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Supporting information for article:

The crystal structure of benzophenone synthase from *Garcinia mangostana* L. pericarps reveals the basis for substrate specificity and catalysis

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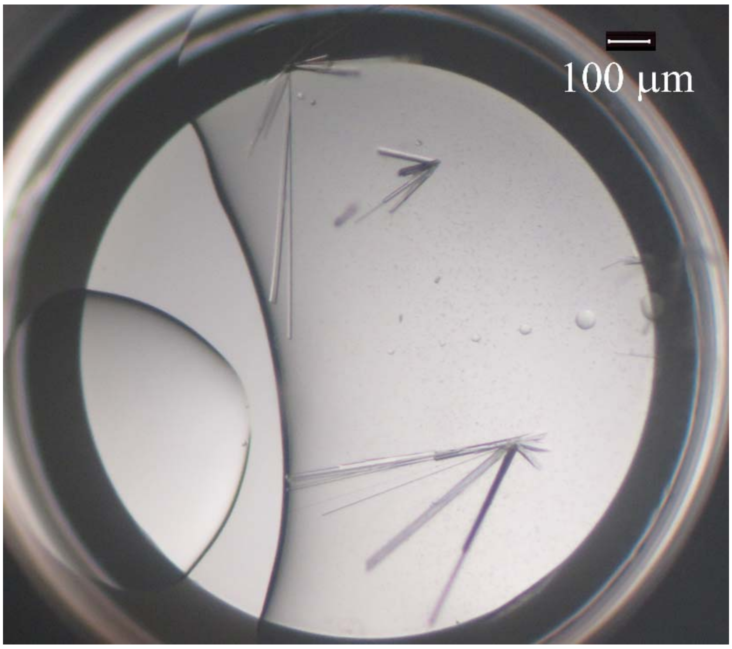

Figure S1 The GmBPS crystals with the average dimension of 200 × 20 × 10 μm^3 were obtained from a precipitant consisting of 0.2 M ammonium iodide, 20% w/v polyethylene glycol 3,350, pH 6.2.

