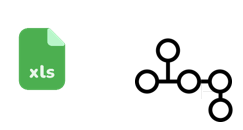
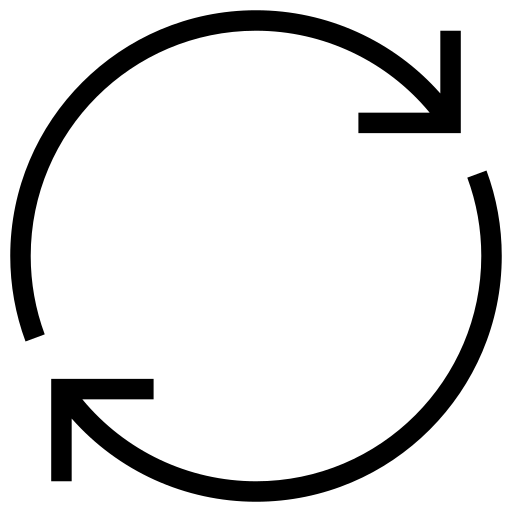
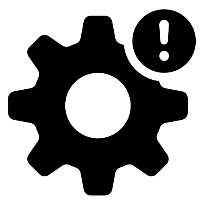
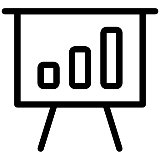
**Data Pre-Processing**

**Data Gathering/Cleaning**

**Drug ID/Side Effect Pairs**







**User Presentation**

**GCN Training**

**Explainable Method Analysis**

WHERE EACH IMAGE IS FROM:

**Drug ID/Side Effect Pairs:** Dissertation poster

**Data Gathering/Cleaning:** <https://www.iconfinder.com/icons/7267712/ext_xls_excel_spreadsheet_microsoft_file_format_extension_document_icon>

**Data Pre-Processing:** <https://www.iconfinder.com/icons/7106332/data_element_infographic_organization_graph_structure_icon>

**GCN Training:**

<https://www.iconfinder.com/icons/3209452/circle_processing_redo_refresh_reload_icon>

**Explainable Method Analysis:**

<https://www.iconfinder.com/icons/6843099/alert_gear_notice_operational_risk_processing_risk_trouble_icon>

**User Presentation:**

<https://www.iconfinder.com/icons/4230550/analytics_board_presentation_icon>

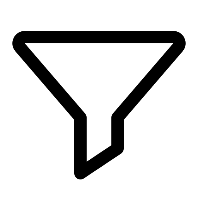
FOR DATA GATHERING AND ANALYSIS:

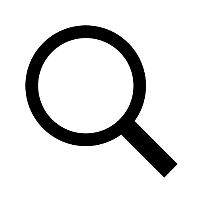
**Remove Non-3D Values**

**Decagon Polypharmacy Dataset**

**Retrieve 3D values from PUG-REST API**







**Filter Side Effects with >4000 Samples**

**Descriptive Analysis**

**Calculate Bond Lengths**

WHERE EACH IMAGE IS FROM:

**Decagon Polypharmacy Dataset:** <https://www.iconfinder.com/icons/7267712/ext_xls_excel_spreadsheet_microsoft_file_format_extension_document_icon>

**Retrieve 3D values from PUG-REST API:**

<https://www.iconfinder.com/icons/532742/api_code_coding_gear_programming_settings_window_icon>

**Remove Non-3D Values:**

<https://www.iconfinder.com/icons/9004715/cross_delete_remove_cancel_icon>

**Calculate Bond Lengths:**

<https://www.iconfinder.com/icons/653269/calculator_accounting_calculate_calculation_math_school_icon>

**Descriptive Analysis:**

<https://www.iconfinder.com/icons/211817/search_strong_icon>

**Filter Pairs with >4000 Samples:**

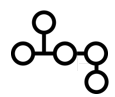
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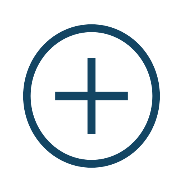
FOR DATA PRE-PROCESSING:

**Compute Features, Edge Indexes and Edge Attributes**

**Create Graph Pairs**

**3D Compound Data**





**Create Data Objects**

**Concatenate Graph Information**

**3D Compound Data:**

<https://www.iconfinder.com/icons/7267712/ext_xls_excel_spreadsheet_microsoft_file_format_extension_document_icon>

