

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072722\
 Data File : BF129381.D
 Acq On : 27 Jul 2022 17:44
 Operator : CG\JU
 Sample : N3861-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-19D

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.504	543	547	551	rBV	3571238	3392996	39.49%	7.273%
2	6.510	713	718	721	rBV	2486485	2426276	28.24%	5.201%
3	6.881	777	781	784	rBV	1868611	1485803	17.29%	3.185%
4	6.940	787	791	798	rBV	164108	186281	2.17%	0.399%
5	7.451	871	878	881	rBV	4516132	5070945	59.01%	10.870%
6	8.163	994	999	1003	rBV	2221419	2010506	23.40%	4.310%
7	9.245	1176	1183	1186	rBV	8348792	8593024	100.00%	18.420%
8	9.922	1292	1298	1302	rBV	2588448	2286476	26.61%	4.901%
9	10.716	1424	1433	1437	rBV	5477525	5740631	66.81%	12.305%
10	11.410	1546	1551	1555	rBV	2280655	2216143	25.79%	4.750%
11	11.651	1586	1592	1601	rBV5	47869	135241	1.57%	0.290%
12	11.792	1613	1616	1620	rBV	328031	262509	3.05%	0.563%
13	11.933	1636	1640	1644	rBV	92041	109685	1.28%	0.235%
14	12.480	1726	1733	1734	rBV3	121946	205788	2.39%	0.441%
15	12.504	1734	1737	1740	rVB	711201	594432	6.92%	1.274%
16	12.586	1748	1751	1755	rVB	242164	193809	2.26%	0.415%
17	12.651	1758	1762	1765	rVB	305987	251233	2.92%	0.539%
18	13.004	1817	1822	1825	rBV	8085784	7989307	92.97%	17.126%
19	13.910	1969	1976	1993	rBV4	161353	518945	6.04%	1.112%
20	14.057	1997	2001	2005	rBV	1862573	1622030	18.88%	3.477%
21	14.898	2141	2144	2149	rVB	119432	117883	1.37%	0.253%
22	15.545	2249	2254	2264	rVB	960322	1241397	14.45%	2.661%

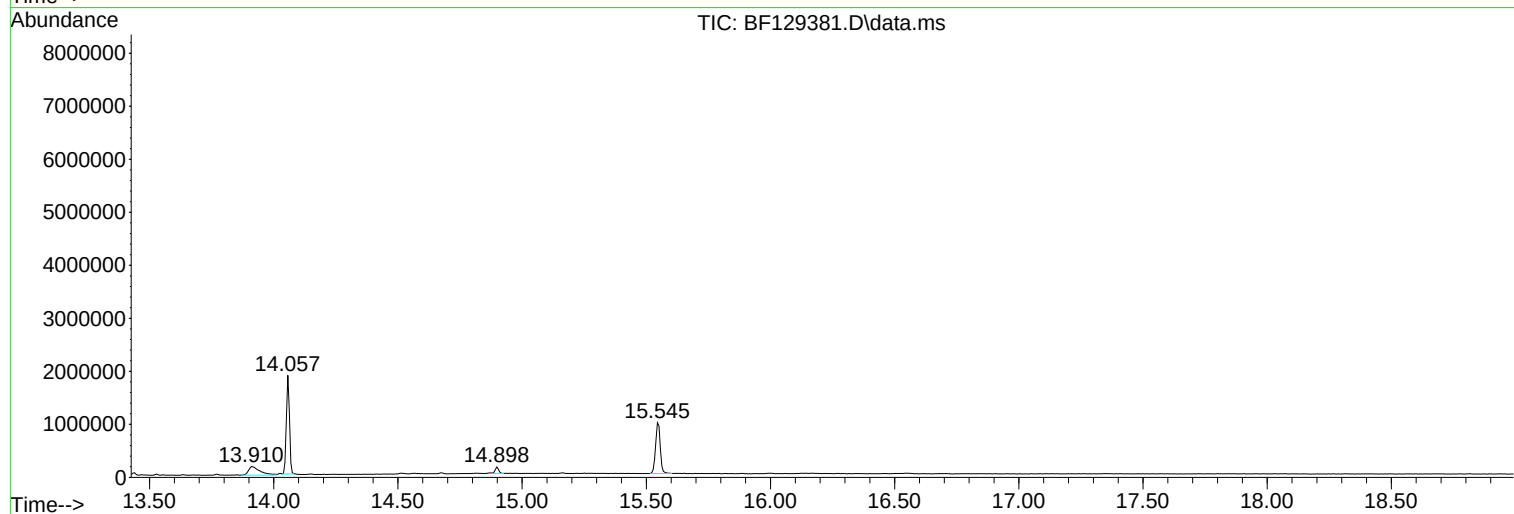
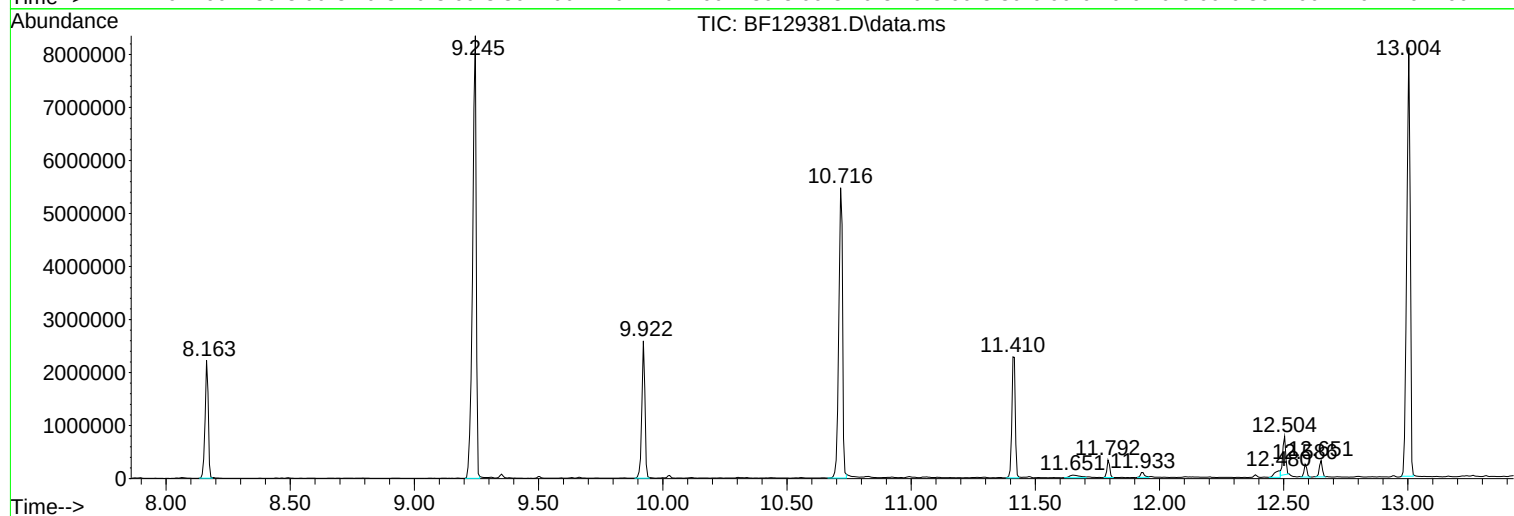
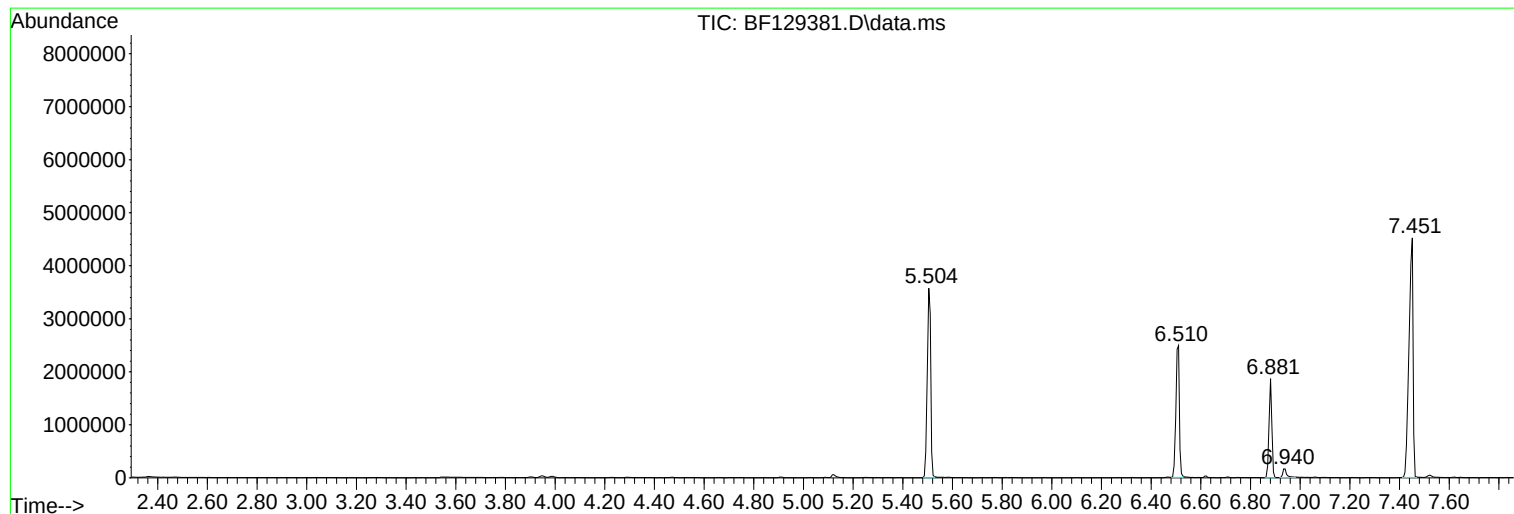
