Drug design
Drug repositioning
Virtual screening

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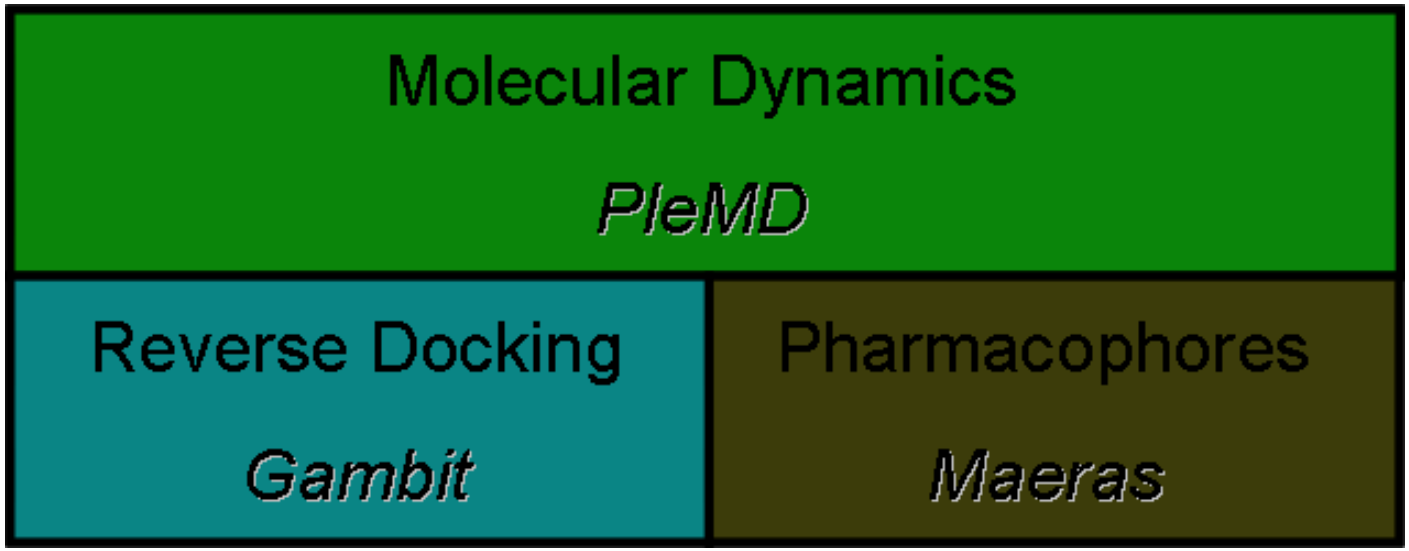
Plebiotic services

- Drug design & re-design
- Drug repositioning
- Virtual screening
- Homology modeling
- Library generation (combinatorial chemistry)
- Docking
- Molecular dynamics
- Enzymes design
- Biotechnological consulting

Plebiotic has a strong biology and computer science team that has created proprietary Molecular Dynamics, reverse docking and pharmacophores products. In combination with a high biotechnological expertise and deep customer commitment, we can help your company in the early stages of molecular design and testing

Plebiotic portfolio

- Molecular Dynamics (PleMD)
- Reverse docking (Gambit)
- Pharmacophores (Maeras)



Plebiotic differential aspects

- Propietary products
  - Molecular Dynamics (PleMD)
  - Reverse Docking (Gambit)
  - Pharmacophores (Maeras)
- Ultra fast Molecular Dynamics solution (PleMD)
  - Best *speed & quality/price* ratio in the market
  - Allows for very long simulations with standard GPU hardware
  - Allowing the understanding of the action mechanism of drugs
  - Very accurate – backed up by *in vitro* and *in vivo* testing
- Unique Reverse Docking product (Gambit)
  - In combination with pharmacophores (Maeras) and molecular dynamics (PleMD), constitutes a perfect platform for drug repositioning
- Gives a flexible, end to end service to customers
  - Outstanding biology and computer science professionals

What is Molecular Dynamics?

Molecular Dynamics (MD) simulates dynamic interactions among atoms in complex life molecules

- Docking is static, thus gives false positives. It has to be complemented with a dynamic analysis: Molecular Dynamics. With MD we understand the action mechanism of drugs with direct application on these key areas:
  - Drug re-design and reprofiling: MD gives qualitative and quantitative information on how drugs work and we can optimize their design.
  - Effective Virtual Screening: Avoiding false positives or negatives.
  - Reduction of side effects: Detailed toxicity analysis.

MD is a fast and effective solution to understand how drugs work with applications to drug design and Virtual Screening

Who can use Molecular Dynamics

Molecular Dynamics (MD) is a novel technique already in use in many drug discovery processes

Plebiotic increases usability of MD:

- Dramatically increasing the speed of the simulations
- Improving the results analysis
- New models allow MD for extremely big proteins
- Integrating MD with other Plebiotic and standard tools
- Offering end to end customer services to our customers

MD has already proven its value in many Drug Discovery processes.

Drug discovery successes based on Molecular Dynamics[1,2,3]

Examples of commercial AIDS drugs designed with MD

Commercial name	Pharma Company	Indication
Zidovudine	Bristol-Myers Squibb	AIDS
Viracept	Agouron Pharmaceuticals	
Crixivan	Merck	
Amprenavir	Glaxo Wellcome	

Other drugs designed with MD

Commercial Name	Pharma Company	Indication
Zomig	Astra Zeneca	Migraine
Trusopt	Merck	Glaucoma
Noroxin	Kyorin Pharmaceuticals	Urinary Tract Infection
Aricept	Eisai	Alzheimer´s disease
Viagra	Pfizer	Impotence

1. Schlick, T. (2010). *Molecular Modeling and Simulation: An Interdisciplinary Guide: An Interdisciplinary Guide* (Vol. 21). Springer.
2. Schlick, T., Collepardo-Guevara, R., Halvorsen, L. A., Jung, S., & Xiao, X. (2011). *Biomolecular modeling and simulation: a field coming of age. Quarterly reviews of biophysics*, *44*(2), 191-228.
3. Talele, T. T., Khedkar, S. A., & Rigby, A. C. (2010). *Successful applications of computer aided drug discovery: moving drugs from concept to the clinic*. *Current topics in medicinal chemistry*, *10*(1), 127-141.

Other reference:

- Molecular dynamics simulations and drug discovery, Jacob D Durrant and J Andrew McCammon, BMC Biology 2011,9:71

Reverse docking

- Reverse docking
  - Given a ligand, we look for other targets suited for it
  - Direct application on drug repositioning
- Plebiotic reverse docking platform (Gambit)
  - Novel technique
  - Makes use of the biggest collection of human proteins
  - In combination with pharmacophores and molecular dynamics, it is a very strong tool for drug repositioning

Use of Plebiotic products

Plebiotic has worked or is currently working on customer projects in the following areas:

- ***Virtual Screening (VS) of a compound library***
- ***Better understanding mechanisms of action of drugs***
- ***Drug reprofiling by combinatorial chemistry and VS***
- ***Drug reprofiling by analysis of the active zone***
- ***Drug reprofiling by pharmacophores and reverse docking***
- ***Toxicity analysis***

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