FEBRUARY 2021

IREADRX

Applied Research Organization in Life Sciences

Application of AI to understand Chemistry & Biology at Scale

The technology in iReadRx is about understanding drugs and their behaviour with the human (or animal) body. Our Core Hyphothesis is leverage ***Deep Neural Networks*** to extract patterns from images and text to solve novel domain-specific optimization problems.

We build tools and techniques that aid personalised medicine. We understand compound chemistry and its biological significance.

NATURAL LANGUAGE PROCESSING, DEEP NEURAL NETWORKS

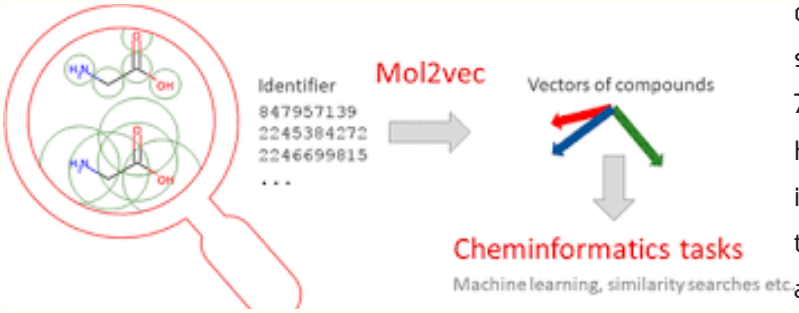
DEEPCHEM

AUTOML

RDKIT, MOL2VEC

Application Areas

1. **Understanding drugs :** When understanding drugs at a fundamental level levraging ***RDKit*** to **mol2vec** to **DeepChem**. .
2. **Other Drugs :** Search & Standardisation to extract Drug Data from other drug / chemical databases & create a homogenous drug (molecule) representation across multiple companies.
3. **Drug Interactions :** Chemical compounds that form a drug will have various reactions when combined with other chemicals in other drugs. Understanding the complex relationship between multiple drugs.



4. **Drug Research Database :** Information about chemical compounds might be present in the various documents such as scientific journals, patents or company documents. Parsing such documents and build a knowledge graph that can harness the information easily and extensively.

