LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090418\
Data File : BG036533.D
Acq On : 4 Sep 2018 15:52
Operator : JU/SJ
Sample : J4748-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12

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-BG082318.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	5.163	312	319	326	rBV2	56106	85322	1.78%	0.317%
2	5.627	389	398	411	rBV	1301070	2068609	43.09%	7.675%
3	7.214	660	668	680	rBV	1335403	2325467	48.44%	8.628%
4	7.590	723	732	739	rBV	1251333	2137712	44.53%	7.932%
5	8.060	803	812	819	rBV	213116	362767	7.56%	1.346%
6	8.383	858	867	878	rVB	893696	1573884	32.78%	5.840%
7	9.217	1001	1009	1023	rBV	782172	1397477	29.11%	5.185%
8	10.863	1281	1289	1297	rVB	297767	520963	10.85%	1.933%
9	13.307	1698	1705	1715	rBV	2047946	3197045	66.59%	11.862%
10	14.129	1837	1845	1851	rBV	413084	596816	12.43%	2.214%
11	14.682	1929	1939	1947	rBV2	478596	744321	15.50%	2.762%
12	16.168	2185	2192	2201	rBV	1799442	2660067	55.41%	9.870%
13	17.425	2399	2406	2415	rBV	669026	991683	20.66%	3.679%
14	18.313	2551	2557	2566	rBV	123738	189786	3.95%	0.704%
15	20.034	2843	2850	2862	rBV	3630886	4801032	100.00%	17.813%
16	21.344	3068	3073	3096	rBV4	156267	465939	9.70%	1.729%
17	21.691	3125	3132	3145	rVB	674402	1157445	24.11%	4.294%
18	21.891	3161	3166	3171	rVB2	63855	94403	1.97%	0.350%
19	22.502	3265	3270	3274	rBV	61060	94286	1.96%	0.350%
20	23.201	3383	3389	3395	rVB	57438	103664	2.16%	0.385%
21	24.000	3519	3525	3532	rBV4	45011	97188	2.02%	0.361%
22	24.899	3668	3678	3696	rVB2	390548	1186766	24.72%	4.403%
23	26.086	3869	3880	3890	rBV5	29789	99526	2.07%	0.369%

