LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018644.D
Acq On : 11 Sep 2015 18:09
Operator : UM/IZ
Sample : G3612-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-22

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-BG091115.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	2.890	5	9	17	rVB2	36681	45453	1.09%	0.174%
2	2.967	17	22	39	rVB	2036028	2818300	67.53%	10.790%
3	3.102	41	45	53	rBV3	40816	72995	1.75%	0.279%
4	3.184	53	59	70	rVB	656184	936556	22.44%	3.586%
5	5.105	381	386	398	rVB	383842	578267	13.86%	2.214%
6	5.575	459	466	475	rBV	847966	1323721	31.72%	5.068%
7	7.168	729	737	751	rBV	894285	1487639	35.64%	5.696%
8	7.538	792	800	808	rBV	867239	1454215	34.84%	5.568%
9	8.008	873	880	886	rVB	199031	338481	8.11%	1.296%
10	8.331	924	935	942	rBV	640829	1089285	26.10%	4.170%
11	9.165	1069	1077	1088	rVB	508467	907229	21.74%	3.473%
12	10.810	1349	1357	1366	rBV	272110	487615	11.68%	1.867%
13	13.255	1764	1773	1782	rBV	1518659	2284576	54.74%	8.747%
14	14.077	1907	1913	1920	rBV	403524	567306	13.59%	2.172%
15	14.629	2001	2007	2016	rVB2	475718	767128	18.38%	2.937%
16	16.116	2251	2260	2270	rBV	1412651	2110015	50.56%	8.079%
17	16.333	2292	2297	2299	rBV	39419	46733	1.12%	0.179%
18	17.126	2427	2432	2436	rBV	35910	49629	1.19%	0.190%
19	17.373	2467	2474	2482	rBV2	767677	1130244	27.08%	4.327%
20	18.255	2620	2624	2634	rBV	102067	180653	4.33%	0.692%
21	19.982	2912	2918	2924	rBV	3214796	4173564	100.00%	15.979%
22	21.286	3134	3140	3150	rBV3	47472	152515	3.65%	0.584%
23	21.627	3192	3198	3205	rBV	828244	1357626	32.53%	5.198%
24	23.302	3476	3483	3495	rBV2	212171	405992	9.73%	1.554%
25	24.823	3730	3742	3753	rBV	469824	1353135	32.42%	5.181%

Sum of corrected areas: 26118872

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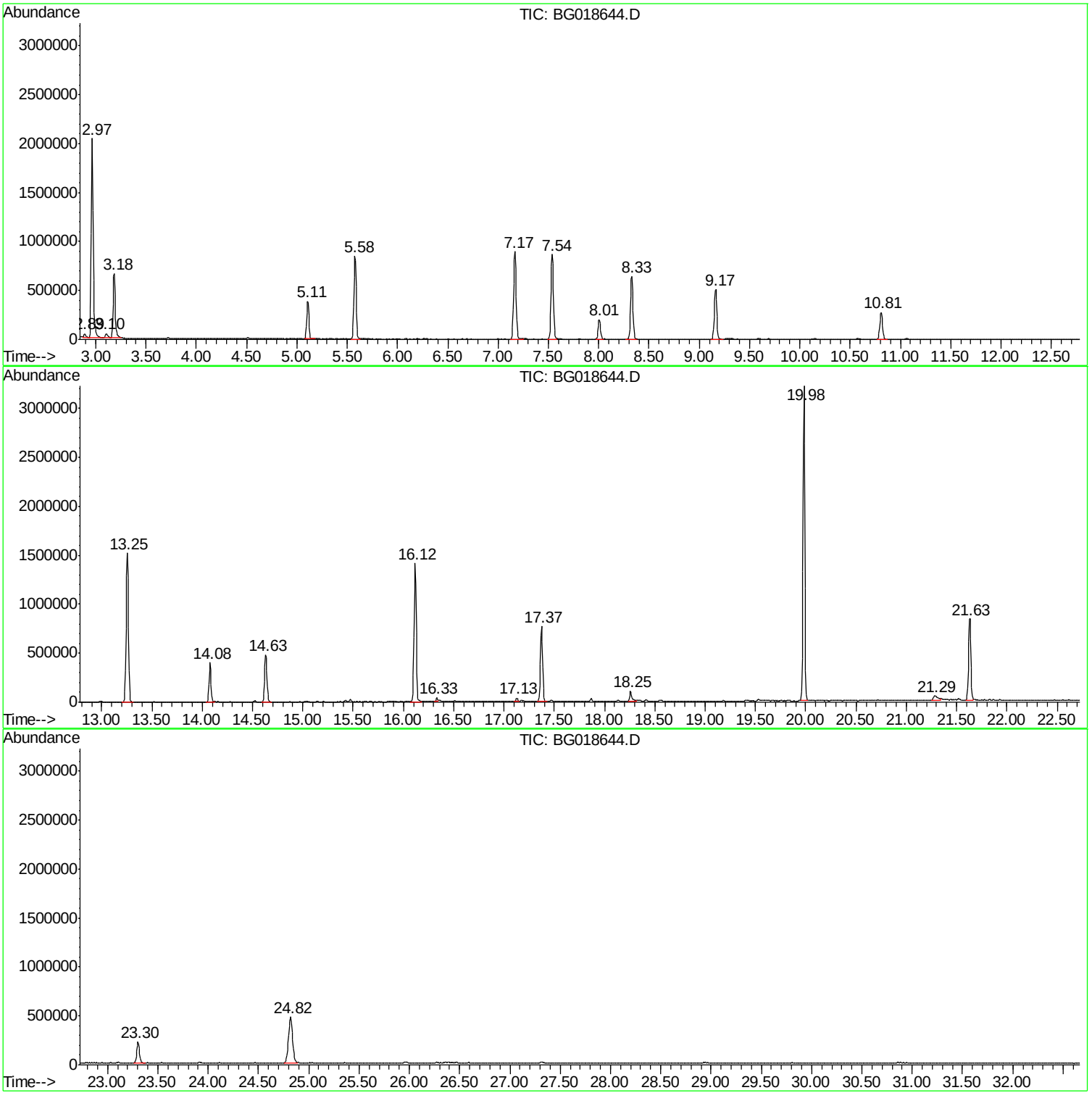
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-22

