

Supplementary Information

Computational Study on Selective PDE9 inhibitors on PDE9-Mg/Mg, PDE9-Zn/Mg, and PDE9-Zn/Zn systems

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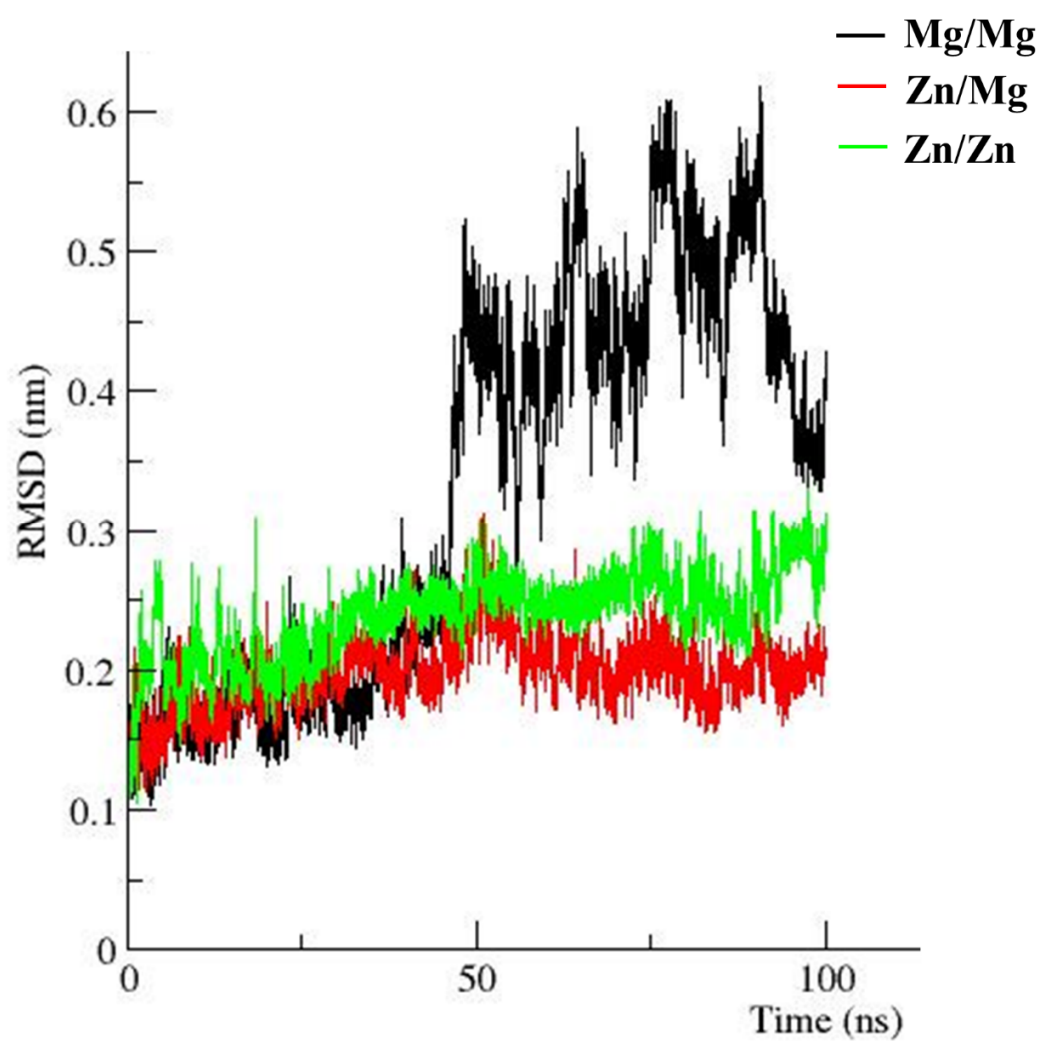


Figure
Figure S1. C-alpha RMSD plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-1R.

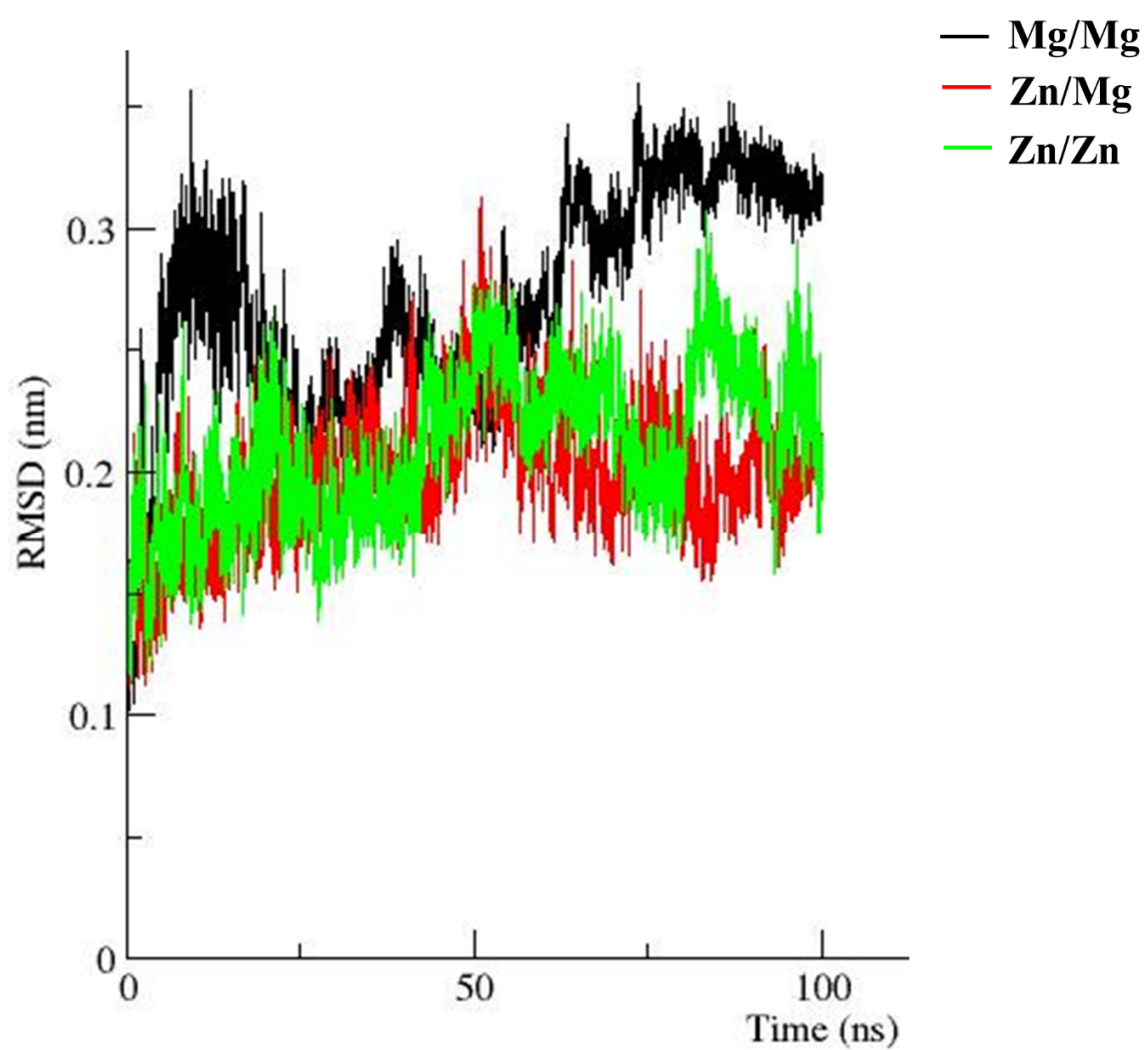


Figure S2. C-alpha RMSD plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-1S.

