

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
 Data File : BF132718.D
 Acq On : 09 Mar 2023 15:10
 Operator : CG\JU
 Sample : 01834-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-9

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132718.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.210	441	446	454	rVB	1490328	1738686	46.09%	6.362%
2	5.610	510	514	530	rBV	3771730	3349086	88.78%	12.255%
3	6.610	680	684	687	rBV	3747264	3300516	87.49%	12.077%
4	6.981	743	747	750	rBV	1250377	1024483	27.16%	3.749%
5	7.539	838	842	846	rBV	2337516	2202849	58.39%	8.061%
6	8.263	962	965	969	rBV	1669220	1313440	34.82%	4.806%
7	9.339	1144	1148	1151	rBV	4724861	3772417	100.00%	13.804%
8	10.022	1261	1264	1268	rBV	1572165	1387748	36.79%	5.078%
9	10.739	1382	1386	1389	rVB	201297	177232	4.70%	0.649%
10	10.816	1395	1399	1409	rBV	2059573	1888994	50.07%	6.912%
11	11.521	1515	1519	1522	rBV	1388021	1198366	31.77%	4.385%
12	12.033	1602	1606	1616	rBV2	100863	155409	4.12%	0.569%
13	12.974	1761	1766	1771	rBV	49233	68285	1.81%	0.250%
14	13.110	1785	1789	1793	rBV	3239221	2822097	74.81%	10.327%
15	13.998	1936	1940	1950	rBV	181341	328816	8.72%	1.203%
16	14.180	1967	1971	1974	rBV	1245556	1070080	28.37%	3.916%
17	14.268	1981	1986	1992	rBV	460196	484633	12.85%	1.773%
18	15.033	2113	2116	2121	rBV	48796	50430	1.34%	0.185%
19	15.721	2228	2233	2242	rVB	768963	994287	26.36%	3.638%

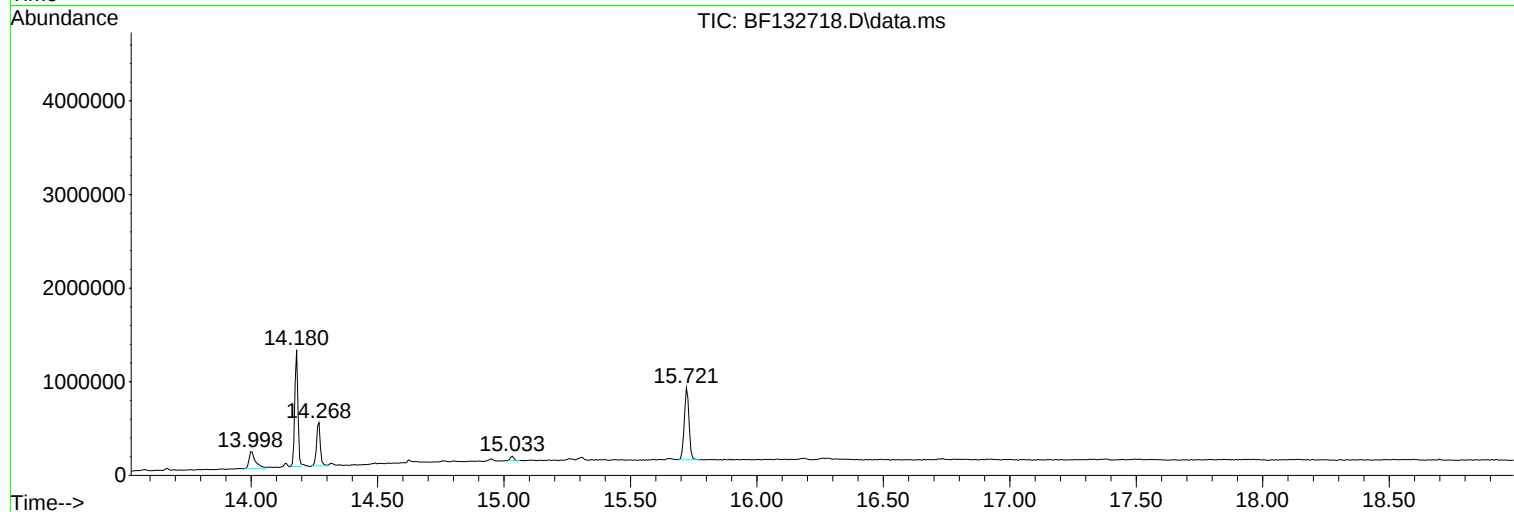
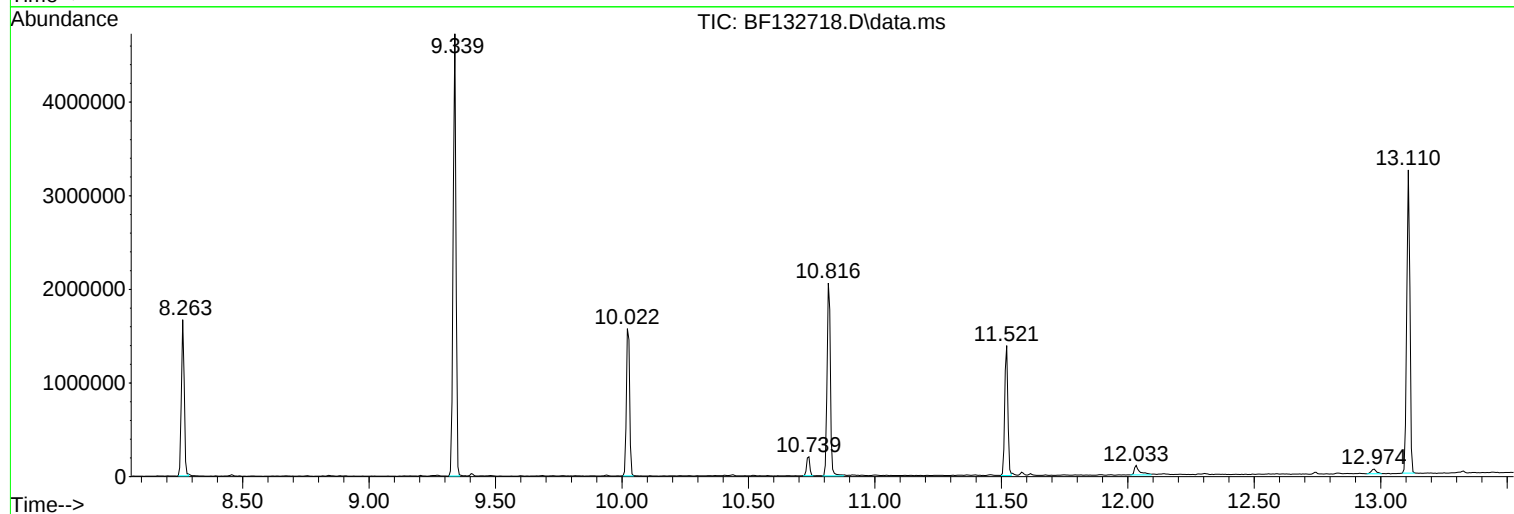
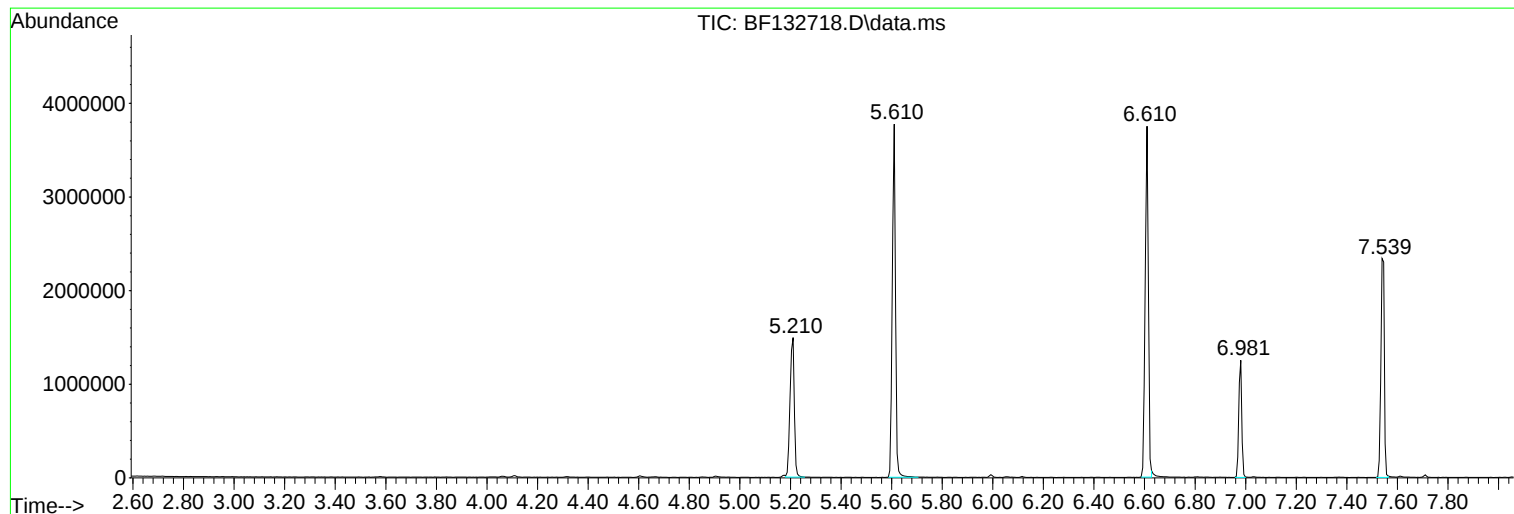
