

Supplementary Information

Molecular docking, dynamics simulation, DFT, MEP, PASS and ADMET approaches to methyl α -D-glucopyranoside derivatives for potential inhibitors of chikungunya virus

Nazia Islam^a, Supriyo Saha^b & Sarkar M A Kawsar^{*a}

^a Laboratory of Carbohydrate and Nucleoside Chemistry (LCNC), Department of Chemistry, Faculty of Science, University of Chittagong, Chittagong-4331, Bangladesh

^b Department of Pharmaceutical Chemistry, Uttarakhal Institute of Pharmaceutical Sciences, Uttarakhal University, Dehradun 248 007, Uttarakhand, India

E-mail: akawsarabe@yahoo.com

Received 31 May 2025; accepted (revised) 4 December 2025

$$\text{Gap } (\Delta E) = [\varepsilon\text{LUMO} - \varepsilon\text{HOMO}]$$

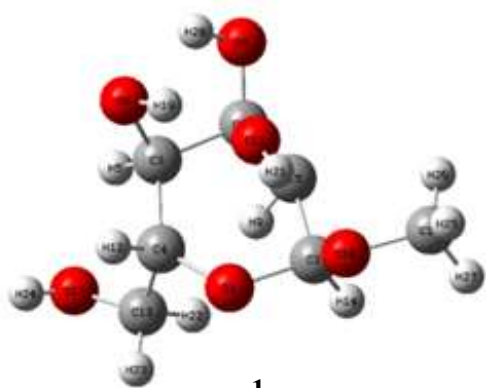
$$\eta = \frac{[\varepsilon\text{LUMO} - \varepsilon\text{HOMO}]}{2}$$

$$S = \frac{1}{2\eta}$$

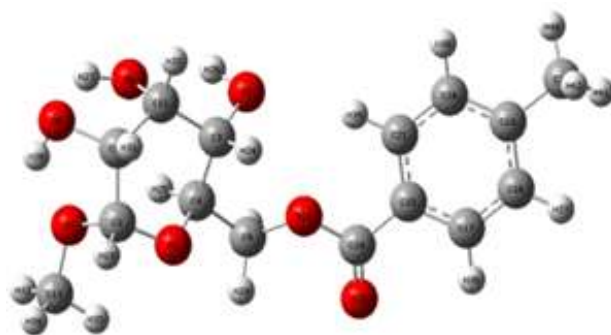
$$\mu = \frac{[\varepsilon\text{LUMO} + \varepsilon\text{HOMO}]}{2}$$

