Supplementary Information (SI) for Journal of Materials Chemistry B.

Emissive and Photothermal PNPM-immobilized-carbon-nanodots with Thermoresponsive Drug Release Property

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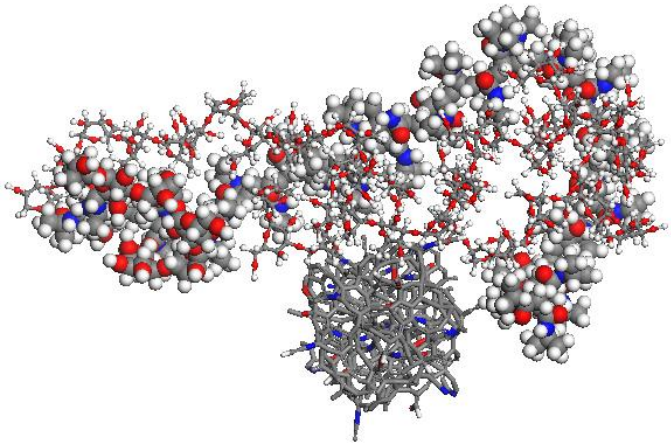

Figure S1. Representation of the simulated model: PNM chain is depicted using the CPK model, agarose is illustrated in ball-and-stick representation and the central carbon dot is displayed using a stick. Water molecules are omitted for clarity.

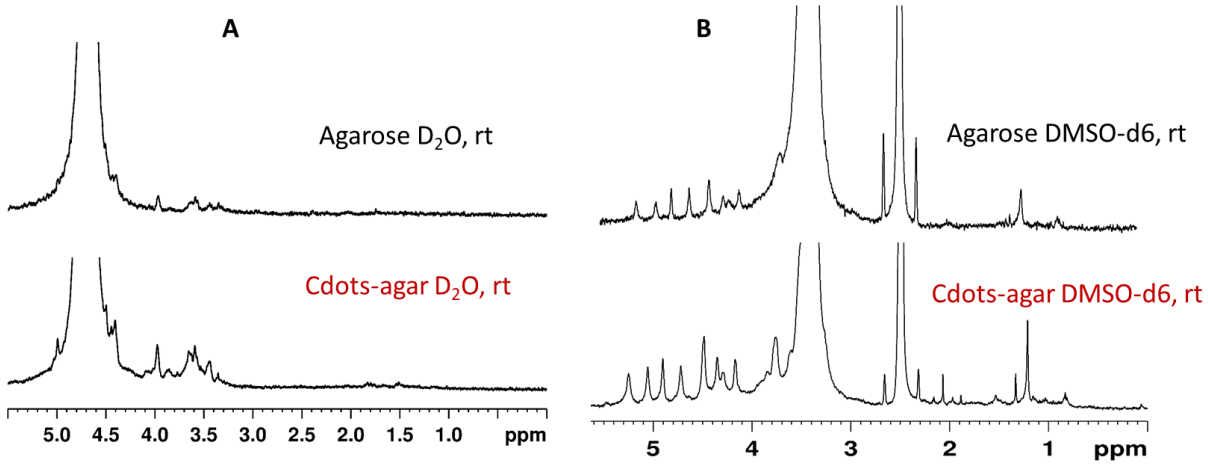

Figure S2. [1]H-NMR spectra (400.13 MHz, 25 °C) of agarose and Cdots-agar in: A) D_2O and B) DMSO-*d6* at 25 °C.

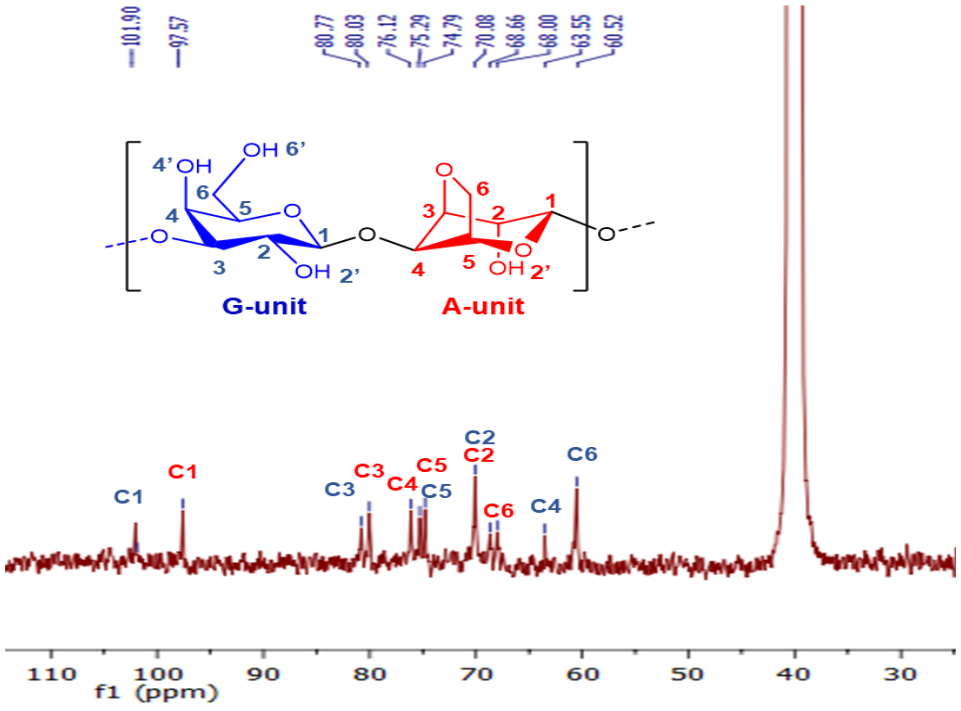

Figure S3. [13]C-NMR spectrum of Cdots-agar in DMSO-*d6* at 37°C (AvanceNEO 400 MHz spectrometer).

