LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

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-BG012015.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	2.826	19	23	27	rBV4	84931	126190	1.33%	0.261%
2	2.902	32	36	40	rBV	149801	163080	1.72%	0.338%
3	4.812	355	361	367	rBV	223805	302107	3.19%	0.626%
4	5.282	432	441	449	rBV	1948006	2854849	30.14%	5.913%
5	6.868	702	711	721	rBV	2141078	3461450	36.55%	7.170%
6	7.221	762	771	780	rBV	2041443	3162202	33.39%	6.550%
7	7.685	842	850	857	rBV	407411	650881	6.87%	1.348%
8	8.002	897	904	910	rVB	1464261	2274287	24.01%	4.711%
9	8.843	1038	1047	1053	rBV	1299124	2140882	22.60%	4.435%
10	10.470	1317	1324	1330	rBV	545269	899545	9.50%	1.863%
11	12.944	1739	1745	1755	rBV	3352015	5039901	53.21%	10.439%
12	13.790	1883	1889	1896	rBV	112648	163960	1.73%	0.340%
13	14.330	1975	1981	1988	rBV2	950613	1407617	14.86%	2.916%
14	15.693	2209	2213	2219	rVB	158555	213338	2.25%	0.442%
15	15.823	2229	2235	2246	rBV	3600387	5071739	53.55%	10.505%
16	17.080	2443	2449	2453	rBV	1356734	1888934	19.94%	3.913%
17	17.121	2453	2456	2461	rVB	127592	168761	1.78%	0.350%
18	17.985	2599	2603	2612	rBV	555677	911930	9.63%	1.889%
19	19.148	2794	2801	2812	rBV2	637604	1254710	13.25%	2.599%
20	19.272	2818	2822	2828	rBV5	301721	487119	5.14%	1.009%
21	19.507	2858	2862	2867	rVB	225209	276020	2.91%	0.572%
22	19.712	2892	2897	2904	rBV	7459471	9470877	100.00%	19.617%
23	20.981	3110	3113	3120	rBV6	265507	422640	4.46%	0.875%
24	21.181	3144	3147	3150	rVB3	131786	126869	1.34%	0.263%
25	21.269	3156	3162	3166	rBV	2030736	2765558	29.20%	5.728%
26	22.321	3337	3341	3343	rVB5	148519	187946	1.98%	0.389%
27	23.525	3540	3546	3556	rVB2	1208250	2384440	25.18%	4.939%

