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Supplemental Information

Integrative Modeling of a Sin3/HDAC

Complex Sub-structure

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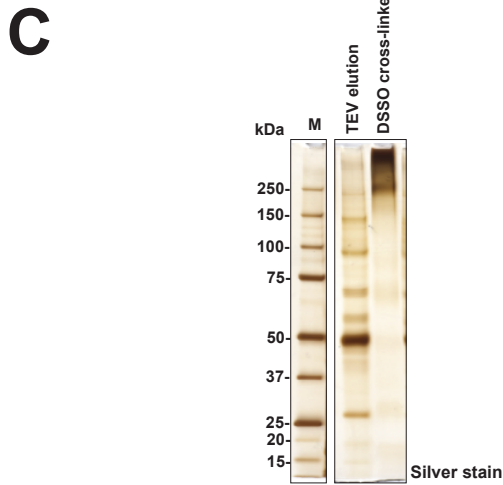
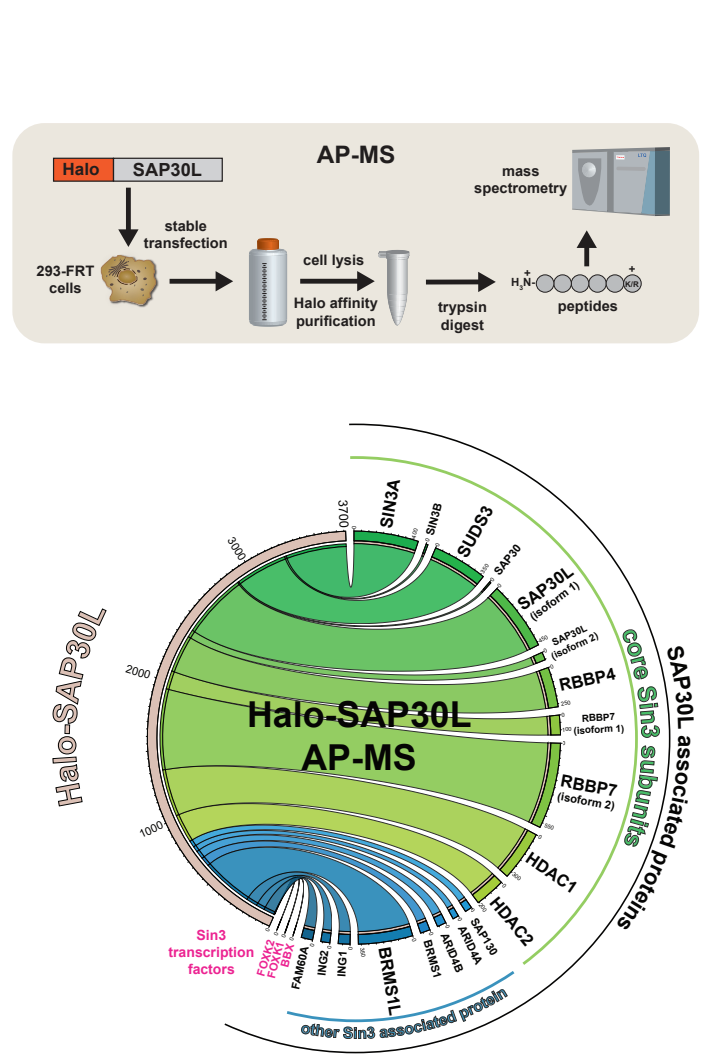
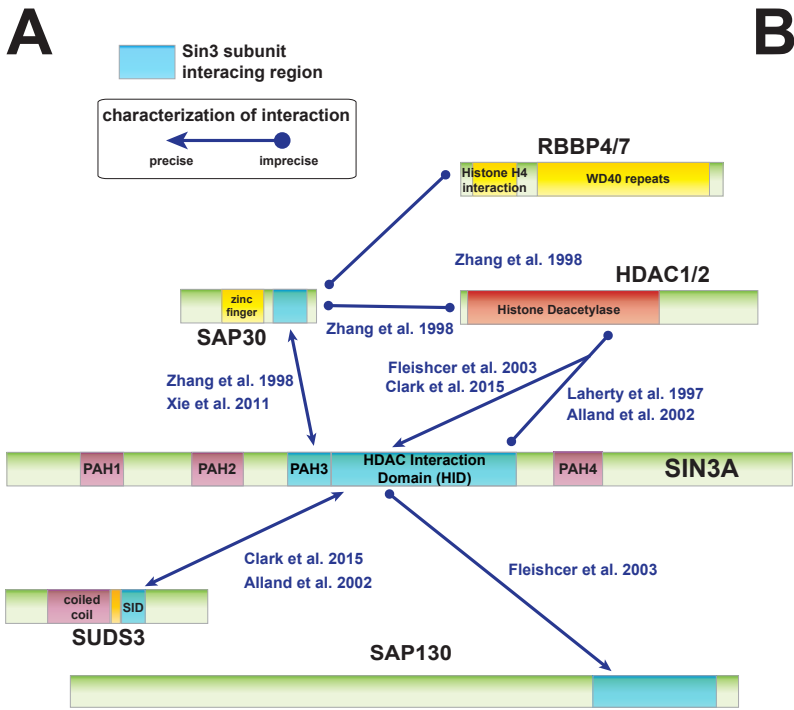


