LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032242.D
Acq On : 23 Jan 2018 21:41
Operator : SJ/JU
Sample : J1238-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-05-9.0-10.0

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-BG011218.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	3.376	11	15	25	rVB5	11048	23762	1.04%	0.157%
2	3.470	25	31	47	rVB	352267	556779	24.28%	3.671%
3	5.650	395	402	411	rBV2	27461	48797	2.13%	0.322%
4	6.161	481	489	504	rBV	551779	942369	41.10%	6.213%
5	7.841	767	775	789	rBV	568695	1067302	46.54%	7.036%
6	8.241	835	843	853	rBV	609035	1081452	47.16%	7.130%
7	8.729	919	926	933	rBV	117542	212162	9.25%	1.399%
8	9.063	975	983	992	rBV	418300	758522	33.08%	5.001%
9	9.921	1118	1129	1142	rBV	341141	634474	27.67%	4.183%
10	11.607	1408	1416	1426	rBV	168274	314843	13.73%	2.076%
11	13.987	1813	1821	1831	rBV	936630	1517529	66.18%	10.005%
12	14.786	1946	1957	1963	rBV	103319	162470	7.09%	1.071%
13	15.203	2022	2028	2032	rBV2	28975	38029	1.66%	0.251%
14	15.362	2048	2055	2064	rVB2	305341	509957	22.24%	3.362%
15	16.143	2184	2188	2194	rVB2	35072	48148	2.10%	0.317%
16	16.837	2298	2306	2317	rBV	1002888	1563595	68.19%	10.308%
17	17.001	2329	2334	2343	rVB	26315	43928	1.92%	0.290%
18	18.094	2512	2520	2530	rBV2	419339	668959	29.17%	4.410%
19	18.917	2655	2660	2671	rBV3	69442	118269	5.16%	0.780%
20	20.150	2866	2870	2875	rBV3	28631	41029	1.79%	0.270%
21	20.632	2946	2952	2962	rVB	1701744	2293106	100.00%	15.118%
22	20.867	2986	2992	2994	rBV6	17170	26404	1.15%	0.174%
23	21.966	3174	3179	3191	rBV2	143976	261361	11.40%	1.723%
24	22.424	3249	3257	3267	rBV2	483504	905150	39.47%	5.967%
25	23.300	3393	3406	3418	rBV4	81758	259410	11.31%	1.710%
26	24.998	3687	3695	3702	rBV6	27170	72397	3.16%	0.477%
27	25.080	3704	3709	3716	rVB6	14876	37625	1.64%	0.248%
28	26.120	3872	3886	3899	rBV2	257694	930924	40.60%	6.137%
29	27.424	4100	4108	4109	rBV7	16625	29703	1.30%	0.196%

