LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120318\
Data File : BG038311.D
Acq On : 3 Dec 2018 22:19
Operator : JU/SJ
Sample : J6179-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S2-0-0.5-BGS

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-BG111318.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	5.155	313	318	323	rBV	14083	22848	1.21%	0.266%
2	5.619	391	397	410	rVB	271092	486693	25.67%	5.665%
3	7.223	663	670	681	rBV	306550	614059	32.39%	7.147%
4	7.599	727	734	747	rBV	282339	540054	28.49%	6.286%
5	8.075	808	815	828	rBV	64013	120761	6.37%	1.406%
6	8.398	863	870	880	rBV	244052	431908	22.78%	5.027%
7	9.250	1008	1015	1026	rBV	193827	389937	20.57%	4.538%
8	10.895	1288	1295	1306	rBV	86496	164692	8.69%	1.917%
9	13.334	1703	1710	1721	rBV	520339	837457	44.17%	9.747%
10	14.156	1844	1850	1858	rBV	69118	108293	5.71%	1.260%
11	14.714	1937	1945	1953	rVB2	157097	272282	14.36%	3.169%
12	16.201	2191	2198	2214	rBV	535890	854705	45.08%	9.948%
13	17.458	2405	2412	2424	rVB2	291689	461333	24.33%	5.369%
14	18.316	2553	2558	2567	rBV2	59670	100184	5.28%	1.166%
15	19.585	2769	2774	2780	rBV4	28752	48364	2.55%	0.563%
16	20.061	2849	2855	2861	rBV	1443912	1895784	100.00%	22.065%
17	21.342	3067	3073	3086	rBV2	44297	106802	5.63%	1.243%
