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# Artificial Intelligence in Drug Discovery

Nathan Brown Benevolent AI, London, UK

## Synopsis

Due to significant advances in Deep Learning and related areas, artificial intelligence methods are increasingly utilised in drug discovery to tackle challenges that have hitherto been difficult to solve, such as predicting properties, designing molecules, and optimising synthetic routes. Artificial Intelligence in Drug Discovery comprehensively covers artificial intelligence and machine learning tools and techniques; covering specific challenges such as learning from chemical data, designing new molecular structures, predictive modelling in both ligand and structure-space, synthesis planning, and molecular simulations. The book tackles real-world challenges in drug discovery ensuring context of application is preserved and disseminated by world leaders in the field.

## Brief Contents

- The History of Artificial Intelligence and Chemistry
- Chemical Topic Modelling – An Unsupervised Approach Originating from Text-mining to Organize Chemical Data
- Deep Learning and Chemical Data Concepts and Applications of Conformal Prediction in Computational Drug Discovery
- Non-applicability Domain. The Benefits of Defining “I don’t know” in Artificial Intelligence
- Predicting Protein-Ligand Binding-Affinities
- Machine Learning in the Area of Molecular Dynamics Simulations

Series: Drug Discovery

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Pages: 500

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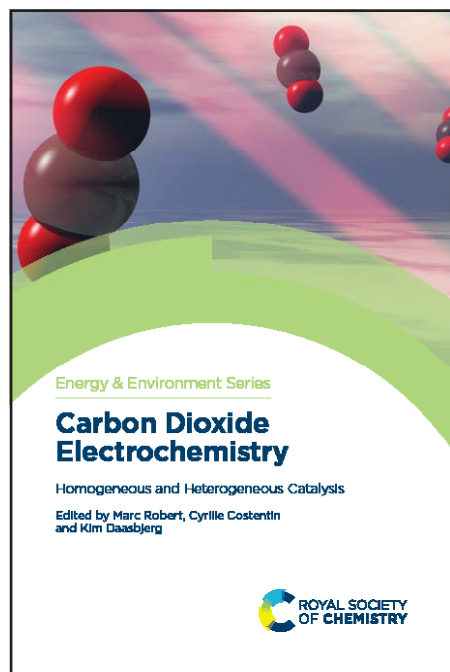
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# Carbon Dioxide Electrochemistry

## Homogeneous and Heterogeneous Catalysis

**Marc Robert** Université Paris Diderot, France

**Cyrille Costentin** Université Paris Diderot, France

**Kim Daasbjerg** Aarhus University, Denmark

### Synopsis

Conversion of light and electricity to chemicals is an important component of a sustainable energy system. Carbon Dioxide Electrochemistry showcases different advances in the field, and bridges the two worlds of homogeneous and heterogeneous catalysis that are often perceived as in competition in research. Written and edited by internationally recognised scientists, this title will appeal to students and researchers working in energy, catalysis, chemical engineering and physical chemistry.

### Brief Contents

- Approaches to Controlling Homogeneous Electrochemical Reduction of Carbon Dioxide
- Homogeneous Electrochemical Reduction of CO<sub>2</sub>: From Homogeneous to Supported Systems
- Heterogeneous Electrochemical CO<sub>2</sub> Reduction
- Nanostructures for CO<sub>2</sub> reduction: from theoretical insight to material design
- Bridging Homogeneous and Heterogeneous Systems: Atomically Dispersed Metal Atoms in Carbon Matrices for Electrocatalytic CO<sub>2</sub> Reduction

Series: **Energy and Environment Series**  
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Publisher: **Royal Society of Chemistry**  
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Edition: **1**  
Size: **234 x 156mm**  
Pages: **450**  
BIC: **PNRD, PNRH, RNU**

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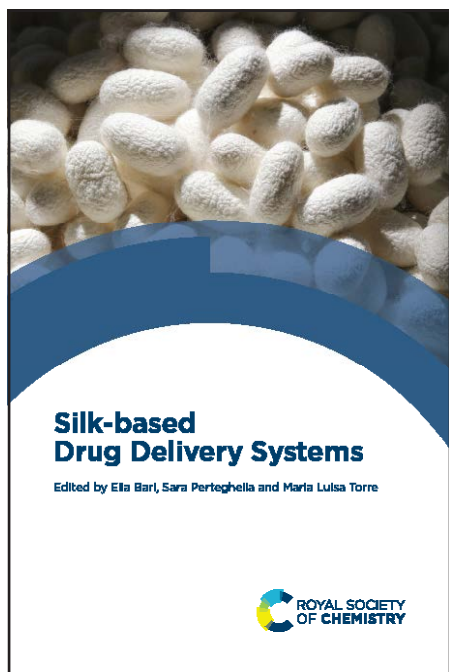
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## Silk-based Drug Delivery Systems

