

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
 Data File : BM038747.D
 Acq On : 15 Feb 2023 14:26
 Operator : CG/JU
 Sample : 01537-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TEST-PIT-1-(TP1)-COMP-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-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038747.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	298	305	321	rVB	245270	338724	9.21%	2.132%
2	5.452	379	385	397	rBV	731490	1038187	28.22%	6.535%
3	7.069	653	660	671	rBV	700869	1087054	29.54%	6.843%
4	7.893	794	800	808	rVB	207697	314327	8.54%	1.979%
5	9.069	992	1000	1007	rBV	435159	673923	18.32%	4.242%
6	10.704	1271	1278	1285	rBV	250851	415926	11.30%	2.618%
7	13.163	1689	1696	1704	rBV	1437718	1984463	53.93%	12.492%
8	14.539	1923	1930	1936	rBV	434613	632153	17.18%	3.979%
9	15.898	2151	2161	2169	rBV	103480	140562	3.82%	0.885%
10	16.027	2176	2183	2195	rBV	1277436	1663221	45.20%	10.470%
11	17.280	2390	2396	2401	rBV	579983	778854	21.17%	4.903%
12	18.168	2541	2547	2557	rBV	233278	359894	9.78%	2.266%
13	19.333	2741	2745	2750	rVB	47242	70019	1.90%	0.441%
14	19.439	2759	2763	2771	rBV	120163	169347	4.60%	1.066%
15	19.698	2804	2807	2816	rVB	48059	62853	1.71%	0.396%
16	19.904	2835	2842	2847	rBV	3106285	3679422	100.00%	23.162%
17	21.151	3050	3054	3064	rVB2	213524	297265	8.08%	1.871%
18	21.356	3086	3089	3093	rBV	101522	106486	2.89%	0.670%
19	21.456	3101	3106	3111	rBV	794803	1023940	27.83%	6.446%
20	23.839	3504	3511	3523	rVB2	537413	1049205	28.52%	6.605%

