

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072423\
 Data File : BF134452.D
 Acq On : 25 Jul 2023 03:40
 Operator : CG\JU
 Sample : 03653-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP20

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-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134452.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	23	rVB	188103	267557	13.70%	1.950%
2	5.475	572	576	590	rBV	2101169	1953445	100.00%	14.240%
3	6.475	742	746	749	rBV	1855881	1835531	93.96%	13.380%
4	6.834	803	807	818	rBV	484668	387174	19.82%	2.822%
5	7.398	899	903	906	rBV	1482933	1216516	62.28%	8.868%
6	8.110	1021	1024	1037	rBV	644184	528663	27.06%	3.854%
7	9.192	1204	1208	1211	rBV	2120450	1879474	96.21%	13.701%
8	9.586	1271	1275	1279	rBV	56823	49815	2.55%	0.363%
9	9.869	1319	1323	1327	rBV	576916	456559	23.37%	3.328%
10	10.663	1454	1458	1468	rBV	1549213	1359872	69.61%	9.913%
11	11.363	1574	1577	1580	rBV	599866	491160	25.14%	3.580%
12	11.892	1664	1667	1680	rBV	187801	190627	9.76%	1.390%
13	12.586	1782	1785	1788	rBV	44291	39797	2.04%	0.290%
14	12.680	1798	1801	1809	rBV2	48772	63212	3.24%	0.461%
15	12.816	1820	1824	1828	rBV	30272	30455	1.56%	0.222%
16	12.963	1844	1849	1852	rBV	2263659	1914850	98.02%	13.959%
17	13.886	1997	2006	2022	rBV7	31896	112445	5.76%	0.820%
18	14.027	2026	2030	2034	rBV	431379	400937	20.52%	2.923%
19	15.151	2218	2221	2225	rVB2	23471	27750	1.42%	0.202%
20	15.527	2281	2285	2297	rBV	295350	404647	20.71%	2.950%
21	16.004	2361	2366	2375	rBV2	23362	45074	2.31%	0.329%
