Supplementary Information

Green synthesis of zinc oxide nanoparticles: Exploring catalytic and antibacterial potential

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1. Experimental.

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4.1 ^{1}H-NMR and ^{13}C-NMR.

1. Experimental

1.1 Materials and Methods:

All chemicals utilized were of analytical grade and employed without any additional purification. Deionized water (DI) was consistently used throughout the experiment. The biosynthesized ZnO NPs were used to explore their surface, structural and optical properties and catalytic activity. The biosynthesized ZnO NPs were first characterized by UV-vis absorption spectroscopy (Shimadzu UV-3600, Japan). The functional groups of the ZnO NPs were recorded by using Fourier Transform-Infrared (FT-IR) spectrometer (Bruker ALPHA). The crystalline nature of the ZnO NPs synthesized using *Thevetia peruviana* (*T. peruviana*) was studied by X-ray diffraction (XRD) spectroscopy (AXS-D8 Advance, Bruker Ltd Germany). Morphological and elemental compositions of prepared ZnO NPs were studied by Field Emission-Scanning Electron Microscopy (FE-SEM) (MIRA3 LMH, TESCAN, Brno, Czech Republic, EU) integrated Energy-despersive X-ray (EDX) spectroscopy. The size and morphologies of ZnO NPs were analyzed by High Resolution-Transmission Electron Microscope (HR-TEM) (JEOL JEM2100F) and selected area diffraction (SAED) pattern were also achieved. The particle size of synthesized ZnO NPs was calculated using ImageJ software. The progress of the reaction was monitored by Thin Layer Chromatography (TLC). The ^{1}H and ^{13}C spectra of isolated compounds were recorded by the 400 MHz Jeol solid state spectrometer in $CDCl_3$ solvent at room temperature and the use of TMS as an internal standard. Melting points were determined using the Lab Star apparatus.

2. General procedure for synthesis of Zinc Oxide Nanoparticles (ZnO NPs)

Here, the biosynthetic method was used to synthesize ZnO NPs. 25 mL of 0.5 M $ZnSO_4.5H_2O$, was added drop-wise into the 25 mL of plant extract for 15 min with continuous stirring at room temperature and basic pH. The color of the solution was changed from brown to soft grayish, it was indicated that the ZnO NPs were synthesized in that reaction mixture. The solution was aged for 12 hrs at room temperature, centrifuged at 6000 rpm for 15 min and washed with (3 X 25 mL) Deionized water (DI) and with ethanol (1 X 20 mL), and then catalyst was dried in an oven at 80 °C for 1 hr. The dried powder was transferred to a crucible and calcinated at 400 °C for 2 hrs. The obtained product was white in color, which stored for further applications.

3. General procedure for synthesis of xanthene derivatives

An oven-dried Schlenk flask, equipped with a magnetic stir bar was charged with aromatic aldehyde (1.0 mmol), dimedone (2.0 mmol), and ZnO nanocatalyst (25 mol%) in ethanol-water (90:10) solvent system was stirred at room temperature. After consumption of starting materials as determined by TLC analysis [Petrolium ether:ethyl acetate (7:3)], the reaction mixture was extracted with ethyl acetate (3 X 5.0 mL). The combined organic layer was collected, dried over anhydrous Na_2SO_4 and concentrated in a vacuum to afford the product which was purified by silica gel column chromatography (eluent: n-hexane/ethyl acetate). The structure of organic product was confirmed by the analysis of using varied spectral techniques including ^1H, ^{13}C-NMR and mass spectra.

4. Characterization and spectral analysis of novel xanthene derivative.

4.1. 9-(3-Benzyloxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H) dione

(Table 2, entry 17)**:** The compound 3q is prepared using the usual procedure.

Yield: 98%; **Melting Point:** 170-172 ^0C;

^1H NMR (400 MHz, $CDCl_3$): δppm= 0.999 (s, 6H, CH_3), 1.02 (s, 6H, CH_3), 2.19 (s, 2H, $2CH_2$), 5. 01 (s, 1H, CH), 4.74 (s, 2H, $2CH_2$), 6.72–7.41 (m, Ar-CH)

^{13}C NMR (400 MHz, $CDCl_3$): δppm= 27.72, 29.41, 32.03, 32. 41, 41.10, 51.00, 70.16, 77. 25,113. 09, 115.72, 121.52, 137.50, 128.74, 129.15, 145.95, 58.94, 162.47, 196.62 ppm.

MS (EI), m/z: 265 [M^+].

