

XII ENCONTRO NACIONAL DE QUÍMICA-FÍSICA  
I SIMPÓSIO DE QUÍMICA COMPUTACIONAL

JUNHO 2016  
UNIVERSIDADE DE ÉVORA

<sup>a,b</sup>Bebiana Pinto, <sup>c</sup>Ana S. Viana, <sup>a</sup>M. Helena Garcia, <sup>b</sup>Paulo J. Mendes, <sup>a</sup>Andreia Valente

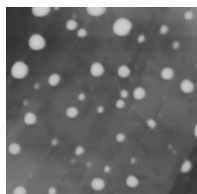
<sup>a</sup>Centro de Química Estrutural, Faculdade de Ciências da Universidade de Lisboa, Lisboa, Portugal, [bebianapinto9@gmail.com](mailto:bebianapinto9@gmail.com)

<sup>b</sup>Departamento de Química, Escola de Ciências e Tecnologia, Centro de Química de Évora, Instituto de Investigação e Formação Avançada, Universidade de Évora, Évora, Portugal

<sup>c</sup>Centro de Química e Bioquímica, Faculdade de Ciências da Universidade de Lisboa, Lisboa, Portugal

Cancer is a leader cause of death worldwide. One of the problems associated with the current chemotherapeutic options is the noxious side effects caused by the lack of selectivity. In this frame, our research group has been committed to the development of a new Ru and Fe macrometallodrugs.[1] The data obtained so far shows that these compounds present an intrinsic selectivity towards cancer cells (relatively to healthy cells) due to the incorporation of polymeric ligands that promote a passive targeting through the cancer cell membrane. These results prompted us to the development of new macrometallodrugs bearing bioessential metals such as Fe, Zn and Co. We used a 'M(bipy)<sub>3</sub>' scaffold (bipy = 2,2'-bipyridine derivatives) for the synthesis of the new compounds due to the promising cytotoxicity results observed for related compounds.[2] As polymeric ligands we have chosen the polylactide-co-polyethylene glycol amphiphilic copolymer that is able to self-assemble into micelles in water, keeping the metal center hidden, like a Trojan horse. We will present the synthesis and characterization of the new compounds and some preliminary data on their ability to form stable micelles (Figure 1).

*The authors thank the COST action CM1302 (SIPs) and The Portuguese Foundation for Science and Technology (as well as POPH and FSE), within the scope of the projects IF/01302/2013 and UID/QUI/00100/2013.*



**Figure 1.** AFM image of the new iron macrometallodrug obtained in a highly oriented pyrolytic graphite surface ( $3 \times 3 \mu\text{m}^2$ ;  $z = 35 \text{ nm}$ ).

[1] a) A. Valente, M.H. Garcia, F. Marques, Y. Miao, C. Rousseau, P. Zinck, J. Inorg. Biochem., **127**, 79-81 (2013). b) M.H. Garcia, A. Valente, T.S. Morais, A.I. Tomaz, Patent Application PCT/IB2015/002312.

[2] K.W. Tan, H.L. Seng, F.S. Lim, S.-C. Cheah, C.H. Ng, K.S. Koo, M.R. Mustafa, S.W. Ng, M.J. Maah, Polyhedron, **38**, 275–84 (2012).