

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
 Data File : BM039284.D
 Acq On : 03 Apr 2023 18:13
 Operator : CG/JU
 Sample : 02161-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

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_M\Methods\8270-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039284.D\data.ms

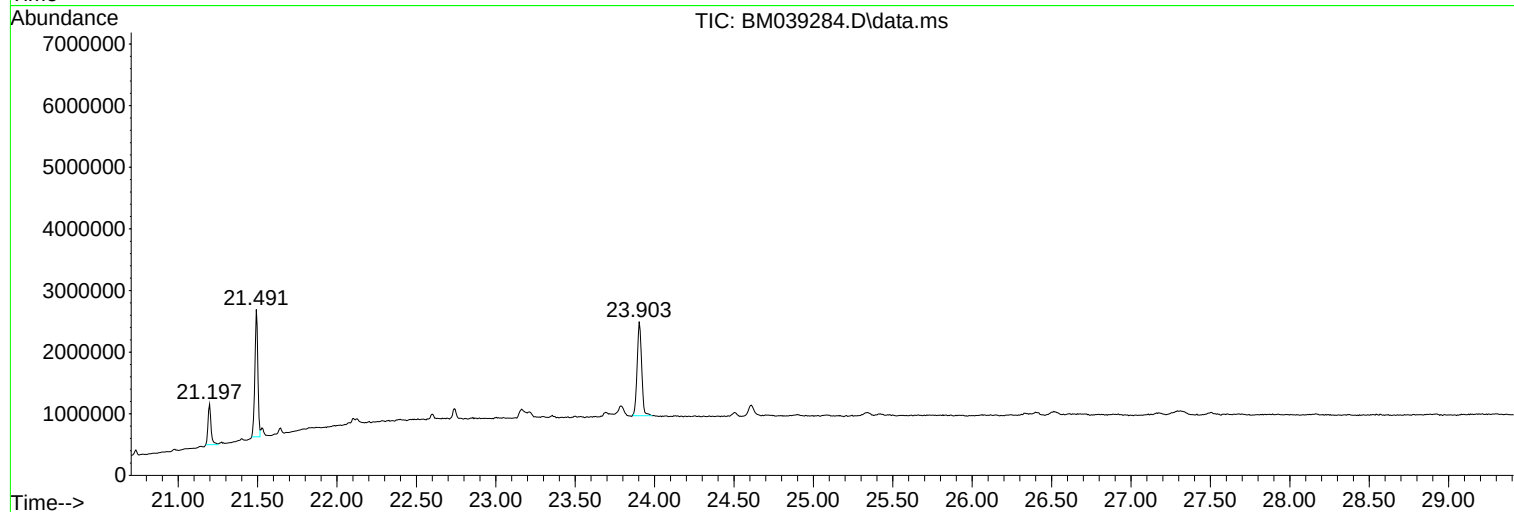
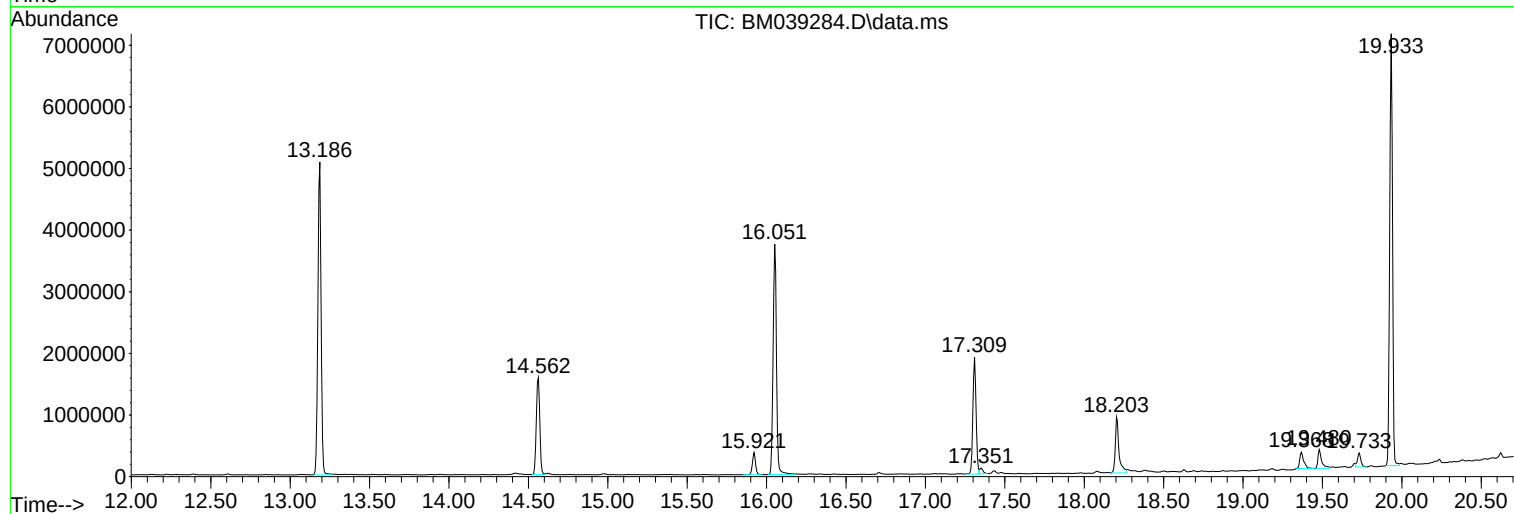
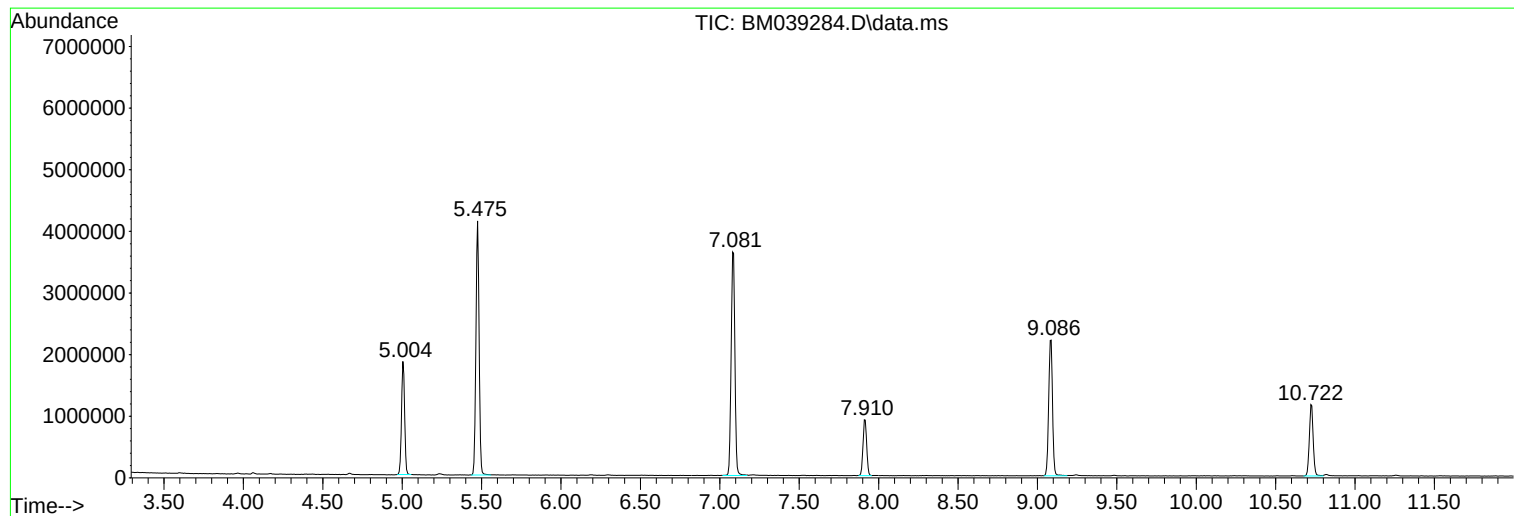
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	286	292	301	rVB	1837814	2488482	29.21%	4.331%
2	5.475	365	372	386	rBV	4124630	5826431	68.40%	10.141%
3	7.081	634	645	660	rBV	3626953	5836905	68.52%	10.159%
4	7.910	780	786	794	rVB	907000	1453028	17.06%	2.529%
