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Computer-Aided Drug Discovery

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¹Solutions

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dx.doi.org/10.17504/protocols.io.dm6gpb918lp/v1

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Computer-aided drug design (CADD) is a widely used technology using computational tools and resources for the storage, management, analysis and modeling of compounds. It relies on digital repositories for the study of designing compounds with physicochemical characteristics, predicting whether a given molecule will be combined with the target, and if so how strongly. [Computer-based methods](#) can help us to search new hits in drug discovery, screening many irrelevant compounds at the same time and study the structure-activity relationship of drug molecules.

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<https://www.solutions.bocsci.com/computational-chemistry.htm>

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