

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090523\
 Data File : BF135115.D
 Acq On : 06 Sep 2023 02:48
 Operator : CG\JU
 Sample : 04203-03
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3(12-12.5)

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: BF135115.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	15	rVB	31483	43626	1.99%	0.276%
2	5.004	493	496	507	rVB	65524	85008	3.87%	0.537%
3	5.404	559	564	567	rBV	2364542	2163817	98.63%	13.670%
4	6.416	731	736	739	rBV	2184904	2157581	98.35%	13.631%
5	6.604	765	768	777	rBV	108602	98294	4.48%	0.621%
6	6.775	793	797	800	rBV	762648	672055	30.63%	4.246%
7	7.334	887	892	895	rBV	1407508	1346188	61.36%	8.505%
8	8.051	1010	1014	1017	rBV	1103003	870364	39.67%	5.499%
9	9.134	1193	1198	1201	rBV	2355299	2193854	100.00%	13.860%
10	9.245	1214	1217	1222	rVB	57903	54699	2.49%	0.346%
11	9.810	1309	1313	1316	rBV	1057631	867254	39.53%	5.479%
12	10.598	1443	1447	1462	rBV	1240593	1152570	52.54%	7.282%
13	11.298	1563	1566	1570	rBV	831932	741794	33.81%	4.686%
14	11.839	1654	1658	1668	rBV	118538	142362	6.49%	0.899%
15	12.627	1788	1792	1796	rBV2	23838	29044	1.32%	0.183%
16	12.898	1834	1838	1841	rBV	2107087	1785684	81.39%	11.281%
17	13.810	1989	1993	2000	rBV	121524	159396	7.27%	1.007%
18	13.957	2014	2018	2025	rVB	713483	648821	29.57%	4.099%
19	14.816	2161	2164	2168	rBV	51663	56083	2.56%	0.354%
20	15.427	2263	2268	2273	rBV	399677	535386	24.40%	3.382%
21	15.910	2348	2350	2357	rVB7	16697	24746	1.13%	0.156%

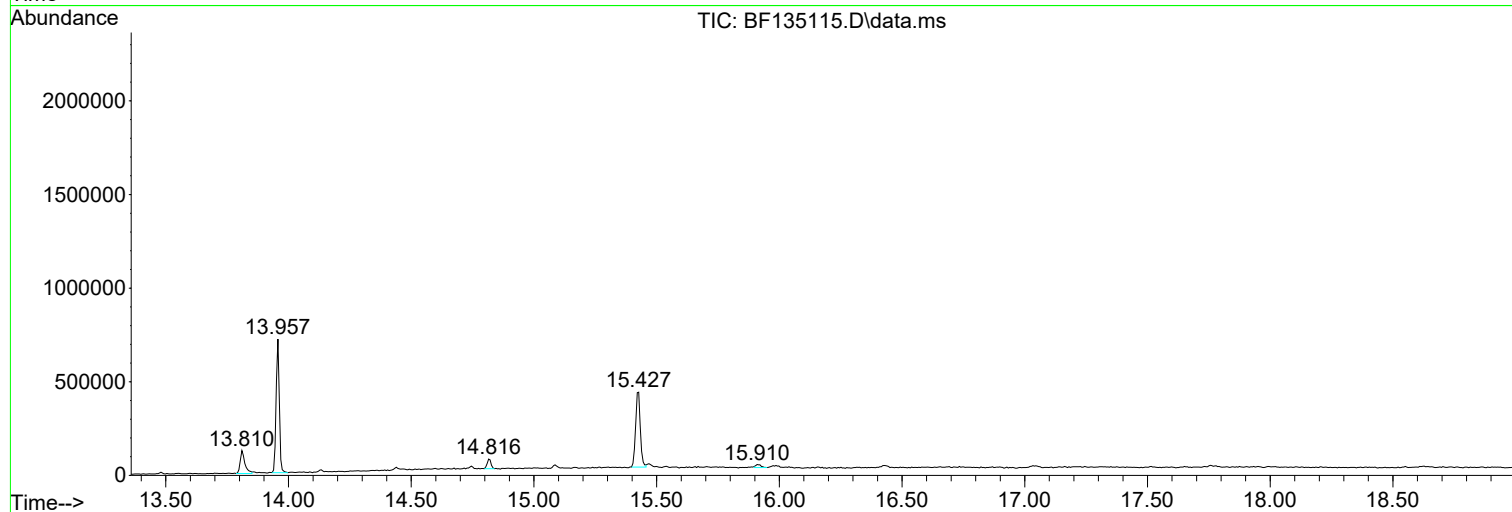