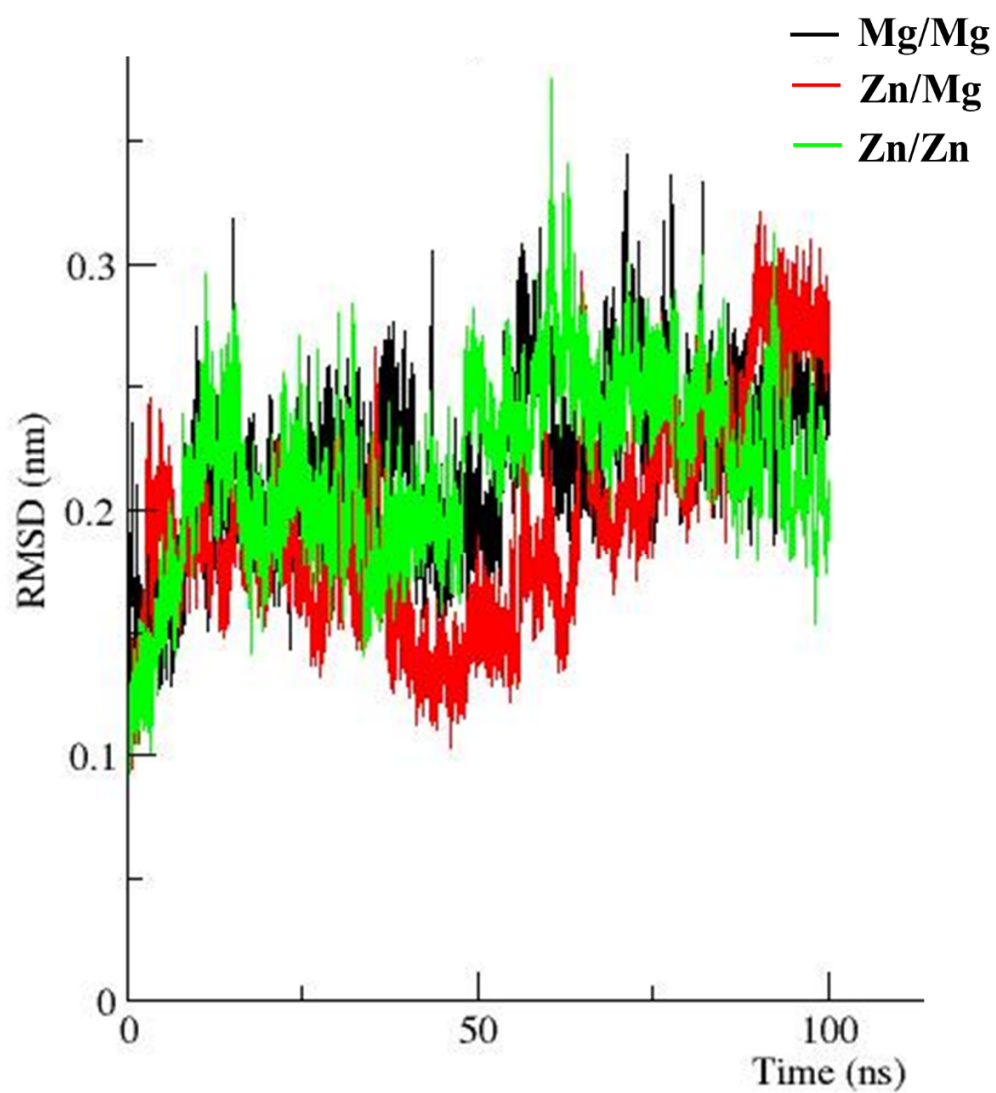


Figure S3.

Figure S3. C-alpha RMSD plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-2R.

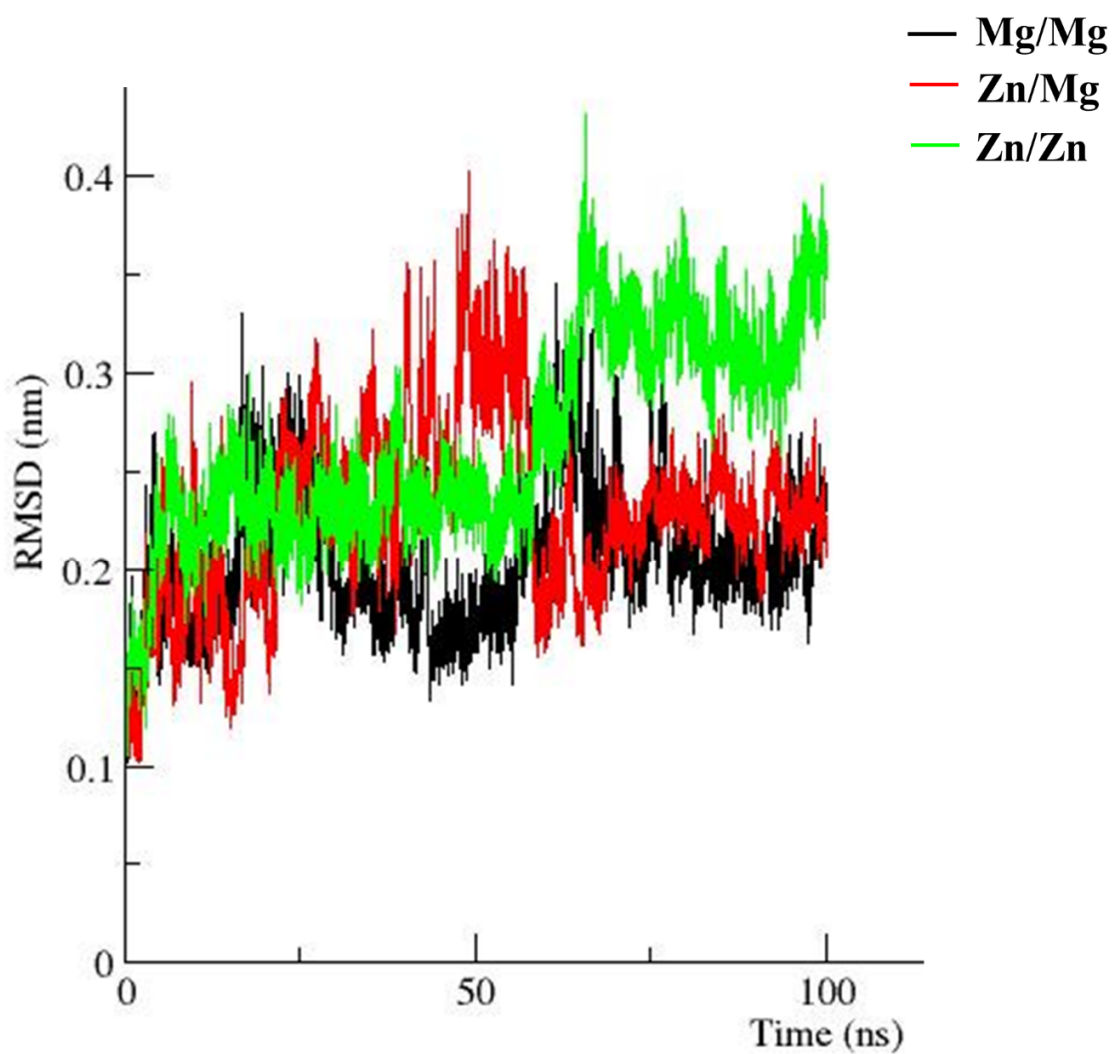


Figure S4. C-alpha RMSD plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-2S.