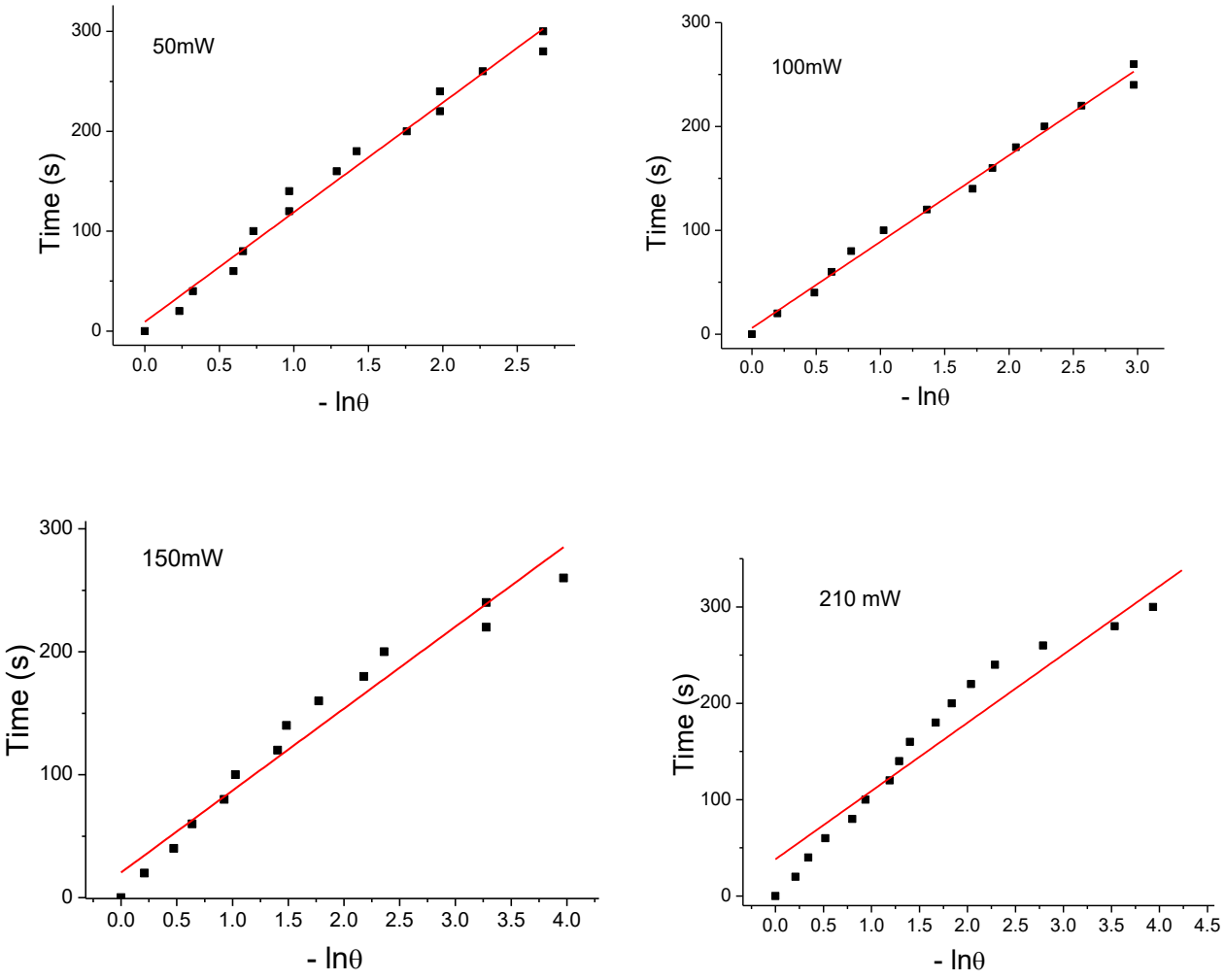

Figure S4. Linear relationship between time (sec) and -ln(θ), the slope is the time constant (τ_s) for different photothermal experiments.

