

Figure S1. MS Analysis of MbtI +/- inhibitor Mass spectrometry analysis of MbtI. A) m/z calcd for recombinant MbtI = [native-MbtI + MGSSHHHHHHSSGLVPRGSH (amino acid sequence introduced from pET19) – N-terminal methionine]: 50787, found: 50785. B) Recombinant MbtI treated with **2**. m/z calcd for [protein + 4 × **2**] 51751, found: 51751.

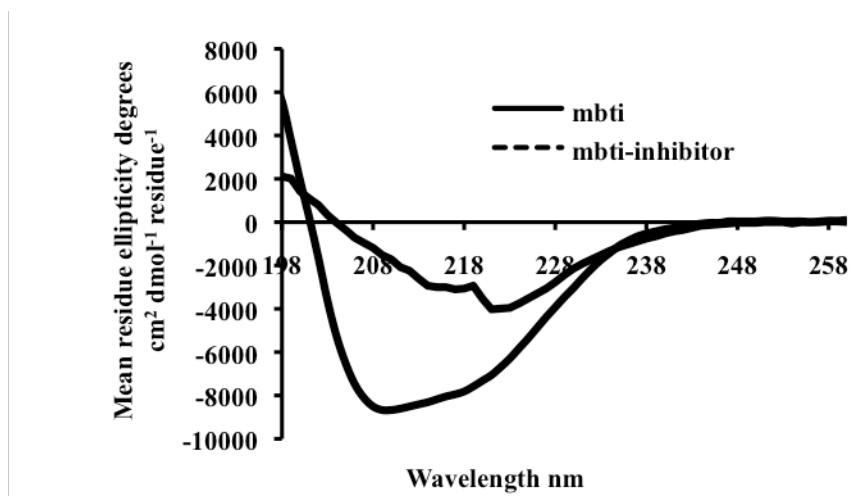


Figure S2. CD Spectra of MbtI +/- inhibitor. MbtI (12 μM) in 20 mM phosphate buffer (pH 7.4) (solid line) and MbtI incubated with benzisothiazolone **2** (hashed line).

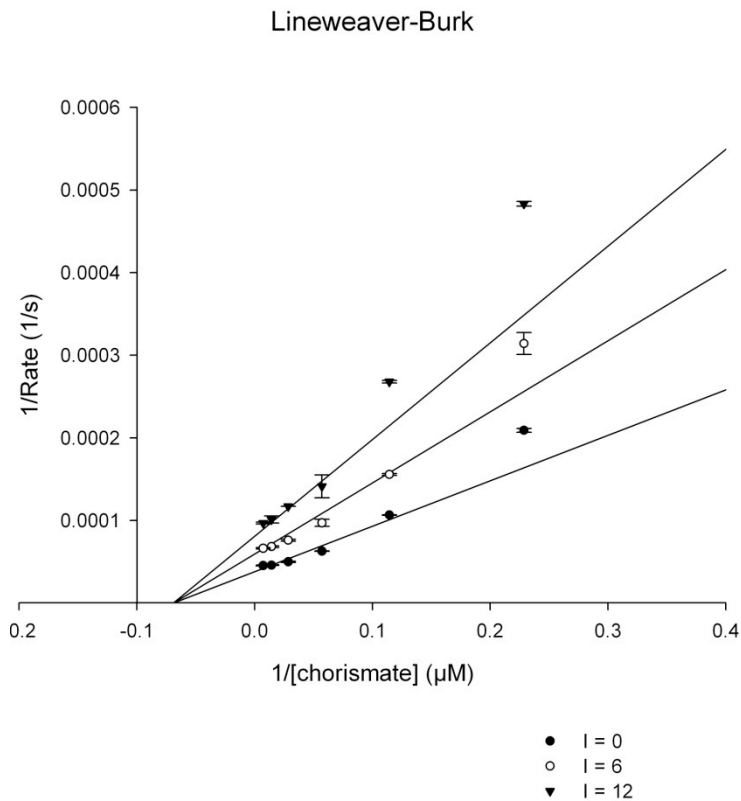


Figure S3. Lineweaver-Burk Plot for compound 4. Double reciprocal plot of initial velocity versus salicylic acid at different concentration of **4**: 0 μM (●), 6 μM (○), 12 μM (▼). The data were fit to a noncompetitive inhibition model with $K_i = 10.6 \pm 0.65$, $\alpha = 1$.