Supplemental

Fig. 1. CPK mode diagram of structure of CyPA in complex with substrate peptide suc-AAPF-NA (PDB code: 1RMH). The bound substrate peptide is shown in golden. The CyPA residue R55 is shown in green, residues R69, H70 and T107 is shown in red, residues F60 and H126 is shown in magenta, and the loop consisting residues 118-125 is shown in cyan.

Figure 1

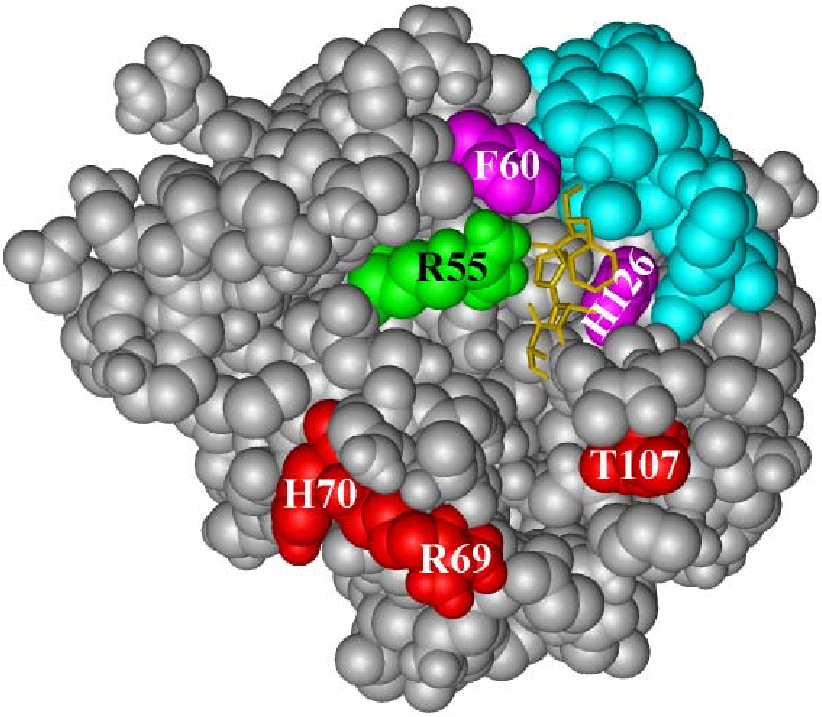

Fig. 2. An overlay of 2D ^{1}H-^{15}N HSQC spectra of CyPA^{R55A} (A), CyPA^{R69A} (B), CyPA^{H70A} (C), CyPA^{T107A} (D), CyPA^{F60A} (E) and CyPA^{H126A} (F) (red) with that of CyPA^{WT} (blue). For CyPA^{R55A}, CyPA^{R69A}, CyPA^{H70A}, CyPA^{T107A}, only NH signals from residues close to the mutation sites are affected. For CyPA^{F60A} and CyPA^{H126A}, much more residues exhibit NH signal shift, indicating for more significant structural perturbation. Residues displaying significant NH chemical shift are indicated by the one-letter amino acid code and residue number in A-D.

Figure 2