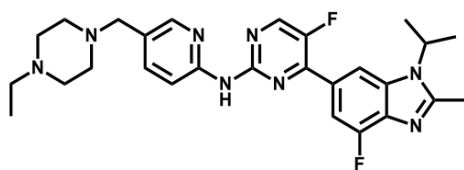


# Abemaciclib



**Alt Names:** Verzenio, Verzenios

**MW:**

**Brutto:** C<sub>27</sub>H<sub>32</sub>F<sub>2</sub>N<sub>8</sub>

**Approved for clinical use:** Advanced (Metastatic) Breast Cancer

**Approval Jurisdiction:** 2017 FDA

**InChI:** InChI=1S/C27H32F2N8/c1-5-35-8-10-36(11-9-35)16-19-6-7-24(30-14-19)33-27-31-15-22(29)25(34-27)20-12-21(28)26-23(13-20)37(17(2)3)18(4)32-26/h6-7,12-15,17H,5,8-11,16H2,1-4H3,(H,30,31,33,34)

**InChI Key:** UZWDCWONPYILKI-UHFFFAOYSA-N

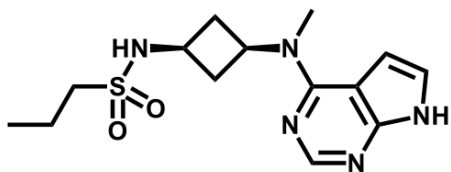
**SMILES:**

CCN1CCN(CC1)CC2=CN=C(C=C2)NC3=NC=C(C(=N3)C4=CC5=C(C(=C4)F)N=C(N5C(C)C)C)F

**PubChem CID:** 46220502

**CAS:** 1231929-97-7

# Abrocitinib



**Alt Names:** PF-04965842, Cibinqo

**MW:** 323.42

**Brutto:** C<sub>14</sub>H<sub>21</sub>N<sub>5</sub>O<sub>2</sub>S

**Approved for clinical use:** Atopic Dermatitis

**Approval Jurisdiction:** 2022 FDA

**InChI:** InChI=1S/C14H21N5O2S/c1-3-6-22(20,21)18-10-7-11(8-10)19(2)14-12-4-5-15-13(12)16-9-17-14/h4-5,9-11,18H,3,6-8H2,1-2H3,(H,15,16,17)

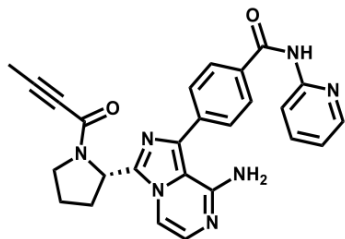
**InChI Key:** IUEWXNHSKRWHDY-UHFFFAOYSA-N

**SMILES:** CCCS(=O)(=O)NC1CC(C1)N(C)C2=NC=NC3=C2C=CN3

**PubChem CID:** 78323835

**CAS:** 1622902-68-4

# Acalabrutinib



**Alt Names:** ACP-196, Calquence

**MW:** 465.50

**Brutto:** C<sub>26</sub>H<sub>23</sub>N<sub>7</sub>O<sub>2</sub>

**Approved for clinical use:** Mantle Cell Lymphoma, CLL

**Approval Jurisdiction:** 2017 FDA 2018 EMA

**InChI:** InChI=1S/C26H23N7O2/c1-2-6-21(34)32-15-5-7-19(32)25-31-22(23-24(27)29-14-16-33(23)25)17-9-11-18(12-10-17)26(35)30-20-8-3-4-13-28-20/h3-4,8-14,16,19H,5,7,15H2,1H3,(H2,27,29)(H,28,30,35)/t19-/m0/s1

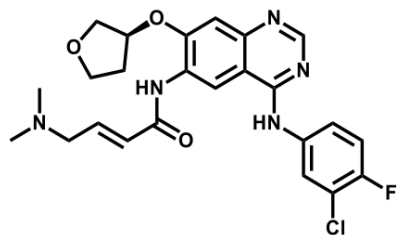
**InChI Key:** WDENQIQQYWYTPO-IBGZPJMESA-N

**SMILES:** CC#CC(=O)N1CCCC1C2=NC(=C3N2C=CN=C3N)C4=CC=C(C=C4)C(=O)NC5=CC=CC=N5

**PubChem CID:** 71226662

**CAS:** 1420477-60-6

# Afatinib



**Alt Names:**

**MW:** 485.90

**Brutto:** C<sub>24</sub>H<sub>25</sub>ClFN<sub>5</sub>O<sub>3</sub>

**Approved for clinical use:** NSCLC With EGFR Mutations

**Approval Jurisdiction:** 2013 FDA 2013 EMA

**InChI:** InChI=1S/C24H25ClFN5O3/c1-31(2)8-3-4-23(32)30-21-11-17-20(12-22(21)34-16-7-9-33-13-16)27-14-28-24(17)29-15-5-6-19(26)18(25)10-15/h3-6,10-12,14,16H,7-9,13H2,1-2H3,(H,30,32)(H,27,28,29)/b4-3+/t16-/m0/s1

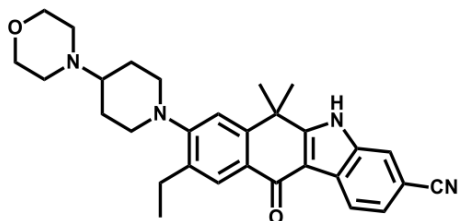
**InChI Key:** ULXXDDBFHOBEGA-CWDCEQMOSA-N

**SMILES:** CN(C)CC=CC(=O)NC1=C(C=C2C(=C1)C(=NC=N2)NC3=CC(=C(C=C3)F)Cl)OC4CCOC4

**PubChem CID:** 10184653

**CAS:** 850140-72-6

# Alectinib



**Alt Names:** Alecensa, AF-802

**MW:** 482.60

**Brutto:** C<sub>30</sub>H<sub>34</sub>N<sub>4</sub>O<sub>2</sub>

**Approved for clinical use:** NSCLC With ALK Translocations

**Approval Jurisdiction:** 2014 Japan 2015 FDA 2017 EMA

**InChI:** InChI=1S/C30H34N4O2/c1-4-20-16-23-24(17-26(20)34-9-7-21(8-10-34)33-11-13-36-14-12-33)30(2,3)29-27(28(23)35)22-6-5-19(18-31)15-25(22)32-29/h5-6,15-17,21,32H,4,7-14H2,1-3H3

**InChI Key:** KDGFLJKFZUIJMX-UHFFFAOYSA-N

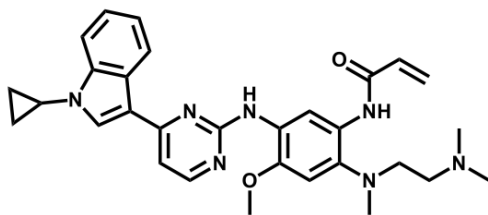
**SMILES:**

CCC1=CC2=C(C=C1N3CCC(CC3)N4CCOCC4)C(C5=C(C2=O)C6=C(N5)C=C(C=C6)C#N)(C)C

**PubChem CID:** 49806720

**CAS:** 1256580-46-7

# Almonertinib



**Alt Names:** HS-10296, Aumolertinib, Ameile

**MW:** 525.60

**Brutto:** C<sub>30</sub>H<sub>35</sub>N<sub>7</sub>O<sub>2</sub>

**Approved for clinical use:** Advanced Mutation +Ve NSCLC

**Approval Jurisdiction:** 2020 China

**InChI:** InChI=1S/C30H35N7O2/c1-6-29(38)32-24-17-25(28(39-5)18-27(24)36(4)16-15-35(2)3)34-30-31-14-13-23(33-30)22-19-37(20-11-12-20)26-10-8-7-9-21(22)26/h6-10,13-14,17-20H,1,11-12,15-16H2,2-5H3,(H,32,38)(H,31,33,34)

**InChI Key:** DOEOECWDNSEFDN-UHFFFAOYSA-N

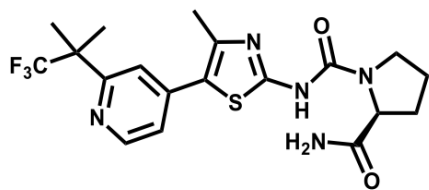
**SMILES:**

CN(C)CCN(C)C1=CC(=C(C=C1NC(=O)C=C)NC2=NC=CC(=N2)C3=CN(C4=CC=CC=C43)C5CC5)OC

**PubChem CID:** 121280087

**CAS:** 1899921-05-1

# Alpelisib



**Alt Names:** BYL-719, BYL719, Piqray

**MW:** 441.50

**Brutto:** C<sub>19</sub>H<sub>22</sub>F<sub>3</sub>N<sub>5</sub>O<sub>2</sub>S

**Approved for clinical use:** Breast Cancer, HR+Ve, HER2-Ve

**Approval Jurisdiction:** 2019 FDA

**InChI:** InChI=1S/C19H22F3N5O2S/c1-10-14(11-6-7-24-13(9-11)18(2,3)19(20,21)22)30-16(25-10)26-17(29)27-8-4-5-12(27)15(23)28/h6-7,9,12H,4-5,8H2,1-3H3,(H2,23,28)(H,25,26,29)/t12-/m0/s1

**InChI Key:** STUWGJZDJHPWGZ-LBPRGKRZSA-N

**SMILES:** CC1=C(SC(=N1)NC(=O)N2CCCC2C(=O)N)C3=CC(=NC=C3)C(C)(C)C(F)(F)F

**PubChem CID:** 56649450

**CAS:** 1217486-61-7

Amivantamab

## Monoclonal antibody

**Alt Names:**

**MW:**

**Brutto:**

**Approved for clinical use:** NSCLC

**Approval Jurisdiction:** 2021 FDA

**InChI:**

**InChI Key:**

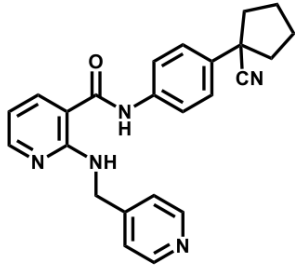
**SMILES:**

**PubChem CID:**

**CAS:** 2171511-58-1

Apatinib





**Alt Names:** rivocecranib

**MW:** 397.50

**Brutto:** C<sub>24</sub>H<sub>23</sub>N<sub>5</sub>O

**Approved for clinical use:** Gastric Cancer, NSCLC

**Approval Jurisdiction:** 2014 China 2018FDA

**InChI:** InChI=1S/C24H23N5O/c25-17-24(11-1-2-12-24)19-5-7-20(8-6-19)29-23(30)21-4-3-13-27-22(21)28-16-18-9-14-26-15-10-18/h3-10,13-15H,1-2,11-12,16H2,(H,27,28)(H,29,30)

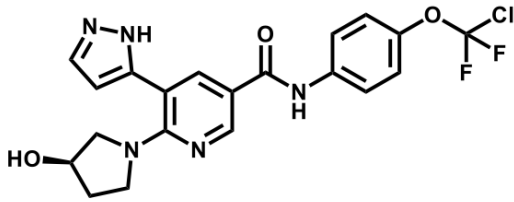
**InChI Key:** WPEWQEMJFLWMLV-UHFFFAOYSA-N

**SMILES:** C1CCC(C1)(C#N)C2=CC=C(C=C2)NC(=O)C3=C(N=CC=C3)NCC4=CC=NC=C4

**PubChem CID:** 11315474

**CAS:** 811803-05-1

Asciminib



**Alt Names:** ABL-001, ABL001

**MW:** 449.80

**Brutto:** C<sub>20</sub>H<sub>18</sub>ClF<sub>2</sub>N<sub>5</sub>O<sub>3</sub>

**Approved for clinical use:** Chronic Myelogenous Leukemia

**Approval Jurisdiction:** 2021 FDA

**InChI:** InChI=1S/C20H18ClF2N5O3/c21-20(22,23)31-15-3-1-13(2-4-15)26-19(30)12-9-16(17-5-7-25-27-17)18(24-10-12)28-8-6-14(29)11-28/h1-5,7,9-10,14,29H,6,8,11H2,(H,25,27)(H,26,30)/t14-/m1/s1

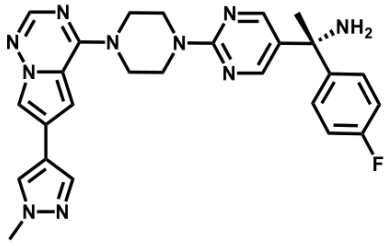
**InChI Key:** VOVZXURTCKPRDQ-CQSZACIVSA-N

**SMILES:** C1CN(CC1O)C2=C(C=C(C=N2)C(=O)NC3=CC=C(C=C3)OC(F)(F)Cl)C4=CC=NN4

**PubChem CID:** 72165228

**CAS:** 1492952-76-7

Avapritinib



**Alt Names:** 1703793-34-3, BLU-285, Ayvakit

**MW:** 498.60

**Brutto:** C<sub>26</sub>H<sub>27</sub>FN<sub>10</sub>

**Approved for clinical use:** PDGFR Exon 18 Mutation (Incl D842V)+Ve

**Approval Jurisdiction:** 2020 FDA

**InChI:** InChI=1S/C26H27FN10/c1-26(28,20-3-5-22(27)6-4-20)21-13-29-25(30-14-21)36-9-7-35(8-10-36)24-23-11-18(16-37(23)33-17-31-24)19-12-32-34(2)15-19/h3-6,11-17H,7-10,28H2,1-2H3/t26-/m0/s1

**InChI Key:** DWYRIWUZIJKQKQ-SANMLTNESA-N

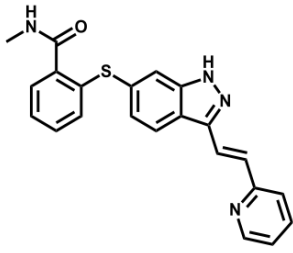
**SMILES:**

CC(C1=CC=C(C=C1)F)(C2=CN=C(N=C2)N3CCN(CC3)C4=NC=NN5C4=CC(=C5)C6=CN(N=C6)C)N

**PubChem CID:** 118023034

**CAS:**

Axitinib



**Alt Names:** Inlyta, Axinix

**MW:**

**Brutto:** C<sub>22</sub>H<sub>18</sub>N<sub>4</sub>OS

**Approved for clinical use:** Renal Cell Carcinoma

**Approval Jurisdiction:** 2012 FDA, EMA, MHRA, TGA

**InChI:** InChI=1S/C22H18N4OS/c1-23-22(27)18-7-2-3-8-21(18)28-16-10-11-17-19(25-26-20(17)14-16)12-9-15-6-4-5-13-24-15/h2-14H,1H3,(H,23,27)(H,25,26)/b12-9+

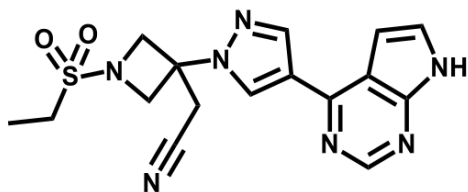
**InChI Key:** RITAVMQDGBJQJZ-FMIVXFBMSA-N

**SMILES:** CNC(=O)C1=CC=CC=C1SC2=CC3=C(C=C2)C(=NN3)C=CC4=CC=CC=N4

**PubChem CID:** 6450551

**CAS:** 319460-85-0

Baricitinib



**Alt Names:** Olumiant

**MW:**

**Brutto:** C<sub>16</sub>H<sub>17</sub>N<sub>7</sub>O<sub>2</sub>S

**Approved for clinical use:** Rheumatoid Arthritis

**Approval Jurisdiction:** 2017 EMA, 2018 FDA

**InChI:** InChI=1S/C16H17N7O2S/c1-2-26(24,25)22-9-16(10-22,4-5-17)23-8-12(7-21-23)14-13-3-6-18-15(13)20-11-19-14/h3,6-8,11H,2,4,9-10H2,1H3,(H,18,19,20)

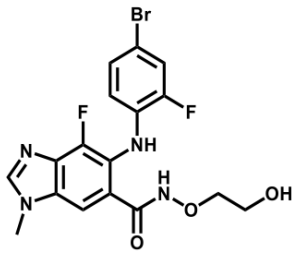
**InChI Key:** XUZMWHLSFXCVMG-UHFFFAOYSA-N

**SMILES:** CCS(=O)(=O)N1CC(C1)(CC#N)N2C=C(C=N2)C3=C4C=CNC4=NC=N3

**PubChem CID:** 44205240

**CAS:** 1187594-09-7

Binimetinib



**Alt Names:** MEK162, ARRY-162, Mektovi

**MW:** 441.20

**Brutto:** C<sub>17</sub>H<sub>15</sub>BrF<sub>2</sub>N<sub>4</sub>O<sub>3</sub>

**Approved for clinical use:** BRAF Mutant Melanoma

**Approval Jurisdiction:** 2018 FDA 2018 EMA

**InChI:** InChI=1S/C17H15BrF2N4O3/c1-24-8-21-16-13(24)7-10(17(26)23-27-5-4-25)15(14(16)20)22-12-3-2-9(18)6-11(12)19/h2-3,6-8,22,25H,4-5H2,1H3,(H,23,26)

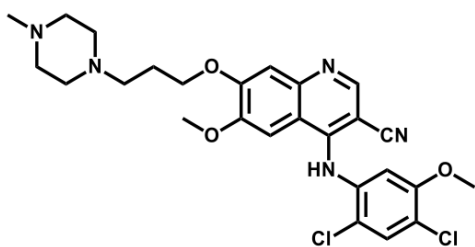
**InChI Key:** ACWZRVQXLIRSDF-UHFFFAOYSA-N

**SMILES:** CN1C=NC2=C1C=C(C(=C2F)NC3=C(C=C(C=C3)Br)F)C(=O)NOCCO

**PubChem CID:** 10288191

**CAS:** 606143-89-9

Bosutinib



**Alt Names:** SKI606, SKI-606, SKI 606

**MW:** 530.45

**Brutto:** C<sub>26</sub>H<sub>29</sub>Cl<sub>2</sub>N<sub>5</sub>O<sub>3</sub>

**Approved for clinical use:** Chronic Myelogenous Leukemia

**Approval Jurisdiction:** 2012 FDA, 2013 EMA

**InChI:** InChI=1S/C26H29Cl2N5O3/c1-32-6-8-33(9-7-32)5-4-10-36-25-13-21-18(11-24(25)35-3)26(17(15-29)16-30-21)31-22-14-23(34-2)20(28)12-19(22)27/h11-14,16H,4-10H2,1-3H3,(H,30,31)

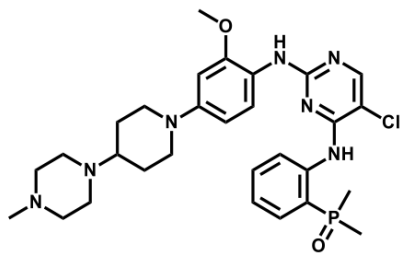
**InChI Key:** UBPYILGKFZZVDX-UHFFFAOYSA-N

