Development of novel biochar derived from *Bacopa monnieri* leaves for adsorptive removal of pendimethalin herbicide from binary and ternary pesticide mixture

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Supplementary Information

Table S.1 Adsorption kinetic models equations and their parameters

Kinetic models	Linear	Non-linear	Kinetic parameters
PFO	$log(q_e - q_t) = logq_e - \frac{k_1}{2.303}$	$q_t = q_e - (1 - e^{k_1 t})$	q_t = Adsorbed amount at time t (mg g^{-1}) q_e = Adsorbed amount at equilibrium (mg g^{-1}) K_1 = Pseudo-first-order rate constant (min^{-1}) T = Time (min)
PSO	$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t$	$q_t = \frac{k_2 q_e^2 t}{1 + k_2 q_e t}$	q_t = Adsorbed amount at time t (mg g-1) q_e = Adsorbed amount at equilibrium (mg g-1) K_2 = Pseudo-second-order rate constant (g mg^{-1} min^{-1}) T = Time (min)
IPD	$q_t = C + K_{int} t^{1/2}$	$q_t = C + K_{int} t^{1/2}$	q_t = Adsorbed amount at time t (mg g^{-1}) K_{int} = Intra-particle diffusion rate constant (mg g^{-1} $min^{0.5}$) C = Boundary layer thickness (mg g-1) t = Time (min)

Table S.2 Adsorption isotherm models equations and their parameters

Isotherm models	Linear	Non-linear	Isotherm parameters
Langmuir isotherm	$\frac{1}{q_e} = \frac{1}{Q_0} + \frac{1}{Q_0 K_L C_e}$	$q_e = q_m K_L \frac{C_e}{1 + K_L C_e}$	q_e = Amount of PND adsorbed per gram of adsorbent at equilibrium (mg g^{-1}) Q_0/q_m = Maximum adsorption capacity K_L = Adsorption capacity constant Ce = adsorbent's equilibrium level (mg L^{-1})
Freundlich isotherm	$logq_e = logK_F + (1/n)logC_e$	$q_e = K_F C_e^{1/n}$	q_e = Quantity of PND absorbed at equilibrium (mg g^{-1}) K_F = Freundlich Contant (L mg^{-1}) Ce = Initial concentration of PND solutions (mg L^{-1}) 1/n = Adsorption intensity
Temkin isotherm	$q_e = \frac{RT}{b_T} ln\, A_T + \frac{RT}{b_T} ln\, C_e$	$q_e = \frac{RT}{b_T} ln A_T C_e$	q_e = Adsorbed amount at equilibrium C_e = Initial equilibrium concentration of the adsorption (mg L^{-1}) A_T = Temkin constant b_T = Related to heat of adsorption R = Universal gas constant T = Temperature (K)

Table S.3 Adsorption isotherm models equations and their parameters

Parameter	Range	Fixed / Variable Conditions	Purpose
Initial PND concentration (mg L^{-1})	30, 40, 50, 60, 70	pH = 6; Dose = 5 mg; Contact time = 150 min	To determine the effect of initial concentration and equilibrium adsorption capacity
Contact time (min)	0, 30, 60, 90, 120, 150	C_0 = 40 mg L^{-1}; pH = 6; Dose = 5 mg	To study adsorption kinetics
Solution pH	2, 4, 6, 8, 10, 12	C_0 = 40 mg L^{-1}; Dose = 10 mg; Time = 150 min	To study effect of surface charge and ionization on adsorption
Adsorbent dosage (mg)	2.5, 5, 10, 15, 20	C_0 = 40 mg L^{-1}; pH = 6; Time = 150 min	To evaluate optimum BMBC amount for maximum removal
Ionic strength	NaCl, KCl, $CaCO_3$, $MgCO_3$, $ZnSO_4$ (1 M)	C_0 = 40 mg L^{-1}; pH = 6; Time = 150 min	To assess the effect of ionic species on adsorption efficiency
Pesticide mixtures	Binary (PND + PFC, PND + H-20); Ternary (PND + PFC + H-20)	20 & 40 mg L^{-1} of each pesticide	To evaluate competitive adsorption in multi-component system

