Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Orbital Energetics and Molecular Recognition AARON GEORGE, Targacept, Inc., REBECCA HARRIS, VISHALI MOGALLAPU, YONAS ABRAHAM, ROBERTO CAR, Princeton University, JEFFREY SCHMITT — We present data demonstrating that orbital eigenenergy fluctuation recorded in the course of ab initio molecular dynamics calculations contains information relevant in determining molecular behavior and recognition. A simple scheme is presented that maps these data to molecular descriptors. Using computational drug design as the context, these descriptors are compared with previous electronic eigenvalue descriptor methods with encouraging results. Finally we discuss further methods of mapping electronic structure based molecular dynamics trajectories to Quantitative Structure Activity Relationships (QSAR).

Aaron George
Targacept, Inc.

Date submitted: 03 Dec 2005 Electronic form version 1.4