

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091622\
 Data File : BF130301.D
 Acq On : 16 Sep 2022 20:58
 Operator : CG\JU
 Sample : N4628-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HW-8

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130301.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.845	465	469	480	rVB	91586	111592	3.62%	0.674%
2	5.263	535	540	543	rBV	1389790	1229815	39.94%	7.429%
3	6.292	711	715	728	rBV	881855	777614	25.25%	4.697%
4	6.669	775	779	782	rBV	618068	534507	17.36%	3.229%
5	7.234	869	875	878	rBV	1862792	1799278	58.43%	10.869%
6	7.692	937	953	958	rBV	110518	224681	7.30%	1.357%
7	7.945	992	996	1000	rBV	763584	677146	21.99%	4.090%
8	9.028	1175	1180	1183	rBV	3759074	3079150	100.00%	18.600%
9	9.698	1289	1294	1297	rBV	827213	670891	21.79%	4.053%
10	10.480	1423	1427	1445	rBV	1578566	1720365	55.87%	10.392%
11	11.174	1541	1545	1548	rBV	678303	520097	16.89%	3.142%
12	11.721	1634	1638	1646	rBV	655863	698116	22.67%	4.217%
13	12.421	1752	1757	1762	rBV7	37655	81061	2.63%	0.490%
14	12.510	1767	1772	1785	rVV	1225840	1490404	48.40%	9.003%
15	12.763	1811	1815	1818	rVB	2435242	1925552	62.54%	11.631%
16	13.804	1988	1992	1995	rBV	442471	423590	13.76%	2.559%
17	15.192	2223	2228	2233	rBV	473444	513279	16.67%	3.100%
18	15.633	2298	2303	2308	rBV2	24794	35861	1.16%	0.217%
19	16.086	2376	2380	2388	rVB4	24046	41919	1.36%	0.253%

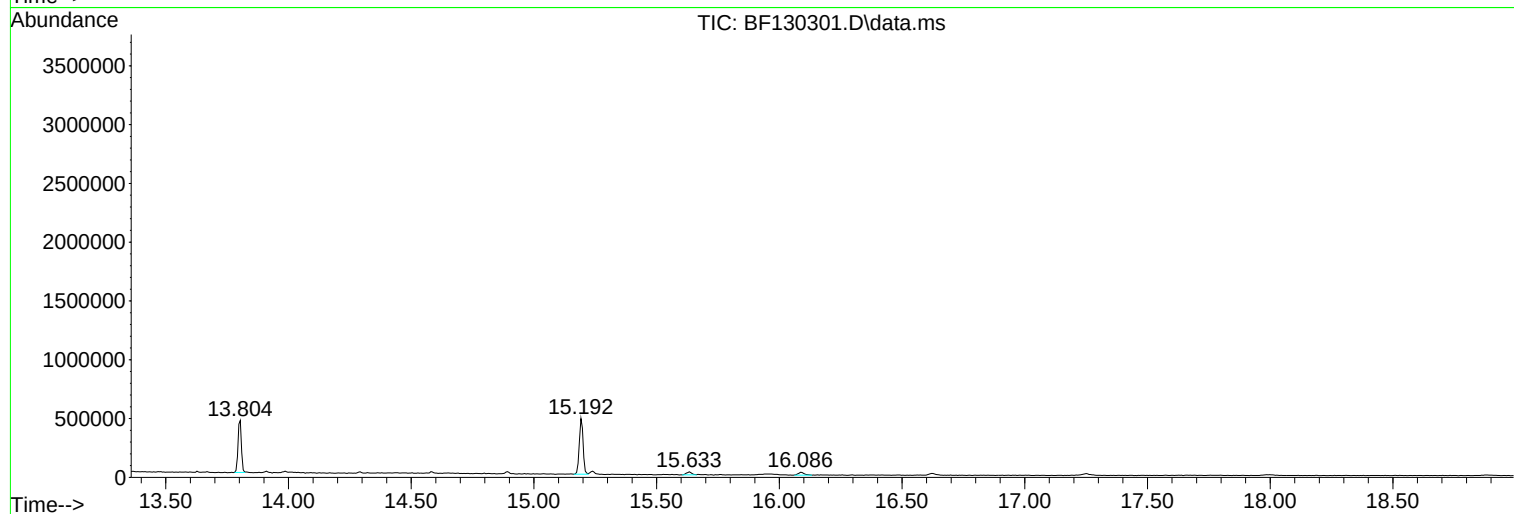
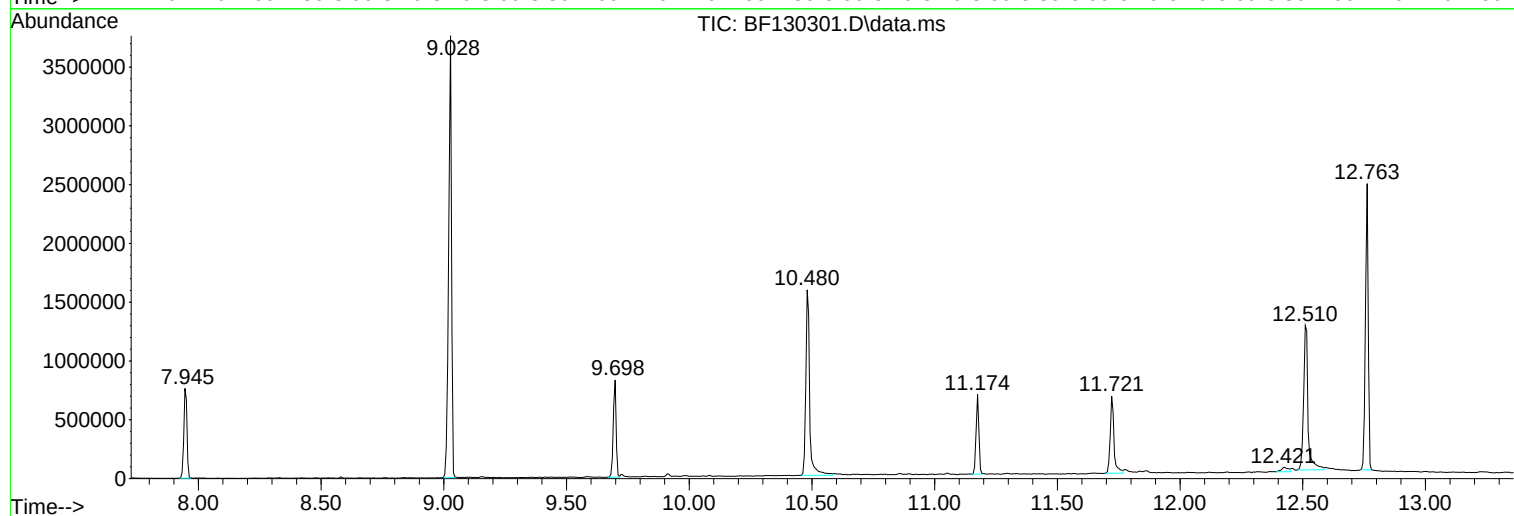
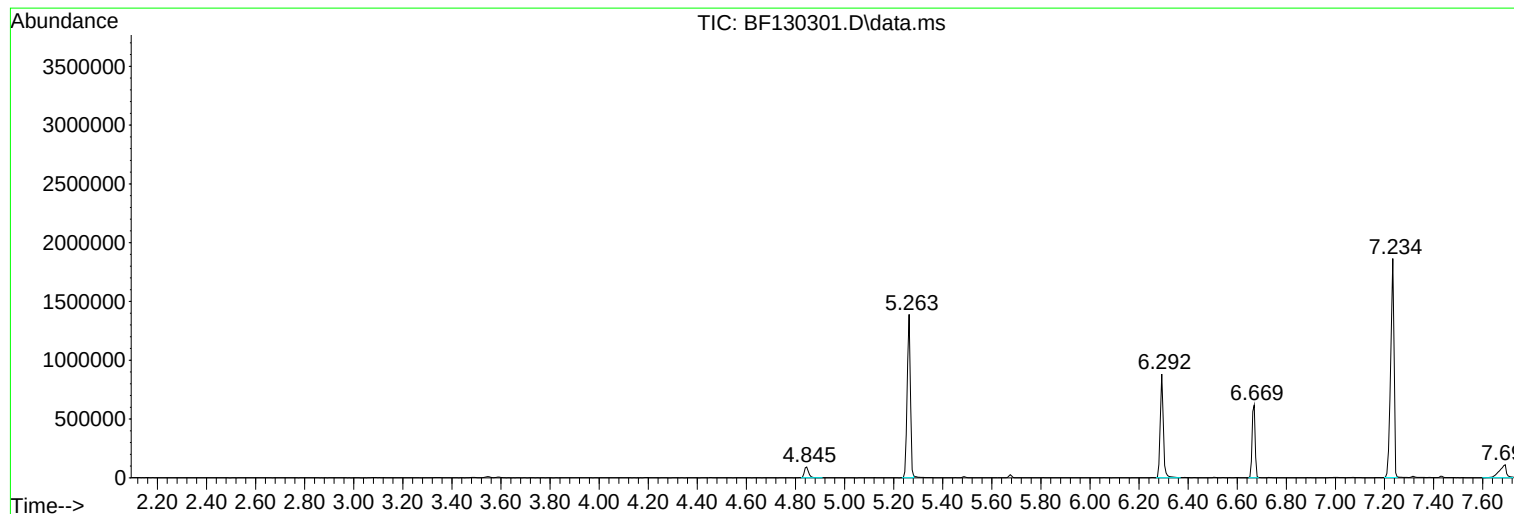
Sum of corrected areas: 16554918

