LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071416\
Data File : BG023106.D
Acq On : 14 Jul 2016 18:13
Operator : UM/SJ
Sample : H3996-29
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B2(5-11)C

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	3.043	30	35	59	rVB	5884916	9355346	100.00%	16.581%
2	5.223	400	406	414	rBV	204654	334932	3.58%	0.594%
3	5.699	478	487	497	rBV	1826145	2945221	31.48%	5.220%
4	7.309	753	761	771	rBV	2083127	3662868	39.15%	6.492%
5	7.685	817	825	834	rBV	1885383	3295339	35.22%	5.840%
6	8.155	898	905	917	rVB	442629	766845	8.20%	1.359%
7	8.478	951	960	969	rBV	1273928	2218403	23.71%	3.932%
8	9.324	1094	1104	1115	rBV	1248147	2352278	25.14%	4.169%
9	10.981	1377	1386	1395	rBV	680115	1241183	13.27%	2.200%
10	13.419	1794	1801	1815	rBV	3308753	5199629	55.58%	9.216%
11	14.242	1935	1941	1947	rBV	640739	938538	10.03%	1.663%
12	14.800	2028	2036	2047	rBV2	1280477	2117439	22.63%	3.753%
13	16.292	2283	2290	2304	rBV	3325629	5198313	55.57%	9.213%
14	16.480	2317	2322	2330	rBV3	54974	109368	1.17%	0.194%
15	17.279	2452	2458	2462	rBV	115005	155645	1.66%	0.276%
16	17.556	2498	2505	2518	rBV	1595831	2599627	27.79%	4.607%
17	18.020	2579	2584	2590	rBV2	85628	119483	1.28%	0.212%
18	18.419	2647	2652	2657	rBV2	187505	262219	2.80%	0.465%
19	19.829	2888	2892	2897	rVB3	105832	120658	1.29%	0.214%
20	20.153	2940	2947	2956	rBV	5695177	7596607	81.20%	13.464%
21	21.469	3166	3171	3179	rBV8	101267	232896	2.49%	0.413%
22	21.862	3230	3238	3247	rBV2	1630375	2913292	31.14%	5.163%
23	25.241	3802	3813	3827	rVB2	889495	2686181	28.71%	4.761%

