SUPPLEMENTAL DATA

STRUCTURAL BASIS OF MOLECULAR RECOGNITION BY LEISHMANIA SMALL HYDROPHILIC ENDOPLASMIC RETICULUM-ASSOCIATED PROTEIN, SHERP, AT MEMBRANE SURFACES

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FIGURE S1 **2D ^{1}H-^{15}N HSQC NMR spectrum of *L. major* SHERP at 4 ^{o}C in the absence of SDS or phospholipids.** The poor amide ^{1}H dispersion is indicative of a lack of tertiary structure.

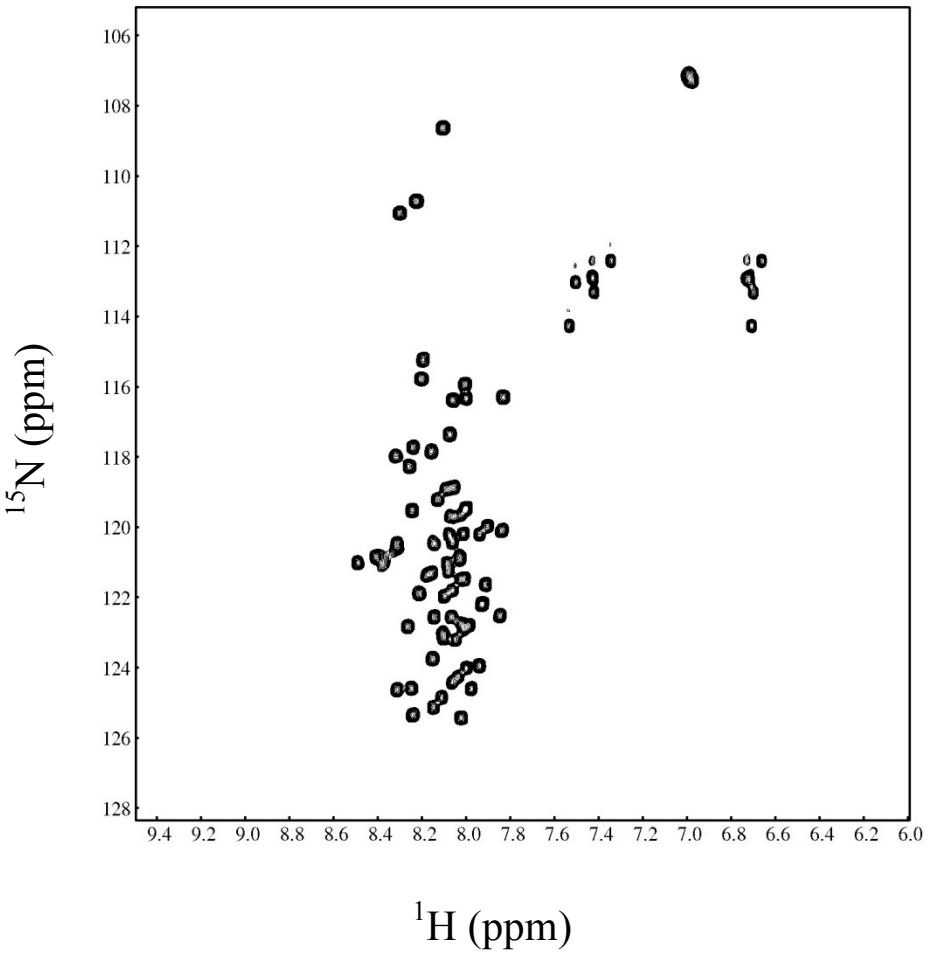

FIGURE S2 **^{1}H-^{15}N heteronuclear NOE spectrum of *L. major* SHERP at 4 ^{o}C in the absence of SDS or phospholipids.** The spectrum shown is a summation of the reference and NOE spectrum corresponding to (0.8 times the reference – NOE spectrum). Residual signals thus correspond to those with a significant ^{1}H-^{15}N NOE contribution arising from extensive internal motion on the ps timescale, which for the free SHERP is observed in essentially all residues (for comparison with Figure S2).

