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Supplemental data

**Combining Metabolite-Based Pharmacophores with Bayesian Machine Learning Models
for *Mycobacterium tuberculosis* Drug Discovery**

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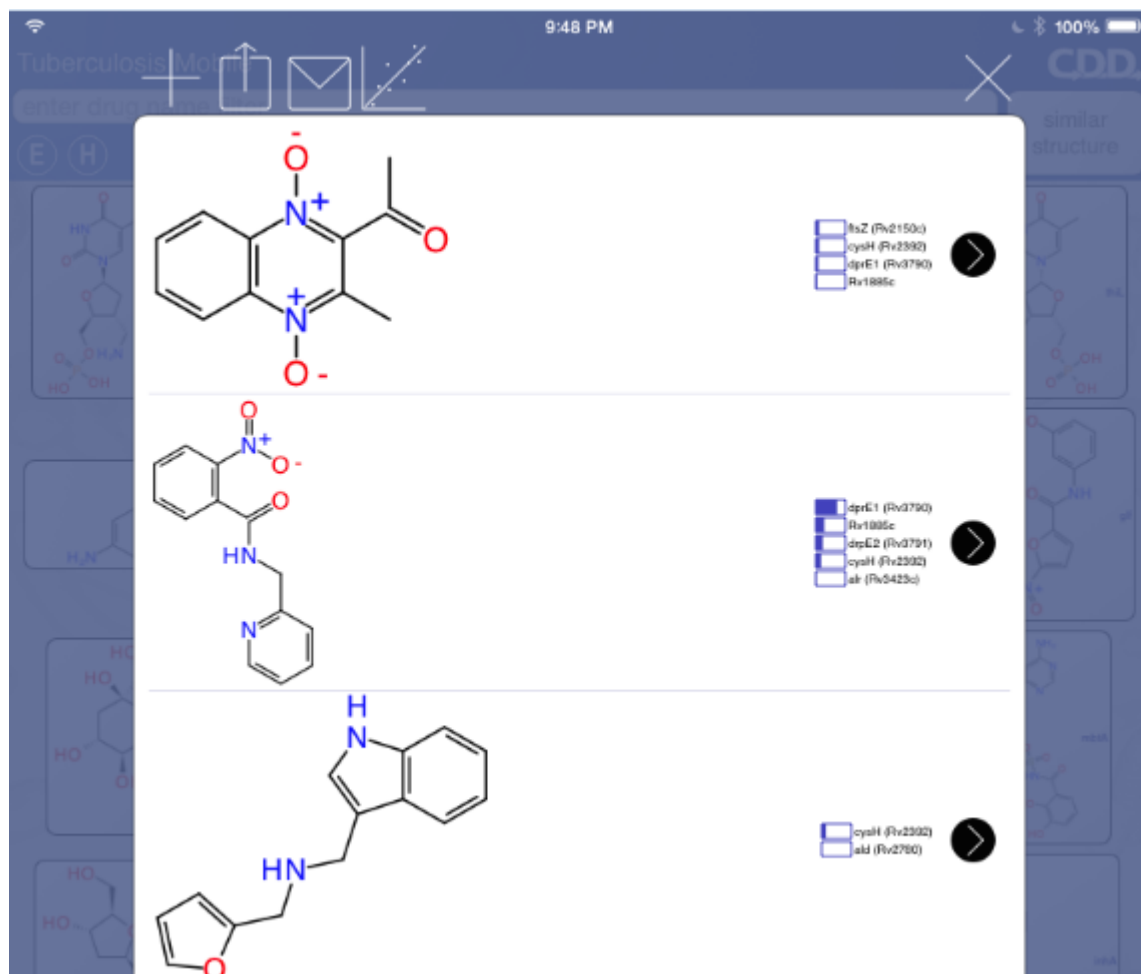
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Figure S4. TB Mobile 2.0 predictions.

