

Dancing with sterols: can antibiotic-sterol interactions explain the selectivity of aromatic analogues of amphotericin B?

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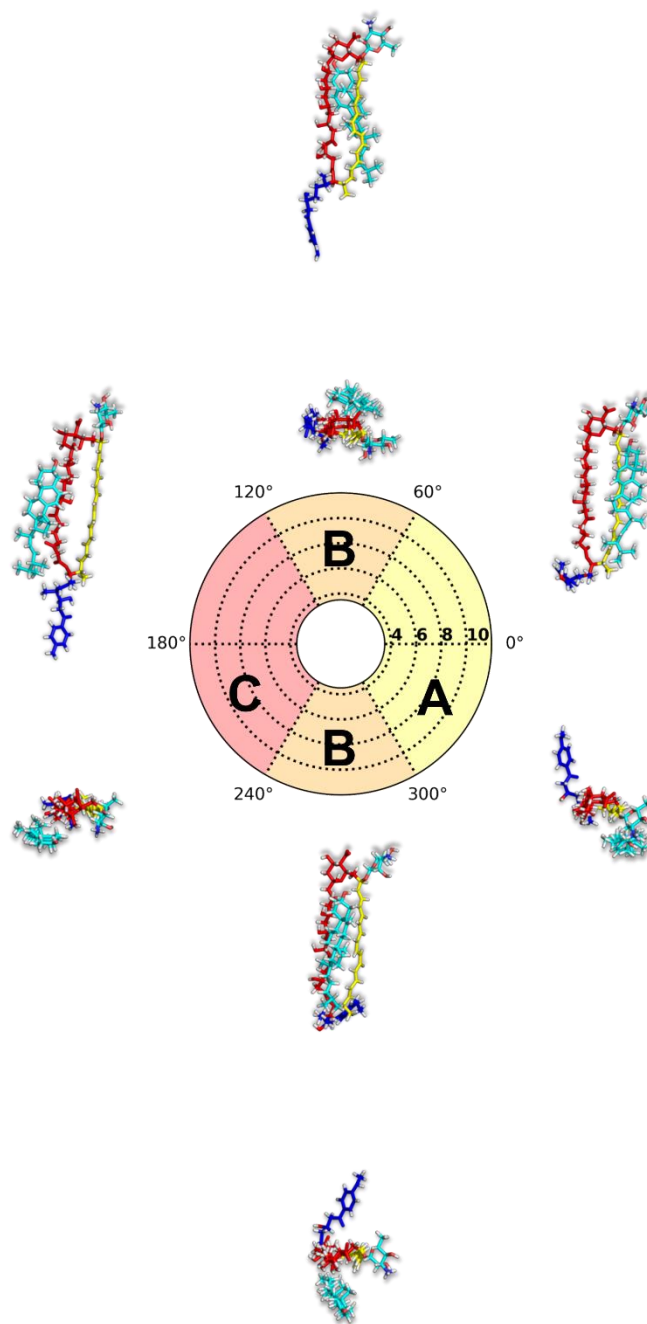


Figure S1. Position of a sterol molecule concerning specific regions of an antibiotic molecule: A) polyene region (yellow color, angles 0-60° and 300-360°), B) in between (orange color, angles 60-120° and 240-300°) and C) polyol region (red color, angle 120-240°) with corresponding binary complex representative structures.

