J Biomol NMR (2007) 38:267
DOI 10.1007/s10858-006-9135-5

LETTER TO THE EDITOR

Automated backbone and side-chain assignment of mitochondrial matrix cyclophilin D

Andreas Schedlbauer · Bernd Hoffmann · Georg Kontaxis · Simon Rüdisser · Ulrich Hommel · Robert Konrat

Received: 18 October 2006 / Accepted: 23 November 2006 / Published online: 25 May 2007

The 17.7 kDa mitochondrial matrix protein cyclophilin D (CycD) is involved in opening of the mitochondrial permeability transition pore which is thought to be a key event in triggering apoptosis of the host cell (Crompton 2000). Low molecular weight ligands binding to CycD can prevent this process and are expected to be useful in the treatment of Parkinson disease (Costantini et al. 2001).

3D HNCA, 3D HNCACB, 3D CBCA(CO)NH, and 3D ^{15}N,^{13}C NOESY-HSQC recorded on ^{15}N,^{13}C labelled recombinant CycD were employed to obtain (a) an essentially complete backbone assignment ($^{1}H^{N}/^{15}N$: 95.6%; $^{13}C^{\alpha}$,$^{1}H^{\alpha}$,$^{13}C^{\beta}$: 90.9%) using a Monte Carlo/Simulated Annealing (MC/SA) program (Hoffmann et al. 2005), and (b) a high extent sidechain assignment (aliphatic $^{1}H/^{13}C$: 87.4%; $^{13}CH_3$ (I,L,V,A,T,M): 87.4%; sidechain aromatic ^{1}H (F,Y,W): 87.5% sidechain amide-$^{15}NH_2$ (N,Q): 61.5%). Allocation of methyl groups and side-chain atoms was achieved applying an automated iterative NOE based side-chain signal assignment approach (to be published). BMRB accession number 7310.

References

Crompton M (2000) Mitochondrial intermembrane junctional complexes and their role in cell death. J Physiol 1:11–21

Hofmann B, Eichmüller C, Kontaxis G, Steinhauser O, Konrat R (2005) Rapid assessment of protein structural stability and fold validation via NMR. MethEnzymol 394:142–174

Costantini LC, Cole D, Isacson O (2001) Immunophilin ligands can prevent progressive dopaminergic degeneration in animal models of Parkinson's disease. Eur J Neurosci 13(6):1085–92

Electronic Supplementary Material The online version of this article (doi:10.1007/s10858-006-9135-5) contains supplementary material, which is available to authorized users.

A. Schedlbauer · B. Hoffmann · G. Kontaxis · R. Konrat (✉)
Department of Biomolecular Structural Chemistry, Max F. Perutz Laboratories, University of Vienna, Vienna Biocenter Campus 5, 1030 Vienna, Austria
e-mail: robert.konrat@univie.ac.at

S. Rüdisser · U. Hommel
Novartis Institutes for BioMedical Research, Basel, Switzerland