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Design and synthesis of potent Cyclin C inhibitors

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The fundamental aspect of cancer is deregulated cell replication leading to tumour formation. Alterations result in the inappropriate proliferation of the apparatus that controls the decision of cells to progress from (G0-G1) resting phase or G1 to S phase leading to tumours (1). Cyclin C is an attractive target operating in G0 – G1 phase of the cell cycle which combines with CDK8/Cdk3 leading to cell division (2). The structure of cyclin C has been evaluated by homology modeling, energy minimised and its active site identified (3). Virtual Screening with CB micro format data bank using Schrodinger Software resulted in a set of novel leads as potent inhibitors for cyclin C protein. The new molecular entities were ascertained based on the Glide score function and QikProp (ADME) properties as substituted barbiturates. Substituted barbiturates are one of the most important structural class of anti-tumour compounds. These compounds act by inhibiting the combination of Cyclin C with CDK3/8 Kinases (3). Further, these chemical entities were synthesised and their cytotoxic studies were performed on HEK 293 cell lines. The new molecular entities have shown promising growth inhibitory (GI) effects.

Key Words

CyclinC; Cyclin Dependant Kinases (CDK); Substituted Barbiturates.

Biography

Dr. P. Sarita Rajender, is a DST – Scientist at The Department of Chemistry, Nizam College, Osmania University since 2009 and has completed Ph. D in Synthetic Organic Chemistry in the year 1996.

She is a post-doctoral research fellow working on novel platforms for finding new leads in Cancer therapy. Patenting process is under progress for promising new lead molecules. Her field of research interest includes identification of new chemical entities (NCE's) using Computational Chemistry, Chemical-Biology and Software tools.

During her teaching tenure, she has mentored PG students in their dissertation work. She is actively organizing Seminars and workshops for students. Dr. P. Sarita Rajender published several research articles in reputed international journals and has presented papers at various International and National Conferences.

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