

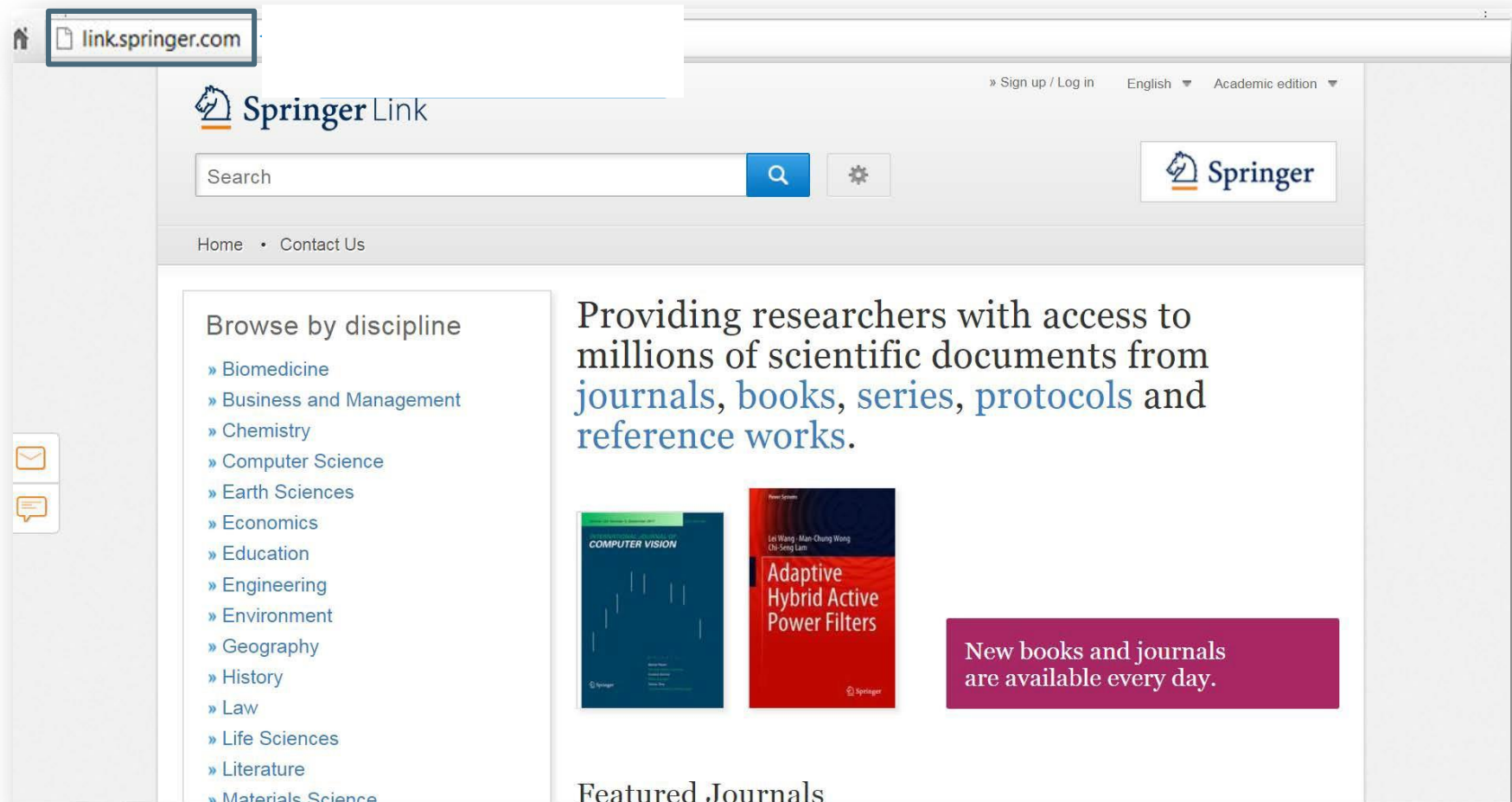
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COMPUTER VISION

