

ANEXO 4

Tabla con valores de pIC₅₀ obtenida experimentalmente por investigadores de la Facultad de Farmacia de la Universidad de Tübingen, los valores de calculados de pIC₅₀ y los valores Z para los 39 ligandos incluidos en el modelo.

ID	pIC ₅₀	\$PRED	\$Z-SCORE
L01	6.76	7.076532	0.925169
L02	7.003	6.959548	0.127002
L03	5.83	6.019441	0.553703
L04	5.241	5.258163	0.050162
L05	5.746	5.883009	0.400456
L06	5.66	5.749195	0.260701
L07	5.44	5.524616	0.247317
L08	7.19	6.597072	1.733026
L09	5.938	6.215816	0.812007
L10	5.051	5.677051	1.829839
L11	5.817	5.938272	0.354455
L12	6.745	6.340012	1.18371
L13	5.879	6.392806	1.501767
L14	6.388	6.485296	0.28438
L17	5.782	5.924737	0.417196
L18	6.482	6.127163	1.037129
L19	5.723	5.748349	0.074089
L20	5.96	6.403843	1.297277
L21	6.892	6.820619	0.208635
L22	7.029	6.95237	0.223975
L23	6.807	7.060899	0.742102
L24	6.742	7.109635	1.074535
L25	6.654	6.472377	0.530853
L26	7.11	6.677198	1.265006
L27	7.12	6.754025	1.069683
L28	6.086	6.113324	0.079863
L29	6.427	6.52228	0.278487
L30	7.441	7.162624	0.813646
L31	6.486	6.802153	0.924059
L32	6.181	6.846357	1.944725
L34	7.374	6.551843	2.403024
L35	7.084	6.824388	0.758802
L37	5.641	6.077967	1.277181
L38	5.758	5.356664	1.173037
L39	6.609	6.017887	1.727724
L40	6.209	5.846003	1.060979
L41	6.842	6.817295	0.072209
L42	5.929	5.89387	0.102679
L43	5.47	5.525305	0.161649