LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031218\
Data File : BG033089.D
Acq On : 12 Mar 2018 14:54
Operator : SJ/JU
Sample : J1868-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 030818-TIDO-F-U-B

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-BG022118.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	3.517	32	39	57	rVB	77981	174225	5.44%	1.268%
2	5.820	425	431	436	rBV	22148	34315	1.07%	0.250%
3	6.325	510	517	528	rBV	246316	434201	13.55%	3.160%
4	7.999	794	802	814	rBV	161184	306481	9.56%	2.230%
5	8.416	866	873	884	rBV	461656	851676	26.58%	6.198%
6	8.910	949	957	965	rBV	136045	241554	7.54%	1.758%
7	9.245	1006	1014	1024	rVB	602814	1111961	34.70%	8.093%
8	10.108	1153	1161	1177	rBV	548079	1020429	31.84%	7.426%
9	11.794	1440	1448	1457	rBV	203218	368998	11.51%	2.685%
10	14.150	1842	1849	1857	rBV	1408972	2262736	70.60%	16.468%
11	14.943	1977	1984	1989	rBV	29917	46007	1.44%	0.335%
12	15.524	2077	2083	2091	rVB2	294051	495445	15.46%	3.606%
13	16.288	2207	2213	2220	rVB2	25204	34873	1.09%	0.254%
14	16.993	2326	2333	2346	rBV	716196	1121926	35.01%	8.165%
15	17.146	2353	2359	2368	rVB	20944	34593	1.08%	0.252%
16	18.250	2540	2547	2556	rBV2	400438	619360	19.33%	4.508%
17	19.049	2676	2683	2687	rBV2	21386	33126	1.03%	0.241%
18	20.770	2969	2976	2986	rBV	2248772	3204796	100.00%	23.324%
19	22.127	3202	3207	3217	rBV7	23418	74908	2.34%	0.545%
20	22.603	3280	3288	3299	rBV2	325631	655425	20.45%	4.770%
21	26.398	3921	3934	3954	rBV2	159651	613475	19.14%	4.465%

