LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023150.D
Acq On : 16 Jul 2016 17:02
Operator : UM/SJ
Sample : H3951-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(0-2ft)

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	2.896	4	10	23	rVB3	158361	435327	3.89%	0.512%
2	3.043	29	35	53	rVB	5860495	9926240	88.68%	11.672%
3	3.190	53	60	69	rVB3	161812	380290	3.40%	0.447%
4	3.813	162	166	173	rBV	72206	122882	1.10%	0.144%
5	5.223	399	406	417	rVB	575816	923421	8.25%	1.086%
6	5.699	480	487	496	rBV	3224488	5346509	47.77%	6.287%
7	7.315	752	762	773	rBV	3558502	6461533	57.73%	7.598%
8	7.685	815	825	837	rBV	3447426	6122390	54.70%	7.199%
9	8.149	897	904	912	rBV	536714	944023	8.43%	1.110%
10	8.478	952	960	968	rVB	2500272	4392679	39.24%	5.165%
11	9.324	1096	1104	1117	rBV	2197160	4155105	37.12%	4.886%
12	9.430	1117	1122	1131	rBV2	81800	157538	1.41%	0.185%
13	10.981	1378	1386	1393	rBV	779787	1423532	12.72%	1.674%
14	13.419	1792	1801	1813	rBV	5568806	8951348	79.97%	10.525%
15	14.242	1934	1941	1947	rBV	2285241	3496887	31.24%	4.112%
16	14.794	2024	2035	2043	rBV2	1168815	2022723	18.07%	2.378%
17	16.293	2283	2290	2305	rBV	4697232	7447584	66.54%	8.757%
18	16.481	2317	2322	2325	rBV3	84518	133852	1.20%	0.157%
19	17.274	2452	2457	2462	rBV	135268	198160	1.77%	0.233%
20	17.550	2498	2504	2509	rBV	1435340	2235571	19.97%	2.629%
21	17.591	2509	2511	2519	rVB	163342	251251	2.24%	0.295%
22	18.020	2580	2584	2588	rVB	118420	146771	1.31%	0.173%
23	18.419	2647	2652	2658	rBV2	690077	1022014	9.13%	1.202%
24	18.619	2681	2686	2690	rBV5	79140	139380	1.25%	0.164%
25	19.600	2848	2853	2858	rVB	523529	770924	6.89%	0.906%
26	19.683	2863	2867	2875	rBV2	367635	559668	5.00%	0.658%
27	19.965	2910	2915	2921	rVB	461048	706875	6.32%	0.831%
28	20.153	2941	2947	2955	rBV	8319310	11193108	100.00%	13.161%
29	21.857	3229	3237	3242	rBV2	1498956	2870823	25.65%	3.376%
30	25.229	3803	3811	3822	rVB2	706035	2106463	18.82%	2.477%

Sum of corrected areas: 85044871

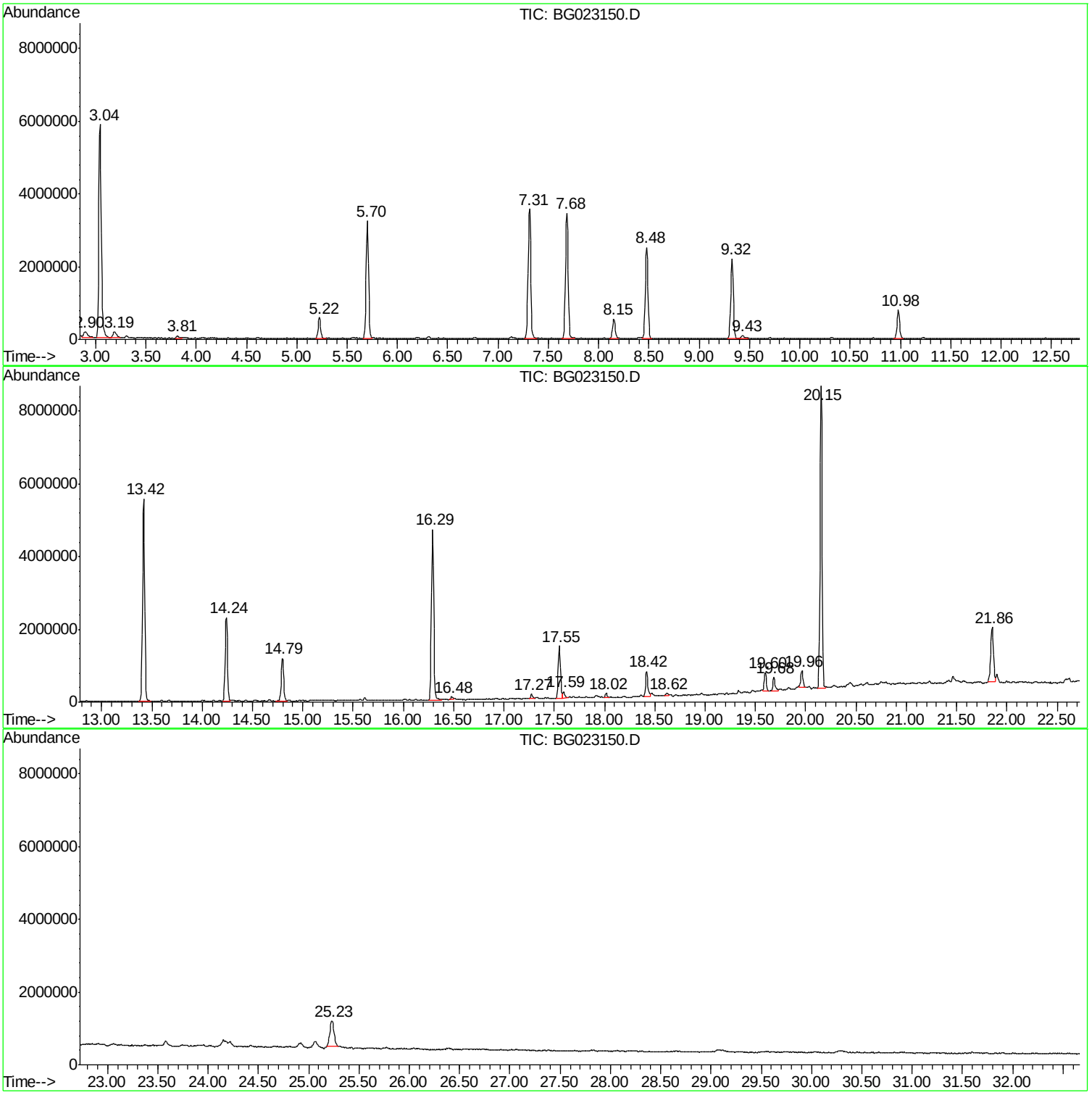
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023150.D
Acq On : 16 Jul 2016 17:02
Operator : UM/SJ
Sample : H3951-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(0-2ft)

