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(54) **HARNESSING NETWORK BIOLOGY TO  
IMPROVE DRUG DISCOVERY**

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(57) **ABSTRACT**

This invention provides principles, methods and compositions for ascertaining the mechanism of action of pharmacologically important compounds in the context of network biology, across the entire scope of the complex pathways of living cells. Importantly, the principles, methods and compositions provided allow a rapid assessment of the on-pathway and off-pathway effects of lead compounds and drug candidates in living cells, and comparisons of lead compounds with well-characterized drugs and toxicants to identify patterns associated with efficacy and toxicity. The invention will be useful in improving the drug discovery process, in particular by identifying drug leads with desired safety and efficacy and in effecting early attrition of compounds with potential adverse effects in man.

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Figure 1 Drugs regulate the behavior of cells within the organs of the body by perturbing cellular networks

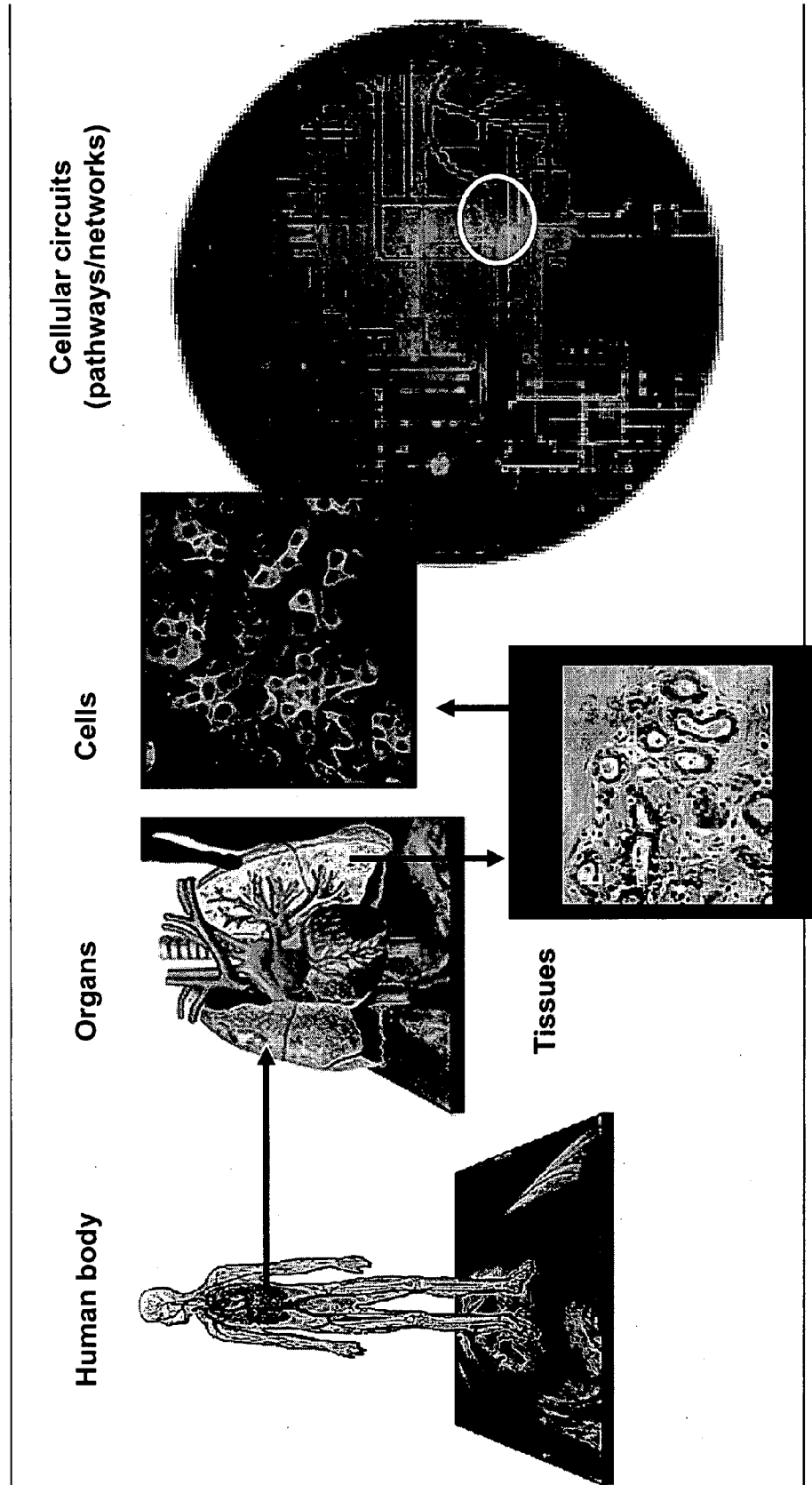


Figure 2. Drugs have known effects (on their intended targets) within cells. Drugs also have unknown effects on other targets and pathways in living cells.

