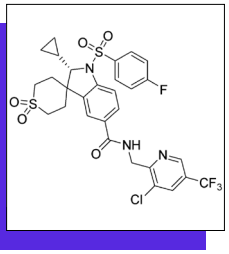
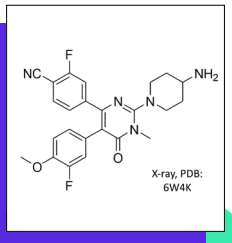
Small Molecules of the Month

October 2020
drughunter.com



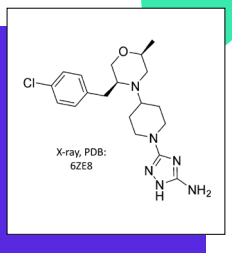
BAY 1214784

Oral hGnRH-R hormone receptor antagonist
To treat of uterine fibroids, Ph. I completed
From cell-based 2.5M cmpd HTS + opt.
J. Med. Chem., Oct. 22, 2020 issue
Bayer AG, Berlin, DE



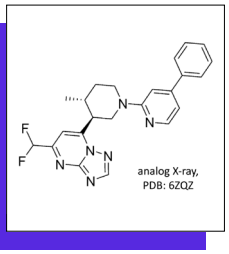
CC-90011

Selective, reversible LSD1 inhibitor
<100 mg orally QW, in Ph. II for 1L ES-SCLC
From 300k+ cmpd HTS, SBDD + opt.
J. Med. Chem., Oct. 9, 2020
Celgene/Bristol Myers Squibb, San Diego, CA



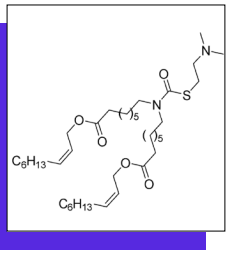
OATD-01

Oral, first-in-class CHIT1/AMCase chitinase inh.
For sarcoidosis/lung fibrosis, Ph. Ib complete
From opt. of literature molecule
J. Med. Chem., Oct. 20, 2020
OncoArendi Therapeutics SA, Warsaw, PL



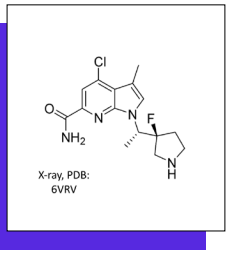
"compound 46"

Oral sel. PDE2A phosphodiesterase inhibitor
For cognition, target engagement in brain
From HTS, SBDD, and FEP calculations
J. Med. Chem., Oct. 26, 2020
Janssen Pharmaceutica NV, Beerse, BE



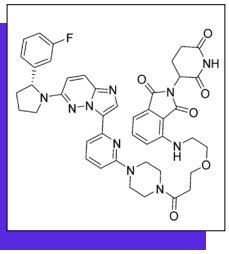
"lipid 10a"

Property-tunable lipid for RNA drug delivery
For lipid nanoparticle delivery of mRNA/siRNA
From empirical optimization of siRNA activity
J. Med. Chem., Oct. 29, 2020
Arcturus Therapeutics, San Diego, CA



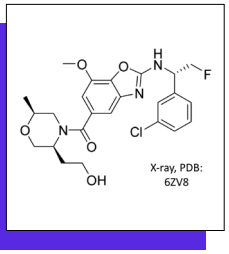
"compound 27"

Potent pan-PIM kinase inhibitor
Oral PD and efficacy in xenograft model
From SBDD of prior lead
Bioorg. Med. Chem. Lett., Oct. 14, 2020
Sanofi, Waltham/Cambridge, MA



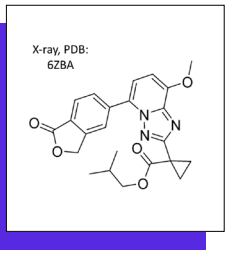
CG428

CRBN-based TRK kinase fusion prot. degrader
Degrad. of mult. TRK fusions (e.g. TPM3-TRKA)
From functionalization of lit. TRK inhibitor
J. Med. Chem., Oct. 15, 2020
Cullgen Inc., San Diego, CA / Shanghai, CN



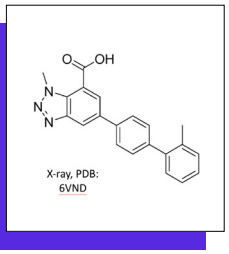
BAY 1217224

Oral non-prodrug thrombin (FIIa) inhibitor
To treat thrombosis, oral bioavailability in HV
From internal library HTS, SBDD, opt. vs. PXR
J. Med. Chem., Oct. 27, 2020
Bayer AG, Wuppertal, DE



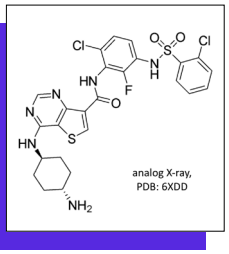
LEO 39652

"Dual-soft" topical PDE4 inhibitor soft drug
To treat atopic dermatitis, lack of PD in Ph. I
From metab. opt. of prev. discont. candidate
J. Med. Chem., Oct. 15, 2020
LEO Pharma, Ballerup, DK



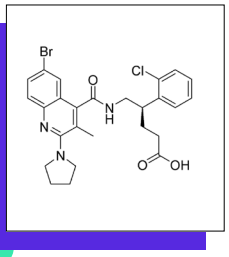
AG-636

Dihydroorotate dehydrogenase inhibitor
In Ph. I for RR-lymphoma
From opt. of literature molecule
Mol. Cancer Ther., Oct. 20, 2020
Agios Pharmaceuticals, Cambridge, MA



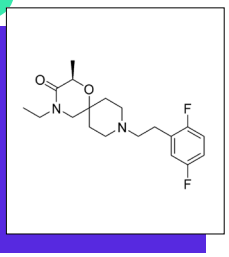
"compound 25"

IRE1α kinase-binding endonuclease inhibitor
Unfolded prot. response disruption for MM
From kinase library screen and SBDD
ACS Med. Chem. Lett, Oct. 16, 2020
Genentech, So. San Francisco, CA / Paraza, QC



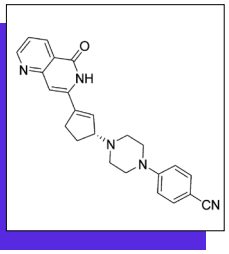
BAY-6672

Oral prostaglandin F receptor GCPR antagonist
To treat IPF, in vivo efficacy in fibrosis model
From ~3M cmpd cell-based HTS and opt.
J. Med. Chem., Oct. 22, 2020 issue
Bayer AG, Wuppertal, DE



"EST73502"

Dual μ-opioid receptor agonist, σ_1 antagonist
Oral analgesia w/ reduced opioid AEs, in Ph. I
From literature cmpd pharmacophore merging
J. Med. Chem., Oct. 16, 2020
ESTEVE Pharmaceuticals SA, Barcelona, ES



"compound 34"

Oral PARP1-selective polymerase inhibitor
Oral efficacy in BRCA1 mutant xenograft
From scaffold hopping from lit. PARP1/2 inh.
Bioorg. Med. Chem., Oct. 6, 2020
Lupin Ltd., Pune, IN

drug hunter