22	17.209	2567	2571	2577	rVB8	15852	25989	1.33%	0.189%
23	17.386	2596	2601	2609	rVB8	14906	36409	1.86%	0.265%

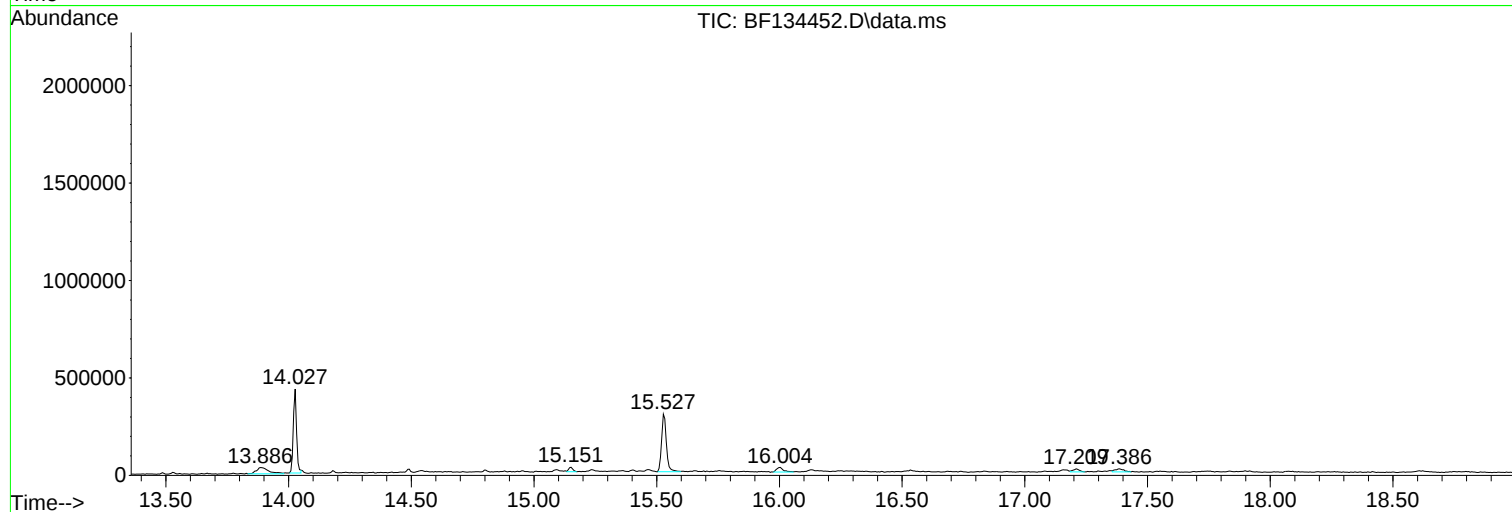
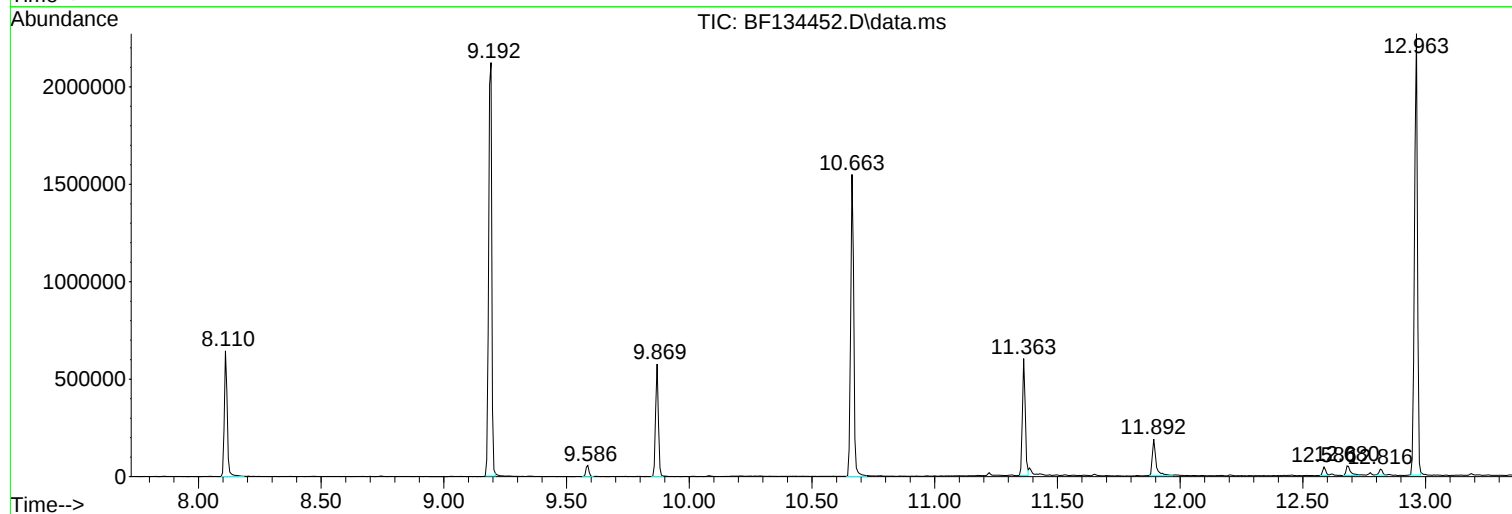
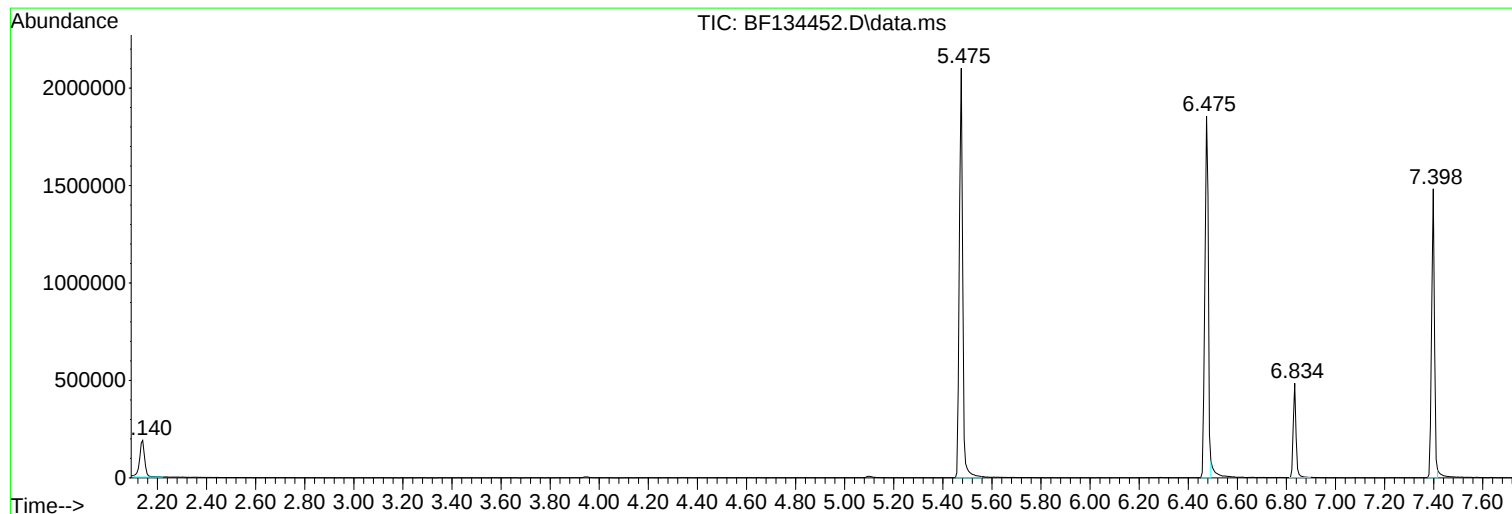
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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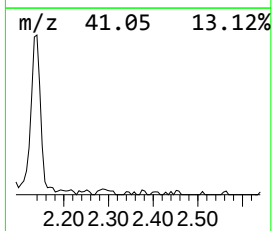
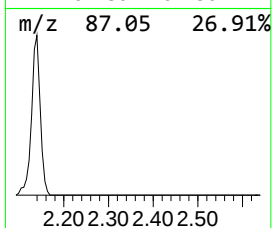
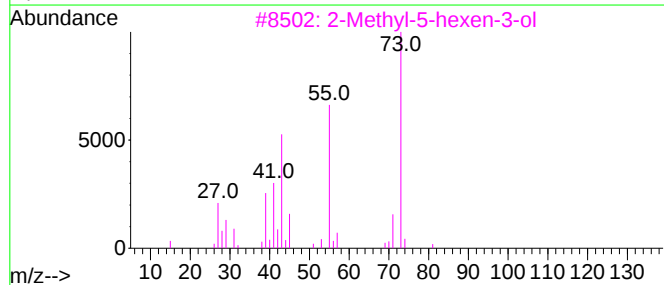
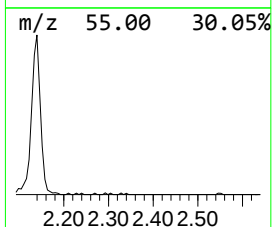
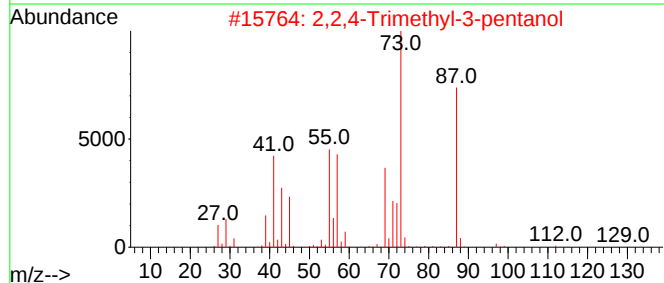
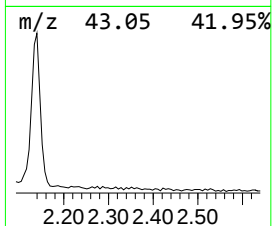
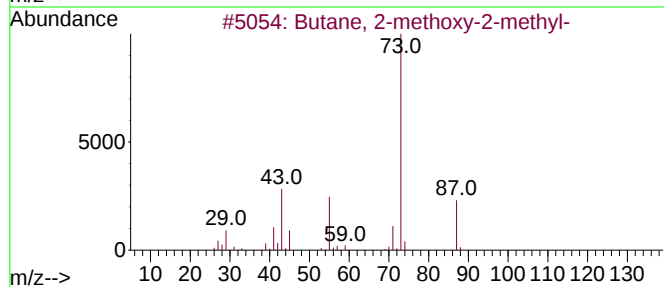
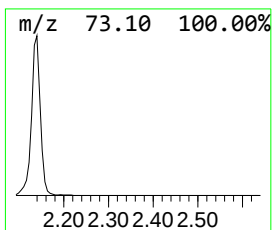
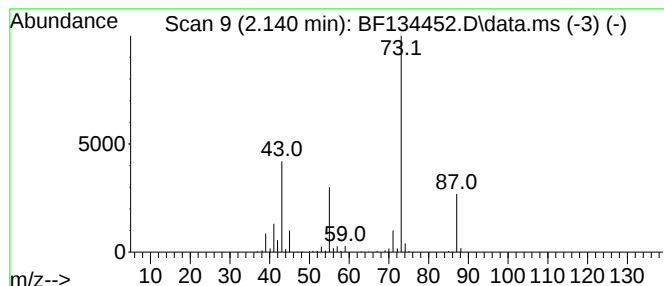
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.140	13.82 ng	267557	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16