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023150.D
Acq On : 16 Jul 2016 17:02
Operator : UM/SJ
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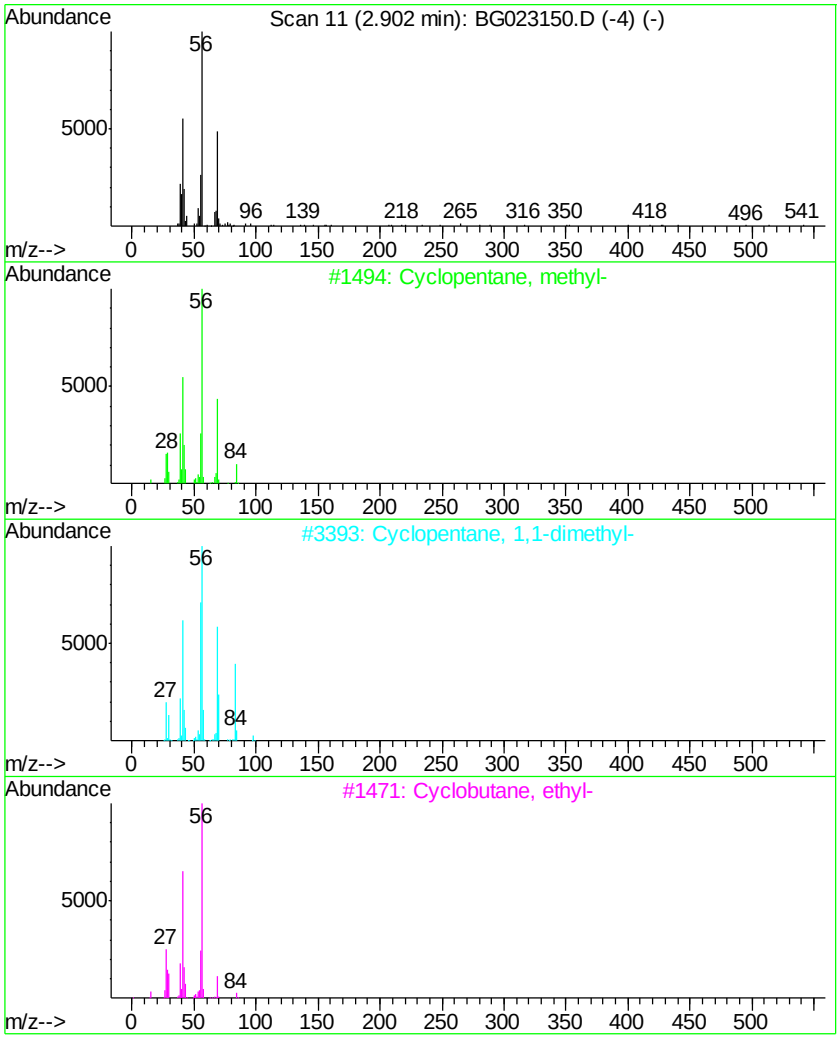
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

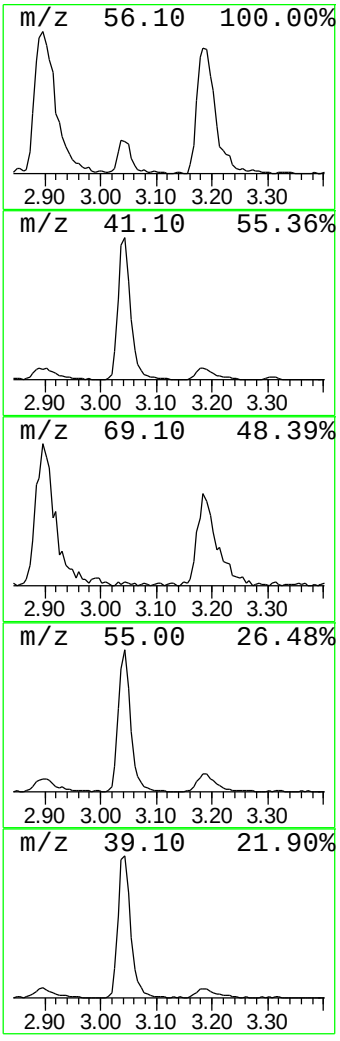
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	9.22 ng	435327	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
2	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	40
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	39
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	39
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023150.D
Acq On : 16 Jul 2016 17:02
Operator : UM/SJ
Sample : H3951-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(0-2ft)

