Supporting Information

Templating Photodimerization of Coumarins Within a Water Soluble Nano Reaction-Vessel

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Contents

^{1}H NMR characterization of the dimers

The regiochemistry of the dimers was assigned based on the chemical shift of the cyclobutane protons reported in the literature.

Syn head-head **(2a) dimer of 1a:** ^{1}H NMR ($CDCl_3$) δ: 4.05-4.1(m, 2H), 4.2-4.25(m, 2H), 6.76-6.8(d, 2H), 6.85-6.95(m, 4H), 7.2-7.24(m, 2H).

Syn head-tail **(3a) dimer of 1a:** ^{1}H NMR ($CDCl_3$) δ: 4.25(m, 4H), 6.6-6.65(m, 2H), 6.9-7.0(m, 2H), 7.2-7.4(m, 4H).

Syn head-head **(2b) dimer of 1b:** ^{1}H NMR ($CDCl_3$) δ: 2.15(s, 6H, $-CH_3$), 4.0-4.05(m, 2H), 4.1-4.15(m, 2H), 6.55(d, 2H), 6.75(d, 2H, J=8.0 Hz), 7.0(m, 2H).

Anti head-head **(4b) dimer of 1b:** ^{1}H NMR ($CDCl_3$) δ: 2.35(s, 6H, $-CH_3$), 3.78-3.80(m, 2H), 3.9-3.92(m, 2H), 6.95(d, 2H), 7.0(d, 2H, J=8.0 Hz), 7.15(m, 2H).

Syn head-head **(2c) dimer of 1c:** ^{1}H NMR ($CDCl_3$) δ: 3.75(s, 6H, $-OCH_3$), 3.99-4.02(m, 2H), 4.06-4.09(m, 2H), 6.43(d, 2H), 6.51-6.54(m, 2H), 6.7(d, 2H, J=8.0 Hz).

Syn head-tail **(3c) dimer of 1c:** ^{1}H NMR ($CDCl_3$) δ: 3.7(s, 6H, $-OCH_3$), 4.15-4.2(m, 2H), 4.22-4.28(m, 2H), 6.2(d, 2H), 6.65-6.72(m, 2H,), 7.05(d, 2H, J=8.3 Hz).

Syn head-head **(2d) dimer of 1d:** ^{1}H NMR ($CDCl_3$) δ: 3.8(s, 6H, $-OCH_3$), 4.01-4.05(m, 2H), 4.19-4.21(m, 2H), 6.38-6.40(d, 2H, J=7 Hz), 6.78-6.80(d, 2H, J=8 Hz), 6.85-6.95(m, 2H).