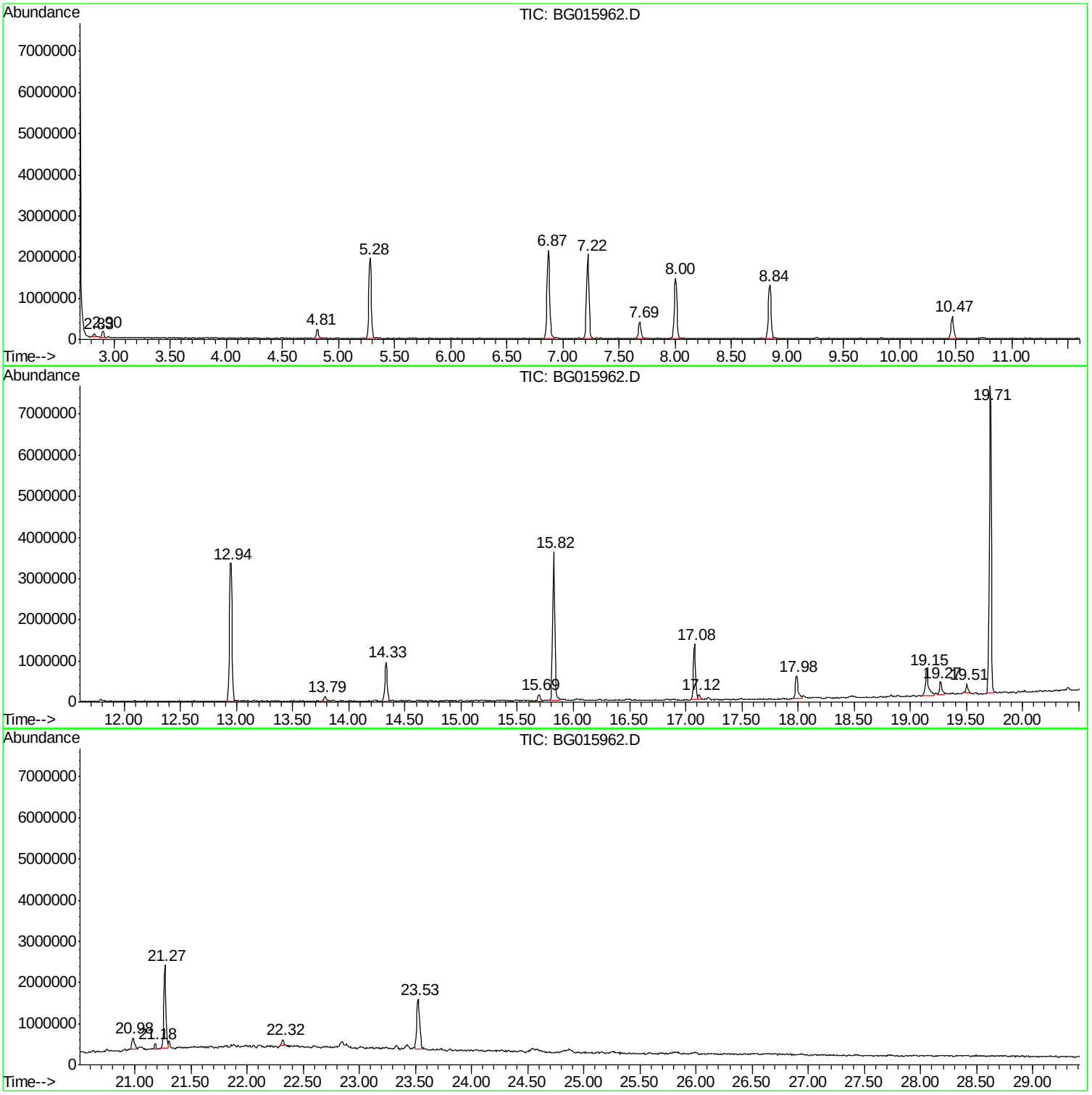
Sum of corrected areas: 48277832

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.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\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

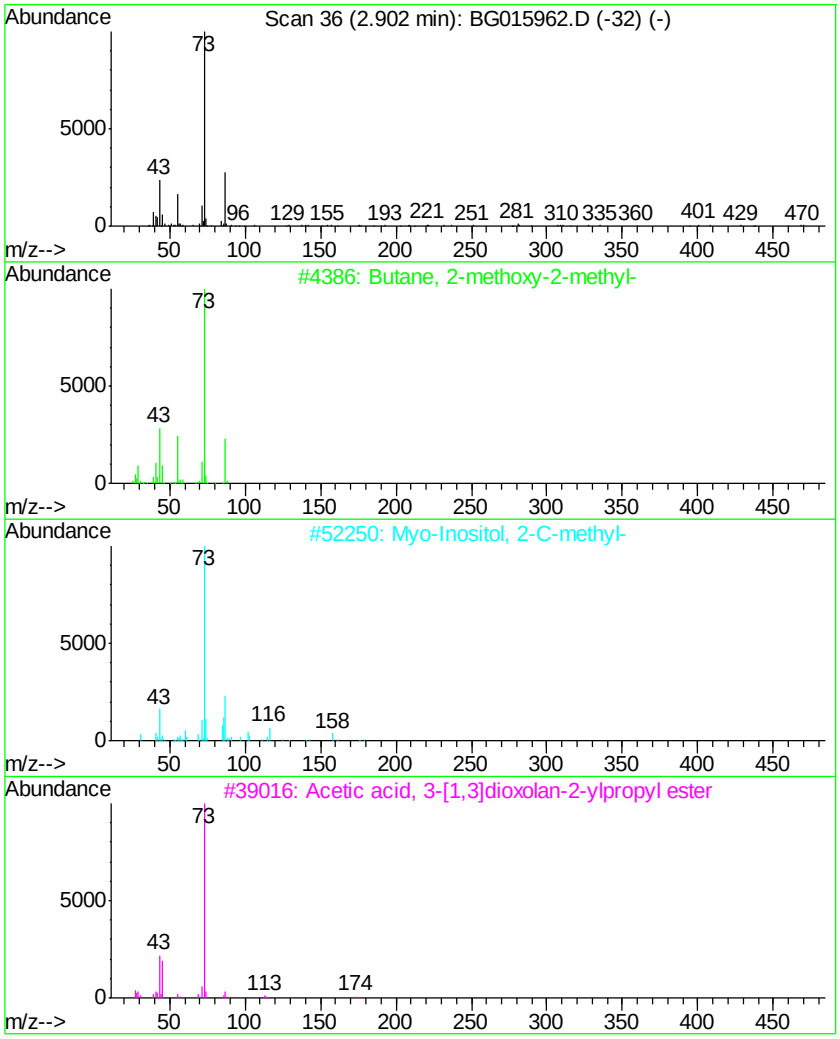
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

