EHzürich

Infozine No. 22

The Magazine for Users of Scientific Information

Information Center in lockdown – but not locked

As the Information Center had developed its plan for the pandemic quite early, there were no issues at all, when the first staff member started working from home already on March 6, 2020. All services were and are continued, except the working and learning spaces which are mostly used by students. It is almost business as usual. only with very short distances from bed to work. We continue to order books and develop our holdings, also to support our mid-sized suppliers. Nevertheless, we are very much looking forward to hopefully reopening the doors of the Information *Center soon, to be a busy place again,* where all learning spaces are used, and communication is not only through Zoom or Skype. We are hoping that also Infozine No. 22 provides you with useful suggestions and information. Many of us are using this time to clean out the house (the corona pandemic is generating record figures of eBay classifieds). Thus, this edition has also some tips for tidying up. We are *looking forward to seeing you – online* - at the 20th series of our Coffee Lectures.

Enjoy reading Infozine No. 22. Your Chemistry | Biology | Pharmacy Information Center.

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2020 is STM Research Data Year

For centuries, researchers have shared their research output through articles in scientific journals, research output that is based on data. For the integrity of research, sharing data is fundamental. But sharing data is also a crucial part of the Open Science concept, as more than ever, research data can be a valuable resource for other scientists. Thus, there is increasing need to ensure the availability, discoverability and re-usability of research data for all stakeholders working across scholarly communications. STM, the International Association of Scientific, Technical and Medical Publishers, has therefore declared 2020 the STM Research Data Year and is working with publishers and others to boost effective sharing of research data:

- SHARE: Increase the number of journals with data policies and articles with Data Availability Statements (DAS)
- LINK: Increase the number of journals that deposit the data links to the SCHOLIX framework
- **CITE:** Increase the citations to datasets along the Joint Declaration of Data Citation Principles



Sharing of research data (those which is worth to be shared!) must be based on the **FAIR** Principles, its needs to be Findable, Accessible, Interoperable and Re-usable (FAIR) both for machines and humans. This is clearly both a challenge and an ongoing process for researchers and publishers and has led to the instigation of several supporting initiatives. Working with publishers and research groups, FAIRsharing.org has co-curated a database of standards, policies and databases. As a result, their website provides an excellent overview of data repositories that journals can recommend to their authors. The database currently consists of a directory of 1460 databases where researchers can upload and share research data. For those interested in the topic, this is the original publication on the FAIR principles: Wilkinson et al. (2016), The FAIR Guiding Principles for scientific data management and stewardship, Scientific Data 3, doi:10.1038/sdata.2016.18.

News from the ETH Library

News from the ETH Library

Visible Body on OVID

Would you like to learn more about basic body functions, physiological processes or common diseases? *Anatomy & Function* and *Physiology Animations* are two new modules from Visible Body that help you understand human biology in detail. You can rotate, zoom in and dissect all the 3D models for a better view.



Thanks to the module *Muscle Premium*, you can examine muscle movements in detail and also expand your knowledge about common injuries and illnesses. Musculoskeletal structures and functions become vivid and comprehensible in 3D animations with rotation and zoom functions. You can also test what you have learned with 1,000 quiz questions.

You can find more medical content on the website of the ETH Library under Resources sorted by subject.

Frankfurter Allgemeine Zeitung

The Frankfurter Allgemeine Zeitung is one of the leading newspapers in Germany. Members of ETH Zurich are now able to access all editions of Frankfurter Allgemeine Zeitung through FAZ Biblionet (but not directly at www.faz.net) dating back to the newspaper's first publication in 1949. Alongside PDF copies of the single pages, featuring the original layout, images and graphics, the individual articles are also available as text-only and PDF files. Once an individual account has been created, readers can also set up watch lists and email notifications for saved search queries.

Frankfurter Allgemeine



In addition, the license also allows access to *Frankfurter Allgemeine* Sonntagszeitung (issues since 1993), all *FAZ.NET* online articles (since 2001), articles featured in the magazines *F.A.Z.-Woche*, *Frankfurter Allgemeine* Quarterly and *Frankfurter Allgemeine* Metropol since 2016), as well as articles appearing in the newspaper's digital magazine *F.A.Z. Einspruch* (since November 2017).



