

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050622\
 Data File : BF128134.D
 Acq On : 06 May 2022 19:56
 Operator : CG\JU
 Sample : N2712-11
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128134.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.487	200	204	221	rBV	10764	28046	1.19%	0.176%
2	5.140	482	485	491	rVB	20744	24534	1.04%	0.154%
3	5.528	547	551	554	rBV	2001663	1836408	77.60%	11.502%
4	6.534	716	722	725	rBV	1847070	1931753	81.63%	12.099%
5	6.904	781	785	788	rBV	583360	470026	19.86%	2.944%
6	7.469	876	881	884	rBV	1352019	1263053	53.38%	7.911%
7	8.187	999	1003	1006	rBV	735028	605030	25.57%	3.789%
8	9.263	1180	1186	1189	rBV	2452043	2157790	91.19%	13.514%
9	9.945	1297	1302	1305	rBV	851690	709641	29.99%	4.445%
10	10.733	1432	1436	1440	rBV	1584852	1489444	62.94%	9.329%
11	11.433	1551	1555	1559	rBV	897456	774350	32.72%	4.850%
12	11.663	1587	1594	1604	rBV6	20107	57978	2.45%	0.363%
13	11.816	1616	1620	1623	rBV	92699	72604	3.07%	0.455%
14	12.498	1729	1736	1737	rBV3	47465	82283	3.48%	0.515%
15	12.522	1737	1740	1748	rVV	334167	305031	12.89%	1.910%
16	12.610	1752	1755	1758	rVB	107402	90159	3.81%	0.565%
17	12.669	1759	1765	1769	rBV2	113731	102850	4.35%	0.644%
18	13.022	1821	1825	1829	rBV	2514540	2366374	100.00%	14.821%
19	13.927	1973	1979	1995	rBV5	82750	258019	10.90%	1.616%
20	14.080	2001	2005	2009	rBV	747022	648092	27.39%	4.059%
21	14.845	2131	2135	2140	rBV	37696	35788	1.51%	0.224%
22	15.192	2190	2194	2198	rVB	35850	41274	1.74%	0.259%
23	15.580	2255	2260	2269	rBV	397608	508775	21.50%	3.187%
24	16.033	2332	2337	2344	rBV2	25927	41081	1.74%	0.257%
25	16.562	2421	2427	2435	rVB3	21043	38810	1.64%	0.243%