Table S.4 Comprehensive Summary of Chemicals used in this study

Chemical / Material	Grade / Purity	Supplier	Application
Bacopa monnieri leaf powder	—	Local market, Patan, Gujarat	Biochar precursor
Pendimethalin (PND)	Commercial formulation	TATA Panida, India	Target pollutant
Profenocombi (PFC: profenofos + cypermethrin)	Commercial	Molraxa Agro Chemicals	Binary/ternary mixture studies
H-Twenty (H-20: chlorpyrifos)	Commercial	Hakuba Organics Pvt. Ltd.	Binary/ternary mixture studies
NaCl	AR grade	SRL Pvt. Ltd.	Ionic strength study
KCl	AR grade	SRL Pvt. Ltd.	Ionic strength study
$CaCO_3$	AR grade	SRL Pvt. Ltd.	Ionic strength study
$MgCO_3$	AR grade	SRL Pvt. Ltd.	Ionic strength study
$ZnSO_4$	AR grade	SRL Pvt. Ltd.	Ionic strength study
HCl (0.1 M)	Analytical grade	SRL Pvt. Ltd.	pH adjustment
NaOH (0.01 M)	Analytical grade	SRL Pvt. Ltd.	pH adjustment

Table S.5 Comprehensive Summary of Instrumentation and Operating Parameters

Instrument	Model / Manufacturer	Operating Parameters	Purpose
Muffle furnace	—	600 °C; 2 h residence; heating rate 10 °C min^{-1}	Biochar synthesis
X-Ray Diffractometer (XRD)	Bruker D8 Advance	2θ: 3–90°; Cu Kα source	Crystallinity & elemental phases
SEM	FEI NOVA NanoSEM 450	Magnification: 25,000× & 100,000×; 20 kV; WD: 7 mm	Morphology, pore structure
FTIR Spectrometer	PerkinElmer S6500	4000–550 cm^{-1}; 16 scans	Functional group analysis
UV–Vis Spectrophotometer	Labman LMSPUV1900	λmax for PND: 452 nm	Concentration measurement
pH Meter	ELICO LI 617	Standard calibration	pH & pHZPC determination
Centrifuge	REMI	5000 rpm; 10 min	Separation of BMBC
Incubator shaker	REMI CIS-24 BL	25 ± 2 °C; 150 rpm	Batch adsorption experiments

Table S.6 Comprehensive Summary of Biochar preparation conditions

Step	Condition / Parameter
Drying	Shade-dried leaves, ground to powder
Sieving	100-mesh stainless steel (<150 μm)
Pyrolysis temperature	600 °C
Heating rate	10 °C min^{-1}
Residence time	2 h
Oxygen availability	Limited (closed crucible)
Pressure	Ambient
Cooling	Natural cooling inside furnace
Final processing	Mild crushing, re-sieving, airtight storage
Biochar yield	21.87%

