

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042123\
 Data File : BM039548.D
 Acq On : 21 Apr 2023 12:30
 Operator : CG/JU
 Sample : 02270-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-17-7-9-20230410

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-BM041723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039548.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.913	313	319	337	rBV	268970	403272	5.73%	1.137%
2	5.384	393	399	420	rBV	2201440	3375008	47.97%	9.514%
3	7.001	667	674	699	rBV	1958624	3520331	50.04%	9.924%
4	7.819	803	813	821	rBV	524806	914731	13.00%	2.579%
5	8.989	1004	1012	1033	rBV	1173437	2206573	31.36%	6.220%
6	10.625	1283	1290	1309	rBV	632346	1217182	17.30%	3.431%
7	13.095	1703	1710	1728	rBV	3337232	5003696	71.12%	14.105%
8	14.471	1938	1944	1960	rBV	985445	1526124	21.69%	4.302%
9	15.842	2170	2177	2190	rBV	83220	154438	2.20%	0.435%
10	15.965	2192	2198	2223	rBV	2020409	3241328	46.07%	9.137%
11	17.224	2406	2412	2431	rBV	1047335	1695942	24.11%	4.781%
12	18.124	2560	2565	2575	rBV	299423	585504	8.32%	1.651%
13	19.406	2779	2783	2800	rBV	180576	383352	5.45%	1.081%
14	19.859	2854	2860	2875	rBV	5541733	7035641	100.00%	19.833%
15	21.136	3072	3077	3088	rBV	267096	593254	8.43%	1.672%
16	21.424	3121	3126	3136	rBV	1220784	1786096	25.39%	5.035%
17	23.783	3521	3527	3541	rVB	883702	1831495	26.03%	5.163%

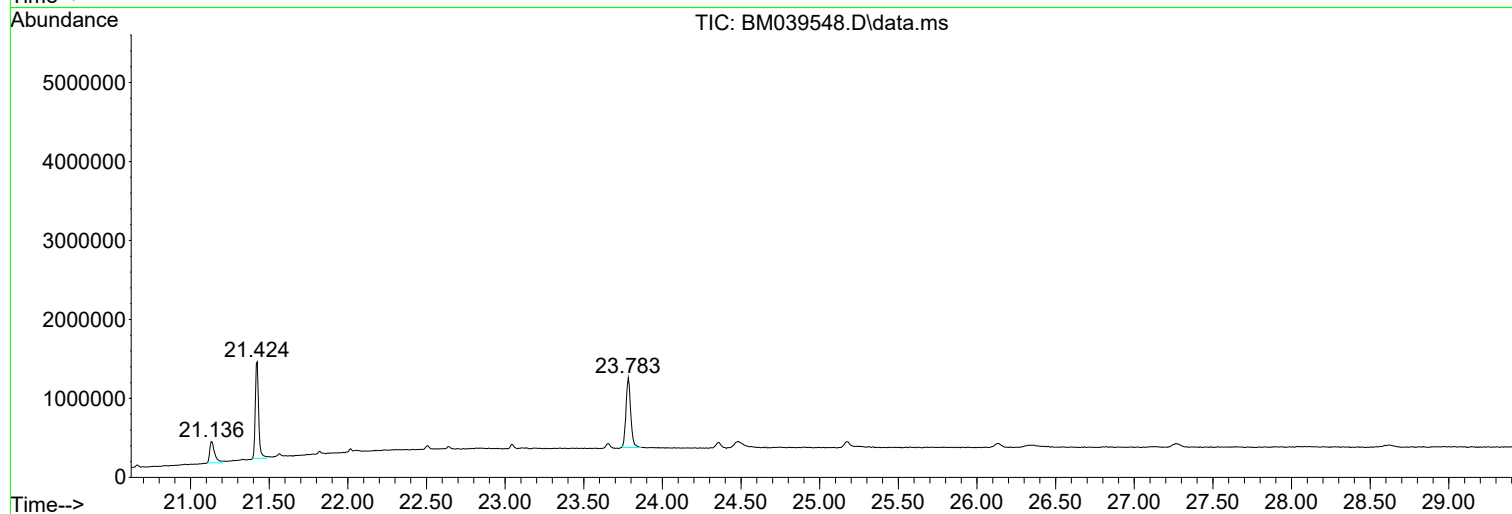
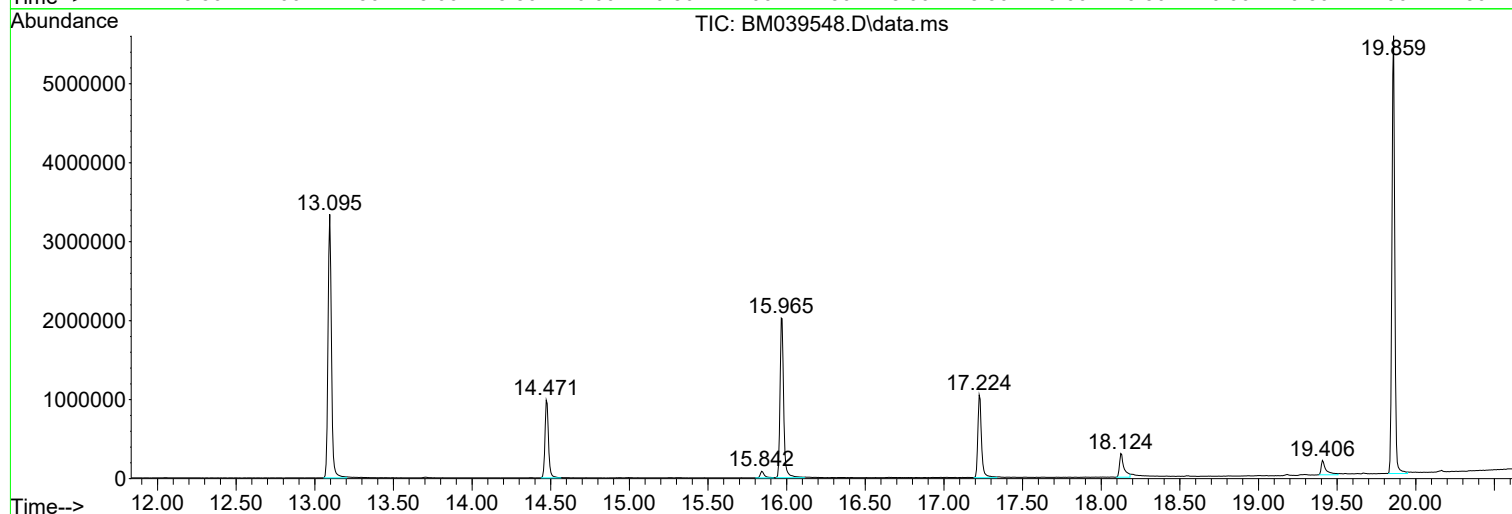