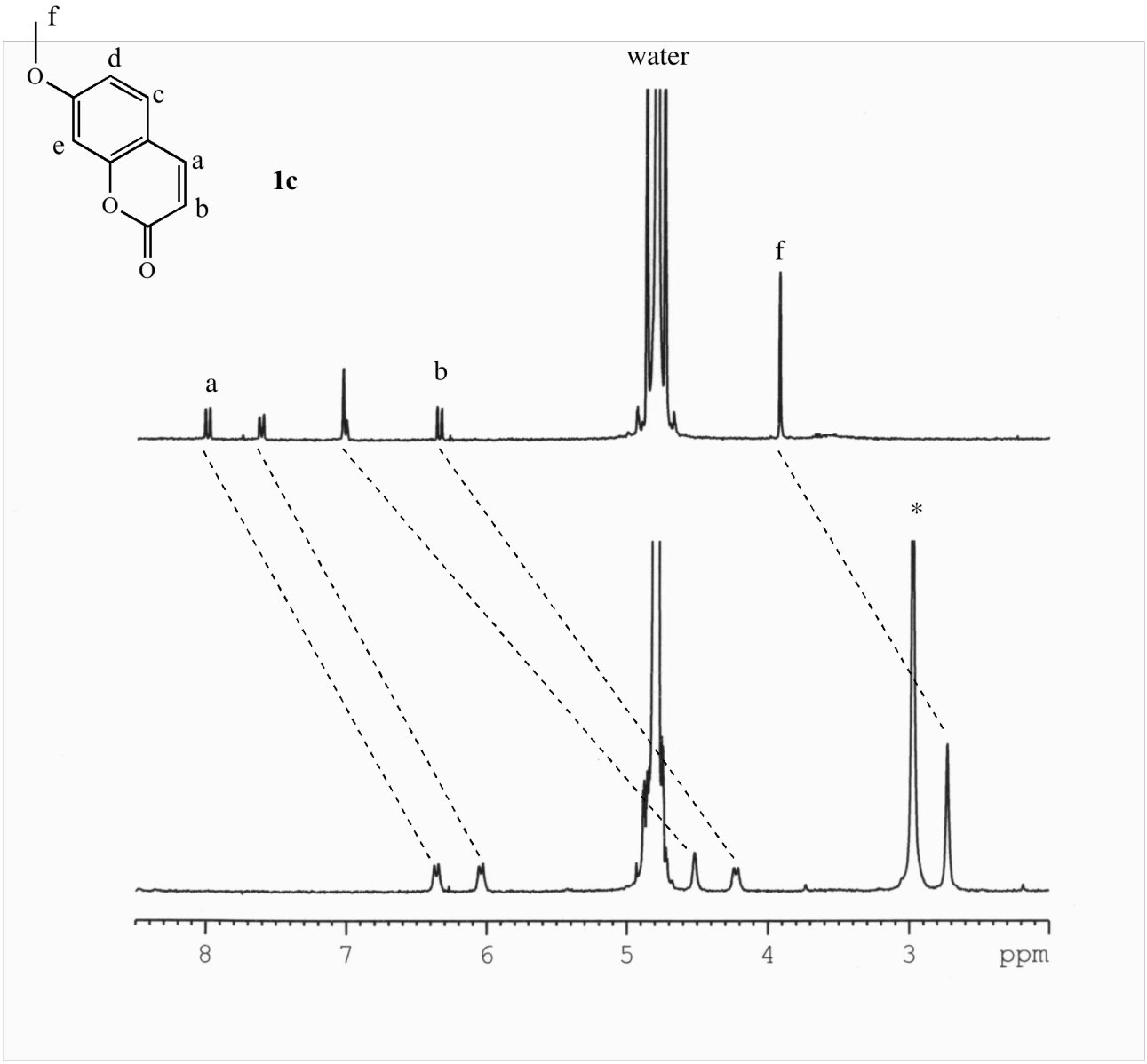

Figure S1 ^{1}H NMR (D_2O) spectra of **1c** in the absence (top) and in the presence of 0.5 equivalents of Pd-nanocage (bottom). The Pd-nanocage signal is indicated by *.

