

Crystal Structure of Calmodulin Binding Domain of Orai1 in Complex with Ca²⁺/Calmodulin Displays a Unique Binding Mode*

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* Running title: Calmodulin and Orai1 form an unusual 1:2 complex

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Supplemental materials

Figure S1. A sample of electron density map of CaM/Orai1-CMBD. A 2Fo-Fc map was contoured around W76 (labeled in black) of Orai1-CMBD at 1.0 σ level using Pymol. The carbon atoms are colored in green for Orai1-CMBD, and in light blue for CaM. The other atoms are colored as: O, red; N, dark blue; S, gold, for both Orai1-CMBD and CaM. The residue numbers of CaM are labeled in blue, and W76 of Orai1-CMBD is labeled in black.

Figure S2. Interaction of Orai1-CMBD with CaM-N of symmetry-related CaM. **A.** Stick and surface representation of the interaction. Residues involved in this interaction are labeled in black for Orai1-CMBD, and in blue for CaM. The two hydrogen bonds are indicated with the dotted lines. **B.** Surface representation of Orai1-CMBD and CaM-C to show the shape complementarity. **C.** Surface representation of Orai1-CMBD and symmetry-related CaM-N to show the shape complementarity. Comparison of B and C shows that Orai1-CMBD and CaM-C have better shape complementarity than Orai1-CMBD and symmetry-related CaM-N. The color schemes are: C, yellow for CaM, and green for Orai1-CMBD; N, blue; O, red; S, gold.

Figure S3. Hydrophobic interactions between CaM and three residues of Orai1-CMBD. **A.** L74; **B.** L79; **C.** Y80. The side chains of Orai1-CMBD residues are shown in green sticks. CaM is shown as ribbon in yellow, with residues interacting with Orai1-CMBD residues shown in sticks. Oxygen atoms are shown in red, and sulfur atoms in gold. Residues of Orai1-CMBD are labeled in black, and residues of CaM are labeled in blue.

Figure S4. NMR ¹⁵N-¹H chemical shift perturbations of CaM and CaM-N due to Orai1-CMBD. **A.** The amide resonances of CaM are shown upon addition of Orai1-CMBD at protein to peptide ratios of 1:0, 1:1, 1:1.5, and 1:2.0. I130 (in red) and A57 (in blue) are highlighted. **B.** The amide resonances of isolated CaM-N are shown upon titration of Orai1-CMBD at protein to peptide ratios of 1:0, 1:0.5, and 1:1. A57 (in blue) is highlighted.

