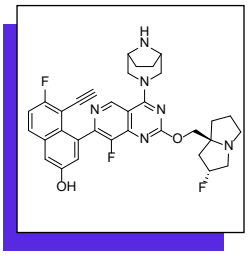
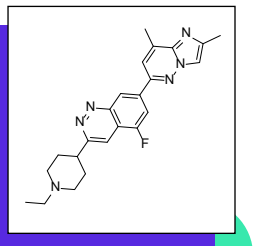
Small Molecules of the Month

December 2021
drughunter.com



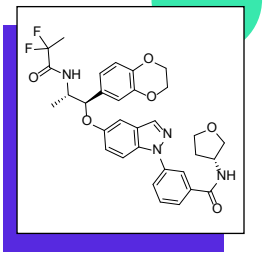
MRTX1133 | KRAS^{G12D}

reversible KRAS^{G12D} inhibitor
preclinical efficacy in cancer model
from SBDD around KRAS^{G12C} inhibitor
Journal of Medicinal Chemistry
Mirati Therapeutics, San Diego, CA



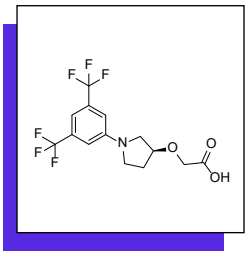
HTT-D3 | HTT

HTT splicing modulator
PD in Huntington's disease model
from HTS and optimization
Nature Communications
PTC Therapeutics, So. Plainfield, NJ



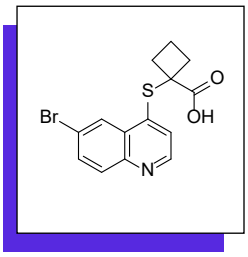
velsecorat | GR

glucocorticoid receptor modulator
phase II candidate for asthma
from soft drug PK optimization
Drug Metabolism and Disposition
AstraZeneca, Gothenburg, SE



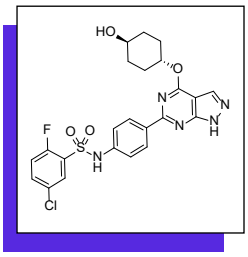
compound 43b | RBP4

RBP4 reducer targeting RBP4/TTR PPI
preclinical, in vivo RBP4 reduction
from HTS and optimization
Bioorganic and Medicinal Chemistry
Takeda, Fujisawa, JP



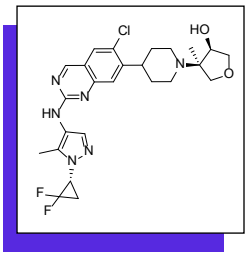
HR11303 | URAT1

human uric acid transporter inhibitor
phase III candidate for hyperuricemia and gout
from pharmacophore-based lead generation
Drug Metabolism and Disposition
Jiangsu Hengrui Medicine Co., Shanghai, CN



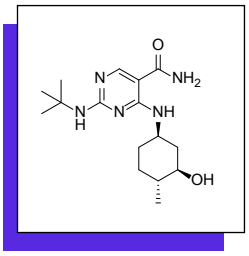
compound 17a | SGK1

SGK1 kinase inhibitor
preclinical activity in osteoarthritis explant model
from DFG-out virtual screening, SBDD and MPO
Journal of Medicinal Chemistry
Sanofi, Frankfurt am Main, DE



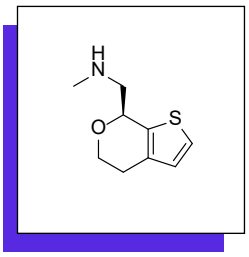
compound 24 | LRRK2

LRRK2 kinase inhibitor
preclinical, brain-penetrant
from rational HTL and structure-guided opt.
Journal of Medicinal Chemistry
Merck & Co., Boston, MA



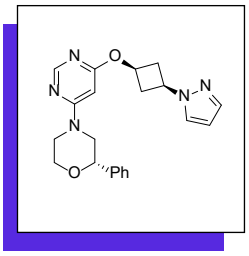
CC-90001 | JNK2

oral JNK2 kinase inhibitor
Ph. II candidate for pulmonary fibrosis
from HTS and SBDD
Journal of Medicinal Chemistry
Celgene (Bristol Myers Squibb), San Diego, CA



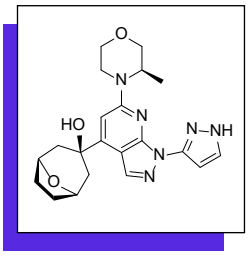
ulotaront | TAAR1

TAAR1 GPCR agonist
phase III candidate for schizophrenia
from in vivo phenotypic screening
ACS Medicinal Chemistry Letters
Sunovion Pharmaceuticals, Marlborough, MA



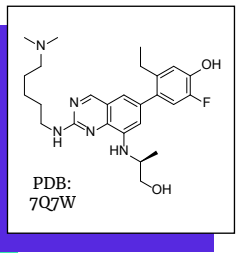
compound 22 | ELOVL1

ELOVL1 fatty acid elongase inhibitor
on-target toxicity suggested
from HTS and property-based optimization
Journal of Medicinal Chemistry
Vertex, Boston, MA



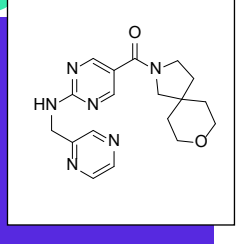
RP-3500 | ATR

ATR kinase inhibitor
phase I/IIa candidate for advanced solid tumors
from lipid-kinase inhibitor scaffold
Molecular Cancer Therapeutics
Repare Therapeutics, Saint-Laurent, CAN



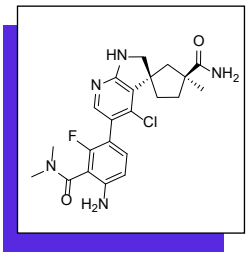
compound 54c | JAK

inhaled JAK inhibitor
reduced AO metabolism in lung
from kinase-focused screening and SBDD
Journal of Medicinal Chemistry
GlaxoSmithKline, Stevenage, UK



compound 3 | Vanin-1

vanin-1 pantetheinase inhibitor
preclinical candidate for IBD
from HTS + SBDD
Journal of Medicinal Chemistry
Pfizer, Cambridge, MA + Groton, CT



compound 25 | HPK1

HPK1 kinase inhibitor
unusual P-loop-folded conformation inhibitor
from HTS + SBDD
ACS Medicinal Chemistry Letters
Genentech, South San Francisco, CA

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