LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042996.D
Acq On : 2 Oct 2019 22:18
Operator : JU
Sample : K5133-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

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-BG092519.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	3.176	9	15	25	rBV2	105802	248239	5.79%	1.018%
2	3.259	25	29	44	rVB	88907	151077	3.52%	0.619%
3	5.656	427	437	448	rBV	987023	1655388	38.58%	6.785%
4	7.242	698	707	717	rBV	1077226	1923077	44.82%	7.883%
5	7.606	760	769	778	rBV	1047065	1823439	42.50%	7.474%
6	8.071	838	848	857	rBV	237491	419586	9.78%	1.720%
7	8.394	894	903	911	rBV	751873	1321686	30.80%	5.418%
8	9.228	1037	1045	1055	rBV	622789	1134575	26.44%	4.651%
9	10.873	1318	1325	1333	rBV	307980	554289	12.92%	2.272%
10	13.311	1732	1740	1748	rBV	1673675	2618339	61.02%	10.733%
11	14.134	1874	1880	1889	rVB	191725	281739	6.57%	1.155%
12	14.686	1966	1974	1981	rBV	540386	845048	19.69%	3.464%
13	16.173	2220	2227	2246	rBV	1567864	2506097	58.41%	10.272%
14	17.430	2433	2441	2451	rBV	706285	1092873	25.47%	4.480%
15	18.317	2587	2592	2602	rBV2	94211	151998	3.54%	0.623%
16	20.039	2878	2885	2893	rBV	3196242	4290820	100.00%	17.588%
17	21.349	3103	3108	3124	rBV5	124336	448548	10.45%	1.839%
18	21.696	3161	3167	3175	rBV	780466	1289281	30.05%	5.285%
19	23.170	3414	3418	3428	rBV7	51327	141897	3.31%	0.582%
20	24.017	3557	3562	3568	rVB4	31646	66913	1.56%	0.274%
21	24.921	3706	3716	3733	rVB3	457221	1431388	33.36%	5.867%

Sum of corrected areas: 24396297

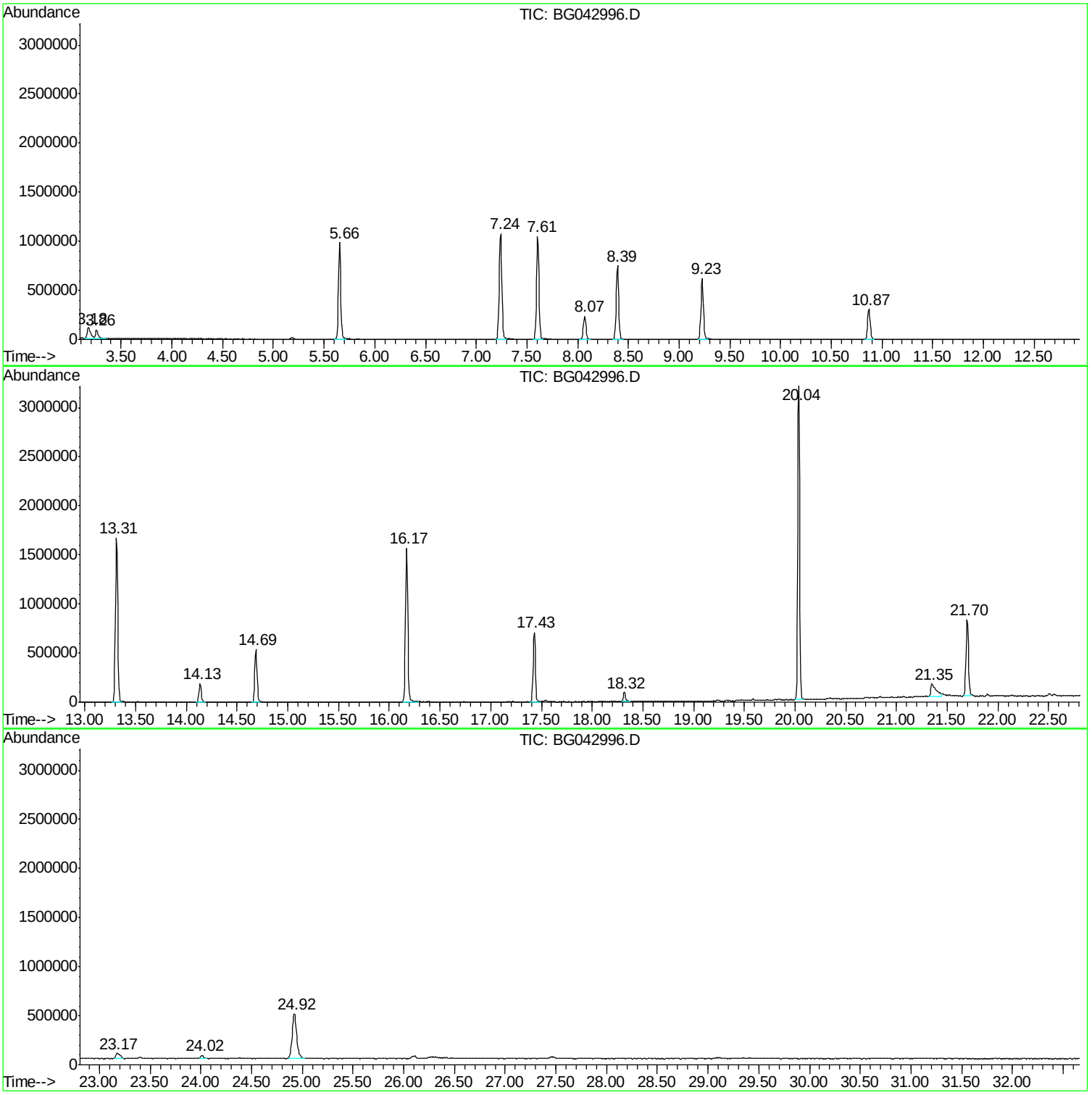
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042996.D
Acq On : 2 Oct 2019 22:18
Operator : JU
Sample : K5133-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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\BG100219\
Data File : BG042996.D
Acq On : 2 Oct 2019 22:18
Operator : JU
Sample : K5133-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

