

Title: Graph theoretical analysis of atom transitions in human dopamine metabolism

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Abstract: Every metabolic network has a corresponding atom transition network where every reactant atom in every reaction is mapped to a product atom. Atom transition networks have several applications in computational biology, in particular in the design and analysis of isotope labeling experiments for intracellular flux estimation. Unlike metabolic networks, atom transition networks are graphs. Standard graph theoretical algorithms can therefore be applied to reveal properties of the corresponding metabolic network. For example, components of atom transition networks represent all possible paths a particular atom can take through a metabolic network, isomorphic components represent chemical moieties, and bridges between components arise from molecular symmetries. We demonstrate these concepts on a small atom transition network corresponding to dopamine metabolism in human cells and investigate the effects of introducing isotopically labeled atoms into the network.