World Data System Webinar Series 2024

Rising Stars: A Webinar on Early Career Researchers' Conference Experiences in Data

27 February 2024
4 AM UTC

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Etiquette

Quick Housekeeping Rules Before We Start

Etiquette Page

- Go to worlddatasystem.org/virtual-meeting-etiquette to view our etiquette rules for virtual meetings including this webinar.
- Please put your questions in the Q&A section.
- This webinar will be recorded.

WDS Virtual Meeting Etiquette

Speakers

Maja Dolinar

Claire Rye

Lianchong Zhang

Maja Dolinar
WDS ECR co-chair
ADP Social Science Data Archives
University of Ljubljana

Reflections on IDW 23

Claire Rye
WDS ECR co-chair
New Zealand eScience Infrastructure
University of Auckland

Synthesis of a series of structurally diverse lignans from a single precursor

THE UNIVERSITY OF AUCKLAND
NEW ZEALAND
Te Whare Wānanga o Tāmaki Makaurau

Claire Rye, David Barker*

University of Auckland, School of Chemistry, Auckland, New Zealand. Email: cwil201@aucklanduni.ac.nz


4,4-di(4-hydroxy-3-methoxyphenyl)-2,3-dimethylbutanol

Kadugunstin J

Talumidin

Fragransin A_2

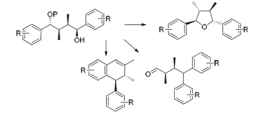
Pycnanthuligene A

Pycnanthuligene B


Introduction

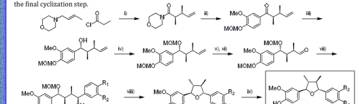
The greatest challenge for chemists who undertake the total synthesis of a natural product is in the conclusion; here success is determined purely by the completion of the molecule. But in some cases the journey can not only demand the use of interesting or novel chemistry but can also lead to unexpected and sometimes exciting side products. This is the story of the side products.

During our work on developing a stereoselective synthesis of manassantin B, a naturally occurring dineolignan which has recently been shown to have potent HIF-1 inhibition (IC_{50} = 3 nM). We carried out model studies which involved synthesizing a series of smaller 2,5-diaryl-3,4-dimethyltetrahydrofuran lignans such as Fragransin A_2 and talaumidin, in order to test the chemistry of the cyclization step which forms the tetrahydrofuran core common to the these lignans. We found differing the substrates and conditions of this cyclization step could significantly change the products formed; and were intrigued that that all the products formed were either natural lignans or derivatives thereof.



Synthesis of fragransin A_2 and talaumidin

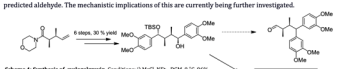
Fragransin A_2 and talaumidin are naturally occurring 2,5-diaryl-3,4-dimethyl tetrahydrofuran lignans both of which have been reported to have interesting biological properties.[2] Our synthesis uses the acyl-Claisen rearrangement as the key transformation to set up the *syn* stereochemistry of the dimethyl substituents. The acyl-Claisen product was found to be a very compatible substrate to which a large variety of lithiates have been added, and thus it was unnecessary to convert the amide to the corresponding aldehyde as we had initially expected, and were pleased with the complete stereocontrol of these additions, which was then maintained in the final cyclization step.



Scheme 1: Synthesis of fragransin A_2 and talaumidin. Conditions: i) 10 mol% AlCl3, crotyl morpholine, iPr2NEt; propionyl chloride, DCM, rt, 24 hours, 93%; ii) 4-bromo-2-methoxy-1-(methoxymethoxy)benzene, t-BuLi, THF, -78 °C, 77%; iii) NaBH4, MeOH, -78 °C, 92%; iv) MOMCl, iPr2NEt, DCM, 0 °C, 91%; v) OsO4, NMO, 1:1 t-BuOH, water, rt, 93%; vi) NaIO4, 3:1 MeOH, water, rt, 82%; vii) R1 =R2 = OCH2O-, 1-bromo-3,4-methylenedioxybenzene, t-BuLi, THF, -78 °C, 46%; R1 = OMOM, R2 = OMe, 4-bromo-2-methoxy-1-(methoxymethoxy)benzene, t-BuLi, THF, -78 °C, 25%; viii) MsCl, NEt_3, DCM, 0 °C, 60-80%; ix) HCl, MeOH, rt 81-83%.

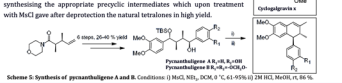
Discovery of further aryltetralone by-products

Keen to take advantage of the modified cyclisation and further elaborate it to the synthesis of a natural product, the cyclisation precursor was synthesised with the aromatic substitution consistent with Kadangustin J. However when the cyclisation was undertaken, another natural product, cyclogalgravin was obtained instead of the predicted aldehyde. The mechanistic implications of this are currently being further investigated.



Scheme 4: Synthesis of cyclogalgravin. Conditions: i) MsCl, NEt_3, DCM, 0 °C, 96%.

Pycnanthuligene A and B were recently isolated from the bark and roots of *Pycnanthus angolensis*, and pycnanthuligene A has been found to have significant antimicrobial activity. With the discovery of being able to synthesize aryltetralones the synthesis of pycnanthuligene A and B were then achieved by synthesising the appropriate precyclic intermediates which upon treatment with MsCl gave after deprotection the natural tetralones in high yield.