$$\chi = -\frac{[\varepsilon\text{LUMO} + \varepsilon\text{HOMO}]}{2}$$

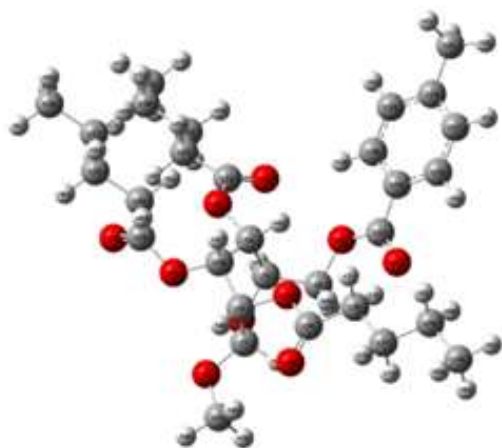
$$\omega = \frac{\mu^2}{2\eta}$$



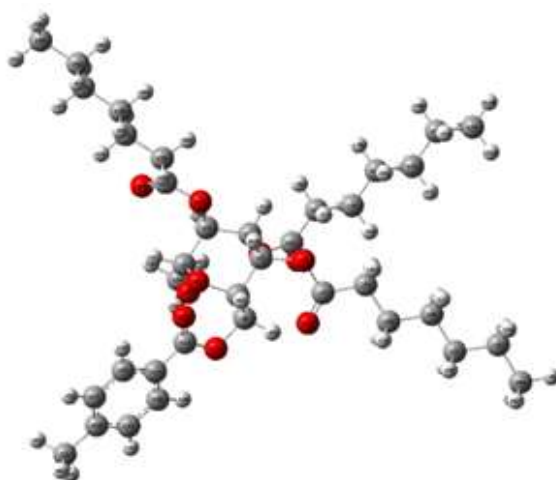
1



2



3



4

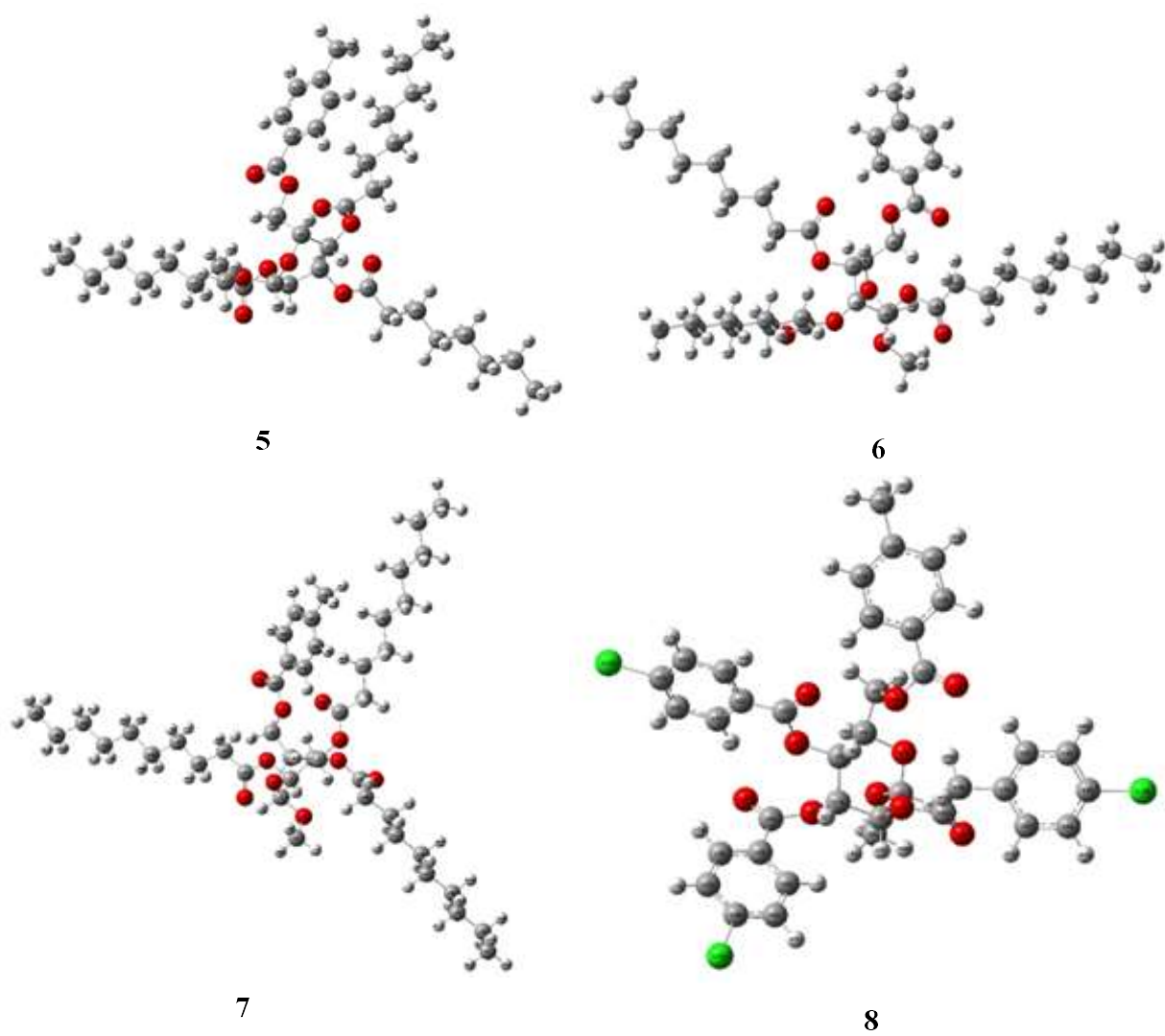
