Electronic supplementary information

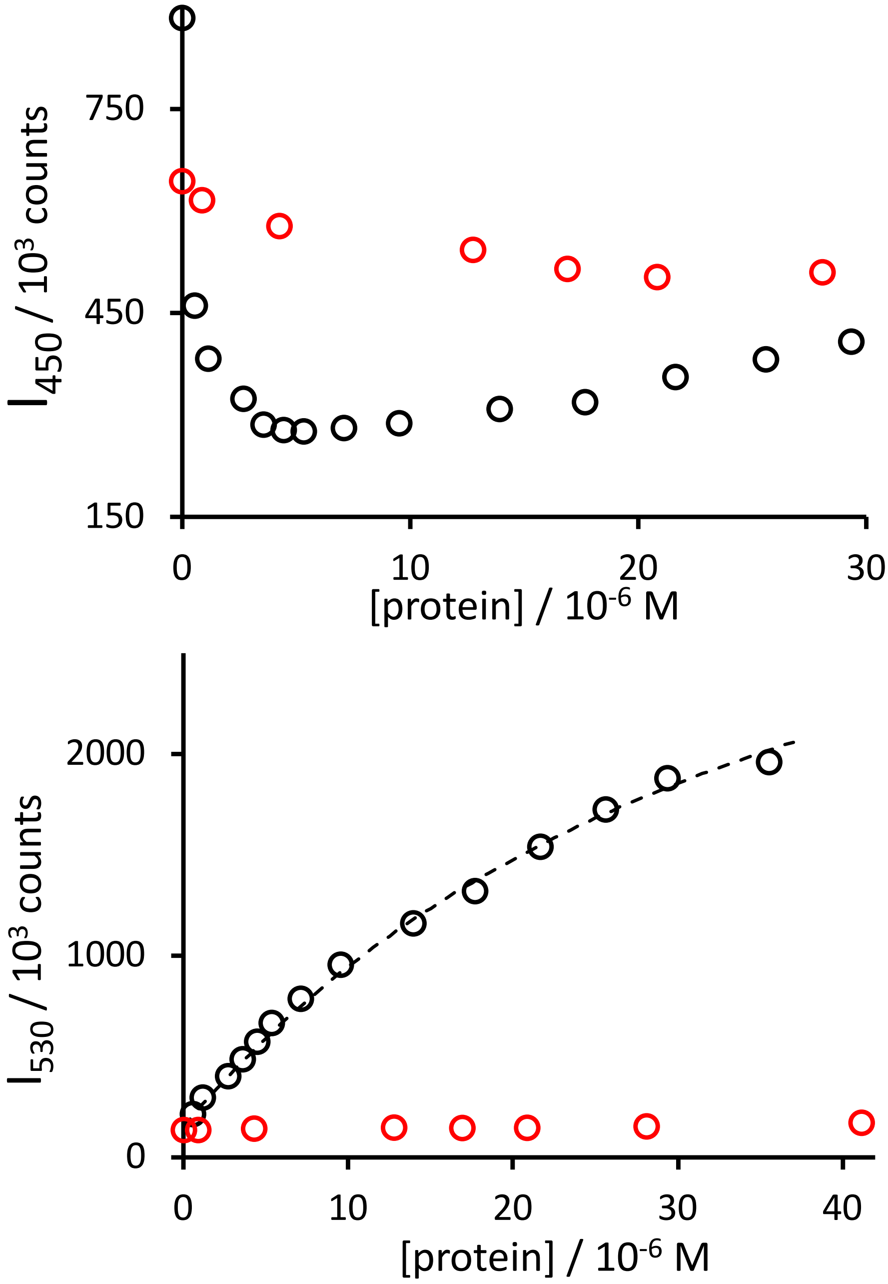

Fig. S1 Emission intensities of compound CHBT at 450 (top) and 530 nm (bottom) as functions of the concentrations of BSA (black circles) and pepsin (red circles). [CHBT] = 5 μM. The dashed curve shows the emission intensity at 530 nm recalculated under the assumption of a 1:1 CHBT/BSA binding stoichiometry, a binding equilibrium constant K_b = 3 x 10^4 M^{-1} and an emission intensity 750 x 10^3 counts at a 1 μM CHBT/BSA complex concentration.

