LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056356.D
Acq On : 19 Jan 2023 21:10
Operator : CG/JU
Sample : 01220-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-G

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-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056356.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.312	3	4	17	rVB	99392	125061	5.57%	1.236%
2	5.345	343	350	359	rVB	90513	140475	6.26%	1.388%
3	5.827	425	432	442	rBV	370668	602639	26.85%	5.956%
4	7.443	700	707	716	rBV	383517	647160	28.83%	6.396%
5	8.306	846	854	863	rBB	114988	194842	8.68%	1.926%
6	9.475	1045	1053	1065	rBB	215982	390381	17.39%	3.858%
7	11.138	1328	1336	1344	rBV	157234	278555	12.41%	2.753%
8	13.541	1738	1745	1757	rBB	847869	1301505	57.98%	12.863%
9	14.916	1972	1979	1988	rVB	306924	476295	21.22%	4.707%
10	16.256	2201	2207	2213	rVB2	19894	30477	1.36%	0.301%
11	16.397	2224	2231	2243	rBV	685153	1017676	45.34%	10.058%
12	17.654	2437	2445	2451	rBV	442056	652618	29.07%	6.450%
13	18.500	2584	2589	2596	rBV	75600	117463	5.23%	1.161%
14	19.752	2799	2802	2807	rBV5	25815	34654	1.54%	0.342%
15	20.051	2849	2853	2858	rVB	18685	29360	1.31%	0.290%
16	20.228	2877	2883	2889	rBV	1736256	2244671	100.00%	22.185%
17	20.892	2989	2996	3005	rBV	196271	280082	12.48%	2.768%
18	21.526	3100	3104	3115	rVB2	82118	135558	6.04%	1.340%
19	21.949	3169	3176	3183	rBV	403467	699097	31.14%	6.909%
20	25.386	3752	3761	3773	rVB	239984	719440	32.05%	7.110%

