

Neural Networks in Chemistry and Drug Design, 2nd Edition

Jure Zupan, Johann Gasteiger



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Neural Networks in Chemistry and Drug Design, 2nd Edition Jure Zupan, Johann Gasteiger The second edition of this highly regarded text has been substantially expanded. Part VI "Applications" is updated from 12 to 21 examples with a new focus on applications in the area of drug design.

From reviews of the first edition:

This book offers a sound introduction to artificial neuronal networks, with insights into their architecture, functioning, and applications, which is intended not only for chemists... The excellent quality of the contents and the presentation should ensure that it reaches a wide international readership. (Angewandte Chemie)

'One of the most useful aspects of the book is a walk-through of the whole process for each application: experimental design, choice and organization of the data, selection of network architecture and parameters, and analysis of the results... The careful approach embodied in this book is an antidote to the hype which has attended neuronal networks in recent years.' (Journal of the American Chemical Society)

'... highly recommended ... could become a scientific bestseller ...' (Spectroscopy Europe)

'The attractive and clear presentation of this book make it recommendable to the complete novice.' (The Analyst)

'We strongly recommend it for library purchase and it will be a useful text for lecture courses.' (Chemistry & Industry)

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