LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024676.D
Acq On : 4 Nov 2016 10:48
Operator : UM/SJ
Sample : H5509-09
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-95-1.0-1.5

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-BG102516.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	3.123	43	48	65	rBV	5715777	9166173	100.00%	15.557%
2	5.326	418	423	432	rBV	476489	764324	8.34%	1.297%
3	5.796	496	503	514	rVB	2179800	3676394	40.11%	6.239%
4	7.406	767	777	788	rBV	2262859	4146555	45.24%	7.037%
5	7.794	832	843	853	rBV	2150946	3843586	41.93%	6.523%
6	8.270	915	924	931	rBV	337811	621033	6.78%	1.054%
7	8.593	972	979	987	rVB	1509582	2714792	29.62%	4.607%
8	9.439	1113	1123	1132	rBV	1385035	2558727	27.91%	4.343%
9	11.090	1397	1404	1413	rBV	470856	874350	9.54%	1.484%
10	13.505	1805	1815	1823	rBV	3089656	4888906	53.34%	8.297%
11	14.321	1945	1954	1960	rBV	1113267	1632232	17.81%	2.770%
12	14.880	2040	2049	2058	rBV	801380	1284155	14.01%	2.179%
13	16.366	2294	2302	2312	rBV	3401465	5429220	59.23%	9.214%
14	16.536	2326	2331	2340	rVB3	78903	133028	1.45%	0.226%
15	17.623	2508	2516	2524	rBV2	1093485	1736868	18.95%	2.948%
16	17.958	2566	2573	2582	rBV	258779	420879	4.59%	0.714%
17	18.464	2655	2659	2669	rBV	205954	329780	3.60%	0.560%
18	19.727	2869	2874	2877	rBV5	69231	95908	1.05%	0.163%
19	20.203	2949	2955	2961	rBV	6423867	8756056	95.53%	14.861%
20	21.495	3170	3175	3186	rBV2	428622	666544	7.27%	1.131%
21	21.918	3240	3247	3256	rVB	1398074	2425530	26.46%	4.117%
22	22.735	3381	3386	3398	rBV8	131753	299648	3.27%	0.509%
23	25.344	3819	3830	3843	rVB	779550	2456743	26.80%	4.170%

Sum of corrected areas: 58921431

LSC Report - Integrated Chromatogram

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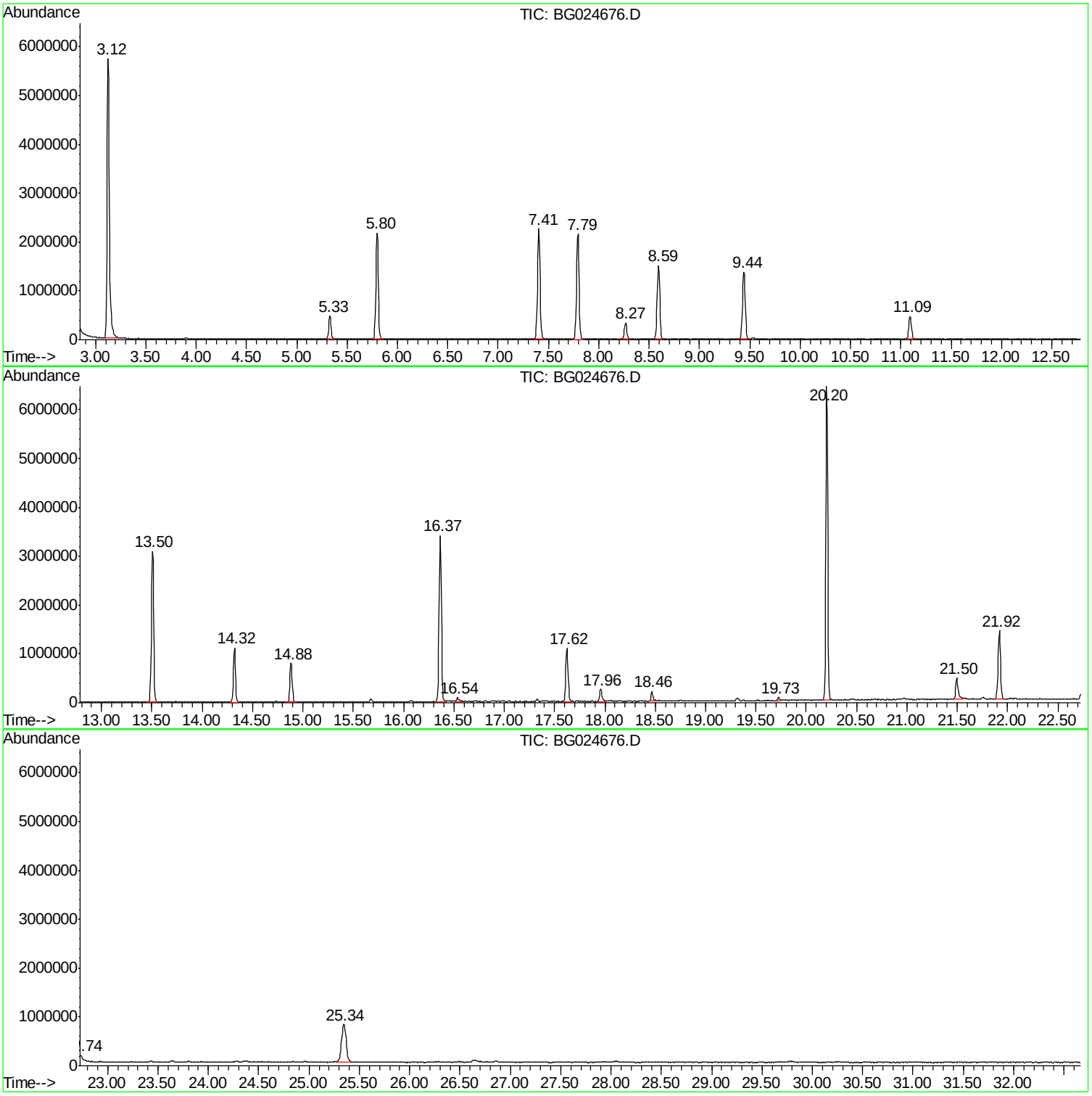
Operator : UM/SJ
Sample : H5509-09
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-95-1.0-1.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024676.D
Acq On : 4 Nov 2016 10:48
Operator : UM/SJ
Sample : H5509-09
Misc :
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Instrument : BNA_G
ClientSampleId : SB-95-1.0-1.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

