

Electronic Supplementary Information

Encapsulation of Oxime Reactivators: Influence of Physiological Conditions on the Stability of Oximes-Cucurbit[7]uril Complexes

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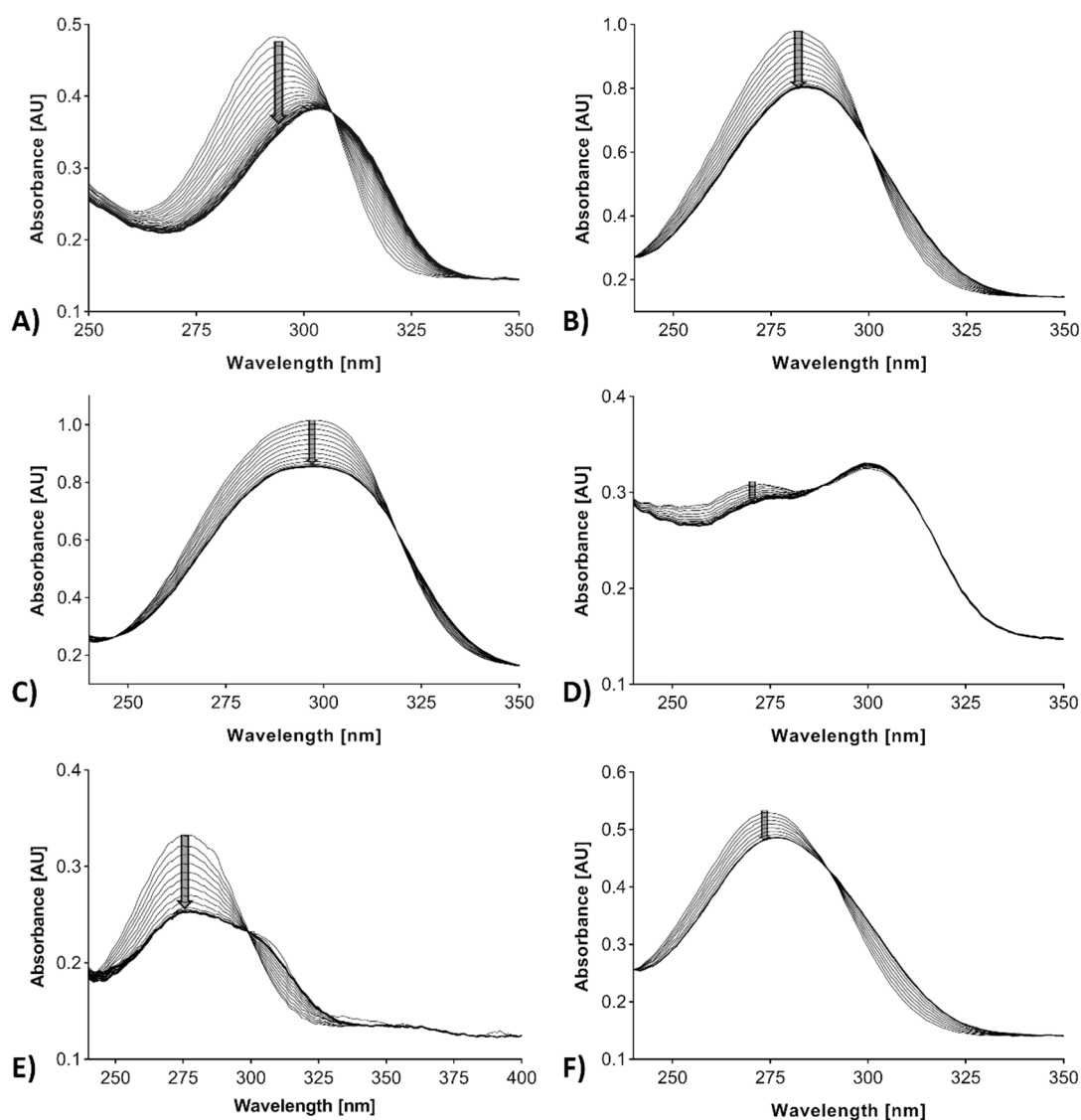


Figure S1: Overlay of the absorption spectra of pralidoxime (A), trimedoxime (B), methoxime (C), asoxime (D), K027 (E) and K048 (F) (30 μ M) measured after consecutive additions of CB[7] (1 μ L of 10 mM) during the titration experiments. Changes in the absorption spectra caused by complexation with the CB[7] host molecule are indicated by arrows.