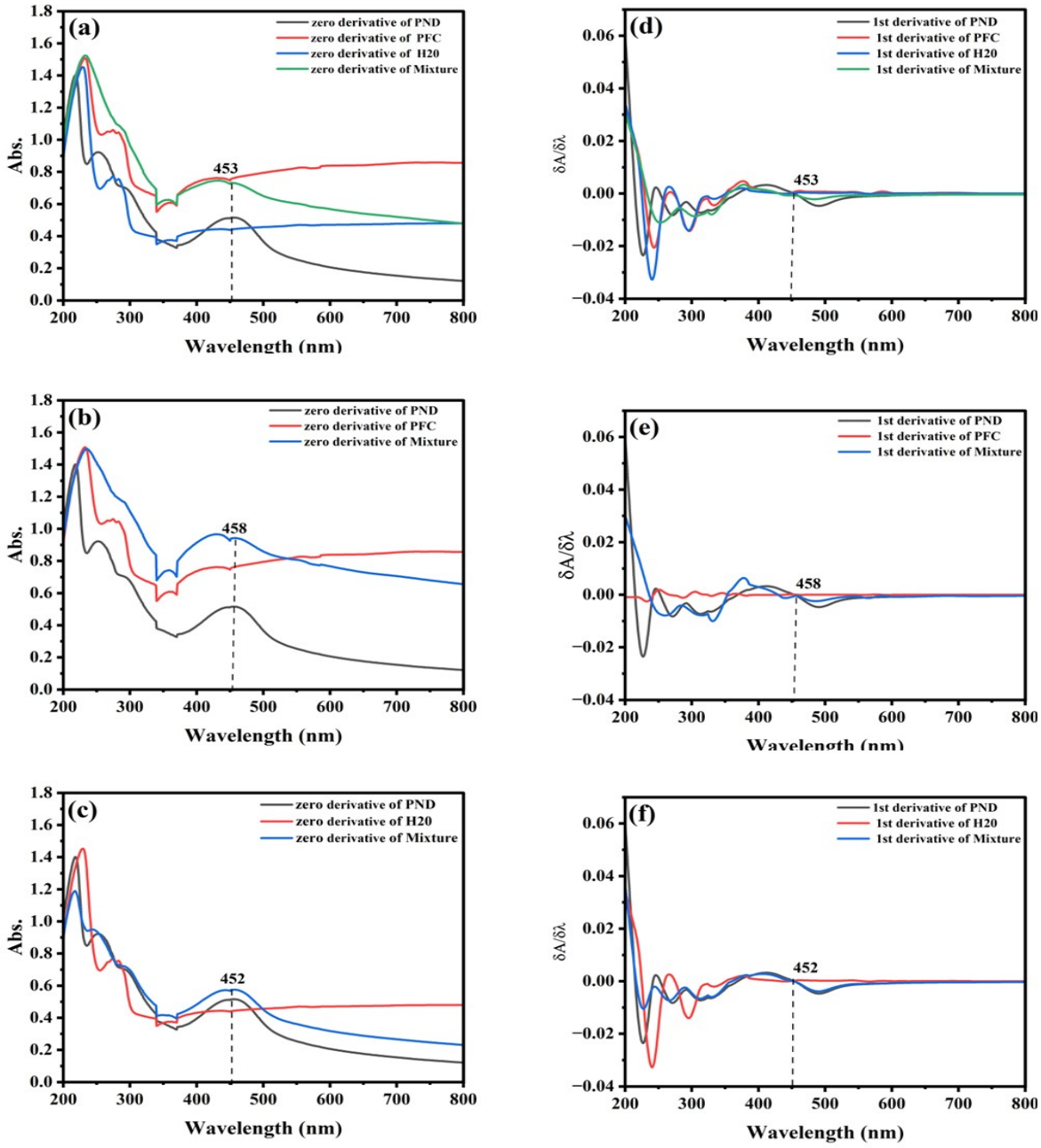

Fig. S1 Zero-derivative UV-Vis spectra (a-c) and first-derivative spectra (d-f) of PND at 20 mg L^{-1} with PFC, H20, and their mixtures.

