

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112423\
 Data File : BF136184.D
 Acq On : 24 Nov 2023 17:37
 Operator : CG\JU
 Sample : 05293-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-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-BF110723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136184.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	14	rVB	397877	511601	6.90%	1.259%
2	5.069	503	507	515	rVB	58584	86661	1.17%	0.213%
3	5.451	566	572	575	rBV	5265711	5491156	74.03%	13.516%
4	6.445	734	741	744	rBV	4722548	5657407	76.27%	13.926%
5	6.804	799	802	806	rVB	992086	798023	10.76%	1.964%
6	7.369	892	898	901	rBV	3353605	3477549	46.88%	8.560%
7	8.081	1015	1019	1023	rBV	1208450	1099050	14.82%	2.705%
8	9.169	1198	1204	1207	rBV	8021239	7417421	100.00%	18.258%
9	9.839	1313	1318	1321	rBV	1687446	1292932	17.43%	3.183%
10	10.639	1448	1454	1457	rBV	4500649	4418115	59.56%	10.875%
11	11.333	1568	1572	1575	rBV	1594233	1293930	17.44%	3.185%
12	11.874	1659	1664	1676	rBV2	319764	345431	4.66%	0.850%
13	12.933	1839	1844	1847	rBV	7421753	7091099	95.60%	17.455%
14	13.845	1995	1999	2013	rBV2	91957	160205	2.16%	0.394%
15	13.980	2018	2022	2026	rBV	947853	802613	10.82%	1.976%
16	15.462	2268	2274	2281	rBV	574580	682457	9.20%	1.680%

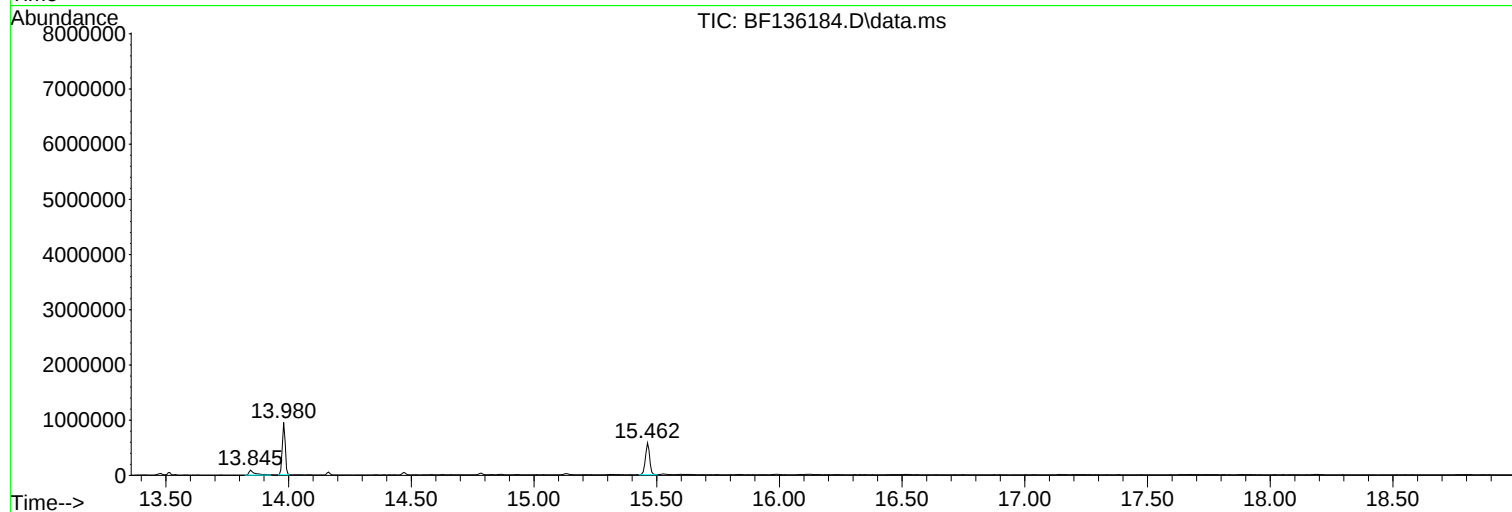
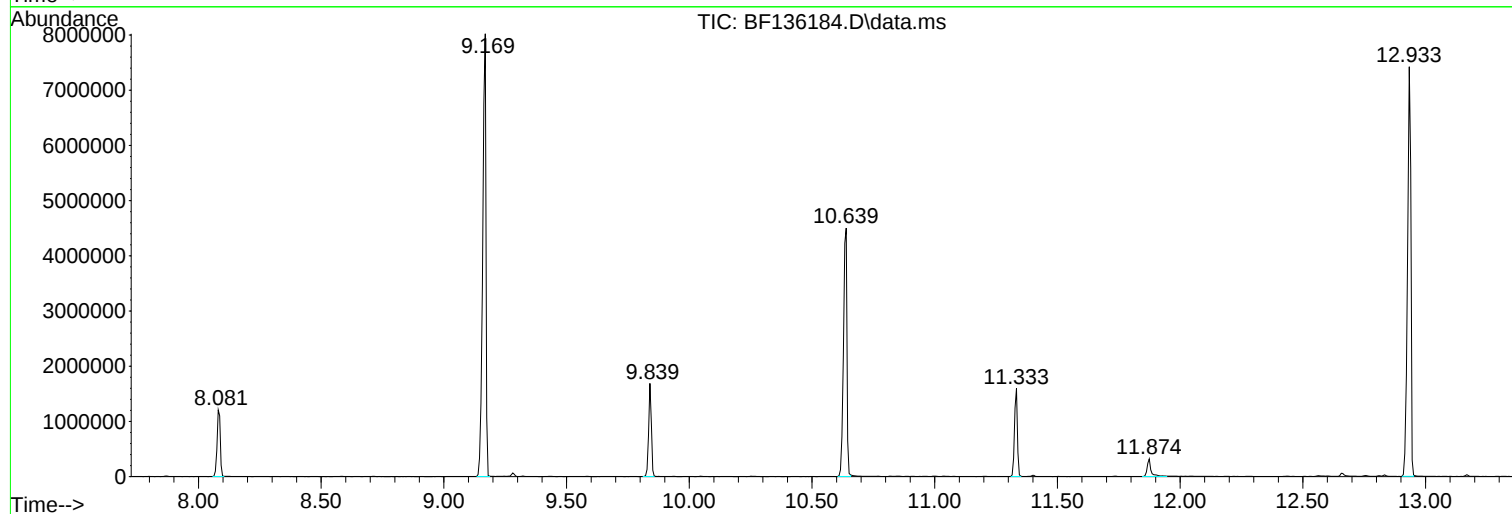
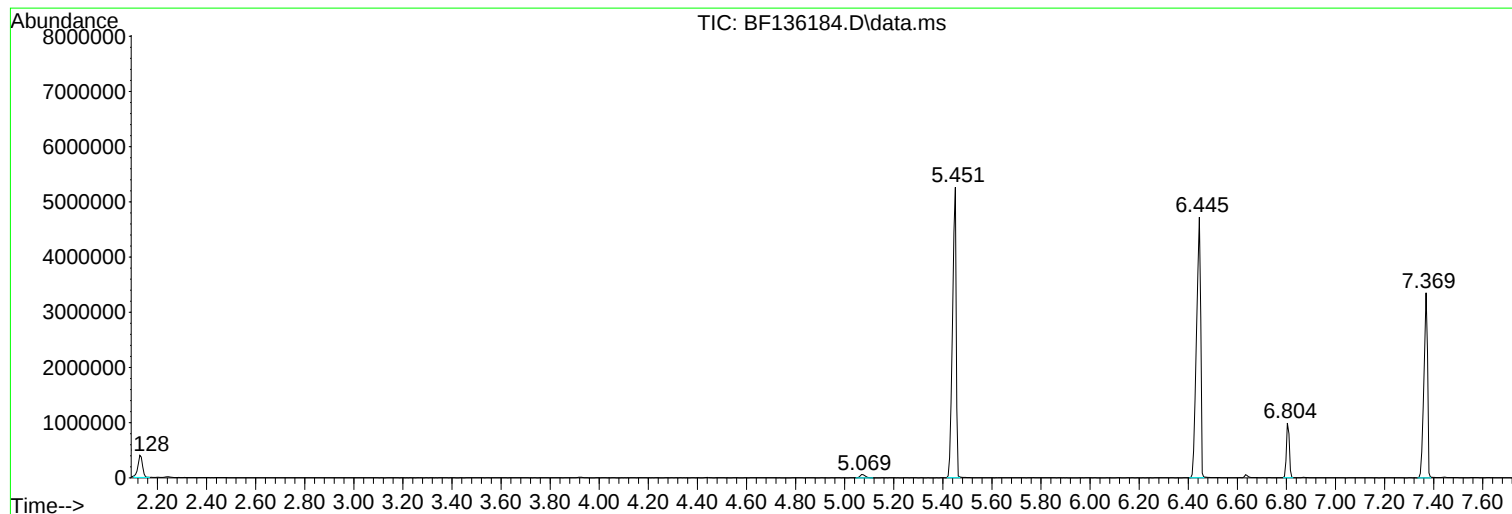
Sum of corrected areas: 40625650

