LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017063.D
Acq On : 11 May 2015 20:56
Operator : TP/IZ
Sample : G2176-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-26(15-20)

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	2.720	3	5	22	rVB	4318988	4821371	100.00%	21.244%
2	2.855	23	28	37	rVB	129187	206443	4.28%	0.910%
3	2.931	37	41	46	rBV	136256	167128	3.47%	0.736%
4	4.864	363	370	376	rVB	64094	91670	1.90%	0.404%
5	5.346	446	452	458	rBV	880372	1268003	26.30%	5.587%
6	6.944	717	724	733	rBV	949646	1431514	29.69%	6.308%
7	7.291	776	783	793	rVB	900800	1383728	28.70%	6.097%
8	7.749	856	861	867	rVB	221407	345967	7.18%	1.524%
9	8.072	907	916	923	rBV	609158	952388	19.75%	4.196%
10	8.913	1051	1059	1066	rBV	516383	853548	17.70%	3.761%
11	10.546	1328	1337	1344	rBV	301196	484391	10.05%	2.134%
12	13.020	1750	1758	1766	rBV	1183768	1723295	35.74%	7.593%
13	13.860	1895	1901	1907	rBV	68720	102487	2.13%	0.452%
14	14.400	1986	1993	2000	rVB2	420010	650020	13.48%	2.864%
15	15.893	2241	2247	2258	rBV	1169261	1673633	34.71%	7.375%
16	17.150	2455	2461	2468	rVB2	649064	889698	18.45%	3.920%
17	17.273	2478	2482	2487	rVB4	38548	54809	1.14%	0.242%
18	18.049	2609	2614	2620	rBV	95148	135526	2.81%	0.597%
19	19.782	2902	2909	2916	rBV	2396598	3098250	64.26%	13.652%
20	21.040	3119	3123	3131	rBV2	89175	123921	2.57%	0.546%
21	21.328	3167	3172	3179	rVB	886646	1072083	22.24%	4.724%
22	22.526	3371	3376	3384	rVB2	89626	145006	3.01%	0.639%
23	23.613	3555	3561	3571	rVB2	535645	1019982	21.16%	4.494%

Sum of corrected areas: 22694861

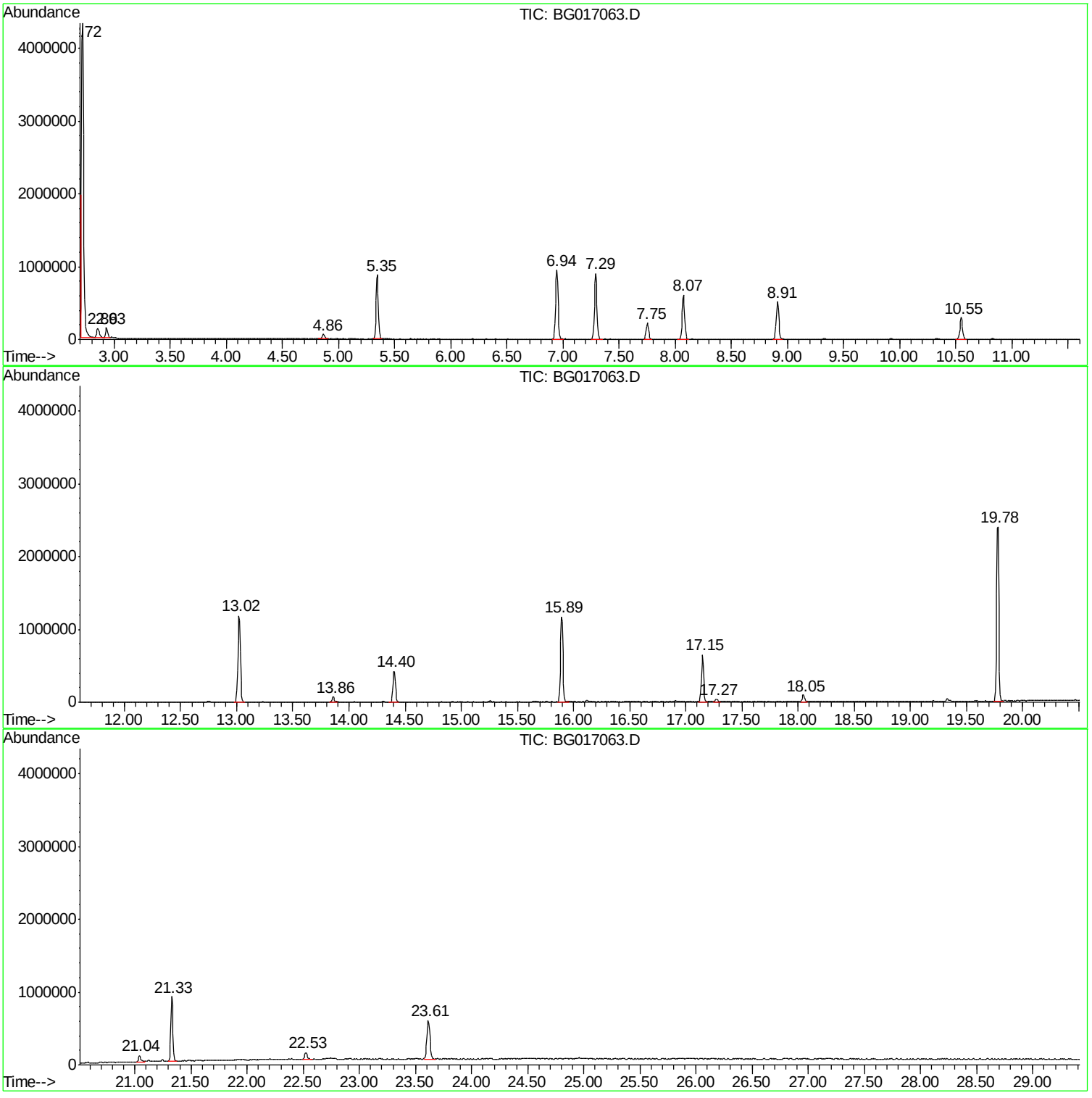
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017063.D
Acq On : 11 May 2015 20:56
Operator : TP/IZ
Sample : G2176-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-26(15-20)

