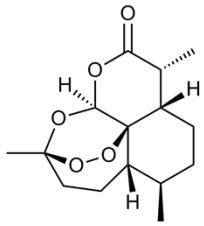
Electronic Supplementary Material (ESI) for Integrative Biology.

Supplemental information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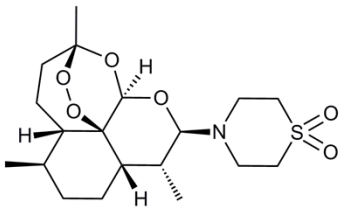
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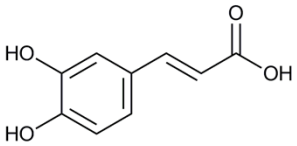
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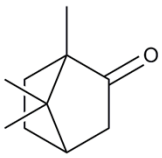
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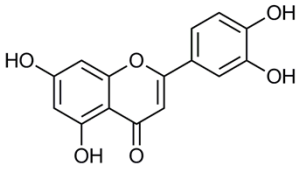
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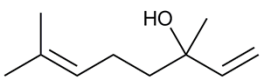
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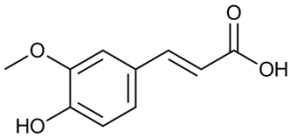
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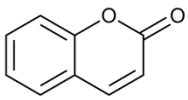
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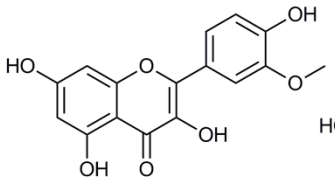
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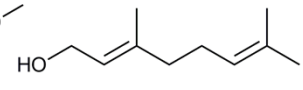
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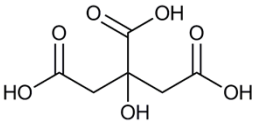
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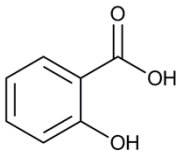
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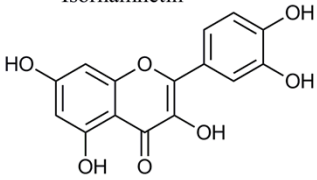
