

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
 Data File : BF137051.D
 Acq On : 12 Jan 2024 16:28
 Operator : CG\JU
 Sample : P1117-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S1-COMPOSITE

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-BF122023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137051.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	18	rBV	11456	19322	1.54%	0.224%
2	5.022	495	499	508	rBV	60347	71676	5.72%	0.830%
3	5.434	565	569	586	rBV	1069223	1047851	83.58%	12.133%
4	6.434	735	739	753	rBV	1180647	1059661	84.52%	12.269%
5	6.781	795	798	802	rBV	411706	339806	27.10%	3.934%
6	7.345	890	894	897	rBV	796295	684144	54.57%	7.921%
7	8.057	1012	1015	1019	rBV	493038	433186	34.55%	5.016%
8	9.139	1194	1199	1202	rBV	1375937	1253779	100.00%	14.517%
9	9.257	1215	1219	1228	rVB2	14632	19491	1.55%	0.226%
10	9.816	1310	1314	1324	rBV	605781	484274	38.63%	5.607%
11	10.610	1446	1449	1462	rBV	717852	715717	57.08%	8.287%
12	11.310	1564	1568	1571	rBV	564684	450729	35.95%	5.219%
13	11.845	1656	1659	1662	rBV	148997	148495	11.84%	1.719%
14	12.533	1773	1776	1779	rBV	36252	35667	2.84%	0.413%
15	12.633	1790	1793	1805	rBV	32805	49279	3.93%	0.571%
16	12.763	1810	1815	1820	rVB	32982	35024	2.79%	0.406%
17	12.904	1835	1839	1842	rBV	1079157	891988	71.14%	10.328%
18	13.886	2000	2006	2011	rBV7	17519	47561	3.79%	0.551%
19	13.969	2016	2020	2024	rBV	360101	322495	25.72%	3.734%
20	14.433	2096	2099	2103	rBV5	12393	13102	1.05%	0.152%
