

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
 Data File : BM038733.D
 Acq On : 14 Feb 2023 16:55
 Operator : CG/JU
 Sample : 01329-11
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-8-BORING-2-21-28

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: BM038733.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	301	306	317	rVB	217791	293584	17.95%	3.091%
2	5.457	380	386	397	rBV	597677	853460	52.19%	8.986%
3	7.075	653	661	677	rBV	560913	853207	52.17%	8.984%
4	7.898	794	801	810	rBV	173946	265422	16.23%	2.795%
5	9.075	994	1001	1013	rBV	323654	517727	31.66%	5.451%
6	10.710	1272	1279	1289	rVB	194877	308931	18.89%	3.253%
7	13.168	1690	1697	1706	rBV	890934	1274236	77.92%	13.417%
8	14.539	1925	1930	1938	rBV	289562	405003	24.77%	4.264%
9	15.898	2156	2161	2167	rVB	38851	53539	3.27%	0.564%
10	16.027	2178	2183	2190	rBV	712639	975491	59.65%	10.271%
11	17.286	2391	2397	2406	rBV	324308	437161	26.73%	4.603%
12	18.168	2542	2547	2556	rBV2	96355	139185	8.51%	1.466%
13	19.445	2759	2764	2772	rBV2	44465	67668	4.14%	0.712%
14	19.721	2805	2811	2816	rBV3	12879	25961	1.59%	0.273%
15	19.903	2836	2842	2847	rBV	1466085	1635343	100.00%	17.219%
16	21.156	3051	3055	3063	rBV5	59650	91034	5.57%	0.959%
17	21.462	3102	3107	3114	rBV	440185	536315	32.80%	5.647%
18	22.333	3252	3255	3260	rVB5	26300	34264	2.10%	0.361%
19	23.844	3506	3512	3523	rVB2	386540	729762	44.62%	7.684%

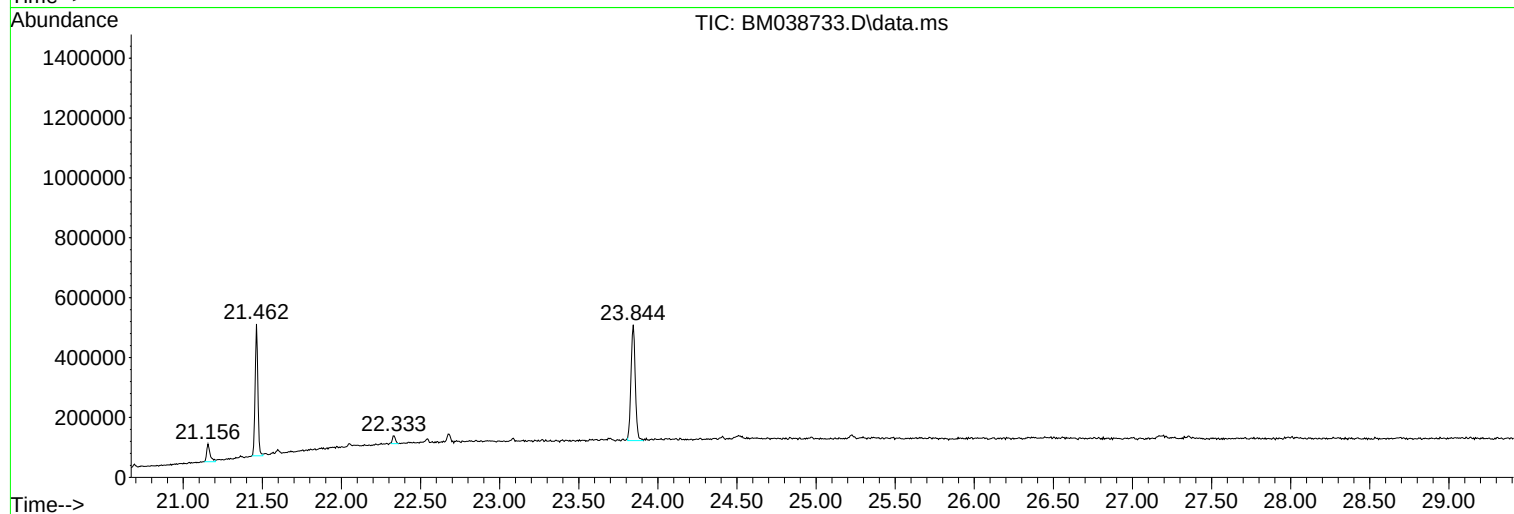
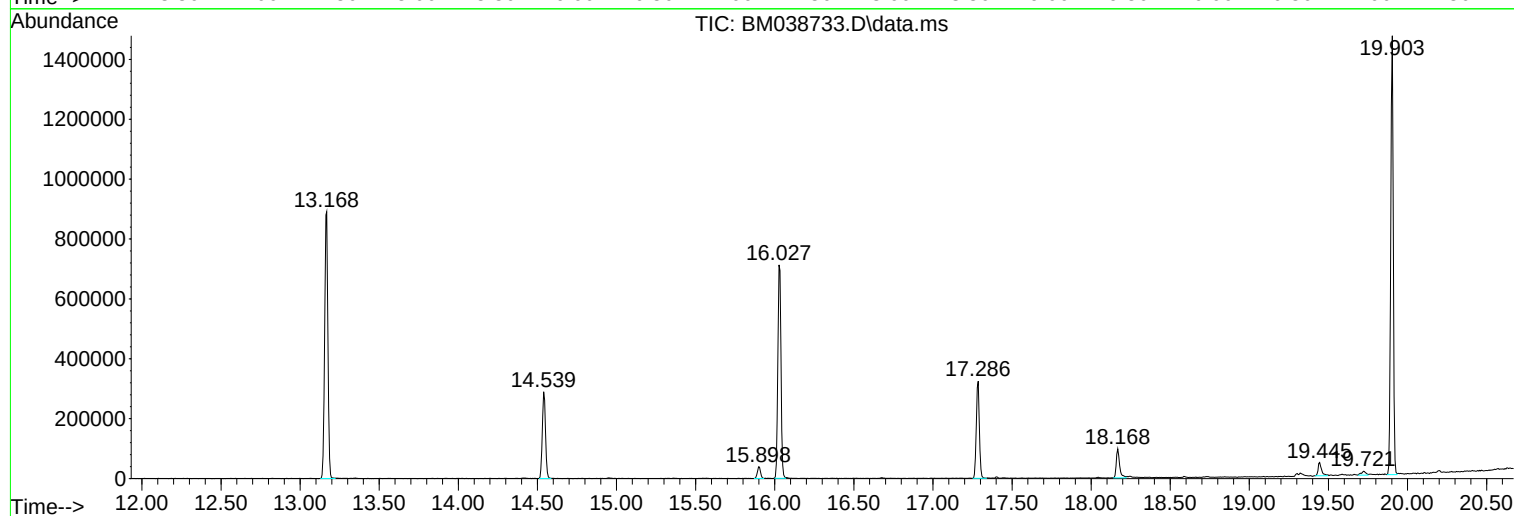
