Examples of MD codes:

LAMMPS

DL_POLY

NAMD & VMD

Materials Studio

GROMACS

AMBER

CHARMM

OPLS

Can use molecular databases of known substances – easy to obtain 'pdb' files, topology files – can then automatically create parameters – and model

drug molecule acts on receptor – both are smaller than cells

PROBLEMS arise – due to unknown drug – receptor interactions or drug-drug interactions or drug – enzyme interactions

Drug/recept/enzyme all are proteins (size)

Drug stability in blood conditions/water/fat etc.

Cancer drugs – gene dependent – population modelling

Drugs – are proteins and if have similar structure can share some effects – so can rule out some drugs that haven't worked before with similar structure? Predict side effects possibly… from structure. – require database 0 use existing literatures.

Modelling of drugs in the body – blood systems.

Drug stability in stomach – acid. Protein could denature due to acid – bad.

Drug pH – ion interactions

Drug – interacts with fat molecules (skin), or with muscles (proteins)

QSAR! – quantitative structure-activity relationships

http://books.google.co.uk/books?hl=en&lr=&id=XZzecES9KZ8C&oi=fnd&pg=PP8&dq=3D%E2%80%90QSAR+tools&ots=2vF58M3WaQ&sig=Fm0tyxgoeBkCn8j8gsvqW4b3iwk#v=onepage&q=3D%E2%80%90QSAR%20tools&f=false

Tripos sell a SYBYL-X product:

http://tripos.com/index.php?family=modules,SimplePage,,,&page=SYBYL-X

http://www.tripos.com/tripos_resources/fileroot/pdfs/TC%20white%20paper_FINAL.pdf

http://tripos.com/index.php?family=modules,SimplePage,tripos_tribune

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some sort of link between molecular and population modelling –

use trends of diseases that affect similar people – identify trends

identify aspects of people which normally react badly to drugs.

Case Studies: