

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111122\
 Data File : BM037466.D
 Acq On : 11 Nov 2022 14:27
 Operator : CG/JU
 Sample : N5530-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-12

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-BM102822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037466.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.381	46	50	56	rVB	139441	153823	1.18%	0.208%
2	4.305	202	207	212	rBV	102300	134315	1.03%	0.181%
3	4.916	305	311	323	rBV	1232195	1674772	12.88%	2.259%
4	5.381	383	390	412	rBV	5611498	8012553	61.61%	10.810%
5	6.993	656	664	683	rBV	5262809	8278841	63.66%	11.169%
6	7.804	795	802	810	rBV	1116897	1707339	13.13%	2.303%
7	8.981	993	1002	1020	rBV	3148053	5304874	40.79%	7.157%
8	10.398	1235	1243	1260	rBV	113165	335930	2.58%	0.453%
9	10.604	1271	1278	1289	rBV	1349529	2289098	17.60%	3.088%
10	13.075	1690	1698	1713	rBV	8504751	12109288	93.12%	16.337%
11	14.451	1926	1932	1944	rBV	1957642	2840048	21.84%	3.832%
12	15.945	2176	2186	2204	rBV	5921274	8431611	64.84%	11.375%
13	17.198	2392	2399	2411	rBV	1906254	2838694	21.83%	3.830%
14	18.092	2546	2551	2561	rBV	449701	834058	6.41%	1.125%
15	19.374	2765	2769	2781	rBV2	270118	545385	4.19%	0.736%
16	19.821	2840	2845	2859	rBV	10681220	13004278	100.00%	17.545%
17	20.586	2972	2975	2978	rBV	122388	137703	1.06%	0.186%
18	21.092	3057	3061	3068	rBV2	324177	478613	3.68%	0.646%
19	21.380	3106	3110	3120	rBV	1842361	2430074	18.69%	3.278%