Fig. S1

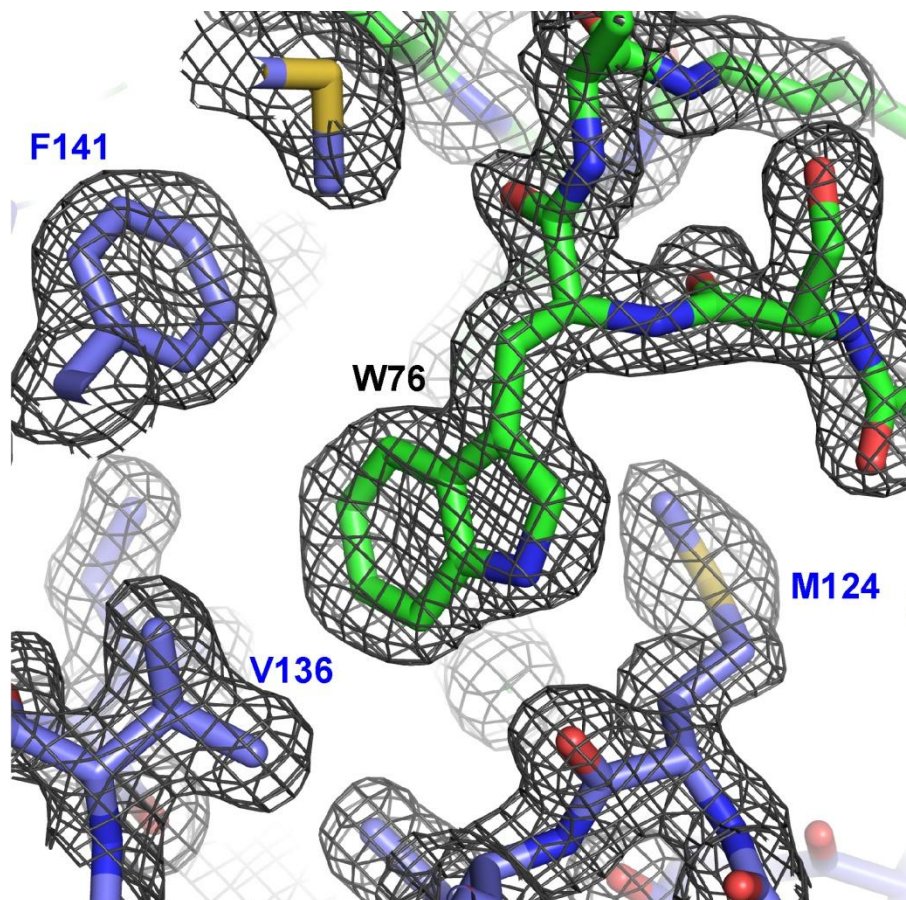


Fig. S2

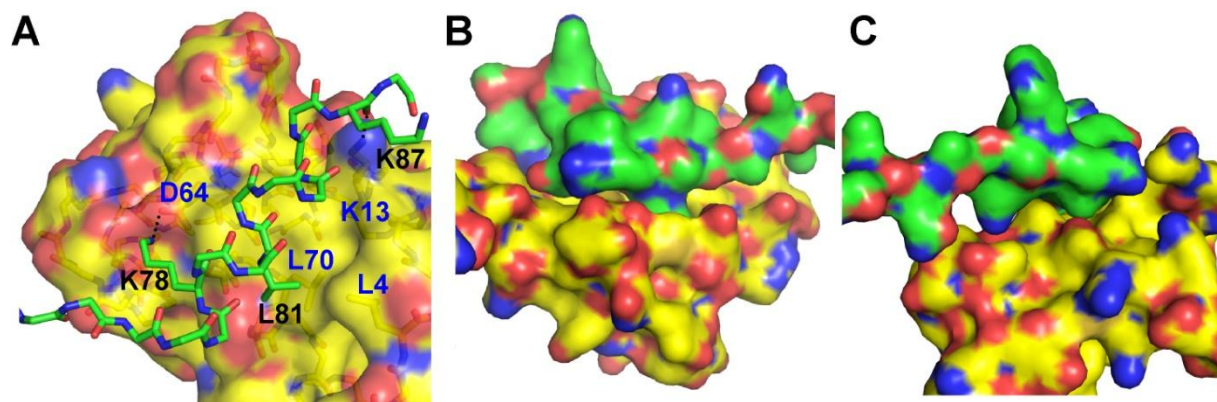


Fig. S3

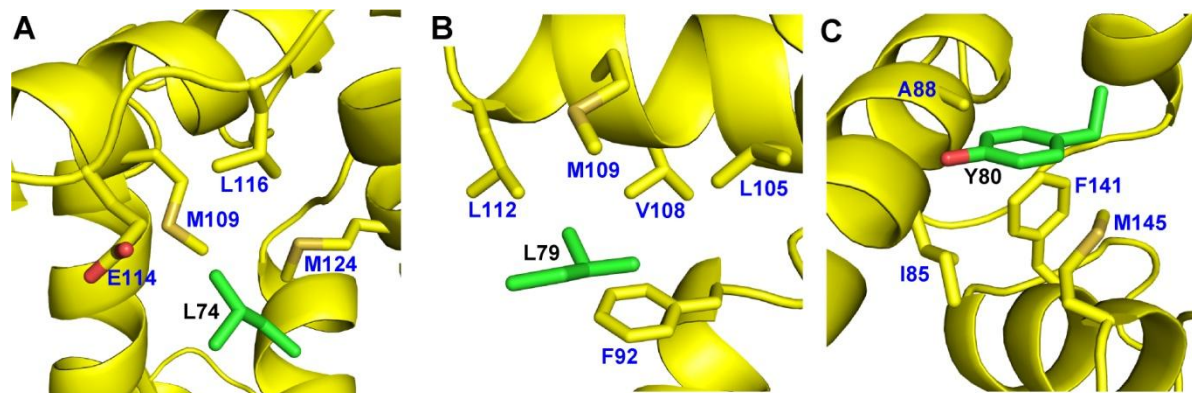


Fig. S4