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.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\BG091215\
Data File : BG018644.D
Acq On : 11 Sep 2015 18:09
Operator : UM/IZ
Sample : G3612-06
Misc :
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Instrument : BNA_G
ClientSampleId : B-22

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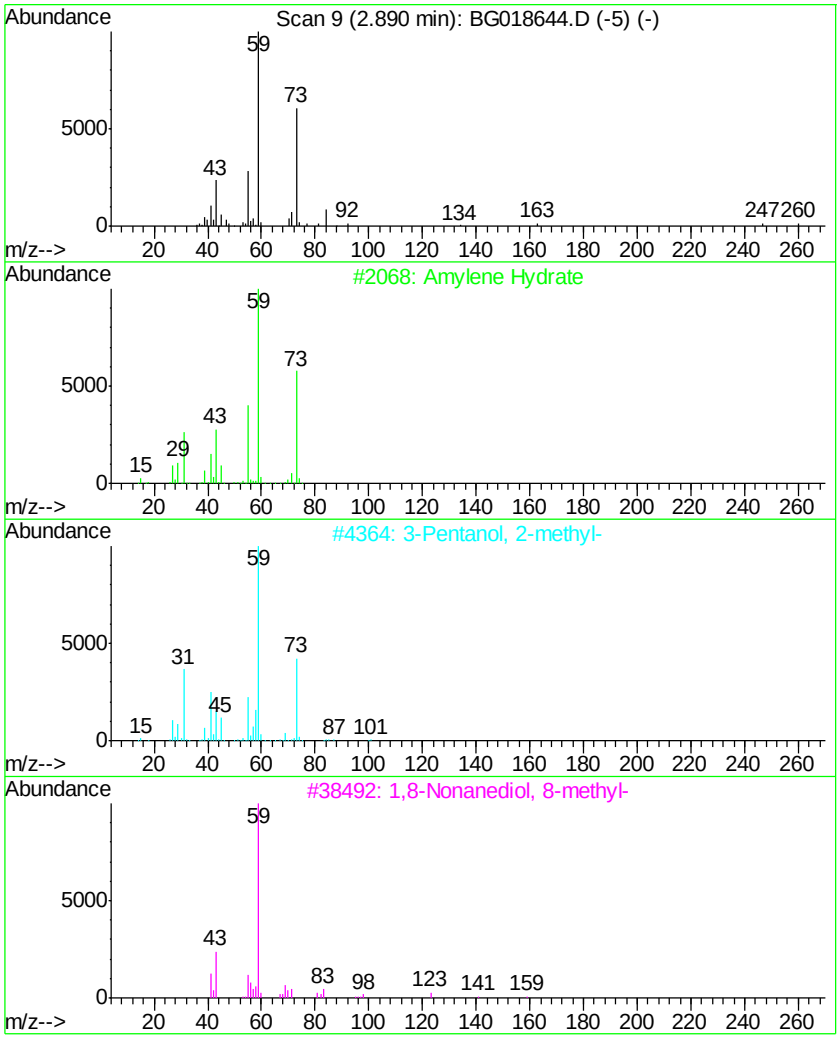
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

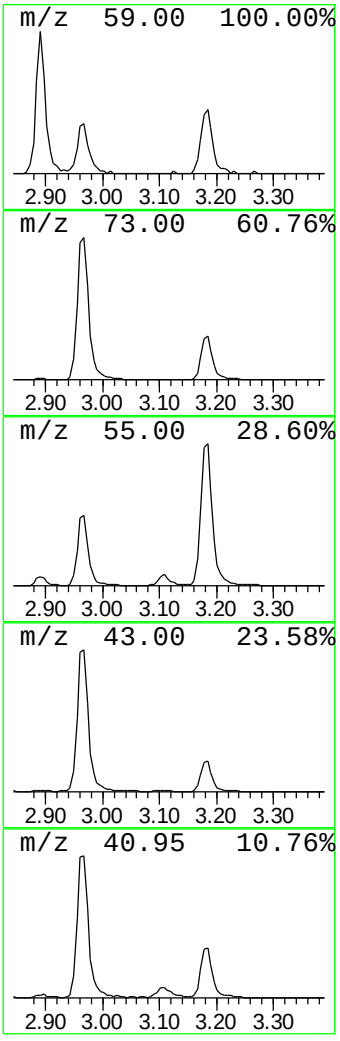
****

Peak Number 1 unknown2.89 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	2.69 ng	45453	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene Hydrate	88	C5H12O	000075-85-4	39
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	36
4	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	9
5	2-Hydroxy-2-methylhept-6-en-3-one	142	C8H14O2	000996-61-2	9





