

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
 Data File : BF135138.D
 Acq On : 07 Sep 2023 17:19
 Operator : CG\JU
 Sample : 04283-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-3

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135138.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	7	11	18	rVB	36980	48084	2.02%	0.296%
2	5.004	492	496	505	rVB	125349	159345	6.71%	0.981%
3	5.404	560	564	567	rBV	2223920	1981189	83.37%	12.202%
4	6.410	730	735	738	rBV	2131126	2073161	87.24%	12.768%
5	6.604	765	768	774	rBV	52369	52465	2.21%	0.323%
6	6.769	793	796	800	rBV	686327	559515	23.54%	3.446%
7	7.333	887	892	895	rBV	1487967	1341035	56.43%	8.259%
8	8.051	1009	1014	1017	rBV	867119	761642	32.05%	4.691%
9	9.127	1192	1197	1200	rBV	2673707	2376442	100.00%	14.636%
10	9.245	1214	1217	1221	rVB	49092	45360	1.91%	0.279%
11	9.810	1308	1313	1316	rBV	985020	847100	35.65%	5.217%
12	10.604	1443	1448	1451	rBV	1415443	1367703	57.55%	8.424%
13	11.298	1563	1566	1570	rBV	903034	825345	34.73%	5.083%
14	11.839	1654	1658	1672	rBV	319955	321037	13.51%	1.977%
15	12.627	1789	1792	1801	rBV	94840	110115	4.63%	0.678%
16	12.898	1834	1838	1841	rBV	2324707	1965560	82.71%	12.106%
17	13.815	1989	1994	2009	rBV	98373	188648	7.94%	1.162%
18	13.956	2014	2018	2025	rVB	582521	503965	21.21%	3.104%
19	14.727	2144	2149	2157	rBV	155905	202869	8.54%	1.249%
20	15.427	2262	2268	2272	rBV	391438	506138	21.30%	3.117%

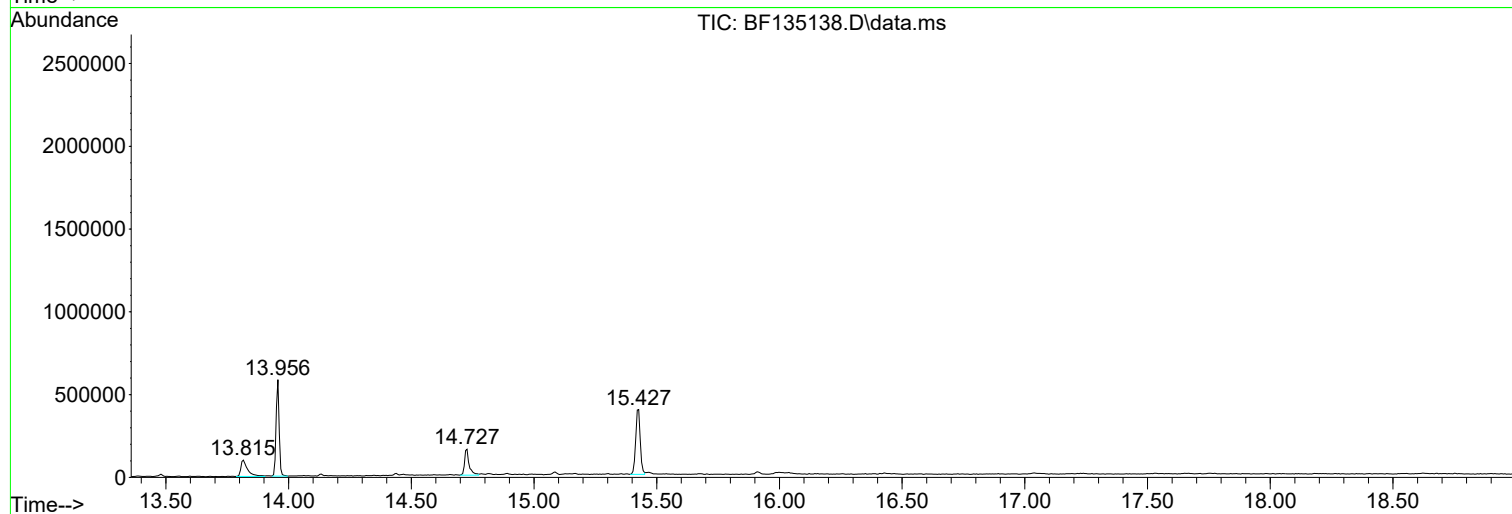
