Supplementary Information

Efficient Removal of H-Acid from Industrial Wastewater via Ag_2ZrO_3 Nanocatalyst-Mediated Advanced Oxidation and Pseudomonas aeruginosa Biodegradation

Sakshi R. Barad[a], G. S. Gaikwad[b], Atul V. Maldhure[c], Atul V. Wankhade[a]*

[a]Department of Chemistry, Visvesvaraya National Institute of Technology (VNIT), Nagpur, 440010, India

[b]Department of Chemistry, Priyadarshini Bhagwati College of Engineering, Nagpur, 440009, India

[c]Water Technology Management Division, CSIR-National Environmental Engineering Research Institute, Nagpur 440020, India

Corresponding author: atulvwankhade007@gmail.com

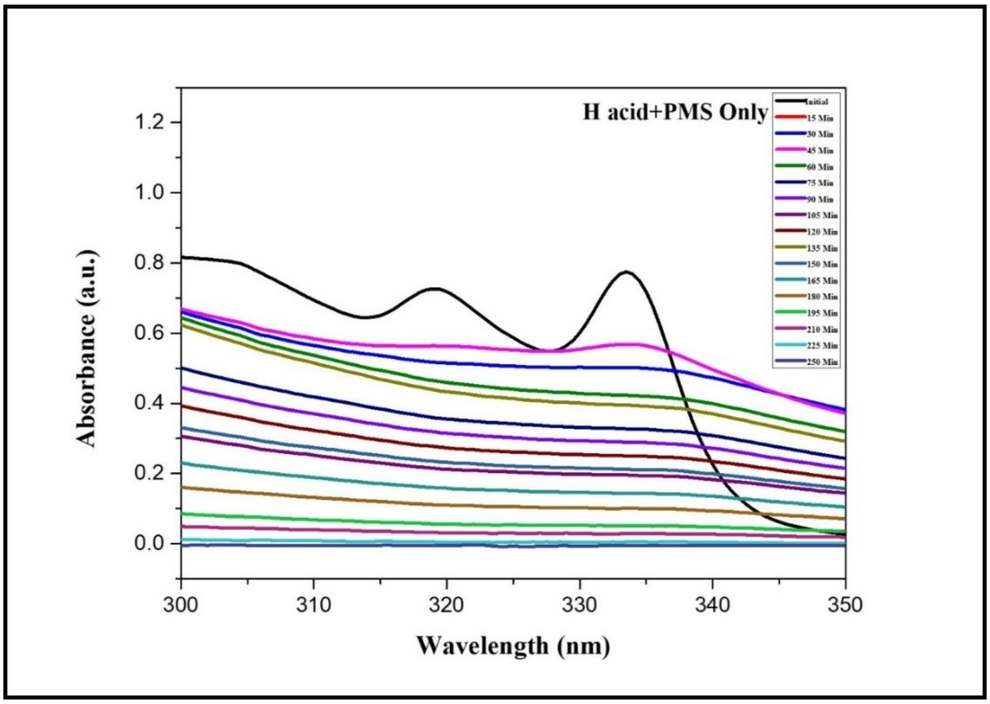


Figure S1. UV-Visible Absorption Spectra of H acid degradation by PMS alone

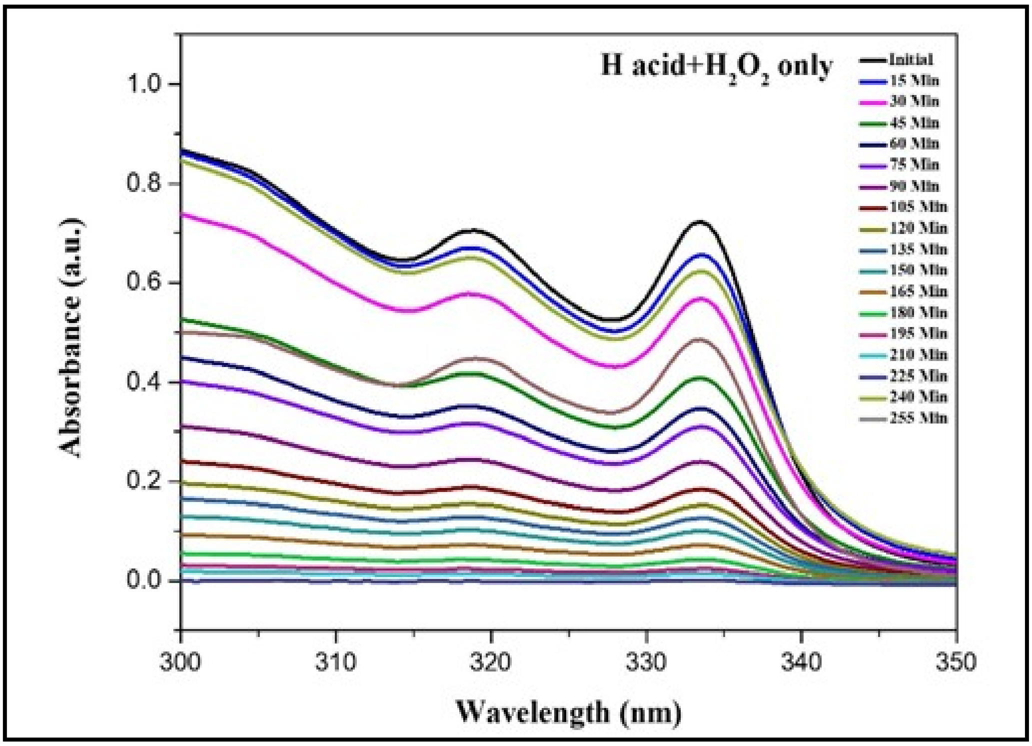
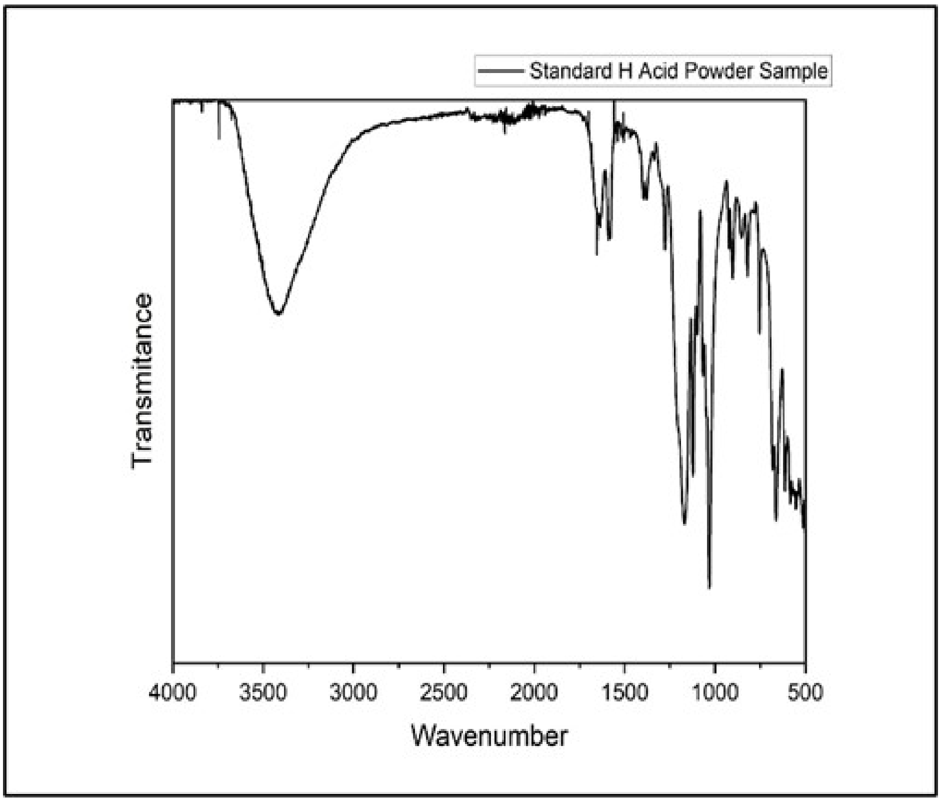


