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Virtual drug screening and repositioning for Mucopolysaccharidoses

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Mucopolysaccharidoses (MPS) are lysosomal storage diseases characterized by defects in the activity of lysosomal hydrolases. In MPS, secondary cell disturbance affects pathways common to cancer. Hence, the study aimed to identify MPS-related drugs targeting oncogenic pathways and identify a list of drugs for repurposing. We used public data from GEO of MPS I and MPS IIIB human datasets. We retrieved drug data from Drugbank. We used STITCH v.5 and Cytoscape v.3.8.2 to the protein-drug network. To improve the interaction networks, we used Omnipath v.2. The network was composed of 244 nodes, 13 of them related to drugs, and 1824 edges. Regarding the Omnipath analysis, the GSE111906 showed 47 enriched drugs in the interaction network. For the GSE23075, there were 31 enriched drugs. Our results suggest that drugs modulating the Axon guidance, EGFR, mTOR, Wnt, and immune system pathways, are particularly promising for intervention. Furthermore, the list of drugs and related MPS enriched genes could be useful as new treatments and considered for pathophysiological studies.

Keywords: lysosomal storage diseases; signaling pathways; drug repurposing; gene expression; network analysis.