**Supplemental Table S2: Similarity measure methods and defined abbreviations of all drug data.**

| **Data of drugs** | **Similarity measure method** | **Defined**  **abbreviation** |
| --- | --- | --- |
| Chemical structures | Tanimoto coefficient | Structures |
| Drug-disease associations | Jaccard similarity | DDA\_Jac |
| Cosine similarity | DDA\_Cos |
| Drug-drug interactions | Jaccard similarity | DDI\_Jac |
| Cosine similarity | DDI\_Cos |
| Drug side effects | Jaccard similarity | SE\_Jac |
| Cosine similarity | SE\_Cos |