26	17.168	2527	2530	2538	rVB4	13885	27362	1.16%	0.171%

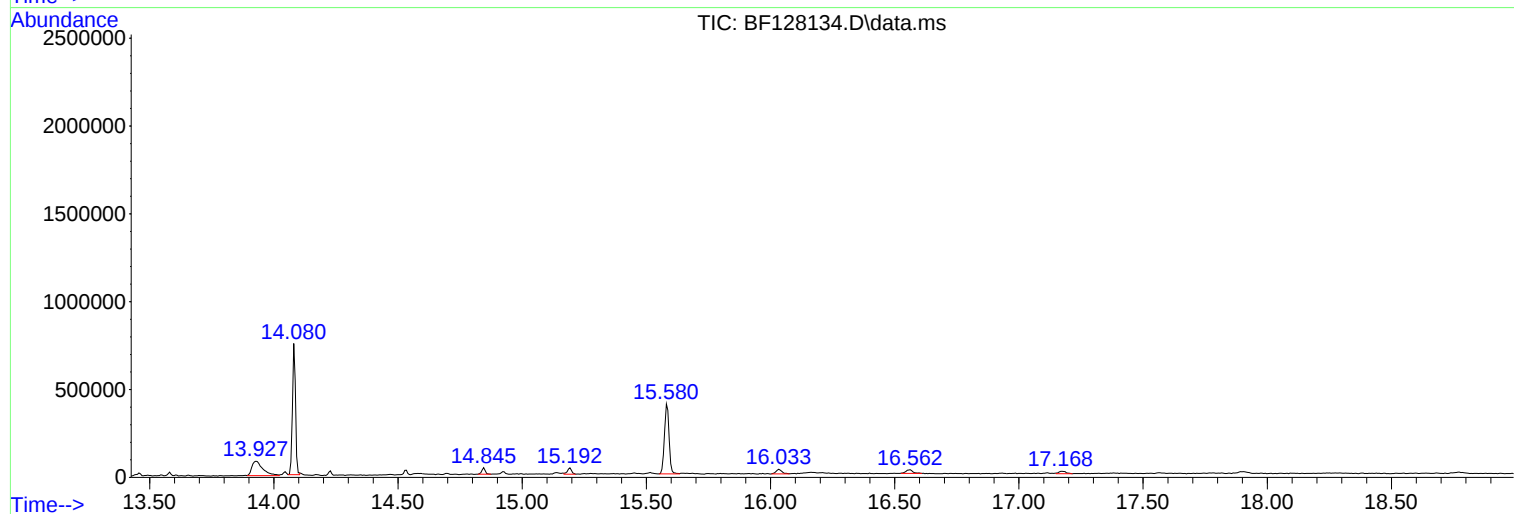
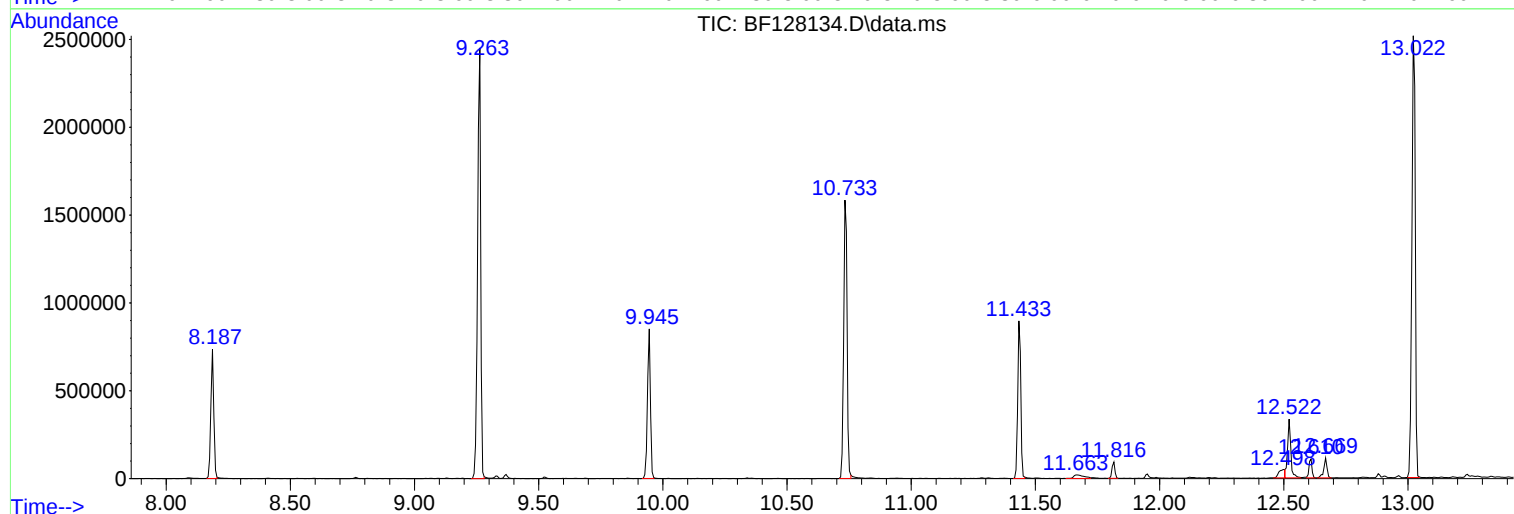
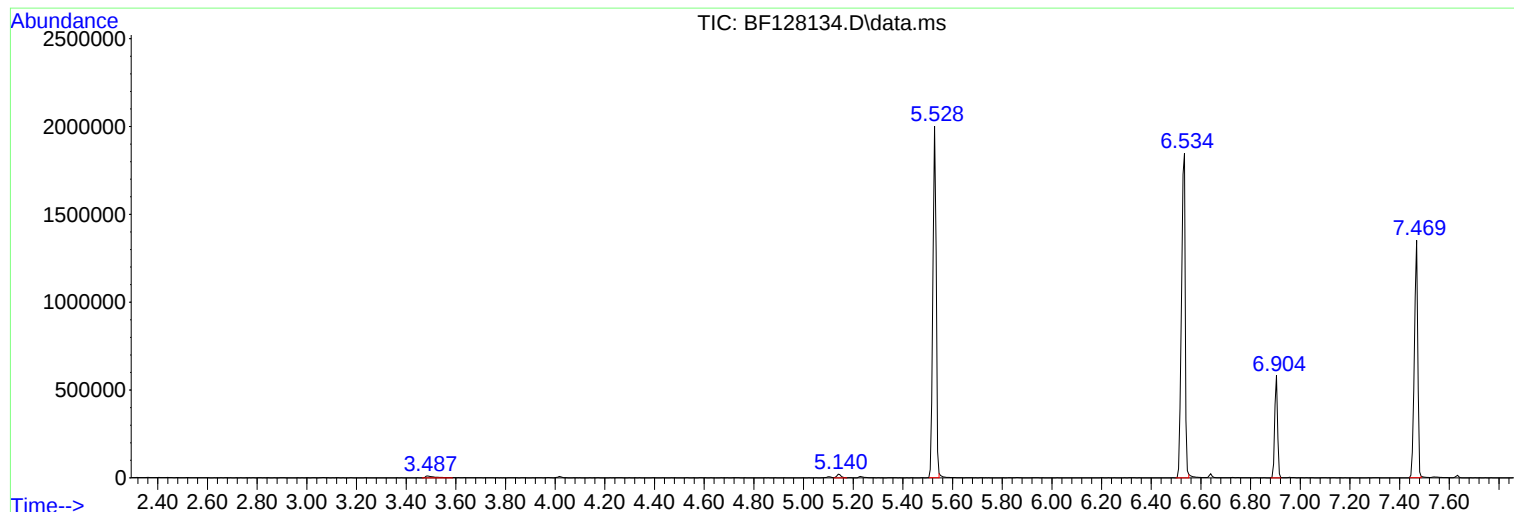
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF128134.D
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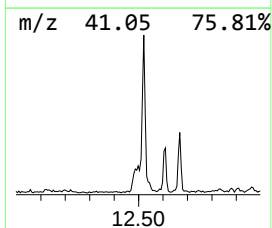
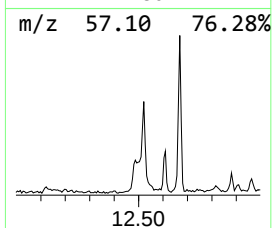
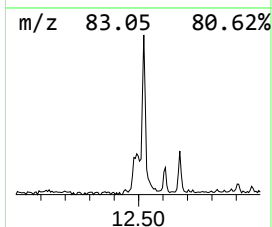
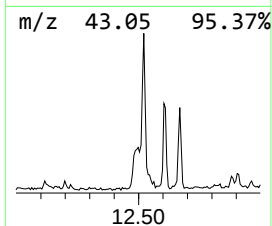
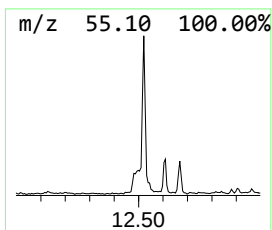
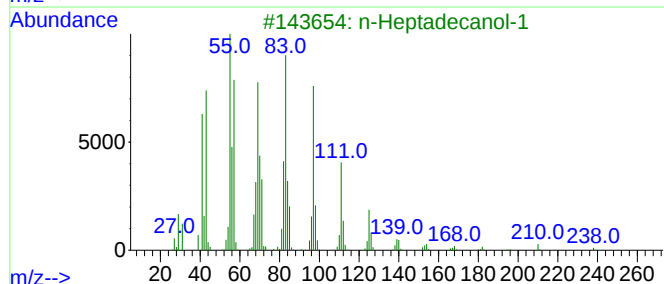
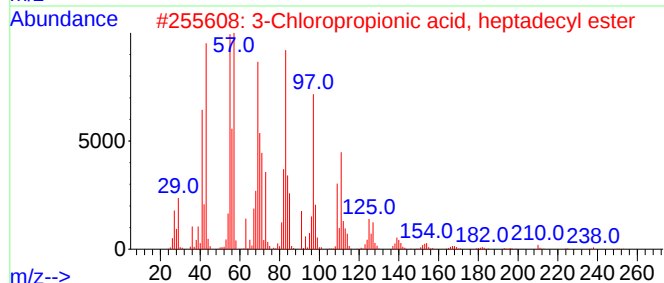
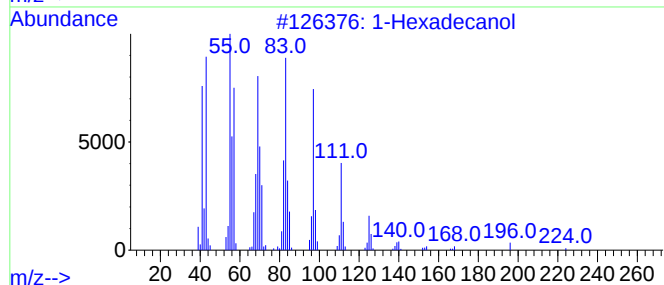
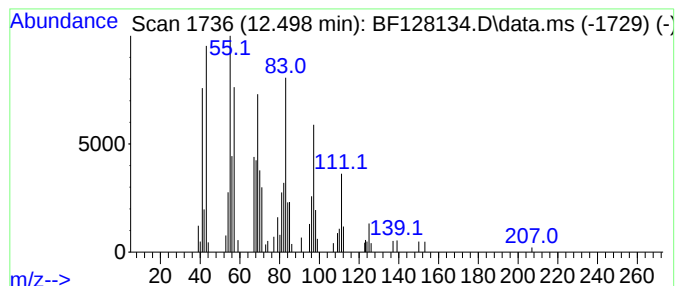
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.498	2.13 ng	82283	Phenanthrene-d10	11.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	76
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	76
