LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016943.D
Acq On : 8 May 2015 4:46
Operator : TP/IZ
Sample : G2084-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9

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	2.788	12	17	34	rVB	2908162	3728058	92.81%	12.798%
2	2.923	35	40	49	rVB2	158278	287562	7.16%	0.987%
3	3.000	49	53	59	rBV	417414	535616	13.33%	1.839%
4	4.921	373	380	390	rBV2	195790	312886	7.79%	1.074%
5	5.379	452	458	467	rBV	1146468	1669791	41.57%	5.732%
6	6.965	720	728	738	rVB	1357448	2104061	52.38%	7.223%
7	7.330	780	790	798	rBV	1225145	1935211	48.18%	6.643%
8	7.800	862	870	876	rBV	294005	484550	12.06%	1.663%
9	8.117	917	924	937	rBV	851033	1346270	33.52%	4.622%
10	8.951	1059	1066	1074	rVB	770352	1265425	31.50%	4.344%
11	10.591	1338	1345	1351	rBV	400319	693618	17.27%	2.381%
12	13.058	1758	1765	1771	rBV	1854248	2651457	66.01%	9.102%
13	13.887	1900	1906	1915	rBV	85184	131333	3.27%	0.451%
14	14.433	1993	1999	2008	rBV2	626678	960843	23.92%	3.299%
15	15.920	2246	2252	2262	rBV	1317131	1855120	46.18%	6.369%
16	16.149	2287	2291	2302	rVB2	30963	53960	1.34%	0.185%
17	17.177	2460	2466	2473	rBV2	810467	1178295	29.33%	4.045%
18	18.076	2613	2619	2625	rBV	109127	169582	4.22%	0.582%
19	19.357	2831	2837	2841	rBV5	47645	70784	1.76%	0.243%
20	19.803	2907	2913	2922	rBV	3070014	4016908	100.00%	13.790%
21	21.067	3124	3128	3139	rBV	476545	621685	15.48%	2.134%
22	21.272	3156	3163	3169	rVB2	92345	198011	4.93%	0.680%
23	21.355	3172	3177	3184	rBV	969754	1240867	30.89%	4.260%
24	21.971	3276	3282	3289	rBV6	55996	122328	3.05%	0.420%
25	22.447	3358	3363	3372	rVV6	26500	78685	1.96%	0.270%
26	22.741	3406	3413	3417	rBV7	29763	60159	1.50%	0.207%
27	23.006	3455	3458	3463	rVB7	28418	45335	1.13%	0.156%
28	23.658	3563	3569	3577	rVB2	610901	1165100	29.00%	4.000%
29	24.316	3676	3681	3690	rBV8	61737	145971	3.63%	0.501%

Sum of corrected areas: 29129471

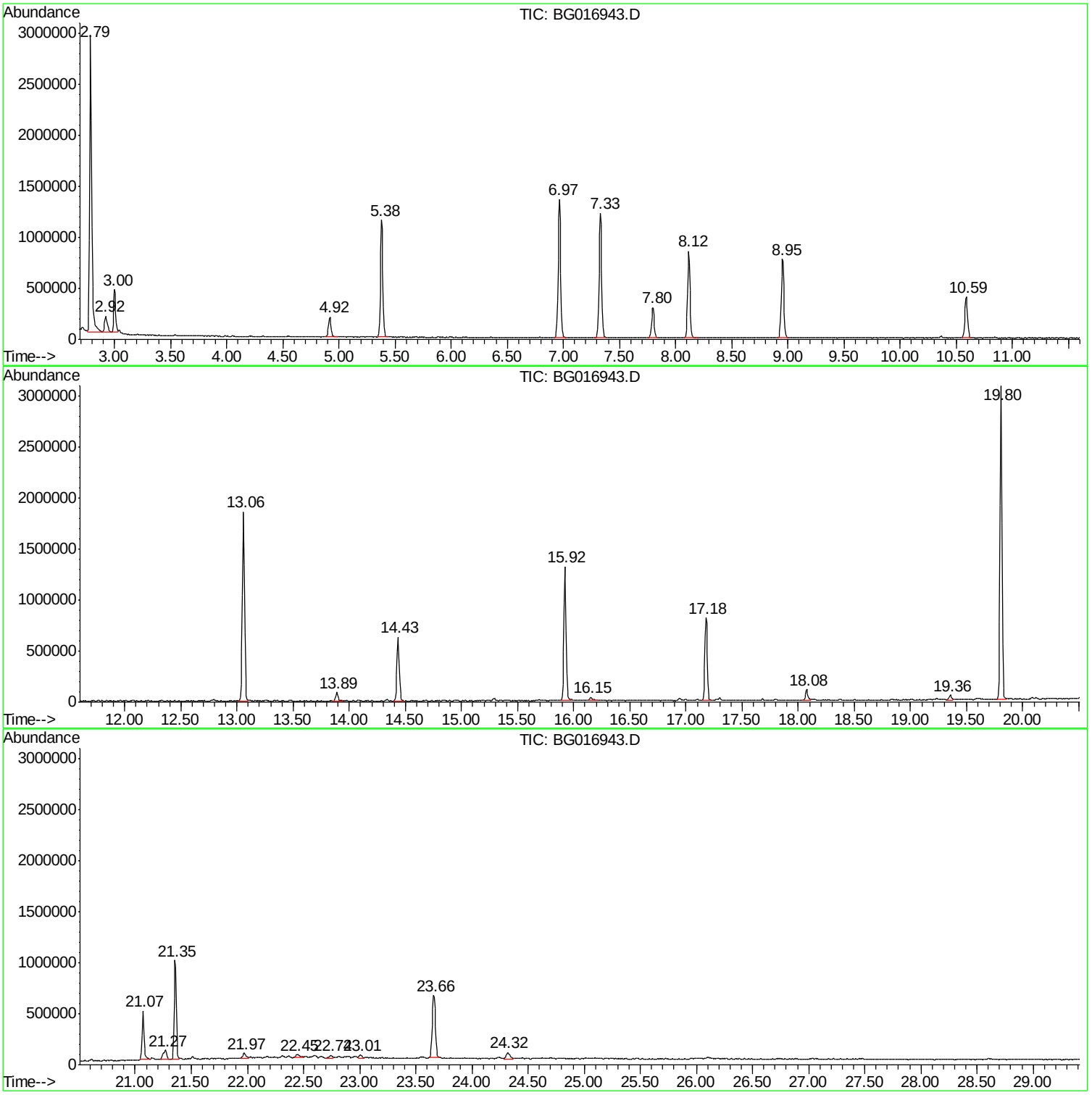
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016943.D
Acq On : 8 May 2015 4:46
Operator : TP/IZ
Sample : G2084-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9