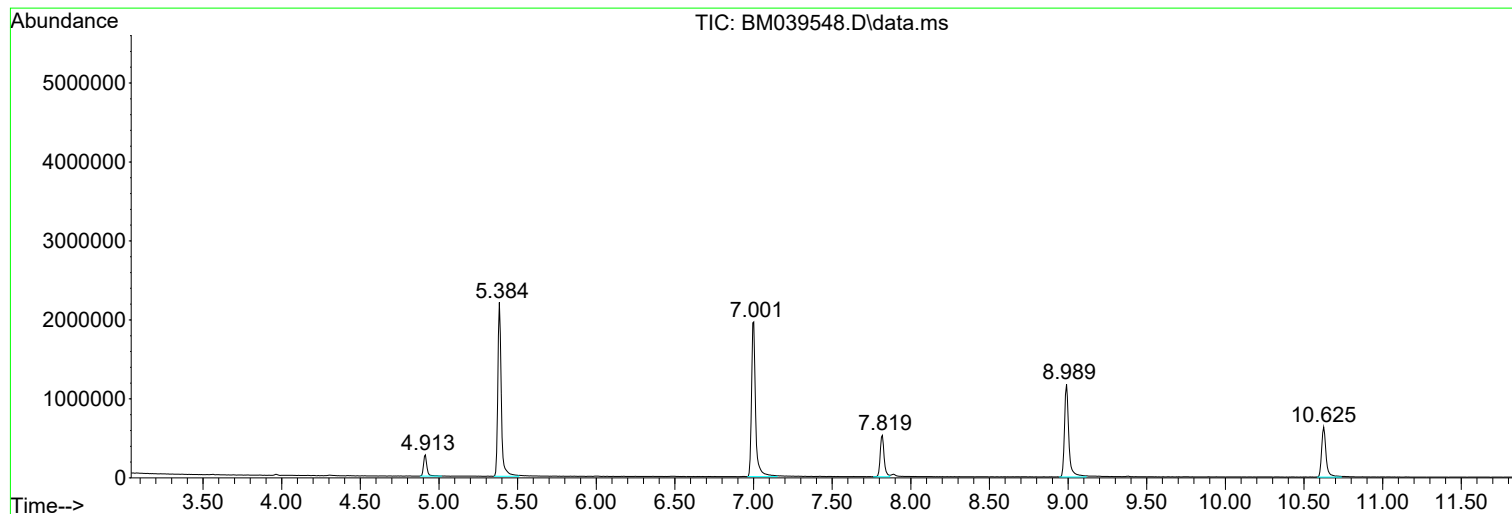
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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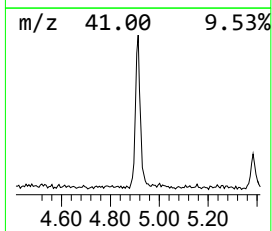
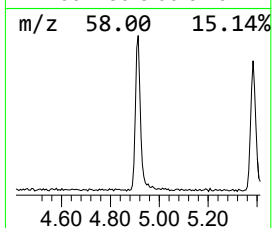
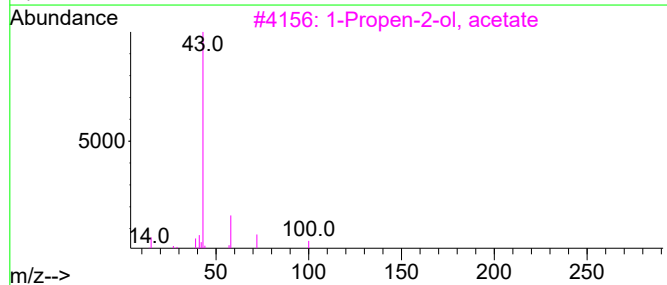
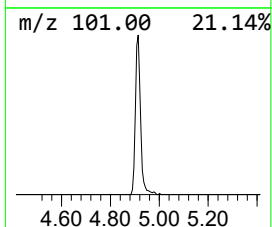
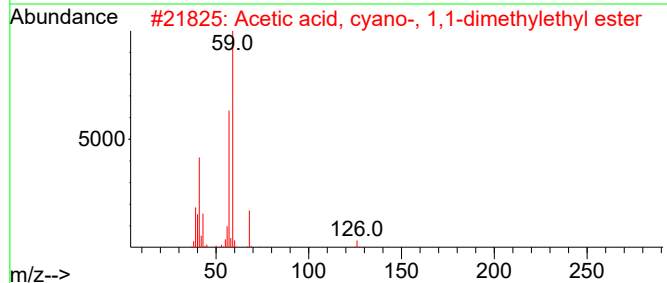
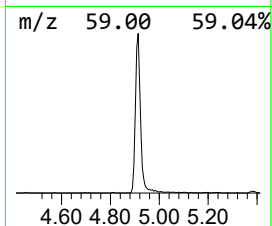
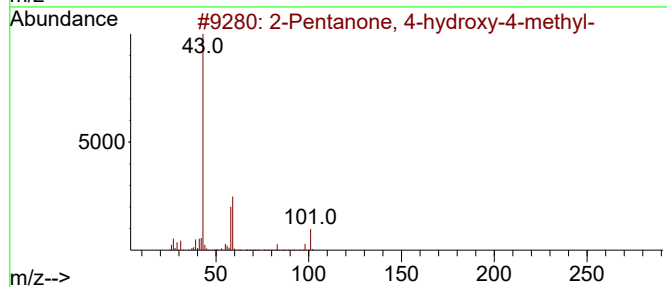
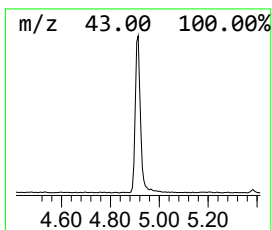
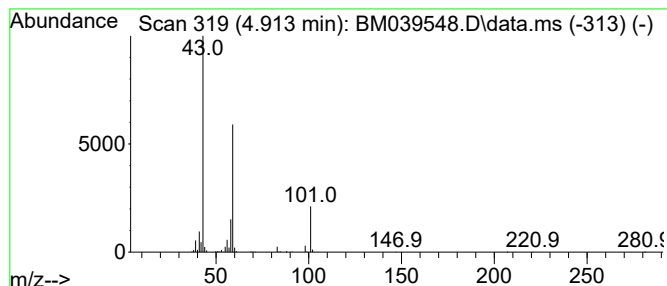
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
4.913	8.82 ng	403272	1,4-Dichlorobenzene-d4	7.819	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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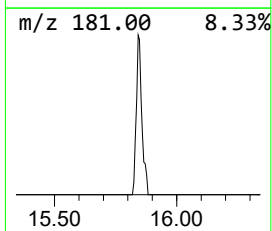
