Target Name	Melatonin receptor type 1B
Target TTD ID	TTDS00422

Target Species	Human
Chemical Type	6-methoxy-1-(2-propionylaminoethyl) indoles
Mode of Action	Ligand
QSAR Model 1	$pRA2 = 0.93(\pm0.12)\ \pi - 0.43(\pm0.08)\ \pi^2 + 0.51(\pm0.20)$ $n = 11 \quad R^2 = 0.89 \quad s = 0.46 \quad F = 31 \quad Q^2 = 0.74\ SDEP = 0.59 \quad Optimal\ \pi = 1.08$
QSAR Model 2	$pRA2 = 0.95(\pm0.09)\ \pi - 0.37(\pm0.07)\ \pi^2 + 1.41(\pm0.56)\ \sigma_m + 0.11(\pm0.22)$ $n = 11 \quad R^2 = 0.94 \quad s = 0.35 \quad F = 36.6 \quad Q^2 = 0.83 \quad SDEP = 0.47$
QSAR Model 3	$pRA2 = 0.98(\pm0.12)\ \pi - 0.32(\pm0.12)\ \pi^2 + 0.40(\pm0.21)$ $n = 10 \quad R^2 = 0.91 \quad s = 0.44 \quad F = 34.2 \quad Q^2 = 0.84\ SDEP = 0.48 \quad Optimal\ \pi = 1.53$
QSAR Model 4	$pRA2 = 0.89(\pm0.09)\ \pi - 0.34(\pm0.06)\ \pi^2 + 1.31(\pm0.51)\ \sigma_m + 0.01(\pm0.20)$ $n = 16 \quad R^2 = 0.90 \quad s = 0.38 \quad F = 36.4 \quad Q^2 = 0.84 \quad SDEP = 0.42$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** π: Aromatic substituent constants for lipophilicity; MR: Molar refractivity; L: Second generation length STERIMOL parameter; B1: Second generation minimum width STERIMOL parameter; B5: Second generation maximum width STERIMOL parameter; Sb: Austel's steric branching parameter; σ_m: Hammett constant for meta substitution; σ_p: Hammett constant for para substitution.
Reference	Synthesis Pharmocological Characterization and QSAR studies of 2-substituted Indole Melatonin Receptor Ligands