

Inovace bakalářského studijního oboru Aplikovaná chemie

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Tento projekt je spolufinancován
Evropským sociálním fondem a státním
rozpočtem České republiky.



evropský
sociální
fond v ČR



EVROPSKÁ UNIE



MINISTERSTVO ŠKOLSTVÍ,
MLÁDEŽE A TĚLOVÝCHOVY



OP Vzdělávání
pro konkurenceschopnost



OKRESNÍ HOSPODÁŘSKÁ
KOMORA OLMOUC

INVESTICE DO ROZVOJE VZDĚLÁVÁNÍ

Odborný článek

Garant: Prof. RNDr. Michal Otyepka, Ph.D.

Vede seminář: Prof. RNDr. Michal Otyepka, Ph.D.

Cvičící: Mgr. Martin Pykal

Odborný článek

- forma vědeckého sdělení
- formát a struktura jsou dané redakcí
- připravuje se ve formě „rukopisu“ (manuscript)

Odborný článek

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- odeslání do odborné redakce (submission)
 - editor (určuje recenzenty), může rukopis vrátit autorům
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- komunikace s tech. redakcí

Recenzní řízení

- recenzní řízení do jisté míry zaručuje (a ověřuje) kvalitu a relevanci publikovaných dat
- „retracted paper“
 - WIKIPEDIA: „In science, a retraction of a published scientific article indicates that the original article should not have been published and that its data and conclusions should not be used as part of the foundation for future research. The common reasons for the retraction of articles are scientific misconduct and serious error.“

Retracted papers (wiki)

- **Retraction for error**

- **2006** Makarova, T. L. et al. *Nature* 413, 716-718 (2001). Set of inconsistencies triggered fraud investigation against first author, but after long investigation all mistakes were admitted by appointed experts as undeliberate and result of negligence or inaccuracy. The paper was retracted by other 7 co-authors. See also Corrigendum published few months prior to retraction where first author admitted personal responsibility for some mistakes. [\[1\]](#)
- **2005** V. Schramke et al. "Retraction: RNA-interference-directed chromatin modification coupled to RNA polymerase II transcription" in *Nature* (volume 437, page 1057). Irreproducible results.
- **2005** R. C. Allshire. "Retraction. Hairpin RNAs and retrotransposon LTRs effect RNAi and chromatin-based gene silencing" in *Science* (volume 310, page 49). Irreproducible results.

Retracted papers (wiki)

- **Retraction for fraud or misconduct**

- **2007** Retraction of several articles written by social psychologist [Jennifer Lerner](#) and colleagues from journals including [Personality and Social Psychology Bulletin](#) and [Biological Psychiatry](#). A graduate student had fabricated data.
- **2006** Retraction of *Patient-specific embryonic stem cells derived from human SCNT blastocysts*. written by [Hwang Woo-Suk](#). Fabrications in the field of stem cell research led to 'indictment on embezzlement and bioethics law violations linked to faked stem cell research'.
- **2003** Numerous articles with questionable data from physicist [Jan Hendrik Schön](#) from many journals including both [Science](#) and [Nature](#) are retracted.

Ukázky podle Am. Chem. Soc.



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Informace pro autory



THE JOURNAL OF
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Information for Authors of Papers (Revised January 2011)

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Typy článků

Articles should report original research that is expected to have a definable impact on the advancement of science and technology. Manuscripts should cover their subjects with thoroughness and clarity but should be as concise as possible. Articles are scheduled for publication in the order of acceptance within limitations of available space. A table of contents (TOC) graphic is required for use in the Web edition of the journal.

Feature Articles are usually published by invitation. However, Authors in important active research fields of interest to physical chemists are encouraged to propose such articles.

Two-page proposals should be sent to the Managing Editor (d_minton@acs.org) for consideration. The Author should provide a clear, concise, and critical status report of the field as an Introduction to the article. The Author's own contribution and its relationship to other work in the field should constitute the main body of the article. Controversies, if they exist, should also be outlined. Possible future directions and the significance of the research area to the field of physical chemistry should be pointed out. Feature Articles are limited to ~8 printed pages (equivalent to ~40 pages of manuscript with figures, tables, references, and double-space-typed text). A brief biography for each Author of the Feature Article should be included. A TOC graphic is required for use in the Web edition of the journal.

