

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101923\
 Data File : BF135886.D
 Acq On : 19 Oct 2023 15:04
 Operator : CG\JU
 Sample : 04788-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PMW-2

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135886.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	485	488	496	rBV	61331	87595	3.84%	0.791%
2	5.375	556	559	576	rBV	687804	870980	38.17%	7.866%
3	6.392	730	732	748	rBV	432747	576865	25.28%	5.210%
4	6.734	787	790	801	rBV	500522	424953	18.63%	3.838%
5	7.304	883	887	901	rBV	1363041	1308195	57.34%	11.815%
6	8.016	1004	1008	1022	rVB	687747	600141	26.30%	5.420%
7	9.092	1187	1191	1194	rBV	2562625	2281549	100.00%	20.606%
8	9.775	1303	1307	1317	rBV	537976	506380	22.19%	4.573%
9	10.575	1439	1443	1455	rBV	1304063	1246112	54.62%	11.254%
10	11.269	1558	1561	1568	rBV	575311	481981	21.13%	4.353%
11	11.804	1648	1652	1666	rBV	138983	163583	7.17%	1.477%
12	12.592	1784	1786	1799	rBV	35780	61749	2.71%	0.558%
13	12.868	1828	1833	1836	rBV	1598734	1556876	68.24%	14.061%
14	13.827	1990	1996	2005	rBV8	25779	71685	3.14%	0.647%
15	13.933	2011	2014	2019	rBV	362953	378072	16.57%	3.415%
16	15.415	2261	2266	2272	rBV	333558	455794	19.98%	4.116%

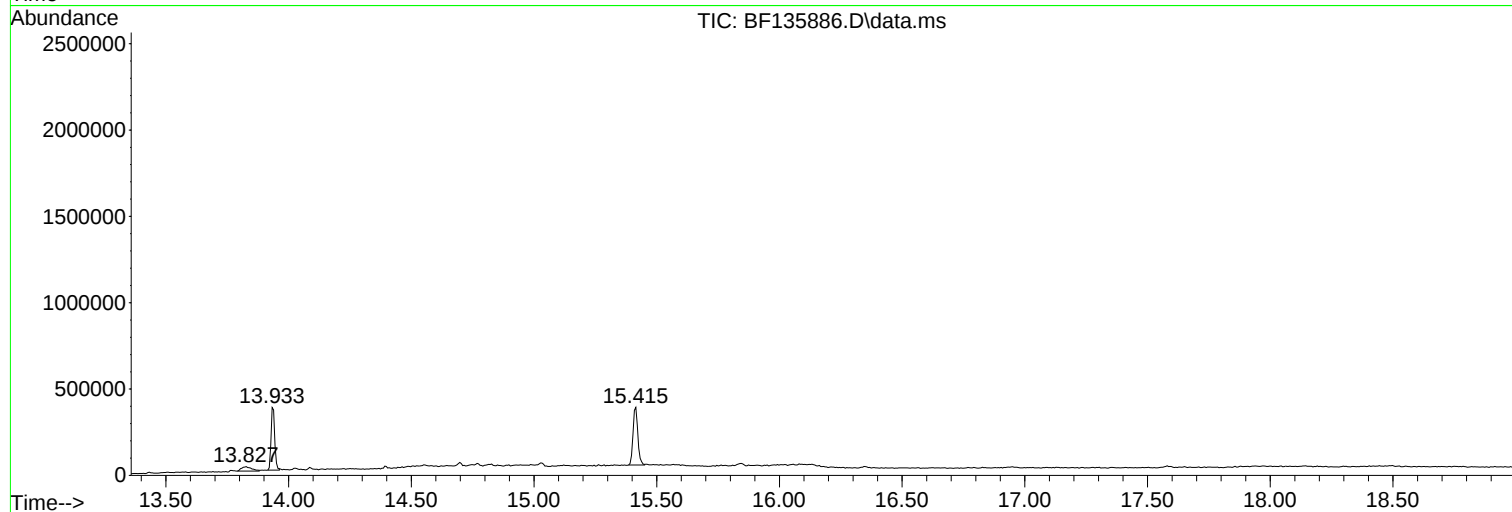
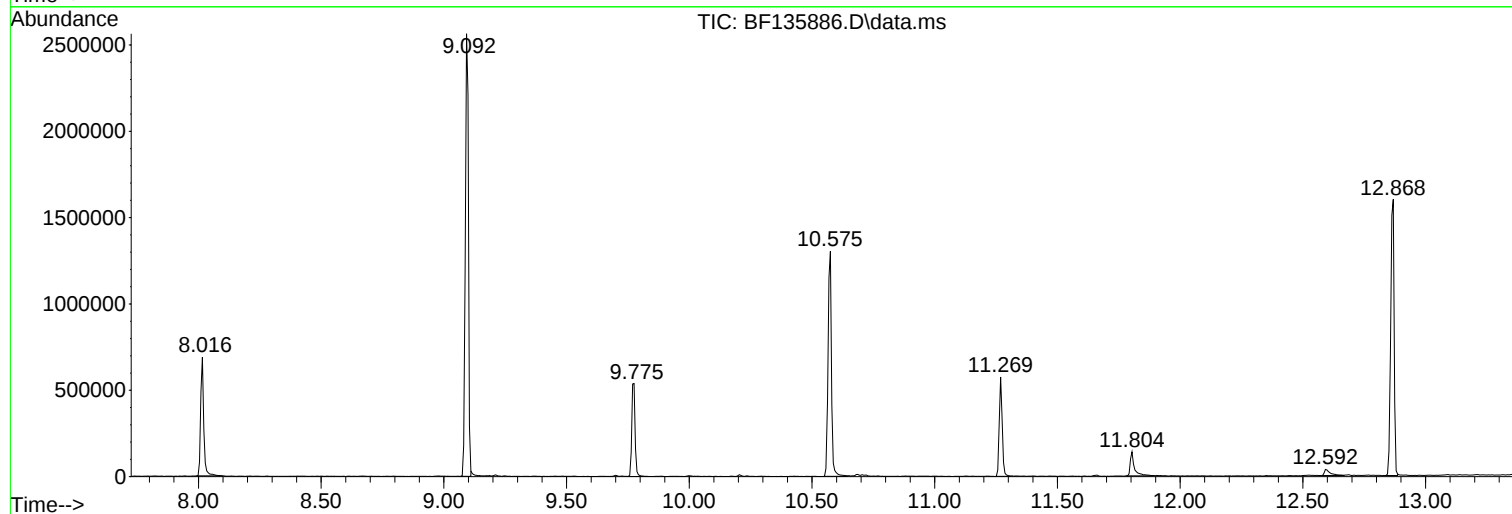
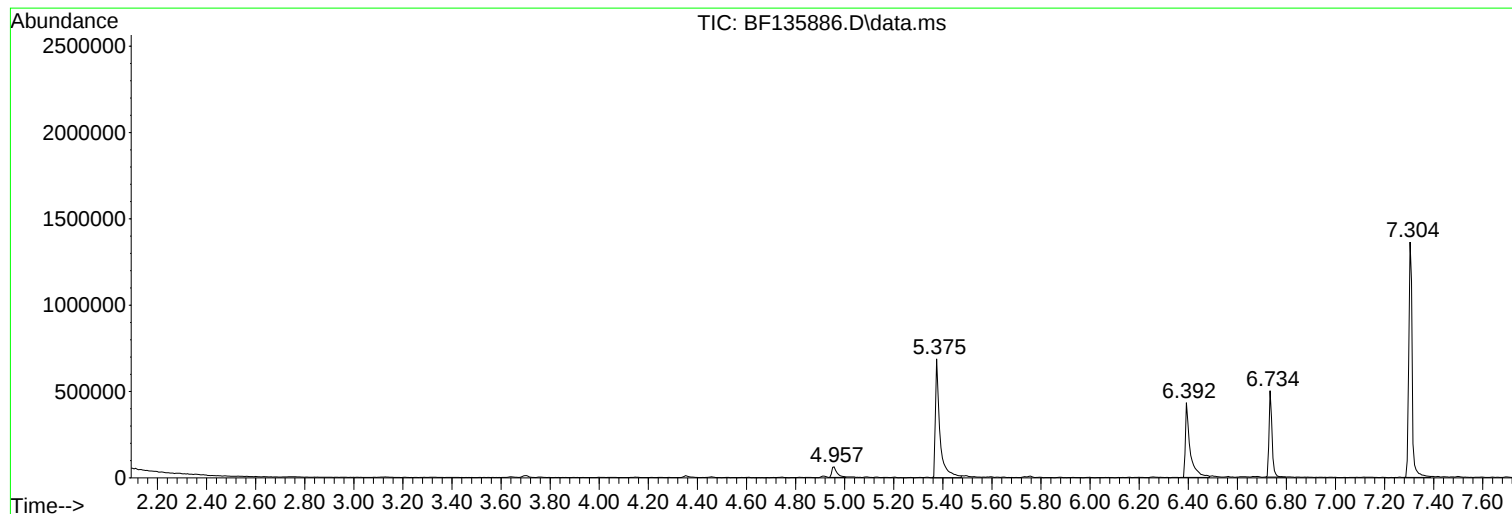
Sum of corrected areas: 11072510

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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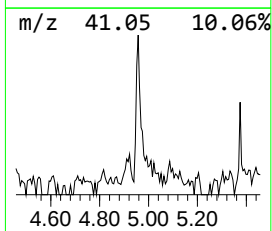
