

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
 Data File : BF135136.D
 Acq On : 07 Sep 2023 16:09
 Operator : CG\JU
 Sample : 04283-06
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-1

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: BF135136.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	6	10	18	rVB	21874	29554	1.58%	0.218%
2	4.998	492	495	503	rVB	43656	56976	3.05%	0.420%
3	5.404	559	564	567	rBV	1666599	1615048	86.57%	11.912%
4	6.410	730	735	738	rBV	1720198	1595823	85.54%	11.770%
5	6.769	793	796	800	rBV	692948	550149	29.49%	4.058%
6	7.333	887	892	895	rBV	1149844	1028693	55.14%	7.587%
7	8.051	1009	1014	1017	rBV	803199	743149	39.83%	5.481%
8	9.127	1193	1197	1200	rBV	2228294	1865598	100.00%	13.760%
9	9.245	1214	1217	1223	rVB	25317	24325	1.30%	0.179%
10	9.810	1308	1313	1316	rBV	917169	819051	43.90%	6.041%
11	10.598	1443	1447	1461	rBV	1248785	1168167	62.62%	8.616%
12	11.298	1563	1566	1570	rBV	905270	790194	42.36%	5.828%
13	11.839	1653	1658	1668	rBV	190737	213203	11.43%	1.573%
14	12.627	1789	1792	1806	rBV	64730	86166	4.62%	0.636%
15	12.898	1834	1838	1841	rBV	1879281	1559738	83.61%	11.504%
16	13.815	1988	1994	2006	rBV2	60905	109257	5.86%	0.806%
17	13.957	2014	2018	2025	rBV	492555	460239	24.67%	3.395%
18	14.721	2145	2148	2159	rBV	283936	354153	18.98%	2.612%
19	15.421	2262	2267	2273	rBV	377472	488562	26.19%	3.603%

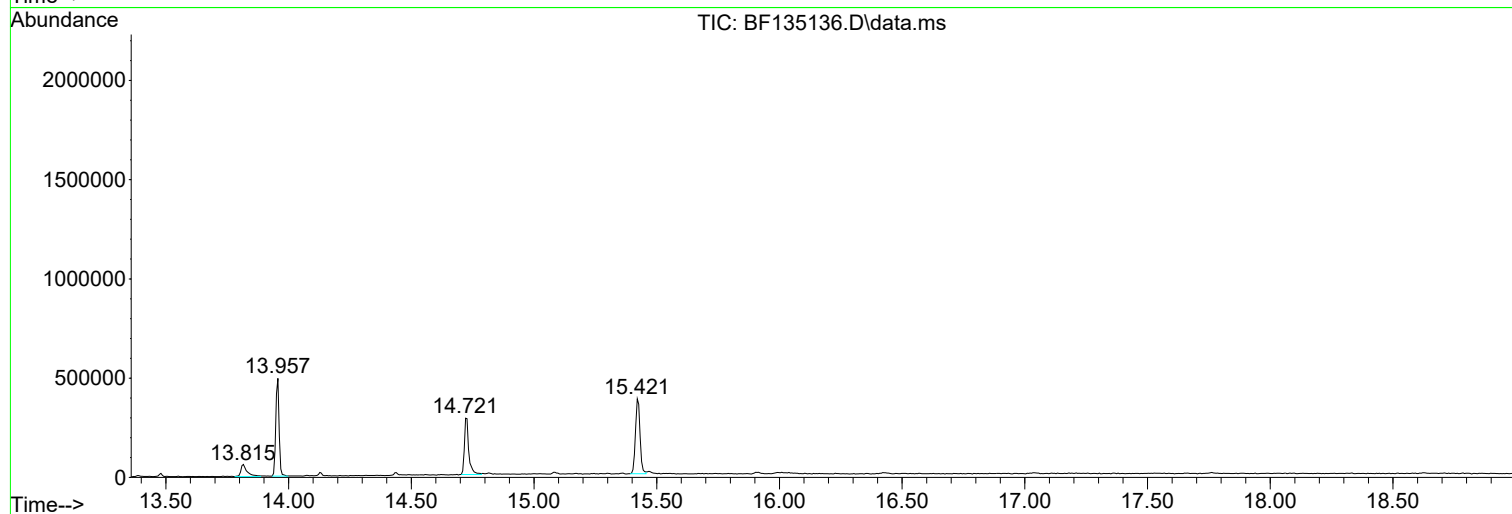
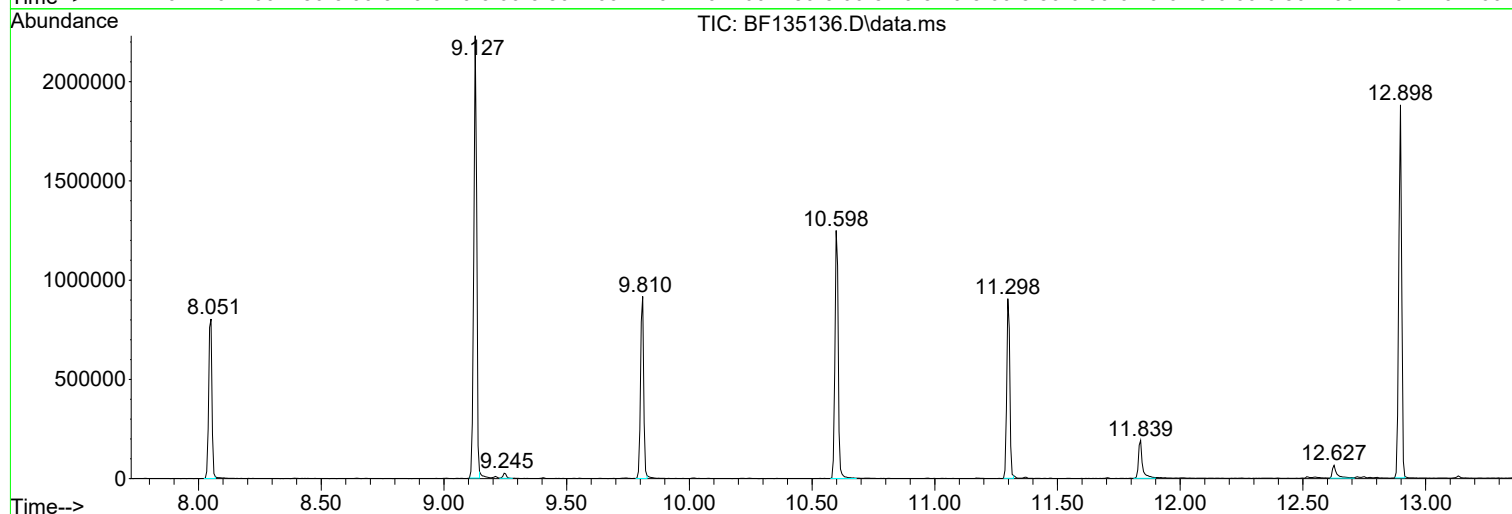
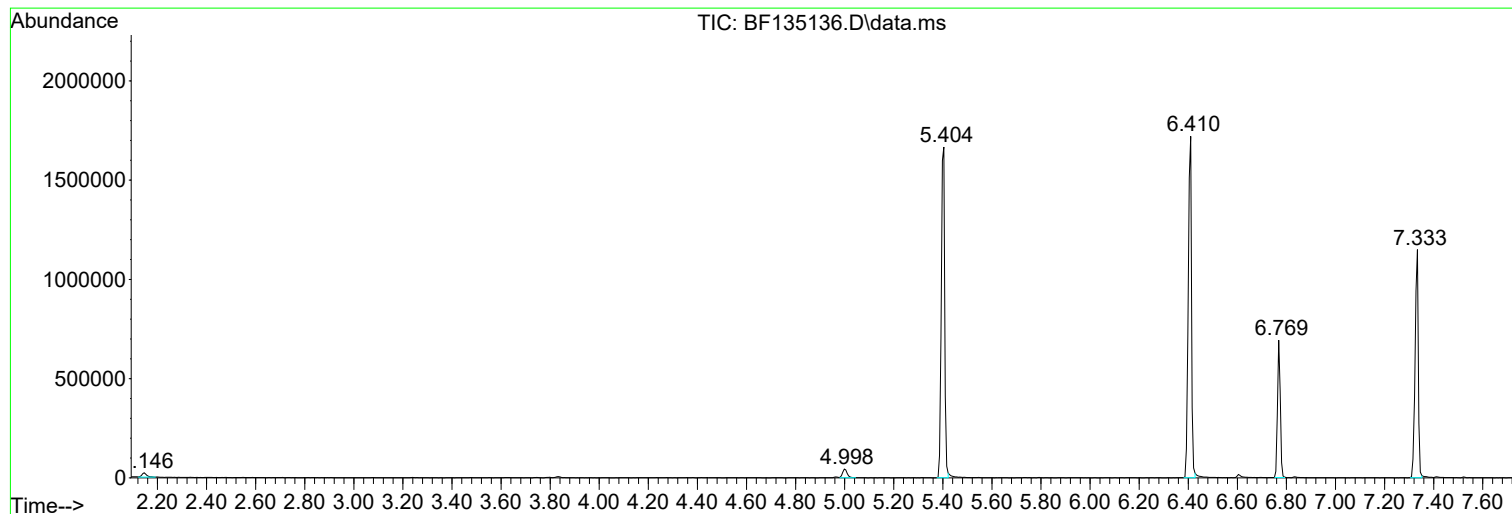
Sum of corrected areas: 13558045

