

Supporting Information

Porous 3-D Honeycomb architecture by self-assembly of helical H-bonded molecular tapes

Arnaud-Pierre Schaffner,^a Gersande Lena,^a Solveig Roussel,^{a,†} Anne Wawrezinieck,^{a,b} André Aubry,^c Jean-Paul Briand,^a Claude Didierjean,^{*c} and Gilles Guichard^{*a}

^a Immunologie et Chimie Thérapeutiques (ICT), UPR CNRS 9021
Institut de Biologie Moléculaire et Cellulaire, 15, rue Descartes, F-67084 Strasbourg (France).
Fax: +33 3 88 61 06 80; Tel: +33 3 88 41 70 25; E-mail: g.guichard@ibmc.u-strasbg.fr

^b Institut Charles Sadron, UPR CNRS 22, 6, rue Boussingault , BP 40016, F-67083
Strasbourg Cedex

^c LCM3B, UMR-CNRS 7036, Groupe Biocristallographie, Université Henri Poincaré, BP
239, 54506 Vandoeuvre (France). E-mail: Claude.Didierjean@lcm3b.uhp-nancy.fr

[†]Present address : Diverchim, Les Marches de l'Oise, 100 rue Louis Blanc, 60765 Montataire, France.

Figure S1. Difference map showing electron density inside the channels in crystals of **1a** grown from a dioxane/diisopropyl ether solution

Figure S2. Thermogravimetric plot showing the weight loss of crystals of **1a** (grown from dioxane/diisopropyl ether) on increasing temperature.

Figure S3. TEM negative stain imaging of **1a** (dioxane solution) deposited on a carbon-coated copper grid.

Figure S4. Concentration dependence of the chemical shifts of the N¹H and N³H protons of **1a** in CDCl₃ at 298K

Figure S5. Concentration dependence of the chemical shifts of the N¹H and N³H protons of **1a** in dioxane-d₈ at 298K

Figure S6. Species in the gas phase as determined by ESI-MS analysis of a solution of **1a**.

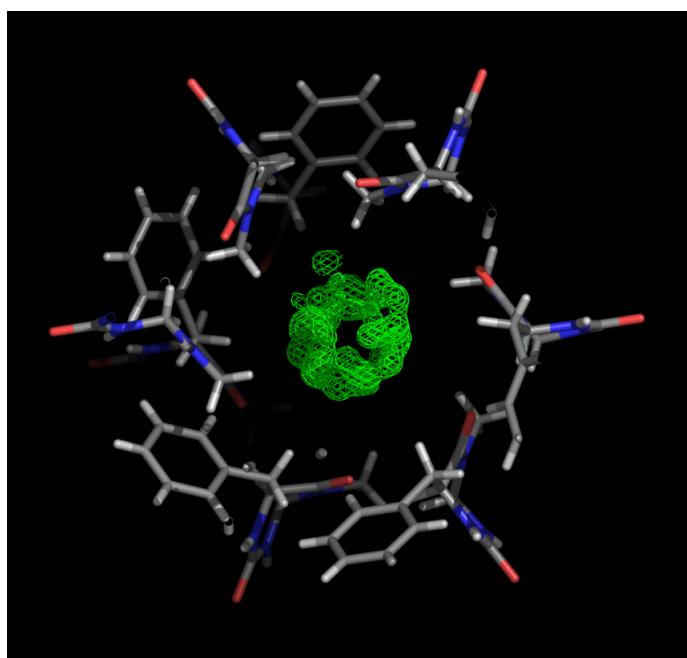


Figure S1. Difference map showing electron density inside the channels in crystals of **1a** grown from a dioxane/diisopropyl ether solution (Figure generated using Pymol, DeLano, W.L. The PyMOL Molecular Graphics System (2002) DeLano Scientific, San Carlos, CA, USA).

