

## Contents of Volume 13, 1999

### Vol. 13 No. 1 1999

#### *Research papers*

|  |       |
|--|-------|
| Improved $^1\text{H}$ -detected triple resonance TROSY-based experiments<br>D. Yang and L.E. Kay   | 3–10  |
| Solution structure of human acidic fibroblast growth factor and interaction with heparin-derived hexasaccharide<br>K. Ogura, K. Nagata, H. Hatanaka, H. Habuchi, K. Kimata, S.-i. Tate, M.W. Ravera, M. Jaye, J. Schlessinger and F. Inagaki | 11–24 |
| Determination of the relative NH proton lifetimes of the peptide analogue viomycin in aqueous solution by NMR-based diffusion measurement<br>M. Liu, H.C. Toms, G.E. Hawkes, J.K. Nicholson and J.C. Lindon                                  | 25–30 |
| Mapping of the detergent-exposed surface of membrane proteins and peptides by $^1\text{H}$ solution NMR in detergent: Application to the gramicidin A ion channel<br>M. Seigneuret and C. Le Guernevé  | 31–41 |
| Half-filter experiments for assignment, structure determination and hydration analysis of unlabelled ligands bound to $^{13}\text{C}/^{15}\text{N}$ labelled proteins<br>C. Dalvit, S. Cottens, P. Ramage and U. Hommel                      | 43–50 |
| Influence of non-bonded parameters on the quality of NMR structures: A new force field for NMR structure calculation<br>J.P. Linge and M. Nilges   | 51–59 |
| <i>Short communications</i>  |       |
| Normalized one-dimensional NOE measurements in isotopically labeled macromolecules using two-way cross-polarization<br>E. Chiarparin, P. Pelupessy, B. Cutting, T.R. Eykyn and G. Bodenhausen  | 61–65 |
| Band-selective editing of exchange-relay in protein-water NOE experiments<br>G. Melacini, R. Boelens and R. Kaptein  | 67–71 |
| Water-protein NOEs: Optimized scheme for selective water excitation<br>E. Liepinsh and G. Otting   | 73–76 |
| Gradient and sensitivity enhancement of 2D TROSY with water flip-back, 3D NOESY-TROSY and TOCSY-TROSY experiments<br>G. Zhu, X. Kong and K. Sze  | 77–81 |
| Reduced spectral density mapping for proteins: Validity for studies of $^{13}\text{C}$ relaxation<br>R.A. Atkinson and J.-F. Lefèvre   | 83–88 |
| <i>Letters to the Editor: New NMR assignments</i>  |       |
| Backbone resonance assignments of human UBC9<br>Q. Liu, B. Shen, D.J. Chen and Y. Chen   | 89–90 |
| $^1\text{H}$ , $^{13}\text{C}$ , and $^{15}\text{N}$ assignments and secondary structure of the high pH form of subunit c of the $\text{F}_1\text{F}_0$ ATP synthase<br>V.K. Rastogi and M.E. Girvin   | 91–92 |
| $^1\text{H}$ , $^{13}\text{C}$ and $^{15}\text{N}$ backbone resonance assignment of <i>Escherichia coli</i> adenylate kinase, a 23.6 kDa protein<br>S. Burlacu-Miron, V. Perrier, A.-M. Gilles, J. Mispelter, O. Bârzu and C.T. Craescu      | 93–94 |