21	14.592	2123	2126	2131	rVB	32610	35293	2.81%	0.409%
22	15.021	2196	2199	2203	rBV	21511	37477	2.99%	0.434%
23	15.086	2207	2210	2213	rVB5	11594	15873	1.27%	0.184%
24	15.333	2249	2252	2257	rVB	12865	18527	1.48%	0.215%
25	15.392	2259	2262	2268	rVB2	19767	27958	2.23%	0.324%
26	15.463	2268	2274	2282	rBV	270476	378253	30.17%	4.380%

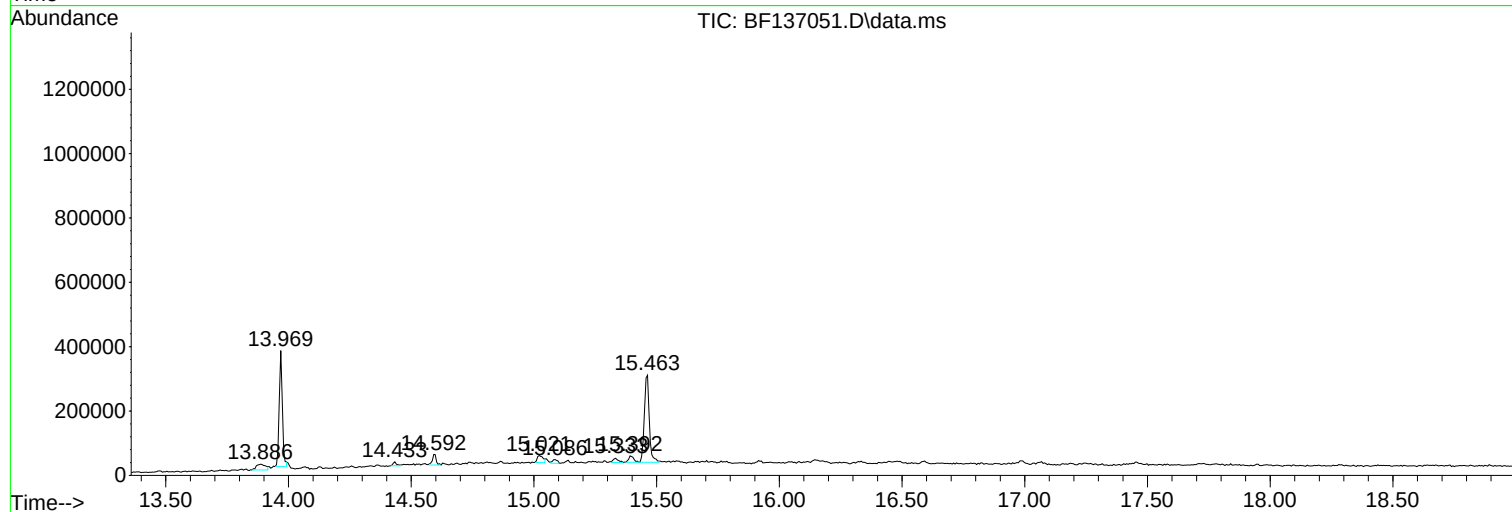
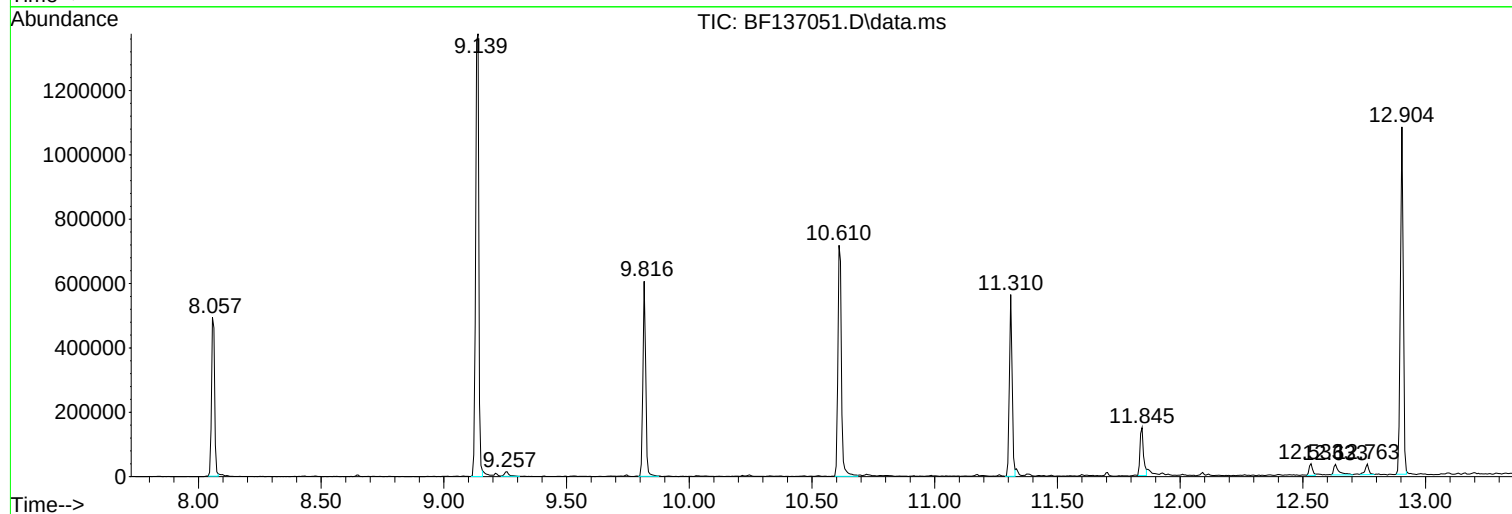
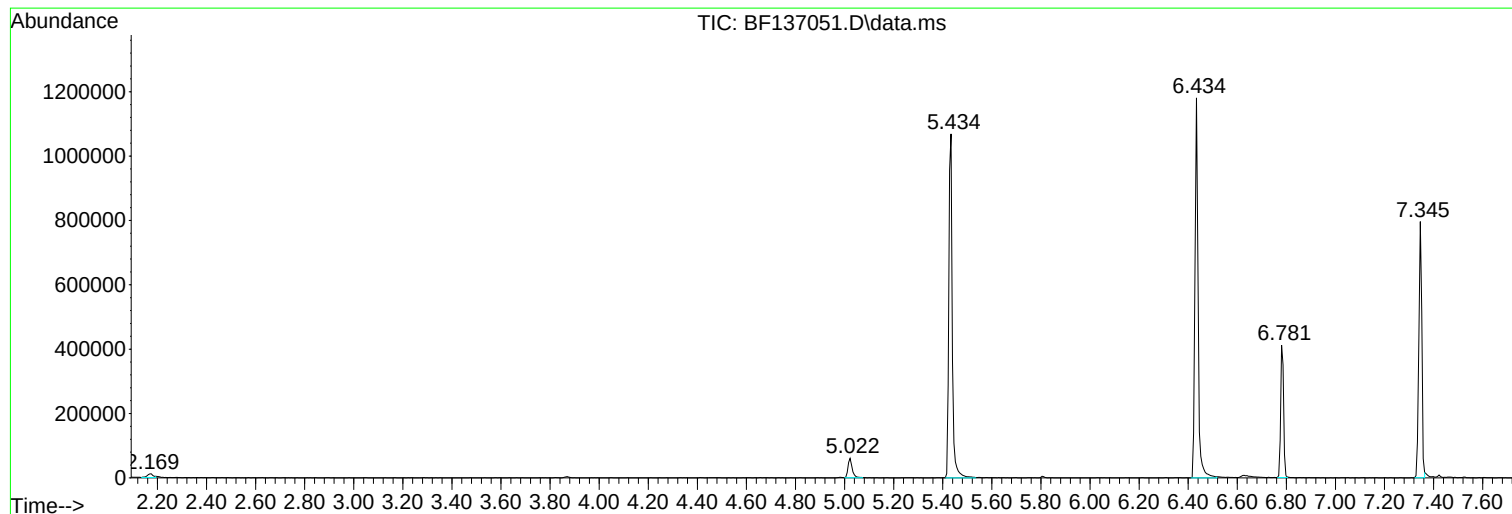
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S1-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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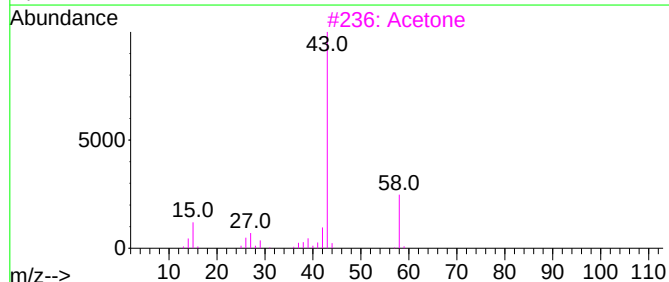
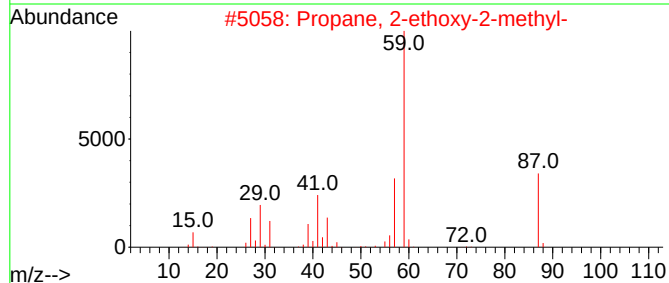
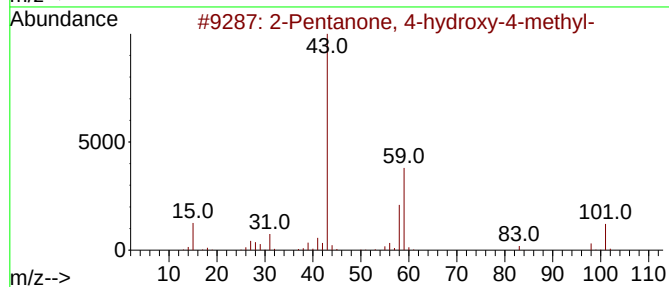
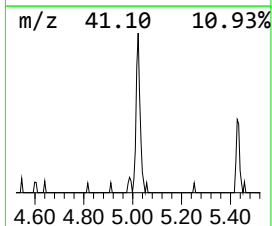