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Operator : UM/IZ
Sample : G3612-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-22

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

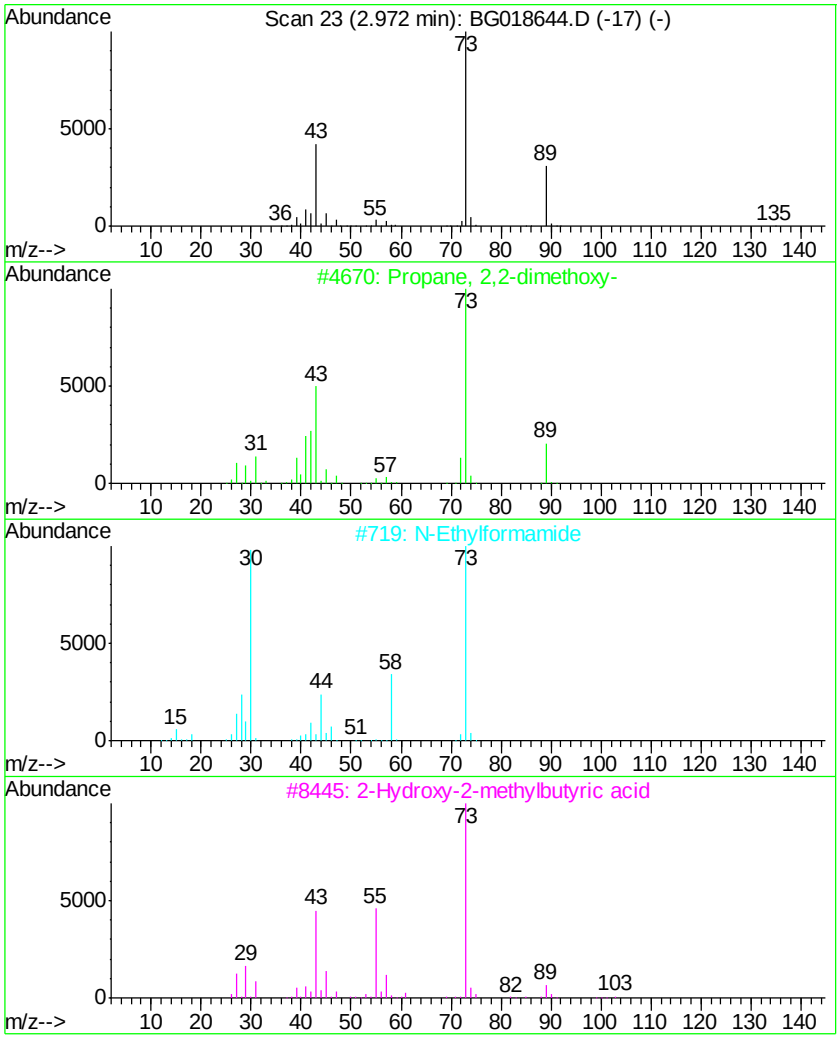
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

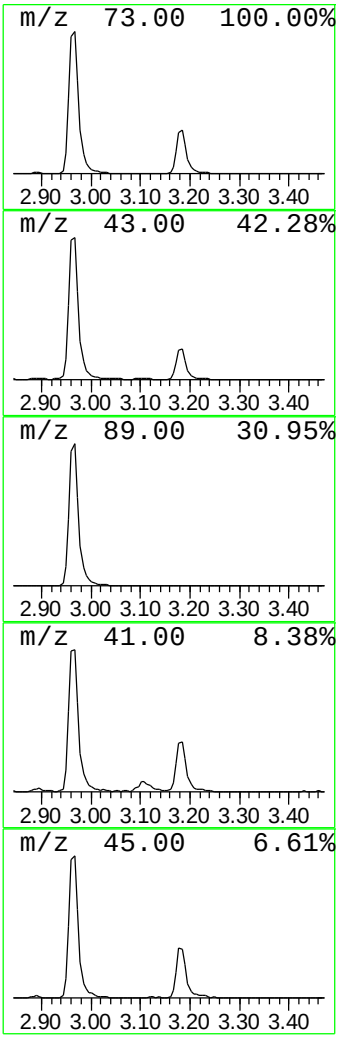
****

Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.97	166.53 ng	2818300	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018644.D
Acq On : 11 Sep 2015 18:09
Operator : UM/IZ
Sample : G3612-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-22

