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# ACCEPTED MANUSCRIPT



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using Instant JChem software [Instant JChem v. 17.17.0, https://chemaxon.com/] and 689 active compounds were retained. Subsequently, drug-like filtering criteria, *e.g.*, HBA (hydrogen bond acceptors) = 3–4, HBD (hydrogen bond donors) = 0–3, MW (molecular weight) = 371–496, RBN (number of rotatable bonds) = 3–6, XLogP = −0.4–3.7, 2dPSA (2d polar surface area) = 60–90 were applied, resulting 179 compounds which have been designated as actives in the evaluation procedure[9-11]. In order to select the decoys, a free on-line automated tool from Directory of Useful Decoys, enhanced (DUD-E), (http://decoys.docking.org), was used[12]. The decoys set was compiled based on the similarities with the compounds used for pharmacophore generation (Table I), employed as queries. Thus, 50 decoys were selected for each query, with the exception of compounds **2** and **22**, (for which 100 decoys were identified for each of them). The extracted decoys have similar physicochemical properties (MW, HBA, HBD, logP and RBN) with queries but dissimilar 2-D topology. Therefore, 179 compounds designated as actives and 1350 decoys entitled as inactive were used for virtual screening (VS) experiments in order to find matches over the obtained pharmacophore hypotheses. The fitness scores were used for the ranking of the compounds over the best pharmacophore hypothesis.

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