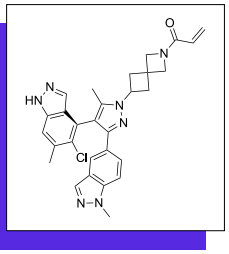
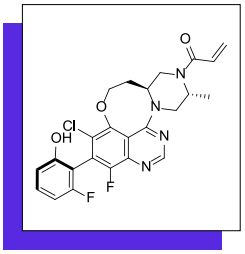
Small Molecules of the Month

April 2022
drughunter.com



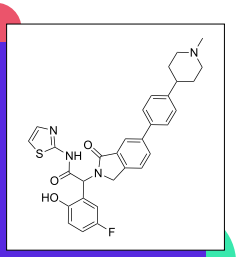
JDQ443 | KRAS^{G12C}

oral KRAS^{G12C} inhibitor
Ph. III candidate for NSCLC
from de novo SBDD in SWII pocket
Cancer Discov.
Novartis, Basel, CH



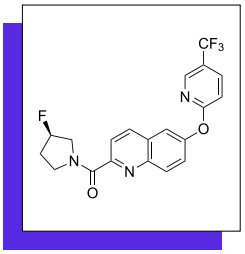
AZD4625 | KRAS^{G12C}

oral KRAS^{G12C} inhibitor
oral efficacy in xenograft mice
from literature starting point and SBDD
J. Med. Chem.
AstraZeneca, Cambridge, UK



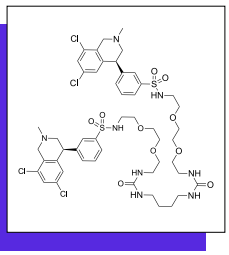
JBJ-09-063 | EGFR

allosteric mutant-EGFR inhibitor
in vivo efficacy in osimertinib-resistant xenograft models
from opt. of prev. disclosed EGFR inhibitor
Nat. Cancer
Dana-Farber Cancer Institute, Boston, MA



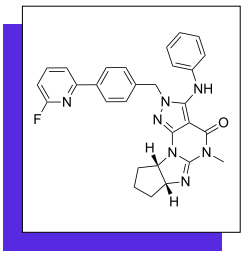
ABBV-318 | NaV1.7/1.8

oral CNS-penetrant Nav1.7/1.8 blocker
in vivo efficacy in rodent pain models
electrophysiology-based HTS and opt.
Bioorg. Med. Chem.
AbbVie, North Chicago, IL



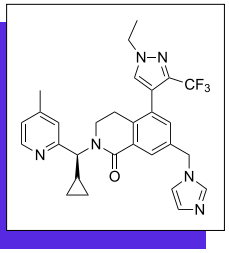
tenapanor | NHE3

oral gut-restricted Na+/H+ exchanger inhibitor
FDA-approved IBS treatment
from literature starting point and opt
ACS Med. Chem. Lett.
Ardelyx Inc., Fremont, CA/Waltham, MA



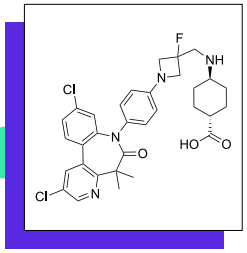
lenrispodun (ITI-214) | PDE1

oral, CNS-penetrant, picomolar PDE1 inhibitor
Ph. I/II in neurology and heart failure
from literature starting point, LBDD and SBDD
Neuropsychopharmacology
Intra-Cellular Therapies, New York, NY



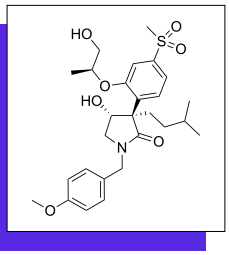
compound 41 | WDR5

oral WDR5 inhibitor
pM Ki, nanomolar in cells
from FBDD, SBDD, and PK opt.
J. Med. Chem.
Vanderbilt University School of Medicine, Nashville, TN



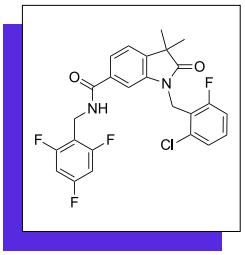
DS69910557 | hPTHR1

oral hPTHR1 GPCR antagonist
calcium-lowering activity in rodent
scaffold-hopping from lit. starting point
Bioorg. Med. Chem.
Daiichi Sankyo, Tokyo, JP



compound 14 | HIV-1 protease

potent HIV-1 protease inhibitor
in vitro activity (IC_{50}= 0.0071 µM, EC_{50}= 0.86 µM)
from "pocket-to-lead" virtual screen and SBDD
J. Med. Chem.
Shionogi, Osaka, JP



compound 53 | STING

non-nucleotide STING agonist
novel mechanism for STING activation
from micromolar HTS hit
Nature
University of Texas Southwestern Medica Center, Dallas, TX