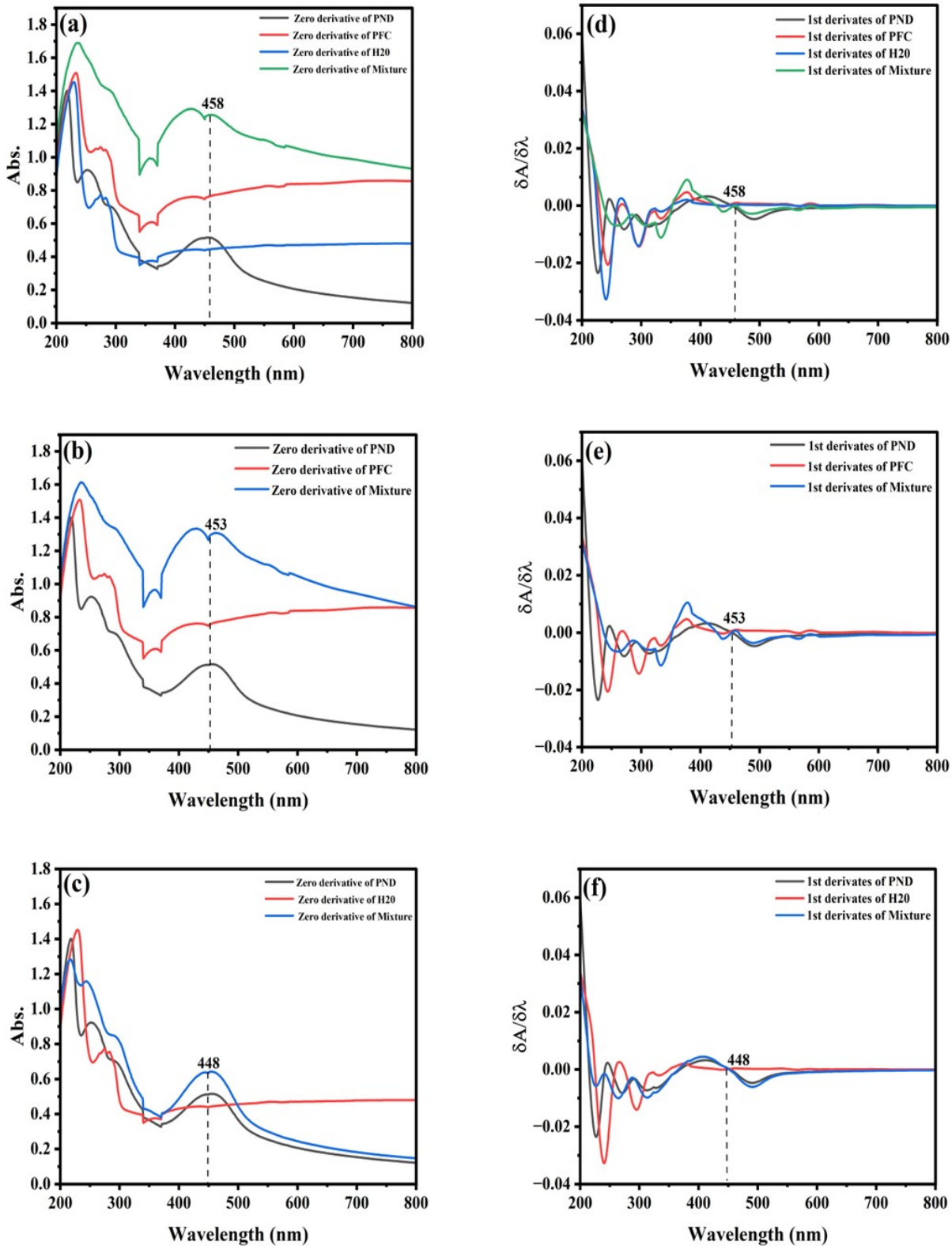

Fig. S2 Zero-derivative UV-Vis spectra (a-c) and first-derivative spectra (d-f) of PND at 40 mg L^{-1} with PFC, H20, and their mixtures.

