Dr. D. James Bound, M.Sc, PhD

Designation: Assistant-Professor

Research Area: Organic & Bio-Organic Chemistry

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Research interests: I am interested in designing and synthesizing target molecules and conducting interdisciplinary research work, spanning Synthetic organic, Carbohydrate chemistry and Biochemistry. My focus is on developing new chemical tools to answer fundamental biological questions. These tools cover a broad range of applications from SAR studies, in order to allow for a deeper understanding of molecular recognition phenomena of particular drug targets and other cellular events. Together with optimizing small molecule hits emerging from screening or from rational drug design approaches. These efforts are strongly connected to the activities of the screening and the drug design of the bio actives synthesized. In this context interested in developing and advancing enabling methodologies for the investigation of unexplored biological targets such as library design, synthetic methodology and fluorescent labeling.

This work embraces the following further areas/fields of interest:

- a) Synthetic methods to access privileged or novel scaffolds useful in drug discovery
- b) To study the *in vitro* antimicrobial, *in vivo* bioavailability, toxicological and antimutagenic attributes of the novel bioactive and its derivatives.

Research Accomplishments:

- Development of efficient microwave assisted protocol to afford t-alkyl, allyl and benzyl
 thiocyanate in excellent yields with formation of thermodynamically stable
 isothiocyanates only in minor proportions.
- A facile, rapid and general synthetic procedure developed for 2,3-unsaturated and 2,3-dideoxy 1-O-glucosides of terpene phenols, especially sterically hindered ones, and terpene alcohols.

- First report of microwave assisted and Zinc-bromide catalyzed Ferrier reaction.
- Novel glucoside derivatives of carvacrol, thymol and perillyl alcohol synthesized.
- Evaluated *in vitro* antimicrobial activity against four food borne pathogens *B.cereus*, *S.aureus*, *E.coli* and *Y.enterocolitica* and established 2,3-unsaturated 1-*O*-glucosides were more effective than parent compounds.
- The time-kill and bacteriolysis assays were performed to demonstrate the mode of action of novel glucosides with *S. aureus* as the model.
- Evaluated *in vitro* antifungal activity against four food borne pathogens *A. flavus*, *A. ochraceus*, *F.oxysporum*, *S.cerevisiae* and *C.albicans* and established 2,3-unsaturated 1-O-glucosides were more effective than parent compounds.
- Assessment of the antitoxigenic effects of carvacrol, thymol, perillyl alcohol and their deoxyglucosides against *A. ochraceus* and *A. flavus*. Effectively inhibiting the production of Ochratoxin and Aflatoxin-B1.
- Selected terpene phenol/alcohols and their 2,3-dideoxy glucosides as bioactive compounds, the production of **Aflatoxin B1, B2** and **Ochratoxin-A1** produced by *A. flavus* and *A.ochraceus* respectively, were evaluated and estimated.
- Evaluated the effect of carvacrol and its 2,3-unsaturated 1-*O*-glucoside on the fungal membrane integrity of *C.albicans* using Propidium Iodide (PI) Influx assay.
- The anti-quorum sensing properties of terpene phenols/alcohols and their deoxyglucosides derivatives were evaluated against G^{-ve} bacteria *Pseudomonas aeruginosa* and *Chromobacterium violaceum*.
- Extraction and quantification of pyocyanin and violacein secondary metabolite important virulence and pro-inflammatory factor produced by *P. aeruginosa and C.violaceum* respectively.
- Demonstrated 2,3-unsaturated 1-O-glucosides of carvacrol, thymol, exhibited superior antimutagenic properties in comparison to parent molecules against MMS induced mutation in Salmonella typhimurium TA 1538.

- Bioavailability, pharmacokinetics and toxicology studies of carvacrol, thymol, perillyl alcohol and their novel glycosides were conducted on mice model.
- Bio-analytical method development for identification and quantification of 2,3-dideoxy 1-*O*-glucosides of Carvacrol, Thymol, S(-)Perillyl alcohol by HPLC.
- *In vitro* quantitative determination of creatinine, urea, and activities of enzymes like ALP, LDH, SGOT and SGPT in serum and plasma.

Technical Skills:

- Synthesis and characterization of Glyco-conjugates of terpene phenols and alcohols and evaluating bio-activity of theglucosides.
- Design, method development and optimization of novel synthetic protocol for target molecules using Microwave Assisted Organic Synthesis (MAOS).
- Skill in handling both single and multi-mode microwave reactors.
- Good knowledge of organic reaction mechanisms, designing multistep organic synthesis, purification using chromatographic techniques and characterization using analytical methods of 1D (¹H,¹³C) and 2D NMR (HSQC, HMBC, HETCOR, ¹H-¹H COSY) IR, UV, Mass Spectrometry, HPLC, LC-MS and GC-MS.
- Evaluation of antibacterial, antifungal, antiquorum sensing and antimutagenic attributes of the 2,3-dideoxyglucosides prepared and studying their mode of action.
- Isolation and quantification of Aflatoxin (B1, B2, G1 & G2) and Ochratoxin produced by the respective fungal cultures.
- Designing and planning of animal experiments to evaluate bioavailability and toxicology of the target molecules synthesised.

Research Publications:

1. D. James Bound, P. S. Negi, Pushpa S. Murthy, P.Srinivas. Evaluation of antiquorum sensing and antimutagenic activity of 2,3-unsaturated and 2,3-dideoxyglucosides of selected terpene alcohols and phenols.

2. D. James Bound, Pushpa S. Murthy, P.Srinivas. 2,3-dideoxygluco- sides of terpene phenols and alcohols as potent antifungal compounds.

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Food Chemistry, 2016; 210, 371-380. (Impact Factor: 6.306)
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3. D. James Bound, Pushpa S. Murthy, P.Srinivas. Synthesis and anti-bacterial properties of 2,3-dideoxyglucosides of terpene alcohols and phenols.

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Food Chemistry, 2015; 185, 192-199. (Impact Factor: 6.306)
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4. D. James Bound, B. K. Bettadaiah, P.Srinivas. ZnBr₂-Catalysed and Microwave Assisted Synthesis of 2,3-Unsaturated Glucosides of Hindered Phenols and Alcohols.

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Synthetic Communications, 2014; 44, 2565-2576. (Impact Factor: 1.796)
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5. D. James Bound, B. K.Bettadaiah, P.Srinivas. Microwave Assisted Synthesis of Alkyl Thiocyanates.

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Synthetic Communications, 2013; 43, 1138-1144. (Impact Factor: 1.796)
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6. D. James Bound, R. Arun Kumar, V. Baskaran, P.Srinivas. Bioavailability and acute toxicology studies of novel 2,3-dideoxyglucosides of carvacrol, thymol and perillyl alcohol in mice model.

(Manuscript under Preparation)

Conference Presentations:

- **D. James Bound,** B. K. Bettadaiah and P.Srinivas. "Synthesis of 2,3-unsaturated 1-O-Glucopyranosides of Terpene Alcohols from Spices and Herbs" at National Carbohydrate Conference, Carbo- XXVII organised at CSIR-CFTRI, Mysore. Abstract no: PP 18, page no 54.
- D. James Bound, Pushpa S. Murthy and P.Srinivas. "Synthesis and anti-quorum sensing inhibitory activity of terpene alcohol/phenols and their glucoside derivatives" at 7th International Food Convention (IFCON-2013), organised at CSIR-CFTRI, Mysore from 18 to 21st December 2013.