

In Vitro Biological Evaluation of Aprepitant Based ^{177}Lu -Radioconjugates

Paweł K. Halik ^{1,*}, Przemysław Koźmiński ¹, Joanna Matalińska ², Piotr F. J. Lipiński ², Aleksandra Misicka ^{2,3} and Ewa Gniazdowska ¹

¹ Centre of Radiochemistry and Nuclear Chemistry, Institute of Nuclear Chemistry and Technology,
03-195 Warsaw, Poland; p.kozminski@ichtj.waw.pl (P.K.);
e.gniazdowska@ichtj.waw.pl (E.G.)

² Department of Neuropeptides, Mossakowski Medical Research Institute, Polish Academy of Sciences,
02-106 Warsaw, Poland; jmatalinska@imdik.pan.pl (J.M.); plipinski@imdik.pan.pl (P.F.J.L.);
misicka@chem.uw.edu.pl (A.M.)

³ Faculty of Chemistry, University of Warsaw, 02-093 Warsaw, Poland

* Correspondence: p.halik@ichtj.waw.pl; Tel.: +48-22-504-13-16

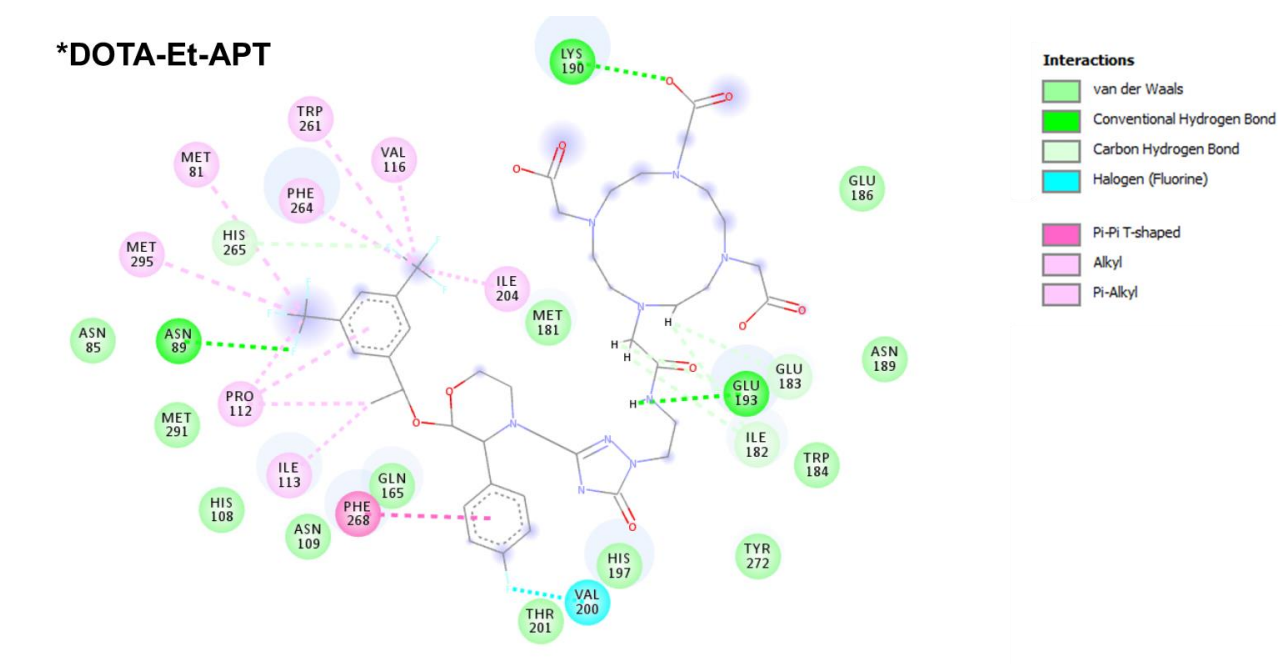


Figure S1. Scheme of the interactions of *DOTA-Et-APT with the NK1R. Interaction types are shown in the legend (top right corner).

