

Withania somnifera Phytochemicals Confer Neuroprotection by Inhibition of Rho-associated Kinase-2 Catalytic Domain †

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Abstract: Cerebral Stroke is the leading cause of death and disability worldwide. Brain damage by ischemic stroke is led by a complex cascade of events. The Rho-associated kinase-2 (ROCK2) plays an important role in cerebral vasospasm, vascular remodeling, and inflammation. It is activated in cerebral ischemia, and its inhibition leads to a neuroprotective effect. The present study is designed to identify potential inhibitors of ROCK2 using a molecular docking approach. We docked phytochemicals of *Withania somnifera* (WS) into the catalytic site of ROCK2 and compared results with inhibitor Y-27632. ADME and drug-likeness properties of WS phytochemicals were also analyzed. Results suggest that 11 phytochemicals exhibited higher binding affinity toward the ROCK2 catalytic domain compared to Y-27632 inhibitor. These phytochemicals formed H-bonding and established hydrophobic contacts with catalytic residues of ROCK2. These results provide strong evidence that WS phytochemicals confer neuroprotection by inhibition of ROCK2 during ischemic insult. Thus, our findings suggest that WS phytochemicals can be developed as a therapeutic agent to combat cerebral stroke.

Keywords: Cerebral Stroke; *Withania somnifera*; Rho-associated Kinase-2 inhibition;

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Conflicts of Interest

The authors declare no conflict of interest.