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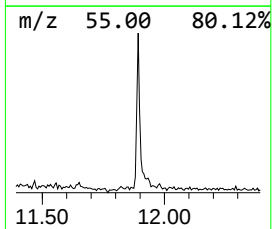
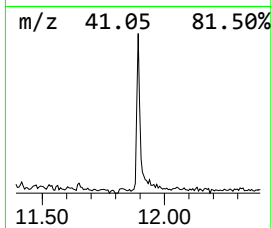
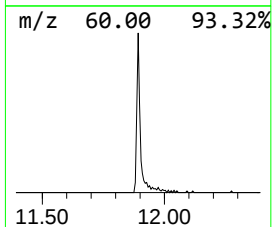
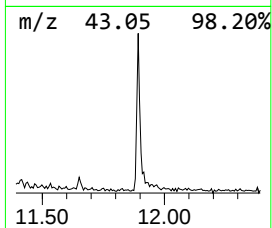
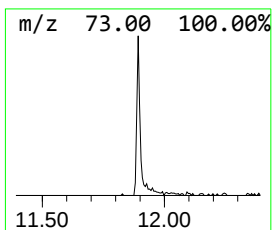
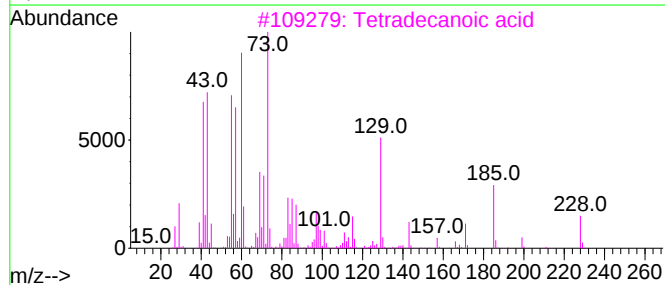
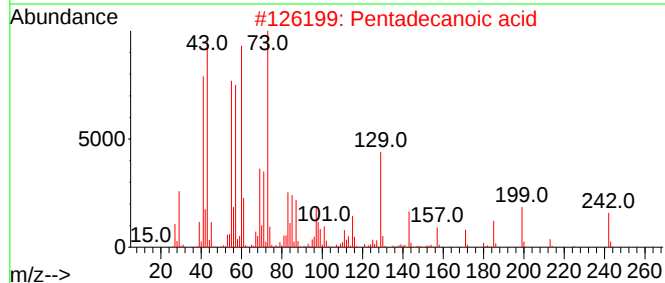
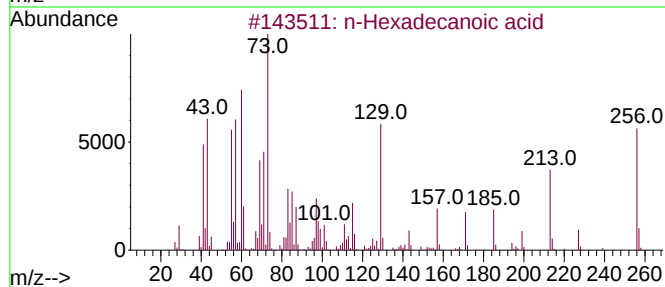
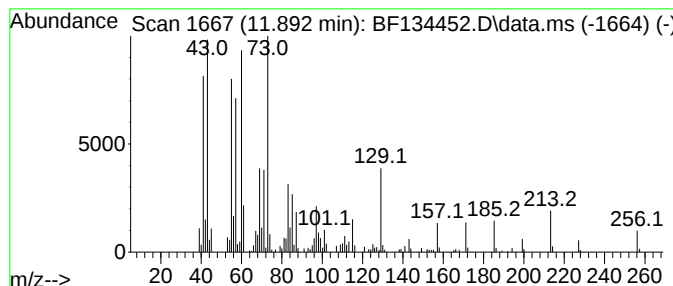
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	7.76 ng	190627	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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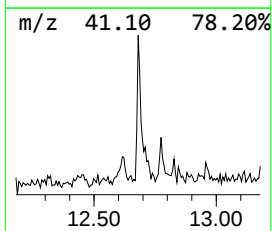
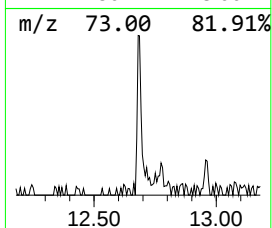
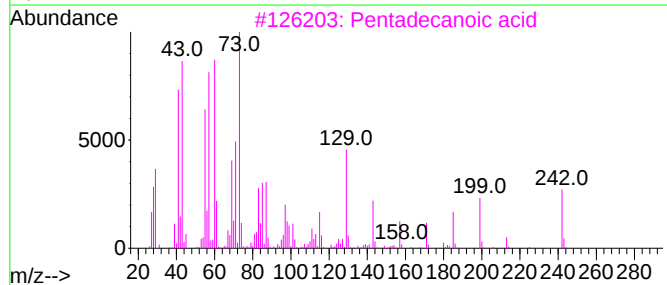
