LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081024\
Data File : BF138916.D
Acq On : 10 Aug 2024 18:22
Operator : RC/JU
Sample : P3457-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
932-K1-WS-080224

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_F\Methods\8270-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138916.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	500	504	518	rVB	18160	26942	1.73%	0.382%
2	5.469	569	574	595	rBV	379626	528865	34.02%	7.497%
3	6.481	742	746	771	rBB	229502	330836	21.28%	4.690%
4	6.839	802	807	814	rBB	190507	235633	15.16%	3.340%
5	7.404	897	903	916	rBV	669873	887394	57.08%	12.579%
6	8.122	1019	1025	1036	rBV	235316	303392	19.51%	4.301%
7	8.439	1074	1079	1094	rVB	31878	49480	3.18%	0.701%
8	9.192	1201	1207	1212	rBV	1257694	1554662	100.00%	22.038%
9	9.869	1317	1322	1332	rBV	268057	342241	22.01%	4.851%
10	10.663	1452	1457	1471	rBV	639471	830842	53.44%	11.778%
11	11.357	1570	1575	1588	rVB	265675	328845	21.15%	4.662%
12	11.880	1659	1664	1681	rBV2	16428	36040	2.32%	0.511%
13	12.751	1808	1812	1817	rVB	24579	29153	1.88%	0.413%
14	12.939	1838	1844	1849	rBV	893905	1110454	71.43%	15.741%
15	13.457	1927	1932	1936	rBV	13959	16794	1.08%	0.238%
16	13.827	1990	1995	2011	rBV2	26517	57676	3.71%	0.818%
17	13.998	2019	2024	2032	rVB	135708	173417	11.15%	2.458%
18	15.462	2267	2273	2282	rBV	135337	211724	13.62%	3.001%

Sum of corrected areas: 7054390

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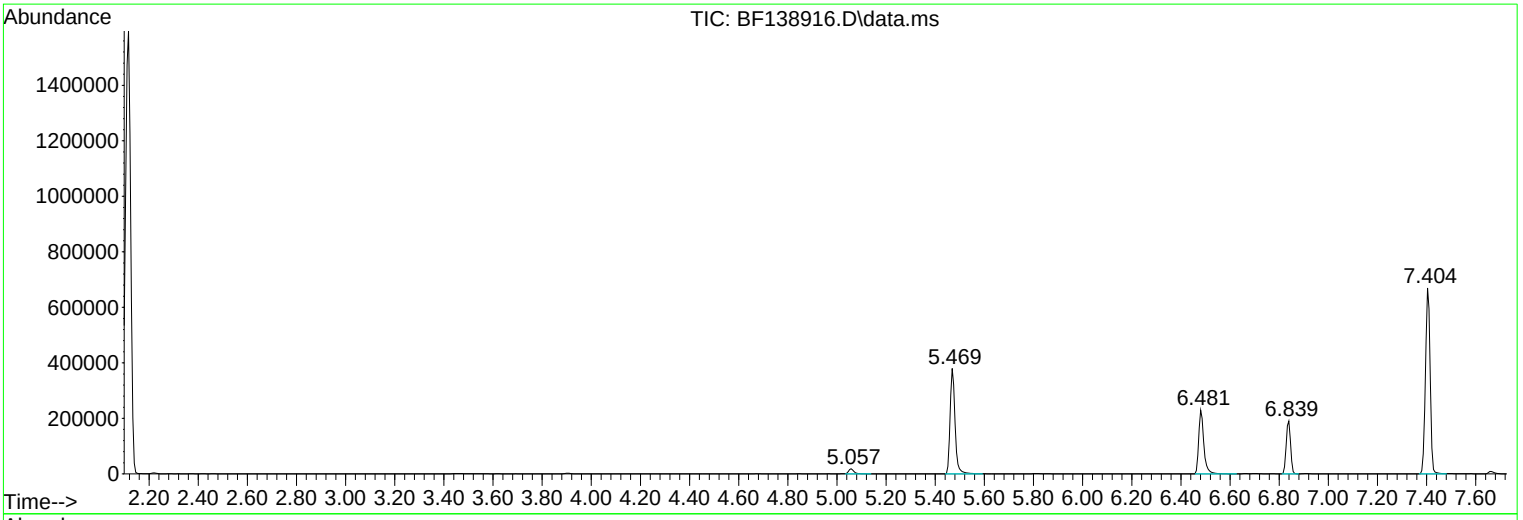
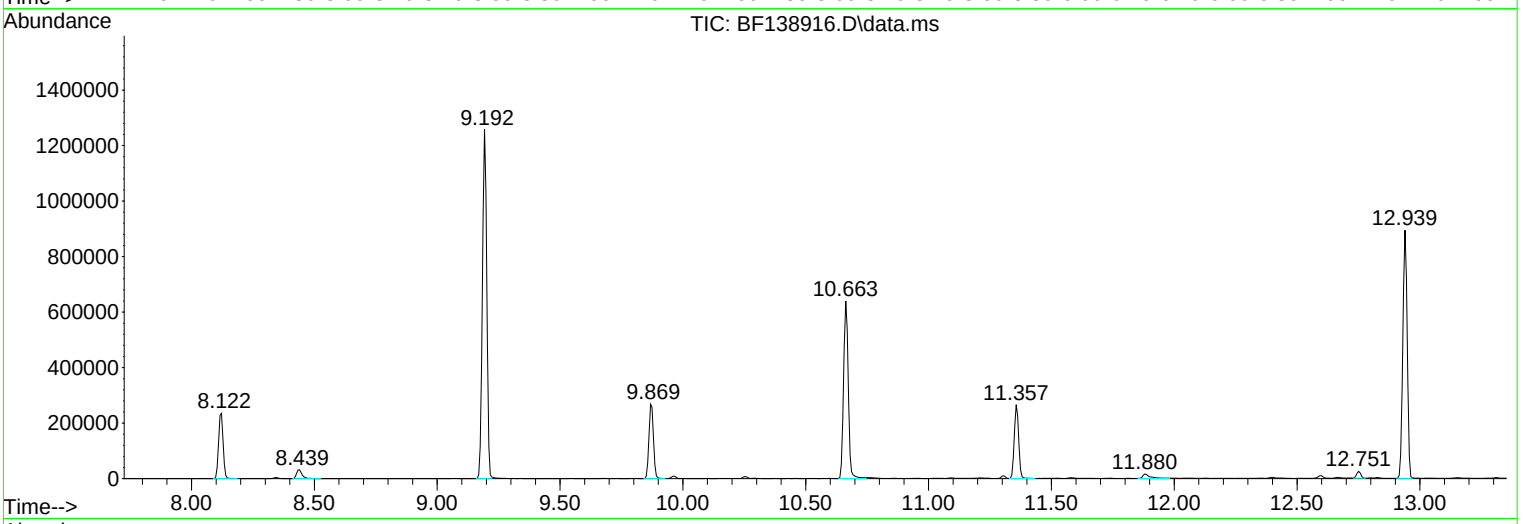
