

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112423\
 Data File : BF136188.D
 Acq On : 24 Nov 2023 19:45
 Operator : CG\JU
 Sample : 05468-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-9

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-BF110723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136188.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	14	rVB	493413	611609	7.98%	1.465%
2	5.057	500	505	517	rVB	653903	900199	11.75%	2.157%
3	5.451	566	572	575	rBV	5317173	5494685	71.72%	13.165%
4	6.446	734	741	744	rBV	4752010	5608172	73.20%	13.437%
5	6.804	799	802	806	rBV	984117	770905	10.06%	1.847%
6	7.369	892	898	901	rBV	3431228	3513668	45.86%	8.419%
7	8.081	1015	1019	1023	rBV	1220855	1060682	13.84%	2.541%
8	9.169	1197	1204	1206	rBV	7685233	7661540	100.00%	18.357%
9	9.281	1219	1223	1231	rVB	82418	79022	1.03%	0.189%
10	9.839	1313	1318	1321	rBV	1571247	1235524	16.13%	2.960%
11	10.633	1448	1453	1456	rBV	4525726	4317184	56.35%	10.344%
12	11.328	1568	1571	1575	rBV	1403675	1223503	15.97%	2.931%
13	11.869	1659	1663	1674	rBV2	323160	350026	4.57%	0.839%
14	12.657	1794	1797	1806	rBV	110581	126947	1.66%	0.304%
15	12.933	1839	1844	1847	rBV	7637136	6989840	91.23%	16.748%
16	13.845	1996	1999	2015	rBV	126371	213133	2.78%	0.511%
17	13.980	2018	2022	2028	rVB	833068	737567	9.63%	1.767%
18	15.463	2268	2274	2281	rBV	554650	687834	8.98%	1.648%
19	18.186	2729	2737	2745	rVB8	59878	154392	2.02%	0.370%

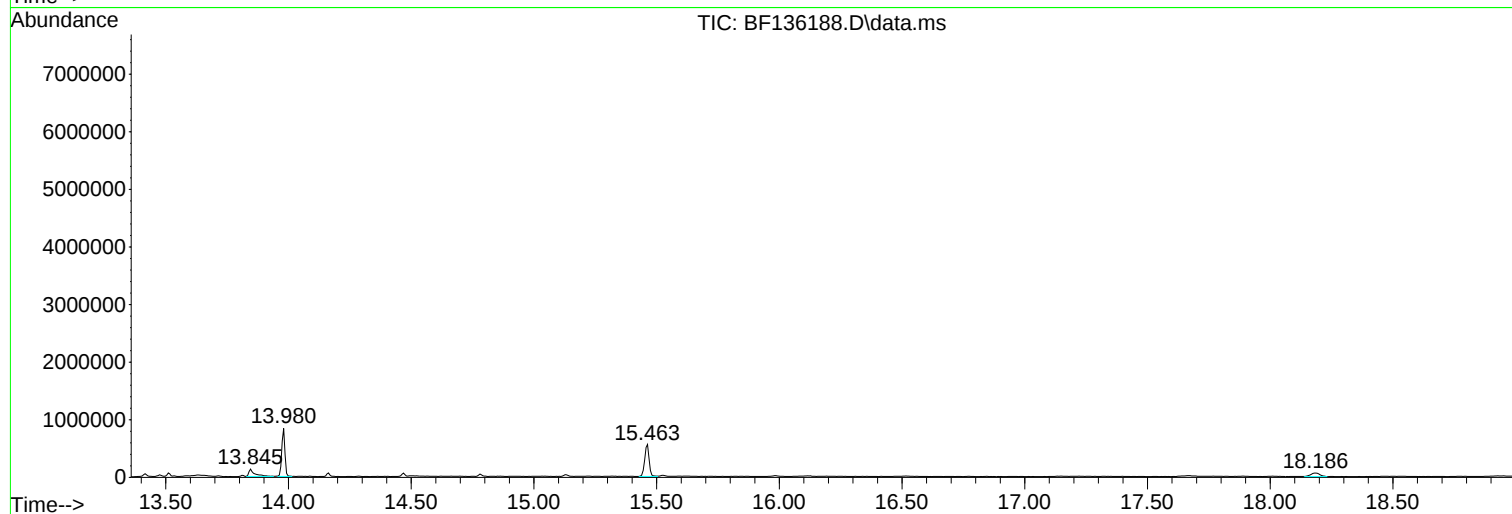
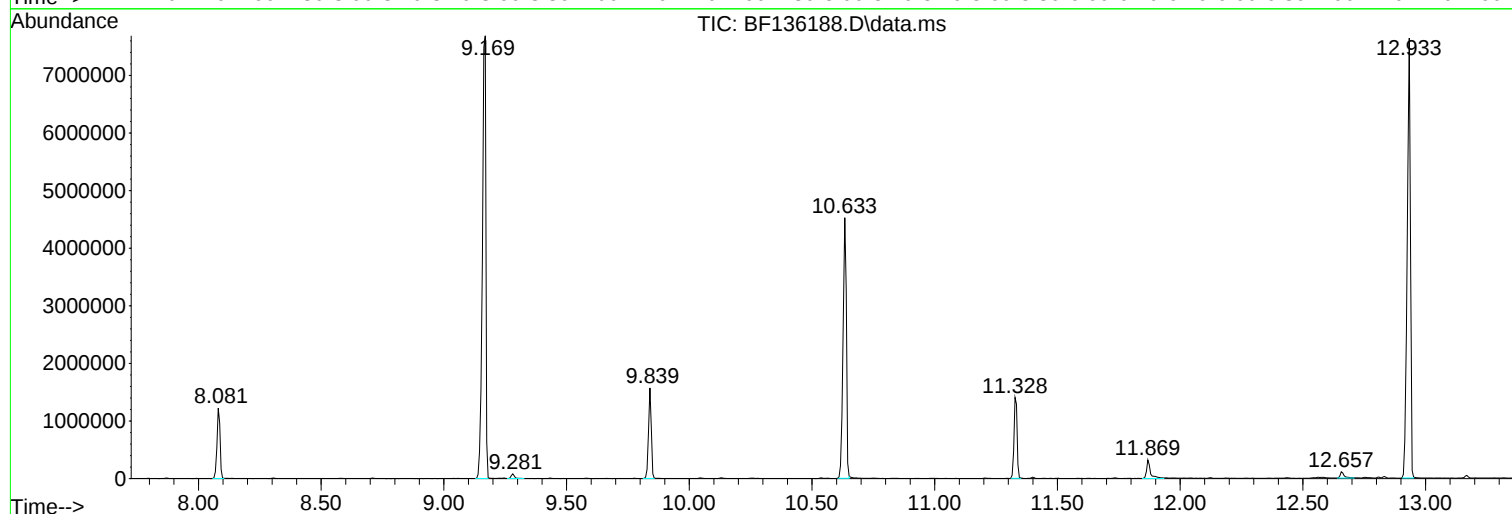
