LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023090.D
Acq On : 14 Jul 2016 5:53
Operator : UM/SJ
Sample : H4005-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 071116-P41-E-U-M

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	4.612	296	302	314	rVB	1683605	2483222	25.42%	5.278%
2	5.223	400	406	416	rVB	1477578	2251657	23.05%	4.786%
3	5.699	481	487	495	rBV	654150	1042738	10.67%	2.216%
4	6.310	585	591	600	rVB	333609	520081	5.32%	1.105%
5	7.309	755	761	768	rBV	493549	861443	8.82%	1.831%
6	7.685	817	825	831	rBV	1148966	2025502	20.73%	4.305%
7	8.155	896	905	913	rVB	400495	691448	7.08%	1.470%
8	8.478	951	960	968	rBV	1386286	2474093	25.32%	5.259%
9	9.330	1097	1105	1113	rBV	1441406	2571085	26.32%	5.465%
10	10.981	1380	1386	1394	rBV	592992	1079043	11.05%	2.293%
11	11.774	1512	1521	1530	rBV	309642	641839	6.57%	1.364%
12	13.072	1735	1742	1752	rBV3	359843	617160	6.32%	1.312%
13	13.425	1793	1802	1809	rBV	3893538	6193042	63.39%	13.163%
14	14.806	2028	2037	2047	rBV2	1096565	1880392	19.25%	3.997%
15	16.292	2283	2290	2301	rBV	2429861	3985152	40.79%	8.470%
16	17.555	2497	2505	2512	rBV	1510638	2415459	24.72%	5.134%
17	18.419	2647	2652	2657	rBV3	117816	174506	1.79%	0.371%
18	19.688	2863	2868	2875	rBV6	81423	130350	1.33%	0.277%
19	20.158	2942	2948	2956	rBV	7303193	9769375	100.00%	20.764%
20	21.862	3231	3238	3246	rBV2	1560820	2727586	27.92%	5.797%
21	25.241	3803	3813	3824	rBV2	809415	2513389	25.73%	5.342%

Sum of corrected areas: 47048562

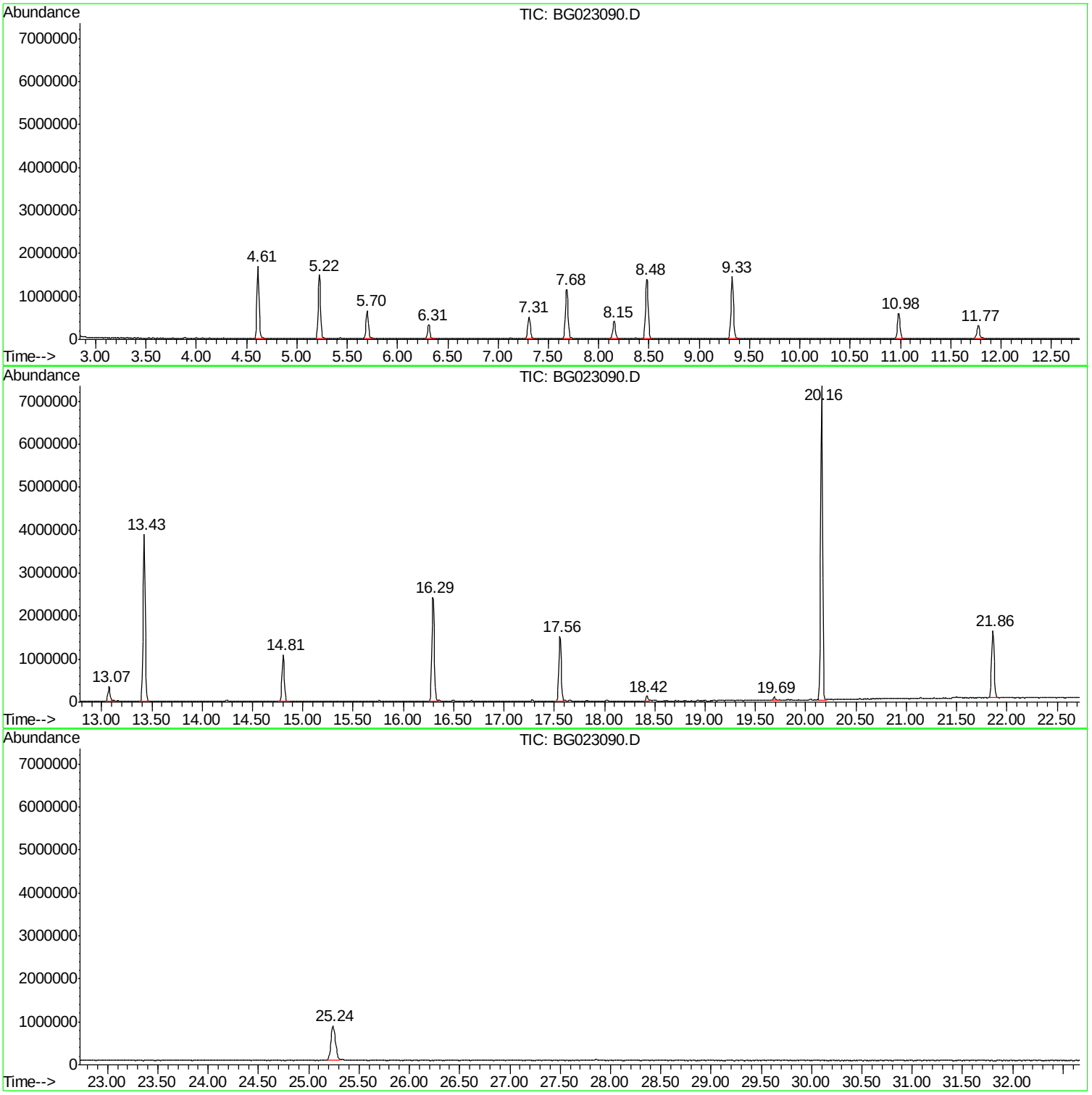
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023090.D
Acq On : 14 Jul 2016 5:53
Operator : UM/SJ
Sample : H4005-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 071116-P41-E-U-M