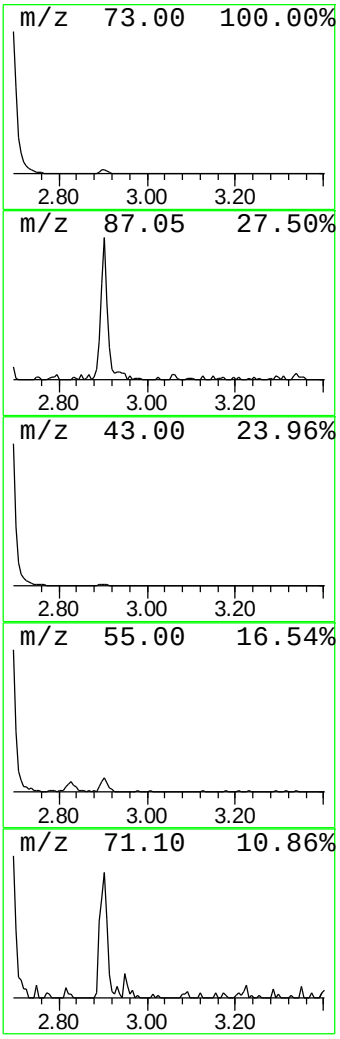
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	5.01 ng	163080	1,4-Dichlorobenzene-d4	7.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	33
3	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	10
4	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9
5	.alpha.-D-Mannofuranoside, 1-O-h...	278	C13H26O6	111570-47-9	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

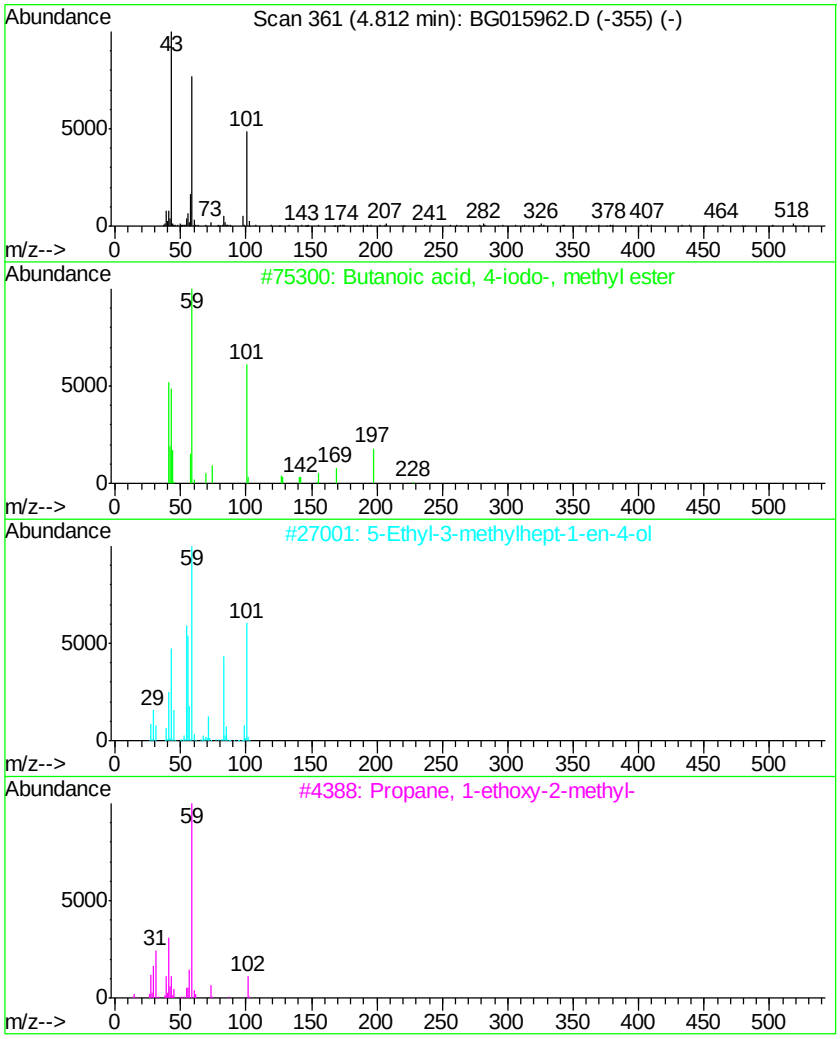
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

