Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supporting Information (SI)

Comparative analysis of cobalt ferrite and iron oxide nanoparticles using bimodal hyperthermia, along with photophysical and *in-silico* interaction with human hemoglobin

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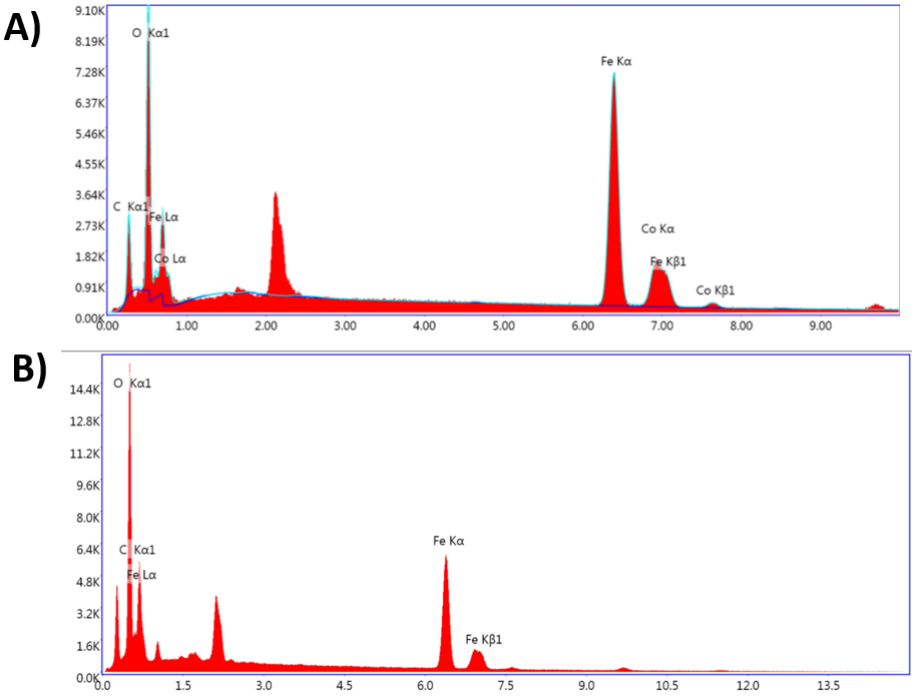


Figure S1: EDAX plot of A) PAA-CFNP B) PAA-IONP.

