LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

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-BG051315.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	2.799	13	19	23	rBV4	55279	85997	2.33%	0.413%
2	2.869	27	31	37	rVV	518225	599362	16.22%	2.877%
3	2.922	37	40	47	rVB	39466	51392	1.39%	0.247%
4	4.209	254	259	264	rBV	116800	149607	4.05%	0.718%
5	4.808	354	361	367	rBV2	200519	341000	9.23%	1.637%
6	5.302	438	445	452	rBV	1152832	1569944	42.48%	7.536%
7	6.906	712	718	732	rBV	1171912	1815317	49.12%	8.714%
8	7.247	769	776	784	rBV	1109764	1722018	46.59%	8.266%
9	7.705	846	854	861	rBV	202394	319066	8.63%	1.532%
10	8.022	901	908	916	rBV	704015	1114489	30.15%	5.350%
11	8.868	1044	1052	1059	rBV	631793	1061524	28.72%	5.096%
12	10.496	1323	1329	1338	rBV	262848	444293	12.02%	2.133%
13	12.981	1745	1752	1758	rBV	1545644	2165450	58.59%	10.395%
14	13.821	1889	1895	1899	rBV	56968	82260	2.23%	0.395%
15	14.362	1980	1987	1995	rBV2	405527	618910	16.75%	2.971%
16	15.854	2234	2241	2254	rBV	1481669	2064322	55.85%	9.910%
17	17.106	2447	2454	2461	rBV	588228	823298	22.28%	3.952%
18	18.010	2604	2608	2613	rBV2	97241	128401	3.47%	0.616%
19	19.291	2820	2826	2831	rBV2	37593	52931	1.43%	0.254%
20	19.744	2896	2903	2909	rBV	2983735	3695929	100.00%	17.742%
21	21.007	3114	3118	3125	rBV2	104247	143171	3.87%	0.687%
22	21.289	3161	3166	3172	rBV	730293	920889	24.92%	4.421%
23	23.557	3545	3552	3560	rVB2	467852	862125	23.33%	4.139%