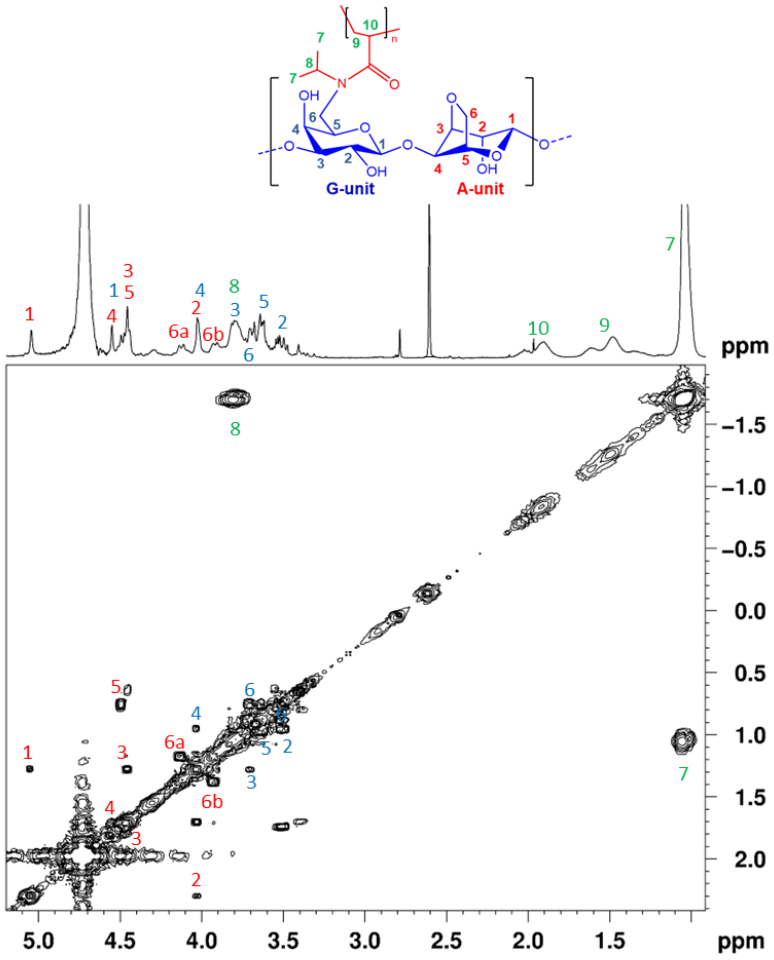

Figure S5. 2D-COSY NMR spectrum of Cdots-agar-PNM in D2O at 25 °C (Bruker Avance 400^{TM}, 400.13 MHz).

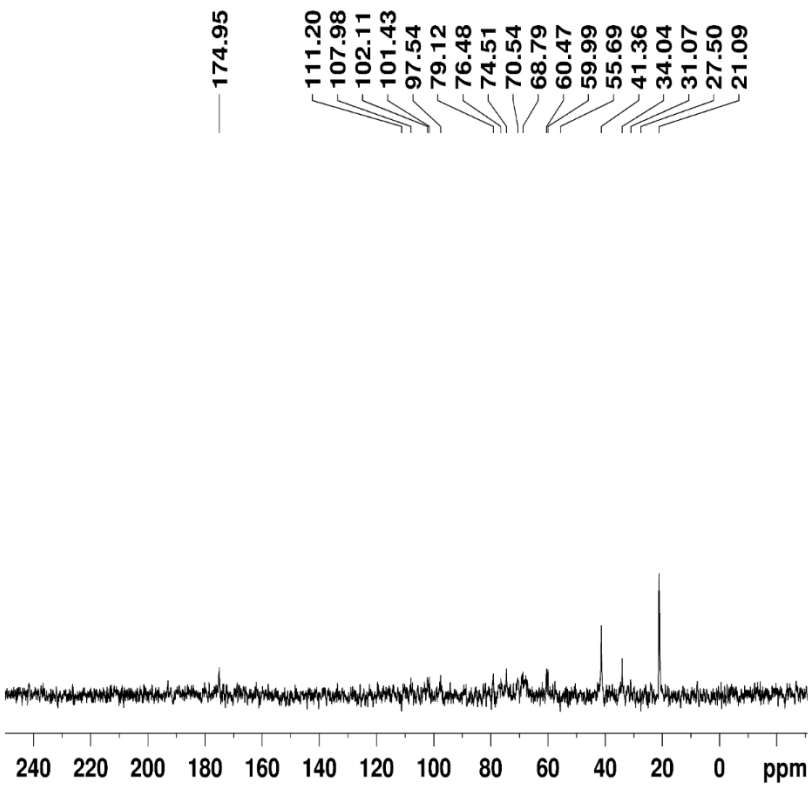

Figure S6. ^{13}C-NMR spectrum of Cdots-agar-PNM in D2O at 25 °C (Bruker Avance 400^{TM} spectrometer).