18	21.741	3133	3141	3151	rBV	320449	574131	30.28%	6.682%
19	23.204	3385	3390	3396	rBV6	10651	22008	1.16%	0.256%
20	25.061	3688	3706	3718	rBV	171912	539490	28.46%	6.279%

Sum of corrected areas: 8591785

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Misc :
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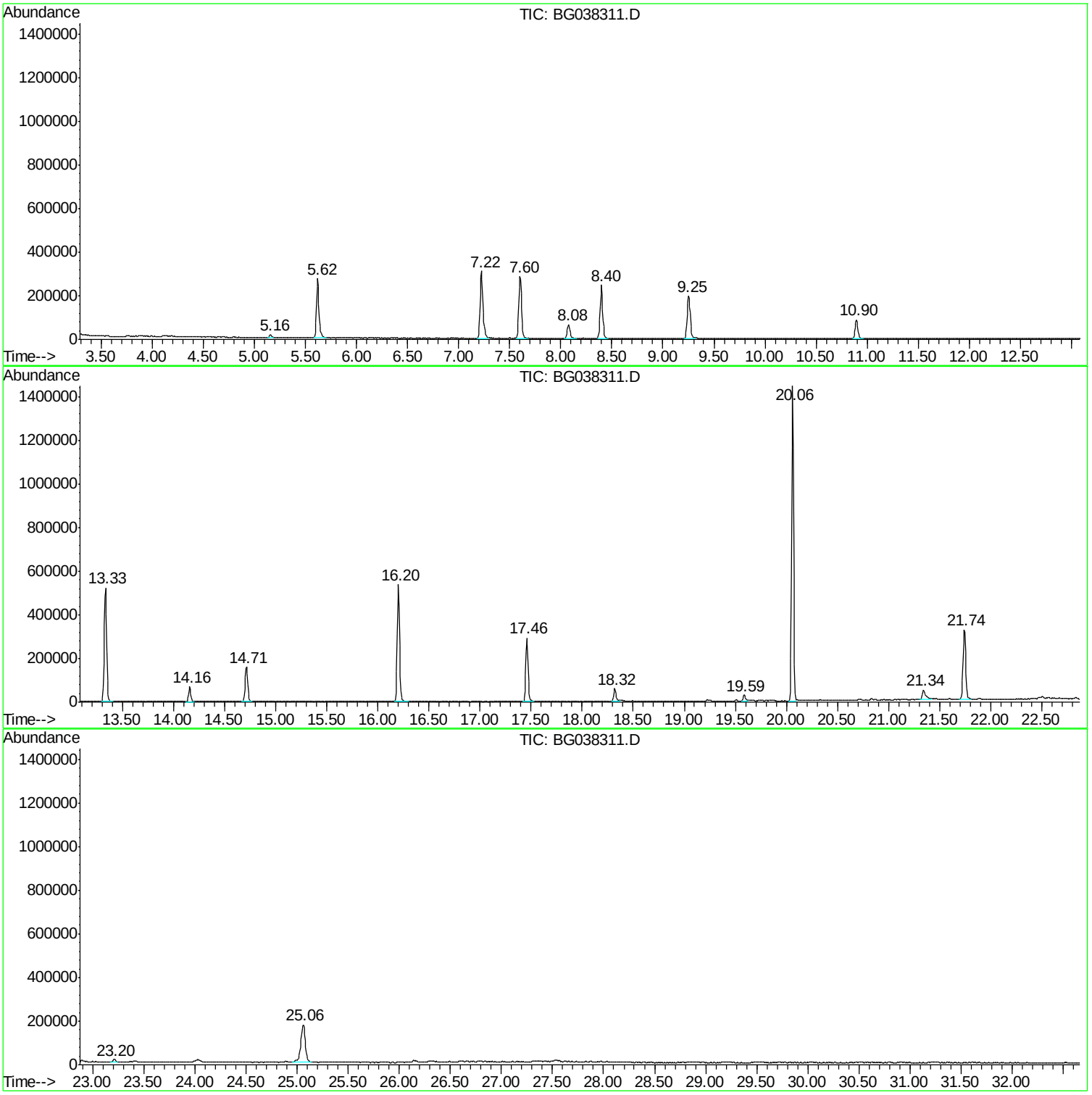
Instrument :
BNA_G
ClientSampleId :
S2-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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

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Data File : BG038311.D
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Misc :