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.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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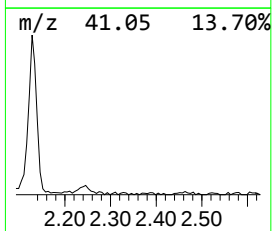
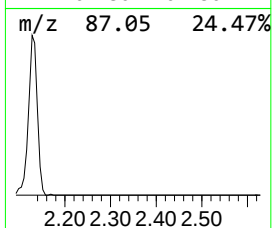
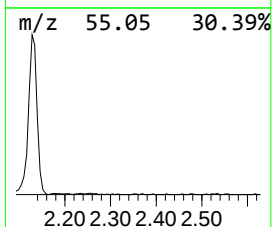
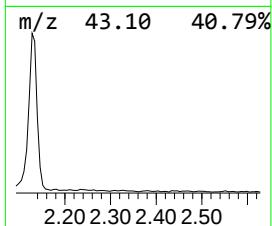
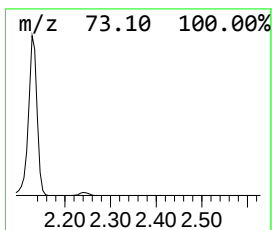
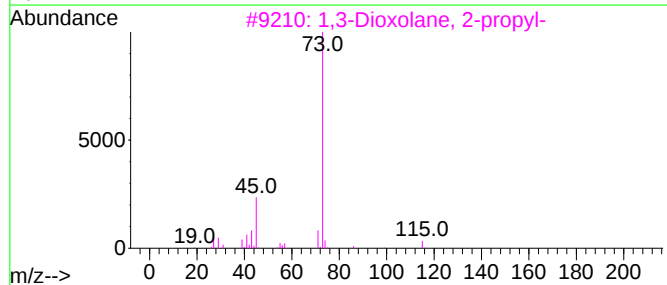
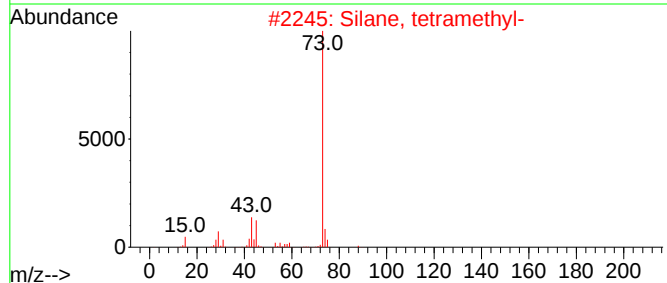
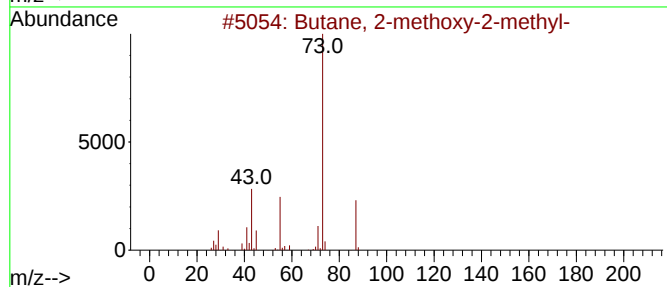
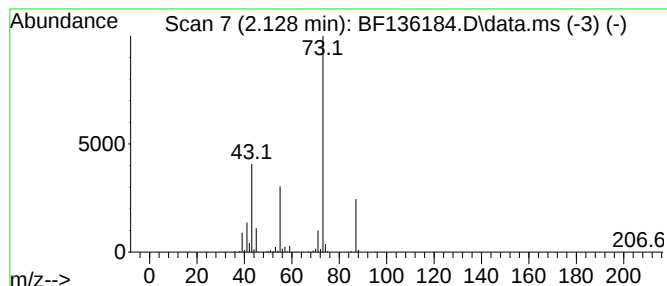
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	12.82 ng	511601	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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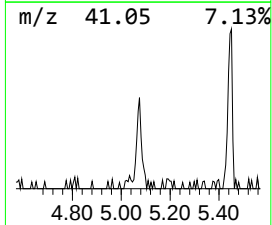
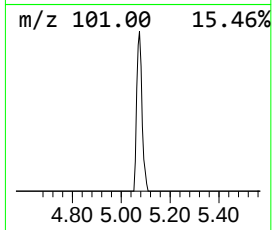
