

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
 Data File : BF132277.D
 Acq On : 02 Feb 2023 00:17
 Operator : CG\JU
 Sample : 01333-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-I

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132277.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.307	415	420	429	rVB	971220	1218371	33.72%	4.914%
2	5.690	480	485	489	rBV	2879303	2985347	82.63%	12.040%
3	6.684	648	654	657	rBV	2884431	2935808	81.26%	11.840%
4	7.072	716	720	723	rVB	1026548	897733	24.85%	3.621%
5	7.631	811	815	818	rBV	2224684	1925117	53.28%	7.764%
6	8.354	935	938	941	rBV	1481352	1159837	32.10%	4.678%
7	9.431	1117	1121	1124	rBV	4385836	3613073	100.00%	14.572%
8	9.501	1127	1133	1136	rBV	49590	48605	1.35%	0.196%
9	10.119	1234	1238	1242	rVB	1478347	1172010	32.44%	4.727%
10	10.831	1356	1359	1363	rVB	152310	122152	3.38%	0.493%
11	10.913	1369	1373	1376	rBV	2251236	1955322	54.12%	7.886%
12	11.013	1386	1390	1400	rVB7	20300	46194	1.28%	0.186%
13	11.619	1489	1493	1496	rBV	1250880	1048540	29.02%	4.229%
14	12.125	1576	1579	1585	rBV	488323	437968	12.12%	1.766%
15	12.919	1710	1714	1720	rBV	158860	188399	5.21%	0.760%
16	13.072	1737	1740	1742	rBV2	74257	67433	1.87%	0.272%
17	13.213	1760	1764	1767	rBV	3485868	2954702	81.78%	11.917%
18	14.107	1913	1916	1929	rBV4	173906	436305	12.08%	1.760%
19	14.242	1937	1939	1941	rVB	88570	60269	1.67%	0.243%
20	14.277	1942	1945	1949	rVV	873817	824511	22.82%	3.325%
21	15.871	2212	2216	2225	rVB	491388	697187	19.30%	2.812%

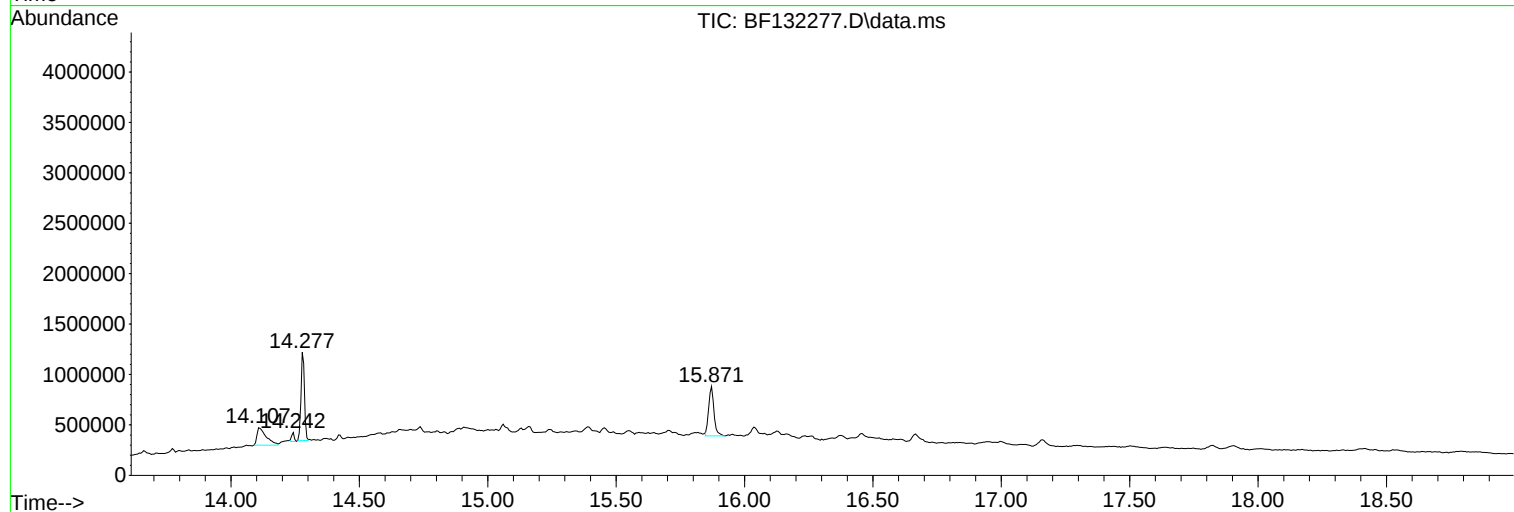
