

Supplementary Material

An O-Demethylation Metabolite of Rabeprazole Sulfide by *Cunninghamella blakesleeana* 3.970 Biotransformation

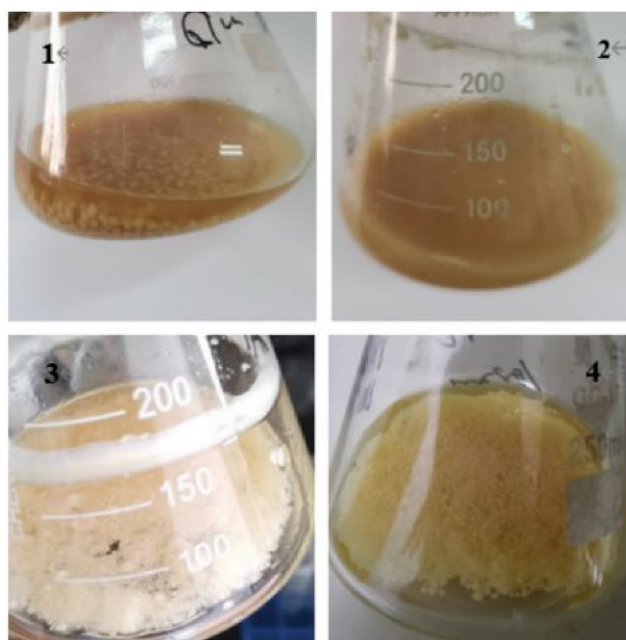


Figure S1. Growth of *Cunninghamella blakesleeana* 3.970 in 4 different transformation media formula

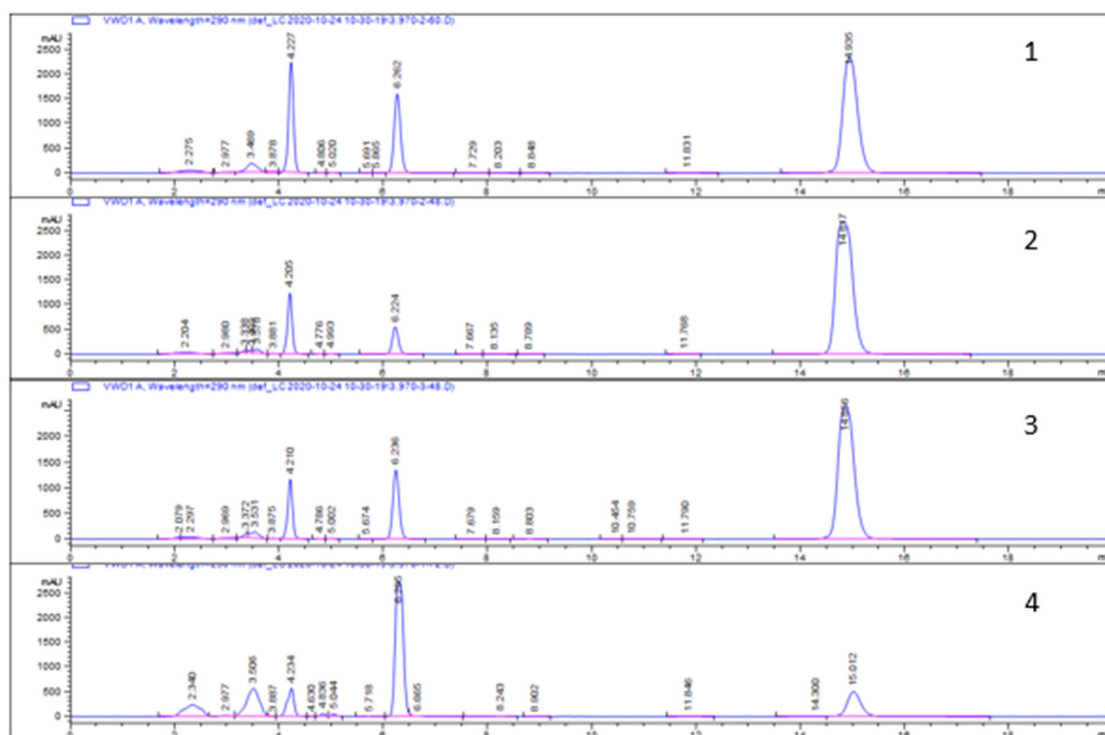


Figure S2. HPLC detection results of *Cunninghamella blakesleeana* 3.970 in 4 different transformation media formula