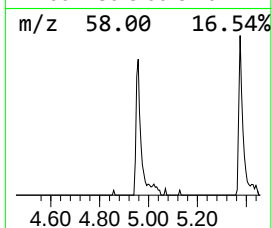
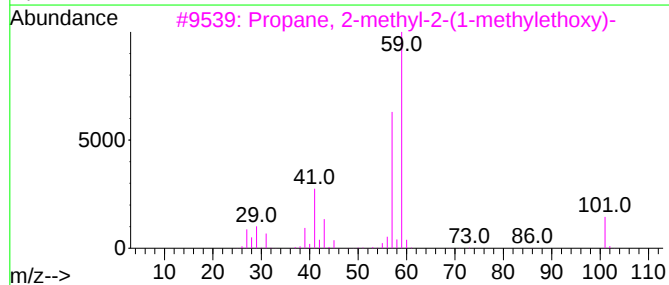
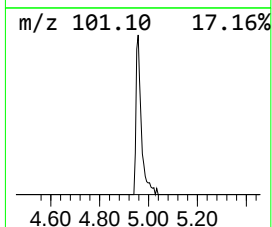
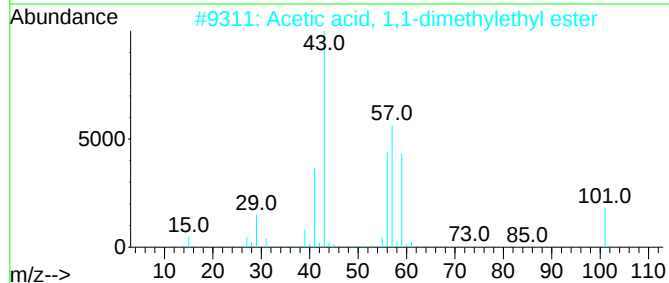
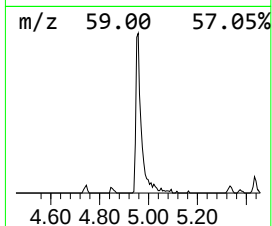
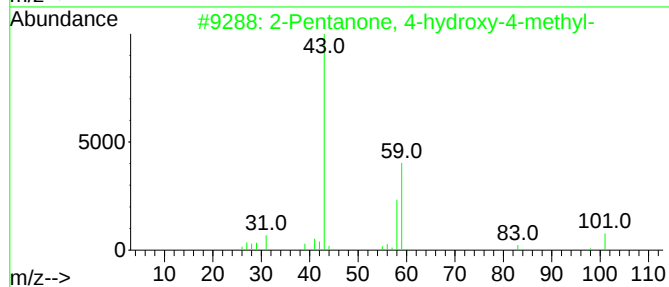
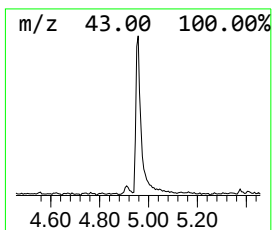
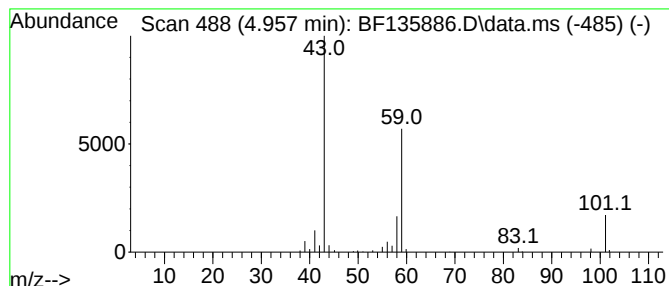
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	4.12 ng	87595	1,4-Dichlorobenzene-d4	6.734

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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		



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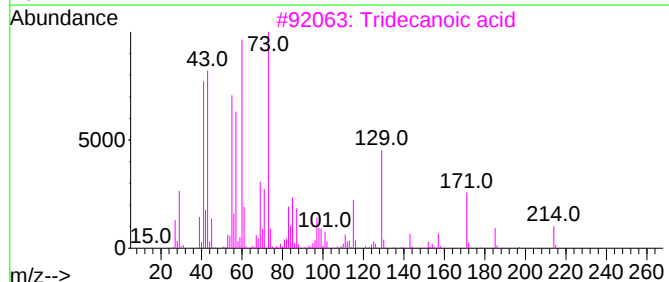
