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Antiviral activity of squalamine: Role of electrostatic membrane binding BERNARD BECKERMAN, WEI QU, Northwestern University, ABHIJIT MISHRA, UCLA, MICHAEL ZASLOFF, Georgetown University, GERARD WONG, UCLA, ERIK LUIJTEN, Northwestern University — Recent work[1] has demonstrated that squalamine, a molecule found in the liver of sharks, exhibits broad-spectrum antiviral properties. It has been proposed that this activity results from the charge-density matching of squalamine and phospholipid membranes, causing squalamine to bind to membranes and displace proteins such as Rac1 that are crucial for the viral replication cycle. Here we investigate this hypothesis by numerical simulation of a coarse-grained model for the competition between Rac1 and squalamine in binding affinity to a flat lipid bilayer. We perform free-energy calculations to test the ability of squalamine to condense stacked bilayer systems and thereby displace bulkier Rac1 molecules. We directly compare our findings to small-angle x-ray scattering results for the same setup.

[1]M. Zasloff *et al.*, Proc. Nat. Acad. Sci. (USA) **108**, 15978 (2011).

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