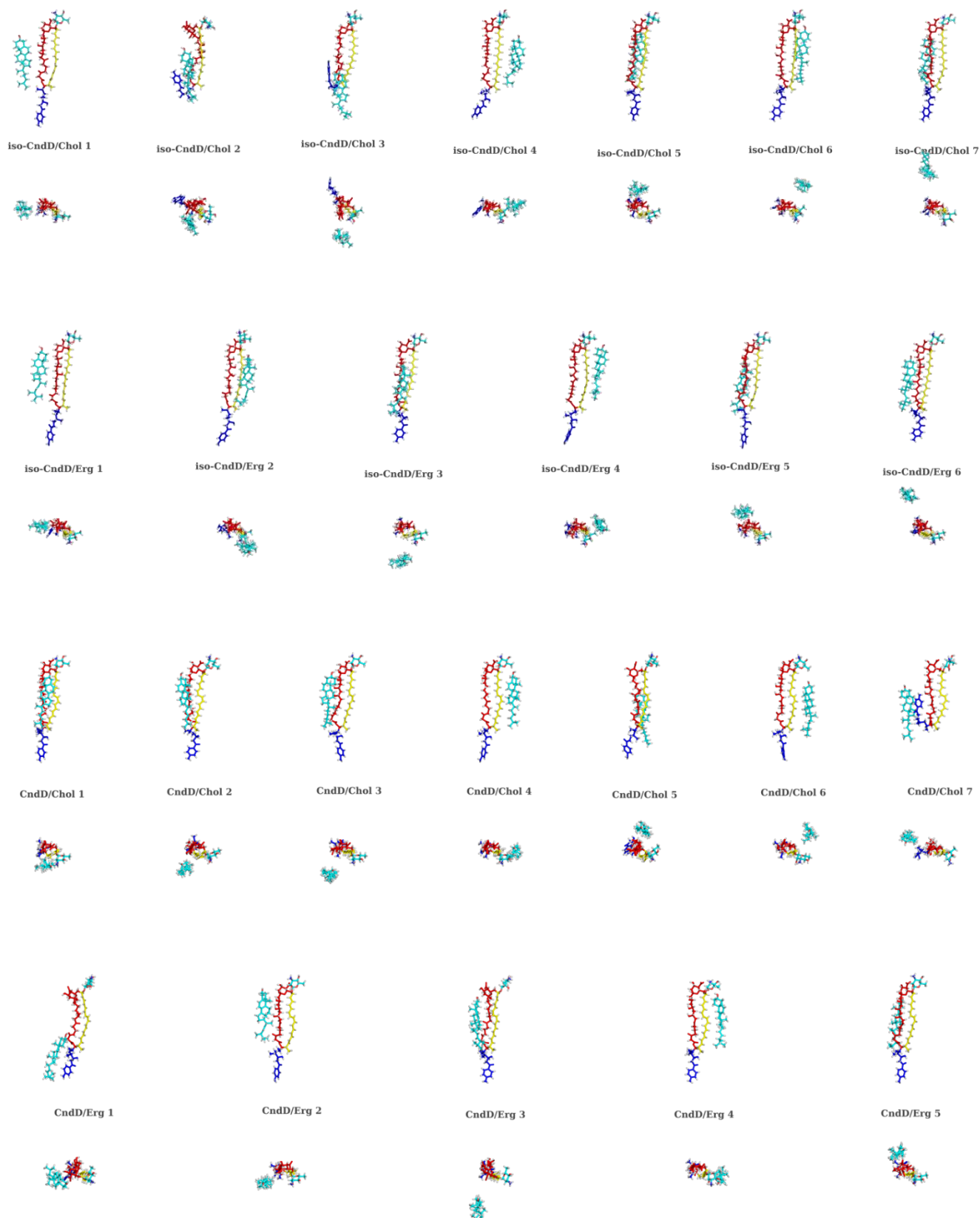


Figure S2. All representative structures of binary complexes extracted from energetic minima via cluster analysis for Candicidin D.