5	9.086	978	986	1003	rBV	2201033	3704510	43.49%	6.448%
6	10.722	1256	1264	1277	rBV	1158648	1960055	23.01%	3.411%
7	13.186	1676	1683	1696	rBV	5076794	7189879	84.41%	12.514%
8	14.562	1910	1917	1924	rBV	1575152	2361128	27.72%	4.109%
9	15.921	2136	2148	2157	rBV	360888	505161	5.93%	0.879%
10	16.051	2163	2170	2192	rBV	3743721	5522755	64.83%	9.612%
11	17.309	2374	2384	2389	rBV	1901136	2628299	30.85%	4.574%
12	17.351	2389	2391	2398	rVV	92012	120489	1.41%	0.210%
13	18.203	2530	2536	2547	rBV	905720	1471280	17.27%	2.561%
14	19.368	2729	2734	2748	rVB	264836	449879	5.28%	0.783%
15	19.480	2749	2753	2764	rBV	303775	497204	5.84%	0.865%
16	19.733	2792	2796	2804	rVB	226435	334992	3.93%	0.583%
17	19.933	2824	2830	2839	rBV	7012275	8518306	100.00%	14.826%
18	21.197	3041	3045	3054	rBV	655568	859399	10.09%	1.496%
19	21.491	3090	3095	3099	rBV	2068916	2731950	32.07%	4.755%
20	23.903	3499	3505	3519	rVB2	1525666	2995627	35.17%	5.214%

Sum of corrected areas: 57455759

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



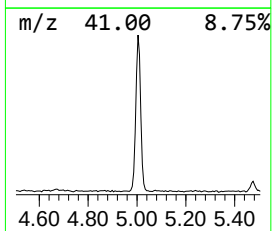
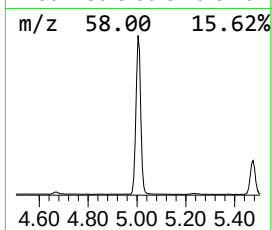
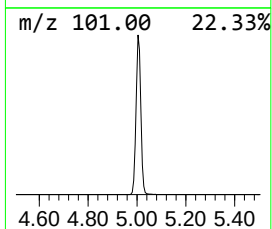
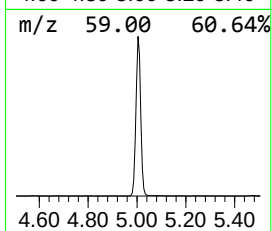
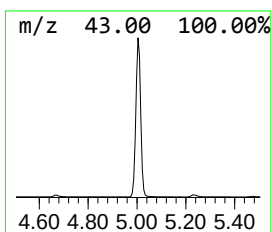
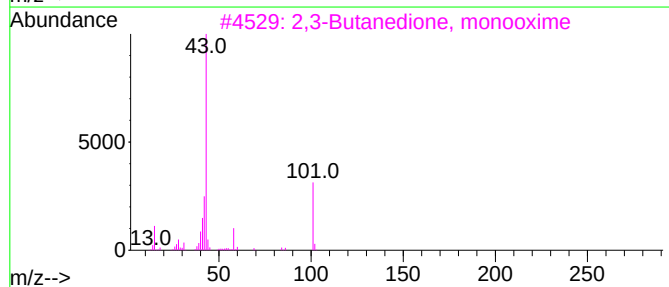
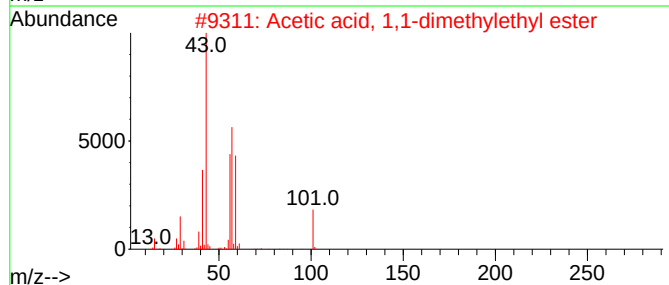
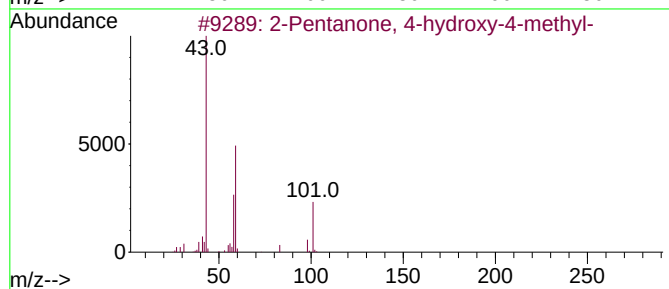
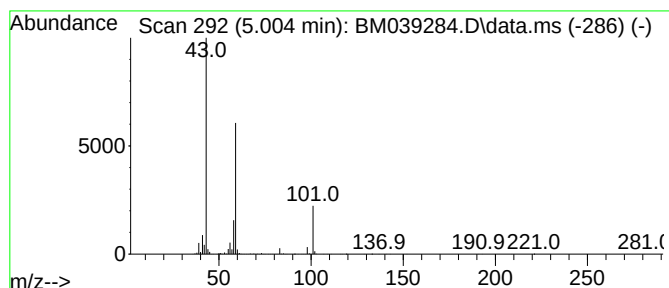
