

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
 Data File : BF136345.D
 Acq On : 01 Dec 2023 19:06
 Operator : CG\JU
 Sample : 05525-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP12

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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136345.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	1587187	1535791	28.15%	6.140%
2	5.440	566	570	573	rBV	1478017	1244356	22.81%	4.975%
3	6.434	735	739	748	rVB	978644	802006	14.70%	3.206%
4	6.804	798	802	805	rBV	1036411	804550	14.75%	3.217%
5	7.369	892	898	901	rBV	2664022	2751056	50.43%	10.999%
6	7.457	908	913	922	rBV	55036	79356	1.45%	0.317%
7	7.810	968	973	979	rBV	46105	58566	1.07%	0.234%
8	8.081	1015	1019	1022	rBV	1353640	1094101	20.06%	4.374%
9	8.428	1073	1078	1085	rBV	120550	154919	2.84%	0.619%
10	9.163	1197	1203	1206	rBV	6103727	5455260	100.00%	21.811%
11	9.839	1314	1318	1321	rBV	1484043	1200457	22.01%	4.800%
12	10.222	1380	1383	1386	rBV	136095	102549	1.88%	0.410%
13	10.263	1386	1390	1393	rBV	2130721	1928875	35.36%	7.712%
14	10.633	1448	1453	1456	rBV	1870169	1762834	32.31%	7.048%
15	11.327	1567	1571	1574	rBV	1176524	991050	18.17%	3.962%
16	11.869	1659	1663	1667	rBV	175054	198819	3.64%	0.795%
17	12.657	1794	1797	1808	rBV2	56791	72022	1.32%	0.288%
18	12.927	1838	1843	1846	rBV	3916764	3387662	62.10%	13.544%
19	13.921	2006	2012	2018	rBV9	23866	68539	1.26%	0.274%
20	13.980	2018	2022	2031	rVB	653984	609082	11.17%	2.435%
21	15.463	2268	2274	2281	rBV2	547375	710046	13.02%	2.839%