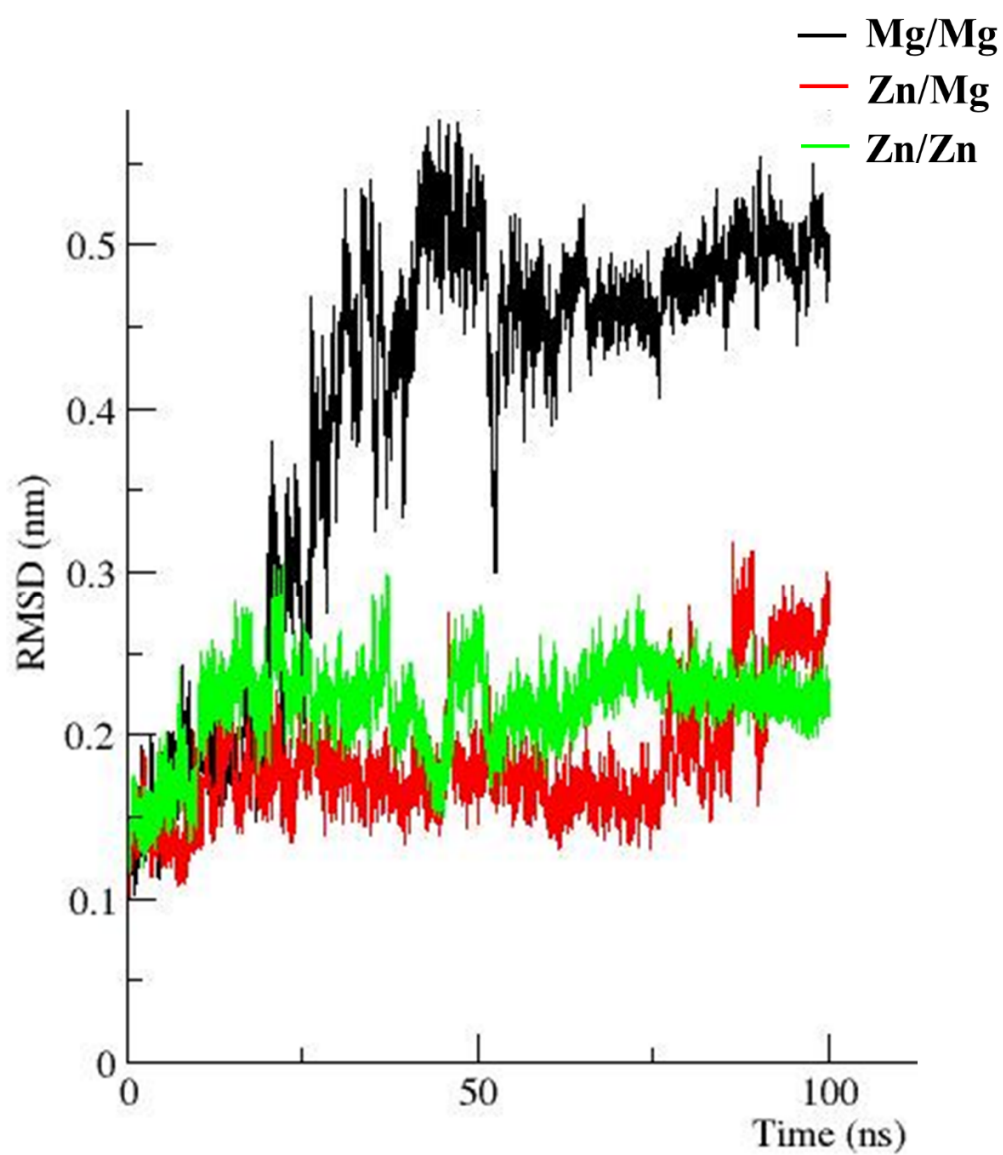


Figure S5.

Figure S5. C-alpha RMSD plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-3R.

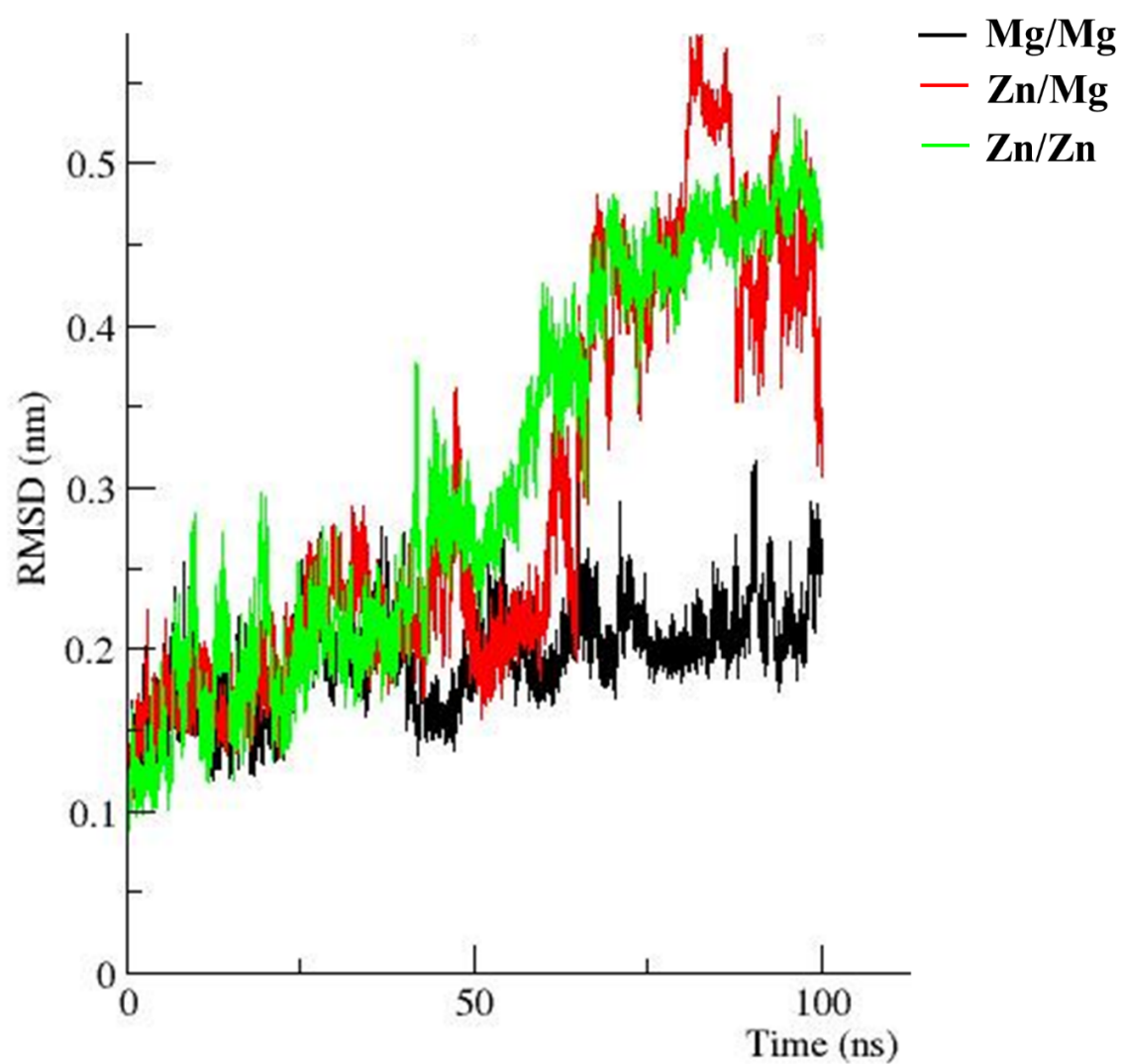


Figure S6. C-alpha RMSD plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-3S.

