

Supporting information

Molecular docking and simulation analysis for elucidation of toxic effects of Dicyclohexyl phthalate (DCHP) in glucocorticoid receptor-mediated adipogenesis

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Table S1: General properties and uses of DCHP and MCHP.

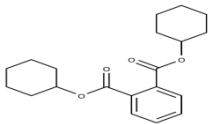
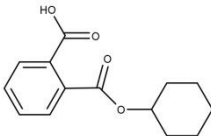
Properties	DCHP	MCHP
Molecular weight	330.424 g/mol	248.278 g/mol
Molecular formula	C ₂₀ H ₂₆ O ₄	C ₁₄ H ₁₆ O ₄
Molecular Structure		
Uses	1. Used in cosmetic products 2. Plasticizer ingredient in nitrocellulose, ethyl cellulose, vinyl cellulose, and resins 3. Added with poly (methyl Methacrylate) in amorphous thermoplastics	

Table S2: Average RMSD, RMSF, and radius of gyration (Rg) values of the DEX-hGR, DCHP-hGR and MCHP-hGR complexes. Resultant average RMSD, RMSF, and Rg values of variation in hGR backbone on the binding of DEX, DCHP, and MCHP are mentioned.

S.no	Compound	Average RMSD (nm)	Average RMSF (nm)	Average Rg (nm)	Intra H Bond (numbers)
1.	DEX	0.144	0.093	1.836	1250.9
2.	DCHP	0.186	0.101	1.835	1250.6
3.	MCHP	0.197	0.097	1.829	1254.7