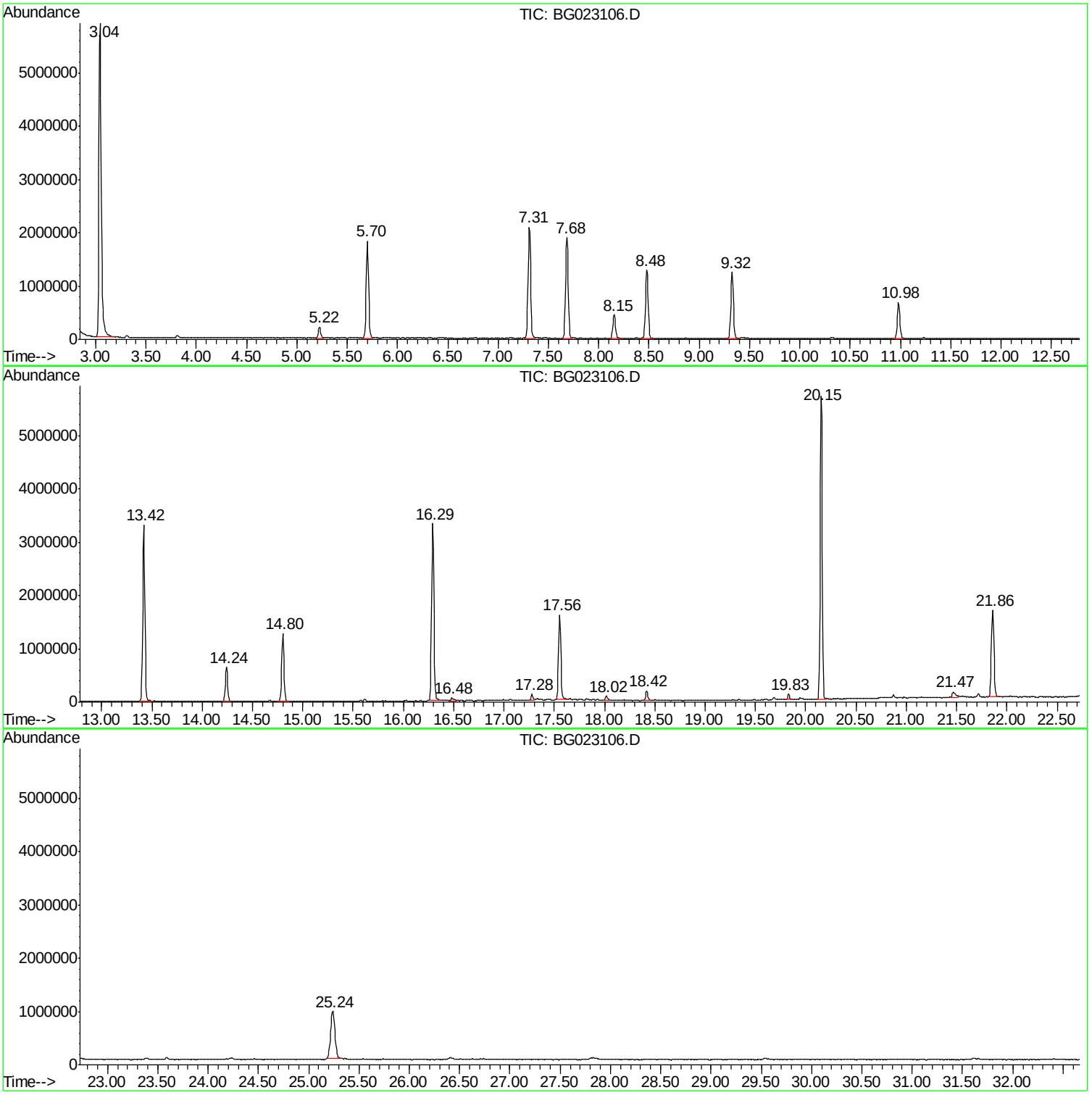
Sum of corrected areas: 56422310

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071416\
Data File : BG023106.D
Acq On : 14 Jul 2016 18:13
Operator : UM/SJ
Sample : H3996-29
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
D8-B2(5-11)C

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\BG071416\
Data File : BG023106.D
Acq On : 14 Jul 2016 18:13
Operator : UM/SJ
Sample : H3996-29
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B2(5-11)C

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

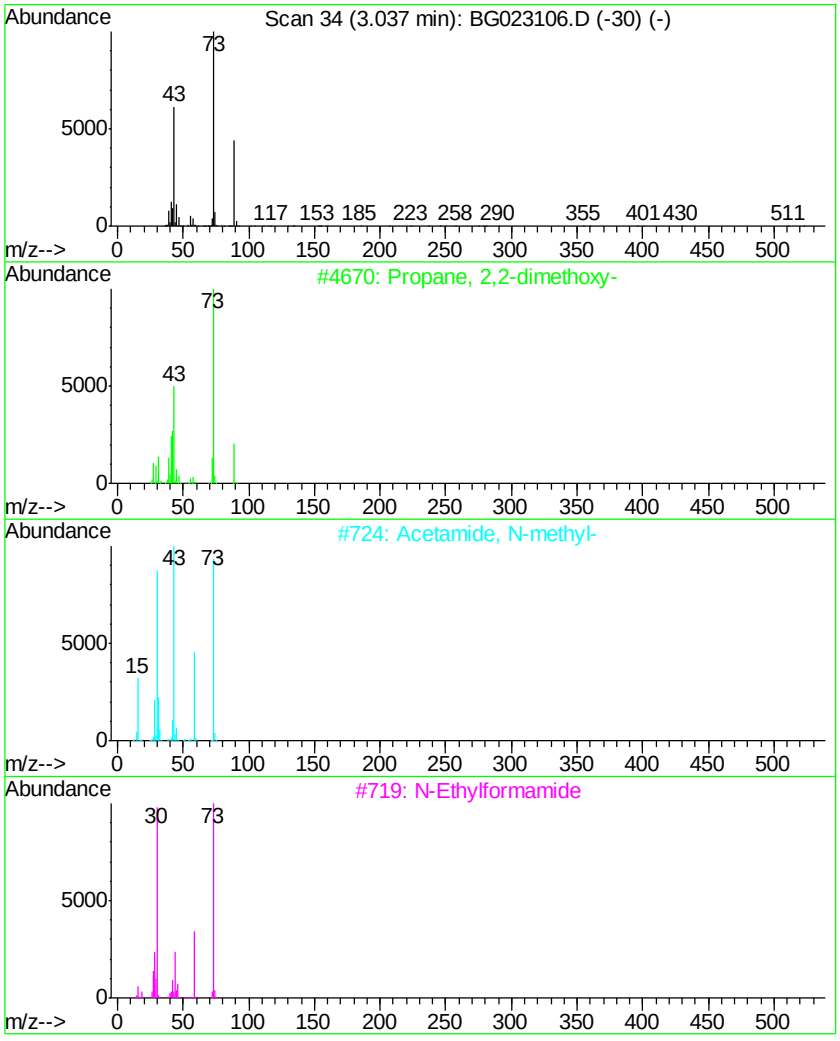
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

