Supplementary Materials: Multiscale Interactome–Based Prioritization of Candidate Herbs and Active Compounds for Bronchiectasis

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Supplementary Figures S1–S5

Tables S1–S6 are provided in a separate Excel file (Bronchiectasis_IJMS_Supplementary_Tables_S1-S6.xlsx).

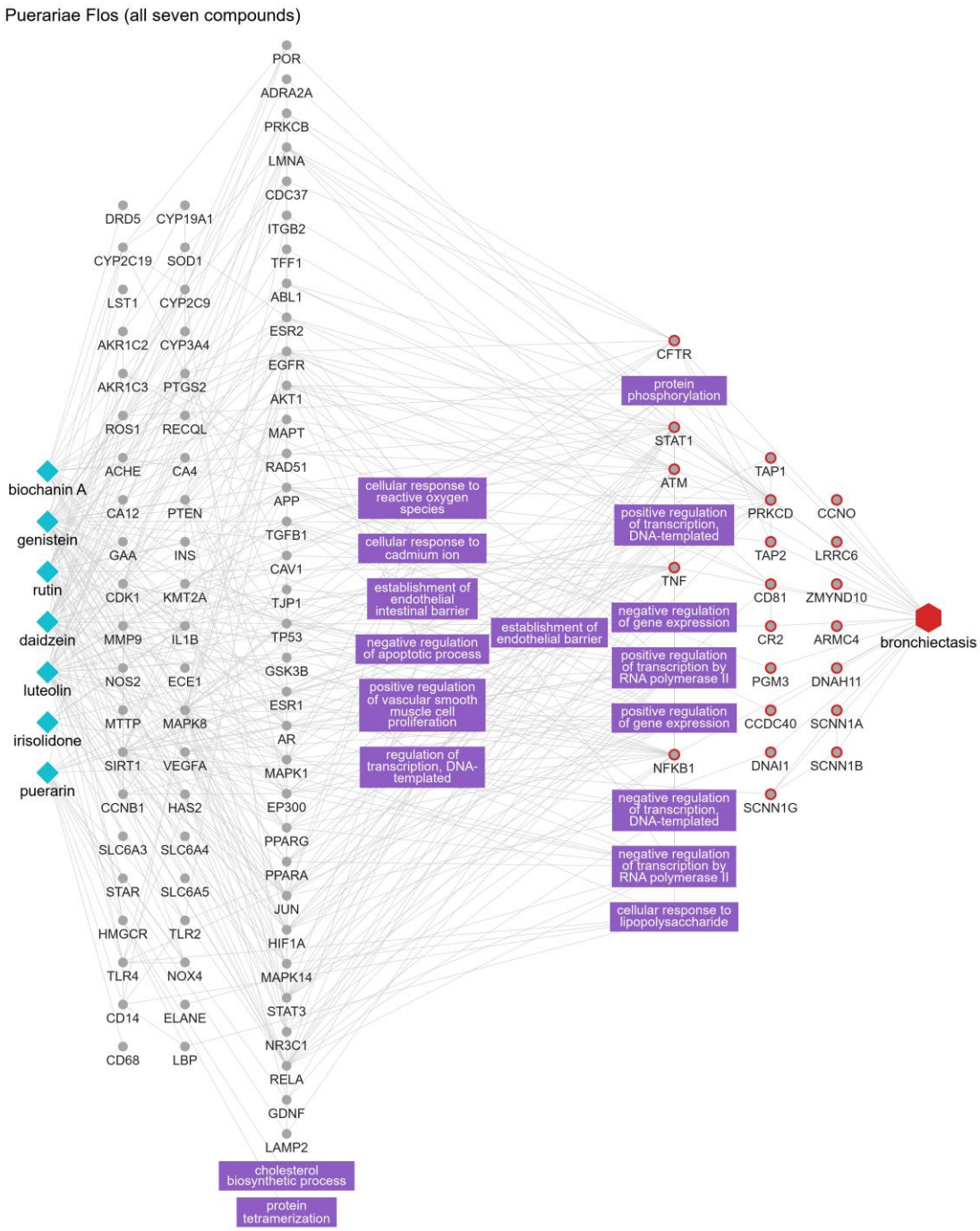

Figure S1. Compound–disease subnetwork of Puerariae Flos (Table 1 rank 5) with all seven compounds meeting the compound-level criterion; it contains the three compounds of Puerariae Radix (Figure 5B). Diamonds, compounds; circles, proteins; boxes, enriched biological functions; hexagon, disease. Disease-associated proteins are outlined in red.

