

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041423\
 Data File : BM039437.D
 Acq On : 14 Apr 2023 17:51
 Operator : CG/JU
 Sample : 02347-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 20230333-COMP-11

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-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039437.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.940	292	298	312	rBV	888781	1236957	14.09%	2.345%
2	5.422	374	380	402	rBV	3668250	5616380	63.96%	10.648%
3	6.028	478	483	495	rVB	59201	94542	1.08%	0.179%
4	7.045	649	656	682	rBV	3348022	5708201	65.00%	10.822%
5	7.851	785	793	806	rBV	575903	991544	11.29%	1.880%
6	9.022	983	992	1017	rBV	1966022	3567042	40.62%	6.762%
7	10.663	1261	1271	1284	rBV	705155	1305597	14.87%	2.475%
8	13.127	1683	1690	1712	rBV	4570772	6954134	79.19%	13.184%
9	14.510	1918	1925	1942	rBV	1031479	1643971	18.72%	3.117%
10	15.868	2148	2156	2172	rBV	647538	980983	11.17%	1.860%
11	16.004	2172	2179	2203	rBV	3683870	5578284	63.53%	10.575%
12	17.256	2386	2392	2404	rBV	1211789	1837628	20.93%	3.484%
13	18.162	2540	2546	2555	rBV	1105025	1948092	22.18%	3.693%
14	19.439	2758	2763	2779	rBV	629112	1248618	14.22%	2.367%
15	19.886	2834	2839	2852	rBV	6880218	8781231	100.00%	16.648%
16	20.686	2972	2975	2979	rBV2	89419	105714	1.20%	0.200%
17	21.150	3050	3054	3062	rBV	775348	1049564	11.95%	1.990%
18	21.444	3100	3104	3117	rBV	1416962	2013847	22.93%	3.818%
19	23.827	3504	3509	3519	rVB2	1022408	2085562	23.75%	3.954%