ETH Library pays open access fees for COVID-19 pandemic related articles

ETH Library supports the dissemination of knowledge related to the COVID-19 pandemic. Researchers at ETH Zurich can now apply for special open access funding, which the library makes available during the COVID-19 pandemic.

The funding covers open access fees for articles in Gold open access journals and in Hybrid journals. The research depicted in funded articles has to be related to the current crisis. This includes all aspects related to the COVID-19 pandemics such as medical, economic, policy and social studies.

The requirement for funding is for the first or corresponding author of the article to be a member of ETH Zurich. More information on how to proceed can be found here.

New E-Journals

Die ETH Library has subscribed to the following scientific journals:

- The American Journal of Surgical Pathology
- Praxis: Schweizerische Rundschau für Medizin
- Project Management Journal
- Gastronomica The Journal of Critical Food Studies
- Nature Food



Coffee Lectures at ETH Library

ETH Library is offering now again Coffee Lectures. Their Coffee Lectures take place at 15:15 on Wednesday afternoon and last 10 minutes. The topics for this spring semester are:

- How to use the new PubMed, May 27, 2020
- Unpaywall & Co. read research papers for free, June 3, 2020
- eresearchcenter your portal for standards (DIN, ISO, and others), June 10, 2020
- Be aware: predatory publishers, June 17, 2020
- Creative Commons how to license your publications and research data for reuse, June 24, 2020

Registration is not required. These are online sessions held via Zoom: https://ethz.zoom.us/j/99585769649



Durable Lego bricks

In your home office you might stumble over Lego bricks from time to time. Did you know that Lego bricks can survive in the sea for up to 1300 years? A publication by the University of Plymouth in *Environmental Pollution* compared the mass of individual bricks found on beaches with unused new bricks and estimated that they could survive between 100 and 1,300 years.

SciFinderⁿ (1): ChemPlanner

The first implementation of Sci-Finderⁿ's synthesis planning tool Chem-Planner could only handle literatureknown compounds ("experimental mode") and was therefore mainly a tool for exploring different synthetic approaches. Now ChemPlanner also features a "predictive mode" (right figure), which means it can draw analogies from similar reactions, adapt them to unknown problems and rank the different solutions. For each step, the output contains a list of potential disconnections, including links to references and expected yield. These abilities could be useful for generating new, non-obvious ideas.

However, if you want to perform a head-to-head comparison of synthetic routes, the AI-driven planner is still a black box of limited use. No basis for the ranking order is provided, *e.g.* reactions with low precedence and moderate yields may have a good ranking, while other promising candidates may have a bad ranking.



As shown in a recent CAS video (https://t1p.de/t3sc), a number of different criteria are used behind the scenes to assess synthetic routes. Among them are complexity reduction, availability and cost of starting materials, overall yields, confidence with respect to literature, convergence and waste.

In order to be more than a tool for ideation and thinking of alternatives, ChemPlanner must become more transparent and provide detailed information on the ranking process as well as additional options to analyse the results. This way, chemists will be able to assess and compare the proposed steps and eventually take informed decisions. The chemical literature is an exponentially growing pile of papers. With more transparency, ChemPlanner has the potential to help us deal with this information overload. Otherwise, the tool may just remain an interesting gimmick.





Clarivate Integrity becomes Cortellis Drug Discovery Intelligence

Researchers at ETH Zurich are in a unique position because they can get access to a drug pipeline database with information on drugs under development: Clarivate's Integrity. The database has been rebranded at the beginning of the year and is now called Cortellis Drug Discovery Intelligence.

Web interface and chemical structure editor have received the long-awaited overhaul, and now one can draw structures with modern, embedded editors such as ChemDraw JS, Marvin JS or Elemental. This update is accompanied by a slightly changed user philosophy with differences in functionality. It seems that due to a lesser degree of linking, possibilities for traditional pharmaceutical type problems have slightly deteriorated, whereas the tool might have become more adept at addressing structure related questions. Only time will tell, if these suspicions are correct (figure above).

Those who already had accounts in the previous Integrity and have not changed yet to Cortellis, should check out their Mailbox for access data and have a look at this documentation.