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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Data File : BG016943.D
Acq On : 8 May 2015 4:46
Operator : TP/IZ
Sample : G2084-09
Misc :
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Instrument : BNA_G
ClientSampleId : 9

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

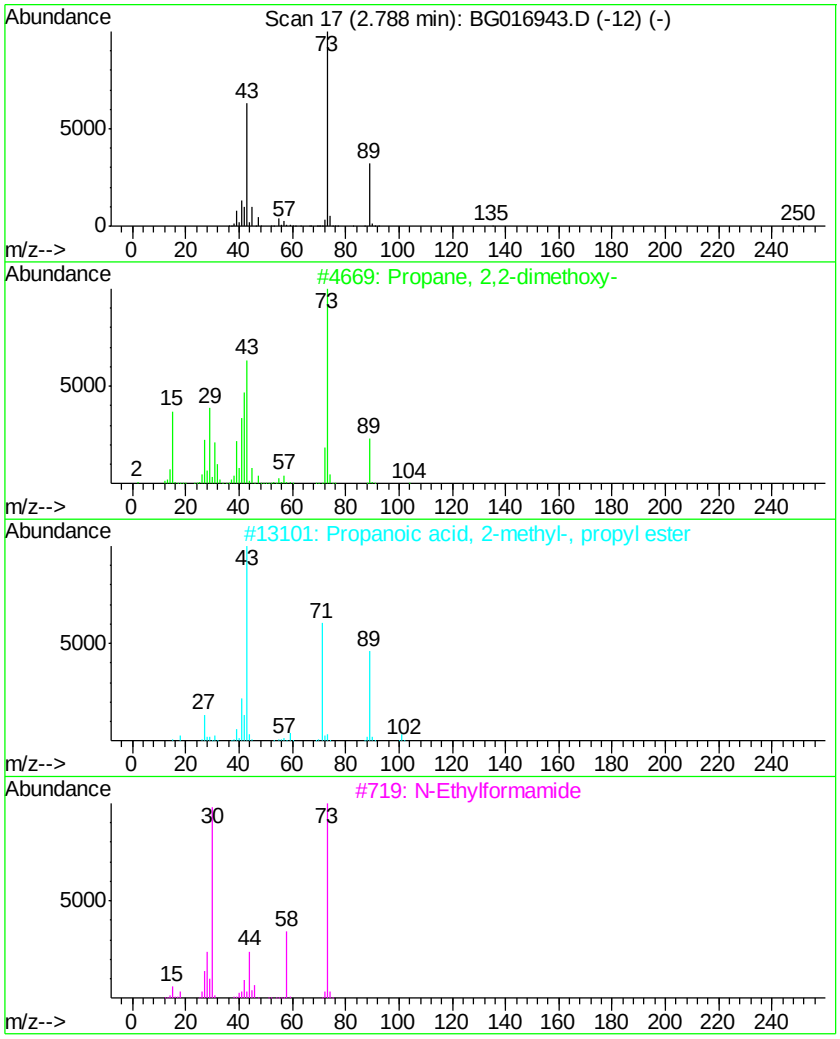
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

