

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111122\
 Data File : BM037476.D
 Acq On : 11 Nov 2022 20:41
 Operator : CG/JU
 Sample : N5531-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-33

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: BM037476.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.916	305	311	324	rBV	1142457	1566228	11.07%	2.197%
2	5.381	383	390	405	rBV	5306370	7766243	54.88%	10.892%
3	6.987	656	663	682	rBV	4949148	7969240	56.31%	11.177%
4	7.804	795	802	810	rBV	949790	1481779	10.47%	2.078%
5	8.975	993	1001	1018	rBV	3006886	5088695	35.96%	7.137%
6	10.398	1235	1243	1263	rBV4	74934	265308	1.87%	0.372%
7	10.604	1271	1278	1291	rBV	1183551	1972455	13.94%	2.766%
8	13.074	1690	1698	1714	rBV	8040954	11398498	80.54%	15.986%
9	14.451	1925	1932	1943	rBV	1626561	2467013	17.43%	3.460%
10	15.939	2174	2185	2204	rBV	5623359	8559868	60.49%	12.005%
11	17.192	2392	2398	2412	rBV	1700614	2627057	18.56%	3.684%
12	18.092	2546	2551	2562	rBV	233371	504939	3.57%	0.708%
13	19.374	2765	2769	2781	rBV2	144232	309699	2.19%	0.434%
14	19.821	2840	2845	2862	rBV	11732819	14151776	100.00%	19.848%
15	20.586	2972	2975	2978	rBV	139124	148868	1.05%	0.209%
16	21.091	3057	3061	3071	rBV2	332472	558748	3.95%	0.784%
17	21.380	3106	3110	3119	rBV	1777885	2308197	16.31%	3.237%
18	23.721	3502	3508	3522	rVB2	1061912	2157157	15.24%	3.025%

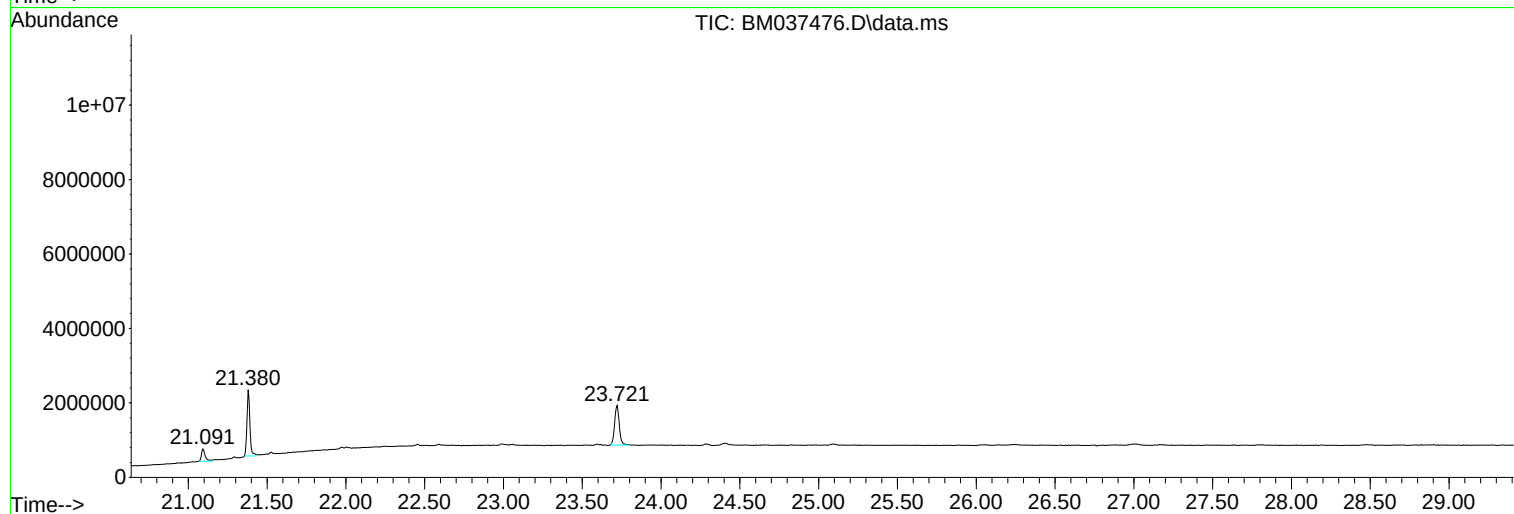
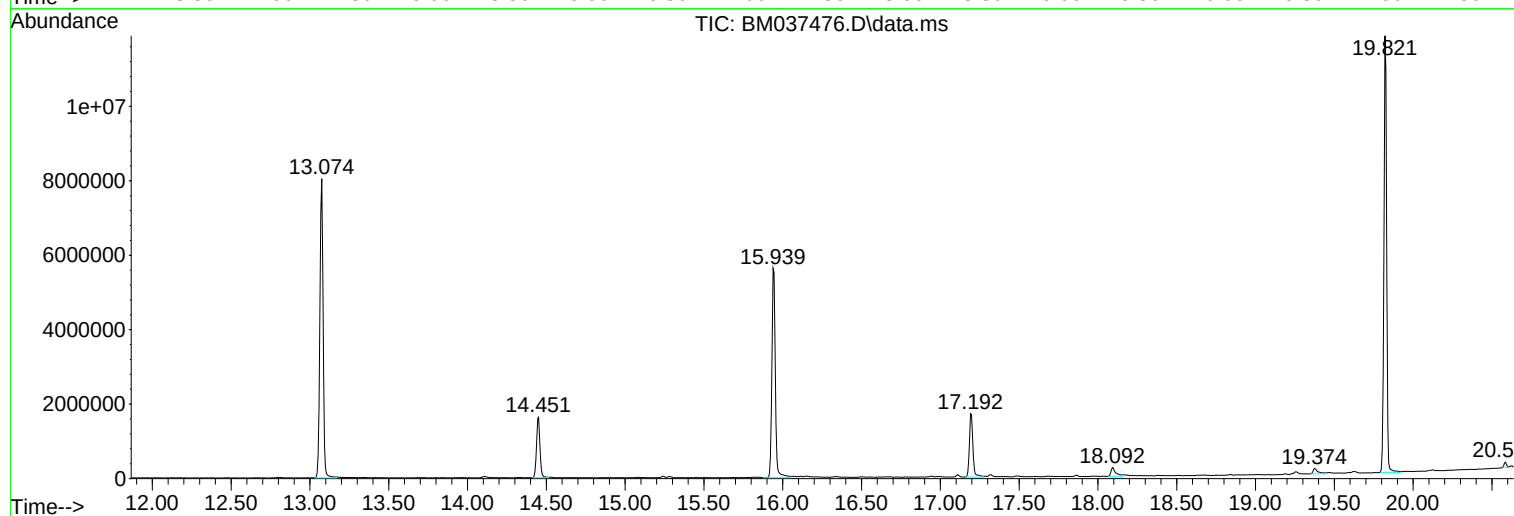