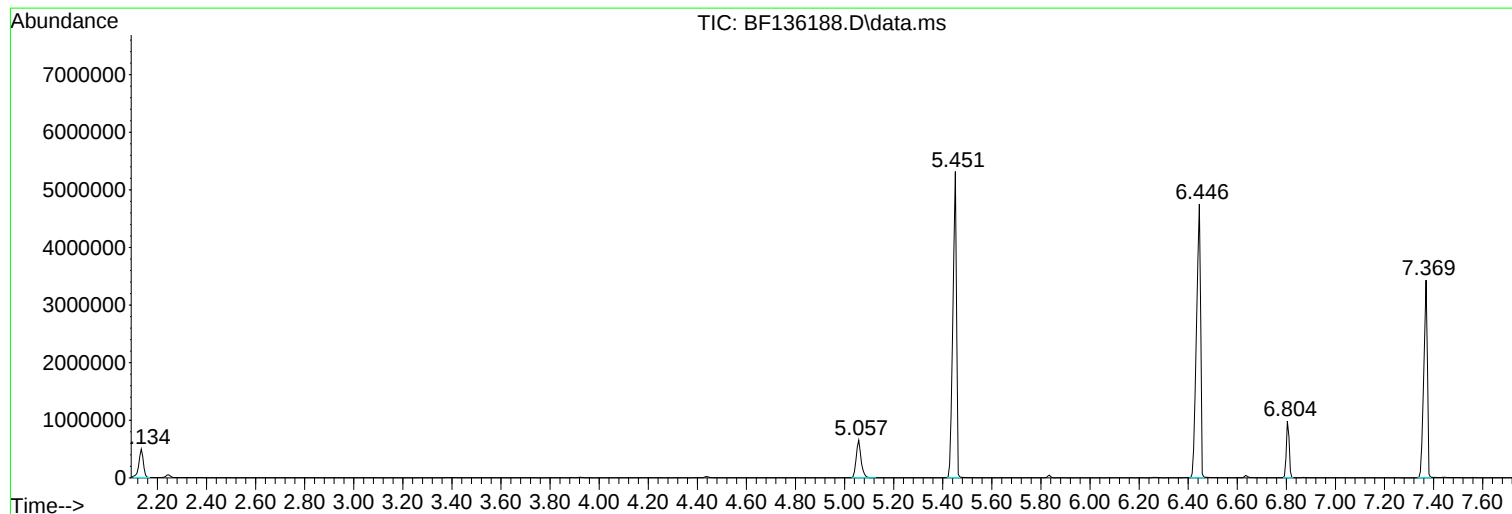
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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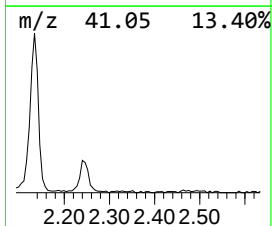
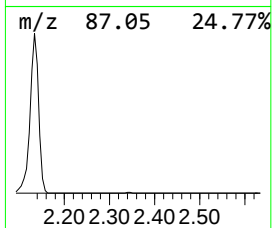
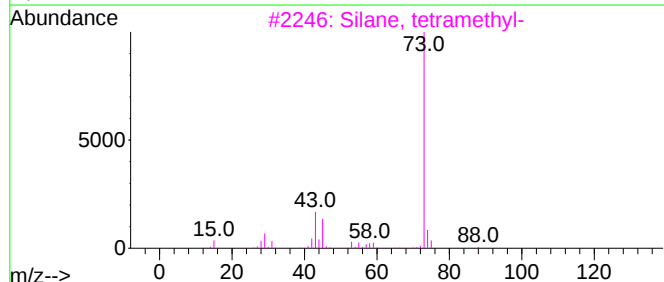
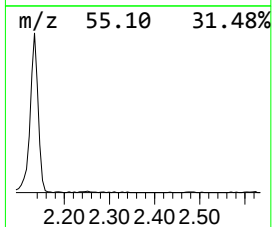
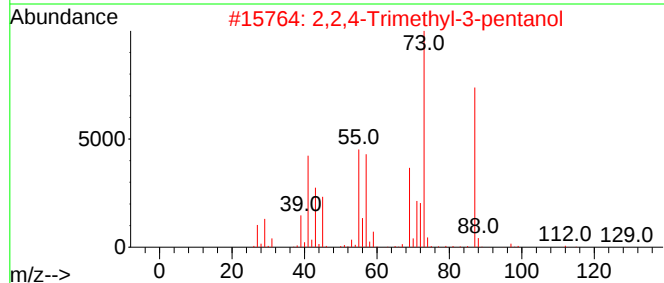
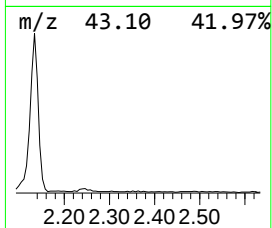
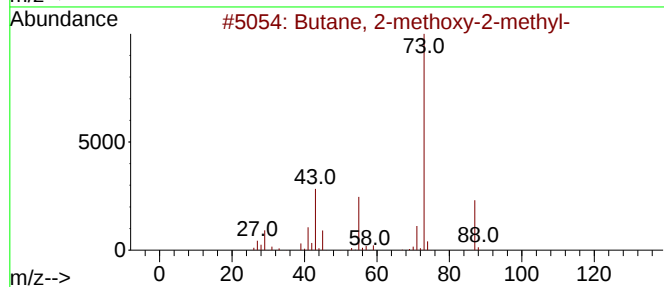
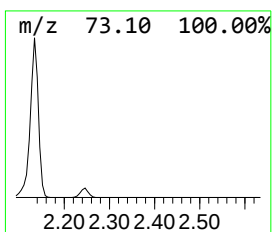
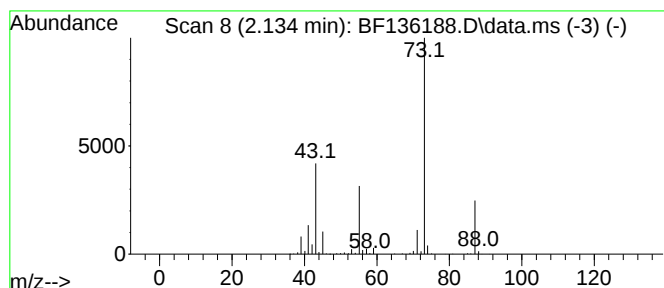
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	15.87 ng	611609	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	17
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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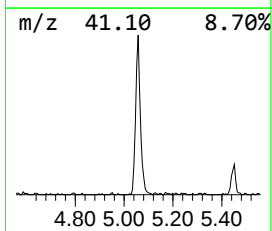