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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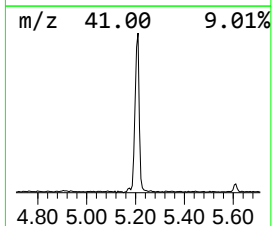
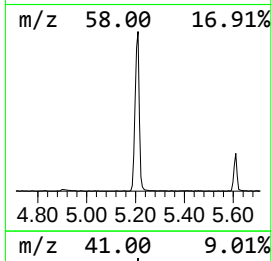
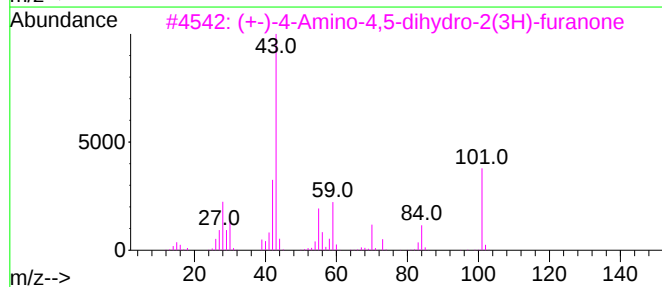
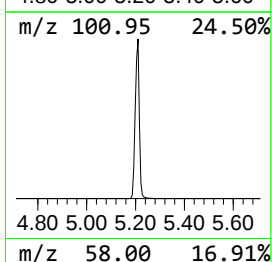
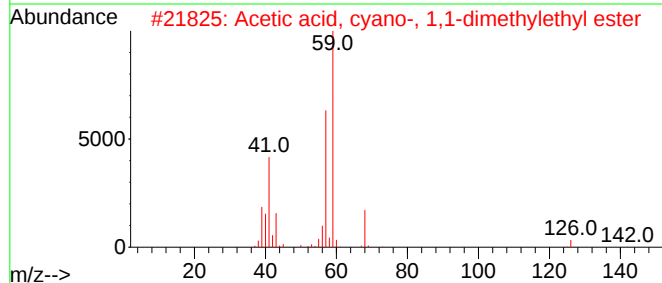
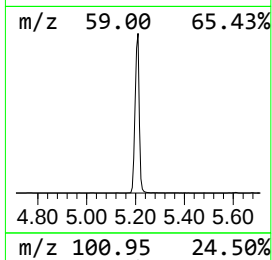
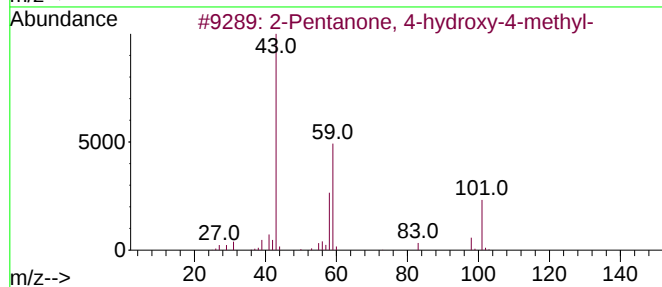
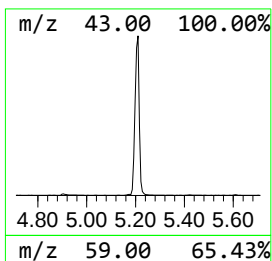
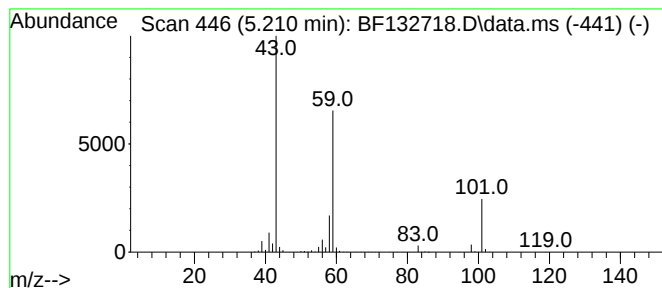
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	33.94 ng	1738690	1,4-Dichlorobenzene-d4	6.981

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Guanidine	59	CH5N3	000113-00-8	9		



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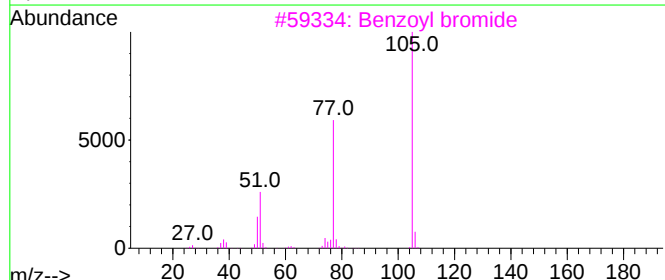
