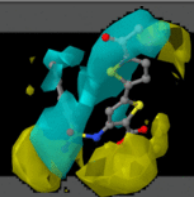


Pharmacophoric Model:LigandScout

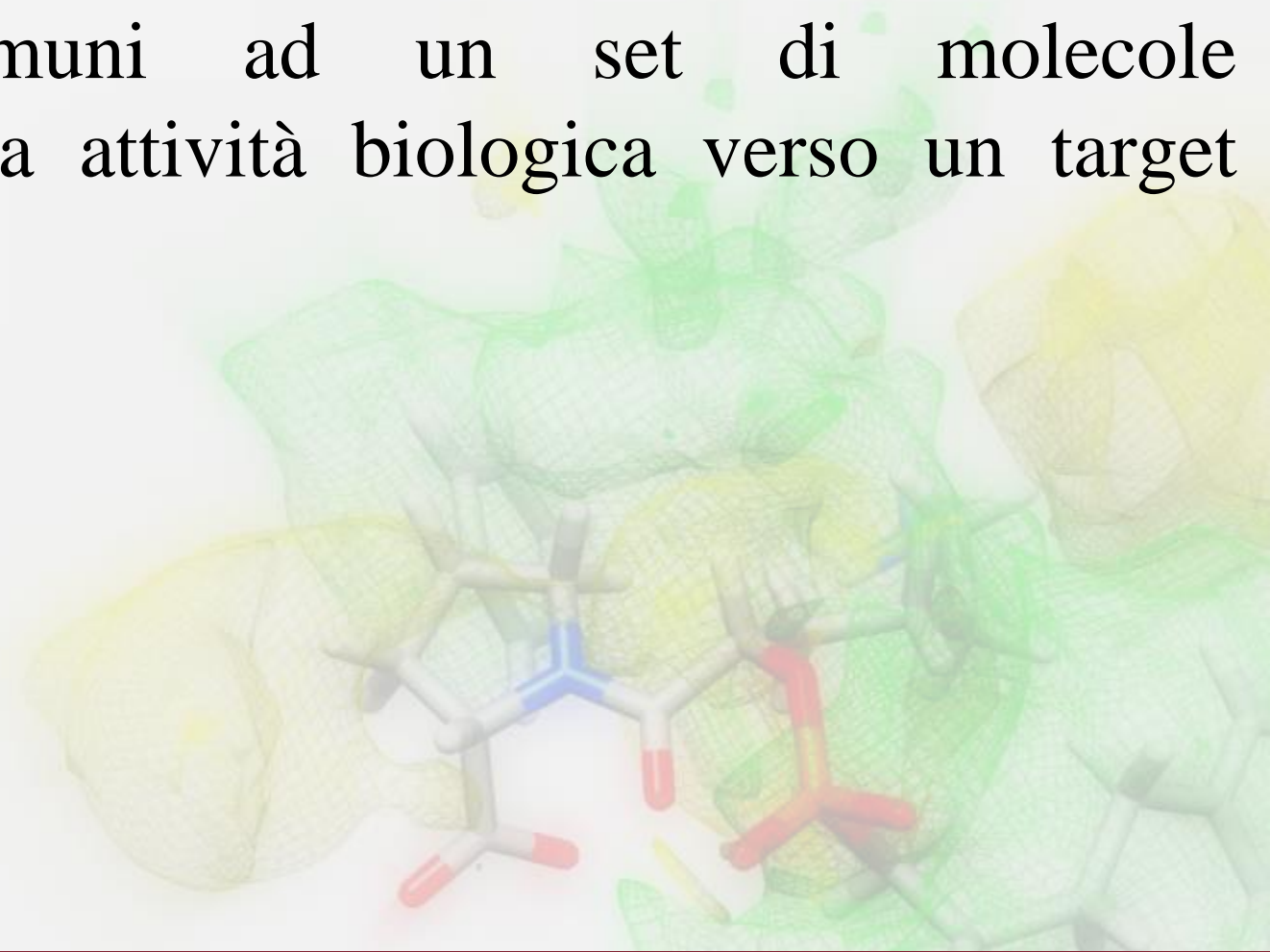


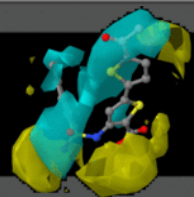
SAPIENZA
UNIVERSITÀ DI ROMA



COS'È UN FARMACOFORO?

