Spectroscopy of Proteins — Insights from Molecular Simulations

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Computational spectroscopy based on hybrid quantum mechanics/molecular mechanics (QM/MM) methods is an effective and reliable research tool that is becoming increasingly popular in proteins' spectroscopy studies. This approach has been used to address the following research challenges:

(i) elucidating the source of an exceptionally high quantum yield in rhodopsin [1],

(ii) characterizing the unusual electronic structure of highly fluorescent neorhodopsin [2],

(iii) identifying and characterizing the structural and electronic factors that modulate the two- and three-photon absorption processes in fluorescent proteins [3].

References

[1] X. Yang, M. Manathunga, S. Gozem, J. Leonard, T. Andruniów, M. Olivucci, *Nat. Chem.* 14 (**2022**) 441–449; [2] M. Broser et al. *J. Phys. Chem. Lett.* 14 (**2022**) 441–449; [3] D. Grabarek, T. Andruniów, *J. Chem. Theory Comput.* 16 (**2020**) 6439–6455.