

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101623\
 Data File : BF135783.D
 Acq On : 16 Oct 2023 18:45
 Operator : CG\JU
 Sample : 04656-21
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-102S

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135783.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	34	39	51	rVB2	25893	46726	1.38%	0.236%
2	4.957	485	488	499	rBV	98709	143108	4.22%	0.722%
3	5.369	555	558	592	rBV	1259983	1658999	48.88%	8.367%
4	6.387	728	731	758	rBV	883334	1104558	32.54%	5.570%
5	6.592	763	766	776	rBV	24621	59584	1.76%	0.300%
6	6.734	787	790	800	rVB	755576	662355	19.52%	3.340%
7	7.304	883	887	902	rBV	2134080	2137859	62.99%	10.782%
8	8.016	1005	1008	1028	rBV	1025099	871821	25.69%	4.397%
9	8.433	1076	1079	1091	rBV	222693	254600	7.50%	1.284%
10	9.098	1188	1192	1195	rBV	3753590	3394038	100.00%	17.117%
11	9.216	1208	1212	1224	rVB	879381	869824	25.63%	4.387%
12	9.775	1303	1307	1321	rVB	1129087	942384	27.77%	4.753%
13	10.575	1439	1443	1458	rBV	2015182	2093630	61.69%	10.559%
14	11.269	1558	1561	1569	rBV	1141797	993755	29.28%	5.012%
15	11.804	1648	1652	1672	rBV	133426	199749	5.89%	1.007%
16	12.374	1747	1749	1751	rVB	55417	41004	1.21%	0.207%
17	12.598	1783	1787	1796	rBV2	29700	54833	1.62%	0.277%
18	12.868	1828	1833	1836	rBV	3162048	2977930	87.74%	15.018%
19	13.874	1995	2004	2008	rBV8	25999	80282	2.37%	0.405%
20	13.933	2011	2014	2025	rVB	581741	601525	17.72%	3.034%
21	15.409	2261	2265	2282	rBV	441840	640179	18.86%	3.229%

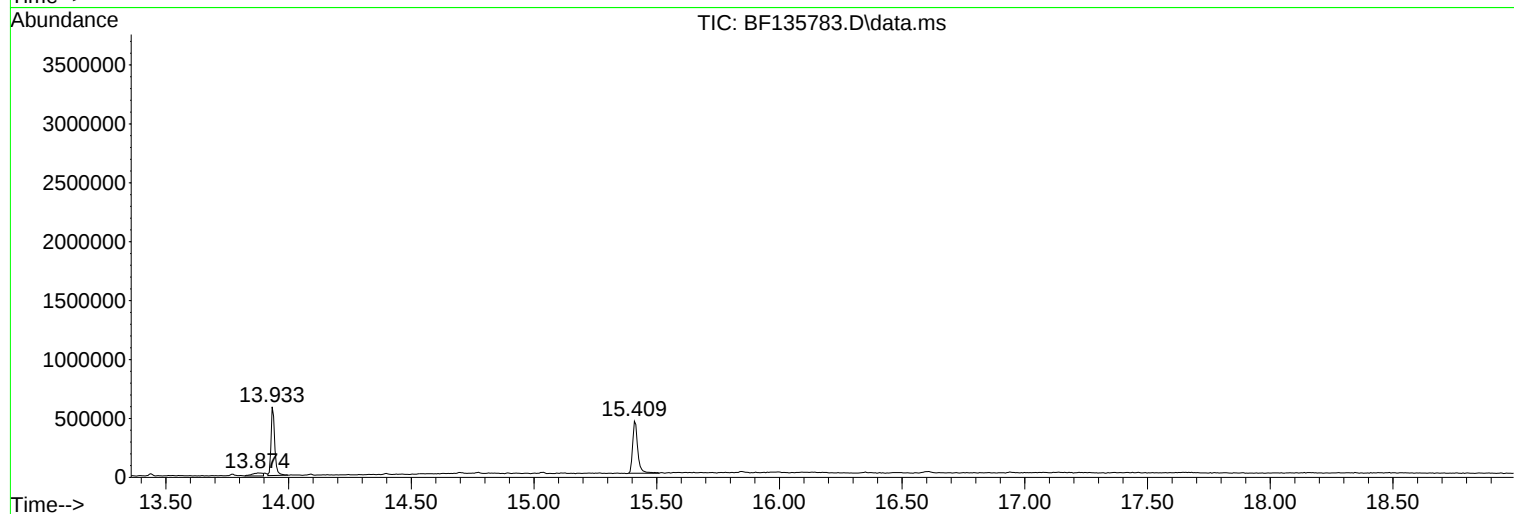
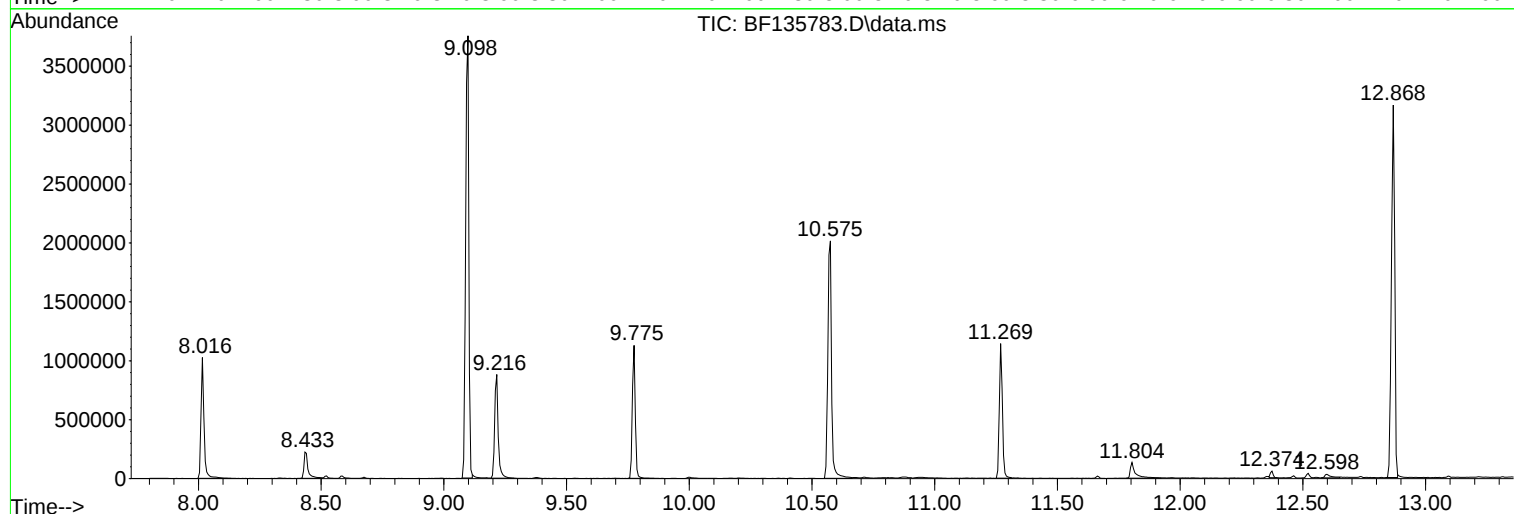
