



STRUCTURAL BIOLOGY
COMMUNICATIONS

Volume 78 (2022)

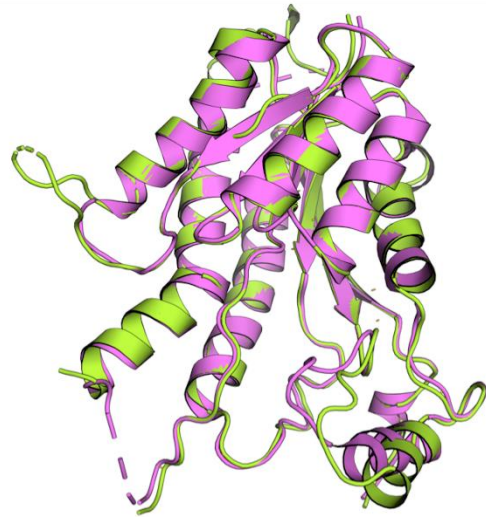
Supporting information for article:

Crystal structure of the ternary complex of *Leishmania major* pteridine reductase 1 with the cofactor NADP⁺/NADPH and the substrate folic acid

Lucia Dello Iacono, Flavio Di Pisa and Stefano Mangani

	1	10	20	30	40	
Leishmania	MTAPT	PVAIVTGA	AKRGRS	EGLEHAP	GVVCHYHRS	SAAPN
Trypanosoma	...MEAP	PAIVTGA	AKRGRS	FAVLEHQT	GVVCHYHRS	SAEAV
	50	60	70	80	90	
Leishmania	ALGAT	LNARFNS	AVTVOAD	LENVAT	APVSGADG	SAPVTFTRCA
Trypanosoma	SLADE	LNKRSNS	AVVCGAD	LENVAT	APVSGADG	SAPVTFTRCA
	100	110	120	130		
Leishmania	ELVAAC	THGRCD	VLVNNAS	FYPTPL	LRNDE	GHEPCVGDREA
Trypanosoma	ELVNS	CHGRCD	VLVNNAS	FYPTPL	LRNDE	GHEPCVGDREA
	140	150	160	170	180	
Leishmania	MEATAD	IFCSNA	IAPVFL	IKAFH	RFACTPA	KHRGTNVSINNV
Trypanosoma	VETQVA	ELIHCNA	IAPVFL	IKAFH	RFACTPA	KHRGTNVSINNV
	190	200	210	220		
Leishmania	DAMTN	QPLIC	YTIY	VMKCAL	BGLTR	SAALELAPLQIRVNGVCPG
Trypanosoma	DAMVD	QPLIC	YTIY	VMKCAL	BGLTR	SAALELAPLQIRVNGVCPG
	230	240	250	260	270	
Leishmania	ISWLV	DDMP	PAVNR	GHRSK	VPIYCR	SSAABVSDVVIPLCSKAK
Trypanosoma	VSHLP	VAMG	EEEKL	KWR	RRKVP	LRREASAEQIADAVIFIVSGSAQ
	280					
Leishmania	YITC	CKK	VDDG	YSI	ITIA	
Trypanosoma	YITC	CKK	VDDG	YSI	ITIA	

(a)



(b)

Fig. S1: (a) Sequence alignment of PTR1 from *Leishmania major* (UniProtKB entry Q01782) and *Trypanosoma brucei* (UniProtKB entry O76290) using Clustal Omega (<https://www.ebi.ac.uk/Tools/msa/clustalo/>; Sievers et al., 2011). The figure was generated using ESPript 3.0 (<https://esprict.ibcp.fr/ESPript/ESPript/>; Robert et al., 2014). The numbering system is based on *Lm*PTR1 sequence. Residues conserved in both sequences are colored in white and highlighted in red, while similar residues are colored in red. Green triangular arrows indicate the residues of the catalytic triad. (b) Structural superposition between our *Lm*PTR1 structure (green) and *Tb*PTR1 structure (pink, PDB code 3BMC). The figure was generated using Pymol (PyMOL Molecular Graphics System, Version 1.8 Schrödinger, LLC).