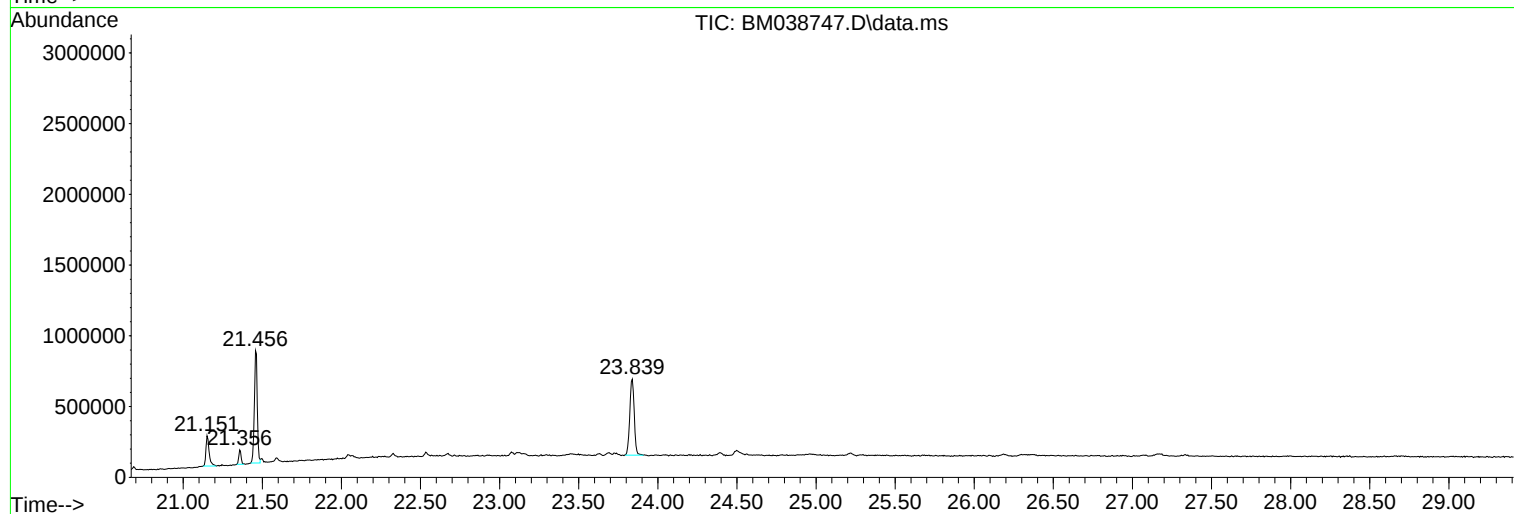
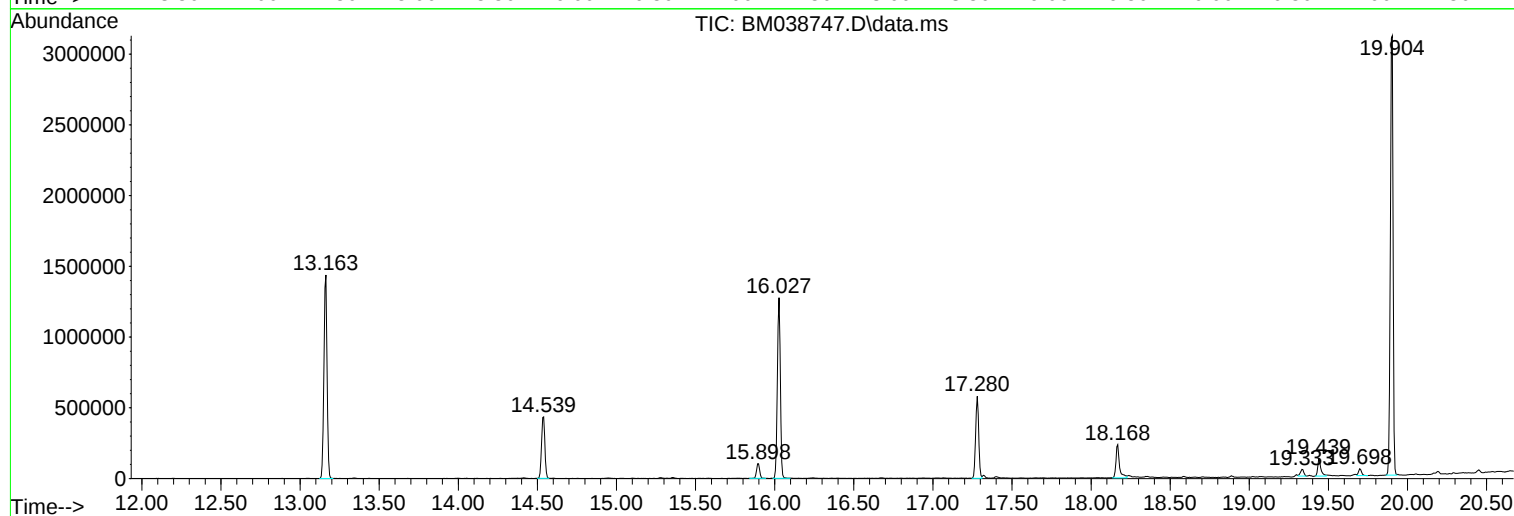
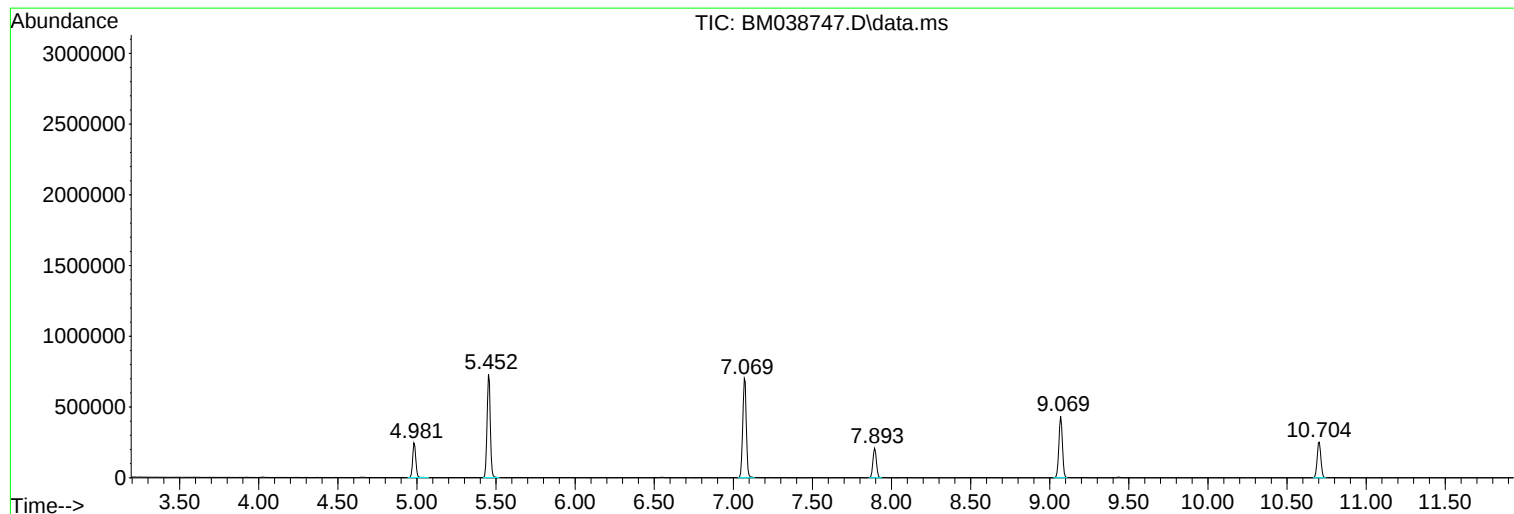
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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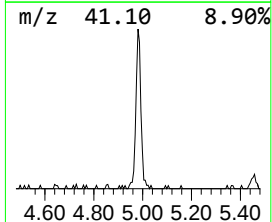
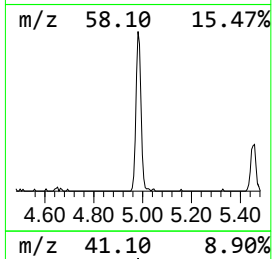
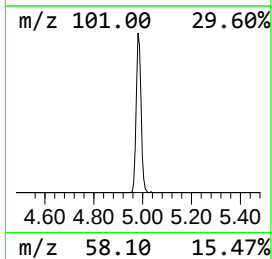
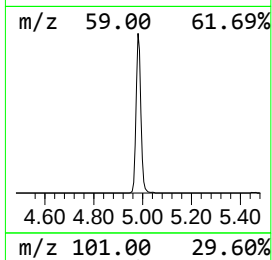
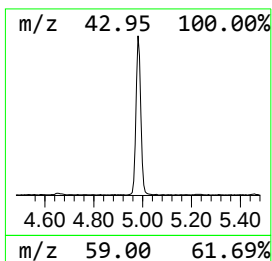
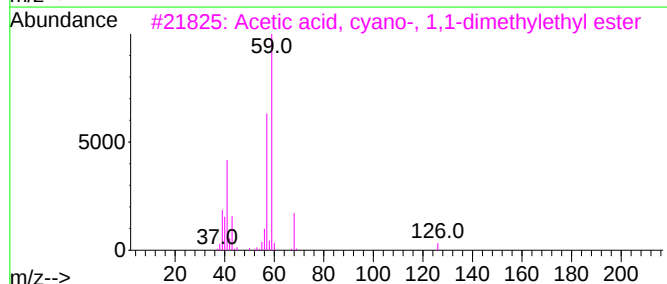
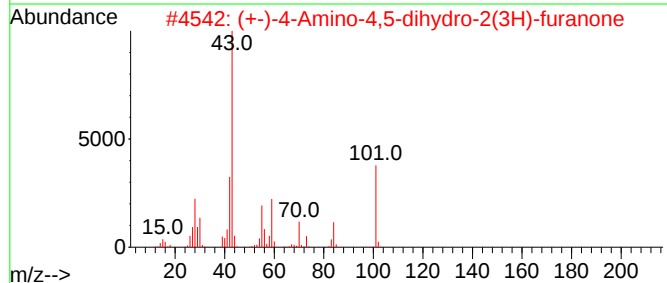
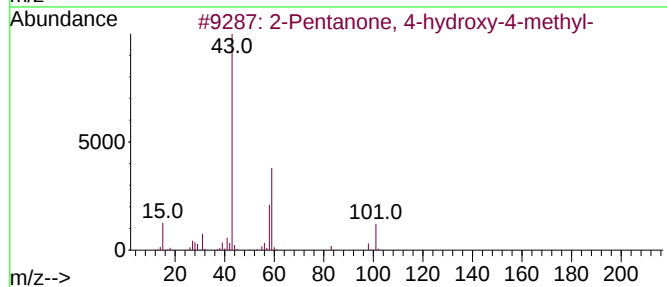
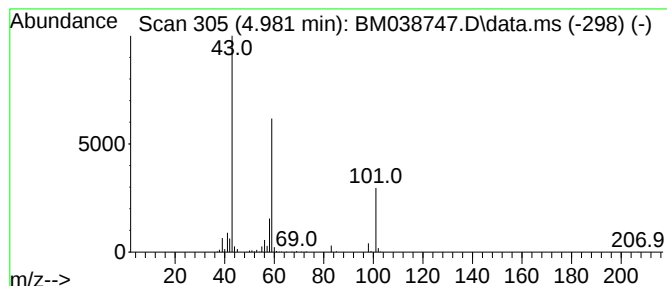
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.981	21.55 ng	338724	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			2,4-Pentanedione, 3-(1-methyleth...	