Electronic Supplementary Material (ESI) for RSC Advances.

Structural exploration of Acid Sphingomyelinase at different physiological pH through molecular dynamics and docking studies.

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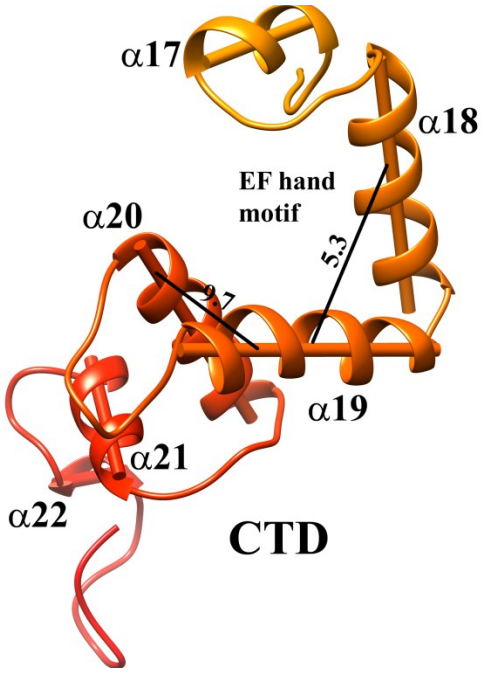
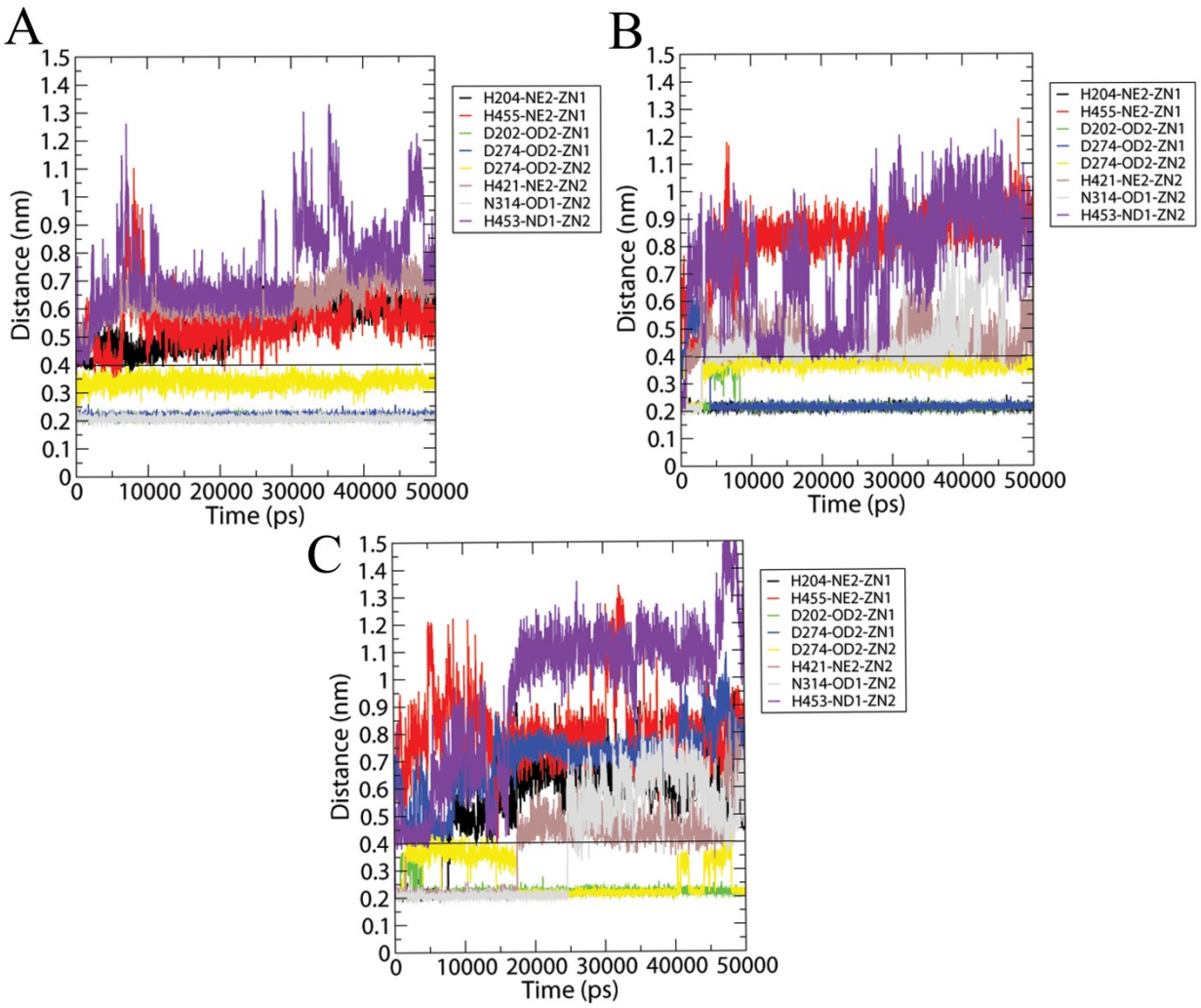
Supplementary Information