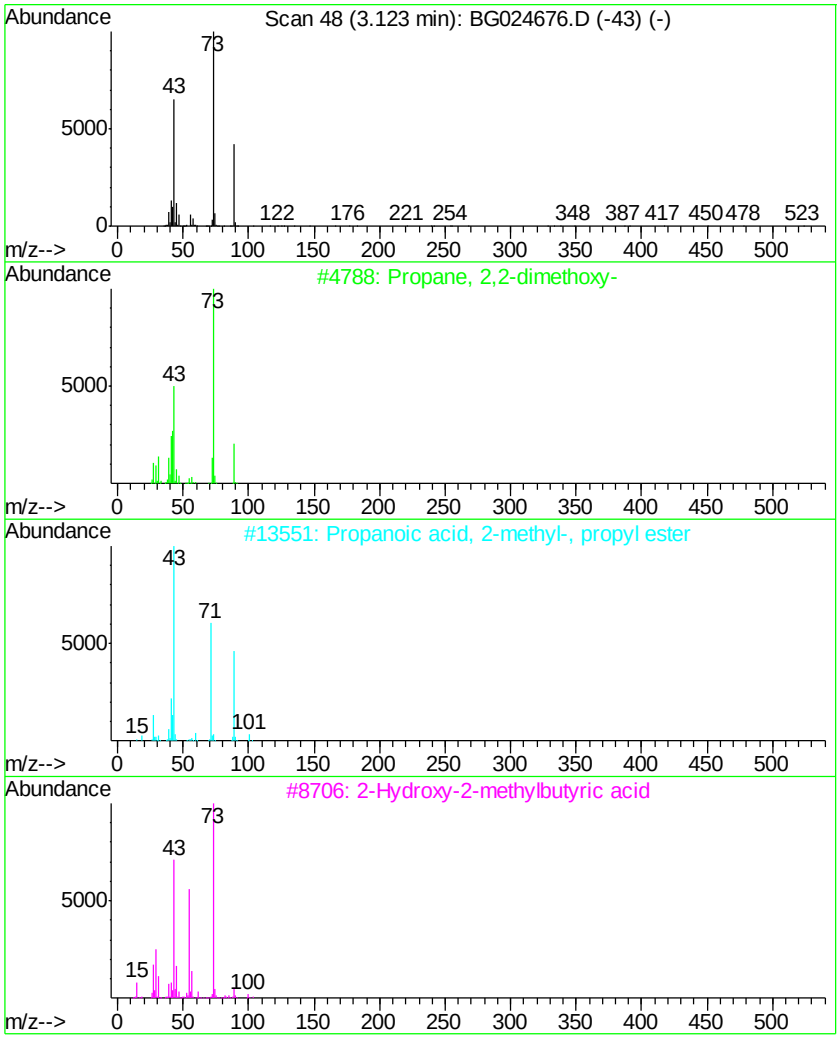
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

