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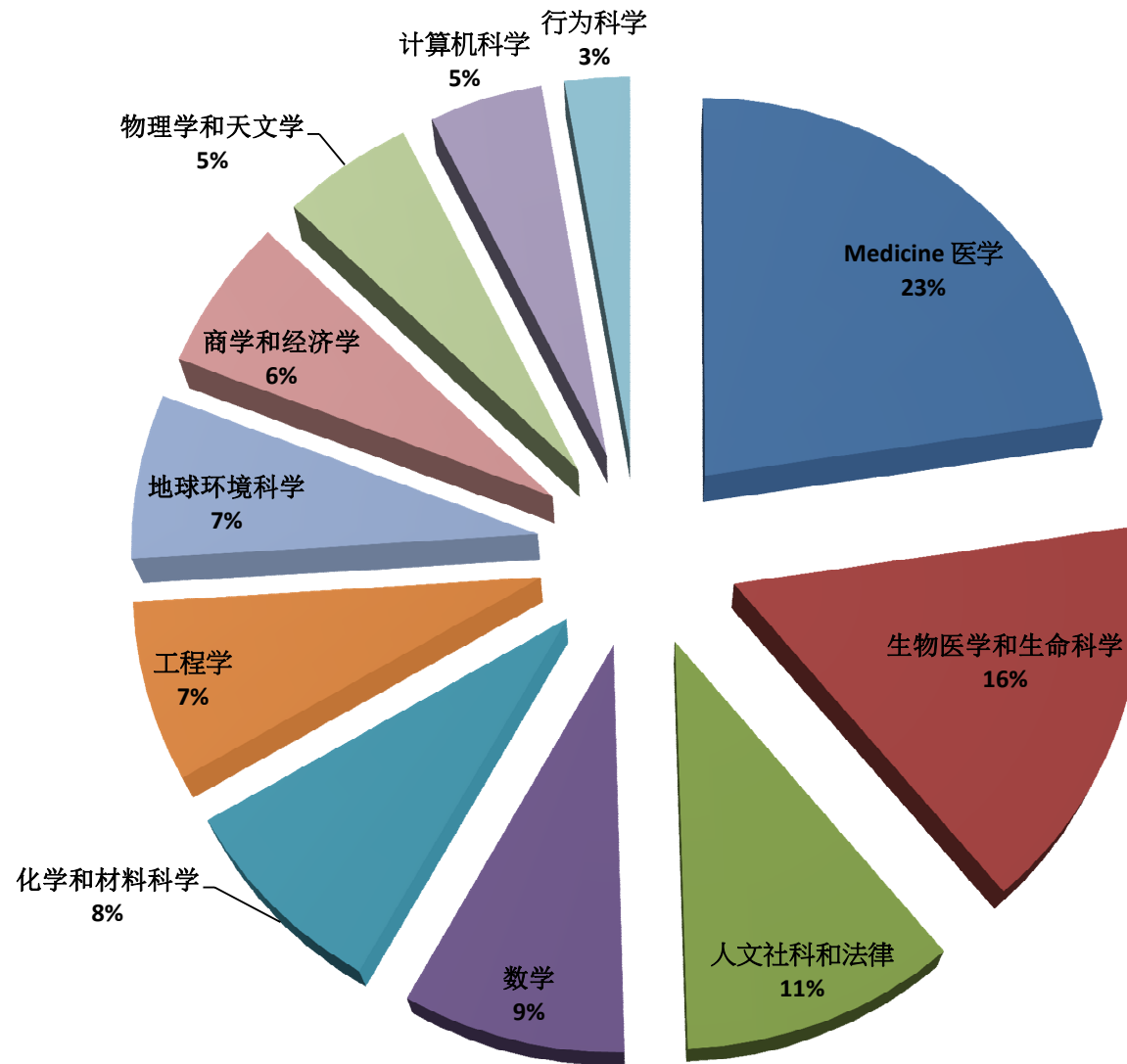
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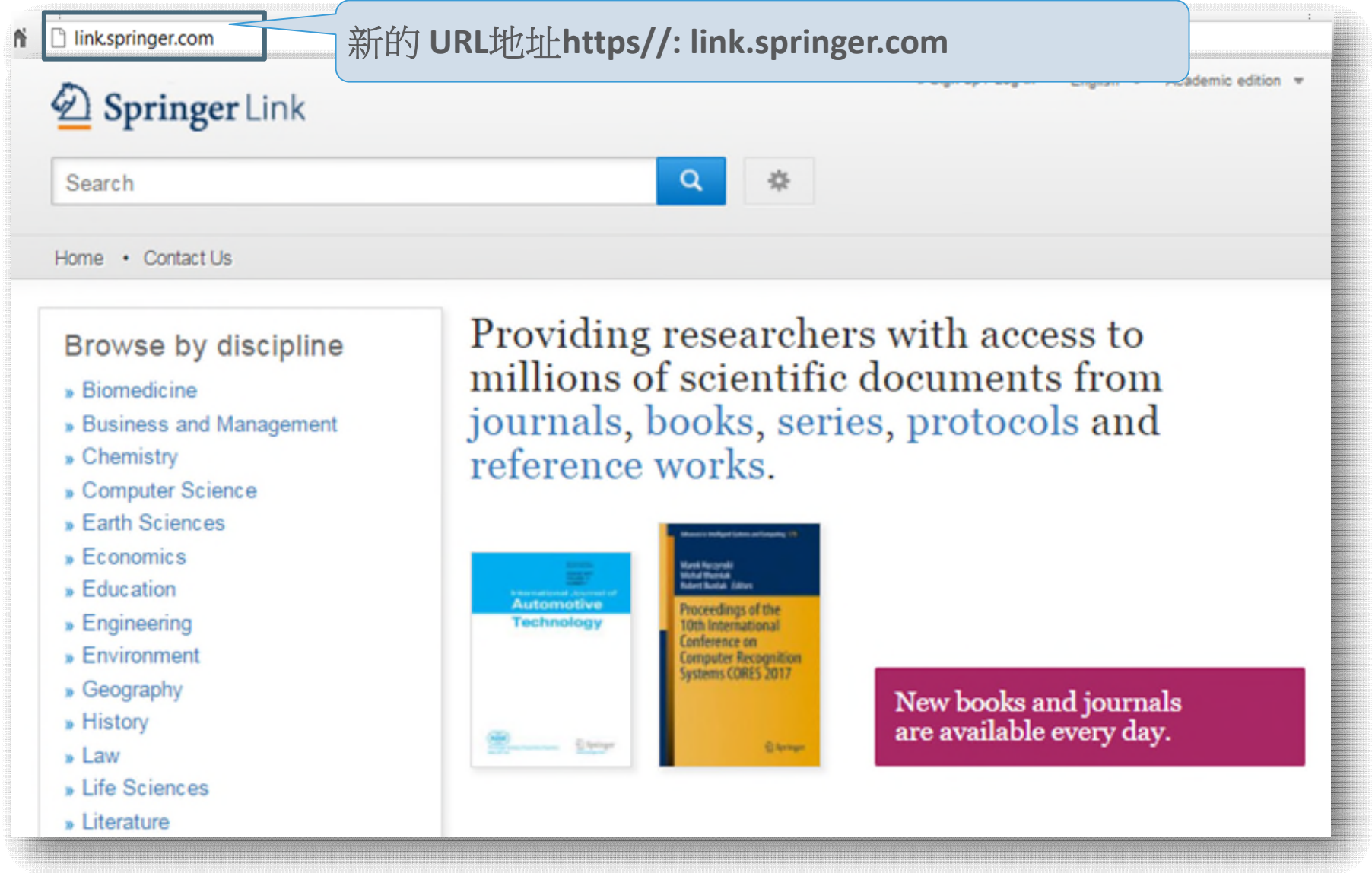
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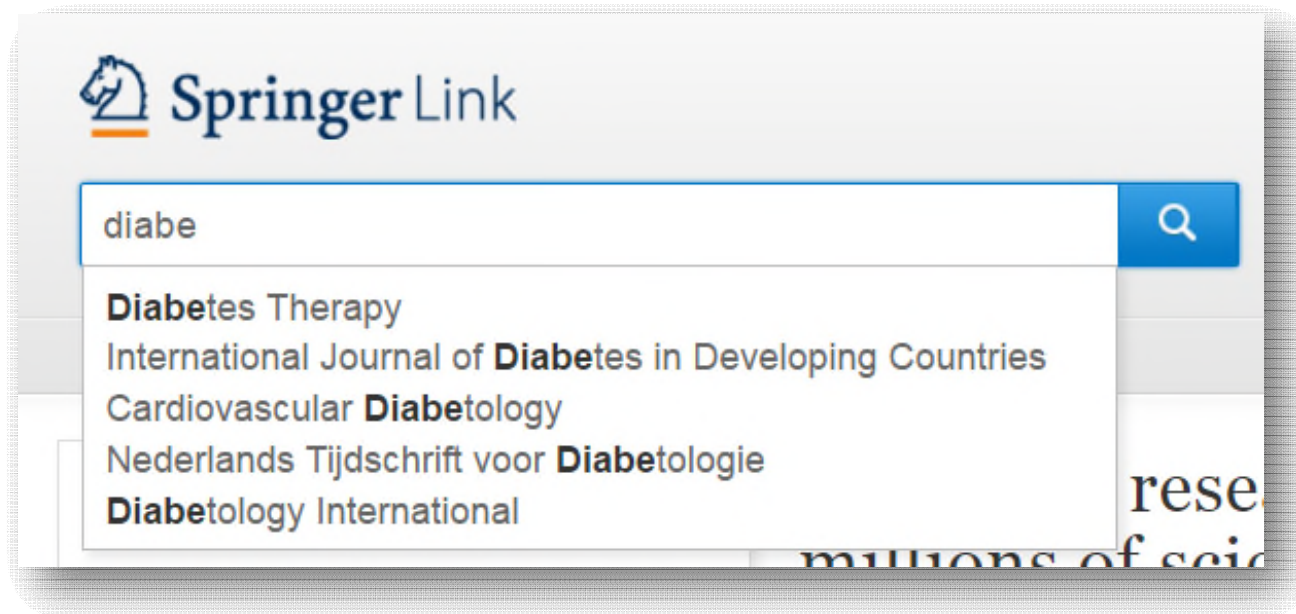