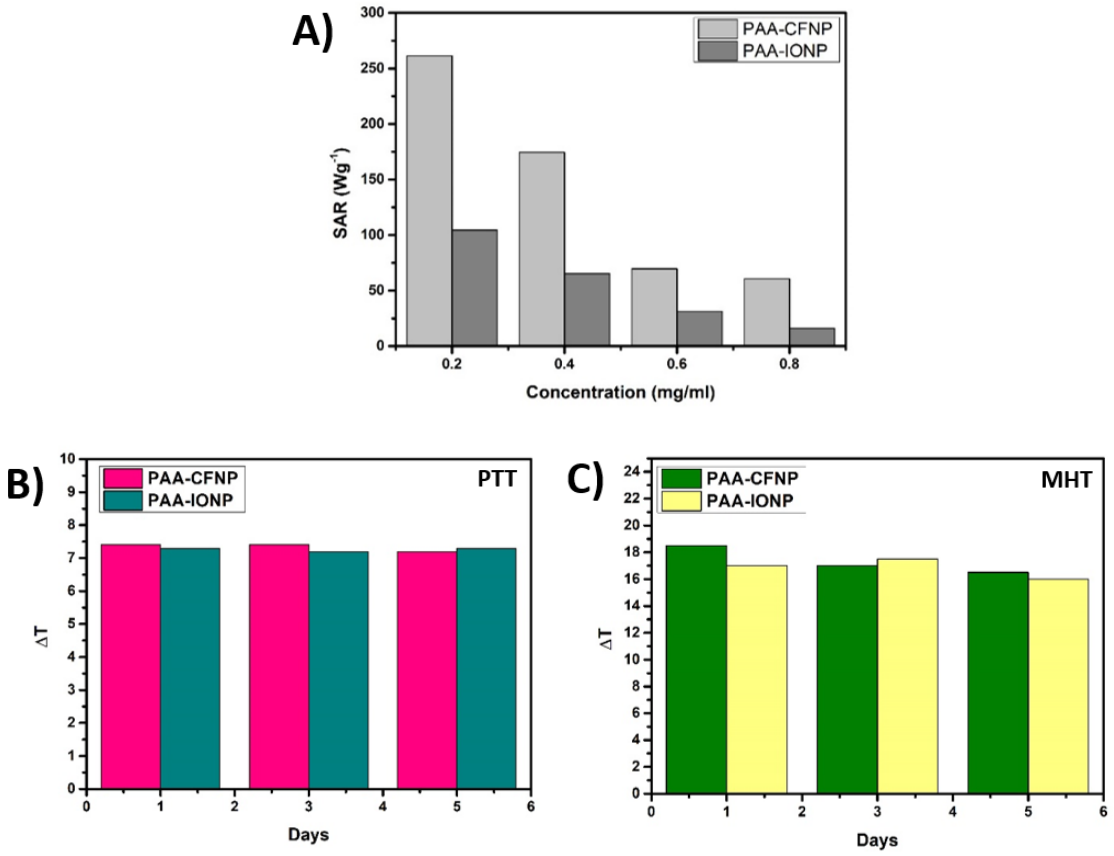


Figure S2: A) SAR plot of PAA-CFNP and PAA-IONP at different concentration. B) Reusability of PAA-CFNP and PAA-IONP as photothermal agents. C) Reusability of PAA-CFNP and PAA-IONP as magnetic hyperthermia agents.

