

DYNEVA: Electronic Eigenvalue descriptors derived from quantum molecular dynamics

Aaron George, Rebecca Harris, Vishali Mogallapu,
Yonas Abraham, Lee Atkinson, Jeffrey D. Schmitt

*Targacept, Inc. 200 East First Street Suite 300
Winston-Salem NC 27101*

Roberto Car

*Chemistry Department, Princeton University
Princeton, NJ 08544*

We present a method of generating quality chemical descriptors derived from quantities fundamental to *ab-initio* quantum molecular dynamics (QMD). A generalizable method of generating descriptors is presented, with a specific example utilizing electronic eigenvalues. Preliminary results indicate that dynamical eigenvalue descriptors contain more information than their static counterparts based on quantitative structure-activity models of nicotinic acetylcholine receptor binding and net oral bioavailability (the well known Topliss dataset).