Biosynthesized $\delta$-Bi$_2$O$_3$ Nanoparticles from Crinum viviparum Flower Extract for Photocatalytic Dye Degradation and Molecular Docking

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ABSTRACT: Bioinspired delta-bismuth oxide nanoparticles ($\delta$-Bi$_2$O$_3$ NPs) have been synthesized using a greener reducing agent and surfactant via co-precipitation method. The originality of this work is the use of Crinum viviparum flower extract for the first time for the fabrication of NPs, which were further calcined at 800 °C to obtain $\delta$-Bi$_2$O$_3$ NPs. Physicochemical studies such as FTIR spectroscopy and XPS confirmed the formation of Bi$_2$O$_3$ NPs, whereas XRD and Raman verified the formation of the cubic delta ($\delta$) phase of Bi$_2$O$_3$ NPs. However, HRTEM revealed the spherical shape with diameter 10–20 nm, while BET studies expose mesoporous nature with a surface area of 71 m$^2$/gm. The band gap for $\delta$-Bi$_2$O$_3$ NPs was estimated to be 3.45 eV, which ensured $\delta$-Bi$_2$O$_3$ to be a promising photocatalyst under visible-light irradiation. Therefore, based on the results of physicochemical studies, the bioinspired $\delta$-Bi$_2$O$_3$ NPs were explored as active photocatalysts for the degradation of toxic dyes, viz., Thymol blue (TB) and Congo red (CR) under visible-light irradiation. The study showed 98.26% degradation of TB in 40 min and 69.67% degradation of CR in 80 min by $\delta$-Bi$_2$O$_3$ NPs. The photogenerated holes and electrons were found responsible for this enhancement. Furthermore, molecular docking investigations were also performed for $\delta$-Bi$_2$O$_3$ NPs to understand its biological function as New Delhi metallo-$\beta$-lactamase 1 (NDM-1) [PDB ID 5XP9] enzyme inhibitor, and studies revealed good interaction with various amino acid residues and found good hydrogen bonding with a fine pose energy of $-3.851$ kcal/mole.

INTRODUCTION

The biogenic synthesis of nanomaterials is laudable and challengeable because it lessens the employment of toxic chemicals. Diverse bioinspired syntheses were developed employing microorganisms and plant extracts (i.e., flowers, leaves, fruits, peels, seed, roots, and stem). Among these, plant-mediated synthesis of nanomaterials is a faster, straightforward, inexpensive, and harmless technique. However, the complexity of the extracts is due to the presence of several types of phytochemicals that require an exhaustive characterization of new nanomaterials obtained.1 Interestingly, the phytochemicals present in plant extracts (i.e., terpenoids, alkaloids, phenols, tannins, flavonoids, saponins, secondary metabolites, etc.) would play different roles during the synthesis like surfactant, reducing, capping, and stabilizing agents. According to recent literature investigations, phytochemicals are involved in the synthesis of ultrasmall particles. Indeed, biogenic syntheses of various metal/metal oxide nanoparticles were widely reported.2–8 However, there are no reports on the biogenic synthesis of Bi$_2$O$_3$ NPs; therefore, the present work focuses on the bioinspired synthesis of Bi$_2$O$_3$ NPs using the flower extract of Crinum viviparum as a green reducer and surfactant.

As per reports, several semiconductor-based materials have been applied as photocatalysts in diverse applications.9–18 Among semiconducting materials, Bi$_2$O$_3$ nanomaterials are gaining significant interest in the areas of fuel cells, ceramics, sensors, optoelectronics, energy storage, and photocatalysis as they have a large band gap, ionic conductivity, dielectric-permittivity, photoconductivity, morphology, and so forth.19–24 Basically, Bi$_2$O$_3$ occurs in six polymorphs with different band gaps: monoclinic $\alpha$-Bi$_2$O$_3$ (stable at 730 °C), face-centered cubic $\delta$-Bi$_2$O$_3$ (stable at 730–825 °C), tetragonal $\beta$-Bi$_2$O$_3$, BCC $\gamma$-Bi$_2$O$_3$, triclinic $\epsilon$-Bi$_2$O$_3$, and orthorhombic $\omega$-Bi$_2$O$_3$.25 The $\delta$-Bi$_2$O$_3$ has an FCC arrangement with fluorite.