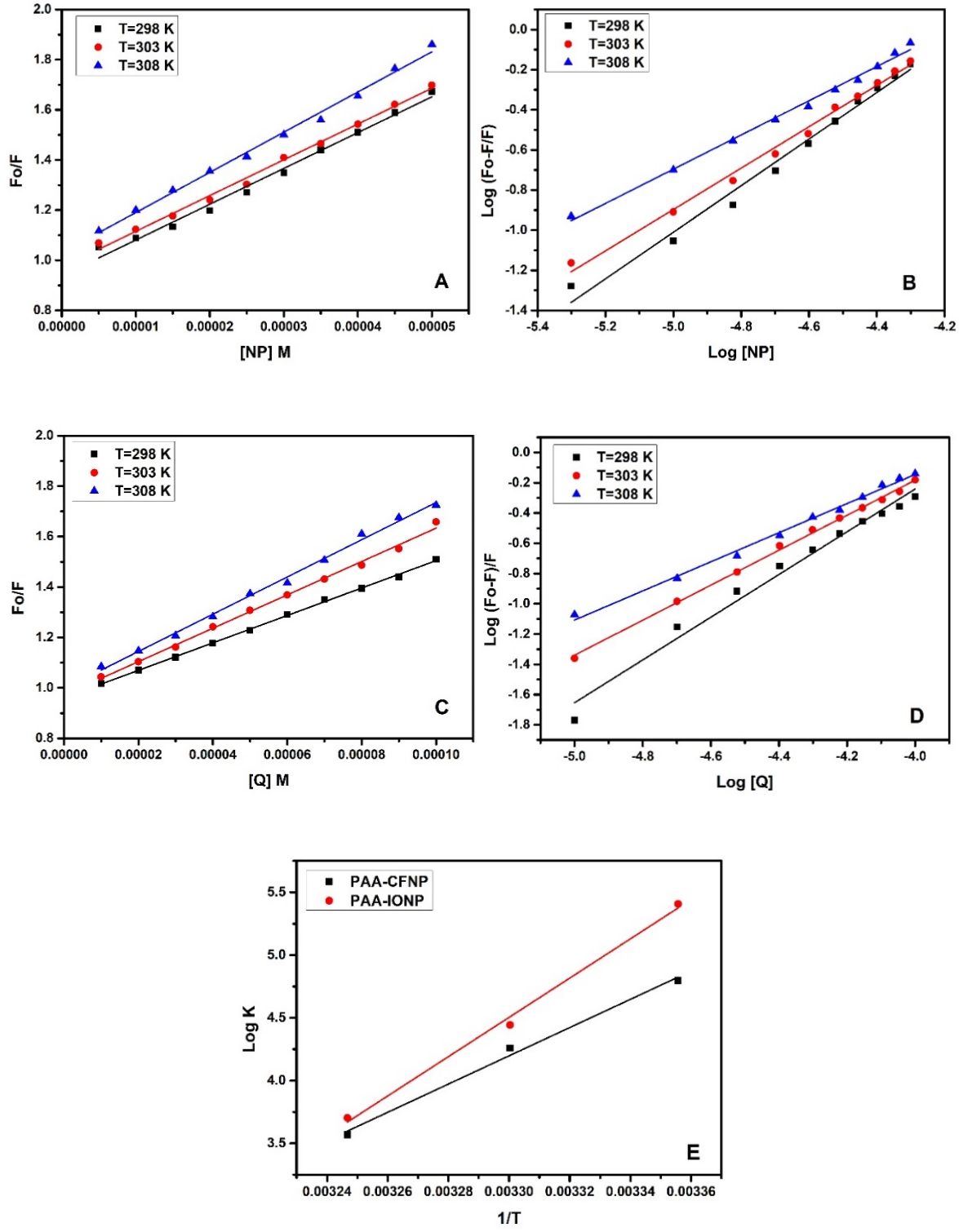


Figure S3: Stern Volmer plot of (Fo/F vs [NP]) for calculating quenching constant A) PAA-CFNP C) PAA-IONP. Modified Stern Volmer plot (Log Fo-F/F vs Log [NP]) for calculating Binding constant B) PAA-CFNP D) PAA-IONP. E) Van't Hoff plot (Log K vs 1/T) for calculating thermodynamic parameters.

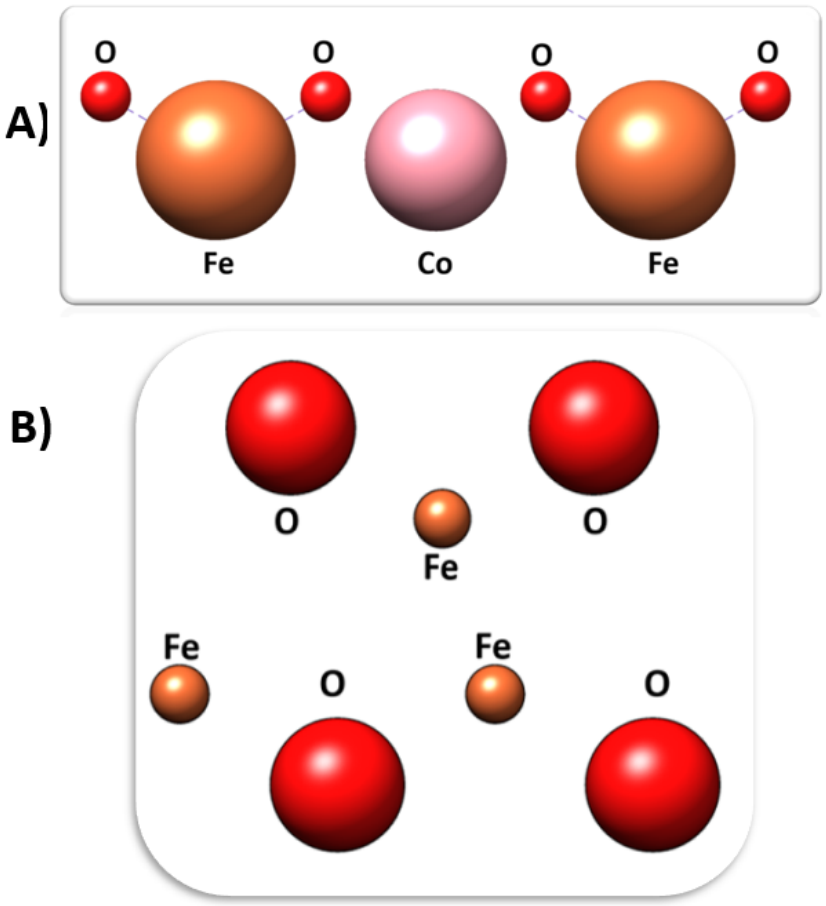


Figure S4: Structure depiction with all atoms labelled A) Cobalt ferrite B) Iron oxide.