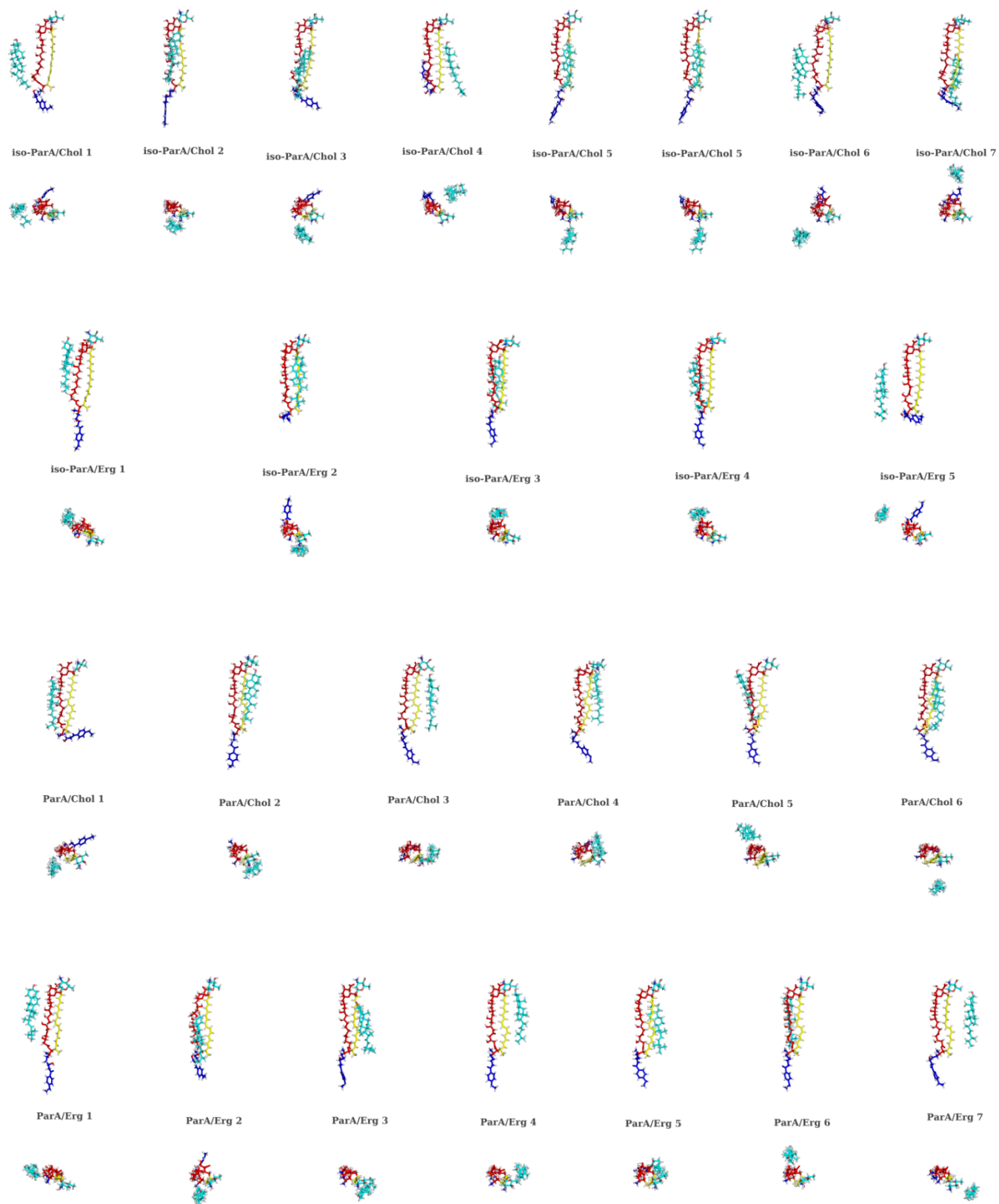


Figure S3. All representative structures of binary complexes extracted from energetic minima via cluster analysis for Partricin A.

