Electronic Supplementary Material (ESI) for Energy & Environmental Science

Supporting Information

Experimental and Theoretical Studies of the Acid-Catalyzed Conversion of Furfuryl Alcohol to Levulinic Acid in Aqueous Solution

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NMR Spectra

Figure S 1. ^{1}H NMR spectra for intermediate A. This spectrum was referenced to diethyl ether that was part of the isolation process (2.2 – 3.0 ppm)

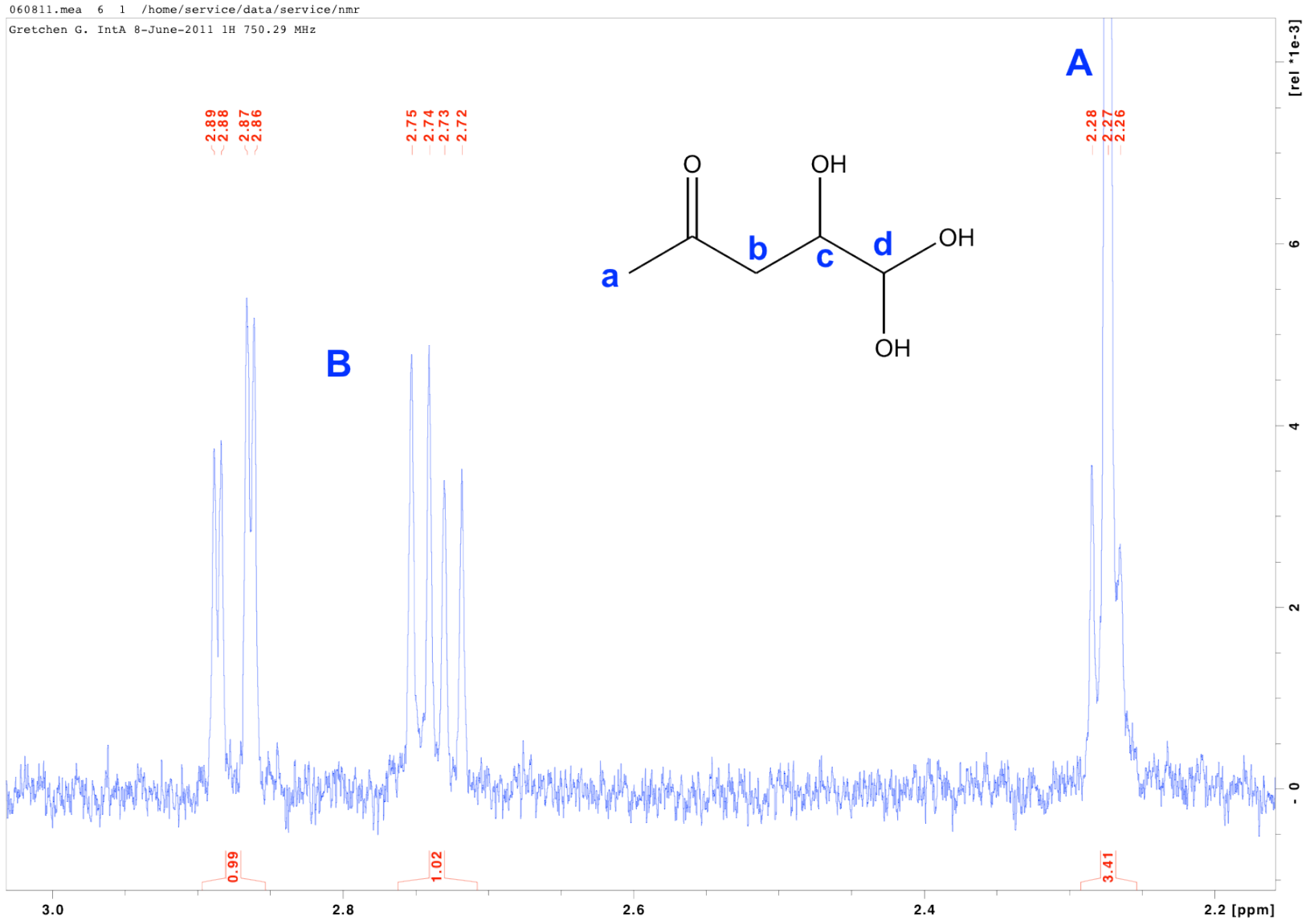


Figure S 2. ^{1}H NMR spectra for intermediate A. This spectrum was referenced to diethyl ether that was part of the isolation process (3.9 – 5.0 ppm)

