

Hormonal-mediated *Cicer arietinum* L. Leaf Extract Assisted Synthesis of Ternary g-C₃N₄/ZrTiO₄/V₂O₅ Nanocomposite for Photocatalytic Remediation of Organic Pollutants

Aakash Venkatesan ^a, Aatika Nizam ^{a*}, Letcy V Theresa ^a, Jobi Xavier ^b, Nagaraju G ^c

^a Department of Chemistry, Christ University, Hosur Road, Bangalore

^b Department of Life Sciences, Christ University, Hosur Road, Bangalore

^c Energy Materials Research Laboratory, Department of Chemistry, Siddaganga Institute of Technology, Tumakuru-572103, India

Corresponding author

Email ID: aatika.nizam@christuniversity.in

3. Results and Discussions

3.1. Plant Extract Characterizations

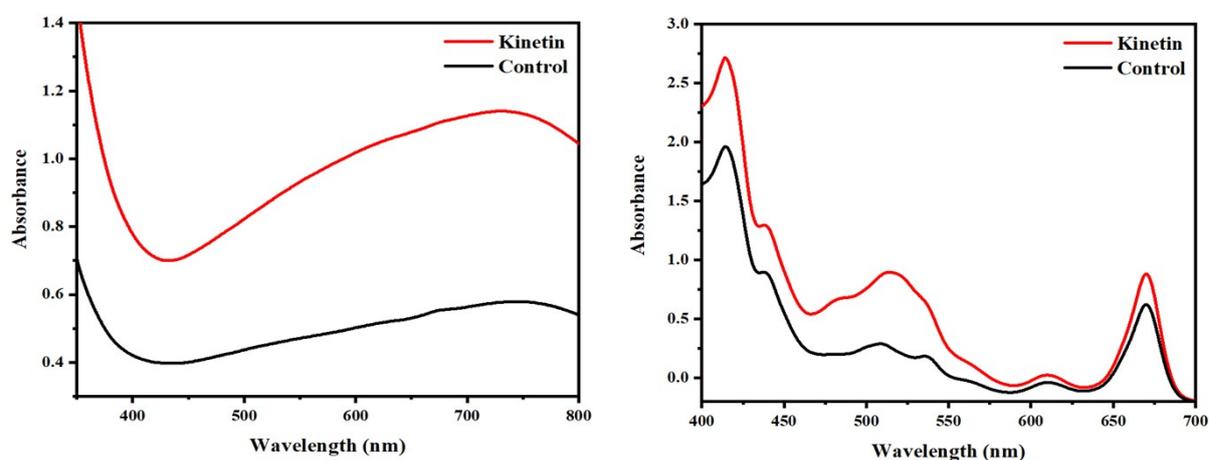


Figure S1: UV-Vis spectrum of (a) Total Phenol content estimation (b) Proline content estimation

3.2. Nanocomposite Characterization

3.2.3. UV-Vis analysis

Table S1: Optical band gap, valence band, and conduction band energies with respect to NPs

| Type of Nanoparticle | Optical band gap energy (eV) | Valence band energy (eV) | Conduction band energy (eV) |
|----------------------|------------------------------|--------------------------|-----------------------------|
| g-ZTC | 4.04 | 2.95 | -1.09 |
| g-ZTK | 3.75 | 2.81 | -0.95 |

3.3. Photo-Catalytic studies of g-ZTK

3.3.1. Photodegradation of organic dyes

3.3.1.2. Kinetic Studies

Table S2: Rate constant values (k) for varying (a) Dyes (b) Catalytic dosage (c) Dye concentration (d) pH Value

| <i>Dyes</i> | <i>Acriflavine Hydrochloride</i> | <i>Rose Bengal</i> | <i>Indigo Carmine</i> | <i>Methylene Blue</i> |
|-----------------------------------|----------------------------------|------------------------|-----------------------|-----------------------|
| <i>k value (min⁻¹)</i> | 4.35×10^{-3} | 12.75×10^{-3} | 1.56×10^{-3} | 1.26×10^{-3} |

| <i>Catalytic Dosage (mg)</i> | <i>10</i> | <i>20</i> | <i>30</i> | <i>40</i> |
|-----------------------------------|------------------------|-----------------------|-----------------------|-----------------------|
| <i>k value (min⁻¹)</i> | 12.75×10^{-3} | 5.57×10^{-3} | 5.15×10^{-3} | 4.24×10^{-3} |

| <i>Dye Concentration (ppm)</i> | <i>10</i> | <i>20</i> | <i>30</i> | <i>40</i> |
|-----------------------------------|-----------------------|------------------------|-----------------------|-----------------------|
| <i>k value (min⁻¹)</i> | 8.77×10^{-3} | 12.75×10^{-3} | 4.61×10^{-3} | 3.46×10^{-3} |

| <i>pH values</i> | <i>5</i> | <i>7</i> | <i>9</i> |
|-----------------------------------|------------------------|------------------------|-----------------------|
| <i>k value (min⁻¹)</i> | 13.34×10^{-3} | 12.75×10^{-3} | 5.85×10^{-3} |