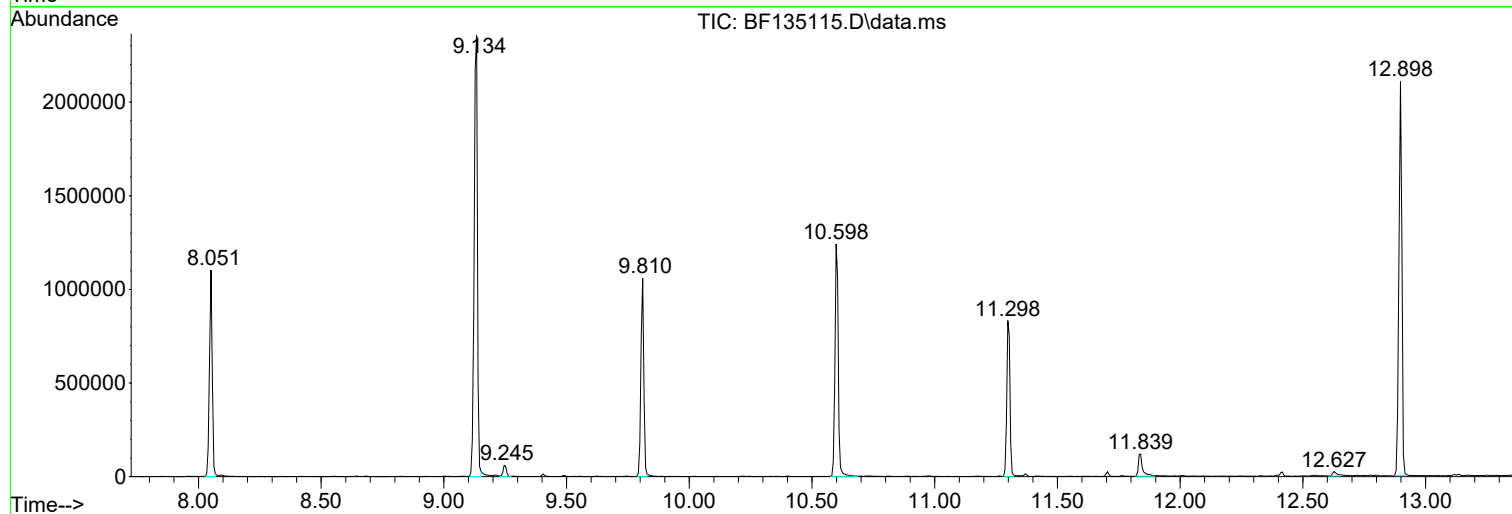
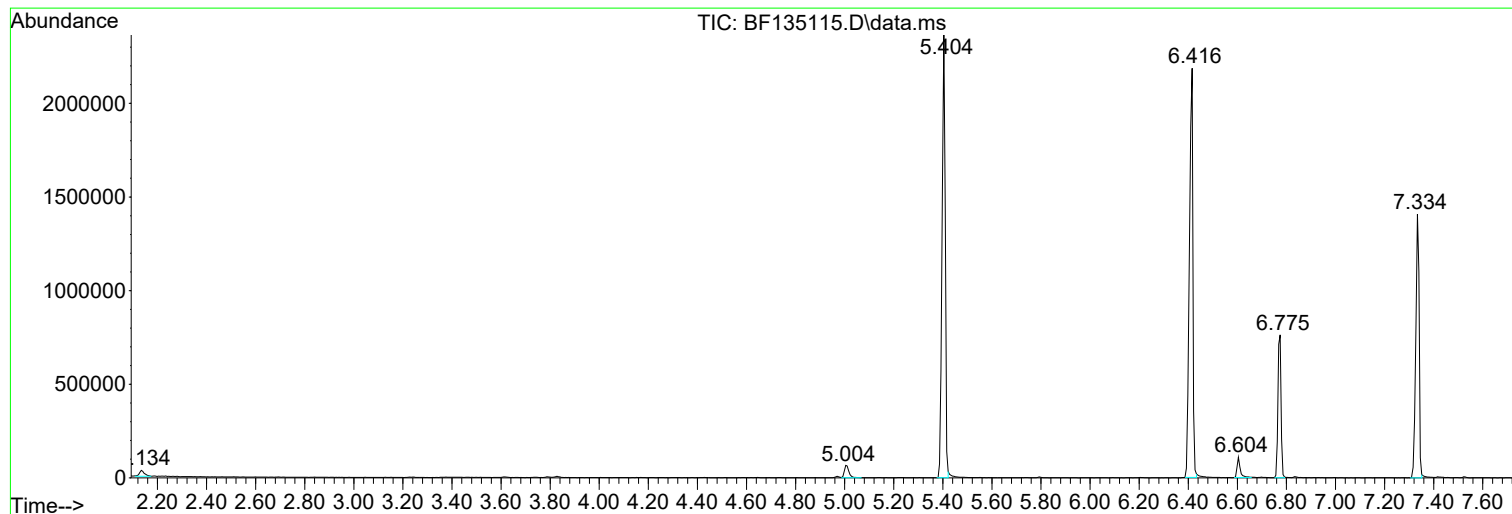
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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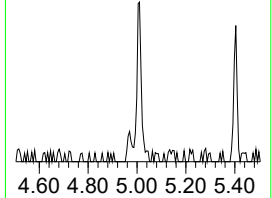
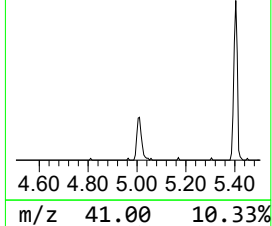
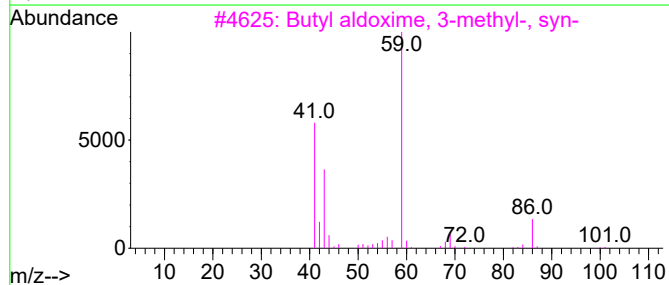
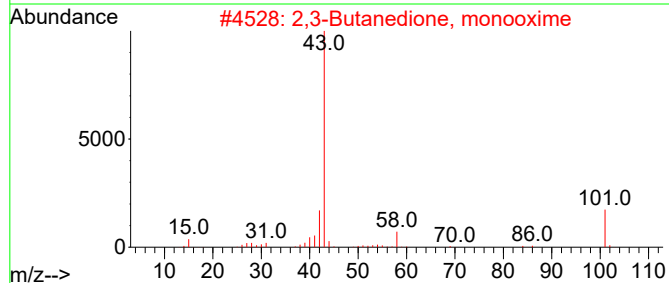
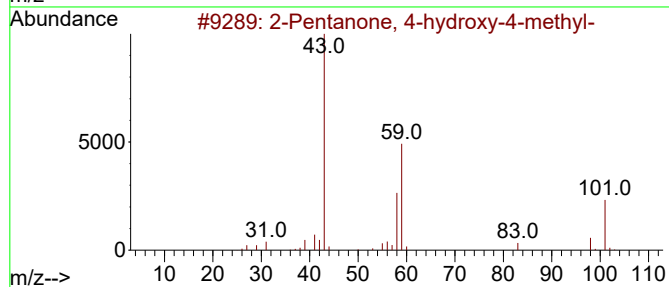
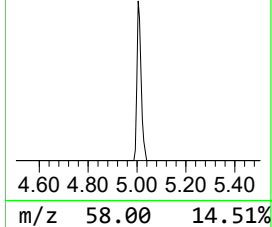
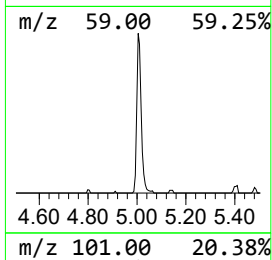
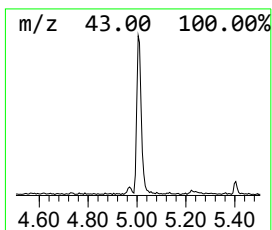
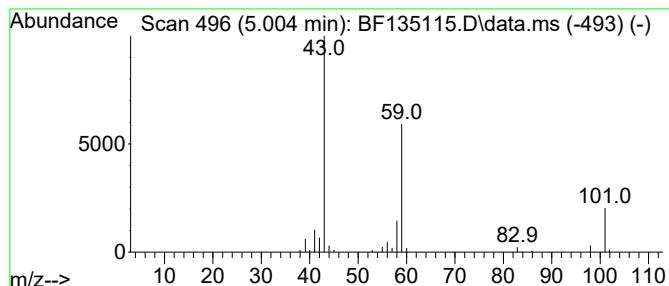
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.53 ng	85008	1,4-Dichlorobenzene-d4	6.775

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	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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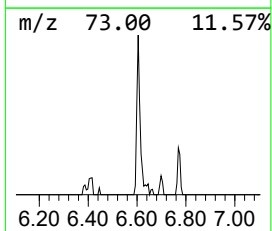