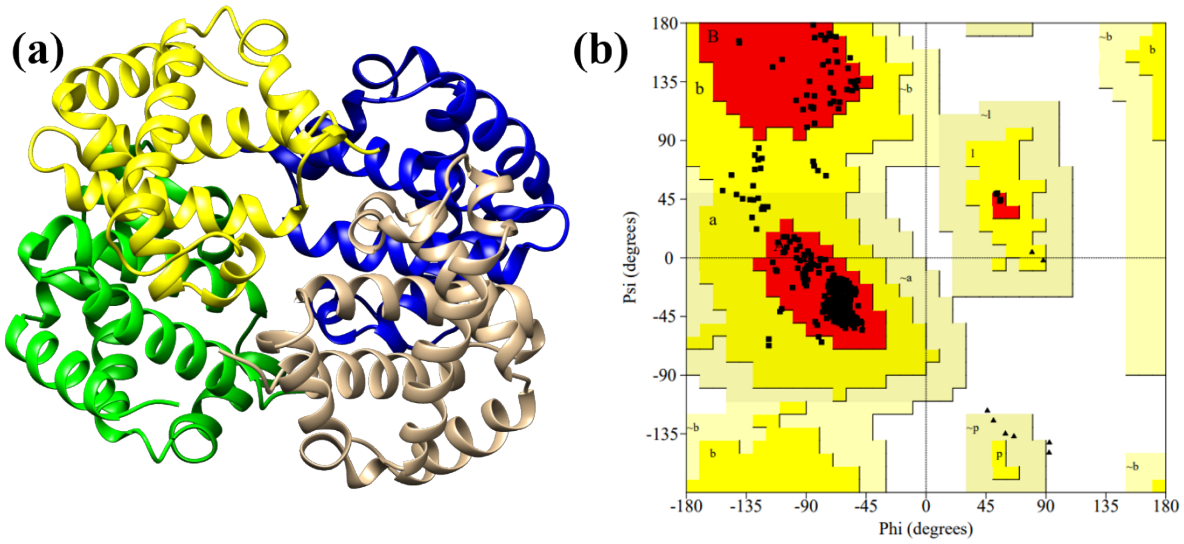


Figure S5: a) 3D structure of haemoglobin. b) Ramachandran plot analysis of 3D structure of haemoglobin.

	Temperature (K)	PAA-CFNP	PAA-IONP
Stern Volmer Constant K_{sv} (M^{-1})	298	1.4275 X 10^4	0.5437 X 10^4
	303	1.4364 X 10^4	0.6615 X 10^4
	308	1.6025 X 10^4	0.7382 X 10^4
Quenching Constant K_q (M^{-1} s^{-1})	298	1.4275 X 10^{12}	0.5437 X 10^{12}
	303	1.4364 X 10^{12}	0.6615 X 10^{12}
	308	1.6025 X 10^{12}	0.7382 X 10^{12}
Binding constant K_b	298	0.62517 X 10^5	2.5537 X 10^5
	303	0.18142 X 10^5	0.2776 X 10^5
	308	0.03703 X 10^5	0.0504 X 10^5
Number of binding sites N	298	1.1613	1.4122
	303	1.0312	1.1567
	308	0.8529	0.9621

Table S1: Binding constants for interaction of Hb with PAA-CFNP and PAA-IONP at 298K, 303K and 308 K.

Nanoparticles	ΔG (kJ/mol)	ΔH (kJ/mol)	TΔS (kJ/mol)
PAA-CFNP	-11.6986	-93.539	-81.890
PAA-IONP	-13.609	-130.127	-116.518

Table S2: Thermodynamic parameters of interaction of Hb with PAA-CFNP and PAA-IONP.