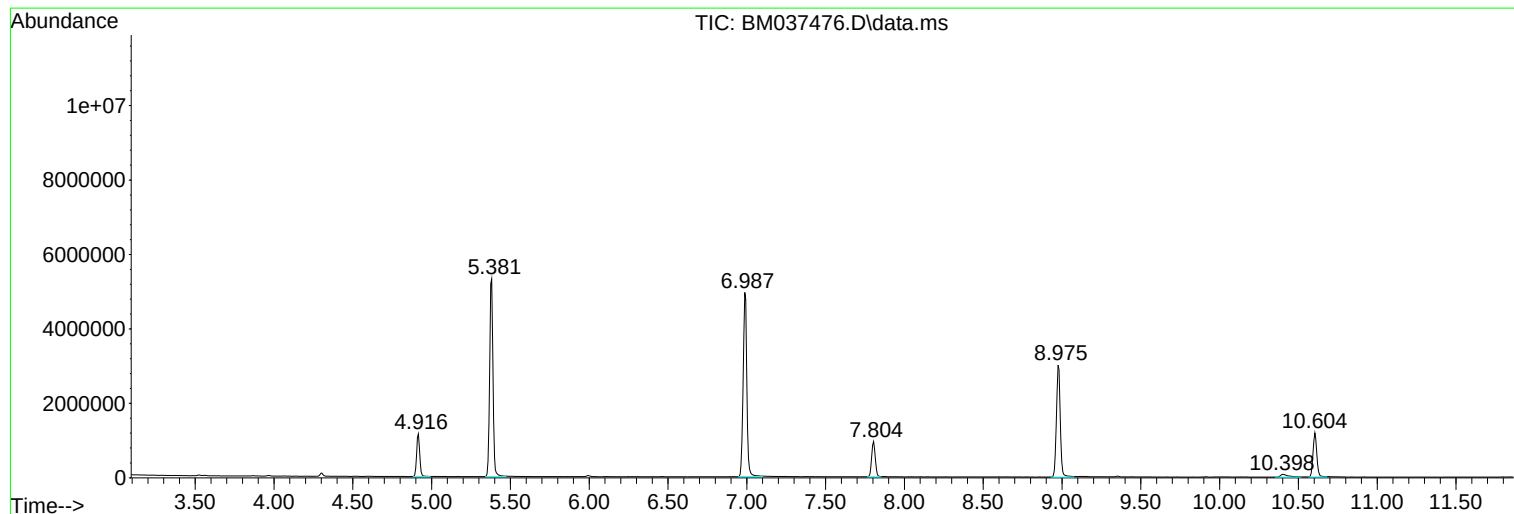
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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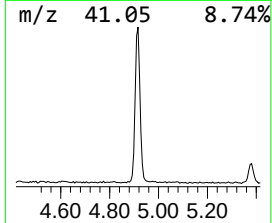
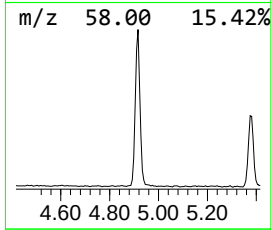
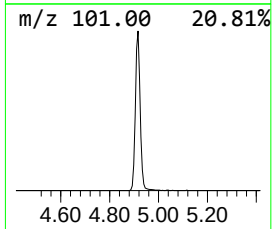
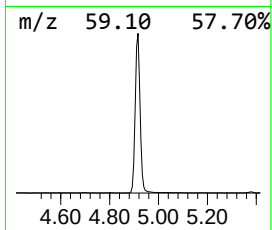
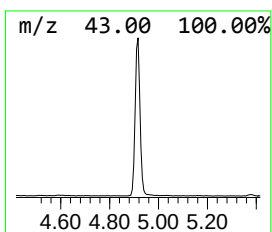
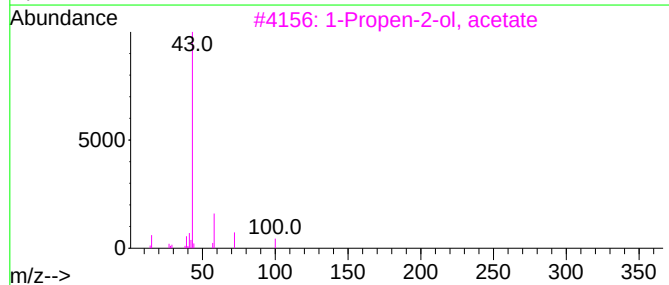
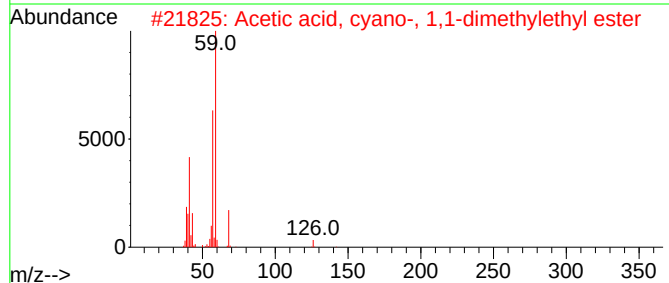
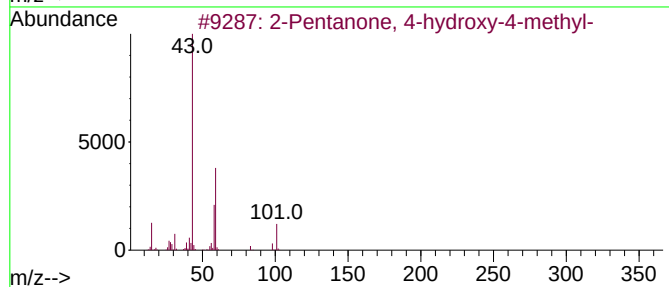
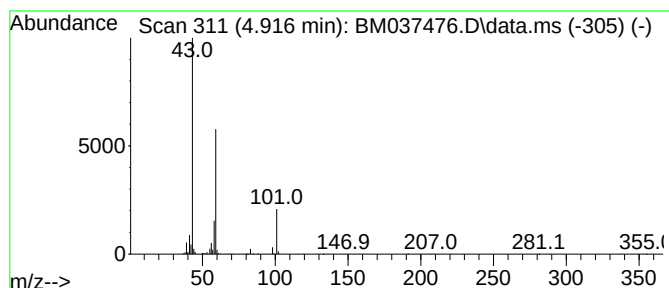
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	21.14 ng	1566230	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	47		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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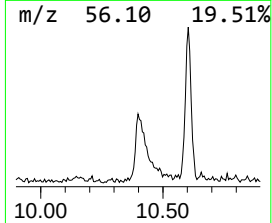
