S6 Fig. Electrostatic potentials of Taspase1 and location of the Taspase1 loop.

(a) Electrostatic potentials were calculated using the Adaptive Poisson-Boltzmann Solver (APBS) applying the YAMBER2 force field. Positive, neutral, and negative charges are displayed in blue, gray, and red, respectively. The surface charge of the Taspase1 alpha-subunit C-terminus is visualized for our proposed loop model and reveals a positive charge. **(b)** The surface charge of the Taspase1 core is visualized for the crystal structure of one active Taspase1 heterodimer (PDB 2a8j). The active site (dashed line) is also positively charged. **(c)** Location of the loop in the functional homodimer of Taspase1. Our proposed loop structure was modeled on both monomers of the Taspase1 proenzyme (PDB 2a8i). Monomer 1 is depicted in orange with its loop in green, monomer 2 in red with its loop in blue.