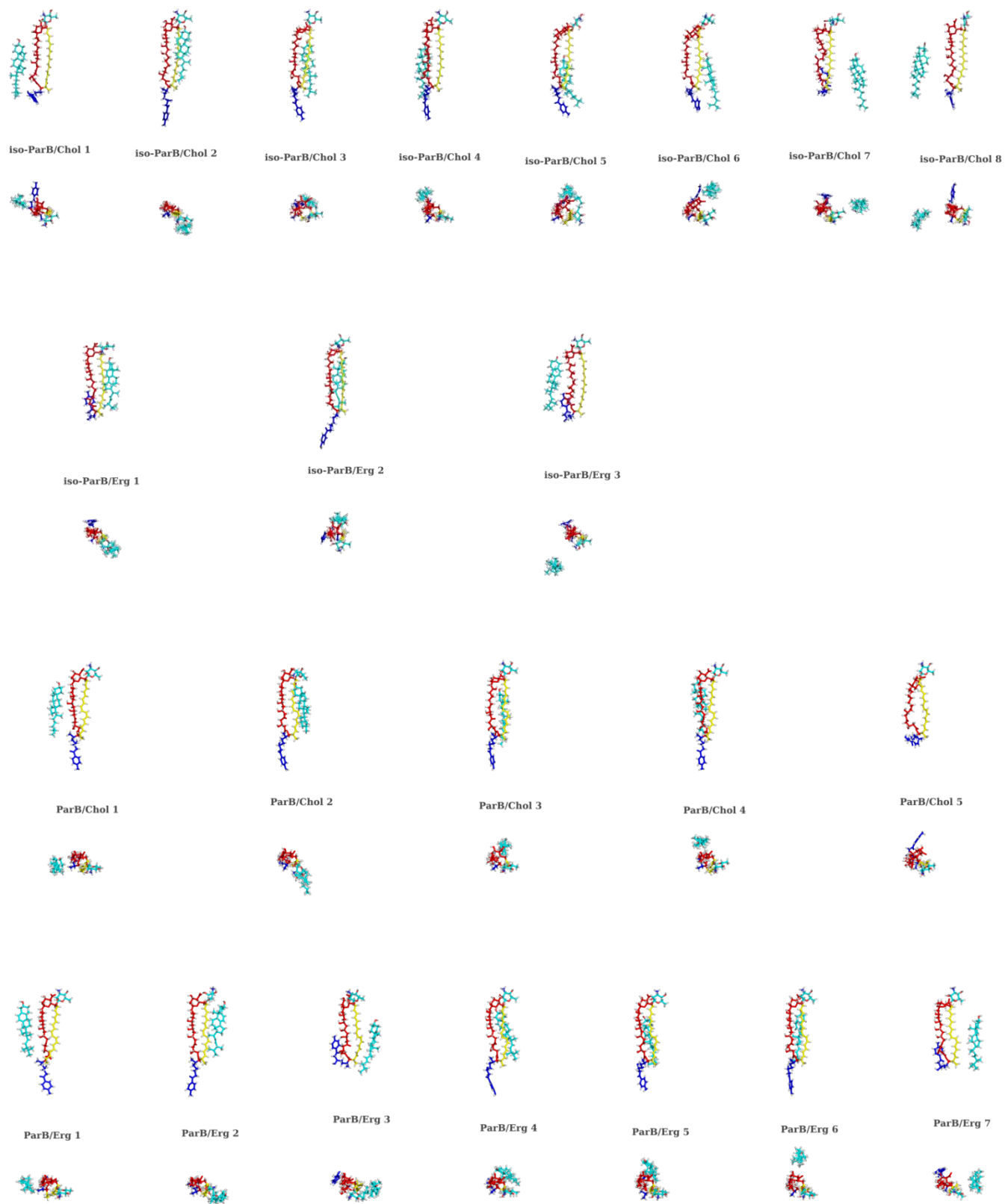


Figure S4. All representative structures of binary complexes extracted from energetic minima via cluster analysis for Partricin B.

