

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121821\
 Data File : BM033525.D
 Acq On : 18 Dec 2021 18:50
 Operator : CG/JU
 Sample : M5115-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-1

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-BM121621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033525.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.031	300	305	318	rVB	81659	121930	3.24%	0.908%
2	5.496	377	384	395	rBV	368146	577817	15.36%	4.305%
3	6.113	483	489	497	rVB	27123	41841	1.11%	0.312%
4	7.096	650	656	672	rBV	221099	391946	10.42%	2.920%
5	7.931	791	798	808	rBV	120982	206475	5.49%	1.538%
6	9.101	988	997	1007	rBV	557140	957304	25.46%	7.132%
7	10.736	1267	1275	1287	rBV	161044	287323	7.64%	2.141%
8	13.201	1687	1694	1705	rBV	1453271	2103905	55.94%	15.674%
9	14.577	1922	1928	1934	rBV	274314	409552	10.89%	3.051%
10	16.066	2175	2181	2198	rBV	1297823	1918346	51.01%	14.292%
11	17.324	2389	2395	2402	rBV	367945	547898	14.57%	4.082%
12	18.212	2541	2546	2551	rBV2	50034	71754	1.91%	0.535%
13	19.489	2758	2763	2770	rBV3	35738	54990	1.46%	0.410%
14	19.948	2834	2841	2851	rBV	2913292	3760691	100.00%	28.017%
15	20.730	2970	2974	2980	rBV	757238	781493	20.78%	5.822%
16	21.201	3051	3054	3060	rBV3	59372	78885	2.10%	0.588%
17	21.500	3100	3105	3110	rBV	462424	609111	16.20%	4.538%
18	23.912	3509	3515	3524	rVB	242598	501644	13.34%	3.737%

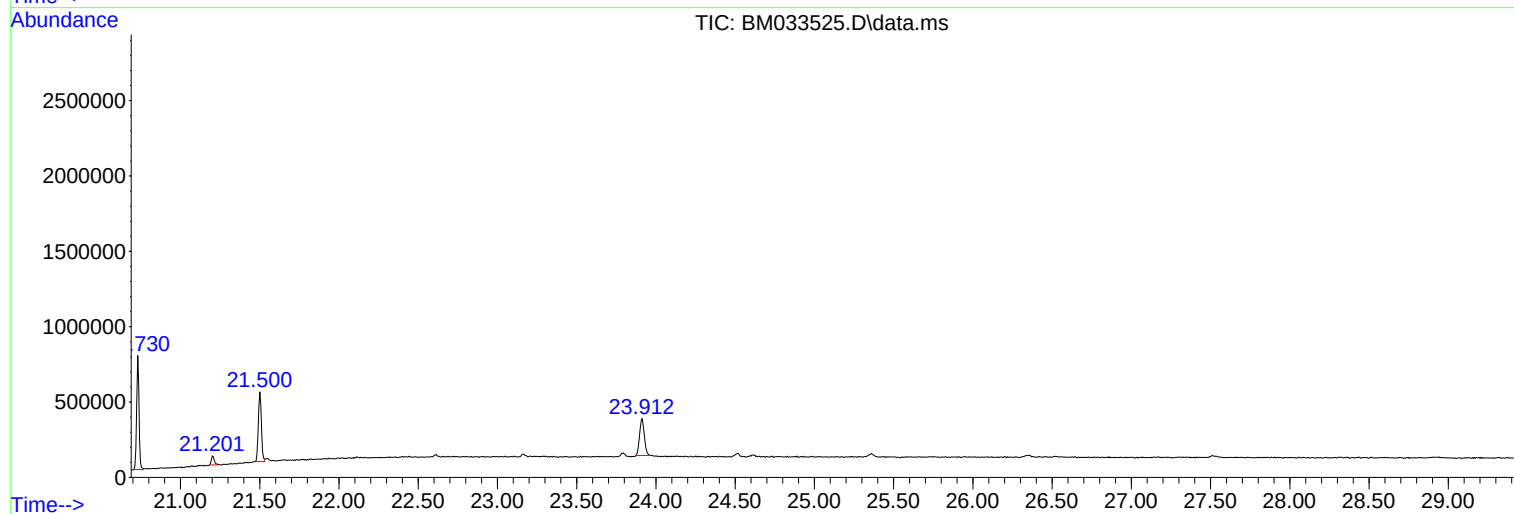
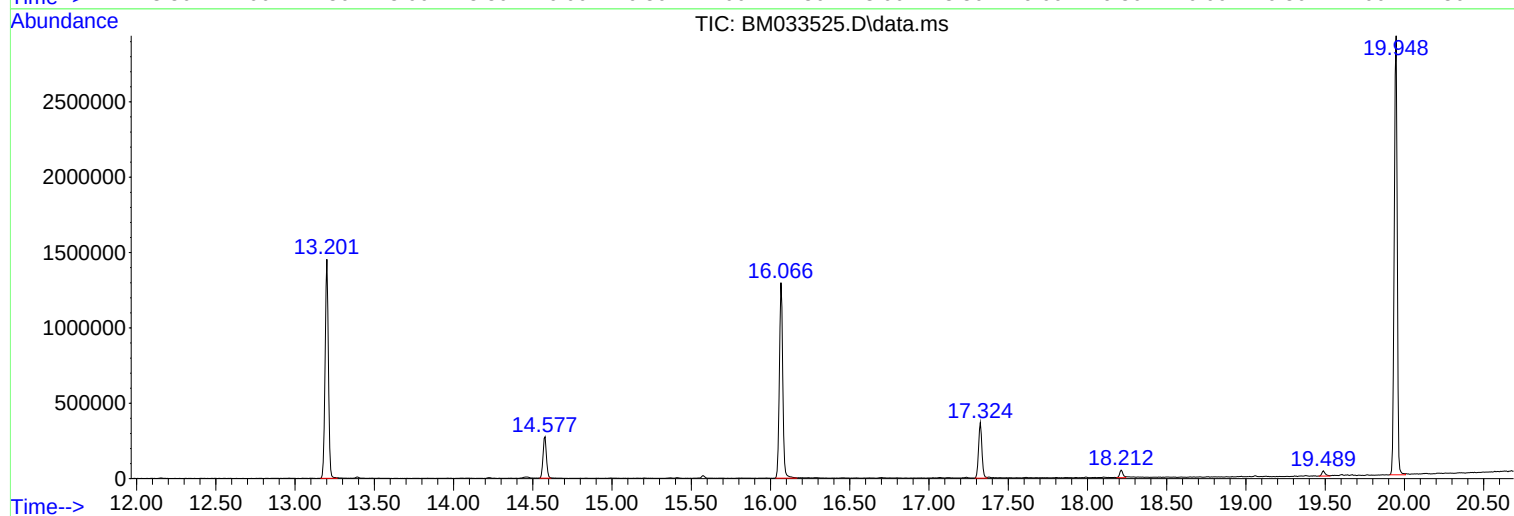
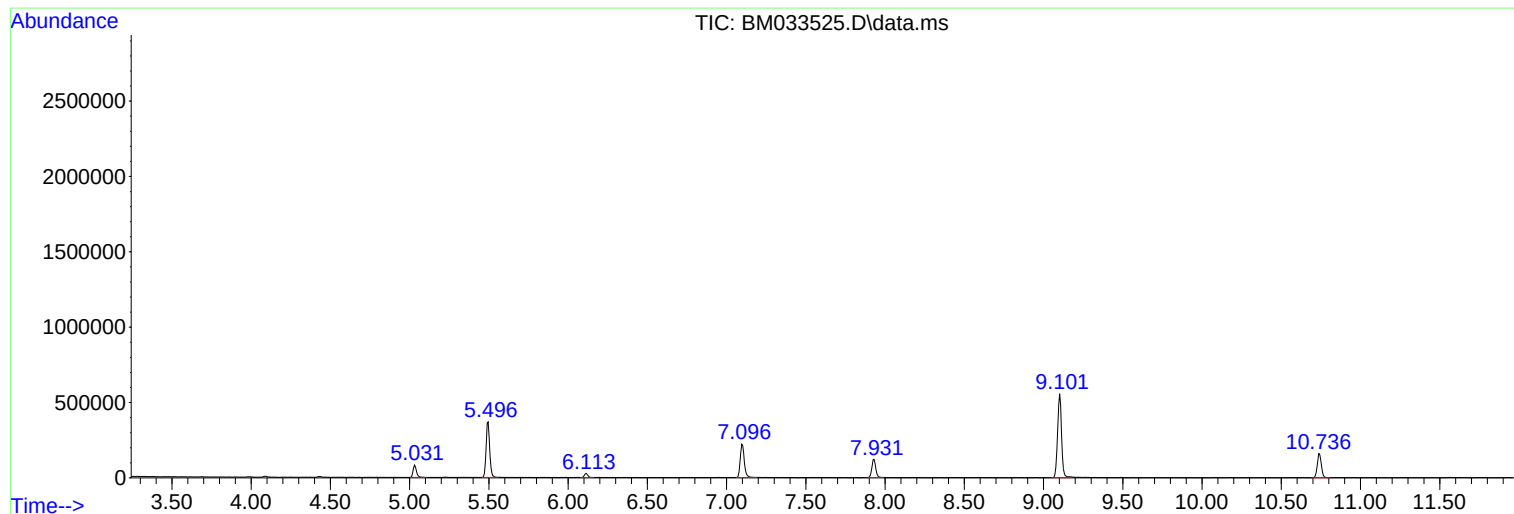
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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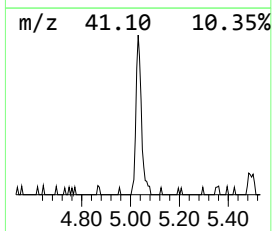