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

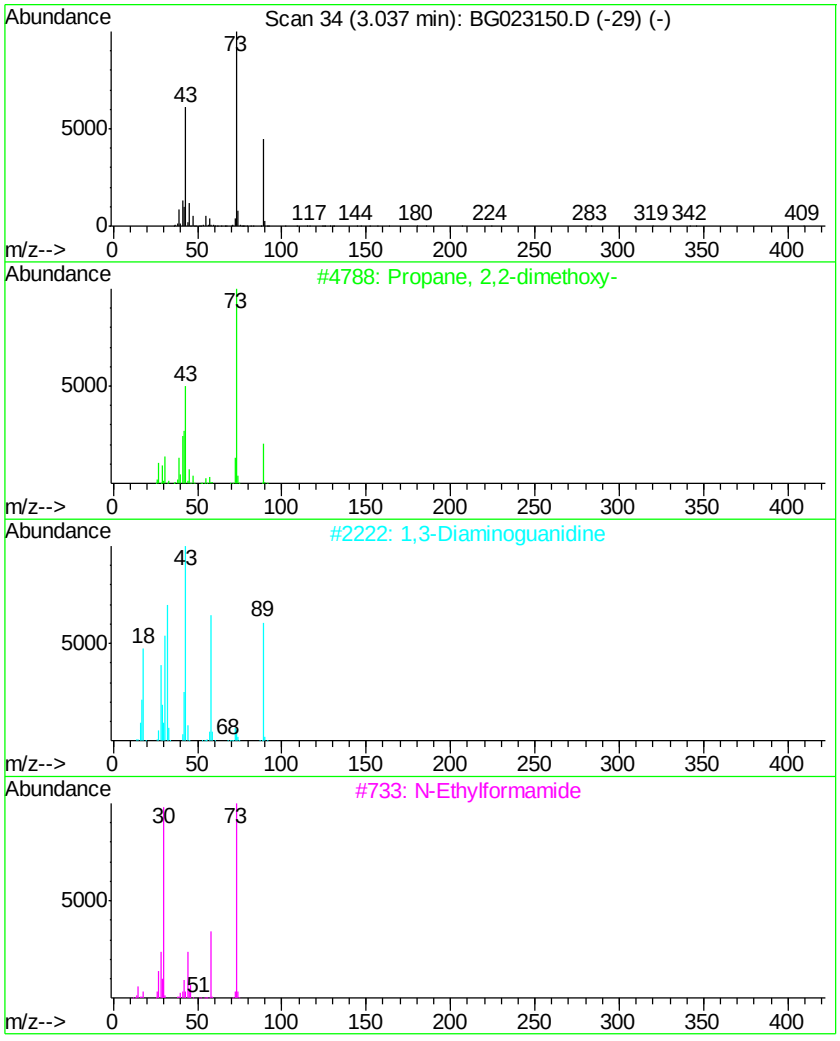
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

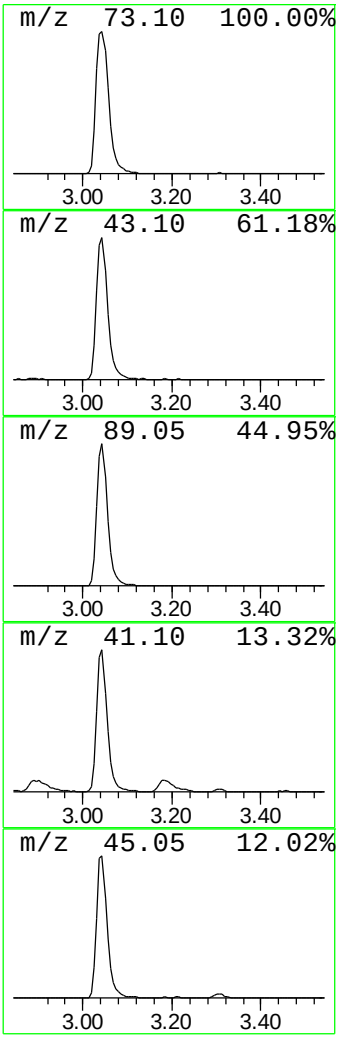
****

Peak Number 2 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	210.30 ng	9926240	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	40
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023150.D
Acq On : 16 Jul 2016 17:02
Operator : UM/SJ
Sample : H3951-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LSS-SB-SB01(0-2ft)

