

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
 Data File : BG055633.D
 Acq On : 15 Nov 2022 22:32
 Operator : CG/JU
 Sample : N5431-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DISSOLVED-20221176-COMP-11-MODIFIED-ELUTRIATE

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-BG110922.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055633.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.690	233	238	244	rBV	15317	22929	1.10%	0.227%
2	5.307	337	343	351	rBV	44738	69704	3.34%	0.689%
3	5.783	417	424	432	rBV	246804	404179	19.39%	3.996%
4	7.387	690	697	711	rVB	200781	354769	17.02%	3.508%
5	8.256	837	845	851	rBV	140917	238768	11.45%	2.361%
6	9.425	1036	1044	1052	rVB	299713	523651	25.12%	5.178%
7	11.082	1316	1326	1334	rBV	195355	353648	16.96%	3.497%
8	11.729	1429	1436	1443	rBV	12814	21766	1.04%	0.215%
9	13.503	1730	1738	1745	rBV	810283	1228330	58.92%	12.145%
10	14.314	1871	1876	1881	rBV	23259	32976	1.58%	0.326%
11	14.878	1965	1972	1979	rVB	347349	533317	25.58%	5.273%
12	16.358	2216	2224	2233	rBV	728994	1161924	55.73%	11.489%
13	17.616	2431	2438	2445	rBV	499305	733230	35.17%	7.250%
14	18.256	2543	2547	2552	rBV	36455	43311	2.08%	0.428%
15	18.479	2580	2585	2595	rBV	127328	215322	10.33%	2.129%
16	19.414	2741	2744	2748	rVB	60787	66475	3.19%	0.657%
17	19.543	2762	2766	2772	rBV	23953	30542	1.46%	0.302%
18	19.619	2772	2779	2789	rBV	12061	40159	1.93%	0.397%
19	19.737	2795	2799	2808	rBV	70412	114280	5.48%	1.130%
20	20.207	2873	2879	2884	rBV	1553140	2084840	100.00%	20.614%