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Instrument : BNA_G
ClientSampleId : S2-0-0.5-BGS

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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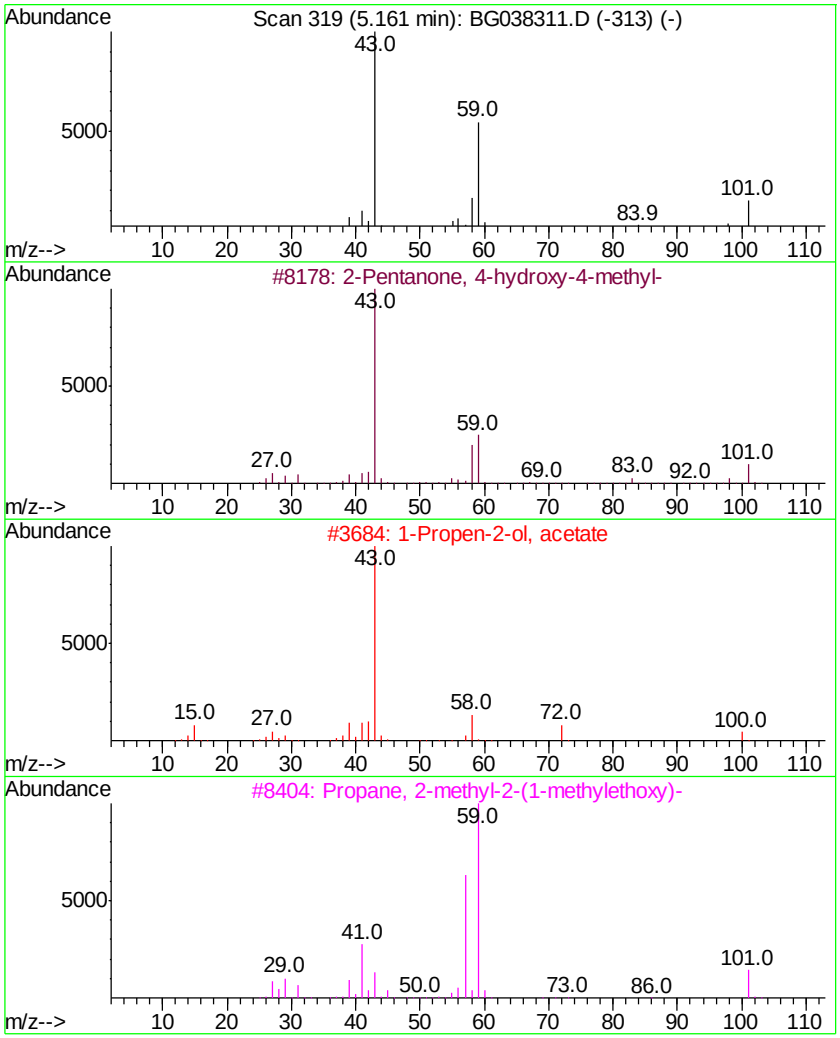
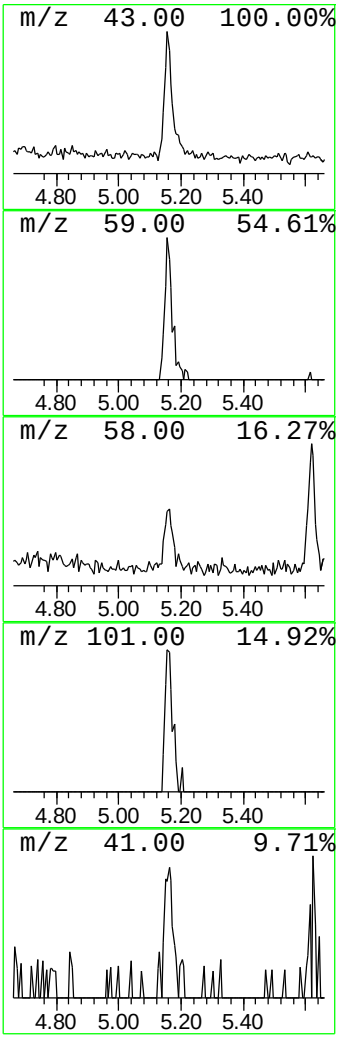
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	3.78 ng	22848	1,4-Dichlorobenzene-d4	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
4	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : S2-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
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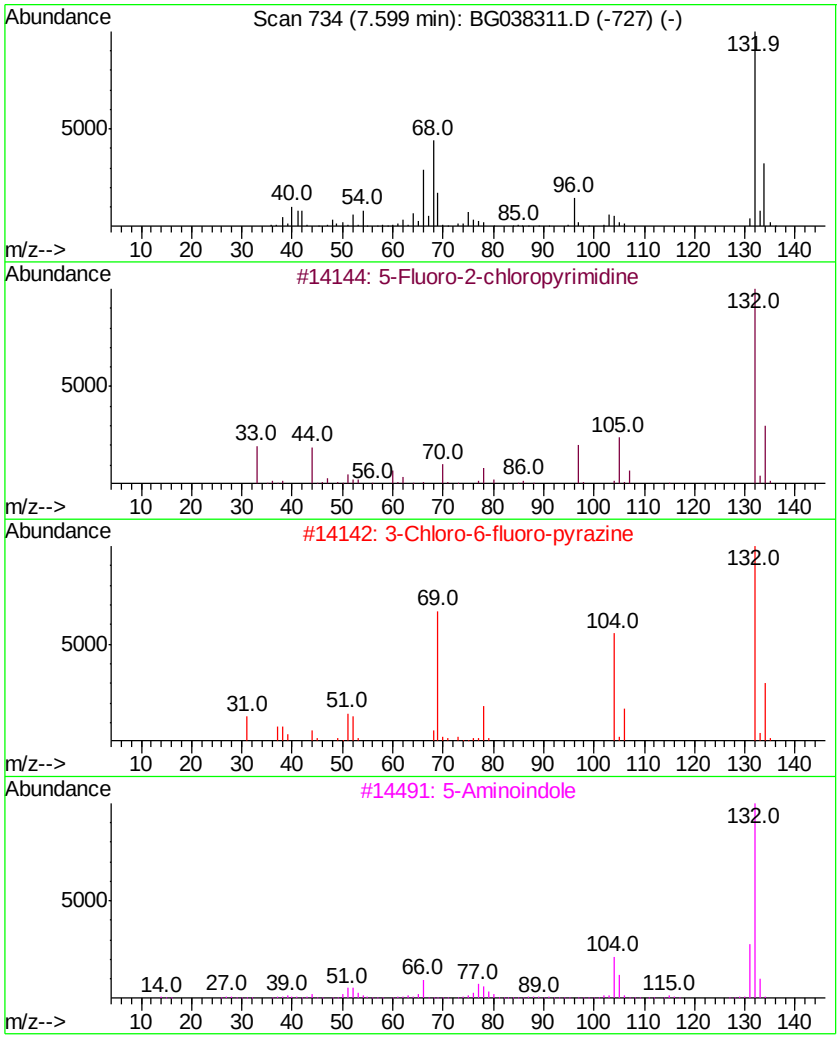