20	23.721	3502	3508	3520	rVB2	1265721	2580306	19.84%	3.481%

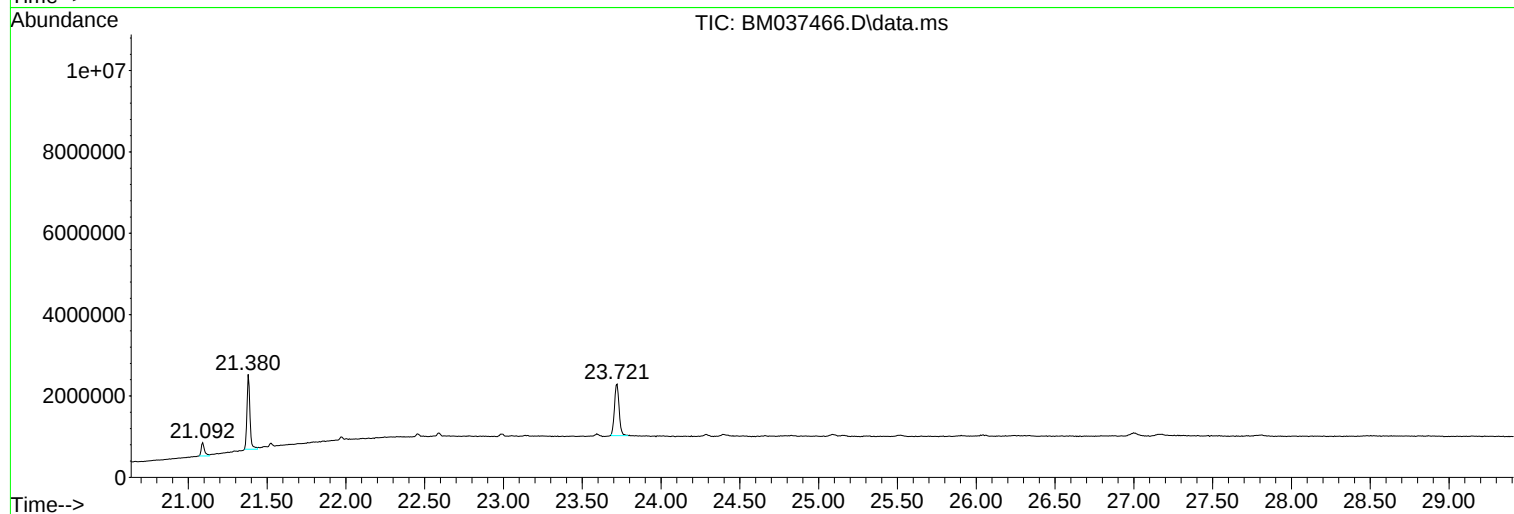
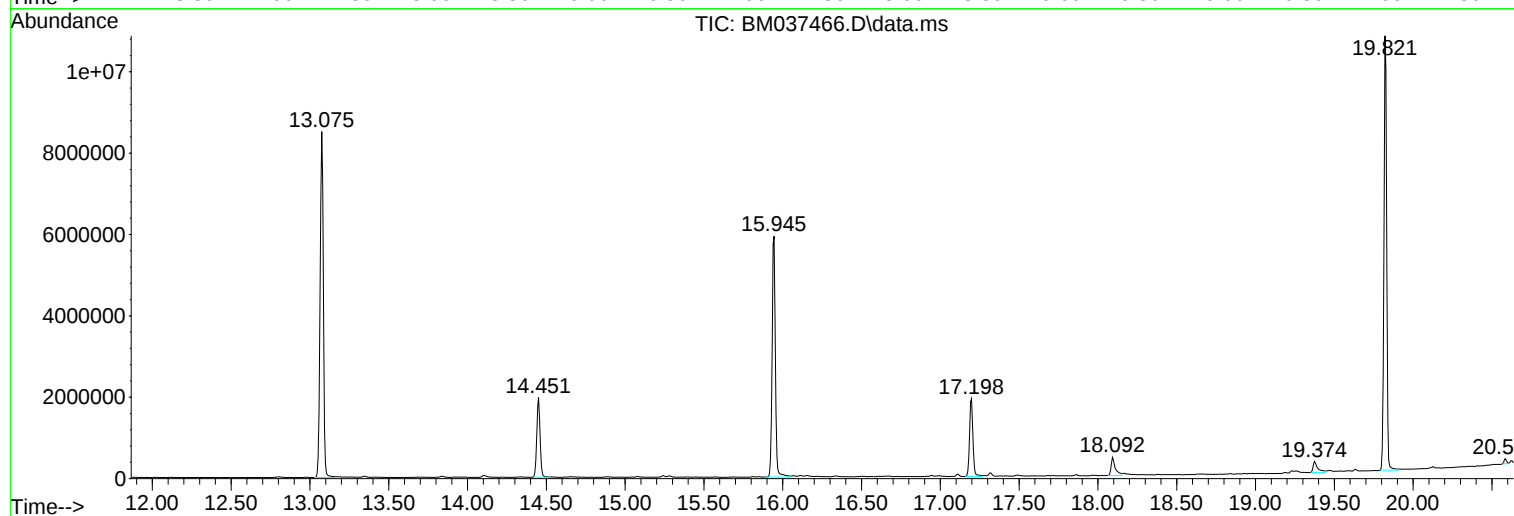
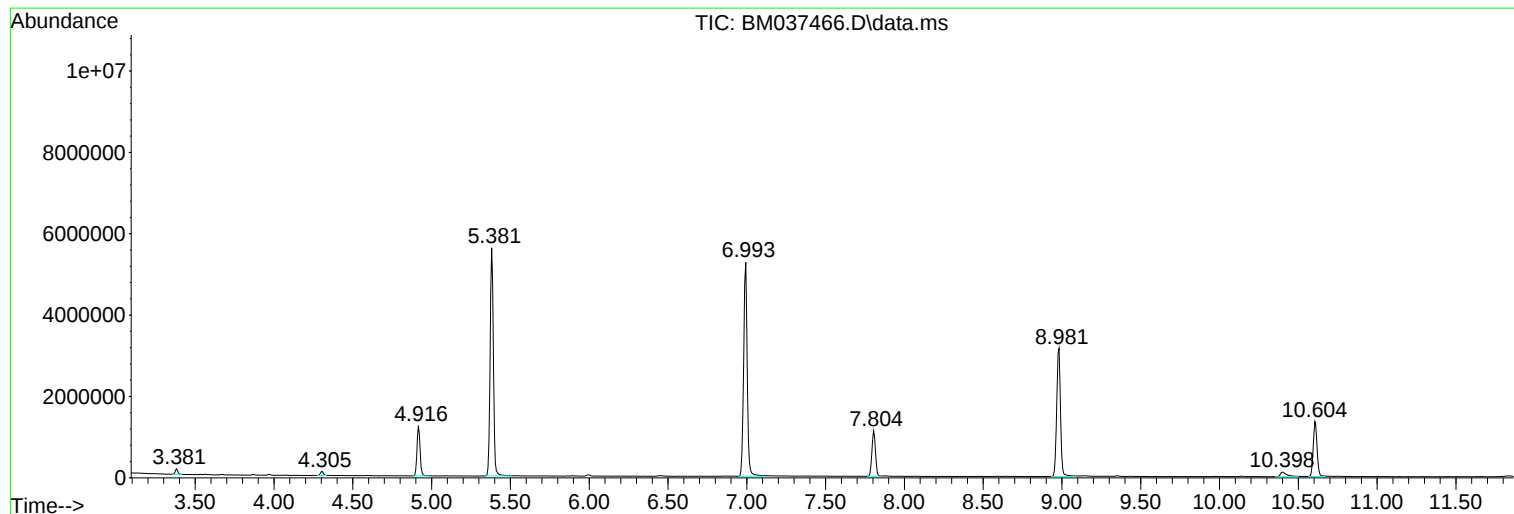
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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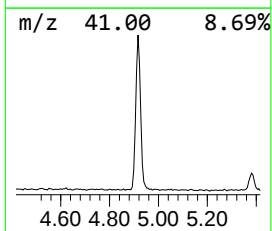
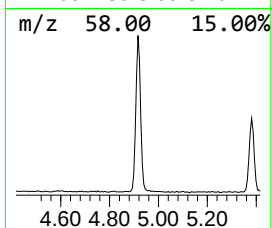
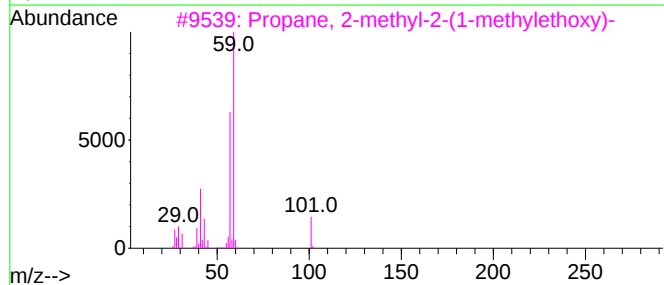
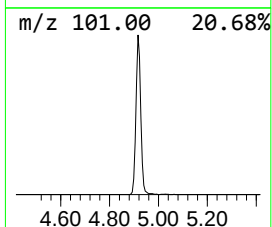
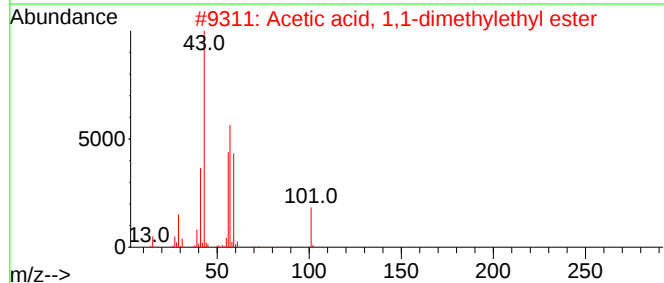
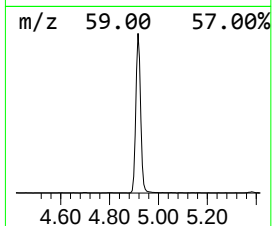
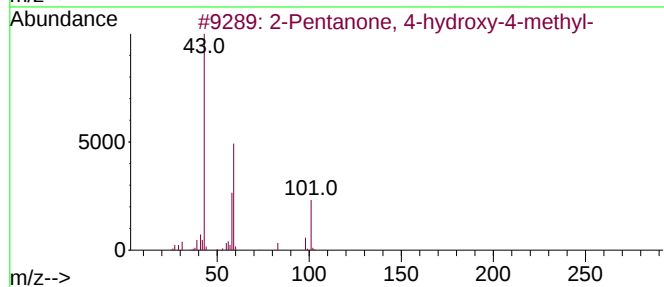
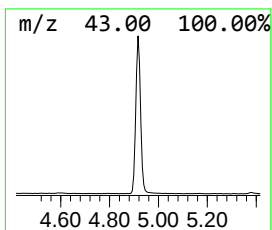
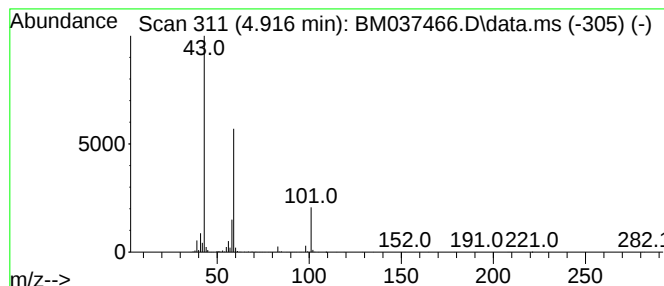