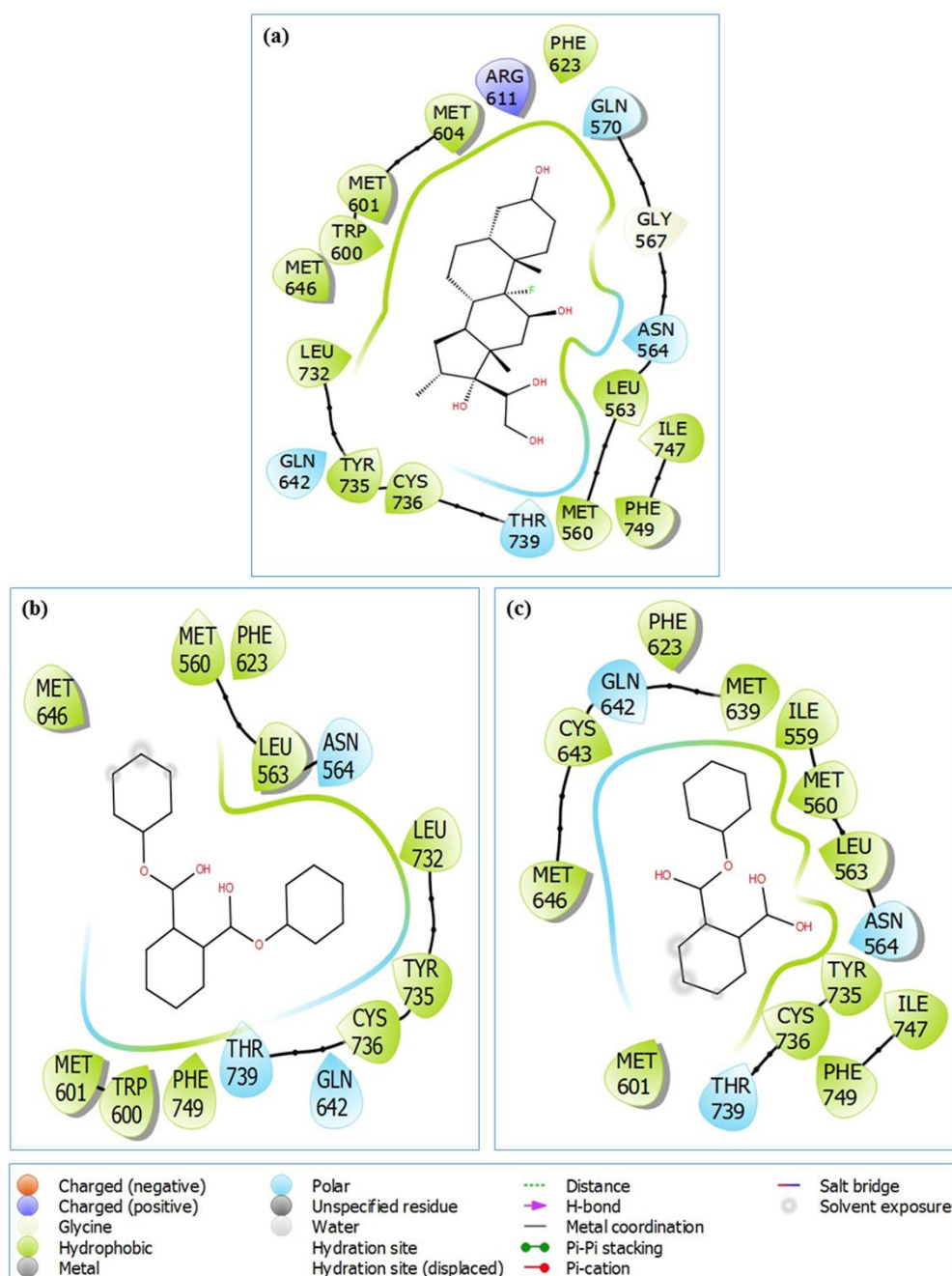


Figure S1. Pictographic representation of hydrophobic interaction involved in DEX-hGR, DCHP- hGR and its metabolite MCHP-hGR complex formation using Maestro 11.2 (a) DEX, (b) DCHP, and (c) MCHP. All the aromatic rings of DCHP and MCHP are deeply embedded into the hydrophobic pockets of hGR. Hydrophobic interactions are shown in green color.

