Electronic Supplementary Material

Novel green-emissive carbon dots as a dual-purpose fluorometric tool for sensitive vismodegib detection and pharmacokinetic analysis

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Instruments

Transmission electron microscopy (TEM) was conducted using a JEOL JEM-100CX II microscope (JEOL Ltd., USA). X-ray photoelectron spectroscopy (XPS) data were acquired with a Thermo Scientific ESCALAB 250Xi system (Thermo Fisher Scientific, USA). Particle size distribution and surface charge (zeta potential) were analyzed via dynamic light scattering (DLS) using a ZEN 3600 Nano ZS analyzer (Malvern Instruments, UK). Fluorescence measurements were performed on a Shimadzu RF-5301 PC spectrofluorometer, while UV–Vis absorption spectra were recorded using a Shimadzu UV-1601 PC spectrophotometer (Tokyo, Japan). Fourier-transform infrared (FT-IR) spectra were obtained with a Nicolet™ iS™10 spectrometer (Thermo Fisher Scientific, USA), and X-ray diffraction (XRD) patterns were collected using a PW 1710 diffractometer (Philips-FEI, Netherlands).

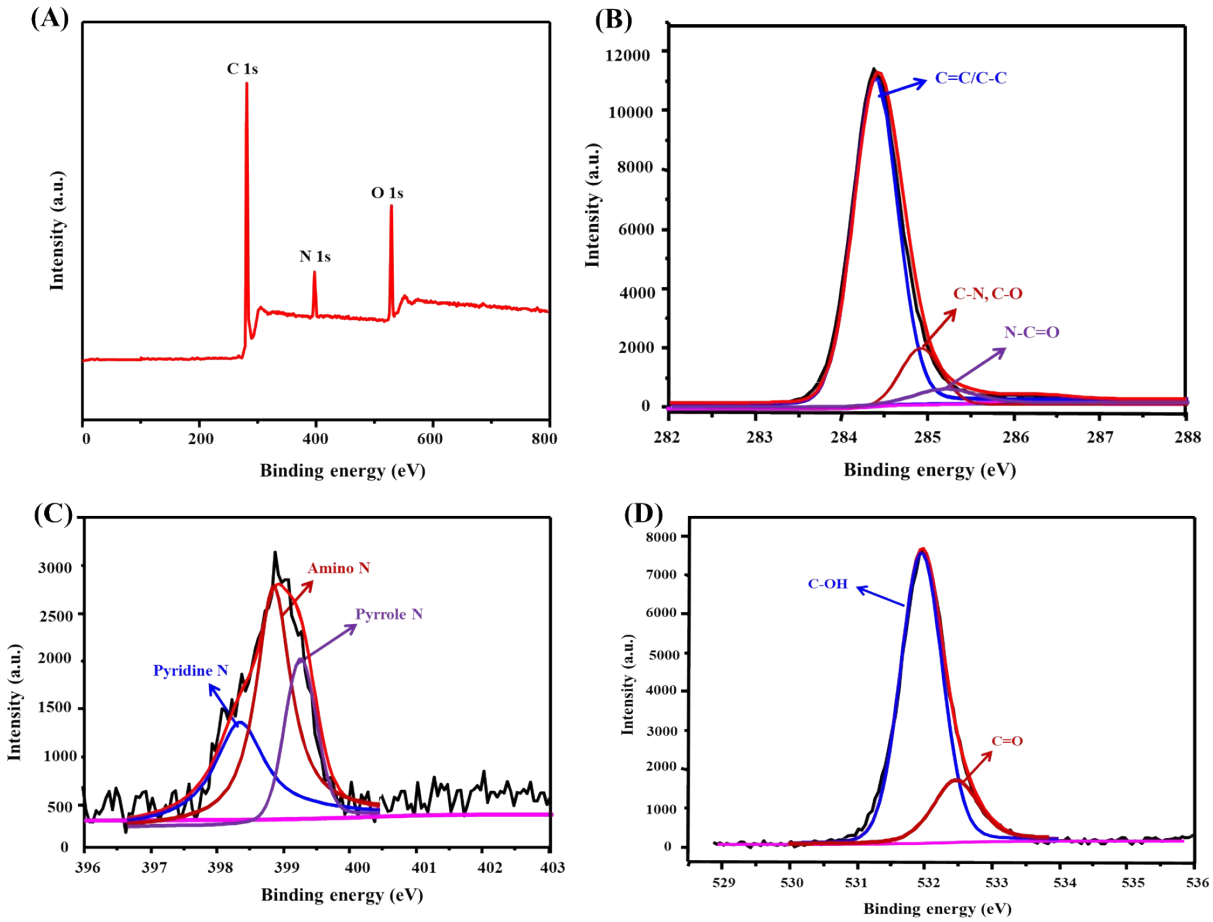

Fig. S1 (A) XPS survey of G-N@CDs and (B-D) are high resolution XPS spectra of (B) C 1s, (C) N 1s, and (D) O 1s.