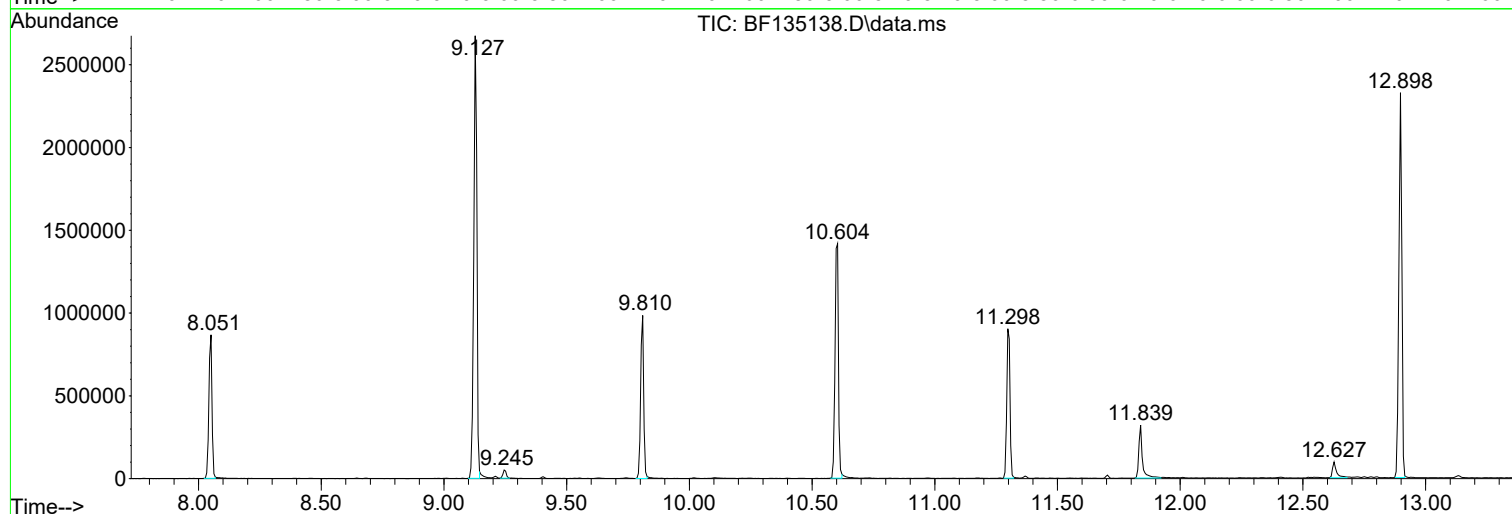
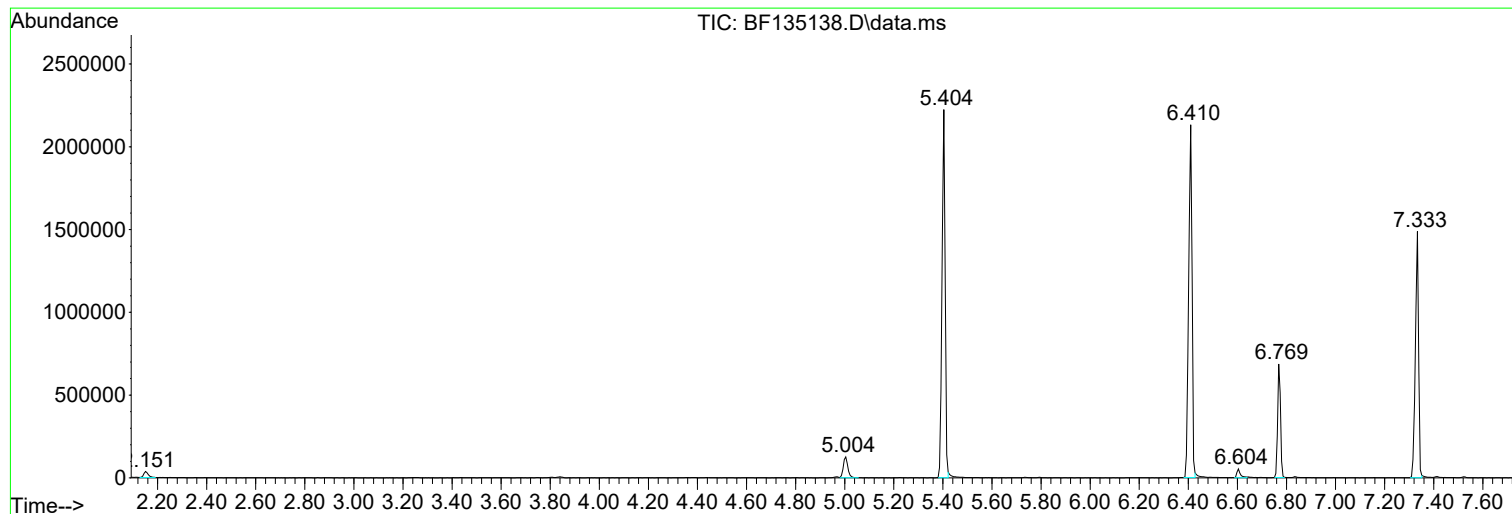
Sum of corrected areas: 16236718

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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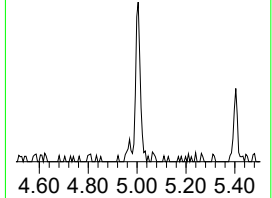
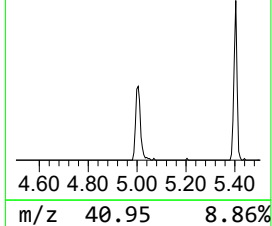
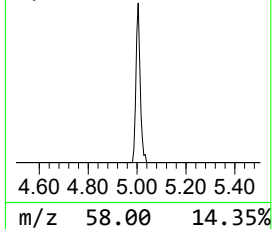
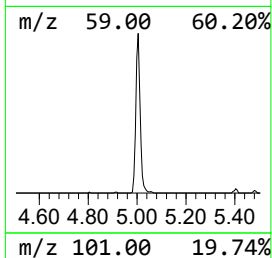
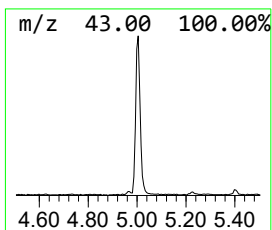
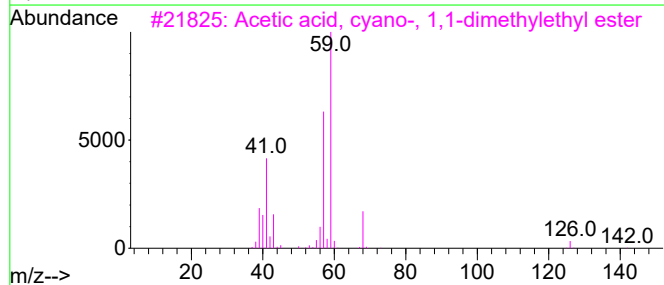
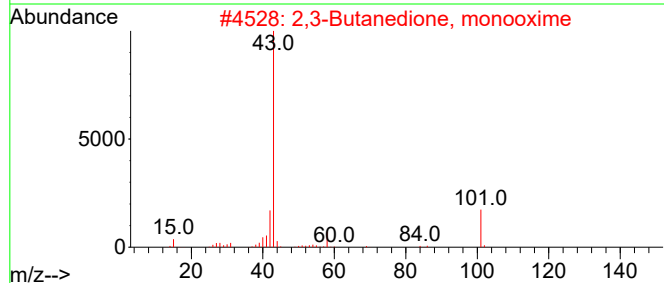
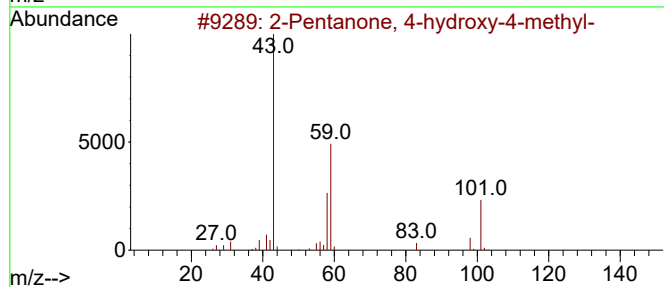
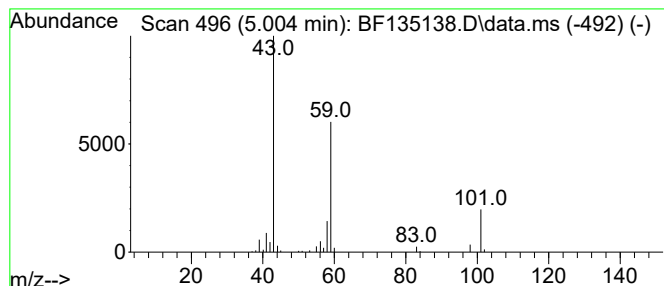
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	5.70 ng	159345	1,4-Dichlorobenzene-d4	6.769