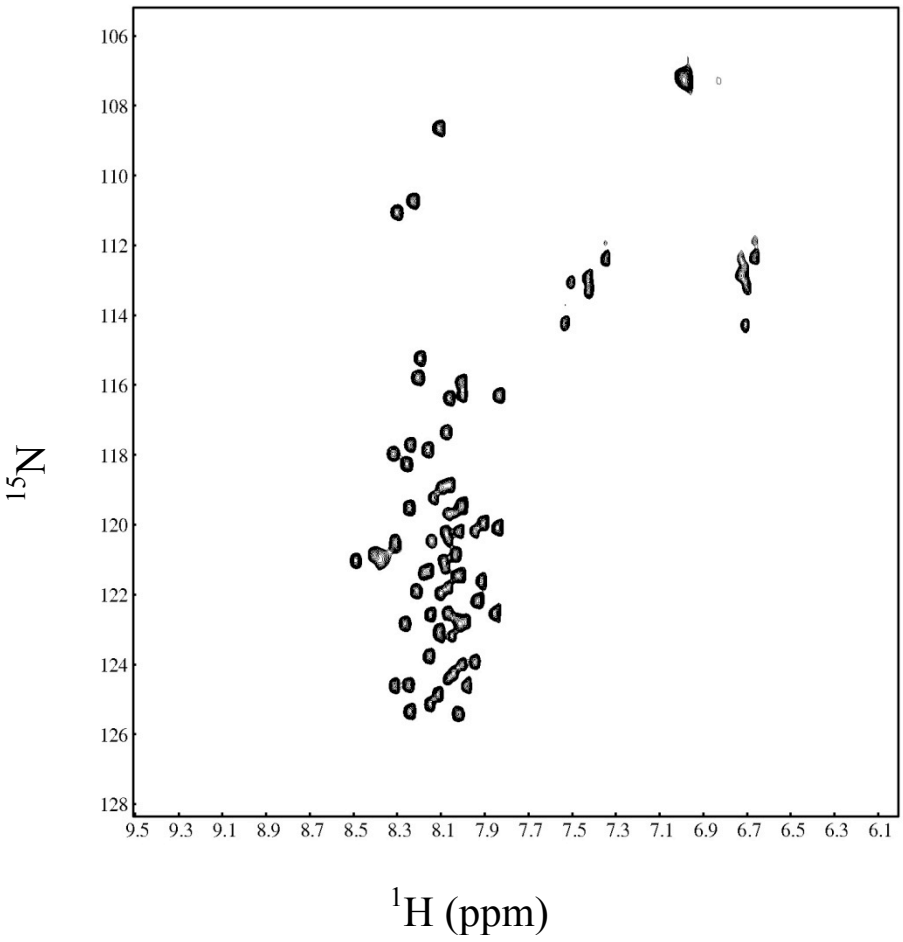

FIGURE S3 **SDS-PAGE avidin-column fractions analyzed to identify SHERP-SBED complexes containing a biotinylated label.** Lanes labeled correspond to the flow-through (FT), wash (W) and elution (E) fractions. Bands labeled with numbers correspond to sample numbers shown in Table S1 below.

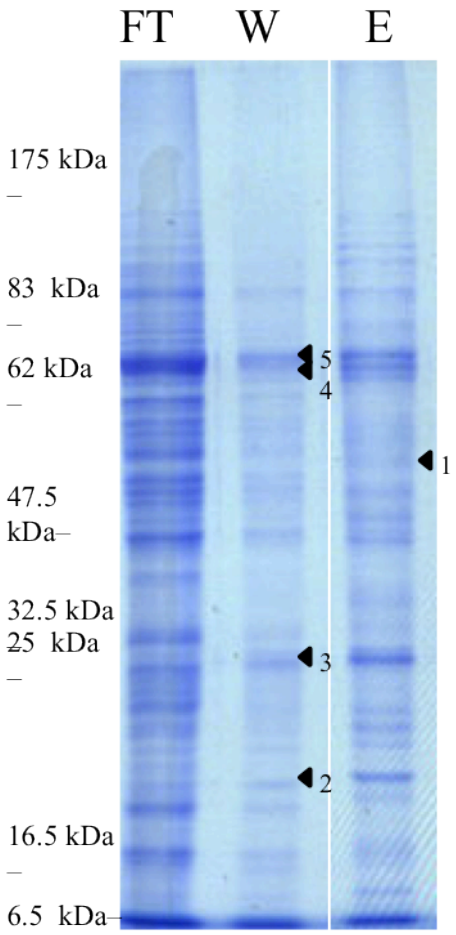

FIGURE S4 **Amino acid sequence alignment between the *L. major* and *T. thermophilus* V-ATPase subunit B.** A ClustalW2 alignment is shown. Identical residues (blue), conserved substitutions (green) and semi-conserved substitutions (yellow) are colored according to ClustalW2 conventions (see http://www.ebi.ac.uk/Tools/clustalw2/index.html and Larkin M.A., et al. (2007) *Bioinformatics* **23**, 2947-2948).