Sum of corrected areas: 10118009

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Instrument :
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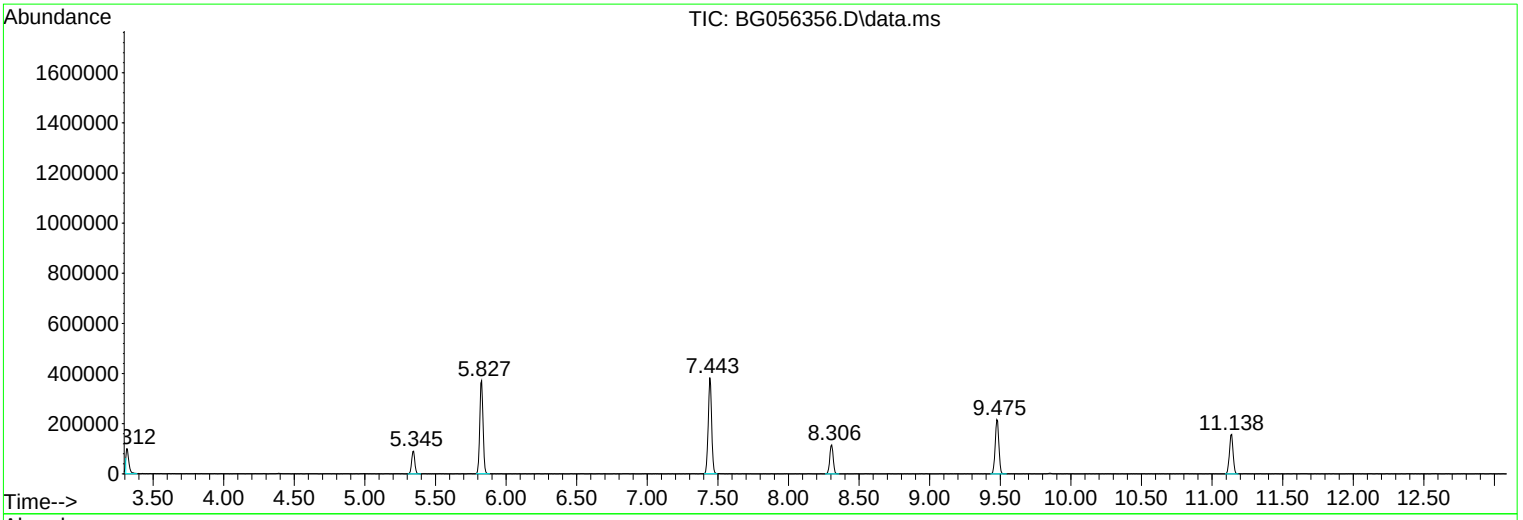
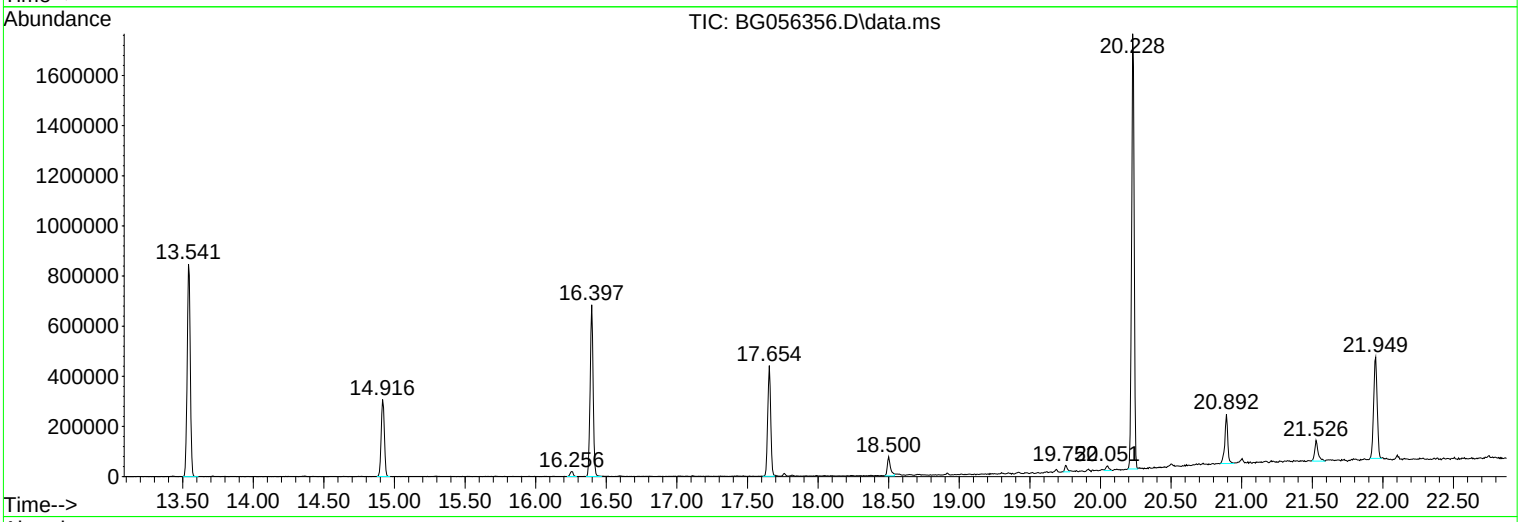
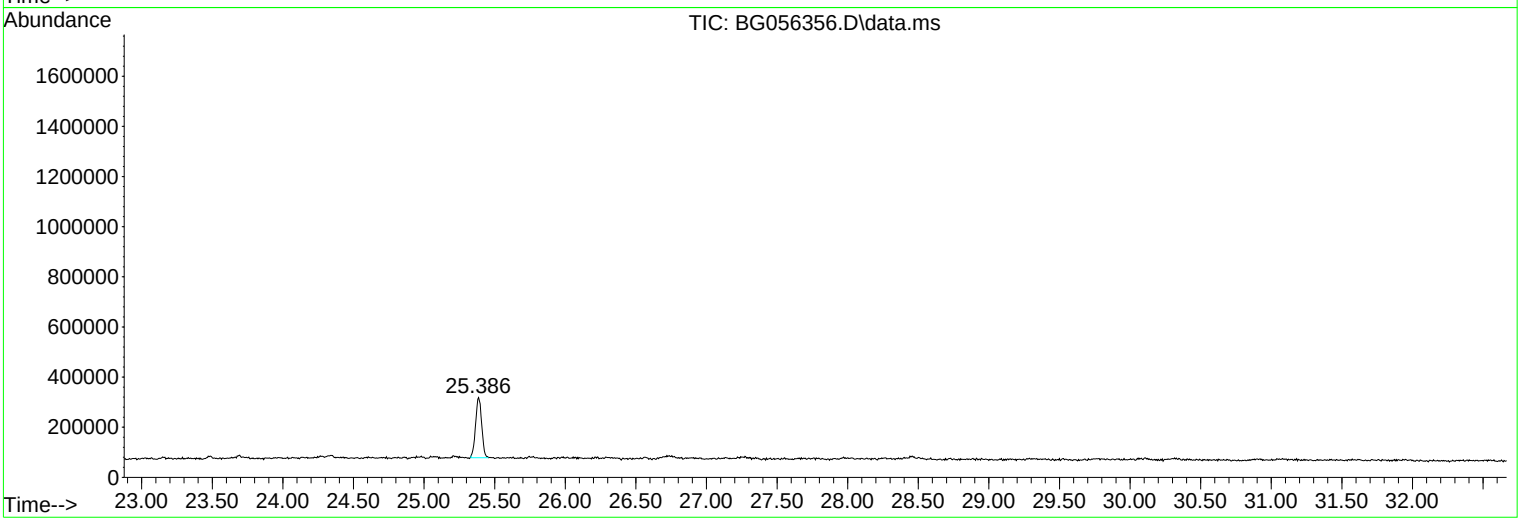
ClientSampleId :
TP-G