Farmacoforo è l'insieme degli elementi strutturali o funzionali comuni ad un set di molecole caratterizzate da attività biologica verso un target biologico





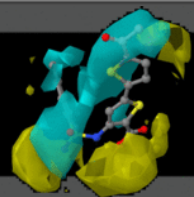
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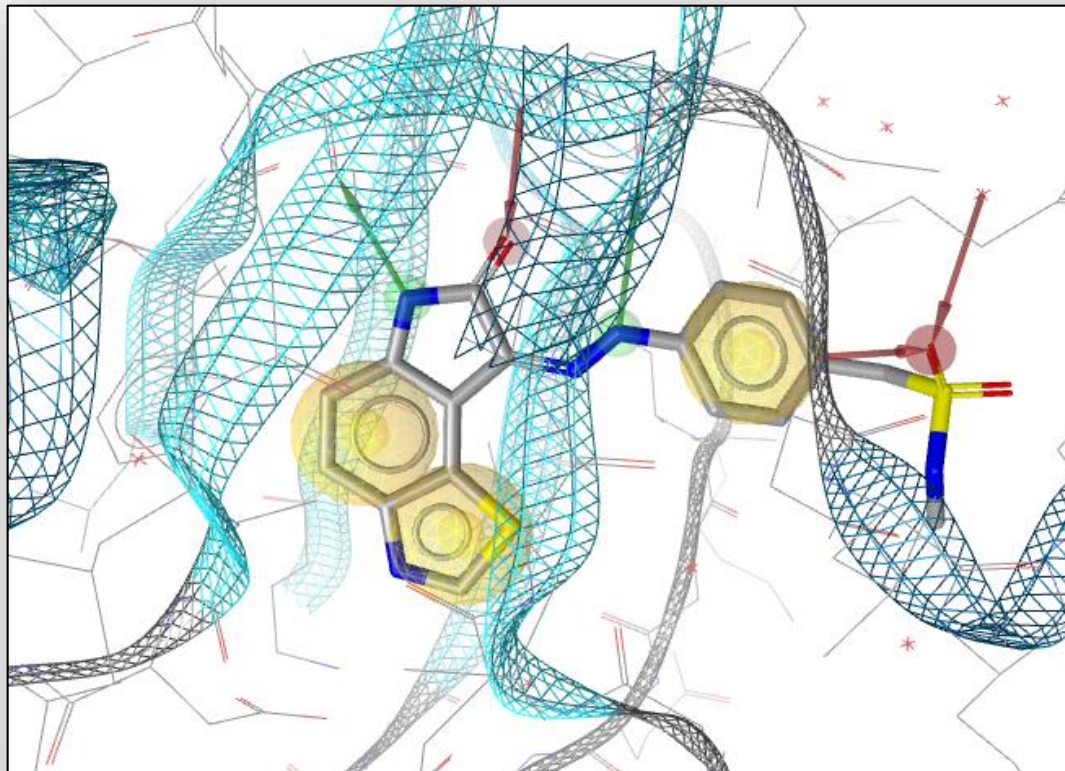


1998
Camille Wermuth

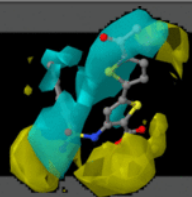
Farmacoforo è l'insieme delle features steriche ed elettrostatiche necessarie a garantire un'interazione intra-molecolare ligando-recettore tale da scatenare una risposta biologica.



COS'È UN FARMACOFORO?