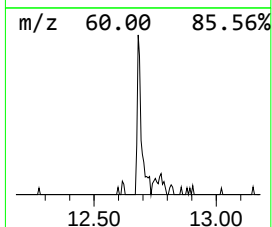
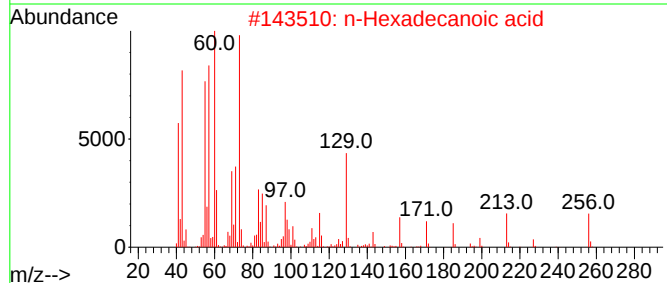
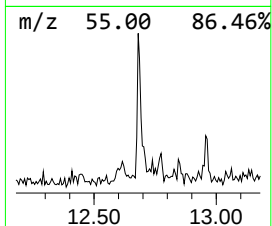
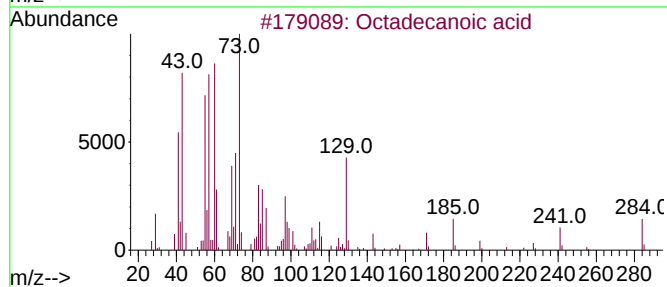
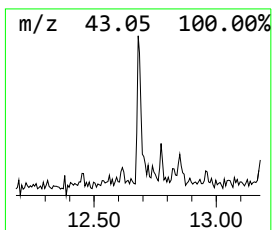
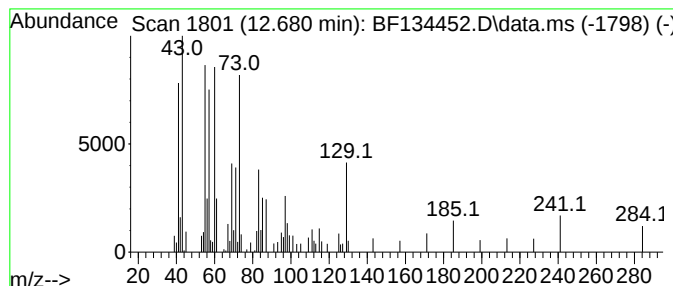
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.57 ng	63212	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5			Docosyl propyl ether	368	C25H52O	1000406-28-2	38



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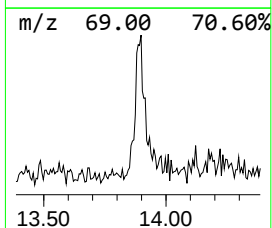
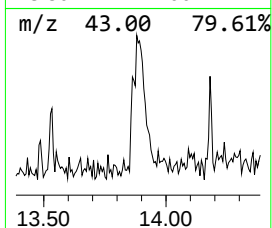
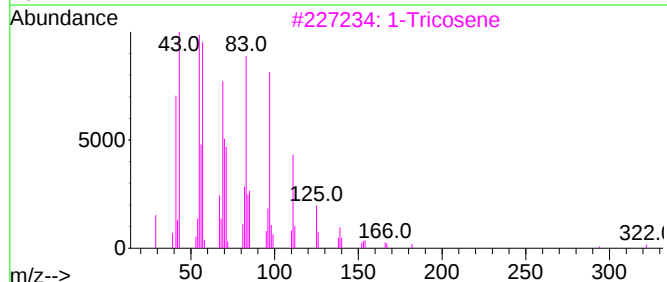
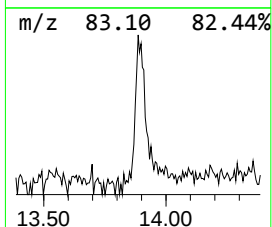
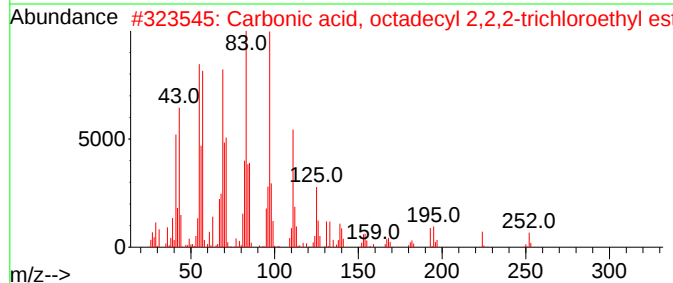
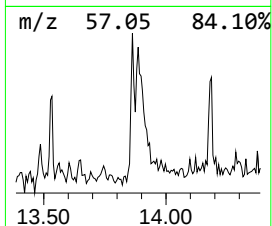
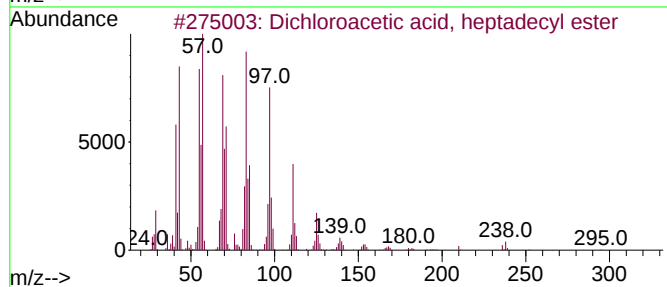
