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MDPI

Supplementary Materials

Elucidation of the Conformational Transition of Oligopeptidase B by an Integrative Approach Based on the Combination of X-Ray, SAXS and Essential Dynamics Sampling Simulation

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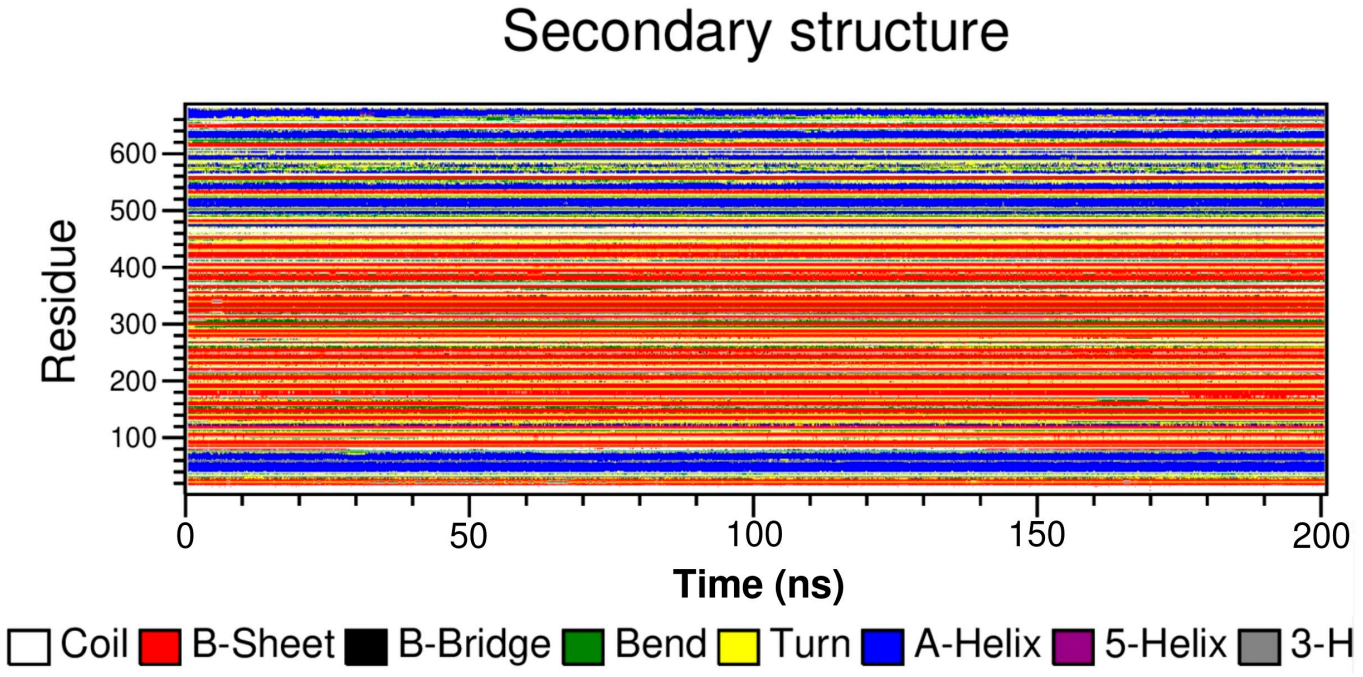

Figure S1. Evolution of secondary structure of the SpOPB during the classical MD simulation calculated by DSSP algorithm.

