



Dedication to Dr. Thomas Baillie in recognition of his scientific career

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Professor Thomas Baillie has left a lasting impact on the field of drug metabolism, influencing both the academic circle and the pharmaceutical industry; the first, as a professor at the University of Washington mentoring graduate students and postdoctoral fellows in the emerging field of

drug metabolism and its biological consequences, and the latter, as Vice President of the Drug Metabolism & Pharmacokinetics (DMPK) department at Merck, setting strategies and establishing DMPK as an integral partner in drug discovery. This special issue of *Medicinal Chemistry Research* is dedicated to honoring Dr. Baillie, with articles showcasing significant discoveries in drug metabolism and reflecting directly or indirectly to his contributions.

As a practicing academician, Professor Baillie has imparted extensive knowledge and expertise to students, inspiring and guiding them to pursue careers in the pharmaceutical sciences. Through his engaging lectures and mentorship, he has nurtured a deep understanding and appreciation for the complexities of drug metabolism among aspiring scientists. We have vivid recollections of his captivating lectures on the practical applications of mass spectrometry and stable isotopes in the pharmaceutical sciences, which had a remarkable ability to stimulate new students and to re-ignite the passion of those who had already taken the course. His studies have provided crucial insights into novel metabolic pathways, the role of specific enzymes, the formation of chemically reactive metabolites that can lead to toxicity, and in the design of covalent inhibitors leading to prolonged efficacy. Of no less value is Professor Baillie's influence on his colleagues within the scientific community. His groundbreaking research, innovative methods in mechanistic drug metabolism, and insightful findings have earned him respect and admiration from fellow researchers. He actively collaborates with other experts, fostering an environment of collective learning that

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pushes the boundaries of scientific enquiry. This is evident in his collaboration with many professors and industrial scientists whose work is captured in this review.

Dr. Baillie has made an indelible impact on the pharmaceutical industry, in part by establishing DMPK as a pivotal partner in the drug discovery process. DMPK, in many ways, was previously looked upon as a support group to the biology therapeutic area and the Medicinal Chemistry function; Dr. Baillie successfully established the role of DMPK as an equal voice in the drug discovery paradigm by becoming involved as early as compound design in terms of optimizing safety and absorption, distribution, metabolism and excretion (ADME) properties. He was one of the first to make teams practice routinely the art of mechanistic biotransformation studies with the end goal of rational derisking of compounds, be it in drug-induced liver injury (DILI), poor clearance or mutagenic liabilities. Such integration of chemistry and analytical mass spectrometry in DMPK shaped a field in itself, influencing a generation of scientists of which the three of us are beneficiaries. His insights on circulating metabolites in the context of drug

safety have shaped industry practices in the drug development phase, leading to the “Metabolites In Safety Testing (MIST)” regulatory guidance. His seminal work on the application of protein covalent binding for the assessment of DILI hazard in a compound has led to decades of scientific exploration and provided the first quantitation of this elusive risk parameter. His expertise and scientific acumen have made him a trusted advisor and consultant to pharmaceutical companies and regulatory agencies since his retirement from Merck.

Professor Baillie’s impact crosses many boundaries – whether in his role as a professor, colleague, or a pharmaceutical industry leader, he has left a lasting imprint on the realms of DMPK and drug-induced toxicity. Through his guidance, collaborative efforts, and exceptional leadership, he has served as an inspiration to many, influencing the trajectory of pharmaceutical sciences and driving progress in drug discovery, safety, and personalized medicine. We consider ourselves incredibly fortunate to have had the opportunity to work with Professor Baillie, to learn from his expertise, and to grow as researchers.