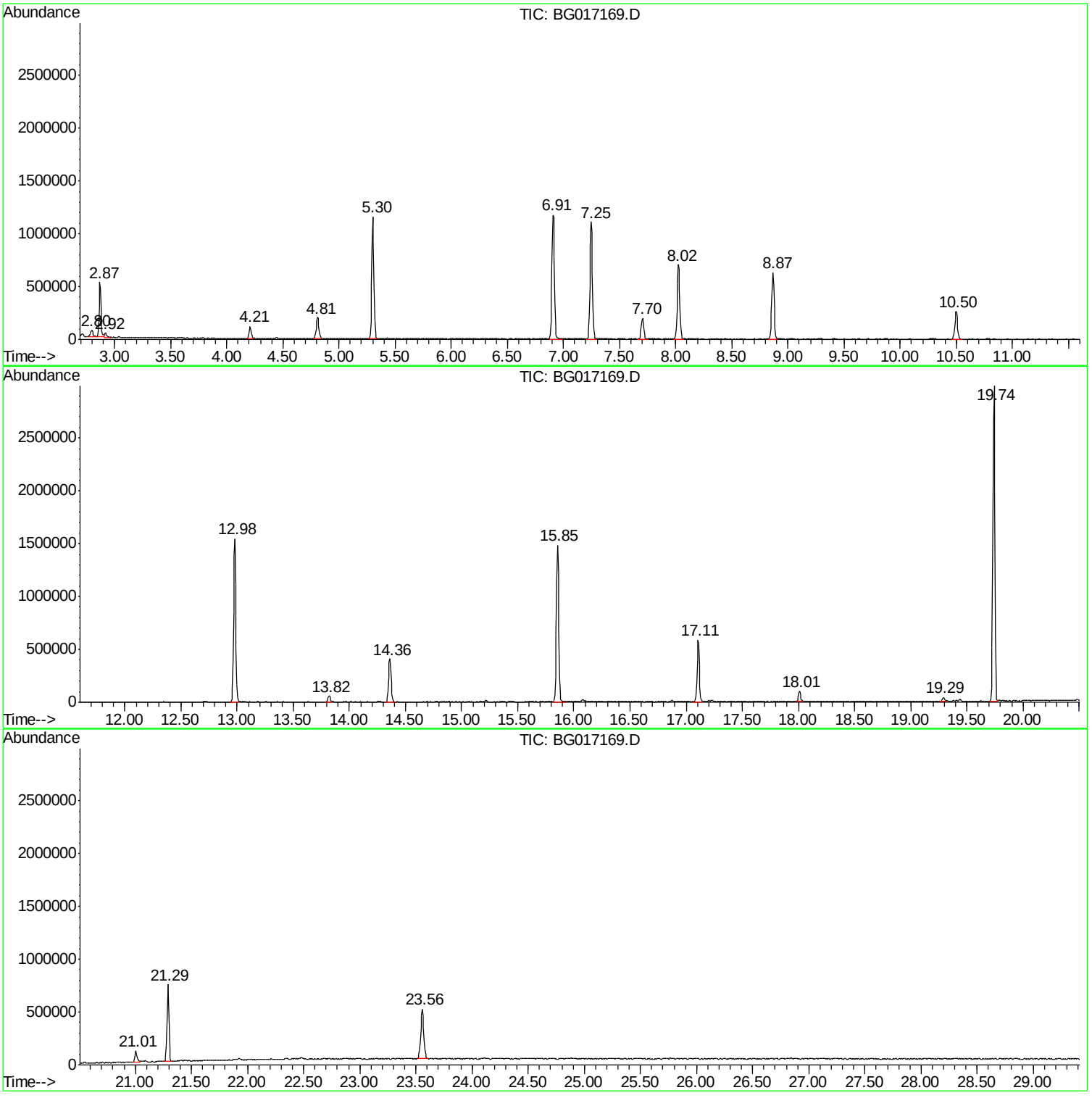
Sum of corrected areas: 20831695

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.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\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

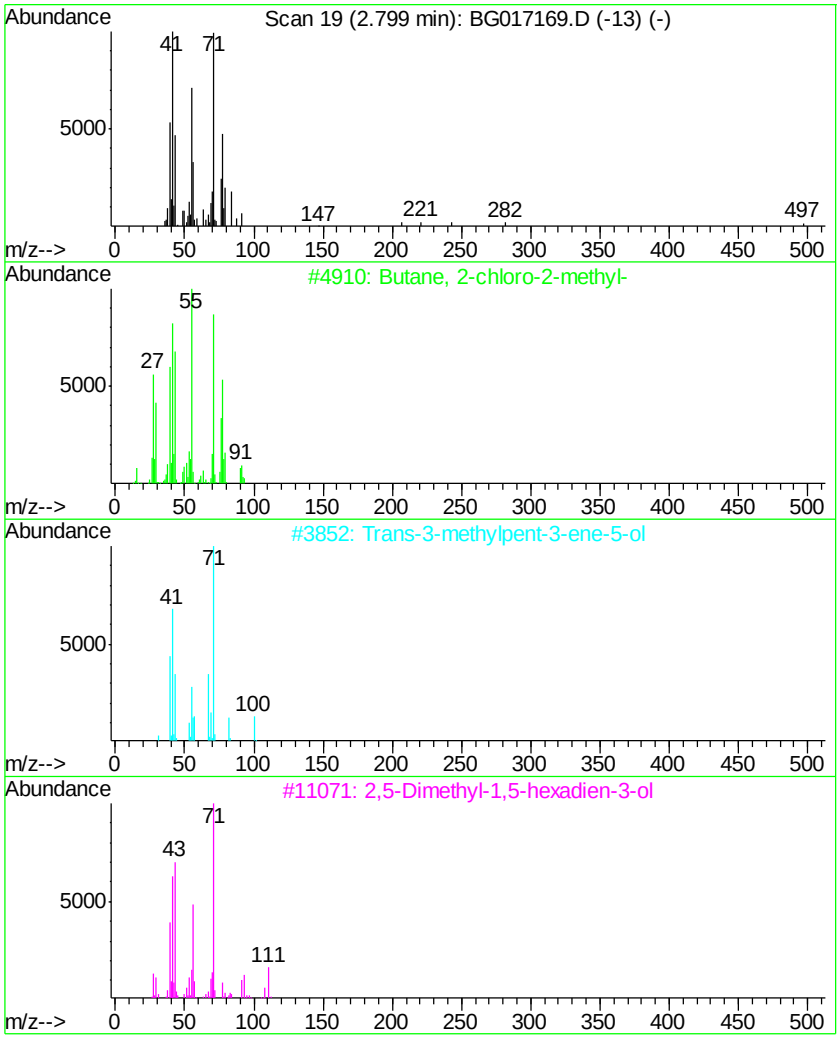
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

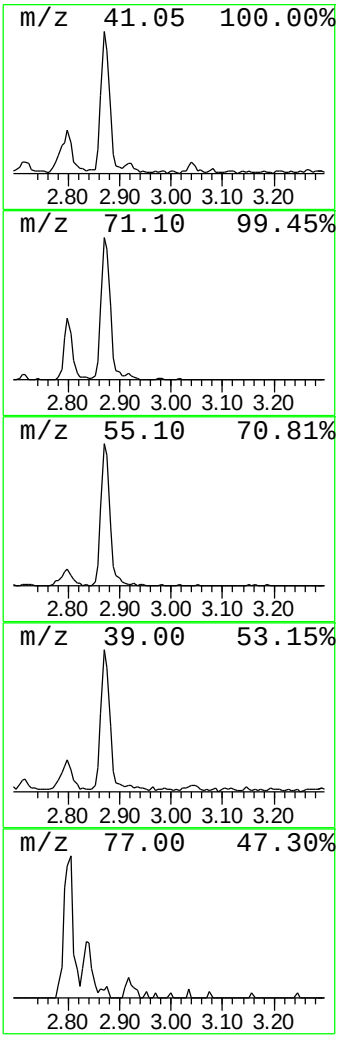
****

Peak Number 1 unknown2.80 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.80	5.39 ng	85997	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	35
2	Trans-3-methylpent-3-ene-5-ol	100	C6H12O	030801-95-7	25
3	2,5-Dimethyl-1,5-hexadien-3-ol	126	C8H14O	017123-63-6	23
4	2-Furancarboxylic acid, 2-tetrah...	196	C10H12O4	004623-04-5	16
5	Butyric acid, 2-pentadecyl ester	298	C19H38O2	107853-73-6	16