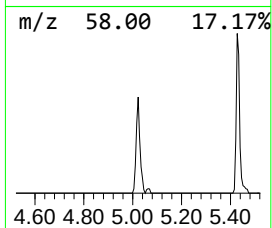
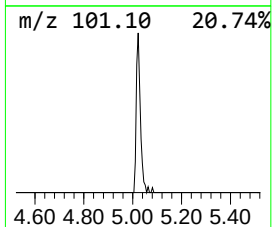
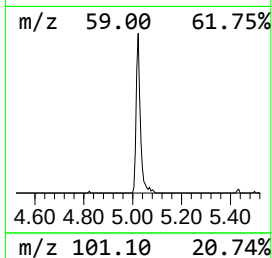
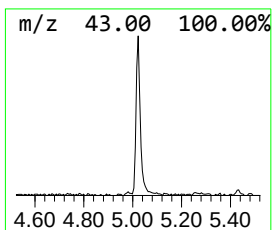
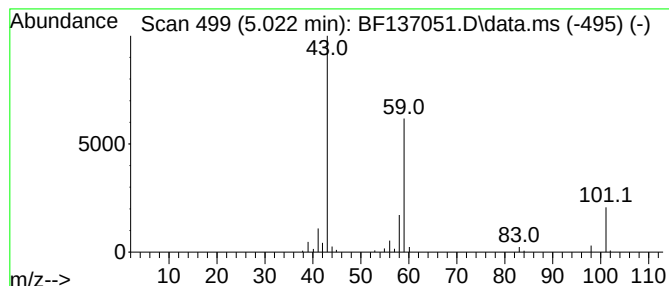
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	4.22 ng	71676	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
3			Acetone	58	C3H6O	000067-64-1	9
4			Pentane, 2-methoxy-	102	C6H14O	006795-88-6	9
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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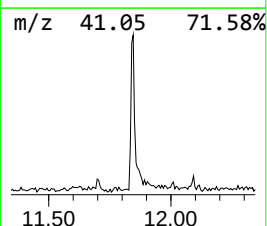
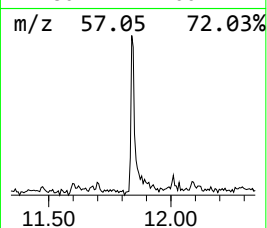
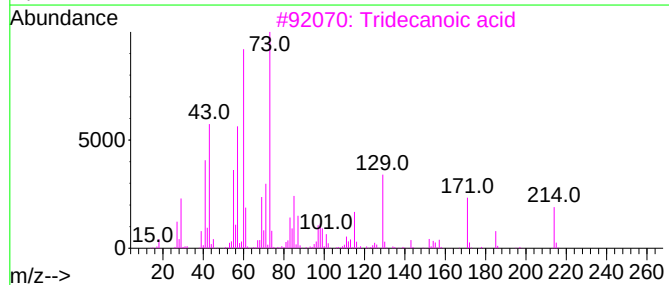
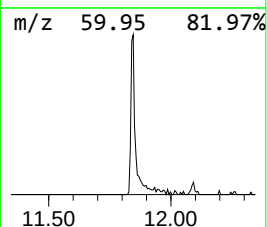
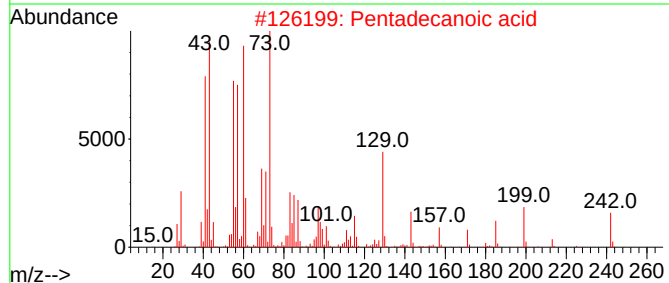