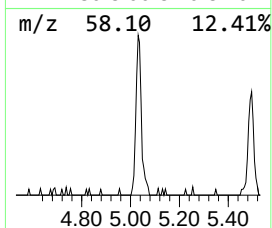
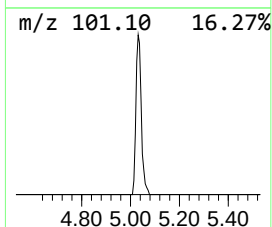
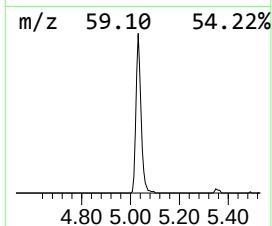
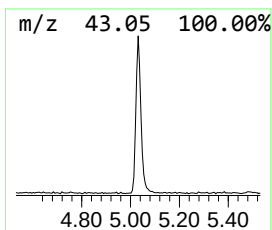
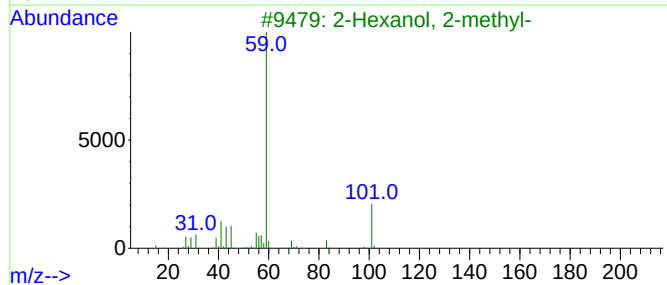
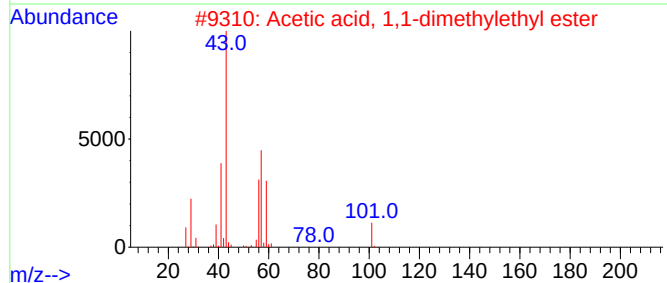
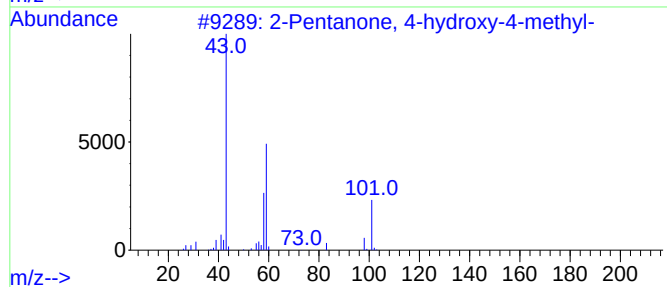
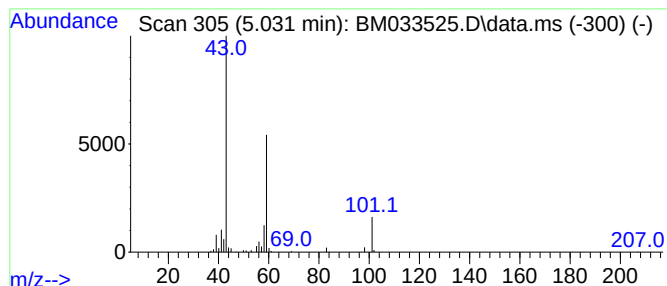
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.031	11.81 ng	121930	1,4-Dichlorobenzene-d4	7.931

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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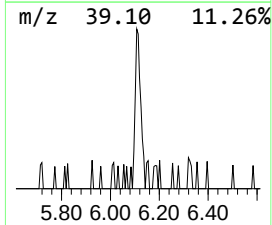
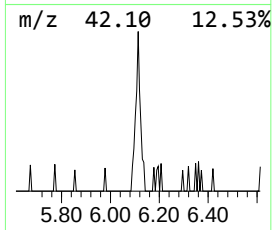
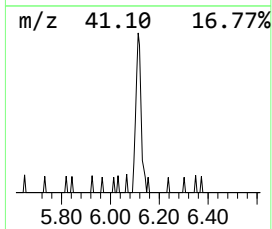
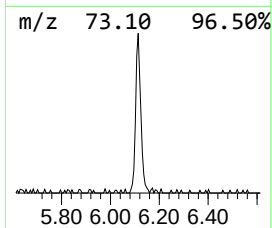
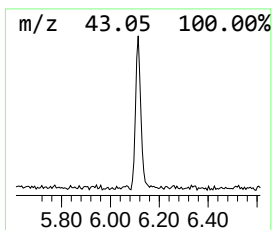
