

Target Name	Phosphodiesterase 5
Target TTD ID	TTDS00296

Target Species	Human
Chemical Type	Pyridopurinone derivatives
Mode of Action	Inhibitor
QSAR Model 1	Activity: $(6.19 \times 10^3) + (-1.54 \times 10^2)[EEeCH] + (-3.43)[AIC1] + (3.23 \times 10^1)[RNOA]$ $+ (-1.08 \times 10^{-2})[EWPNSA] + (7.29 \times 10) \times [MeRIC]$
QSAR Model 2	Biological Activity: $(6.1881 \times 10^3) + (-3.4269)[AIC1] + (1.5357 \times 10^1)[EEeCH] + (3.2264 \times 10^1)[RNOA]$ $+ (-1.0776 \times 10^{-2})[EWPNSA] + (7.2946 \times 10^1)[MeRIC]$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: MoDel and e-dragon Relative number of oxygen atoms, RNOA; Average information content, AIC1; Exch. eng. + e-e rep. for a C-H bond, EEeCH, ESP-WNSA-1 Weighted PNSA (PNSA1*TMSA/1000) EWPNSA, and min-1 electron reaction index for a C atom, MeRIC) descriptors
Reference	Molecular modeling studies of pyridopurinone derivatives-Potential phosphodiesterase 5 inhibitors. <i>Journal of Molecular Graphics and Modelling</i> 26 (2007) 378–390