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	35		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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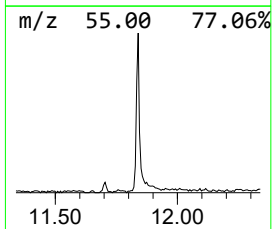
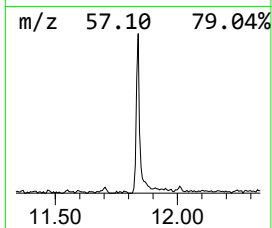
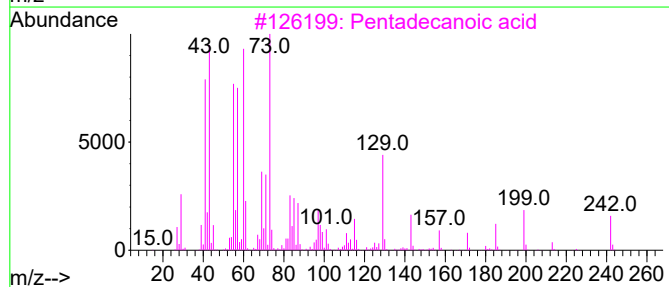
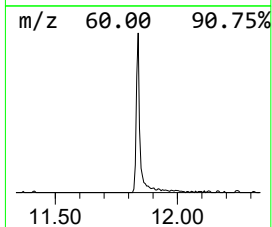
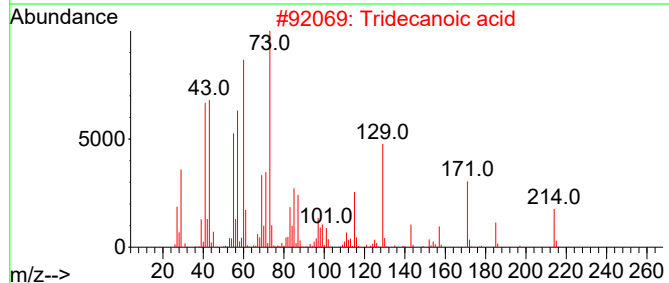
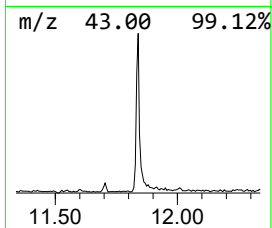
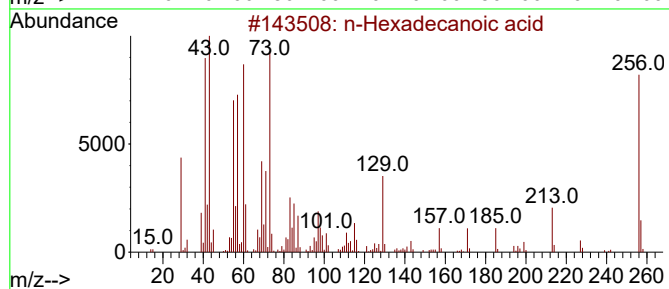
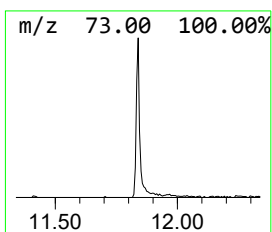
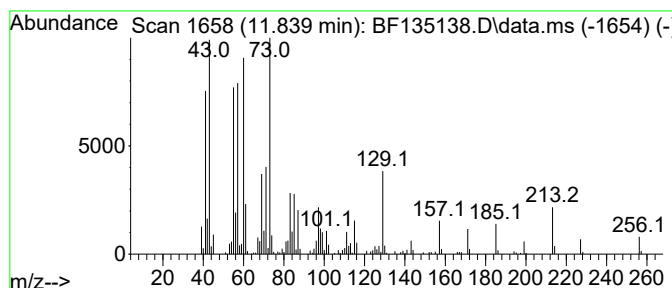
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	7.78 ng	321037	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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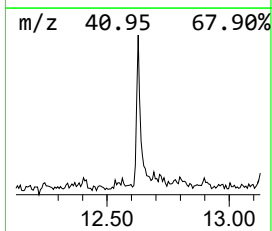