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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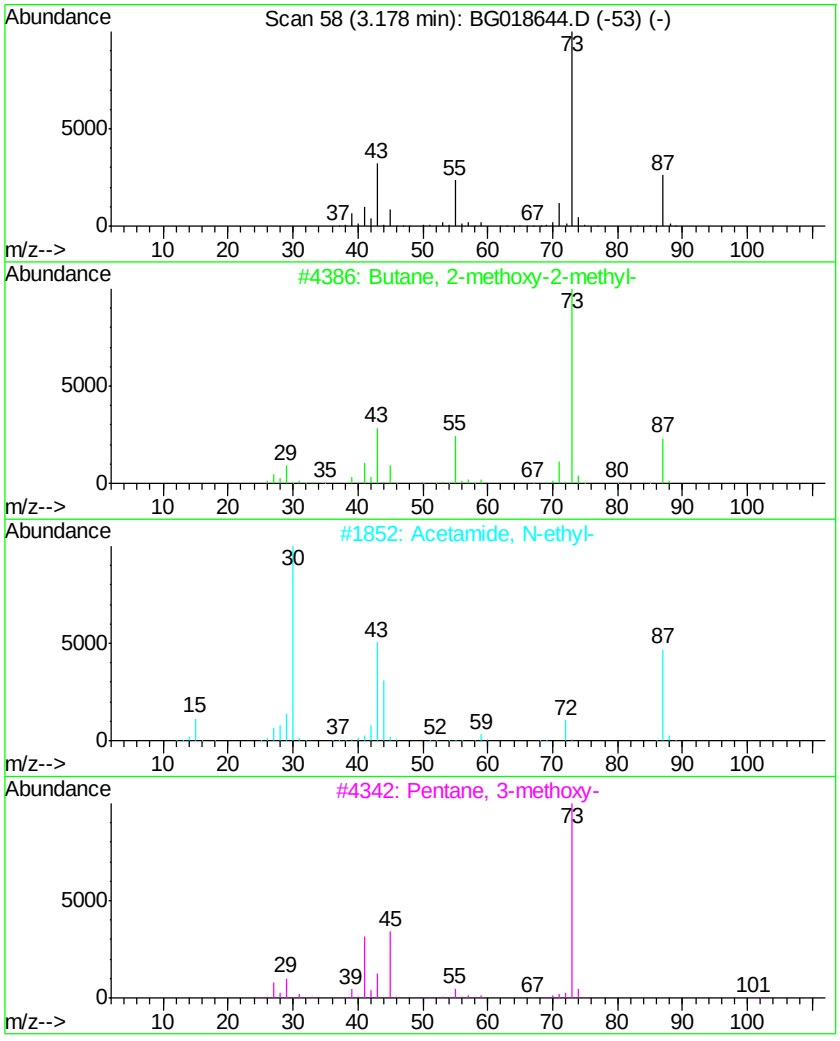
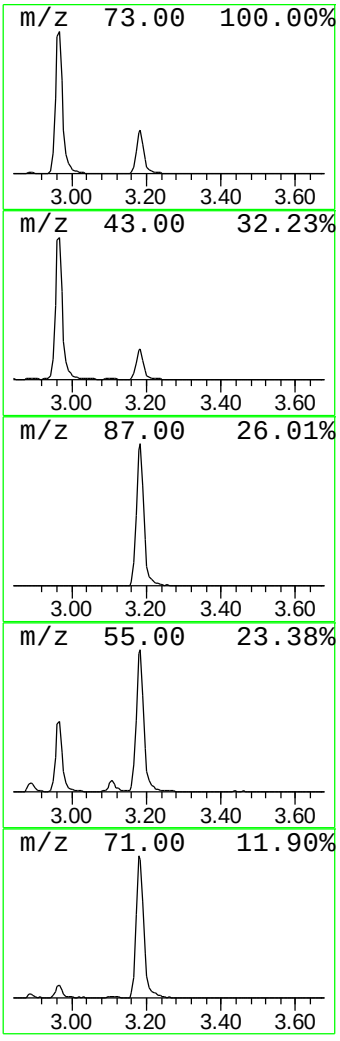
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	55.34 ng	936556	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018644.D
Acq On : 11 Sep 2015 18:09
Operator : UM/IZ
Sample : G3612-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-22

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

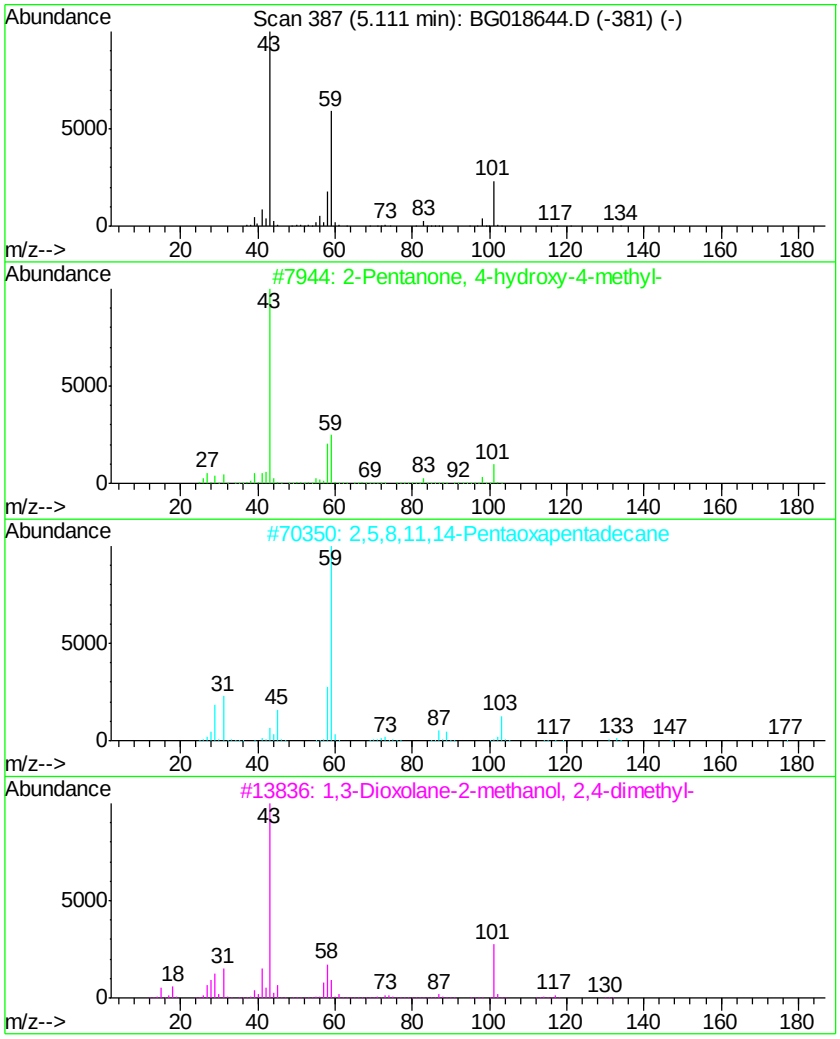
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