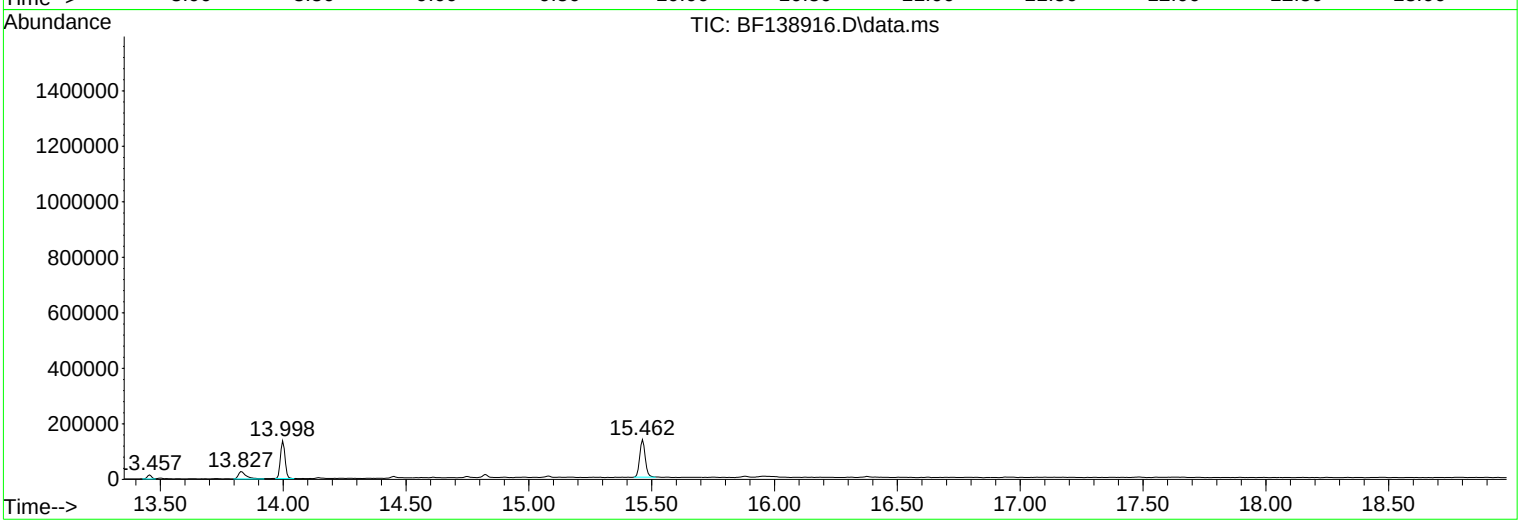
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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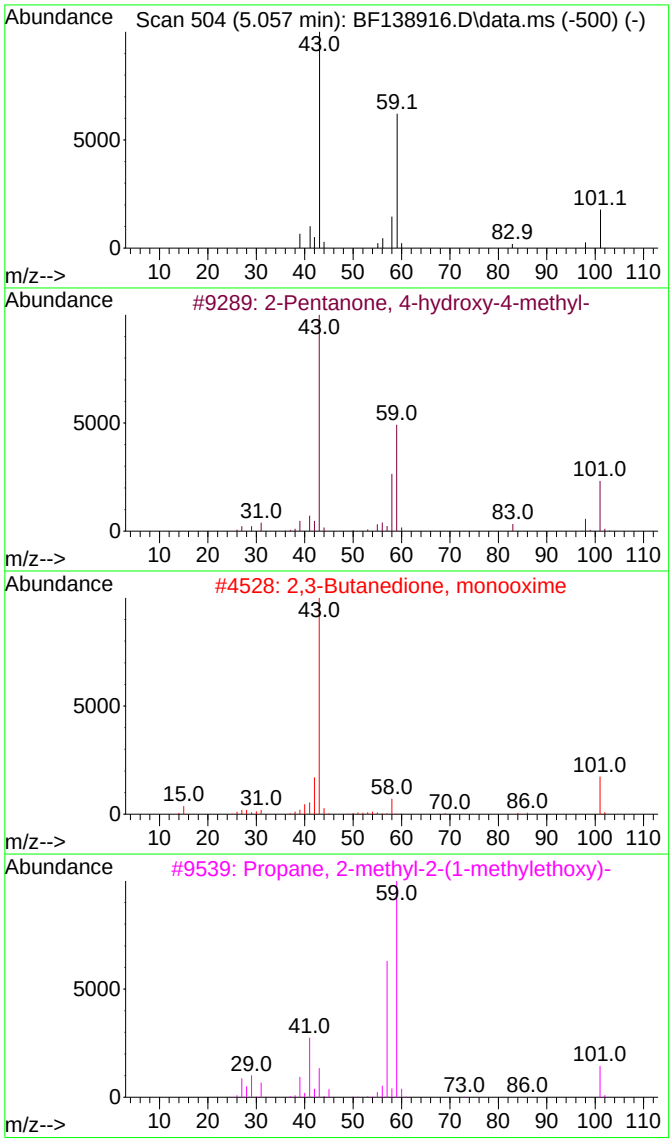
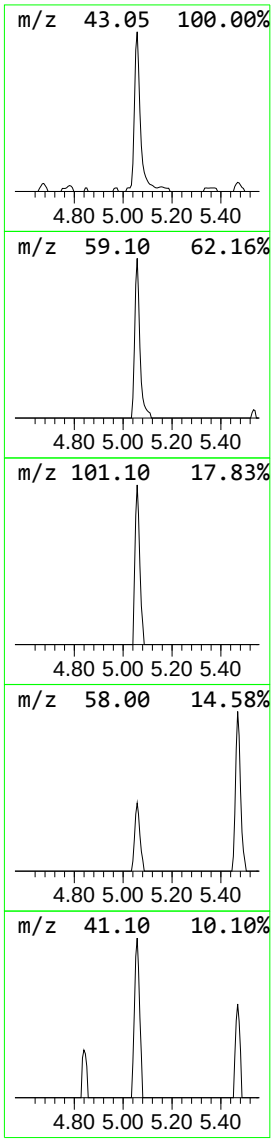
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	2.29 ng	26942	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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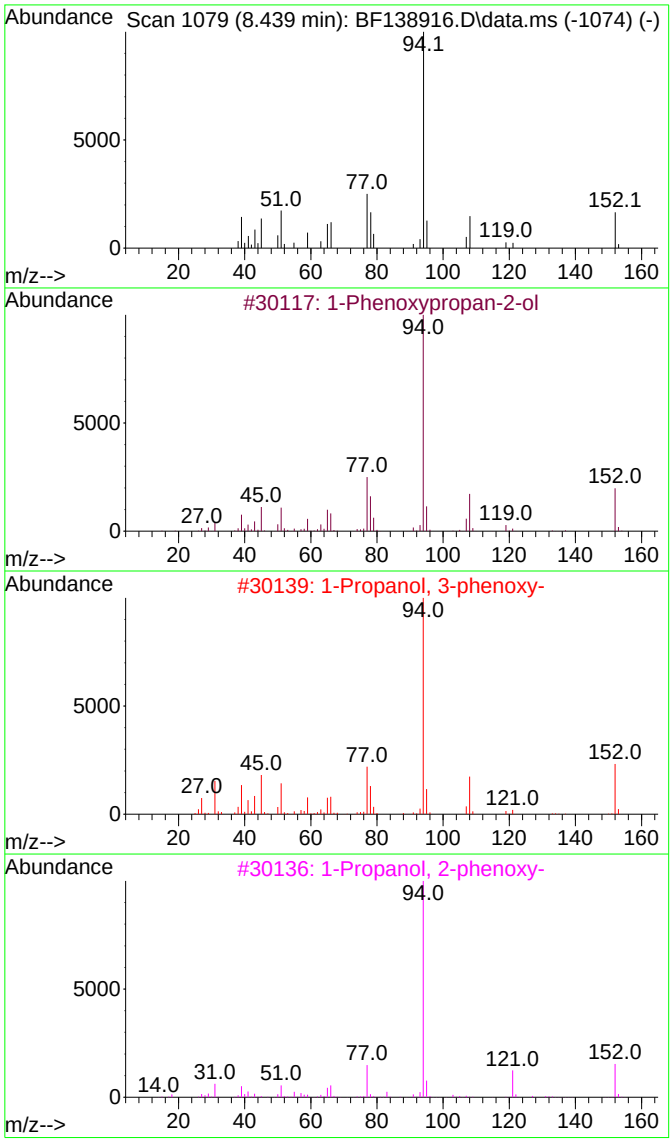
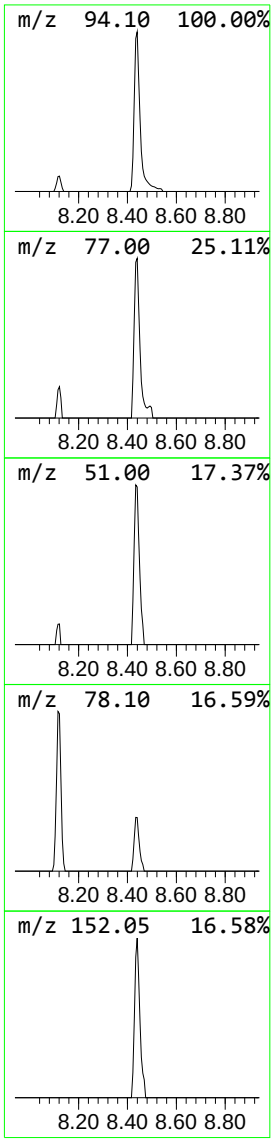
