

from many large bilateral donors outside the United States has plummeted by 57% over the past decade. Overall, in 2021, international resources available for HIV were 6% lower than in 2010, according to UNAIDS. On this basis, an expensive new drug will not be affordable, researchers and campaigners are arguing.

In an open letter to Deborah Waterhouse, who is ViiV's chief executive, a group of more than 70 politicians, civil-society activists, researchers and heads of philanthropic organizations urged the company to set the price of cabotegravir "as close as possible" to that of existing HIV prevention medicines, which they say is around \$60 per person per year – equivalent to \$10 per cabotegravir dose.

A ViiV spokesperson said in an e-mail to

*Nature* that a \$10 price is not realistic because cabotegravir is more complex and therefore more expensive than "a simple white tablet". Moreover, a low price could prevent generics manufacturers from coming forward. "It's important not to stifle generic interest in development and manufacture through the voluntary licence agreement we have just finalized by setting unrealistic expectations on price now."

The spokesperson said all manufacturers can apply to make generic copies of the drug, and that three licences will be awarded in the first instance. "We have the ability to increase the number of sub-licences in future if we think the demand signals are supportive and there is a need," the spokesperson added.

concern for the 992 entries implicated in the preprint and has removed 12 structures that were described in 9 papers that have been retracted. Because the investigation is still ongoing, 277 of the flagged structures were omitted from the latest desktop data update in mid-June. If publishers decide to retract a paper, the data will also be retracted. "We mirror the literature," says Sophie Bryant, marketing manager at the CCDC in Cambridge, UK.

### Ongoing investigations

Affected journals are also investigating the preprint's allegations. Chris Graf, director of research integrity at Springer Nature, says that it is investigating the concerns in 157 papers published in at least 5 of its journals. "Should these concerns turn out to be well founded, they would very much support the need for the publishing industry to work collaboratively to address the issue of paper mills," Graf says. (*Nature's* news team is editorially independent of Springer Nature, its publisher.)

Publisher Wiley says that it has already retracted two articles from the *Journal of the Chinese Chemical Society*, both of which were listed in Bimler's preprint. It is investigating a further 50 articles published in at least 15 journals – more than the 25 papers that were flagged in the preprint. Elsevier, which published 88 of the papers in at least 4 journals, says that it is investigating and will report its findings in due course. A spokesperson for Taylor & Francis, which published 204 of the papers in at least 2 journals, says that it is actively investigating a large number of articles. "Our investigation originated with an internal audit we ran in 2021 and was expanded following concerns raised to us by researchers," the spokesperson says.

Chemist Filipe Almeida Paz at the University of Aveiro in Portugal is shocked by the situation. Researchers use the CCDC's database to inform drug discovery, he says, and incorrect data will ultimately waste time, so it is important that the database is not "contaminated with wrong information".

"It creates the possibility that people are wasting their time looking at materials that have never been made," says Randall Snurr, a chemical engineer at Northwestern University in Evanston, Illinois.

Jon Clardy, a biological chemist at Harvard Medical School in Boston, Massachusetts, says that the paper mill has been "extraordinarily clever" to combine metal-organic frameworks with applications such as cancer immunotherapy, because the chances that people have studied both topics in depth are slim.

The CCDC is now looking at whether its processes need to change. Discussions are continuing about developing more automated screening to help its integrity team to identify and prioritize what to look at more closely, says Suzanna Ward, head of the CCDC's database.

# MAJOR CHEMICAL DATABASE INVESTIGATES SUSPICIOUS STRUCTURES

Hundreds of entries are undergoing extra checks amid fears that they are based on bogus data.

By Holly Else

**T**he Cambridge Crystallographic Data Centre (CCDC), a go-to resource for chemists seeking information on crystal structures, is reviewing almost 1,000 database entries after a research-integrity sleuth flagged the underlying scientific papers as potentially coming from paper mills – businesses that sell fake scientific papers to researchers who want them for their CVs.

The CCDC's database, called the Cambridge Structural Database, has never before seen such a large number of entries flagged as suspicious. The centre says that 992 entries are potentially affected, but that these represent a "very small amount of the total".

The CCDC has been collating data on the crystal structures of small organic and metal-organic molecules since 1965, and currently lists more than one million structures. Its database is accessible online and through a desktop app, and is an important resource for chemists and biochemists. Many journals in the field of crystallography require researchers to deposit their structural data with the CCDC.

The Cambridge Structural Database does retract entries from time to time, when individual papers get retracted from the literature. In 2010, it retracted 70 entries because of falsified data. But fewer than 300 structures have been retracted during its lifetime.

The latest expressions of concern were prompted by a preprint on the Research Square repository that flagged more than 800 questionable papers published in crystallography and exotic-chemistry journals between 2015 and 2022 (D. Bimler Preprint at Research Square <https://doi.org/hrzg:2022>). Many of the papers propose medical applications for metal-organic frameworks, a class of sponge-like materials that comprise both metal ions and organic molecules. The author of the preprint, retired psychology researcher David Bimler, noted that, in these papers, images and spectra had been repeated. The

**"It creates the possibility that people are wasting their time looking at materials that have never been made."**

papers also bear the hallmarks of having been produced by a paper mill, including recycled and irrelevant references, suspicious e-mail addresses and strange turns of phrase.

CCDC staff members do tests to scrutinize the submitted data and hand check each entry. Some were already suspicious of a handful of structures on Bimler's list before the preprint was posted. When they saw his analysis, they launched an investigation.

So far, the CCDC has issued expressions of