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 : BG017063.D
Acq On : 11 May 2015 20:56
Operator : TP/IZ
Sample : G2176-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-26(15-20)

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

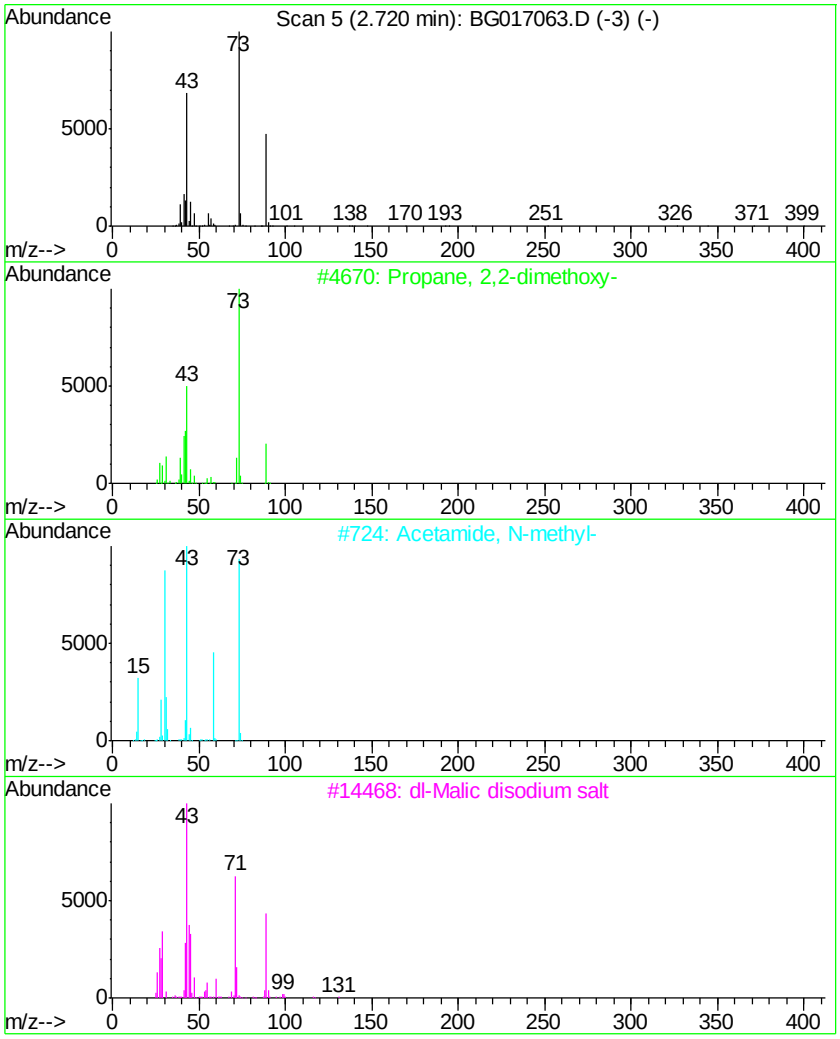
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

