

Supporting Information for: Conformation and Domain Movement Analysis of Human Matrix Metalloproteinase-2: role of associated Zn²⁺ and Ca²⁺ ions.

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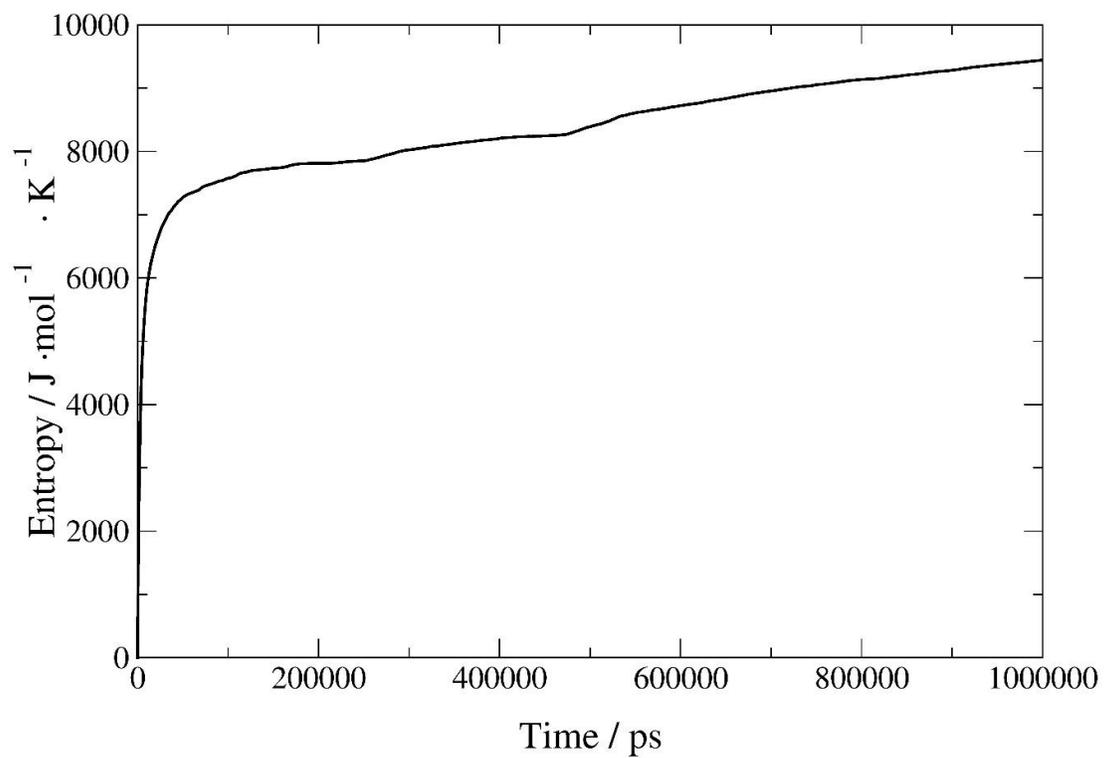


Figure S1. Configurational entropy of MMP-2 (calculated from the C α -trace, Zn²⁺ and Ca²⁺ coordinates) as a function of time, demonstrating the 200000 ps necessary for system equilibration.