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.004	34.25 ng	2488480	1,4-Dichlorobenzene-d4	7.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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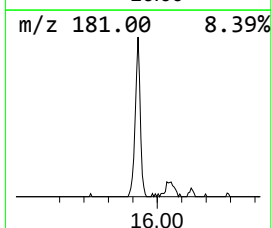
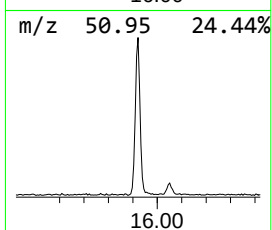
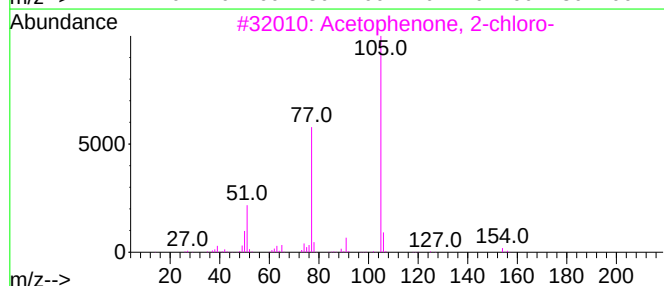
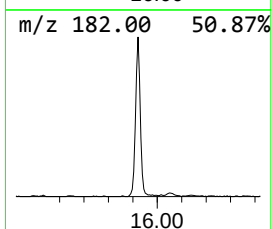
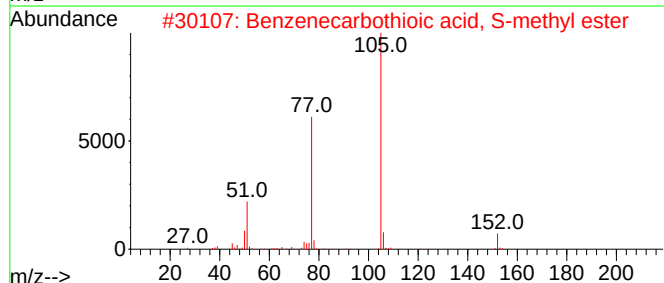
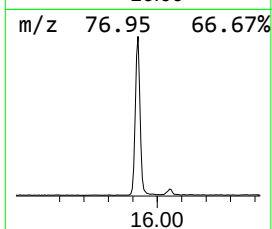
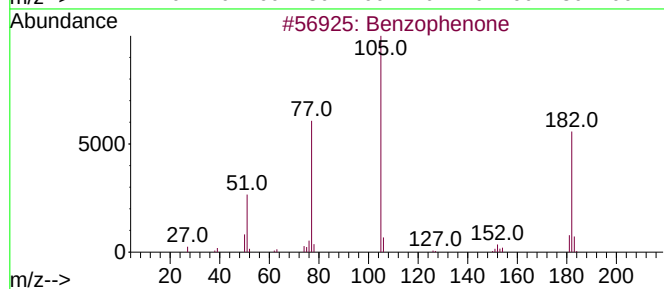
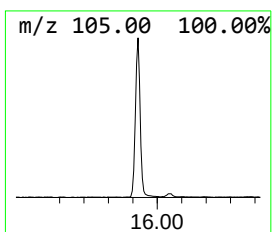
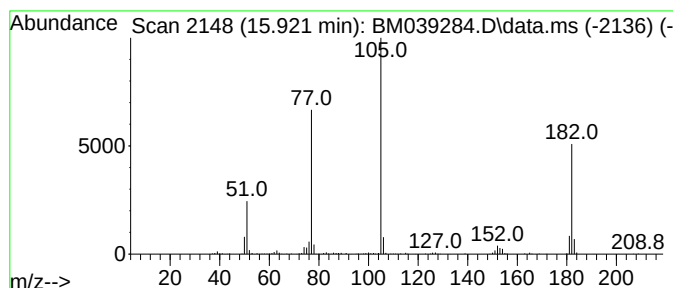
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	4.28 ng	505161	Acenaphthene-d10	14.563

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4		N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
5		acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47