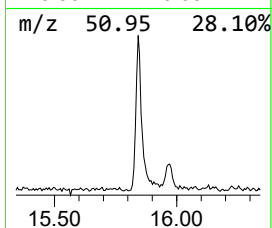
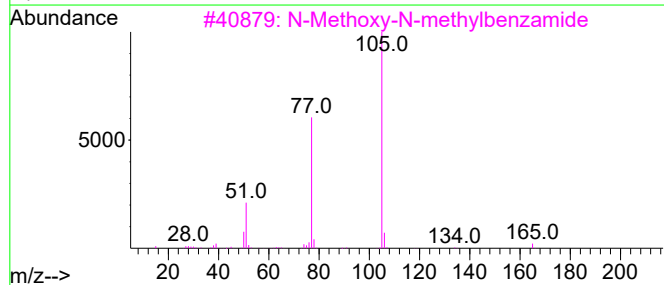
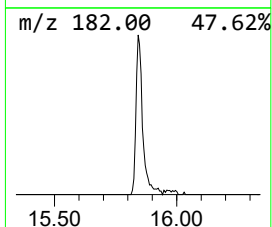
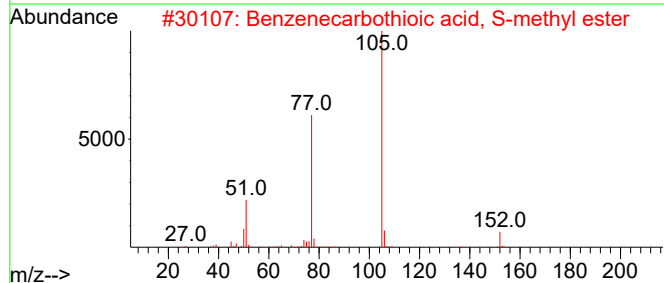
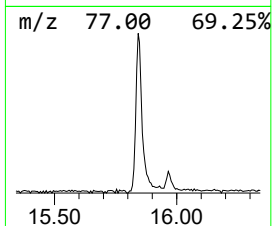
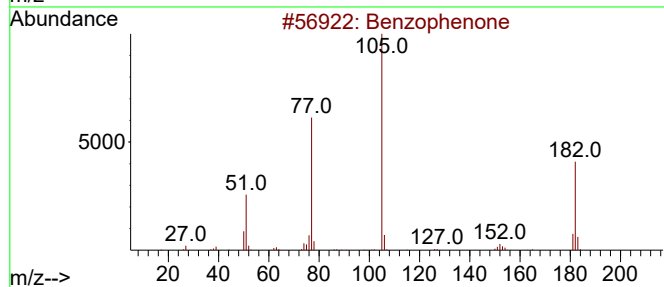
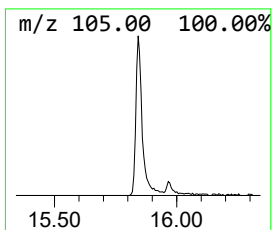
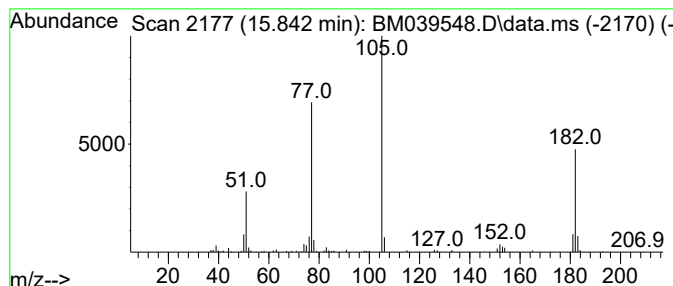
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.842	2.02 ng	154438	Acenaphthene-d10	14.471

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			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			2-(2-Oxo-2-phenyl-ethyl)-malon...	184	C11H8N2O	1000296-76-9	47
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47



