

Halogen-Enriched Fragment Library

Unique fragment compounds for FBDD!

As a Director of Otava Ltd. I would like to offer you our new Halogen-Enriched Fragment Library that comprises 430 brominated fragments. The library is intended for rapid hit evolution and more effective identification of the fragment bound in the active site of a drug target by X-ray crystallography.

Halogen bonds have recently attracted increased interest in molecular design offering alternatives to classical polar interactions such as hydrogen bonds. Halogen-Enriched Fragment Library designed by Otava uses criteria for fragment selection similar to the "rule of three" but employing an upper limit of the number of heavy atoms (up to 22) rather than the original molecular weight-based criterion (MW \leq 300). As an additional cheminformatics selection rule, the molecules were required to contain at least one bromine atom.

All compounds are in stock (20mg min. amount).

The library has the following characteristics:

Parameter	Value	
Number of Heavy Atoms	< 22	
ClogP	< 3	
Number of Rotatable Bonds	≤ 3	
Number of H Donors	≤ 3	
Number of H Acceptors	≤ 4	
PSA	< 80	
Number of Rings	> 0	
LogSw	> -5	
Number of Bromine Atoms	> 0	
Compounds with "undesirable" functionalities	Removed	
Compound amount in stock	> 20mg	

Find out more...

Our price is **ONLY \$9.8** per 1mg (if more than 500 compounds are ordered)

Example price list in USD:

Num. of compounds ordered	1-20	21- 50	51- 100	101- 500	501- 1000
Price for 1mg	\$32.0	\$25.0	\$19.0	\$13.9	\$9.8

All compounds are in stock (20mg min. amount).

The library is for prompt delivery, cherry-picking is available.

Feel free to contact me if you are interested to obtain this library or if you need more information. I am looking forward to your reply.

Best regards,

Andriy Dmytrenko, MBA
Director of Business Development and Marketing

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