LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-A2

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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	5.137	344	349	357	rBV	23588	39427	2.40%	0.413%
2	5.607	422	429	444	rBV	370768	632250	38.50%	6.627%
3	7.211	693	702	716	rBV	408066	776258	47.27%	8.137%
4	7.581	756	765	775	rBV	367019	667934	40.67%	7.001%
5	8.057	839	846	854	rBV	78341	140252	8.54%	1.470%
6	8.374	893	900	909	rBV	271434	494773	30.13%	5.186%
7	9.232	1038	1046	1058	rBV	237778	449206	27.35%	4.709%
8	10.872	1315	1325	1342	rBV	105014	197920	12.05%	2.075%
9	13.310	1732	1740	1749	rBV	590014	960920	58.51%	10.072%
10	14.138	1876	1881	1891	rVB	35545	52764	3.21%	0.553%
11	14.691	1968	1975	1985	rVB2	177101	301252	18.34%	3.158%
12	16.183	2222	2229	2239	rBV	531222	843670	51.37%	8.843%
13	17.440	2435	2443	2454	rBV2	259606	415203	25.28%	4.352%
14	18.298	2583	2589	2599	rBV2	24476	40807	2.48%	0.428%
15	19.779	2837	2841	2844	rBV2	21956	23935	1.46%	0.251%
16	20.043	2880	2886	2895	rBV	1207148	1642352	100.00%	17.215%
17	20.308	2926	2931	2937	rBV	40200	47209	2.87%	0.495%
18	20.801	3011	3015	3020	rVB	56488	66825	4.07%	0.700%
19	21.312	3097	3102	3111	rBV	115557	185571	11.30%	1.945%
20	21.718	3164	3171	3181	rBV2	271409	468717	28.54%	4.913%
21	21.859	3185	3195	3205	rBV2	65355	104678	6.37%	1.097%
22	22.470	3292	3299	3305	rBV2	61952	113498	6.91%	1.190%
23	23.169	3412	3418	3428	rVB	50403	100017	6.09%	1.048%
24	23.363	3444	3451	3457	rBV2	15847	36018	2.19%	0.378%
25	23.980	3546	3556	3563	rBV3	44292	106896	6.51%	1.120%
26	24.937	3710	3719	3724	rBV2	33276	84220	5.13%	0.883%
27	25.014	3724	3732	3744	rVB2	150564	444003	27.03%	4.654%
28	26.083	3904	3914	3925	rVB3	22834	70200	4.27%	0.736%
29	27.458	4139	4148	4157	rVB4	10764	33309	2.03%	0.349%