Sum of corrected areas: 13740510

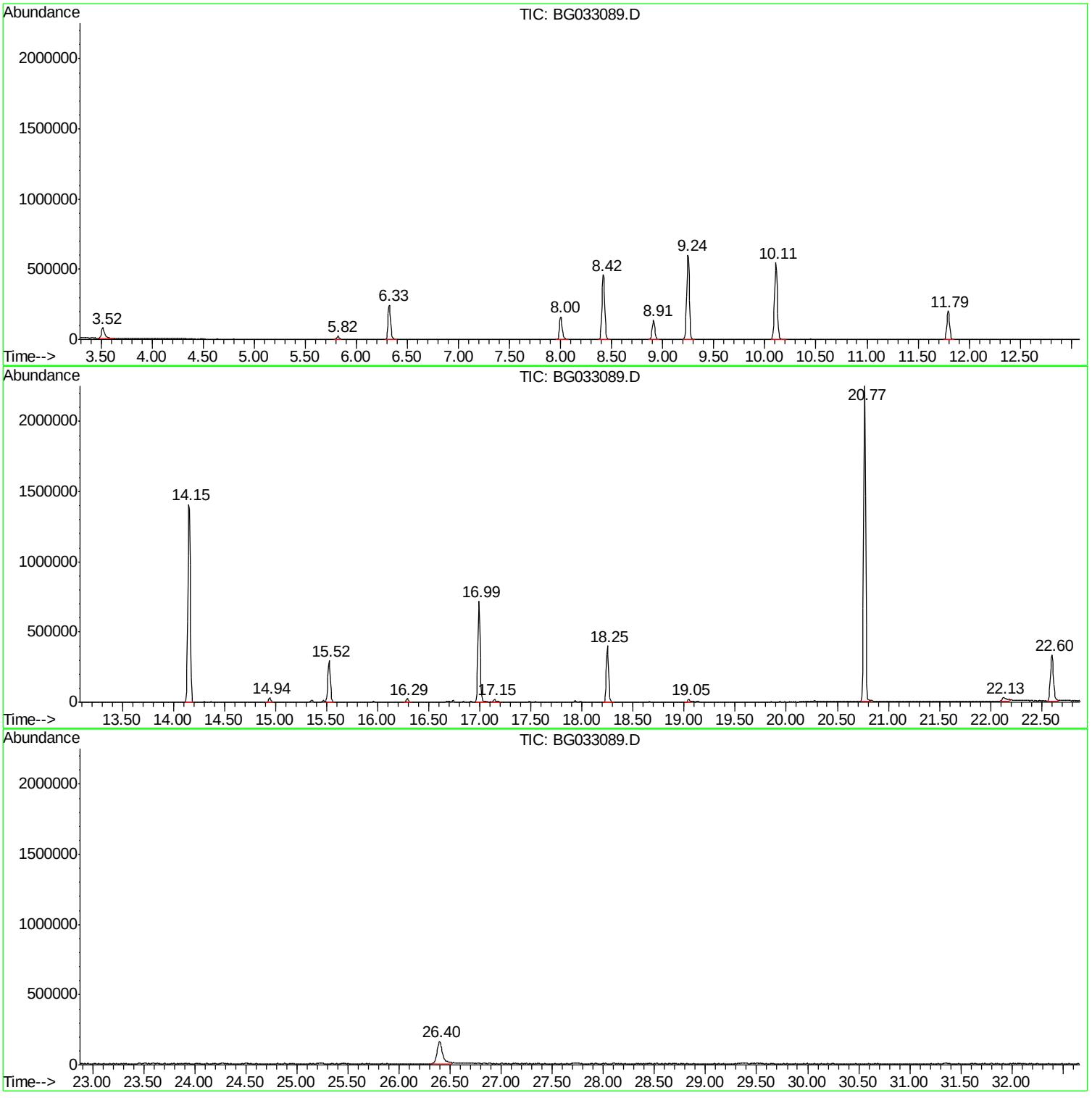
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031218\
Data File : BG033089.D
Acq On : 12 Mar 2018 14:54
Operator : SJ/JU
Sample : J1868-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 030818-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.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\BG031218\
Data File : BG033089.D
Acq On : 12 Mar 2018 14:54
Operator : SJ/JU
Sample : J1868-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 030818-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

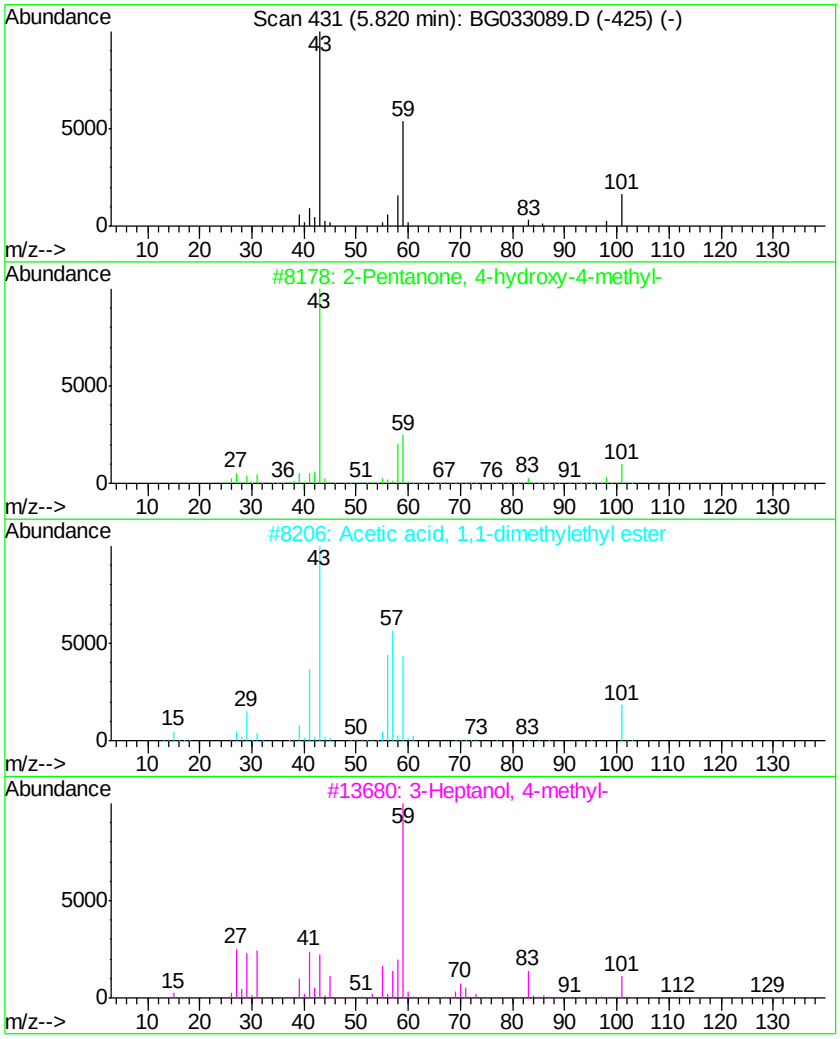
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

