LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017058.D
Acq On : 11 May 2015 18:01
Operator : TP/IZ
Sample : G2176-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-29(20-25)

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-BG050515.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	2.718	3	5	22	rVB	5771364	7058076	100.00%	22.783%
2	2.859	24	29	37	rVV	273749	473512	6.71%	1.528%
3	2.935	38	42	46	rVB	168133	194312	2.75%	0.627%
4	4.868	365	371	382	rVB	81186	120252	1.70%	0.388%
5	5.344	446	452	466	rVB	1298468	1863514	26.40%	6.015%
6	6.948	718	725	733	rBV	1390531	2090926	29.62%	6.749%
7	7.295	775	784	791	rBV	1325830	2023853	28.67%	6.533%
8	7.753	853	862	868	rBV	236992	370404	5.25%	1.196%
9	8.070	908	916	923	rBV	856518	1372926	19.45%	4.432%
10	8.910	1052	1059	1070	rBV	761958	1271935	18.02%	4.106%
11	10.550	1328	1338	1345	rVB	305564	509295	7.22%	1.644%
12	13.023	1751	1759	1765	rBV	1810061	2632238	37.29%	8.497%
13	13.857	1896	1901	1908	rBV	162305	235136	3.33%	0.759%
14	14.404	1984	1994	2001	rBV2	470963	715563	10.14%	2.310%
15	15.896	2241	2248	2255	rBV	1764546	2503742	35.47%	8.082%
16	17.154	2454	2462	2469	rBV	627739	924416	13.10%	2.984%
17	18.047	2610	2614	2621	rBV2	145099	206377	2.92%	0.666%
18	19.333	2828	2833	2835	rBV3	60922	81763	1.16%	0.264%
19	19.780	2904	2909	2915	rVB	3296678	4082056	57.84%	13.177%
20	21.043	3120	3124	3133	rVB3	98909	147313	2.09%	0.476%
21	21.331	3168	3173	3181	rBV	854799	1067172	15.12%	3.445%
22	23.622	3556	3563	3573	rVB	528359	1034826	14.66%	3.340%