Farmacoforo Structure-based



Download
complesso

Verifica
correttezza
del dato

Analisi punti
farmacoforici

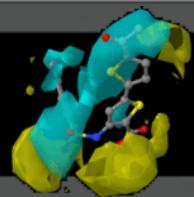
Gruppi
potenziali

Interazioni
potenziali

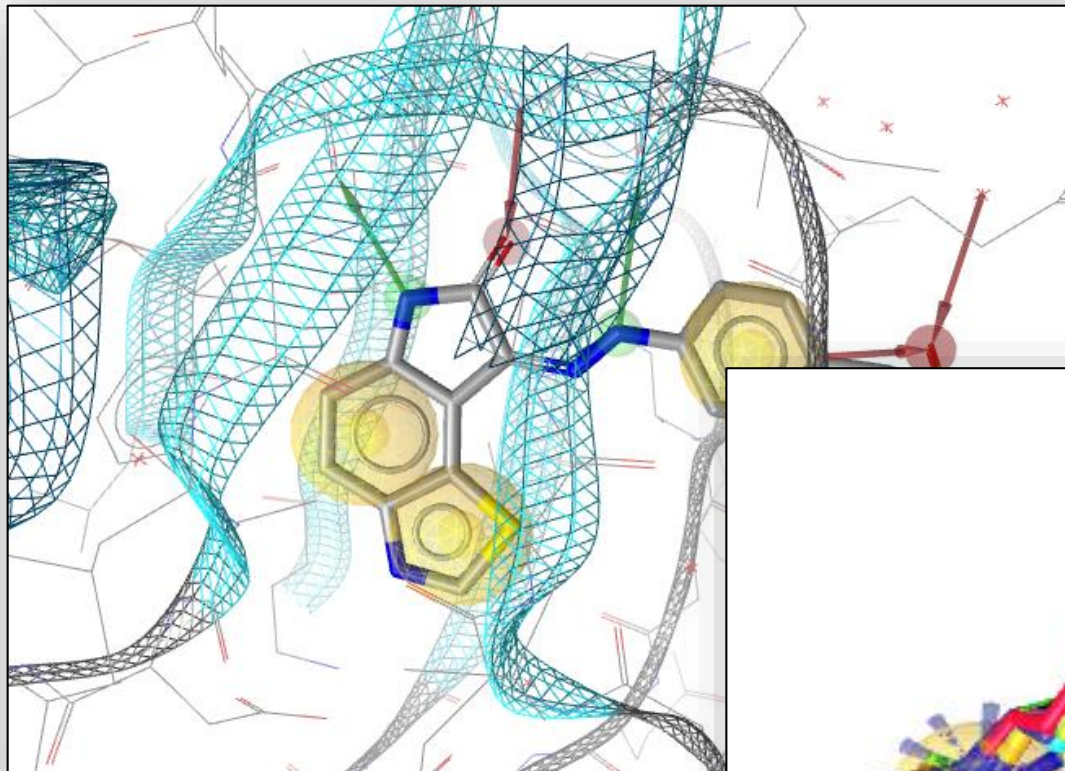
Posizionamento
delle features

Verifica
dei
requisiti
geometrici

Inserimento
delle sfere di
esclusioni

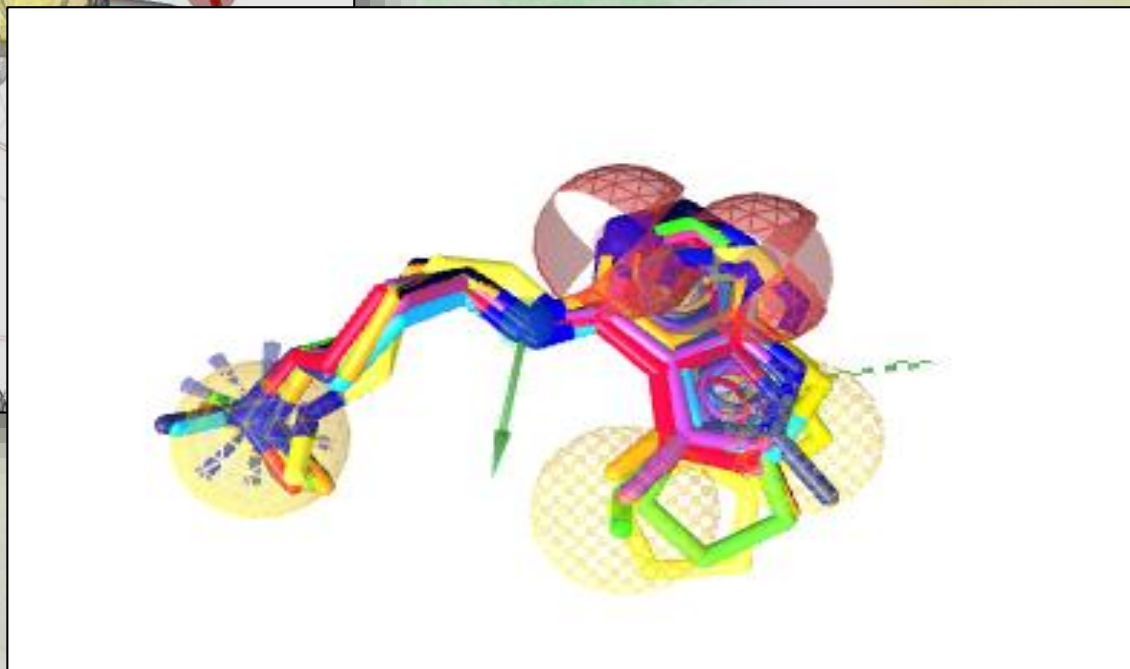


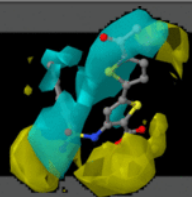
COS'È UN FARMACOFORO?



