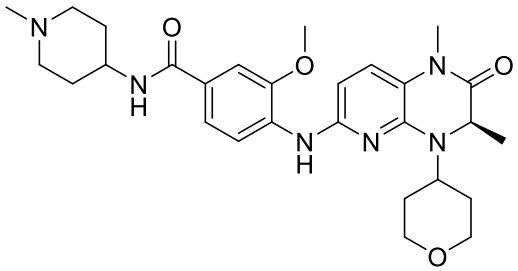
## TAF1-Compound 31



Chemical Formula: $C_{28}H_{38}N_6O_4$
Molecular Weight: 522.65

| Category | Parameter | Description |
|---|---|---|
| Compound | Name | **TAF1-compound 31** |
| | Citation | *ACS Med Chem Lett* **2019**, 10(10), 1443-1449 https://doi.org/10.1021/acsmedchemlett.9b00243 |
| | Chemical descriptors | O=C1N(C)C2=CC=C(NC3=CC=C(C(NC4CCN(C)CC4)=O)C=C3OC)N=C2N(C5CCOCC5)[C@@H]1C |
| | Chemical name | (*R*)-4-((1,3-dimethyl-2-oxo-4-(tetrahydro-2*H*-pyran-4-yl)-1,2,3,4-tetrahydropyrido[2,3-*b*]pyrazin-6-yl)amino)-3-methoxy-*N*-(1-methylpiperidin-4-yl)benzamide |
| | Availability | Gray Laboratory |
| | Additional comments | Dual TAF1 BRD4 inhibitor, Low (>10uM) PLK1 inhibition |
| *In vitro* profiling | Target (potency) | TAF1(2nd BRD): <10nM (AlphaScreen) |
| | Target (potency) | BRD4(1st BRD): 49nM (AlphaScreen) |
| | Selectivity | BRPF1 Bromodomain activity at 1uM (BromoScan assay panel) |
| | Potential reactivity | None |
| | SAR | Extension pyridopiperazone amide methyl to 1-butenyl group increases TAF1 selectivity. |
| | Mechanism of inhibition | Acetyl-lysine competitive bromodomain inhibition |
| | Structure of target-probe complex | N/A |
| Cellular profiling | Validation of cellular target | N/A |
| | Validation of cellular specificity | N/A |
| Pharmacodynamics | | N/A |
| Pharmacokinetics | | N/A |

Synthetic scheme