Supporting Information for: Ultrafast *trans*→*cis* Photoisomerization Dynamics of Alkyl-Substituted Stilbenes in a Supramolecular Capsule

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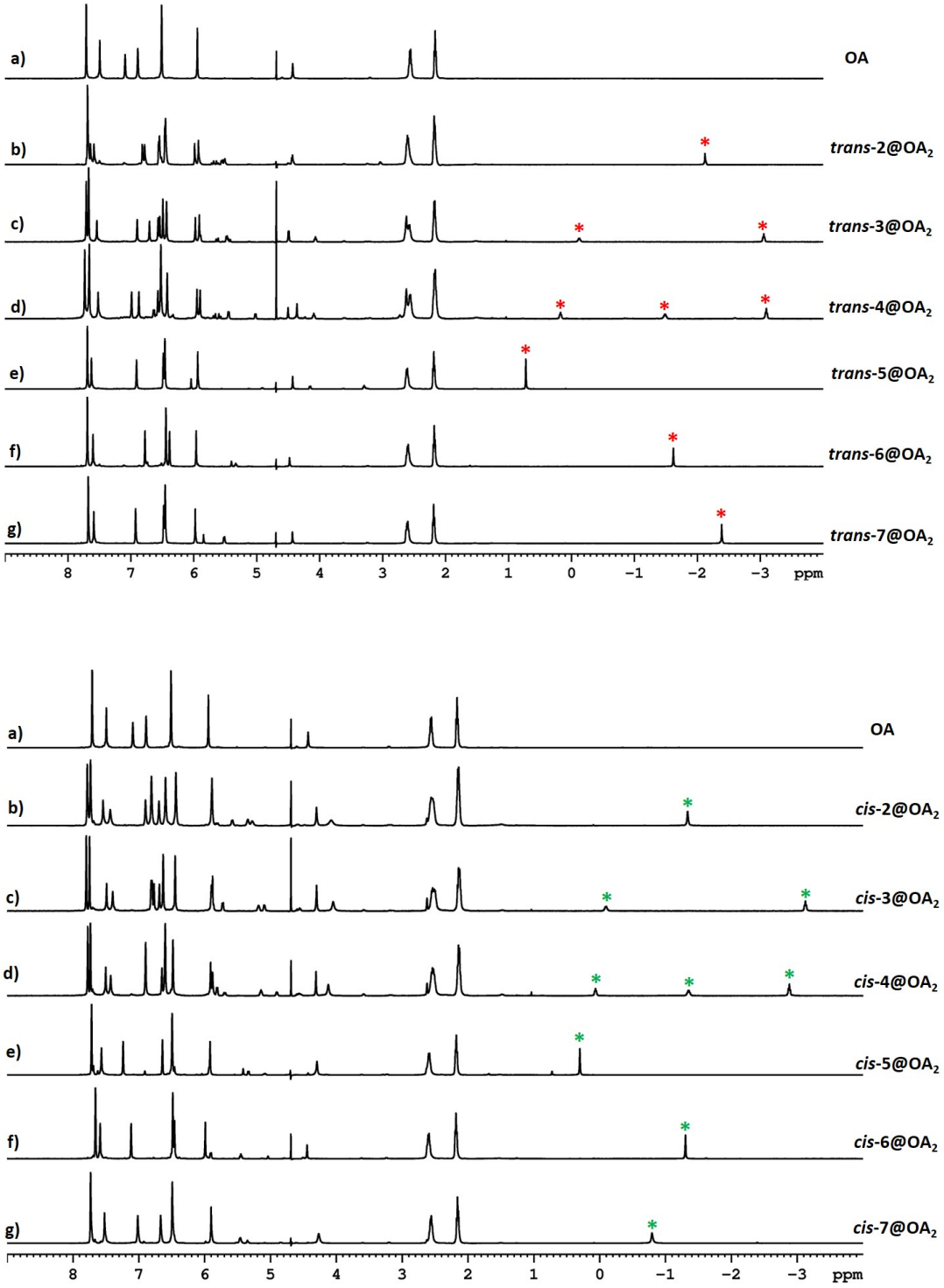

Figure S1: NMR spectra for *trans* (top) and *cis* (bottom) isomers of all six alkyl-substituted stilbenes in the OA_2 capsule. The spectrum of OA is included in both panels for comparison.