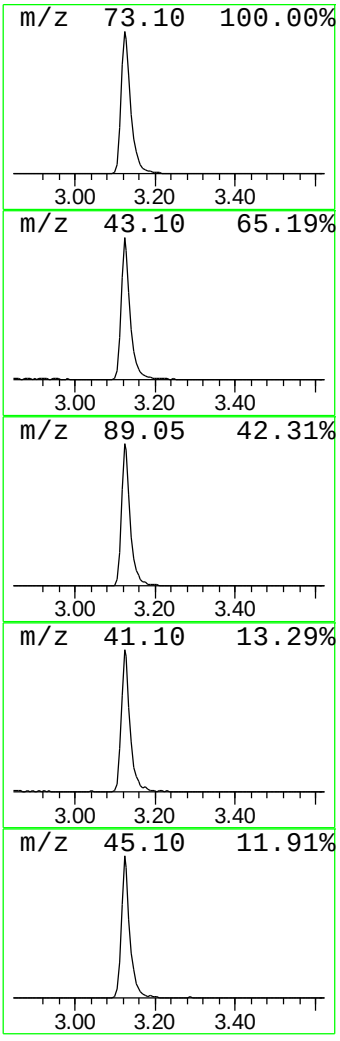
****

Peak Number 1 unknown3.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	295.19 ng	9166170	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	40
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	38
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





Library Search Compound Report

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Data File : BG024676.D
Acq On : 4 Nov 2016 10:48
Operator : UM/SJ
Sample : H5509-09
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-95-1.0-1.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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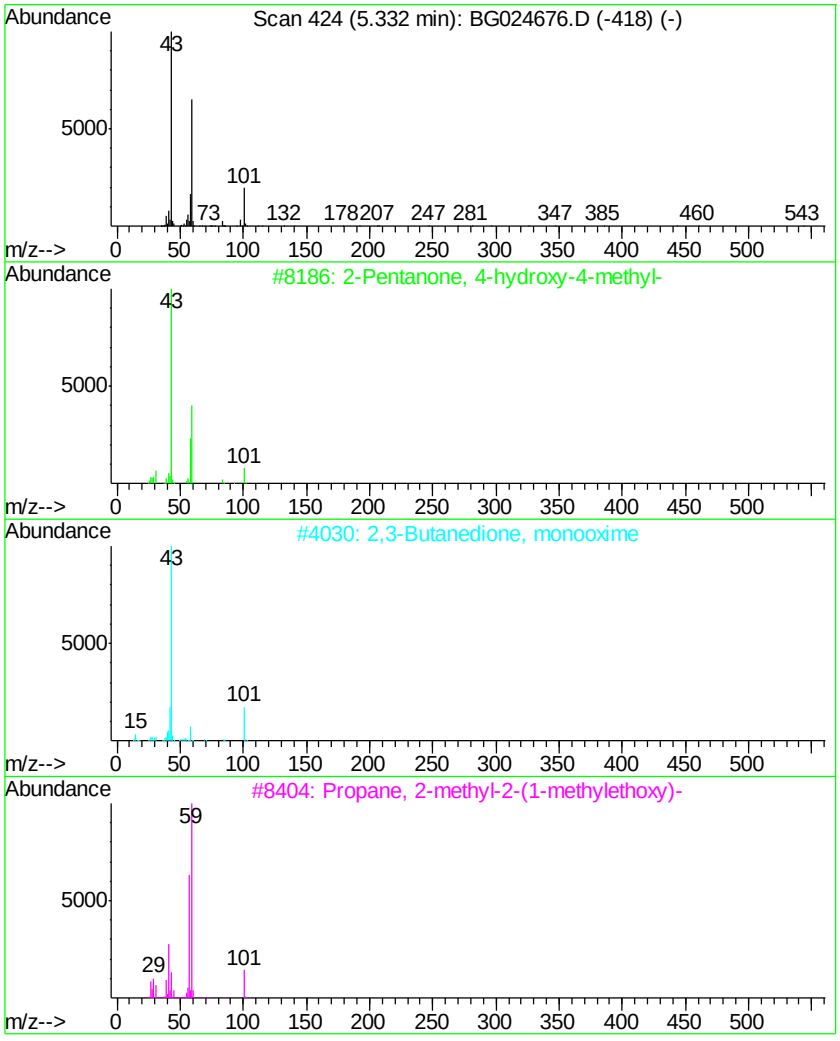
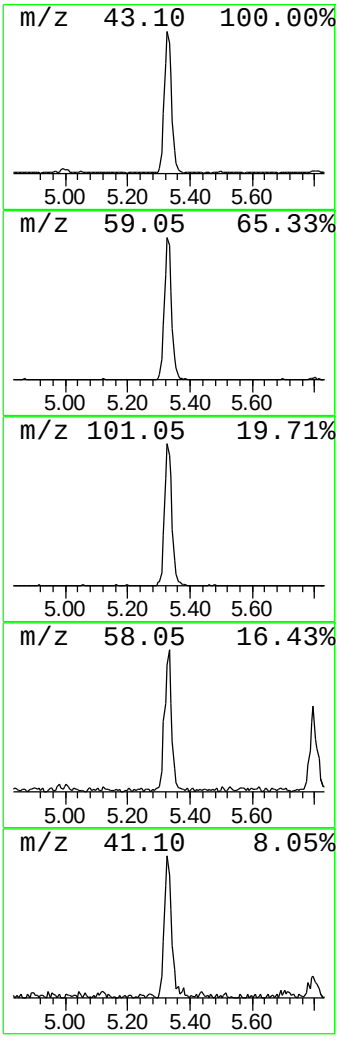
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	24.61 ng	764324	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024676.D
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Operator : UM/SJ
Sample : H5509-09
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-95-1.0-1.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

