

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
 Data File : BM038798.D
 Acq On : 20 Feb 2023 22:04
 Operator : CG/JU
 Sample : 01593-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SED-2

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-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038798.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	294	301	309	rVB	200799	265154	23.95%	2.975%
2	5.428	375	381	391	rBV	628303	852201	76.99%	9.562%
3	7.051	650	657	667	rBV	573727	856800	77.41%	9.614%
4	7.875	790	797	804	rVB	164977	248428	22.44%	2.787%
5	9.051	988	997	1008	rBV	348064	546889	49.41%	6.136%
6	10.686	1268	1275	1289	rVB	199559	319802	28.89%	3.588%
7	13.151	1688	1694	1703	rBV	772900	1043815	94.30%	11.712%
8	14.527	1919	1928	1936	rBV	283200	416302	37.61%	4.671%
9	15.892	2153	2160	2166	rBV	57288	73644	6.65%	0.826%
10	16.021	2176	2182	2194	rBV	813862	1106898	100.00%	12.420%
11	17.280	2390	2396	2407	rBV	338738	460985	41.65%	5.172%
12	18.168	2542	2547	2557	rBV	103423	147992	13.37%	1.661%
13	18.592	2615	2619	2625	rVB4	12132	14626	1.32%	0.164%
14	19.339	2741	2746	2750	rVB	24146	35197	3.18%	0.395%
15	19.445	2760	2764	2771	rBV	61847	82906	7.49%	0.930%
16	19.704	2804	2808	2814	rVV4	22729	34977	3.16%	0.392%
17	19.904	2836	2842	2849	rBV	966019	1106634	99.98%	12.417%
18	21.156	3052	3055	3066	rVB4	52864	73761	6.66%	0.828%
19	21.462	3102	3107	3112	rBV	464218	580414	52.44%	6.512%
