



SUPPLEMENTARY MATERIAL TO
Natural flavonoids in *Delonix regia* leaf as an antimycobacterial agent: An *in silico* study

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TABLE S-I. Chemical Interaction of natural flavonoid against *MtKasA*

Id compound	Interaction	
	Amino acid and type bond	Distance of hydrogen bond (Å)
TLM	Cys171 (HB), His311, Pro280, Phe237, Phe404 Flavonoid compounds	3.54
F1	Pro316 (HB), Val278 (HB), Thr313 (HB), Thr315 (HB), Pro280 (HB), His276 (HB)	3.37, 3.26, 2.62, 2.39, 3.54, 2.89
F2	Arg214 (HB); Met213 (HB); Met212 (HB)	3.02, 2.78, 2.31
F3	Thr315 (HB), Pro280 (HB), Ala215 (HB), Met213 (HB), His345 (HB)	4.12, 3.75, 3.50, 2.89, 2.72
F4	Phe402 (HB), Ala215 (HB), Met213 (HB), Pro280 (HB), Ile317 (HB), Cys171, His311, Phe404,	3.43, 3.23, 2.28, 2.17, 2.92
F5	Gly406 (HB), Asp273 (HB), His311 (HB), Arg214 (HB), Thr313 (HB), Pro280	3.45, 2.50, 3.27, 2.56, 3.10
F6	Thr315 (HB), His311 (HB), Asn408 (HB), Asp273 (HB), Pro280 (HB)	4.13, 2.30, 2.33, 2.67, 3.51
F7	Thr315 (HB), Ala215 (HB), His276 (HB), Pro280	4.14, 3.53, 3.43
F8	Thr315 (HB), Thr313 (HB), Gly318 (HB), Pro280, Phe404	2.26, 2.92, 3.70
F9	Met213 (HB)	2.56
F10	Arg214 (HB), Thr315 (HB), Pro280, Phe404	2.36, 3.99
F11	Ala215 (HB), Met213 (HB), Pro280, His311	3.70, 2.56
F12	Gly406 (HB), Thr313 (HB), Cys171, Pro280	3.31, 4.05
F13	Thr313 (HB), Gly406 (HB), Asn408 (HB), Cys171, Pro280, Phe404	4.06, 3.27, 1.55

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*HB = Hydrogen Bond

TABLE S-II. Chemical Interaction of natural flavonoid against *MtDprE1*

Id compound	Interaction	
	Amino acid and type bond	Distance of hydrogen bond (Å)
OT4	Val365 (HB), Cys387 (HB), Lys134 (HB), Gly117 (HB), Leu363, Gly133 Flavonoid compounds	2.49, 3.22, 2.98, 3.73
F1	Ser246 (HB), Ser228 (HB), Tyr314 (HB), Lys134, Val365	3.71, 3.29, 2.20
F2	Ser228 (HB), Tyr60 (HB), Asn385 (HB), Val365	2.31, 2.63, 2.86
F3	Ser228 (HB), His132 (HB), Gln336 (HB), Tyr60 (HB), Cys387 (HB), Lys134, Val365	3.66, 2.76, 2.76, 2.85, 3.68
F4	Trp230 (HB), Ser228 (HB), Lys134 (HB), Gly133 (HB), Pro116 (HB), His132 (HB), Tyr60 (HB), Cys387 (HB), Val365	3.02, 3.40, 3.20, 3.21, 3.35, 2.37, 3.10, 3.53
F5	Gly117 (HB), Tyr314 (HB), Ser228 (HB), His132 (HB), Gln336 (HB), Val365, Cys387, Lys134, Gly133	3.17, 2.05, 3.03, 2.27, 2.47
F6	Trp230 (HB), Lys134 (HB), Tyr60 (HB), Asp389 (HB), Ser228 (HB), Val365	3.04, 3.26, 2.79, 3.71, 3.32
F7	Ser228 (HB), Tyr60 (HB), Gln336 (HB), Asn385 (HB), Val365, Lys134, Cys387	3.35, 2.85, 3.28, 2.62
F8	Phe313 (HB), Thr314 (HB), Tyr60 (HB), Cys387 (HB), His315 (HB), Ser228 (HB), Val365, Leu363	2.42, 2.94, 2.83, 2.35, 3.76, 3.21
F9	Asn385 (HB), His315 (HB), Gly117 (HB), Ser228 (HB), His132 (HB), Val365, Lys134, Cys387, Leu363	2.89, 2.55, 2.73, 2.88, 2.56
F10	Asn385 (HB), Lys134 (HB), Tyr314 (HB), Ser228 (HB), Tyr60 (HB), Cys387 (HB), Gly117 (HB), Val365	2.80, 2.94, 2.39, 3.13, 2.89, 4.14, 3.10
F11	Gln336 (HB), Asn385 (HB), Cys387 (HB), His132 (HB), Tyr60 (HB), Val365, Leu363	2.80, 3.07, 3.37, 3.06, 2.43
F12	Lys418 (HB), His132 (HB), Ser228 (HB), Val365, Cys387, Lys134,	3.31, 2.70, 3.58
F13	Lys134 (HB), Ser228 (HB), Trp230 (HB), Val365	3.11, 3.48, 3.08