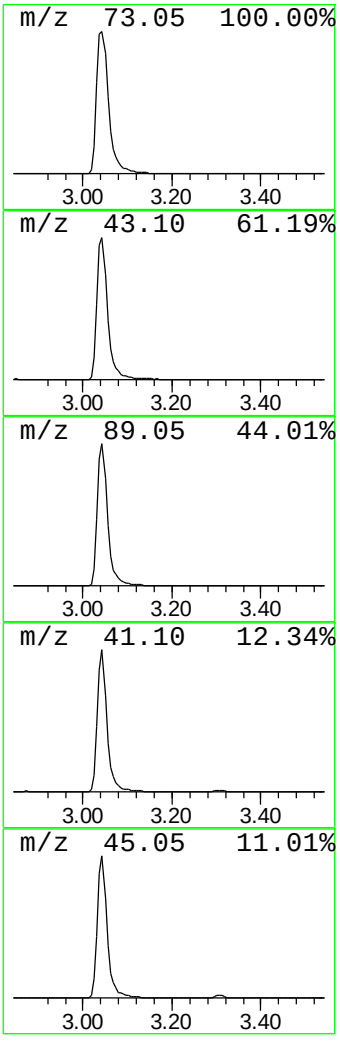
****

Peak Number 1 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	244.00 ng	9355350	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	38
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071416\
Data File : BG023106.D
Acq On : 14 Jul 2016 18:13
Operator : UM/SJ
Sample : H3996-29
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B2(5-11)C