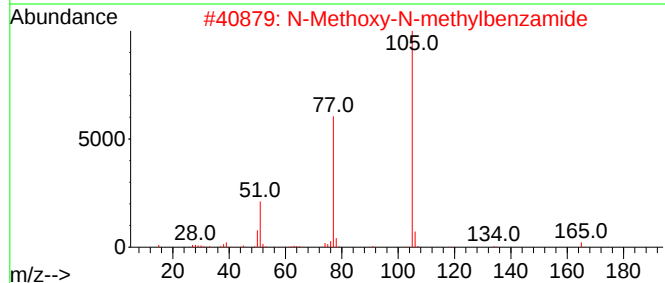
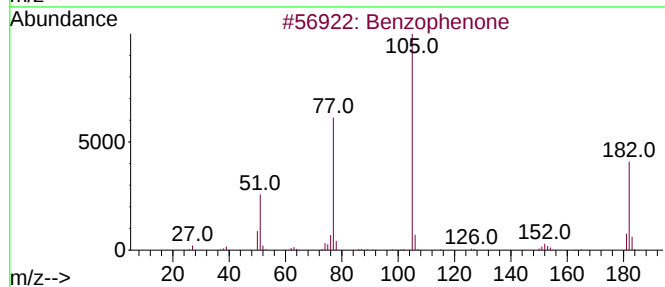
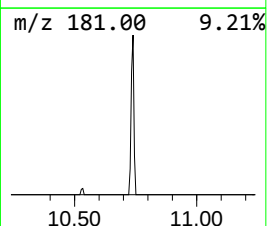
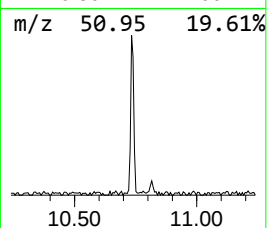
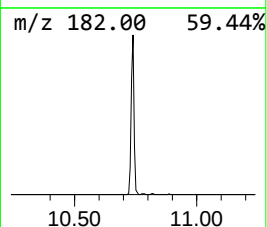
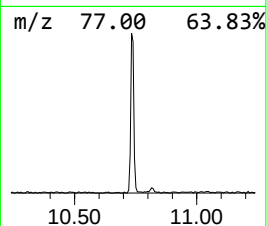
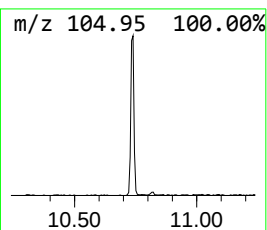
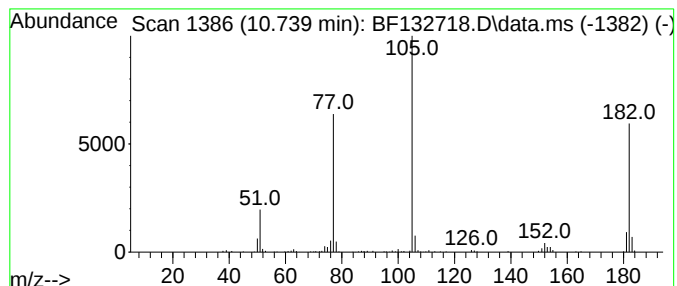
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	2.55 ng	177232	Acenaphthene-d10	10.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
3			Benzoyl bromide	184	C7H5BrO	000618-32-6	47
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47



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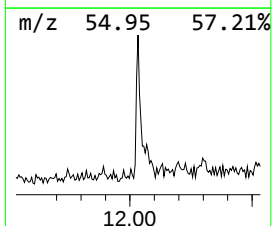
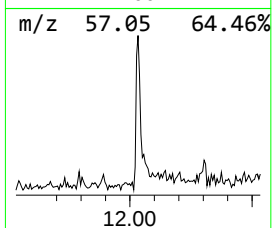
