Supporting Information

Intracellular binding/unbinding kinetics of approved drugs to carbonic anhydrase II observed by in-cell NMR

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Supplementary Figures S1, S2

Supplementary Figures

Figure S1

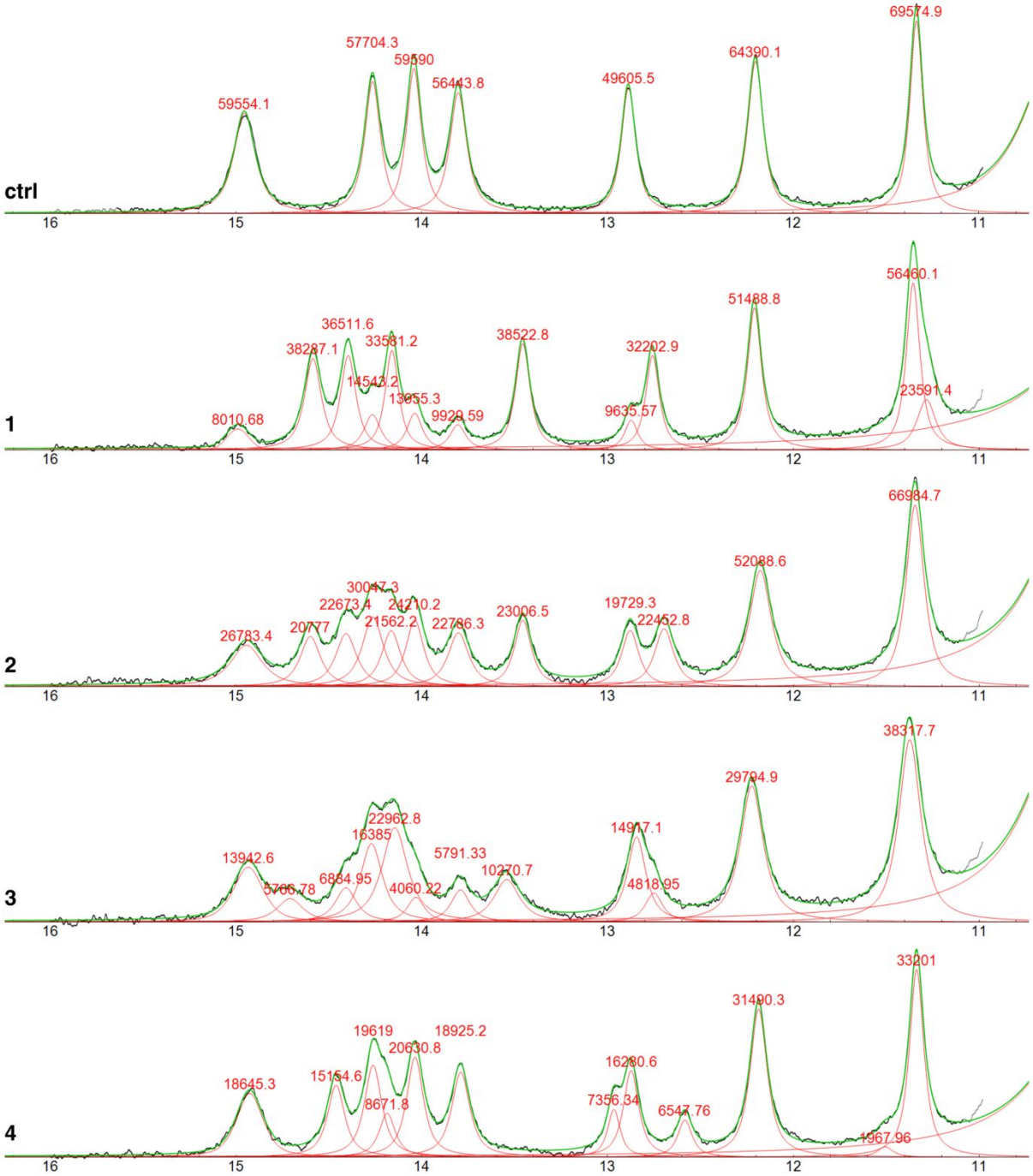

Figure S1 (cont.)