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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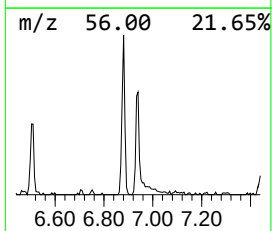
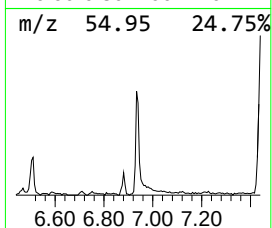
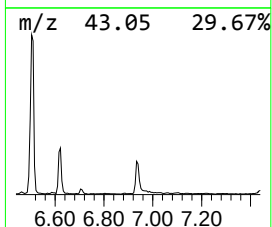
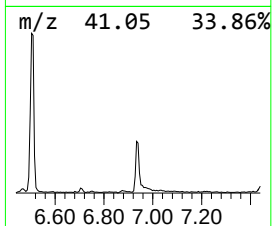
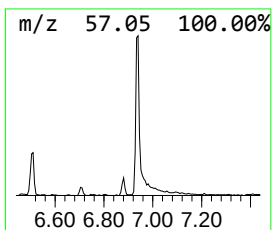
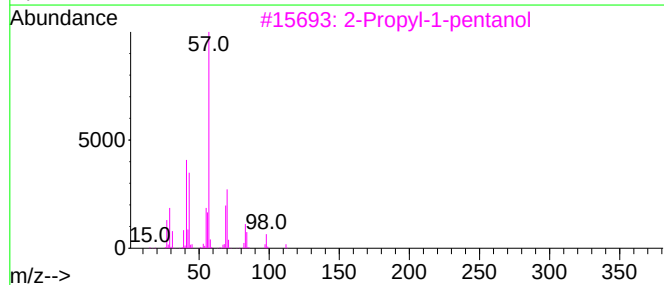
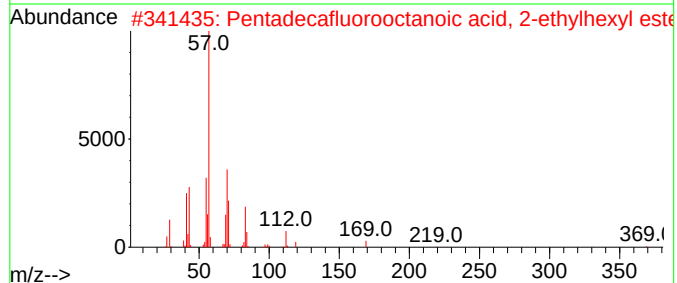
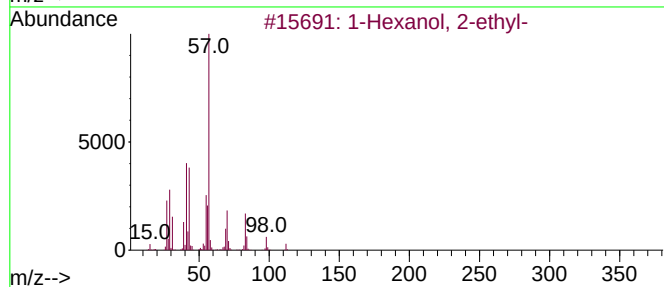
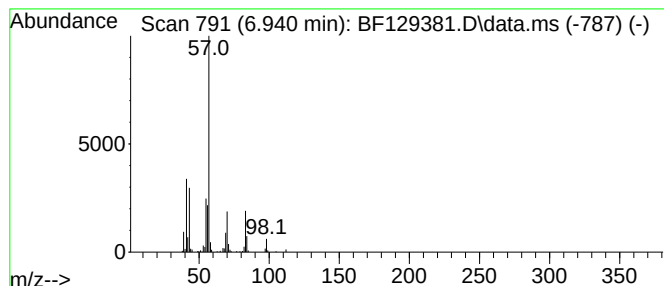
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.940	2.51 ng	186281	1,4-Dichlorobenzene-d4	6.881

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4		Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47
5		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	47



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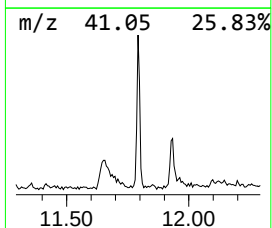