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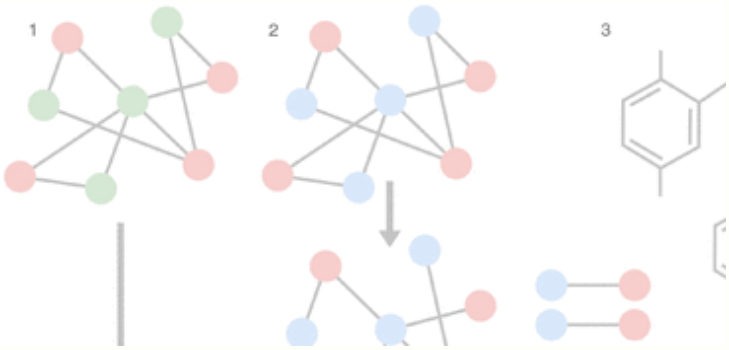
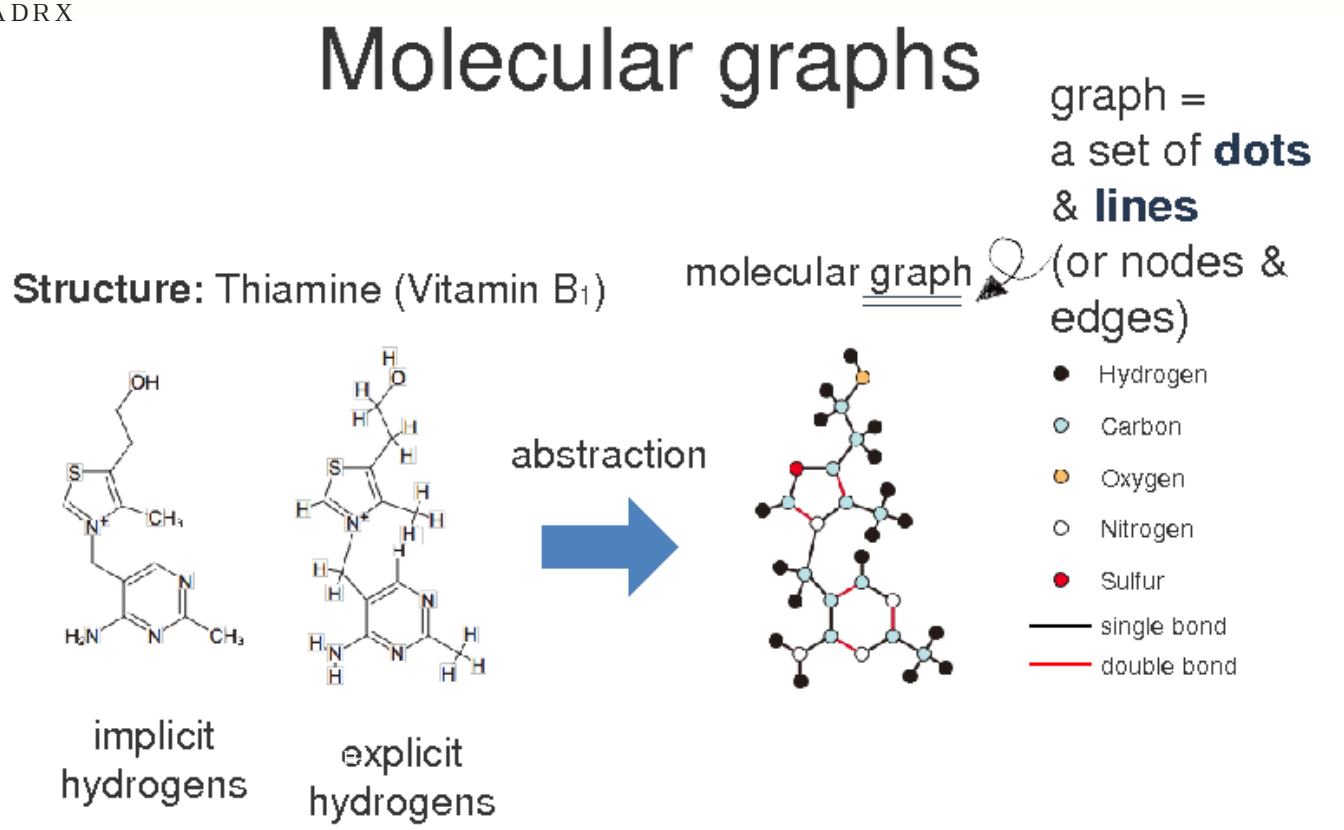
5. **Drug Research / Discovery :** Our ability to parse diverse (unstructured) documents into standardized document structure accelerates drug discovery and drug research. Information on any chemical compound would be immediately searchable and any information related to drug w.r.t side effects / benefits etc. will be automatically associated
6. **Biology of Clinical Trial Humans :** With the latest deep learning models, we can understand biological reactions for each drug / chemical compound. We have technology that can allow structured storage and retrieval of such interactions
7. **Drug Relationship Extraction :** We would have systems and tools that can capture the interaction between clinical trial humans and the drug development process. With predictive algorithms, we can also optimise the clinical trial process.



CURRENT PROJECTS

1. Automation in Drug Data Extraction & application of AI in Determinining Relevant Compounds from a Universe of Chemical Compounds
2. Molecular Data Organiser using Content Swamp & Data Lakes



8. **Biology of Real World Humans :** We have known cases where real world data isincreasingly becoming different from the clinical trial sampling of population. Minor genetic mutations among the human population and lifestyle habits have made human bodies react differently to different drugs. Storing large volumes of data for large populations can be computationally challenging. But, with the right tools, this challengeis not insurmountable. With our technological capability, we can offer pharma companiesto scale their analytics to terabytes.

9. **Drug Interactions on RWD :**Fitness gadgets or Fitness applications are capturing key metrics from larger populations using newer technology. All the big-data collected cannot be processed through conventional analytics tools. Our custom solutions can scale and give great insights into the drug behaviour on real world data. With stricter standards in pharmacovigilance, these techniques might be mandatory soon.

10. Bridging the gap between clinical trials and real world : The ultimate aim of pharma is personalisation of medicines. Every human body is different in its own way. Hence, it's important to have a good representation of all humans in the clinical trial phase to achieve personalization of medicine. We can capture the nuance in biology and help continuously improve the trials.

APPLIED RESEARCH AREAS

- Deep learning for molecular design —a review of the state of the art
- Deep Learning for Computational Chemistry
- Deep learning framework for repurposing drugs
- Machine Learning Methods in Drug discovery
- SMILES Transformer: Pre-trained Molecular Fingerprint for Low Data Drug Discovery