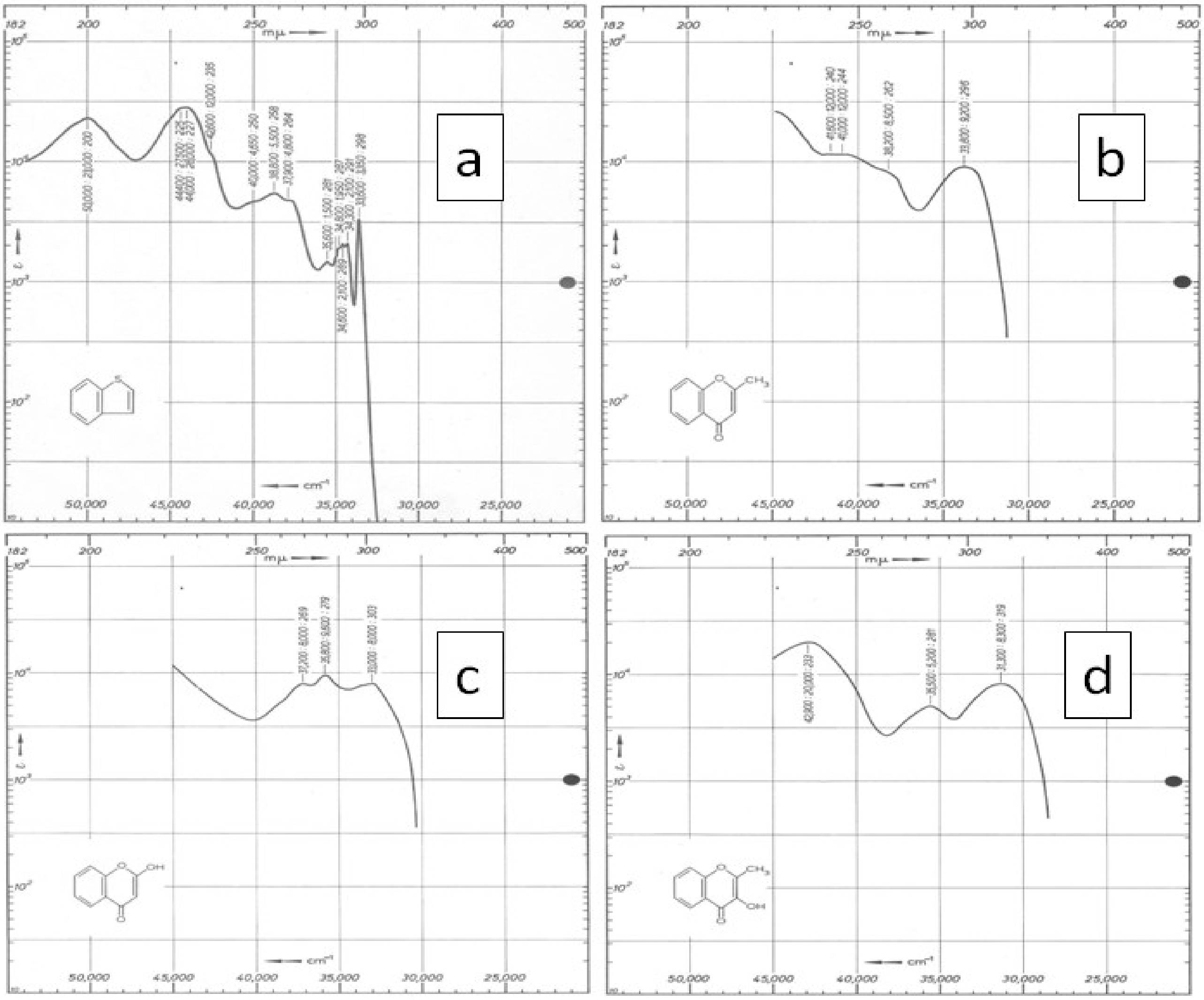

Fig. S2 UV spectra of benzothiophene (a) and three simple chromenones in light petroleum (b-d) (from the UV Atlas of Organic Compounds, Verlag Chemie, 1966).

