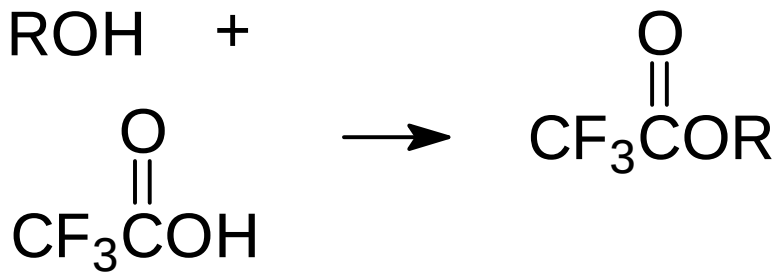
Kinetics data for reaction of alcohols with trifluoroacetic acid

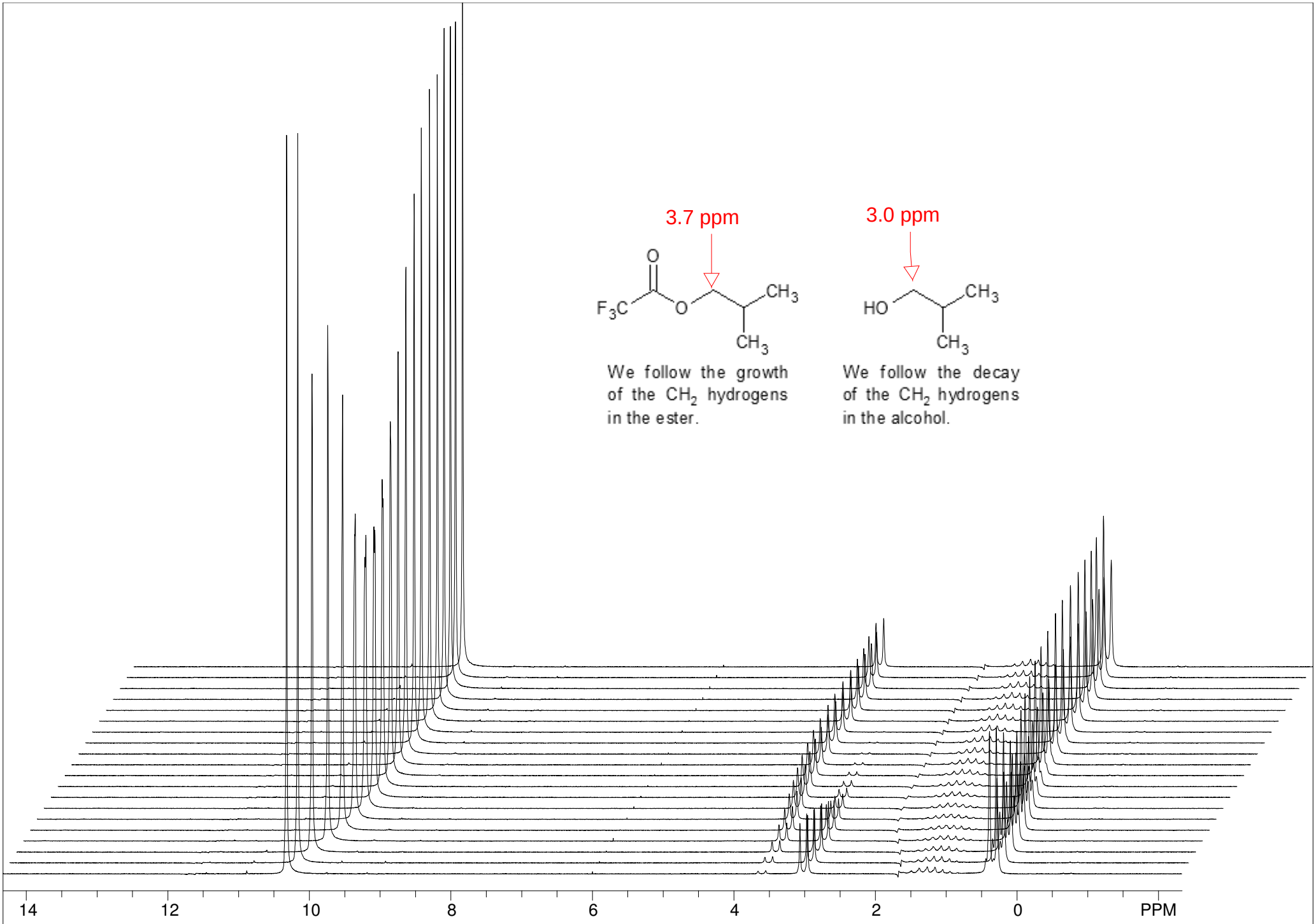
We obtain the kinetics data by taking a series of 1H NMR scans over time, as the reaction progresses. We can follow a product peak as it grows in, or a reactant peak as it decays away.