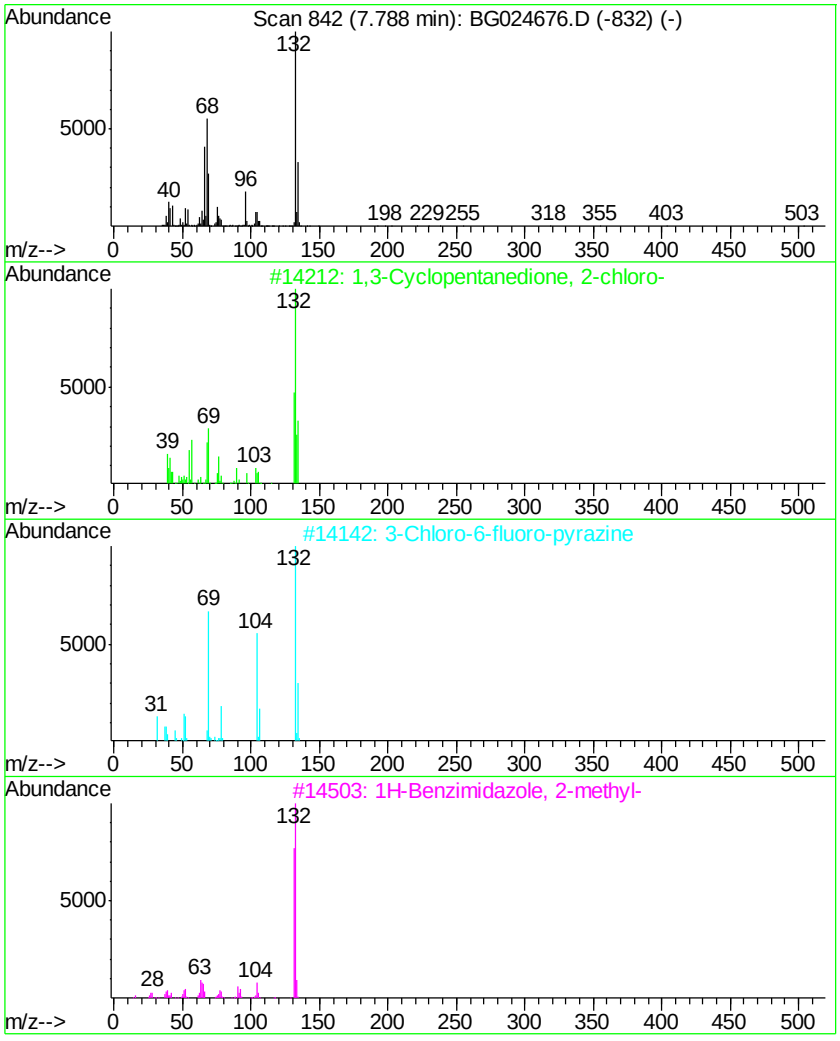
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

