

Supplementary Information

Selective and sensitive on-site colorimetric detection of 4,4' - Isopropylidenediphenol using non-enzymatic molecularly imprinted graphitic carbon nitride hybrids in milk and water samples

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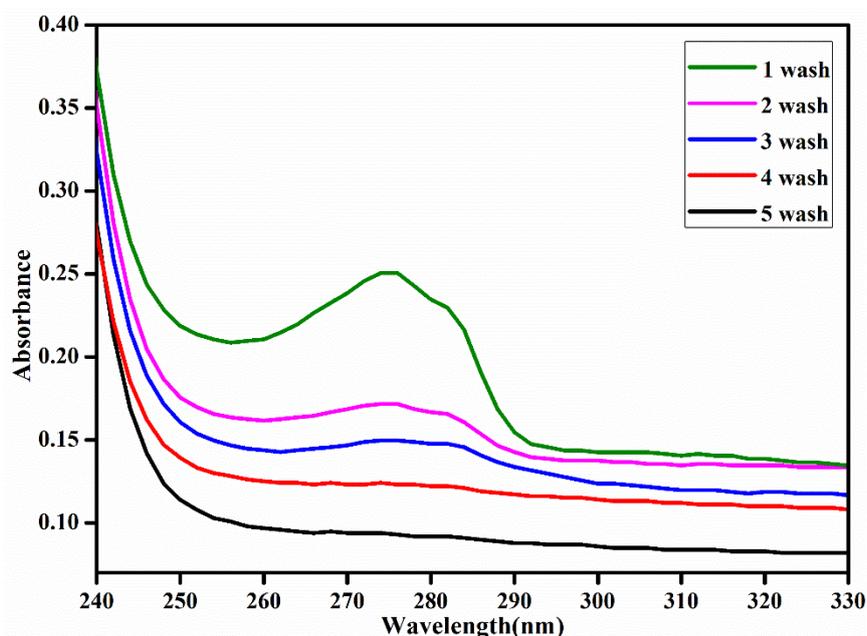


Fig. S1 Extraction of the template (BPA) from MIP@g-C₃N₄.

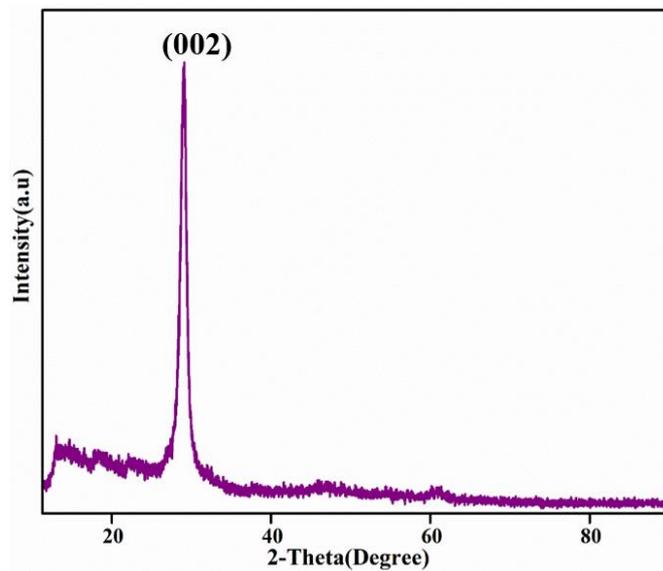


Fig. S2 XRD spectrum of g-C₃N₄.