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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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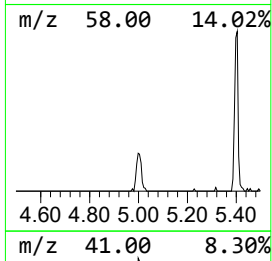
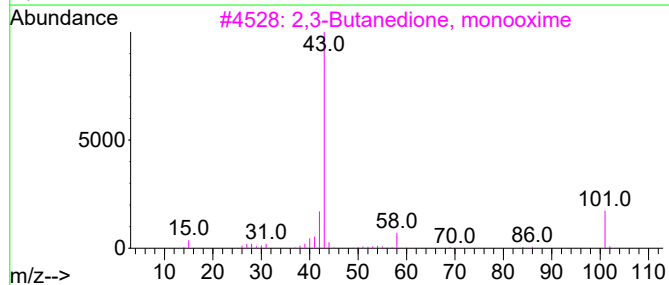
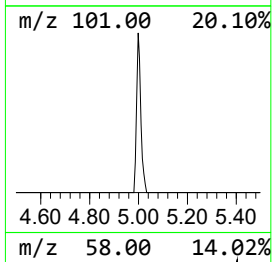
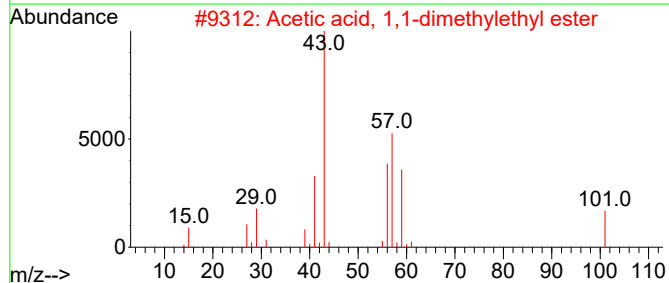
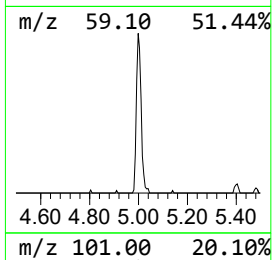
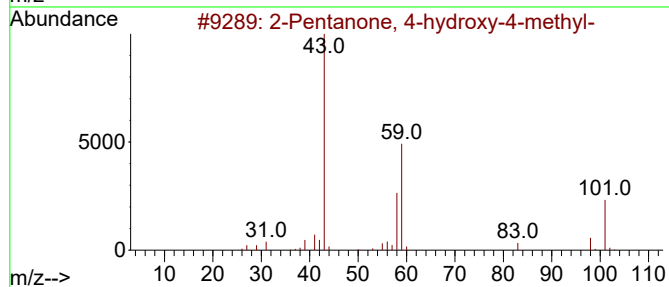
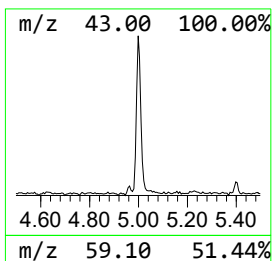
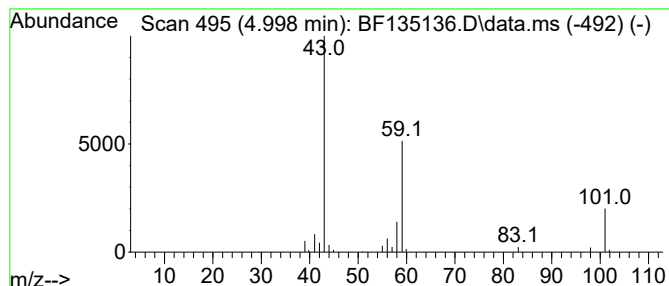
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	2.07 ng	56976	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	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	3-Octanol	130	C8H18O	000589-98-0	9		



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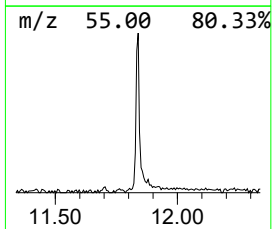