Sum of corrected areas: 15168455

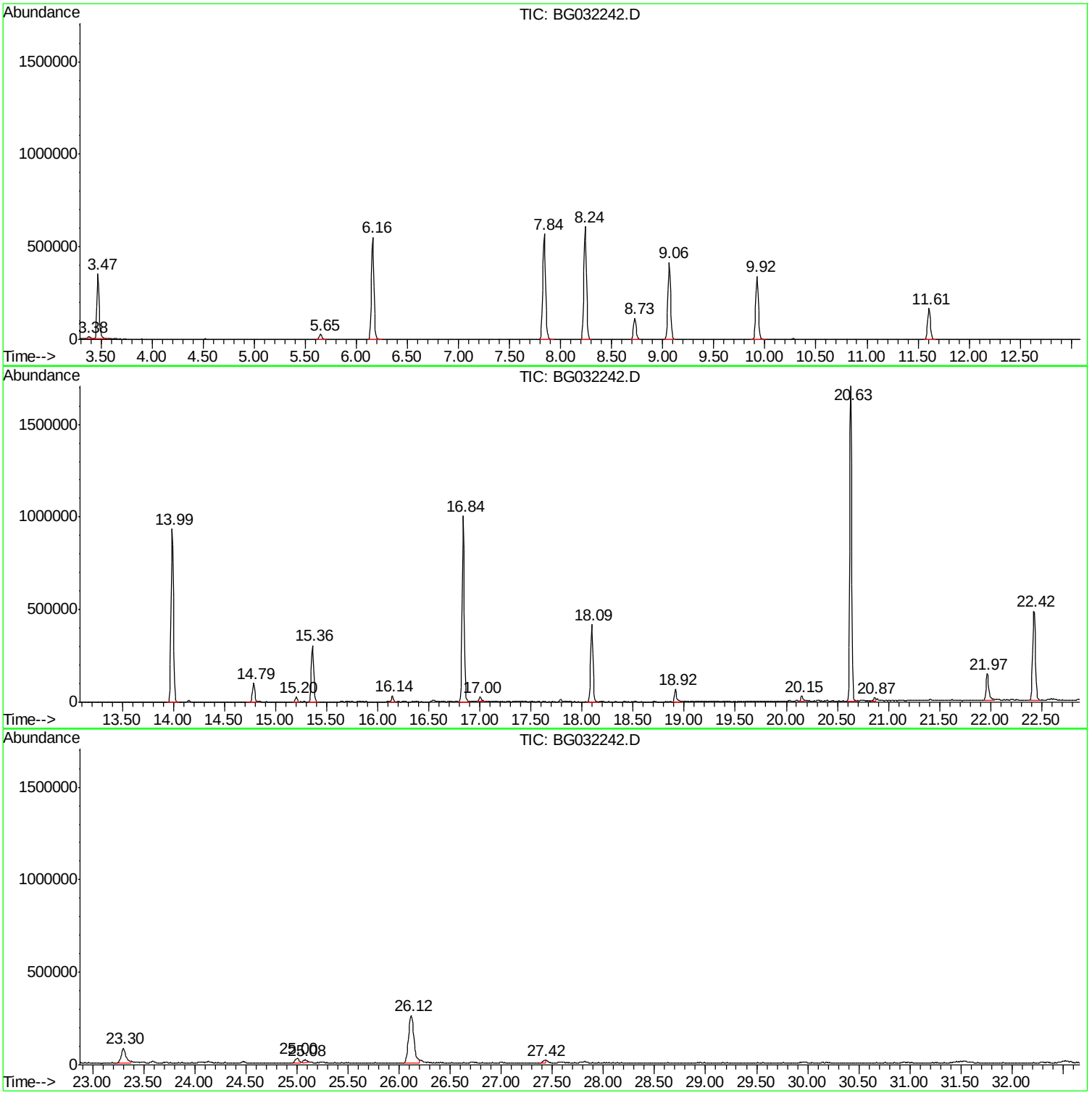
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032242.D
Acq On : 23 Jan 2018 21:41
Operator : SJ/JU
Sample : J1238-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-05-9.0-10.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032242.D
Acq On : 23 Jan 2018 21:41
Operator : SJ/JU
Sample : J1238-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-05-9.0-10.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

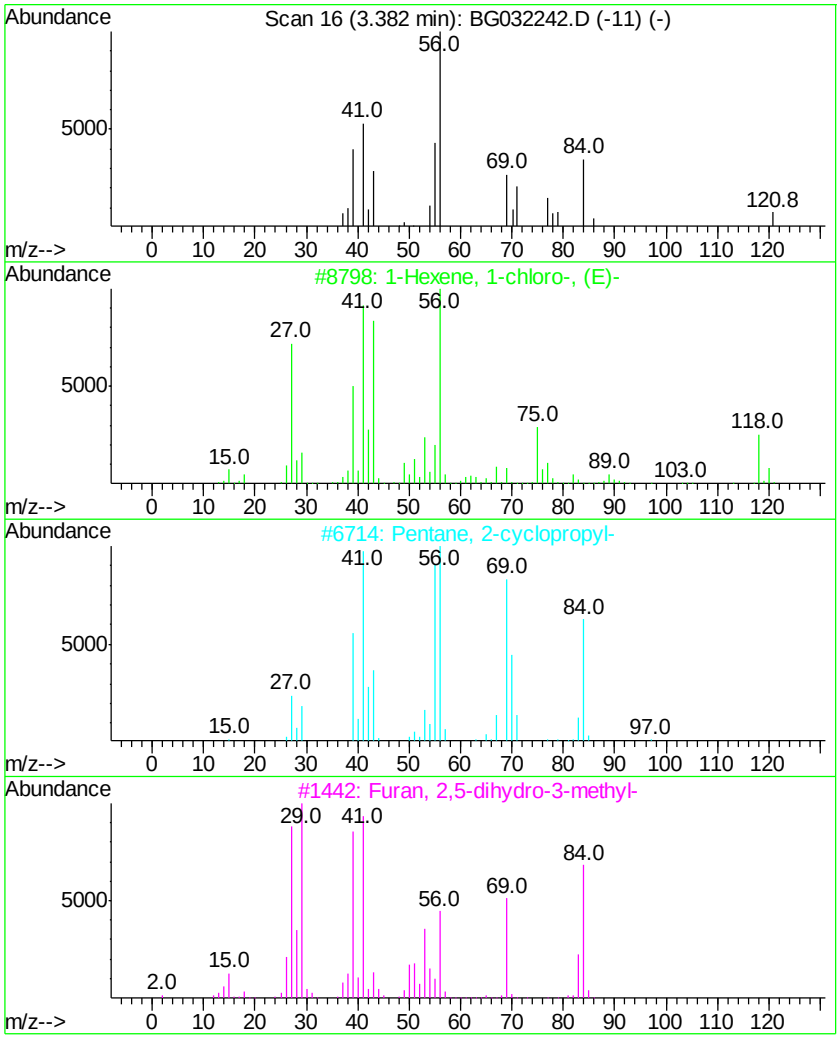
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

