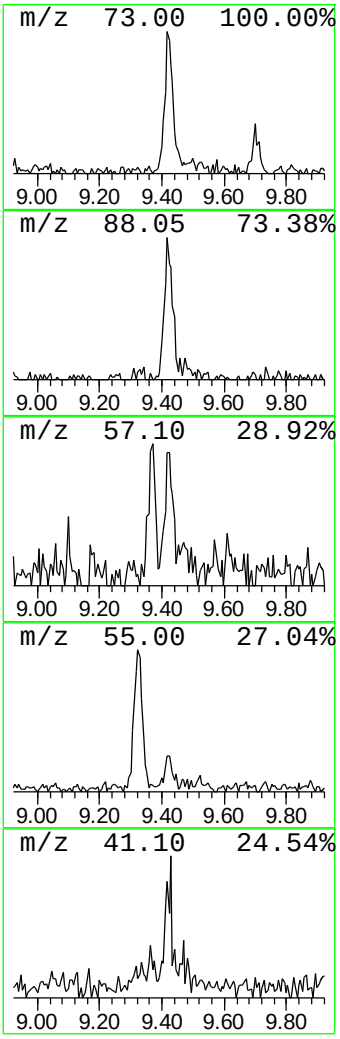
****

Peak Number 7 Heptanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	2.10 ng	72183	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	72
2	Methyl 6-O-acetyl-2,3,4,7-tetra-...	322	C14H26O8	084564-15-8	59
3	5-(Methylamino)-1,2,3,4-thiatria...	116	C2H4N4S	052098-72-3	59
4	Decanoic acid, ethyl ester	200	C12H24O2	000110-38-3	53
5	Dodecanoic acid, 2,6-dimethyl-, ...	242	C15H30O2	055955-75-4	53





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Sample : H4017-03
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Instrument : BNA_G
ClientSampleId : C5-13

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

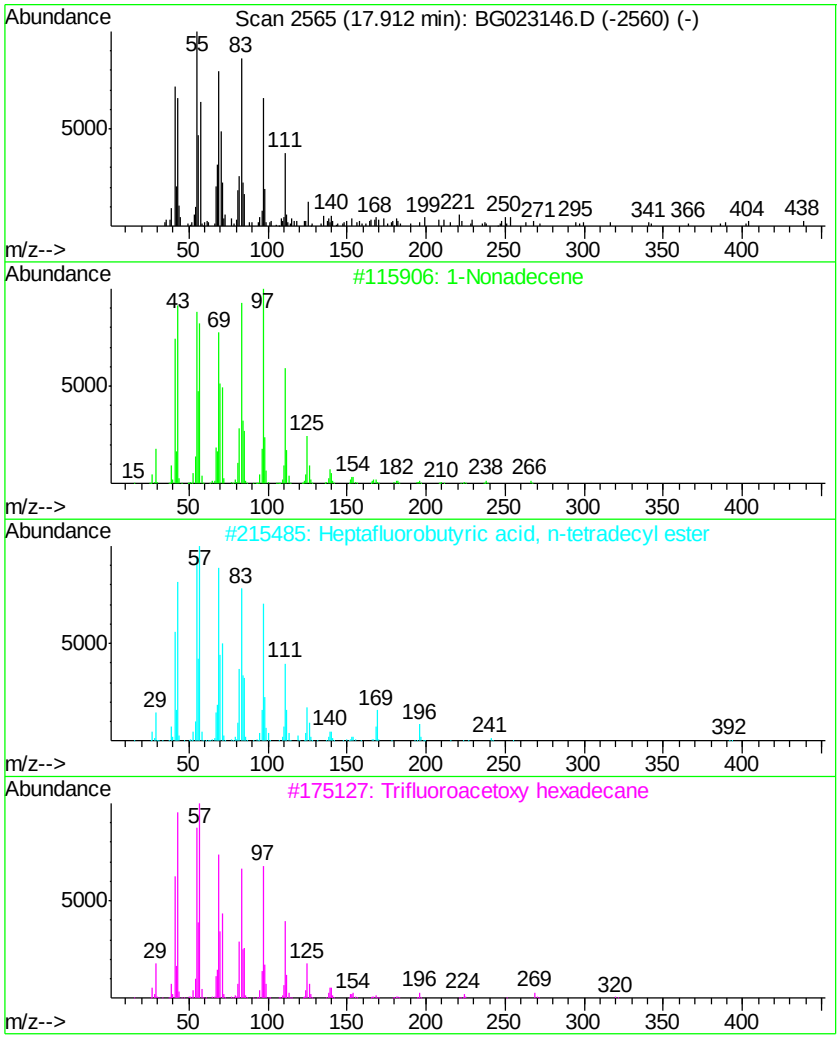
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

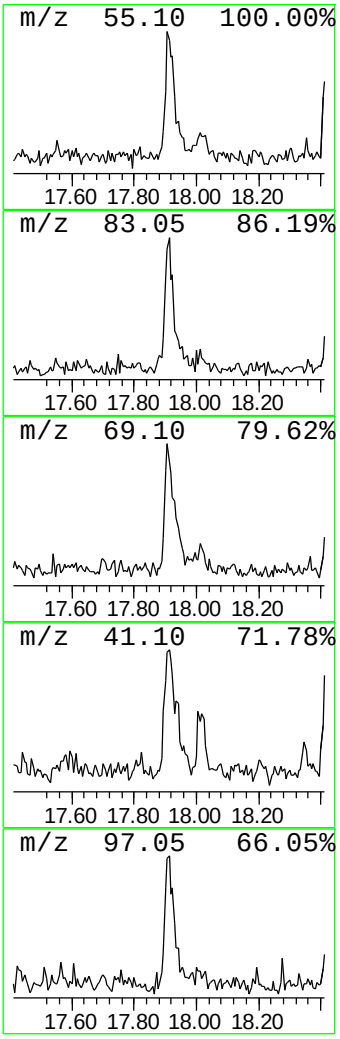
****

Peak Number 8 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	2.11 ng	227207	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	90
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	86
5	Cyclooctane, methyl-	126	C9H18	001502-38-1	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023146.D
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Sample : H4017-03
Misc :
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Instrument : BNA_G
ClientSampleId : C5-13

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, 1,1...	2.89	36.3	ng	1250830	1	8.15	688477	20.0
Propane, 2,2-dime...	3.04	173.7	ng	5980630	1	8.15	688477	20.0
2-Pentanone, 4-hy...	5.22	11.4	ng	392159	1	8.15	688477	20.0
unknown7.68	7.68	94.1	ng	3238890	1	8.15	688477	20.0
Heptanoic acid, 2...	9.42	2.1	ng	72183	1	8.15	688477	20.0
1-Nonadecene	17.91	2.1	ng	227207	4	17.55	2151600	20.0