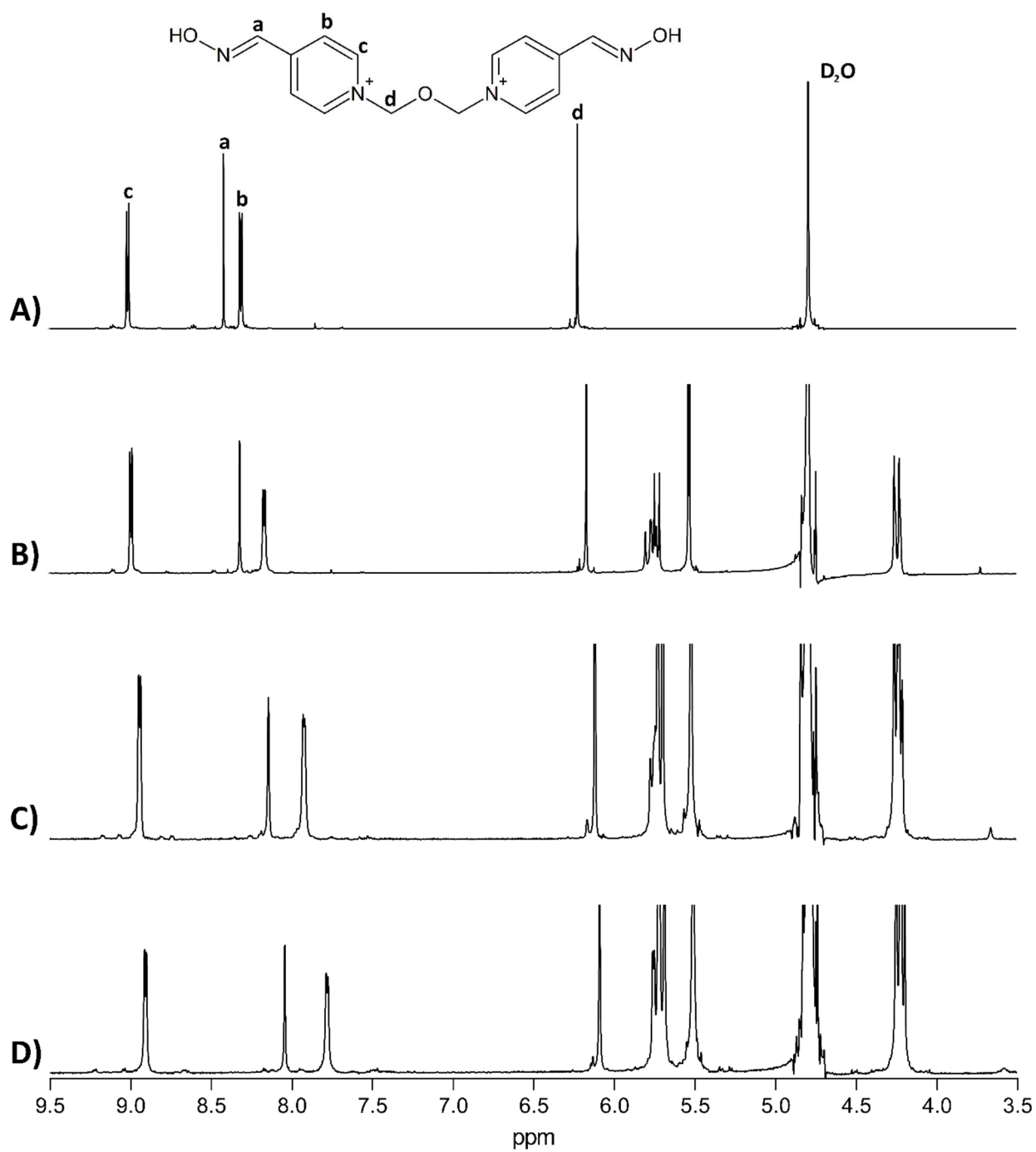


Figure S2: ^1H NMR spectra (500 MHz, D_2O) of obidoxime/CB[7] solutions: 1:0 (A), 1:0.5 (B), 1:1 (C), and 1:1.5 (D) molar ratio.

