Istraživački podaci u praksi

Milica Ševkušić
Institut tehničkih nauka SANU

Upravljanje otvorenim istraživačkim podacima za istraživače

Institut za biološka istraživanja „Siniša Stanković“, 8. jul 2020.

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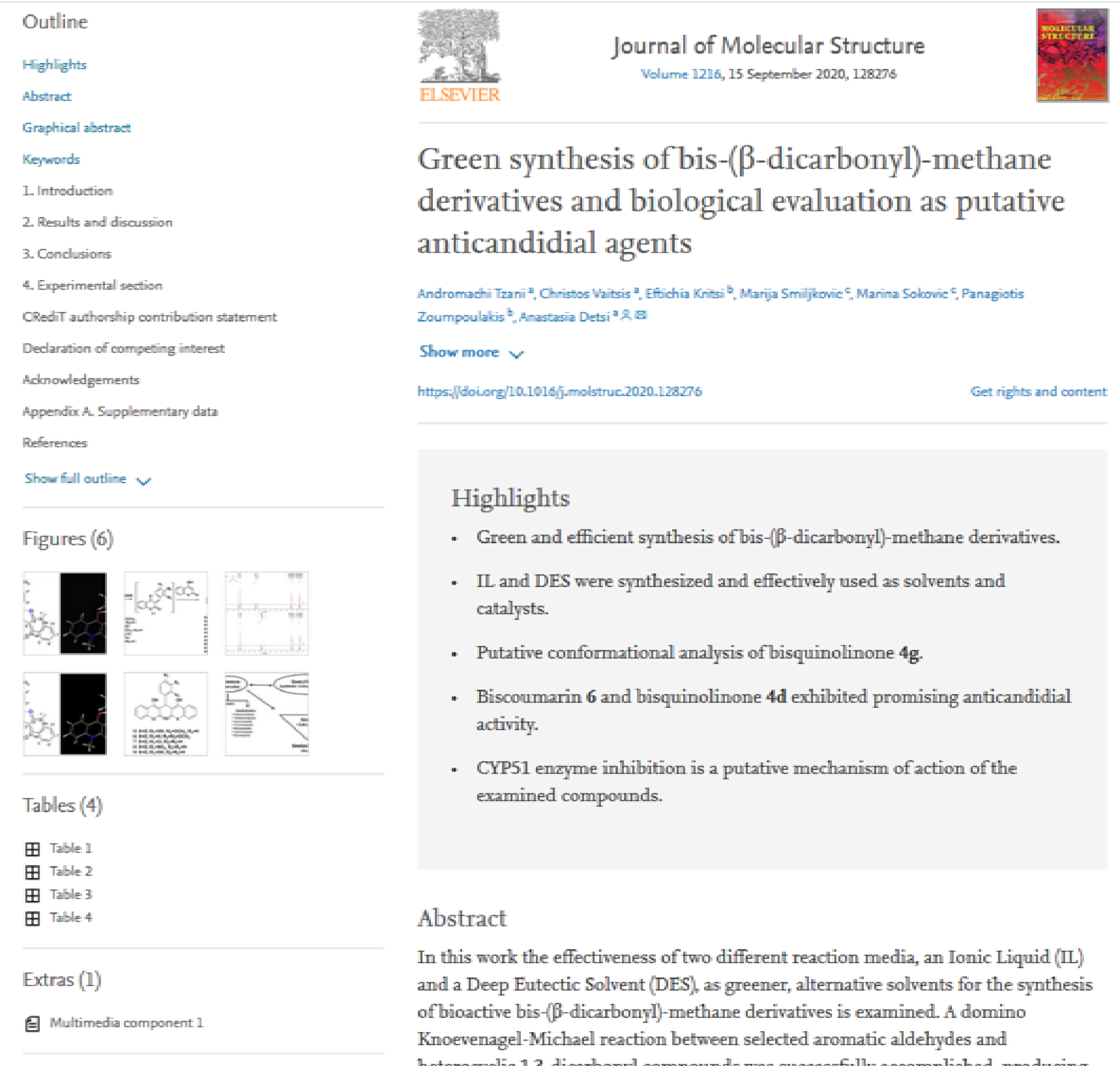

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ELSEVIER
Journal of Molecular Structure
Volume 1216, 15 September 2020, 128276

Green synthesis of bis-(β-dicarbonyl)-methane derivatives and biological evaluation as putative anticandidial agents

Andromachi Tzani [a], Christos Vaitsis [a], Efthichia Kritsi [b], Marija Smiljkovic [c], Marina Sokovic [c], Panagiotis Zoumpoulakis [b], Anastasia Detsi [a]

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https://doi.org/10.1016/j.molstruc.2020.128276

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Highlights

- Green and efficient synthesis of bis-(β-dicarbonyl)-methane derivatives.
- IL and DES were synthesized and effectively used as solvents and catalysts.
- Putative conformational analysis of bisquinolinone **4g**.
- Biscoumarin **6** and bisquinolinone **4d** exhibited promising anticandidial activity.
- CYP51 enzyme inhibition is a putative mechanism of action of the examined compounds.

Abstract

In this work the effectiveness of two different reaction media, an Ionic Liquid (IL) and a Deep Eutectic Solvent (DES), as greener, alternative solvents for the synthesis of bioactive bis-(β-dicarbonyl)-methane derivatives is examined. A domino Knoevenagel-Michael reaction between selected aromatic aldehydes and

- Dodatni materijal (Supplementary data) je nedostupan
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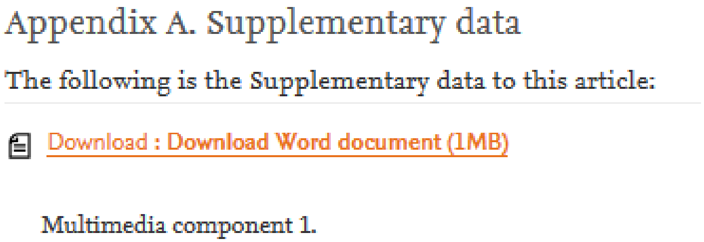

Appendix A. Supplementary data

The following is the Supplementary data to this article:

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Multimedia component 1.

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Green synthesis of bis-(β-dicarbonyl)-methane derivatives and biological evaluation as putative anticandidial agents

Andromachi Tzani,[1] Christos Vaitsis,[1] Eftichia Kritsi,[2] Marija Smiljkovic,[3] Marina Sokovic,[3] Panagiotis Zoumpoulakis[2] and Anastasia Detsi[1]*

Email: Anastasia Detsi - adetsi@chemeng.ntua.gr

* Corresponding author

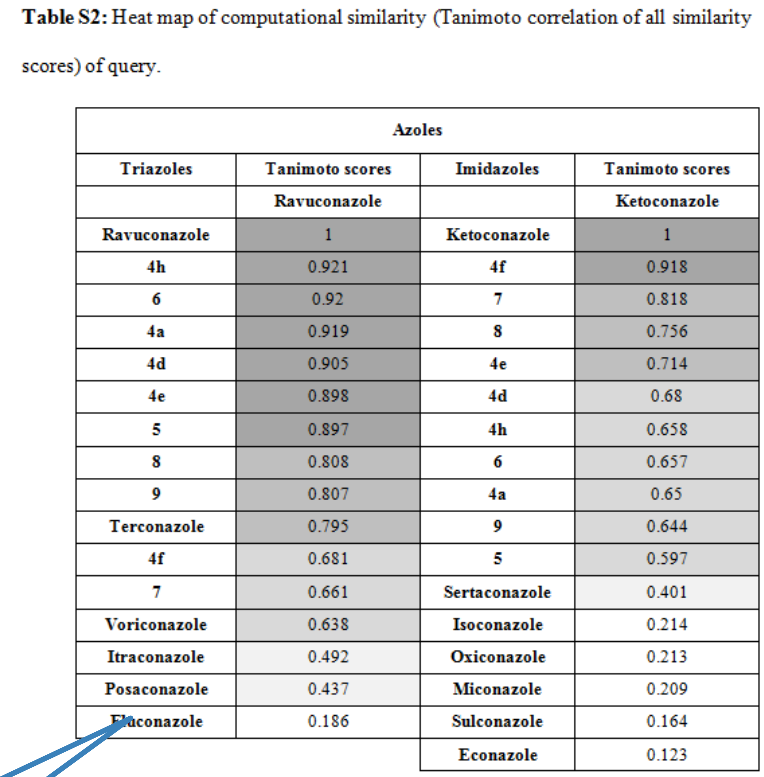

Table S2: Heat map of computational similarity (Tanimoto correlation of all similarity scores) of query.