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	76
4	1-Heneicosanol	312	C21H44O	015594-90-8	76
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	74



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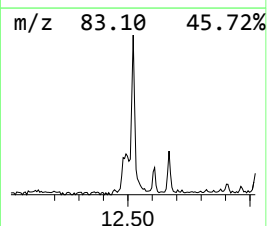
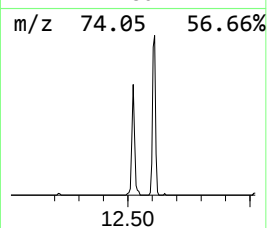
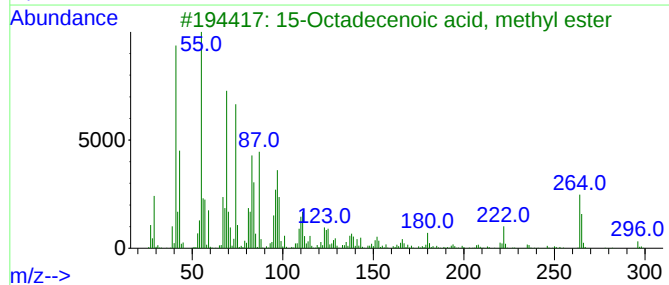
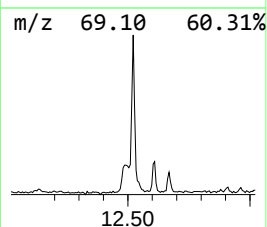
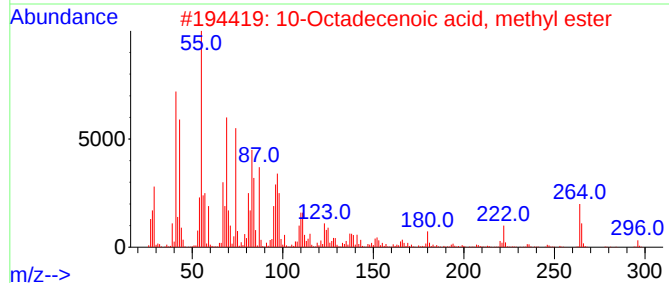
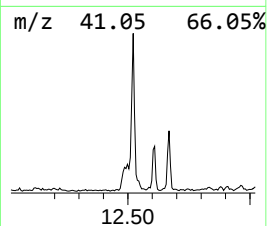
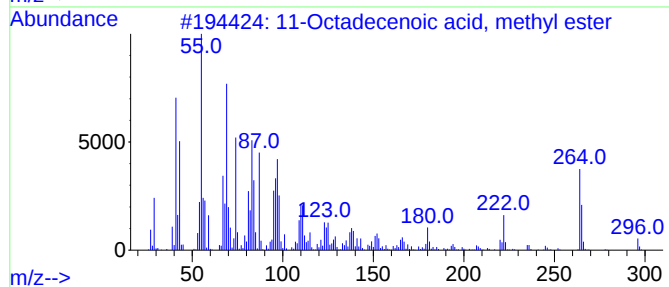
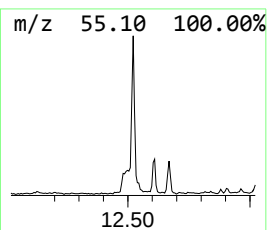
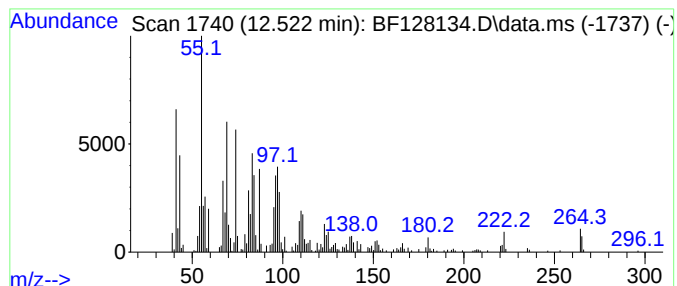
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 11-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.522	7.88 ng	305031	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
4			9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