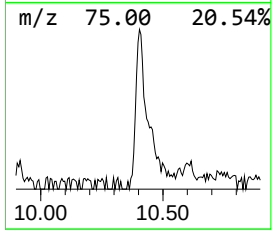
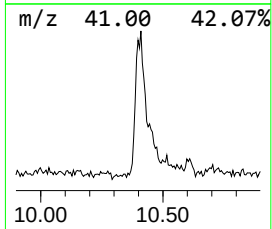
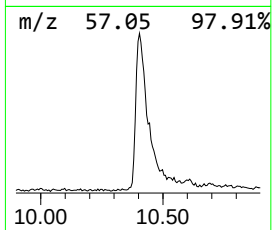
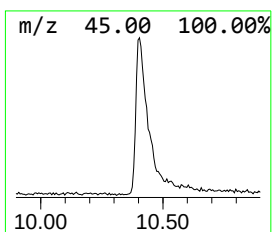
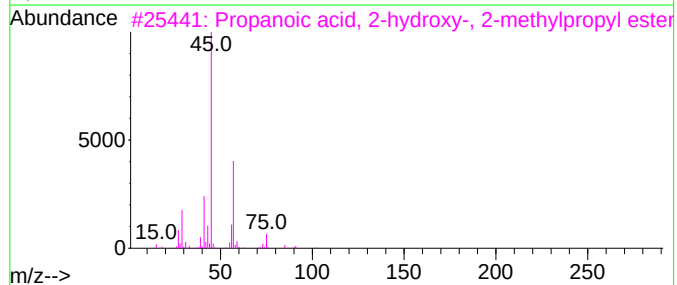
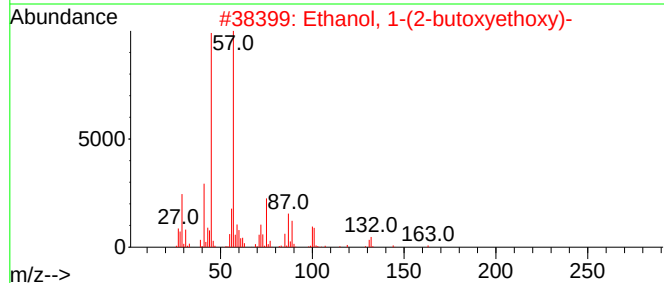
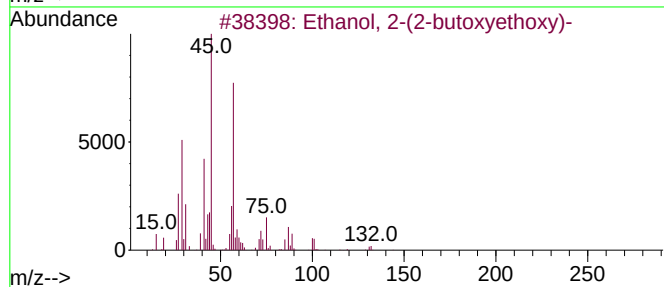
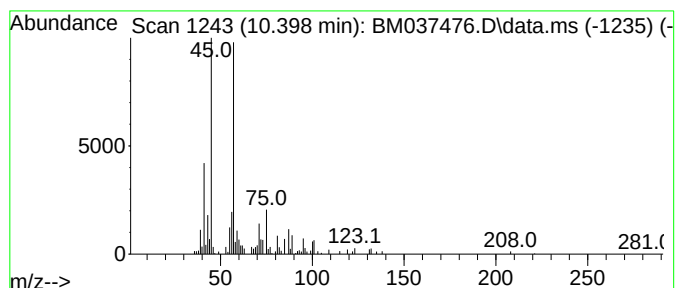
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.398	2.69 ng	265308	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	80
3	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	72
4	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	53
5	Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	53