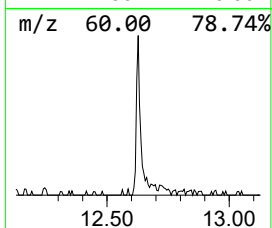
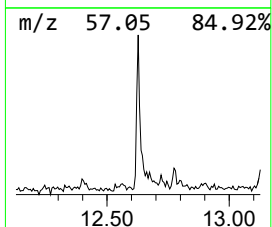
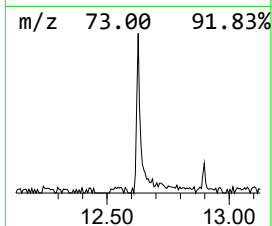
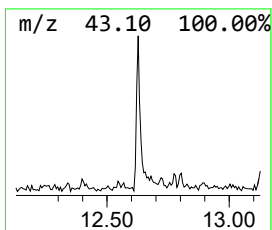
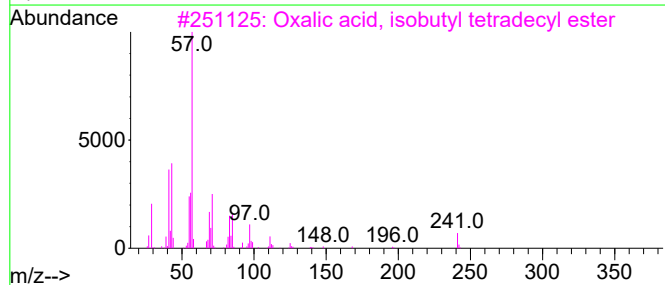
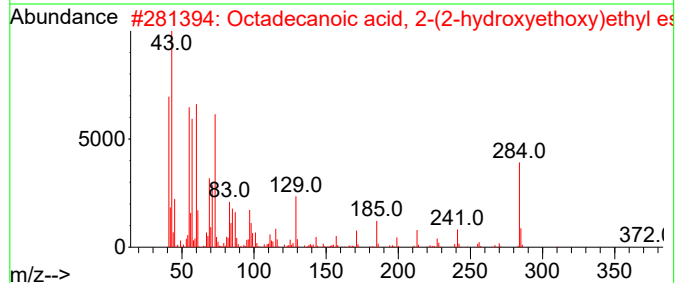
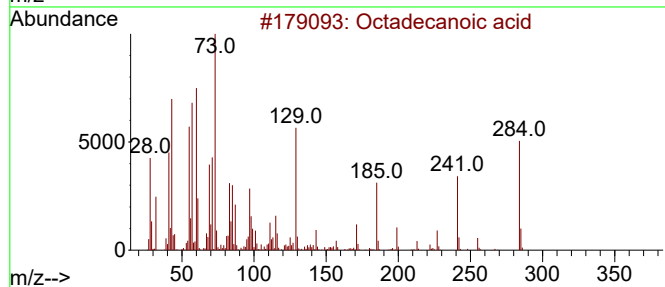
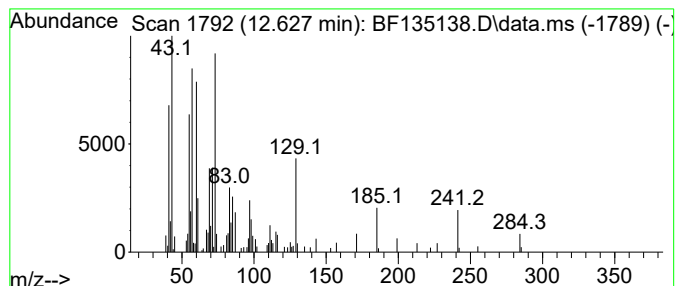
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	2.67 ng	110115	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	25
4			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	18
5			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	18



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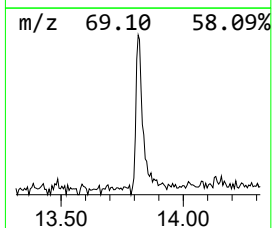
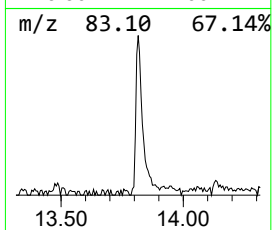
