

## Synthesis and spectral studies of some bio-active aryl bis-enones

P Gayathri<sup>†a</sup>, P Mayavel<sup>a,b</sup>, I Muthuvel<sup>a,c</sup>, S Balasundari<sup>a</sup>, P Sudha<sup>a</sup>, V Usha<sup>d</sup>, K Ranganathan<sup>e</sup>, V Sathiyendiran<sup>f</sup>, B Krishnakumar<sup>†g,h,i</sup>, S Rajasri<sup>j</sup>, K Veeravelan<sup>k</sup> & G Thirunarayanan<sup>\*a</sup>

<sup>a</sup>Department of Chemistry, Annamalai University, Annamalainagar 608 002, Tamil Nadu, India

<sup>b</sup>Department of Chemistry, Government Arts College, Ariyalur 613 204, Tamil Nadu, India

<sup>c</sup>Department of Chemistry, M. R. Government Arts College, Mannargudi 614 001, Tamil Nadu, India

<sup>d</sup>Department of Chemistry, University College of Engineering Panruti, Panruti 607 106, Tamil Nadu, India

<sup>e</sup>Department of Chemistry, P. T. Lee Chengalvaraya Naicker College of Engineering and Technology, Kanchipuram 631 502, Tamil Nadu, India

<sup>f</sup>Department of Chemistry, Saurashtra College, Madurai 625 004, Tamil Nadu, India

<sup>g</sup>Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences (SIMATS), Chennai 602 105, Tamil Nadu, India

<sup>h</sup>Department of Civil Engineering, Yeungnam University, Gyeongsan 38541, Republic of Korea

<sup>i</sup>Centre for Research Impact and Outcome, Chitkara University Institute of Engineering and Technology, Chitkara University, Rajpura 140 401, Punjab, India

<sup>j</sup>Department of Chemistry, Raak College of Engineering and Technology, G. N. Palayam, Villiyanur, Puducherry 605 110, India

<sup>k</sup>Department of Science and Humanities, Vel Tech Multi Tech Dr. Rangarajan Dr. Sakunthala Engineering College (Autonomous), Avadi, Chennai 600 055, Tamil Nadu, India

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

Received 5 November 2025; accepted (revised) 30 January 2026

Seven series of bis-chalcones have been synthesized *via* the Claisen-Schmidt condensation between various aromatic aldehydes and ketones under conventional heating conditions, utilizing nano fly ash-supported  $H_3PO_4$  as a catalyst in an ethanol medium. The reaction affords yields exceeding 60%. The resulting bis-chalcones have been characterized based on their physical properties, elemental (micro) analyses, and spectroscopic data. The characteristic infrared absorption frequencies ( $\nu$ ,  $cm^{-1}$ ) corresponding to C=O and  $\nu_{C=C}$  (vinyl) groups, along with the NMR chemical shifts ( $\delta$ , ppm) of vinyl protons, carbons, and carbonyl carbons in the bis-enones, have been correlated using Hammett substituent constants ( $\sigma$ ,  $\sigma^+$ ,  $\sigma_1$ ,  $\sigma_R$ ), field (F) and resonance (R) parameters, as well as Swain-Lupton constants through single and multiple regression analyses. The statistical results have been used to establish quantitative structure-activity relationships (QSAR) for the substituent effects. Molecular docking studies have been further performed to evaluate the protein-ligand interactions of the synthesized bis-chalcones with a target protein. The *in vitro* antimicrobial potential of compounds **8-13** has been determined using the Bauer-Kirby disc diffusion assay, while their antimalarial efficacy has been assessed against *Plasmodium falciparum*.

**Keywords:** Aryl bis-enones, nano Fly-ash: $H_3PO_4$ , NMR spectra, Hammett correlation, Molecular docking, Bio-activities