BIOMIMETIC OXIDATION OF CARBAMAZEPINE WITH HYDROGEN PEROXIDE CATALYZED BY A MANGANESE PORPHYRIN

Cláudia M. B. Neves, Mário M. Q. Simões*, Fernando M. J. Domingues, M. Graça P. M. S. Neves e José A. S. Cavaleiro Departamento de Química, QOPNA, Universidade de Aveiro, 3810-193 Aveiro, Portugal



Figure 1S. TLC of the free-base 5,10,15,20-tetrakis(2,6-dichlorophenyl)porphyrin (1) after crystallization using CH₂Cl₂ as eluent

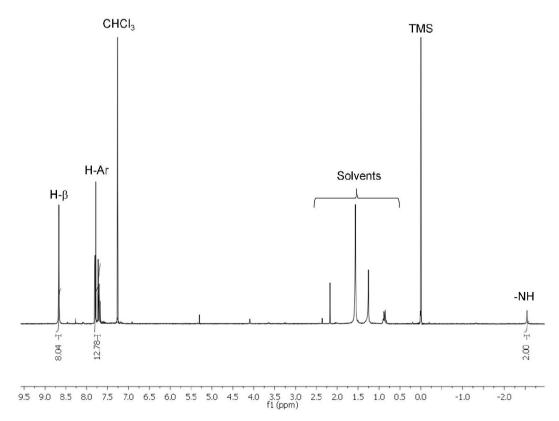


Figure 2S. ¹H NMR spectrum of the 5,10,15,20-tetrakis(2,6-dichlorophenyl)porphyrin (1) using CDCl₃ as solvent

Neves et al.

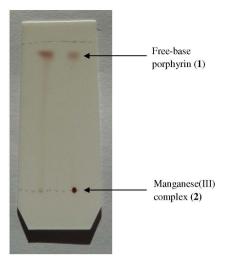


Figure 3S. Monitoring of the reaction progress (session 2) by TLC after one hour. A new red spot of manganese(III) complex (2) can be observed at the base, in contrast with the brown spot of the free-base porphyrin (1) in the top of the TLC plate, using CH_2Cl_2 as eluent

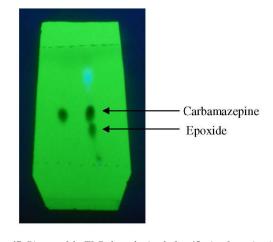


Figure 4S. Picture of the TLC plate obtained after 45 min of reaction (session 3). The carbamazepine spot is at the left and the reaction mixture is at the right, with the formation of a new spot corresponding to the epoxide product, using ethyl acetate as eluent

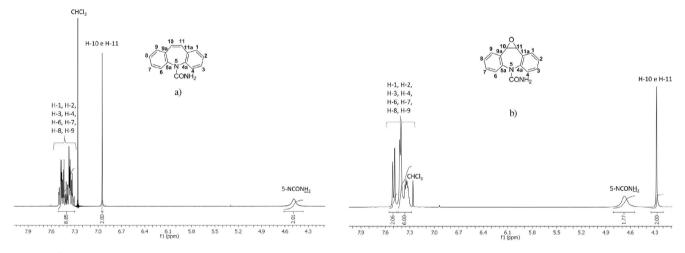


Figure 5S. ¹H NMR spectra (CDCl₃) of a) carbamazepine (3); b) carbamazepine 10,11-epoxide (4)