

Description of Additional Supplementary Files

File Name: Supplementary Movie 1

Description: Overview of the catalytic pocket of the Mtb – ER module

The ER module of Mtb FAS-I is shown in grey surface representation. The FMN cofactor is shown in cyan-colored sticks, docked at the catalytic cleft. The movie shows a 30° rotational tilt of the structure.

File Name: Supplementary Movie 2

Description: Overview of the catalytic pocket of the Fungal – ER module

The ER module of fungal FAS-I (PDB code: 4V59) is shown in pink surface representation. Both the FMN and NADPH co-factors are shown as sticks in cyan and green, respectively. The movie shows a 30° rotational tilt of the structure.

File Name: Supplementary Movie 3

Description: Overview of the catalytic pocket of the Mtb – KR module

The KR module of Mtb FAS-I is shown in grey surface representation. The NADPH cofactor from the fungal FAS-I (PDB code: 4V59, shown as green spheres) is included to help visualize the catalytic cleft. A loop that partially conceals the catalytic cleft and changes conformation in respect to the fungal KR (residues 2237-2248) is highlighted in black. The movie shows a 30° rotational tilt of the structure.

File Name: Supplementary Movie 4

Description: Overview of the catalytic pocket of the Fungal – KR module

The KR module of fungal FAS-I (PDB code: 4V59) is shown in grey surface representation. The NADPH co-factor is shown as green spheres. A loop that partially conceals the catalytic cleft and changes conformation in respect to the Mtb KR (residues 750-761) is highlighted in hot pink. The movie shows a 30° rotational tilt of the structure.

File Name: Supplementary Movie 5

Description: Overview of the catalytic pocket of the Mtb – DH module

The DH module of Mtb FAS-I is shown in grey surface representation. The catalytic histidine is shown in blue inside the cleft. The movie shows a 30° rotational tilt of the structure.

File Name: Supplementary Movie 6

Description: Overview of the catalytic pocket of the Fungal – DH module

The DH module of fungal FAS-I (PDB code: 4V59) is shown in pink surface representation. The catalytic histidine is shown in blue inside the cleft. The movie shows a 30° rotational tilt of the structure.

File Name: Supplementary Movie 7

Description: Overview of the catalytic pocket of the Mtb – KS module

The KS module of Mtb FAS-I is shown in grey surface representation. The catalytic histidine and lysine residues are shown in blue inside the cleft. A long loop projected from the KR module and forms part of the ACP interaction surface is colored black. The movie shows a 30° rotational tilt of the structure.

File Name: Supplementary Movie 8

Description: Overview of the catalytic pocket of the Fungal – KS module

The KS module of fungal FAS-I is shown in pink surface representation. The catalytic histidine and lysine residues are shown in blue inside the cleft. The short equivalent loop to the Mtb-KR loop is colored hot pink. The movie shows a 30° rotational tilt of the structure.

File Name: Supplementary Movie 9

Description: Overview of the KR projecting loop near the KS active site

The Mtb-KR loop is shown in blue. The histidine and lysine catalytic residues of the KS module are shown in red and density for the ACP domain is shown in purple. A 360° rotation is shown to illustrate how the loop will affect the binding of the ACP domain.