

### 2025 ACS Green Chemistry Institute Pharmaceutical Roundtable Research Grant Towards More Sustainable Catalysis

The <u>ACS Green Chemistry Institute Pharmaceutical Roundtable</u> (GCIPR) is a partnership between the ACS Green Chemistry Institute<sup>®</sup> and pharmaceutical-related corporations united by a shared commitment to integrate the principles of green chemistry and engineering into the business of drug discovery and production. Current members are AbbVie, Amgen, AstraZeneca, Bayer, Biogen, Biohaven, Boehringer-Ingelheim, Bristol-Myers Squibb, F. Hoffmann-La Roche Ltd., Ferring, Gilead, GSK, Ipsen, Johnson & Johnson, Lilly, Merck & Co., Merck KGaA, Darmstadt, Germany, Neurocrine, Novartis, Novo Nordisk, Pfizer, Sanofi, Takeda, UCB Pharma, Vertex, and the ACS Green Chemistry Institute<sup>®</sup>. Associate members are Asymchem, Axplora, Bachem, CatSci, ChemExpress, Codexis, EuroAPI, Hikal, Hongene, Hovione, InnoSyn, Nitto Avecia, PharmaBlock, Pharmaron, Polypeptide, Porton, Sai Life Sciences, ST Pharm, Syngene, and WuXi AppTec. Affiliate members are Aralez Bio, Corteva Agriscience, FMC, PHT and Zoetis.

The ACS GCI Pharmaceutical Roundtable is seeking a one-year R&D commitment to assist the Roundtable's green chemistry initiative to **develop strategies to employ earth-abundant or sustainable organic catalysts** to enable organic synthesis of pharmaceutically relevant scaffolds and/or **devising methods to enhance the sustainability of existing catalytic processes** by way of solvent/reagent modulation/recycling. Proposals are invited from public and private institutions of higher education worldwide. This collaborative project is intended for a student within the selected Principal Investigator's research group. One grant is planned to be awarded, and the total award is limited to \$80,000 for a grant period of 12 months. Interested PIs are required to provide a written proposal describing the investigator's capability to carry out the Roundtable's proposed research. Deadline for receipt of proposals is **May 16, 2025, at 11:59 p.m. EDT**. All submissions must be made in our application portal: <a href="https://gci.acs.org">https://gci.acs.org</a>. The Principal Investigator with the selected proposal will be notified by **September 1, 2025**. It is expected that research will commence in the principal investigator's lab no later than **October 2025** and last 12 months.

### **Requirements for Submission**

Proposals will only be accepted from public and private institutions of higher education. The grant is not limited to institutions in the United States. <u>Proposals must be submitted in our application portal https://gci.acs.org through the appropriate institutional office for external funding. For international submissions, if there is no comparable office, submit a PDF of a letter signed by an appropriate university official recognizing the terms of the grant.</u>

**Detailed Project Description:** Catalysis is a cornerstone of modern organic synthesis and in particular, provides industry with the tools to facilitates the production of APIs and agrochemicals in the most expedient manner. Developments in transition metal catalysis, photocatalysis, and organocatalysis have been enabling for end-to-end product development. These technologies have provided medicinal chemists with the tools to more rapidly interrogate SAR as well as drastically shorten the synthetic sequences that process chemists use in production campaigns. Despite initiatives and advances in enhancing their sustainable profile, the majority of catalytic paradigms largely use the

same sets of catalysis, ligands, and solvents that were in use over a decade ago. As such, the ACS GCIPR would like to divert some funding back to the development of sustainable platforms for catalysis, broadly defined. Representative key areas include (but are not limited to):

- 1) Expanding knowledge around abundant metal catalysis (e.g., iron, nickel, copper, etc.)
- 2) Improving conditions for established transition metal-catalyzed transformations by employing more sustainable solvents or solvent-free
- 3) Devising alternatives for super stoichiometric inorganic bases
- 4) Improving methods of immobilization of catalysts to enable reuse/recycle

Based on a generalized need for innovation in this area, the GCIPR seeks proposals that fall within the general framework of enhancing the sustainable profile of the workhorses of organic synthesis: **Photocatalysis, Transition-Metal Mediated Catalysis, and Organocatalysis.** Proposed areas of research should be practical in nature and have some definable metric for scoring improvement of sustainability (e.g., Carbon Economy or Environmental Factor, etc.). Further, submissions should make clear how the developed processes can be used to advance drug discovery and/or agrochemical efforts. Topical areas of interest include (but are not limited to):

- Identification of novel earth-abundant catalysts for photocataylsis and/or transition metal cross-coupling (e.g. Fe, Co, Cu, etc.) that facilitate C-C, C-N, C-O or C-F bond construction. In particular, such methods should retain tolerance towards heterocyclic scaffolds and/or provide access to chemical space where entry is currently limited.
- Design and implementations of ligands derived directly from sustainable sources that reduce the synthetic burden for assembly while maintaining comparable or better catalytic activity to traditional ligands (e.g. Buchwald, Fu, Davies etc.)
- Utilization of sustainable (non-petroleum derived) substrates that allow for rapid increases in molecular complexity
- Design and development of readily accessible, sustainable organocatalysts with high recyclability rate that enable C-C, C-N, C-O or C-F bond construction with stereocontrol where applicable
- Implementation of solvent (or solvent combinations) that provide equivalent (or better) efficacy for existing catalytic systems including processes performed in aqueous media with surfactants
- Replacement of non-sustainable additives critical for reaction success and commonly employed by existing processes (e.g. bases or salts)
- More sustainable photochemical activation by way of novel photocatalysts, catalysts that use lower energy wavelengths, or processes in which the substrates are themselves photoactivated
- Use of computational models (i.e. machine learning) to better understand solvent/catalyst interplay to guide screening efforts towards appropriate sustainable solvents