Sum of corrected areas: 30979607

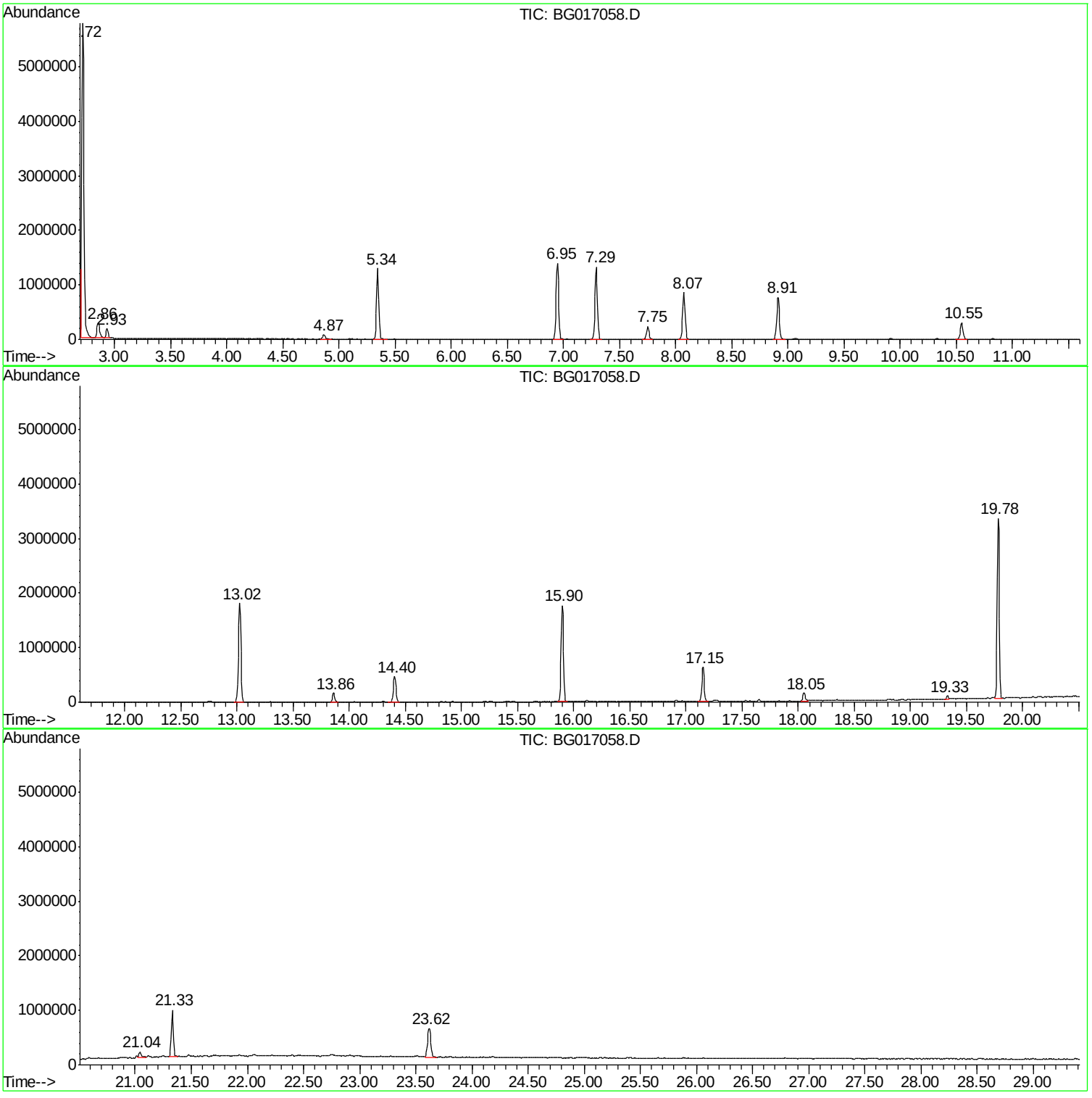
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017058.D
Acq On : 11 May 2015 18:01
Operator : TP/IZ
Sample : G2176-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-29(20-25)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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\BG051115\
Data File : BG017058.D
Acq On : 11 May 2015 18:01
Operator : TP/IZ
Sample : G2176-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-29(20-25)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

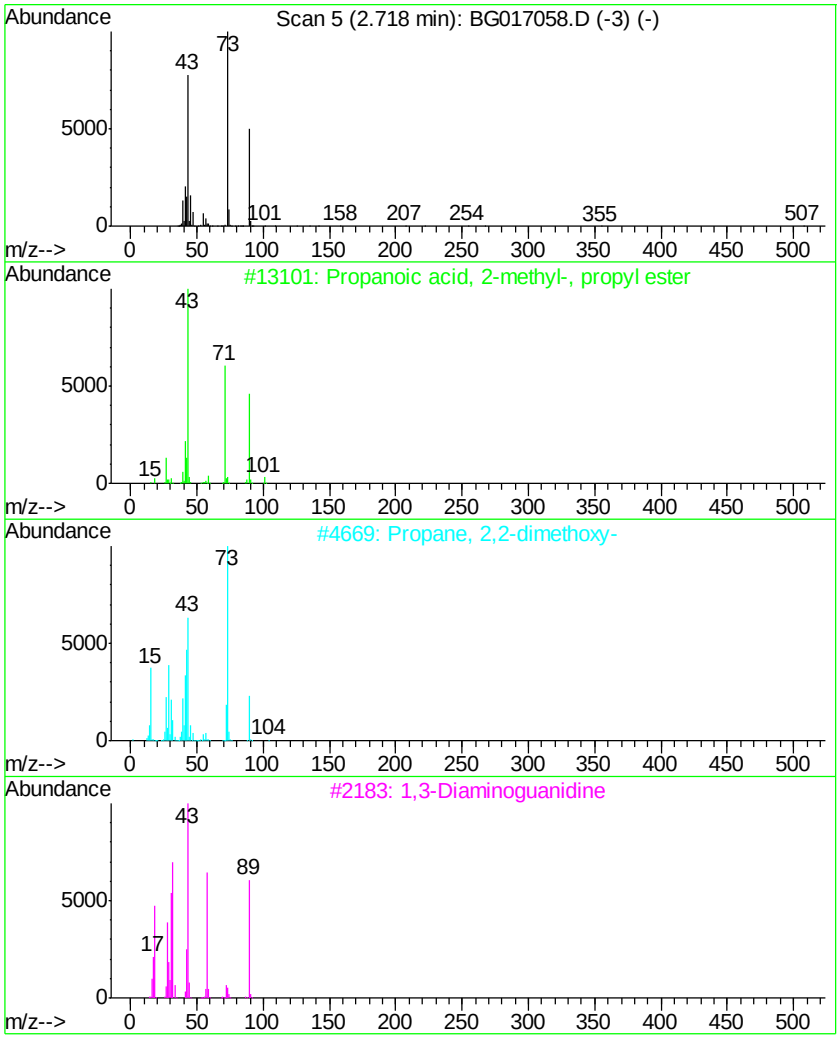
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