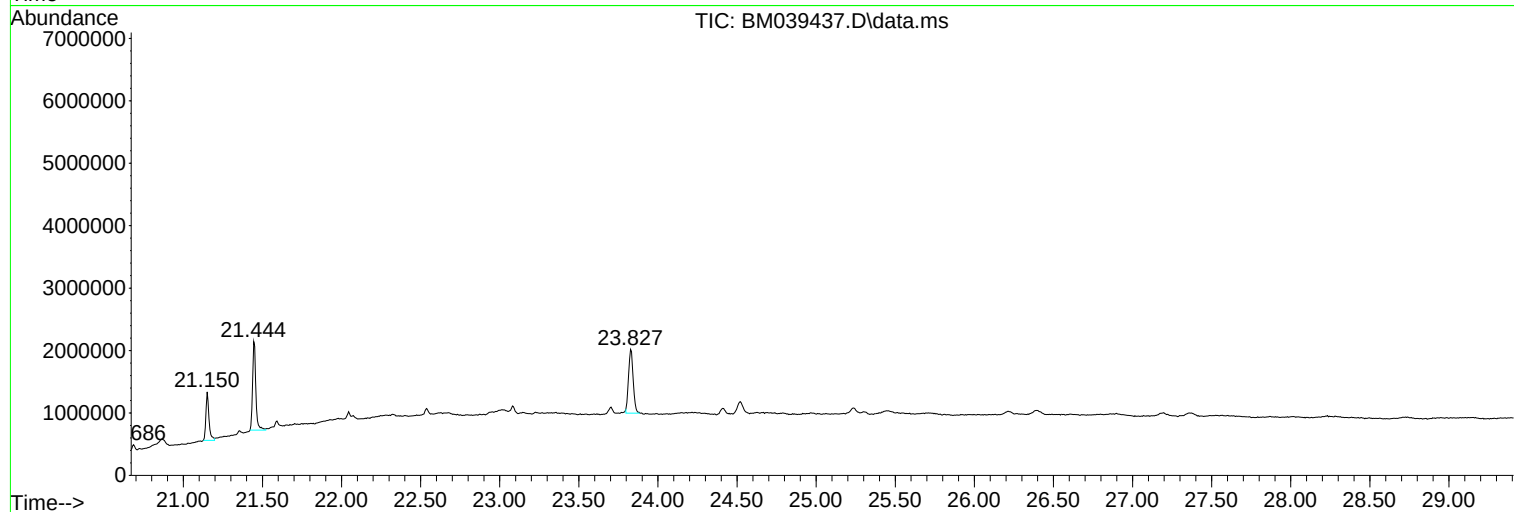
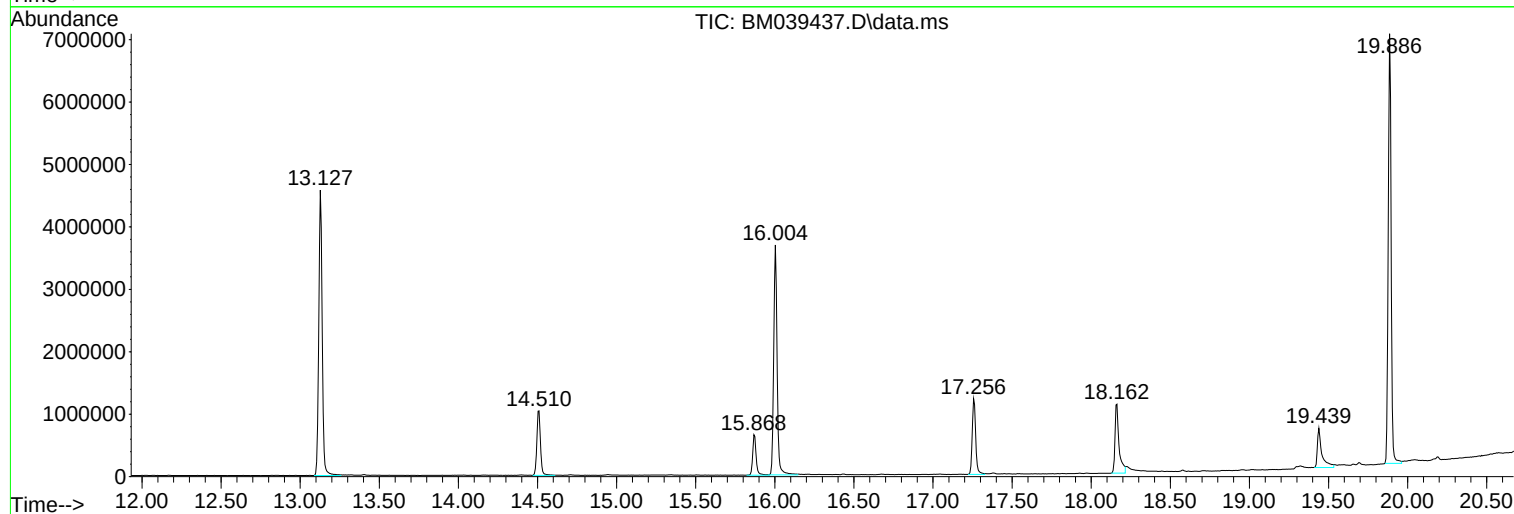
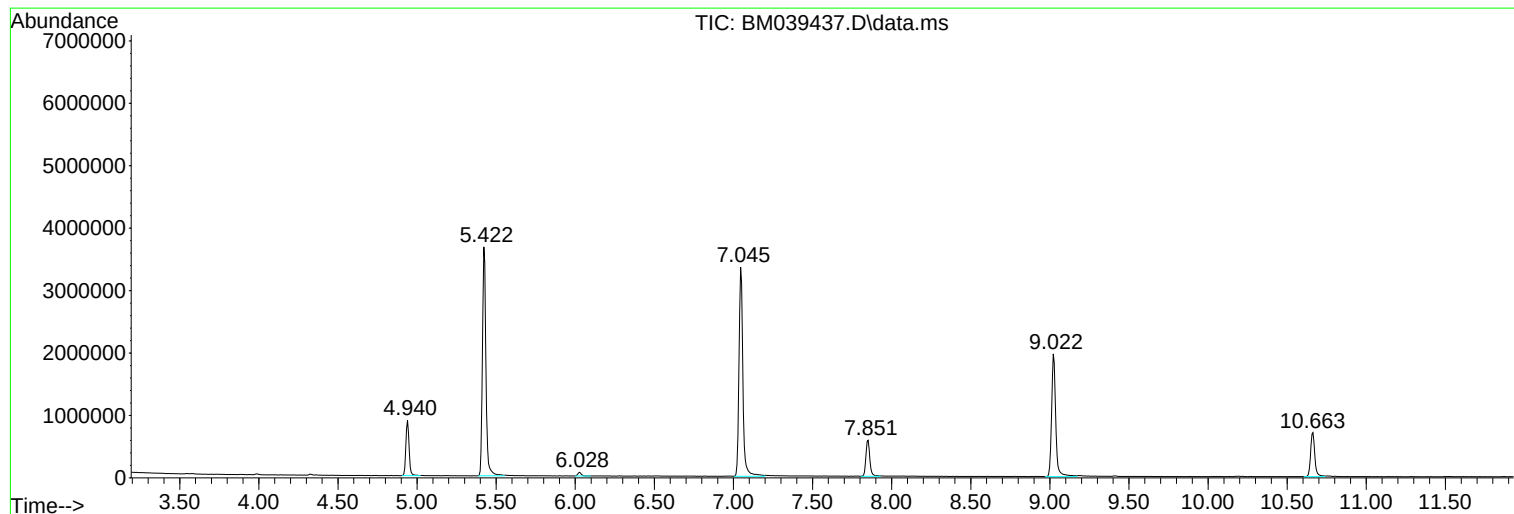
Sum of corrected areas: 52747891

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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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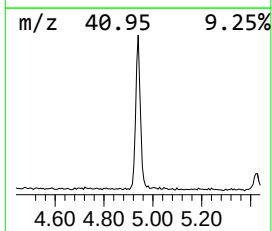
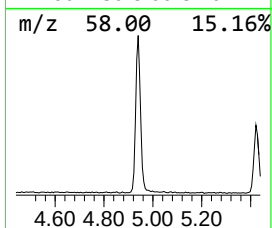
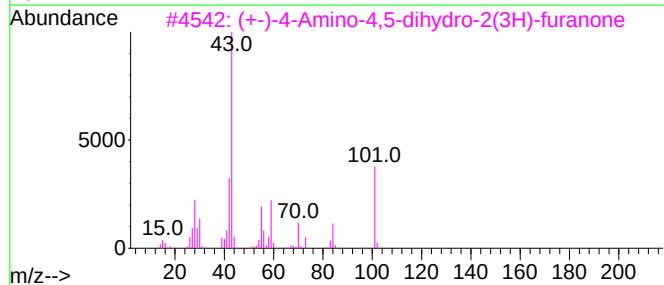
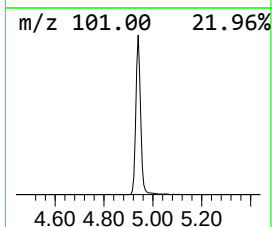
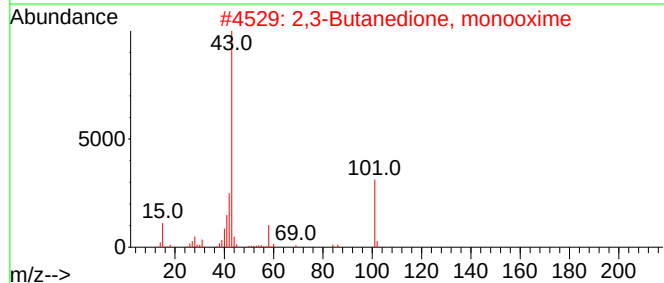
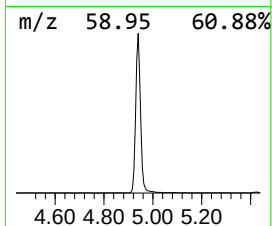
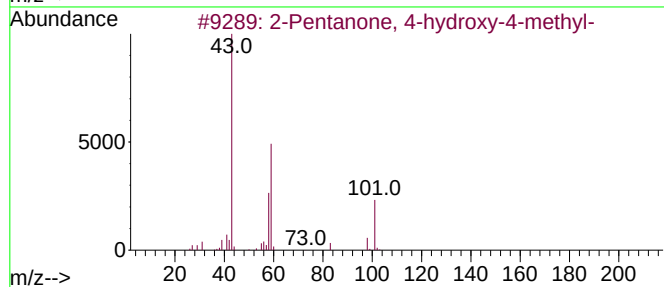
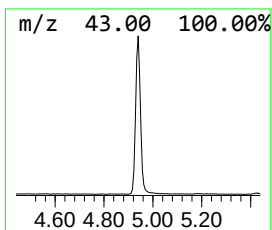
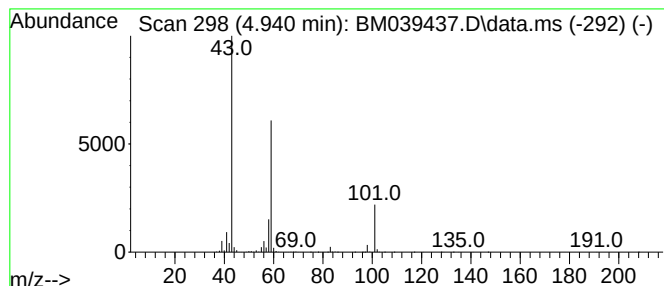
