

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
 Data File : BM038746.D
 Acq On : 15 Feb 2023 13:49
 Operator : CG/JU
 Sample : 01539-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-7

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: BM038746.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	295	305	317	rVB	241094	329078	9.86%	2.132%
2	5.451	379	385	398	rBV	731487	1017561	30.50%	6.591%
3	7.069	653	660	669	rBV	701571	1046817	31.38%	6.781%
4	7.892	793	800	807	rBV	196307	294423	8.83%	1.907%
5	9.069	993	1000	1010	rBV	412121	647888	19.42%	4.197%
6	10.704	1270	1278	1285	rBV	237979	390906	11.72%	2.532%
7	13.163	1689	1696	1703	rBV	1334534	1850896	55.48%	11.989%
8	14.533	1923	1929	1939	rVB	408595	592048	17.75%	3.835%
9	15.898	2156	2161	2166	rVB	65098	86475	2.59%	0.560%
10	16.027	2176	2183	2195	rVB	1368510	1768617	53.01%	11.456%
11	17.280	2390	2396	2402	rBV	539969	727969	21.82%	4.716%
12	18.168	2541	2547	2557	rBV	479035	660539	19.80%	4.279%
13	19.321	2741	2743	2751	rVB7	21830	37222	1.12%	0.241%
14	19.439	2759	2763	2775	rBV	198347	293812	8.81%	1.903%
15	19.898	2836	2841	2849	rBV	2915532	3336125	100.00%	21.610%
16	21.150	3050	3054	3065	rBV	224651	357467	10.72%	2.316%
17	21.456	3101	3106	3112	rBV	748424	924139	27.70%	5.986%
18	23.839	3504	3511	3521	rVB2	557958	1075767	32.25%	6.968%

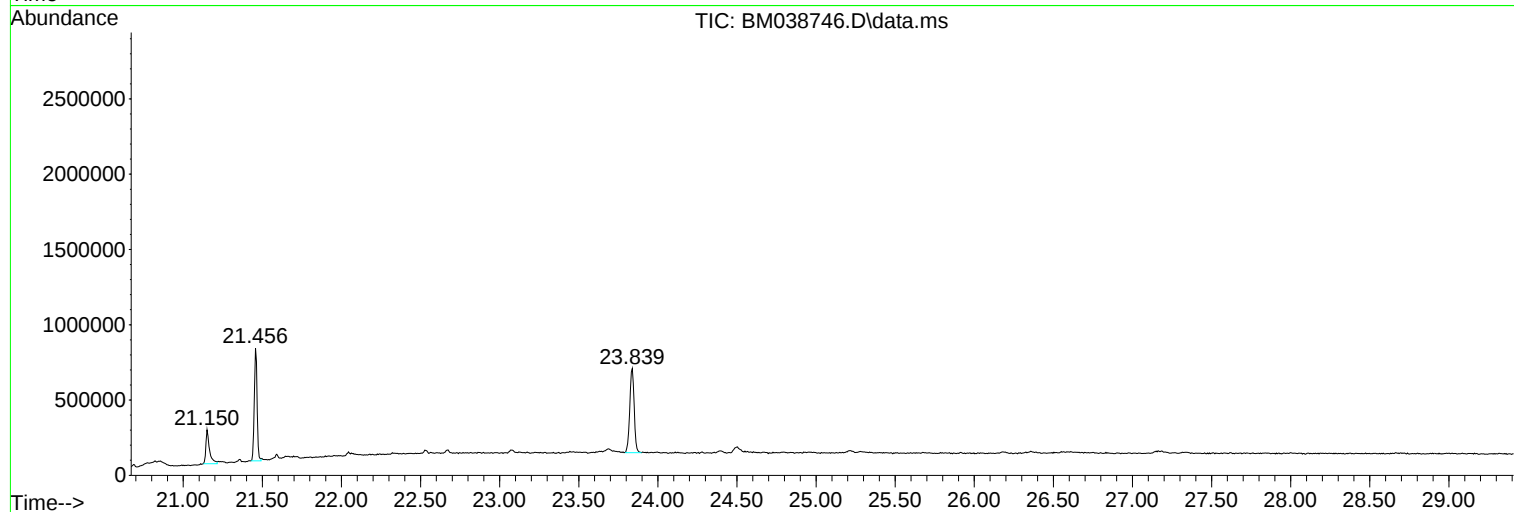
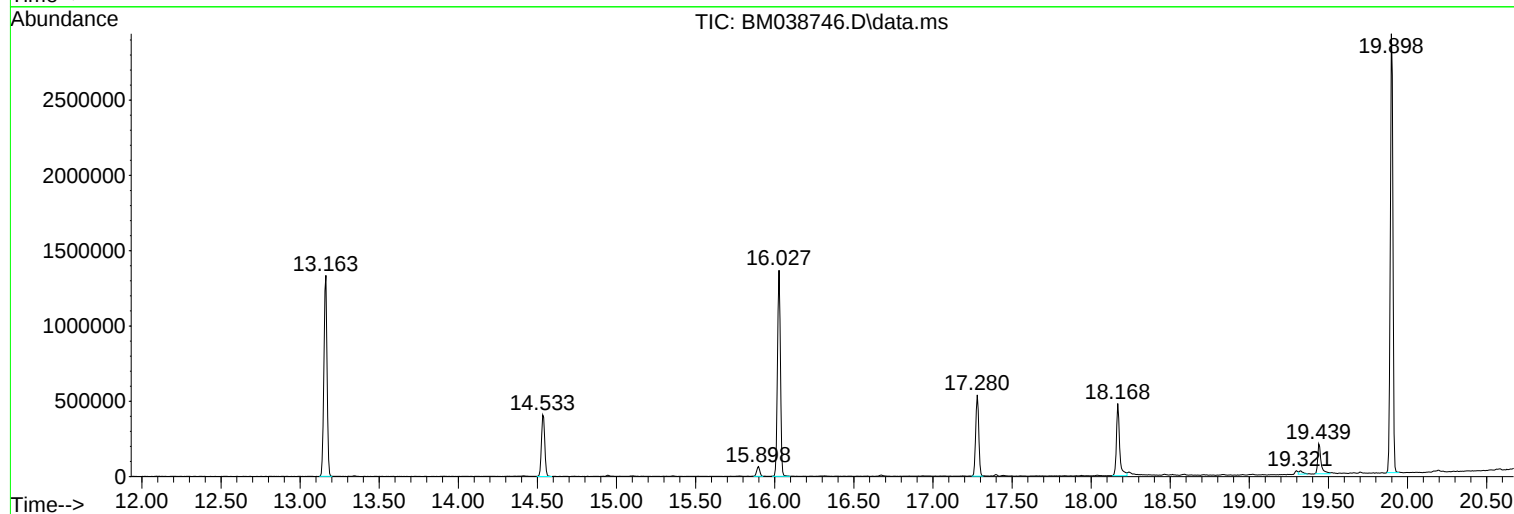
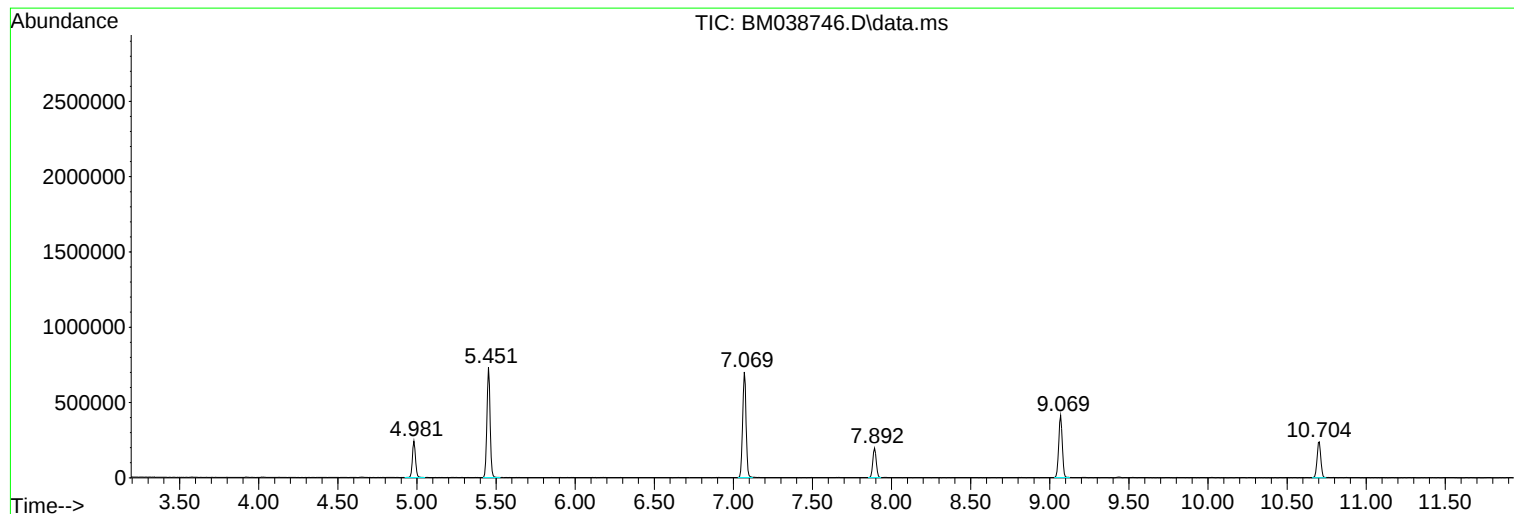
