SARS-CoV-2 Spike Protein Interaction with Monoamine Oxidase B: Implications for Neurodegeneration

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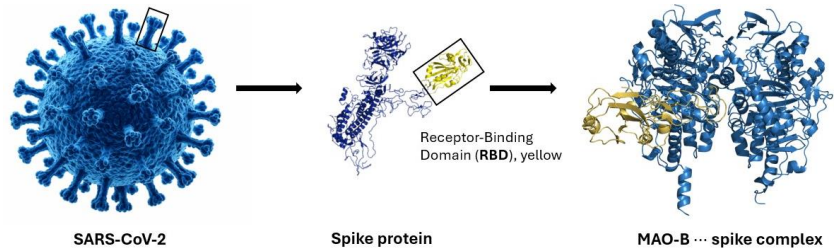
COVID-19, caused by **SARS-CoV-2**, is primarily a respiratory disease but is also associated with neurological complications. One proposed mechanism involves interactions between viral components and monoamine oxidase (**MAO**) enzymes [1]. Here, we investigate the binding of the SARS-CoV-2 spike protein to monoamine oxidase B (**MAO-B**), hypothesizing disruption of monoaminergic homeostasis and potential links to neurodegeneration [2].

An integrated computational approach combining molecular docking, molecular dynamics (**MD**) simulations, and **MM-GBSA** calculations was used to characterize MAO-B· · · spike interactions. Multiple high-affinity binding sites were identified, with stable binding observed in MD simulations and significant effects on binding energetics of substrates and inhibitors, suggesting interference with MAO-B function.

Overall, the findings indicate a potential molecular basis for SARS-CoV-2-induced disruption of monoaminergic signaling, warranting further investigation [3,4].



Research Rationale

Spike protein can bind to **MAO-B**, impacting its activity and altering neurotransmitter levels. This disruption suggests increased risk for neurodegenerative diseases.

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References:

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