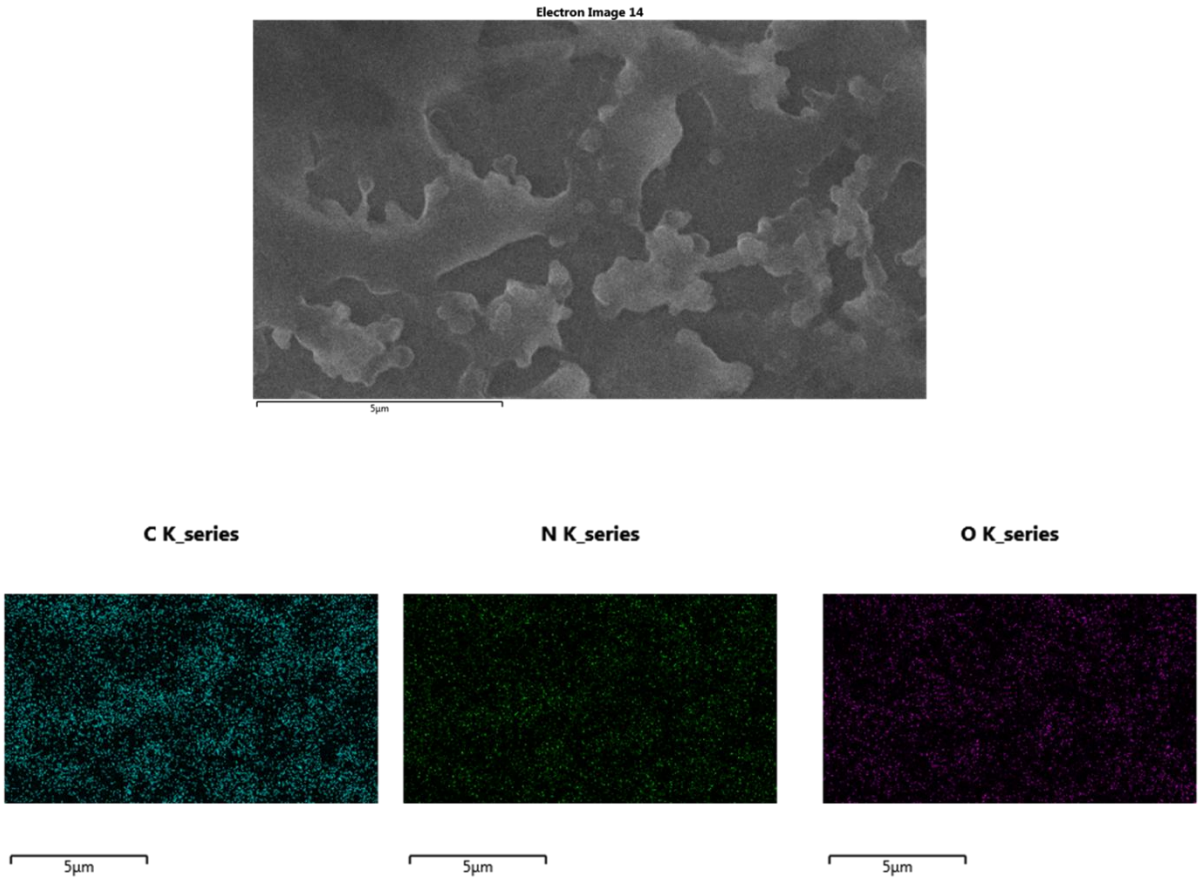

Figure S7. EDX-maps for A) CDs-agar-PNM and B) CDs-agar nanostructures on Si substrate

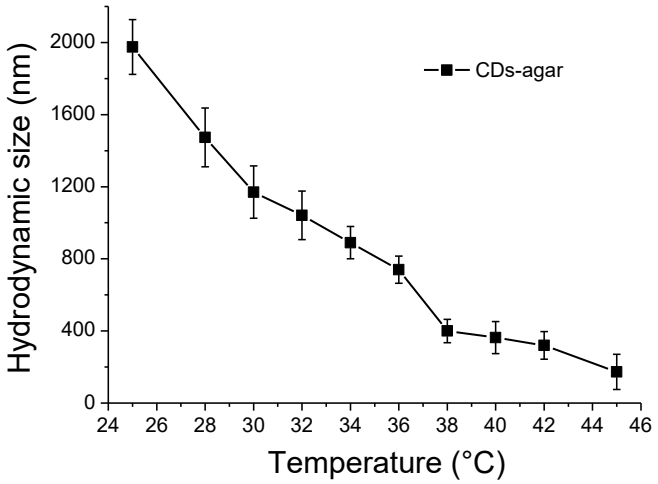

Figure S8. CDs-agar: DLS measurements for CDs-agar aqueous dispersion (2 mg mL^{-1}) at pH 7.0 and at various temperatures: 25, 28, 30, 32, 34, 36, 38, 40, 42 and 45 °C.

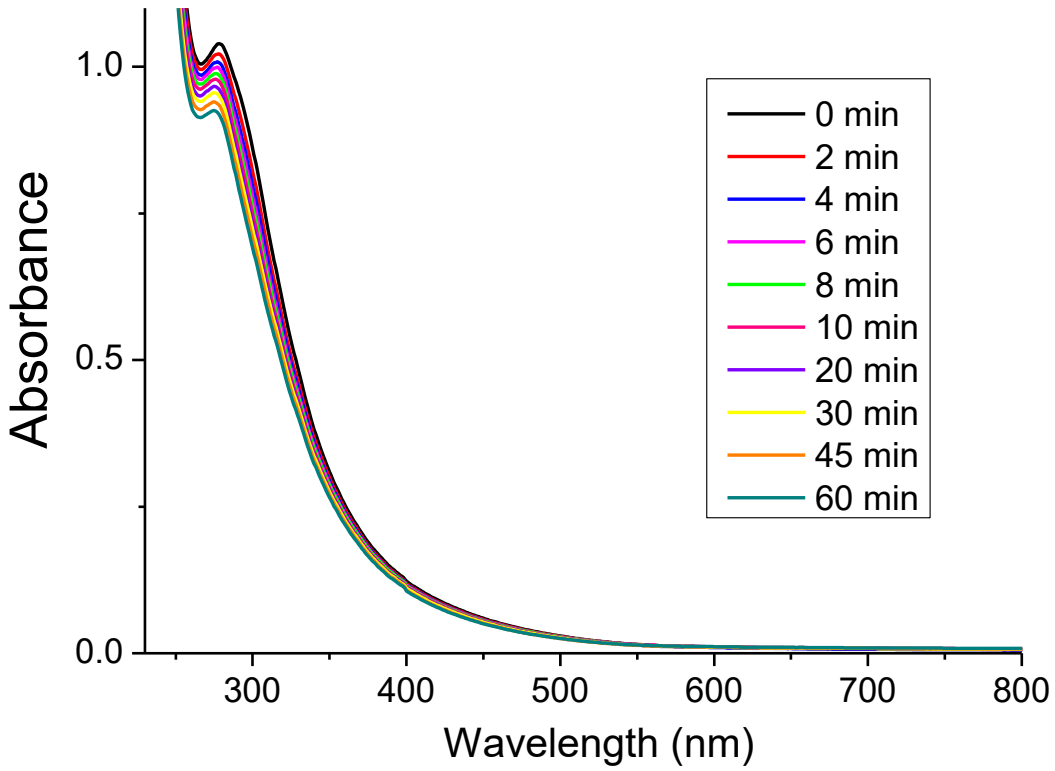

Figure S9. optical spectra changes of CDs-agar-PNM/gold precursor dispersion at different time on dark condition.