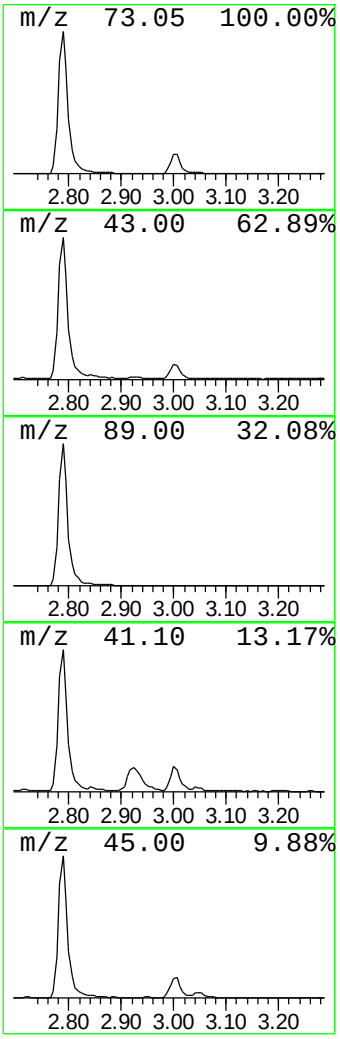
****

Peak Number 1 unknown2.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	153.88 ng	3728060	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	17
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016943.D
Acq On : 8 May 2015 4:46
Operator : TP/IZ
Sample : G2084-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9

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

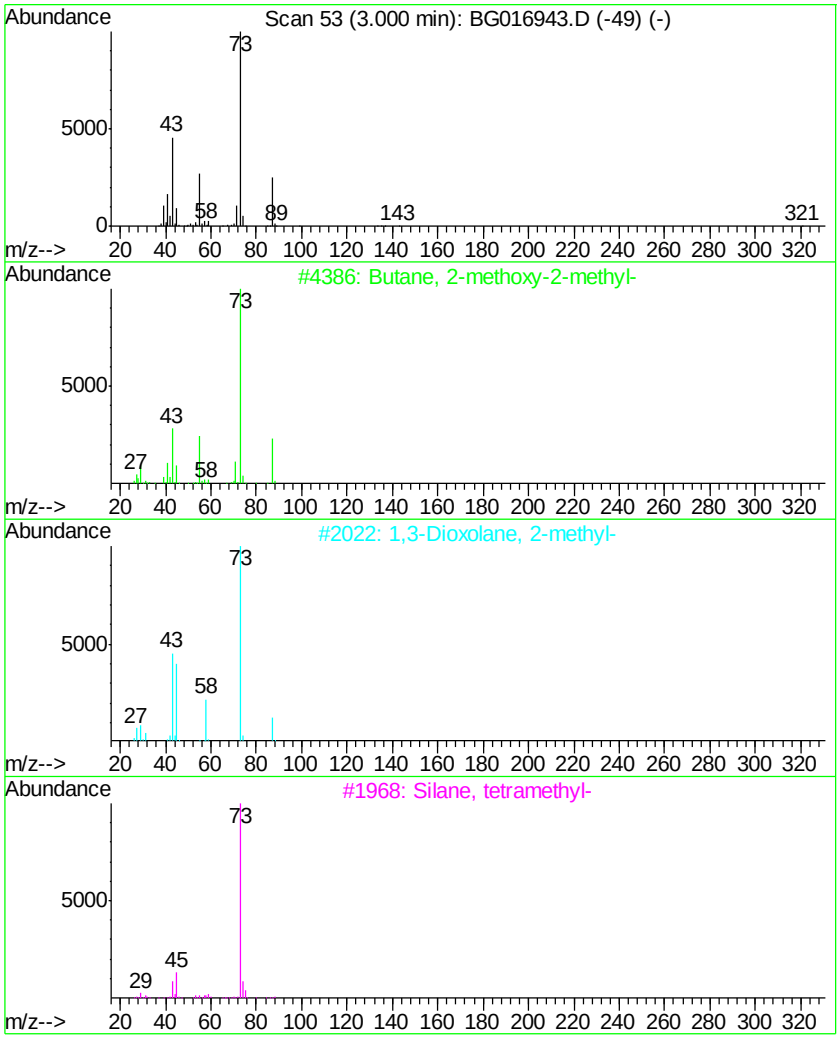
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