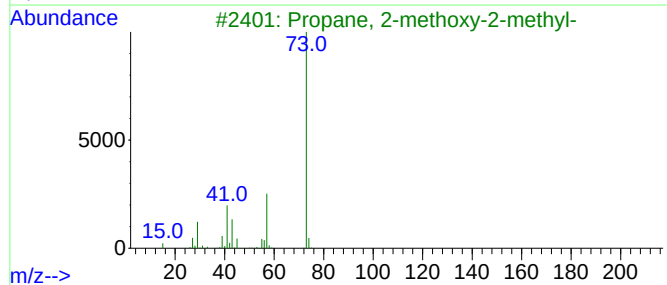
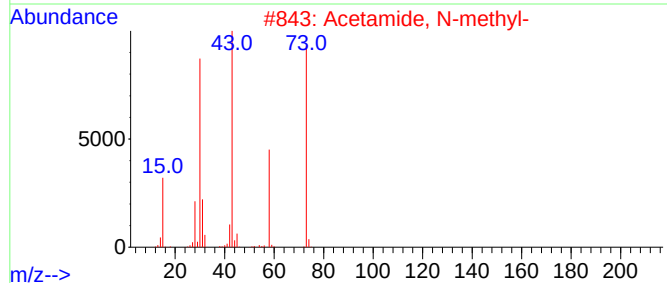
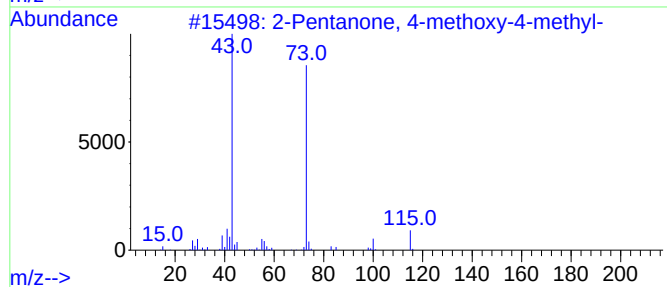
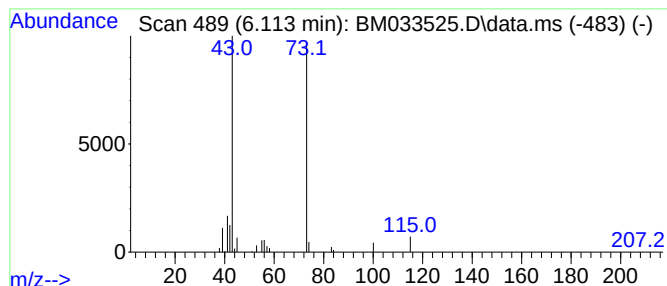
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.113	4.05 ng	41841	1,4-Dichlorobenzene-d4	7.931

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	42
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	23
4		Guanidine, methyl-	73	C2H7N3	000471-29-4	9
5		2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9



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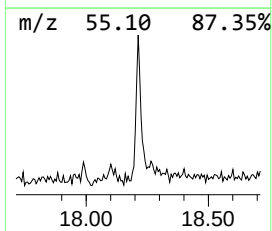
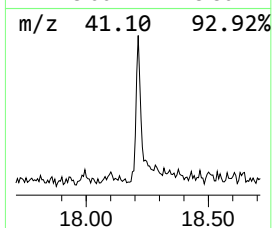
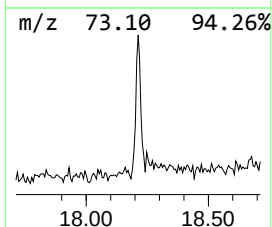
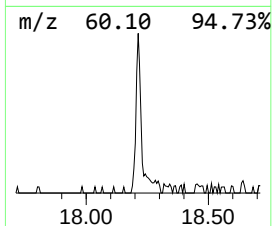
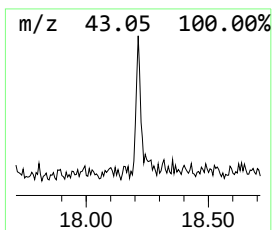
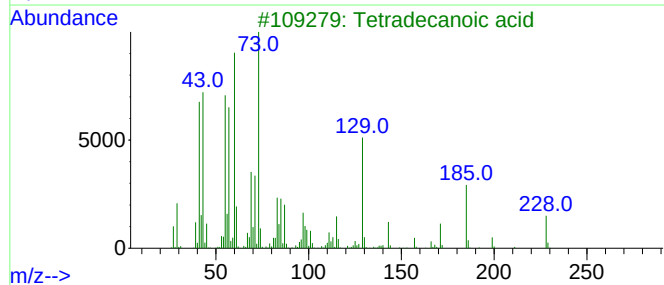