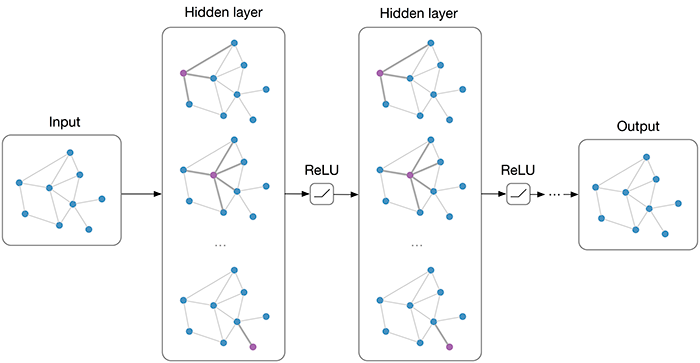
**Create Graph Pairs:** <https://www.iconfinder.com/icons/7106332/data_element_infographic_organization_graph_structure_icon>

**Compute Features, Edge Indexes and Edge Attributes**

<https://www.iconfinder.com/icons/653269/calculator_accounting_calculate_calculation_math_school_icon>

**Concatenate Graph Information;**

<https://www.iconfinder.com/icons/1814113/add_more_plus_icon>



[Input Data] -> [GCN Layer 1] -> [ReLU] -> [GCN Layer 2] -> [ReLU] -> [GCN Layer 3] -> [ReLU] -> [Attention Mechanism] -> [Pooling] -> [Fully Connected Layer] -> [Log Softmax] -> [Output Probabilities]

**ReLu**

**ReLu**

**ReLu**

**Attention Mechanism**

**Hidden Layer**

**Hidden Layer**

**Hidden Layer**

**Input**

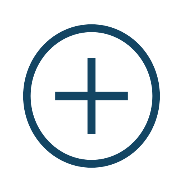
**Pooling**

**Output**

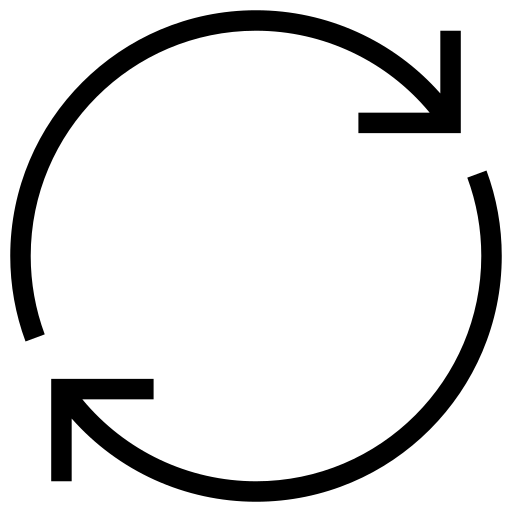
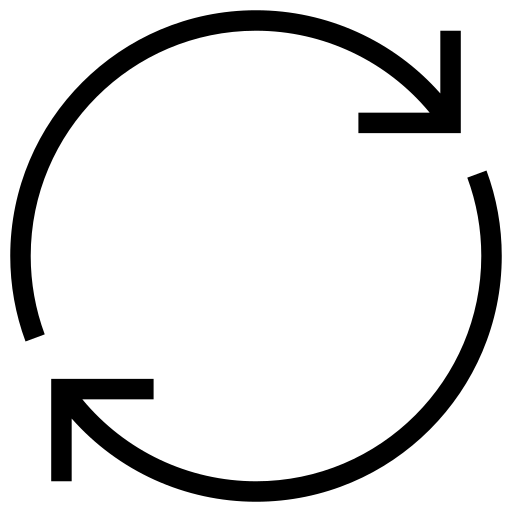
**Fully Connected Layer**



**SMILES Strings**



**Concatenate SMILES**



**LSTM Model**

**2D-GCN Model**

**SMILES Strings:**

<https://www.iconfinder.com/icons/7267712/ext_xls_excel_spreadsheet_microsoft_file_format_extension_document_icon>

**Concatenate SMILES:**

<https://www.iconfinder.com/icons/1814113/add_more_plus_icon>

**Models:**

<https://www.iconfinder.com/icons/3209452/circle_processing_redo_refresh_reload_icon>