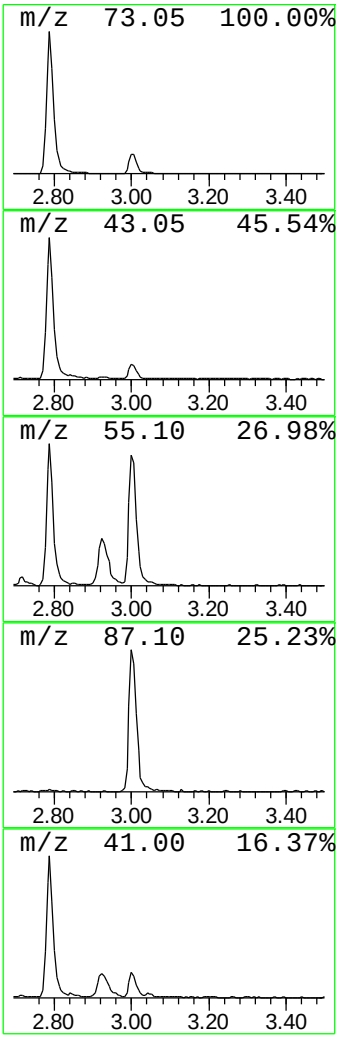
****

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	22.11 ng	535616	1,4-Dichlorobenzene-d4	7.79

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	23
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016943.D
Acq On : 8 May 2015 4:46
Operator : TP/IZ
Sample : G2084-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9

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

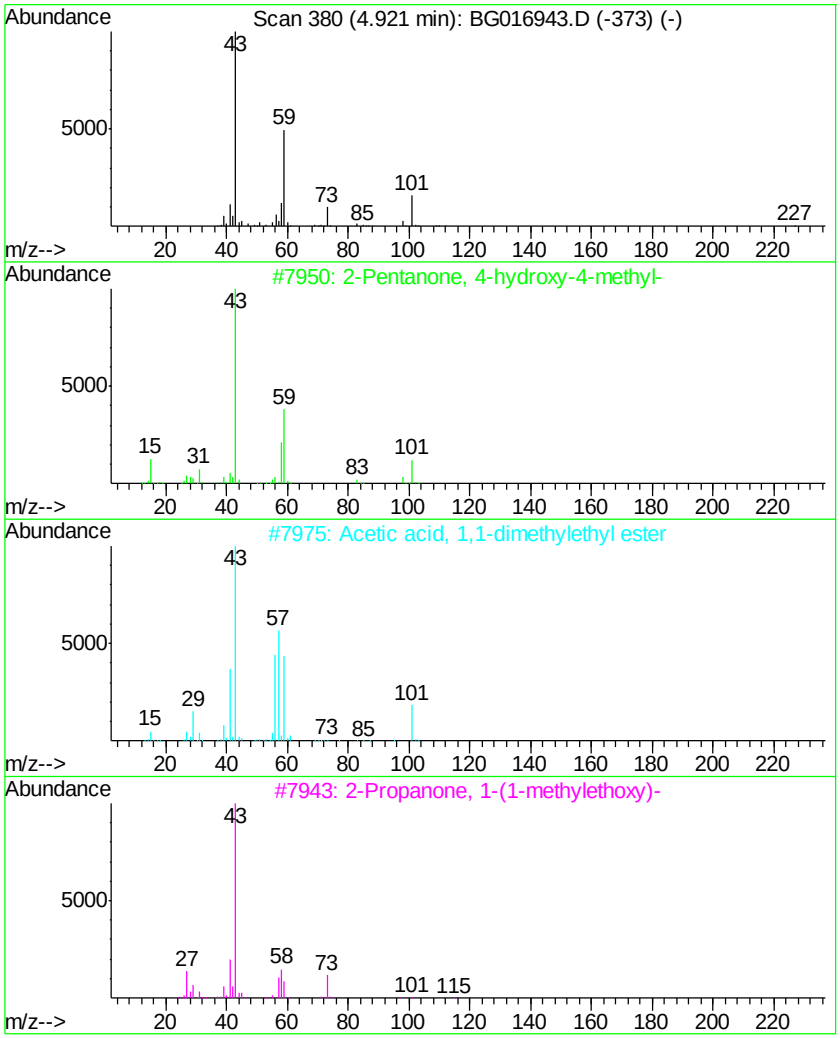
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

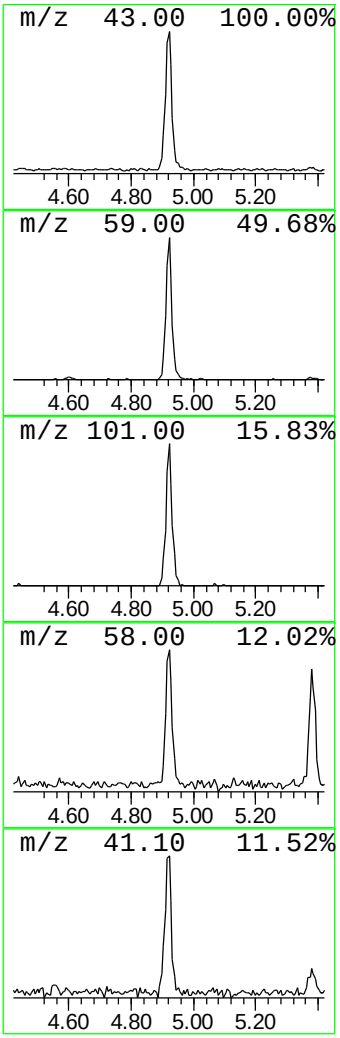
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	12.91 ng	312886	1,4-Dichlorobenzene-d4	7.79

