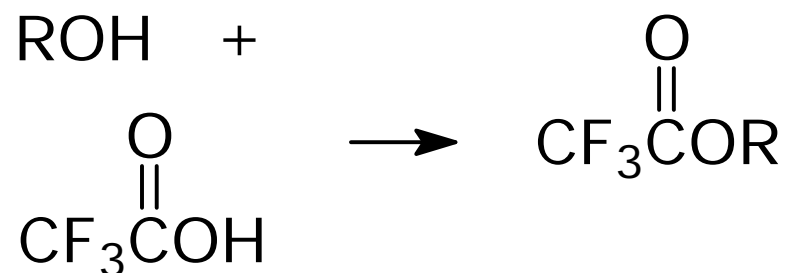


Kinetics data for reaction of alcohols with trifluoroacetic acid

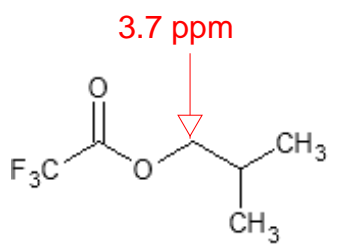
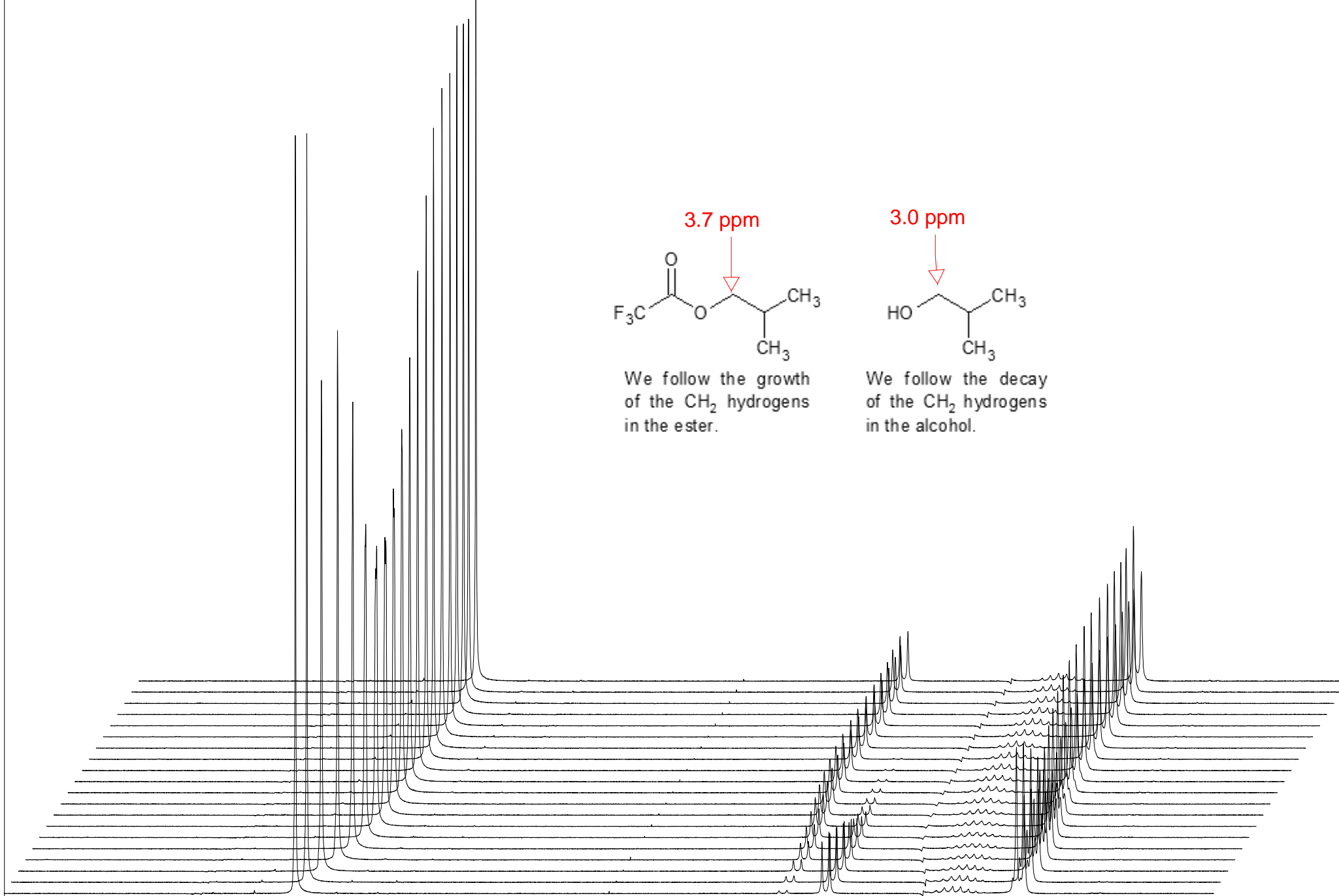
We obtain the kinetics data by taking a series of ^1H NMR scans over time, as the reaction progresses. We can follow a product peak as it grows in, or a reactant peak as it decays away.