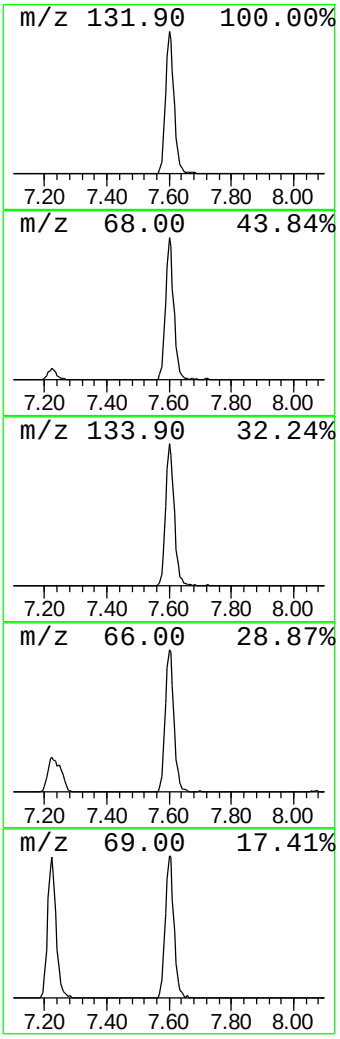
Peak Number 2 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	89.44 ng	540054	1,4-Dichlorobenzene-d4	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	10





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Sample : J6179-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S2-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
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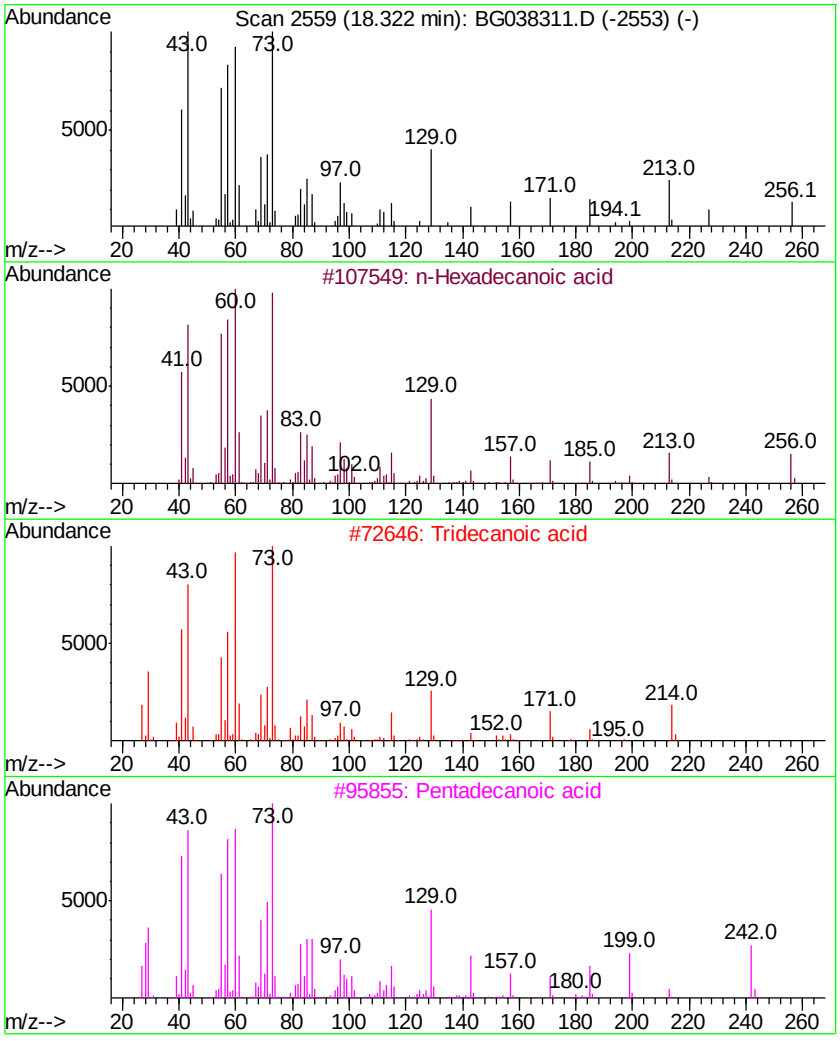
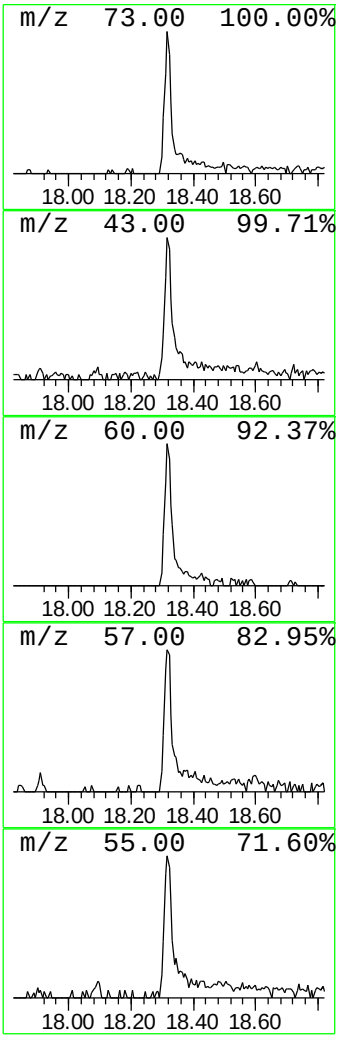
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	4.34 ng	100184	Phenanthrene-d10	17.46