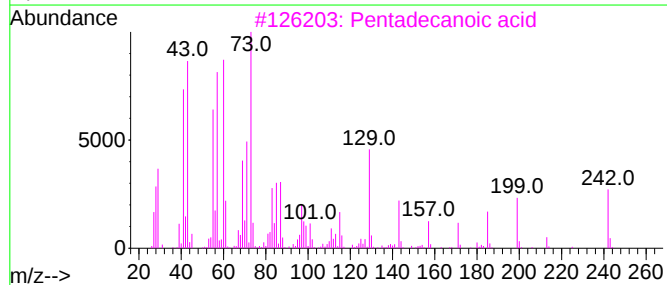
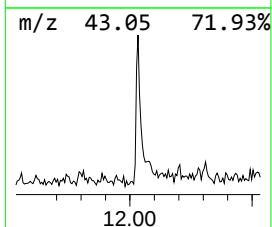
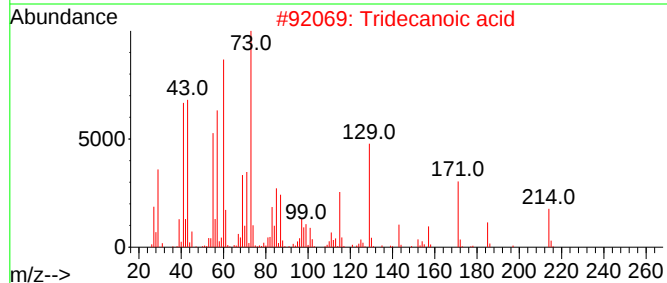
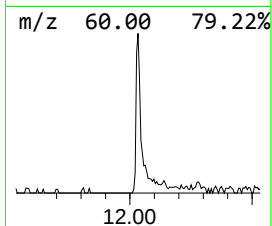
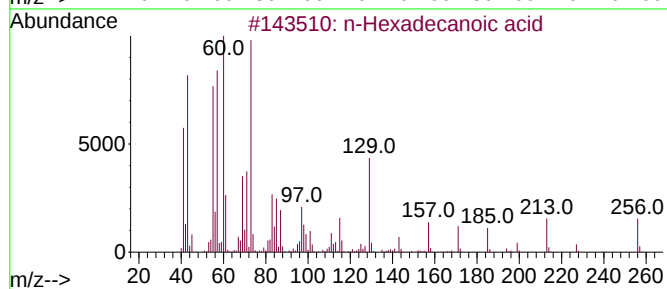
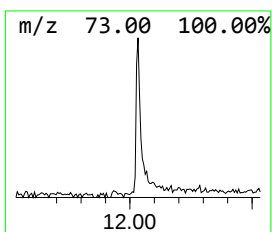
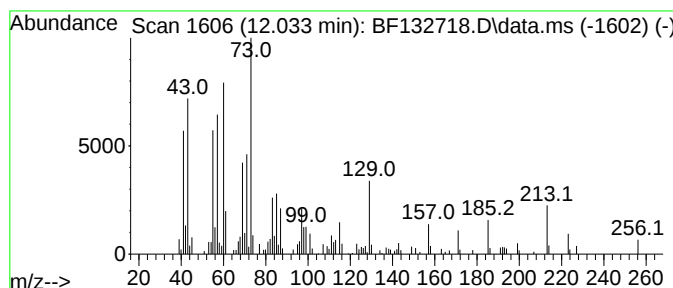
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	2.59 ng	155409	Phenanthrene-d10	11.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Dodecanoic acid	200	C12H24O2	000143-07-7	53
5			Undecanoic acid	186	C11H22O2	000112-37-8	43



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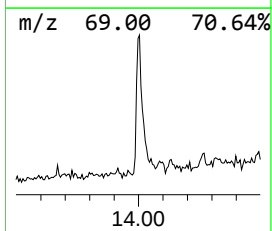
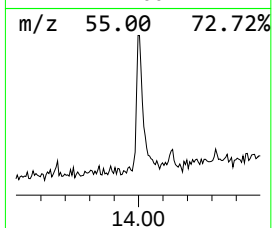
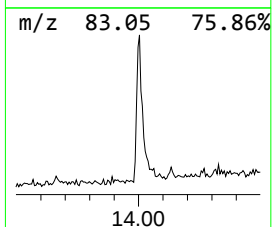
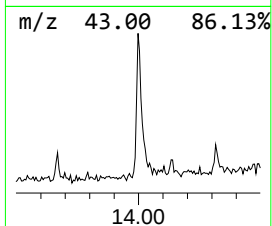
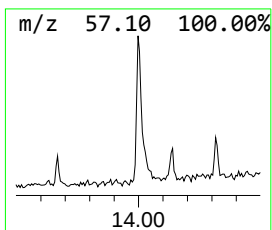