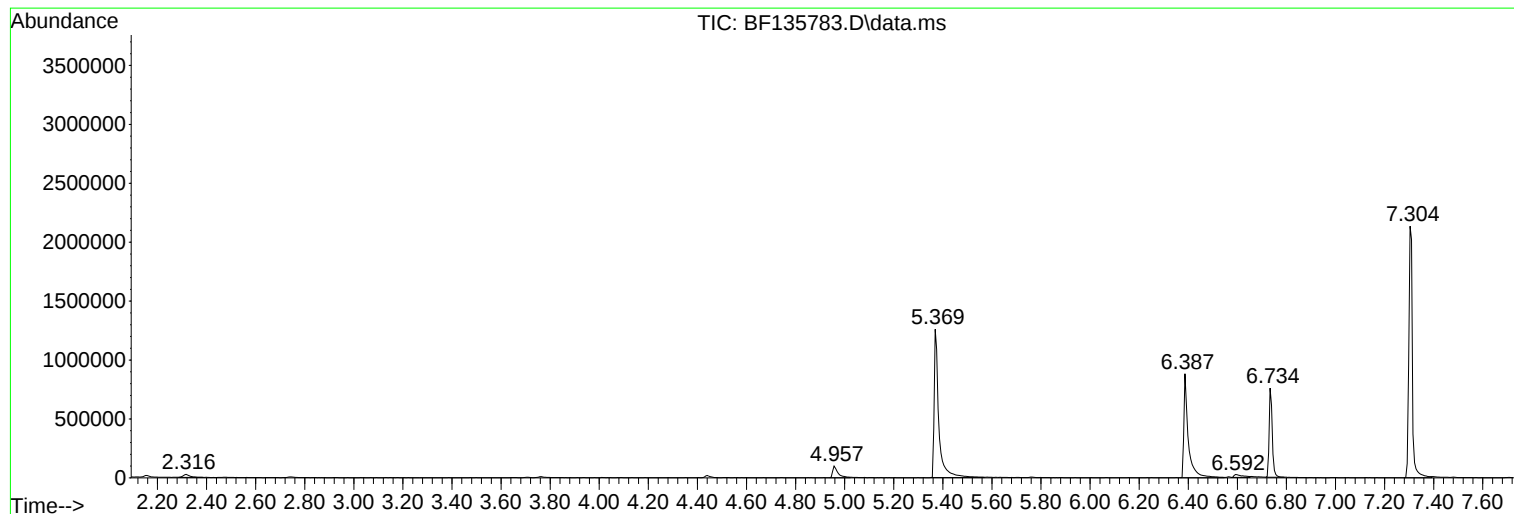
Sum of corrected areas: 19828743

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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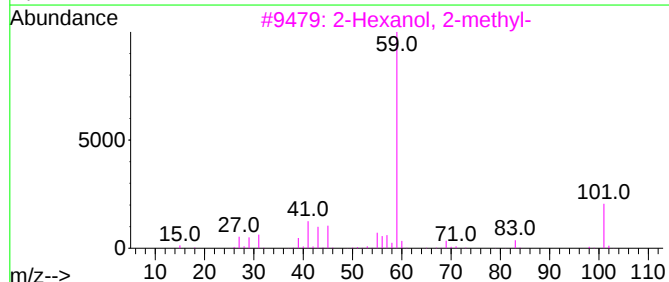
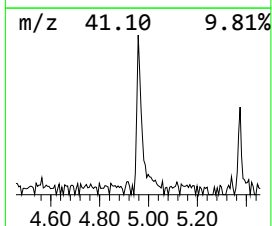
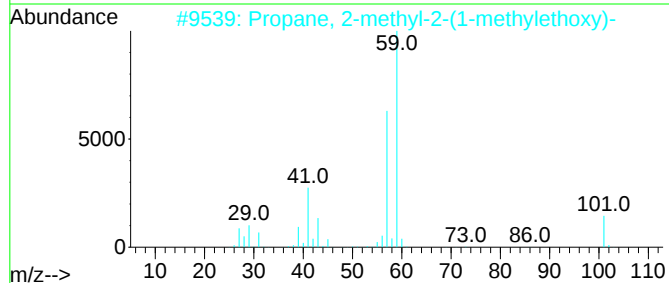
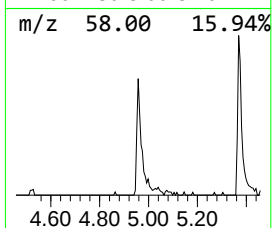
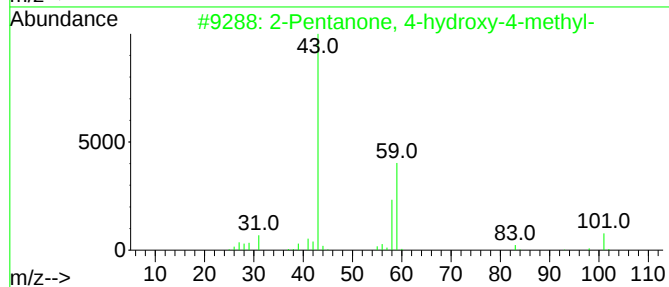
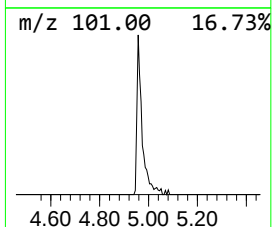
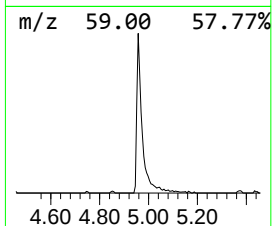
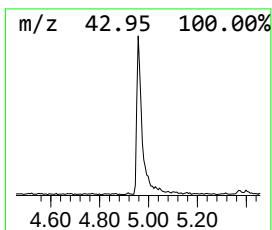
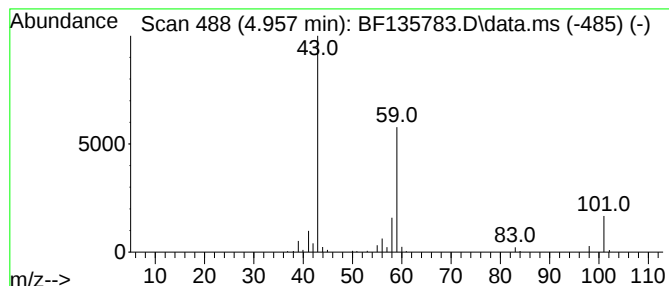
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	4.32 ng	143108	1,4-Dichlorobenzene-d4	6.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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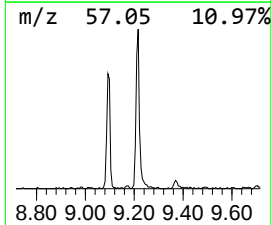