*HB = Hydrogen Bond

Table S-III. Chemical Interaction of natural flavonoid against *MtPank*

Id compound	Interaction	
	Amino acid and type bond	Distance of hydrogen bond (Å)
ZVT	Arg238 (HB), Tyr235 (HB), Asn277 (HB), Lys147 (HB), Met242, Phe254, Phe239, Ile272, Leu203, Leu132, Ile276	3.13, 1.94, 2.46, 2.74
	Flavonoid compounds	
F1	Tyr182 (HB), Tyr235 (HB), Asn277 (HB), Lys147 (HB), Phe254, Ile272	4.11, 3.80, 2.46, 2.98
F2	Tyr257 (HB), Tyr182 (HB), Lys147 (HB), Tyr153 (HB), His179 (HB), Tyr235 (HB), Phe254, Ile272, Ile276	3.17, 3.98, 2.14, 2.29, 2.41, 3.14
F3	Tyr235 (HB), Tyr153 (HB), Ile272, Phe254, Met242	3.86, 2.42
F4	Glu201 (HB), Gly148 (HB), Asn277 (HB), Tyr182 (HB), Tyr235 (HB), His179 (HB), Leu203, Met242	3.46, 3.54, 2.74, 3.54, 3.73, 2.87
F5	Asn277 (HB), Tyr235 (HB)	2.55, 2.29
F6	Tyr235 (HB), Arg238 (HB), Tyr177 (HB), Tyr153 (HB), Ile272, Met242	3.87, 3.21, 3.06, 3.10
F7	Asp129 (HB), Gly148 (HB), Asn277 (HB), Lys103 (HB), Leu203, Leu132	2.63, 3.58, 2.34, 3.39
F8	Tyr235 (HB), Met242 (HB), Tyr153 (HB), Lys103 (HB), Lys147 (HB), Ile272, Ile276, Leu203 (HB), Asp129 (HB), Tyr182 (HB), Phe239, Lys147	3.13, 2.77, 2.11, 3.13, 2.34
F9	Tyr235 (HB), Asn277 (HB), His179 (HB), Tyr182 (HB), Lys147, Phe254	2.97, 2.81, 2.15, 2.49
F10	Tyr235 (HB), His179 (HB), Tyr182 (HB), Glu201 (HB), Phe254, Ile272, Met242, Leu203	3.90, 2.62, 3.04, 2.75
F11	Tyr153 (HB), Tyr235 (HB), Asn277 (HB), Lys147	2.38, 2.25, 3.16
F12	Tyr153 (HB), Asn277 (HB), Tyr235 (HB), Lys147	2.48, 3.08, 2.64
F13		

*HB = Hydrogen Bond