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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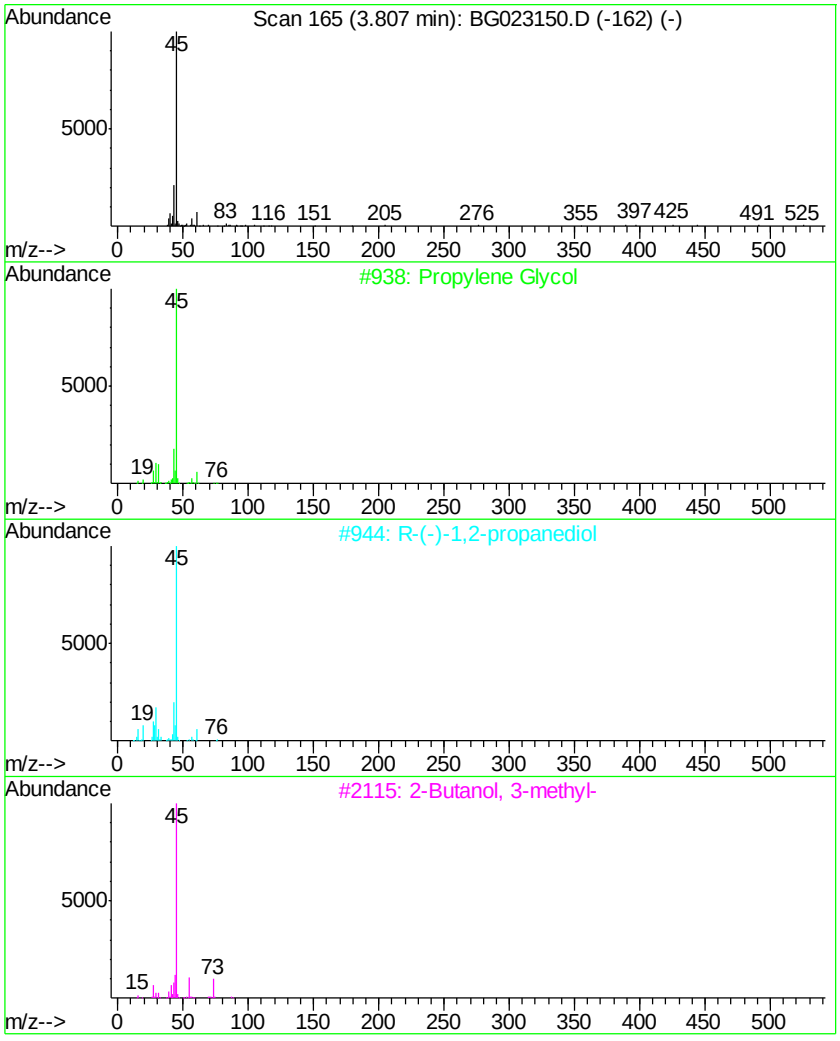
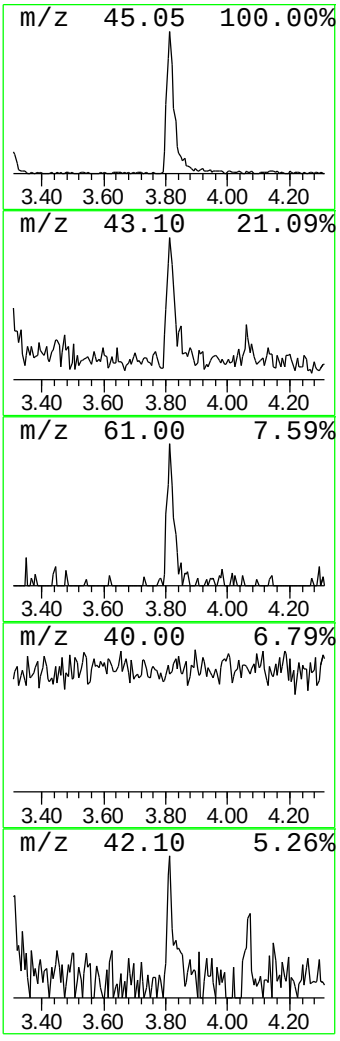
Peak Number 4 Propylene Glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.81	2.60 ng	122882	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	50
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	39
3	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	38
4	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	38
5	2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	38





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023150.D
Acq On : 16 Jul 2016 17:02
Operator : UM/SJ
Sample : H3951-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(0-2ft)