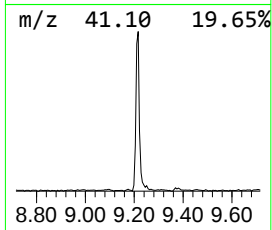
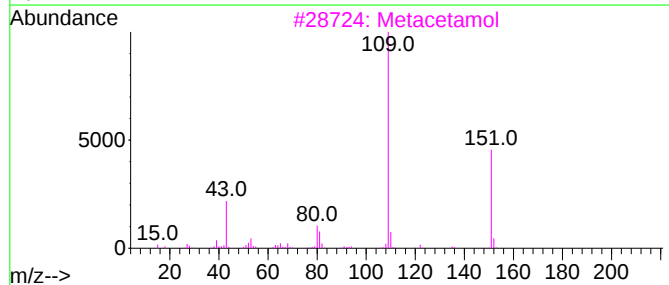
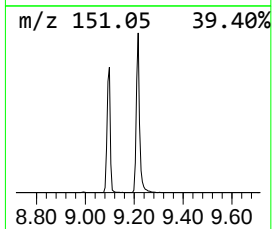
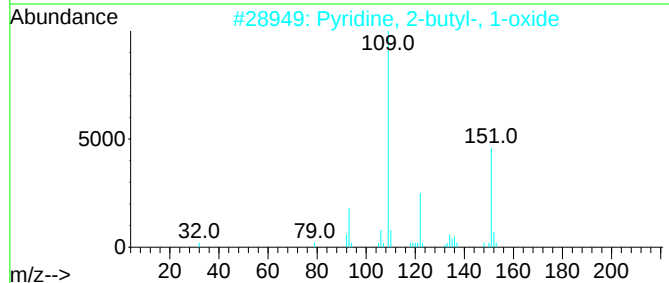
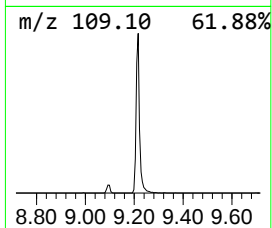
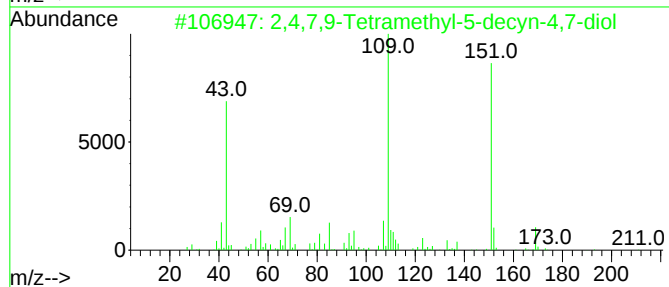
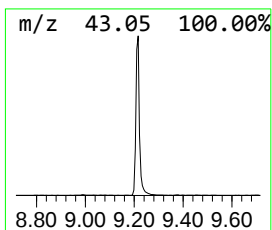
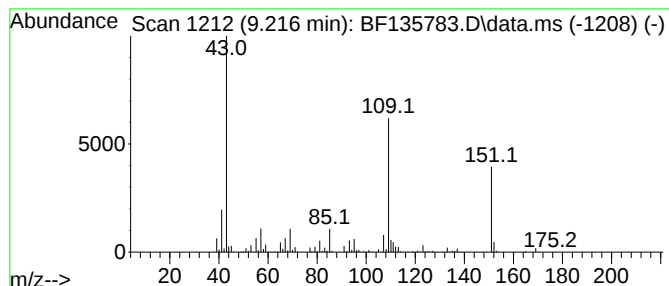
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	18.46 ng	869824	Acenaphthene-d10	9.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	90
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	59
3	Metacetamol	151	C8H9NO2		000621-42-1	53
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3		1000107-08-7	42
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O		000116-02-9	38



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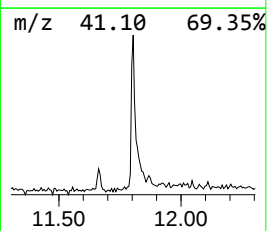