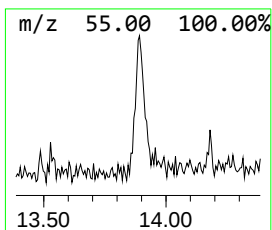
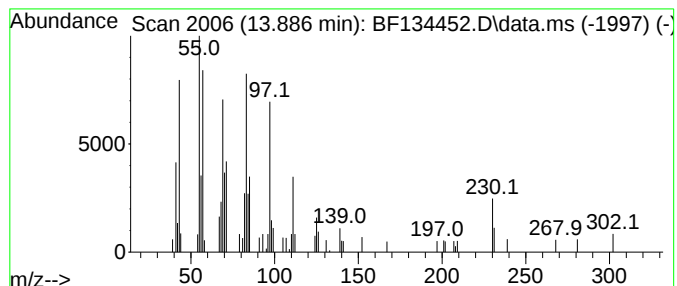
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Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	5.61 ng	112445	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
2			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	87
3			1-Tricosene	322	C23H46	018835-32-0	87
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	83



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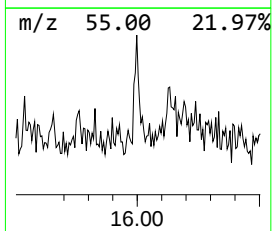
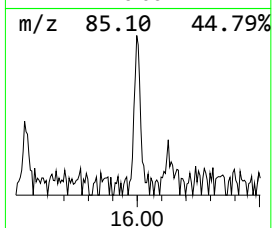
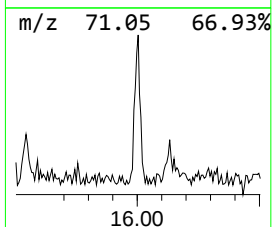
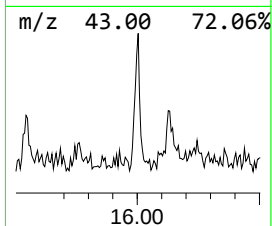
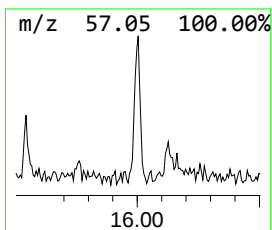
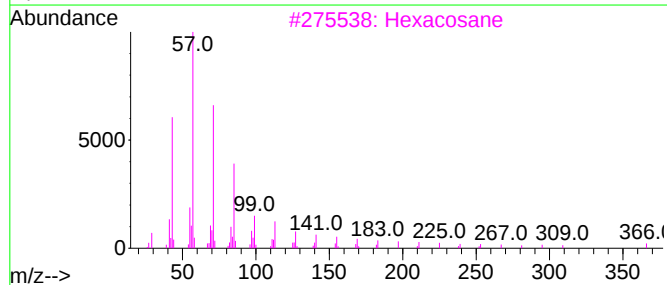
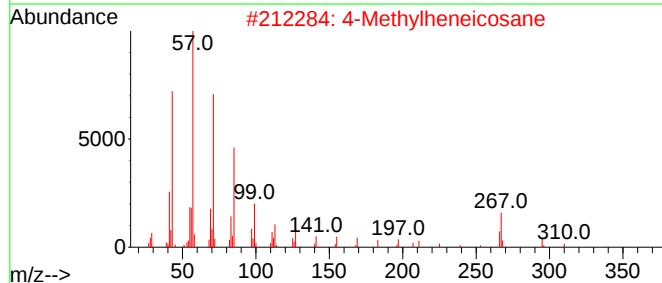
