



VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI / INVITATION TO THE
LECTURE WITHIN DOCTORAL PROGRAMME IN
CHEMICAL SCIENCES

Dr. Volker Derdau

*Sanofi Germany, R&D, Integrated Drug Discovery,
Isotope Chemistry, Industriepark Höchst, Frankfurt*

z naslovom / title:

**Chasing the miracles of Science with
Hydrogen Isotopes**

v sredo, 9. 4. 2025 ob 15. uri
v predavalnici 1 v 1. nadstropju Fakultete za kemijo
in kemijsko tehnologijo, Večna pot 113 /
on Wednesday, 9. 4. 2025 at 15.00
in lecture room 1, 1st floor at the Faculty of
Chemistry and Chemical Technology, Večna pot 113

Vljudno vabljeni! / Kindly invited!

Abstract:

One of the major motivations in pharma industry is to improve the life of patients using efficient drug treatments. Due to the complexity of biological processes in living creatures the number of scientific tools and experiments required to understand the nature of a disease is very high. One of these tools is the use of isotopically labeled compounds.^[1] They contribute significantly to the deeper understanding of metabolism and the improved safety profile of drugs. While applications such as classical radioactive immune assays or nuclear magnetic resonance (NMR) structure elucidations lost their attractiveness due to other more accurate, simpler or faster methods, uses of isotopically labeled compounds have increased.

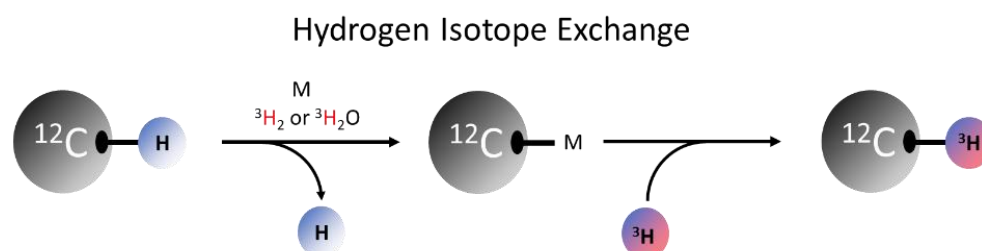


Figure 1. Schematic explanation of hydrogen isotope exchange (HIE)

In recent years C-H functionalization of complex molecules has become a strong tool in lead optimization of bioactive molecules in the life science industry. To achieve this at the latest possible serial step is a convenient way to increase speed and to decrease costs and resources in drug discovery research. This concept is also followed in the Hydrogen Isotope Exchange (HIE^[2]) reaction (figure 1). The HIE reaction can be considered as the most fundamental of all C-H functionalization's as the proton is just substituted by its isotopes. In the lecture several concepts of HIE will be discussed with recent examples from the group and an outlook will be given how this isotope chemistry knowledge on CH-functionalization can foster lead optimization in drug discovery.

References (reviews)

1. a) J. Atzrodt, V. Derdau, W.J. Kerr, M. Reid, *Angew. Chem. Int. Ed.* **2018**, *57*, 1758-1784; b) V. Derdau, C. S. Elmore, T. Hartung, B. McKillican, T. Mejuch, C. Rosenbaum, C. Wiebe, Christine, *Angew. Chem. Int. Ed.* **2023**, e202306019.
2. a) J. Atzrodt, V. Derdau, M. Reid, W. J. Kerr *Angew. Chem. Int. Ed.* **2018**, *57*, 3022-3047; b) J. Atzrodt, V. Derdau, T. Fey, J. Zimmermann *Angew. Chem. Int. Ed.* **2007**, *46*, 7744-7765; c) Voges, R.; Heys, J. R.; Moenius, T. Preparation of Compounds Labeled with Tritium and Carbon-14; John Wiley & Sons, **2009**; d) S. Kopf, F. Bourriquen, W. Li, H. Neumann, K. Junge, M. Beller *Chem. Rev.* **2022**, *122*, 6, 6634-6718; e) Q.-K. Kang, H. Shi, *Synlett* **2022**, *33*, 329-338; f) V. Derdau **2022** in Handbook of CH-Functionalization (ISBN 9783527834242. Ed. A. Maiti).