

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
 Data File : BM047271.D
 Acq On : 20 Aug 2024 14:46
 Operator : RC/JU
 Sample : P3643-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 924-K1-SD-0-0.5-081524

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: BM047271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.569	279	286	295	rVB	131709	199068	1.90%	0.403%
2	5.016	355	362	377	rBV	2361734	3555433	33.97%	7.205%
3	6.575	620	627	642	rBV	2328572	3808327	36.39%	7.717%
4	7.357	752	760	770	rBV	753796	1161973	11.10%	2.355%
5	8.504	947	955	969	rBV	1498675	2478805	23.68%	5.023%
6	10.116	1221	1229	1241	rBV	931126	1550198	14.81%	3.141%
7	10.881	1352	1359	1368	rBV2	65535	142739	1.36%	0.289%
8	12.627	1648	1656	1670	rBV	3574108	5552087	53.05%	11.251%
9	14.016	1886	1892	1903	rBV	1458005	2214620	21.16%	4.488%
10	14.257	1926	1933	1934	rBV	541711	743872	7.11%	1.507%
11	14.274	1934	1936	1947	rVB	696903	820175	7.84%	1.662%
12	15.527	2142	2149	2163	rBV	3738022	5599492	53.50%	11.347%
13	16.780	2356	2362	2375	rBV	1892673	2843098	27.16%	5.761%
14	17.721	2517	2522	2535	rBV	326952	563386	5.38%	1.142%
15	19.021	2739	2743	2755	rBV2	146331	270778	2.59%	0.549%
16	19.451	2810	2816	2827	rBV	8742317	10466468	100.00%	21.210%
17	20.762	3034	3039	3050	rBV	469780	822604	7.86%	1.667%
18	21.021	3078	3083	3092	rBV	2444315	3407178	32.55%	6.904%
19	23.721	3534	3542	3558	rVB	1328678	3147481	30.07%	6.378%

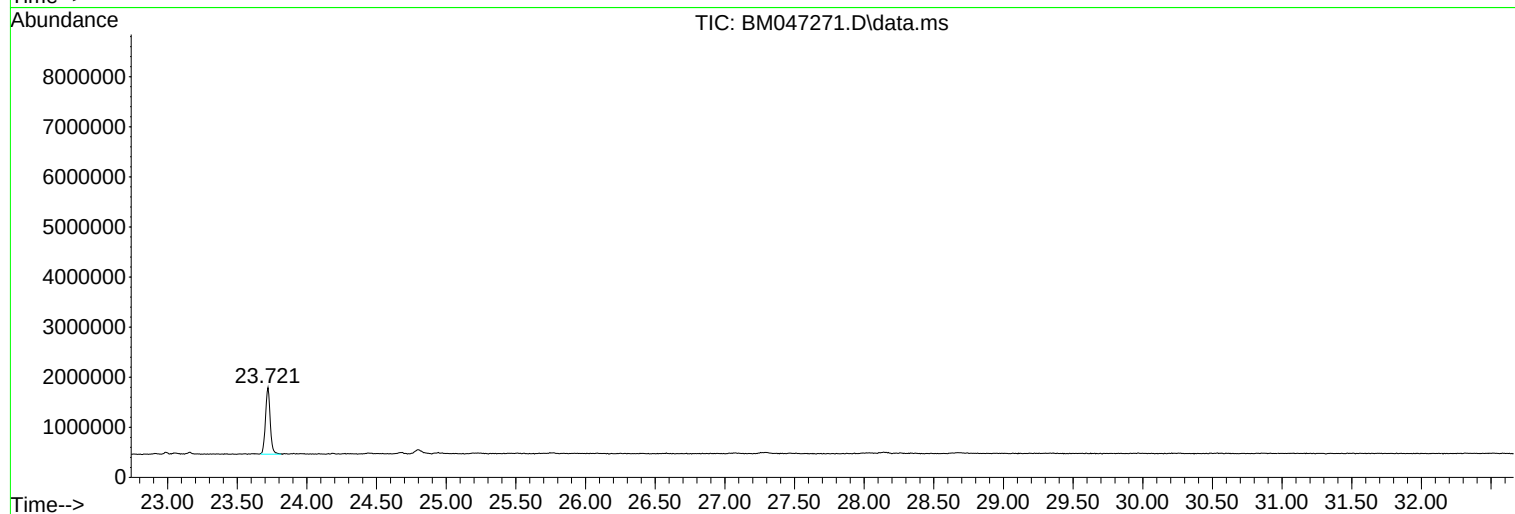
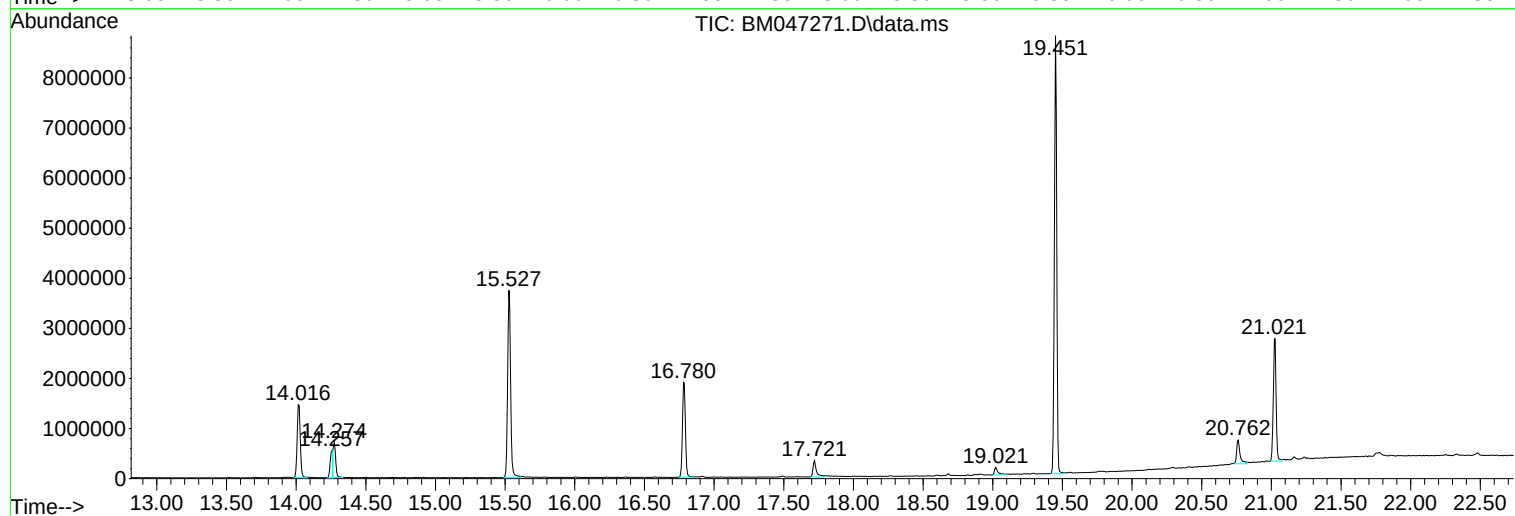
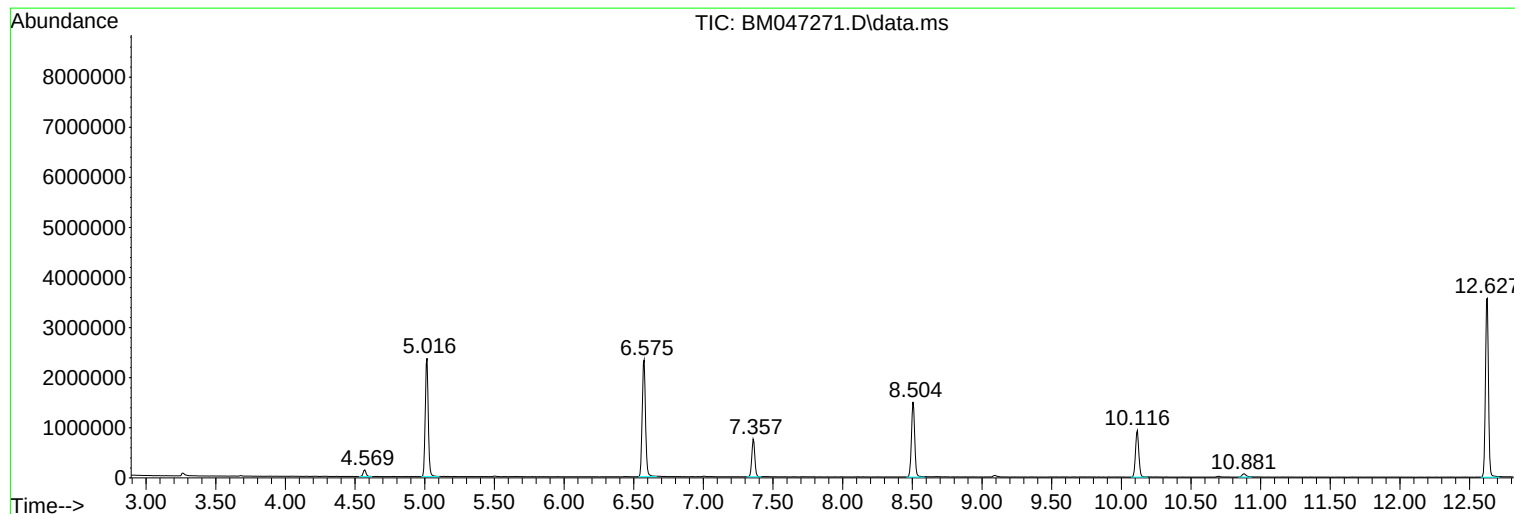
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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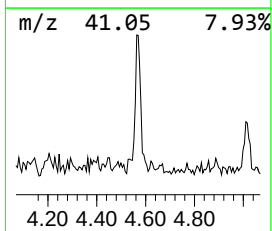
