



# COMPOSITION OF THE F2X-UNIVERSAL AND F2X-ENTRY FRAGMENT LIBRARIES

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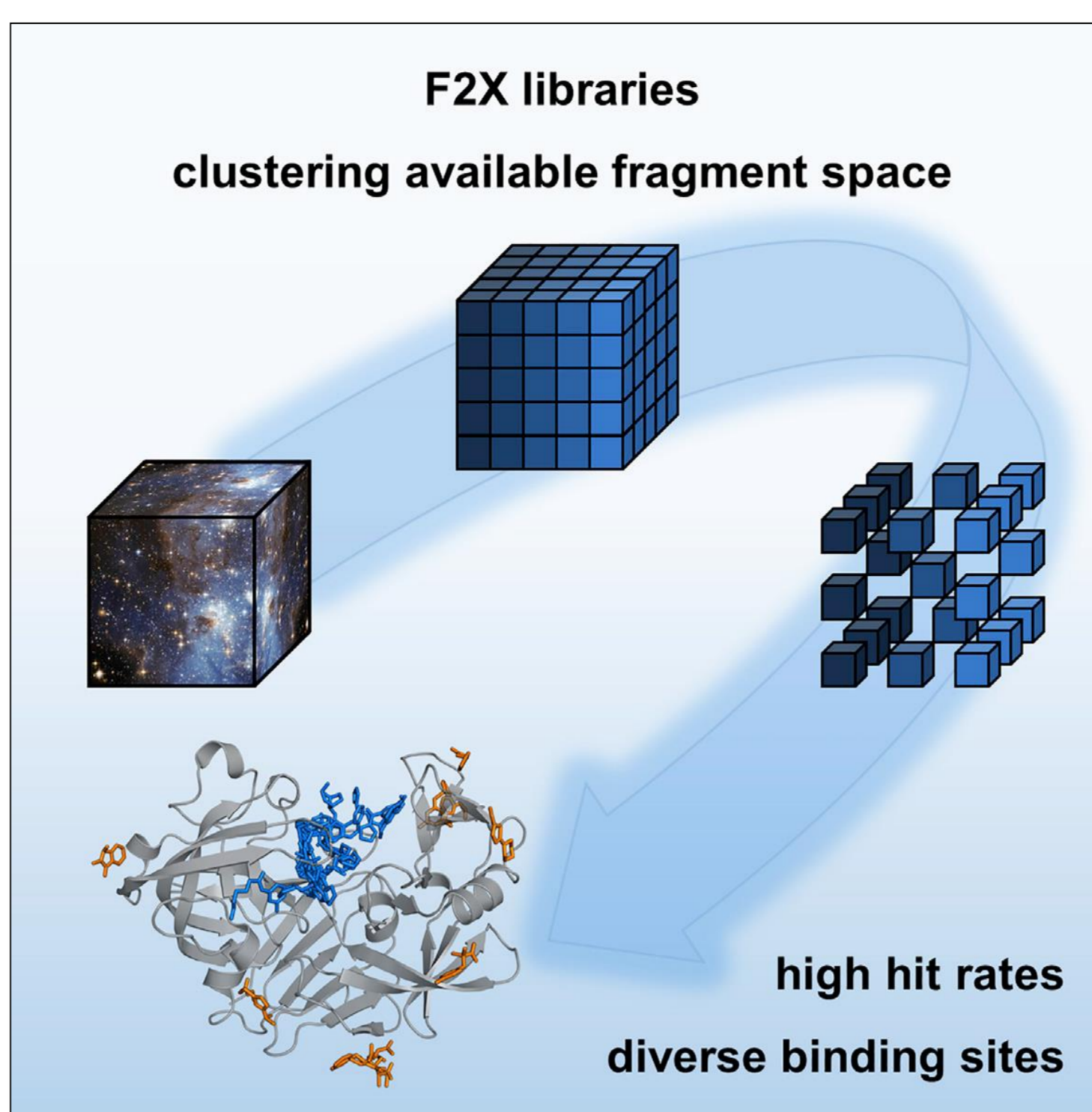
