

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101923\
 Data File : BF135892.D
 Acq On : 19 Oct 2023 18:12
 Operator : CG\JU
 Sample : 04908-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135892.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	484	488	501	rBV	465629	633940	33.96%	4.879%
2	5.375	556	559	589	rBV	1395168	1565645	83.86%	12.049%
3	6.392	729	732	755	rBV	1652849	1576012	84.42%	12.129%
4	6.733	787	790	800	rVB	462969	387681	20.77%	2.984%
5	7.304	883	887	900	rBV	1070952	928017	49.71%	7.142%
6	8.016	1004	1008	1021	rBV	492508	445659	23.87%	3.430%
7	9.092	1187	1191	1194	rBV	2359638	1866955	100.00%	14.368%
8	9.210	1208	1211	1216	rVB	28369	25856	1.38%	0.199%
9	9.769	1303	1306	1315	rBV	656241	575184	30.81%	4.427%
10	10.568	1438	1442	1458	rBV	1249093	1132370	60.65%	8.715%
11	11.268	1557	1561	1571	rBV	657107	567945	30.42%	4.371%
12	11.804	1648	1652	1664	rBV	335764	381567	20.44%	2.937%
13	12.592	1783	1786	1798	rBV	67755	94598	5.07%	0.728%
14	12.862	1828	1832	1836	rBV	1798855	1585675	84.93%	12.203%
15	13.768	1979	1986	1988	rBV	25303	32850	1.76%	0.253%
16	13.821	1988	1995	2006	rVV6	37167	135651	7.27%	1.044%
17	13.933	2011	2014	2025	rVV	414144	408551	21.88%	3.144%
18	14.698	2140	2144	2147	rBV2	22570	23502	1.26%	0.181%
19	14.768	2152	2156	2160	rVB	165593	172602	9.25%	1.328%
20	15.027	2197	2200	2205	rVB3	28598	34585	1.85%	0.266%
21	15.409	2261	2265	2273	rBV	313609	418859	22.44%	3.224%

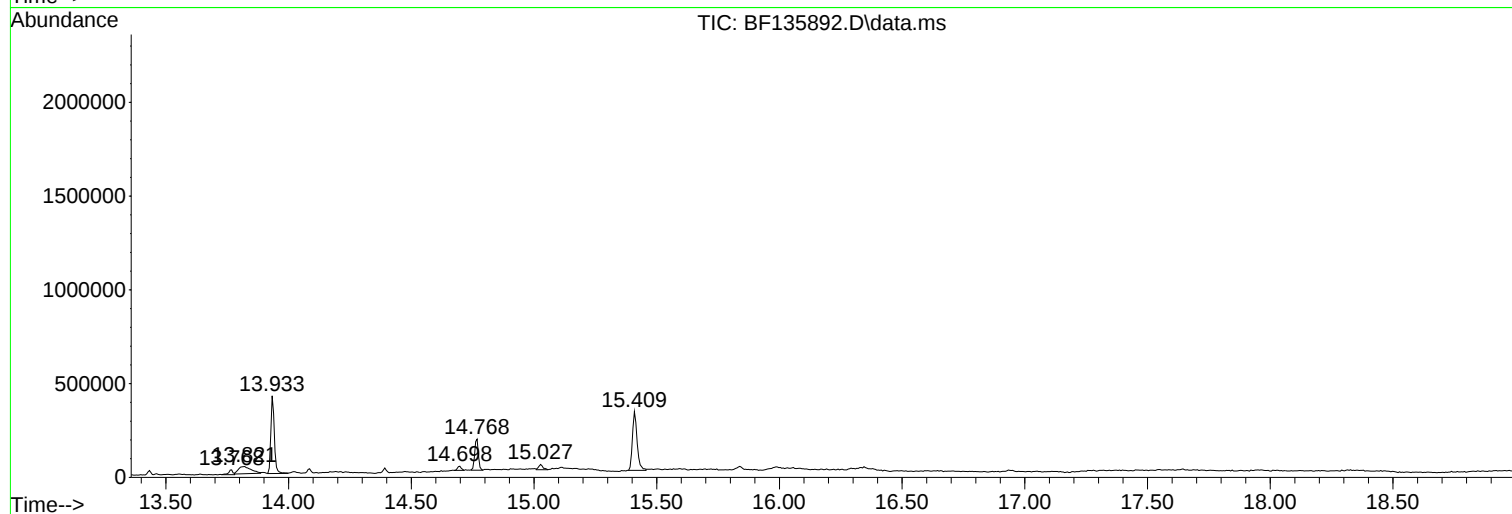