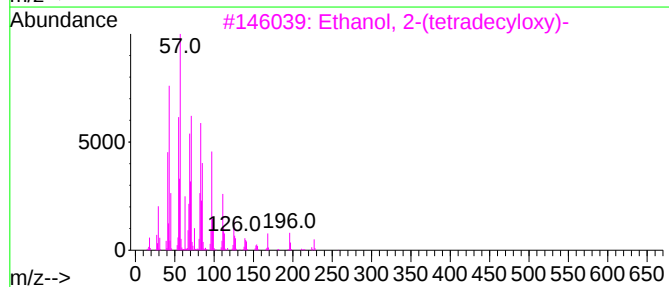
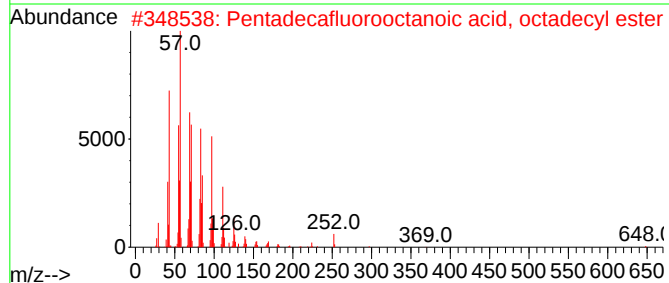
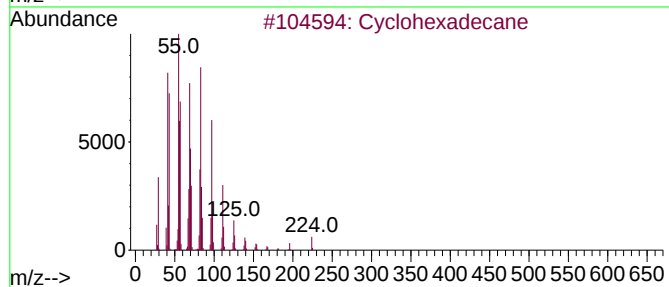
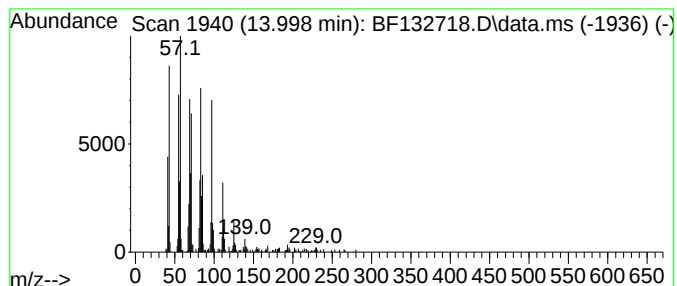
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Peak Number 4 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	6.15 ng	328816	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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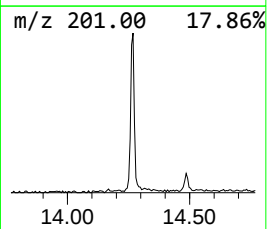
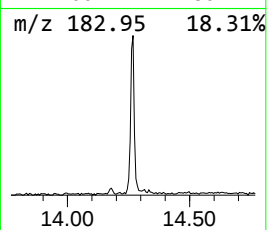
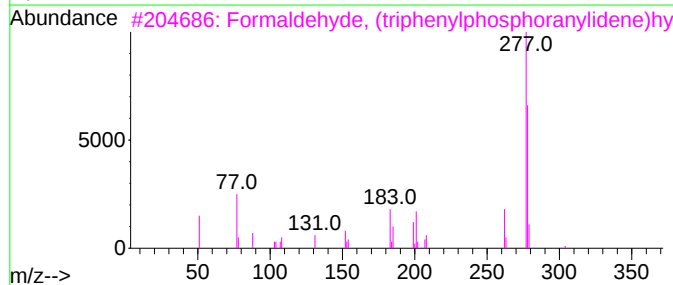
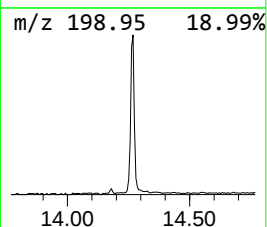
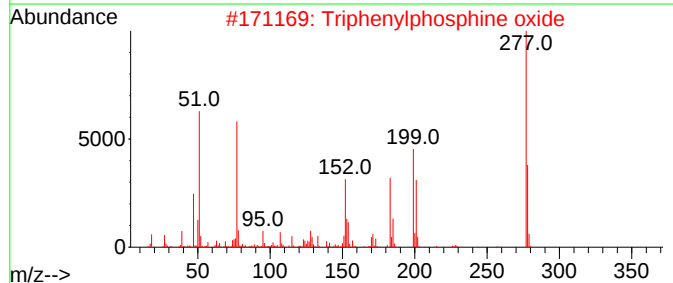
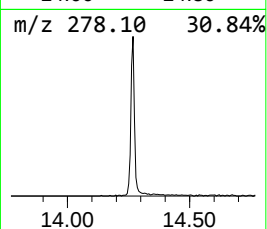
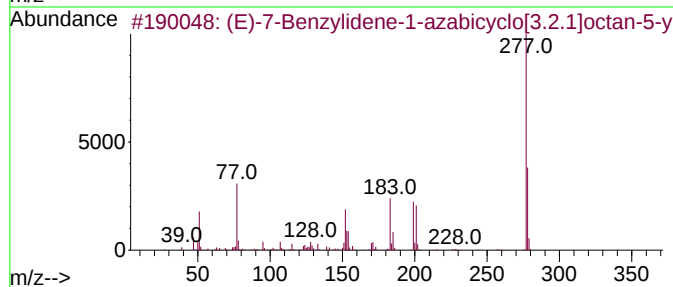
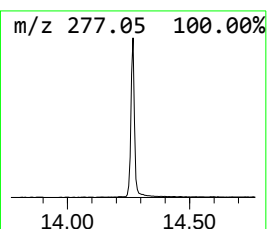