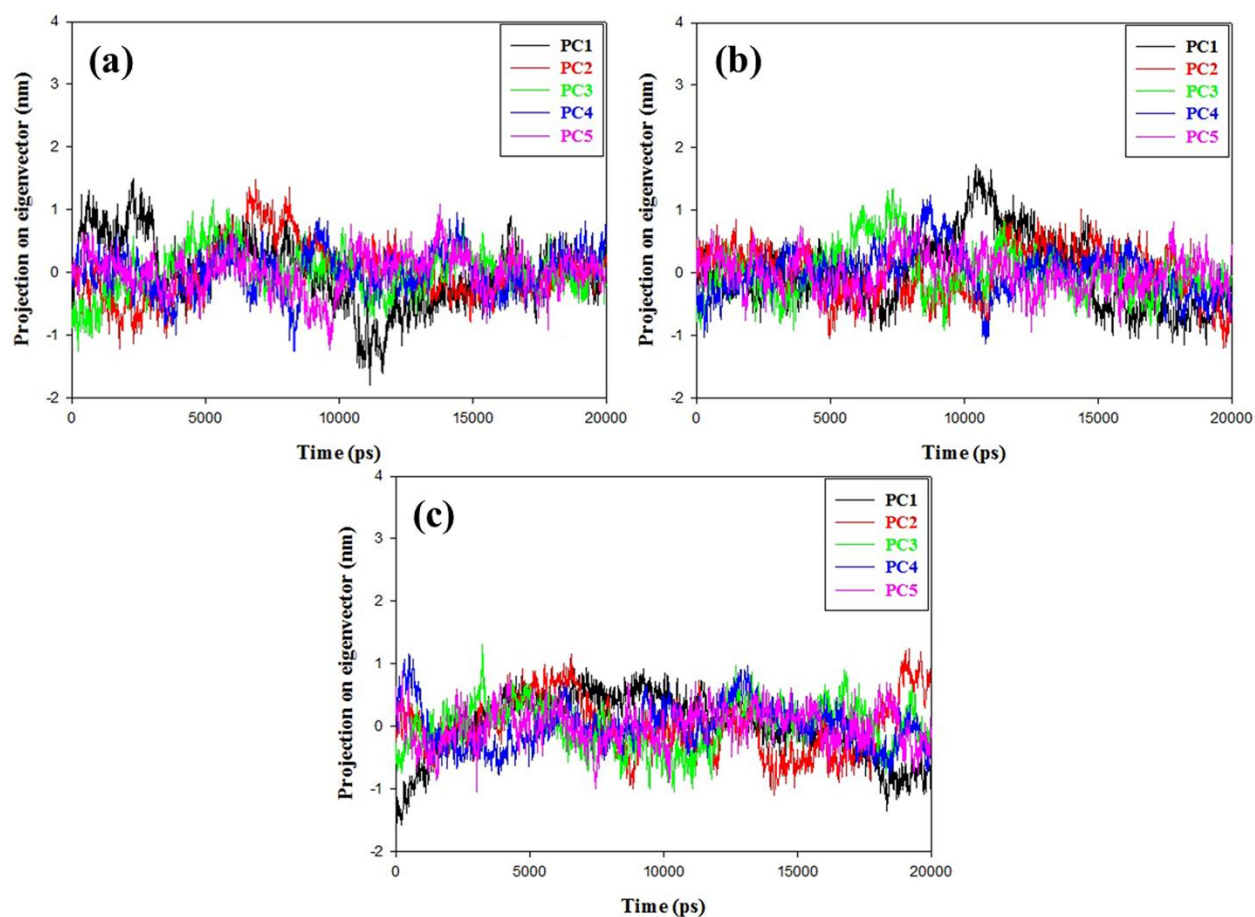


Figure S2. Principal component analysis along top five eigenvectors for DEX-hGR and PAEs-hGR complexes. The motion along PC1, PC2, PC3, PC4 and PC5 for DEX-hGR (a), DCHP-hGR, (b) and MCHP-hGR, and (c) complexes.

