ATLAS OF STEREOCHEMISTRY

Absolute Configurations of Organic Molecules

Second Edition

SUPPLEMENT

J. Buckingham

and

R.A. Hill

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LONDON NEW YORK
CHAPMAN AND HALL

First published in 1986 by
Chapman and Hall Ltd
11 New Fetter Lane, London EC4P 4EE
Published in the USA by
Chapman and Hall
29 West 35th Street, New York NY 10001

Printed in Great Britain at the
University Press, Cambridge

ISBN 0 412 26000 X

British Library Cataloguing in Publication Data

Klyne, William
Atlas of stereochemistry: absolute configurations of organic molecules.—2nd ed. supplement
1. Stereochemistry—Atlases
I. Title, II. Buckingham, J. III. Hill, R.A. 547.1'223
QD481

ISBN 0–412–26000–X

Library of Congress Cataloging in Publication Data

Buckingham, J.
Atlas of stereochemistry, absolute configurations of organic molecules, second edition. Supplement.

Supplement to: Atlas of stereochemistry: absolute configurations of organic moleculares/W. Klyne and J. Buckingham. 2nd ed. London, 1978.
Bibliography: p.
Includes indexes.
1. Stereochemistry—Atlases. I. Hill, R.A., 1951–
II. Klyne, William. Atlas of stereochemistry.
III. Title.
QD481.K64 1978 Suppl. 541.2'23 85–12825
ISBN 0–412–26000–X

Preface to the Supplement

The determination of absolute configurations is now a central and routine part of research in organic chemistry and biochemistry. Since the publication of the second edition of the *Atlas* in 1978, many hundred further important determinations have been carried out, more than justifying the present publication of an extensive supplement.

Despite some expectations to the contrary, direct Bijvoet X-ray determinations have not completely dominated the field in the last seven years. Chemical correlations continue to be the method of choice for most types of compound except complex natural products; the correlation charts which are the *raison d'être* of this publication continue to prosper, as perusal of the pages of this supplement will show.

Once again, our thanks to those reviewers and correspondents who have sent in their comments on published correlations. There have been relatively few absolute configuration reversals during the last seven years, leading to the presumption that the vast majority of the determinations so far recorded in the *Atlas* will stand the test of time.

J. Buckingham
R.A. Hill

Key to the Supplement

Scope

The coverage of the Supplement corresponds with that of the Second Edition main volumes, except that organometallic compounds have been omitted.

Literature coverage

The literature has been scanned to the end of 1982, and a few important references from 1983 have been included. There are also a considerable number of pre-1976 correlations included for the first time.

Numbering of formulae and cross-references

The arrangement of chapters is the same as in the Main Work. In the supplement each compound reference carries a second prime. Thus A32.2 refers to volume 1 of the Main Work, A'32.2 to volume 2, and A''32.2 to the Supplement.

Important general literature references

Proposals modifying the Cahn–Ingold–Prelog system of configurational notation have been put forward by V. Prelog and G. Helmchen (*Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 567).

1977 saw the publication of the major work *Stereochemistry Fundamentals and Methods*, Georg Thieme Verlag. In particular volume 3 is entitled 'Determination of Configurations by Chemical Methods' and volume 4, by J. Jaques, C. Cross and S. Bourcier gives the absolute configurations of 6000 selected compounds with one chiral carbon atom in tabular form.

For a discussion of the Bijvoet X-ray anomalous dispersion method, see D. Rogers, *Acta Crystallogr. Sect. B.*, 1979, **35**, 2823.

The publication of the series *Atlas of Three-dimensional structure of drugs* (Janssen Research Foundation Series) began in 1979 with Vol. 1 edited by J.P. Tolleaere, H. Moereels and L.A. Raymaekers, published by Elsevier, Amsterdam.

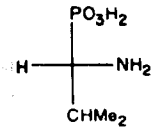
The theory of 'hyperchirality' advanced by J. Dugundy, D. Marquarding and I. Ugi (*Chem. Scr.* 1976, **9**, 74; 1977, **11**, 17), seems to have passed into the limbo of history (W. Hasselbarth, *ibid*, 1976, **10**, 96; 1977, **11**, 148; C.A. Mead, *ibid*, 1976, **10**, 101; 1977, **11**, 145).

