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Supplementary Materials

Computational Studies

Molecular Docking (MD) Calculations

Auto Dock Tools-1.5.7 software was used for dsDNA and MAL docking. Gauss View 5.0 and Gaussian 09 programs were used to draw and optimize the three-dimensional structure of MAL, respectively. Then Viewer Lite 5.0 program was used to prepare input files of Auto Dock Tools-1.5.7 software in pdb format. The three-dimensional structure of dsDNA with the code 423D was downloaded from Protein Data Bank (PDB) (http://www.rcsb.org). Other ligands and water molecules were removed from the dsDNA structure. To prepare MAL and dsDNA input files in pdbqt format, Auto Dock Tools-1.5.7 software was used. Colony charges were added to dsDNA and its non-polar hydrogens were also incorporated. The interaction points were set on dsDNA and MAL in dimensions of 55 × 45 × 61 Å with a grid spacing of 0.4 Å. The genetic algorithm parameters were set to 100 cycles and 150 population. Docking energy of dsDNA and MAL was obtained using Auto Dock Tools-1.5.7 software, and the three-dimensional structure obtained from MD was observed and analyzed with Discovery Studio 2016 Client software.

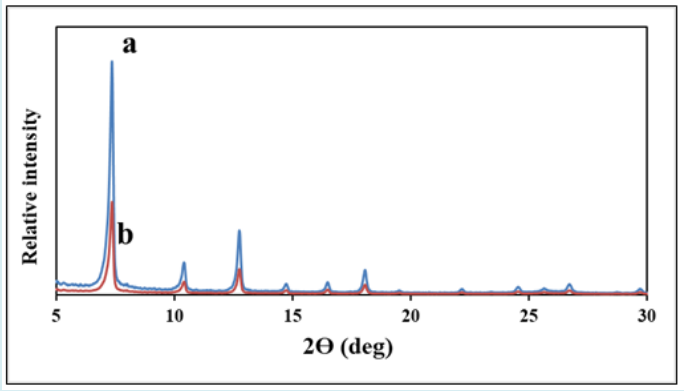

Figure S1: X-ray diffraction (XRD) patterns of ZIF-8 (a) and ZIF-8/CNT (b).

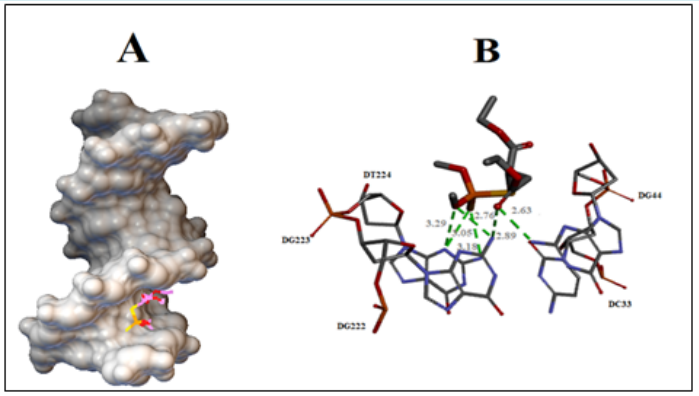

Figure S2: Location of MAL in the minor groove of dsDNA (A) and 3D structure of the MAL–dsDNA interaction (B).

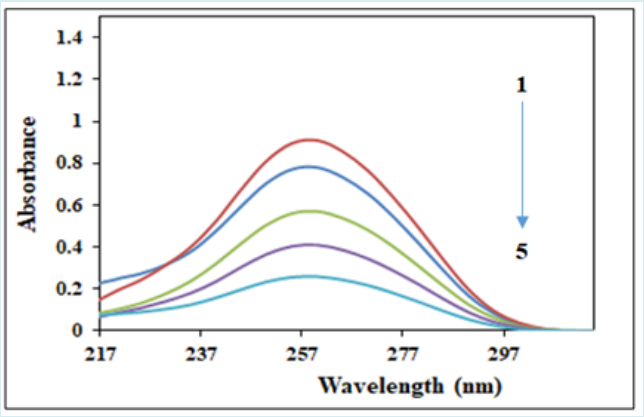

Figure S3: UV–visible spectrum of 140.00 µM dsDNA with increasing concentrations of MAL from 1 to 5.

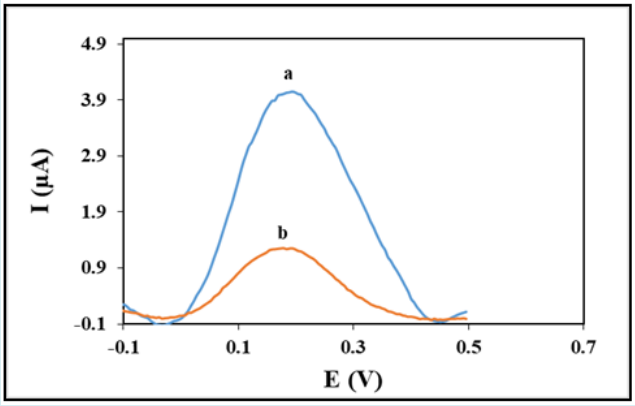

Figure S4: Differential pulse voltammetry (DPV) curves of ZIF-8/CNT/dsDNA/GCE (a) and ZIF-8/CNT/GCE (b) in 0.1 M phosphate buffer with pH = 7.0 after incubation in 2.00 µM MAL solution.

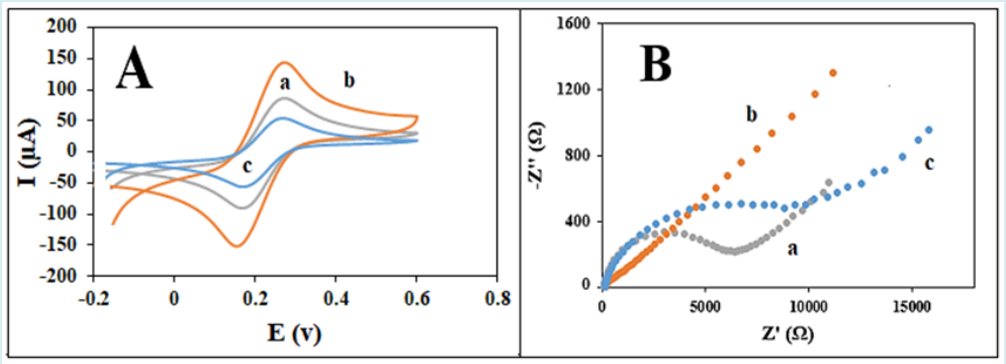

Figure S5: (A) Cyclic voltammograms (CVs) of bare GCE (a), ZIF-8/CNT-GCE (b), and ZIF-8/CNT/dsDNA-GCE (c) in 6 mmol L–1 [Fe(CN)6]3–/4– and 0.1 M KCl with a scan rate of 100 mV s–1.
(B) Electrochemical impedance spectroscopy (EIS) diagrams of bare GCE (a), ZIF-8/CNT-GCE (b), and ZIF-8/CNT/dsDNA-GCE (c) in 6 mmol L–1 [Fe(CN)6]3–/4– and 0.1 M KCl with a frequency range of 0.0001 to 10 kHz and an amplitude of 0.2 V.

Pesticide	Tolerance concentration (μM)
CPF	50
DZN	90
DLM	7.5
FNT	16

Table S1: The effect of interfering species on the measurement of MAL (2.00 μM).