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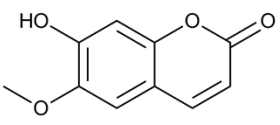
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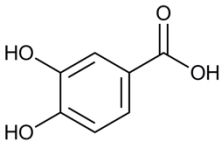
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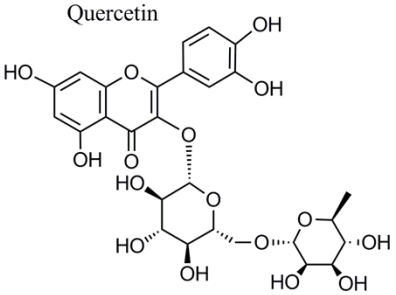
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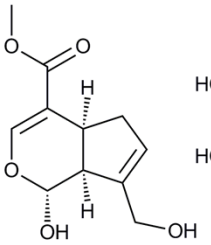
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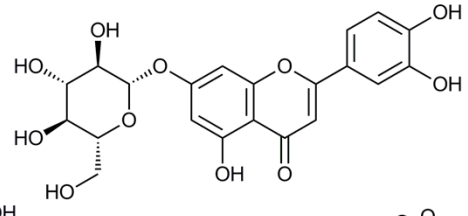
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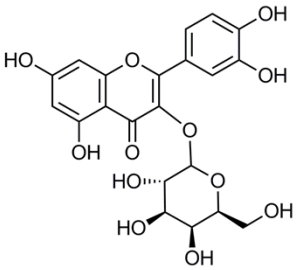
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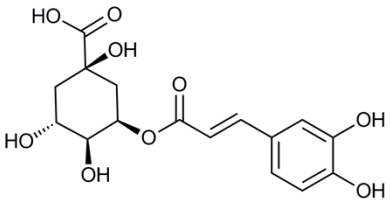
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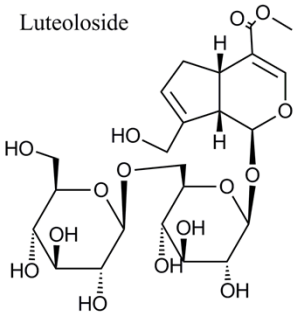
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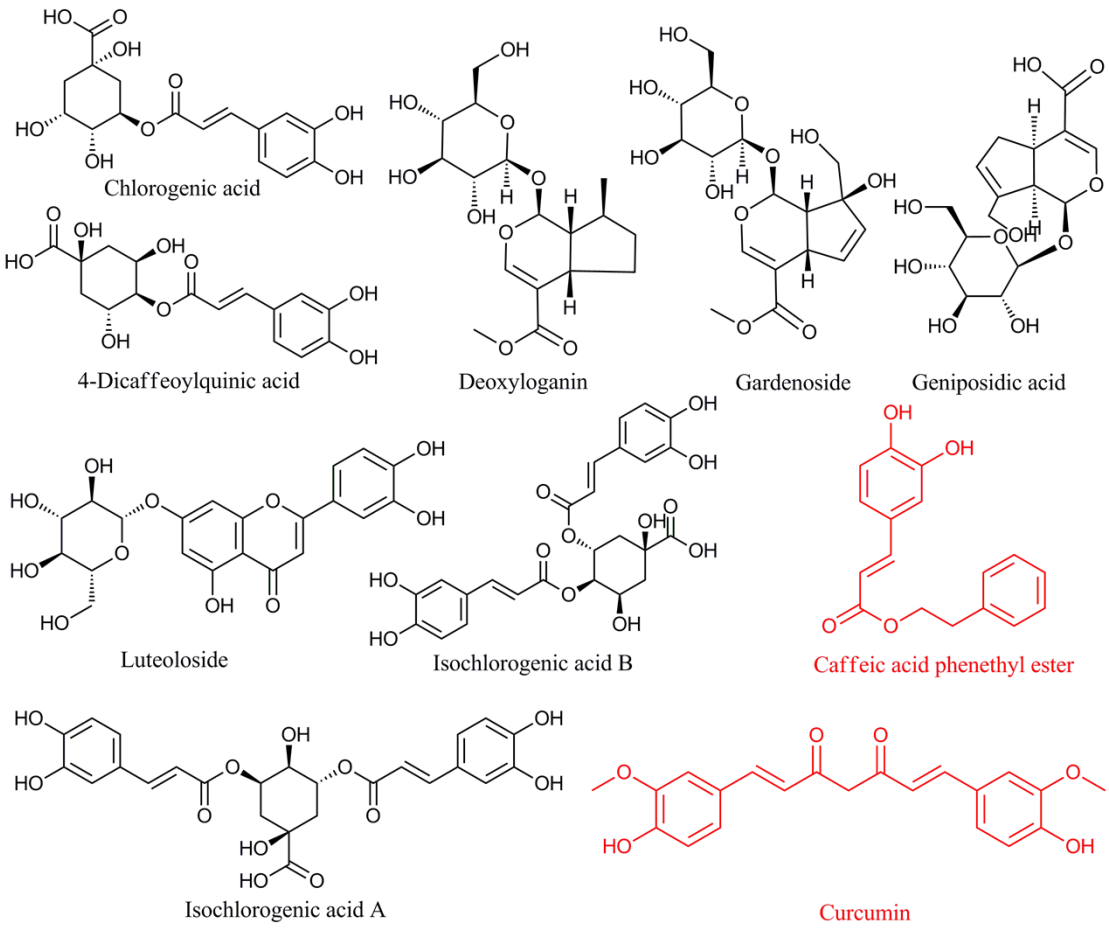
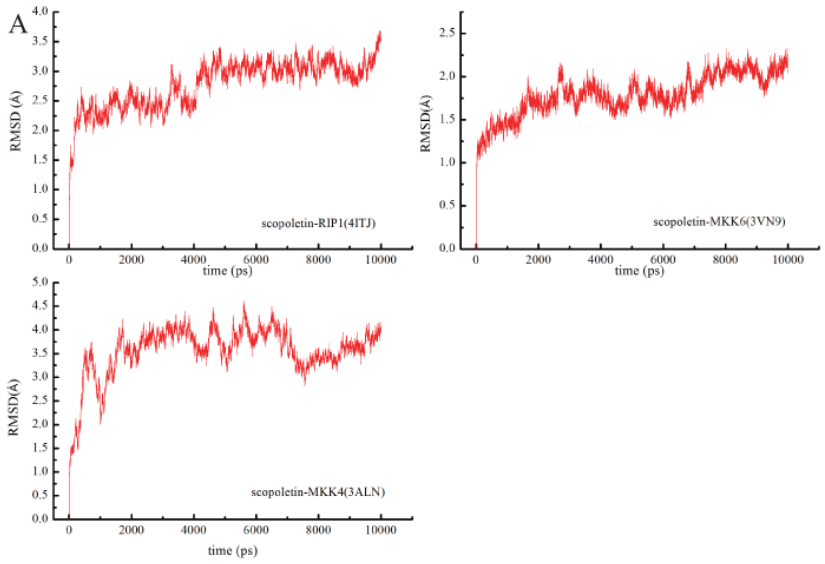


Figure S1. Two dimensional structures of all compounds and two known inhibitor for molecular docking. Caffeic acid phenethyl ester and curcumin were two known inhibitors(Kumar and Bora, 2012; Natarajan, et al., 1996) for AP-1 (PDB ID: 1FOS) and NF-kB (PDB ID: 3GUT). The structure related to Table 1.