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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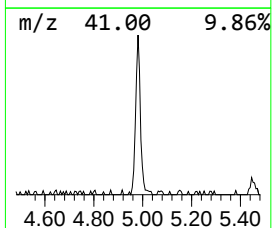
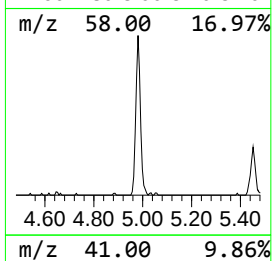
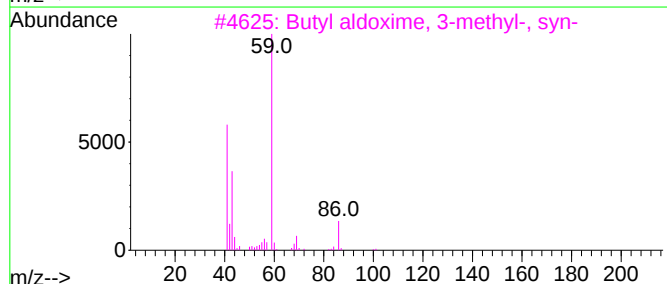
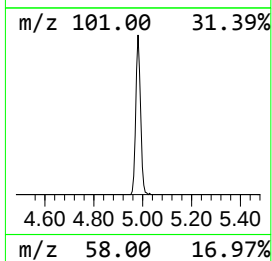
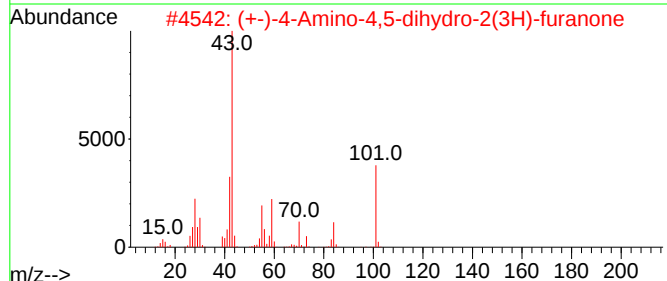
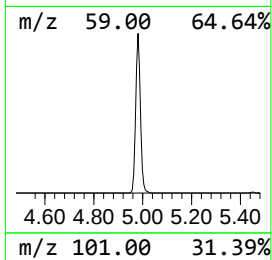
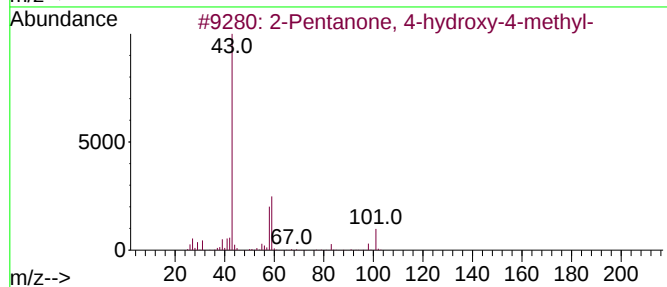
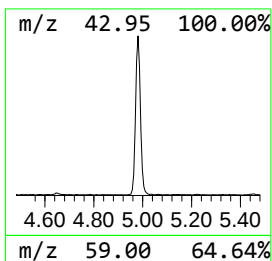
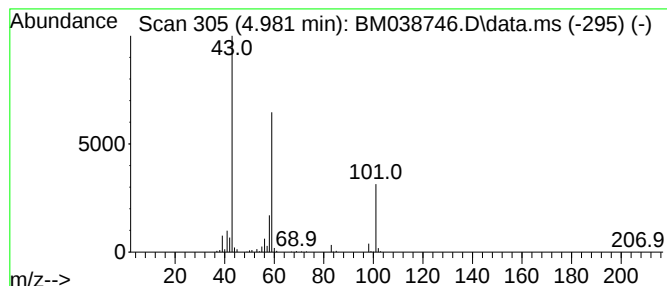
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	22.35 ng	329078	1,4-Dichlorobenzene-d4	7.892

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	43		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	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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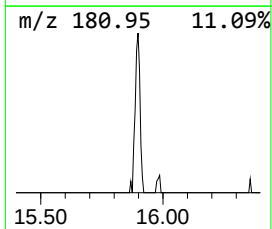
