Hit#1: Leupeptin bound to SARS-CoV-2 MPro, PDB: 6YZ6

Synonyms: Leupeptin, Ac-Leu-Leu-Arg-H, Ac-Leu-Leu-Argininal

PubChem CID: 72429

CAS: 55123-66-5

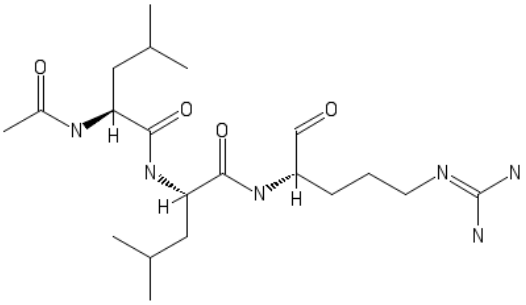
Molecular weigth: 426.6 g/mol

Binding type: covalent, hemithioacetal

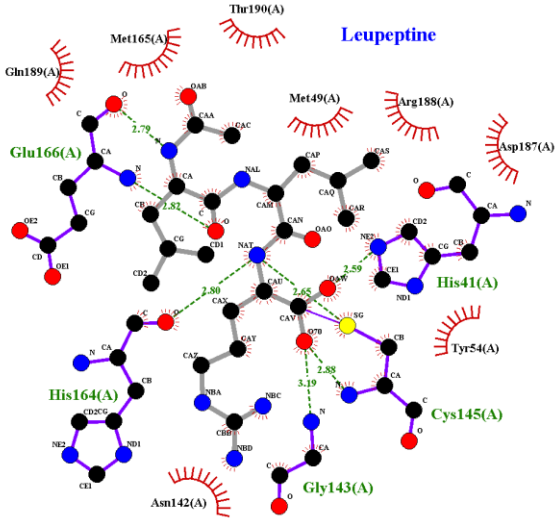
Binding location: Cystein 145

Screen compound ID: - (positive control)

Original compound:



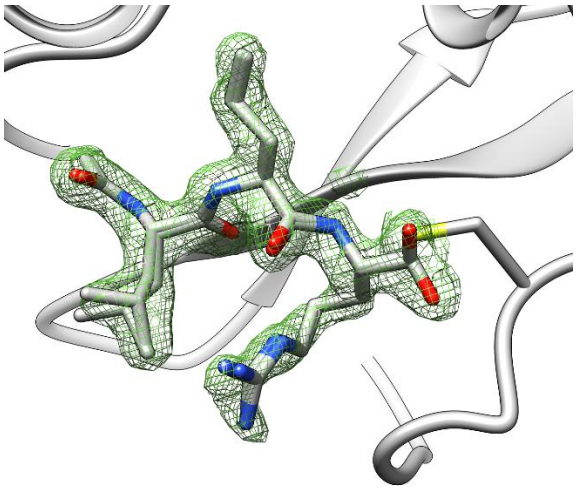
Lig-Plot interaction network

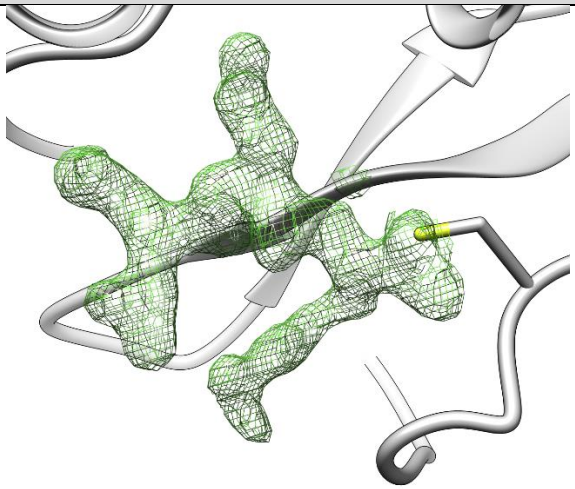


Isomeric smiles:
CC(C)C[C@@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCCN=C(N)N)C=O)NC(=O)C

Refinement 2Fo-Fc map, 1.2 σ-level

note





PDB structure code: 6YZ6

PDB Ligand code: AR7

Resolution: 1.7 Å

R_{work}/R_{free}: 0.17/0.22

Occupancy: 0.73, 0.21

Ligand RSCC/RSR: 0.86/0.19, 0.86/0.19

Biochemistry & Cell biology

Anti viral activity EC_{50}: N.a.

vRNA yield EC_{50}: N.a.

Anti viral activity EC_{90}: N.a.

vRNA yield EC_{90}: N.a.

Cytotoxicity CC_{50}: N.a.

SI CC50/EC50: N.a.

Native MS adduct saturation: N.a.

Native MS adduct size: N.a.

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Hit#2: Calpeptin bound to SARS-CoV-2 MPro, PDB: 7AKU

Synonyms: Calpeptin, N-Cbz-leu-nleu-al, Benzylcarbonyl-leu-nleu-H

PubChem CID: 73364

CAS: 117591-20-5

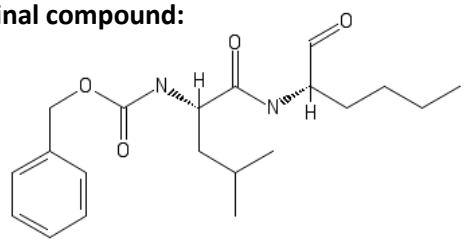
Molecular weigth: 362.5 g/mol

Binding type: covalent, hemithioacetal

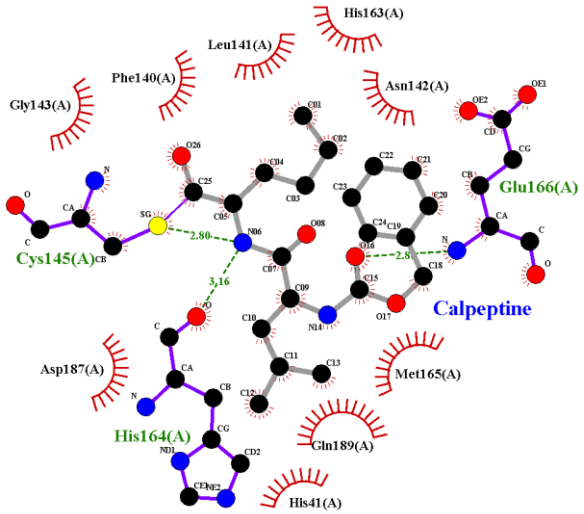
Binding location: Cystein 145

Screen compound ID: SPE_K26134695

Original compound:

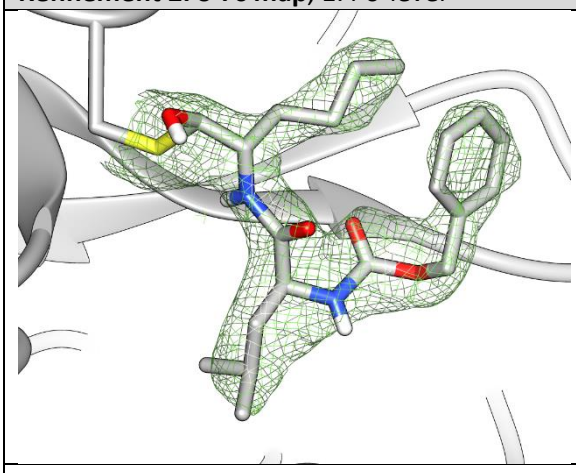


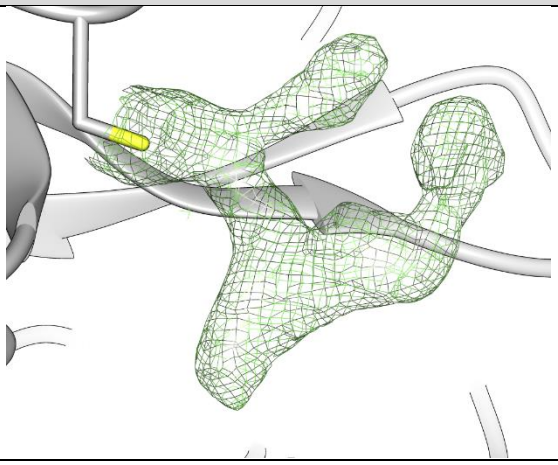
Lig-Plot interaction network



Isomeric smiles: CCCC[C@@H](C=O)NC(=O)[C@H](CC(C)C)NC(=O)OCC1=CC=CC=C1

Refinement 2Fo-Fc map, 1.4 σ-level





PDB structure code: 7AKU	**PDB Ligand code:** RN2
Resolution: 2.5 Å	**R_{work}/R_{free}:** 0.19/0.24
Occupancy: 1.0	**Ligand RSCC/RSR:** 0.94/0.16
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 82% (5 / 27 68)	**Native MS adduct size:** 362.5 Da

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Hit#3: HEAT bound to SARS-CoV-2 MPro, PDB: 6YNQ

Synonyms: HEAT, BE-2254, 2-(beta-(4-Hydroxyphenyl)ethylaminomethyl)tetralone

PubChem CID: 34772

CAS: 40077-13-2

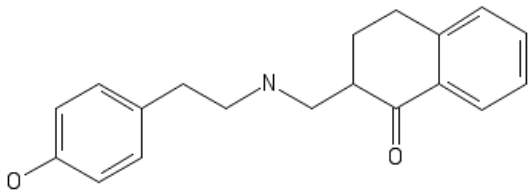
Molecular weigth: 295.4 g/mol

Binding type: covalent, thioether

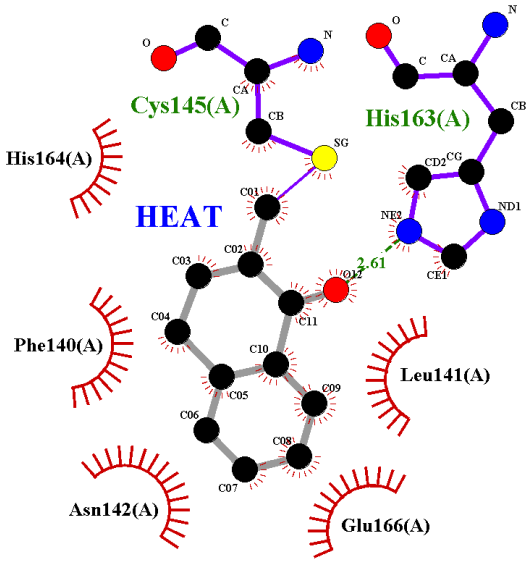
Binding location: Cystein 145

Screen compound ID: SPE_A24429032

Original compound:

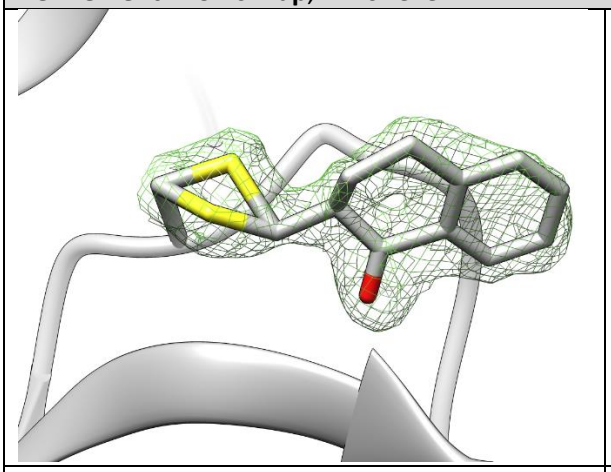


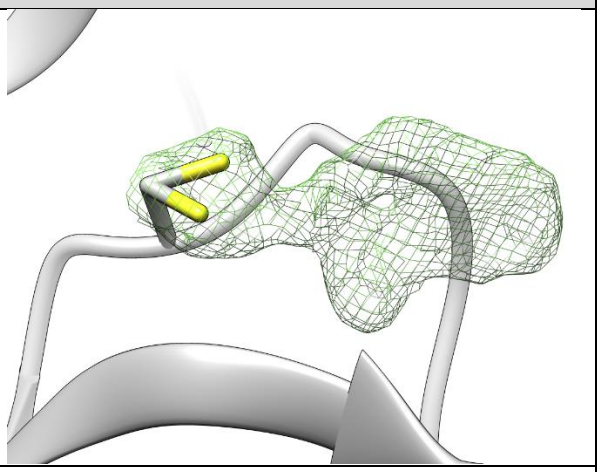
Lig-Plot interaction network



Isomeric smiles: C1CC2=CC=CC=C2C(=O)C1CNCCC3=CC=C(C=C3)O

Refinement 2Fo-Fc map, 1.4 σ-level





PDB structure code: 6YNQ	**PDB Ligand code:** P6N
Resolution: 1.8 Å	**R_{work}/R_{free}:** 0.19/0.23
Occupancy: 1.0	**Ligand RSCC/RSR:** 0.92/0.11
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 43% (39/37/24)	**Native MS adduct size:** 181 Da

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Hit#4: Tolperisone HCl bound to SARS-CoV-2 MPro, PDB: 7ADW

Synonyms: Tolperisone, Mydeton, Mydocalm, Mideton

PubChem CID: 5511

CAS: 728-88-1

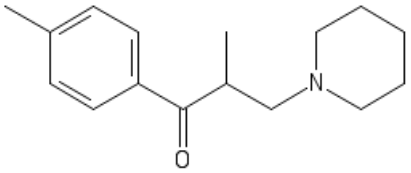
Molecular weigth: 245.36 g/mol

Binding type: covalent, thioether

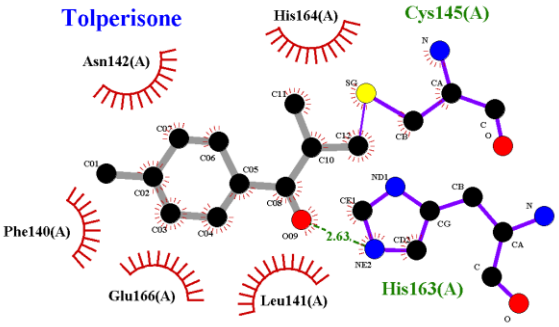
Binding location: Cystein 145

Screen compound ID: SPE_A27732521

Original compound:

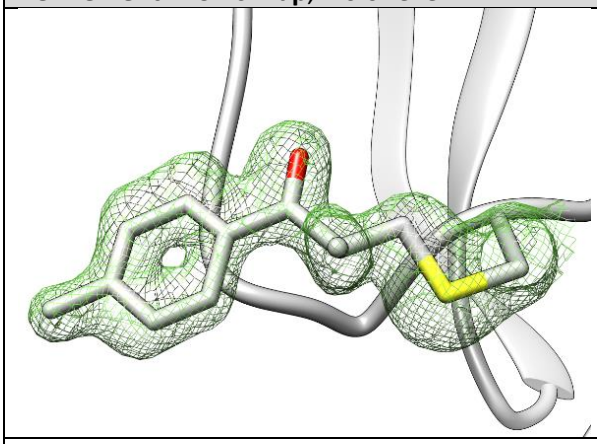


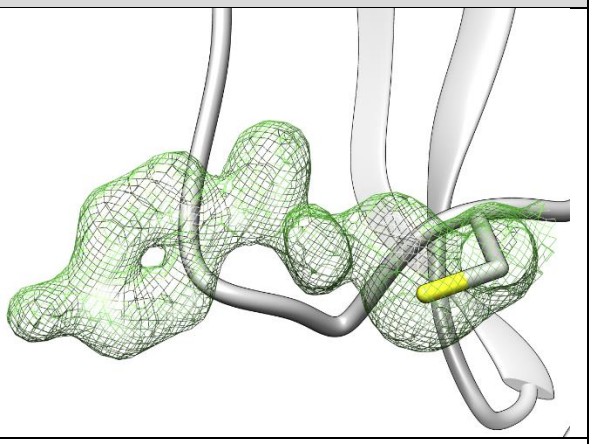
Lig-Plot interaction network



Isomeric smiles: CC1=CC=C(C=C1)C(=O)C(C)CN2CCCCC2

Refinement 2Fo-Fc map, 1.0 σ-level





PDB structure code: 7ADW	**PDB Ligand code:** R7Q
Resolution: 1.62 Å	**R_{work}/R_{free}:** 0.20/0.23
Occupancy: 1.0	**Ligand RSCC/RSR:** 0.87/0.11
Biochemistry & Cell biology	
Anti viral activity EC_{50}: 17.16 ± 1.76 µM	**vRNA yield EC_{50}:** 22.42 ± 2.25 µM
Anti viral activity EC_{90}: 29.68 ± 2.32 µM	**vRNA yield EC_{90}:** 34.65 ± 3.76 µM
Cytotoxicity CC_{50}: > 100 µM	**SI CC50/EC50:** > 5.83
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

Hit#5: Maleate (Quipazine) bound to SARS-CoV-2 MPro, PDB: 7AHA

Synonyms: Maleic acid, cis-butenedioic acid, 110-16-7, Toxilic acid, Maleinic acid

PubChem CID: 444266 (Maleate) / 5011 (Quip.)

