

Advanced in silico drug design

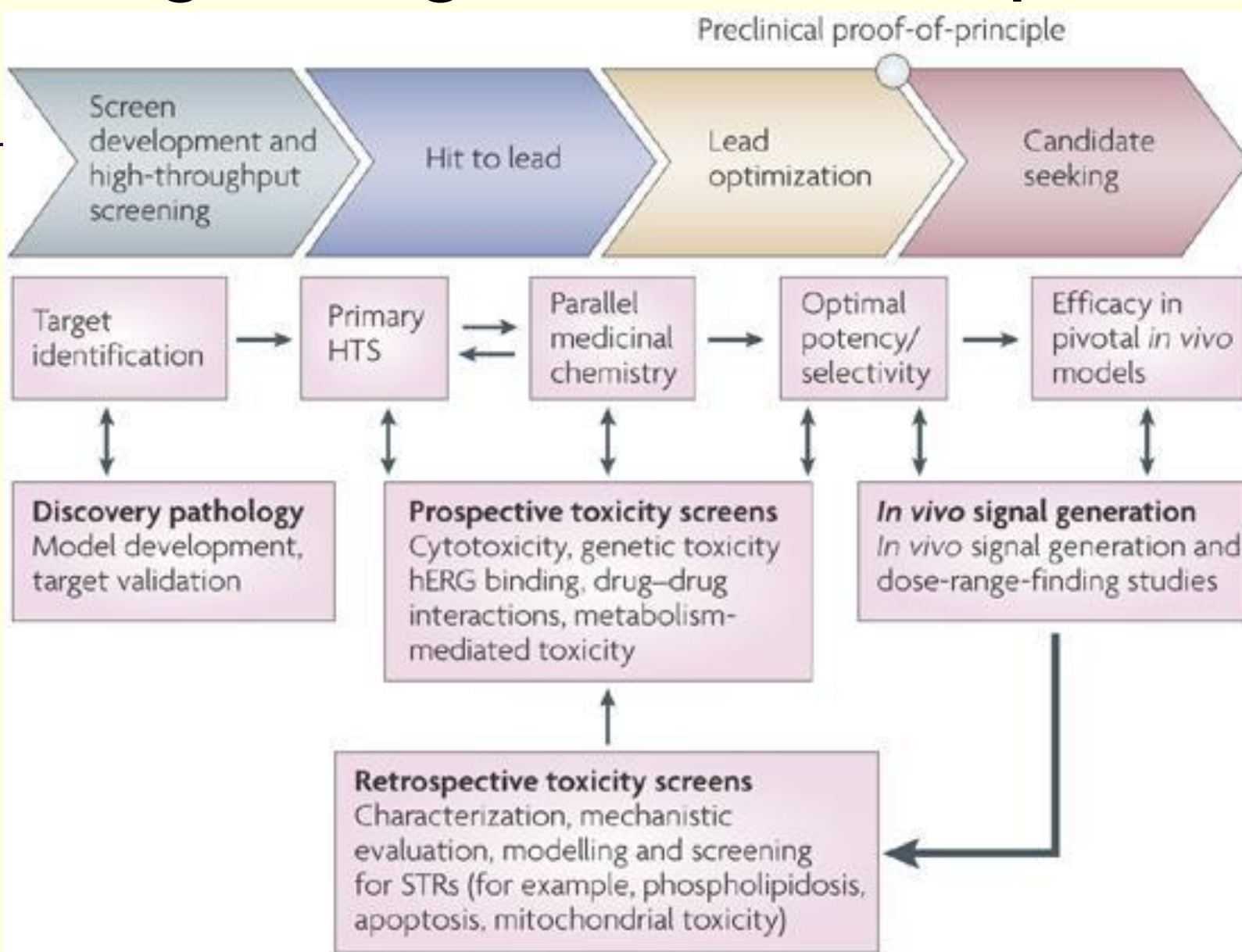
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Lecture: Future of Drug Design