Review Articles are on active and rapidly changing fields. They are ~8 pages long (~40 typed pages). Authors are encouraged to submit two-page proposals to the Managing Editor (d_minton@acs.org) for consideration. A brief biography for each Author of the Review Article should be included. A TOC graphic is required for use in the Web edition of the journal.

Comments are significant remarks on work previously published (usually in *JPC A/B/C*) and are restricted to approximately one page (1000 words or equivalent) including tables, figures, and text. There is no abstract. Comments are subject to critical review. If the Comments are concerned with the work of other Authors, the Editors will generally permit these Authors to reply if approved by the Reviewers.

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Special Issues are published throughout the year. These issues can be a Memorial, a Festschrift, or a collection of papers from a Symposium. *JPC A/B/C* also publishes Special Sections, which

Odeslání do redakce

SUBMISSION OF MANUSCRIPTS

Manuscripts must be submitted via the ACS Paragon Plus Environment (<http://paragonplus.acs.org/login>). Complete instructions and an overview of the electronic

The screenshot shows the ACS Paragon Plus Environment submission interface. The browser window title is "ScholarOne Manuscripts - Windows Internet Explorer". The address bar shows the URL "https://acs.manuscriptcentral.com/acs". The page header includes "ACS PUBLICATIONS HIGH QUALITY. HIGH IMPACT." and "ACS PARAGON PLUS ENVIRONMENT". The user is logged in as "Dr. Michal Otyepka". The main content area displays "Personal publishing activity for Dr. Michal Otyepka" with links for "Edit Your Account" and "Log Out". Below this, there is a section for "To submit a NEW manuscript" with a dropdown menu for "Select a journal..." and a "GO" button. A "My Authoring Activity" section shows a list of manuscript statuses: 1 Invited Manuscript, 0 Incomplete Manuscript Submissions, 0 Unsubmitted Manuscripts, 0 Submitted to Editorial Office, 0 Forms Awaiting Completion, 0 Revisions and Resubmissions Requested by Editorial Office, 0 Incomplete Revisions and Resubmissions, 0 Revisions and Resubmissions Received by Editorial Office, 0 Accepted Manuscripts, 0 Proof Ready for Review, 0 Proof Comments Received, 0 Expired Revisions and Manuscripts No Longer Under Consideration, and 6 Recently Published Articles. A sidebar on the right provides "Authoring & Review Support" links: "Submission & Authoring in ACS Paragon Plus", "Peer Review in ACS Paragon Plus", "Tools & Forms for ACS Paragon Plus", and "System Requirements for ACS Paragon Plus".

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Multiple Reporting of Research. It is improper for an Author to submit manuscripts describing essentially the same research to more than one journal.

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Coauthorship. The submitting Author must obtain consent of coauthorship from all Coauthors listed prior to submitting the manuscript and must include as Coauthors all individuals who made significant scientific contributions to the work. Any disagreement between the Corresponding Author and Coauthor(s) after submission will cause review of the manuscript to cease. Removal or addition of Coauthor(s) after submission of the manuscript requires confirmation in writing by the respective Coauthor(s).

The complete document “Ethical Guidelines to Publication of Chemical Research” is available via <http://pubs.acs.org/ethics>.

Information on the ACS Journal Publishing Agreement may be found below in the section entitled “Journal Publishing Agreement” and at <http://pubs.acs.org/page/4authors/jpa/index.html>.

Příprava rukopisu

Manuscript Format

Manuscripts must be prepared using accepted word-processing software, and all parts must be double-spaced. All pages must be numbered consecutively starting with the title page and including tables and figures. A standard font, in a size of 12 points or greater, must be used. Templates and instructions for software, including Tex/LaTex, are available on the Web.

Standard American English usage is required. Authors who are not familiar with standard American English are urged to seek assistance; deficiencies in grammar may be a serious hindrance during the review process. For more information, Authors may visit the [Language Editing Services](#) listed under the Publishing Tools tab of the Author & Reviewer Resource Center.