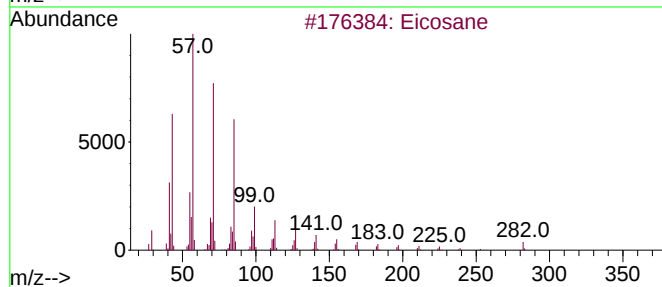
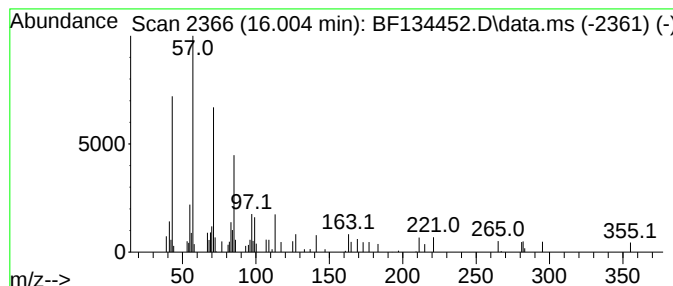
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Peak Number 5 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	2.23 ng	45074	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	90
2			4-Methylheneicosane	310	C22H46	025117-29-7	72
3			Hexacosane	366	C26H54	000630-01-3	72
4			Heptacosane	380	C27H56	000593-49-7	72
5			Octacosane	394	C28H58	000630-02-4	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.140	13.8	ng	267557	1	6.834	387174	20.0
n-Hexadecanoic ...	11.892	7.8	ng	190627	4	11.363	491160	20.0
Octadecanoic acid	12.680	2.6	ng	63212	4	11.363	491160	20.0
Dichloroacetic ...	13.886	5.6	ng	112445	5	14.027	400937	20.0
Eicosane	16.004	2.2	ng	45074	6	15.527	404647	20.0