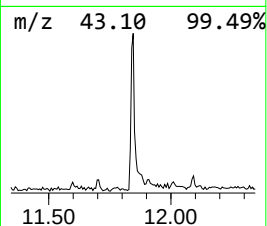
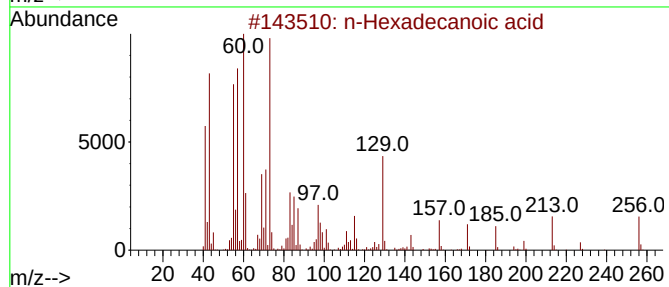
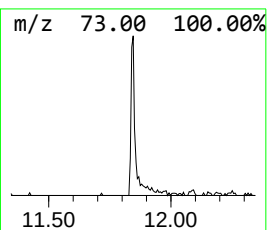
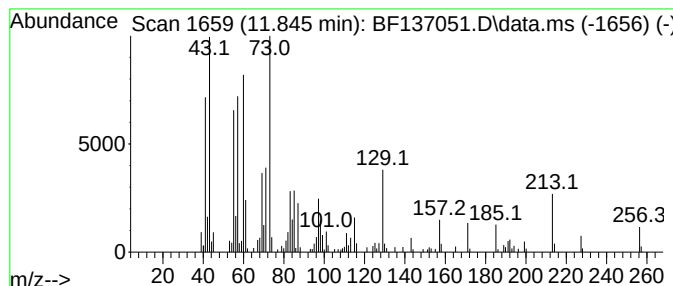
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	6.59 ng	148495	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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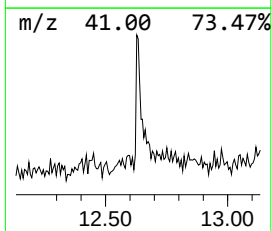
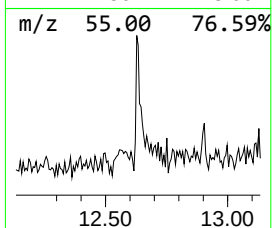
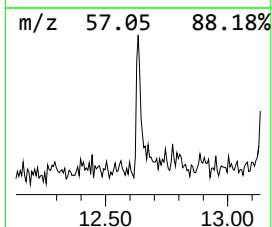
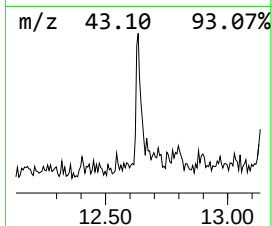
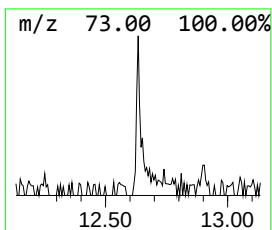
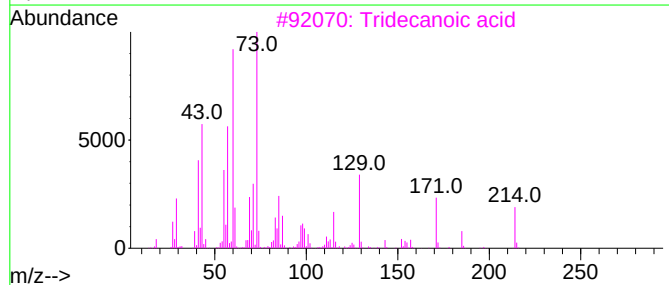
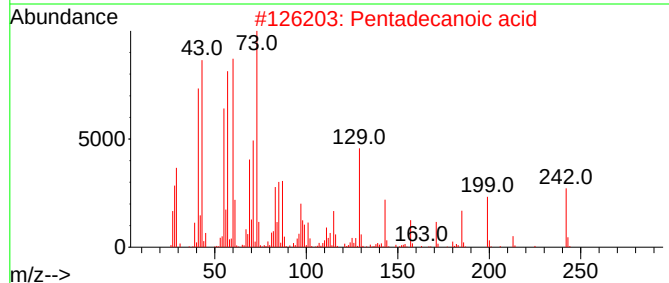
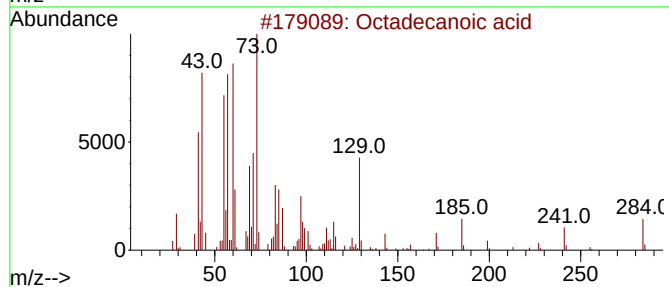
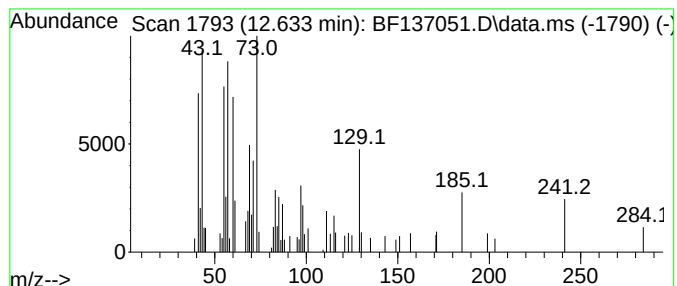