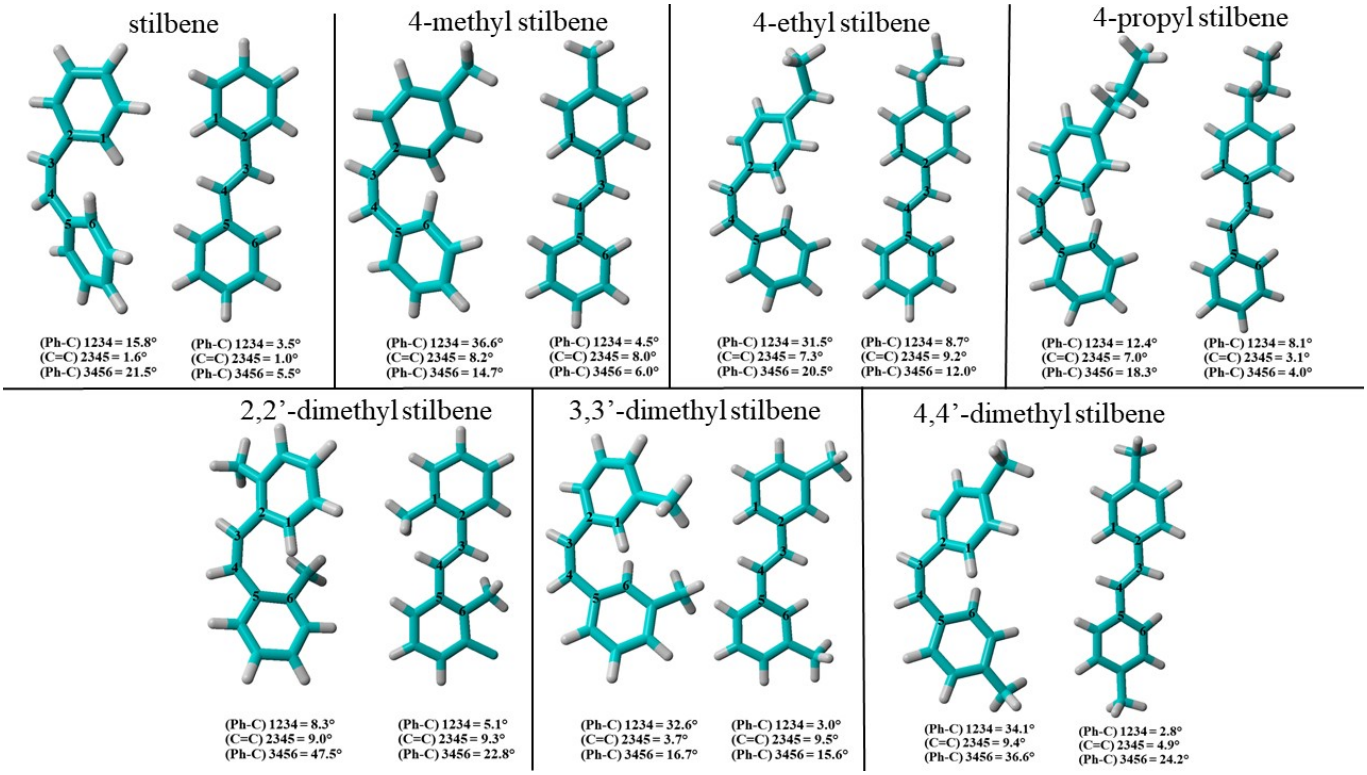

Figure S2: Geometries of encapsulated molecules from MD simulations.

