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Pathway-based technologies for early drug discovery

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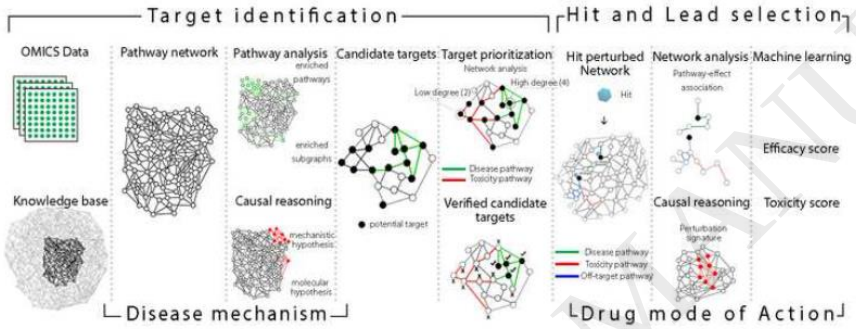
Graphical abstract



Highlights:

- The reductionist drug discovery approach entails high attrition rates.
- Topology-based pathway analysis can unravel the disease mechanism(s).
- Candidate targets can be prioritized based on their network effects.
- Pathway-based technologies can help predict a hit's side-effects and efficacy.

Teaser: Pathway-based technologies can improve drug discovery efficiency by matching the disease mechanism(s) to the signaling footprint of the drug or target.

Although the traditional drug discovery approach has led to the development of many successful drugs, the attrition rates remain high. Recent advances in systems-oriented approaches (systems-biology and/or pharmacology) and 'omics technologies has led to a plethora of new computational tools that promise to enable a more-informed and successful implementation of the reductionist, one drug for one target for one disease, approach. These tools, based on biomolecular pathways and interaction networks, offer a systematic approach to unravel the mechanism(s) of a disease and link them to the chemical space and network footprint of a drug. Drug discovery can draw upon this holistic approach to identify the most-promising targets and compounds during the early phases of development.

Keywords: drug discovery; multi-omics data; pathway analysis; systems pharmacology; network pharmacology.

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