4D APSY-HBCB(CG)CDHD experiment for automated assignment of aromatic amino acid side chains in proteins

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A four-dimensional (4D) APSY (automated projection spectroscopy)-HBCB(CG)CDHD experiment is presented. This 4D experiment correlates aromatic with aliphatic carbon and proton resonances from the same amino acid side chain of proteins in aqueous solution. It thus allows unambiguous sequence-specific assignment of aromatic amino acid ring signals based on backbone assignments. Compared to conventional 2D approaches, the inclusion of evolution periods on (1)H(?) and (13)C(?) efficiently removes overlaps, and provides two additional frequencies for consequent automated or manual matching. The experiment was successfully applied to three proteins with molecular weights from 6 to 13ăkDa. For the complementation of the assignment of the aromatic resonances, TOCSY- or COSY-based versions of a 4D APSY-HCCH(aro) sequence are proposed.

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