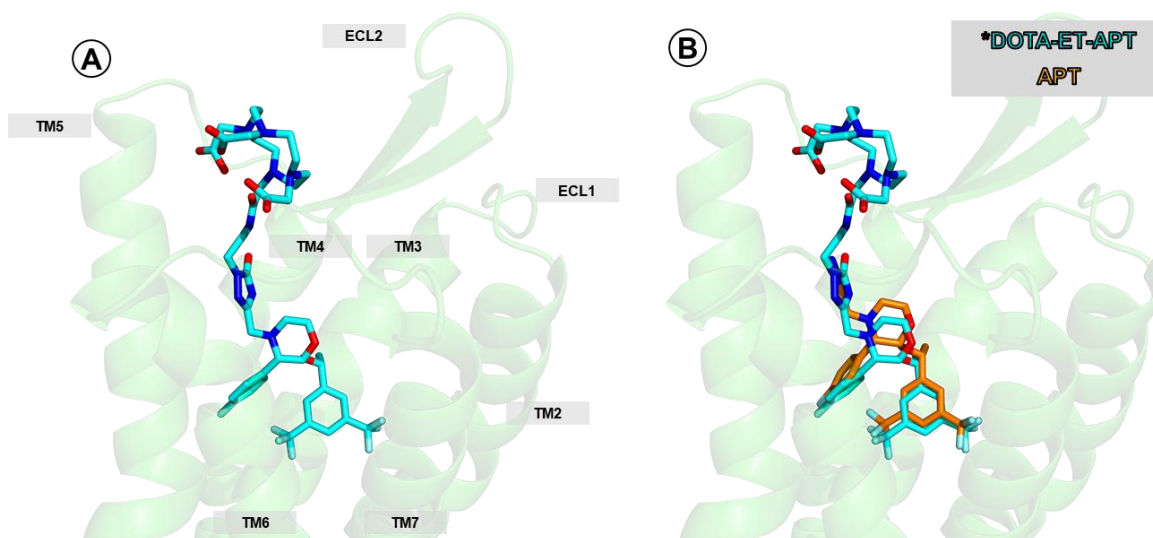


Figure S2. Binding mode of *DOTA-Et-APT in the NK1R (general view). **A)** the ligand alone or **B)** superposed on the crystallographic position of aprepitant (APT). *DOTA-Et-APT shown as cyan sticks. APT shown as orange sticks. Hydrogen display is suppressed. The receptor is shown in a simplified manner as green helices. TM1 not shown.

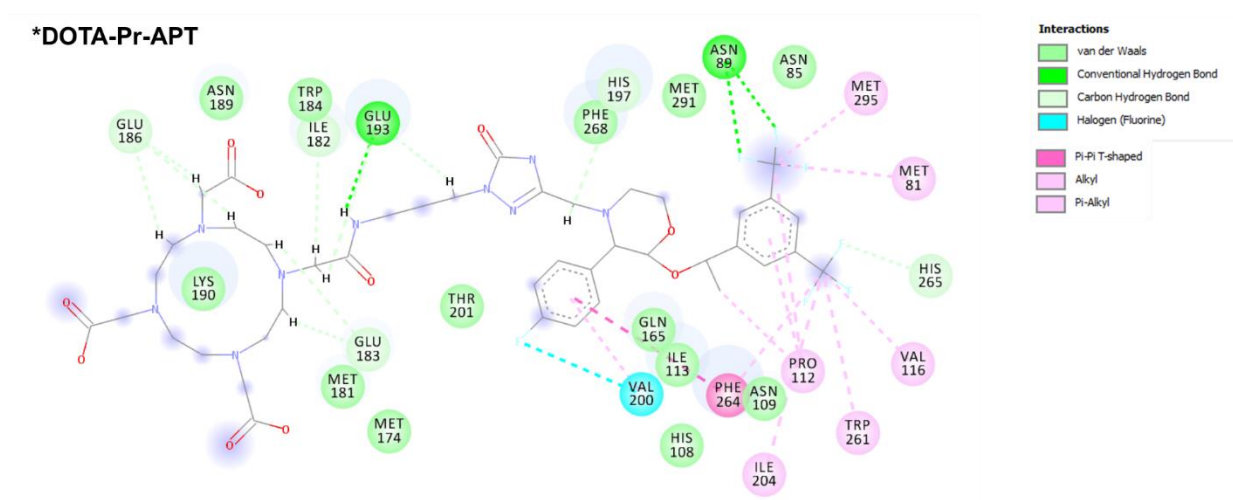


Figure S3. Scheme of the interactions of *DOTA-Pr-APT with the NK1R. Interaction types are shown in the legend (top right corner).