The ACS Style Guide (3rd ed., 2006; ISBN 13:9780841239999) is available from <http://pubs.acs.org/page/books/index.html>. The Third Edition is the definitive source for all information needed to write, review, submit, and edit scholarly and scientific manuscripts. Refer to a current issue of the Journals for general style.

Příprava rukopisu

The various sections of the manuscript should be assembled in the following sequence:

- Title, Authorship, and Affiliations (single page)
- Author Biographies (Feature Articles & Review Articles)
- Abstract and Keywords (single page)
- Introduction
- Experimental Methods
- Results
- Discussion
- Conclusions
- Acknowledgment/Dedication
- Supporting Information Description
- References
- Tables
- Figure Captions
- Figures
- Table of Contents Image
- [Supporting Information: submitted as separate files and not repeated in the manuscript (proposed cover art images should be submitted as Supporting Information for Review Only)]

Příprava rukopisu

Title

The title should be specific and informative. Keywords in the title assist in effective literature retrieval. The title, authorship, and institutional affiliations should be included on a single page.

Authorship

Be consistent in authorship designation on the manuscript and on all correspondence. First name, middle initial, and last name are needed for correct identification, but omit titles. Give the complete mailing address of the institution where the work was conducted and identify the affiliation of each Author. If the current address of an Author is different, include it in a footnote on the title page. The Corresponding Author to whom inquiries about the paper should be addressed must be marked with an asterisk; provide the telephone number, fax number, and e-mail address of this correspondent.

Author Biographies

Feature Articles and Review Articles include a brief biography for each Author of the paper. Biographies should contain approximately four to five sentences describing the Author's education, previous and current positions, and scientific interests. Photograph(s) are optional but are welcome. Photos of Authors posed individually are acceptable; however, if more than five Authors wish to include photographs, a group picture is required. Biographies (and photographs) are to be submitted as part of the manuscript.

Abstract

The abstract should be a clear, concise, one paragraph summary (100–150 words). It should be informative rather than descriptive, giving scope, purpose, experimental approach, significant

Příprava rukopisu

Keywords

Identify four to six keywords to assist in indexing your paper, and list these on a separate line beginning with “Keywords” on the abstract page. Do not use words contained in the title.

Introduction

Discuss relationships of the study to previously published work, but do not reiterate or attempt to provide a complete literature survey. The purpose or reason for the research being reported and its significance, originality, or contribution to new knowledge in the field should be clearly and concisely stated. Do not include or summarize current findings in this section.

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General Information. Complicated chemical equations, schemes, and structures should be supplied as furnished artwork, ready for publication. Schemes and charts should be numbered consecutively with Arabic numbers. Mathematical expressions and chemical formulas with unavailable symbols and letters should be clearly identified. Capital, lowercase, and Greek letters should be easily discernible or identified if ambiguity might result. Complicated superscripts and subscripts should be avoided. Fractional exponents should be used instead of root signs.

Authors should consult a current copy of the Journal and [*The ACS Style Guide*](#) for examples of style and general recommendations. See also: Mills, I.; et al. *Quantities, Units and Symbols in Physical Chemistry*, 2nd ed.; Blackwell Scientific Publications: Oxford, U.K., 1993.

Hazards. Any unusual hazards in the chemicals, equipment, or procedures used in an investigation should be clearly identified.

Příprava rukopisu

Results/Discussion

Results and Discussion may be presented in separate sections or combined into a single section, whichever format conveys the results in the most lucid fashion. The Author should discuss the significance of observations, measurements, or computations and should also point out how they contribute to the scientific objectives indicated in the Introduction.

Conclusions

A brief summary should be given for the principal conclusions of the work.

Acknowledgment/Dedication

Acknowledgments of financial assistance for the conduct of research, citations of theses, or indications of presentation at a research meeting should be brief and placed in this section.

Dedications are not generally recommended and must reference scientific contributions without being overtly personal. Statements deemed inappropriately personal will be removed by the Journal office staff. If a dedication is included in a manuscript, the Author needs to notify the Journal office in the cover letter. In the case of a Dedication for a Special Issue, the Author should refrain from starting the Dedication with “Dedicated to the honoree on the occasion of ...”