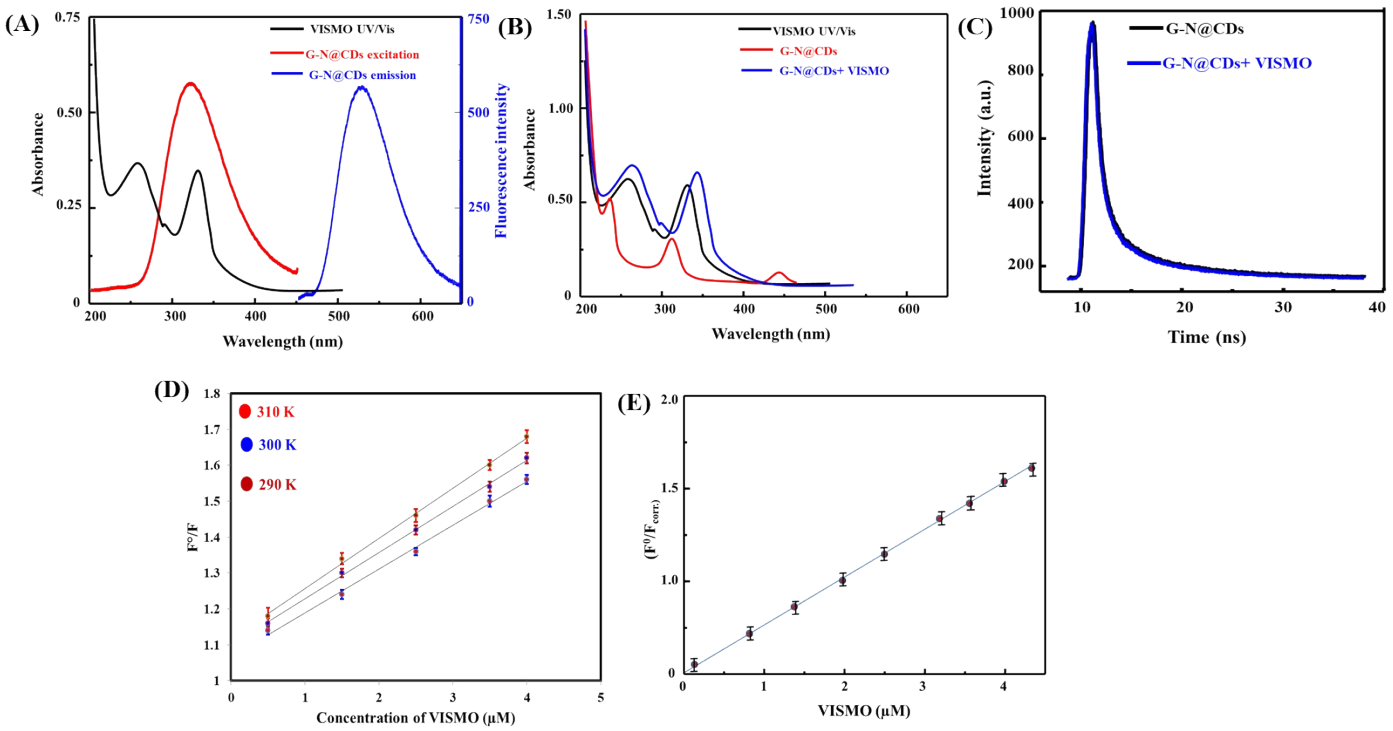

Fig. S2(A) UV–Vis absorption spectrum of VISMO, and fluorescence excitation and emission spectra of G-N@CDs; (B) Fluorescence lifetime decay curves of G-N@CDs before and after VISMO addition; (C) UV–Vis absorption spectra of VISMO, G-N@CDs, and G-N@CDs + ISQ; (D) Stern–Volmer plots for G-N@CDs with increasing VISMO concentrations at different temperatures; (E) IFE-corrected Stern–Volmer plot ($F^0/F_{corr.}$ vs. [VISMO]) for the G-N@CDs–VISMO system.

