

Contents of Volume 33, 2005

Vol. 33 No. 1 September 2005

Articles

Optimization of resolution and sensitivity of 4D NOESY using multi-dimensional decomposition	
T. Luan, V. Jaravine, A. Yee, C. H. Arrowsmith and V. Yu. Orekhov	1–14
An AMBER/DYANA/MOLMOL phosphorylated amino acid library set and incorporation into NMR structure calculations	
J.W. Craft and G.B. Legge	15–24
Comparison of $^{13}\text{CH}_3$, $^{13}\text{CH}_2\text{D}$, and $^{13}\text{CHD}_2$ methyl labeling strategies in proteins	
J.E. Ollerenshaw, V. Tugarinov, N.R. Skrynnikov and L.E. Kay	25–41
Fast assignment of ^{15}N-HSQC peaks using high-resolution 3D HNcocaNH experiments with non-uniform sampling	
Z.-Y.J. Sun, D.P. Frueh, P. Selenko, J.C. Hoch and G. Wagner	43–50
<i>NMR structure notes</i>	
Solution structure of MTH0776 from <i>Methanobacterium thermoautotrophicum</i>	
G. Amegbey, P. Stothard, E. Kuznetsova, A.Yee, C.H. Arrowsmith and D.S. Wishart	51–56
Solution structure of a novel C₂-symmetrical bifunctional bicyclic inhibitor based on SFTI-1	
A.M. Jaulent, A.B.E. Brauer, S.J. Matthews, R.J. Leatherbarrow	57–62
Refinement of the solution structure of rat Olfactory Marker Protein (OMP)	
N.T. Wright, J.W. Margolis, F.L. Margolis and D.J. Weber	63–68
Solution structure of human dihydrofolate reductase in its complex with trimethoprim and NADPH	
N.V. Kovalevskaya, Y.D. Smurnyy, V.I. Polshakov, B. Birdsall, A.F. Bradbury, T. Frenkel and J. Feeney	69–72
<i>Letters to the Editor: New NMR assignments</i>	
NMR assignment of the backbone resonances of the firefly luciferase C-terminal 14.3 KDa domain	
B.R. Branchini, S.A. Gonzalez and R.A. Magyar	73
NMR assignment of protein Rv1980c from <i>Mycobacterium tuberculosis</i>	
J.M. Danahy, B.M. Potter, B.V. Geisbrecht and J.H. Laity	73
^1H, ^{13}C and ^{15}N NMR assignments for AlgH, a putative transcriptional regulator from <i>Pseudomonas aeruginosa</i>	
A.B. Cowley, R.J. Bieber Urbauer and J.L. Urbauer	74
^1H, ^{13}C and ^{15}N resonance assignments of the AT-Rich Interaction Domain (ARID) of Jumonji	
H. Kusunoki, T. Hasegawa, C. Komatsu, T. Takeuchi and T. Kohno	74

Backbone ^1H, ^{13}C, and ^{15}N resonance assignment of the 46 kDa dimeric GAF A domain of Phosphodiesterase 5	
M.R. Sekharan, P. Rajagopal and R.E. Klevit	75
NMR assignment of the DNA binding domain A of RPA from <i>S. cerevisiae</i>	
C.-J. Park, J.-H. Lee and B.-S. Choi	75
Resonance assignments of 30 kDa complexes of TFIID subunit TAF1 with TATA-binding protein	
T.K. Mal, D. Liu, Y. Masutomi, L. Zheng, Y. Nakatani, T. Kokubo and M. Ikura	76
^1H, ^{15}N and ^{13}C resonance assignments of the Domain III of the Dengue Virus Envelope Protein	
C.-W. Wu, Y.-T. Lin, K.-C. Huang and J.-W. Cheng	76
Instructions for Authors	77–82

Vol. 33 No. 2 October 2005

Articles

Estimating the accuracy of protein structures using residual dipolar couplings	
K. Simon, J. Xu, C. Kim and N.R. Skrynnikov	83–93
Heterologous expression of hen egg white lysozyme and resonance assignment of tryptophan side chains in its non-native states	
C. Schlörb, K. Ackermann, C. Richter, J. Wirmer and H. Schwalbe	95–104
Accurate determination of leucine and valine side-chain conformations using U-[$^{15}\text{N}/^{13}\text{C}/^2\text{H}$]/[$^1\text{H}$-(methine/methyl)-Leu/Val] isotope labeling, NOE pattern recognition, and methine $\text{C}_\gamma\text{--H}_\gamma/\text{C}_\beta\text{--H}_\beta$ residual dipolar couplings: application to the 34-kDa enzyme IIA_{Chitobiose}	
C. Tang, J. Iwahara and G.M. Clore	105–121
Definition of a new information-based per-residue quality parameter	
S.B. Nabuurs, E. Krieger, C.A.E.M. Spronk, A.J. Nederveen, G. Vriend and G.W. Vuister	123–134
<i>Letters to the Editor: New NMR assignments</i>	
^1H, ^{13}C and ^{15}N resonance assignments of URNdesign, a computationally redesigned RRM protein	
N. Dobson, G. Dantas and G. Varani	135
Backbone and side-chain ^1H, ^{15}N and ^{13}C assignments for the <i>cis</i> conformer of the β domain of the bacterial cell division protein DivIB	
S.A. Robson and G.F. King	135
Backbone NMR assignment of the low-molecular-weight protein tyrosine phosphatase (MPtpA) from <i>Mycobacterium tuberculosis</i>	
K. Saxena, B. Elshorst, H. Berk, M. Betz, S. Grimme, T. Langer, B. Pescatore, U. Schieborr, M. Vogtherr and H. Schwalbe	136
NMR assignment of the N-terminal domain <i>a</i> of the glycoprotein chaperone ERp57	
L. Silvennoinen, P. Koivunen, J. Myllyharju, I. Kilpeläinen and P. Permi	136