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\BG071316\
Data File : BG023090.D
Acq On : 14 Jul 2016 5:53
Operator : UM/SJ
Sample : H4005-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 071116-P41-E-U-M

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

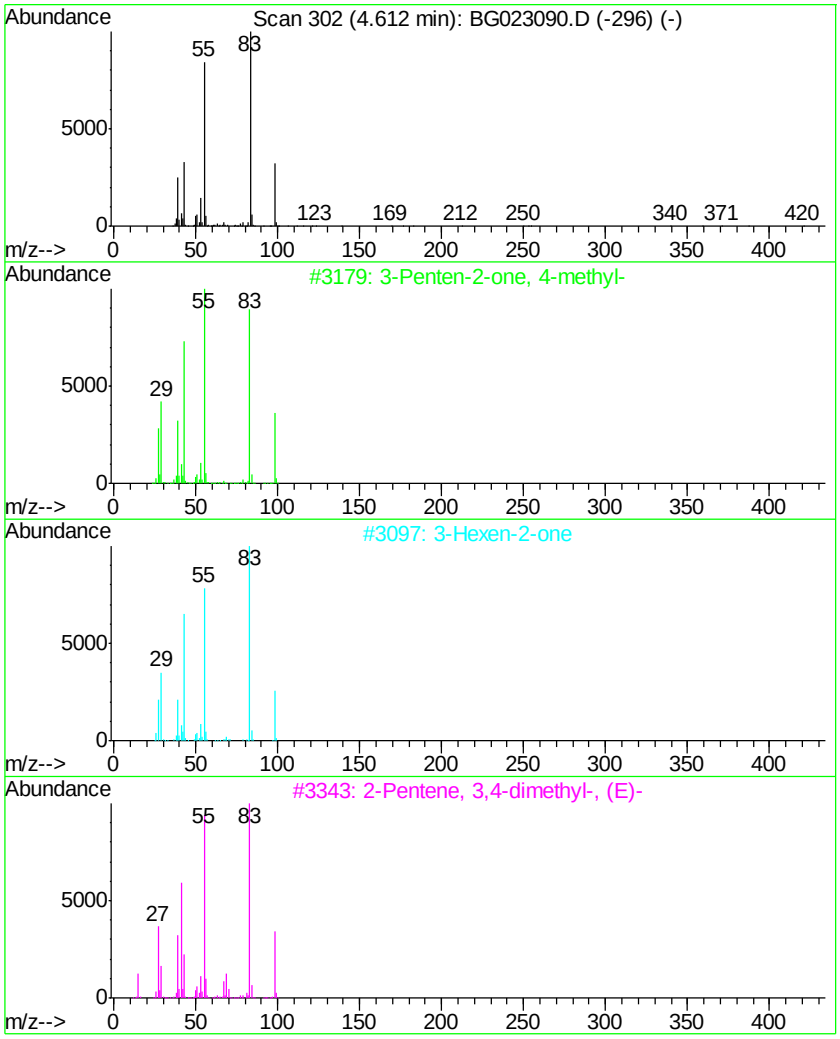
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