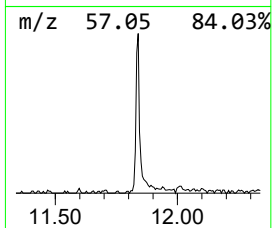
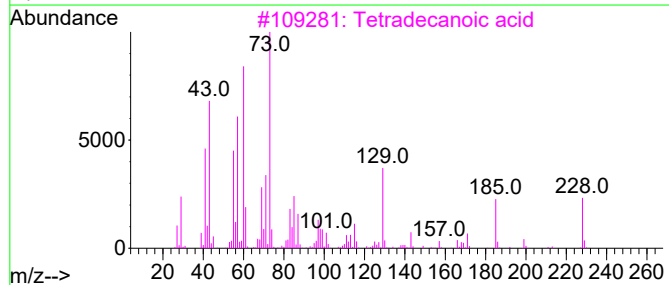
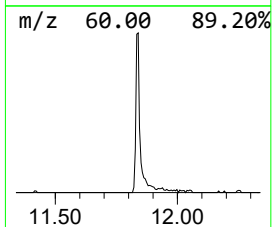
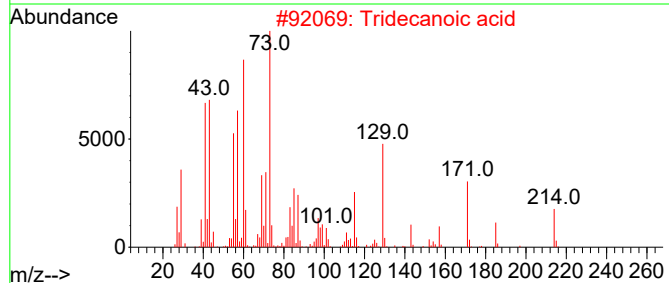
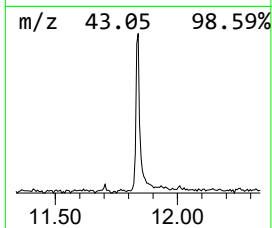
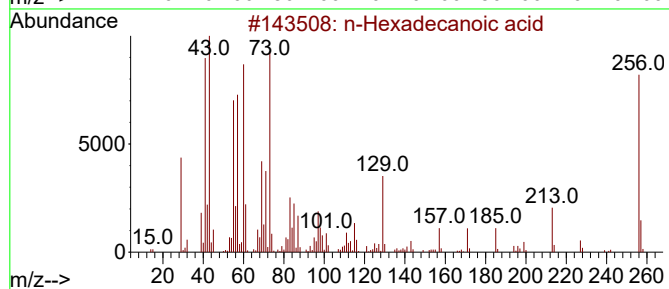
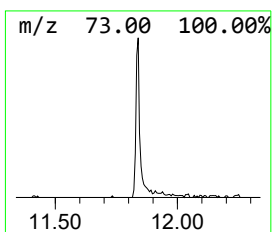
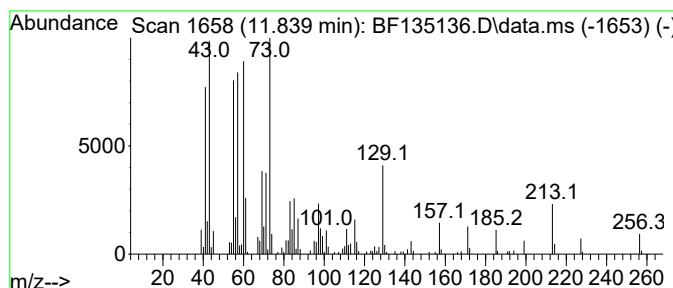
Instrument :
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.839	5.40 ng	213203	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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60



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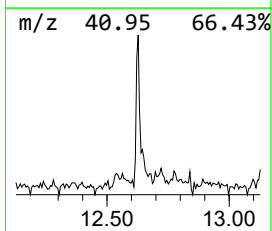
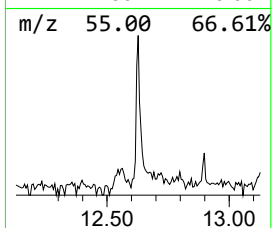
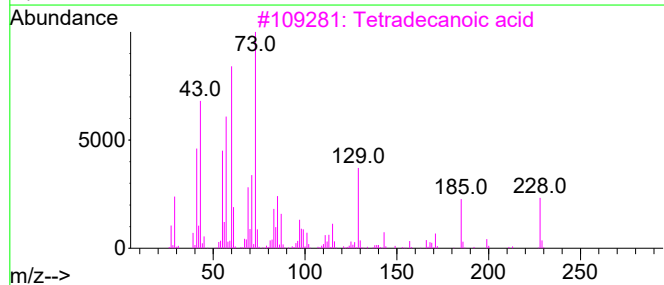