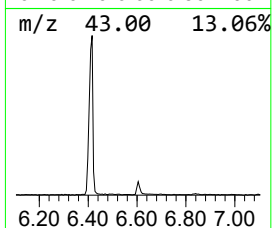
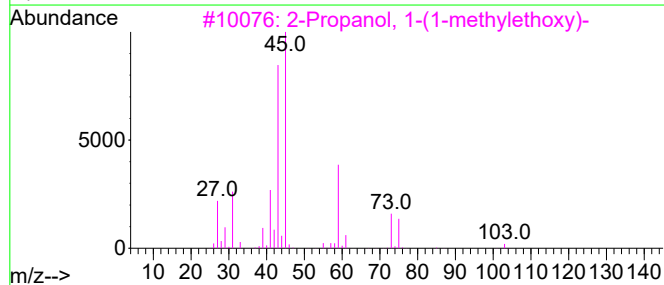
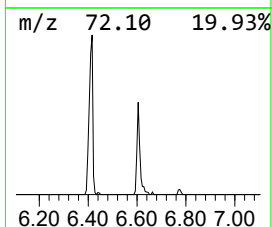
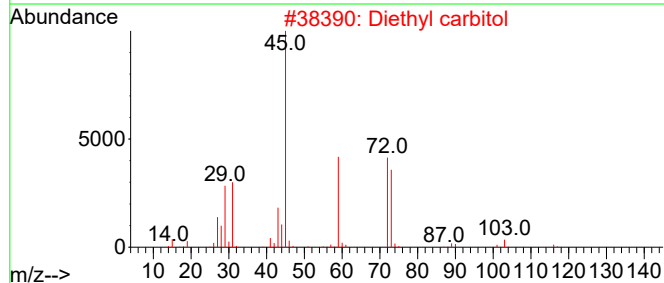
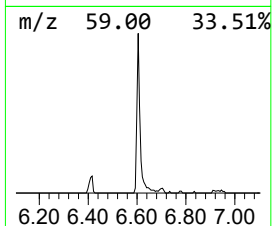
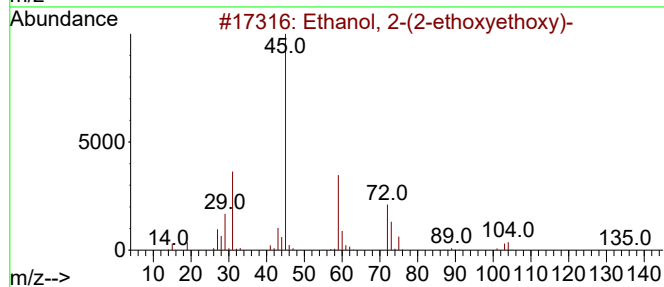
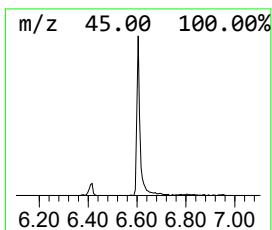
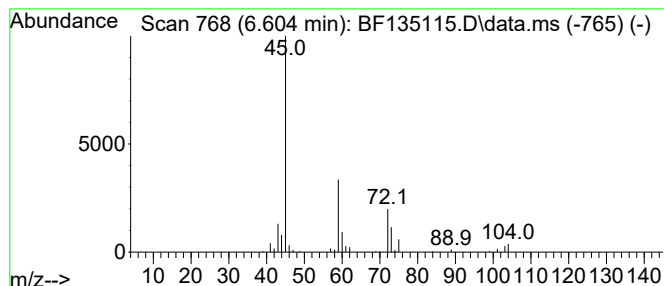
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Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	2.93 ng	98294	1,4-Dichlorobenzene-d4	6.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
4			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	38
5			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	36