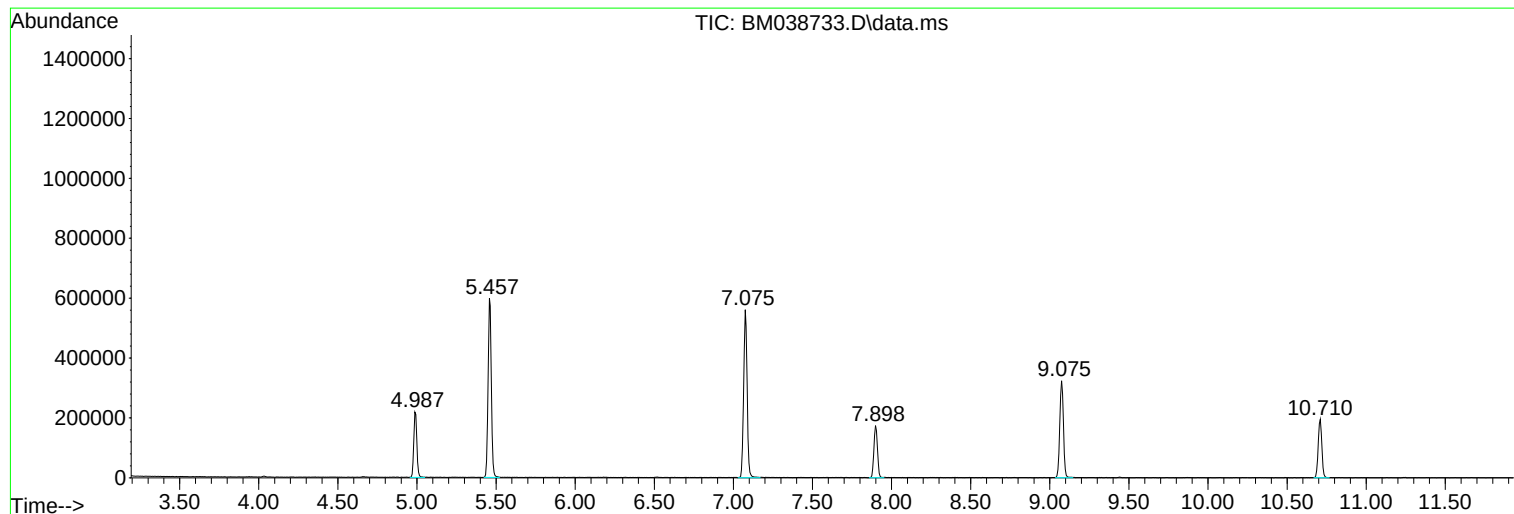
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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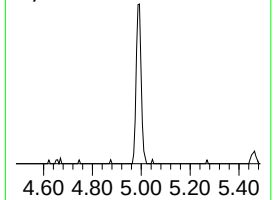
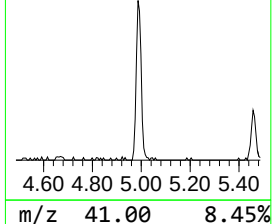
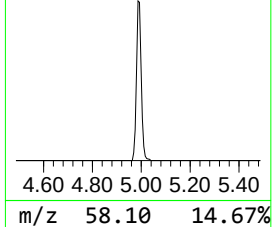
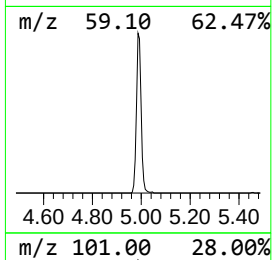
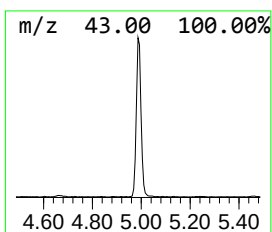
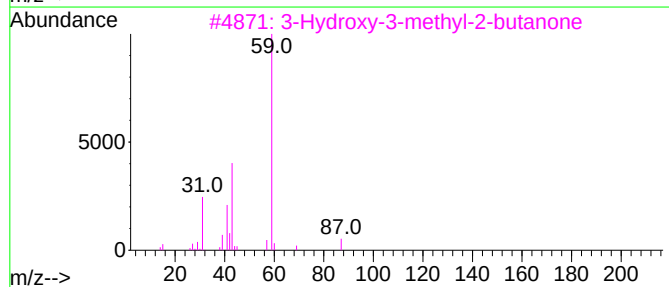
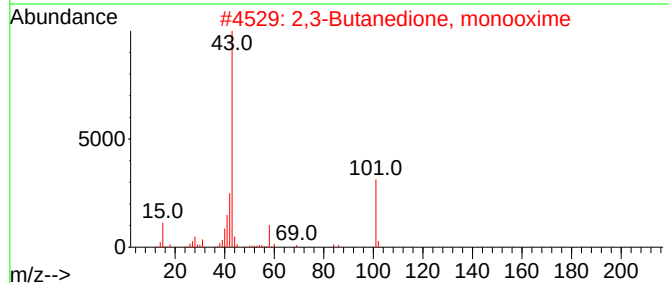
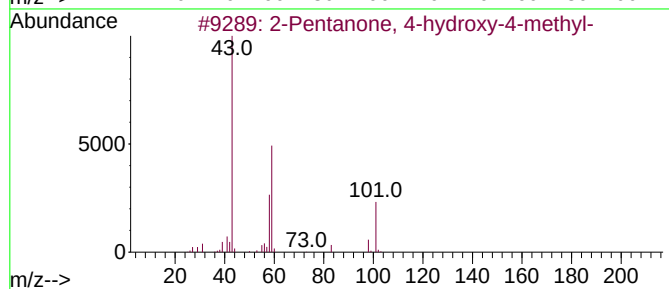
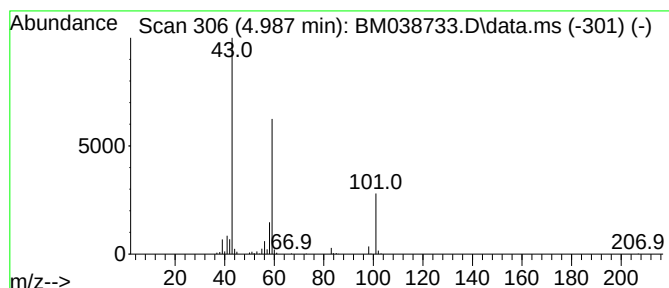
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	22.12 ng	293584	1,4-Dichlorobenzene-d4	7.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
