

Bibliography

- [1] P. Atkinson. *Feedback Control Theory for Engineers*. Heineman Educational Books, 1974.
- [2] J. Barkhuijsen, R. de Beer, W.M.M.J. Bovée, and D. van Ormondt. Retrieval of frequencies, amplitudes, damping factors, and phases from time-domain signals using a linear least-squares procedure. *Journal of Magnetic Resonance*, 61:465, 1985.
- [3] C. Bartels, M. Billeter, P. Güntert, and K. Wüthrich. Automated sequence-specific NMR assignment of homologous proteins using the program GARANT. *Journal of Biomolecular NMR*, 7:207–213, 1996.
- [4] C. Bartels, T. Xia, M. Billeter, P. Güntert, and K. Wüthrich. The program XEASY for computer-supported NMR spectral analysis of biological macromolecules. *Journal of Biomolecular NMR*, 5:1–10, 1995.
- [5] A. Bax, G. M. Clore, and A. M. Gronenborn. ^1H - ^1H correlation via isotropic mixing of ^{13}C magnetisation, a new three-dimensional approach for assigning ^1H and ^{13}C spectra of ^{13}C enriched proteins. *Journal of Magnetic Resonance*, 88:425–431, 1990.
- [6] R. Bernstein, C. Cieslar, A. Ross, H. Oschkinat, J. Freund, and T.A. Holak. Computer-assisted assignment of multidimensional NMR spectra of proteins: Applications 3D NOESY-HMQC and TOCSY-HMQC spectra. *Journal of Biomolecular NMR*, 3:245–252, 1993.
- [7] M. Billeter. New interactive and automatic algorithms for the assignment of NMR spectra. *NATO ASI*, 225(Ser. A):279–290, 1991.
- [8] W. Braun. Distance geometry and related methods for protein structure determination from NMR data. *Quarterly Review of Biophysics*, 19(3/4):115–157, 1987.
- [9] N. E. G. Buchler, E. R. P. Zuiderweg, H. Wang, and R. A. Golstein. Protein heteronuclear NMR experiments using mean-field simulated annealing. *Journal of Magnetic Resonance*, 125:34–42, 1997.
- [10] J. Cavanagh, W. J. Fairbrother, A. G. Palmer III, and N. J. Skelton. *Protein NMR spectroscopy, principles and practice*. Academic Press, 1996.
- [11] K. O. Cho, A. Hunt, and M. Kennedy. The rat brain postsynaptic density fraction contains a homologue of the drosophila discs-large tumor suppressor protein. *Biochemistry*, 9:929–942, 1992.
- [12] C. Cieslar, G. Marius Clore, and A.N. Gronenborn. Computer-aided sequential assignment of protein ^1H NMR spectra. *Journal of Magnetic Resonance*, 80:119–127, 1988.
- [13] S.A. Corne, P. Johnson, and J. Fisher. An artificial neural network for classifying cross peaks in two-dimensional NMR spectra. *Journal of Magnetic Resonance*, 100:256–266, 1992.
- [14] V. Dötsch, R. E. Oswald, and G. Wagner. Amino-acid-type-selective triple-resonance experiments. *Journal of Magnetic Resonance*, 110(Series B):107–111, 1996.

- [15] V. Dötsch, R. E. Oswald, and G. Wagner. Selective identification of threonine, valine, and isoleucine sequential connectivities with a TVI-CBCACONH experiment. *Journal of Magnetic Resonance*, 110(Series B):304–308, 1996.
- [16] C.D. Eads and J.D. Kuntz. Programs for computer-assisted sequential assignment of proteins. *Journal of Magnetic Resonance*, 82:467–482, 1989.
- [17] C. Eccles, P. Güntert, M. Billeter, and K. Wüthrich. Efficient analysis of protein 2D NMR spectra using the software package EASY. *Journal of Biomolecular NMR*, 1:111–130, 1991.
- [18] U. Eggenburger and G. Bodenhausen. Analysis of two-dimensional nuclear magnetic resonance spectra with relayed proton-proton-carbon magnetisation transfer: a step towards automated structure elucidation. *Anal. Chem.*, 61:2298–2306, 1989.
- [19] S. W. Fesik, H. L. Eaton, E. T. Olejniczak, R. P. Zuiderweg, P. McIntosh, and F. W. Dahlquist. 2D and 3D spectroscopy employing ^{13}C - ^{13}C magnetization transfer by isotropic mixing. Spin system identification in large proteins. *Journal of the American Chemical Society*, 112:886–888, 1990.
- [20] S. W. Fesik and E. R. P. Zuiderweg. Homonuclear three-dimensional NMR spectroscopy. *Journal of Magnetic Resonance*, 78:588–593, 1988.