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

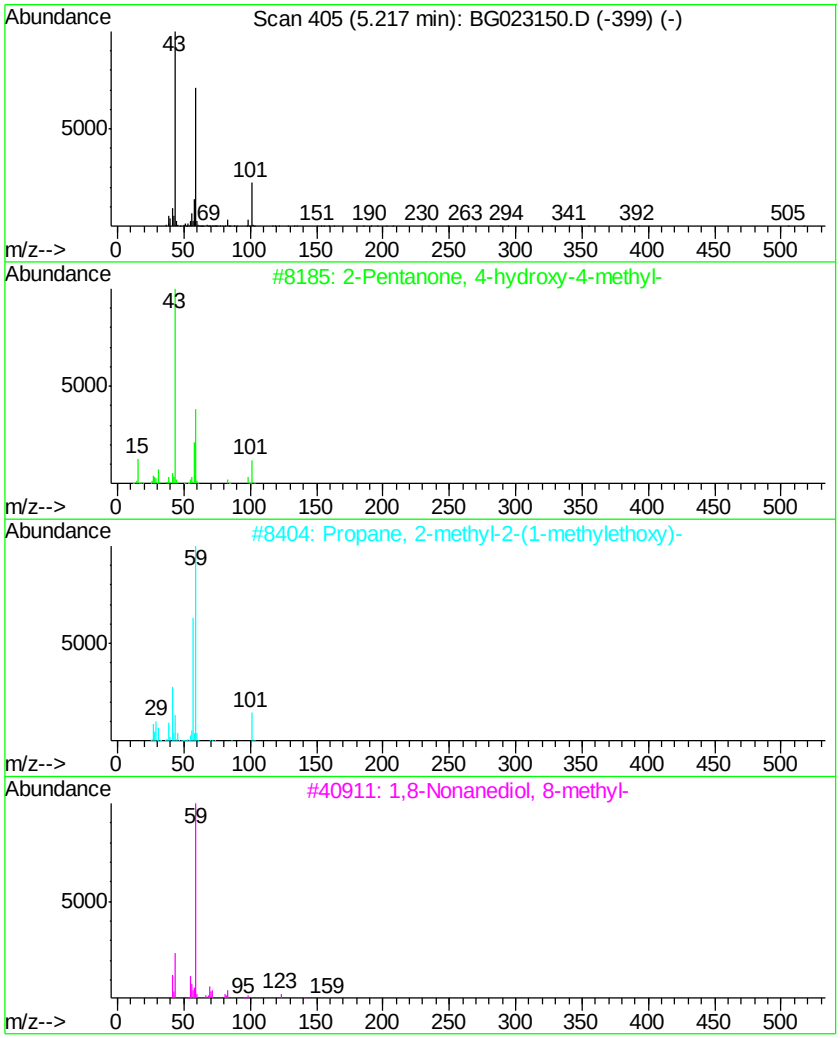
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

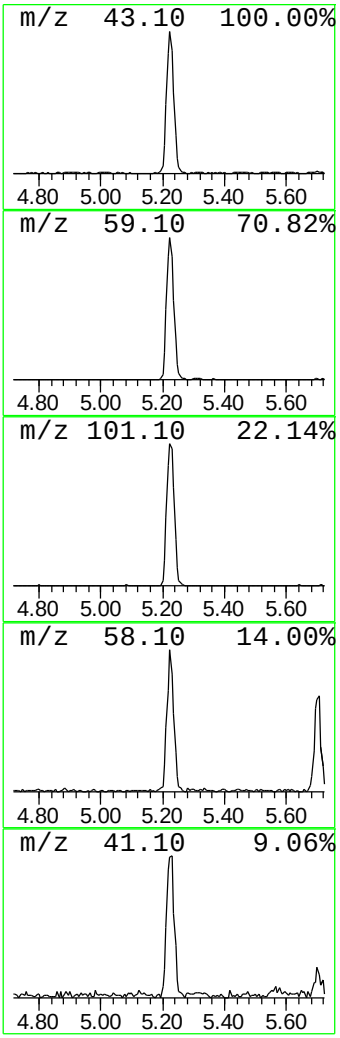
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	19.56 ng	923421	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023150.D
Acq On : 16 Jul 2016 17:02
Operator : UM/SJ
Sample : H3951-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LSS-SB-SB01(0-2ft)

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

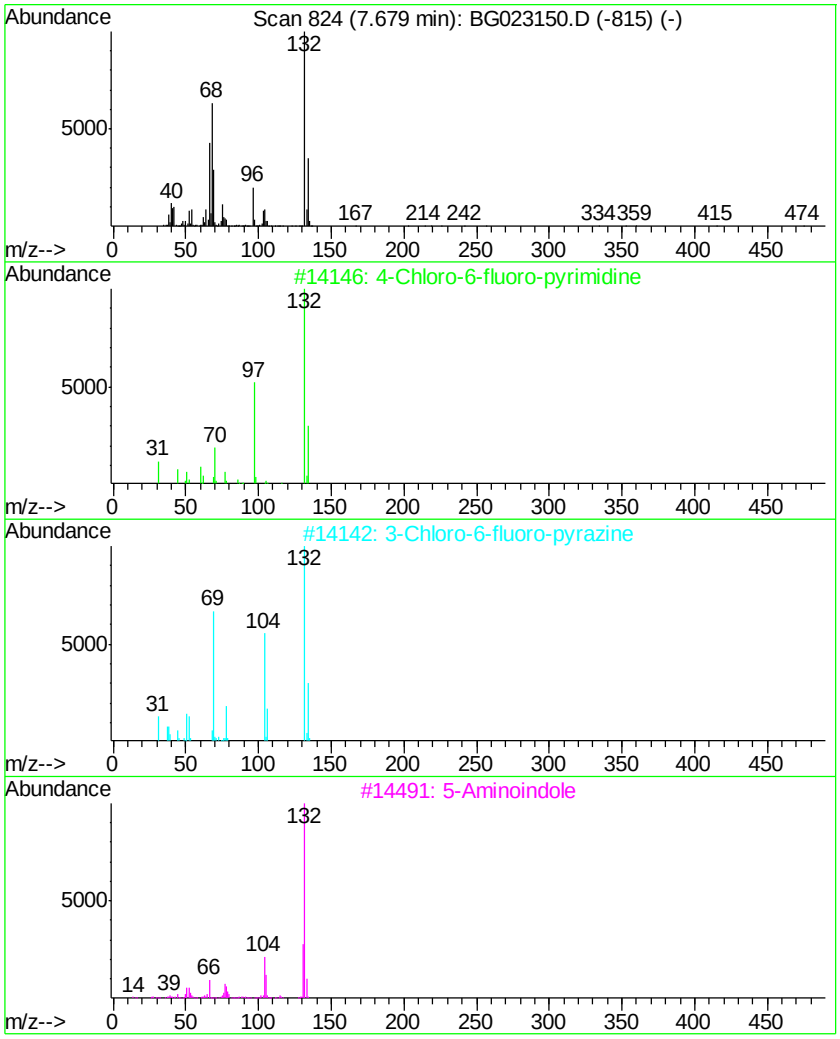
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