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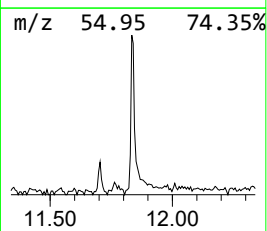
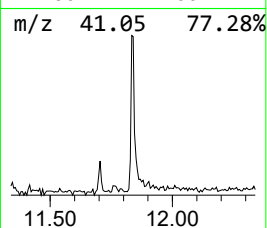
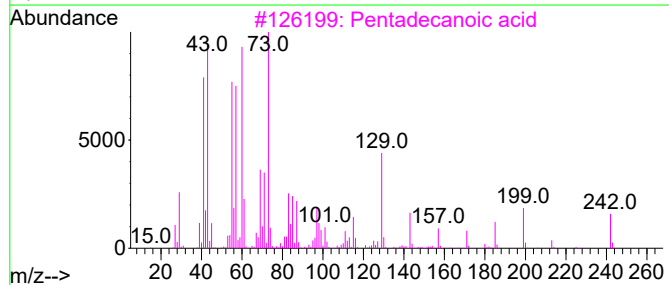
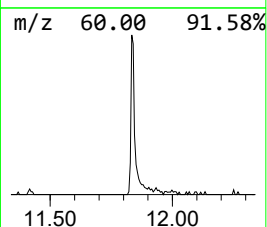
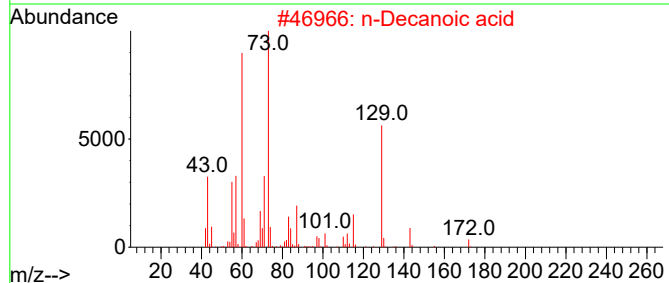
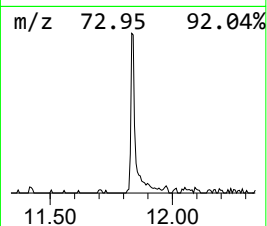
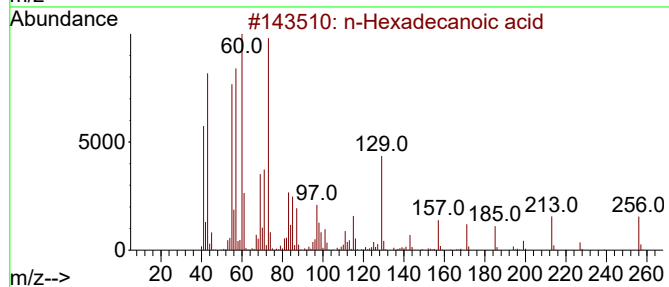
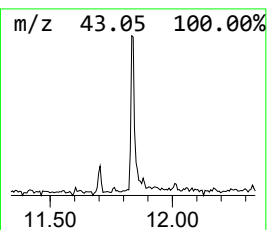
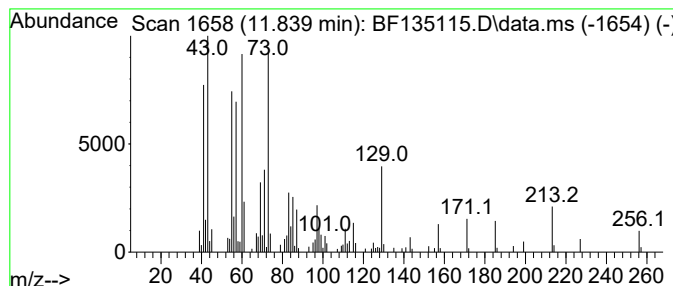
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	3.84 ng	142362	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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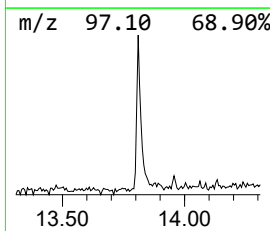
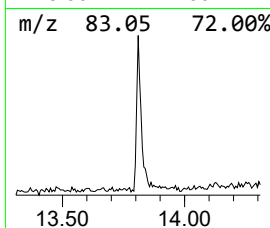
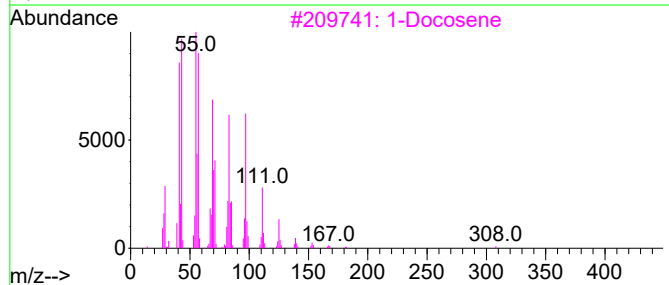
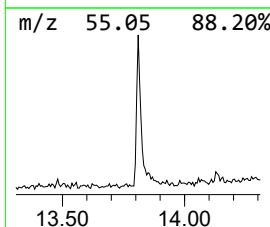
