

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
 Data File : BF135131.D
 Acq On : 07 Sep 2023 13:16
 Operator : CG\JU
 Sample : 04256-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-4-6

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_F\Methods\8270-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135131.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	6	10	20	rVB	49534	64014	2.25%	0.343%
2	5.016	495	498	508	rVB	40395	55115	1.93%	0.295%
3	5.404	560	564	567	rBV	2513764	2526720	88.63%	13.531%
4	6.416	730	736	739	rBV	2385427	2535531	88.94%	13.578%
5	6.604	765	768	775	rBV	73912	74527	2.61%	0.399%
6	6.769	793	796	801	rVB	689250	553273	19.41%	2.963%
7	7.334	887	892	895	rBV	1682363	1624898	56.99%	8.701%
8	8.051	1009	1014	1017	rBV	878100	752319	26.39%	4.029%
9	9.133	1192	1198	1201	rBV	3042839	2850983	100.00%	15.267%
10	9.245	1214	1217	1222	rVB	40791	38622	1.35%	0.207%
11	9.810	1308	1313	1316	rBV	937813	839086	29.43%	4.493%
12	10.604	1443	1448	1451	rBV	1940486	1835842	64.39%	9.831%
13	11.298	1562	1566	1570	rBV	912117	809917	28.41%	4.337%
14	11.839	1653	1658	1674	rBV	443565	472119	16.56%	2.528%
15	12.539	1771	1777	1784	rBV10	14051	38830	1.36%	0.208%
16	12.627	1787	1792	1799	rBV	124977	151387	5.31%	0.811%
17	12.898	1834	1838	1842	rBV	2481550	2331113	81.77%	12.483%
18	13.810	1989	1993	2005	rVB	123728	179439	6.29%	0.961%
19	13.957	2014	2018	2023	rVB	488810	458824	16.09%	2.457%
20	15.427	2263	2268	2273	rBV	374381	481307	16.88%	2.577%