****

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.439	3.26 ng	49480	Naphthalene-d8	8.122

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59





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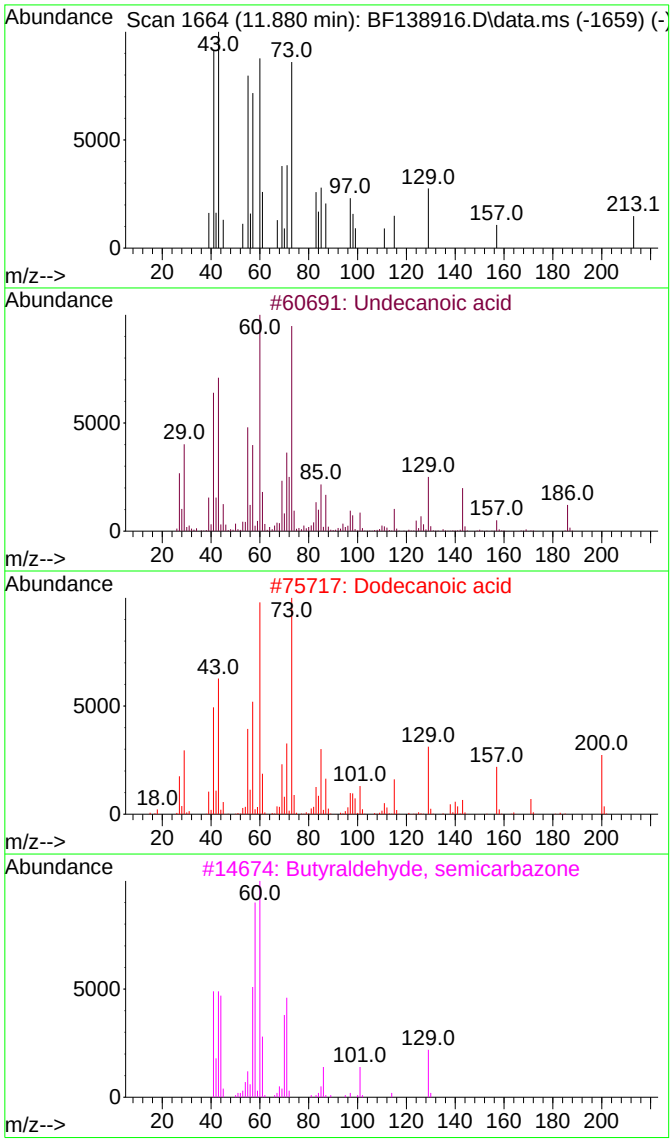
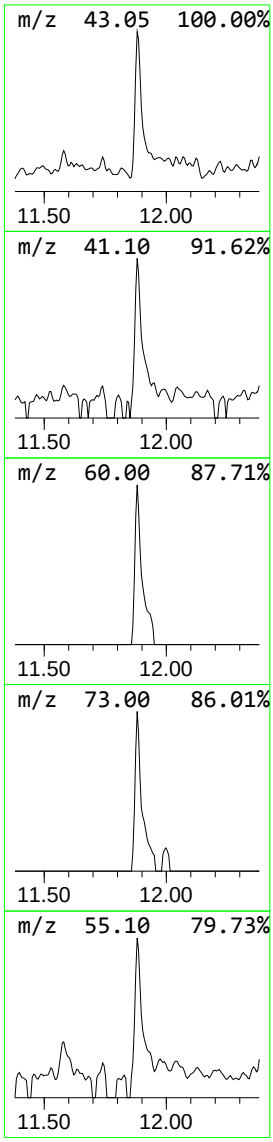
****

Peak Number 3 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	2.19 ng	36040	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	50
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	38
5	Melezitose	504	C18H32O16	000597-12-6	38





