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## Biophysical Properties of the Essential Flavaglines as Antiviral

Agents JINSEO LEE, RICHARD KYUNG, CRG-NJ — Instead of synthetic polymers and other inorganic particulates, scientists are now focusing on multimodal nano-scaled molecules as antiviral agents. The new molecules can reduce the Reactive Oxygen Species (ROS) in affected cells which can have detrimental effects, such as stressing and damaging the cell structures. In this paper, Flavaglines, which is a common name of cyclopenta[b]benzofurans found in plants of the genus Aglaia, were theoretically and computationally analyzed to assess their pharmacological activities. Antiviral effects against several types of viruses including severe acute respiratory syndrome coronavirus were also biophysically studied. To find optimized energy of the molecules, an auto optimize tool which continuously optimizes molecular geometry through molecular mechanics was employed. Also the electrostatic potential maps were calculated to visualize charge distribution and other charge related properties of molecules. Finally, dipole moments which are caused by different values of electronegativity of different atoms in a molecule were calculated. Calculations show a few compounds converge easily, which makes them suitable to use as biochemical compounds in the antiviral agents.

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