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Revisiting INH: QSAR-based design of new anti-tubercular compounds

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Tuberculosis (TB) ranks as the second leading cause of death from a single infectious agent, the *Mycobacterium tuberculosis* (*Mtb*). WHO reports 8.6 million new TB cases and 1.3 million deaths worldwide in 2012. The emergence of multidrug resistant (MDR-TB) and extensively drug-resistant tuberculosis (XDR-TB) has reduced considerably the number of available drugs for treatment, making the quest for "new", effective and non-toxic drugs a major concern. Despite the significant progresses made in the last ten years in the development of new anti-TB drugs, with several compounds reaching phases 2 and 3 of the clinical pipeline, the truth is that isoniazid (INH), firstly synthesized in 1952, remains one of the most effective drugs to treat TB. Any new compound derived from INH that proves to be active against several forms of tuberculosis, would certainly be less problematical than totally new compounds with unknown long-term effects as those recently introduced in therapeutic combination regimens. In this work we show how a judicious and well-validated QSAR methodology can be used to successfully design new INH-based derivatives with better activitiesthan the parent compound against both susceptible and resistant *Mtb* strains. Also, some evidences will be presented that question the putative increase in resistance of *katG* (S315T) towards INH, when compared with *wtkatG*.

Biography

Filomena Martins has obtained her PhD at the University of Lisbon in 1993. She did postdoctoral work with Prof. Michael Abraham at the University College London and Dr. Robert Mitchell at SmithKline Beecham Pharmaceuticals at Welwyn, Hertfordshire, UK. She is currently Assistant Professor at the University of Lisbon where she is responsible for the Structure and Reactivity Group of the Chemistry and Biochemistry Centre. Her present research interests include the development of judicious and well validated quantitative structure-property relationships (QSPRs) to design (and synthesize) new molecules with better biological or physicochemical performance. She has more than 40 publications in the areas of Physical and Medicinal Chemistry.

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