Secondary structures	Details of secondary	Percentage content of

	structures	secondary structure	
		Hb	1:3 PAA-CFNP
Helix	Helix 1 (Regular)	9.4	2.7
	Helix 2 (Distorted)	6.3	0.0
Antiparallel	Anti 1 (Left-twisted)	2.8	6.1
	Anti 2 (Relaxed)	10.4	17.8
	Anti 3 (Right twisted)	14.5	17.1
Parallel		9.8	0.0
Turns		13.7	14.5
Others		33.2	41.8

Table S3: Percentage content of secondary structure of protein for Hb only and Hb with PAA-CFNP (1:3).

Secondary structures	Details of secondary structures	Percentage content of secondary structure	
		Hb	1:3 PAA-IONP
Helix	Helix 1 (Regular)	10.2	2.9
	Helix 2 (Distorted)	6.6	0.0
Antiparallel	Anti 1 (Left-twisted)	2.6	6.2
	Anti 2 (Relaxed)	11.2	18.1
	Anti 3 (Right twisted)	14.6	17.2
Parallel		10.0	0.0
Turns		14.0	14.6
Others		30.6	41.0

Table S4: Percentage content of secondary structure of protein for Hb only and Hb with PAA-IONP (1:3).

Index	Interactions	Å
1.	**Hydrophobic interactions**	94C-ASP-2.59
2.	**Hydrogen bonds**	37B-TRP-3.43 94C-ASP-3.75 102B-ASN-2.65
3.	**Hydrogen bonds**	42C-TYR-3.25 92C-ARG-3.11 94C-ASP-3.33 102B-ASN-2.67

Table S5: The molecular binding analysis of cobalt ferrite and haemoglobin interaction profiler evaluation

Calculations of photothermal efficiency (PCE)

0.5 mg/ml of PAA-CFNP and PAA-IONP, were irradiated by 635 nm (350 mW) and 808 nm (1200 mW) laser until the steady state temperature reached. The diode laser was switched off and the solution was allowed to cool down. The following formula was used to calculate PCE (η):

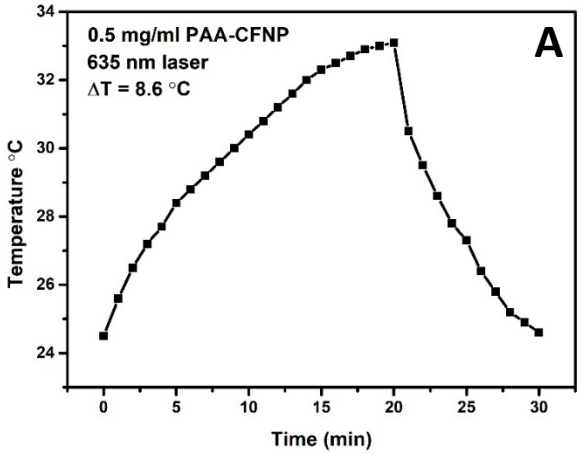
$$\eta = \frac{hS(Tmax - Tsurr) - Qo}{I(1 - 10 - A)} \quad (1)$$

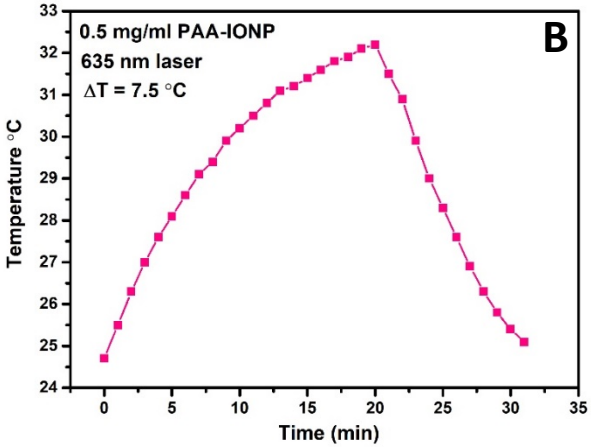
where h is heat transfer coefficient, S is the surface area, T_{max} and T_{surr} are the maximum temperature and surrounding temperature respectively. Q_o and I are the heat absorbed by the tube and the laser power density, whereas the optical density of each material denoted by A. The value of hS can be obtained using equation (2)