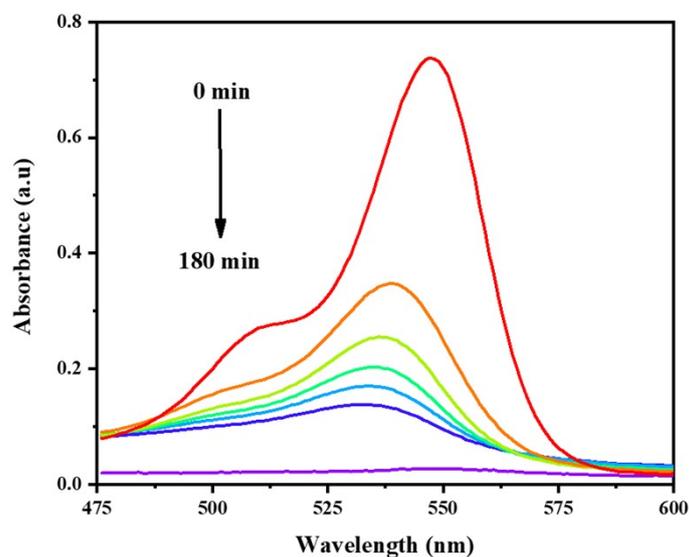


Figure S2: Absorption spectra of optimized photocatalytic degradation of Rose Bengal dye by g-ZTK NPs