Received: March 23, 2022
Accepted: May 25, 2022
Published: June 8, 2022
structure, wherein 75% oxygen occupied in a tetrahedral manner. The remaining 25% vacant space provides an exceptionally high ionic conductivity to the $\delta$-$\text{Bi}_2\text{O}_3$ phase. Therefore, among the polymorphs, $\delta$-$\text{Bi}_2\text{O}_3$ is a promising contender for photocatalyst.\(^{26}\) Besides, it possesses the highest conductivity compared to any other metal oxide materials. This allows an efficient movement of photoexcited charge carriers from the bulk via redox reactions.\(^{27}\) Of course, efficient photocatalysis could be possible because of the effective migration of charge carriers. An efficient visible-light photocatalytic performance of material also depends on the surface morphology, crystallographic phase, and manufacturing techniques. Also, another important factor is the porous nature of the material because of the associated advantages such as large surface area and porous network, which makes them a potential candidate for various applications. As in the field of photocatalysis, a large surface area provides a large number of surface sites and improves mass transfer.\(^{28-33}\)

There are numerous reports documented on conventionally synthesized different phases of $\alpha$, $\beta$, $\gamma$, and $\delta$-$\text{Bi}_2\text{O}_3$ nanoparticles for photocatalytic degradation of toxic dyes;\(^{34-39}\) however, there are no reports available on bioinspired $\delta$-$\text{Bi}_2\text{O}_3$.

Figure 1. Schematic route for the biosynthesis of $\delta$-$\text{Bi}_2\text{O}_3$ NPs using the flower extract of C. viviparum.

Figure 2. (a) XRD pattern, (b) Raman spectrum, (c) FT-IR spectrum, and (d) DRS; the inset is the Kubelka–Munk plot for the band gap estimation of $\delta$-$\text{Bi}_2\text{O}_3$ NPs.
NPs for photocatalytic application. Keeping this perspective in mind, this is the first time we reported bioinspired \textit{C. viviparum}-assisted $\delta$-Bi$_2$O$_3$ NPs (Figure 1) for visible-light-driven photocatalytic degradation of toxic dyes. Also, $\delta$-Bi$_2$O$_3$ NPs have been widely applied for biological activities; therefore, to evaluate $\delta$-Bi$_2$O$_3$ NPs for biological functions, molecular docking investigation has been performed on protein crystal structure (NDM-1) PDB ID 5XP9 having natural inhibitor Bi$^{+++}$ (ligand BS3). It was found that Bi (III) exerts anti-MBL activity in vitro and also it had good interaction with amino acid residues 512 THR, 82 GLN, 189 VAL, 121 THR, 131 LEU, 192 VAL, 91 GLN, 82 ILE, 111 SER, 199 LEV, 142 VAL, and 143 ALA, all having a hydrogen-bonding distance of about 2.0 Å, showing good interaction property with the best ligand pose energy of $-3.851$ kcal/mole.

### RESULTS AND DISCUSSION

Exploring Structural Composition of Biosynthesized $\delta$-Bi$_2$O$_3$ NPs. The X-ray diffraction (XRD) pattern of $\delta$-Bi$_2$O$_3$ (Figure 2a) has sharp peaks at $2\theta = 27$, 46, and 55° corresponding to $(hkl)$ values (111), (220), and (311), confirming the existence of cubic delta ($\delta$) phase of Bi$_2$O$_3$. The additional peaks that were obtained might be due to the plant extract impurity. The crystallite size of $\delta$-Bi$_2$O$_3$ was estimated at about ~12 nm using the Debye–Scherer equation. The Raman spectrum (Figure 2b) shows the characteristic peak positioned at 619 cm$^{-1}$ assigned to the $\delta$-phase of Bi$_2$O$_3$ with fluorite structure, which is well supported by XRD data. The peak positioned at 116, 221, and 315 cm$^{-1}$ can be assigned to bismuth–oxygen–bismuth (Bi–O–Bi) and bismuth–oxygen (Bi–O) of Bi$_2$O$_3$ NPs. FT-IR spectrum