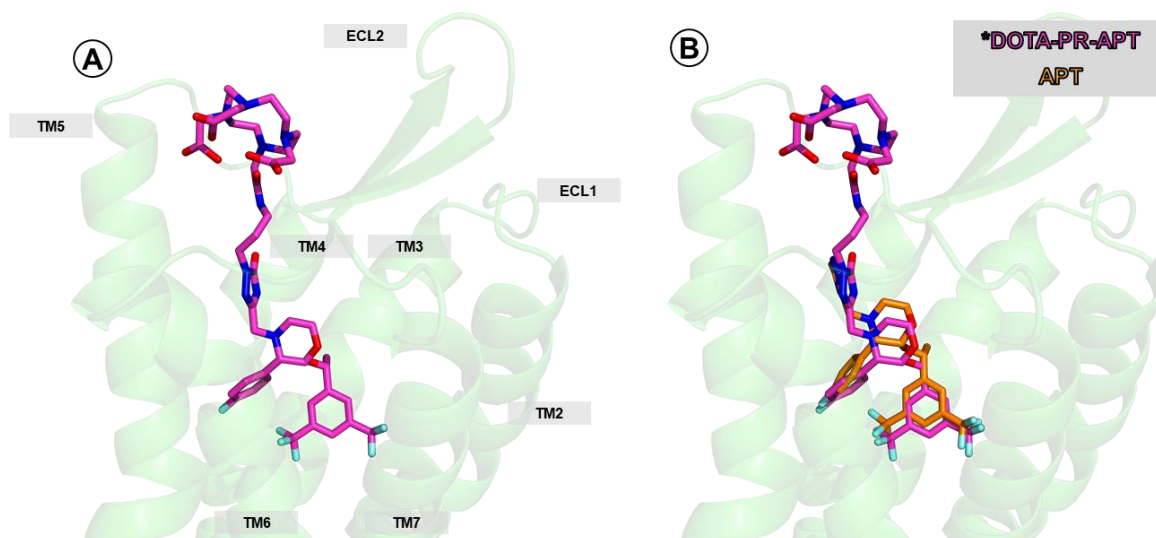


Figure S4. Binding mode of *DOTA-Pr-APT in the NK1R (general view). **A)** the ligand alone or **B)** superposed on the crystallographic position of aprepitant (APT). *DOTA-Pr-APT shown as magenta sticks. APT shown as orange sticks. Hydrogen display is suppressed. The receptor is shown in a simplified manner as green helices. TM1 not shown.