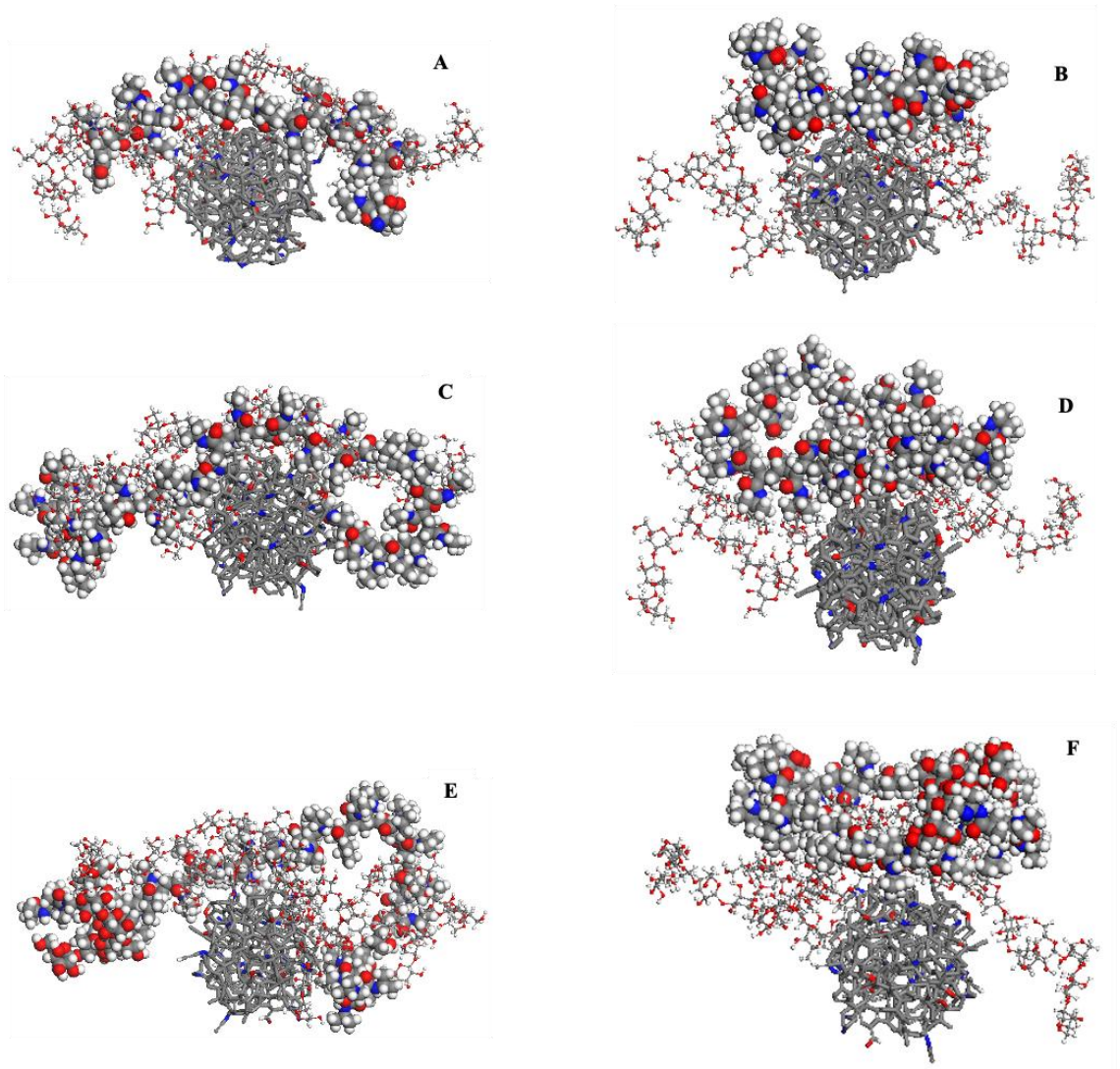

Figure S10. Snapshots taken at 70 ns and 160 ns for CDs-agar-PNM-24 (A,B), CDs-agar-PNM-32 (C,D) and CDs-agar-PNM-42 (E,F); PNM chain is depicted using the CPK model, agarose is illustrated in ball-and-stick representation and the central carbon dot is displayed using a stick. Water molecules are omitted for clarity.