Scheme 5: Synthesis of pycnanthuligene A and B. Conditions: i) MsCl, NEt_3, DCM, 0 °C, 61-95%; ii) 2M HCl, MeOH, rt, 86 %.

References

1. Nicolaou, K. C.; Montagnon, T. *Molecules that changed the world*. Wiley-VCH: Weinheim, **2008**; 2-8.
2. Rye, C. E.; Barker, D. *Synlett* **2009**, 20, 3315-3319.
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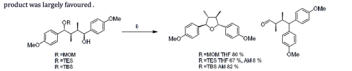
4. Gao, X.-M.; Pu, J.-X.; Huang, S.-X.; Yang, L.-M.; Huang, H.; Xiao, W.-L.; Zheng, Y.-T.; Sun, H.-D. *J. Nat. Prod.* **2008**, 71, 558.
5. Nono, E. C. N.; Mkounga, P.; Kuete, V.; Marut, K.; Hultin, P. G.; Nkengfack, A. E. *J. Nat. Prod.* **2010**, 73, 213.

Acknowledgements

The authors gratefully acknowledge The Royal Society of New Zealand Marsden Fund and The University of Auckland Doctoral Scholarship (CR) for funding this work.

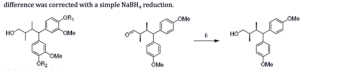
Discovery of diaryl butanol by-products

In order to further investigate the cyclisation step and stereochemistry of the resultant tetrahydrofuran ring, the cyclisation step was attempted with different protecting groups on the nucleophilic oxygen. We found that when we used a TBS protecting group, instead of the tetrahydrofuran ring being formed, aldehyde was instead. Further to this when TES protecting group was used, both products **1** and **2** were observed, although the tetrahydrofuran product was largely favoured.



Scheme 2: Synthesis of Conditions: i) MsCl, NEt_3, DCM, 0 °C, 60-80%.

Kadangustin J, K, and the unnamed *Schisandra* lignan are related naturally occurring neolignans, which have been recently isolated from two plant species within the *Schisandraceae* family. The structural similarities to aldehyde are unmistakeable, differing only in oxidation state and aromatic substitution. The oxidation state difference was corrected with a simple $NaBH_4$ reduction.



Scheme 3: Synthesis of Conditions: i) $NaBH_4$, MeOH, 64 %.

Comparing the ^{1}H-NMR data of alcohol **A** to the data of the neolignans **B** and **C**, we were able to determine that it matched the combined data **B** suggesting that the relative stereochemistry of all three compounds is *syn*, the signals are significantly different from **C** which suggests that it is in fact *anti*.

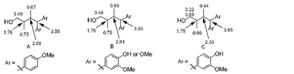
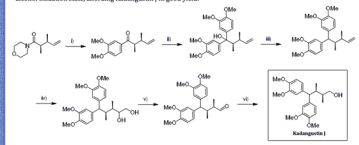


Figure 2. Selected ^{1}H-NMR resonances from alcohol (A) , kadangustin J and K (B) and the unnamed *Schisandra* lignan (C).

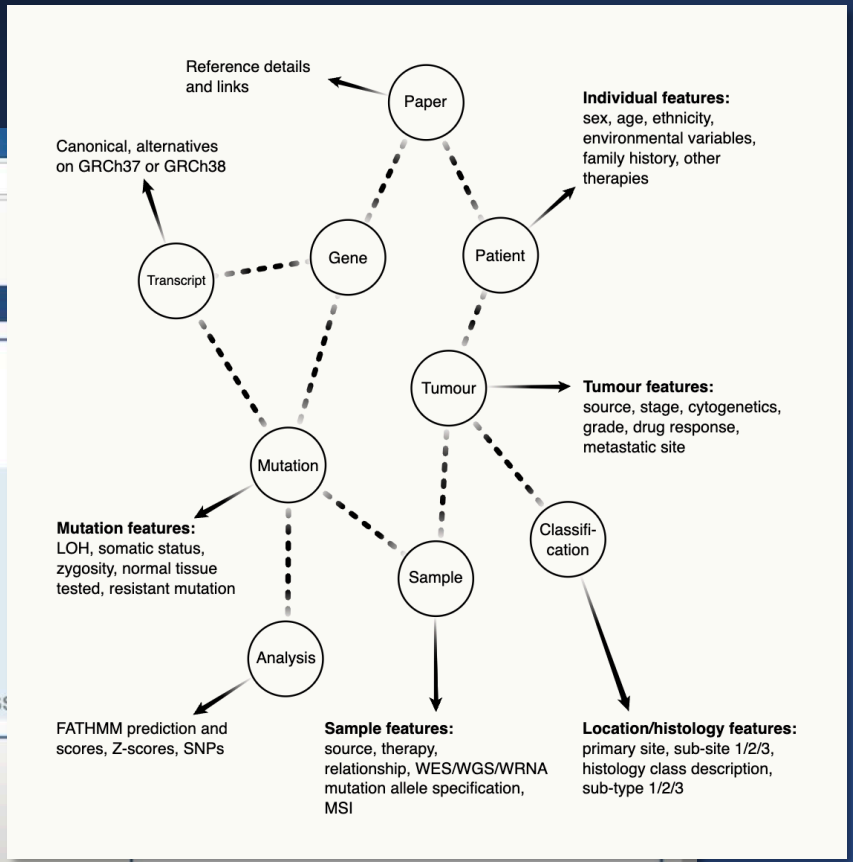
Synthesis of Kadangustin J

A new synthetic strategy was developed for Kadangustin J, this still used the acyl-Claisen derived aromatic ketone, which underwent a second addition of lithiated bromide to afford the corresponding tertiary alcohol. This achieved the desired 1,1-bis aryl system of the kadangustins, which after removal of the tertiary alcohol and manipulation of the terminal alkene gave the corresponding aldehyde. Finally, the aldehyde was reduced to the alcohol oxidation state, affording Kadangustin J in good yield.



