Description of Additional Supplementary Files

File name: Supplementary Data 1
Description: Gromacs *mdp input file for the production run.

File name: Supplementary Data 2
Description: Representative snapshot after 250ns production run for antagonist bound APJR.

File name: Supplementary Data 3
Description: Representative snapshot after 250ns production run for apo APJR.

File name: Supplementary Data 4
Description: Representative snapshot after 250ns production run for AP13 bound APJR.