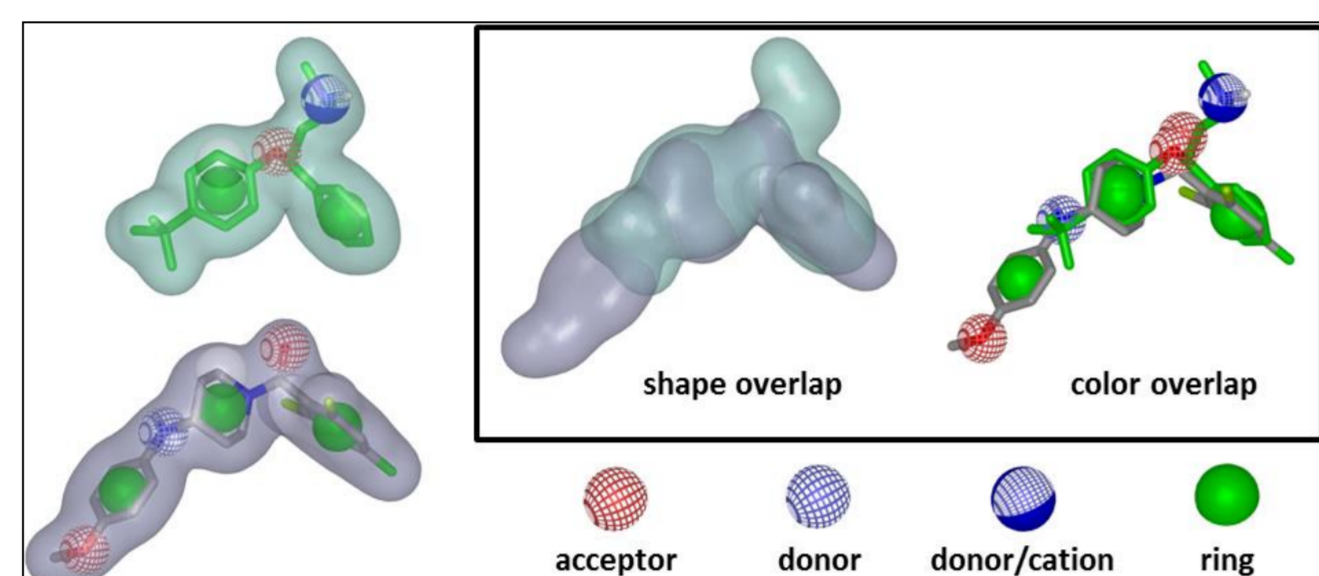
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## Representing the Available Fragment Space