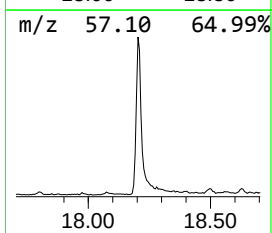
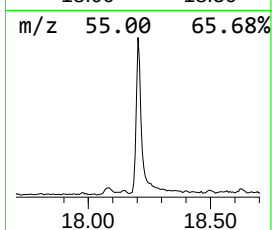
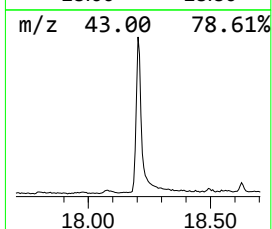
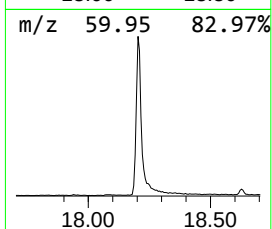
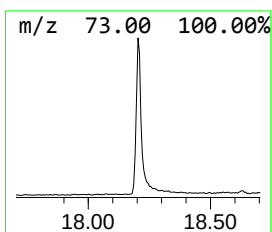
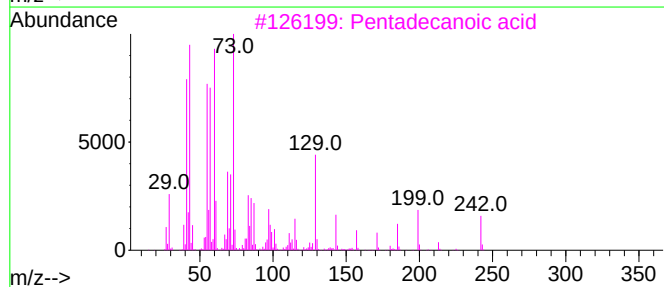
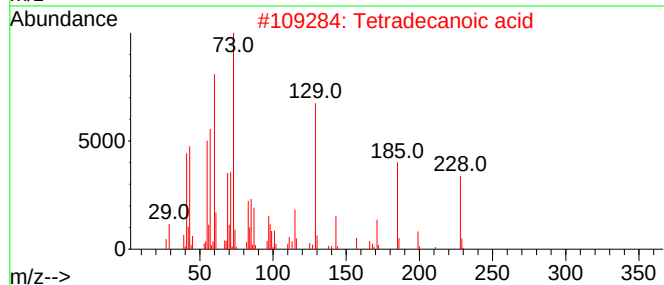
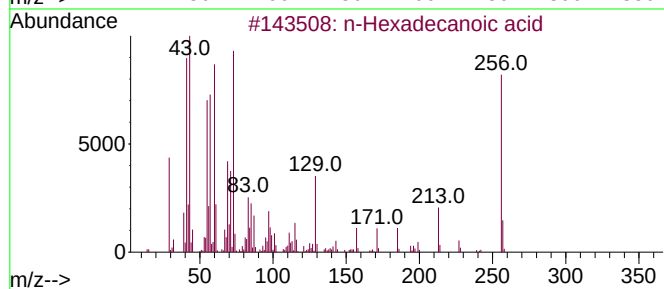
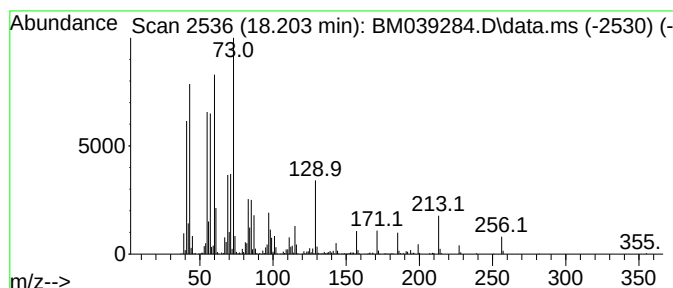
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.203	11.20 ng	1471280	Phenanthrene-d10	17.309	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	81



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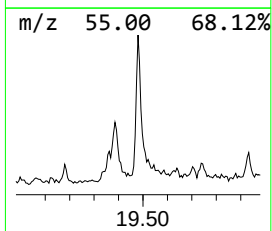
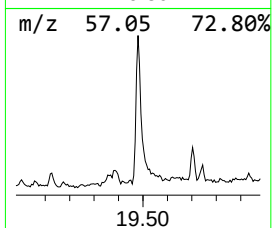
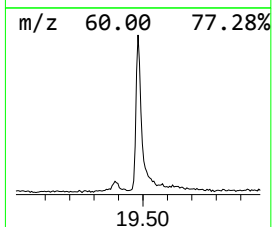