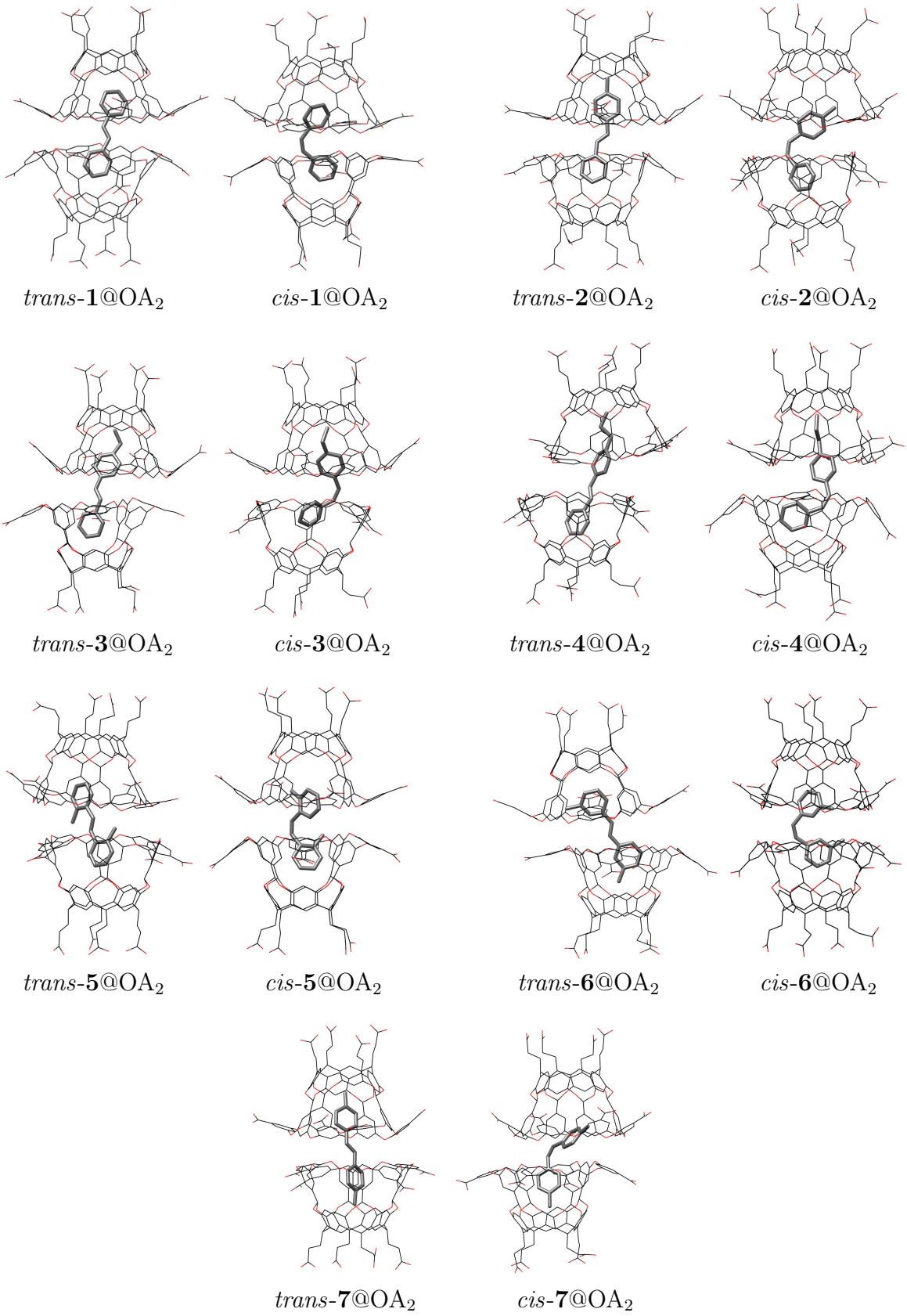

Figure S3: Structures of guest@OA_2 complexes from MD simulations.