Contents

A″

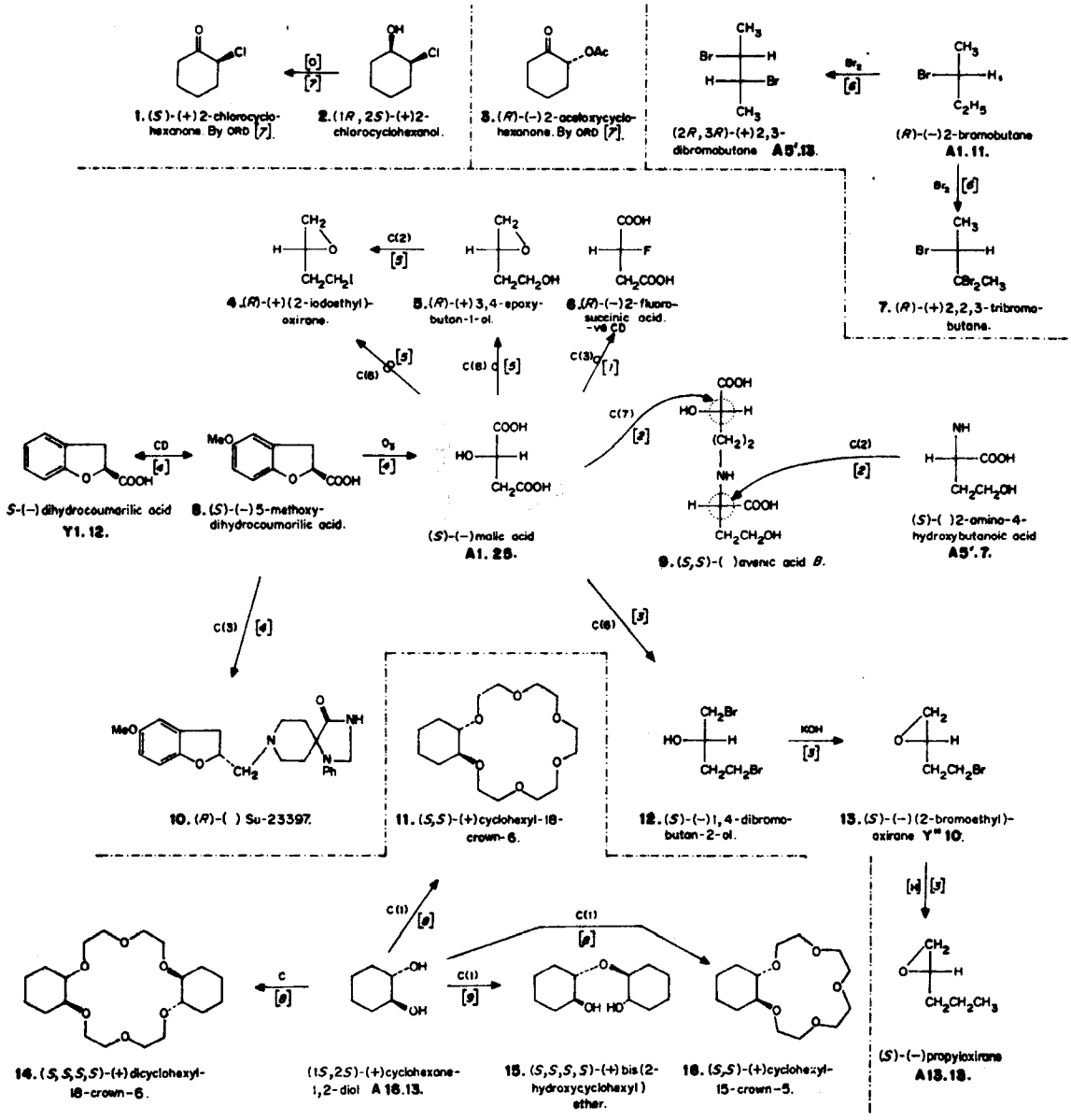
Fundamental Chiral Compounds

Sub-classification of compounds in chapter A″

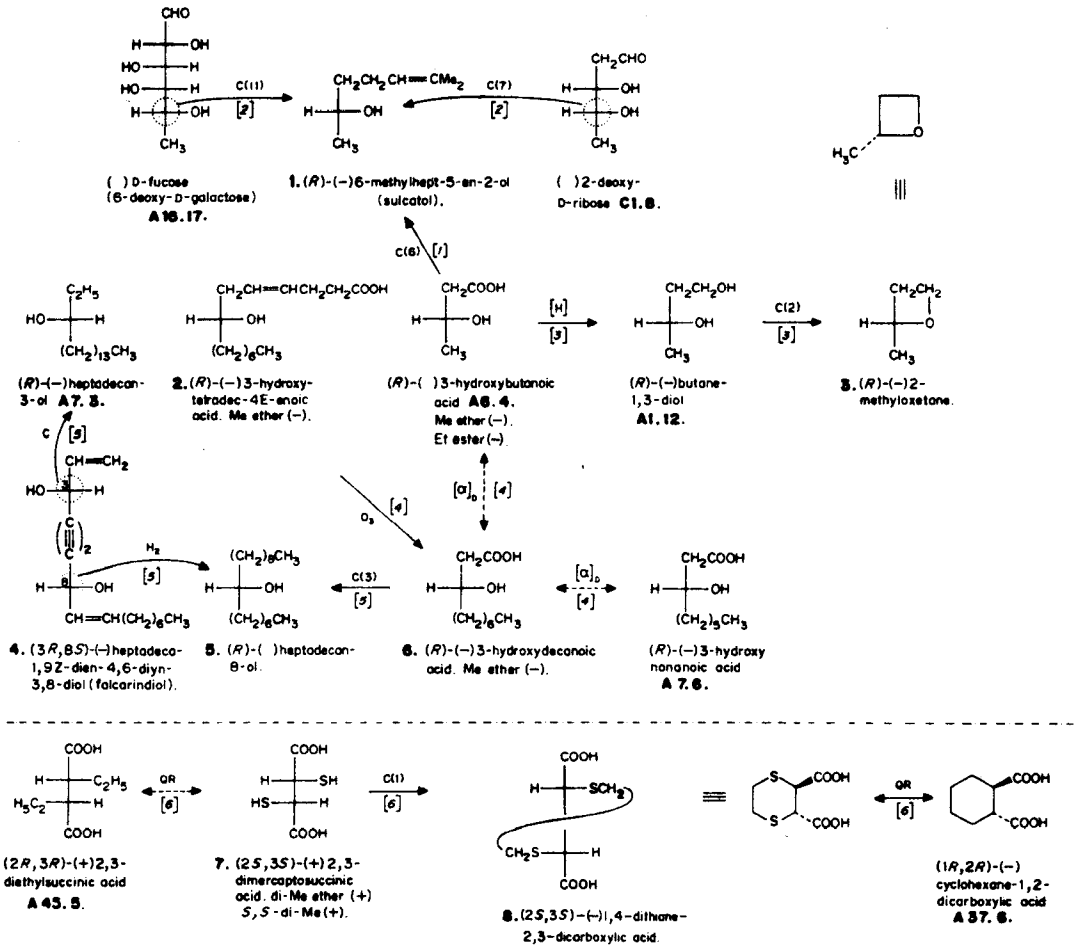


(*S*)-(−)1-amino-2-methylpropanephosphonic acid
Abs. X-ray [*1*]