*DOTA-Bu-APT

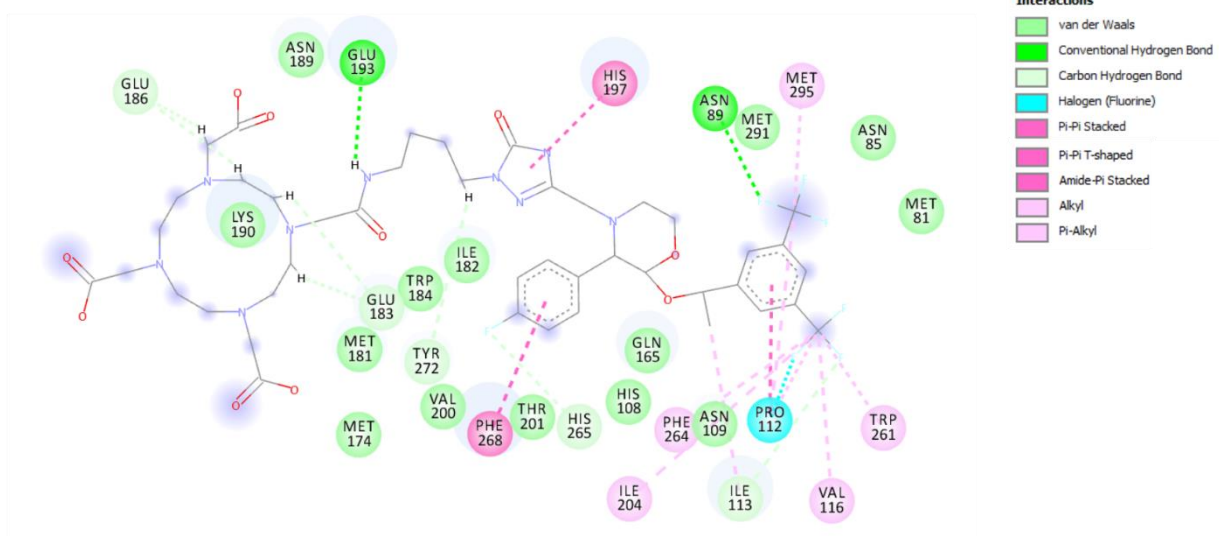


Figure S5. Scheme of the interactions of *DOTA-Bu-APT with the NK1R. Interaction types are shown in the legend (top right corner).

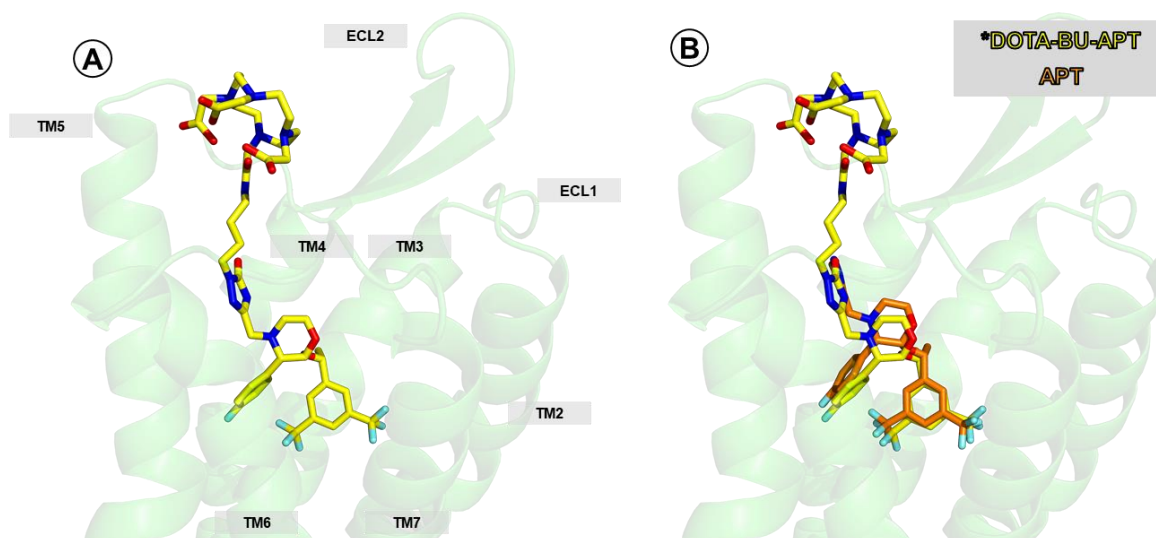


Figure S6. Binding mode of *DOTA-Bu-APT in the NK1R (general view). **A)** the ligand alone or **B)** superposed on the crystallographic position of aprepitant (APT). *DOTA-Bu-APT shown as yellow sticks. APT shown as orange sticks. Hydrogen display is suppressed. The receptor is shown in a simplified manner as green helices. TM1 not shown.