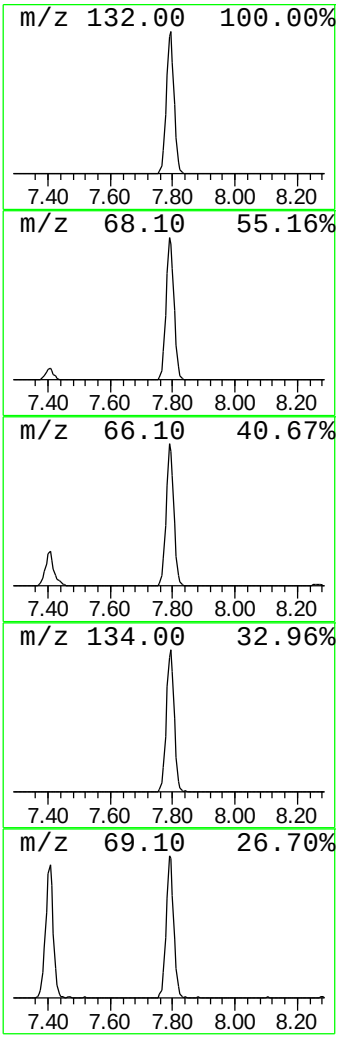
****

Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	123.78 ng	3843590	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024676.D
Acq On : 4 Nov 2016 10:48
Operator : UM/SJ
Sample : H5509-09
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-95-1.0-1.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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TIC Library : C:\DATABASE\NIST11.L
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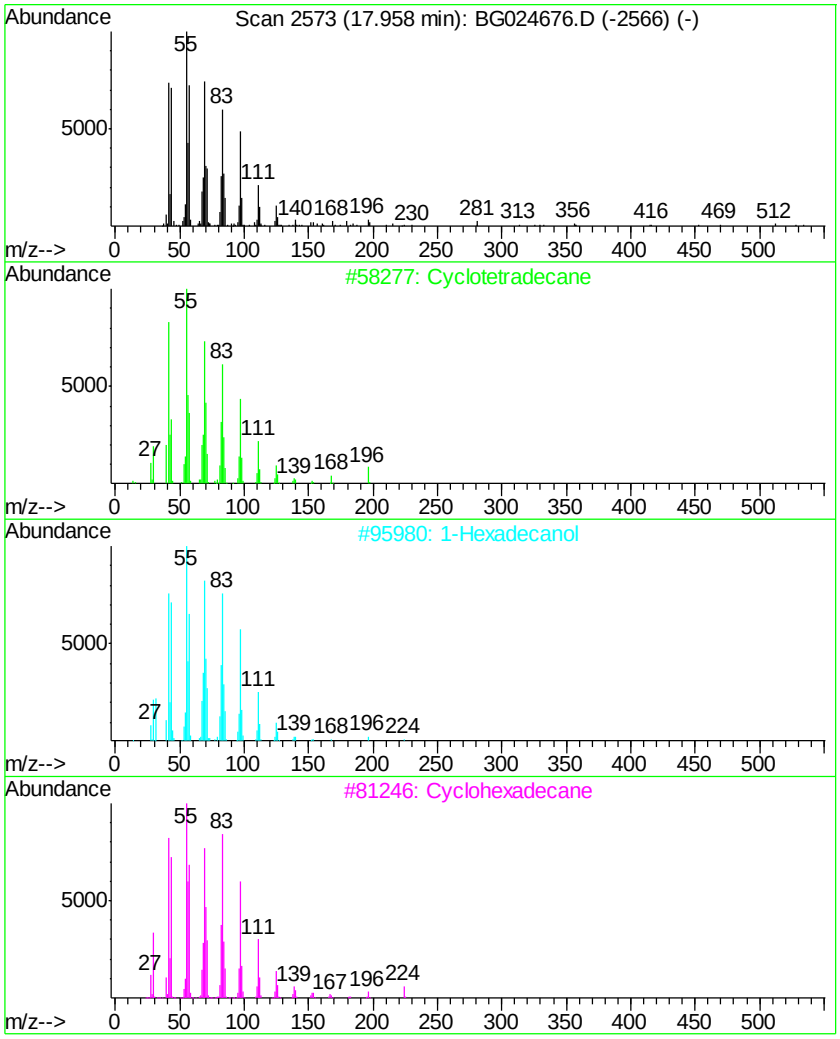
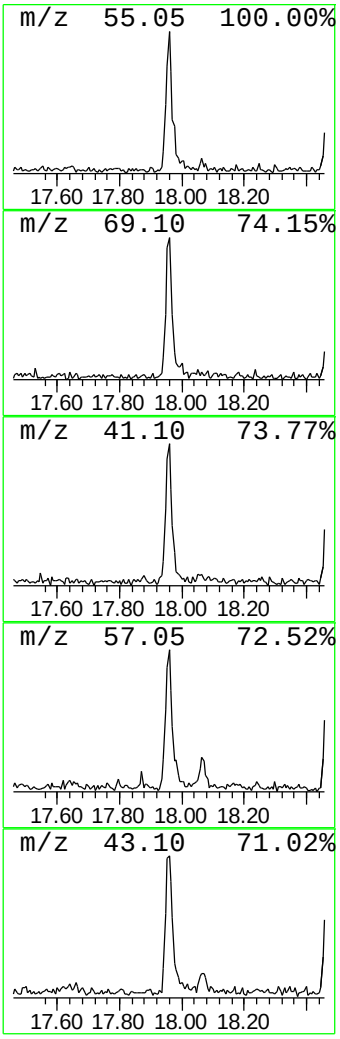
****