Figure S1, related to Figure 1. A Previously characterized interactions between Sin3 subunits. Regions important for interactions between Sin3 subunits are shown in blue, for interaction with DNA/nucleosomes in yellow, for histone deacetylase activity in red, and other structurally defined regions in purple. **B** Relative abundance of Sin3 complex subunits copurifying with the Halo-SAP30L subunit determined by AP-MS. Values for each subunit are 1000 x mean dNSAF (data and experimental details previously published in Banks et al. 2018). **C** Halo-SAP30L purified complexes treated with or without DSSO cross-linking. Samples purified from Flp-In™-293 cells stably expressing Halo-SAP30L as described in methods were treated with or without 5 mM DSSO for 40 minutes at room temperature, boiled in sample buffer and separated by SDS-PAGE. Proteins were visualized by silver staining.

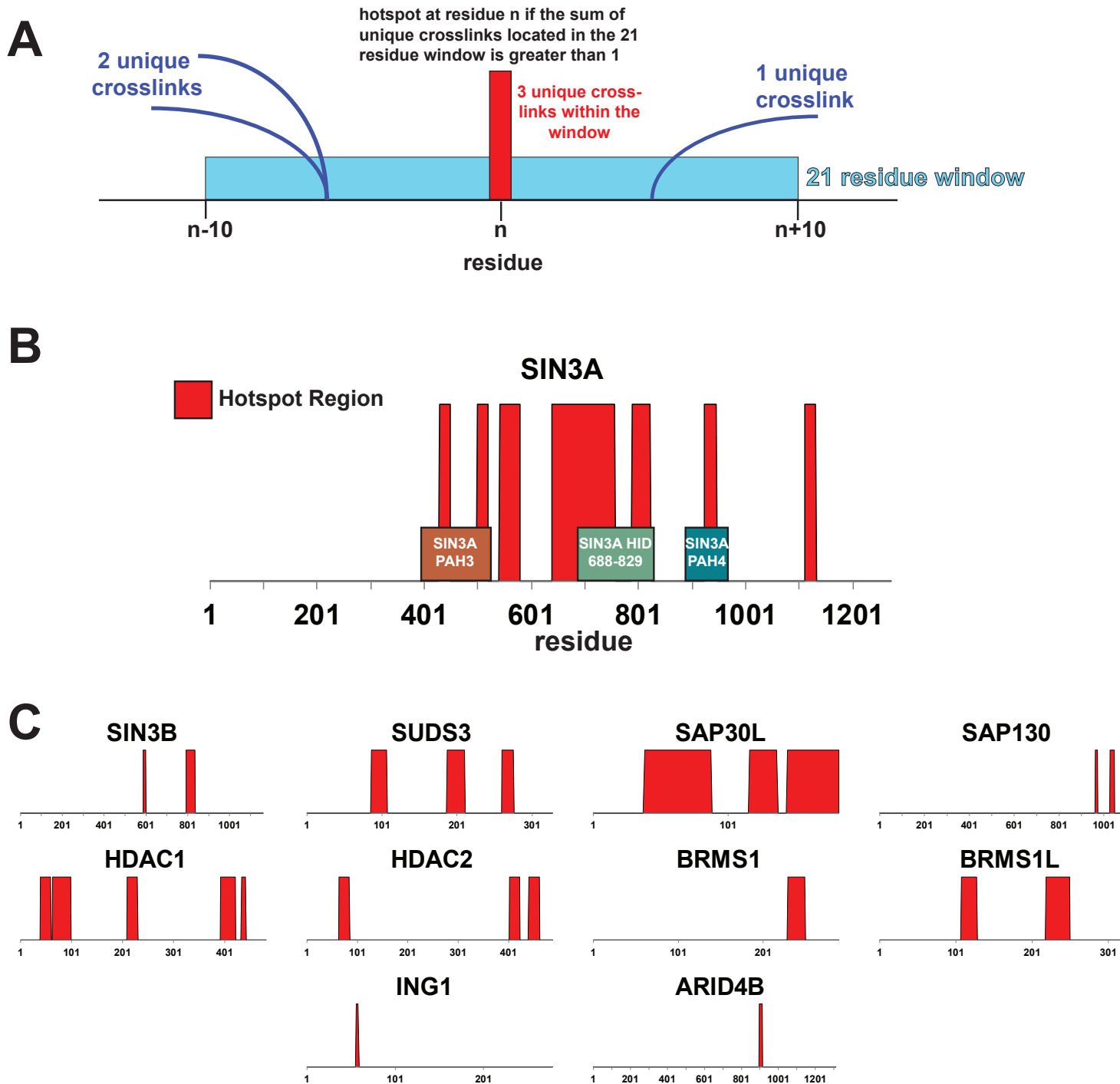


Figure S2. Crosslink hotspot regions, related to Figure 1. A Defining crosslink hotspot regions. Residue n of a protein resides within a hotspot region if there is more than 1 unique crosslink within a 21 residue window centered on residue n . **B** Hotspot regions within SIN3A. Regions of SIN3A deleted for the analysis of Figure 3 are indicated (SIN3A PAH3, SIN3A HID 688-829, and SIN3A PAH4). **C** Hotspot regions for other SIN3 complex subunits. No hotspot regions were detected for ARID4A and RBBP7.

