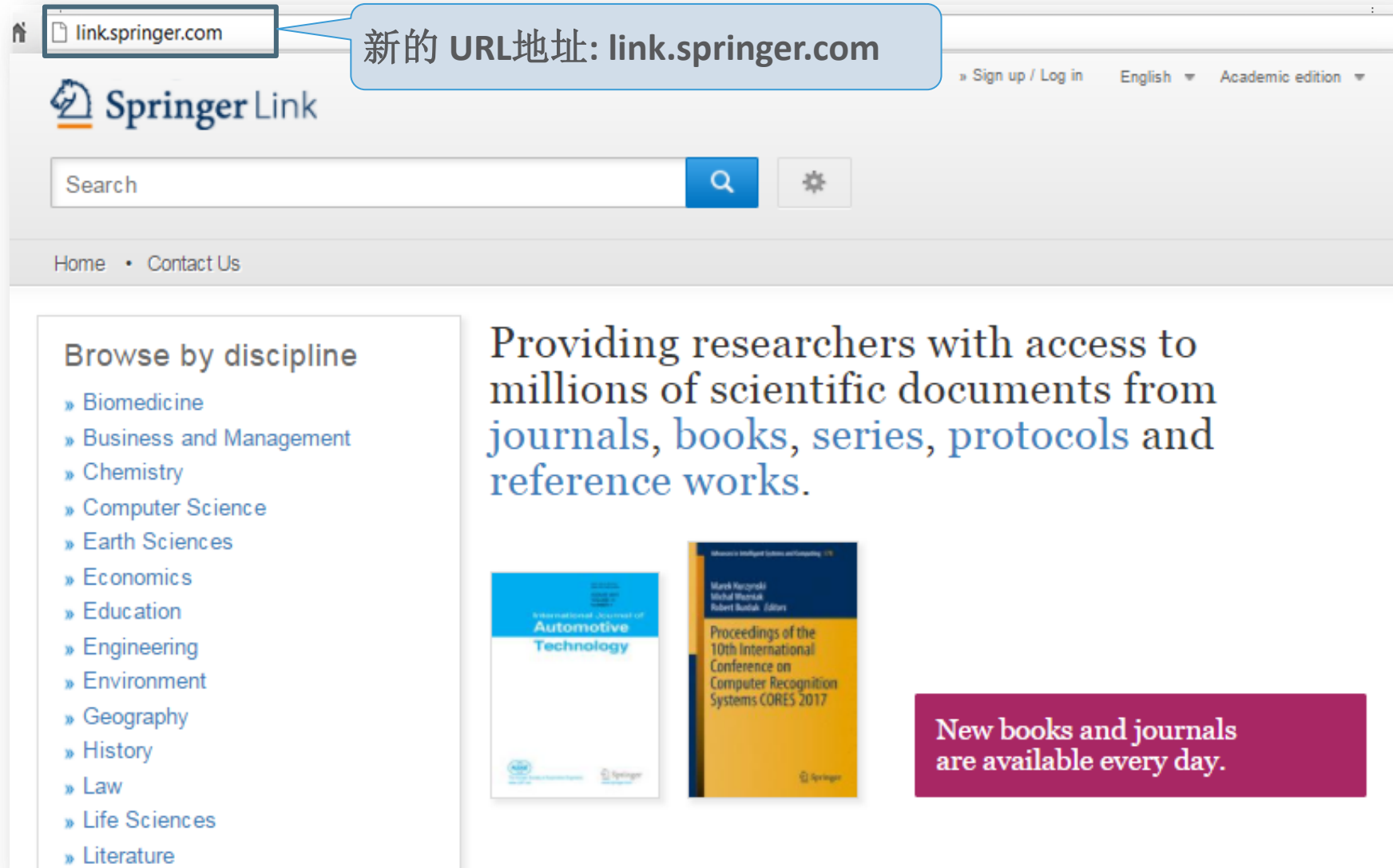


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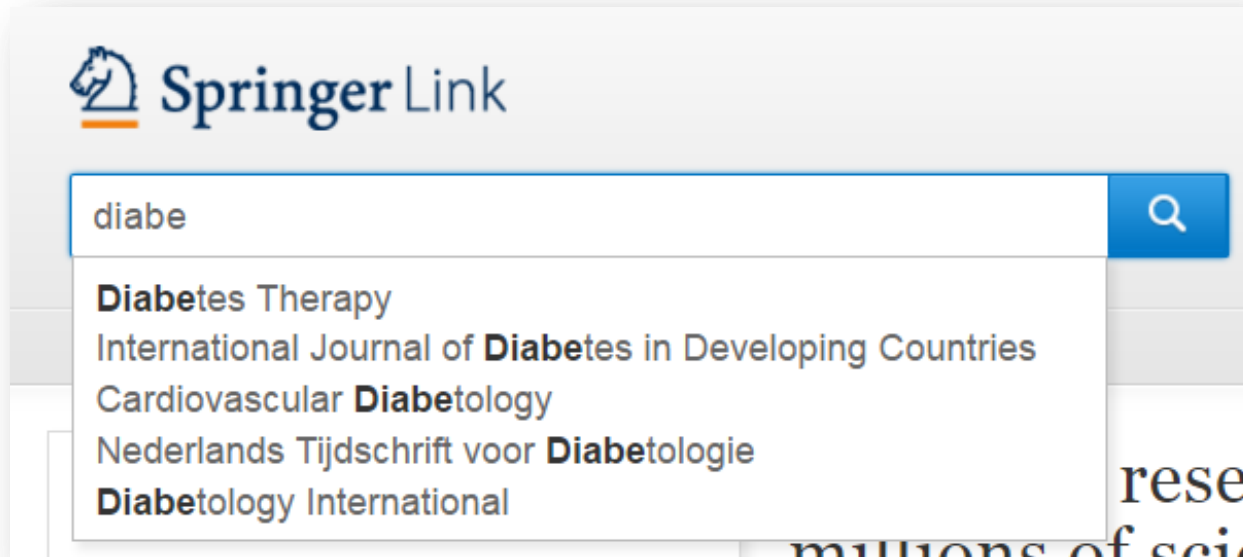
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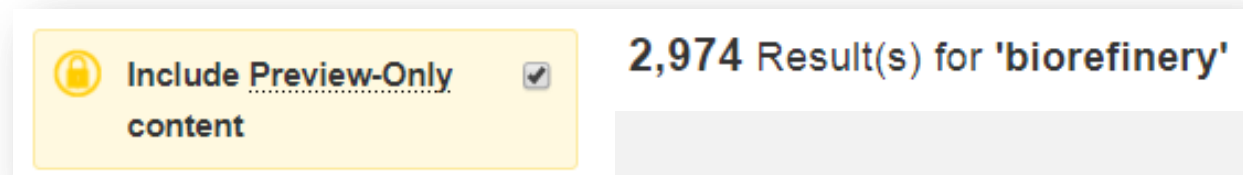
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Article Title: Validation of macromolecular flexibility in solution by small-angle X-ray scattering (SAXS)

