

Natural Product-like Fragment Library

A remarkable structural diversity and drug-likeness of molecular scaffolds identified in natural compounds provide a basis for the design of novel natural product-derived compound libraries for drug discovery [1,2]. Implementation of natural product-like frameworks into fragment-based drug discovery (FBDD) might benefit from using biologically validated areas of chemical space not occupied by average synthetic molecules [3,4].

Life Chemicals presents a proprietary Collection of Natural Product-like Fragments generated via the Scaffold Tree approach [5]. The resulting Screening Library comprises over **3,800** synthetic fragments similar to natural compounds as promising starting points for FBDD within an attractive chemical space.

Compound selection

Over 17,000 level-two and level-three scaffolds were extracted from the Universal Natural Product Database and COCONUT online: Collection of Open Natural Products database (comprising over 406, 000 structures in its current version) [6, 11] using scaffold tree analysis. The selection has been made with substructure search for natural-like scaffolds and most relevant groups: coumarins, urolithins, flavonoids, aurones, alkaloids, bile acids, aryl benzothiazole, benzofuran, benzoxazole, carbohydrate, arylpiperazine, arylpiperidine, benzodiazepine, benzothiophene, benzylpiperidine, indole, indoline, indolizine, isoquinoline, purine, quinazolinone, quinoline, quinoxaline, steroids, tetrahydroisoquinoline, chromone, tetrahydroquinoline, etc., that were presented in the databases.

After excluding undesirable and primitive chemotypes, the remaining ca. 4,000 structures were used for substructure search within the Life Chemicals [HTS Compound Collection](#) and [General Fragment Library](#). In addition to that, fragment-like molecules derived from scaffolds showing over 85 % similarity with the natural product-derived scaffold set mentioned above were included as well. Finally, additional structural filtering was performed.



The compound selection can be customized based on your requirements, cherry-picking is available.



Please, contact us at orders@lifechemicals.com for any additional information and price quotations.

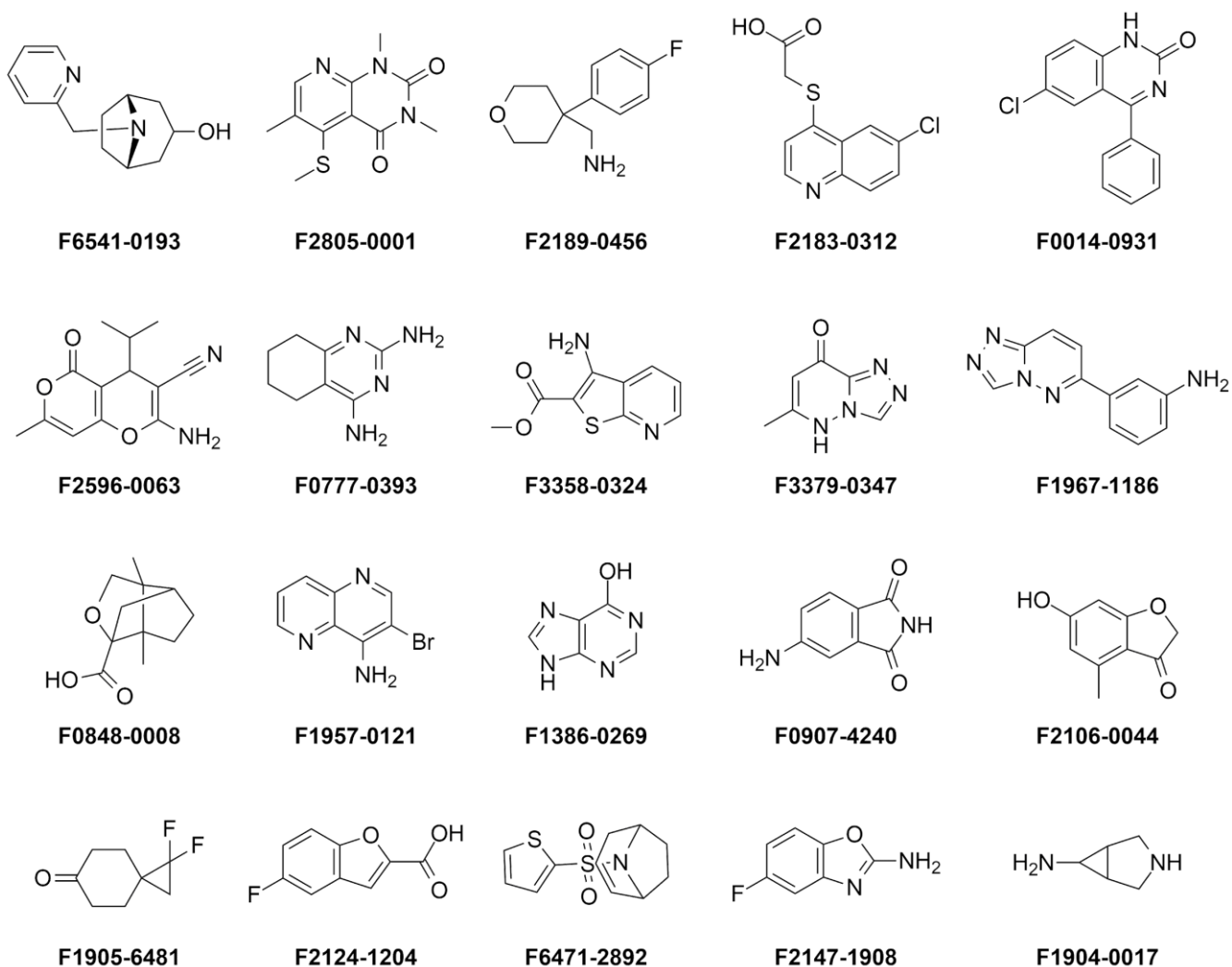


Figure 1. Representative compounds from Natural Product-like Fragment Library

References

1. Grabowski K.; Schneider G. *Curr. Chem. Biol.* 2007, 10, 115–127
2. Rizzo S.; Waldmann H. *D. Chem. Rev.* 2014, 114, 4621–4639.
3. Rodrigues T. et al. *Nature Chem.* 2016, 8, 531–541.
4. Over, B. et al. *Nature Chem.* 2013, 5, 21–28.
5. Schuffenhauer A. et al. *J Chem Inf Model.* 2007, 47, 47–58.
6. Gu J.; Gui Y.; Chen L.; Yuan G.; Lu H.-Z.; Xu X. *PLoS ONE*, 2013, 8, e62839.
7. Liu M, Quinn RJ. *Expert Opin Drug Discov.* 2019 Dec;14(12):1283–1295.
8. Ertl P, Schuhmann T. *J Nat Prod.* 2019 May 24;82(5):1258–1263.
9. Foley DJ et al. *Chemistry.* 2017 Oct 26;23(60):15227–15232.
10. Prescher H, Koch G et al. *Bioorg Med Chem.* 2017 Feb 1;25(3):921–925.
11. Sorokina M, et al. *J Cheminform.* 2021;13(1):2.