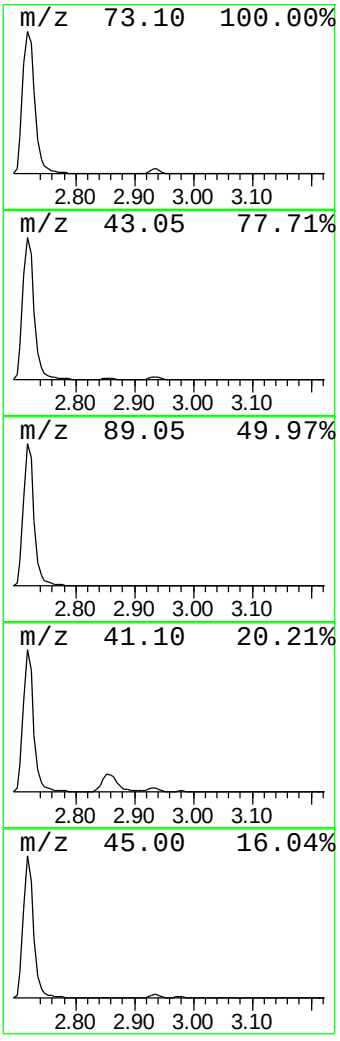
****

Peak Number 1 Propanoic acid, 2-methyl-, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.72	381.10 ng	7058080	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	50
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	36
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	33
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	23





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017058.D
Acq On : 11 May 2015 18:01
Operator : TP/IZ
Sample : G2176-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-29(20-25)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

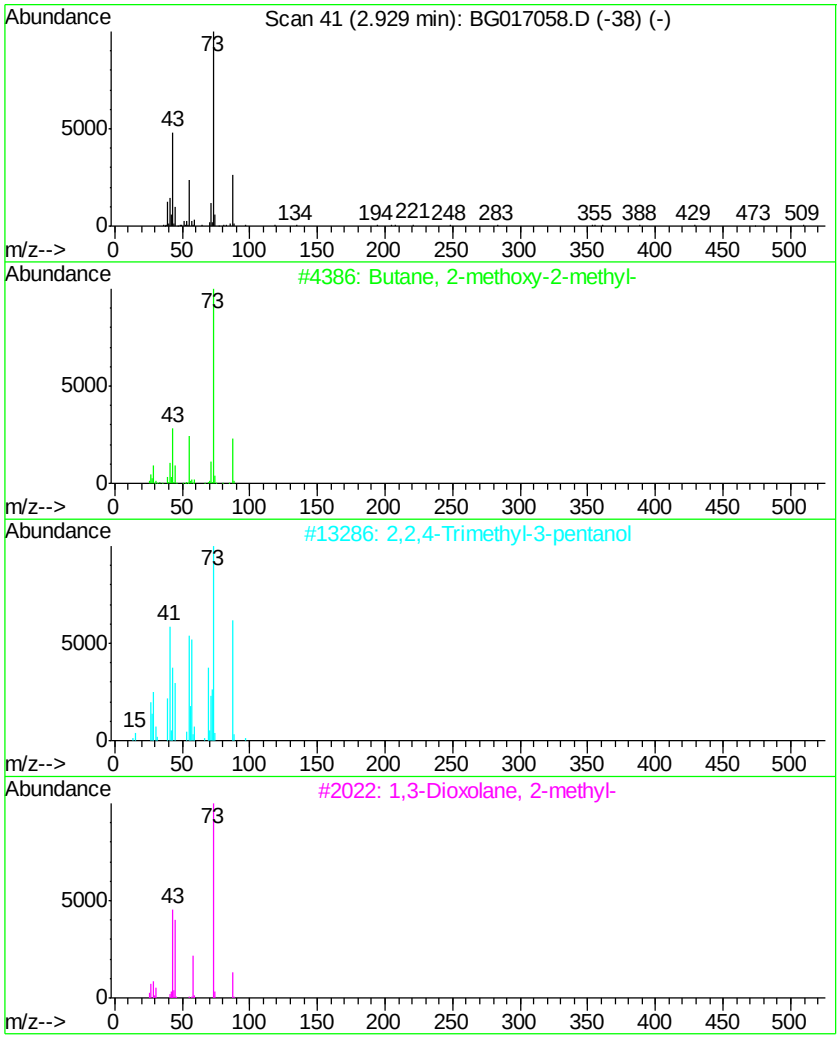
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