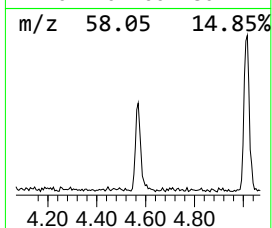
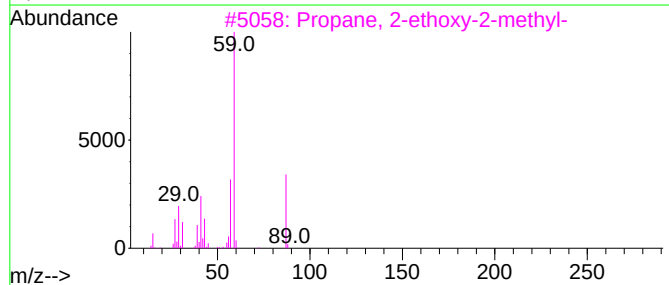
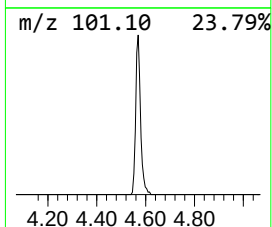
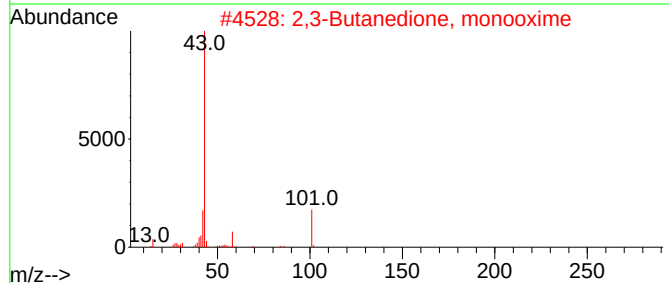
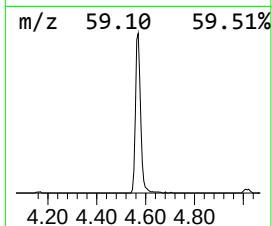
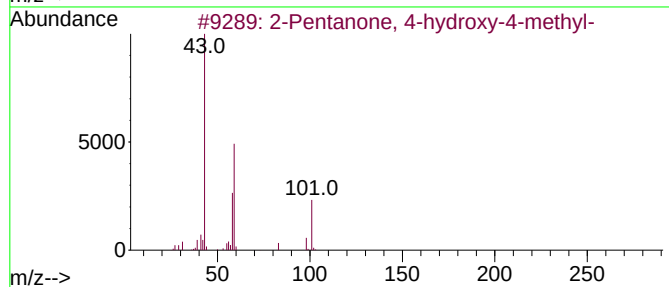
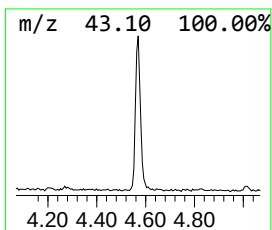
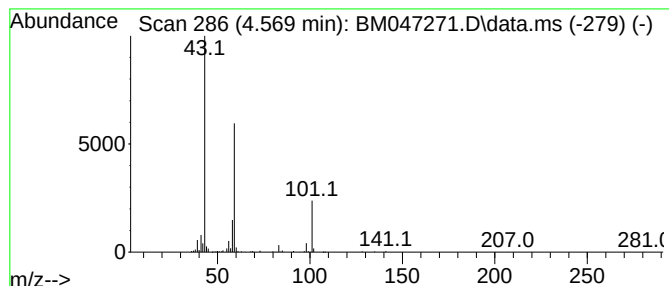
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	3.43 ng	199068	1,4-Dichlorobenzene-d4	7.357

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35	
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17	
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	17	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	



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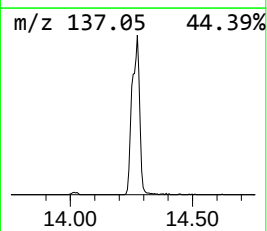
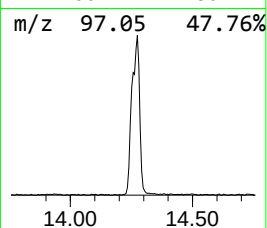
