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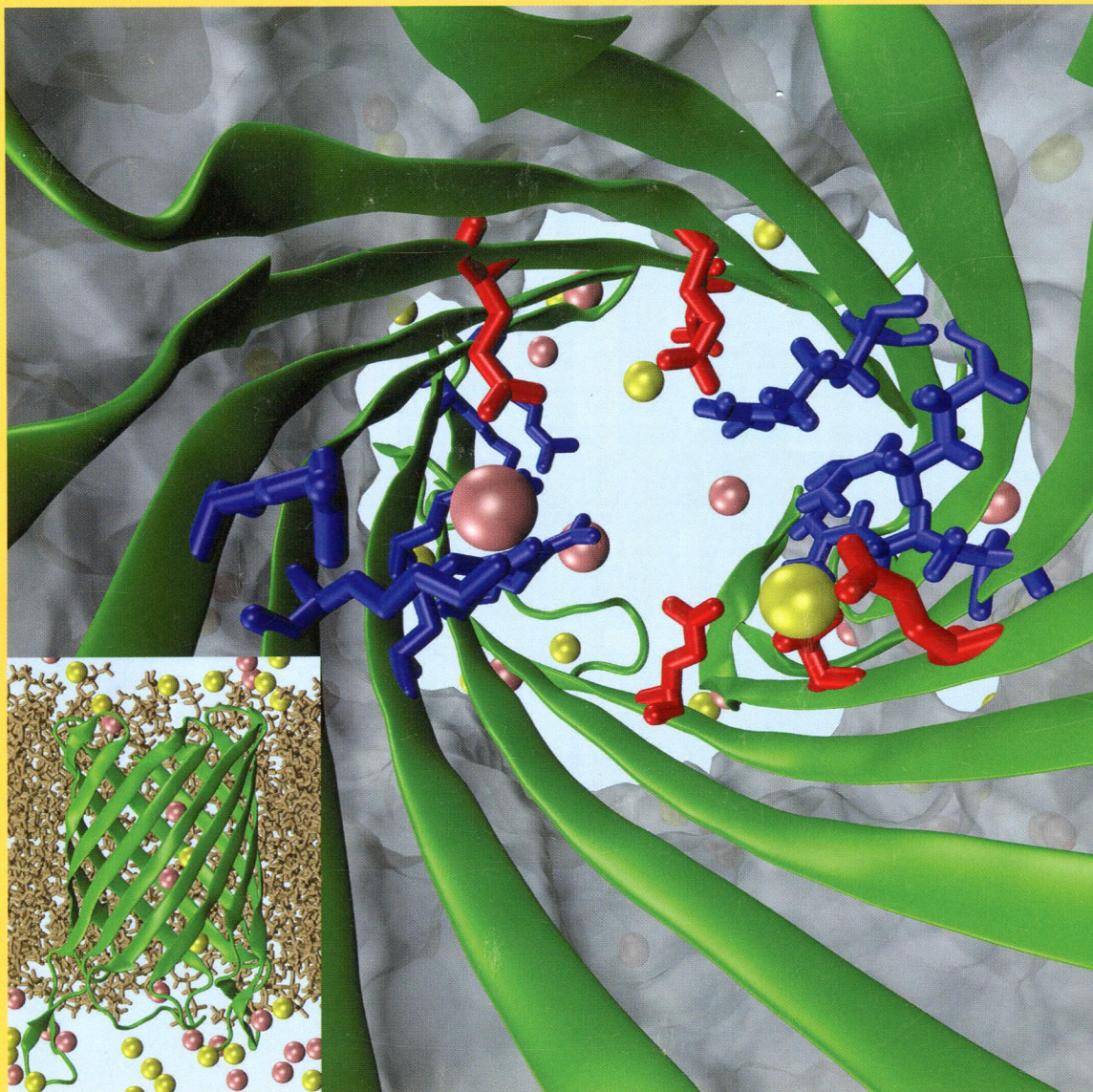
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B

Atomic Details of
Ion Transport through
NanC Revealed by
Molecular Dynamics
Simulations
(see page 5A)



BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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ON THE COVER: Atomic details of ion transport through NanC revealed by molecular dynamics simulations. Ion transport through the *N*-acetylneuraminic acid-inducible channel (NanC) is studied using molecular dynamics simulations. Applied-field simulations recover the asymmetric conductance property and the anion selectivity in agreement with experiments. The particular distribution of charged residues at the inner channel walls leads to a faster permeation of Cl ions compared with K ions, resulting in the anion selectivity of NanC. In addition, the channel can be engineered by mutations, leading to enhanced asymmetric conductances and anion selectivities. See page 15966.

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Interaction of Cationic Protoberberine Alkaloids with Human Serum Albumin. No Spectroscopic Evidence on Binding to Sudlow's Site 1
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Synthesize Multiblock Copolymers via Complex Formations between β -Cyclodextrin and Adamantane Groups Terminated at Diblock Copolymer Ends: A Brownian Dynamics Simulation Study

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Role of Absorbed Solvent in Polymer Pen Lithography

Daniel J. Eichelsdoerfer, Keith A. Brown, Mary X. Wang, and Chad A. Mirkin*

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