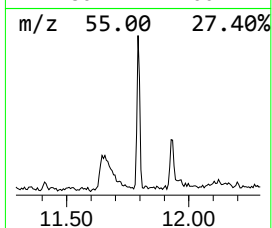
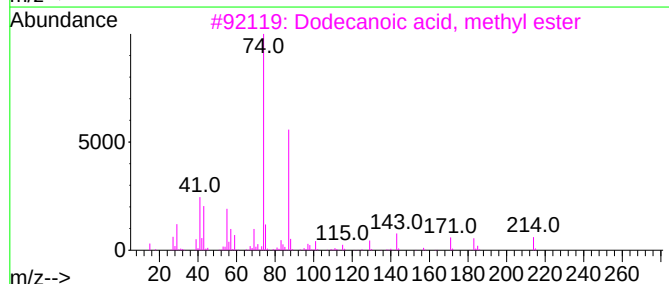
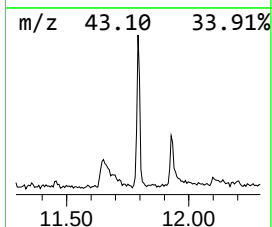
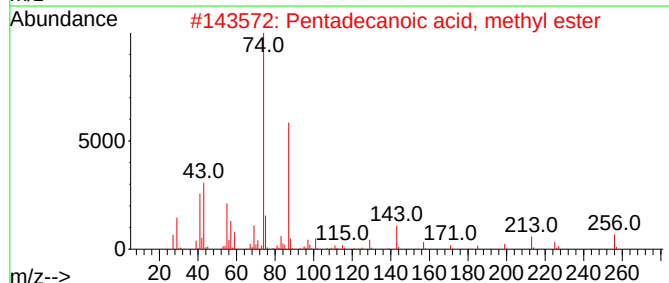
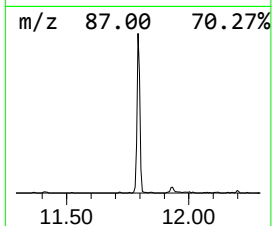
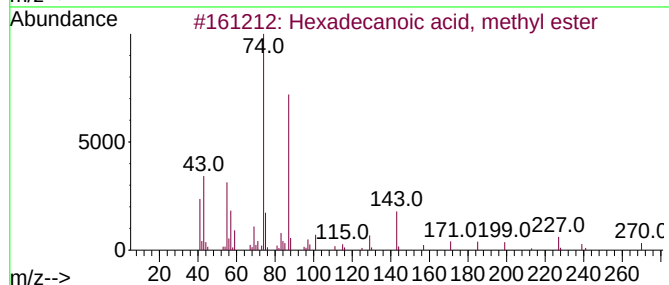
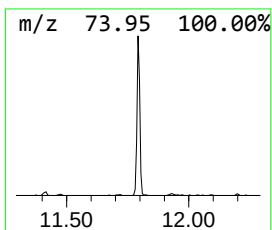
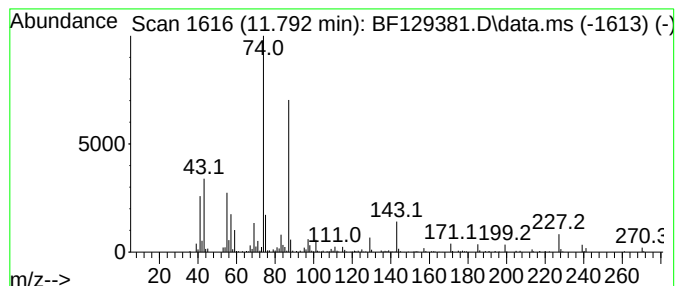
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	2.37 ng	262509	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
2			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	86
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86



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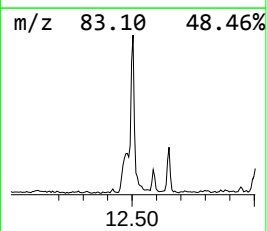
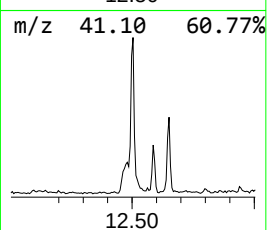
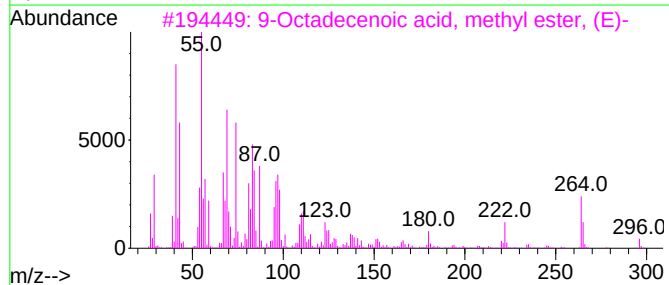
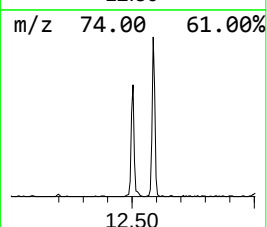