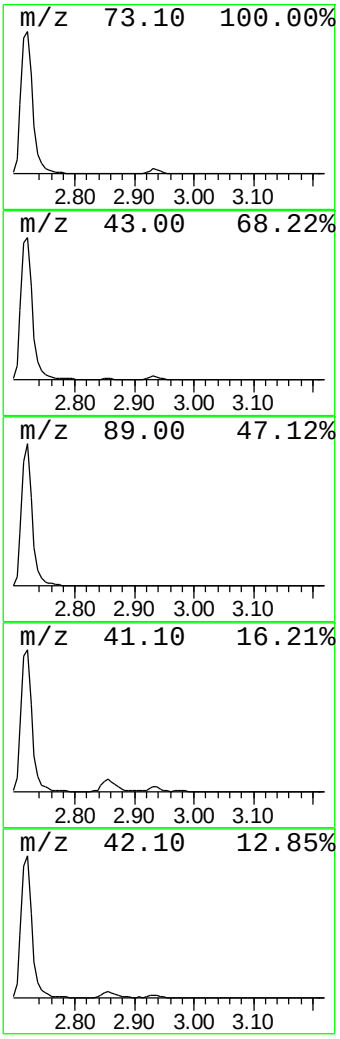
****

Peak Number 1 unknown2.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.72	278.72 ng	4821370	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	33
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
3	dl-Malic disodium salt	134	C4H6O5	000617-48-1	9
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	7





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017063.D
Acq On : 11 May 2015 20:56
Operator : TP/IZ
Sample : G2176-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-26(15-20)

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

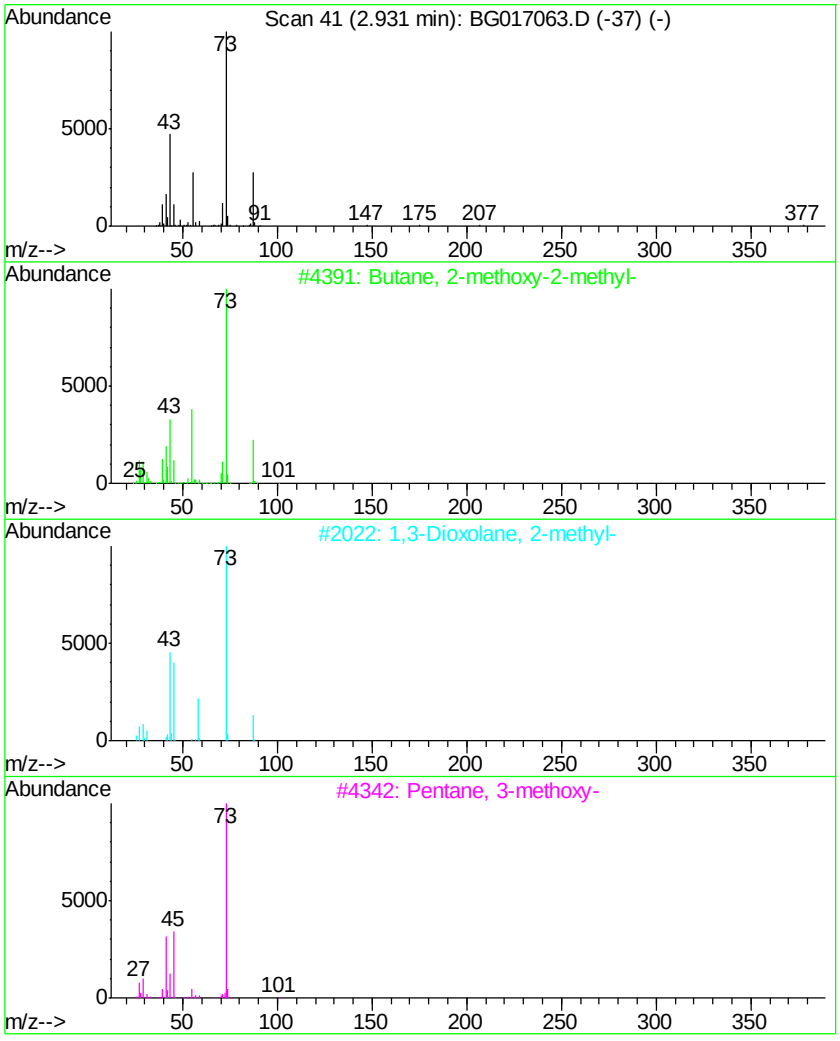
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