20	23.844	3505	3512	3520	rVB2	332764	644916	58.26%	7.236%

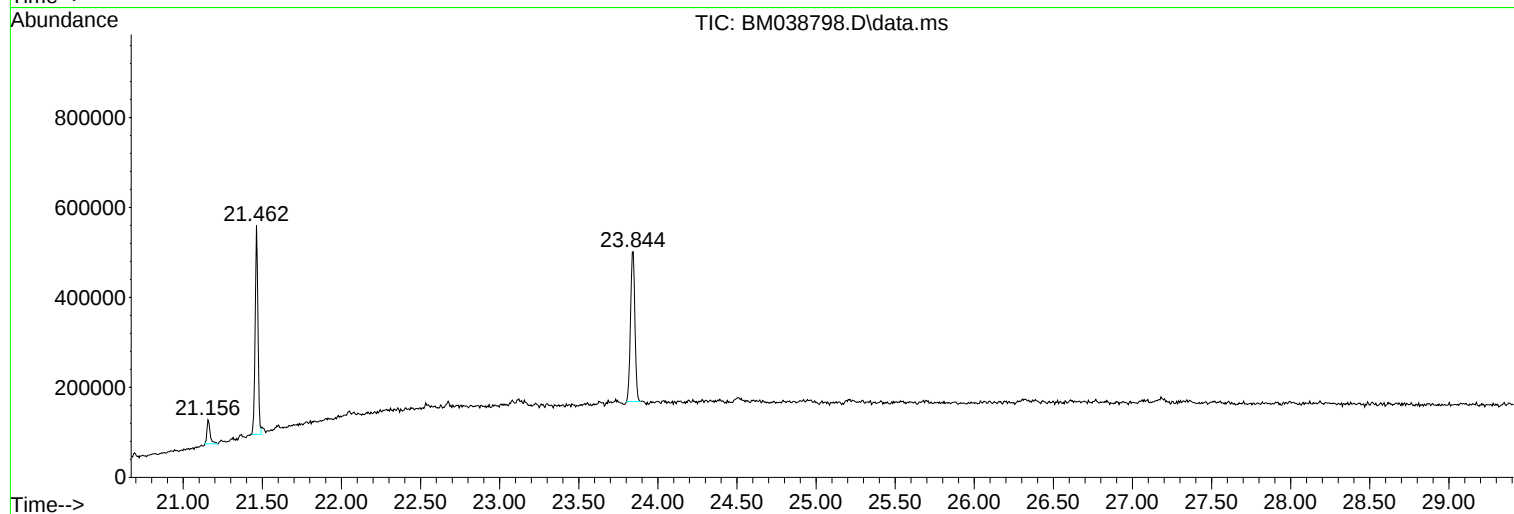
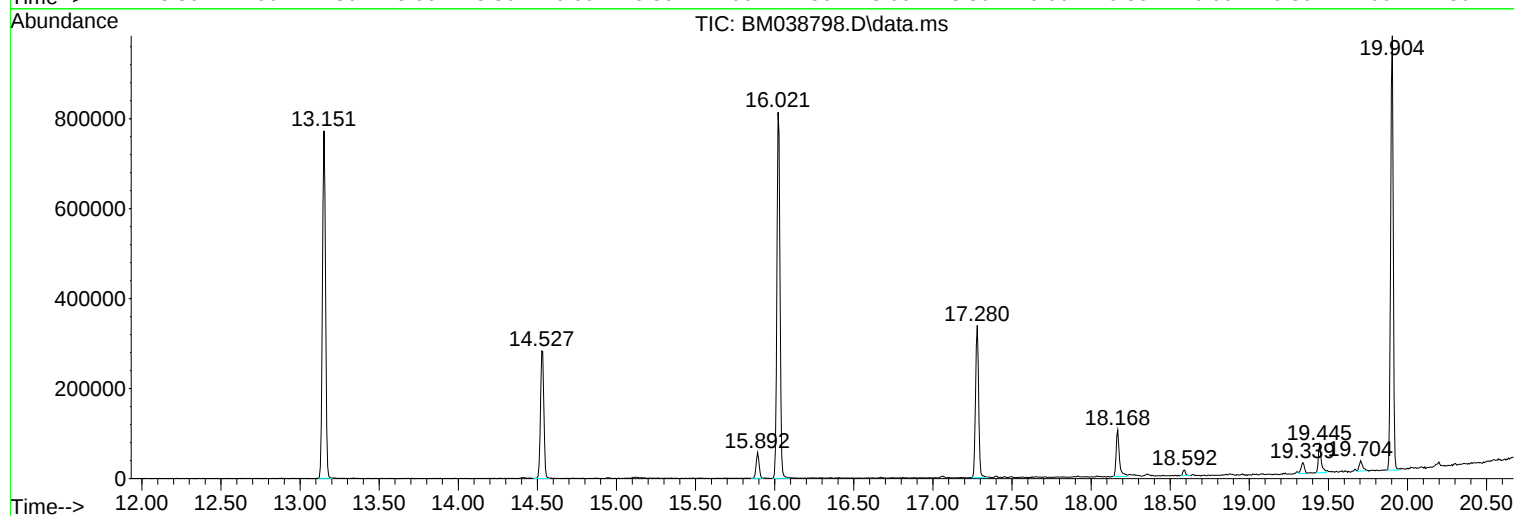
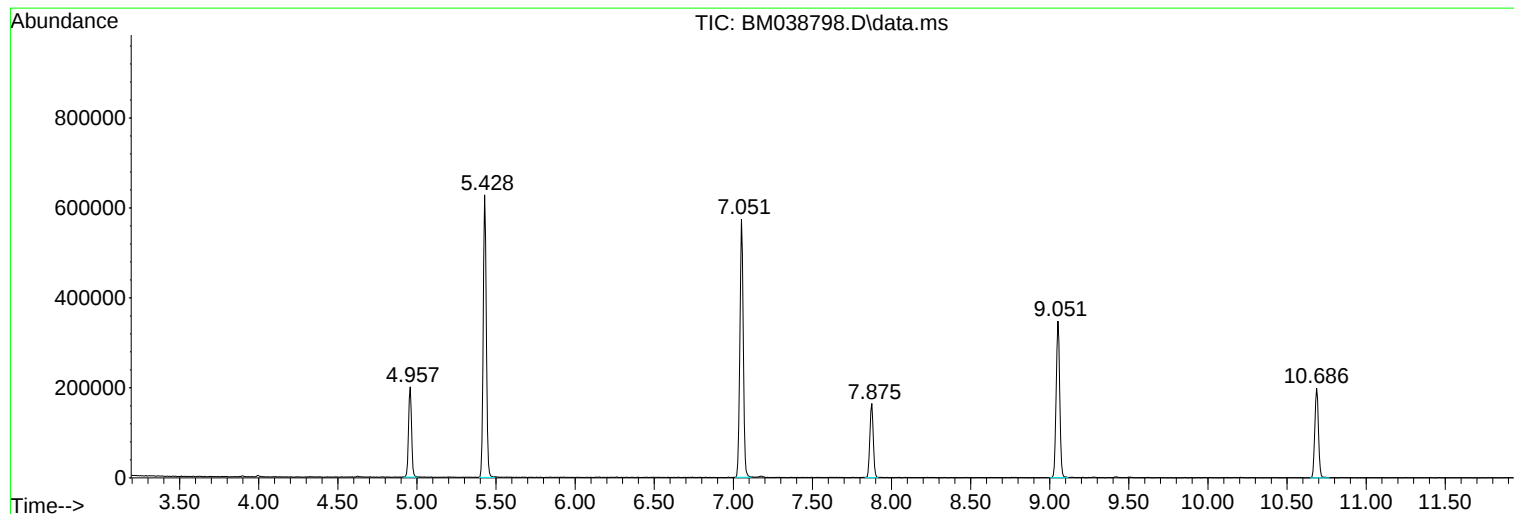
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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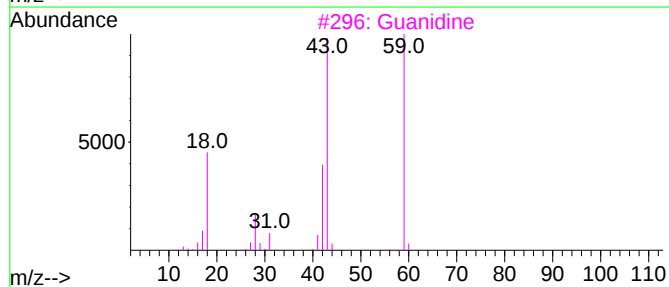
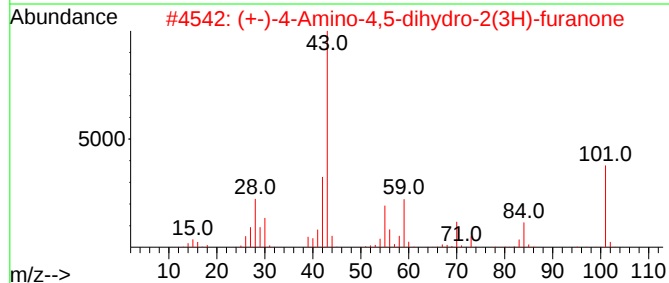
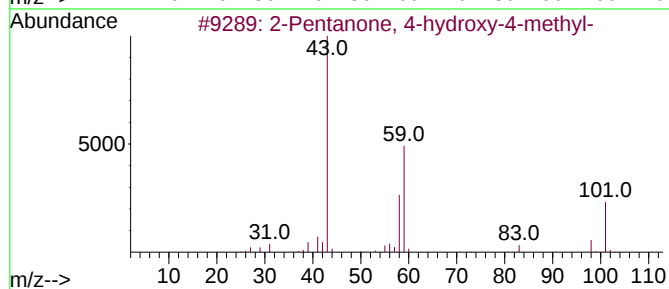
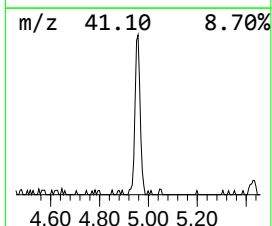
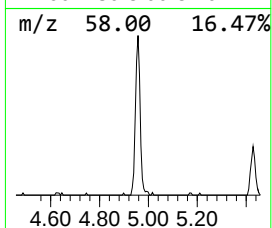
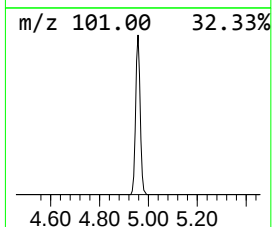
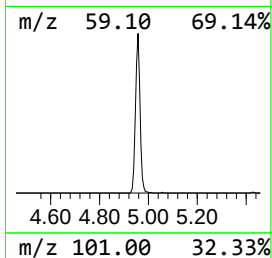
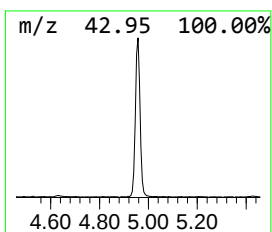
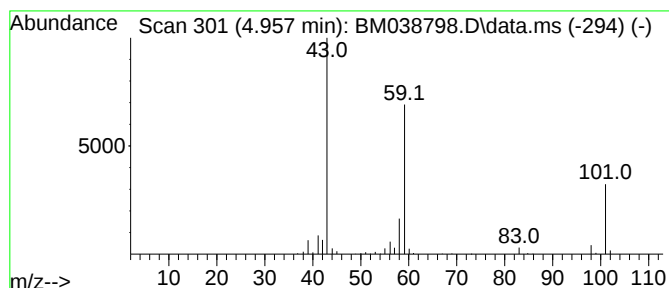
TIC Library : C:\Database\NIST20.L

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.