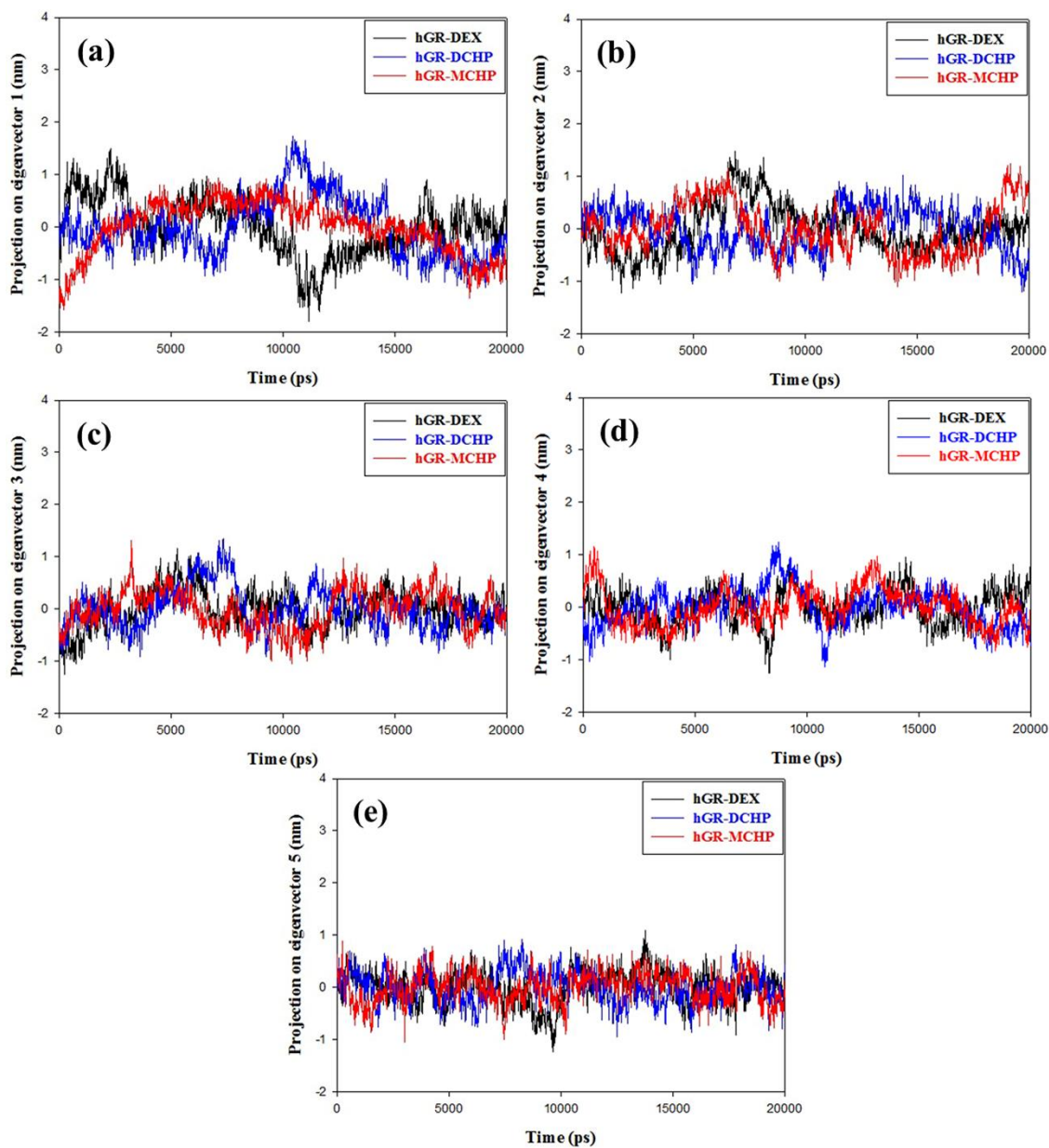


Figure S3. Principal component analysis along top five eigenvectors (PC1, PC2, PC3, PC4 and PC5) for simulation period of 20ns. PCA plot for DEX-hGR, DCHP-hGR, and MCHP-hGR along, (a) eigenvectors 1, (b) eigenvectors 2, (c) eigenvectors 3, (d) eigenvectors 4, and (e) eigenvectors 5.

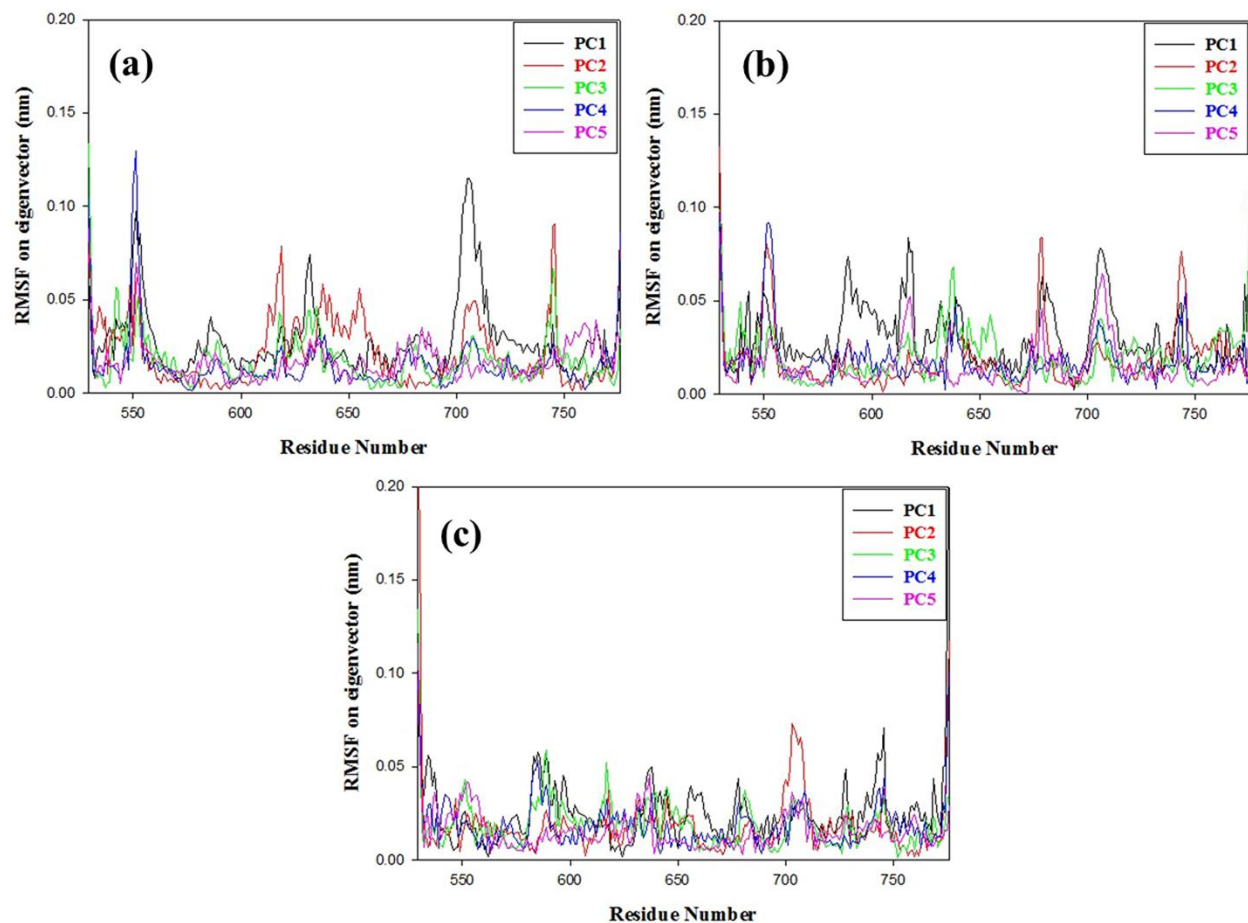


Figure S4. Root mean square fluctuation (RMSF) along different eigenvectors during 20 ns. RMSF along PC1, PC2, PC3, PC4 and PC5 for: (a) DEX-hGR, (b) DCHP-hGR, and (c) MCHP-hGR, respectively.