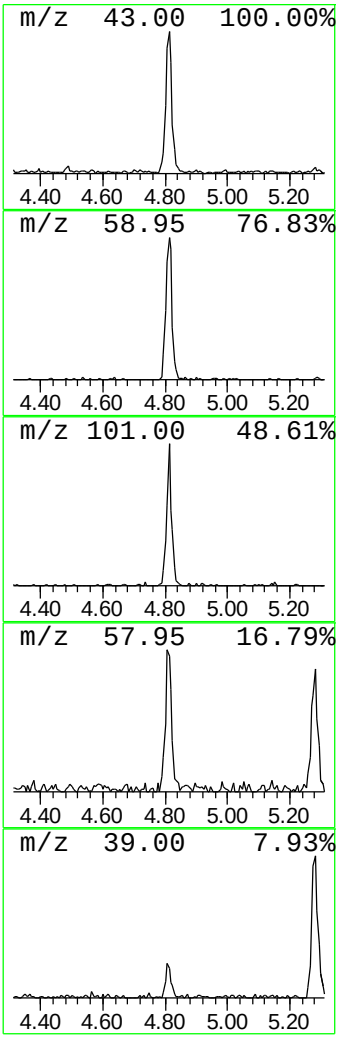
****

Peak Number 3 unknown4.81 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	9.28 ng	302107	1,4-Dichlorobenzene-d4	7.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-iodo-, methyl e...	228	C5H9IO2	014273-85-9	40
2	5-Ethyl-3-methylhept-1-en-4-ol	156	C10H20O	286424-80-4	40
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	37
4	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	37
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

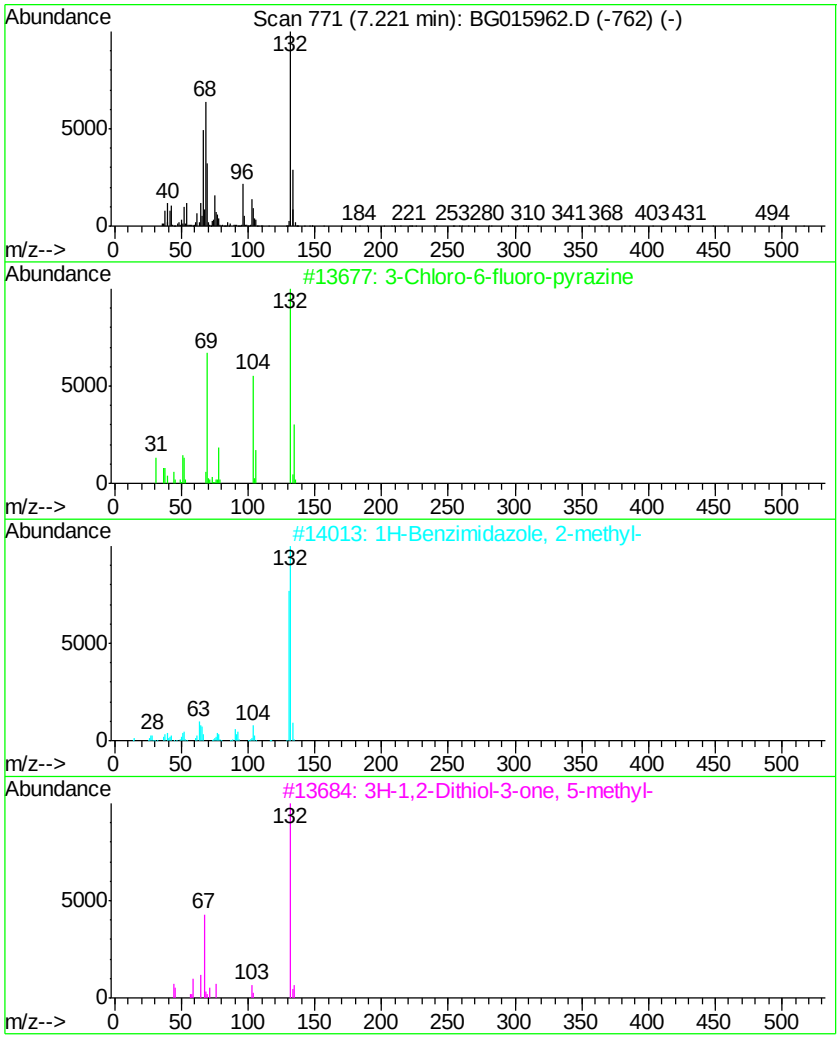
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

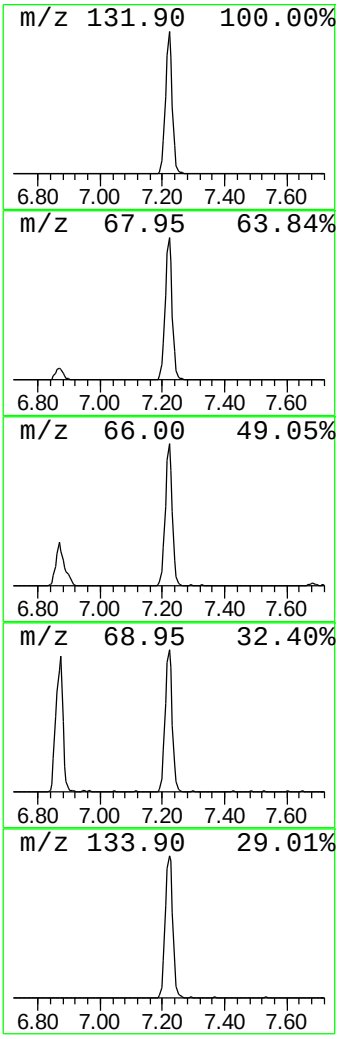
****

Peak Number 4 unknown7.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	97.17 ng	3162200	1,4-Dichlorobenzene-d4	7.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	10
5	1H-Indenol	132	C9H8O	056631-57-3	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