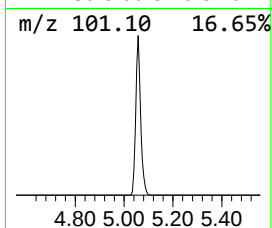
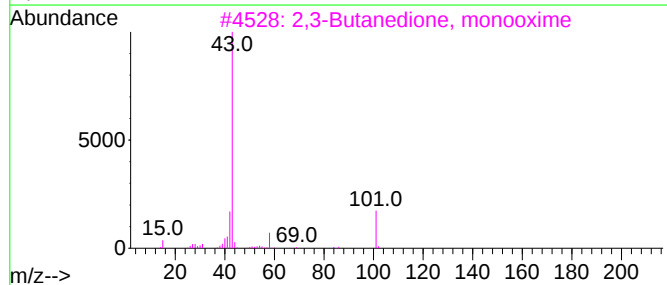
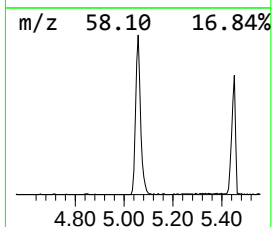
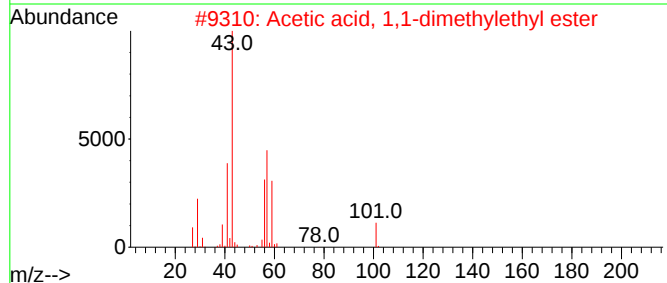
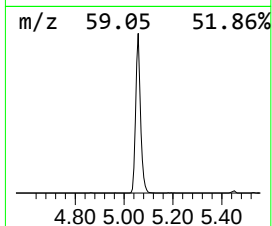
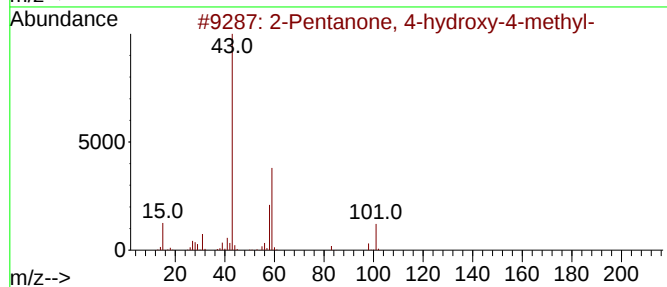
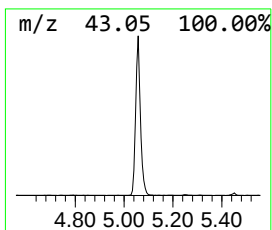
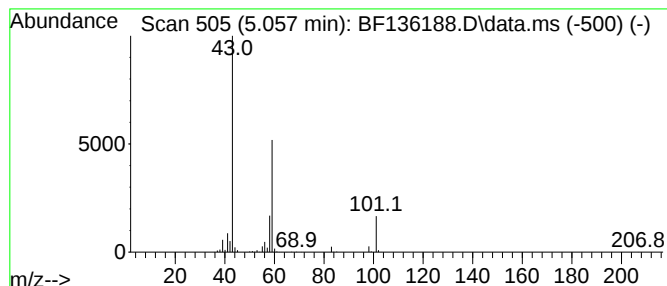
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.057	23.35 ng	900199	1,4-Dichlorobenzene-d4	6.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Acetone	58	C3H6O	000067-64-1	12



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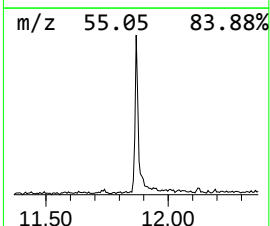
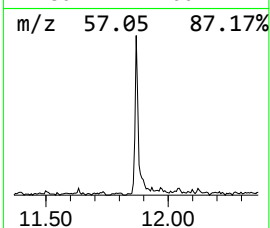
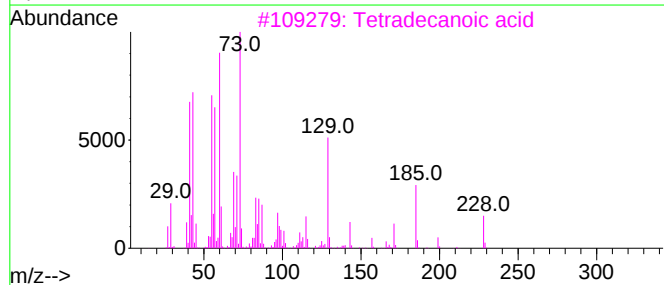
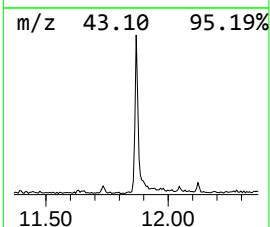