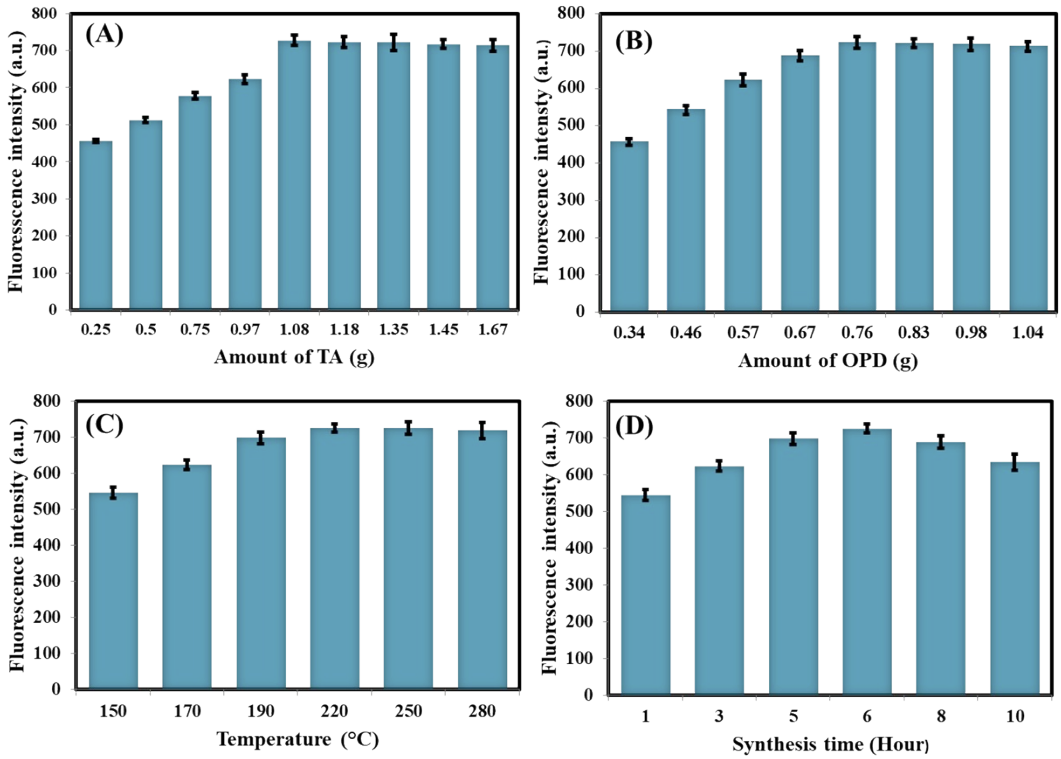

Fig. S3 Influence of amounts of TA (A) and OPD (B), synthesis temperature (C), synthesis time (D) on the fluorescence emission of G-N@CDs.