Typical data for methanol, ethanol, isopropyl alcohol and isobutyl alcohol are shown on the attached pages. If we zoom in on the peak of interest, the NUTS software will calculate a "T1" value that represents the reciprocal of the rate constant.

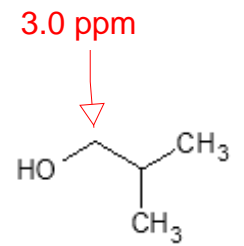
T1 values for the alcohols of interest to us are shown in the spreadsheet [kinetics.xls](#).



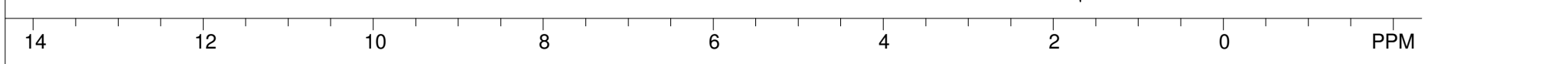
We follow hydrogens on the "R" group of the alcohol.



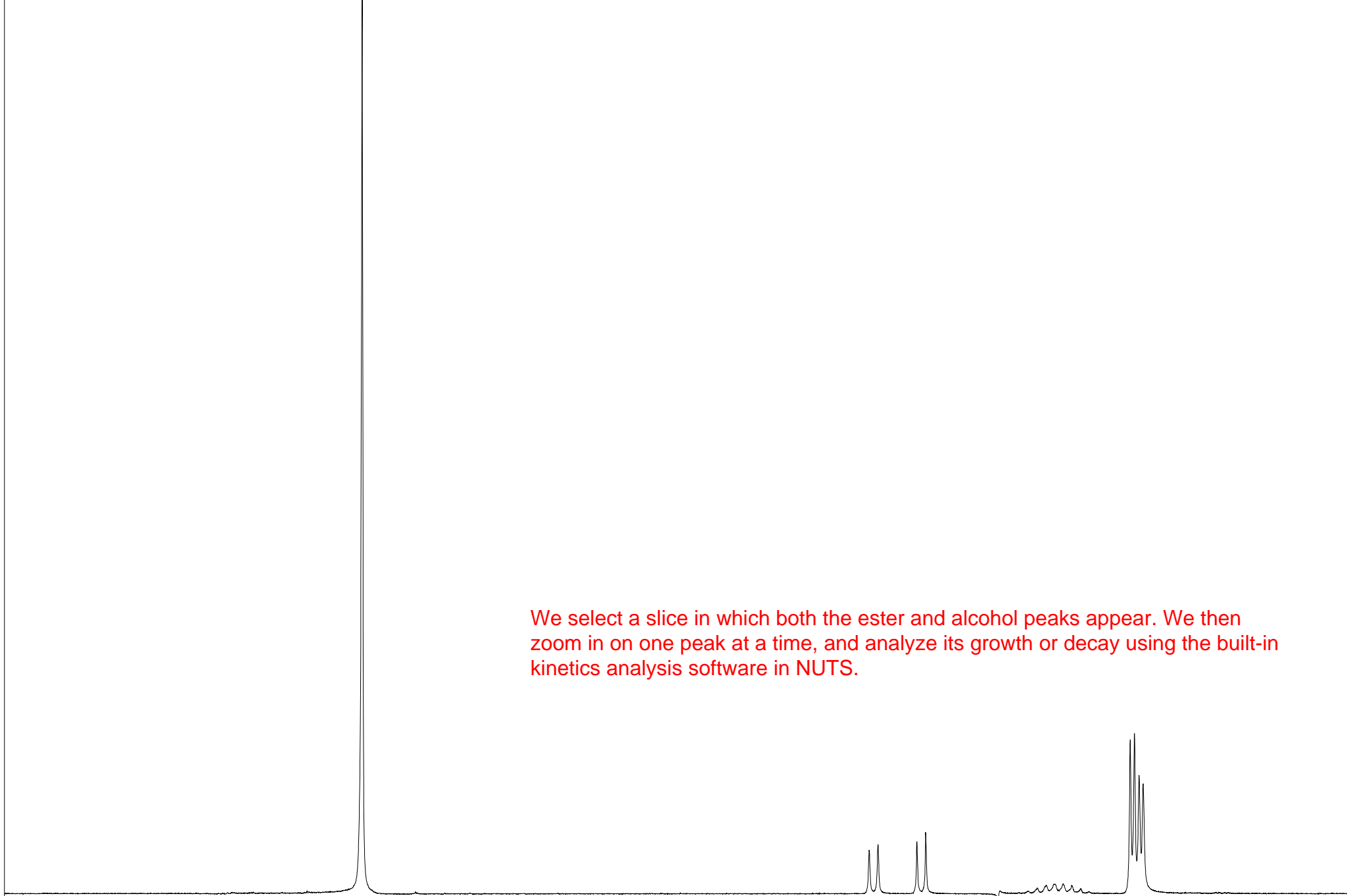
We follow the growth of the CH₂ hydrogens in the ester.