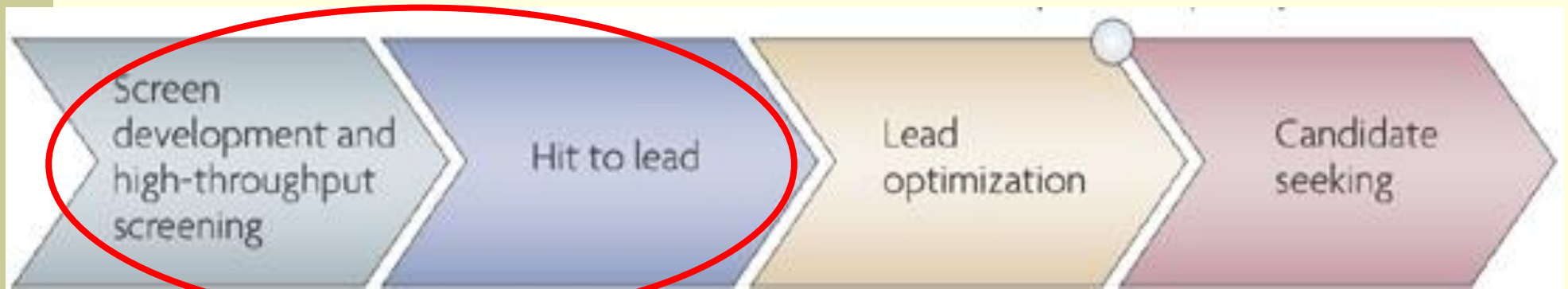
Outline

1. Drug Development Challenges
2. New Diseases, New Targets
3. New/Old Drugs

Drug Design and Development



Drug Design and Development



Biophysics

Pharma

Pharmacology
Chemiinformatics



Academy

Management
Economics

Pharma Industry Under Pressure

- costly animal, clinical trials (3 rounds) + safety precautions
- 15 years of development, $>10^9$ USD
- high attrition rate, high risk
- few blockbusters
- 20 years for patent, then generics

- New drugs/year – ca. 20 but declining
- Simple targets solved – Difficult target challenging