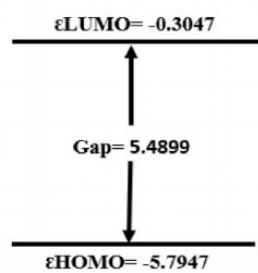
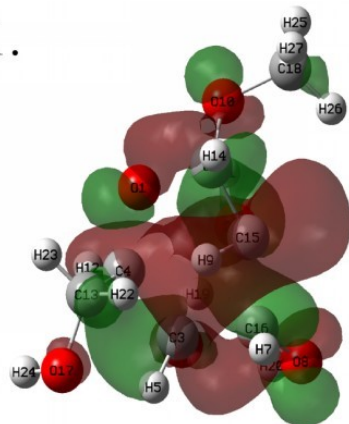
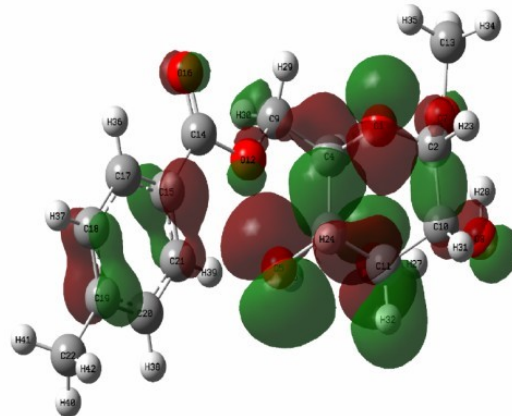
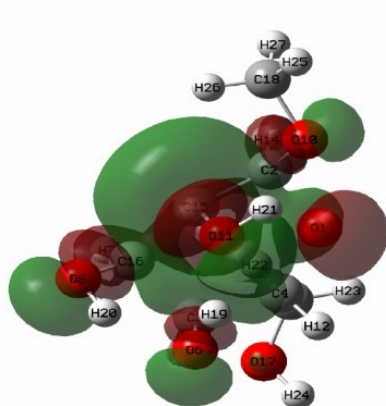
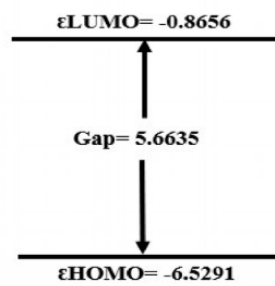
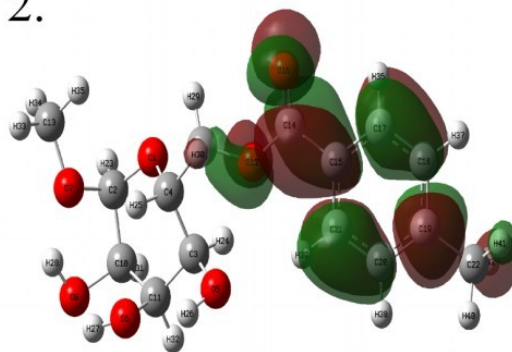