**SMILES:** CN1CCN(CC1)CCCOC2=C(C=C3C(=C2)N=CC(=C3NC4=CC(=C(C=C4Cl)Cl)OC)C#N)OC

**PubChem CID:** 5328940

**CAS:** 380843-75-4

Brigatinib



**Alt Names:** ALUNBRIG, AP-26113

**MW:** 584.10

**Brutto:** C<sub>29</sub>H<sub>39</sub>ClN<sub>7</sub>O<sub>2</sub>P

**Approved for clinical use:** ALK-Rearranged Metastatic NSCLC

**Approval Jurisdiction:** 2017 FDA 2018 EMA

**InChI:** InChI=1S/C29H39ClN7O2P/c1-35-15-17-37(18-16-35)21-11-13-36(14-12-21)22-9-10-24(26(19-22)39-2)33-29-31-20-23(30)28(34-29)32-25-7-5-6-8-27(25)40(3,4)38/h5-10,19-21H,11-18H2,1-4H3,(H2,31,32,33,34)

**InChI Key:** AILRADAXUVEEIR-UHFFFAOYSA-N

**SMILES:**

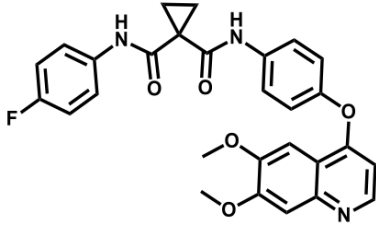
CN1CCN(CC1)C2CCN(CC2)C3=CC(=C(C=C3)NC4=NC=C(C(=N4)NC5=CC=CC=C5P(=O)(C)C)Cl)O

**PubChem CID:** 68165256

**CAS:** 1197953-54-0



# Cabozantinib



**Alt Names:** Cabometyx, Cometriq, Cabozanix

**MW:**

**Brutto:** C<sub>28</sub>H<sub>24</sub>FN<sub>3</sub>O<sub>5</sub>

**Approved for clinical use:** Medullary Thyroid Cancer

**Approval Jurisdiction:** 2012 FDA

**InChI:** InChI=1S/C28H24FN3O5/c1-35-24-15-21-22(16-25(24)36-2)30-14-11-23(21)37-20-9-7-19(8-10-20)32-27(34)28(12-13-28)26(33)31-18-5-3-17(29)4-6-18/h3-11,14-16H,12-13H2,1-2H3,(H,31,33)(H,32,34)

**InChI Key:** ONIQOQHATWINJY-UHFFFAOYSA-N

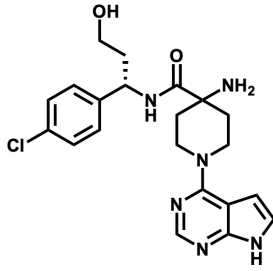
**SMILES:**

COC1=CC2=C(C=CN=C2C=C1OC)OC3=CC=C(C=C3)NC(=O)C4(CC4)C(=O)NC5=CC=C(C=C5)F

**PubChem CID:** 25102847

**CAS:** 849217-68-1

# Capivasertib



**Alt Names:** capivasertib, AZD5363, 1143532-39-1, AZD-5363, AZD 5363

**MW:** 428.90

**Brutto:** C<sub>21</sub>H<sub>25</sub>ClN<sub>6</sub>O<sub>2</sub>

**Approved for clinical use:** HR+ And PI3K Mutation Breast Cancer

**Approval Jurisdiction:** 2023 FDA

**InChI:** InChI=1S/C21H25ClN6O2/c22-15-3-1-14(2-4-15)17(6-12-29)27-20(30)21(23)7-10-28(11-8-21)19-16-5-9-24-18(16)25-13-26-19/h1-5,9,13,17,29H,6-8,10-12,23H2,(H,27,30)(H,24,25,26)/t17-/m0/s1

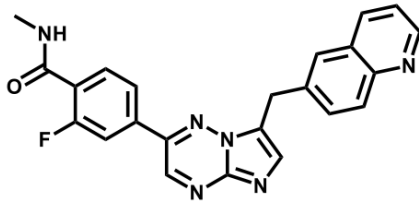
**InChI Key:** JDUBGYFRJFOXQC-KRWDZBQOSA-N

**SMILES:** ClC1=CC=C([C@H](CCO)NC(C2(CCN(C3=C4C(NC=C4)=NC=N3)CC2)N)=O)C=C1

**PubChem CID:** 25227436

**CAS:** 1143532-39-1

# Capmatinib



**Alt Names:** Tabrecta, INCB28060, INC280

**MW:** 412.40

**Brutto:** C<sub>23</sub>H<sub>17</sub>FN<sub>6</sub>O

**Approved for clinical use:** MET Mutation+Ve NSCLC

**Approval Jurisdiction:** 2020 FDA

**InChI:** InChI=1S/C23H17FN6O/c1-25-22(31)18-6-5-16(11-19(18)24)21-13-28-23-27-12-17(30(23)29-21)10-14-4-7-20-15(9-14)3-2-8-26-20/h2-9,11-13H,10H2,1H3,(H,25,31)

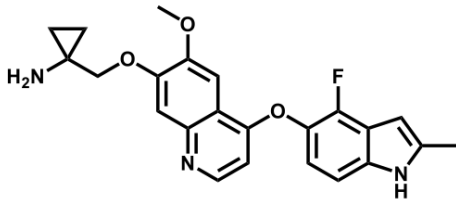
**InChI Key:** LIOLIMKSCNQPLV-UHFFFAOYSA-N

**SMILES:** CNC(=O)C1=C(C=C(C=C1))C2=NN3C(=CN=C3N=C2)CC4=CC5=C(C=C4)N=CC=C5)F

**PubChem CID:** 25145656

**CAS:** 1029712-80-8

# Catequentinib



**Alt Names:** Anlotinib, AL3818, AL-3818

**MW:** 407.40

**Brutto:** C<sub>23</sub>H<sub>22</sub>FN<sub>3</sub>O<sub>3</sub>

**Approved for clinical use:** NSCLC

**Approval Jurisdiction:** 2018 China

**InChI:** InChI=1S/C23H22FN3O3/c1-13-9-15-16(27-13)3-4-19(22(15)24)30-18-5-8-26-17-11-21(20(28-2)10-14(17)18)29-12-23(25)6-7-23/h3-5,8-11,27H,6-7,12,25H2,1-2H3

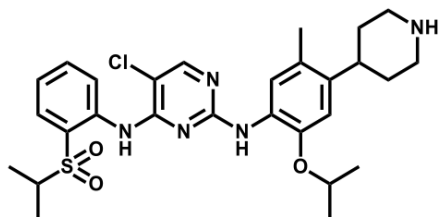
**InChI Key:** KSMZEXLVHXZPEF-UHFFFAOYSA-N

**SMILES:** CC1=CC2=C(N1)C=CC(=C2F)OC3=C4C=C(C(=CC4=NC=C3)OCC5(CC5)N)OC

**PubChem CID:** 25017411

**CAS:** 1058156-90-3

# Ceritinib



**Alt Names:** LDK378, ZYKADIA, LDK-378

**MW:** 558.10

**Brutto:** C<sub>28</sub>H<sub>36</sub>ClN<sub>5</sub>O<sub>3</sub>S

**Approved for clinical use:** NSCLC With ALK Translocations

**Approval Jurisdiction:** 2014 FDA 2015 EMA

**InChI:** InChI=1S/C28H36ClN5O3S/c1-17(2)37-25-15-21(20-10-12-30-13-11-20)19(5)14-24(25)33-28-31-16-22(29)27(34-28)32-23-8-6-7-9-26(23)38(35,36)18(3)4/h6-9,14-18,20,30H,10-13H2,1-5H3,(H2,31,32,33,34)

**InChI Key:** VERWOWGGCGHDQE-UHFFFAOYSA-N

**SMILES:**

CC1=CC(=C(C=C1C2CCNCC2)OC(C)C)NC3=NC=C(C(=N3)NC4=CC=CC=C4S(=O)(=O)C(C)C)Cl

**PubChem CID:** 57379345

**CAS:** 1032900-25-6

Cetuximab

## Monoclonal antibody

**Alt Names:**

**MW:**

**Brutto:**

**Approved for clinical use:** EGFR Colorectal Cancer

**Approval Jurisdiction:** 2004 FDA 2004 EMA

**InChI:**

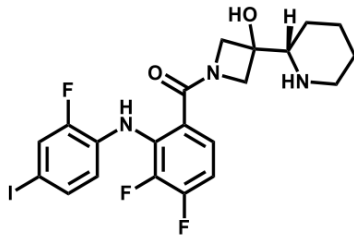
**InChI Key:**

**SMILES:**

**PubChem CID:**

**CAS:** 205923-56-4

Cobimetinib



**Alt Names:** GDC-0973, XL518, Cotellic

**MW:** 531.30

**Brutto:** C<sub>21</sub>H<sub>21</sub>F<sub>3</sub>IN<sub>3</sub>O<sub>2</sub>

**Approved for clinical use:** Melanoma, Breast Cancer

**Approval Jurisdiction:** 2015 FDA 2015 EMA

**InChI:** InChI=1S/C21H21F3IN3O2/c22-14-6-5-13(19(18(14)24)27-16-7-4-12(25)9-15(16)23)20(29)28-10-21(30,11-28)17-3-1-2-8-26-17/h4-7,9,17,26-27,30H,1-3,8,10-11H2/t17-/m0/s1

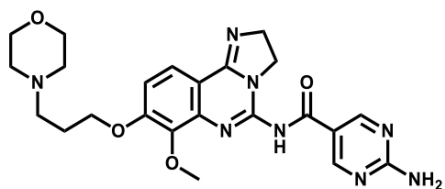
**InChI Key:** BSMCAPRUBJMWDF-KRWDZBQOSA-N

**SMILES:** C1CCN[C@@H](C1)C2(CN(C2)C(=O)C3=C(C(=C(C=C3)F)F)NC4=C(C=C(C=C4)I)F)O

**PubChem CID:** 16222096

**CAS:** 934660-93-2

Copanlisib



**Alt Names:** Aliqopa

**MW:**

**Brutto:** C<sub>23</sub>H<sub>28</sub>N<sub>8</sub>O<sub>4</sub>

**Approved for clinical use:** Follicular Lymphoma

**Approval Jurisdiction:** 2017 FDA

**InChI:** InChI=1S/C23H28N8O4/c1-33-19-17(35-10-2-6-30-8-11-34-12-9-30)4-3-16-18(19)28-23(31-7-5-25-20(16)31)29-21(32)15-13-26-22(24)27-14-15/h3-4,13-14H,2,5-12H2,1H3,(H2,24,26,27)(H,28,29,32)

**InChI Key:** PZBCKZWLPJMAO-UHFFFAOYSA-N

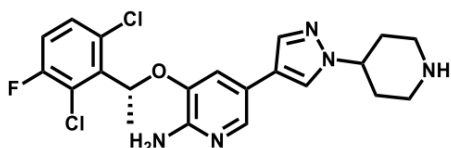
**SMILES:** COC1=C(C=CC2=C1N=C(N3C2=NCC3)NC(=O)C4=CN=C(N=C4)N)OCCCN5CCOCC5

**PubChem CID:** 24989044

**CAS:** 1032568-63-0

Crizotinib





**Alt Names:** Xalkori, Crizonix

**MW:**

**Brutto:** C<sub>21</sub>H<sub>22</sub>Cl<sub>2</sub>FN<sub>5</sub>O

**Approved for clinical use:** NSCLC With Alkmutation

**Approval Jurisdiction:** 2011 FDA

**InChI:** InChI=1S/C21H22Cl2FN5O/c1-12(19-16(22)2-3-17(24)20(19)23)30-18-8-13(9-27-21(18)25)14-10-28-29(11-14)15-4-6-26-7-5-15/h2-3,8-12,15,26H,4-7H2,1H3,(H2,25,27)/t12-/m1/s1

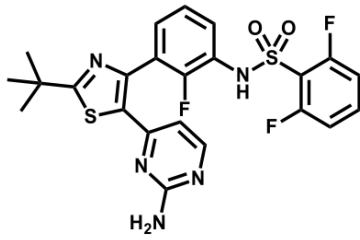
**InChI Key:** KTEIFNKAUNYNJU-GFCCVEGCSA-N

**SMILES:** CC(C1=C(C=CC(=C1Cl)F)Cl)OC2=C(N=CC(=C2)C3=CN(N=C3)C4CCNCC4)N

**PubChem CID:** 11626560

**CAS:** 877399-52-5

Dabrafenib



**Alt Names:** Tafinlar

**MW:**

**Brutto:** C<sub>23</sub>H<sub>20</sub>F<sub>3</sub>N<sub>5</sub>O<sub>2</sub>S<sub>2</sub>

**Approved for clinical use:** Skin Cancer

**Approval Jurisdiction:** 2013 FDA

**InChI:** InChI=1S/C23H20F3N5O2S2/c1-23(2,3)21-30-18(19(34-21)16-10-11-28-22(27)29-16)12-6-4-9-15(17(12)26)31-35(32,33)20-13(24)7-5-8-14(20)25/h4-11,31H,1-3H3,(H2,27,28,29)

**InChI Key:** BFSMGDJOXZAERB-UHFFFAOYSA-N

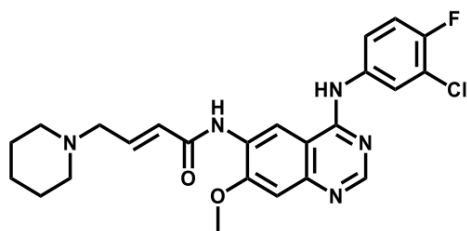
**SMILES:**

CC(C)(C)C1=NC(=C(S1)C2=NC(=NC=C2)N)C3=C(C(=CC=C3)NS(=O)(=O)C4=C(C=CC=C4F)F)F

**PubChem CID:** 44462760

**CAS:** 1195765-45-7

Dacomitinib



**Alt Names:** PF-00299804, PF299804

**MW:** 469.90

**Brutto:** C<sub>24</sub>H<sub>25</sub>ClFN<sub>5</sub>O<sub>2</sub>

**Approved for clinical use:** NSCLC With EGFR Mutations

**Approval Jurisdiction:** 2018 FDA 2019 EMA

**InChI:** InChI=1S/C24H25ClFN5O2/c1-33-22-14-20-17(24(28-15-27-20)29-16-7-8-19(26)18(25)12-16)13-21(22)30-23(32)6-5-11-31-9-3-2-4-10-31/h5-8,12-15H,2-4,9-11H2,1H3,(H,30,32)(H,27,28,29)/b6-5+

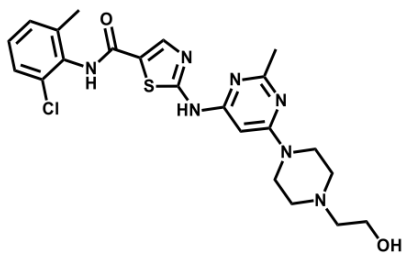
**InChI Key:** LVXJQMNHJWSHET-AATRIKPKSA-N

**SMILES:** COC1=C(C=C2C(=C1)N=CN=C2NC3=CC(=C(C=C3)F)Cl)NC(=O)C=CCN4CCCCC4

**PubChem CID:** 11511120

**CAS:** 1110813-31-4

Dasatinib



**Alt Names:** Sprycel, Dasanix

**MW:** 487.00

**Brutto:** C<sub>22</sub>H<sub>26</sub>ClN<sub>7</sub>O<sub>2</sub>S

**Approved for clinical use:** Chronic Myelogenous Leukemia, ALL

**Approval Jurisdiction:** 2006 FDA, EMA

**InChI:** InChI=1S/C22H26ClN7O2S/c1-14-4-3-5-16(23)20(14)28-21(32)17-13-24-22(33-17)27-18-12-19(26-15(2)25-18)30-8-6-29(7-9-30)10-11-31/h3-5,12-13,31H,6-11H2,1-2H3,(H,28,32)(H,24,25,26,27)

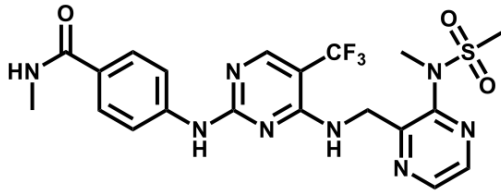
**InChI Key:** ZBNZXTGUTAYRHI-UHFFFAOYSA-N

**SMILES:** CC1=C(C(=CC=C1)Cl)NC(=O)C2=CN=C(S2)NC3=CC(=NC(=N3)C)N4CCN(CC4)CCO

**PubChem CID:** 3062316

**CAS:** 302962-49-8

Defactinib



**Alt Names:**

**MW:** 510.50

**Brutto:** C<sub>20</sub>H<sub>21</sub>F<sub>3</sub>N<sub>8</sub>O<sub>3</sub>S

**Approved for clinical use:** Solid Tumours

**Approval Jurisdiction:** 2022 FDA

**InChI:** InChI=1S/C20H21F3N8O3S/c1-24-18(32)12-4-6-13(7-5-12)29-19-28-10-14(20(21,22)23)16(30-19)27-11-15-17(26-9-8-25-15)31(2)35(3,33)34/h4-10H,11H2,1-3H3,(H,24,32)(H2,27,28,29,30)

**InChI Key:** FWLMVFUGMHIOAA-UHFFFAOYSA-N

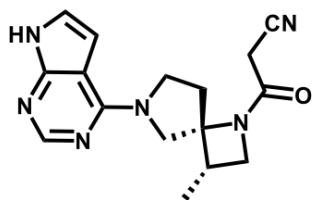
**SMILES:**

CNC(=O)C1=CC=C(C=C1)NC2=NC=C(C(=N2)NCC3=NC=CN=C3N(C)S(=O)(=O)C)C(F)(F)F

**PubChem CID:** 25117126

**CAS:** 1073154-85-4

Delgocitinib



**Alt Names:** JTE-052, JTE-052A, Corectim

**MW:** 310.35

**Brutto:** C<sub>16</sub>H<sub>18</sub>N<sub>6</sub>O

**Approved for clinical use:** Atopic Dermatitis

**Approval Jurisdiction:** 2020 Japan

**InChI:** InChI=1S/C16H18N6O/c1-11-8-22(13(23)2-5-17)16(11)4-7-21(9-16)15-12-3-6-18-14(12)19-10-20-15/h3,6,10-11H,2,4,7-9H2,1H3,(H,18,19,20)/t11-,16-/m0/s1

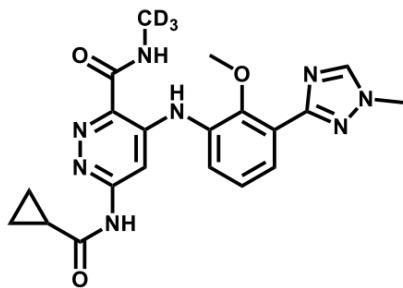
**InChI Key:** LOWWYYZBZNSPDT-ZBEGNZNMSA-N