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	2.19 ng	49279	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
3			Tridecanoic acid	214	C13H26O2	000638-53-9	50
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5			n-Decanoic acid	172	C10H20O2	000334-48-5	43



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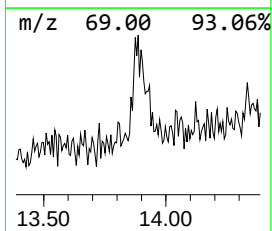
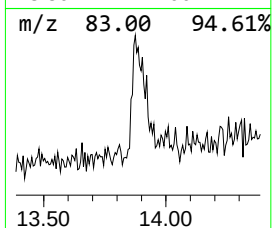
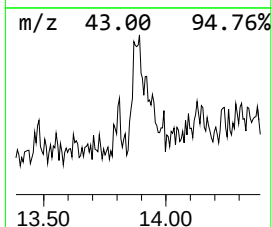
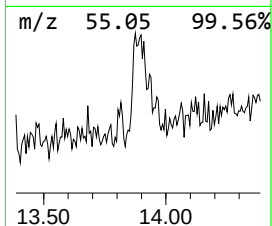
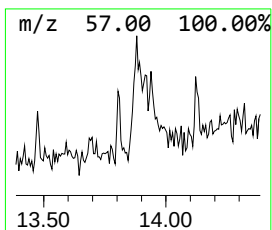
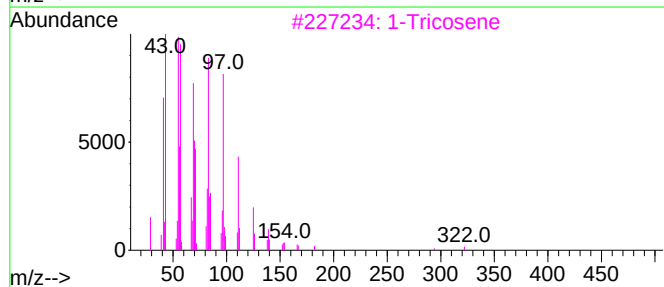
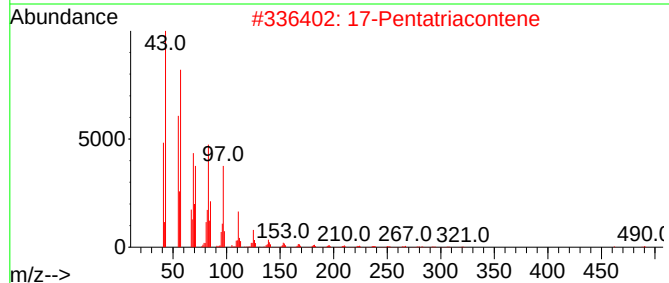
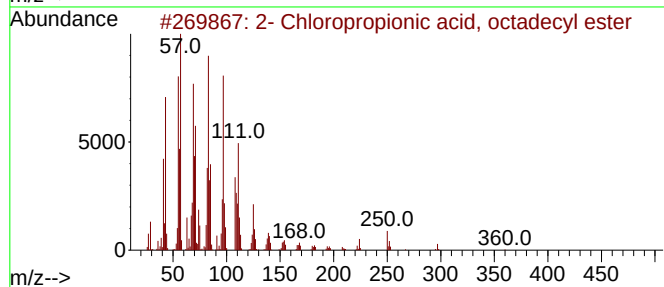
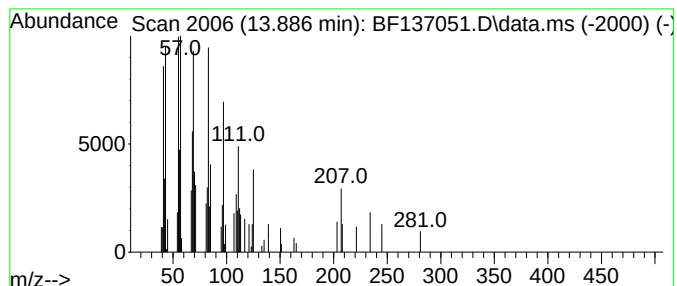