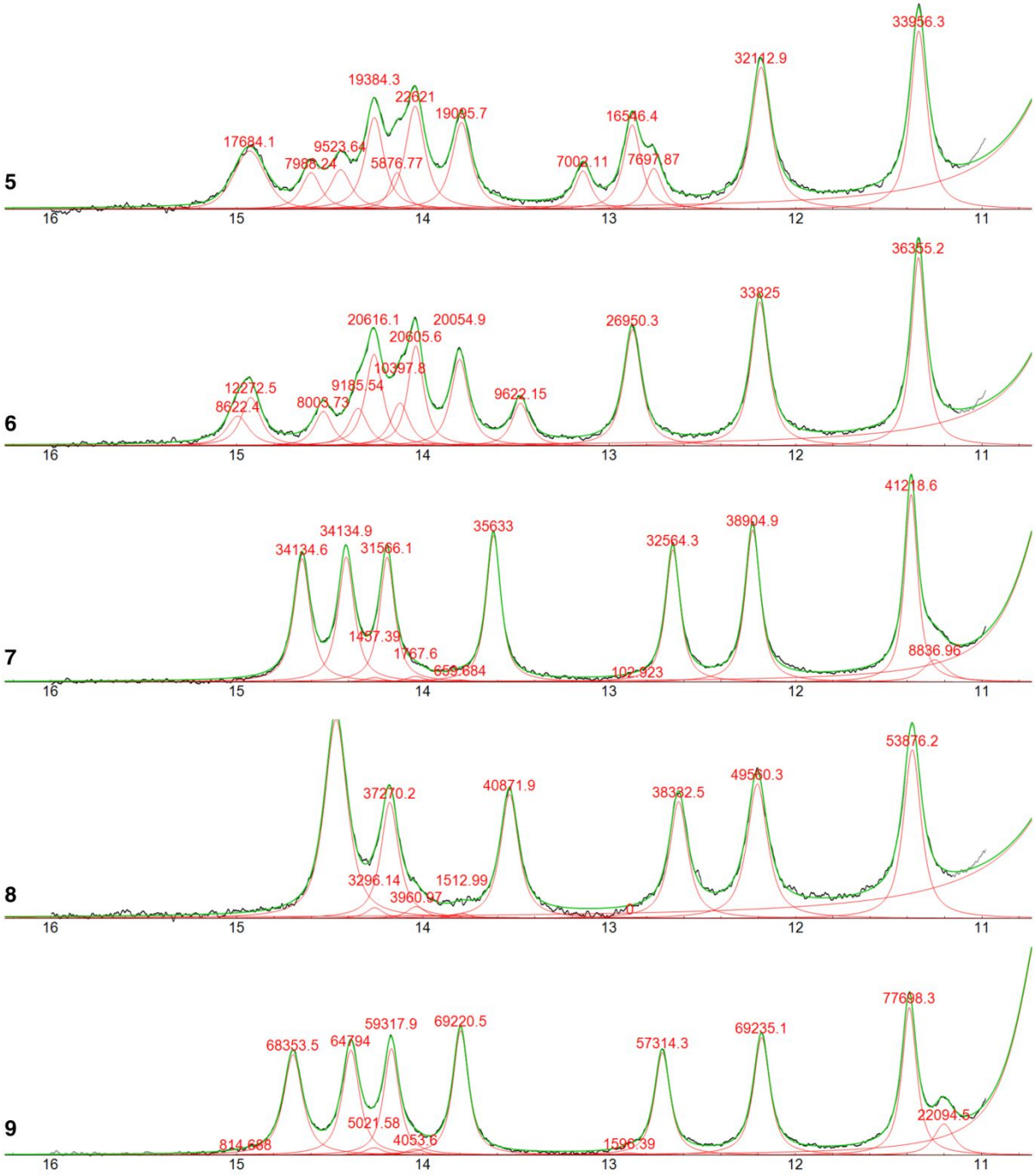

Figure S1. Spectral deconvolution in the imino region of 1D ^{1}H NMR spectra of cells expressing CA II both untreated (**ctrl**) and treated for 1 hour with 100 μM of each compound (**1-9**). The raw NMR data (black), the Pseudo-Voigt functions of each peak (red) and the overall sum (green) are shown. Peak areas are indicated in red. In some instances, peaks with non-ideal shapes were fitted as the sum of two Pseudo-Voigt functions (e.g. **6**). An additional