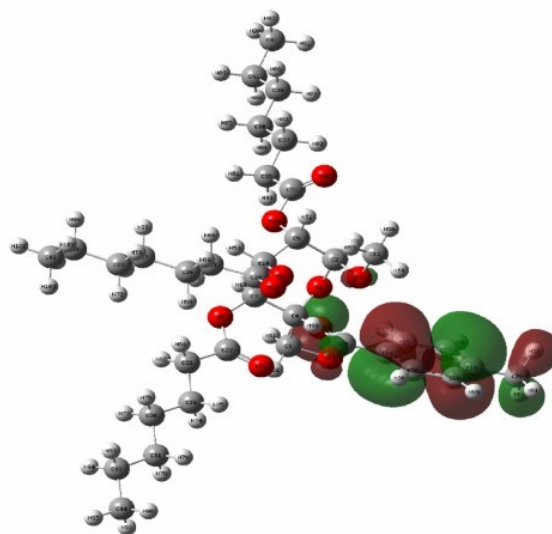
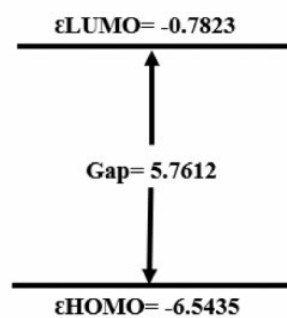
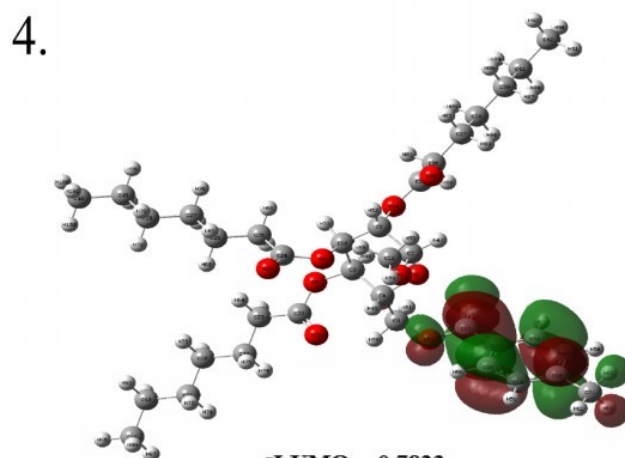
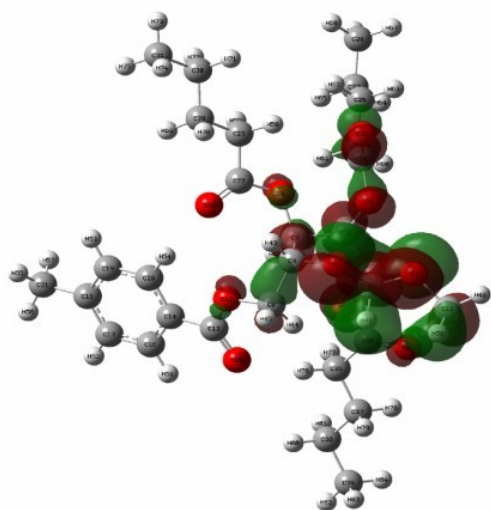
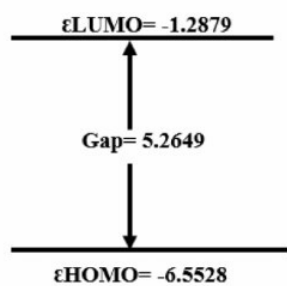
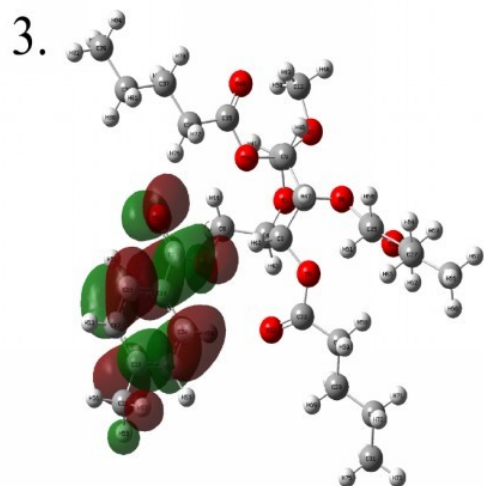
Fig. 1S — 3D optimized structures of methyl α -D-glucopyranoside (**1**) and its derivatives (**2-8**)

