

Supplemental Table 3. GLP-1R systems prepared and simulated in the present work.

Besides the GLP-1R:Gs protein complexes bound to TT-OAD2 (GLP-1R:TT-OAD2:Gs) and GLP-1 (GLP-1R:GLP-1:Gs), the two corresponding complex without Gs protein (GLP-1R:TT-OAD2 and GLP-1R:GLP-1, respectively) and the two apo receptors (apo-GLP-1R (TT-OAD2) and apo-GLP-1R (GLP-1), respectively) were prepared as described above and subject to four MD replicas each.

GLP-1R System	Number of replicas	Total MD simulation time
GLP-1R:TT-OAD2:Gs	4	2 μ s
GLP-1R:TT-OAD2	4	4 μ s
Apo-GLP-1R (TT-OAD2)	4	4 μ s
GLP-1R:GLP-1:Gs	4	2 μ s
GLP-1R:GLP-1	4	4 μ s
Apo-GLP-1R (GLP-1)	4	4 μ s