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.940	24.95 ng	1236960	1,4-Dichlorobenzene-d4	7.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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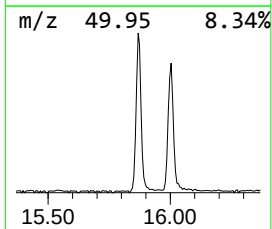
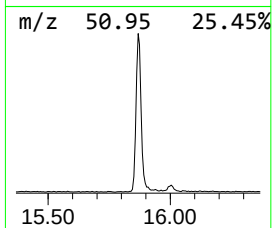
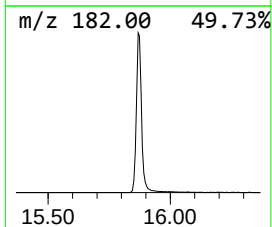
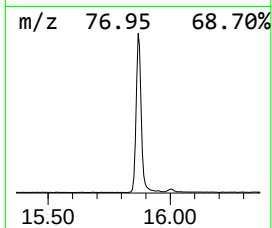
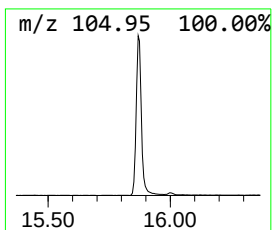
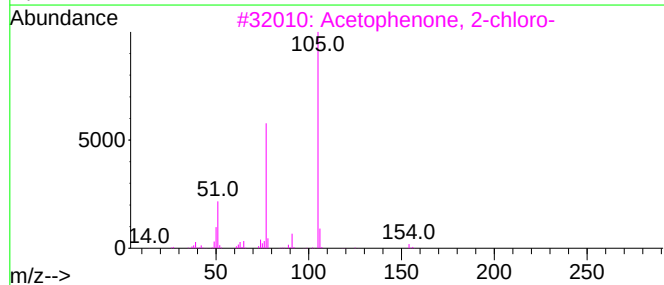
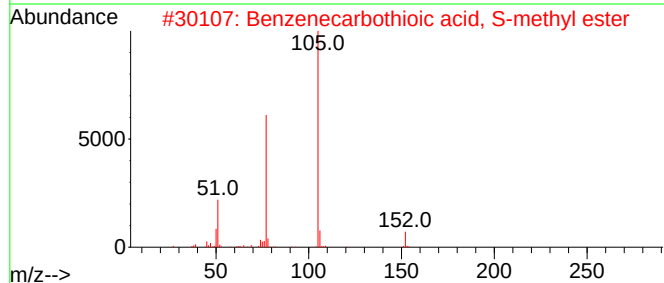
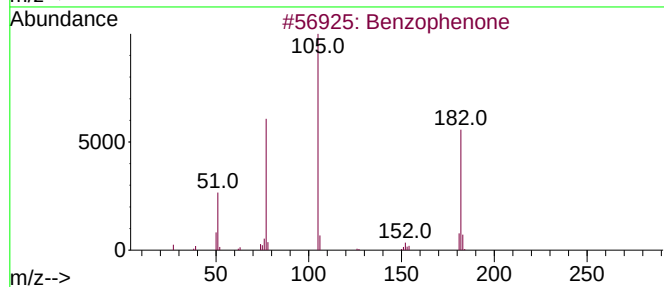
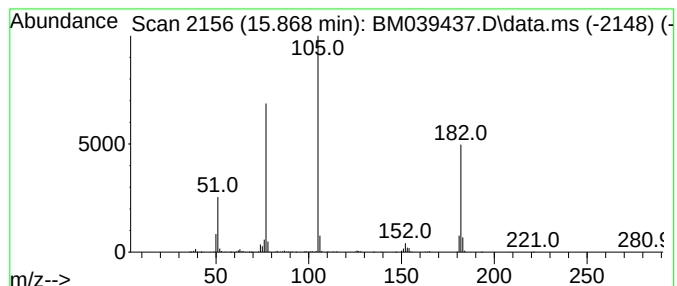
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.868	11.93 ng	980983	Acenaphthene-d10	14.509

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	52
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	47