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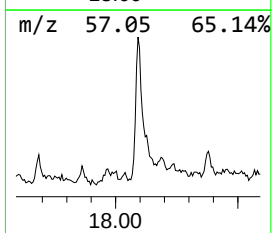
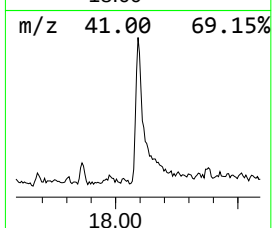
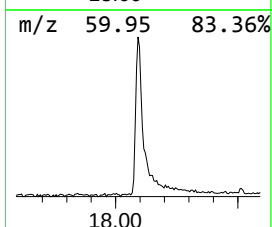
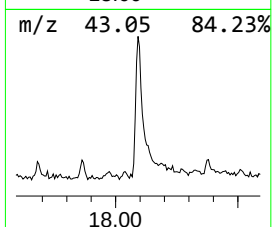
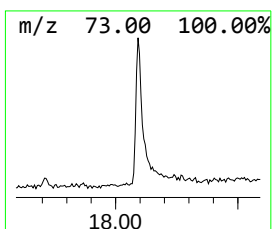
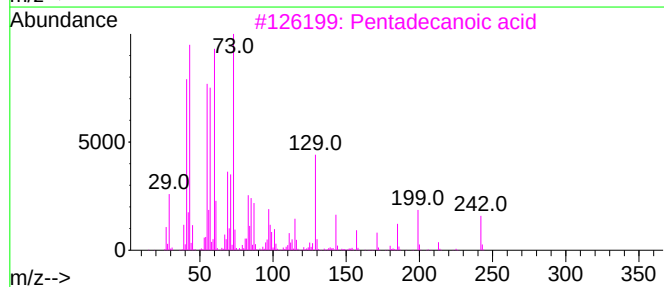
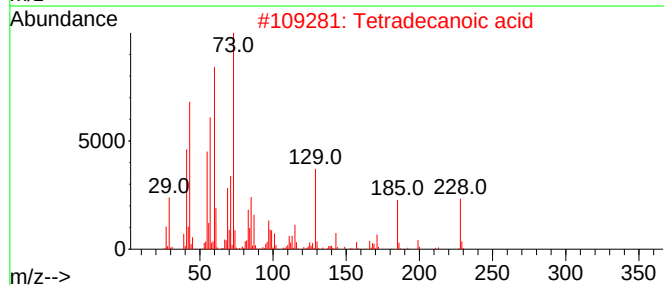
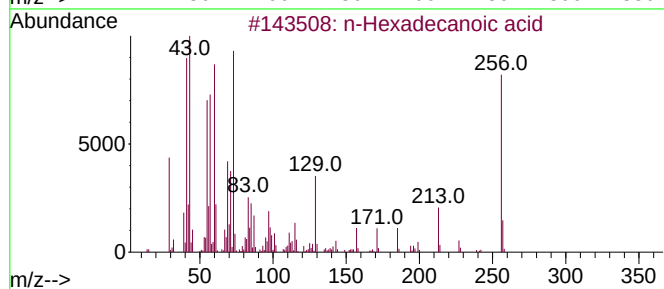
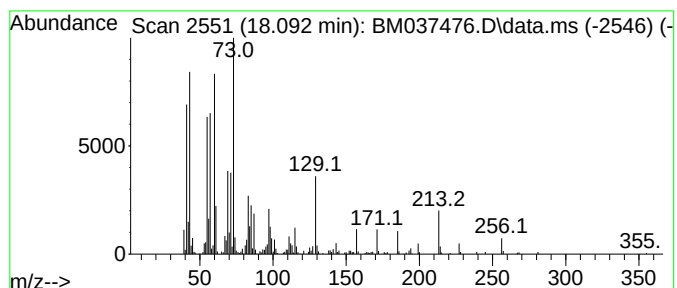
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	3.84 ng	504939	Phenanthrene-d10	17.192

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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Octadecanoic acid	284	C18H36O2	000057-11-4	53



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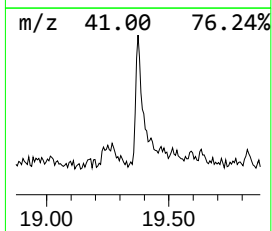
