

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
 Data File : BG055688.D
 Acq On : 18 Nov 2022 13:01
 Operator : CG/JU
 Sample : N5607-07
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-38

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_G\Methods\8270-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055688.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.302	337	343	353	rBV	73626	121265	7.26%	1.187%
2	5.784	417	425	440	rBV	505654	874923	52.41%	8.564%
3	7.394	690	699	711	rBV	523701	923833	55.34%	9.043%
4	8.252	834	845	851	rBV	153077	269653	16.15%	2.639%
5	9.421	1036	1044	1055	rBV	312714	558850	33.48%	5.470%
6	10.825	1277	1283	1293	rBV	40432	82540	4.94%	0.808%
7	11.078	1319	1326	1334	rVB	214910	387237	23.20%	3.790%
8	13.499	1729	1738	1747	rBV	850811	1303164	78.07%	12.755%
9	14.509	1902	1910	1920	rBV4	7675	18590	1.11%	0.182%
10	14.874	1965	1972	1979	rBV	339505	530539	31.78%	5.193%
11	16.354	2218	2224	2236	rBV	607218	961645	57.61%	9.413%
12	17.494	2414	2418	2427	rBV5	11950	17288	1.04%	0.169%
13	17.612	2431	2438	2444	rBV	407008	615441	36.87%	6.024%
14	18.252	2543	2547	2552	rVB	21883	28853	1.73%	0.282%
15	18.481	2581	2586	2596	rBV2	74502	229910	13.77%	2.250%
16	19.409	2741	2744	2747	rVB3	18129	20082	1.20%	0.197%
17	19.739	2795	2800	2818	rVB2	130992	339702	20.35%	3.325%
18	20.203	2873	2879	2884	rVB	1226550	1669319	100.00%	16.339%
19	21.525	3100	3104	3114	rVB4	52844	117361	7.03%	1.149%
20	21.912	3164	3170	3176	rVB	371936	610949	36.60%	5.980%
21	25.326	3744	3751	3762	rVB2	177867	535383	32.07%	5.240%

