Schrödinger

Introduction to Schrödinger and the IMMERSE Initiative

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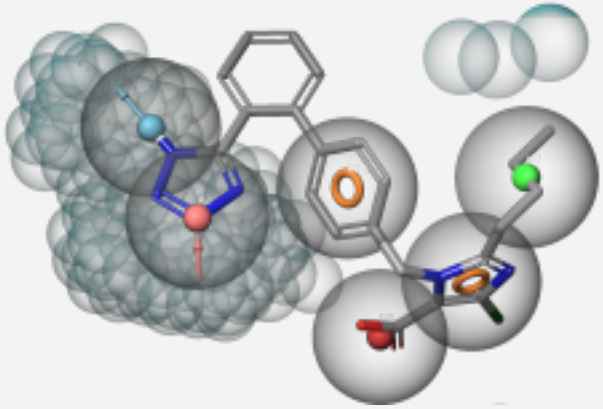
Introducing Schrödinger

Maestro

Small Molecule Drug Discovery & Design

proteins



ligands (small molecules)

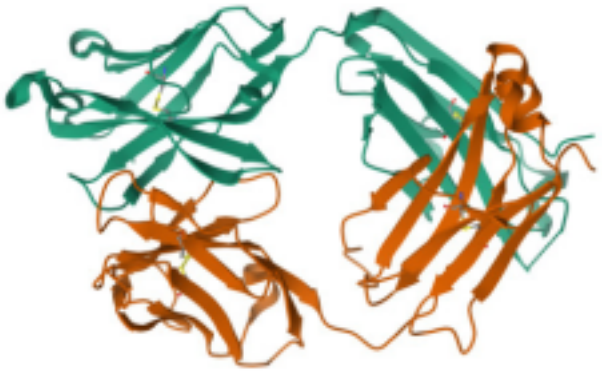
We use Schrödinger's technology platform to design molecules

Schrödinger

Results of molecular design – Therapeutics

Pills

Vaccines



Antibodies

Results of molecular design – Materials

What is modeling and how does it help us?

Models are essential tools for thinking

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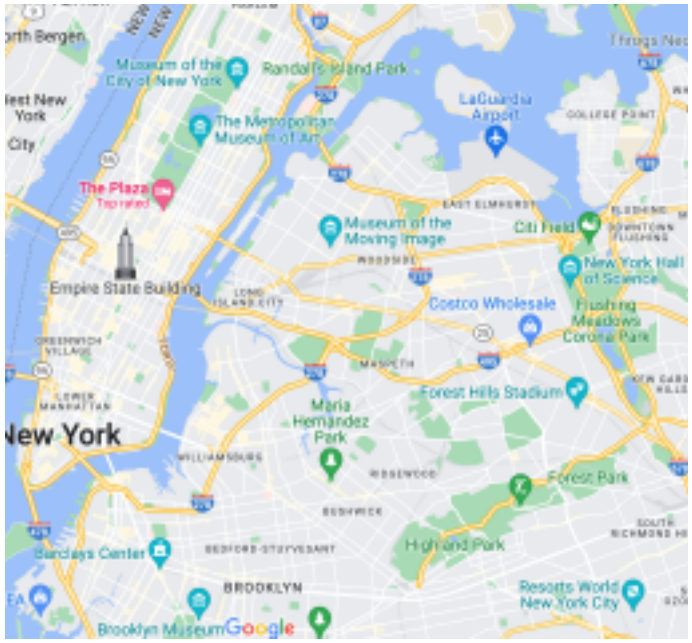