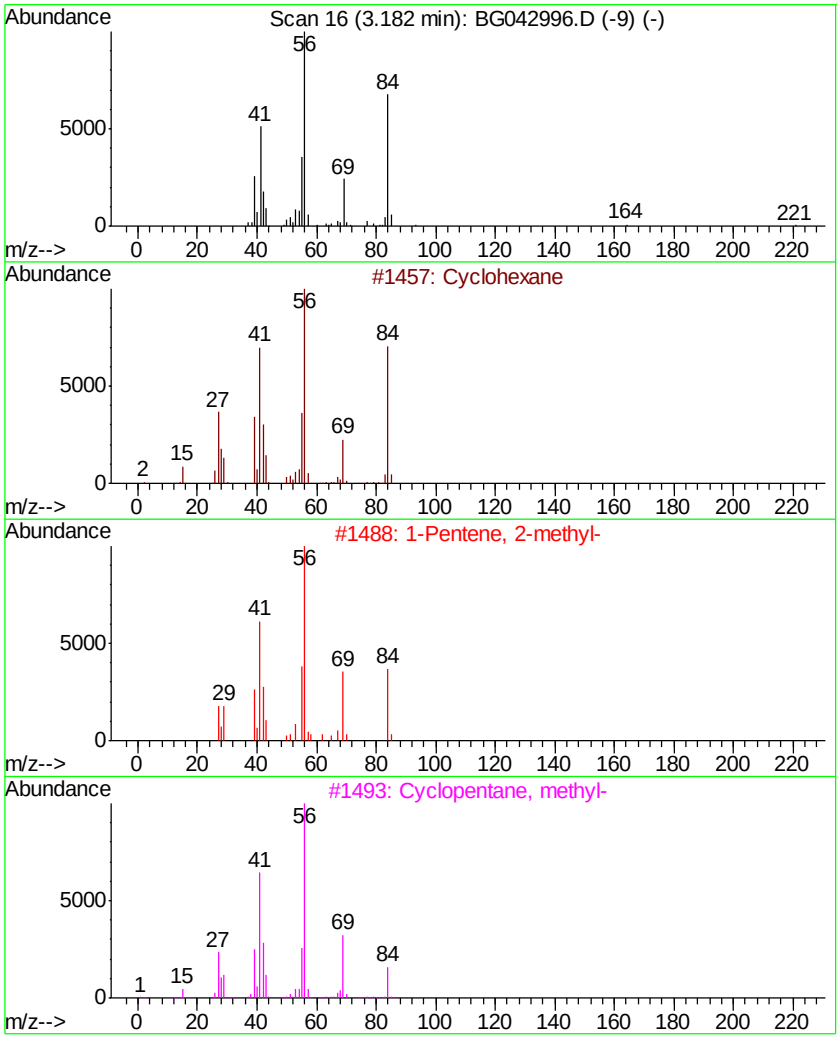
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