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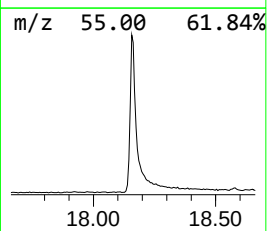
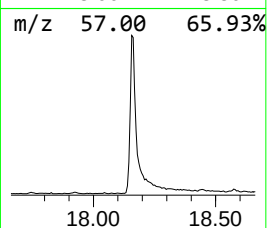
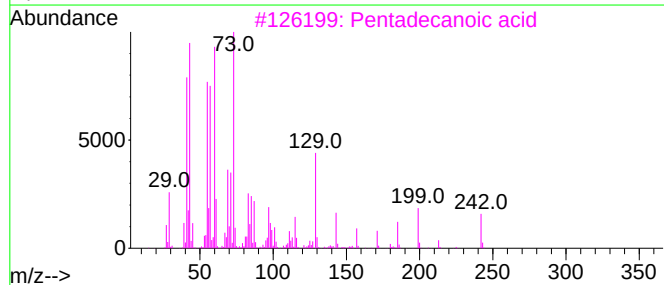
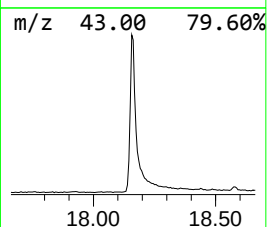
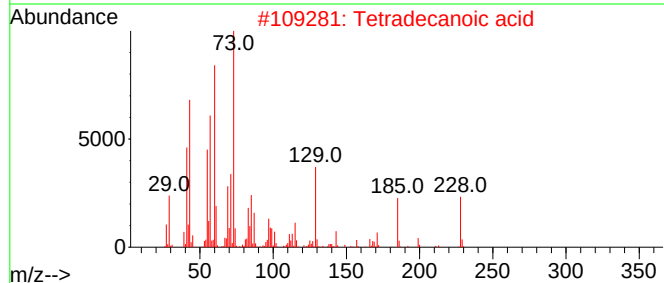
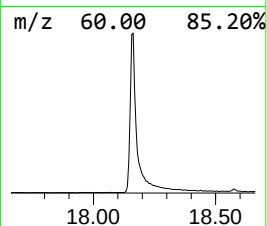
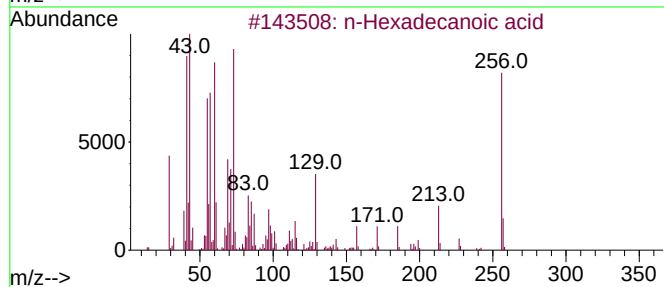
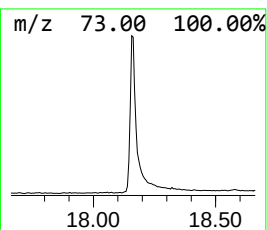
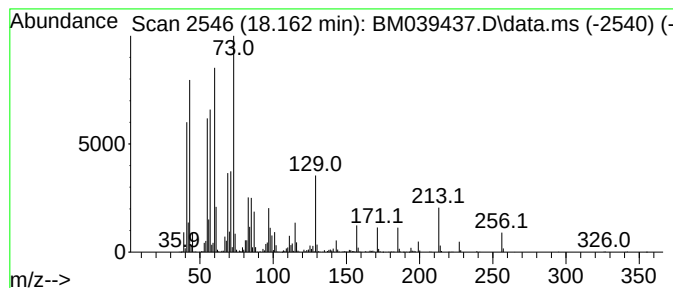
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.162	21.20 ng	1948090	Phenanthrene-d10	17.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	89
5			Octadecanoic acid	284	C18H36O2	000057-11-4	81



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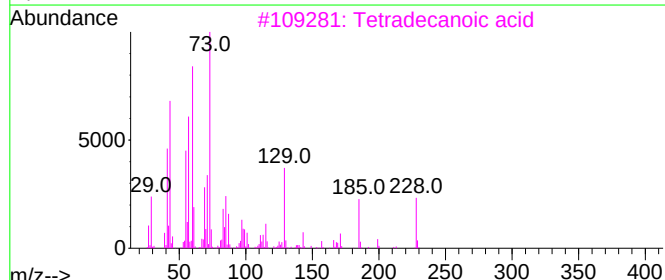