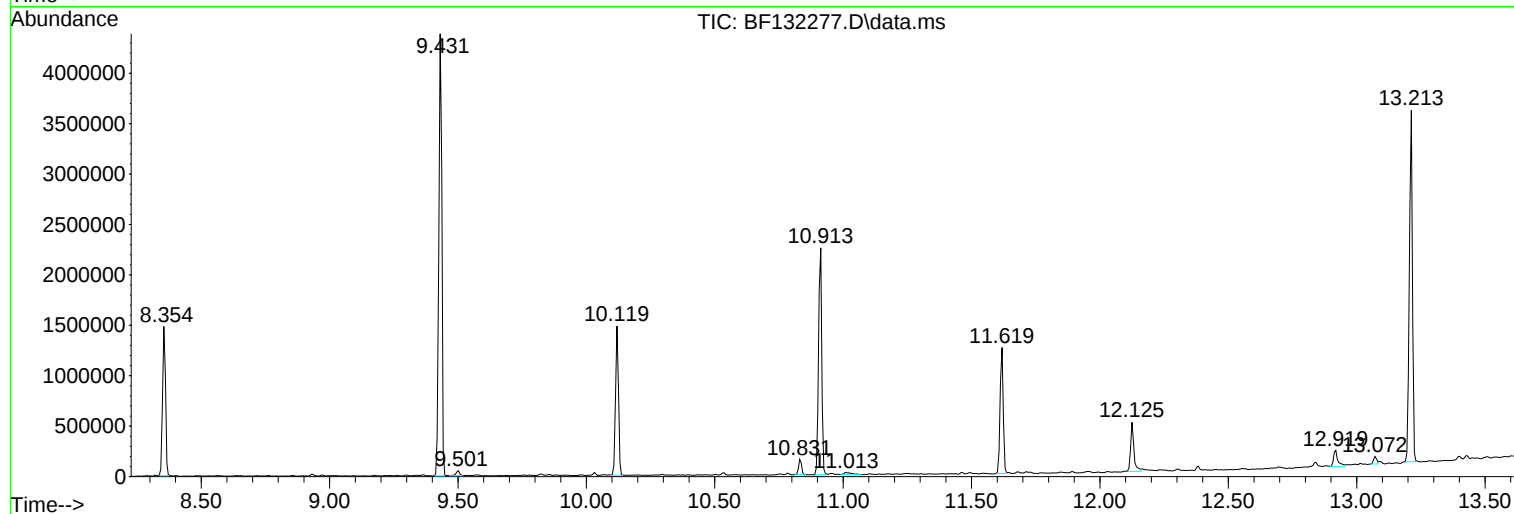
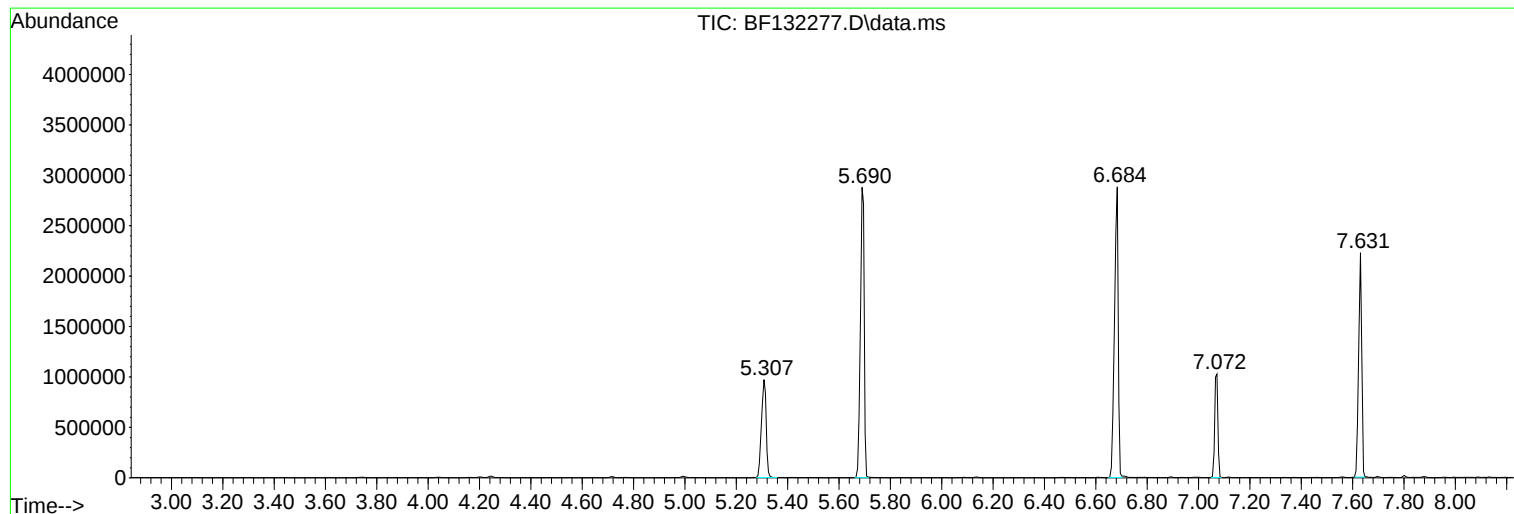
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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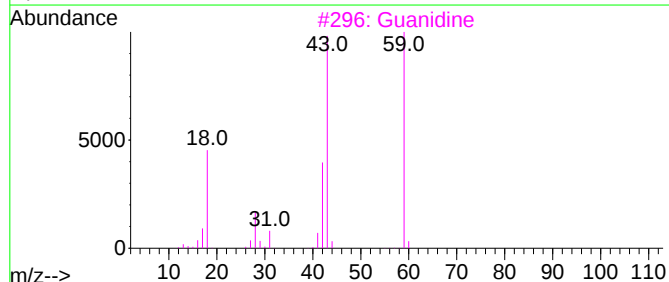
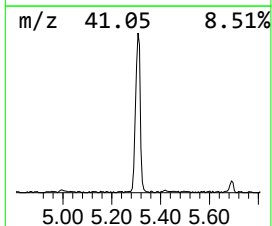
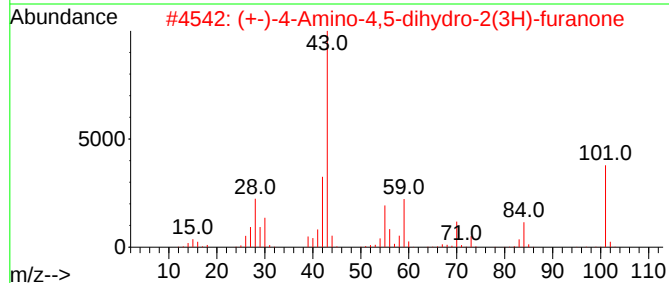
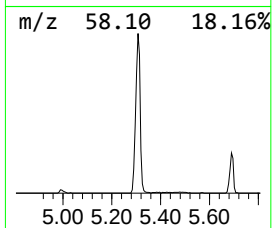
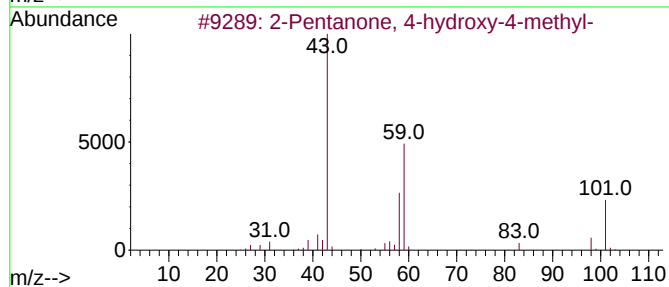
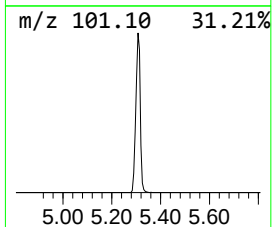
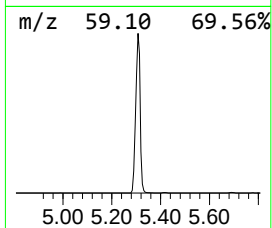
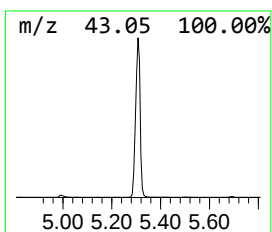
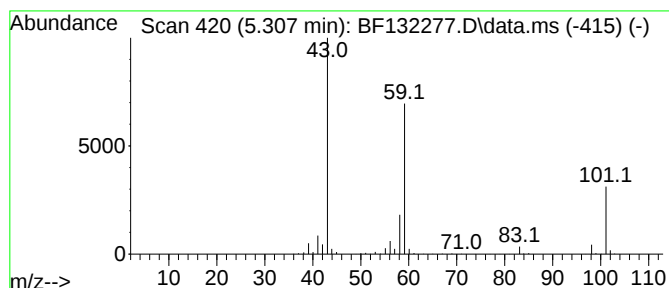
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.307	27.14 ng	1218370	1,4-Dichlorobenzene-d4	7.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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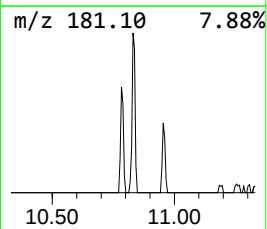