Journal: European Biophysics Journal

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

Authors: Michal Hammel

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

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Abstract

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

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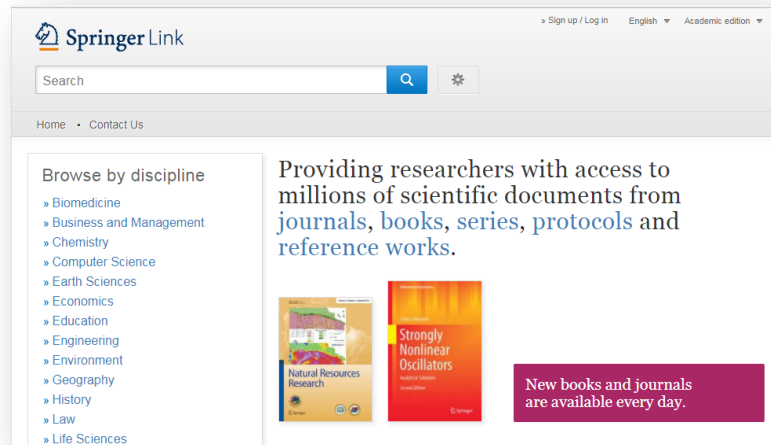
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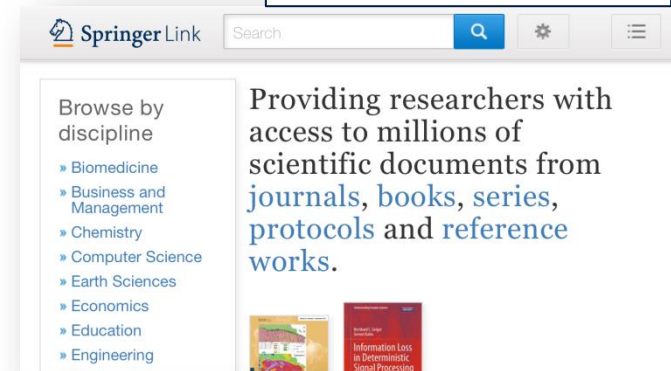
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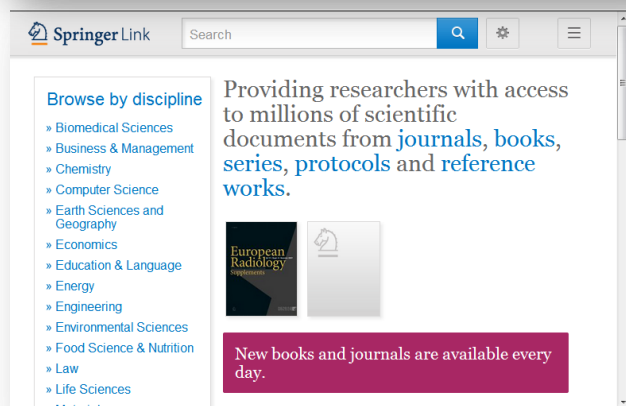
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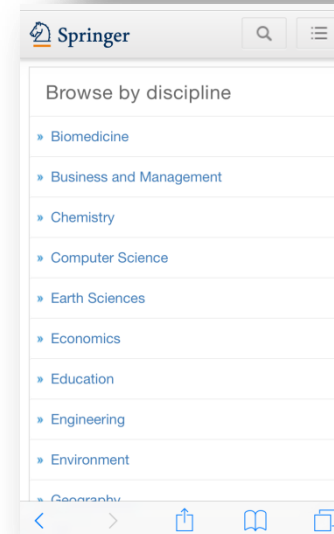
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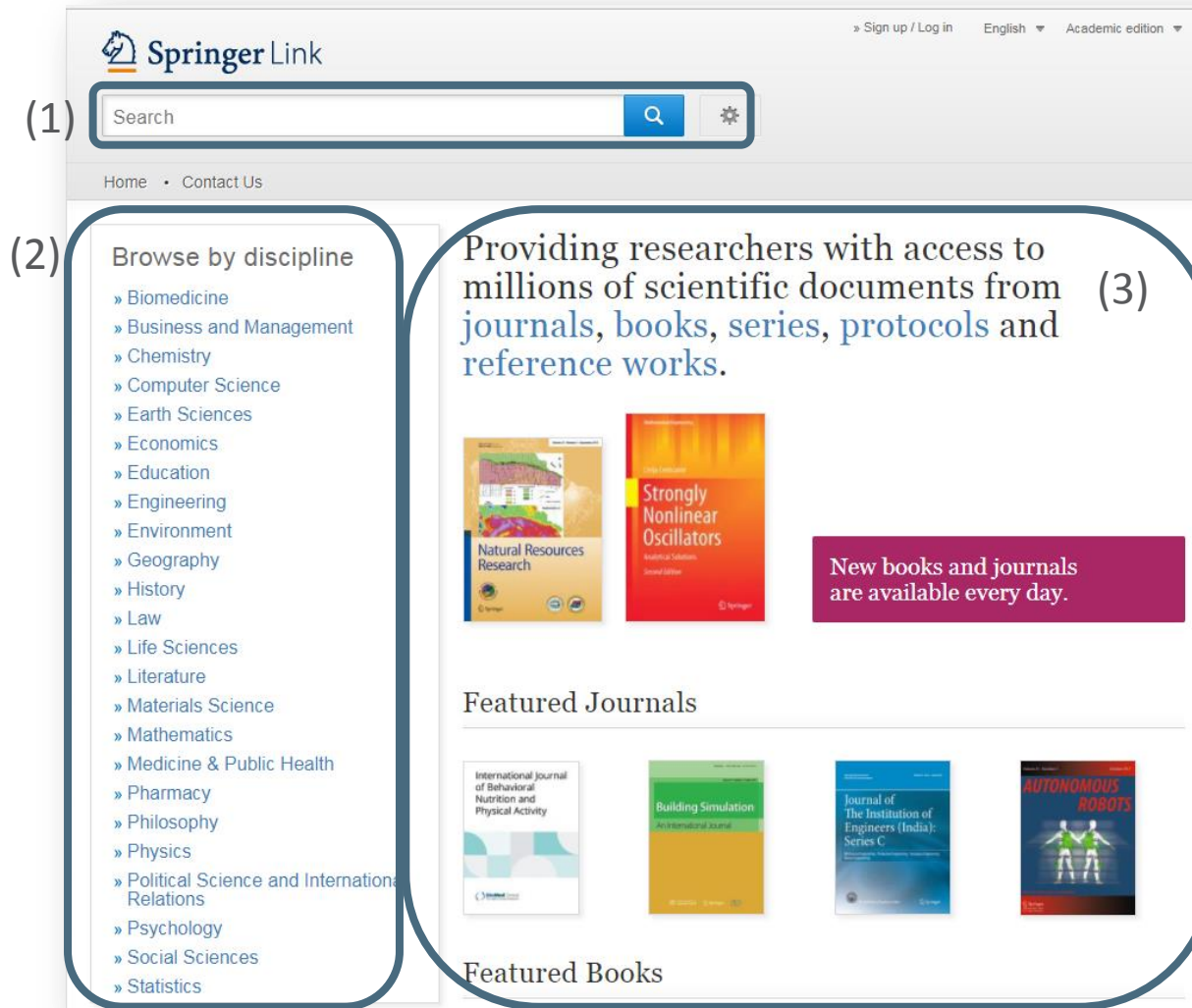