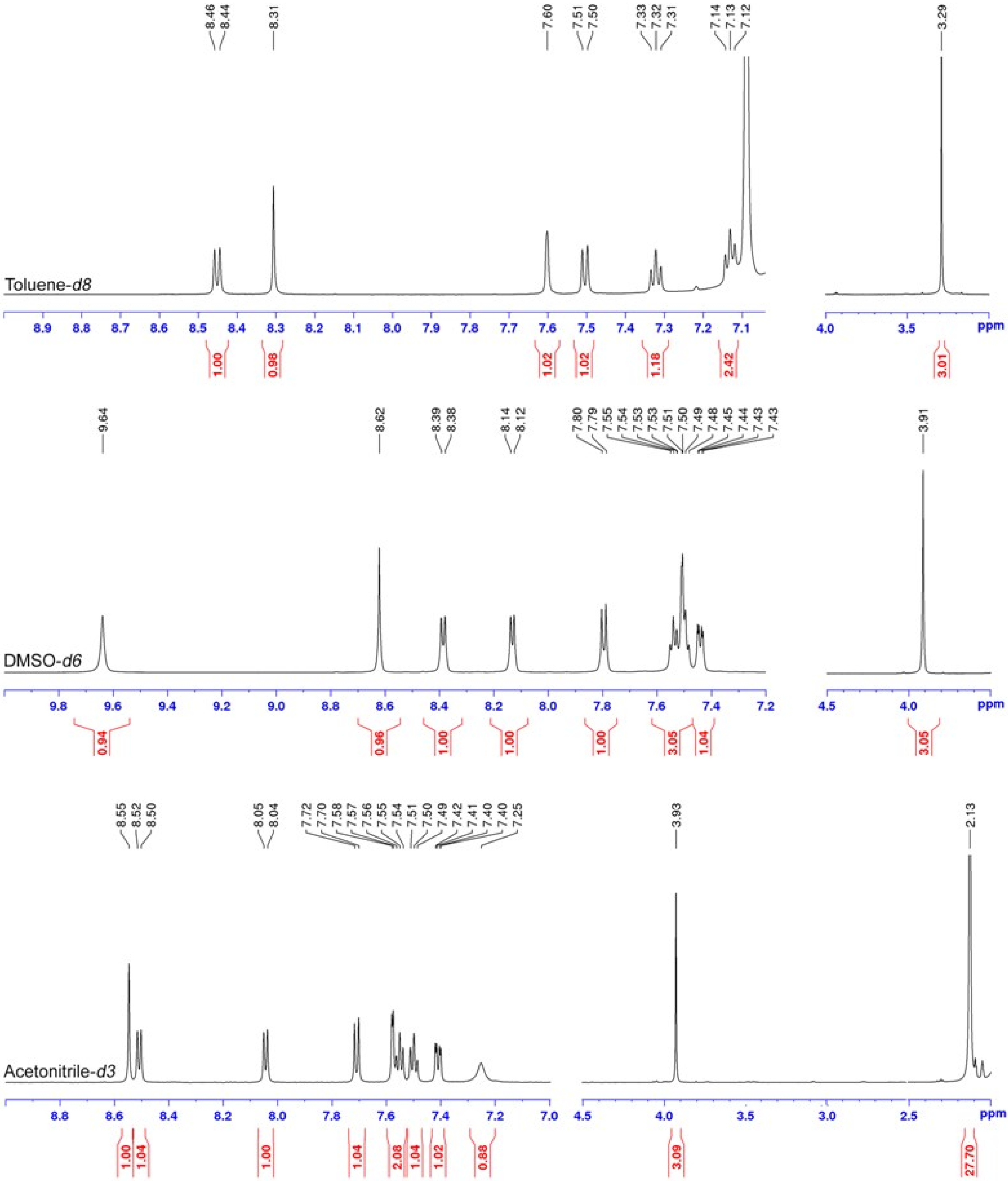

Fig. S3 ^{1}H-NMR spectra of compound CHBT in deuterated toluene, DMSO and acetonitrile.

