Supplemental Data

Structure and Site-Specific Recognition of Histone H3 by the PHD Finger of Human Autoimmune Regulator

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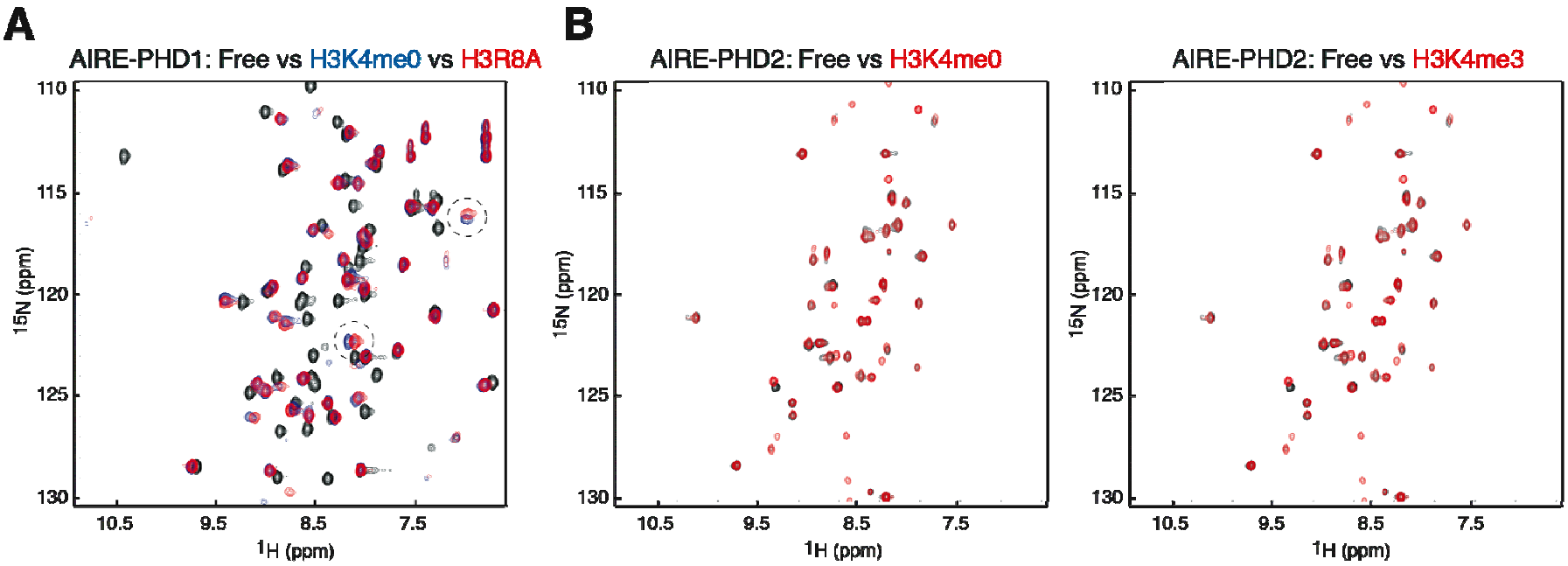

Figure S1. NMR Analysis of Histone H3 Binding by the Two AIRE PHD Fingers

(A) Comparison of ^{1}H-^{15}N HSQC spectra of AIRE-PHD1 (0.5 mM) between its free form (black) and that in presence of a wild-type H3 peptide (residue 1-11 plus Cys, blue) or a H3R8A mutant peptide (residues 1-11 plus Cys, red). The molar ratio of protein to peptide was kept at 1:5 in the experiments.

(B) Comparison of ^{1}H-^{15}N HSQC spectra of AIRE-PHD2 (0.5 mM) between its free form (black, left and right) and that in presence of a H3 peptide (residue 1-11 plus Cys, red)(left) and H3K4me3 residues 1-11 plus Cys, red). The molar ratio of protein to peptide was kept at 1:5 in the experiments.