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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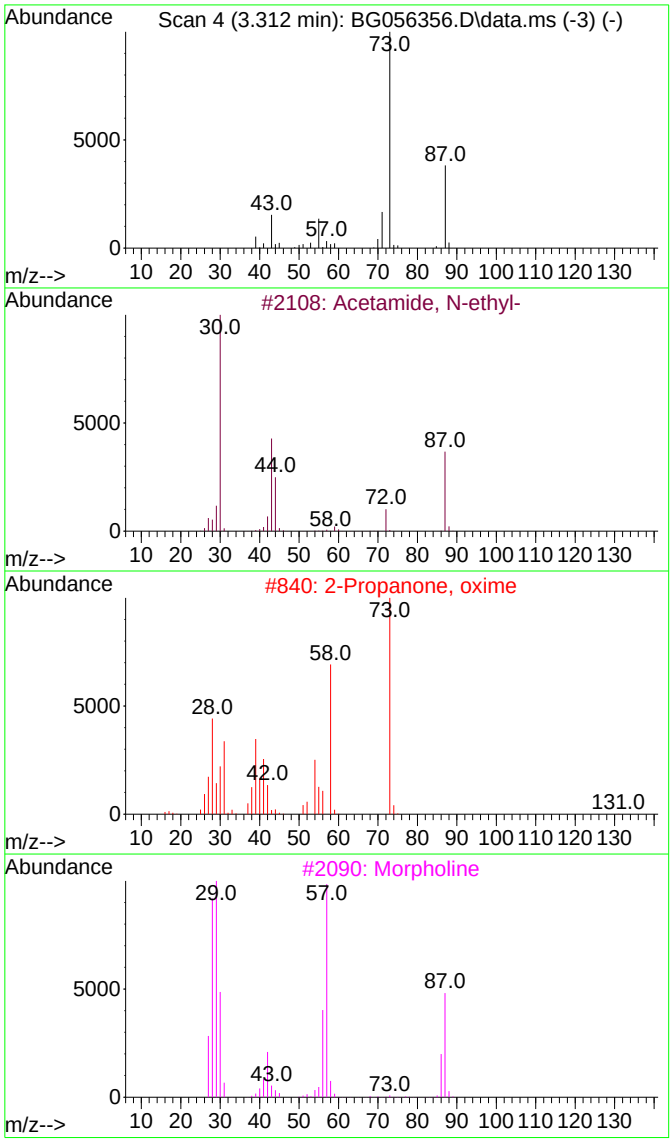
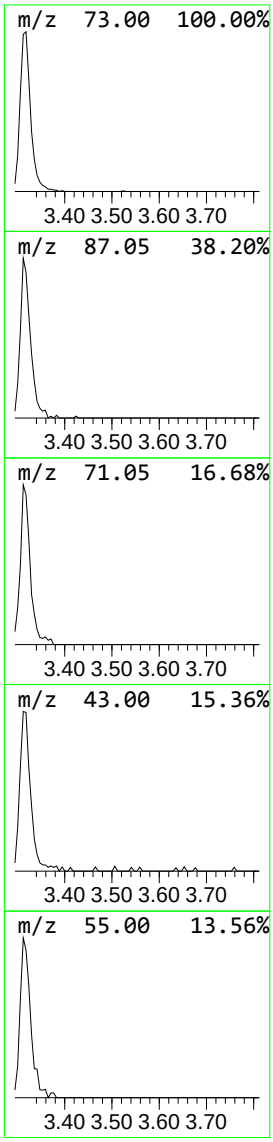
****

