

Electronic Supplementary Information

Superstructure Based on β -CD Self-Assembly Induced by Small Guest Molecule

*Frederico B. De Sousa^{a,b}, Ana C. Lima^a, Ângelo M. L. Denada^c, Cleber P. A. Anconi^d,
Wagner B. De Almeida^e, Willian T. G. Novato^d, Hélio F. Dos Santos^d, Chester L Drum^b,
Robert Langer^{b*}, and Rubén D. Sinisterra^{a*}.*

^aLaboratório de Encapsulamento Molecular e Biomateriais (LEMB) – Departamento de Química, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais (UFMG), Belo Horizonte, 31270-901, MG, Brazil.

^bDepartment of Chemical Engineering, Massachusetts Institute of Technology (MIT), Cambridge, MA, 02139, USA.

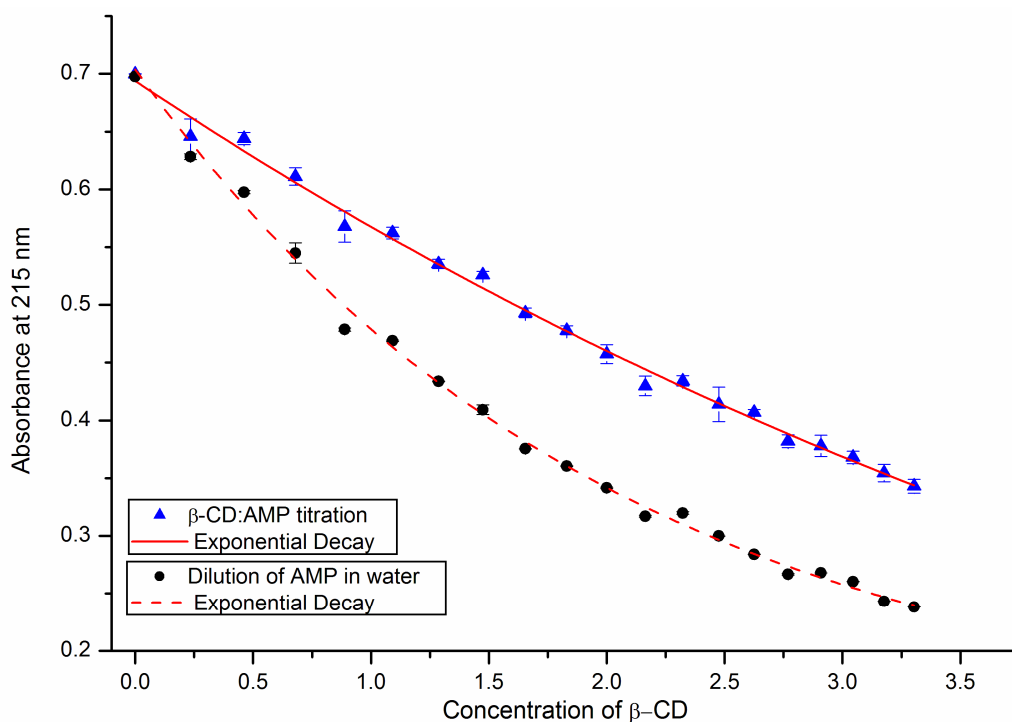
^cCentro Federal de Educação Tecnológica (CEFET-MG), Campus VII, Timóteo, MG, Brazil 35183-006.

^dNúcleo de Estudos em Química Computacional (NEQC), Departamento de Química, Instituto de Ciências Exatas, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora 36036-330, MG, Brazil.

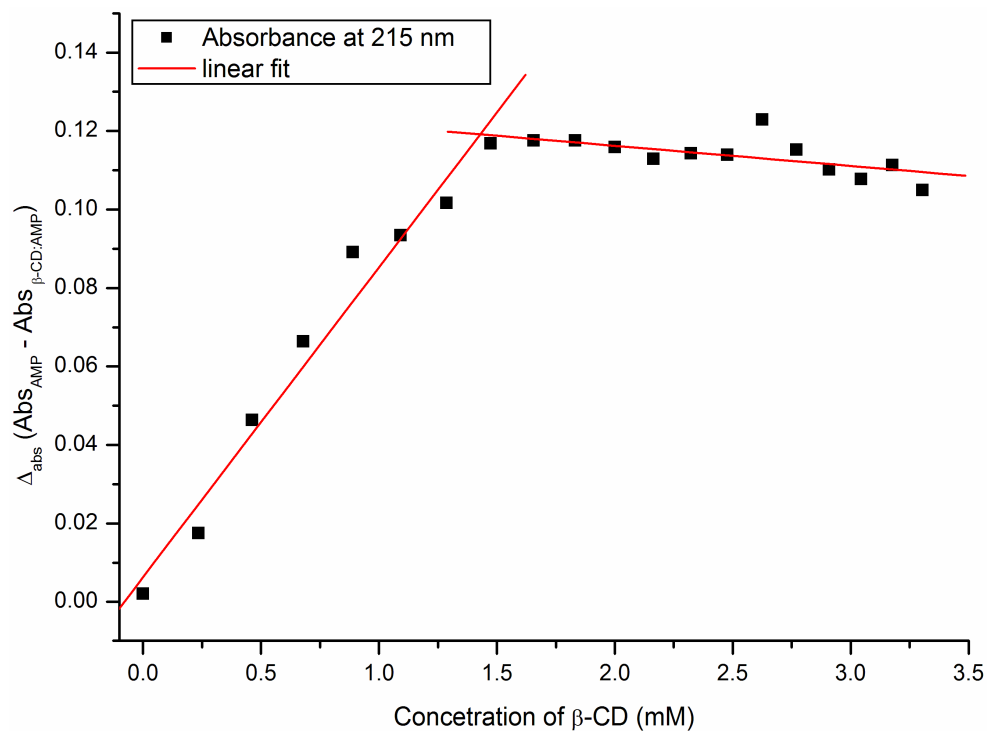
^eLaboratório de Química Computacional e Modelagem Molecular (LQC-MM), Departamento de Química, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais (UFMG), Belo Horizonte, 31270-901, MG, Brazil.