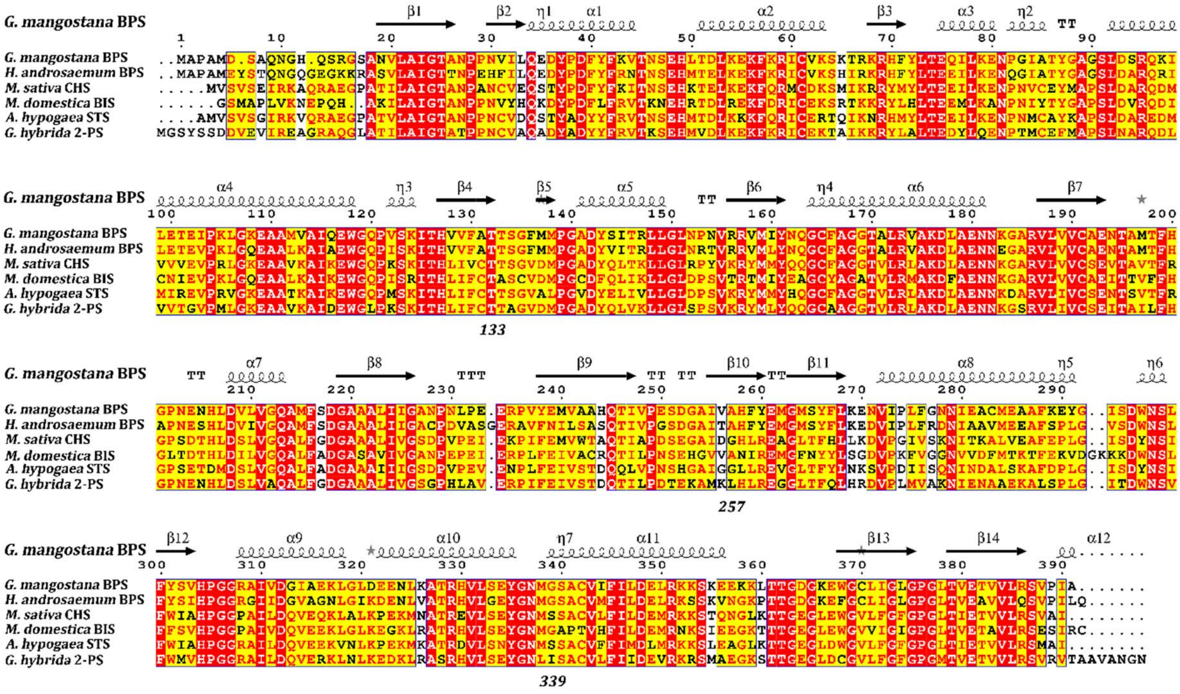

Figure S2 Sequence and secondary structure comparison of Type III PKS enzymes. The amino acid sequence of *G. mangostana* BPS (PDB code 7CBF) was aligned with *H. androsaemum* BPS (PDB code 5UCO), *M. sativa* CHS (PDB code 1CGK), *M. domestica* BIS (PDB code 5W8Q), *A. hypogaea* STS (PDB code 1Z1E) and *G. hybrida* 2-PS (PDB code 1EE0). The secondary structure of *G. mangostana* BPS is displayed as a diagram above the alignment and its mutated residues are marked in italics, according to the sequence numbering of *G. mangostana* BPS. The α helices and β strands are displayed as squiggles and arrows, respectively. TT indicates strict β-turn. Grey star which is above residues is modelled with alternate conformations. Residues printed as white characters in red frames are strictly conserved. Residues marked as red characters are designated as similar.

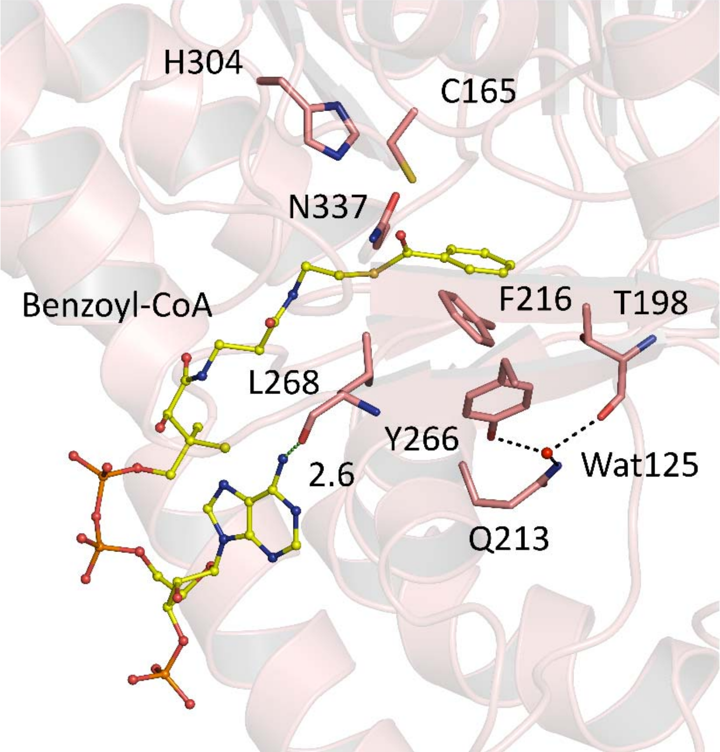

Figure S3 The molecule of benzoyl-CoA docked to GmBPS (PDB entry 7CBF). The labelled amino acid residues are shown as stick models with carbon in salmon, sulfur in yellow, nitrogen in blue and oxygen in red. The benzoyl-CoA modelled in the structure of GmBPS is shown as ball-and-stick model with carbon in yellow, nitrogen in blue and oxygen in red. The predicted hydrogen bond is shown as green dashed line. Black dashed lines represent hydrogen bonds formed in the crystal structure of GmBPS with their distances given in Å.

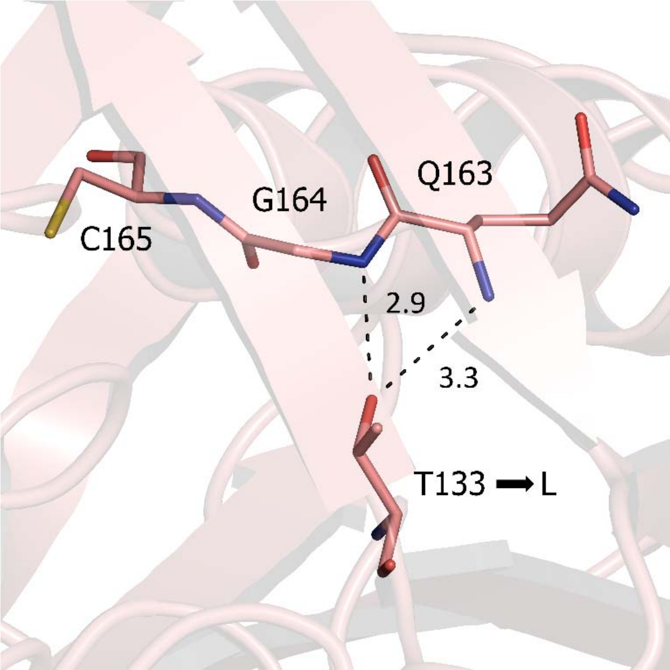

Figure S4 Hydrogen bonds between side-chain oxygen of Thr133 and the peptide amino hydrogens of Gln163 and Gly164. The structure of GmBPS is shown as ball-and-stick model with carbon in salmon and oxygen in red. Black dashed lines represent hydrogen bonds formed in the crystal structure of GmBPS with their distances given in Å.