3.3.1.4. Recyclability and Photostability studies

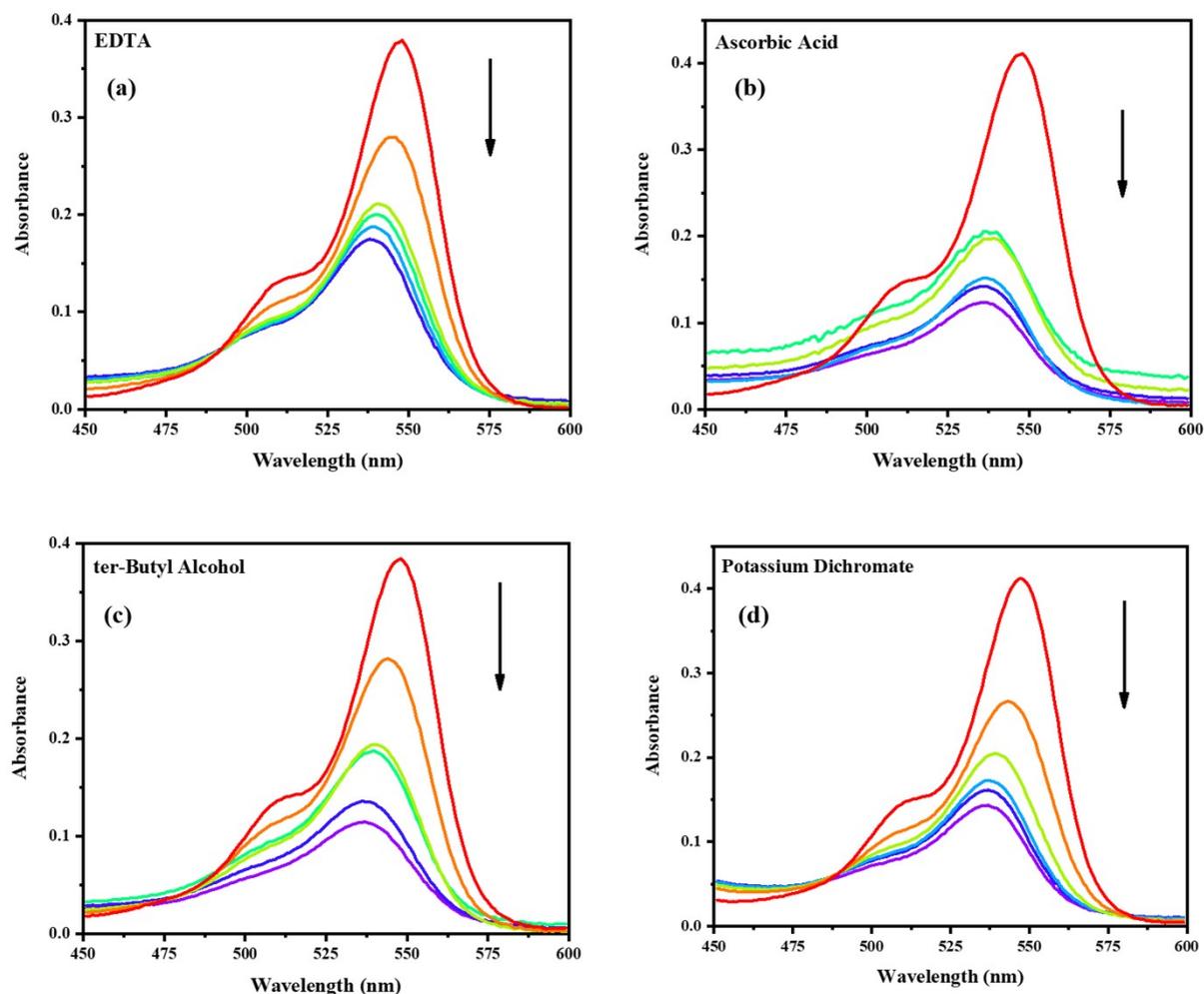


Figure S3: Absorption spectra of Scavengers Studies (a) EDTA (b) Ascorbic Acid (c) TBA (d) Potassium dichromate

3.3.2. Photooxidation of Aromatic Alcohols

Spectral data of substituted aldehyde compounds

Compound 3a: Colourless liquid, bp = 177-178 °C.

Compound 3b: Light yellow powder, $^1\text{H-NMR}$: δ , ppm (DMSO- d_6): 8.186-8.164 (d, 2H), 8.419-8.440 (d, 2H), 10.175 (s, 1H).

Compound 3c: Colourless liquid, $^1\text{H-NMR}$: δ , ppm (DMSO- d_6): 3.809-3.875 (q, 3H), 7.083-7.118 (m, 2H), 7.840-7.875 (m, 2H), 9.868 (s, 1H).

Compound 3d: White powder, $^1\text{H-NMR}$: δ , ppm (DMSO- d_6): 3.050 (s, 6H), 6.778-6.814 (m, 2H), 7.674-7.710 (m, 2H), 9.676 (s, 1H).

Compound 3e: White powder, $^1\text{H-NMR}$: δ , ppm (DMSO- d_6): 7.680-7.712 (m, 2H), 7.925-7.958 (m, 2H), 10.013 (s, 1H).

Compound 3f: Colourless liquid, $^1\text{H-NMR}$: δ , ppm (DMSO- d_6): 7.505-7.542 (t, 1H), 7.594-7.710 (q, 2H), 7.853-7.872 (d, 1H).

Compound 3g: Colourless liquid, $^1\text{H-NMR}$: δ , ppm (DMSO- d_6): 7.385-7.429 (q, 2H), 7.968-8.004 (m, 2H), 9.976 (s, 1H).

Compound 3h: Colourless liquid, $^1\text{H-NMR}$: δ , ppm (DMSO- d_6): 6.930-7.011 (m, 2H), 7.485-7.652 (m, 1H), 7.656-7.676 (t, 1H), 10.261 (s, 1H), 10.716 (s, 1H).

Compound 3i: White crystalline powder, $^1\text{H-NMR}$: δ , ppm (DMSO- d_6): 6.979-7.001 (d, 1H), 7.646-7.675 (q, 1H), 7.719-7.725 (d, 1H), 10.217 (s, 1H), 10.990 (s, 1H).

Compound 3j: Brown liquid, $^1\text{H-NMR}$: δ , ppm (DMSO- d_6): 6.770-6.783 (q, 1H), 7.529-7.539 (q, 1H), 8.092-8.096 (t, 1H), 9.620-9.621 (d, 1H).