Adaptive Hybrid Active Power Filters

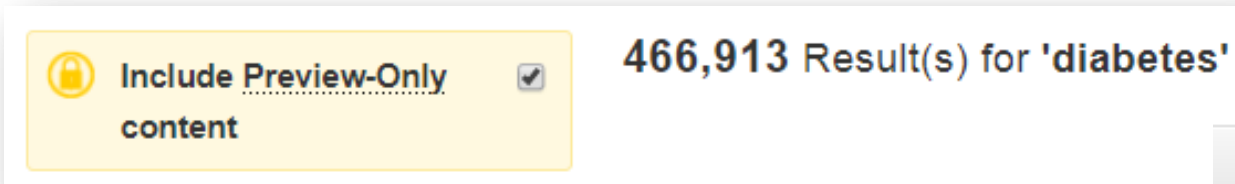
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僅顯示機構有訪問權的查詢
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European Biophysics Journal
October 2012, Volume 41, Issue 10, pp 789-799 | [Cite as](#)

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

Authors Authors and affiliations
Michel Hammel

Open Access | Review
First Online: 26 May 2012

2.2k Downloads 54 Citations

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

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

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Article

Abstract

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Conclusions and prospects

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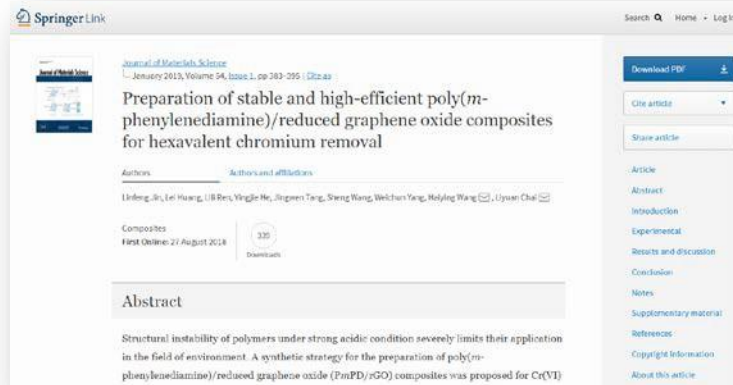
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Abstract

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.

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Tablet



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- (1) Search:** A search bar with a magnifying glass icon and a settings gear icon.
- (2) Browse by discipline:** A list of academic disciplines including Biomedicine, Business and Management, Chemistry, Computer Science, Earth Sciences, Economics, Education, Engineering, Environment, Geography, History, Law, Life Sciences, Literature, Materials Science, Mathematics, Medicine & Public Health, Pharmacy, Philosophy, Physics, Political Science and International Relations, Psychology, Social Sciences, and Statistics.
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Below the featured journals, there is a section for 'Featured Books'.

首頁分成三個部分:

1) 搜索功能

2) 瀏覽功能

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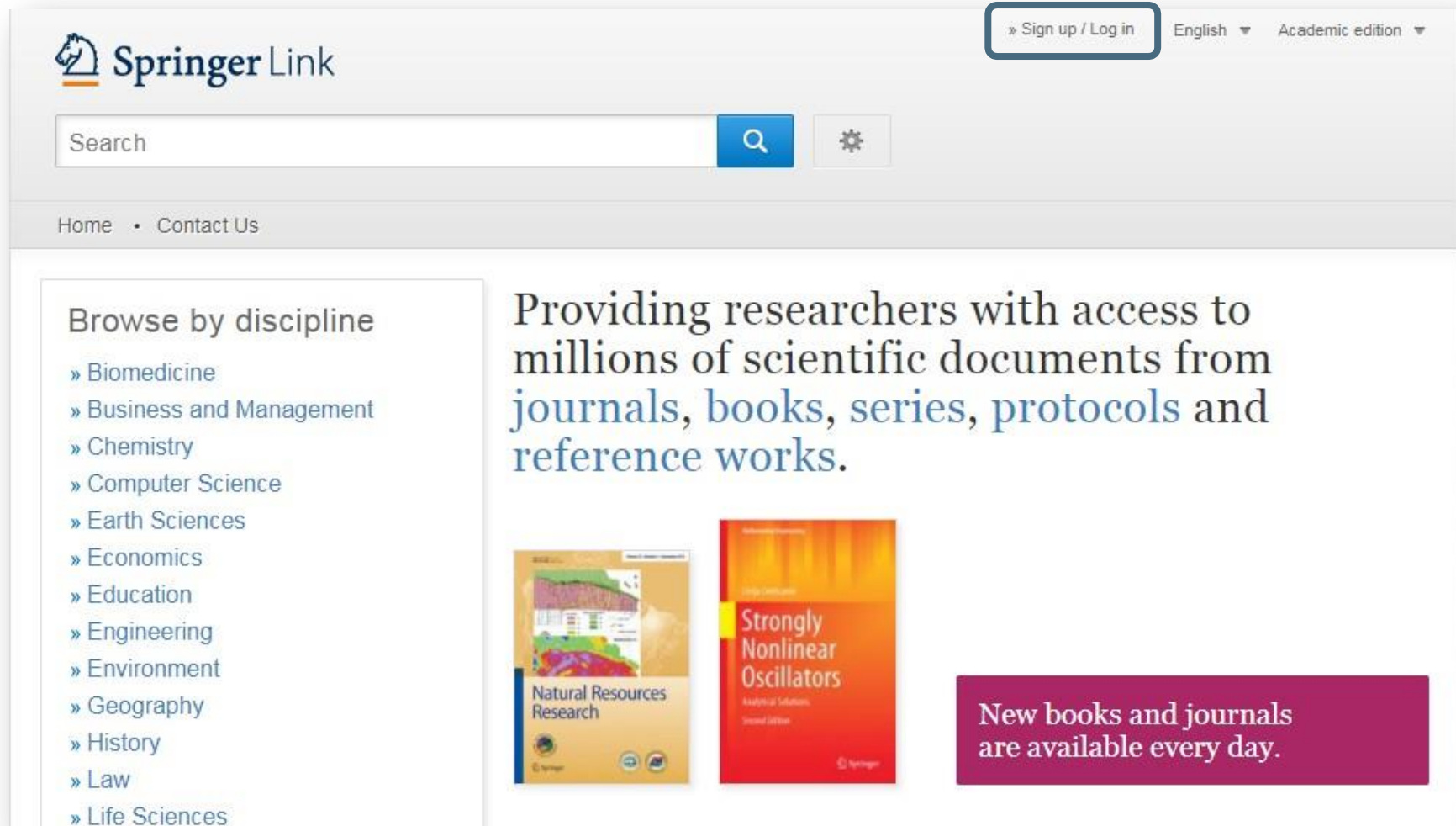
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- » Biomedicine
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- » Economics
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- » Engineering
- » Environment
- » Geography
- » History
- » Law
- » Life Sciences

On the right, a large text block reads: "Providing researchers with access to millions of scientific documents from **journals, books, series, protocols** and reference works." Below this text are two book covers: "Natural Resources Research" and "Strongly Nonlinear Oscillators: Analytical Solutions, Second Edition". To the right of the book covers, a purple box contains the text: "New books and journals are available every day."