Scheme 6: Synthesis of kadangustin J. Conditions: i) 4-bromoveratrole, t-BuLi, THF, -78 °C, 81%; ii) 4-bromoveratrole, t-BuLi, THF, -78 °C, 68%; iii) Et_3SiH, $BF_3.OEt_2$, DCM, 97%; iv) OsO_4, NMO, 1:1 t-BuOH, water, rt, 96%; v) $NaIO_4$, 3:1 MeOH, water, rt, 98%; vi) $NaBH_4$, MeOH, -78 °C, 92%.


PHOX2B Hallmarks of Ca
cancer.sanger.ac.uk/cosmic/census-page/PHOX2B
COSMIC
Catalogue Of Somatic Mutations In Cancer
Projects
Data
Tools
News
Help
About
Genome Version
Search COSMIC...
SEARCH
PHOX2B
switch view
paired-like homeobox 2b
Function summary
neuronal-type-specific transcription factor [Pubmed];
upregulates ALK transcription by directly binding its promoter
[Pubmed]
Promotes
PHOX2B
Suppress
Role in cancer
TSG
Differentiation and development
controls the differentiation of noradrenergic neurons during embryogenesis [Pubmed]
Impact of mutation on function
overexpression of wild-type PHOX2B in neuroblastoma cell lines suppresses cell proliferation and synergizes with all-trans retinoic acid to promote differentiation, mutant protein retains the ability to suppress cellular proliferation, but is not able to promote differentiation or activate expression of a known PHOX2B target gene in vitro [Pubmed]


Reference details and links
Paper
Individual features: sex, age, ethnicity, environmental variables, family history, other therapies
Canonical, alternatives on GRCh37 or GRCh38
Transcript
Gene
Patient
Tumour
Tumour features: source, stage, cytogenetics, grade, drug response, metastatic site
Mutation
Mutation features: LOH, somatic status, zygosity, normal tissue tested, resistant mutation
Classifi-cation
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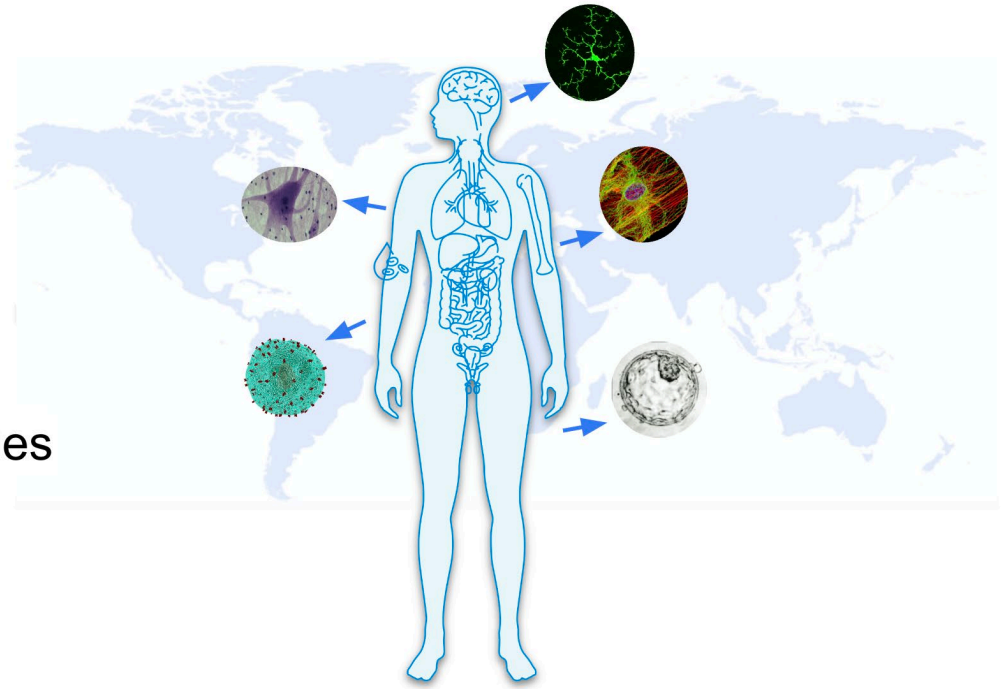
Analysis
FATHMM prediction and scores, Z-scores, SNPs
Sample features: source, therapy, relationship, WES/WGS/WRNA mutation allele specification, MSI
Location/histology features: primary site, sub-site 1/2/3, histology class description, sub-type 1/2/3

The HCA community is profiling millions of diverse human cells

Global effort requiring:

- Hundreds of labs
- Organ-specific data
- Disparate experimental techniques and data types