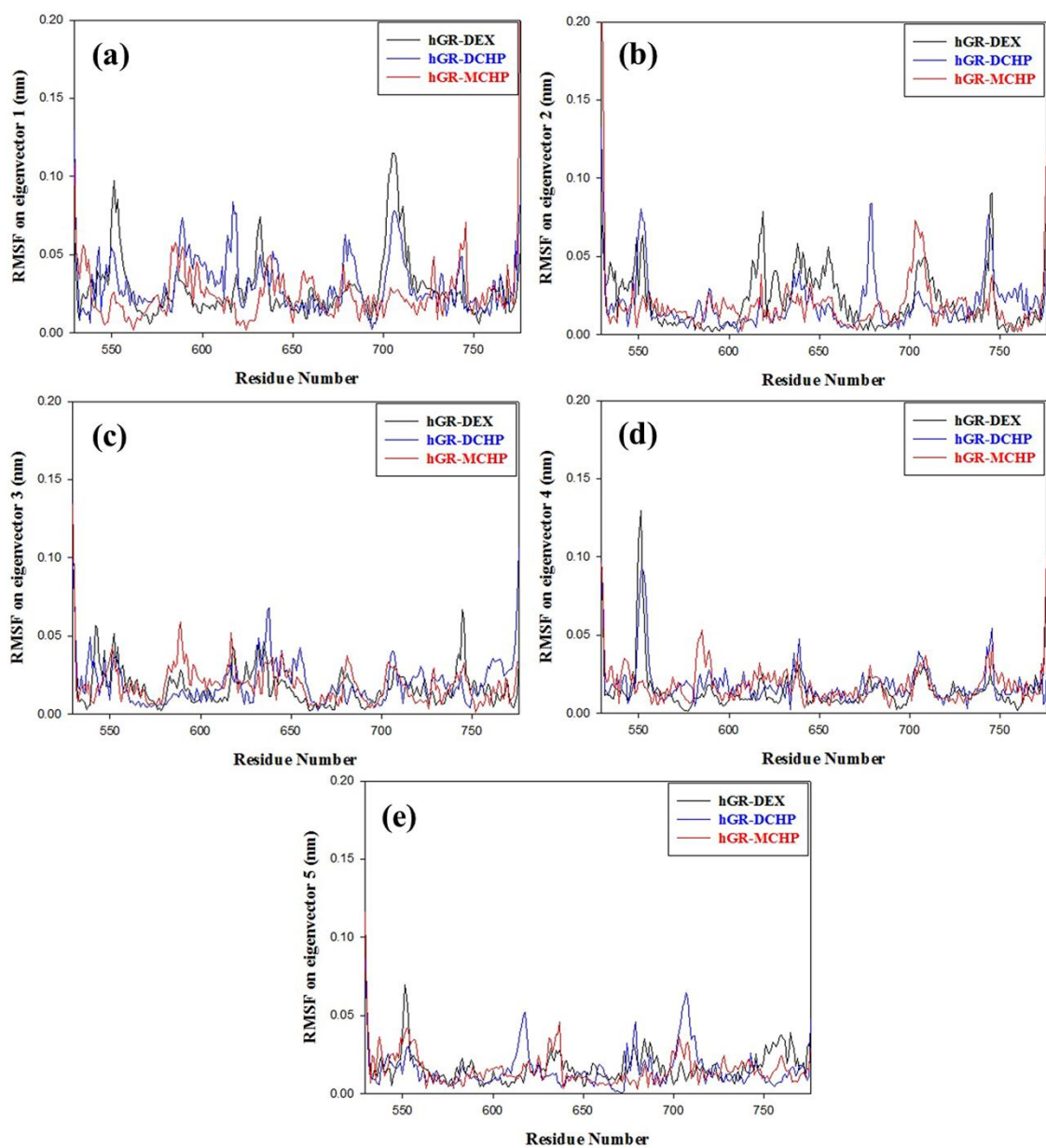


Figure S5. Root mean square fluctuation (RMSF) on eigenvectors for DEX-hGR, DCHP-hGR and MCHP-hGR complexes. RMSF on different eigenvectors, (a) eigenvector 1, (b) eigenvector 2, (c) eigenvector 3, (d) eigenvector 4, and (e) eigenvector 5.