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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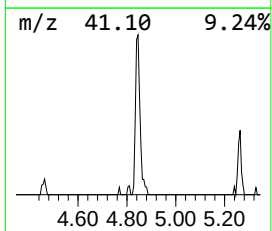
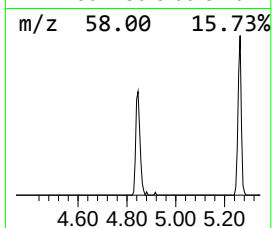
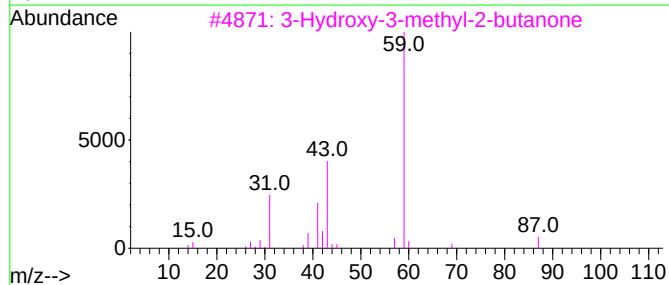
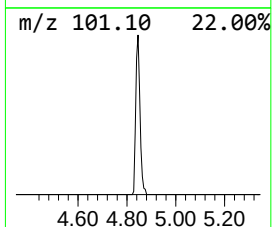
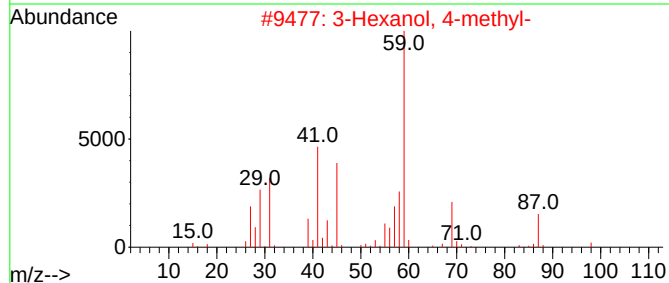
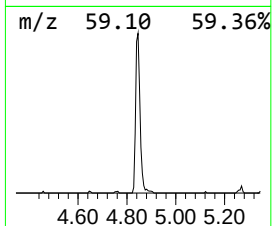
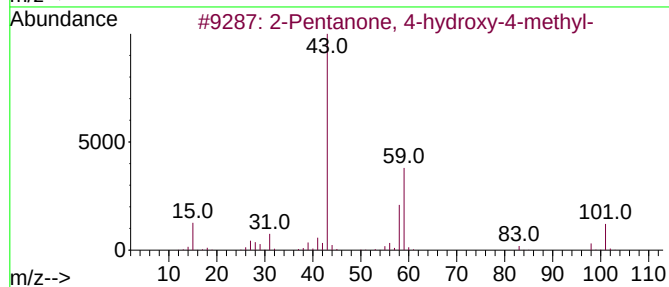
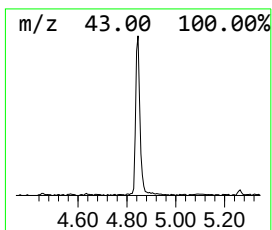
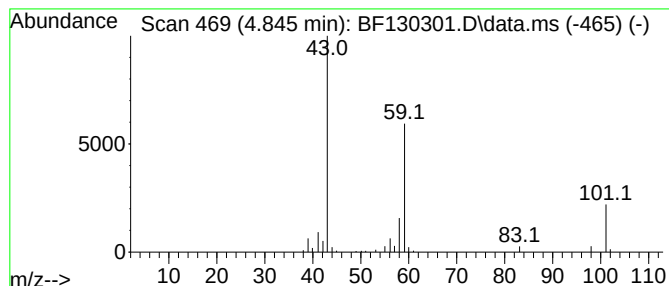
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.845	4.18 ng	111592	1,4-Dichlorobenzene-d4	6.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
4	Acetone	58	C3H6O	000067-64-1	9		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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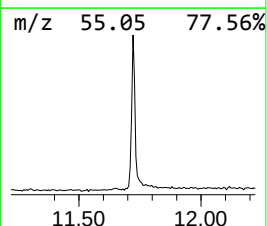
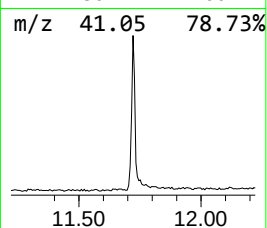
