

Supplementary material

***N*-(3-{4-[3-(trifluoromethyl)phenyl]piperazin-1-yl}propyl)-1*H*-indazole-3-carboxamide
(D2AAK3) as a potential antipsychotic: *in vitro*, *in silico* and *in vivo* evaluation of a
multi-target ligand**

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Figures S1-S4

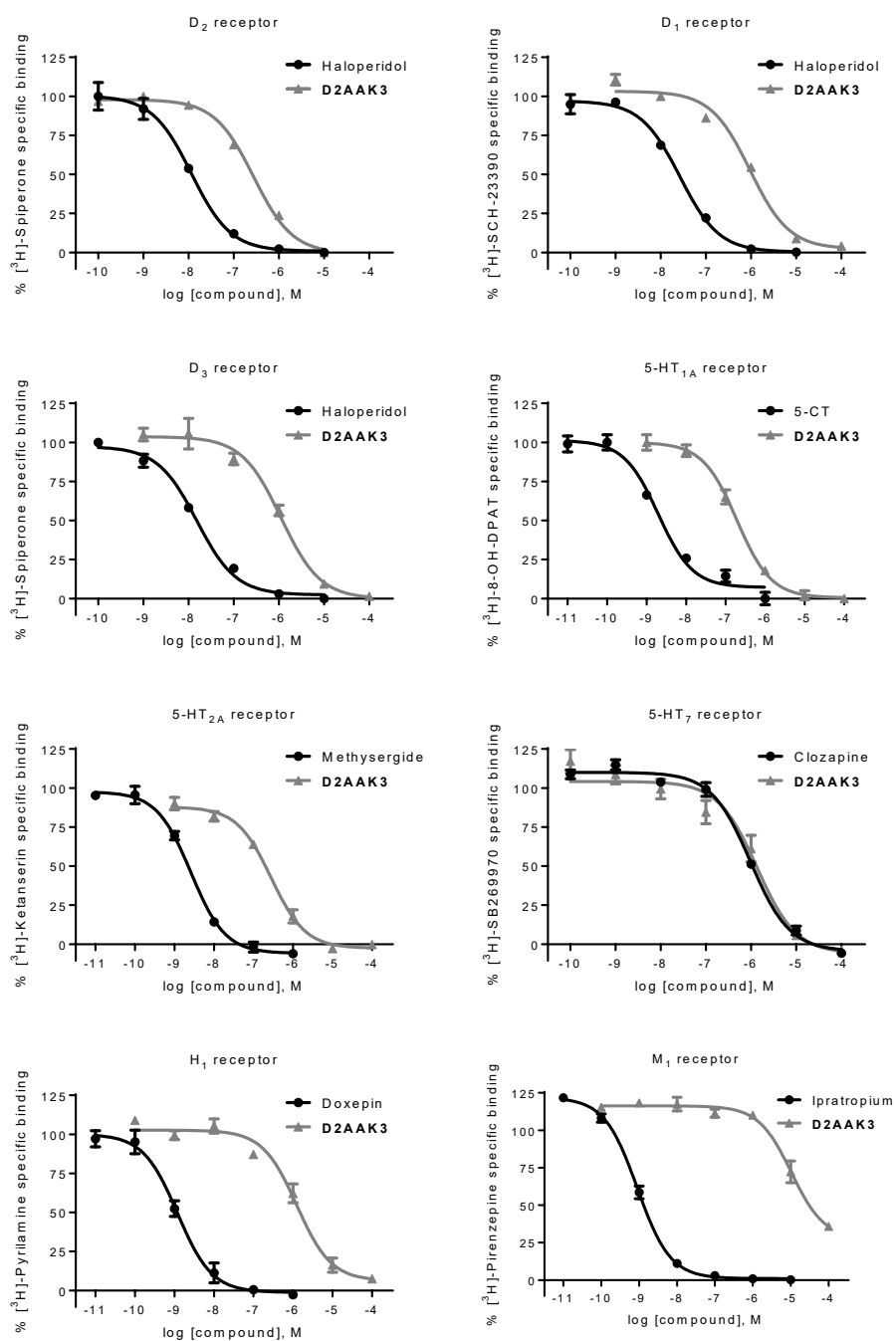


Fig. S1. Competition binding curves of D2AAK3 in radioligand binding assays at the indicated receptors. Concentration-dependent displacement of the specific radioligand binding by compounds D2AAK3 and corresponding reference compound at the human cloned receptors indicated. The graphs show the data (media \pm SEM) of a representative experiment out of 2-3 independent experiments performed in duplicate.