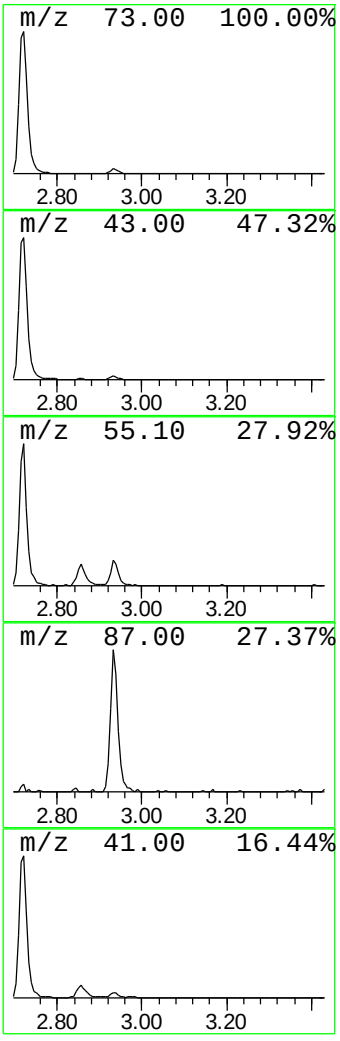
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	9.66 ng	167128	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017063.D
Acq On : 11 May 2015 20:56
Operator : TP/IZ
Sample : G2176-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-26(15-20)

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

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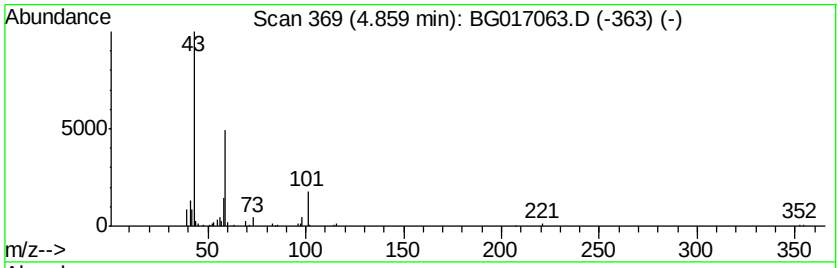
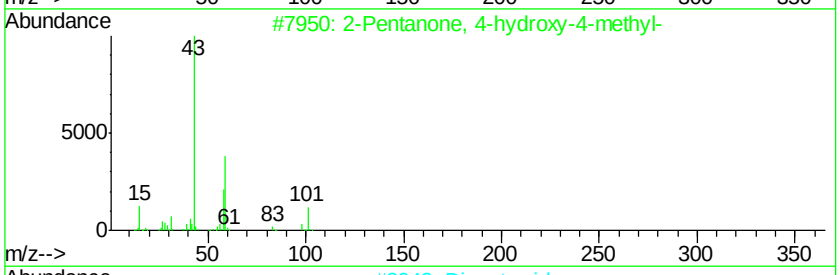
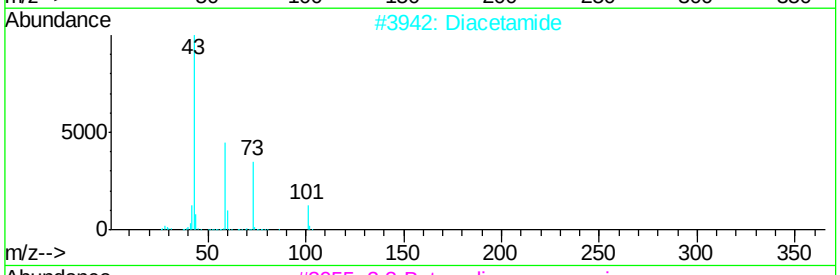
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