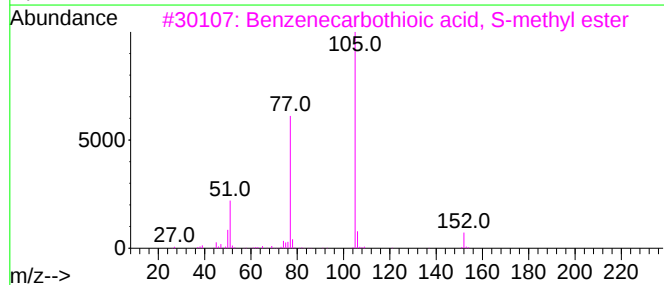
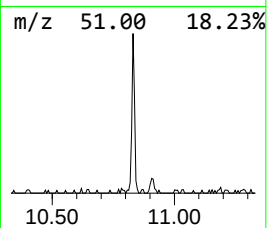
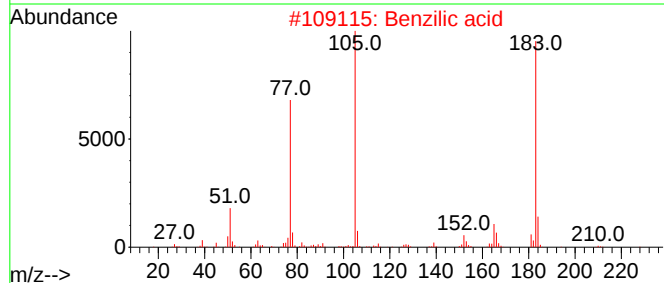
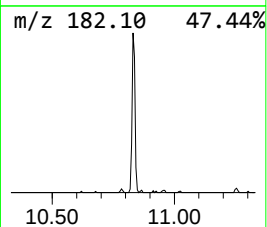
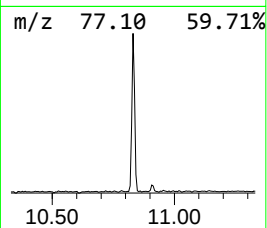
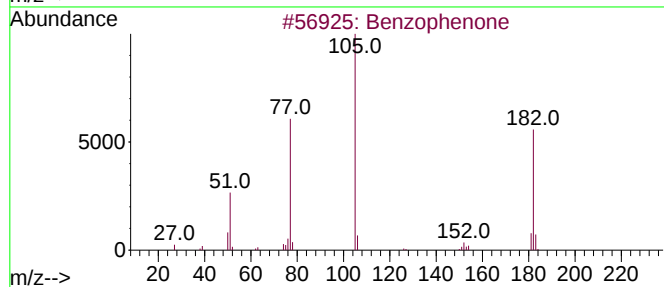
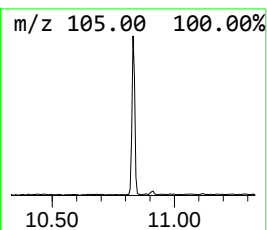
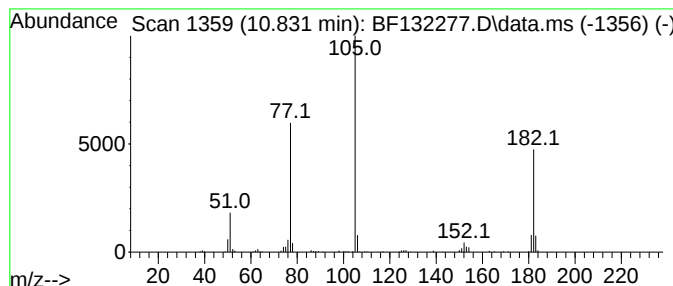
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.831	2.08 ng	122152	Acenaphthene-d10	10.119

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzilic acid	228	C14H12O3	000076-93-7	50
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
4			N-Benzoylimidazole	172	C10H8N2O	010364-94-0	43
5			5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	43