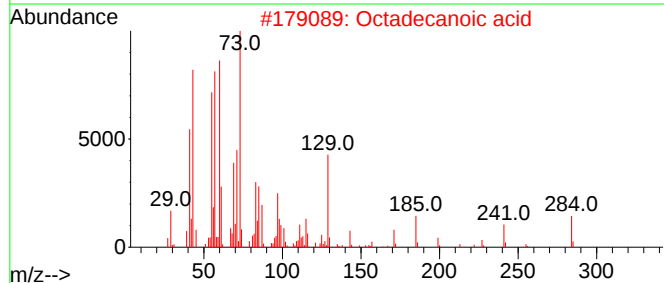
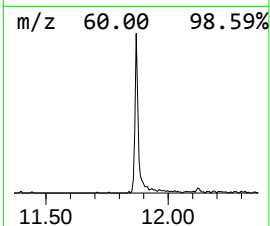
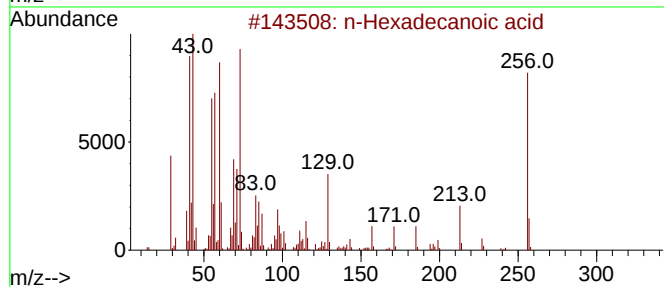
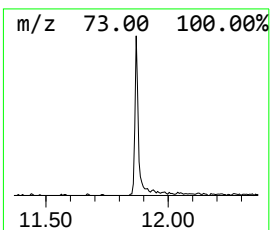
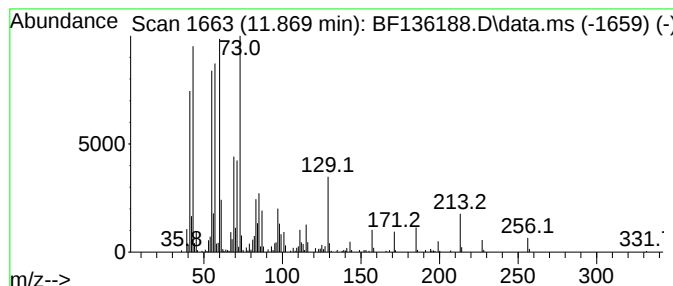
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	5.72 ng	350026	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5			Tridecanoic acid	214	C13H26O2	000638-53-9	81



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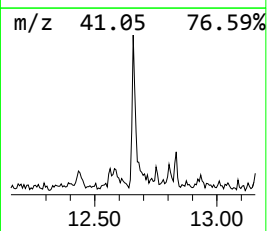
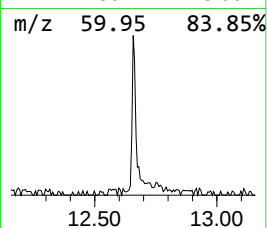
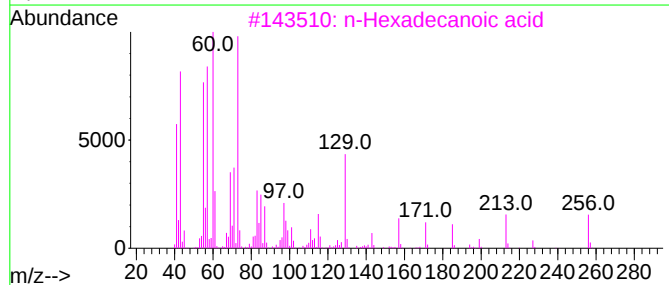
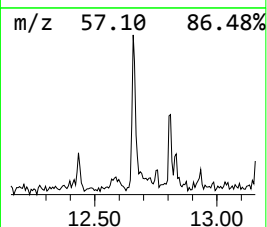
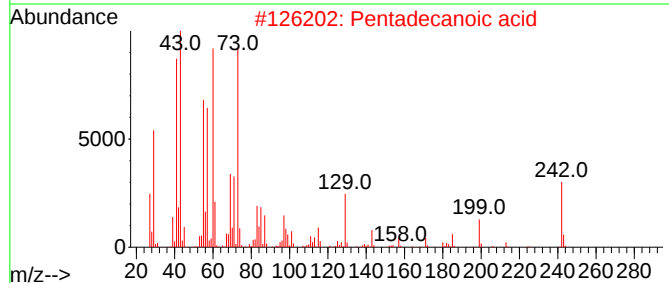
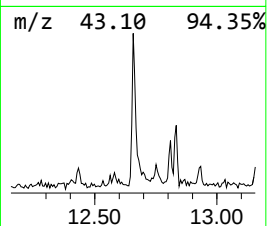
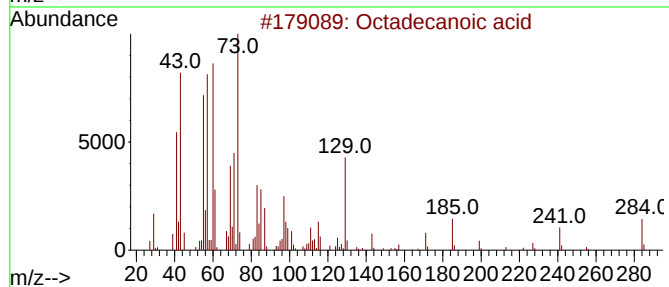
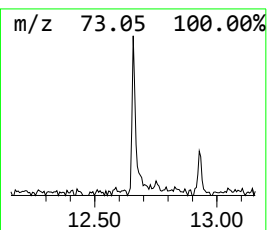
