Table S1: Stability data of 5-AIQ in human plasma (n = 5).

Stability	Nominal concentration (ng/mL) (n=6)	Precision (RSD, %)	Bias (RE, %)
Short-term (8 h)			
	50	1.7	–2.6
	500	3.3	7.4
Freeze thaw (3 cycle)			
	50	3.8	–4.1
	500	4.2	–13.5
Autosampler (24 h at 15°C)			
	50	10.5	5.7
	500	7.2	7.6
2 month at −70°C			
	50	7.9	–10.1
	500	3.6	–8.3

Table S2: ADME properties of 5-AIQ screened by SwissADME software.

Physicochemical Properties	
Formula	C9H8N2
Molecular weight	144.17 g/mol
Num. heavy atoms	11
Num. arom. heavy atoms	10
Fraction Csp3	0.00
Num. rotatable bonds	0
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	46.15
TPSA	38.91 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.27
Log $P_{o/w}$ (XLOGP3)	1.42
Log $P_{o/w}$ (WLOGP)	1.82
Log $P_{o/w}$ (MLOGP)	0.92
Log $P_{o/w}$ (SILICOS-IT)	1.77
Consensus Log $P_{o/w}$	1.44
Water Solubility	
Log *S* (ESOL)	-2.30
Solubility	7.21e-01 mg/ml ; 5.00e-03 mol/l
Class	Soluble
Log *S* (Ali)	-1.84
Solubility	2.08e+00 mg/ml ; 1.44e-02 mol/l
Class	Very soluble
Log *S* (SILICOS-IT)	-3.32
Solubility	6.93e-02 mg/ml ; 4.81e-04 mol/l
Class	Soluble
Pharmacokinetics	
GI absorption	High

BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-6.17 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 2 violations: MW<160, #atoms<20
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: MW<200
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: aniline
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	1.00