Azoles			
Triazoles	**Tanimoto scores**	**Imidazoles**	**Tanimoto scores**
	Ravuconazole		**Ketoconazole**
Ravuconazole	1	**Ketoconazole**	1
4h	0.921	**4f**	0.918
6	0.92	**7**	0.818
4a	0.919	**8**	0.756
4d	0.905	**4e**	0.714
4e	0.898	**4d**	0.68
5	0.897	**4h**	0.658
8	0.808	**6**	0.657
9	0.807	**4a**	0.65
Terconazole	0.795	**9**	0.644
4f	0.681	**5**	0.597
7	0.661	**Sertaconazole**	0.401
Voriconazole	0.638	**Isoconazole**	0.214
Itraconazole	0.492	**Oxiconazole**	0.213
Posaconazole	0.437	**Miconazole**	0.209
Fluconazole	0.186	**Sulconazole**	0.164
		Econazole	0.123

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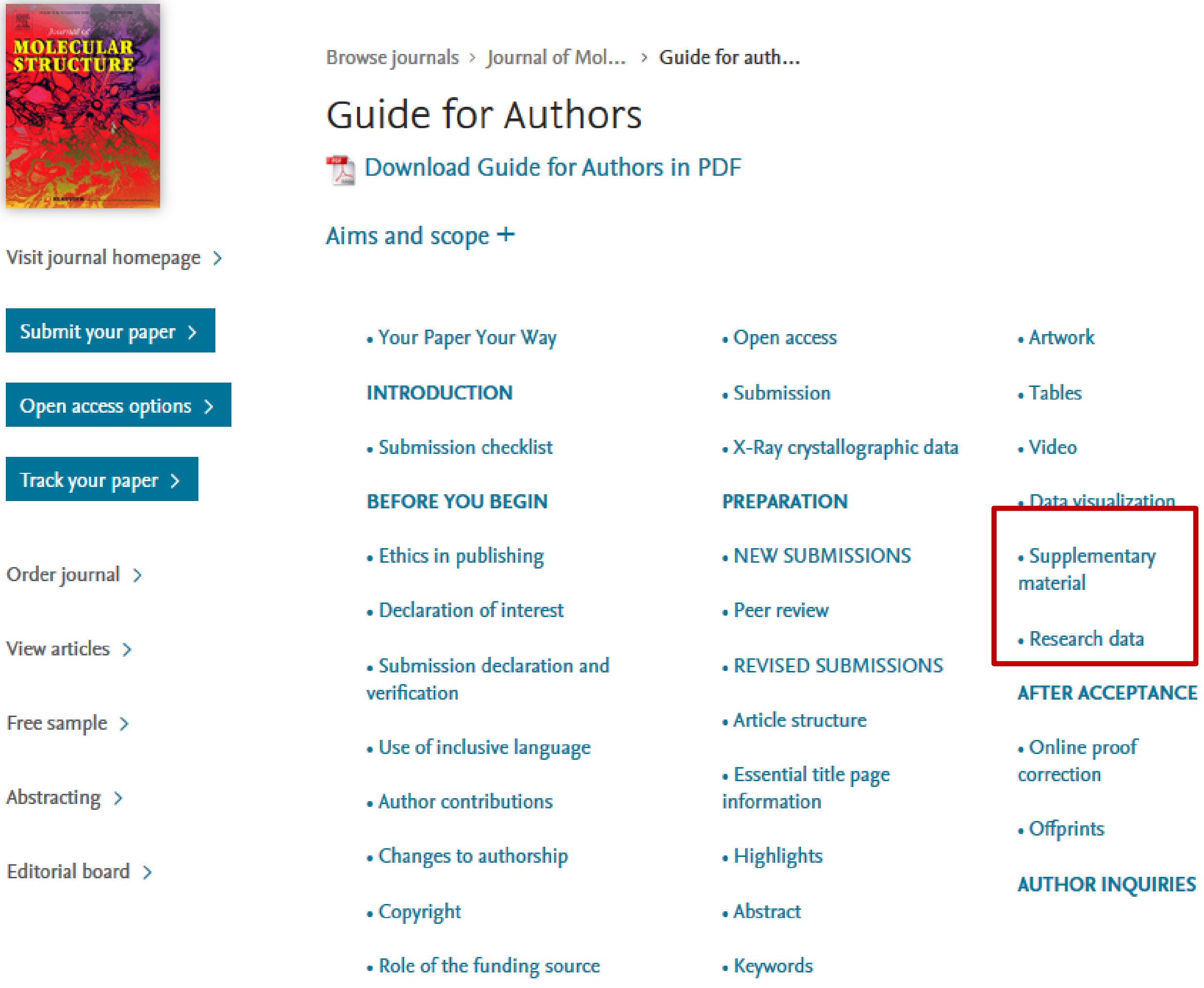

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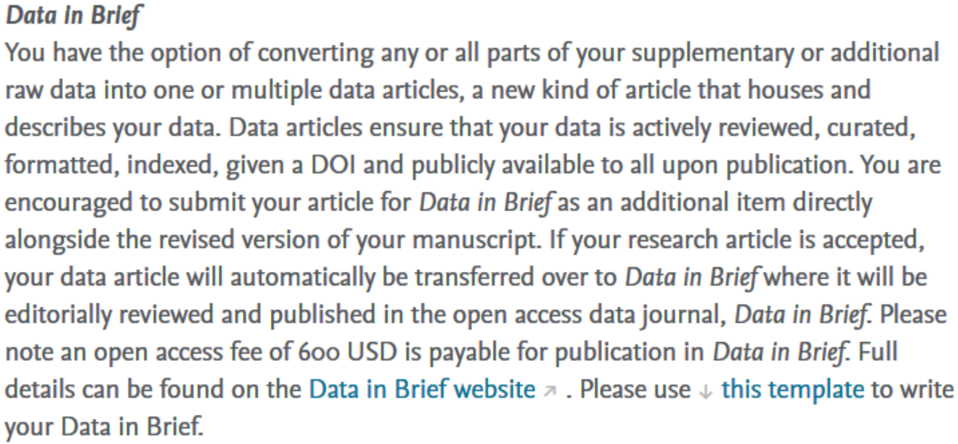

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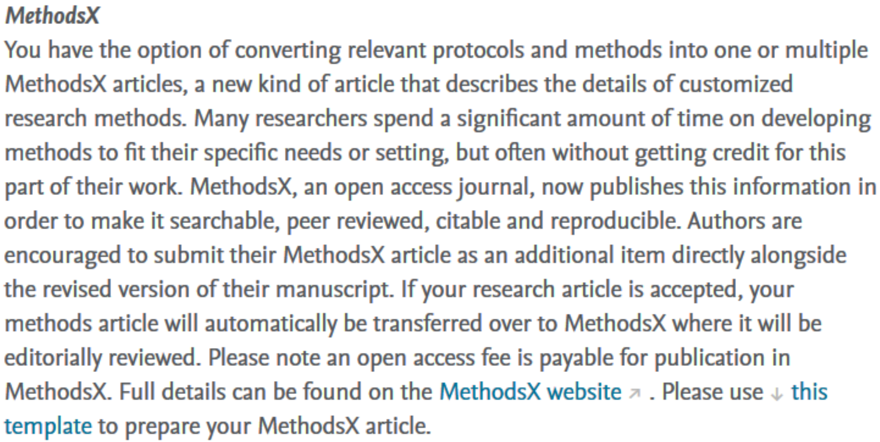

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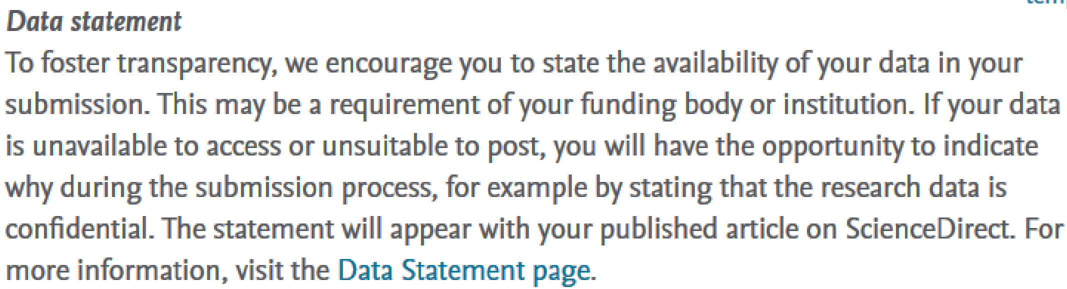