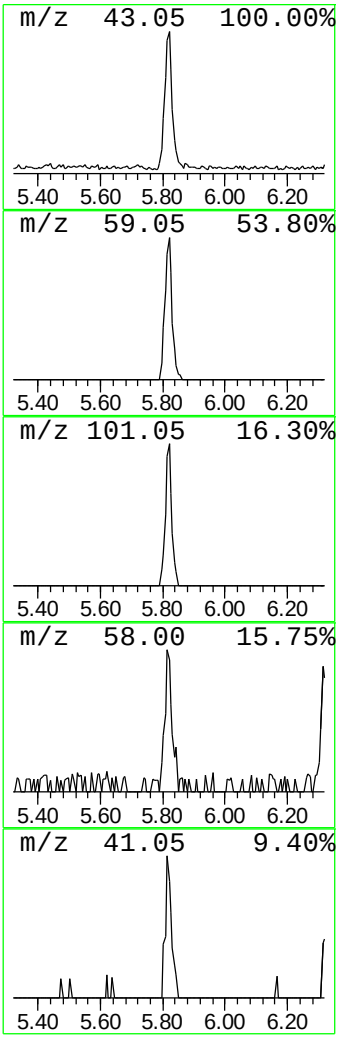
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	2.84 ng	34315	1,4-Dichlorobenzene-d4	8.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031218\
Data File : BG033089.D
Acq On : 12 Mar 2018 14:54
Operator : SJ/JU
Sample : J1868-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 030818-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

