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Data Mining & *In silico* Research

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About Data Mining & *In silico* Research

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Data Mining and *in silico* Research Group (DMR) utilizes computational modeling, online bioinformatics and scientific databases to identify novel compounds that may potentially improve function, folding, trafficking, channel gating, or the membrane stability of

misfolded F508del-CFTR. Along with CFTR, DMR evaluates targets within the CFTR interactome, a diverse array of proteins involved in CFTR folding, trafficking and stabilization that have been shown to modulate CFTR activity. Compounds selected using modeling and bioinformatic tools are then screened in appropriate *in vitro* assays to measure their effects on CFTR function. DMR Team members further apply in-silico modeling and ligand-based or protein structure-based models to guide development of SAR (Structure-Activity Relationships), and to accelerate lead compound optimization. These approaches have yielded a variety of novel lead compounds that increase F508del-CFTR activity.

Our computational tools

- Aid in creating SAR (Structure Activity Relationships)
- Perform protein-ligand binding simulations
- Find novel drug scaffolds through pharmacophores
- Enable statistical data analysis

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We’d love to hear it!

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