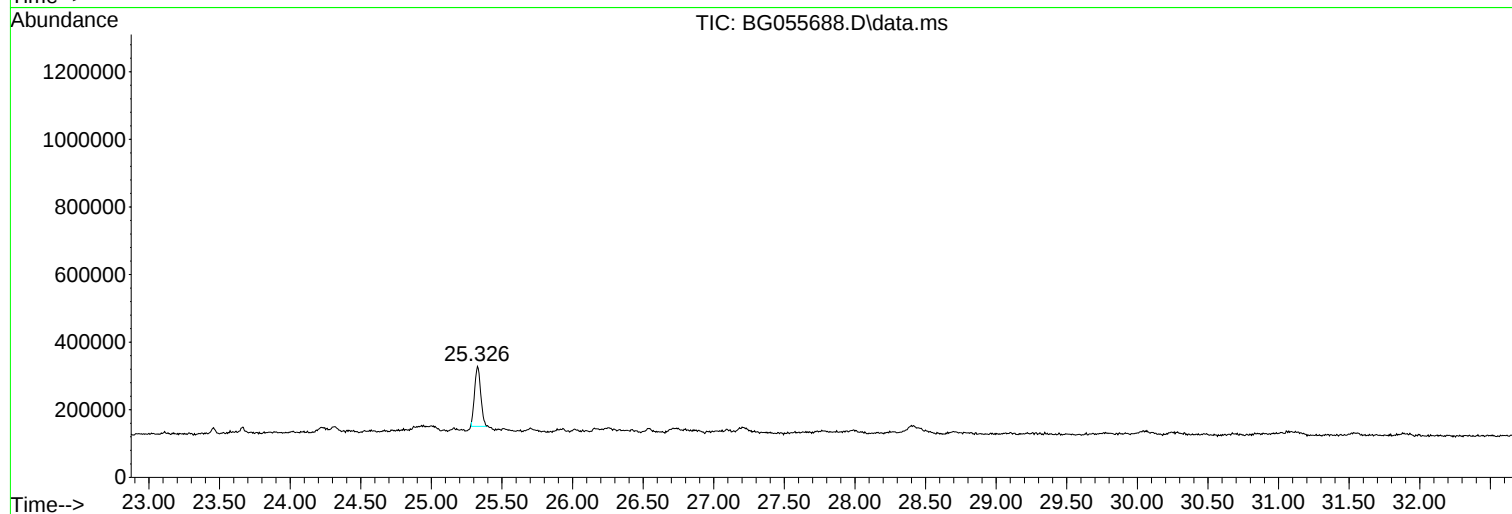
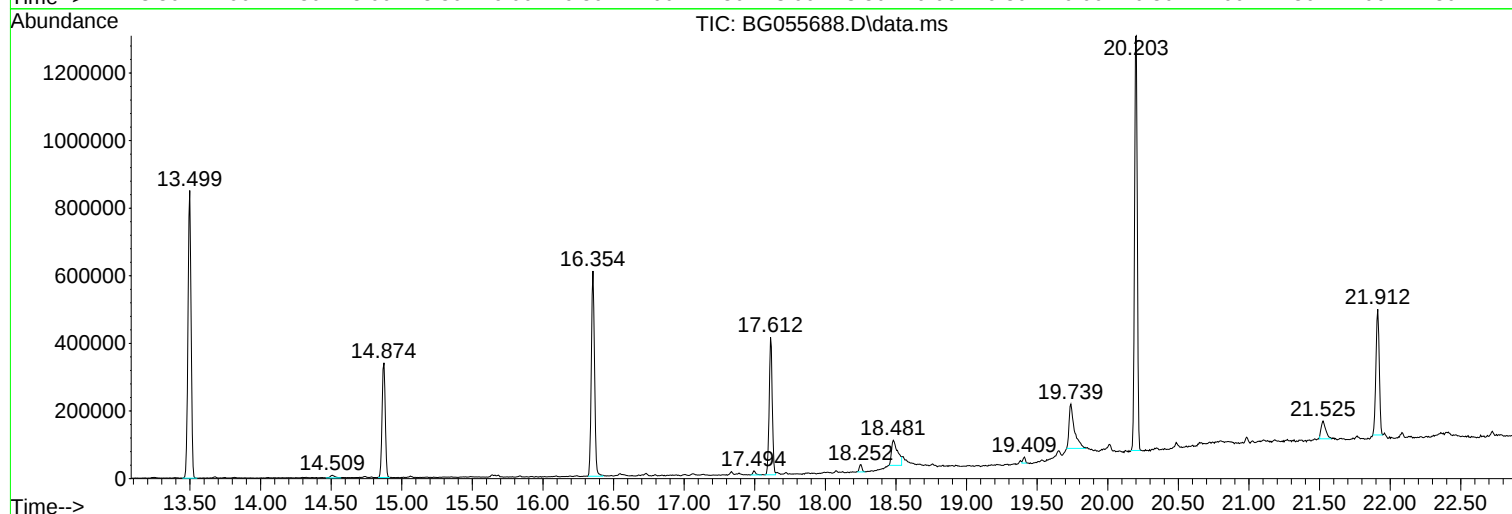
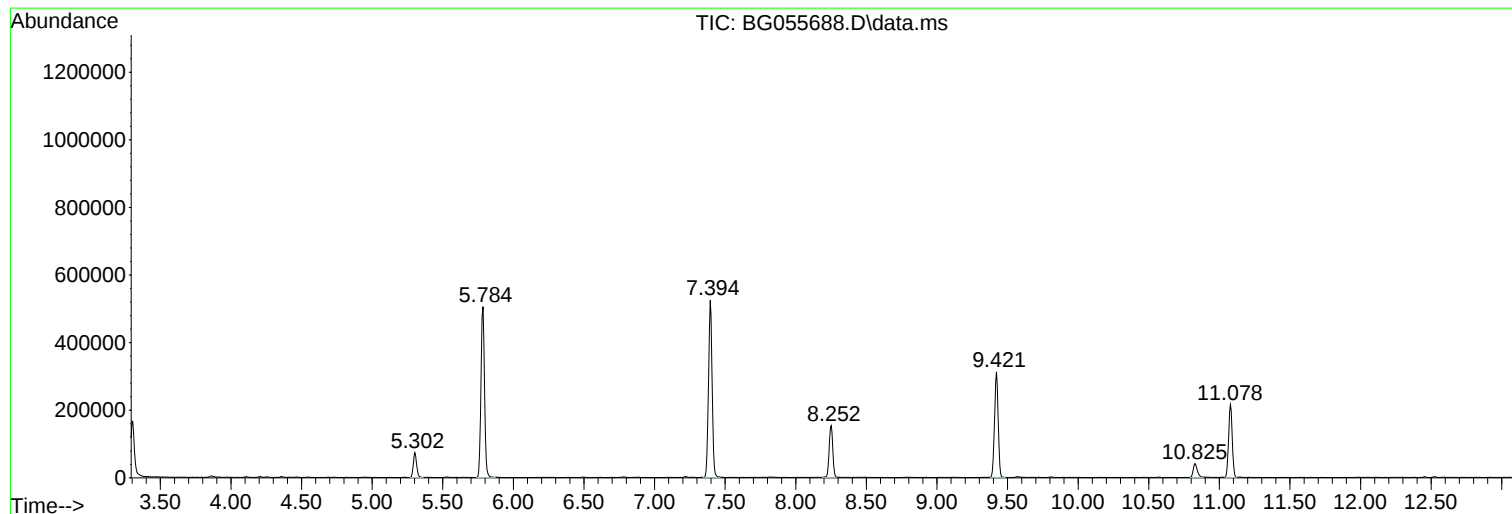
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG055688.D
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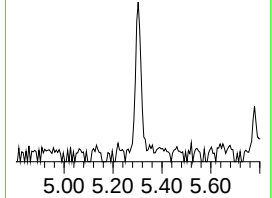
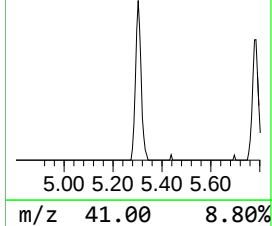
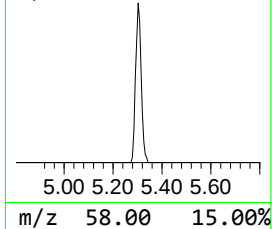
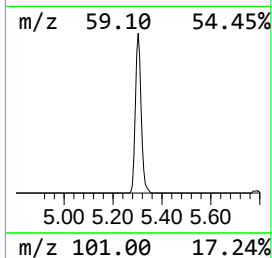
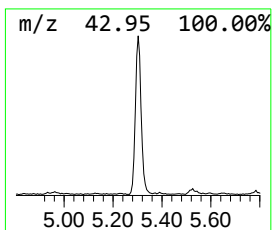
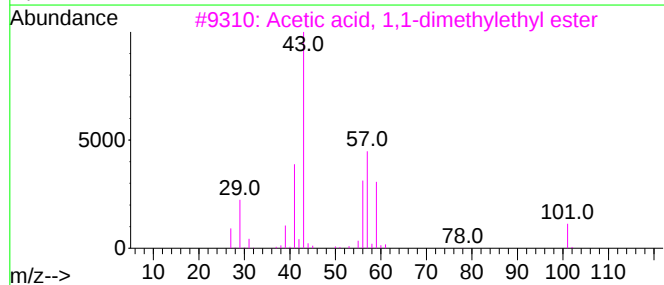
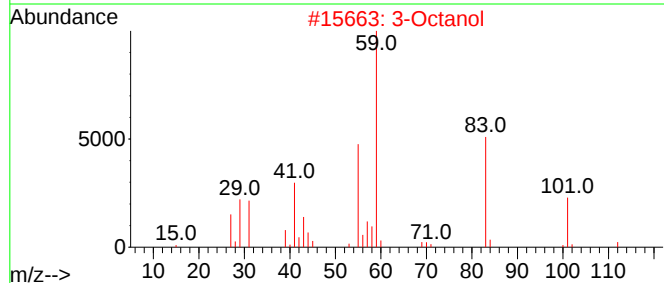
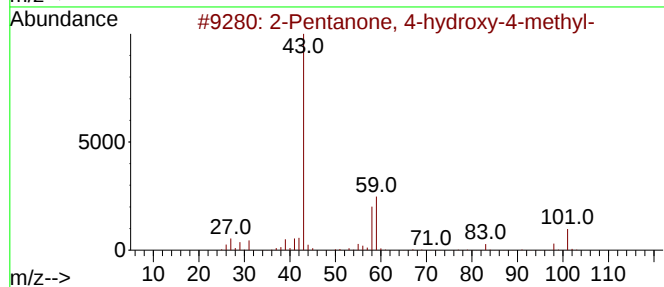
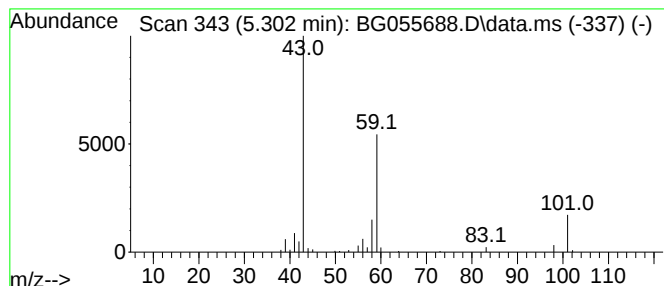
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.302	8.99 ng	121265	1,4-Dichlorobenzene-d4	8.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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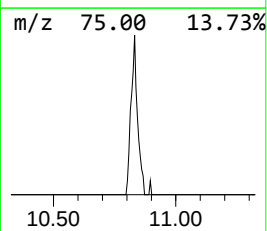