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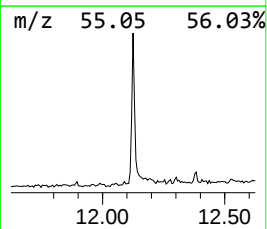
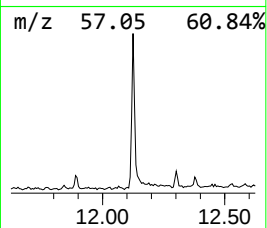
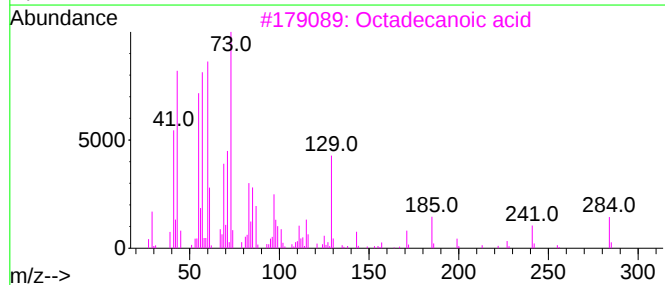
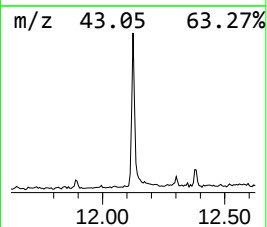
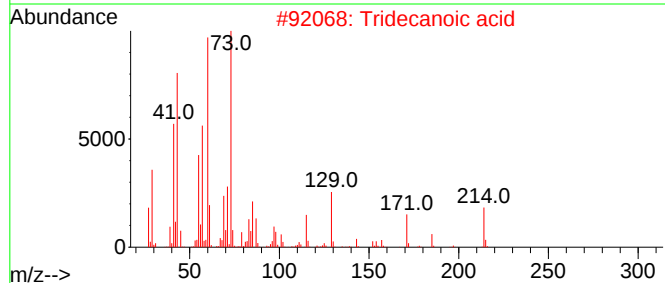
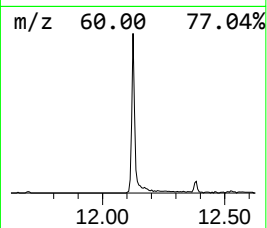
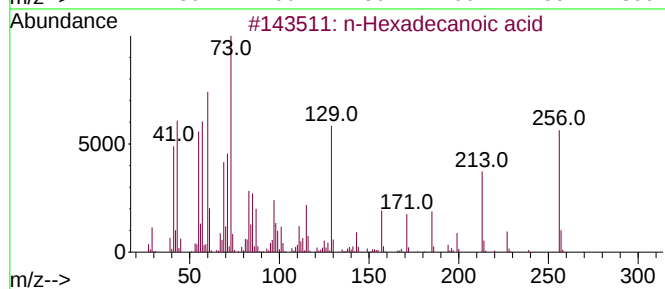
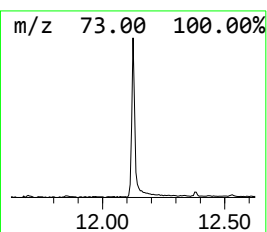
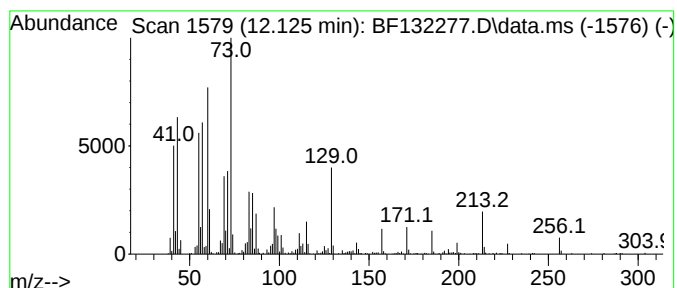
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TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.125	8.35 ng	437968	Phenanthrene-d10		11.619	
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	91
3	Octadecanoic acid		284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	80



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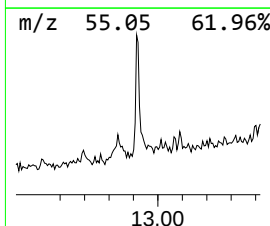