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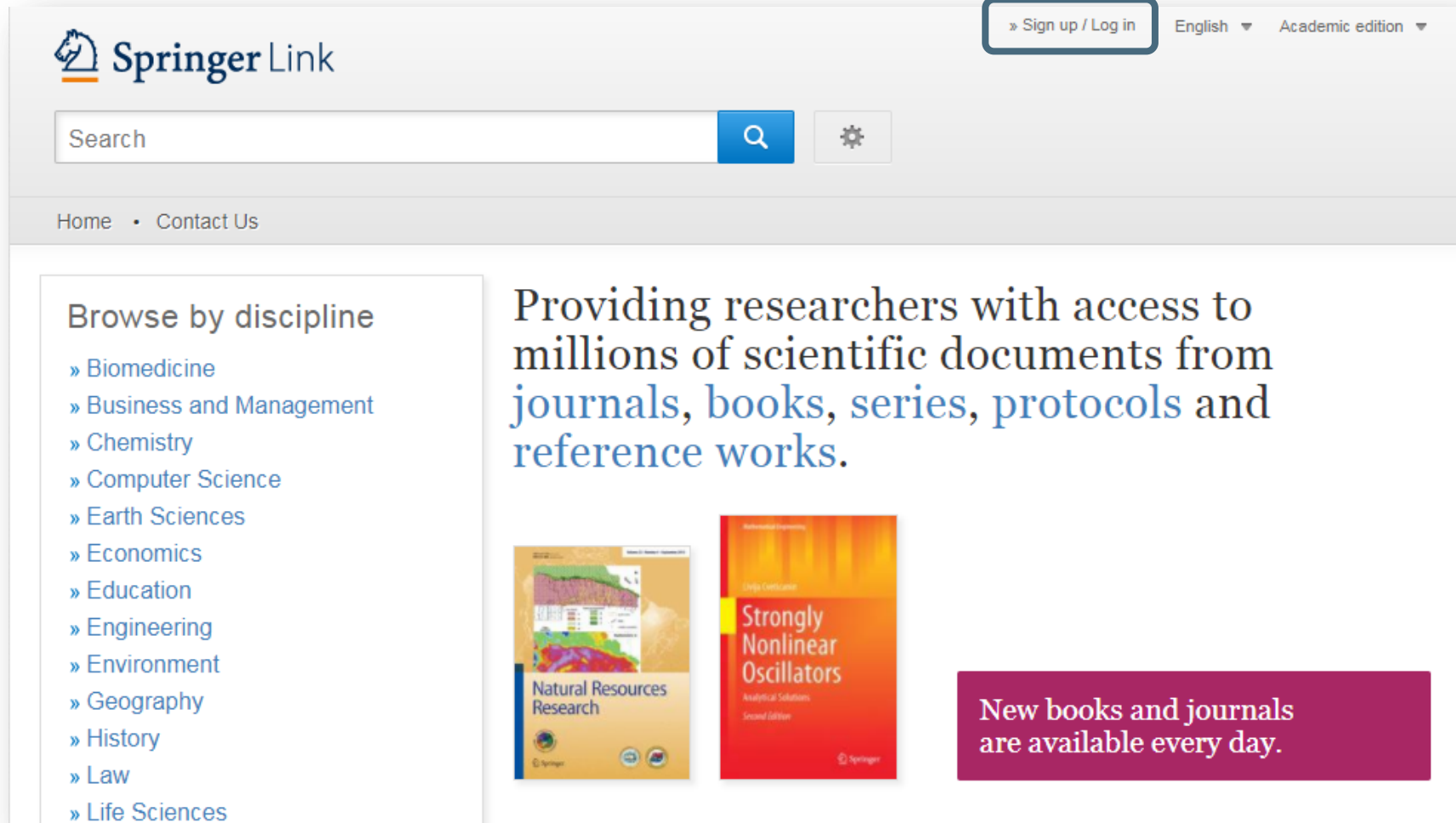
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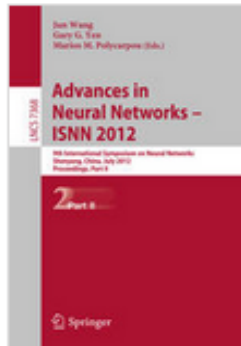
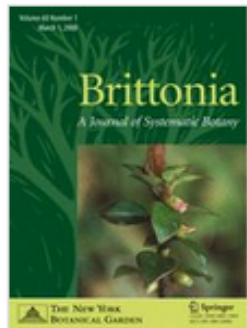
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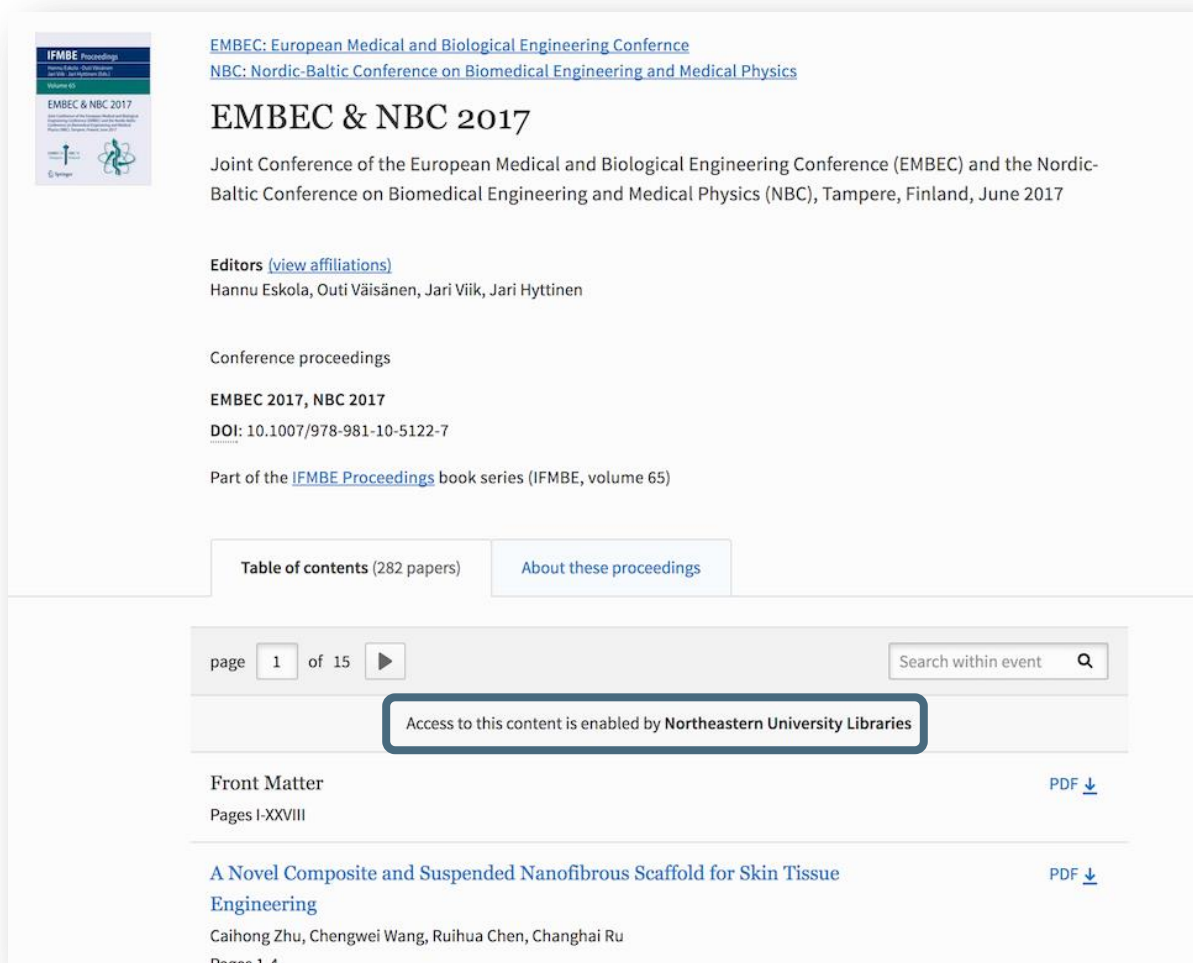
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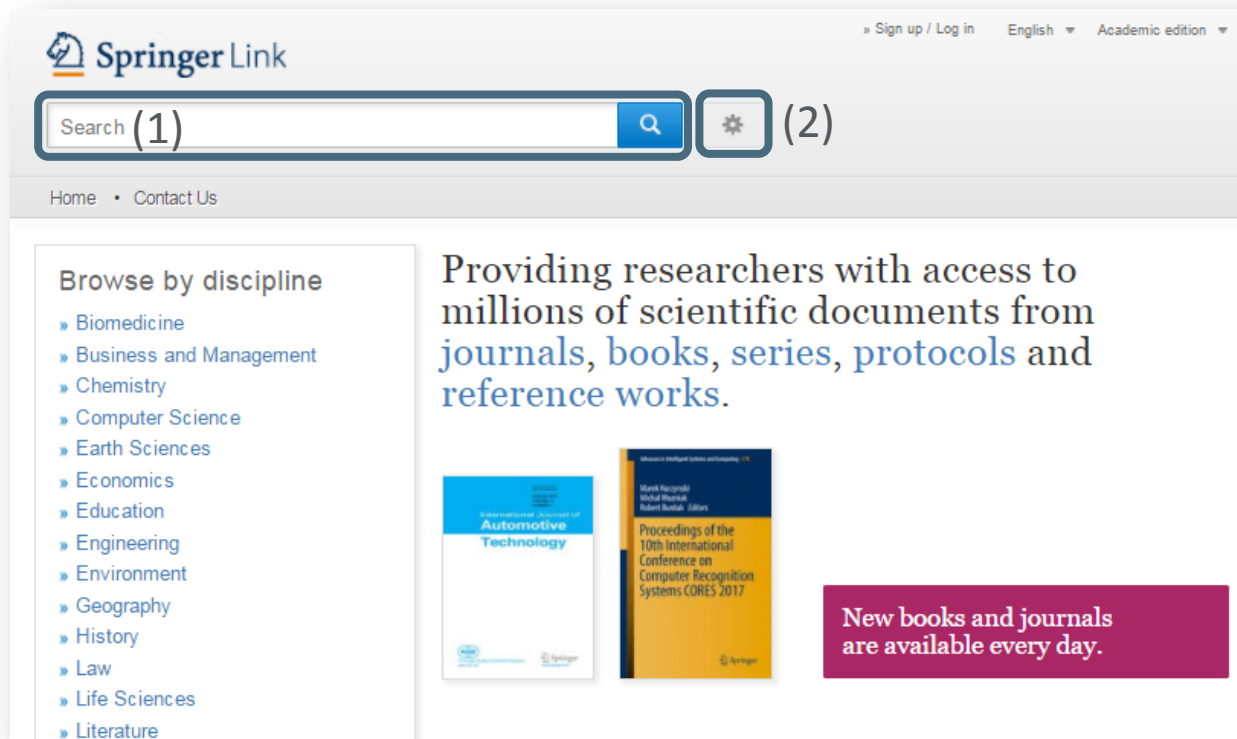
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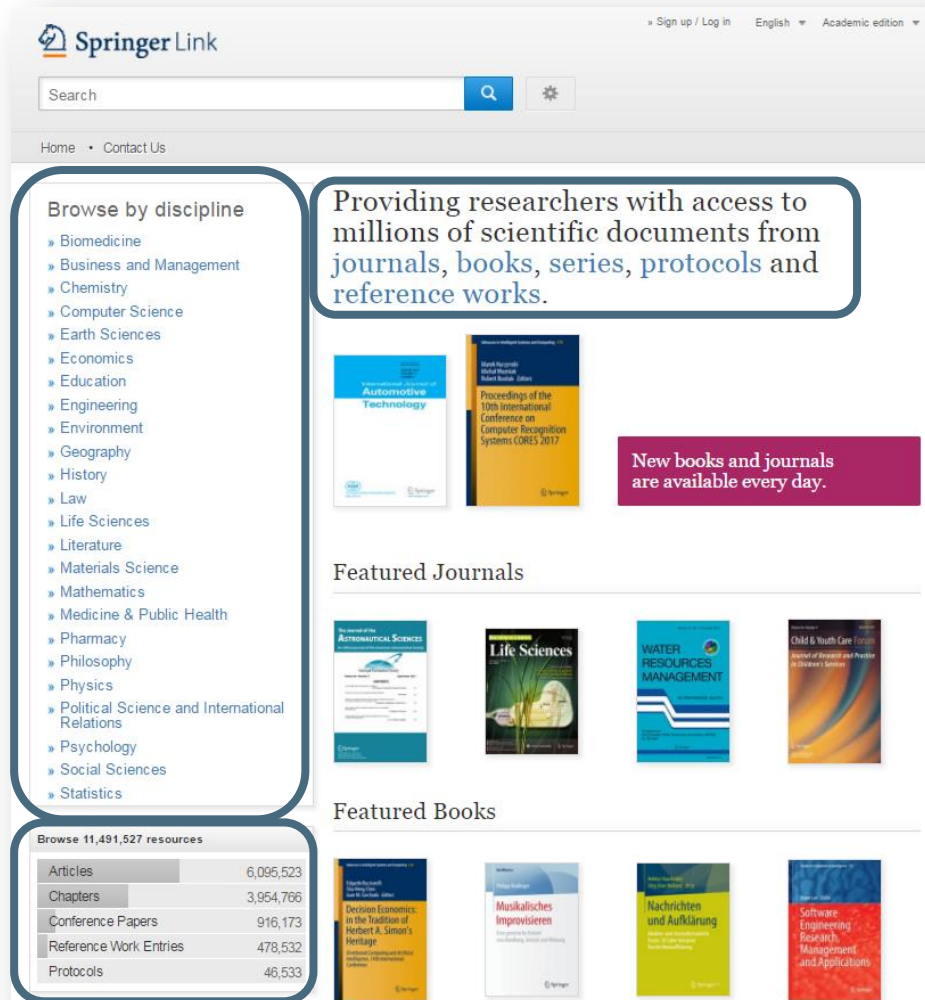
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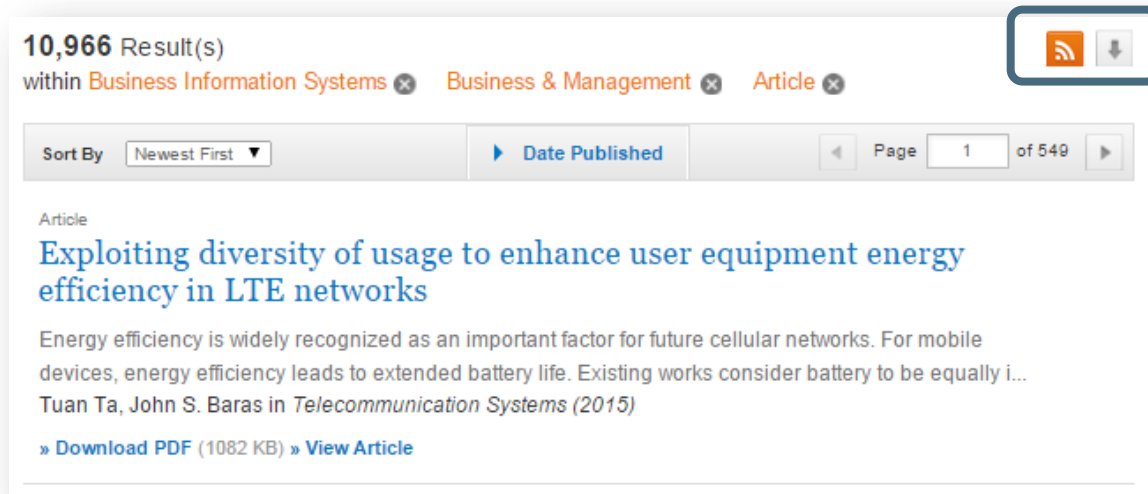
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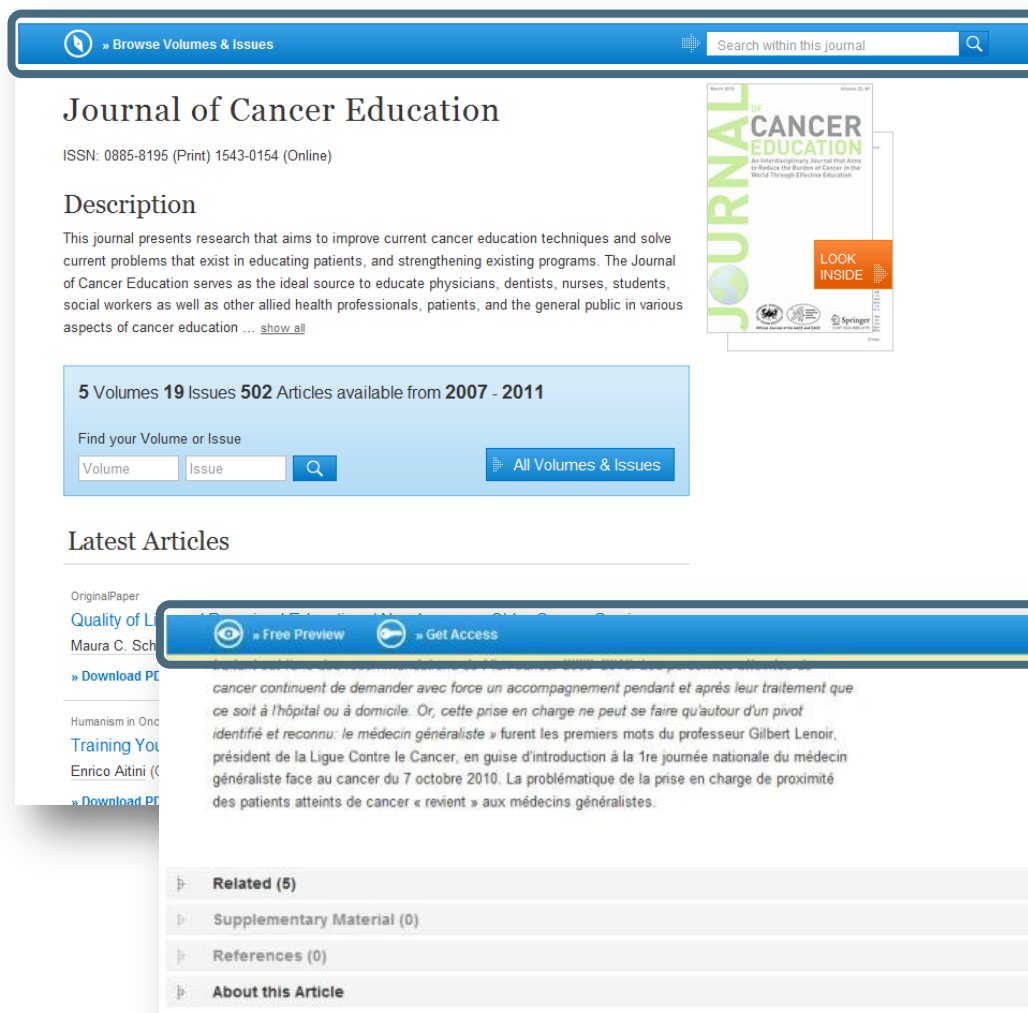
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A Framework for Durability Design with Strain-Hardening Cement-Based Composites (SHCC)