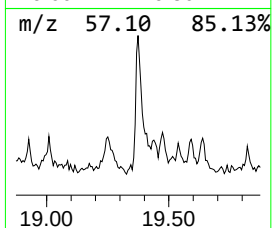
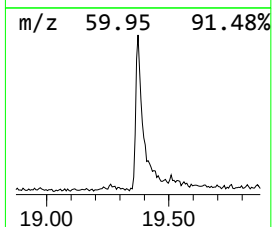
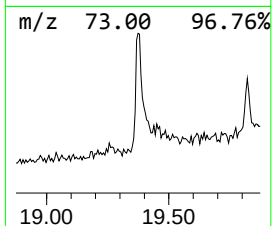
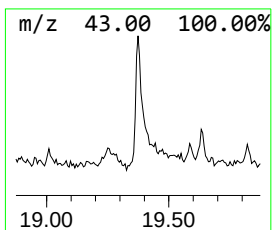
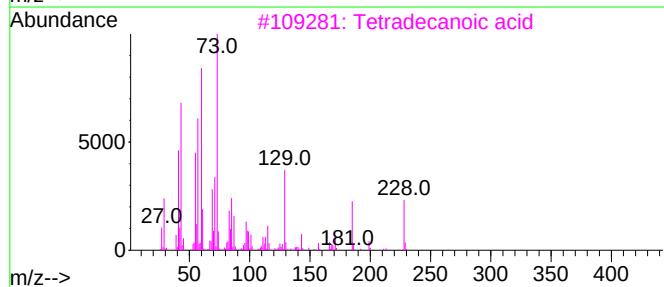
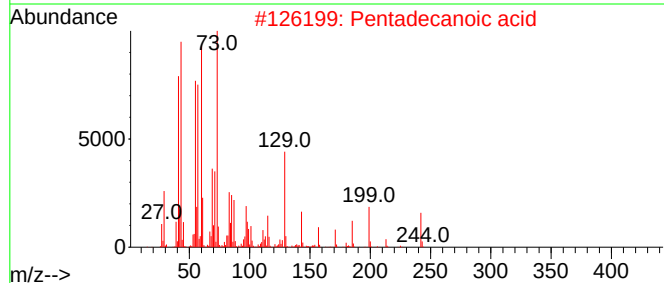
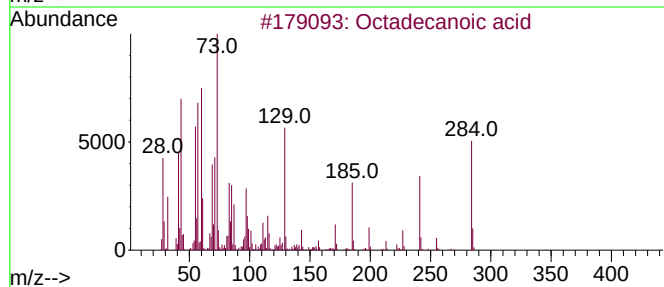
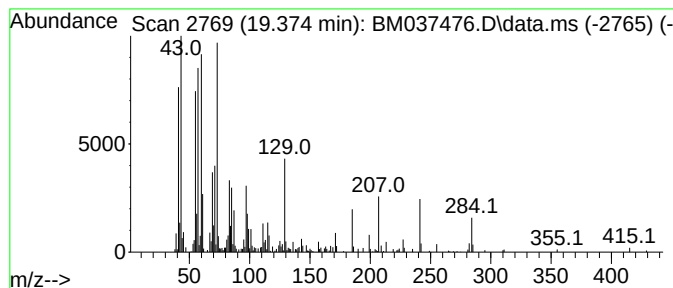
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.374	2.68 ng	309699	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	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



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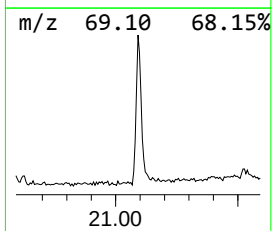
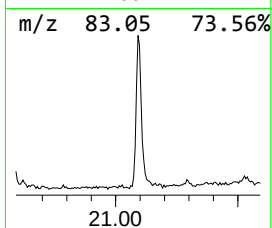
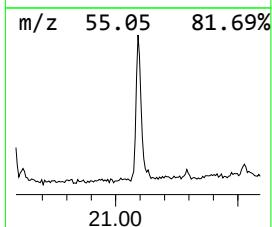
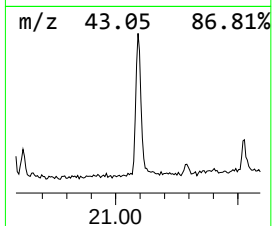