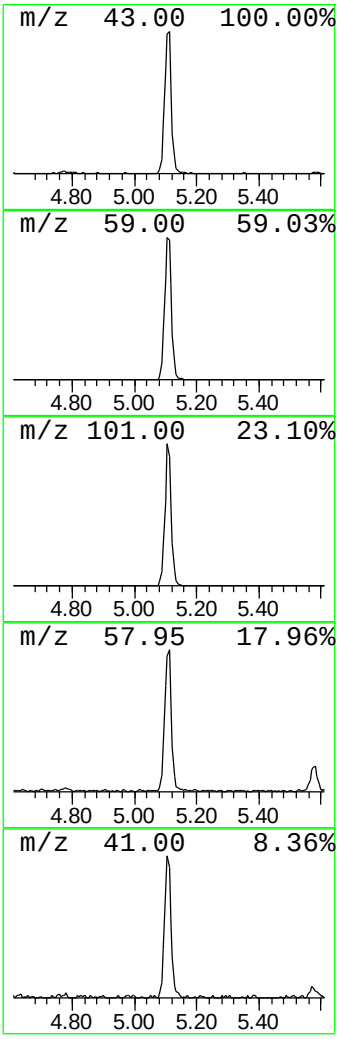
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	34.17 ng	578267	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	25
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Operator : UM/IZ
Sample : G3612-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-22

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
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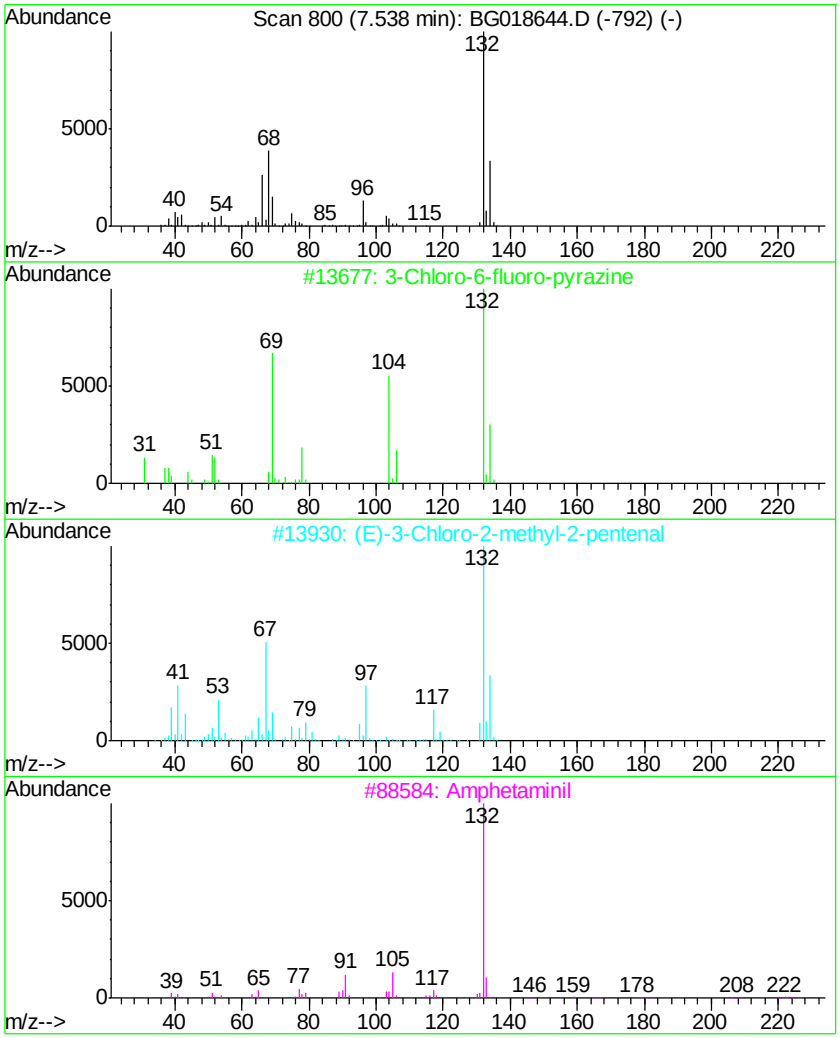
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

