Target Name	Melatonin receptor type 1A
Target TTD ID	TTDS00393

Target Species	Human
Chemical Type	6-methoxy-1-(2-propionylaminoethyl) indoles
Mode of Action	Ligand
QSAR Model 1	$pRA1 = 0.90(\pm0.17)\ \pi - 0.58(\pm0.12)\ \pi^2 + 0.74(\pm0.30)$ $n = 11 \quad R^2 = 0.80 \quad s = 0.67 \quad F = 16.5 \quad Q^2 = 0.38 \quad SDEP = 1.01 \quad Optimal\ \pi = 0.78$
QSAR Model 2	$pRA1 = 0.93(\pm0.15)\ \pi - 0.51(\pm0.11)\ \pi^2 + 1.81(\pm0.90)\ \sigma_m + 0.23(\pm0.36)$ $n = 11 \quad R^2 = 0.88 \quad s = 0.57 \quad F = 16.5 \quad Q^2 = 0.53 \quad SDEP = 0.88$
QSAR Model 3	$pRA1 = 0.87(\pm0.15)\ \pi - 0.48(\pm0.11)\ \pi^2 + 2.10(\pm0.89)\ \sigma_m + 0.05(\pm0.34)$ $n = 16 \quad R^2 = 0.79 \quad s = 0.65 \quad F = 15.1 \quad Q^2 = 0.64 \quad SDEP = 0.74$
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