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A text-mining based comparison of RNAi screening assays to NIH chemical probes

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The NIH (National Institutes of Health) Molecular Libraries and Imaging (MLI) initiative was funded as a cross-institutional effort to identify novel chemical compounds-probes that can interact with a cell or cell byproduct with precision. Between 2004 and 2013, MLI funded ten high-throughput Screening Centers resulting in the deposition of 5677 assays into PubChem and the nomination of 240 publicly available chemical probes. About 25% of these probes were found to be undesirable by a crowd-sourcing effort suggesting more rigorous probe evaluation methods are appropriate. In this study, we offer two in silico evaluation methods for probe quality assessment. In the first method, we annotated the 149 NIH probes and the 81 Bioassays with biomedical concepts using their probe synonyms and assay text descriptions. 8 of the 149 MLP probes are confirmed by this biomedical term matching method. For these 8 probes, overlapping concept identifiers might point to an agonist or antagonist related information revealing potential target protein-ligand information through the semantic ties. 4 of these 8 probes have been assessed medium-high reliable in an earlier crowd-sourced study. This is a promising support for text-mining based probe filtering as an in silico tool to include in future drug discovery initiatives. In the second part, we computed the percentage of probes that targets the same gene with an RNAi assay. An earlier study reported that 40% of the targets had no active probe compounds with potency better than 10mM. When no such potent chemical exist, these targets could be alternatively silenced by RNA interference suggesting a potential to develop more potent drugs through the combined efforts of medicinal chemistry and siRNA therapeutics approaches. Among 240 existing chemical probes in PubChem, 8 of the targets were found active in an RNAi screening Bioassay.

Biography

Tugba Suzek completed her Undergraduate from Middle East Technical University, Faculty of Engineering and Computer Engineering in the year 1997. She finished her Masters from Johns Hopkins University, Whiting School of Engineering in Computer Science in the year 2000. Later she pursued for PhD from George Mason University, School of Systems Biology Bioinformatics and Computational Biology and successfully completed it in the year 2012. Currently she is working as an Assistant Professor at Mugla University, Turkey. She has many important publications on her name and also have major association with NCBI/NIH.

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