21	21.546	3100	3107	3122	rBV8	42322	169186	8.12%	1.673%
22	21.917	3163	3170	3179	rBV2	469945	802385	38.49%	7.934%
23	23.679	3466	3470	3477	rVB4	19309	40782	1.96%	0.403%
24	25.330	3741	3751	3762	rVB2	285957	827039	39.67%	8.178%

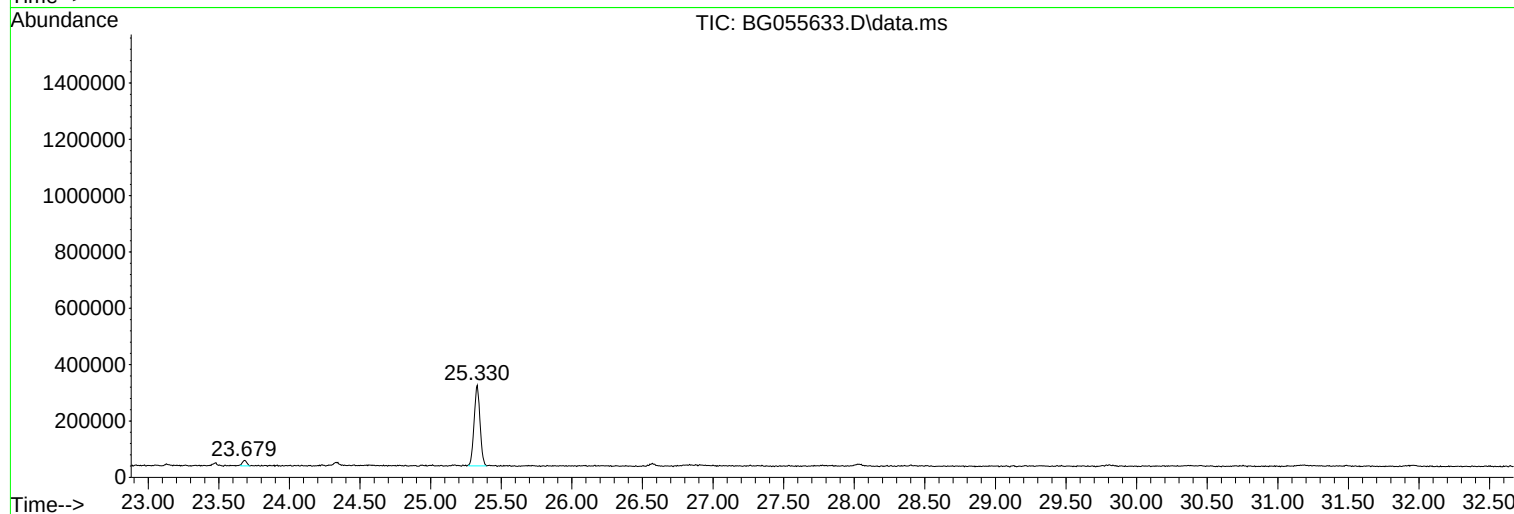
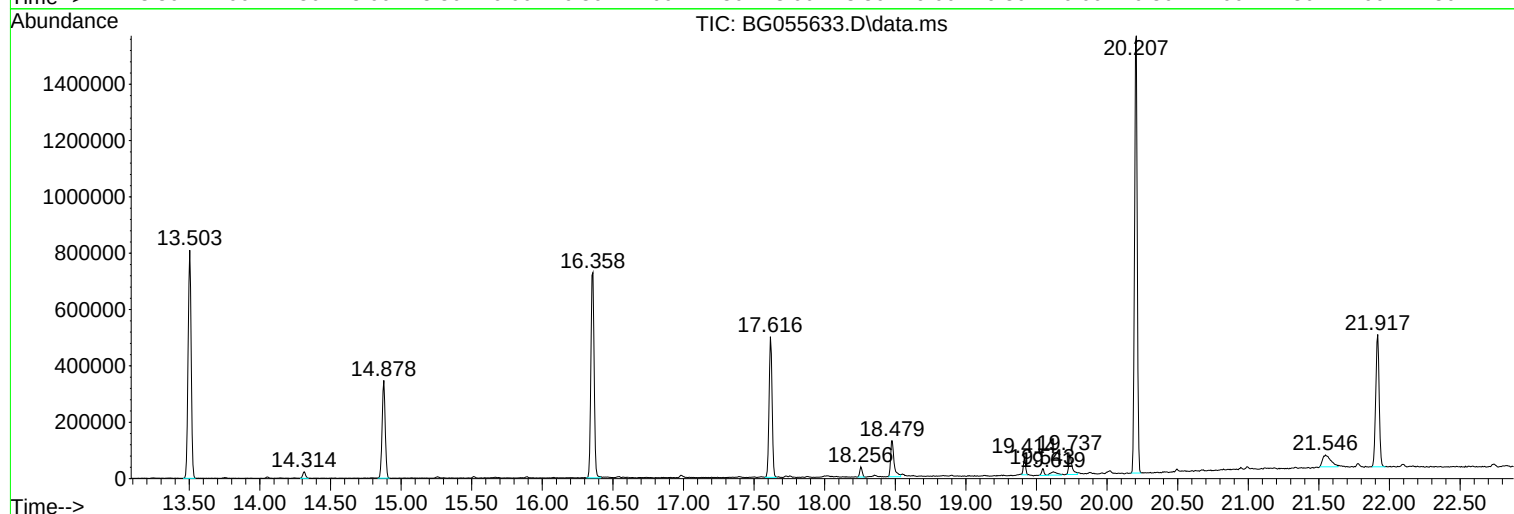
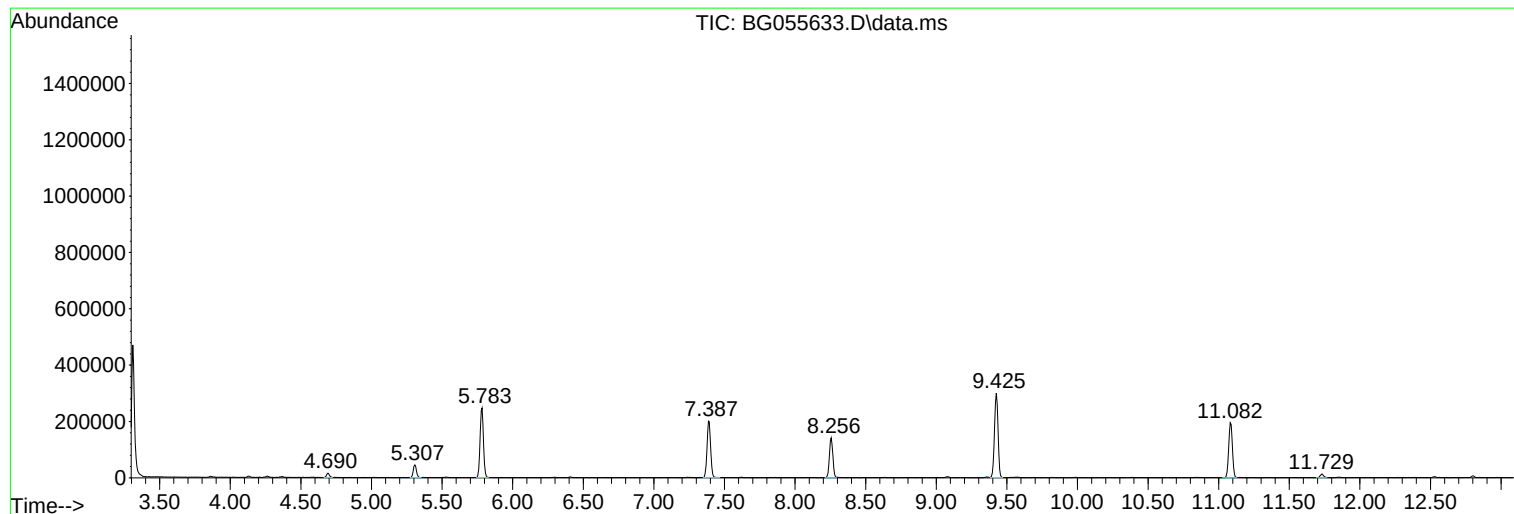
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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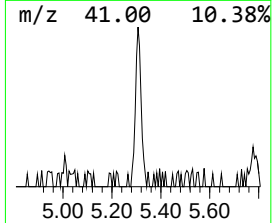
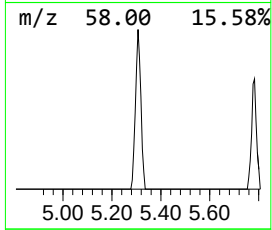
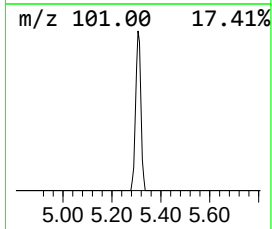
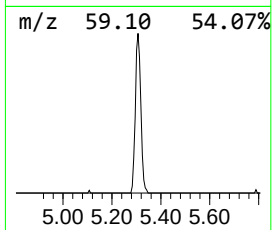
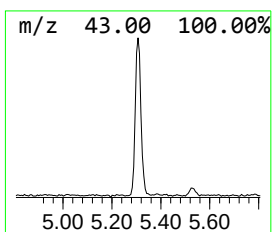
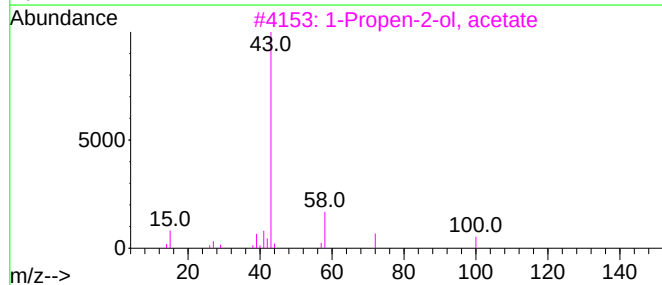
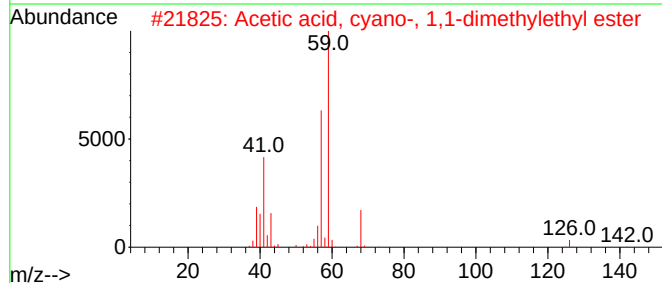
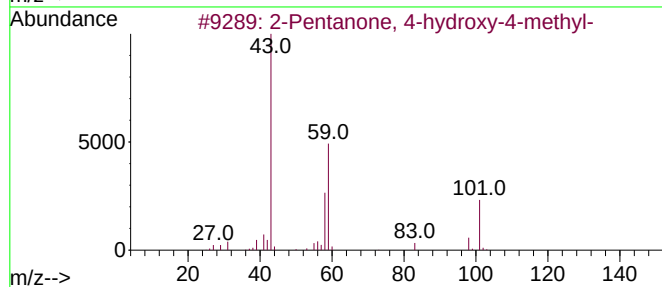