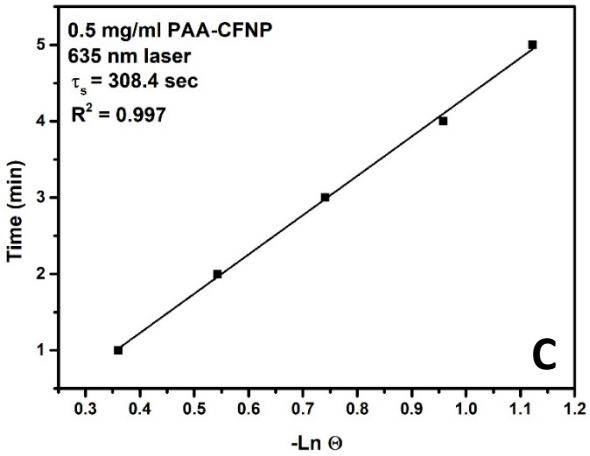
$$hS = \frac{mDCD}{\tau s} \quad (2)$$

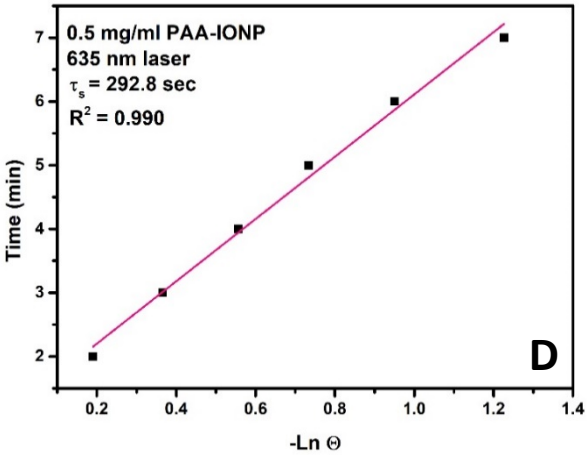
where m_D is mass and C_D is heat capacity of H_2O (4.2 J/g°C), while τ_s is the heat dissipation time constant. It can be calculated using equation (3)

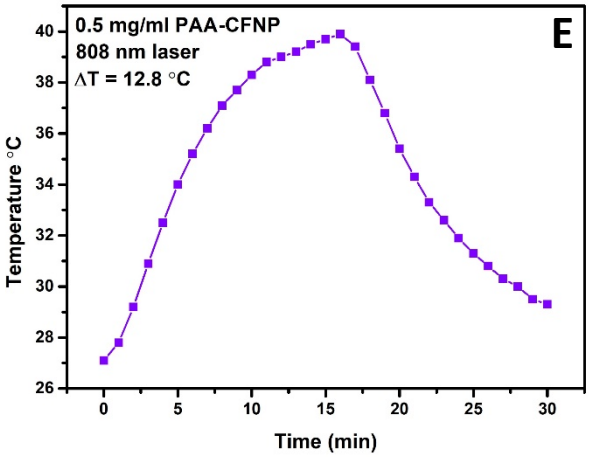
$$t = -\tau_s \ln\Theta = \tau_s \ln \frac{T - Tsurr}{Tmax - Tsurr} \quad (3)$$

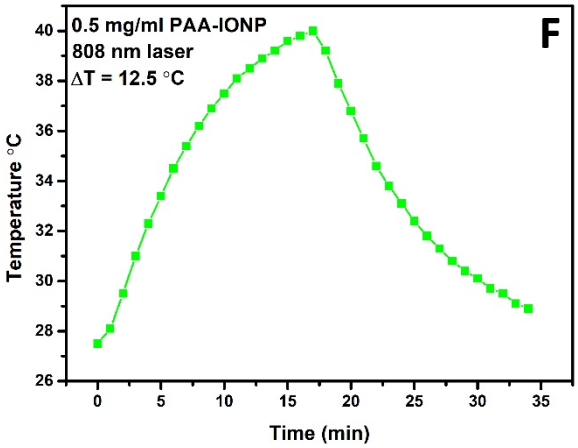

0.5 mg/ml PAA-CFNP
635 nm laser
ΔT = 8.6 °C
A
Temperature °C
Time (min)