Crystallographic fragment screening (CFS) provides excellent starting points for drug discovery or biochemical tool compound development. A prerequisite for effective CFS is a versatile fragment library. Here, we present the assembly of the 1,103-compound F2X-Universal Library and its 96-compound sub-selection, the F2X-Entry Screen. Both represent the available fragment space and are highly diverse in terms of their 3D-pharmacophore variations.

Pharmacophore diversity was achieved by hierarchical clustering based on ROCS similarity.

fastROCS, OpenEye Scientific Software. <http://www.eyesopen.com>.



## Results of Screening Campaign

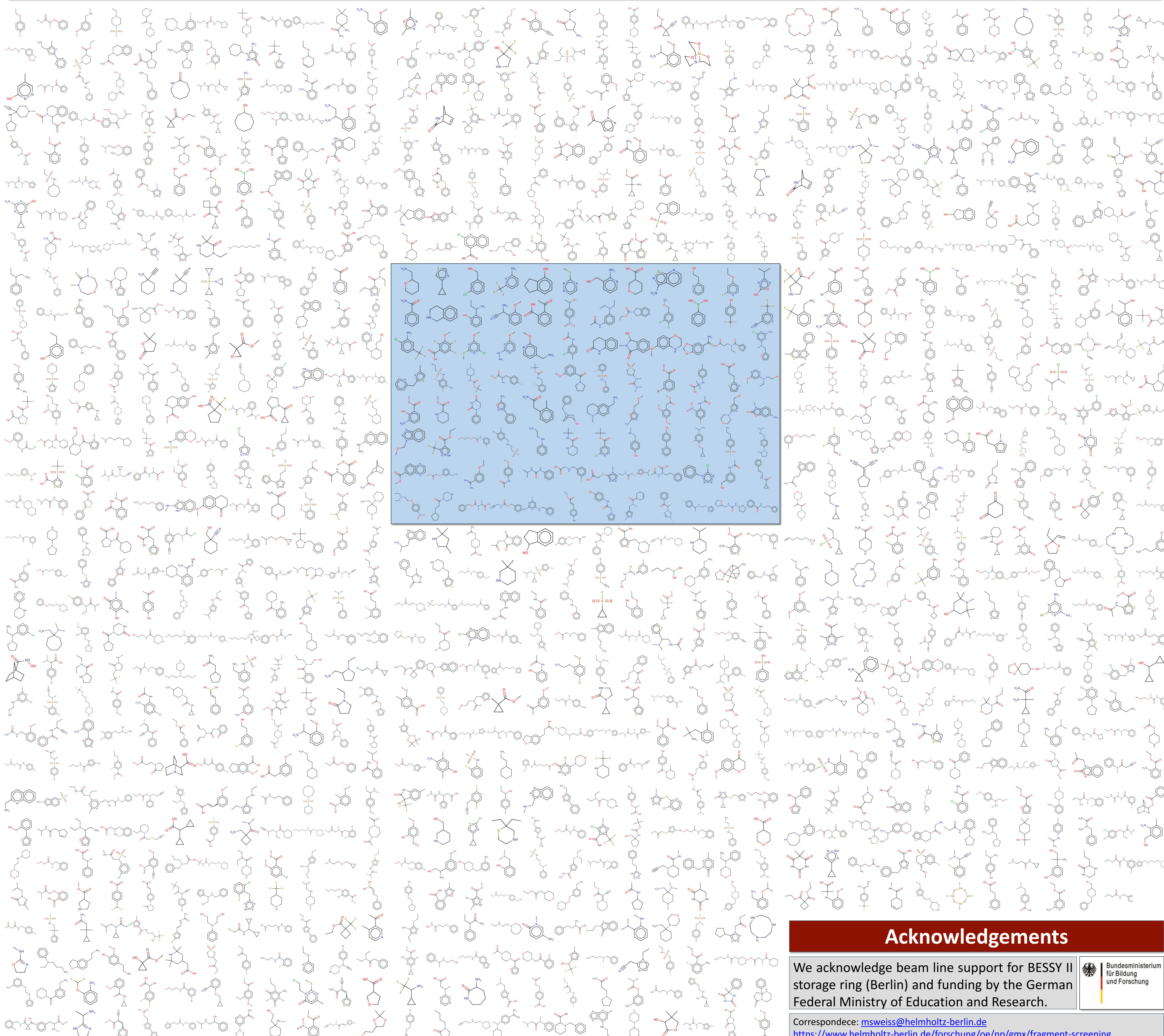
- F2X-Entry Screen validated by two crystallographic fragment-screening campaigns
- High hit rates: 30% versus endothiapepsin and 21% versus the Aar2/RNaseH protein complex
- Formulation as immobilized, dry compounds allows for soaking with and without DMSO

Wollenhaupt and Metz et al.,  
*Structure* 2020, 28, 694.

For crystal structures & details see  
**Poster of Jan Wollenhaupt**

At present, the F2X-Universal Library and the F2X-Entry Screen are available for users of the macromolecular crystallography beamlines of the BESSY II synchrotron in Berlin free-of-charge on the basis of a collaboration contract. Moreover, the F2X-Entry Screen will be made available to everyone on the basis of a material transfer agreement.

## All 1103 Fragments Contained in the F2X-Universal Library and the F2X-Entry Sub-Selection (central box)



## Acknowledgements

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<https://www.helmholtz-berlin.de/forschung/oe/np/gmx/fragment-screening>