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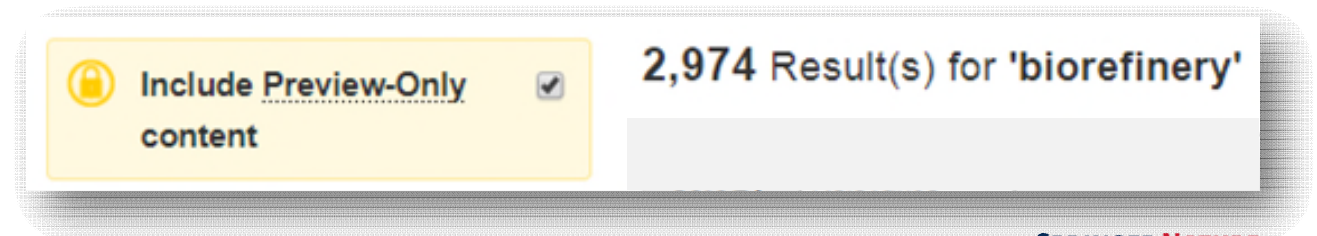


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European Biophysics Journal
October 2012, Volume 41, Issue 10, pp 789–799

Validation of macromolecular flexibility in solution by small-angle X-ray scattering (SAXS)

Authors: Michal Hammel

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First Online: 26 May 2012
DOI: 10.1007/s00249-012-0820-x

Cite this article as:
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The dynamics of macromolecular conformations are critical to the action of cellular networks. Solution X-ray scattering studies, in combination with macromolecular X-ray crystallography (MX) and nuclear magnetic resonance (NMR), strive to determine complete and accurate states of macromolecules, providing novel insights describing allosteric mechanisms, supramolecular complexes, and dynamic molecular machines. This review addresses theoretical and practical concepts, concerns, and considerations for using these techniques in conjunction with computational methods to productively combine solution-scattering data with high-resolution structures. I discuss the principal means of direct identification of macromolecular flexibility from SAXS data followed by critical concerns about the methods used to calculate theoretical SAXS profiles from high-resolution structures. The SAXS profile is a direct interrogation of the thermodynamic ensemble and techniques such as, for example, minimal ensemble search (MES), enhance interpretation of SAXS experiments by describing the SAXS profiles as population-weighted thermodynamic ensembles. I discuss recent developments in computational techniques used for conformational sampling, and how these techniques provide a basis for assessing the level of the flexibility within a sample. Although these approaches sacrifice atomic detail, the knowledge gained from ensemble analysis is often appropriate for developing hypotheses and guiding biochemical experiments. Examples of the use of SAXS and combined approaches with X-ray crystallography, NMR, and computational methods to characterize dynamic assemblies are presented.

Keywords

Small-angle X-ray scattering (SAXS) Macromolecular flexibility Rigid-body modeling Ensemble analysis

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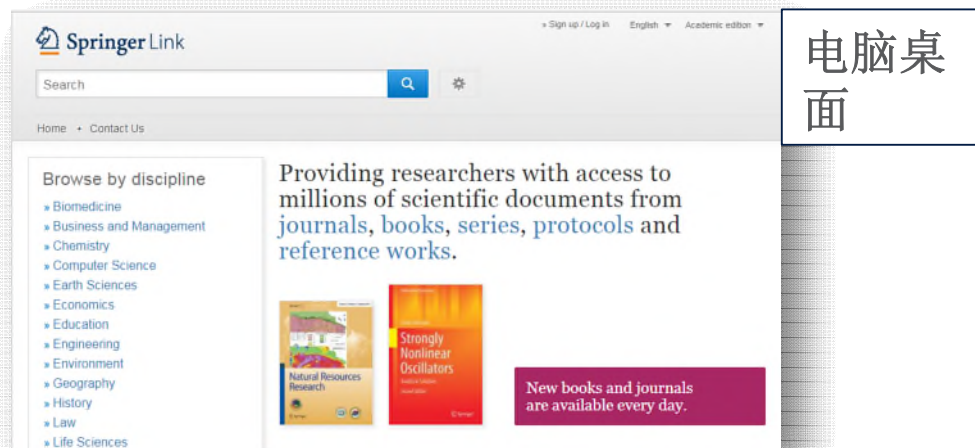
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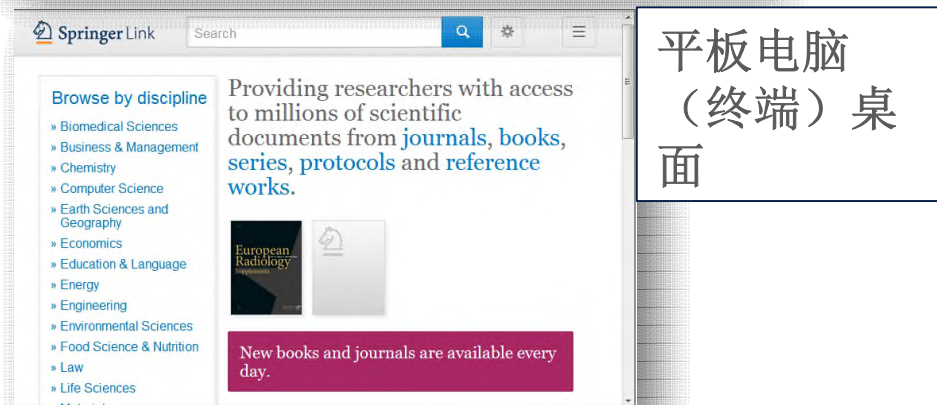
