

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
 Data File : BM047298.D
 Acq On : 21 Aug 2024 15:06
 Operator : RC/JU
 Sample : P3596-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 918-J-WS-081324-FD

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047298.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.011	355	361	374	rBV	1298134	1951491	13.39%	3.600%
2	6.569	619	626	641	rBV	793838	1303680	8.94%	2.405%
3	7.352	752	759	769	rBV	676806	1061839	7.28%	1.959%
4	8.499	946	954	973	rBV	1717562	2864392	19.65%	5.284%
5	10.110	1221	1228	1239	rBV	847459	1415776	9.71%	2.611%
6	10.875	1348	1358	1370	rBV	83752	190201	1.30%	0.351%
7	12.622	1646	1655	1676	rBV	4477909	6770956	46.45%	12.489%
8	14.016	1885	1892	1910	rBV	1333861	2010644	13.79%	3.709%
9	14.251	1926	1932	1933	rBV	1491751	1784846	12.24%	3.292%
10	14.269	1933	1935	1951	rVB	1766014	2286735	15.69%	4.218%
11	15.522	2142	2148	2161	rBV	4831922	7391274	50.70%	13.634%
12	16.780	2356	2362	2371	rBV	1755864	2545827	17.46%	4.696%
13	17.716	2516	2521	2530	rBV	454595	712973	4.89%	1.315%
14	18.674	2681	2684	2688	rVB	171859	194969	1.34%	0.360%
15	19.015	2738	2742	2750	rBV	183036	292740	2.01%	0.540%
16	19.451	2810	2816	2827	rBV	11599354	14577128	100.00%	26.888%
17	20.757	3034	3038	3045	rBV2	263729	450181	3.09%	0.830%
18	21.021	3078	3083	3092	rBV	2347062	3183222	21.84%	5.872%
19	23.715	3533	3541	3555	rVB	1403272	3224558	22.12%	5.948%

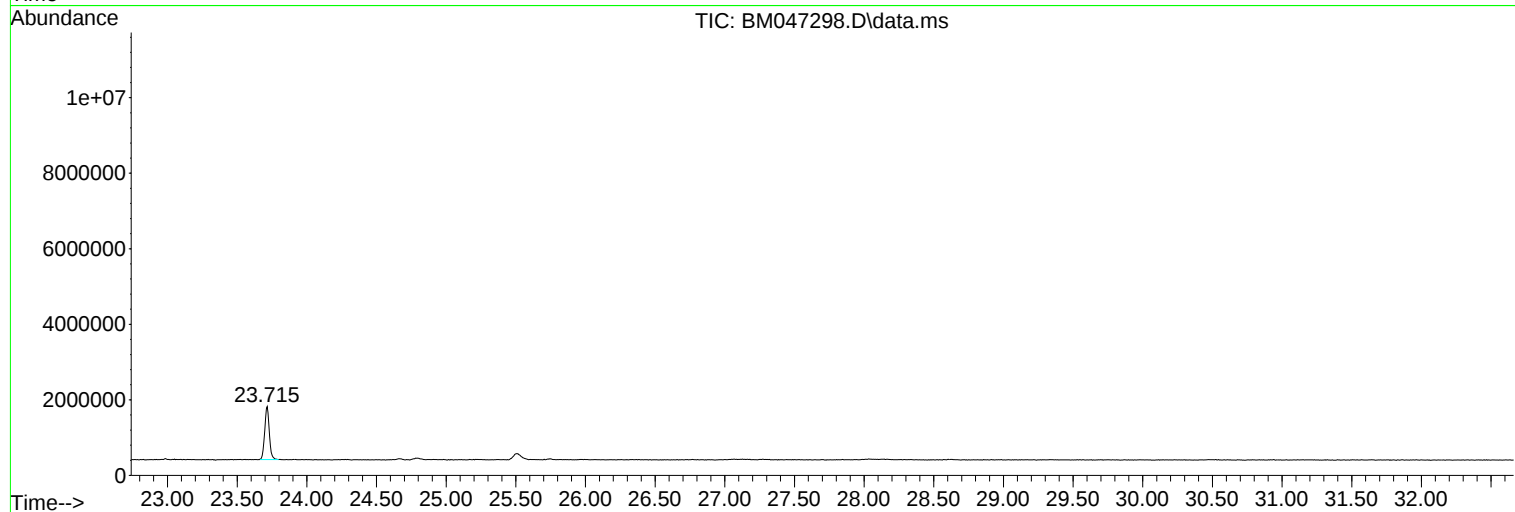
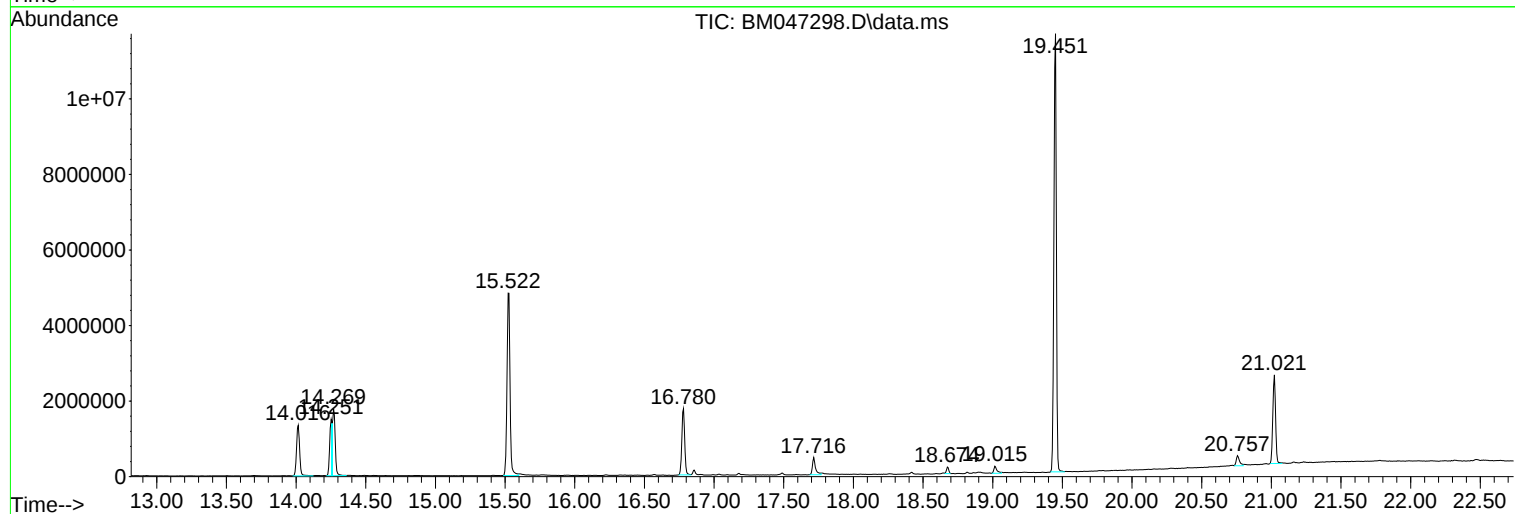
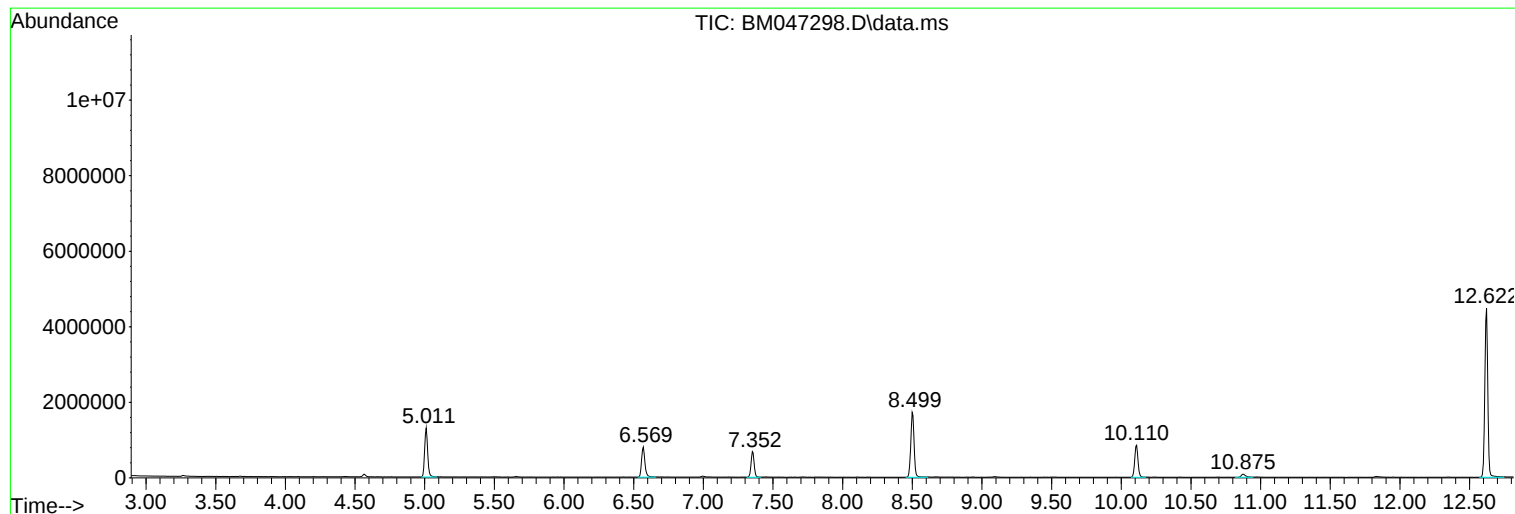
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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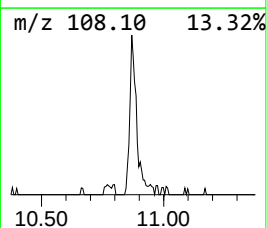