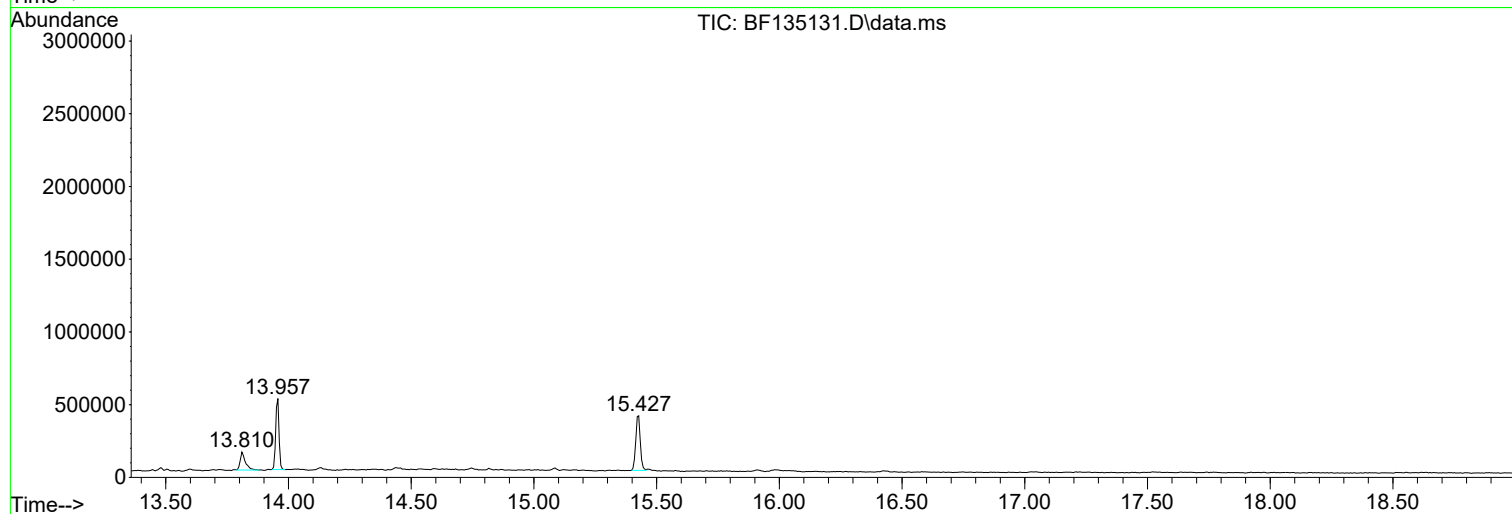
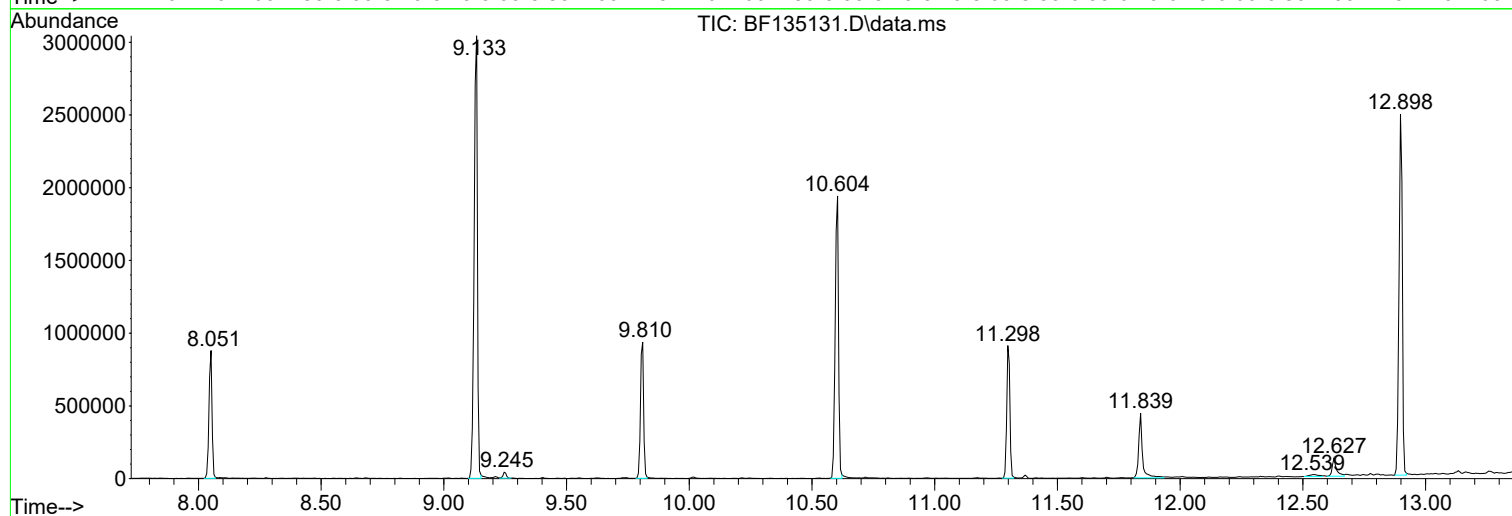
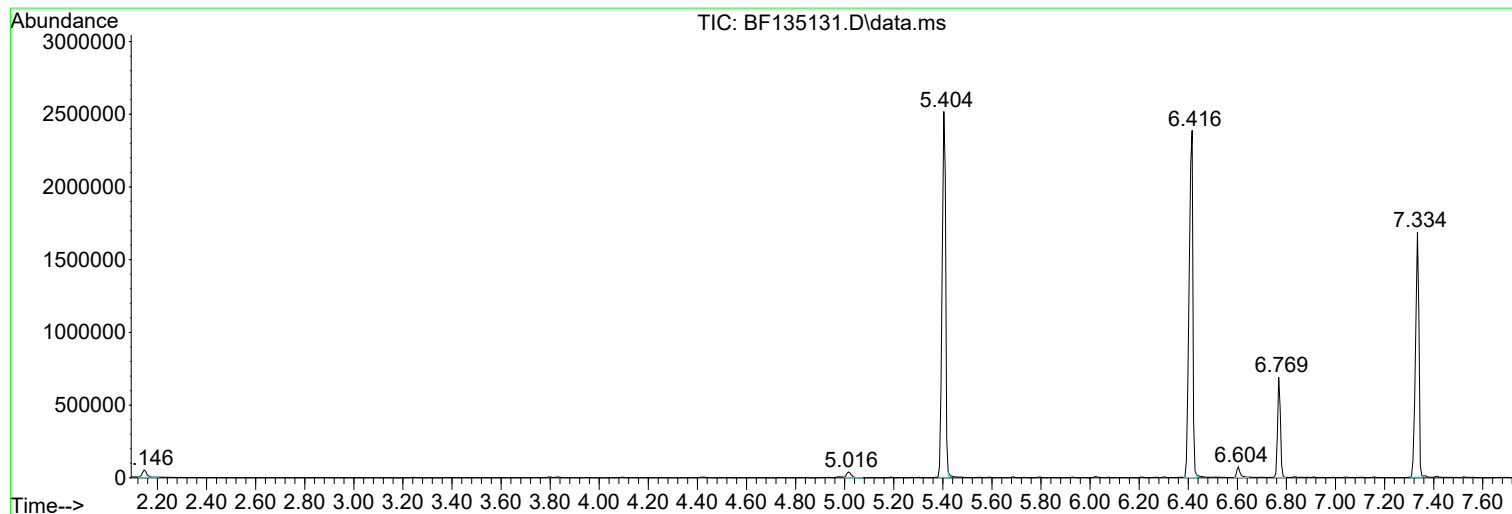
Sum of corrected areas: 18673866

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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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Data File : BF135131.D
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Instrument :
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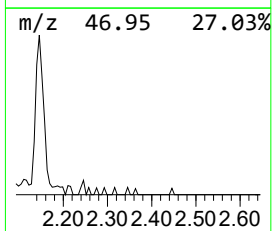
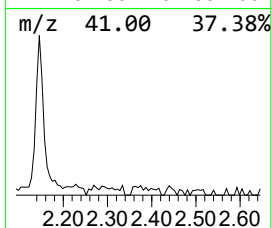
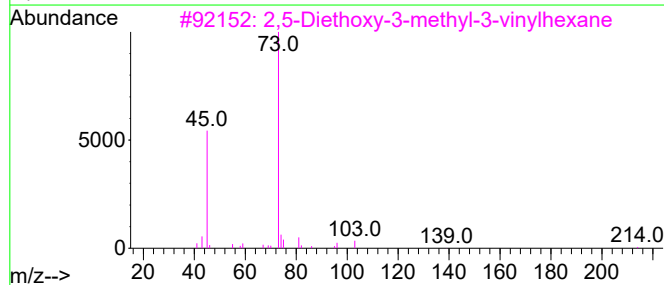
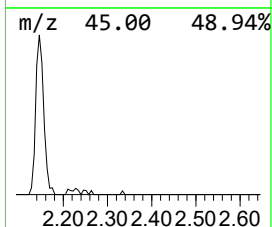
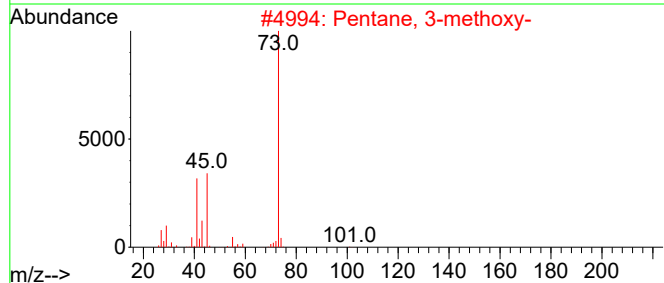
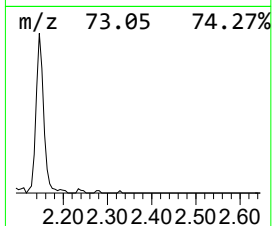
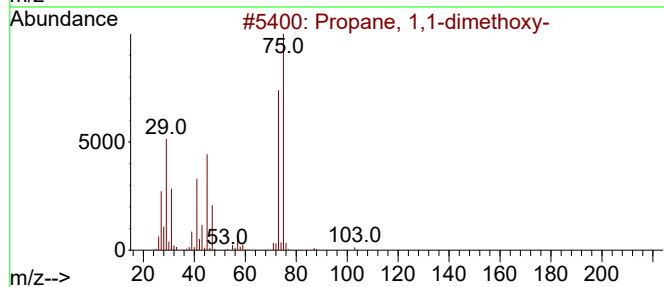
