



**Laudatio for the Award Ceremony
of the Prix Schläfli Chemistry 2022
of the Swiss Academy of Sciences (SCNAT)
for Dr Philippe Schwaller**

The jury of the Prix Schläfli 2022 in Chemistry of the Swiss Academy of Sciences (SCNAT) consisting of Christian Bochet (U. Fribourg), Rebecca Buller (ZHAW), Catherine Housecroft (U. Basel), Thomas Bürgi (U. Geneva), Klemens Koch (PH Bern), Laura Nyström (ETHZ), Patrick Steinegger (Paul Scherrer Institute), Shana Sturla (ETHZ) and Oliver Wenger (U. Basel) has evaluated seven high quality applications and proposed to award the prize to Philippe Schwaller for his publication entitled 'Extraction of organic chemistry grammar from unsupervised learning of chemical reactions.' (Sci. Adv. 2021, 7(15),4166).

Philippe Schwaller received his Bachelor and Master degrees in Materials Science and Engineering from EPFL. He then moved to the University of Cambridge for a Master in Physics. After that he joined the group of Prof. Jean-Louis Reymond at the University of Bern for a PhD in Chemistry and Molecular Sciences. During his thesis he was co-supervised by Dr. Teodoro Laino at IBM Zurich. After a postdoc at IBM Research Philippe Schwaller took up a Tenure Track Professorship of Digital Chemistry at EPFL.

Philippe Schwaller pioneered the use of transformer models, which are neural networks, in the field of chemical reactions. His 'Molecular Transformer' model is a landmark contribution to the field of computer-assisted synthesis planning (CASP). The study presented by Philippe Schwaller describes a method for automated atom mapping, which is indispensable for developing computer-assisted synthesis planning. Atom mapping of a chemical reaction is a mapping between the atoms in the reactant molecules and the atoms in the product molecules. Atom mapping is extremely tedious and, up to his publication, could not be convincingly automated.

The jury of the Prix Schläfli was particularly impressed by the originality of the work, which represents a milestone contribution in automated synthesis planning.

Thy jury would like to congratulate again Philippe Schwaller on his excellent work, and wish him the best of luck for the future.

Prof. Thomas Bürgi, president of the jury of the Prix Schläfli Chemistry 2022

Award ceremony, 3 October 2022 in Zurich, ETHZ