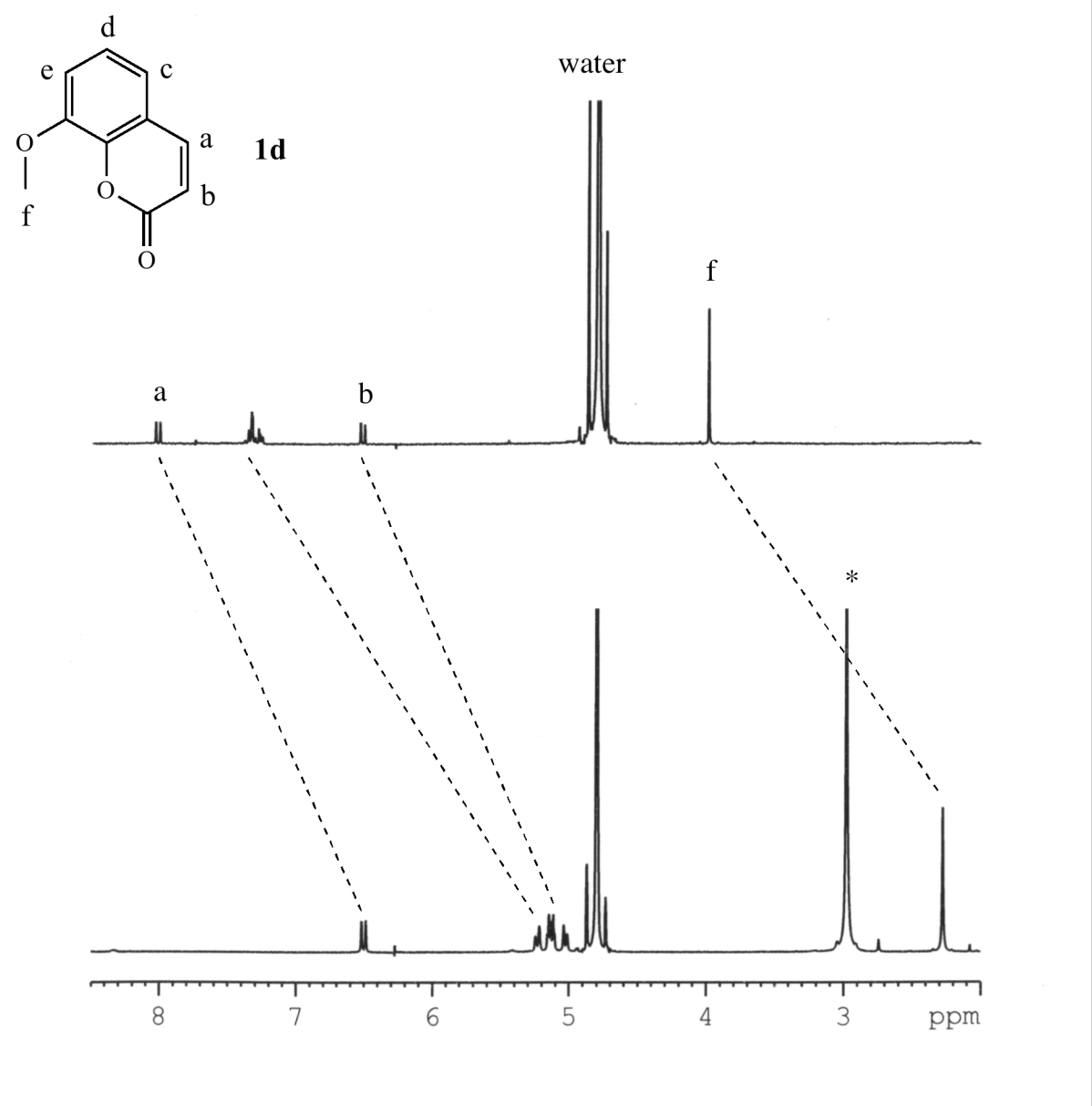

Figure S2 ^{1}H NMR (D_2O) spectra of **1d** in the absence (top) and in the presence of 0.5 equivalents of Pd-nanocage (bottom). The Pd-nanocage signal is indicated by *.

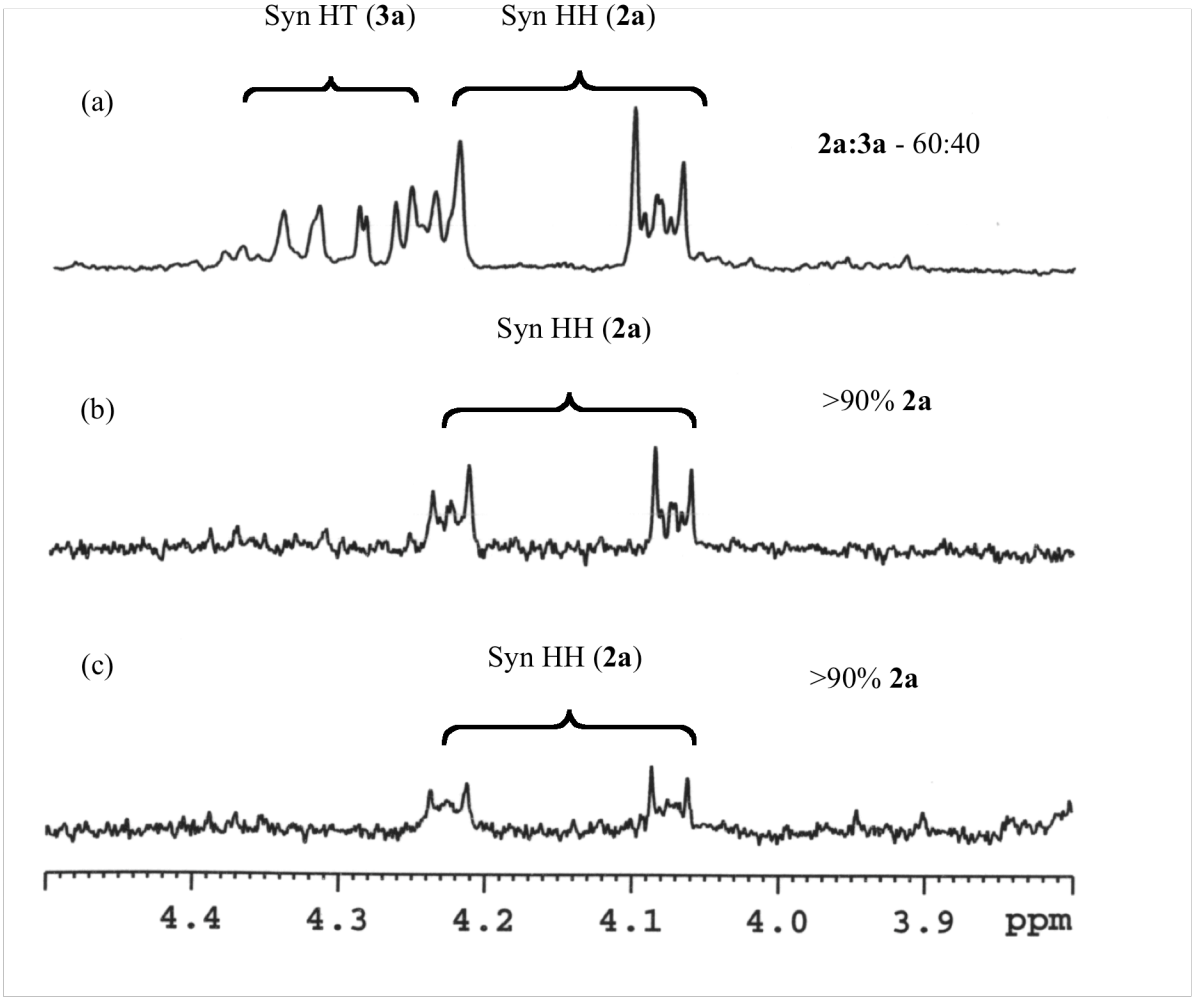

Figure S3 ^{1}H NMR ($CDCl_3$) spectra showing the cyclobutane region of the dimer obtained upon irradiation of **1a** in (a) water and as a host-guest complex having H:G ratios of (b) 1:6 and (c) 1:2.