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

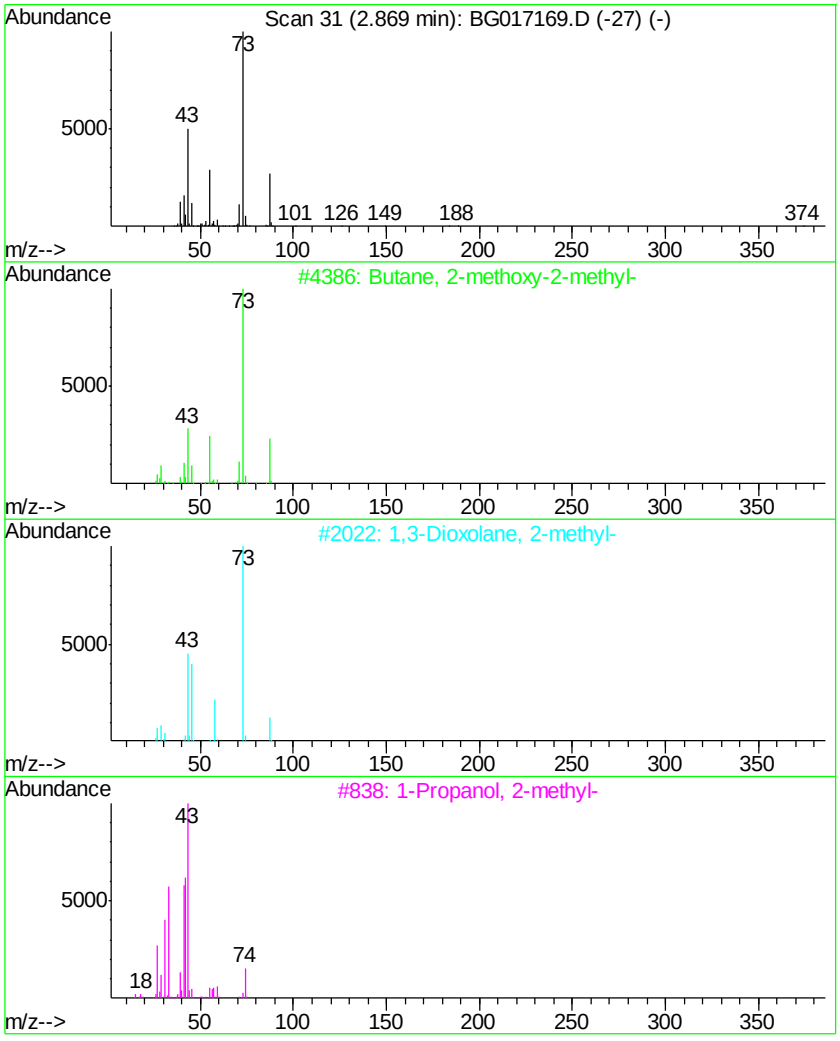
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

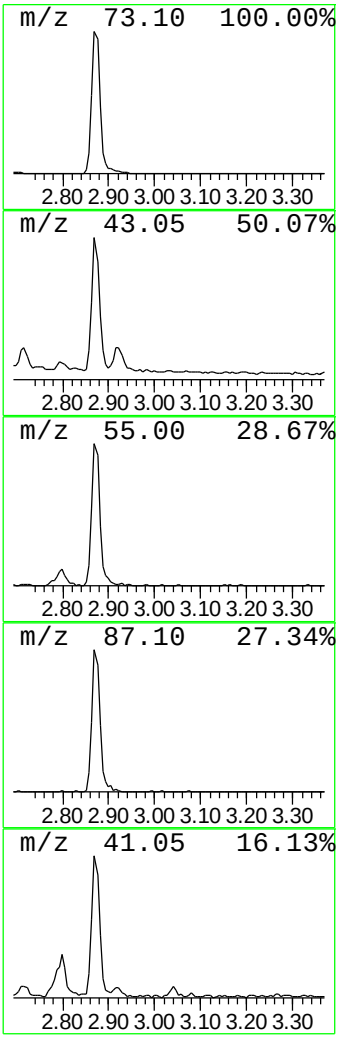
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	37.57 ng	599362	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