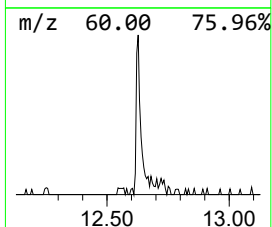
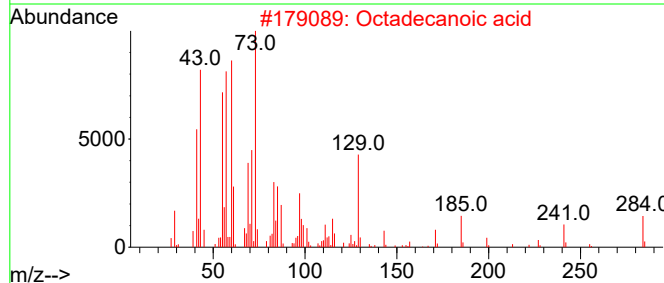
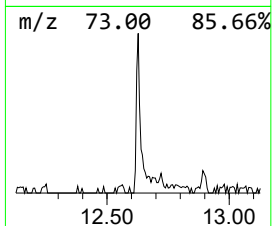
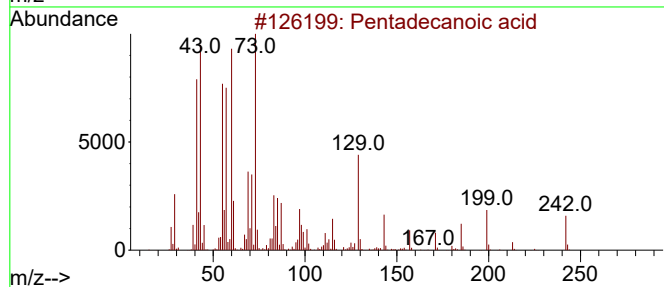
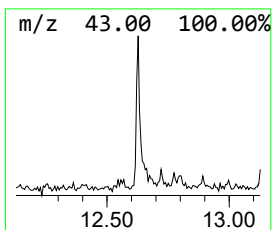
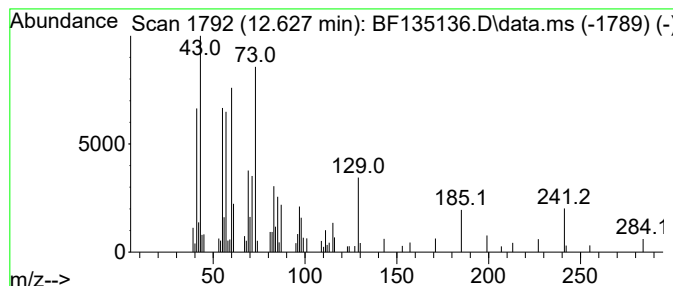
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Peak Number 3 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	2.18 ng	86166	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2			Octadecanoic acid	284	C18H36O2	000057-11-4	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	53
5			Dodecanoic acid	200	C12H24O2	000143-07-7	50



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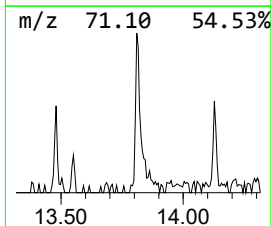
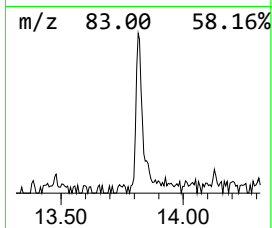
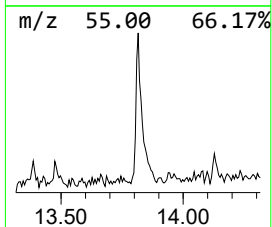
