

# Supporting Information for: Conformation and Domain Movement Analysis of Human Matrix Metalloproteinase-2: role of associated Zn<sup>2+</sup> and Ca<sup>2+</sup> ions.

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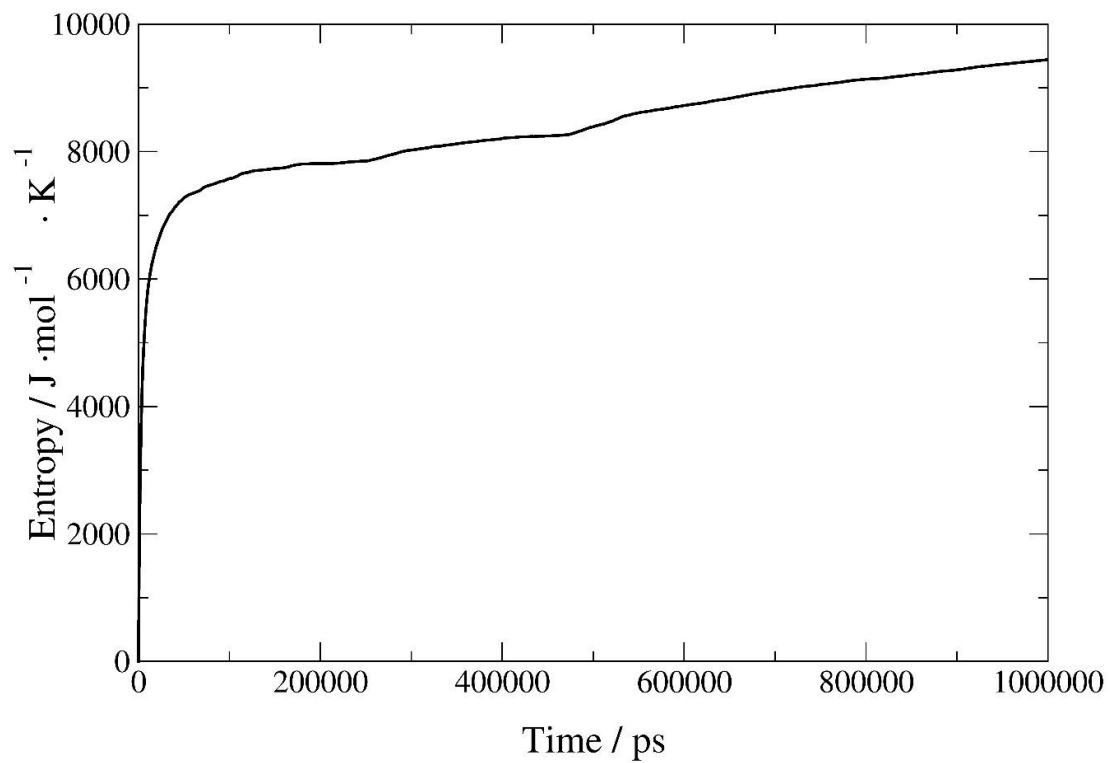
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**Figure S1.** Configurational entropy of MMP-2 (calculated from the C $\alpha$ -trace, Zn<sup>2+</sup> and Ca<sup>2+</sup> coordinates) as a function of time, demonstrating the 200000 ps necessary for system equilibration.