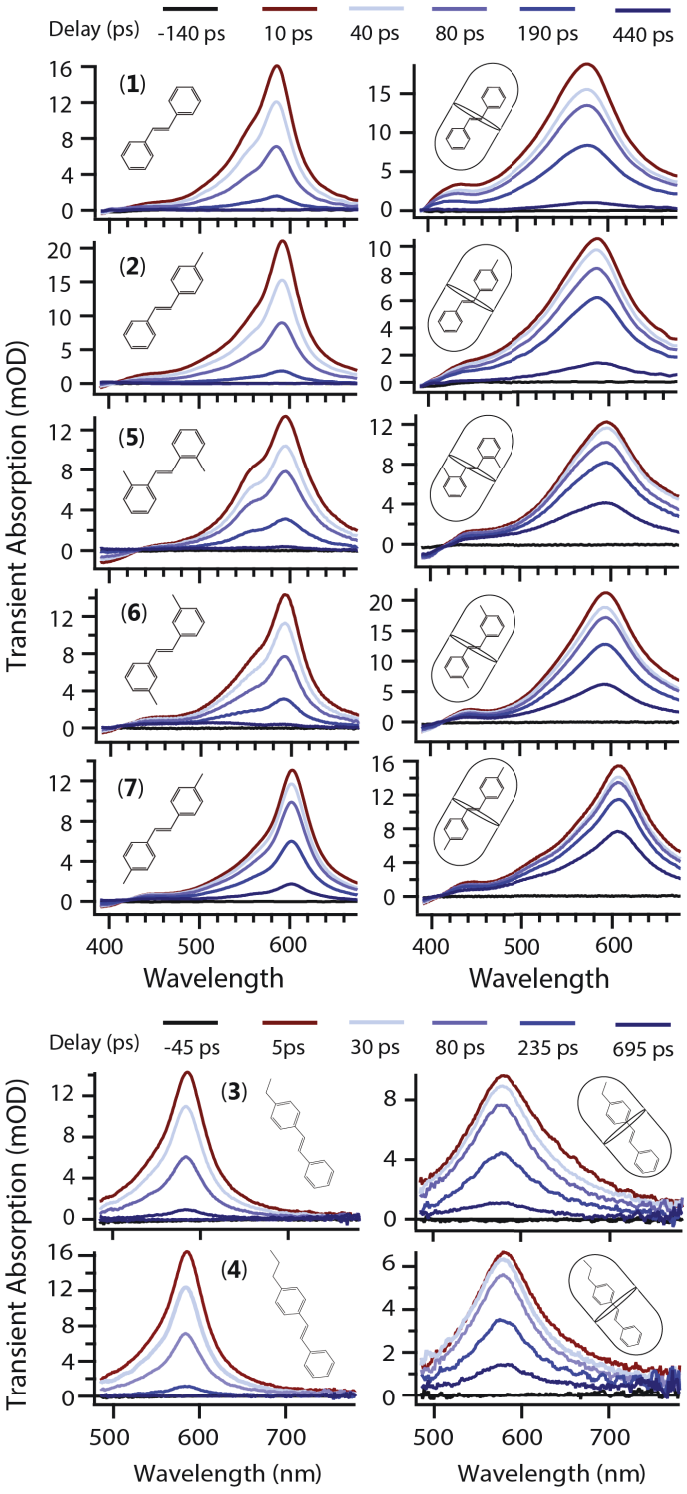

Figure S4: Transient absorption spectra for all seven stilbene derivatives in solution (left) and in the OA_2 capsule (right). Note the different range of probe wavelengths for compounds **3** and **4**.