Peak Number 1 unknown3.312 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.312	12.84 ng	125061	1,4-Dichlorobenzene-d4	8.306

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
2	2-Propanone, oxime	73	C3H7NO	000127-06-0	7
3	Morpholine	87	C4H9NO	000110-91-8	5
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	4





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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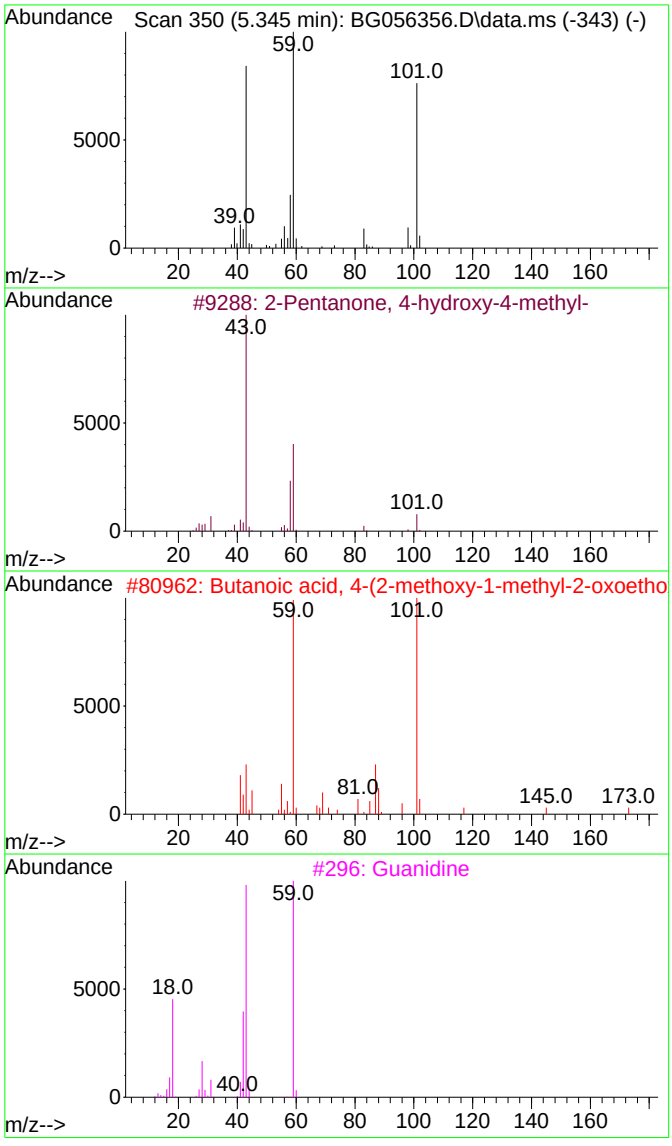
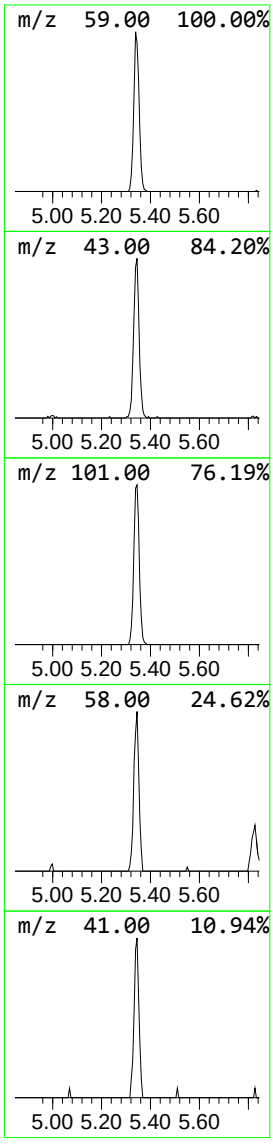
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.345	14.42 ng	140475	1,4-Dichlorobenzene-d4	8.306