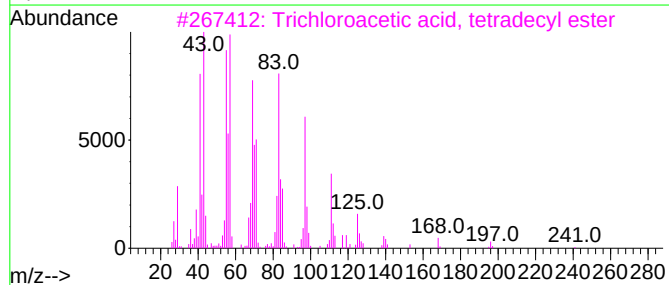
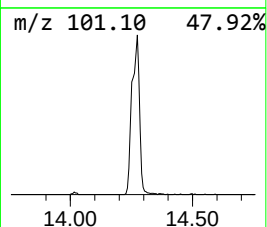
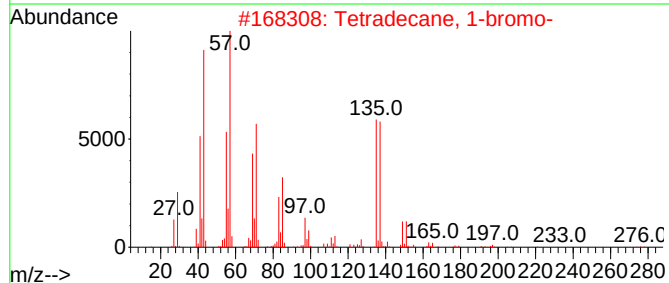
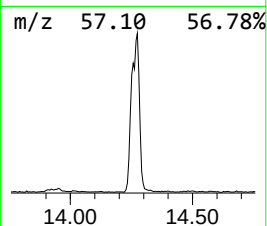
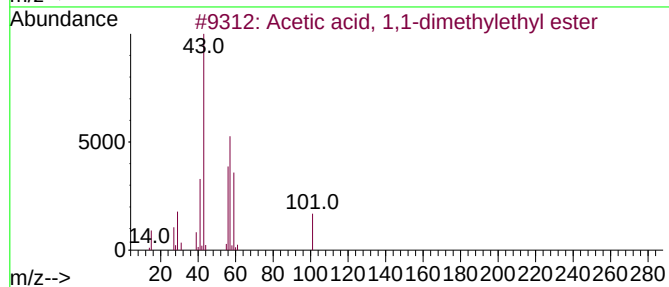
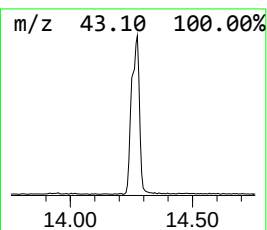
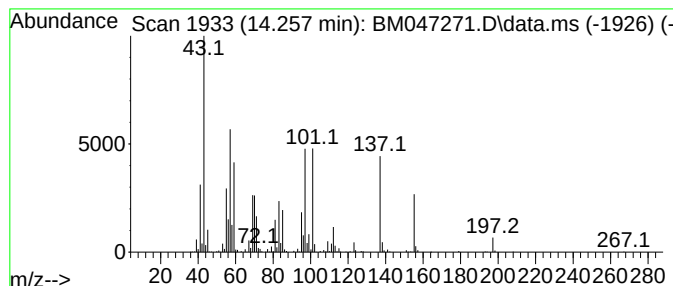
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown14.257 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	6.72 ng	743872	Acenaphthene-d10	14.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
2			Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	14
3			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	12
4			6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	12
5			Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	10



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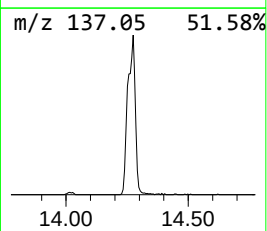