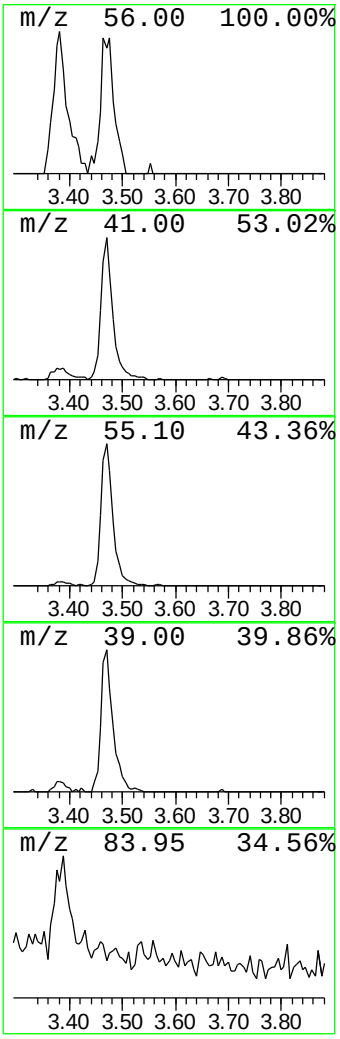
****

Peak Number 1 unknown3.38 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	2.24 ng	23762	1,4-Dichlorobenzene-d4	8.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 1-chloro-, (E)-	118	C6H11Cl	050586-19-1	38
2	Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	37
3	Furan, 2,5-dihydro-3-methyl-	84	C5H8O	001708-31-2	27
4	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	25
5	(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032242.D
Acq On : 23 Jan 2018 21:41
Operator : SJ/JU
Sample : J1238-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-05-9.0-10.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

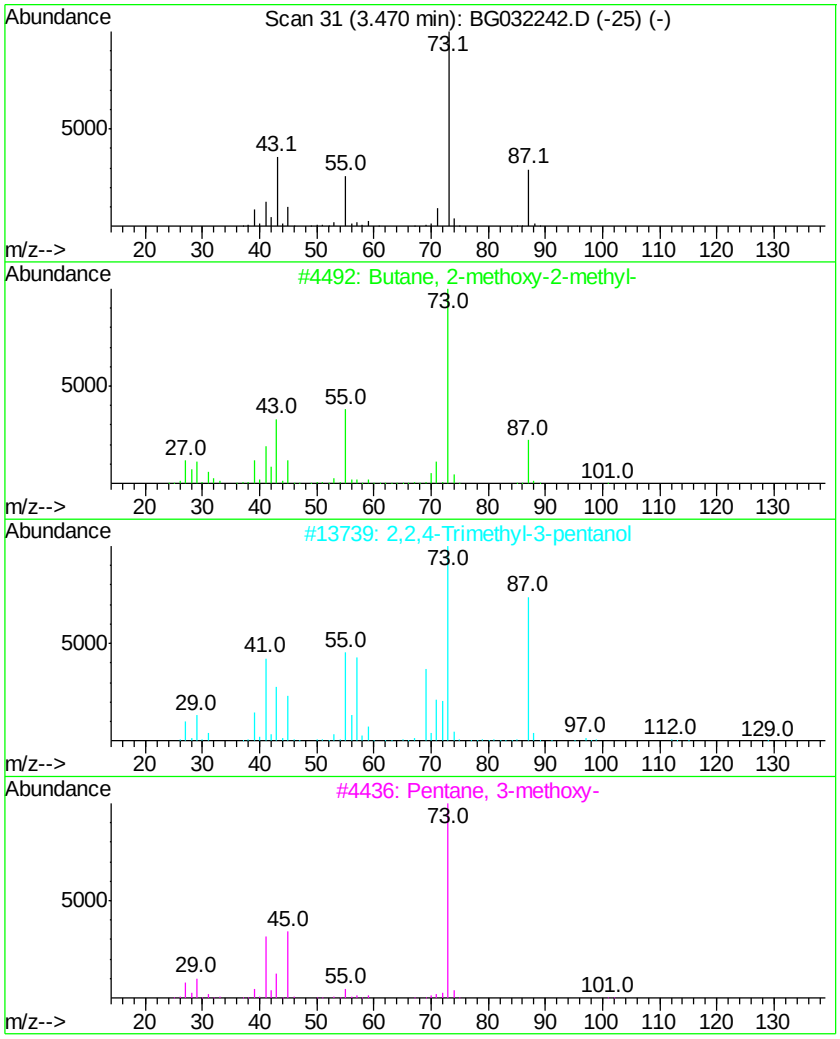
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