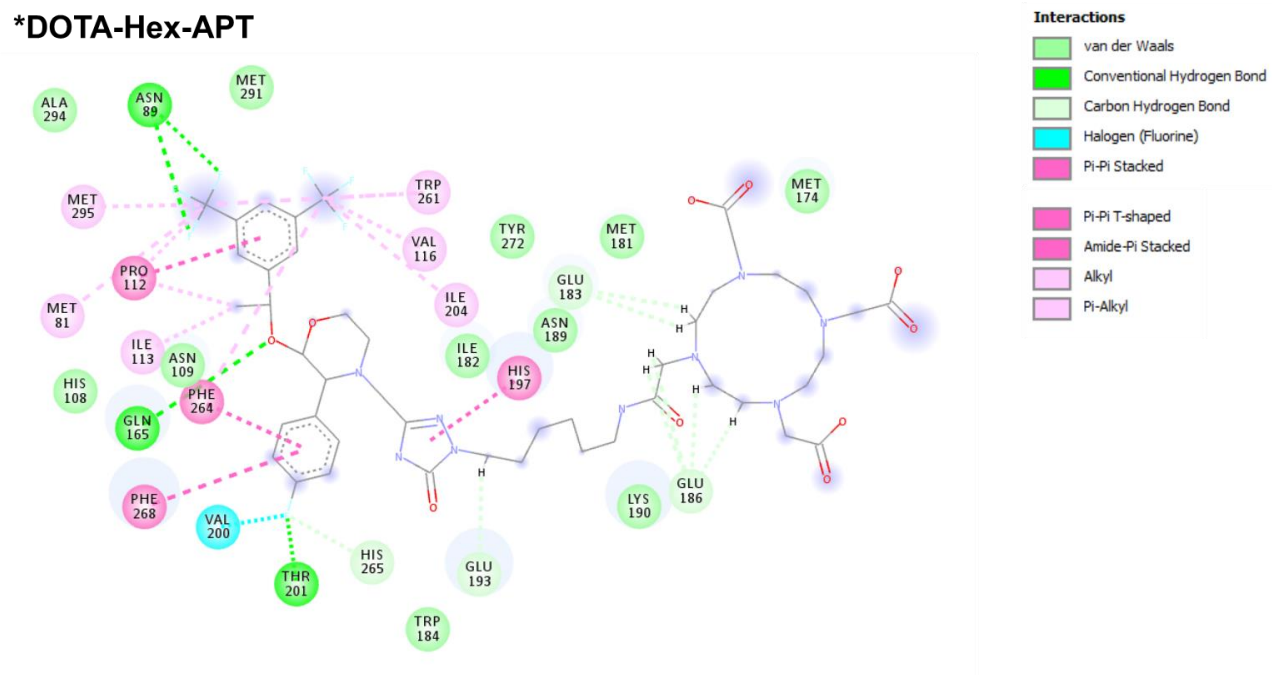


Figure S7. Scheme of the interactions of *DOTA-Hex-APT with the NK1R. Interaction types are shown in the legend (top right corner).