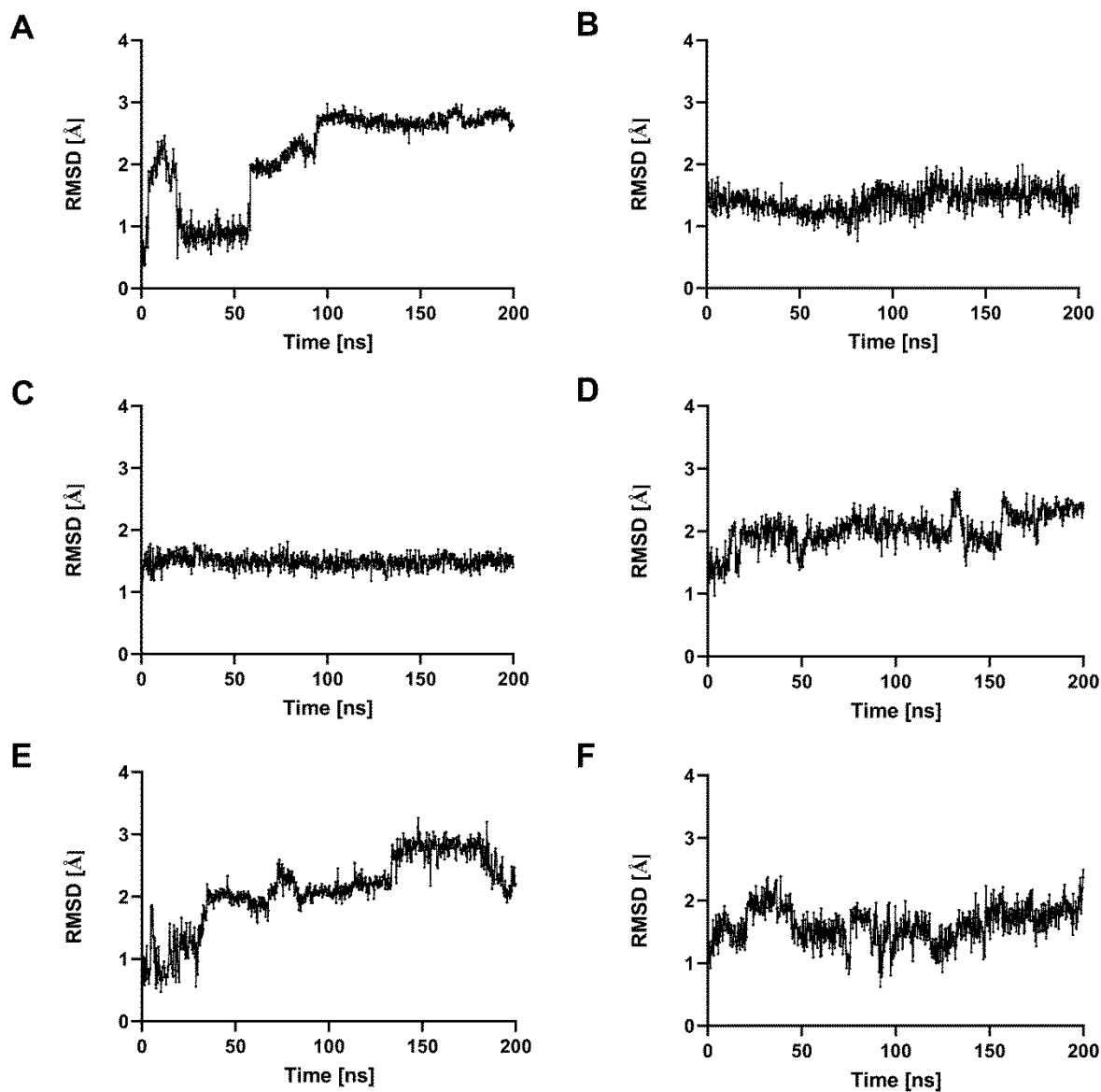


Fig. S2. Ligand RMSD values during 200 ns molecular dynamics simulations for D2AAK3 in complex with dopamine D₁ (A), D₂ (B), D₃ (C) and serotonin 5-HT_{1A} (D), 5-HT_{2A} (E) and 5-HT₇ (F) receptors.