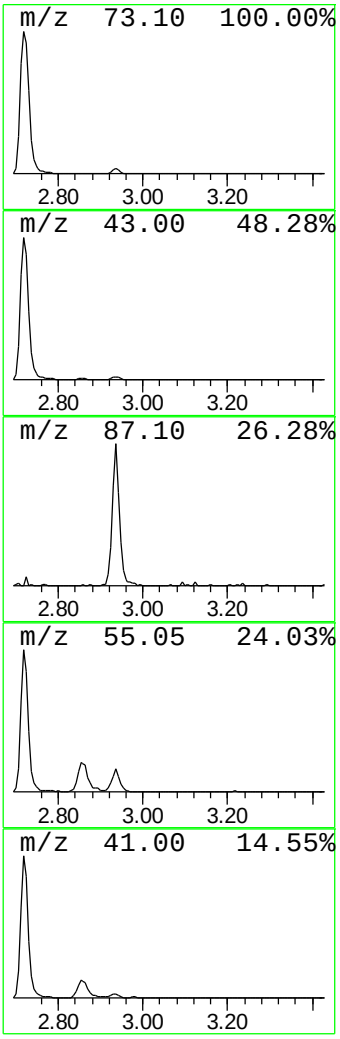
****

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	10.49 ng	194312	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017058.D
Acq On : 11 May 2015 18:01
Operator : TP/IZ
Sample : G2176-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-29(20-25)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

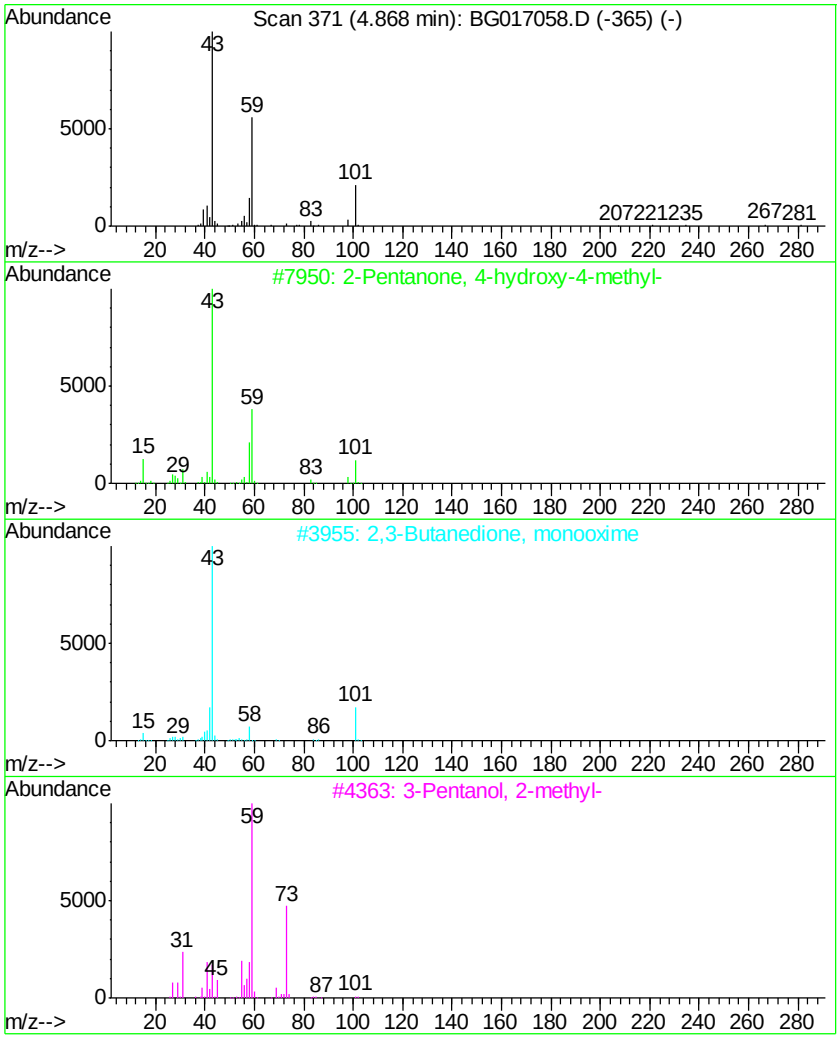
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