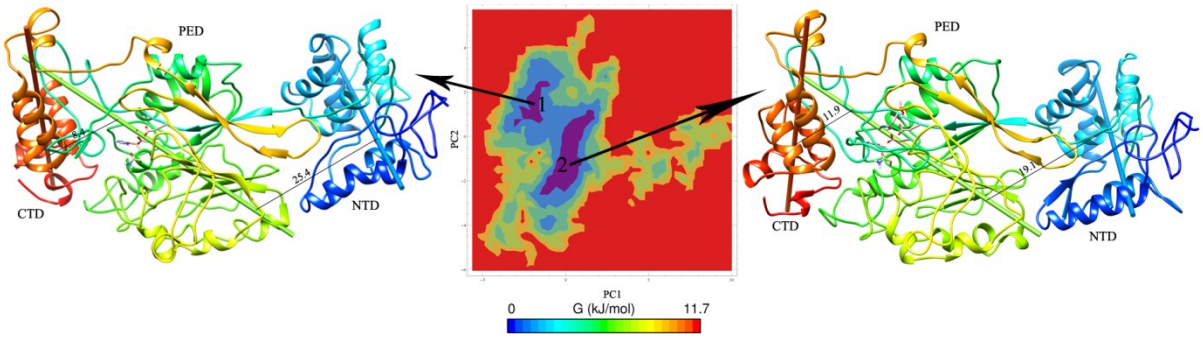
Supplementary Fig. 1: Three dimensional representation of C-terminal domain of ASM contains six helices (α17-α22). The α18 and α19 forms EF hand like motif and is placed equatorial to each other with distance and angle of 5.3 Å and 72.0° respectively. Helices α19-α20 are placed bisectionally (Angle: 48.3°) with a distance of 9.7 Å.



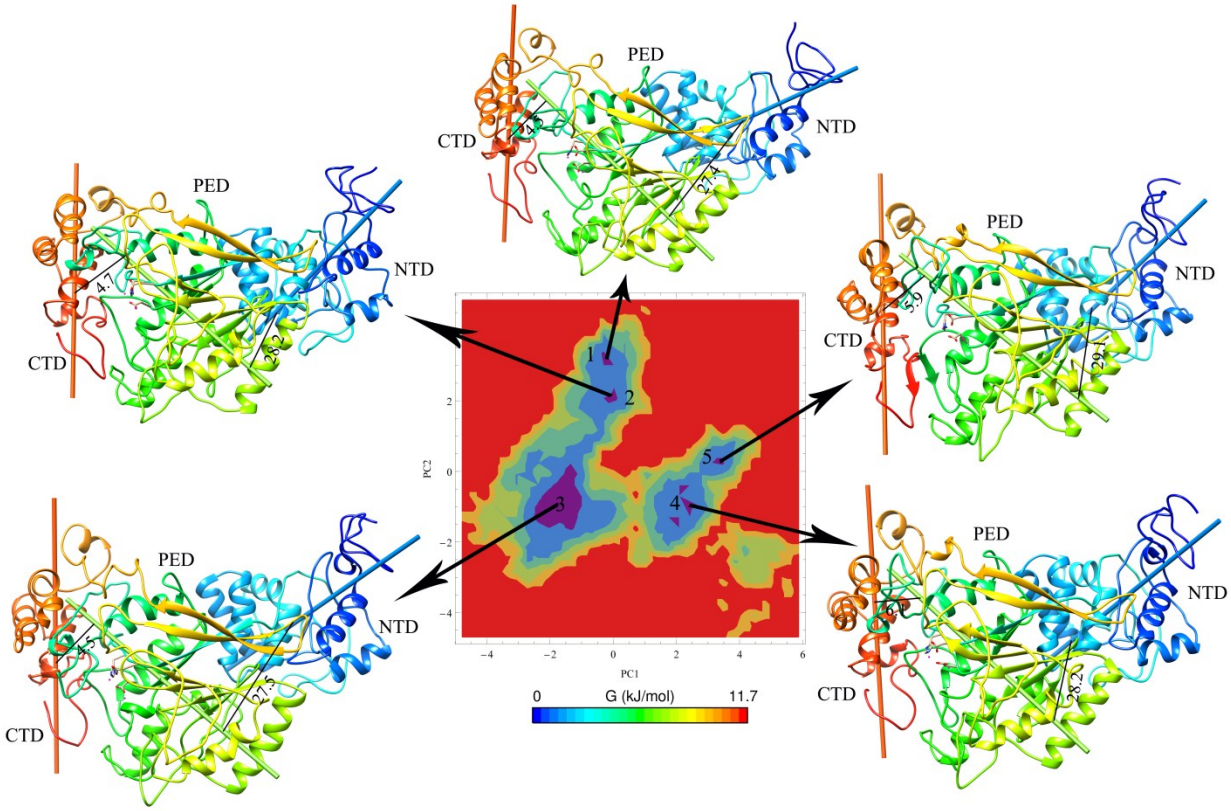
Supplementary Fig. 2: The metal co-ordination interactions throughout the simulation period. The coordination interaction formed between the Zn1 and Zn2 with the residues of A) neutral ASM B) pH3.0 ASM C) pH 5.0 ASM.



Supplementary Fig. 3: The free energy landscape of neutral ASM structure has shown the function of first two principal components whose cosine content is less than 2.0 using projection eigenvector of PCA. There are two representative structures identified and extracted from the most populated free energy minimum clusters and displayed with the details of domain-domain distance acquired based on the domain axis.



Supplementary Fig. 4: The free energy landscape of pH3.0 ASM structure derived based on the function of first two principal component whose cosine content less than 2.0 using projection eigenvector of PCA. There are five representative structures were identified and extracted from the most populated free energy minimum clusters and displayed with the details of domain-domain distance acquired based on the domain axis.



Supplementary Fig. 5: Helical orientation of CTD and loop region of ASM structures at A) neutral B) pH 3.0 C) pH 5.0.