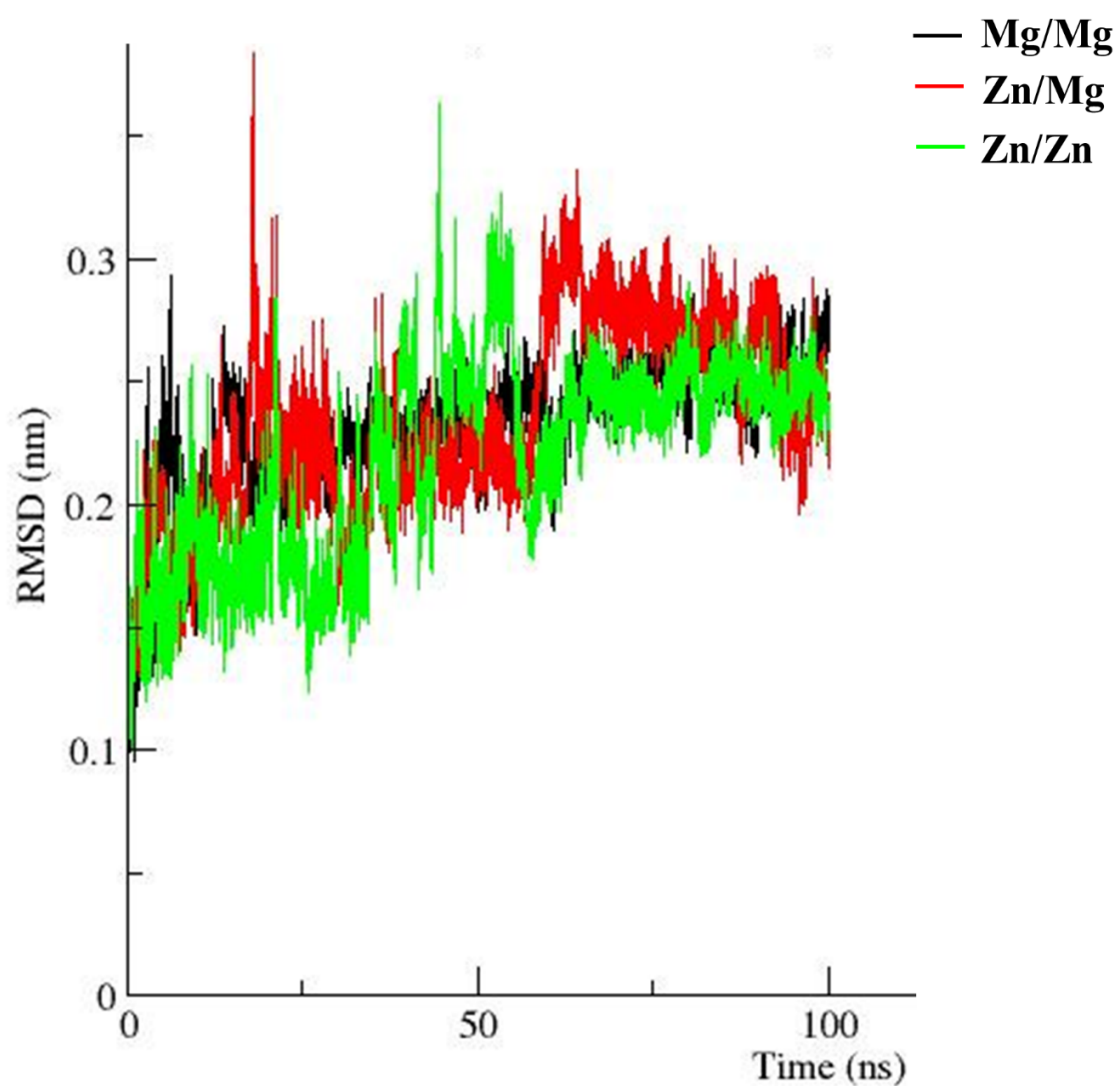


Figure S7. C-alpha RMSD plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-4.

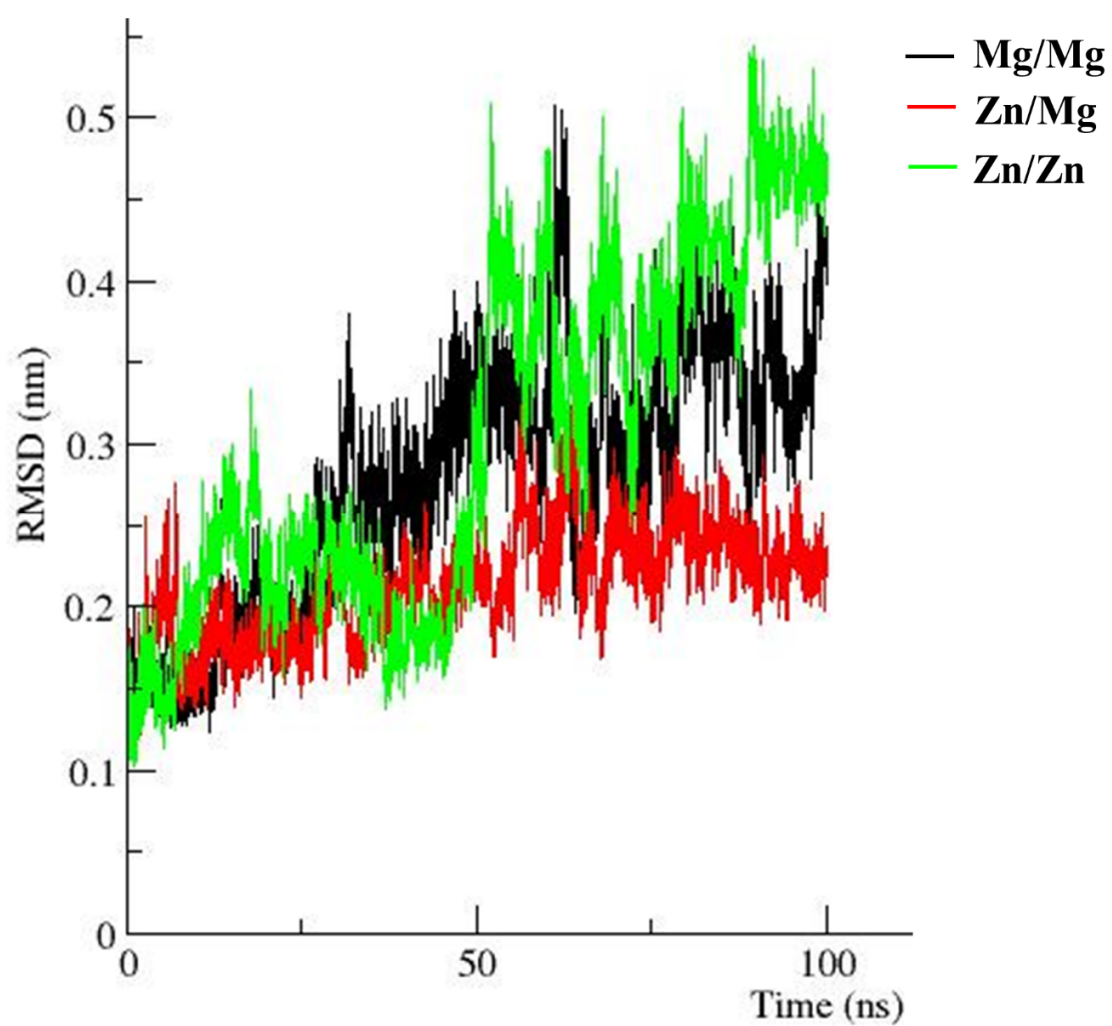


Figure S8. C-alpha RMSD plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-5.