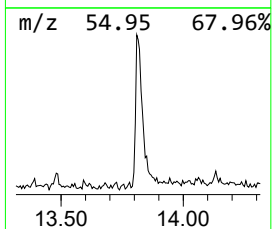
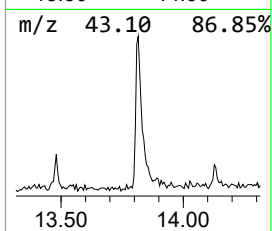
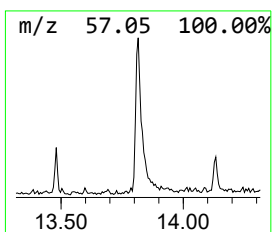
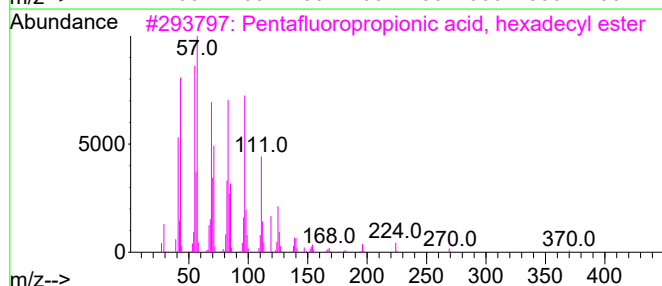
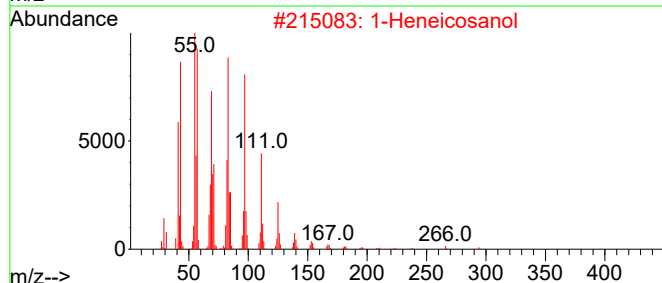
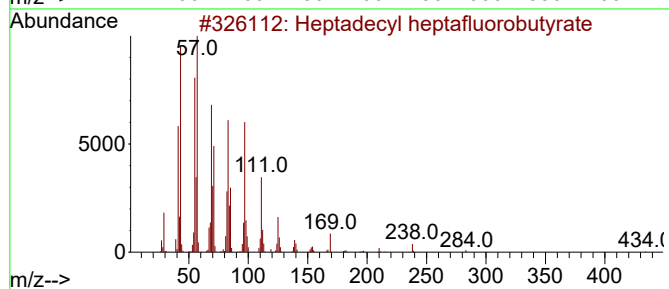
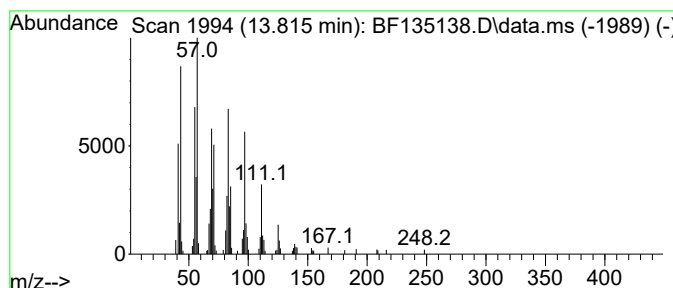
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.815	7.49 ng	188648	Chrysene-d12	13.957	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



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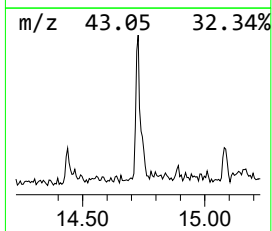
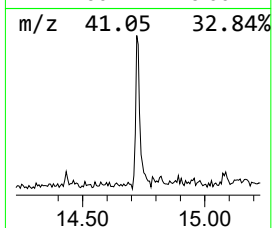
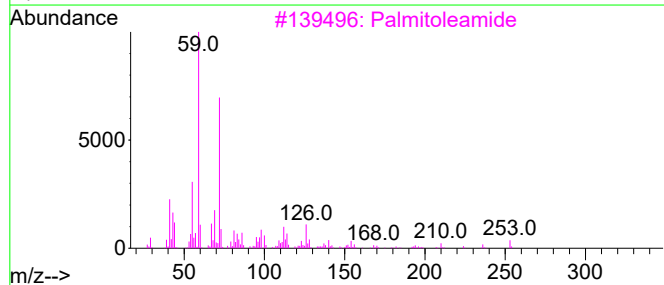
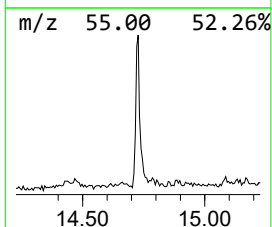
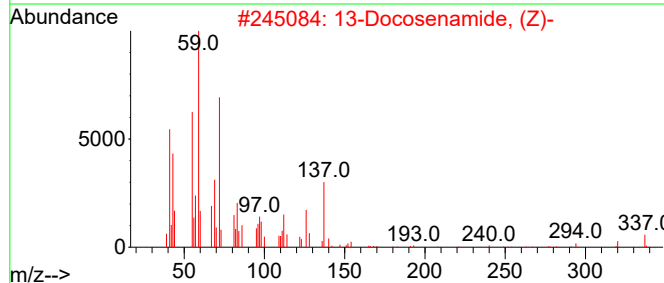