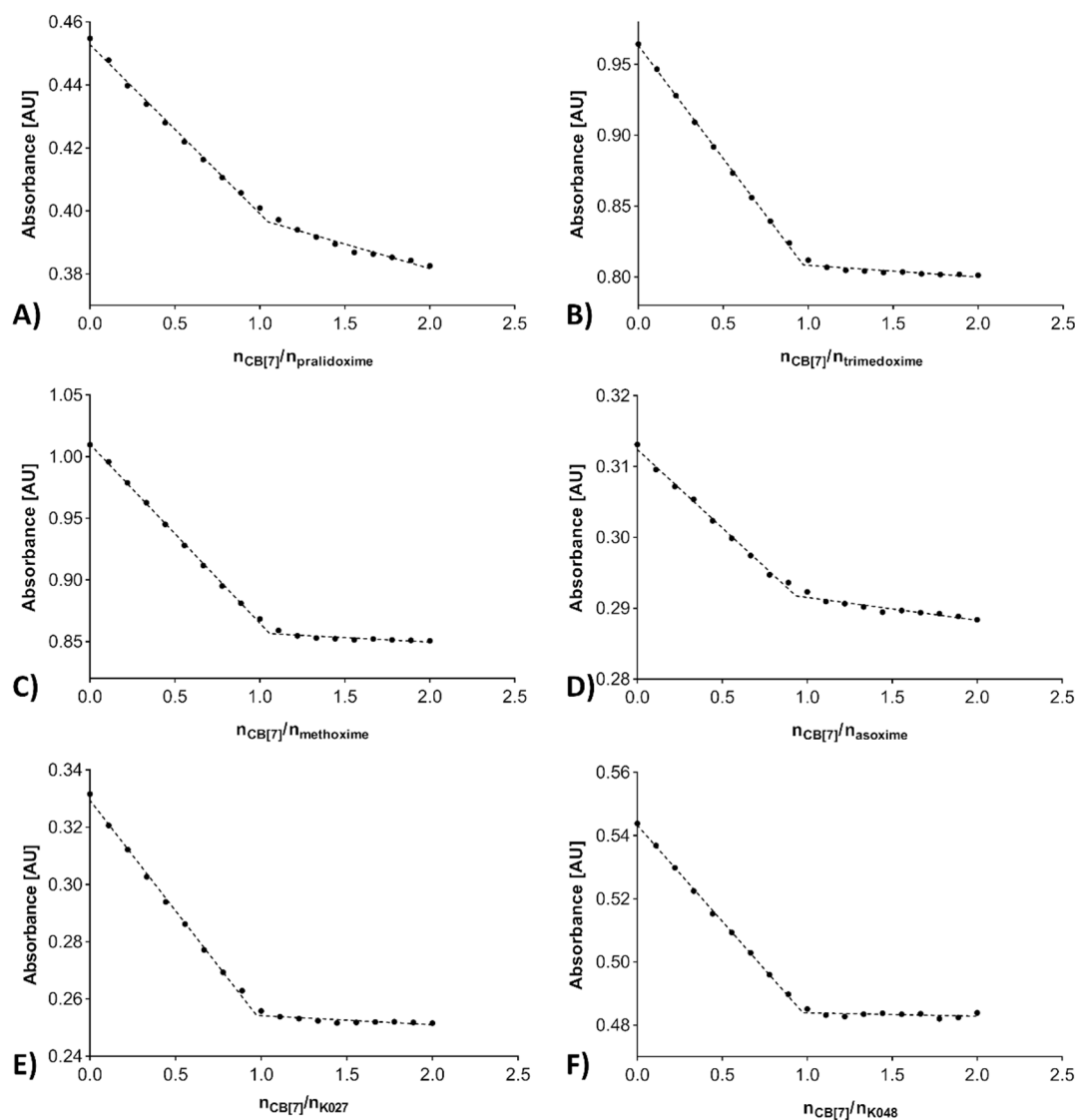


Figure S3: Determination of the complex stoichiometry ratio from the titration experiments. Dependence of the absorbance of pralidoxime (293 nm) (A), trimedoxime (282 nm) (B), methoxime (290 nm) (C), asoxime (272 nm) (D), K027 (276 nm) (E) and K048 (274 nm) (F) on the CB[7]/oxime mole ratio during the titration experiment showing the 1:1 stoichiometry of the complexes.

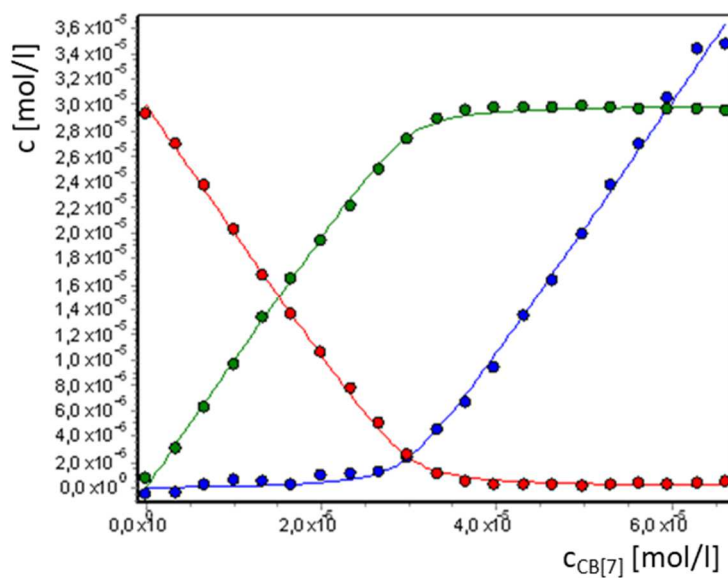


Figure S4: Concentrations of K027 (red), CB[7] (blue), and K027-CB[7] complex (green) from the titration experiment used for the determination of complex stability. Concentrations were calculated using Datan 5 software (MultiD Analyses AB, Göteborg, Sweden).