142	C8H14O2	001540-38-1	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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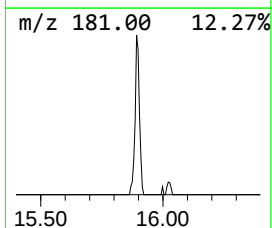
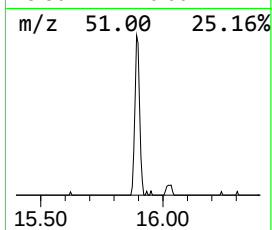
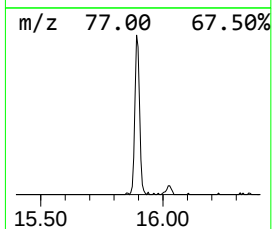
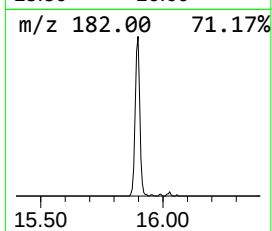
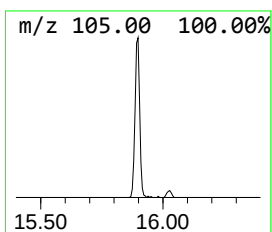
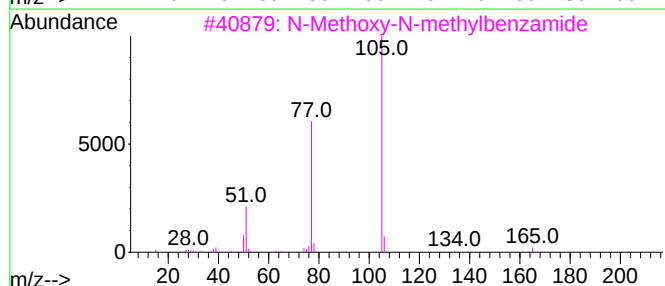
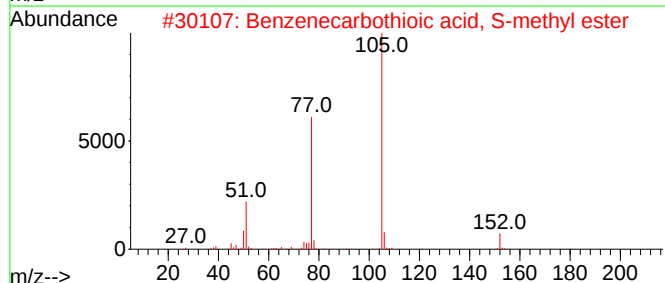
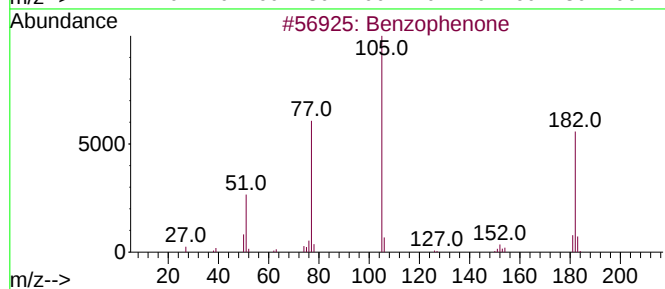
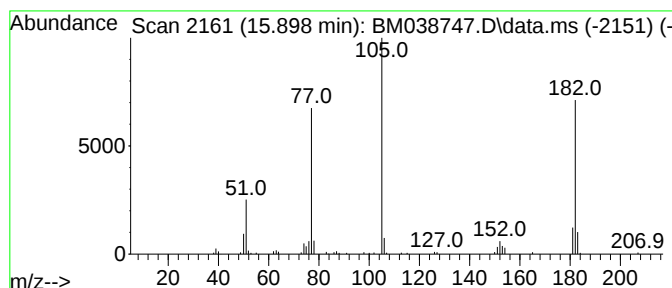
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	4.45 ng	140562	Acenaphthene-d10	14.533

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	53
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	46
4			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	43