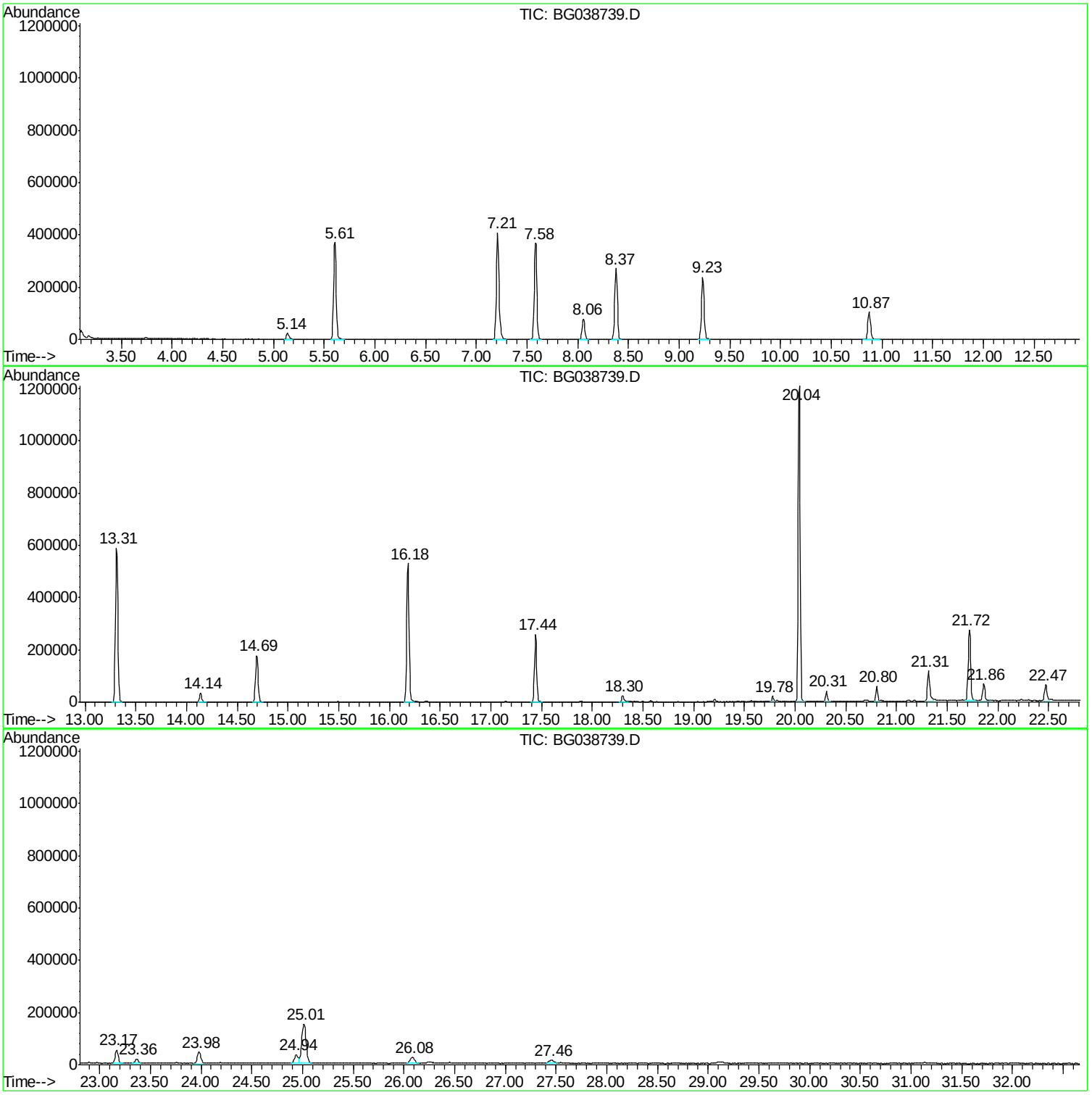
Sum of corrected areas: 9540084

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-A2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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:\SVOASRV\HPCHEM1\BNA G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-A2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

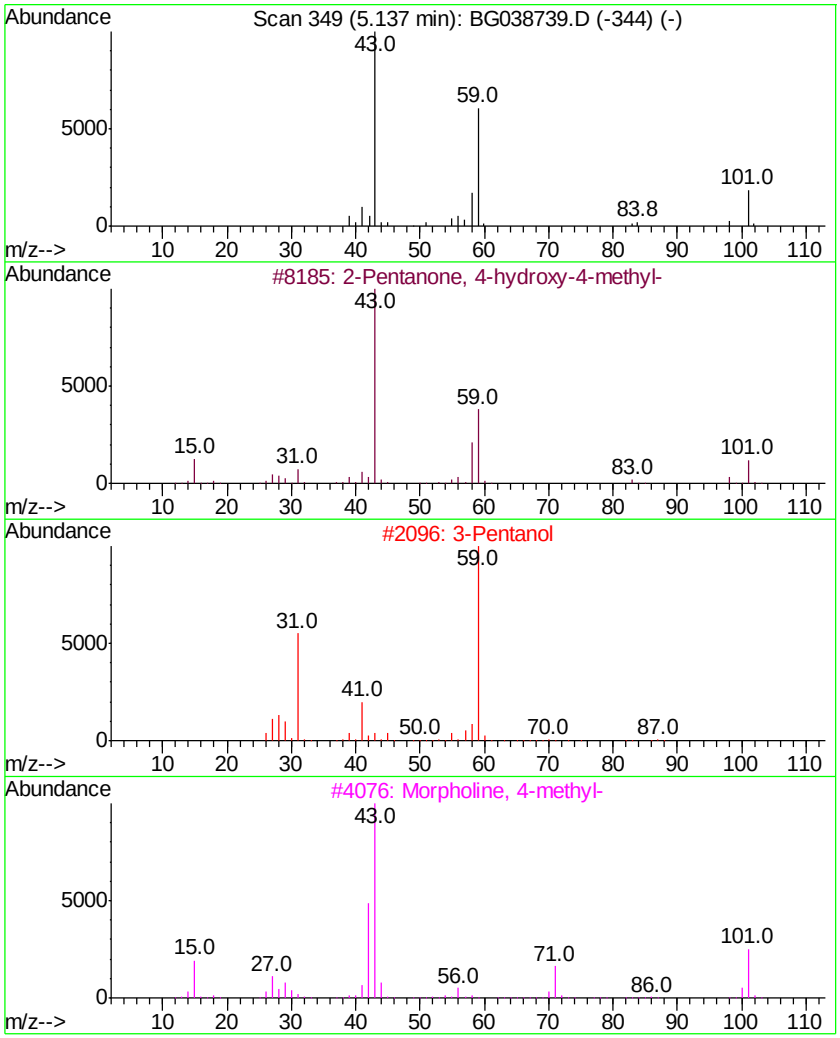
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