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

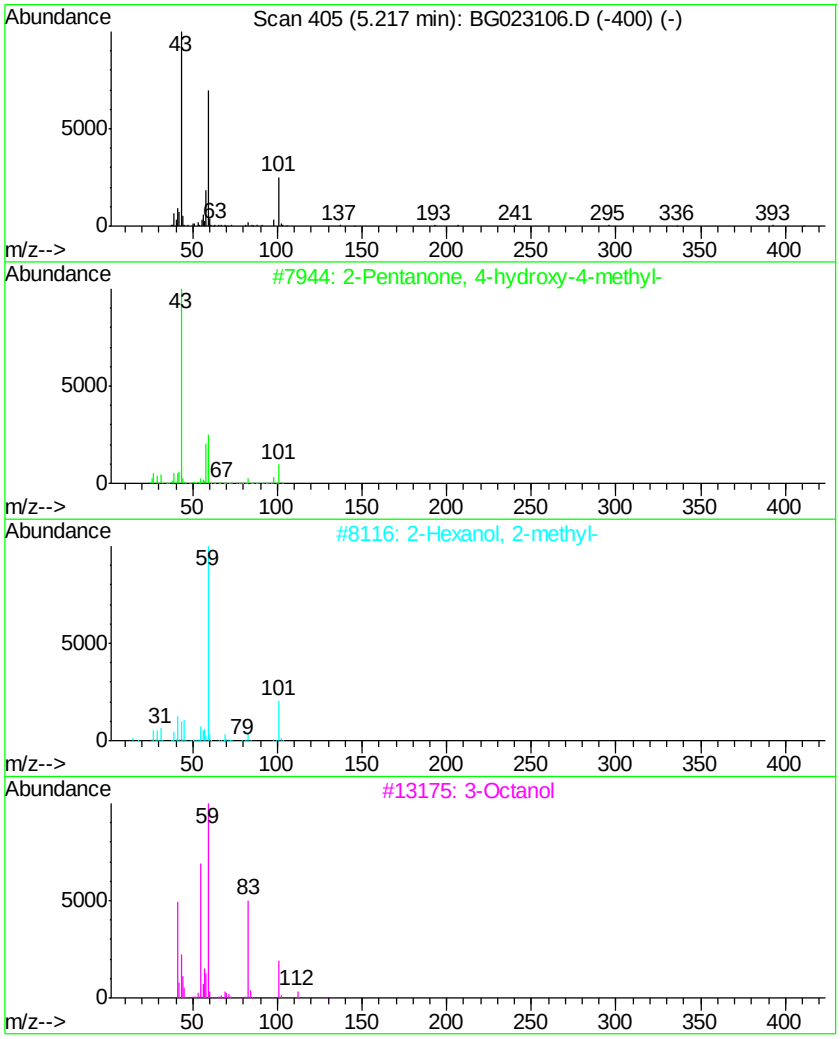
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

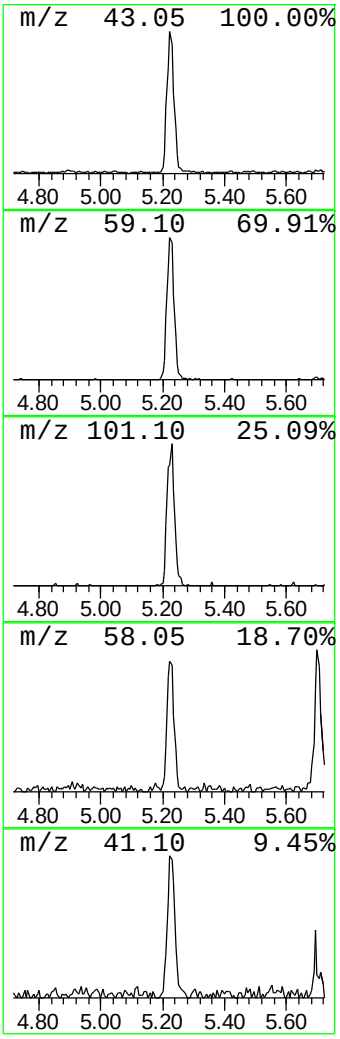
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	8.74 ng	334932	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	42
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
3	3-Octanol	130	C8H18O	020296-29-1	33
4	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	28
5	3-Octanol	130	C8H18O	000589-98-0	25





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071416\
Data File : BG023106.D
Acq On : 14 Jul 2016 18:13
Operator : UM/SJ
Sample : H3996-29
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B2(5-11)C

