Catalytic Mechanism of Class A β-lactamase:
Role of Lysine 73 and C3-carboxyl group of the substrate
pen G in the deacylation step

Yasuyuki Fujii, Masayuki Hata, Tyuji Hoshino and Minoru Tsuda

Supporting Information

Fig.S1: Structures of extended model I. The atoms which are also used in Fig.1(b) are shown with circles.
Fig. S2: Structures of extended model II.
Fig. S3: Energy diagrams with the extended model I and II, which were obtained by potential energy calculation at B3LYP/6-31G** level. Vertical axis represents absolute value of potential energy in kcal/mol. Relative values to A2-I or A2-II are shown in parenthesis.