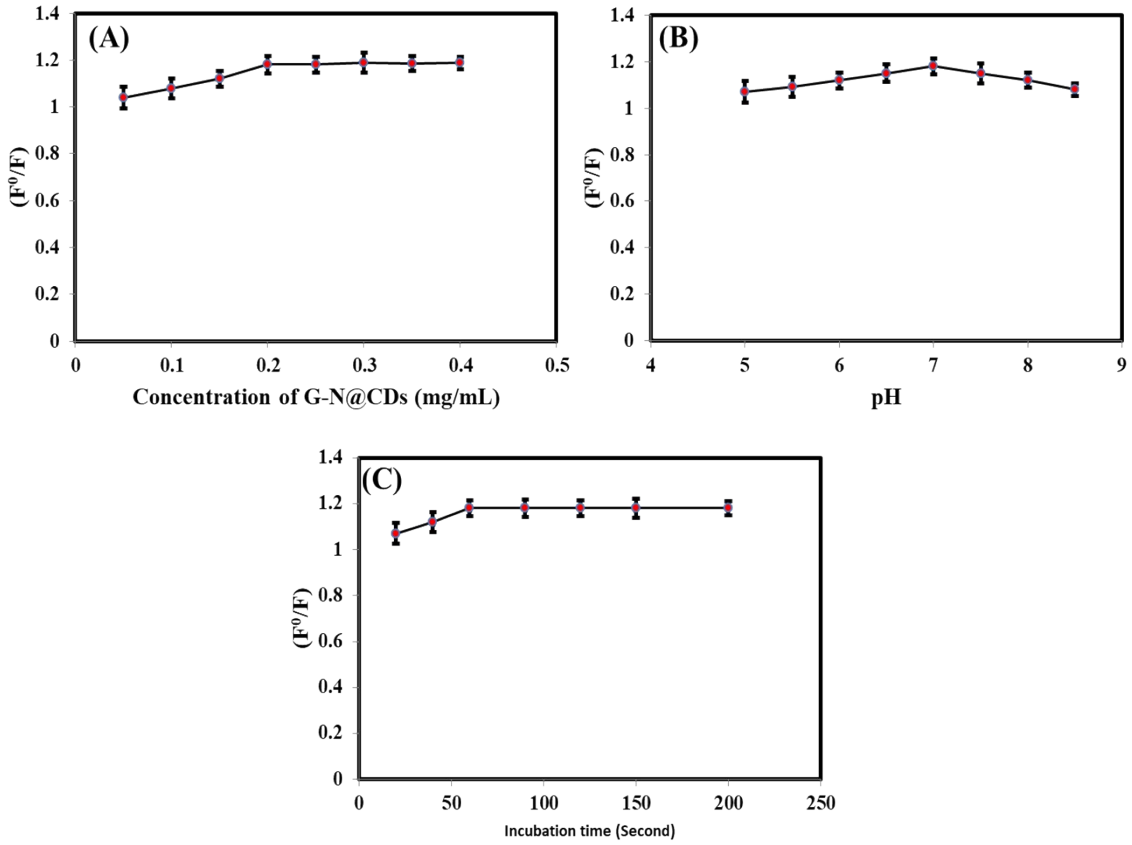

Fig. S4 Influence of G-N@CDs concentration (A), pH value (B), and incubation time (C) on the detection of 20 μM VISMO.