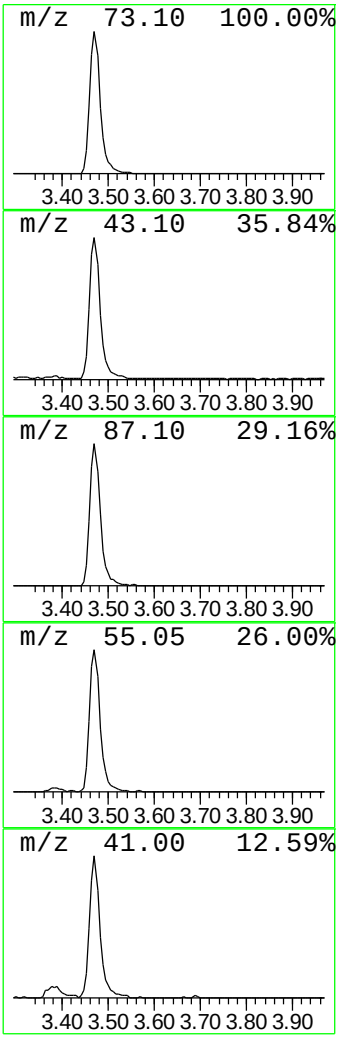
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.47	52.49 ng	556779	1,4-Dichlorobenzene-d4	8.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032242.D
Acq On : 23 Jan 2018 21:41
Operator : SJ/JU
Sample : J1238-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-05-9.0-10.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

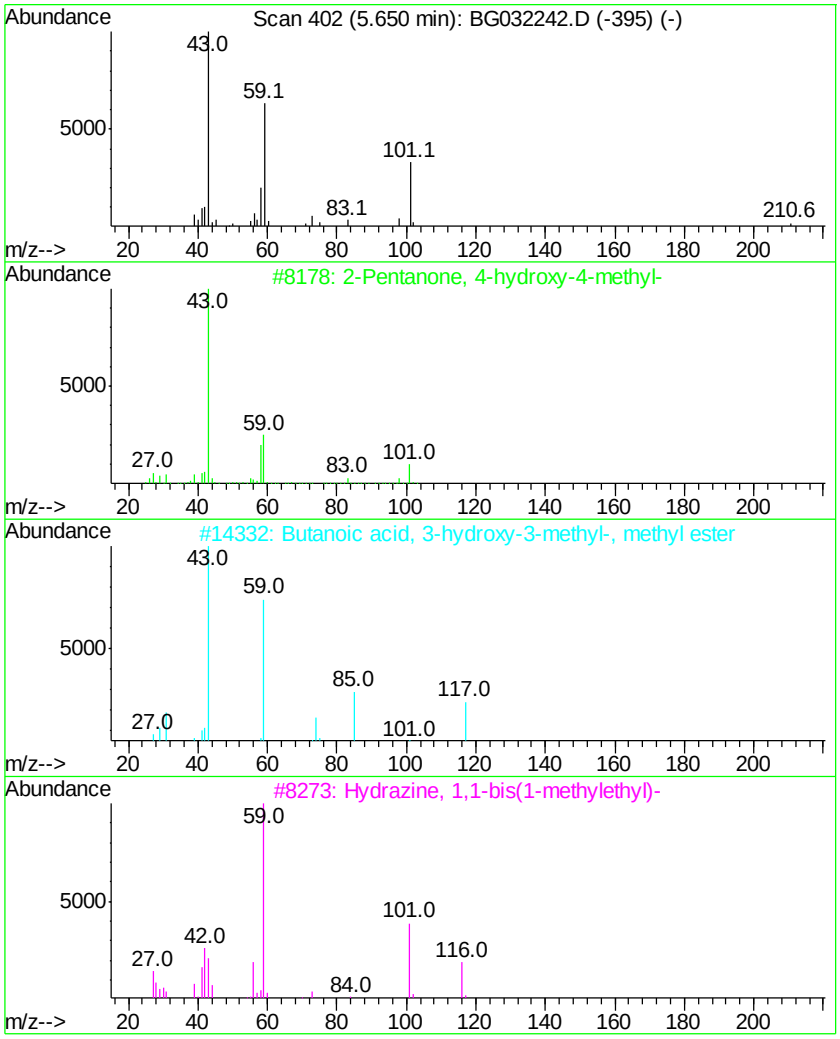
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