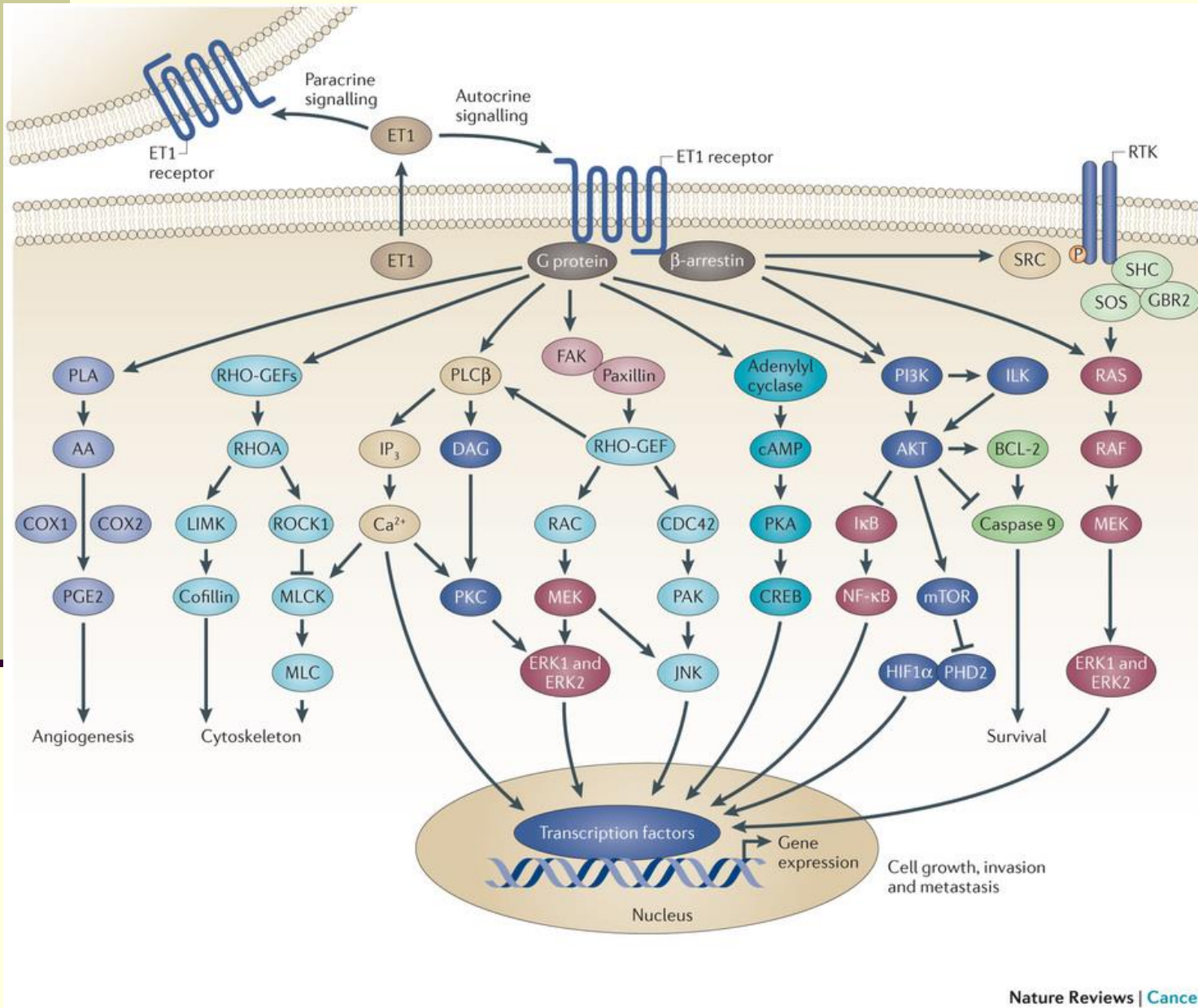
New Ideas
Academic Research

New Diseases, New Targets

- **traveling**: viruses: Zika, Ebola, Flu, SARS
- Standard techniques
- **ageing**: cancer, neurological disorders
- complex networks, specificity (=off-target activities), toxicity
- blood-brain barrier
- **treatment**: resistance
- compounds become ineffective