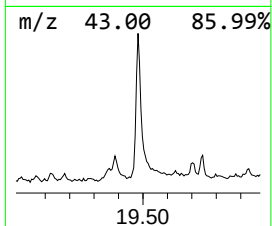
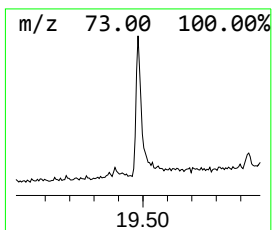
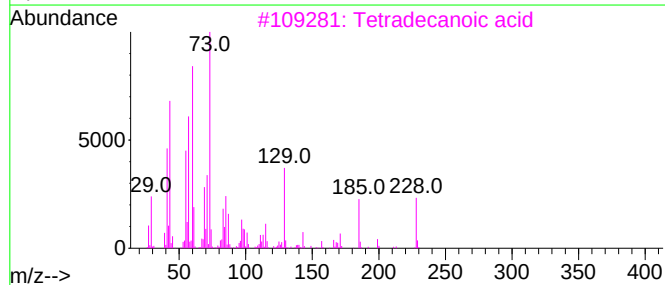
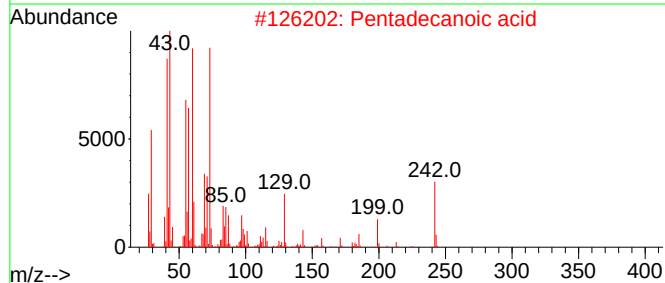
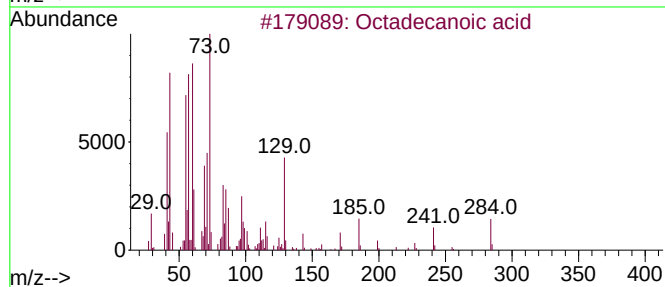
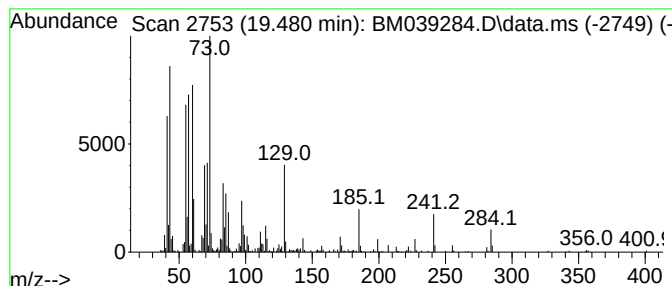
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	3.64 ng	497204	Chrysene-d12	21.491

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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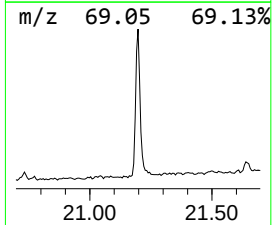
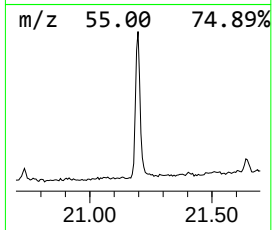
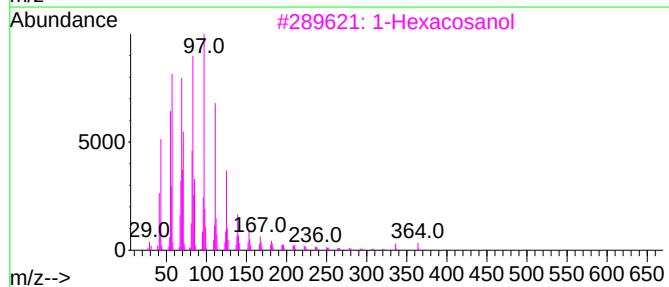
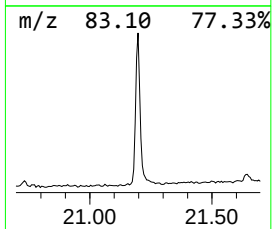
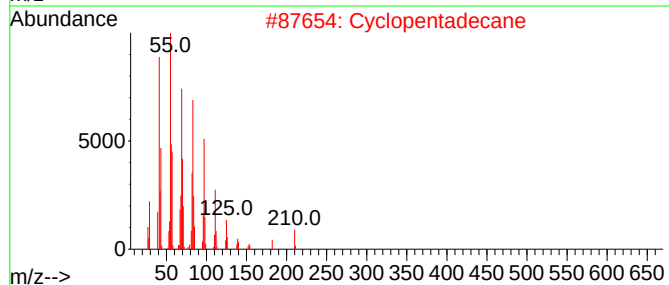
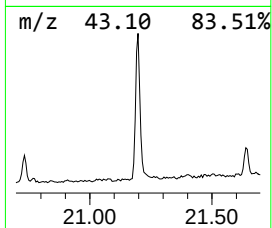
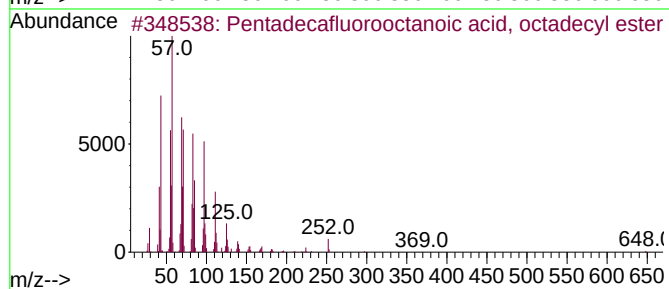