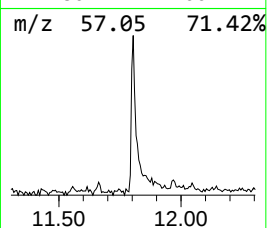
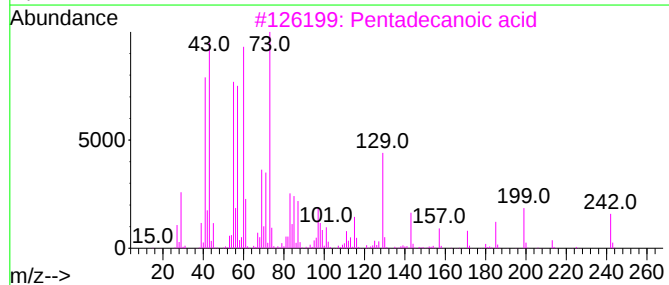
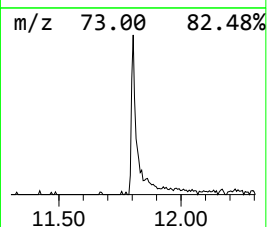
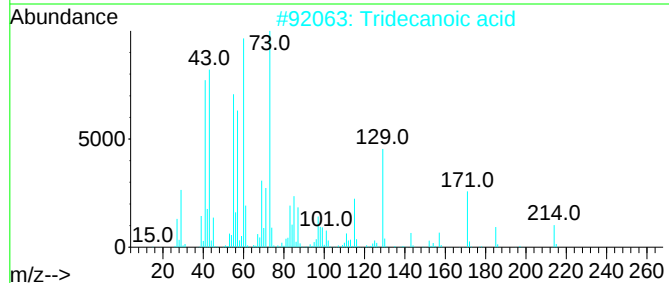
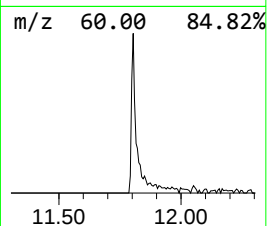
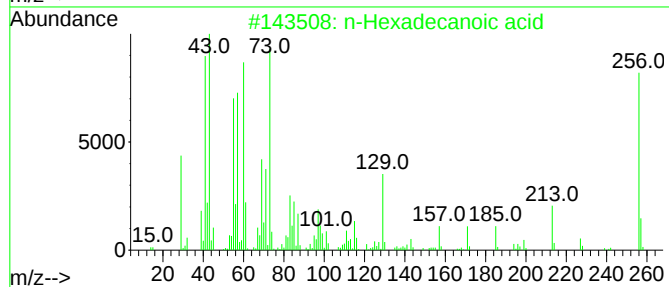
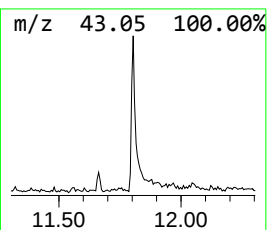
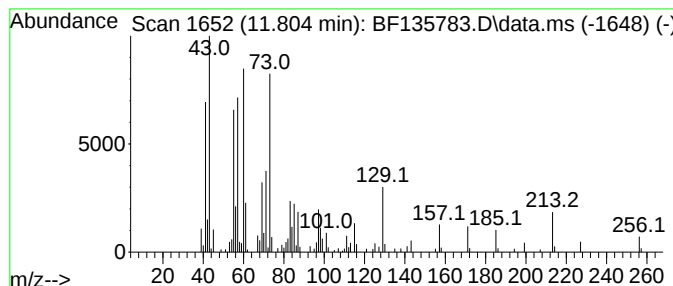
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	4.02 ng	199749	Phenanthrene-d10	11.269

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Nonanoic acid	158	C9H18O2	000112-05-0	60



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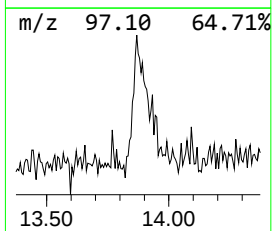
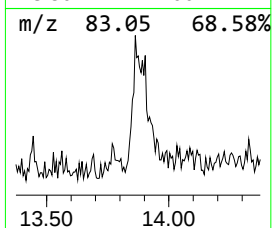
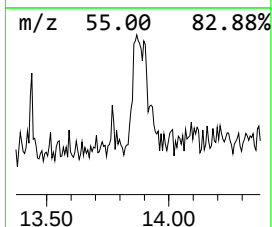
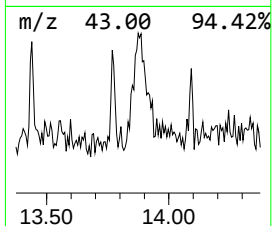
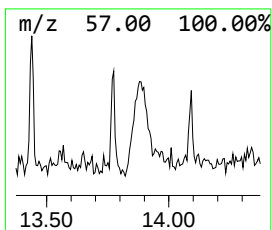