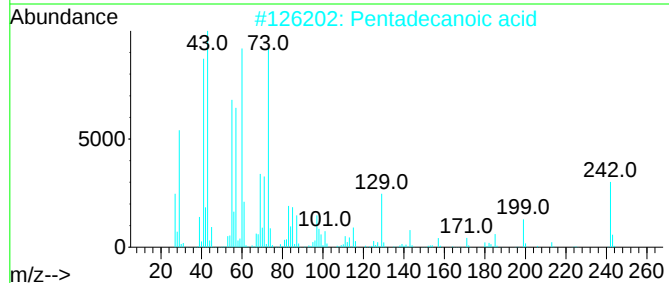
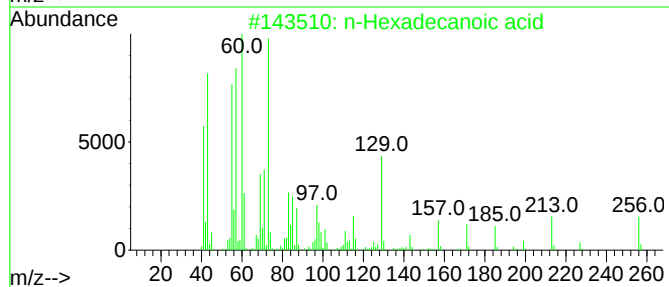
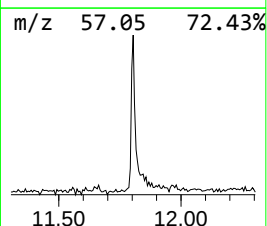
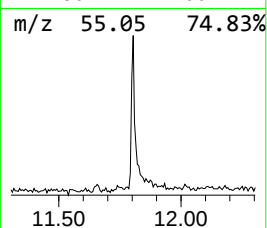
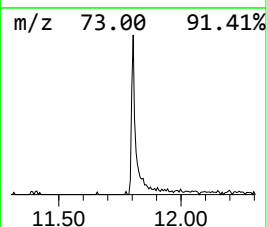
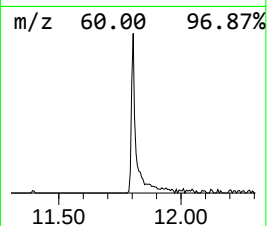
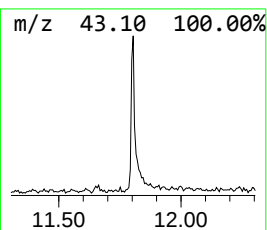
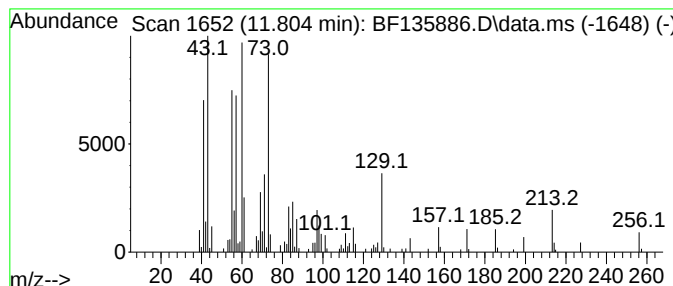
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	6.79 ng	163583	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Nonanoic acid	158	C9H18O2	000112-05-0	55



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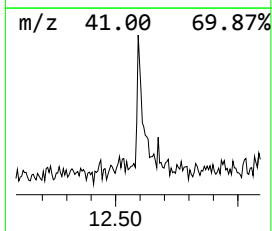
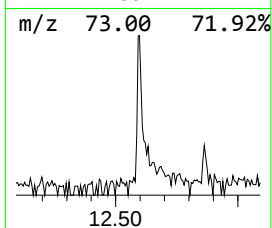
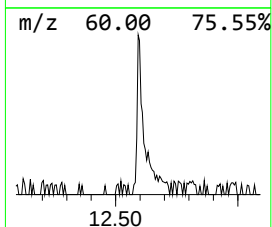
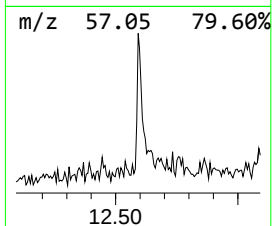
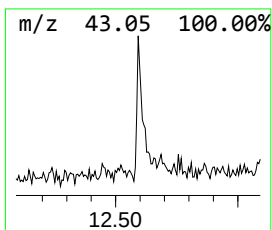
