COMPUTER SOFTWARE USED IN PHARMACY AND PHARMACEUTICAL RESEARCH

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Software and computer based programs used during new drug discovery and development

Software for Pharmacokinetic parameters

Software name	Major use
DDPlus	Dissolution and disintegration study
GastroPlus	In vitro and in vivo correlation for various formulations
Map Chek	Compare dose or fluency measurement

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2.ligand interactions and molecular dynamic

Sr.no	Software name	Major use
1	Auto Dock	Evaluate the ligand –protein interaction
2	Schrodinger	Ligand –receptor docking
3	GOLD	Protein –ligand docking
4	bio Suite	Genome analysing and sequence analysing

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3. Molecular modelling and structural activity relationship

Sr no	Software name	use
1	Maestro	Molecular modelling analysis
2	PASS	Create and analysis of SAR models
3	GRAMM	Protein –protein docking and protein ligand docking

Data analysis

REST 2009 software	Analysis of gene expression data

Behavioural study	
Ethowatcher	Behaviour analysis
MARS(multimodal animal rotation system)	Animal activity tracing, enzyme activity

Computer aided techniques used in drug design and discovery

TECHNIQUE	ROLES IN DRUG DESIGN AND DISCOVERY
Docking	Predict binding mode and approximate binding energy of compound to a target
Structural based virtual screening	Identify active compounds for a specific target from a chemical library based on docking techniques
Pharmacophore modelling	Perceive and provide description of molecular features necessary for molecular ligand by a biological macromolecule
ADMET prediction	Prediction of ADMET of chemical substances in the human body to avoid costly later stage failure drug development

Computers in pharmaceutical analysis

- Analytical instruments use computer designed software.

- Data storage and processing

- Building up libraries

- HPLC(Wincarts Software) , IR(Lab solution) Spectrophotometers and all other instruments.

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Informatics pharmacist

Pharmacist who serve as a translational bridge between IT staff and clinicians, and are experts in health information system and technology.

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New uses for computer in medical education ,clinical practice, And patient safety in the US and Japan

- Rapid expansion of computer use in medicine medical education at all levels ,point of service medical information (diagnostic , treatment , and medications) ,medical research , electronic billing, electronic prescribing, and the collection of data to determine quality of care .

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Clinical Software

These software consist of integrated suits of application s that support clinical research process, including various ways of data collection, data enter , batch data load.

Some example of software –

> 1-oracle clinical V4IR from Oracle Corporation

> Data labsXCR from data labs, Inc.

> Cliniplus R Data management from DZC software solution, Inc.

> Openclinica by AKARA Research (Cambridge, MA)

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Approach for Pharmacokinetic study with help of software

There are different approaches to pharmacokinetic study using differential equation with the help of software

➤ NONLIN is software which allow to perform statistical regression analysis to estimate the value of parameters for linear function.

➤ KINPAK is software used to obtain AUC, Cmax (peak plasma concentration),tmax(peak plasma time).

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conclusion

- Software used for pharmacokinetic profile
- Ligand interaction and molecular dynamic used in GOLD and SCHRODINGER Software
- Data analysis for REST 2009 software
- Computer aided drug design and discovery used in techniques .
- Pharmaceutical analysis used in software .
- HPLC (Lab solution)
- Pharmacokinetic used in NONLIN and KINPAK software.

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