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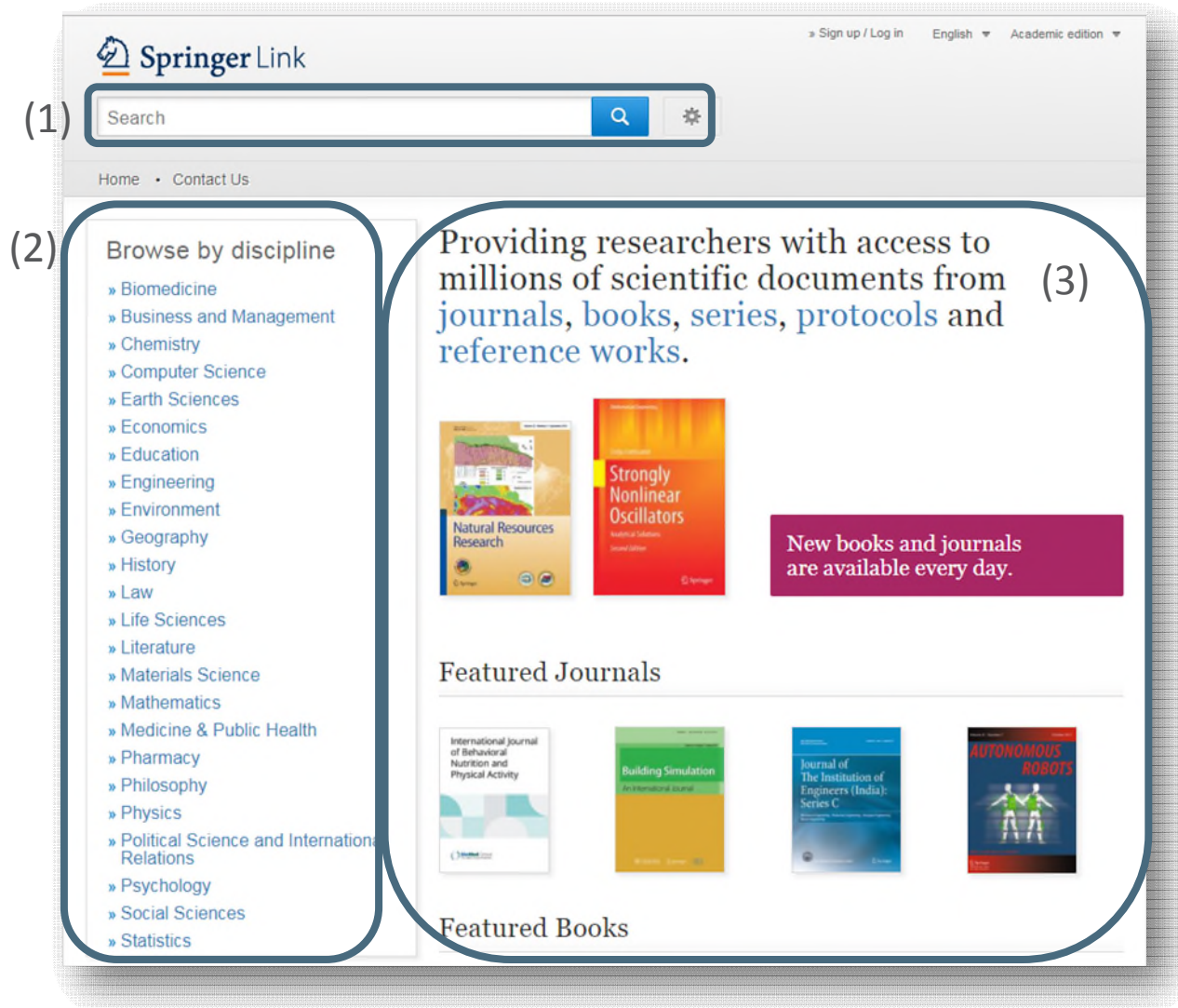
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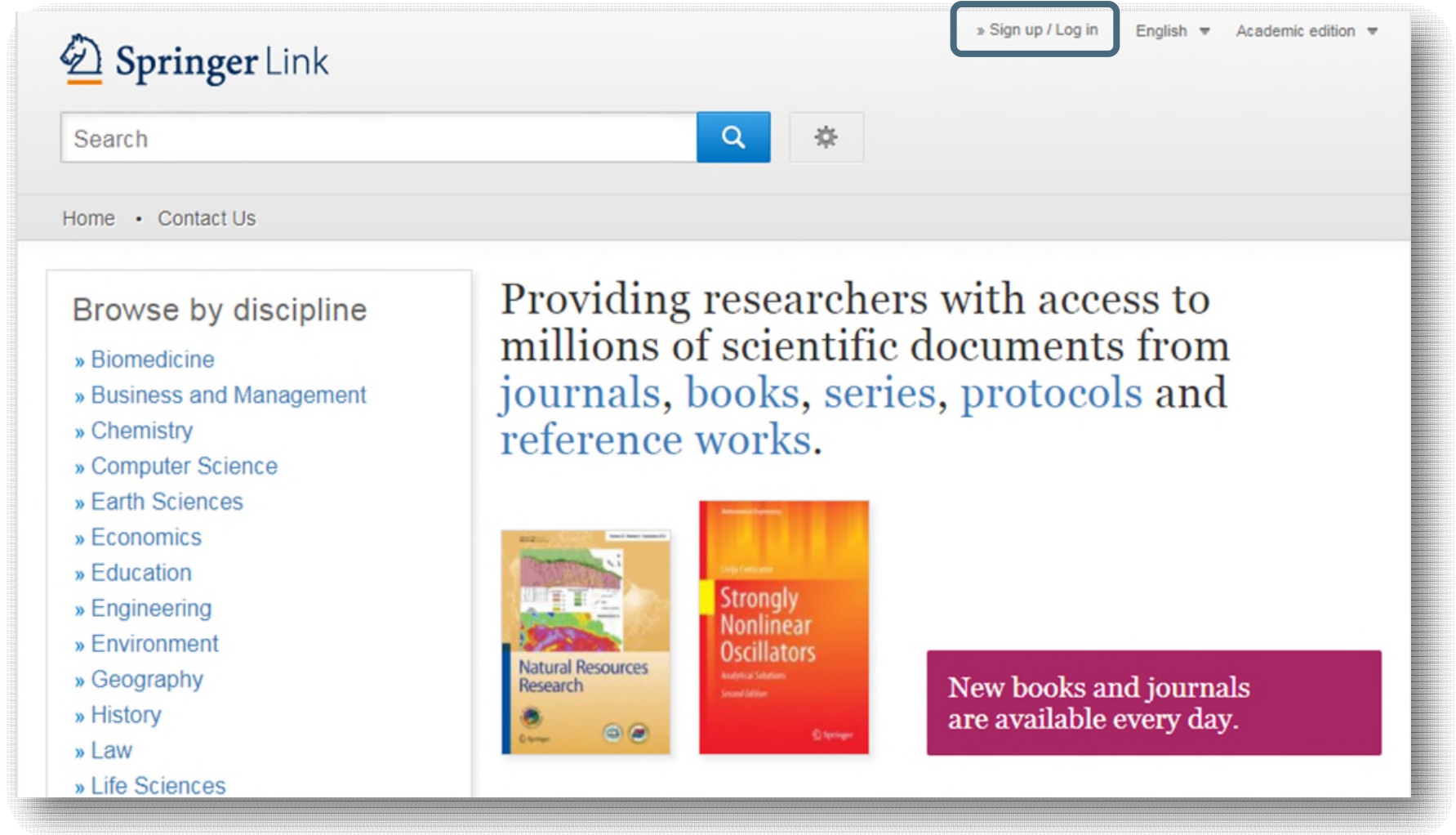
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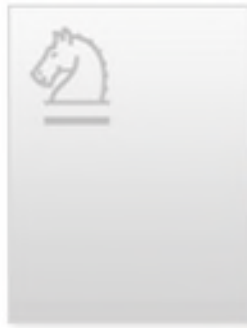
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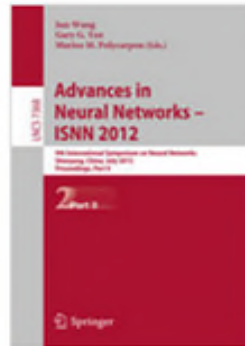