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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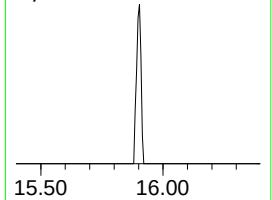
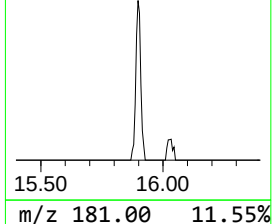
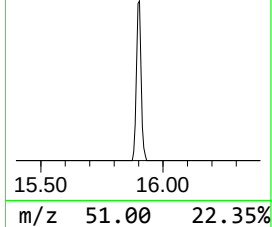
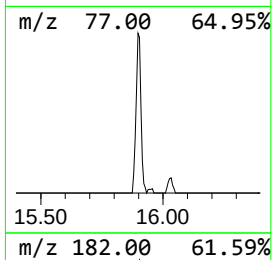
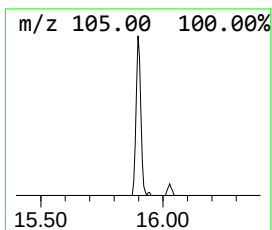
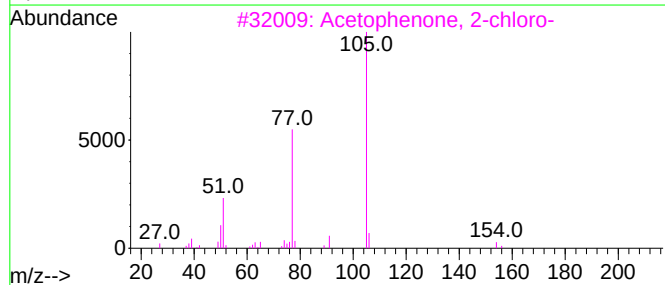
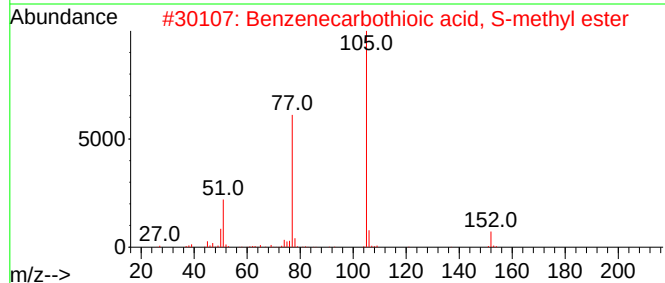
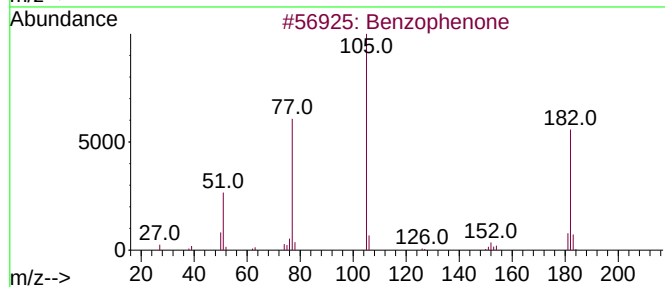
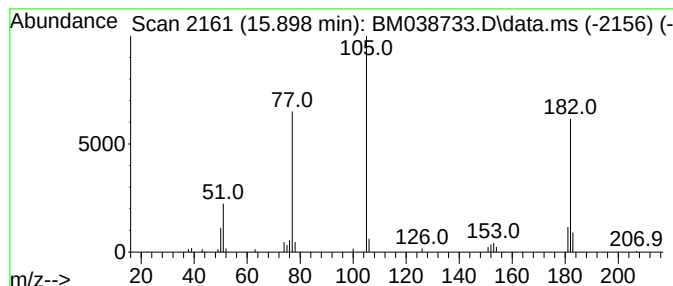
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	2.64 ng	53539	Acenaphthene-d10	14.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			Glyoxylohydroximoyl chloride, 2-...	183	C8H6ClNO2	004937-87-5	46
5			Ethanone, 2-(5-nitrotetrazol-2-y...	233	C9H7N5O3	1000310-77-2	43