State-of-the-Art Report of the RILEM Technical Committee 240-FDS

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Paul McMahon

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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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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

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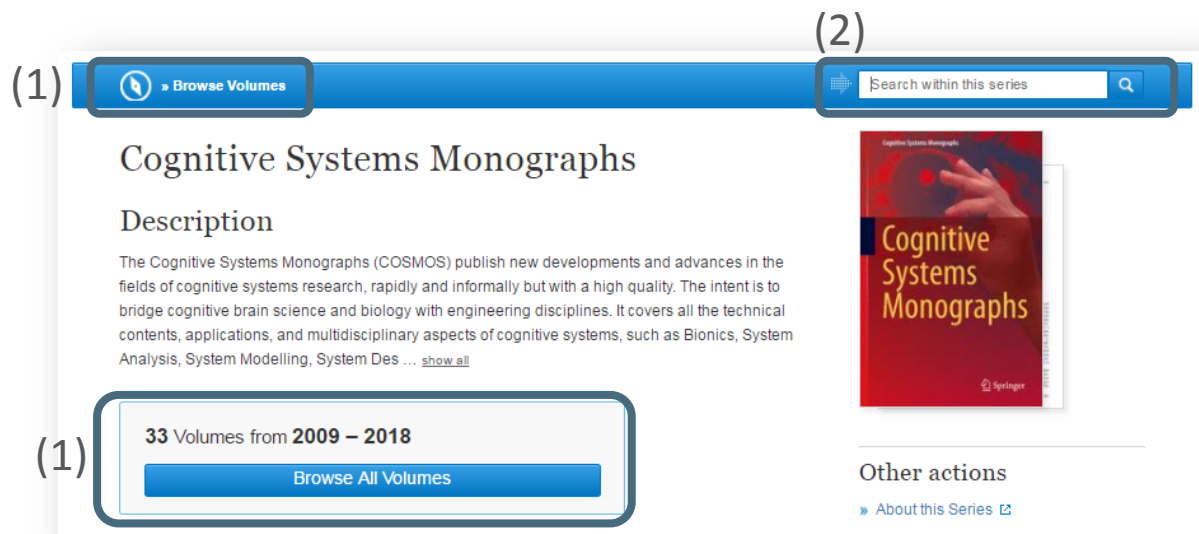