Příprava rukopisu

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Unnecessarily long lists of references, including excessive self-citation, are to be avoided; however, Authors must provide references to all relevant publications in which portions of the present work have appeared. Citation of recent papers published in physical chemistry and chemical physics journals that highlight the significance of work to the general readership is encouraged.

Journal references should contain author names, abbreviated journal title, year, volume, and pages (first–last). An example is provided below.

Habenicht, B. F.; Prezhdo, O. V. *J. Phys. Chem. C* 2009, 113, 14067–14070.

Book references should contain author names, book title (written in title case), publisher, city, and year. An example is provided below.

Datta, S. *Electronic Transport in Mesoscopic Systems*; Cambridge University Press: Cambridge, U.K., 1995.

In literature references, journal abbreviations should be those used by Chemical Abstracts Service [see *Chemical Abstracts Service Source Index (CASSI) 1907–2004*]. For references to *JPC A/B/C*, part A, B, or C must be specified for papers published in 1997 forward.

Příprava rukopisu

Tables

Tables should be numbered consecutively with Arabic numbers. Each table must have a brief title that describes its contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Tables should be used when the data cannot be presented clearly as narrative, when many numbers must be presented, or when more meaningful interrelationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise.

Column headings should be lowercase, except for symbols and proper names. Define nonstandard abbreviations in footnotes. Footnotes in tables should be given letter designations and be cited in the table by italic superscript letters. The sequence of letters should proceed by line rather than by column. If a reference is cited both in the text and in a table, a lettered footnote that refers to the numbered reference in the text should be inserted in the table.

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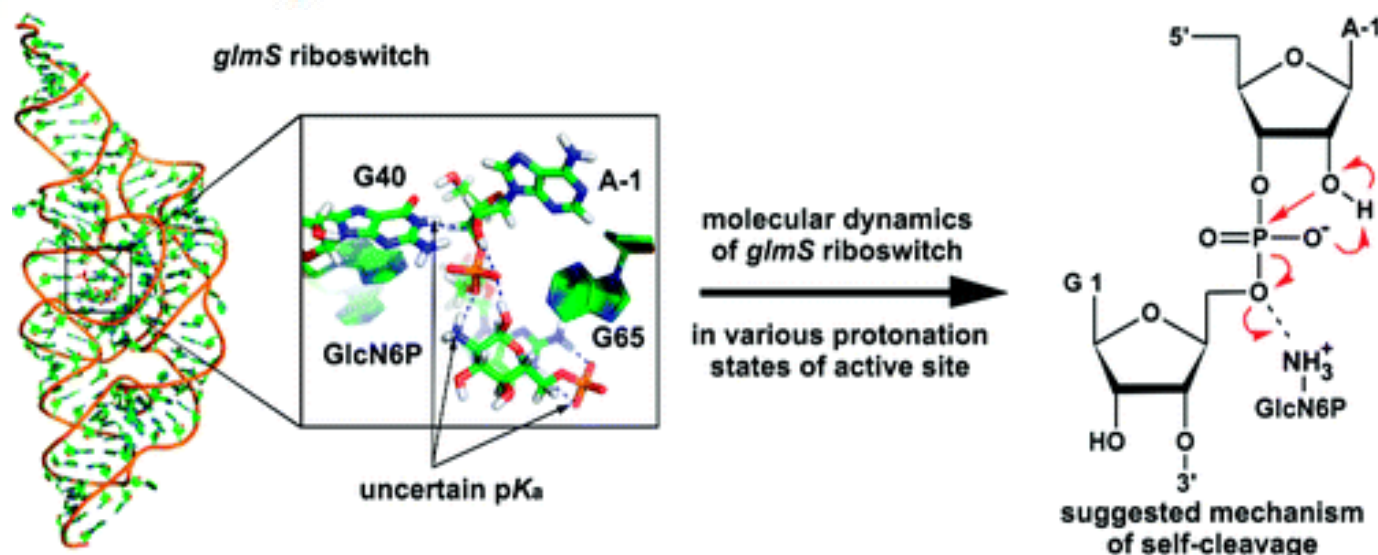
Figures

All figures must be mentioned in the text in consecutive order and must be numbered with Arabic numbers. If symbols are used, it is preferable to place a key in the artwork itself, not in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the figures. Remove all color from graphics, except those graphics to be considered for publication in color. See more detailed information on submission of graphics under [Artwork](#) below.