Figure S2. UV-Visible absorption Spectra of H acid degradation by H_2O_2 alone



Figu

re S3. FTIR Spectra of Standard H-acid Powder Sample

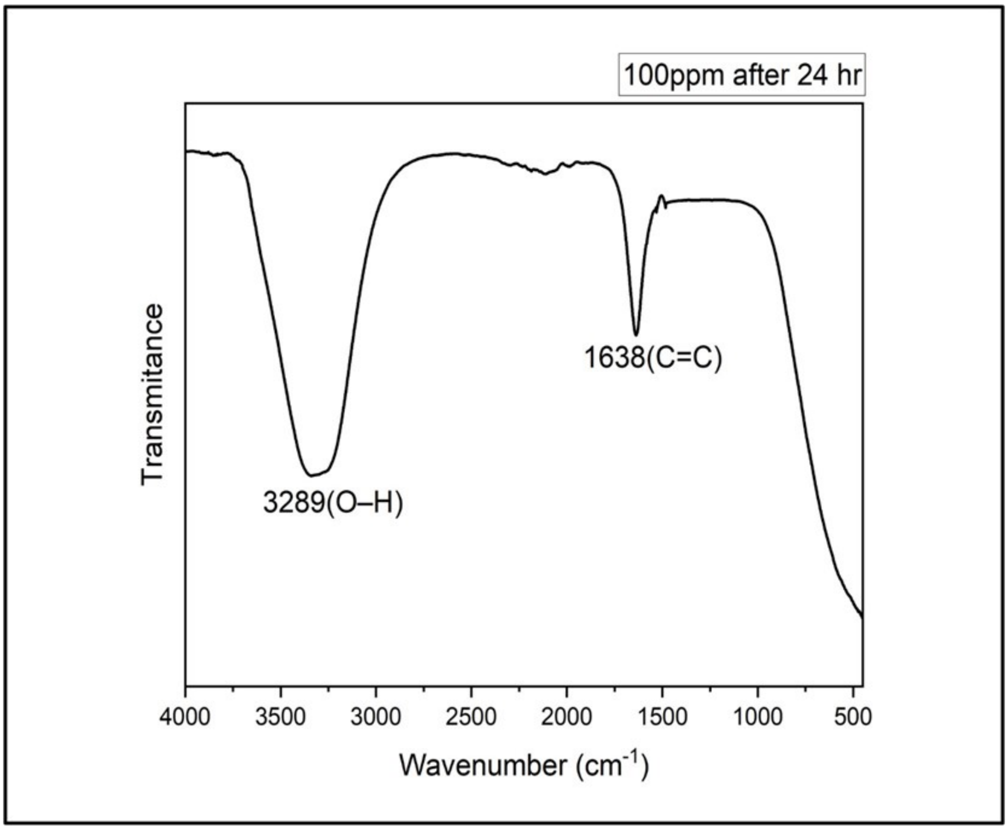


Figure S4. FTIR Spectra of H-acid degradation by Pseudomonas aeruginosa

Fourier-transform infrared (FTIR) spectroscopy was employed to analyse structural modifications in the degraded samples (Figure S4.). Post-biodegradation FTIR spectra displayed a broad peak at 3289 cm^{-1}, attributed to O–H stretching vibrations, indicating the presence of hydroxyl or phenolic groups. A distinct peak observed at 1638 cm^{-1} may correspond to C=C or C=O stretching, suggesting the formation of unsaturated or carbonyl-containing degradation products. Notably, the characteristic sulfonic group peaks observed around 1040–1180 cm^{-1} in the parent compound were absent, confirming desulfonation. Additionally, a weak shoulder near 2350 cm^{-1} may indicate trace amounts of CO_2 formation, implying partial mineralization. These FTIR observations are consistent with the proposed microbial degradation pathway and support the formation of low-molecular-weight carboxylic acids and aldehydes as end-products. Overall, the combination of pathway analysis and FTIR data confirms the ability of Pseudomonas aeruginosa to efficiently degrade H-acid via enzymatic transformation, ring cleavage, and further mineralization. These findings highlight its potential application in the bioremediation of sulfonated aromatic pollutants from industrial wastewater.