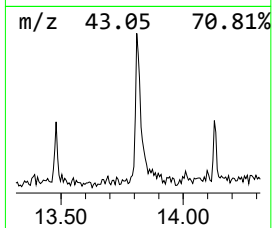
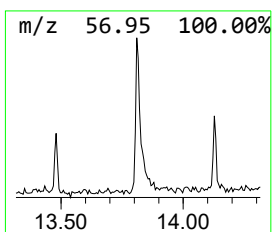
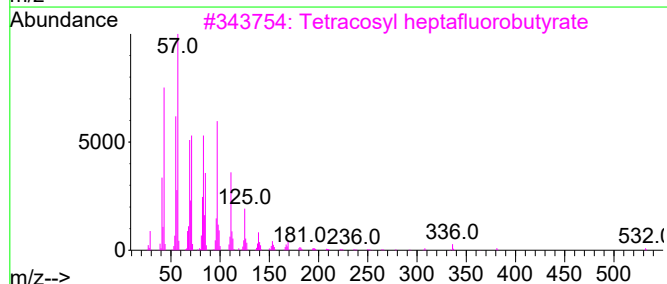
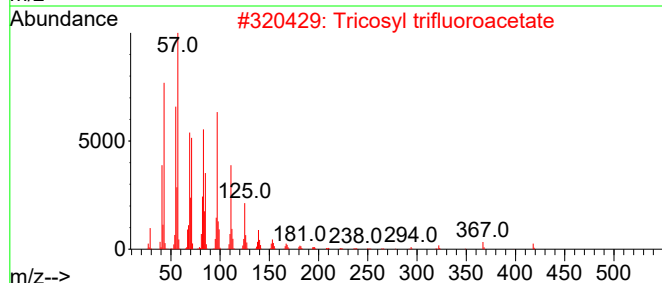
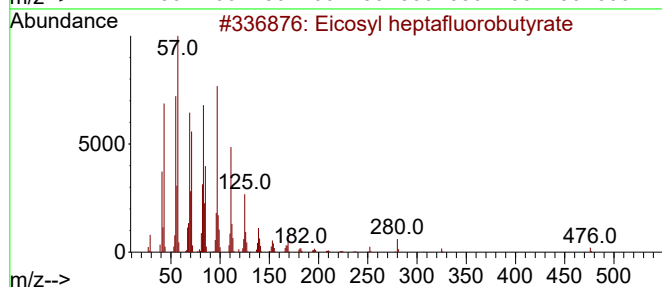
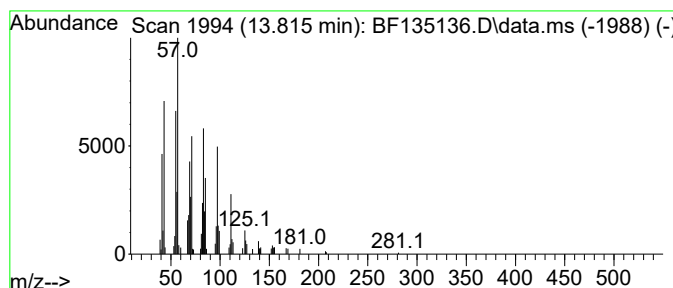
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Peak Number 4 Eicosyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	4.75 ng	109257	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
2			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5			Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91



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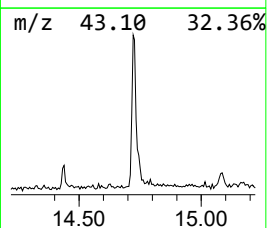
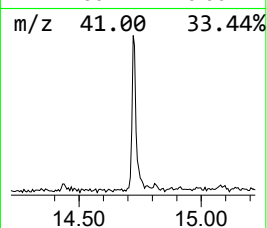
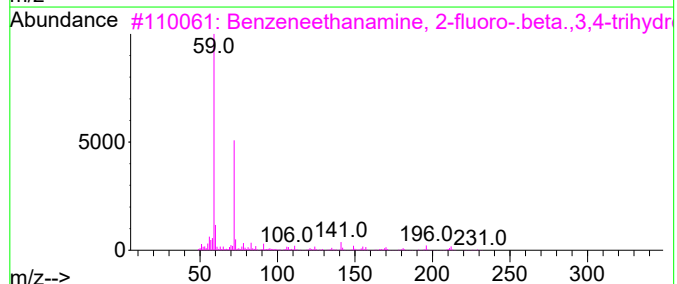
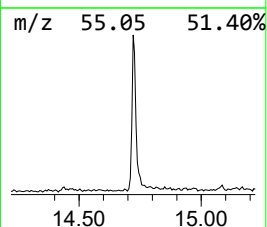