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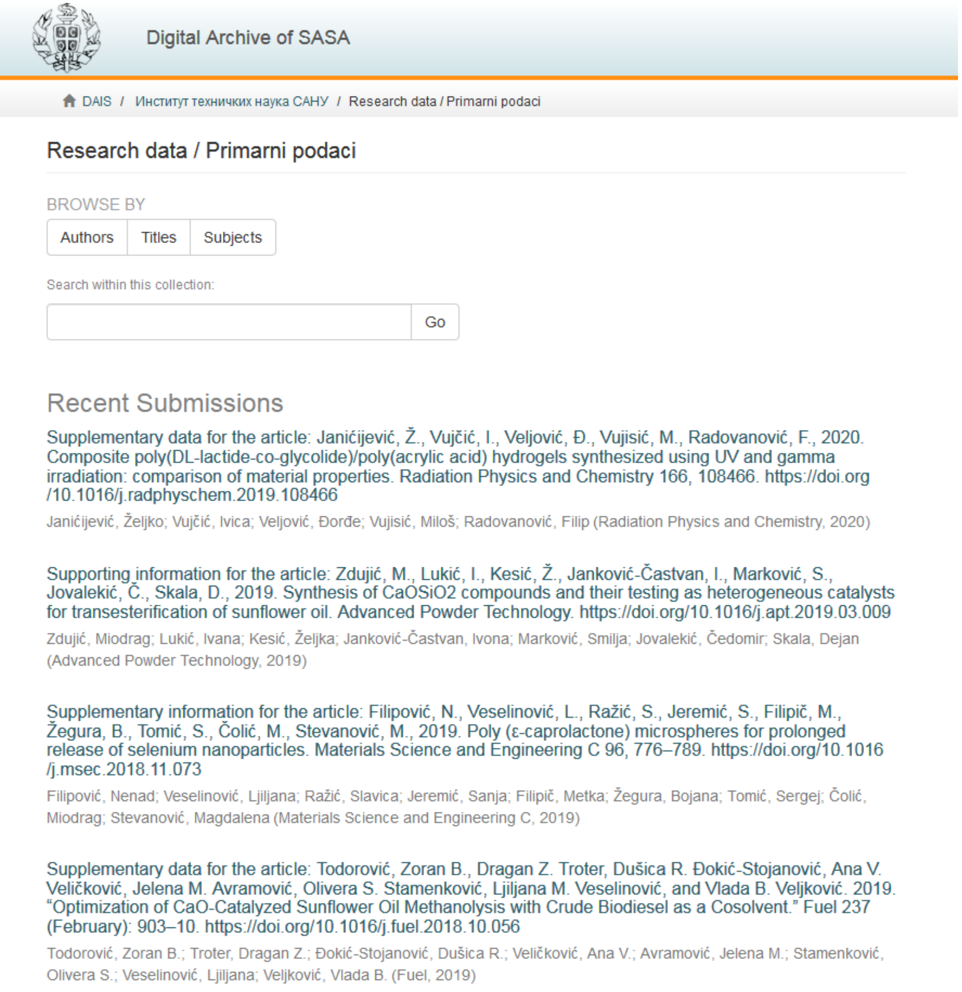

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Janićijević, Željko; Vujčić, Ivica; Veljović, Đorđe; Vujisić, Miloš; Radovanović, Filip (Radiation Physics and Chemistry, 2020)

Supporting information for the article: Zdujić, M., Lukić, I., Kesić, Ž., Janković-Častvan, I., Marković, S., Jovalekić, Č., Skala, D., 2019. Synthesis of CaOSiO2 compounds and their testing as heterogeneous catalysts for transesterification of sunflower oil. Advanced Powder Technology. https://doi.org/10.1016/j.apt.2019.03.009

Zdujić, Miodrag; Lukić, Ivana; Kesić, Željka; Janković-Častvan, Ivona; Marković, Smilja; Jovalekić, Čedomir; Skala, Dejan (Advanced Powder Technology, 2019)

Supplementary information for the article: Filipović, N., Veselinović, L., Ražić, S., Jeremić, S., Filipič, M., Žegura, B., Tomić, S., Čolić, M., Stevanović, M., 2019. Poly (ε-caprolactone) microspheres for prolonged release of selenium nanoparticles. Materials Science and Engineering C 96, 776–789. https://doi.org/10.1016/j.msec.2018.11.073

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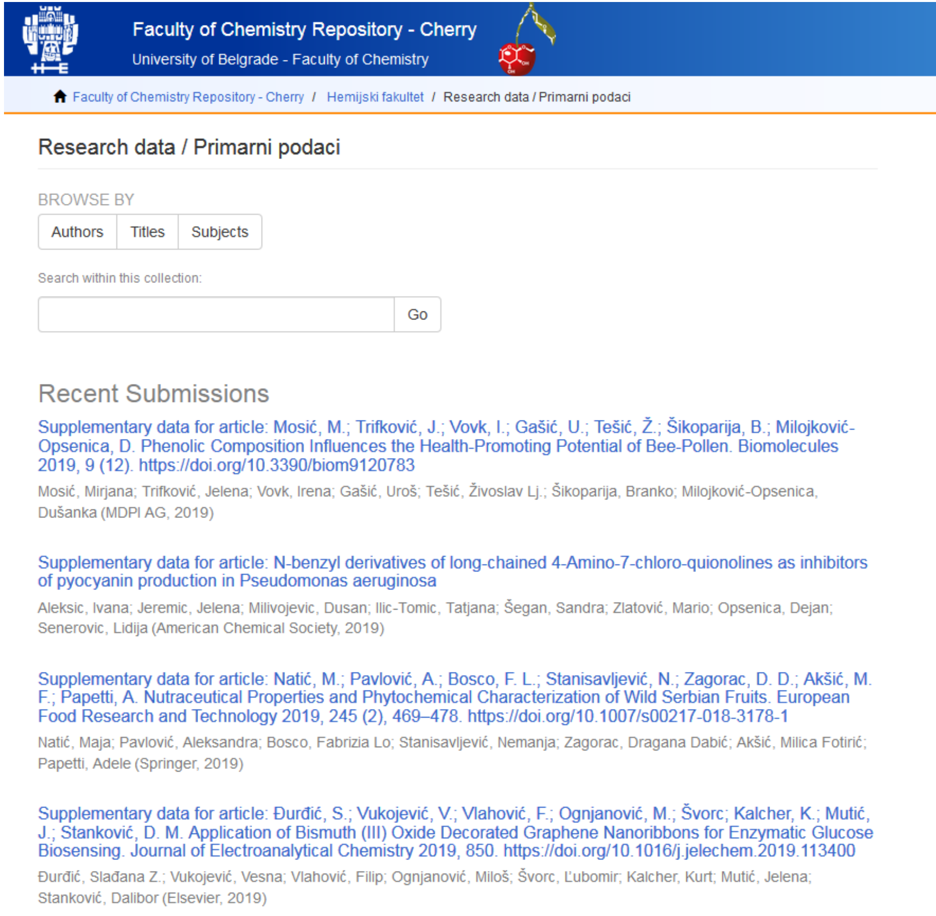
Supplementary data for the article: Todorović, Zoran B., Dragan Z. Troter, Dušica R. Đokić-Stojanović, Ana V. Veličković, Jelena M. Avramović, Olivera S. Stamenković, Ljiljana M. Veselinović, and Vlada B. Veljković. 2019. "Optimization of CaO-Catalyzed Sunflower Oil Methanolysis with Crude Biodiesel as a Cosolvent." Fuel 237 (February): 903–10. https://doi.org/10.1016/j.fuel.2018.10.056

Todorović, Zoran B.; Troter, Dragan Z.; Đokić-Stojanović, Dušica R.; Veličković, Ana V.; Avramović, Jelena M.; Stamenković, Olivera S.; Veselinović, Ljiljana; Veljković, Vlada B. (Fuel, 2019)



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Mosić, Mirjana; Trifković, Jelena; Vovk, Irena; Gašić, Uroš; Tešić, Živoslav Lj.; Šikoparija, Branko; Milojković-Opsenica, Dušanka (MDPI AG, 2019)

Supplementary data for article: N-benzyl derivatives of long-chained 4-Amino-7-chloro-quionolines as inhibitors of pyocyanin production in Pseudomonas aeruginosa

Aleksic, Ivana; Jeremic, Jelena; Milivojevic, Dusan; Ilic-Tomic, Tatjana; Šegan, Sandra; Zlatović, Mario; Opsenica, Dejan; Senerovic, Lidija (American Chemical Society, 2019)