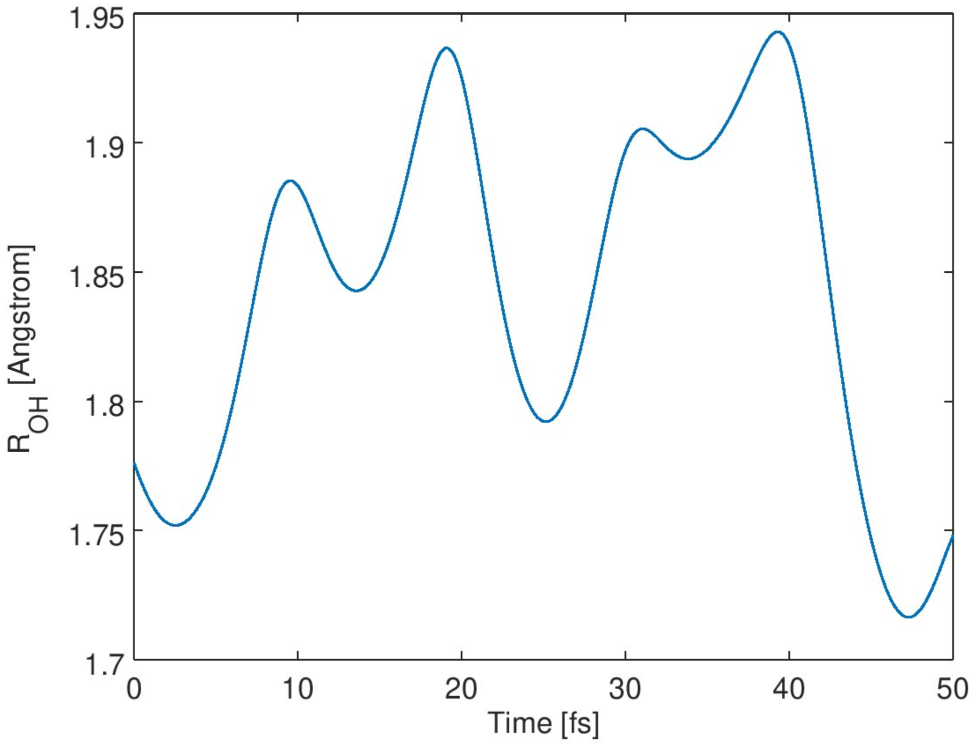

Fig. S4 Time evolution of the O (carbonyl)-H distance obtained in the molecular dynamics run performed by initially assigning zero-point vibrational energies to all vibrational modes (condition *a* in the Computational section).