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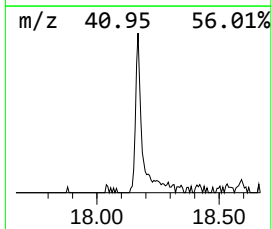
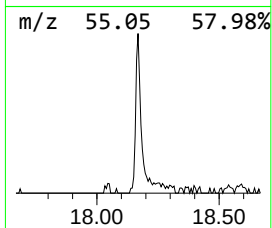
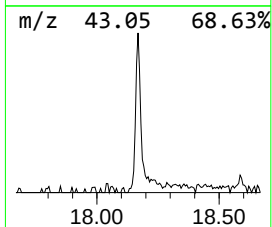
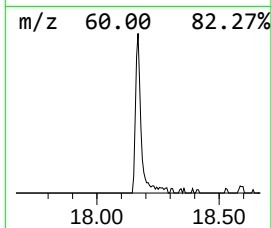
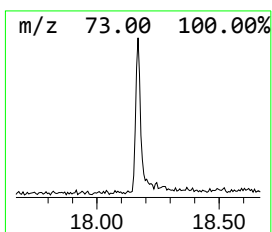
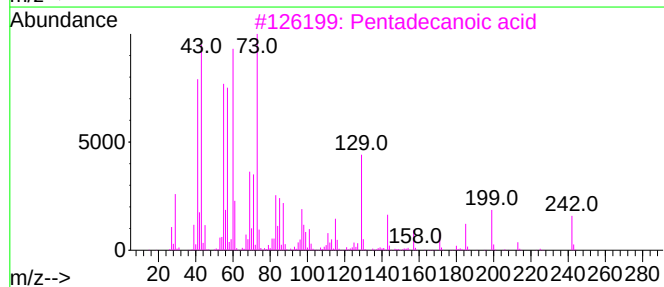
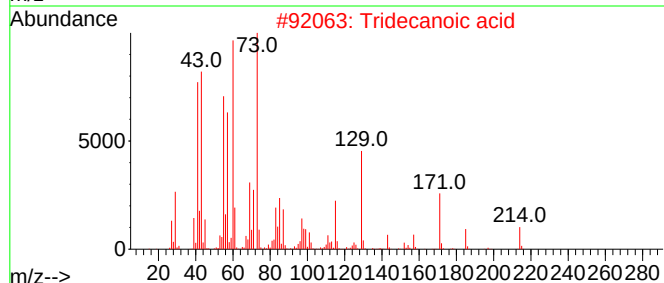
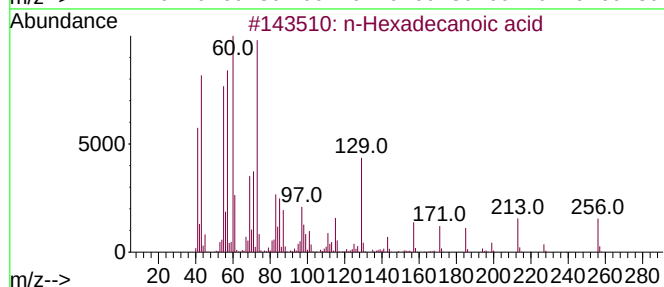
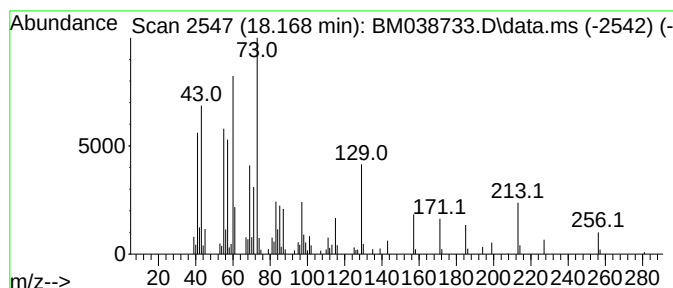
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.168	6.37 ng	139185	Phenanthrene-d10	17.286	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



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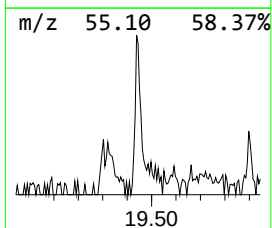
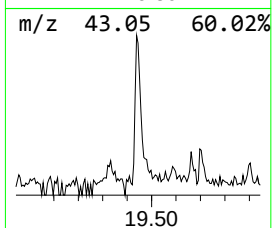
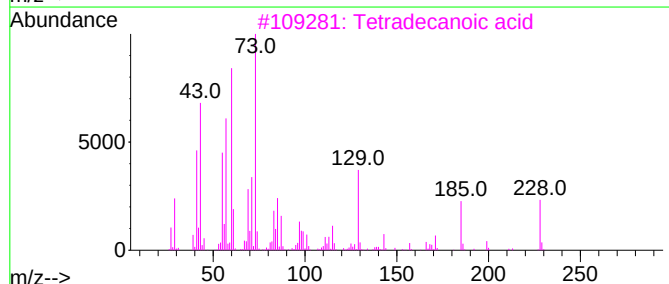