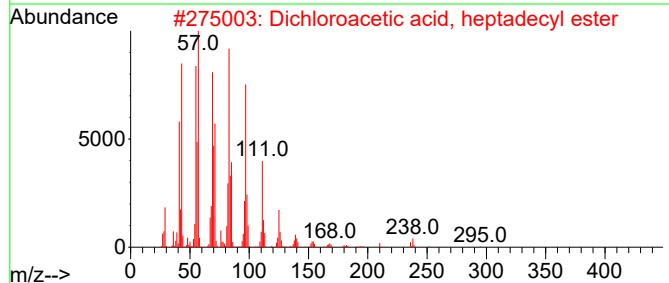
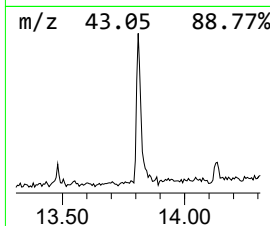
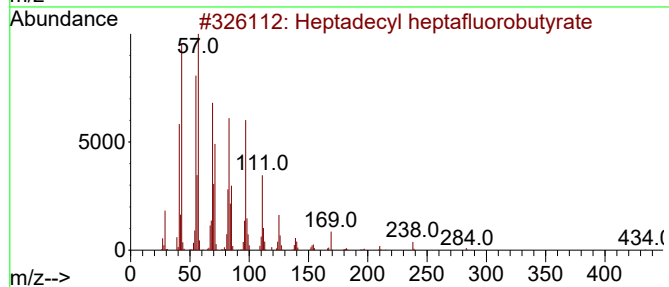
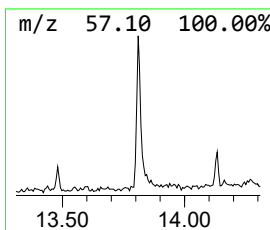
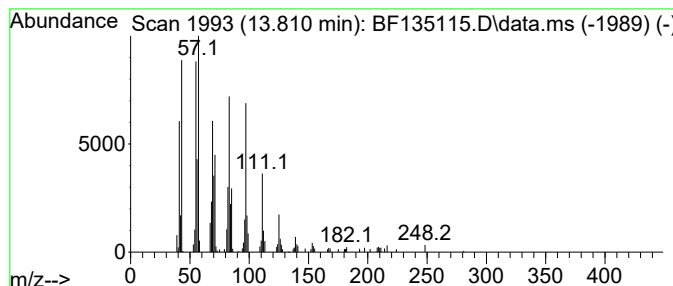
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	4.91 ng	159396	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3			1-Docosene	308	C22H44	001599-67-3	94
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94



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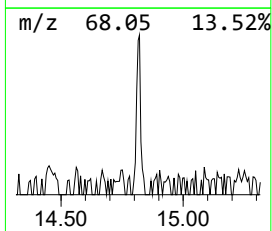
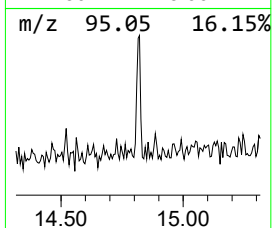
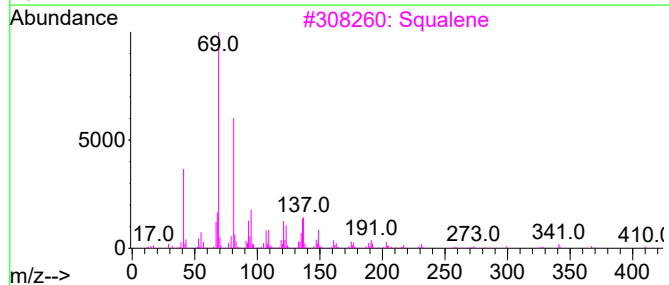
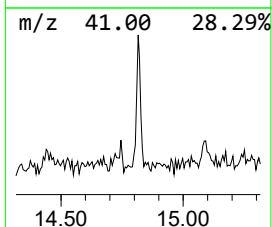
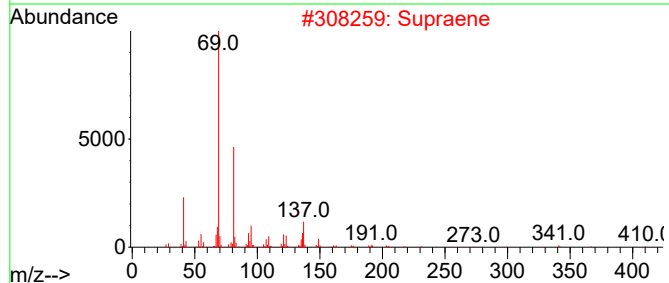
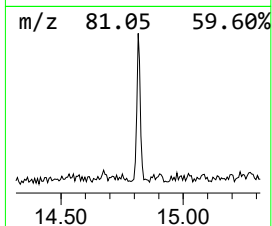
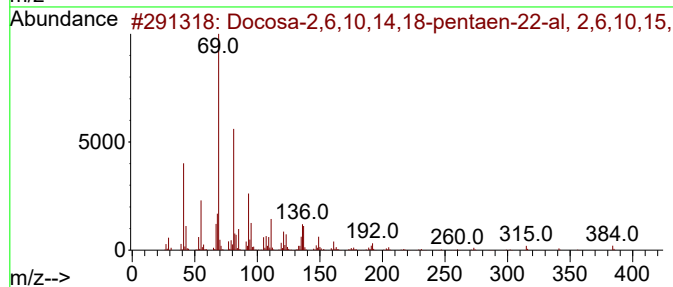