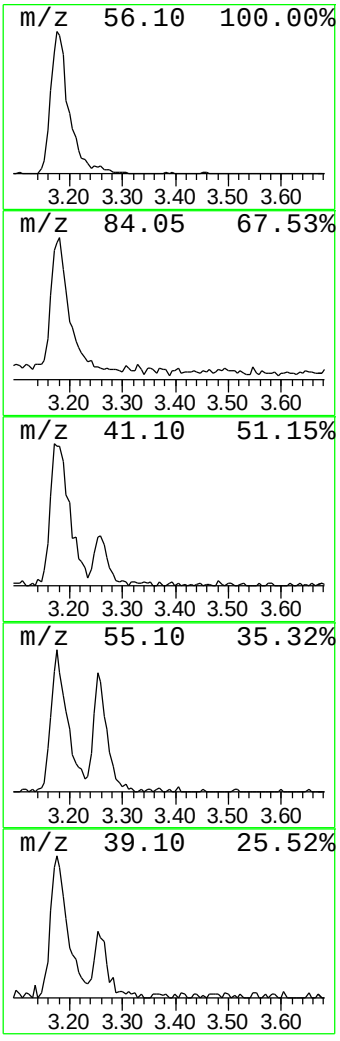
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	11.83 ng	248239	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	86
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4	Pyridine-D5-	84	C5D5N	007291-22-7	64
5	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	56





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042996.D
Acq On : 2 Oct 2019 22:18
Operator : JU
Sample : K5133-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

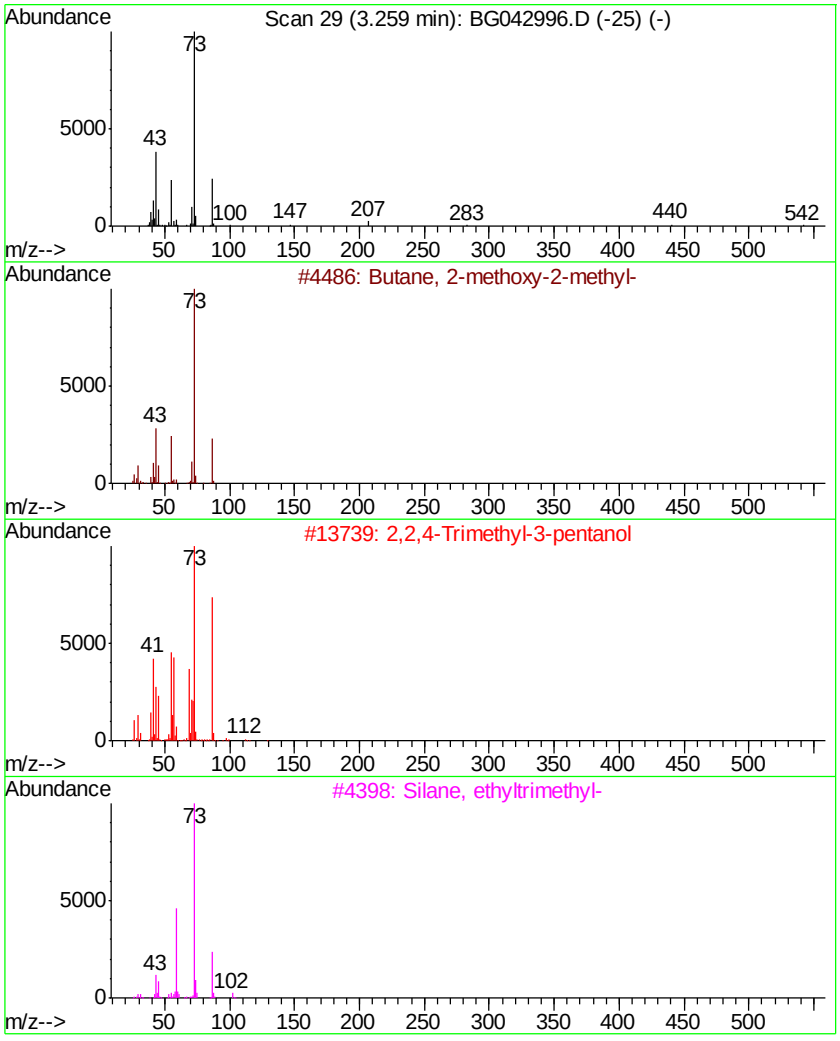
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

