## SUPPLEMENTARY MATERIALS

# In Silico Development of Novel Benzofuran-1,3,4-Oxadiazoles Lead Inhibitors of M. tuberculosis Polyketide Synthase13 Enzyme

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**Table S1:** The binding affinities of benzofuran-1,3,4-oxadiazoles **BF10-BF16** with the Mtb Pks13 enzyme.

| Benzofuran-1,3,4-oxadiazoles | Binding Affinities with Pks13 |
|---|---|
| **BF10** | -11.49 kcal/mol |
| **BF11** | -10.94 kcal/mol |
| **BF12** | -11.10 kcal/mol |
| **BF13** | -10.90 kcal/mol |
| **BF14** | -12.01 kcal/mol |
| **BF15** | -11.08 kcal/mol |
| **BF16** | -12.39 kcal/mol |
| **TAM-16** | -14.61 kcal/mol |

**Table S2:** ADMET profiles of the synthesized benzofuran-1,3,4-oxadiazoles **BF10-16 and TAM-16**

| Compounds | Carcinogenicity | HIA+ Values | Lipophilicity (iLogP) | CYP450 3A4 Inhibitor/Substrate | Log S (ESOL) $H_2O$ Solubility | P-gp Substrate | Renal OCTs |
|---|---|---|---|---|---|---|---|
| **BF10** | None | 1.00 | 2.73 | Substrate | -5.52 Moderately Soluble | No | Non-inhibitor |
| **BF11** | None | 1.00 | 2.79 | Substrate | -3.29 Soluble | No | Non-inhibitor |
| **BF12** | None | 1.00 | 3.28 | Substrate | -5.07 Moderately Soluble | No | Non-inhibitor |
| **BF13** | None | 1.00 | 3.54 | Substrate | -4.54 Moderately Soluble | No | Non-inhibitor |
| **BF14** | None | 1.00 | 3.68 | Substrate | -4.77 Moderately Soluble | No | Non-inhibitor |
| **BF15** | None | 1.00 | 3.57 | Substrate | -5.07 Moderately Soluble | No | Non-inhibitor |
| **BF16** | None | 1.00 | 3.48 | Substrate | -3.75 Soluble | No | Non-inhibitor |
| **TAM-16 (Standard)** | None | 0.993 | 2.48 | Substrate | -3.72 Moderately Soluble | Yes | Non-inhibitor |

**Table S3.** Drug-likeness and Medicinal chemistry profiles of benzofuran-1,3,4-oxadiazoles **BF10-16** and **TAM-16**

| Compounds | Bioavailability Score | PAINS Alerts | Accept Lipinski's Rule Yes/No | Pfizer Rule | Golden Triangle Rule | TPSA |
|---|---|---|---|---|---|---|
| **BF10** | 0.55 | None | Yes | complied | Accepted | 106.46 Å² |
| **BF11** | 0.55 | None | Yes | complied | Accepted | 118.93 Å² |
| **BF12** | 0.55 | None | Yes | complied | Accepted | 106.46 Å² |
| **BF13** | 0.55 | None | Yes | complied | Accepted | 115.69 Å² |
| **BF14** | 0.55 | None | Yes | complied | Accepted | 115.69 Å² |
| **BF15** | 0.55 | None | Yes | complied | Accepted | 106.46 Å² |
| **BF16** | 0.55 | None | Yes | complied | Accepted | 97.67 Å² |
| **TAM-16** | 0.55 | 1-alert | Yes | complied | Accepted | 85.94 Å² |