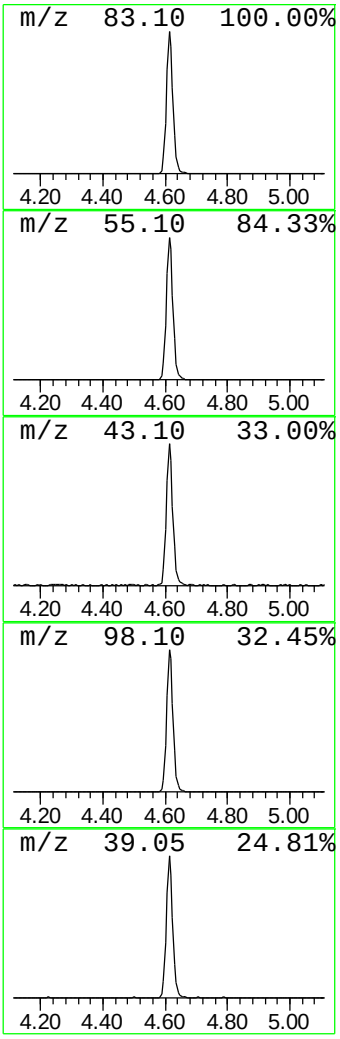
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	71.83 ng	2483220	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023090.D
Acq On : 14 Jul 2016 5:53
Operator : UM/SJ
Sample : H4005-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 071116-P41-E-U-M

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

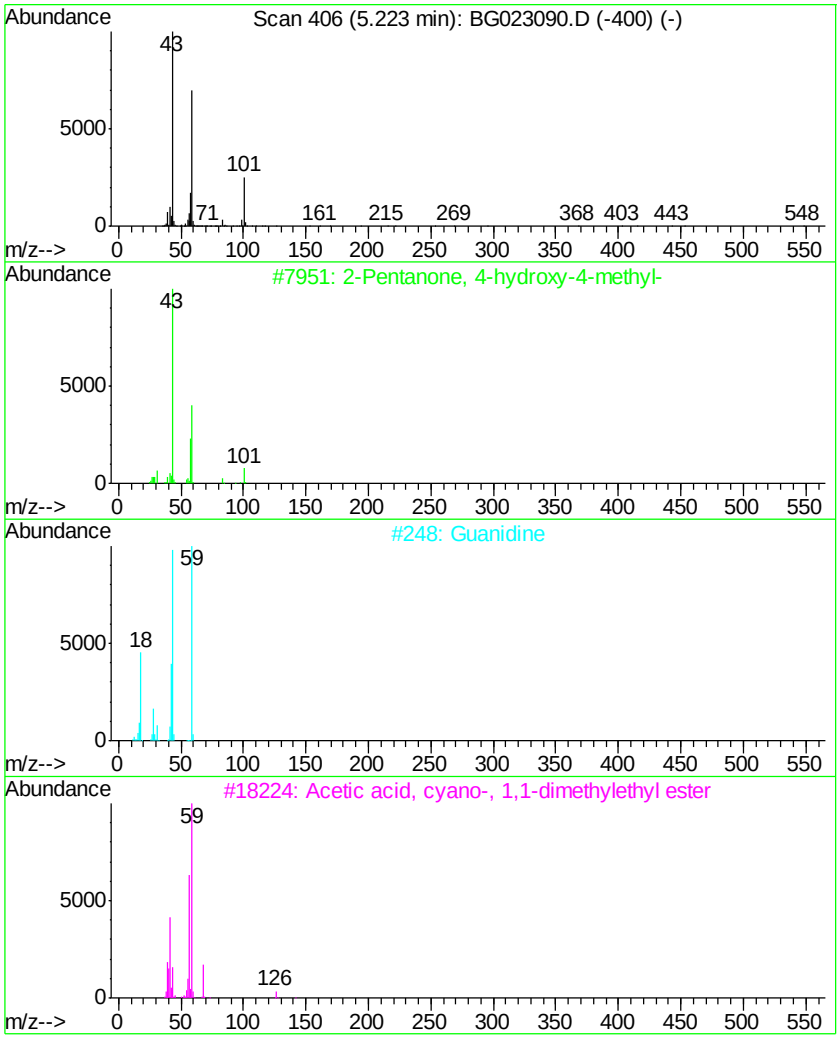
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