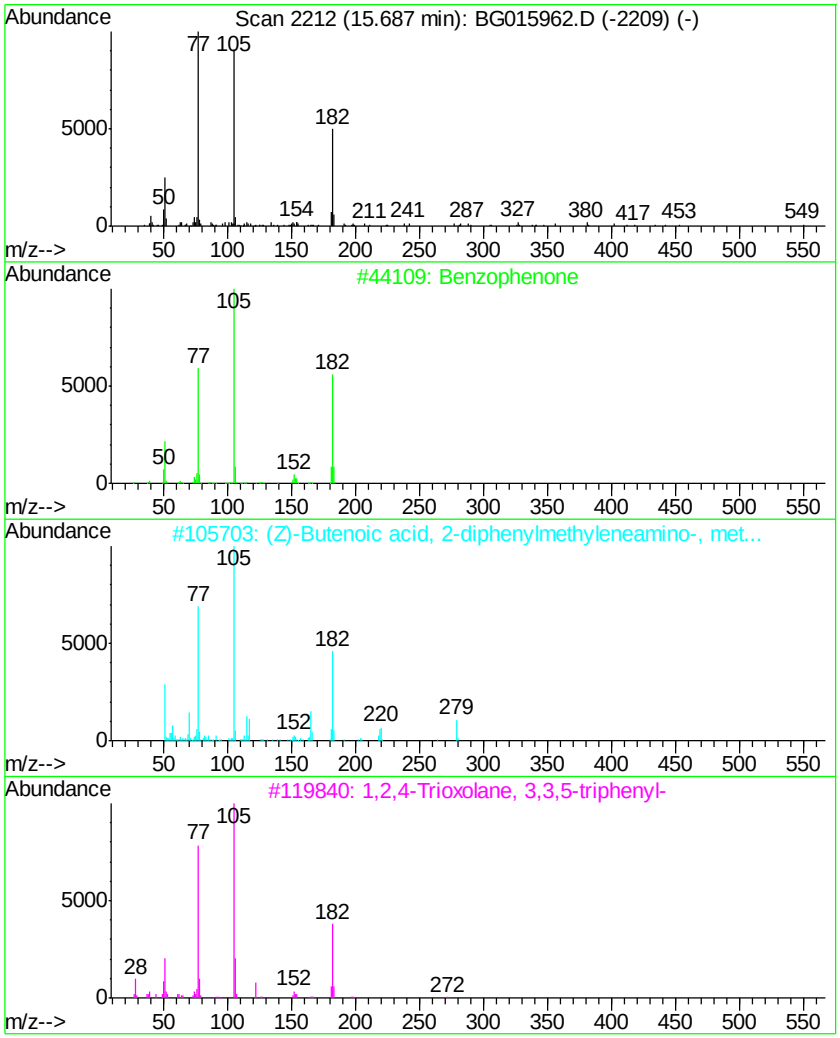
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

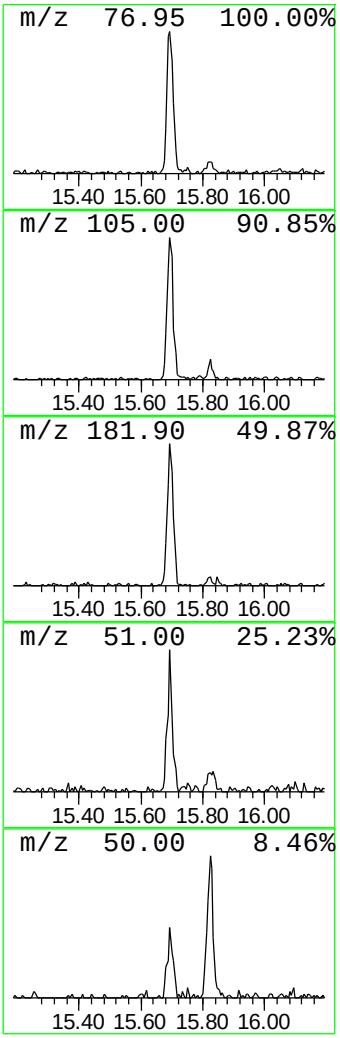
****

Peak Number 6 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	3.03 ng	213338	Acenaphthene-d10	14.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	86
2	(Z)-Butenoic acid, 2-diphenylmet...	279	C18H17NO2	120238-59-7	64
3	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
4	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	50
5	Azobenzene	182	C12H10N2	000103-33-3	45





