

Target Name	K ⁺ channel
Target TTD ID	TTDS00431

Target Species	Human
Chemical Type	Dequalinium analogues
Mode of Action	Blocker
QSAR Model 1	$pEMR = -1.16 (\pm 0.38) \sigma_p - 1.05 (\pm 0.17)$ $n = 7, r = -0.80, s = 0.317$
QSAR Model 2	$pEMR = 1.43 (\pm 1.27) \sigma_I - 0.97 (\pm 0.30)$ $n = 7, r = 0.45, s = 0.477$
QSAR Model 3	$pEMR = 1.43 (\pm 1.27) \sigma_I - 0.97 (\pm 0.30)$ $n = 7, r = 0.45, s = 0.477$
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: MoDel and e-dragon</p> <p>σ_p: Hammett constant for “para” substitution; n is the number of compounds; r is the correlation coefficient; s is the standard deviation. σ_p: a descriptor of the overall electronic effect of R⁴; This is separated in to its inductive and resonance components as represented by σ_I^{16} and σ_R^{16}.</p>
Reference	Synthesis and QSAR of dequalinium analogues as K ⁺ channel blockers. Investigations on the role of the 4-amino group. <i>Bioorganic & Medicinal Chemistry Letters</i> , Vol. 5, No. 6, pp. 559-562. 1995