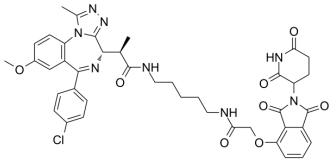
XY-06-007

Cat. No.:	HY-145226
CAS No.:	2757045-94-4
Molecular Formula:	$C_{41}H_{41}ClN_8O_8$
Molecular Weight:	809.27
Target:	PROTACs; Epigenetic Reader Domain
Pathway:	PROTAC; Epigenetics
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	XY-06-007 is a selective and potent bump-and-hole (B&H)-PROTAC $BRD4_{BD1}$L94V degrader. XY-06-007 shows a $DC_{50,\ 6\ h}$ of 10 nM against $BRD4_{BD1}$L94V with no degradation of off-targets. XY-06-007 demonstrates suitable pharmacokinetics for in vivo studies[1].
IC_{50} & Target	Cereblon
In Vitro	XY-06-007 shows a half-degradation concentration (DC50, 6 h) of 10.2±1.8 nM against $BRD4_{BD1}$L94V with no degradation of off-targets, as assessed by whole proteome mass spectrometry[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	XY-06-007 has favorable pharmacokinetic profile, including good plasma concentration, area under the curve (AUC), and bioavailability. XY-06-007 exhibits short elimination half-life (0.515 h) due to relatively low clearance (21.9 mL/min/kg) following intravenous administration (2.0 mg/kg). XY-06-007 exhibits short elimination half-life (0.721 h) due to the C_{max} (6.10 μM) and T_{max} (0.25 h) following intraperitoneal injection (10 mg/kg)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Six to eight weeks old male C57BL/6 mice[1]
Dosage:	2 mg/kg (iv) or 10 mg/kg (ip) (Pharmacokinetic Analysis)
Administration:	Administered via tail vein injection or via intraperitoneal injection. Approximately 110 μL of blood/time point was collected into the K2EDTA tube via facial vein for bleeding for the time points: 0.083, 0.25, 0.5, 1, 2, 4, 8, and 24 h.
Result:	Maintained above its DC50, 6h of 10 nM for approximately 6 h when dosed at 10 mg/kg via intraperitoneal injection (IP), indicating that such in vivo degradation experiment would result in a favorable outcome.

REFERENCES

[1]. Radosław P Nowak, et al. Structure-Guided Design of a "Bump-and-Hole" Bromodomain-Based Degradation Tag. J Med Chem. 2021 Aug 12;64(15):11637-11650.

Caution: Product has not been fully validated for medical applications. For research use only.

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