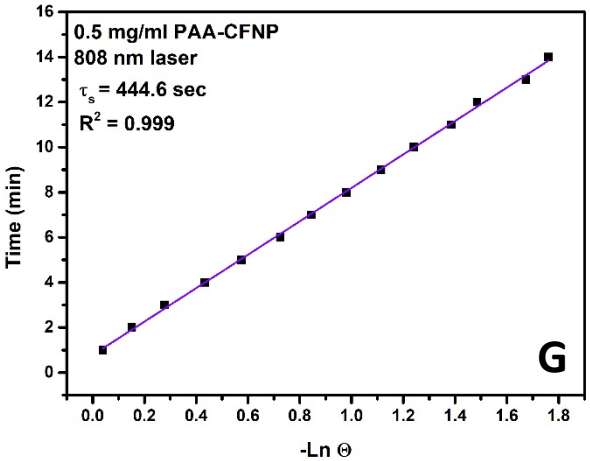

0.5 mg/ml PAA-IONP
635 nm laser
ΔT = 7.5 °C
B
Temperature °C
Time (min)


0.5 mg/ml PAA-CFNP
635 nm laser
τs = 308.4 sec
R2 = 0.997
C
Time (min)
-Ln Θ


0.5 mg/ml PAA-IONP
635 nm laser
τs = 292.8 sec
R2 = 0.990
D
Time (min)
-Ln Θ


0.5 mg/ml PAA-CFNP
808 nm laser
ΔT = 12.8 °C
E
Temperature °C
Time (min)


0.5 mg/ml PAA-IONP
808 nm laser
ΔT = 12.5 °C
F
Temperature °C
Time (min)


0.5 mg/ml PAA-CFNP
808 nm laser
τs = 444.6 sec
R2 = 0.999
G
Time (min)
-Ln Θ

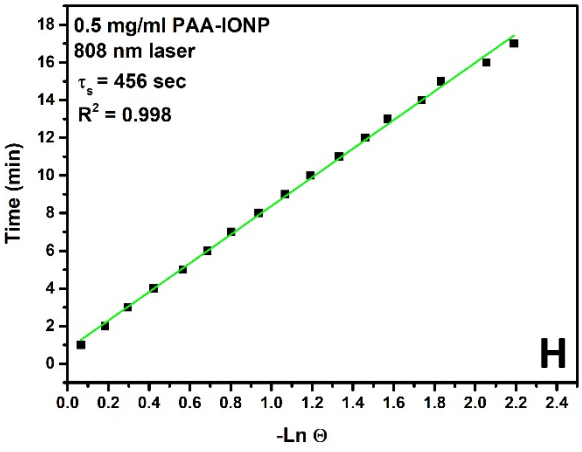

0.5 mg/ml PAA-IONP
808 nm laser
τs = 456 sec
R2 = 0.998
H
Time (min)
-Ln Θ

Figure S6: Photothermal conversion efficiency. (A-B and E-F) PCE calculations using 635 nm and 808 nm. (C-D and G-H) Plot of negative logarithm of cooling period with time (min) to calculate heat dissipation time constant of each sample.

S. No.	Nanoparticle	Concentration (mg/ml)	Size (nm)	Amplitude (kA/m)	Frequency (kHz)	SAR (W/g)	ILP (nHm^2/kg)	Ref.
1.	PAA-CFNPs	0.2	17	8.7	465.6	261.2	7.41	This study
		0.4				174.5	4.95	
		0.6				69.6	1.97	
		0.8				60.7	1.72	
2.	PMAO-CFNPs		13	23.9	450	297.4	1.16	25
3.	CFNPs		9	37.3	500	609	0.88	26
4.	CFNPs		9.7	24.8	700	577	1.34	27
5.	PAA-IONPs	0.2	18	8.7	465.6	104.5	2.96	This study
		0.4				65.3	1.85	
		0.6				31.3	0.88	
		0.8				16.1	0.45	
6.	PMA-IONP	0.5	8 ± 3	15.3	522.5	41.0	0.3	29
7.	PMA-ATA-IONP	0.5	8 ± 2	15.3	522.5	41.0	0.3	

*ATA- aminoterephthalic acid

* PMA- pyromellitic acid

Table S6: Comparison of SAR and ILP of CFNPs and IONPs at different magnetic field