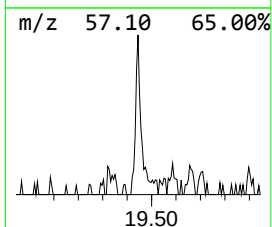
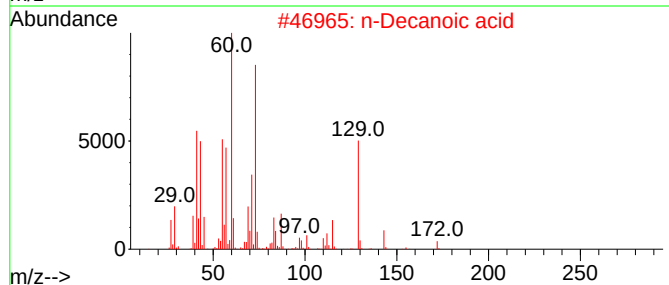
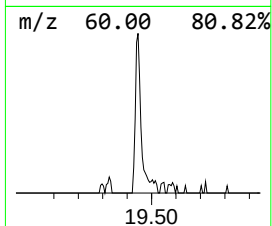
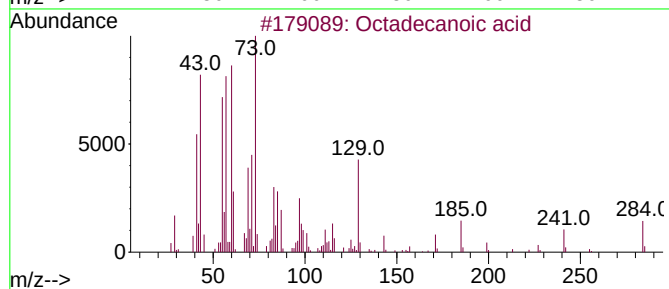
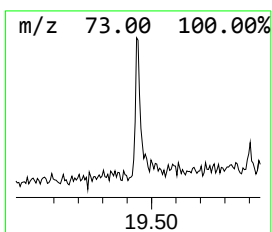
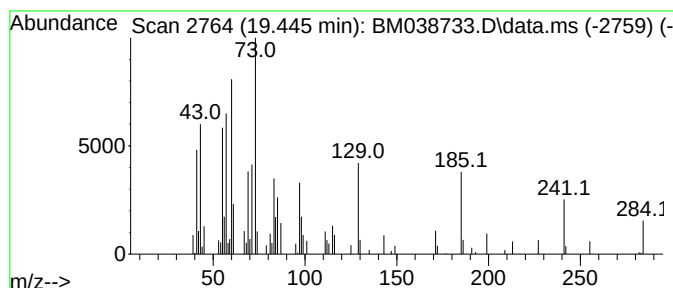
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	2.52 ng	67668	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			n-Decanoic acid	172	C10H20O2	000334-48-5	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53



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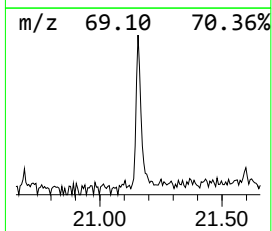
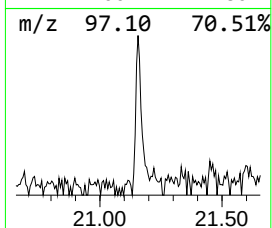
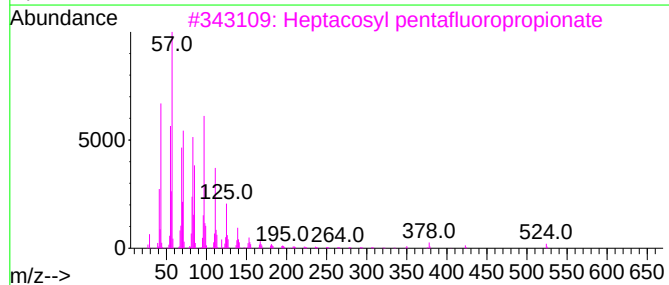
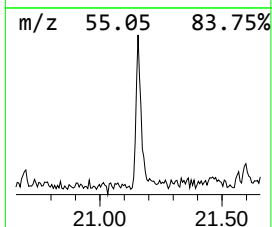
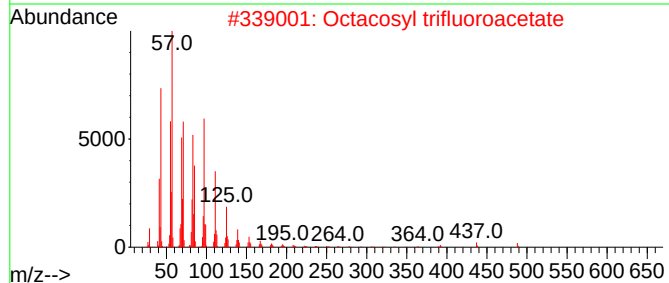