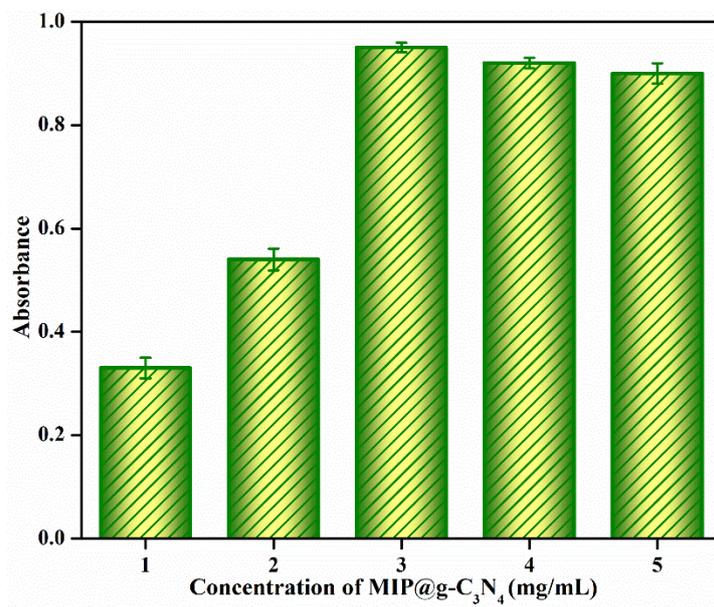


Fig. S3 Effect of the concentration of MIP@g-C₃N₄.

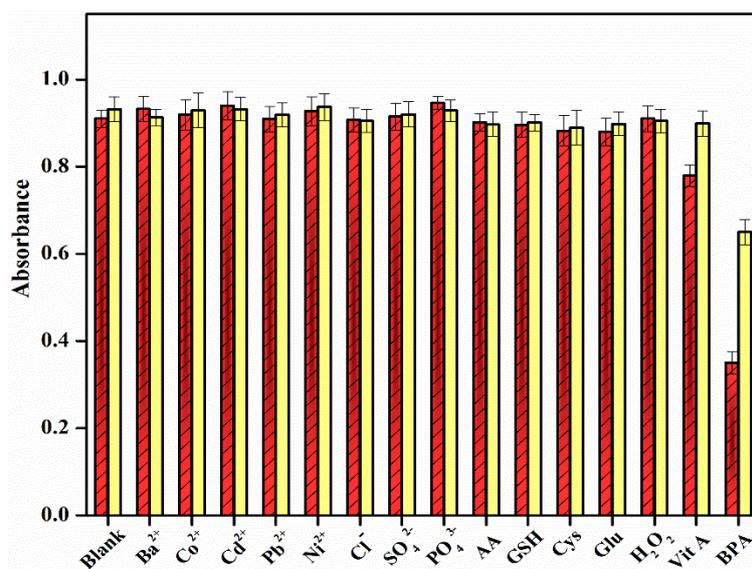


Fig. S4 Selectivity of MIP@g-C₃N₄ (red bar) and NIP@g-C₃N₄ (yellow bar) with BPA and interfering species.

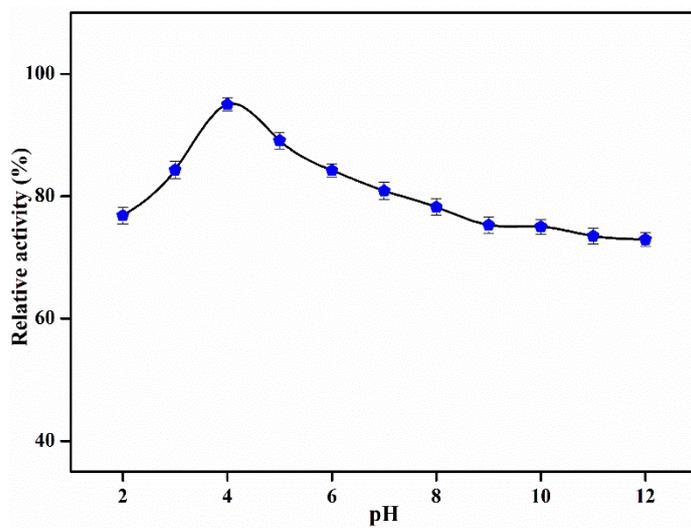


Fig S5. Stability analysis of MIP@g-C₃N₄ in different pH.

