New Results

Hijacking SARS-Cov-2/ACE2 receptor interaction by natural and semi-synthetic steroidal agents acting on functional pockets on receptor binding region

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Abstract

The coronavirus disease 2019 (COVID-19) is a respiratory tract infection caused by the severe acute respiratory syndrome coronavirus (SARS)-CoV-2. In the light of the urgent need to identify novel approaches to be used in the emergency phase, a largely explored strategy has been the repurpose of clinically available drugs as new antivirals, by targeting different viral proteins. In this paper, we describe a drug repurposing strategy based on a virtual screening of druggable pockets located in the central β-sheet core of the SARS-CoV-2 Spike protein RBD supported by in vitro tests identifying several steroidal derivatives as SARS-CoV-2 entry inhibitors. Our results demonstrate that several potential binding sites exist in the SARS CoV-2 S protein, and that the occupancy of these pockets reduces the ability of the S protein RBD to bind to the ACE2 consensus in vitro. In particular, natural occurring and clinically available steroids as

load. All together, these results might help to define novel approaches to reduce the viral load by using SARS-CoV-2 entry inhibitors.

Competing Interest Statement

This paper was supported by a research grant by BAR Pharmaceuticals S.r.L. to the Department of Pharmacy of the University of Napoli Federico II and to the Department of Surgical and Biomedical Sciences, University of Perugia. The authors declare the following competing financial interest(s): S.F., A.Z. and B.C. have filed an Italian patent application no.102020000011092 in the name of BAR Pharmaceuticals S.r.L. on the compounds described in this paper.

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