Supplementary Information

Single-Component, Low Molecular Weight Organic Supergelators based on Chiral Barbiturate Scaffolds

Daniel T. Seidenkranz, Kurt A. Langworthy, Lev N. Zakharov, Michael D. Pluth*

Department of Chemistry and Biochemistry Materials Science Institute University of Oregon Eugene, OR 97403

Contact Information: Michael D. Pluth pluth@uoregon.edu

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Scheme S1. Synthesis of dibromomethylbinapthalene with (*R*)-stereochemistry shown.

NMR Spectra of Compounds 1-3

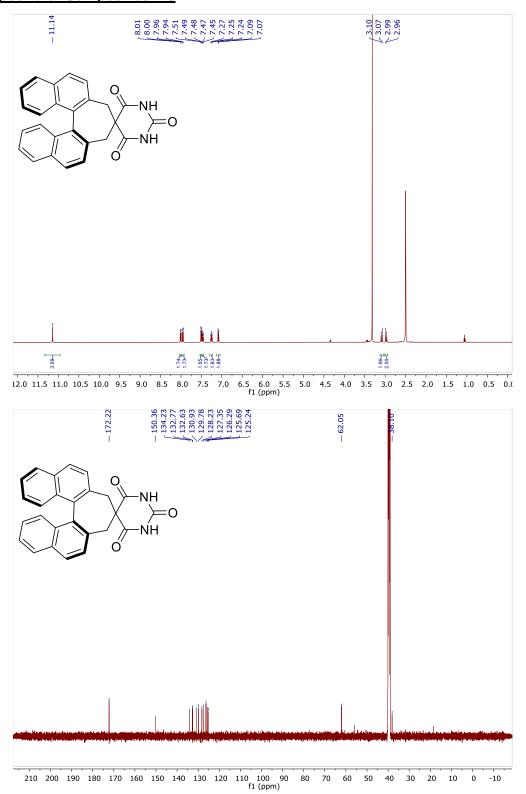


Figure S1. 1 H (500 MHz) and 13 C{ 1 H} (126 MHz) NMR spectra of **1a** in d_{6} -DMSO.

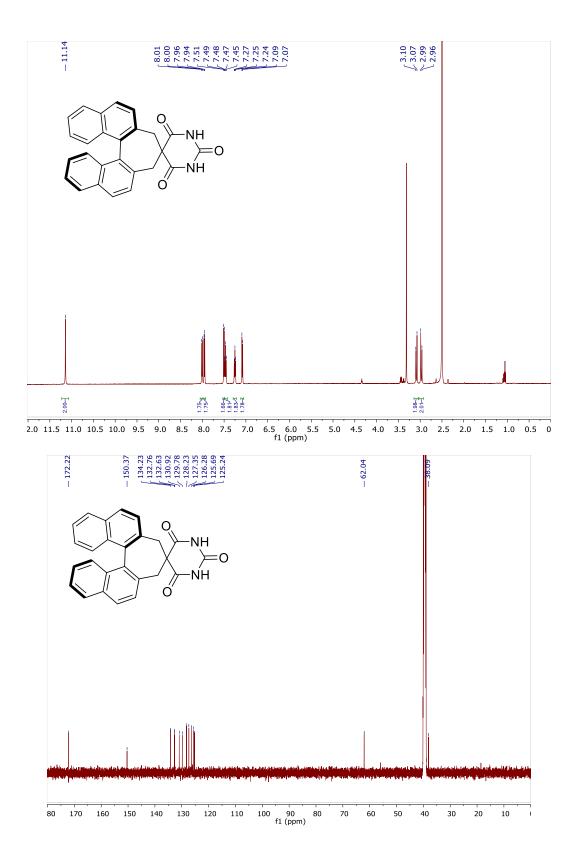


Figure S2. 1 H (500 MHz) and 13 C{ 1 H} (126 MHz) NMR spectra of 1b in d_{6} -DMSO.