5			8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99



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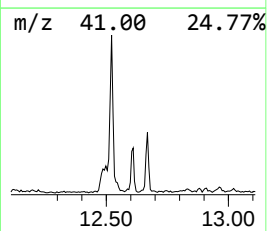
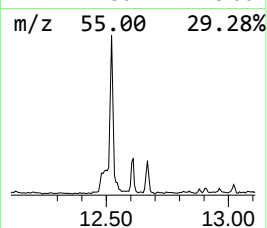
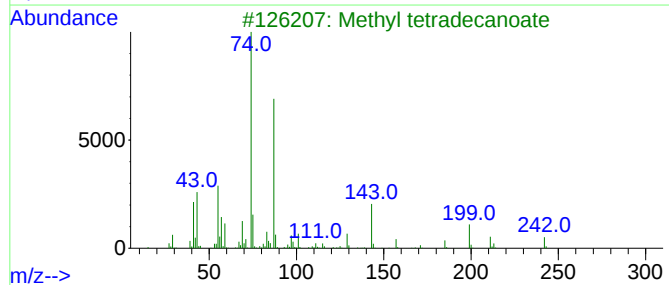
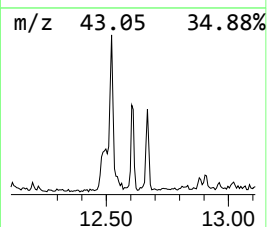
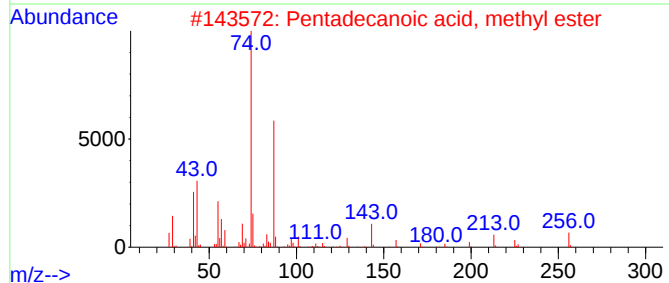
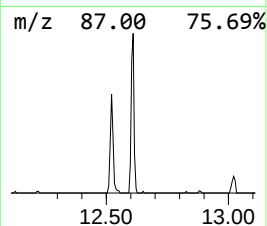
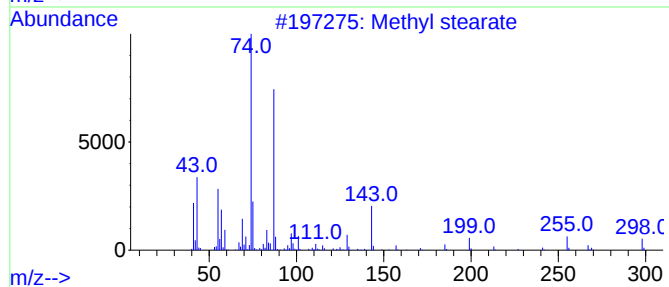
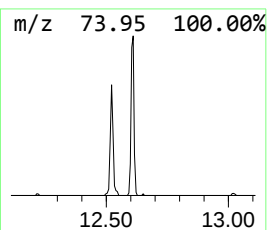
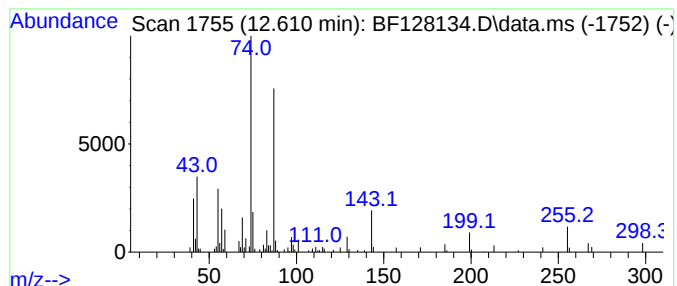
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	2.33 ng	90159	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
4			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80



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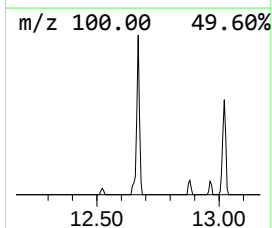
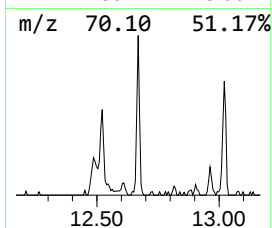
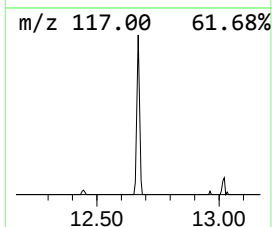