Sum of corrected areas: 26952168

LSC Report - Integrated Chromatogram

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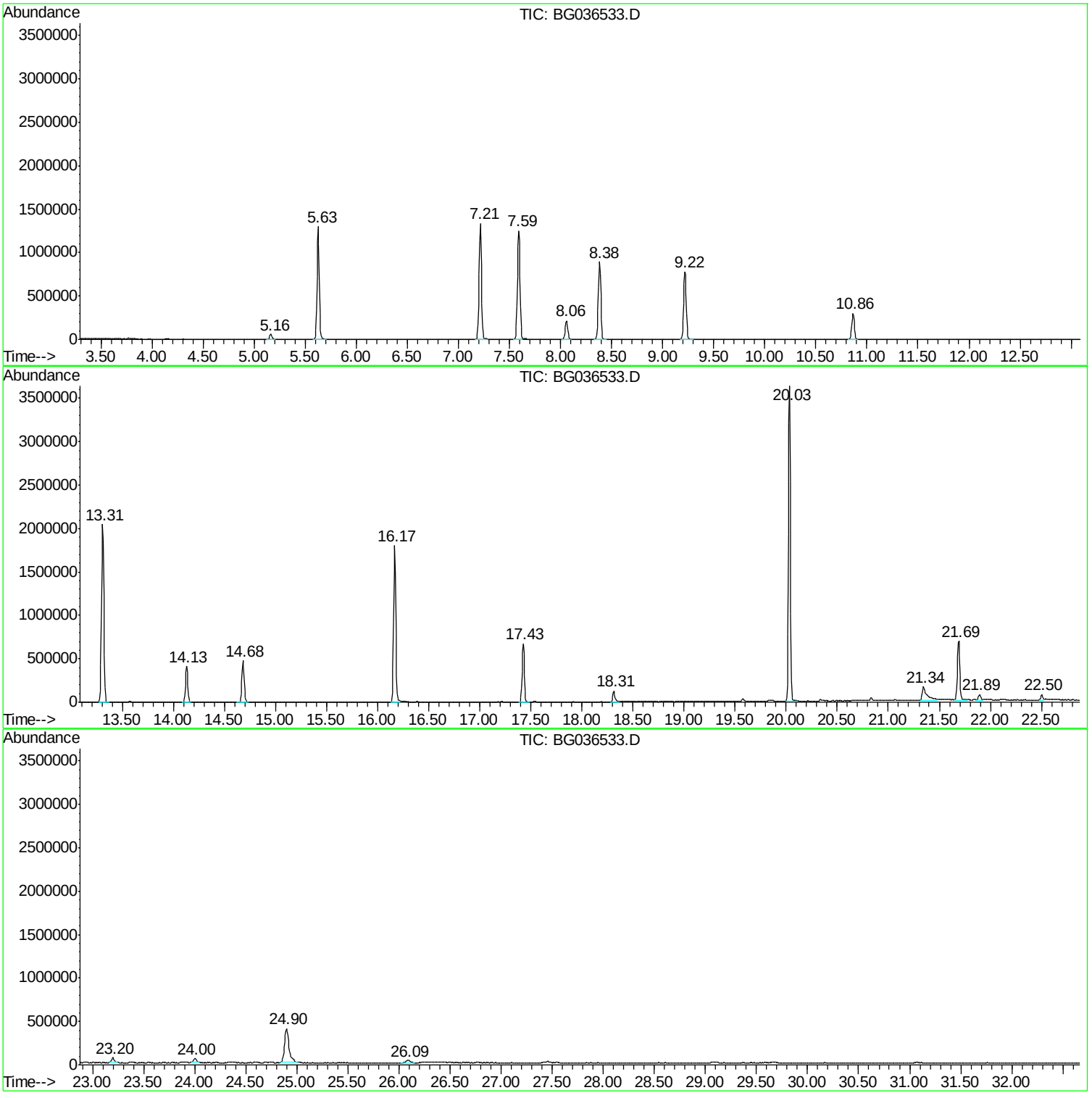
Instrument : BNA_G
ClientSampleId : SB-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG036533.D
Acq On : 4 Sep 2018 15:52
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Instrument : BNA_G
ClientSampleId : SB-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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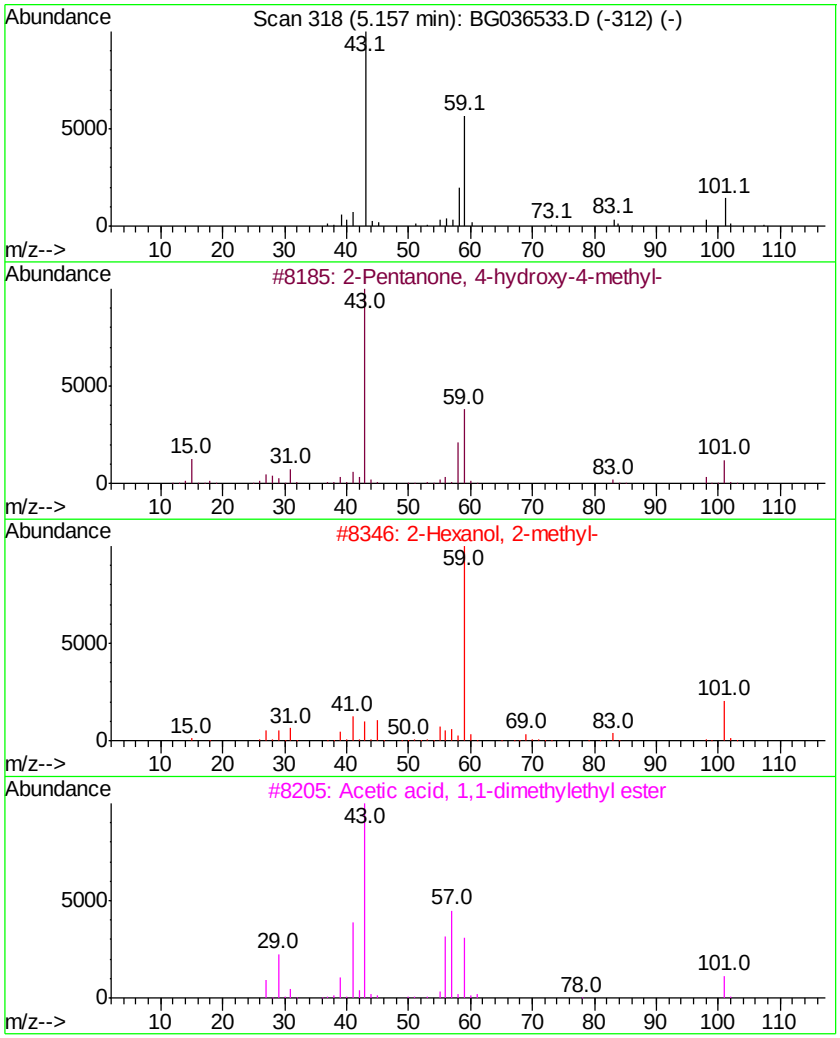
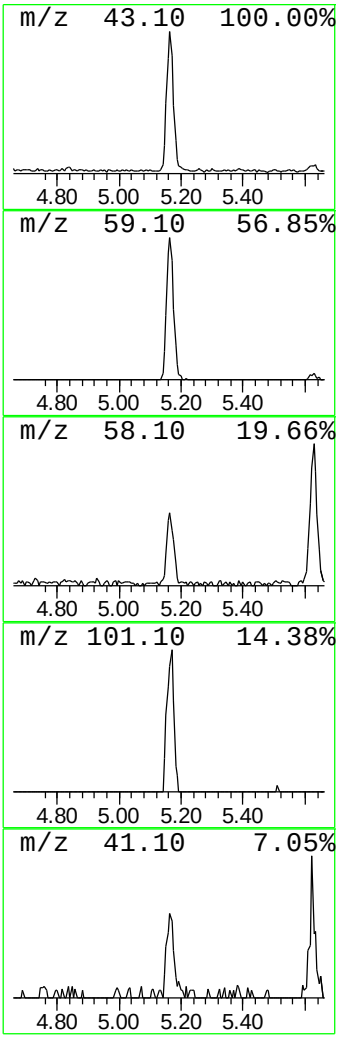
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	4.70 ng	85322	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	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Library Search Compound Report