CAS: 110-16-7 (Maleate) / 5786-68-5

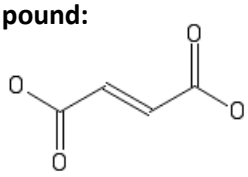
Molecular weigth: 116.07 g/mol (Maleate)

Binding type: covalent, thioether

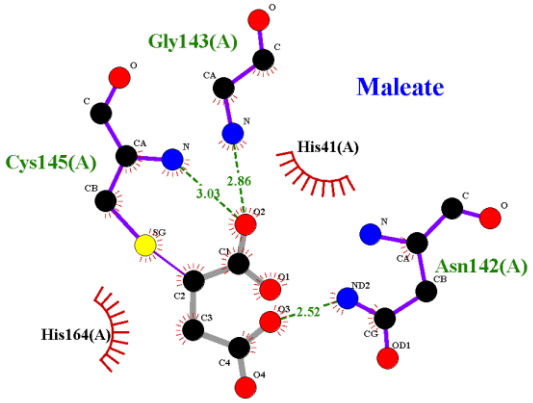
Binding location: Cystein 145

Screen compound ID: SPE_K77925998

Original compound:

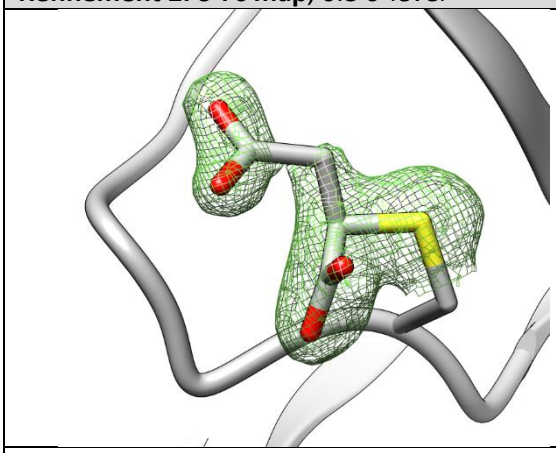


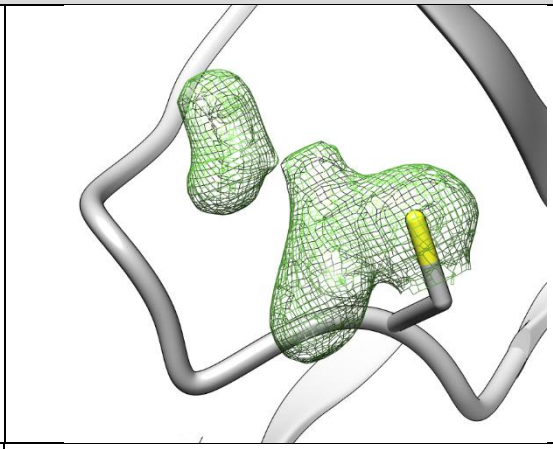
Lig-Plot interaction network



Isomeric smiles: C(=C\C(=O)[O-])\C(=O)[O-] (Maleate)

Refinement 2Fo-Fc map, 0.8 σ-level





PDB structure code: 7AHA	**PDB Ligand code:** SIN
Resolution: 1.68 Å	**R_{work}/R_{free}:** 0.17/0.20
Occupancy: 1.0	**Ligand RSCC/RSR:** 0.89/0.16
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

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Hit#6: Isofloxythepin bound to SARS-CoV-2 MPro, PDB: 7AY7

Synonyms: Isofloxythepin, EINECS 275-028-1, 70931-18-9

PubChem CID: 115193

CAS: 70931-18-9

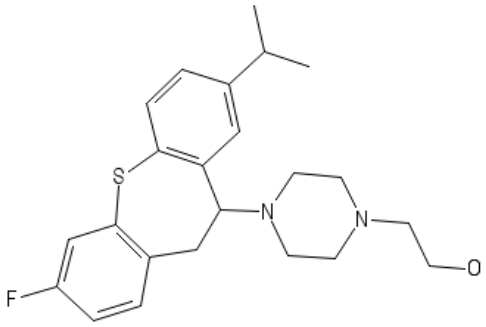
Molecular weigth: 400.6 g/mol

Binding type: covalent, thioether

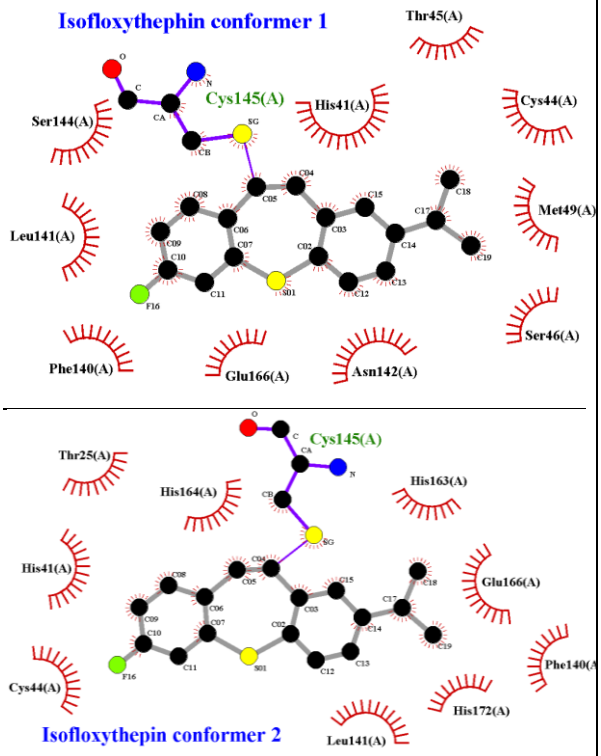
Binding location: Cystein 145

Screen compound ID: DOM_SIM_130

Original compound:

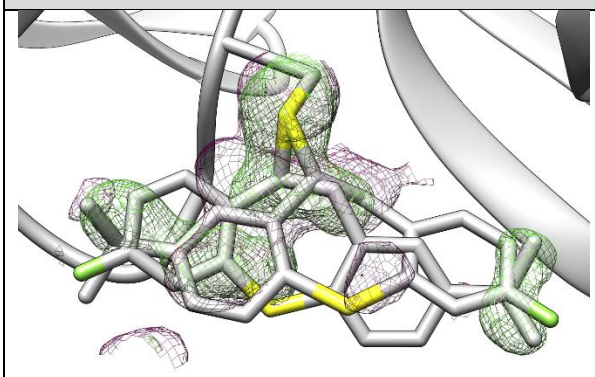


Lig-Plot interaction network

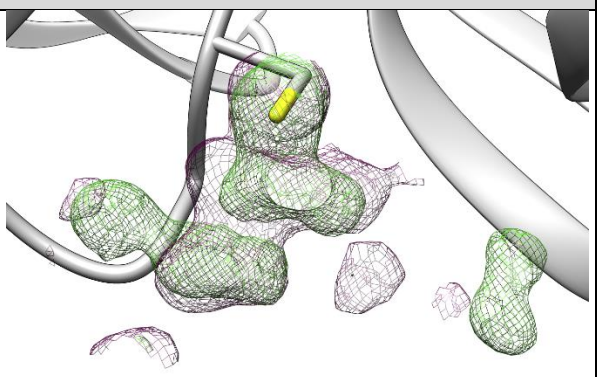


Isomeric smiles: CC(C)C1=CC2=C(C=C1)SC4=C(CC2N3CCN(CC3)CCO)C=CC(=C4)F

Refinement 2Fo-Fc map, 0.7 σ-level, **PanDDA event map BDC 0.15** , 1.4 σ-level



2Fo-Fc map, PanDDA event map



PDB structure code: 7AY7	**PDB Ligand code:** S8T
Resolution: 1.55 Å	**R_{work}/R_{free}:** 0.17/0.20
Occupancy: 0.30, 0.38	**Ligand RSCC/RSR:** 0.60/0.51, 0.72/43
Biochemistry & Cell biology	
Anti viral activity EC_{50}: 4.82 ± 0.33 µM	**vRNA yield EC_{50}:** 4.94 ± 0.58 µM
Anti viral activity EC_{90}: 7.21 ± 0.31 µM	**vRNA yield EC_{90}:** 7.52 ± 0.56 µM
Cytotoxicity CC_{50}: 14.49 ± 3.57 µM	**SI CC50/EC50:** > 4.04
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

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Hit#7: Triglycidyl isocyanurate bound to SARS-CoV-2 MPro, PDB: 7AQJ

Synonyms: Triglycidyl isocyanurate, 2451-62-9, 1,3,5-Triglycidyl isocyanurate, Teroxirone

PubChem CID: 17142

CAS: 6990-06-3

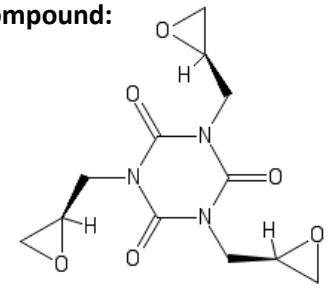
Molecular weigth: 297.26 g/mol

Binding type: covalent, thioether

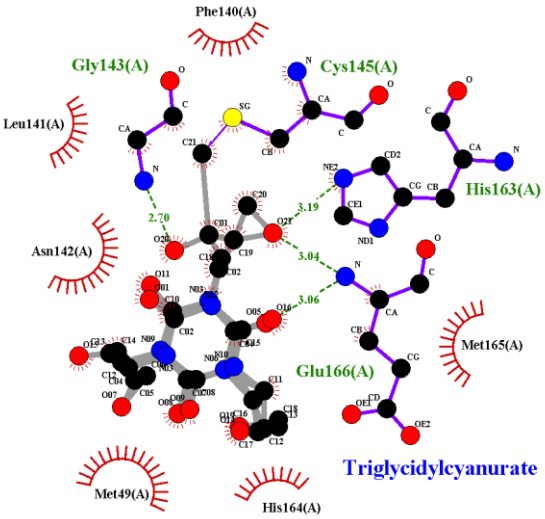
Binding location: Cystein 145

Screen compound ID: SPE_A06935312

Original compound:

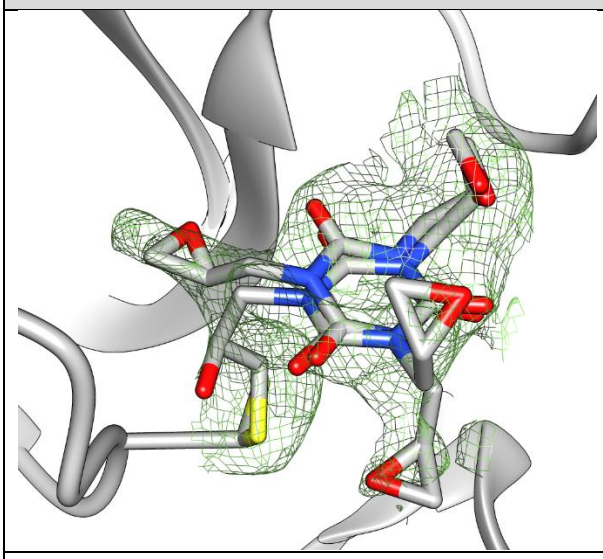


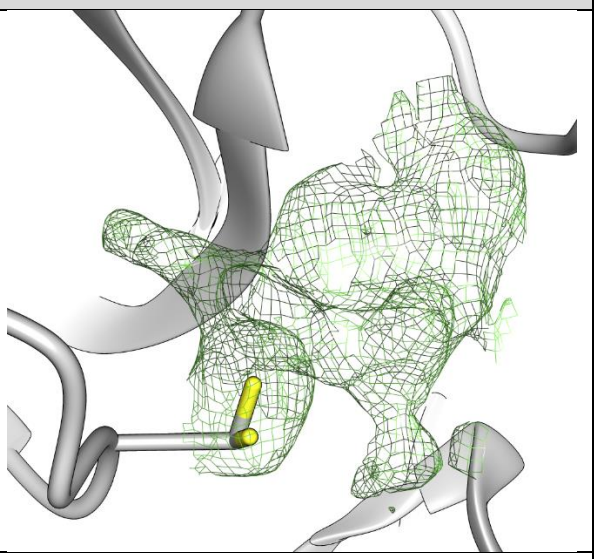
Lig-Plot interaction network



Isomeric smiles: C1[C@H](O1)CN2C(=O)N(C(=O)N(C2=O)C[C@@H]3CO3)C[C@@H]4CO4

Refinement 2Fo-Fc map, 0.7 σ-level





PDB structure code: 7AQJ	**PDB Ligand code:** RV8, S7H
Resolution: 2.59 Å	**R_{work}/R_{free}:** 0.22/0.26
Occupancy: 0.4 / 0.47	**Ligand RSCC/RSR:** 0.78/0.27, 0.84/0.22
Biochemistry & Cell biology	
Anti viral activity EC_{50}: 35.68 ± 10.87 µM	**vRNA yield EC_{50}:** 37 ± 5.35 µM
Anti viral activity EC_{90}: 48.08 ± 9.57 µM	**vRNA yield EC_{90}:** 50.25 ± 4.14 µM
Cytotoxicity CC_{50}: > 100 µM	**SI CC50/EC50:** > 2.8
Native MS adduct saturation: 72% (8/38/53)	**Native MS adduct size:** 297 Da

Hit#8: MUT056399 acid bound to SARS-CoV-2 MPro, PDB: 7AP6

Synonyms: MUT056399, 1269055-85-7, FAB-001, 4-(4-ethyl-5-fluoro-2-hydroxyphenoxy)-3-fluorobenzamide

PubChem CID: 44208849

CAS: 1269055-85-7

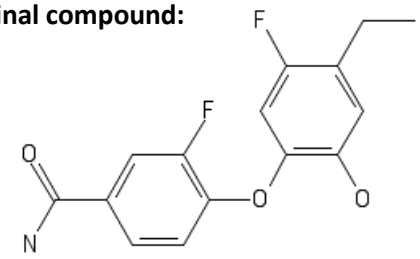
Molecular weigth: 293.26 g/mol

Binding type: non-covalent

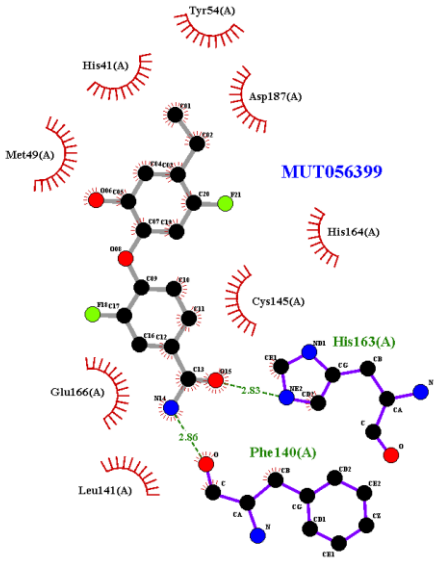
Binding location: active site pocket

Screen compound ID: SPE_K72078047

Original compound:

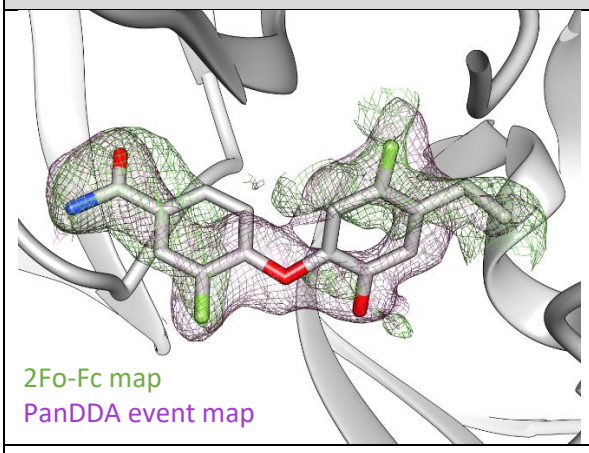


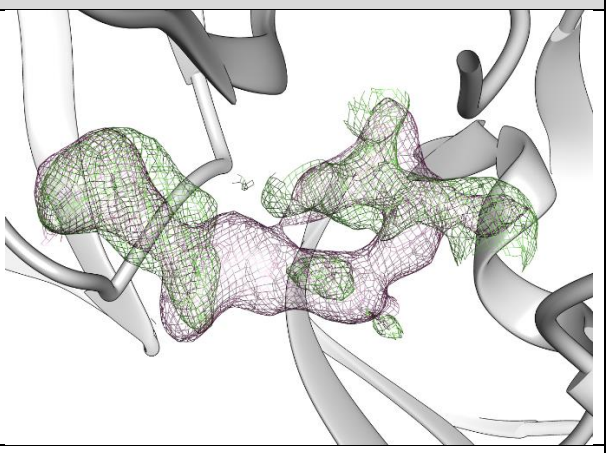
Lig-Plot interaction network



Isomeric smiles: CCC1=CC(=C(C=C1F)OC2=C(C=C(C=C2)C(=O)N)F)O

Refinement 2Fo-Fc map, 0.7 σ-level, **PanDDA event map BDC 0.18** , 1.4 σ-level





PDB structure code: 7AP6	**PDB Ligand code:** RQN
Resolution: 1.78 Å	**R_{work}/R_{free}:** 0.20/0.23
Occupancy: 0.44	**Ligand RSCC/RSR:** 0.64/0.54
Biochemistry & Cell biology	
Anti viral activity EC_{50}: 43.27 ± 0.59 µM	**vRNA yield EC_{50}:** 42.18 ± 3.86 µM
Anti viral activity EC_{90}: 54.05 ± 0.48 µM	**vRNA yield EC_{90}:** 54.27 ± 2.27 µM
Cytotoxicity CC_{50}: > 100 µM	**SI CC50/EC50:** > 2.31
Native MS adduct saturation: 6% (83/17/0)	**Native MS adduct size:** 293 Da

Hit#9: Pelitinib bound to SARS-CoV-2 MPro, PDB: 7AXM

Synonyms: Pelitinib, 257933-82-7, EKB-569

PubChem CID: 6445562

CAS: 257933-82-7

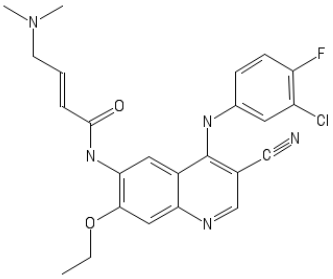
Molecular weigth: 467.9 g/mol

Binding type: non-covalent

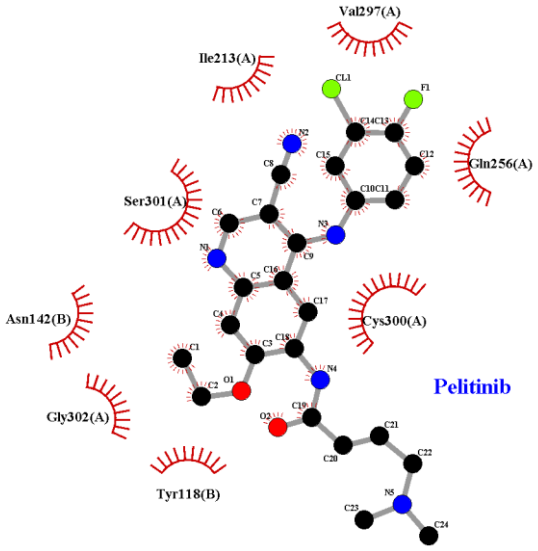
Binding location: allosteric site I

Screen compound ID: DOM_SIM_123

Original compound:

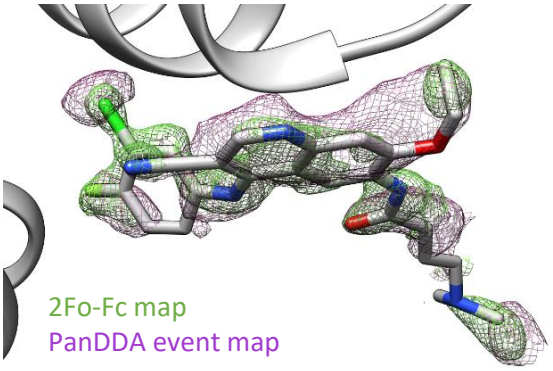


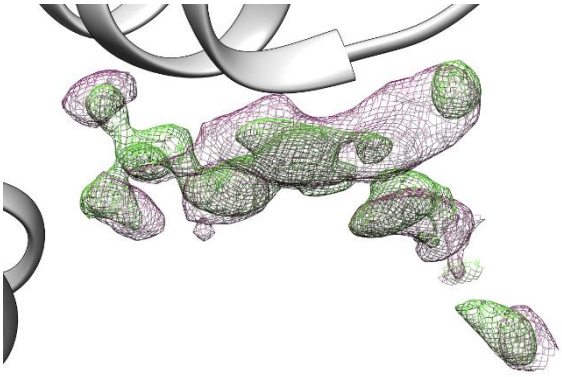
Lig-Plot interaction network



Isomeric smiles: CCOC1=C(C=C2C(=C1)N=CC(=C2NC3=CC(=C(C=C3)F)Cl)C#N)NC(=O)/C=C/CN(C)C

Refinement 2Fo-Fc map, 0.6 σ-level, **PanDDA event map BDC 0.18** , 1.0 σ-level





PDB structure code: 7AXM	**PDB Ligand code:** 93J
Resolution: 1.4 Å	**R_{work}/R_{free}:** 0.14/0.20
Occupancy: 0.61	**Ligand RSCC/RSR:** 0.61/0.28
Biochemistry & Cell biology	
Anti viral activity EC_{50}: 1.25 ± 0.02 µM	**vRNA yield EC_{50}:** 1.21 ± 0.1 µM
Anti viral activity EC_{90}: 2.13 ± 0.12 µM	**vRNA yield EC_{90}:** 2.32 ± 0.1 µM
Cytotoxicity CC_{50}: > 100 µM	**SI CC50/EC50:** 11.17
Native MS adduct saturation: 12% (88/12/0)	**Native MS adduct size:** 467 Da

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Hit#10: Ifenprodil bound to SARS-CoV-2 MPro, PDB: 7AQI

Synonyms: Ifenprodil, 23210-56-2, ifenprodil tartrate, Vadilex, Dilvax

PubChem CID: 3689

CAS: 23210-56-2

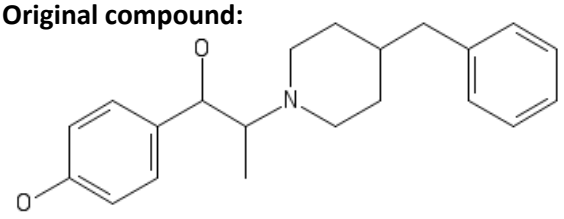
Molecular weigth: 325.4 g/mol

Binding type: non-covalent

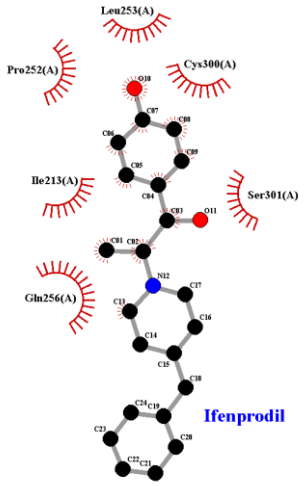
Binding location: allosteric site I

Screen compound ID: SPE_A06935312

Original compound:

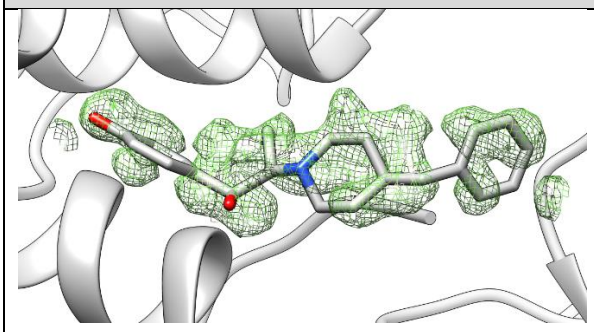


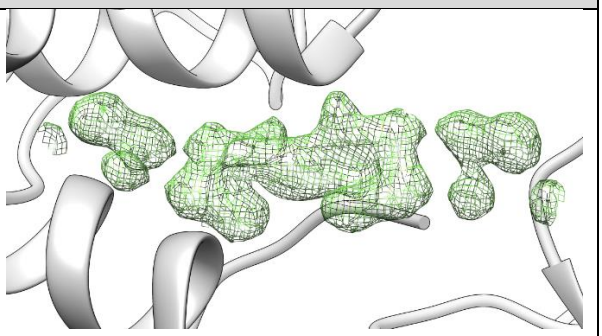
Lig-Plot interaction network



Isomeric smiles: CC(C(C1=CC=C(C=C1)O)O)N2CCC(CC2)CC3=CC=CC=C3

Refinement 2Fo-Fc map, 0.7 σ-level





PDB structure code: 7AQI	**PDB Ligand code:** QEL
Resolution: 1.7 Å	**R_{work}/R_{free}:** 0.23/0.26
Occupancy: 0.5 + 0.5	**Ligand RSCC/RSR:** 0.80/0.19

Biochemistry & Cell biology

Anti viral activity EC_{50}: 43.37 ± 2.99 µM	**vRNA yield EC_{50}:** 44.96 ± 5.52 µM
Anti viral activity EC_{90}: 51.25 ± 2.34 µM	**vRNA yield EC_{90}:** 53.73 ± 1.74 µM
Cytotoxicity CC_{50}: > 100 µM	**SI CC50/EC50:** > 2.31
Native MS adduct saturation: 27% (61/24/15)	**Native MS adduct size:** 126 Da

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Hit#11: RS102895 bound to SARS-CoV-2 MPro, PDB: 7ABU

Synonyms: RS102895, GTPL779, CHEMBL1593104, SCHEMBL9972649

PubChem CID: 10000456

CAS: 1173022-16-6

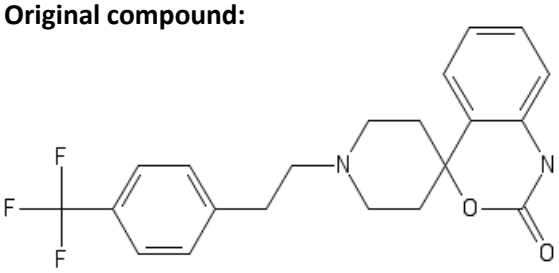
Molecular weigth: 390.4 g/mol

Binding type: non-covalent

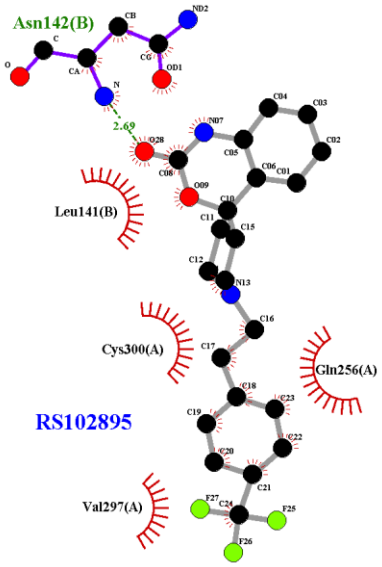
Binding location: allosteric site I

Screen compound ID: SPE_K83063356

Original compound:

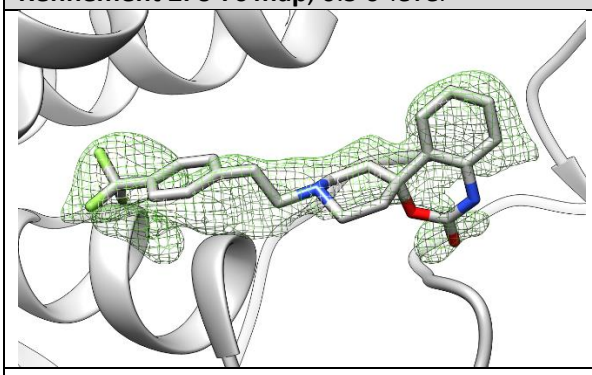


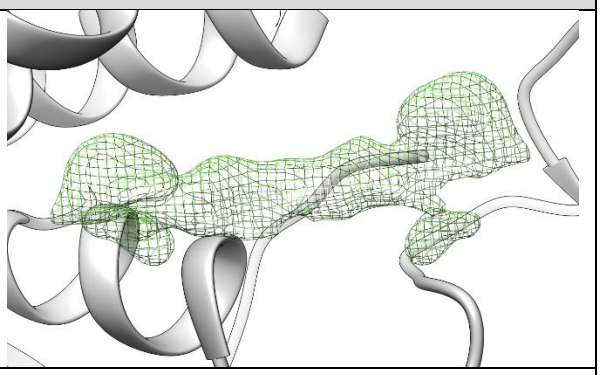
Lig-Plot interaction network



Isomeric smiles: C1CN(CCC12C3=CC=CC=C3NC(=O)O2)CCC4=CC=C(C=C4)C(F)(F)F

Refinement 2Fo-Fc map, 0.5 σ-level





PDB structure code: 6ABU	**PDB Ligand code:** R6Q
Resolution: 1.6 Å	**R_{work}/R_{free}:** 0.18/0.22
Occupancy: 0.48 + 0.48	**Ligand RSCC/RSR:** 0.74/0.22
Biochemistry & Cell biology	
Anti viral activity EC_{50}: 19.92 ± 0.21 µM	**vRNA yield EC_{50}:** 16.76 ± 3.65 µM
Anti viral activity EC_{90}: 23.29 ± 0.15 µM	**vRNA yield EC_{90}:** 22.3 ± 1.38 µM
Cytotoxicity CC_{50}: 51.5 ± 0.62 µM	**SI CC50/EC50:** 2.59
Native MS adduct saturation: 3% (94/6/0)	**Native MS adduct size:** 390 Da

Hit#12: AT7519 bound to SARS-CoV-2 MPro, PDB: 7AGA

Synonyms: AT7519, 844442-38-2

PubChem CID: 11338033

CAS: 844442-38-2

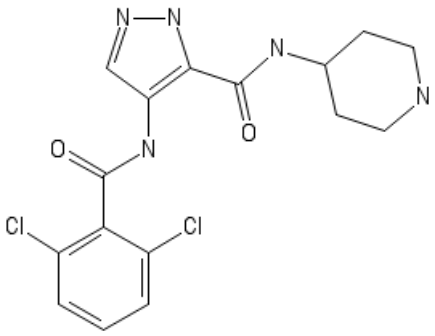
Molecular weigth: 382.2 g/mol

Binding type: non-covalent

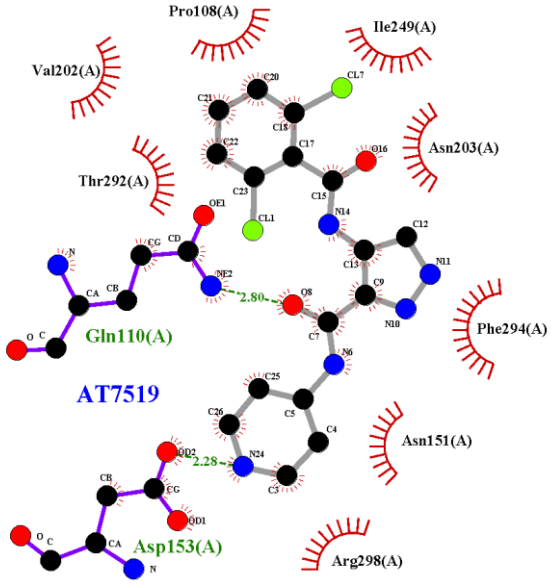
Binding location: allosteric site II

Screen compound ID: DOM_SIM_132

Original compound:

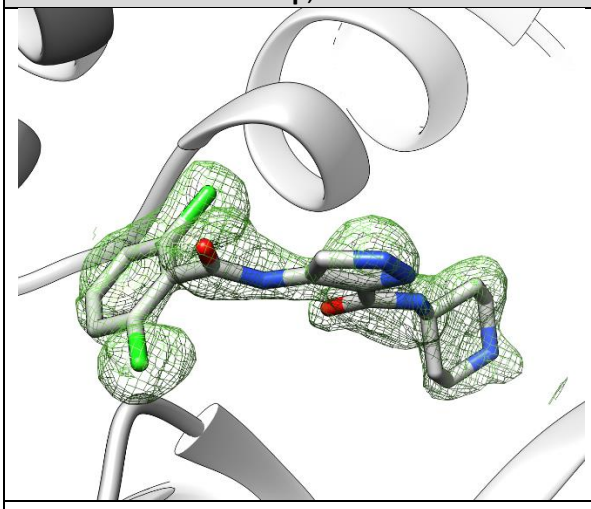


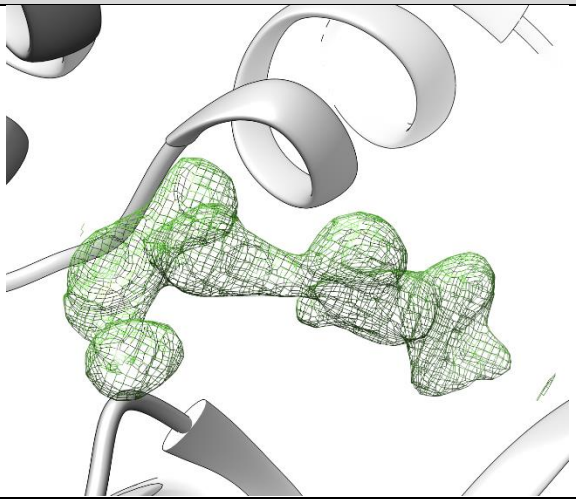
Lig-Plot interaction network



Isomeric smiles: C1CNCCC1NC(=O)C2=C(C=NN2)NC(=O)C3=C(C=CC=C3Cl)Cl

Refinement 2Fo-Fc map, 0.6 σ-level





PDB structure code: 7AGA	**PDB Ligand code:** LZE
Resolution: 1.68 Å	**R_{work}/R_{free}:** 0.19/0.23
Occupancy: 0.72	**Ligand RSCC/RSR:** 0.80/0.16
Biochemistry & Cell biology	
Anti viral activity EC_{50}: 27.5 ± 2.83 µM	**vRNA yield EC_{50}:** 43.66 ± 6.32 µM
Anti viral activity EC_{90}: 45.47 ± 2.64 µM	**vRNA yield EC_{90}:** 74.93 ± 5.39 µM
Cytotoxicity CC_{50}: > 100 µM	**SI CC50/EC50:** > 3.64
Native MS adduct saturation: 21% (65/28/7)	**Native MS adduct size:** 382 Da

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Hit#13: Zinc pyrithion bound to SARS-CoV-2 MPro, PDB: 6YT8

Synonyms: Zinc pyrithione, Zinc Omadine,

PubChem CID: 26041

CAS: 13463-41-7

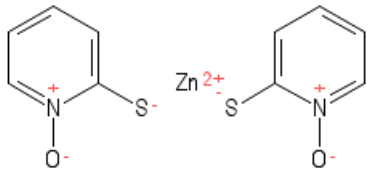
Molecular weigth: 317.7 g/mol

Binding type: Covalent, complex bond

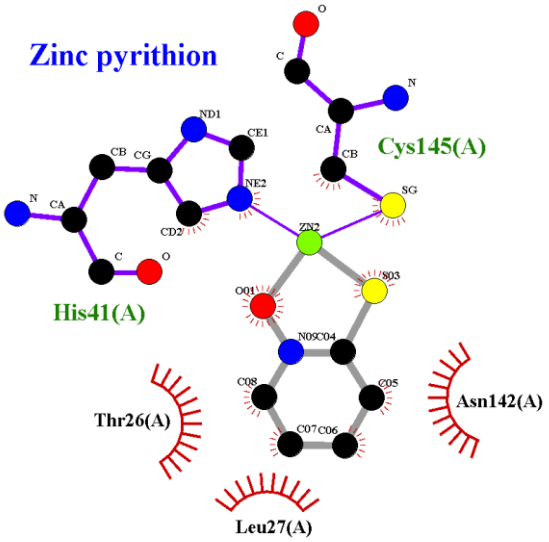
Binding location: Cystein 145, Histidine 41

Screen compound ID: SPE_K16136380

Original compound:

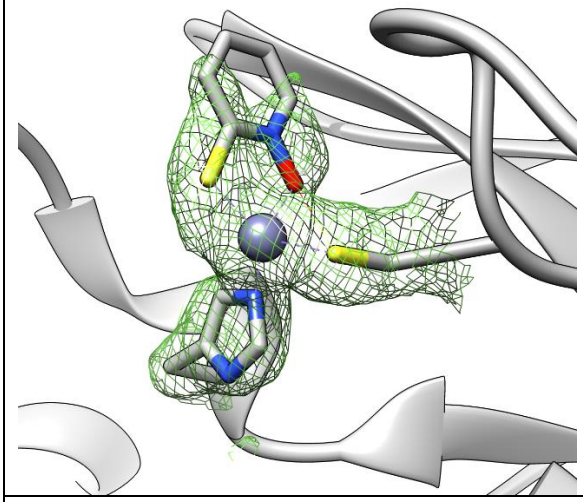


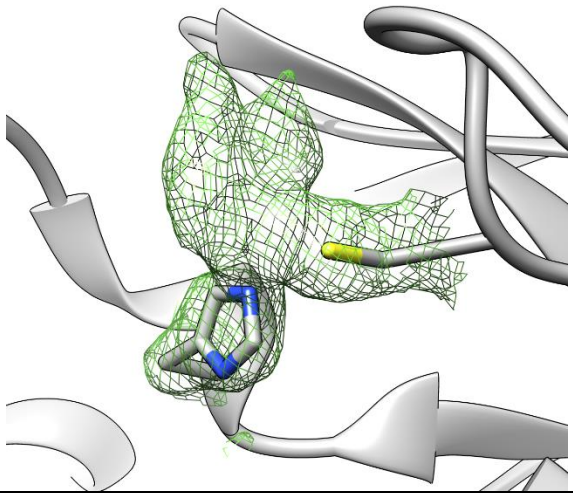
Lig-Plot interaction network



Isomeric smiles: C1=CC=[N+](C(=C1)[S-])[O-].C1=CC=[N+](C(=C1)[S-])[O-].[Zn+2]