SI 1

UV-visible measurements for β -CD-Ampicillin system



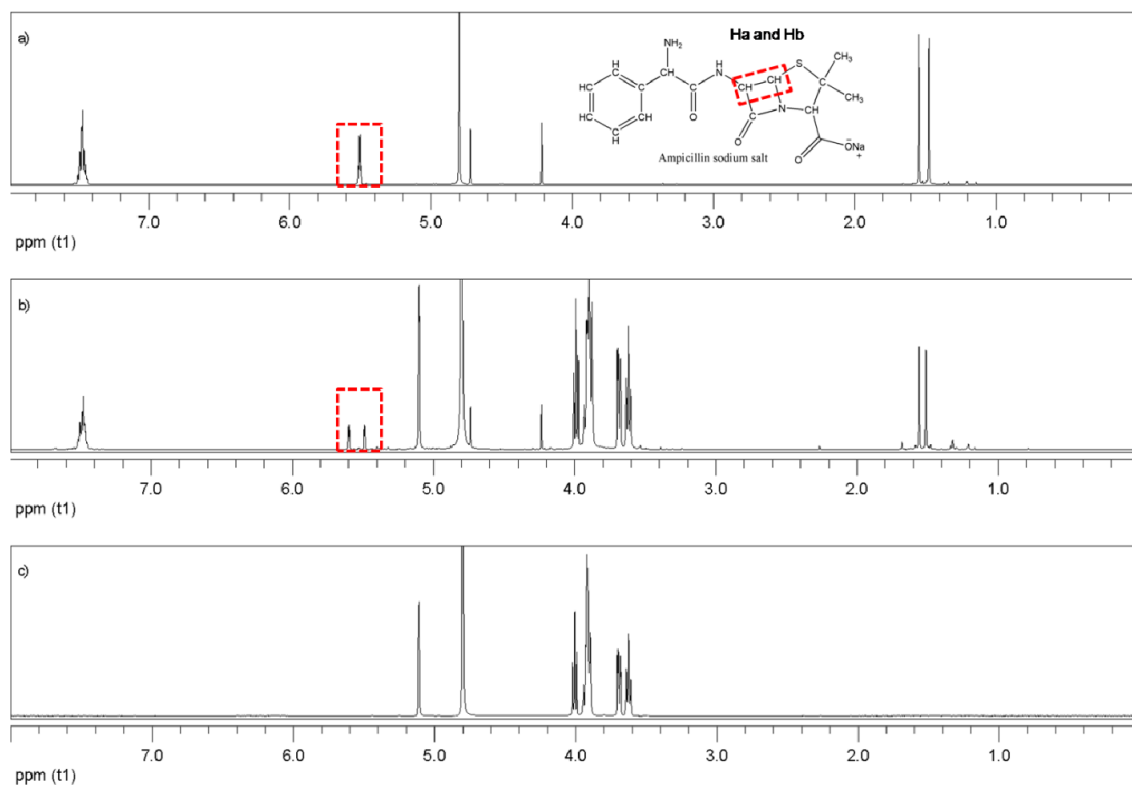
Titration curves and exponential decay adjust of: β -CD (12 mM) in AMP (6.7×10^{-2} mM) and AMP dilution process in water.



Δ_{abs} curve at 215 nm from β -CD (12.0 mM) titration in AMP (6.7×10^{-2} mM).

SI 2

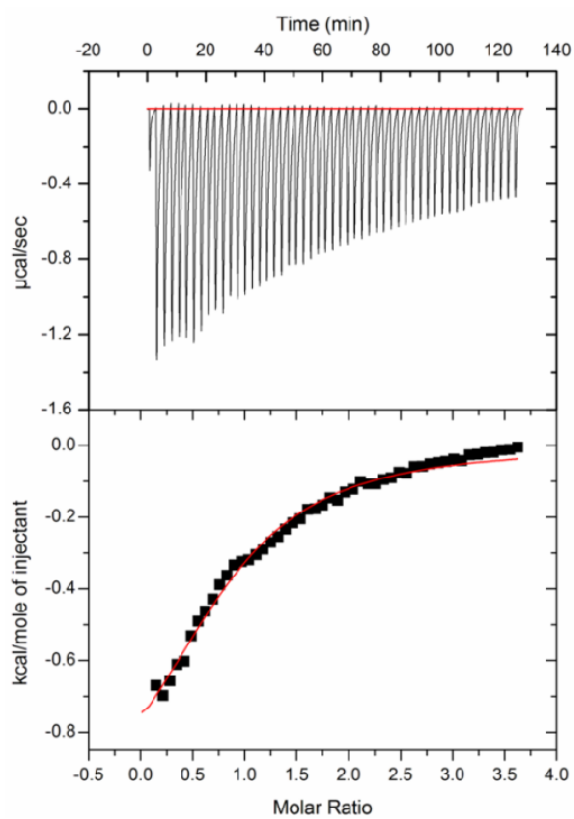
Nuclear Magnetic Resonance



^1H NMR spectra at 600 MHz in D_2O at 30 °C to: a) Ampicillin sodium salt, b) β -CD and c) β -CD:AMP at 1:1 molar ratio.

SI 3

Isothermal Titration Calorimetry



ITC final figure for AMP at 20.0 mM and β -CD at 1.0 mM titration at 25 °C.

SI 4

Distinct arrangement for β -CD:AMP considered in the present work as starting structures for MD simulation.

