Czech Chemical Society Lecture

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University Campus Bohunice, Kamenice 5, Building B11/room 132

Towards Supramolecular Systems for Small-Molecule Diagnostics in Biofluids.

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Supramolecular systems hold great promise for future use in molecular diagnostics applications due to their potentially superior robustness, cost-efficiency, and response time compared to biosensors.[1] New technologies that allow for targeted detection of small biomarkers, such as metabolites, are of particular interest, as their detection is often not possible with antibody-based sensors and cumbersome with chromatographic methods. However, major challenges remain to be solved before the use of synthetic supramolecular systems can become a general option for molecular diagnostics. Simply speaking, current synthetic receptors, nanosensors, and probes still display significant shortcomings both in terms of binding strength and selectivity for small molecule analytes such as amino acids, biogenic amines, or neurotransmitters.

We show here novel supramolecular systems, including macrocyclic chemosensors (**Fig. 1**) and hybrid-material nanozeolites, that offer new ways to address the binding affinity- and analyte-distinction challenges.[2-4] Moreover, proof-of-concept examples for detecting metabolites and drugs at a physiologically relevant concentration range in biofluids such as human urine, saliva, or blood are showcased. Finally, we would also like to invite the community to contribute to the open-access SupraBank repository that makes both structures and physicochemical properties of non-covalent systems accessible and findable in a machine-readable format.[5]

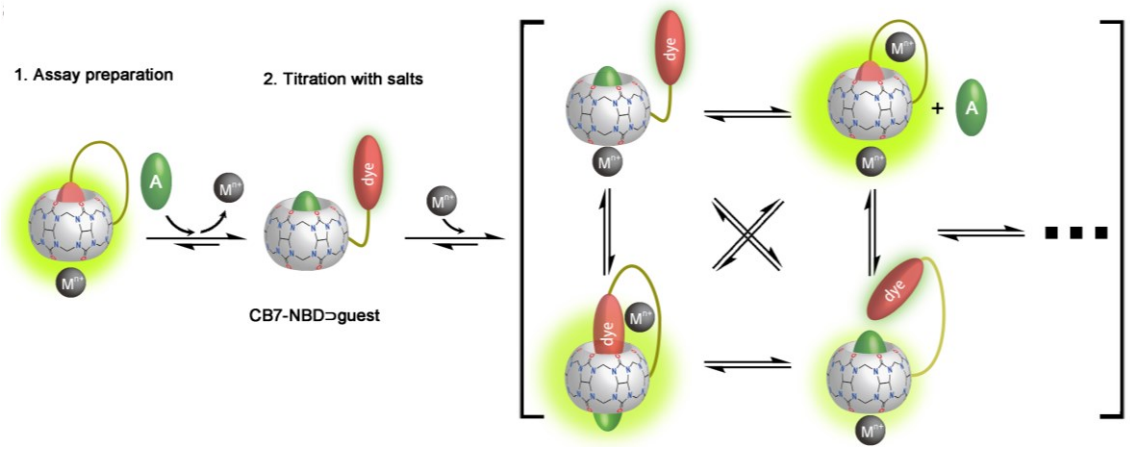

Figure 1: Schematic representation of supramolecular sensing strategies which enable *in situ* analyte identification through a salt-induced chemosensor response.

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[1] Krämer J., Kang R., Grimm L. M., De Cola L., Picchetti P., Biedermann F., *Chem. Rev.*, **2022**, *122*, 3459-3636.
[2] Hu C., Jochmann T., Chakraborty P., Neumaier M., Levkin P. A., Kappes M. M., Biedermann F., *J. Am. Chem. Soc.* **2022**, *144*, 13084-13095.
[3] Grimm L. M., Sinn S., Krstić M., D'Este E., Sonntag I., Prasetyanto E. A., Kuner T., Wenzel W., De Cola L., Biedermann F., *Adv. Mater.*, **2021**, *33*, 2104614.
[4] Hu C., Grimm L., Prabodh A., Baksi A., Siennicka A., Levkin P. A., Kappes M. M., Biedermann F., *Chem. Sci.*, **2020**, *11*, 1114-11153.
[5] https://suprabank.org/