Elia Bari University of Pavia, Italy

Sara Perteghella University of Pavia, Italy

Maria Luisa Torre University of Pavia, Italy

### Synopsis

Covering spider silk and silk worm cocoons, the editors elucidate the extraction, structure and properties of silk sericin and silk fibroin. Showing how these proteins are employed in micro and nano drug delivery systems, their use in pre-clinical and clinical trials, and closing with chapter on sustainability- driven innovation in the pharma industry, this book is ideal for graduates and researchers in biomaterials science and pharmaceutical science.

### Brief Contents

- Micro and Nano-Drug Delivery Systems
- Silk-Fibroin Micro-Drug Delivery Systems
- Silk-Fibroin Nano-Drug Delivery Systems
- Silk-Sericin Micro-Drug Delivery Systems
- Silk-Sericin Nano-Drug Delivery Systems
- Physico-Chemical Characterisation of Silk-Based Materials
- From Bench to Bedside: the Long Way Towards GMP Scale-Up, Preclinical and Clinical Trials for Silk-Based Drug Delivery Systems
- From Textile to Pharmaceutical and Cosmetic Industry: Circular Economy Applied to Silk Manufacturing Wastes

Series:

ISSN:

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Publishing date: 28/10/2020

Target Audience: Professional and scholarly

Format: Hardback

Edition: 1

Size: 234 x 156mm

Pages: 275

BIC: PHFC1, PNNP, TDCP

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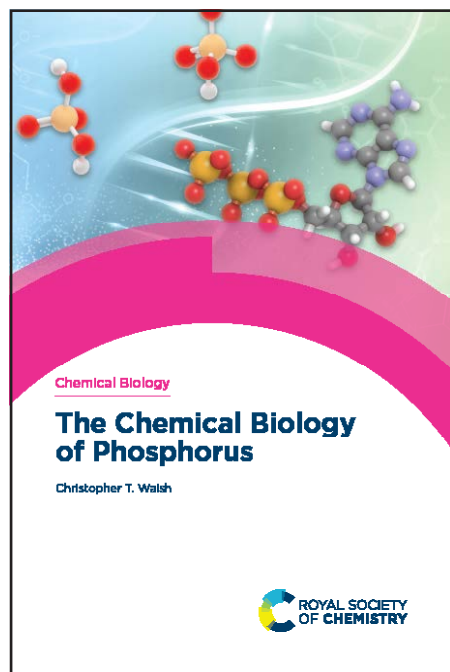
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# The Chemical Biology of Phosphorus

Christopher T Walsh Stanford University, USA

## Synopsis

Phosphorus chemical biology underlies most of life's reactions and processes, from the covalent bonds that hold RNA and DNA together, to the making and spending 75 kg of ATP every day, required to run almost all metabolic and mechanical events in cells. Authored by a renowned biochemist, *The Chemical Biology of Phosphorus* provides an in-depth, unifying chemical approach to the logic and reactivity of inorganic phosphate and its three major derivatives (anhydrides, mono- and diesters) throughout biology to examine why life depends on phosphorus. Covering the breadth of phosphorus chemistry in biology, this book is ideal for biochemistry students, postgraduates and researchers interested in the chemical logic of phosphate metabolites, energy generation, biopolymer accumulation and phosphoproteomics.

## Brief Contents

- Introduction to Phosphorus Chemical Biology
- Inorganic Phosphate, Pyrophosphate and Polyphosphate
- ATP as the Premier Biologic Phosphoryl Transfer Reagent
- Nucleotidyl Transfers (ATPs and NTPs)
- Pyrophosphoryl and Adenosyl Transfers from Mg-ATP
- Activated Phosphoryl Groups and Biosynthetic Paths to ATP
- Phosphomonoesters: Enzymatic Formation and Decomposition
- Phosphodiester and Phosphotriester; Phosphorylases: Inorganic Phosphate as Oxygen Nucleophile
- N-P Bond Chemical Biology