**SMILES:** CC1CN(C12CCN(C2)C3=NC=NC4=C3C=CN4)C(=O)CC#N

**PubChem CID:** 50914062

**CAS:** 1263774-59-9

Deucravacitinib



**Alt Names:** BMS-986165, Tyk2-IN-4, Sotyktu

**MW:** 425.50

**Brutto:** C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>3</sub>

**Approved for clinical use:** Psoriasis

**Approval Jurisdiction:** 2022 FDA

**InChI:** InChI=1S/C20H22N8O3/c1-21-20(30)16-14(9-15(25-26-16)24-19(29)11-7-8-11)23-13-6-4-5-12(17(13)31-3)18-22-10-28(2)27-18/h4-6,9-11H,7-8H2,1-3H3,(H,21,30)(H2,23,24,25,29)/i1D3

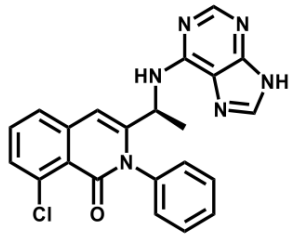
**InChI Key:** BZZKEPGENYLQSC-FIBGUPNXSA-N

**SMILES:** CNC(=O)C1=NN=C(C=C1NC2=CC=CC(=C2OC)C3=NN(C=N3)C)NC(=O)C4CC4

**PubChem CID:** 134821691

**CAS:** 1609392-27-9

Duvelisib



**Alt Names:** IPI-145, INK-1197

**MW:** 416.90

**Brutto:** C<sub>22</sub>H<sub>17</sub>ClN<sub>6</sub>O

**Approved for clinical use:** CLL, SLL, FL

**Approval Jurisdiction:** 2018 FDA

**InChI:** InChI=1S/C22H17ClN6O/c1-13(28-21-19-20(25-11-24-19)26-12-27-21)17-10-14-6-5-9-16(23)18(14)22(30)29(17)15-7-3-2-4-8-15/h2-13H,1H3,(H2,24,25,26,27,28)/t13-/m0/s1

**InChI Key:** SJVQHLPISAIATJ-ZDUSSCGKSA-N

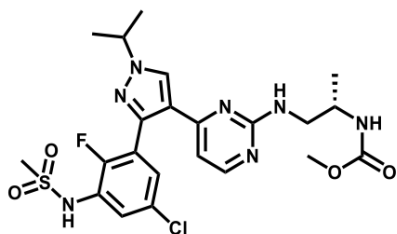
**SMILES:** CC(C1=CC2=C(C(=CC=C2)Cl)C(=O)N1C3=CC=CC=C3)NC4=NC=NC5=C4NC=N5

**PubChem CID:** 50905713

**CAS:** 1201438-56-3

Encorafenib





**Alt Names:** LGX818, LGX-818, Braftovi

**MW:** 540.00

**Brutto:** C<sub>22</sub>H<sub>27</sub>ClFN<sub>7</sub>O<sub>4</sub>S

**Approved for clinical use:** BRAF Mutant Melanoma

**Approval Jurisdiction:** 2018 FDA 2018 EMA

**InChI:** InChI=1S/C22H27ClFN7O4S/c1-12(2)31-11-16(17-6-7-25-21(28-17)26-10-13(3)27-22(32)35-4)20(29-31)15-8-14(23)9-18(19(15)24)30-36(5,33)34/h6-9,11-13,30H,10H2,1-5H3,(H,27,32)(H,25,26,28)/t13-/m0/s1

**InChI Key:** CMJCYNUCSMDBY-ZDUSSCGKSA-N

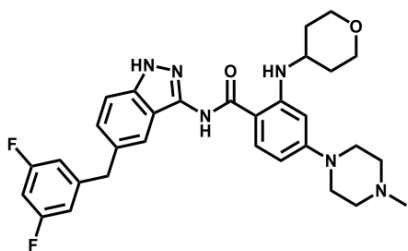
**SMILES:**

CC(C)N1C=C(C(=N1)C2=C(C(=CC(=C2)Cl)NS(=O)(=O)C)F)C3=NC(=NC=C3)NCC(C)NC(=O)OC

**PubChem CID:** 50922675

**CAS:** 1269440-17-6

# Entrectinib



**Alt Names:** RXDX-101, NMS-E628, Rozlytrek

**MW:** 560.60

**Brutto:** C<sub>31</sub>H<sub>34</sub>F<sub>2</sub>N<sub>6</sub>O<sub>2</sub>

**Approved for clinical use:** ROS1+Ve NSCLC, Solid Tumors NTRK+Ve

**Approval Jurisdiction:** 2019 FDA

**InChI:** InChI=1S/C31H34F2N6O2/c1-38-8-10-39(11-9-38)25-3-4-26(29(19-25)34-24-6-12-41-13-7-24)31(40)35-30-27-17-20(2-5-28(27)36-37-30)14-21-15-22(32)18-23(33)16-21/h2-5,15-19,24,34H,6-14H2,1H3,(H2,35,36,37,40)

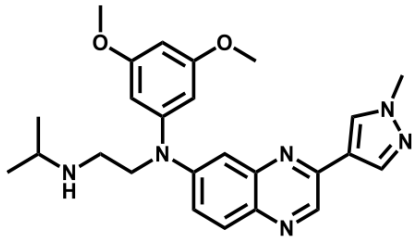
**InChI Key:** HAYYBYPASCDWEQ-UHFFFAOYSA-N

**SMILES:** CN1CCN(CC1)C2=CC(=C(C=C2)C(=O)NC3=NNC4=C3C=C(C=C4)CC5=CC(=CC(=C5)F)F)NC6CCOCC6

**PubChem CID:** 25141092

**CAS:** 1108743-60-7

# Erdafitinib



**Alt Names:** JNJ-42756493, Balversa

**MW:** 446.50

**Brutto:** C<sub>25</sub>H<sub>30</sub>N<sub>6</sub>O<sub>2</sub>

**Approved for clinical use:** Advanced Metastatic Urothelial Carcinoma

**Approval Jurisdiction:** 2019 FDA

**InChI:** InChI=1S/C25H30N6O2/c1-17(2)26-8-9-31(20-10-21(32-4)13-22(11-20)33-5)19-6-7-23-24(12-19)29-25(15-27-23)18-14-28-30(3)16-18/h6-7,10-17,26H,8-9H2,1-5H3

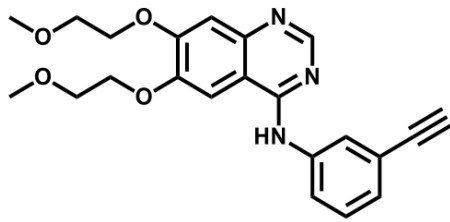
**InChI Key:** OLAHOMJCDNXHFI-UHFFFAOYSA-N

**SMILES:** CC(C)NCCN(C1=CC2=NC(=CN=C2C=C1)C3=CN(N=C3)C)C4=CC(=CC(=C4)OC)OC

**PubChem CID:** 67462786

**CAS:** 1346242-81-6

# Erlotinib



**Alt Names:** Tarceva

**MW:**

**Brutto:** C<sub>22</sub>H<sub>23</sub>N<sub>3</sub>O<sub>4</sub>

**Approved for clinical use:** Pancreatic Cancer

**Approval Jurisdiction:** 2004 NSCLC

**InChI:** InChI=1S/C22H23N3O4/c1-4-16-6-5-7-17(12-16)25-22-18-13-20(28-10-8-26-2)21(29-11-9-27-3)14-19(18)23-15-24-22/h1,5-7,12-15H,8-11H2,2-3H3,(H,23,24,25)

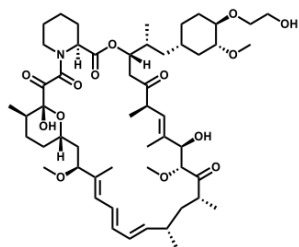
**InChI Key:** AAKJLRGGTJKAMG-UHFFFAOYSA-N

**SMILES:** COCCOC1=C(C=C2C(=C1)C(=NC=N2)NC3=CC=CC(=C3)C#C)OCCOC

**PubChem CID:** 176870

**CAS:** 183321-74-6

# Everolimus



**Alt Names:** Afinitor, Zortress

**MW:**

**Brutto:** C<sub>53</sub>H<sub>83</sub>NO<sub>14</sub>

**Approved for clinical use:** Renel Cell Carcinoma

**Approval Jurisdiction:** 2009 FDA

**InChI:** InChI=1S/C53H83NO14/c1-32-16-12-11-13-17-33(2)44(63-8)30-40-21-19-38(7)53(62,68-40)50(59)51(60)54-23-15-14-18-41(54)52(61)67-45(35(4)28-39-20-22-43(66-25-24-55)46(29-39)64-9)31-42(56)34(3)27-37(6)48(58)49(65-10)47(57)36(5)26-32/h11-13,16-17,27,32,34-36,38-41,43-46,48-49,55,58,62H,14-15,18-26,28-31H2,1-10H3/b13-11+,16-12+,33-17+,37-27+/t32-,34-,35-,36-,38-,39+,40+,41+,43-,44+,45+,46-,48-,49+,53-/m1/s1

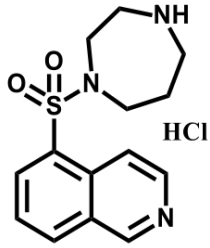
**InChI Key:** HKVAMNSJSFKALM-GKUWKFKPSA-N

**SMILES:** CC1CCC2CC(C(=CC=CC=CC(C(C(=O)C(C(C(=CC(C(=O)CC(OC(=O)C3CCCCN3C(=O)C(=O)C1(O2)O)C(C)CC4CCC(C(C4)OC)OCCO)C)C)O)OC)C)C)OC

**PubChem CID:** 6442177

**CAS:** 159351-69-6

# Fasudil



**Alt Names:** Eril

**MW:** 291.10

**Brutto:** C<sub>14</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub>S

**Approved for clinical use:** Cerebral Vasospasm PAH

**Approval Jurisdiction:** 1995 Japan, China

**InChI:** InChI=1S/C14H17N3O2S/c18-20(19,17-9-2-6-15-8-10-17)14-4-1-3-12-11-16-7-5-13(12)14/h1,3-5,7,11,15H,2,6,8-10H2

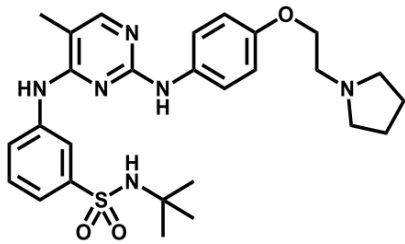
**InChI Key:** NGOGFTYYXHNFQH-UHFFFAOYSA-N

**SMILES:** C1CNCCN(C1)S(=O)(=O)C2=CC=CC3=C2C=CN=C3

**PubChem CID:** 3547

**CAS:** 103745-39-7

# Fedratinib



**Alt Names:** Tg-101348, TG101348, SAR302503

**MW:** 524.70

**Brutto:** C<sub>27</sub>H<sub>36</sub>N<sub>6</sub>O<sub>3</sub>S

**Approved for clinical use:** Myelofibrosis

**Approval Jurisdiction:** 2019 FDA 2021EMA

**InChI:** InChI=1S/C27H36N6O3S/c1-20-19-28-26(30-21-10-12-23(13-11-21)36-17-16-33-14-5-6-15-33)31-25(20)29-22-8-7-9-24(18-22)37(34,35)32-27(2,3)4/h7-13,18-19,32H,5-6,14-17H2,1-4H3,(H2,28,29,30,31)

**InChI Key:** JOOXLOJCABQBSG-UHFFFAOYSA-N

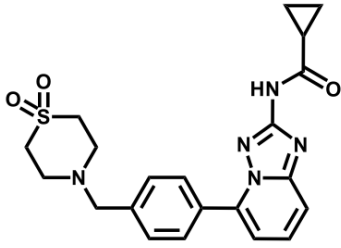
**SMILES:**

CC1=CN=C(N=C1NC2=CC(=CC=C2)S(=O)(=O)NC(C)(C)C)NC3=CC=C(C=C3)OCCN4CCCC4

**PubChem CID:** 16722836

**CAS:** 936091-26-8

# Filgotinib



**Alt Names:** GLPG0634

**MW:** 425.50

**Brutto:** C<sub>21</sub>H<sub>23</sub>N<sub>5</sub>O<sub>3</sub>S

**Approved for clinical use:** Rheumatoid Arthritis

**Approval Jurisdiction:** 2020 EMA 2020 Japan

**InChI:** InChI=1S/C21H23N5O3S/c27-20(17-8-9-17)23-21-22-19-3-1-2-18(26(19)24-21)16-6-4-15(5-7-16)14-25-10-12-30(28,29)13-11-25/h1-7,17H,8-14H2,(H,23,24,27)

**InChI Key:** RIJLVEAXPNLDTC-UHFFFAOYSA-N

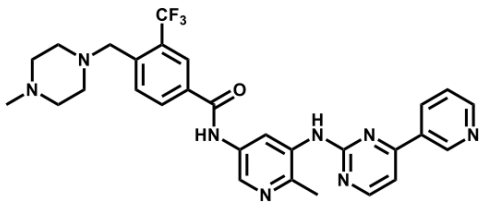
**SMILES:** C1CC1C(=O)NC2=NN3C(=N2)C=CC=C3C4=CC=C(C=C4)CN5CCS(=O)(=O)CC5

**PubChem CID:** 49831257

**CAS:** 1206101-20-3



# Flumatinib



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**Alt Names:** HH-GV678, HHGV678, flumbatinib

**MW:** 562.60

**Brutto:** C<sub>29</sub>H<sub>29</sub>F<sub>3</sub>N<sub>8</sub>O

**Approved for clinical use:** Chronic Myelogenous Leukemia

**Approval Jurisdiction:** 2019 China

**InChI:** InChI=1S/C29H29F3N8O/c1-19-26(38-28-34-9-7-25(37-28)21-4-3-8-33-16-21)15-23(17-35-19)36-27(41)20-5-6-22(24(14-20)29(30,31)32)18-40-12-10-39(2)11-13-40/h3-9,14-17H,10-13,18H2,1-2H3,(H,36,41)(H,34,37,38)

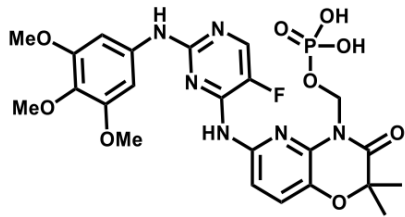
**InChI Key:** BJCJYEYYYGBROF-UHFFFAOYSA-N

**SMILES:** CC1=C(C=C(C=N1)NC(=O)C2=CC(=C(C=C2)CN3CCN(CC3)C)C(F)(F)F)NC4=NC=CC(=N4)C5=CN=CC=C5

**PubChem CID:** 46848036

**CAS:** 895519-90-1

# Fostamatinib



**Alt Names:** R788, Tavalisse

**MW:** 580.50

**Brutto:** C<sub>23</sub>H<sub>26</sub>FN<sub>6</sub>O<sub>9</sub>P

**Approved for clinical use:** Autoimmune Thrombocyto-Penia

**Approval Jurisdiction:** 2018 FDA 2020 EMA

**InChI:** InChI=1S/C23H26FN6O9P/c1-23(2)21(31)30(11-38-40(32,33)34)20-14(39-23)6-7-17(28-20)27-19-13(24)10-25-22(29-19)26-12-8-15(35-3)18(37-5)16(9-12)36-4/h6-10H,11H2,1-5H3,(H2,32,33,34)(H2,25,26,27,28,29)

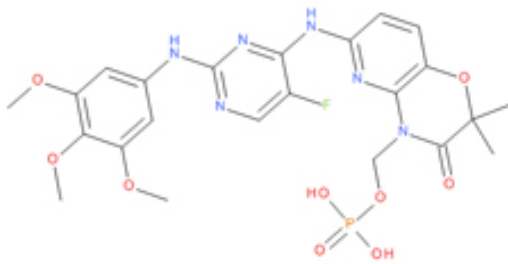
**InChI Key:** GKDRMWXFWHEQQT-UHFFFAOYSA-N

**SMILES:** CC1(C(=O)N(C2=C(O1)C=CC(=N2)NC3=NC(=NC=C3F)NC4=CC(=C(C(=C4)OC)OC)OC)COP(=O)(O)O)C

**PubChem CID:** 11671467

**CAS:** 901119-35-5

# Fostamatinib



**Alt Names:** R788, Tavalisse

**MW:** 580.46

**Brutto:** C<sub>23</sub>H<sub>26</sub>FN<sub>6</sub>O<sub>9</sub>P

**Approved for clinical use:** Chronic Immune Thrombocytopenia

**Approval Jurisdiction:** 2018 FDA

**InChI:** InChI=1S/C23H26FN6O9P/c1-23(2)21(31)30(11-38-40(32,33)34)20-14(39-23)6-7-17(28-20)27-19-13(24)10-25-22(29-19)26-12-8-15(35-3)18(37-5)16(9-12)36-4/h6-10H,11H2,1-5H3,(H2,32,33,34)(H2,25,26,27,28,29)

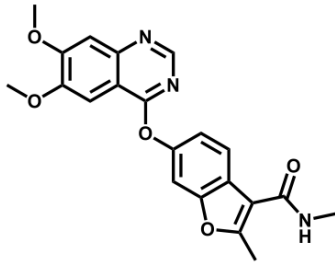
**InChI Key:** GKDRMWXFWHEQQT-UHFFFAOYSA-N

**SMILES:** CC1(C(=O)N(c2c(ccc(n2)Nc3c(cnc(n3)Nc4cc(c(c(c4)OC)OC)OC)F)O1)COP(=O)(O)O)C

**PubChem CID:** 11671467

**CAS:** 901119-35-5

# Fruquintinib



**Alt Names:** HMPL-013, HMPL013

**MW:** 393.40

**Brutto:** C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>

**Approved for clinical use:** Metastatic Colorectal Cancer

**Approval Jurisdiction:** 2018 China

**InChI:** InChI=1S/C21H19N3O5/c1-11-19(20(25)22-2)13-6-5-12(7-16(13)28-11)29-21-14-8-17(26-3)18(27-4)9-15(14)23-10-24-21/h5-10H,1-4H3,(H,22,25)

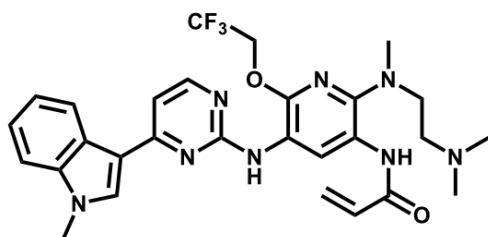
**InChI Key:** BALLNEJQLSTPIO-UHFFFAOYSA-N