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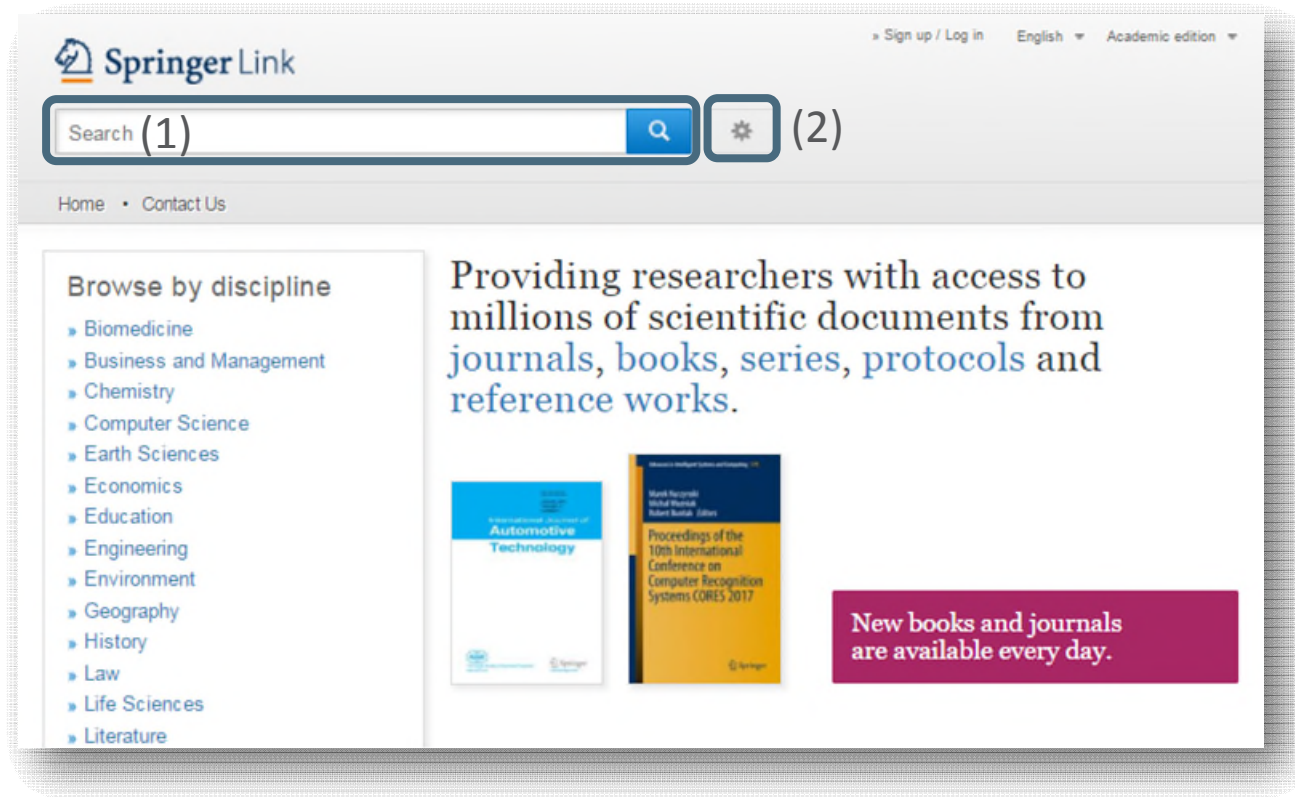
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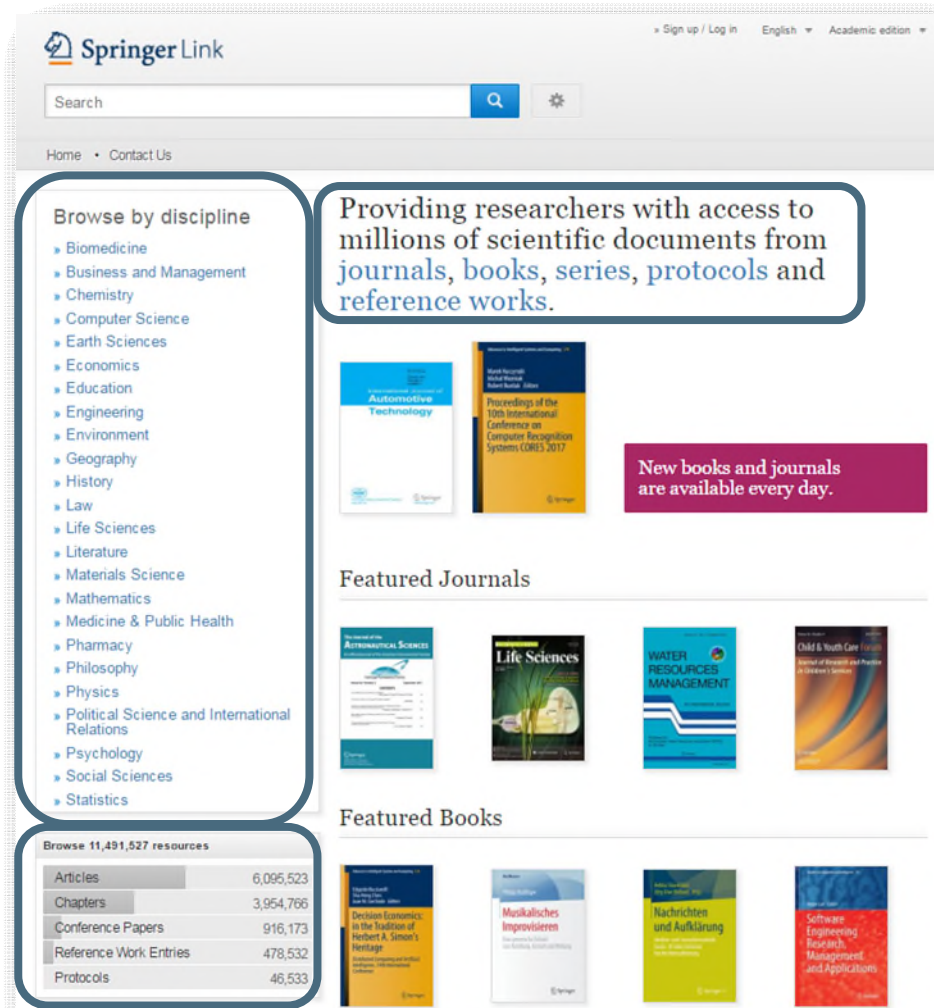
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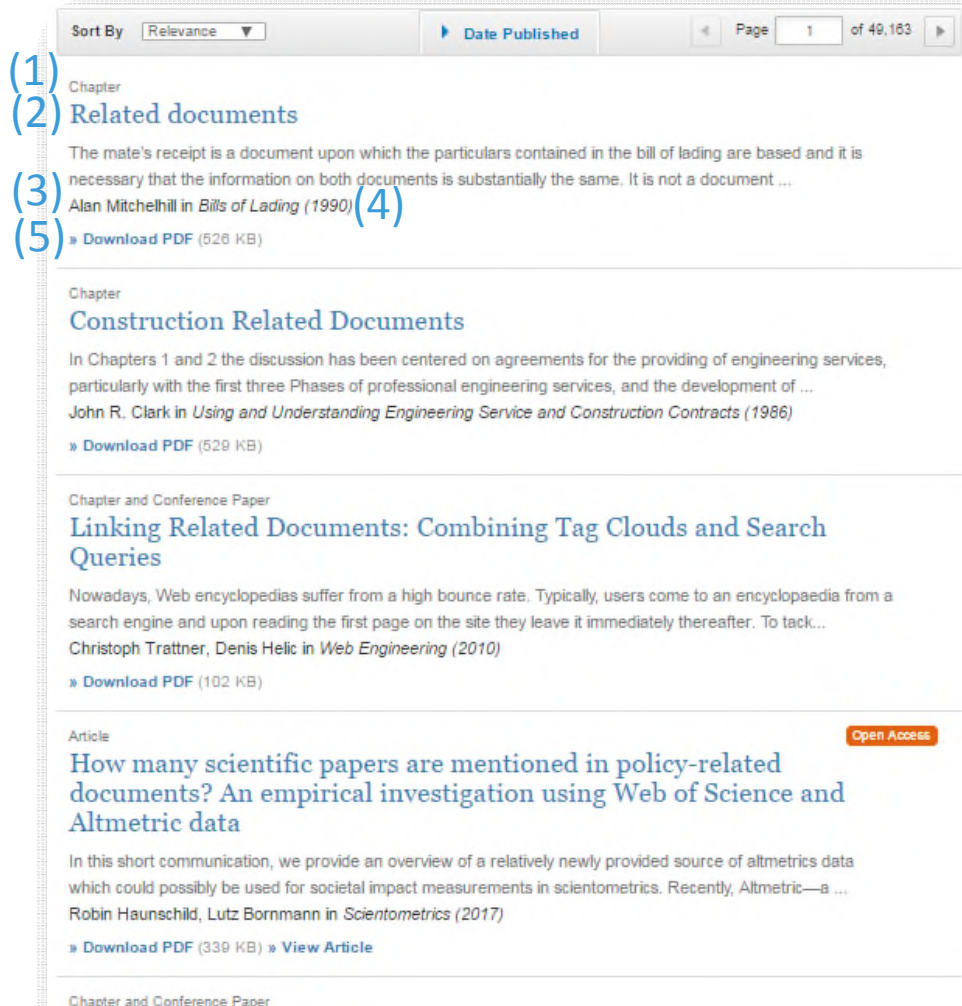