Peak Number 5 Cyclotetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	4.85 ng	420879	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	96
2	1-Hexadecanol	242	C16H34O	036653-82-4	94
3	Cyclohexadecane	224	C16H32	000295-65-8	91
4	Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	91
5	Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	91





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
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Acq On : 4 Nov 2016 10:48
Operator : UM/SJ
Sample : H5509-09
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-95-1.0-1.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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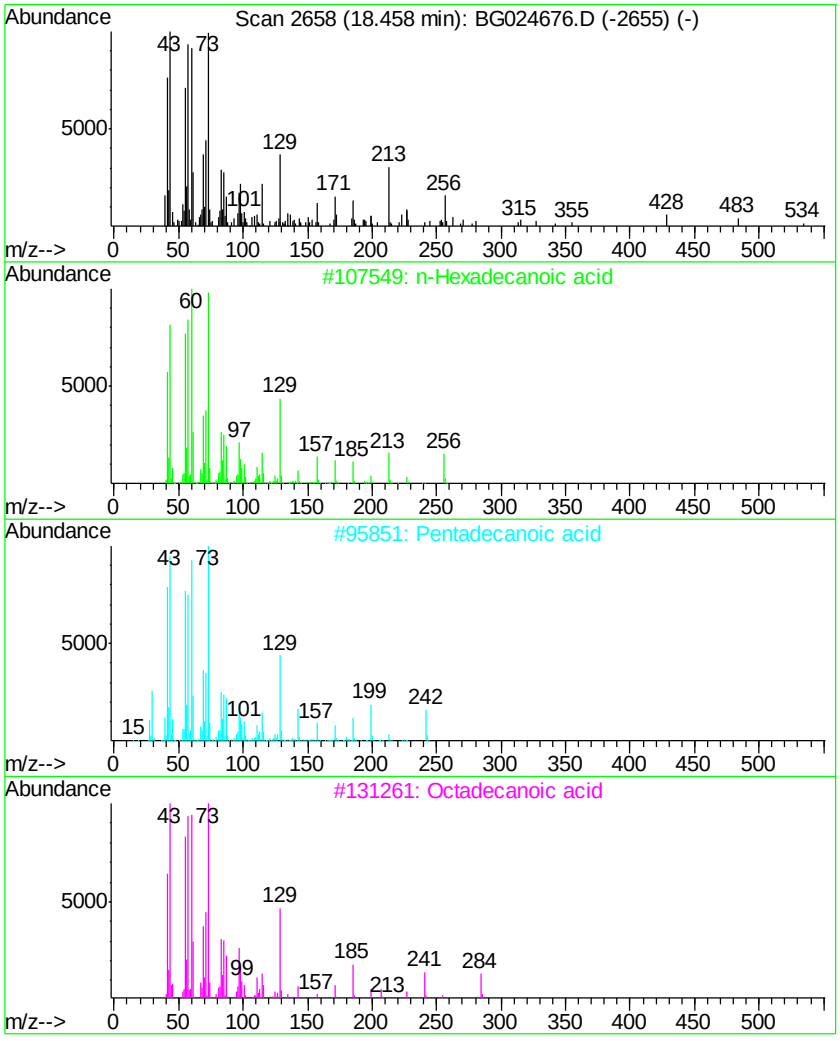
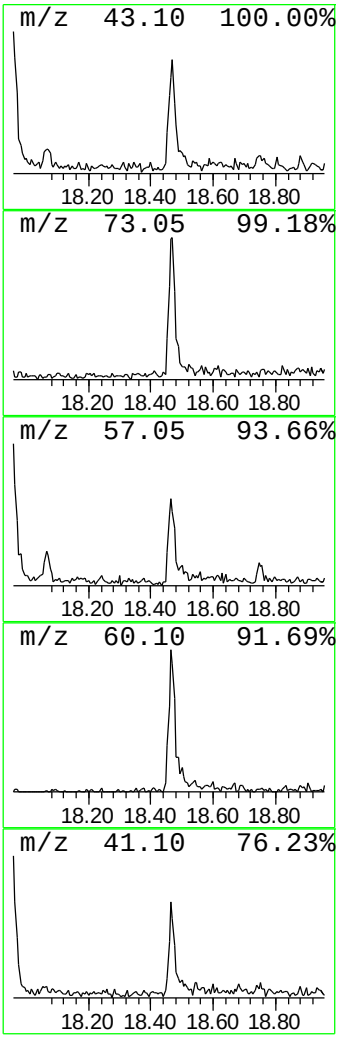
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.46	3.80 ng	329780	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Octadecanoic acid	284	C18H36O2	000057-11-4	78
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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Instrument : BNA_G
ClientSampleId : SB-95-1.0-1.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