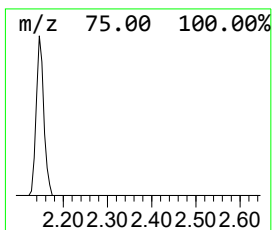
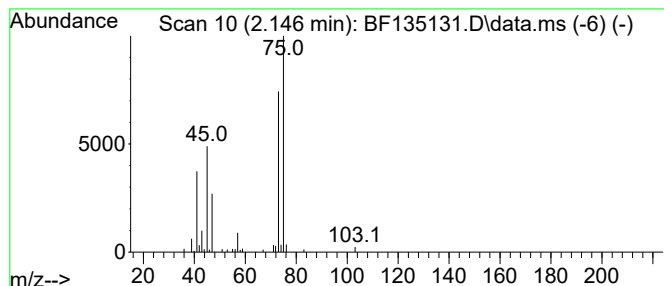
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	2.31 ng	64014	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3			2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	16
4			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
5			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



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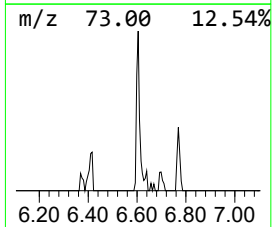
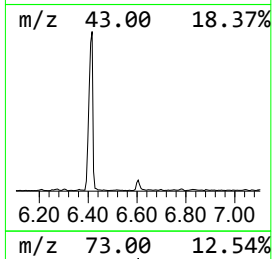
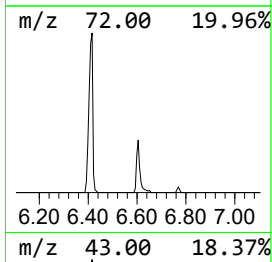
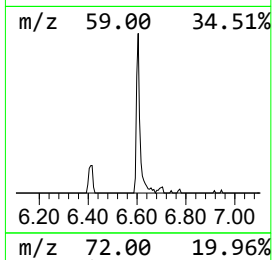
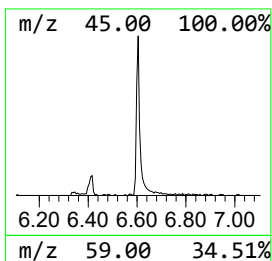
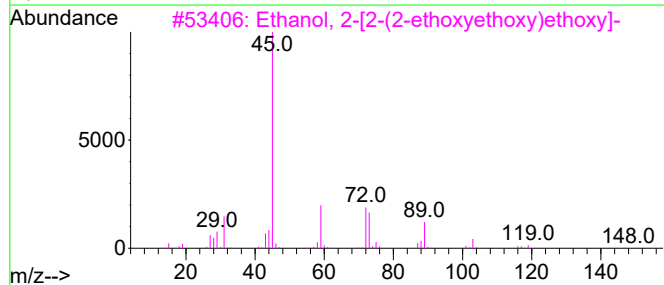
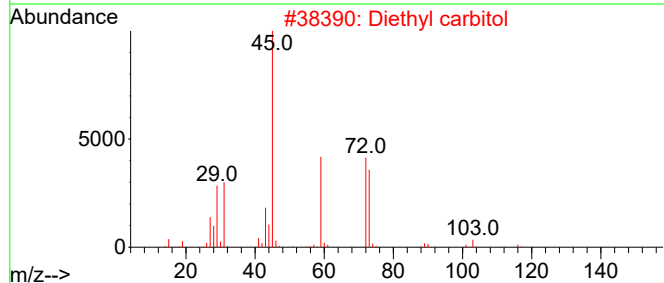
