Title: Rubrofusarin as a Dual Protein Tyrosine Phosphate 1B and Human Monoamine Oxidase-A Inhibitor: An In Vitro and In Silico Study

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Supplementary Table 1. Drug-likeness and ADME characteristics as determined by PreADMET.

compounds	drug-likeness		ADME characteristics					
	MDDR-like rule	Lipinski's rule	Log $P_{o/w}$ [a]	PPB [b]	HIA [c]	in vitro Caco2 permeability (nm/sec) [d]	in vitro MDCK cell permeability (nm/s) [e]	in vivo BBB penetration ([brain]/[blood]) [f]
rubrofusarin	mid-structure	suitable	2.89	85.78%	93.22%	19.31	45.39	0.64
2	drug-like	violated	-0.85	34.48%	13.23%	9.89	0.32	0.03

[a] The log of the coefficient of solvent partitioning between 1-octanol and water.

[b] Plasma protein binding (PPB) (< 90% represents weak binding and > 90% represents strong binding).

[c] Human intestinal absorption (HIA) (0-20% is poorly absorbed, 20-70% is moderately absorbed and 70-100% is well-absorbed).

[d] 0-10 nm/sec is low permeability, 10-100 nm/sec is medium permeability and > 100 nm/sec is high permeability.

[e] Permeability across MDCK cells.

[f] < 0.1 is low absorption by the central nervous system, 0.1-2.0 is middle absorption and > 2.0 is high absorption.

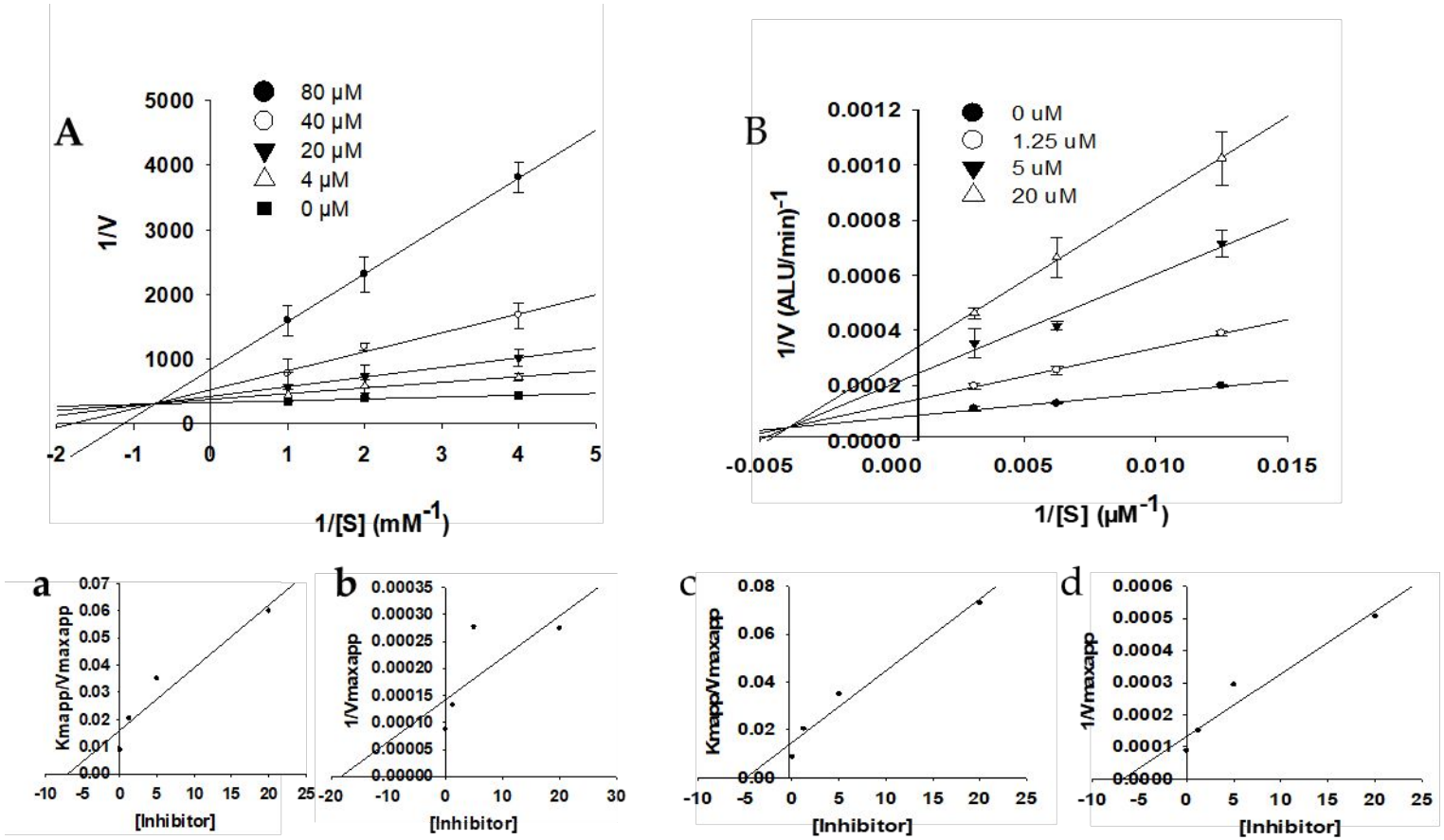

Figure S1. Lineweaver-Burk plots for PTP1B (**A**) and *h*MAO-A (**B**) inhibition by rubrofusarin. PTP1B inhibition was tested in the presence of 0.25 mM, 0.5 mM and 1 mM concentrations of substrate, *p*NPP. *h*MAO-A inhibition was tested with 80, 160 and 320 µM *h*MAO substrate. Graphs below Lineweaver-Burk plots represent secondary plots for PTP1B (**a** and **b**) and *h*MAO-A (**c** and **d**) inhibition by rubrofusarin.