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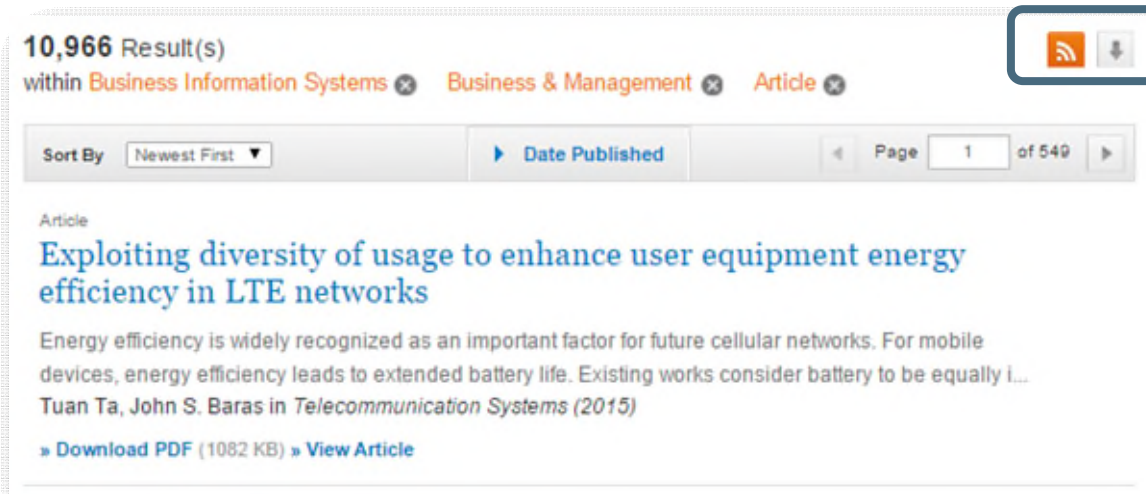
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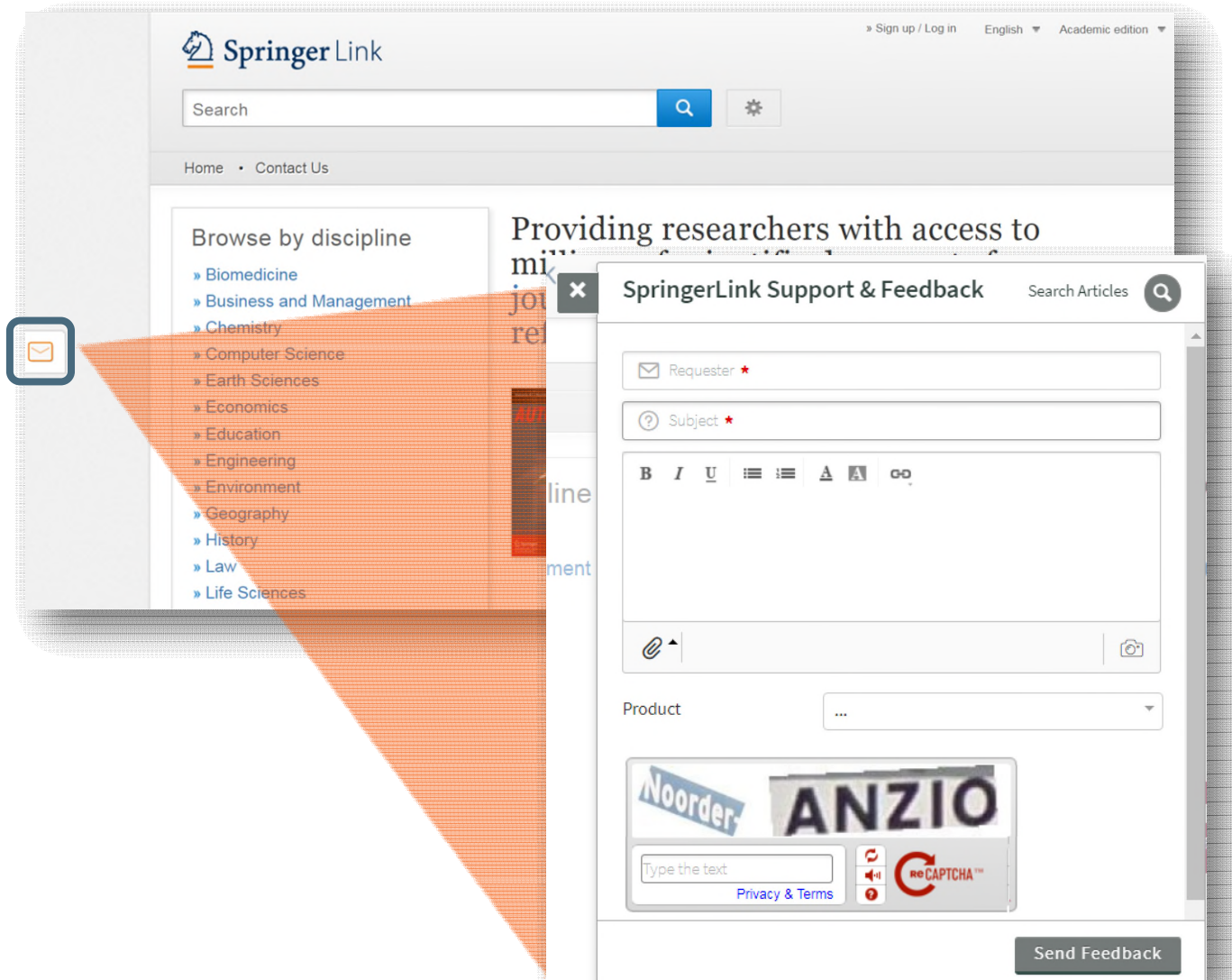
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October 2012, Volume 41, Issue 10, pp 789–799