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.916	19.62 ng	1674770	1,4-Dichlorobenzene-d4	7.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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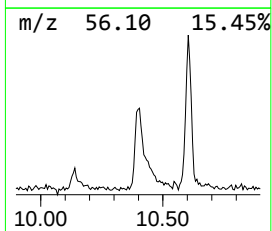
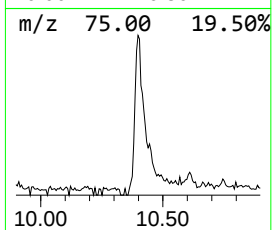
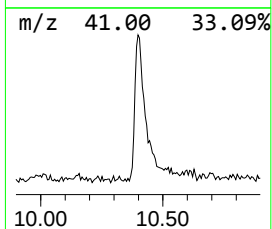
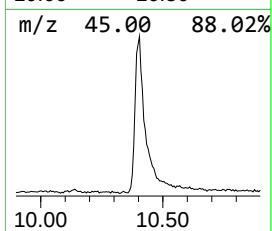
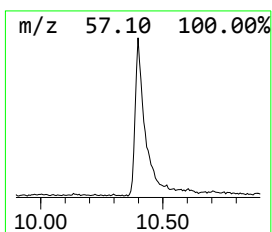
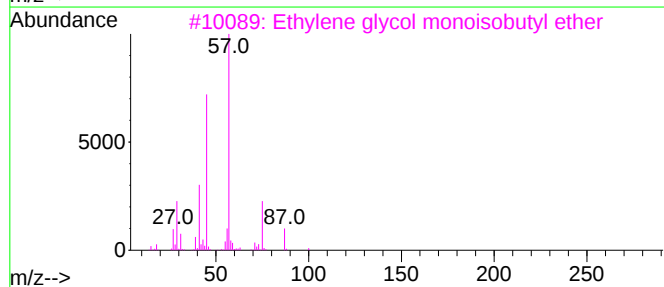
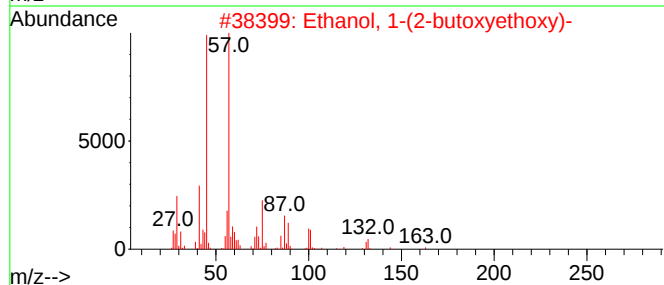
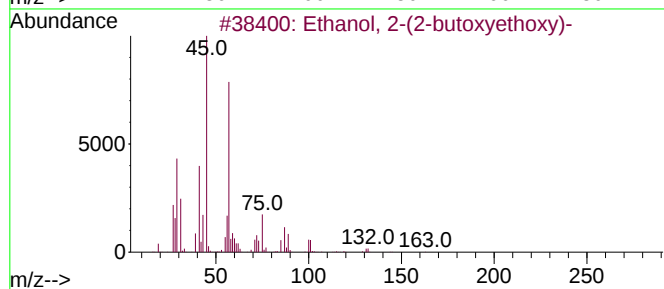
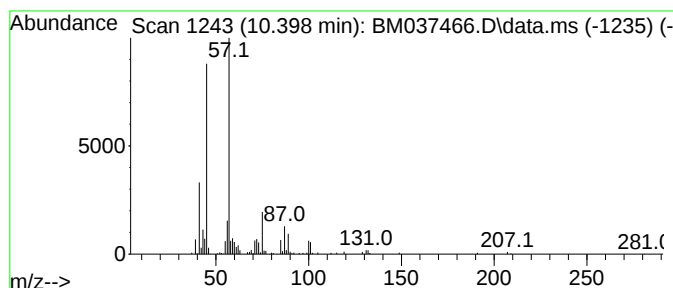
Instrument :
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ClientSampleId :
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.398	2.94 ng	335930	Naphthalene-d8	10.604	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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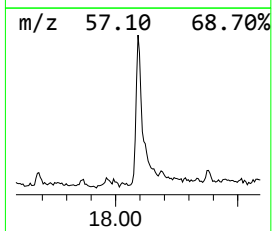