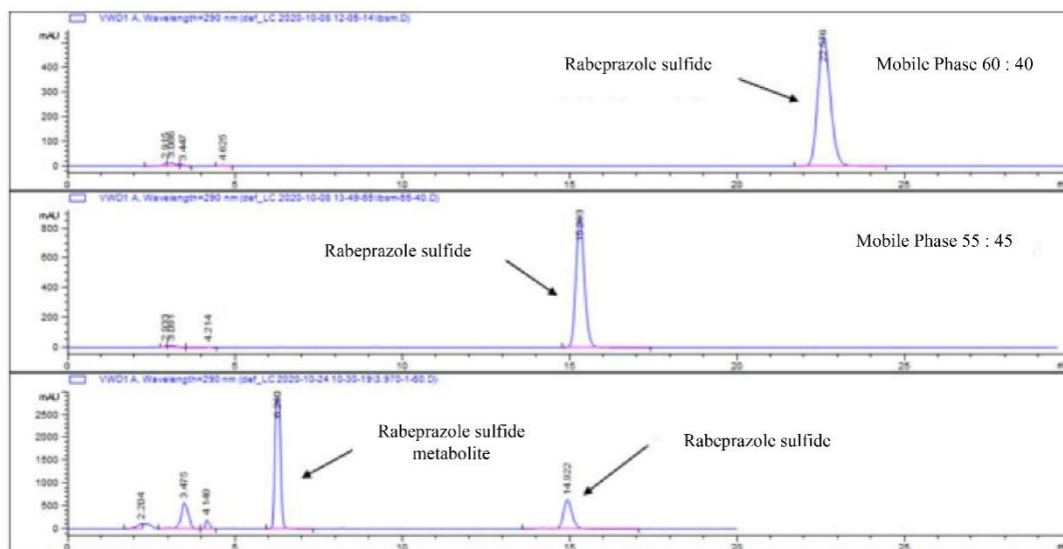


Figure S3. HPLC detection results of rabeprazole sulfide and its metabolites.

HPLC detection for the rabeprazole sulfide biotransformation

When the mobile phase ingredients change from (0.015mol/L NaHPO₄: Acetonitrile = 60:40, v/v) to (0.015 mol/L NaHPO₄: Acetonitrile = 55:45, v/v), the retention time of substrate rabeprazole decreased from 22.4 min to 15.08 min, and the retention time of targeted metabolite is 6.26 min, as Figure S3 indicated.

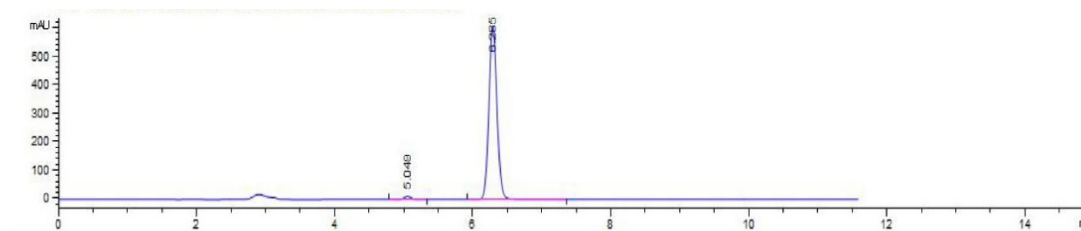


Figure S4. HPLC detection results of rabeprazole sulfide metabolites for MS and NMR analysis.

Semi-preparative HPLC isolation for the rabeprazole sulfide biotransformation

After optimization, the mobile phase ingredients is consisted of Acetonitrile:H₂O = 30:70, v/v, loading volume is 100 μ L, elution speed is 4ml/min, detection wave length is 290 nm, and the column temperature is 30 $^{\circ}$ C. The retention time for the target metabolite is 21.5 min. All the proper eluant were collected and the purity detected by HPLC is 99.2%, Figure 10.