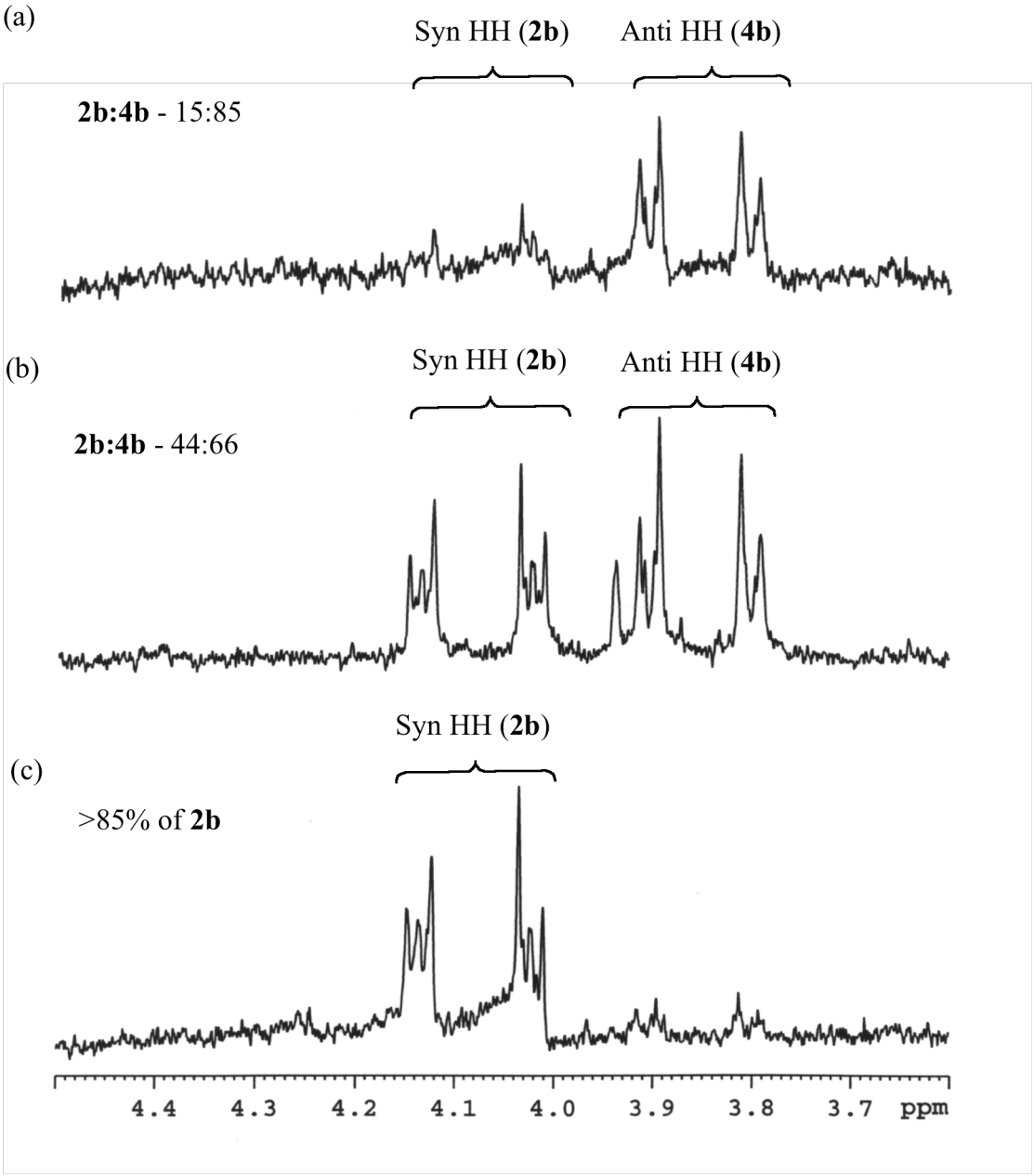

Figure S4 ^{1}H NMR ($CDCl_3$) spectra showing the cyclobutane region of the dimer obtained upon irradiation of **1b** in (a) water and as a host-guest complex having H:G ratios of (b) 1:6 and (c) 1:2.