Supplementary data for article: Natić, M.; Pavlović, A.; Bosco, F. L.; Stanisavljević, N.; Zagorac, D. D.; Akšić, M. F.; Papetti, A. Nutraceutical Properties and Phytochemical Characterization of Wild Serbian Fruits. European Food Research and Technology 2019, 245 (2), 469–478. https://doi.org/10.1007/s00217-018-3178-1

Natić, Maja; Pavlović, Aleksandra; Bosco, Fabrizia Lo; Stanisavljević, Nemanja; Zagorac, Dragana Dabić; Akšić, Milica Fotirić; Papetti, Adele (Springer, 2019)

Supplementary data for article: Đurđić, S.; Vukojević, V.; Vlahović, F.; Ognjanović, M.; Švorc; Kalcher, K.; Mutić, J.; Stanković, D. M. Application of Bismuth (III) Oxide Decorated Graphene Nanoribbons for Enzymatic Glucose Biosensing. Journal of Electroanalytical Chemistry 2019, 850. https://doi.org/10.1016/j.jelechem.2019.113400

Đurđić, Slađana Z.; Vukojević, Vesna; Vlahović, Filip; Ognjanović, Miloš; Švorc, Ľubomir; Kalcher, Kurt; Mutić, Jelena; Stanković, Dalibor (Elsevier, 2019)

Kosanović, D., Blagojević, V.A., Maričić, A., Aleksić, S., Pavlović, V.P., Pavlović, V.B., Vlahović, B., 2018. Influence of mechanical activation on functional properties of barium hexaferrite ceramics. Ceramics International 44, 6666–6672. https://doi.org/10.1016/j.ceramint.2018.01.078: Supplement

2018

1-s2.0-S0272884218300919-mmc1.pdf (413.4Kb)

Authors

Kosanović, Darko
Blagojević, Vladimir A.
Maričić, Aleksa
Aleksić, S.
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Rietveld analysis of XRD patterns of mechanically activated Fe:BaTiO3 powder mixtures sintered at 1200°C

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Ceramics International, 2018, 44, 6

Projects:

- United States National Aeronautics and Space Administration (NASA), Grant NNX09AV07A
- Directed synthesis, structure and properties of multifunctional materials (RS-172057)
- Serbian Academy of Sciences and Arts, Project F-178
- United States National Science Foundation (NSF) / Centers of Research Excellence in Science and Technology (CREST), Grant HRD-0833184
- United States National Science Foundation (NSF) / Partnerships for Research and Education in Materials (PREM), Grant 1523617

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Metapodaci

Schriml, L.M., Chuvochina, M., Davies, N., Eloe-Fadrosh, E.A., Finn, R.D., Hugenholtz, P., Hunter, C.I., Hurwitz, B.L., Kyrpides, N.C., Meyer, F., et al. (2020). COVID-19 pandemic reveals the peril of ignoring metadata standards. Scientific Data *7*, 188.

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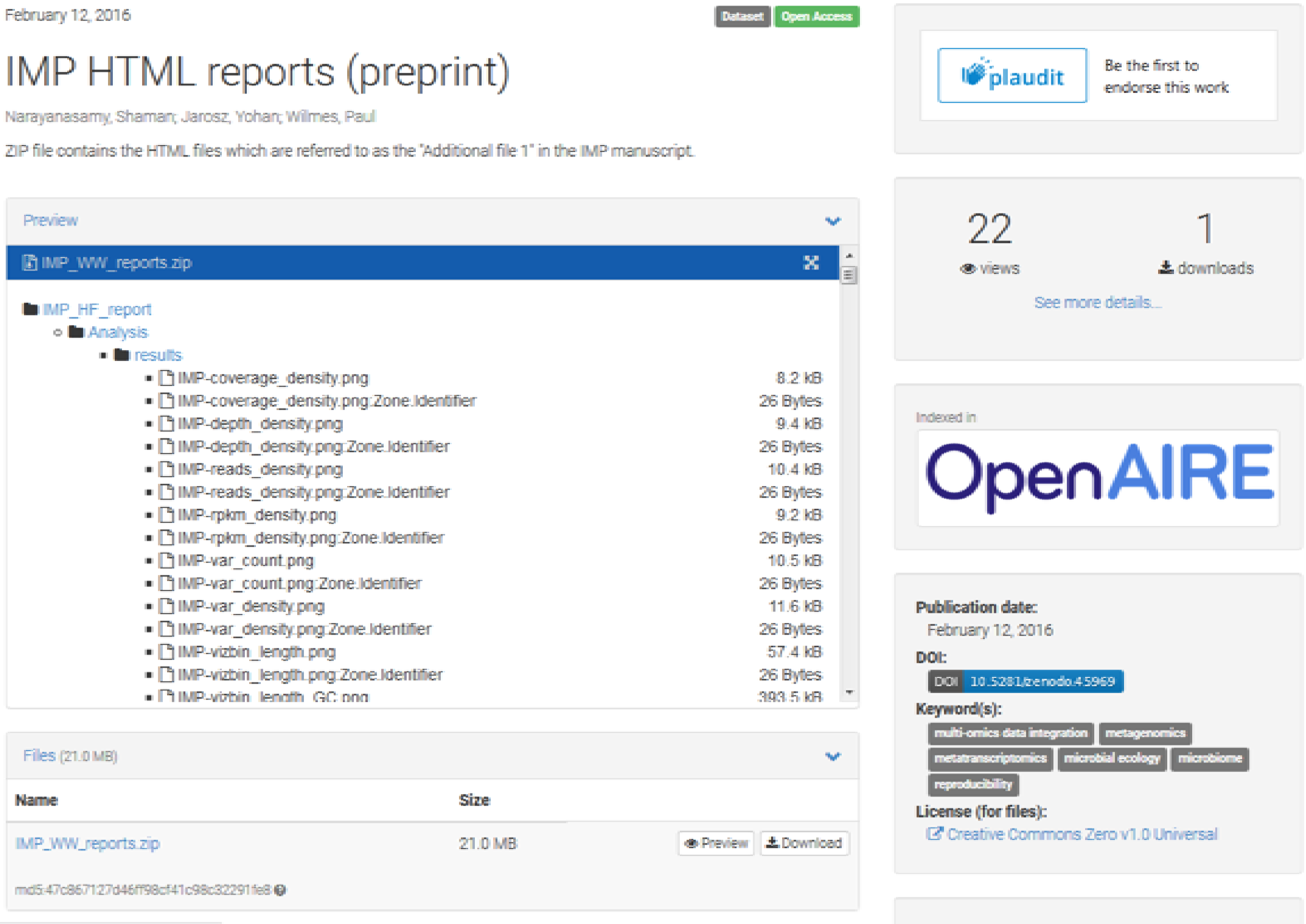

February 12, 2016

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Keyword(s):
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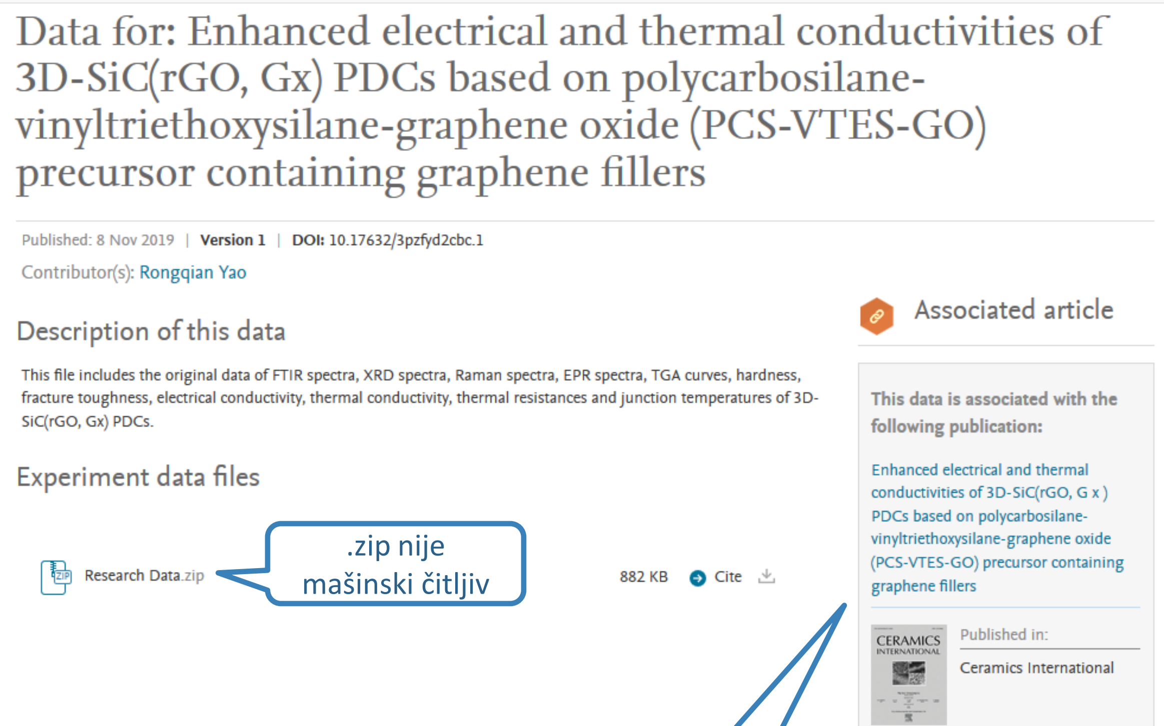

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Published: 8 Nov 2019 | **Version 1** | **DOI:** 10.17632/3pzfyd2cbc.1

Contributor(s): Rongqian Yao

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This file includes the original data of FTIR spectra, XRD spectra, Raman spectra, EPR spectra, TGA curves, hardness, fracture toughness, electrical conductivity, thermal conductivity, thermal resistances and junction temperatures of 3D-SiC(rGO, Gx) PDCs.