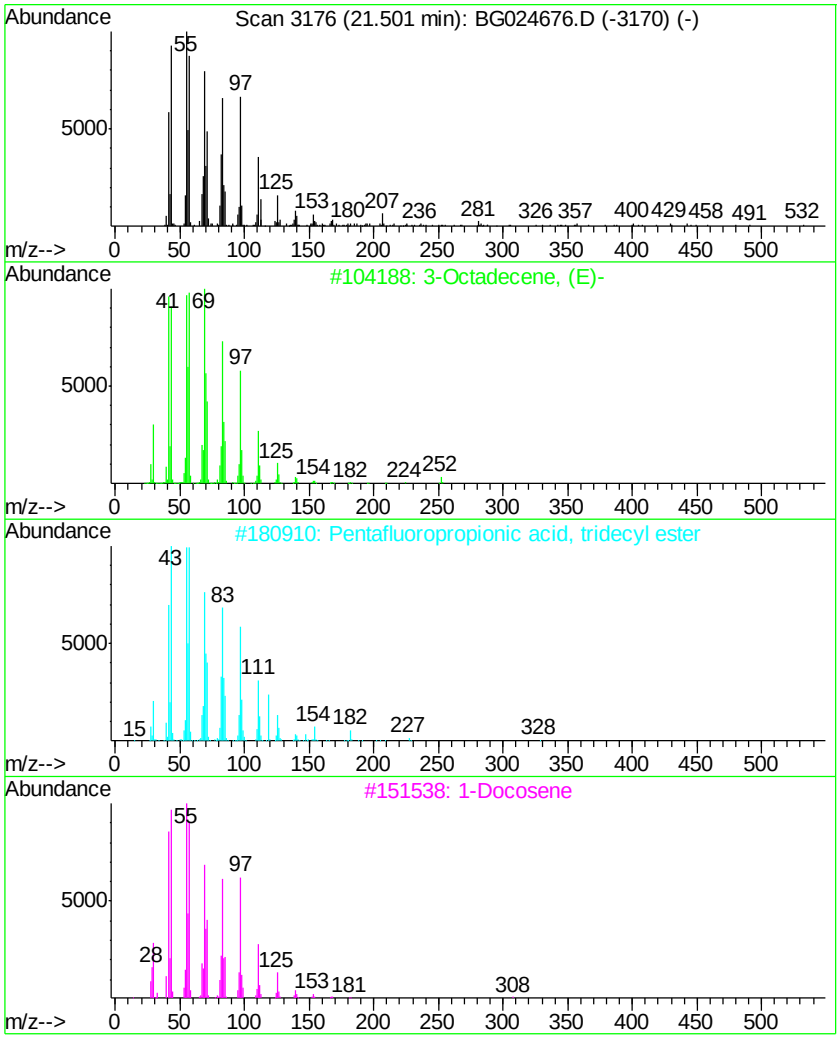
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

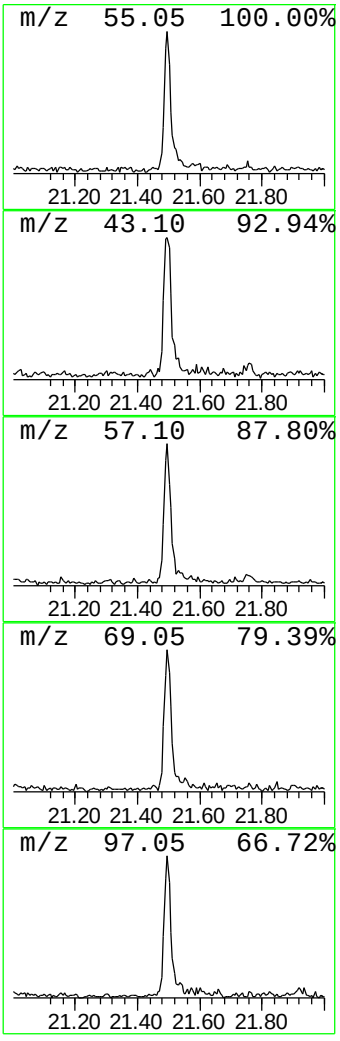
****

Peak Number 7 3-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	5.50 ng	666544	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	93
2	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	90
3	1-Docosene	308	C22H44	001599-67-3	90
4	Cyclooctacosane	392	C28H56	000297-24-5	90
5	Behenic alcohol	326	C22H46O	000661-19-8	90





