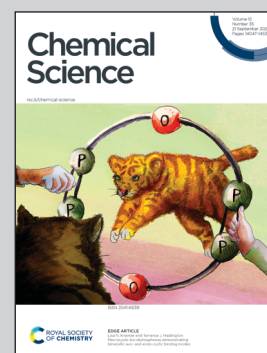


Showcasing research from Professor Jean-Philip Piquemal's group, Department of Chemistry, Sorbonne Université, Paris, France, and from Qubit Pharmaceuticals, Paris, France.

Water-glycan interactions drive the SARS-CoV-2 spike dynamics: insights into glycan-gate control and camouflage mechanisms

To elucidate the molecular mechanisms of SARS-CoV-2 spike dynamics, we performed μs -long allatom AMOEBA high-resolution polarizable adaptive sampling molecular dynamics simulations, zooming into the interaction interface in its both open and closed states. Our findings revealed a sophisticated protein-solvent-glycan polarization network essential for stabilizing the open state. Additionally, we demonstrated that the glycan shield consistently preserves viral camouflage across both conformations, effectively protecting the virus from immune detection. These insights not only deepen our understanding of viral behavior but also pave the way for further exploration of viral evasion strategies.

As featured in:



See Louis Lagardère,
Jean-Philip Piquemal *et al.*,
Chem. Sci., 2024, 15, 14177.