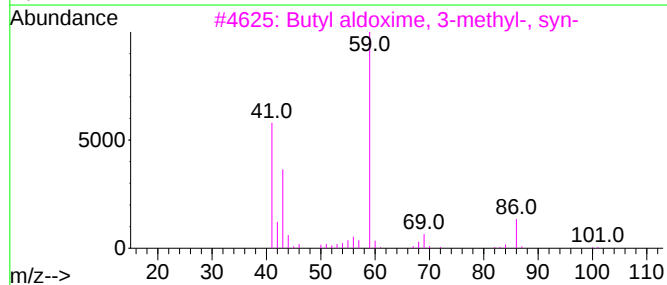
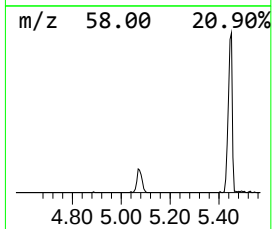
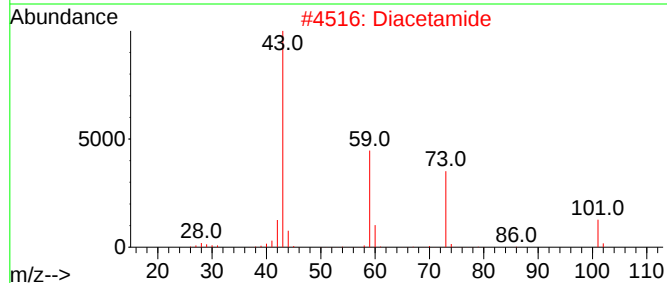
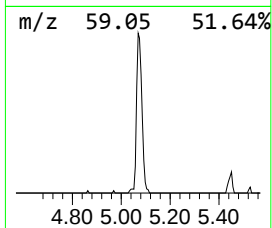
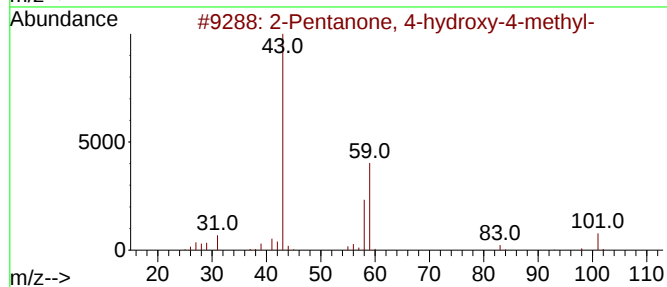
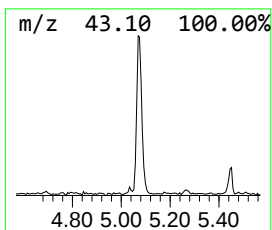
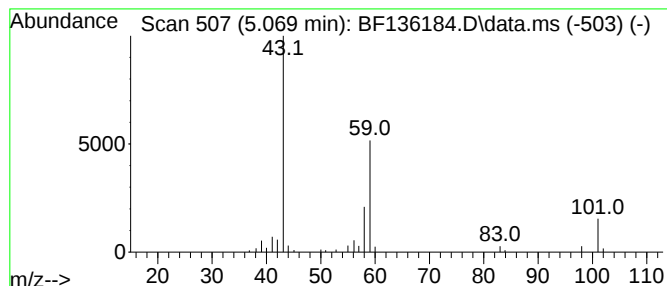
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	2.17 ng	86661	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Diacetamide	101	C4H7NO2	000625-77-4	33		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	16		



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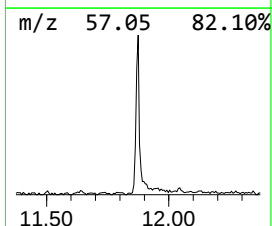
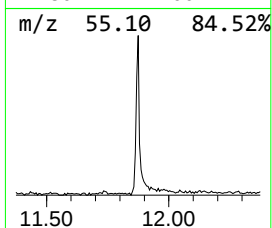
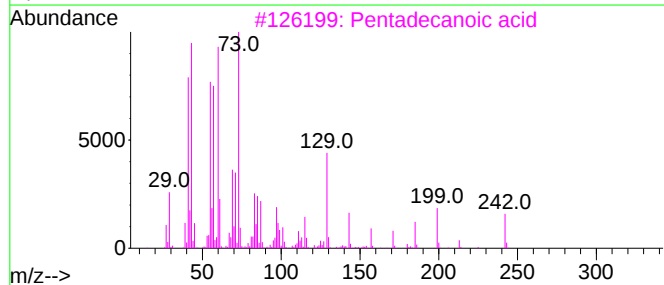
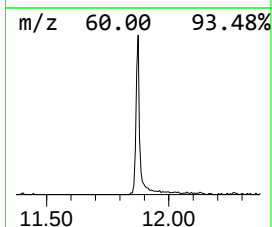