NMR resonance assignments of the NEAT (NEAr Transporter) domain from the <i>Staphylococcus aureus</i> lsdH protein	137
R.M. Pilpa and R.T. Clubb	
Backbone and side-chains ^1H, ^{13}C and ^{15}N NMR assignment of human β-parvalbumin	137
E. Babini, I.C. Felli, M. Lelli, C. Luchinat and R. Pierattelli	
Resonance assignments of <i>Escherichia coli</i> AlkB: a key 2-oxoglutarate and Fe(II)-dependent dioxygenase of the adaptive DNA-repair response	138
T. Shivarattan, H.A. Chen, P. Simpson, B. Sedgwick and S. Matthews	
Backbone ^1H, ^{13}C, and ^{15}N resonance assignments for the two 13 kD Ras associating domains (RA1 and RA2) from phospholipase Cϵ	138
R. Harris, T.D. Bunney, M. Katan and P.C. Driscoll	

Vol. 33 No. 3 November 2005

Articles

Automated protein NMR structure determination using wavelet de-noised NOESY spectra	139–152
F. Dancea and U. Günther	
Applications of variable-angle sample spinning experiments to the measurement of scaled residual dipolar couplings and ^{15}N CSA in soluble proteins	153–161
N. Lancelota, K. Elbayed and M. Piotto	
Determination of ^{13}C CSA tensors: Extension of the model-independent approach to an RNA kissing complex undergoing anisotropic rotational diffusion in solution	163–174
S. Ravindranathan, C.-H. Kim and G. Bodenhausen	
Describing partially unfolded states of proteins from sparse NMR data	175–186
G. Fuentes, A.J. Nederveen, R. Kaptein, R. Boelens and A.M.J.J. Bonvin	
Unambiguous assignment of NMR protein backbone signals with a time-shared triple-resonance experiment	187–196
D.P. Frueh, H. Arthanari and G. Wagner	

Letters to the Editor: New NMR assignments

^1H, ^{13}C, and ^{15}N resonance assignments for the protein coded by gene locus BB0938 of <i>Bordetella bronchiseptica</i>	197
P. Rossi, T. Ramelot, R. Xiao, C.K. Ho, L.-C. Ma, T.B. Acton, M.A. Kennedy and G.T. Montelione	
^1H, ^{13}C, and ^{15}N resonance assignments for <i>Escherichia coli</i> ytfP, a member of the broadly conserved UPF0131 protein domain family	197
J.M. Aramini, G.V.T. Swapna, Y.J. Huang, P.K. Rajan, R. Xiao, R. Shastry, T.B. Acton, J.R. Cort, M.A. Kennedy and G.T. Montelione	
^1H, ^{13}C and ^{15}N resonance assignments of the cytosolic domain of Tom20 from <i>Arabidopsis thaliana</i>	198
A.J. Perry, J.M. Hulett, T. Lithgow and P.R. Gooley	
^1H, ^{15}N and ^{13}C assignments of an intramolecular Lhx3:ldb1 complex	198
C. Lee, A.L. Nancarrow, I. Bach, J.P. Mackay and J.M. Matthews	

Articles

SOFAST-HMQC experiments for recording two-dimensional heteronuclear correlation spectra of proteins within a few seconds P. Schanda, E. Kupče and B. Brutscher	199–211
Chemical shifts provide fold populations and register of β hairpins and β sheets R.M. Fesinmeyer, F.M. Hudson, K.A. Olsen, G.W.N. White, A. Euser and N.H. Andersen	213–231
Effects of protein–pheromone complexation on correlated chemical shift modulations C. Perazzolo, J. Wist, K. Loth, L. Poggi, S. Homans and G. Bodenhausen	233–242
Extended flip-back schemes for sensitivity enhancement in multidimensional HSQC-type out-and-back experiments T. Diercks, M. Daniels and R. Kaptein	243–259
CASA: An efficient automated assignment of protein mainchain NMR data using an ordered tree search algorithm J. Wang, T. Wang, E.R.P. Zuiderweg and G.M. Crippen	261–279
<i>Letters to the Editor: New NMR Assignments</i>	
^1H, ^{13}C and ^{15}N backbone and side chain resonance assignments of <i>Haloferax volcanii</i> DHFR1 B. Binbuga and J.K. Young	281
NMR Assignment of HI1506, a novel two-domain protein from <i>Haemophilus influenzae</i> N. Sari, D.C. Yeh, V. Doseeva, K. Surabian, O. Herzberg, and J. Orban	281
Backbone resonance assignments for the Fv fragment of catalytic antibody 6D9 complexed with a transition state analogue M. Sakakura, H. Takahashi, H. Terasawa, K. Takeuchi, I. Fujii and I. Shimada	282
Resonance assignments of the two N-terminal RNA recognition motifs (RRM) of the human heterogeneous nuclear ribonucleoprotein F (HnRNP F) C. Dominguez and F.H.-T. Allain	282
Author Index	283–284
Keyword Index	285–286
Volume Contents	287–290