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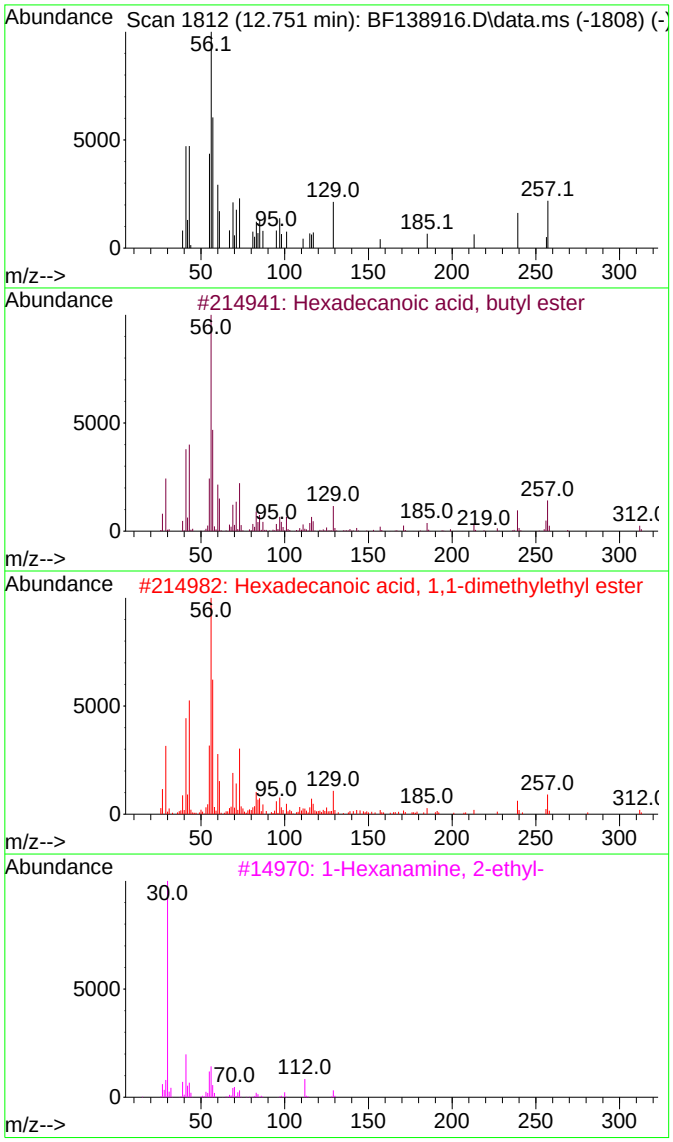
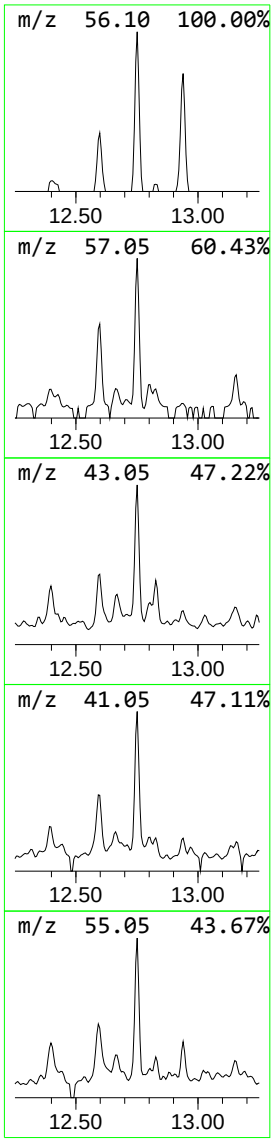
****

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	3.36 ng	29153	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3	1-Hexanamine, 2-ethyl-	129	C8H19N	000104-75-6	37
4	Pentanoic acid, butyl ester	158	C9H18O2	000591-68-4	28
5	2-Methyl-1-tetradecene	210	C15H30	052254-38-3	25





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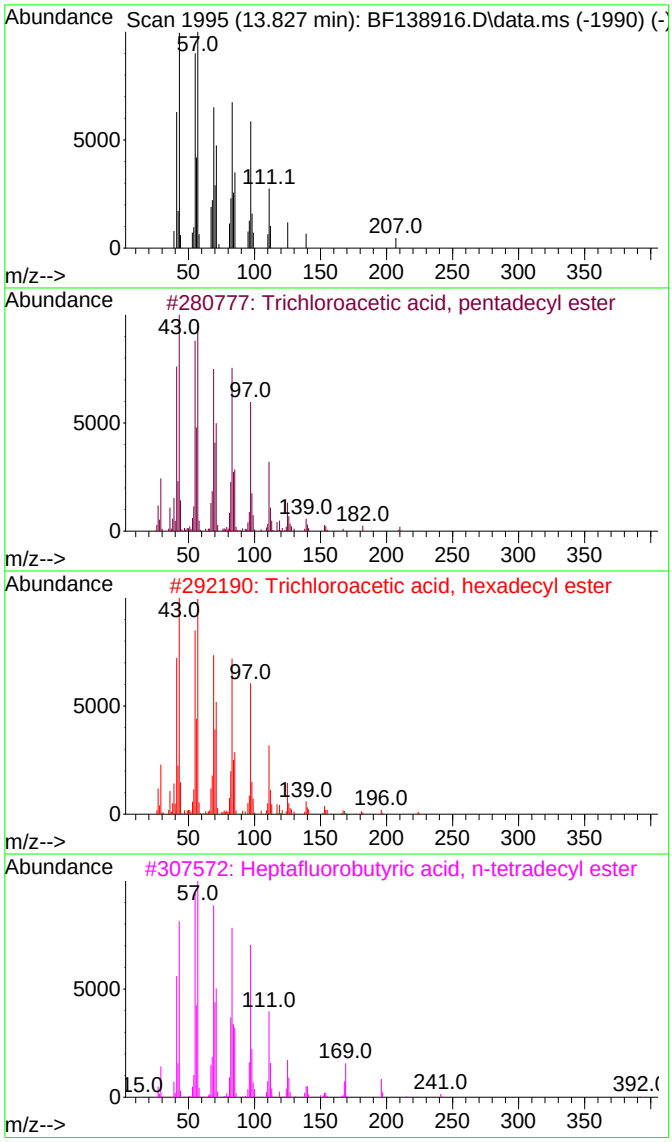