Farmacoforo Structure-based

Farmacoforo Ligand-based





FARMACOFORO LIGAD-BASED

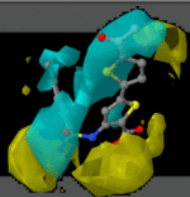
Ottenimento
del data set

Analisi
conformazion
ale

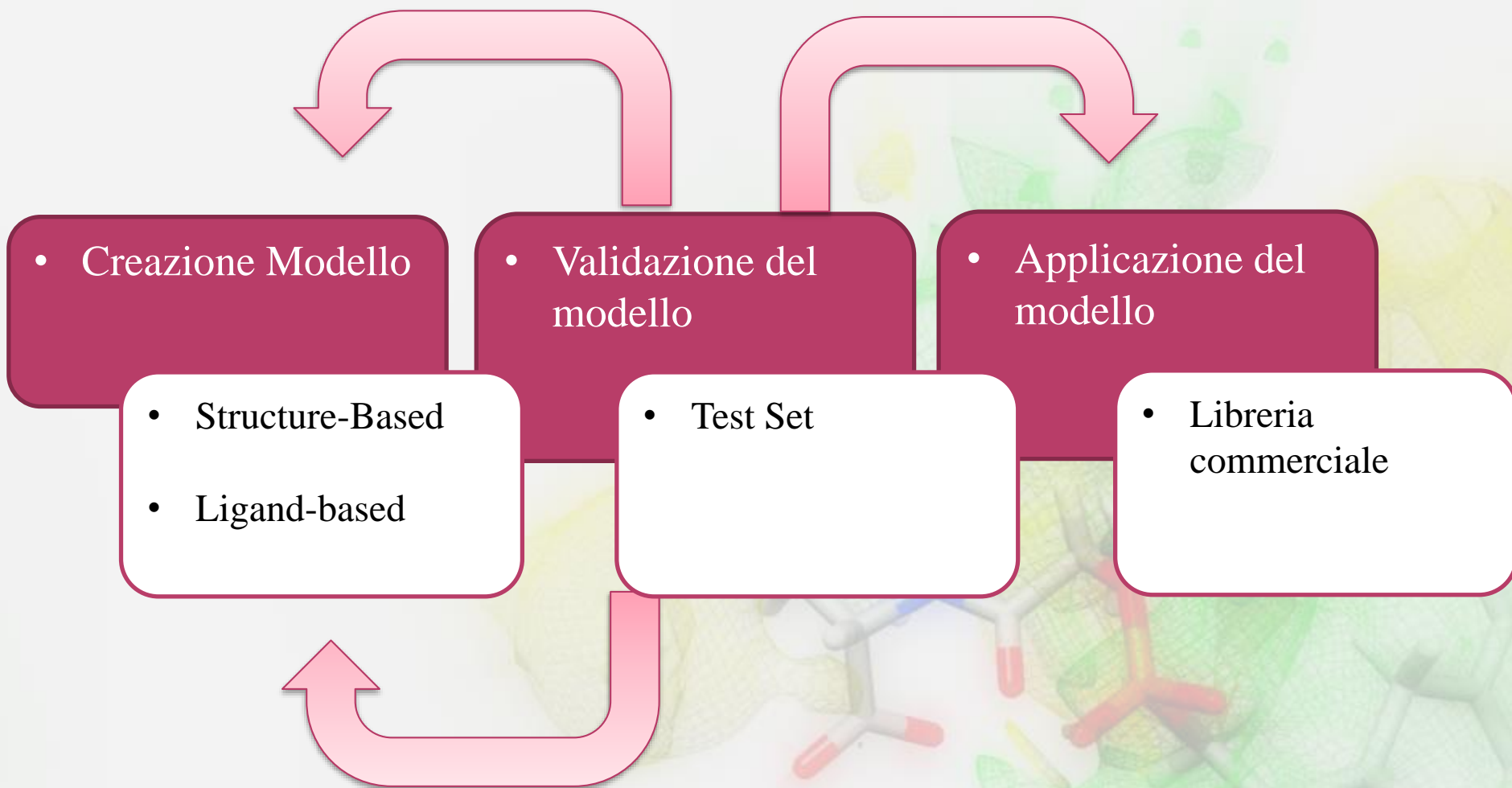
Creazione
modelli
farmacoforici

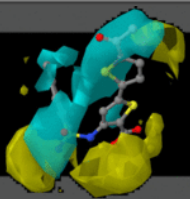
Allineamento
dei modelli
farmacoforici

Ottenimento
dei modelli
ottimali

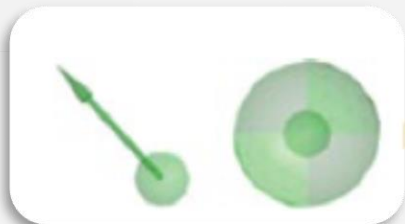


WORKFLOW

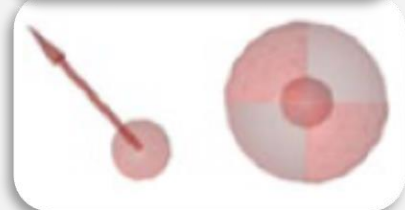




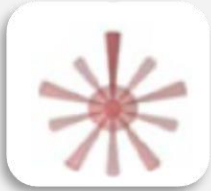
PUNTI FARMACOFORICI