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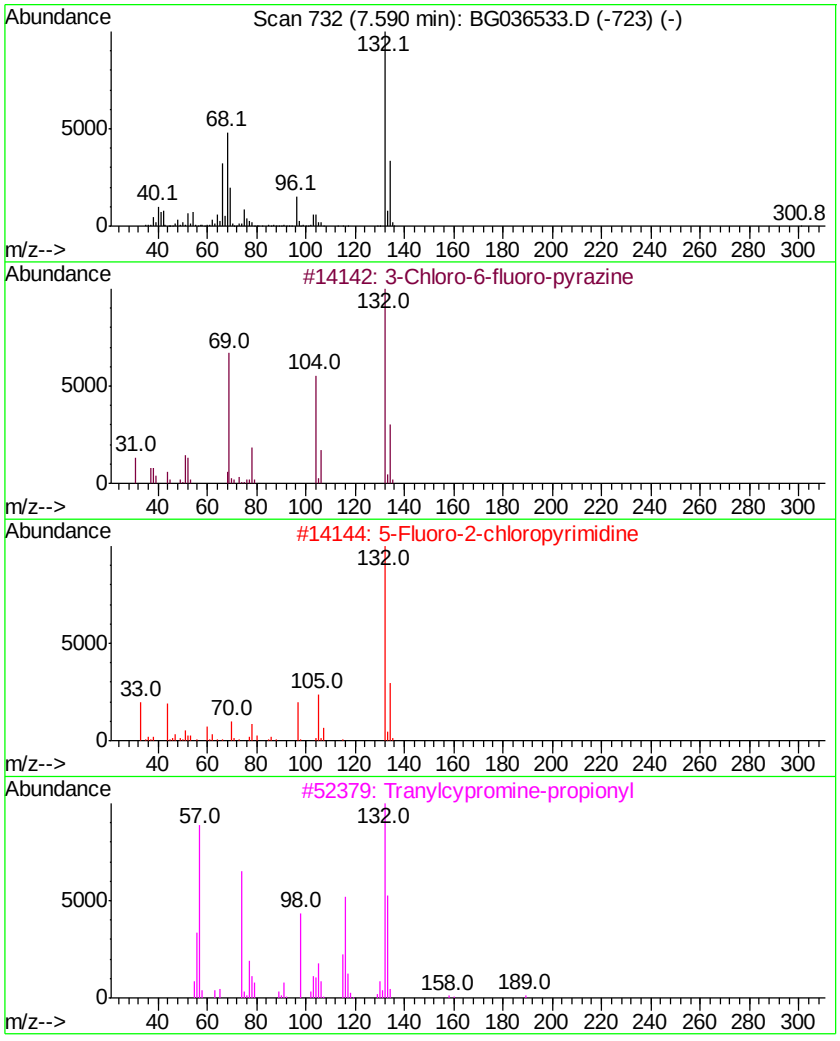
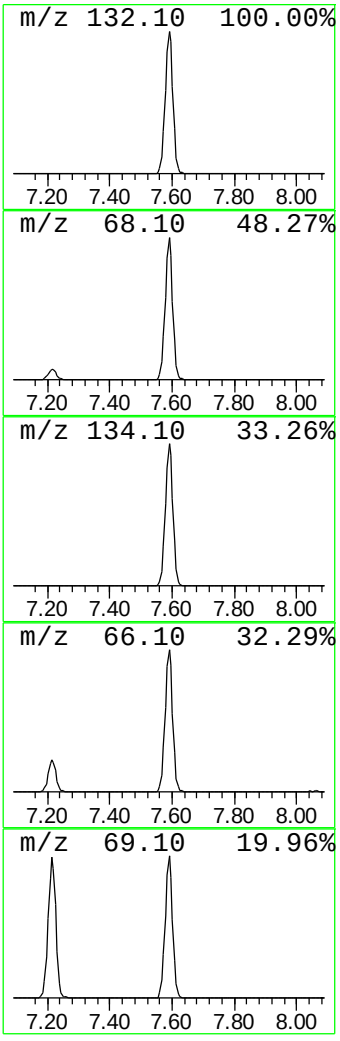
****

Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	117.86 ng	2137710	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
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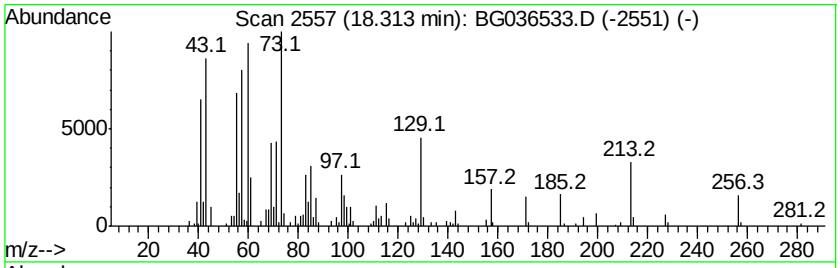
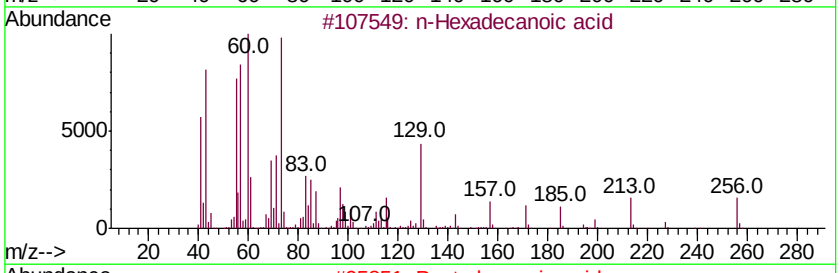
****

