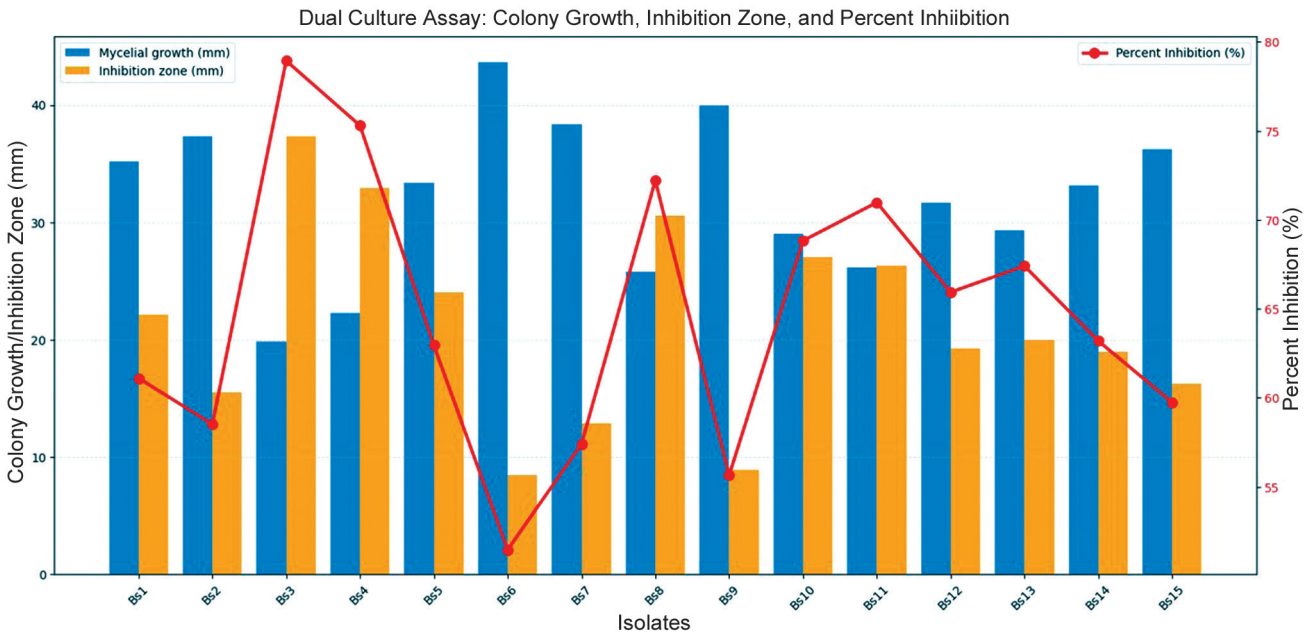
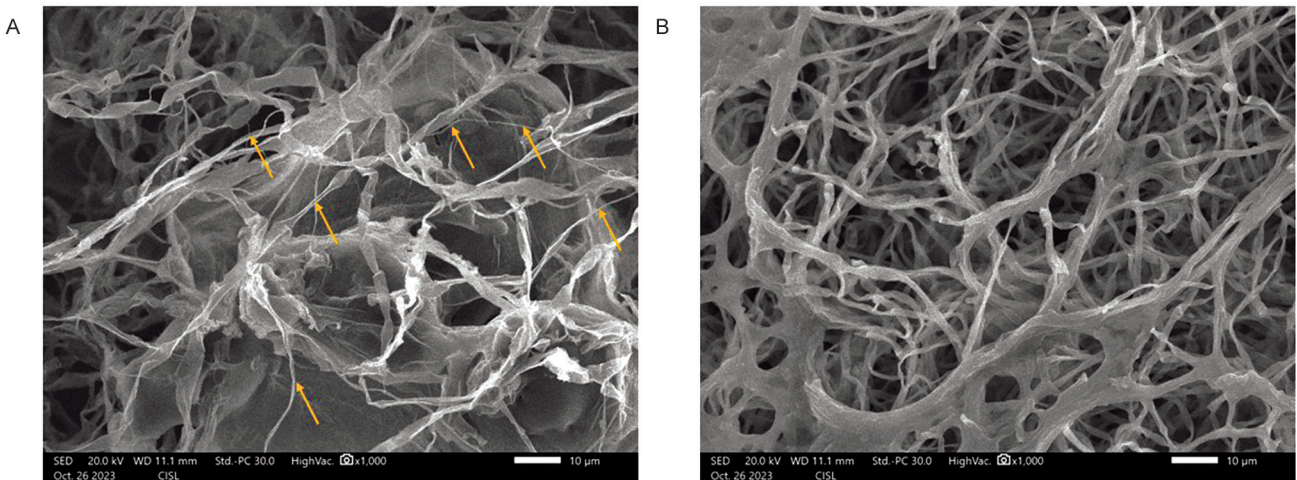