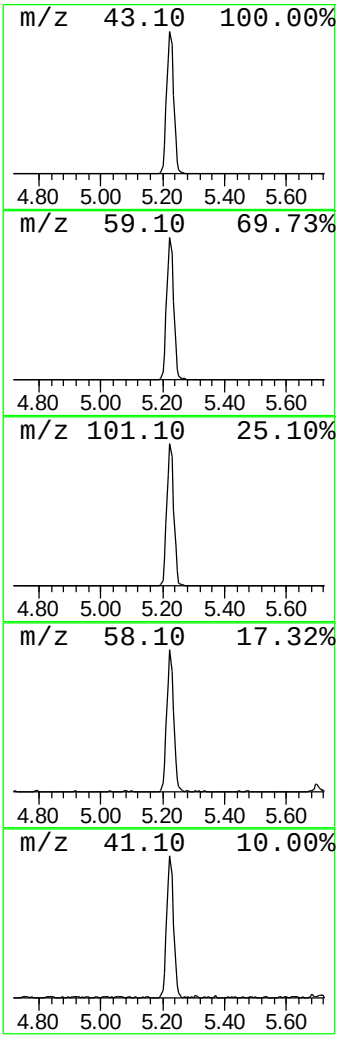
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	65.13 ng	2251660	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	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023090.D
Acq On : 14 Jul 2016 5:53
Operator : UM/SJ
Sample : H4005-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 071116-P41-E-U-M

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

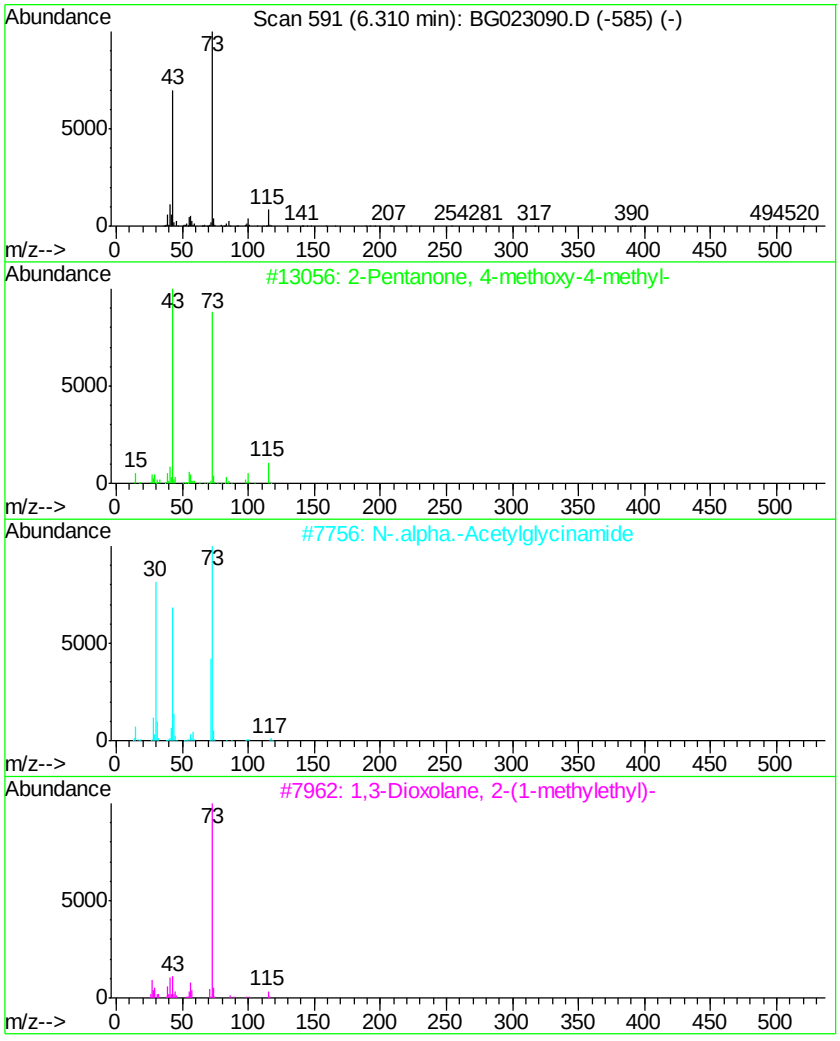
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

