

Table SI. Binding affinity scores and interacting residues of filtered compounds docked to the  $\gamma$ -aminobutyric acid B receptor.

PubChem identification	Binding energy (Kcal/mol)	Interacting residues
Baclofen	-7.9	Ser153, Ser130, Tyr250, Gln349
5281795	-8.2	Tyr250, Glu251, Trp278, His176
10394	-7.7	Ser153, Ser130, Tyr250
6448	-7.6	Ser130, Ser153, Tyr250, Gly151
7393172	-7.4	Ser130, Ser153, His170
699414	-7.3	Ser153
582	-7.2	Ser153
6057	-7.2	Ser153, Ser130, Tyr250, Phe249
9457	-7.2	Ser153, Gly151
2556155	-7.2	Trp64, Trp278, Glu251
31226	-7.2	Ser153, Ser130, Tyr250
450432	-7.1	Tyr250, Gly151, Ser153, Ser130
441457	-7.1	Ser153, Ser130, Tyr250
637542	-7.0	No hydrogen bond
6931754	-6.9	Ser153, Gly151
637541	-6.8	Ser130, Ser153
6918907	-6.7	No hydrogen bond
450502	-6.1	Tyr279, Gln348, Phe347, Gly346