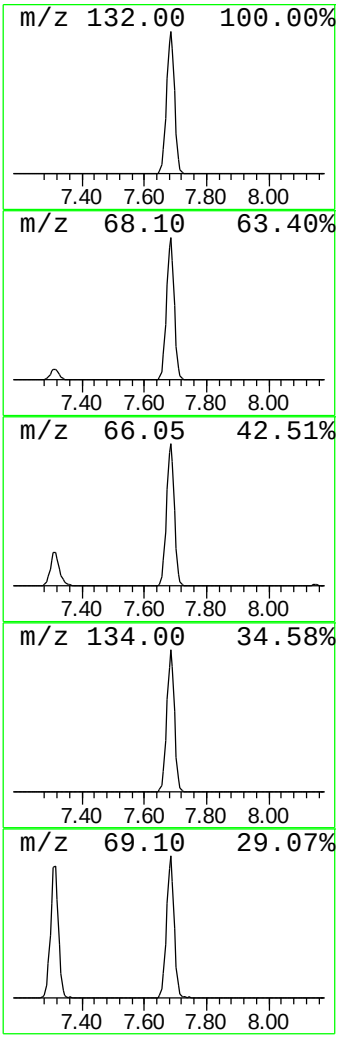
****

Peak Number 6 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	129.71 ng	6122390	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	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10





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Operator : UM/SJ
Sample : H3951-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(0-2ft)

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

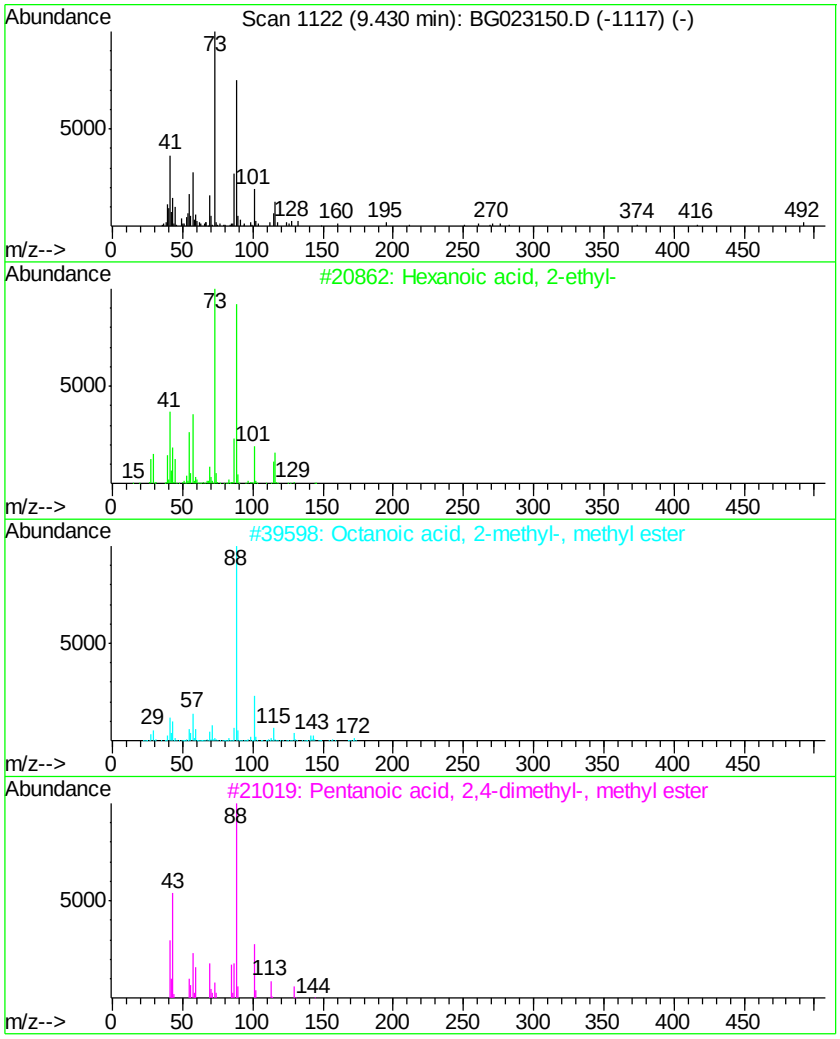
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