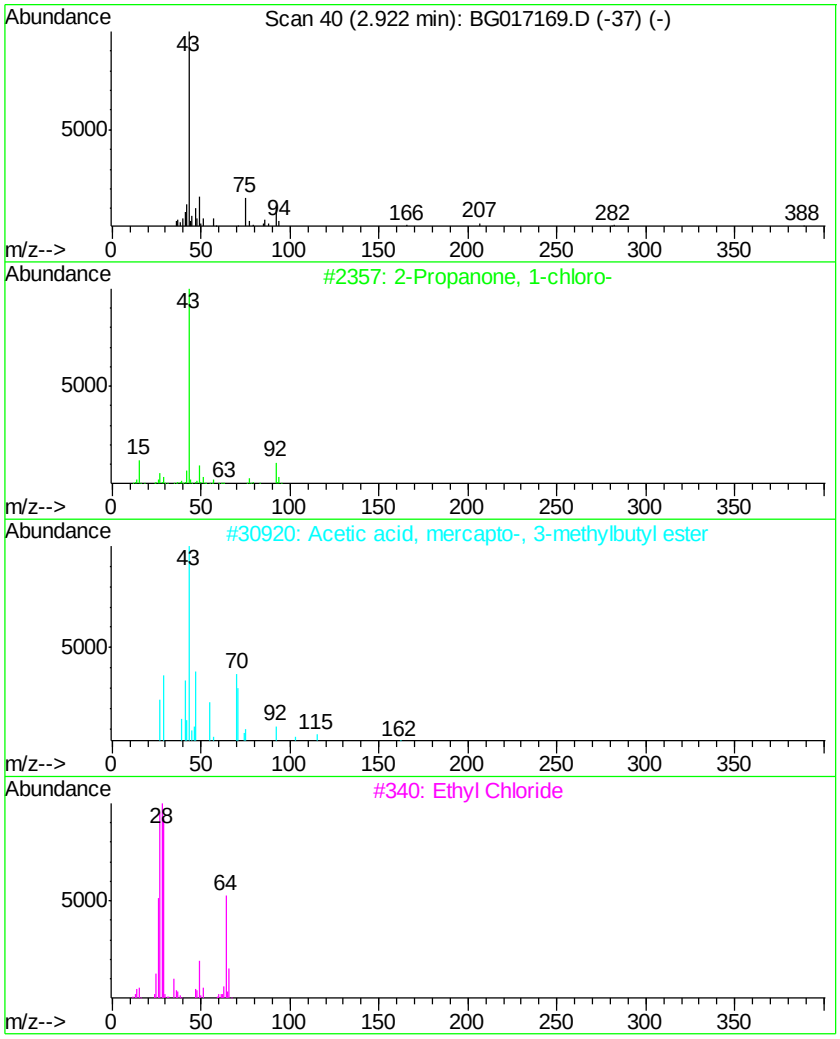
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

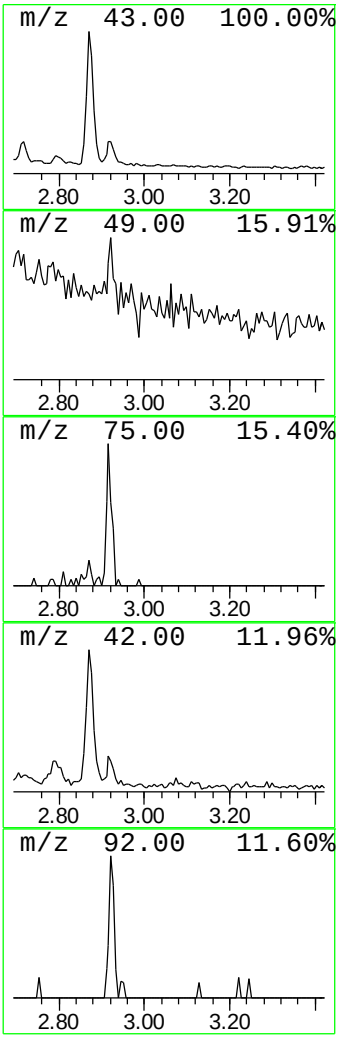
****

Peak Number 3 unknown2.92 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.92	3.22 ng	51392	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-chloro-	92	C3H5ClO	000078-95-5	27
2	Acetic acid, mercapto-, 3-methyl...	162	C7H14O2S	016849-97-1	9
3	Ethyl Chloride	64	C2H5Cl	000075-00-3	9
4	cis-2-Chlorovinylacetate	120	C4H5ClO2	103659-54-7	9
5	trans-2-Chlorovinylacetate	120	C4H5ClO2	1000288-27-5	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