Cortellis

Cortellis Drug Discovery Intelligence Glossary and Help File

A limited number of seats is still available. If you are interested, please do get in touch with Dr. Oliver Renn.

English Edition

SciFinderⁿ(2): New Features

Since last December, SciFinderⁿ has added a number of useful new features. Check here (https://t1p.de/fta0) for the complete list.

The possibility to combine saved search queries with Boolean operations (AND, OR, NOT) and then set alerts for the resulting query can be a big timesaver. Instead of combining static answer sets, already the questions can be combined and can be rerun periodically to find new hits. Previously, one had to manually select all the hits returned by a search and save them, which was cumbersome with large hit sets. A "save all hits" option is still missing.

There is a new filter "Non-Participating Functional Groups" to search for reactions wherein certain additional structural motives survive the reaction conditions.

The filter "concepts" was extended to MeSH terms and MEDLINE supplementary concepts. Previously, only CAplus concepts were available.

The use of wildcards and phrase search was extended from abstracts only to also include concepts and chemical names.

Substances can be sorted by molecular weight, by their registry number or by the number of respective publications. This function had disappeared with the transition from the old SciFinder and is now available again.

It is now possible to perform structure searches for deuterium (D) and tritium (T). In substructures, these nuclides may be attached to single-atom variables, but not to generic groups.



When reading Infozine online – on screen – you can click or tap on the blue hyperlinks to go to the references.

Happy Birthday SoS

Science of Synthesis (SoS) celebrates its 20th anniversary this year. In the year 2000. SoS started out both in print as well as online. SoS has permanently filled a gap in the organic chemistry database world with curated and regularly updated content, and their unique hierarchical organization according to functional groups. Once or twice a year, SoS releases what they call "Special Topics" volumes. These stand-alone books provide current and comprehensive reviews on selected areas of interest. The latest volumes are already available online: "Organoboron Chemistry" https://t1p.de/t6t3 and "Dual Catalysis" https://t1p.de/oz8m.



KnowItAll AnyWare goes Wiley

At ETH Zurich, you have access to the spectral database KnowItAll AnyWare via the Information Center. KnowItAll provides a variety of spectra: proton and carbon NMR, IR, Raman, MS and UV-VIS are covered. Key features are the search for specific peaks and upload of spectra for identifying unknown substances as well as spectral mixture analysis. Bio-Rad, the provider of KnowItAll was recently acquired by large publisher Wiley. Let's hope that the database will now finally receive a well-deserved makeover of the old-fashioned user interface.

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How to search for information on COVID 19 or SARS-CoV-2 with Qinsight

If you are working on a treatment or a vaccine against SARS-CoV-2, or are just generally interested, you may want to use Qinsight, the AI-based biomedical Search Engine. Quertle, the provider of Qinsight – which has been licensed for ETH Zurich by us – has put up some suggestions for your literature discovery on Qinsight's web site:

- SARS-CoV-2 is the official name of the virus. Qinsight will automatically find all the older names as well, such as 2019-nCoV. Since SARS-CoV-2 is the sole cause of the disease COVID-19, a search for the virus will also bring up articles about the disease.
- **COVID-19** is the official name of the **disease** caused by SARS-CoV-2. Use this search term when you want to focus on the aspects of the disease rather than the biology of the causative virus.
- Coronaviruses in general may be useful to look at for comparison. Qinsight will recognize all CoV strains. You could also look for the genus **Betacoronaviruses** (group 2) or the subgenus **Sarbecovirus** containing SARS-CoV-2.

For some additional advice on how to use Qinsight to discover more about COVID-19 and related concepts, Quertle has put together an informal 26.5 min-webinar on the Quertle YouTube site: Qinsight[™] COVID-19 webinar (you may need to put this in YouTube's Theatre Mode for better quality). This covers general coronavirus searching, drug repurposing, and finding new targets (and has an added bonus at the end of the video – due to its having been created in home office).

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opnMINER – a free semantic search tool from Boehringer Ingelheim

opnMINER is a free semantic search tool from the pharmaceutical company Boehringer Ingelheim for searching information on therapeutic properties of pharmaceutical substances, chemicals and biologics in PubMed Central, Medline, patents (EPO, USPTO, WIPO), Expression Data, FDA's Drug Labels, NIH grant applications, and Clinical Trials. One of its strongest features is that it performs a full-text search using concepts and subconcepts rather than just simple text.

opnMINER offers three search strategies: Basic Search, Compound Search, and Search for Co-occurrences.