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Associated article

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Enhanced electrical and thermal conductivities of 3D-SiC(rGO, G x) PDCs based on polycarbosilane-vinyltriethoxysilane-graphene oxide (PCS-VTES-GO) precursor containing graphene fillers

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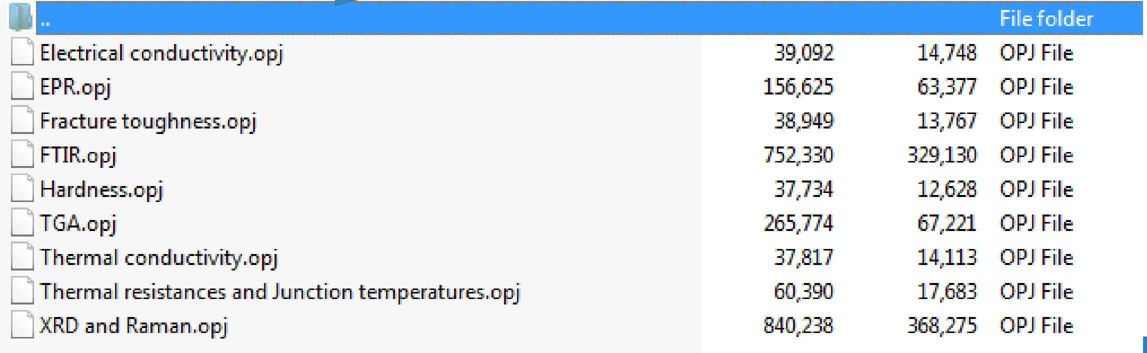

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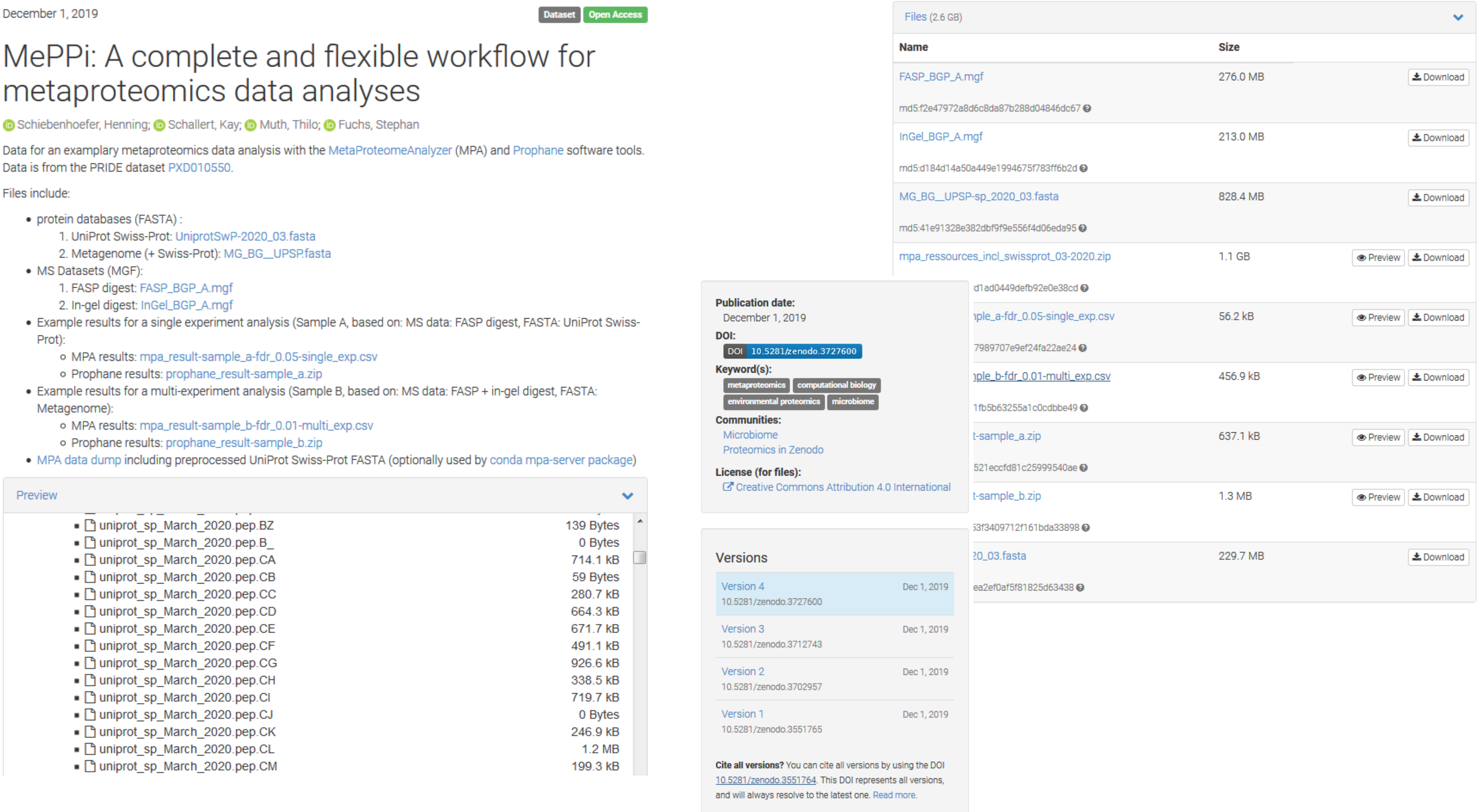

December 1, 2019

MePPi: A complete and flexible workflow for metaproteomics data analyses

Schiebenhoefer, Henning; Schallert, Kay; Muth, Thilo; Fuchs, Stephan

Data for an examplary metaproteomics data analysis with the MetaProteomeAnalyzer (MPA) and Prophane software tools. Data is from the PRIDE dataset PXD010550.

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  2. Metagenome (+ Swiss-Prot): MG_BG__UPSP.fasta
- MS Datasets (MGF):
  1. FASP digest: FASP_BGP_A.mgf
  2. In-gel digest: InGel_BGP_A.mgf
- Example results for a single experiment analysis (Sample A, based on: MS data: FASP digest, FASTA: UniProt Swiss-Prot):
  - MPA results: mpa_result-sample_a-fdr_0.05-single_exp.csv
  - Prophane results: prophane_result-sample_a.zip
- Example results for a multi-experiment analysis (Sample B, based on: MS data: FASP + in-gel digest, FASTA: Metagenome):
  - MPA results: mpa_result-sample_b-fdr_0.01-multi_exp.csv
  - Prophane results: prophane_result-sample_b.zip
- MPA data dump including preprocessed UniProt Swiss-Prot FASTA (optionally used by conda mpa-server package)

Preview

uniprot_sp_March_2020.pep.BZ	139 Bytes
uniprot_sp_March_2020.pep.B_	0 Bytes
uniprot_sp_March_2020.pep.CA	714.1 kB
uniprot_sp_March_2020.pep.CB	59 Bytes
uniprot_sp_March_2020.pep.CC	280.7 kB
uniprot_sp_March_2020.pep.CD	664.3 kB
uniprot_sp_March_2020.pep.CE	671.7 kB
uniprot_sp_March_2020.pep.CF	491.1 kB
uniprot_sp_March_2020.pep.CG	926.6 kB
uniprot_sp_March_2020.pep.CH	338.5 kB
uniprot_sp_March_2020.pep.CI	719.7 kB
uniprot_sp_March_2020.pep.CJ	0 Bytes
uniprot_sp_March_2020.pep.CK	246.9 kB
uniprot_sp_March_2020.pep.CL	1.2 MB
uniprot_sp_March_2020.pep.CM	199.3 kB

Publication date:
December 1, 2019
DOI:
DOI 10.5281/zenodo.3727600
Keyword(s):
metaproteomics, computational biology, environmental proteomics, microbiome
Communities:
Microbiome
Proteomics in Zenodo

Versions

Version 4 10.5281/zenodo.3727600	Dec 1, 2019
Version 3 10.5281/zenodo.3712743	Dec 1, 2019
Version 2 10.5281/zenodo.3702957	Dec 1, 2019
Version 1 10.5281/zenodo.3551765	Dec 1, 2019

Cite all versions? You can cite all versions by using the DOI 10.5281/zenodo.3551764. This DOI represents all versions, and will always resolve to the latest one. Read more.