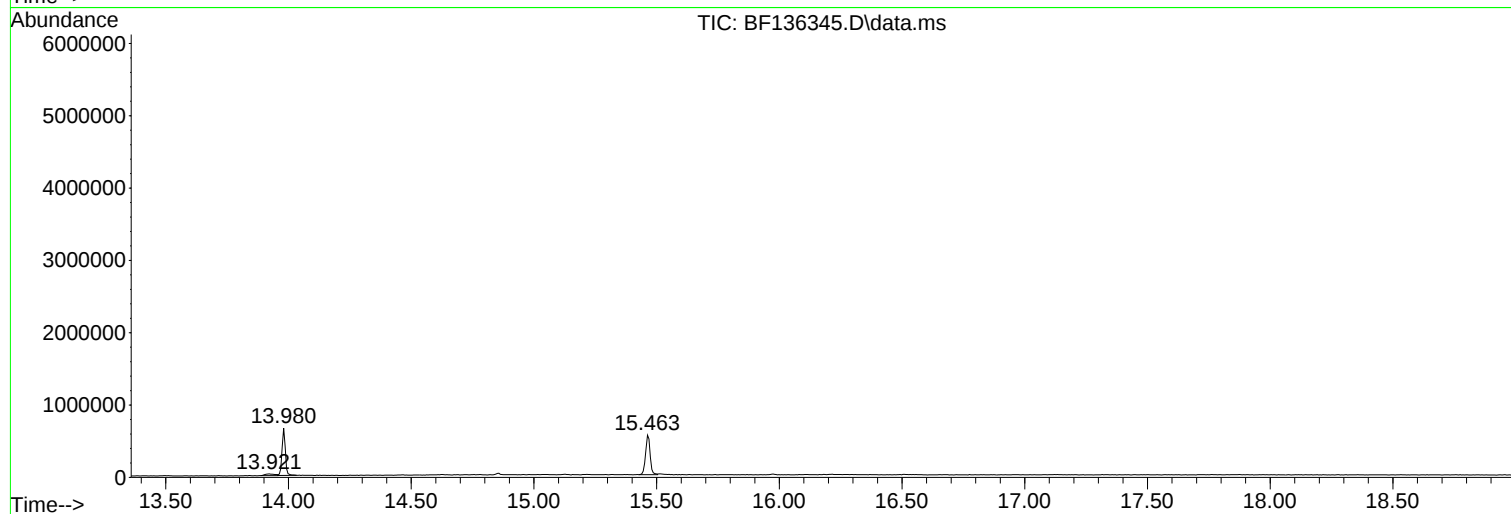
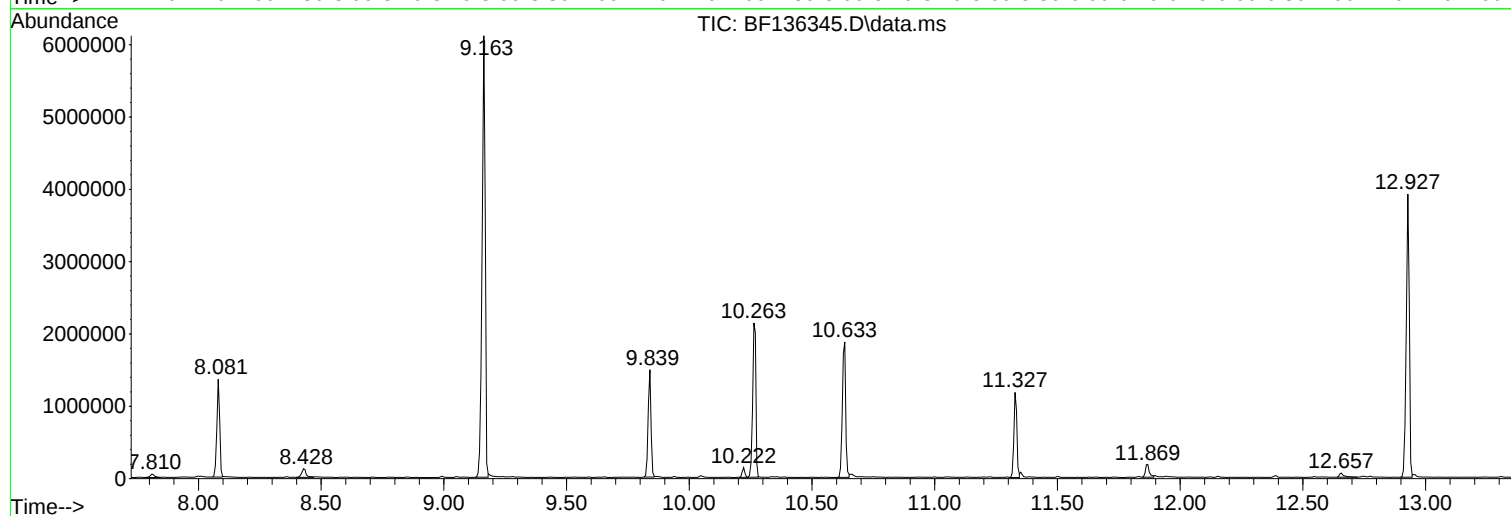
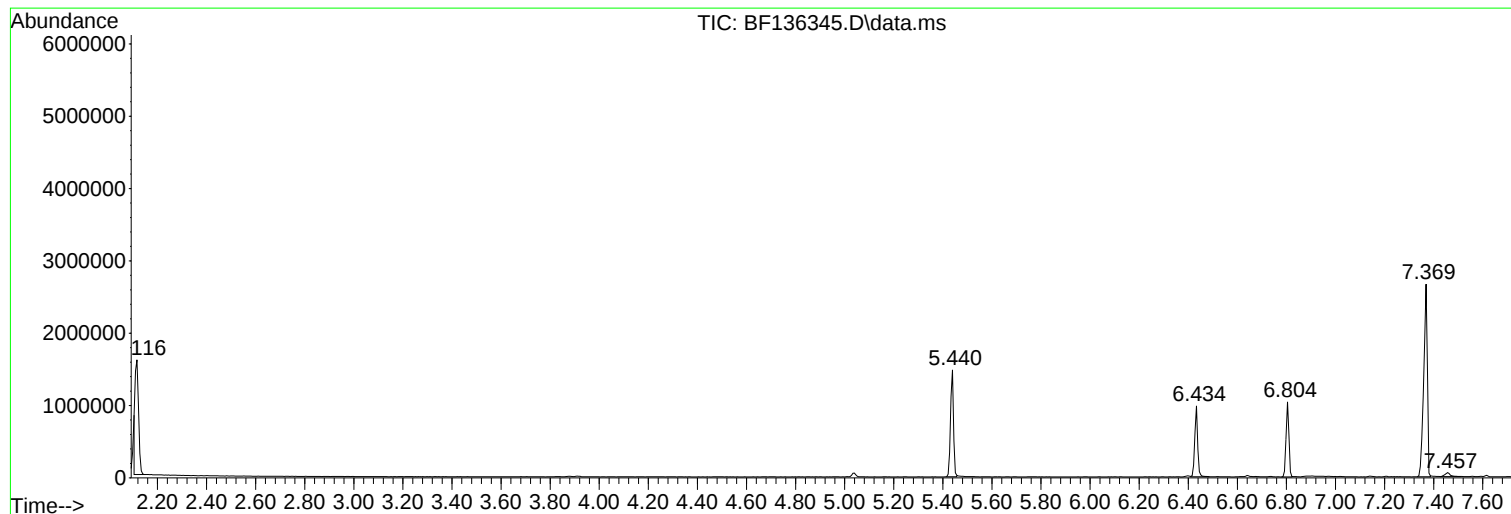
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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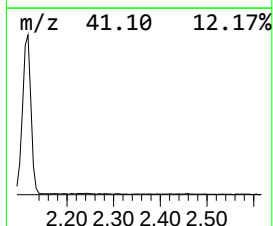
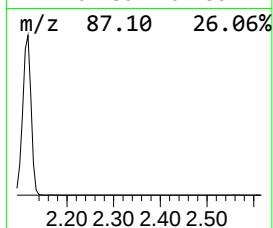
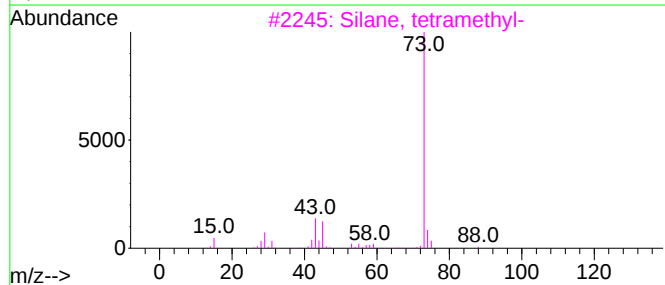
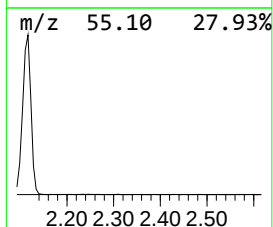
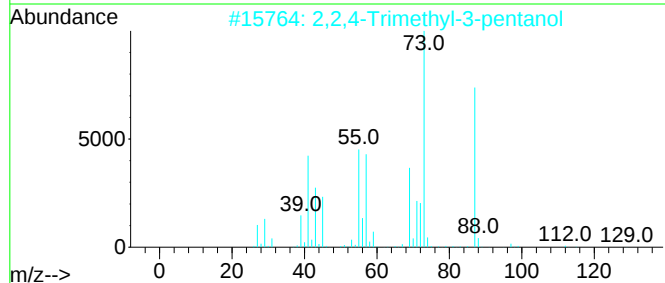
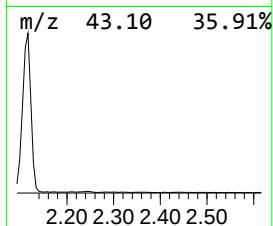
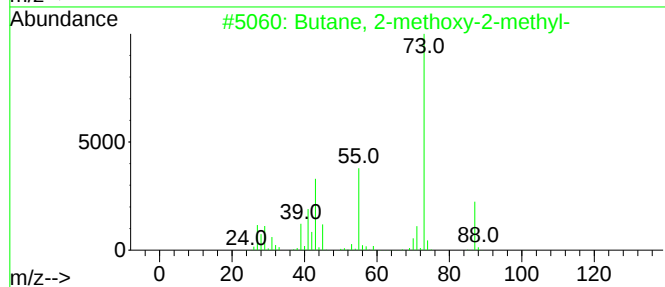
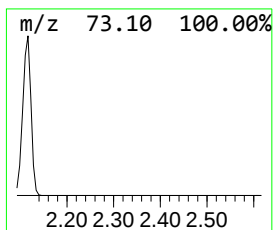
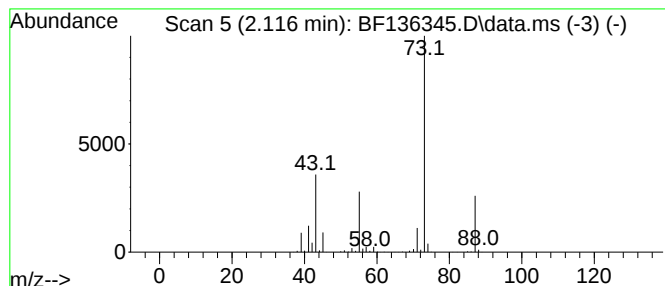
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	38.18 ng	1535790	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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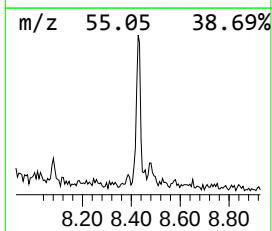
