

Q5: Are we confident that quantum spin microscopy will work?

A5: Newly feasible is end-to-end HWIL of (e.g.) the anti-HIV drug Nevirapine

Assessing the Capabilities of Quantum Microscopy for Drug Development: Nevirapine as a Case Study and Design Target

Christian K. Kikuchi^{*1}, Jonathan P. Jacky², Joseph L. Garbini², Joseph R. Malcomb², Anthony G. Norman³, John A. Sidles⁴

December 18, 2005

The recent demonstration of single-spin resolution in magnetic resonance force microscopy has stimulated quantum system engineering groups around the world to begin designing next-generation quantum microscopes whose design goal is to image macromolecular ensembles with single-atom resolution. Central to this design effort is detailed modeling and simulation of quantum microscope performance. In order to define a specific target for the design of next-generation quantum microscopes, and also in order to begin defining more clearly how quantum microscopes might be used in practice, this article considers the suitability of the HIV reverse transcriptase inhibitor Nevirapine as a design target. The literature from 1990–1994 is reviewed, spanning the period from the discovery of Nevirapine's anti-HIV activity to the elucidation of the structural basis for this activity. An analysis of this literature indicates that quantum microscopy could significantly shorten the duration and improve the reliability of Nevirapine-type drug development. From a physics point of view, Nevirapine's carbon-carbon nuclear dipole interactions are shown to be well-matched to testing and developing next-generation quantum simulation algorithms, being neither unrealistically simple nor intractably complex. It is noted that if the present rapid pace of advance in *ab initio* quantum chemical calculations continues, such that these calculations can be interfaced to the pipeline of structural information emerging from quantum microscopes, a new resource frontier will be opened biological science and medicine.

DoD Modeling and Simulation (M&S)
Glossary



January 1998

Under Secretary of Defense for
Acquisition Technology

