A Nudged Elastic Band Study on the N-terminal Domain Conformational Pathways of Annexin A1 from a Buried State to an Exposed State

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Table S1. Unscaled Energies (Kcal/mol) from the NEB (IMP 1, IMP 2, IMP 3) Simulations and MMGBSA Analysis, both with (MMGBSA-NM) and without (MMGBSA) Normal Mode Analysis.

Structure	IMP 1	IMP 2	IMP 3	MMGBSA	MMGBSA-NM
1	-11515.2	-11520.3	-11522.2	-5861.5	-9655.8
2	-11431.8	-11492.3	-11484.7		
3	-11400.0	-11473.1	-11436.7		
4	-11364.5	-11433.5	-11432.3	-5781.5	-9582.8
5	-11379.6	-11440.2	-11421.3		
6	-11351.7	-11436.6	-11398.3		
7	-11308.0	-11441.2	-11418.9	-5787.7	-9604.6
8	-11322.7	-11409.5	-11384.8		
9	-11305.8	-11383.8	-11286.7		
10	-11321.2	-11375.8	-11263.5	-5756.9	-9567.7
11	-11280.8	-11313.1	-11260.9		
12	-11212.4	-11338.5	-11263.5		
13	-11204.4	-11333.6	-11247.7	-5766.8	-9578.2
14	-11199.0	-11285.1	-11248.7		
15	-11199.8	-11285.7	-11301.8		
16	-11215.0	-11349.2	-11258.6	-5758.7	-9571.4
17	-11201.7	-11303.8	-11283.6		
18	-11201.8	-11328.9	-11254.1		
19	-11215.4	-11300.6	-11295.1	-5773.8	-9599.8
20	-11202.4	-11302.9	-11288.0		
21	-11236.7	-11334.8	-11316.0		
22	-11283.0	-11362.0	-11318.6	-5768.7	-9589.0
23	-11337.5	-11413.0	-11421.8		
24	-11350.9	-11443.7	-11538.0		
25	-11409.8	-11479.0	-11488.8	-5794.3	-9618.8
26	-11432.6	-11461.7	-11475.6		
27	-11446.6	-11460.4	-11492.1		
28	-11476.8	-11467.3	-11490.7	-5818.4	-9635.5
29	-11480.2	-11472.8	-11490.8		
30	-11502.7	-11445.2	-11447.7		
31	-11472.2	-11447.0	-11446.2		
32	-11519.9	-11522.2	-11525.8	-5793.4	-9637.8