Data Article

Molecular dynamics simulation dataset of a microtubule ring in electric field

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A R T I C L E   I N F O

A B S T R A C T

We present molecular dynamics (MD) trajectories of a single ring of B-lattice microtubule ring consisting of 13 tubulin heterodimers. The data contain trajectories of this molecular system ran under various conditions (two temperature values, three ionic strength values, three values of electric field (including no field), and four electric field orientations). Our data enable us to analyze the effects of the electric field on microtubule under a variety of conditions. This data set was a basis of our *in silico* discovery, which demonstrates that the electric field can open microtubule lattice [1].

Specifications Table

Subject	Chemistry, Biology
Specific subject area	Computational Molecular biophysics
Type of data	Molecular Dynamics (MD) simulations
How data were acquired	Classical MD simulation in explicit solvent
Data format	Amber trajectory (.mdcrd)

Parameters for data collection	NVT ensemble
Description of data collection	Data were obtained from molecular dynamics simulations ran on 1GPU PC with AMBER software.
Data source location	Institution: Institute of Photonics and Electronics of the Czech Academy of Sciences City/Town/Region: Prague Country: Czechia
Data accessibility	Data is stored in a publicly accessible link Direct URL to data: http://hdl.handle.net/20.500.12618/0000-e7879093-4d84-47e9-bdce-13c87bef96e6
Related research article	Authors: Jiří Průša, Ahmed T. Ayoub, Djamel E. Chafai, Daniel Havelka, Michal Cifra Title: Electro-opening of a microtubule lattice *in silico* Journal: *Computational and Structural Biotechnology Journal* Volume 19, 2021, Pages 1488–1496, DOI 10.1016/j.csbj.2021.02.007

Value of the Data

- Data enable understanding of the influence of nano-second scale electric field on the structure of microtubule
- Computational chemists, physical chemists, chemical biologists, bioelectromagnetic engineers and biophysicists can benefit from the data
- The data can be further used for a further analysis of the structural and dynamics effects of electric field on microtubule structure at the atomic level

1. Data Description

The raw data (355 GB) are available in archive files under this permanent link http://hdl.handle.net/20.500.12618/0000-e7879093-4d84-47e9-bdce-13c87bef96e6

The archives, once unpacked, contains four folders:

1. 100 MV - contains trajectories for 100 MV/m electric field condition separated to folders according to the direction of field in x(x),y(y),-x(xrev) and -y(yrev) directions and also the trajectories with lower (lion) and higher (hion) ionic concentration respectively same as trajectories for lower temperature (low_temp). Each folder contains three trajectories.
2. 50 MV - contains trajectories for 50 MV/m electric field condition. There are four subfolders for x(x),y(y),-x(xrev) and -y(yrev) directions of the field each holding one trajectory file with exceptions of xrev for which there are three trajectories and x folder where the trajectory is separated into two files (field_x011_part1.mdcrd and field_x011_part2.mdcrd, respectively).
3. NO_FIELD contains trajectory without the field and is separated into three Afiles (nf_part1.mdcrd, nf_part2.mdcrd and nf_part3.mdcrd).
4. TOPO - contains appropriate topologies. top.prmtop is a standard topology for our system. The system with lower and higher ion concentrations corresponds to different topologies lion.parm7 and mm.parm7, respectively

2. Experimental Design, Materials and Methods

2.1. Molecular structure

The simulated molecular system consists of a ring of 13 tubulin heterodimers (Fig. 1). The system was solvated and equilibrated. We exploited the symmetry of the system (the ring and the solvent) and utilized the effect of periodic boundary conditions to multiply the ring in all directions, so that we could obtain an arbitrary number of arbitrarily long microtubules in the
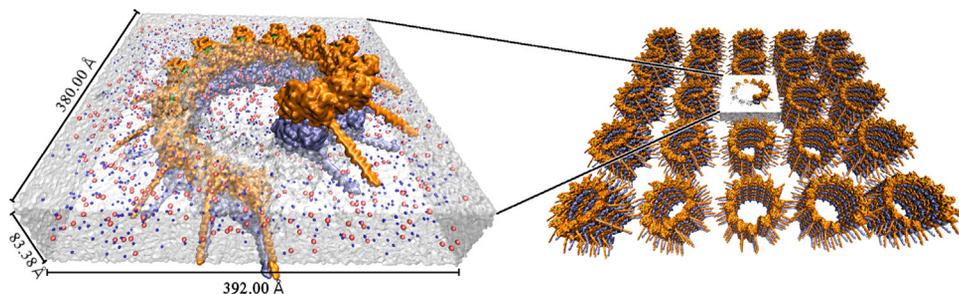
Fig. 1. The microtubule ring system before equilibration. Limited number of periodic images is displayed in the *x, y* and *z* directions.

Table 1
Number of atoms in our simulation system for various ion concentration.

Ionic concentration	Number of Na+ ions	Number of Cl- ions	Number of water atoms	Number of protein atoms (including GTP cofactor)	Total number of atoms
low	663	0	1053312	179972	1233947
normal	1296	633	1053312	179972	1235213
high	1929	1266	1048368	179972	1231535

B-lattice form. We based our system on the one from our previous work [2], where we obtained the binding energy between adjacent tubulin heterodimers using a similar setting.

The C-terminus is not resolved in the original crystal structure of tubulin. Therefore, in the current work, we added the C-terminal tail to each tubulin heterodimer because there is evidence that the C-terminus has an important contribution to the overall tubulin electric charge [3] and affects the response of tubulin to external electric fields [4,5]. α-tubulin C-terminal tails sequence of amino acids was and GVDSVEGEGEEEGEEY and QDATADEQGEFEEEGEEDEA for β-tubulin The α and β tubulin protein sequences totaled 451 and 445 residues, respectively.

2.2. MD simulations

All molecular dynamics trajectories were produced utilizing CUDA-accelerated version of AMBER software [6,7]. The parameters set used was Amber ff14SB for the protein part, TIP3P [8] for water solvent, Joung and Cheatham parameters for ions [9] and parameters derived by Meagher et al. [10] for the GTP cofactor. As a starting structure we have used MT ring structure from our previous publication [2]. This time we also attached C-terminus tails as unstructured chains to that well-equilibrated MT ring. After this procedure we solvated the system in 380 × 392 × 83.88 Å water box with ions. We prepare the system in three different ionic concentrations so the number of ions and water molecules varies through these different systems (see Table 1). For each of these systems we let them settle into a local minima of potential energy. Firstly by a steepest descent algorithm followed by a conjugate gradient algorithm. Thereafter we let the system evolve under constant pressure to reach the velocity distribution of particles corresponding to equilibrated thermodynamic temperature of 310 K. Thereafter we let the system to well equilibrate for another 5 ns in NpT conditions. The coordinates derived after this equilibration part were used as a starting point for the main production run. Before we applied an electric field in main production run we assign a random velocities to all particles in our system from Maxwell-Boltzmann velocity distribution corresponding to 310 K and let the system evolve for 500 ps (250,000 steps) to reach slightly different point in possible phase space for our system. During the production run system propagates by Langevin integrator with 2-fs time step and

constrained all hydrogen bonds (SHAKE algorithm [11]) under constant volume and temperature (2 ps-1 frequency of collision). All our MD runs used periodic boundary conditions and long-range electrostatic forces were treated by particle-mesh Ewald method. For a non-bonded integration we used a cut-off distance of 10Å. The rest of parameters were kept at Amber default values.

Declaration of Competing Interest

Hereby we declare that we are not aware of any conflict of interest.

Acknowledgments

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