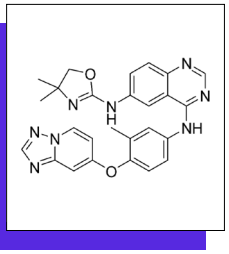
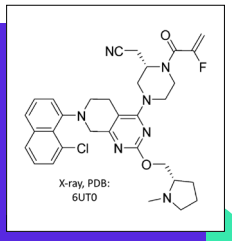
Small Molecules of the Month

April 2020
drughunter.com



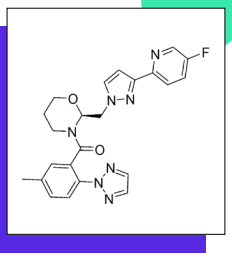
tucatinib

EGFR-sparing HER2 kinase inhibitor
Approved in met. HER2+ BC incl. w/ brain met.
From optimization of known TKIs
Mol. Cancer Ther., Apr. 1, 2020
Array / Cascadian Tx / Seattle Genetics



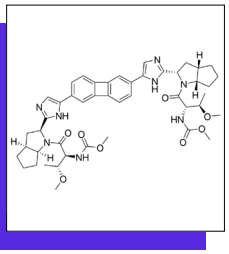
MRTX849

Covalent KRASG12C inhibitor
In clinical development for KRASG12C+ cancers
From optimization of known starting point
J. Med. Chem., Apr. 6, 2020
Array / Mirati Therapeutics



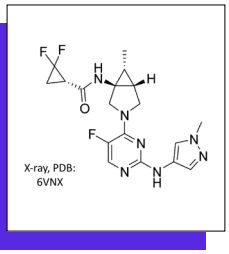
ORN0829

Short $T_{½}$ dual orexin 1/2 receptor antagonist
In clinical dev. for insomnia (Ph. II)
From ligand-based drug design
Bioorg. Med. Chem., Apr. 11, 2020
Taisho Pharmaceutical Co., Saitama, JP



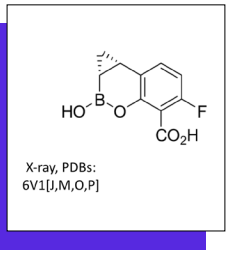
GSK2818713

Broad geno. HCV NS5A repl. complex inhibitor
Low Cl and orally available in higher species
From rational design from known ligand
J. Med. Chem., Apr. 23, 2020
GlaxoSmithKline, Research Triange Park, NC



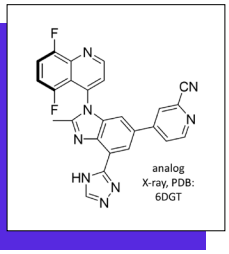
"Compound 19"

JAK1/TYK2-selective dual kinase inhibitor
Oral activity in arthritis model
From SBDD of prior internal matter
Bioorg. Med. Chem. Lett., Mar. 31, 2020
Pfizer, Cambridge, MA and Groton, CT



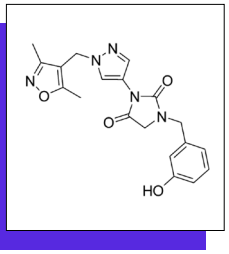
QPX7728

Serine and metallo-β-lactamase inhibitor
Oral activity in resistant infection model
From optimization of literature starting point
J. Med. Chem., Apr. 2, 2020
Qpex Biopharma, San Diego, CA



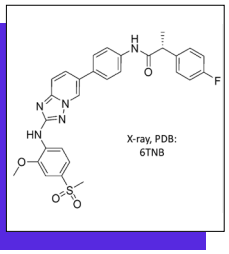
"Compound (P)-14"

Atropisomeric PI3Kβ-selective inhibitor
Off-target tox. in higher species, discontinued
From rational design of known starting point
J. Med. Chem., Apr. 15, 2020
Gilead Sciences, Seattle, WA + Foster City, CA



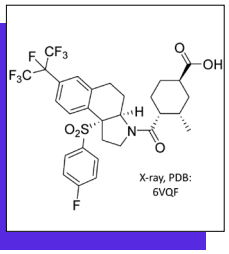
S6821

Potent and selective TAS2R8 GPCR antagonist
Approved non-systemic bitter taste blocker
From 200k cmpd cell-based screen and opt.
J. Med. Chem., Apr. 24, 2020
Firmenich SA, San Diego, CA



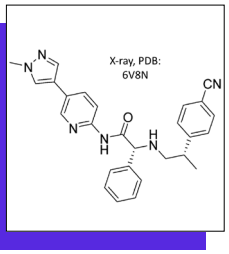
BAY1161909

Pro-mitotic selective MPS1 kinase inhibitor
Dev. paused for 2nd candidate (BAY1217389)
From 2M cmpd biochem. HTS and SBDD
J. Med. Chem., Apr. 27, 2020
Bayer AG, Berlin, DE



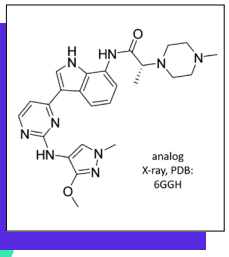
BMS-986251

Selective RORγt inverse agonist
Entered clinical dev. (psoriasis), discontinued
From HTS and SBDD
ACS Med. Chem. Lett., Apr. 10, 2020
Bristol Myers Squibb, Princeton, NJ



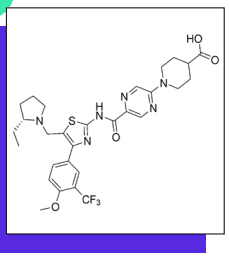
CPI-1612

Bioavailable EP300/CBP HAT inhibitor
Brain penetrant, orally efficacious in xeno.
From HTS and SBDD
ACS Med. Chem. Lett., Apr. 27, 2020
Constellation Pharma., Cambridge, MA



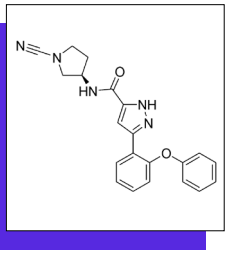
AZD4205

JAK1-selective kinase inhibitor
In clinical development for cancer
From HTS and SBDD of promiscuous hit
J. Med. Chem., Apr. 28, 2020
AstraZeneca, Waltham, MA



"Compound 9"

M3-selective positive allosteric modulator
Oral bioavailability in rodent
From HTS and optimization
Bioorg. Med. Chem. Apr. 23, 2020
Astellas Pharma, Tsukuba, JP



FT385

USP30-sel. covalent DUB enzyme inhibitor
Active in cells and selective vs. DUB panel
Undisclosed, related to lit. DUB inhibitors
BioRXiV, Apr. 20, 2020
FORMA Therapeutics / U. Liverpool

drug hunter