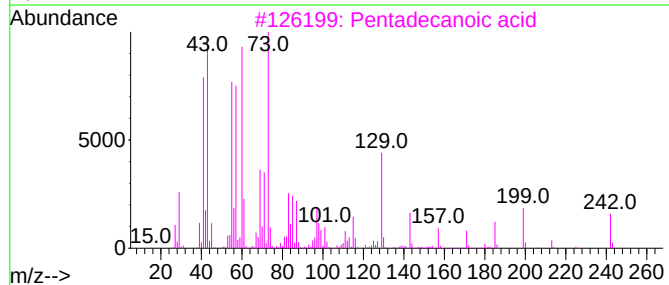
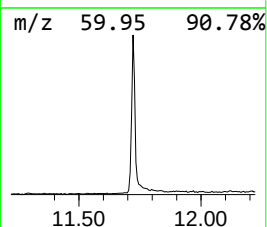
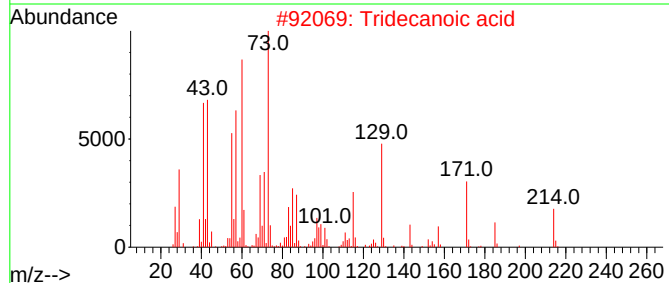
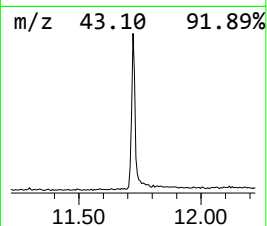
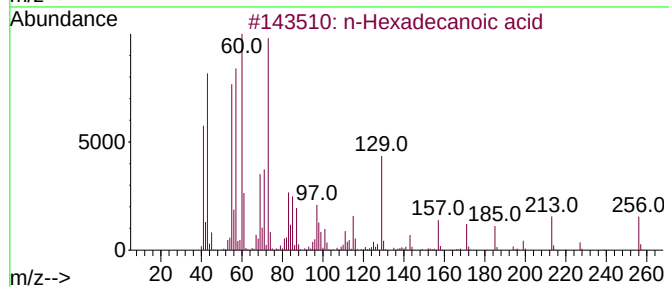
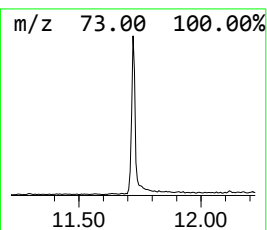
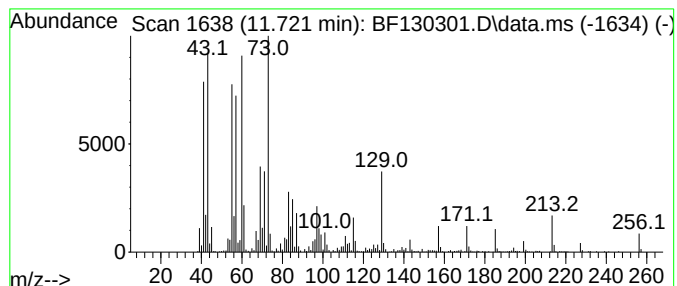
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.722	26.85 ng	698116	Phenanthrene-d10	11.174

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	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Nonanoic acid	158	C9H18O2	000112-05-0	53



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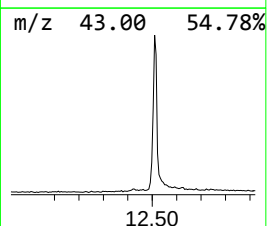
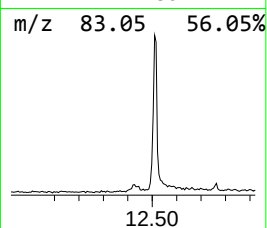
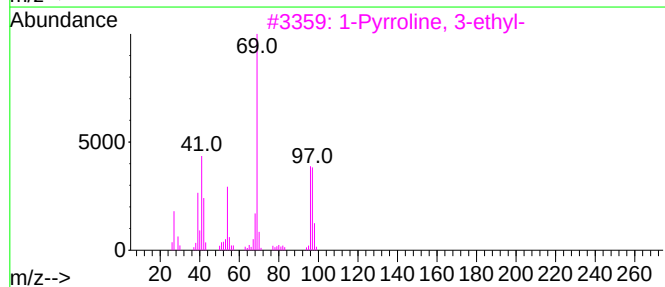
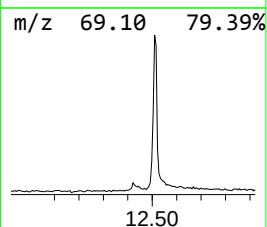
