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**Supporting information for article:**

**Structural insights into novel inhibition mechanism of *Trypanosoma cruzi* spermidine synthase**

**Yasushi Amano, Ichiji Namatame, Yukihiro Tateishi, Kazuya Honbo, Eiki Tanabe, Tatsuya Niimi and Hitoshi Sakashita**

**Table S1** List of the amino acid residues in outliers of Ramachandran plot.

Compound	dcSAM	dcSAM + 4MCHA	dcSAM + Fragment 1	dcSAM + Fragment 2	dcSAM + Fragment 3	dcSAM + Fragment 4	dcSAM + Fragment 5	dcSAM + Fragment 6
PDB ID	4YUV	4YUW	4YUX	4YUY	4YUZ	4YU0	4YU1	4YU2
Ramachandran plot (%)								
Preferred	95.6	96.2	95.5	95.4	96.1	96.4	96	95
Allowed	3.8	3.1	3.6	4.1	3.3	3	3.3	4.6
Outliers	0.5	0.7	0.9	0.5	0.6	0.6	0.6	0.4
Residues in outliers	A, K87	A, K87	A, G3	A, E203	A, K87	A, K87	A, K87	A, E70
(Chain ID, Residue ID)	A, E203	A, E203	A, K87	B, K87	A, E203	A, E203	A, E203	A, E203
	B, E203	B, K87	A, E203	B, E203	A, V253	B, E203	B, E203	
		B, E203	B, K87		C, K30	C, S8	C, Q18	
			B, E203		C, K87	C, E203	C, K87	
					C, E203	D, T170	C, E203	
						D, E203		

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TcSpdSyn      1  -----MPGSELI SGWFREENDQWPGQAMSLRV
TbSpdSyn      1  -----MPGPGLLADGWFREENGOWPGQAMSEKRV
LmSpdSyn      1  -----MPGPGLLPD GWFREESTMWPQQAQGLKRV
PfSpdSyn      1  MDKLI SNNK LKLSV VLLGGLCS LAYYHLK NKFHLSQ FCF S KKW FSEFS IMWPQQA FSLKI
HsSpdSyn      1  -----MEPGPDGPAASGPAATREGWFRETCSLWPGQALSLOV
MmSpdSyn      1  -----MEPGPDGPAAPGPAATREGWFRETCSLWPGQALSLOV

TcSpdSyn      29  EKVL YDAPT KFOHL TIFESD PKGPWGTVMALDGC IQVTDY DEFVYHEV L GHTSLCSHPKP
TbSpdSyn      29  EEVL HDTPTKFOHLS IFETDPK GPWGTVM TLDGCIQLTD FDEFVYHEML SHTPLCAHPDP
LmSpdSyn      29  EKVL YDQPT EFOHL TVFESD PS GPWGTVM TLDGAIQLTD YDEFVYHEMLAN LSLACHHKP
PfSpdSyn      61  KKIL YETKSKYQNV LVFESTY G---KVL VLDGVIQLTEK DEFAYHEMTH VPMTVSKEP
HsSpdSyn      38  EQLL HRRRSRYQDI LVFRSKTYG ---NVL VLDGVIQCTER DEFYSYQEMIAN LPLCSHPNP
MmSpdSyn      38  EQLL HRRRSRYQDI LVFRSKTYG ---NVL VLDGVIQCTER DEFYSYQEMIAN LPLCSHPNP

TcSpdSyn      89  ERVLI IGGDGGV LREVL RHG----TVEHCDLVDID GEVMEQSKQH FPOISRSLADPRA
TbSpdSyn      89  VDVL IGGDGGV MREVL RHG----TVKRCVLVDID GDVIEASKKY FPOISSGFSDPRA
LmSpdSyn      89  ERVL IGGDGGV VREVL RHKSEKDG VVQSVELVDID GAVMQQSKKH FPOVACGFANPCV
PfSpdSyn      118  KNLV VGGDGGI IRELCKYK ----SVENIDI CEIDETVIEVSKI YFKNISCGYEDKRV
HsSpdSyn      95  RKVL IGGDGGV LREVVKHP ----SVESV VQCEIDEDVIOVSKKFL PGM AIGYSSSKL
MmSpdSyn      95  RKVL IGGDGGV LREVVKHP ----SVESV VQCEIDEDVIEVSKKFL PGM AVGFSSSKL

TcSpdSyn      144  TVR VGDGLAFVRQ TPDNTY DVV IIDTTDPAGPASKLFG EA FYKDVLRI LKPDGICCNQGE
TbSpdSyn      144  DVR VGDGVAFVREAASESFDV V IIDTTDPDGPAAELFGEK FYRDVLRILKPRGICCNQGE
LmSpdSyn      149  TAT VGDGAAFVRNVPDSVY DVIIIDTTDPKGPASELFGAD FYTNVLRILRPGGVVCNQGE
PfSpdSyn      173  NVF IEDASKFLENVTN -TYDV IIVDSSDPI GPAETL FNQNFY EK IYNAL KPNGYCV AQCE
HsSpdSyn      150  TLH VGDGF EFMKQND -AFDV IITDSSDPMGPAESL FKES Y YQLMKTAL KEDGVLCCQGE
MmSpdSyn      150  TLH VGDGF EFMKQND -AFDV IITDSSDPMGPAESL FKES Y YQLMKTAL KEDGILCCQGE

TcSpdSyn      204  SIWLD LELIEKMSRFIR -ETGFASVQYALMHV PTPYPCGSIGTLVCSKKA GVDVTKPLRPV
TbSpdSyn      204  SVWLN RNLIEGMADFIKNKVG FASVKYAM IYTPYPCGSIGSLICSKVAGVDVTPVVRPV
LmSpdSyn      209  SVWL HRPLIEKMMGFLK KDIGFATVKYAM IYIPTYPCGSIGTLVCAK SADTDVTVPMRPV
PfSpdSyn      232  SLW LHVGTIKNMIGYAK --KLFKKVEYANIS IPTYPCGCIGILCCSKT -DTGLTKPNKKL
HsSpdSyn      209  CQWLH LDLIKEMRQFCQ --SLFPV VAYAYCTIPTYPSGOIGFMLCSKNPSTNFQEPVQPL
MmSpdSyn      209  CQWLH LDLIKEMRHFC K--SLFPV VDYAYCS IPTYPSGOIGFMLCSKNPSTNFRFPVQPL

TcSpdSyn      263  EDMP FAK-DLKYD SEMHKAS FALPRFARH INNSE-
TbSpdSyn      264  ESMP FAG-ELKYD SDVHKA AFVLP RFARHINQ NYS
LmSpdSyn      269  ESL GFAD-QLKYYS DMHKA AFVLP RF A AHLNE ---
PfSpdSyn      289  ESKE FAD--LKYYN YENHSA AFKLP AFLLKEI ENI-
HsSpdSyn      267  TQQQV AQMQLKYYS DVHRA AFVLP EFARKALNDVS
MmSpdSyn      267  TQAQVEQMQLKYYS DMHRA AFVLP EFTRKALNDIS

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**Figure S1** Sequence alignment of SpdSyn from *Trypanosoma cruzi* (Tc), *Trypanosoma brucei* (Tb),

*Leishmania major* (Lm), *Plasmodium falciparum* (Pf), human (Hs), and mouse (Mm). Identical residues are boxed in black and similar residues are boxed in gray.