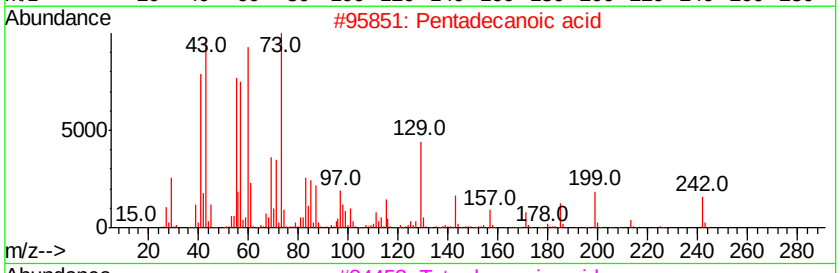
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

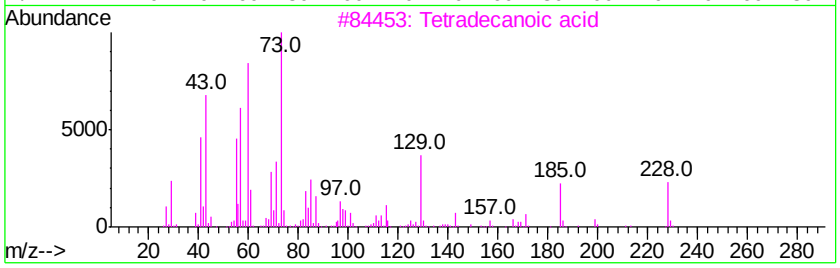
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	3.83 ng	189786	Phenanthrene-d10	17.43

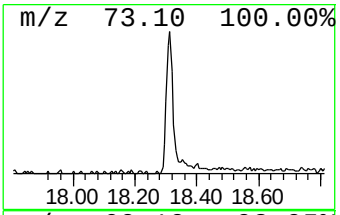
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62