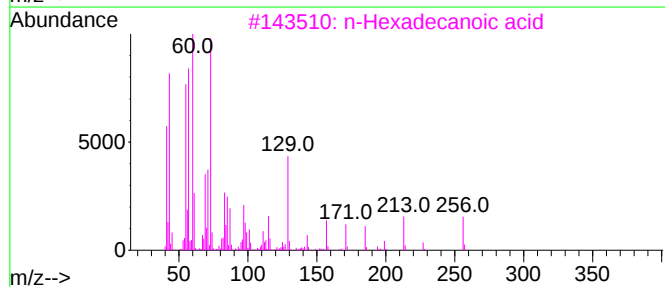
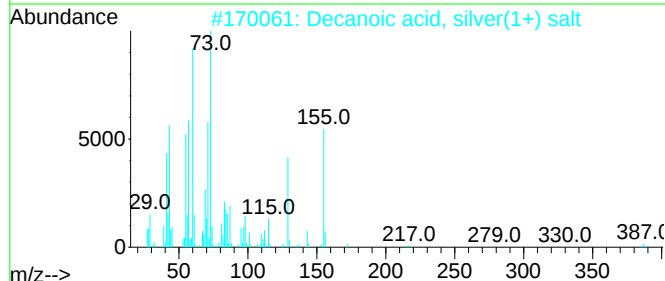
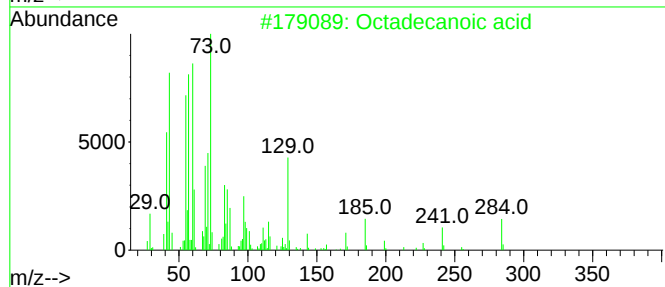
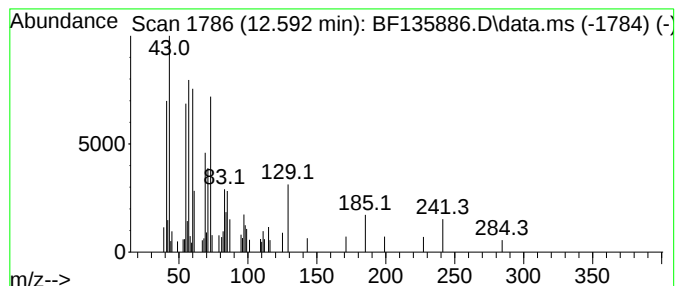
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	2.56 ng	61749	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	91
2			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5			Isobutyl octadecyl ether	326	C22H46O	1000406-32-9	22



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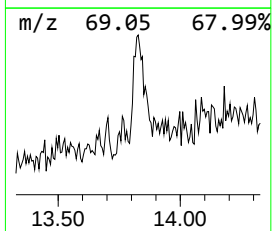
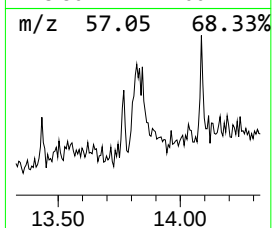
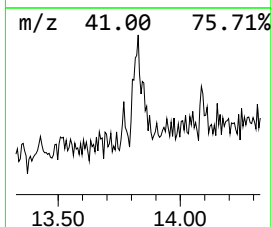
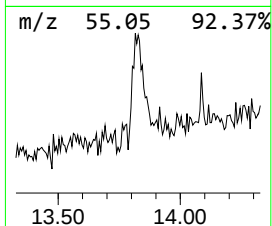
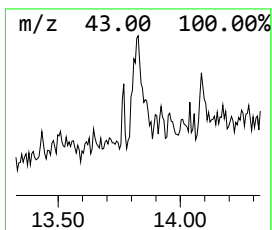
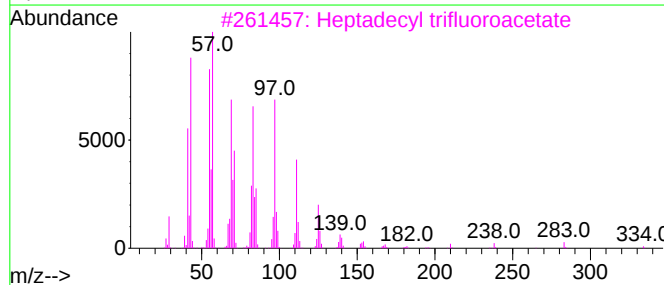