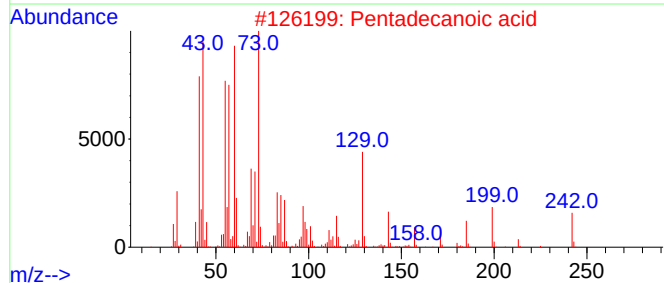
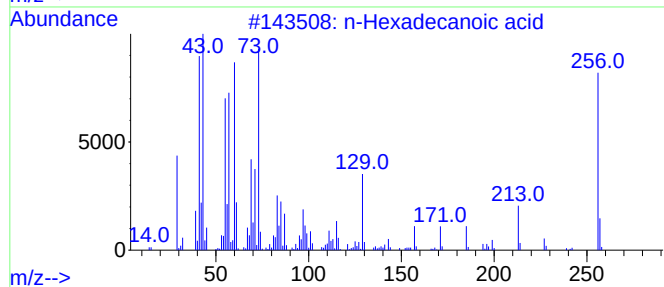
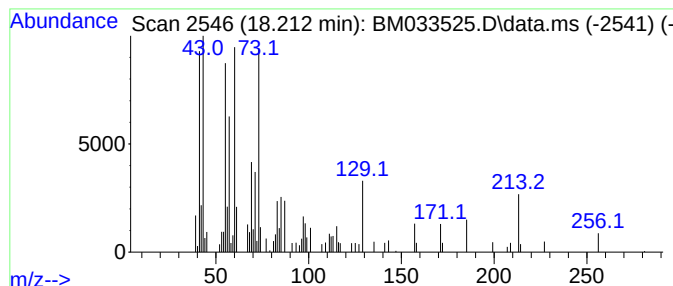
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	2.62 ng	71754	Phenanthrene-d10	17.324

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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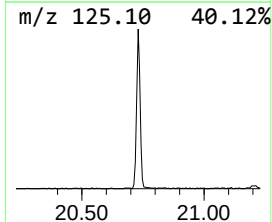
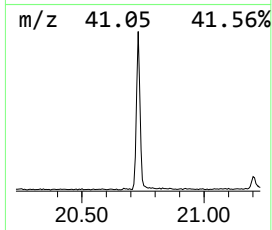
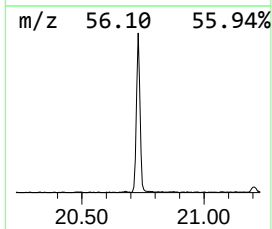
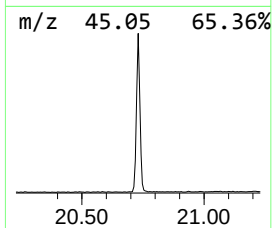
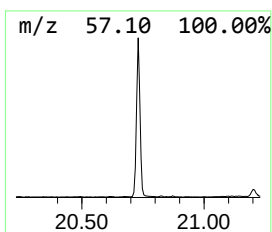
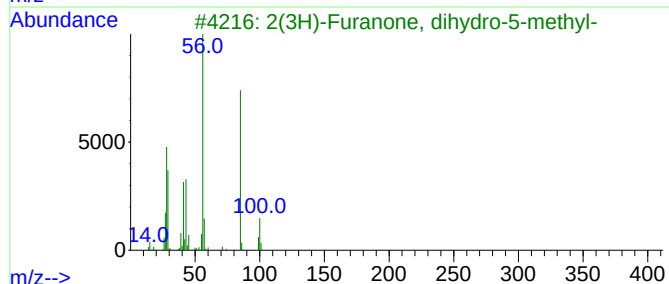
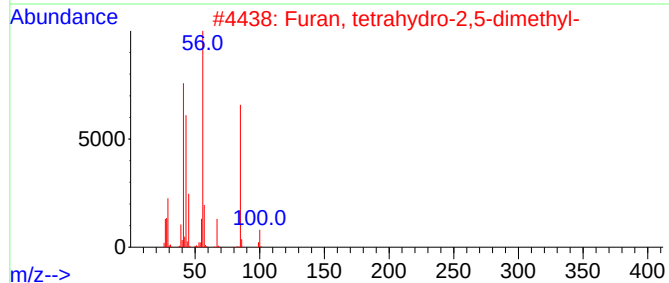
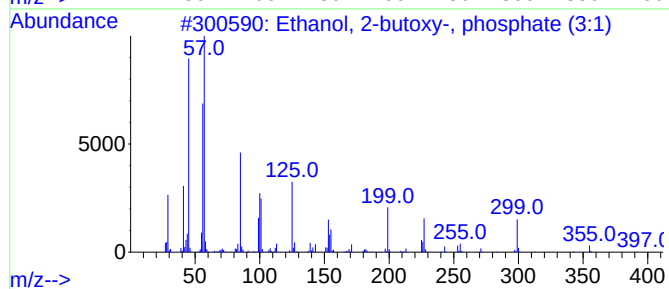
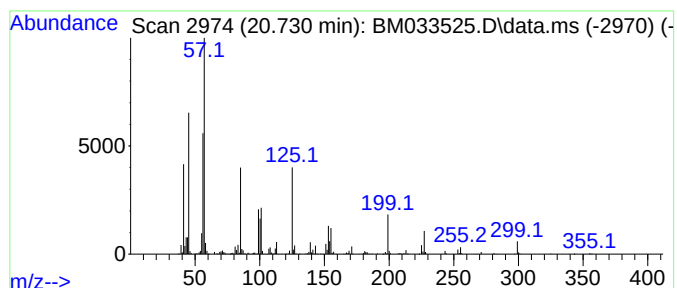
