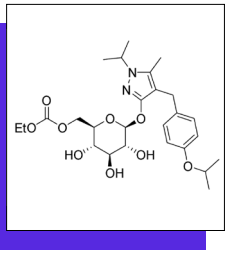
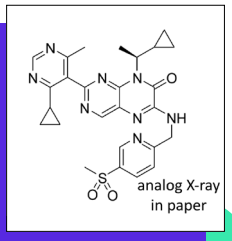
Small Molecules of the Month

January 2021
drughunter.com



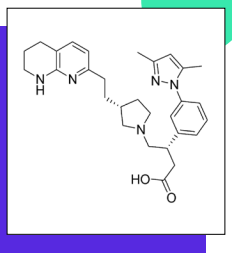
remogliflozin etabonate

SGLT1-sparing oral SGLT2 inhibitor prodrug
Launched in India for diabetes, 100 mg BID
From mouse urine drug metabolite and opt.
Bioorg. Med. Chem., Jan. 22, 2021
Kissei Pharma / Toho University, JP



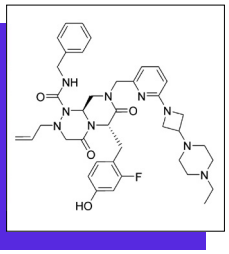
BI 730357

Oral RORγ nuclear receptor antagonist
On-going Ph. II for psoriasis (QD dosing)
50k cmpd high-conc. frag. screen + scaff. hop
ACS Med. Chem. Lett., Jan. 5, 2021
Boehringer Ingelheim, Ridgefield, CT



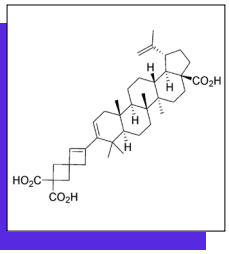
GSK 3008348 ("cmpd 1")

αvβ6 integrin inhibitor + lysosomal degrader
In vitro degradation, Ph. I completed, discont.
Derived from prior integrin inhibitors
J. Pharmacol. Exp. Ther., Jan. 26, 2021
GlaxoSmithKline, Stevenage, UK



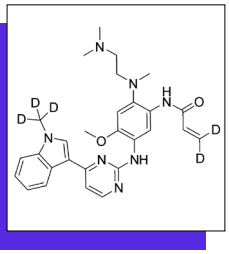
E7386

Oral, selective β-catenin/CBP PPI inhibitor
Synergy w/ PD-1i in model, in Ph.I for cancer
Opt. of prior peptidomimetic candidate
Cancer Res., Jan. 6, 2021
Eisai Co., Ltd., Tsukuba, JP



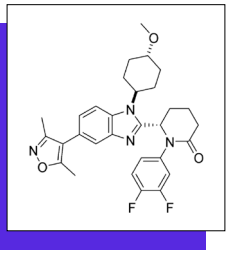
"compound 16"

Nanomolar HIV-1 maturation inhibitor
Interesting structure
Derivative of GSK3532795/BMS955176
Bioorg. Med. Chem. Lett., Jan. 26, 2021
Bristol Myers Squibb, CT + NJ



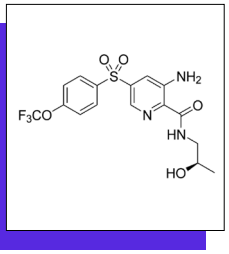
dosimertinib

Deuterated covalent mut. EGFR inhibitor
Wider TI in model, Ph. I in China
Deuteration reduces less sel. metabolite
J. Med. Chem., Jan. 18, 2021
ZZU / HNU / Henan Genuine Biotech Co., CN



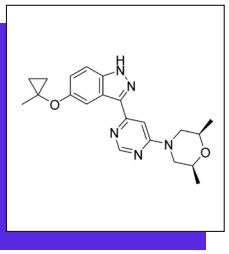
CCS1477

p300/CBP bromodomain inhibitor
PD observed in serial biopsies from Ph.I
50 mg QD, 3-d-on-4-off; origin not discussed
Cancer Discovery, Jan. 11, 2021
ICR / Royal Marsden / CellCentric, UK



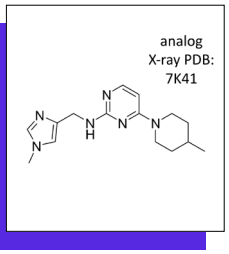
GLPG2451

Oral CFTR ABC transporter potentiator
Ph. II for cystic fibrosis (5-80 mg QD), discont.
Similarity screen of 589 cmpds + scaffold hop
J. Med. Chem., Jan. 5, 2021
Galapagos NV, Mechelen, BE



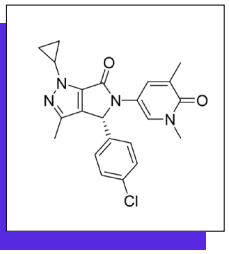
MLi-2

Oral, brain-penetrant LRRK2 kinase inhibitor
Recapitulated LRRK2 lung tox. in model
Discovery details manuscript in preparation
J. Pharmacol. Exp. Ther., Jan. 28, 2021
Merck & Co., Inc., Boston, MA



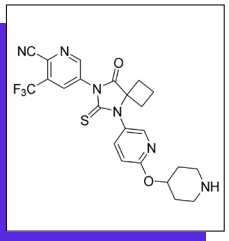
"compound 5i"

Oral, brain-penetrant O-GlcNAcase (OGA) inh.
Structurally distinct in vivo tool
From virtual screen of 100k cmpd, testing 2681
J. Med. Chem., Jan. 6, 2021
Takeda Pharmaceutical, Fujisawa, JP



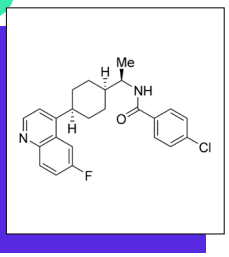
NVS-BET-1

BRD4 (BD1/2) BET bromodomain inhibitor
Wound-heal. at 1 mpk QD, bell-shaped pharm.
From phenotypic screen (MDM2 inhibitor hit)
Nat. Chem. Biol., Jan. 18, 2021
Novartis (NIBR), Basel, CH



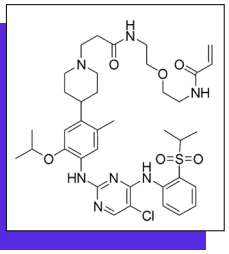
JNJ-63576253 / TRC-253

Oral WT and F877L mut. AR inhibitor
Completed Ph. I/II trial in mCPRC
No hepatotox. vs. bioactivated prior lead
J. Med. Chem., Jan. 20, 2021
Janssen R&D, Spring House, PA



BMS-986242

Oral IDO1 inhibitor
Clinical candidate in Ph. I/II combo for cancer
Reversed amide of linrodostat
ACS Med. Chem. Lett., Jan. 28, 2021
Bristol Myers Squibb, Lawrence Township, NJ



Con B-1

Covalent inh. of remote ALK kinase cysteine
Thought-provoking proposed MoA
From ceritinib and linker opt.
J. Med. Chem., Jan. 20, 2021
Sichuan University / Tsinghua University, CN

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