Refinement 2Fo-Fc map, 1.4 σ-level





PDB structure code: 6YT8	**PDB Ligand code:** PK8
Resolution: 2.05 Å	**R_{work}/R_{free}:** 0.20/0.23
Occupancy: 0.83	**Ligand RSCC/RSR:** 0.96/0.16
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 72% (11/34/55)	**Native MS adduct size:** 128 Da

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Hit#14: TH-302 bound to SARS-CoV-2 MPro, PDB: 7AWS

Synonyms: Evofosfamide, TH-302, 918633-87-1, TH302

PubChem CID: 11984561

CAS: 918633-87-1

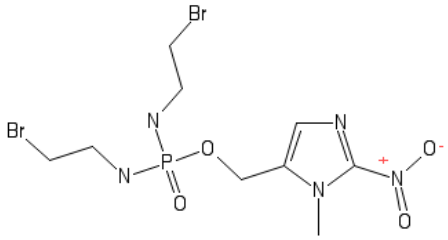
Molecular weigth: 449.04 g/mol

Binding type: covalent, thioether

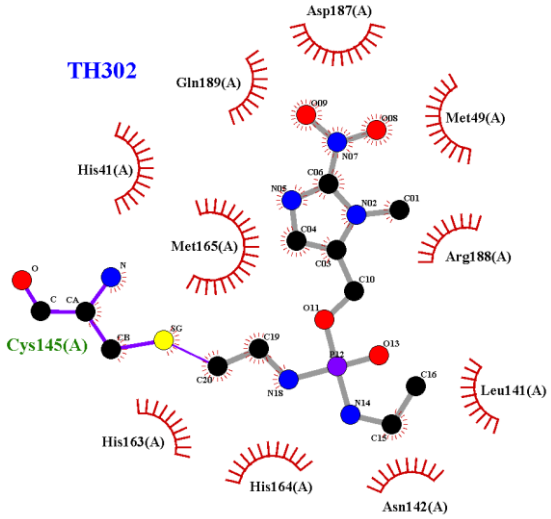
Binding location: Cystein 145

Screen compound ID: SPE_K20958582

Original compound:

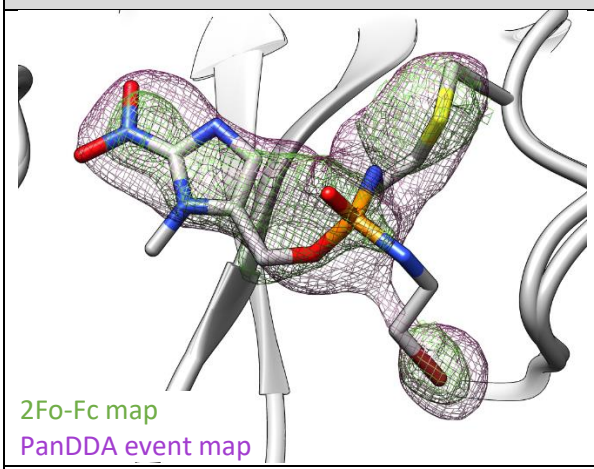


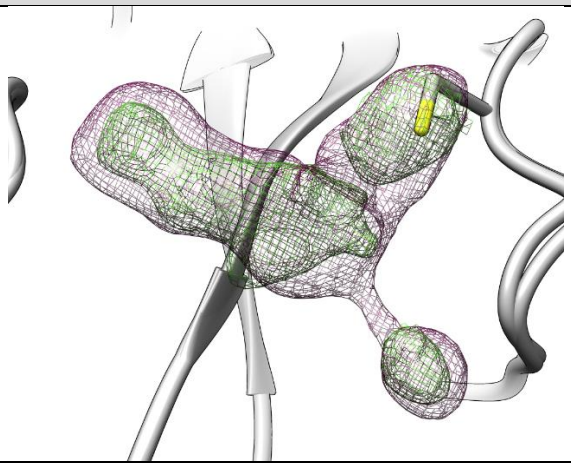
Lig-Plot interaction network



Isomeric smiles: CN1C(=CN=C1[N+](=O)[O-])COP(=O)(NCCBr)NCCBr

Refinement 2Fo-Fc map, 1.0 σ-level, **PanDDA event map BDC 0.18** , 2.0 σ-level





PDB structure code: 7AWS	**PDB Ligand code:** S8E
Resolution: 1.81 Å	**R_{work}/R_{free}:** 0.20/0.24
Occupancy: 0.56	**Ligand RSCC/RSR:** 0.64/0.27
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 25% (59/30/7)	**Native MS adduct size:** 365 Da

Hit#15: Methazolamide bound to SARS-CoV-2 MPro, not deposited

Synonyms: Methazolamide, Neptazane, Methenamide, Neptazaneat

PubChem CID: 4100

CAS: 554-57-4

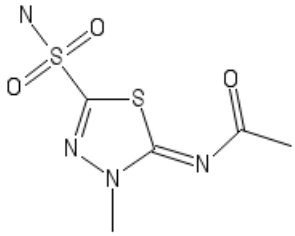
Molecular weigth: 236.3 g/mol

Binding type: binding mode undefined

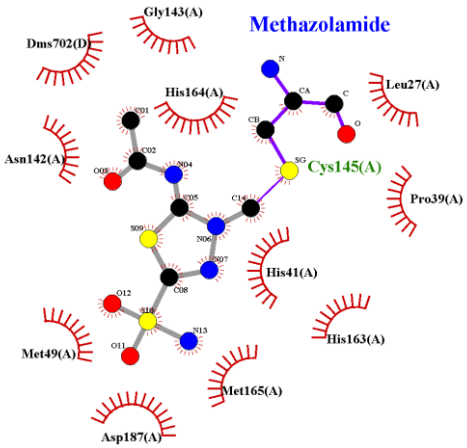
Binding location: active site pocket

Screen compound ID: SPE_K13356952

Original compound:

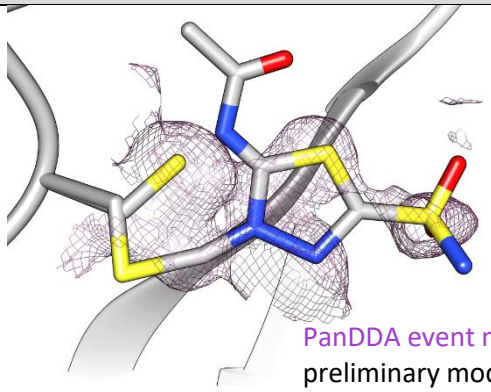


Lig-Plot interaction network

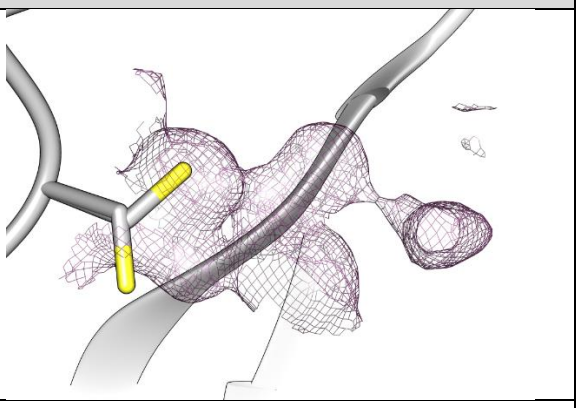


Isomeric smiles: CC(=O)N=C1N(N=C(S1)S(=O)(=O)N)C

PanDDA event map BDC 0.18, 1.2 σ-level



PanDDA event map, preliminary model



PDB structure code: -	**PDB Ligand code:** -
Resolution ohh my god Resolution: 1.65 Å	**R_{work}/R_{free}:** -
Occupancy: -	**Ligand RSCC/RSR:** -
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

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Hit#16: Fusidic acid bound to SARS-CoV-2 MPro, PDB: 7A1U

Synonyms: Fusidic acid, Fusidine, Ramycin, Fucithalmic

PubChem CID: 3000226

CAS: 6990-06-3

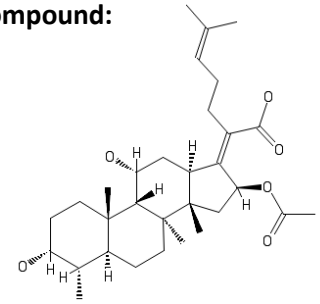
Molecular weigth: 516.7 g/mol

Binding type: non-covalent

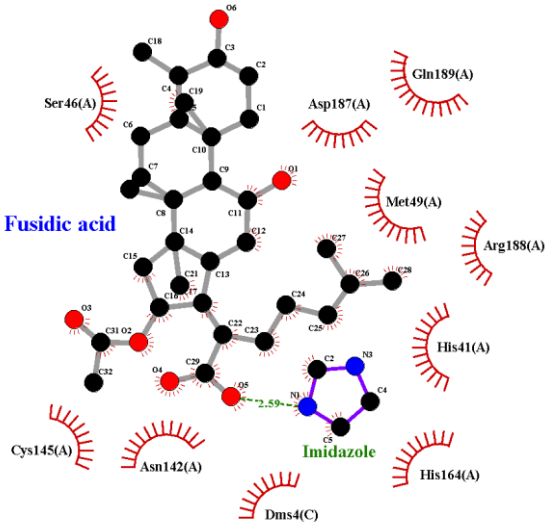
Binding location: active site pocket

Screen compound ID: SPE_A06935312

Original compound:

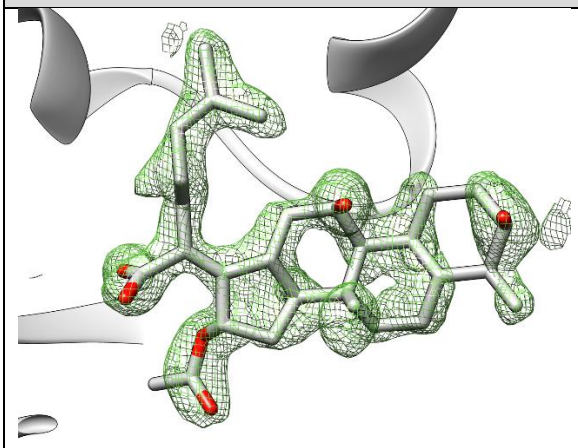


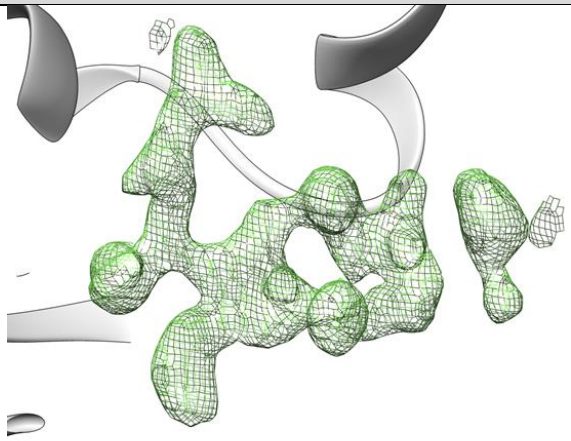
Lig-Plot interaction network



Isomeric smiles:
C[C@H]1[C@@H]2CC[C@]3([C@H]([C@]2(CC[C@H]1O)C)[C@@H](C[C@@H]\4[C@@]3(C[C@@H](/C4=C(/CCC=C(C)C)\C(=O)O)OC(=O)C)C)O)C

Refinement 2Fo-Fc map, 0.7 σ-level





PDB structure code: 7A1U	**PDB Ligand code:** FUA
Resolution: 1.8 Å	**R_{work}/R_{free}:** 0.19/0.23
Occupancy: 0.8	**Ligand RSCC/RSR:** 0.69/0.18
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 14% (78/18/5)	**Native MS adduct size:** 516 Da

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Hit#17: UNC-2327 bound to SARS-CoV-2 MPro, PDB: 7AQE

Synonyms: UNC-2327**,** CHEMBL2325198, BDBM50427787

PubChem CID: 71583615

CAS: 5057

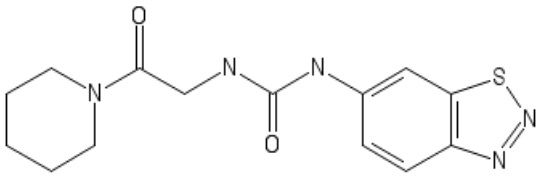
Molecular weigth: 319.38 g/mol

Binding type: non-covalent

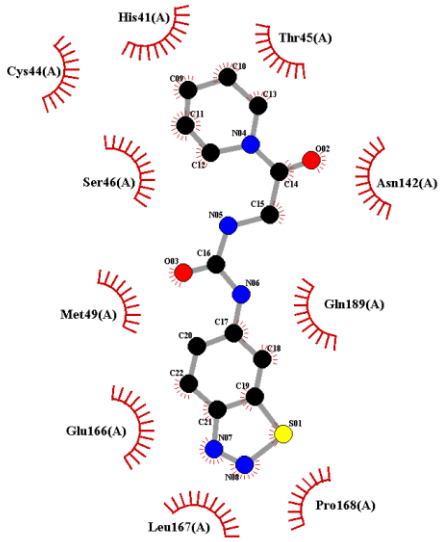
Binding location: active site pocket

Screen compound ID: SPE_K60635008

Interaction:

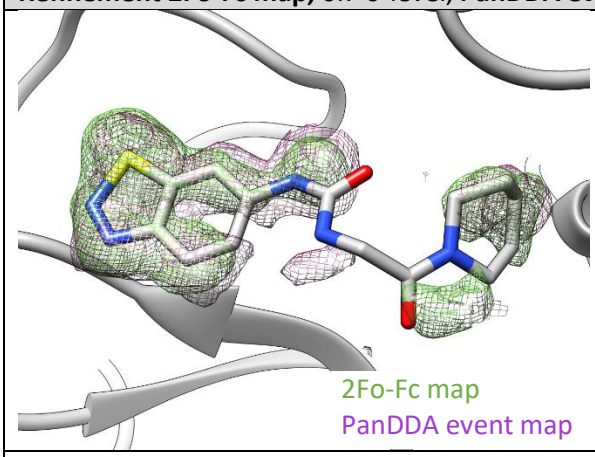


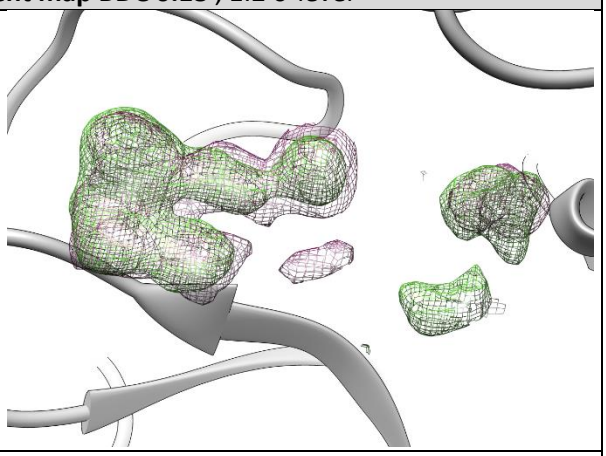
Lig-Plot interaction network



Isomeric smiles: C1CCN(CC1)C(=O)CNC(=O)NC2=CC3=C(C=C2)N=NS3

Refinement 2Fo-Fc map, 0.7 σ-level, **PanDDA event map BDC 0.18** , 1.2 σ-level





PDB structure code: 7AQE	**PDB Ligand code:** RV5
Resolution: 1.5 Å	**R_{work}/R_{free}:** 0.20/0.24
Occupancy: 0.82	**Ligand RSCC/RSR:** 0.67/0.34
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 12% (76/24/0)	**Native MS adduct size:** 319 Da

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Hit#18: Glycitein bound to SARS-CoV-2 MPro, not deposited

Synonyms: Glycitein, 40957-83-3, 7,4'-Dihydroxy-6-methoxyisoflavone

PubChem CID: 5317750

CAS: 956128-01-1

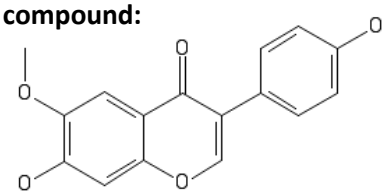
Molecular weigth: 284.26 g/mol

Binding type: binding mode undefined

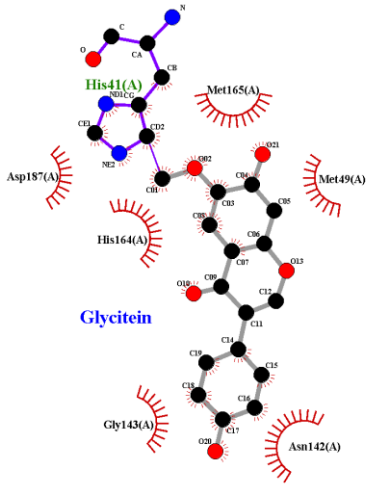
Binding location: active site pocket

Screen compound ID: SPE_K78303961

Original compound:



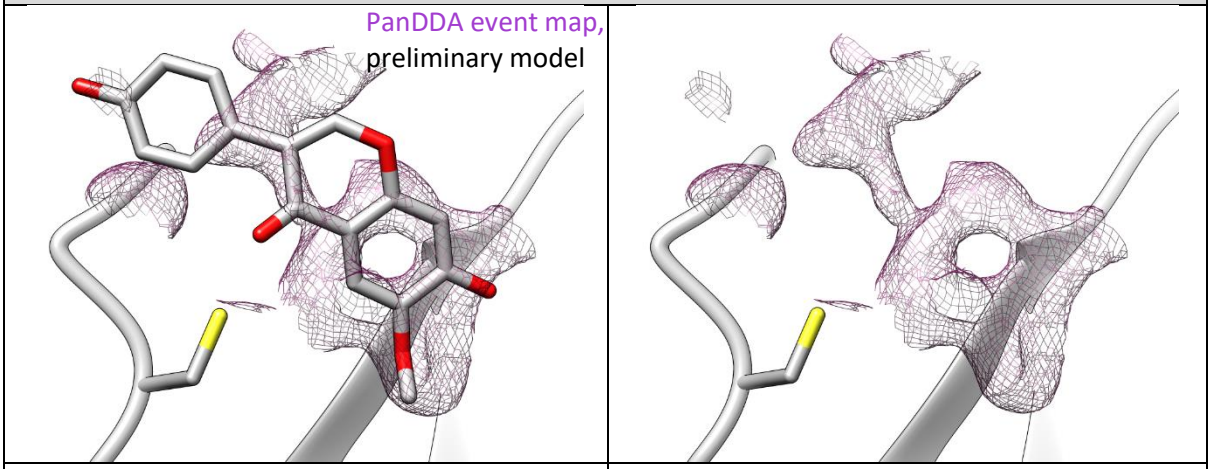
Lig-Plot interaction network



Isomeric smiles: COC1=C(C=C2C(=C1)C(=O)C(=CO2)C3=CC=C(C=C3)O)O

Pandda event-map, 1.0 σ-level

PanDDA event map, preliminary model



PDB structure code: -	**PDB Ligand code:** -
Resolution: 1.7 Å	**R_{work}/R_{free}:** -
Occupancy: -	**Ligand RSCC/RSR:** -
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