4.957	21.35 ng	265154	1,4-Dichlorobenzene-d4	7.875

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	43
3		Guanidine	59	CH5N3	000113-00-8	43
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17



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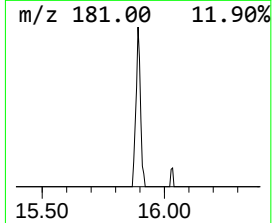
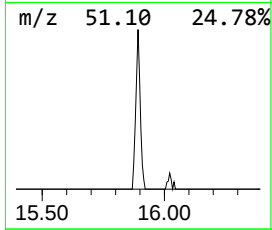
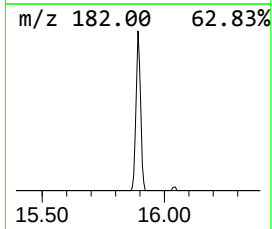
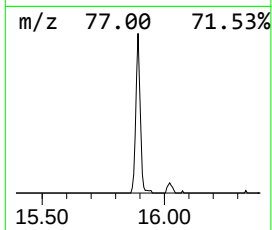
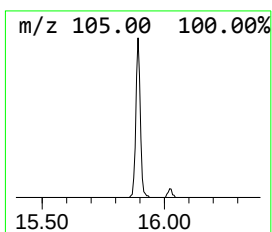
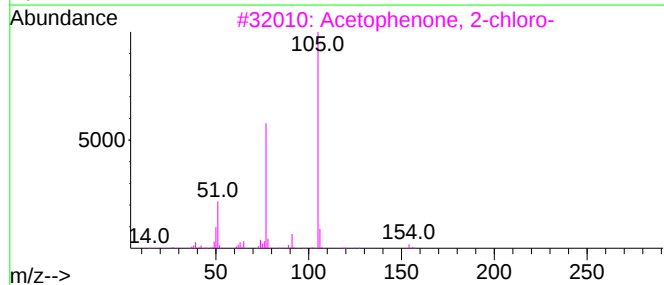
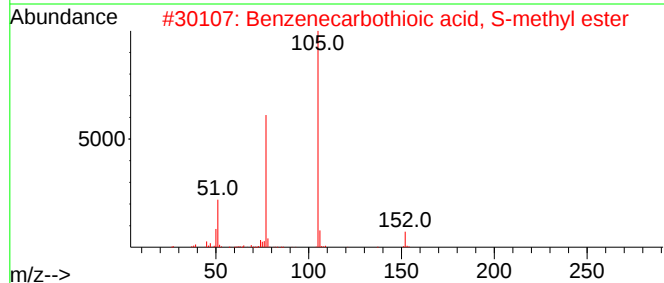
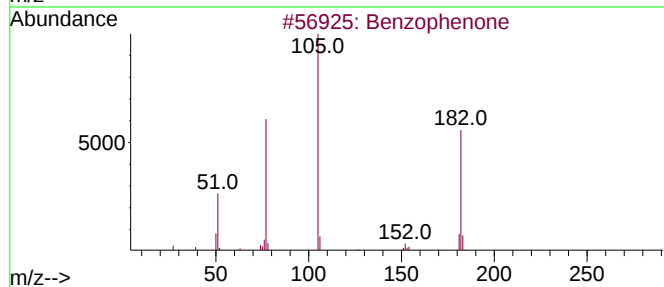
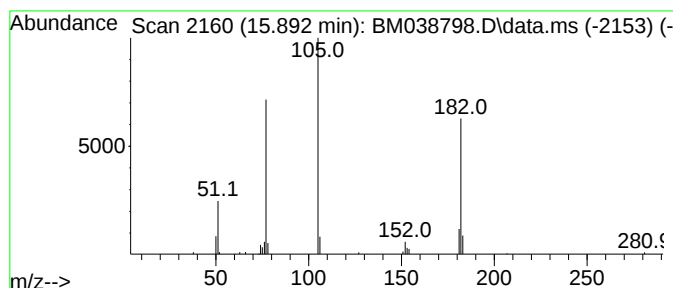
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	3.54 ng	73644	Acenaphthene-d10	14.527