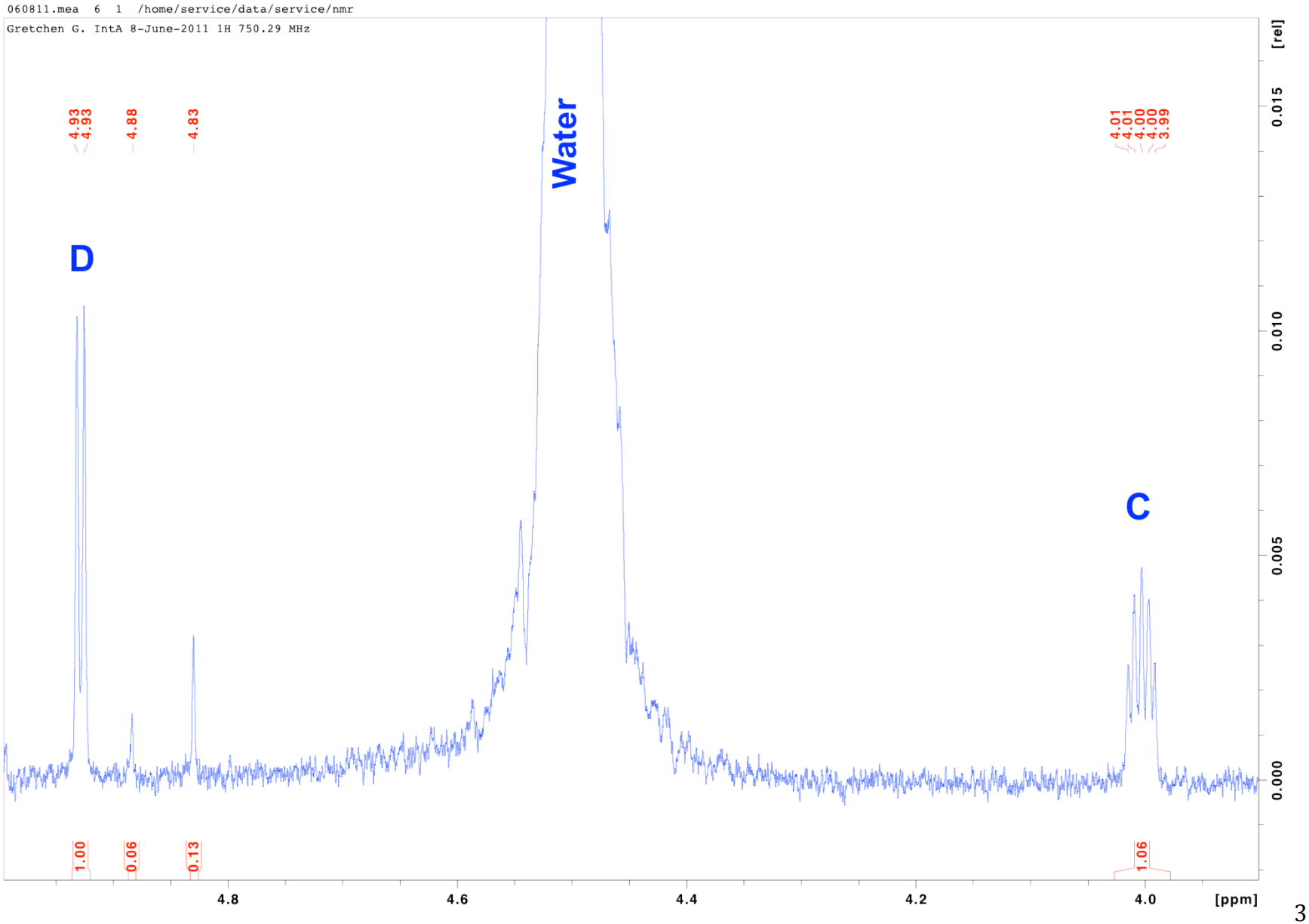


Figure S 3. Intermediate B ^{1}H NMR (referenced to external DSS)

