Master Thesis proposal
Investigating the structure and organization of a
drug-target network

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This proposal is for a Master thesis in in the field of Systems Biology.
In databases such as DrugBank (www.drugbank.ca/), all currently known annotation of
the effects of a drug on its molecular targets is publicly available and can be queried. In
particular, the DrugBank database is a unique bioinformatics and cheminformatics resource
containing 7,680 drug entries (small molecules, peptides, nutraceuticals and over 6,000 experi-
mental drugs) and 4,270 non-redundant drug targets (e.g. enzymes, ion channels, receptors).
Each DrugCard entry contains more than 200 data fields, among which there is often a field
describing whether the drug acts as an agonist (activator) or as an antagonist (inhibitor)
on a target. The objective of the proposed thesis is to construct a drug-target network, i.e.,
a bipartite graph in which one type of nodes are the drugs and the other the targets, see
[4, 1] for examples. The edges we are interested in are those carrying information on the
agonistic/antagonistic nature of the drug-target interactions. The bipartite graph that we
intend to construct is therefore a signed bipartite graph. This type of graph is related to a
so-called “spin glass” in Statistical Physics, a prototype “disordered system”. The plan for
the thesis is to study a series of properties related to the ordered or disordered organization
of the resulting network (in the style of [3, 2], where analogous concepts are used in different
contexts), and to apply them to the understanding of drug synergies and drug repurposing.

The ideal candidate for the thesis will have a curriculum in Engineering or Computer
Science or Bioinformatics. Given that the nature of the work is essentially computational, a
background in Biology is not strictly necessary, although willingness to acquire some basic
notions is a prerequisite.

References
8(5):e1002503, 05 2012.