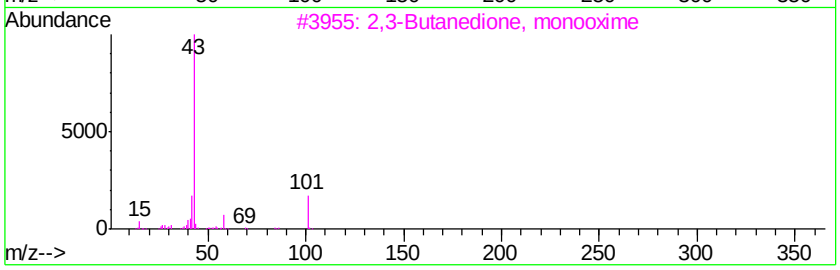
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	5.30 ng	91670	1,4-Dichlorobenzene-d4	7.75

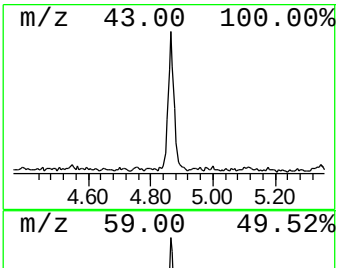
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Diacetamide	101	C4H7NO2	000625-77-4	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	000100-79-8	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	7

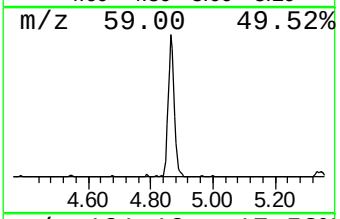


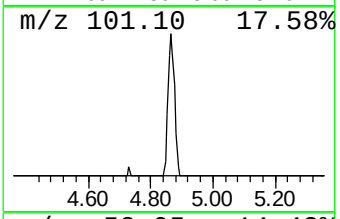


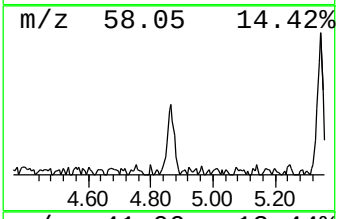


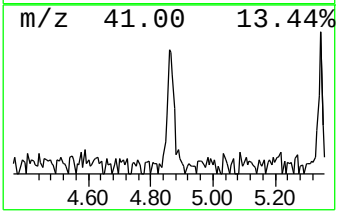












Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
Data File : BG017063.D
Acq On : 11 May 2015 20:56
Operator : TP/IZ
Sample : G2176-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-26(15-20)

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

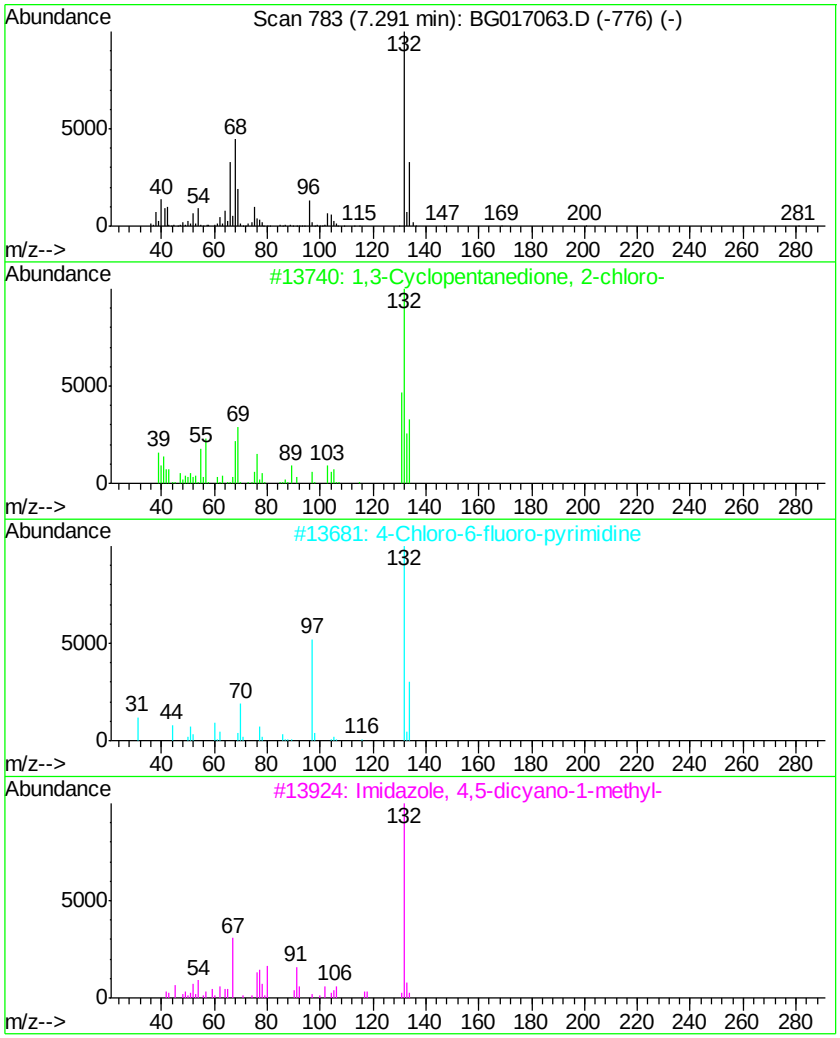
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