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 2- Chloropropionic acid, oc... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.886	2.95 ng	47561	Chrysene-d12	13.969	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	72
2	17-Pentatriacontene	491	C35H70	006971-40-0	68
3	1-Tricosene	322	C23H46	018835-32-0	64
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	49
5	1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	49



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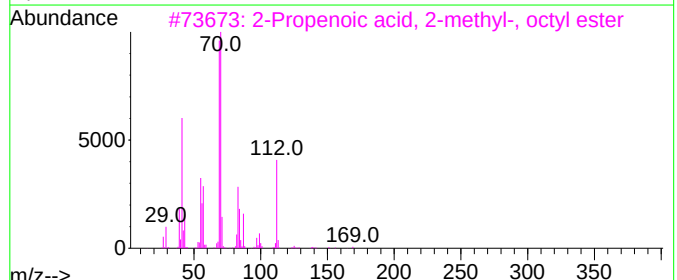
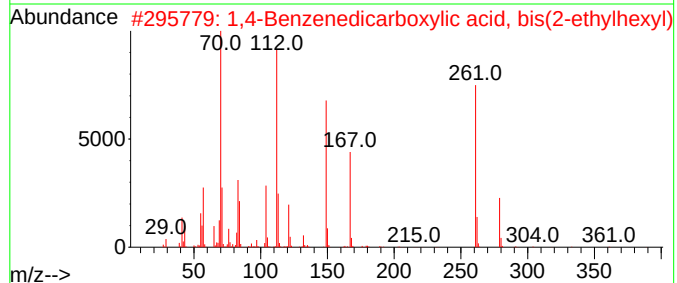
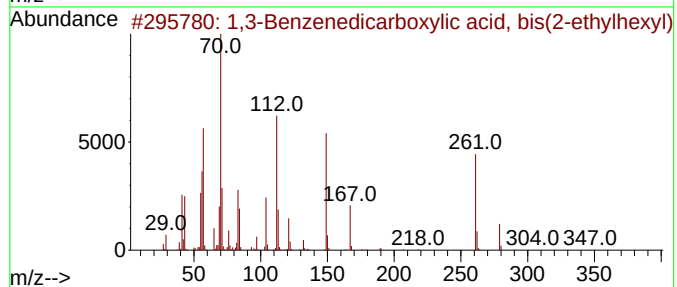
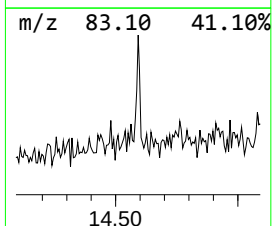
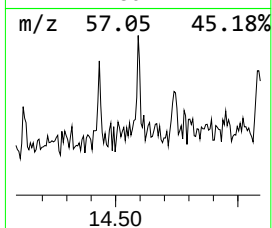
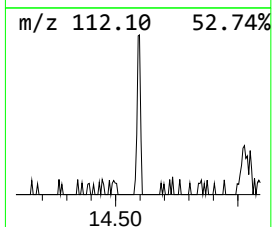
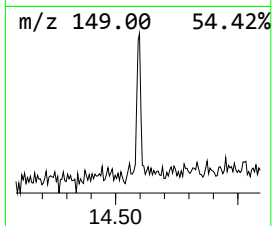
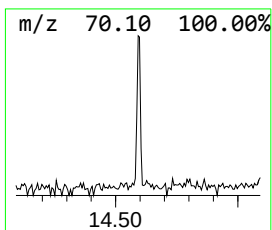