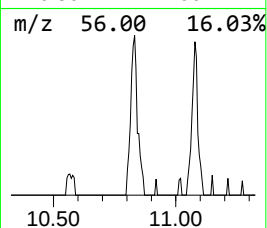
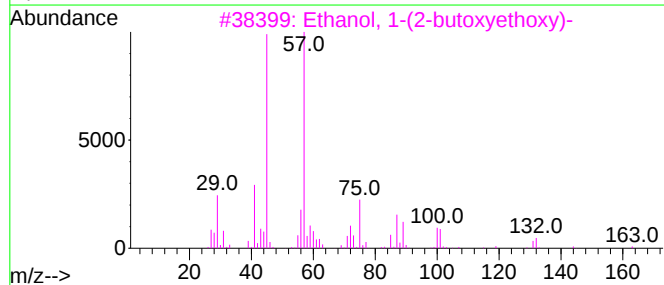
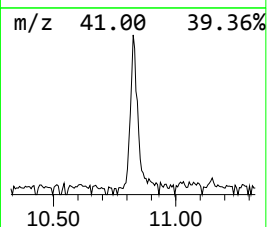
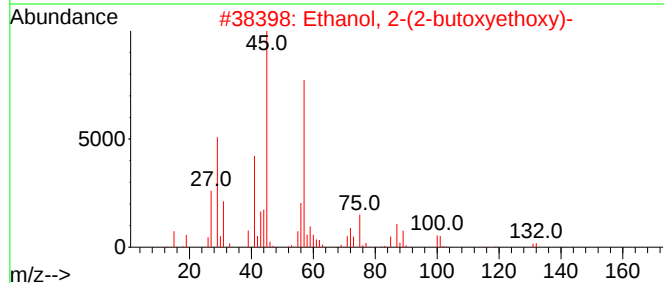
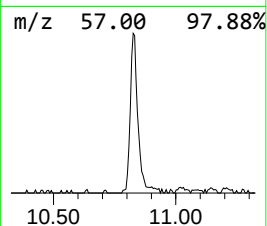
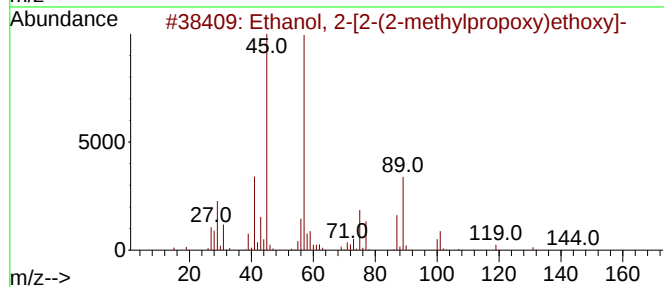
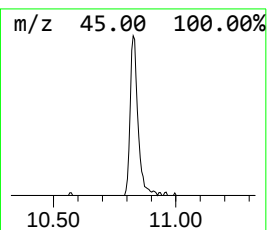
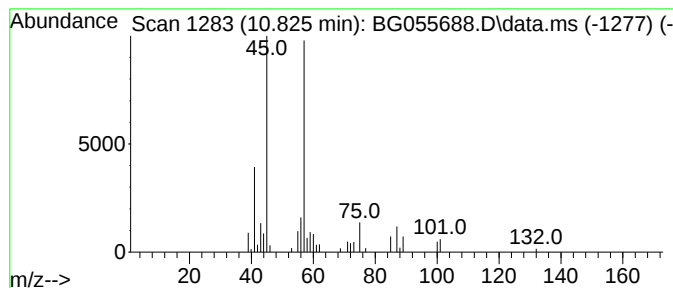
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-[2-(2-methylprop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.825	4.26 ng	82540	Naphthalene-d8	11.078

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	74
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47



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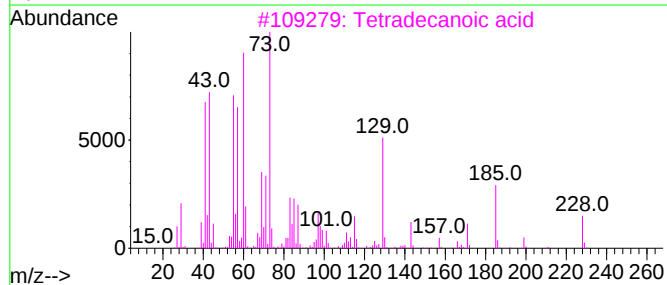