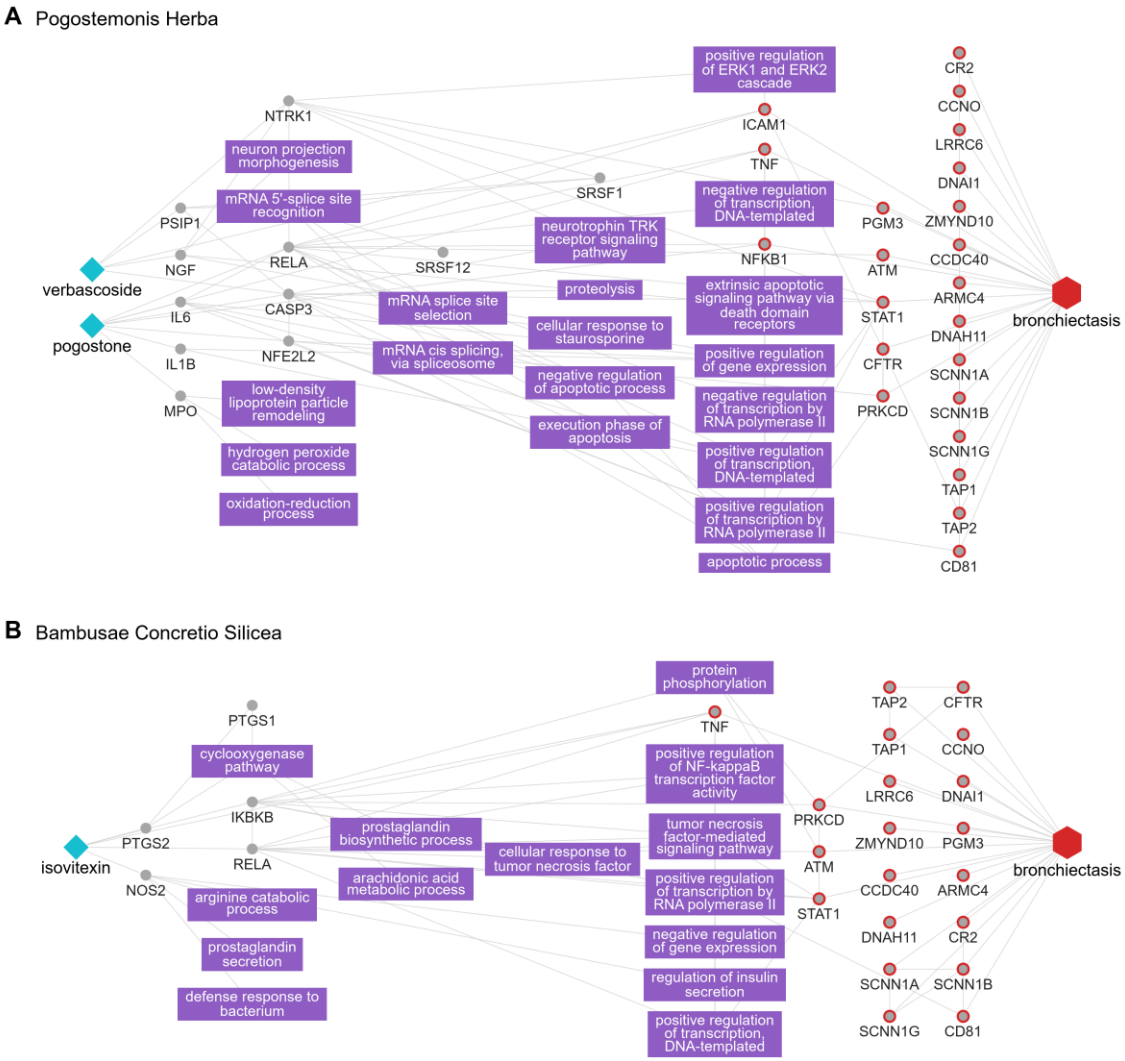

Figure S2. Compound–disease subnetworks of the remaining novel candidate herbs for bronchiectasis. (A) Pogostemonis Herba. (B) Bambusae Concretio Silicea. Diamonds, compounds; circles, proteins; boxes, enriched biological functions; hexagon, disease. Disease-associated proteins are outlined in red.