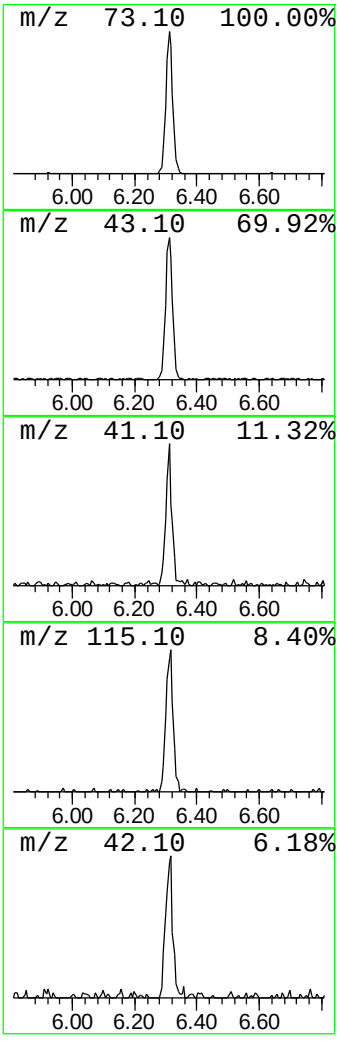
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.31	15.04 ng	520081	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	43
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4	N-Formylmorpholine	115	C5H9NO2	004394-85-8	12
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023090.D
Acq On : 14 Jul 2016 5:53
Operator : UM/SJ
Sample : H4005-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 071116-P41-E-U-M

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

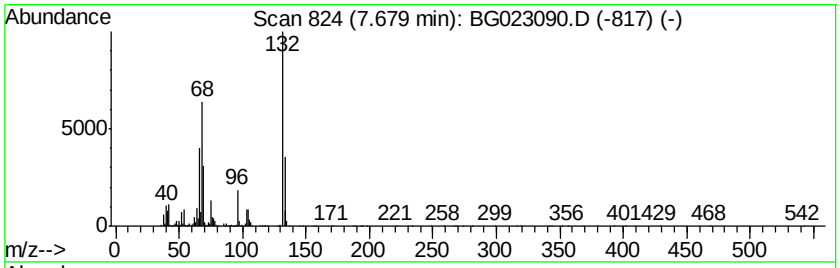
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

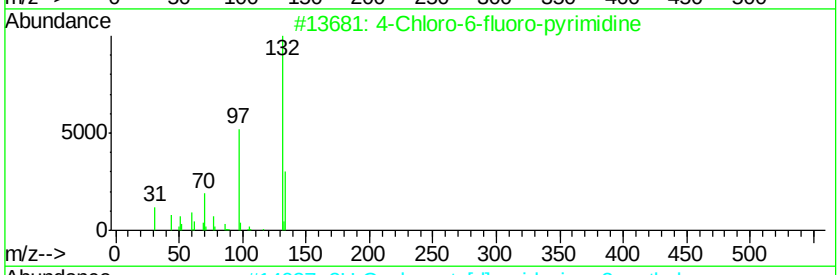
****

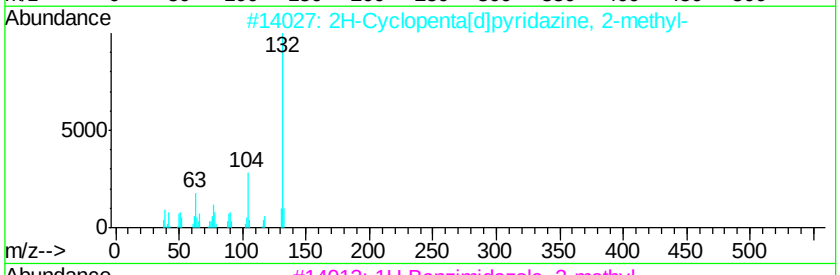
Peak Number 4 unknown7.68 Concentration Rank 4

