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, isoproxy 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.

\[
\text{ROH} + \quad \text{CF}_3\text{COH} \quad \rightarrow \quad \text{CF}_3\text{COR}
\]

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.
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.
T2 = 1152.278564 sec

Decay of the alcohol peak

T2 = 1152.278564 sec

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Nuts - temp
Growth of the ester peak

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