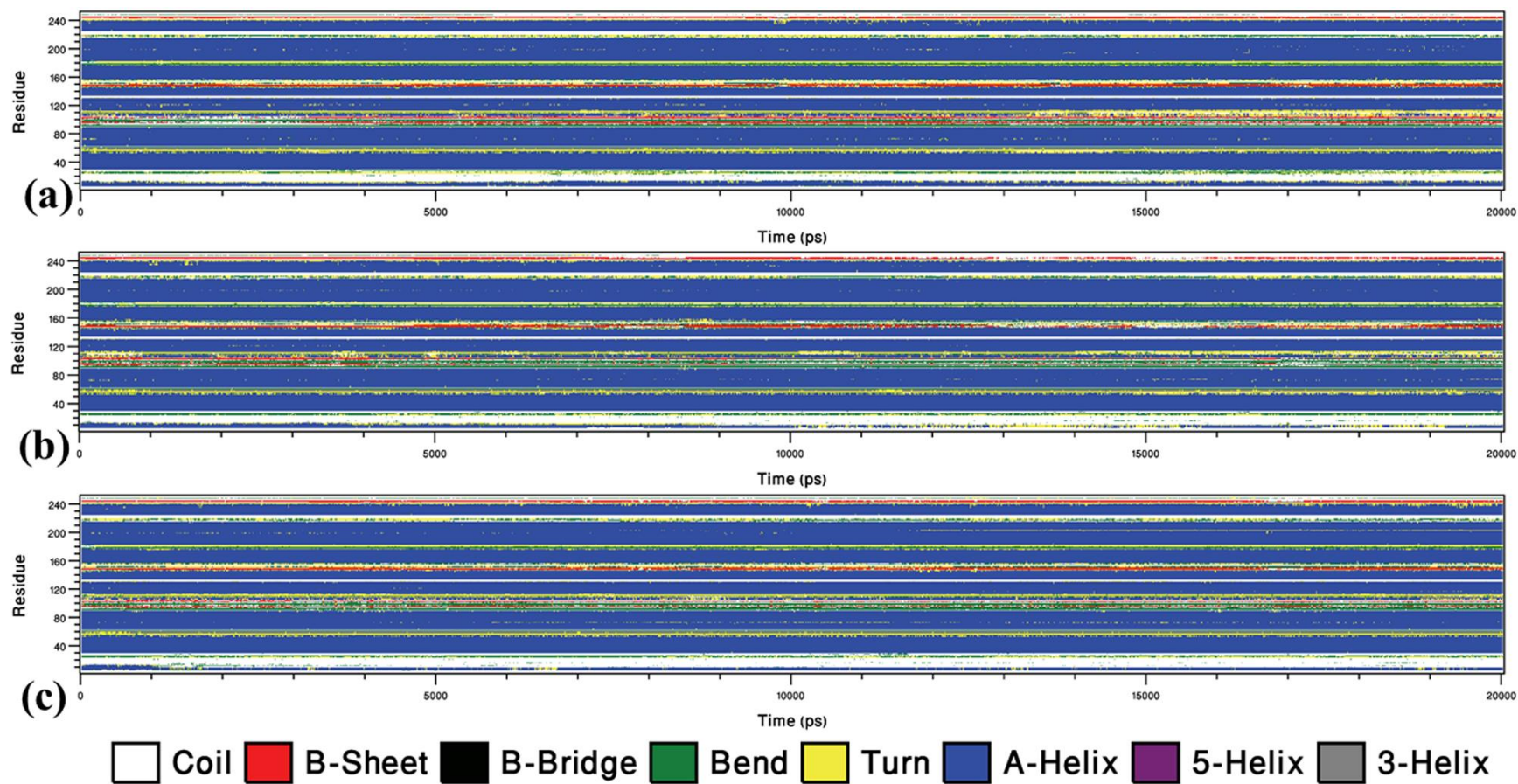


Figure S6. Define Secondary structure of proteins (DSSP) analysis of DEX - hGR and PAEs - hGR complexes during the simulation period of 20 ns. (a) DEX - hGR, (b) DCHP - hGR, and (c) MCHP - hGR.