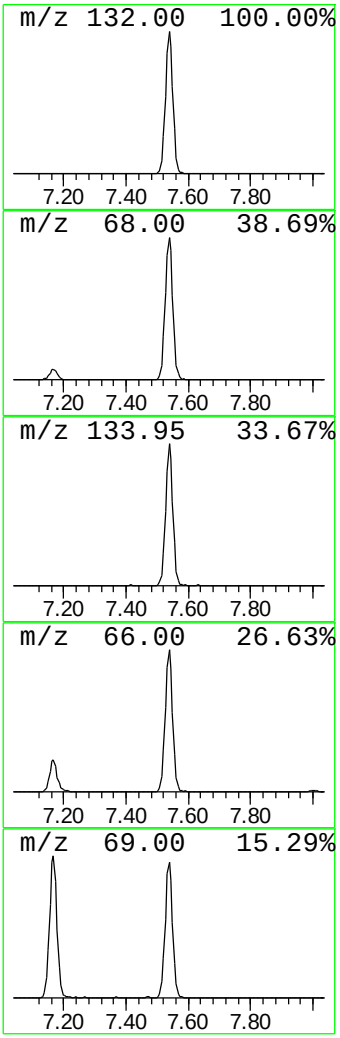
****

Peak Number 6 unknown7.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	85.93 ng	1454220	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Amphetaminil	250	C17H18N2	017590-01-1	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Aminoindole	132	C8H8N2	005192-03-0	10





Library Search Compound Report

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Sample : G3612-06
Misc :
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Instrument : BNA_G
ClientSampleId : B-22

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

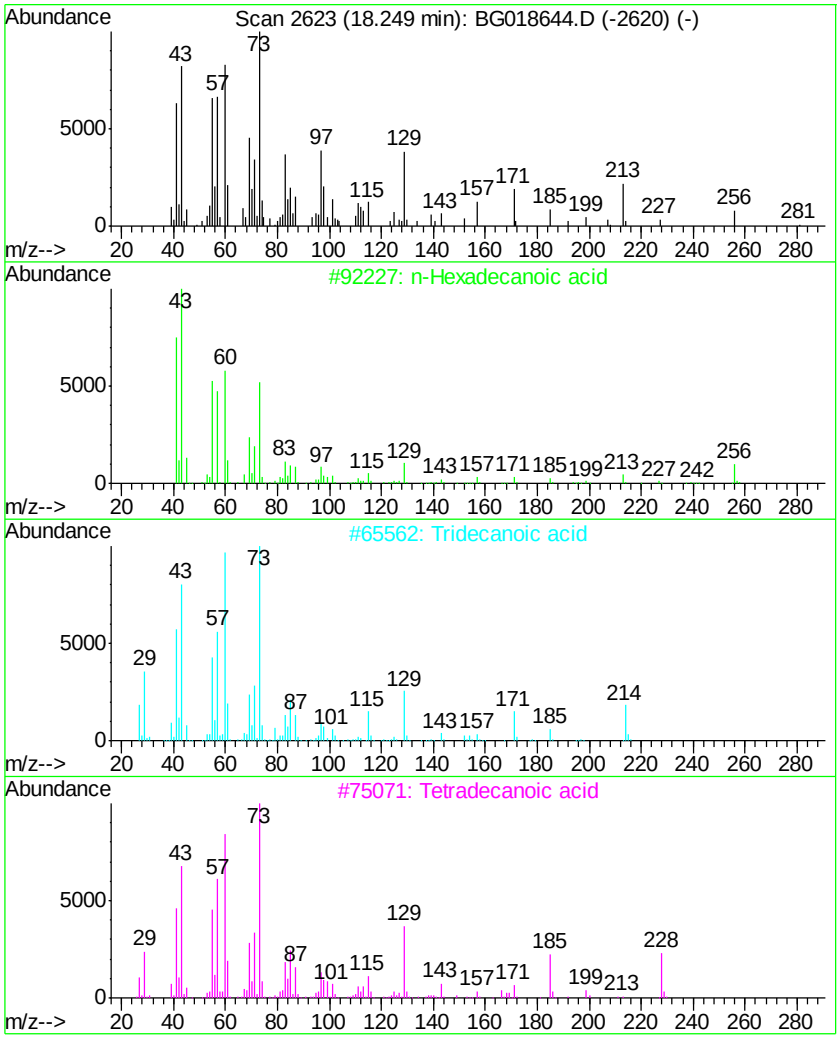
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