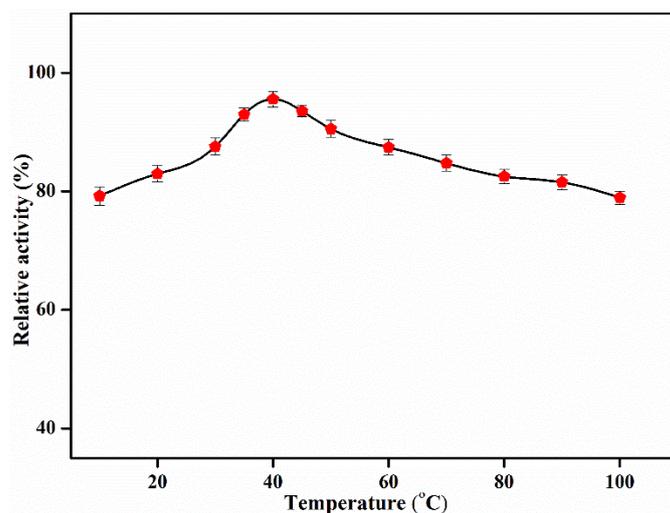


Fig S6. Stability analysis of MIP@g-C₃N₄ in different temperatures.

Kinetic analysis:

Kinetics studies were performed by determining the A₆₅₂ nm with respect to reaction time. In order to quantify the catalytic efficiency and affinity for TMB, steady-state kinetic parameters, including Michaelis-Menten's constant (K_m), [S] was the concentration of the substrate, and the maximum initial velocity value V_{max} , were calculated using a double-reciprocal method ($1/V = (K_m/V_{max}) \times (1/[S]) + 1/V_{max}$).¹ The K_m value and the V_{max} value of the MIP@g-C₃N₄ have been given in Table 1. The lower the K_m value is, the higher the affinity of the simulated object to the substrate. The higher the V_{max} value is, the higher the saturation reaction rate. Moreover, the obtained K_m value and the V_{max} value have been compared with other reported enzymes in order to show the efficiency of the MIP@g-C₃N₄ hybrid nanocomposite which is shown below:

Table S1 Comparison of K_m and V_{max} with other previously reported literature

Catalyst	Substrate	K_m (mM)	V_{max}	Reference
HRP	TMB	0.275	$1.24 (10^{-8} \text{ Ms}^{-1})$	2
	H_2O_2	0.214	$2.46 (10^{-8} \text{ Ms}^{-1})$	
g- C_3N_4	TMB	0.031	$1.35 (10^4 \text{ Ms}^{-1})$	3
	H_2O_2	4.565	$1.72 (10^4 \text{ Ms}^{-1})$	
MnSe-g- C_3N_4	TMB	0.137	$2.40 (10^{-3} \text{ s}^{-1})$	4
	H_2O_2	0.623	$2.85 (10^{-3} \text{ s}^{-1})$	
MIP@g- C_3N_4	TMB	0.122	$1.39 (10^{-8} \text{ Ms}^{-1})$	Current work
	H_2O_2	0.402	$1.9 (10^{-8} \text{ Ms}^{-1})$	

Detection of BPA in real samples

To determine BPA, we used this colorimetric detection platform in real-world samples such as human serum samples. The human serum samples were collected from a nearby healthcare clinic. The serum samples were diluted to 500- fold and then it was spiked with different concentrations of BPA. In addition, a recovery experiment using the standard addition approach was conducted, in which different BPA concentrations were introduced into the samples for analysis.

Table S2 Investigation of BPA detection in the human blood serum samples.

Sample	Spiked (nM)	Detected \pm SD	Recovery (%)
		BPA	BPA
Serum	5	$4.85^x \pm 0.3^y$	95.7
	10	$9.91^x \pm 0.15^y$	98.5