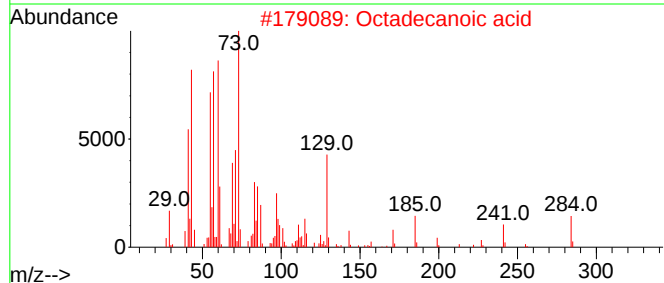
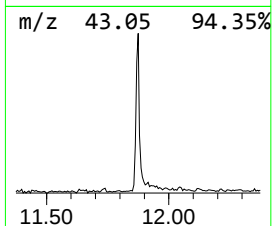
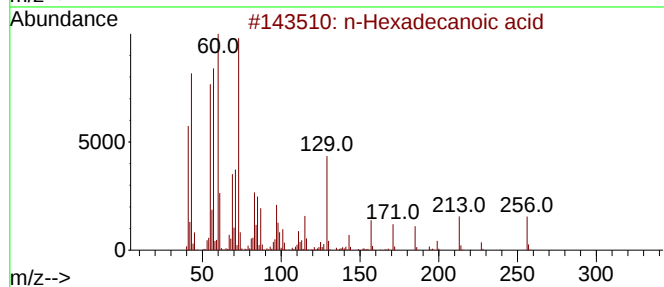
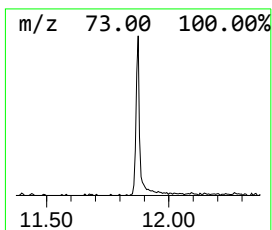
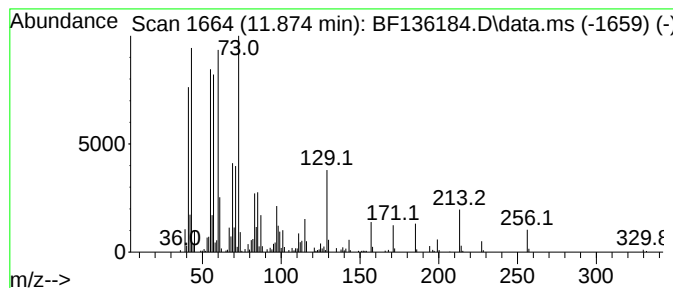
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	5.34 ng	345431	Phenanthrene-d10	11.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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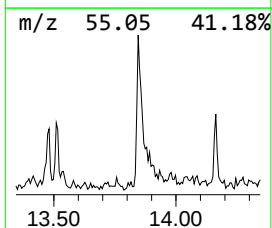
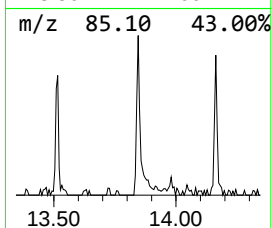
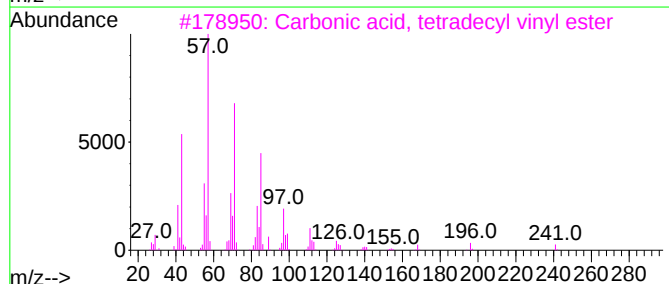
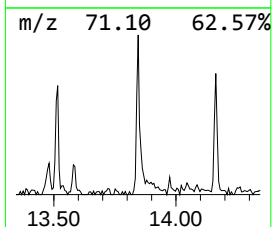
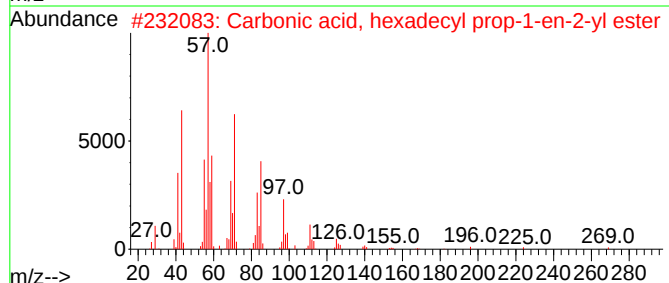
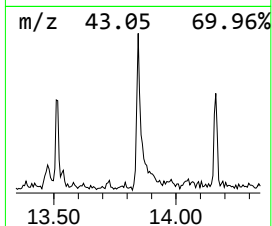
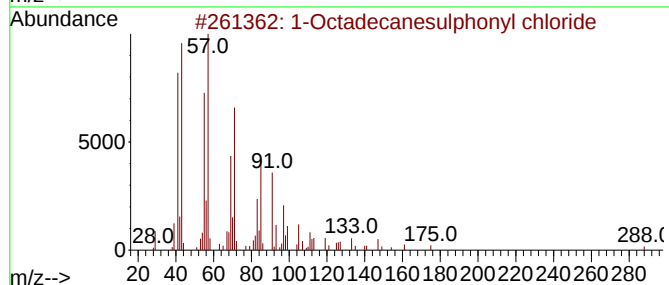
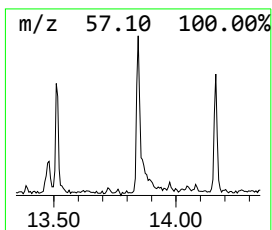
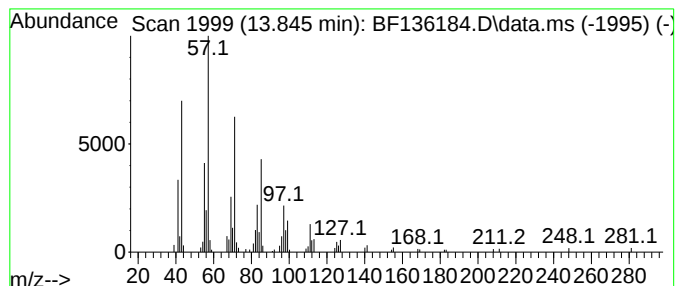
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Peak Number 4 1-Octadecanesulphonyl chloride Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.845	3.99 ng	160205	Chrysene-d12	13.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
2	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
3	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	91
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1010309-12-5	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	12.8	ng	511601	1	6.804	798023	20.0
2-Pentanone, 4-...	5.069	2.2	ng	86661	1	6.804	798023	20.0
n-Hexadecanoic ...	11.874	5.3	ng	345431	4	11.333	1293930	20.0
1-Octadecanesul...	13.845	4.0	ng	160205	5	13.980	802613	20.0