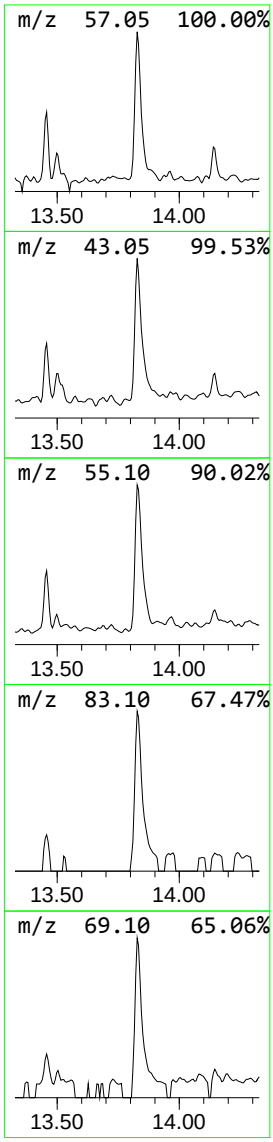
****
Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	6.65 ng	57676	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	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-...	5.057	2.3	ng	26942	1	6.839	235633	20.0
1-Phenoxypropan...	8.439	3.3	ng	49480	2	8.122	303392	20.0
Undecanoic acid	11.880	2.2	ng	36040	4	11.357	328845	20.0
Hexadecanoic ac...	12.751	3.4	ng	29153	5	13.998	173417	20.0
Trichloroacetic...	13.827	6.7	ng	57676	5	13.998	173417	20.0