1.

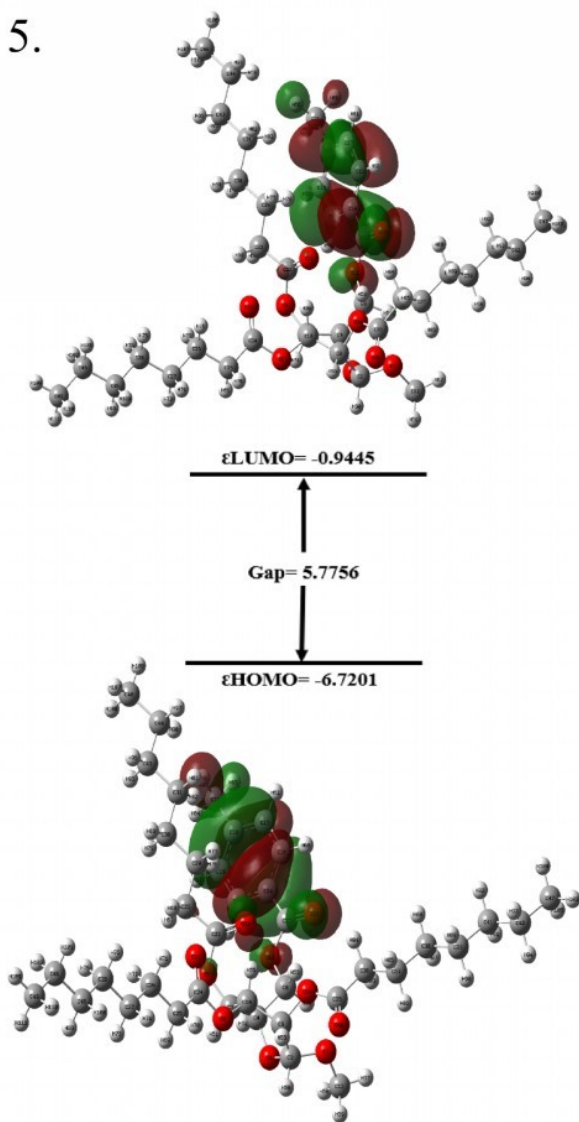


2.

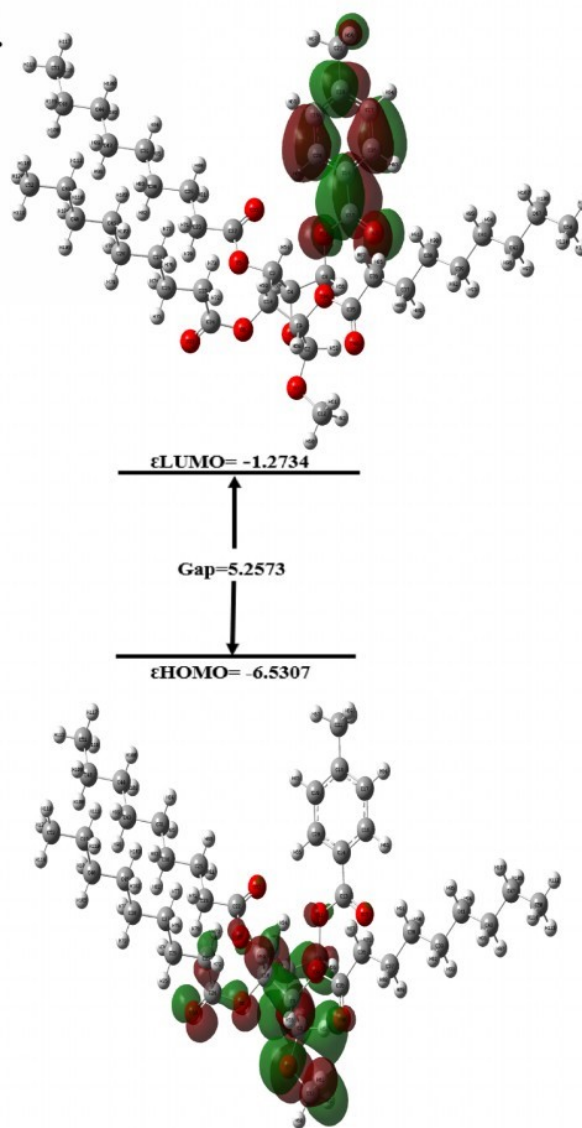




5.



6.