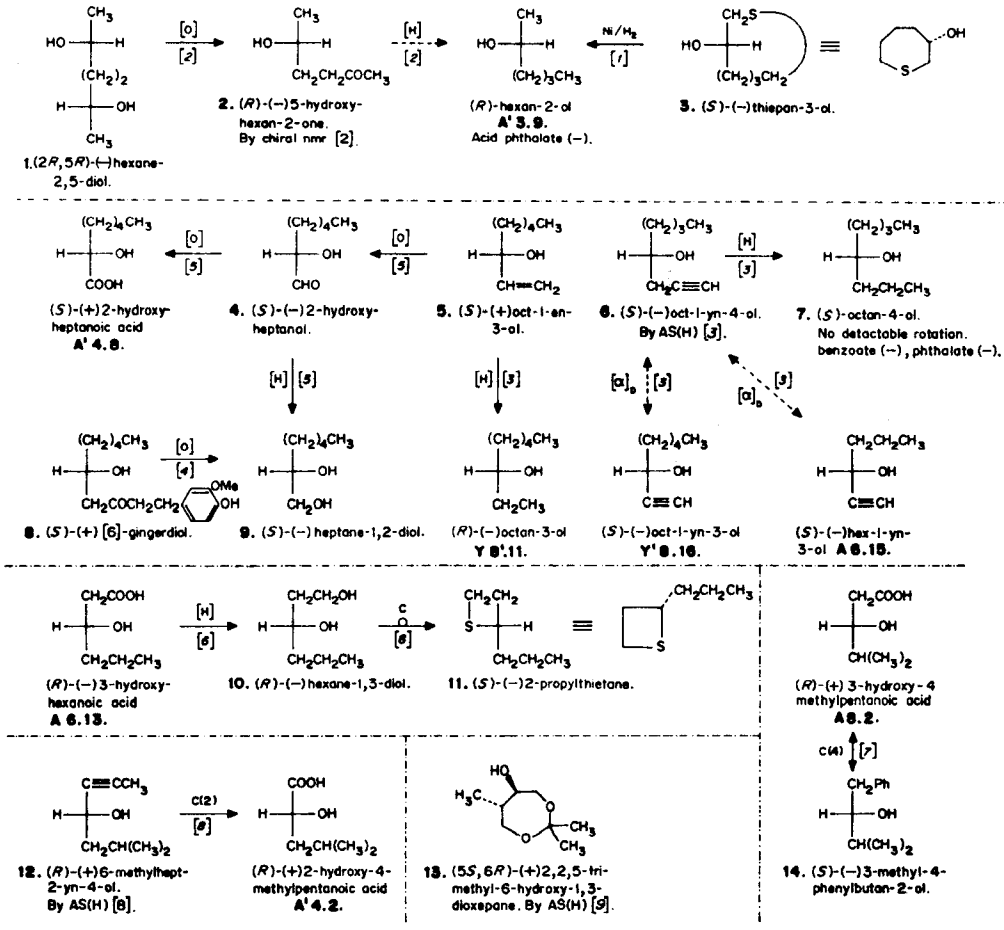
1. T. Głowiak, W. Sawka-Dobrowalska, J. Kowalik, P. Mastalerz, M. Soroka and J. Zon, *Tetrahedron Lett.*, 1977, 3965.