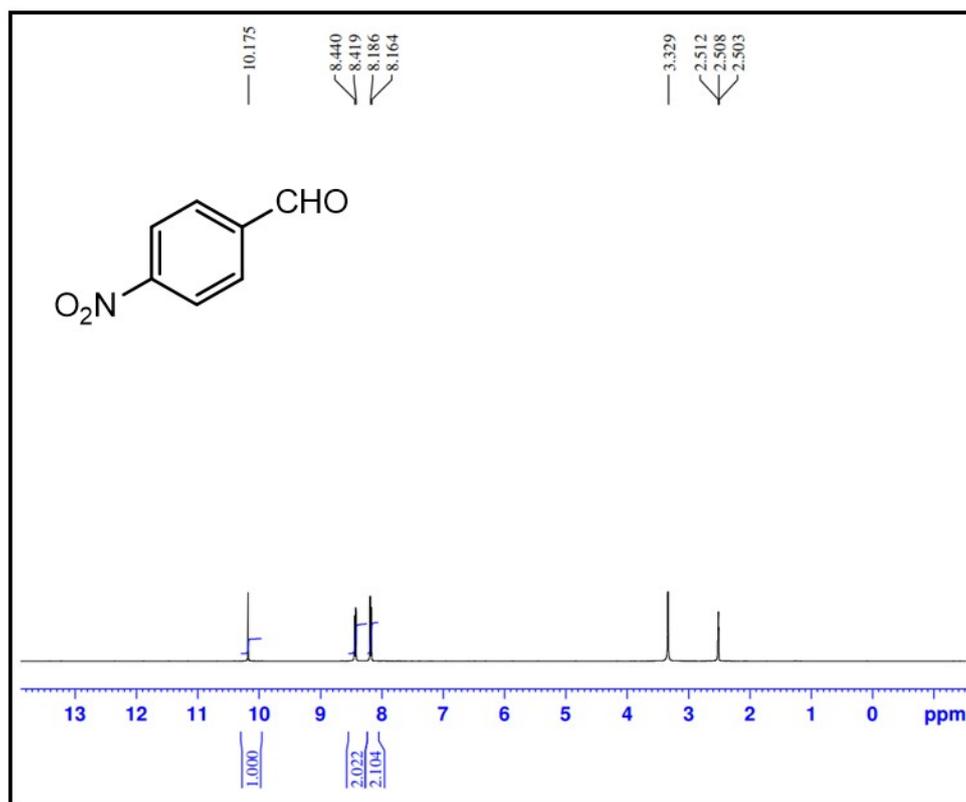


Figure S4: $^1\text{H-NMR}$ Spectrum of Compound 3b

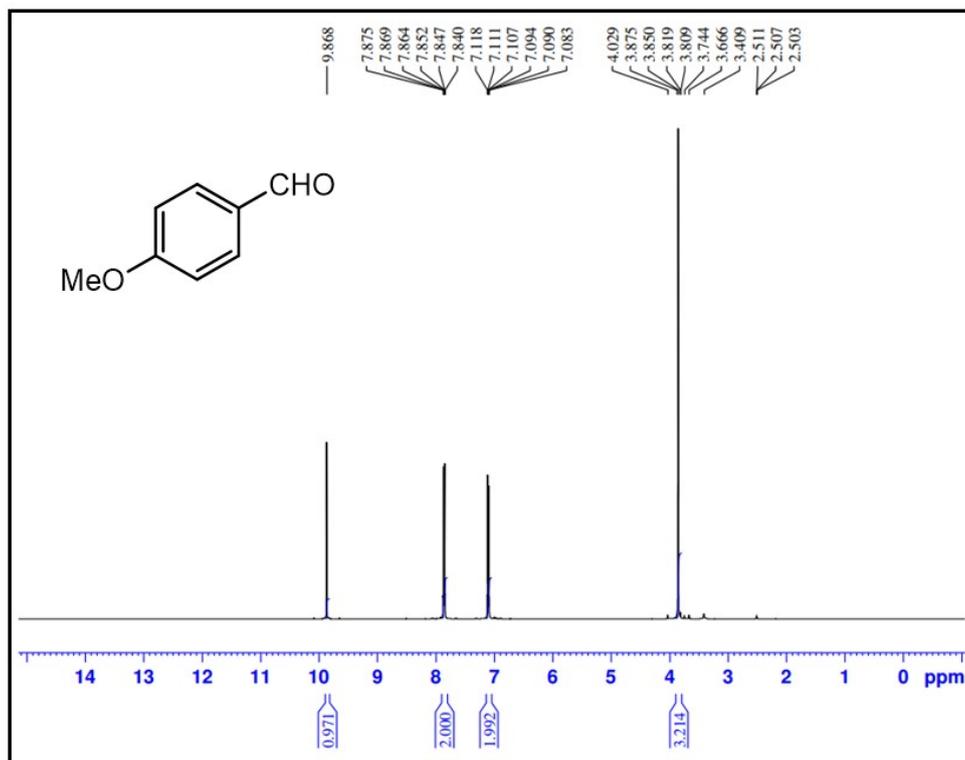


Figure S5: $^1\text{H-NMR}$ Spectrum of Compound 3c

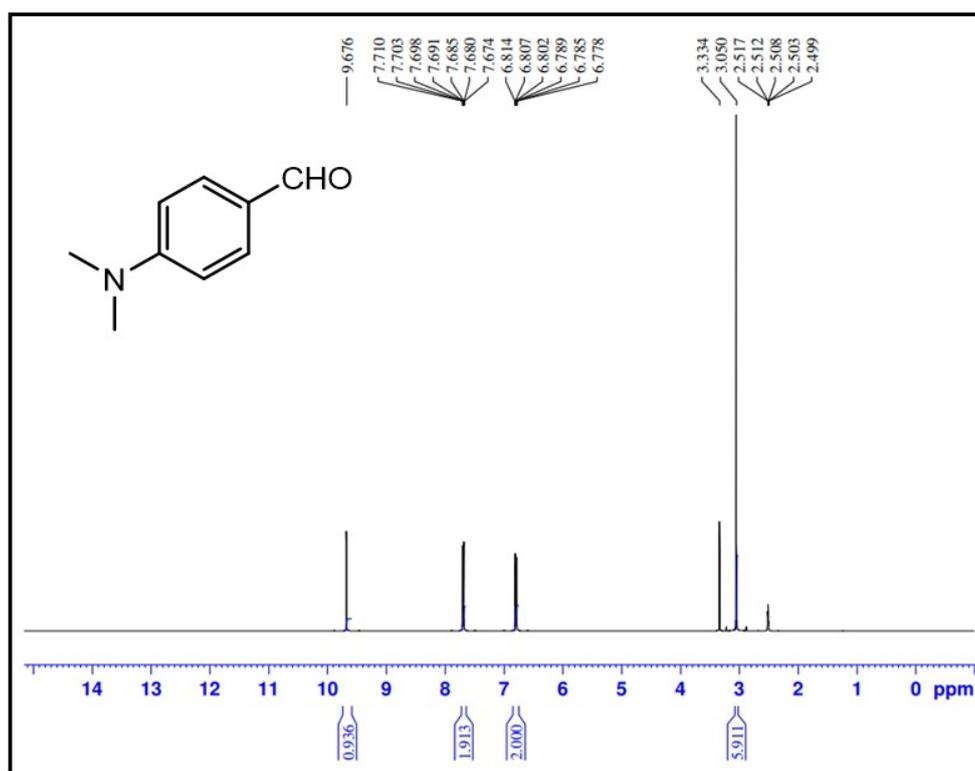


Figure S6: $^1\text{H-NMR}$ Spectrum of Compound 3d

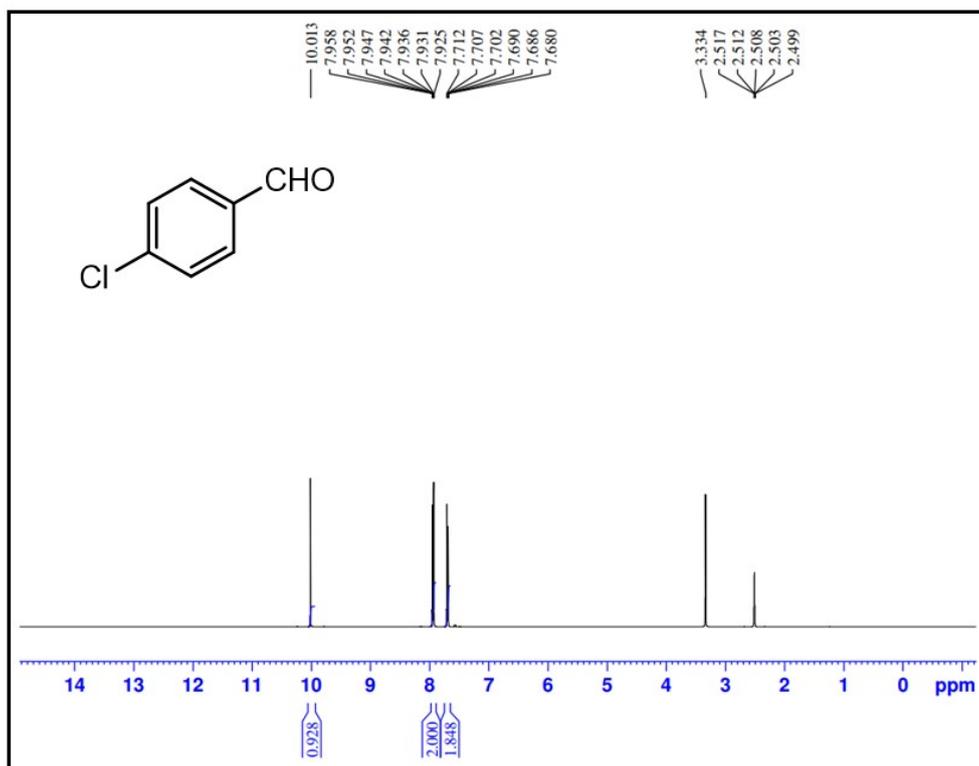