Validation of macromolecular flexibility in solution by small-angle X-ray scattering (SAXS)

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Michal Hammel ✉

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First Online: 26 May 2012

DOI: 10.1007/s00249-012-0820-x

Cite this article as:

Hammel, M. Eur Biophys J (2012) 41: 789. doi:10.1007/s00249-012-0820-x

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QTL for root angle and number in a population developed from bread wheats (*Triticum aestivum*) with contrasting adaptation to water-limited environments

Authors: Jack Christopher, Mandy Christopher, Raelen Jennings, Shirley Jones, Susan Fletcher, Andrew Borrell, Ahmad M. Manschadi, David Jordan, Emma Mace, Graeme Hammer

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First Online: 24 March 2013

DOI: 10.1007/s00122-013-2074-0

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June 2013, Volume 126, [Issue 6](#), pp 1563–1574

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Challenges and Opportunities for the World's Forests in the 21st Century
Volume 81 of the series Forestry Sciences pp 23-35
Date: 12 October 2013


A Burning Issue: Tropical Forests and the Health of Global Ecosystems

Paul McMahon

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(4) Abstract

Tropical forests are in the front line of efforts to tackle climate change. This article provides an overview of the ecosystem services that tropical forests provide, the way in which rates of deforestation have changed over the past 20 years, and the economic drivers of tropical deforestation around the world. It describes recent intergovernmental efforts to reduce deforestation, both through a proposed UNFCCC REDD+ mechanism and through interim finance or 'Fast Start' partnerships that seek to achieve results between now and 2020. There has never been a better opportunity to forge international cooperation on this important environmental issue, but progress so far has been slow.

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A Framework for Durability Design with Strain-Hardening Cement-Based Composites (SHCC)
Volume 22 of the series RILEM State-of-the-Art Reports pp 1-26

Date: 08 January 2017

Introduction: Crack Distribution and Durability of SHCC

Gideon P. A. G. van Zijl, William P. Boshoff, Christian Wagner, Volker Slowik

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Abstract

Inherent crack control to fine widths in strain-hardening cement-based composites (SHCC) suggests that structural elements produced from SHCC or steel-reinforced SHCC (R/SHCC) may be rendered durable by limiting the ingress rates of potentially deleterious substances. Recently, it has been reported that, while the average crack width in SHCC is maintained up to large tensile strains in excess of 3‰, the maximum crack width may equal or exceed those are considered to be limiting in terms of durability. Also, the typical range in SHCC average crack width, from 50 to 100 µm, has been shown to be a threshold in water permeability, at which width permeability is restricted to several orders lower than that expected for crack widths ranging from 0.2 to 0.3 mm — a typical reinforced concrete crack width limit in durability standards. However, it has recently been shown that capillary absorption in dry, pre-cracked SHCC is a quick process, with water penetrating into fine cracks within minutes of exposure. In addition to describing these findings, this chapter sets the scene for later chapters on improved ingress rate characterisation and the actual deterioration of cracked SHCC or R/SHCC. Guidelines for the pre-cracking of SHCC towards durability testing are derived, based on the results of recent comparative testing. These include the specimen shape, size, test set-up, crack measurement to sufficient resolution, and crack width distribution presentation. Finally, the field performance of repairs, structures and structural elements produced from SHCC and R/SHCC in the past decade is reported.

