Supplementary Material 1

Supplementary Table 1. ***In silico*** **ADME data from QikPro 3.1 software (Schrödinger) for PQM130**

ADME parameter	Description of predicted parameters	PQM130	Reference value*
Reactive FG	Number of reactive functional groups; the specific groups are listed in the jobname.out file. The presence of these groups can lead to false positives in HTS assays and to decomposition, reactivity, or toxicity problems in vivo. See Appendix 5 of the QikProp User Manual for a complete list	1	0 – 2
CNS	Predicted CNS activity on a –2 (inactive) to +2 (active) scale	1	-2 – +2
mol_MW	molecular weight	381.471	130 – 725
donorHB	Estimated number of hydrogen bonds that would be donated by the solute to water molecules in an aqueous solution. Values are averages taken over a number of configurations, so they can be non-integer	1	0 – 6
accptHB	Estimated number of hydrogen bonds that would be accepted by the solute from water molecules in an aqueous solution. Values are averages taken over a number of configurations, so they can be non-integer	5.5	2.0 – 20.0
QPlogPo/w	Predicted octanol/water partition coefficient	4.356	-2 – 6.5
QPlogS	Predicted aqueous solubility, log S. S in mol dm–3 is the concentration of the solute in a saturated solution that is in equilibrium with the crystalline solid	-5.118	-6.5 – 0.5
QPlogHERG	Predicted IC50 value for blockage of HERG K+ channels	-7.39	< -5
QPPCaco	Predicted apparent Caco-2 cell permeability in nm/sec. Caco-2 cells are a model for the gut-blood barrier. QikProp predictions are for non-active transport	275.881	< 25 poor >500 great
QPlogBB	Predicted brain/blood partition coefficient	-0.688	-3 – 1.2
QPlogKhsa	Prediction of binding to human serum albumin	0.708	-1.5 – 1.5
Hum Oral Absorp	Predicted qualitative human oral absorption	3	1: low 2: medium 3: high
% Hum Oral Absorp	Predicted human oral absorption on 0 to 100% scale	96.134	>80%: high <25%: poor
PSA	Van der Waals surface area of polar nitrogen and oxygen atoms.	70.453	7.0 – 200.0
Rule of Five	Number of violations of Lipinski's rule of five. The rules are: mol_MW < 500, QPlogPo/w < 5, donorHB ≤ 5, accptHB ≤ 10. Compunds that satisfy these rules are considered drug-like.	0	Max 4
Rule of Three	Number of violations of Jorgensen's rule of three. The three rules are: , QPlogS > -5.7, QPPCaco > 22 nm/s, # Primary Metabolites < 7. Compounds with fewer (and preferably no) violations of these rules are more likely to be orally available.	0	Max 3

*gap or recommended value for 95% of known drugs (source: QikProp 3.1 Manual User - Schrödinger Software)