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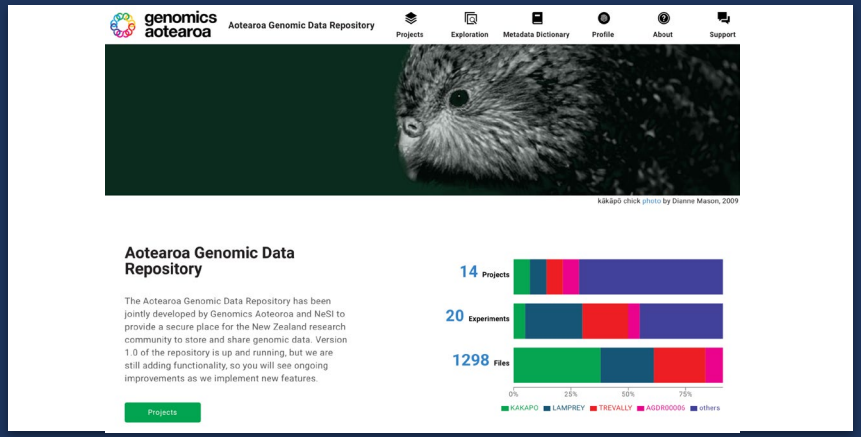
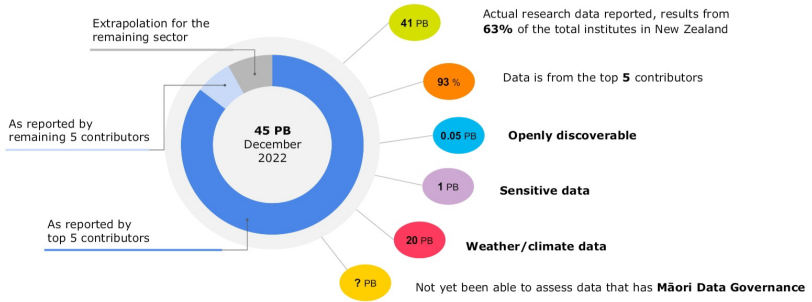
GENOMICS PLATFORM





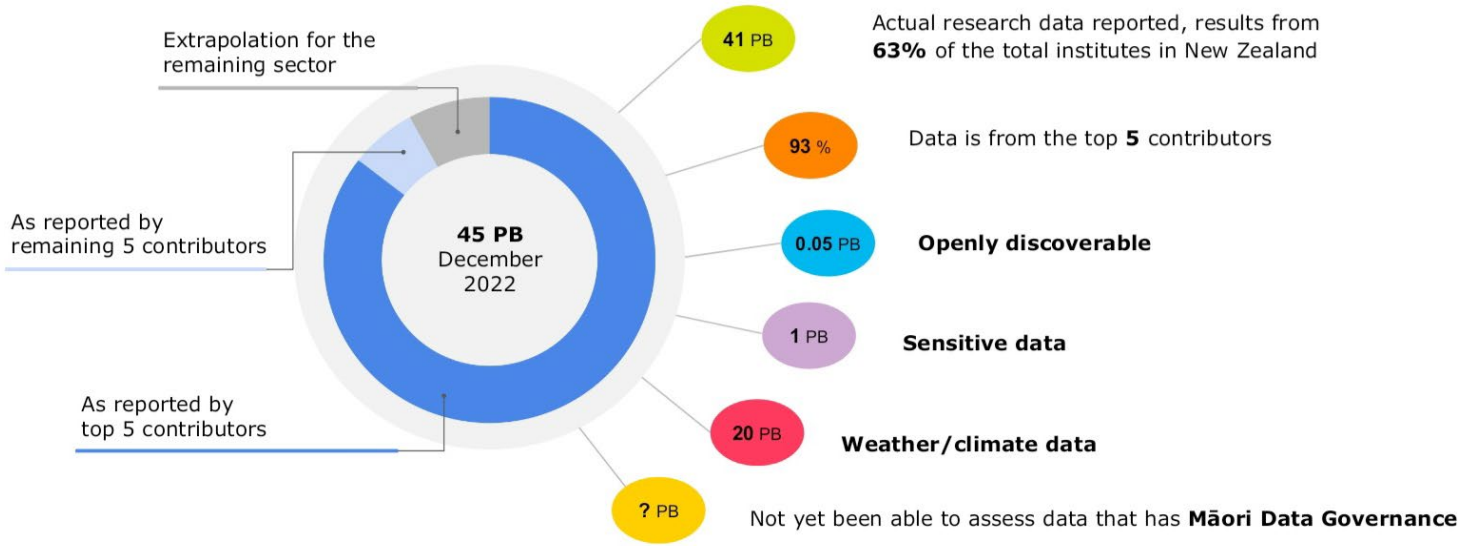
IDW23

- Networking opportunities
- Presenting your work
- Fitting your research into the landscape
- Understanding more about how WDS, RDA and CoData work


A first count of research data at scale
SciDataCon 2023
organized by
CODATA
as part of
International Data Week