5			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	43



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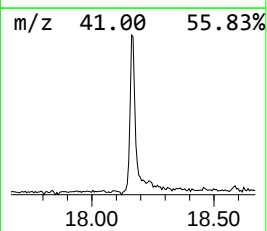
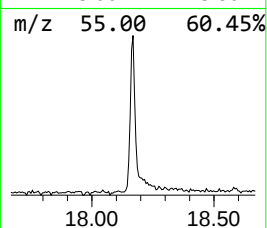
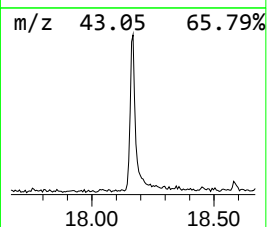
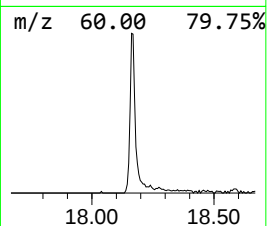
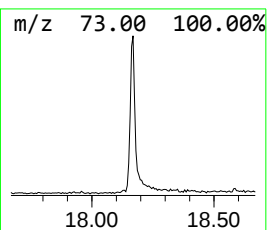
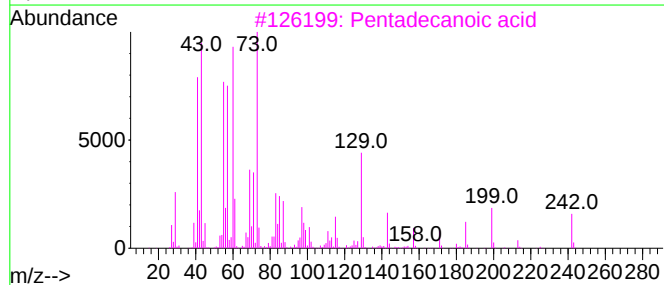
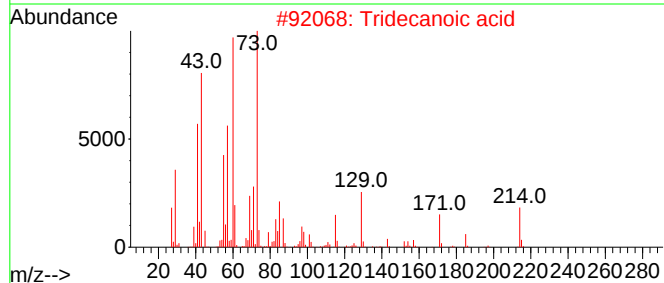
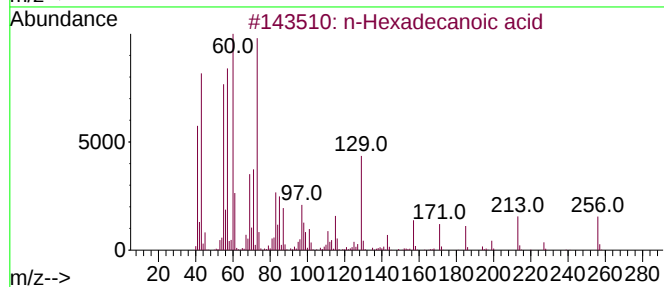
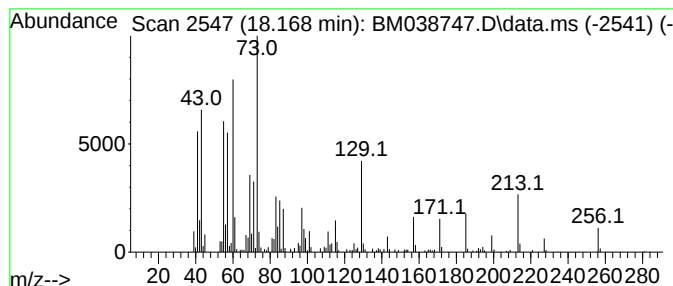
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BNA_M
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.168	9.24 ng	359894	Phenanthrene-d10	17.280	
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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