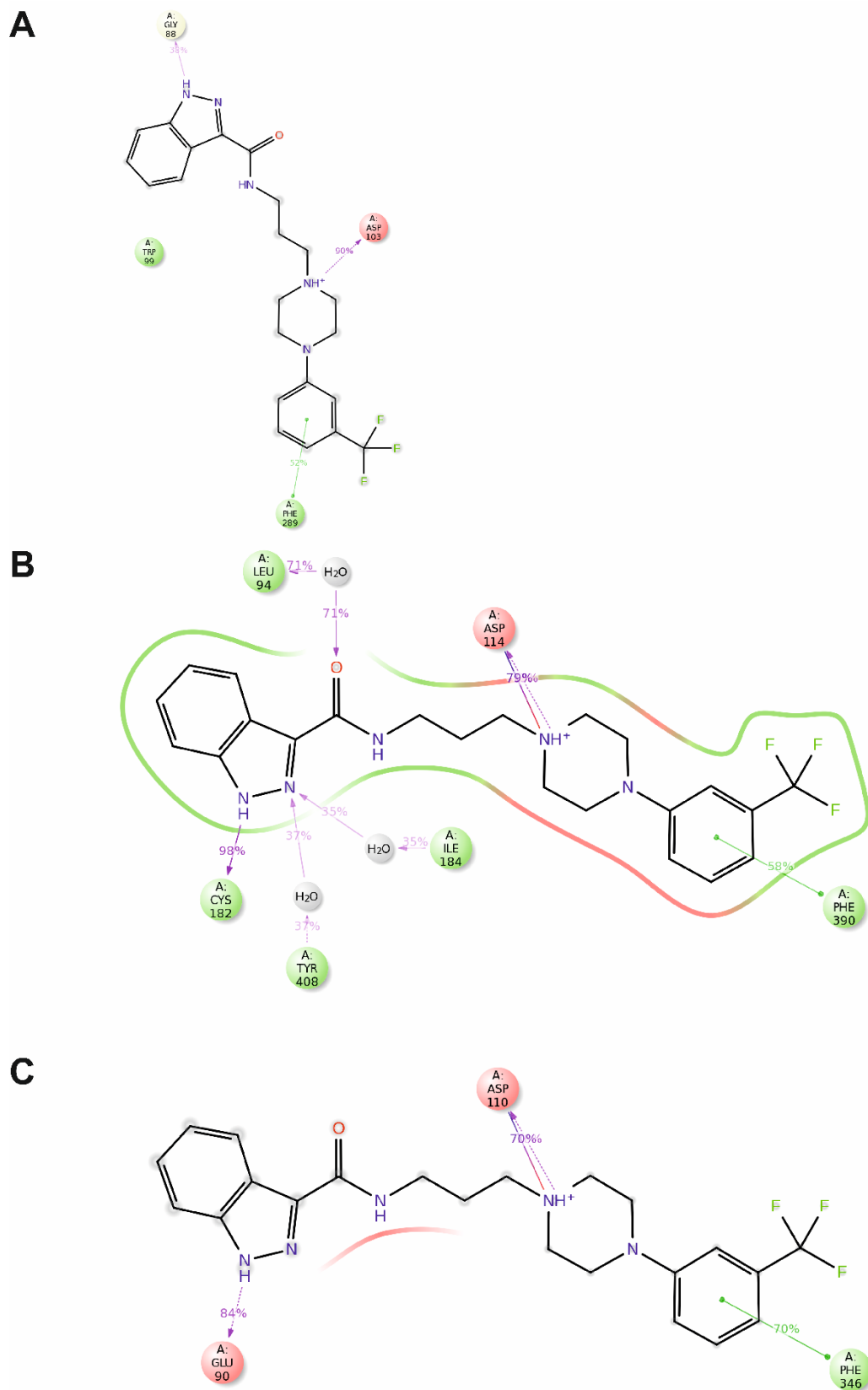


Fig. S3. Molecular interactions of D2AAK3 with human dopamine D₁ (A), D₂ (B) and D₃ (C) receptor during 200 ns molecular dynamics simulations: summary of contacts. Interactions that occur more than 30% of the simulation time in the selected trajectory (0 through 200 ns) are shown.

