

**10th International Conference on
Genomics and Molecular Biology**

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**6th International Conference on
Integrative Biology**

May 21-23, 2018 Barcelona, Spain

Onco-Plus: an integrated database and computational protocol for discovery of lead molecules targeting unique DNA**Akhilesh Mishra, Pradeep Pant and B Jayaram**
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The specific binding of transcription factors (TFs) to specific DNA sequences make the DNA motifs promising drug targets for the coordinated regulation of gene expression. Here, we present Onco-Plus, an integrated database of regulatory motifs of cancer genes clubbed with Unique Sequence Predictor (USP) (<http://www.scfbio-iitd.res.in/software/onco/NavSite/index.htm>) and a software suite for targeting DNA for drug discovery. USP identifies unique sequences (i.e. these sequences occur only once in the entire genome and if targeted would presumably show no off-target binding /side effects) for each of the identified regulatory DNA motifs at the specified position in the genome by extending a given DNA motif, in 5'→3' or 3'→5' or in both directions. For each identified motif, three possible unique sequences could be generated. Taking off from the identified unique sequences as drug targets, a rapid virtual screening against a million-compound library could be performed (<http://www.scfbio-iitd.res.in/PSDDF/tool4.php>) to generate a list of hit molecules (potential candidate drugs) with their predicted binding free energies. This methodology is demonstrated on E2F transcription factor binding site for the WNT10B gene, implicated in breast and endometrial cancers and a few small molecules are proposed as potential drug candidates. Being fast and cost effective, this protocol could be of considerable value in generating new potential drug candidates to inhibit desired sequences for further experimental studies.

Biography

Akhilesh Mishra has done his Master's in Bioinformatics from Jamia Millia Islamia, New Delhi, India. He is pursuing his PhD from Indian Institute of Technology, New Delhi. He is the Recipient of CSIR-UGC-SRF and BINC award from the Department of Biotechnology, India. He has published many research articles in reputed peer reviewed journals.

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