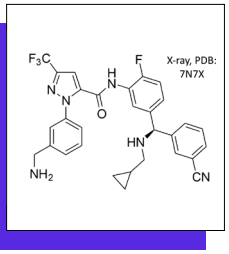
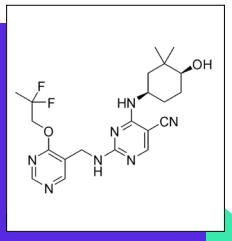
Small Molecules of the Month

August 2021
drughunter.com



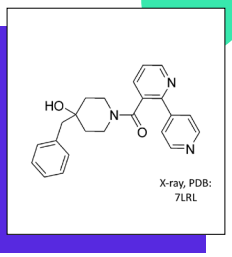
berotralstsat | kallikrein

Oral plasma kallikrein serine protease inhibitor
Approved for prevention of HAE attacks
From structure-based drug design
Journal of Medicinal Chemistry
BioCryst, Birmingham, AL, USA



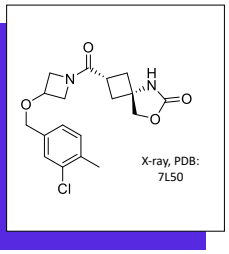
CC-90005 | PKCθ

Oral, selective PKCθ kinase inhibitor
Ph. I candidate for Psoriasis
From screen of internal library and SBDD
Journal of Medicinal Chemistry
Celgene/BMS, San Diego, CA, USA



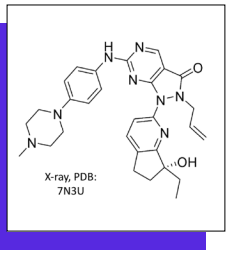
soticlestat | CH24H

Brain-penetrant CH24H inhibitor
Ph. 2 for epilepsies (up to 300 mg PO QD)
From SBDD
Journal of Medicinal Chemistry
Takeda, Fujisawa, Japan



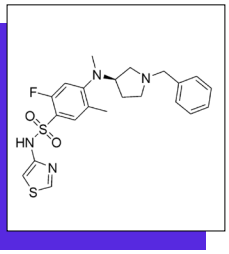
"compound 4f" | MAGL

Oral, brain-penetrant, reversible MAGL inh.
in vivo PK/PD in CNS (0.3-10 mpk PO)
from HTS and SBDD
Journal of Medicinal Chemistry
Takeda, Fujisawa, Japan



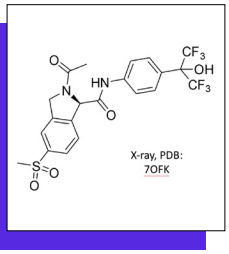
ZN-c3 | Wee1

Selective oral Wee1 kinase inh. (300 mg QD)
Ph. II candidate for uterine serous carcinoma
From literature starting point
Journal of Medicinal Chemistry
Zentalis Pharmaceuticals, San Diego, CA, USA



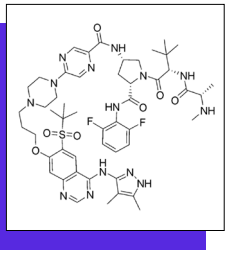
NBI-921352 | NaV1.6

Highly selective NaV1.6 sodium channel inh.
Entering Ph. II for seizures (100 mg TID)
Arylsulfonamide class
bioRxiv
Xenon Pharmaceuticals, Burnaby, Canada



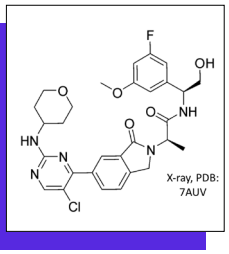
AZD0284 | RORC2

Oral RORC2 inverse agonist for psoriasis
100 mg PO BID, Ph. I term. due to preclin. data
From opt. of lit. inverse agonist
Journal of Medicinal Chemistry
AstraZeneca, Gothenburg, Sweden



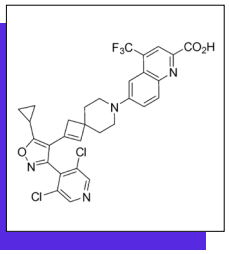
"compound 20" | RIPK2

Long-acting RIPK2 degrader (SC admin.)
In vivo degradation of RIPK2 over 60 days
IAP binder linked to RIPK2 binder
Journal of Medicinal Chemistry
GlaxoSmithKline, Stevenage, UK



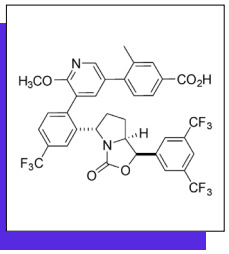
ASTX029 | ERK1/2

Oral ERK1/2 kinase and phosphorylation inhib.
Ph. 1/2 candidate for solid tumors
from SBDD from prior lead
Journal of Medicinal Chemistry
Astex Pharmaceuticals, Cambridge, UK



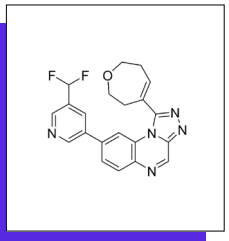
BMS-986318 | FXR

Oral FXR agonist for NASH
Robust in vivo PD, phase I HV study withdrawn
From prior FXR agonists
ACS Med. Chem. Lett
Bristol Myers Squibb, Princeton, NJ, USA



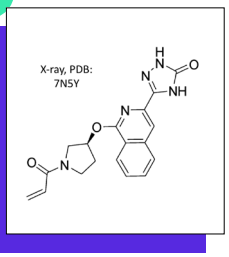
MK-8262 | CETP

Potential best-in-class CETP inh. (<1 mg QD)
Completed Ph. I in HV; discont. as backup
From anacetrapib
Journal of Medicinal Chemistry
Merck & Co., Kenilworth, NJ, USA



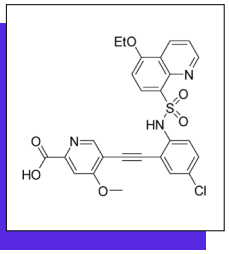
BAY-8400 | DNA-PK

Oral selective DNA-PK kinase inhibitor
Synergy with radiotherapy in model
From library screen
Journal of Medicinal Chemistry
Bayer AG, Berlin, Germany



TAK-020 | BTK

Oral covalent BTK inhibitor
>80% BTK occupancy <5 mg (Ph. I dose esc.)
From fragment-based screen of 11k cmpds
Journal of Medicinal Chemistry
Takeda, San Diego, CA, USA



"compound 18n" | MCT4

Monocarboxylate transporter 4 inhibitor
In vivo PD but limited eff. in xenograft model
From cell-based screen and opt.
Journal of Medicinal Chemistry
Merck Healthcare KGaA, Darmstadt, Germany

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