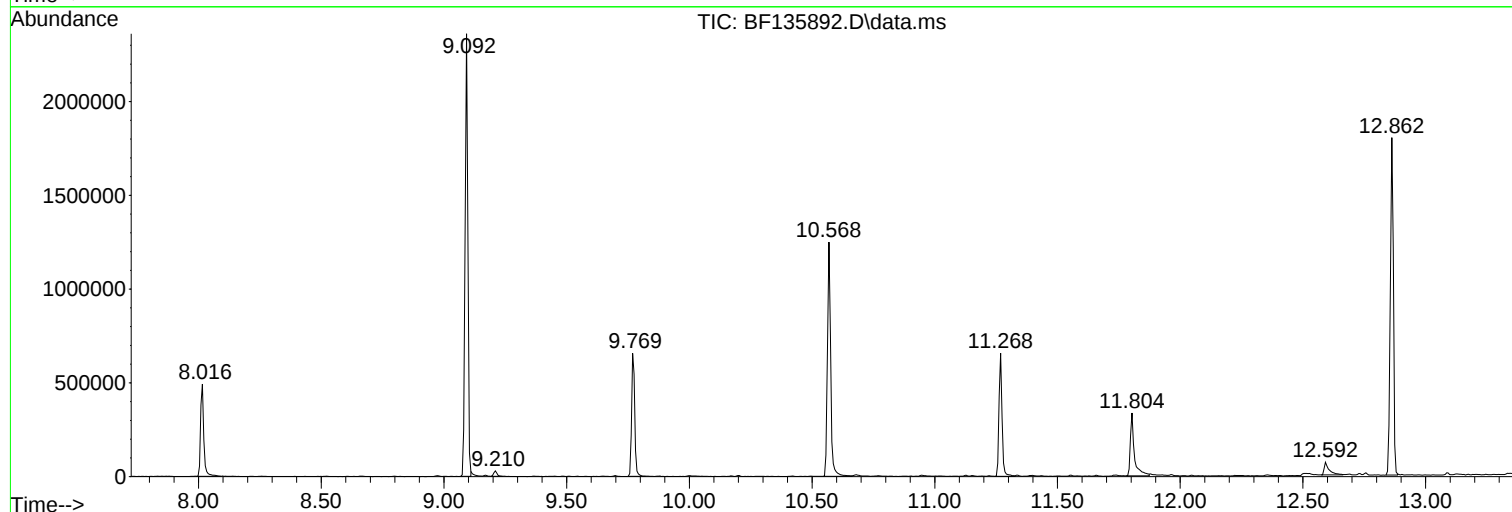
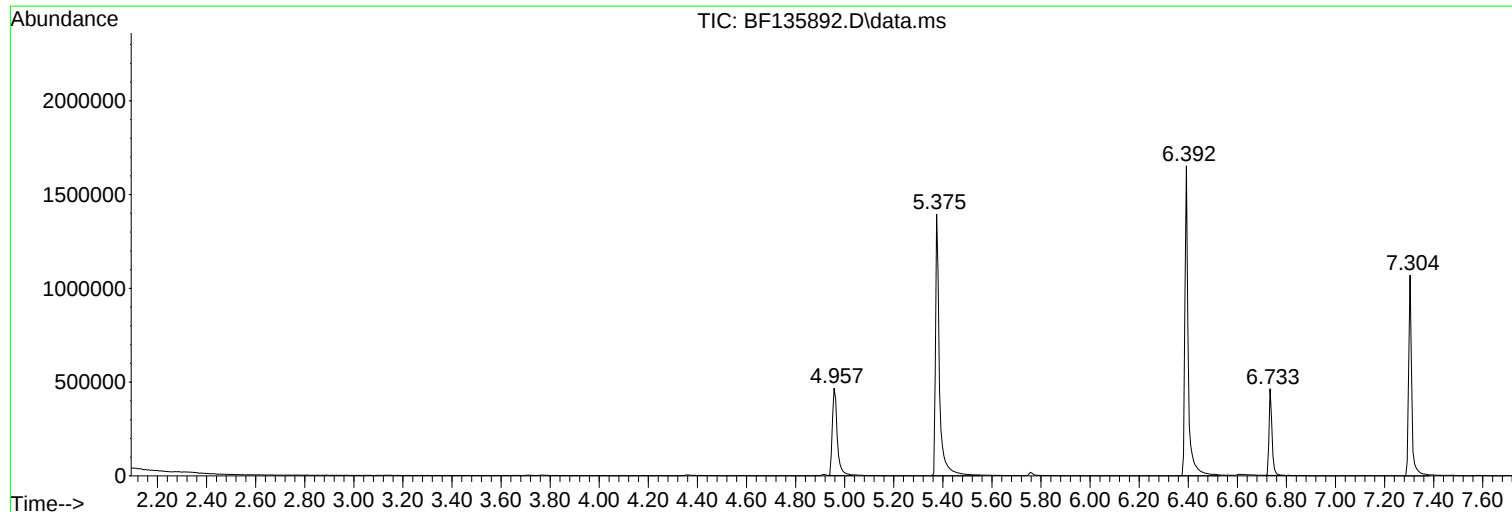
Sum of corrected areas: 12993704

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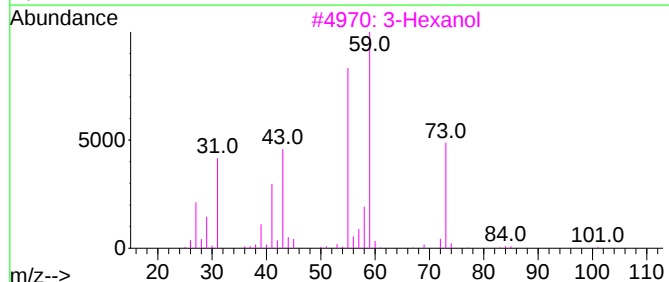
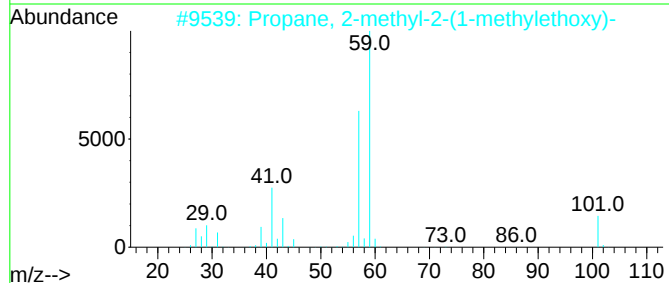
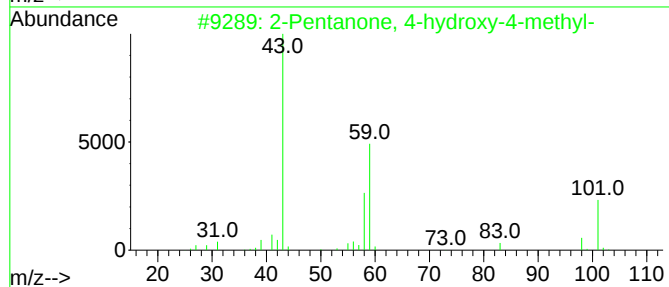
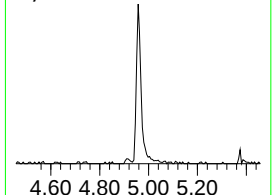
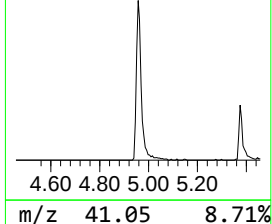
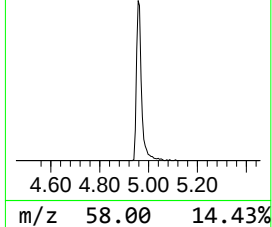
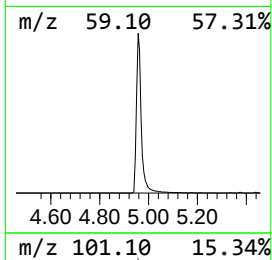
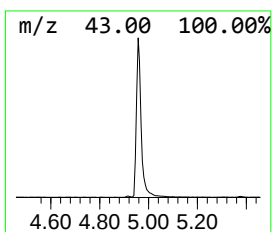
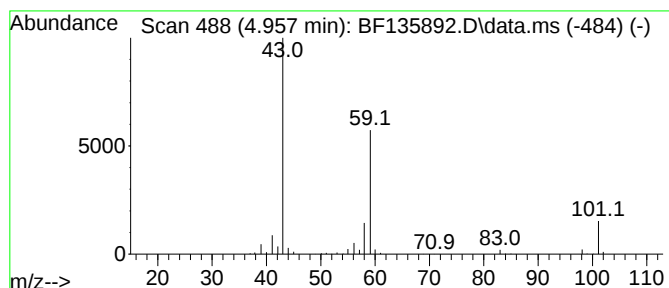
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	32.70 ng	633940	1,4-Dichlorobenzene-d4	6.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	3-Hexanol	102	C6H14O	000623-37-0	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		