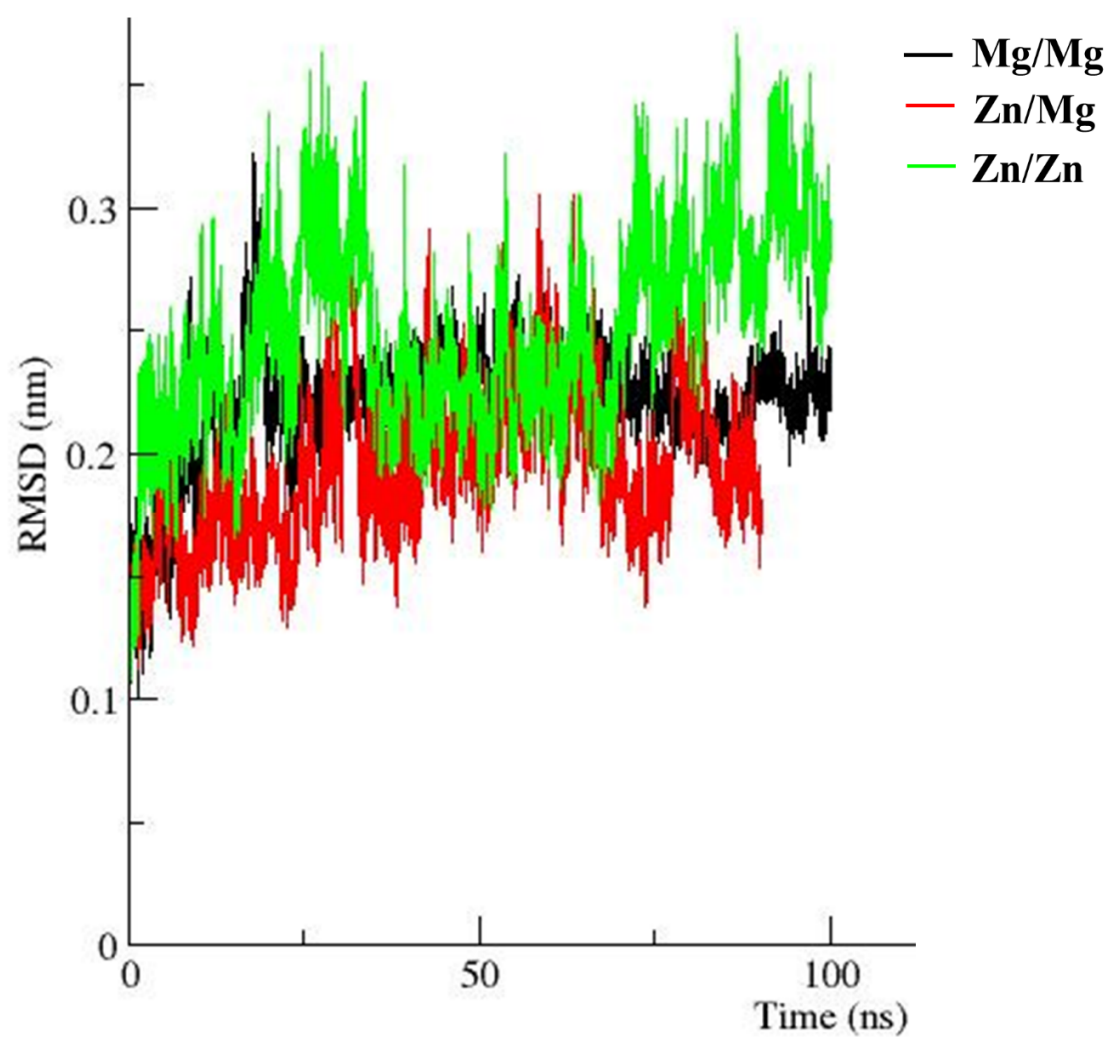


Figure S9. C-alpha RMSD plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

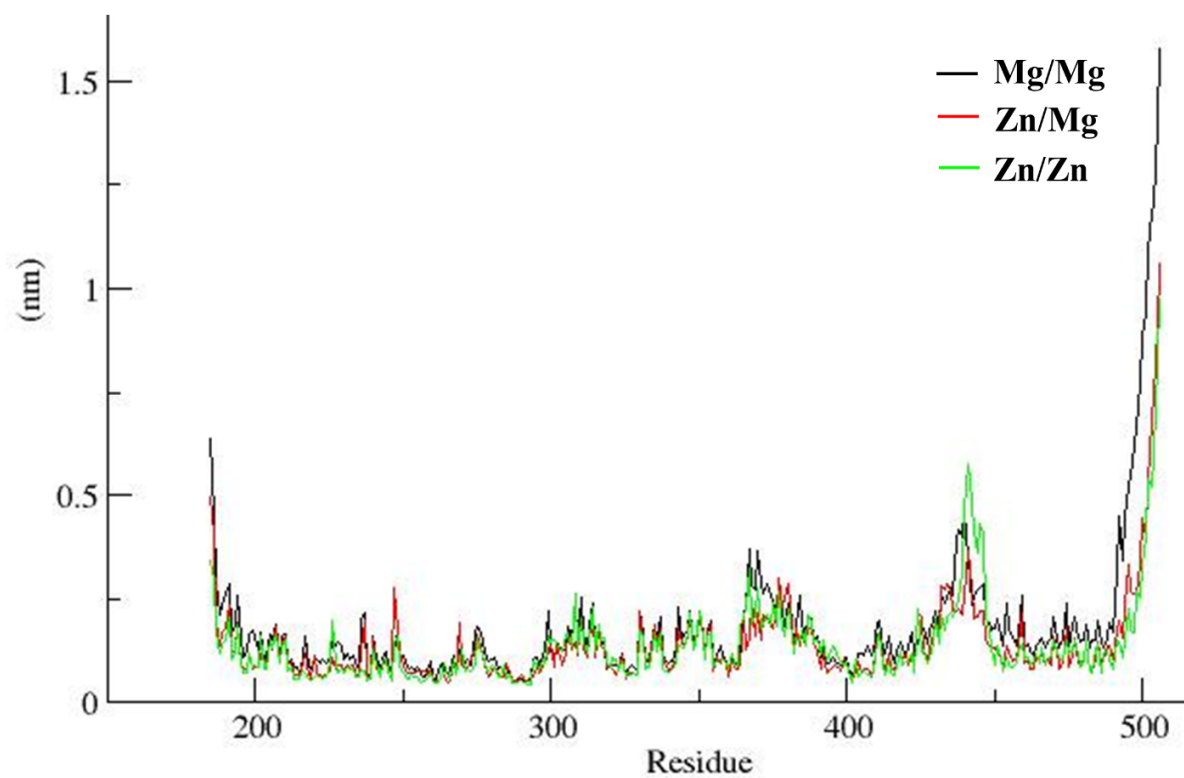


Figure S10. Protein RMSF plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

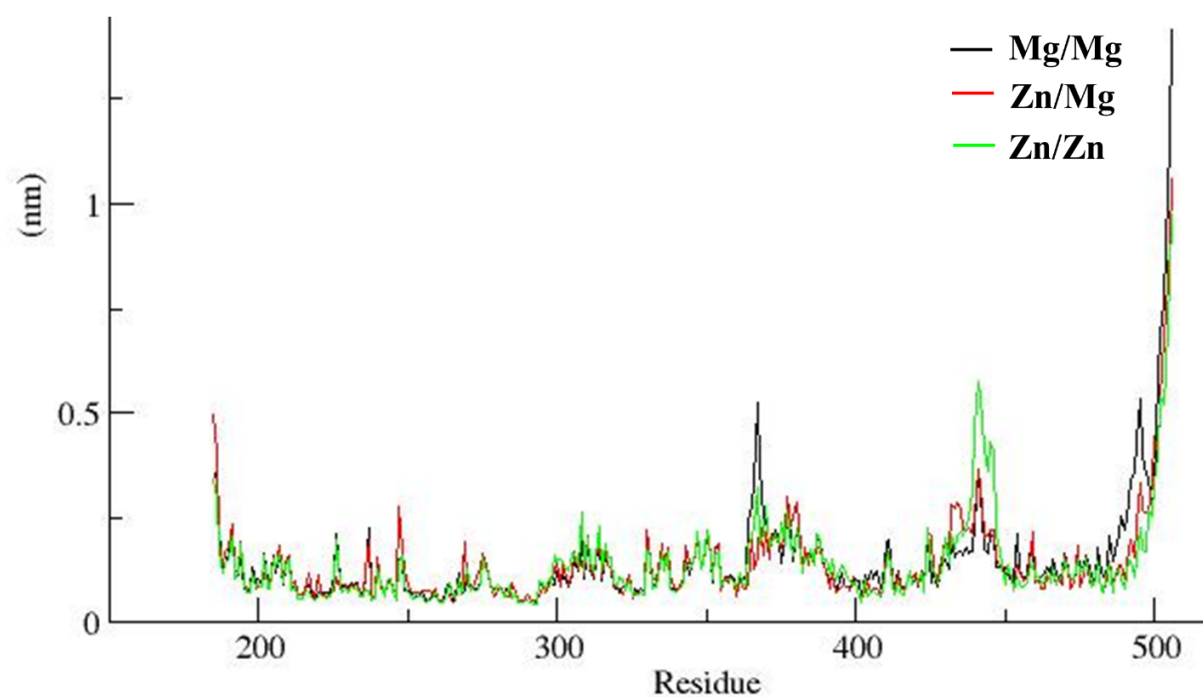


Figure S11. Protein RMSF plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

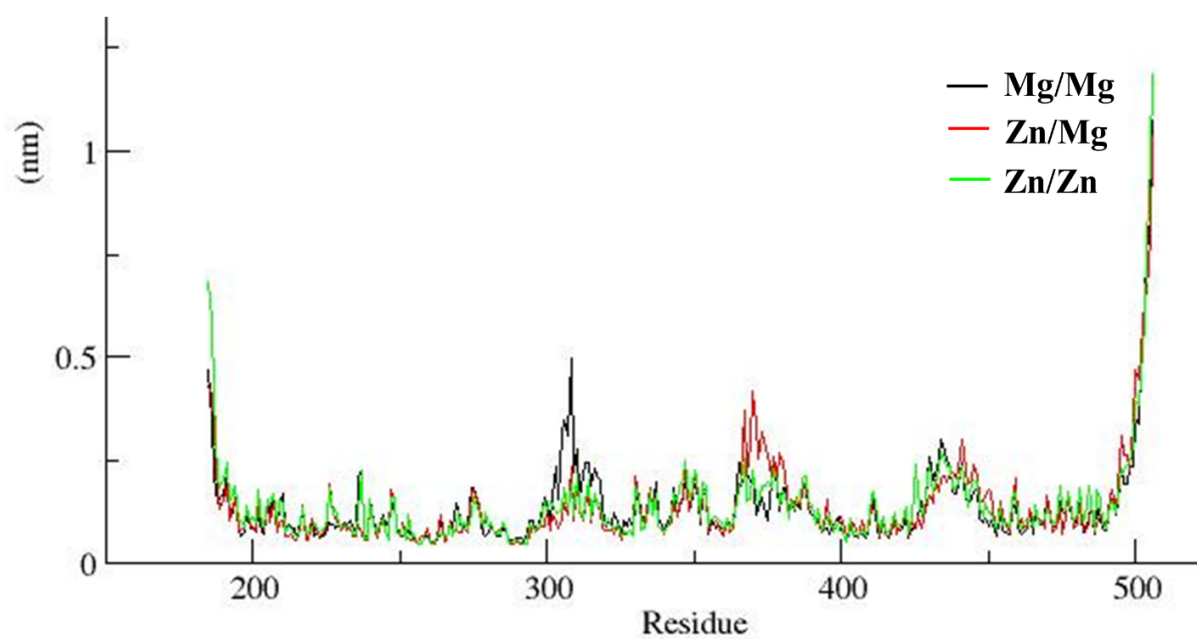