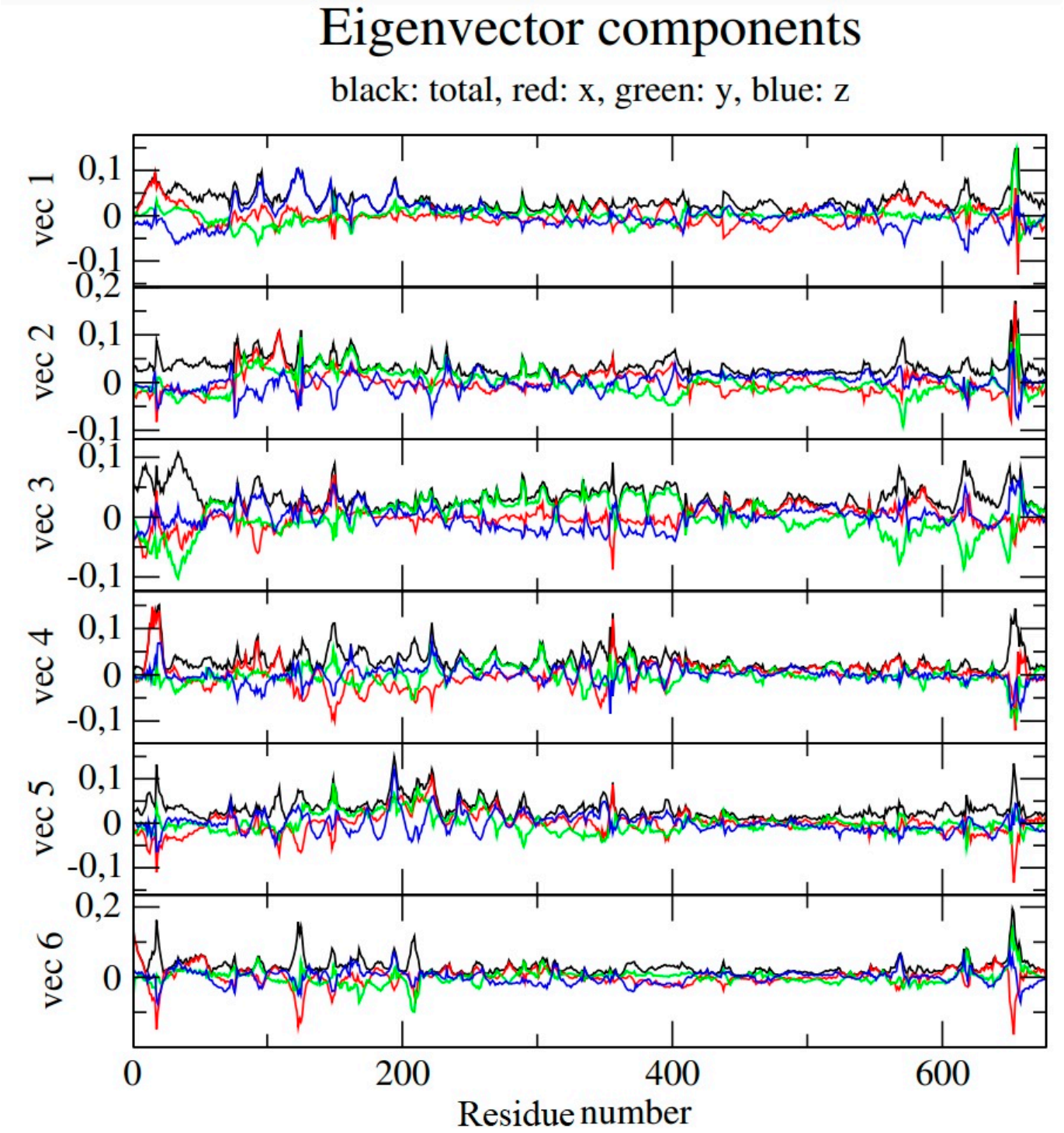

Figure S2. Components of the first six eigenvectors from covariance analysis of the classical MD trajectory.

