Tetrahydroisoquinoline analogues as potential antimalarials: synthesis, *in vitro* antiplasmodial activity and *in silico* pharmacokinetics evaluation

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Electronic Supplementary Information

Table S1 Selected computed ADMET-related descriptors and their recommended ranges for 95% of known drugs

Property	Description	Recommended range
S_{mol}	the total solvent-accessible molecular surface, in Å^2 (probe radius 1.4 Å).	300 to 1000 Å^2
$S_{mol,hfob}$	the hydrophobic portion of the solvent-accessible molecular surface, in Å^2 (probe radius 1.4 Å).	0 to 750 Å^2
V_{mol}	the total volume of molecule enclosed by solvent-accessible molecular surface, in Å^3 (probe radius 1.4 Å).	500 to 2000 Å^3
log S_{wat}	the logarithm of aqueous solubility.[1,2]	−6.0 to 0.5
log K_{HSA}	the logarithm of predicted binding constant to human serum albumin.[3]	−1.5 to 1.2
log *B/B*	the logarithm of predicted blood/brain barrier partition coefficient.[4-6]	−3.0 to 1.0
BIP_{caco-2}	the predicted apparent Caco-2 cell membrane permeability, in nm s^{-1} (in Boehringer–Ingelheim scale).[7-9]	< 5 low, > 100 high
MDCK	the predicted apparent Madin-Darby canine kidney cell permeability in nm s^{-1}.[8]	< 25 poor, > 500 great
Ind_{coh}	the index of cohesion interaction in solids, calculated from the number of hydrogen bond acceptors (HBA), donors (HBD) and the surface area accessible to the solvent, SASA (S_{mol}) by the relation $Ind_{coh} = HBA \times \sqrt{HBD}/S_{mol}$.[10]	0.0 to 0.05
Glob	the globularity descriptor, Glob = $(4\pi r^2)/S_{mol}$, where r is the radius of the sphere whose volume is equal to the molecular volume.	0.75 to 0.95
QP_{polrz}	the predicted polarizability.	13.0 to 70.0
log *HERG*	the predicted IC_{50} value for blockage of HERG K^+ channels.[11,12]	concern < −5
log K_p	the predicted skin permeability.[13,14]	−8.0 to −1.0
#metab	the number of likely metabolic reactions	1 to 8

Notes and references

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