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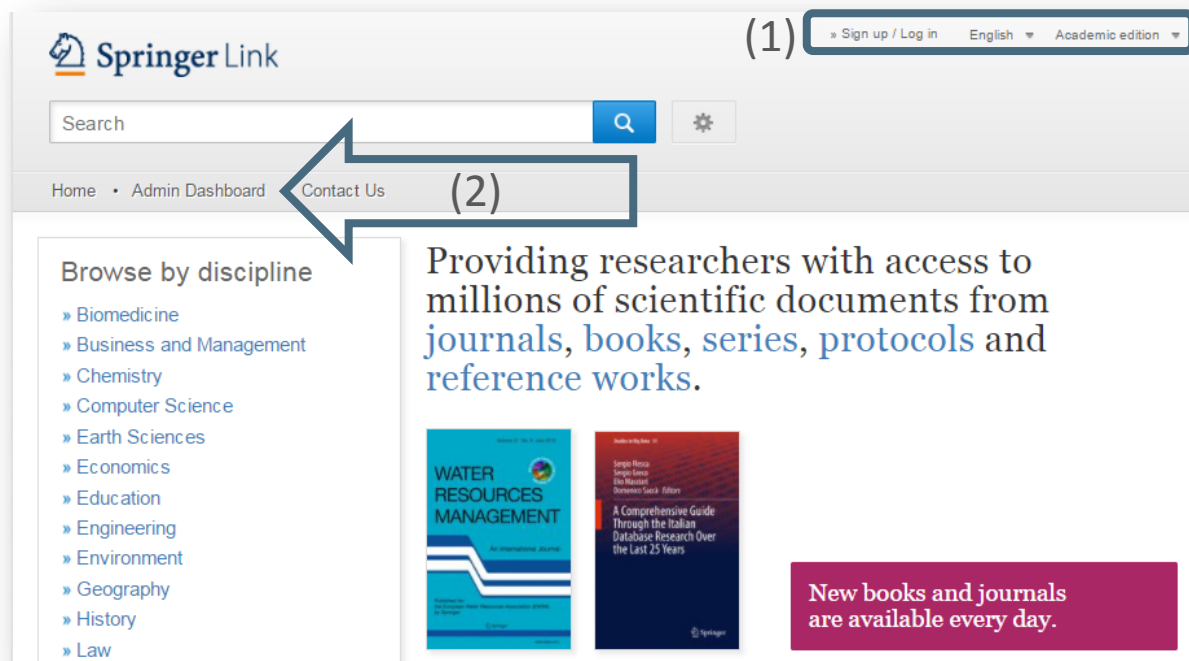
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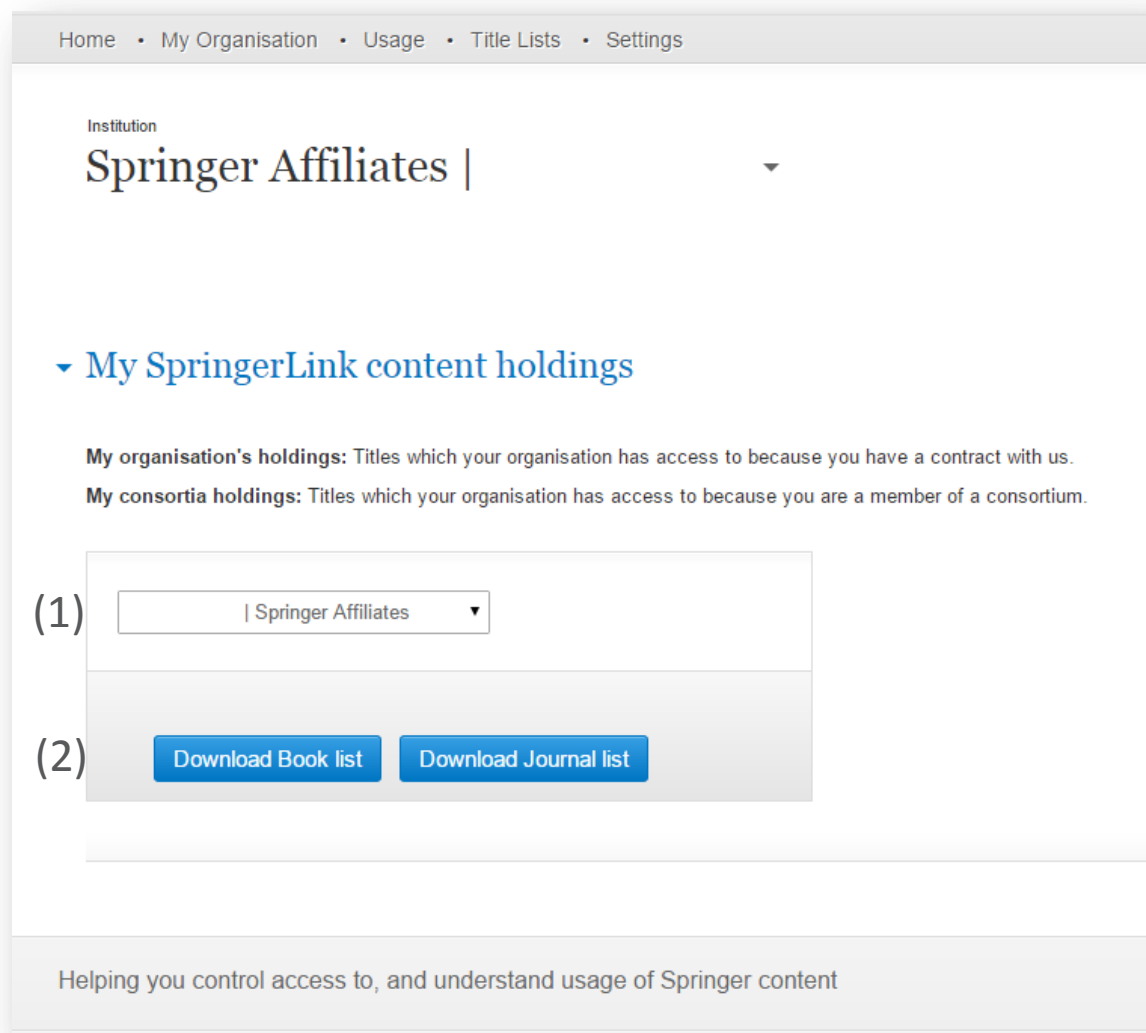
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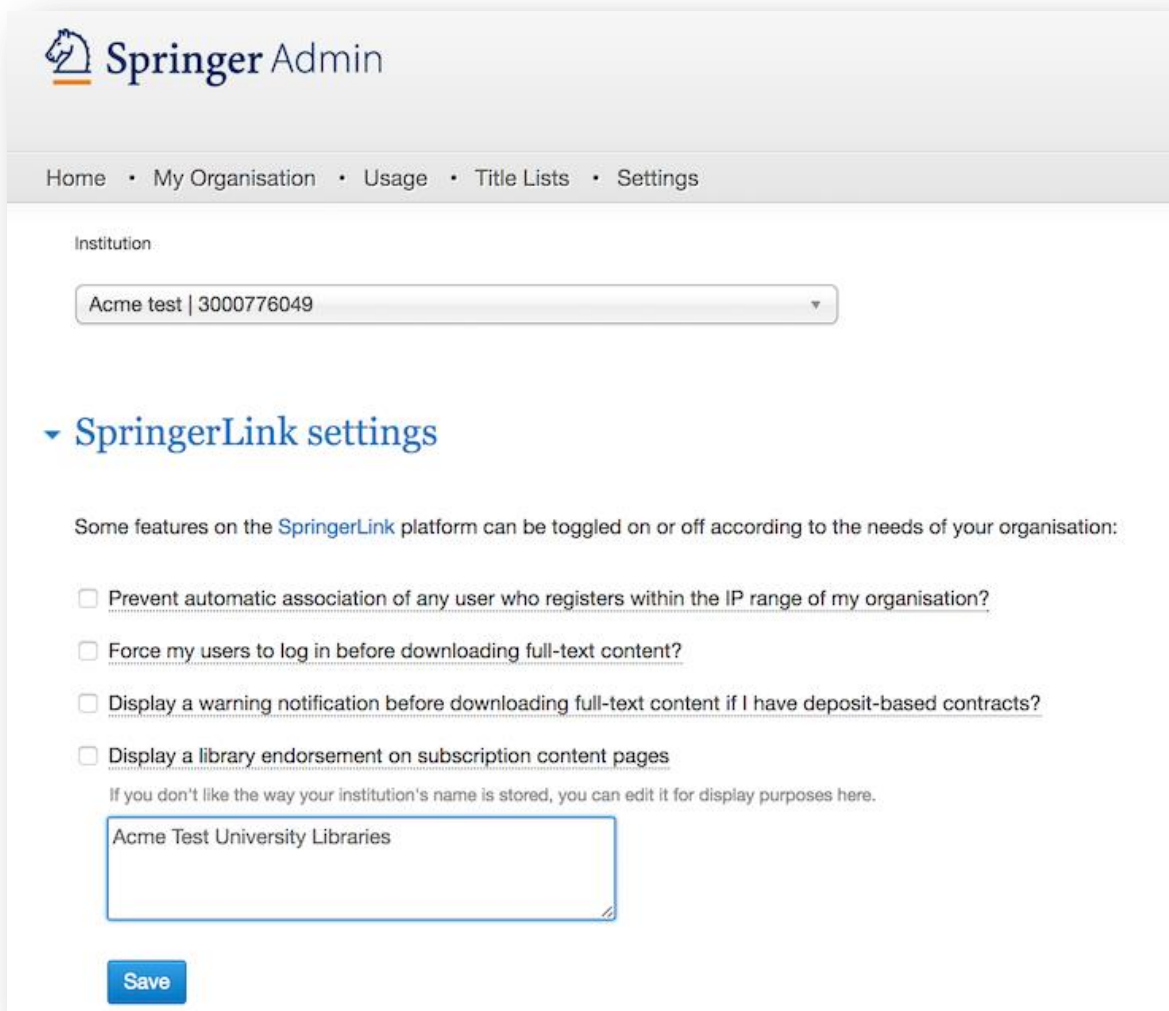
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Title Lists

