

## **NFDI4Chem, Chemistry Consortium in the NFDI**

Activity Update

**Analysis of the Landscape of Repositories for Chemistry in re3data**

TA3 – Repositories

Lead Institution: FIZ Karlsruhe

TA lead: Felix Bach (FIZ)

Contributing partner(s): FIZ Karlsruhe, IPB Halle & JGU Mainz

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Authors of this report: Christian Bonatto Minella (FIZ), Tillmann Fischer (IPB), John Jolliffe (JGU)

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## Detailed report on the activity

In Summer 2023, we carried out an analysis of repositories for chemistry data in re3data [1]. When applying the filters “Chemistry” and “Worldwide” **252** repositories were listed. Subsequently, additional filters were applied: after filtering for “Database Access: Open”, **220** repositories remained, after applying “Content Types: raw data”, **100** repositories were displayed and finally, only **98** repositories resulted after applying the filter “Repository Languages: English”.

However, we quickly realised that while the repositories provided raw data, the ingestion of these raw data was not possible or only possible for a selected group of users (e.g. for institutional repositories). Re3data does not currently provide a field that allows it to filter for repositories that allow ingestion of data submitted by anyone in the world.

We were therefore forced to apply the following filters manually:

- Ingestion of raw data possible
- Submission of raw data not restricted to a selected group of users (i.e. open to anyone)
- Submission possible independent of the country of origin

After applying these two filters manually, only **12** repositories remained which are as follows:

#	Name	Homepage	re3data	In federation of NFDI4Chem repositories?
1	Chemotion	<a href="https://www.chemotion-repository.net/welcomee">https://www.chemotion-repository.net/welcomee</a>	<a href="https://www.re3data.org/repository/r3d100010748">https://www.re3data.org/repository/r3d100010748</a>	Yes
2	Environmental Data Initiative Repository	<a href="https://portal.edirepository.org/nis/home.jsp">https://portal.edirepository.org/nis/home.jsp</a>	<a href="https://www.re3data.org/repository/r3d100010272">https://www.re3data.org/repository/r3d100010272</a>	No
3	European MassBank	<a href="https://massbank.eu/MassBank/">https://massbank.eu/MassBank/</a>	<a href="https://www.re3data.org/repository/r3d100011839">https://www.re3data.org/repository/r3d100011839</a>	Yes
4	Materials Cloud Archive	<a href="https://archive.materialscloud.org/">https://archive.materialscloud.org/</a>	<a href="https://www.re3data.org/repository/r3d100012611">https://www.re3data.org/repository/r3d100012611</a>	No
5	NoMaD Repository & Archive	<a href="https://nomad-lab.eu/services/repo-ar">https://nomad-lab.eu/services/repo-ar</a>	<a href="https://www.re3data.org/repository">https://www.re3data.org/repository</a>	Yes

		<a href="#">ch</a>	<a href="#">/r3d100011583</a>	
<b>6</b>	nmrXiv	<a href="https://nmrxiv.org/">https://nmrxiv.org/</a>	<a href="https://www.re3data.org/repository/r3d100014211">https://www.re3data.org/repository/r3d100014211</a>	<b>Yes</b>
<b>7</b>	Protein Data Bank in Europe	<a href="https://www.ebi.ac.uk/pdbe/">https://www.ebi.ac.uk/pdbe/</a>	<a href="https://www.re3data.org/repository/r3d100010538">https://www.re3data.org/repository/r3d100010538</a>	No
<b>8</b>	ProteomeXchange	<a href="http://www.proteomexchange.org/">http://www.proteomexchange.org/</a>	<a href="https://www.re3data.org/repository/r3d100010692">https://www.re3data.org/repository/r3d100010692</a>	No
<b>9</b>	RADAR4Chem	<a href="https://radar.products.fiz-karlsruhe.de/en/radarabout/radar4chem">https://radar.products.fiz-karlsruhe.de/en/radarabout/radar4chem</a>	<a href="https://www.re3data.org/repository/r3d100014010">https://www.re3data.org/repository/r3d100014010</a>	<b>Yes</b>
<b>10</b>	SABIO-RK	<a href="http://sabiork.h-its.org/">http://sabiork.h-its.org/</a>	<a href="https://www.re3data.org/repository/r3d100011052">https://www.re3data.org/repository/r3d100011052</a>	No
<b>11</b>	STRENDA DB	<a href="https://www.beilstein-strenda-db.org/strenda/">https://www.beilstein-strenda-db.org/strenda/</a>	<a href="https://www.re3data.org/repository/r3d100012329">https://www.re3data.org/repository/r3d100012329</a>	<b>Yes</b>
<b>12</b>	The Cambridge Structural Database	<a href="https://www.ccdc.cam.ac.uk/solutions/csd-system/components/csd/">https://www.ccdc.cam.ac.uk/solutions/csd-system/components/csd/</a>	<a href="https://www.re3data.org/repository/r3d100010197">https://www.re3data.org/repository/r3d100010197</a>	<b>Yes</b>

Of these 12 repositories, **7** are part of the NFDI4Chem federation [2].

Concluding, NFDI4Chem currently provides a valuable service to the chemistry community (at least according to the re3data analysis) with few alternatives and for specific data types, there are, at the moment, no other options to the repositories included within the NFDI4Chem federation.

## References

[1] <https://www.re3data.org/>

[2] [https://knowledgebase.nfdi4chem.de/knowledge\\_base/docs/choose\\_repository/](https://knowledgebase.nfdi4chem.de/knowledge_base/docs/choose_repository/)