A first count of research data at scale

The characterisation experiences from Australia and Aotearoa New Zealand



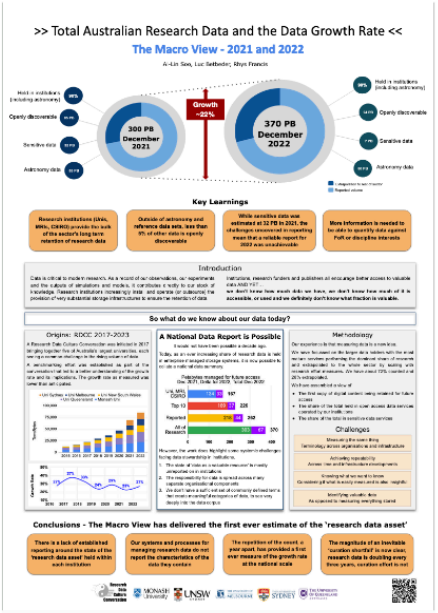
Key Learnings: **We don't know much about the research data we keep!**

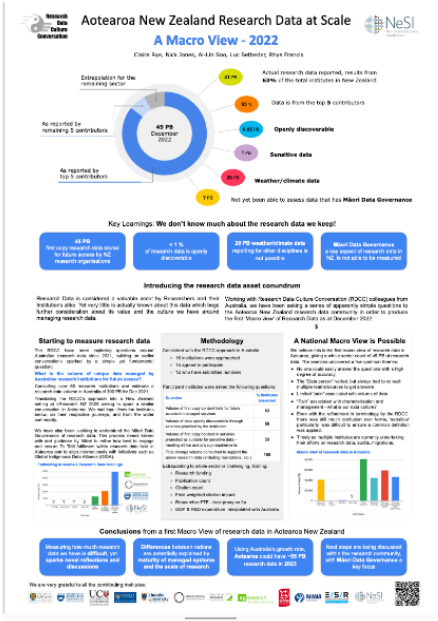
45 PB
first copy research data stored for future access by NZ research organisations

< 1 %
of research data is openly discoverable

20 PB weather/climate data
reporting for other disciplines is not possible

Māori Data Governance
a key aspect of research data in NZ, is not able to be measured





Thank You

The Macro View of Research Data in Australia and Aotearoa New Zealand

claire.rye@auckland.ac.nz

Research Data Culture Conversation

NeSI New Zealand eScience Infrastructure

[DSWS-2023] International Symposium on Data Science 2023

Lianchong Zhang
WDS ECR co-chair
Aerospace Information Research Institute
Chinese Academy of Sciences

International Symposium on Data Science
(DSWS -2023)

– Building an Open Data Collaborative network in the Asia-Oceania area –

11 ～ 15 December 2023

Science Council of Japan
Roppongi, Minato-ku, Tokyo, Japan
(hybrid type conference)

大学共同利用機関法人 情報・システム研究機構 Research Organization of Information and Systems
大学共同利用機関法人 情報・システム研究機構 データサイエンス共同利用基盤施設 Joint Support-Center for Data Science Research (ROIS-DS)
DDBJ
WORLD DATA SYSTEM
CODATA

Dates	Morning (10:00-12:00)	Lunch Time (12:15-14:00)	Afternoon-1 (14:00-15:30)	Afternoon-2 (16:00-17:30)	Dinner Time (19:00-)
11 DEC (MON)			Registration	Registration	Ice breaker dinner
12 DEC (TUE)	Registration		Public Lectures (in Japanese)	Public Lectures (in Japanese)	Reception
13 DEC (WED)	Opening session, Keynote talks	Poster Session (Lightning talks 1; 11:50-12:05) (Core time 1; 13:00-14:00)	Session 1: Challenges of data systems and networks	Session 2: Open Science and the FAIR Principles	Banquet
14 DEC (THU)	Session 3: Lessons learned fron COVID-19 data	Poster Session (Lightning talks 2; 12:00-12:15) (Core time 2; 13:00-14:00)	Session 4: Recent developments in data science	Session 5: Involvement of early career researchers and scientists	Working dinner
15 DEC (FRI))	Session 6: Asia-Oceania data forum	Poster Session (Lightning talks 3; 12:00-12:15) (Core time 3; 13:00-14:00)	Session 7: GEO variables and data mapping for Cold Regions	Strategic discussion, Closing remark	

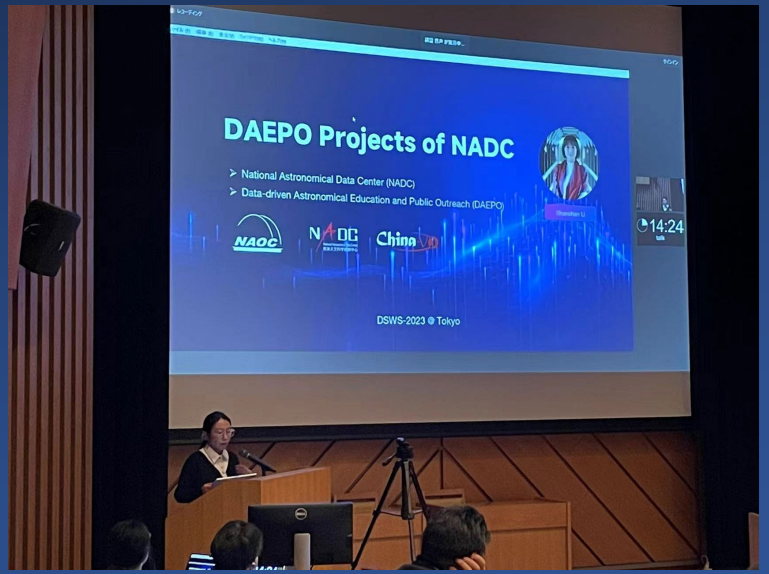
International Symposium on Data Science 2023 (DSWS-2023)

11-15 December 2023
Science Council of Japan

Asia-Oceania data forum

1. The session is an attempt of networking of data repositories and data sciences in the Asia-Oceania area, including WDS, CODATA and other international activities.