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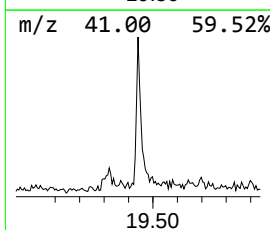
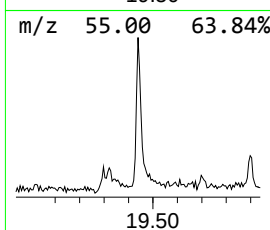
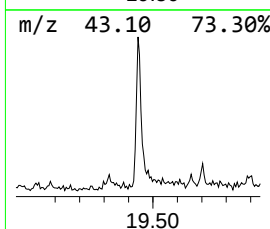
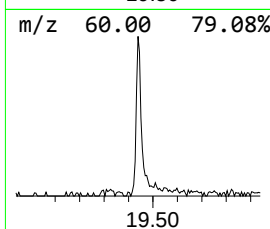
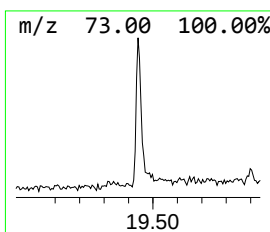
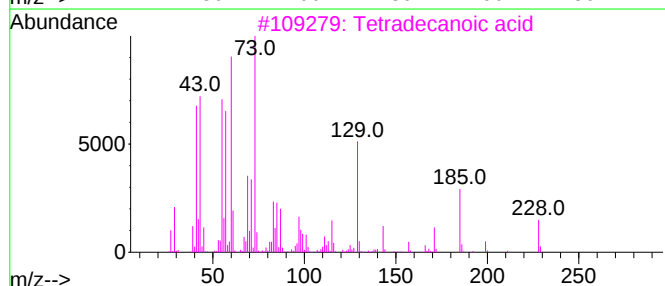
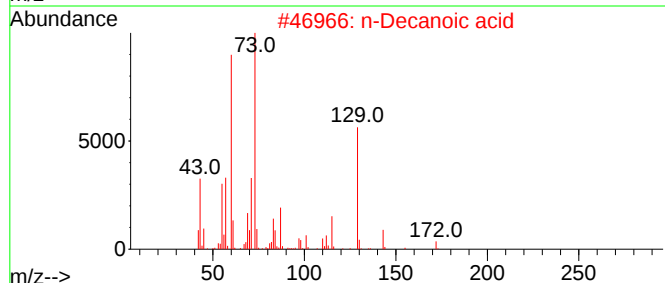
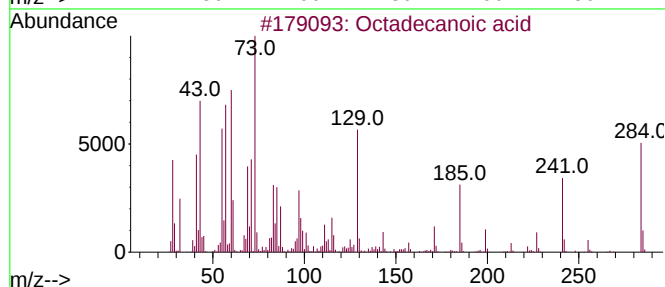
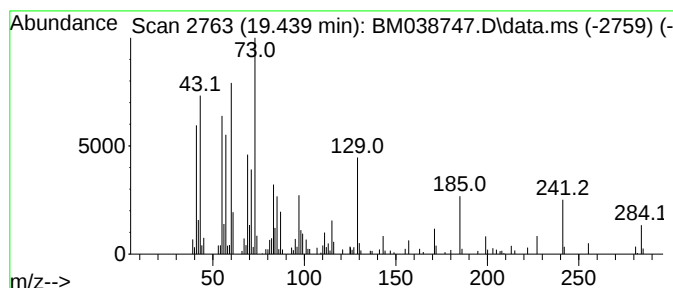
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	3.31 ng	169347	Chrysene-d12	21.456

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	86
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5		Undecanoic acid	186	C11H22O2	000112-37-8	81



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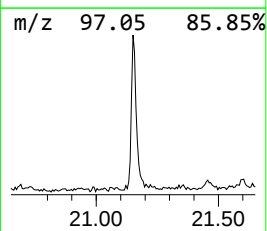
