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A THEORETICAL INVESTIGATION OF CALIXARENE-BASED SUPRAMOLECULAR SYSTEMS FOR VOC DETECTION

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Introduction. Volatile organic compounds (VOCs) serve as critical biomarkers for early lung cancer detection, driving demand for developing selective sensor materials. Calixarenes – macrocyclic molecules with tunable cavities and host-guest capabilities – are promising candidates for such applications due to their ability to recognize small organic analytes through non-covalent interactions. While computational methods, including those based on density functional theory (DFT) reliably model these interactions and correlate well with experimental binding trends [2], their predictive accuracy to a significant extent depends on the choice of functional and the specific physicochemical properties of the system. This study evaluates three DFT functionals to identify the optimal approach for modeling calixarene-VOC interactions.

Main part. 11 calixarene derivatives were evaluated for their ability to bind two clinically relevant lung cancer-associated VOCs: propanol-1 and acetonitrile. Host-guest interactions were modeled using density functional theory (DFT) to compute molecular descriptors (e.g., dipole moments, molecular area2) and Gibbs free energy (ΔG) of complex formation. Three hybrid DFT functionals – B3LYP, PBE0, and r²SCAN – were tested to assess their performance in predicting calixarene-VOC binding.

Conclusion. In this study, analyte-specific behavior of calixarene derivatives was analyzed in order to select optimum functional for modelling calixarene-VOC interaction. In future, the described functional-dependent variance will provide a roadmap for descriptor-driven screening of calixarene-VOC supramolecular systems.

References:

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