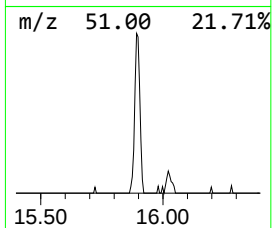
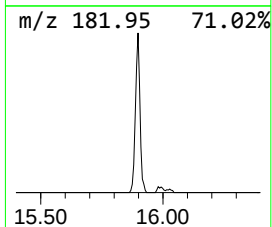
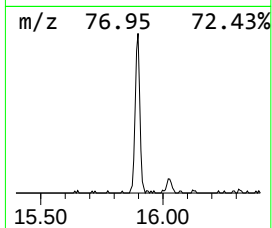
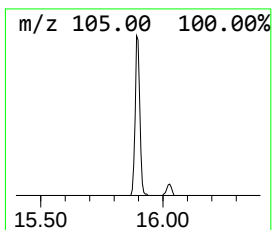
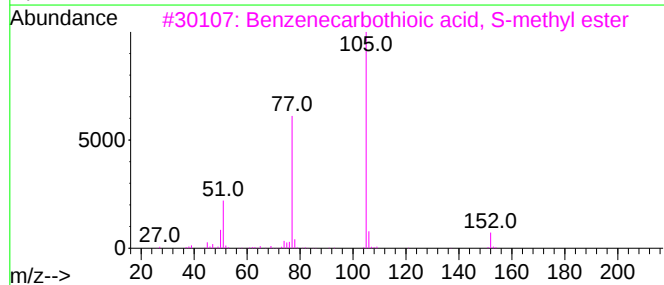
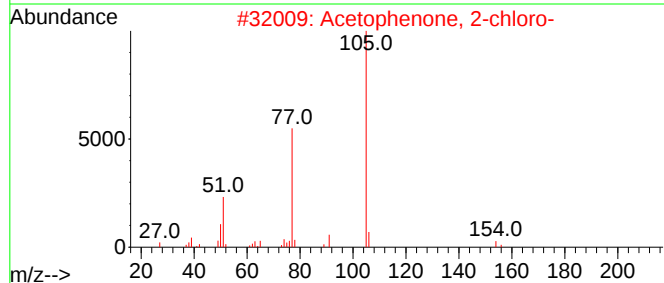
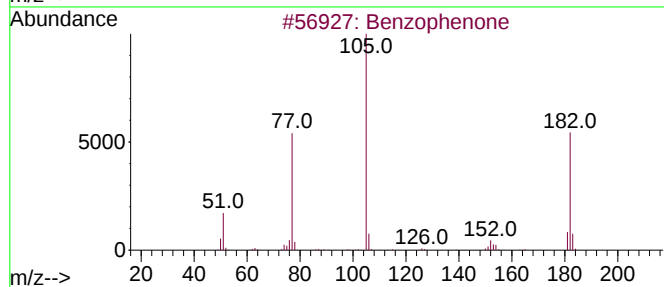
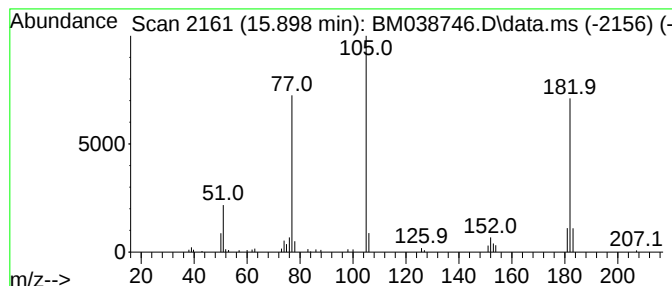
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	2.92 ng	86475	Acenaphthene-d10	14.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
4			Ethyl 2-benzoyl-4-cyanobutanoate	245	C14H15NO3	1000486-83-9	43
5			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	43



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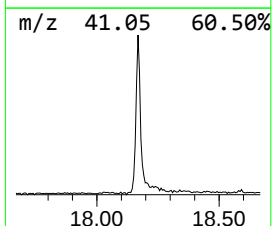
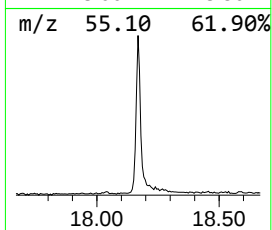
