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Exploiting the Catenane Mechanical Bond Effect for Selective Halide Anion Transmembrane Transport

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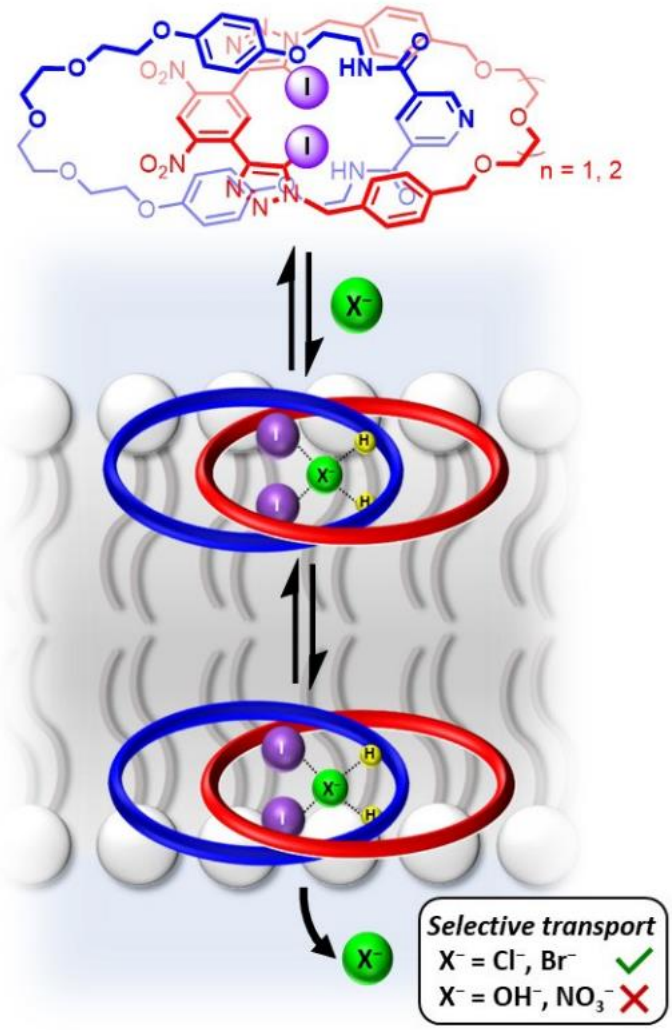

Who are the corresponding authors and what are their research areas?

Matthew J. Langton:

He and his group mainly focus on molecular devices working in the lipid bilayer membranes that enable ion transport across membrane systems responsive to external stimulus.

Paul D. Beer：

Studying the biological way of molecular recognition and applying them in artificial systems with macrocylic or interlocked structures, the main field of him is the host-guest supramolecular chemistry system.

What is the main claim of the article?

The authors reported the first example of a [2]catenane carrier selective for Cl^- across the membrane, due to the mechanical bond effect.

How is it demonstrated?

First, 1D/2D NMR are used to understand the interlocked structure especially the cavity of the synthesized carrier.

Also, NMR titration studies is used to understand the binding affinity and also selectivity.

Then for the anion transport study, the HPTS assay was carried out with and without FCCP to demonstrate that the [2]catenane has a stronger activity than the macrocycle analogue and showed preference for Cl^- anion over NO_3^-.

A mobile carrier mechanism was demonstrated by DPPC assay with lost activity at 25 °C and restored activity at 40 °C. And according to the liner dependence of the transport rate on the concentration of the carrier, the mechanism was suggested to be unimolecular.

What are the typical experimental conditions?

For binding affinity, the NMR solution is 95:5 acetone-d_6/D_2O or 90:10 system. Binding constants were calculated using Bindfit with a 1:1 host–guest binding model.

For the HPTS assay, the concentration of POPC LUVs is 31 μM, containing 1 mM HPTS, 100 mM internal and external NaCl, buffered with 10 mM HEPES at pH 7.0. carriers were added in DMSO (10 mol% with respect to lipid). FCCP was also added in DMSO (0.8 mol%). The concentration of the NaOH pulse is 5 mM. For HPTS, λem =510 nm; λex1=405 nm, λex2=460 nm.

Which are the key related papers?

Anti-Hofmeister Anion Selectivity via a Mechanical Bond Effect in Neutral Halogen-Bonding [2]Rotaxanes. A. Docker, Y. C. Tse, H. M. Tay, A. J. Taylor, Z. Zhang, P. D. Beer, *Angew. Chem. Int. Ed*. **2022**, 61, e202214523.

A Photo-responsive Transmembrane Anion Transporter Relay. T. G. Johnson, A. Sadeghi-Kelishadi, M. J. Langton*. *J. Am. Chem. Soc.* **2022**, 144 (23), 10455–10461.

Multistate Redox-Switchable Ion Transport Using Chalcogen-Bonding Anionophores. A. Docker, T. G. Johnson, H. Kuhn, Z. Zhang, M. J. Langton*. *J. Am. Chem. Soc.* **2023**, 145 (4), 2661-2668.

Halogen bonding relay and mobile anion transporters with kinetically controlled chloride selectivity. T. G. Johnson, A. Docker, A. Sadeghi-Kelishadi, M. J. Langton*. *Chem. Sci.*, **2023**, 14, 5006-5013.