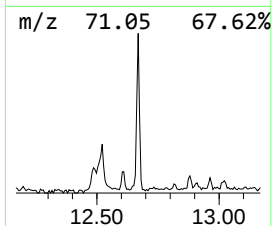
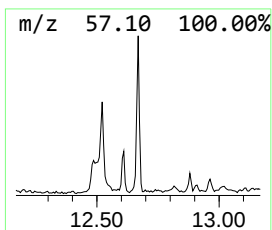
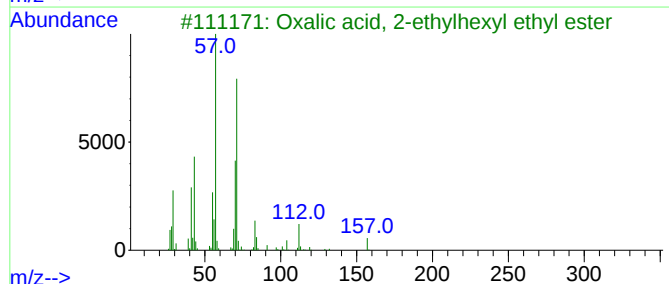
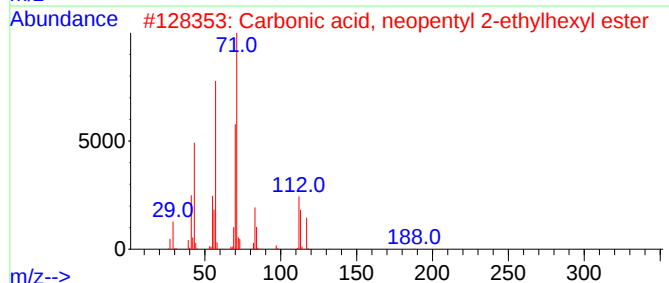
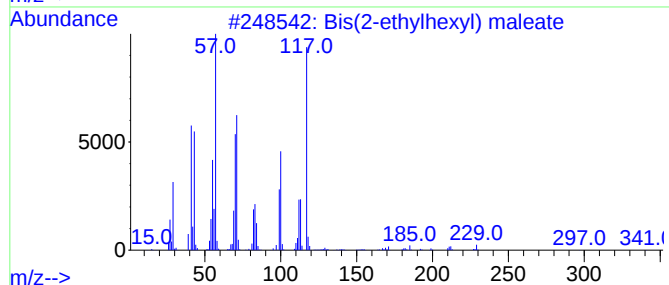
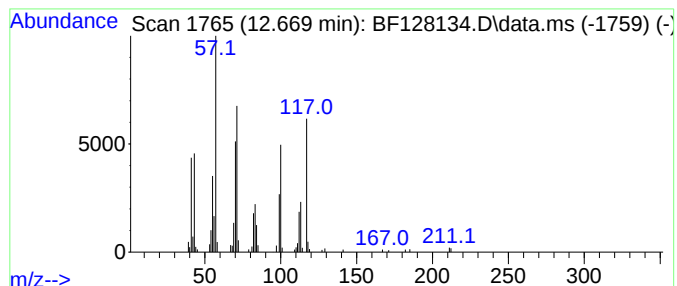
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Bis(2-ethylhexyl) maleate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.669	2.66 ng	102850	Phenanthrene-d10	11.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	81
2	Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	38
3	Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	38
4	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	35
5	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	35



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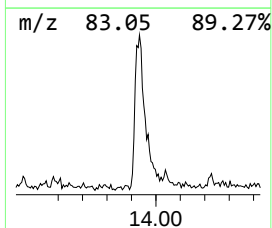