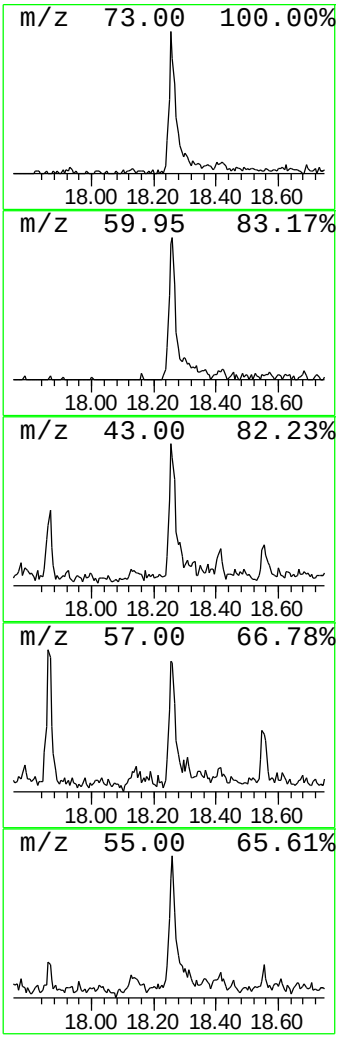
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.25	3.20 ng	180653	Phenanthrene-d10	17.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	3,7-Dimethyl-8-oxo-1,5-dioxa-spi...	256	C13H20O5	1000193-79-8	44
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	43





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Instrument : BNA_G
ClientSampleId : B-22

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

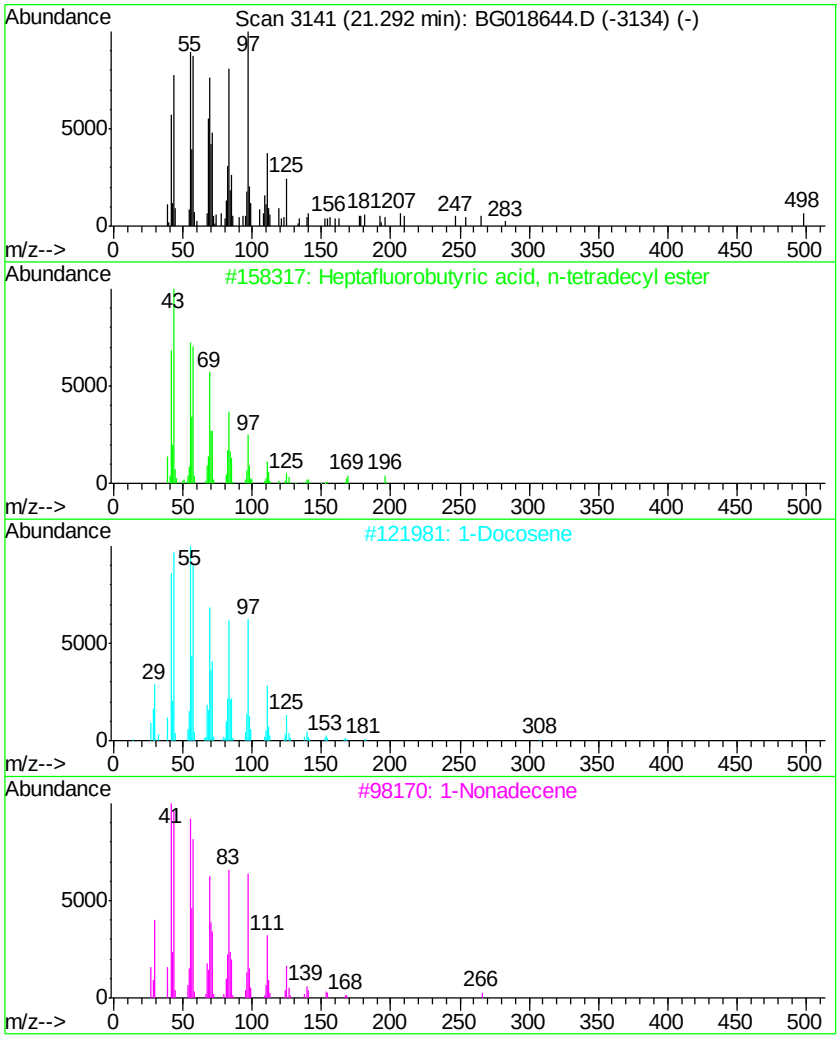
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

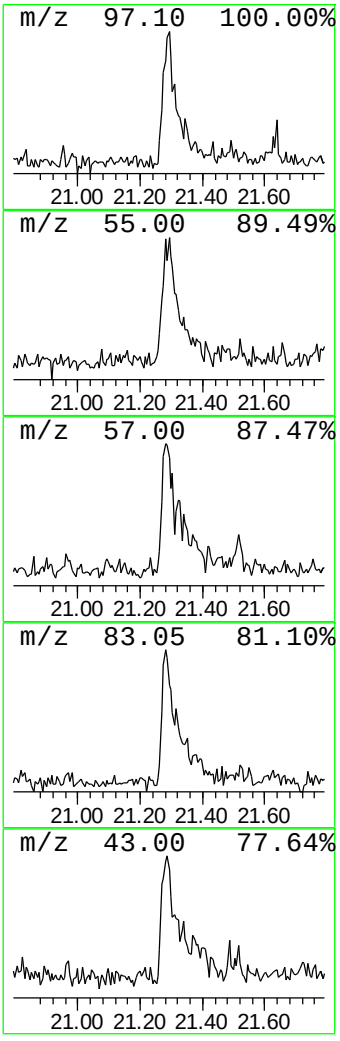
****

Peak Number 9 Heptafluorobutyric acid, n-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	2.25 ng	152515	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
2	1-Docosene	308	C22H44	001599-67-3	87
3	1-Nonadecene	266	C19H38	018435-45-5	87
4	1-Eicosanol	298	C20H42O	000629-96-9	86
5	Cyclotetracosane	336	C24H48	000297-03-0	86