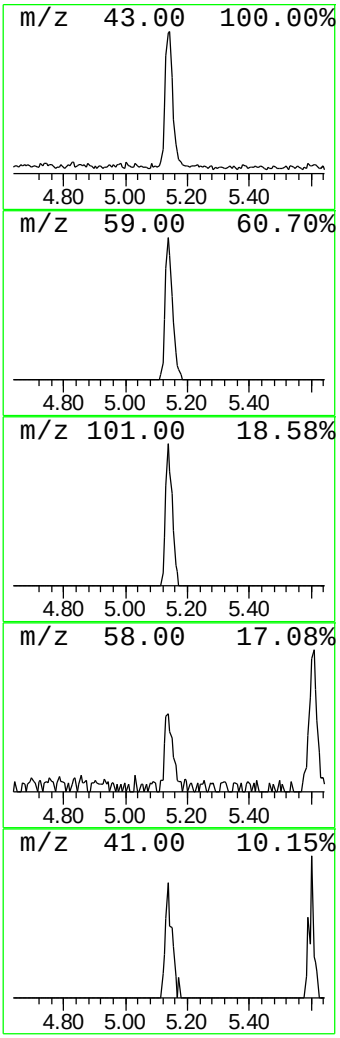
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	5.62 ng	39427	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	3-Pentanol	88	C5H12O	000584-02-1	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Acetone	58	C3H6O	000067-64-1	9
5	3-Octanol	130	C8H18O	000589-98-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-A2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

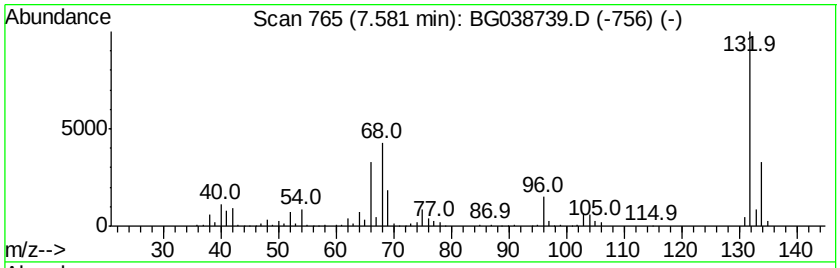
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

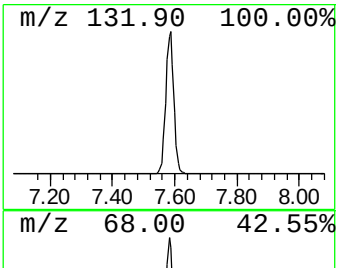
****

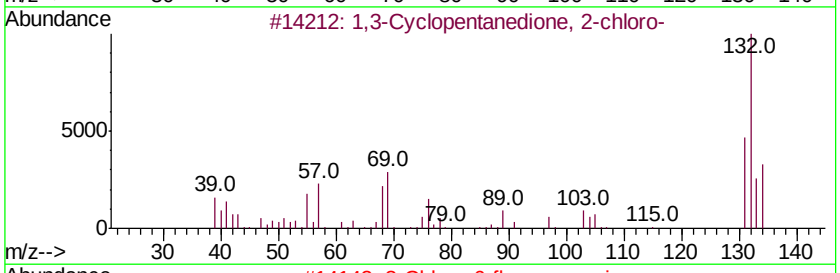
Peak Number 2 unknown7.58 Concentration Rank 1

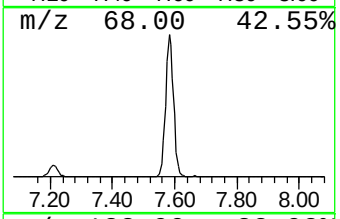
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	95.25 ng	667934	1,4-Dichlorobenzene-d4	8.06

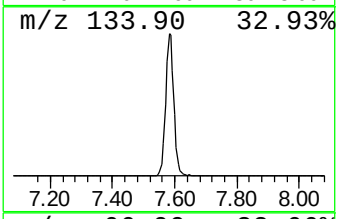
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	28
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	5-Aminoindole	132	C8H8N2	005192-03-0	27
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12