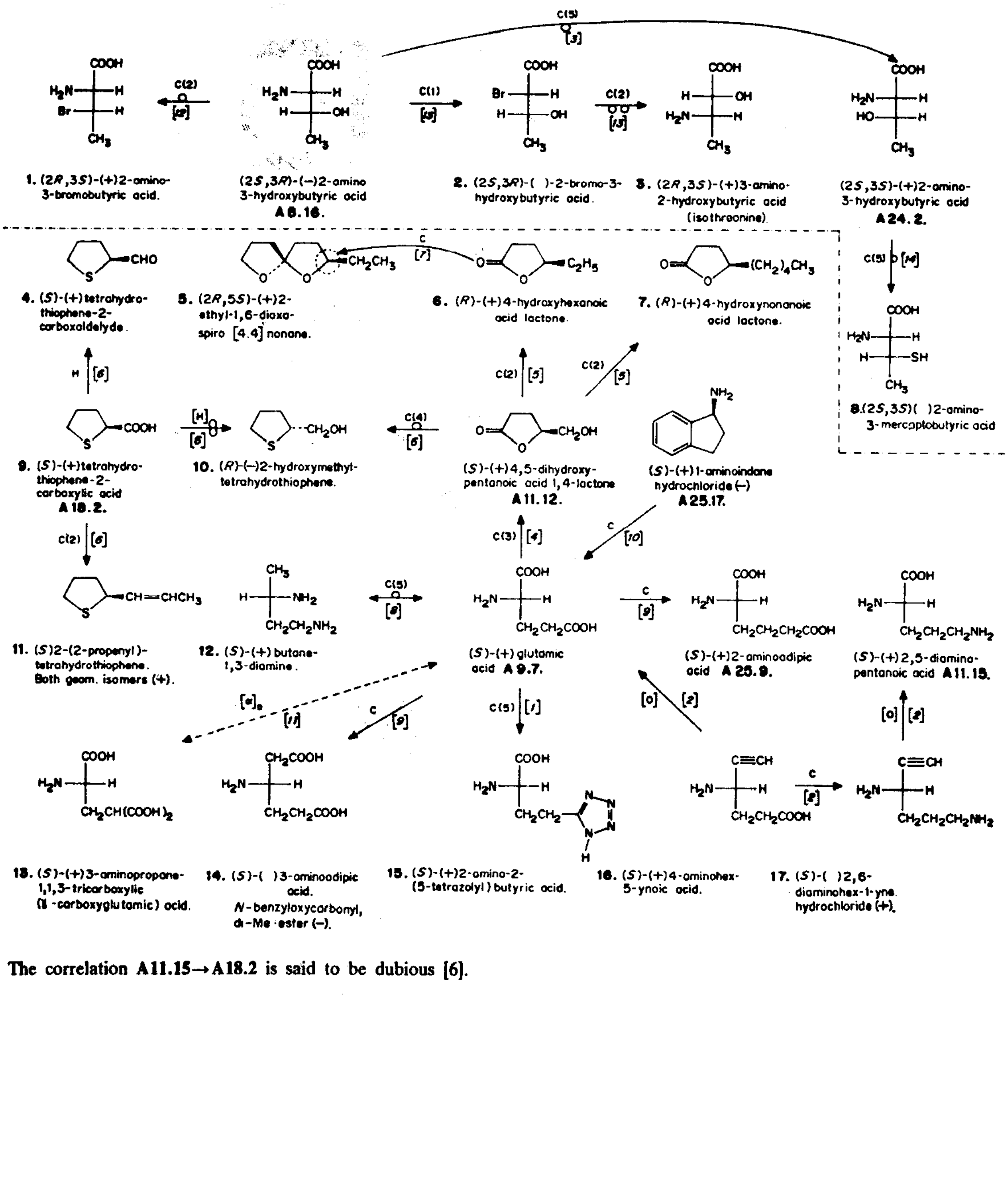
1. G. Lowe and B.V.L. Potter, *J. Chem. Soc., Perkin Trans. 1*, 1980, 2029.
2. S. Fushiya, Y. Sato and S. Nozoe, *Chem. Lett.* 1980, 1215.
3. B. Seuring and D. Seebach, *Helv. Chim. Acta*, 1977, **60**, 1175.
4. N.K. Chauduri, T.J. Ball and N. Finch, *Experientia*, 1977, **33**, 575.
5. D.L. Boger and J.S. Panek, *J. Org. Chem.*, 1981, **46**, 1208.
6. D.D. Tanner, G.V. Blackburn, Y. Kosugi and T.C.S. Rao, *J. Am. Chem. Soc.*, 1977, **99**, 2714.
7. R.L. Coumbie, D.D. Ridley and G.W. Simpson, *Chem. Comm.*, 1977, 315.
8. R.C. Hayward, C.H. Overton and G.H. Whitham, *J. Chem. Soc., Perkin Trans. 1*, 1976, 2413.
9. P.G. Barili, G. Bellucci, G. Ingrosso and A. Vatteroni, *Gazz. Chim. Ital.*, 1977, **107**, 147.



1. K. Mori, *Tetrahedron*, 1981, **37**, 1341.
2. H.R. Schuler and K.N. Slessor, *Can. J. Chem.*, 1977, **55**, 3280.
3. M. Segi, T. Takebe, S. Masuda, T. Nakajima and S. Suga, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 167.
4. J.H. Cardellina, D. Dalietos, F.-J. Marner, J.S. Mynderse and R.E. Moore, *Phytochemistry*, 1978, **17**, 2091.
5. E. Lemmich, *Phytochemistry*, 1981, **20**, 1419.
6. M.O. Hedblom, *Ark. Kemi*, 1969, **31**, 489.