**SMILES:** CC1=C(C2=C(O1)C=C(C=C2)OC3=NC=NC4=CC(=C(C=C43)OC)OC)C(=O)NC

**PubChem CID:** 44480399

**CAS:** 1194506-26-7

# Furmonertinib



**Alt Names:** Alflutinib, AST2818, AST-2818

**MW:** 568.60

**Brutto:** C<sub>28</sub>H<sub>31</sub>F<sub>3</sub>N<sub>8</sub>O<sub>2</sub>

**Approved for clinical use:** NSCLC

**Approval Jurisdiction:** 2021 China

**InChI:** InChI=1S/C28H31F3N8O2/c1-6-24(40)33-21-15-22(26(41-17-28(29,30)31)36-25(21)38(4)14-13-37(2)3)35-27-32-12-11-20(34-27)19-16-39(5)23-10-8-7-9-18(19)23/h6-12,15-16H,1,13-14,17H2,2-5H3,(H,33,40)(H,32,34,35)

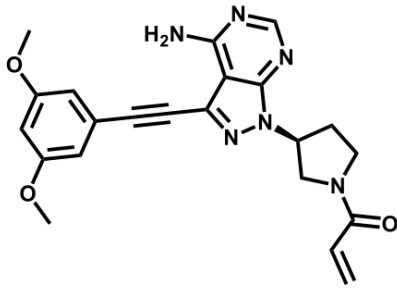
**InChI Key:** GHKOONMJXNWOIW-UHFFFAOYSA-N

**SMILES:** CN1C=C(C2=CC=CC=C21)C3=NC(=NC=C3)NC4=C(N=C(C(=C4)NC(=O)C=C)N(C)CCN(C)C)OCC(F)(F)F

**PubChem CID:** 118861389

**CAS:** 1869057-83-9

# Futibatinib



**Alt Names:** TAS-120, TAS120

**MW:** 418.40

**Brutto:** C<sub>22</sub>H<sub>22</sub>N<sub>6</sub>O<sub>3</sub>

**Approved for clinical use:** Cholangiocarcinoma

**Approval Jurisdiction:** 2022 FDA

**InChI:** InChI=1S/C22H22N6O3/c1-4-19(29)27-8-7-15(12-27)28-22-20(21(23)24-13-25-22)18(26-28)6-5-14-9-16(30-2)11-17(10-14)31-3/h4,9-11,13,15H,1,7-8,12H2,2-3H3,(H2,23,24,25)/t15-m/s1

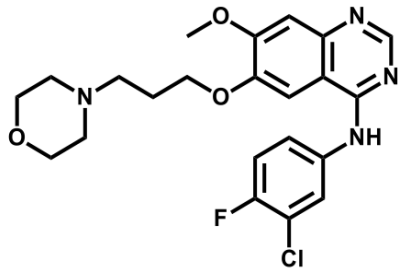
**InChI Key:** KEIPNCCJPRMIAX-HNNXBMFYSA-N

**SMILES:** COC1=CC(=CC(=C1)C#CC2=NN(C3=NC=NC(=C23)N)C4CCN(C4)C(=O)C=C)OC

**PubChem CID:** 71621331

**CAS:** 1448169-71-8

# Gefitinib



**Alt Names:** Iressa

**MW:**

**Brutto:** C<sub>22</sub>H<sub>24</sub>ClFN<sub>4</sub>O<sub>3</sub>

**Approved for clinical use:** NSCLC

**Approval Jurisdiction:** 2002 Japan, 2003 FDA

**InChI:** InChI=1S/C22H24ClFN4O3/c1-29-20-13-19-16(12-21(20)31-8-2-5-28-6-9-30-10-7-28)22(26-14-25-19)27-15-3-4-18(24)17(23)11-15/h3-4,11-14H,2,5-10H2,1H3,(H,25,26,27)

**InChI Key:** XGALLCVXEZPNRQ-UHFFFAOYSA-N

**SMILES:** COC1=C(C=C2C(=C1)N=CN=C2NC3=CC(=C(C=C3)F)Cl)OCCCN4CCOCC4

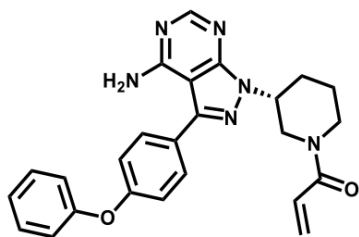
**PubChem CID:** 123631

**CAS:** 184475-35-2





# Ibrutinib



**Alt Names:**

**MW:** 440.50

**Brutto:** C<sub>25</sub>H<sub>24</sub>N<sub>6</sub>O<sub>2</sub>

**Approved for clinical use:** Mantle Cell Lymphoma

**Approval Jurisdiction:** 2013 FDA 2013 EMA

**InChI:** InChI=1S/C25H24N6O2/c1-2-21(32)30-14-6-7-18(15-30)31-25-22(24(26)27-16-28-25)23(29-31)17-10-12-20(13-11-17)33-19-8-4-3-5-9-19/h2-5,8-13,16,18H,1,6-7,14-15H2,(H2,26,27,28)/t18-/m1/s1

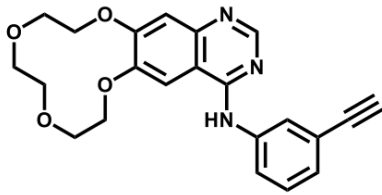
**InChI Key:** XYFPWWZEPKGCCK-GOSISDBHSA-N

**SMILES:** C=CC(=O)N1CCCC(C1)N2C3=NC=NC(=C3C(=N2)C4=CC=C(C=C4)OC5=CC=CC=C5)N

**PubChem CID:** 24821094

**CAS:** 936563-96-1

# Icotinib



**Alt Names:** Conmana

**MW:** 391.40

**Brutto:** C<sub>22</sub>H<sub>21</sub>N<sub>3</sub>O<sub>4</sub>

**Approved for clinical use:** NSCLC

**Approval Jurisdiction:** 2012 China

**InChI:** InChI=1S/C22H21N3O4/c1-2-16-4-3-5-17(12-16)25-22-18-13-20-21(14-19(18)23-15-24-22)29-11-9-27-7-6-26-8-10-28-20/h1,3-5,12-15H,6-11H2,(H,23,24,25)

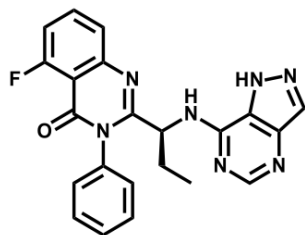
**InChI Key:** QQLKULDARVNMAL-UHFFFAOYSA-N

**SMILES:** C#CC1=CC(=CC=C1)NC2=NC=NC3=CC4=C(C=C32)OCCOCCOCCO4

**PubChem CID:** 22024915

**CAS:** 610798-31-7

# Idelalisib



**Alt Names:** CAL-101, Zydelig, GS-1101

**MW:** 415.40

**Brutto:** C<sub>22</sub>H<sub>18</sub>FN<sub>7</sub>O

**Approved for clinical use:** Chronic Lymphocytic Leukemia

**Approval Jurisdiction:** 2014 FDA 2014 EMA

**InChI:** InChI=1S/C22H18FN7O/c1-2-15(28-20-18-19(25-11-24-18)26-12-27-20)21-29-16-10-6-9-14(23)17(16)22(31)30(21)13-7-4-3-5-8-13/h3-12,15H,2H2,1H3,(H2,24,25,26,27,28)/t15-/m0/s1

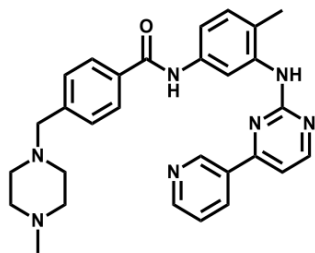
**InChI Key:** IFSDAJWBUCMOAH-HNNXBMFYSA-N

**SMILES:** CCC(C1=NC2=C(C(=CC=C2)F)C(=O)N1C3=CC=CC=C3)NC4=NC=NC5=C4NC=N5

**PubChem CID:** 11625818

**CAS:** 870281-82-6

# Imatinib



**Alt Names:** Imatinib Methansulfonate, sti-571 , Cgp 57148 , Imatinib free base, Gleevec

**MW:** 493.60

**Brutto:** C<sub>29</sub>H<sub>31</sub>N<sub>7</sub>O

**Approved for clinical use:** Chronic Myelogenous Leukemia

**Approval Jurisdiction:** 2001 FDA

**InChI:** InChI=1S/C29H31N7O/c1-21-5-10-25(18-27(21)34-29-31-13-11-26(33-29)24-4-3-12-30-19-24)32-28(37)23-8-6-22(7-9-23)20-36-16-14-35(2)15-17-36/h3-13,18-19H,14-17,20H2,1-2H3,(H,32,37)(H,31,33,34)

**InChI Key:** KTUFNOKKBVMGRW-UHFFFAOYSA-N

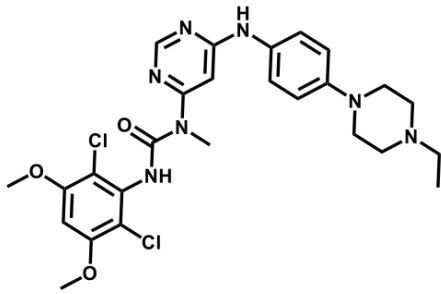
**SMILES:**

CC1=C(C=C(C=C1)NC(=O)C2=CC=C(C=C2)CN3CCN(CC3)C)NC4=NC=CC(=N4)C5=CN=CC=C5

**PubChem CID:** 5291

**CAS:** 152459-95-5

# Infigratinib



**Alt Names:** NVP-BGJ398, BGJ398, BGJ-398

**MW:** 560.50

**Brutto:** C<sub>26</sub>H<sub>31</sub>Cl<sub>2</sub>N<sub>7</sub>O<sub>3</sub>

**Approved for clinical use:** Cholangiocarcinoma

**Approval Jurisdiction:** 2021 FDA

**InChI:** InChI=1S/C26H31Cl2N7O3/c1-5-34-10-12-35(13-11-34)18-8-6-17(7-9-18)31-21-15-22(30-16-29-21)33(2)26(36)32-25-23(27)19(37-3)14-20(38-4)24(25)28/h6-9,14-16H,5,10-13H2,1-4H3,(H,32,36)(H,29,30,31)

**InChI Key:** QADPYRIHXKWUSV-UHFFFAOYSA-N

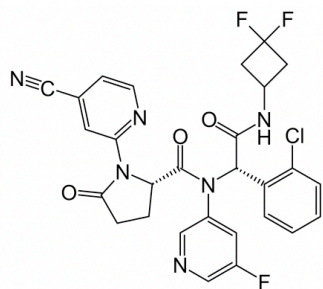
**SMILES:**

CCN1CCN(CC1)C2=CC=C(C=C2)NC3=CC(=NC=N3)N(C)C(=O)NC4=C(C(=CC(=C4Cl)OC)OC)Cl

**PubChem CID:** 53235510

**CAS:** 872511-34-7

# Ivosidenib



**Alt Names:** AG-120, Tibsovo

**MW:** 583.00

**Brutto:** C<sub>28</sub>H<sub>22</sub>ClF<sub>3</sub>N<sub>6</sub>O<sub>3</sub>

**Approved for clinical use:** Acute Myeloid Leukemia (AML) And Cholangiocarcinoma

**Approval Jurisdiction:** 2018 FDA, 2023 EMA

**InChI:** InChI=1S/C28H22ClF3N6O3/c29-21-4-2-1-3-20(21)25(26(40)36-18-11-28(31,32)12-18)37(19-10-17(30)14-34-15-19)27(41)22-5-6-24(39)38(22)23-9-16(13-33)7-8-35-23/h1-4,7-10,14-15,18,22,25H,5-6,11-12H2,(H,36,40)/t22-,25-/m0/s1

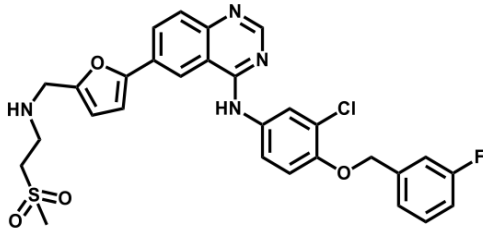
**InChI Key:** WIJZXSJMHAVGX-DHLKQENFSA-N

**SMILES:** C1CC(=O)N([C@@H]1C(=O)N(C2=CC(=CN=C2)F)[C@@H](C3=CC=CC=C3Cl)C(=O)NC4CC(C4)(F)F)C5=NC=CC(=C5)C#N

**PubChem CID:** 71657455

**CAS:** 1448347-49-6

# Lapatinib



**Alt Names:** Tykerb, Tyverb

**MW:**

**Brutto:** C<sub>29</sub>H<sub>26</sub>ClFN<sub>4</sub>O<sub>4</sub>S

**Approved for clinical use:** Breast Cancer

**Approval Jurisdiction:** 2007 FDA

**InChI:** InChI=1S/C29H26ClFN4O4S/c1-40(36,37)12-11-32-16-23-7-10-27(39-23)20-5-8-26-24(14-20)29(34-18-33-26)35-22-6-9-28(25(30)15-22)38-17-19-3-2-4-21(31)13-19/h2-10,13-15,18,32H,11-12,16-17H2,1H3,(H,33,34,35)

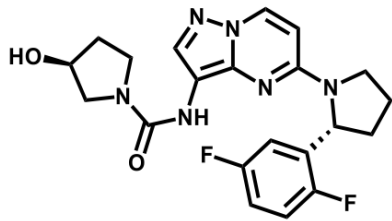
**InChI Key:** BCFGMOOMADDAQU-UHFFFAOYSA-N

**SMILES:** CS(=O)(=O)CCNCC1=CC=C(O1)C2=CC3=C(C=C2)N=CN=C3NC4=CC(=C(C=C4)OCC5=C(C=CC=C5)F)Cl

**PubChem CID:** 208908

**CAS:** 388082-78-8

# Larotrectinib



**Alt Names:** LOXO-101, ARRY-470, Vitrakvi

**MW:** 428.40

**Brutto:** C<sub>21</sub>H<sub>22</sub>F<sub>2</sub>N<sub>6</sub>O<sub>2</sub>

**Approved for clinical use:** Solid Tumours With NTRK Fusions

**Approval Jurisdiction:** 2018 FDA

**InChI:** InChI=1S/C21H22F2N6O2/c22-13-3-4-16(23)15(10-13)18-2-1-7-28(18)19-6-9-29-20(26-19)17(11-24-29)25-21(31)27-8-5-14(30)12-27/h3-4,6,9-11,14,18,30H,1-2,5,7-8,12H2,(H,25,31)/t14-,18+/m0/s1

**InChI Key:** NYNZQNWKBUAII-KBXCAEBGSA-N

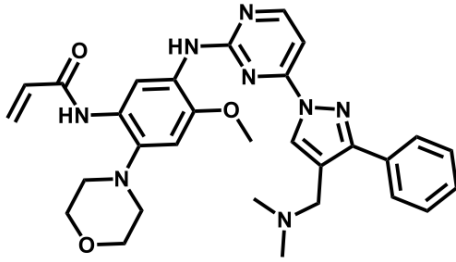
**SMILES:** C1CC(N(C1)C2=NC3=C(C=NN3C=C2)NC(=O)N4CCC(C4)O)C5=C(C=CC(=C5)F)F

**PubChem CID:** 46188928

**CAS:** 1223403-58-4



# Lazertinib



**Alt Names:** YH-25448, GNS-1480, YH25448

**MW:** 554.60

**Brutto:** C<sub>30</sub>H<sub>34</sub>N<sub>8</sub>O<sub>3</sub>

**Approved for clinical use:** NSCLC

**Approval Jurisdiction:** 2021 S.Korea

**InChI:** InChI=1S/C30H34N8O3/c1-5-28(39)32-23-17-24(26(40-4)18-25(23)37-13-15-41-16-14-37)33-30-31-12-11-27(34-30)38-20-22(19-36(2)3)29(35-38)21-9-7-6-8-10-21/h5-12,17-18,20H,1,13-16,19H2,2-4H3,(H,32,39)(H,31,33,34)

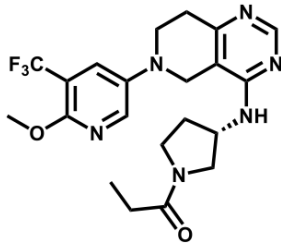
**InChI Key:** RRMJMHOQSALEJJ-UHFFFAOYSA-N

**SMILES:** CN(C)CC1=CN(N=C1C2=CC=CC=C2)C3=NC(=NC=C3)NC4=C(C=C(C(=C4)NC(=O)C=C)N5CCOCC5)OC

**PubChem CID:** 121269225

**CAS:** 1903008-80-9

# Leniolisib



**Alt Names:** CDZ173

**MW:** 450.50

**Brutto:** C<sub>21</sub>H<sub>25</sub>F<sub>3</sub>N<sub>6</sub>O<sub>2</sub>

**Approved for clinical use:** APDS PASLI Disease

**Approval Jurisdiction:** 2019 FDA

**InChI:** InChI=1S/C21H25F3N6O2/c1-3-18(31)30-6-4-13(10-30)28-19-15-11-29(7-5-17(15)26-12-27-19)14-8-16(21(22,23)24)20(32-2)25-9-14/h8-9,12-13H,3-7,10-11H2,1-2H3,(H,26,27,28)/t13-/m0/s1

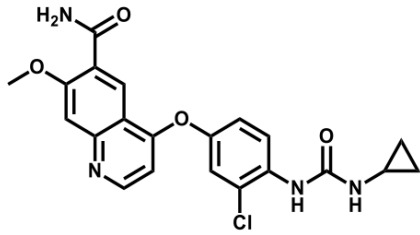
**InChI Key:** MWKYMZXCGYXLPL-ZDUSSCGKSA-N

**SMILES:** CCC(N(CC1)C[C@H]1NC2=C(C3)C(CCN3C4=CC(C(F)(F)F)=C(OC)N=C4)=NC=N2)=O

**PubChem CID:** 57495353

**CAS:** 1354690-24-6

# Lenvatinib



**Alt Names:** E7080, Lenvima, E7080 (Lenvatinib)

**MW:** 426.90

**Brutto:** C<sub>21</sub>H<sub>19</sub>ClN<sub>4</sub>O<sub>4</sub>

**Approved for clinical use:** Thyroid Cancer (DTC) Kidney Cancer

**Approval Jurisdiction:** 2015 FDA 2015 EMA

**InChI:** InChI=1S/C21H19ClN4O4/c1-29-19-10-17-13(9-14(19)20(23)27)18(6-7-24-17)30-12-4-5-16(15(22)8-12)26-21(28)25-11-2-3-11/h4-11H,2-3H2,1H3,(H2,23,27)(H2,25,26,

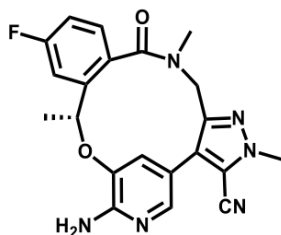
**InChI Key:** WOSKHXYHFSIKNG-UHFFFAOYSA-N