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Hit#19: Bromebric-acid bound to SARS-CoV-2 MPro, not deposited

Synonyms: Bromebric acid, Bromebrinsaeure, Acido bromebrico, Acidum bromebricum

PubChem CID: 5358572

CAS: 21739-91-3

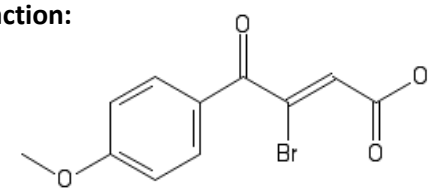
Molecular weigth: 285.09 g/mol

Binding type: non-covalent

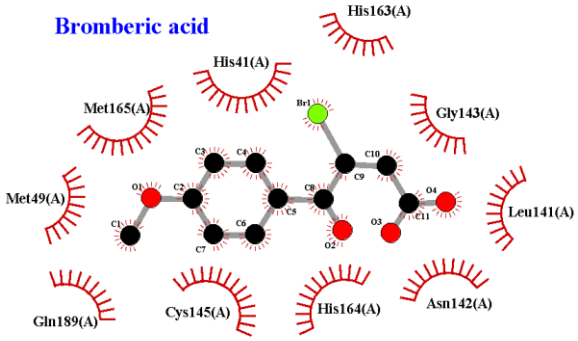
Binding location: active site pocket

Screen compound ID: SPE_K17874929

Interaction:

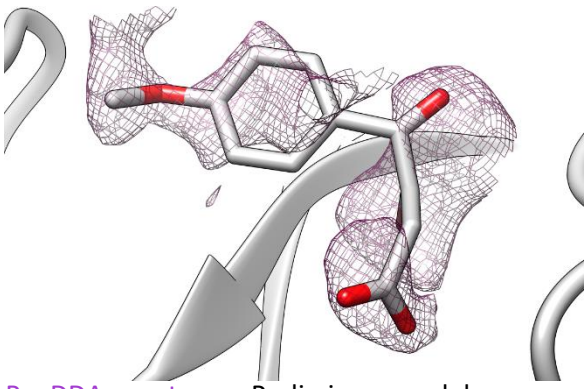


Lig-Plot interaction network

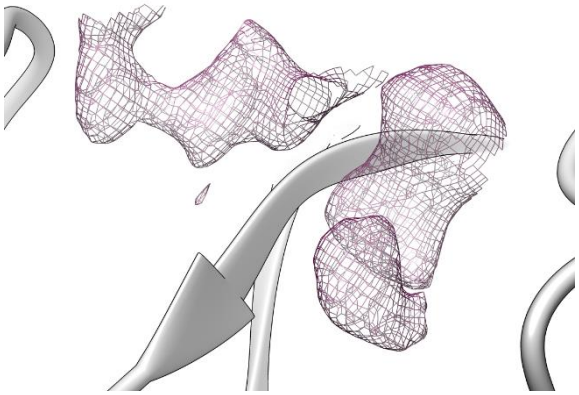


Isomeric smiles: COC1=CC=C(C=C1)C(=O)/C(=C\C(=O)O)/Br

PanDDA event map BDC 0.16 , 1.2 σ-level



PanDDA event map, Preliminary model



PDB structure code: -

PDB Ligand code: -

Resolution: 1.7 Å

R_{work}/R_{free}: -

Occupancy: -

Ligand RSCC/RSR: -

Biochemistry & Cell biology

Anti viral activity EC_{50}: N.a.

vRNA yield EC_{50}: N.a.

Anti viral activity EC_{90}: N.a.

vRNA yield EC_{90}: N.a.

Cytotoxicity CC_{50}: N.a.

SI CC50/EC50: N.a.

Native MS adduct saturation: N.a.

Native MS adduct size: N.a.

Hit#20: Aurothioglucose bound to SARS-CoV-2 MPro, PDB: 7ARF

Synonyms: Aurothioglucose, Gold thioglucose, Solganal

PubChem CID: 454937

CAS: 12192-57-3

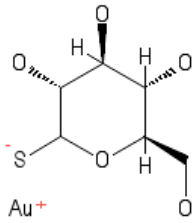
Molecular weigth: 392.18 g/mol

Binding type: Sulfinic acid Cys145, covalent disulfide Cys156

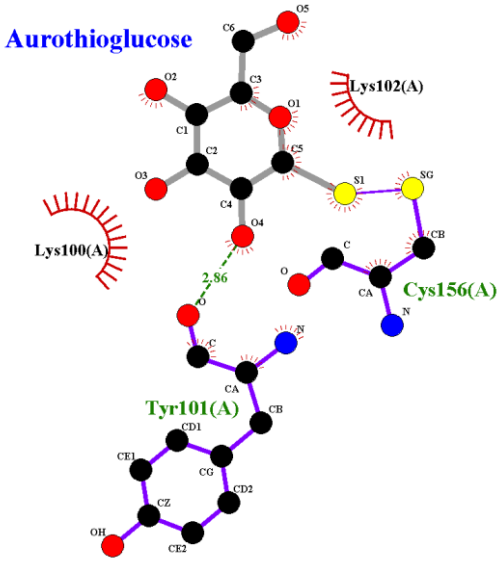
Binding location: active site Cys145, surface Cys 156

Screen compound ID: SPE_A89825407

Original compound:

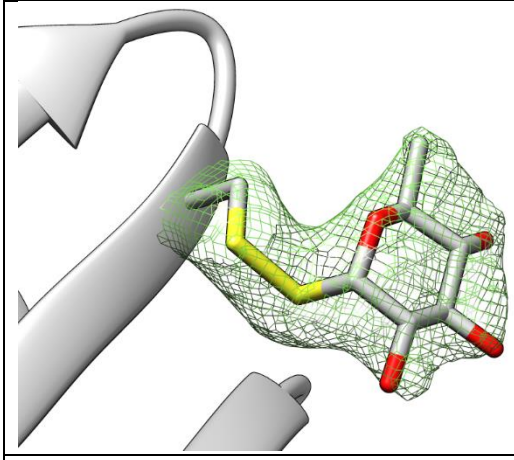


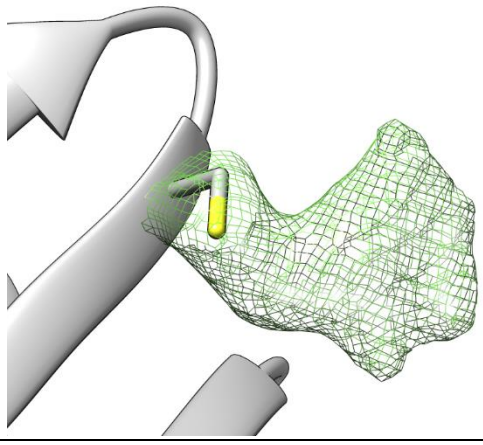
Lig-Plot interaction network



Isomeric smiles: C([C@@H]1[C@H]([C@@H]([C@H](C(O1)[S-])O)O)O)O.[Au+]

Refinement 2Fo-Fc map, 1.2 σ-level





PDB structure code: 7ARF

PDB Ligand code: RVW

Resolution: 2.0 Å

R_{work}/R_{free}: 0.21/0.25

Occupancy: 1.0

Ligand RSCC/RSR: 0.93/0.16

Biochemistry & Cell biology

Anti viral activity EC_{50}: N.a.

vRNA yield EC_{50}: N.a.

Anti viral activity EC_{90}: N.a.

vRNA yield EC_{90}: N.a.

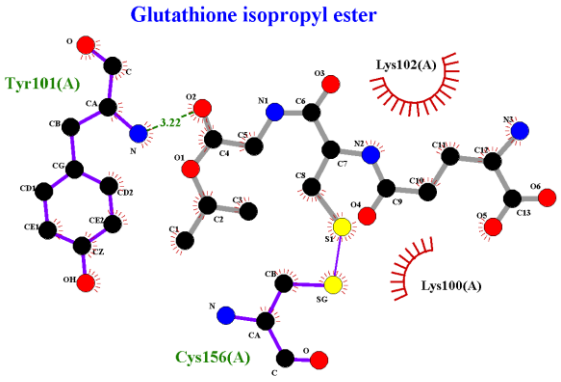
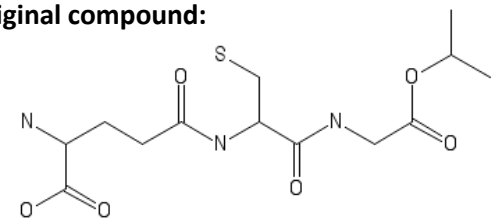
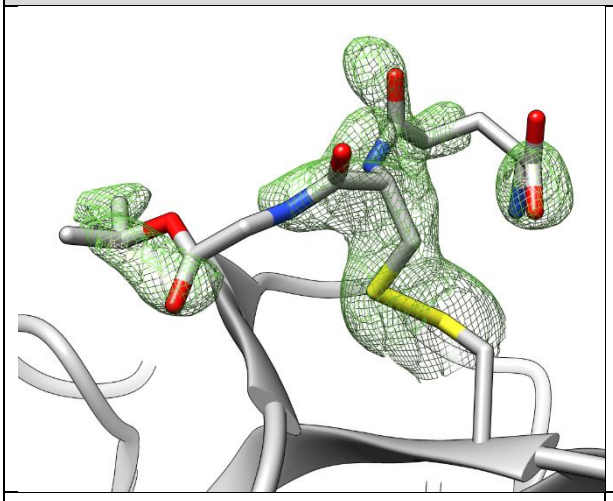
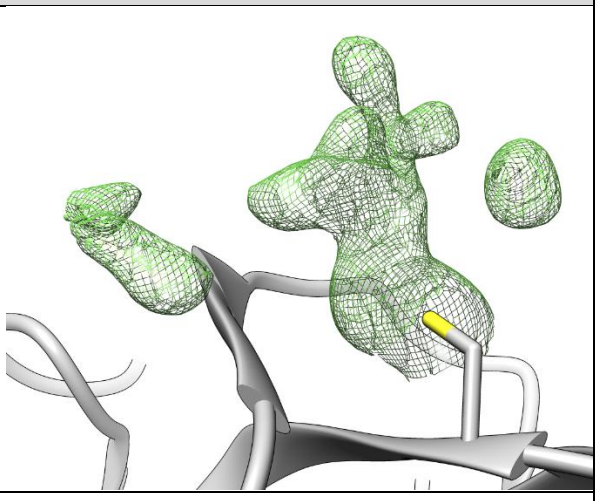
Cytotoxicity CC_{50}: N.a.

SI CC50/EC50: N.a.

Native MS adduct saturation: N.a.

Native MS adduct size: N.a.

Hit#21: Glutathione isopropyl ester bound to SARS-CoV-2 MPro, PDB: 7AX6

Synonyms: Glutathione monoisopropyl ester, Glutathione isopropyl ester, H-Glu(cys-gly-isopropyl ester)-OH	Lig-Plot interaction network
PubChem CID: 114894	
CAS: 97451-46-2	
Molecular weigth: 349.41 g/mol	
Binding type: covalent, disulfide bond	
Binding location: Cystein 156	
Screen compound ID: SPE_K58937086	
Original compound: 	
Isomeric smiles: CC(C)OC(=O)CNC(=O)C(CS)NC(=O)CCC(C(=O)O)N	
Refinement 2Fo-Fc map, 0.7 σ-level	
	
PDB structure code: 7AX6	**PDB Ligand code:** S8H
Resolution: 1.95 Å	**R_{work}/R_{free}:** 0.19/0.25
Occupancy: 0.6	**Ligand RSCC/RSR:** 0.85/0.24
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 24% (62/28/10)	**Native MS adduct size:** 126/188 Da

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Hit#22: LSN-2463359 bound to SARS-CoV-2 MPro, PDB: 7AWU

Synonyms: N-Isopropyl-5-(pyridin-4-ylethynyl)picolinamide, LSN2463359, CHEMBL2431212

PubChem CID: 72551298

CAS: -

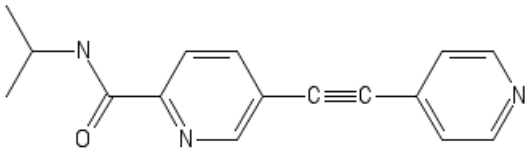
Molecular weigth: 265.31 g/mol

Binding type: Non-covalent

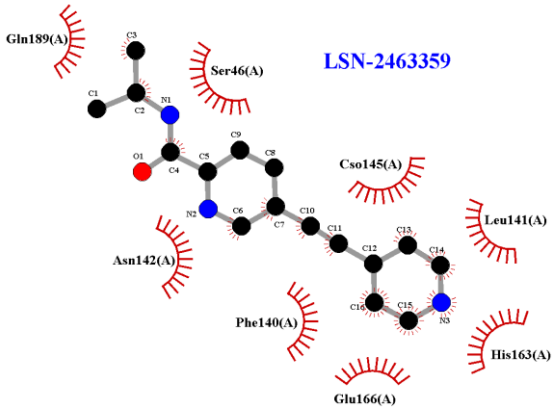
Binding location: Active site pocket

Screen compound ID: SPE_A06935312

Original compound:

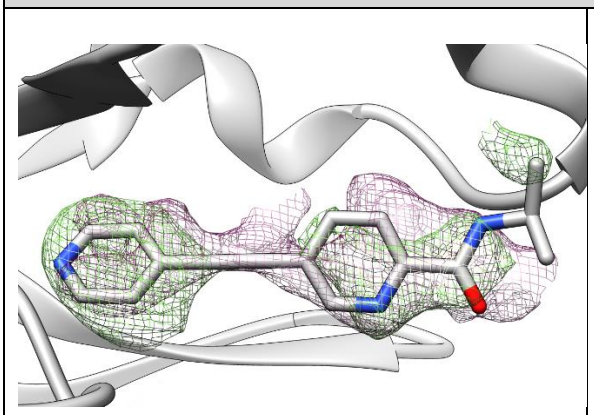


Lig-Plot interaction network

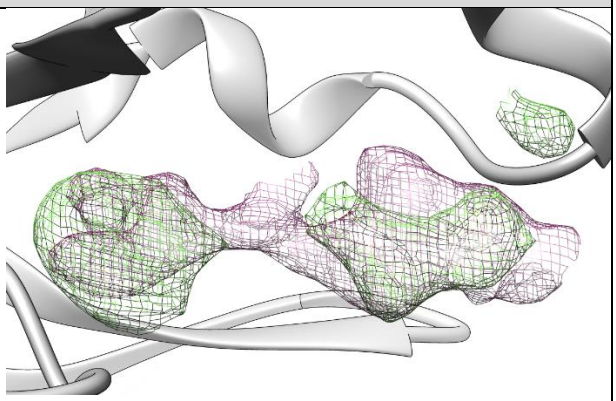


Isomeric smiles: CC(C)NC(=O)C1=NC=C(C=C1)C#CC2=CC=NC=C2

Refinement 2Fo-Fc map, 0.6 σ-level, **PanDDA event map BDC 0.18** , 1.6 σ-level



2Fo-Fc map, PanDDA event map



PDB structure code: 7AWU

PDB Ligand code: S8B

Resolution: 2.07 Å

R_{work}/R_{free}: 0.21/0.26

Occupancy: 0.75

Ligand RSCC/RSR: 0.73/0.44

Biochemistry & Cell biology

Anti viral activity EC_{50}: N.a.

vRNA yield EC_{50}: N.a.

Anti viral activity EC_{90}: N.a.

vRNA yield EC_{90}: N.a.

Cytotoxicity CC_{50}: N.a.

SI CC50/EC50: N.a.

Native MS adduct saturation: N.a.

Native MS adduct size: N.a.

Hit#23: SUN-B-8155 bound to SARS-CoV-2 MPro, not deposited

Synonyms: SUN-B 8155, 345893-91-6, 5-[1-[(2-Aminophenyl)imino]ethyl]-1,6-dihydroxy-4-methyl-2(1H)-pyridone, ZINC9129

PubChem CID: 135484493

CAS: 6990-06-3

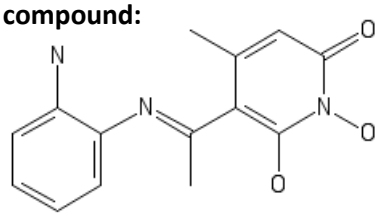
Molecular weigth: 273.29 g/mol

Binding type: binding mode undefined

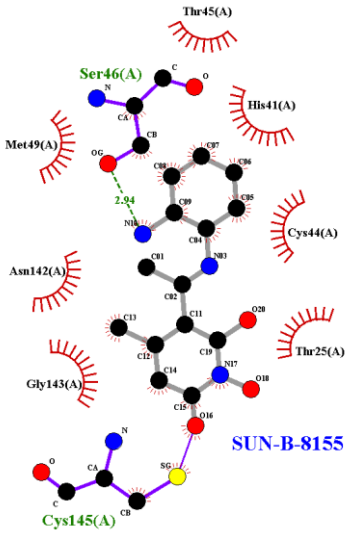
Binding location: active site pocket

Screen compound ID: SPE_K79239947

Original compound:

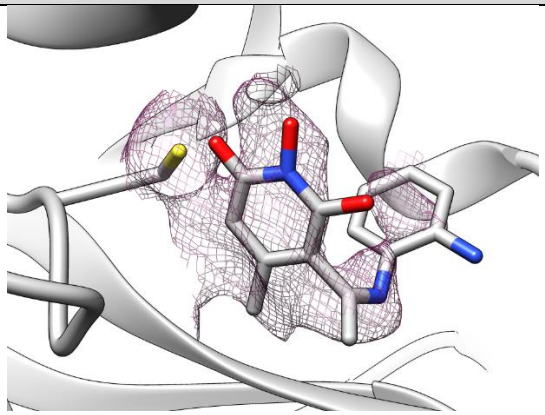


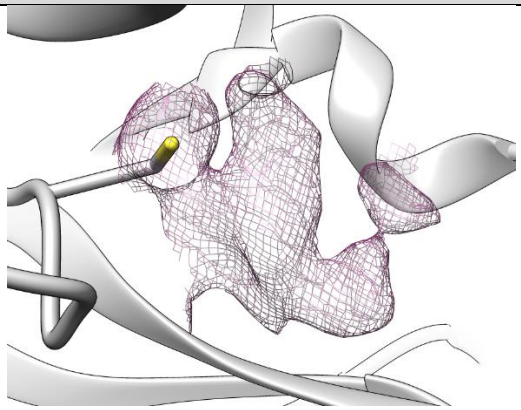
Lig-Plot interaction network



Isomeric smiles: CC1=CC(=O)N(C(=C1C(=NC2=CC=CC=C2N)C)O)O

PanDDA event map BDC 0.18 , 1.2 σ-level





PanDDA event Map, preliminary model

PDB structure code: -	**PDB Ligand code:** -
Resolution: 1.7 Å	**R_{work}/R_{free}:** -
Occupancy: -	**Ligand RSCC/RSR:** -
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
In vitro inhibition IC50: N.a.	**Native mass spectrometry:** N.a.