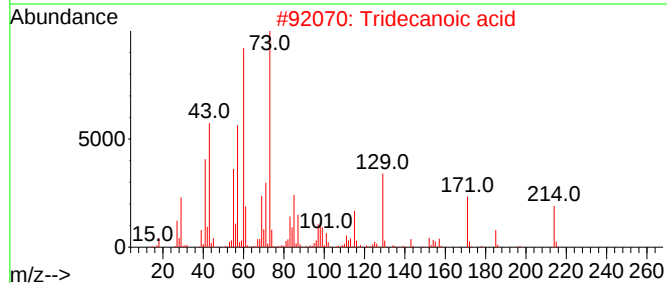
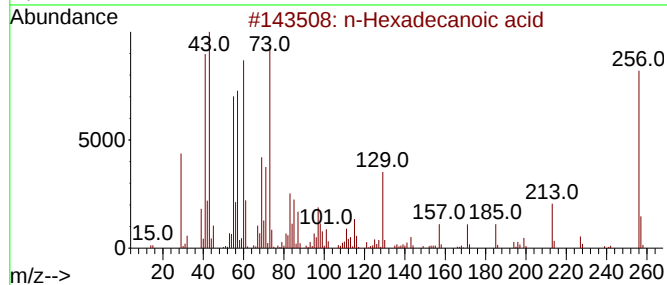
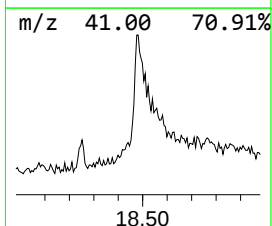
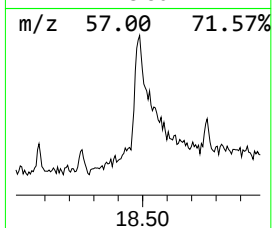
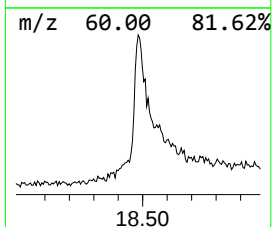
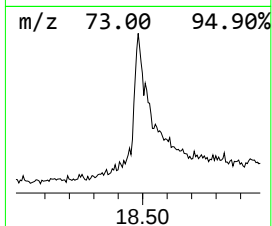
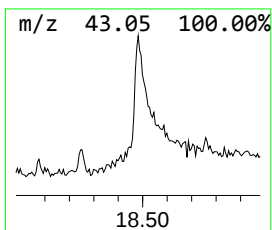
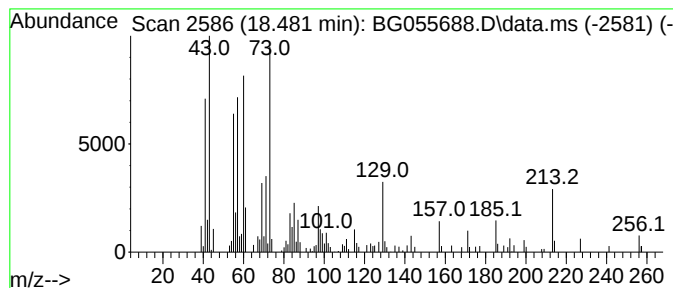
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.481	7.47 ng	229910	Phenanthrene-d10	17.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	70



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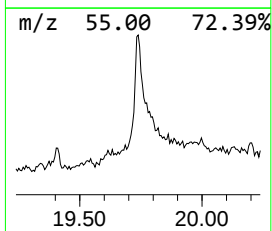
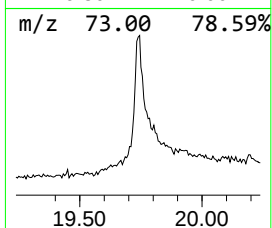
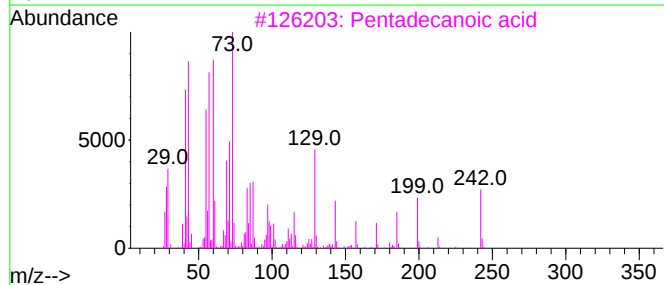
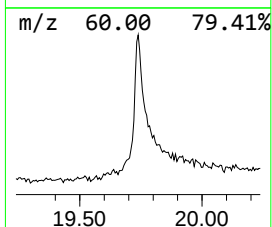
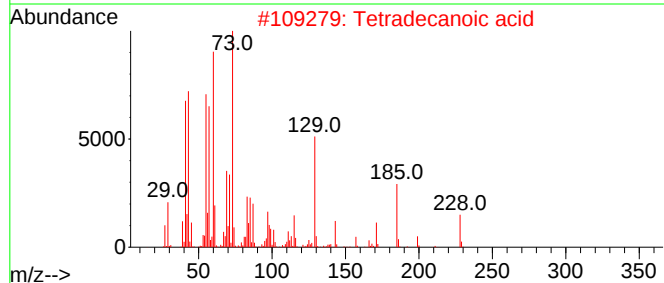