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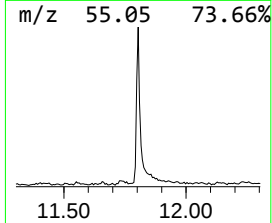
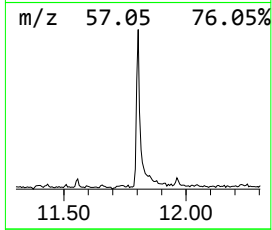
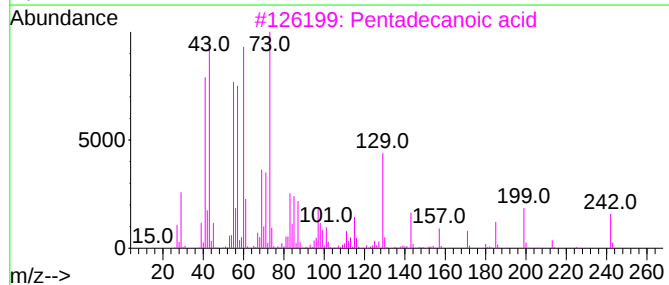
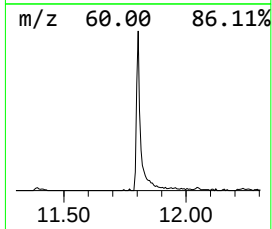
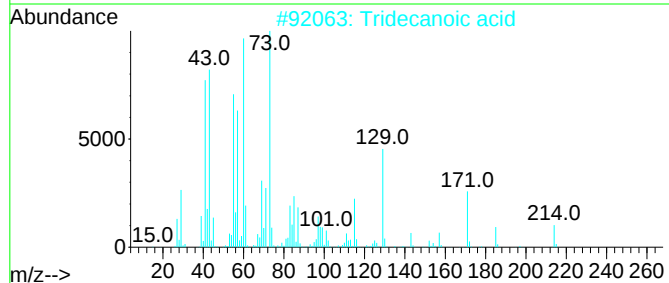
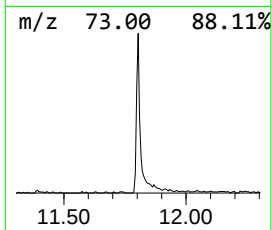
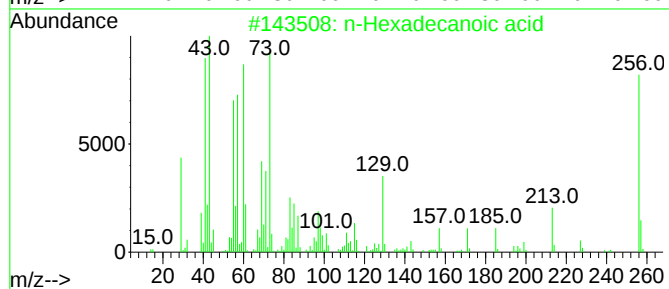
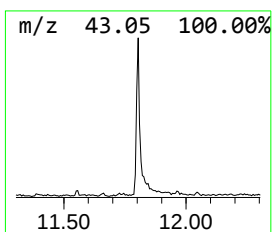
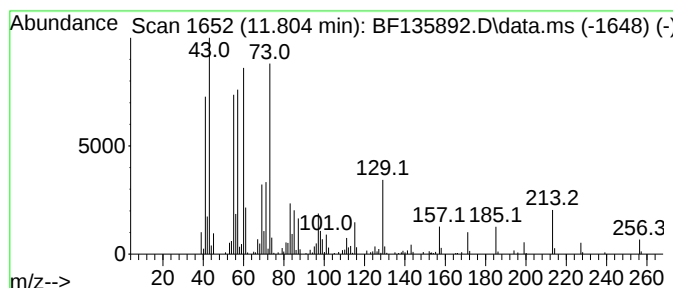
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	13.44 ng	381567	Phenanthrene-d10	11.268

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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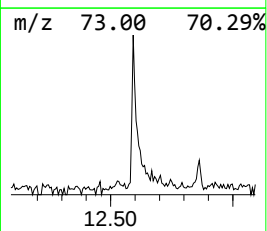
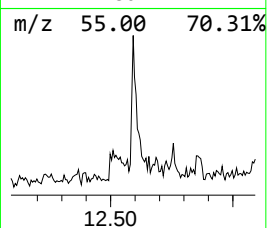