2. Discussions on current status and future of open data/science infrastructures in the Asia-Oceania region, as well as in context of international global science data platform.



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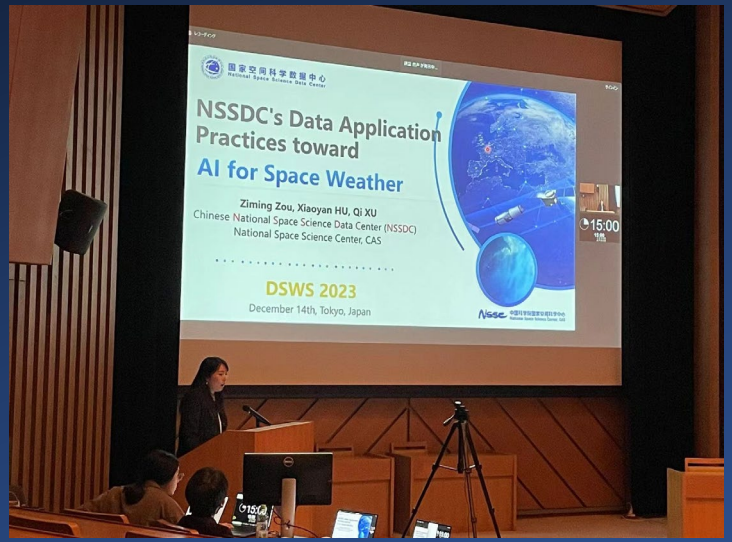
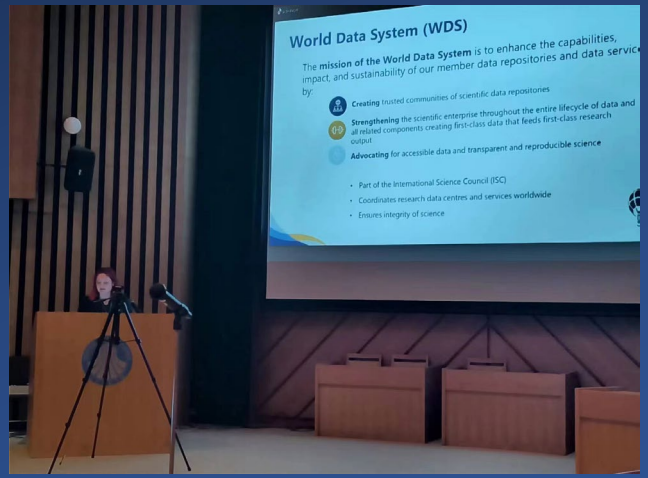
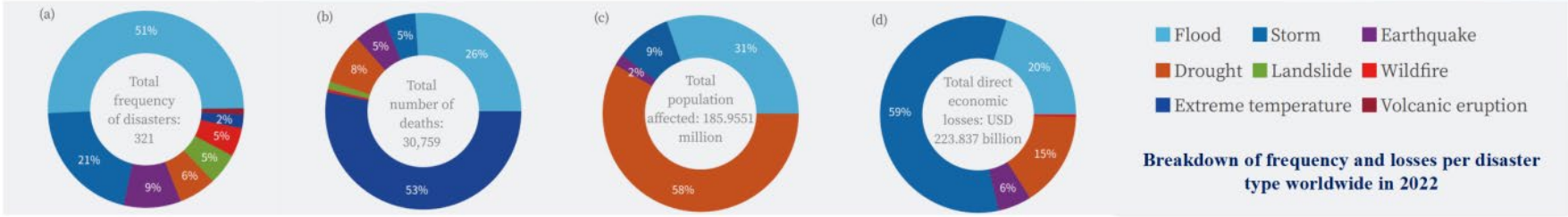


Involvement of early career researchers and scientists

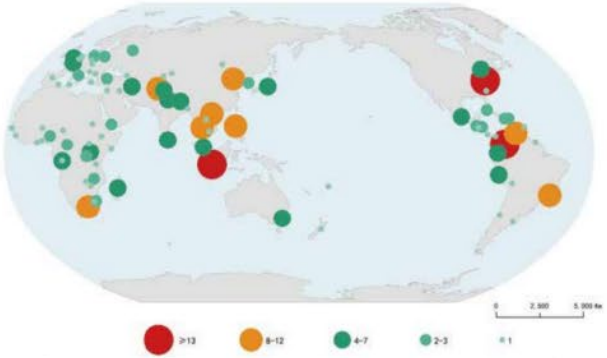
1. A forum for young-generation researchers and scientists in the Asia-Oceania area to identify current and future societal challenges. This session is led by the WDS Early Career Researchers (ECR) Network.

2. Developing proposals on training and activities aimed at increasing engagement of young researchers and scientists in the broad data science community.

