Supplementary information

Concurrent ultrafast twisting and proton transfer photoreactions in new pyrano[2,3-c]pyrazole derivatives

Marius Navickas, ^{*a} Karolis Gineitis,^a Arminas Urbonavičius,^b Sonata Krikštolė,^c Vytas Martynaitis,^c Eglė Arbačiauskienė,^c Miglė Dagilienė,^b Algirdas Šačkus,^{b,c} and Mikas Vengris^a

^{*a*}Vilnius University, Laser Research Center, Saulėteko av. 10, LT-10223 Vilnius, Lithuania; E-mail: marius.navickas@ff.vu.lt

^bKaunas University of Technology, Institute of Synthetic Chemistry, K. Baršausko str. 59, Kaunas LT-51423, Lithuania

^cKaunas University of Technology, Department of Organic Chemistry, Radvilėnų rd. 19, Kaunas LT-50254, Lithuania



Fig. S1. (a) Target evolution model of M2 in MeOH used in global analysis and (b) the SADS retrieved from the global analysis. Panel (c) shows the quality of the fits obtained by the kinetic scheme depicted in (a).



Fig. S2. (a) Target evolution model of M2 in CHCl₃ used in global analysis and (b) the SADS retrieved from the global analysis. Panel (c) shows the quality of the fits obtained by the kinetic scheme depicted in (a).



Fig. S3. The SE kinetics of M1 in MeOH and MeOH-glycerol solutions.



Fig.S4 (a) The kinetic model for the M1 compound in both pure methanol (MeOH) and a methanol/glycerol (MeOH/Glyc) mixture. The time values indicated in parentheses represent those obtained for the MeOH/Glyc mixture. Panel (b) shows the SADS from the time-resolved spectra of M1 in methanol (solid lines) and a methanol/glycerol mixture (dash-dotted lines). Panel (c) presents kinetic traces of M1 in MeOH/Glyc solution that demonstrate the quality of the fits.



Fig S5. (a) Target evolution model of M1 pump-dump-probe dynamics in MeOH used in global analysis. SADS retrieved from the global analysis with (b) absence and (c) presence of SE dumping pulse, arriving at 550 ps. Panel (d) presents the pump-dump-probe kinetic traces, illustrating the quality of the fits obtained from the kinetic scheme shown in (a).





Fig S6. (a) The evolution model of M1 pump-dump-probe dynamics in CHCl3 is used for global analysis, and (b) the SADS retrieved from this global analysis. Panel (c) shows the quality of the fits obtained through the kinetic scheme depicted in (a).