**SMILES:** COC1=CC2=NC=CC(=C2=C1C(=O)N)OC3=CC(=C(C=C3)NC(=O)NC4CC4)Cl

**PubChem CID:** 9823820

**CAS:** 417716-92-8

# Lorlatinib



**Alt Names:**

**MW:** 406.40

**Brutto:** C<sub>21</sub>H<sub>19</sub>FN<sub>6</sub>O<sub>2</sub>

**Approved for clinical use:** ALK+Ve Met NSCLC

**Approval Jurisdiction:** 2018 FDA 2019 EMA

**InChI:** InChI=1S/C21H19FN6O2/c1-11-15-7-13(22)4-5-14(15)21(29)27(2)10-16-19(17(8-23)28(3)26-16)12-6-18(30-11)20(24)25-9-12/h4-7,9,11H,10H2,1-3H3,(H2,24,25)/t11-/m1/s1

**InChI Key:** IIXWYSCJSQVBQM-LLVKDONJSA-N

**SMILES:** CC1C2=C(C=CC(=C2)F)C(=O)N(CC3=NN(C(=C3C4=CC(=C(N=C4)N)O1)C#N)C)C

**PubChem CID:** 71731823

**CAS:** 1454846-35-5

Margetuximab

## Monoclonal antibody

**Alt Names:**

**MW:**

**Brutto:**

**Approved for clinical use:** MHER2-Positive Breast Cancer

**Approval Jurisdiction:** 2020 FDA

**InChI:**

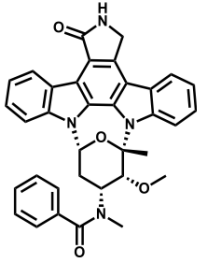
**InChI Key:**

**SMILES:**

**PubChem CID:**

**CAS:** 1350624-75-7

Midostaurin



**Alt Names:** PKC412, Cgp 41251, PKC-412

**MW:** 570.60

**Brutto:** C<sub>35</sub>H<sub>30</sub>N<sub>4</sub>O<sub>4</sub>

**Approved for clinical use:** Acute Myeloid Leukemia (FLT3 Mutation-Positive)

**Approval Jurisdiction:** 2017 FDA 2017 EMA

**InChI:** InChI=1S/C35H30N4O4/c1-35-32(42-3)25(37(2)34(41)19-11-5-4-6-12-19)17-26(43-35)38-23-15-9-7-13-20(23)28-29-22(18-36-33(29)40)27-21-14-8-10-16-24(21)39(35)31(27)30(28)38/h4-16,25-26,32H,17-18H2,1-3H3,(H,36,40)/t25-,26-,32-,35+/m1/s1

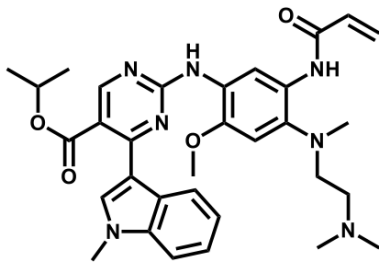
**InChI Key:** BMGQWWVMWDBQGC-IIFHNQTCSA-N

**SMILES:** CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CC=CC=C9)OC

**PubChem CID:** 9829523

**CAS:** 120685-11-2

# Mobocertinib



**Alt Names:** TAK-788, AP32788, Exkivity

**MW:** 585.70

**Brutto:** C<sub>32</sub>H<sub>39</sub>N<sub>7</sub>O<sub>4</sub>

**Approved for clinical use:** NSCLC With EGFR Mutations

**Approval Jurisdiction:** 2021 FDA

**InChI:** InChI=1S/C32H39N7O4/c1-9-29(40)34-24-16-25(28(42-8)17-27(24)38(6)15-14-37(4)5)35-32-33-18-22(31(41)43-20(2)3)30(36-32)23-19-39(7)26-13-11-10-12-21(23)26/h9-13,16-20H,1,14-15H2,2-8H3,(H,34,40)(H,33,35,36)

**InChI Key:** AZSRSNUQCUDCGG-UHFFFAOYSA-N

**SMILES:** CC(C)OC(=O)C1=CN=C(N=C1C2=CN(C3=CC=CC=C32)C)NC4=C(C=C(C(=C4)NC(=O)C=C)N(C)CCN(C)C)OC

**PubChem CID:** 118607832

**CAS:** 1847461-43-1

Necitumumab

## Monoclonal antibody

**Alt Names:** Portrazza, IMC-11F8

**MW:**

**Brutto:**

**Approved for clinical use:** NSCLC

**Approval Jurisdiction:** 2015 FDA 2015 EMA

**InChI:**

**InChI Key:**

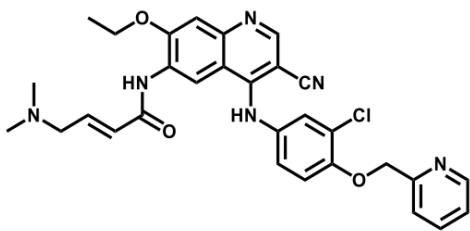
**SMILES:**

**PubChem CID:**

**CAS:** 906805-06-9

Neratinib





**Alt Names:** HKI-272, Nerlynx

**MW:** 557.00

**Brutto:** C<sub>30</sub>H<sub>29</sub>ClN<sub>6</sub>O<sub>3</sub>

**Approved for clinical use:** HER2-Positive Breast Cancer

**Approval Jurisdiction:** 2017 FDA 2018 EMA

**InChI:** InChI=1S/C30H29ClN6O3/c1-4-39-28-16-25-23(15-26(28)36-29(38)9-7-13-37(2)3)30(20(17-32)18-34-25)35-21-10-11-27(24(31)14-21)40-19-22-8-5-6-12-33-22/h5-12,14-16,18H,4,13,19H2,1-3H3,(H,34,35)(H,36,38)/b9-7+

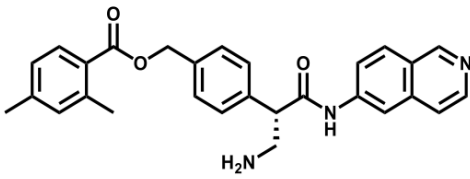
**InChI Key:** JWNPDZNEKVCWMY-VQHVLOKHS-A-N

**SMILES:** CCOC1=C(C=C2C(=C1)N=CC(=C2NC3=CC(=C(C=C3)OCC4=CC=CC=N4)Cl)C#N)NC(=O)C=CCN(C)C

**PubChem CID:** 9915743

**CAS:** 698387-09-6

# Netarsudil



**Alt Names:** Rhopressa

**MW:**

**Brutto:** C<sub>28</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub>

**Approved for clinical use:** Glaucoma (Topical)

**Approval Jurisdiction:** 2017 FDA

**InChI:** InChI=1S/C28H27N3O3/c1-18-3-10-25(19(2)13-18)28(33)34-17-20-4-6-21(7-5-20)26(15-29)27(32)31-24-9-8-23-16-30-12-11-22(23)14-24/h3-14,16,26H,15,17,29H2,1-2H3,(H,31,32)/t26-/m1/s1

**InChI Key:** OURRXQUGYQRVML-AREMUKBSSA-N

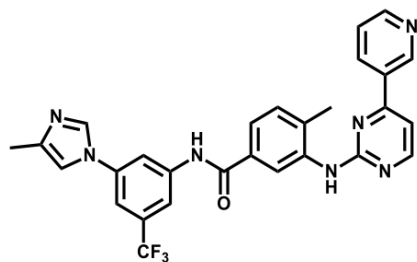
**SMILES:**

CC1=CC(=C(C=C1)C(=O)OCC2=CC=C(C=C2)C(CN)C(=O)NC3=CC4=C(C=C3)C=NC=C4)C

**PubChem CID:** 66599893

**CAS:** 1254032-66-0

# Nilotinib



**Alt Names:** Tassigna

**MW:**

**Brutto:** C<sub>28</sub>H<sub>22</sub>F<sub>3</sub>N<sub>7</sub>O

**Approved for clinical use:** Chronic Myelogenous Leukemia

**Approval Jurisdiction:** 2007 FDA

**InChI:** InChI=1S/C28H22F3N7O/c1-17-5-6-19(10-25(17)37-27-33-9-7-24(36-27)20-4-3-8-32-14-20)26(39)35-22-11-21(28(29,30)31)12-23(13-22)38-15-18(2)34-16-38/h3-16H,1-2H3,(H,35,39)(H,33,36,37)

**InChI Key:** HHZIURLSWUIHRB-UHFFFAOYSA-N

**SMILES:** CC1=C(C=C(C=C1)C(=O)NC2=CC(=CC(=C2)C(F)(F)F)N3C=C(N=C3)C)NC4=NC=CC(=N4)C5=CN=CC=C5

**PubChem CID:** 644241

**CAS:** 641571-10-0

Nimotuzumab

## Monoclonal antibody

**Alt Names:**

**MW:**

**Brutto:**

**Approved for clinical use:** Cell Carcinomas Of The Head And Neck

**Approval Jurisdiction:** 2014 China, India

**InChI:**

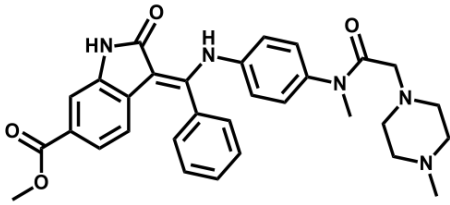
**InChI Key:**

**SMILES:**

**PubChem CID:**

**CAS:** 780758-10-3

Nintedanib



**Alt Names:** Intedanib, Vargatef, BIBF-1120

**MW:** 539.60

**Brutto:** C<sub>31</sub>H<sub>33</sub>N<sub>5</sub>O<sub>4</sub>

**Approved for clinical use:** Idiopathic Pulmonary Fibrosis

**Approval Jurisdiction:** 2014 FDA 2014 EMA

**InChI:** InChI=1S/C31H33N5O4/c1-34-15-17-36(18-16-34)20-27(37)35(2)24-12-10-23(11-13-24)32-29(21-7-5-4-6-8-21)28-25-14-9-22(31(39)40-3)19-26(25)33-30(28)38/h4-14,19,33,38H,15-18,20H2,1-3H3

**InChI Key:** CPMDPSXJELVGJG-UHFFFAOYSA-N

**SMILES:** CN1CCN(CC1)CC(=O)N(C)C2=CC=C(C=C2)N=C(C3=CC=CC=C3)C4=C(NC5=C4C=CC(=C5)C(=O)OC)O

**PubChem CID:** 135423438

**CAS:** 656247-17-5

Olaratumab

# Monoclonal antibody

**Alt Names:** Lartruvo, IMC-3G3

**MW:**

**Brutto:**

**Approved for clinical use:** Soft Tissue Sarcoma

**Approval Jurisdiction:** 2016 DFA 2016 EMA

**InChI:**

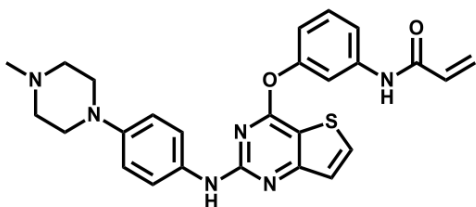
**InChI Key:**

**SMILES:**

**PubChem CID:**

**CAS:** 1024603-93-7

Olmutinib



**Alt Names:** HM61713, BI 1482694

**MW:** 486.60

**Brutto:** C<sub>26</sub>H<sub>26</sub>N<sub>6</sub>O<sub>2</sub>S

**Approved for clinical use:** T790M+Ve NSCLC

**Approval Jurisdiction:** 2016 S.Korea

**InChI:** InChI=1S/C26H26N6O2S/c1-3-23(33)27-19-5-4-6-21(17-19)34-25-24-22(11-16-35-24)29-26(30-25)28-18-7-9-20(10-8-18)32-14-12-31(2)13-15-32/h3-11,16-17H,1,12-15H2,2H3,(H,27,33)(H,28,29,30)

**InChI Key:** FDMQDKQUTRLUBU-UHFFFAOYSA-N

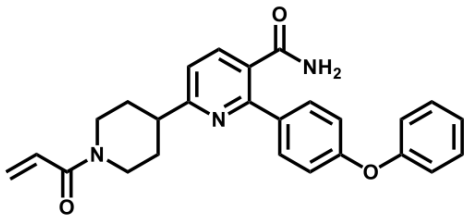
**SMILES:**

CN1CCN(CC1)C2=CC=C(C=C2)NC3=NC4=C(C(=N3)OC5=CC=CC(=C5)NC(=O)C=C)SC=C4

**PubChem CID:** 54758501

**CAS:** 1353550-13-6

Orelabrutinib



**Alt Names:** ICP-022, ICP022

**MW:** 427.50

**Brutto:** C<sub>26</sub>H<sub>25</sub>N<sub>3</sub>O<sub>3</sub>

**Approved for clinical use:** Mantle Cell Lymphoma CLL, SLL

**Approval Jurisdiction:** 2020 China

**InChI:** InChI=1S/C26H25N3O3/c1-2-24(30)29-16-14-18(15-17-29)23-13-12-22(26(27)31)25(28-23)19-8-10-21(11-9-19)32-20-6-4-3-5-7-20/h2-13,18H,1,14-17H2,(H2,27,31)

**InChI Key:** MZPVEMOYADUARK-UHFFFAOYSA-N

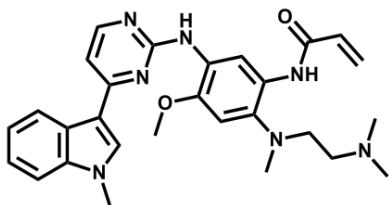
**SMILES:** C=CC(=O)N1CCC(CC1)C2=NC(=C(C=C2)C(=O)N)C3=CC=C(C=C3)OC4=CC=CC=C4

**PubChem CID:** 91667513

**CAS:** 1655504-04-3

Osimertinib





**Alt Names:** AZD-9291, AZD9291, Mereletinib

**MW:** 499.60

**Brutto:** C<sub>28</sub>H<sub>33</sub>N<sub>7</sub>O<sub>2</sub>

**Approved for clinical use:** T790M+Ve NSCLC

**Approval Jurisdiction:** 2015 FDA 2016 EMA

**InChI:** InChI=1S/C28H33N7O2/c1-7-27(36)30-22-16-23(26(37-6)17-25(22)34(4)15-14-33(2)3)32-28-29-13-12-21(31-28)20-18-35(5)24-11-9-8-10-19(20)24/h7-13,16-18H,1,14-15H2,2-6H3,(H,30,36)(H,29,31,32)

**InChI Key:** DUYJMQONPNNFPI-UHFFFAOYSA-N

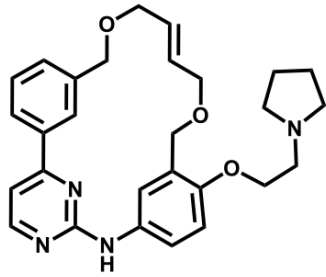
**SMILES:**

CN1C=C(C2=CC=CC=C21)C3=NC(=NC=C3)NC4=C(C=C(C(=C4)NC(=O)C=C)N(C)CCN(C)C)OC

**PubChem CID:** 71496458

**CAS:** 1421373-65-0

# Pacritinib



**Alt Names:** SB1518, SB-1518

**MW:** 472.60

**Brutto:** C<sub>28</sub>H<sub>32</sub>N<sub>4</sub>O<sub>3</sub>

**Approved for clinical use:** Myelofibrosis

**Approval Jurisdiction:** 2022 FDA

**InChI:** InChI=1S/C28H32N4O3/c1-2-13-32(12-1)14-17-35-27-9-8-25-19-24(27)21-34-16-4-3-15-33-20-22-6-5-7-23(18-22)26-10-11-29-28(30-25)31-26/h3-11,18-19H,1-2,12-17,20-21H2,(H,29,30,31)/b4-3+

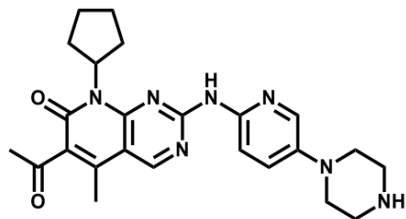
**InChI Key:** HWXVIOGONBBTBY-ONEGZZNKSA-N

**SMILES:** C1CCN(C1)CCOC2=C3COCC=CCOCC4=CC(=CC=C4)C5=NC(=NC=C5)NC(=C3)C=C2

**PubChem CID:** 46216796

**CAS:** 937272-79-2

# Palbociclib



**Alt Names:** Ibrance, PD-0332991, PD0332991

**MW:** 447.50

**Brutto:** C<sub>24</sub>H<sub>29</sub>N<sub>7</sub>O<sub>2</sub>

**Approved for clinical use:** Advanced (Metastatic) Breast Cancer

**Approval Jurisdiction:** 2015 FDA 2016 EMA

**InChI:** InChI=1S/C24H29N7O2/c1-15-19-14-27-24(28-20-8-7-18(13-26-20)30-11-9-25-10-12-30)29-22(19)31(17-5-3-4-6-17)23(33)21(15)16(2)32/h7-8,13-14,17,25H,3-6,9-12H2,1-2H3,(H,26,27,28,29)

**InChI Key:** AHJRHEGDXXFFMBM-UHFFFAOYSA-N

**SMILES:** CC1=C(C(=O)N(C2=NC(=NC=C12)NC3=NC=C(C=C3)N4CCNCC4)C5CCCC5)C(=O)C

**PubChem CID:** 5330286

**CAS:** 571190-30-2

Panitumumab

## Monoclonal antibody

**Alt Names:**

**MW:**

**Brutto:**

**Approved for clinical use:** EGFR Colorectal Cancer

**Approval Jurisdiction:** 2006 FDA 2007 EMA

**InChI:**

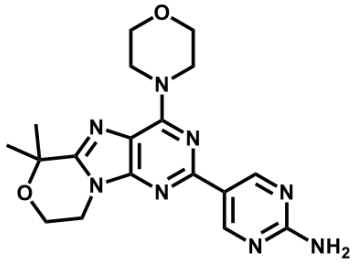
**InChI Key:**

**SMILES:**

**PubChem CID:**

**CAS:** 339177-26-3

Paxalisib



**Alt Names:** GDC0084, GDC-0084

**MW:** 382.40

**Brutto:** C<sub>18</sub>H<sub>22</sub>N<sub>8</sub>O<sub>2</sub>

**Approved for clinical use:** Malignant Glioblastoma

**Approval Jurisdiction:** 2020 FDA

**InChI:** InChI=1S/C18H22N8O2/c1-18(2)16-22-12-14(25-3-6-27-7-4-25)23-13(11-9-20-17(19)21-10-11)24-15(12)26(16)5-8-28-18/h9-10H,3-8H2,1-2H3,(H2,19,20,21)

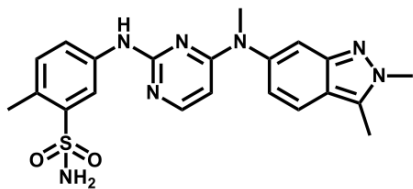
**InChI Key:** LGWACEZVCMBKW-UHFFFAOYSA-N

**SMILES:** CC1(C2=NC3=C(N2CCO1)N=C(N=C3N4CCOCC4)C5=CN=C(N=C5)N)C

**PubChem CID:** 57384863

**CAS:** 1382979-44-3

Pazopanib



**Alt Names:** Votrient

**MW:**

**Brutto:** C<sub>21</sub>H<sub>24</sub>ClN<sub>7</sub>O<sub>2</sub>S

**Approved for clinical use:** Renal Cancer

**Approval Jurisdiction:** 2009 FDA, 2010 EMA, MHRA, TGA

**InChI:** InChI=1S/C21H23N7O2S.ClH/c1-13-5-6-15(11-19(13)31(22,29)30)24-21-23-10-9-20(25-21)27(3)16-7-8-17-14(2)28(4)26-18(17)12-16;/h5-12H,1-4H3,(H2,22,29,30)(H,23,24,25);1H

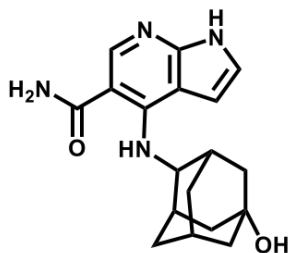
**InChI Key:** MQHIQUBXFFAOMK-UHFFFAOYSA-N

**SMILES:** CC1=C(C=C(C=C1)NC2=NC=CC(=N2)N(C)C3=CC4=NN(C(=C4C=C3)C)C)S(=O)(=O)N.Cl

**PubChem CID:** 11525740

**CAS:** 635702-64-6

Peficitinib



**Alt Names:** ASP015K, ASP-015K

**MW:** 326.40

**Brutto:** C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>

**Approved for clinical use:** Rheumatoid Arthritis

**Approval Jurisdiction:** 2021 Japan

**InChI:** InChI=1S/C18H22N4O2/c19-16(23)13-8-21-17-12(1-2-20-17)15(13)22-14-10-3-9-4-11(14)7-18(24,5-9)6-10/h1-2,8-11,14,24H,3-7H2,(H2,19,23)(H2,20,21,22)/t9?,10-,11+,14?,18?