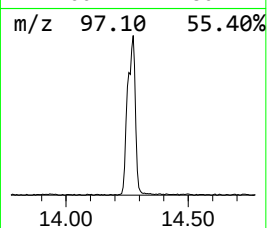
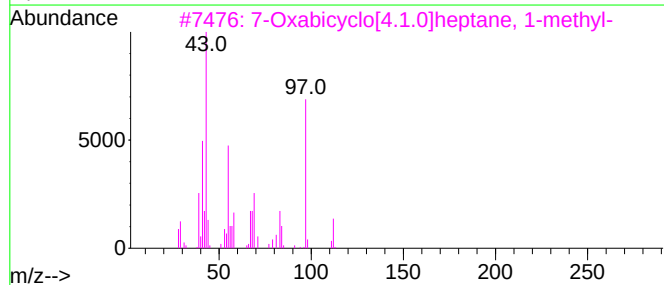
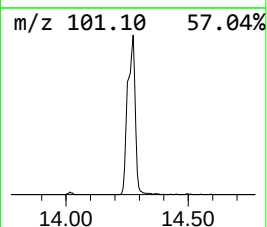
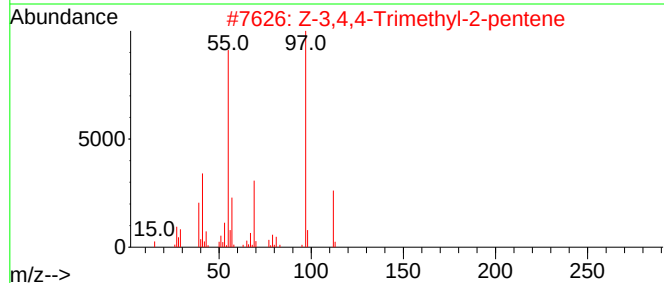
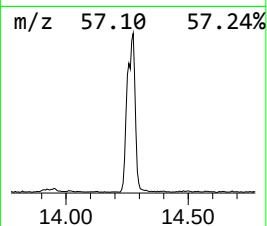
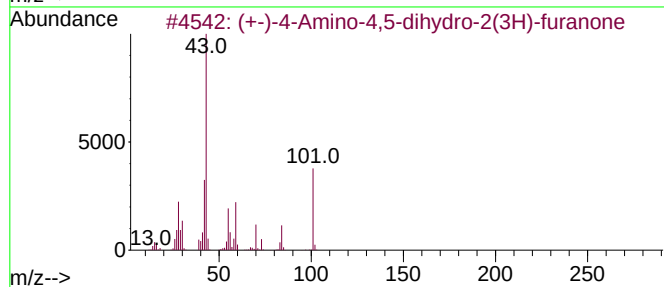
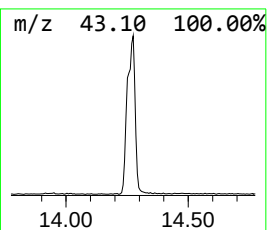
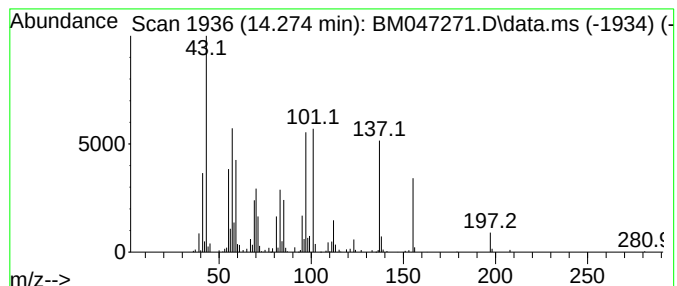
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Peak Number 3 unknown14.274 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.274	7.41 ng	820175	Acenaphthene-d10	14.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	22		
2	Z-3,4,4-Trimethyl-2-pentene	112	C8H16	039761-64-3	11		
3	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	11		
4	Succinic acid, hexadecyl 2,2,2-t...	472	C22H39Cl3O4	1000349-17-9	10		
5	2-Pyrazoline, 1,4,5-trimethyl-	112	C6H12N2	007423-11-2	10		