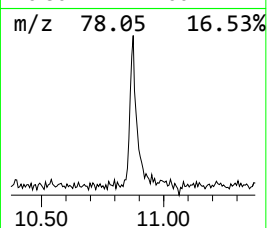
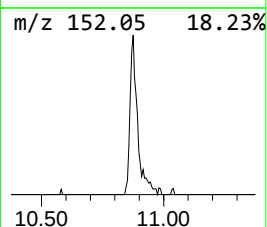
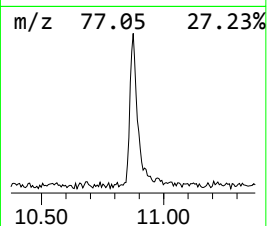
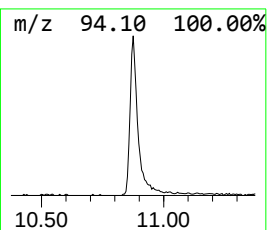
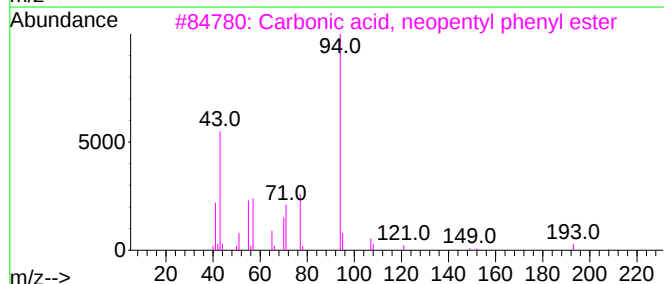
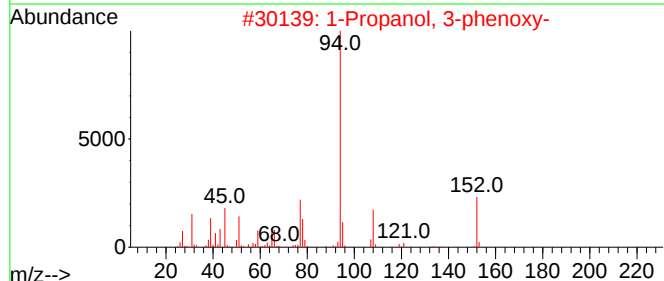
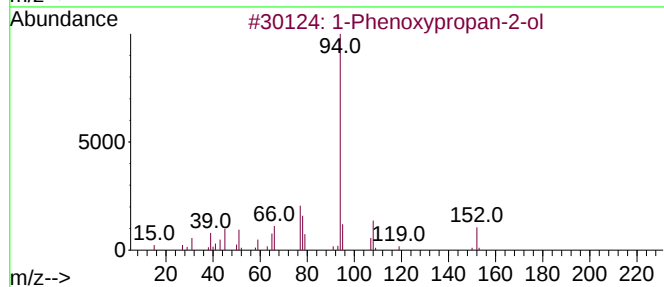
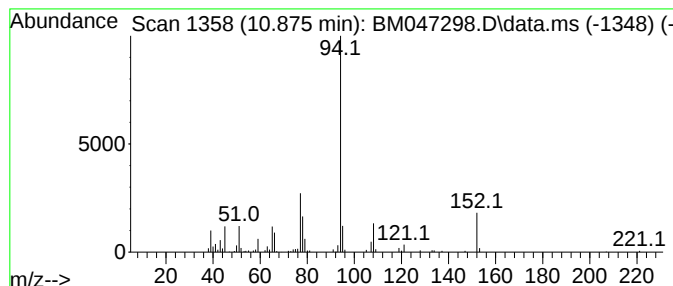
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	2.69 ng	190201	Naphthalene-d8	10.110

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3		Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5		Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	59



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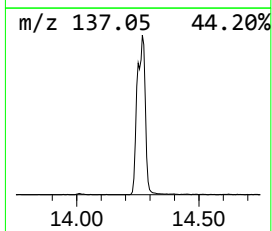
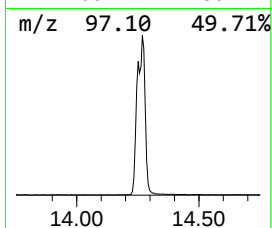
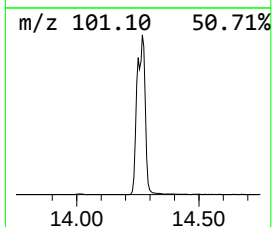
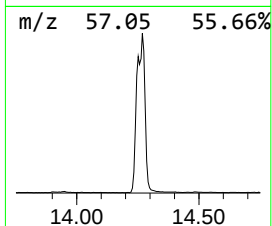