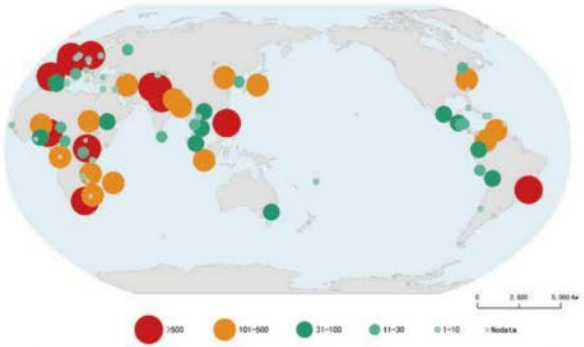




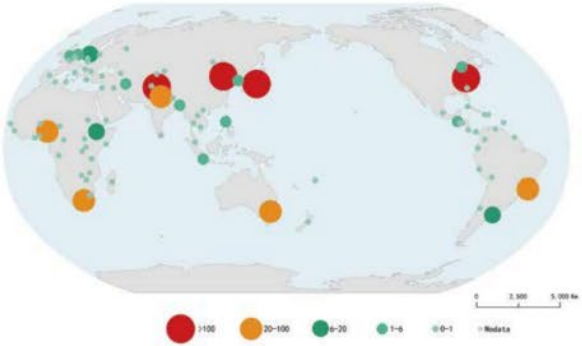
Breakdown of frequency and losses per disaster type worldwide in 2022



Spatial distribution of the frequency of natural disasters by country/region, globally in 2022



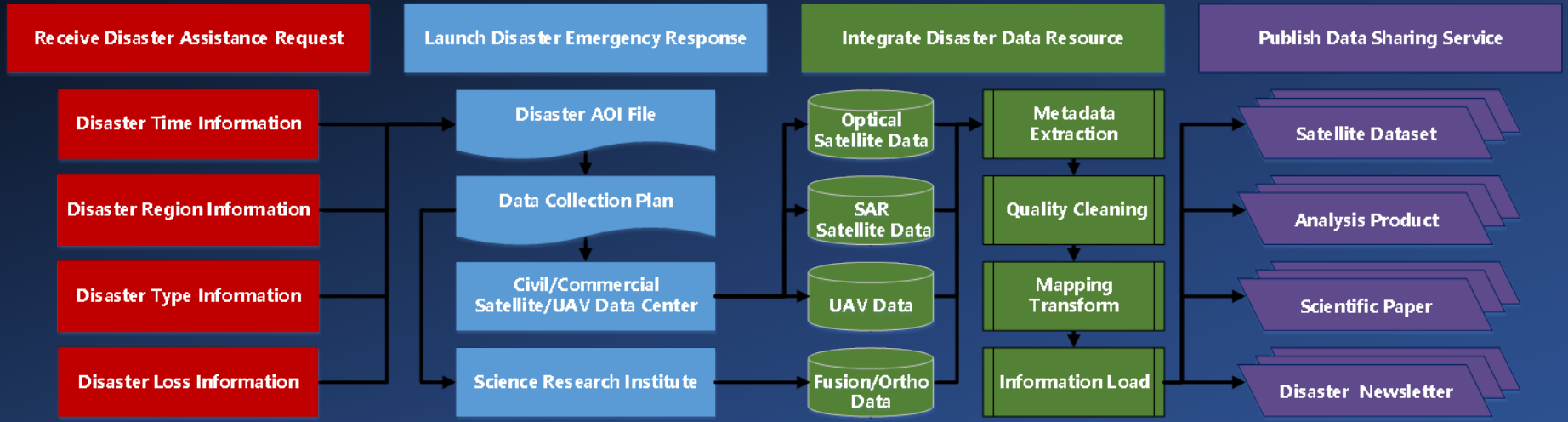
Spatial distribution of the death toll from natural disasters by country/region, globally in 2022



Spatial distribution of direct economic losses from natural disasters by country/region, globally in 2022