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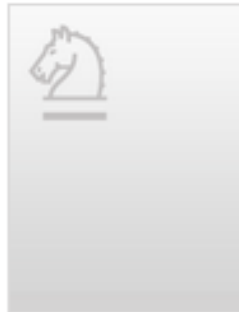
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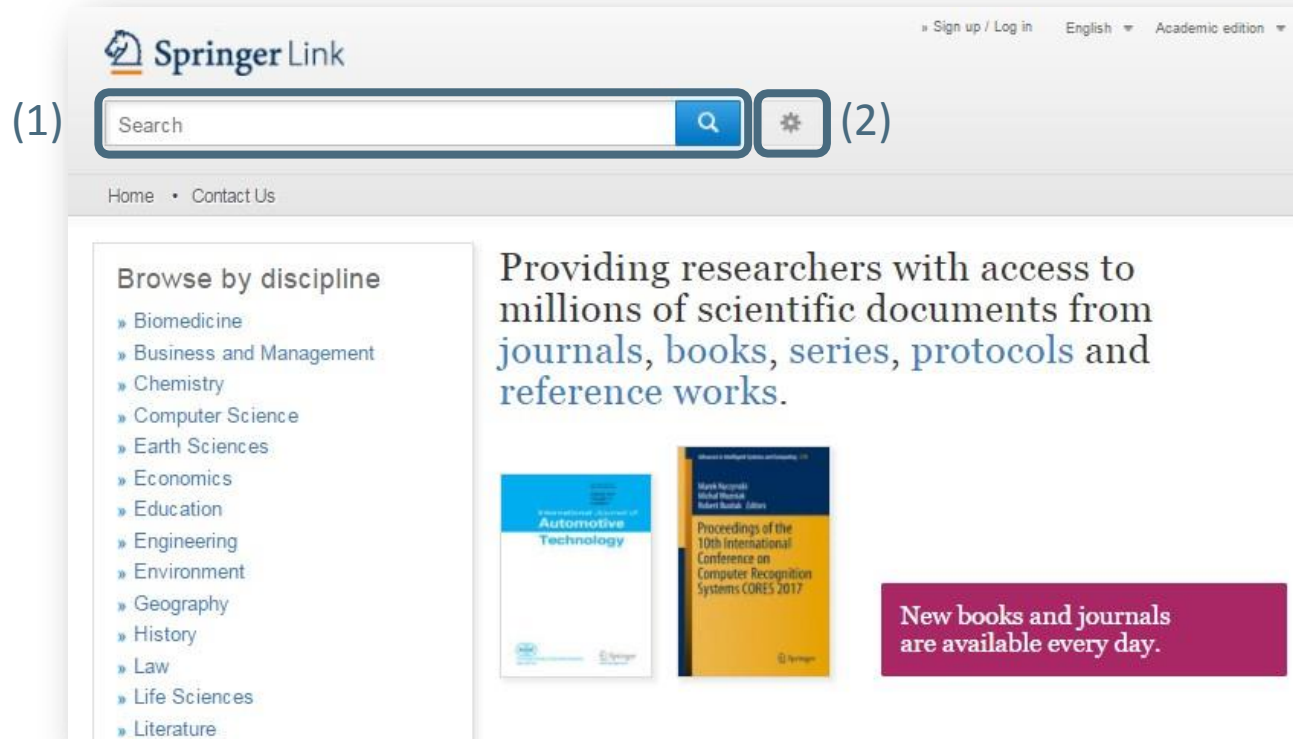


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Springer Link

Search

Home • Contact Us

Advanced Search

Find Resources

with all of the words

with the exact phrase

with at least one of the words

without the words

where the title contains

e.g., "Cassini at Saturn" or Saturn

where the author / editor is

e.g., "H.G.Kennedy" or Elvis Morison

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By default, searches on our site will return only results containing all words entered into the search box, without case sensitivity or spell-checking, and without regard to your access rights to the content.

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- Browse by discipline:** A list of 20 disciplines including Biomedicine, Business and Management, Chemistry, Computer Science, Earth Sciences, Economics, Education, Engineering, Environment, Geography, History, Law, Life Sciences, Literature, Materials Science, Mathematics, Medicine & Public Health, Pharmacy, Philosophy, Physics, Political Science and International Relations, Psychology, Social Sciences, and Statistics.
- Providing researchers with access to millions of scientific documents from journals, books, series, protocols and reference works.** A banner with a blue border.
- New books and journals are available every day.** A purple banner.
- Featured Journals:** A grid of journal covers including 'Journal of Materials Science', 'Advanced Optical Methods for Brain Imaging', 'International Journal of Thermophysics', 'SCIENCE CHINA', 'IEEE TECHNICAL JOURNAL OF TRENDS AND ADVANCE', and 'LMP: Letters in Mathematical Physics'.
- Featured Books:** A grid of book covers including 'Information Technology and Applied Mathematics', 'GCEC 2017', 'Wireless Communication Networks and Internet of Things', and 'Fluid-Structure-Sound Interactions and Control'.
- Browse 12,126,496 resources:** A table showing the number of resources for different document types.