Basic Search retrieves documents that contain the search terms. If a search term is part of the opnMINER knowledge domains (chemistry, companies, diseases, drugs, effects, methods, proteins, species, polymers, and toxicology), the search automatically includes all the synonyms and sub-concepts; otherwise, the search returns resources with exactly matched terms. For example, searching for coronavirus infections in the NIH grants from 2019 and 2020 results in 12 documents that contain the term in the full text, and 7 documents where the term is present in the abstract.

Compound search features Marvin JS that enables drawing of chemical compounds. Substructure and similarity searches are also possible. The result is a compound hit list providing quick access to the documents that contain the searched structure.

The Search for Co-occurrences allows searching for sentences that contain two concepts of interest. For example, if you are interested in the relation between *inhibition of microtubule polymerization or depolymerization* and *cancer* you can put those in the search fields Concept 1 and Concept 2, and select a repository, e.g. PubMed Central. The result is a graphical representation, depicting the frequency of these co-occurrences by the size of the nodes in the interaction map. While the interaction map is interesting for exploring the relationships between different concepts and sub-concepts, the frequencies alone can be misleading and should not be compared, as not all the co-occurrences are equally meaningful. The sentences that gave rise to the co-occurrences are listed beneath the graph, unfortunately without links to the respective publications. OpnMINER is part of OpnMe, the Open Innovation Portal of Boehringer Ingelheim. There you will also find **Molecules for free.** Collaborations for Science. In the spirit of collaboration, our molecules are provided to the scientific community to help unlock and fulfil their full potential. These molecules are either freely available or applied for via scientific research submissions. Also, scientific experts are enlisted for advice on key biologic issues.



Open Access: Agreement with Springer Nature

After one and a half years of negotiations, swissuniversities and Springer Nature have now signed a Memorandum of Understanding for a new Read & Publish agreement. Authors in Switzerland will have the option to publish their articles in more than 2.200 hybrid journals - as long as their research institution is part of the Swiss swissuniversities. consortium The articles will be immediately and freely accessible from the point of publication. In addition, researchers will have access to all research results published on SpringerLink. The contract with Springer Nature is to be signed by summer 2020.

SPRINGER NATURE

swissuniversities

Next level Open Access: Open Peer Review for RCS Chemical Biology

In April 2020, *RSC Chemical Biology* was launched as a Gold Open Access journal (no APCs until mid-2022). For the first time, authors may opt voluntarily for publishing the complete peer review process under a CC BY 4.0 license. Referees will remain anonymous, unless they choose to sign their referee reports.

The first issue of the journal is comprised of three articles, only one of which contains the referee reports. Ironically, it's not the contribution by editorial board chair Hiroaki Suga.

Having peer review reports publicly available is not only a great step for open science, but in the long run it might also have tremendous benefits for teaching critical reviewing skills and the scientific method to students and young researchers.

Publishing Open Access in Elsevier journals

Academics at ETH Zurich can now publish free open-access articles in Elsevier journals with immediate effect. The prerequisite for this is that the corresponding author of the submitted article is employed at ETH Zurich. When submitting the manuscript, the ETH email address must be used. This agreement applies to all Elsevier journals including gold open-access. The Cell Press journals, The Lancet" and selected society journals are not included in the agreement. Therefore, please consult the above list before choosing a journal to publish open access.

This agreement with Elsevier, negotiated by swissuniversities, is the second "Read & Publish" deal for ETH Zurich besides the agreement with the Royal Society of Chemistry. It combines elec-



tronic access to all Elsevier journals with the possibility of open-access publishing in the form of a combined contract model. This represents an important step for ETH

Zurich in the successful implementation of its open-access policy and national open access strategy (German only).

Please contact the ETH Library's E-Publishing Group with any questions regarding the Elsevier agreement.

There are also selected journals of the Royal Society of Chemistry (RSC), Wiley and the Public Library of Sciences (PLOS) where publishing open access is possible with no additional cost. For the complete list of publishers and detailed information check here: (http://u.ethz.ch/AiAHR).

