

The investigation of interaction competition between ATP with N-DIPP-AA, N-Boc-AA and AA

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Abstract

Protein kinases, which is one of the largest families of enzymes and structurally diverse, catalyze and the transfer the γ -phosphoryl group of ATP to the amino acid residues in their target proteins^[1]. The phosphorylation of protein is one of the major posttranslational modifications required for regulation of cellular activities, so the study of detailed chemical mechanism for the phosphoryl-transfer step is of profound importance. It is well known that electrospray ionization mass spectrometry (ESI-MS) is a powerful method to observe the intact non-covalent complexes between biomolecules and small molecular^[2,3]. In this paper, the interactions of ATP with N-DIPP-AA, N-Boc-AA and AA were studied by ESI-MS. Shown as Fig.1 (Ala was as the example), the complex of ATP and Boc-Ala or DIPP-Ala was clearly observed, while that of ATP and Ala could not be found in the spectrum. The parameter of capillary exit on which the complex disappeared gives a proof that the interaction between ATP and DIPP-Ala was stronger than that between ATP and Boc-Ala. The binding energy of ATP with Ala, Boc-Ala and DIPP-Ala was computed using the software Sybyl 7.1. From all the data, it can be concluded that DIPP-Ala is the winner in the competition for ATP.

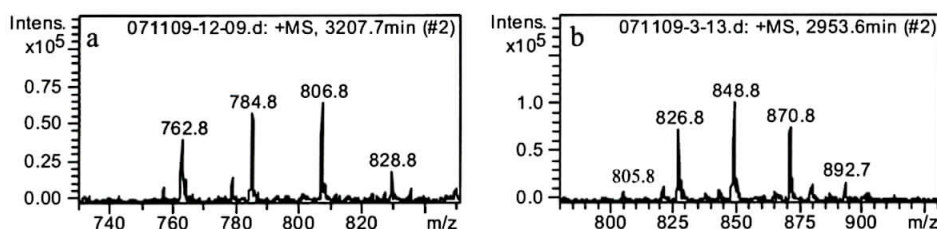


Fig. 1 The ESI-MS spectra of the interaction of ATP-2Na with Boc-Ala(a), DIPP-AA(b) (a: 763: [ATP-2Na+Boc-Ala+Na]⁺, 785: [ATP-3Na+Boc-Ala+Na]⁺; 807: [ATP-4Na+Boc-Ala+Na]⁺; 829: [ATP-4Na+Boc-Ala+2Na]⁺. b: 805: [ATP-2Na+DIPP-Ala+H]⁺, 827: [ATP-2Na+DIPP-Ala+Na]⁺, 849: [ATP-3Na+DIPP-Ala+Na]⁺, 871: [ATP-4Na+DIPP-Ala+Na]⁺, 893: [ATP-4Na+DIPP-Ala+2Na]⁺)

Table 1. The data of Capillary Exit on which the complex disappeared and Binding energy from Sybyl 7.1

Copound name	Capillary Exit on which the complex disappeared (Volt)	Binding energy(kJ/mol)
L-Ala	/	-6.555
Boc-L-Ala	236.6	-15.634
DIPP-L-Ala	>320	-35.407

Reference:

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