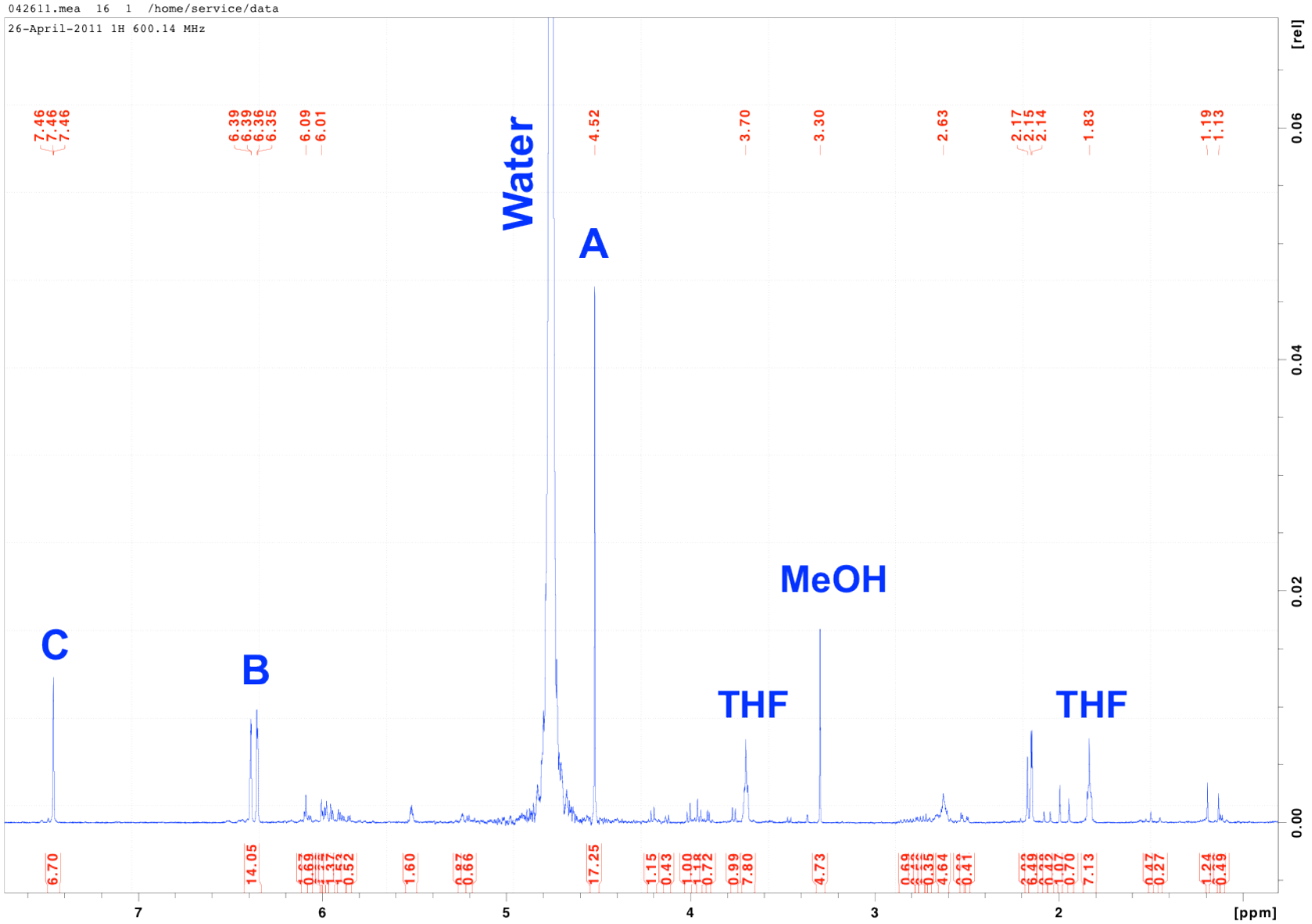


Figure S 4. FAL ^{1}H NMR standard in D_2O (referenced to external DSS)