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	36
3	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	12
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9





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Data File : BG016943.D
Acq On : 8 May 2015 4:46
Operator : TP/IZ
Sample : G2084-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9

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

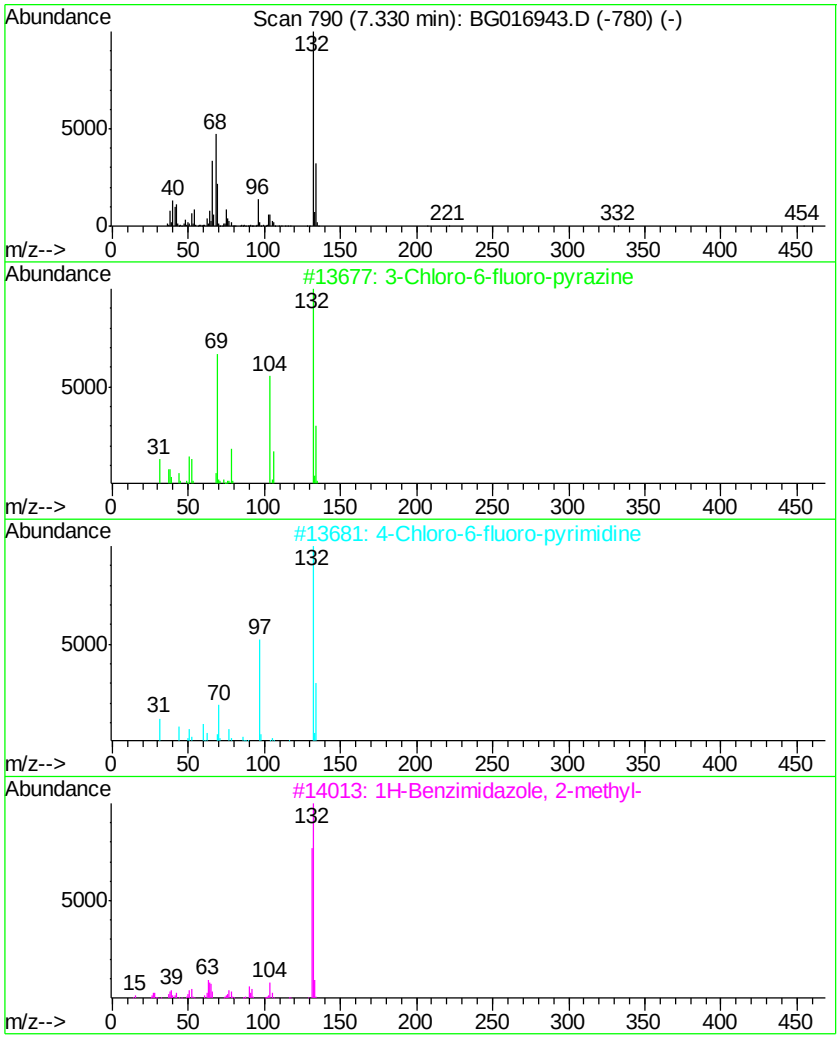
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

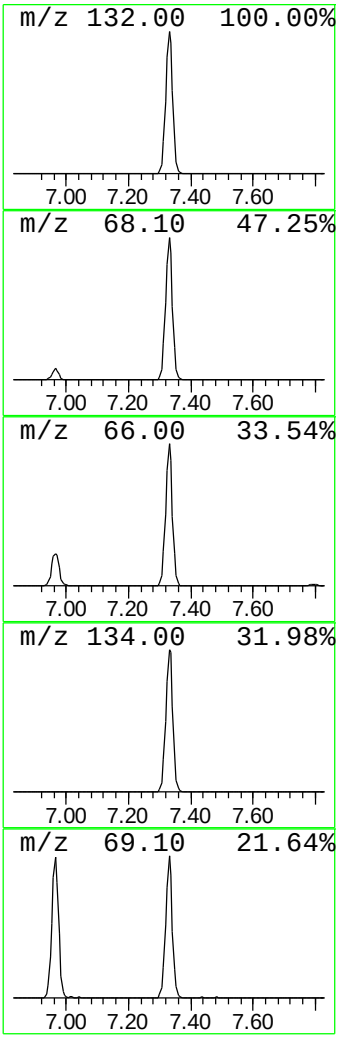
****

Peak Number 5 unknown7.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	79.88 ng	1935210	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





