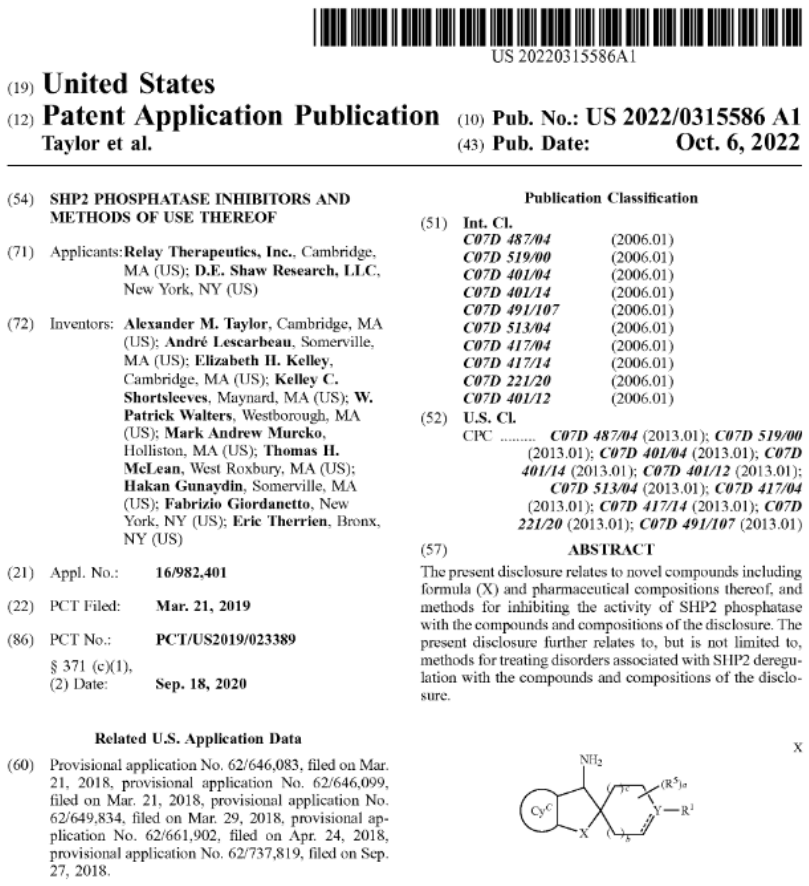
Organizing and Manipulating Chemical Information

Pat Walters

RCSB PDB Crash Course

May 1, 2025

Chemical Patents Protect Intellectual Property



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(19) **United States**

(12) **Patent Application Publication** (10) **Pub. No.: US 2022/0315586 A1**

Taylor et al. (43) **Pub. Date: Oct. 6, 2022**

(54) **SHP2 PHOSPHATASE INHIBITORS AND METHODS OF USE THEREOF**

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(72) Inventors: **Alexander M. Taylor**, Cambridge, MA (US); **André Lescarbeau**, Somerville, MA (US); **Elizabeth H. Kelley**, Cambridge, MA (US); **Kelley C. Shortsleeves**, Maynard, MA (US); **W. Patrick Walters**, Westborough, MA (US); **Mark Andrew Murcko**, Holliston, MA (US); **Thomas H. McLean**, West Roxbury, MA (US); **Hakan Gunaydin**, Somerville, MA (US); **Fabrizio Giordanetto**, New York, NY (US); **Eric Therrien**, Bronx, NY (US)

(21) Appl. No.: **16/982,401**

(22) PCT Filed: **Mar. 21, 2019**

(86) PCT No.: **PCT/US2019/023389**

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Related U.S. Application Data

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C07D 401/04	(2006.01)
C07D 401/14	(2006.01)
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C07D 513/04	(2006.01)
C07D 417/04	(2006.01)
C07D 417/14	(2006.01)
C07D 221/20	(2006.01)
C07D 401/12	(2006.01)

(52) **U.S. Cl.**

CPC ***C07D 487/04*** (2013.01); ***C07D 519/00*** (2013.01); ***C07D 401/04*** (2013.01); ***C07D 401/14*** (2013.01); ***C07D 401/12*** (2013.01); ***C07D 513/04*** (2013.01); ***C07D 417/04*** (2013.01); ***C07D 417/14*** (2013.01); ***C07D 221/20*** (2013.01); ***C07D 491/107*** (2013.01)

(57) **ABSTRACT**

The present disclosure relates to novel compounds including formula (X) and pharmaceutical compositions thereof, and methods for inhibiting the activity of SHP2 phosphatase with the compounds and compositions of the disclosure. The present disclosure further relates to, but is not limited to, methods for treating disorders associated with SHP2 deregulation with the compounds and compositions of the disclosure.