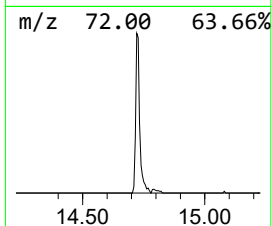
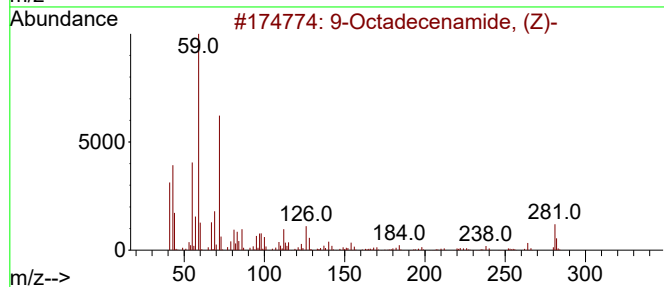
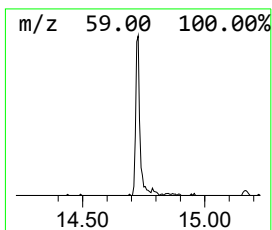
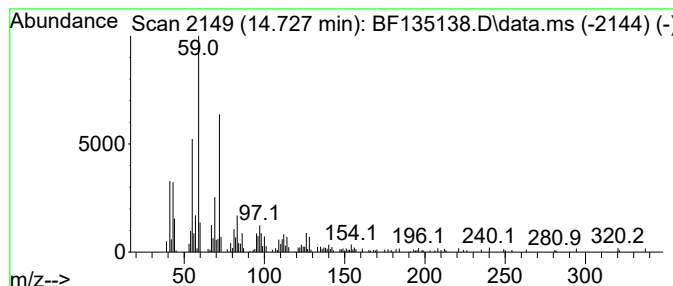
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	8.02 ng	202869	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3			Palmitoleamide	253	C16H31NO	106010-22-4	80
4			Dodecanamide	199	C12H25NO	001120-16-7	50
5			2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.004	5.7	ng	159345	1	6.769	559515	20.0
n-Hexadecanoic ...	11.839	7.8	ng	321037	4	11.298	825345	20.0
Octadecanoic acid	12.627	2.7	ng	110115	4	11.298	825345	20.0
Heptadecyl hept...	13.815	7.5	ng	188648	5	13.957	503965	20.0
9-Octadecenamid...	14.727	8.0	ng	202869	6	15.427	506138	20.0