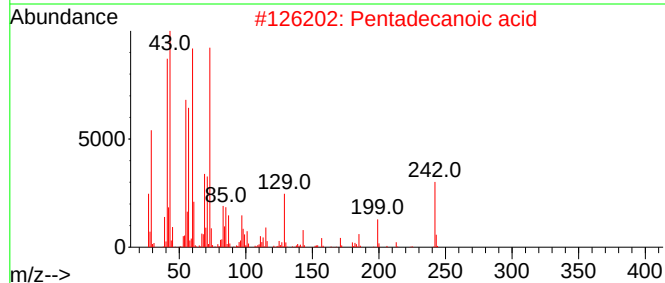
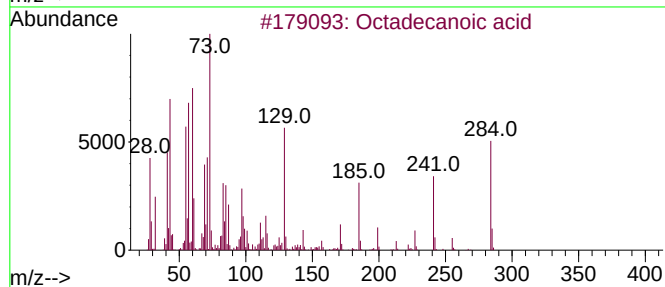
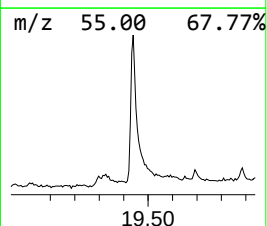
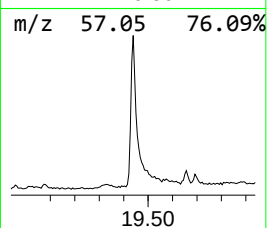
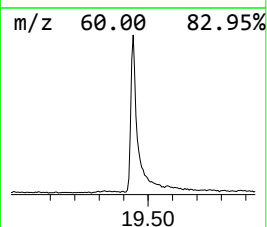
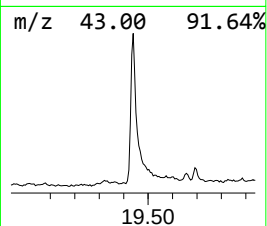
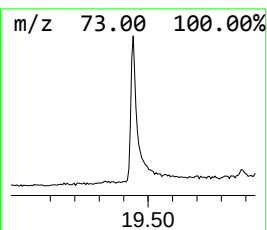
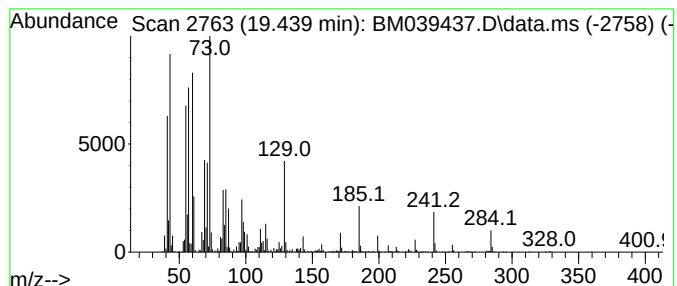
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	12.40 ng	1248620	Chrysene-d12	21.444

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83



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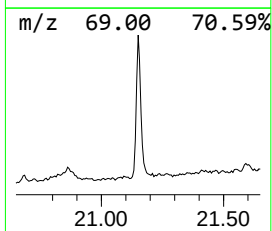
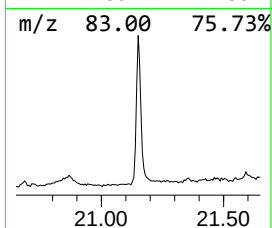
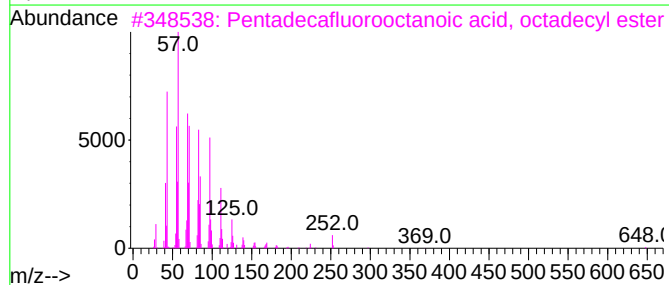
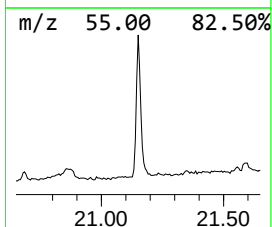
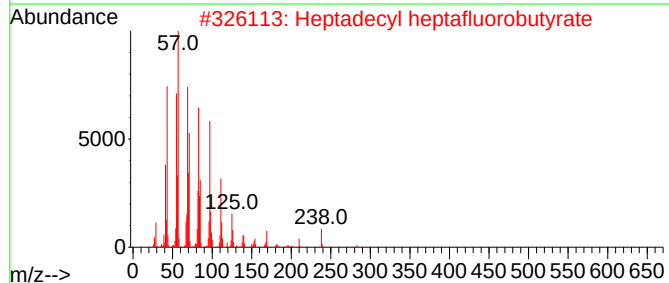