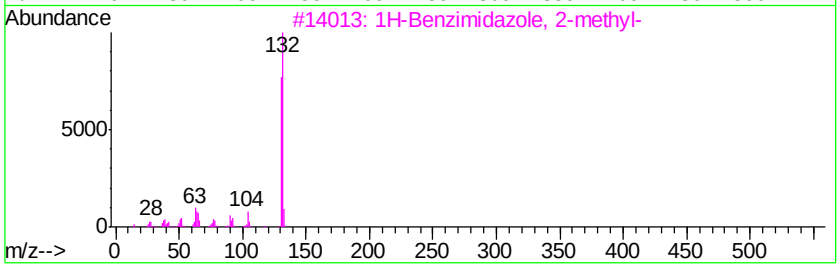
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	58.59 ng	2025500	1,4-Dichlorobenzene-d4	8.15

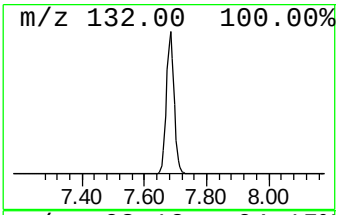
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10

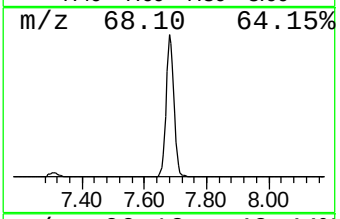


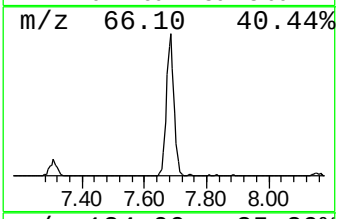


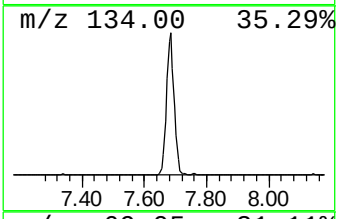


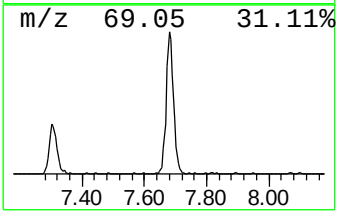












Library Search Compound Report

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Acq On : 14 Jul 2016 5:53
Operator : UM/SJ
Sample : H4005-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 071116-P41-E-U-M