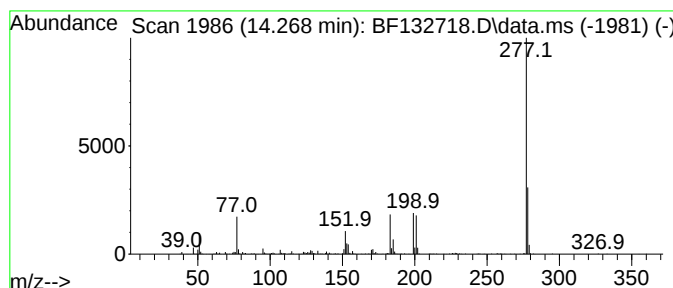
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Peak Number 5 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	9.06 ng	484633	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	89		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	39		
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28		
5	2-Indolinone, 2TMS derivative	277	C14H23NOSi2	010416-65-6	9		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.210	33.9	ng	1738690	1	6.981	1024480	20.0
Benzophenone	10.739	2.5	ng	177232	3	10.022	1387750	20.0
n-Hexadecanoic ...	12.033	2.6	ng	155409	4	11.521	1198370	20.0
Cyclohexadecane	13.998	6.2	ng	328816	5	14.180	1070080	20.0
(E)-7-Benzylide...	14.268	9.1	ng	484633	5	14.180	1070080	20.0