Supplementary Information

DENSITY FUNCTIONAL THEORY STUDY OF INTERMOLECULAR INTERACTION BETWEEN AMYLUM AND CELLULOSE

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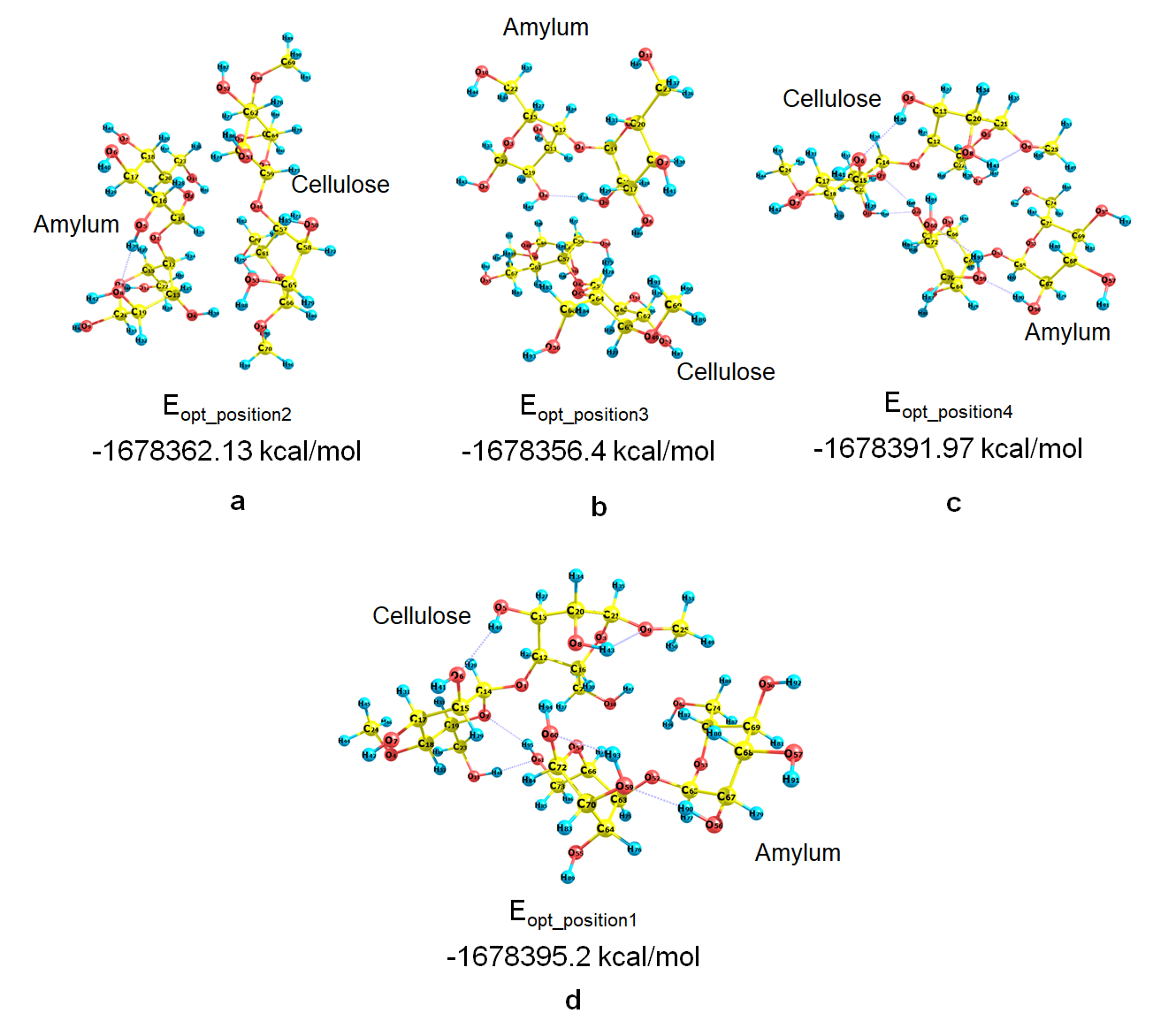
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Table

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CP: critical point; BCP: Bond critical point; : Electron density (a.u.); ﻿∇2ρ: Laplacian of electron density (a.u); G: Lagrangian kinetic energy (a.u); H: Hamiltonian kinetic energy or electronic energy density (a.u); V: Potential energy density (a.u); ε: Ellipticity of electron density (a.u); λ1, λ2, λ3 : Components of Laplacian in x/y/z (a.u); EHB: Hydrogen bond energy (kcal/mol).

**Table S1** Topological parameters of the complex cellulose-amylum.



**Figure S1** Energy optimization of various positions of cellulose-amylum complexes: a) position2, b) position3, c) position4, d) position1.