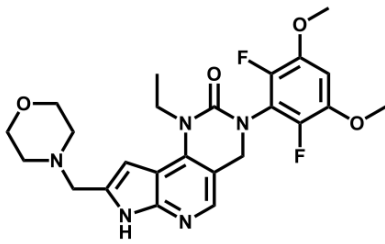
**InChI Key:** DREIJXJRTLTGJC-JQCLMNFQSA-N

**SMILES:** C1C2CC3CC(C2)(CC1C3NC4=C5C=CNC5=NC=C4C(=O)N)O

**PubChem CID:** 57928403

**CAS:** 944118-01-8

Pemigatinib



**Alt Names:** Pemazyre, INCB054828

**MW:** 487.50

**Brutto:** C<sub>24</sub>H<sub>27</sub>F<sub>2</sub>N<sub>5</sub>O<sub>4</sub>

**Approved for clinical use:** Cholangiocarcinoma With FGFR2 Fusion

**Approval Jurisdiction:** 2020 FDA

**InChI:** InChI=1S/C24H27F2N5O4/c1-4-30-21-14(11-27-23-16(21)9-15(28-23)13-29-5-7-35-8-6-29)12-31(24(30)32)22-19(25)17(33-2)10-18(34-3)20(22)26/h9-11H,4-8,12-13H2,1-3H3,(H,27,28)

**InChI Key:** HCDMJFOHIXMBOV-UHFFFAOYSA-N

**SMILES:** CCN1C2=C3C=C(NC3=NC=C2CN(C1=O)C4=C(C(=CC(=C4F)OC)OC)F)CN5CCOCC5

**PubChem CID:** 86705695

**CAS:** 1513857-77-6

Pertuzumab



## Monoclonal antibody

**Alt Names:** Perjeta, Omnitarg

**MW:**

**Brutto:**

**Approved for clinical use:** HER2-Positive Breast Cancer

**Approval Jurisdiction:** 2012 FDA 2013 EMA

**InChI:**

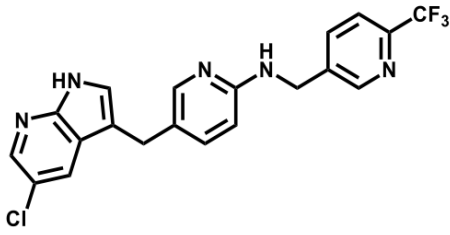
**InChI Key:**

**SMILES:**

**PubChem CID:**

**CAS:** 380610-27-5

Pexidartinib



**Alt Names:** PLX3397, PLX-3397, Turalio

**MW:** 417.80

**Brutto:** C<sub>20</sub>H<sub>15</sub>ClF<sub>3</sub>N<sub>5</sub>

**Approved for clinical use:** Tenosynovial Giant Cell Tumour

**Approval Jurisdiction:** 2019 FDA

**InChI:** InChI=1S/C20H15ClF3N5/c21-15-6-16-14(10-28-19(16)29-11-15)5-12-2-4-18(26-7-12)27-9-13-1-3-17(25-8-13)20(22,23)24/h1-4,6-8,10-11H,5,9H2,(H,26,27)(H,28,29)

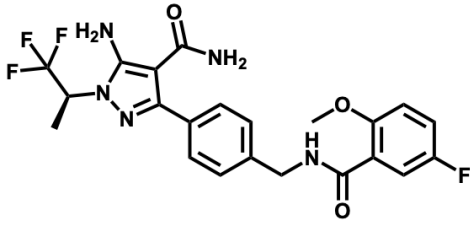
**InChI Key:** JGWRKYUXBBNENE-UHFFFAOYSA-N

**SMILES:** C1=CC(=NC=C1CC2=CNC3=C2C=C(C=N3)Cl)NCC4=CN=C(C=C4)C(F)(F)F

**PubChem CID:** 25151352

**CAS:** 1029044-16-3

Pirtobrutinib



**Alt Names:**

**MW:** 479.40

**Brutto:** C<sub>22</sub>H<sub>21</sub>F<sub>4</sub>N<sub>5</sub>O<sub>3</sub>

**Approved for clinical use:** Mantle Cell Lymphoma

**Approval Jurisdiction:** 2023 FDA

**InChI:** InChI=1S/C22H21F4N5O3/c1-11(22(24,25)26)31-19(27)17(20(28)32)18(30-31)13-5-3-12(4-6-13)10-29-21(33)15-9-14(23)7-8-16(15)34-2/h3-9,11H,10,27H2,1-2H3,(H2,28,32)(H,29,33)/t11-/m0/s1

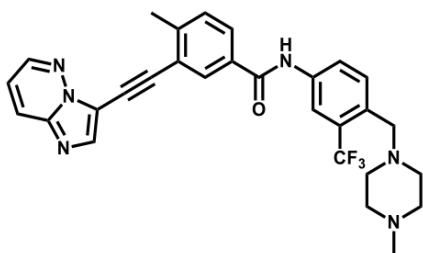
**InChI Key:** FWZAWAUZYCBKZ-NSHDSACASA-N

**SMILES:** CC(C(F)(F)F)N1C(=C(C(=N1)C2=CC=C(C=C2)CNC(=O)C3=C(C=CC(=C3)F)OC)C(=O)N)N

**PubChem CID:** 129269915

**CAS:** 2101700-15-4

Ponatinib



**Alt Names:** Iclusig, AP24534

**MW:**

**Brutto:** C<sub>29</sub>H<sub>27</sub>F<sub>3</sub>N<sub>6</sub>O

**Approved for clinical use:** Chronic Myelogenous Leukemia, ALL

**Approval Jurisdiction:** 2012 FDA

**InChI:** InChI=1S/C29H27F3N6O/c1-20-5-6-22(16-21(20)8-10-25-18-33-27-4-3-11-34-38(25)27)28(39)35-24-9-7-23(26(17-24)29(30,31)32)19-37-14-12-36(2)13-15-37/h3-7,9,11,16-18H,12-15,19H2,1-2H3,(H,35,39)

**InChI Key:** PHXJVRSECIGDHY-UHFFFAOYSA-N

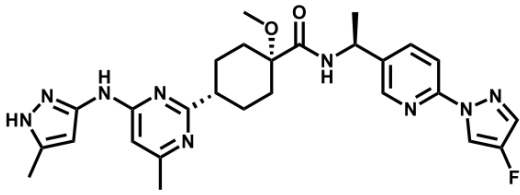
**SMILES:**

CC1=C(C=C(C=C1)C(=O)NC2=CC(=C(C=C2)CN3CCN(CC3)C)C(F)(F)F)C#CC4=CN=C5N4N=CC=C5

**PubChem CID:** 24826799

**CAS:** 943319-70-8

# Pralsetinib



**Alt Names:** BLU-667, Gavreto

**MW:** 533.60

**Brutto:** C<sub>27</sub>H<sub>32</sub>FN<sub>9</sub>O<sub>2</sub>

**Approved for clinical use:** Met RET Fusion +Ve NSCLC MTC

**Approval Jurisdiction:** 2020 FDA

**InChI:** InChI=1S/C27H32FN9O2/c1-16-11-22(33-23-12-17(2)35-36-23)34-25(31-16)19-7-9-27(39-4,10-8-19)26(38)32-18(3)20-5-6-24(29-13-20)37-15-21(28)14-30-37/h5-6,11-15,18-19H,7-10H2,1-4H3,(H,32,38)(H2,31,33,34,35,36)/t18-,19?,27?/m0/s1

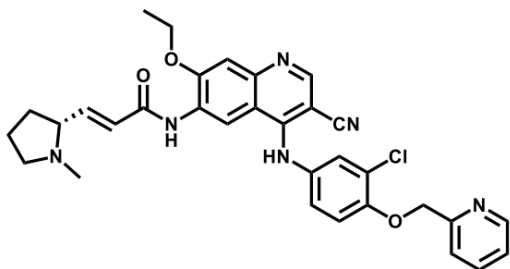
**InChI Key:** GBLBJPZSROAGMF-SIYOEGHSA-N

**SMILES:** CC1=CC(=NN1)NC2=NC(=NC(=C2)C)C3CCC(CC3)(C(=O)NC(C)C4=CN=C(C=C4)N5C=C(C=N5)F)OC

**PubChem CID:** 129073603

**CAS:** 2097132-94-8

# Pyrotinib



**Alt Names:** SHR-1258, UNII-CJN36EQM0H, CJN36EQM0H

**MW:** 583.10

**Brutto:** C<sub>32</sub>H<sub>31</sub>ClN<sub>6</sub>O<sub>3</sub>

**Approved for clinical use:** Breast Cancer

**Approval Jurisdiction:** 2020 China

**InChI:** InChI=1S/C32H31ClN6O3/c1-3-41-30-17-27-25(16-28(30)38-31(40)12-10-24-8-6-14-39(24)2)32(21(18-34)19-36-27)37-22-9-11-29(26(33)15-22)42-20-23-7-4-5-13-35-23/h4-5,7,9-13,15-17,19,24H,3,6,8,14,20H2,1-2H3,(H,36,37)(H,38,40)/b12-10+/t24-/m1/s1

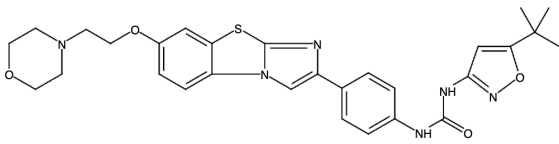
**InChI Key:** SADXACCFNXBCFY-IYNHSRRRSA-N

**SMILES:** CCOC1=C(C=C2C(=C1)N=CC(=C2NC3=CC(=C(C=C3)OCC4=CC=CC=N4)Cl)C#N)NC(=O)C=CC5CCCN5C

**PubChem CID:** 51039030

**CAS:** 1269662-73-8

# Quizartinib



**Alt Names:** AC220, AC010220, Vanflyta

**MW:** 560.67

**Brutto:** C<sub>29</sub>H<sub>32</sub>N<sub>6</sub>O<sub>4</sub>S

**Approved for clinical use:** Acute Myeloid Leukemia

**Approval Jurisdiction:** 2019 Japan, 2023 FDA

**InChI:** InChI=1S/C29H32N6O4S/c1-29(2,3)25-17-26(33-39-25)32-27(36)30-20-6-4-19(5-7-20)22-18-35-23-9-8-21(16-24(23)40-28(35)31-22)38-15-12-34-10-13-37-14-11-34/h4-9,16-18H,10-15H2,1-3H3,(H2,30,32,33,36)

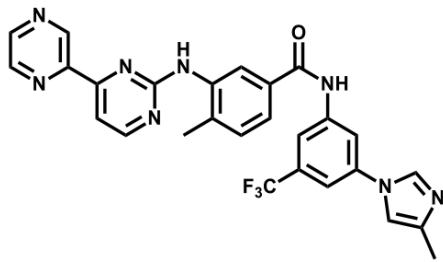
**InChI Key:** InChIKey=CVWXJKQAOSCOAB-UHFFFAOYSA-N

**SMILES:** O(CCN1CCOCC1)C=C=C3C(N4C(S3)=NC(=C4)C5=CC=C(NC(NC=6C=C(C(C)(C)C)ON6)=O)C=C5)=CC2

**PubChem CID:** 24889392

**CAS:** 950769-58-1

# Radotinib



**Alt Names:** Supect

**MW:**

**Brutto:** C<sub>27</sub>H<sub>21</sub>F<sub>3</sub>N<sub>8</sub>O

**Approved for clinical use:** Chronic Myelogenous Leukemia

**Approval Jurisdiction:** 2012 FDA

**InChI:** InChI=1S/C27H21F3N8O/c1-16-3-4-18(9-23(16)37-26-33-6-5-22(36-26)24-13-31-7-8-32-24)25(39)35-20-10-19(27(28,29)30)11-21(12-20)38-14-17(2)34-15-38/h3-15H,1-2H3,(H,35,39)(H,33,36,37)

**InChI Key:** DUPWHXBITIZIKZ-UHFFFAOYSA-N

**SMILES:** CC1=C(C=C(C=C1)C(=O)NC2=CC(=CC(=C2)C(F)(F)F)N3C=C(N=C3)C)NC4=NC=CC(=N4)C5=NC=CN=C5

**PubChem CID:** 16063245

**CAS:** 926037-48-1



Ramucirumab

## Monoclonal antibody

**Alt Names:** LY3009806, Cyramza

**MW:**

**Brutto:**

**Approved for clinical use:** MNSCLC Colorectal Cancer

**Approval Jurisdiction:** 2014 FDA 2014 EMA

**InChI:**

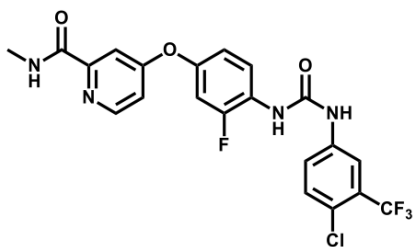
**InChI Key:**

**SMILES:**

**PubChem CID:**

**CAS:** 947687-13-0

Regorafenib



**Alt Names:** Stivarga , Regonix

**MW:**

**Brutto:** C<sub>21</sub>H<sub>15</sub>ClF<sub>4</sub>N<sub>4</sub>O<sub>3</sub>

**Approved for clinical use:** Clorectal Cancer GIST, HCC

**Approval Jurisdiction:** 2012 FDA

**InChI:** InChI=1S/C21H15ClF4N4O3/c1-27-19(31)18-10-13(6-7-28-18)33-12-3-5-17(16(23)9-12)30-20(32)29-11-2-4-15(22)14(8-11)21(24,25)26/h2-10H,1H3,(H,27,31)(H2,29,30,32)

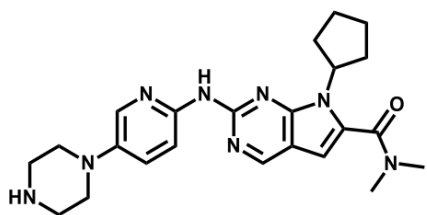
**InChI Key:** FNHKPVJBJVTLMP-UHFFFAOYSA-N

**SMILES:** CNC(=O)C1=NC=CC(=C1)OC2=CC(=C(C=C2)NC(=O)NC3=CC(=C(C=C3)Cl)C(F)(F)F)

**PubChem CID:** 11167602

**CAS:** 755037-03-7

Ribociclib



**Alt Names:** LEE011, LEE-011

**MW:** 434.50

**Brutto:** C<sub>23</sub>H<sub>30</sub>N<sub>8</sub>O

**Approved for clinical use:** Advanced (Metastatic) Breast Cancer HR+, HER2-Ve

**Approval Jurisdiction:** 2017 FDA 2017 EMA

**InChI:** InChI=1S/C23H30N8O/c1-29(2)22(32)19-13-16-14-26-23(28-21(16)31(19)17-5-3-4-6-17)27-20-8-7-18(15-25-20)30-11-9-24-10-12-30/h7-8,13-15,17,24H,3-6,9-12H2,1-2H3,(H,25,26,27,28)

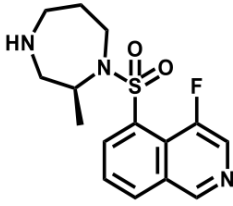
**InChI Key:** RHXHGRAEPCAFML-UHFFFAOYSA-N

**SMILES:** CN(C)C(=O)C1=CC2=CN=C(N=C2N1C3CCCC3)NC4=NC=C(C=C4)N5CCNCC5

**PubChem CID:** 44631912

**CAS:** 1211441-98-3

Ripasudil



**Alt Names:**

**MW:** 323.40

**Brutto:** C<sub>15</sub>H<sub>18</sub>FN<sub>3</sub>O<sub>2</sub>S

**Approved for clinical use:** Glaucoma Ocular Hypertension

**Approval Jurisdiction:** 2014 Japan

**InChI:** InChI=1S/C15H18FN3O2S/c1-11-8-17-6-3-7-19(11)22(20,21)14-5-2-4-12-9-18-10-13(16)15(12)14/h2,4-5,9-11,17H,3,6-8H2,1H3/t11-/m0/s1

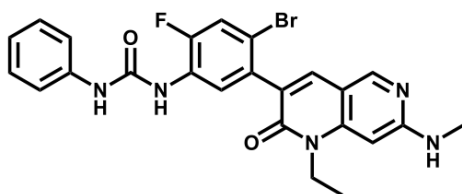
**InChI Key:** QSKQVZWVLOIIEV-NSHDSACASA-N