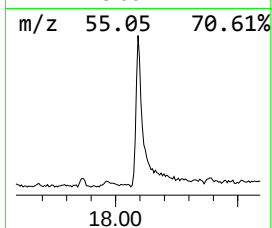
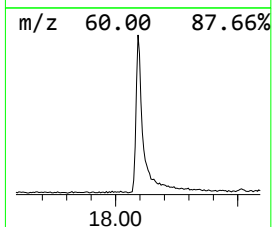
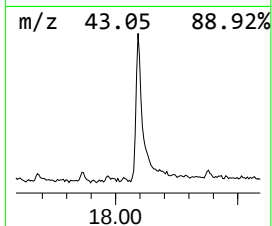
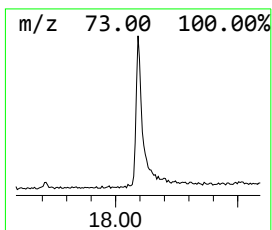
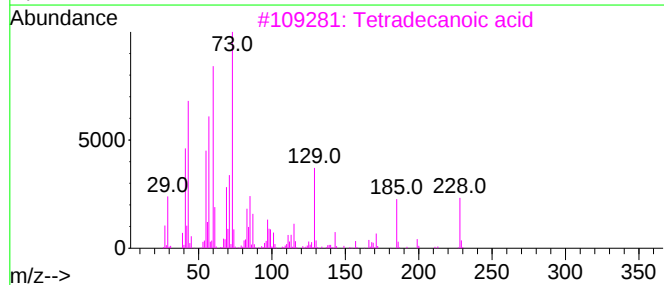
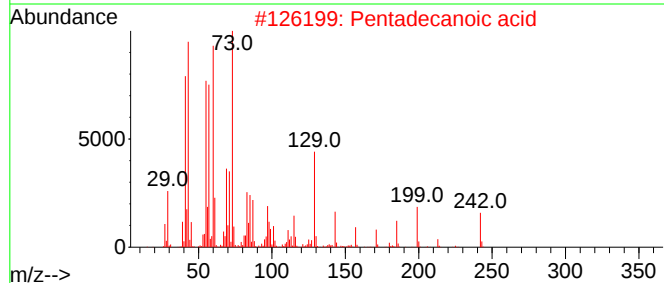
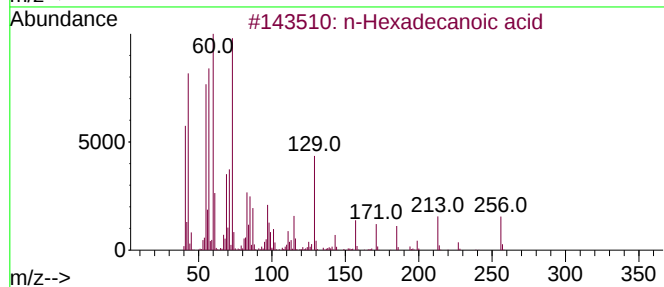
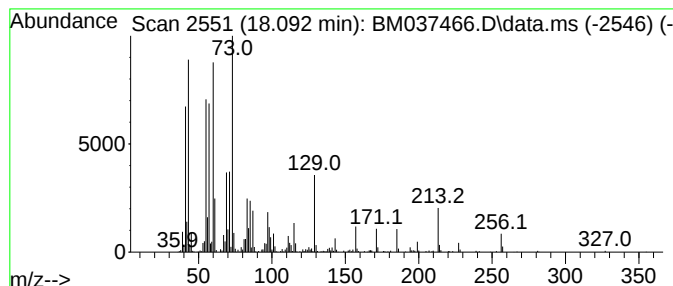
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	5.88 ng	834058	Phenanthrene-d10	17.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Octadecanoic acid	284	C18H36O2	000057-11-4	64



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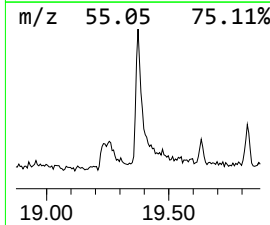
