In Silico Molecular Docking and ADMET analysis of compounds isolated from Neocarya macrophylla against three targets of SARS CoV-2 coronavirus

Amina Yusuf Jega¹, Musa Ismail Abdullahi¹, Aliyu Muhammad Musa¹, Hassan Abubakar², Abubakar Muhammad Amali¹

¹Department of Pharmaceutical and Medicinal Chemistry, Usman Danfodiyo University, Sokoto, Nigeria
²Department of Pharmacology and Toxicology, Ahmadu Bello University, Zaria, Nigeria

Introduction
The novel corona virus disease (COVID-19) which emerged in China is a highly transmittable and pathogenic viral infection caused by the SARS-CoV-2; the disease has been declared by WHO as a public health emergency of international concern. The unavailability of approved therapeutic agents or vaccines is of great concern. The aim of this study was to perform molecular docking and ADMET analysis of some compounds isolated from Neocarya macrophylla against three targets of SARS CoV-2 proteins (3C-like protease, spike protein and papain-like protease).

Materials and Methods

Results and Discussion

Molecular docking
The four compounds (catechin, catechin-3-rhamnoside, epicatechin and quercetin) isolated from N. macrophylla were screened against three important protein targets of SARS CoV-2 including main protease, spike protein and papain-like protease by conducting a molecular docking analysis using AutoDock Vina tools in PyRx. The docking scores and interactions of the four ligands at the active site of the three proteins are shown in Table 1 and Figures 1 – 3. The ADMET and drug-likeness results indicated that all the compounds have satisfied the limitations and drug-likeness.

Table 1: Docking scores of the compounds against three targets proteins of SARS CoV-2

<table>
<thead>
<tr>
<th>Compound name</th>
<th>Compound ID</th>
<th>Main protease</th>
<th>Spike protein</th>
<th>Papain-like protease</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catechin</td>
<td>9064</td>
<td>-7.0</td>
<td>-6.6</td>
<td>-6.4</td>
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<td>Catechin-3-rhamnoside</td>
<td>21626704</td>
<td>-8.0</td>
<td>-7.1</td>
<td>-6.9</td>
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<td>Epicatechin</td>
<td>72276</td>
<td>-6.9</td>
<td>-6.3</td>
<td>-7.1</td>
</tr>
<tr>
<td>Quercetin</td>
<td>528043</td>
<td>-6.9</td>
<td>-6.7</td>
<td>-7.0</td>
</tr>
</tbody>
</table>

Some References
3. Peterson L. In Silico Molecular Dynamics Docking of Drugs to the Inhibitory Active Site of SARS-CoV-2 Protease and Their Predicted Toxicology and ADME. Preprint at RR. 2820. doi:10.13140/RS.2.2.17897.83045.