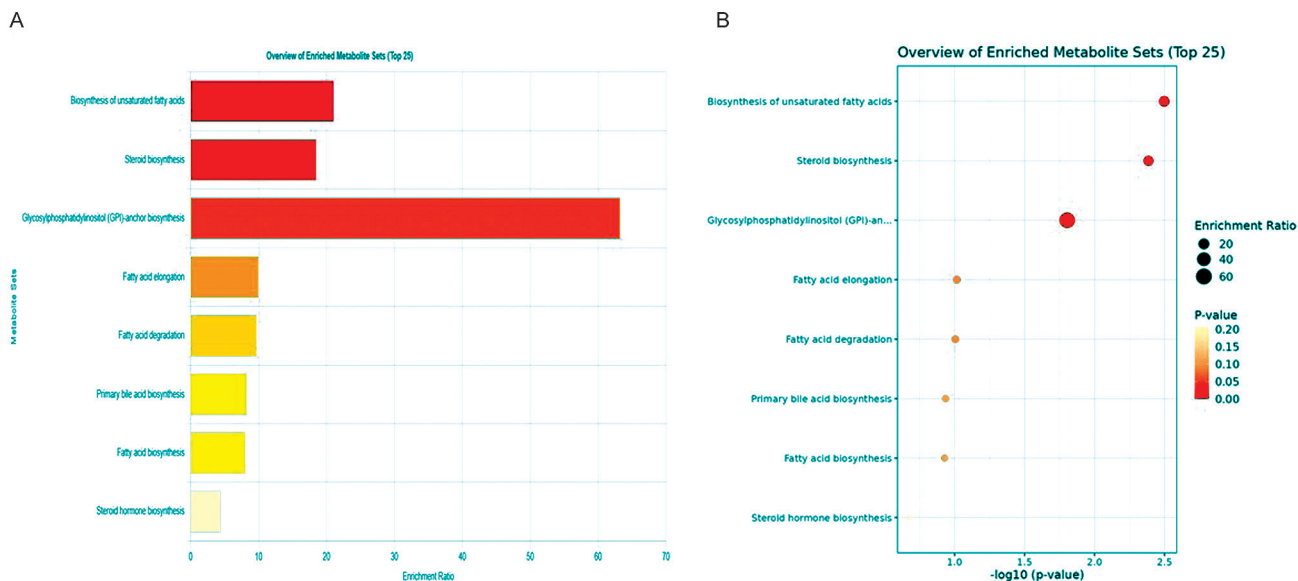
Supplementary Fig. 1 Phylogenetic tree of *Bacillus* spp. constructed based on 16S rRNA gene sequences using MEGA 12 software, showing the genetic relationship among the bacterial isolates and reference strains.