- 1) 浏览本校或者本联盟的购买内容清单
- 2) 下拉菜单所选产品的贵校已采购清单

管理员账户



The screenshot shows the Springer Admin interface. At the top, there is a header with the Springer logo and the text "Springer Admin". Below the header is a navigation bar with links: Home, My Organisation, Usage, Title Lists, and Settings. The main content area is titled "Institution" and shows a dropdown menu with the selected option "Acme test | 3000776049". Below this, there is a section titled "SpringerLink settings" with a blue arrow icon. The text below this section states: "Some features on the SpringerLink platform can be toggled on or off according to the needs of your organisation:". There are four checkboxes with labels: "Prevent automatic association of any user who registers within the IP range of my organisation?", "Force my users to log in before downloading full-text content?", "Display a warning notification before downloading full-text content if I have deposit-based contracts?", and "Display a library endorsement on subscription content pages". Below these checkboxes, there is a text input field with the value "Acme Test University Libraries" and a "Save" button.

Springer Admin

Home • My Organisation • Usage • Title Lists • Settings

Institution

Acme test | 3000776049

▼ SpringerLink settings

Some features on the SpringerLink platform can be toggled on or off according to the needs of your organisation:

- ☐ Prevent automatic association of any user who registers within the IP range of my organisation?
- ☐ Force my users to log in before downloading full-text content?
- ☐ Display a warning notification before downloading full-text content if I have deposit-based contracts?
- ☐ Display a library endorsement on subscription content pages

If you don't like the way your institution's name is stored, you can edit it for display purposes here.

Acme Test University Libraries

Save

设置栏

当你移动鼠标时，选项会更详细地解释，包括显示机构名称和图书馆品牌。

脚注

- 功能概述

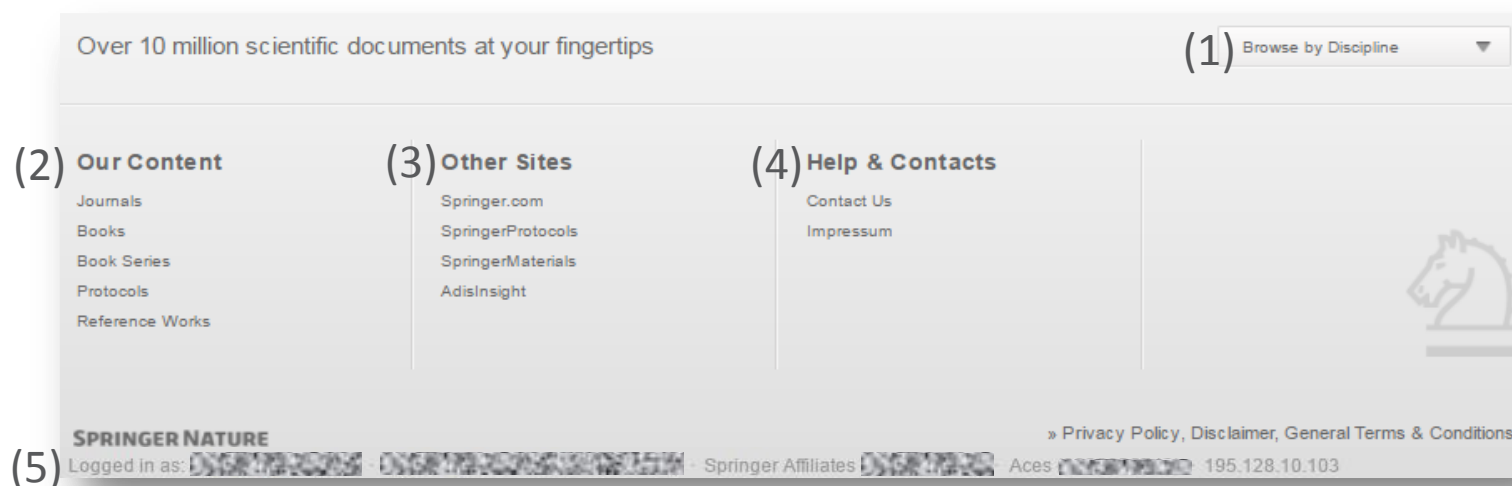
8.0

脚注

概述

浏览内容可分为：

- 1) 行业
- 2) 内容类型
- 3) 其他Springer链接
- 4) 协助和联系方式
- 5) 已认证的机构和商业伙伴的电话号码



Questions?

Visit [springer.com/librarians](https://www.springer.com/librarians) for more information