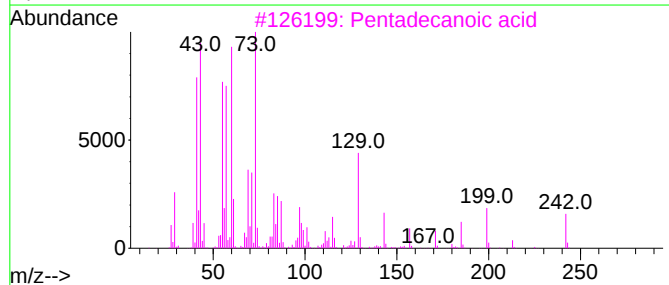
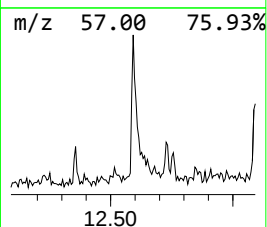
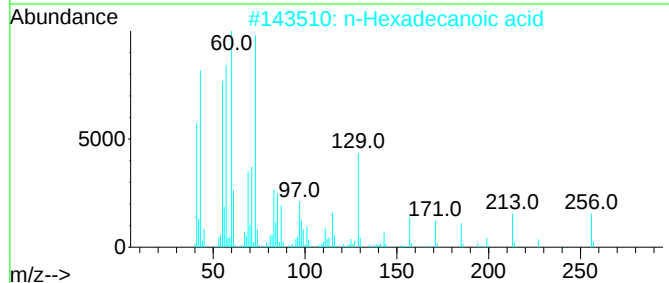
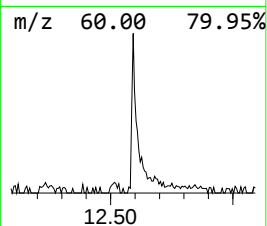
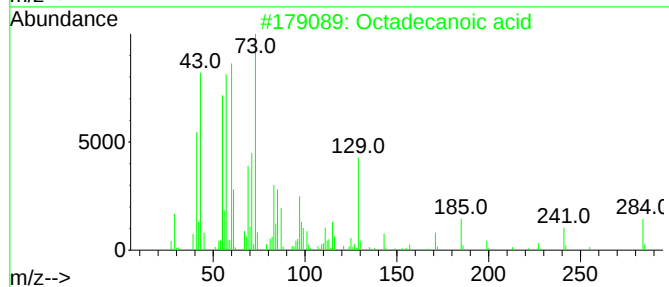
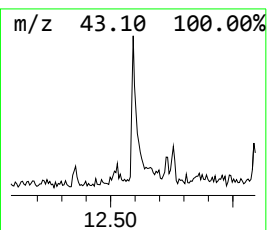
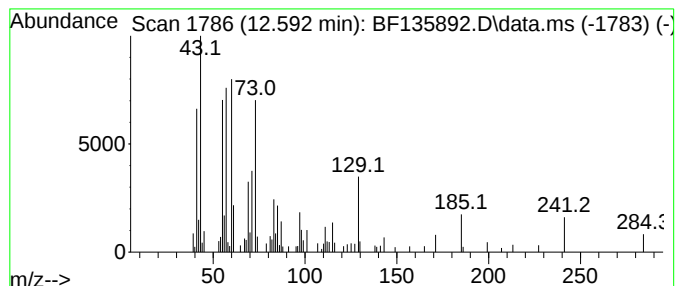
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	3.33 ng	94598	Phenanthrene-d10	11.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	62



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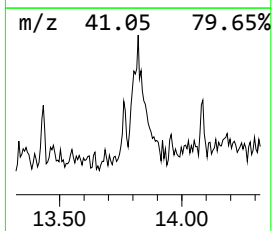
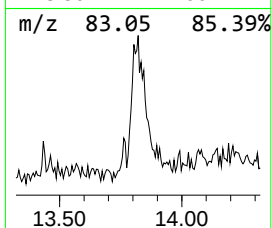
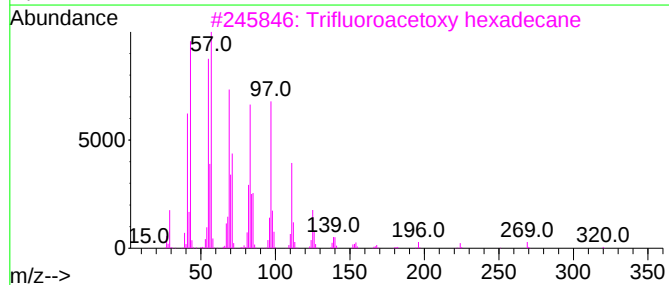
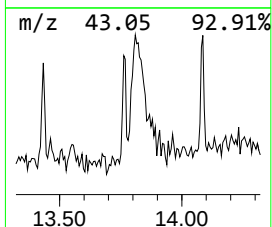
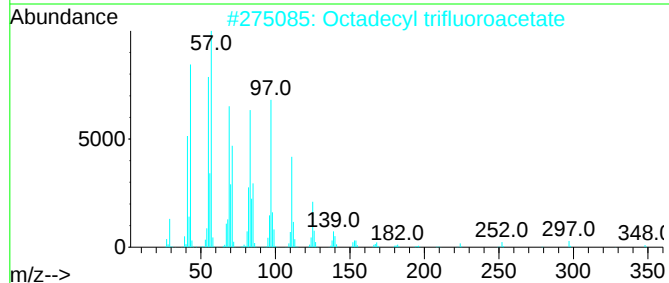
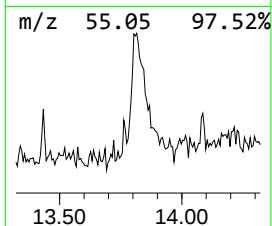