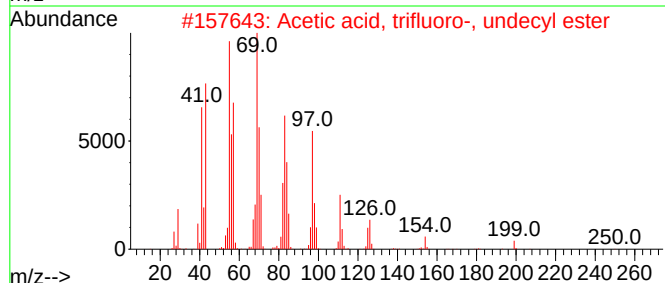
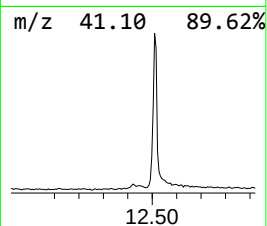
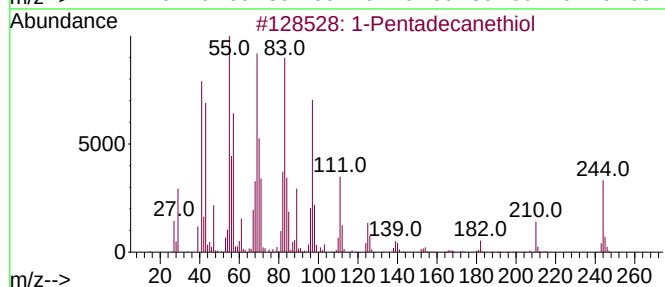
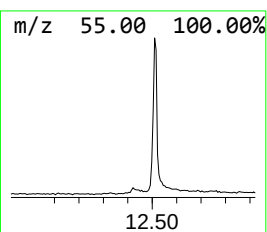
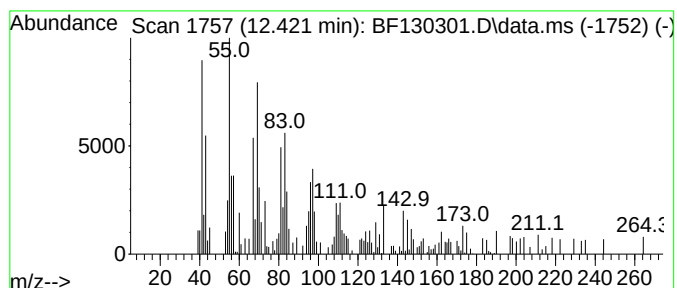
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Peak Number 3 unknown12.421 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	3.12 ng	81061	Phenanthrene-d10	11.174

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentadecanethiol	244	C15H32S	025276-70-4	49
2		Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	49
3		1-Pyrroline, 3-ethyl-	97	C6H11N	1000073-06-0	46
4		4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	46
5		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	43



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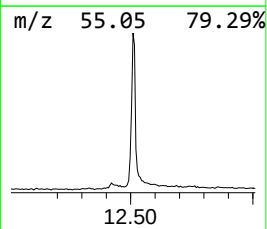