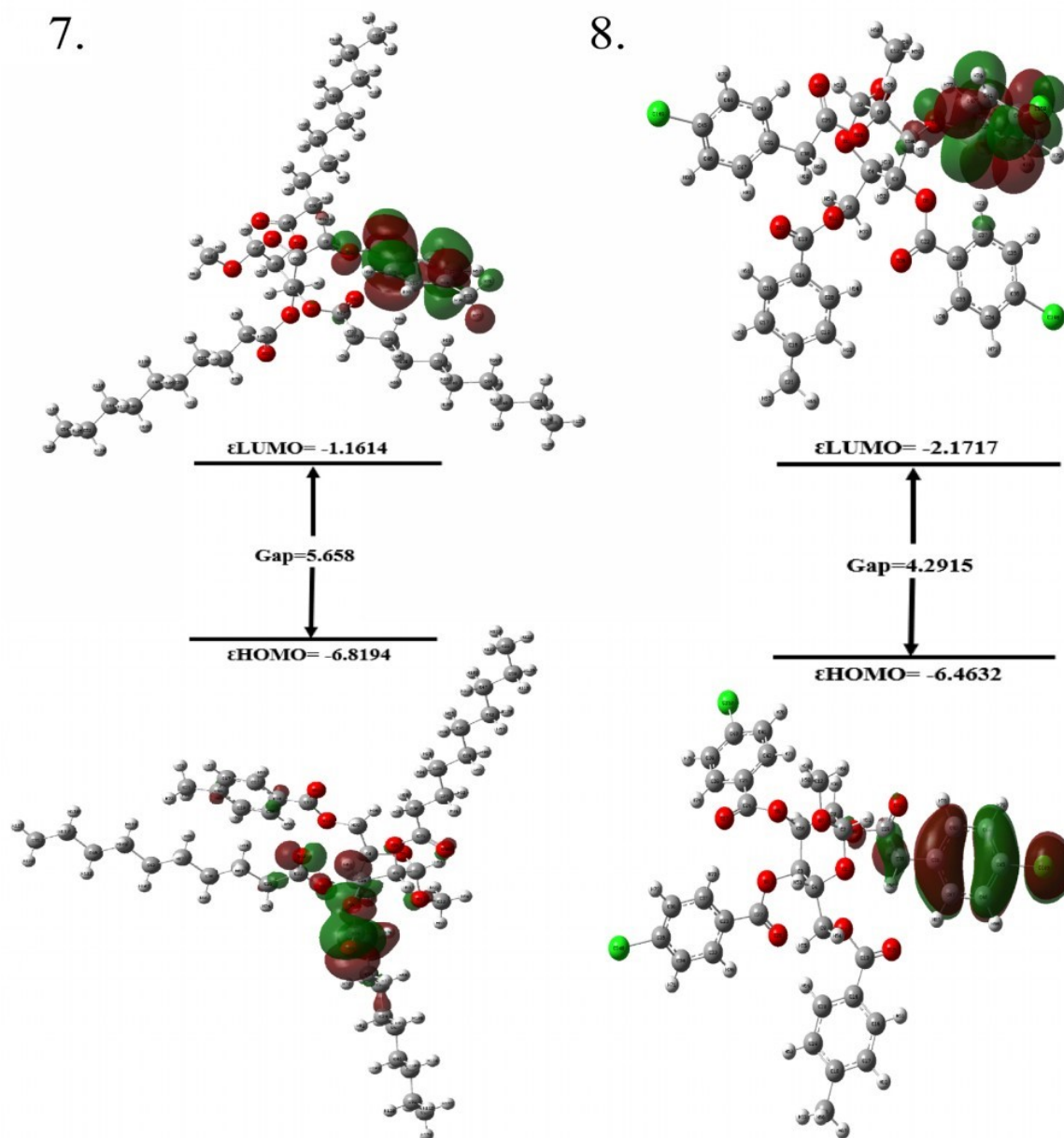
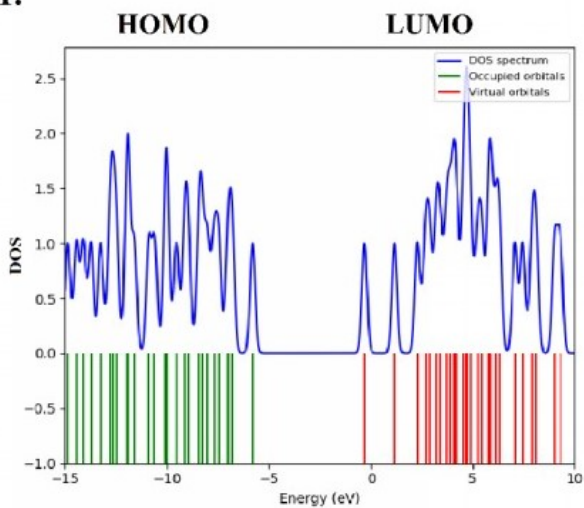
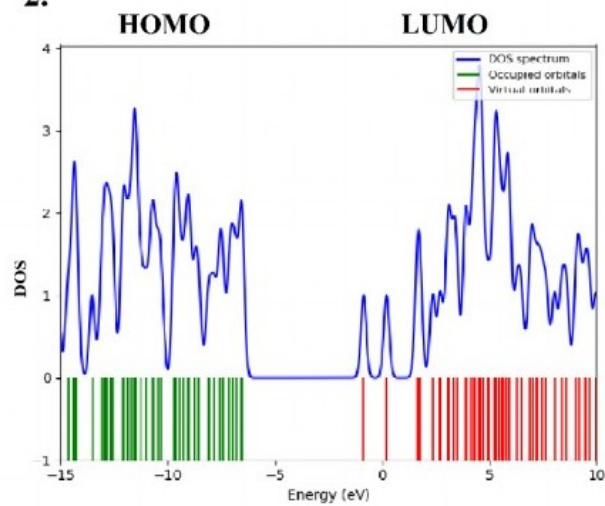