![Figure 3. XPS (a) survey spectrum, (b) Bi 4f spectrum, (c) C 1s spectrum, and (d) O 1s spectrum of $\delta$-Bi$_2$O$_3$ NPs.](image)

![Figure 4. (a) SEM and (b) HRTEM micrographs and (c) N$_2$ adsorption/desorption isotherm of $\delta$-Bi$_2$O$_3$ NPs; the inset is the pore size distribution curve.](image)
(Figure 2c) shows broad peaks at 750 and 400 cm\(^{-1}\), which can be ascribed to bismuth–oxygen–bismuth (Bi–O–Bi) and bismuth–oxygen (Bi–O) vibrations, respectively. The weak peak observed at 1415 cm\(^{-1}\) might be due to the plant extract impurity. The diffuse reflectance spectrum (Figure 2d) mainly exhibited absorption at 413 nm that confirmed the δ-Bi\(_2\)O\(_3\) material. The Kubelka–Munk plot was adopted to estimate the band gap of NPs, which is shown as an inset in Figure 2d, and the band gap was estimated to be 3.45 eV, indicating that the δ-Bi\(_2\)O\(_3\) material can be a promising photocatalyst under visible-light irradiation.

Next, the spectra obtained from XPS study are presented in Figure 3a–d, to explore the chemical composition and oxidation states of biosynthesized material. Figure 3a shows the obtained survey spectrum for the biosynthesized δ-Bi\(_2\)O\(_3\) NPs, and peaks were obtained for Bi, O, and C which reveals that these are the main elements making the chemical composition of the biosynthesized δ-Bi\(_2\)O\(_3\) NPs. The XPS spectrum of Bi4f shown in Figure 3b contains two peaks at 158.7 and 163.8 eV, which correspond to the binding energies of Bi 4f\(_{7/2}\) and Bi 4f\(_{5/2}\) of Bi\(_2\)O\(_3\).\(^{41}\) Accordingly, the O1s XPS spectrum (Figure 3d) has a peak at 529.6 eV, which confirmed the existence of Bi–O linkage in Bi\(_2\)O\(_3\) that is also supported by FT-IR spectra.\(^{41}\) In addition, Figure 3c shows the C 1s XPS spectrum, having a peak at 284.6 eV, which corresponds to C–C,\(^{42}\) that may be present due to the plant extract impurity or the advantages of carbon.
Detailed Morphology Investigation of Biosynthesized δ-Bi₂O₃ NPs. The surface behavior, particle sizes, surface topography, surface area, and porosity of the biosynthesized light-yellow-colored cubic δ-Bi₂O₃ material were examined by SEM, TEM, and BET techniques. SEM micrographs obtained for the δ-Bi₂O₃ material are shown in Figure 4a, which reveals the small rock-type microstructure morphology containing a number of holes. Several microscopic holes are present on the surface of the microstructure, and these holes were found to have a nonuniform size of about 5–8 µm. These microscopic holes on the material surface were generated during the biosynthesis with the assistance of several phytochemicals present in the flower extract, which acted as surfactants and stabilizing agents. This microscopic hole formation on the material surfaces may also depend on the period of aging and calcination. It might be possible due to the orientation, interaction, and fusion of materials with phytochemicals surfactants that lead to microscopic hole formations. The development of nonuniform microscopic holes on the material surfaces can also be due to the homogeneous nucleation with constant and prolonged heating at higher temperatures. In the conventional heating mode, time for nucleation might be sufficient, but varied heat zones led to the formation of bigger particles and wider distribution. Conceivably, this could be possible due to capping, surfactants, structure-directing, and protecting agents present in the flower extract. Besides, the hole-formatted materials are more active for catalytic and adsorption activity. It is already well known.