We follow the decay of the CH₂ hydrogens in the alcohol.

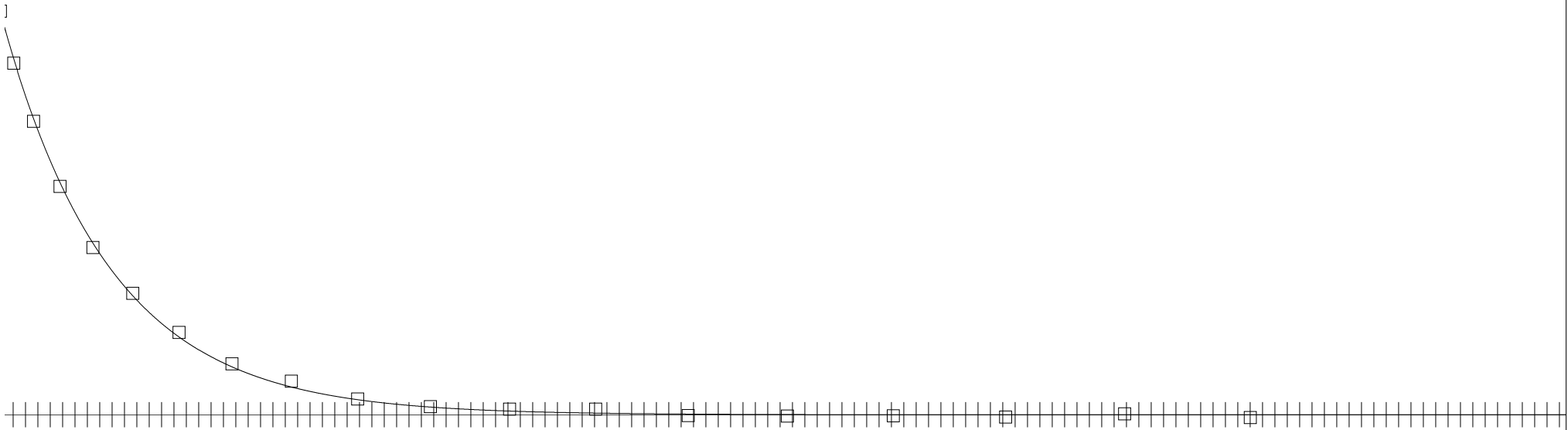


USER: -- DATE: 01/28/11 (11:33)							
F1: 60.010	SW1: 1000	SW2: 0	OF1: 360.0	OF2: 0.0	PTS1d: 8192	PTS2d: 1 , 20	
EX: c:\eft\H1\KINETIC.ppg	PW: 7.8 us	PD: 0.0 sec	NA: 1	LB: 0.0	Nuts - temp		



We select a slice in which both the ester and alcohol peaks appear. We then zoom in on one peak at a time, and analyze its growth or decay using the built-in kinetics analysis software in NUTS.

