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Theoretical study on a newly approved pharmaceutical formulation active components-Indacaterol and Roflumilast

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Indacaterol (In) is 5-[(1R)-2-[(5,6-diethyl-2,3-dihydro-1H-inden-2-yl)amino]-1-hydroxyethyl]-8-hydroxy-2(1H)-quinolinone maleate. Roflumilast (Ro) (3-cyclopropylmethoxy-4-difluoromethoxy-N-[3,5-dichloropyridyl]-benzamide) (Fig. 1). They have been approved for chronic obstructive pulmonary disease (COPD) [1]. According to the World Health Organization (WHO), more than 200 million people have moderate-to-severe COPD worldwide [2]. It is in urgent need of the theoretical properties and structure-activity relationship information for Indacaterol and Roflumilast. These are searched by DFT method with Gaussian09 program (B3LYP/6-311++G(d,p)).

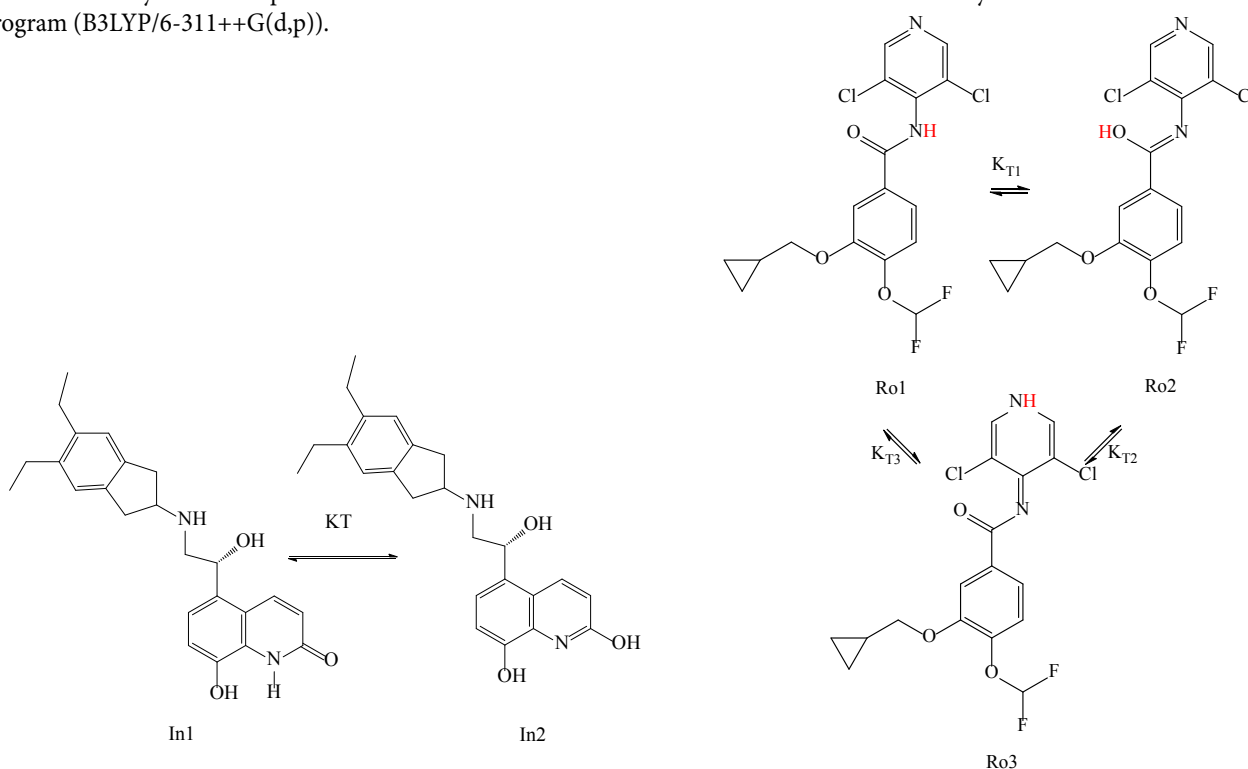


Fig. 1. Chemical structure of Indacaterol (In), Roflumilast (Ro) and their tautomers.

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