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SUPPLEMENTARY MATERIAL TO

Ligand- and structure-based virtual screening of 16-((diiso-butylamino)methyl)-6*α*-hydroxyvouacapane-7*β*,17*β*-lactone, a compound with potential anti-prostate cancer activity

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TABLE S-I. Virtual bases used in the research and the number of structures in each

Data base	Number of structures
Chembridge, Diverset™ EXPRESS - Pick™	49 998
Chembridge, DIVERSet CORE Library	49 908
ZINC drug database	3 404
ZINC naturals stock	111 572
Drug@FDA BindingDB	24 040
TOTAL	238 922

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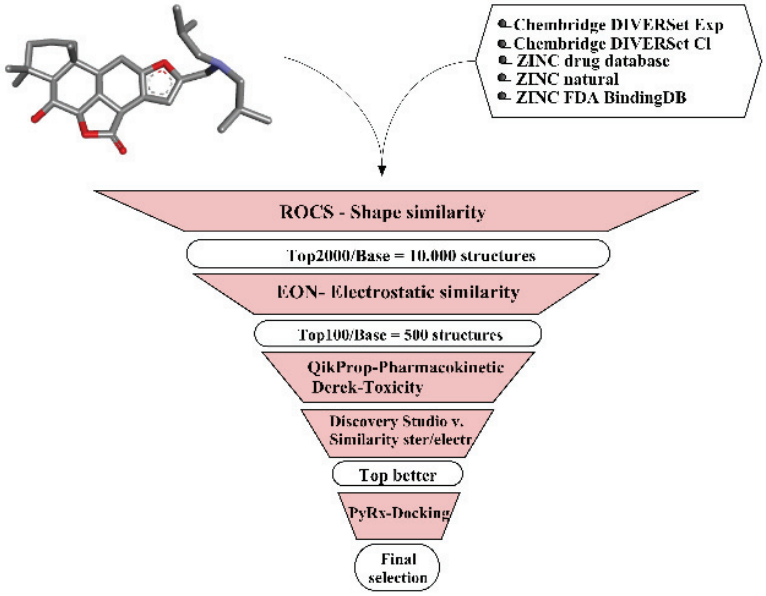

Fig. S-1. Virtual screening ligand-based (eon and rocs), pharmacokinetic and toxicity predictions, overlap similarity 50 %ster/electr and molecular docking.