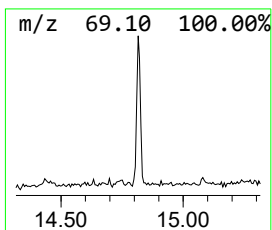
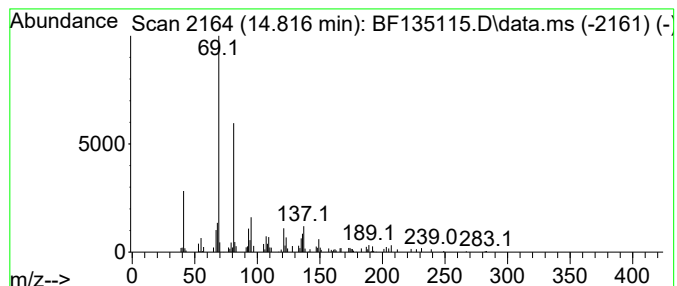
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Docosa-2,6,10,14,18-pentaen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.10 ng	56083	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	91		
2	Supraene	410	C30H50	007683-64-9	91		
3	Squalene	410	C30H50	000111-02-4	91		
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83		
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.004	2.5	ng	85008	1	6.775	672055	20.0
Ethanol, 2-(2-e...	6.604	2.9	ng	98294	1	6.775	672055	20.0
n-Hexadecanoic ...	11.839	3.8	ng	142362	4	11.298	741794	20.0
Heptadecyl hept...	13.810	4.9	ng	159396	5	13.957	648821	20.0
Docosa-2,6,10,1...	14.816	2.1	ng	56083	6	15.427	535386	20.0