

<https://doi.org/10.7124/bc.000B67>

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UNIVERSAL IN SILICO ALGORITHM FOR 3D-MODELING AND PRINTING OF MACROMOLECULAR COMPLEXES: CASE STUDY OF MITOCHONDRIAL ELECTRON TRANSPORT CHAIN

Aim. Membrane complexes of organelles are exceptionally challenging to perceive spatially and to study, which leads to oversimplified views of their structure and function. Modern databases contain comprehensive information on molecular structure; The aim of this work was to develop and validate a universal algorithm for converting bioinformatic data into physically accurate, SLA-printable 3D models, using the mitochondrial electron transport chain as a case study. **Methods.** The first step involved retrieving the required structures in .pdb format from the PDB and PubChem databases, followed by optimization of lipid and small molecule conformations in Avogadro2 using the MMFF94 force field. In the second step, molecular structures were adapted for SLA printing within the ChimeraX environment. The third step involved spatial modeling in Blender: constructing membrane topology with physiological curvature (radius ~17 nm) and procedural lipid placement. Post-processing of printed parts included washing in isopropyl alcohol, support removal, and final UV polymerization. **Results.** Application of the proposed algorithm enabled successful modeling and printing of a mitochondrial crista fragment containing ETC complexes and an ATP synthase dimer. Using Blender's procedural modeling, lipids were distributed across the prepared membrane topology in proportions close to physiological levels (42:42:16 for phosphatidylcholine, phosphatidylethanolamine, and cardiolipin, respectively). Additionally, to visualize chemical gradients (pH) and differences in ATP/ADP pools without overloading the geometry of the main model, lithophane was used, where varying light intensity depending on polymer thickness renders the image. **Conclusions.** The developed data transfer algorithm (PDB/OPM → Avogadro2 → ChimeraX → Blender → SLA printing) is a universal and efficient tool for rapid physical prototyping of complex biomolecular systems. The proposed methodology allows the model to be adapted to the capabilities of 3D printing technology while preserving scientific accuracy (stoichiometry, positioning, and conformation). This algorithm can be directly applied to the modeling and printing of other multicomponent biological objects such as viral envelopes, chloroplast thylakoids, or bacterial membranes substantially expanding the toolkit of structural biology.

Keywords: electron transport chain, 3D printing, SLA.

Received: 08.06.2026; Accepted: 08.09.2026; Published: 29.09.2026

Citation: Vernoslov D.M., Zavalska Ya.B., Khomichenko D.S., Stepanenko V.V., Vilshanskyi D.O., Shpylchyn V.V. (2026) Universal in silico algorithm for 3D-modeling and printing of macromolecular complexes: case study of mitochondrial electron transport chain. *Biopolymers & Cell*, Special issue(42), 45. <https://doi.org/10.7124/bc.000B67>

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