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	36
3	Guanidine	59	CH5N3	000113-00-8	17
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	16
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16





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Operator : CG/JU
Sample : 01220-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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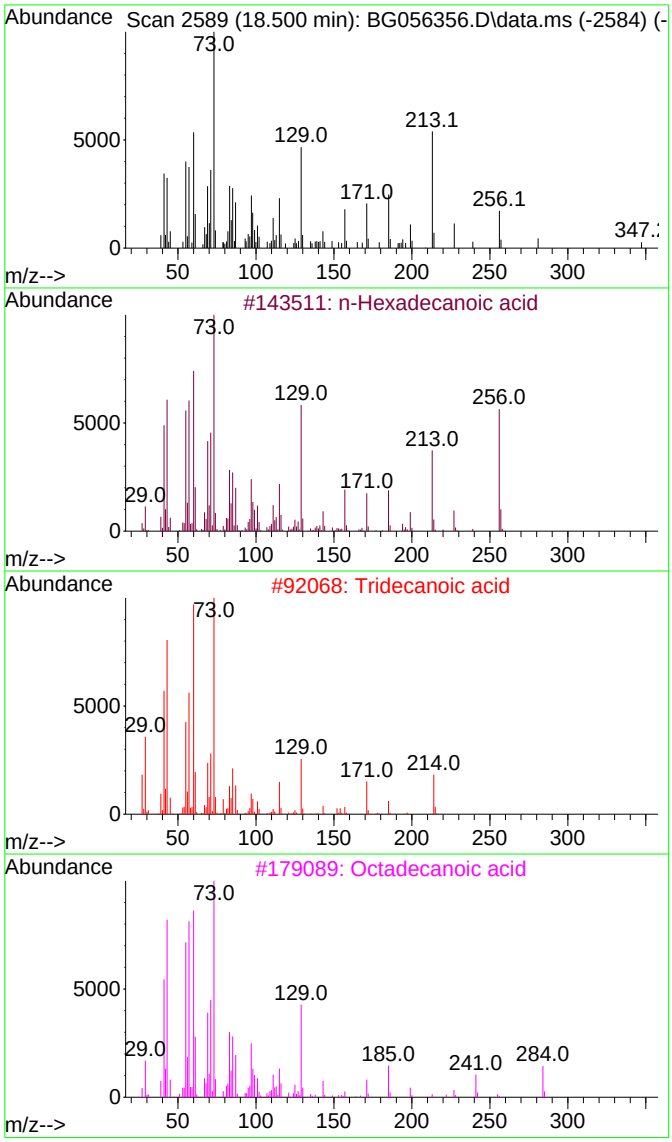
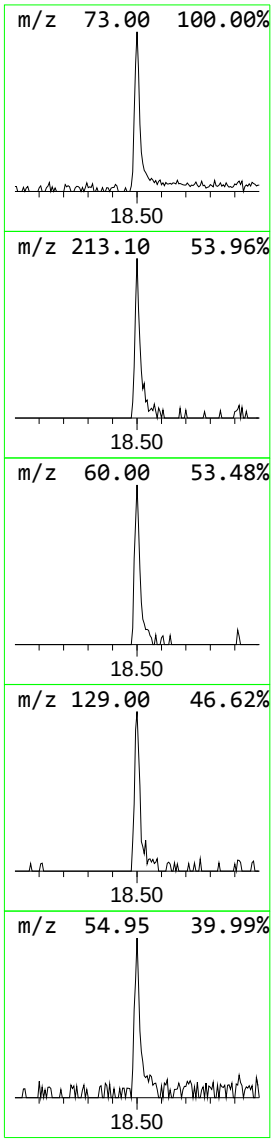
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.500	3.60 ng	117463	Phenanthrene-d10	17.654