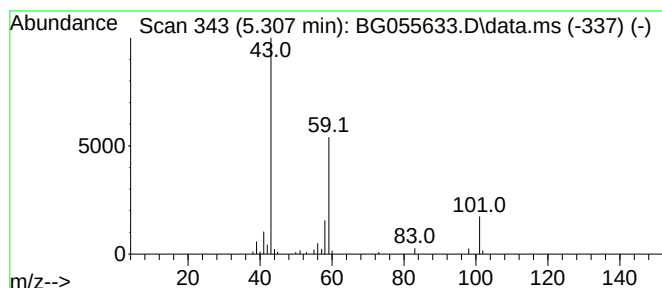
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.307	5.84 ng	69704	1,4-Dichlorobenzene-d4	8.256

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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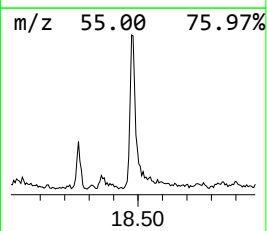
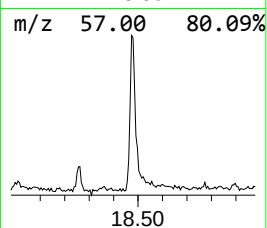
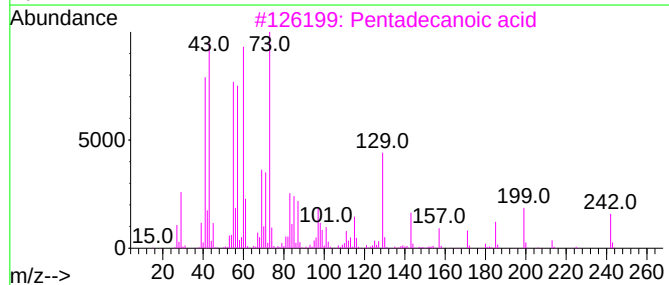
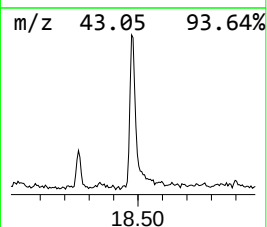
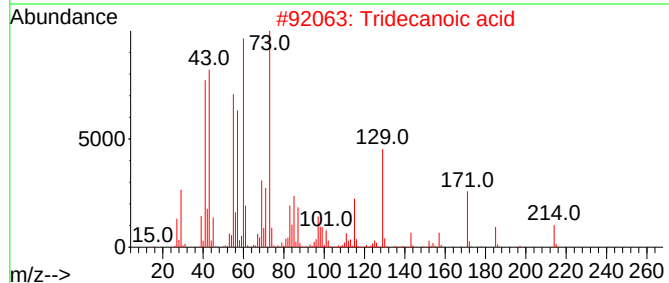
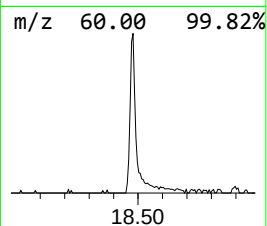
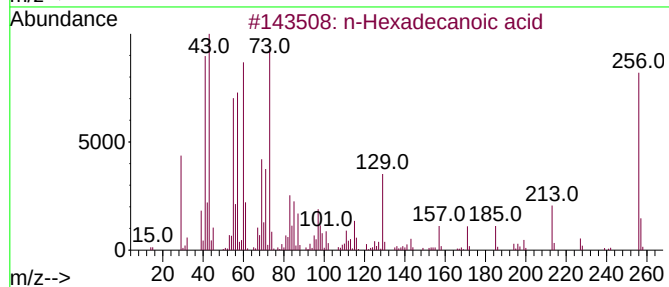
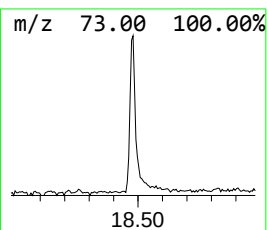
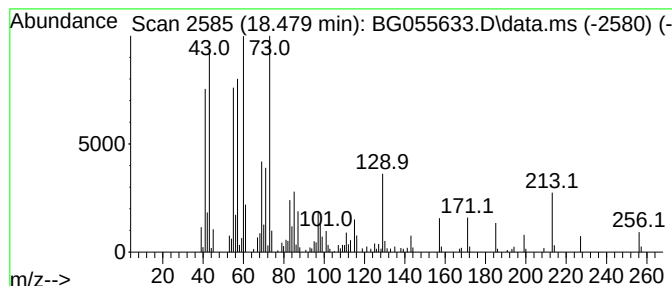
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.480	5.87 ng	215322	Phenanthrene-d10	17.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	80