Pseudo-Voigt function was used to correct for baseline distortion, the area of which was not used in the normalization process.

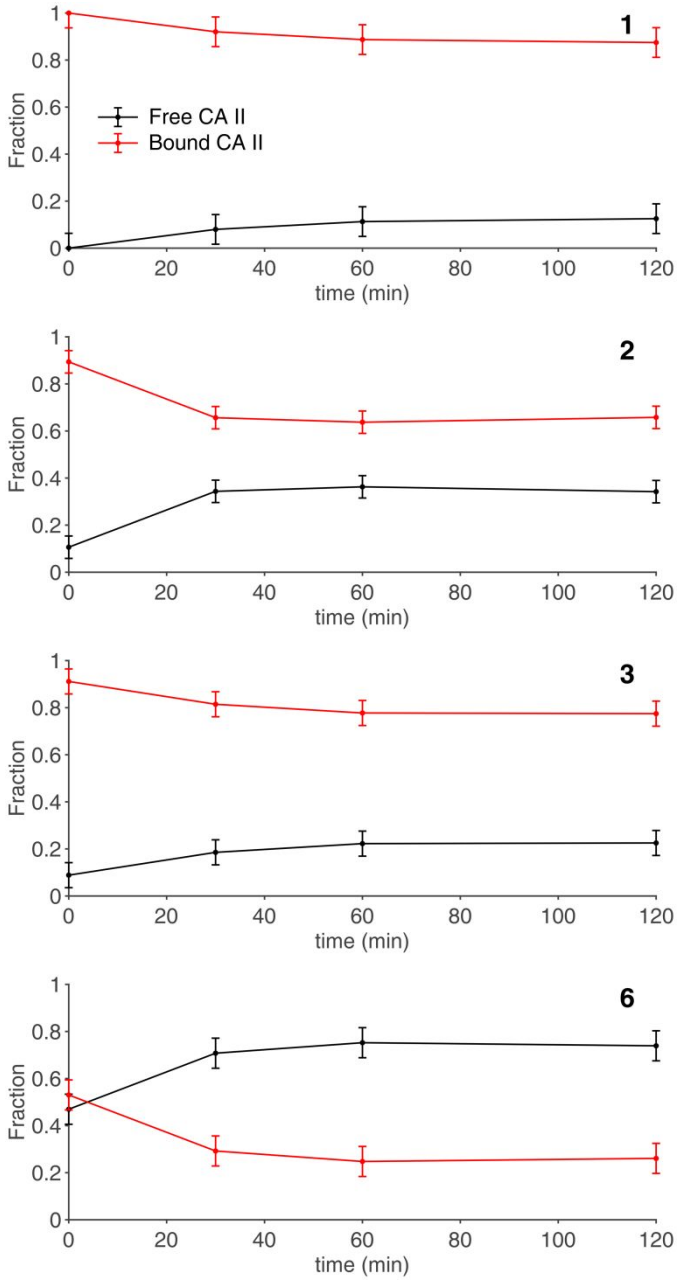

Figure S2. Time-dependence of free (black) and bound (red) CA II in cell lysates from cells treated for 1 hour with 100 μM of compounds **1-3** and **6** and subsequently washed and incubated in the absence of compound for different times. Error bars were obtained from the MCR-ALS global fitting as follows: err = 2 × [lack of fit(%)]/100.