Data Path : Z:\HPCHEM1\BNA G\DATA\BG050715\
Data File : BG016943.D
Acq On : 8 May 2015 4:46
Operator : TP/IZ
Sample : G2084-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9

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

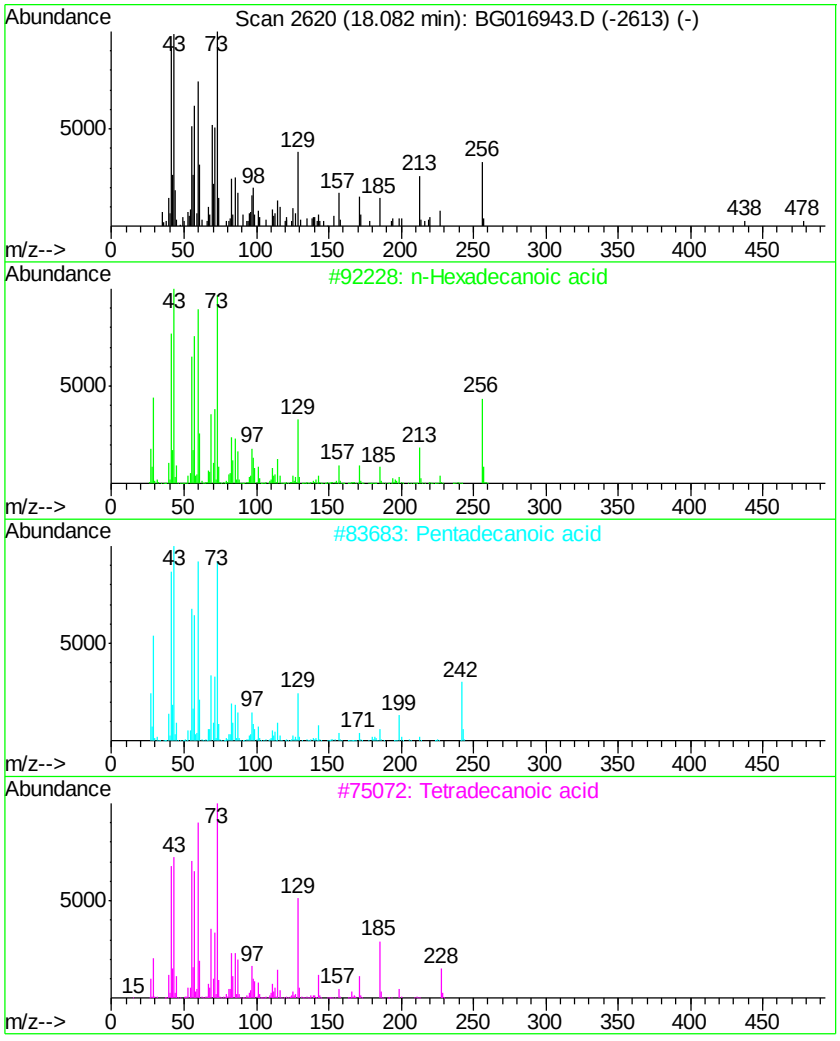
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

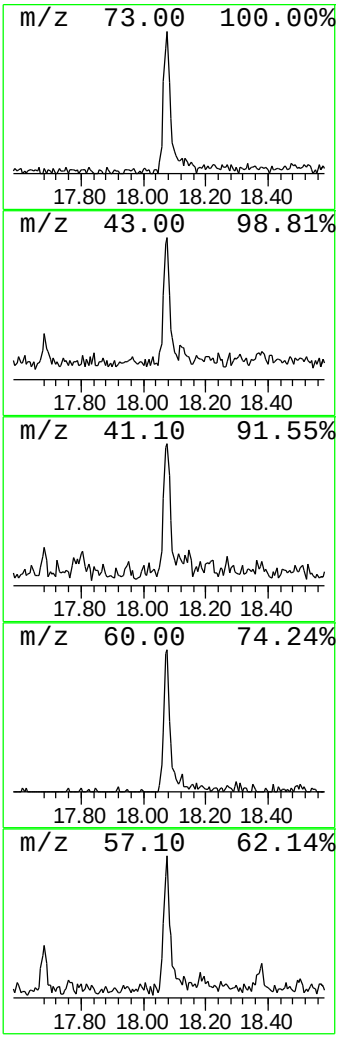
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	2.88 ng	169582	Phenanthrene-d10	17.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Undecanoic acid	186	C11H22O2	000112-37-8	52
5	Tridecanoic acid	214	C13H26O2	000638-53-9	52