Typical data for methanol, ethanol, isopropy 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**.

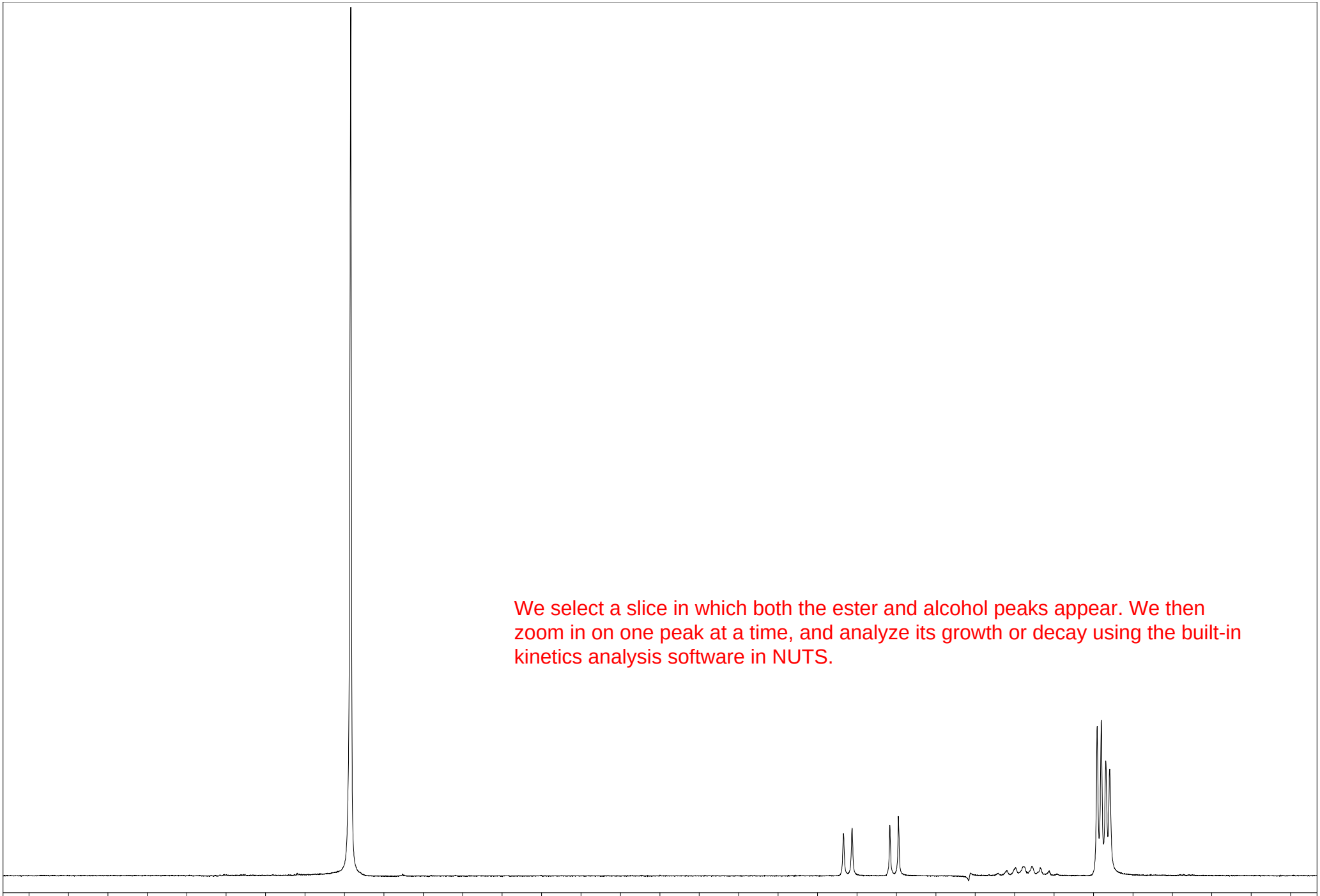


We follow hydrogens on the "R" group of the alcohol.