Files (2.6 GB)

Name	Size	
FASP_BGP_A.mgf md5:f2e47972a8d6c8da87b288d04846dc67	276.0 MB	Download
InGel_BGP_A.mgf md5:d184d14a50a449e1994675f783ff6b2d	213.0 MB	Download
MG_BG__UPSP-sp_2020_03.fasta md5:41e91328e382dbf9f9e556f4d06eda95	828.4 MB	Download
mpa_ressources_incl_swissprot_03-2020.zip d1ad0449defb92e0e38cd	1.1 GB	Preview Download
nple_a-fdr_0.05-single_exp.csv 7989707e9ef24fa22ae24	56.2 kB	Preview Download
nple_b-fdr_0.01-multi_exp.csv 1fb5b63255a1c0cdbbe49	456.9 kB	Preview Download
t-sample_a.zip 521eccfd81c25999540ae	637.1 kB	Preview Download
t-sample_b.zip 53f3409712f161bda33898	1.3 MB	Preview Download
20_03.fasta ea2ef0af5f81825d63438	229.7 MB	Download

https://doi.org/10.5281/zenodo.3551764

Data from: Target enrichment of ultraconserved elements from arthropods provides a genomic perspective on relationships among Hymenoptera

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Branstetter, Michael G., Smithsonian Institution
White, Noor D., University of Maryland, College Park, Smithsonian Institution
Brady, Séan G., Smithsonian Institution

Publication date: September 19, 2014
Publisher: Dryad
https://doi.org/10.5061/dryad.46195

Data Files

› September 19, 2014

Metrics

677 views

620 downloads

1 citations

Citation

Faircloth, Brant C.; Branstetter, Michael G.; White, Noor D.; Brady, Séan G. (2014), Data from: Target enrichment of ultraconserved elements from arthropods provides a genomic perspective on relationships among Hymenoptera, Dryad, Dataset, https://doi.org/10.5061/dryad.46195

Keywords

Stenamma felixi
Nasonia giraulti
Aporus niger
Arthropods
Harpegnathos saltator
Ceratosolen solmsi
Acromyrmex echinatior
Orthogonalys pulchella
Apis mellifera
Aphaenogaster megommata
baits

Abstract

Gaining a genomic perspective on phylogeny requires the collection of data from many putatively independent loci across the genome. Among insects, an increasingly common approach to collecting this class of data involves transcriptome sequencing, because few insects have high-quality genome sequences available; assembling new genomes remains a limiting factor; the transcribed portion of the genome is a reasonable, reduced subset of the genome to target; and the data collected from transcribed portions of the genome are similar in composition to the types of data with which biologists have traditionally worked (e.g. exons). However, molecular techniques requiring RNA as a template, including transcriptome sequencing, are limited to using very high-quality source materials, which are often unavailable from a large proportion of biologically important insect samples. Recent research suggests that DNA-based target enrichment of conserved genomic elements offers another path to collecting phylogenomic data across insect taxa, provided that conserved elements are present in and can be collected from insect genomes. Here, we identify a large set (n = 1510) of ultraconserved elements (UCEs) shared among the insect order Hymenoptera. We used in silico analyses to show that these loci accurately reconstruct relationships among genome-enabled hymenoptera, and we designed a set of RNA baits (n = 2749) for enriching these loci that researchers can use with DNA templates extracted from a variety of sources. We used our UCE bait set to enrich an average of 721 UCE loci from 30 hymenopteran taxa, and we used these UCE loci to reconstruct phylogenetic relationships spanning very old (≥220 Ma) to very young (≤1 Ma) divergences among hymenopteran lineages. In contrast to a recent study addressing hymenopteran phylogeny using transcriptome data, we

Usage Notes

hymenoptera-uce-probes.fasta
FASTA file containing target enrichment bait sequences for UCE loci in hymenoptera.

in-silico-NOTES
NOTES describing the pipeline steps used to analyze the in silico data.

in-silico-contigs.tar.gz
UCE contigs sliced from available hymenopteran genomes.

in-silico-uce-probes-to-contigs.lastz.tar.gz
LASTZ files showing mapping of UCE probes onto in silico genome slices AND probe.matches.sqlite database.

in-silico-taxon-set-alignment-data.tar.gz
Archive file containing nested directories of in-silico alignment and analysis data. See overall README or file-specific README.

hymenoptera-data-sets.conf
Top level file defining taxon sets used in analyses (e.g. ABYSS and TRINITY, with and without sawflies.

abyss-NOTES
NOTES describing the pipeline steps used to analyze the ABYSS data.

abyss-contigs.tar.gz
UCE contigs enriched from hymenopteran taxa and assembled using ABySS.

abyss-uce-probes-to-contigs.lastz.tar.gz
LASTZ files showing mapping of UCE probes onto in ABySS contigs AND probe.matches.sqlite database.

abyss-probe-alignment-logs.tar.gz
Log files from ABySS probe alignment.

abyss-taxon-set-alignment-data.tar.gz
Archive file containing nested directories of ABySS alignment and analysis data. See overall README or file-specific README.