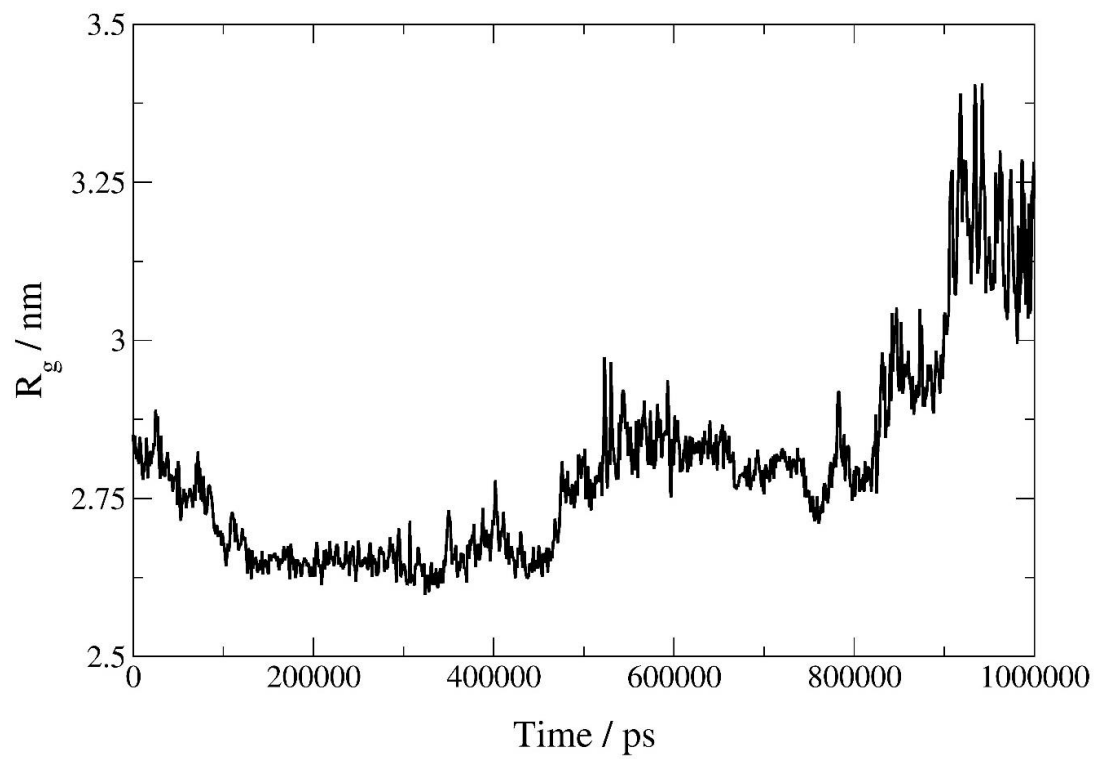
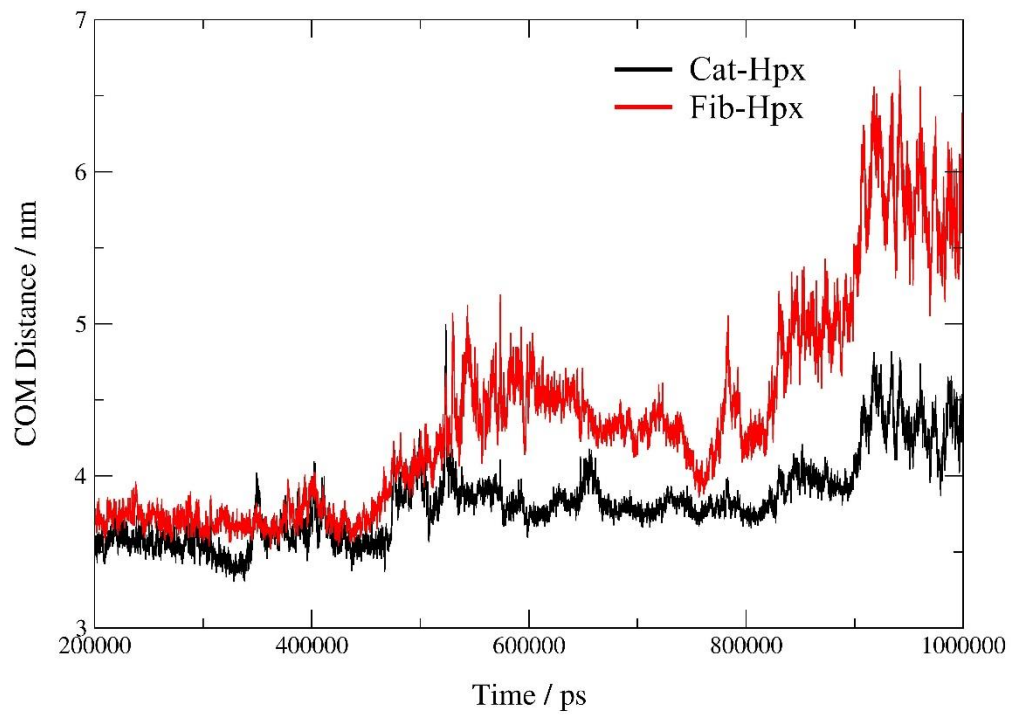
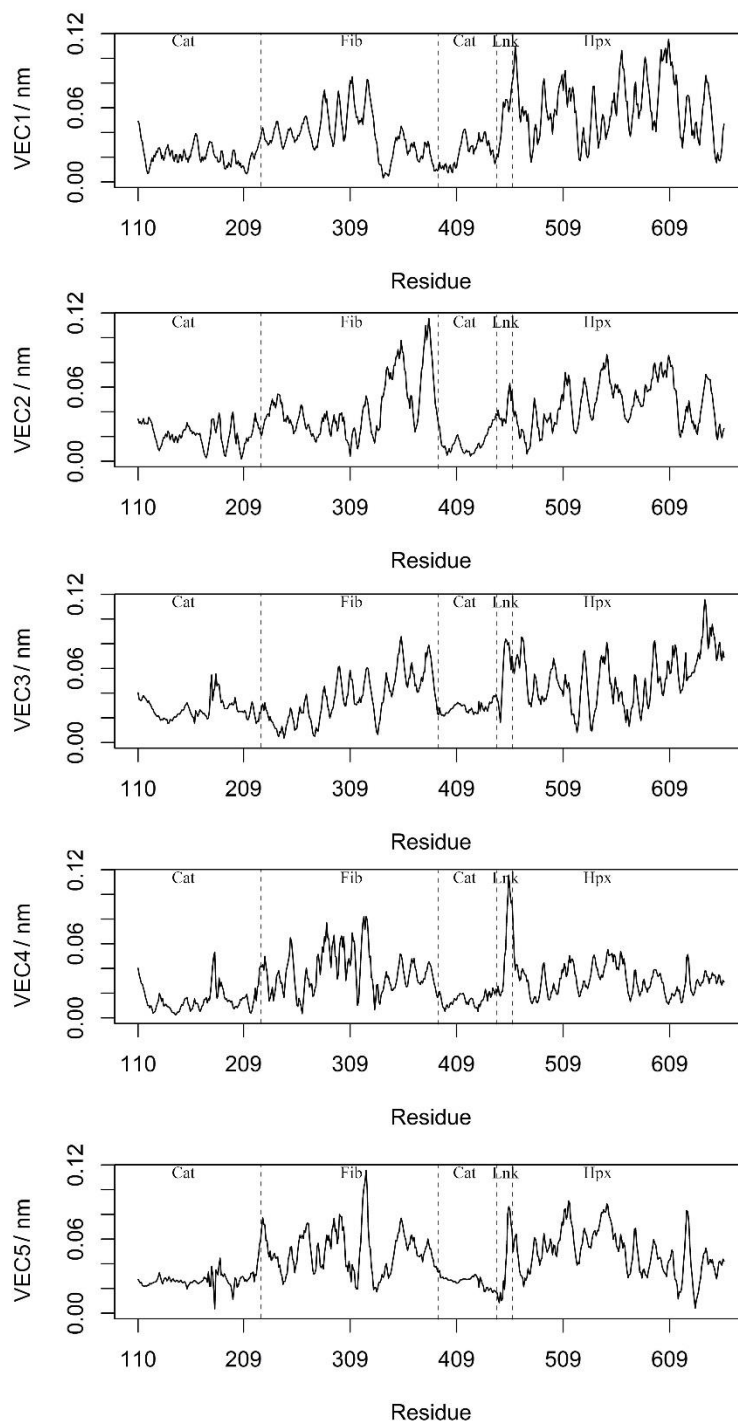


Figure S2. The radius of gyration ( $R_g$ ) as a function of time.



**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.**  $\alpha$ -trace RMSF plots of the top 5 eigenvectors.