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

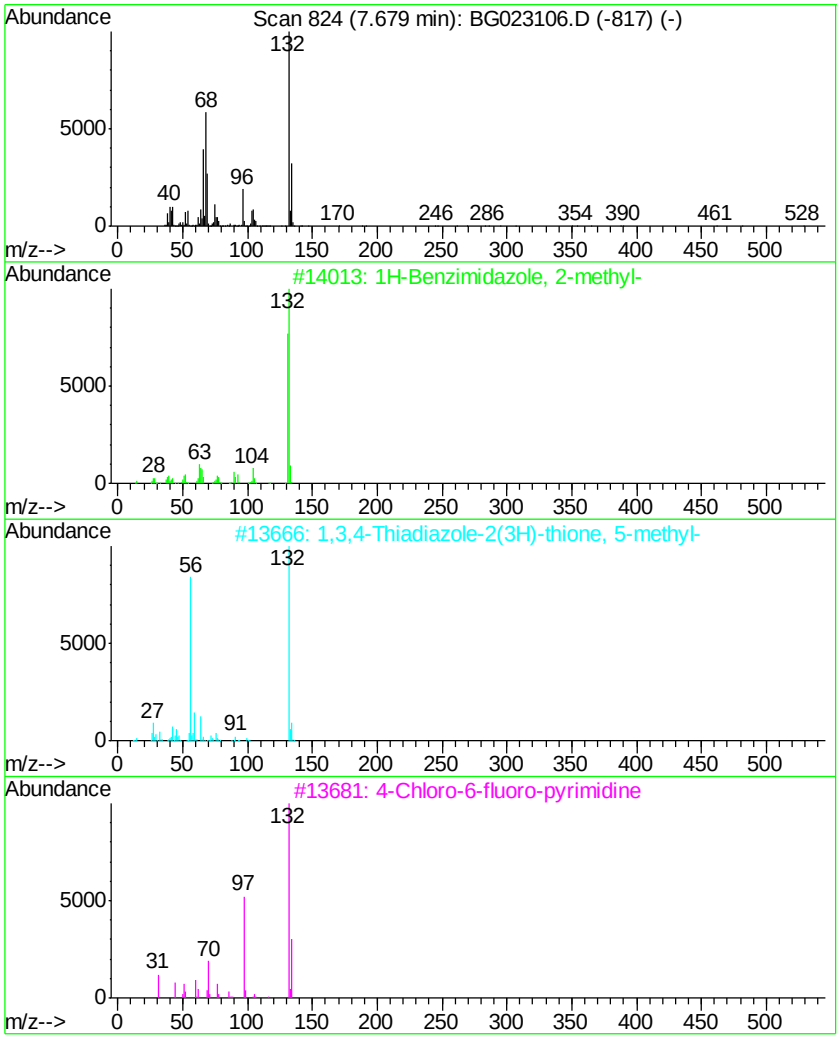
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

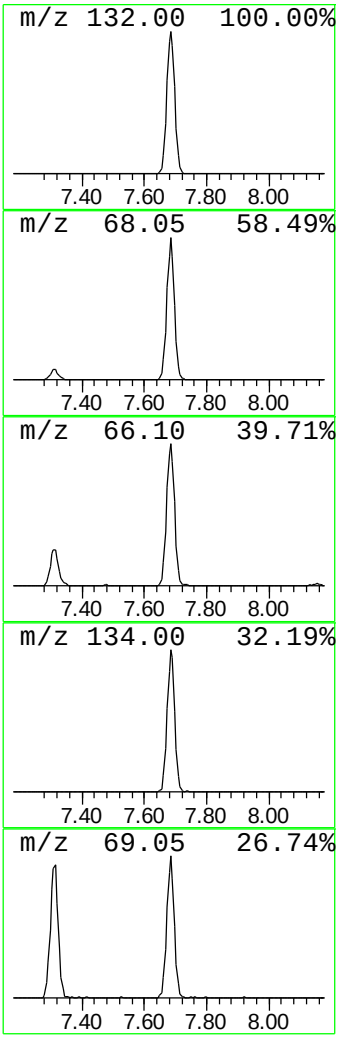
****

Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	85.95 ng	3295340	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	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG071416\
Data File : BG023106.D
Acq On : 14 Jul 2016 18:13
Operator : UM/SJ
Sample : H3996-29
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B2(5-11)C