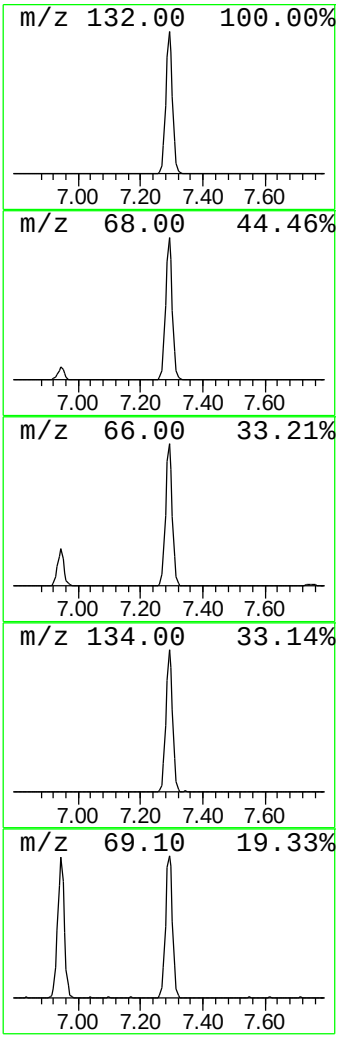
****

Peak Number 5 unknown7.29 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	79.99 ng	1383730	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	32
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22





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Instrument : BNA_G
ClientSampleId : PS-26(15-20)

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

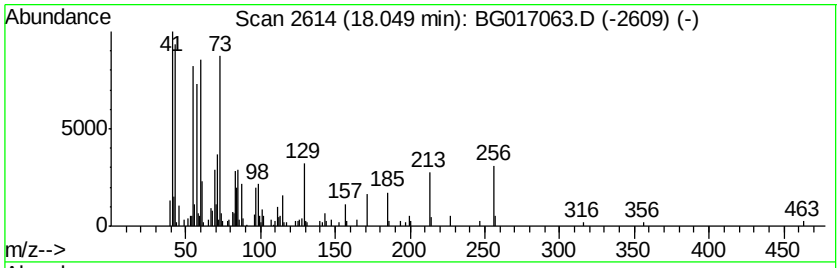
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

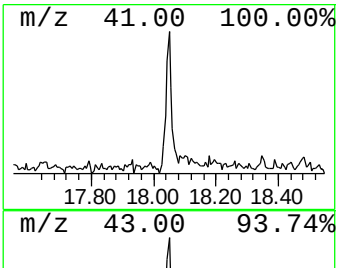
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	3.05 ng	135526	Phenanthrene-d10	17.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Tridecanoic acid	214	C13H26O2	000638-53-9	47
5	Octanoic Acid	144	C8H16O2	000124-07-2	43





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Data File : BG017063.D
Acq On : 11 May 2015 20:56
Operator : TP/IZ
Sample : G2176-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PS-26(15-20)

