Supplementary Data

This supplementary data is a part of paper entitled "Density Functional Theory Study of Intermolecular Interactions between Amylum and Cellulose".

Table S1. Topological parameters of the complex cellulose-amylum

BCP	Point	ρ(BCP)	λ1	λ2	λ3	$\nabla^2\rho$	G(BCP)	V(BCP)	H(BCP)	|V/G|	ε (BCP)	EHB (kcal/mol)
Amylum-Cellulose												
143	H29…O60	0.008	-0.006	0.038	-0.003	0.029	0.006	-0.006	0.001	0.858	0.296	-1.079
125	H95…O2	0.024	0.013	0.073	-0.015	0.07	0.018	-0.019	-0.001	1.051	0.019	-4.560
174	H94…O8	0.017	0.08	-0.008	-0.019	0.053	0.013	-0.014	0.000	1.011	0.059	-3.008
134	H84…H29	0.007	0.008	0.024	-0.005	0.027	0.005	-0.004	0.001	0.724	0.770	-0.882
138	O61…H37	0.012	0.052	-0.005	-0.011	0.036	0.009	-0.009	0.000	0.968	0.065	-1.985
220	O62…H50	0.005	0.008	-0.002	0.012	0.018	0.004	-0.003	0.001	0.758	0.625	-0.310
227	H82…C25	0.005	0.021	-0.002	0.000	0.018	0.003	-0.002	0.001	0.656	1.895	-0.324
233	H88…H50	0.005	0.004	0.012	0.002	0.019	0.003	-0.002	0.001	0.641	0.374	-0.326
246	O58…H49	0.016	0.018	0.044	-0.018	0.044	0.011	-0.012	0.000	1.034	0.040	-2.825
177	O54…H30	0.015	0.072	-0.014	-0.012	0.047	0.011	-0.011	0.000	0.976	0.125	-2.569
181	H78…O10	0.015	0.053	-0.015	0.003	0.041	0.011	-0.011	0.000	1.034	0.051	-2.579
206	O62…H47	0.017	-0.016	0.091	-0.018	0.057	0.014	-0.014	0.000	0.992	0.120	-3.038
154	H94…O1	0.014	0.007	0.007	0.031	0.045	0.011	-0.011	0.000	0.988	0.096	-2.361
120	O61…H48	0.034	-0.026	0.163	-0.045	0.092	0.024	-0.025	-0.001	1.047	0.042	-6.791
153	O54…O1	0.011	0.022	0.022	-0.008	0.036	0.009	-0.009	0.000	0.980	0.064	-1.636

CP: critical point; BCP: Bond critical point; ρ: Electron density (a.u.); $\nabla^2\rho$: 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.); λ_1, λ_2, λ_3: Components of Laplacian in x/y/z (a.u.); E_{HB}: Hydrogen bond energy (kcal/mol)

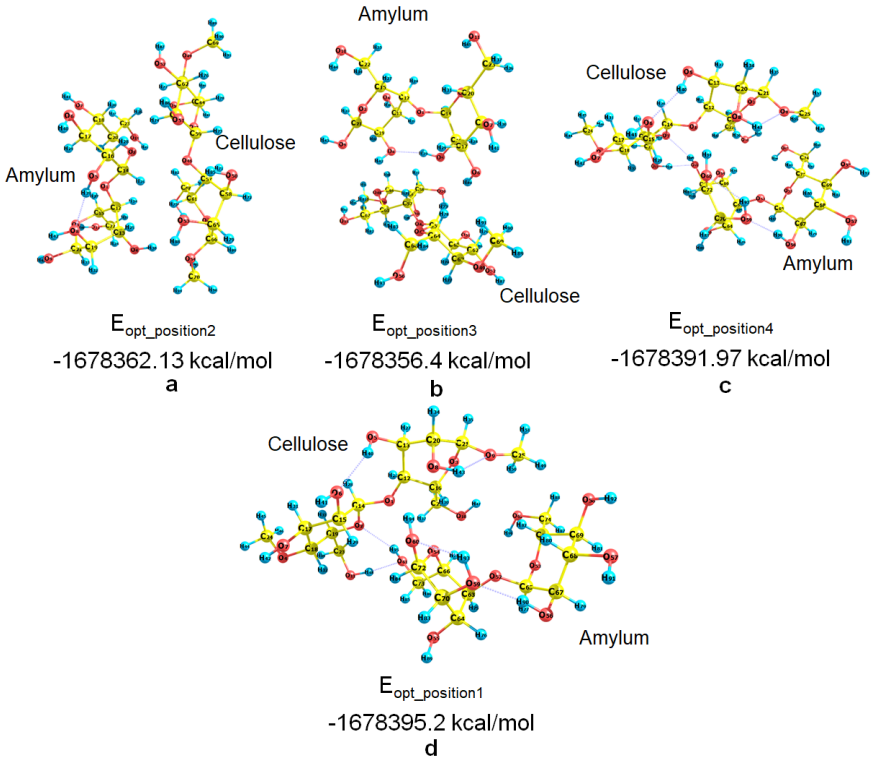

Fig S1. Energy optimization of various positions of cellulose-amylum complexes: (a) position2, (b) position3, (c) position4, (d) position1