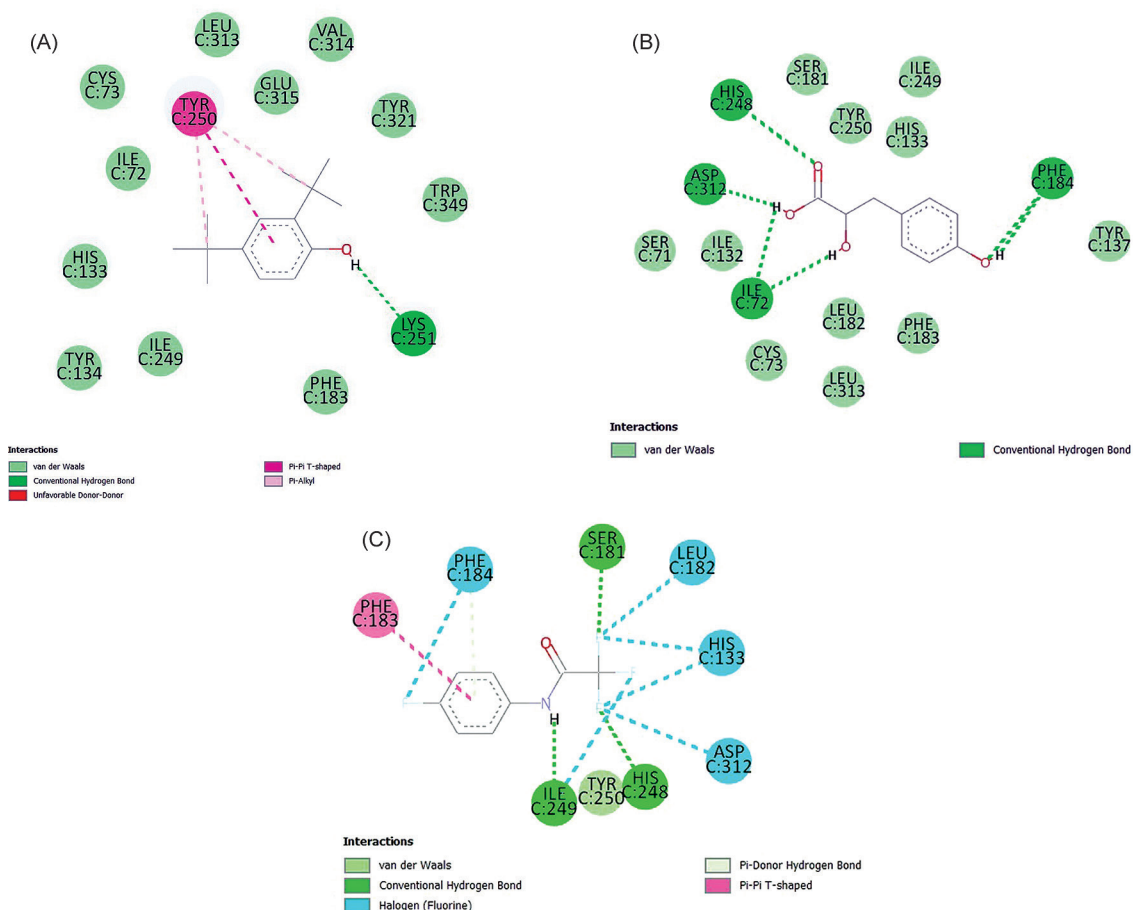
Supplementary Fig. 2 Dual culture assay showing mycelial growth, inhibition zone, and percent inhibition of *Sclerotium rolf sii* by bacterial isolates.



Supplementary Fig. 3 Microscopic observation of the antagonistic interaction between *Bacillus subtilis* Bs<sub>3</sub> and *Sclerotium rolf sii* isolate Sr<sub>10</sub> on potato dextrose agar (PDA) under dual culture conditions. (A) Normal, intact mycelial growth of *S. rolf sii* observed after three days of incubation (B) Severe mycelial shrinkage, distortion, and hyphal disintegration observed after seven days of incubation in the presence of *Bacillus subtilis* Bs<sub>3</sub>, indicating a strong antagonistic effect.



Supplementary Fig. 4 Pathway enrichment analysis of secondary metabolites identified from *B. subtilis* Bs-3 based on GC-MS data, highlighting significantly affected metabolic pathways.



Supplementary Fig. 5 2D interactions of A) Ligand (squalene); B) Ligand (cyclohexasiloxane); C) Ligand [ergost-5-en-3-ol(beta)]- protein complex docking on 4YLD protein

Supplementary Table 1 *In silico* binding analysis and therapeutic potential of major secondary metabolites

S.No.	Bioactive compounds	Binding score	Mode of action	Biological function	Reference
1	Squalene	-6.17 kcal/mol	Antimicrobial	Disrupts fungal cell membrane integrity and interferes with lipid metabolism, leading to reduced pathogen growth and virulence	Lou-Bonafonte <i>et al.</i> (2018), Talan <i>et al.</i> (2023)
2	Cyclohexasiloxane	-5.91 kcal/mol	Antimicrobial	Alters membrane permeability and inhibits essential enzymatic functions, thereby suppressing fungal proliferation	Micah (2025)
3	Ergost-5-en-3-ol (beta)	-5.53 kcal/mol	Antifungal, Antimicrobial	Targets ergosterol-associated pathways, causing membrane destabilization and inhibition of fungal growth	Majolagbe <i>et al.</i> (2024)