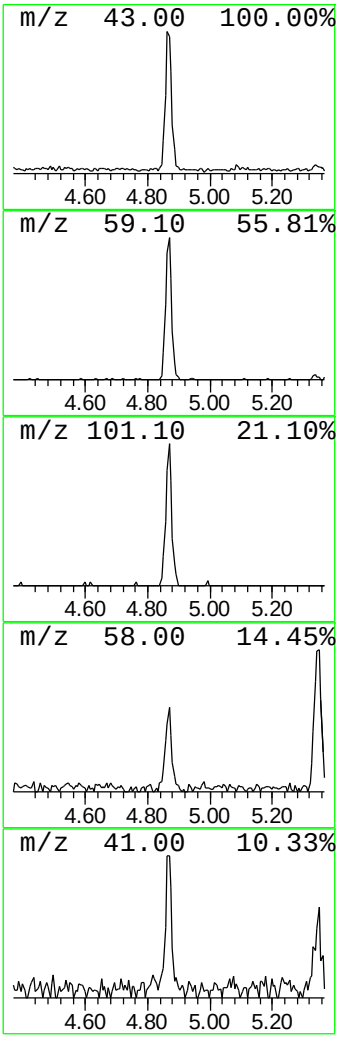
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	6.49 ng	120252	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Dimethadione	129	C5H7NO3	000695-53-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017058.D
Acq On : 11 May 2015 18:01
Operator : TP/IZ
Sample : G2176-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-29(20-25)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

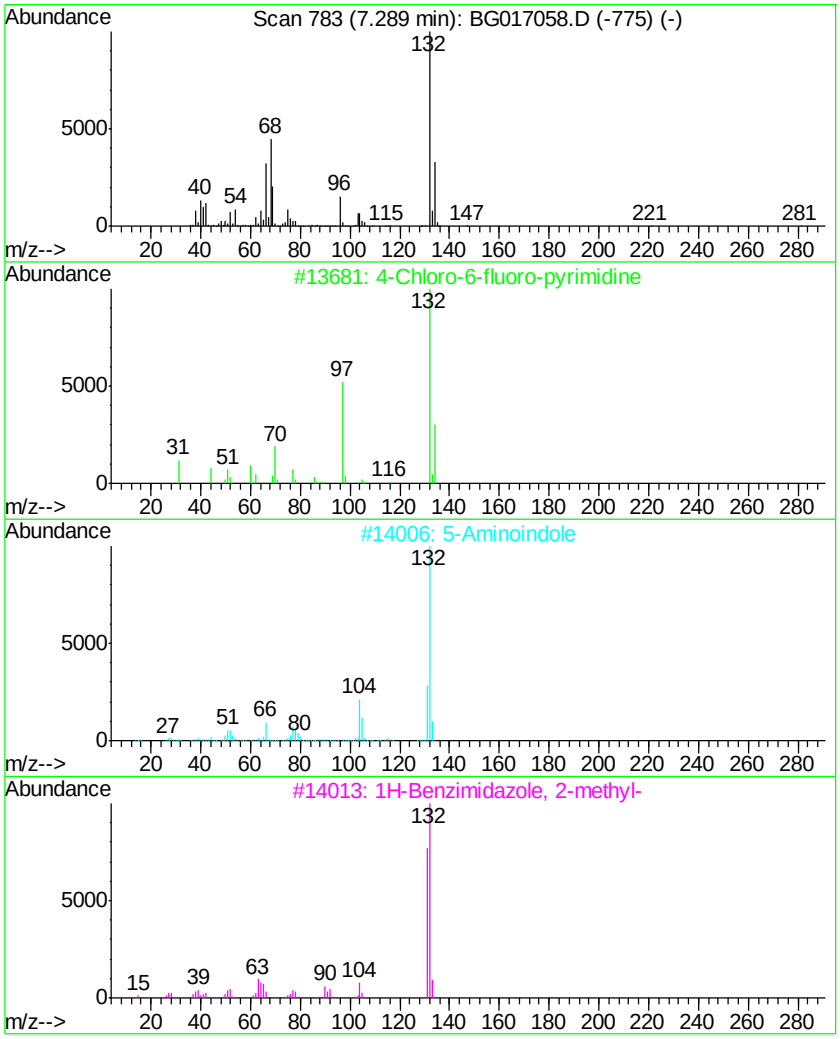
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