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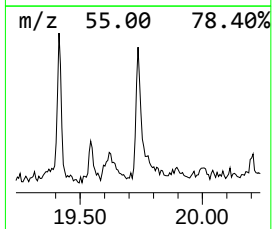
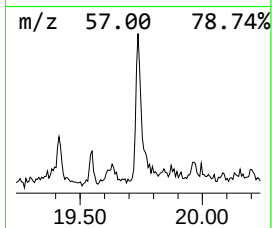
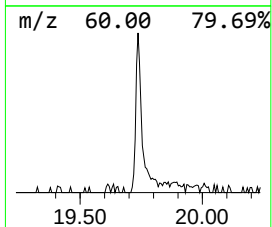
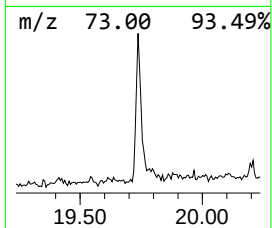
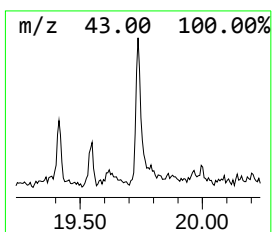
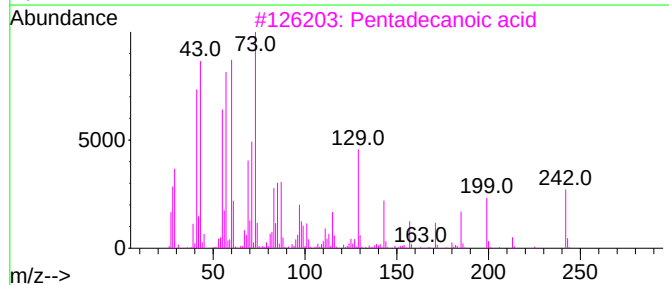
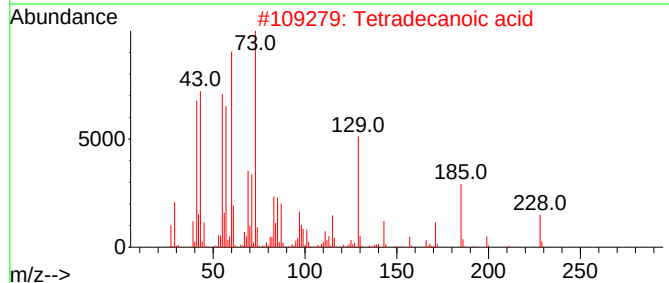
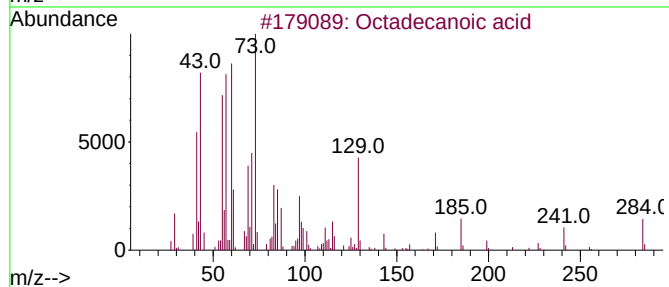
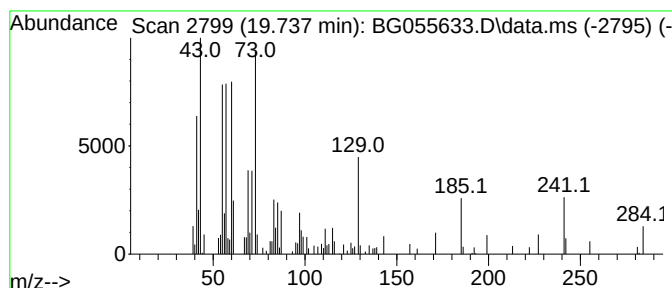
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.737	3.12 ng	114280	Phenanthrene-d10	17.616	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	62



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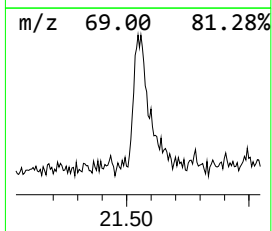
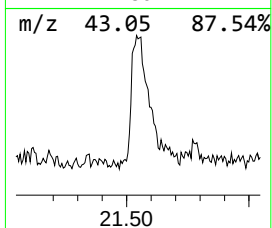
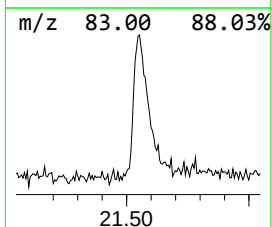