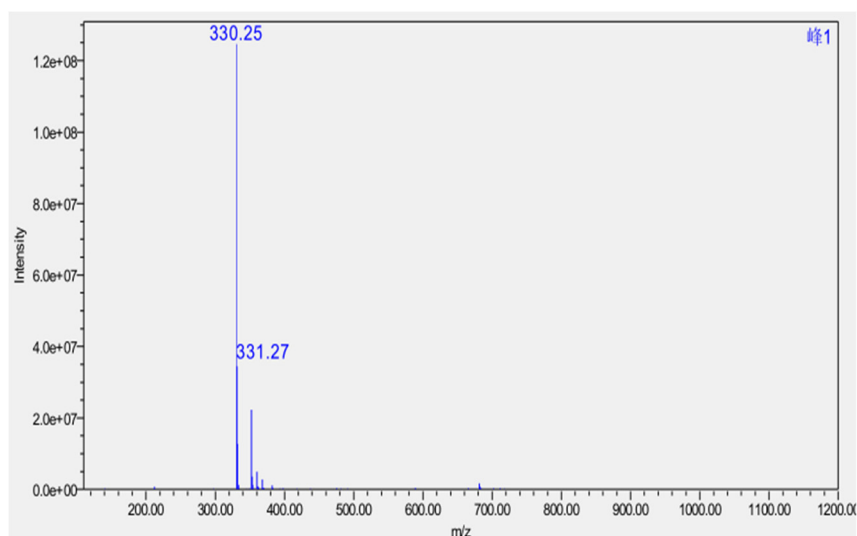


Figure S5. MS (ESI) $m/z[M+H]^+$ diagram for the metabolite

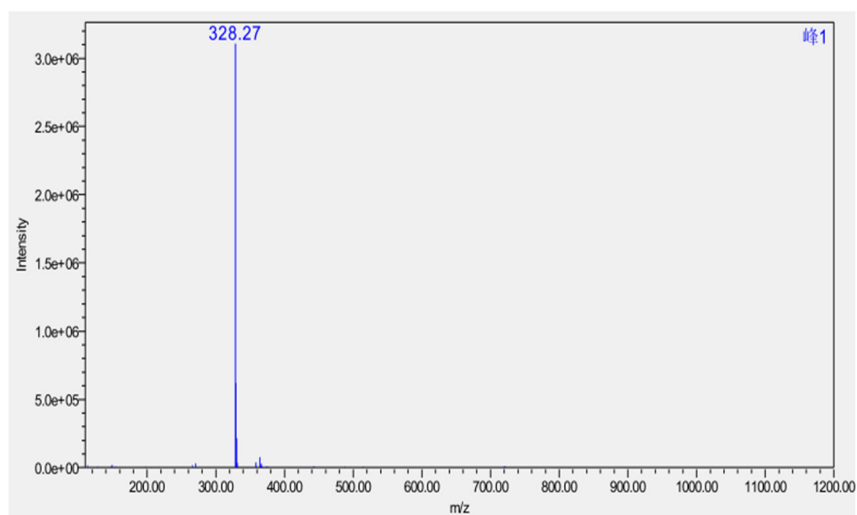


Figure S6. MS (ESI) $m/z[M+H]^-$ diagram for the metabolite

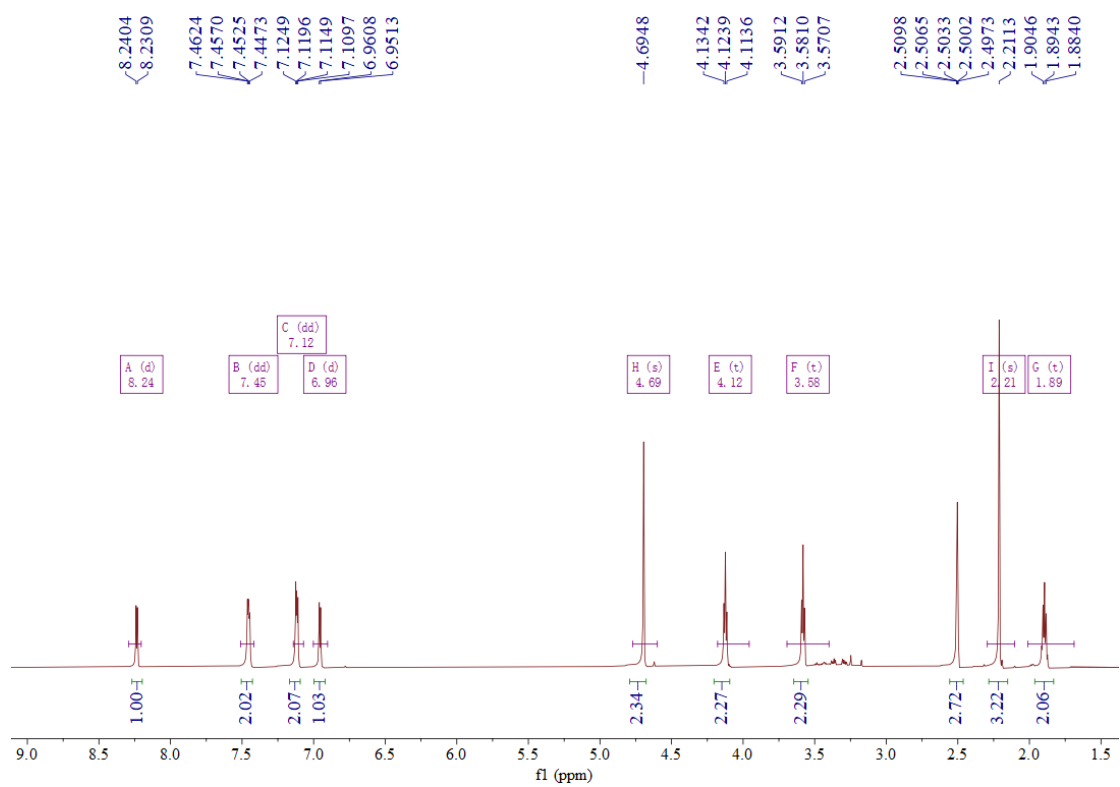


Figure S9. ¹H NOESY diagram for the *O*-demethyl rabeprazole sulfide