X

375 pages

https://patentimages.storage.googleapis.com/4b/b8/a2/bbf9ac18c23f35/US20220315586A1.pdf

Why Are Patents Important?

1. Allow inventors to claim intellectual property (IP)
2. Enable companies to avoid competitors' IP
3. Enable companies to learn from competitors’ IP
4. Provide a great way to learn about Medicinal Chemistry

Why Is Patent Data Difficult?

- Key information is not available electronically
- Chemical structures are not downloadable from USPTO
- Chemical structures and data are separate
- Patent documents span hundreds of pages
- Data is often obfuscated

Patents Can Contain 100s of Structures

TABLE 1-continued

Representative Compounds of the disclosure.

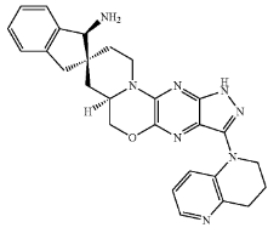
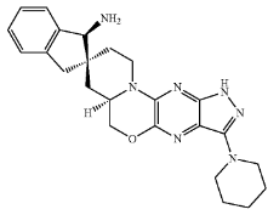
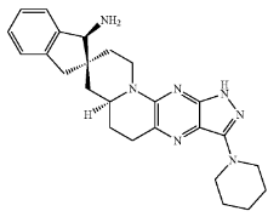
Example	Structure
7	 $C_{27}H_{28}N_8O$
8	 $C_{24}H_{29}N_7O$
9	 $C_{24}H_{31}N_7$

TABLE 1-continued

Representative Compounds of the disclosure.

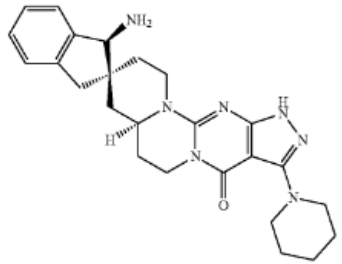
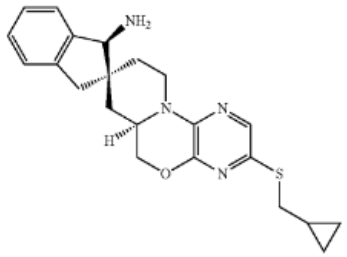
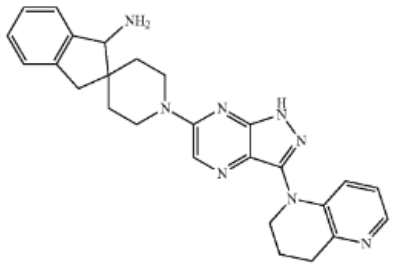
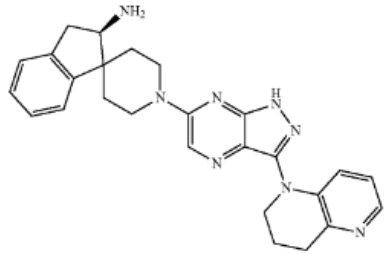
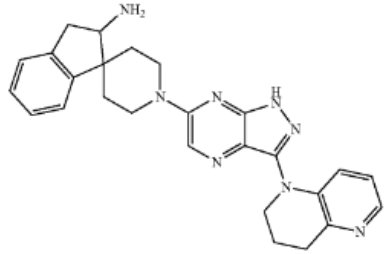
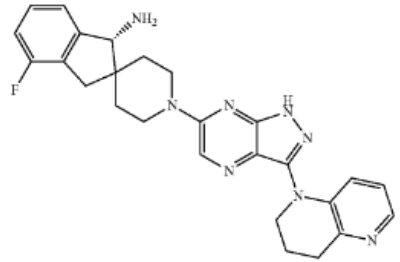
Example	Structure
10	 $C_{25}H_{31}N_7O$
11	 $C_{22}H_{26}N_4OS$
12	 $C_{28}H_{28}N_8$

TABLE 1-continued

Representative Compounds of the disclosure.