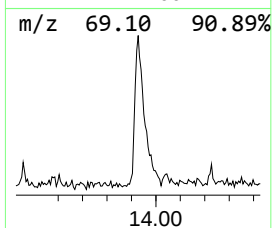
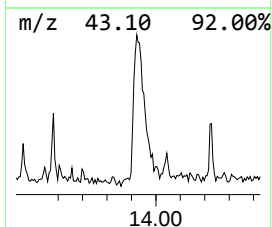
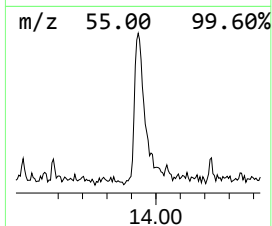
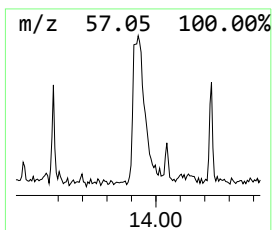
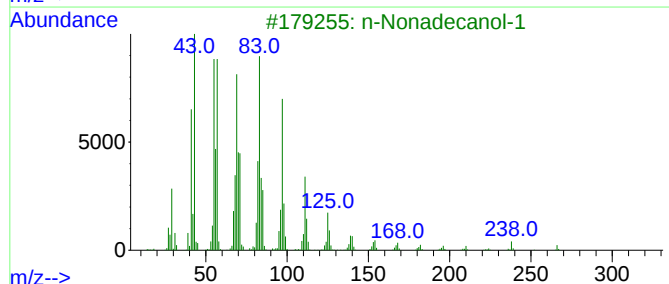
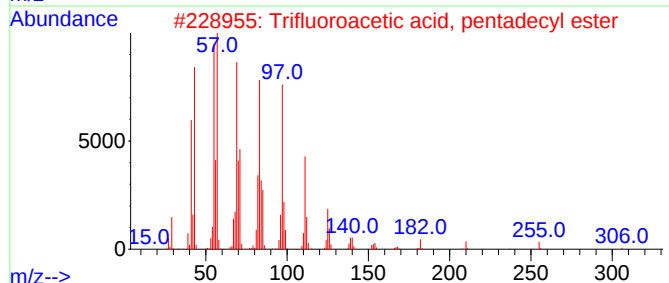
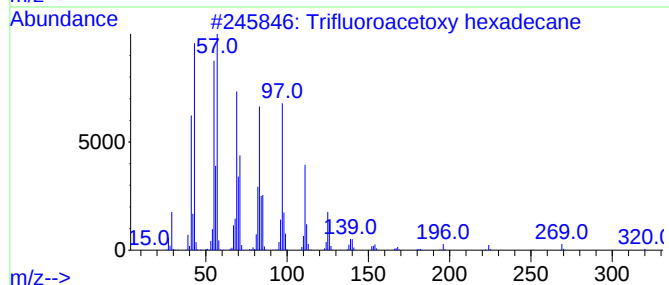
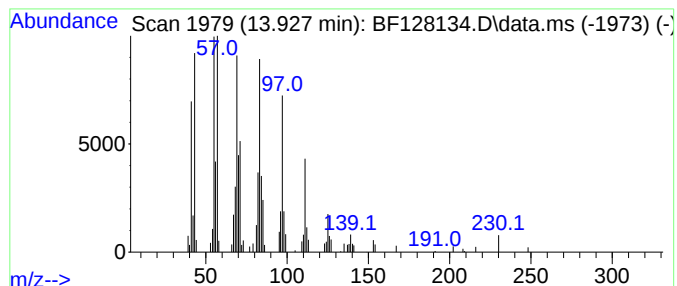
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	7.96 ng	258019	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			n-Heptadecanol-1	256	C17H36O	001454-85-9	93
5			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexadecanol	12.498	2.1	ng	82283	4	11.433	774350	20.0
11-Octadecenoic...	12.522	7.9	ng	305031	4	11.433	774350	20.0
Methyl stearate	12.610	2.3	ng	90159	4	11.433	774350	20.0
Bis(2-ethylhexy...	12.669	2.7	ng	102850	4	11.433	774350	20.0
Trifluoroacetox...	13.927	8.0	ng	258019	5	14.080	648092	20.0