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pH detection in biological samples by 1D and 2D ^{1}H-^{31}P NMR

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Abstract

The chemical shifts of several important endogenous phosphorus compounds under different pH conditions were explored, including adenosine-5'-triphosphate, adenosine-5'-diphosphate, adenosine-5'-monophosphate, phosphorylcholine and phosphorylethanolamine. Their ^{31}P-NMR and ^{1}H-NMR chemical shifts were all pH-sensitive in the similar pH range. Two dimensional (2D) ^{1}H-^{31}P NMR spectra were found helpful to identify these endogenous phosphorus markers in biological samples from rather complicated NMR spectra. Herein, for the first time, a pH sensor based on 2D ^{1}H-^{31}P NMR was established and applied to biological samples analysis with pH values determined in good agreement with those by potentiometric method. Apart from being simple, green, rapid and less sample-consuming, information concerning both the endogenous phosphorus markers and pH status could be attained in a single NMR run, which demonstrated the great potential of this method in rare sample analysis and even disease diagnosis.

Graphical abstract

The chemical shifts of several important endogenous phosphorus compounds were explored in different pH condition, including adenosine 5'- triphosphate, adenosine-5'-di-phosphate, adenosine-5'-monophosphate, phosphorylcholine and phosphoylethanolamine. Their ^{31}P-NMR and ^{1}H-NMR chemical shifts were both pH-sensitive in a similar range. 2D ^{1}H-^{31}P NMR spectra were helpful to recognize endogenous phosphorus markers in very complex NMR spectra of biological samples. A pH sensor based on 2D ^{1}H-^{31}P NMR was established and applied. The measured pH values agreed well with the results by potentiometric method.