

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
 Data File : BP011822.D
 Acq On : 27 Sep 2022 18:55
 Operator : CG/JU
 Sample : N4839-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 5592-1

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_P\Methods\8270E-BP092122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011822.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.046	6	10	34	rVB	8209699	12830617	54.53%	12.048%
2	5.469	415	422	439	rBV	2505221	3914776	16.64%	3.676%
3	7.069	685	694	710	rBV	1428281	2391228	10.16%	2.245%
4	7.910	830	837	845	rBV	1222128	1994392	8.48%	1.873%
5	9.075	1027	1035	1055	rBV	4066558	6816919	28.97%	6.401%
6	10.499	1271	1277	1296	rBV	235657	532650	2.26%	0.500%
7	10.716	1306	1314	1328	rBV	1669998	2930216	12.45%	2.752%
8	13.175	1725	1732	1747	rBV	10170358	15682818	66.66%	14.727%
9	14.551	1957	1966	1982	rBV	2705733	4036349	17.16%	3.790%
10	16.045	2213	2220	2237	rBV	8319171	11928762	50.70%	11.201%
11	17.310	2428	2435	2447	rBV	3417150	4914112	20.89%	4.614%
12	18.186	2580	2584	2594	rBV	211100	435433	1.85%	0.409%
13	19.422	2790	2794	2810	rBV	361579	809333	3.44%	0.760%
14	19.863	2863	2869	2883	rBV	18555713	23528290	100.00%	22.094%
15	21.098	3075	3079	3090	rBV	307284	641590	2.73%	0.602%
16	21.392	3124	3129	3135	rBV	4047534	5374365	22.84%	5.047%
17	21.516	3145	3150	3160	rBV	1237323	2055921	8.74%	1.931%
18	23.833	3537	3544	3561	rVB2	2840147	5675963	24.12%	5.330%

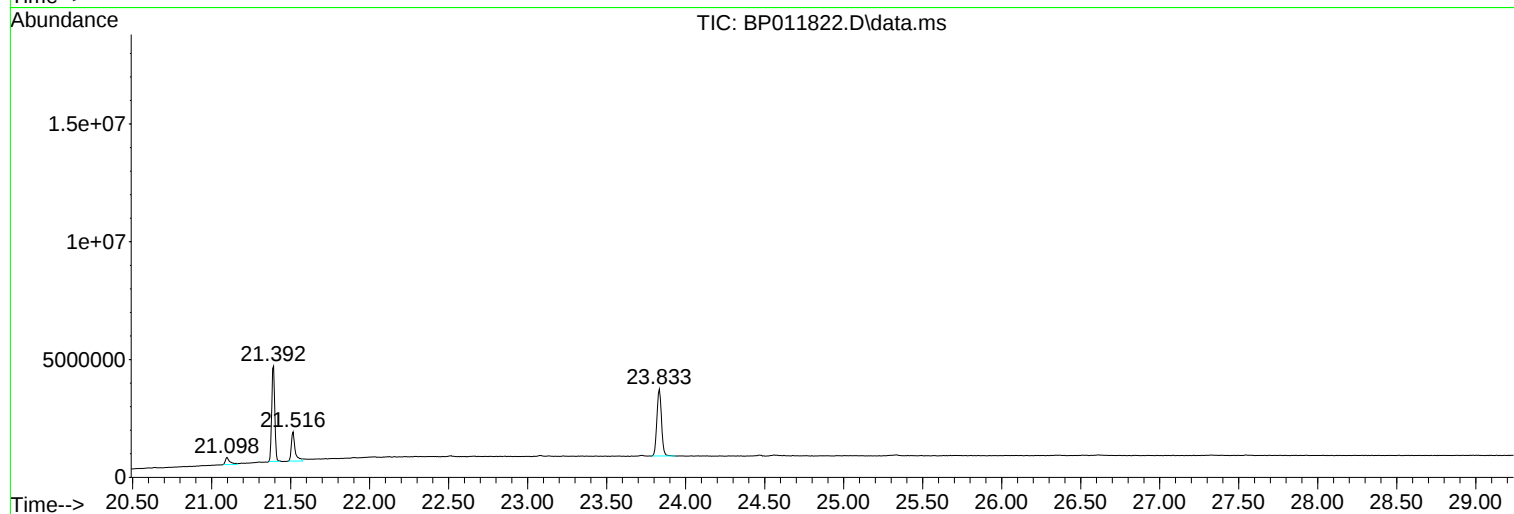