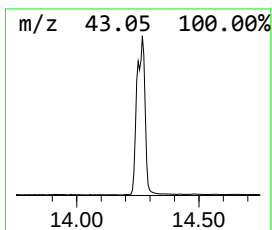
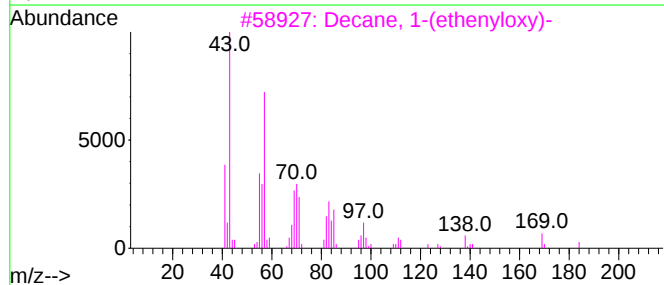
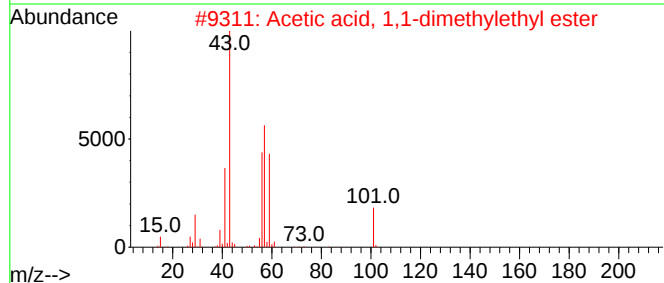
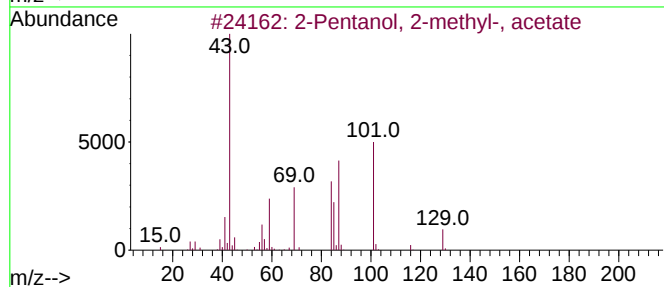
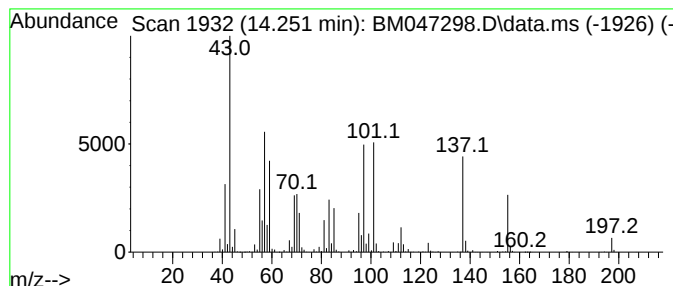
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown14.251 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.251	17.75 ng	1784850	Acenaphthene-d10		14.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-, acetate	144	C8H16O2		034859-98-8	14
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2		000540-88-5	10
3	Decane, 1-(ethenyloxy)-	184	C12H24O		000765-05-9	10
4	2,2,3,4-Tetramethylhex-5-en-3-ol	156	C10H20O		1010191-06-9	10
5	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3		058002-07-6	10



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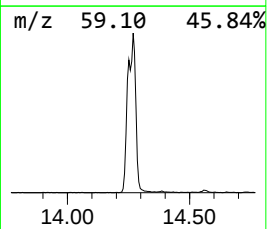