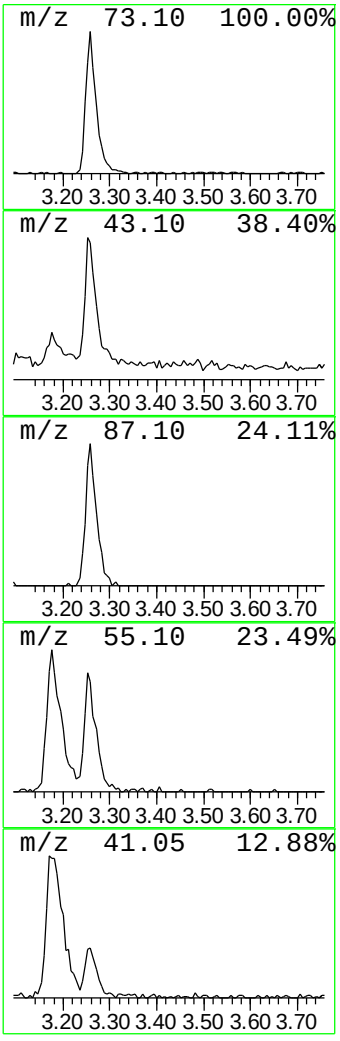
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	7.20 ng	151077	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	28
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042996.D
Acq On : 2 Oct 2019 22:18
Operator : JU
Sample : K5133-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

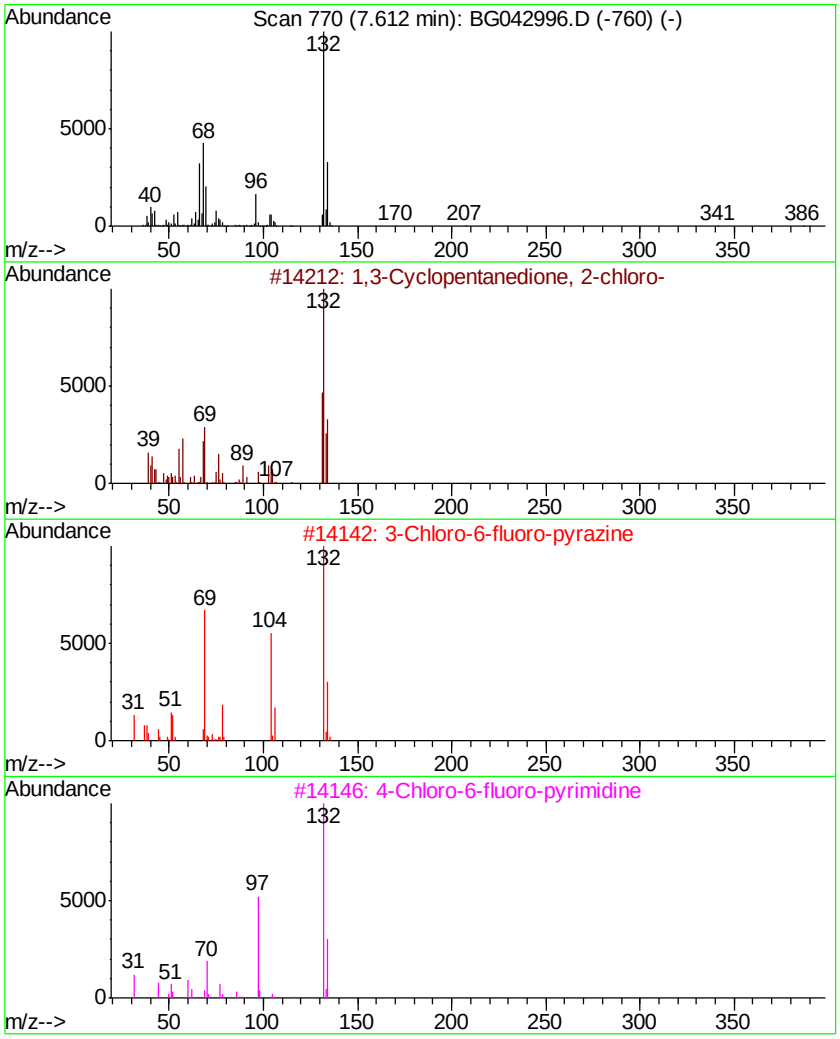
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

