

Greener synthesis, spectroscopical relationships, molecular docking analysis, antimicrobial, antimalarial activities of aryl *E*-imines and X-ray crystal structure of (*E*)-*N*-(4-nitrobenzylidene)-2-(trifluoromethyl)aniline

P Gayathri^a, P Mayavel^{a,b}, I Muthuve^{1a,c}, S Balasundari^a, P Sudha^a, J Divya^{a,d}, D Govindarajan^c, B Krishnakumar^{f,g,h}, K Ranganathanⁱ, V Usha^j, K Devika^k & G Thirunarayanan^{*a}

^a Department of Chemistry, Annamalai University, Annamalinagar 608 002, Tamil Nadu, India

^b Department of Chemistry, Government Arts College, Ariyalur 621 713, Tamil Nadu, India (Affiliated to Bharathidasan University, Tiruchirppalli 620 024, Tamil Nadu, India)

^c Department of Chemistry, M. R. Government Arts College, Mannargudi 614 001, Tamil Nadu, India

^d Department of Chemistry, Indra Ganesan College of Engineering College, College, Manikandam, Tiruchirappalli 620 012, Tamilnadu, India

^e Department of Physics, Annamalai University, Annamalinagar 608 002, Tamil Nadu, India

^f Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences (SIMATS), Chennai 602 105, India.

^g Department of Civil Engineering, Yeungnam University, Gyeongsan 38541, Republic of Korea.

^h Center for Research Impact and Outcome, Chitkara University Institute of Engineering and Technology, Chitkara University, Rajpura 140 401, Punjab, India

ⁱ Department of Chemistry, P. T. Lee Chengalvaraya Naickar College of Engineering & Technology, Kanchipuram 631 502, Tamil Nadu, India.

^j Department of Chemistry, University College of Engineering Panruti, Panruti 607 106, Tamil Nadu, India

^k Department of Chemistry, Thiru. Vi. Ka. Government Arts College, Thiruvavur 610 003, Tamil Nadu, India. (Affiliated to Bharathidasan University, Tiruchirppalli 620 024, Tamil Nadu, India)

E-mail: drgtnarayanan@gmail.com, thirunarayanan.g.10313@annamalaiuniversity.ac.in

Received 2 February 2026; accepted (revised) 7 April 2026

Three series of *E*-imines such as (*E*)-*N*-(substituted benzylidene)-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amines, (*E*)-[4-(substituted benzylideneamino) phenyl] (phenyl) methanones and (*E*)-*N*-(substituted benzylidene)-2-(trifluoromethyl)anilines have been synthesized by sulfated fly-ash:SnO₂ catalyst assisted condensation of 2,3-dihydro(*b*)[1,4]dioxin-6-amine, 4-benzoylaniline, 2-trifluoromethylaniline and substituted benzaldehydes under microwave irradiation conditions. This condensation gives more than 70% yield. Physicochemical constants, elemental analysis, and spectroscopical information have been applied for the characterization of synthesized *E*-imines. The X-ray single crystal structure of (*E*)-*N*-(4-nitrobenzylidene)-2-(trifluoromethyl) aniline (**27**) has been established. Specific spectroscopical wave numericals of the imines have been applied for QSAR linear statistical investigations. Based on the outcomes of linear QSAR computations, the influence of auxiliaries on specified spectroscopical data has been investigated. Resonance and inductive properties of the auxiliaries yield satisfactory correlations ($r > 0.900$). In molecular-docking analysis, the *E*-imines **4**, **7**, **10**, **11**, **13**, **16**, **17** and **22** show high protein-ligand interaction binding energy. The imines **5-7** and **10** show good antibacterial actions in contrast to *S. aureus*, *E. coli* and *P. aeruginosa* strains. In the serial dilution method, all compounds are active against their antibacterial strains. The imines **2-9**, **24** and **26** are active with MICs of 9.5-16.5 against *A. niger* microbes. Imines **4**, **5**, **14-16** and **22** exhibit good antimalarial activities against *P. falciparum* strain.

Keywords: Environmentally benign synthesis, Sulfated fly-ash:SnO₂, *E*-imines, XRD spectra, Spectral QSAR, Biological activities