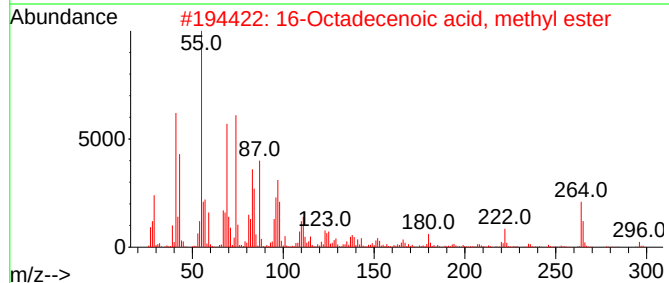
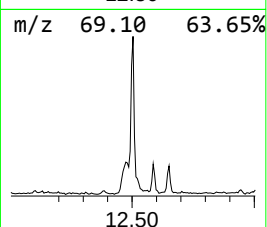
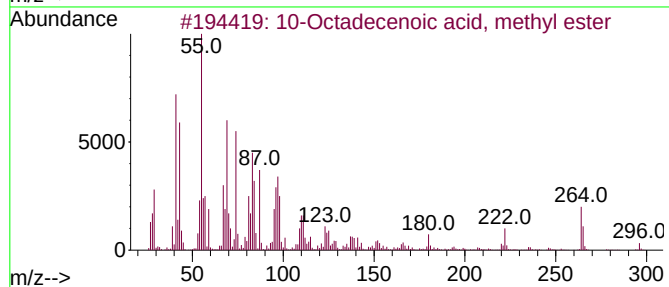
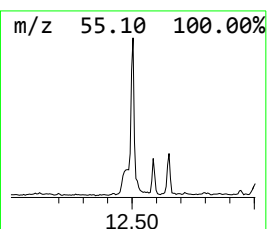
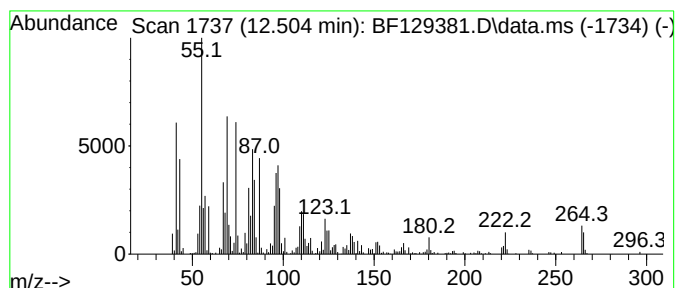
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 10-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.504	5.36 ng	594432	Phenanthrene-d10	11.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
2		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3		9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
4		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
5		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99



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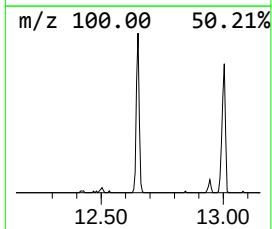
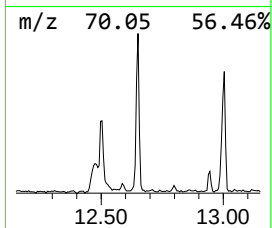
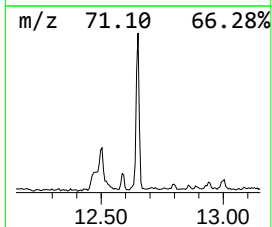