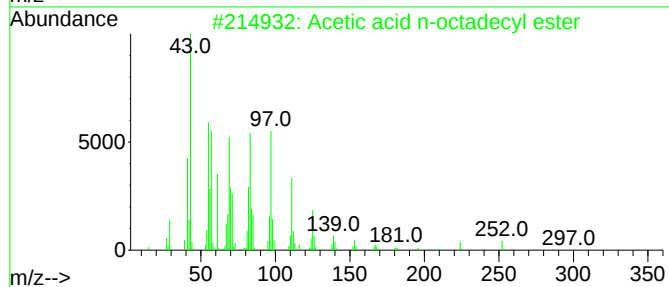
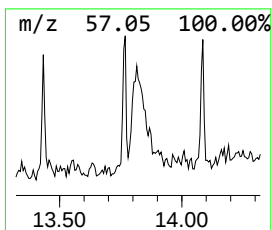
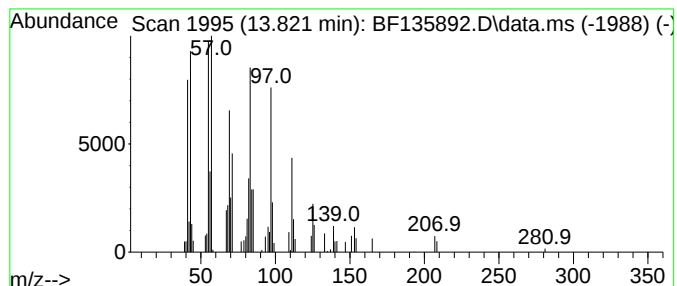
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Acetic acid n-octadecyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.821	6.64 ng	135651	Chrysene-d12	13.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	91
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91



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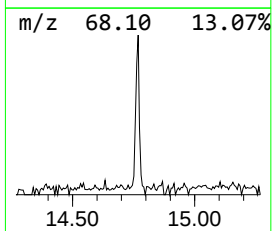
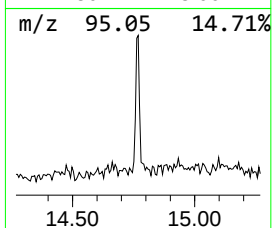
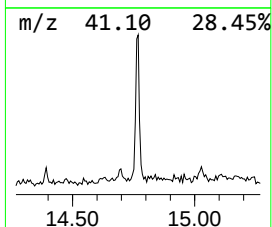
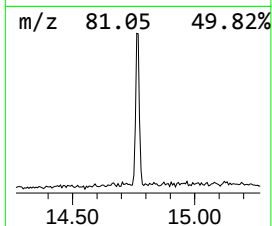
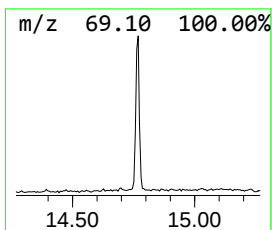
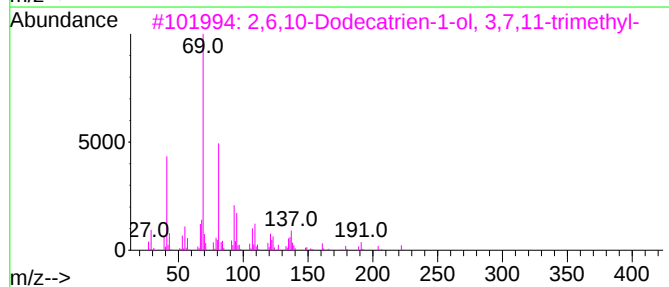