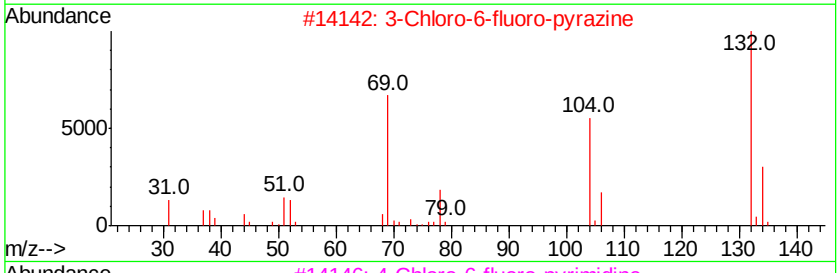


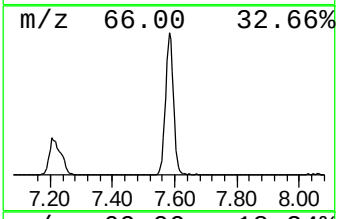


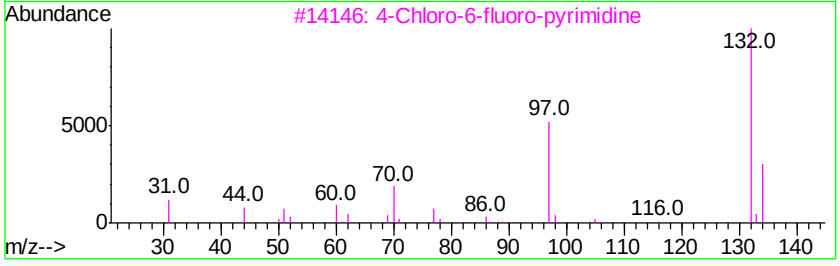


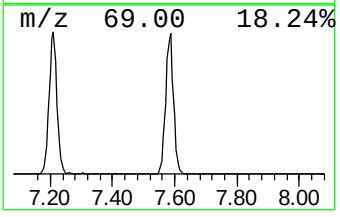












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-A2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

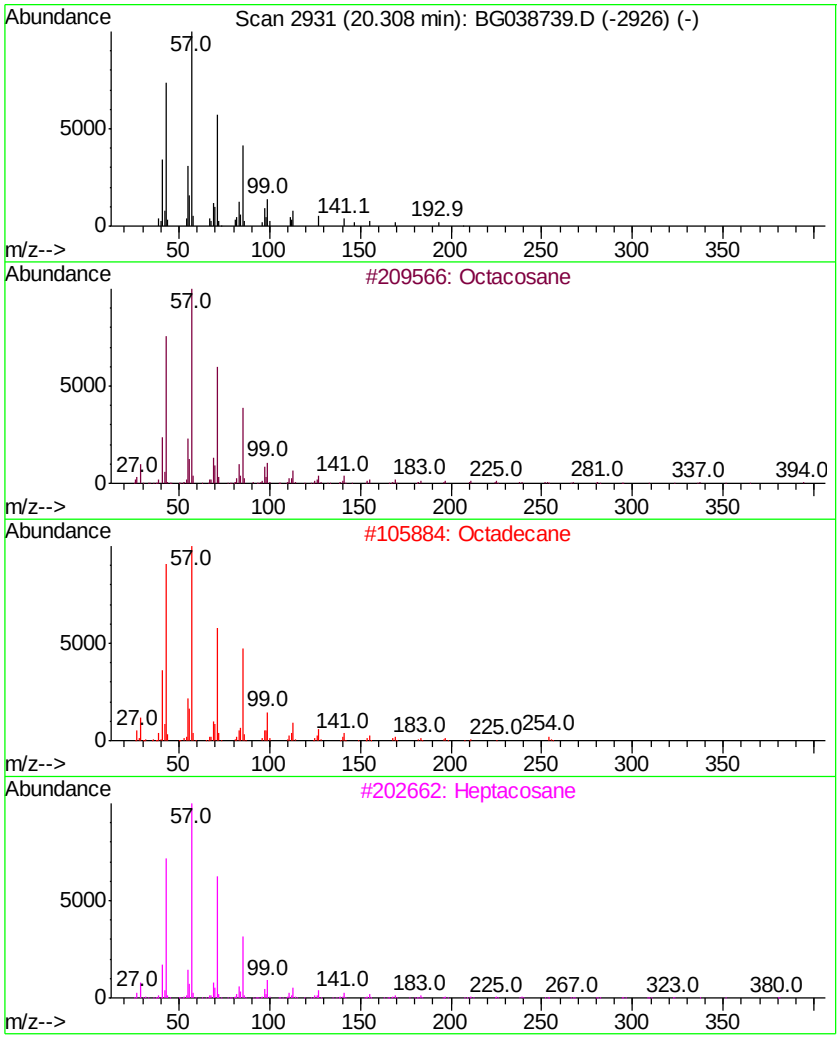
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