Figure S12. Protein RMSF plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

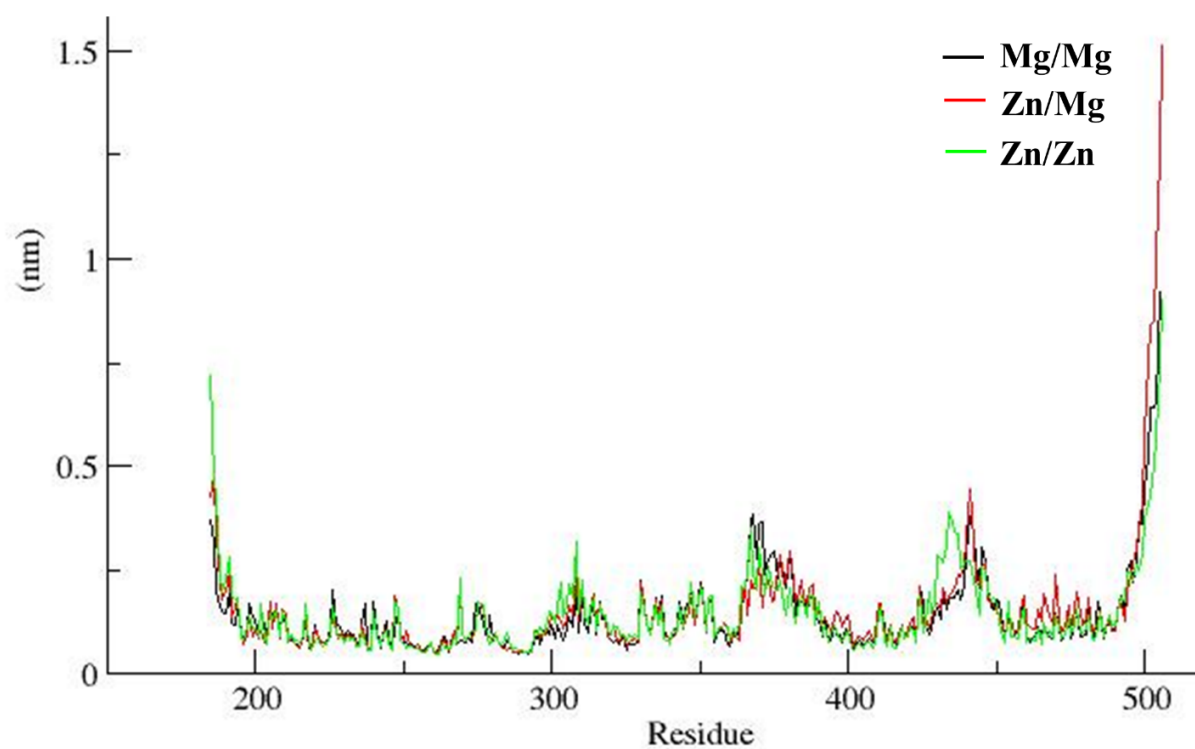


Figure S13. Protein RMSF plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

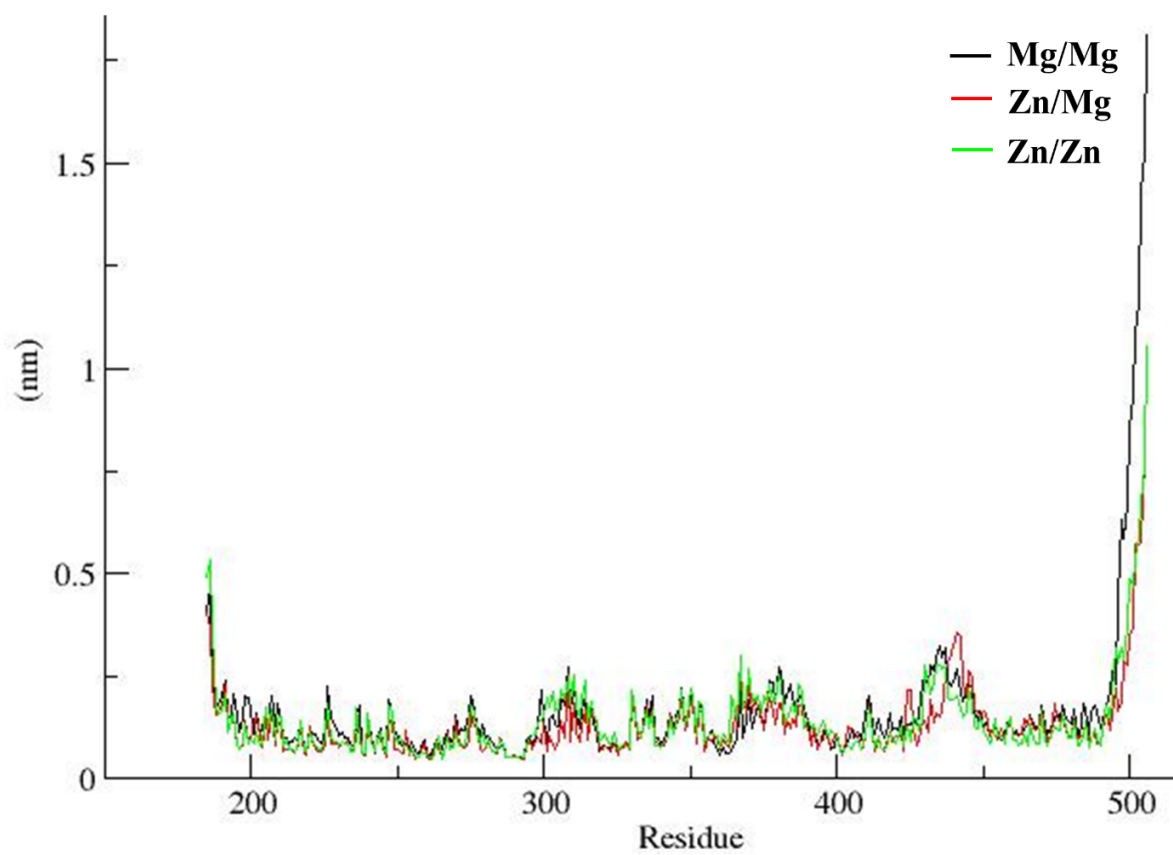


Figure S14. Protein RMSF plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

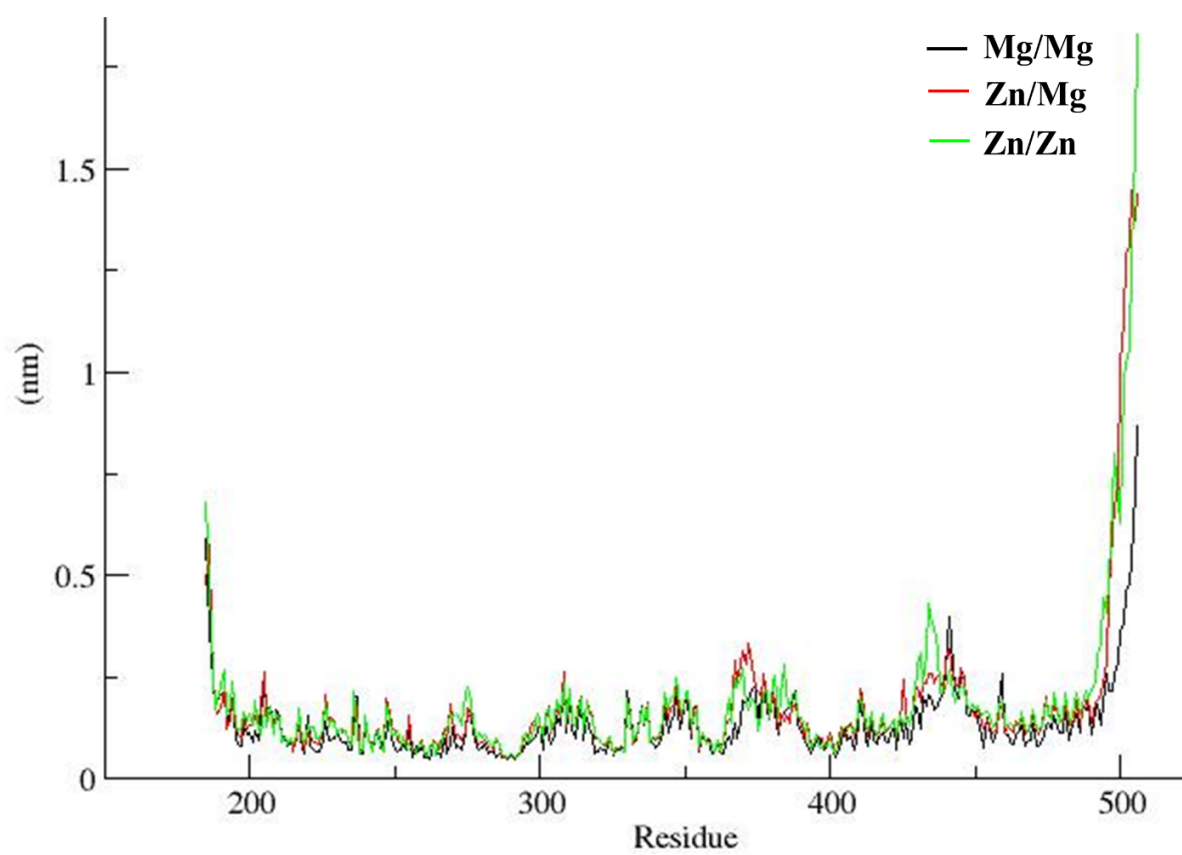


Figure S15. Protein RMSF plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