Figure S7: ¹H-NMR Spectrum of Compound 3e

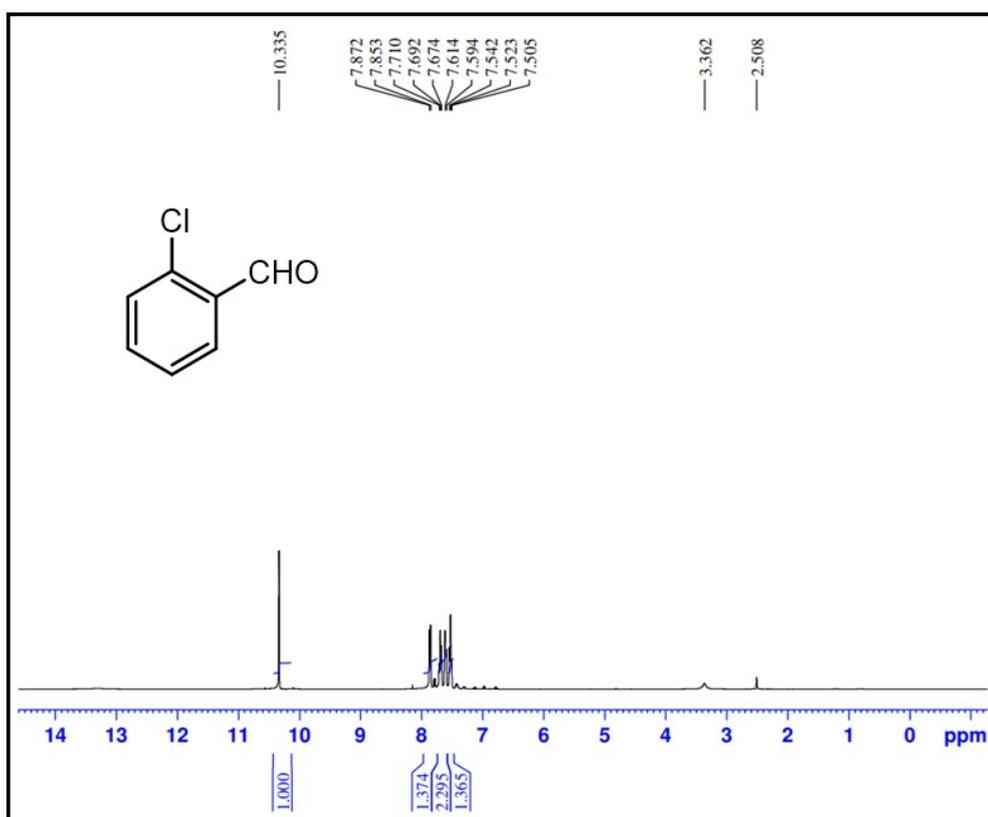


Figure S8: ¹H-NMR Spectrum of Compound 3f

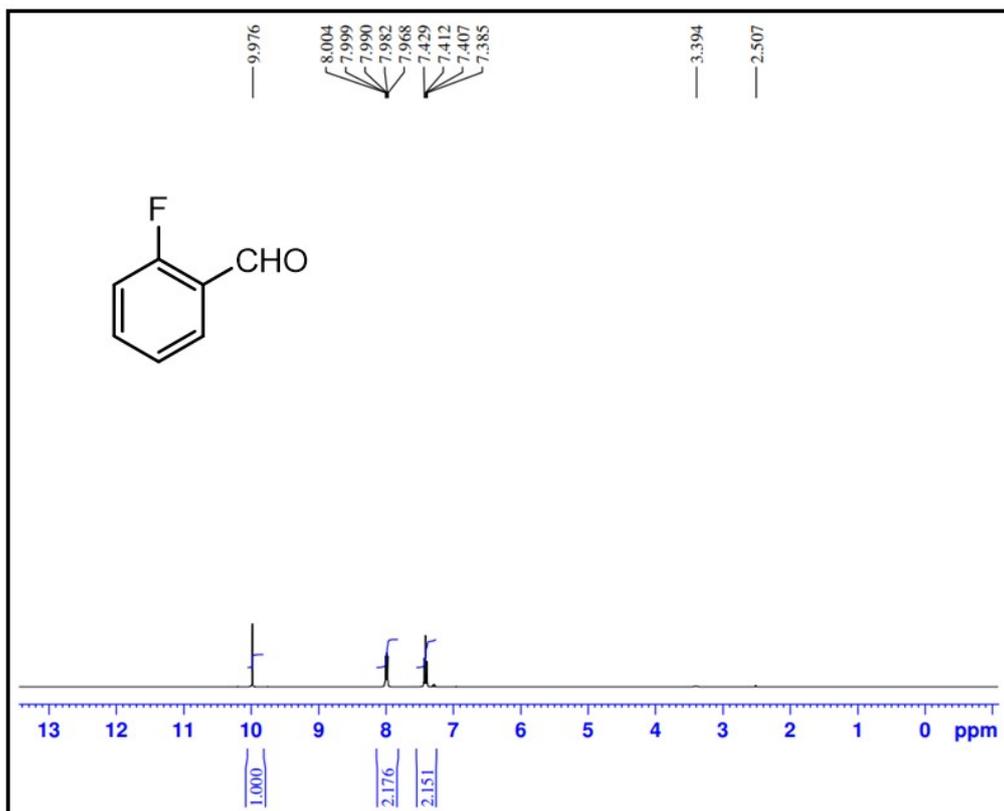


Figure S9: $^1\text{H-NMR}$ Spectrum of Compound 3g

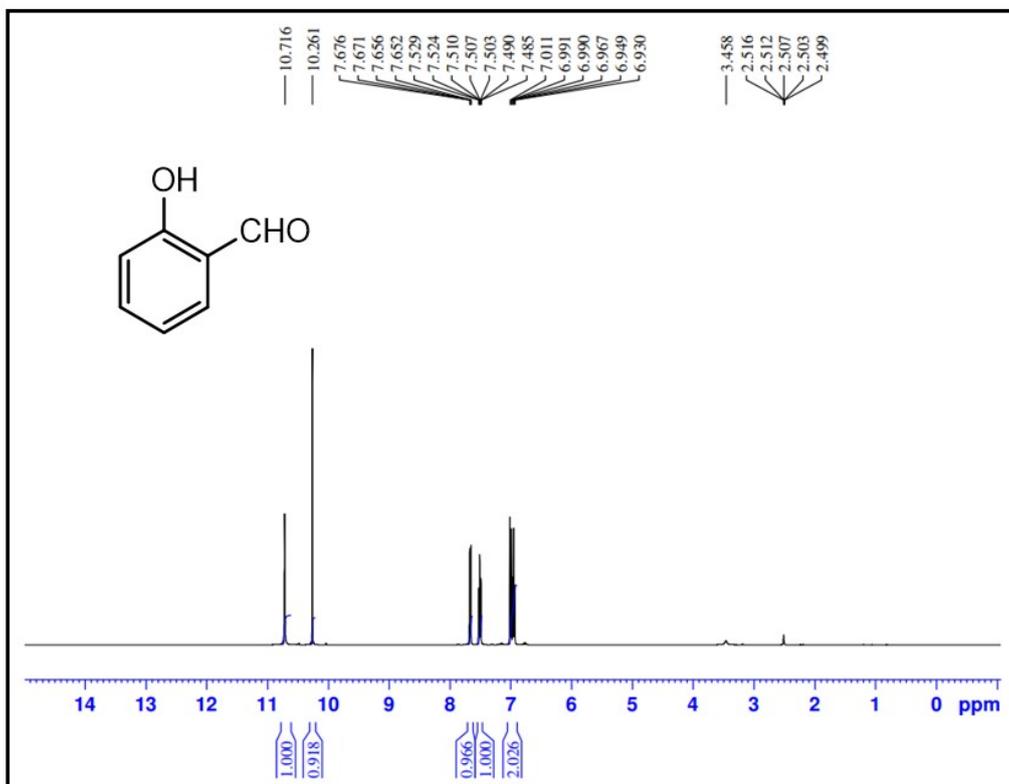


Figure S10: $^1\text{H-NMR}$ Spectrum of Compound 3h