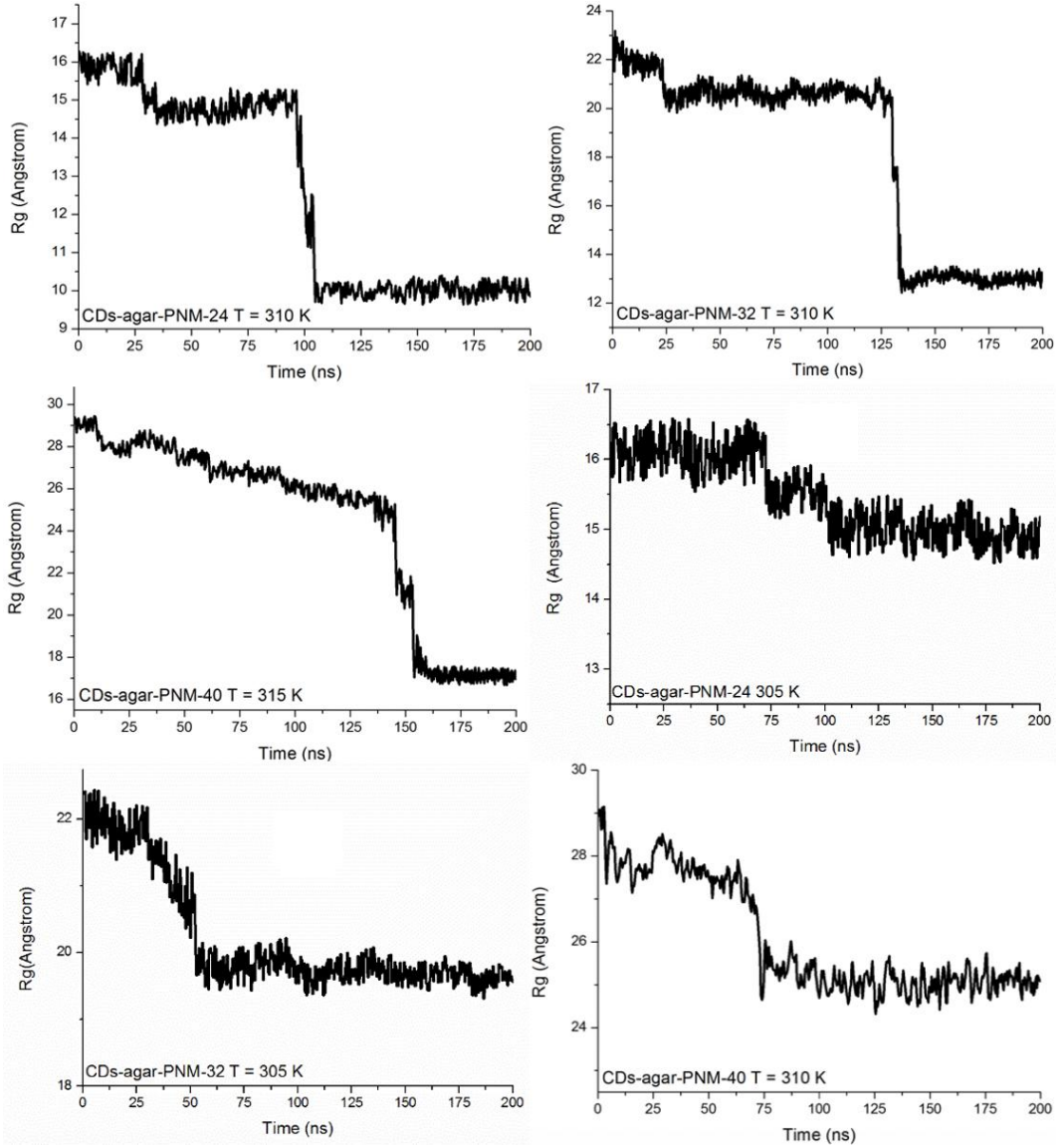

Figure S11. Rg trends for the investigated models, at 305, 310 and 315 K.