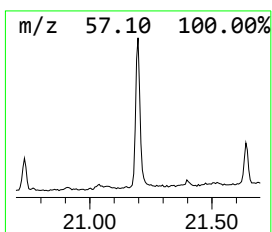
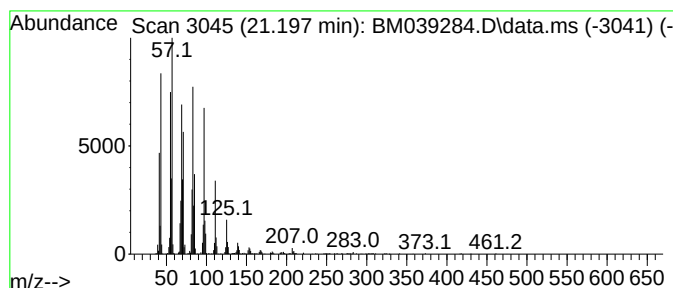
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.197	6.29 ng	859399	Chrysene-d12	21.491

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Cyclopentadecane	210	C15H30	000295-48-7	93
3			1-Hexacosanol	382	C26H54O	000506-52-5	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			1-Hexacosene	364	C26H52	018835-33-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.004	34.3	ng	2488480	1	7.916	1453030	20.0
Benzophenone	15.921	4.3	ng	505161	3	14.563	2361130	20.0
n-Hexadecanoic ...	18.203	11.2	ng	1471280	4	17.309	2628300	20.0
Octadecanoic acid	19.480	3.6	ng	497204	5	21.491	2731950	20.0
Pentadecafluoro...	21.197	6.3	ng	859399	5	21.491	2731950	20.0