Příprava rukopisu

Table of Contents (TOC) Image

A TOC graphic is required for Articles, Feature Articles, and Review Articles. TOC graphics will appear only in the Web edition of the journal. The illustration should capture the Reader's attention and, in conjunction with the manuscript title, should give the Reader a quick visual impression of the essence of the paper without providing specific results. The graphic should be in the form of a structure, graphical image, photograph, reaction scheme, or equation. The Author must submit the graphic in the actual size to be used for the TOC, fitting in an area 1.375 in. high and 3.5 in. wide (3.6 cm × 8.9 cm). Larger images will be reduced to fit within those dimensions. The type size of labels and other symbols within the graphic must be legible. Tables and spectra are not acceptable. Provide the TOC graphic upon submission of the paper as the last page of the manuscript.



Příprava rukopisu

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	single (preferred)	double
width		
minimum		10.5 cm (4.13 in.)
maximum	8.25 cm (3.25 in.)	17.78 cm (7 in.)
maximum depth	24 cm (9.5 in.)	24 cm (9.5 in.)

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Příprava rukopisu

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fixed length	14.4 pt (0.508 cm, 0.2 in.)
bold width	2.0 pt (0.071 cm, 0.0278 in.)
line width	0.6 pt (0.021 cm, 0.0084 in.)
margin width	1.6 pt (0.056 cm, 0.0222 in.)
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(2) As text settings select:

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size	10 pt

(3) Under the preferences choose:

Units	points
Tolerances	5 pixels

(4) Under page setup choose:

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**Inovace bakalářského studijního
oboru Aplikovaná chemie**

Cíle odborného článku

- sdělit komunitě své poznatky, myšlenky, představit nové výsledky
- ucelené pojednání
- úvod
 - zasazuje do širšího kontextu
 - uvádí motivaci a cíle práce
- metody
 - velmi stručně, ale zásadní postupy jsou uvedeny (podle metod by se měly dát výsledky reprodukovat)

Cíle odborného článku

- Výsledky
 - přehled a popis dosažených výsledků, využívají se grafy a tabulky
- Diskuze
 - na začátku se zopakuje motivace
 - rozbor dosažených výsledků, jejich souvislosti, soulad/nesoulad s hypotézami a dostupnou literaturou
- Závěr(y)
 - stručné shrnutí nejvýznamnějších zjištění a výsledků

Protonation States of the Key Active Site Residues and Structural Dynamics of the *glmS* Riboswitch As Revealed by Molecular Dynamics

Pavel Banáš,^{†,‡} Nils G. Walter,[§] Jiří Šponer,^{*,†,‡} and Michal Otyepka^{*,†,‡}

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The *glmS* catalytic riboswitch is part of the 5′-untranslated region of mRNAs encoding glucosamine-6-phosphate (GlcN6P) synthetase (*glmS*) in numerous Gram-positive bacteria. Binding of the cofactor GlcN6P induces site-specific self-cleavage of the RNA. However, the detailed reaction mechanism as well as the protonation state of the *glmS* reactive form still remains elusive. To probe the dominant protonation states of key active site residues, we carried out explicit solvent molecular dynamic simulations involving various protonation states of three crucial active site moieties observed in the available crystal structures: (i) guanine G40 (following the *Thermoanaerobacter tengcongensis* numbering), (ii) the GlcN6P amino/ammonium group, and (iii) the GlcN6P phosphate moiety. We found that a deprotonated G40[−] seems incompatible with the observed *glmS* active site architecture. Our data suggest that the canonical form of G40 plays a structural role by stabilizing an in-line attack conformation of the cleavage site A-1(2′-OH) nucleophile, rather than a more direct chemical role. In addition, we observe weakened cofactor binding upon protonation of the GlcN6P phosphate moiety, which explains the experimentally observed increase in K_m with decreasing pH. Finally, we discuss a possible role of cofactor binding and its interaction with the G65 and G1 purines in structural stabilization of the A-1(2′-OH) in-line attack conformation. On the basis of the identified dominant protonation state of the reaction precursor, we propose a hypothesis of the self-cleavage mechanism in which A-1(2′-OH) is activated as a nucleophile by the G1(*pro*-R_p) nonbridging oxygen of the scissile phosphate, whereas the ammonium group of GlcN6P acts as the general acid protonating the G1(O5′) leaving group.