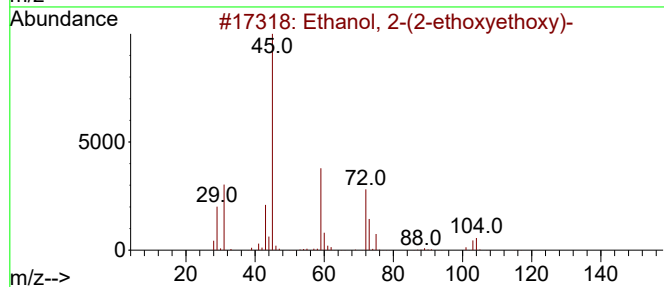
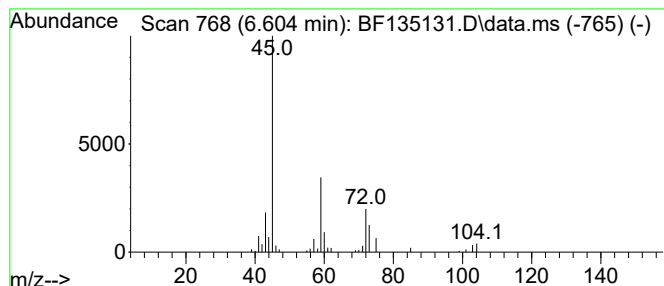
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	2.69 ng	74527	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	64
4			Ethyl ether	74	C4H10O	000060-29-7	40
5			2-Pentanol	88	C5H12O	006032-29-7	38



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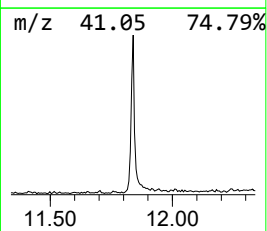
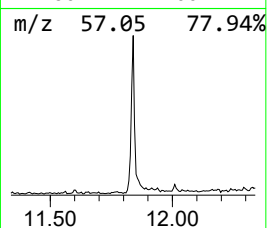
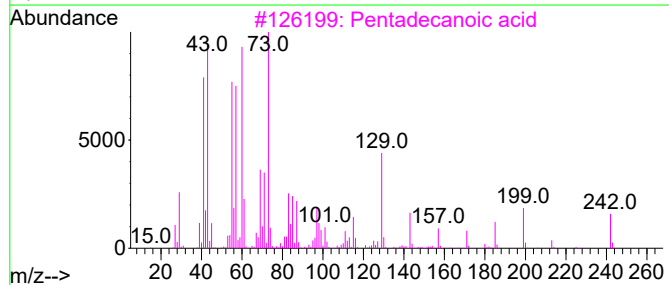
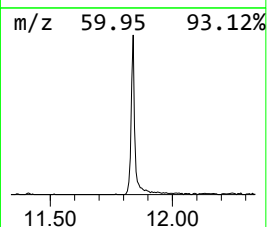
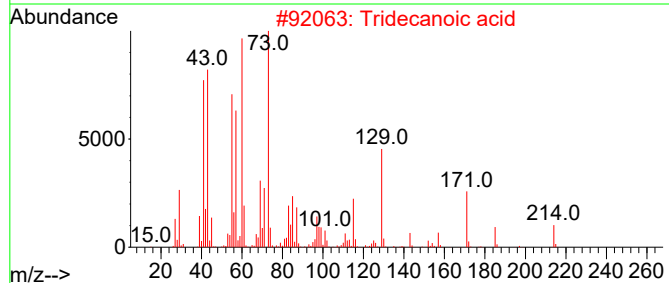
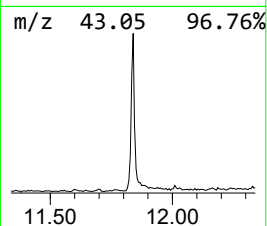
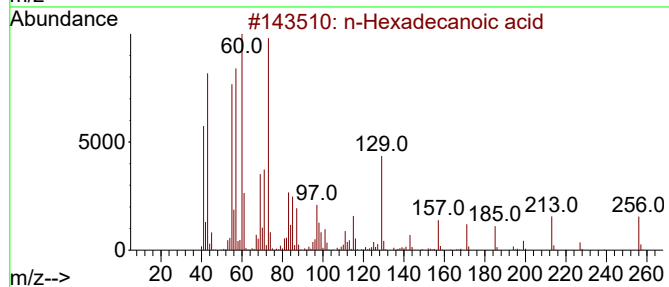
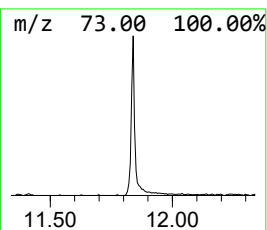
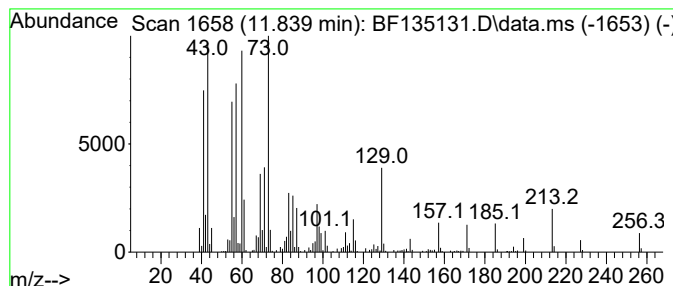
