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When designing small molecules to interact with these targets, one should consider stereoselectivity. As considerations for exploring structure space evolve, chirality is increasingly important. Binding affinity for a chiral drug can differ for diastereomers and

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From exploration of structure space to governmental regulations it is clear that the question of chirality in drug design is of vital importance. Keywords: Chiral, virtual screening, drug design, drug discovery, FDA guidelines, enantiomer,

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Chirality and drug development The importance of chiral drugs in the drug development space cannot be

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understated. In pharmaceutical industries, 56% of the drugs currently in use are chiral molecules and 88% of the last ones are marketed as racemates (or racemic mixtures), consisting of an equimolar mixture of two enantiomers.

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Most pharmaceutically active compounds possess a chirality that greatly influences their pharmacological properties. Since all pharmaceutical products nowadays are produced in chirally pure form, this places huge demands on the technology used for drug synthesis, purification, analysis and testing.

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enantiomer of a chiral drug often differs significantly in its pharmacological, toxicological, pharmacodynamic, and pharmacokinetic [4,5] properties.

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Chirality in drug design and development by Indra K. Reddy, 2004, Marcel Dekker edition, in English

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For the virtual screening and computational design stage of drug development, this problem can be compounded by incomplete stereochemical information in structure libraries leading to a "coin toss" as to whether or not the "ideal" chiral structure is present.

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