

## Quantum Drug Discovery

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### **HEALTH-2009-4.3.1-1: Discovery and development of new vaccines or drugs for helminth infections**

We perform quantum drug discovery. Our technology is based on a unique, proprietary method to determine essential, rigorous, easily computable molecular attributes that describe chemical activity. It has been successfully applied to diverse biochemical phenomena, against targets ranging from a single macromolecule to a whole organism, with success rates that exceed the industry standards by orders of magnitude. *In vitro* or *in vivo* testing of the compounds identified by our *in silico* predictive molecular modeling readily confirms its accuracy.

Quantum mechanics is fundamental to a full understanding of molecular interactions. However standard quantum chemical calculations demand exorbitant computational capabilities to be truly useful for new drug discovery within acceptable timeframes.

We have therefore developed a set of fast algorithms that apply quantum theory to identify and then optimize new compounds on a large scale.

We have a well-documented capability in discovering new therapeutic leads against serious infectious diseases. We are willing to join a consortium planning a submission of a project related to **HEALTH-2009-4.3.1-1: Discovery and development of new vaccines or drugs for helminth infections.**

Snet is a Micro Enterprise (3 people) specializing in computer modeling for Diagnostics and Drug Discovery.

**HEALTH-2009-4.2-1: Adapting off-patent medicines to the specific needs of paediatric populations.**

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Our *in silico* modeling capabilities allow us to optimize patient-specific pharmacokinetics, formulations and other properties based on multiple pharmaceutical factors. We are willing to join a consortium planning a submission of a project related to **HEALTH-2009-4.2-1: Adapting off-patent medicines to the specific needs of paediatric populations.**

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**HEALTH-2009-2.4.4-2: Preclinical development of substances with a clear potential as orphan drugs.**

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We have therefore developed a set of fast algorithms that apply quantum theory to identify and then optimize new compounds on a large scale.

Low cost, high speed and high success rate make our drug discovery and optimization platform well suited for orphan drugs and diseases because we can also optimize *in silico* the ADMIN-TOX properties. We are willing to join a consortium planning a submission of a project related to **HEALTH-2009-2.4.4-2: Preclinical development of substances with a clear potential as orphan drugs.**

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**HEALTH-2009-2.2.1-4: Understanding the blood brain barrier (BBB) to improve drug delivery to the brain.**

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Quantum mechanics is fundamental to a full understanding of molecular interactions. However standard quantum chemical calculations demand exorbitant computational capabilities to be truly useful for new drug discovery within acceptable timeframes.

We have therefore developed a set of fast algorithms that apply quantum theory to identify and then optimize new compounds on a large scale.

We have also developed statistically validated, predictive *in silico* models for BBB permeability. (We believe we can predict chemically dissimilar compounds with mechanistic hypothesis for interaction). We are willing to join a consortium planning a submission of a project related to **HEALTH-2009-2.2.1-4: Understanding the blood brain barrier (BBB) to improve drug delivery to the brain.**

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**HEALTH-2009-2.4.5-2: Cellular and molecular mechanisms of the development of chronic kidney disease (CKD)**

We have developed a cost-effective, non-invasive, software-based diagnostic methodology to identify bio-molecular relationships that define specific disease states. We use a data-driven process that generates predictive profiles from the totality of information contained within the input data. Unlike other methodologies forced to rely on only a limited number of data points, our proprietary software and algorithms analyze the entire data sequence to identify all pertinent bio-predictors and include their concomitant linkages and relationships. This generates unique, accurate and internally consistent diagnostic profiles which are then cross-validated with accepted statistical re-sampling procedures. Our technology has been successfully applied to a wide array of diseases as well as to a variety of biological samples and data, including gene expression, proteomics, and metabolomics. Where datasets are sufficiently large and diverse, the resulting diagnostic profiles exhibit near-perfect specificity and sensitivity for both symptomatic and asymptomatic patients. Moreover, the exceptional discrimination of our diagnostic profiles establishes them as a powerful tool for monitoring the progress and effectiveness of treatment protocols.

We have extensive expertise in modeling kidney-specific bio-molecular processes. Combined with our ability to discover and characterize accurate composite biomarkers from simple blood and urine data, we offer novel insights into renal failure and we are willing to join a consortium with a project targeted at **HEALTH-2009-2.4.5-2: Cellular and molecular mechanisms of the development of chronic kidney disease (CKD)** planned for submission.

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**HEALTH-2009-2.3.1-3: Clinical evaluation of point-of-care diagnostic tests for microbial detection and identification, antibiotic susceptibility determination and biomarkers**

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We think our technology fully fits some of the goals of **HEALTH-2009-2.3.1-3: Clinical evaluation of point-of-care diagnostic tests for microbial detection and identification, antibiotic susceptibility determination and biomarkers** and we are willing to join a consortium with a project planned for submission.

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