- [21] D.S. Garrett, R. Powers, A.M. Gronenborn, and G.M. Clore. A common sense approach to peak picking in two-, three-, and four-dimensional spectra using automatic computer analysis of contour diagrams. *Journal of Magnetic Resonance*, 95:214–220, 1991.
- [22] S. Glaser and R. Kalbitzer. Improvement of two-dimensional NMR spectra by weighted mean t_1 -ridge subtraction and antidiagonal reduction. *Journal of Magnetic Resonance*, 68:350–354, 1986.
- [23] K-H. Groß and H.R. Kalbitzer. Distribution of chemical shifts in ^1H nuclear magnetic resonance spectra of proteins. *Journal of Magnetic Resonance*, 76:87–99, 1988.
- [24] J.C. Hoch, C. Redfield, and A.S. Stern. Computer aided analysis of protein NMR spectra. *Current Op. in Struct. Biol.*, 1:1036–1041, 1991.
- [25] M. Ikura, L. E. Kay, and A. Bax. Improved three-dimensional ^1H - ^{13}C - ^1H correlation spectroscopy of a ^{13}C labelled protein using constant-time evolution. *Journal of Biomolecular NMR*, 1:299–304, 1991.
- [26] H.R. Kalbitzer, K-P. Neidig, and W. Hengstenberg. Structure determination of polypeptides and proteins by two-dimensional nuclear magnetic resonance spectroscopy. *Physica*, 164(B):180–192, 1990.
- [27] L. E. Kay, M. Ikura, and A. Bax. Proton-proton correlation via carbon-carbon couplings: a three-dimensional NMR approach for the assignment of aliphatic resonances in proteins labelled with carbon-13. *Journal of the American Chemical Society*, 112:888–889, 1990.
- [28] L. E. Kay, M. Ikura, R. Tschudin, and A. Bax. Three-dimensional triple-resonance NMR spectroscopy of isotopically enriched proteins. *Journal of Magnetic Resonance*, 89:496–514, 1990.
- [29] J. Kemmink, N. J. Darby, K. Dijkstra, M. Nilges, and T. E. Creighton. Structure determination of the N-terminal thioredoxin-like domain of protein disulfide isomerase using multidimensional heteronuclear $^{13}\text{C}/^{15}\text{N}$ NMR spectroscopy. *Biochemistry*, 35:7684–7691, 1996.
- [30] J. Kemmink, N. J. Darby, K. Dijkstra, R. M. Scheek, , and T. E. Creighton. Nuclear Magnetic Resonance Characterisation of the N-Terminal thioredoxin-like domain of protein disulfide isomerase. *Protein Science*, 4:2587–2593, 1995.
- [31] H. Kessler, M. Gehrke, and C. Griesinger. Two-dimensional NMR spectroscopy: background and overview of the experiments. *Angw. Chem. Int. Ed. Engl.*, 27:490–536, 1988.

- [32] M. Kjaer and F.M. Poulsen. Identification of 2D 1H NMR antiphase cross peaks using a neural network. *Journal of Magnetic Resonance*, 94:659–663, 1991.
- [33] G.J. Kleijwegt. *Computer-assisted assignment of 2D and 3D NMR spectra of proteins*. PhD thesis, Rijksuniversiteit te Utrecht, Holland, 1991.
- [34] G.J. Kleijwegt, R. Boelens, M. Cox, M. Llinás, and R. Kaptein. Computer assisted assignment of 2D 1H NMR spectra of proteins: Basic algorithms and application to phorataxin B. *Journal of Biomolecular NMR*, 1:23–47, 1991.
- [35] G.J. Kleijwegt, R. Boelens, and R. Kaptein. A versatile approach towards the partially automatic recognition of cross peaks in 2D 1H NMR spectra. *Journal of Magnetic Resonance*, 88:601–608, 1990.
- [36] P.J. Kraulis. ANSIG: a program for the assignment of protein 1H NMR Spectra by Interactive Computer Graphics. *Journal of Magnetic Resonance*, 84:627–633, 1989.
- [37] Z.L. Mádi and R.R. Ernst. Computer analysis of two-dimensional NMR spectra. Estimation of spectral parameters by least squares approximation. *Journal of Magnetic Resonance*, 79:513–527, 1988.
- [38] D. Marion, P. C. Driscoll, L. E. Kay, P. T. Wingfield, A. Bax, A. M. Gronenborn, and G. M. Clore. Overcoming the overlap problem in the assignment of 1H NMR spectra of larger proteins by use of three-dimensional heteronuclear 1H - ^{15}N Hartmann-Hahn-multiple quantum coherence and nuclear-Overhauser-multiple quantum coherence spectroscopy: application to Interleukin 1β . *Biochemistry*, 28:6150–6156, 1989.
- [39] J. L. Markley and M. Kainosho. Stable isotope labelling and resonance assignments in larger proteins. In G. C. K. Roberts, editor, *NMR of Macromolecules*. IRC Press, 1993.