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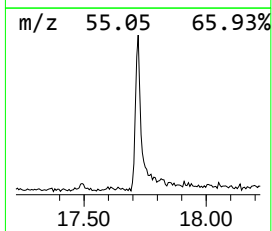
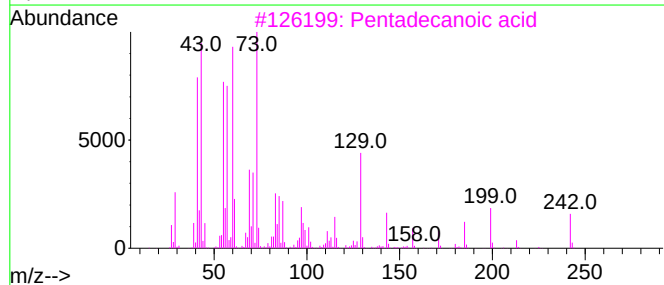
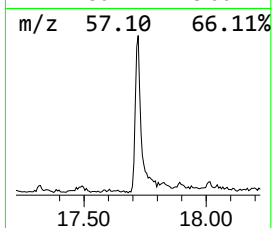
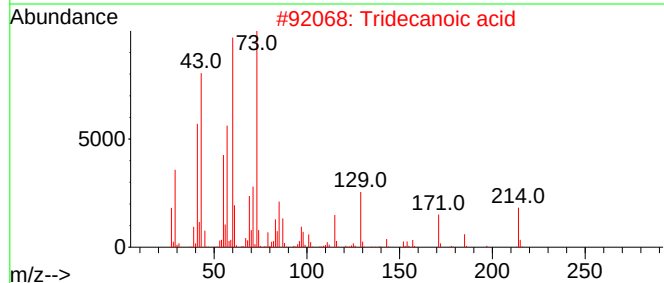
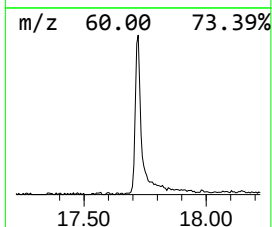
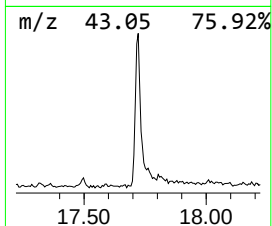
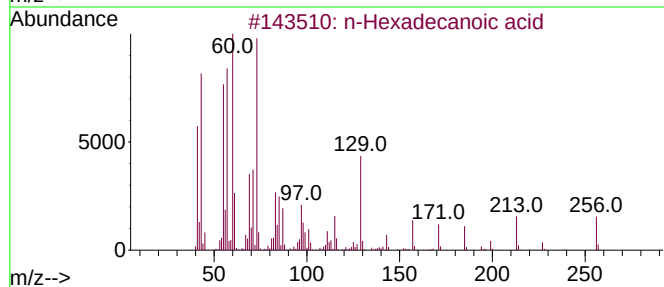
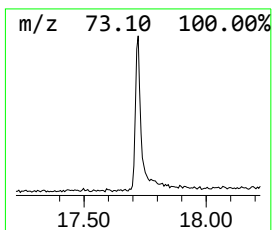
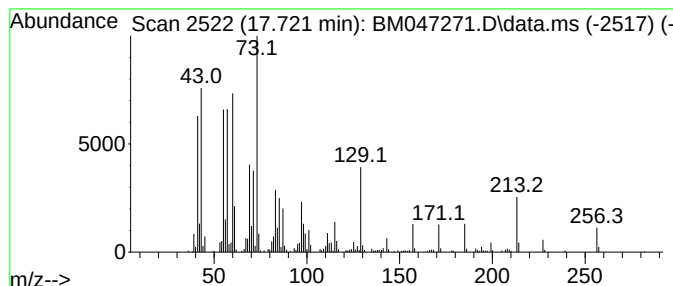
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	3.96 ng	563386	Phenanthrene-d10	16.786

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	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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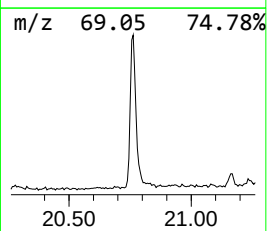
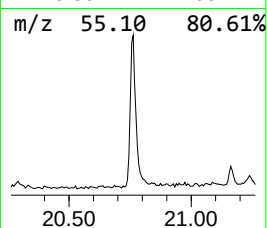
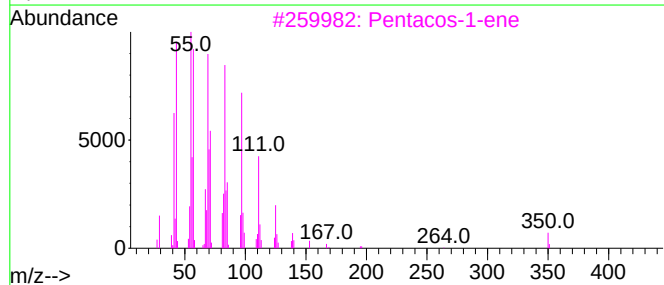
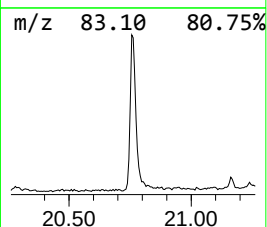