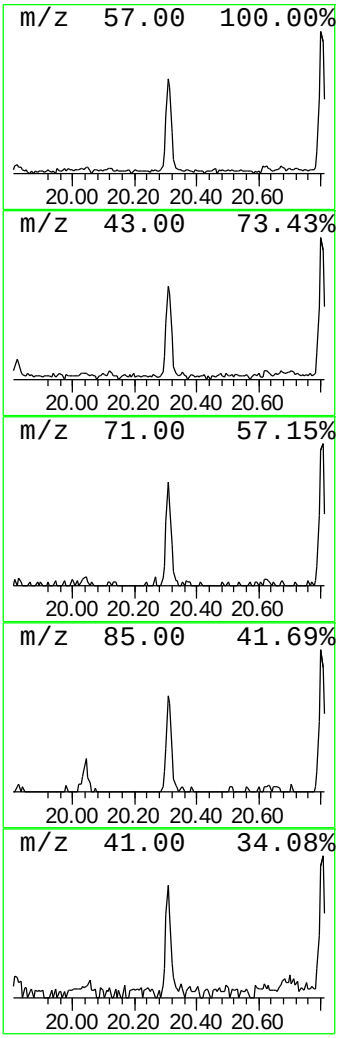
****

Peak Number 4 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.31	2.01 ng	47209	Chrysene-d12	21.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-A2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

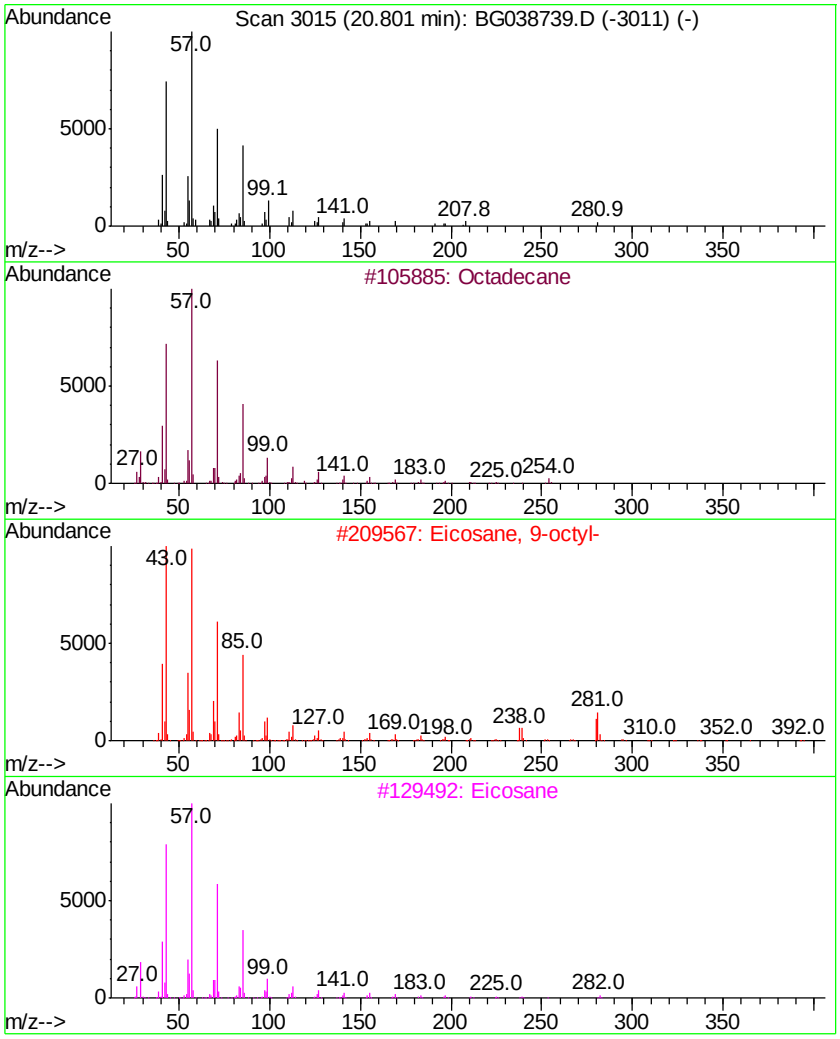
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

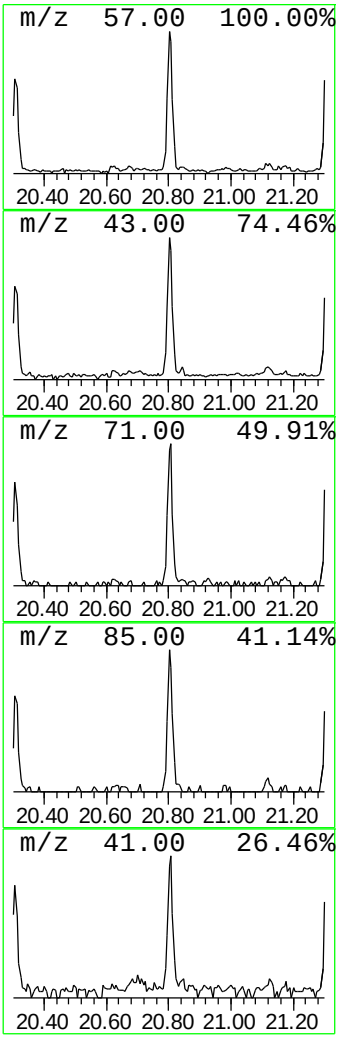
****

Peak Number 5 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.80	2.85 ng	66825	Chrysene-d12	21.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Eicosane, 9-octyl-	394	C28H58	013475-77-9	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Docosane	310	C22H46	000629-97-0	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-A2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

