# Synthesis of boronic acid derivatives designed as SARS-CoV-2 MPro inhibitors

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## Abstract

Identification of new targets for SARS-CoV-2 virus allow the development of novel therapeutic approaches [1]. Among those targets, the inhibition of the main cysteine protease, named Mpro (3CLpro), interfered in the viral replication and transcription [2]. FL-166, a bi-functionalized boronic acid derivative, exhibited potent inhibition of SARS-CoV Mpro (Ki = 0,04 μM) [3]. Considering the similarity between SARS-CoV-2 and SARS-CoV MPro, in this work we designed new boronic acid derivates in order to investigate their role as inhibitors of SARS-CoV-2 Mpro. Exploring molecular optimization assisted by molecular modelling, we have synthesized four main class of compounds: amides, esters, carbonyl-alpha-beta-unsaturated and N-acyl hydrazones. All compounds were synthesized at yields ranging from 12 to 30 % and characterized by analytical methods. Docking studies have shown docking scores values ranging from -4.30 to -5.11. All these data suggest that boronic acid derivatives could be explored as prototypes to design new SARS-Cov-2 Mpro inhibitors



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## Keywords

boronic acids

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