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	52





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Sample : J6179-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S2-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
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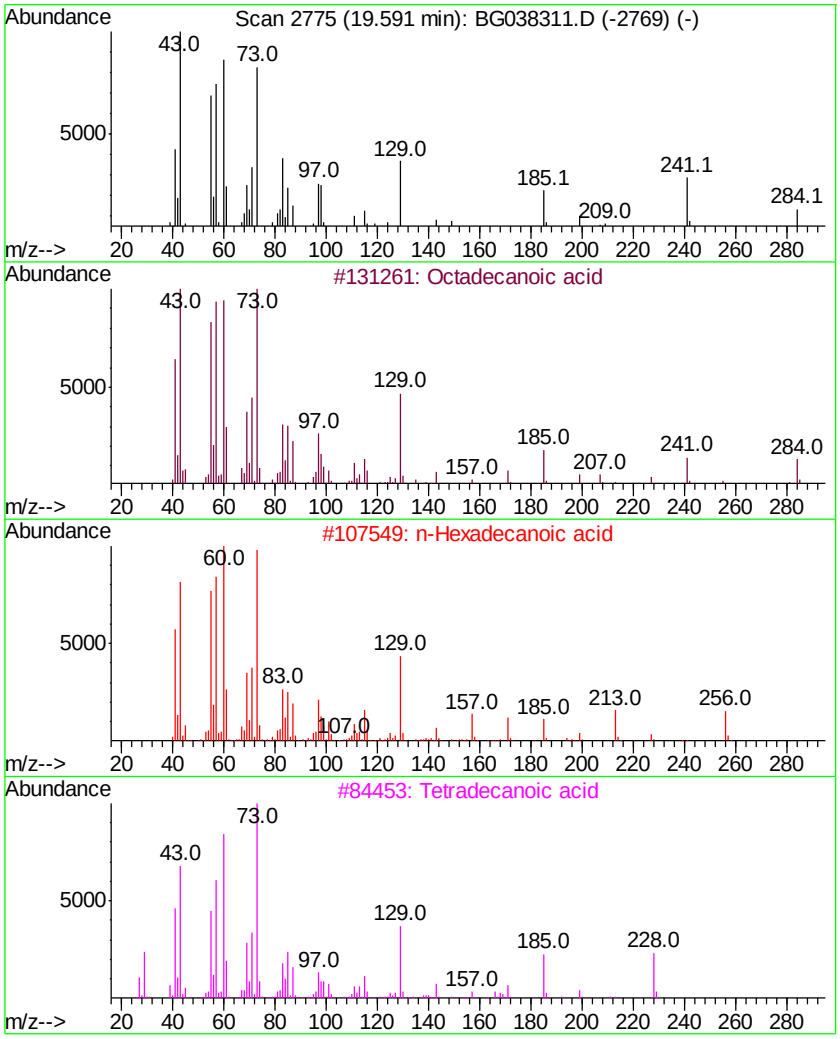
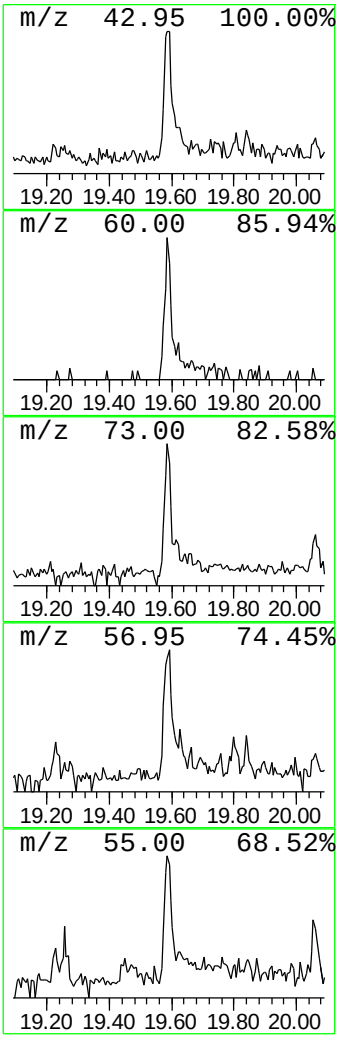
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	2.10 ng	48364	Phenanthrene-d10	17.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S2-0-0.5-BGS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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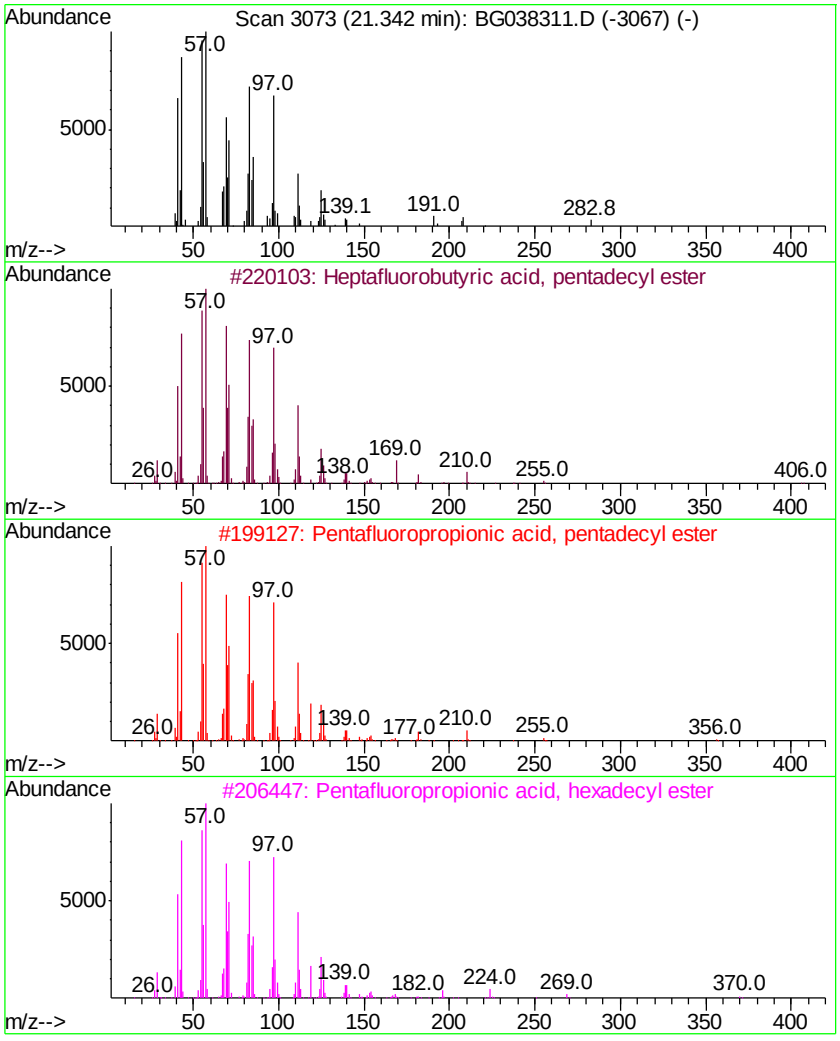