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

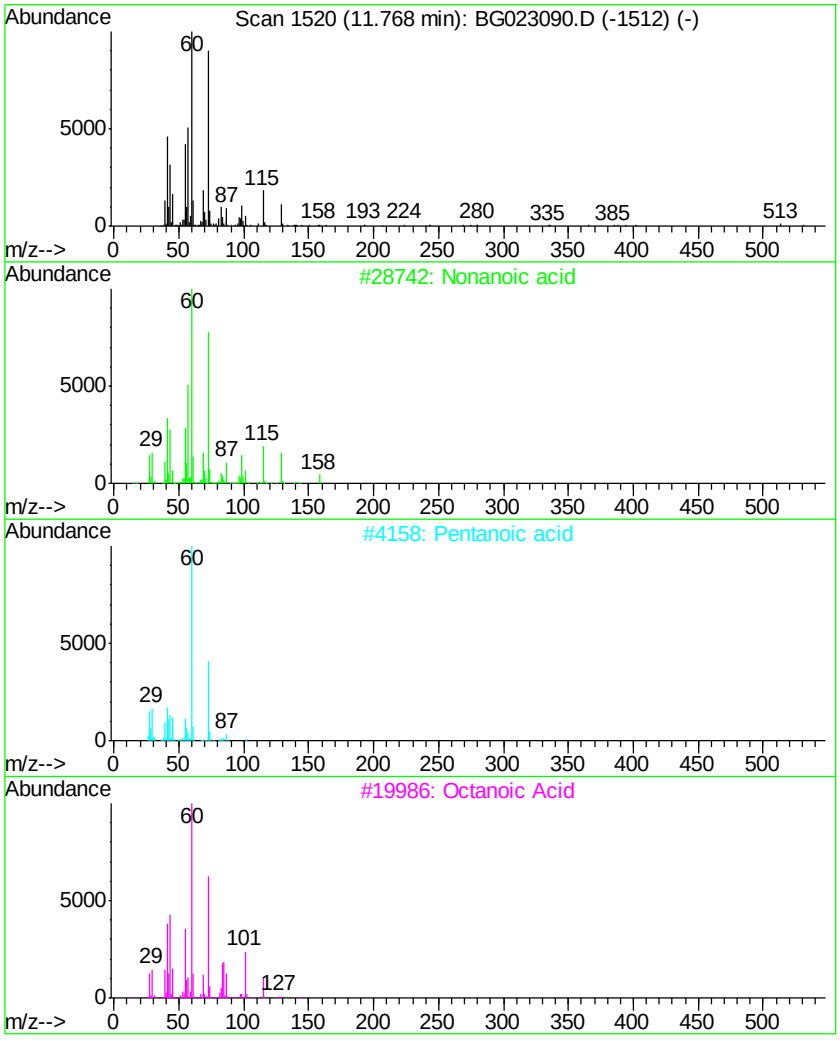
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

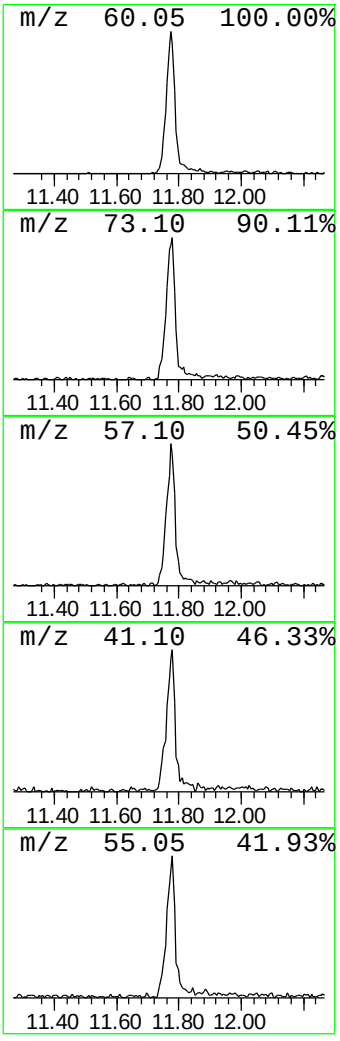
****

Peak Number 6 Nonanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	11.90 ng	641839	Naphthalene-d8	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	86
2	Pentanoic acid	102	C5H10O2	000109-52-4	53
3	Octanoic Acid	144	C8H16O2	000124-07-2	50
4	Hexanoic acid	116	C6H12O2	000142-62-1	49
5	n-Decanoic acid	172	C10H20O2	000334-48-5	45





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023090.D
Acq On : 14 Jul 2016 5:53
Operator : UM/SJ
Sample : H4005-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 071116-P41-E-U-M

