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Computational modeling of hepatocellular carcinoma associated PARP-1 protein and structure base screening of potential inhibitor

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Hepatocellular carcinoma is one of the hard-treating and high mortality cancers for which novel therapies are very much in need. There are many complications and side-effects in present available treatment modalities, there is only one drug that is in use (Sorafenib) and many are under clinical trials. So, some proteins were found which were responsible for causing Hepatocellular carcinoma. One of these proteins was selected and targeted, and its inhibitors were found, which inhibit the activity of that protein to cause HCC. Here, *in silico* approach was directed to find the novel inhibitor as potential candidate therapy for HCC. Here, Poly[ADP-ribose]polymerase-1 (PARP-1) was used as druggable target. Total 20 inhibitors of PARP-1 in 91 conformations were used for standard precision computational docking. On the basis of docking score and glide score, suitable inhibitors were identified. These selected inhibitors can be used as lead molecules for the designing of inhibitor based drugs. Lead molecules were further characterised by ADMET analysis, which include Lipinski's rule, Jorgensen's rule, blood-brain barrier penetration, Skin permeability, Human intestinal absorption and oral absorption. $C_{15}H_{19}N_3O_2$+ was found to be best inhibitor of PARP-1 among all the inhibitors with best ADMET properties. So it may be a better alternative for the inhibition of PARP-1and preventing from HCC. Present study focuses on the importance of structure based *in silico* drug design which takes less time and is cost effective.

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Enhancing the solubility of a drug using novel formulations

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Use of inorganic mesoporous silica substances in formulation to improve the dissolution of poorly water soluble drugs is a fast developing area in pharmaceutical drug research. In this research, three different mesoporous silica (silica gel, syloid AL 1 FP and syloid XDP 3050) micro particles were utilized in enhancing the solubility of phenylbutazone. They were formulated by means of wet mixtures using water as a solvent at different drug/excipient mass ratios of 50:50 (w/w), 60:40 (w/w), 70:30 (w/w) for silica gel and syloid AL 1 FP, while syloid XDP 3050 was formulated at 50:50 (w/w), 40:60 (w/w) and 30:70 (w/w) drug/excipient mass ratios. All the particles before and after formulation were investigated for their morphology and size distribution via microscopy and malvern mastersizer. *In vitro* dissolution analysis was carried out in order to investigate their pharmaceutical performance. This analysis demonstrated that the release of phenylbutazone in the samples prepared with syloid XDP 3050 was 85.13±2.55% in 15 minutes and 99.62±2.95% in 30 minutes. Upon all formulations investigated, this release was the best and the greatest achieved during this study in comparison to only 24.57±1.40% and 43.66±2.25% release of the pure phenylbutazone over the same period. Drug formulation with silica gel exhibited the slowest release in comparison to the formulations with two syloid silicas, this deviation is thought to be as a result of a larger particle size of the silica gel and also during the formulation, drug crystals and silica gel particles did not mix well together due to the large mass of drug used.

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