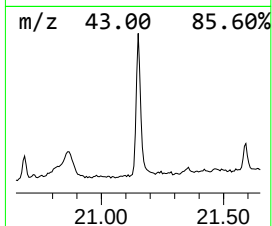
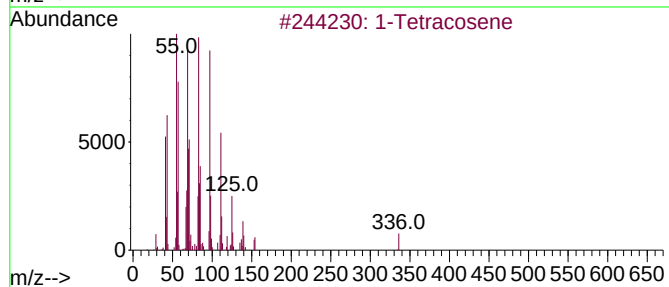
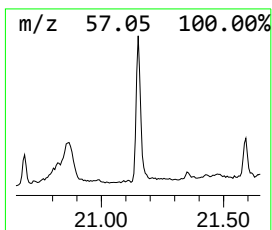
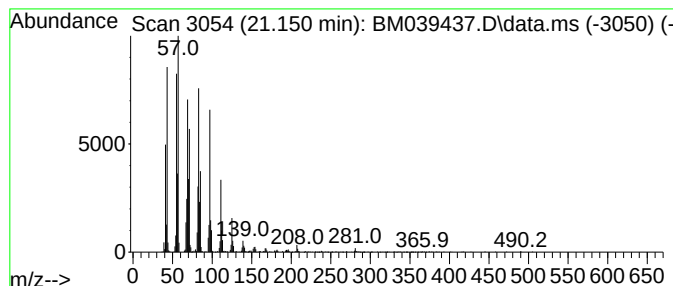
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Peak Number 5 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.150	10.42 ng	1049560	Chrysene-d12	21.444	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	97
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.940	24.9	ng	1236960	1	7.851	991544	20.0
Benzophenone	15.868	11.9	ng	980983	3	14.509	1643970	20.0
n-Hexadecanoic ...	18.162	21.2	ng	1948090	4	17.256	1837630	20.0
Octadecanoic acid	19.439	12.4	ng	1248620	5	21.444	2013850	20.0
1-Tetracosene	21.150	10.4	ng	1049560	5	21.444	2013850	20.0