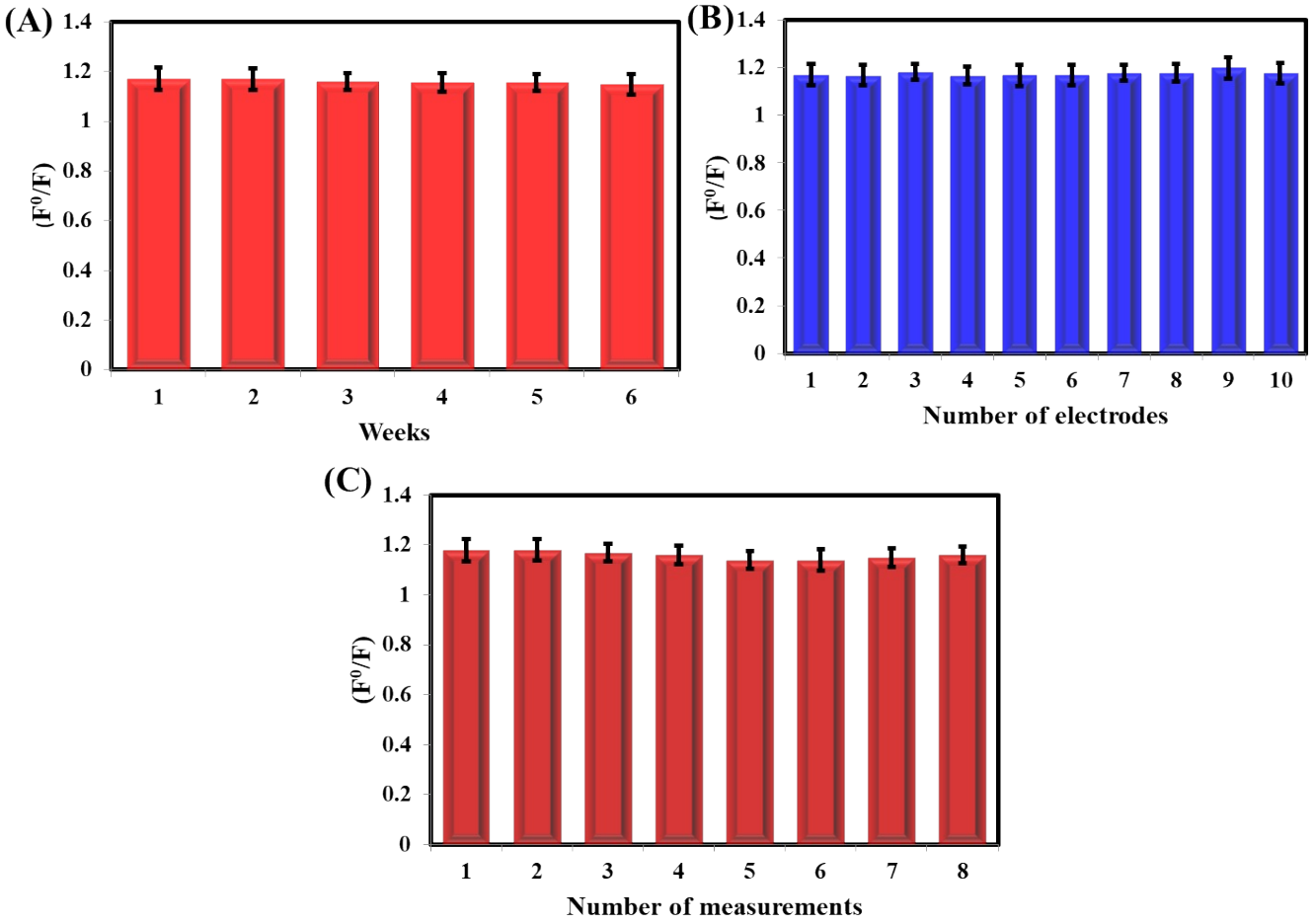

Fig. S5 Stability (A), reproducibility (B), and repeatability (C) of the G-N-CDs for measuring 20 µM VISMO.

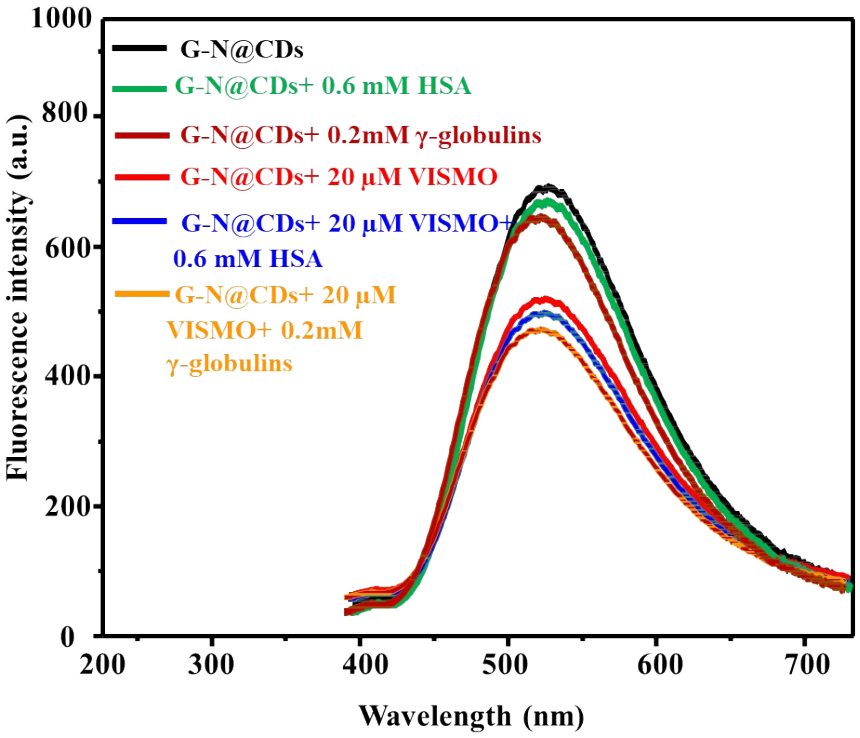

Fig. S6 Selectivity of the G-N-CDs probe for measuring 20 μM VISMO, 0.6 mM HAS, 0.2 mM γ-globulins, and mixtures of them.