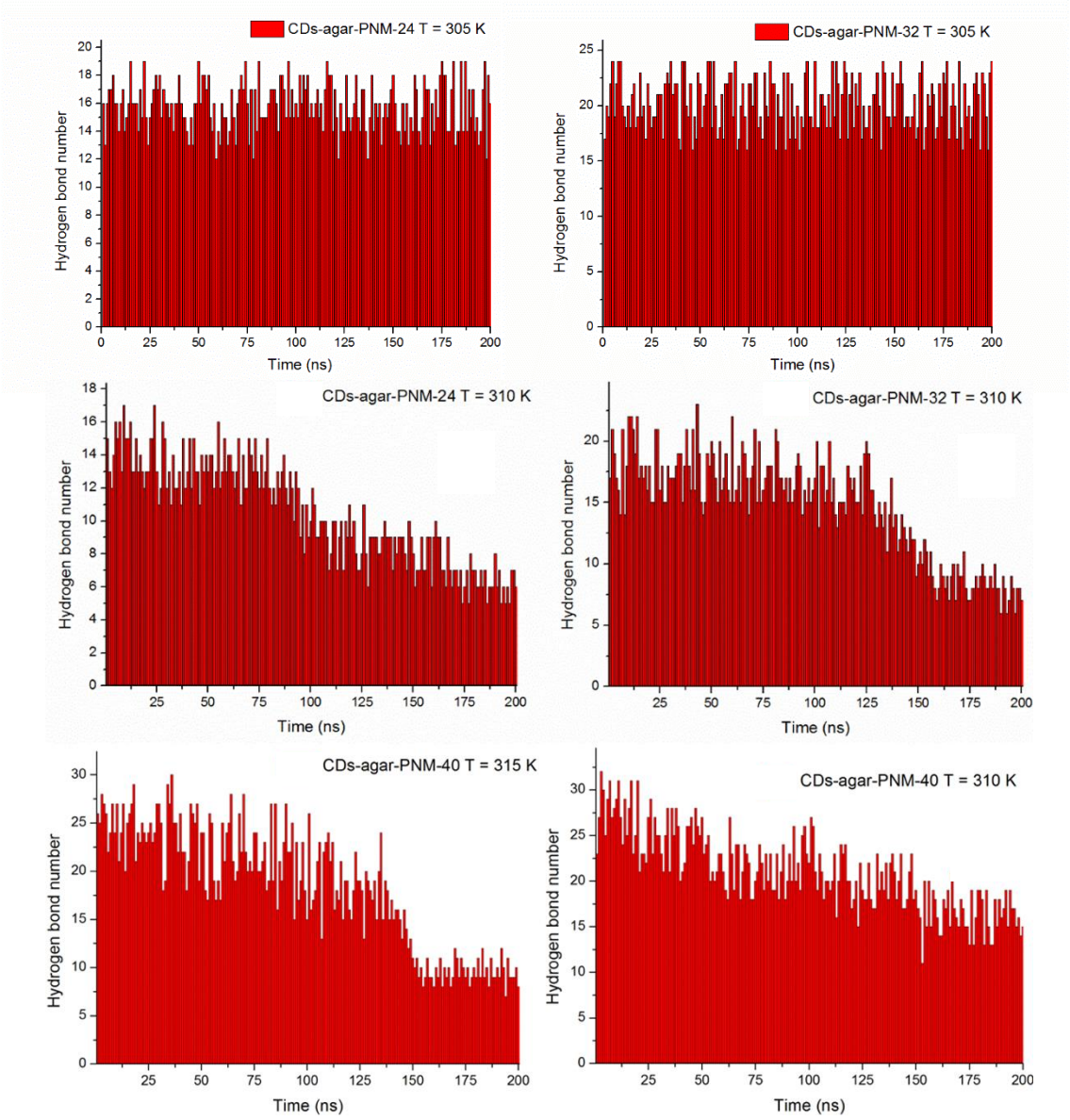

Figure S12. Number of hydrogen bonds formed during the simulations at 305, 310 and 315 K.