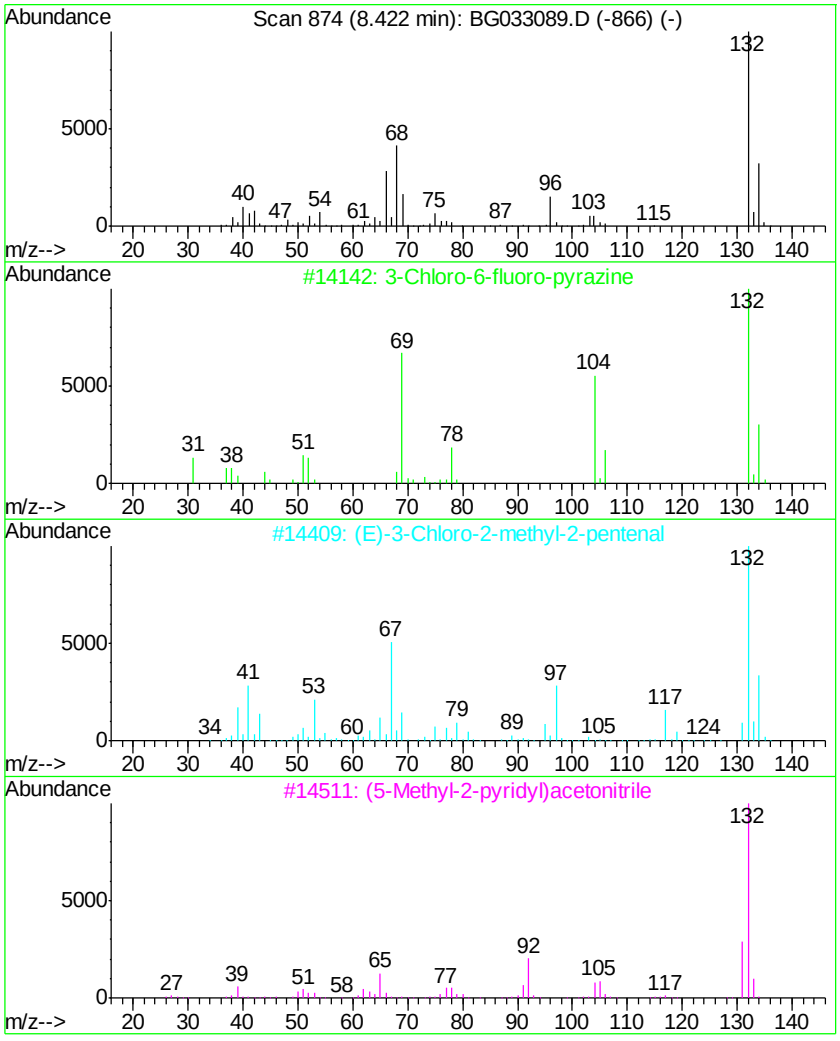
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

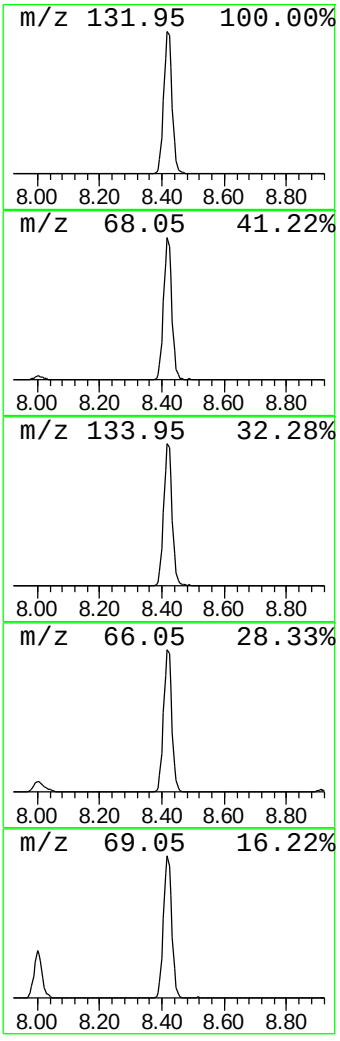
****

Peak Number 3 unknown8.42 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	70.52 ng	851676	1,4-Dichlorobenzene-d4	8.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031218\
Data File : BG033089.D
Acq On : 12 Mar 2018 14:54
Operator : SJ/JU
Sample : J1868-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 030818-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

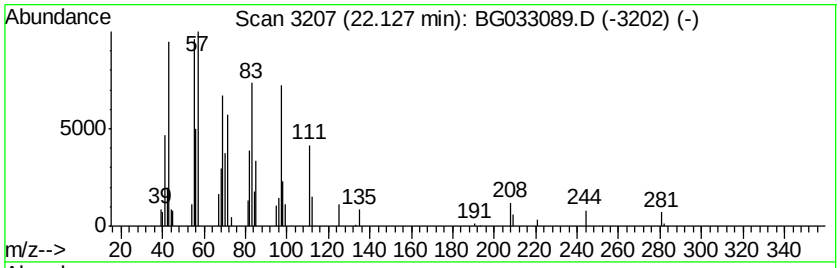
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