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

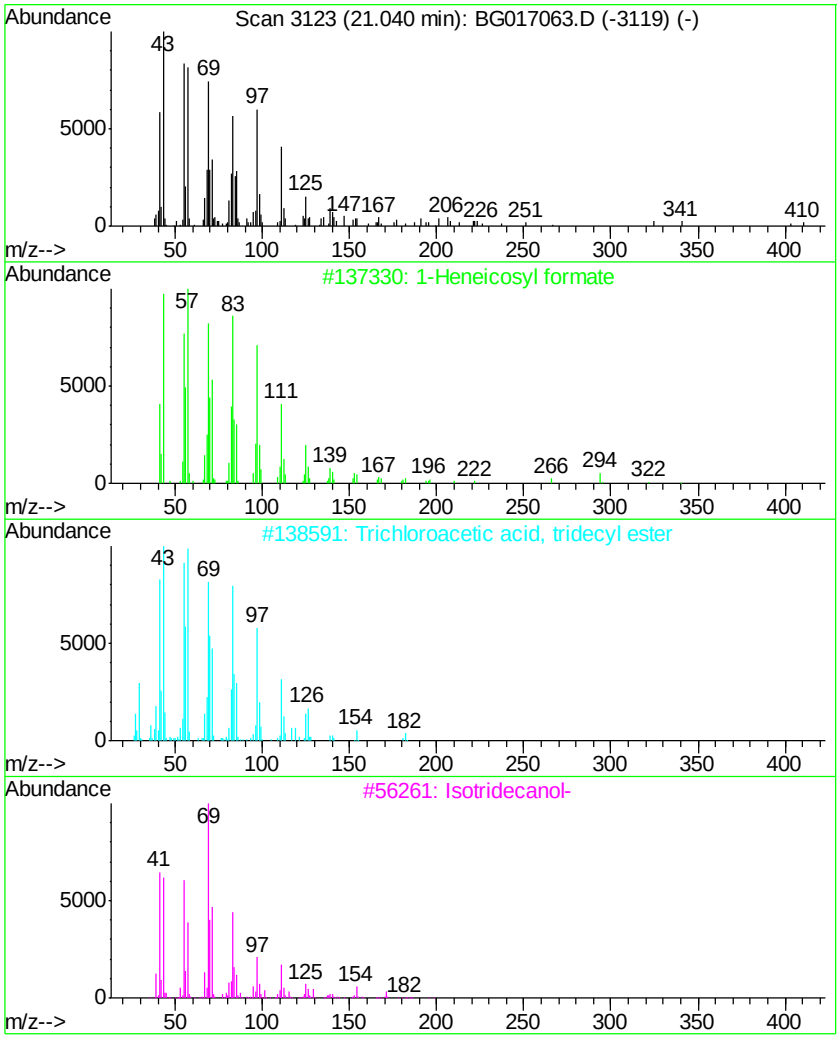
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

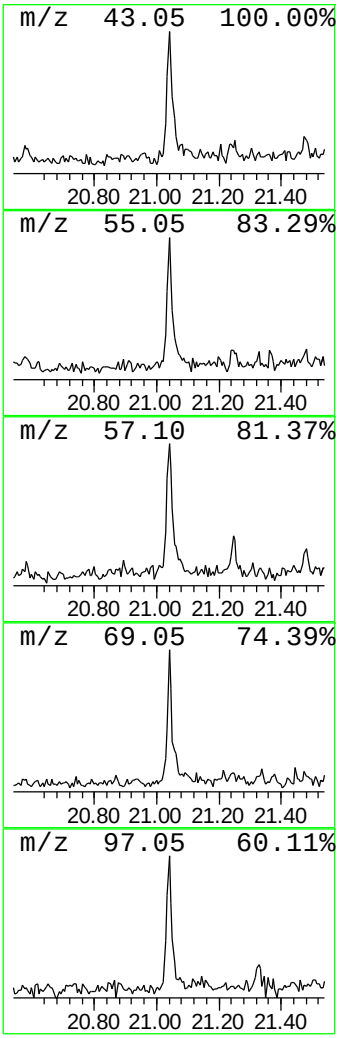
****

Peak Number 8 1-Heneicosyl formate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	2.31 ng	123921	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	80
2	Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	80
3	Isotridecanol-	200	C13H28O	027458-92-0	74
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	72
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	64





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Instrument : BNA_G
ClientSampleId : PS-26(15-20)