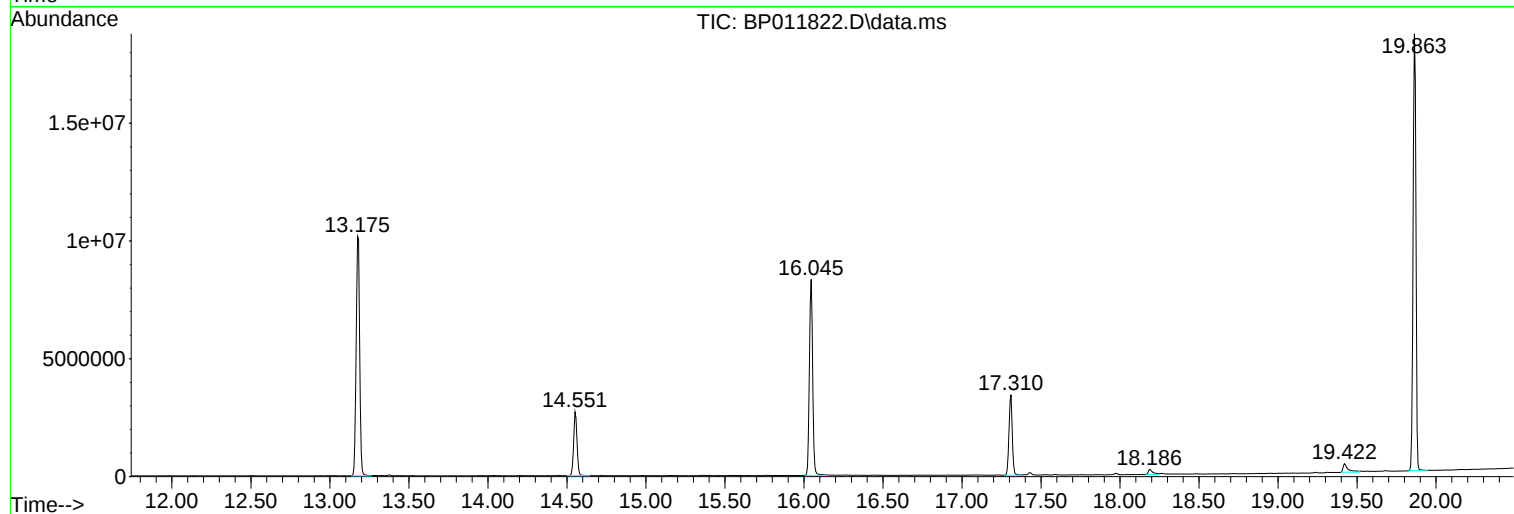
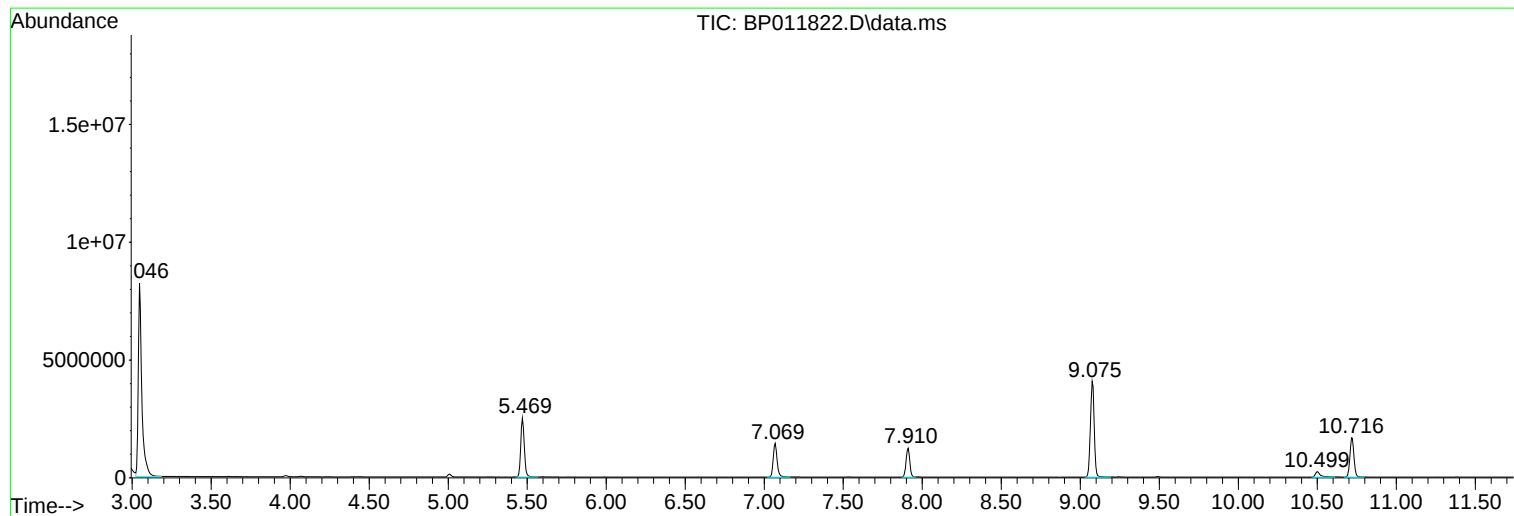
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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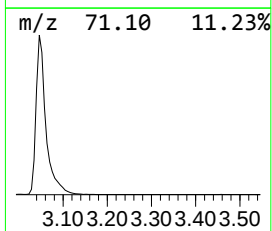
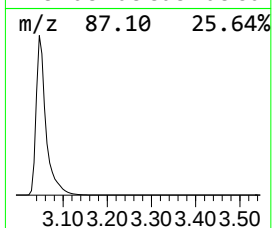
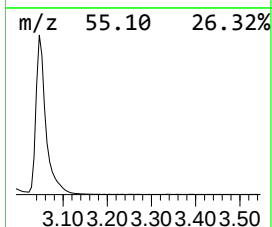
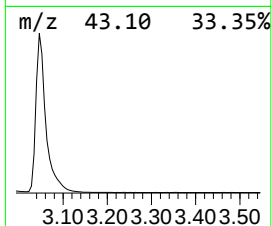
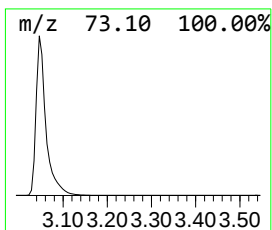
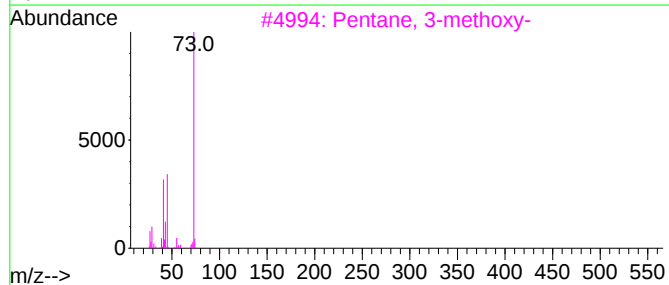
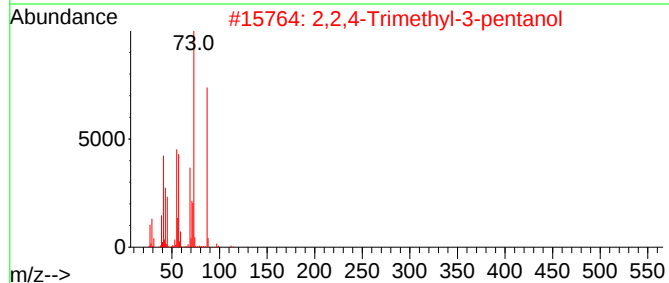
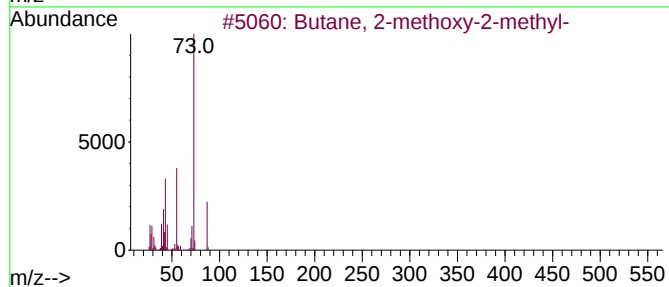
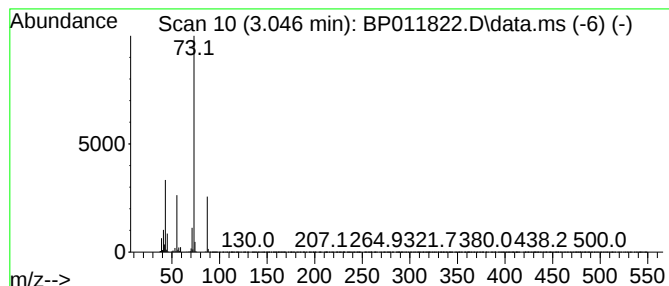
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.046	128.67 ng	12830600	1,4-Dichlorobenzene-d4	7.910