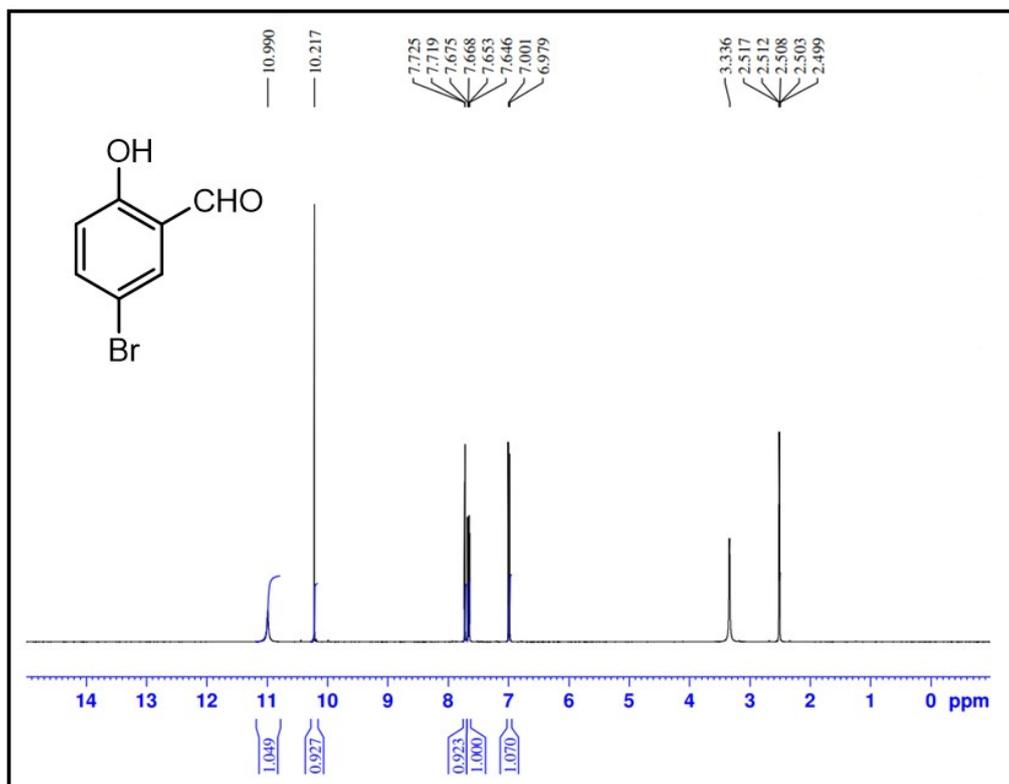


Figure S11: $^1\text{H-NMR}$ Spectrum of Compound 3i

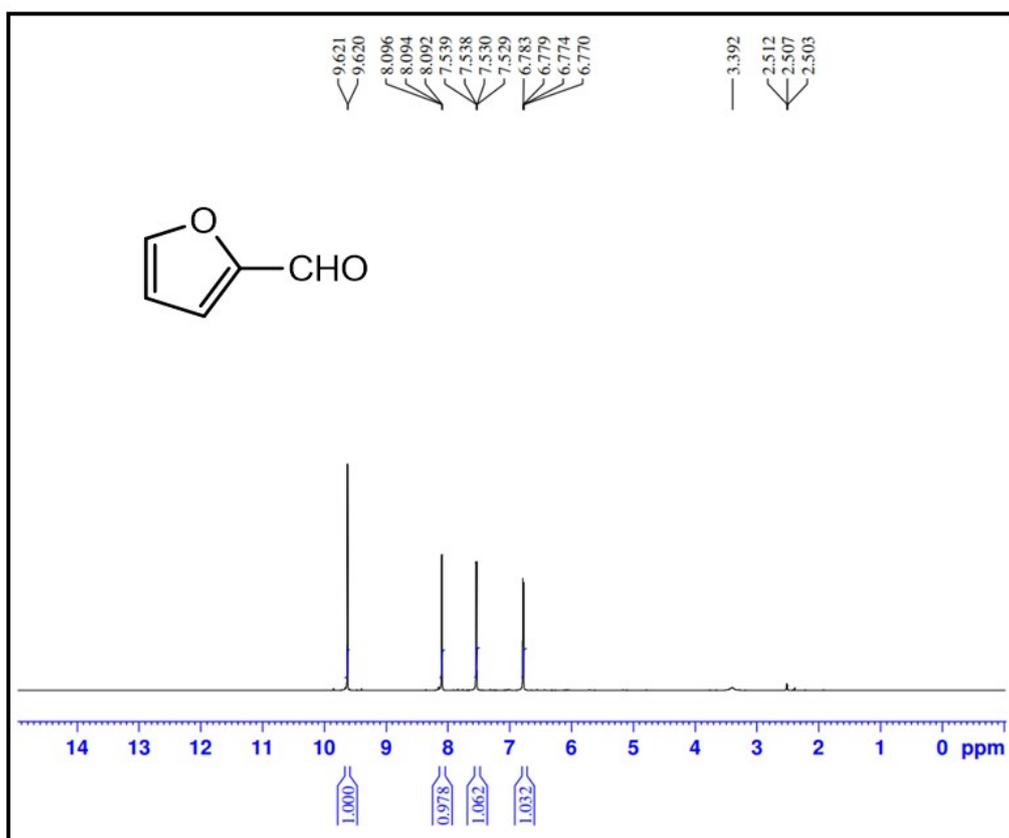
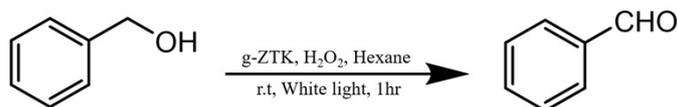


Figure S12: $^1\text{H-NMR}$ Spectrum of Compound 3j

3.3.2.2. Green Chemistry Metrics



Catalyst Mass = 0.030 g

