Selective virtual screening for partial and full agonists in the beta2 adrenergic receptor crystal structure

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The recently solved high-resolution X-ray structure of the beta2 adrenergic receptor has been challenged for its ability to discriminate inverse agonists/antagonists from partial/full agonists. Whereas the X-ray structure of the ground state receptor was unsuitable to distinguish true ligands with different functional effects, modifying this structure to reflect early conformational events in receptor activation led to a model able to selectively retrieve full and partial agonists by structure-based virtual screening.