With many publishers, APCs are still not covered by ETH and the only option to go open access is by paying them yourself or at a marginal ETH Zurich discount. Sadly enough, among these publishers/journals are the American Chemical Society (ACS), Science Advances (AAAS), Proceedings of the National Academy of Sciences (PNAS) and Acta Crystallographica Section E.

Lynda is now LinkedIn Learning

Members of the American Chemical Society have recently been invited to gain free access until 2020 to LinkedIn Learning as part of their ACS membership. LinkedIn Learning used to be named Lynda, but was acquired in 2016 by Microsoft, which end of 2016 also acquired LinkedIn. Now, those two Microsoft products have been merged. However, at ETH Zurich you do not need to be an ACS member to get access. LinkedIn Learning is now available at the ETH Zurich IT Shop, although for a little fee of 40 CHF annually (charged on your cost center).



With LinkedIn Learning, you get:

- Access to more than 15,000 on-demand video tutorials covering software training, design skills, web design, business skills, study skills, photography, musical trainings, and much more.
- **Personalized recommendations:** Explore the most in-demand skills based on your experience.
- **Expert instructors:** Learn from industry leaders, all in one place.
- **Convenient learning:** Access courses on your schedule, from any desktop or mobile device.

• Helpful resources and recognition: Reinforce new knowledge with quizzes and exercise files. The access to LinkedIn Learning for the undergraduate

students is still being negotiated.

Breaking News Meme Generator

If you want to create your own Breaking News, with header and image of your choice, this is the tool for you.



App Tip (1)

Flatastic – the flat sharing App



You love your flat mates, but you are annoyed when the toilet paper is always out, the shower drain is clogged with hair, the kitchen is a mess - and, once again, it was no one's fault? Then you have made similar experiences as the Swiss Malik El Bay: His shared flat broke up because of such arguments. To prevent this, he developed *Flatastic* together with

Clemens Bachmair and Moritz von Hase. The app shows who has to do specific tasks at a certain time, and reminds you when the next task is due. Everyone receives a

notification acknowledging the completion of the task. Then, the next one in the list moves up. In addition, the app can be used to create shopping lists, manage finances or make announcements. Of course, it does not solve every problem. Some shared flats are just hopeless.

Apple App Store and Google Play.

ChemDraw 19.1

ChemDraw Version 19.1 is freshly available for download from https://t1p.de/r27k. It's only a minor update with some bugfixes and cosmetics, but nevertheless has a few useful additions. Keyboard shortcuts enable rapid rotation of a molecule using [ALT] + [arrow keys] by either 15° [up] and [down] or 1° [left] and [right]. The new functional group hotkeys for generating a cyclopropyl or a cyclobutyl group are [v] and [u], respectively. When drawing a molecule with a repeat-unit, one can draw it in the abridged version and add square brackets and the correct subscript. ChemDraw will recognize the correct molecular weight for this depiction, and moreover, the repeat-unit can be expanded to the full structure using "expand generic structure".

Cluster Searching with Carrot²

The open source search engine Carrot² clusters results from various sources (e.g. PubMed, Bing Search API, OpenSearch) automatically into thematic categories using different algorithms such as Suffix Tree Clustering (STC) and Lingo. Carrot² is implemented in Java and allows the user to add more functions or document sources. The commercial spin-off "Carrot Search" offers more features, and the developer hub "Carrot Search Labs" comprises several independent open source projects based on Carrot². If you would like to experiment with Carrot²'s different cluster visualizations (i.e., Folders, Treemap and Piechart), then follow this link.



PubChem links to physical property data from SpringerMaterials

More than 32,000 compounds in the open access chemistry database PubChem now have links to critically evaluated chemical and physical properties from the Springer-Materials database. The SpringerMaterials property data can be found on the "Chemical and Physical Properties" tab of PubChem, in the special SpringerMaterials Properties section. Clicking on any of the properties from this list will direct the users to the SpringerMaterials platform, which is licensed by the ETH Library.

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Fun signs made easily

The web service Kennzeichengenerator was probably programmed for model railroaders, but you can use this website also to generate all kinds of plates for other purposes, such as road signs and danger signs from Germany, Austria and Switzerland (and Liechtenstein), but also for license plates of your choice for a car, e.g. for California. The system does not check if your entry makes sense and the image file can be downloaded free of charge and used privately. Made with Love in Austria.