***DOTA-Oct-APT**

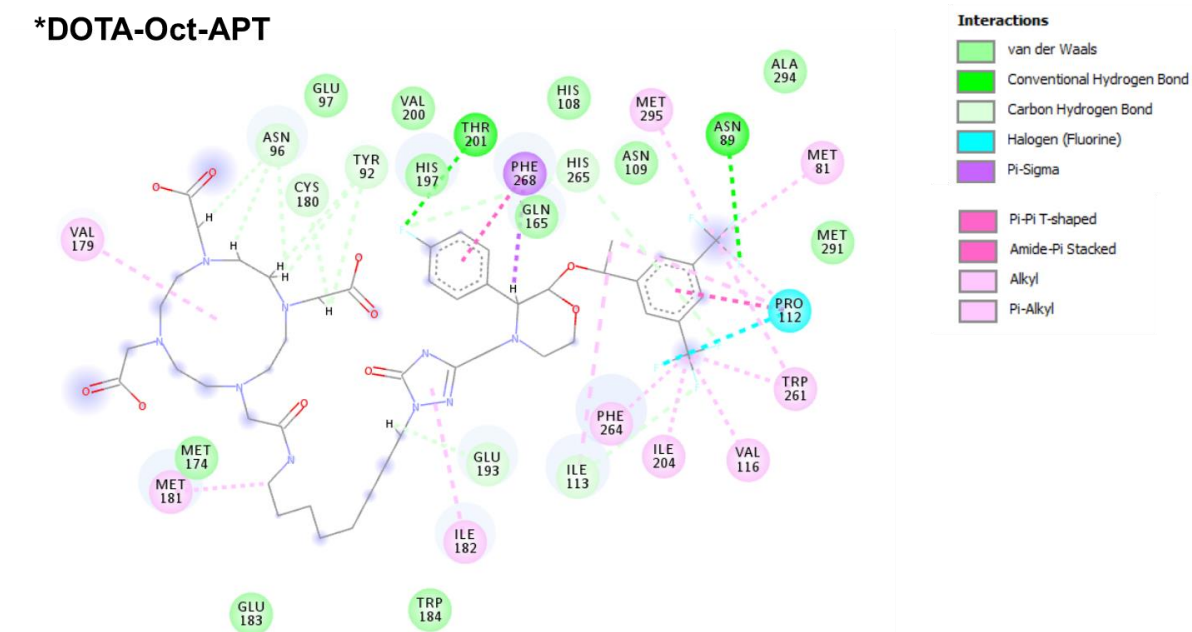


Figure S8. Scheme of the interactions of ***DOTA-Oct-APT** with the NK1R. Interaction types are shown in the legend (top right corner).

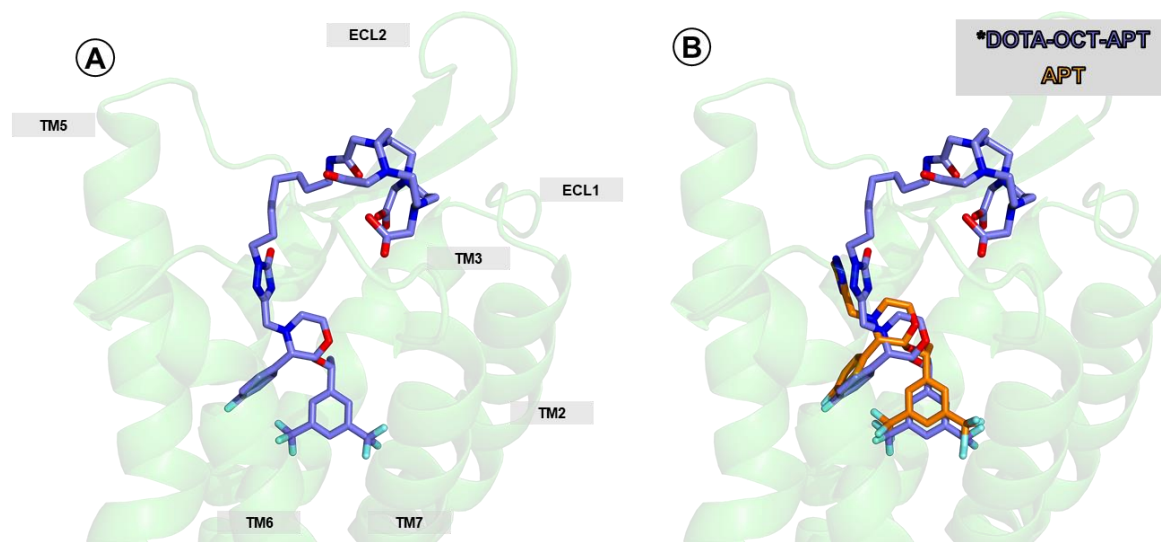


Figure S9. Binding mode of ***DOTA-Oct-APT** in the NK1R (general view). **A)** the ligand alone or **B)** superposed on the crystallographic position of aprepitant (APT). ***DOTA-Oct-APT** shown as slate blue sticks. APT shown as orange sticks. Hydrogen display is suppressed. The receptor is shown in a simplified manner as green helices. TM1 not shown.