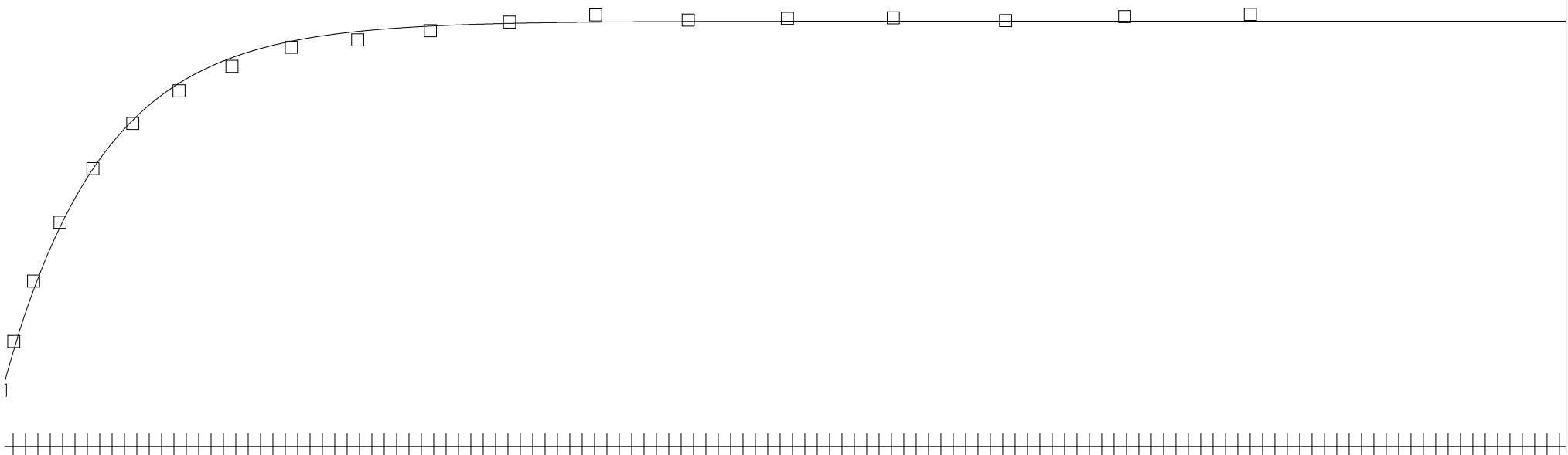
USER: -- DATE: 01/28/11 (11:33)							
F1: 60.010		SW1: 1000	SW2: 0	OF1: 360.0	OF2: 0.0	PTS1d: 8192	PTS2d: 1 , 20
EX: c:\eft\H1\KINETIC.ppg		PW: 7.8 us	PD: 0.0 sec	NA: 1	LB: 0.0		Nuts - temp



Decay of the alcohol peak

T2 = 1152.278564 sec

		USER: -- DATE: 01/28/11 (11:33)					
: 60.010		SW1: 1000	SW2: 0	OF1: 360.0	OF2: 0.0	PTS1d: 8192	PTS2d: 1, 20
ζ: c:\left\H1\KINETIC.ppg		PW: 7.8 us	PD: 0.0 sec	NA: 1	LB: 0.0	Nuts - temp	



Growth of the ester peak

T1 = 1050.496582 sec
 A(inf) = 375.20 K
 Inversion = 0.00 %

USER: -- DATE: 01/28/11 (11:33)

: 60.010	SW1: 1000	SW2: 0	OF1: 360.0	OF2: 0.0	PTS1d: 8192	PTS2d: 1	20
ζ: c:\left\H1\KINETIC.ppg	PW: 7.8 us	PD: 0.0 sec	NA: 1	LB: 0.0	Nuts - temp		