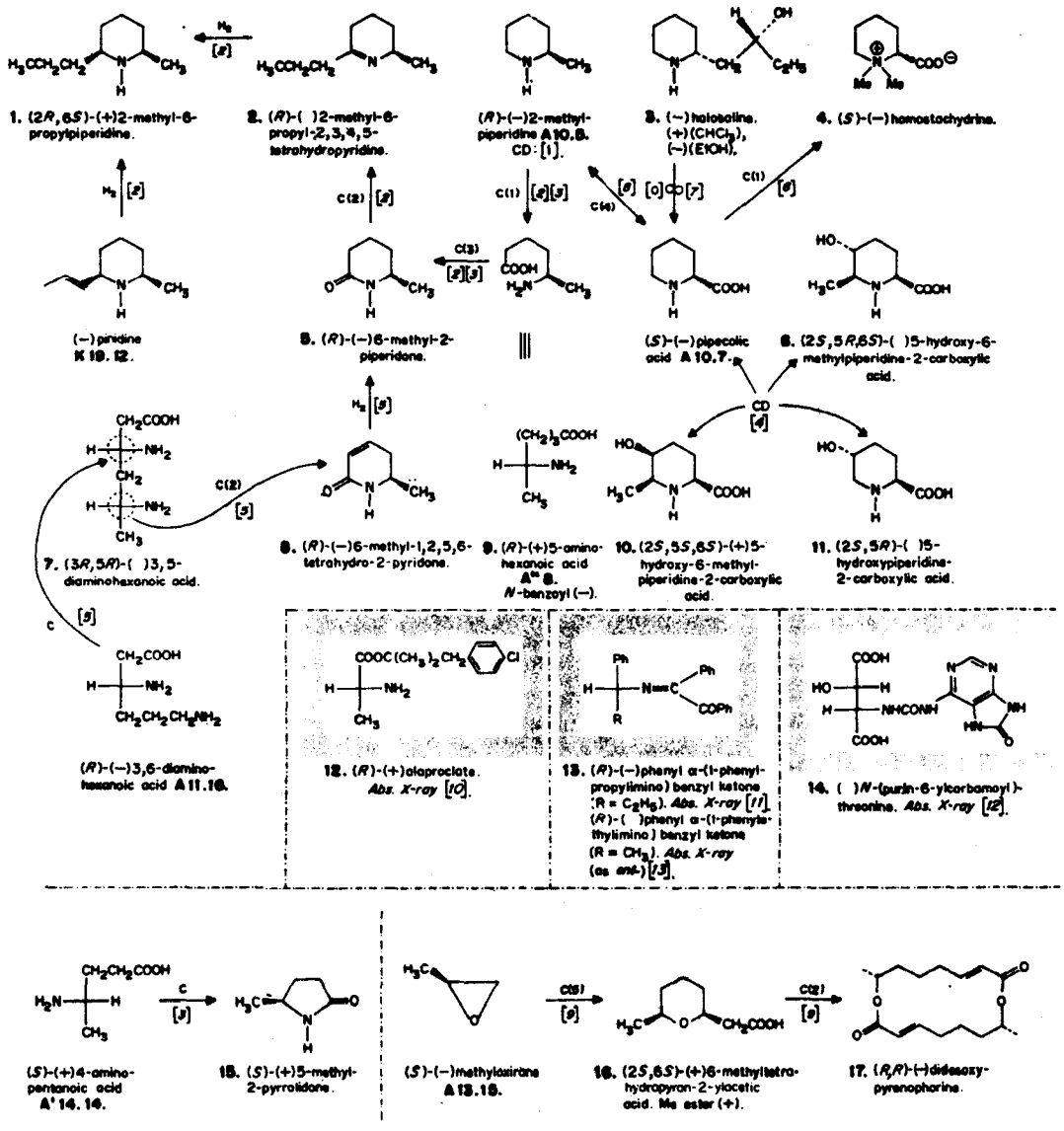


1. J.B. Jones and H.M. Schwartz, *Can. J. Chem.*, 1981, **59**, 1574.
2. B.R. Davis, G.W. Rewcastle, R.J. Stevenson and P.D. Woodgate, *J. Chem. Soc., Perkin Trans. 1*, 1977, 2148.
3. W.J. McGahren, K.J. Sax, M.P. Kunstmann and G.A. Ellestad, *J. Org. Chem.*, 1977, **42**, 1659.
4. D.W. Connell and M.D. Sutherland, *Aust. J. Chem.*, 1969, **22**, 1033.
5. P.A. Levene and A. Walti, *J. Biol. Chem.*, 1931, **94**, 593.
6. D.R. Crump, *Aust. J. Chem.*, 1982, **35**, 1945.
7. J.P. Vigneron, M. Dhaenens and A. Horeau, *Tetrahedron*, 1977, **33**, 507.
8. K. Chan, N. Cohen. J.P. DeNoble, A.C. Specian and G. Sauey, *J. Org. Chem.*, 1976, **41**, 3497.
9. W.J. Elliott and J. Fried, *J. Org. Chem.*, 1976, **41**, 2469.



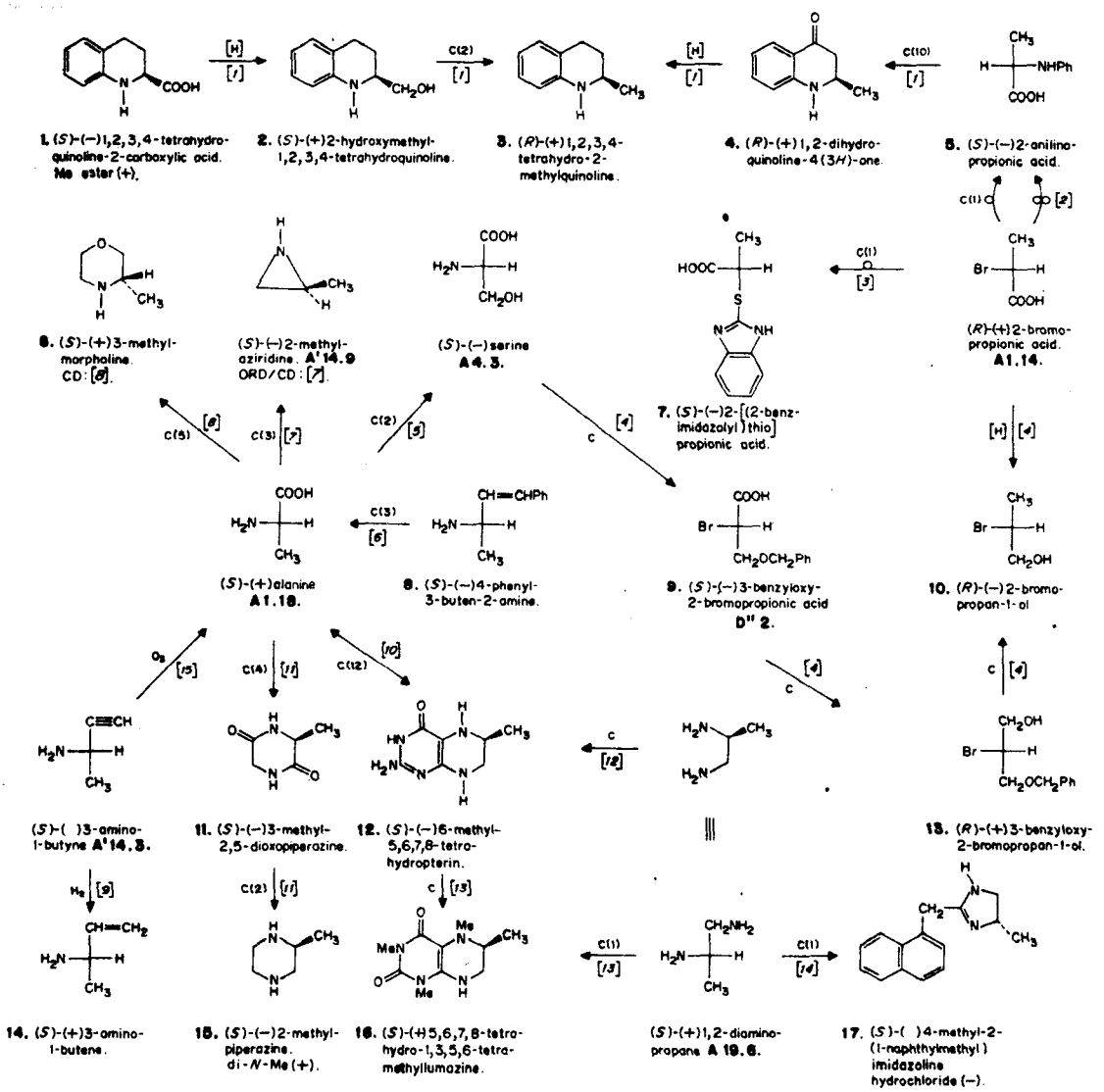
The correlation **A11.15→A18.2** is said to be dubious [6].