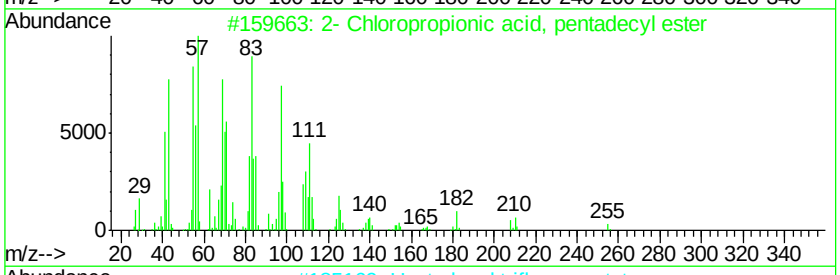
****

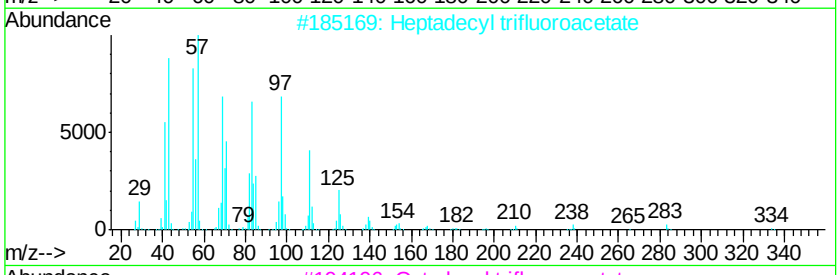
Peak Number 5 2- Chloropropionic acid, pe... Concentration Rank 5

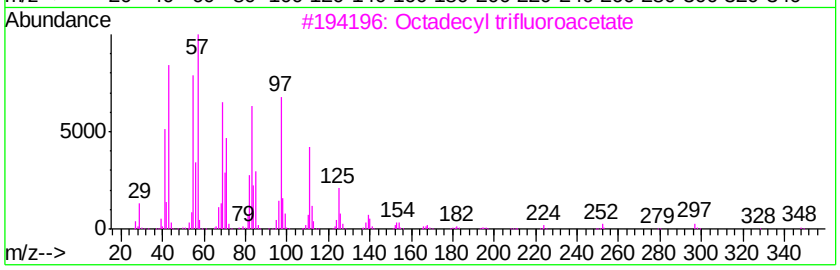
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.13	2.29 ng	74908	Chrysene-d12	22.60

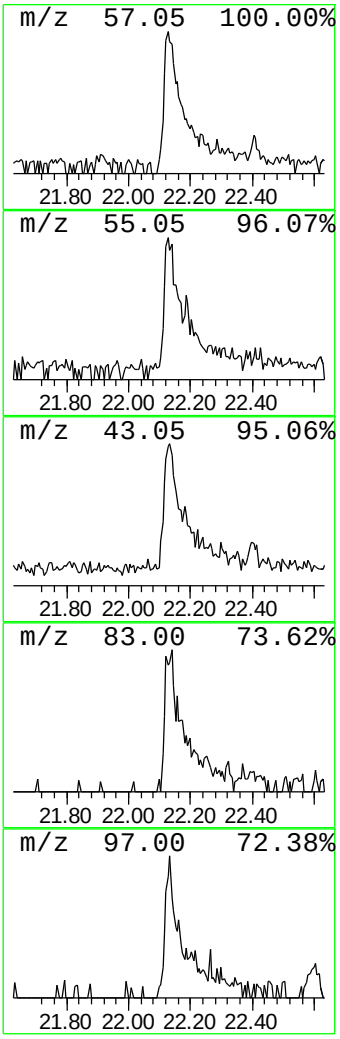
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
4	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	90
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG031218\
Data File : BG033089.D
Acq On : 12 Mar 2018 14:54
Operator : SJ/JU
Sample : J1868-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 030818-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.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...	5.82	2.8	ng	34315	1	8.91	241554	20.0
unknown8.42	8.42	70.5	ng	851676	1	8.91	241554	20.0
2- Chloropropioni...	22.13	2.3	ng	74908	5	22.60	655425	20.0