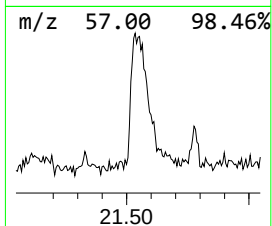
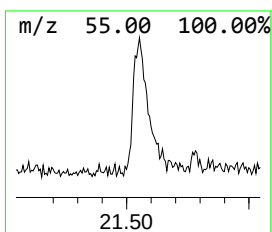
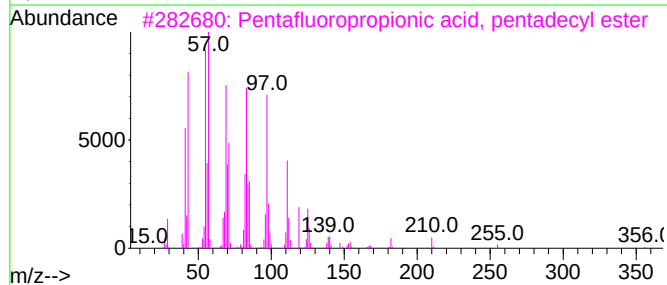
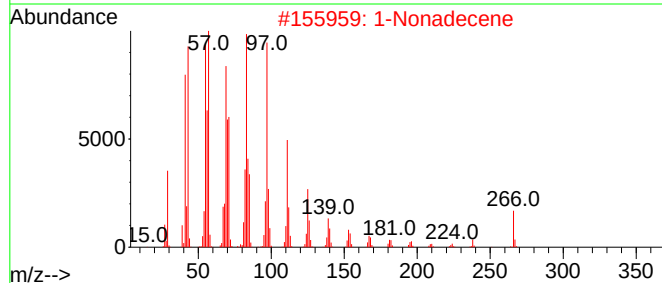
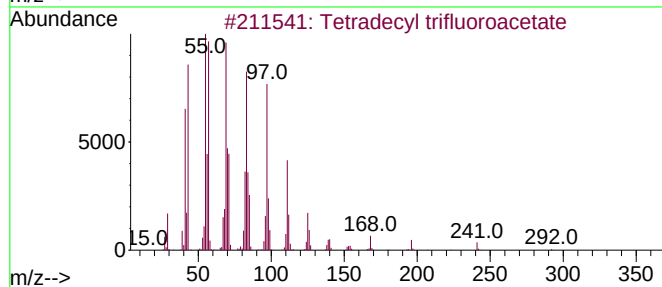
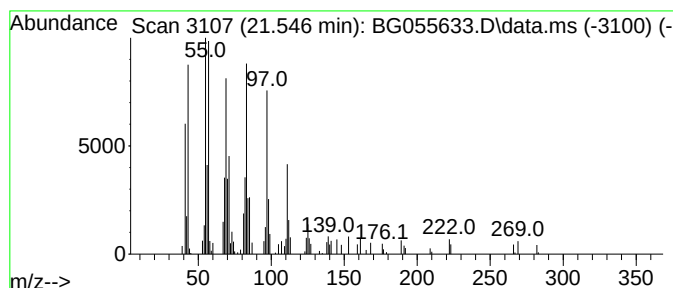
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Peak Number 4 Tetradecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.547	4.22 ng	169186	Chrysene-d12	21.917	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	95
2	1-Nonadecene	266	C19H38	018435-45-5	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.307	5.8	ng	69704	1	8.256	238768	20.0
n-Hexadecanoic ...	18.480	5.9	ng	215322	4	17.616	733230	20.0
Octadecanoic acid	19.737	3.1	ng	114280	4	17.616	733230	20.0
Tetradecyl trif...	21.547	4.2	ng	169186	5	21.917	802385	20.0