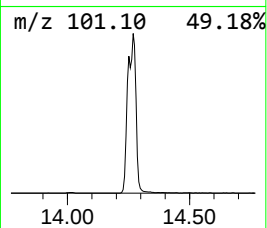
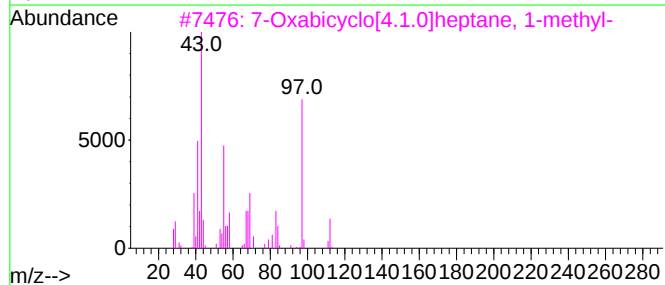
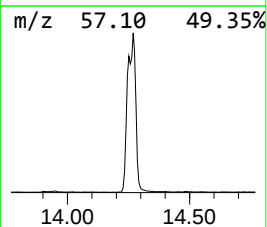
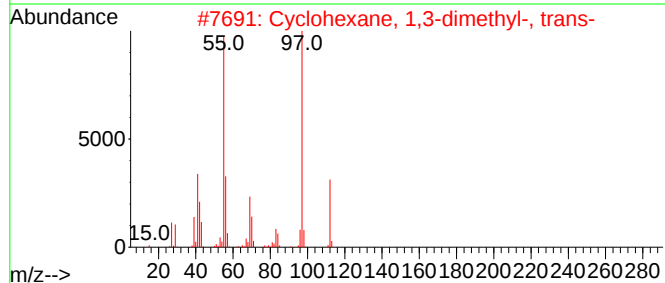
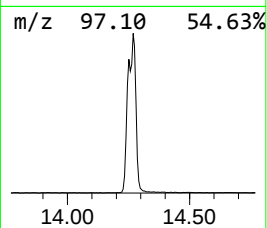
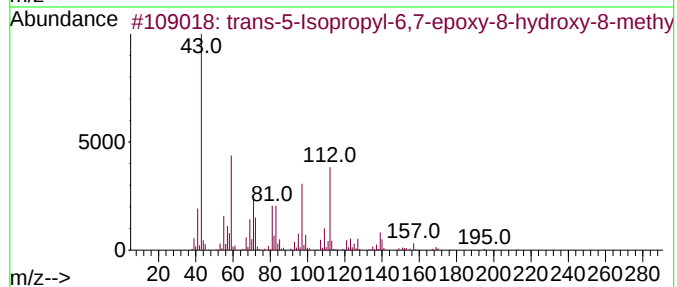
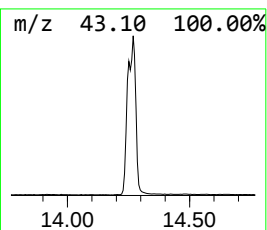
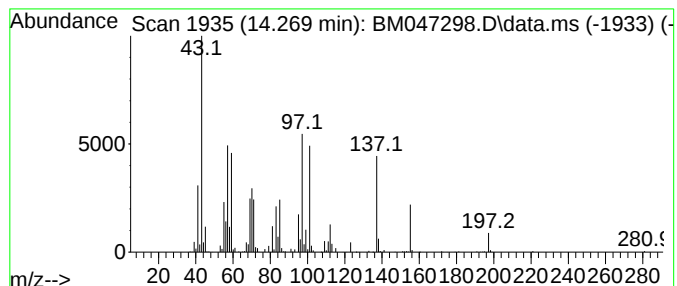
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Peak Number 3 unknown14.269 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	22.75 ng	2286740	Acenaphthene-d10	14.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	16
2			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	11
3			7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	11
4			2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10
5			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	10