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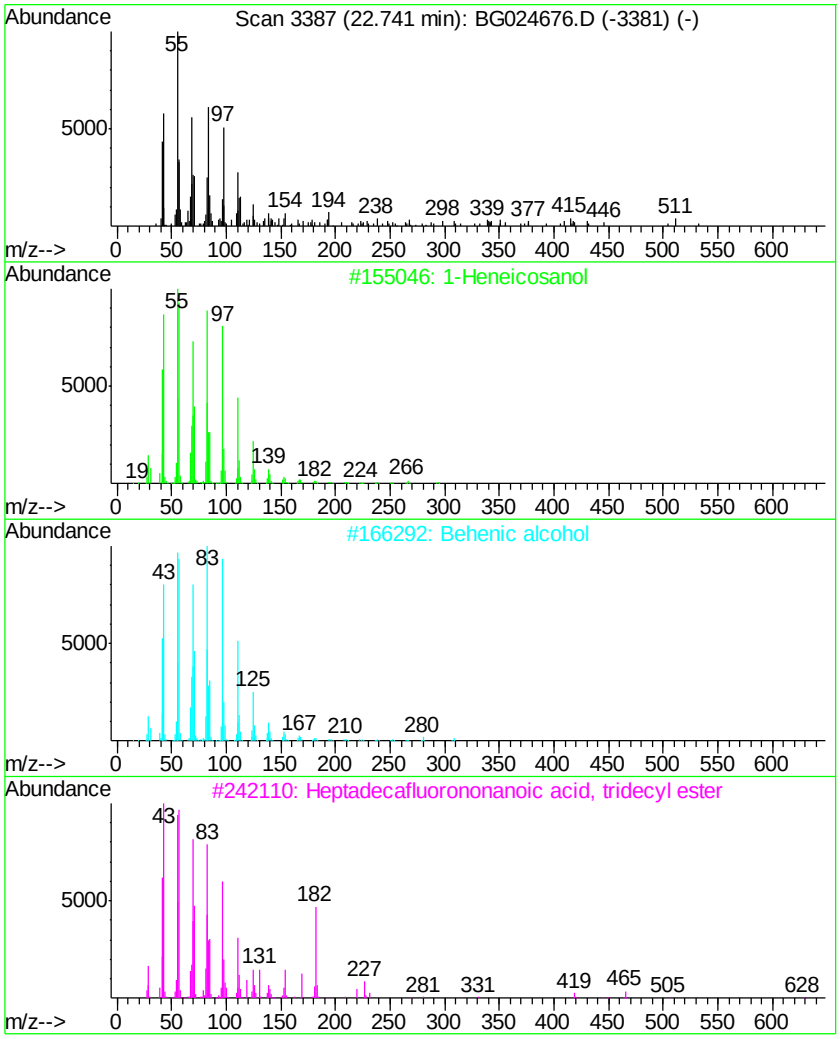
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

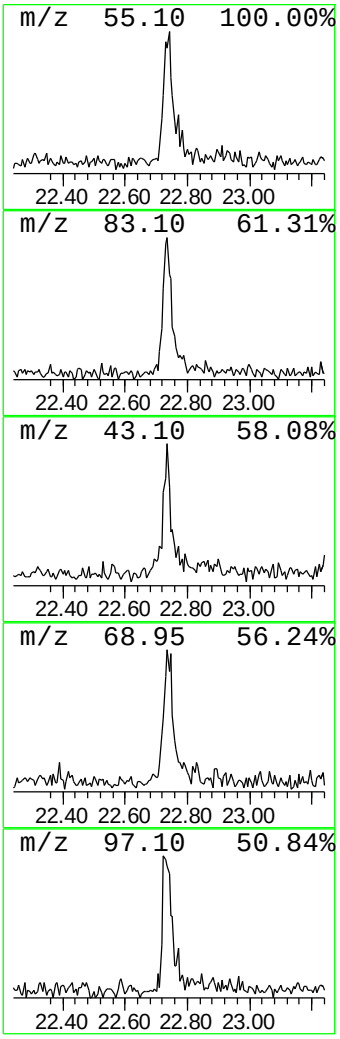
****

Peak Number 8 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.74	2.47 ng	299648	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Heptadecafluorononanoic acid, tr...	646	C22H27F17O2	1000356-02-9	76
4	1-Heptadecene	238	C17H34	006765-39-5	74
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.12	3.12	295.2	ng	9166170	1	8.27	621033	20.0
2-Pentanone, 4-hy...	5.33	24.6	ng	764324	1	8.27	621033	20.0
unknown7.79	7.79	123.8	ng	3843590	1	8.27	621033	20.0
Cyclotetradecane	17.96	4.8	ng	420879	4	17.62	1736870	20.0
n-Hexadecanoic acid	18.46	3.8	ng	329780	4	17.62	1736870	20.0
3-Octadecene, (E)-	21.50	5.5	ng	666544	5	21.92	2425530	20.0
1-Heneicosanol	22.74	2.5	ng	299648	5	21.92	2425530	20.0