1. T.T. Van, E. Kojro and Z. Grzonka, *Tetrahedron*, 1977, **33**, 2299.
2. P. Casara, C. Danzin, B.W. Metcalf and M.J. Jung, *Chem. Comm.*, 1982, 1190.
3. J.L. Morell, P. Fleckenstein and E. Gron, *J. Org. Chem.*, 1977, **42**, 355.
4. See p. **A11**.
5. U. Ravid, R.M. Silverstein and L.R. Smith, *Tetrahedron*, 1978, **34**, 1449.
6. G. Stork and A.F. Kreft, *J. Am. Chem. Soc.*, 1977, **99**, 3851.
7. L.R. Smith, H.J. Williams and R.M. Silverstein, *Tetrahedron Lett.*, 1978, 3231.
8. E. Balieu, P.M. Boll and E. Larsen, *Acta Chem. Scand.*, 1969, **23**, 2191.
9. C.T. Clarke and J.H. Jones, *Tetrahedron Lett.*, 1977, 2367, and refs therein.
10. J.H. Brewster, *Helv. Chim. Acta*, 1982, **65**, 317, and refs. therein; V. Ghislandi and D. Vercesi, *Boll. Chem., Farm.*, 1976, **115**, 489.
11. W. Marki and R.S. Schwyzer, *Helv. Chim. Acta*, 1976, **59**, 1591.
12. T. Wieland, D. Schermer, G. Rohr and H. Faulstich, *Justus Liebigs Ann. Chem.*, 1977, 806.
13. Y. Shimohigashi, M. Waki and N. Izumiya, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 949.

