



## Concept of a Robot Computational Chemist

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The objective of the proposed project is to develop and implement an artificial intelligence approach to planning, conducting, and understanding of computational studies in quantum chemistry. Key to this approach will be the integration of general background knowledge with specific problem-solving experience from computational chemistry. The proposed evolutionary decision support (EDS) system will provide non-expert users with guidance in selecting physically correct models that are amenable to computation and help them to avoid results of unspecified reliability. Capitalising on recent advances in artificial intelligence, the EDS architecture will be built based on a flexible methodology for knowledge-intensive case-based reasoning. To facilitate extensibility and address maintenance issues, the system will be designed around multiple knowledge repositories. Effective and efficient decision support will be achieved through the use and integration of various concepts from machine learning, soft computing, and information fusion. The system to be developed has a high potential to become the first safe and reliable tool for computational studies in chemistry for non-expert users in academia and in particular in chemical and pharmaceutical industry.