Ligand Docking of Lincomycin and *Escherichia Tenella*

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Abstract: *Escherichia Tenella* is a parasite derived from class Sporozoa. It causes cecal Coccidiosis in poultry. Coccidiosis causes economic loss in the poultry industry because it causes death in young chickens that are raised for meat consumption. Lincomycin is a lincosamide antibiotic that comes from the actinomyces *Streptomyces lincolnensis*. It can be administered in pure form or with a combination of water or feed. It is known to effectively treat Coccidiosis. Ligand docking is the process of building a molecular complex with two molecules. Ligand binding has brought about many advances to drug design. Specifically, it contributes to creating visualizations for biologists to discover new drugs for diseases, and it also helps test current drugs and their effects on developing diseases.

Introduction:

Coccidiosis

- Caused by *Escherichia Tenella*
- One major factor of economic loss in the poultry industry
- Prevalent among herd-raised animals

Lincomycin

- Lincosamide antibiotic
- Multiple forms of dosage
- Effective treatment of Coccidiosis

Ligand Docking

- Molecular complex of two molecules
- Lock-and-key system
- Based on the Free Energy Function

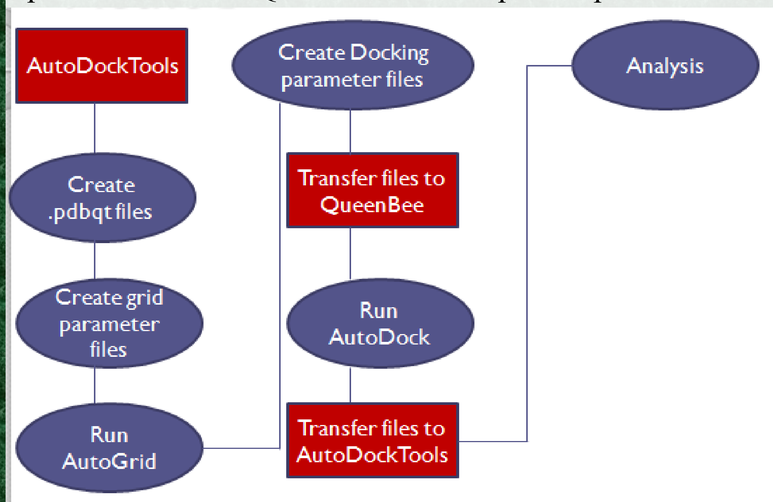
Free Energy Function

- Semiempirical free-energy force field to evaluate conformations during docking simulations
- Evaluates dispersion/repulsion, hydrogen bonding, electrostatics, and desolvation

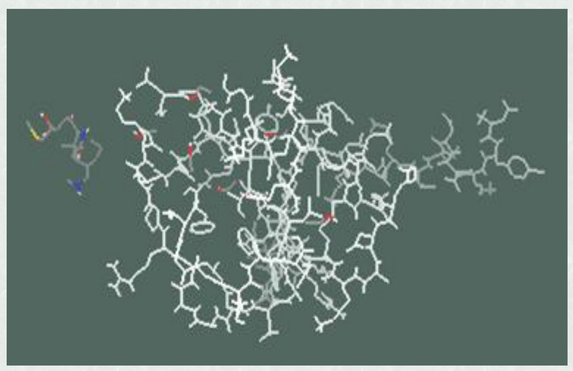
$$\Delta G = (V^{L-L}_{\text{bound}} - V^{L-L}_{\text{unbound}}) + (V^{P-P}_{\text{bound}} - V^{P-P}_{\text{unbound}}) + (V^{P-L}_{\text{bound}} - V^{P-L}_{\text{unbound}} + \Delta S_{\text{conf}})$$

$$V = W_{\text{vdw}} \sum_{i,j} \left(\frac{A_{ij}}{r^{12}_{ij}} - \frac{B_{ij}}{r^{6}_{ij}} \right) + W_{\text{hbond}} \sum_{i,j} E(t) \left(\frac{C_{ij}}{r^{12}_{ij}} - \frac{D_{ij}}{r^{10}_{ij}} \right) + W_{\text{elec}} \sum_{i,j} \frac{q_i q_j}{\varepsilon(r_{ij}) r_{ij}} + W_{\text{sol}} \sum_{i,j} (S_i V_j + S_j V_i) e^{(-r^2_{ij}/2\sigma^2)}$$

Experiment: AutoDock and AutoDockTools Software was utilized to conduct this simulation. The software was created by the Scripps Research Institute. Docking was performed on the QueenBee HPC Supercomputer.

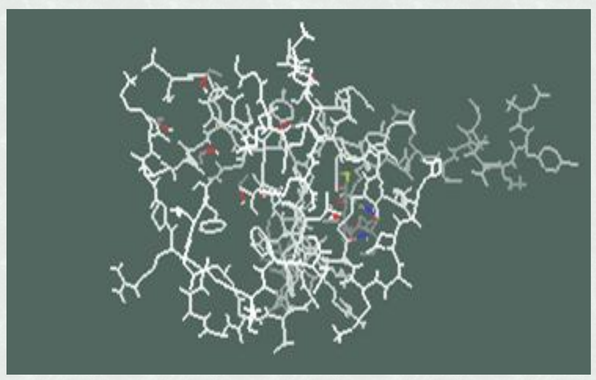


Results: Lincomycin (**multi-colored molecule**) successfully docked to *Eischerichia Tenella* (**white molecule**).



Before docking simulation

After docking simulation



Docking confirmation

```
binding_energy=22.51
ligand_efficiency=0.83
intermol_energy=18.04
vdw_hb_desolv_energy=18.45
electrostatic_energy=-0.41
moving_ligand_fixed_receptor=18.04
moving_ligand_moving_receptor=0.08
total_internal=0.0
ligand_internal=0.0
torsional_energy=4.47
unbound_energy=0.0
filename=C:/Documents and Settings/Paige Northern\1HKYÿÿÿÿ.dlg
clRMS=23.154
refRMS=n/a
rseed1=None
rseed2=None
```

Docking Confirmation:

- Binding energy (Kcal/mol) is the sum of the intermolecular energy and the torsional free-energy penalty.
- Docking energy is the sum of the intermolecular energy and the ligand's internal energy.
- Torsional energy is the number of active torsions.

Conclusion and Future Work: Ligand docking is able to give a qualitative visualization of Lincomycin treating Coccidiosis. Through this visualization, scientists are able to see a precise pathway of Lincomycin affecting the parasite in an effort to treat it. Although the length of treatment can not be determined at this time, the results can contribute to future work with Molecular Dynamics (MD) simulation. This type of simulation will generate accurate and quantitative results than with Ligand Docking.

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