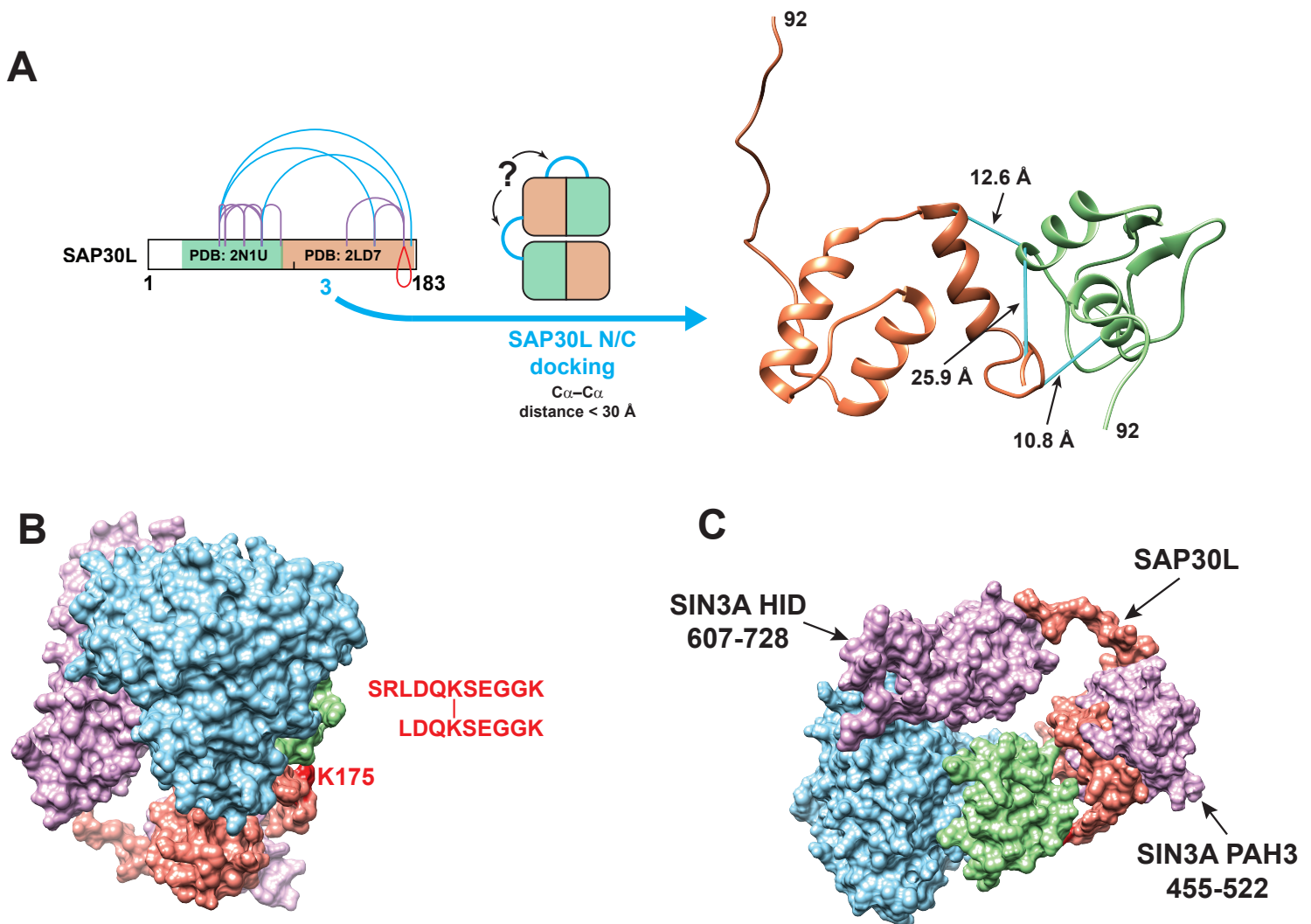


Figure S3. Docking Sin3 structures, related to Figure 4. A Docking structures mapping to SAP30L. SAP30 structure 2LD7 was mapped to the homologous protein SAP30L using SWISS-MODEL. A cross-link with overlapping peptides (red) is consistent with a SAP30L homodimer. The self cross-links shown in blue were then used as docking restraints to assemble the structures using the HADDOCK platform, leaving unresolved the question as to whether the docked structures represent regions of the same SAP30L molecule or two different SAP30L molecules. B Residue SAP30L K175 is exposed and accessible for interaction with a second SAP30L molecule. The crosslinked SAP30L peptides shown have overlapping sequence consistent with a crosslink between two different SAP30L molecules. Docking SAP30L, HDAC1 and SIN3A structures (Figure 4B) does not occlude K175. C Position of the SIN3A PAH3 domain (previously modeled relative to SAP30 in the structure 2LD7) relative to SAP30L and the SIN3A HID. N.B. although HDAC1 cross-links to the SIN3A PAH3 domain at K439 (lower blue cross-link, Fig. 3B), this cross-link does not map to the part of the PAH3 structure shown here.