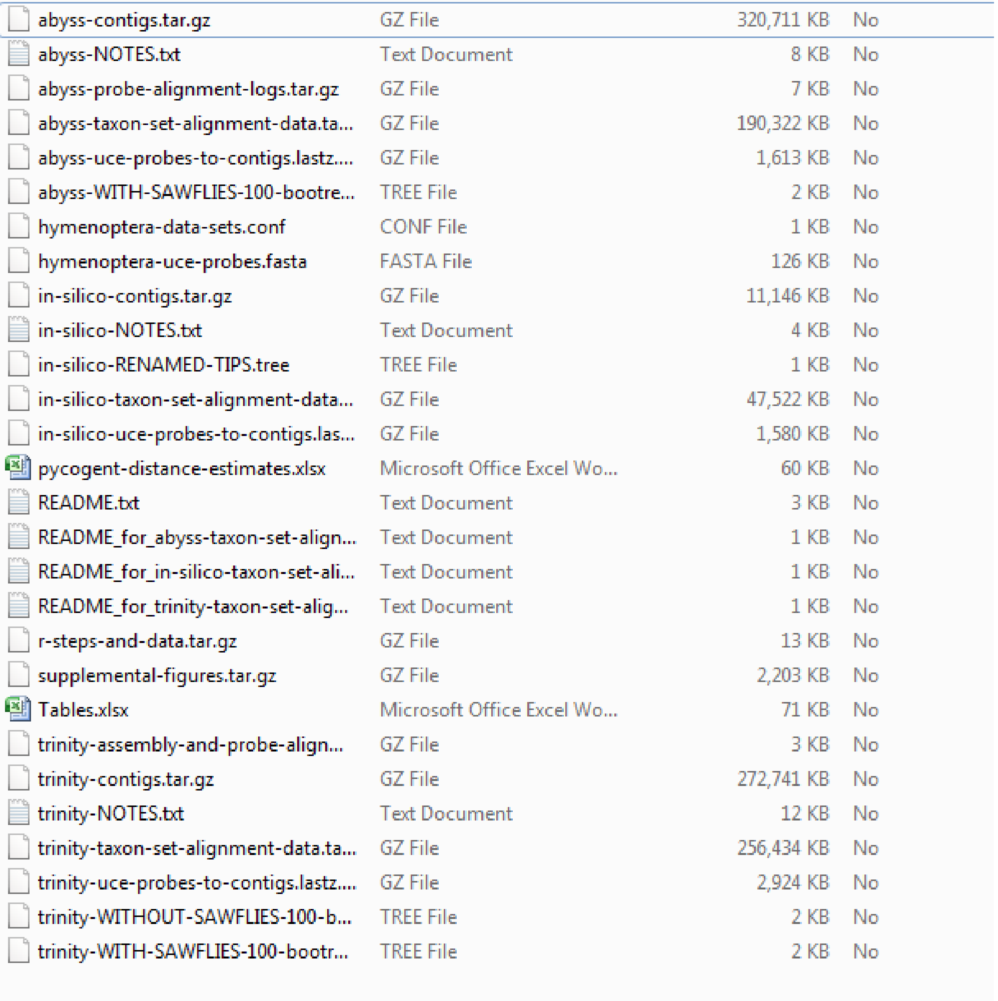
trinity-NOTES

References

This dataset is supplement to https://doi.org/10.1111/1755-0998.12328

This dataset is supplemented by http://dx.doi.org/10.6084/m9.figshare.1173286

License



abyss-contigs.tar.gz	GZ File	320,711 KB	No
abyss-NOTES.txt	Text Document	8 KB	No
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abyss-taxon-set-alignment-data.ta...	GZ File	190,322 KB	No
abyss-uce-probes-to-contigs.lastz....	GZ File	1,613 KB	No
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hymenoptera-data-sets.conf	CONF File	1 KB	No
hymenoptera-uce-probes.fasta	FASTA File	126 KB	No
in-silico-contigs.tar.gz	GZ File	11,146 KB	No
in-silico-NOTES.txt	Text Document	4 KB	No
in-silico-RENAMED-TIPS.tree	TREE File	1 KB	No
in-silico-taxon-set-alignment-data...	GZ File	47,522 KB	No
in-silico-uce-probes-to-contigs.las...	GZ File	1,580 KB	No
pycogent-distance-estimates.xlsx	Microsoft Office Excel Wo...	60 KB	No
README.txt	Text Document	3 KB	No
README_for_abyss-taxon-set-align...	Text Document	1 KB	No
README_for_in-silico-taxon-set-ali...	Text Document	1 KB	No
README_for_trinity-taxon-set-alig...	Text Document	1 KB	No
r-steps-and-data.tar.gz	GZ File	13 KB	No
supplemental-figures.tar.gz	GZ File	2,203 KB	No
Tables.xlsx	Microsoft Office Excel Wo...	71 KB	No
trinity-assembly-and-probe-align...	GZ File	3 KB	No
trinity-contigs.tar.gz	GZ File	272,741 KB	No
trinity-NOTES.txt	Text Document	12 KB	No
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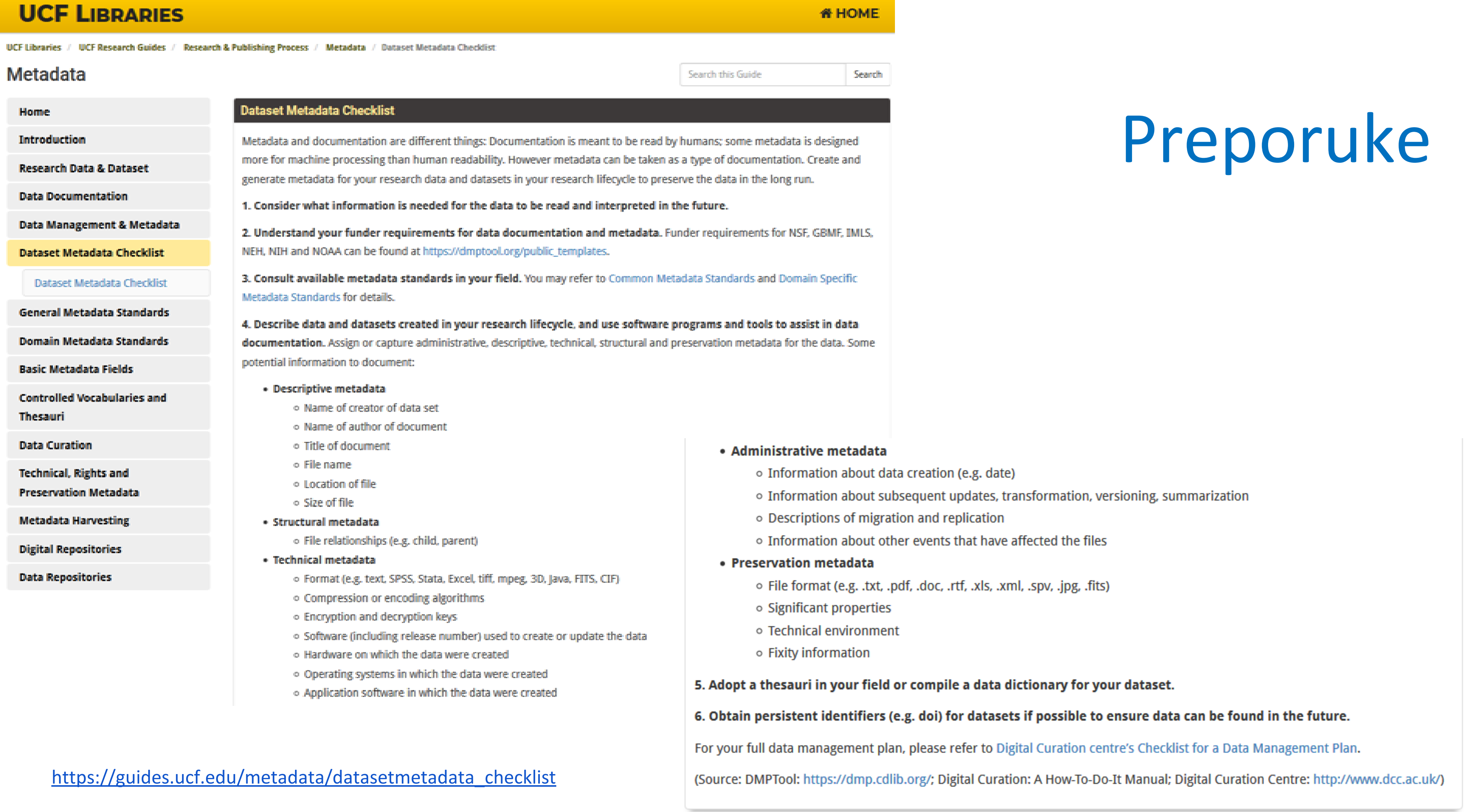
trinity-uce-probes-to-contigs.lastz....	GZ File	2,924 KB	No
trinity-WITHOUT-SAWFLIES-100-b...	TREE File	2 KB	No
trinity-WITH-SAWFLIES-100-bootr...	TREE File	2 KB	No

- Publikacija i podaci su povezani
- U metapodacima je ukratko opisan sadržaj datoteka
- Dodatne informacije su date i u README datotekama
- Formati datoteka nisu optimalni (npr. xlsx)
-
- U bazi podataka DRYAD proverava se da li metapodaci zadovoljavaju minimalne uslove
- Deponovanje nije besplatno
- Obavezna je CC 0 licenca

https://doi.org/10.5061/dryad.46195

Preporuke



Metadata

Dataset Metadata Checklist

Metadata and documentation are different things: Documentation is meant to be read by humans; some metadata is designed more for machine processing than human readability. However metadata can be taken as a type of documentation. Create and generate metadata for your research data and datasets in your research lifecycle to preserve the data in the long run.

1. Consider what information is needed for the data to be read and interpreted in the future.

2. Understand your funder requirements for data documentation and metadata. Funder requirements for NSF, GBMF, IMLS, NEH, NIH and NOAA can be found at https://dmptool.org/public_templates.

3. Consult available metadata standards in your field. You may refer to Common Metadata Standards and Domain Specific Metadata Standards for details.

