opnMe by Boehringer Ingelheim

Boehringer's SMART Kit

How would your novel synthetic methodology perform against 96 pharma-relevant aryl bromides at Boehringer Ingelheim?

Answers to this question including a brief outline of the proposed methodology, can only be considered if they arrive no later than November 10, 2026, 11:59 pm PST.

Boehringer Ingelheim

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Summary

Boehringer Ingelheim invites academic researchers to test their newly developed synthetic method (including catalysts and reagents) across a curated panel of 96 medicinal chemistry-relevant building blocks – the **Boehringer Ingelheim's SMART Kit** (B-SMART: Boehringer's Synthesis Methodology Assessment and Reactivity Test). Selected proposals will be evaluated in-house at Boehringer Ingelheim under standardized high-throughput experimentation (HTE) conditions by our Medicinal Chemistry Technologies Group, generating a comprehensive, publication-ready dataset on method generality, robustness, and substrate-dependent limitations – free of charge.

In return, you keep full ownership of your data and any resulting IP and are free to publish independently. **Please note: this call does not provide monetary funding; the benefit consists exclusively of free access to experimental data and publication rights** (see "What benefits do we offer to you?" below).

Submit your proposal, specifying the coupling partner(s) you wish to have assessed, no later than **November 10, 2026, 11:59 pm PST**.

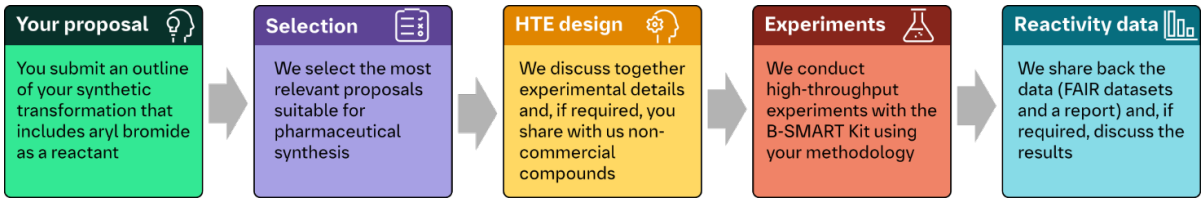
Background

The discovery of new chemical transformations continues to expand the toolbox of synthetic chemistry. Yet for many promising methodologies, the true scope, robustness, and practical applicability remain insufficiently explored – especially across the diverse chemical space encountered in medicinal chemistry. Systematic reaction scope evaluation has therefore become an active area of interest, including Merck's chemistry informer libraries, Glorius' substrate-selection strategy for reducing bias in reaction generality assessment, Doyle's data-guided aryl bromide scope analysis for Ni/photoredox catalysis, and our own recently shared Boehringer Ingelheim ChemKit.[1-4]

The **B-SMART Kit** builds on this movement by combining curated, medicinal chemistry-relevant building blocks with standardized high-throughput experimentation (HTE). Rather than treating an extended substrate scope as a single demonstration for one method, its central concept is to apply the same representative set of building blocks systematically across multiple emerging methodologies and reaction parameters – catalysts, ligands, or activation modes alike. This generates comparable, cross-method datasets that reveal reactivity trends, substrate-dependent limitations, and optimization opportunities, helping to assess the real-world applicability of new methodologies in medicinal chemistry synthesis and to support future predictive models for synthesis planning. The current B-SMART Kit comprises (hetero)aryl bromides (featuring C(sp^2)–Br bonds) with a strong emphasis on heterocyclic cores that are abundant in marketed drugs and therefore highly relevant to medicinal chemistry synthesis (e.g., bromo-azoles, azines, 5,6- and 6,6-fused heteroaromatic cycles). The complete list of B-SMART Kit compounds, including their structures and identifiers, is available for download here.

Through this opnMe call, we invite academic researchers who develop innovative reaction methodologies, catalysts, activation modes, or synthesis technologies to submit a non-confidential outline of their proposed research, specifying the coupling partner(s) (if applicable) they wish to have assessed. Experimental conditions, including catalyst structures, do not need to be disclosed at the proposal stage. Selected contributors will provide their experimental conditions and/or catalysts/reagents, which will be evaluated in-house at Boehringer Ingelheim's Medicinal Chemistry Technologies Group in Biberach an der Riss, Germany, using the B-SMART platform (96 (hetero)aryl bromides, micromolar scale).

In return, contributors gain access to comprehensive reaction scope data that would be difficult to generate within a typical academic environment – free of charge, and free to publish. Beyond advancing individual methodologies, this collaborative effort aims to build valuable, comparable datasets that improve our collective understanding of reaction generality and accelerate the development of AI-guided synthesis planning tools. Ultimately, the combination of innovative academic chemistry, systematic HTE data generation, and predictive modeling has the potential to meaningfully accelerate medicinal chemistry and drug discovery by enabling faster identification of reliable, scalable synthetic routes.



What proposals could be in scope?

In scope are novel (ideally unpublished) transformations in which the B-SMART Kit's (hetero)aryl bromides serve as substrates/building blocks for method evaluation.

- The methodologies may include new catalysts/ligands and/or other reagents.
- Proposed reactions may include but are not limited to C–C/C–X cross-coupling reactions, C–H functionalization, and radical, organo-, or biocatalytic methods applicable to heteroaryl bromides – provided that the required experimental conditions and any commercially unavailable materials (sufficient for at least 100 reactions at 1 µmol scale) are supplied by you once your proposal has been selected. The proposed reactions may be air sensitive.
- Photoredox catalysis and electrocatalysis as standalone technologies are of particular interest.

What proposals would be out of scope?

- Proposals addressing any objective other than extending the scope of novel chemical transformations. This specifically excludes any medicinal chemistry proposals that aim to use subsets of the B-SMART Kit for drug discovery or drug design purposes.