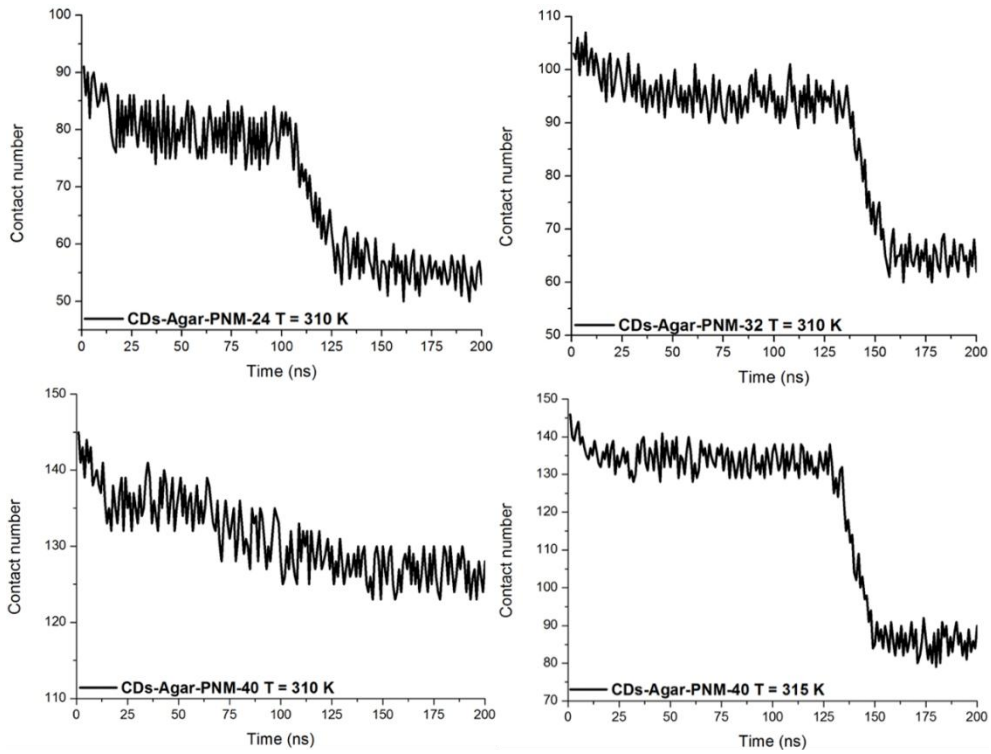

Figure S13. Atom contact number between PNM and agarose

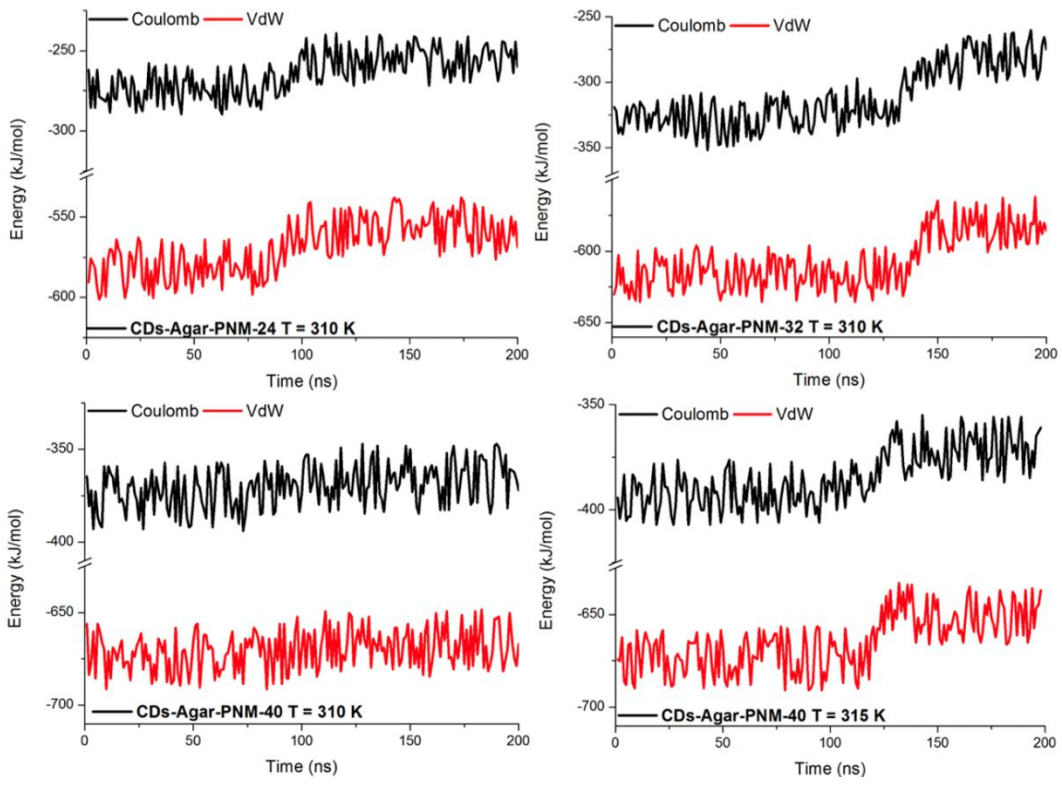

Figure S14. Interaction energies between PNM and agarose. VdW and Coulomb indicate van der Waals and Coulomb energies, respectively

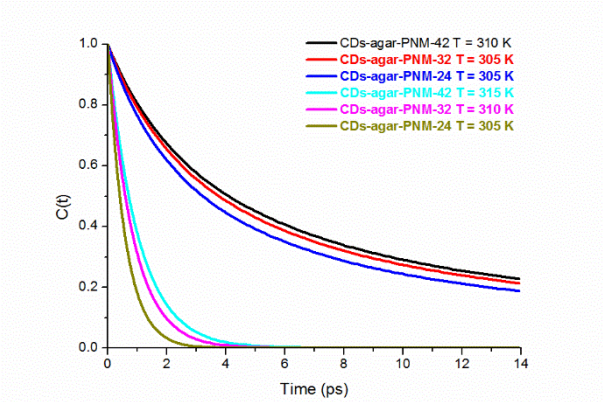

Figure S15. *c(t)* autocorrelation function for hydrogen bond involving PNM acceptor groups and hydrogen atom donors from the –OH groups on agarose.

Table S1. Cytotoxicity test. Statistical analysis with *Two-stage linear step-up procedure of Benjamini, Krieger and Yekutieli*

Two-stage linear step-up procedure of Benjamini, Krieger and Yekutieli	Mean Diff,	Discovery?	P Value
Untreated vs. 400 ug	20,52	Yes	<0,0001
Untreated vs. 40 ug	-0,452	No	0,8291
Untreated vs. 4 ug	2,995	No	0,1602
Untreated vs. 0.4 ug	4,115	No	0,0577
Untreated vs. 0.04 ug	2,259	No	0,2856

Table S2. Chemical shifts (ppm) of proton and carbon signals for Cdots-agar in DMSO-*d6* at 70 °C.

	H1	H2	H3	H4	H5	H6
G	4.32	3.45	3.55	3.84	3.44	3.54
A	5.08	3.83	4.22	4.53	4.35	3.92
	C1	**C2**	**C3**	**C4**	**C5**	**C6**
G	101.9	68.66	80.77	63.55	75.92	60.52
A	97.57	70.08	80.03	76.12	74.79	68.00

Photothermal conversion efficiency (η).

Photothermal measurements were performed irradiating a volume of 100 μL of CDs-agar-PNM deionized water dispersion in a glass tube (diameter 3 mm), using continuous wave with excitation wavelength 405 nm. A standard infrared thermal imaging camera was used to measure the temperature of solution every 20 seconds, during the heating and cooling processes. The photothermal conversion efficiency (η) was calculated according to equation (1) introduced by Roper

$$\eta = \frac{hA\,(T_{max} - T_{surr}) - Q_{Dis}}{I(1 - 10^{-A})} \quad (1)$$

Where Tmax and Tsurr represents the max photothermal temperature and the ambient temperature respectively, I is the incident laser power and A is the absorbance value of Cds-agar-PNM dispersion at the wavelength excitation .The equations (2) and (3) were introduced to calculate the parameter hA.

$$\theta = \frac{T - T_{surr}}{T_{max} - T_{surr}} \quad (2)$$

$$\tau = \frac{M_D\, C_D}{hA} \quad (3)$$

where MD and CD are the mass (0.1 g) and heat capacity (4.2 J g^{-1}) of water respectively, and τs is the time constant, calculated by the equation (4).

$$t = -\tau(ln\theta) \quad (4)$$

Table S2 Photothermal experiments data of CDs-agar-PNM at different laser power.

Laser λ (nm)	**Laser Power (mW)**	**Abs $_{exc\ nm}$**	**τ_s (s)**	**η (%)**	**η (%)** **mean ± std dev**
405	50	0.336	109.7	41.2	**38.8 ±2.8 %**
	100		83.1	36.6	
	150		66.6	41.3	
	210		70.8	36.1	