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	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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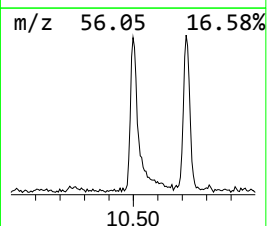
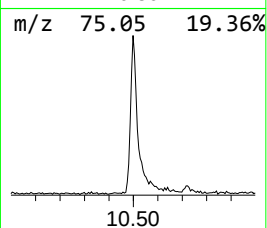
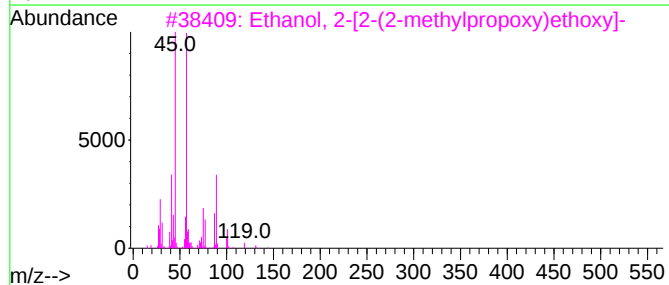
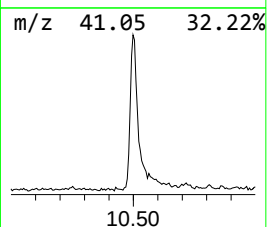
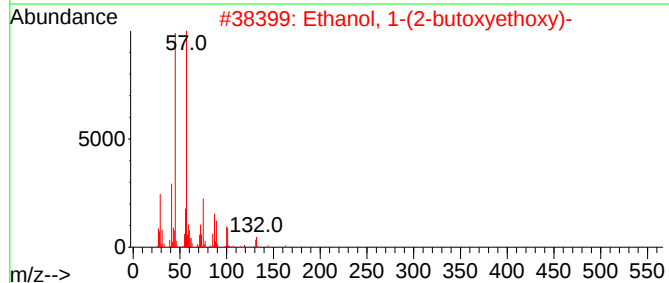
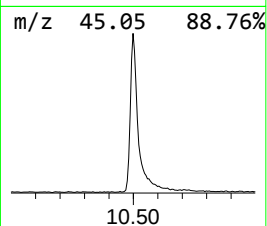
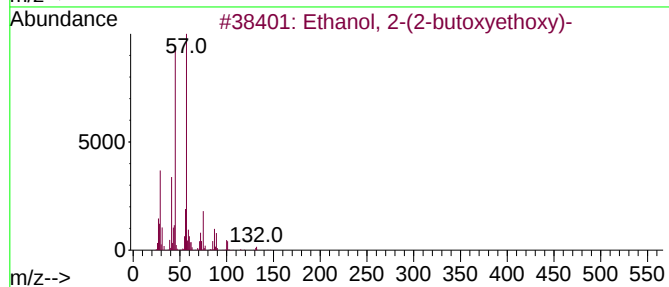
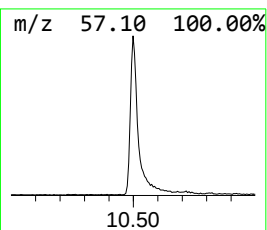
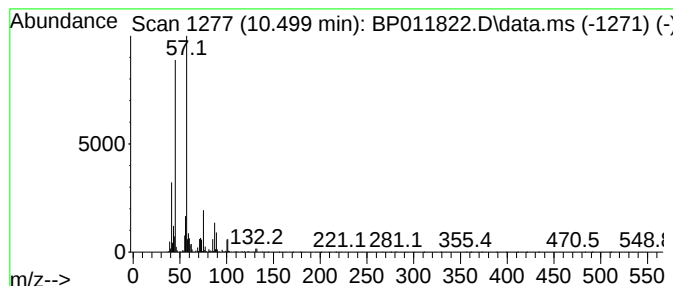
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.499	3.64 ng	532650	Naphthalene-d8	10.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53



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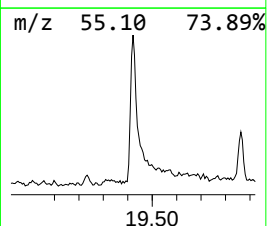
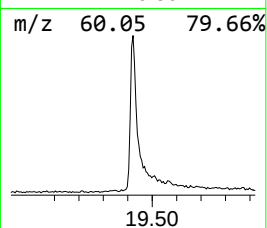
