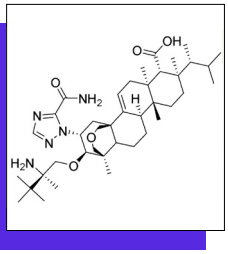
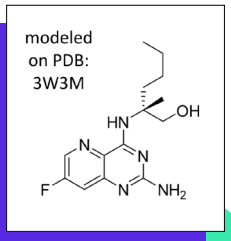
Small Molecules of the Month

June 2020
drughunter.com



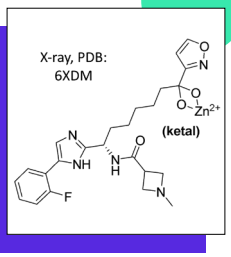
MK-5204

Orally active β-1,3-glucan synthesis inhibitor
Eff. in fungal infect. model, discont. for alt.
From semisynthetic mod. of enfumafungin
Bioorg. Med. Chem. Lett., Jun. 19, 2020
Merck & Co., Kenilworth, NJ / Scynexis



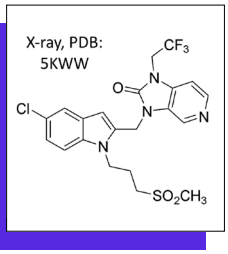
GS-9688 (selgantolimod)

Pre-systemic oral toll-like receptor 8 agonist
In multiple Ph. II studies for chron. hep. B
From optimization of lit. dual TLR7/8 agonists
J. Med. Chem., Jun. 3, 2020
Gilead Sciences, Foster City, CA



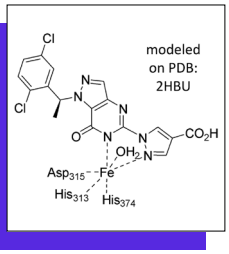
"Compound 10"

Class I sel. histone deacetylase (HDAC) inhib.
In vitro HIV reactivation for HIV eradication
From structure-based design of prior ligand
ACS Med. Chem. Lett., Jun. 22, 2020
Merck & Co., Kenilworth, NJ / West Point



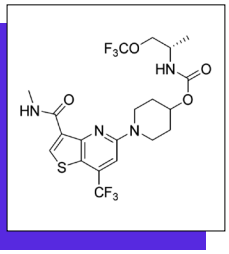
JNJ-53718678

Potent, oral fusion inhibitor of RSV virus
Efficacious in Ph. 2a challenge study in HV
From scaffold hop from known inhibitor
J. Med. Chem., Jun. 15, 2020
Janssen Pharmaceutica NV, Beerse, BE



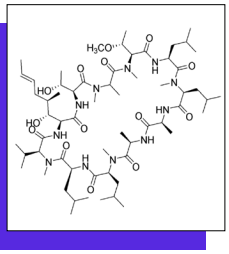
"Compound 19"

HIF prolyl hydroxylase domain inhibitor
Orally active in anemia model
From structure-based scaffold hop and opt.
ACS Med. Chem. Lett., Jun. 4, 2020
Mitsubishi Tanabe Pharma, Yokohama, JP



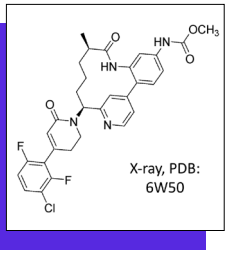
"Compound 19"

Brain pen. UGT8 galactosyltransferase inh.
Excellent oral PK/PD in brain model
From 30k cmpd cellular MTS and optimization
J. Med. Chem., Jun. 26, 2020
Sanofi R&D, Waltham, MA



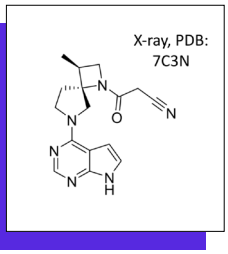
ASP5286

Non-immunosuppressive cyclophilin inhibitor
Oral activity in humanized HCV model
From semisynthetic deriv. of FR901459
Bioorg. Med. Chem. Lett., Jun. 2, 2020
Astellas Pharma, Ibaraki, JP



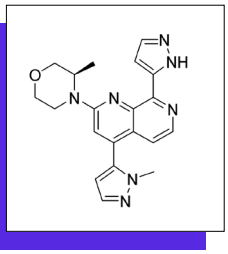
"Compound 6f"

Selective factor XIa serine protease inhibitor
Oral in higher species, eff. in thrombosis model
From PK optimization of prior series
J. Med. Chem., May 26, 2020
Bristol Myers Squibb, Princeton, NJ



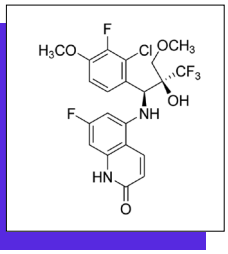
JTE-052 (delgocitinib)

Topical Janus kinase (JAK) family inhibitor
Approved for atopic dermatitis in JP
From scaffold hop from known JAK inhibitor
J. Med. Chem., Jun. 8, 2020
Japan Tobacco, Osaka, JP



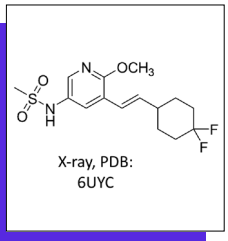
BAY 1895344

Selective oral ATR kinase inhibitor
In Ph. I for adv. solid tumors and lymphomas
From HTS and modeling on PI3Kg structure
J. Med. Chem., Jun. 5, 2020
Bayer AG, Berlin, DE



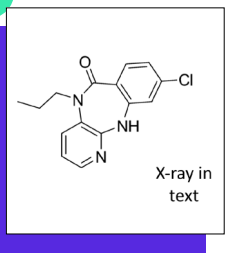
BAY 1003803

Non-steroid glucocorticoid receptor modulator
Completed Ph. I as topical agent in psoriasis
From optimization of prior lead
Bioorg. Med. Chem. Lett., Jun. 1, 2020
Bayer AG, Berlin, DE / AstraZeneca



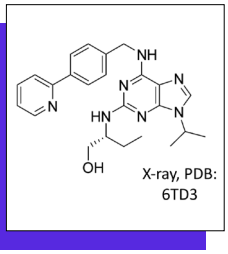
"Compound 2"

TEAD transcription factor lipidation modulator
Orally active in xenograft model
From 1M cmpd biochemical HTS and opt.
Cell Reports, Jun. 23, 2020
Genentech, South San Francisco, CA



BI-0115

Selective LOX-1 lectin inhibitor/tetramerizer
In vitro activity and co-crystallized in tetramer
From 1M cmpd cellular HTS
Commun. Chem., Jun. 10, 2020
Boehringer Ingelheim, Biberach, DE



(R)-CR8

CDK inhib. and mol. glue degrader of cyclin K
Selective degradation of cyclin K in cells
From characterization of 4.5k known cmpds
Nature, Jun. 3, 2020
Broad Institute / Friedrich Miescher Institute

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