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	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Thiophene, 2,3-dimethyl-4-cyano-...	256	C14H12N2OS	313533-21-0	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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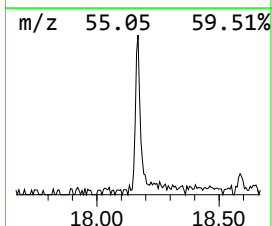
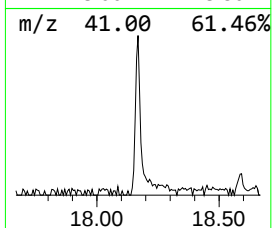
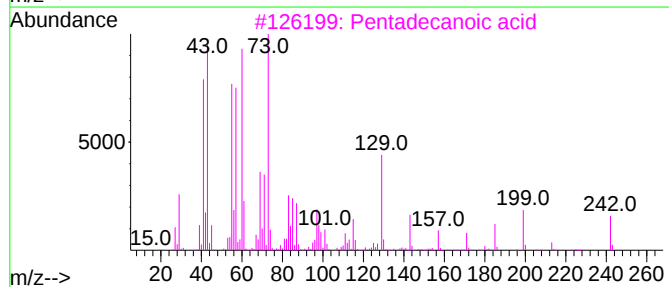
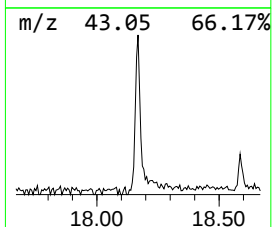
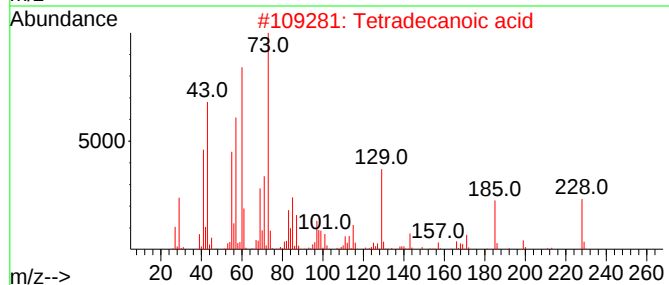
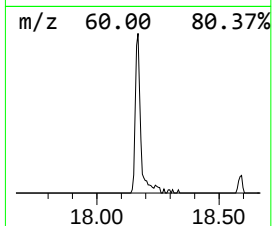
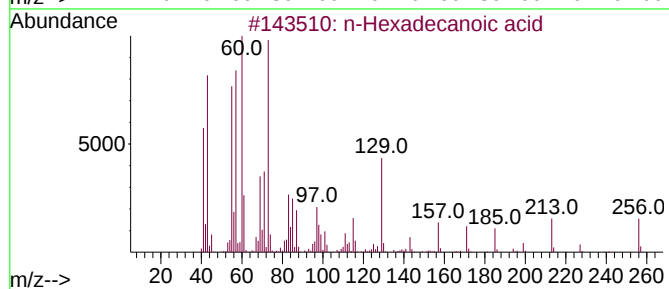
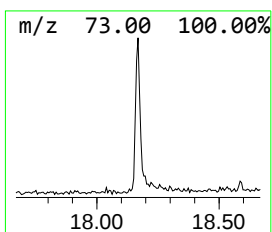
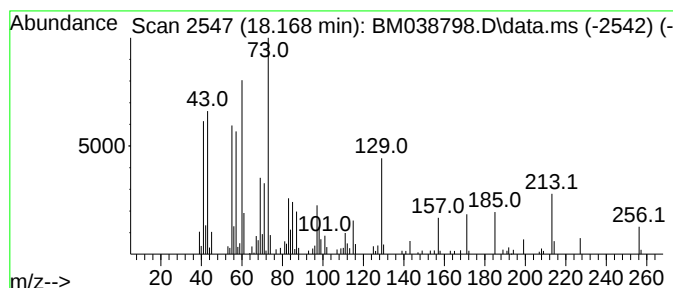
Instrument :
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.168	6.42 ng	147992	Phenanthrene-d10	17.280	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	60
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