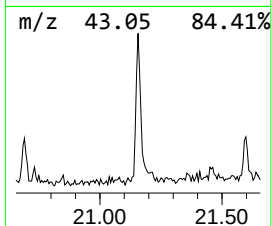
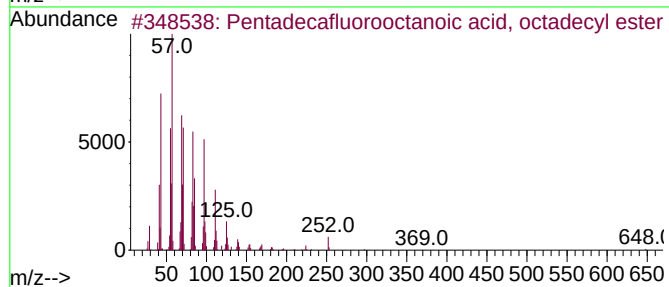
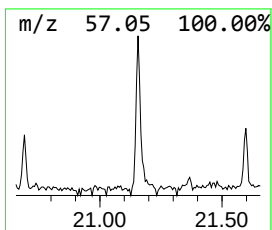
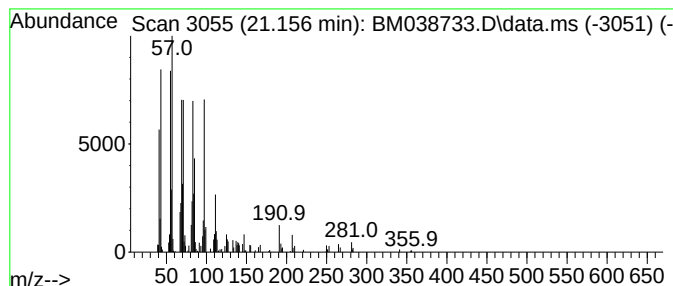
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	3.39 ng	91034	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	76
3			Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	62
4			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	62
5			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	22.1	ng	293584	1	7.898	265422	20.0
Benzophenone	15.898	2.6	ng	53539	3	14.539	405003	20.0
n-Hexadecanoic ...	18.168	6.4	ng	139185	4	17.286	437161	20.0
Octadecanoic acid	19.445	2.5	ng	67668	5	21.462	536315	20.0
Pentadecafluoro...	21.156	3.4	ng	91034	5	21.462	536315	20.0