**SMILES:** CC1CNCCCN1S(=O)(=O)C2=CC=CC3=CN=CC(=C32)F

**PubChem CID:** 9863672

**CAS:** 223645-67-8

Ripretinib



**Alt Names:** DCC-2618

**MW:** 510.40

**Brutto:** C<sub>24</sub>H<sub>21</sub>BrFN<sub>5</sub>O<sub>2</sub>

**Approved for clinical use:** Advanced GIST Mastocytosis

**Approval Jurisdiction:** 2020 FDA

**InChI:** InChI=1S/C24H21BrFN5O2/c1-3-31-21-12-22(27-2)28-13-14(21)9-17(23(31)32)16-10-20(19(26)11-18(16)25)30-24(33)29-15-7-5-4-6-8-15/h4-13H,3H2,1-2H3,(H,27,28)(H2,29,30,33)

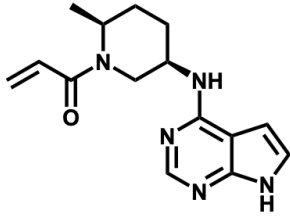
**InChI Key:** CEFJVGZHQAGLHS-UHFFFAOYSA-N

**SMILES:** CCN1C2=CC(=NC=C2C=C(C1=O)C3=CC(=C(C=C3Br)F)NC(=O)NC4=CC=CC=C4)NC

**PubChem CID:** 71584930

**CAS:** 1442472-39-0

Ritlecitinib



**Alt Names:**

**MW:**

**Brutto:** C<sub>15</sub>H<sub>19</sub>N<sub>5</sub>O

**Approved for clinical use:** Severe Alopecia

**Approval Jurisdiction:** 2023 FDA

**InChI:** InChI=1S/C15H19N5O/c1-3-13(21)20-8-11(5-4-10(20)2)19-15-12-6-7-16-14(12)17-9-18-15/h3,6-7,9-11H,1,4-5,8H2,2H3,(H2,16,17,18,19)/t10-,11+/m0/s1

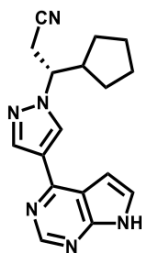
**InChI Key:** CBRJPGIXUFMTM-WDEREUQCSA-N

**SMILES:** O=C(C=C)N(C1)[C@@H](C)CC[C@H]1NC2=C3C(NC=C3)=NC=N2

**PubChem CID:** 118115473

**CAS:** 1792180-81-4

Ruxolitinib



**Alt Names:** Jakafi, Jakavi, INCB18424

**MW:** 306.37

**Brutto:** C<sub>17</sub>H<sub>18</sub>N<sub>6</sub>

**Approved for clinical use:** Myelofibrosis

**Approval Jurisdiction:** 2011 FDA, 2012 EMA

**InChI:** InChI=1S/C17H18N6/c18-7-5-15(12-3-1-2-4-12)23-10-13(9-22-23)16-14-6-8-19-17(14)21-11-20-16/h6,8-12,15H,1-5H2,(H,19,20,21)/t15-/m1/s1

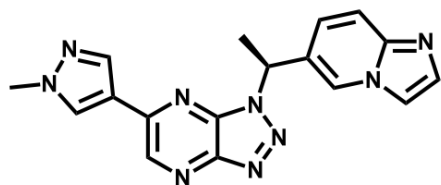
**InChI Key:** HFNKQEVNSGCOJV-OAHLLOKOSA-N

**SMILES:** C1CCC(C1)C(CC#N)N2C=C(C=N2)C3=C4C=CNC4=NC=N3

**PubChem CID:** 25126798

**CAS:** 941678-49-5

Savolitinib



**Alt Names:** Volitinib, AZD-6094, HMPL-504

**MW:** 345.40

**Brutto:** C<sub>17</sub>H<sub>15</sub>N<sub>9</sub>

**Approved for clinical use:** Adenocarcinoma, NSCLC

**Approval Jurisdiction:** 2021 China

**InChI:** InChI=1S/C17H15N9/c1-11(12-3-4-15-18-5-6-25(15)10-12)26-17-16(22-23-26)19-8-14(21-17)13-7-20-24(2)9-13/h3-11H,1-2H3/t11-/m0/s1

**InChI Key:** XYDNMOZJKOGZLS-NSHDSACASA-N

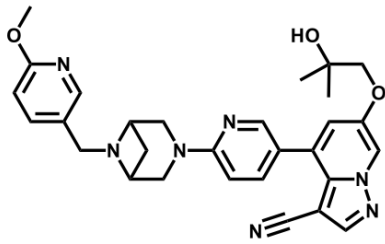
**SMILES:** CC(C1=CN2C=CN=C2C=C1)N3C4=NC(=CN=C4N=N3)C5=CN(N=C5)C

**PubChem CID:** 68289010

**CAS:** 1313725-88-0

Selpercatinib





**Alt Names:** LOXO-292, Retevmo

**MW:** 525.60

**Brutto:** C<sub>29</sub>H<sub>31</sub>N<sub>7</sub>O<sub>3</sub>

**Approved for clinical use:** NSCLC, MTC, Thyroid Cancers

**Approval Jurisdiction:** 2020 FDA

**InChI:** InChI=1S/C29H31N7O3/c1-29(2,37)18-39-24-9-25(28-21(10-30)13-33-36(28)17-24)20-5-6-26(31-12-20)34-15-22-8-23(16-34)35(22)14-19-4-7-27(38-3)32-11-19/h4-7,9,11-13,17,22-23,37H,8,14-16,18H2,1-3H3

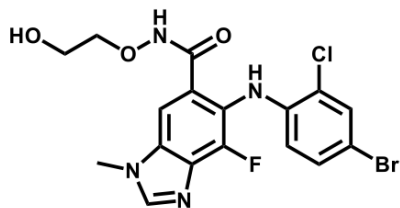
**InChI Key:** XIIOFHFUYBLOLW-UHFFFAOYSA-N

**SMILES:** CC(C)(COC1=CN2C(=C(C=N2)C#N)C(=C1)C3=CN=C(C=C3)N4CC5CC(C4)N5CC6=CN=C(C=C6)OC)O

**PubChem CID:** 134436906

**CAS:** 2152628-33-4

# Selumetinib



**Alt Names:** AZD6244, ARRY-142886, AZD 6244

**MW:** 457.70

**Brutto:** C<sub>17</sub>H<sub>15</sub>BrClFN<sub>4</sub>O<sub>3</sub>

**Approved for clinical use:** Neurofibromatosis Type 1

**Approval Jurisdiction:** 2020 FDA

**InChI:** InChI=1S/C17H15BrClFN4O3/c1-24-8-21-16-13(24)7-10(17(26)23-27-5-4-25)15(14(16)20)22-12-3-2-9(18)6-11(12)19/h2-3,6-8,22,25H,4-5H2,1H3,(H,23,26)

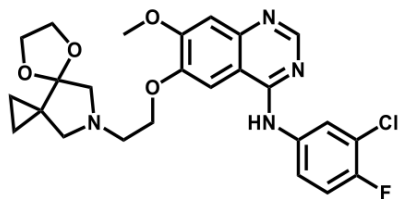
**InChI Key:** CYOHGALHFOKKQC-UHFFFAOYSA-N

**SMILES:** CN1C=NC2=C1C=C(C(=C2F)NC3=C(C=C(C=C3)Br)Cl)C(=O)NOCCO

**PubChem CID:** 10127622

**CAS:** 606143-52-6

# Simotinib



**Alt Names:** UNII-58K797D5IK, 58K797D5IK, SIM-6802

**MW:** 500.90

**Brutto:** C<sub>25</sub>H<sub>26</sub>ClFN<sub>4</sub>O<sub>4</sub>

**Approved for clinical use:** Solid Tumours

**Approval Jurisdiction:** 2018 China

**InChI:** InChI=1S/C25H26ClFN4O4/c1-32-21-12-20-17(23(29-15-28-20)30-16-2-3-19(27)18(26)10-16)11-22(21)33-7-6-31-13-24(4-5-24)25(14-31)34-8-9-35-25/h2-3,10-12,15H,4-9,13-14H2,1H3,(H,28,29,30)

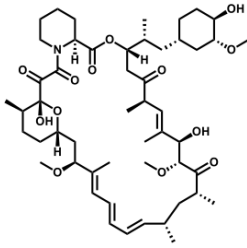
**InChI Key:** OXWUWXCJDBRCCG-UHFFFAOYSA-N

**SMILES:** COC1=C(C=C2C(=C1)N=CN=C2NC3=CC(=C(C=C3)F)Cl)OCCN4CC5(CC5)C6(C4)OCCO6

**PubChem CID:** 16735117

**CAS:** 944258-89-3

# Sirolimus



**Alt Names:** Rapamycin, Rapamune , WY-090217, AY-22989, CHEBI:9168, Antibiotic AY 22989

**MW:** 914.20

**Brutto:** C<sub>51</sub>H<sub>79</sub>NO<sub>13</sub>

**Approved for clinical use:** Kidney Transplantation

**Approval Jurisdiction:** 1999 FDA

**InChI:** InChI=1S/C51H79NO13/c1-30-16-12-11-13-17-31(2)42(61-8)28-38-21-19-36(7)51(60,65-38)48(57)49(58)52-23-15-14-18-39(52)50(59)64-43(33(4)26-37-20-22-40(53)44(27-37)62-9)29-41(54)32(3)25-35(6)46(56)47(63-10)45(55)34(5)24-30/h11-13,16-17,25,30,32-34,36-40,42-44,46-47,53,56,60H,14-15,18-24,26-29H2,1-10H3/b13-11+,16-12+,31-17+,35-25+/t30-,32-,33-,34-,36-,37+,38+,39+,40-,42+,43+,44-,46-,47+,51-/m1/s1

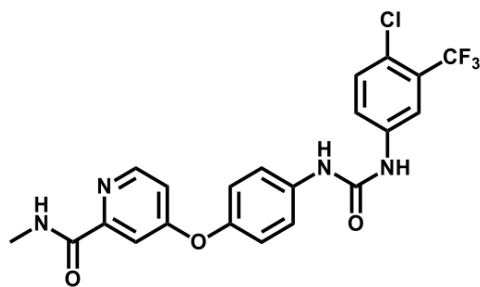
**InChI Key:** QFJCIRLUMZQUOT-HPLJQQBZSA-N

**SMILES:** CC1CCC2CC(C(=CC=CC=CC(C(C(=O)C(C(C(=CC(C(=O)CC(OC(=O)C3CCCCN3C(=O)C(=O)C1(O2)O)C(C)CC4CCC(C(C4)OC)O)C)C)O)OC)C)C)OC

**PubChem CID:** 5284616

**CAS:** 53123-88-9

# Sorafenib



**Alt Names:** Sorafenib, Kinome\_766, AC1L50CF, ChEMBL1336, BAY-439006, BAY 439006, BAY439006, Nexavar

**MW:** 464.80

**Brutto:** C<sub>21</sub>H<sub>16</sub>ClF<sub>3</sub>N<sub>4</sub>O<sub>3</sub>

**Approved for clinical use:** Renal Cancer HCC

**Approval Jurisdiction:** 2005 FDA, 2006 EMA

**InChI:** InChI=1S/C21H16ClF3N4O3/c1-26-19(30)18-11-15(8-9-27-18)32-14-5-2-12(3-6-14)28-20(31)29-13-4-7-17(22)16(10-13)21(23,24)25/h2-11H,1H3,(H,26,30)(H2,28,29,31)

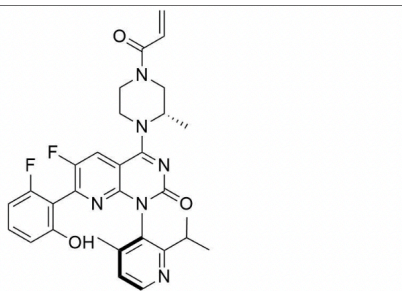
**InChI Key:** MLDQJTXFUGDVEO-UHFFFAOYSA-N

**SMILES:** CNC(=O)C1=NC=CC(=C1)OC2=CC=C(C=C2)NC(=O)NC3=CC(=C(C=C3)Cl)C(F)(F)F

**PubChem CID:** 216239

**CAS:** 284461-73-0

# Sotorasib



**Alt Names:** AMG-510, AMG510, Lumakras

**MW:** 560.60

**Brutto:** C<sub>30</sub>H<sub>30</sub>F<sub>2</sub>N<sub>6</sub>O<sub>3</sub>

**Approved for clinical use:** KRAS Non-Small-Cell Lung Cancer

**Approval Jurisdiction:** 2021 FDA, 2022 EMA

**InChI:** InChI=1S/C30H30F2N6O3/c1-6-23(40)36-12-13-37(18(5)15-36)28-19-14-21(32)26(24-20(31)8-7-9-22(24)39)34-29(19)38(30(41)35-28)27-17(4)10-11-33-25(27)16(2)3/h6-11,14,16,18,39H,1,12-13,15H2,2-5H3/t18-/m0/s1

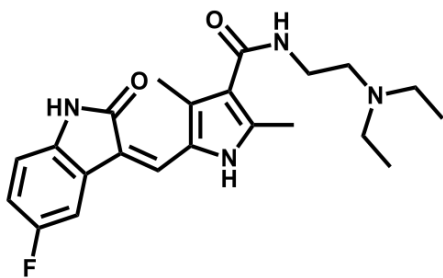
**InChI Key:** NXQKSXLFSAEQCZ-SFHVURJKSA-N

**SMILES:** CC1CN(CCN1C2=NC(=O)N(C3=NC(=C(C=C32)F)C4=C(C=CC=C4F)O)C5=C(C=CN=C5C(C)C)C(=O)C=C

**PubChem CID:** 137278711

**CAS:** 2296729-00-3

# Sunitinib



**Alt Names:** GSK-R, sunitinibum, Sutent , SU-11248

**MW:** 398.47

**Brutto:** C<sub>22</sub>H<sub>27</sub>FN<sub>4</sub>O<sub>2</sub>

**Approved for clinical use:** Renal Cancer, Imatinib Resistant GIST

**Approval Jurisdiction:** 2006 FDA

**InChI:** InChI=1S/C22H27FN4O2/c1-5-27(6-2)10-9-24-22(29)20-13(3)19(25-14(20)4)12-17-16-11-15(23)7-8-18(16)26-21(17)28/h7-8,11-12,25H,5-6,9-10H2,1-4H3,(H,24,29)(H,26,28)/b17-12-

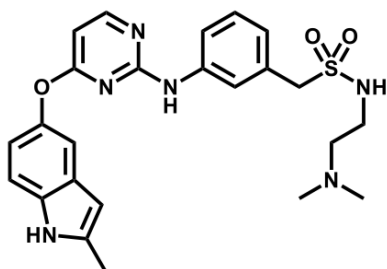
**InChI Key:** WINHZLLDWRZWRT-ATVHPVEESA-N

**SMILES:** CCN(CC)CCNC(=O)C1=C(NC(=C1C)C=C2C3=C(C=CC(=C3)F)NC2=O)C

**PubChem CID:** 5329102

**CAS:** 341031-54-7

# Surufatinib



**Alt Names:** Sulfatinib, HMPL-012

**MW:** 480.60

**Brutto:** C<sub>24</sub>H<sub>28</sub>N<sub>6</sub>O<sub>3</sub>S

**Approved for clinical use:** Advanced Pancreatic NET

**Approval Jurisdiction:** 2021 China

**InChI:** InChI=1S/C24H28N6O3S/c1-17-13-19-15-21(7-8-22(19)27-17)33-23-9-10-25-24(29-23)28-20-6-4-5-18(14-20)16-34(31,32)26-11-12-30(2)3/h4-10,13-15,26-27H,11-12,16H2,1-3H3,(H,25,28,29)

**InChI Key:** TTZSNFLLYPYKIL-UHFFFAOYSA-N

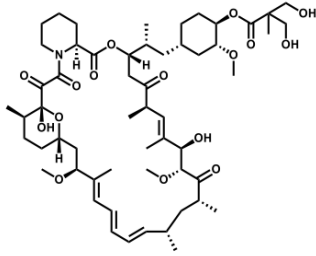
**SMILES:** CC1=CC2=C(N1)C=CC(=C2)OC3=NC(=NC=C3)NC4=CC=CC(=C4)CS(=O)(=O)NCCN(C)C

**PubChem CID:** 52920501

**CAS:** 1308672-74-3



# Temsirolimus



**Alt Names:** Torisel

**MW:**

**Brutto:** C<sub>56</sub>H<sub>87</sub>NO<sub>16</sub>

**Approved for clinical use:** Advanced Renal Cell Carcinoma

**Approval Jurisdiction:** 2007 FDA, EMA

**InChI:** InChI=1S/C56H87NO16/c1-33-17-13-12-14-18-34(2)45(68-9)29-41-22-20-39(7)56(67,73-41)51(63)52(64)57-24-16-15-19-42(57)53(65)71-46(30-43(60)35(3)26-38(6)49(62)50(70-11)48(61)37(5)25-33)36(4)27-40-21-23-44(47(28-40)69-10)72-54(66)55(8,31-58)32-59/h12-14,17-18,26,33,35-37,39-42,44-47,49-50,58-59,62,67H,15-16,19-25,27-32H2,1-11H3/b14-12+,17-13+,34-18+,38-26+/t33-,35-,36-,37-,39-,40+,41+,42+,44-,45+,46+,47-,49-,50+,56-/m1/s1

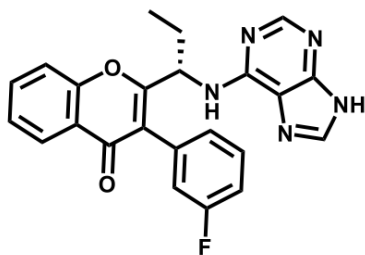
**InChI Key:** CBPNZQVSJQDFBE-FUXHJELOSA-N

**SMILES:** CC1CCC2CC(C(=CC=CC=CC(C(C(=O)C(C(C(=CC(C(=O)CC(OC(=O)C3CCCCN3C(=O)C(=O)C1(O2)O)C(C)CC4CCC(C(C4)OC)OC(=O)C(C)(CO)CO)C)C)O)OC)C)C)OC

**PubChem CID:** 6918289

**CAS:** 162635-04-3

# Tenalisib



**Alt Names:** RP6530, RP-6530

**MW:** 415.40

**Brutto:** C<sub>23</sub>H<sub>18</sub>FN<sub>5</sub>O<sub>2</sub>

**Approved for clinical use:** PTCL, Brest Cancer

**Approval Jurisdiction:** 2019 FDA

**InChI:** InChI=1S/C23H18FN5O2/c1-2-16(29-23-19-22(26-11-25-19)27-12-28-23)21-18(13-6-5-7-14(24)10-13)20(30)15-8-3-4-9-17(15)31-21/h3-12,16H,2H2,1H3,(H2,25,26,27,28,29)/t16-/m0/s1

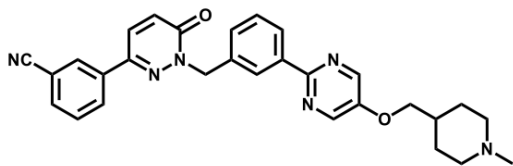
**InChI Key:** HDXDQPRPFRKGGKZ-INIZCTEOSA-N