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

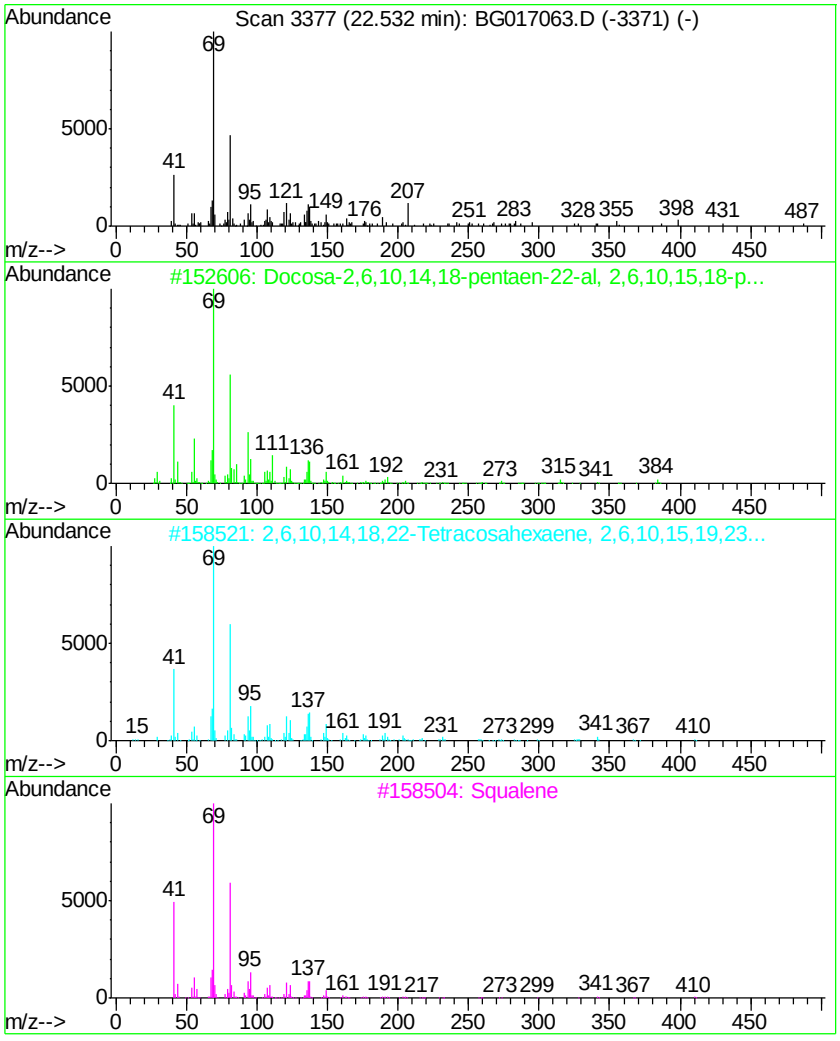
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

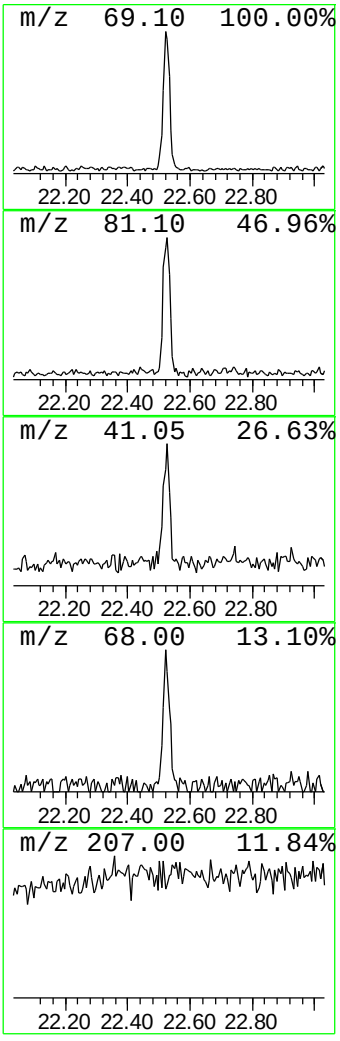
****

Peak Number 9 Docosa-2,6,10,14,18-pentaen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.53	2.84 ng	145006	Perylene-d12	23.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	87
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87
3	Squalene	410	C30H50	007683-64-9	86
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051115\
Data File : BG017063.D
Acq On : 11 May 2015 20:56
Operator : TP/IZ
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.72	2.72	278.7	ng	4821370	1	7.75	345967	20.0
Butane, 2-methoxy...	2.93	9.7	ng	167128	1	7.75	345967	20.0
2-Pentanone, 4-hy...	4.86	5.3	ng	91670	1	7.75	345967	20.0
unknown7.29	7.29	80.0	ng	1383730	1	7.75	345967	20.0
n-Hexadecanoic acid	18.05	3.0	ng	135526	4	17.15	889698	20.0
1-Heneicosyl formate	21.04	2.3	ng	123921	5	21.33	1072080	20.0
Docosa-2,6,10,14,...	22.53	2.8	ng	145006	6	23.61	1019980	20.0