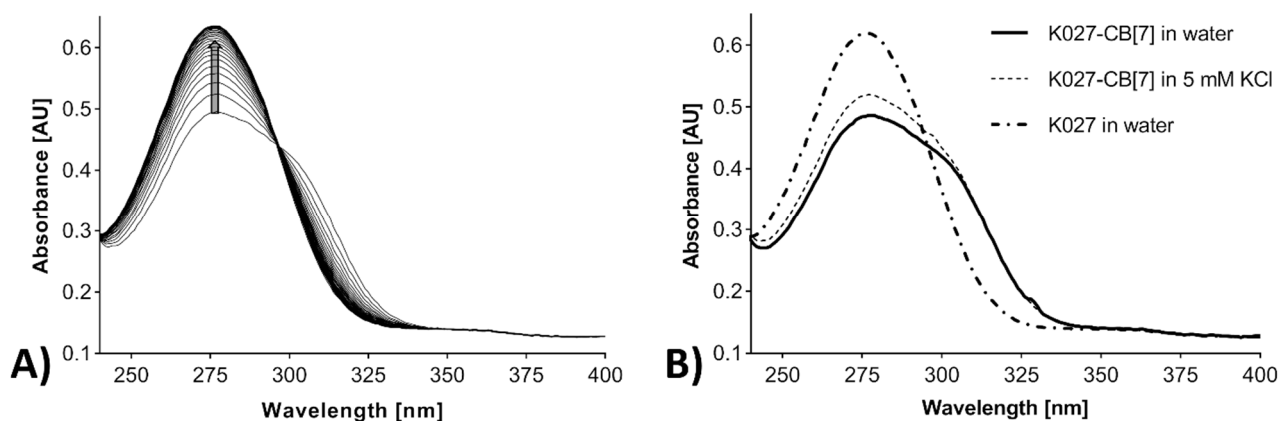


Figure S5: Effect of potassium cations on the stability of the K027-CB[7] complex. (A) Overlay of the absorption spectra of the K027-CB[7] complex solution (30 μM) measured after consecutive additions of KCl (10 μL of 4.5 M). The arrow indicates the increase in absorbance of the solution with the concentration of cation corresponding to the partial displacement of the oxime from the complex. (B) Absorption spectra of free K027 (30 μM) in water, K027-CB[7] complex (30 μM) in 5 mM KCl and K027-CB[7] complex (30 μM) in deionized water.

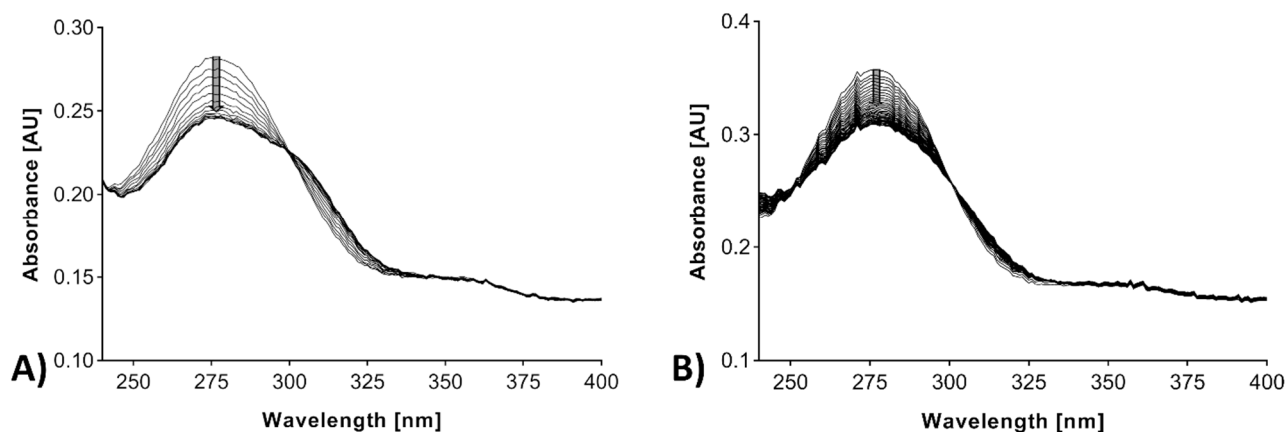


Figure S6: Effect of organic solvent on complexation of the oxime into CB[7]. Overlay of the absorption spectra of K027 (30 μ M) measured after consecutive additions of CB[7] (1 μ L of 10 mM) during the titration experiments in 20% methanol (A) and 20% acetonitrile (B). Changes in the absorption spectra caused by the complexation with the CB[7] host molecule are indicated by the arrow.