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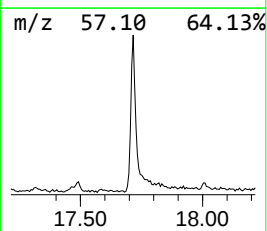
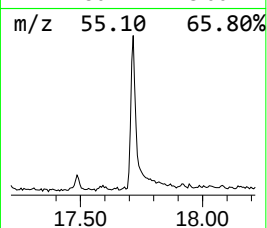
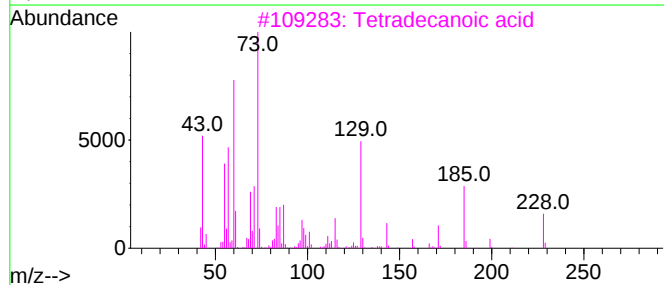
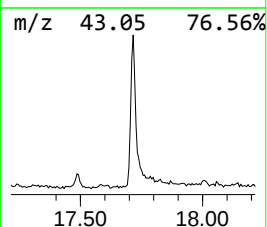
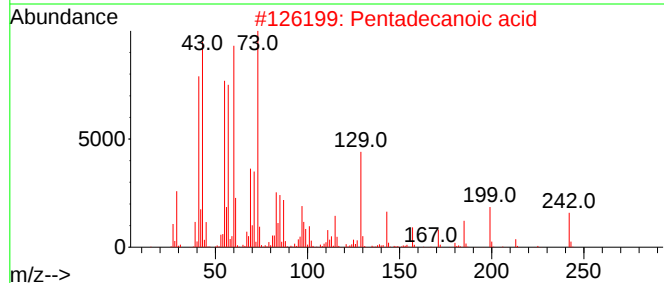
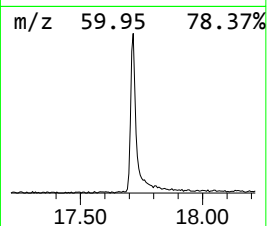
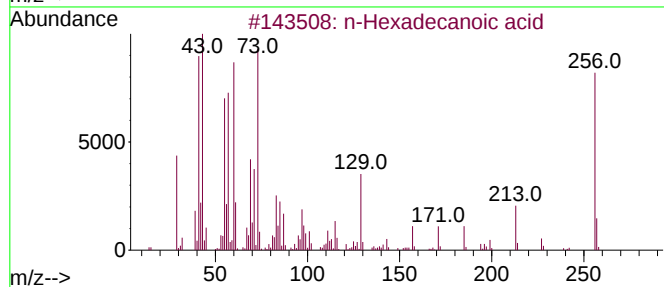
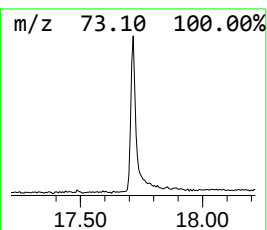
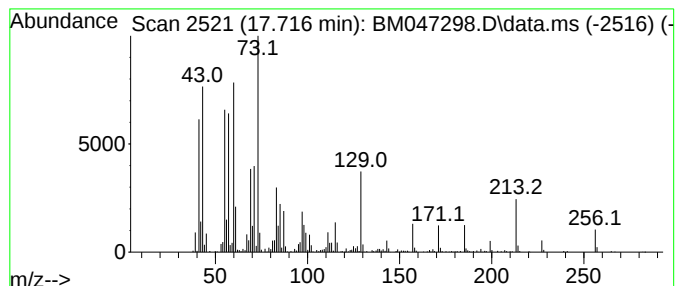
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.716	5.60 ng	712973	Phenanthrene-d10	16.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46



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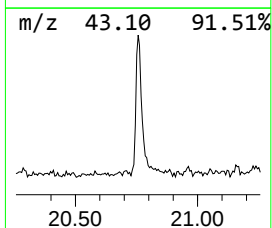
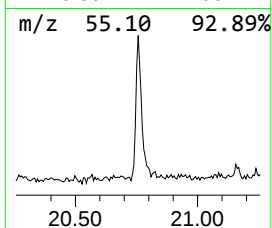
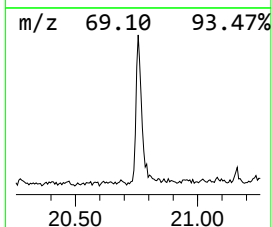
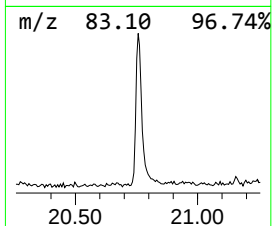
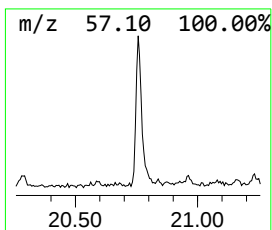
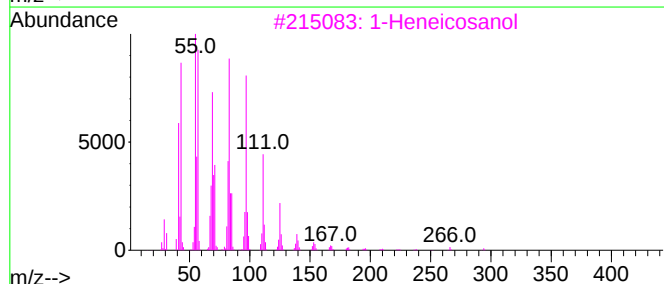