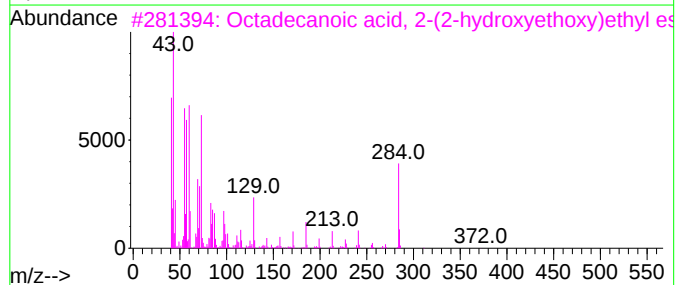
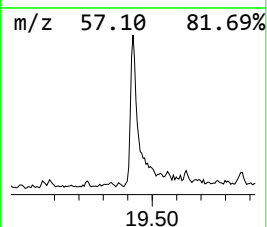
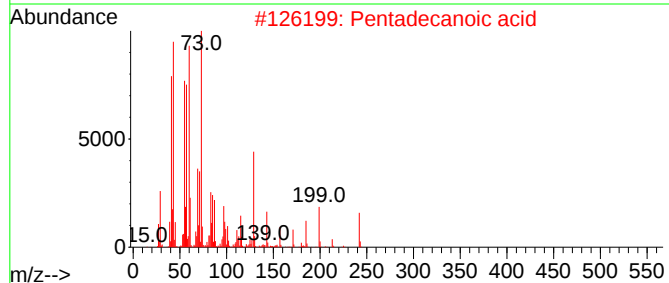
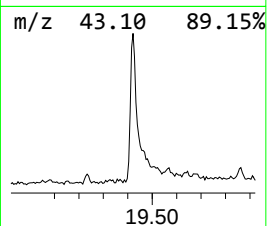
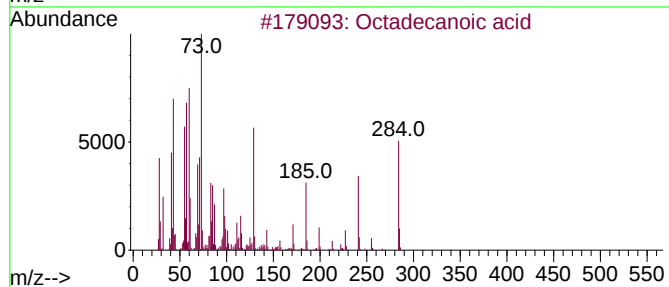
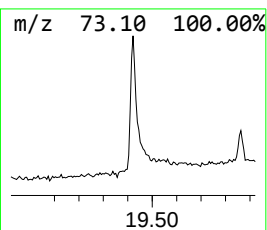
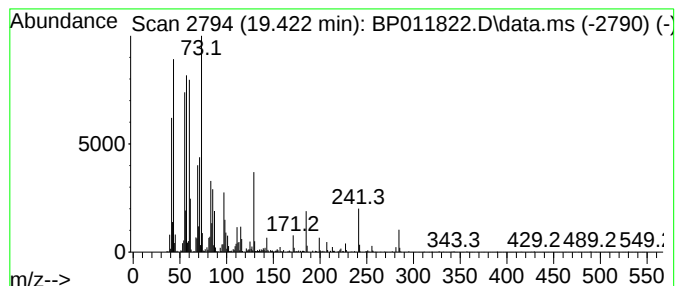
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.422	3.01 ng	809333	Chrysene-d12	21.392	
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	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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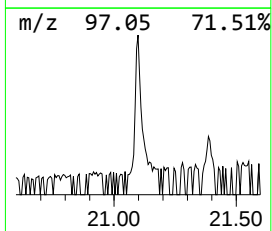
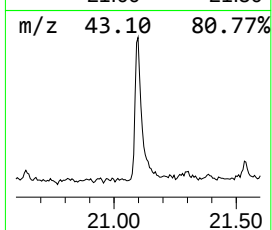
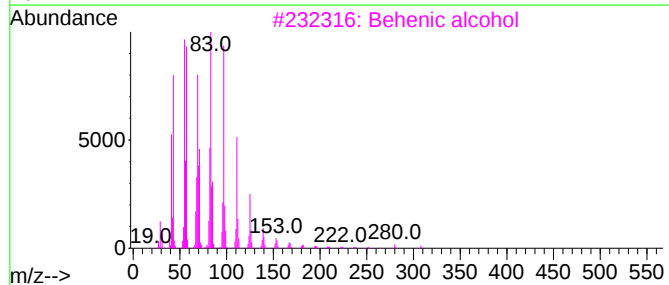
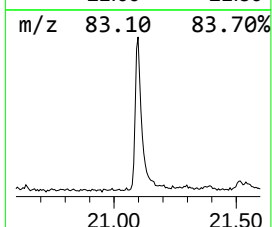
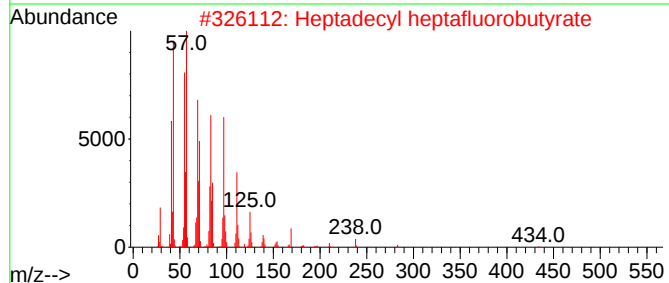
