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Synthesis, characterization, and *in silico* analysis against SARS CoV-2 of novel benzimidazolium salts

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Abstract. In acute conditions, vaccines are very important, although they provide antibodies for fighting against COVID-19 for a certain period. It is necessary to produce an anti-viral agent for a usual healing process against SARS CoV-2 which is responsible the pandemic we are living in. Many drugs with benzimidazole main scaffold are still used in a wide variety of treatment procedures. In this case, substituted benzimidazole structures could be good candidates for fighting against COVID-19. Theoretical calculation methods could be a key tool for overcome the difficulties of individual analyzing of each new structure. In this study, new benzimidazole structures were synthesized and characterized for *in silico* evaluation as anti-viral agent. The molecules were optimized and analyzed for reactivity with Koopmans Theorem. Also, molecular docking simulations were performed for SARS coronavirus main peptidase (PDB ID: 2GTB), COVID-19 main protease (PDB ID: 5R82), and papain-like protease of SARS CoV-2 (PDB ID: 6W9C) crystals.

***Keywords*:** benzimidazolium; molecular docking; COVID-19; global reactivity descriptors.

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