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Peak Number 4 Ethanol, 2-butoxy-, phospho... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.730	25.66 ng	781493	Chrysene-d12	21.500

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	80
2			Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	22
3			2(3H)-Furanone, dihydro-5-methyl-	100	C5H8O2	000108-29-2	22
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	12
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	10



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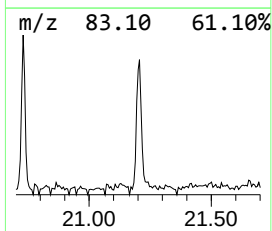
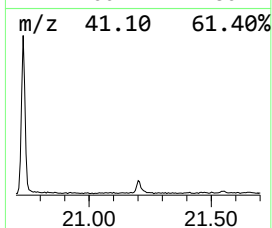
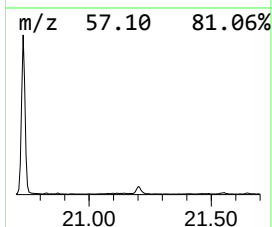
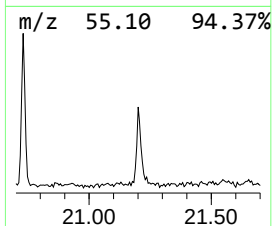
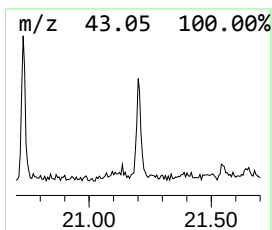
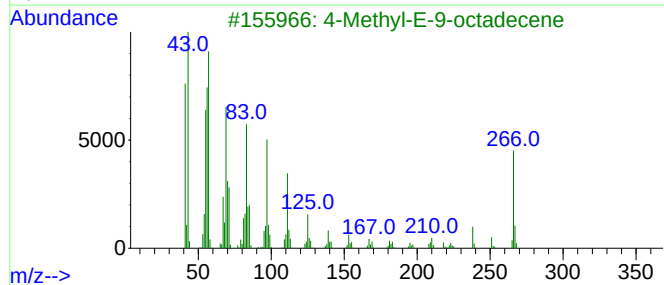
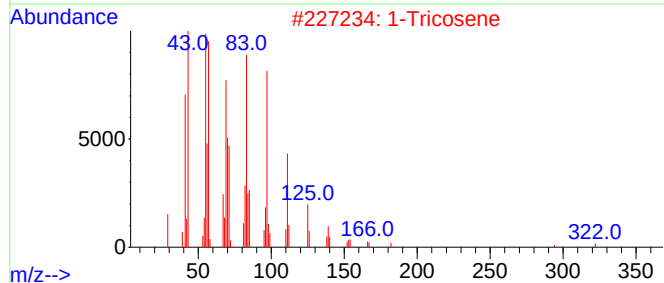
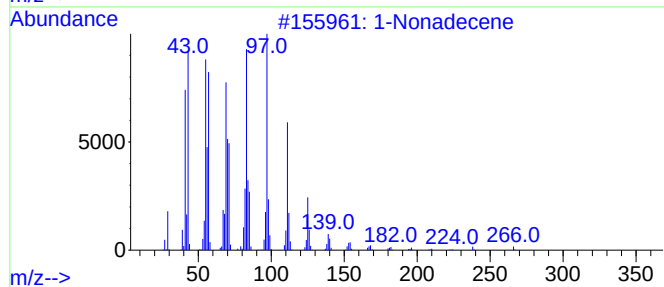