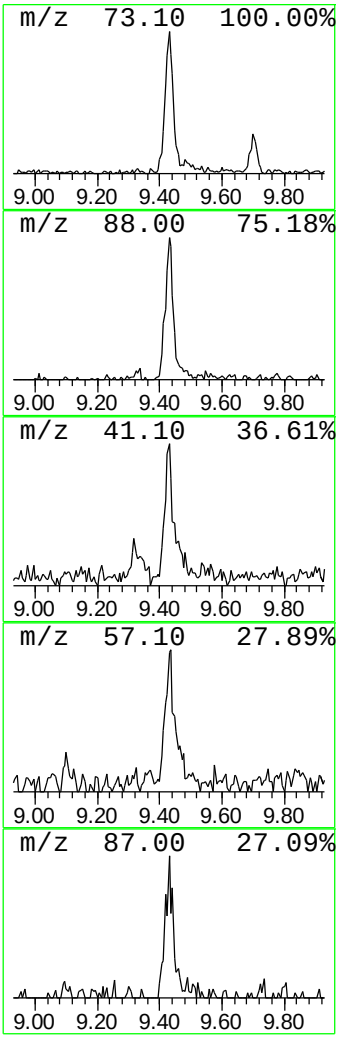
****

Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.43	3.34 ng	157538	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	47
3	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	42
4	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-44-6	42
5	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023150.D
Acq On : 16 Jul 2016 17:02
Operator : UM/SJ
Sample : H3951-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(0-2ft)

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

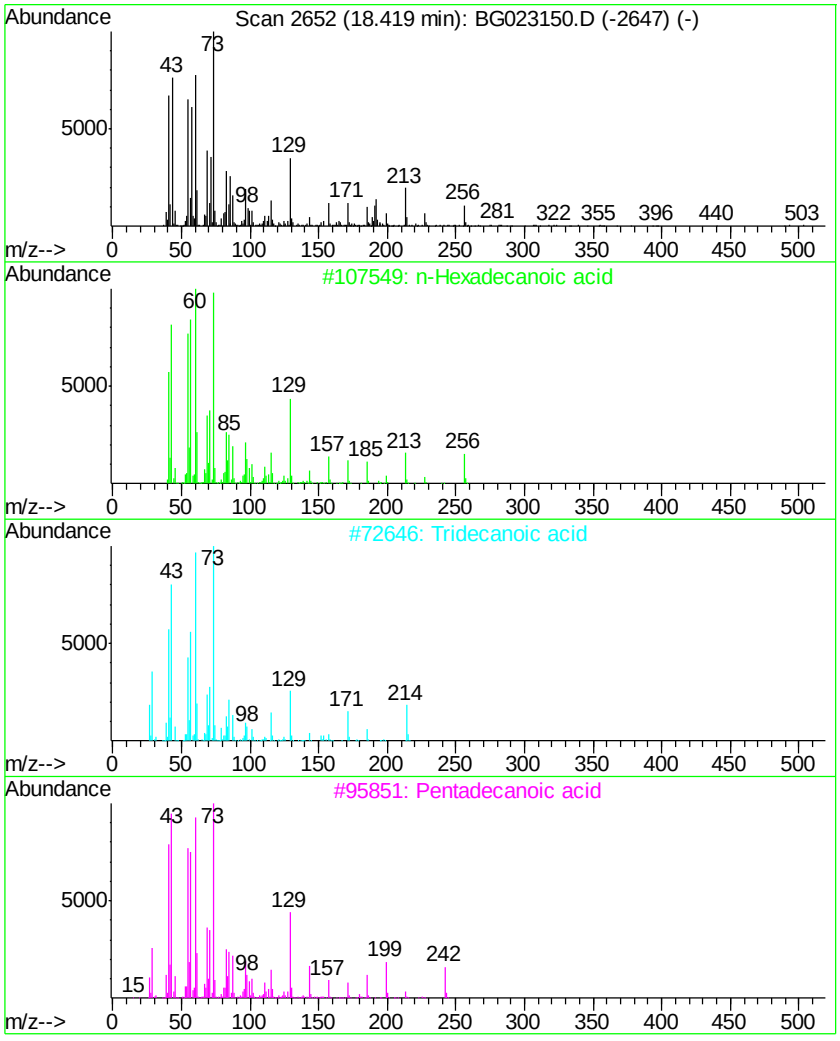
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

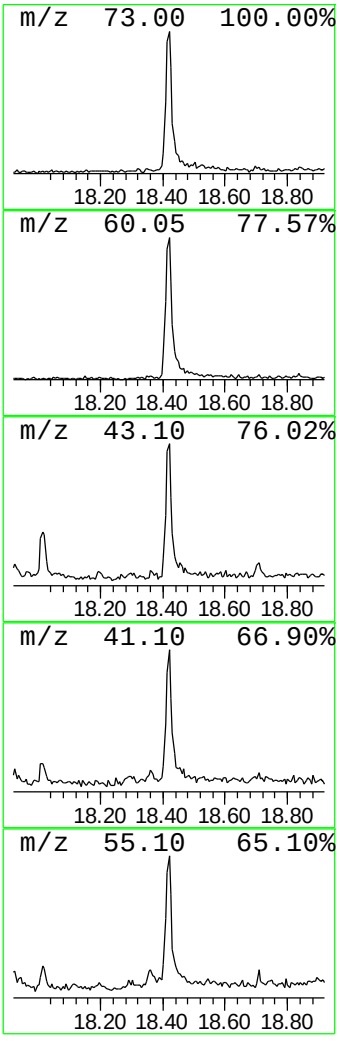
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	9.14 ng	1022010	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Octadecanoic acid	284	C18H36O2	000057-11-4	58