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

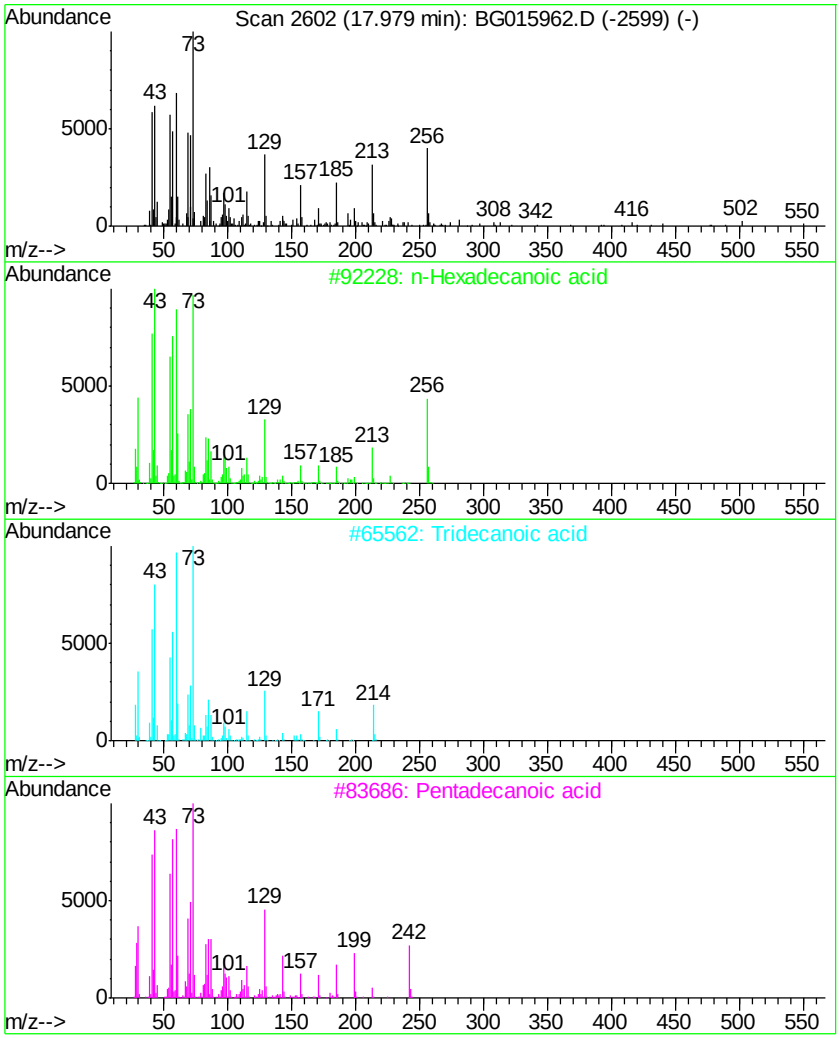
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

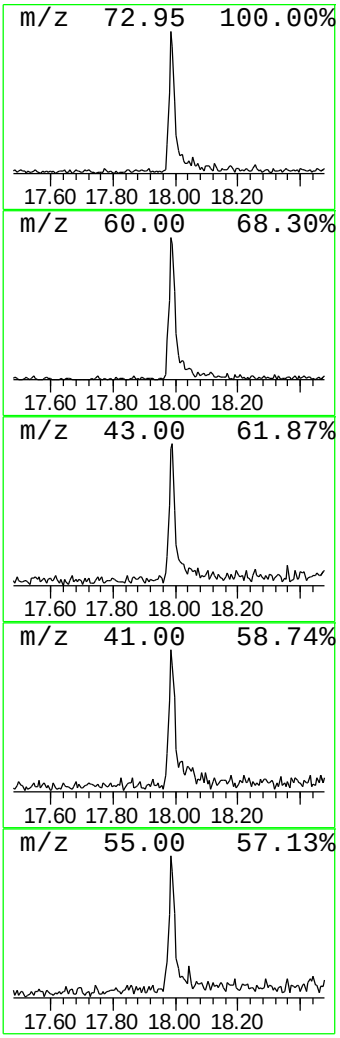
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	9.66 ng	911930	Phenanthrene-d10	17.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	Undecanoic acid	186	C11H22O2	000112-37-8	40
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	38