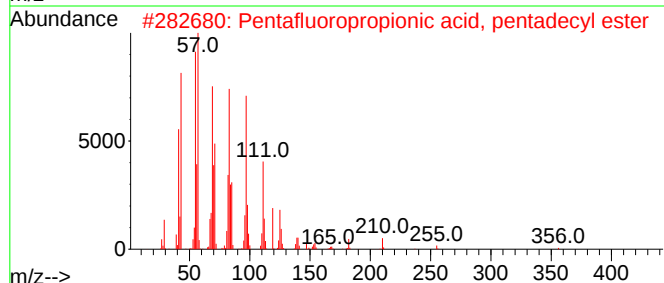
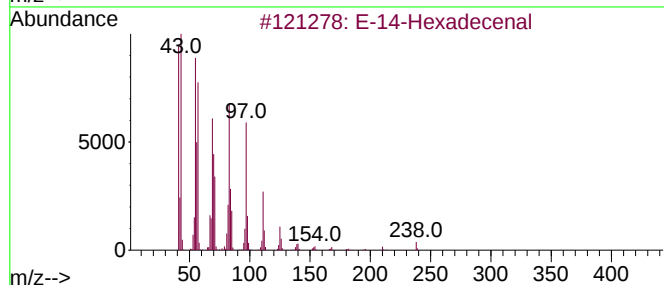
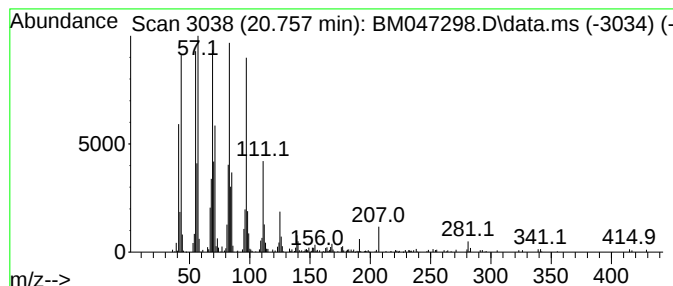
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Peak Number 5 E-14-Hexadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.757	2.83 ng	450181	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-14-Hexadecenal	238	C16H30O	330207-53-9	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	94
4			1-Heptacosanol	396	C27H56O	002004-39-9	94
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Phenoxypropan...	10.875	2.7	ng	190201	2	10.110	1415780	20.0
unknown14.251	14.251	17.8	ng	1784850	3	14.016	2010640	20.0
unknown14.269	14.269	22.8	ng	2286740	3	14.016	2010640	20.0
n-Hexadecanoic ...	17.716	5.6	ng	712973	4	16.780	2545830	20.0
E-14-Hexadecenal	20.757	2.8	ng	450181	5	21.021	3183220	20.0