Figure 6. (a) Optimization of CR concentration, (b) catalyst dose optimization, (c) rate constant, (d) degradation efficiency, (e) changes in UV–vis absorption pattern of CR with respect to time, and (f) scavenging study of δ-Bi₂O₃ NPs under visible irradiation.
that a hole-formatted material always enhances the degradation activity of dyes, as it uses inner–outer surfaces.46

Further, the HRTEM image (Figure 4b) revealed the nearly monodispersed spherical shape of nanoparticles with a diameter of 10–20 nm. Further, lattice sizes were found to be 0.21 and 0.28 nm. The particle sizes of the material were absolutely harmonized with crystallite sizes. Further, Figure 4c consists of a N₂ adsorption/desorption isotherm for the biosynthesized material, and the inset image shows the pore size distribution for the δ-Bi₂O₃ material. The study revealed the mesoporous nature of the material as it has pores with a diameter size of 11 nm, while the surface area is 71 m²/gm. The multilayer adsorption is followed by capillary condensation, ensuing IV isotherm pattern. The porosity plot reveals the nearly monodispersed behavior of the material with the nonuniform holes on the material surfaces with pore diameter sizes around 11 and 22 nm. The presence of nonuniform holes on the material surface is also supported by SEM. However, the material was found to be mesoporous, which indicates the nanoscale behavior with good catalytic adsorption property. Moreover, the surface area of the material was also good; hence, it indicated the effective catalytic and adsorption properties of the material. Most importantly, it might be due to the material having a tunable band gap energy. Therefore, keeping this in our mind, we carried out the photocatalytic degradation of Thymol blue and Congo red dyes in visible-light irradiation using biosynthesized δ-Bi₂O₃ NPs.

**Photodegradation of Toxic Dyes Using Biosynthesized δ-Bi₂O₃ NPs.** Further, δ-Bi₂O₃ NPs were employed to investigate the photocatalytic activity of TB and CR dyes under visible-light irradiation. Primarily, concentration optimization of TB (Figure 5a) and CR (Figure 6a) were performed at constant loading of photocatalyst (10 mg, 25 ± 2 °C, pH: 7.0). TB exhibited maximum degradation efficiency at 15 ppm concentration, while CR exhibited at 20 ppm; thus, they were fixed as stock solutions. The influence of photocatalyst dose on the photodegradation of both dyes is shown in Figures 5b and 6b, as an initial increase in photocatalyst doses increased the rate of photodegradation due to more effective active pores and holes on the surface of photocatalyst.47 However, subsequent increases in the concentration of photocatalyst (30 mg) decrease the rate of photodegradation, as the deactivation of photocatalyst’s active sites due to the catalyst’s aggregation and low absorption. The time-dependent experiment shows (Figure 5c) rapid photodegradation of TB in 40 min at 15 ppm than its counterpart.

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**Table 1.** Comparison of Photocatalytic Performance of δ-Bi₂O₃ NPs with Other Photocatalytic Systems

| s. no. | materials | photocatalytic performance | refs |
|--------|-----------|----------------------------|------|
| 1      | CuO/Bi₂O₃ nanocomposite | at acidic pH and 0.2 g/L catalyst, degradation was higher (87.76%) | 50   |
| 2      | β-Bi₂O₃ microflakes | indigo carmine and acid violet 7 dyes were 99 and 87% degraded, respectively, within 15 min of irradiation. whereas only 21% degradation was obtained for Rhodamine B dye. | 51   |
| 3      | α/β-Bi₂O₃ composite | In a solution having a mixture of indigo carmine and rhodamine B, the catalyst selectively degraded Indigo carmine first, and after its complete degradation, rhodamine B degradation initiated. | 52   |
| 4      | ACF-Bi₂O₃ composite | 25.47% removal was obtained for rhodamine B, 25.44% removal was obtained for methylene blue, and 14.47% removal was obtained for reactive black B. | 53   |
| 5      | β-Bi₂O₃/GR composite | catalyst having 7 wt % graphene content degraded 65% of methylene blue after 240 min irradiation | 54   |
| 6      | α-Bi₂O₃ and β-Bi₂O₃ Nanowires | more than 90% orange-G was degraded by β-Bi₂O₃ nanowires (NWs) after 15 h irradiation, and the photocatalytic activity of β-Bi₂O₃ NWs was ~1.3 times higher than that of α-Bi₂O₃ NWs. | 56   |
| 7      | Bi@Bi₂O₃ microspheres | ~96.6% rhodamine B and 100% Methyl orange were photodegraded after 4 h. | 55   |
| 8      | La/Er-doped Bi₂O₃ | 3% La-doped Bi₂O₃ degraded 88% acid yellow 29, 96% brilliant blue G250 and 90% acid green 25 in 120 min irradiation, whereas 0.9% Er-doped Bi₂O₃ degraded 83% acid yellow 29, 86% brilliant blue G250, and 84.6% acid green 25 in 120 min of irradiation. | 22   |
| 9      | α-Bi₂O₃ nanorods | rhodamine B dye was degraded 97% in 45 min and 2,4,6-trichlorophenol degraded 88% in 180 min. | 56   |
| 10     | δ-Bi₂O₃ NPs | 98.26% photocatalytic degradation of TB in 40 min and 69.67% photocatalytic degradation of CR in 80 min. | this work |