Example	Structure
14	 $C_{26}H_{28}N_8$
15	 $C_{26}H_{28}N_8$
16	 $C_{26}H_{27}FN_8$

Patent Data is Typically Separate From Structures

Data is often categorized

TABLE 2-continued

Results of SHP2 allosteric inhibition assay.

Example	SHP2 IC_{50}
74	A
75	A
76	A
77	A
78	A
79	A
80	A
80	A
81	A
82	A
84	A
84	A
86	A
87	A
88	A
89	A
90	B
91	C
92	A

[1324] Results of the SHP2 allosteric inhibition assay are depicted in the table below. Compounds designated as "A" have an IC_{50} value less than or equal to 50 nM; compounds designated as "B" have an IC_{50} value greater than 50 nM but less than or equal to 1 uM; compounds designated as "C" have an IC_{50} value greater than 1 uM but less than or equal to 10 uM; and compounds designated as "D" have an IC_{50} value greater than 10 uM.

BindingDB Curates Papers and Patents

3.0M BIOLOGICAL DATAPOINTS

1.3M COMPOUNDS

9.5K BIOLOGICAL TARGETS

HTTPS://BINDINGDB.ORG

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(19) **United States**

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(43) **Pub. Date: Sep. 5, 2024**

(54) **PROTEASE INHIBITORS AND METHODS OF USE**

(71) Applicant: **The Cleveland Clinic Foundation**, Cleveland, OH (US)

(72) Inventors: **Shaun R. Stauffer**, Cleveland, OH (US); **Jonathan D. Macdonald**, Cleveland, OH (US); **Alice Hooper**, Cleveland, OH (US); **Sang Hoon Han**, Cleveland, OH (US); **Dhiraj P. Sanawane**, Cleveland, OH (US); **Matthew R. Porter**, Cleveland, OH (US); **Joshua Maw**, Cleveland, OH (US); **Steven Martinez**, Cleveland, OH (US); **Joseph Alvarado**, Cleveland, OH (US)

(21) Appl. No.: **18/570,520**

(22) PCT Filed: **Jun. 16, 2022**

(86) PCT No.: **PCT/US22/33861**

§ 371 (c)(1),
(2) Date: **Dec. 14, 2023**

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A61K 31/444	(2006.01)
A61K 31/4725	(2006.01)
A61K 31/496	(2006.01)
A61K 31/497	(2006.01)
A61K 31/498	(2006.01)
A61K 31/501	(2006.01)
A61K 31/502	(2006.01)
A61K 31/5025	(2006.01)
A61P 31/14	(2006.01)
C07D 217/16	(2006.01)
C07D 401/12	(2006.01)
C07D 401/14	(2006.01)
C07D 403/12	(2006.01)
C07D 413/12	(2006.01)
C07D 471/04	(2006.01)
C07D 487/04	(2006.01)