Series: **Chemical Biology**

ISSN: 2055-1975

Publisher: Royal Society of Chemistry

ISBN: 9781839162022

Price: £179.00 | \$250.00

Publishing date: 20/10/2020

Target Audience: College/higher education

Format: **Hardback**

Edition: 1

Size: 234 x 156mm

Pages: 400

BIC: PNN, PSBZ, PSD

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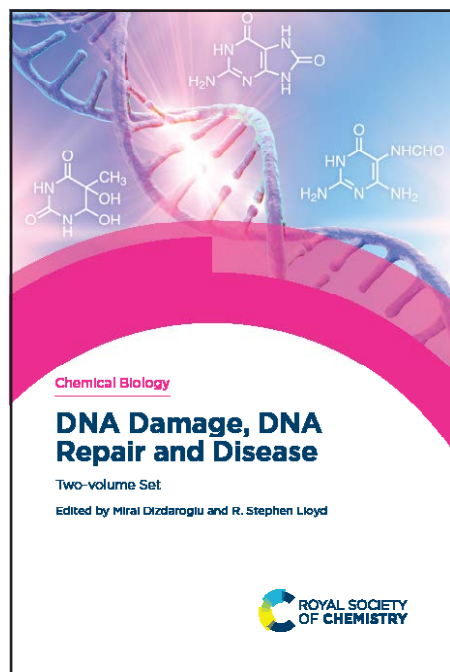
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# DNA Damage, DNA Repair and Disease

## Two-volume Set

Miral Dizdaroglu  
R Stephen Lloyd

### Synopsis

The DNA of all organisms is constantly being damaged by endogenous and exogenous sources. Oxygen metabolism generates reactive species that can damage DNA, proteins and other organic compounds in living cells. These books provide a comprehensive overview of the interdisciplinary area of DNA damage and DNA repair, and their relevance to disease pathology. Edited by recognised leaders in the field, this two-volume set is an appealing resource to a variety of readers including chemists, chemical biologists, geneticists, cancer researchers and drug discovery scientists.

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Series: **Chemical Biology**

ISSN: **2055-1975**

Publisher: **Royal Society of Chemistry**

ISBN: **9781839162527**

Price: **£310.00 | \$435.00**

Publishing date: **19/11/2020**

Target Audience: **College/higher education**

Format: **Hardback**

Edition: **1**

Size: **234 x 156mm**

Pages: **839**

BIC: **PNN, PSAK1, PSB**

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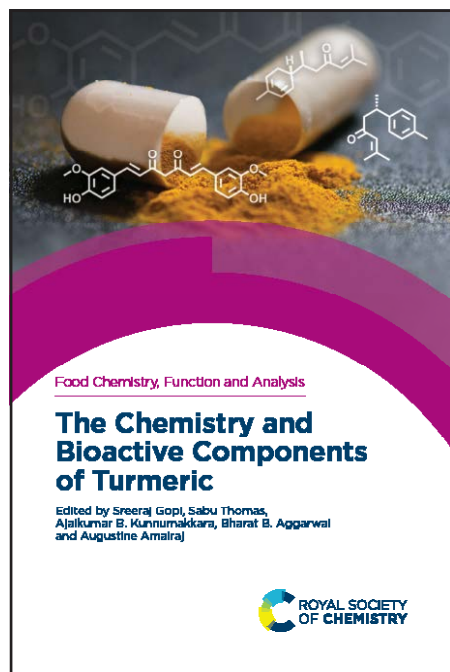
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## The Chemistry and Bioactive Components of Turmeric

**Sreeraj Gopi** Aurea Biolabs Private Limited, India

**Sabu Thomas** Mahatma Gandhi University, India

**Ajai Kumar B Kunnumakkara** Indian Institute of Technology Guwahati, India

**Bharat B Aggarwal** Anti-inflammation Research Institute, USA

**Augustine Amalraj** Aurea Biolabs Private Limited, India

### Synopsis

Turmeric is cultivated in tropical and sub-tropical regions around the world and used extensively as a colouring and flavouring agent. It is also one of the most popular medicinal herbs, with a wide range of pharmacological activities attributed mainly to curcuminoids and two related compounds, demethoxycurcumin and bisdemethoxycurcumin. This book brings together the research carried out in the products and nutraceuticals and food chemists.

### Brief Contents

- Turmeric - The Miraculous Herb from Ancient India and its Historical Background
- Chemistry of Turmeric
- Geographical Variations of Turmeric and Curcumin
- Turmeric - Active Ingredients Other than Curcuminoids
- Curcuminoids - Isolation, Formulations and the Bioavailability Problems
- Curcumin Pharmacokinetics and Plasma Determination
- Curcumin: A Potential Molecule for the Prevention and Treatment of Inflammatory Disorders

Series: Food Chemistry, Function and Analysis

ISSN: 2398-0656

Publisher: Royal Society of Chemistry

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Target Audience: Professional and scholarly

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Edition: 1

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Pages: 450

BIC: MBNH3, PSB, TDCT

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