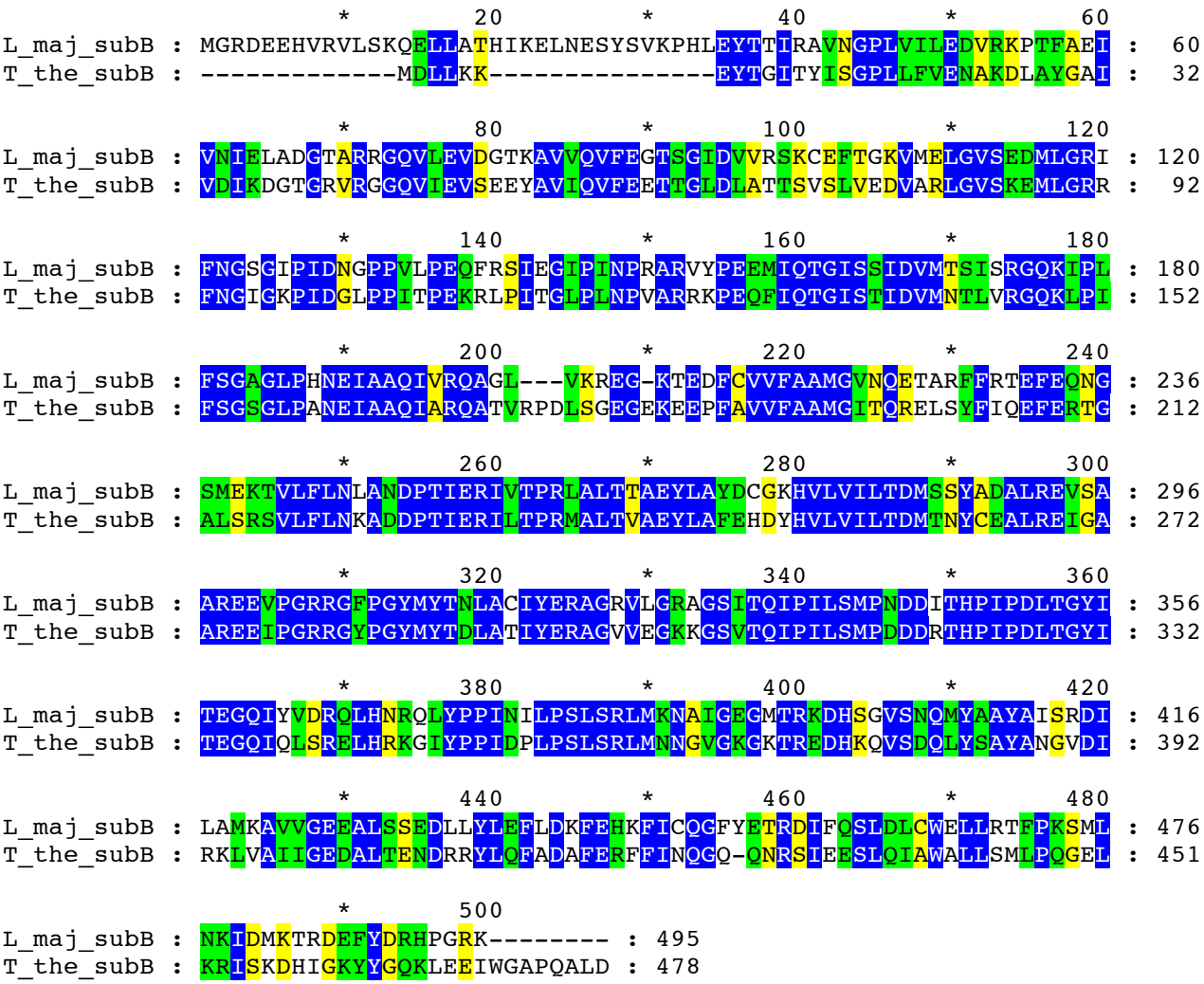

FIGURE S5 **Recombinant *L. major* SHERP binding to *T. thermophilus* V-ATPase demonstrated by surface plasmon resonance.** *T. thermophilus* V-ATPase at 0.2 mg/ml in 10 mM sodium acetate buffer, pH 5.0 was immobilized to a CM5 chip by amine coupling. Injection of *L. major* SHERP at a flow rate of 5 ul/min is shown for concentrations ranging from 0.5 µM (red) to 15 µM (dark blue) are shown along with the associated fits (dashed lines) to the raw data based upon a 1:1 Langmuir binding model. Binding was measured as response units over time. See main article for more details on the experimental data and analysis.