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



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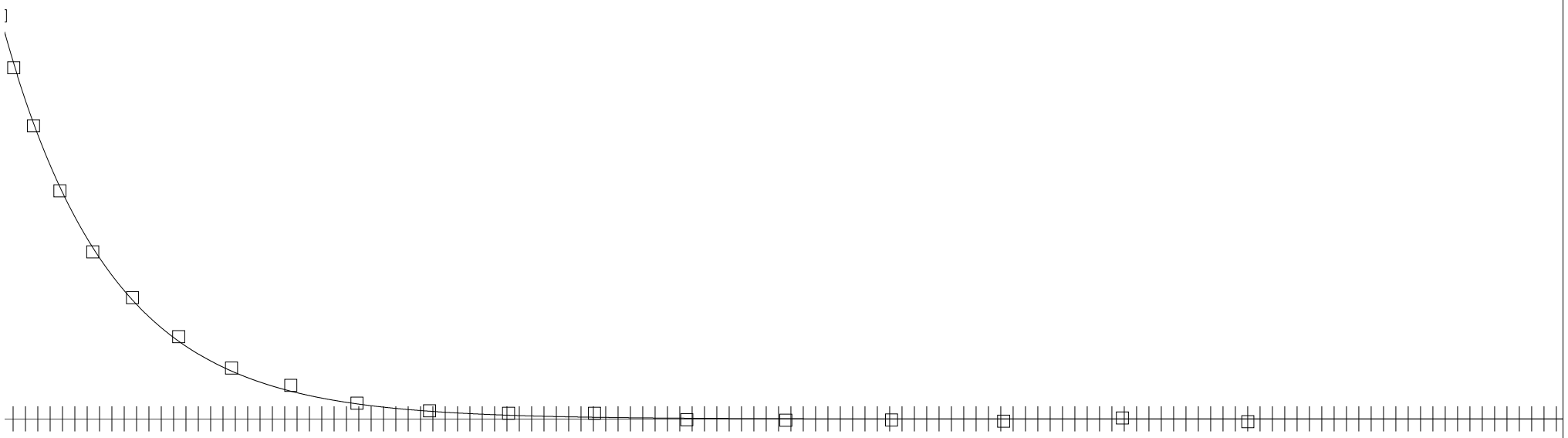
F1: 60.010		SW1: 1000	SW2: 0	OF1: 360.0	OF2: 0.0	PTS1d: 8192	PTS2d: 1 , 20
EX: c:\eft\H1\KINETIC.ppg		PW: 7.8 us	PD: 0.0 sec	NA: 1	LB: 0.0		Nuts - temp



Decay of the alcohol peak

T2 = 1152.278564 sec

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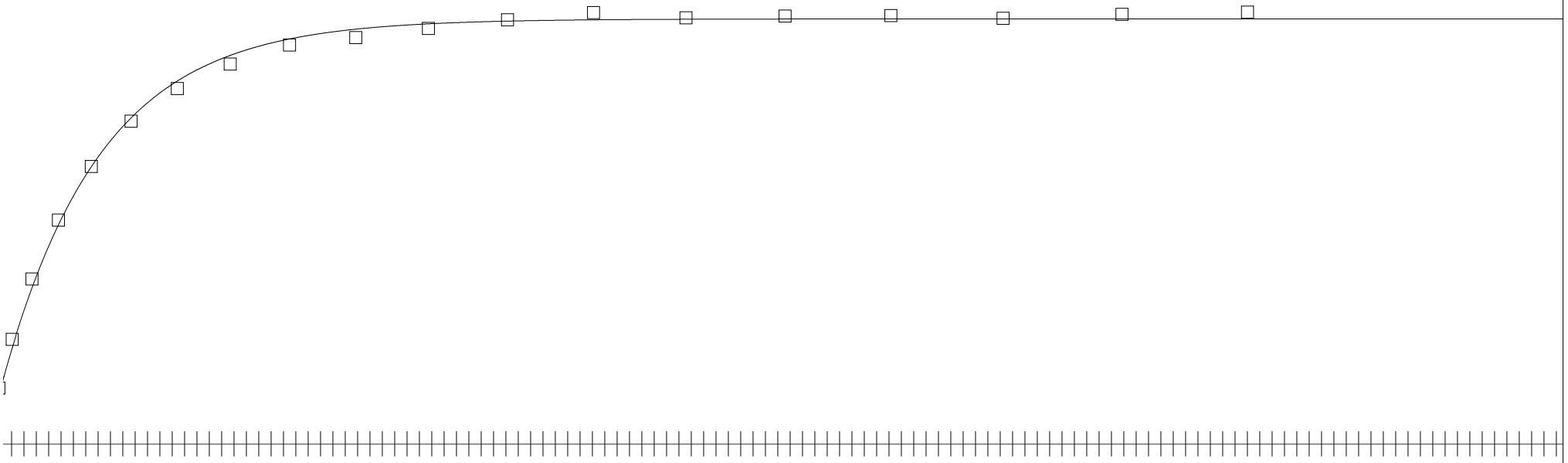
: 60.010		SW1: 1000	SW2: 0	OF1: 360.0	OF2: 0.0	PTS1d: 8192	PTS2d: 1 , 20
ζ: c:\eft\H1\KINETIC.ppg		PW: 7.8 us	PD: 0.0 sec	NA: 1	LB: 0.0		Nuts - temp



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:\eft\H1\KINETIC.ppg		PW: 7.8 us	PD: 0.0 sec	NA: 1	LB: 0.0		Nuts - temp