• Systems that can be implemented to improve recycling of catalyst by way of isolation/regeneration of catalysts or via catalyst immobilization

## **Project Goal**

Render tools to reduce or eliminate the dependency on non-sustainable catalysts for catalytic systems by way of identification of new catalysts or remediation of current platforms.

### **Project Timeline**

It is expected that one year of research support will be sufficient to provide progress toward intended goals.

### **Proposal Format**

Please be prepared to provide the following information in the application portal:

- 1. Name and email of grant officer
- 2. Name, title, phone, email and address of the Principal Investigator
- 3. Project Title
- 4. Research Group website
- 5. PDF of Proposed Plan of Work (2 pages, 12 pt font, 1-inch margins)
  - Objectives: Briefly state the project objectives
  - Project Approach: Include specific aims and investigations planned
  - Proposed milestone deliveries with brief description of the manner in which the researcher intends to achieve them
  - Brief description of the PI's research facilities and summary of the student's (undergraduate, graduate student and /or postdoc) capabilities to perform the proposed work
  - References (does not count toward your page limit)

Note: The PI should list any existing background intellectual property and/or collaborations they are aware of that might limit the freedom to operate any of the results arising from any research funded by ACS GCIPR. The priority of the Roundtable is to encourage research utilizing reaction conditions that are commercially available with the freedom to use.

- 6. PDF of Detailed Estimated Budget: The total amount requested would include all direct costs, student assistantships, etc. The total award is limited to \$80,000 for a grant period of up to 12 months.
  - Institutional overhead costs (indirect costs) should not be more than 10% of the total budget.
  - Post-doctoral associate salary and benefits are supported.
  - Student stipend and benefits are supported. Proposals for support of advanced graduate students are highly favored.

- PI salary supplements will not be supported.
- Laboratory supplies and instrument use charges are supported.
- No funds may be allocated for travel, equipment purchase or repair, or administrative support.
- 7. Curriculum Vitae of Project Team Members: Please submit a curriculum vitae of each project team member (up to two pages per team member, combined into one document). This does not count toward your page limit.

# **Report Requirements**

- Progress reports or updates are due monthly or bi-monthly from initiation of research and will be discussed in arranged web-conferences. Reports will be shared with the member companies of the Roundtable.
- Reports are to include research milestones/significant outcomes, summary of progress to date noting any deviations from the proposal, and research plans for upcoming months.
- A final comprehensive report is due one month after the end of the grant period. This report must be submitted as a PDF document electronically to gcipr@acs.org. In addition, the content of the report should be targeted for publication in a peer-reviewed technical journal. The paper will be co-authored by the principal investigator and student(s) performing the work with the guidance of member companies of the ACS GCIPR. Representatives of member companies who make intellectual contributions to the project should be recognized as authors.

# Intellectual Property, Publication Acknowledgement, and Terms of the Grant

- The primary purpose of this grant is the public dissemination of research through publication.
- Every patent, United States or foreign, that results from research funded (in part or in its <u>entirety</u>) by the ACS GCIPR Research Grant shall be immediately dedicated to the public, royalty free.
- Publication of results is expected within 6 months of work completion.
- Each publication prepared in connection with the ACS GCIPR Research Grant shall make acknowledgement in the following manner: "This manuscript was developed with the support of the American Chemical Society Green Chemistry Institute Pharmaceutical Roundtable (www.acsgcipr.org). The ACS GCI is a not-for-profit organization whose mission is to catalyze and enable the implementation of green and sustainable chemistry throughout the global chemistry enterprise. The ACS GCI Pharmaceutical Roundtable, composed of pharmaceutical and related industries, was established in 2005 to encourage innovation while catalyzing the integration of green chemistry and green engineering in the global pharmaceutical industry. The activities of the Roundtable reflect its member's

shared belief that the pursuit of green chemistry and engineering is imperative for business and environmental sustainability."

- Acceptance of a Roundtable Grant will be conditional upon agreement by the grantee institution that in the event the Principal Investigator is unable for any reason to conduct the research proposed, the funds, if previously paid by the Roundtable, shall, upon demand, be returned in full to the Roundtable, and further, that in the event the PI is unable for any reason to continue with the research after it has commenced, this grant shall be terminated forthwith and the unexpended and unencumbered balance of any funds theretofore advanced shall be returned to the Roundtable.
- The grantee institution, by acceptance of this grant, provides assurance that support normally provided by the institution for research of the faculty member will not be diminished.
- Applicants may have only one research grant with the ACS GCIPR at a time. In order to close a grant, the ACS GCIPR must receive and approve the required reports.

### For additional information:

Website: <u>www.acsgcipr.org</u> Email: <u>gcipr@acs.org</u>