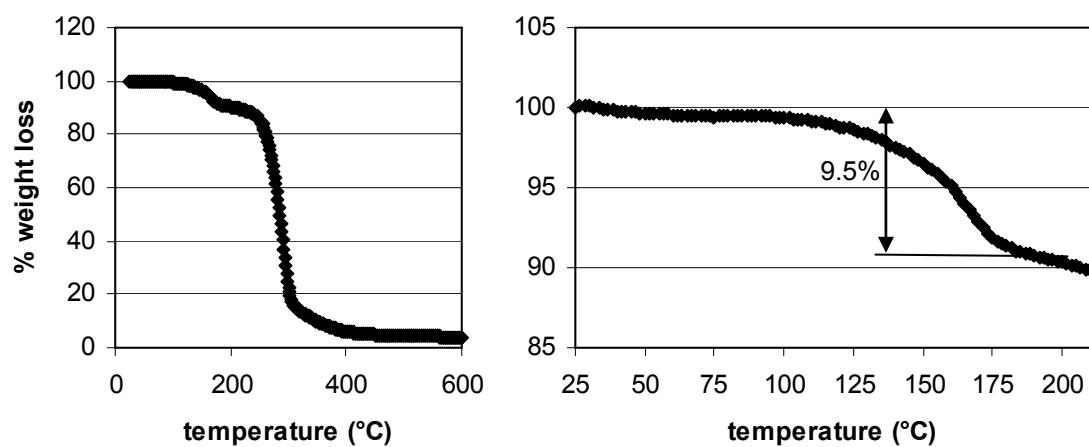


Figure S2. Thermogravimetric plot showing the weight loss of crystals of **1a** (grown from dioxane/diisopropyl ether) on increasing temperature. TGA analysis show a weight loss of 9.5 % in the temperature range of 25-195°C

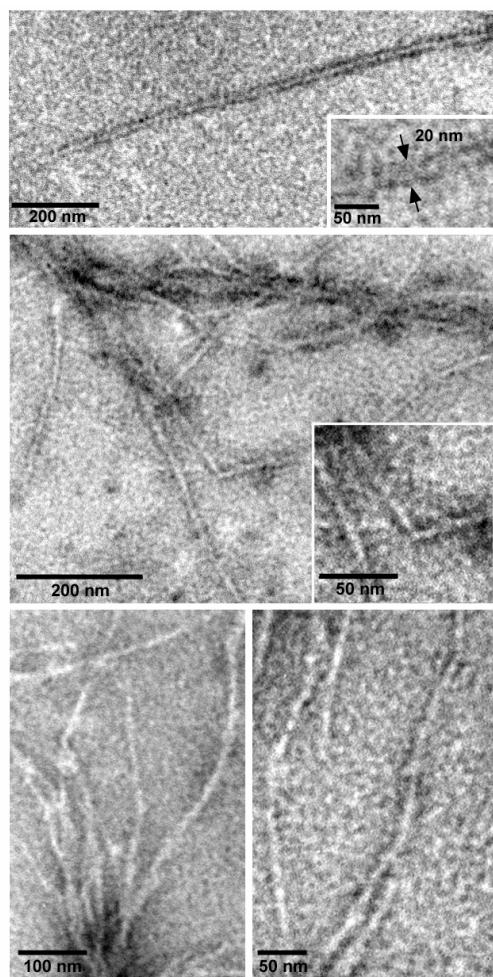


Figure S3. TEM negative stain imaging of **1a** (dioxane solution) deposited on a carbon-coated copper grid.
A $5\mu\text{L}$ drop of a 1mg/mL dioxane solution of **1a** was deposited on a carbon-coated copper grid and allowed to air-dry for 5 minutes. The sample was negatively stained with uranyl acetate before observation by transmission electron microscopy using a Phillips CM12 operating at 120kV (Amsterdam, The Netherlands)