Bayesian models

A



In app similarity predictions

B

Tuberculosis Mobile 9:48 PM 100%

enter drug name filter

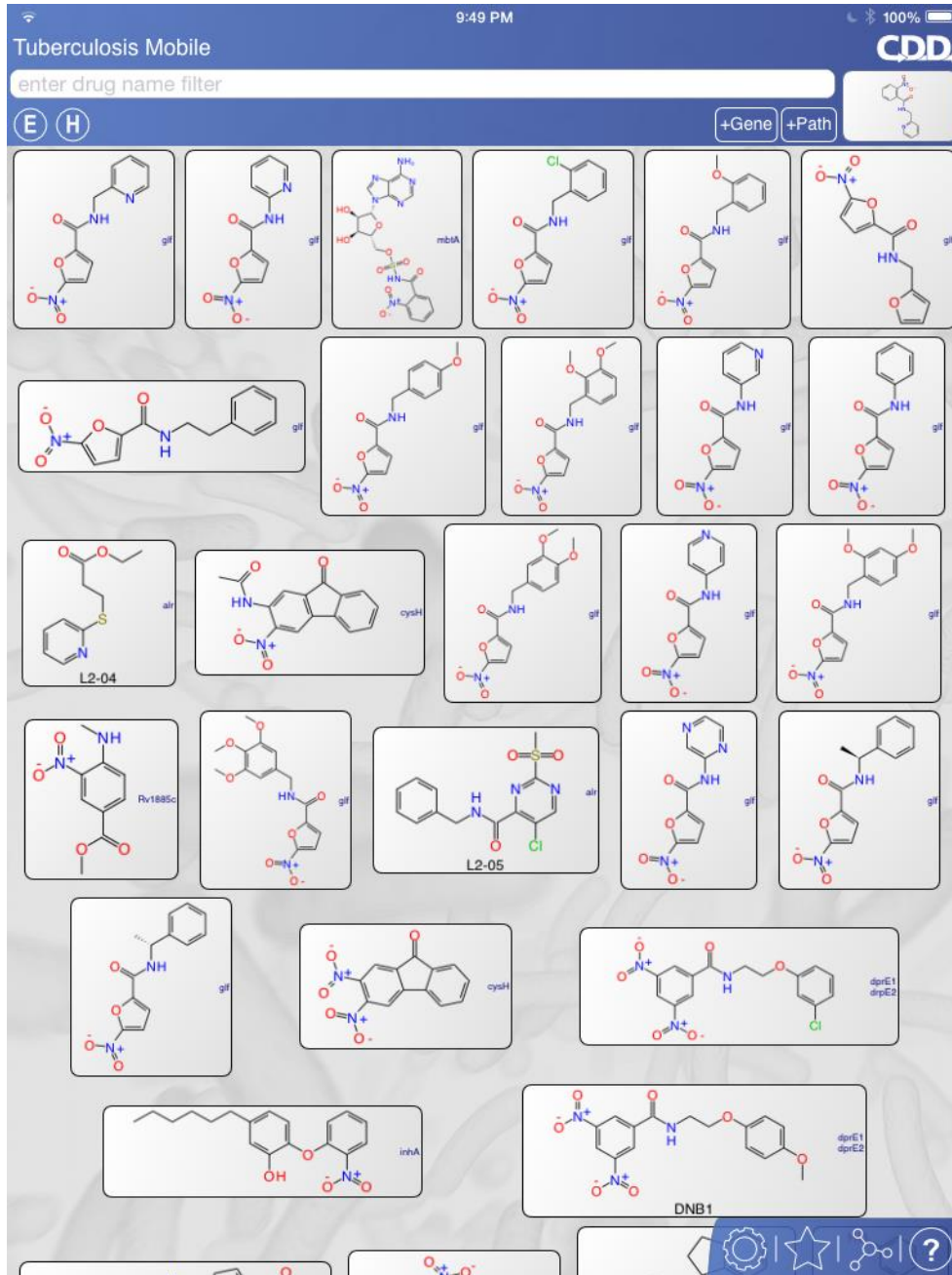
+Gene +Path

The screenshot displays a grid of chemical structures for various drugs, each labeled with its name and target. The drugs shown include:

- cysS**: A long-chain bis-benzimidazole derivative.
- dapA**: A pyridine derivative with a methyl ester group.
- cysH**: A complex polycyclic structure with a nitro group.
- inhA**: Multiple structures, including a piperazine derivative and a piperidine derivative.
- glt**: Several structures, including a pyridine derivative with a nitro group and a piperazine derivative.
- salH**: Nicotinamide.
- fabH**: A thiazolidine derivative with a hydroxyl group.
- L2-04**: A pyridine derivative with a thioether group.
- Krieger 4**: A complex structure with a bromine atom and multiple hydroxyl groups.
- ilvG**: A complex structure with a pyridine ring and a thioether group.

Navigation icons at the bottom: Settings (gear), Favorites (star), Home (molecule), and Help (question mark).

C



D

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+Gene +Path

The screenshot displays a grid of chemical structures for various drugs used in tuberculosis treatment. The drugs are labeled with gene names: inhA, gif, plpB, ndhA, fbpC, and cysH. The interface includes a search bar, navigation buttons, and a bottom menu with icons for settings, favorites, and help.

Chemical structures shown include:

- inhA: A complex molecule with a benzimidazole core and a carboxylic acid group.
- gif: A molecule with a furfuryl ring and a nitro group.
- plpB: A large, complex molecule with multiple amide and ester groups.
- ndhA: A molecule with a quinoline ring and a sulfonamide group.
- fbpC: A molecule with a benzimidazole core and a phosphate group.
- cysH: A molecule with a naphthalene ring and a nitro group.