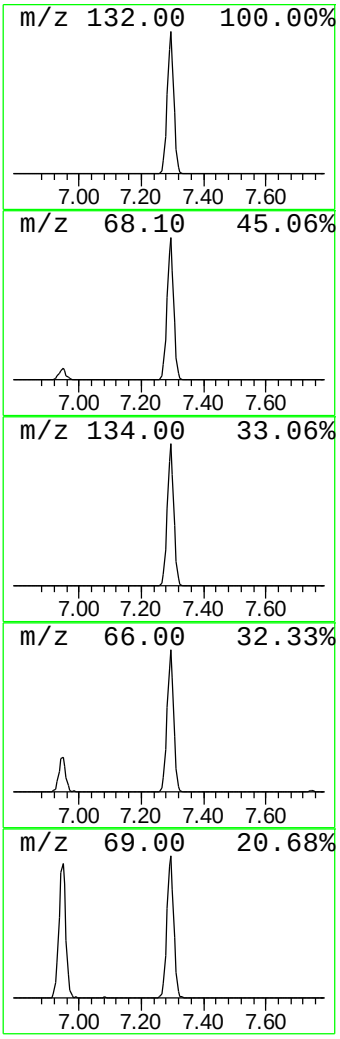
****

Peak Number 5 unknown7.29 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	109.28 ng	2023850	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Benzene, 1-methyl-4-(1-methyleth...	132	C10H12	001195-32-0	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017058.D
Acq On : 11 May 2015 18:01
Operator : TP/IZ
Sample : G2176-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-29(20-25)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