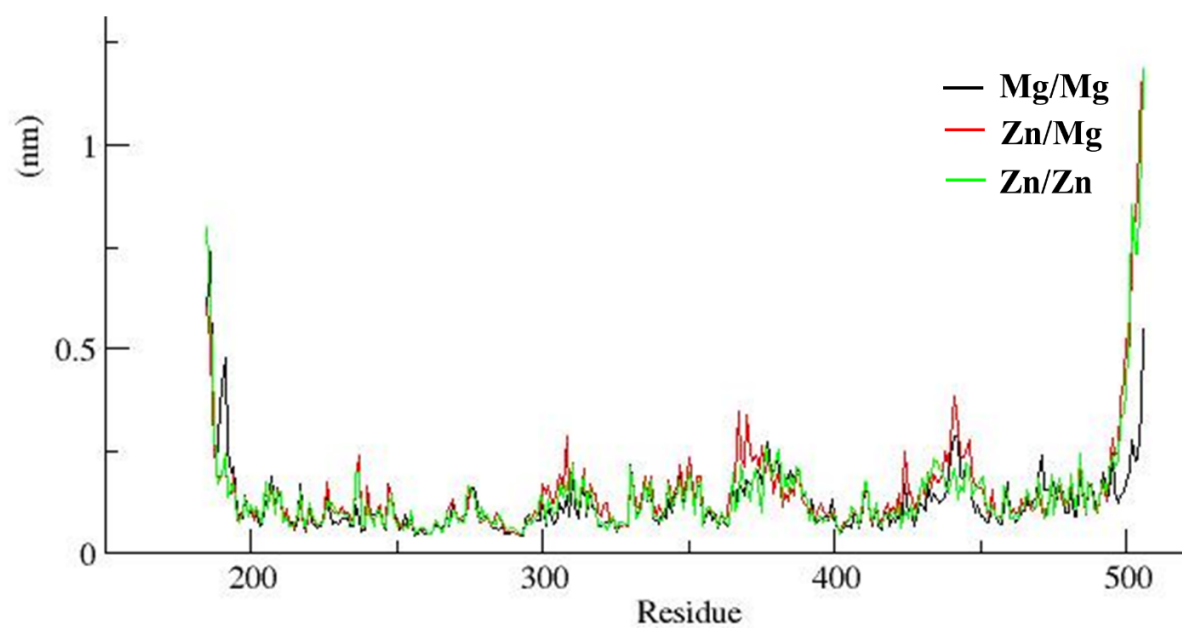


Figure S16. Protein RMSF plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

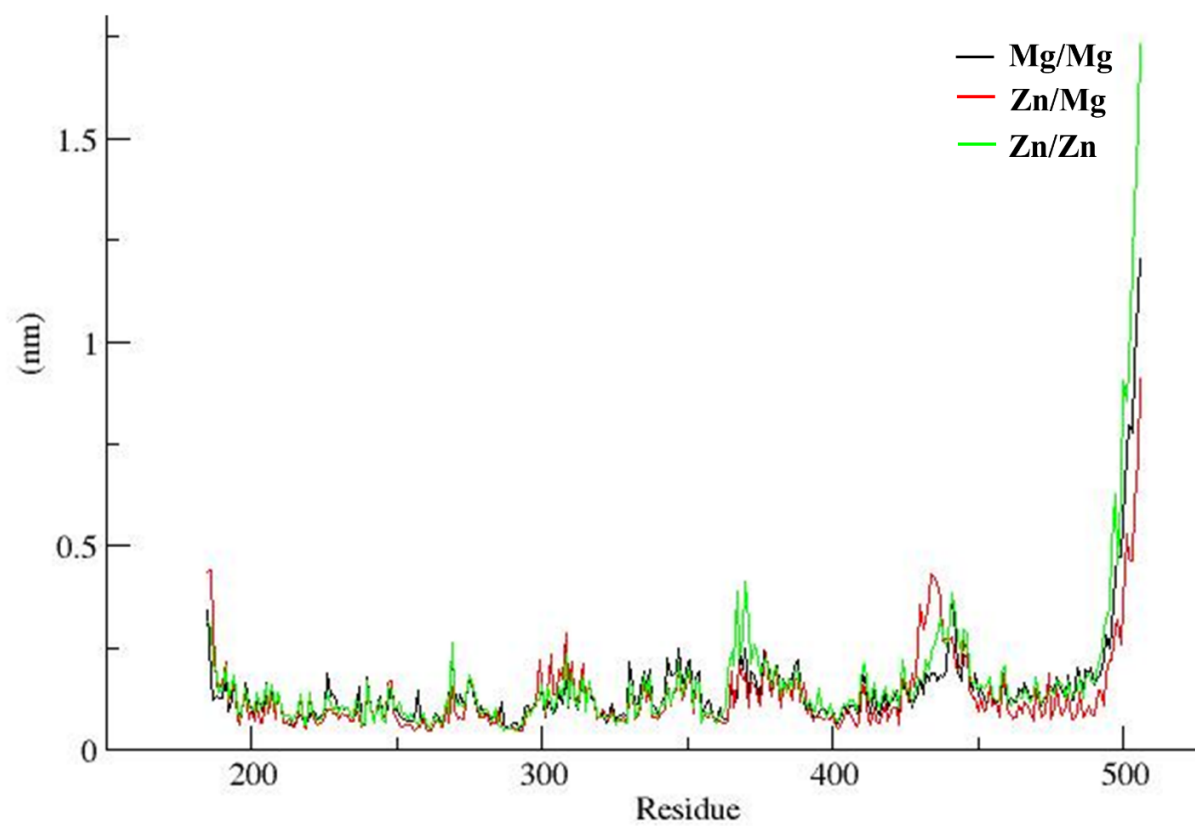


Figure S17. Protein RMSF plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

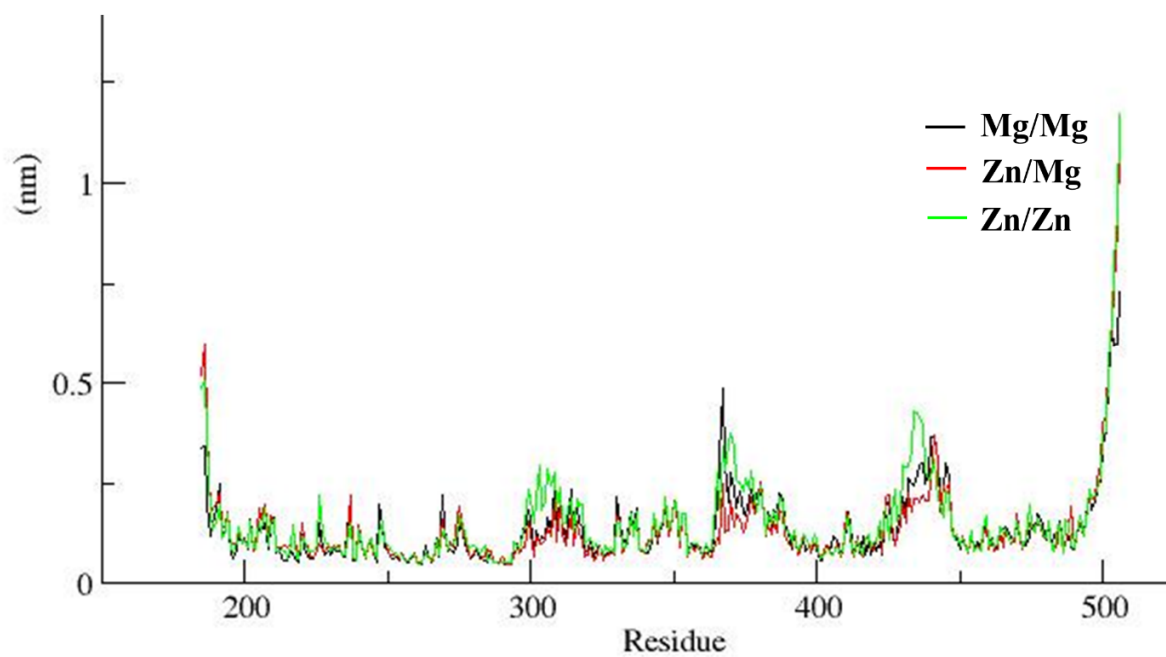


Figure S18. Protein RMSF plot of PDE-9 (Mg/Mg, Zn/Mg, Zn/Zn) in complexed with compound-6.

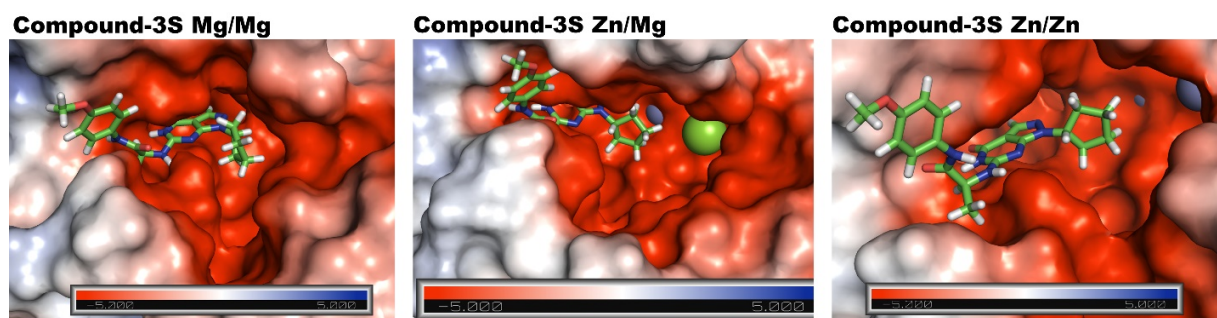
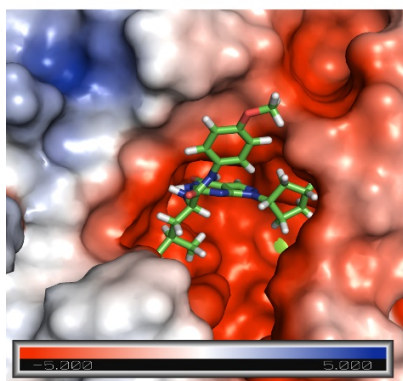