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**Figure 7.** (a) Photocatalytic stability of δ-Bi₂O₃ NPs and (b) XRD pattern of recycled δ-Bi₂O₃ NPs.
CR (Figure 6c): hence, photodegradation reaction follows pseudo-first-order kinetics. Consequently, noteworthy photodegradation progress of both dyes was studied by changing the absorption spectrum as a function of time for the dye solution (Figures 5d and 6d). Fascinatingly, it was observed that with an increased visible-light radiation time, the absorption climax reduces and became flat in 40 min with 98.26% degradation of TB (Figure 5e), while CR degraded 69.67% in 80 min (Figure 6e). Further, the photocatalytic performance obtained for δ-Bi2O3 NPs has also been compared with other systems in Table 1. The regeneration and reuse of δ-Bi2O3 NPs were performed after the complete degradation of dyes. δ-Bi2O3 NPs were recovered by vacuum filtration, washed two times, dried at 75 °C, and re-tested. This sequence was repeated with five cycles to check the stability of the material, and the results are presented in Figure 7a. And the stability of the reused material was evaluated by XRD (Figure 7b). Additionally, the scavenging assays were executed for both dyes to seek out the formation of radicals during photocatalysis. The scavenging tests were carried out using potassium bromide (KB), potassium iodide (KI), and ethylenediaminetetraacetic acid (EDTA) as scavengers (Figures 5f and 6f). It was found that the photodegradation of TB is completely affected when KB and EDTA were employed as scavenging agents. Basically, in the mechanism of photocatalytic reaction, the photogenerated holes (h+) are initially amenable to the degradation of dyes. However, hydroxyl (OH) and superoxide (O2−) also played important roles in photocatalytic reactions (Figure 8). The important participation of (OH, h+ and O2−) in the reaction further confirms that photogenerated holes and electrons are responsible for the photocatalytic reaction.48,49

![Figure 8. Possible photodegradation mechanism of dyes using δ-Bi2O3 NPs including CB/VB levels and redox potentials.](image-url)

In conclusion, the present study is based on a greener synthesis of δ-Bi2O3 NPs, for which C. viivaram flower extract was used for the first time, followed by calcination at 800 °C resulting in delta-Bi2O3 NPs. The biosynthesized δ-Bi2O3 NPs were confirmed through various physicochemical analytical techniques. Morphology was studied via SEM and TEM techniques, whereas the BET study showed that δ-Bi2O3 NPs had a surface area of 71 m²/gm with mesoporous nature. The estimated band gap (3.45 eV) indicated δ-Bi2O3 NPs to be a promising photocatalyst under visible-light irradiation. Therefore, when bioinspired δ-Bi2O3 NPs were employed as a photocatalyst for the photocatalytic degradation of TB and CR dyes under visible-light irradiation, enhanced photocatalytic degradation was obtained. The study demonstrated 98.26% degradation of TB in 40 min while 69.67% degradation of CR in 80 min by δ-Bi2O3 NPs, and photogenerated holes and electrons were found responsible for this enhancement. Furthermore, results from molecular docking revealed that δ-Bi2O3 NPs were found as an effective inhibitor to protein (NDM-1) PDB ID 5XP9 with good hydrogen-bonding interactions. In brief, biosynthesized δ-Bi2O3 NPs are an excellent photocatalyst and a true candidate as a future antimicrobial agent.