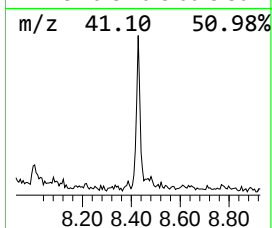
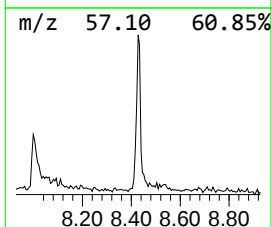
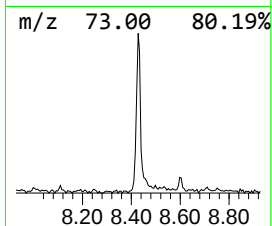
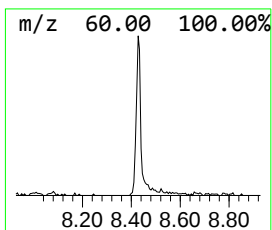
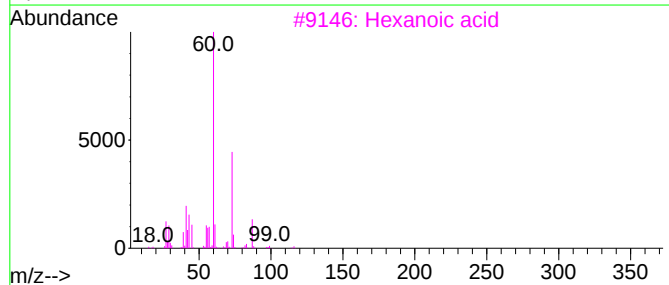
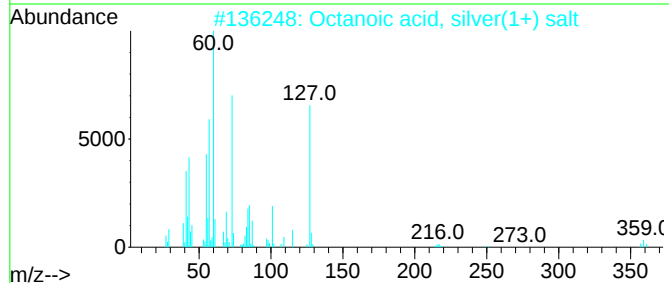
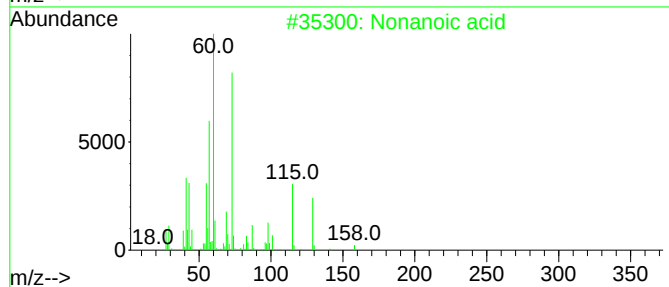
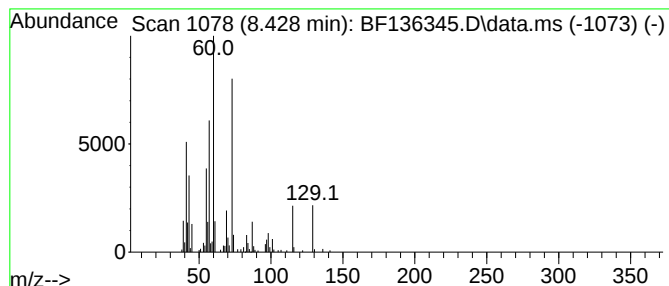
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Peak Number 2 Nonanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.428	2.83 ng	154919	Naphthalene-d8	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	90
2			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	58
3			Hexanoic acid	116	C6H12O2	000142-62-1	47
4			Heptanoic acid	130	C7H14O2	000111-14-8	47