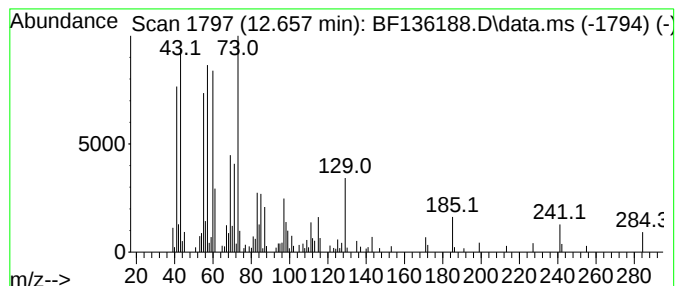
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	3.44 ng	126947	Chrysene-d12	13.980

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	80
4			n-Decanoic acid	172	C10H20O2	000334-48-5	49
5			n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25



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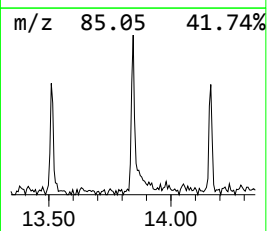
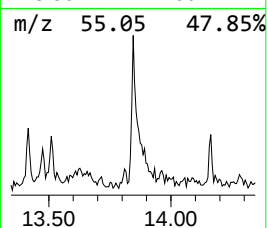
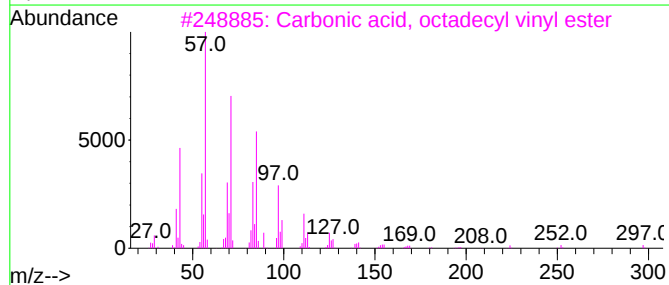
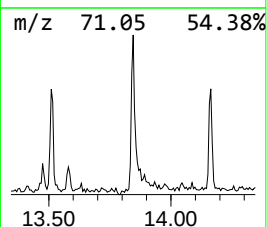
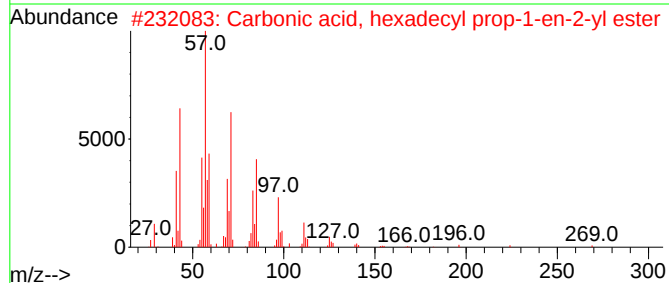
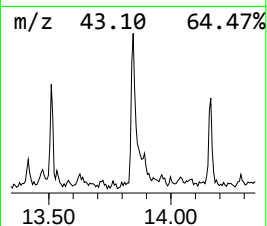
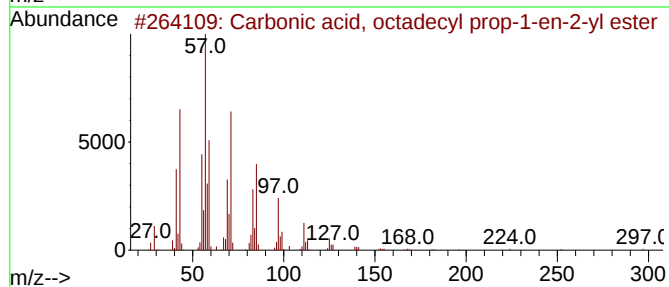
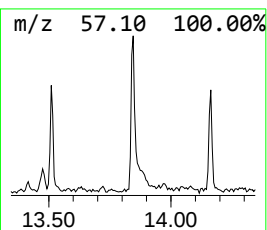
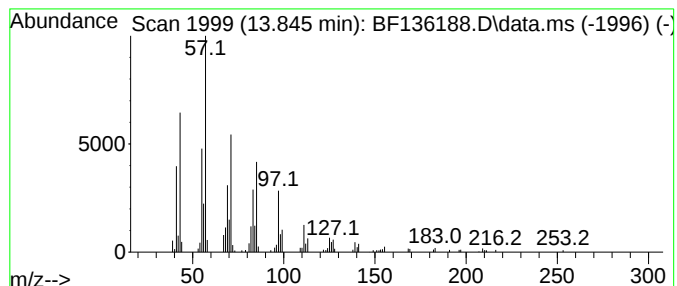
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Peak Number 5 Carbonic acid, octadecyl pr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.78 ng	213133	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
2			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
3			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	87
4			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	83
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.134	15.9	ng	611609	1	6.804	770905	20.0
2-Pentanone, 4-...	5.057	23.4	ng	900199	1	6.804	770905	20.0
n-Hexadecanoic ...	11.869	5.7	ng	350026	4	11.328	1223500	20.0
Octadecanoic acid	12.657	3.4	ng	126947	5	13.980	737567	20.0
Carbonic acid, ...	13.845	5.8	ng	213133	5	13.980	737567	20.0
Lup-20(29)-en-3...	18.186	4.5	ng	154392	6	15.463	687834	20.0