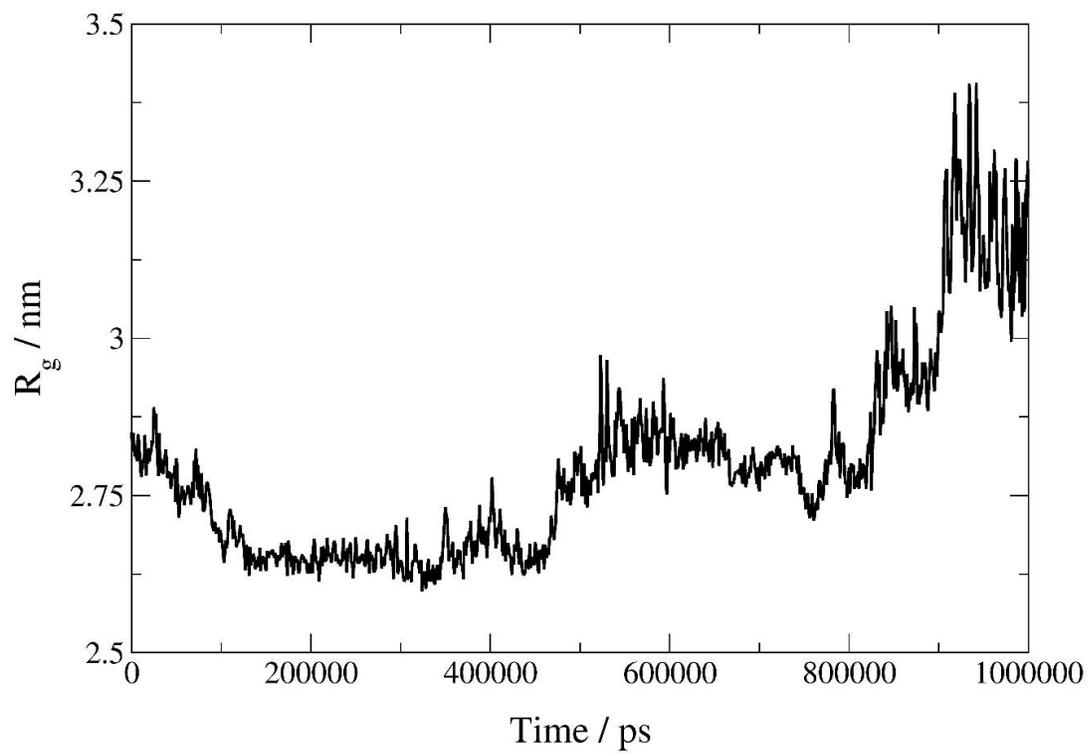


Figure S2. The radius of gyration (R_g) as a function of time.

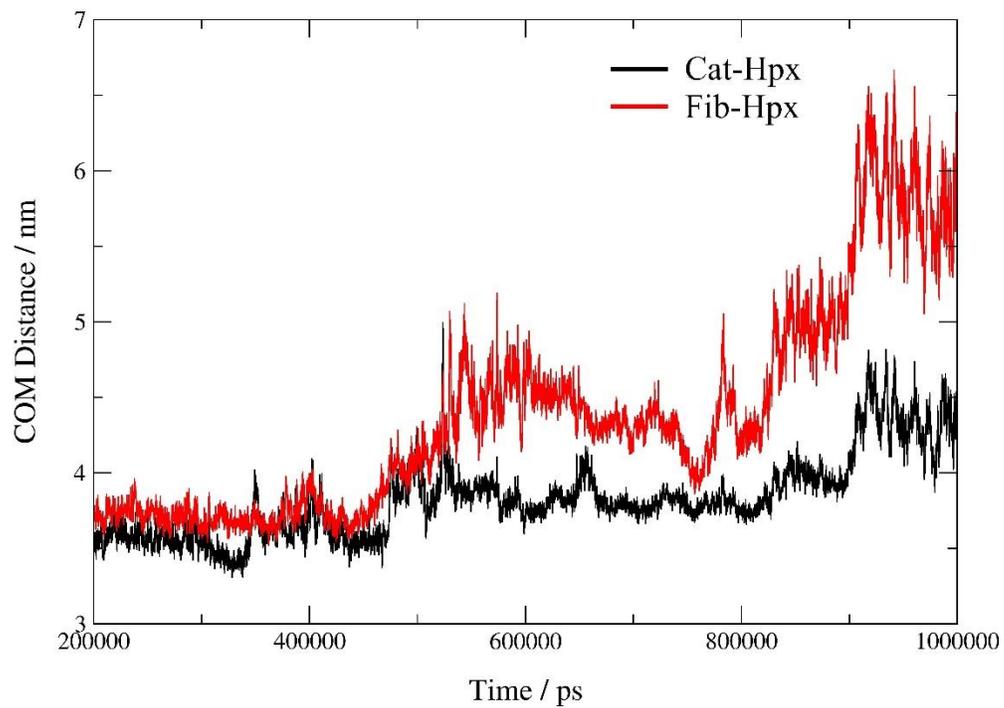


Figure S3. The Center of mass (COM) distance as a function of time between the Cat and Hpx (black) and Fib and Hpx (red) domains, respectively.