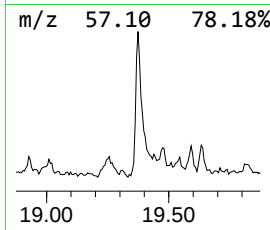
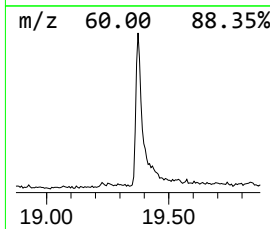
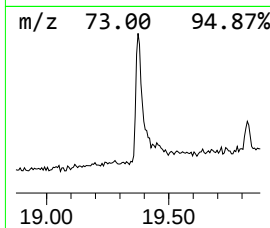
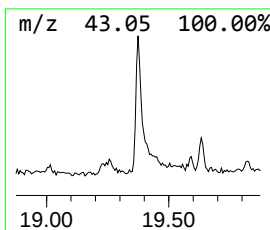
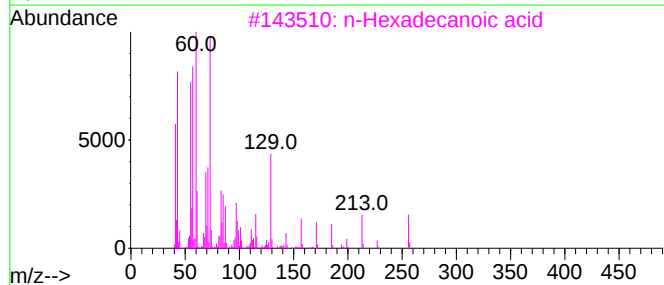
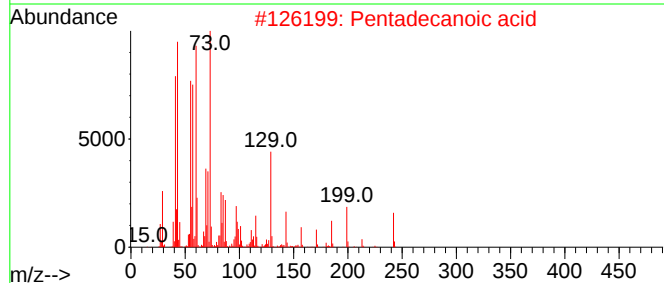
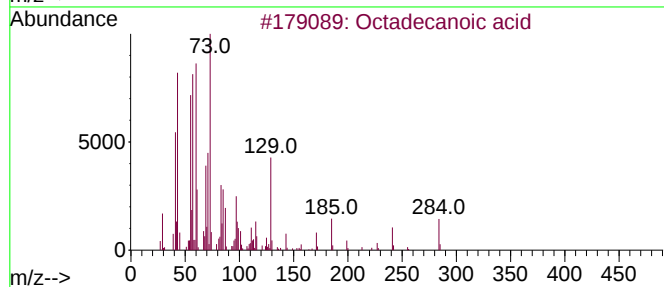
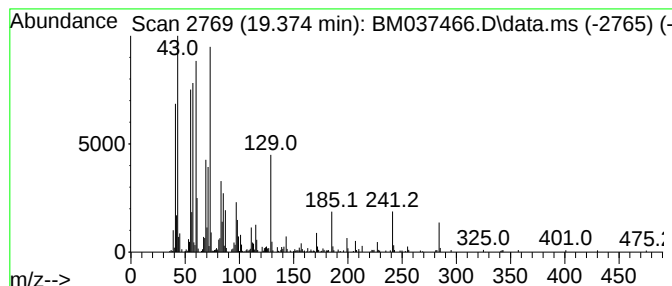
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.374	4.49 ng	545385	Chrysene-d12	21.380

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			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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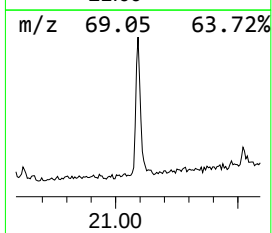
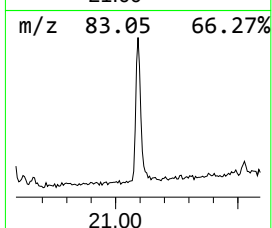
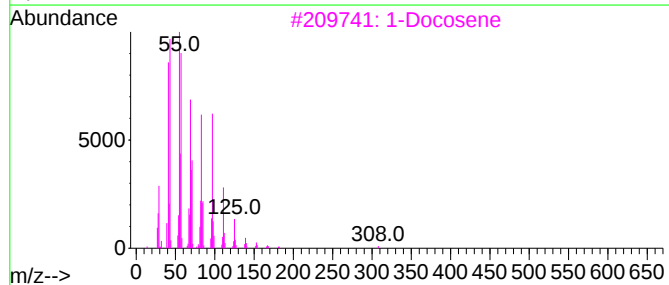
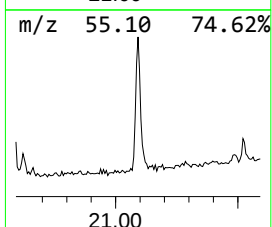