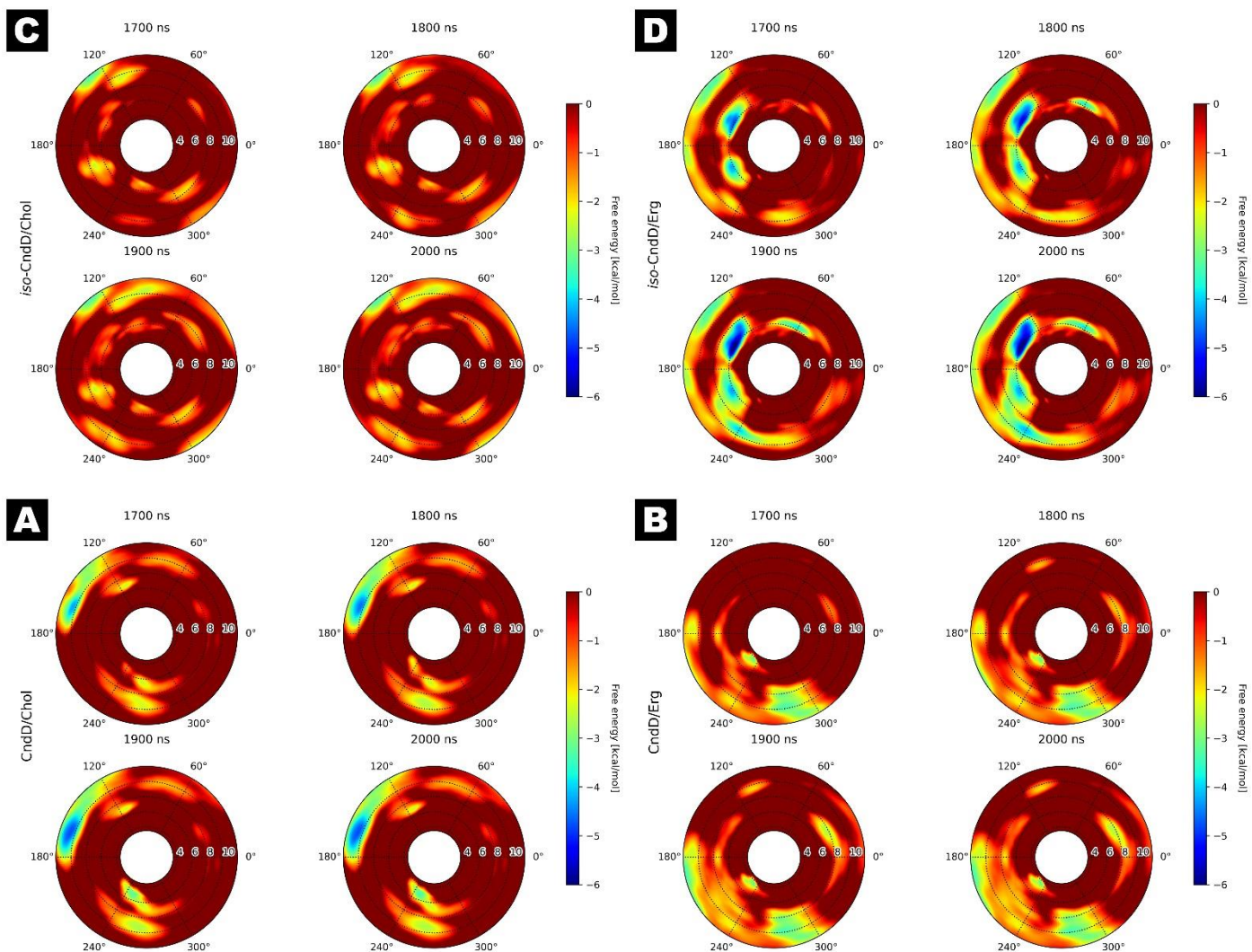


Figure S5. Convergence of free energy landscapes for Candidicin D: A) native with Chol, B) native with Erg, C) isomer with Chol, D) isomer with Erg.