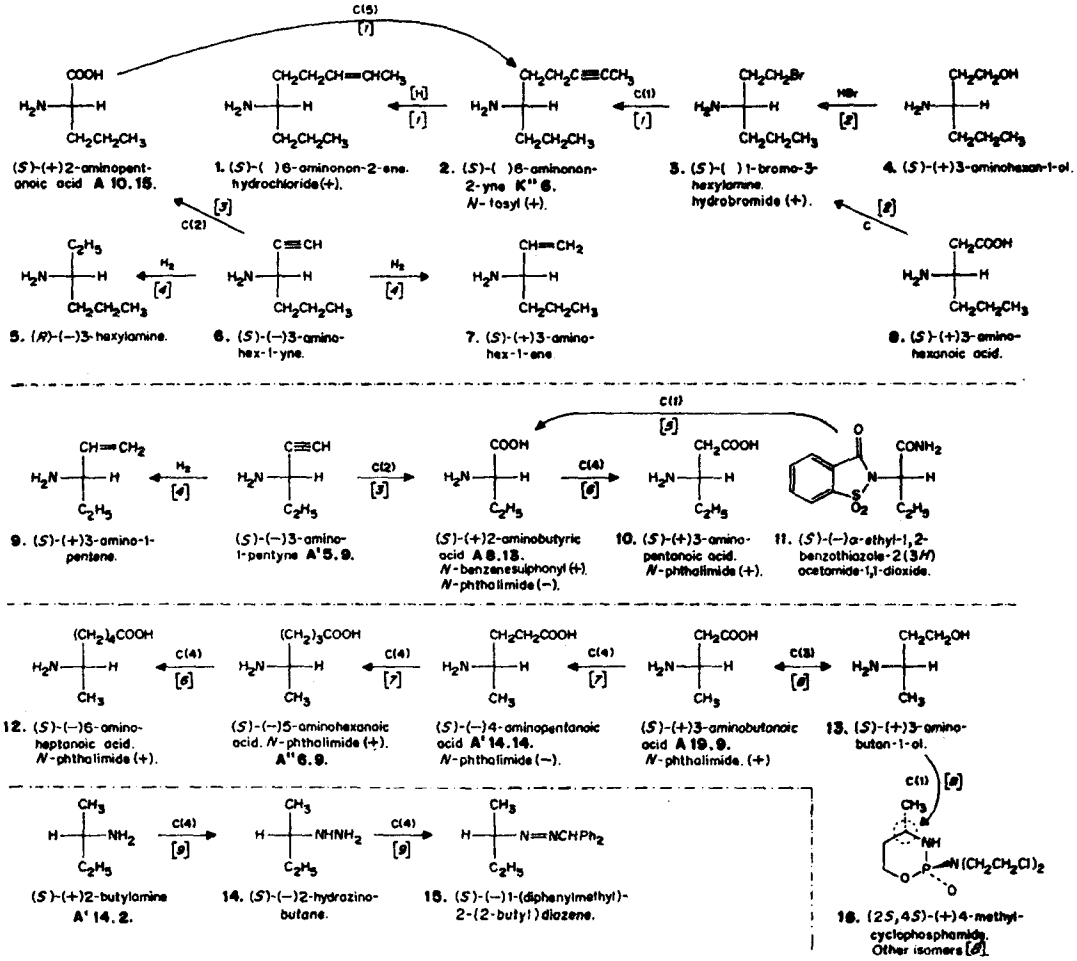


CD of 2-substituted piperidines: [*1*].

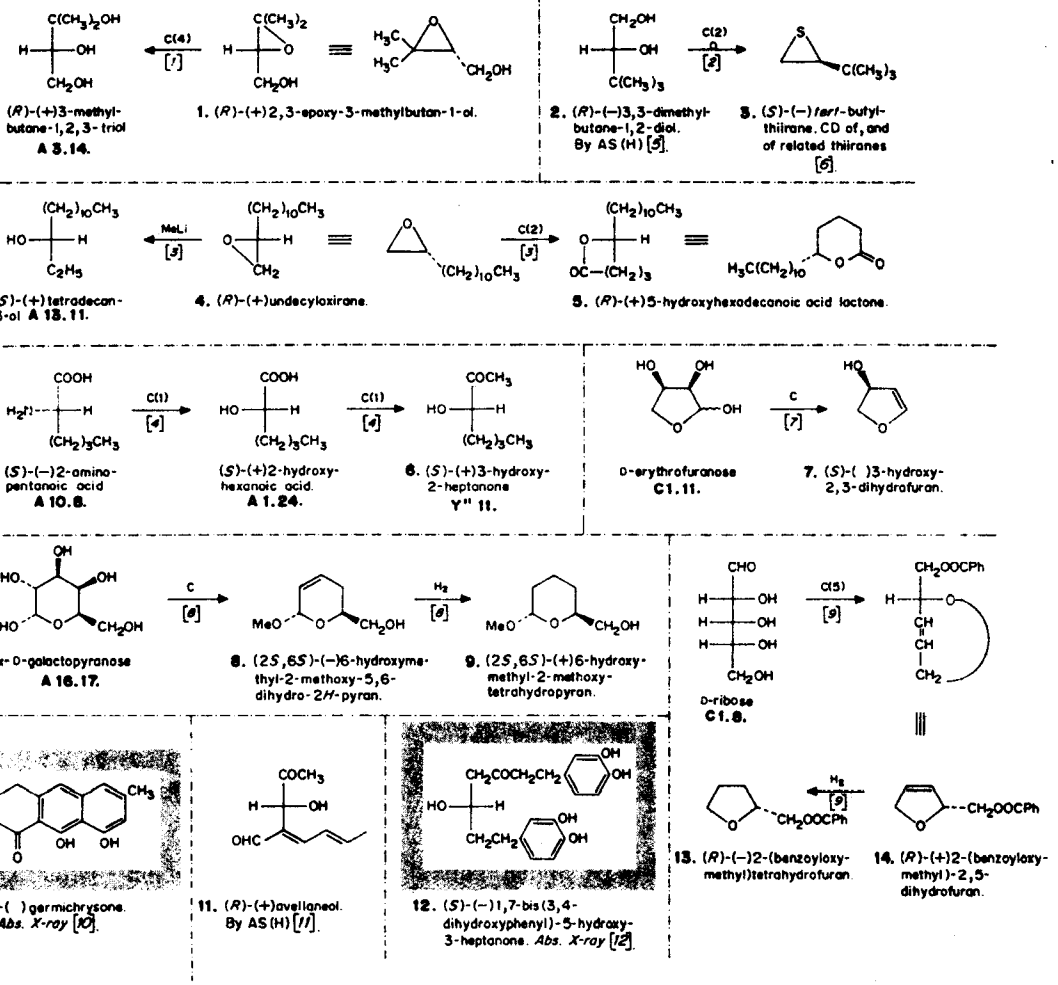
1. J.C. Craig, S-Y.C. Lee, W.E. Pereira, H.C. Beyerman and L. Maat, *Tetrahedron*, 1978, **34**, 501.
2. R.H. Hill and T. Yuri, *Tetrahedron*, 1977, **33**, 1569.
3. O. Cervinka, A. Fabryova and V. Novak, *Collect. Czech. Chem. Commun*, 1965, **30**, 1742.
4. I. Kristensen, P.O. Larsen and C.E. Olsen, *Tetrahedron*, 1976, **32**, 2799.
5. F. Kunz, J. Rétey, D. Arigoni, L. Tsai and T.C. Stadtman, *Helv. Chim. Acta*, 1978, **61**, 1139.
6. A.V. Robertson and L. Marion, *Can. J. Chem.*, 1959, **37**, 829.
7. K-H. Michel, F. Sandberg, F. Haglid, T. Norin, R.P.K. Chan and J.C. Craig, *Acta Chem. Scand.*, 1969, **23**, 3479.
8. See p. **A10**.
9. D. Seebach and M. Pohmakotr, *Helv. Chim. Acta.*, 1979, **62** 843.
10. A. Wägner, *Acta Crystallogr. Sect. B*, 1980, **36**, 77.
11. I. Fonseca, S. Martinez-Carrera and S. Garcia-Blanco, *Acta Crystallogr., Sect. B*, 1982, **38**, 2735.
12. R. Parthasarathy, J.M. Ohrt and G.B. Chheda, *J. Am. Chem. Soc.*, 1974, **96**, 8087.
13. I. Fonseca, S. Martinez-Carrera and S. Garcia-Blanco, *Acta Crystallogr.*, 1979, **35**, 2643.



