Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Using Electronic Properties of Adamantane Derivatives to Analyze their Ion Channel Interactions: Implications for Alzheimer's Disease[1]

JASON BONACUM, Indiana State University — The derivatives of adamantane, which is a cage-like diamondoid structure, can be used as pharmaceuticals for the treatment of various diseases and disorders such as Alzheimer's disease. These drugs interact with ion channels, and they act by electronically and physically hindering the ion transport. The electronic properties of each compound influence the location and level of ion channel hindrance, and the specific use of each compound depends on the functional groups that are attached to the adamantane base chain. Computational analysis and molecular simulations of these different derivatives and the ion channels can provide useful insight into the effect that the functional groups have on the properties of the compounds. Using this information, conclusions can be made about the pharmaceutical mechanisms, as well as how to improve them or create new beneficial compounds. Focusing on the electronic properties, such as the dipole moments of the derivatives and amino acids in the ion channels, can provide more efficient predictions of how these drugs work and how they can be enhanced.

[1]Department of Energy Grant DE-FG02-06ER46304

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Date submitted: 31 Oct 2012 Electronic form version 1.4