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

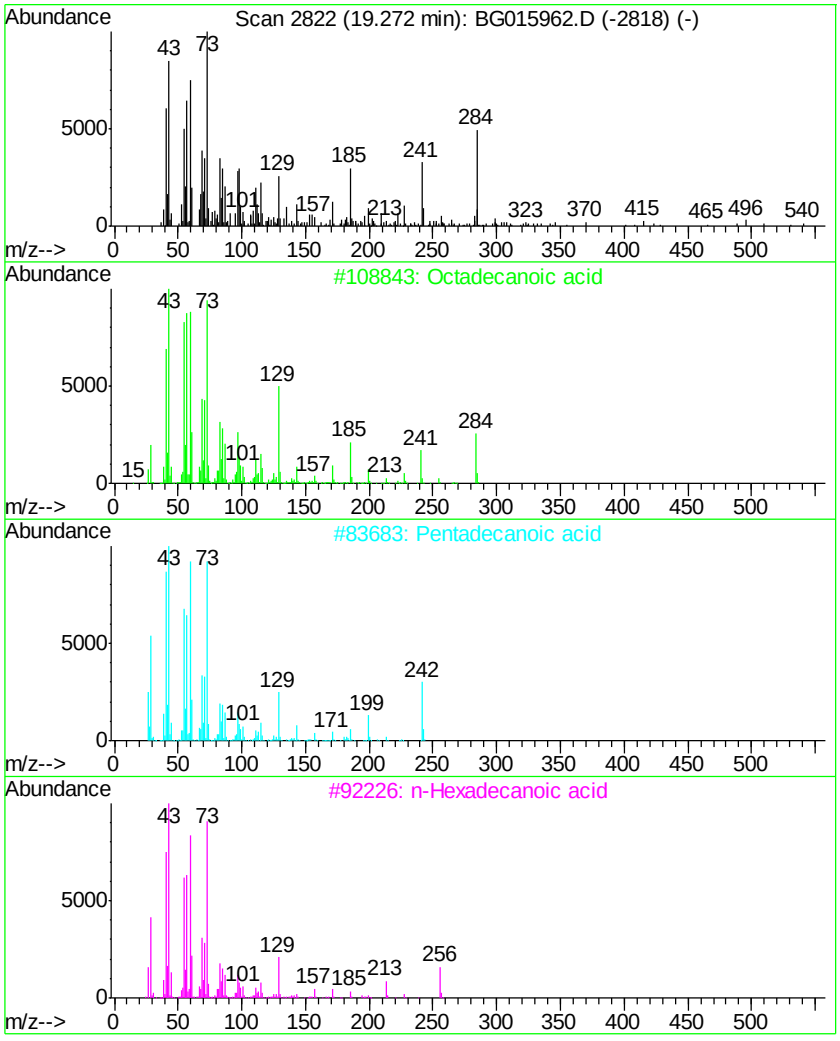
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

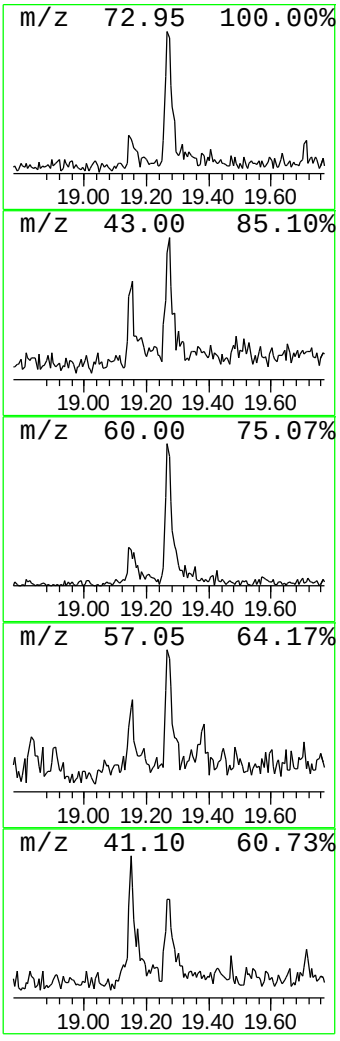
****

Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	3.52 ng	487119	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	42
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