Nature ranks universities

The Nature Index 2020 Annual Tables highlight the institutions that dominated high quality research in the natural sciences in 2019. ETH Zurich is ranked 15^{th} , compared to 10^{th} in the 2019 annual table.



ChemDraw 19.0 for Mac supports both PDF and ESP for import of cycles in vector format. In Windows, import is only possible via a rastered png, which can make the cycles slightly blurry. Hopefully ChemDraw will fix this soon.

The corresponding paper can be found in the journal Organometallics.

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Coffee Lectures by the Information Center

The 20th series of our Coffee Lectures has already started–join us online! Since May 26th, and for three weeks, we again offer a small bite of knowledge for your coffee break every Tuesday, Wednesday and Thursday. Due to the circumstances this series has to take place online – join us at https://ethz.zoom.us/j/92636472246.

The lectures -10 minutes at max – will be given during this series in English only and will present databases and tools that help you work with scientific information and knowledge.

The dates of the nine Coffee Lectures can be found on our website. Using our Event Calendar, you can import any lecture with one click into your personal calendar, no matter if you are using a PC, Mac, smartphone or tablet. The flyer (PDF) for the 20th Series with all links can be found here. For a short period of time, a recording of the Coffee Lectures will be made available on our Youtube channel and as IGTV video on our Instagram account.

Farewell from the Information Center

At the end of January 2020, Dr. Joachim Schnabl left the Chemistry | Biology | Pharmacy Information Center and ETH Zurich to co-found a biotech company, Athebio in Schlieren (ZH). Joachim Schnabl was active in both the Information Center and in Science Communication D-CHAB and made a strong impact in both units. The visualization of D-CHAB's research areas and the list of scientific publications on the D-CHAB website would not have been possible without him. We will also miss his contribution to the lecture Scientific Information Retrieval & Management in Life Sciences and Chemistry on 2D and 3D visualization of molecules and the pipelining tool KNIME, just to name a few. We thank him for his support over the last five years, wish him a lot of success and a happy hand in developing the start-up Athebio. His position is vacant in both areas, and as a contact person for questions regarding Science Communication D-CHAB remains Dr. Oliver Renn, the Head of Science Communication. Since November 2019 Oliver Renn is also responsible for Public Relations D-CHAB (in addition to his remaining responsibility for the Chemistry | Biology | Pharmacy Information Center).

"Alles Open oder was?"

For the May issue of *Nachrichten aus der Chemie*, the journal of the German Society of Chemists (GDCh), the editors have – for the very first time – compiled a special issue with a particular focus on Switzerland as a neighboring country. All articles from and about the country can also be found in a special digital edition. There is also an article by Dr. Leo Betschart and Dr. Oliver Renn. "Alles open oder was?" is, of course, published open access and gives (in German) an overview of the development of scientific publishing and scientific communication.



Imprint

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Take authorship of your publications in the Research Collection – the benefits of ORCID

Being forced to work in your home office may give you time for some housekeeping you never found time to do. Do you have an ORCID iD? If no, then now is the time to register at ORCID.org (its free and has many advantages – most publishers require an ORCID iD when submitting a paper). If yes, did you link our ORCID iD to your ETH profile? Then you can avoid that your author search results look like this in the ETH Zurich Research Collection:

Filter by: Author / Creator

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Five identities for J. Dolenc? Publications are assigned to multiple name variants; some might even be falsely assigned to you or some of your publications assigned to someone else. With little effort and in no time, you can get rid of multiple identities and split-up publications lists and avoid them in the future:

Step 1: If you haven't done so yet: link your ORCID iD with your ETH profile at www.addresses.ethz.ch and wait until the next day for this to apply. Step 2: Sign in at www.researchcollection.ethz.ch/ and go to "Assign ORCID ID". Assign or dismiss publications using the checkboxes. Done! The result is visible immediately. Now there is just one J. Dolenc with 32 papers and a trustworthy identity.

Dolenc, Irena (1)	
Dolenc, Jozica (1) (32)	

More detailed instructions can be found at Research Collections Online Manual.