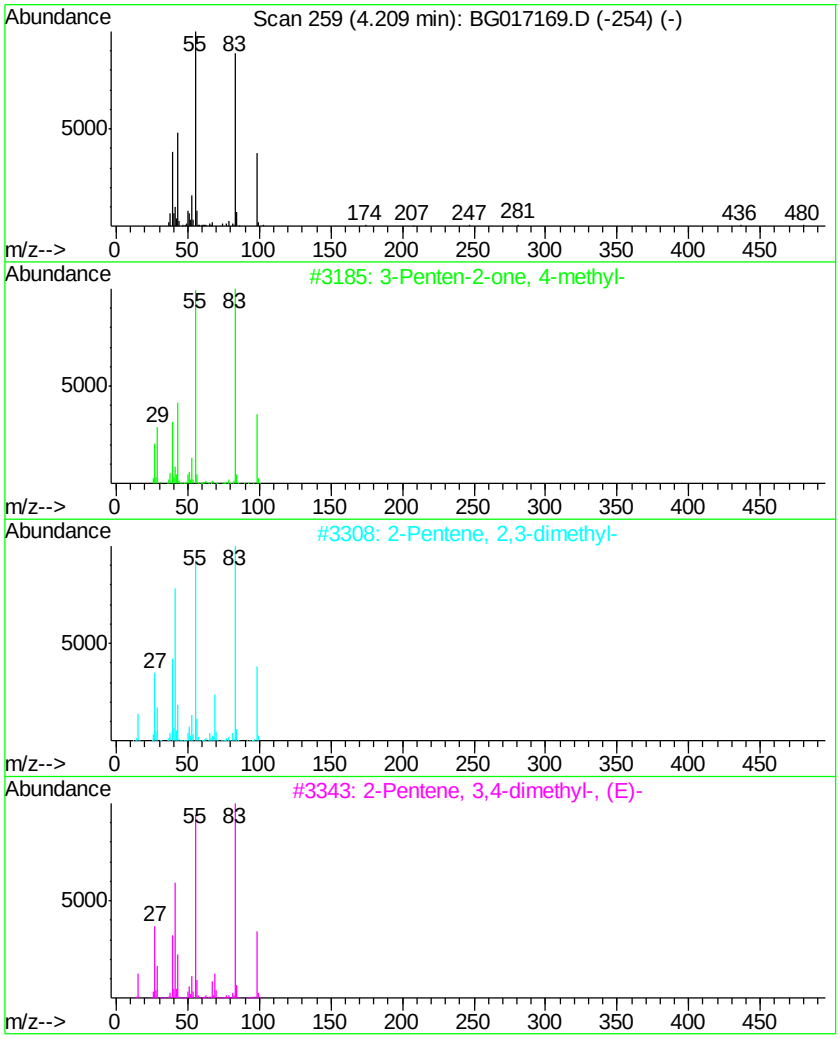
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

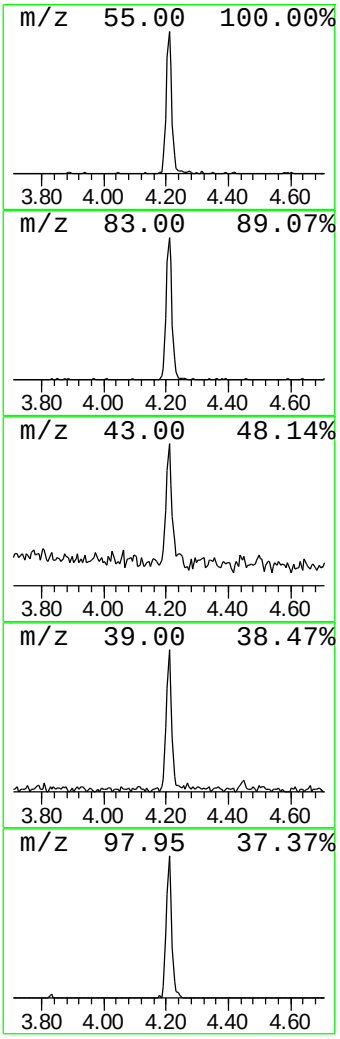
****

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.21	9.38 ng	149607	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	93
2	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	58
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	58
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	53





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

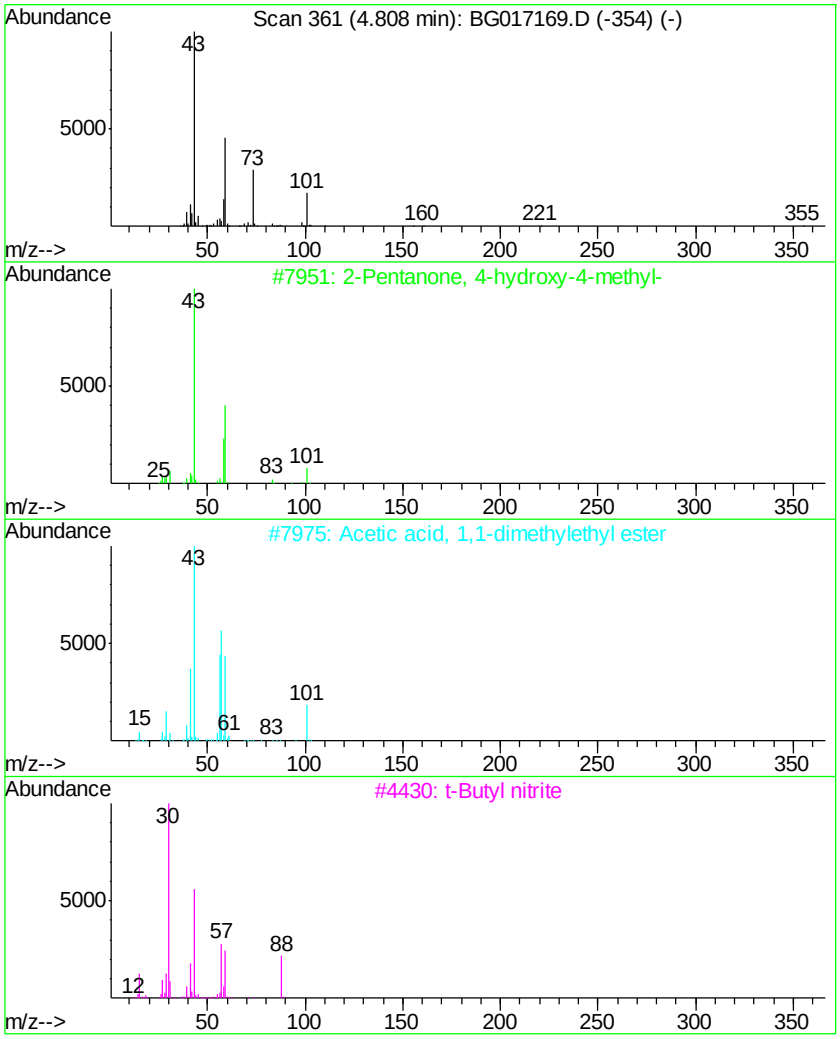
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