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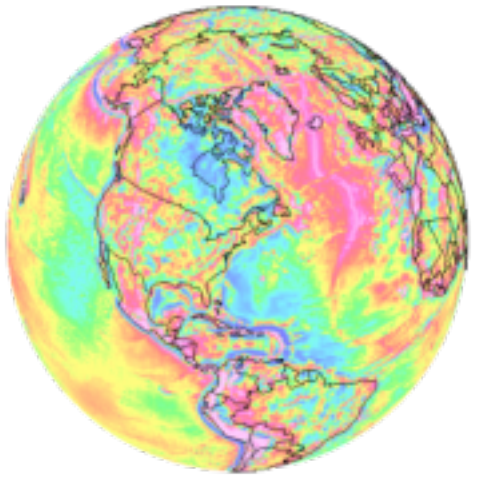
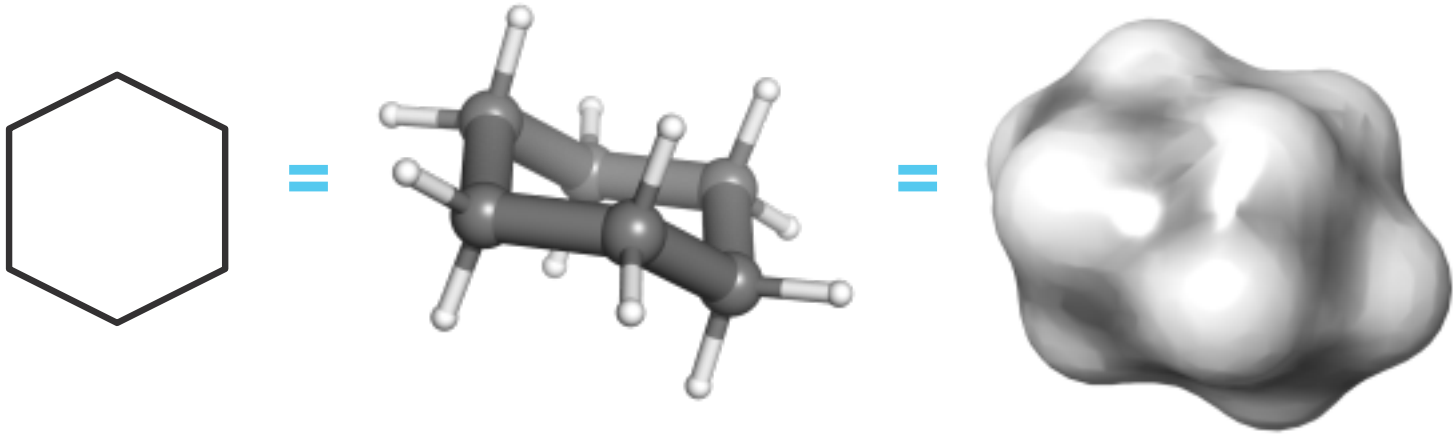
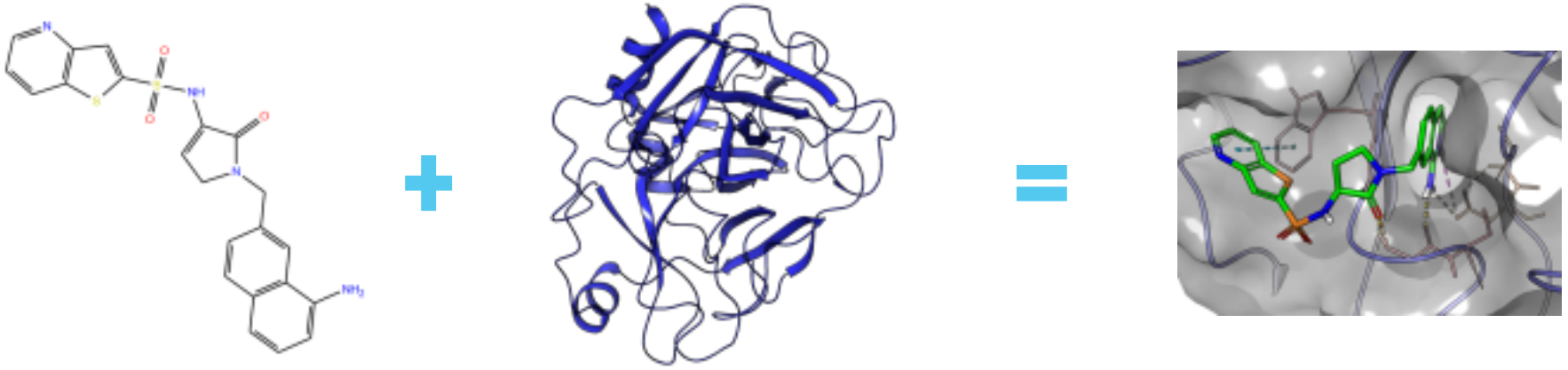


Models are essential tools for thinking about molecules



Common questions in drug design



Does this ligand fit into the target?

Which interactions in the pocket drive potency?

Which of these ligands is the tightest binder?

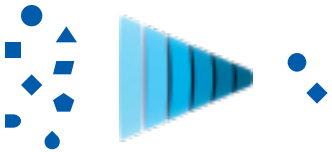
Why does this tiny change impact potency so much?

Which differences between target and off-target pocket can we use?

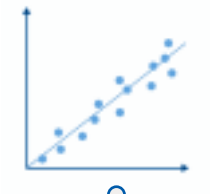
Different goals, methods, and challenges over time

Target selection + enablement | Hit identification | Lead optimisation | Candidate selection | Clinical trials

Where in the biochemical pathway of the disease do we interfere?



Which molecular scaffolds are promising “tools” to make the target behave?



How can we understand and leverage the structure-activity relationship?

Have we found a compound that’s good enough to invest in?

Does it actually work?

An increasing industry shift towards integrated digital chemistry

Schrödinger Announces Collaboration with AstraZeneca to Deploy Advanced Computing Technology for Drug Discovery

Takeda and Schrodinger Announce Multi-Year, Multi-Target Research Collaboration

Schrödinger and Bayer Collaborate to Co-Develop de novo Design Technology to Accelerate Drug Discovery

Strategic Collaboration with Thermo Fisher Scientific to Expand Structure-Based Drug Discovery to Novel Targets Using Cryo-EM

Schrodinger Announces a Multi-Target Drug Discovery, Development and Commercialization Collaboration with Bristol Myers Squibb

Schrödinger Expands Discovery Efforts for COVID-19 Alliance with Advanced Molecular Simulation Leveraging High-Powered Parallel Computing on Google Cloud