Reaction Solvent Mass = 3.274 g

By-products: H₂O

Yield: 92 %

$$\text{Atom Economy (AE): } \frac{106.12 \text{ g/mol}}{(108.14 + 34.01) \text{ g/mol}} \times 100 = 77.8 \%$$

$$\text{Generalized reaction mass efficiency (gRME): } \frac{0.1061 \text{ g}}{0.1489 \text{ g}} \times 100 = 71.3 \%$$

$$\text{E-factor: } \frac{0.1489 - 0.1061 \text{ g}}{0.1061 \text{ g}} = 0.40$$

Carbon Efficiency: 100 %

TON: 27.9

TOF: 27.9 h⁻¹

Eco-scale: 81

3.3.2.3. Reusability of g-ZTK Nano-catalyst

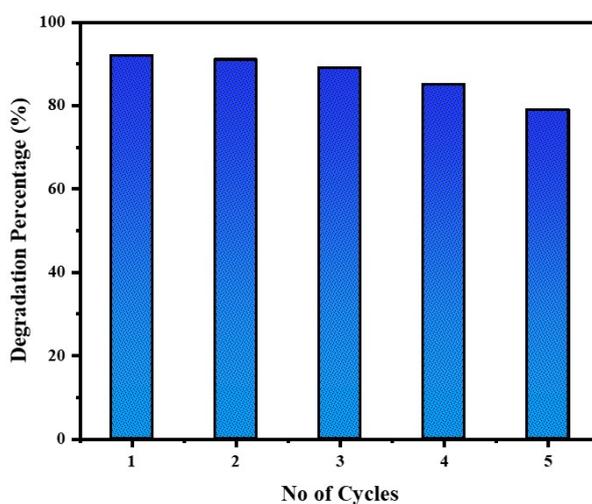


Figure S13: Reusability of g-ZTK catalyst for the model reaction under the same reaction conditions.