5			Butanoic acid	88	C4H8O2	000107-92-6	43



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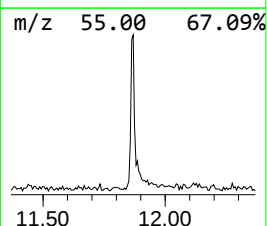
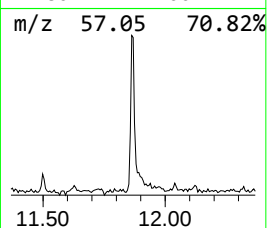
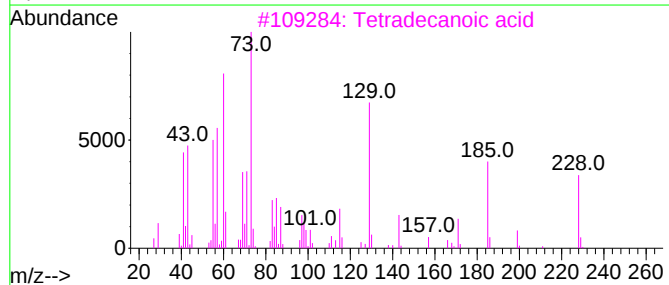
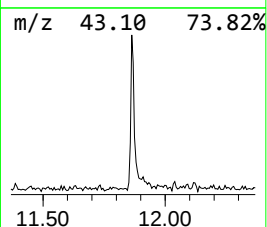
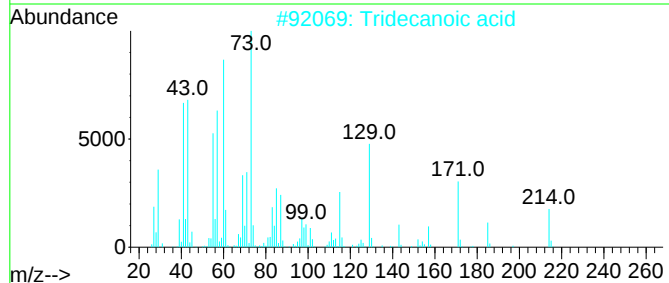
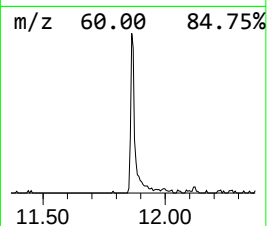
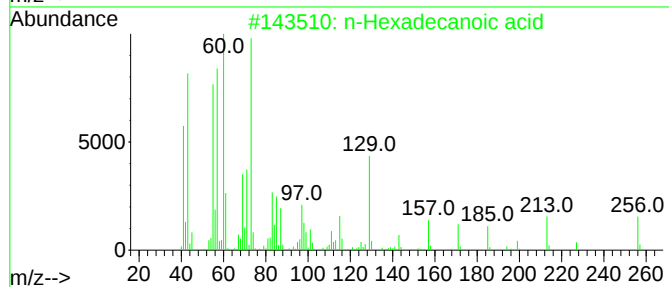
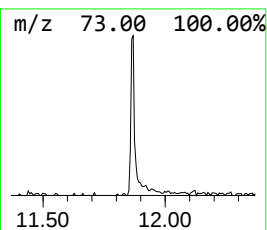
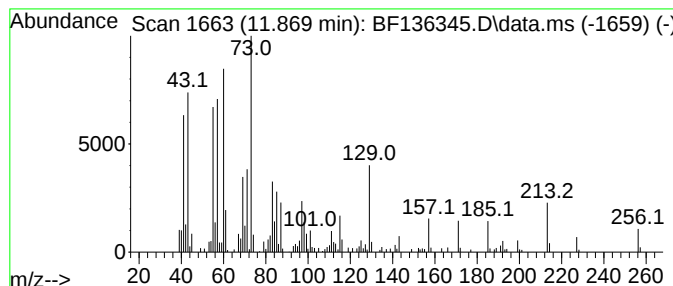
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	4.01 ng	198819	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Undecanoic acid	186	C11H22O2	000112-37-8	83



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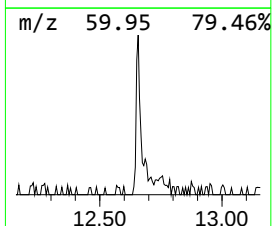