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	50
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





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TIC Library : C:\Database\NIST20.L
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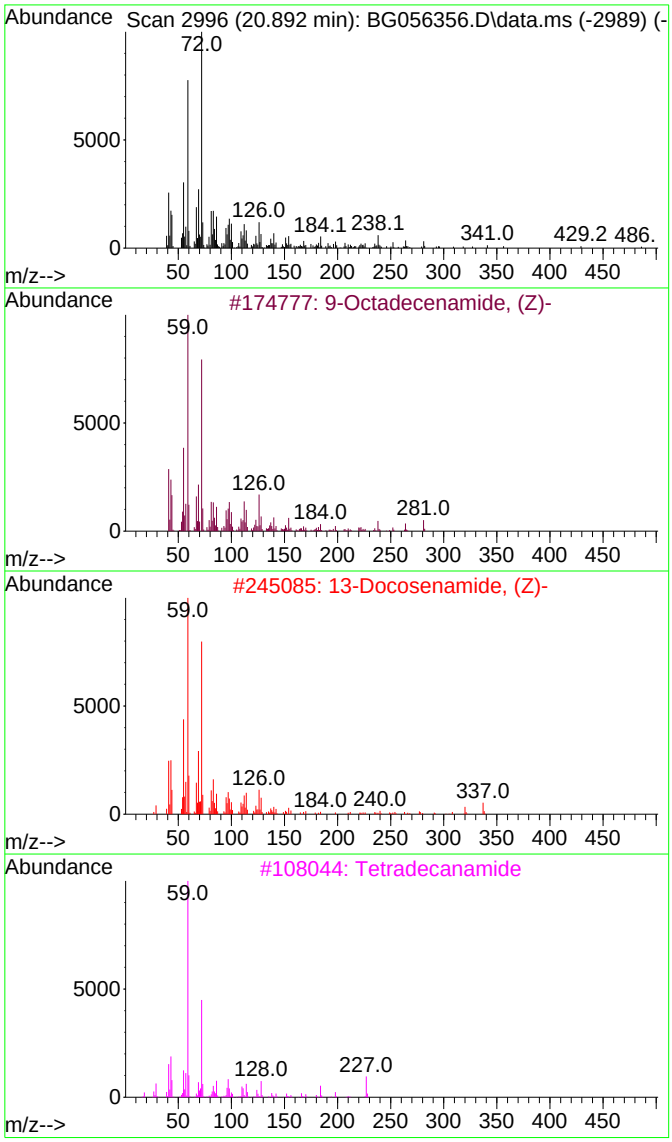
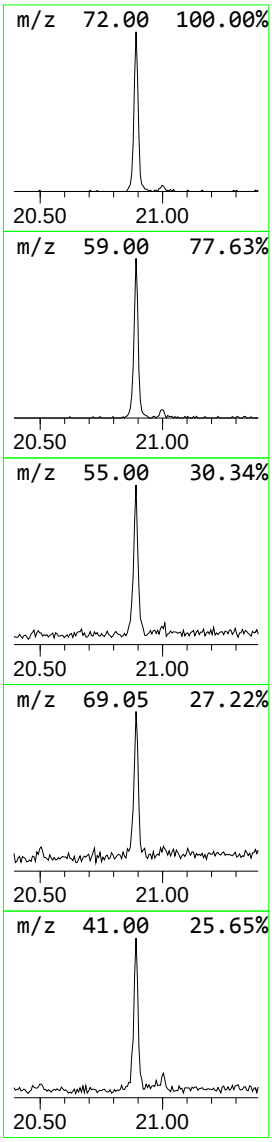
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	8.01 ng	280082	Chrysene-d12	21.949

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	52
3	Tetradecanamide	227	C14H29NO	000638-58-4	43
4	Dodecanamide	199	C12H25NO	001120-16-7	41
5	Octanamide	143	C8H17NO	000629-01-6	38