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

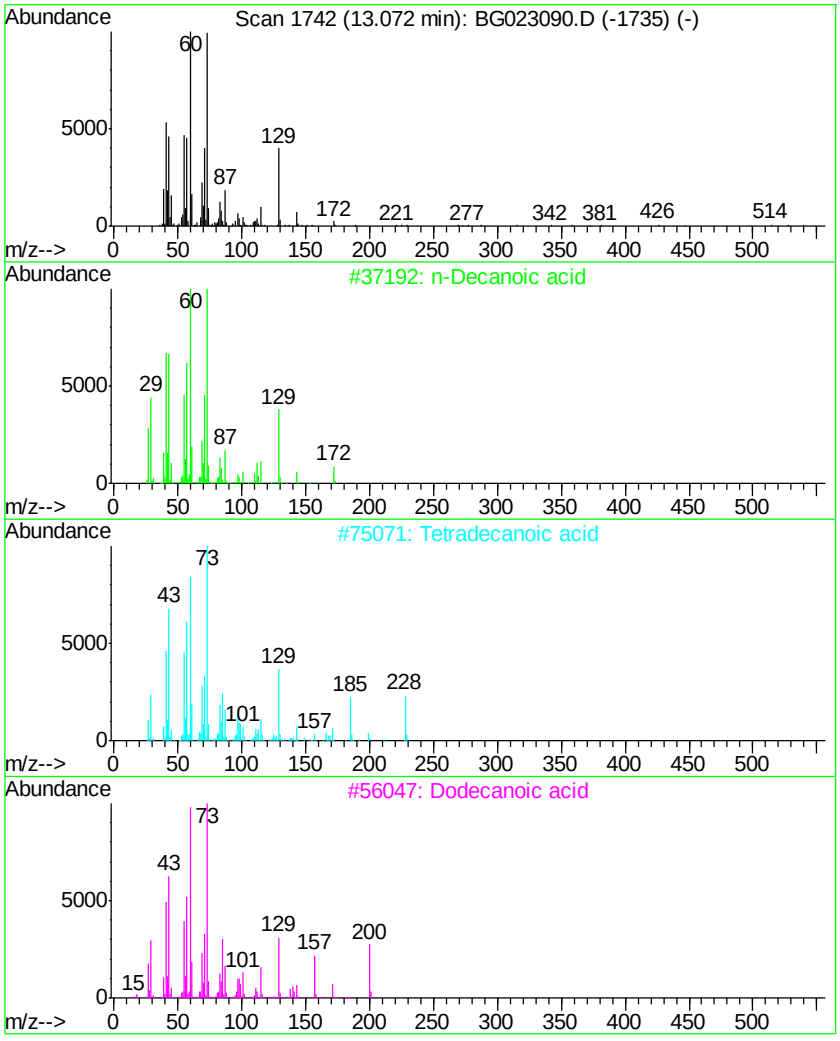
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

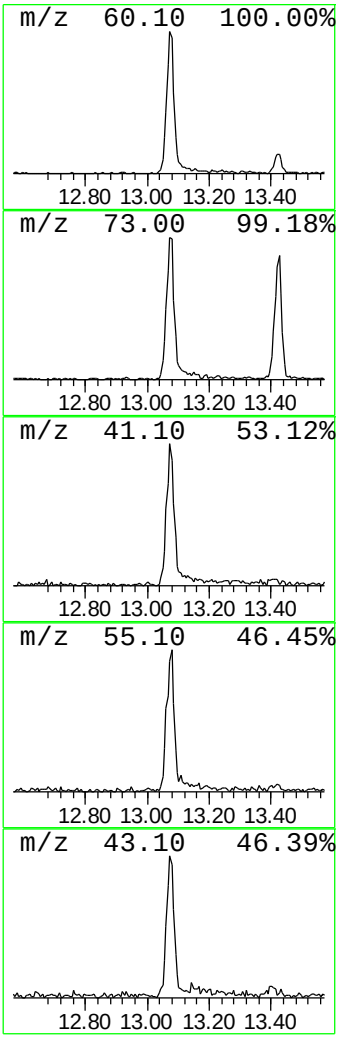
****

Peak Number 7 n-Decanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.07	6.56 ng	617160	Acenaphthene-d10	14.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Dodecanoic acid	200	C12H24O2	000143-07-7	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	56
5	Heptanoic acid	130	C7H14O2	000111-14-8	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071316\
Data File : BG023090.D
Acq On : 14 Jul 2016 5:53
Operator : UM/SJ
Sample : H4005-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 071116-P41-E-U-M

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.61	71.8	ng	2483220	1	8.15	691448	20.0
2-Pentanone, 4-hy...	5.22	65.1	ng	2251660	1	8.15	691448	20.0
2-Pentanone, 4-me...	6.31	15.0	ng	520081	1	8.15	691448	20.0
unknown7.68	7.68	58.6	ng	2025500	1	8.15	691448	20.0
Nonanoic acid	11.77	11.9	ng	641839	2	10.99	1079040	20.0
n-Decanoic acid	13.07	6.6	ng	617160	3	14.81	1880390	20.0