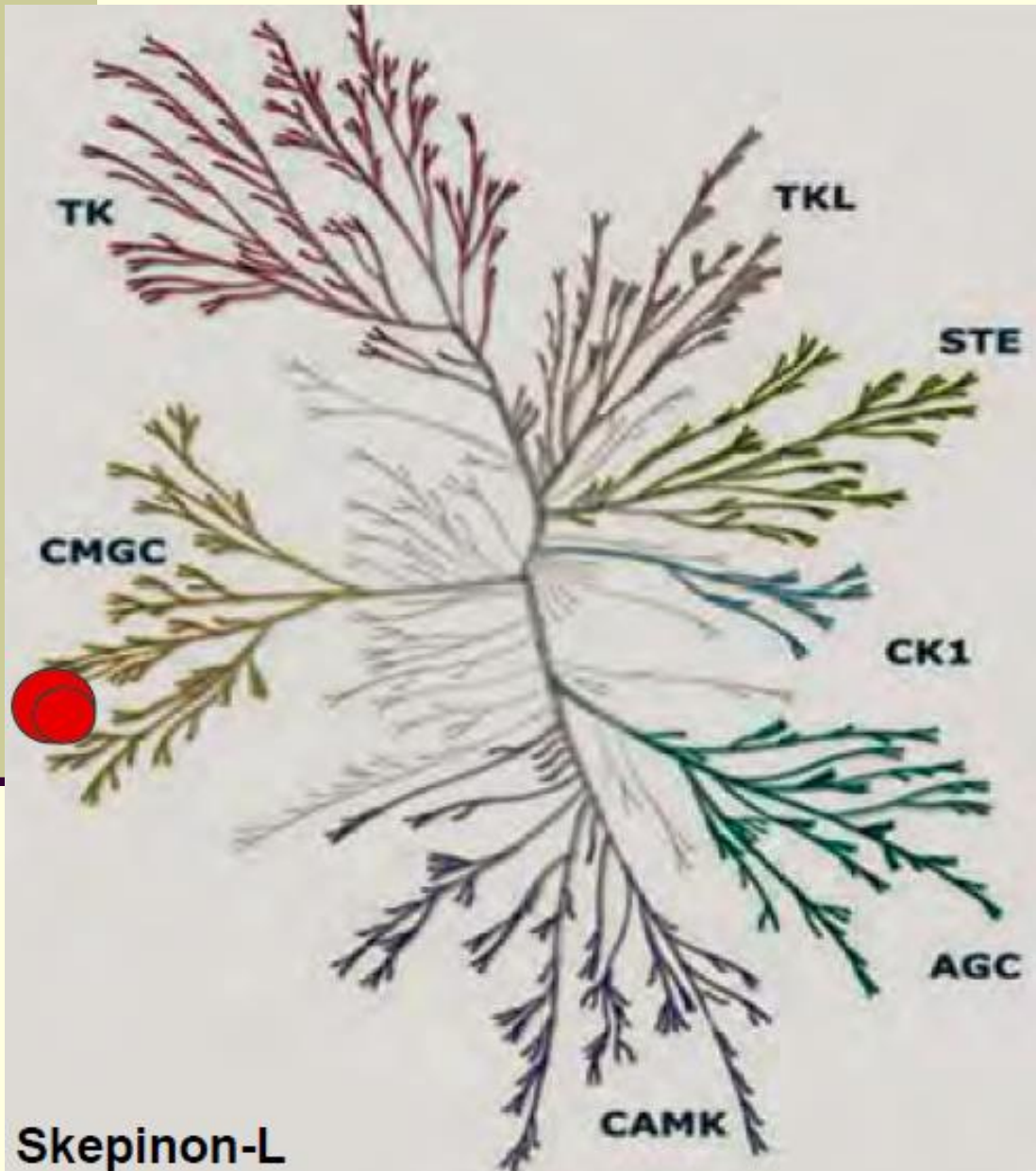
Complex networks

- Hitting other pathways
- Signalling pathway redundancy



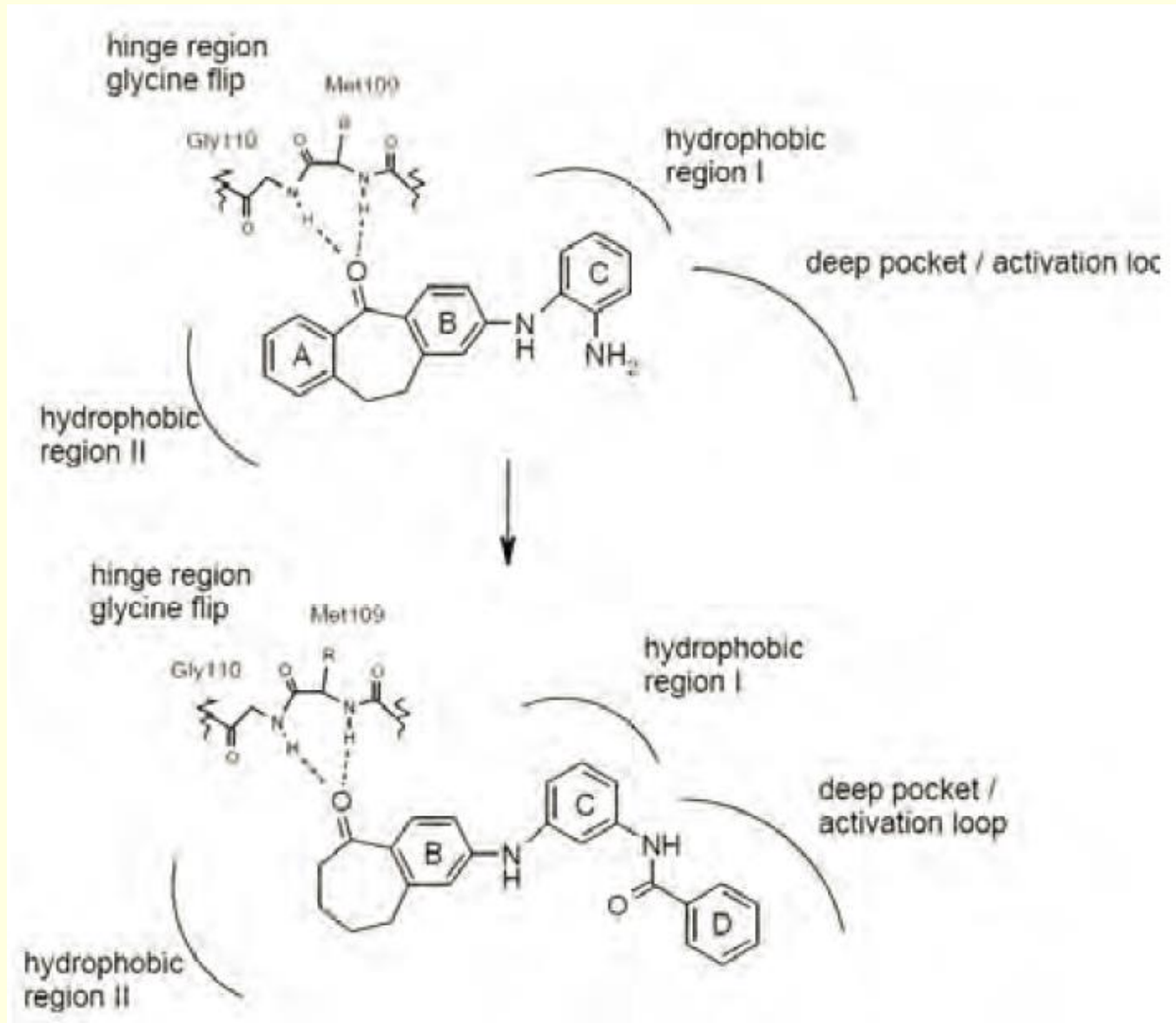
Kinome Cross-reactivity

- Specific, bifunctional, pan-kinase



Allosteric Inhibitors

- Reduced toxicity



New Drugs

- Small-molecule vs. Biologics
- Allosteric, Covalent, Prodrugs, Fragment-based design,
- Druggability, Protein-protein Interactions
- Resistance-Evading (Enthalpy, backbone)

Old Drugs-New Indications (=Repurposing)

- Optimized ADME-Tox properties

Outlook

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**Bright Future for the drug design fields and
for your research !!!**