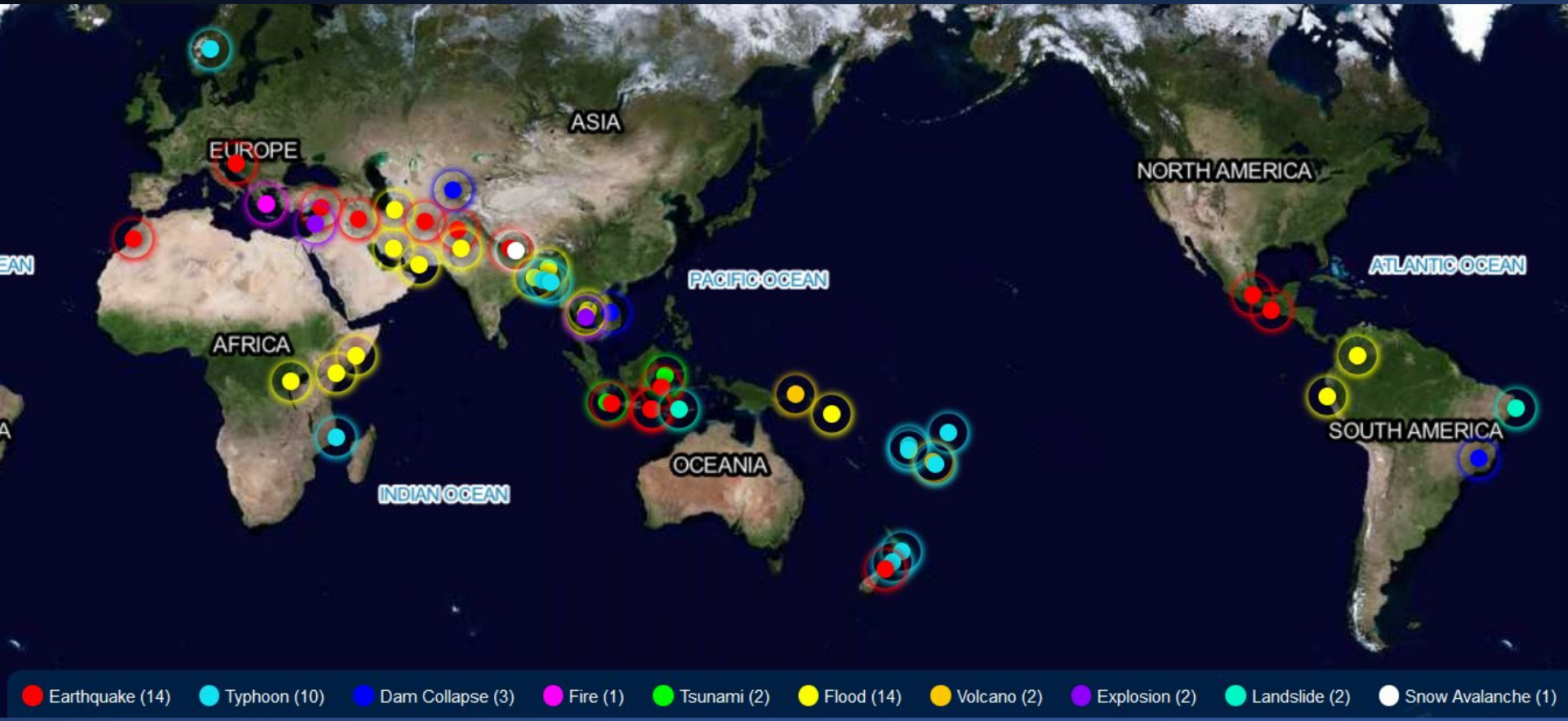
Source: global natural disaster assessment report 2022

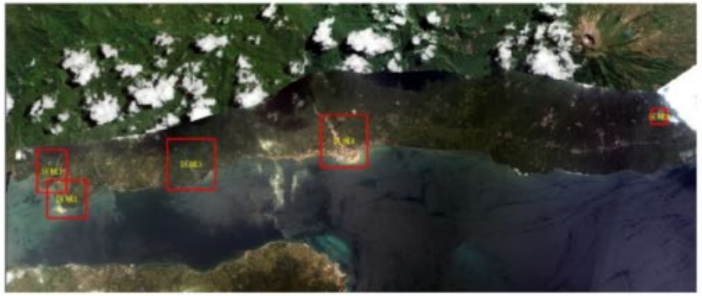
Collaborative network of Disaster Data Response (CDDR)



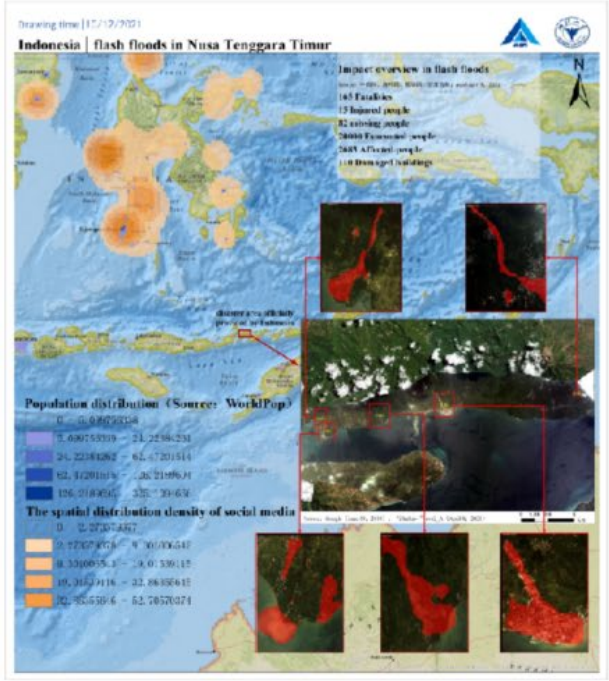
NODA 中国·GEO AIR NSMC UNITED NATIONS ESCAP unitar United Nations Institute for Training and Research

IRDR Integrated Research on Disaster Risk Tonkin+Taylor CODATA 理化学研究所 HOT Humanitarian Open Street Map Team


ASIA
EUROPE
NORTH AMERICA
PACIFIC OCEAN
ATLANTIC OCEAN
AFRICA
SOUTH AMERICA
OCEANIA
INDIAN OCEAN
Earthquake (14)
Typhoon (10)
Dam Collapse (3)
Fire (1)
Tsunami (2)
Flood (14)
Volcano (2)
Explosion (2)
Landslide (2)
Snow Avalanche (1)



Landslide distribution



Remote sensing

- Zhuhai No. 1 (OSH-2C, OSH-3B, OSH-3C)
- Planet

Media data

- Twitter
- News

Auxiliary data

- Population distribution data
- NAdministrative Division Data
- Disaster loss statistics

Comprehensive mapping of disaster analysis

Q&A

Please type your questions in Q&A

Your Opinion is Our Progress

Help Shape Our Future with Your Feedback!

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