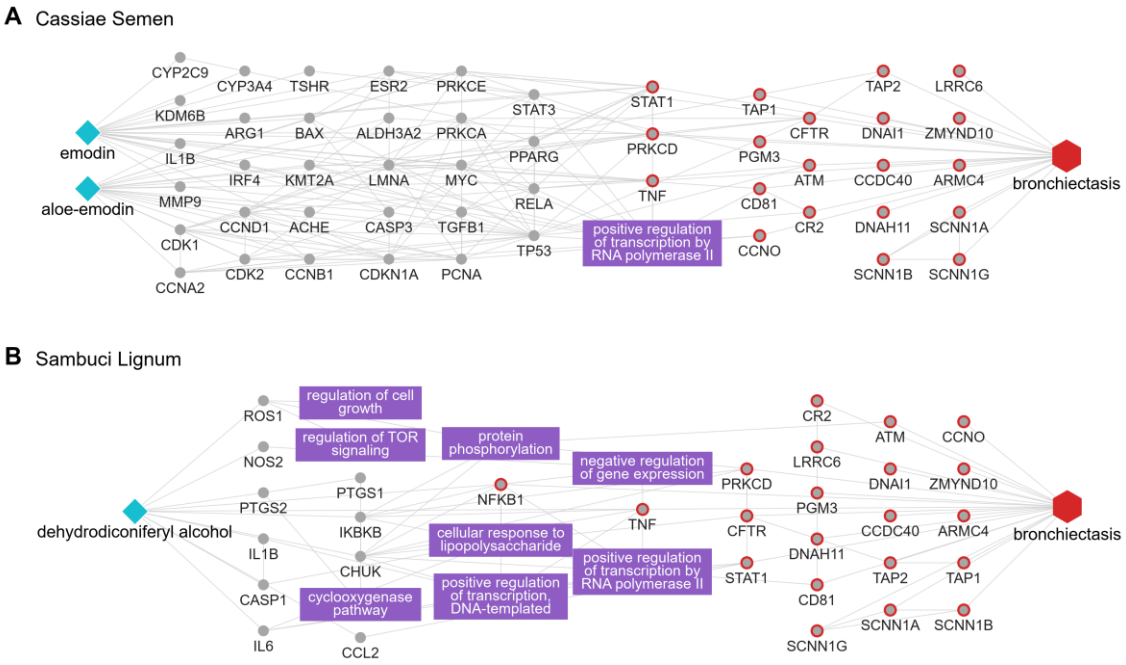

Figure S3. Compound–disease subnetworks of the remaining novel candidate herbs for bronchiectasis. (A) Cassiae Semen. (B) Sambuci Lignum. Diamonds, compounds; circles, proteins; boxes, enriched biological functions; hexagon, disease. Disease-associated proteins are outlined in red.

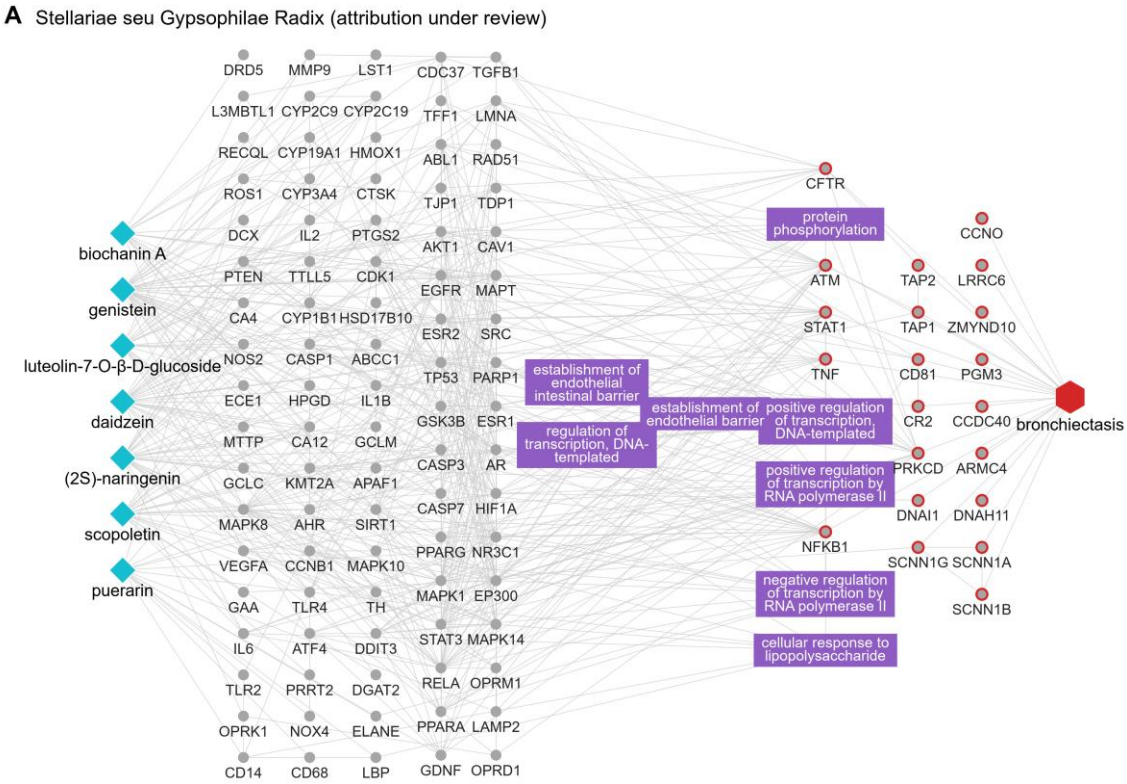

Figure S4. Compound–disease subnetwork of Stellariae seu Gypsophilae Radix (ranked tenth in Table 1), whose annotated isoflavones probably reflect database misattribution (see Section 2.6 of the main text). Representation as in Figure 5.