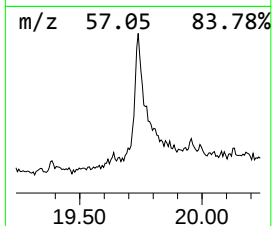
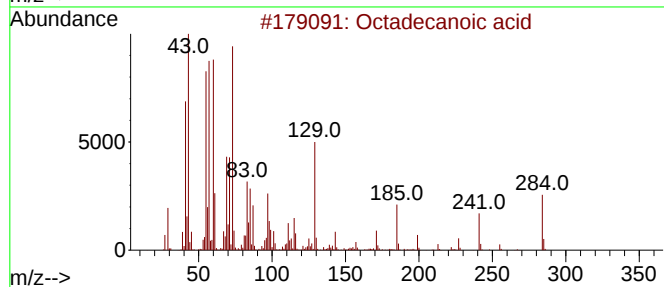
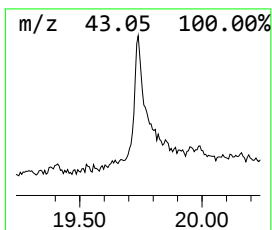
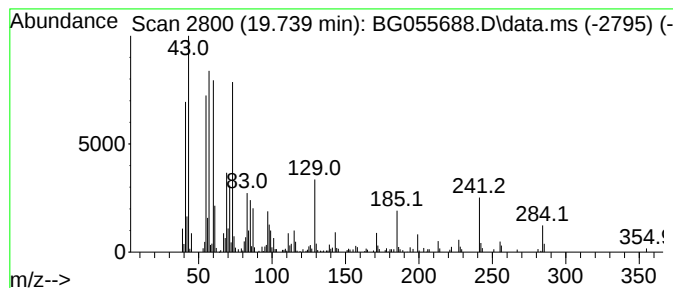
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.738	11.04 ng	339702	Phenanthrene-d10	17.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	78
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	74



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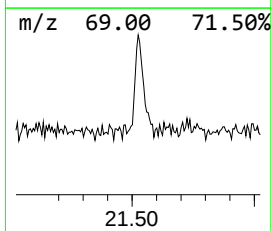
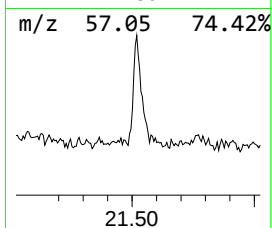
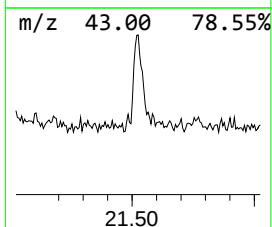
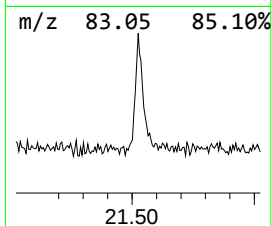
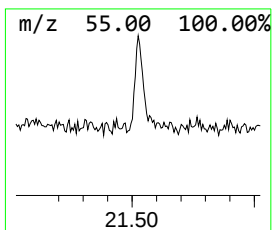
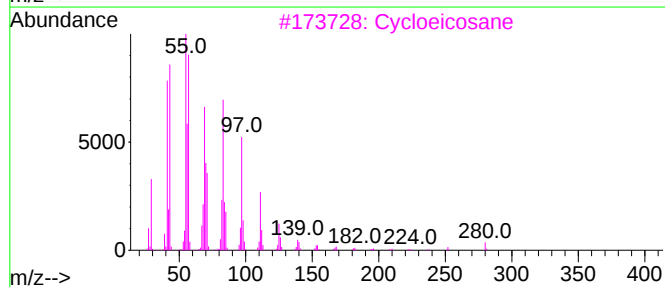
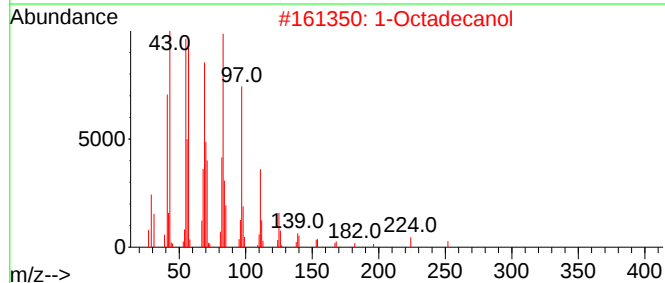
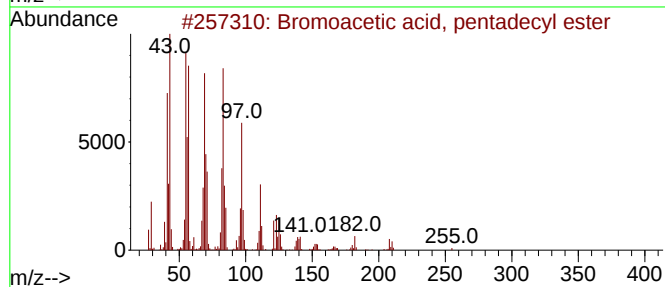