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Sample : G2084-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
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TIC Library : C:\DATABASE\NIST02.L
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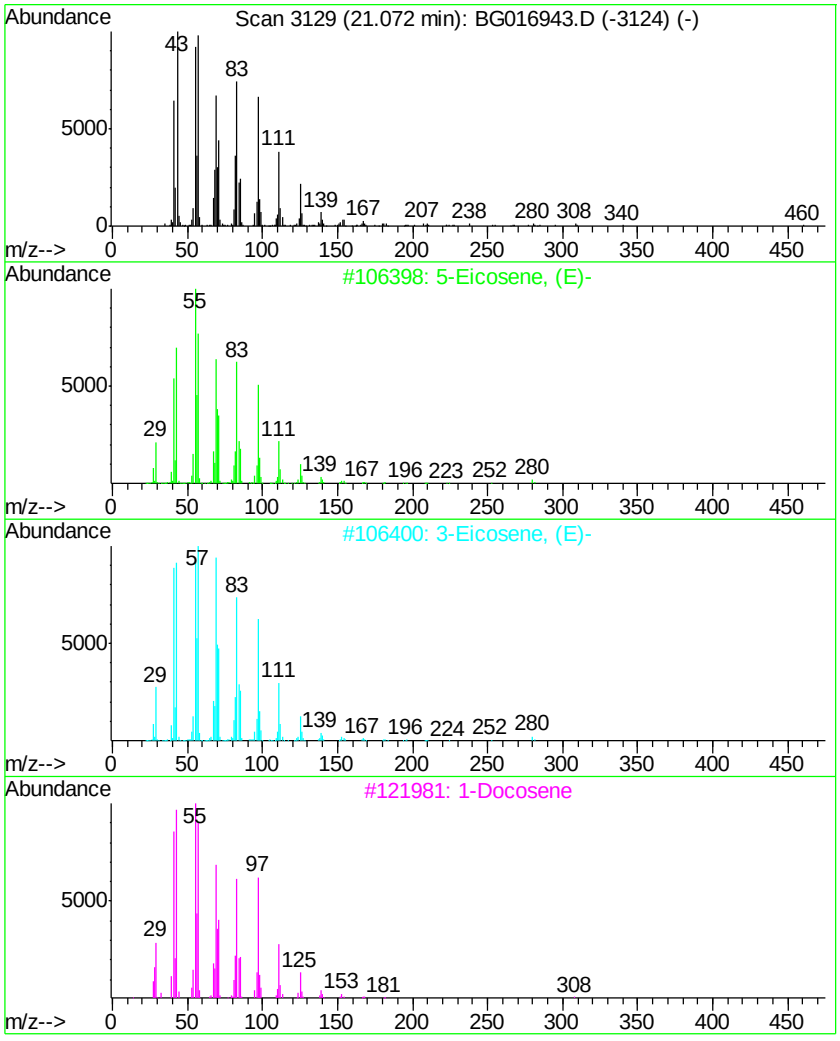
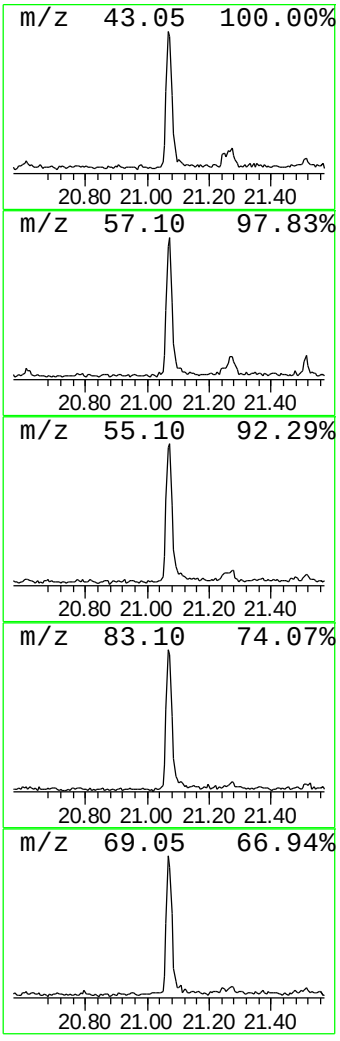
****

Peak Number 8 5-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.07	10.02 ng	621685	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	99
3	1-Docosene	308	C22H44	001599-67-3	95
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91