*DOTA-Dec-APT

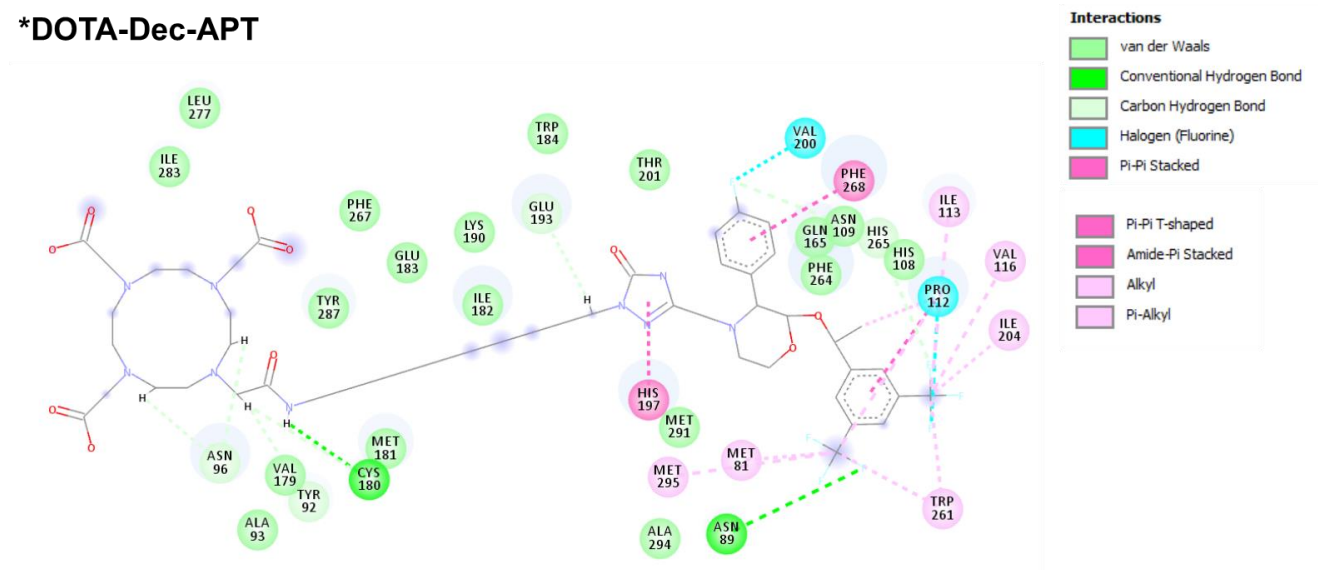


Figure S10. Scheme of the interactions of *DOTA-Dec-APT with the NK1R. Interaction types are shown in the legend (top right corner).

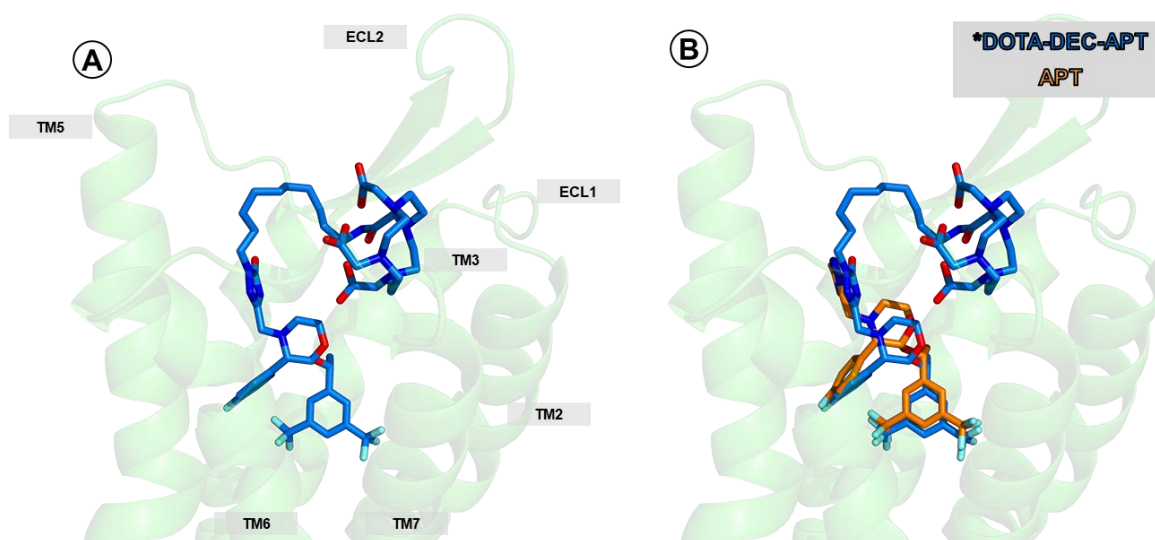


Figure S11. Binding mode of *DOTA-Dec-APT in the NK1R (general view). **A)** the ligand alone or **B)** superposed on the crystallographic position of aprepitant (APT). *DOTA-Dec-APT shown as marine-blue sticks. APT shown as orange sticks. Hydrogen display is suppressed. The receptor is shown in a simplified manner as green helices. TM1 not shown.