Resource Type	Count
Articles	6,384,670
Chapters	4,157,590
Conference Papers	1,017,082
Reference Work Entries	516,618
Protocols	50,536

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Book	3

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Subdiscipline see all

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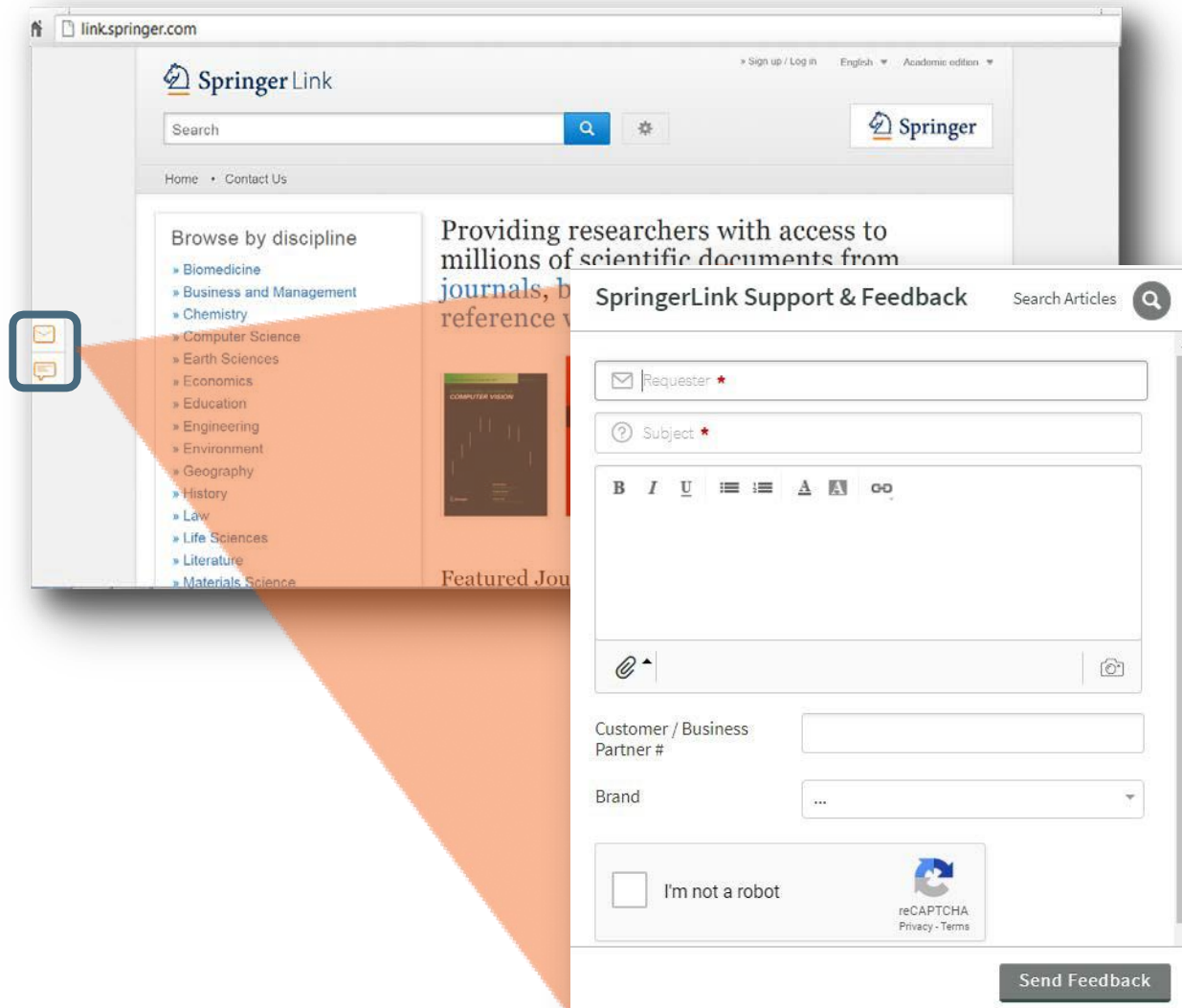
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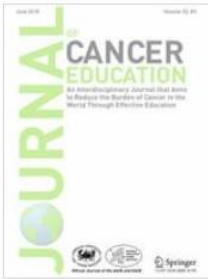