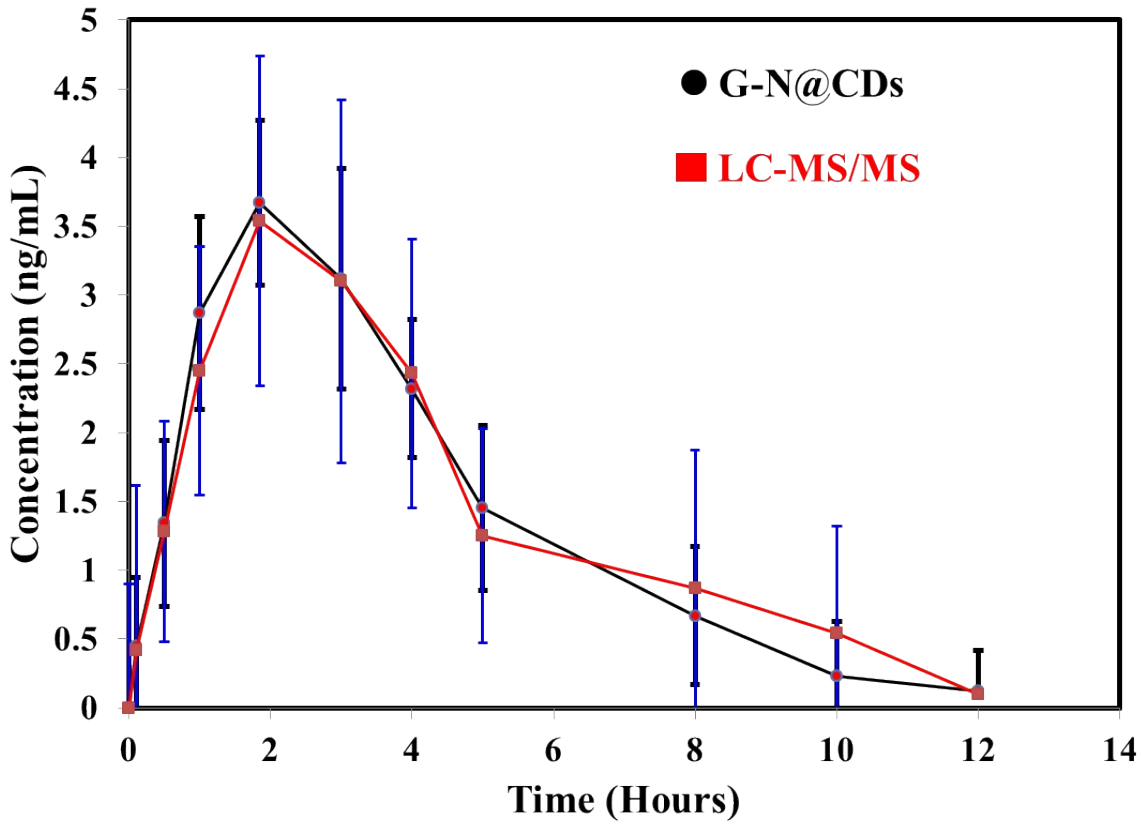

Fig. S7 Pharmacokinetic profile of VISMO in SCLC patients using proposed G-N@CDs and LC-MS/MS methods. Number of replicates is four.

Table S1 Summary of the pharmacokinetic parameters of VISMO in the plasma of SCLC patients.

Parameter	SCLC
C_{max} (ng/mL)	3.670
T_{max} (Hour)	1.85
$AUC_{0–48h}$ (ng.h/mL)	4,767.89
λz (terminal slope) (h^{-1})	0.07530
t½ = ln2/λz (h)	16.878
AUC_{extra} (Clast/λz) (ng.h/mL)	332.88
$AUC_{0–\infty}$ (ng.h/mL)	5,765.34
%AUC extrapolated (%)	8.68
$AUMC_{0–\infty}$ ($ng.h^2/mL$)	76.758.31
MRT = AUMC/AUC (h)	15.098
CL($L.h^{-1}.m^{-2}$)	5.648
Vz = CL/λz ($L.m^{-2}$)	223.52
Vss ($L.m^{-2}$)	156.87

C_{max}: Maximum plasma concentration; T_{max} = time of C_{max}; $AUC_{0–48}$: area under the concentration–time curve from 0 to 48 h; λz = terminal elimination rate constant; t½ = terminal half-life (= ln2/λz); AUCextra = extrapolated AUC beyond last time point (= C_last/λz); $AUC_{0–\infty}$ = total AUC to infinity (= AUC0–t + AUCextra); %AUC extrapolated = 100 × AUCextra/$AUC_{0–\infty}$; AUMC0–∞ = area under the first-moment curve to infinity; MRT = mean residence time (= AUMC0–∞/AUC0–∞); CL = systemic clearance (dose-normalized; = Dose/AUC0–∞); Vz = apparent volume of distribution in the terminal phase (= CL/λz); Vss = steady-state volume of distribution.