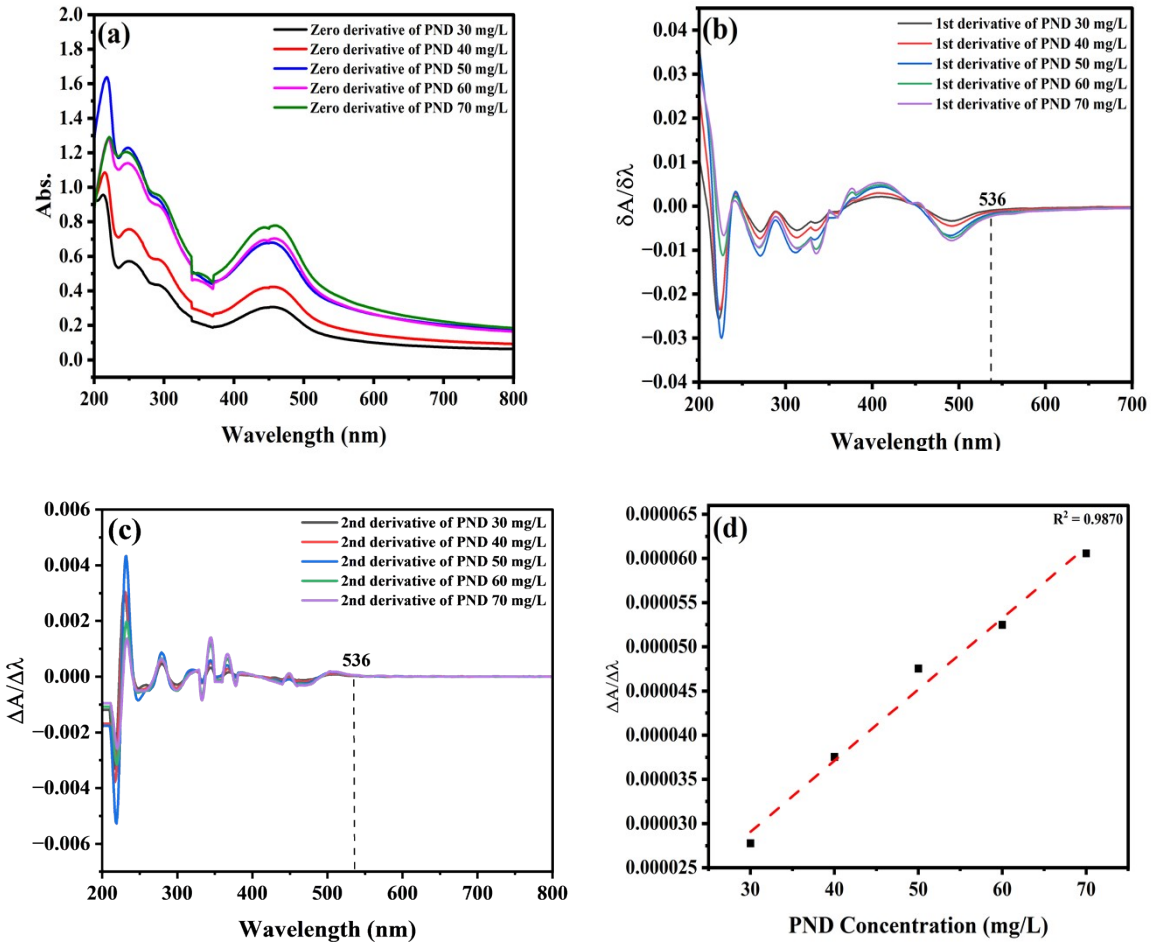

Fig. S3 Zero-derivative UV-Vis spectra (a), first-derivative spectra (b), second-derivative spectra (c), and calibration curve (d) for PND at various concentrations.

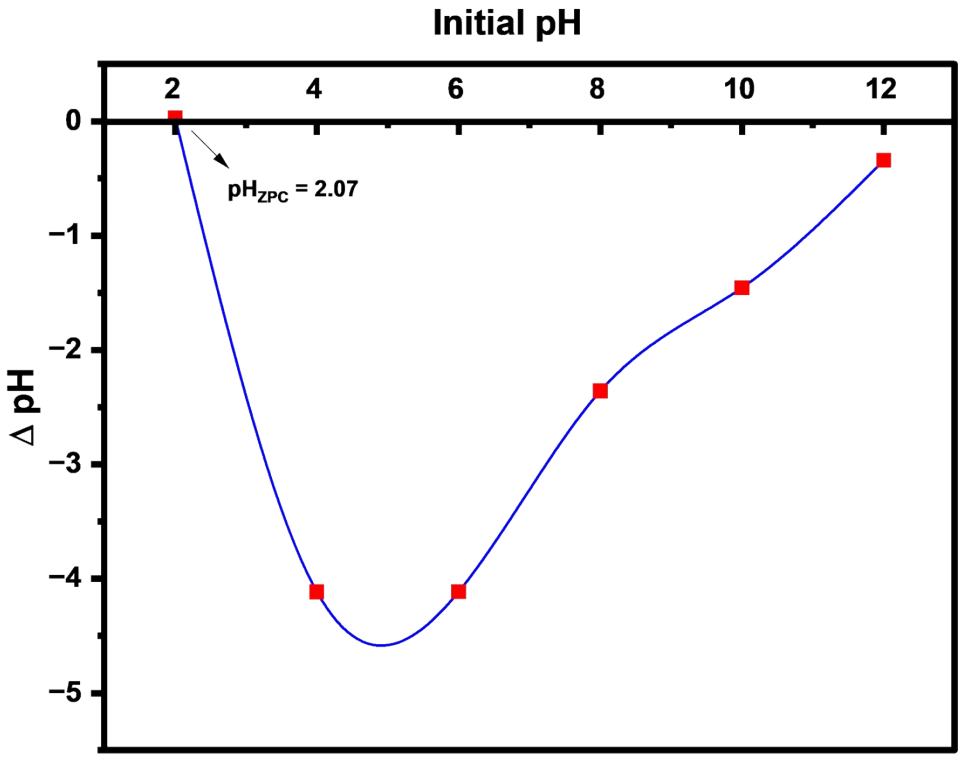

Fig. S4. pH_{ZPC} of BMBC using pH drift method.