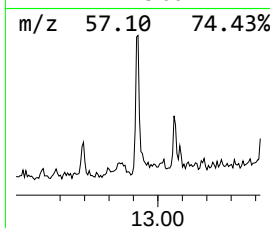
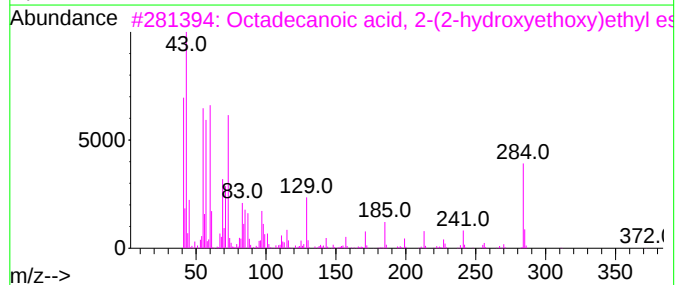
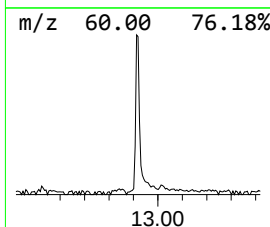
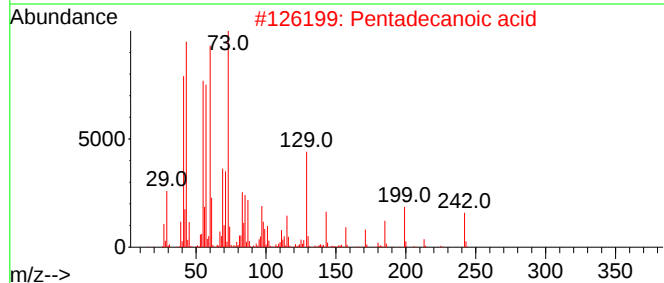
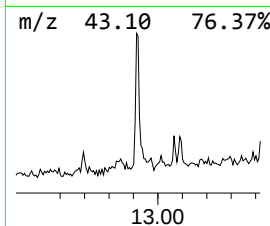
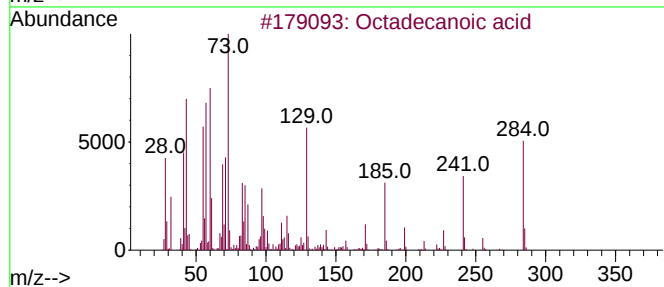
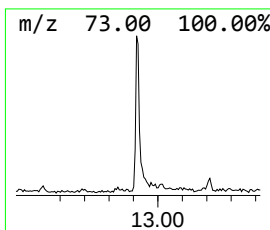
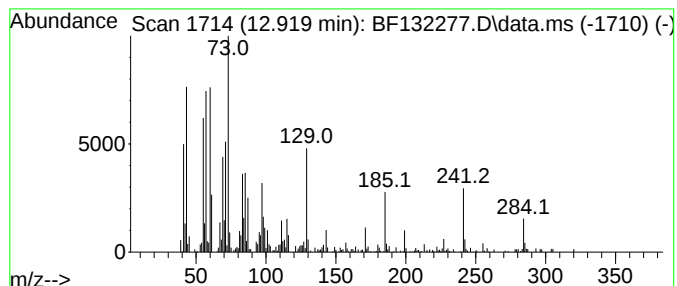
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.919	3.59 ng	188399	Phenanthrene-d10	11.619

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	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50



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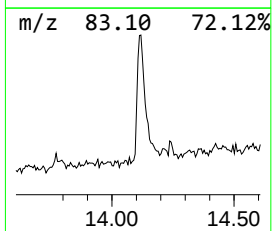
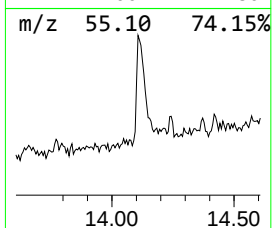
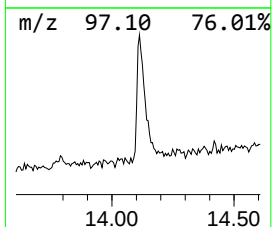
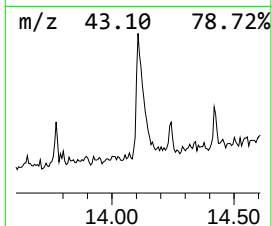