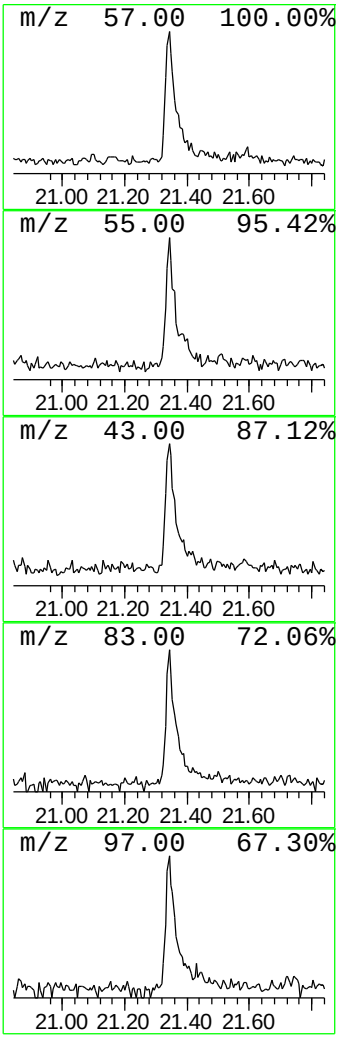
Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.34	3.72 ng	106802	Chrysene-d12	21.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Tentatively Identified Compound (LSC) summary

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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...	5.16	3.8	ng	22848	1	8.08	120761	20.0
unknown7.60	7.60	89.4	ng	540054	1	8.08	120761	20.0
n-Hexadecanoic acid	18.32	4.3	ng	100184	4	17.46	461333	20.0
Octadecanoic acid	19.59	2.1	ng	48364	4	17.46	461333	20.0
Heptafluorobutyri...	21.34	3.7	ng	106802	5	21.74	574131	20.0