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

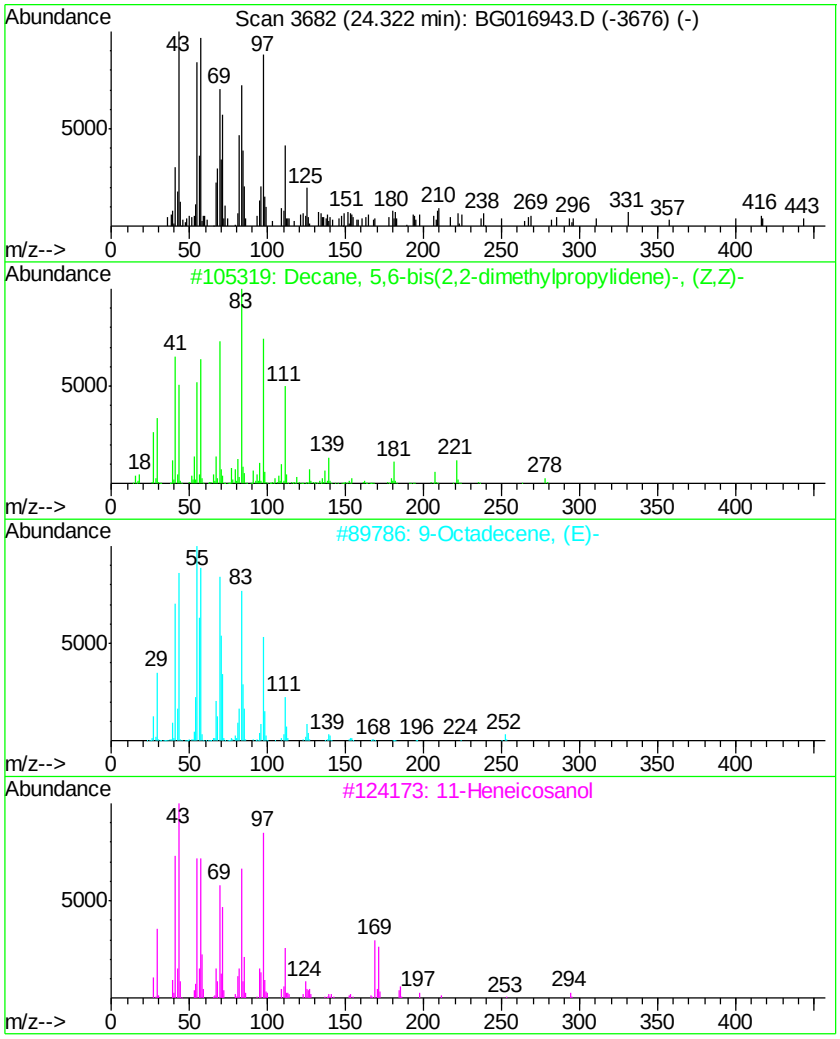
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

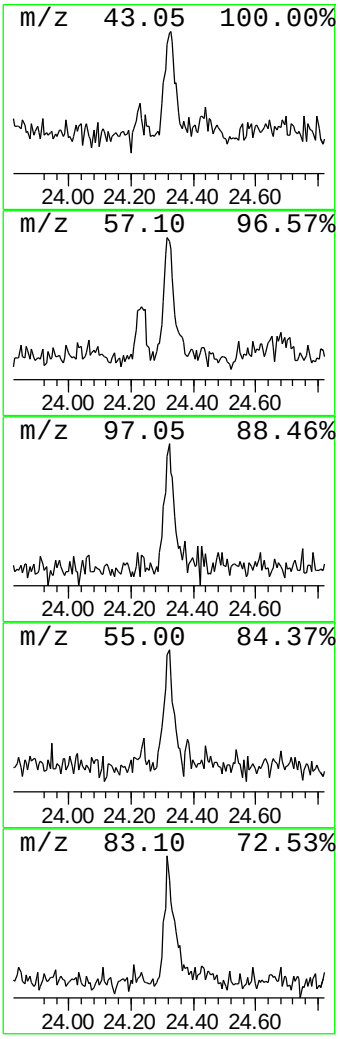
****

Peak Number 9 unknown24.32 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.32	2.51 ng	145971	Perylene-d12	23.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 5,6-bis(2,2-dimethylprop...	278	C20H38	073002-85-4	41
2	9-Octadecene, (E)-	252	C18H36	007206-25-9	38
3	11-Heneicosanol	312	C21H44O	003381-26-8	35
4	cis-Inositol tri-methylboronate	252	C9H15B3O6	1000064-40-1	35
5	1H-Imidazole, 1-(cyclohexylacetyl)-	192	C11H16N2O	093383-50-7	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050715\
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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
unknown2.79	2.79	153.9	ng	3728060	1	7.79	484550	20.0
Butane, 2-methoxy...	3.00	22.1	ng	535616	1	7.79	484550	20.0
2-Pentanone, 4-hy...	4.92	12.9	ng	312886	1	7.79	484550	20.0
unknown7.33	7.33	79.9	ng	1935210	1	7.79	484550	20.0
n-Hexadecanoic acid	18.08	2.9	ng	169582	4	17.18	1178300	20.0
5-Eicosene, (E)-	21.07	10.0	ng	621685	5	21.35	1240870	20.0
unknown24.32	24.32	2.5	ng	145971	6	23.66	1165100	20.0