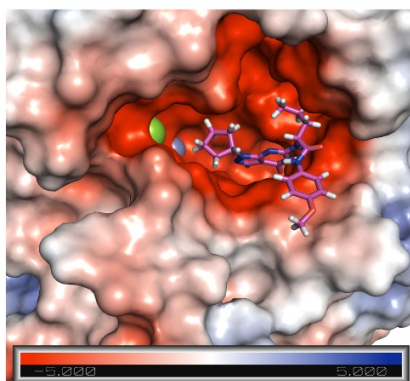


Figure S19. Electrostatic interaction map using APBS calculation for the Compound-3S in all three different metal systems (Mg/Mg, Zn/Mg, Zn/Zn).

Compound-6 Mg/Mg



Compound-6 Zn/Mg



Compound-6 Zn/Zn

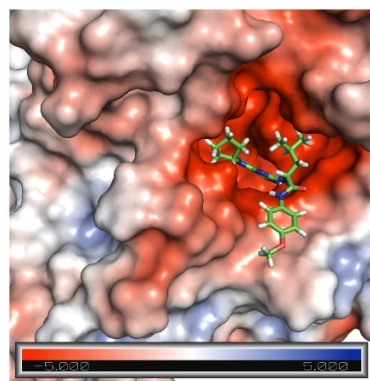


Figure S20. Electrostatic interaction map using APBS calculation for the Compound-6 in all three different metal systems (Mg/Mg, Zn/Mg, Zn/Zn).