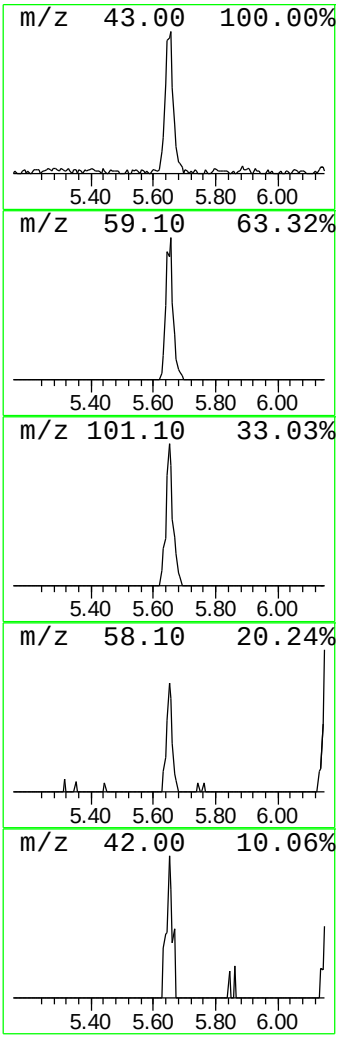
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.65	4.60 ng	48797	1,4-Dichlorobenzene-d4	8.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Butanoic acid, 3-hydroxy-3-methy...	132	C6H12O3	006149-45-7	38
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	32
5	Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032242.D
Acq On : 23 Jan 2018 21:41
Operator : SJ/JU
Sample : J1238-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-05-9.0-10.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

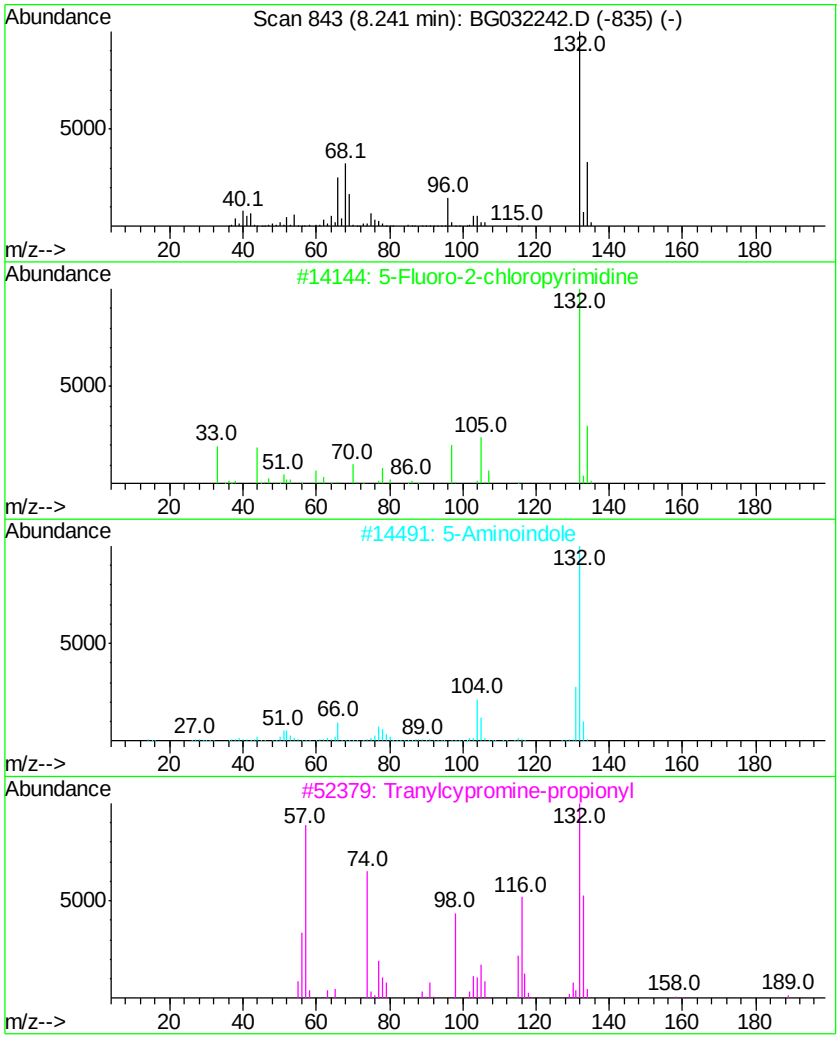
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

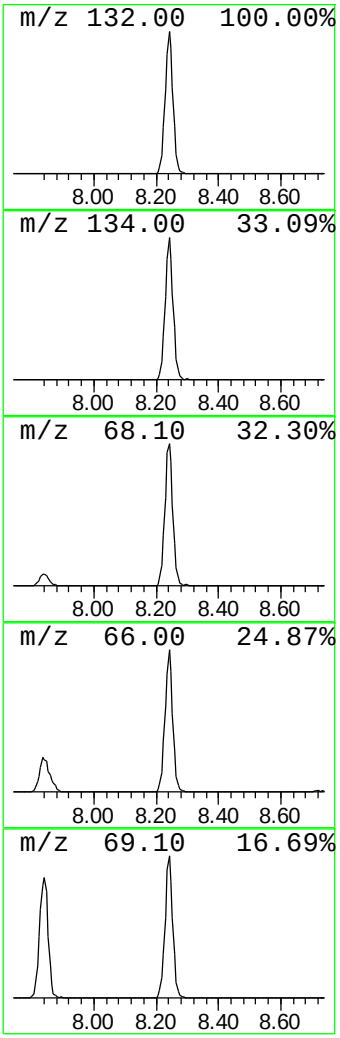
****

Peak Number 4 unknown8.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.24	101.95 ng	1081450	1,4-Dichlorobenzene-d4	8.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032242.D
Acq On : 23 Jan 2018 21:41
Operator : SJ/JU
Sample : J1238-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-05-9.0-10.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