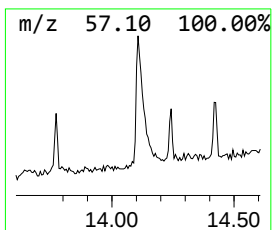
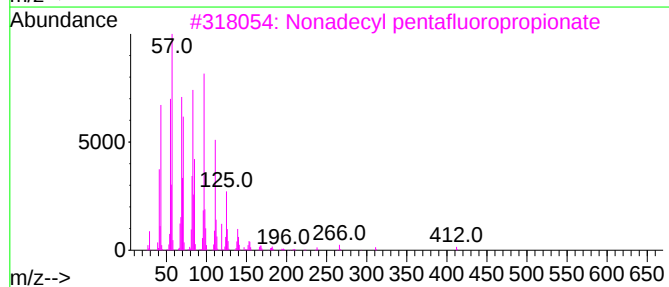
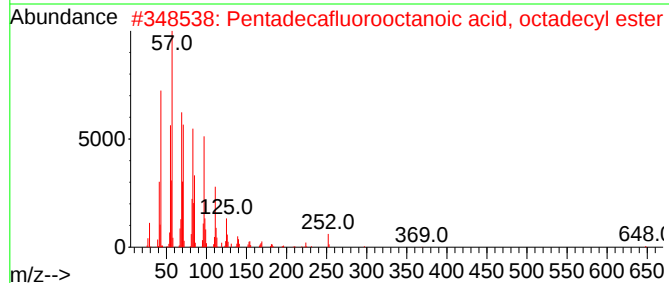
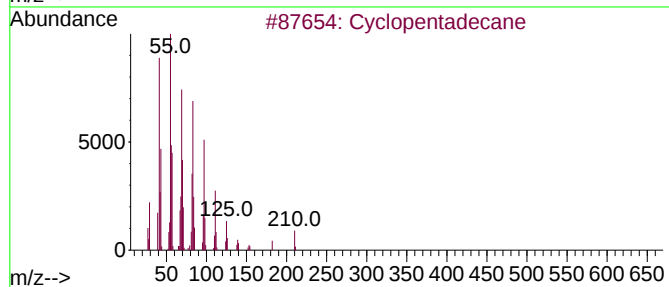
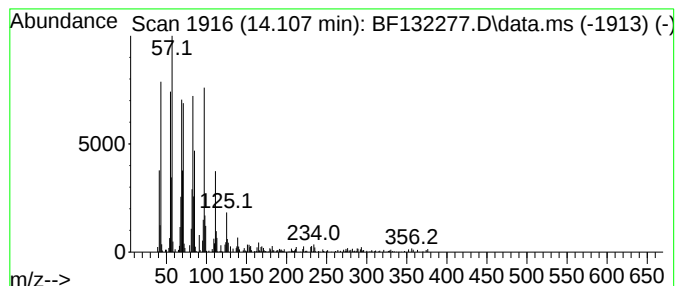
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Peak Number 5 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.107	10.58 ng	436305	Chrysene-d12	14.277

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	95
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.307	27.1	ng	1218370	1	7.072	897733	20.0
Benzophenone	10.831	2.1	ng	122152	3	10.119	1172010	20.0
n-Hexadecanoic ...	12.125	8.3	ng	437968	4	11.619	1048540	20.0
Octadecanoic acid	12.919	3.6	ng	188399	4	11.619	1048540	20.0
Cyclopentadecane	14.107	10.6	ng	436305	5	14.277	824511	20.0