

The isoleucine at position 118 in transmembrane 2 is responsible for the selectivity of xamoterol, nebivolol and ICI89406 for the human β 1-adrenoceptor. Lim, Proudman, Monteleone, Kolb, Baker. Molecular Pharmacology MOLPHARM-AR-2022-000583

Supplementary Figure 1

Representative pose of ICI89406 (magenta carbons) and H93 from (a) active (59.9% of simulated frames) and (b) inactive state (84.3% of simulated frames) of β 2-AR MD simulations.