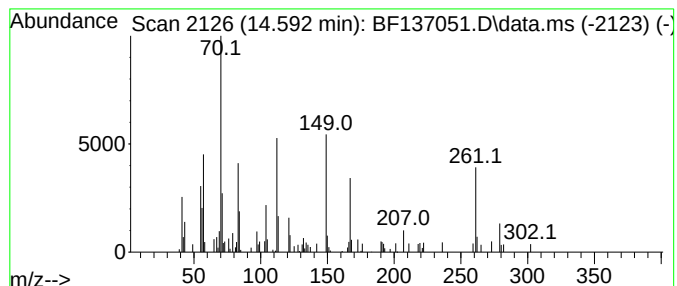
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,3-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.592	2.19 ng	35293	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
3			2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	32
4			9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42C12N4O3	1000111-04-6	22
5			Mono(2-ethylhexyl) phthalate	278	C16H22O4	004376-20-9	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	4.2	ng	71676	1	6.781	339806	20.0
n-Hexadecanoic ...	11.845	6.6	ng	148495	4	11.310	450729	20.0
Octadecanoic acid	12.633	2.2	ng	49279	4	11.310	450729	20.0
2- Chloropropio...	13.886	3.0	ng	47561	5	13.969	322495	20.0
1,3-Benzenedica...	14.592	2.2	ng	35293	5	13.969	322495	20.0