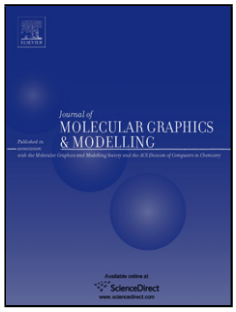

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Proposal of potent inhibitors for vitamin-D receptor based on *ab initio* fragment molecular orbital calculations

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Graphical abstract

Figure 7 in our paper

Interacting structures between VDR residues (Tyr143, Asp144, Arg274 and His305) and the novel derivative D5b proposed in the present study; green and blue dashed lines indicate hydrogen-bonding and CH-π interactions, respectively.