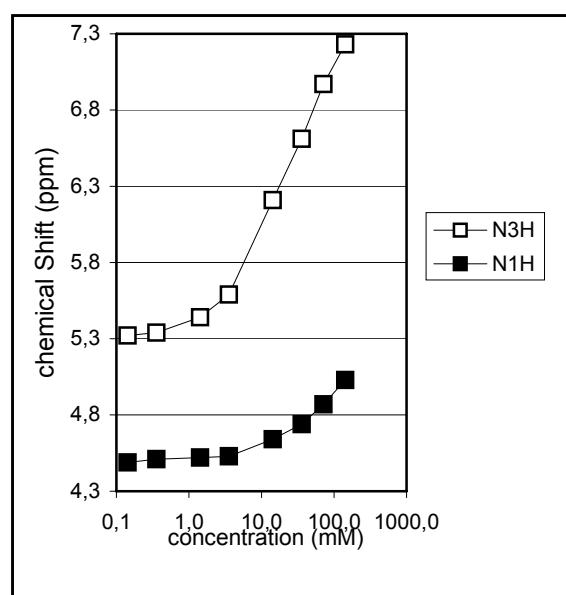


Figure S4. Concentration dependence of the chemical shifts of the N¹H and N³H protons of **1a** in CDCl₃ at 298K

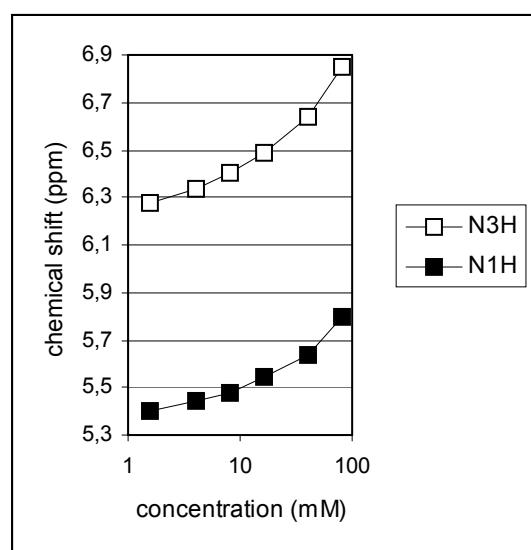


Figure S5. Concentration dependence of the chemical shifts of the N¹H and N³H protons of **1a** in dioxane-*d*₈ at 298K

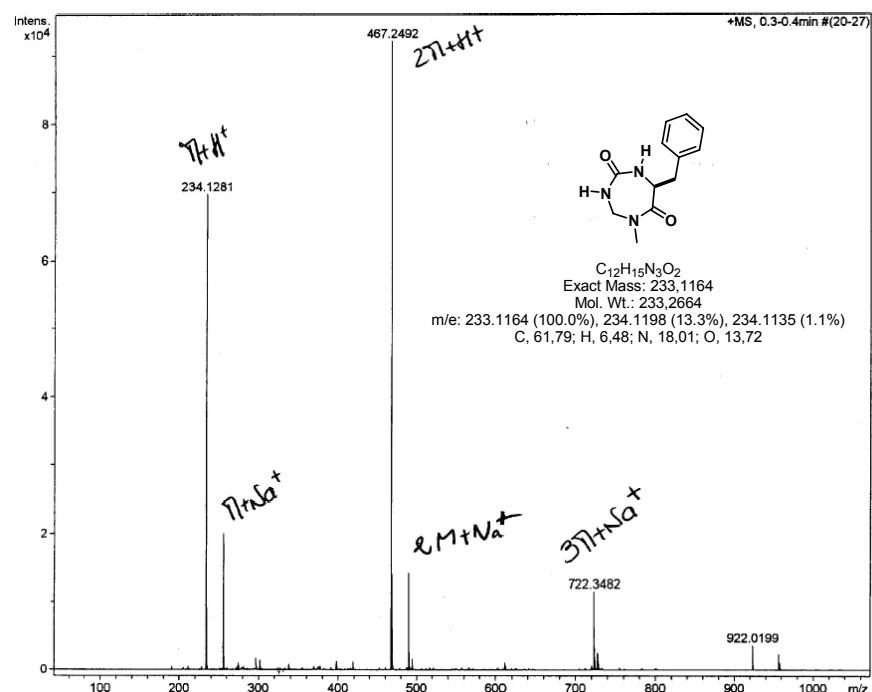


Figure S6. Species in the gas phase as determined by ESI-MS analysis of a solution of **1a**.