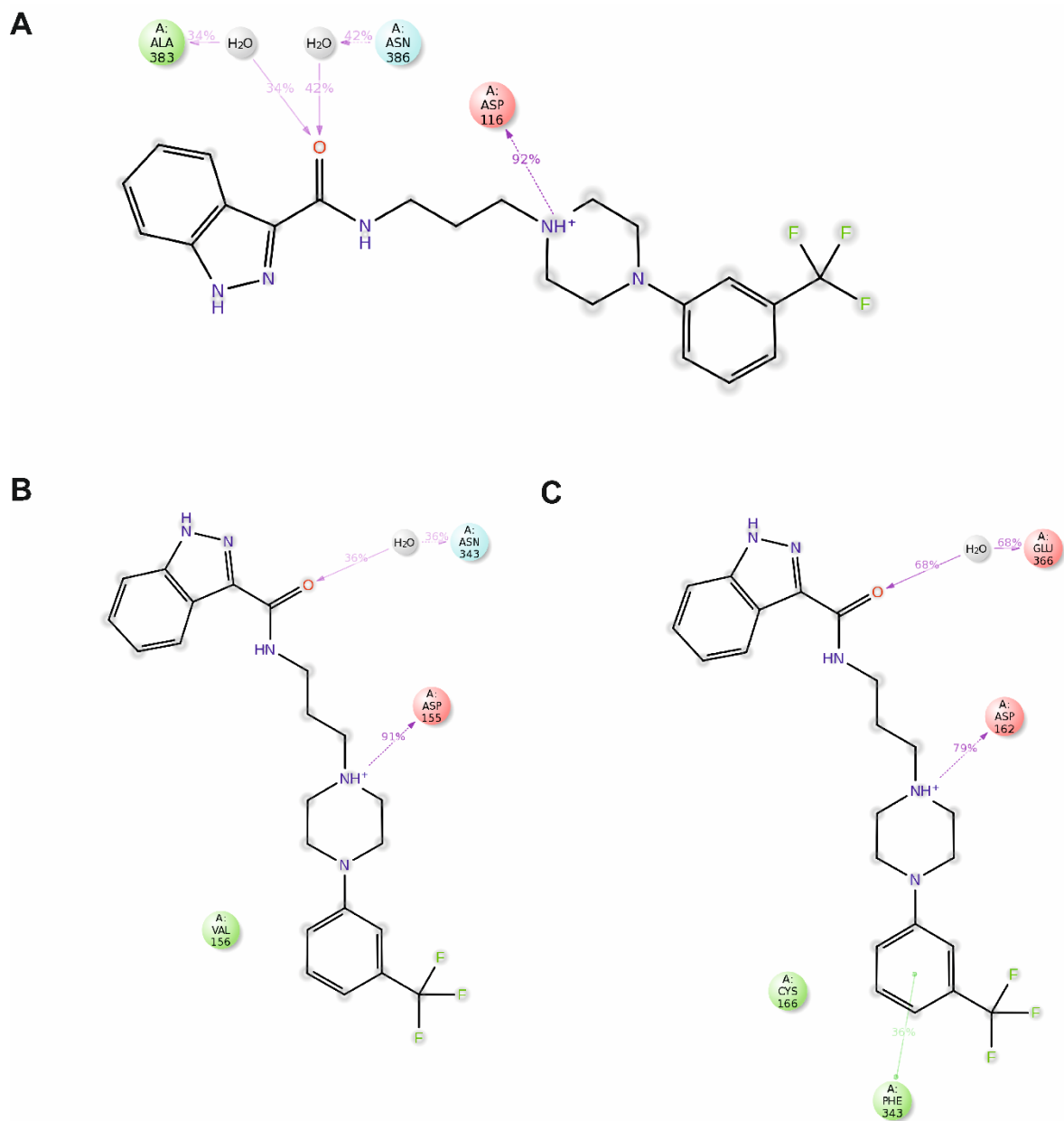


Fig. S4. Molecular interactions of D2AAK3 with human serotonin 5-HT_{1A} (A), 5-HT_{2A} (B) and 5-HT₇ (C) receptor during 200 ns molecular dynamics simulations: summary of contacts. Interactions that occur more than 30% of the simulation time in the selected trajectory (0 through 200 ns) are shown.