**CONCLUSIONS**

In conclusion, the present study is based on a greener synthesis of δ-Bi2O3 NPs, for which C. viivaram flower extract was used for the first time, followed by calcination at 800 °C resulting in delta-Bi2O3 NPs. The biosynthesized δ-Bi2O3 NPs were confirmed through various physicochemical analytical techniques. Morphology was studied via SEM and TEM techniques, whereas the BET study showed that δ-Bi2O3 NPs had a surface area of 71 m²/gm with mesoporous nature. The estimated band gap (3.45 eV) indicated δ-Bi2O3 NPs to be a promising photocatalyst under visible-light irradiation. Therefore, when bioinspired δ-Bi2O3 NPs were employed as a photocatalyst for the photocatalytic degradation of TB and CR dyes under visible-light irradiation, enhanced photocatalytic degradation was obtained. The study demonstrated 98.26% degradation of TB in 40 min while 69.67% degradation of CR in 80 min by δ-Bi2O3 NPs, and photogenerated holes and electrons were found responsible for this enhancement. Furthermore, results from molecular docking revealed that δ-Bi2O3 NPs were found as an effective inhibitor to protein (NDM-1) PDB ID 5XP9 with good hydrogen-bonding interactions. In brief, biosynthesized δ-Bi2O3 NPs are an excellent photocatalyst and a true candidate as a future antimicrobial agent.

**EXPERIMENTAL SECTION**

**Materials and General Methods.** Bi(NO3)3·5H2O, nitric acid (HNO3), hydrochloric acid (HCl), sodium hydroxide (NaOH), potassium chloride (KCl), Congo red (CR), and Thymol blue (TB) were procured from Merck (India) Chemicals. The scavenging tests were carried out using
potassium bromide (KB), potassium iodide (KI), and ethylenediaminetetraacetic acid (EDTA) as scavengers.

C. viviparum flowers were collected from Gorewada National Park, Nagpur (India). The precursor was used without further purification.

Figure 9. (a) Photoluminescence (PL) and (b) time-resolved transient absorption spectra of δ-Bi₂O₃ NPs.

Table 2. Lifetimes and Relative Intensities of the Biosynthesized δ-Bi₂O₃ NPs

| material  | τ₁ (ns)/Int. (%) | τ₂ (ns)/Int. (%) |
|-----------|-----------------|-----------------|
| δ-Bi₂O₃   | 0.11/95         | 1.23/6          |

Figure 10. (a) 3D ball-and-stick model of δ-Bi₂O₃ NPs, (b) δ-Bi₂O₃ structures dock with protein via CPK mode surrounded by hydrogen-bonding residues, and (c–f) translucent surface images, with NPs fitted at the center of the protein.
Table 3. Hydrogen-Bond Distances in Selected Amino Acids Using δ-Bi2O3 NPs

| amino acid residues | hydrogen bond in Å |
|---------------------|--------------------|
| 512 THR, 82 GLN,189 VAL | 2.246154, 2.23721, 2.319003 |
| 121 THR,131 LEU,192 VAL | 2.251422, 2.2 7152 |
| 91 GLN, 82 ILE | 2.2242 |
| 111 SER,199 LEV | 2.24253 |
| 142 VAL, 143 ALA | 2.246238 |

**Characterization Techniques.** XRD of the biosynthesized material was carried out by an Advance diffractometer (Bruker AXS D8) in the 2θ range of 2 − 80°. FT-IR spectrum was recorded in the range of 800 − 1200 cm⁻¹ at 4.0 cm⁻¹ resolution by a Bruker IFS 66v spectrophotometer using KBr pellets. UV−visible absorption spectra were examined using a Shimadzu 1800 UV−visible spectrophotometer (SL171 Minispec). Raman spectra were acquired using a JY Horiba (HR-800) spectrophotometer, and XPS spectra were recorded on an ESCALAB 250 XPS with a monochromatic Al Kα X-ray source (150 W). The BET analysis was performed at liquid nitrogen temperature using a Micromeritics ASAP-2010 analyzer. During adsorption/desorption measurements, the samples were degassed for 2 h at 200 °C under vacuum. SEM (JEOL-JSM-690LV) and TEM (JEOL-JEM 100SX) were used for obtaining the micrographs to find the morphology of the biosynthesized material.