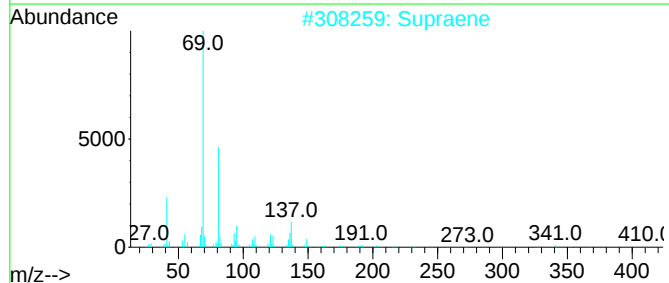
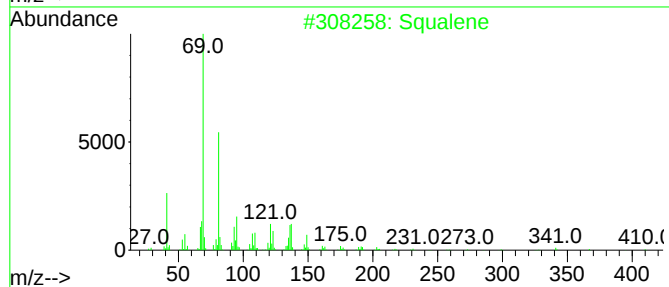
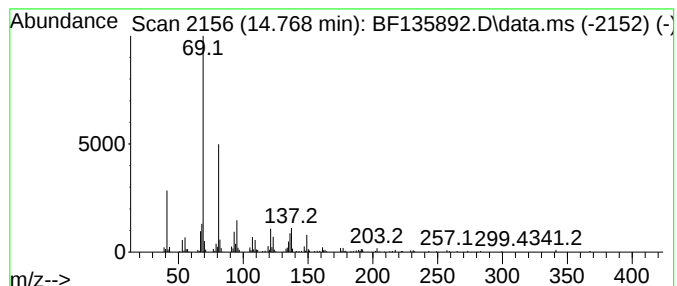
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	8.24 ng	172602	Perylene-d12	15.409

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	91
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
4			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
5			trans-Farnesol	222	C15H26O	000106-28-5	64



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	32.7	ng	633940	1	6.733	387681	20.0
n-Hexadecanoic ...	11.804	13.4	ng	381567	4	11.268	567945	20.0
Octadecanoic acid	12.592	3.3	ng	94598	4	11.268	567945	20.0
Acetic acid n-o...	13.821	6.6	ng	135651	5	13.933	408551	20.0
Squalene	14.768	8.2	ng	172602	6	15.409	418859	20.0