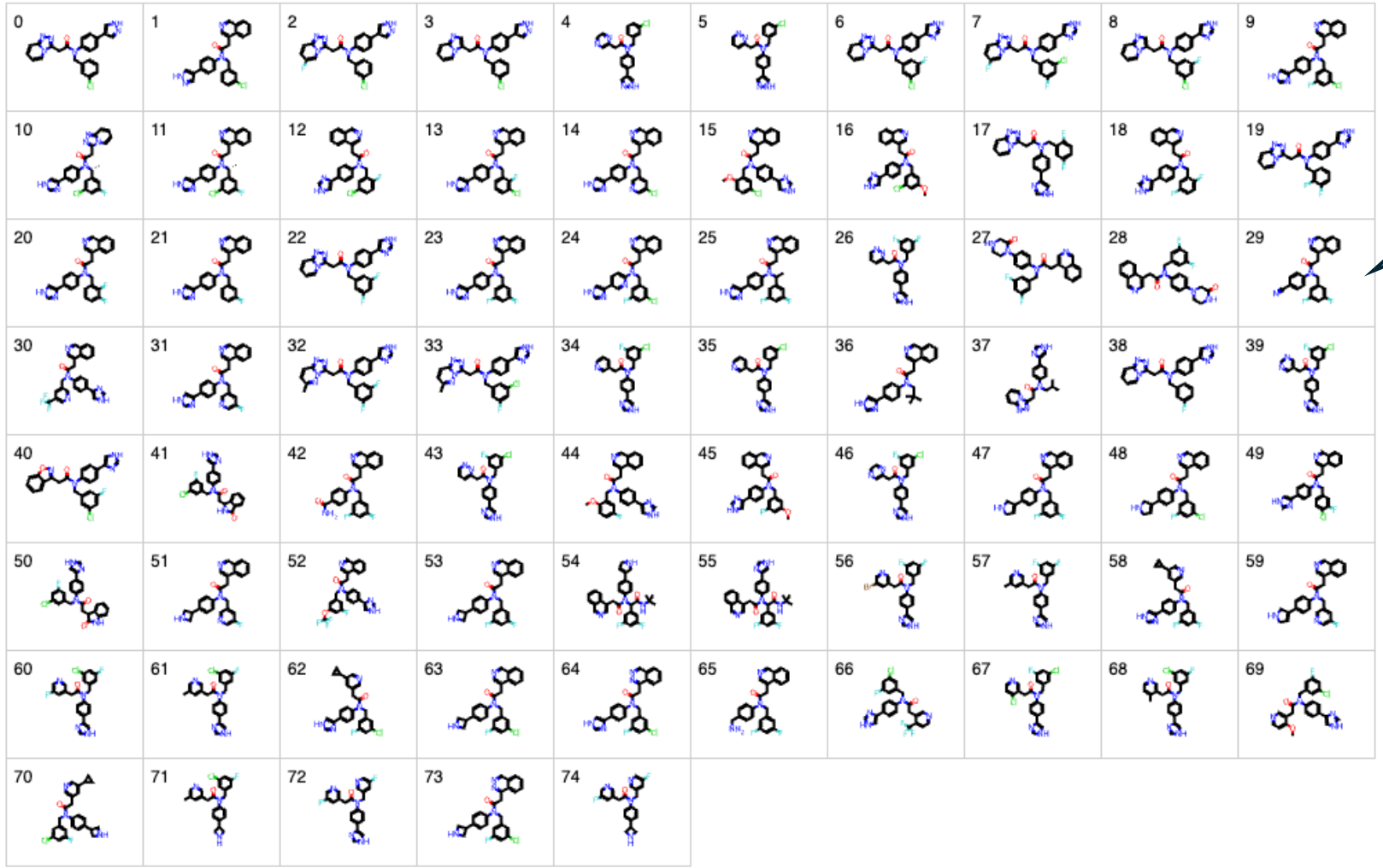
(52) **U.S. Cl.**

CPC ***A61K 31/437*** (2013.01); ***A61K 31/423*** (2013.01); ***A61K 31/4439*** (2013.01); ***A61K 31/444*** (2013.01); ***A61K 31/4725*** (2013.01); ***A61K 31/496*** (2013.01); ***A61K 31/497*** (2013.01); ***A61K 31/498*** (2013.01); ***A61K 31/501*** (2013.01); ***A61K 31/502*** (2013.01); ***A61K 31/5025*** (2013.01); ***A61P 31/14*** (2018.01); ***C07D 217/16*** (2013.01); ***C07D 401/12*** (2013.01); ***C07D 401/14*** (2013.01); ***C07D 403/12*** (2013.01); ***C07D 413/12*** (2013.01); ***C07D 471/04*** (2013.01); ***C07D 487/04*** (2013.01)