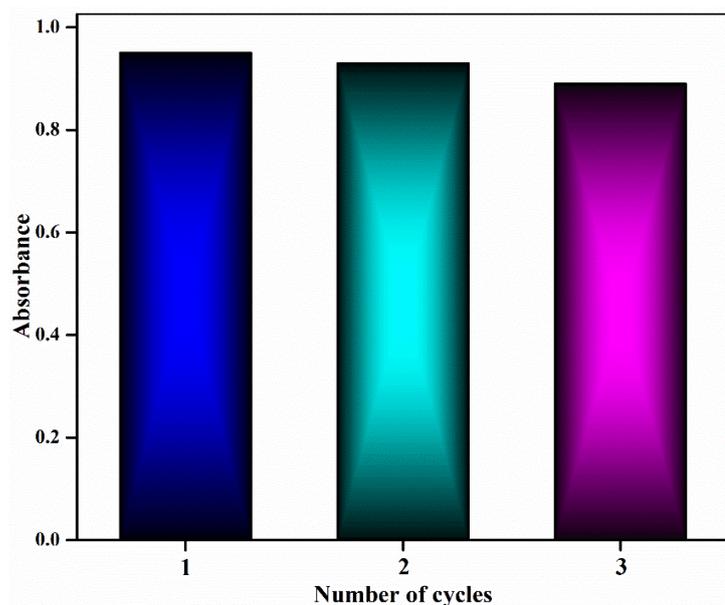


Fig. S7 Reproducibility of MIP@g-C₃N₄ nanocomposite colorimetric system.

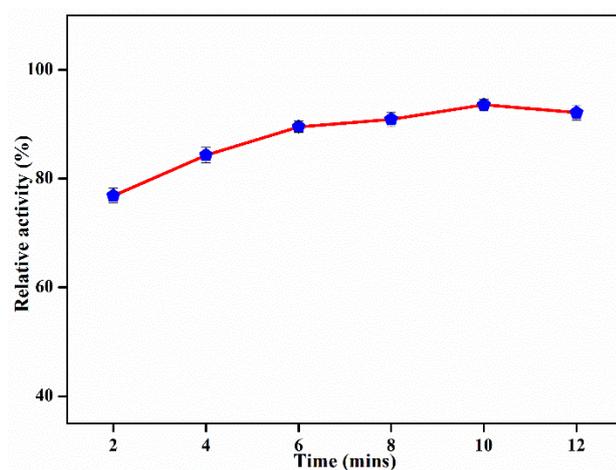


Fig. S8 Effect of the time

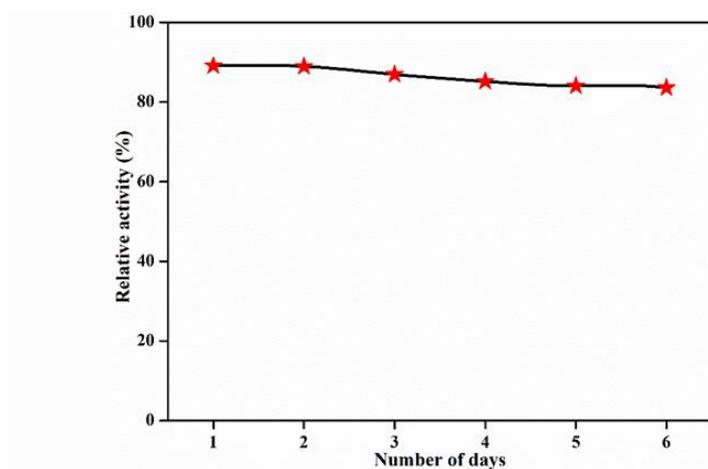


Fig. S9 Stability analysis of MIP@g-C₃N₄ in a number of days.

References:

1. C. Song, W. Ding, W. Zhao, H. Liu, J. Wang, Y. Yao and C. Yao, *Biosens. Bioelectron.*, 2020, **151**, 111983.
2. Y. Song, K. Qu, C. Zhao, J. Ren and X. Qu, *Adv. Mater.*, 2010, **22**, 2206–2210.
3. J. Tian, Q. Liu, A. M. Asiri, A. H. Qusti, A. O. Al-Youbi and X. Sun, *Nanoscale*, 2013, **5**, 11604–11609.
4. F. Qiao, Q. Qi, Z. Wang, K. Xu and S. Ai, *Sensors Actuators, B Chem.*, 2016, **229**, 379–386.