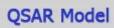
## **Therapeutic Targets Database**





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 (± 1.27) $\sigma_I$ - 0.97 (± 0.30) n = 7, r = 0.45, s = 0.477
QSAR Model 3	pEMR = 1.43 (± 1.27) $\sigma_{I}$ - 0.97 (± 0.30) n = 7, r = 0.45, s = 0.477
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: MoDel and e-dragon $\sigma_P$ : Hammett constant for "para" substitution; $n$ is the number of compounds; $r$ is the correlation coefficient; $s$ is the standard deviation. $\sigma_P$ : a descriptor of the overall electronic effect of $R^4$ ; This is separated in to its inductive and resonance components as represented by $\sigma_I^{16}$ and $\sigma_R^{16}$ .
Reference	Synthesis and QSAR of dequalinium analogues as K+ channel blockers. Investigations on the role of the 4-amino group. <i>Bioorganic &amp; Medicinal Chemistry Letters</i> , Vol. 5, No. 6, pp. 559-562. 1995