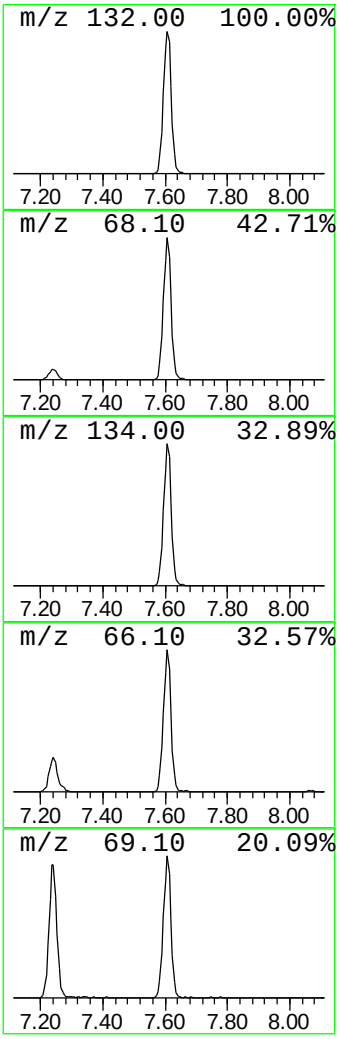
****

Peak Number 3 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	86.92 ng	1823440	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Aminoindole	132	C8H8N2	005192-03-0	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042996.D
Acq On : 2 Oct 2019 22:18
Operator : JU
Sample : K5133-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

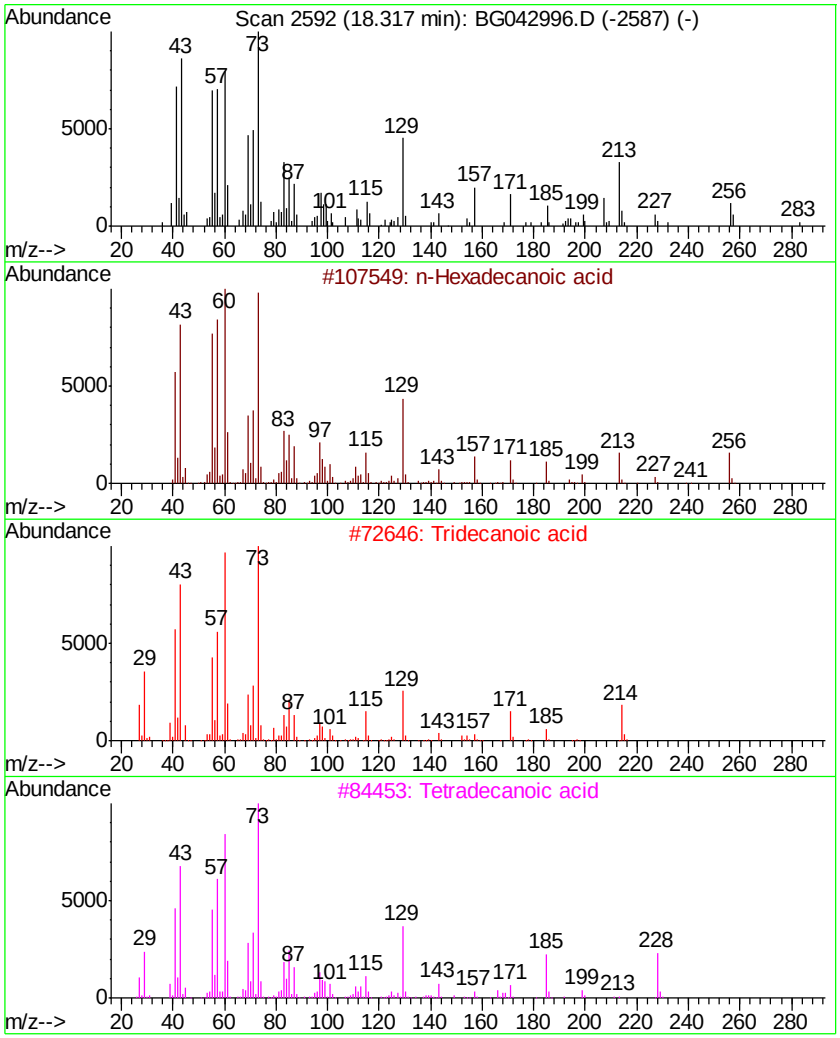
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