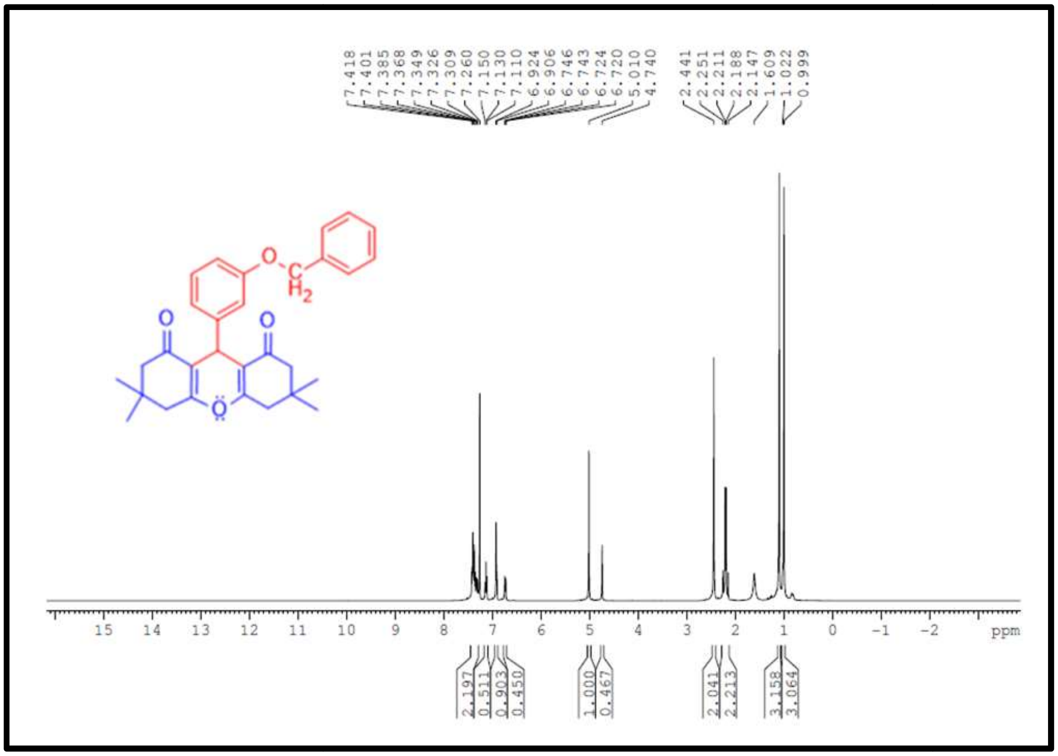

Fig. S1. ^{1}H Spectrum of Entry 3q

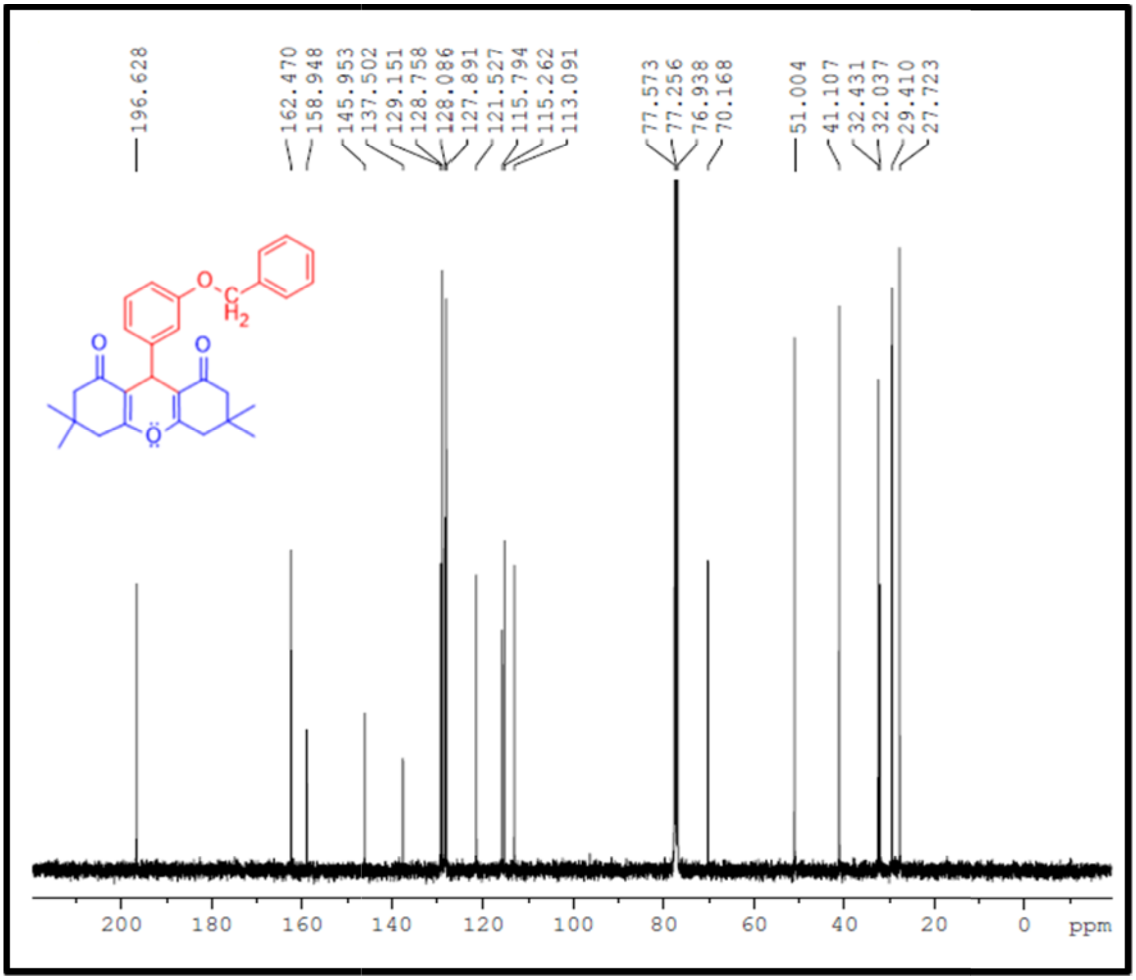

