

Target Name	Na^+ / Ca^{2+} exchanger
Target TTD ID	TTDR00490

Target Species	Human
Chemical Type	6-{4-[(3-fluorobenzyl)oxy]phenoxy} nicotinamide derivatives
Mode of Action	Inhibitor
QSAR Model 1	$pIC_{50} = -0.624(\pm 0.300)\pi - 0.085(\pm 0.038)MR + 6.268(\pm 0.360)$ $n = 15, \quad r = 0.879, \quad r^2 = 0.773, \quad s = 0.352, \quad F = 20.4$
QSAR Model 2	$pIC_{50} = -0.471(\pm 0.276)\pi - 0.538(\pm 0.211)L + 7.490(\pm 0.766)$ $n = 15, \quad r = 0.900, \quad r^2 = 0.809, \quad s = 0.322, \quad F = 25.5$
QSAR Model 3	$pIC_{50} = -0.560(\pm 0.236)\pi - 0.552(\pm 0.179)B_{IV} + 6.788(\pm 0.418)$ $n = 15, \quad r = 0.926, \quad r^2 = 0.857, \quad s = 0.279, \quad F = 36.0$
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: MoDel and e-dragon</p> <p>Hansch substituent parameters: π (hydrophobicity), MR (steric bulk), σ_m (electronic property); Verloop parameters: L (length), $B_i - B_{IV}$ (shape of each substituent)</p>
Reference	Synthesis and structure–activity relationships of 6-{4-[(3-fluorobenzyl)oxy]phenoxy}nicotinamide derivatives as a novel class of NCX inhibitors: a QSAR study. <i>Bioorganic & Medicinal Chemistry</i> 13 (2005) 717–724