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Editorial

Data Mining in Drug Discovery

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DATA MINING

Today, within the modern business world the financial crisis has increased the main target on Business Intelligence. The giants that pioneered Business Intelligence (BI) made a crucial discovery that the trail to true business intelligence passes through a knowledge Warehouse. "A data warehouse may be a subject-oriented, integrated, time variant and non-volatile collection of knowledge in support of management deciding process. Automated data collection tools and mature database technology cause tremendous amounts of knowledge stored in databases, data warehouses and other information repositories. The answer for the info explosion problem is data processing. Data processing is that the Knowledge Discovery within the databases that's the Extraction of interesting (non-trivial, implicit, previously unknown and potentially useful) information or patterns from data in large databases. Data processing is that the process of extracting hidden patterns from large amounts of knowledge.

"Drug Discovery today conceptualizes on the involvement of chemo informatics to beat the shortcomings of the normal Drug development process. Drug Discovery with the utilization of Chemo informatics and data processing generates large numbers of related chemical compounds. It accelerates the drug discovery in two ways: It can generate several million structurally related chemical molecules. By increasing the chemicals available for testing, the probabilities of finding a drug lead could also be higher. If you recognize the biological effects of various molecules, you'll combine them to form chemicals with particular designed biological effects.

Chemo informatics (Chemical Informatics) is that the use of Computer and knowledge Technology, applied to a variety of problems within the field of Chemistry. It transforms the info into information and knowledge into knowledge for the intended purpose of creating better decisions faster within the area of drug identification and optimization. With data processing, throughout drug discovery, data is collected relating chemical structures to every other. The info Mining Technique "Clustering Process" divides the databases of unknown drugs in clusters supported their similarity. It makes use of Lipinski Rule which defines those compounds as Drug like which have properties implicit to drug likeness like log p, relative molecular mass , Number of chemical bond acceptors and donors during a molecule etc. The clusters of unknown similar drugs are evaluated and compared with the clusters of some specific (e.g. HIV) drugs to get from unknown drugs those drugs that are similar in properties with the known drugs.

Drug discovery using data processing

An Active Pharmaceutical Ingredient is employed to develop the code, algorithms and therefore the interface. Microsoft Access is employed because the backend for storing the drugs. The system would allow the user to seek out the clusters of unknown similar drugs and compare them with the clusters of some specific (e.g. HIV) drugs to get from unknown drugs those drugs that are similar in properties with the known drugs. The access rights aren't a problem because this software is made keeping in mind the freeware concept. The summary of the main functions the software will perform are:

Creating of DNS directly if the database is already attached or browse for data marts if not already uploaded.

After the DNS creation, the info marts are often integrated into a knowledge Warehouse.

Cleaning are often done on the info Warehouse to get rid of noisy and inconsistent data.

Clustering are often done to seek out clusters of medicine similar in chemical properties.

Pattern evaluation is often done using Tanimoto Coefficient and structural similarity.

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