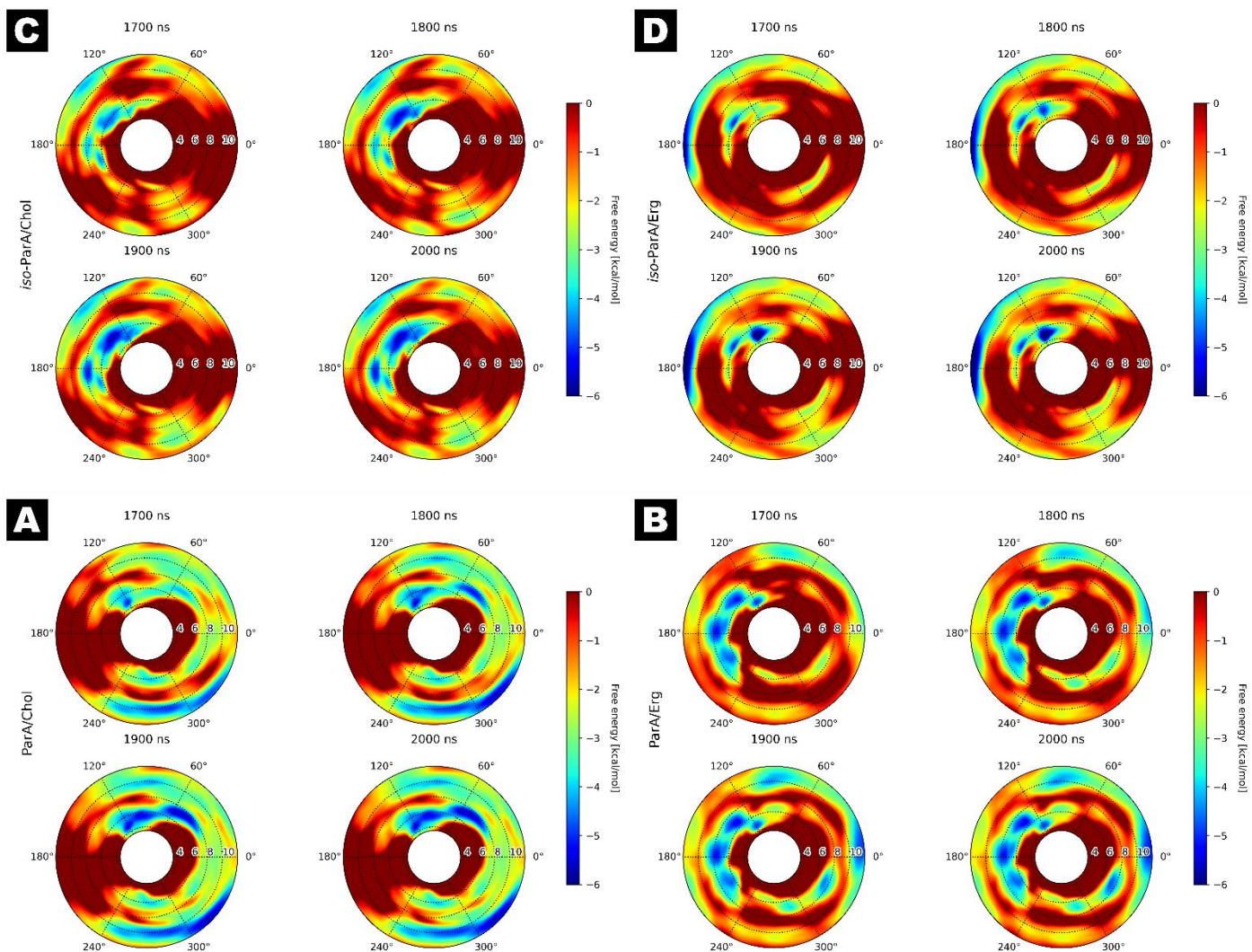


Figure S6. Convergence of free energy landscapes for Partricin A: A) native with Chol, B) native with Erg, C) isomer with Chol, D) isomer with Erg.

