

PLOS ONE

Supplemental data

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

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B

iPad 4:24 PM 89%

Tuberculosis Mobile CDD

enter drug name filter

E H +Gene +Path

The screenshot displays the Tuberculosis Mobile application interface. At the top, it shows the device name 'iPad', time '4:24 PM', and battery level '89%'. The app title 'Tuberculosis Mobile' and the CDD logo are visible. Below the title bar is a search bar with the placeholder text 'enter drug name filter'. Navigation buttons for 'E' and 'H' are present, along with '+Gene' and '+Path' options. The main area contains a grid of chemical structures for various drugs, each with its name and associated target genes:

- glt** (multiple structures)
- Nicotinamide** (target: *sahH*)
- Isoniazid** (target: *inhA*, *katA*, *dhx*)
- Flv1885c** (target: *Flv1885c*)
- Ethionamide** (target: *inhA*)
- Prothionamide** (target: *sahH*)
- p-Aminosalicylic acid** (target: *IsIP1*, *IsIP2*)

C

iPad 4:26 PM 89%

Tuberculosis Mobile

enter drug name filter

E H +Gene +Path

The screenshot displays the Tuberculosis Mobile application interface. At the top, it shows the device status (iPad, 4:26 PM, 89% battery) and the app title. Below the title is a search bar with the placeholder text "enter drug name filter". To the right of the search bar are buttons for "+Gene" and "+Path", and a small thumbnail of a chemical structure. Below the search bar are two tabs, "E" and "H", and a grid of drug cards. Each card contains a chemical structure and a gene target. The drugs shown include:

- Nicotinamide (target: *sahH*)
- Isoniazid (target: *inhA*, *kasA*, *dirA*)
- Ethionamide (target: *inhA*)
- Prothionamide (target: *sahH*)
- C215 (target: *mmpL3*)
- Other drugs with targets: *glt*, *inhL*, and *inhA*.