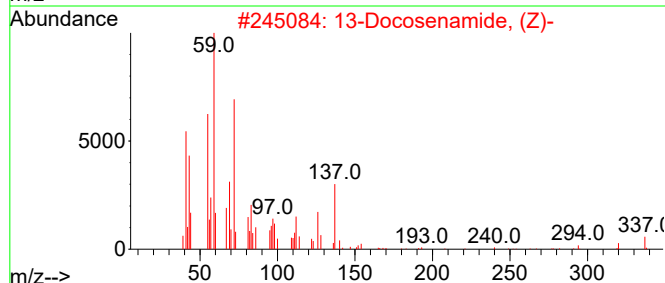
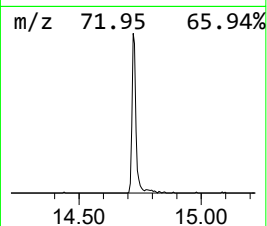
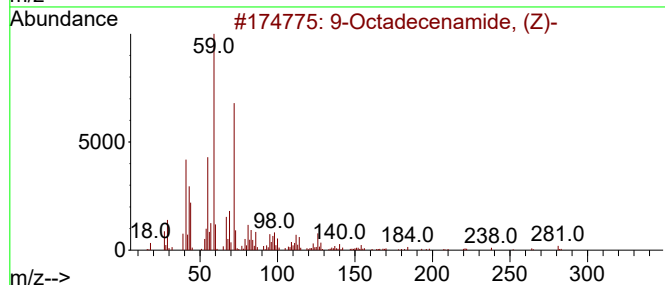
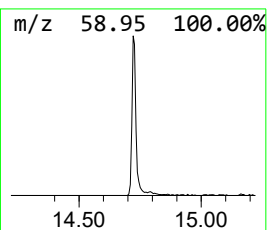
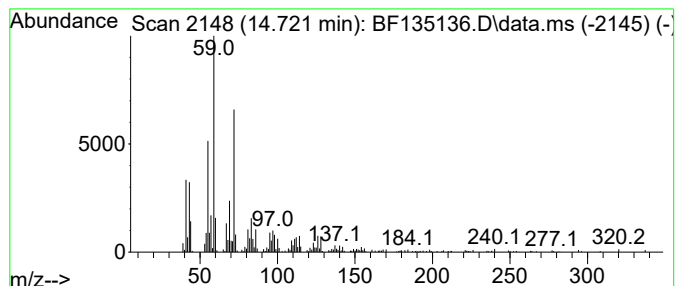
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	14.50 ng	354153	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
4			Dodecanamide	199	C12H25NO	001120-16-7	53
5			Octadecanamide	283	C18H37NO	000124-26-5	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.998	2.1	ng	56976	1	6.769	550149	20.0
n-Hexadecanoic ...	11.839	5.4	ng	213203	4	11.298	790194	20.0
Pentadecanoic acid	12.627	2.2	ng	86166	4	11.298	790194	20.0
Eicosyl heptafl...	13.815	4.8	ng	109257	5	13.957	460239	20.0
9-Octadecenamid...	14.721	14.5	ng	354153	6	15.421	488562	20.0