**Vol. 13 No. 2 1999***Research papers*

- Assessing potential bias in the determination of rotational correlation times of proteins by NMR relaxation  
A.L. Lee and A.J. Wand 101–112
- Characterization of the solution properties of *Pichia farinosa* killer toxin using PGSE NMR diffusion measurements  
W.S. Price, F. Tsuchiya, C. Suzuki and Y. Arata 113–117
- Restrained molecular dynamics of solvated duplex DNA using the particle mesh Ewald method  
D.E. Konerding, T.E. Cheatham III, P.A. Kollman and T.L. James 119–131
- Determination of order parameters and correlation times in proteins: A comparison between Bayesian, Monte Carlo and simple graphical methods  
M.T. McMahon and E. Oldfield 133–137
- The effect of noncollinearity of  $^{15}\text{N}$ - $^1\text{H}$  dipolar and  $^{15}\text{N}$  CSA tensors and rotational anisotropy on  $^{15}\text{N}$  relaxation, CSA/dipolar cross correlation, and TROSY  
D. Fushman and D. Cowburn 139–147
- Production of large quantities of isotopically labeled protein in *Pichia pastoris* by fermentation  
M.J. Wood and E.A. Komives 149–159
- Conformational flexibility in calcitonin: The dynamic properties of human and salmon calcitonin in solution  
P. Amodeo, A. Motta, G. Strazzullo and M.A. Castiglione Morelli 161–174
- Short communications*
- A doublet-separated sensitivity-enhanced HSQC for the determination of scalar and dipolar one-bond J-couplings  
F. Cordier, A.J. Dingley and S. Grzesiek 175–180
- Analysis of deuterium relaxation-derived methyl axis order parameters and correlation with local structure  
A. Mittermaier, L.E. Kay and J.D. Forman-Kay 181–185
- Bicelle-based liquid crystals for NMR-measurement of dipolar couplings at acidic and basic pH values  
M. Ottiger and A. Bax 187–191
- Letters to the Editor: New NMR assignments*
- Backbone and  $\text{C}^\beta$  assignments of the anti-gp120 antibody Fv fragment complexed with an antigenic peptide  
V. Tugarinov, R. Levy, A. Dahan-Schokoroy and J. Anglister 193–194
- Sequence-specific  $^1\text{H}$ ,  $^{15}\text{N}$  and  $^{13}\text{C}$  assignment of adenylate kinase from *Escherichia coli* in complex with the inhibitor AP<sub>5</sub>A  
E. Meirovitch, M.A. Sinev and E.V. Sineva 195–196
- Expression and assignment of the  $^1\text{H}$ ,  $^{15}\text{N}$ , and  $^{13}\text{C}$  resonances of the C-terminal domain of the diphtheria toxin repressor  
P.D. Twigg, G.P. Wylie, G. Wang, D.L.D. Caspar, J.R. Murphy and T.M. Logan 197–198

**Vol. 13 No. 3 1999**

|  |         |
|--|---------|
| $C^\alpha$ and $C^\beta$ carbon-13 chemical shifts in proteins from an empirical database<br>M. Iwadate, T. Asakura and M.P. Williamson  | 199–211 |
| Heteronuclear relaxation in time-dependent spin systems: $^{15}\text{N}-\text{T}_{1\rho}$ dispersion during adiabatic fast passage<br>R. Konrat and M. Tollinger   | 213–221 |
| Protein-ligand interactions measured by $^{15}\text{N}$ -filtered diffusion experiments<br>M.L. Tillett, M.A. Horsfield, L.-Y. Lian and T.J. Norwood   | 223–232 |
| High resolution solution structure of apo calycyclin and structural variations in the S100 family of calcium-binding proteins<br>L. Mäler, B.C.M. Potts and W.J. Chazin  | 233–247 |
| The solution structure of the N-terminal zinc finger of GATA-1 reveals a specific binding face for the transcriptional co-factor FOG<br>K. Kowalski, R. Czolij, G.F. King, M. Crossley and J.P. Mackay                                 | 249–262 |
| Alternative E.COSY techniques for the measurement of $^3J(\text{C}'_{i-1}, \text{C}_i^\beta)$ and $^3J(\text{H}_i^N, \text{C}_i^\beta)$ coupling constants in proteins<br>F. Löhr and H. Rüterjans                                     | 263–274 |
| Microsecond time scale dynamics in the RXR DNA-binding domain from a combination of spin-echo and off-resonance rotating frame relaxation measurements<br>F.A.A. Mulder, P.J.A. van Tilborg, R. Kaptein and R. Boelens                 | 275–288 |
| Protein backbone angle restraints from searching a database for chemical shift and sequence homology<br>G. Cornilescu, F. Delaglio and A. Bax  | 289–302 |
| <i>Letters to the Editor: New NMR assignments</i>  |         |
| Sequence-specific $^1\text{H}$ , $^{13}\text{C}$ and $^{15}\text{N}$ assignment of the single-stranded DNA binding protein of the bacteriophage $\phi 29$<br>A. Pineda-Lucena, G.W. Vuister and C.W. Hilbers                           | 303–304 |
| Sequence-specific resonance assignments for the NADP(H)-binding component (domain III) of proton-translocating transhydrogenase from <i>Rhodospirillum rubrum</i><br>M. Jeeves, K.J. Smith, P.G. Quirk, N.P.J. Cotton and J.B. Jackson | 305–306 |
| $^1\text{H}$ , $^{15}\text{N}$ and $^{13}\text{C}$ resonance assignments for the catalytic core of $\gamma\delta$ resolvase<br>B. Pan and G.P. Mullen  | 307–308 |
| $^1\text{H}$ , $^{15}\text{N}$ and $^{13}\text{C}$ resonance assignments for the 22 kDa LC1 light chain from <i>Chlamydomonas</i> outer arm dynein<br>H. Wu, M.W. Maciejewski, S.E. Benashski, G.P. Mullen and S.M. King               | 309–310 |