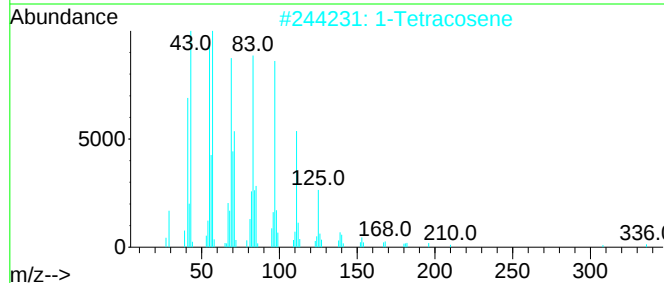
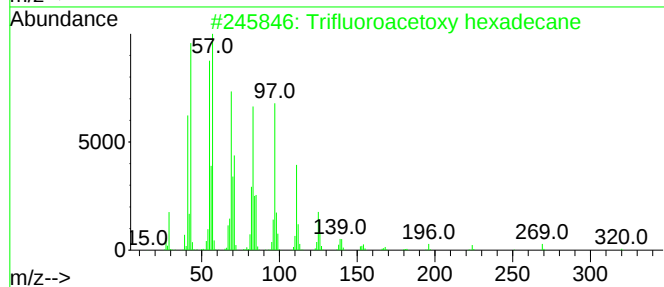
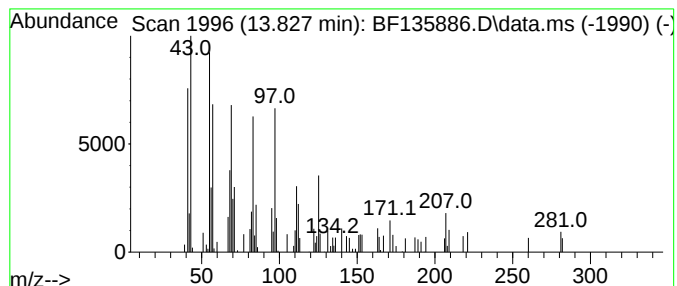
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	3.79 ng	71685	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	58
2			1-Tetracosene	336	C24H48	010192-32-2	58
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	58
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	58
5			1-Hexacosene	364	C26H52	018835-33-1	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	4.1	ng	87595	1	6.734	424953	20.0
n-Hexadecanoic ...	11.804	6.8	ng	163583	4	11.269	481981	20.0
Octadecanoic acid	12.592	2.6	ng	61749	4	11.269	481981	20.0
Trifluoroacetox...	13.827	3.8	ng	71685	5	13.933	378072	20.0