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	11.66 ng	472119	Phenanthrene-d10	11.298

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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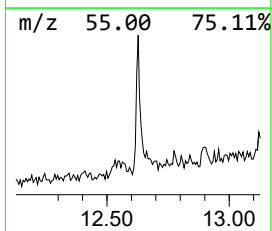
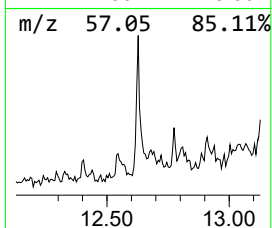
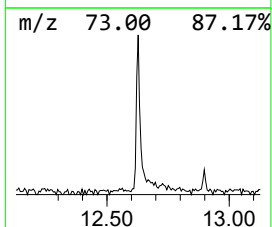
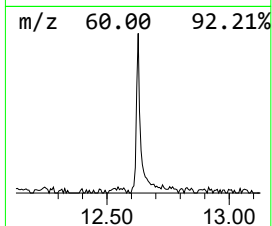
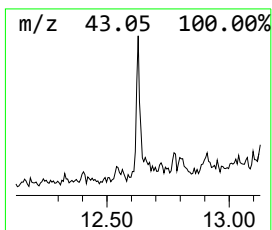
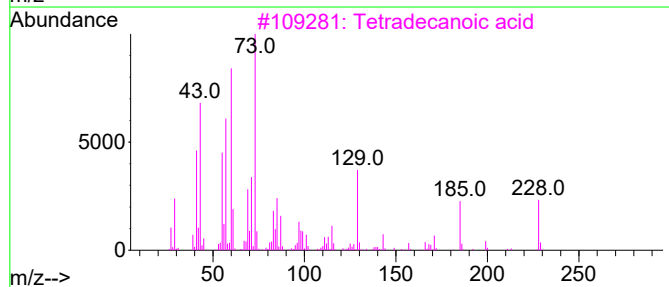
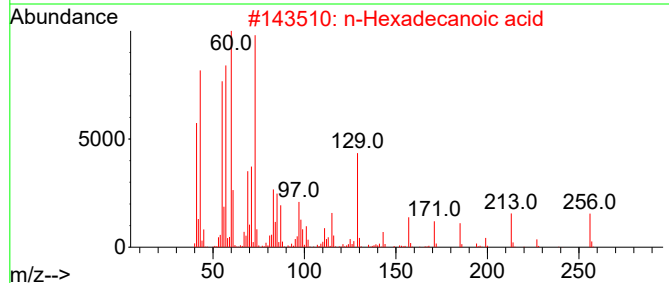
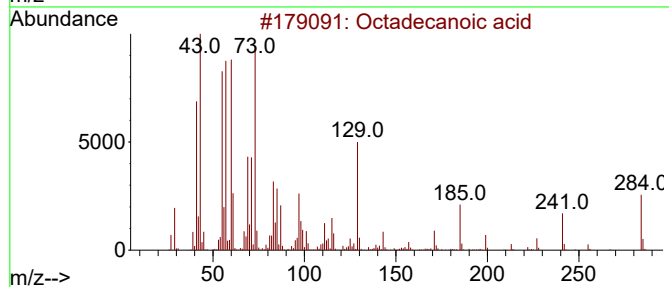
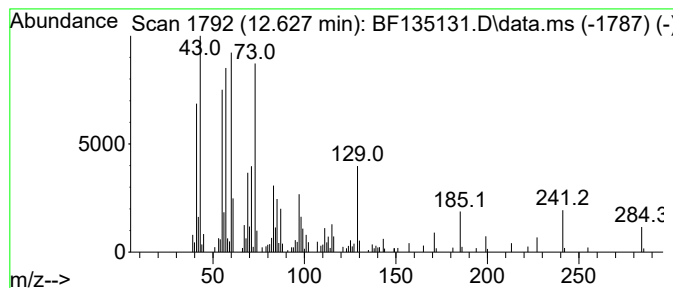
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	3.74 ng	151387	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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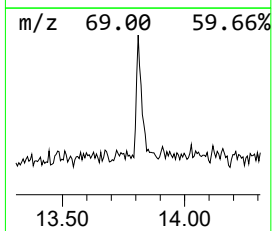