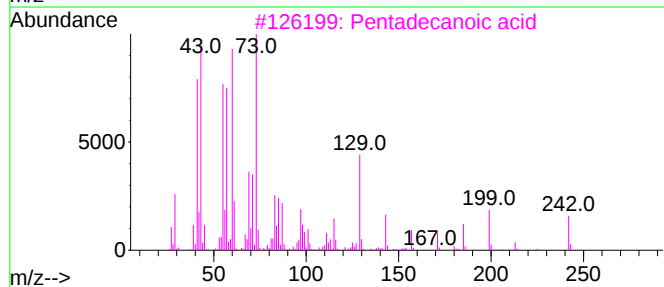
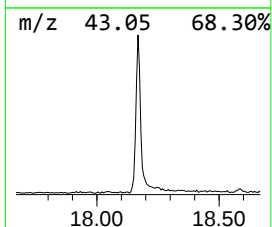
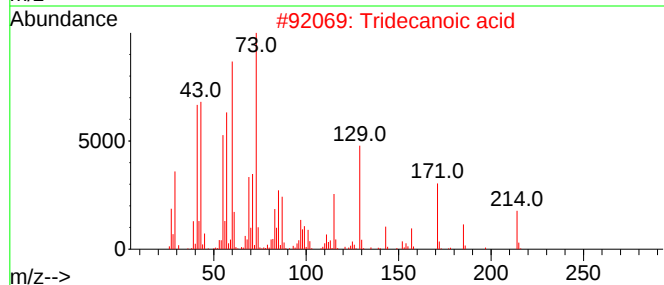
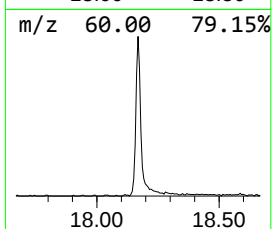
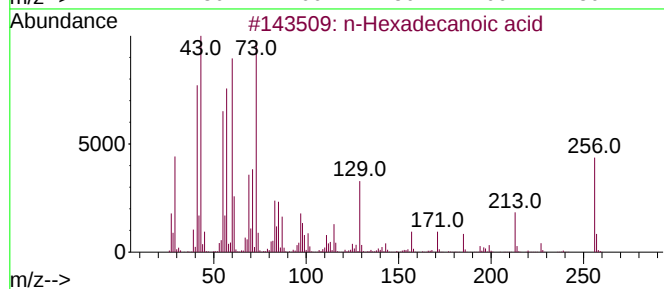
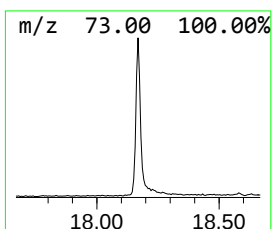
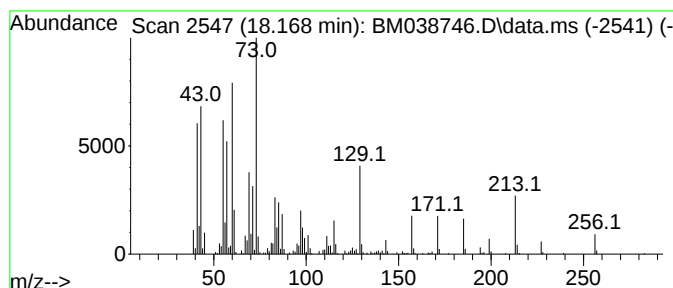
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TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.168	18.15 ng	660539	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	93
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	53



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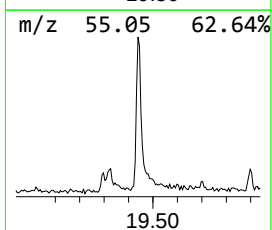
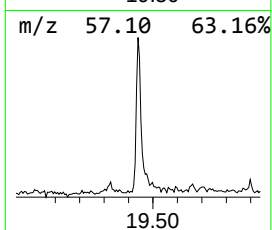
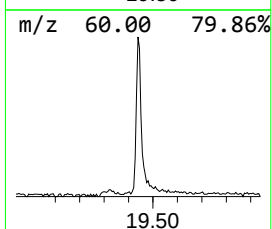
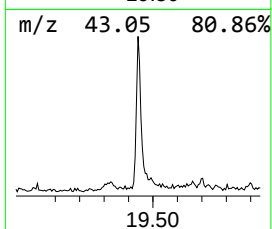