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Instrument :
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ClientSampleId :
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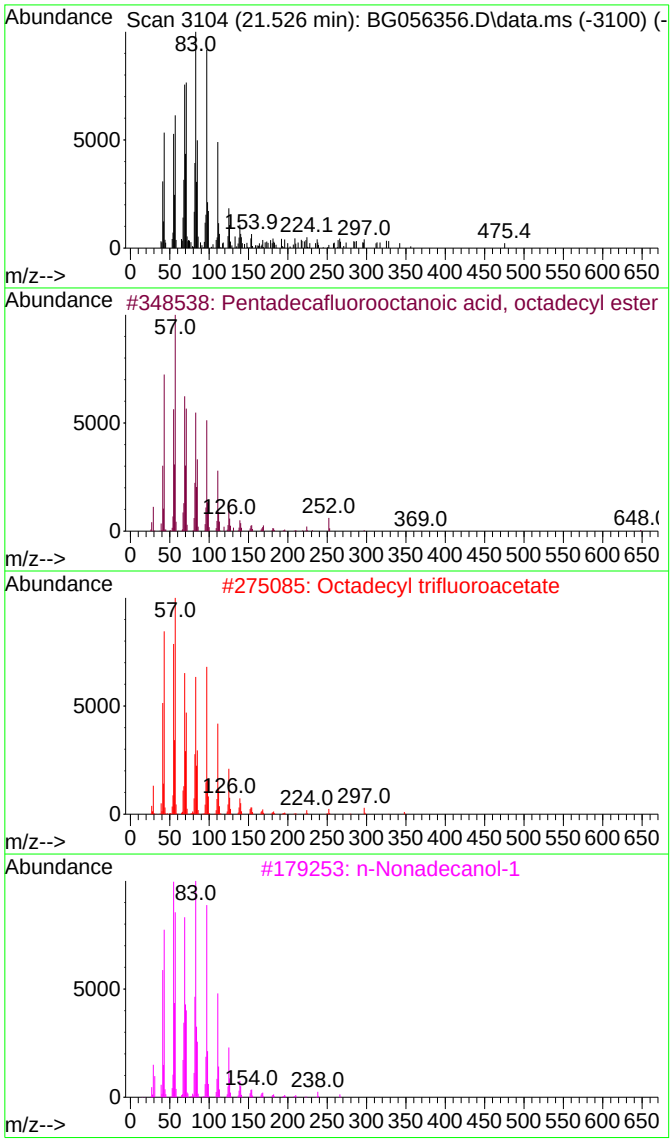
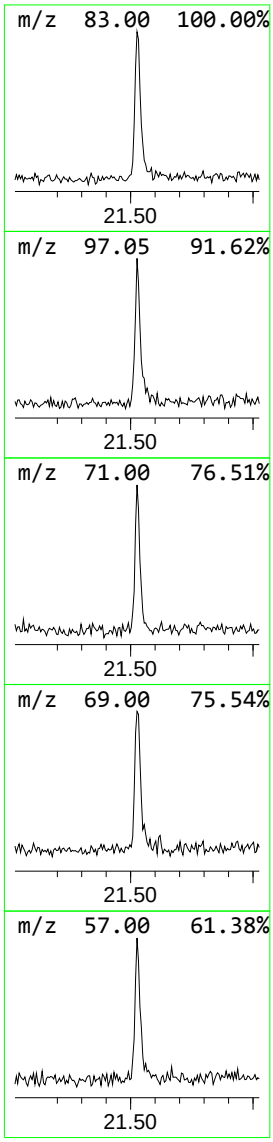
****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.526	3.88 ng	135558	Chrysene-d12	21.949

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	83
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	83
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	83
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	83





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.312	3.312	12.8	ng	125061	1	8.306	194842	20.0
2-Pentanone, 4-...	5.345	14.4	ng	140475	1	8.306	194842	20.0
n-Hexadecanoic ...	18.500	3.6	ng	117463	4	17.654	652618	20.0
9-Octadecenamid...	20.892	8.0	ng	280082	5	21.949	699097	20.0
Pentadecafluoro...	21.526	3.9	ng	135558	5	21.949	699097	20.0