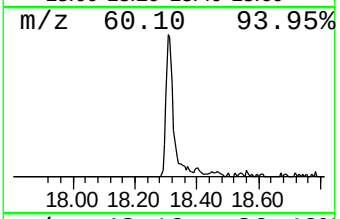


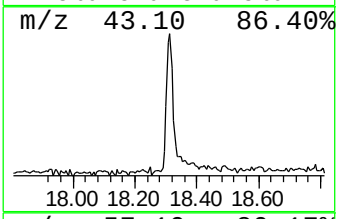


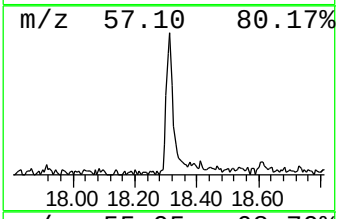


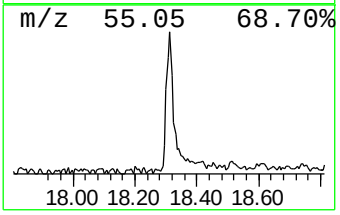












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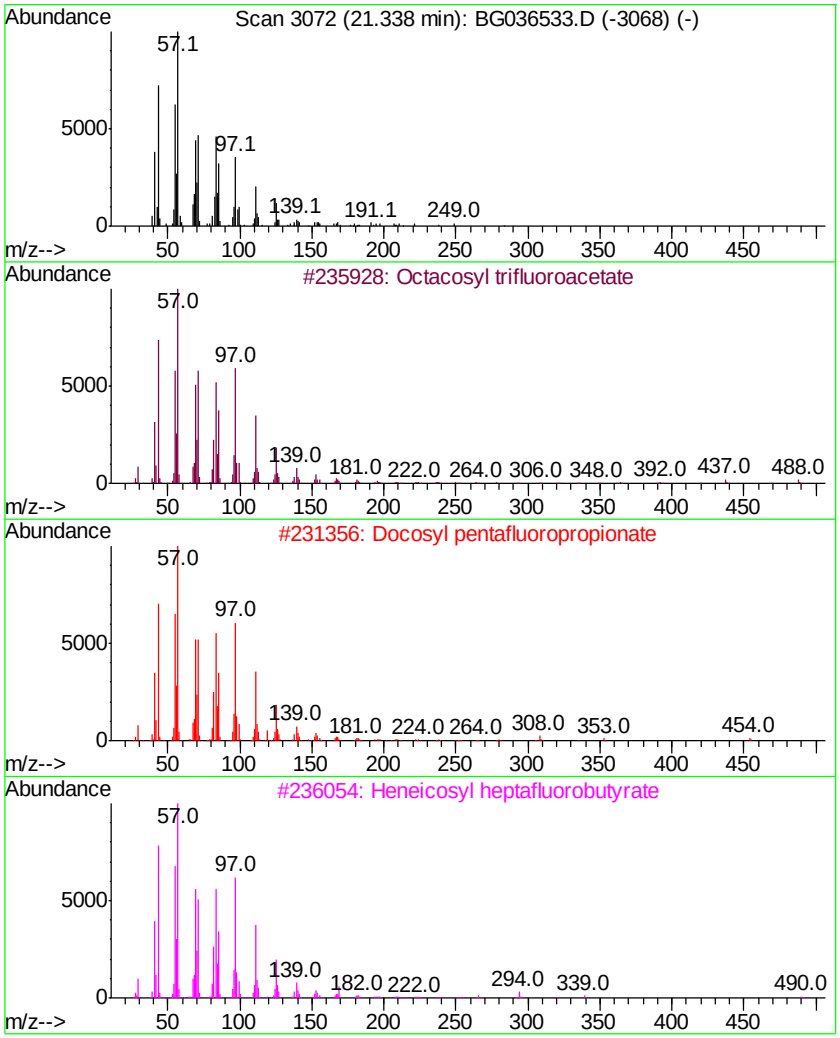
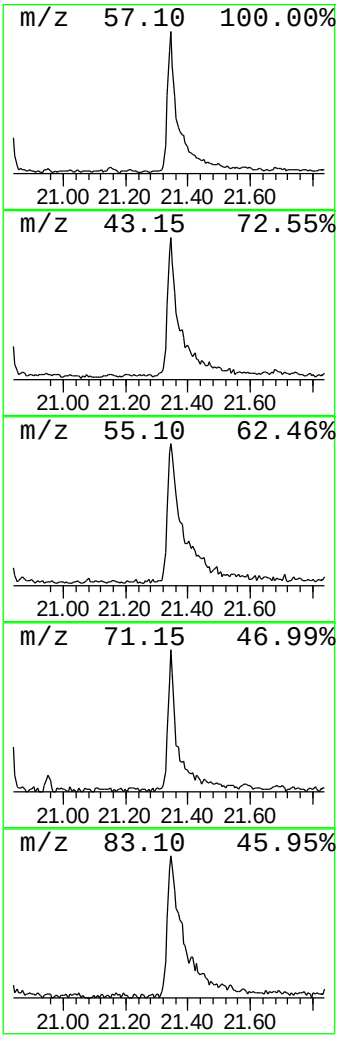
****

Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.34	8.05 ng	465939	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.16	4.7	ng	85322	1	8.06	362767	20.0
unknown7.59	7.59	117.9	ng	2137710	1	8.06	362767	20.0
n-Hexadecanoic acid	18.31	3.8	ng	189786	4	17.43	991683	20.0
Octacosyl trifluo...	21.34	8.1	ng	465939	5	21.69	1157450	20.0