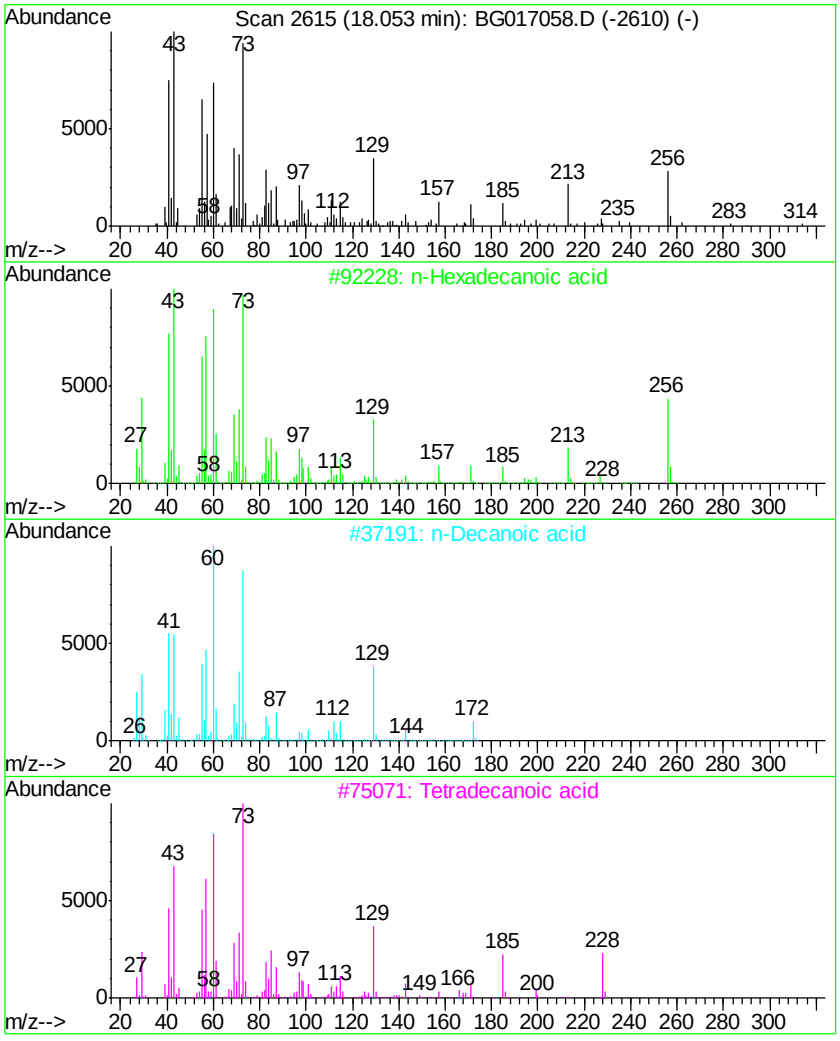
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

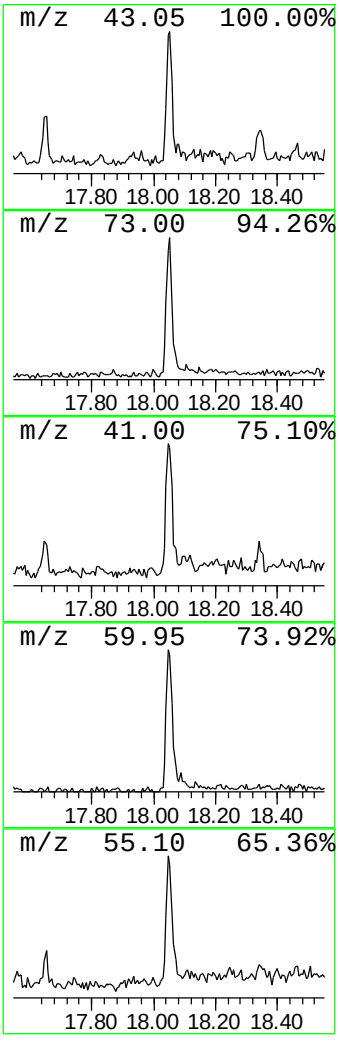
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	4.47 ng	206377	Phenanthrene-d10	17.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	n-Decanoic acid	172	C10H20O2	000334-48-5	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	38
5	Tridecanoic acid	214	C13H26O2	000638-53-9	27





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Operator : TP/IZ
Sample : G2176-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-29(20-25)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