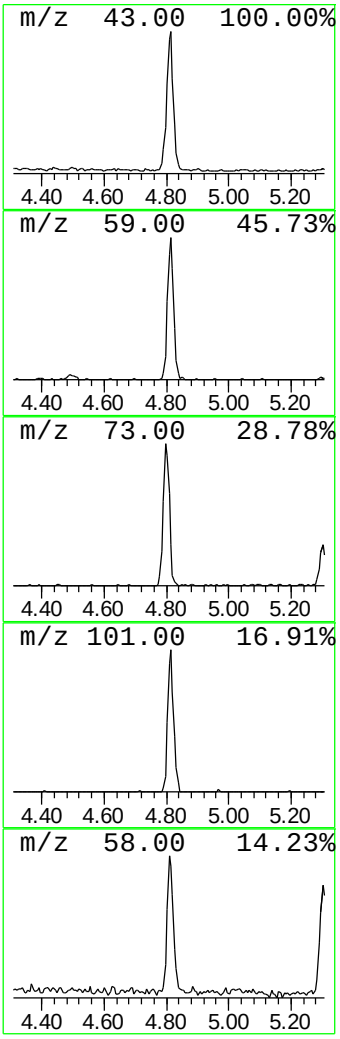
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	21.37 ng	341000	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	33
3	t-Butyl nitrite	103	C4H9NO2	000540-80-7	28
4	Di-n-propyl ether	102	C6H14O	000111-43-3	16
5	1-Butanamine	73	C4H11N	000109-73-9	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

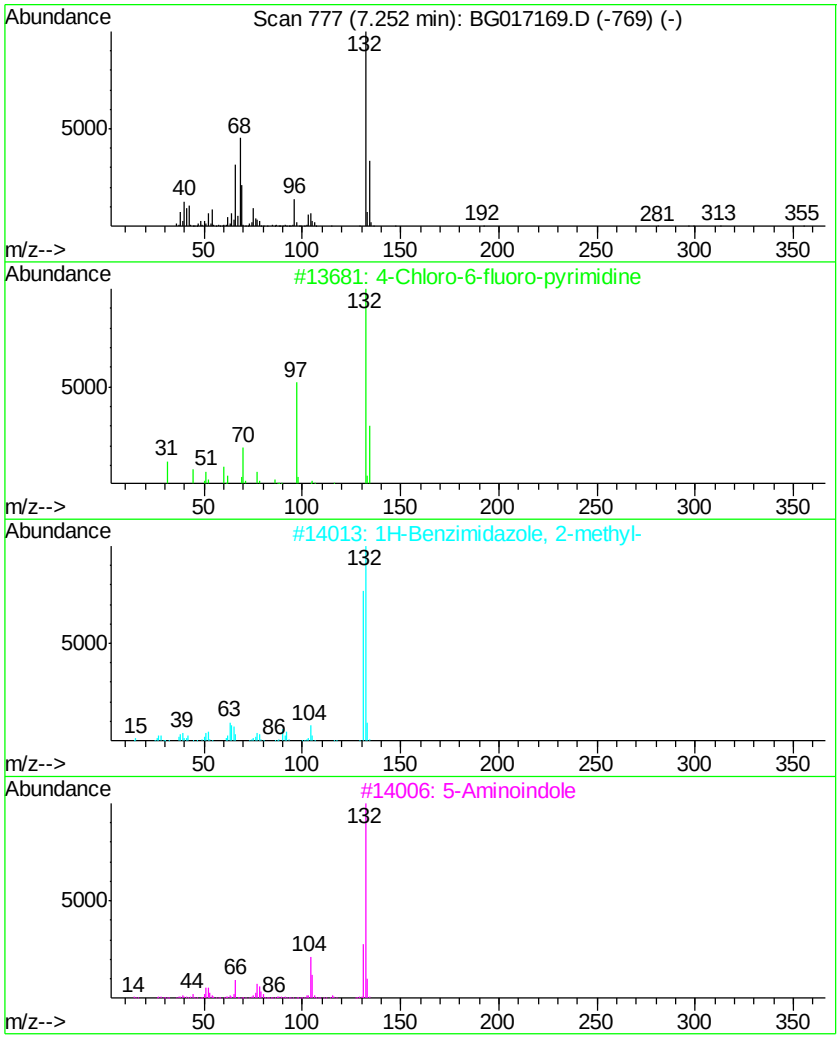
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