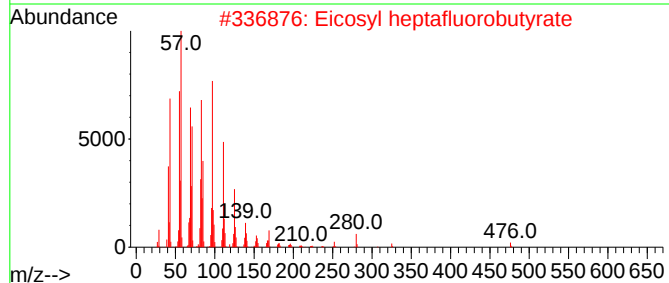
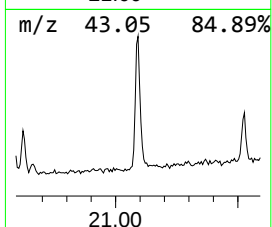
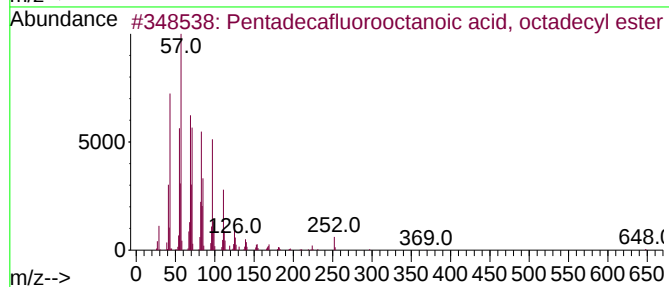
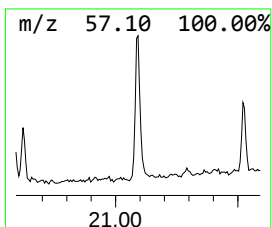
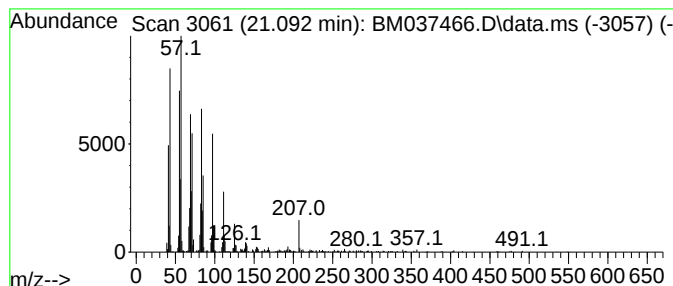
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	3.94 ng	478613	Chrysene-d12	21.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3			1-Docosene	308	C22H44	001599-67-3	89
4			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.916	19.6	ng	1674770	1	7.804	1707340	20.0
Ethanol, 2-(2-b...	10.398	2.9	ng	335930	2	10.604	2289100	20.0
n-Hexadecanoic ...	18.092	5.9	ng	834058	4	17.198	2838690	20.0
Octadecanoic acid	19.374	4.5	ng	545385	5	21.380	2430070	20.0
Pentadecafluoro...	21.092	3.9	ng	478613	5	21.380	2430070	20.0