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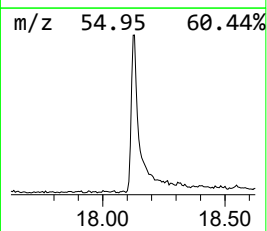
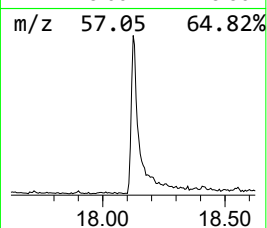
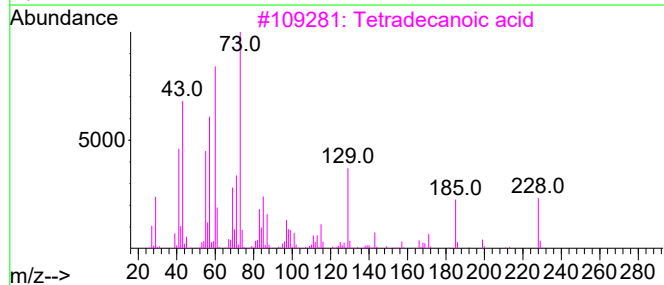
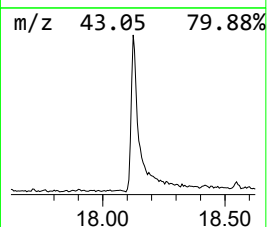
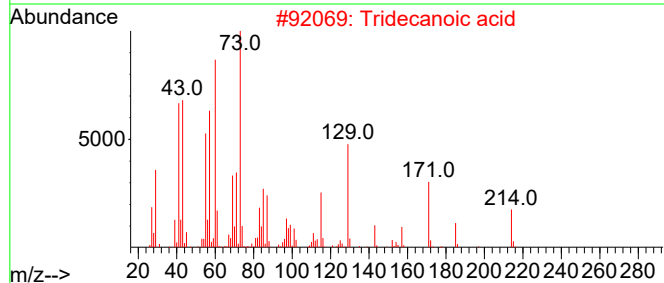
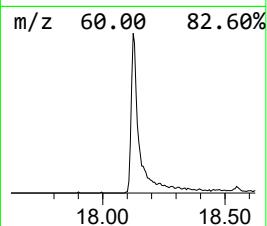
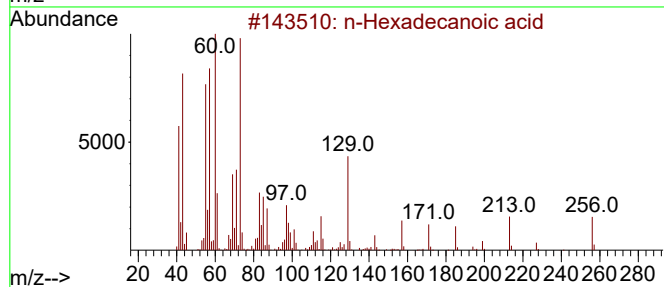
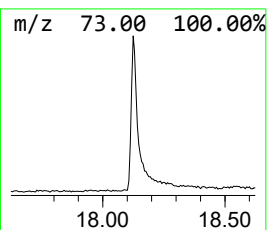
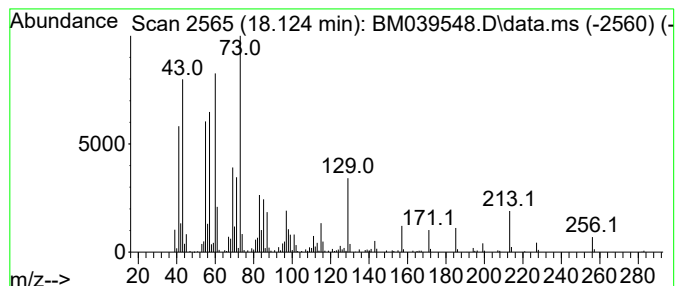
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.124	6.90 ng	585504	Phenanthrene-d10	17.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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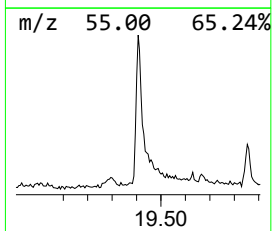
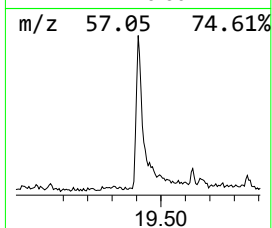