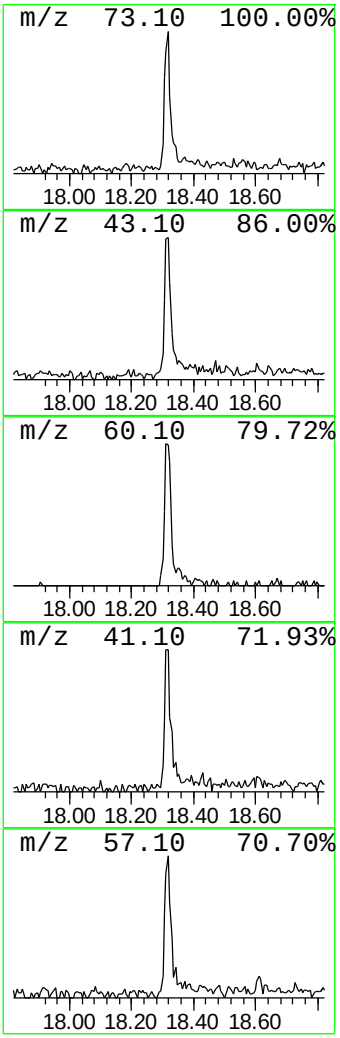
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	2.78 ng	151998	Phenanthrene-d10	17.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	15
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	11





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042996.D
Acq On : 2 Oct 2019 22:18
Operator : JU
Sample : K5133-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