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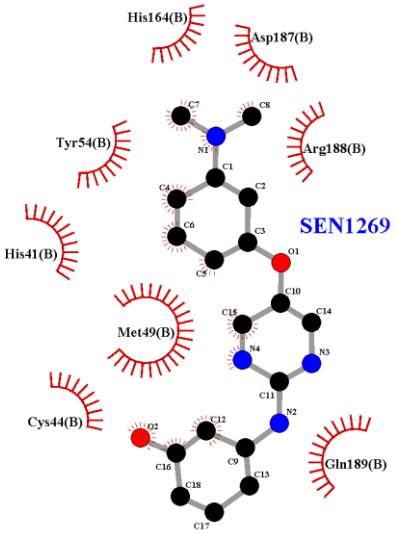
Hit#24: SEN1269 bound to SARS-CoV-2 MPro, PDB: 7AVD

Synonyms: SEN1269, 3-(5-(3-(dimethylamino)phenoxy)pyrimidin-2-ylamino)phenol

Lig-Plot interaction network



PubChem CID: 46835756

CAS: 956128-01-1

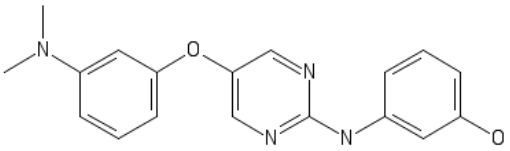
Molecular weigth: 322.36 g/mol

Binding type: Non-covalent

Binding location: Surface

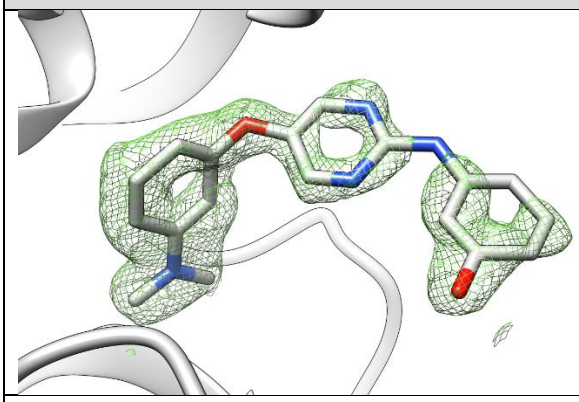
Screen compound ID: SPE_K70614402

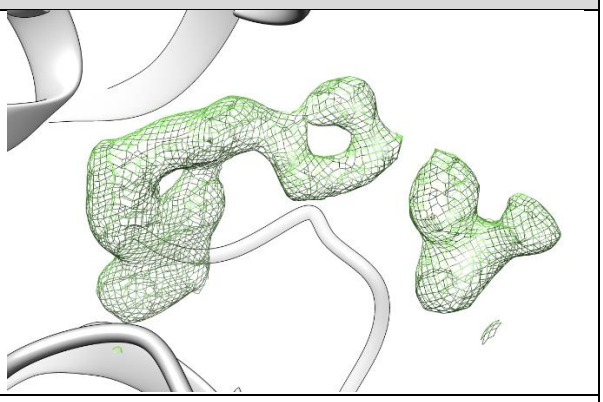
Original compound:



Isomeric smiles: CN(C)C1=CC(=CC=C1)OC2=CN=C(N=C2)NC3=CC(=CC=C3)O

Refinement 2Fo-Fc map, 0.7 σ-level





PDB structure code: 7AVD	**PDB Ligand code:** S1W
Resolution: 1.8 Å	**R_{work}/R_{free}:** 0.19/0.24
Occupancy: 1.0	**Ligand RSCC/RSR:** 0.76/0.27
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
In vitro inhibition IC50: N.a.	**Native mass spectrometry:** N.a.

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Hit#25: PD168568 bound to SARS-CoV-2 MPro, PDB: 7AMJ

Synonyms: PD 168568, 210688-56-5

PubChem CID: 56972231

CAS: 210688-56-5

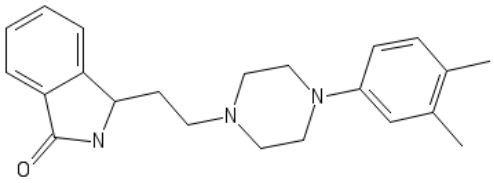
Molecular weigth: 422.4 g/mol

Binding type: non-covalent

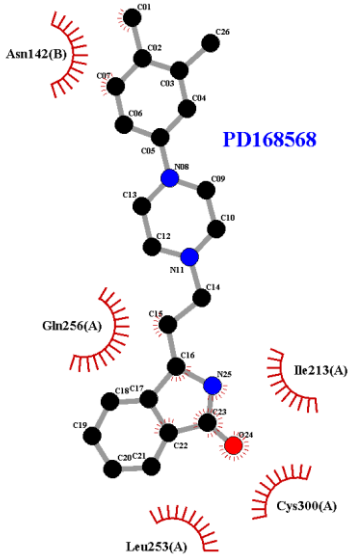
Binding location: allosteric site I

Screen compound ID: SPE_A82013137

Original compound:

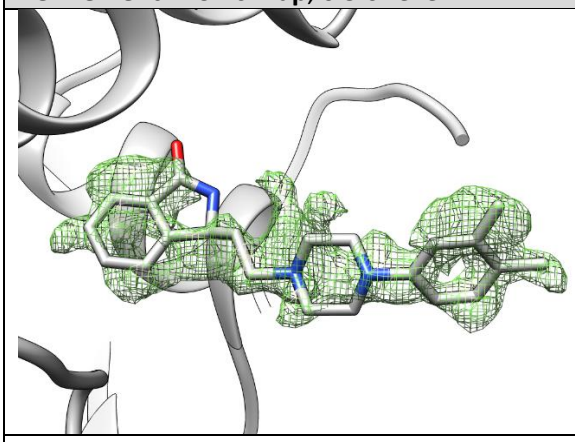


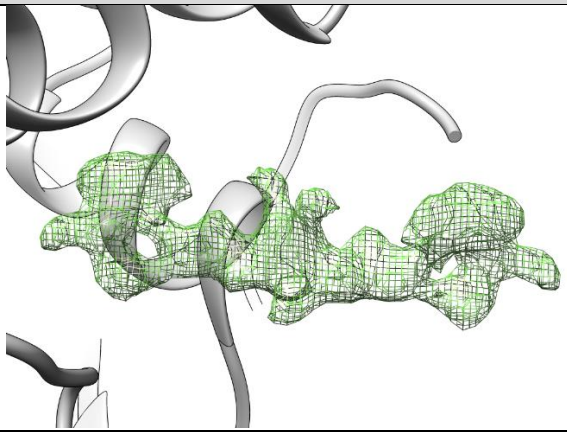
Lig-Plot interaction network



Isomeric smiles: CC1=C(C=C(C=C1)N2CCN(CC2)CCC3C4=CC=CC=C4C(=O)N3)C.Cl.Cl

Refinement 2Fo-Fc map, 0.5 σ-level





PDB structure code: 7AMJ	**PDB Ligand code:** RMZ
Resolution: 1.59 Å	**R_{work}/R_{free}:** 0.17/0.21
Occupancy: 0.42 + 0.42	**Ligand RSCC/RSR:** 0.65/0.27
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 11% (81/16/3)	**Native MS adduct size:** 350 Da

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Hit#26: Tofogliflozin bound to SARS-CoV-2 MPro, PDB: 7APH

Synonyms: Tofogliflozin, 903565-83-3, CSG 452, Tofogliflozin anhydrous, UNII-554245W62T

PubChem CID: 46908929

CAS: 903565-83-3

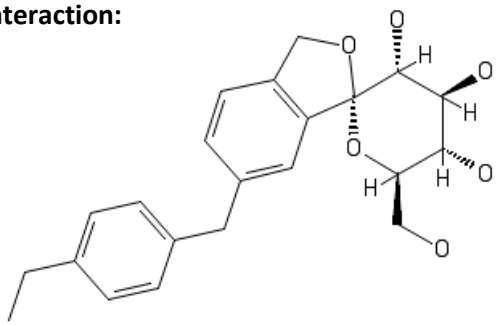
Molecular weigth: 386.4 g/mol

Binding type: non-covalent

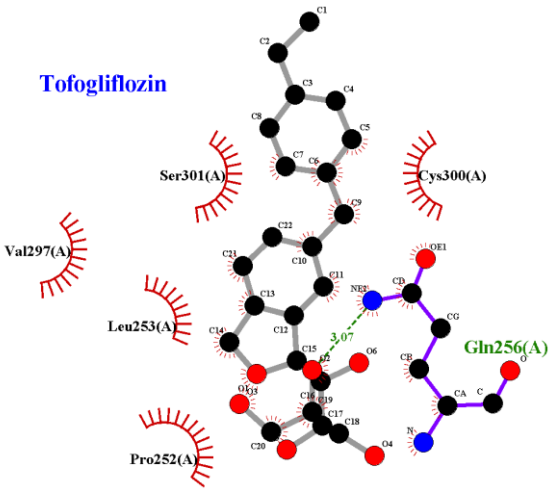
Binding location: allosteric site I

Screen compound ID: SPE_K96344439

Interaction:

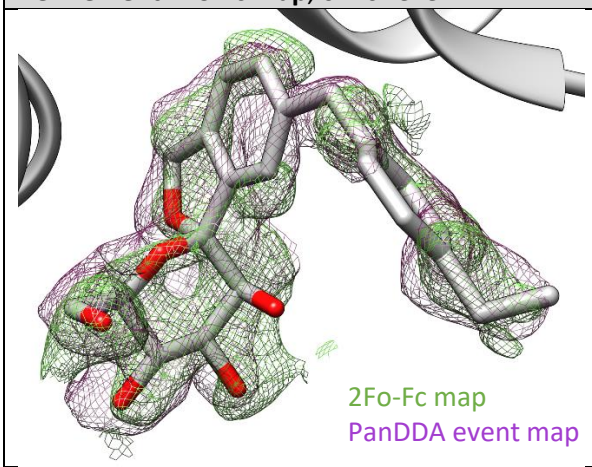


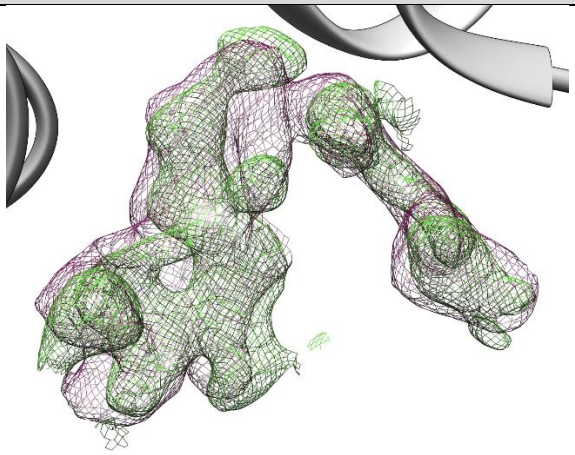
Lig-Plot interaction network



Isomeric smiles:
CCC1=CC=C(C=C1)CC2=CC3=C(CO[C@@]34[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)C=C2

Refinement 2Fo-Fc map, 0.7 σ-level





PDB structure code: 7APH	**PDB Ligand code:** RT2
Resolution: 1.65 Å	**R_{work}/R_{free}:** 0.23/0.27
Occupancy: 0.5	**Ligand RSCC/RSR:** 0.52/0.38
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 9% (82/18/0)	**Native MS adduct size:** 380 Da

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Hit#27: Adrafinil bound to SARS-CoV-2 MPro, PDB: 7ANS

Synonyms: Adrafinil, Olmifon, CRL 40028

PubChem CID: 3033226

CAS: 63547-13-7

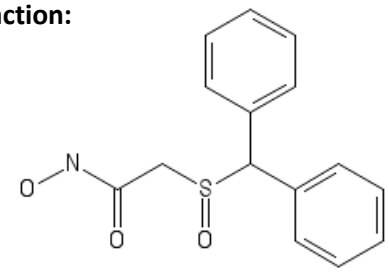
Molecular weigth: 289.4 g/mol

Binding type: non-covalent

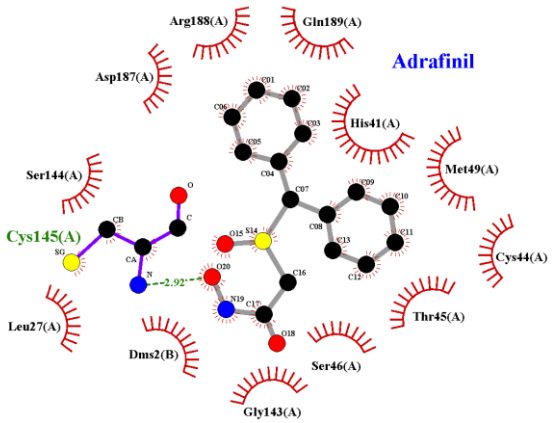
Binding location: active site pocket

Screen compound ID: DOM_SIM_074 & SPE_A90926615

Interaction:

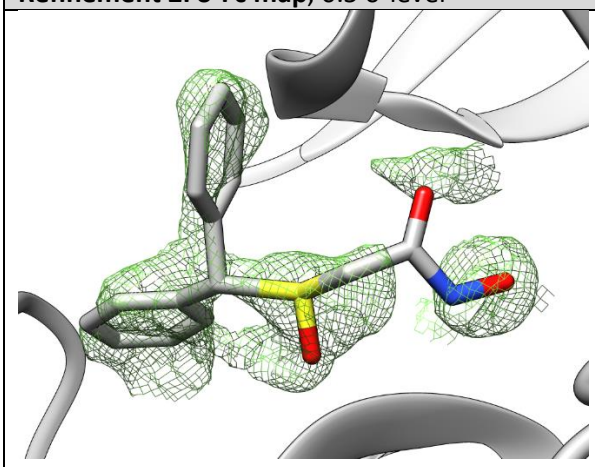


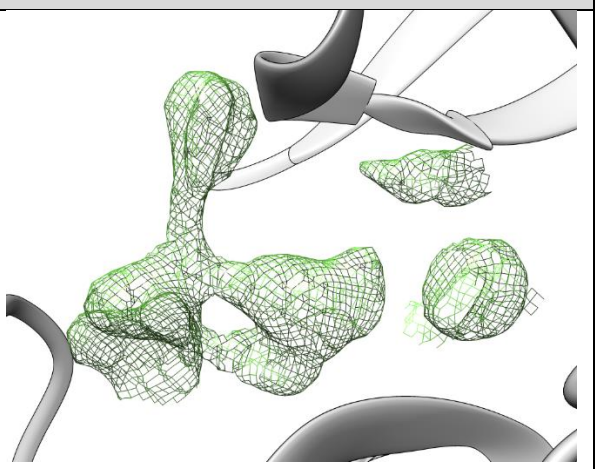
Lig-Plot interaction network



Isomeric smiles: C1=CC=C(C=C1)C(C2=CC=CC=C2)[S](=O)CC(=O)NO

Refinement 2Fo-Fc map, 0.5 σ-level





PDB structure code: 7ANS	**PDB Ligand code:** RNW
Resolution: 1.7 Å	**R_{work}/R_{free}:** 0.18/0.21
Occupancy: 0.65	**Ligand RSCC/RSR:** 0.63/0.28
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 28% (58/28/14)	**Native MS adduct size:** 289 Da

Hit#28: Tretazicar bound to SARS-CoV-2 MPro, PDB: 7AK4

Synonyms: Tretazicar, CB 1954, 21919-05-1

PubChem CID: 89105

CAS: 21919-05-1

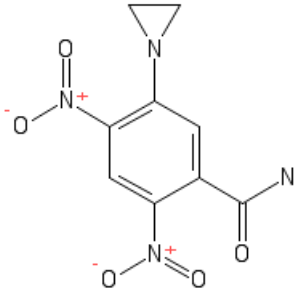
Molecular weigth: 252.18 g/mol

Binding type: non-covalent

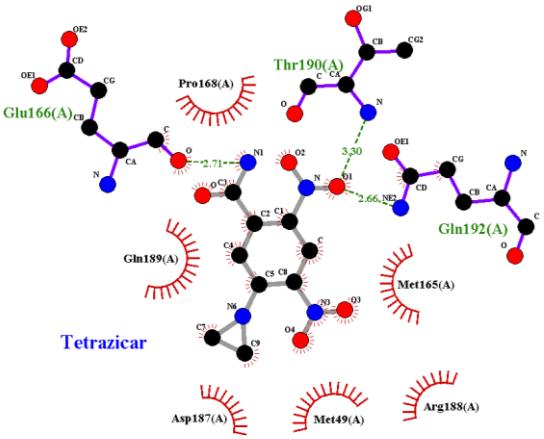
Binding location: active site pocket

Screen compound ID: DOM_SIM_234

Interaction:

