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Chamelogk: a new experimental-chromatographic chameleonicity descriptor

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The increasing interest in Beyond the Rule of 5 (bRo5) molecules in drug discovery is due to the fact that they are proved to act over difficult-to-drug targets, involved in untreated human diseases. Because of their complex and flexible structure, bRo5 compounds are often affected by poor solubility/permeability issues. Chameleonicity describes the capacity of a molecule to adapt to the environment through conformational changes, and designing molecular chameleons could be a smart strategy to simultaneously optimize the solubility/permeability balance. Here we describe Chamelogk, an automated, fast, and cheap chromatographic descriptor of chameleonicity