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
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Operator : UM/SJ
Sample : H3951-02
Misc :
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Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(0-2ft)

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

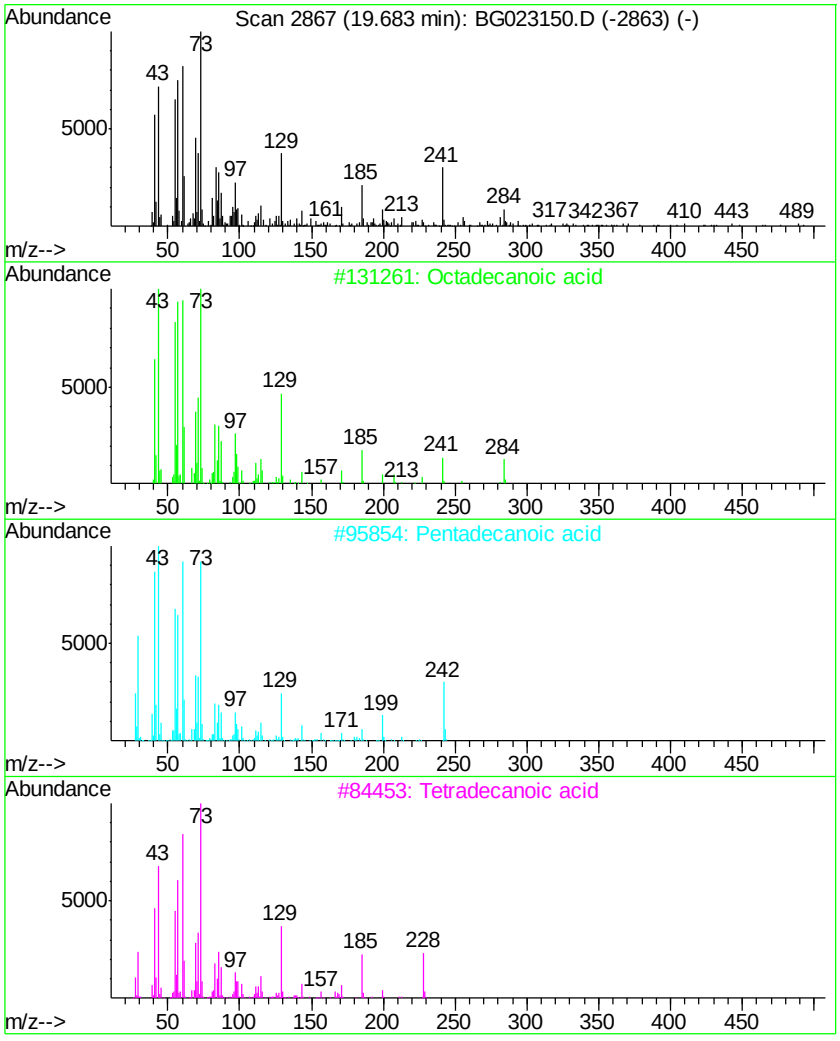
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

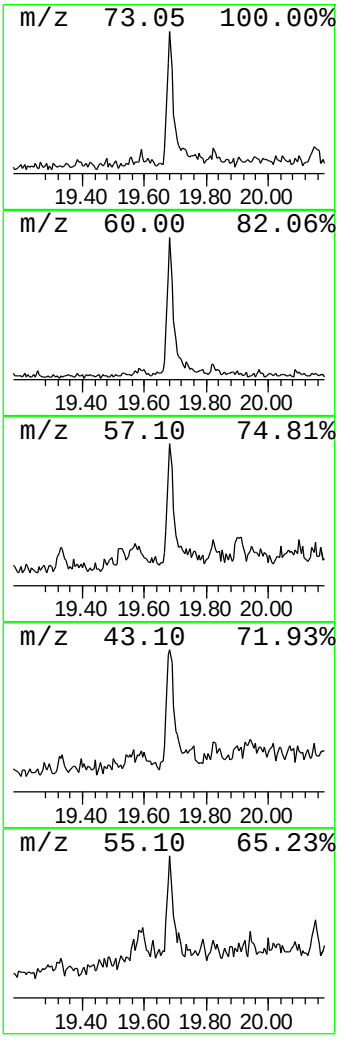
****

Peak Number 10 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	5.01 ng	559668	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023150.D
Acq On : 16 Jul 2016 17:02
Operator : UM/SJ
Sample : H3951-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(0-2ft)

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, met...	2.90	9.2	ng	435327	1	8.15	944023	20.0
unknown3.04	3.04	210.3	ng	9926240	1	8.15	944023	20.0
Propylene Glycol	3.81	2.6	ng	122882	1	8.15	944023	20.0
2-Pentanone, 4-hy...	5.22	19.6	ng	923421	1	8.15	944023	20.0
unknown7.68	7.68	129.7	ng	6122390	1	8.15	944023	20.0
Hexanoic acid, 2-...	9.43	3.3	ng	157538	1	8.15	944023	20.0
n-Hexadecanoic acid	18.42	9.1	ng	1022010	4	17.55	2235570	20.0
Octadecanoic acid	19.68	5.0	ng	559668	4	17.55	2235570	20.0