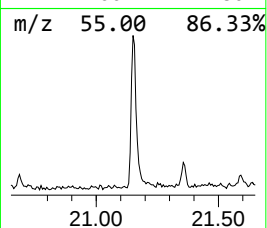
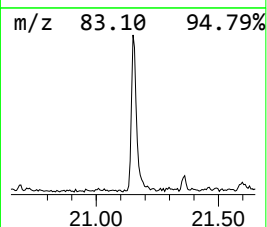
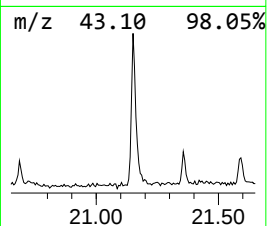
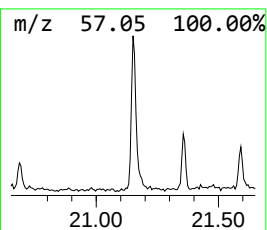
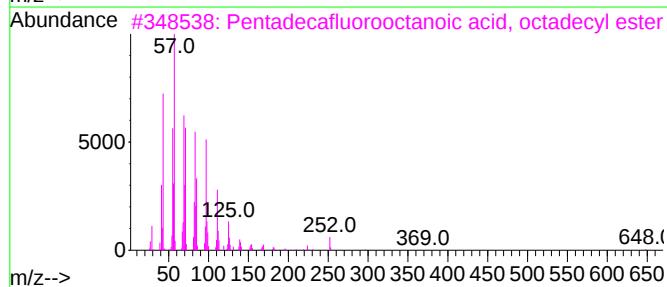
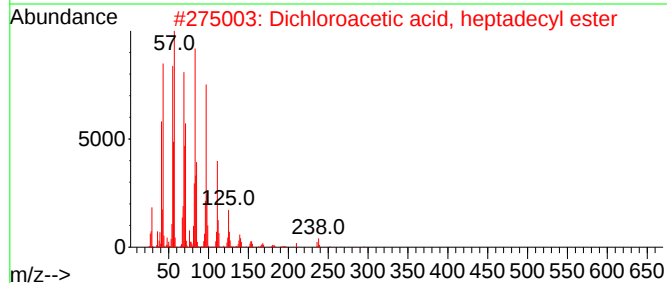
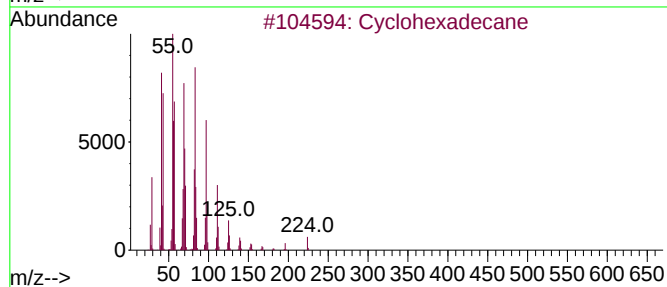
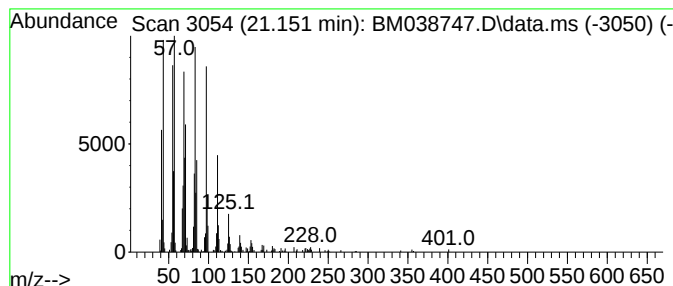
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.151	5.81 ng	297265	Chrysene-d12	21.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.981	21.6	ng	338724	1	7.893	314327	20.0
Benzophenone	15.898	4.5	ng	140562	3	14.533	632153	20.0
n-Hexadecanoic ...	18.168	9.2	ng	359894	4	17.280	778854	20.0
Octadecanoic acid	19.439	3.3	ng	169347	5	21.456	1023940	20.0
Cyclohexadecane	21.151	5.8	ng	297265	5	21.456	1023940	20.0