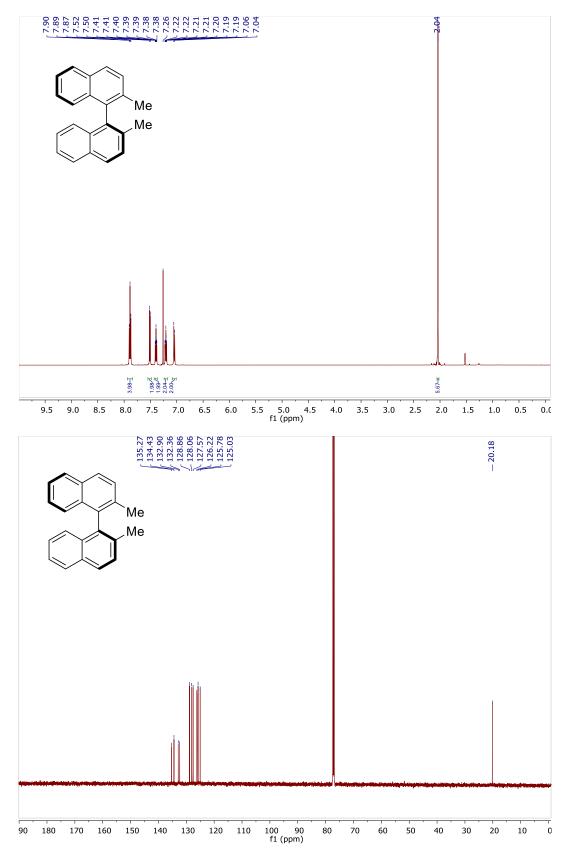


Figure S3. 1 H (500 MHz) and 13 C{ 1 H} (126 MHz) NMR spectra of 2 in CDCl₃.

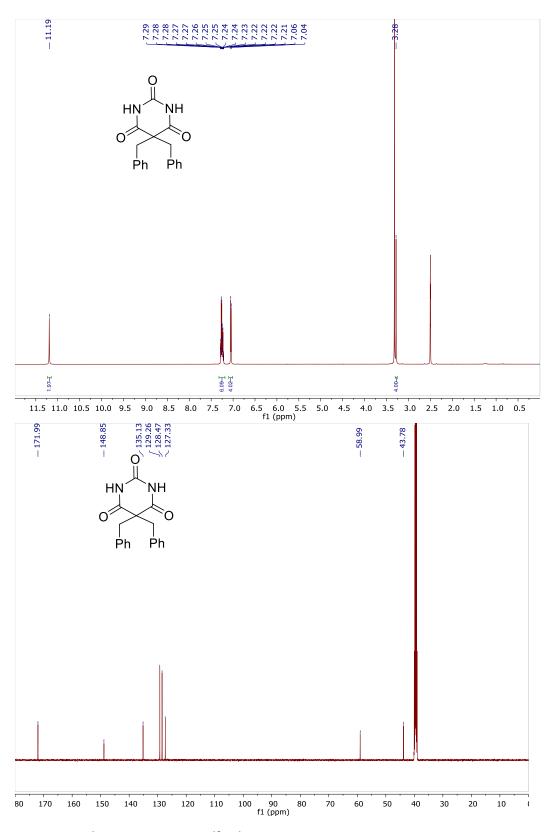


Figure S4. 1 H (500 MHz) and 13 C{ 1 H} (126 MHz) NMR spectra of **3** in d_{6} -DMSO.

Representative DOSY Plots and Fitting

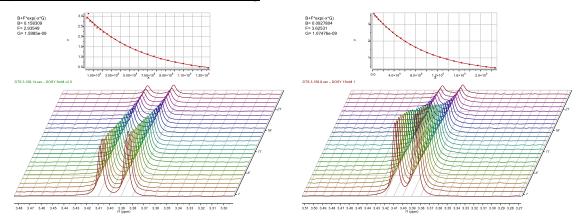


Figure S5: Representative exponential decay plots from DOSY experiments of **1a** at 5 mM (left) and 15 mM (right) showing doublet at 3.40 ppm and the corresponding exponential decay fits.

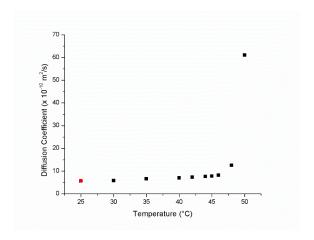


Figure S6. Variable temperature DOSY of a 20 mM gel sample of **1a** in CDCl₃. The black squares represent a sequential increase in temperature until the T_{gel} was reached. The red circle represents the diffusion coefficient after cooling the sample back to 25 °C from 50 °C.

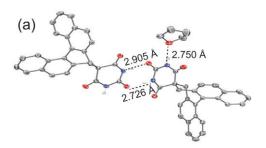


Figure S7. ORTEP representation of smallest repeat unit of **1b**. Thermal ellipsoids shown at 50% probability. Non-H bonding hydrogens omitted for clarity.

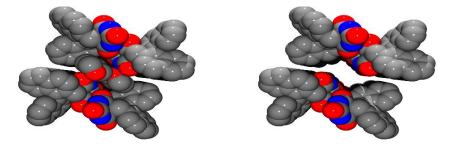


Figure S8. Space-filling representation of columnar stack of **1b** viewed down screw axis with (left) and without (right) THF co-solvent. H bonds omitted for clarity.