4. Describe data and datasets created in your research lifecycle, and use software programs and tools to assist in data documentation. Assign or capture administrative, descriptive, technical, structural and preservation metadata for the data. Some potential information to document:

- **Descriptive metadata**
  - Name of creator of data set
  - Name of author of document
  - Title of document
  - File name
  - Location of file
  - Size of file
- **Structural metadata**
  - File relationships (e.g. child, parent)
- **Technical metadata**
  - Format (e.g. text, SPSS, Stata, Excel, tiff, mpeg, 3D, Java, FITS, CIF)
  - Compression or encoding algorithms
  - Encryption and decryption keys
  - Software (including release number) used to create or update the data
  - Hardware on which the data were created
  - Operating systems in which the data were created
  - Application software in which the data were created
- **Administrative metadata**
  - Information about data creation (e.g. date)
  - Information about subsequent updates, transformation, versioning, summarization
  - Descriptions of migration and replication
  - Information about other events that have affected the files
- **Preservation metadata**
  - File format (e.g. .txt, .pdf, .doc, .rtf, .xls, .xml, .spv, .jpg, .fits)
  - Significant properties
  - Technical environment
  - Fixity information

5. Adopt a thesauri in your field or compile a data dictionary for your dataset.

6. Obtain persistent identifiers (e.g. doi) for datasets if possible to ensure data can be found in the future.

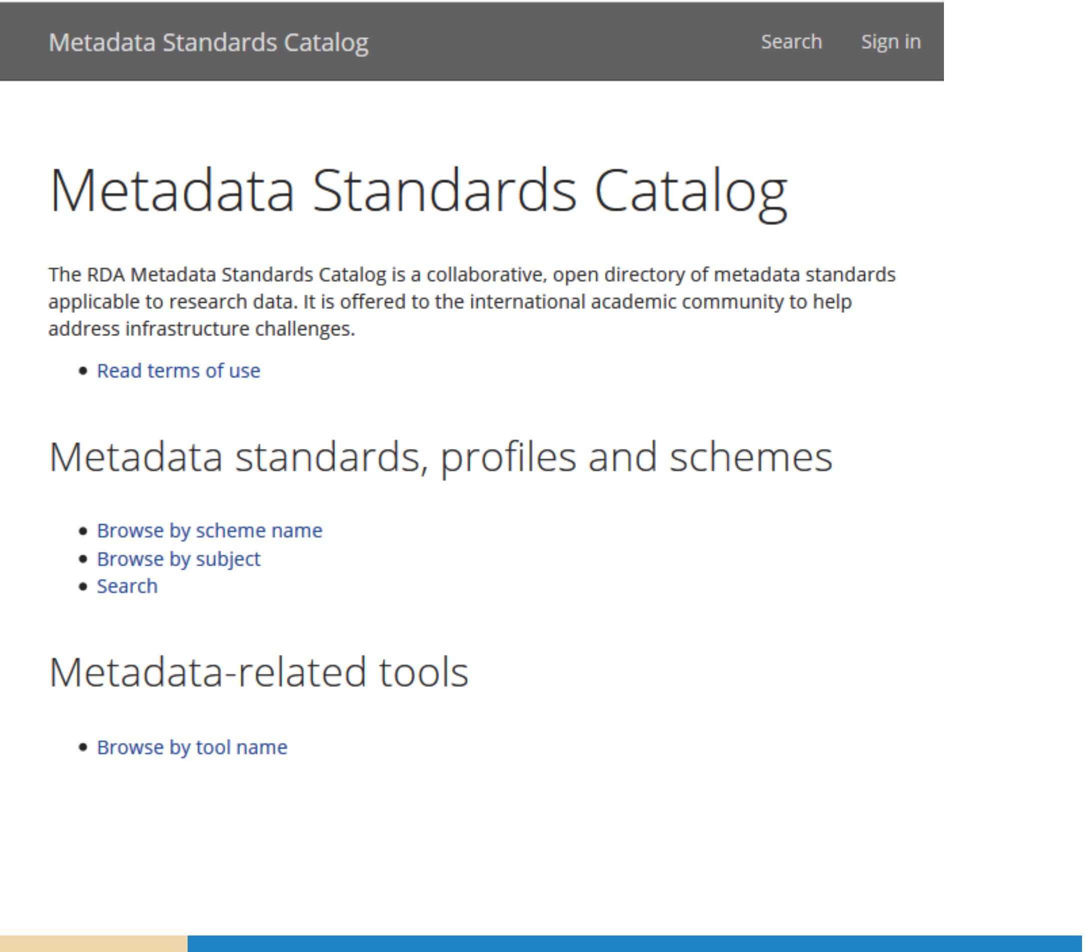
For your full data management plan, please refer to Digital Curation centre's Checklist for a Data Management Plan.

(Source: DMPTool: https://dmp.cdlib.org/; Digital Curation: A How-To-Do-It Manual; Digital Curation Centre: http://www.dcc.ac.uk/)

https://guides.ucf.edu/metadata/datasetmetadata_checklist

Standardi za metapodatke

- http://www.dcc.ac.uk/resources/subject-areas/general-research-data
- http://www.dcc.ac.uk/resources/metadata-standards
- https://guides.ucf.edu/metadata/domMetaStandards
- https://rdamsc.dcc.ac.uk/



Metadata Standards Catalog

The RDA Metadata Standards Catalog is a collaborative, open directory of metadata standards applicable to research data. It is offered to the international academic community to help address infrastructure challenges.

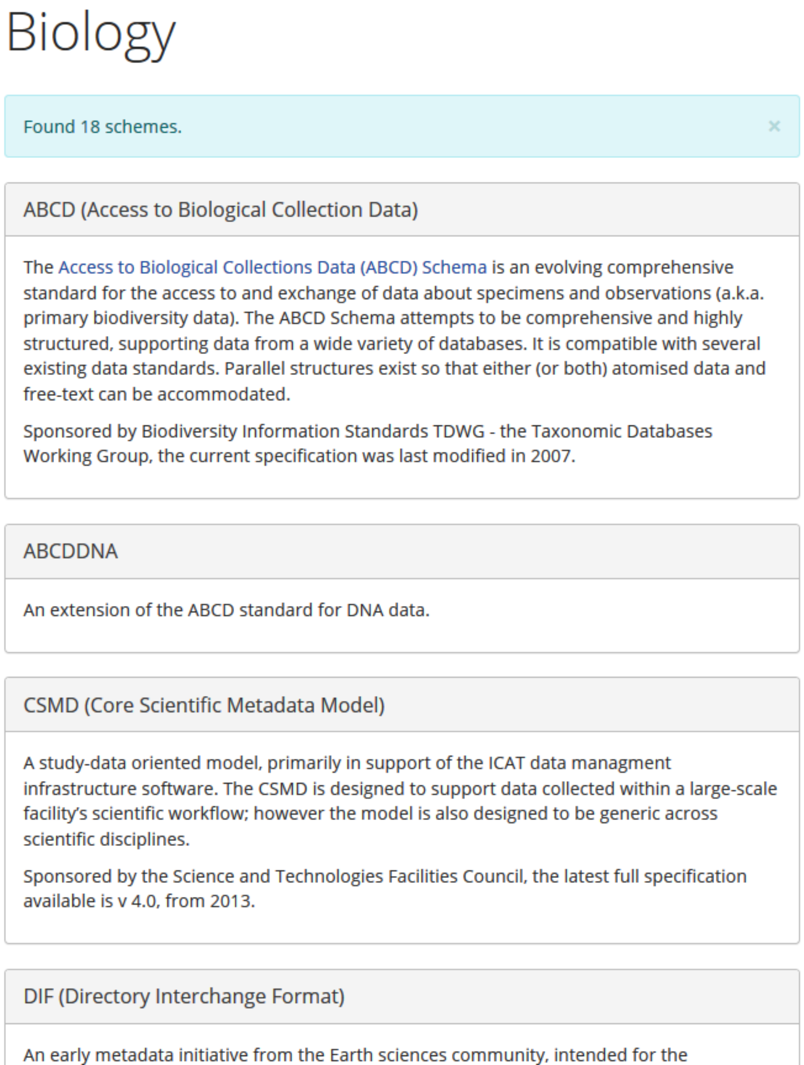
- Read terms of use

Metadata standards, profiles and schemes

- Browse by scheme name
- Browse by subject
- Search

Metadata-related tools

- Browse by tool name



Biology

Found 18 schemes.

ABCD (Access to Biological Collection Data)

The Access to Biological Collections Data (ABCD) Schema is an evolving comprehensive standard for the access to and exchange of data about specimens and observations (a.k.a. primary biodiversity data). The ABCD Schema attempts to be comprehensive and highly structured, supporting data from a wide variety of databases. It is compatible with several existing data standards. Parallel structures exist so that either (or both) atomised data and free-text can be accommodated.

Sponsored by Biodiversity Information Standards TDWG - the Taxonomic Databases Working Group, the current specification was last modified in 2007.

ABCDDNA

An extension of the ABCD standard for DNA data.

CSMD (Core Scientific Metadata Model)

A study-data oriented model, primarily in support of the ICAT data managment infrastructure software. The CSMD is designed to support data collected within a large-scale facility's scientific workflow; however the model is also designed to be generic across scientific disciplines.

Sponsored by the Science and Technologies Facilities Council, the latest full specification available is v 4.0, from 2013.

DIF (Directory Interchange Format)

An early metadata initiative from the Earth sciences community, intended for the

Pitanja?

biblioteka@itn.sanu.ac.rs