Keywords

Crack width – Capillary absorption – Digital image correlation – Durability

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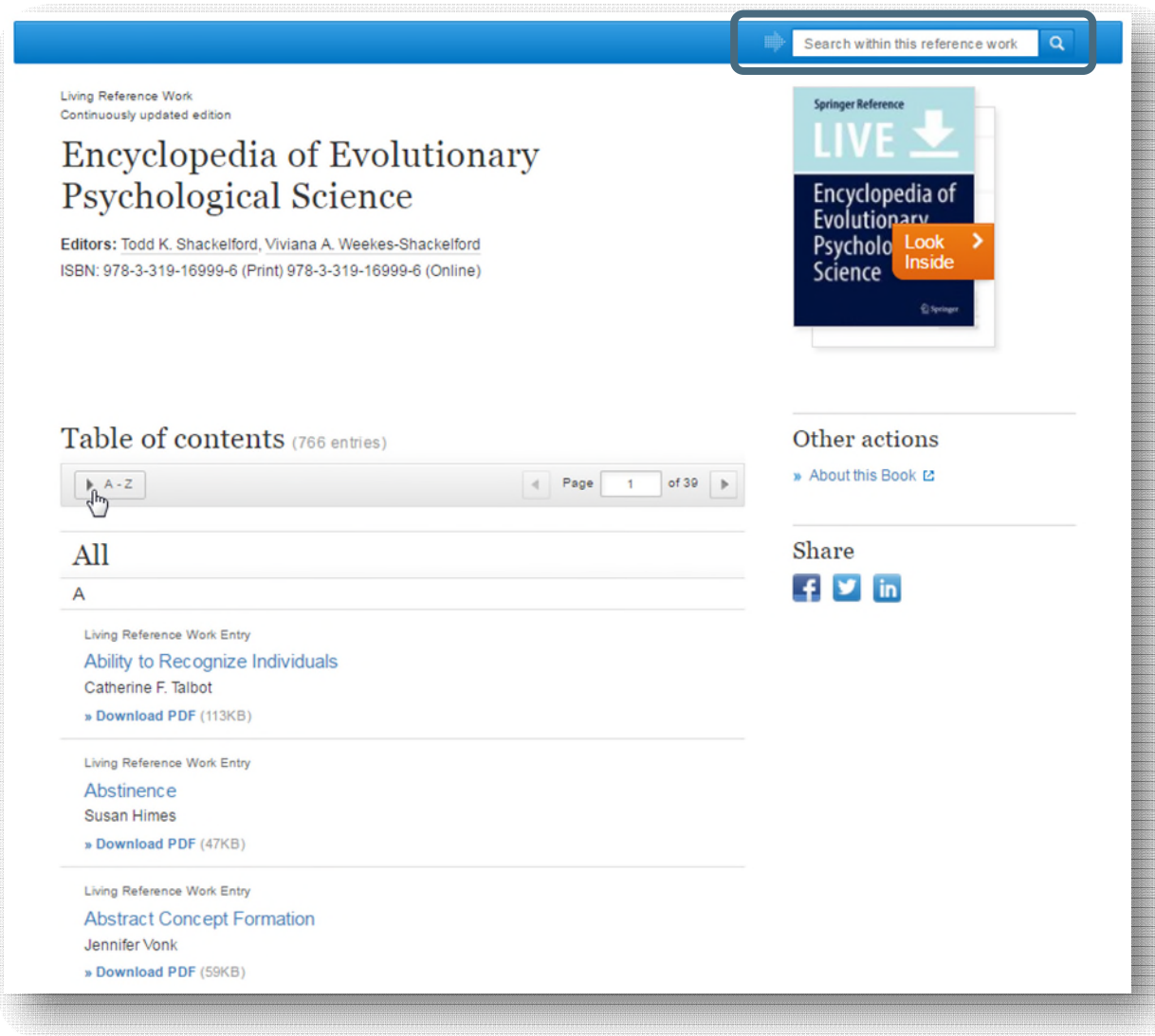
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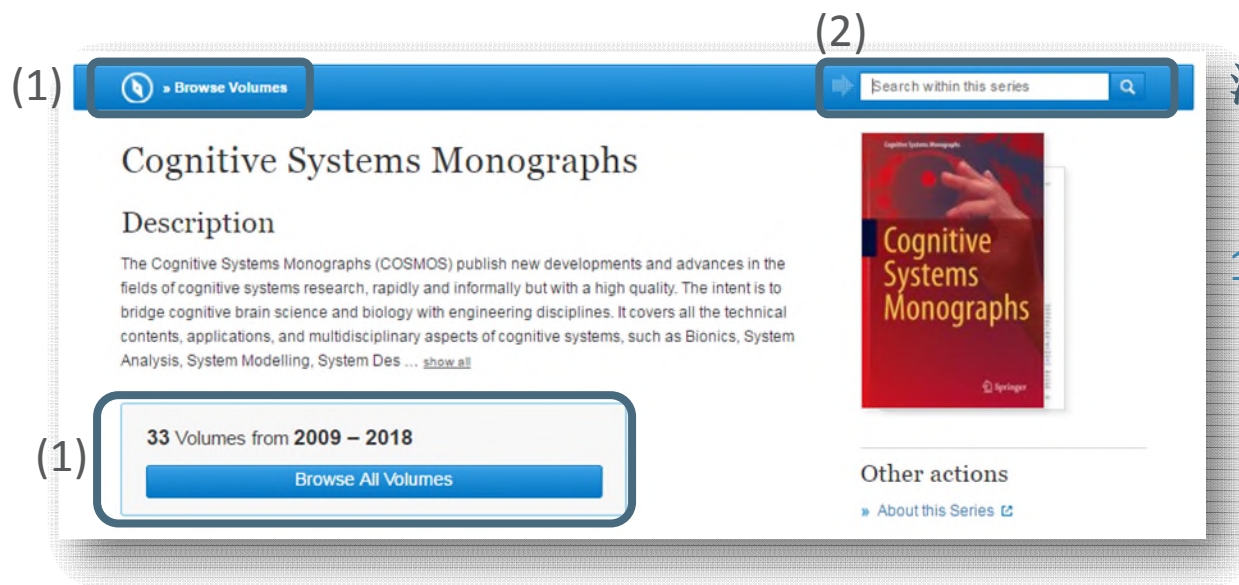
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Decellularization Methods for Scaffold Fabrication

Sweta K. Gupta, Narayan C. Mishra ✉

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Abstract

Decellularization is the process of removal of native cells from tissue, leaving behind a three-dimensional (3D) ultrastructure of extracellular matrix (ECM) proteins while preserving the bioactivity and mechanics of the tissue. It offers a unique top-down approach for fabricating ECM based natural scaffold for tissue engineering application. Herein, this chapter presents the fabrication of decellularized scaffold employing different methods: whole organ perfusion, immersion and agitation, pressure gradient, and supercritical fluid. The decellularized scaffold aims to exploit the nature-designed 3D architecture, a successful platform technology, for creating scaffolding materials for tissue engineering and regenerative medicine.

Keywords

Decellularization – Scaffold – Cells – Extracellular matrix – Tissue engineering



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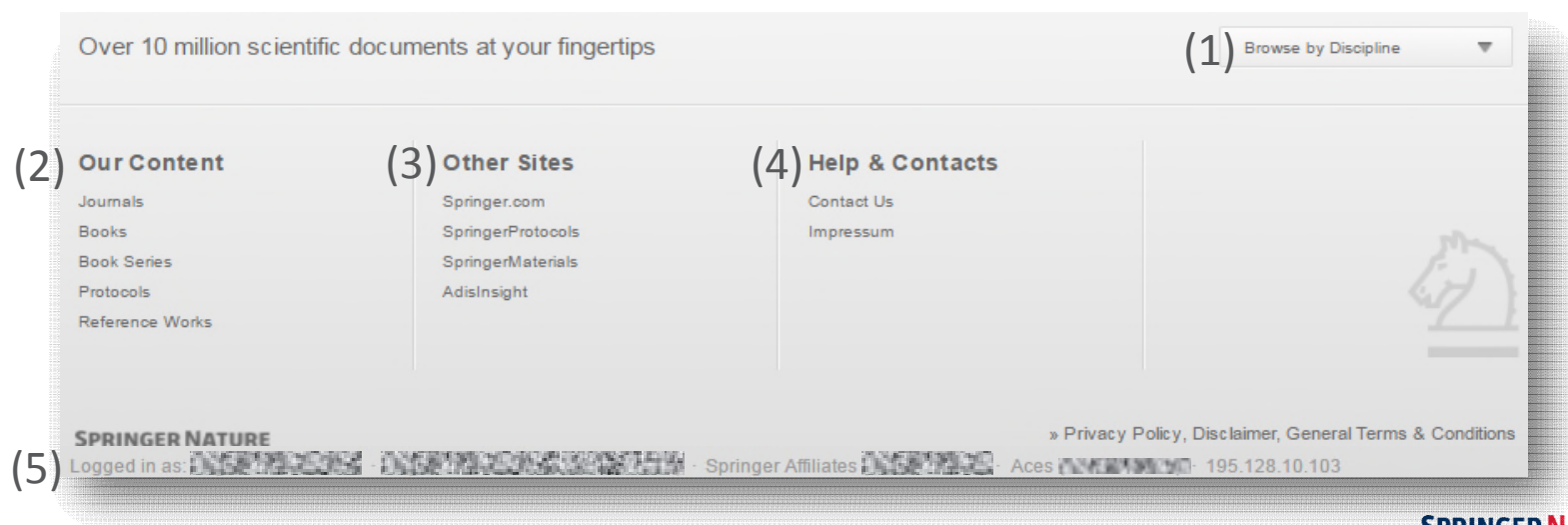
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