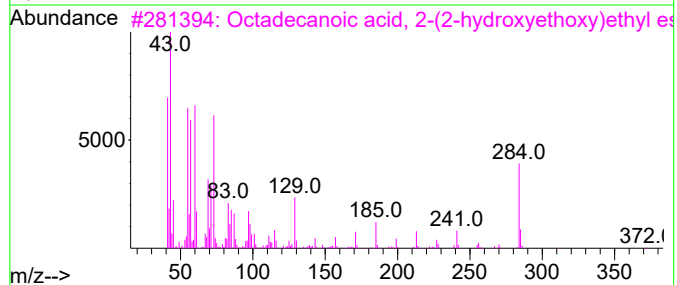
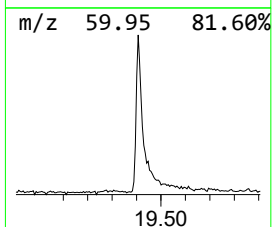
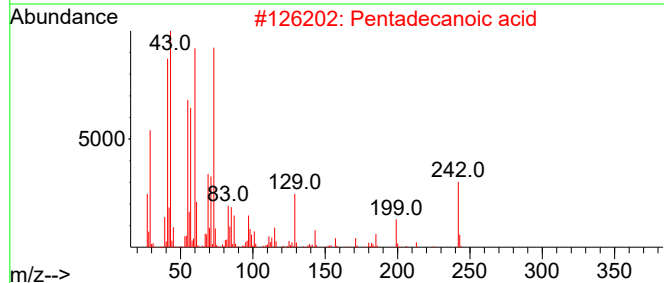
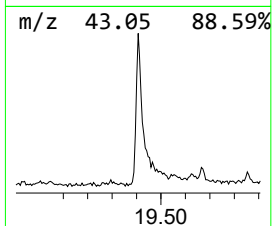
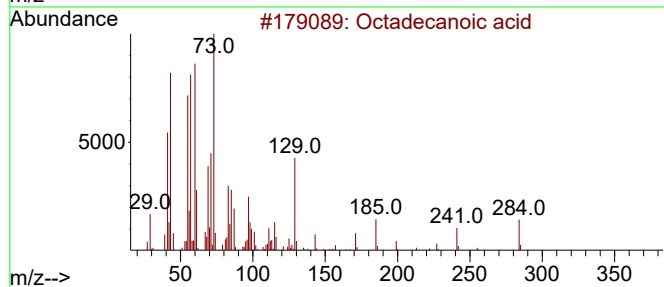
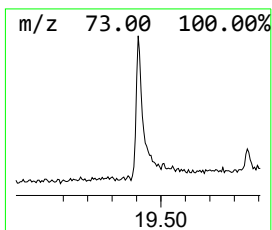
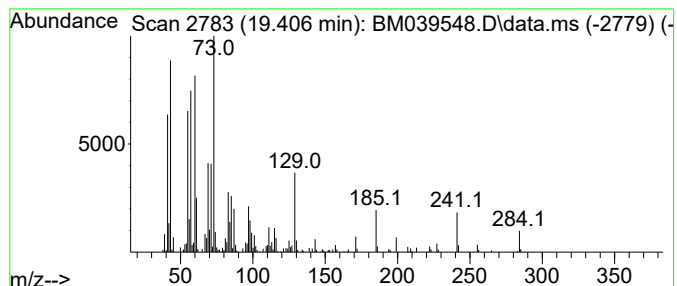
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.406	4.29 ng	383352	Chrysene-d12	21.424

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	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



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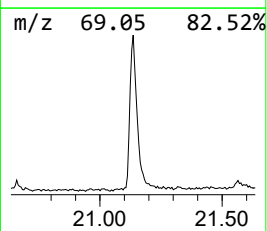
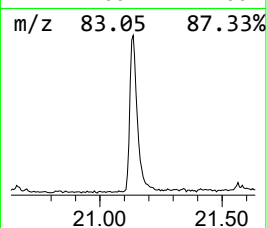
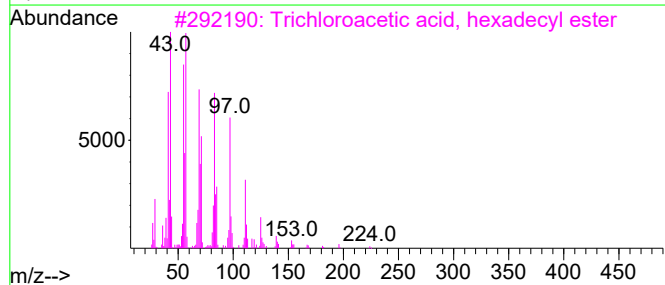
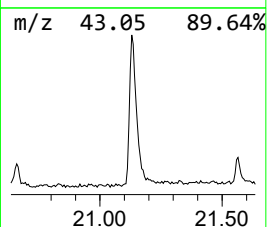