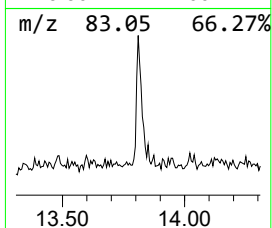
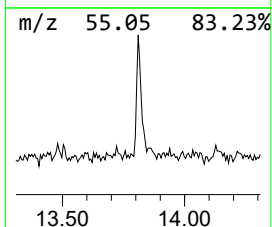
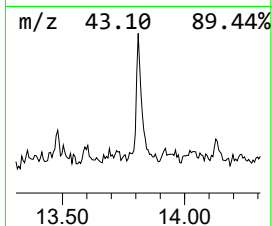
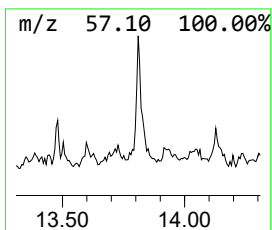
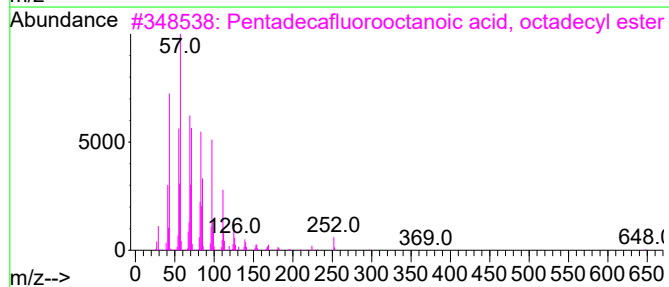
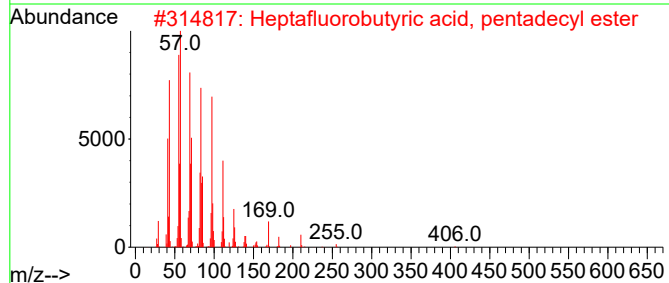
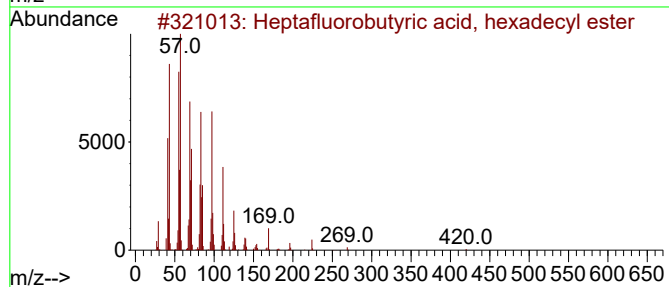
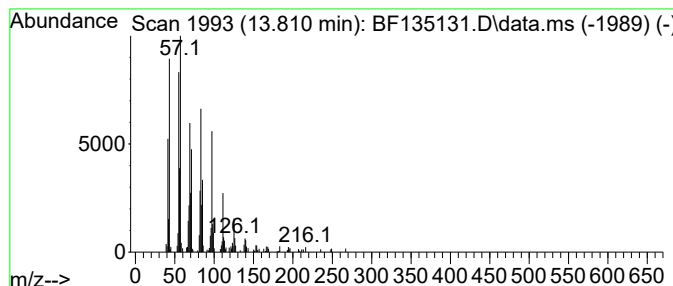
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	7.82 ng	179439	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-di...	2.146	2.3	ng	64014	1	6.769	553273	20.0
Ethanol, 2-(2-e...	6.604	2.7	ng	74527	1	6.769	553273	20.0
n-Hexadecanoic ...	11.839	11.7	ng	472119	4	11.298	809917	20.0
Octadecanoic acid	12.627	3.7	ng	151387	4	11.298	809917	20.0
Heptafluorobuty...	13.810	7.8	ng	179439	5	13.957	458824	20.0