Fig. 2S — Molecular orbital analysis of the HOMO–LUMO energy (eV) and energy gap, hardness (η) and softness (S)

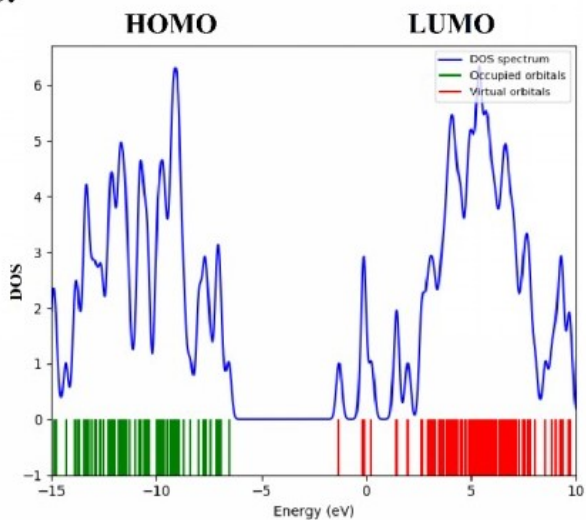
1.



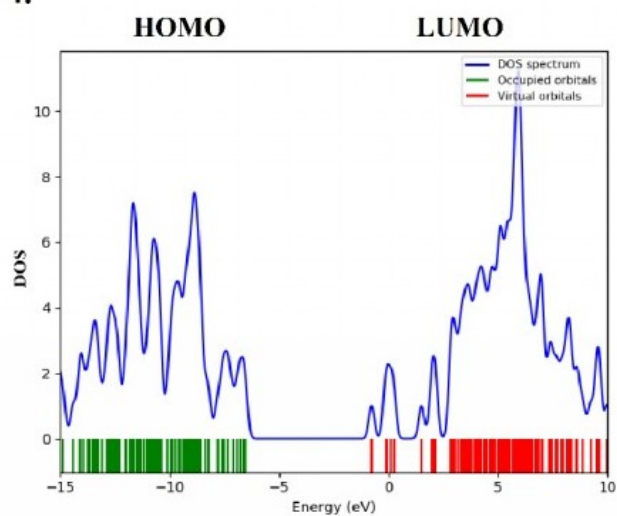
2.



3.



4.