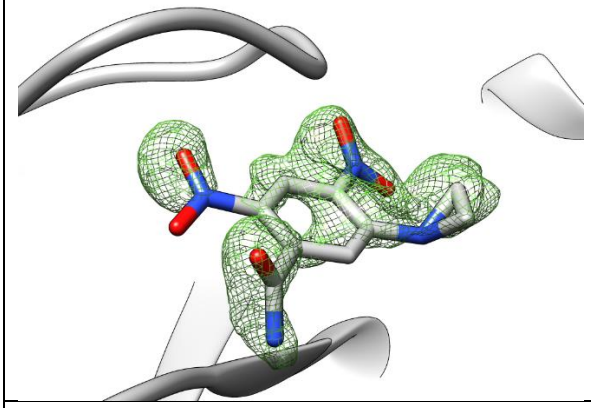


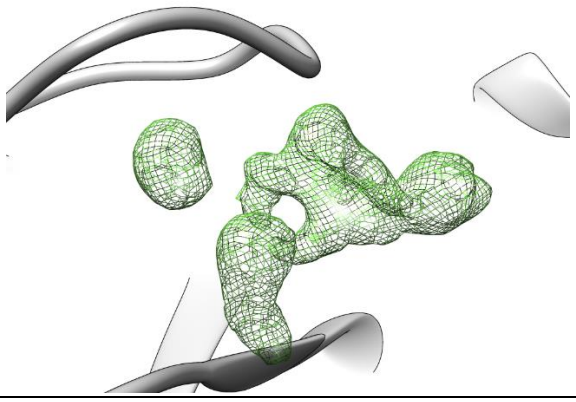
Lig-Plot interaction network



Isomeric smiles: C1CN1C2=C(C=C(C(=C2)C(=O)N)[N+](=O)[O-])[N+](=O)[O-]

Refinement 2Fo-Fc map, 0.7 σ-level





PDB structure code: 7AK4	**PDB Ligand code:** CB1
Resolution: 1.63 Å	**R_{work}/R_{free}:** 0.19/0.22
Occupancy: 0.71	**Ligand RSCC/RSR:** 0.62/0.20
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

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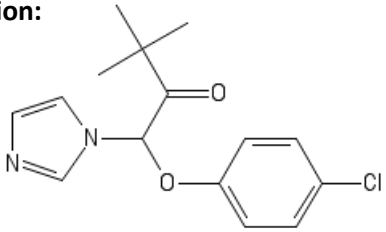
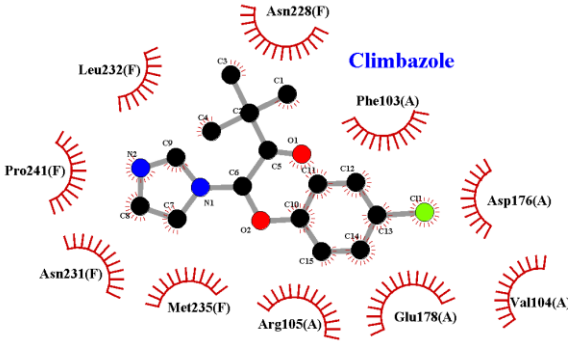
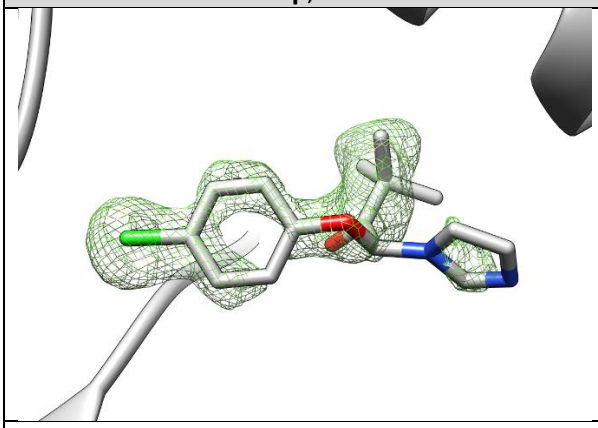
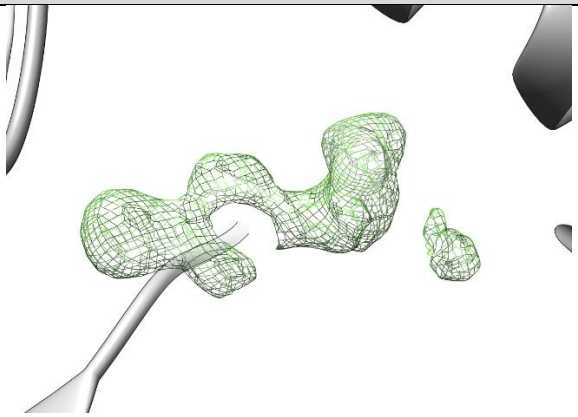
Hit#29: Climbazole bound to SARS-CoV-2 MPro, PDB: 7AOL

Synonyms: Climbazole, 38083-17-9, Baypival, Baysan	Lig-Plot interaction network
PubChem CID: 37907	
CAS: 38083-17-9	
Molecular weigth: 292.76 g/mol	
Binding type: non-covalent	
Binding location: surface	
Screen compound ID: DOM_SIM_072	
Interaction: 	
Isomeric smiles: CC(C)(C)C(=O)C(N1C=CN=C1)OC2=CC=C(C=C2)Cl	

Refinement 2Fo-Fc map, 0.5 σ-level





PDB structure code: 7AOL	**PDB Ligand code:** RQH
Resolution: 1.47 Å	**R_{work}/R_{free}:** 0.17/0.19
Occupancy: 0.65	**Ligand RSCC/RSR:** 0.86/0.26
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

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Hit#30: Dexrazoxane bound to SARS-CoV-2 MPro, not deposited

Synonyms: Dexrazoxane, 24584-09-6, Zinecard, Cardioxane

PubChem CID: 71384

CAS: 24584-09-6

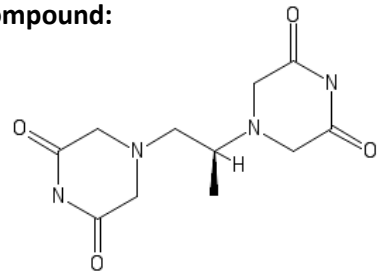
Molecular weigth: 268.27 g/mol

Binding type: binding mode undefined

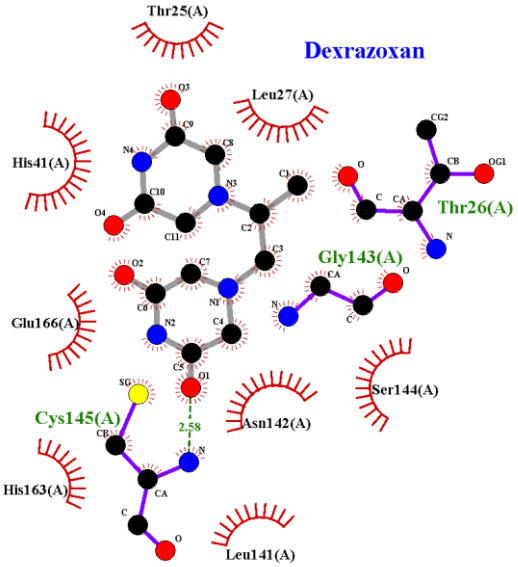
Binding location: active site pocket

Screen compound ID: DOM_SIM_486

Original compound:



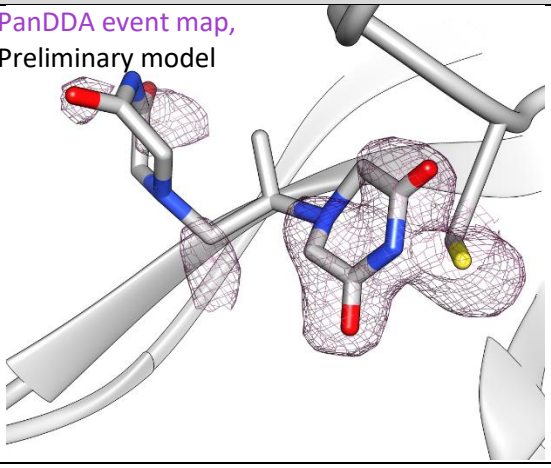
Lig-Plot interaction network

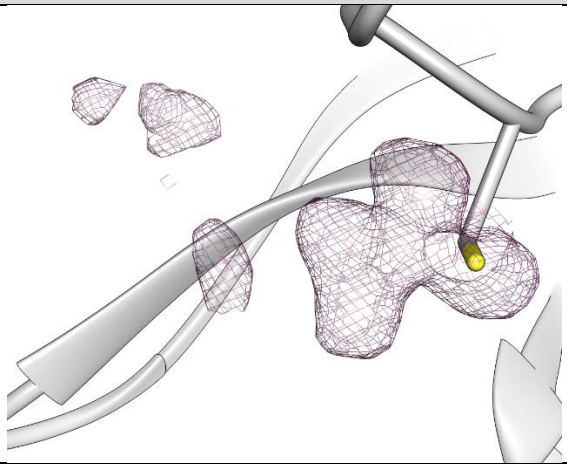


Isomeric smiles: C[C@@H](CN1CC(=O)NC(=O)C1)N2CC(=O)NC(=O)C2

PanDDA event map BDC 0.18 , 1.2 σ-level

PanDDA event map,
Preliminary model





PDB structure code: -	**PDB Ligand code:** -
Resolution: 1.7 Å	**R_{work}/R_{free}:** -
Occupancy: -	**Ligand RSCC/RSR:** -
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 30% (56/29/15)	**Native MS adduct size:** 268 Da

Hit#31: AR-42 bound to SARS-CoV-2 MPro, PDB: 7AXO

Synonyms: AR-42, OSU-HDAC42

PubChem CID: 6918848

CAS: 935881-37-1

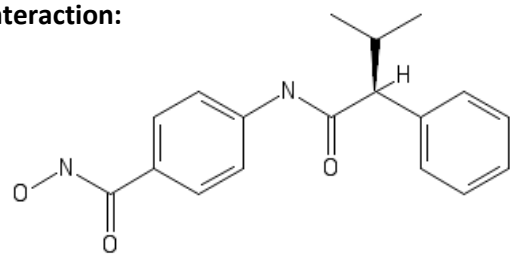
Molecular weigth: 312.4 g/mol

Binding type: non-covalent

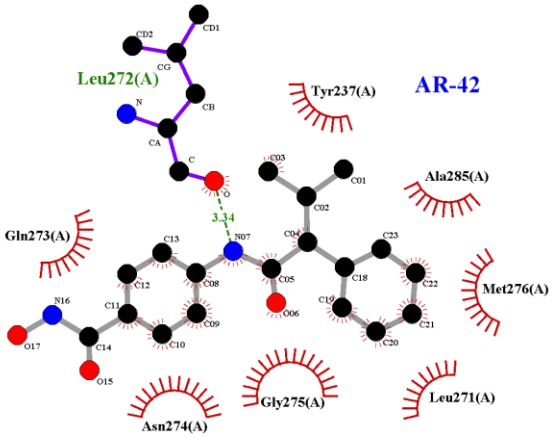
Binding location: surface

Screen compound ID: DOM_SIM_538

Interaction:

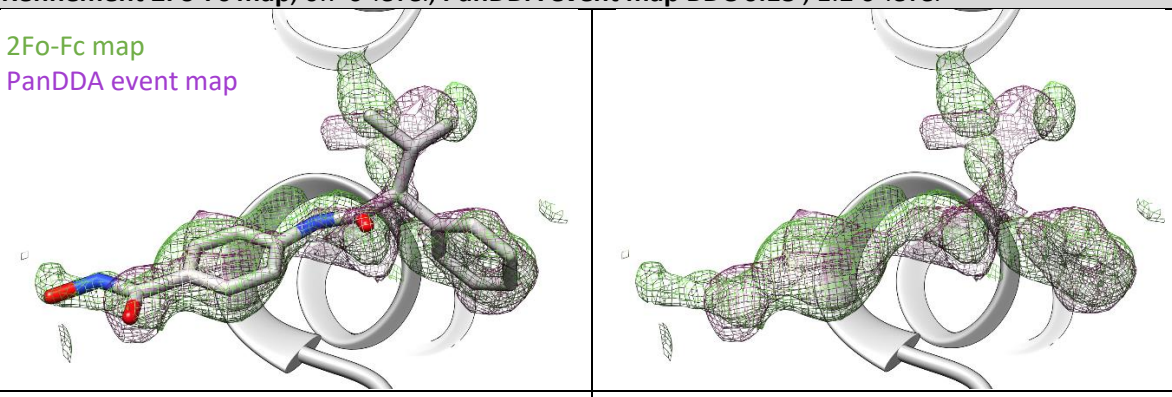


Lig-Plot interaction network



Isomeric smiles: CC(C)[C@@H](C1=CC=CC=C1)C(=O)NC2=CC=C(C=C2)C(=O)NO

Refinement 2Fo-Fc map, 0.7 σ-level, **PanDDA event map BDC 0.18** , 1.2 σ-level



PDB structure code: 7AXO	**PDB Ligand code:** QCP
Resolution: 1.65 Å	**R_{work}/R_{free}:** 0.17/0.20
Occupancy: 0.79	**Ligand RSCC/RSR:** 0.67/0.22
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 13% (78/18/4)	**Native MS adduct size:** 580 Da

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Hit#32: Clonidine bound to SARS-CoV-2 MPro, PDB: 7AWW

Synonyms: Clonidine

PubChem CID: 5358572

CAS: 21739-91-3

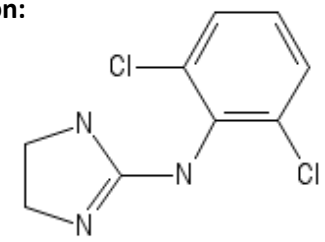
Molecular weigth: 285.09 g/mol

Binding type: non-covalent

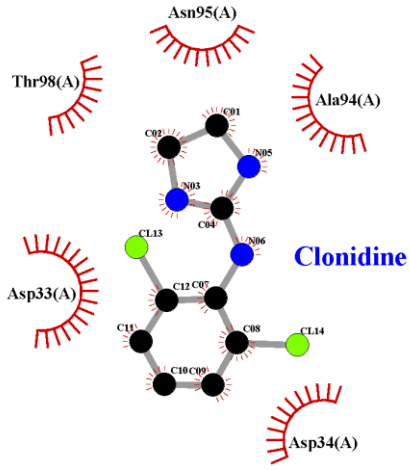
Binding location: active site

Screen compound ID: SPE_K98530306

Interaction:

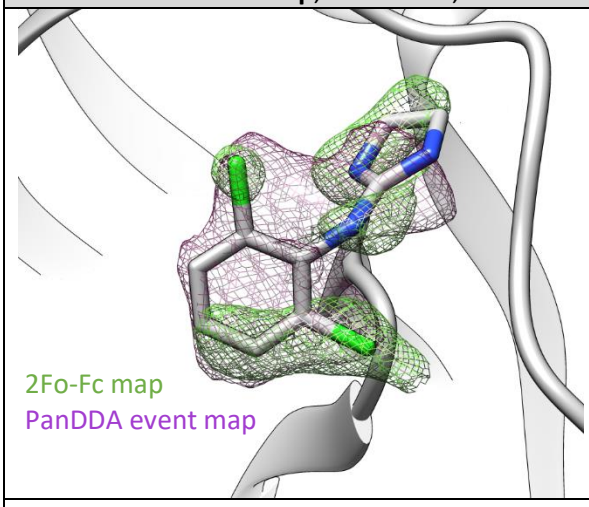


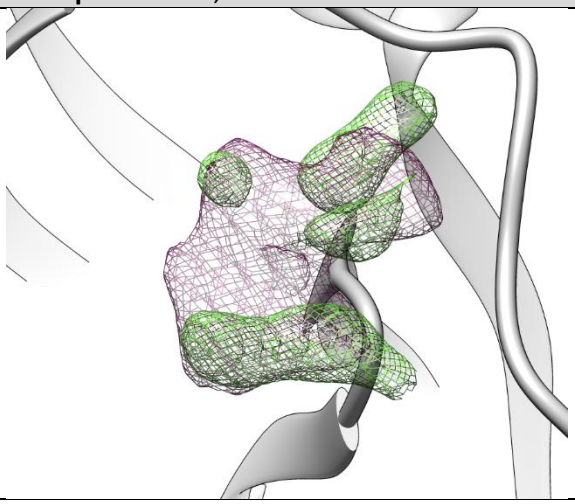
Lig-Plot interaction network



Isomeric smiles: C1CN=C(N1)NC2=C(C=CC=C2Cl)Cl

Refinement 2Fo-Fc map, 0.7 σ-level, **PanDDA event map BDC 0.18** , 1.6 σ-level





PDB structure code: 7AWW	**PDB Ligand code:** CLU
Resolution: 1.65 Å	**R_{work}/R_{free}:** 0.20/0.24
Occupancy: 0.80	**Ligand RSCC/RSR:** 0.40/0.39
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

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Hit#33: Tegafur bound to SARS-CoV-2 MPro, PDB: 7AWR

Synonyms: Tegafur, Ftorafur, 17902-23-7, Futraful, Fluorofur

PubChem CID: 5386

CAS: 6990-06-3

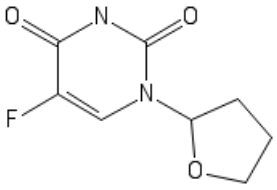
Molecular weigth: 200.17 g/mol

Binding type: non-covalent

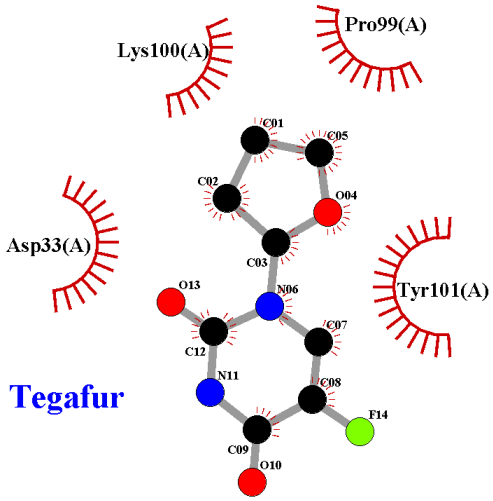
Binding location: surface

Screen compound ID: SPE_A06935312

Original compound:

