

S4 Table Library Bias

Receptor (Max IC ₅₀)	Number of known ligands in ChEMBL19	Number of purchasable known ligands	Number of purchasable analogs of known ligands *
SMO (1 μM)	363	25	2835
ADRB2 (1 μM)	1432	206	21581
HTR2A (1 μM)	3570	397	25390
DRD2 (1 μM)	4939	469	26137

*ECFP4 cut-off = 0.8

ChEMBL 19 (Bento *et al.*, 2014; Gaulton *et al.*, 2012)