**SMILES:** CCC(C1=C(C(=O)C2=CC=CC=C2O1)C3=CC(=CC=C3)F)NC4=NC=NC5=C4NC=N5

**PubChem CID:** 86291103

**CAS:** 1639417-53-0

# Tepotinib



**Alt Names:** EMD-1214063, EMD 1214063

**MW:** 492.60

**Brutto:** C<sub>29</sub>H<sub>28</sub>N<sub>6</sub>O<sub>2</sub>

**Approved for clinical use:** Metastatic NSCLC

**Approval Jurisdiction:** 2020 Japan 2021 FDA

**InChI:** InChI=1S/C29H28N6O2/c1-34-12-10-21(11-13-34)20-37-26-17-31-29(32-18-26)25-7-3-5-23(15-25)19-35-28(36)9-8-27(33-35)24-6-2-4-22(14-24)16-30/h2-9,14-15,17-18,21H,10-13,19-20H2,1H3

**InChI Key:** AHYMHWXQRWRBKT-UHFFFAOYSA-N

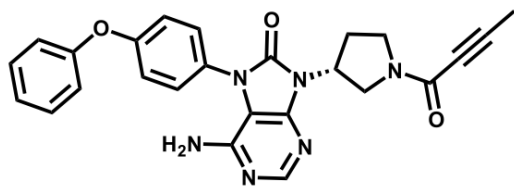
**SMILES:**

CN1CCC(CC1)COC2=CN=C(N=C2)C3=CC=CC(=C3)CN4C(=O)C=CC(=N4)C5=CC=CC(=C5)C#N

**PubChem CID:** 25171648

**CAS:** 1100598-32-0

# Tirabrutinib



**Alt Names:** ONO-4059, GS-4059

**MW:** 454.50

**Brutto:** C<sub>25</sub>H<sub>22</sub>N<sub>6</sub>O<sub>3</sub>

**Approved for clinical use:** Chronic Myelogenous Leukemia

**Approval Jurisdiction:** 2020 Japan

**InChI:** InChI=1S/C25H22N6O3/c1-2-6-21(32)29-14-13-18(15-29)31-24-22(23(26)27-16-28-24)30(25(31)33)17-9-11-20(12-10-17)34-19-7-4-3-5-8-19/h3-5,7-12,16,18H,13-15H2,1H3,(H2,26,27,28)/t18-/m1/s1

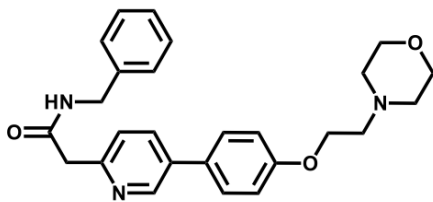
**InChI Key:** SEJLPXCPMNSRAM-GOSISDBHSA-N

**SMILES:** CC#CC(=O)N1CCC(C1)N2C3=NC=NC(=C3N(C2=O)C4=CC=C(C=C4)OC5=CC=CC=C5)N

**PubChem CID:** 54755438

**CAS:** 1351636-18-4

# Tirbanibulin



**Alt Names:** KX2-391, KX-01

**MW:** 431.50

**Brutto:** C<sub>26</sub>H<sub>29</sub>N<sub>3</sub>O<sub>3</sub>

**Approved for clinical use:** Actinic Keratosis

**Approval Jurisdiction:** 2020 FDA

**InChI:** InChI=1S/C26H29N3O3/c30-26(28-19-21-4-2-1-3-5-21)18-24-9-6-23(20-27-24)22-7-10-25(11-8-22)32-17-14-29-12-15-31-16-13-29/h1-11,20H,12-19H2,(H,28,30)

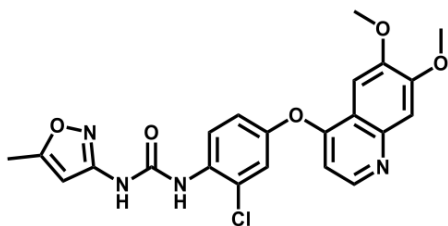
**InChI Key:** HUNGUWOZPQBXGX-UHFFFAOYSA-N

**SMILES:** C1COCCN1CCOC2=CC=C(C=C2)C3=CN=C(C=C3)CC(=O)NCC4=CC=CC=C4

**PubChem CID:** 23635314

**CAS:** 897016-82-9

# Tivozanib



**Alt Names:** AV-951, KRN-951

**MW:** 454.90

**Brutto:** C<sub>22</sub>H<sub>19</sub>ClN<sub>4</sub>O<sub>5</sub>

**Approved for clinical use:** Advanced RCC

**Approval Jurisdiction:** 2017 EMA

**InChI:** InChI=1S/C22H19ClN4O5/c1-12-8-21(27-32-12)26-22(28)25-16-5-4-13(9-15(16)23)31-18-6-7-24-17-11-20(30-3)19(29-2)10-14(17)18/h4-11H,1-3H3,(H2,25,26,27,28)

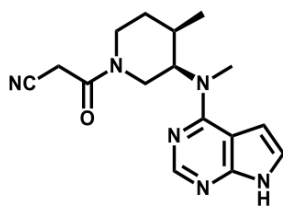
**InChI Key:** SPMVMDHWKHCIDT-UHFFFAOYSA-N

**SMILES:** CC1=CC(=NO1)NC(=O)NC2=C(C=C(C=C2)OC3=C4C=C(C(=CC4=NC=C3)OC)OC)Cl

**PubChem CID:** 9911830

**CAS:** 475108-18-0

# Tofacitinib



**Alt Names:** Tasocitinib

**MW:** 312.37

**Brutto:**

**Approved for clinical use:** Rheumatoid Arthritis

**Approval Jurisdiction:** 2012 FDA 2017 EMA

**InChI:** InChI=1S/C16H20N6O/c1-11-5-8-22(14(23)3-6-17)9-13(11)21(2)16-12-4-7-18-15(12)19-10-20-16/h4,7,10-11,13H,3,5,8-9H2,1-2H3,(H,18,19,20)/t11-,13+/m1/s1

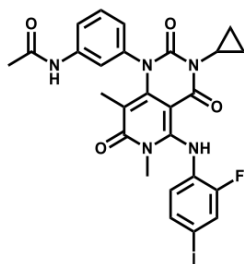
**InChI Key:** UJLAWZDWDVHWOW-YPMHNCESA-N

**SMILES:** CC1CCN(CC1N(C)C2=NC=NC3=C2C=CN3)C(=O)CC#N

**PubChem CID:** 9926791

**CAS:** 477600-75-2

# Trametinib



**Alt Names:** Mekinist, GSK1120212, GSK-1120212

**MW:** 615.40

**Brutto:** C<sub>26</sub>H<sub>23</sub>FIN<sub>5</sub>O<sub>4</sub>

**Approved for clinical use:** M-Melanoma With BRAFV600E

**Approval Jurisdiction:** 2013 FDA 2014 EMA

**InChI:** InChI=1S/C26H23FIN5O4/c1-13-22-21(23(31(3)24(13)35)30-20-10-7-15(28)11-19(20)27)25(36)33(17-8-9-17)26(37)32(22)18-6-4-5-16(12-18)29-14(2)34/h4-7,10-12,17,30H,8-9H2,1-3H3,(H,29,34)

**InChI Key:** LIRYPHYGHXZJBZ-UHFFFAOYSA-N

**SMILES:**

CC1=C2C(=C(N(C1=O)C)NC3=C(C=C(C=C3))F)C(=O)N(C(=O)N2C4=CC=CC(=C4)NC(=O)C)C5CC5

**PubChem CID:** 11707110

**CAS:** 871700-17-3



Trastuzumab

## Monoclonal antibody

**Alt Names:**

**MW:**

**Brutto:**

**Approved for clinical use:** EGFR Breast Cancer

**Approval Jurisdiction:** 1998 FDA 2000 EMA

**InChI:**

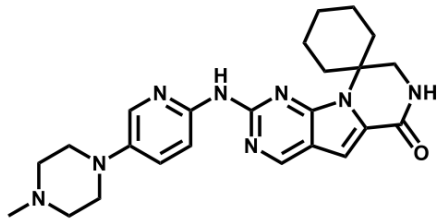
**InChI Key:**

**SMILES:**

**PubChem CID:**

**CAS:** 180288-69-1

Trilaciclib



**Alt Names:** G1T28, Cosela

**MW:** 446.50

**Brutto:** C<sub>24</sub>H<sub>30</sub>N<sub>8</sub>O

**Approved for clinical use:** SCLC Chemo Myelopreservation

**Approval Jurisdiction:** 2021 FDA

**InChI:** InChI=1S/C24H30N8O/c1-30-9-11-31(12-10-30)18-5-6-20(25-15-18)28-23-26-14-17-13-19-22(33)27-16-24(7-3-2-4-8-24)32(19)21(17)29-23/h5-6,13-15H,2-4,7-12,16H2,1H3,(H,27,33)(H,25,26,28,29)

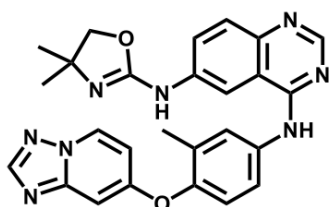
**InChI Key:** PDGKHKMBHVFCMG-UHFFFAOYSA-N

**SMILES:** CN1CCN(CC1)C2=CN=C(C=C2)NC3=NC=C4C=C5C(=O)NCC6(N5C4=N3)CCCCC6

**PubChem CID:** 68029831

**CAS:** 1374743-00-6

Tucatinib



**Alt Names:** Irbinitinib, ONT-380, Tukysa

**MW:** 480.50

**Brutto:** C<sub>26</sub>H<sub>24</sub>N<sub>8</sub>O<sub>2</sub>

**Approved for clinical use:** HER2-Positive Breast Cancer

**Approval Jurisdiction:** 2020 FDA 2021EMA

**InChI:** InChI=1S/C26H24N8O2/c1-16-10-17(5-7-22(16)36-19-8-9-34-23(12-19)28-15-30-34)31-24-20-11-18(4-6-21(20)27-14-29-24)32-25-33-26(2,3)13-35-25/h4-12,14-15H,13H2,1-3H3,(H,32,33)(H,27,29,31)

**InChI Key:** SDEAXTCZPQIFQM-UHFFFAOYSA-N

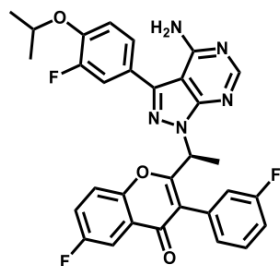
**SMILES:**

CC1=C(C=CC(=C1)NC2=NC=NC3=C2C=C(C=C3)NC4=NC(CO4)(C)C)OC5=CC6=NC=NN6C=C5

**PubChem CID:** 51039094

**CAS:** 937263-43-9

# Umbralisib



**Alt Names:** TGR-1202, rp-5264, TGR1202

**MW:** 571.50

**Brutto:** C<sub>31</sub>H<sub>24</sub>F<sub>3</sub>N<sub>5</sub>O<sub>3</sub>

**Approved for clinical use:** Marginal Zone Lymphoma

**Approval Jurisdiction:** 2019 FDA

**InChI:** InChI=1S/C31H24F3N5O3/c1-15(2)41-24-9-7-18(12-22(24)34)27-26-30(35)36-14-37-31(26)39(38-27)16(3)29-25(17-5-4-6-19(32)11-17)28(40)21-13-20(33)8-10-23(21)42-29/h4-16H,1-3H3,(H2,35,36,37)/t16-/m0/s1

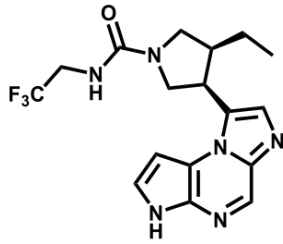
**InChI Key:** IUVCFHHAEHNCFT-INIZCTEOSA-N

**SMILES:** CC(C)OC1=C(C=C(C=C1)C2=NN(C3=NC=NC(=C23)N)C(C)C4=C(C(=O)C5=C(O4)C=CC(=C5)F)C6=CC(=CC=C6)F)F

**PubChem CID:** 72950888

**CAS:** 1532533-67-7

# Upadacitinib



**Alt Names:** ABT-494, Rinvoq

**MW:** 380.40

**Brutto:** C<sub>17</sub>H<sub>19</sub>F<sub>3</sub>N<sub>6</sub>O

**Approved for clinical use:** Rheumatoid Arthritis

**Approval Jurisdiction:** 2019 FDA 2019 EMA

**InChI:** InChI=1S/C17H19F3N6O/c1-2-10-7-25(16(27)24-9-17(18,19)20)8-11(10)13-5-22-14-6-23-15-12(26(13)14)3-4-21-15/h3-6,10-11,21H,2,7-9H2,1H3,(H,24,27)/t10-,11+/m1/s1

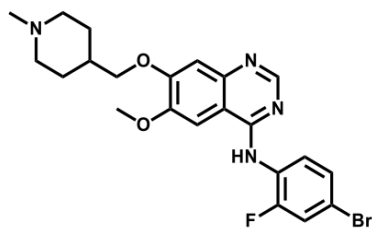
**InChI Key:** WYQFJHHDOKWSHR-MNOVXSKESA-N

**SMILES:** CCC1CN(CC1C2=CN=C3N2C4=C(NC=C4)N=C3)C(=O)NCC(F)(F)F

**PubChem CID:** 58557659

**CAS:** 1310726-60-3

# Vandetanib



**Alt Names:** Zactima, Caprelsa

**MW:**

**Brutto:** C<sub>22</sub>H<sub>24</sub>BrFN<sub>4</sub>O<sub>2</sub>

**Approved for clinical use:** Thyroid Cancer

**Approval Jurisdiction:** 2011 FDA

**InChI:** InChI=1S/C22H24BrFN4O2/c1-28-7-5-14(6-8-28)12-30-21-11-19-16(10-20(21)29-2)22(26-13-25-19)27-18-4-3-15(23)9-17(18)24/h3-4,9-11,13-14H,5-8,12H2,1-2H3,(H,25,26,27)

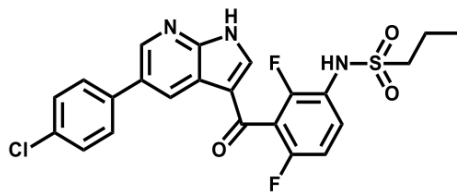
**InChI Key:** UHTHHESEBZOYNR-UHFFFAOYSA-N

**SMILES:** CN1CCC(CC1)COC2=C(C=C3C(=C2)N=CN=C3NC4=C(C=C(C=C4)Br)F)OC

**PubChem CID:** 3081361

**CAS:** 443913-73-3

# Vemurafenib



**Alt Names:** Vemurafenib , Zelboraf , PLX4032, PLX-4032, Zelboraf, PLX 4032

**MW:** 489.92

**Brutto:** C<sub>23</sub>H<sub>18</sub>ClF<sub>2</sub>N<sub>3</sub>O<sub>3</sub>S

**Approved for clinical use:** Metastatic Melanoma BRAFV600E

**Approval Jurisdiction:** 2011 FDA, 2012 EMA

**InChI:** InChI=1S/C23H18ClF2N3O3S/c1-2-9-33(31,32)29-19-8-7-18(25)20(21(19)26)22(30)17-12-28-23-16(17)10-14(11-27-23)13-3-5-15(24)6-4-13/h3-8,10-12,29H,2,9H2,1H3,(H,27,28)

**InChI Key:** GPXBXXGIAQBQNI-UHFFFAOYSA-N

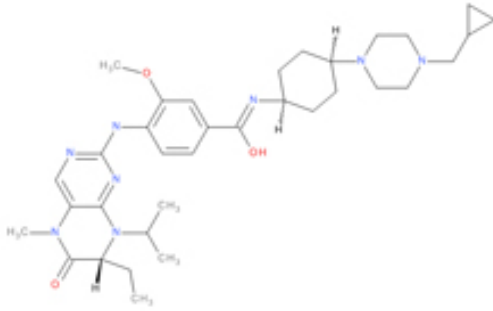
**SMILES:**

CCCS(=O)(=O)NC1=C(C(=C(C=C1)F)C(=O)C2=CNC3=NC=C(C=C23)C4=CC=C(C=C4)Cl)F

**PubChem CID:** 42611257

**CAS:** 1029872-54-5

# Volasertib



**Alt Names:** BI6727, BI 6727, BI-6727

**MW:** 618.81

**Brutto:** C<sub>34</sub>H<sub>50</sub>N<sub>8</sub>O<sub>3</sub>

**Approved for clinical use:** Acute Myeloid Leukemia

**Approval Jurisdiction:** 2014 FDA

**InChI:** InChI=1S/C34H50N8O3/c1-6-28-33(44)39(4)29-20-35-34(38-31(29)42(28)22(2)3)37-27-14-9-24(19-30(27)45-5)32(43)36-25-10-12-26(13-11-25)41-17-15-40(16-18-41)21-23-7-8-23/h9,14,19-20,22-23,25-26,28H,6-8,10-13,15-18,21H2,1-5H3,(H,36,43)(H,35,37,38)/t25?,26?,28-/m1/s1

**InChI Key:** SXNJFOWDRLKDSF-XKHVUIRMSA-N

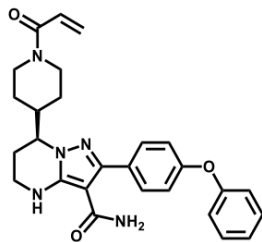
**SMILES:** CCC1C(=O)N(C2=CN=C(N=C2N1C(C)C)NC3=C(C=C(C=C3)C(=O)NC4CCC(CC4)N5CCN(CC5)CC6CC6)OC)C

**PubChem CID:** 10461508

**CAS:** 755038-65-4



# Zanubrutinib



**Alt Names:** Brukinsa, BGB-3111

**MW:** 471.50

**Brutto:** C<sub>27</sub>H<sub>29</sub>N<sub>5</sub>O<sub>3</sub>

**Approved for clinical use:** Mantle Cell Lymphoma

**Approval Jurisdiction:** 2019 FDA

**InChI:** InChI=1S/C27H29N5O3/c1-2-23(33)31-16-13-18(14-17-31)22-12-15-29-27-24(26(28)34)25(30-32(22)27)19-8-10-21(11-9-19)35-20-6-4-3-5-7-20/h2-11,18,22,29H,1,12-17H2,(H2,28,34)/t22-/m0/s1

**InChI Key:** RNOAOAWBMHREKO-QFIPXVFZSA-N

**SMILES:**

C=CC(=O)N1CCC(CC1)C2CCNC3=C(C(=NN23)C4=CC=C(C=C4)OC5=CC=CC=C5)C(=O)N

**PubChem CID:** 135565884

**CAS:** 1691249-45-2