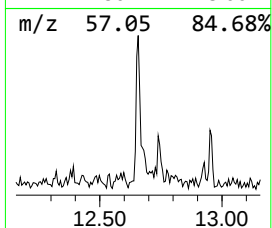
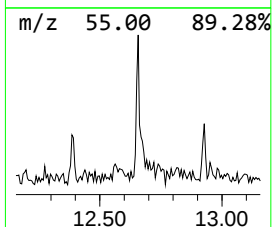
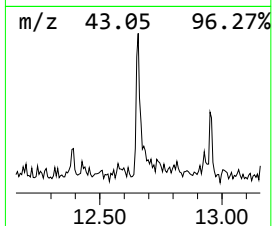
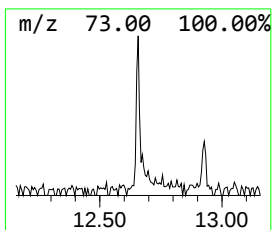
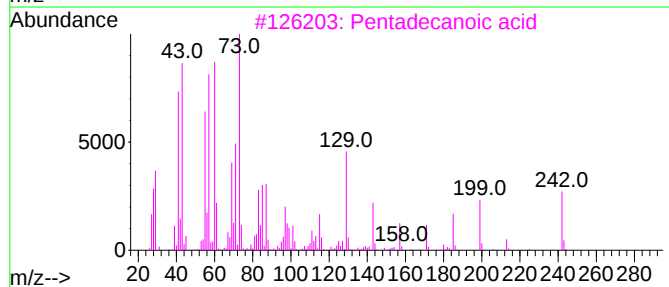
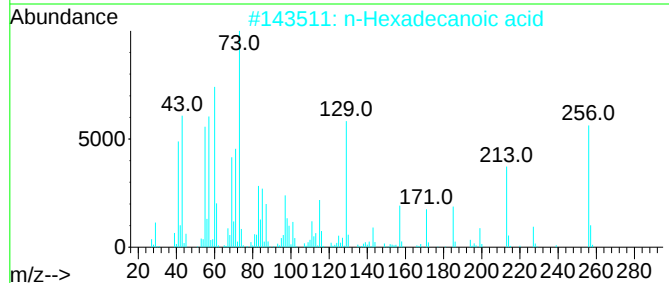
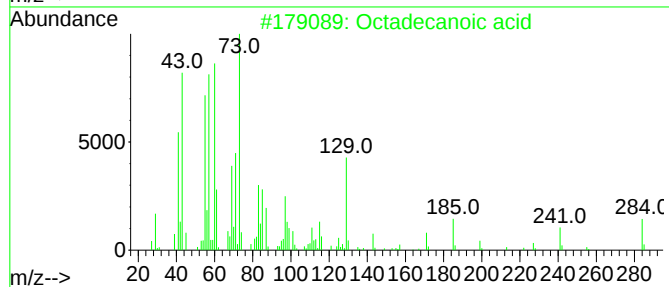
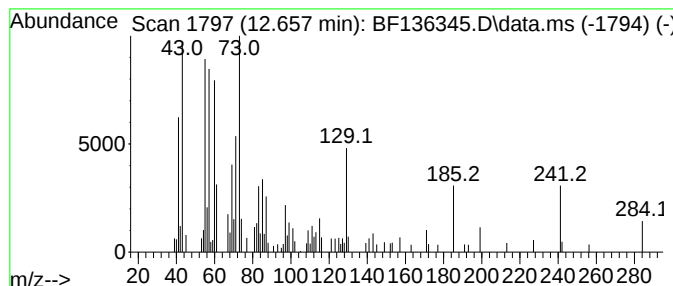
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	2.36 ng	72022	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20



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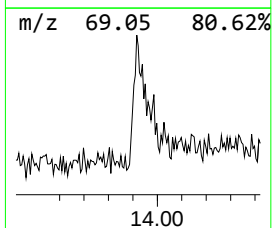
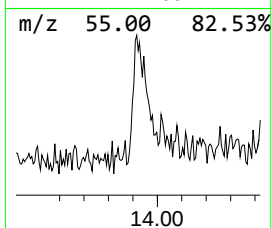
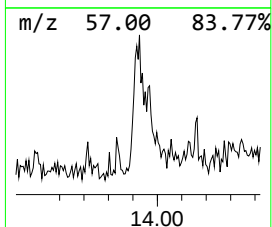
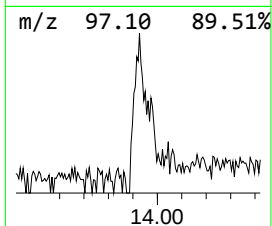
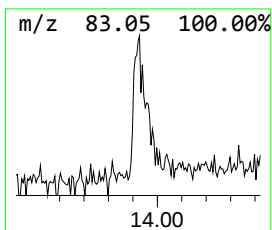
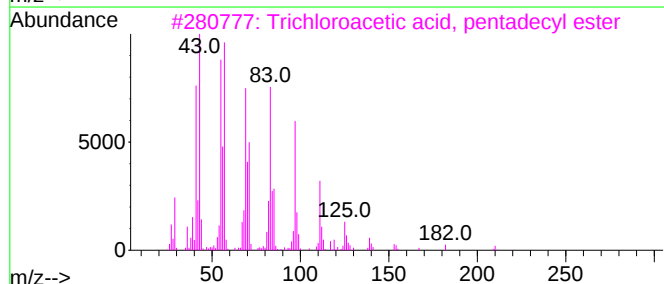
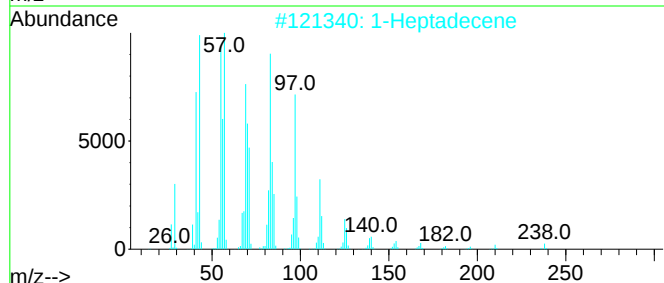
