Jubilant Biosys computational chemistry team excels in drug discovery design efforts in collaboration with medicinal chemistry, structural biology and DMPK teams, by conducting molecular modeling studies - pharmacophore and QSAR modeling, protein structure-based drug design, ligand-based drug design, fragment-based drug design, homology modeling, docking & scoring, chemoinformatics analysis and de novo design. The team of 20 scientists extensively utilizes in-house expertise in software development, chemocuration and structural biology for driving molecular design.

**Achievements**

- The Jubilant modeling group is actively involved in over twenty integrated drug discovery projects and modeling collaborations.
- Molecular modeling and structure-based drug design techniques have been employed in the development of two clinical candidates (GPCR, kinase targets) and a back up candidate (protease target) for clinical trials.
- Jubilant computational chemistry group played a critical role in the design and successful development of multi-kinase inhibitor series for multiple projects:
  - Two different, novel and potent lead series of inhibitors for a dual kinase inhibitor program
  - Two different lead series of novel, potent inhibitors for a triple kinase inhibitor program

**Molecular Design Collaborations (MDC)**

- Jubilant computational chemistry team empowers drug discovery scientists to deploy ready-to-use models and make faster and wiser decisions:
  - Virtual screening
  - Protein-ligand interactions
  - Validated docking models and scoring
  - SAR analysis
  - Selectivity analysis
  - Activity prediction
  - Suggestions for synthesis/testing
  - Template search
  - Validated homology models
  - Sequence analysis
  - Structural analysis
  - Comparison of homologous proteins
  - Analysis of PDGs
  - Compare & characterize binding sites
  - PDB water analysis
  - Calculate ligand properties
  - Correlate activity & properties

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**Docking**

- Virtual screening
- Protein-ligand interactions
- Validated docking models and scoring
- SAR analysis
- Selectivity analysis
- Activity prediction
- Suggestions for synthesis/testing

**Pharmacophore/ QSAR**

- Validated pharmacophore/3D-/2D-QSAR models
- Activity prediction
- SAR analysis
- Selectivity analysis
- Cluster analysis
- Suggestions for synthesis/testing

**Homology modeling**

- Template search
- Validated homology models
- Sequence analysis
- Structural analysis
- Comparison of homologous proteins

**Miscellaneous**

- Analysis of PDGs
- Compare & characterize binding sites
- PDB water analysis
- Calculate ligand properties
- Correlate activity & properties

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**Fragment based drug discovery**

```
Apo enzyme
IC_{50} = x
```

```
IC_{50} > x/1000
```

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