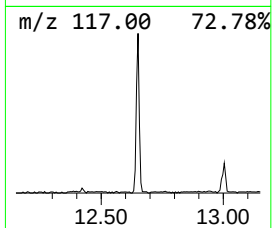
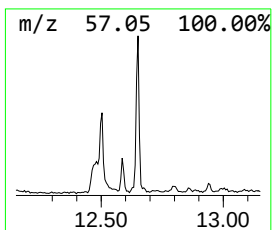
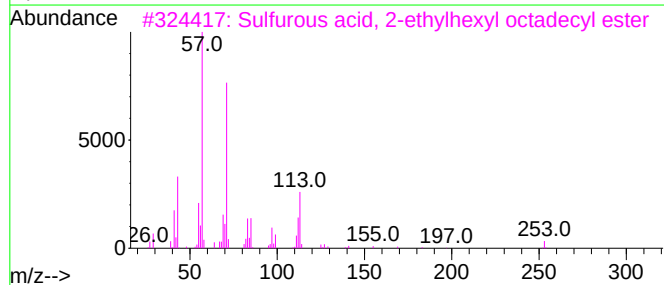
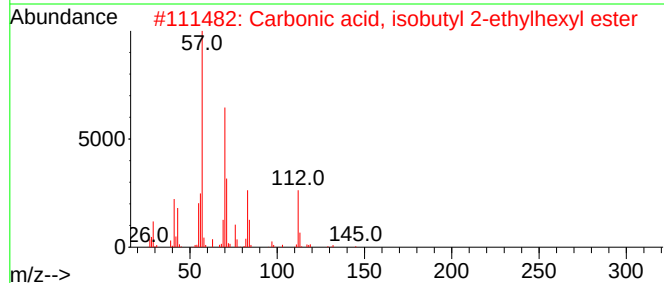
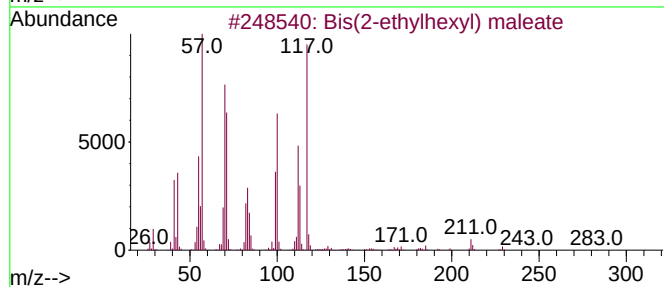
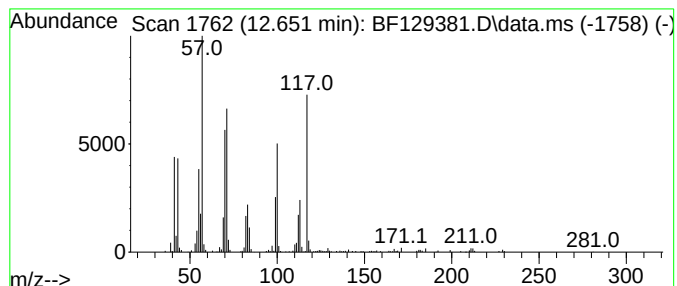
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Bis(2-ethylhexyl) maleate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.651	2.27 ng	251233	Phenanthrene-d10	11.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	91
2	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	35
3	Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	35
4	Dichloroacetic acid, 2-ethylhexy...	240	C10H18Cl2O2	068144-72-9	35
5	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	35



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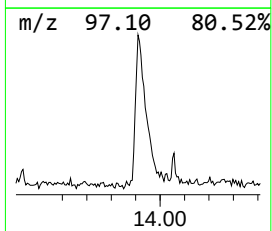