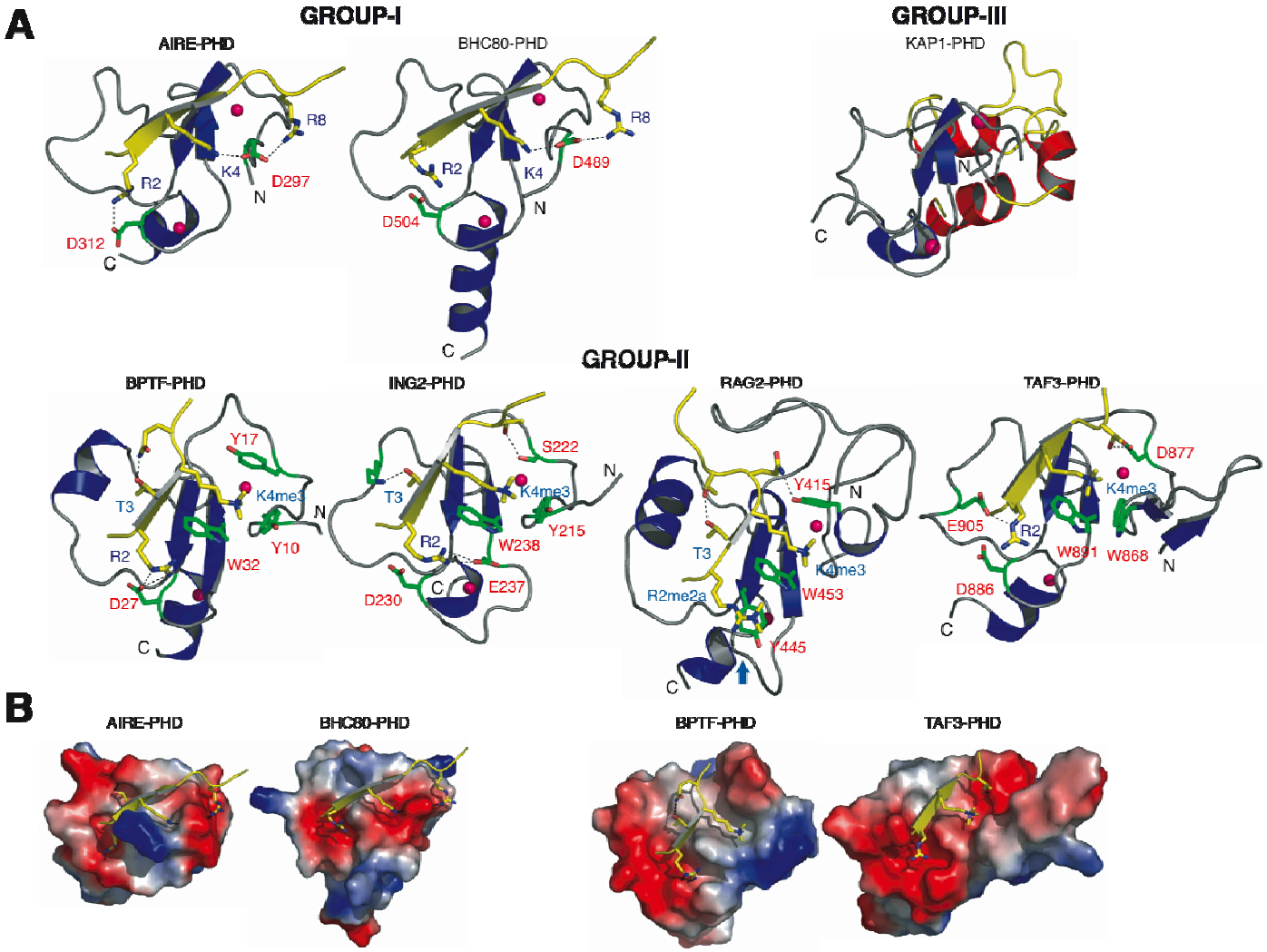

Figure S2. Structural Comparison between AIRE-PHD1 and Other PHD Fingers

(A) All protein modules (green) superimposed on AIRE-PHD finger are viewed showing the histone H3 peptide (yellow) binding site. For the H3Kme0 peptide R2, K4 and R8 are involved in ion-pair interactions, while for the H3K4me3 recognition, the peptide has limited interactions beyond H3T6 with K4me3 and R2 being peptide anchoring residues. The effects of modifications at sites close to H3R8 such as K9 and S10 can be sensed in the Kme0 case. The symbol of ‚' in RAG2 indicates the loss of R2 interacting D/E residue that show a two-fold enhancement of peptide binding on H3R2 to H3R2me2 modification reasoned due to the presence of Tyr 445. The corresponding peptide-binding site in KAP1 is empty and the bromodomain interacting surface is shown behind in the current view. The corresponding secondary structural elements are colored as in Figure 1B and 1C for convenience.

(B) Comparison of electrostatic potential surface (± 70 kT/e isocontour) between AIREPHD1 and BHC80-PHD (left, H3K4me0 case), TAF3-PHD and BPTF-PHD (right, H3K4me3 case).