- Proposals that would require any type of validation as part of *in vitro* or *in vivo* biological experiments.
- Methods that require the use of gaseous reagents, high pressures, or cryogenic temperatures.
- Application of microwave-, mechano-, flow-, or photoelectrochemistry technologies.
- Methods with a clear potential for "dual use."
- Any commercial activities, including contract research or manufacturing organizations.

What benefits do we offer to you in exchange for having submitted a proposal?

Please note: no monetary funding is associated with this call. In its place, we offer the following:

Free experimental evaluation

- If your proposal is shortlisted, our Medicinal Chemistry Technologies group will apply your experimental conditions to the 96 aryl bromides of the B-SMART Kit, following prior discussion of the experimental design with you. Experiments are performed in our laboratories in Biberach/Riss, Germany, entirely free of charge to you.
- Your proposal is treated confidentially and is never shared with other submitting scientists, nor other third parties.

A comprehensive, publication-ready dataset

- You will receive a comprehensive FAIR dataset with reaction information for each well including relative assay yields (HPLC peak areas of the products relative to an internal standard), extending your substrate scope and revealing robustness and performance of your method. While assay yields cannot be compared across different B-SMART Kit products (due to differing absorption coefficients), they reliably indicate whether – and to what extent – a reaction proceeds with a given aryl bromide.
- You will also receive a publication-ready report with product structures and corresponding assay yields that you can use to support publications, conference presentations, grant applications, methodology benchmarking, and data-driven/AI-enabled reaction design.

Ownership, confidentiality, and involvement

- You keep full ownership of all results, data, discoveries, and any IP generated through your work in this project. Boehringer Ingelheim receives only a non-exclusive, internal right to use the results for research purposes, including improving and training its computational and AI models.
- The reaction conditions of your methodology are treated confidentially and are never disclosed to third parties by us.
- You can participate in the experimental design, data interpretation, and decisions on follow-up experiments.

- You are free to use and publish the generated data which belongs to you. We only ask that you acknowledge access to the Boehringer Ingelheim B-SMART Kit through opnMe in any resulting publications, posters, presentations, or grant applications.
- We believe in full transparency: you can review the material transfer agreement in advance to understand the terms that will apply if your proposal is selected.

Key criteria for the selection of proposals

Boehringer Ingelheim is seeking research collaboration proposals that:

- Are highly feasible, novel, and clearly address the in-scope and out-of-scope criteria above.
- Include a brief, non-confidential description of your research and an outline of the proposed methodology, specifying the coupling partner(s) (if applicable). Experimental conditions, including catalyst structures, do not need to be disclosed at the proposal stage.
- Confirm the availability of any required non-commercial catalysts, reagents, or materials in quantities sufficient to complete the evaluation (at least 100 reactions at 1 µmol scale).
- Demonstrate a proven track record in the required field of expertise.

Anticipated Timelines

Phase 1	Please complete your submission by **November 10, 2026, 11:59 pm PST at** the very latest.
Phase 2	Our review of all proposals will be completed by mid-January 2027, and applicants will be informed afterwards.
Phase 3	Selected contributors provide their experimental conditions and/or materials by post, after having signed our MTA.
Phase 4	Experiments are projected to start at Boehringer's medicinal chemistry site in February–March 2027.
Phase 5	Boehringer Ingelheim plans to provide a results dataset and report in the timeframe of two months once the method has been successfully reproduced in-house.

Submitting a proposal

- Check the B-SMART Kit profile on opnMe.com, or alternatively:
- Click the "Download your submission template" banner to access the collaboration submission template (requires login or registration).

- Recommended length of proposals is less than 5 pages (including background information and high-level description of the transformation/method). The use of graphics to convey the proposed concept is highly encouraged.
- Follow the instructions to download the template or upload your submission document.
- If you are selected as a winner, we will ask you to provide the signed Material Transfer Agreement (MTA), which you can find on our website.
- You will be able to access your final submitted collaboration proposal in your personal dashboard and follow its review status.
- Please also visit the FAQ section on opnMe.com to learn more about the call.

What do we need from you if your proposal is selected?

For selected collaborators, the following should be further provided: 1) a comprehensive method description (treated confidentially, under the MTA terms that we encourage you to review prior to submission), 2) non-commercial catalysts, reagents, or other materials required for experimental evaluation, and 3) one to three representative reaction schemes (with specified commercial substrates) to ensure method reproducibility at Boehringer Ingelheim's laboratories.

References

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2. Kariofillis S. K., Jiang S., Żurański A. M., Gandhi S. S., Martinez Alvarado J. I., Doyle A. G. Using Data Science To Guide Aryl Bromide Substrate Scope Analysis in a Ni/Photoredox-Catalyzed Cross-Coupling with Acetals as Alcohol-Derived Radical Sources *J Am Chem Soc*. **2022**, 144(2):1045-1055. DOI: 10.1021/jacs.1c12203, PubMed.
3. Rana D., Pflüger P. M., Hölter N. P., Tan G., Glorius F. Standardizing Substrate Selection: A Strategy toward Unbiased Evaluation of Reaction Generality *ACS Cent Sci*. **2024**, 10(4):899-906. DOI: 10.1021/acscentsci.3c01638, PubMed.
4. Kutchukian P. S., Dropinski J. F., Dykstra K. D., Li B., DiRocco D. A., Streckfuss E. C., Campeau L-C., Cernak T., Vachal P., Davies I. W., Krska S. W., Dreher S. D. Chemistry informer libraries: a chemoinformatics enabled approach to evaluate and advance synthetic methods *Chem Sci*. **2016**, 7(4):2604-2613. DOI: 10.1039/c5sc04751j, PubMed.