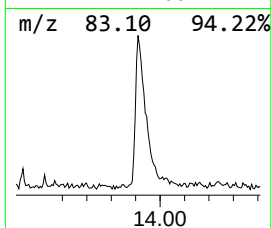
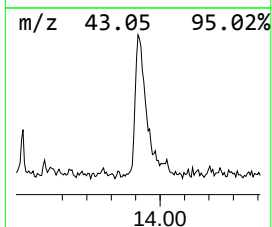
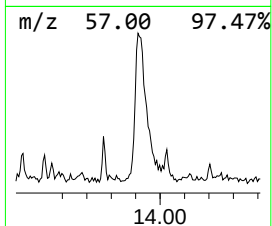
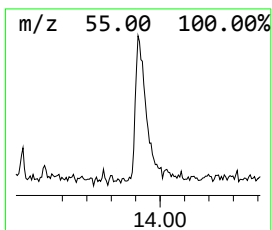
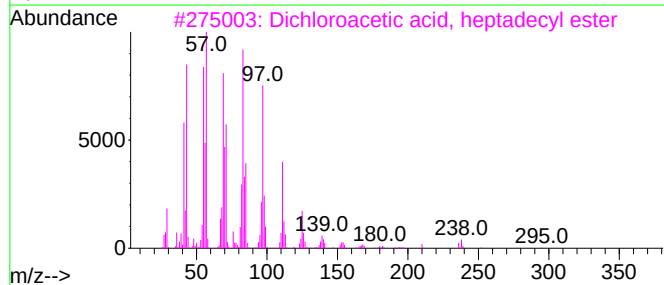
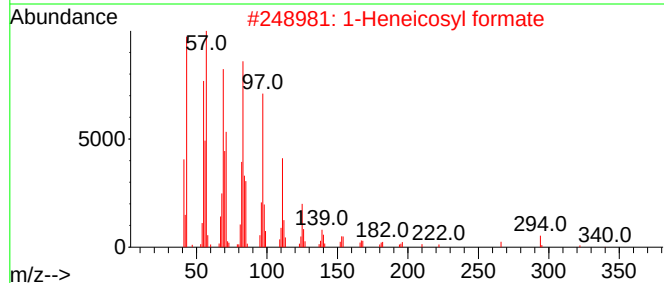
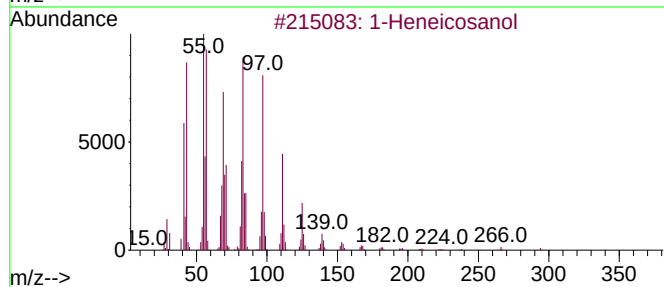
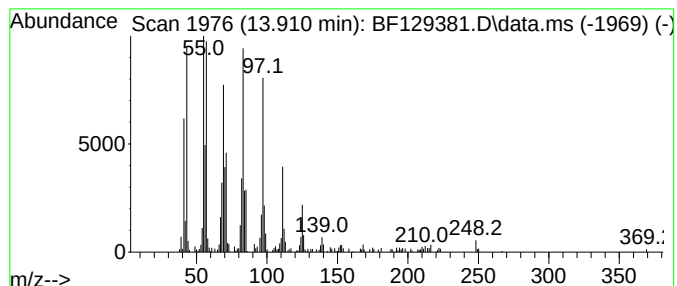
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	6.40 ng	518945	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
4			Cyclopentadecane	210	C15H30	000295-48-7	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	6.940	2.5	ng	186281	1	6.881	1485800	20.0
Hexadecanoic ac...	11.792	2.4	ng	262509	4	11.416	2216140	20.0
10-Octadecenoic...	12.504	5.4	ng	594432	4	11.416	2216140	20.0
Bis(2-ethylhexy...	12.651	2.3	ng	251233	4	11.416	2216140	20.0
1-Heneicosanol	13.910	6.4	ng	518945	5	14.057	1622030	20.0