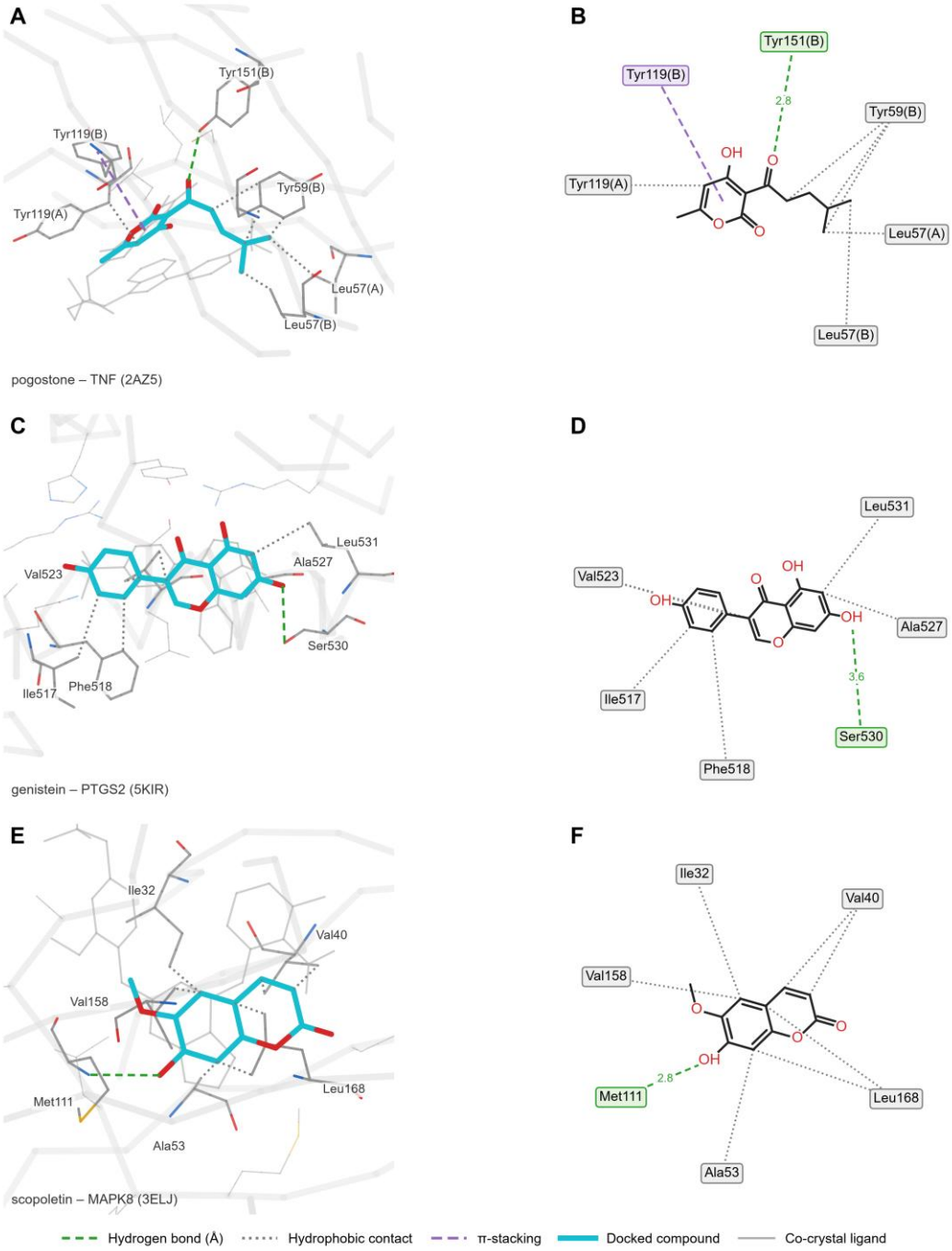

Figure S5. Additional binding modes. (A,B) pogostone in the SPD304 site at the TNF dimer interface (2AZ5, chains A/B). (C,D) genistein in the cyclooxygenase channel of PTGS2/COX-2 (5KIR). (E,F) scopoletin in the ATP pocket of MAPK8/JNK1 (3ELJ). Representation as in Figure 6. Scopoletin is annotated only to Stellariae seu Gypsophilae Radix, whose compound annotation is doubtful (see main text).