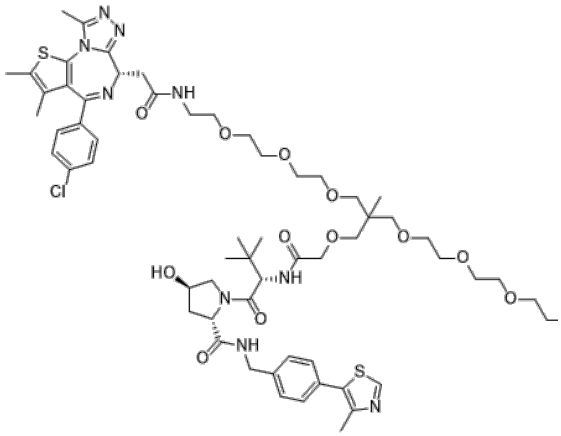
ProbeChem®
*Expedite Your Scientific Research*

WWW.PROBECHEM.COM

# Data Sheet

Global Supplier of Chemical Probes, Inhibitors & Agonists.

| | | |
|---|---|---|
| **Product Name** | : | BET PROTAC SIM1 |
| **Cat. No.** | : | PC-23323 |
| **CAS No.** | : | 2719051-84-8 |
| **Molecular Formula** | : | $C_{79}H_{98}Cl_2N_{14}O_{13}S_3$ |
| **Molecular Weight** | : | 1618.82 |
| **Target** | : | PROTAC |
| **Solubility** | : | 10 mM in DMSO |



## Biological Activity

BET PROTAC SIM1 is a highly potent, von Hippel-Lindau (VHL)-based BET trivalent PROTAC degrader with preference for BRD2 with DC50 of 1.1 nM, 3.3 nM and 0.7 nM for RD2, BRD3, BRD4 in HEK293 cells, potently inhibits cell viability of MV4;11 AML cell line with IC50 of 1.1 nM (48 h).
SIM1 exhibits Dmax50 values of 60-400pM and BET family degradation preference of BRD2>BRD4>BRD3 on both λmax and Dmax50.
SIM1 shows more efficacious apoptosis-induced cytotoxicity in BET-sensitive cancer cell lines than bivalent PROTACs or inhibitors.
SIM1 simultaneously engages with high avidity both BET bromodomains in a cis intramolecular fashion and forms a 1:1:1 ternary complex with VHL, exhibiting positive cooperativity and high cellular stability with prolonged residence time.

## References

Satomi Imaide, et al. Nat Chem Biol. 2021 Nov;17(11):1157-1167.

**Caution: Product has not been fully validated for medical applications. Lab Use Only!**

E-mail: tech@probechem.com