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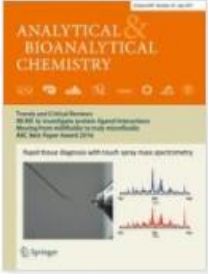
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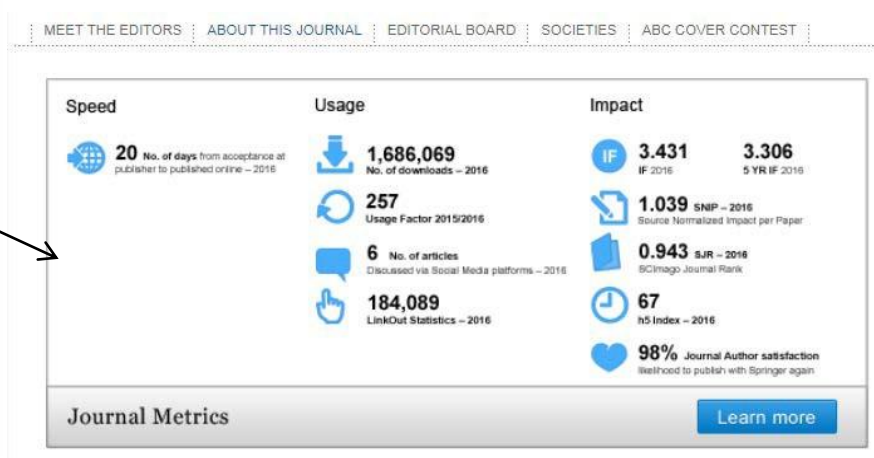
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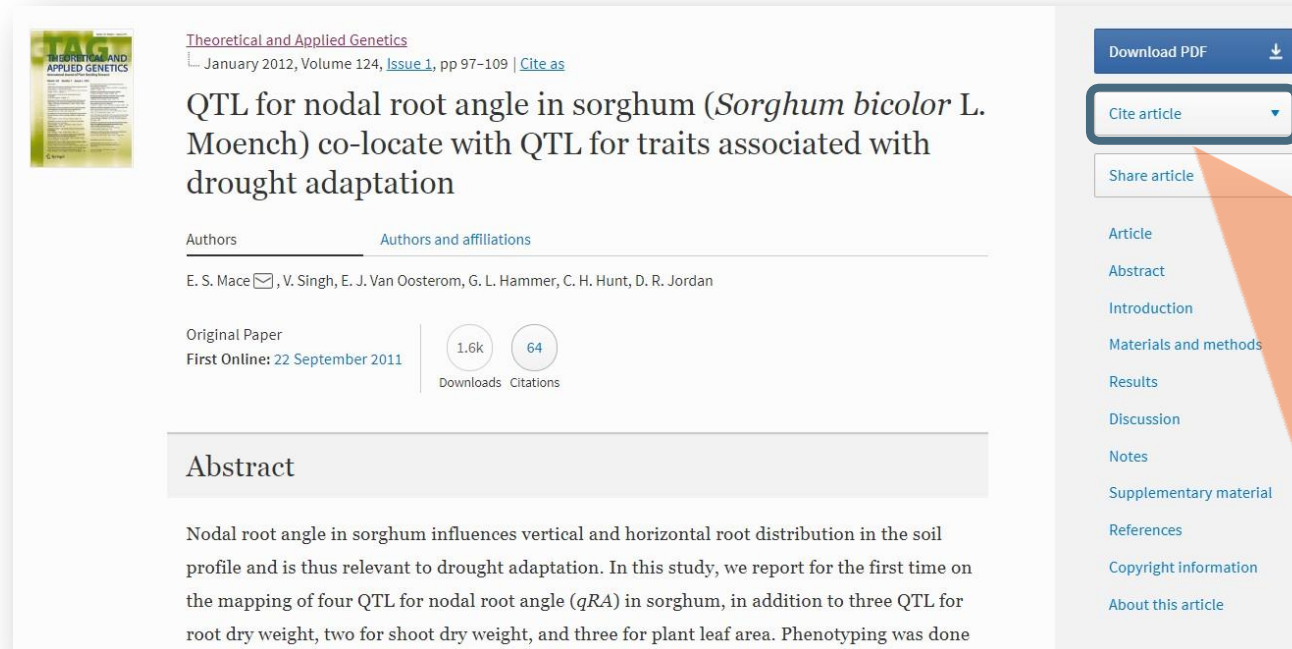
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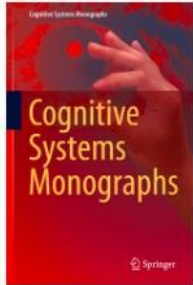
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