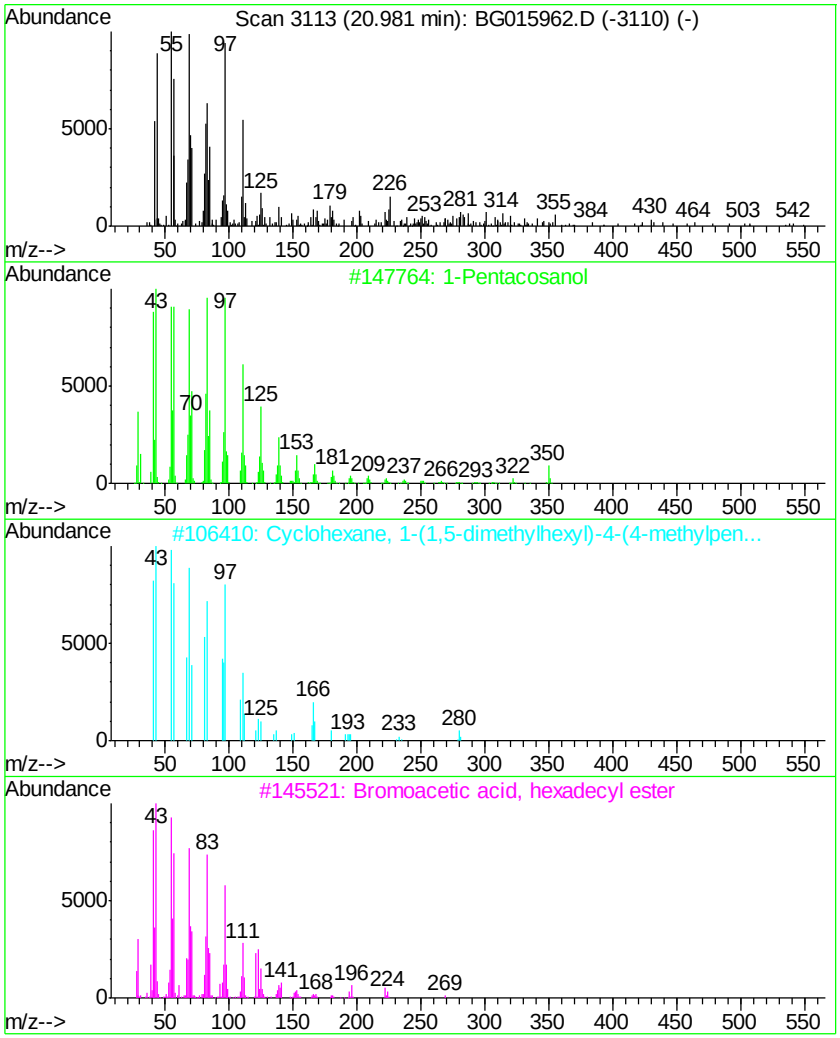
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

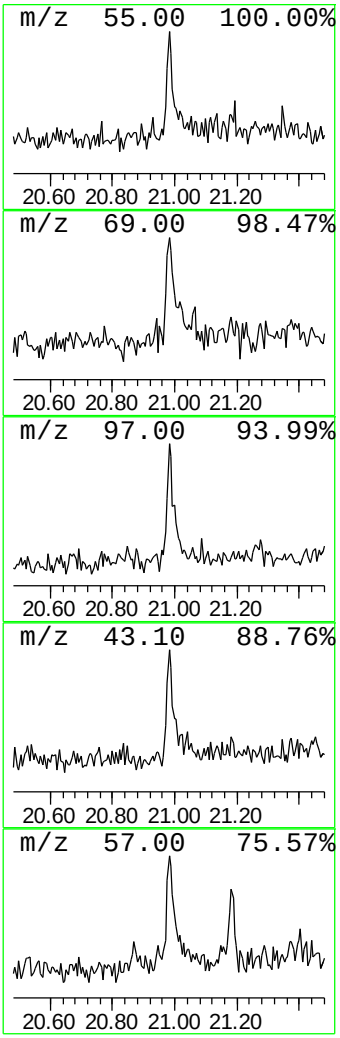
****

Peak Number 9 1-Pentacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.98	3.06 ng	422640	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentacosanol	368	C25H52O	026040-98-2	90
2	Cyclohexane, 1-(1,5-dimethylhexy...	280	C20H40	056009-20-2	64
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	58
4	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	52
5	Hexadecane, 1-(ethenyloxy)-	268	C18H36O	000822-28-6	51





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015962.D
Acq On : 28 Jan 2015 1:27
Operator : TP/IZ
Sample : G1159-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73(14-16)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.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
Butane, 2-methoxy...	2.90	5.0	ng	163080	1	7.68	650881	20.0
unknown4.81	4.81	9.3	ng	302107	1	7.68	650881	20.0
unknown7.22	7.22	97.2	ng	3162200	1	7.68	650881	20.0
Benzophenone	15.69	3.0	ng	213338	3	14.33	1407620	20.0
n-Hexadecanoic acid	17.98	9.7	ng	911930	4	17.08	1888930	20.0
Octadecanoic acid	19.27	3.5	ng	487119	5	21.27	2765560	20.0
1-Pentacosanol	20.98	3.1	ng	422640	5	21.27	2765560	20.0