Donatore Legami idrogeno



Accettore Legami idrogeno



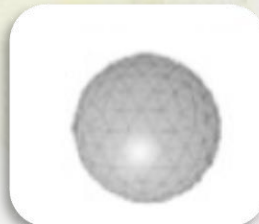
Area ionizzabile



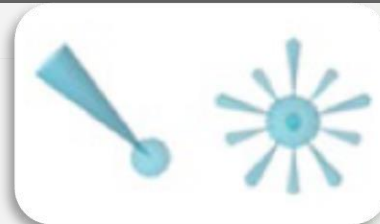
Interazioni idrofobiche



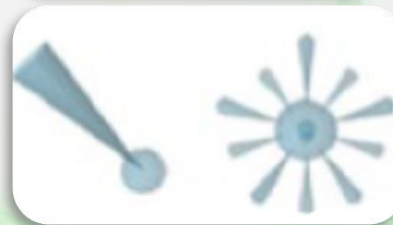
Anelli aromatici



Excluded Volume



Magnesium Binding Location



Zinc Binding Location



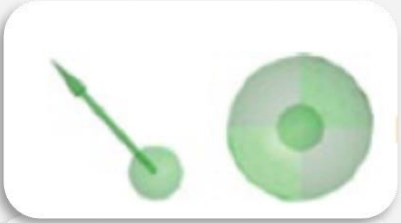
Iron Binding Location



Manganese Binding Location



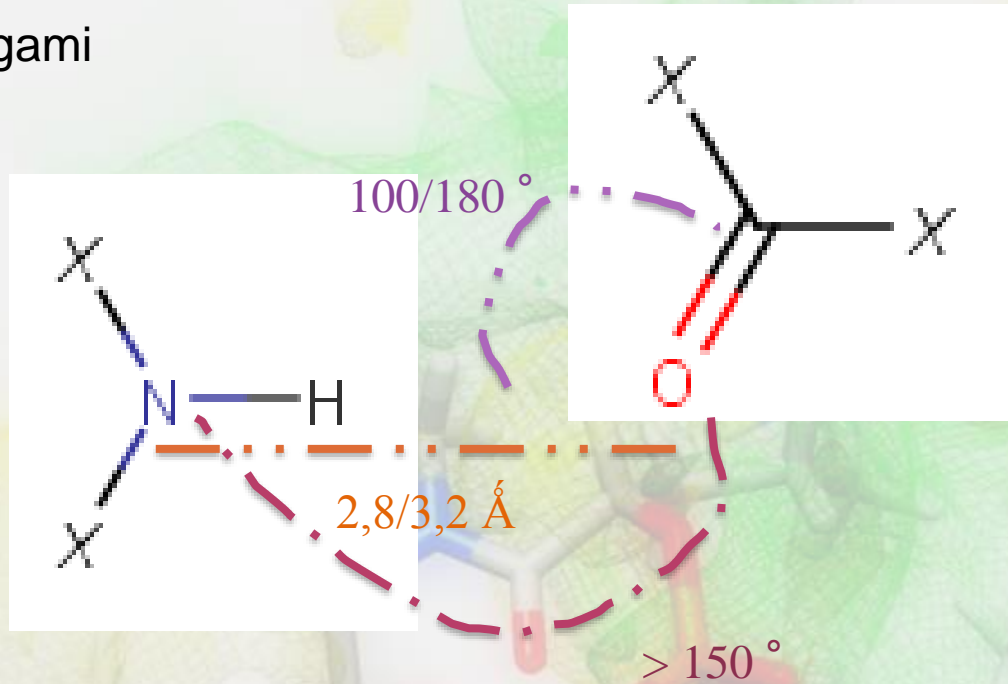
LEGAMI IDROGENO



Donatore Legami
idrogeno



Accettore Legami
idrogeno





Anelli aromatici

