Figure S1. HR-MS (A) and ¹H-NMR (B) spectra of DA-7010. HR-MS spectrum was obtained in positive ESI mode using Thermo Scientific Q Exactive Orbitrap mass spectrometer. Accurate mass of $[M+H]^+$ ion of DA-7010 measured was consistent with calculated mass based on chemical formula of DA-7010 (220.11395 Da). ¹H-NMR spectrum of DA-7010 hydrochloride (in DMSO-*d*6) was obtained using Varian 400 MHz NMR spectrometer.





δ 1.41 (3H, d, *J* = 6.4 Hz), 2.87 (1H, dd, *J* = 13.2, 9.2 Hz), 3.52 (1H, dd, *J* = 13.2, 2.4 Hz), 4.15-4.26 (2H, m), 4.41 (1H, brs), 5.54-5.59 (1H, m), 6.88 (1H, *d*, *J* = 8.4 Hz), 7.14 (1H, *d*, *J* = 7.2 Hz), 7.49 (1H, *t*, *J* = 7.8 Hz), 8.40 (3H, brs)

Figure S2. Full-scan mass spectra of DA-7010 (A) and the IS (B). Spectra were obtained in MS2 scan mode (positive ESI with Fragment voltage of 135V) using an Agilent 6460 triple quadrupole tandem mass spectrometer. $[M+H]^+$ ions of DA-7010 and the IS were indicated by red arrows.



(B)



Figure S3. Representative calibration curves with regression equations for DA-7010 in plasma from various species (mice (A), rats (B) and dogs (C)). Calibration curves over the DA-7010 concentration range of 10–10000 ng/mL were constructed by plotting the peak area ratio of DA-7010 to the IS (y) versus the relative concentration of DA-7010 to the IS (x) with weighted $(1/x \text{ or } 1/x^2)$ least-squares linear regression.