**Preparation of Flower Extracts (C. viviparum).** Petals of C. viviparum flowers were cut into small pieces and dried in shelter, mashed, and stored at room temperature (25 ± 2 °C) until further use. In an Erlenmeyer flask, 10 g of dried flower petals powder and 200 mL of deionized water were added and stirred vigorously using a magnetic stirrer for 20−30 min. Further, the flower petals extract was centrifuged for 15 min at keeping 3000 rpm to remove impurities. The supernatant was filtered by Whatman paper (No. 41). Finally, the filtrate was stored at 4 °C and used for further experiment.

**Biogenic Synthesis of δ-Bi2O3 NPs.** δ-Bi2O3 NPs were fabricated using a greener reducer via the co-precipitation technique. Initially, 20 mL of 0.1 M bismuth nitrate pentahydrates was transferred into an Erlenmeyer flask containing 50 mL of HNO₃ (10%). A hot-plate magnetic stirrer was used to mix the solution thoroughly for 15 min (1080 rpm). About 50 mL of the flower petals extract was added dropwise under constant stirring. The schematic route of synthesis is presented in Figure 1. The reaction was carried out at room temperature, and after 2 h, the obtained chocolate-colored precipitant was centrifuged (4000 rpm), washed with hot water and ethanol, and dried. Afterward, the light-yellow-colored powder was calcined at 800 °C; this higher temperature was chosen to obtain δ-Bi₂O₃ phase NPs with good crystallinity. The as-biosynthesized nanomaterials were characterized by various analytical techniques and utilized for photocatalytic and docking investigation.

**Photocatalytic Performance of Biosynthesized δ-Bi2O3 NPs.** The photocatalytic activity of biosynthesized δ-Bi₂O₃ NPs was assessed for the degradation of 15 ppm aqueous solution of TB and CR dyes. All photocatalytic experiments were carried out under visible-light irradiation using a tungsten lamp (60W, λ = 400−490 nm) kept ~5 cm from the aqueous dye solution. Stock solutions (15 ppm) were prepared and kept in the dark. For each photocatalytic experiment, 100 mL of aqueous dye solution was kept in a borosil beaker having 100 mg of the δ-Bi₂O₃ nanocatalyst under ambient conditions. Before irradiation, the dye/catalyst mixture was thoroughly stirred with a magnetic stirrer in the dark for 30 min so that uniform adsorption equilibrium is achieved. The remaining dye concentration was measured by taking a small aliquot of the reaction mixture at regular time intervals, followed by centrifugation and measuring the clear supernatant’s light absorption at λ_max = 435 nm and 439 nm for TB and CR, respectively.

**Design of Molecular Ligand (δ-Bi2O3 NPs).** Initially, we designed a small molecule called a ligand to study the inhibition of the enzyme. The 3D structures of the molecules were designed by ChemOffice software-12. The finalized 3D structures of ligand were tested for global minima to estimate the minimum energy values. Crystal structure downloaded from online resources. All of the heteroatoms were removed. Kollman charges and solvation parameters were incorporated into the final macromolecule (proteins) structures utilizing an AutoDock. The suitable active site of the enzyme was selected for the docking process to interact with the inhibitor (ligand).

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ACKNOWLEDGMENTS

The authors are thankful to Dr. Subhash Somkuwar, Associate Professor, Dr. Ambedkar College, Deekshabhoomi, Nagpur, for the taxonomical analysis of the plant (C. viviparum), and Dr. Sunil G. Chaudhari, Department of English, N.H. College, Bramhupuri, for editing the manuscript.

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