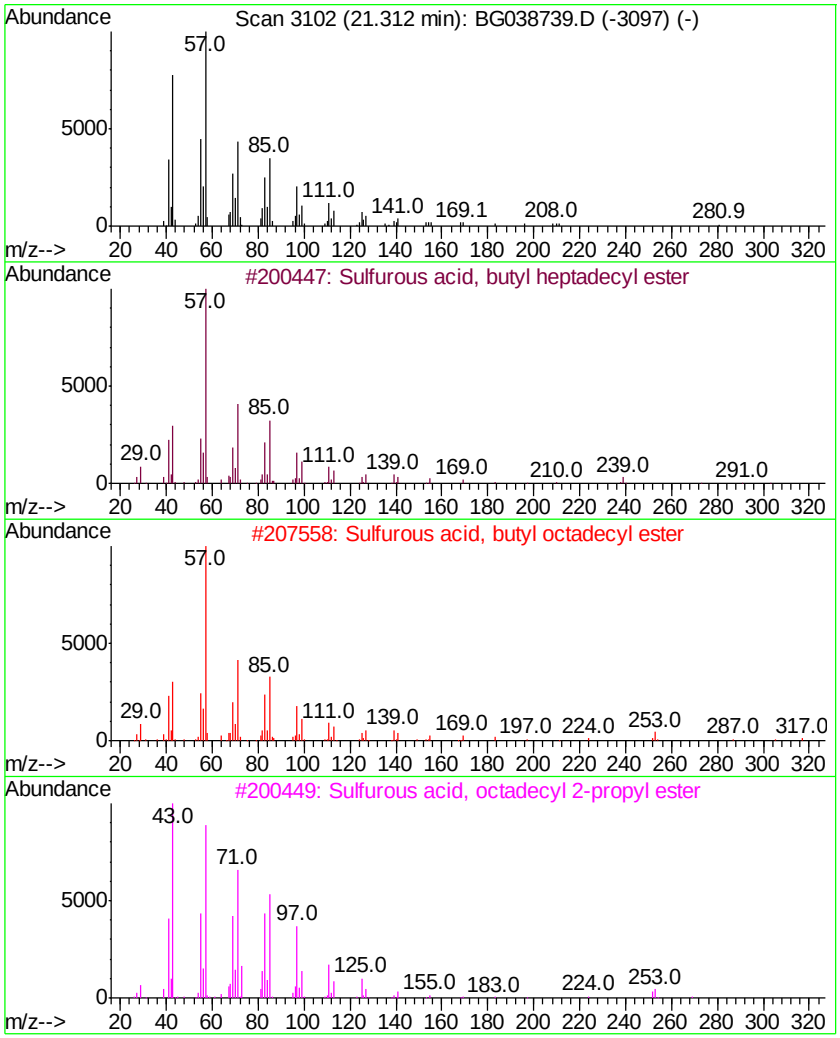
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

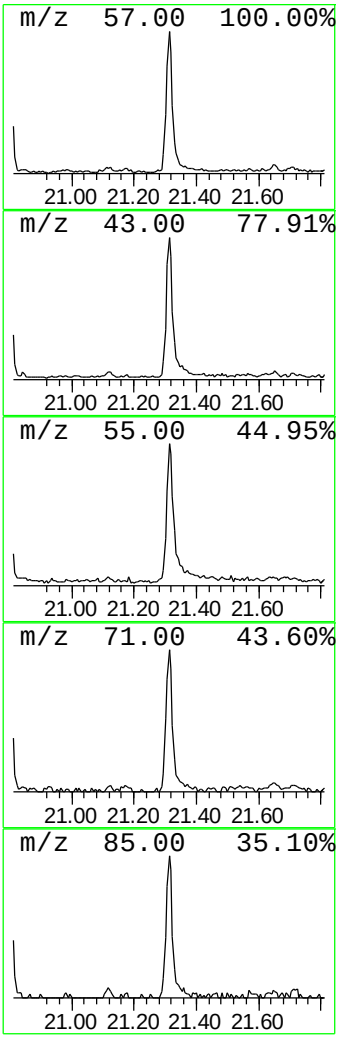
****

Peak Number 6 Sulfurous acid, butyl hepta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	7.92 ng	185571	Chrysene-d12	21.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
2	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	91
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	68
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	68





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-A2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