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

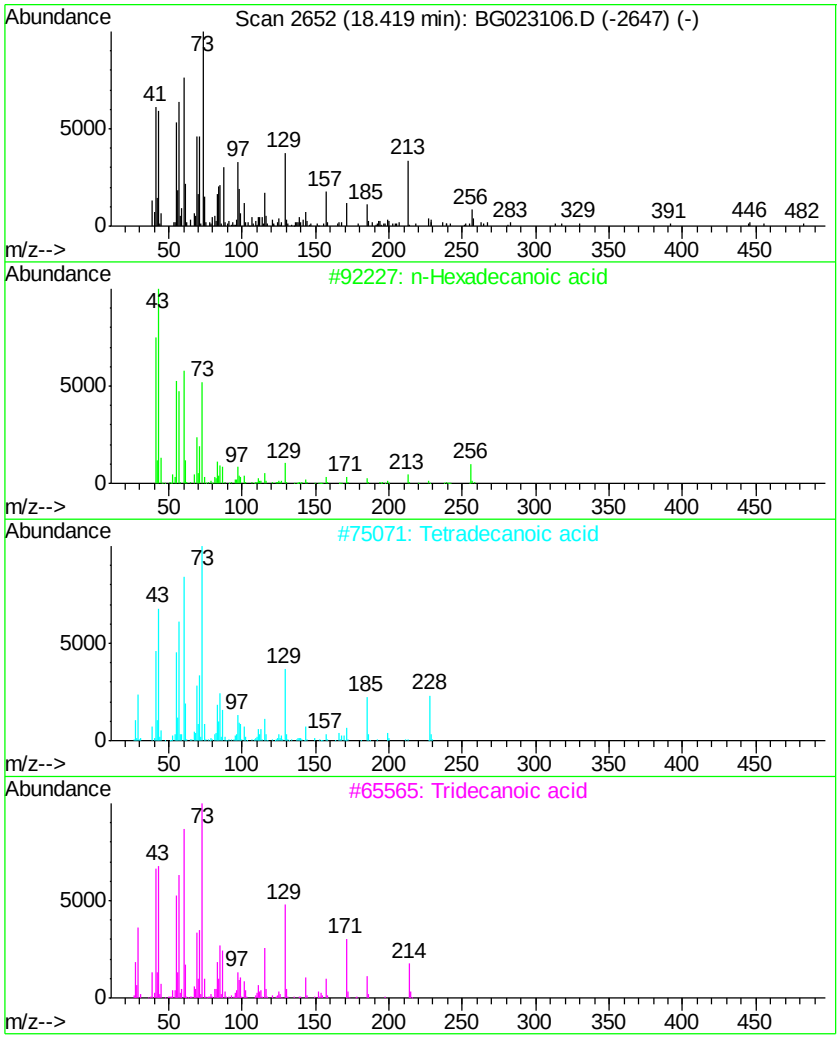
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

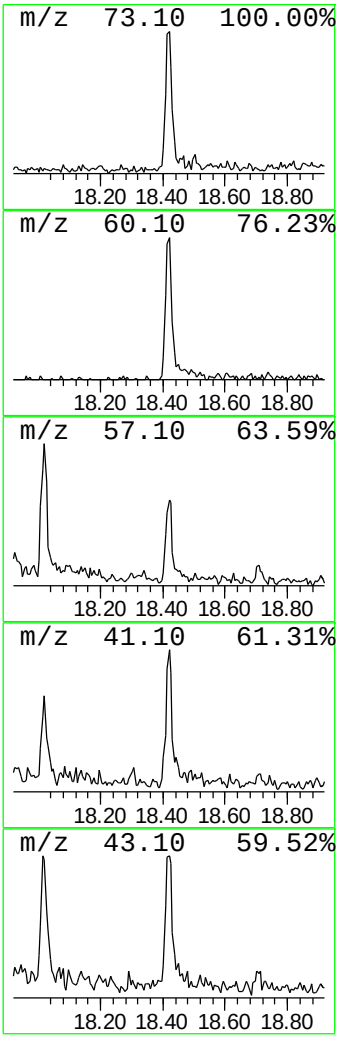
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	2.02 ng	262219	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	56
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3	Tridecanoic acid	214	C13H26O2	000638-53-9	47
4	Nonanoic acid	158	C9H18O2	000112-05-0	43
5	Undecanoic acid	186	C11H22O2	000112-37-8	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071416\
Data File : BG023106.D
Acq On : 14 Jul 2016 18:13
Operator : UM/SJ
Sample : H3996-29
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : D8-B2(5-11)C

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
unknown3.04	3.04	244.0	ng	9355350	1	8.15	766845	20.0
2-Pentanone, 4-hy...	5.22	8.7	ng	334932	1	8.15	766845	20.0
unknown7.68	7.68	86.0	ng	3295340	1	8.15	766845	20.0
n-Hexadecanoic acid	18.42	2.0	ng	262219	4	17.56	2599630	20.0