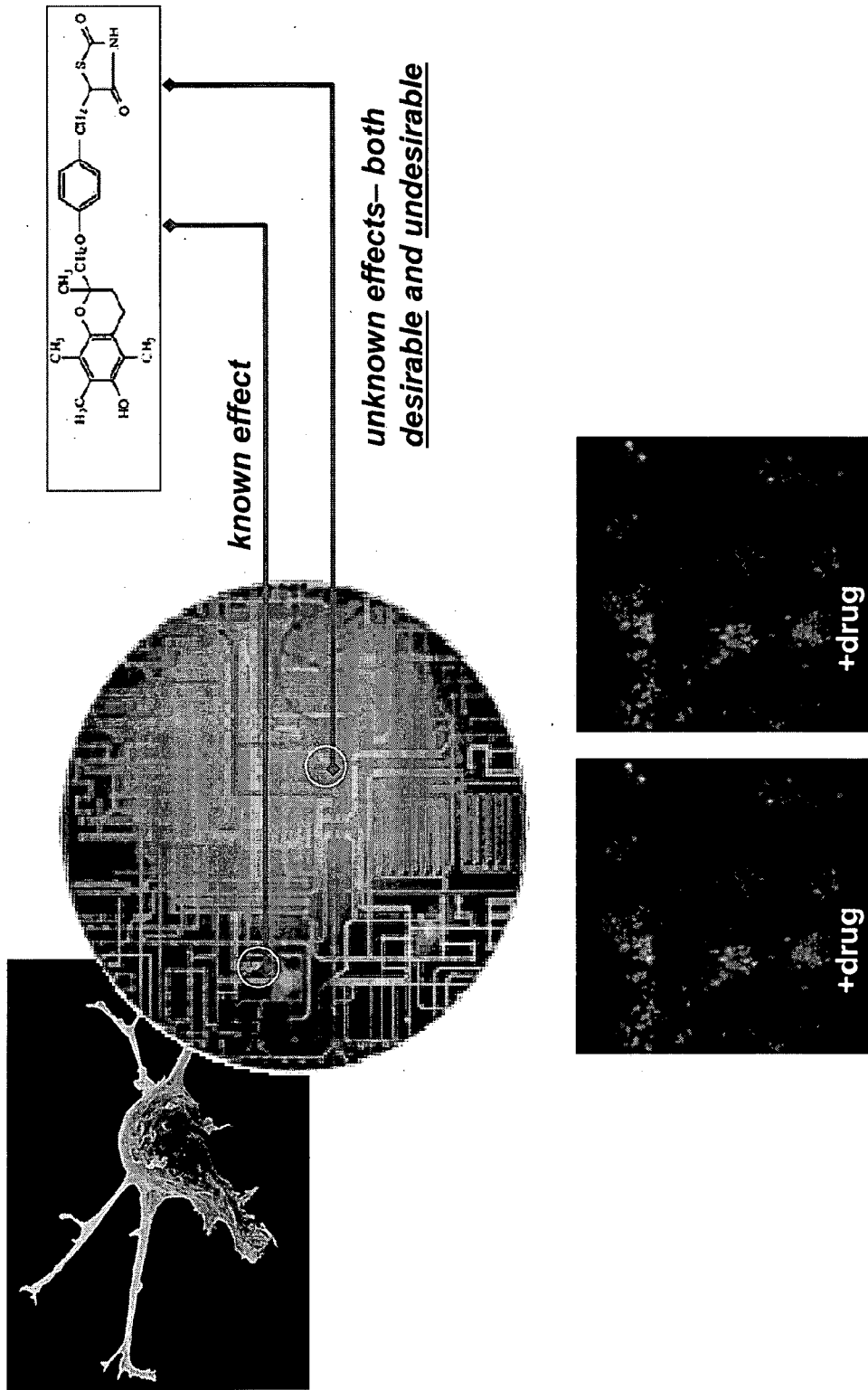
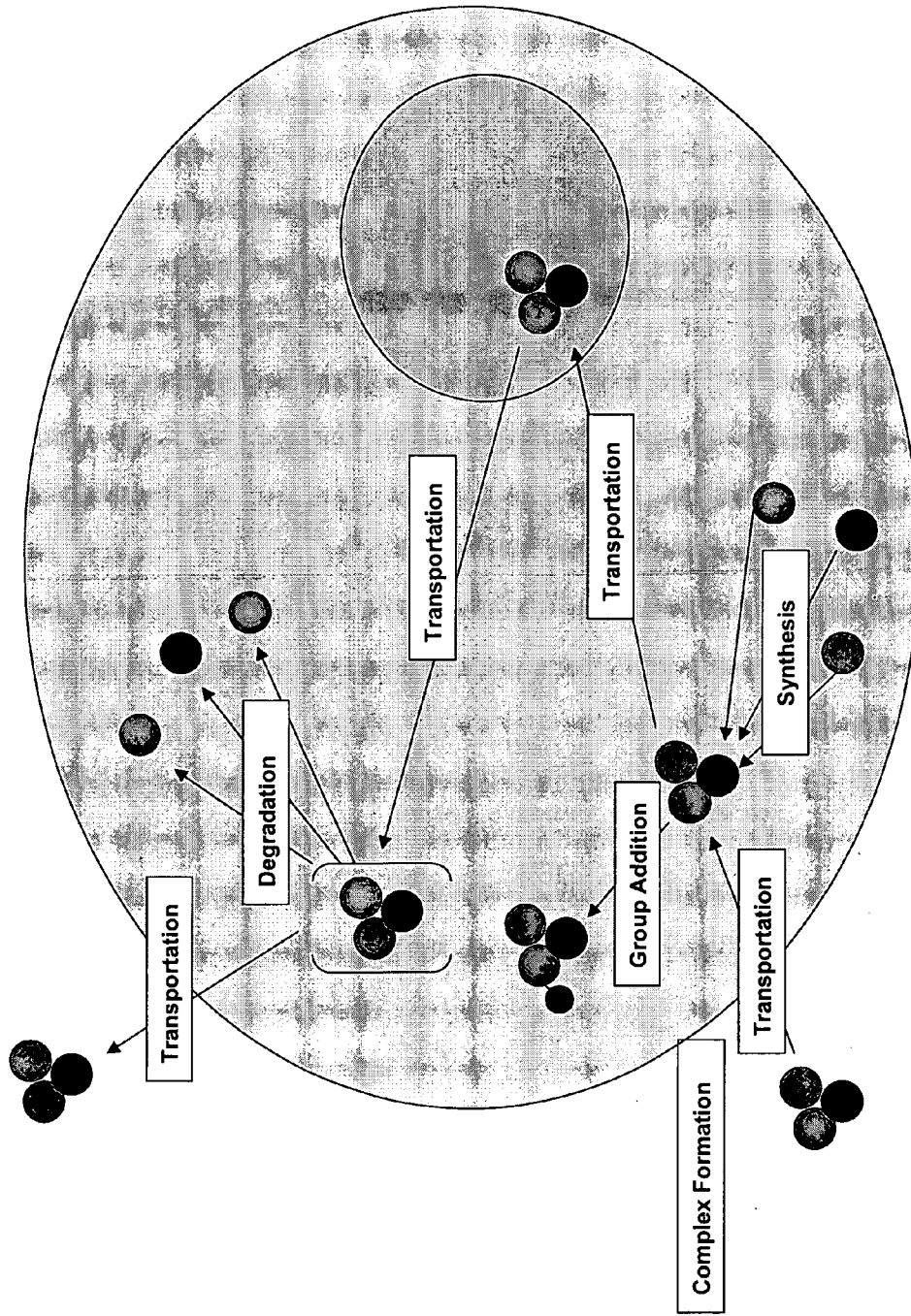
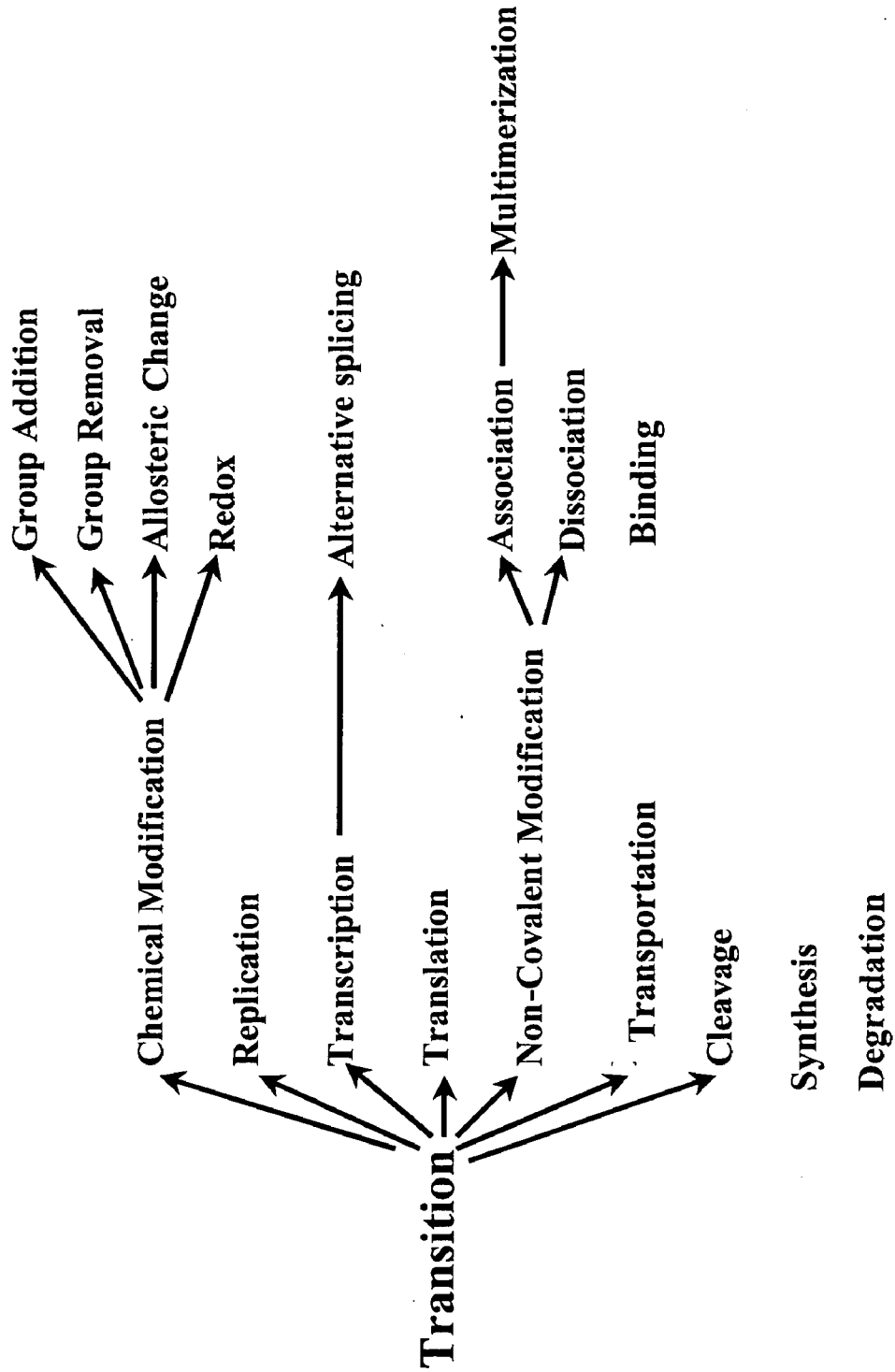


Figure 3. Cellular networks are controlled by molecules that undergo transitions.



From: E. Demir et al. (2002) *Bioinformatics* 18 (7): 996-1003

Figure. 4 Examples of transitions which a molecule may undergo in a cell.



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