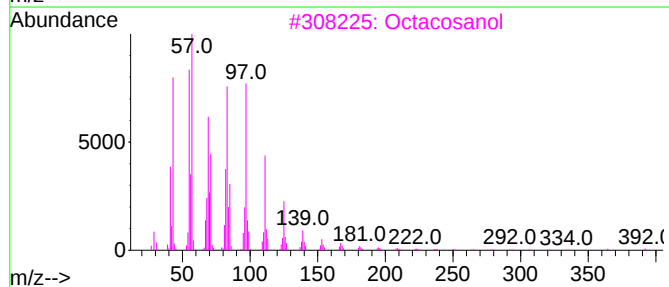
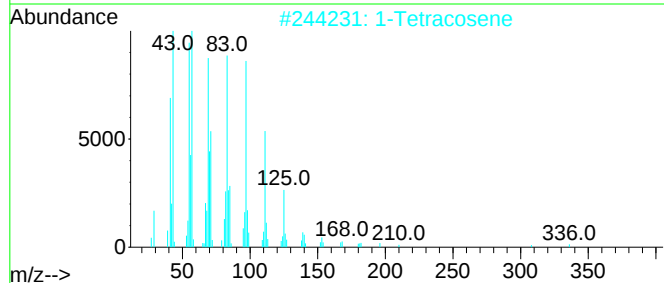
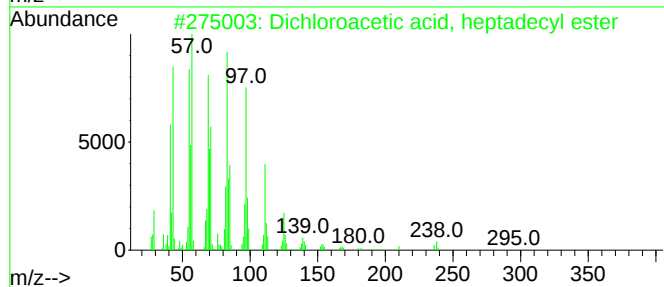
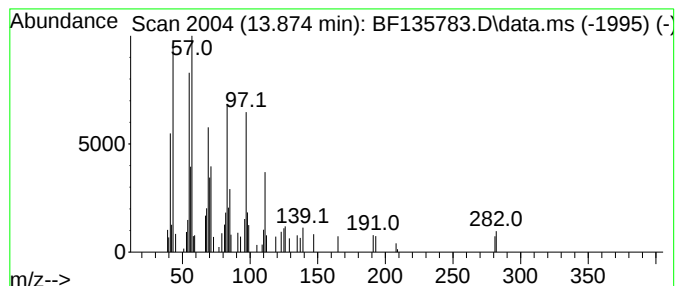
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Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.67 ng	80282	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
2			1-Tetracosene	336	C24H48	010192-32-2	87
3			Octacosanol	410	C28H58O	000557-61-9	86
4			E-15-Heptadecenal	252	C17H32O	1000130-97-9	83
5			1-Nonadecene	266	C19H38	018435-45-5	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	4.3	ng	143108	1	6.734	662355	20.0
2,4,7,9-Tetrame...	9.216	18.5	ng	869824	3	9.775	942384	20.0
n-Hexadecanoic ...	11.804	4.0	ng	199749	4	11.269	993755	20.0
Dichloroacetic ...	13.874	2.7	ng	80282	5	13.933	601525	20.0