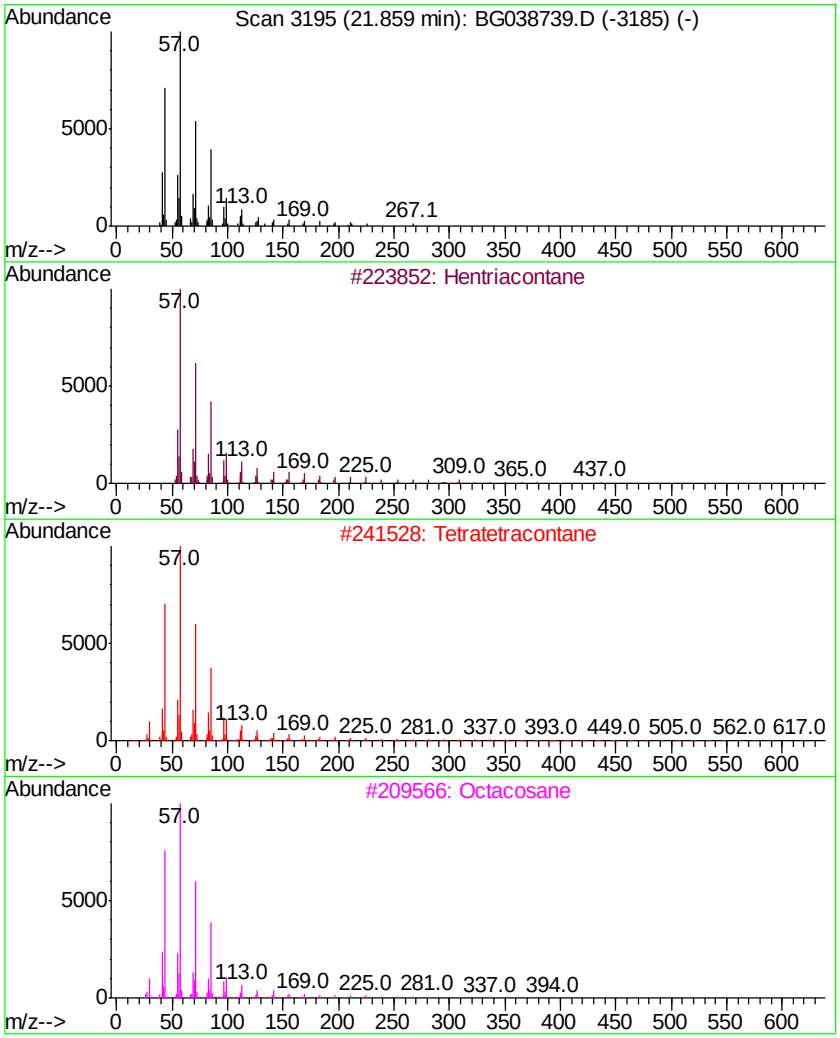
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

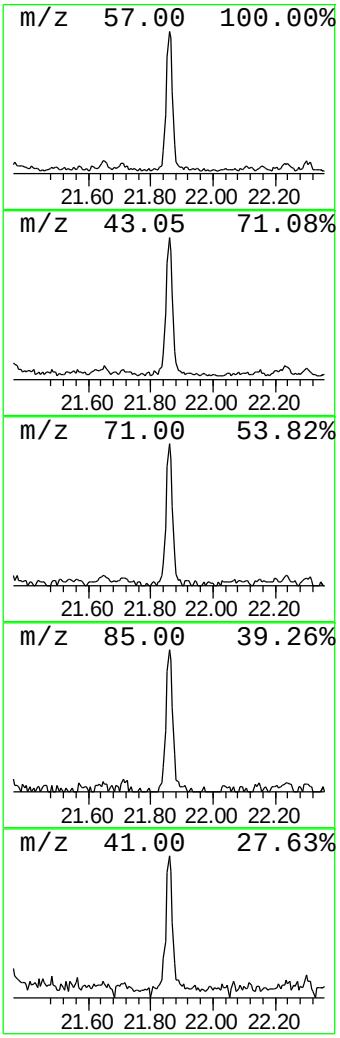
****

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	4.47 ng	104678	Chrysene-d12	21.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-A2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

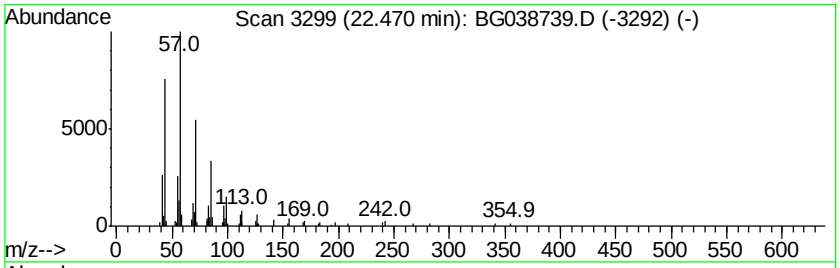
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