Fig. S2. ^{13}C Spectrum of Entry 3q

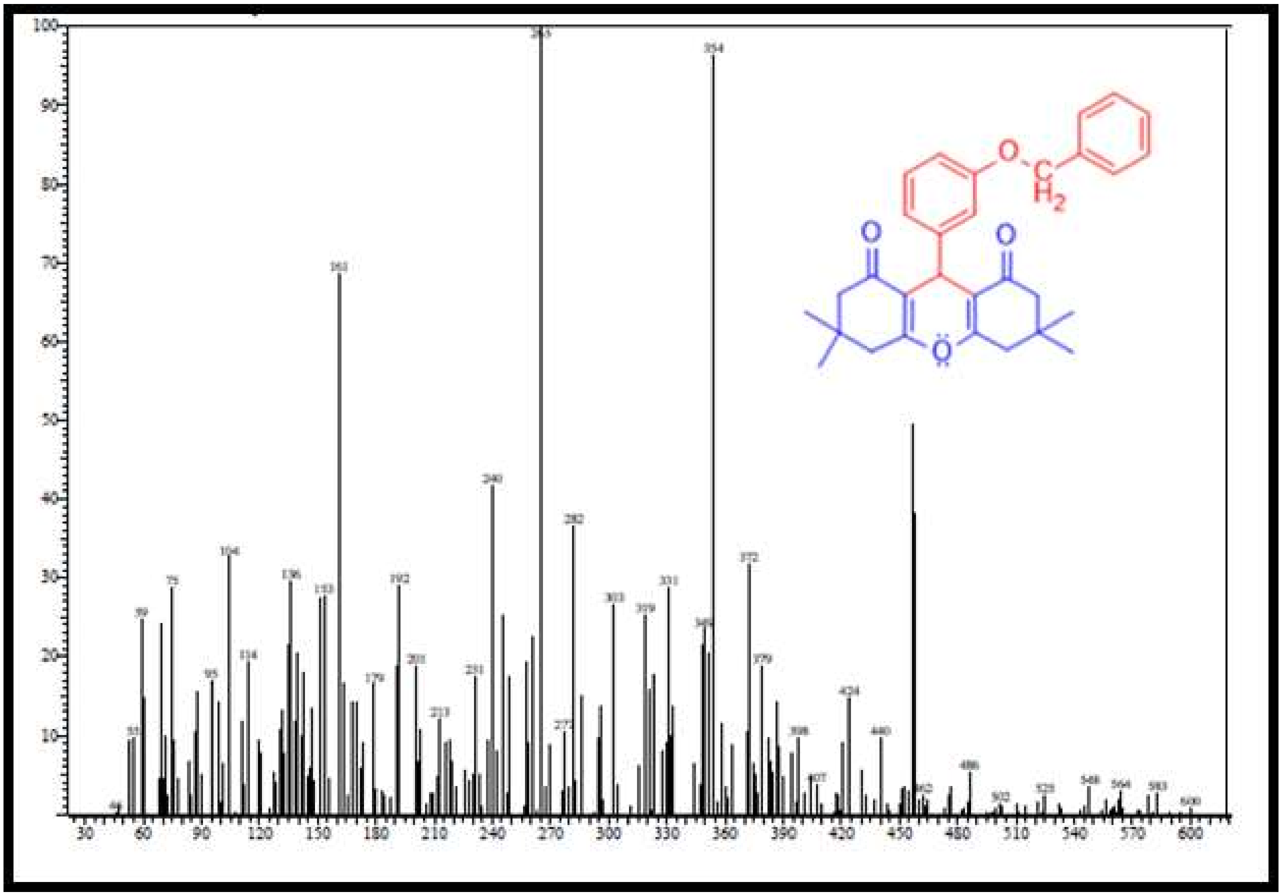

Fig. S3. Mass Spectrum of Entry 3q