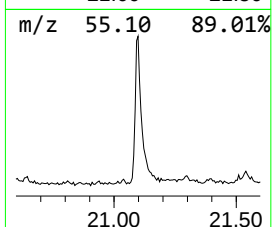
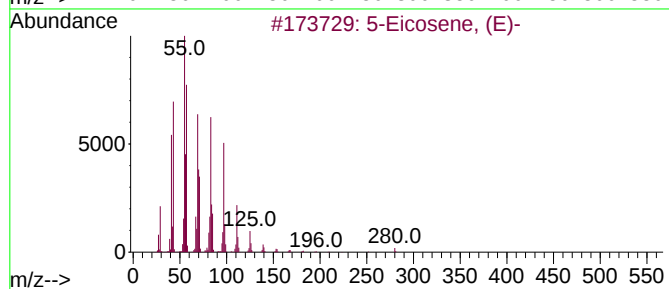
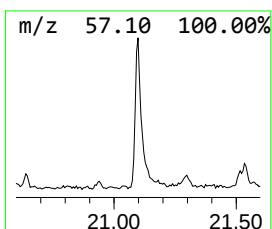
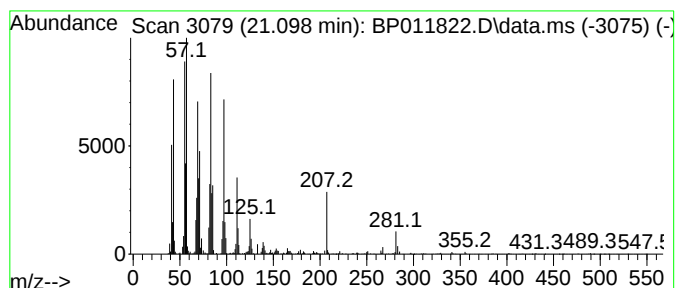
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.098	2.39 ng	641590	Chrysene-d12	21.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5	1-Hexacosene	364	C26H52	018835-33-1	93



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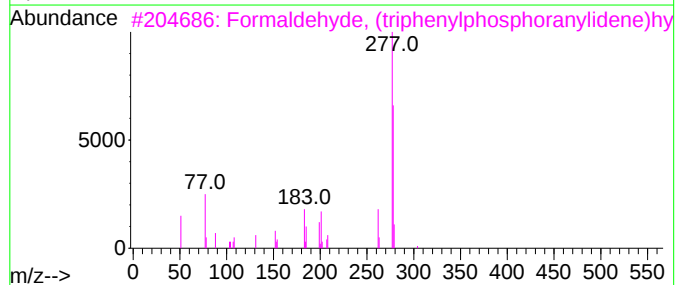
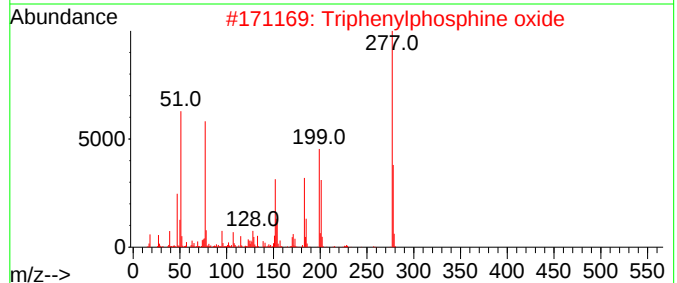
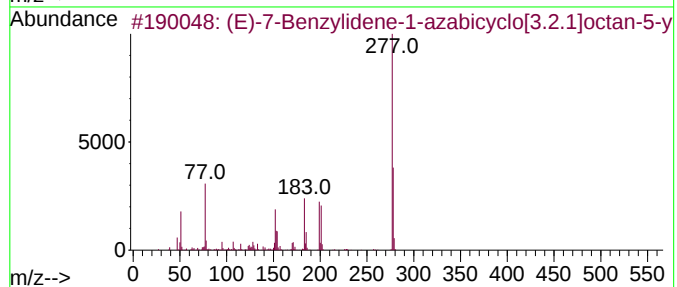
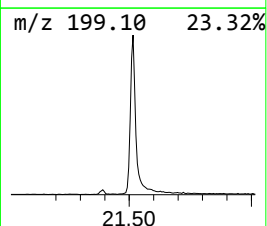
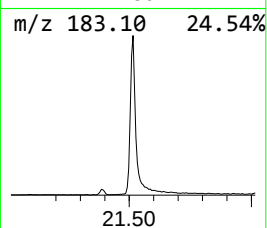
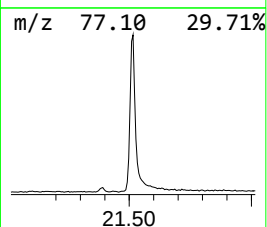
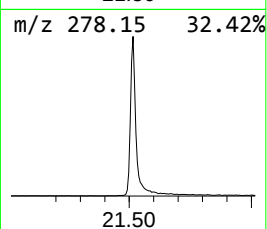
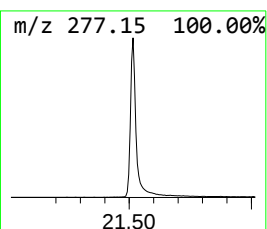