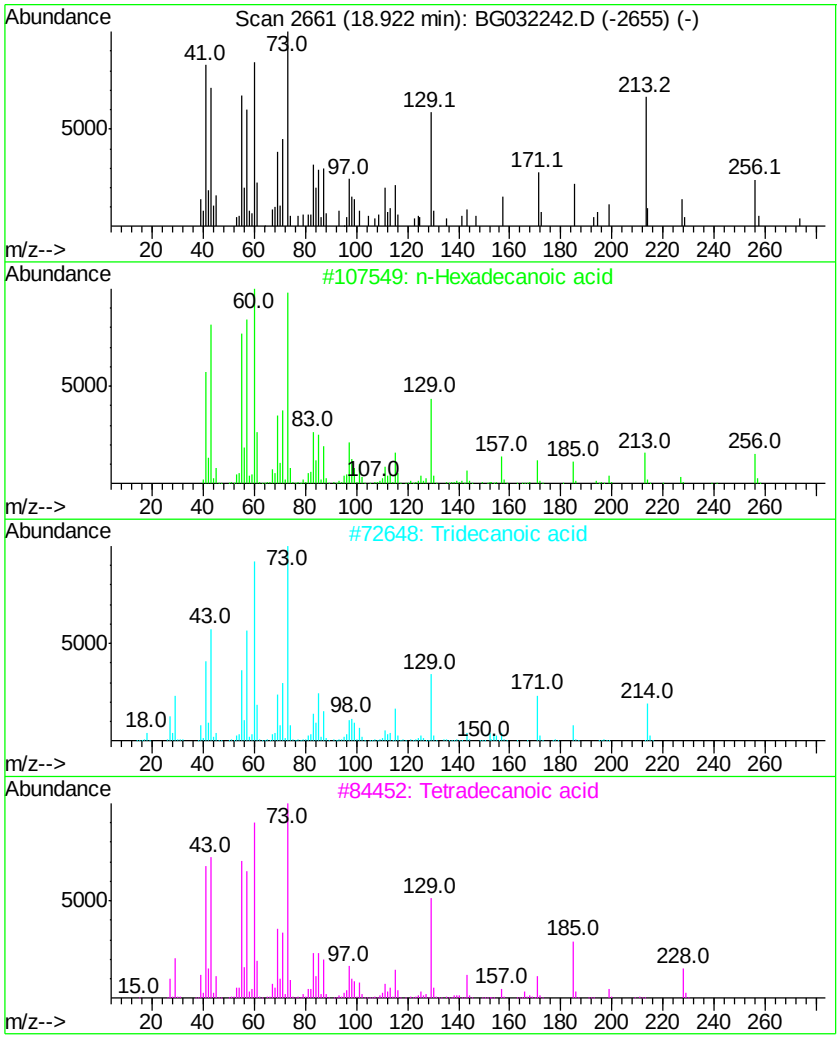
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

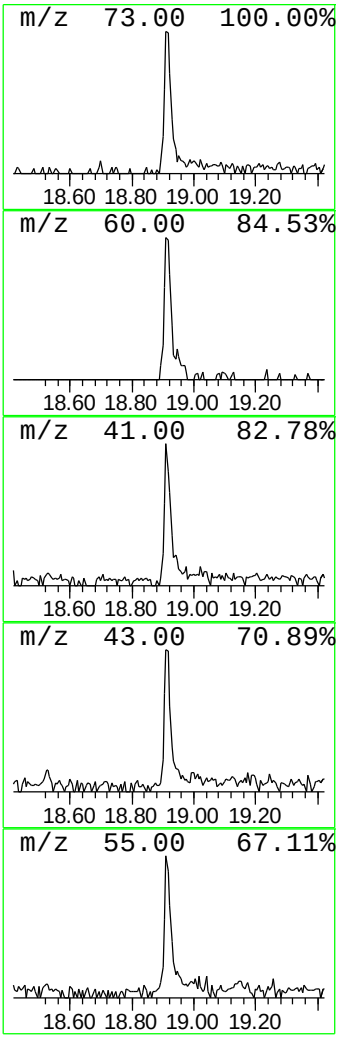
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.92	3.54 ng	118269	Phenanthrene-d10	18.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	Octadecanoic acid	284	C18H36O2	000057-11-4	49