Introduction

Riboswitches are RNA motifs embedded in messenger RNAs (mRNAs) that regulate gene expression in response to binding

5′-OH termini of the reaction products. The same general mechanism is found in all ribozymes classified as “small” with typically less than 100 nucleotides in the catalytic core, yet the details of how the reaction participants are activated differ

Ukázka

protonation states of the essential residues in the AS. MD is suitable to suggest the protonation states of the critical nucleobases corresponding to the crystalline conditions. This was previously shown, for example, for protonated cytosines in a HDV ribozyme and a frameshifting pseudoknot.^{50,55} The aim of our simulations is to suggest dominant protonation states of AS residues, to describe the cofactor binding, and to study the dynamic behavior of AS to get ideas about the plausible reaction state. In particular, our data indicate that G40 is not deprotonated and likely plays a structural role in stabilizing the in-line attack conformation of the cleavage site A-1(2'-OH). We propose that A-1(2'-OH) could be activated as the nucleophile by the G1(*pro-R_p*) nonbridging oxygen of the scissile phosphate, whereas the ammonium group of GlcN6P acts as the general acid that neutralizes the leaving group 5'-oxygen (to avoid any confusion, we will further use terms *pro-S_p* for O1P and *pro-R_p* for O2P nonbridging oxygens according to IUPAC terminology). The presented results should be considered within the context of common limitations (mentioned above) of the contemporary simulation methods.

Methods

Preparation of Starting Structures. The starting geometries were based on the currently available crystal structures. The native

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Supporting Information Available: The content of the Supporting Information includes force field parameters of nonstandard residues, a detailed analysis of the structural dynamic of the *glmS* riboswitch active site, details of the structural dynamics of the *glmS* riboswitch without cofactor, analysis of constant-pH MD simulations using implicit solvent methods, and some other material. This material is available free of charge via the Internet at <http://pubs.acs.org>.

References and Notes

- (1) Mandal, M.; Boese, B.; Barrick, J. E.; Winkler, W. C.; Breaker, R. R. *Cell* **2003**, *113*, 577.
- (2) Tucker, B. J.; Breaker, R. R. *Curr. Opin. Struct. Biol.* **2005**, *15*, 342.
- (3) Winkler, W. C.; Breaker, R. R. *Annu. Rev. Microbiol.* **2005**, *59*, 487.

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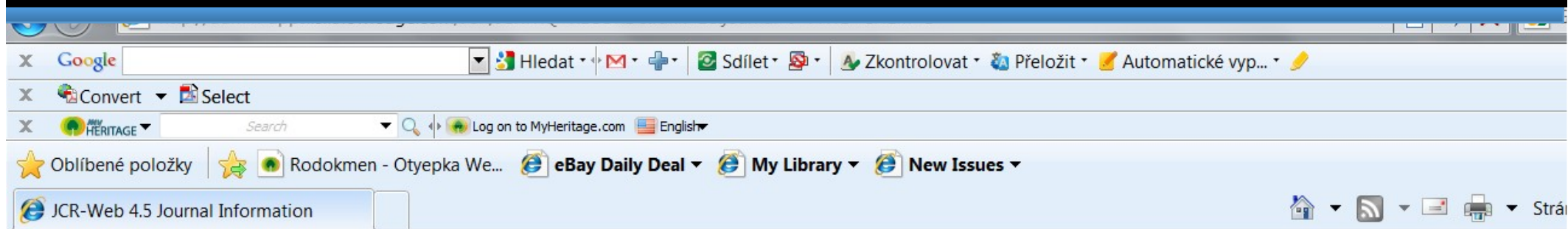
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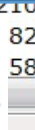
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