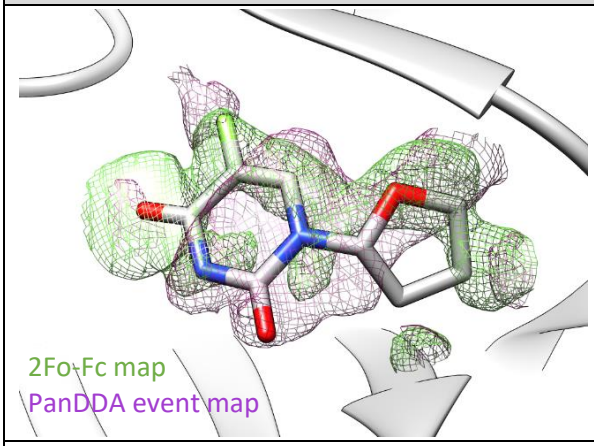


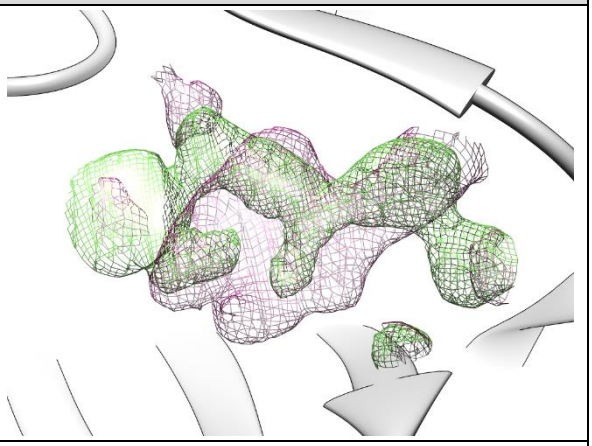
Lig-Plot interaction network



Isomeric smiles: C1CC(OC1)N2C=C(C(=O)NC2=O)F

Refinement 2Fo-Fc map, 0.6 σ-level, **PanDDA event map BDC 0.18** , 1.7 σ-level





PDB structure code: 7AWR	**PDB Ligand code:** S7W
Resolution: 1.65 Å	**R_{work}/R_{free}:** 0.18/0.22
Occupanc	**Ligand RSCC/RSR:** 0.50/0.27
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

Hit#34: Necrostatin-1 bound to SARS-CoV-2 MPro, not deposited

Synonyms: Necrostatin-1, MTH-DL-Tryptophan, Nec-1

PubChem CID: 2828334

CAS: 4311-88-0

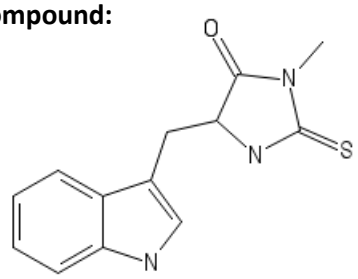
Molecular weigth: 259.33 g/mol

Binding type: non-covalent

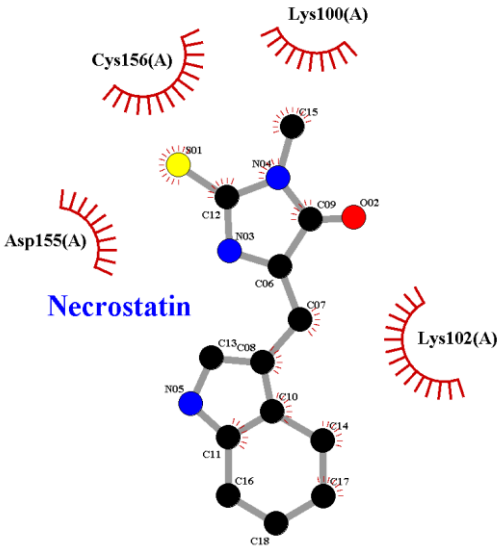
Binding location: surface

Screen compound ID: SPE_A06935312

Original compound:

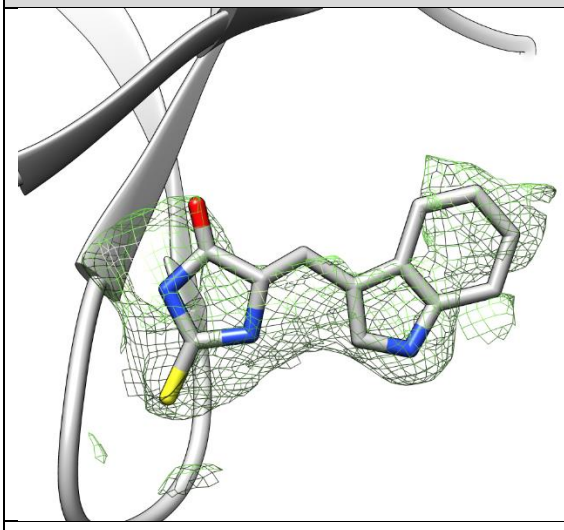


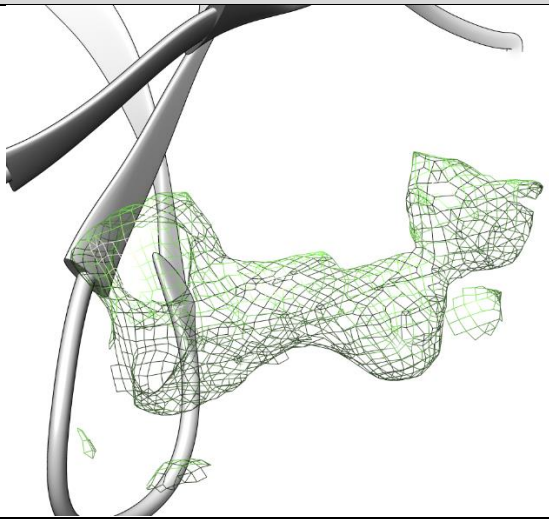
Lig-Plot interaction network



Isomeric smiles: CN1C(=O)C(NC1=S)CC2=CNC3=CC=CC=C32

Refinement 2Fo-Fc map, 0.7 σ-level





PDB structure code: -

PDB Ligand code: -

Resolution: 1.7 Å

R_{work}/R_{free}: -

Occupancy: -

Ligand RSCC/RSR: -

Biochemistry & Cell biology

Anti viral activity EC_{50}: N.a.

vRNA yield EC_{50}: N.a.

Anti viral activity EC_{90}: N.a.

vRNA yield EC_{90}: N.a.

Cytotoxicity CC_{50}: N.a.

SI CC50/EC50: N.a.

Native MS adduct saturation: -

Native MS adduct size: N.a.

Hit#35: Ipidacrine bound to SARS-CoV-2 MPro, PDB: 7AF0

Synonyms: Ipidacrine, Amiridine, 2,3,5,6,7,8-Hexahydro-1H-cyclopenta[b]quinolin-9-ylamine

PubChem CID: 604519

CAS: 62732-44-9

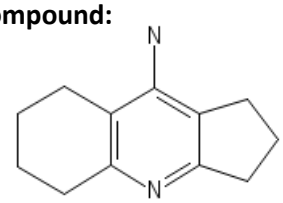
Molecular weigth: 188.27 g/mol

Binding type: non-covalent

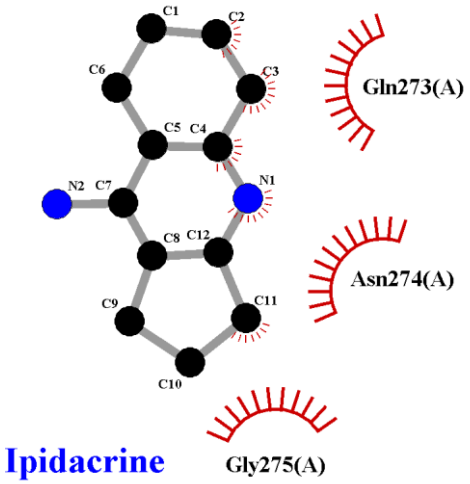
Binding location: surface

Screen compound ID: SPE_K66896231

Original compound:

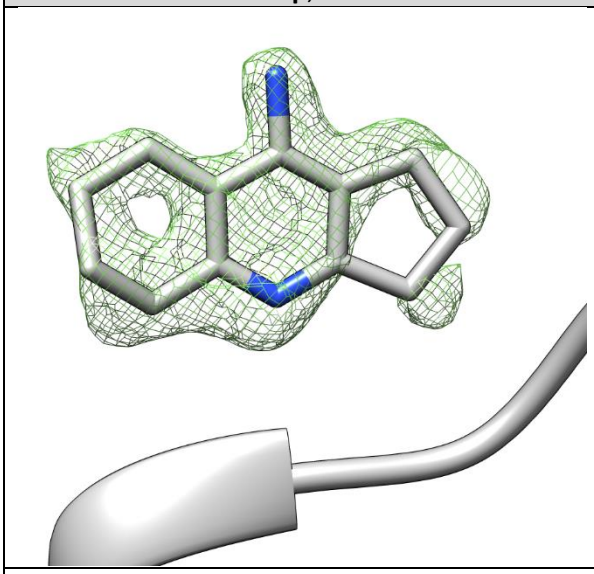


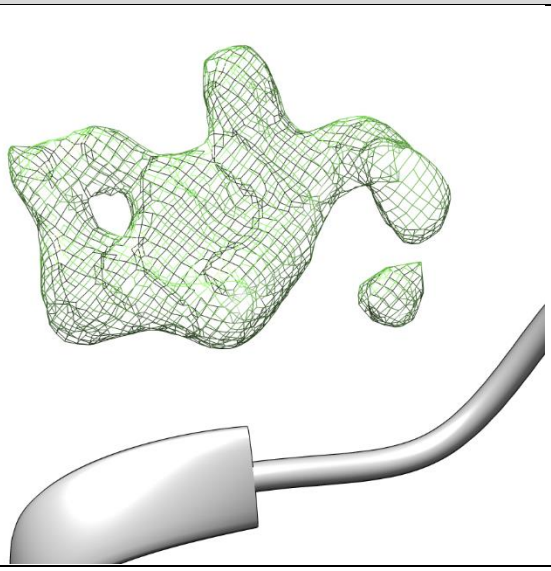
Lig-Plot interaction network



Isomeric smiles: C1CCC2=C(C1)C(=C3CCCC3=N2)N

Refinement 2Fo-Fc map, 0.8 σ-level





PDB structure code: 7AF0	**PDB Ligand code:** R9W
Resolution: 1.7 Å	**R_{work}/R_{free}:** 0.18/0.23
Occupancy: 0.61	**Ligand RSCC/RSR:** 0.74/0.22
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: -	**Native MS adduct size:** N.a.

Hit#36: AZD6482 bound to SARS-CoV-2 MPro, PDB: 6YVF

Synonyms: AZD6482, 1173900-33-8

PubChem CID: 44137675

CAS: 1173900-33-8

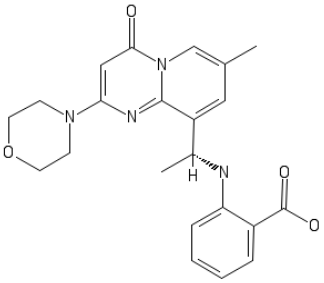
Molecular weigth: 408.4 g/mol

Binding type: non-covalent

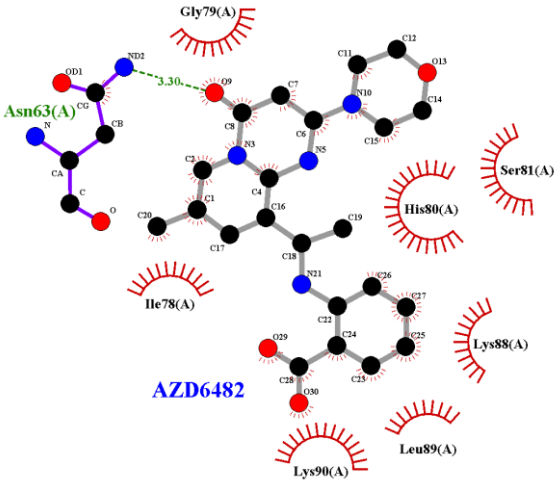
Binding location: surface

Screen compound ID: SPE_K58772419

Interaction:

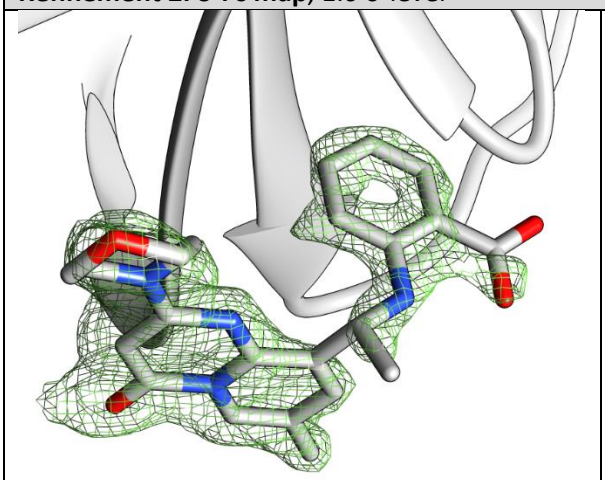


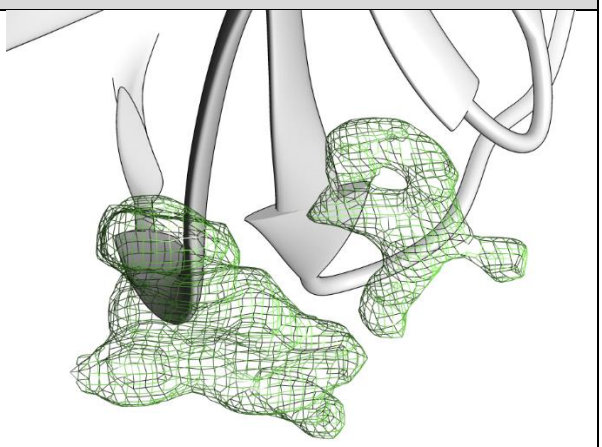
Lig-Plot interaction network



Isomeric smiles: CC1=CN2C(=O)C=C(N=C2C(=C1)[C@@H](C)NC3=CC=CC=C3C(=O)O)N4CCOCC4

Refinement 2Fo-Fc map, 1.0 σ-level





PDB structure code: 6YVF	**PDB Ligand code:** A82
Resolution: 1.63 Å	**R_{work}/R_{free}:** 0.19/0.21
Occupancy: 0.71	**Ligand RSCC/RSR:** 0.81/0.13
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 24% (62/29/9)	**Native MS adduct size:** 408 Da

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Hit#37: Polydatin bound to SARS-CoV-2 MPro, not deposited

Synonyms: Polydatin, Piceid, Trans-Piceid

PubChem CID: 5281718

CAS: 27208-80-6

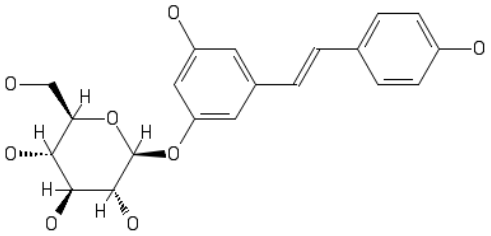
Molecular weigth: 390.4 g/mol

Binding type: Non-covalent

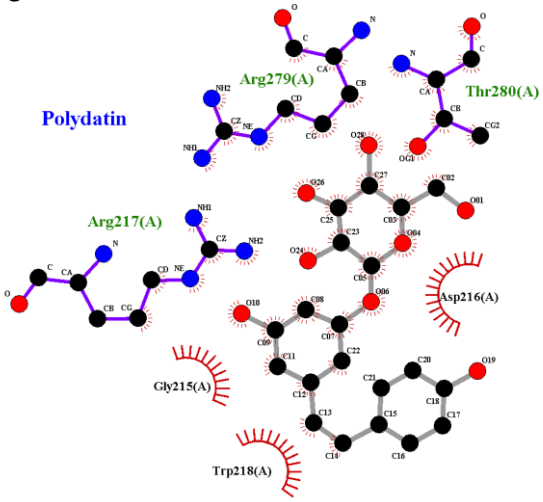
Binding location: surface

Screen compound ID: DOM_SIM_161

Original compound:

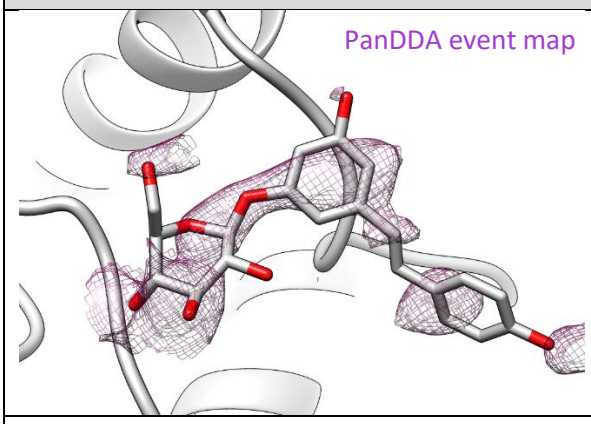


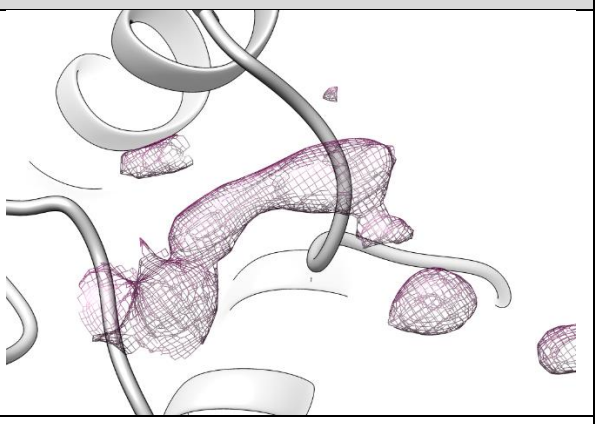
Lig-Plot interaction network



Isomeric smiles:
C1=CC(=CC=C1/C=C/C2=CC(=CC(=C2)O[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O)O)O

PanDDA event map BDC 0.25 , 1.5 σ-level





PDB structure code: -	**PDB Ligand code:** -
Resolution: 1.7 Å	**R_{work}/R_{free}:** -
Occupancy: -	**Ligand RSCC/RSR:** -
Biochemistry & Cell biology	
Anti viral activity EC_{50}: N.a.	**vRNA yield EC_{50}:** N.a.
Anti viral activity EC_{90}: N.a.	**vRNA yield EC_{90}:** N.a.
Cytotoxicity CC_{50}: N.a.	**SI CC50/EC50:** N.a.
Native MS adduct saturation: 5% (91/9/0)	**Native MS adduct size:** 390 Da

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