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
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Acq On : 23 Jan 2018 21:41
Operator : SJ/JU
Sample : J1238-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-05-9.0-10.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

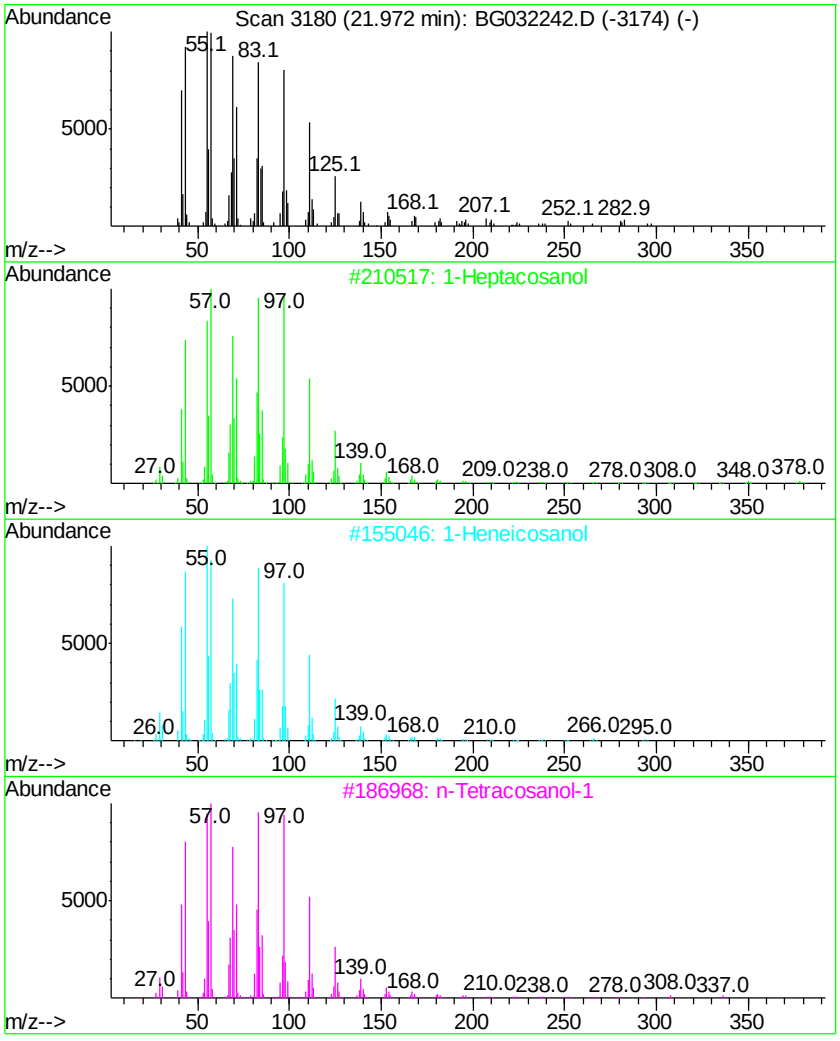
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

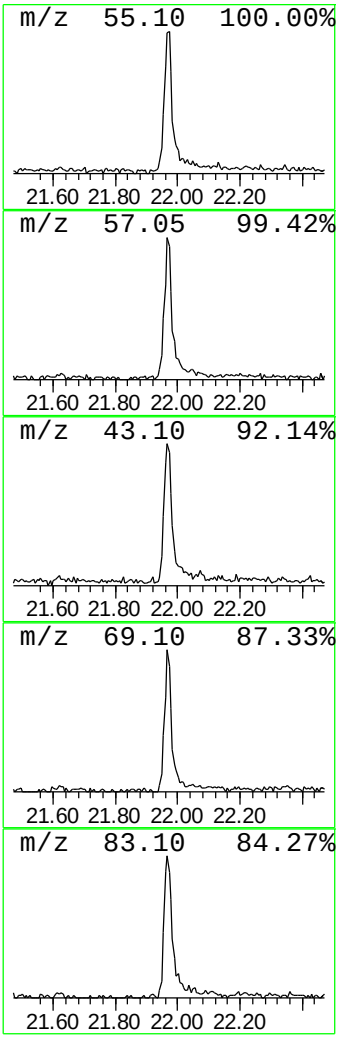
****

Peak Number 7 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.97	5.77 ng	261361	Chrysene-d12	22.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Behenic alcohol	326	C22H46O	000661-19-8	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
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Sample : J1238-16
Misc :
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Instrument : BNA_G
ClientSampleId : SB-05-9.0-10.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