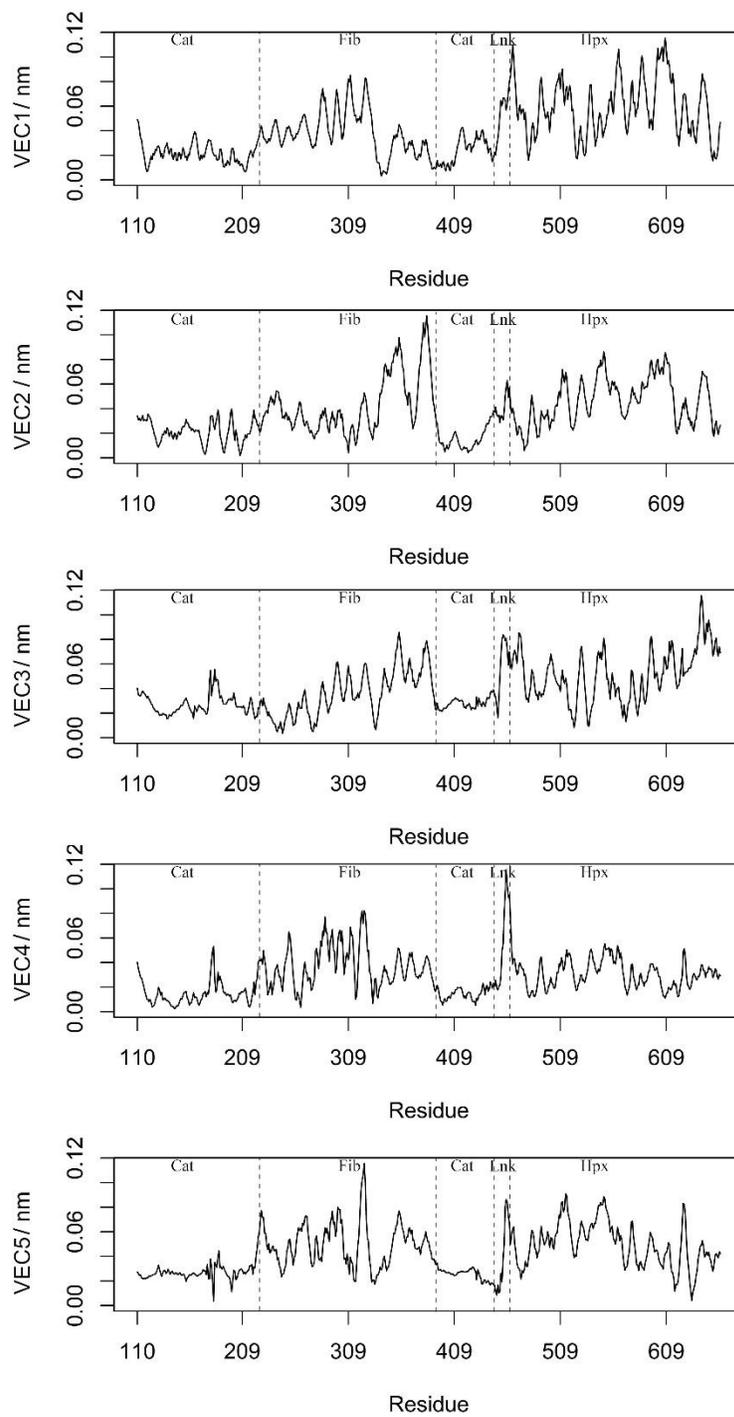


Figure S4. α -trace RMSF plots of the top 5 eigenvectors.