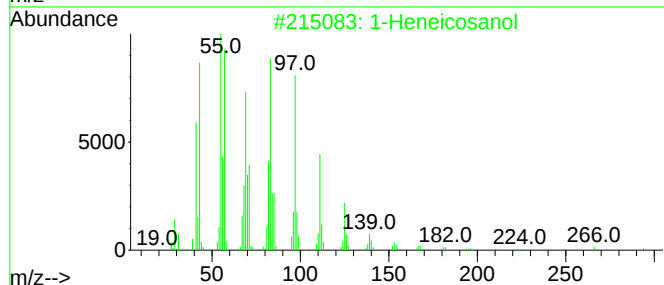
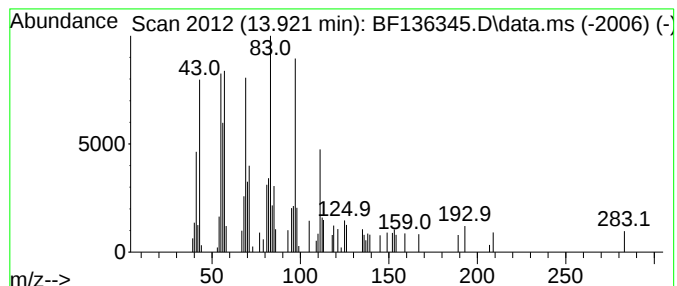
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	2.25 ng	68539	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol			312	C21H44O	015594-90-8	87
2	1-Heptadecene			238	C17H34	006765-39-5	72
3	Trichloroacetic acid, pentadecyl...			372	C17H31Cl3O2	074339-53-0	68
4	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	62
5	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.116	38.2	ng	1535790	1	6.804	804550	20.0
Nonanoic acid	8.428	2.8	ng	154919	2	8.081	1094100	20.0
n-Hexadecanoic ...	11.869	4.0	ng	198819	4	11.328	991050	20.0
Octadecanoic acid	12.657	2.4	ng	72022	5	13.980	609082	20.0
1-Heneicosanol	13.921	2.3	ng	68539	5	13.980	609082	20.0