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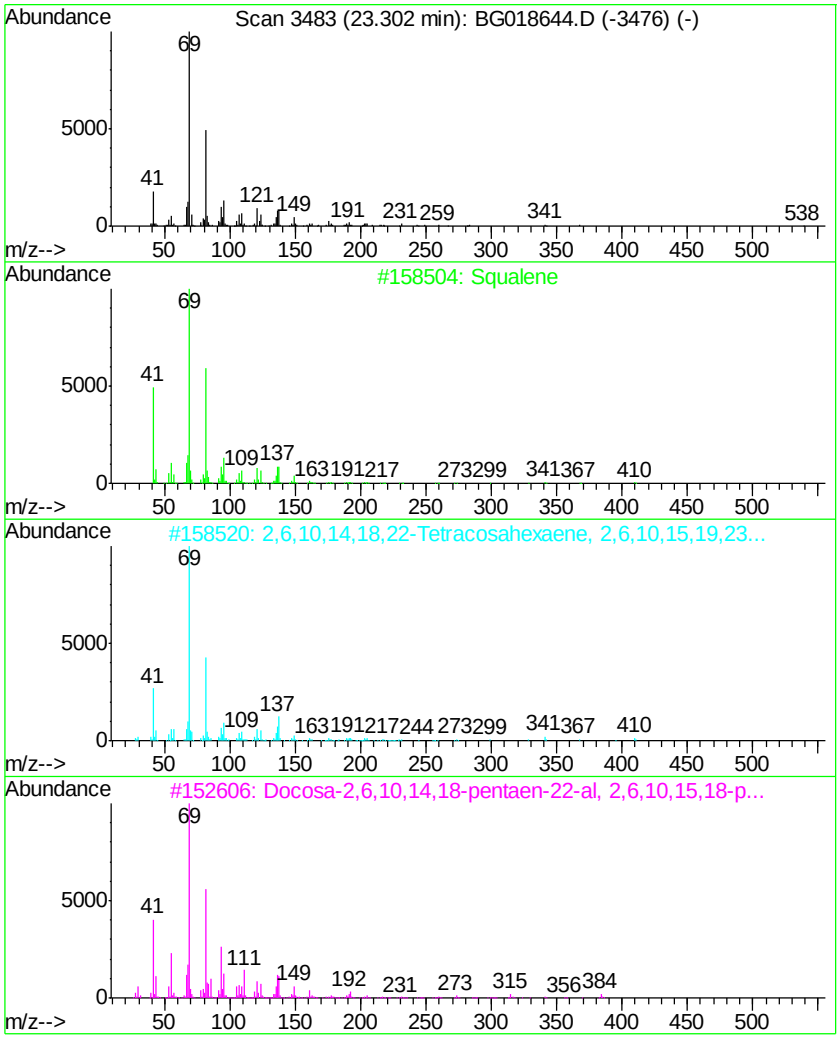
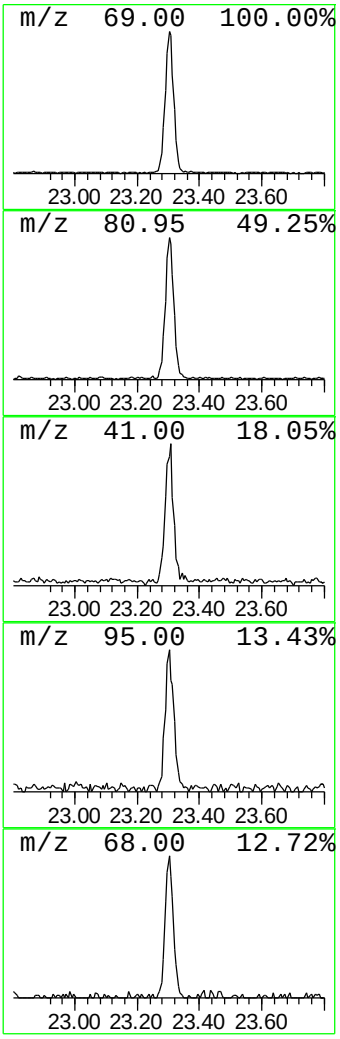
****

Peak Number 10 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	6.00 ng	405992	Perylene-d12	24.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	83
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	80





Tentatively Identified Compound (LSC) summary

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Acq On : 11 Sep 2015 18:09
Operator : UM/IZ
Sample : G3612-06
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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
unknown2.89	2.89	2.7	ng	45453	1	8.01	338481	20.0
Propane, 2,2-dime...	2.97	166.5	ng	2818300	1	8.01	338481	20.0
Butane, 2-methoxy...	3.18	55.3	ng	936556	1	8.01	338481	20.0
2-Pentanone, 4-hy...	5.11	34.2	ng	578267	1	8.01	338481	20.0
unknown7.54	7.54	85.9	ng	1454220	1	8.01	338481	20.0
n-Hexadecanoic acid	18.25	3.2	ng	180653	4	17.37	1130240	20.0
Heptafluorobutyri...	21.29	2.3	ng	152515	5	21.63	1357630	20.0
Squalene	23.30	6.0	ng	405992	6	24.82	1353140	20.0