Supplementary Material

Cellulose-Based Hectocycle Nanopolymers: Synthesis, Molecular Docking and Adsorption of Difenoconazole from Aqueous Medium

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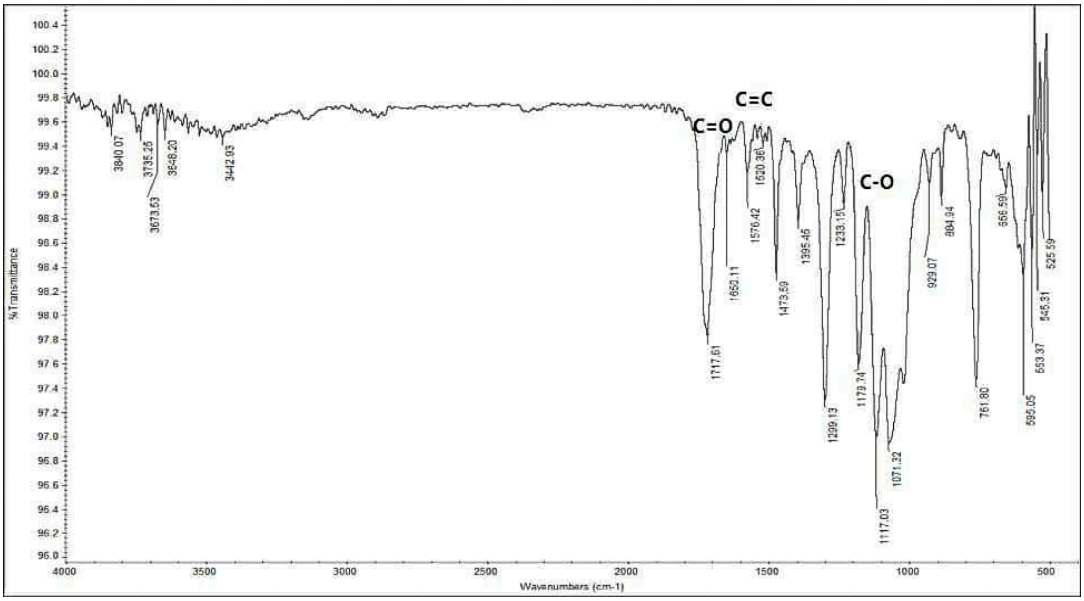

Figure S1. FT-IR analysis for Cell-D.

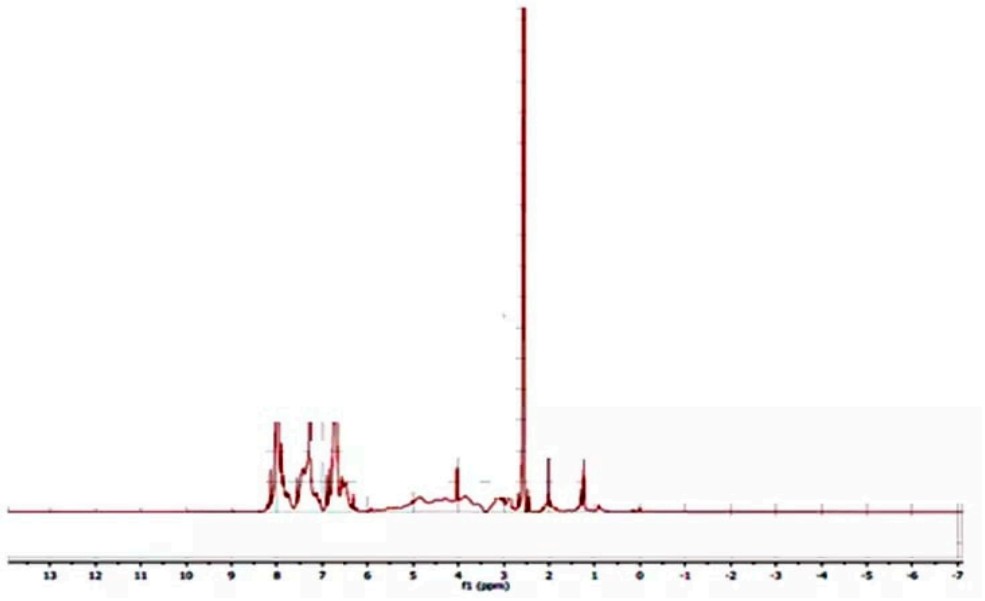

Figure S2. H^1 NMR analysis for Cell-D dissolved in DMSO-d_6.

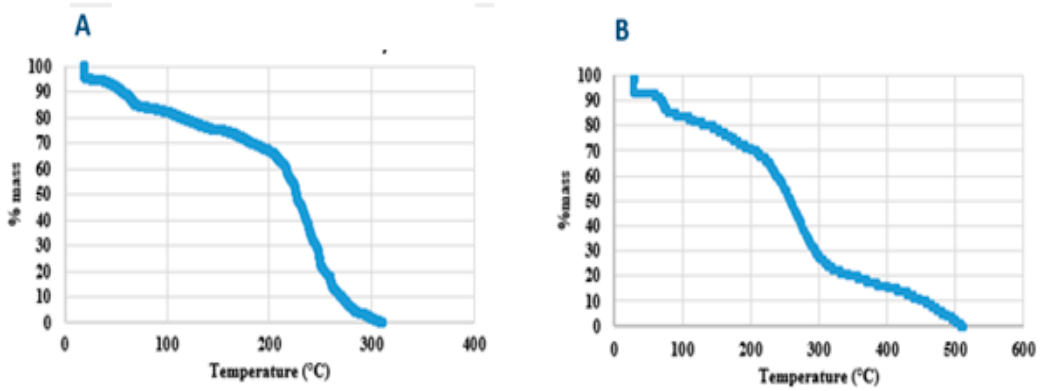

Figure S3. TGA analysis for A: Cell-D and B: Cell-X.

Table S1. Parameters of Langmuir and Freundlich isotherms for Difenoconazole by Cell-X and Cell-D.

Nanopolymer	Langmuir Isotherm		Freundlich Isotherm	
	Q_o (mg/g)	b (L/mg)	K_F (mg/g)	n (g/L)
Cell-D	5.893	2.173	9.270	−4.016
Cell-X	5.447	1.708	9.311	−3.618

Table S2. Pseudo-first-order, pseudo-second-order and intra-particle-diffusion kinetic adsorption parameters of Difenoconazole removal by Cell-X or Cell-D.

Nanopolymer	Pseudo First-Order Kinetics		q_{exp} (mg/g)	Pseudo Second-Order Kinetics		Intra-Particle Diffusion Kinetics	
	q_e (mg/g)	K_1 ($mg.g^{-1}.min^{-1}$)	8.524	q_e (mg/g)	K_2 ($g.mg^{-1}.min^{-1}$)	C (mg/g)	K_p ($mg.g^{-1}.min^{-0.5}$)
Cell-D	1.764	7.83×10^{-3}	8.773	8.849	0.224	7.8276	0.1483
Cel-X	2.016	8.98×10^{-3}	8.745	8.834	0.1396	7.5422	0.1746

Table S3. Thermodynamic parameters of Difenoconazole pesticide adsorption by Cell-X or Cell-D.

Nanopolymer	ΔH (kJ)	ΔG ° (kJ)	ΔS (J/K)
Cell-D	−25.442	−5.312	−68.667
Cell-X	−24.554	−4.013	−70.071