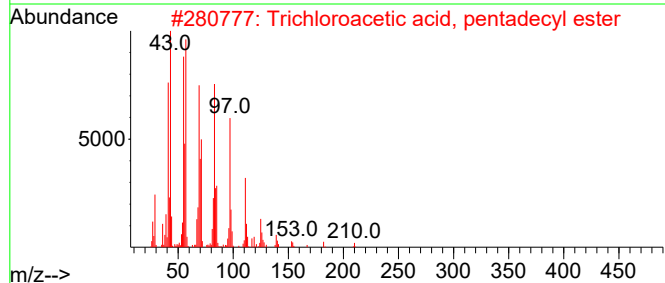
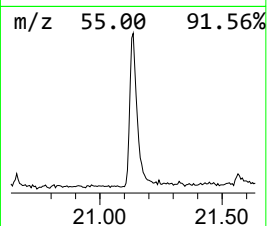
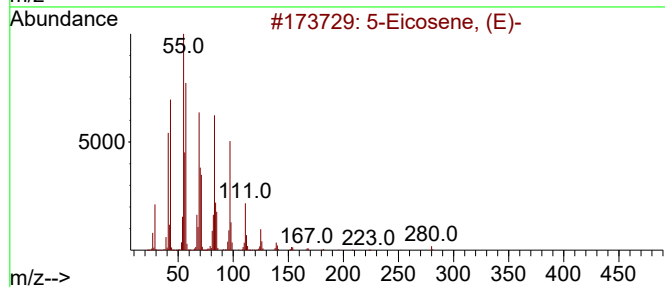
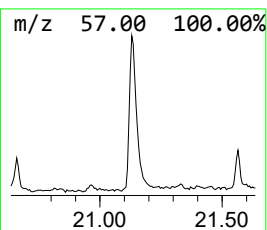
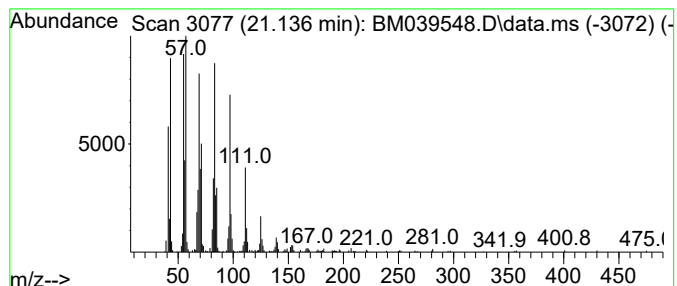
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.136	6.64 ng	593254	Chrysene-d12	21.424

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	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-...	4.913	8.8	ng	403272	1	7.819	914731	20.0
Benzophenone	15.842	2.0	ng	154438	3	14.471	1526120	20.0
n-Hexadecanoic ...	18.124	6.9	ng	585504	4	17.224	1695940	20.0
Octadecanoic acid	19.406	4.3	ng	383352	5	21.424	1786100	20.0
5-Eicosene, (E)-	21.136	6.6	ng	593254	5	21.424	1786100	20.0