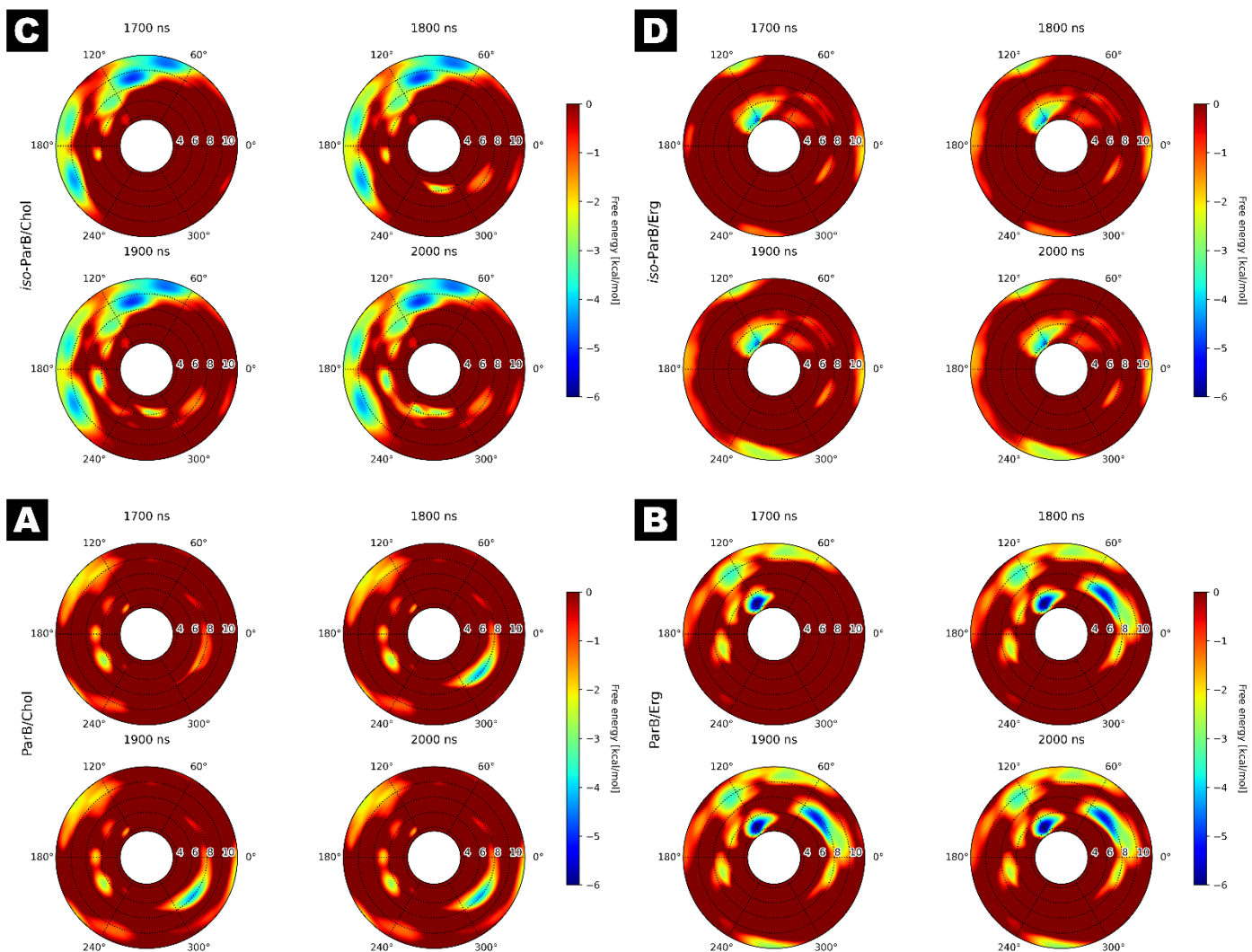


Figure S7. Convergence of free energy landscapes for Partricin B: A) native with Chol, B) native with Erg, C) isomer with Chol, D) isomer with Erg.