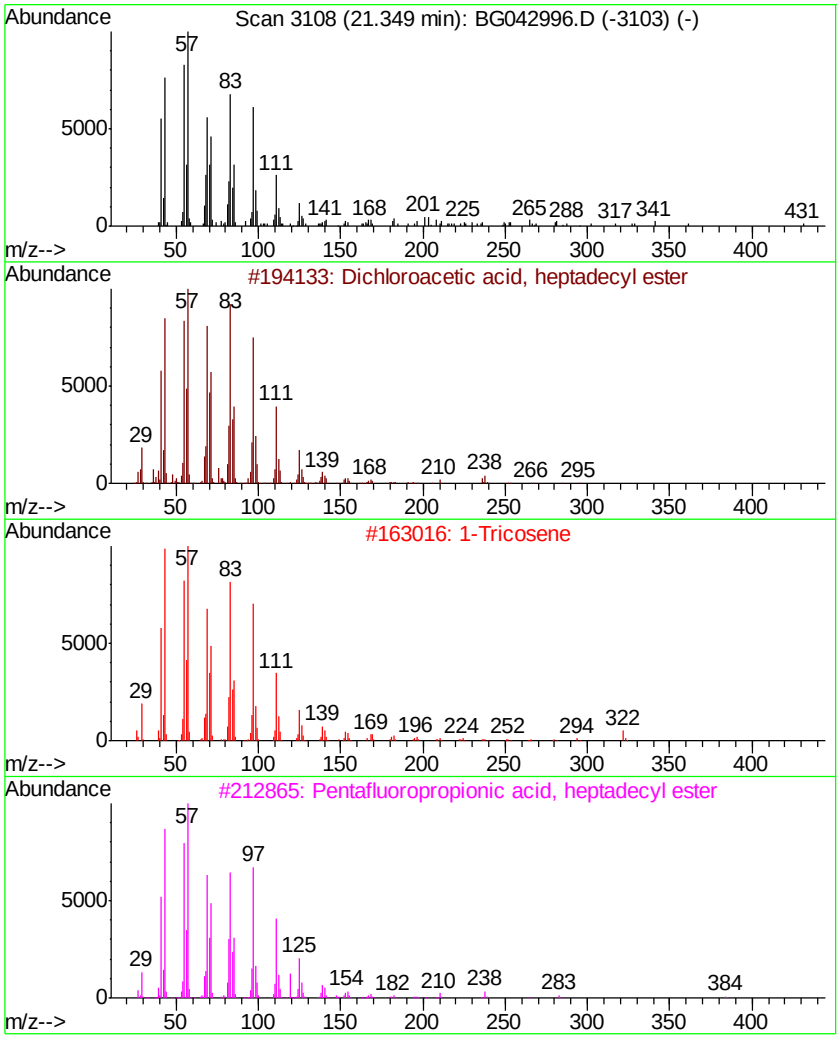
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

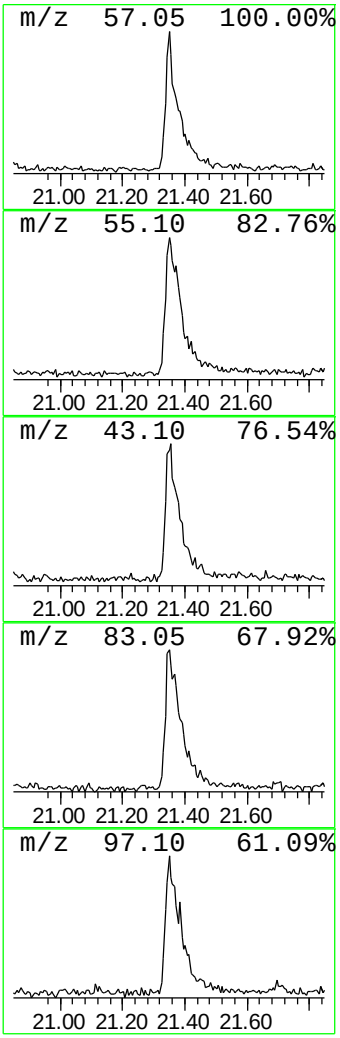
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	6.96 ng	448548	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	1-Tricosene	322	C23H46	018835-32-0	91
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100219\
Data File : BG042996.D
Acq On : 2 Oct 2019 22:18
Operator : JU
Sample : K5133-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