- [40] R. P. Meadows, E. T. Olejniczak, and S. W. Fesik. A computer-based protocol for semiautomated assignments and 3D structure determination of proteins. *Journal of Biomolecular NMR*, 4:79–96, 1994.
- [41] B.U. Meir, Z.L. Mádi, and R.R. Ernst. Computer analysis of nuclear spin systems based on local symmetry in 2D spectra. *Journal of Magnetic Resonance*, 74:565–573, 1987.
- [42] P.A. Mireau. A strategy for NMR structure determination. *Journal of Magnetic Resonance*, 96:480–490, 1992.
- [43] L. Mitschang, C. Cieslar, T.A. Holak, and H. Oschkinat. Application of the Karhunen-Loève transformation to the suppression of undesired resonances in three-dimensional NMR. *Journal of Magnetic Resonance*, 92:208, 1991.
- [44] N. Morelle, B. Brutscher, J.P. Simorre, and D. Marion. Computer assignment of the backbone resonances of labelled proteins using two-dimensional correlation experiments. *Journal of Biomolecular NMR*, 5:154–160, 1995.
- [45] C. Mumenthaler and W. Braun. Automated assignment of simulated and experimental NOESY spectra of proteins by feedback filtering and self-correcting distance geometry. *Journal of Molecular Biology*, 254:465–480, 1995.
- [46] K-P. Neidig and H.R. Kalbitzer. Improved representation of two-dimensional NMR spectra by local rescaling. *Journal of Magnetic Resonance*, 88:155–160, 1990.
- [47] K-P. Neidig, R. Saffrich, M. Lorenz, and H.R. Kalbitzer. Cluster analysis and multiplet pattern recognition in two-dimensional NMR spectra. *Journal of Magnetic Resonance*, 89:543–552, 1990.
- [48] P. Neidig. *AURELIA: Computer aided analysis of 2D and 3D NMR, user's guide*. Brucker Analytische Meßtechnik GmbH, 1992.
- [49] S.J. Nelson, D.M. Schneider, D.L. Di Stefano, and A.J. Wand. Refinement and automation of main chain directed assignment procedure for the analysis of 2-D 1H spectra of proteins. *Bull. Magn. Reson.*, 13:14–21, 1991.

- [50] D. Nietlispach, R. T. Clowes, R. W. Broadhurst, I. Yutaka, J. Keeler, M. Kelly, J. Ashurst, H. Oschkinat, P. J. Dommelle, and E. D. Laue. An approach to the structure determination of larger proteins using triple resonance NMR experiments in conjunction with random fractional deuteration. *Journal of the American Chemical Society*, 118:407–415, 1996.
- [51] M. Nilges. A calculation strategy for the structure determination of symmetric dimers by ^1H NMR. *Proteins: Structure, Function and Genetics*, 17:297–309, 1993.
- [52] M. Nilges. Calculation of protein structures with ambiguous distance restraints. Automated assignment of ambiguous NOE crosspeaks and disulphide connectivities. *Journal of Molecular Biology*, 245:645–660, 1995.
- [53] H. Oschkinat, C. Cieslar, and C. Griesinger. Recognition of secondary structure elements in 3D TOCSY-NOESY spectra of proteins. Interpretation of 3D cross-peak amplitudes. *Journal of Magnetic Resonance*, 86:453–469, 1990.
- [54] H. Oschkinat, T.A. Holak, and C. Cieslar. Assignment of protein NMR spectra in the light of homonuclear 3D spectroscopy: An automatable procedure based on 3D TOCSY-TOCSY and 3D NOESY-NOESY. *Biopolymers*, 31:699–711, 1991.
- [55] H. Oschkinat, T. Müller, and T. Diekmann. Protein structure determination with three- and four-dimensional NMR spectroscopy. *Angw. Chem. Int. Ed. Eng.*, 33:277–293, 1994.
- [56] C.M. Oshiro and I.D. Kuntz. Application of distance geometry to the protein assignment problem. *Biopolymers*, 33:107–115, 1993.
- [57] P. Pfändler and G. Bodenhausen. Topological classification of fragments of coupling networks and multiplet patterns in two-dimensional NMR spectra. *Journal of Magnetic Resonance*, 79:99–123, 1988.
- [58] P. Pfändler and G. Bodenhausen. Automated analysis of 2D correlation spectra. Assembly of fragments into networks of coupled spins. *Journal of Magnetic Resonance*, 87:26–45, 1990.
- [59] R. Powers, D. S. Garrett, C. J. March, E. A. Frieden, A. M. Gronenborn, and G. M. Clore. ^1H , ^{15}N , ^{13}C and ^{13}CO assignments of human interleukin-4 using three-dimensional double- and triple-resonance heteronuclear magnetic resonance spectroscopy. *Biochemistry*, 31:4334–4346, 1992.