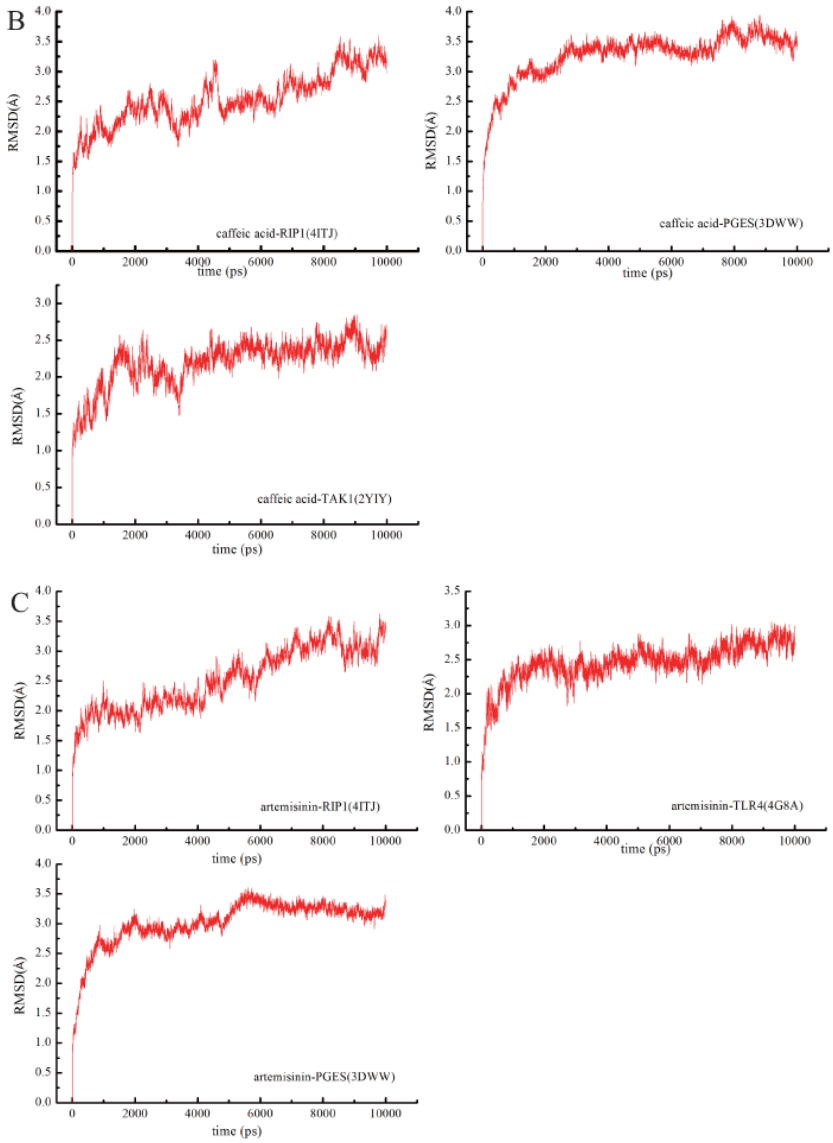
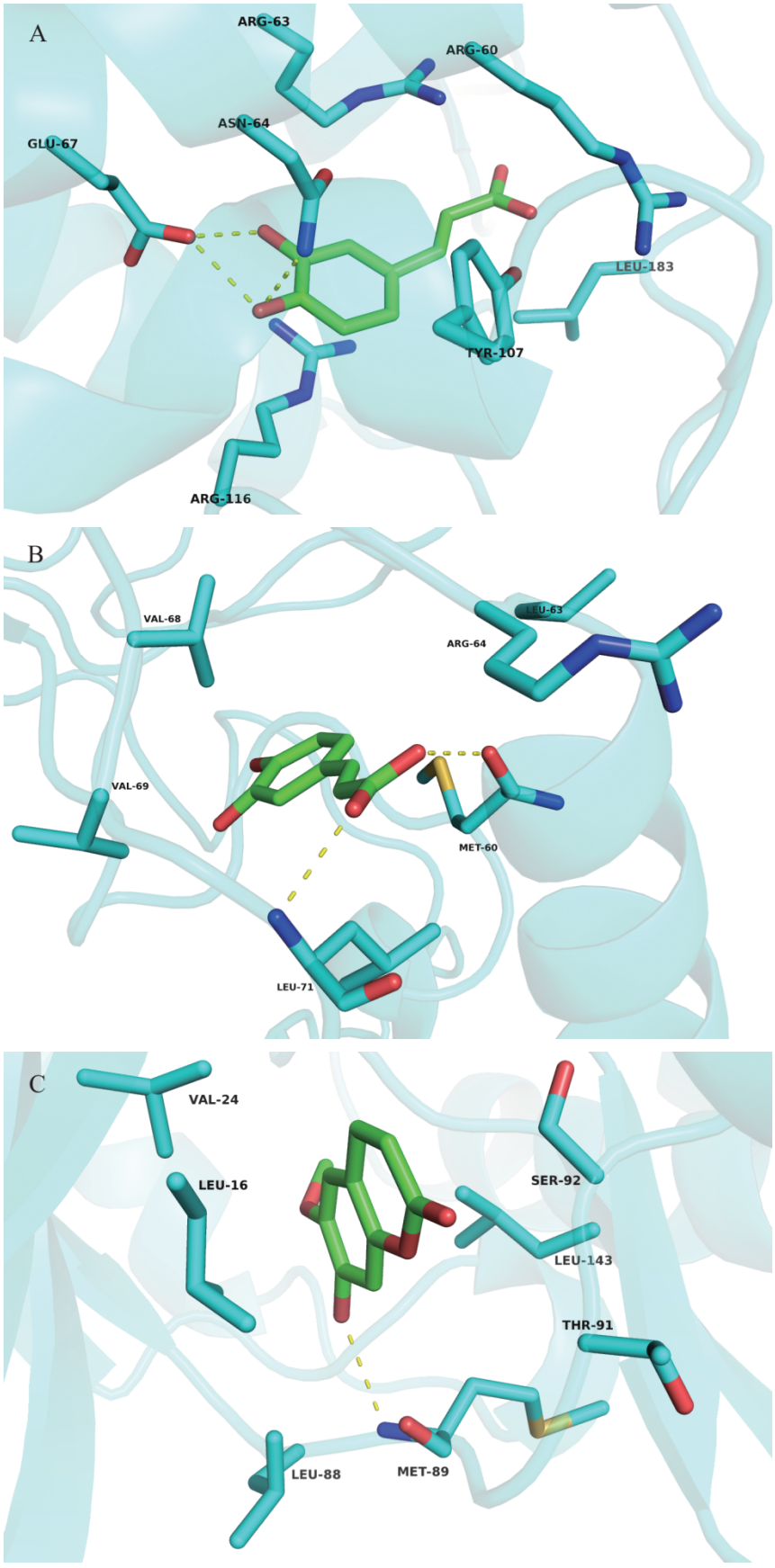


Figure S2. Plots of RMSDs of the top three protein-ligand complexes for most potent compounds during 10 ns of MD simulations. (A) three proteins and scopoletin complex, (B) three proteins and caffeic acid, (C) three proteins and artemisin.