**Vol. 13 No. 4 1999***Research papers*

|  |         |
|--|---------|
| A high quality nuclear magnetic resonance solution structure of peptide deformylase from <i>Escherichia coli</i> : Application of an automated assignment strategy using GARANT<br>J.F. O'Connell, K.D. Pryor, S.K. Grant and B. Leiting | 311–324 |
| Automated detection of problem restraints in NMR data sets using the FINGAR genetic algorithm method<br>D.A. Pearlman  | 325–335 |
| Solid-state NMR triple-resonance backbone assignments in a protein<br>W.M. Tan, Z. Gu, A.C. Zeri and S.J. Opella   | 337–342 |

|  |         |
|--|---------|
| NMR structure of the chimeric hybrid duplex r(gcagggc) · r(gcca)d(CTGC) comprising the tRNA-DNA junction formed during initiation of HIV-1 reverse transcription<br>T. Szyperski, M. Götte, M. Billeter, E. Perola, L. Cellai, H. Heumann and K. Wüthrich  | 343–355 |
| The structure in solution of the <i>b</i> domain of protein disulfide isomerase<br>J. Kemmink, K. Dijkstra, M. Mariani, R.M. Scheek, E. Penka, M. Nilges and N.J. Darby  | 357–368 |
| <i>Short communications</i>  |         |
| A robust and cost-effective method for the production of Val, Leu, Ile ( $\delta$ 1) methyl-protonated $^{15}\text{N}$ -, $^{13}\text{C}$ -, $^2\text{H}$ -labeled proteins<br>N.K. Goto, K.H. Gardner, G.A. Mueller, R.C. Willis and L.E. Kay   | 369–374 |
| Efficient determination of angles subtended by $\text{C}^\alpha\text{-H}^\alpha$ and $\text{N-H}^N$ vectors in proteins via dipole-dipole cross-correlation<br>P. Pelupessy, E. Chiaparin, R. Ghose and G. Bodenhausen   | 375–380 |
| A novel NMR experiment for the sequential assignment of proline residues and proline stretches in $^{13}\text{C}/^{15}\text{N}$ labeled proteins<br>M.J. Bottomley, M.J. Macias, Z. Liu and M. Sattler   | 381–385 |
| Improved low pH bicelle system for orienting macromolecules over a wide temperature range<br>S. Cavagnero, H.J. Dyson and P.E. Wright  | 387–391 |
| <i>Letters to the Editor: New NMR assignments</i>  |         |
| $^1\text{H}$ , $^{15}\text{N}$ , and $^{13}\text{C}$ resonance assignments for the N-terminal 20 kDa domain of the DNA single-strand break repair protein XRCC1<br>A. Marintchev, M.W. Maciejewski and G.P. Mullen   | 393–394 |
| Backbone and side-chain $^1\text{H}$ , $^{15}\text{N}$ , and $^{13}\text{C}$ assignments for the topological specificity domain of the MinE cell division protein<br>G.F. King, B. Pan, M.W. Maciejewski, S.L. Rowland, L.I. Rothfield and G.P. Mullen   | 395–396 |
| $^1\text{H}$ , $^{15}\text{N}$ and $^{13}\text{C}$ assignments of the DNA binding domain of transcription factor Mbp1 from <i>S. cerevisiae</i> in both its free and the DNA bound forms, and $^1\text{H}$ assignments of the free DNA<br>P.B. McIntosh, I.A. Taylor, S.J. Smerdon, T.A. Frenkel and A.N. Lane | 397–398 |
| <i>Author index</i>  | 399–400 |
| <i>Keyword index</i>   | 401–403 |
| <i>Volume contents</i>   | 405–408 |