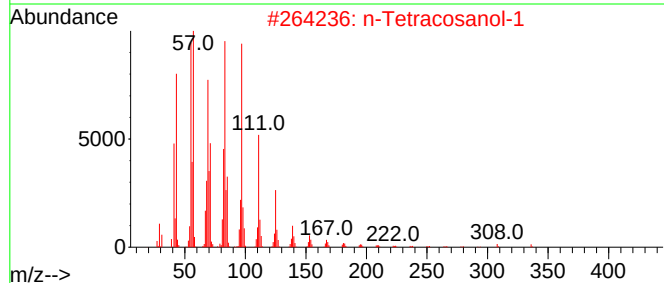
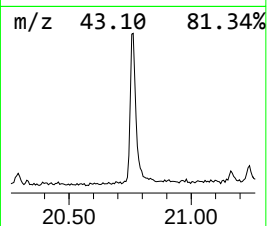
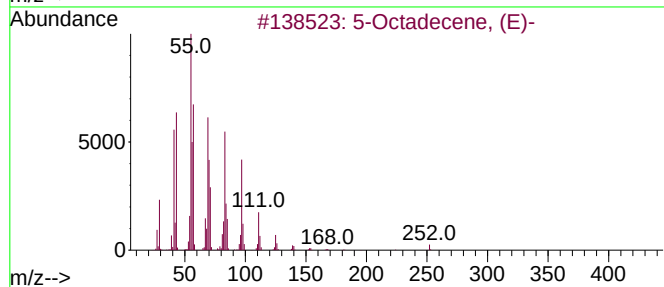
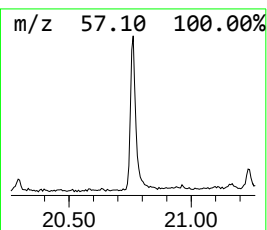
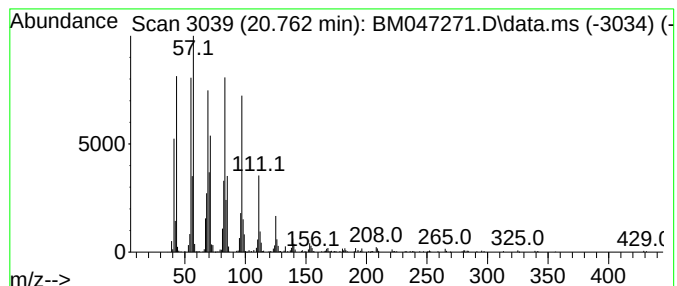
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Peak Number 5 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.762	4.83 ng	822604	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			Heptacos-1-ene	378	C27H54	015306-27-1	94
5			Behenic alcohol	326	C22H46O	000661-19-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.569	3.4	ng	199068	1	7.357	1161970	20.0
unknown14.257	14.257	6.7	ng	743872	3	14.016	2214620	20.0
unknown14.274	14.274	7.4	ng	820175	3	14.016	2214620	20.0
n-Hexadecanoic ...	17.721	4.0	ng	563386	4	16.786	2843100	20.0
5-Octadecene, (E)-	20.762	4.8	ng	822604	5	21.021	3407180	20.0