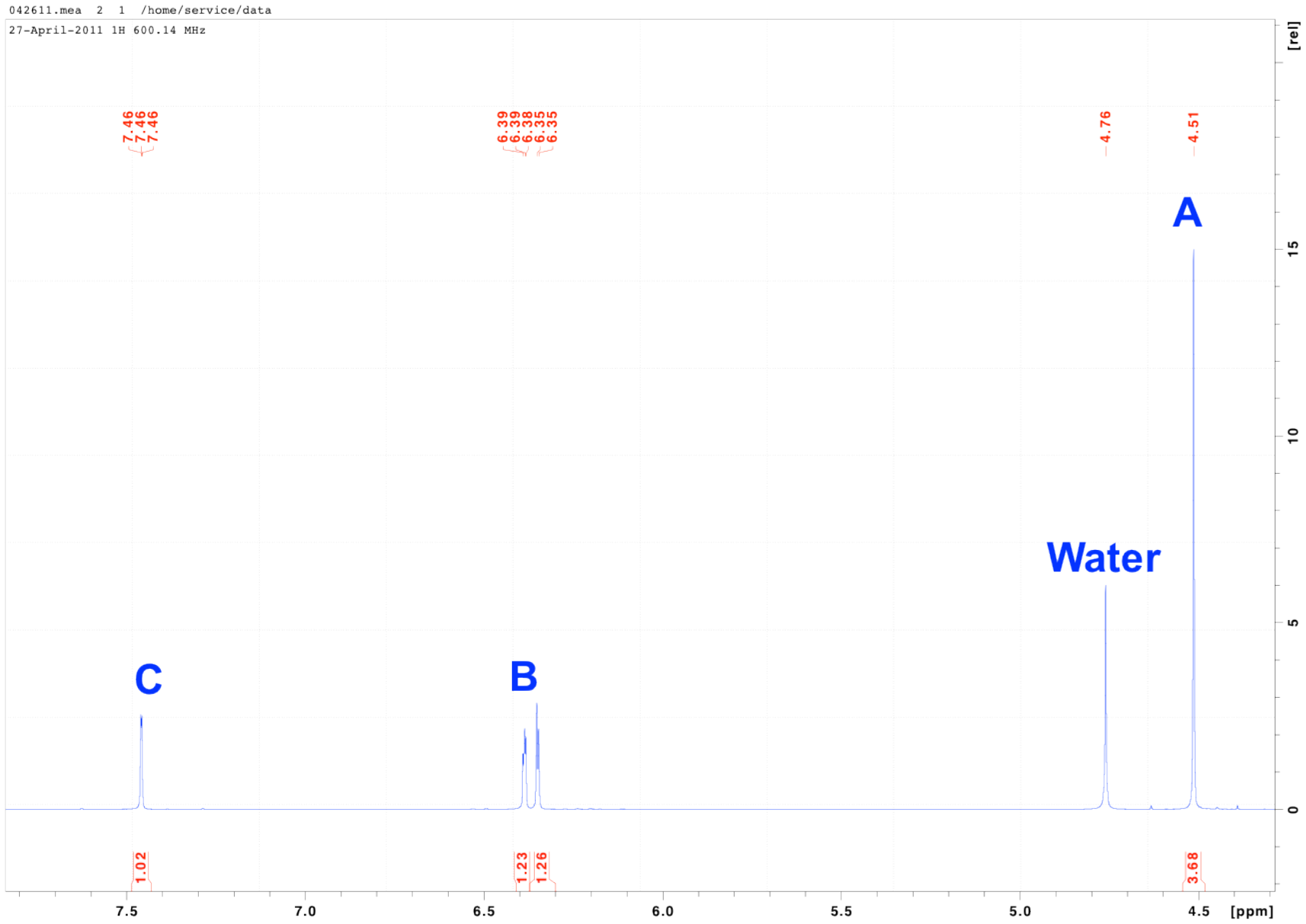


Figure S 3. TOCSY NMR Spectrum of Intermediate A

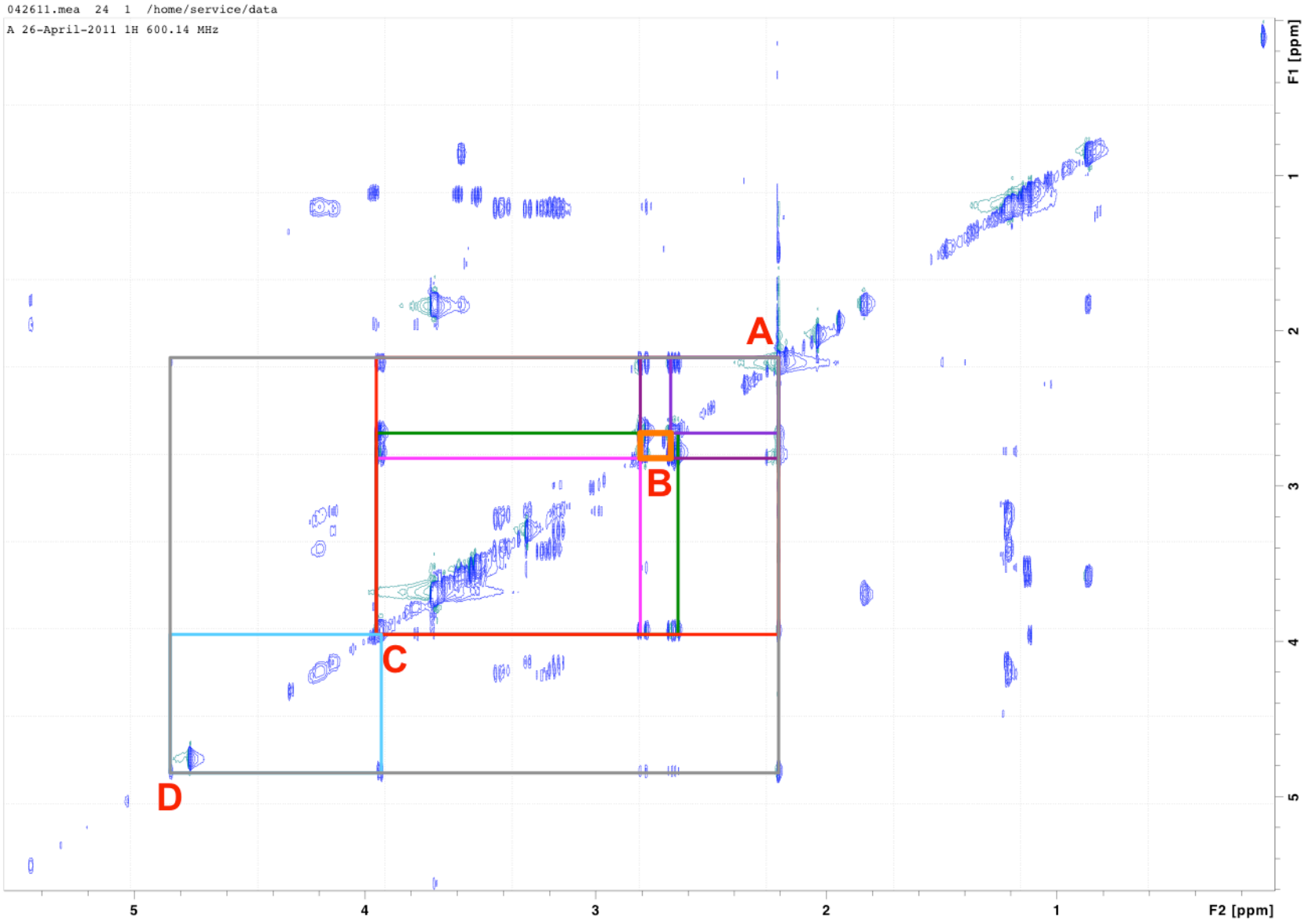


Figure S 4. COSY NMR Spectrum of Intermediate A

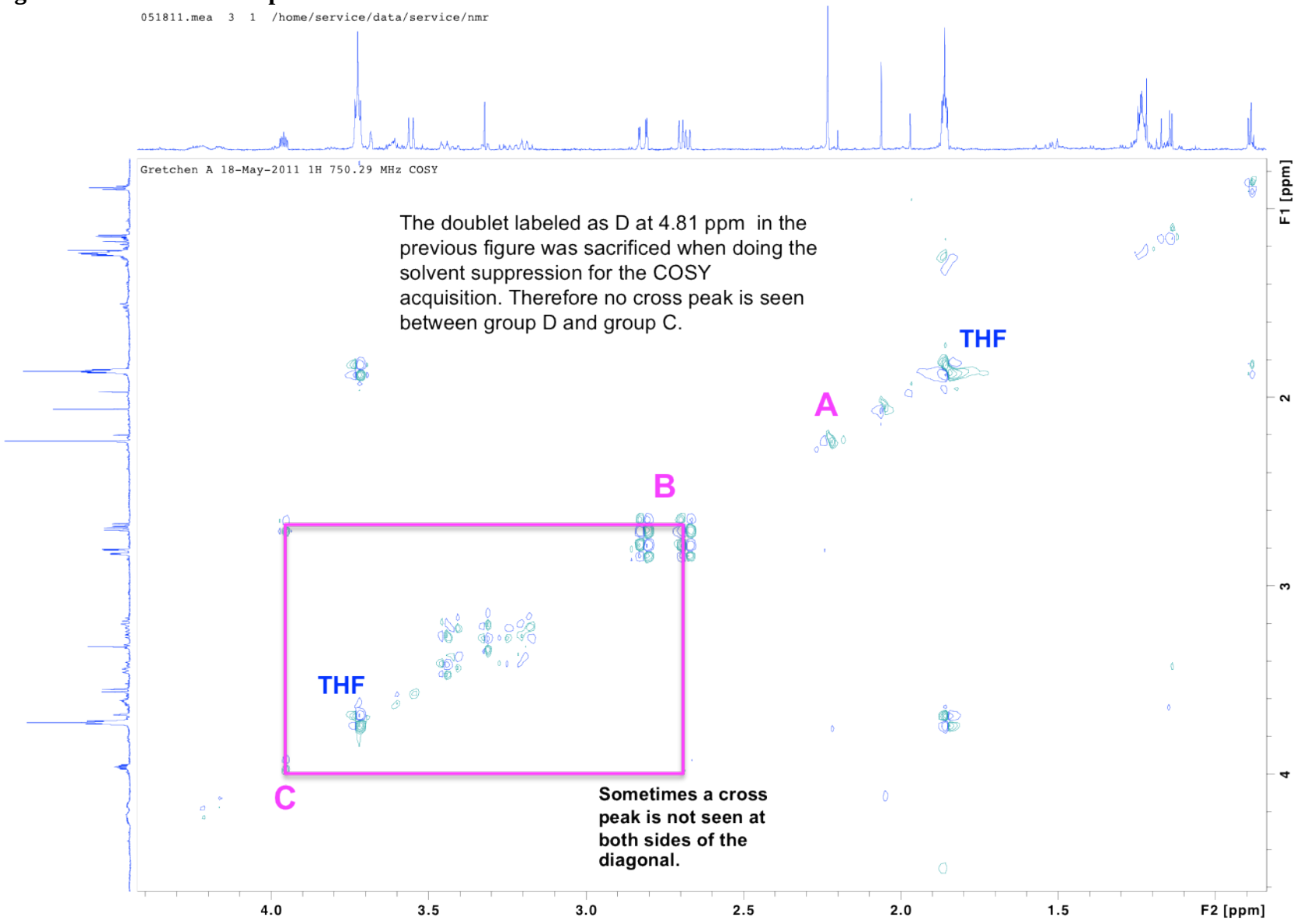
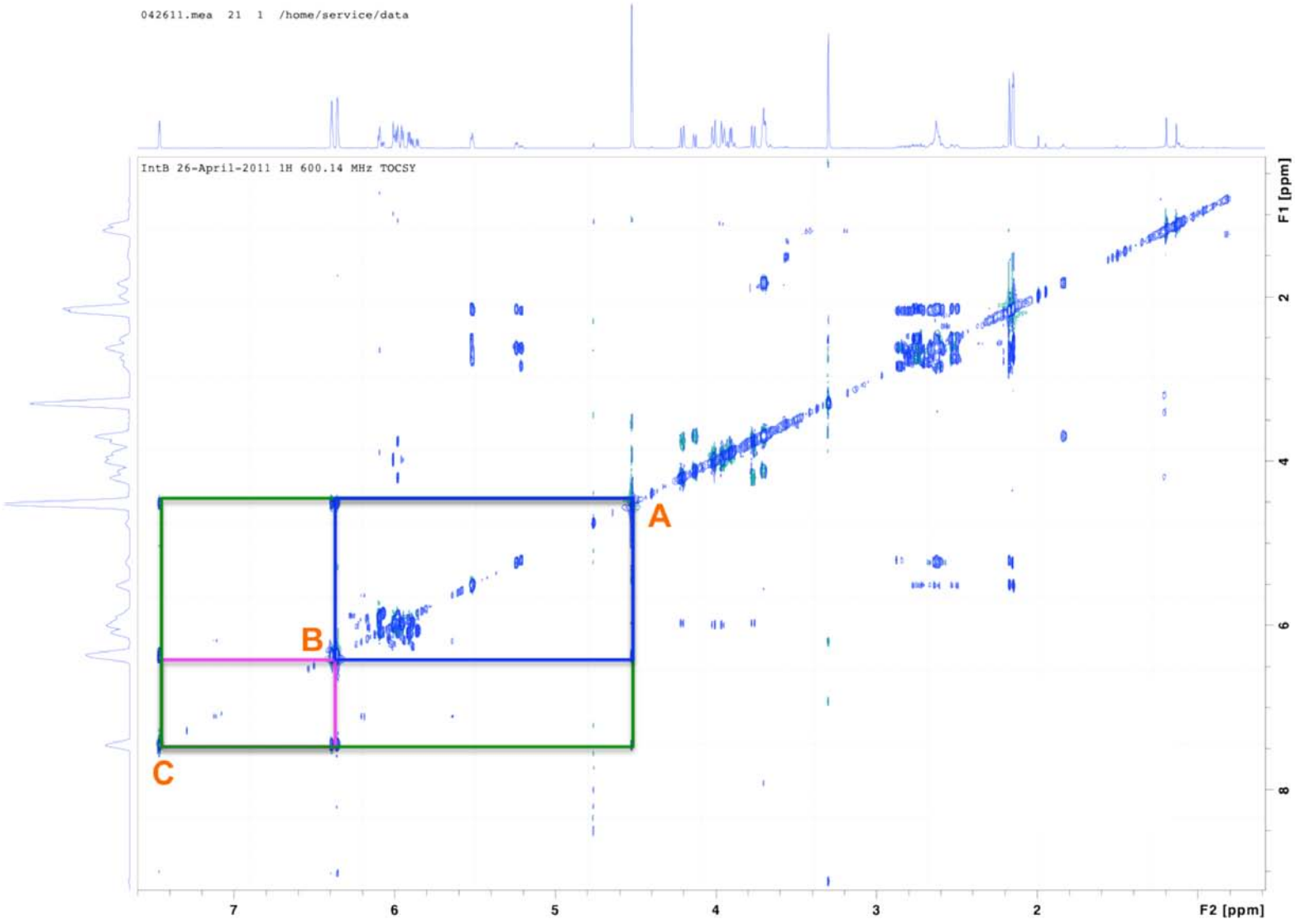


Figure S 5. TOCSY NMR Spectrum of Intermediate B



Computational Studies

1. Protonation of Furfuryl alcohol.

Figure S 4. Computed free energy of protonation of various positions of furfuryl alcohol computed at the G4MP2 level of theory (298 K, in kcal/mol). The solvation free energy contributions were computed using SMD model at the B3LYP/6-31G(2df,p) level of theory. A value of -262.4 kcal/mol is taken into account for the proton solvation energy of aqueous solution.

2. Possible nucleophillic addition reactions with FAL cation

Figure S 5. Computed free energies of addition reactions of FAL cation with water at the B3LYP/6-31G(2df,p) level of theory. The solvation contributions to the free energy are calculated using the SMD model at the same level of theory.