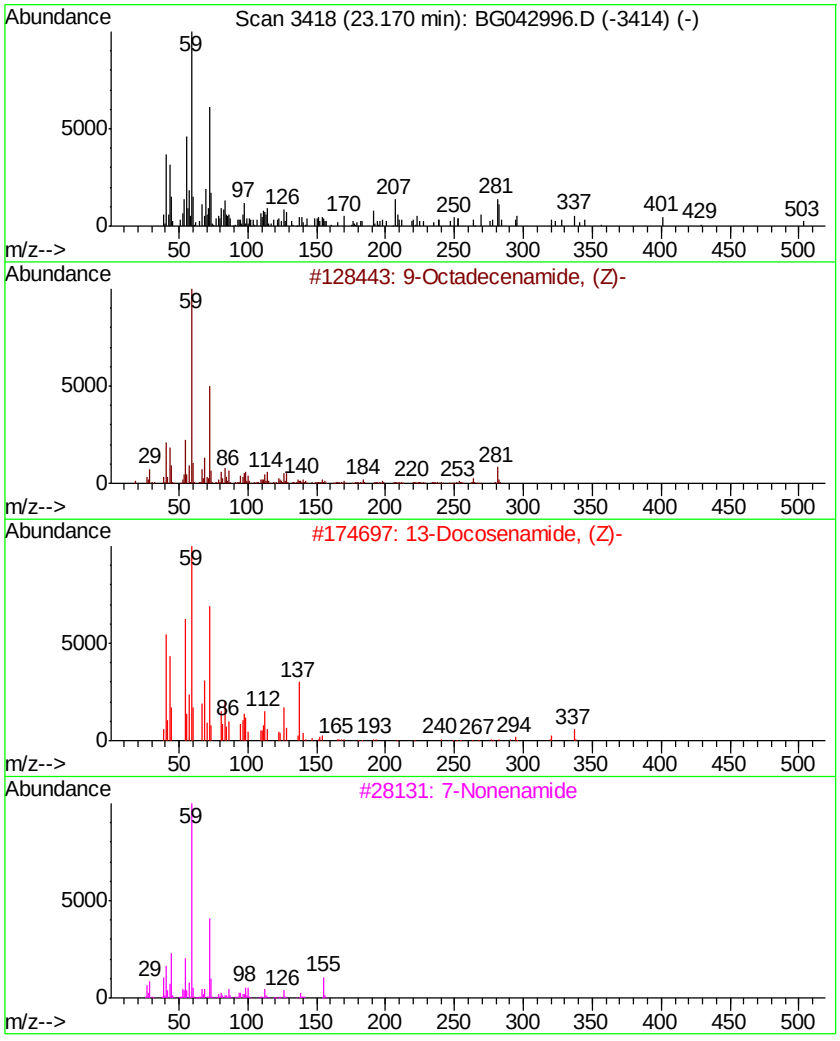
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

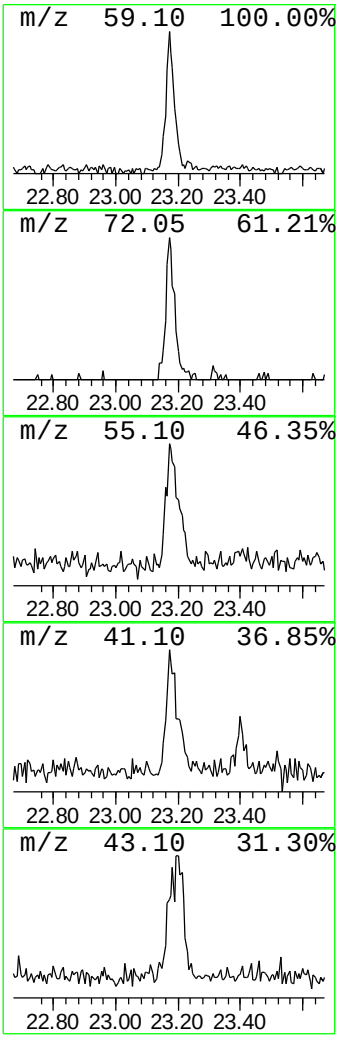
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.17	2.20 ng	141897	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	76
3	7-Nonenamide	155	C9H17NO	090949-53-4	58
4	Tetradecanamide	227	C14H29NO	000638-58-4	47
5	L-Arabinopyranoside phenyl-3,4-O...	282	C14H18O4S	1000163-58-0	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100219\
Data File : BG042996.D
Acq On : 2 Oct 2019 22:18
Operator : JU
Sample : K5133-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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
1-Pentene, 2-methyl-	3.18	11.8	ng	248239	1	8.07	419586	20.0
Butane, 2-methoxy...	3.26	7.2	ng	151077	1	8.07	419586	20.0
unknown7.61	7.61	86.9	ng	1823440	1	8.07	419586	20.0
n-Hexadecanoic acid	18.32	2.8	ng	151998	4	17.43	1092870	20.0
Dichloroacetic ac...	21.35	7.0	ng	448548	5	21.70	1289280	20.0
9-Octadecenamide,...	23.17	2.2	ng	141897	5	21.70	1289280	20.0