

Update on NORMAN Suspect List Exchange (NORMAN-SLE)

Prof. Dr. Emma L. Schymanski
and Hiba Mohammed Taha
(plus many, many colleagues and collaborators!)

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Web: <https://www.uni.lu/lcsb-en/research-groups/environmental-cheminformatics/>

NORMAN Cross Working Group Non-Target Screening
Virtual Meeting, 7 December 2023



Slides available at
DOI: [10.5281/zenodo.10072510](https://doi.org/10.5281/zenodo.10072510)

Updated content: 12 new lists (more coming)



Hiba
Mohammed
Taha

NORMAN-SLE Summary

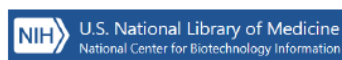
Category	Number	Comment
Number of Lists	111	S0 to S111
Total Unique Compounds	115,669	From PubChem NOR
Total Live Substances	118,557	From PubChem NOR
Total Live Annotations	22,229	From PubChem NOR
Largest List	109,631	S0 NORMAN-SusDa
Smallest List	16	S98 TIRECHEM
Total Views	86,005	From Zenodo (see b
Unique Downloads	76,175	From Zenodo (see b
Citations	61	From Zenodo (see b

S100 PFASREACH List of PFAS identified in REACH 2019	?	↗	432
S101 MTMDUST List of chemicals characterised in indoor dust samples	?	↗	298
S102 PARCPFAS List of PFAS from PARC WP4	?	↗	190
S103 NORMANUVCB NORMAN Dataset of Curated UVCB Mappings	?	↗	417
S104 UKVETMED UK Veterinary Medicines Directorate's List	?	↗	420
S105 P65CHEM Californian Proposition 65 warning list of chemicals	?	↗	749
S106 AQUALity19 EU AQUALity's water analysis list 2019	?	↗	238
S107 AQUALity20 EU AQUALity's water analysis list 2020	?	↗	382
S108 SINLIST SIN (Substitute It Now) list of hazardous chemicals by ChemSec	?	↗	653
S110 DUTCHUSE Dutch Prioritized Chemical Use Categories	?	↗	1,739
S111 PMTPFAS Fluorine-containing Compounds in PMT Suspect Lists	?	↗	180

S109 in progress...

Last updated 3/11/2023. More details per list in [NORMAN-SLE_List_Overview_20220504.csv](#).

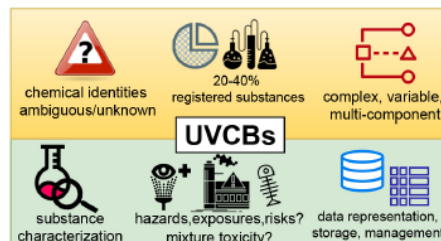
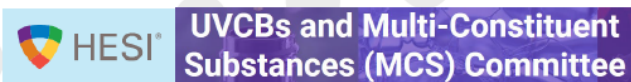
UVCBs are underway ...



Integrating UVCBs and Related Data into Open Chemical Knowledgebases

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National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health



Lai et al. (2022) ES&T DOI: [10.1021/acs.est.2c00321](https://doi.org/10.1021/acs.est.2c00321)

Workshop, 18-19 Sept 2023
(presented remotely)

Slides available at DOI: [10.5281/zenodo.8302440](https://doi.org/10.5281/zenodo.8302440)



Workshop, 18-19 Sept 2023
(presented remotely)

Slides & poster available at
DOI: [10.5281/zenodo.8302440](https://doi.org/10.5281/zenodo.8302440)

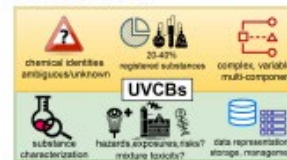


Integrating UVCBs and Related Data into Open Chemical Knowledgebases – PubChem and NORMAN-SLE Examples

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UVCBs are ...



PubChem is ...

- A large open chemical database
- >115 million compounds
- >300 million substances
- >930 data sources
- ...and much, much more

<https://pubchem.ncbi.nlm.nih.gov/>

NORMAN is ...

- A worldwide network on emerging substances of concern, based in Europe
- UVCBs a priority topic since Dec. 2022
- Action via NORMAN Suspect List Exchange
- ...first data @ DOI: [10.5281/zenodo.7414795](https://doi.org/10.5281/zenodo.7414795)

<https://www.norman-network.com/>

Lai et al. (2022) DOI: [10.1021/acs.est.2c00321](https://doi.org/10.1021/acs.est.2c00321); Kim et al. (2023) DOI: [10.1093/nar/nkac956](https://doi.org/10.1093/nar/nkac956); Mohammed Taha et al. (2022) DOI: [10.1186/s12302-022-00680-6](https://doi.org/10.1186/s12302-022-00680-6)

Examples of HESI UVCBs (and associated data) in PubChem

Example UVCBs – PubChem / NORMAN-SLE Efforts

Value Adding UVCB Data

This work was supported in part by the National Center for Biotechnology Information (NCBI) of the National Library of Medicine (NLM), National Institutes of Health (NIH)



NORMAN-SLE Outreach



Hiba Mohammed Taha • 1st

Data enthusiast | Cheminformatics | Data Curation | R |

1w • 🌐

Indeed a memorable day for the records with my little girl....!!!

Honored to have represented NORMAN Suspect List Exchange (SLE) at IDW-SciDataCon WORLDFAIR session with a talk on "NORMAN-SLE -Unleashing the Power of Chemical Data beyond FAIR"

slides here : <https://lnkd.in/exSFWKaN>

Thank you [University of Luxembourg](#) , [Emma Schymanski](#) and the fantastic organizers for this amazing opportunity!

#IDWeek2023 #IDWSalzburg2023 #OpenScience #FAIRChemistry
#Cheminformatics #SessionSpeaker



October 23, 2023 (v2 pdf)

Presentation

Open

NORMAN-SLE: Unleashing the Power of Chemical Data Beyond FAIR

MOHAMMED TAHA, Hiba ; Schymanski, Emma

Talk given by Hiba at IDW-SciDataCon Salzburg 2023

Uploaded on October 23, 2023

1 more versions exist for this record



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Acknowledgements!

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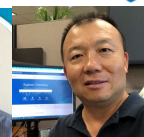
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PubChem

... &
team



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