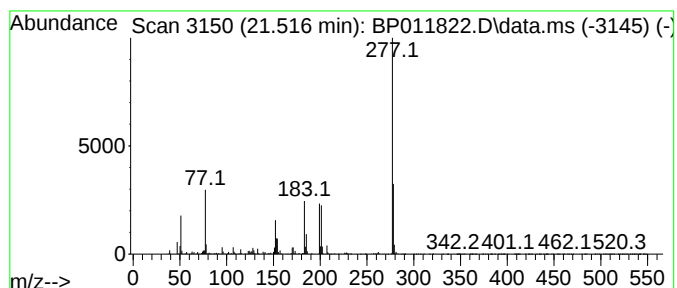
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TIC Integration Parameters: LSCINT.P

Peak Number 5 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.516	7.65 ng	2055920	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	95		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64		
4	Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38		
5	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.046	128.7	ng	12830600	1	7.910	1994390	20.0
Ethanol, 2-(2-b...	10.499	3.6	ng	532650	2	10.722	2930220	20.0
Octadecanoic acid	19.422	3.0	ng	809333	5	21.392	5374370	20.0
5-Eicosene, (E)-	21.098	2.4	ng	641590	5	21.392	5374370	20.0
(E)-7-Benzylide...	21.516	7.7	ng	2055920	5	21.392	5374370	20.0