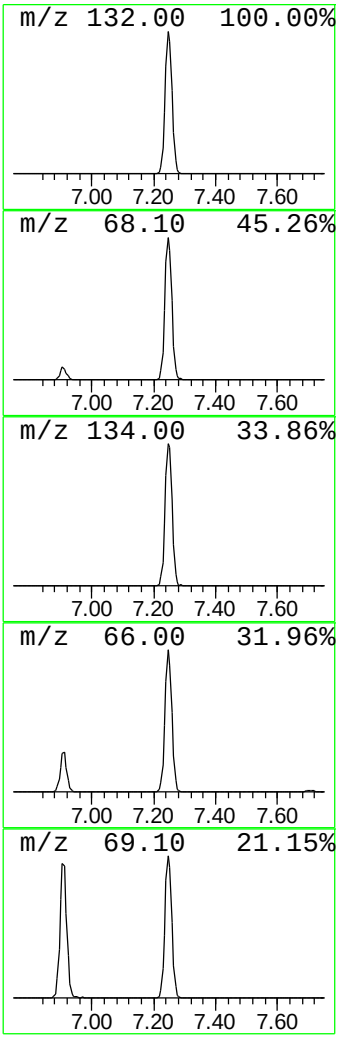
****

Peak Number 6 unknown7.25 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.25	107.94 ng	1722020	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	20
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

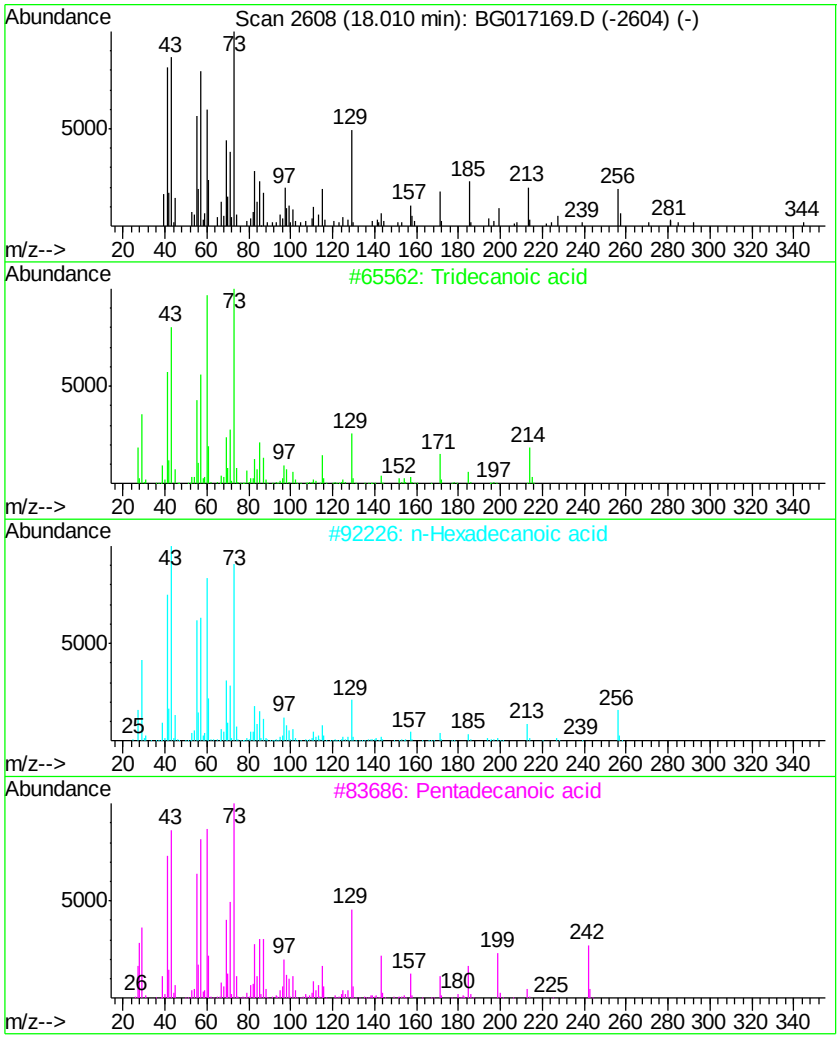
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

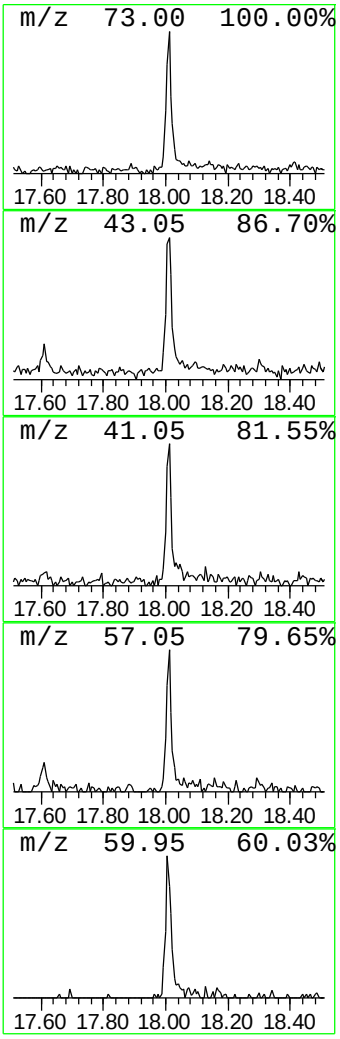
****

Peak Number 8 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.01	3.12 ng	128401	Phenanthrene-d10	17.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	35





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Data File : BG017169.D
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Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