(57) **ABSTRACT**

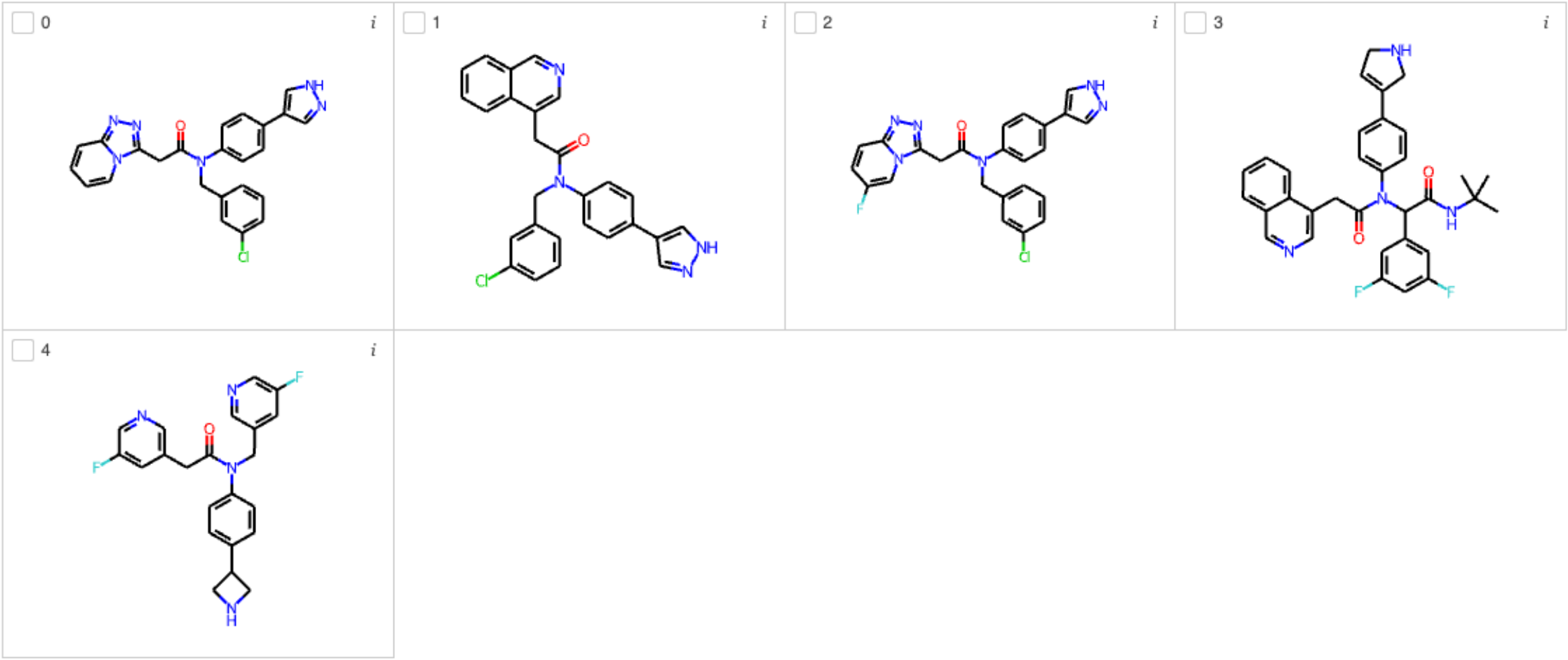
Disclosed herein are compounds that inhibit the 3C-like protease of SARS-CoV-2. Also disclosed herein are pharmaceutical compositions comprising the compounds, and methods of using the compounds, e.g., in a method of treating a viral infection, such as a coronavirus infection.

How Can We Organize the Structures?



75 structures curated by BindingDB

How Do We Select a Representative Subset?



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Pat Walters is Chief Data Officer at Relay Therapeutics in Cambridge, MA. Prior to joining Relay, he spent more than 20 years at Vertex Pharmaceuticals where he was Global Head of Modeling & Informatics. Pat is the 2023 recipient of the Herman Skolnik Award for Chemical Information Science from the American Chemical Society. He is a member of the editorial advisory boards for the Journal of Chemical Information and Modeling and Artificial Intelligence in the Life Sciences, and previously held a similar role with the Journal of Medicinal Chemistry. Pat is co-author of the book "Deep Learning for the Life Sciences", published in 2019 by O'Reilly and Associates. He received his Ph.D. in Organic Chemistry from the University of Arizona where he studied the application of artificial intelligence in conformational analysis. Prior to obtaining his Ph.D., Pat worked at Varian Instruments as both a chemist and a software developer. He received his B.S. in Chemistry from the University of California, Santa Barbara.