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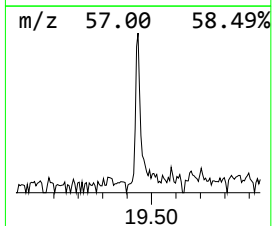
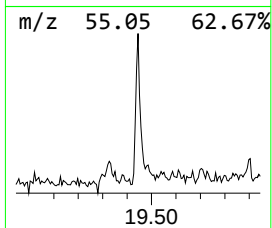
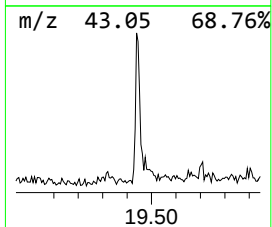
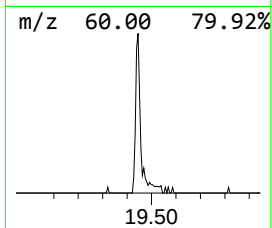
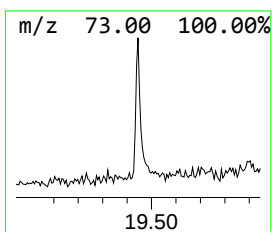
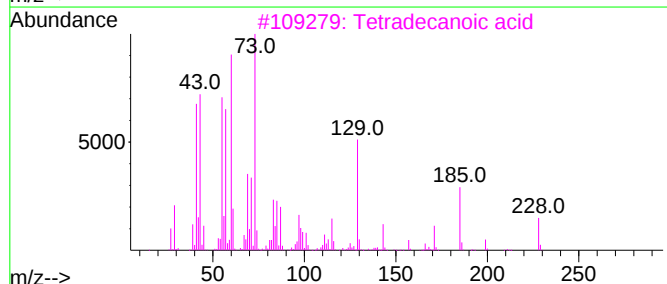
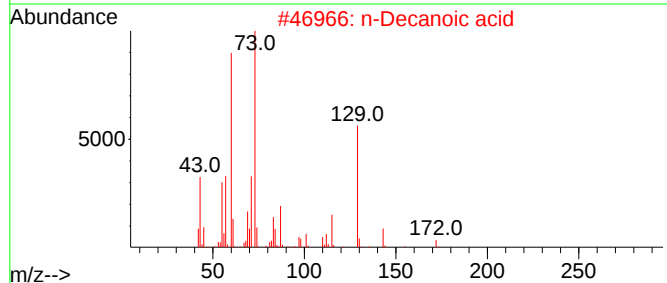
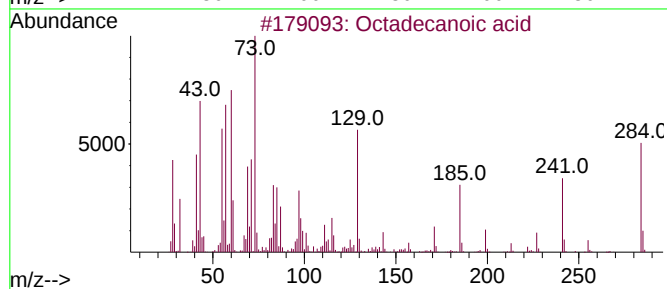
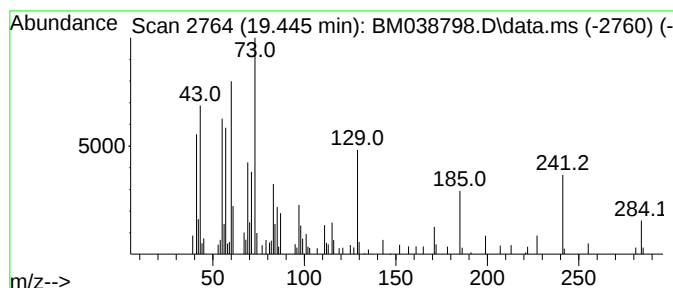
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	2.86 ng	82906	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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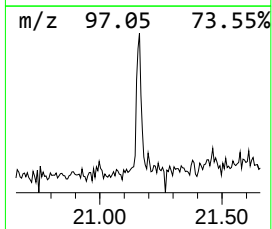
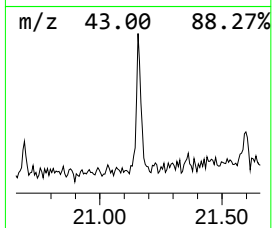
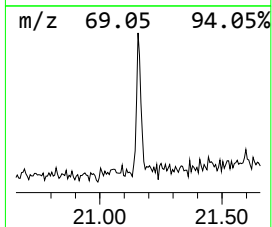
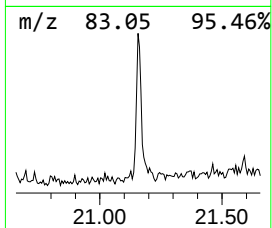
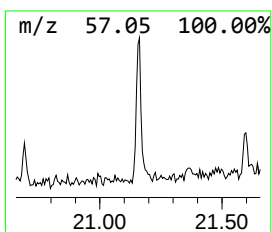