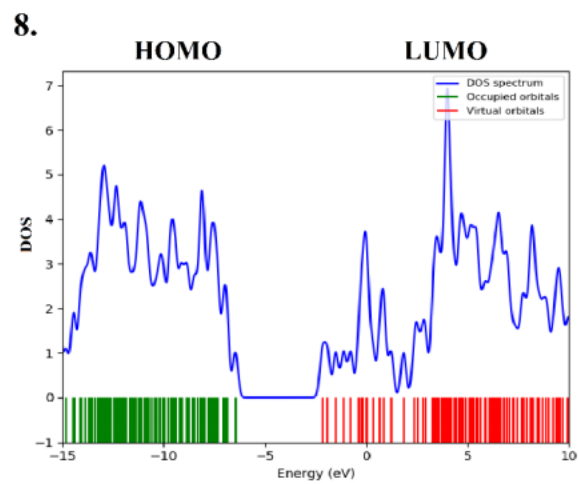
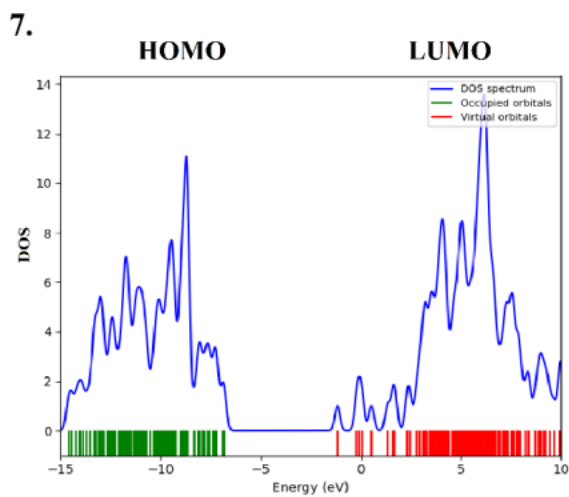
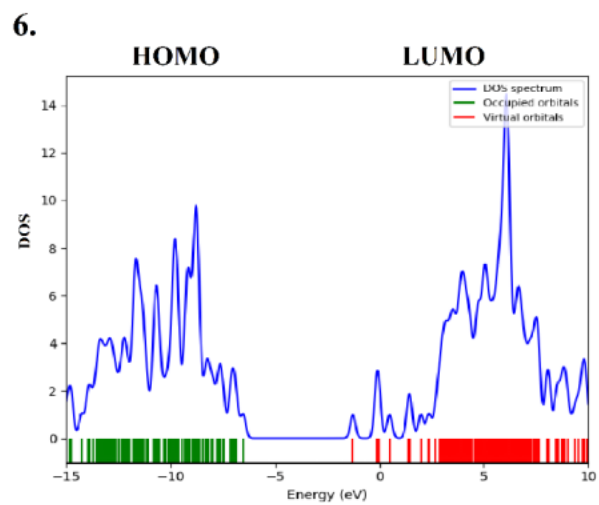
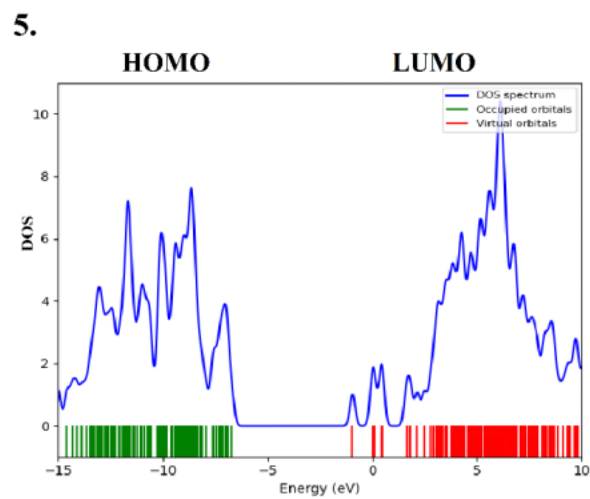


Fig. 3S — DOS plot of the derivatives of methyl α -D-glucopyranoside