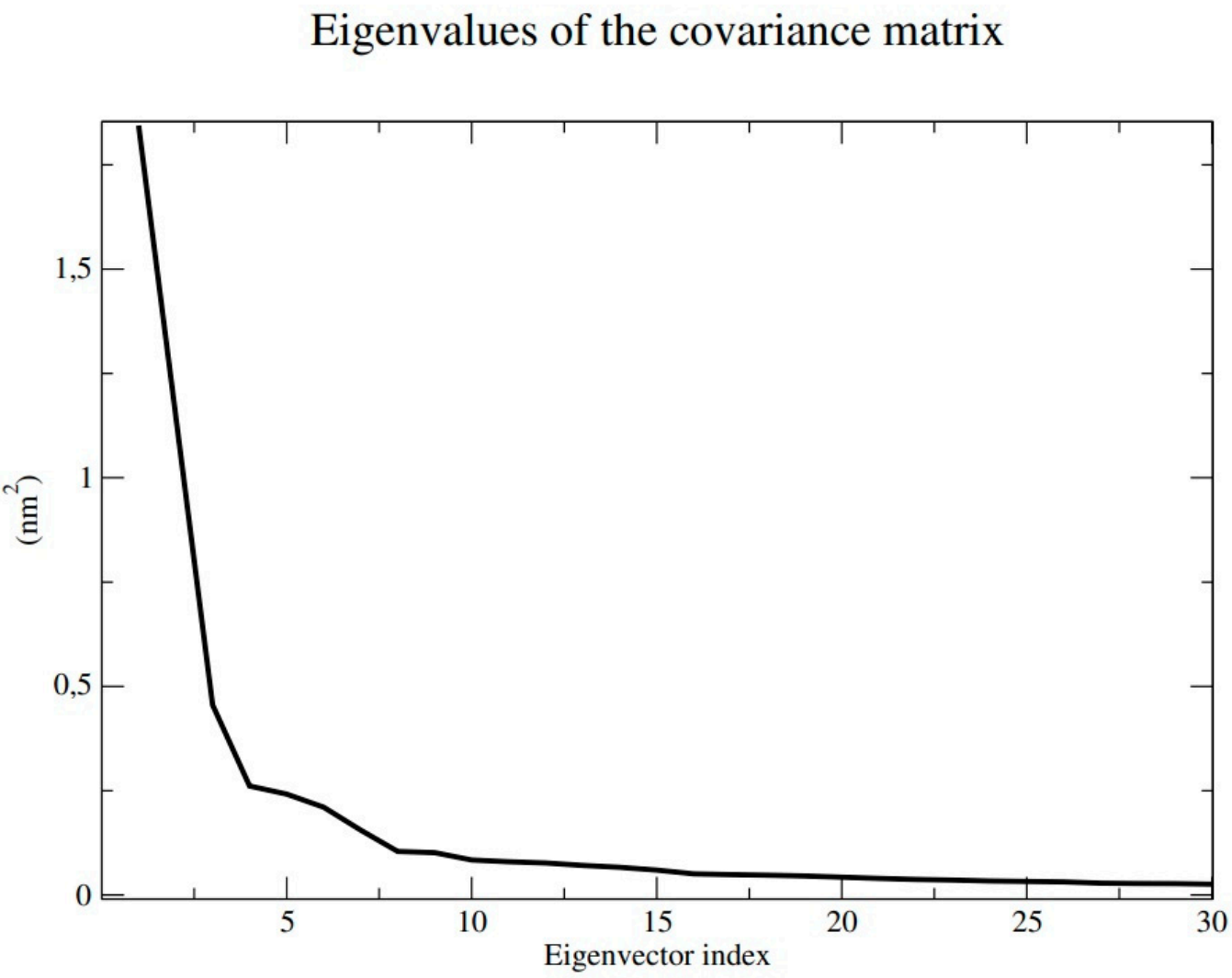

Figure S3. Eigenvalues obtained from covariance analysis of MD trajectories.

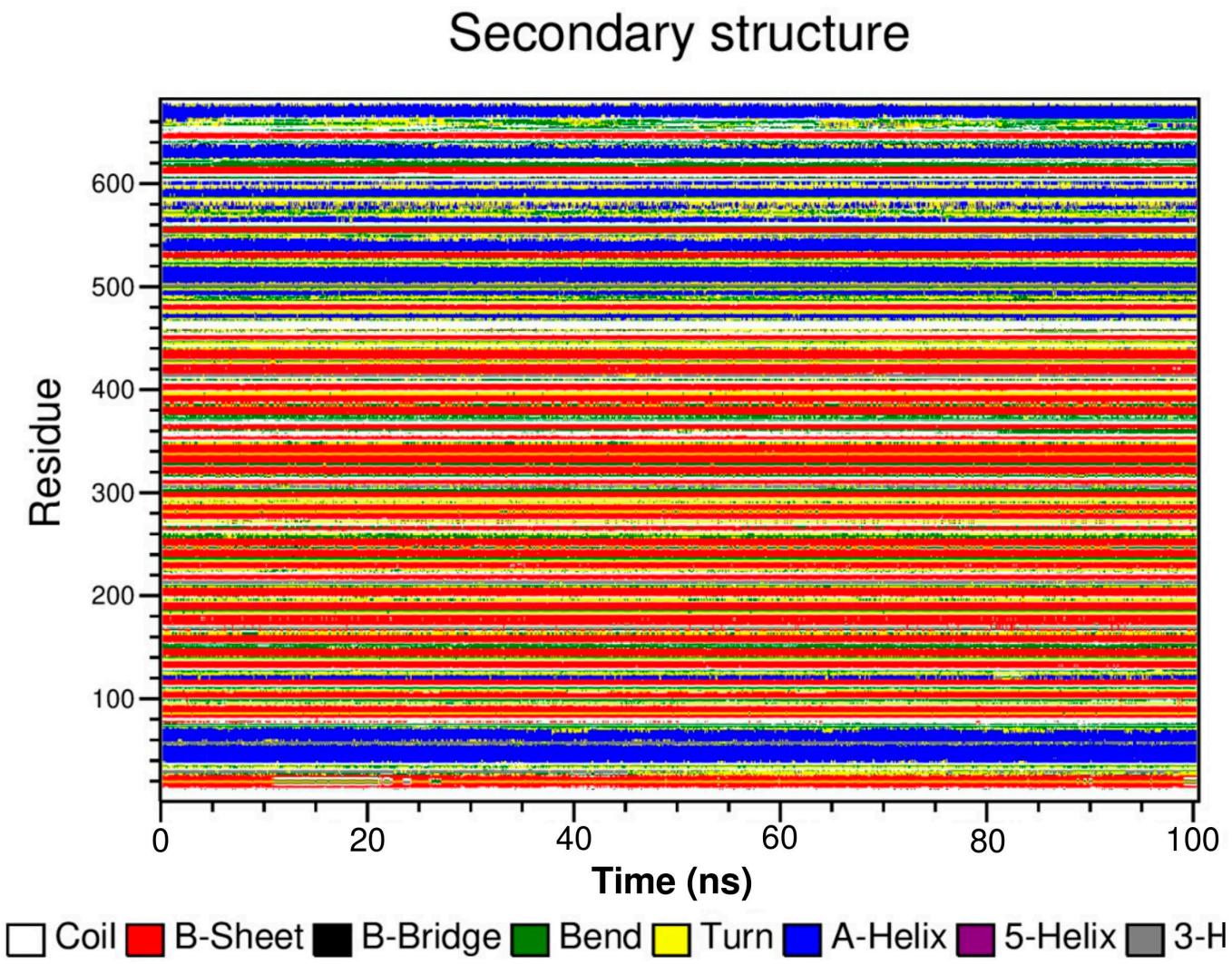

Figure S4. Evolution of secondary structure of the SpOPB during EDS simulation calculated by DSSP algorithm.