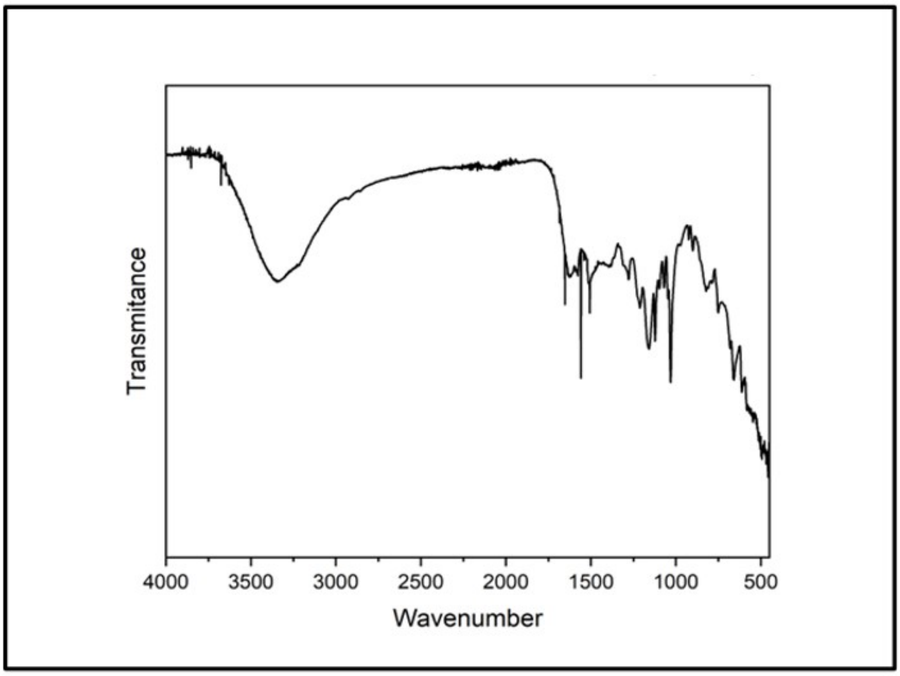


Figure S5. FTIR Spectra of Industrial Effluent

FTIR analysis of a standard H-acid sample reveals several key characteristic peaks (Figure S5.). A strong, broad band observed in the region of 3400-3200 cm^{-1} indicates the presence of intact hydroxyl (O-H) and amino (N-H) groups. A peak around 1700-1600 cm^{-1} is attributed to the stretching vibrations of carbon-carbon double bonds (C=C) within the aromatic rings and any carbonyl (C=O) groups that may be present, confirming the aromatic nature of the compound. The sulfonic acid groups are confirmed by a peak between 1400-1300 cm^{-1}, which corresponds to the stretching vibrations of the sulfur-oxygen double bond (S=O). Furthermore, peaks in the 1200-1000 cm^{-1} region are associated with the stretching of carbon-nitrogen (C-N) and carbon-oxygen (C-O) bonds, reinforcing the presence of the amino and hydroxyl functional groups. Finally, the presence of peaks below 900 cm^{-1}, which are characteristic of out-of-plane C-H bending, confirms the intact naphthalene ring structure of the H-acid molecule.

Industrial effluent is a complex mixture. Therefore, the FT-IR spectrum shows additional peaks from other compounds present. Peaks in the 3000-2800 cm^{-1} range would indicate the presence of aliphatic C-H bonds, suggesting the effluent contains hydrocarbons or other organic matter from manufacturing processes. Peaks in the 500-600 cm^{-1} range could point to the presence of metal oxides or salts, which are common byproducts or contaminants in industrial wastewater, potentially from residual raw materials or the process of wastewater treatment itself. These additional peaks highlight the complexity of the sample and the potential presence of various impurities alongside the target compound, H-acid.

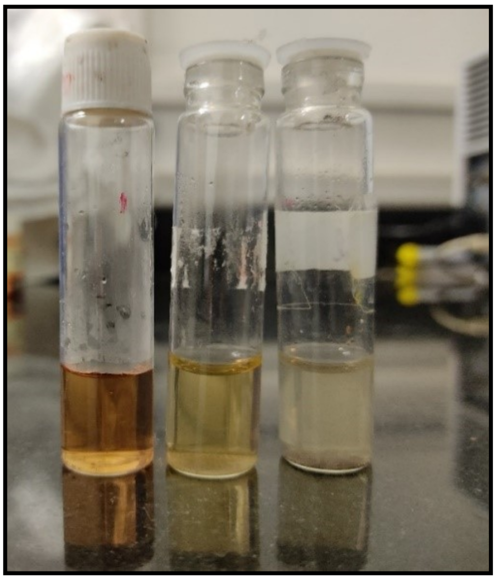


Figure S6. Treated Industrial Effluent