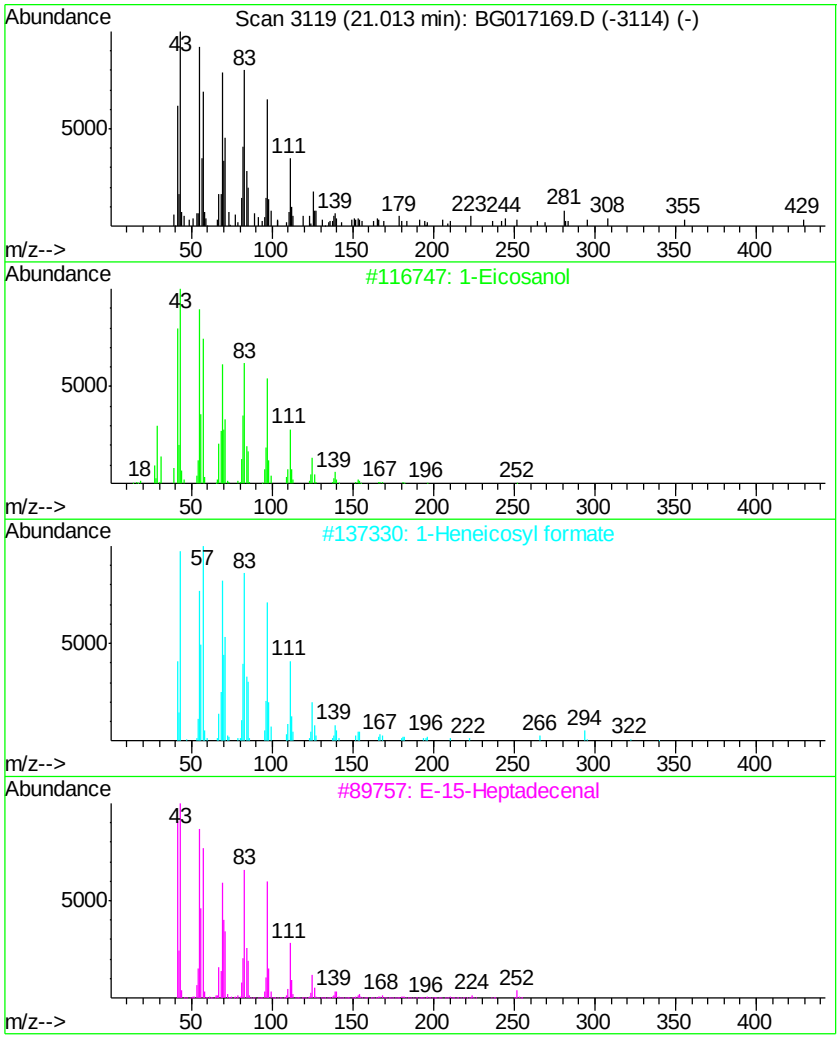
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

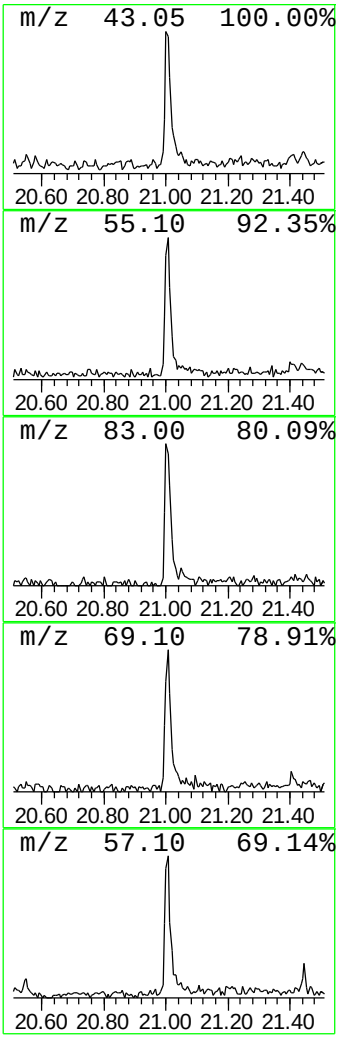
****

Peak Number 9 1-Eicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.01	3.11 ng	143171	Chrysene-d12	21.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	89
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	86
4	1-Octadecene	252	C18H36	000112-88-9	83
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
Data File : BG017169.D
Acq On : 15 May 2015 9:34
Operator : TP/IZ
Sample : G2177-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-30A(5-10)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.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
unknown2.80	2.80	5.4	ng	85997	1	7.70	319066	20.0
Butane, 2-methoxy...	2.87	37.6	ng	599362	1	7.70	319066	20.0
unknown2.92	2.92	3.2	ng	51392	1	7.70	319066	20.0
3-Penten-2-one, 4...	4.21	9.4	ng	149607	1	7.70	319066	20.0
2-Pentanone, 4-hy...	4.81	21.4	ng	341000	1	7.70	319066	20.0
unknown7.25	7.25	107.9	ng	1722020	1	7.70	319066	20.0
Tridecanoic acid	18.01	3.1	ng	128401	4	17.11	823298	20.0
1-Eicosanol	21.01	3.1	ng	143171	5	21.29	920889	20.0