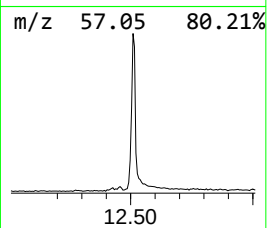
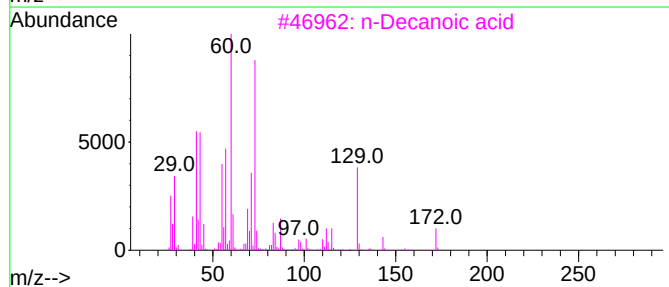
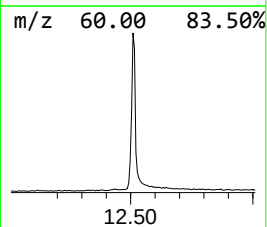
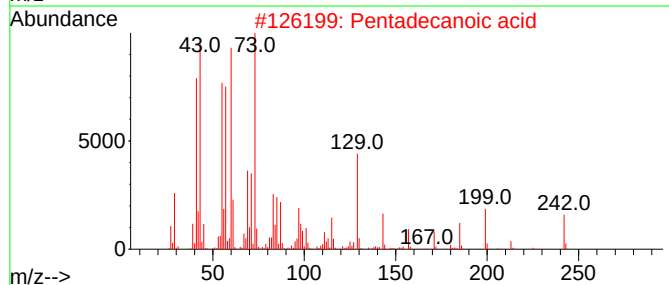
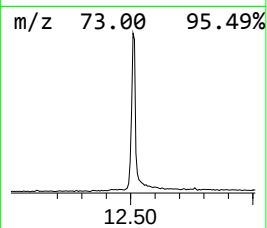
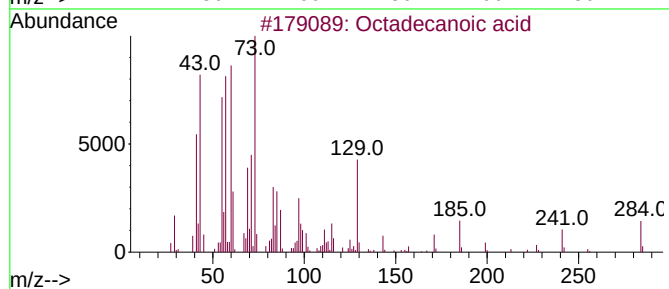
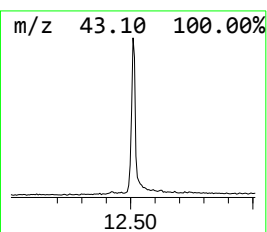
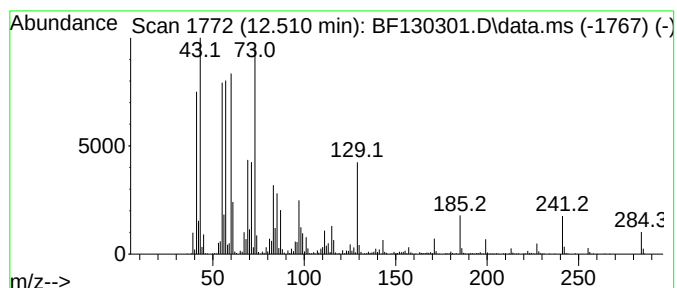
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	70.37 ng	1490400	Chrysene-d12	13.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		n-Decanoic acid	172	C10H20O2	000334-48-5	76
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.845	4.2	ng	111592	1	6.669	534507	20.0
n-Hexadecanoic ...	11.722	26.9	ng	698116	4	11.174	520097	20.0
unknown12.421	12.421	3.1	ng	81061	4	11.174	520097	20.0
Octadecanoic acid	12.510	70.4	ng	1490400	5	13.804	423590	20.0