

Description of Additional Supplementary Files

File Name: Supplementary Movie 1

Description: MD simulation from 0-100ns for micafungin with 3CLpro monomer.

File Name: Supplementary Movie 2

Description: MD simulation from 0-100ns for ivermectin with 3CLpro monomer.

File Name: Supplementary Movie 3

Description: MD simulation from 0-100ns for ivermectin with homodimer of 3CLpro.

File Name: Supplementary Data 1

Description: Data set for Figures 2-5, and Supplementary Figure 2 and 3.

File Name: Supplementary Data 2

Description: Data set for 3CLpro-OTDs docking study

File Name: Supplementary Data 3

Description: Data set for 3CLpro-OTDs docking study

File Name: Supplementary Data 4

Description: Data set for 3CLpro-PIs and VNIs

File Name: Supplementary Data 5

Description: Data set for MD simulation study of 3CLPro homodimer with ivermectin

File Name: Supplementary Data 6

Description: Data set for MD simulation study of 3CLPro monomer with ivermectin

File Name: Supplementary Data 7

Description: Data set for MD simulation study of 3CLPro monomer with micafungin