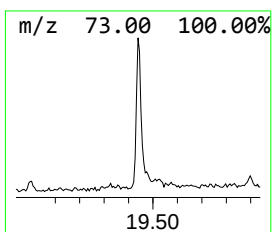
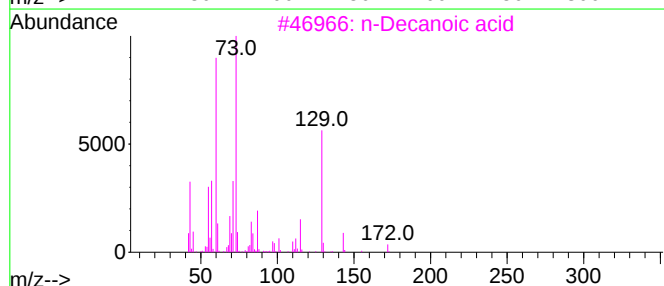
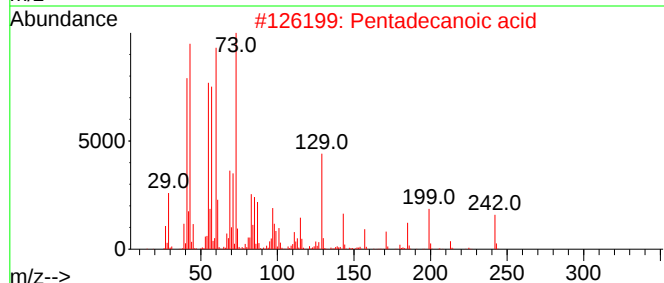
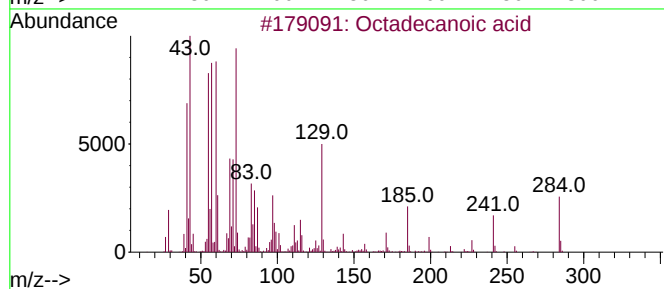
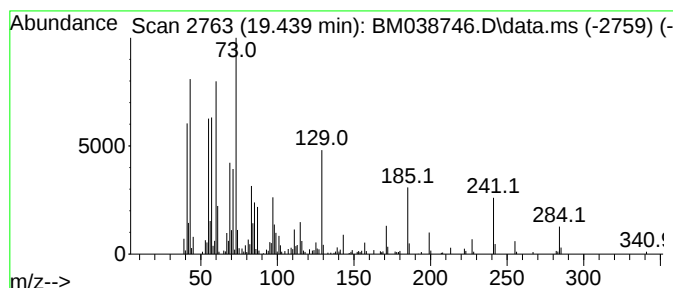
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	6.36 ng	293812	Chrysene-d12	21.456

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			n-Decanoic acid	172	C10H20O2	000334-48-5	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81



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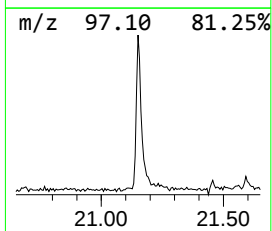
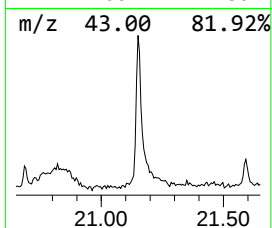
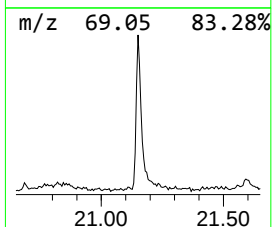
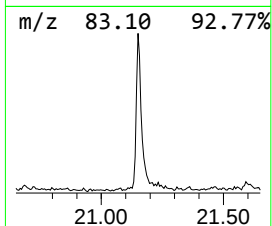
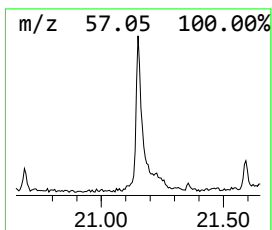
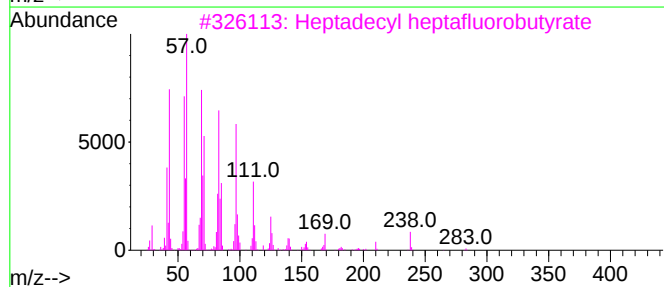
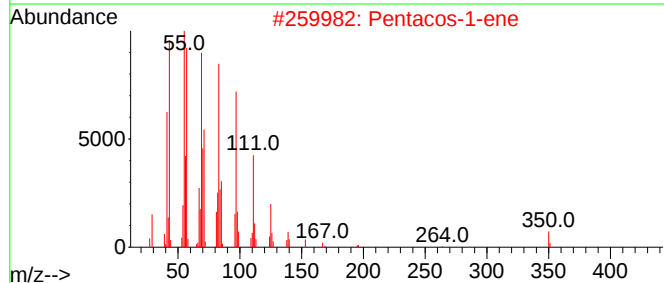
