International Journal of Biomedical Data Mining

ISSN: 2090-4924

OPEN ACCESS Freely available online

Abstract

Spectroscopic evaluation of synthesized 5β-dihydrocortisol and 5β-dihydrocortisol acetate binding mechanism with human serum albumin and their role in anticancer activity

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Our study focus on the biological importance of synthesized 5β-dihydrocortisol (Dhc) and 5β-dihydrocortisol acetate (DhcA) molecules, the cytotoxic study was performed on breast cancer cell line (MCF-7) normal human embryonic kidney cell line (HEK293), the IC50 values for MCF-7 cells were 28 and 25 μM, respectively, whereas no toxicity in terms of cell viability was observed with HEK293 cell line. Further experiment proved that Dhc and DhcA induced 35.6 and 37.7% early apoptotic cells and 2.5, 2.9% late apoptotic cells, respectively, morphological observation of cell death through TUNEL assay revealed that Dhc and DhcA induced apoptosis in MCF-7 cells. The complexes of HSA–Dhc and HSA–DhcA were observed as static quenching, and the binding constants (K) was 4.7 ± .03 × 104 M−1 and 3.9 ± .05 × 104 M−1, and their binding free energies were found to be −6.4 and −6.16 kcal/mol, respectively. The displacement studies confirmed that lidocaine 1.4 ± .05 × 104 M−1 replaced Dhc, and phenylbutazone 1.5 ± .05 × 104 M−1 replaced by DhcA, which explains domain I and domain II are the binding sites for Dhc and DhcA. Further, FT-IR, synchronous spectroscopy, and CD results revealed that the secondary structure of HSA was altered in the presence of Dhc and DhcA. Furthermore, the atomic force microscopy and transmission electron microscopy showed that the dimensions like height and molecular size of the HSA–Dhc and HSA–DhcA complex were larger compared to HSA alone. Detailed analysis through molecular dynamics simulations also supported greater stability of HSA–Dhc and HSA–DhcA complexes, and root-mean-square-fluctuation interpreted the binding site of Dhc as domain IB and domain IIA for DhcA. This information is valuable for further development of steroid derivative with improved pharmacological significance as novel anti-cancer drugs.

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Received: January 18, 2021; **Accepted**: February 4, 2021; **Published:** March 15, 2021

Citation: Monika K. (2021) Spectroscopic evaluation of synthesized 5β-dihydrocortisol and 5β-dihydrocortisol acetate binding mechanism with human serum albumin and their role in anticancer activity. Int J Biomed Data Min 10: 135.