Supplementary Information

Atomic Structure of the *Leishmania spp.* Hsp100 N-Domain

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Fig. S1

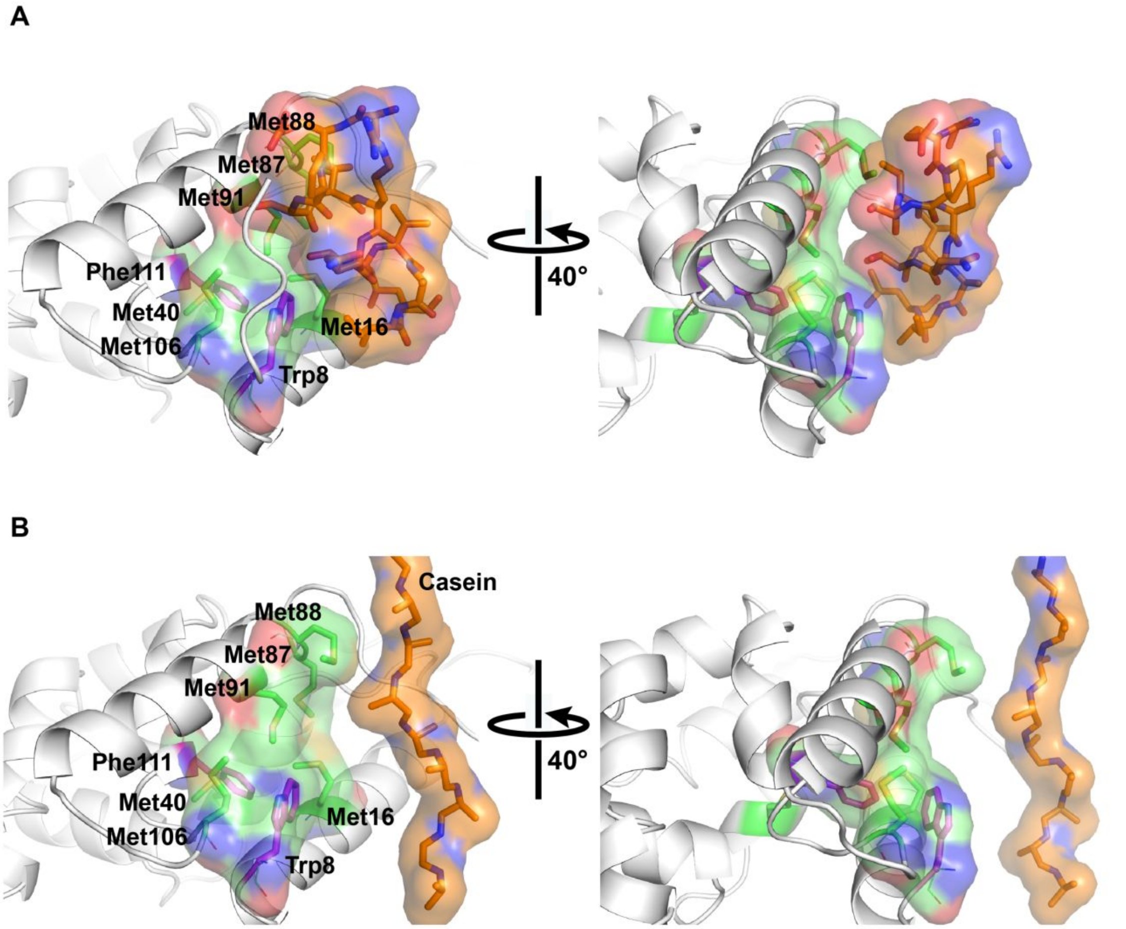

Figure S1: Model of a putative *Lm*Hsp100$_N$-substrate complex. Key residues are labelled and depicted as stick models and surface rendering. **(A)** Superposition of *Lm*Hsp100$_N$ onto the crystal structure of yeast Hsp104$_N$ bound to the C-terminal helix of a neighboring N-domain (PDB: 6AMN) [1]. The C-terminal helix (residues 341-352) of sequence AEPSVRQTVAIL (orange), which mimics a substrate peptide [1], is depicted as stick model and surface representation. The figure highlights the putative interface between the N-domain and substrate. **(B)** Model of *Lm*Hsp100$_N$ bound to casein, an Hsp100 model substrate, depicted as poly-alanine (gold). *Lm*Hsp100$_N$ was superposed onto the 3D structure of the N-domain of an *E. coli* ClpB hexamer bound to casein (PDB: 6OG3_C) [2]. The casein side-chains were not resolved in the cryoEM reconstruction with casein represented as a poly-alanine model [2].

References

1. Lee J, Sung N, Mercado JM, et al. Overlapping and specific functions of the Hsp104 N domain define its role in protein disaggregation. *Sci Rep.* 2017;7:11184.
2. Rizo AN, Lin J, Gates SN, et al. Structural basis for substrate gripping and translocation by the ClpB AAA+ disaggregase. *Nat Commun.* 2019;10(1):2393.