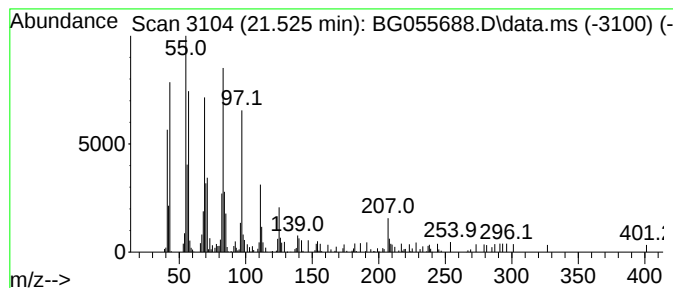
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Bromoacetic acid, pentadecy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.525	3.84 ng	117361	Chrysene-d12	21.912

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87
2		1-Octadecanol	270	C18H38O	000112-92-5	87
3		Cycloeicosane	280	C20H40	000296-56-0	87
4		1-Heptadecene	238	C17H34	006765-39-5	86
5		E-14-Hexadecenal	238	C16H30O	330207-53-9	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.302	9.0	ng	121265	1	8.252	269653	20.0
Ethanol, 2-[2-(...	10.825	4.3	ng	82540	2	11.078	387237	20.0
n-Hexadecanoic ...	18.481	7.5	ng	229910	4	17.612	615441	20.0
Octadecanoic acid	19.738	11.0	ng	339702	4	17.612	615441	20.0
Bromoacetic aci...	21.525	3.8	ng	117361	5	21.912	610949	20.0