|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Receptor type | Ligand | Docking Rank | London dG scoring (kcal/mol) | GBVI/WSA Δ*G* scoring (kcal/mol) | Distance  Asp3.32 Cγ - Lig N1 (Å) | Distance  Asp5.43 Cγ - Lig N2 (Å) |
| hTAAR6active-like | PUT | 4 of 100 | -9,13 | -4,20 | 3,4 | 3,6 |
| CAD | 2 of 100 | -10,13 | -4,54 | 3,2 | 3,5 |
| hTAAR6inactive-like | PUT | 3 of 100 | -9,25 | -3,65 | 3,3 | 3,3 |
| CAD | 5 of 100 | -10,6 | -4,09 | 3,7 | 3,1 |
| hTAAR8active-like | PUT | 6 of 83 | -9,26 | -3,81 | 3,6 | 3,7 |
| CAD | 1 of 100 | -10,12 | -4,28 | 3,3 | 3,4 |
| hTAAR8inactive-like | PUT | 2 of 100 | -8,73 | -3,64 | 3,2 | 3,2 |
| CAD | 7 of 72 | -9,43 | -4,47 | 3,4 | 3,8 |
| zTAAR13cactive-like | CAD | 5 of 100 | -10,21 | -4,32 | 3,2 | 3,0 |
| zTAAR13cinactive-like | CAD | 9 of 62 | -9,02 | -4,09 | 3,4 | 4,1 |