Synthesis, crystal growth, and computational investigation of new tetrahydroisoquinoline derivatives potent against molecule nitric oxide synthases

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Supporting materials

Table S1. Experimental details

Compound	**IVa**	**IVb**
CCDC deposit Number	**2237395**	**2237396**
Chemical formula	$C_{23}H_{25}N_5S_2$	$C_{28}H_{27}N_5S_2$
M_r	435.60	497.66
Crystal system, space group	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$
Temperature (K)	150	150
a, *b*, *c* (Å)	8.5983 (5), 9.0810 (6), 16.091 (1)	9.3158 (2), 9.6035 (2), 15.4342 (3)
α, β, γ (°)	100.356 (2), 98.052 (2), 111.746 (2)	73.957 (1), 87.334 (1), 73.106 (1)
V (Å^3)	1118.23 (12)	1268.91 (5)
Z	2	2
Radiation type	Mo *K*α	Mo *K*α

μ (mm^{-1})	0.26	0.24
Crystal size (mm)	0.39 × 0.34 × 0.20	0.33 × 0.17 × 0.07
Data collection		
Absorption correction	Numerical *SADABS* (Krause *et al.*, 2015)	Numerical *SADABS* (Krause *et al.*, 2015)
T_{min}, T_{max}	0.91, 0.95	0.95, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	99231, 9421, 8447	89674, 8499, 6833
R_{int}	0.026	0.037
$(\sin\theta/\lambda)_{max}$ ($Å^{-1}$)	0.796	0.738
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.089, 1.06	0.043, 0.125, 1.05
No. of reflections	9421	8499
No. of parameters	283	327
No. of restraints	2	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.51, −0.42	0.44, −0.51

Table S2. Metabolism and excretion by the CYP450 isoenzymes inhibition and toxicity endpoints of **IVa** and **IVb** (Note: CYP450 (Cytochrome P450 isoenzymes inhibition), LD50 (Letal dose in 600 mg/kg), - (Inactive toxic class (probability score)) and + (Active toxic class (probability score)).

Metabolism and Excretion									**Toxicity endpoints**	
CY450 Inhibitors										
	1A2	2C19	2C9	2D6	3A4	Hepato	Carcino	Immuno	Mutagen	Cito
1	No	Yes	Yes	No	Yes	-0.57	0.52	-0.99	-0.54	-0.74
2	No	Yes	Yes	No	Yes	-0.56	0.55	-0.99	-0.50	-0.76