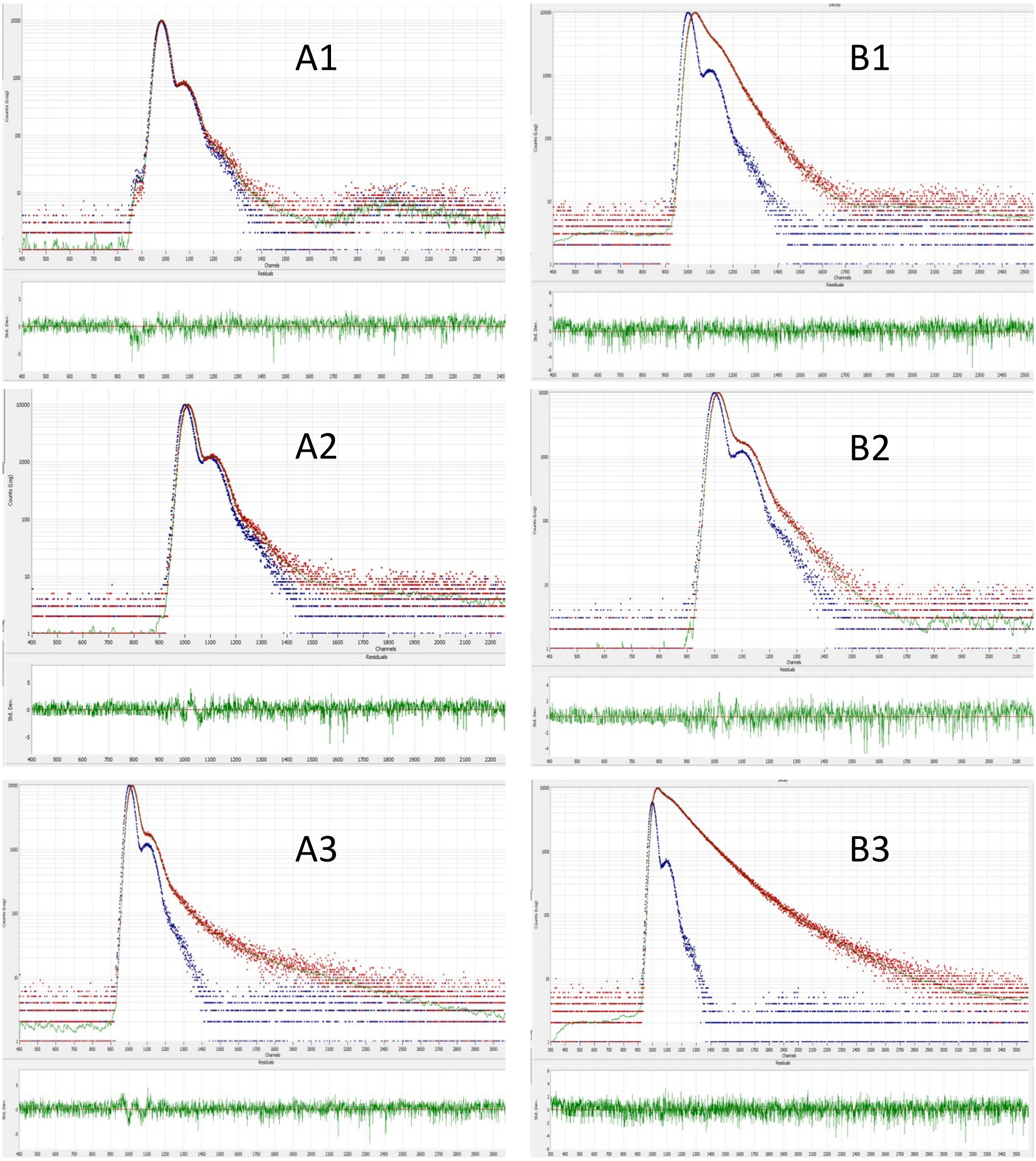

Fig. S5 Semi-log plots of the time-decays of the emission of CHBT in different solvents. Blue dots, scattered excitation pulse; red dots, emission; green line, plot of the fitting curve and of the corresponding residuals. 1 channel ≡ 27 ps. λ_{exc} = 340 nm in all cases. A1, in DMSO, λ_{em} = 430 nm; A2, in acetonitrile-water 1:2 mixture, λ_{em} = 440 nm; A3, in the aqueous buffer, λ_{em} = 425 nm, τ_1 = 0.42 ns (90%), τ_2 = 3 ns (5%), τ_3 = 11 ns (5%). B1, in cyclohexane, λ_{em} = 530 nm, τ_1 = 1.2 ns (85%), τ_2 = 3 ns (15%); B2, in acetonitrile, λ_{em} = 540 nm, τ_1 = 0.17 ns (64%), τ_2 = 0.75 ns (32%); B3, with 25 μM BSA, λ_{em} = 530 nm, τ_1 = 1.15 ns (12%), τ_2 = 3.3 ns (38%), τ_3 = 5.4 ns (40%), τ_4 = 9 ns (10%). The fitting lifetimes of the decays in A1 and A2 are shorter than the instrumental resolution (0.15 ns).