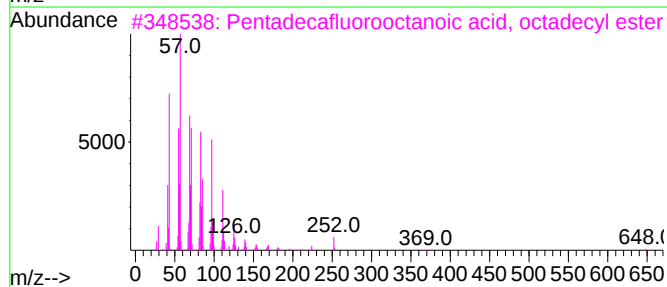
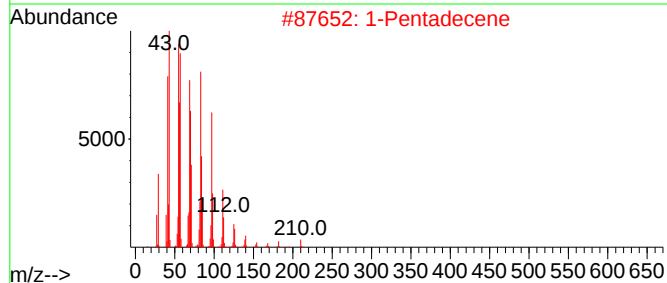
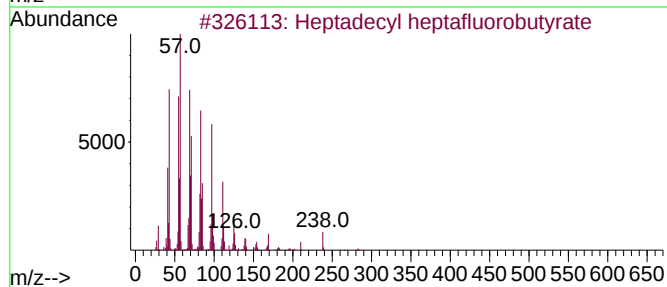
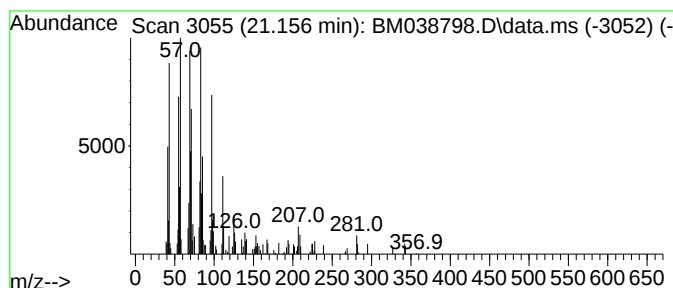
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	2.54 ng	73761	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
2			1-Pentadecene	210	C15H30	013360-61-7	70
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	64
4			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	62
5			1-Docosene	308	C22H44	001599-67-3	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	21.4	ng	265154	1	7.875	248428	20.0
Benzophenone	15.892	3.5	ng	73644	3	14.527	416302	20.0
n-Hexadecanoic ...	18.168	6.4	ng	147992	4	17.280	460985	20.0
Octadecanoic acid	19.445	2.9	ng	82906	5	21.462	580414	20.0
Heptadecyl hept...	21.156	2.5	ng	73761	5	21.462	580414	20.0