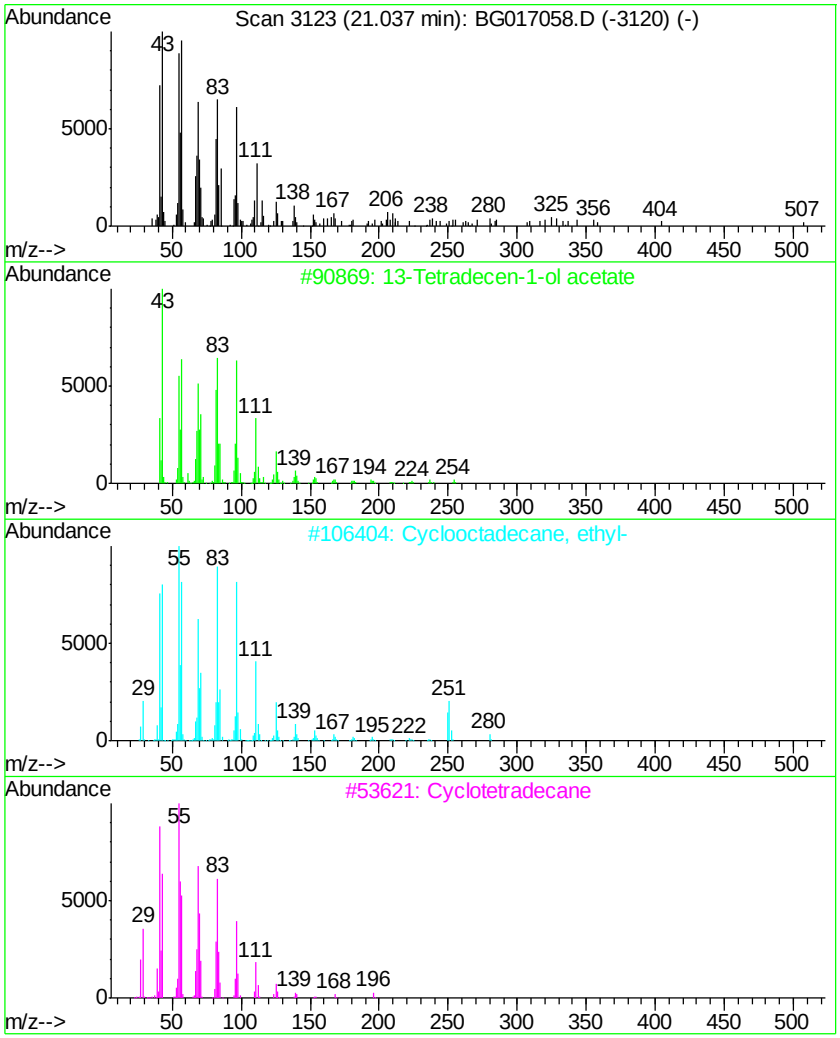
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

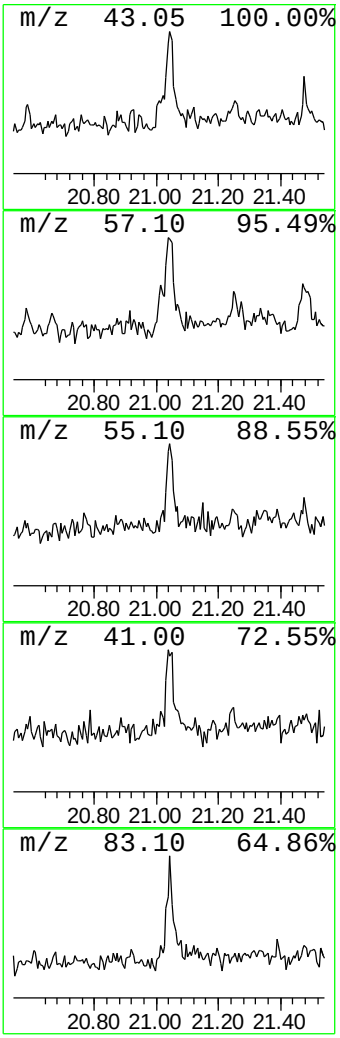
****

Peak Number 8 13-Tetradecen-1-ol acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	2.76 ng	147313	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	70
2	Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	68
3	Cyclotetradecane	196	C14H28	000295-17-0	52
4	Cycloeicosane	280	C20H40	000296-56-0	46
5	Titanium tetrachloride	188	Cl4Ti	007550-45-0	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051115\
Data File : BG017058.D
Acq On : 11 May 2015 18:01
Operator : TP/IZ
Sample : G2176-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-29(20-25)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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
Propanoic acid, 2...	2.72	381.1	ng	7058080	1	7.75	370404	20.0
Butane, 2-methoxy...	2.93	10.5	ng	194312	1	7.75	370404	20.0
2-Pentanone, 4-hy...	4.87	6.5	ng	120252	1	7.75	370404	20.0
unknown7.29	7.29	109.3	ng	2023850	1	7.75	370404	20.0
n-Hexadecanoic acid	18.05	4.5	ng	206377	4	17.15	924416	20.0
13-Tetradecen-1-o...	21.04	2.8	ng	147313	5	21.33	1067170	20.0