- [60] C. Redfield. Resonance assignment strategies for small proteins. In G. C. K. Roberts, editor, *NMR of Macromolecules*. IRC Press, 1993.
- [61] R. J. Schalkoff. *Digital Image Processing and Computer Vision*. John Wiley and Sons, 1989.
- [62] G. L. Shaw, T. Müller, H. R. Mott, H. Oschkinat, I. D. Campbell, and L. Mitschang. Constant-time HMQC experiment for protein NMR spectroscopy. *Journal of Magnetic Resonance*, 124:479–483, 1997.
- [63] M. Spaargaren and J. R. Bischoff. Identification of the guanine nucleotide dissociation stimulator for Ral as a putative effector molecule of R-ras, H-ras, K-ras and Rap. *Proceedings of the National Association of Science*, 91:12609–12613, 1994.
- [64] D.L. Di Stefano and J. Wand. Two dimensional ^1H NMR study of human ubiquitin: a main chain directed assignment and structure analysis. *Biochemistry*, 26:7272–7281, 1987.
- [65] V. Stoven, A. Mikov, D. Piveteau, E. Guittet, and J-Y. Lallemand. PARIS, a program for automatic recognition and integration of 2D NMR spectra. *Journal of Magnetic Resonance*, 82:163–168, 1989.
- [66] J.U. Thomsen and B. Meyer. Pattern recognition of the ^1H NMR spectra of sugar alditols using a neural network. *Journal of Magnetic Resonance*, 84:212–217, 1989.
- [67] F.J.M. van de Ven. PROSPECT, a program for automated interpretation of 2D NMR spectra of proteins. *Journal of Magnetic Resonance*, 86:633–644, 1990.

- [68] G.W. Vuister, B. Boelens, A. Padilla, G.J. Kleijwegt, and R. Kaptein. Assignment strategies in homonuclear 3D 1H NMR spectra of proteins. *Biochemistry*, 29:1829–1839, 1990.
- [69] J. Walter. *Mustererkennung in dreidimensionalen NMR-Spektren von Proteinen zur Automatischen Zuordnung und Strukturbestimmung*. Ruprecht-Karls-Universität, Heidelberg, Germany, 1997.
- [70] S.W. Englander A.J. Wand. Main chain directed strategy for the assignment of 1H NMR spectra of proteins. *Biochemistry*, 26(N19):5953–5958, 1987.
- [71] P.L. Weber, J.A. Malikayil, and L. Mueller. Automated elucidation of J connectivities in 1H NMR spectra. *Journal of Magnetic Resonance*, 82:419–426, 1989.
- [72] J. Wehrens, C. Lucasius, L. Buydens, and G. Kateman. Sequential assignment of 2D NMR spectra of proteins using genetic algorithms. *J. Chem. Inf. Comput. Sci.*, 33:245–251, 1993.
- [73] D. S. Wishart, C. G. Bigham, A. Holm, R. S. Hodges, and B. D. Sykes. 1H , ^{13}C and ^{15}N random coil chemical shifts of the common amino acids. Investigation of nearest neighbour effects. *Journal of Biomolecular NMR*, 5:67–81, 1995.
- [74] D. S. Wishart, B. D. Sykes, and F. M. Richards. Relationship between nuclear magnetic resonance chemical shift and protein secondary structure. *Journal of Molecular Biology*, 222:311–333, 1991.
- [75] K. Wüthrich. *NMR of Proteins and Nucleic Acids*. John Wiley & Sons, 1986.
- [76] K. Wüthrich, G. Wider, G. Wagner, and W. Braun. Sequential resonance assignments as a basis for determination of spatial proton structures by high resolution proton nuclear magnetic resonance. *Journal of Molecular Biology*, 155:311–319, 1982.
- [77] J. Xu, S. K. Straus, B. C. Sanctuary, and L. Trimble. Use of fuzzy mathematics for complete automated assignment of peptide 1H 2D NMR spectra. *Journal of Magnetic Resonance*, 103(Ser. B):53–58, 1994.
- [78] C. Yu, J-F. Hwang, T-B. Chen, and V-W. Soo. RUBIDIUM, a program for computer-aided assignment of two-dimensional NMR spectra of polypeptides. *J. Chem. Inf. Comput. Sci.*, 32:183–187, 1992.
- [79] D. Zimmerman, C. A. Kulikowski, Y. Huang, W. Feng, M. Tashiro, S. Shimotakahara, C. Chien, R. Powers, and G. T. Montelione. Automated analysis of protein NMR assignments using methods from artificial intelligence. *Journal of Molecular Biology*, 269:592–610, 1997.
- [80] D. Zimmerman and G. T. Montelione. Automated analysis of nuclear magnetic resonance assignments for proteins. *Current Opinions in Structural Biology*, 5:664–673, 1995.