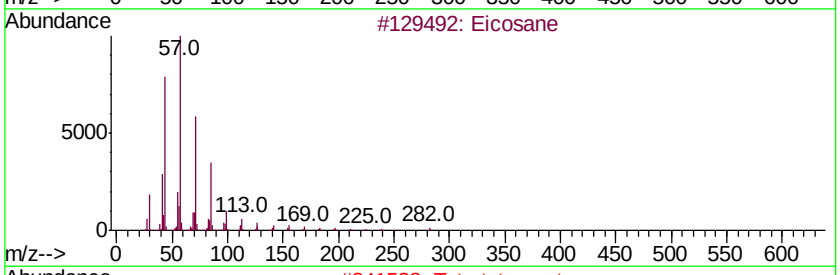
****

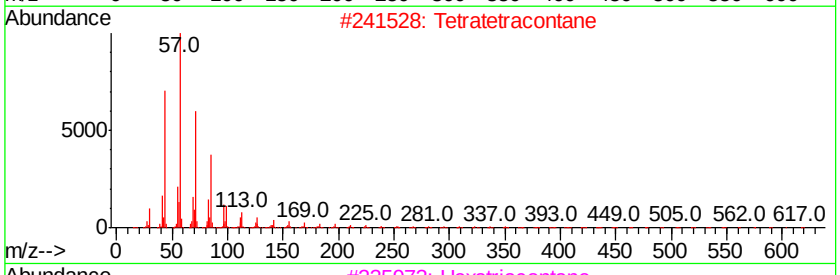
Peak Number 8 Eicosane Concentration Rank 5

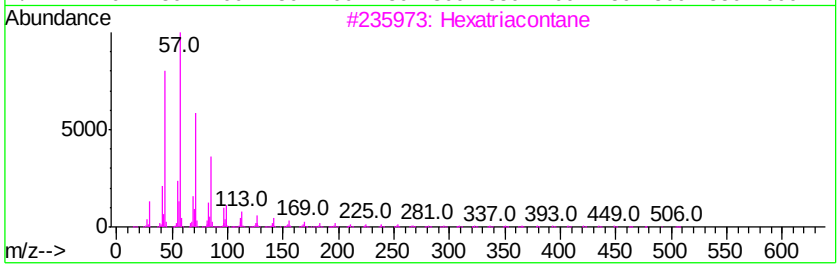
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.47	4.84 ng	113498	Chrysene-d12	21.72

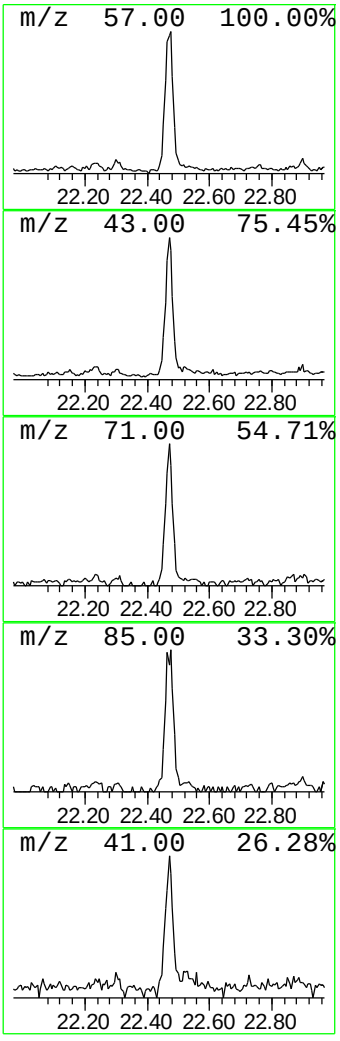
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Hexatriacontane	507	C36H74	000630-06-8	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Heptacosane	380	C27H56	000593-49-7	83











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121918\
Data File : BG038739.D
Acq On : 19 Dec 2018 23:03
Operator : JU/SJ
Sample : J6477-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-A2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
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
2-Pentanone, 4-hy...	5.14	5.6	ng	39427	1	8.06	140252	20.0
unknown7.58	7.58	95.3	ng	667934	1	8.06	140252	20.0
Octacosane	20.31	2.0	ng	47209	5	21.72	468717	20.0
Octadecane	20.80	2.9	ng	66825	5	21.72	468717	20.0
Sulfurous acid, b...	21.31	7.9	ng	185571	5	21.72	468717	20.0
Hentriacontane	21.86	4.5	ng	104678	5	21.72	468717	20.0
Eicosane	22.47	4.8	ng	113498	5	21.72	468717	20.0