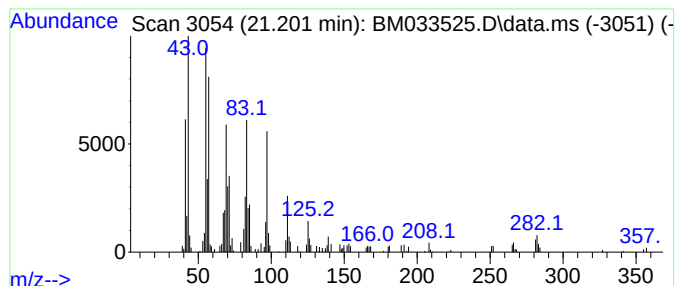
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Peak Number 5 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.201	2.59 ng	78885	Chrysene-d12		21.500	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	97
2	1-Tricosene		322	C23H46	018835-32-0	93
3	4-Methyl-E-9-octadecene		266	C19H38	1000130-87-1	93
4	Acetic acid, chloro-, octadecyl ...		346	C20H39ClO2	005348-82-3	91
5	E-7-Octadecene		252	C18H36	1000130-92-0	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.031	11.8	ng	121930	1	7.931	206475	20.0
2-Pentanone, 4-...	6.113	4.0	ng	41841	1	7.931	206475	20.0
n-Hexadecanoic ...	18.212	2.6	ng	71754	4	17.324	547898	20.0
Ethanol, 2-buto...	20.730	25.7	ng	781493	5	21.500	609111	20.0
1-Nonadecene	21.201	2.6	ng	78885	5	21.500	609111	20.0