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Identification of Potential SARS-CoV-2 Inhibitors: A selected Natural Compounds Targeting RNA-dependent-RNA Polymerase Activity, and Binding Affinity of the Receptor-binding Domain (RBD)

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SUMMARY. **Coronavirus disease (COVID-19) is caused by SARS-CoV-2 and represents the causative agent of a potentially lethal disease. COVID-19 has been described as a significant global public health pandemic by the World Health Organization due to its high mortality rate, rapid spread, and the lack of drugs. Active antiviral drugs are desperately needed to combat the potential return of severe acute respiratory syndrome (SARS). In this study, we selected 39 natural compounds present in plants, algae, and sponges with antiviral activity. Molecular docking was used to screen the compounds' activity on SARS- CoV-2 RNA-dependent-RNA polymerase, receptor-binding domain (RBD), and the human ACE2 receptor. Compounds with binding energy less than -6.5 kcal/mol enter pre-clinical testing using insilco ADME/Tox (absorption, distribution, metabolism, excretion, and toxicity). We found eight potential SARS-CoV-2 inhibitors: (glycyrrhizin, rutin, baicalin, 1, 6-di-O- galloyl-beta-D-glucose, pyropheophorbide A, pheophorbide A, beta-Sitosterol, and vitexin). These outcomes indicate that these compounds could be potential candidates to be utilized for the design and production of the anti-SARS-CoV-2 drug.**

RESUMEN. La enfermedad por coronavirus (COVID-19) es causada por el SARS-CoV-2 y representa el agente causal de una enfermedad potencialmente letal. La COVID-19 ha sido descrita como una importante pandemia mundial de salud pública por la Organización Mundial de la Salud debido a su alta tasa de mortalidad, su rápida propagación y la falta de medicamentos. Se necesitan desesperadamente medicamentos antivirales activos para combatir el posible regreso del síndrome respiratorio agudo severo (SARS). En este estudio, seleccionamos 39 compuestos naturales presentes en plantas, algas y esponjas con actividad antiviral. El acoplamiento molecular se utilizó para evaluar la actividad de los compuestos en la polimerasa de ARN dependiente de ARN del SARS-CoV-2, el dominio de unión al receptor (RBD) y el receptor ACE2 humano. Los compuestos con energía de enlace inferior a -6,5 kcal/mol entran en pruebas preclínicas utilizando insilco ADME/Tox (absorción, distribución, metabolismo, excreción y toxicidad). Encontramos ocho posibles inhibidores del SARS-CoV-2: (glicirricina, rutina, baicalina, 1, 6-di-O-galoil-beta-D-glucosa, pirofeoforbida A, feoforbida A, beta-sitosterol y vitexina). Estos resultados indican que estos compuestos podrían ser candidatos potenciales para ser utilizados en el diseño y la producción del fármaco anti-SARS-CoV-2.

KEY WORDS: antiviral agents, coronavirus, molecular docking, natural compounds, SARS-COV2.

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