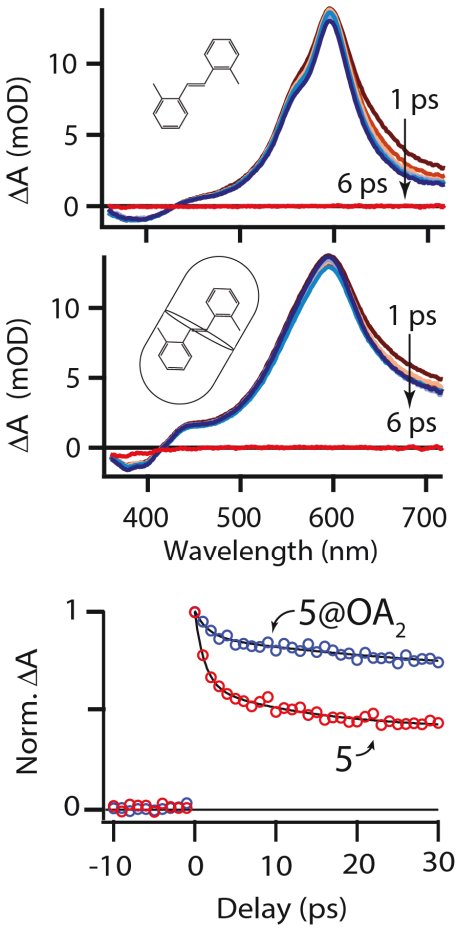

Figure S5: Narrowing of the excited-state absorption band of compound **5** in solution and in OA_2 over the range 1-6 ps. Bottom panel shows the decay of the normalized transient absorption signal at 710 nm, with black lines showing bi-exponential fits to the data.

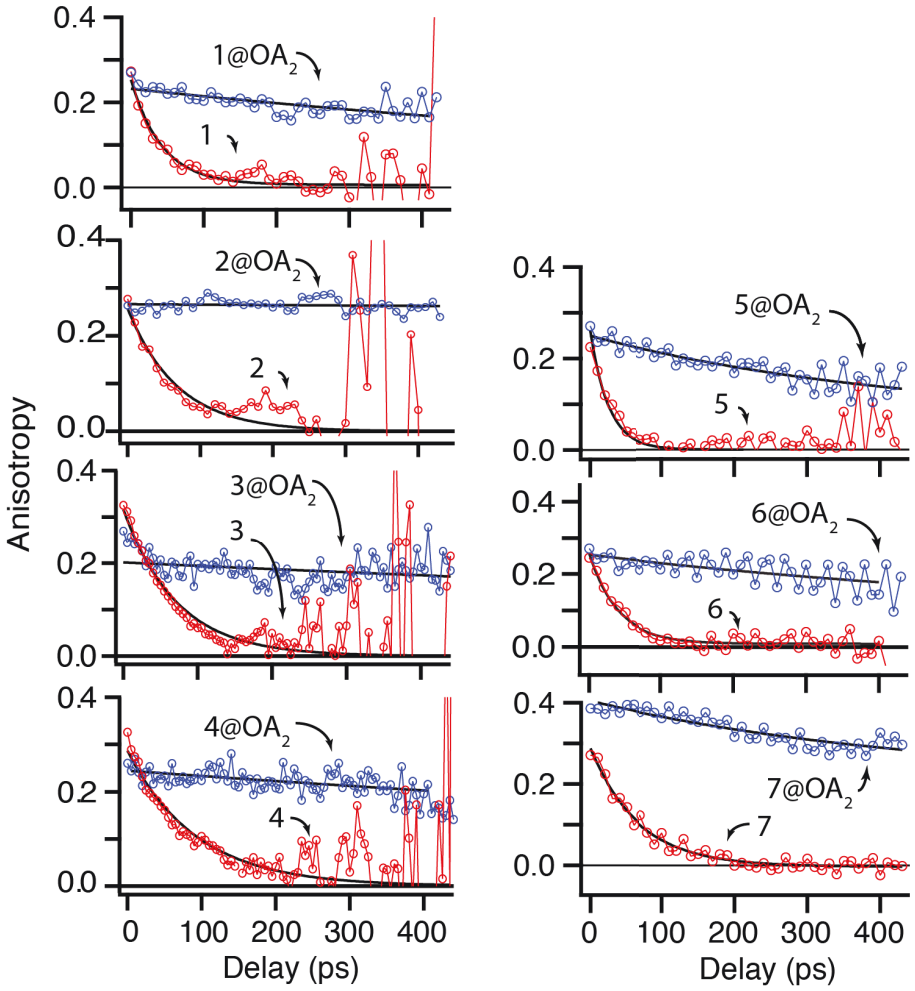

Figure S6: Anisotropy decay of all seven compounds in solution (red) and in the OA_2 capsule (blue). Black lines are single-exponential fits to the data to obtain molecular reorientation times, τ_{rot}, in solution. Fits are insufficient to obtain reorientation times in the capsule, where we estimate a rotation time for the entire guest@OA_2 complex of $\sim$1 ns using a rotational diffusion model (see main text).