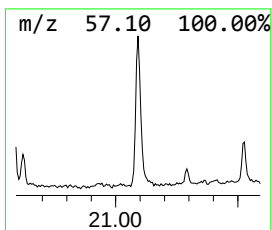
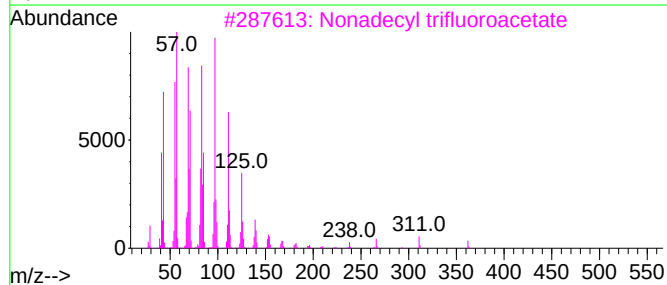
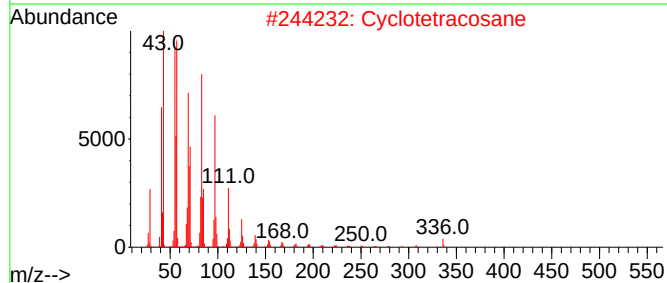
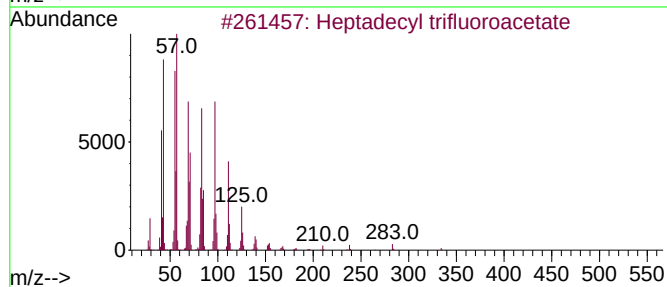
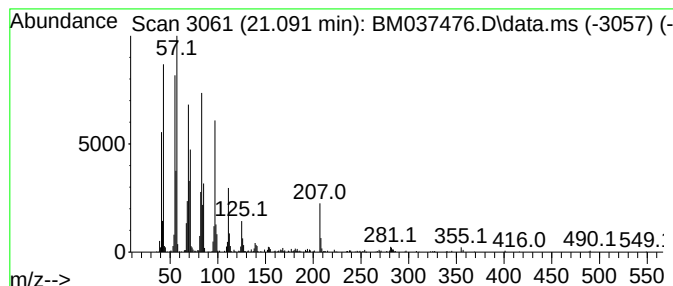
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	4.84 ng	558748	Chrysene-d12	21.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
2			Cyclotetracosane	336	C24H48	000297-03-0	93
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.916	21.1	ng	1566230	1	7.804	1481780	20.0
Ethanol, 2-(2-b...	10.398	2.7	ng	265308	2	10.604	1972460	20.0
n-Hexadecanoic ...	18.092	3.8	ng	504939	4	17.192	2627060	20.0
Octadecanoic acid	19.374	2.7	ng	309699	5	21.380	2308200	20.0
Heptadecyl trif...	21.092	4.8	ng	558748	5	21.380	2308200	20.0