1. M.P. Paradisi and A. Romeo, *J. Chem. Soc., Perkin Trans. 1*, 1977, 596.
2. P.S. Portoghese, *J. Pharm. Sci.*, 1964, **53**, 228.
3. A. Fredga, *Acta Chem. Scand., Ser. B*, 1977, **31**, 869.
4. W.L.F. Armarego, B.A.Milloy and W. Pendergast, *J. Chem. Soc., Perkin Trans. 1.*, 1976, 2229.
5. See p. **A4.**
6. Y. Yamamoto, J. Oda and Y. Inouye. *J. Org. Chem.*, 1976, **41**, 303.
7. L. Maat and R.W. Wulkan, *Recl. Trav. Chim. Pays-Bas*, 1981, **100**, 204.
8. G. Bettoni, C. Franchini, R. Perrone and V. Tortorella, *Tetrahedron*, 1980, **36**, 409.
9. B. Ringdahl and R. Dahlbom, *Chem. Scr.*, 1977, **12**, 47.
10. W.L.F. Armarego, P. Waring and J.W. Williams, *Chem. Commun.*, 1980, 334.
11. W.L.F. Armarego, H. Schou and P. Waring, *J. Chem. Res. (S)*, 1980, 133.
12. S. Matsuura and T. Sugimoto, *Bull. Chem. Soc. Jpn.*, 1981, **54**, 2543.
13. T. Sugimoto and S. Matsuura, *Bull. Chem. Soc. Jpn.*, 1980, **53**, 3385.
14. D.D. Miller, F. Hsu, R.R. Ruffolo and P.N. Patil, *J. Med. Chem.*, 1976, **19**, 1382.
15. A. Lindquist, B. Ringdahl, U. Svensson and R. Dahlbom, *Acta Chem. Scand., Ser. B.*, 1976, **30**, 517.



1. W. Oppolzer and G. Flaskamp, *Helv. Chim. Acta*, 1977, **60**, 204.
2. G. Habermehl and H. Andres, *Justus Liebigs Ann. Chem.*, 1977, 800.
3. B. Ringdahl and R. Dahlbom, *Acta Chem. Scand., Ser. B*, 1976, **30**, 812.
4. B. Ringdahl and R. Dahlbom, *Chem. Scr.*, 1977, **12**, 47.
5. C.M. Svahn and N.A. Jonsson, *Acta Chem. Scand. Ser. B*, 1978, **32**, 137.
6. G. Lucente, G. Piccinni and A. Romeo, *Gazz. Chim. Ital.*, 1966, **96**, 1380.
7. G. Lucente, G. Cagnetta, G. Fiorentini and A. Romeo, *Gazz. Chim. Ital.*, 1965, **95**, 1335.
8. R. Kinas, K. Pankiewicz, W.J. Stec, P.B. Farmer, A.B. Foster and M. Jarman, *J. Org. Chem.*, 1977, **42**, 1650.
9. K.R. Kopecky, P.M. Pope and J.A. Lopez Sastre, *Can. J. Chem.*, 1976, **54**, 2639.



1. S. Yamada, T. Mashiko and S. Terashima, *J. Am. Chem. Soc.*, 1977, **99**, 1988.
2. P. Dumas, N. Spassky and P. Sigwalt, *Makromol. Chem.*, 1972, **156**, 55.
3. J.L. Coke and A.B. Richon, *J. Org. Chem.*, 1976, **41**, 3516.
4. M. Masada and K. Nishimura, *Chem. Lett.*, 1981, 1333.
5. J.P. Guette and N. Spassky, *Bull. Soc. Chim. Fr.*, 1972, 4217.
6. G. Gottarelli, B. Samori, I. Moretti and G. Torre, *J. Chem. Soc., Perkin Trans. 2*, 1977, 1105.
7. R.E. Ireland, C.S. Wilcox and S. Thaisrivongs, *J. Org. Chem.*, 1978, **43**, 786.
8. A. Konowal, J. Jurczak and A. Zamojski, *Tetrahedron*, 1976, **32**, 2957.
9. J. Cléophax and S.D. Géro, *Bull. Soc. Chim. Fr.*, 1967, 1441.
10. H. Noguchi, U. Sankawa and Y. Iitaka, *Acta Crystallogr., Sect. B*, 1978, **34**, 3273.
11. L. Ananthasubramanian, S.T. Carey and M.S.R. Nair, *Tetrahedron Lett.*, 1978, 3527.
12. T. Suga, S. Ohta, T. Hirata and T. Aoki, *Chem. Lett.*, 1982, 895.