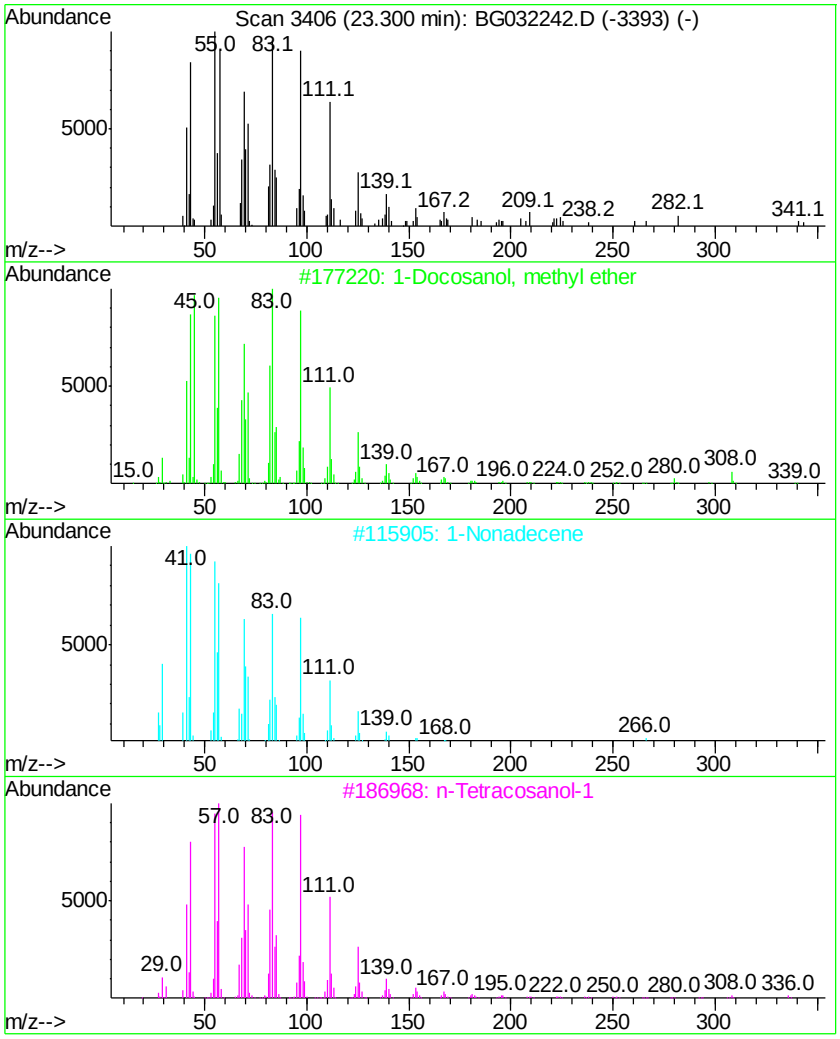
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

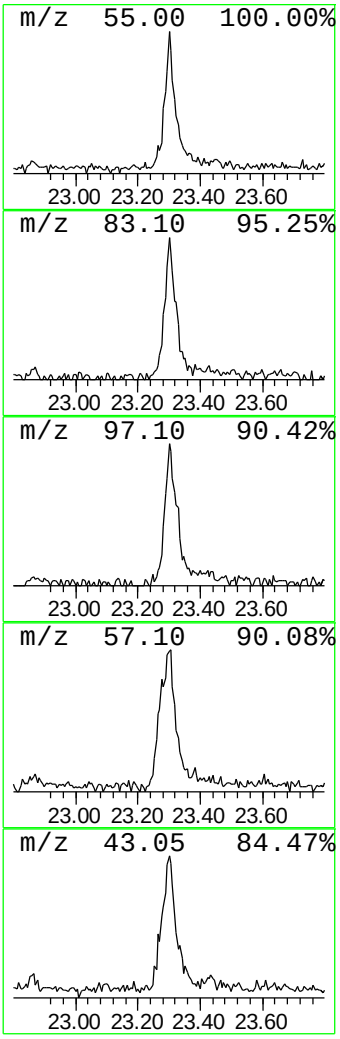
****

Peak Number 8 1-Docosanol, methyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	5.73 ng	259410	Chrysene-d12	22.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	90
2	1-Nonadecene	266	C19H38	018435-45-5	90
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	1-Heptadecene	238	C17H34	006765-39-5	87
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012318\
Data File : BG032242.D
Acq On : 23 Jan 2018 21:41
Operator : SJ/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.38	3.38	2.2	ng	23762	1	8.73	212162	20.0
Butane, 2-methoxy...	3.47	52.5	ng	556779	1	8.73	212162	20.0
2-Pentanone, 4-hy...	5.65	4.6	ng	48797	1	8.73	212162	20.0
unknown8.24	8.24	102.0	ng	1081450	1	8.73	212162	20.0
n-Hexadecanoic acid	18.92	3.5	ng	118269	4	18.09	668959	20.0
1-Heptacosanol	21.97	5.8	ng	261361	5	22.42	905150	20.0
1-Docosanol, meth...	23.30	5.7	ng	259410	5	22.42	905150	20.0