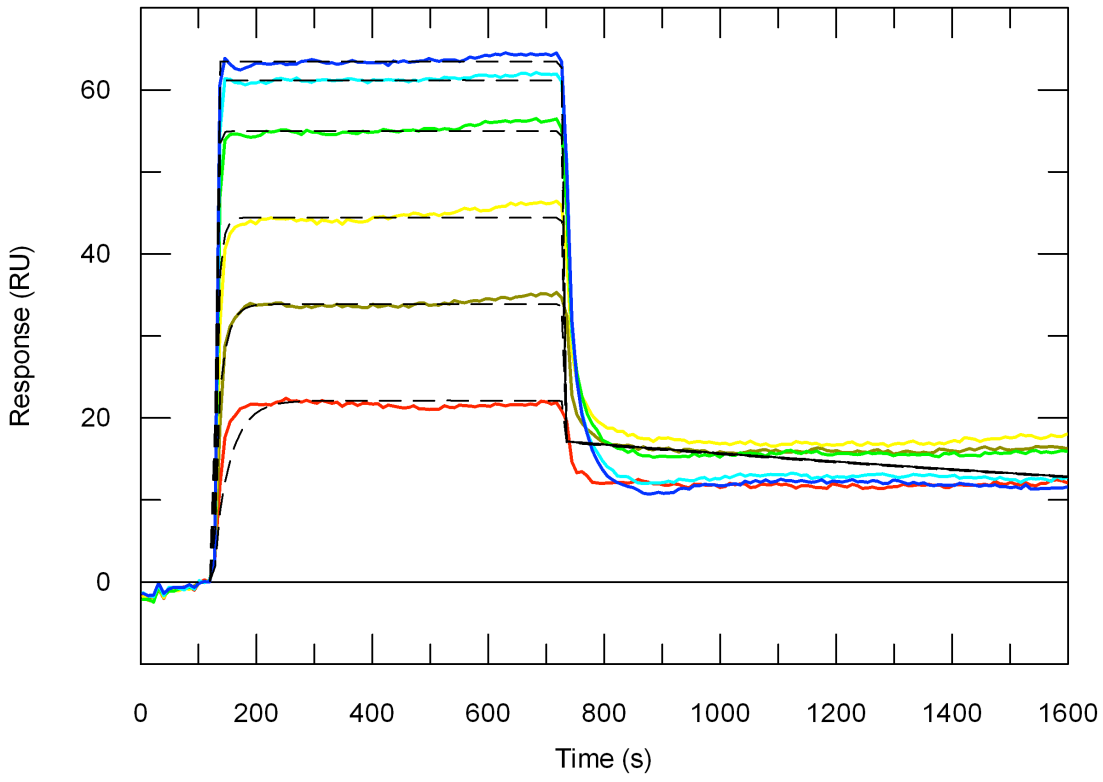

TABLE S1

Summary of mass spectrometric analyses of *Leishmania major* proteins isolated from cross-linking studies with recombinant *L. major* SHERP

Sample No.	Molecular Mass (kDa)	MOWSE Score[a]	GeneDB Identifier	Description
1	**55**	**301**	LmjF28.2430	vacuolar ATP synthase subunit B, putative
2	**25**	**121**	LmjF23.0040	peroxidoxin tryparedoxin peroxidase
3	**27**	**381**	LmjF36.5010	40S ribosomal protein SA, putative
4	**68**	**111**	LmjF29.1760	paraflagellar rod protein 1D, putative
5	**71**	**574**	LmjF28.2780	heat-shock protein hsp70, putative

[a] Pappin, D. J., Hojrup, P., and Bleasby, A. J. (1993) *Curr. Bio.* **3**, 327–332