Table S1
Atomic compositions and properties of different simulation systems

| Simulation system                                      | Number of water molecule | Number of Na⁺ | Number of Cl⁻ | Total number of atoms |
|--------------------------------------------------------|--------------------------|---------------|---------------|-----------------------|
| Apo System                                             |                          |               |               |                       |
| zNOD1-NACHT (336 aa)                                   | 20884                    | 64            | 62            | 66251                 |
| zNOD2-NACHT (324 aa)                                   | 19944                    | 61            | 59            | 63259                 |
| zNOD1-NACHT (336 aa) + ATP (Holo system)               |                          |               |               |                       |
| Complex I                                              | 20862                    | 68            | 62            | 66226                 |
| Complex II                                             | 20859                    | 68            | 62            | 66217                 |
| Complex III                                            | 20883                    | 68            | 62            | 66289                 |
| zNOD2-NACHT (324 aa) + ATP (Holo system)               |                          |               |               |                       |
| Complex I                                              | 19923                    | 65            | 59            | 63237                 |
| Complex II                                             | 19920                    | 65            | 59            | 63228                 |
| Complex III                                            | 19956                    | 65            | 59            | 63336                 |