A
ARG-63
ARG-60
ASN-64
GLU-67
LEU-183
TYR-107
ARG-116
B
VAL-68
LEU-63
ARG-64
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C
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LEU-16
SER-92
LEU-143
THR-91
LEU-88
MET-89

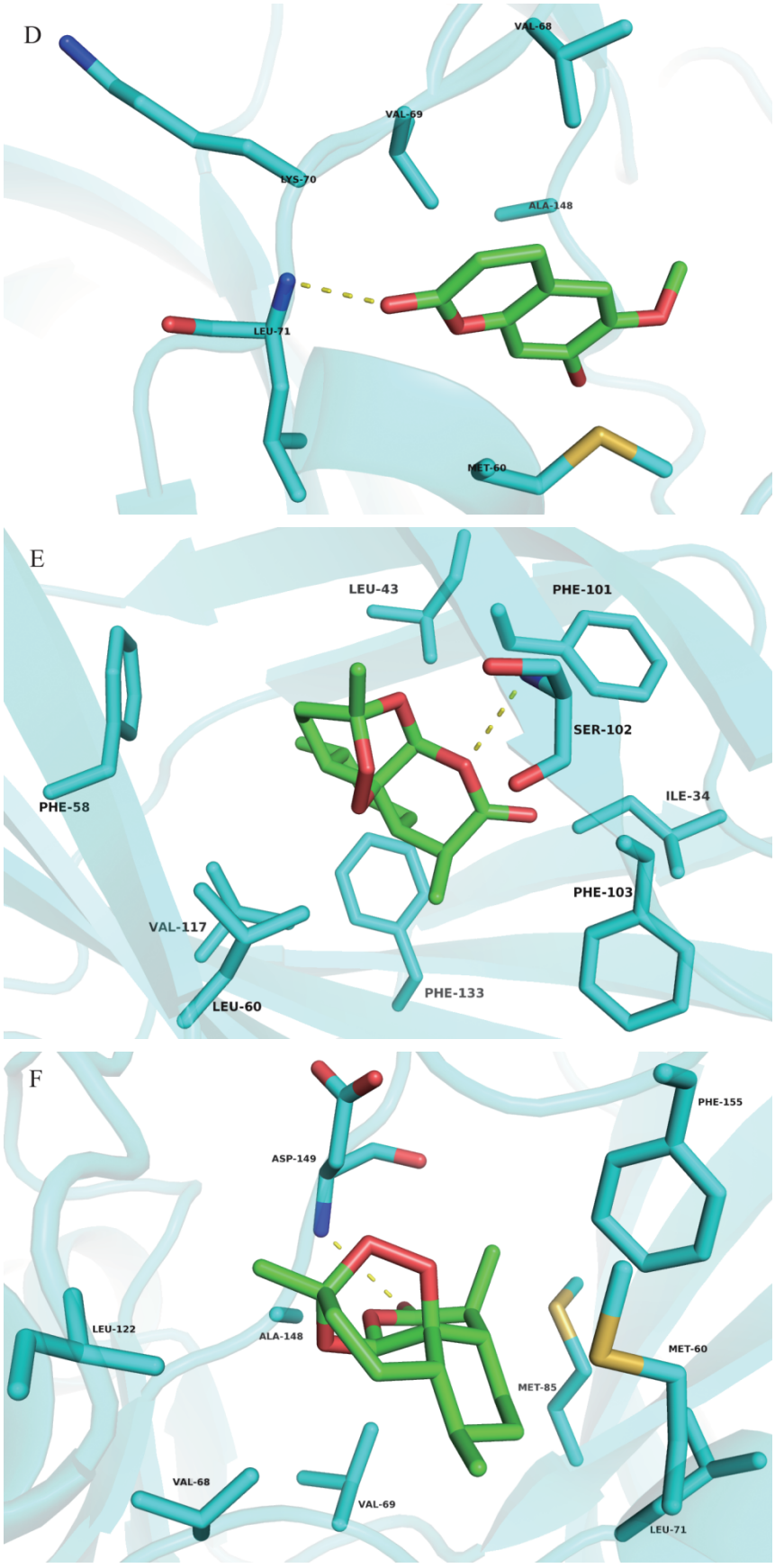

Figure S3. The binding modes of potent compounds with top target proteins after 10

ns MD simulations. (A) complex caffeic acid/PGES (3DWW), (B) complex caffeic acid/RIP1 (4ITJ), (C) complex scopoletin/MKK6 (3VN9), (D) complex scopoletin/RIP1 (4ITJ), (E) complex artemisinin/TLR4 (4G8A), (F) complex artemisinin/RIP1 (4ITJ) Ligands and some important residues are shown in stick, and hydrogen bonds are shown in dashed line (yellow).