Post-Doc Position in Computational Chemistry, Bioinformatics, and Programming at the University of Lübeck (LIED), Germany.

The Institution:

The Position is located at the Lübeck Institute of Experimental Dermatology (LIED) at the University of Lübeck within the facilities of the University Medical Center Schleswig-Holstein – one of the largest university hospitals in Germany. The LIED concentrates excellent research with 8 current research grants from the German Research Foundation (Germ. '*Deutsche Forschungsgemeinschaft*', DFG), 9 Collaborative Research Centers (Germ. '*Sonderforschungsbereich*'), 1 Research Training Group (Germ. '*Graduiertenkolleg*'), and participation in one Excellence Cluster. The LIED offers an interdisciplinary and translational work environment including *in silico*, *in vitro*, and *in vivo* approaches, particularly pre-clinical and clinical studies, supported by large international collaborative networks with work groups, for example, in Australia, Canada, China, Germany, Hungary, India, Norway, and the United States.

The Project:

ABC transporters are large membrane-bound proteins that critically impact drug distribution and pharmacokinetics in the body. Almost each of the 48 transporters is associated with both highly prevalent and orphan human diseases, however, at least 33 ABC transporters can be considered as 'under-studied' and cannot be addressed by small-molecule modulators. The PANABC project (www.panabc.info) seeks to provide pharmacological and medical research with selective and potent modulators (i) to study the physiological and pathological role of these under-studied ABC transporters, but also (ii) as template-molecules for new diagnostics and therapeutics of under-studied ABC transporters-associated diseases. A cutting-edge field in the discovery and optimization of new ABC transporter-addressing agents is the intended design and development of 'polypharmaceutics' which address a proposed 'multitarget-binding site' amongst all/most ABC transporters.

The Task

The successful candidate will apply fragment-based drug discovery methodologies, in particular, Computer-aided Pattern Analysis (C@PA) approaches, including subsequent virtual screening of (ultra-large) compound libraries and chemical

space. Deep knowledge in Similarity Search, Pharmacophore Modelling, and Clustering as well as common fingerprints (path-like, circular, *etc*) and other comparative ligand discovery and preparation tools is assumed. The generation of novel (multitarget) fingerprints, also applying standard programming techniques, is emphasized. In addition, structure-based approaches (*e.g.*, sequence alignment, homology modelling, molecular docking, molecular dynamics simulations, *etc*) will be applied to decipher the proposed multitarget binding site.

Requirements:

- A PhD in cheminformatics, computational chemistry, chemistry, life science informatics or a related field.
- Extensive knowledge and documented experience in computational medicinal chemistry is mandatory.
- Experience in ligand- and structure-based drug design approaches including molecular docking and molecular dynamics is required.
- Familiarity with computational chemistry packages (*e.g.*, Schrödinger, MOE, ChemDraw, *etc*) is expected.
- Familiarity with benchmark databases (*e.g.*, PubMed, PubChem, DrugBank, ChEMBL, DUD, MUV, PDB, UniProt, *etc*) is expected.
- Applicants who have experience in any of the following areas will be prioritized: cheminformatics, AI/ML approaches, and Python programming.
- A track record of excellent publications in high-rank peer-reviewed journals is desired.
- Proficient in oral and written English in order to be able to interact and communicate efficiently with collaborators.

Application

Please send your application including cover letter, 2-page cv and list of all publications and funding to svenmarcel.stefan@uksh.de no later than **October 31**, **2022**.