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Drug target interaction by KEM of Quantum Crystallography

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It is possible to use the full power of ab initio quantum mechanics in application to the interaction of drugs and their molecular targets. Two things advance this perspective: (i) the use of parallel supercomputers, and (ii) the discovery of a quantum formalism called quantum crystallography and the use of quantum kernels, a method that is well suited for parallel computation. The calculations are simplified by adopting an acceptable approximation that allows a full biological molecule to be represented by smaller "kernels"of atoms. The KEM is suggestive that problems in the rational design of drugs, may be illuminated by quantum mechanical analysis. The general case is illustrated by specific examples.

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