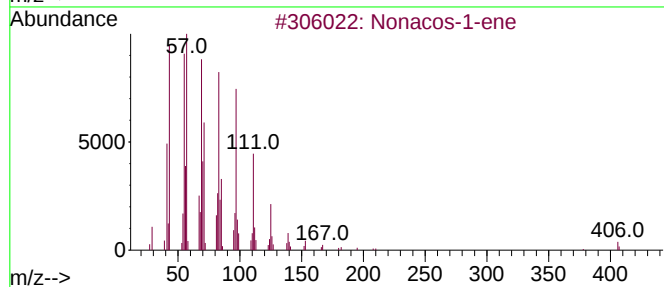
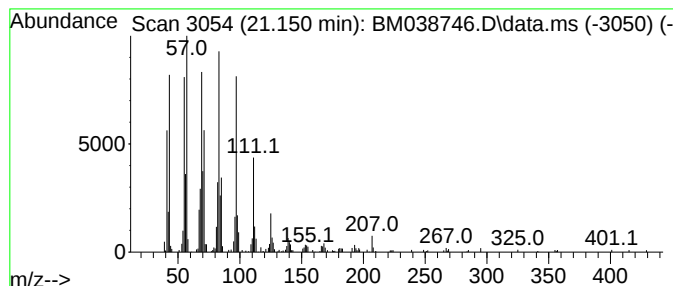
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonacos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.150	7.74 ng	357467	Chrysene-d12	21.456	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacos-1-ene	406	C29H58	018835-35-3	94
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	1-Tetracosene	336	C24H48	010192-32-2	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.981	22.4	ng	329078	1	7.892	294423	20.0
Benzophenone	15.898	2.9	ng	86475	3	14.533	592048	20.0
n-Hexadecanoic ...	18.168	18.1	ng	660539	4	17.280	727969	20.0
Octadecanoic acid	19.439	6.4	ng	293812	5	21.456	924139	20.0
Nonacos-1-ene	21.150	7.7	ng	357467	5	21.456	924139	20.0