

*Supplementary Materials*

# Development of an LC-MS/MS method for ARV-110, a PROTAC molecule, and applications to pharmacokinetic studies

Thi-Thao-Linh Nguyen<sup>1,#</sup>, Jin Woo Kim<sup>2,#</sup>, Hae-in Choi<sup>2</sup>, Han-Joo Maeng<sup>1,\*</sup>, Tae-Sung Koo<sup>2,\*</sup>

<sup>1</sup> College of Pharmacy, Gachon University, 191 Hambakmoe-ro, Yeonsu-gu, Incheon 21936, Republic of Korea

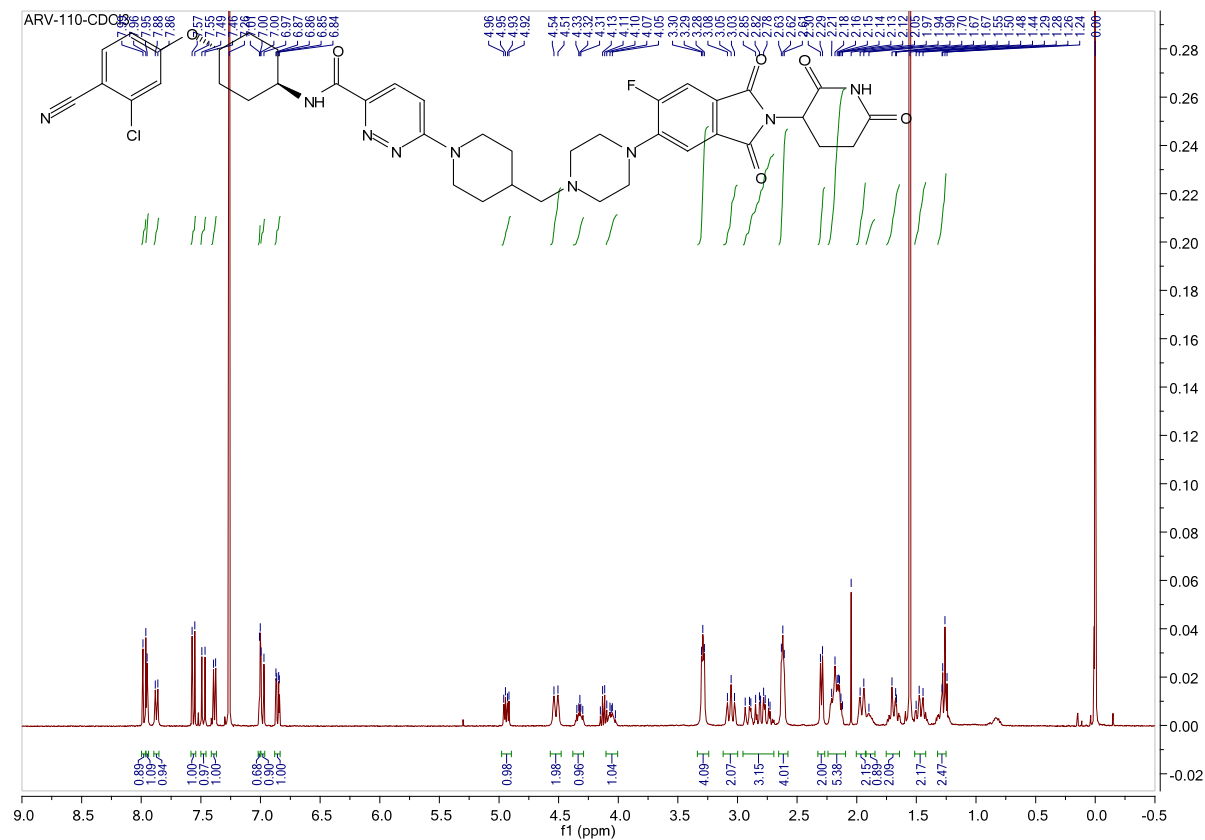
<sup>2</sup> Graduate School of New Drug Discovery and Development, Chungnam National University, Daejeon 34134, Republic of Korea

# These authors contributed equally to this work

\* Correspondence: hjmaeng@gachon.ac.kr (H.-J.M.); kootae@cnu.ac.kr (T.-S.K.); Tel.: +82-32-820-4935 (H.-J.M.); +82-42-821-8628 (T.-S.K.)

**ARV-110:  $^1\text{H}$ -NMR (400 MHz,  $\text{CDCl}_3$ )**

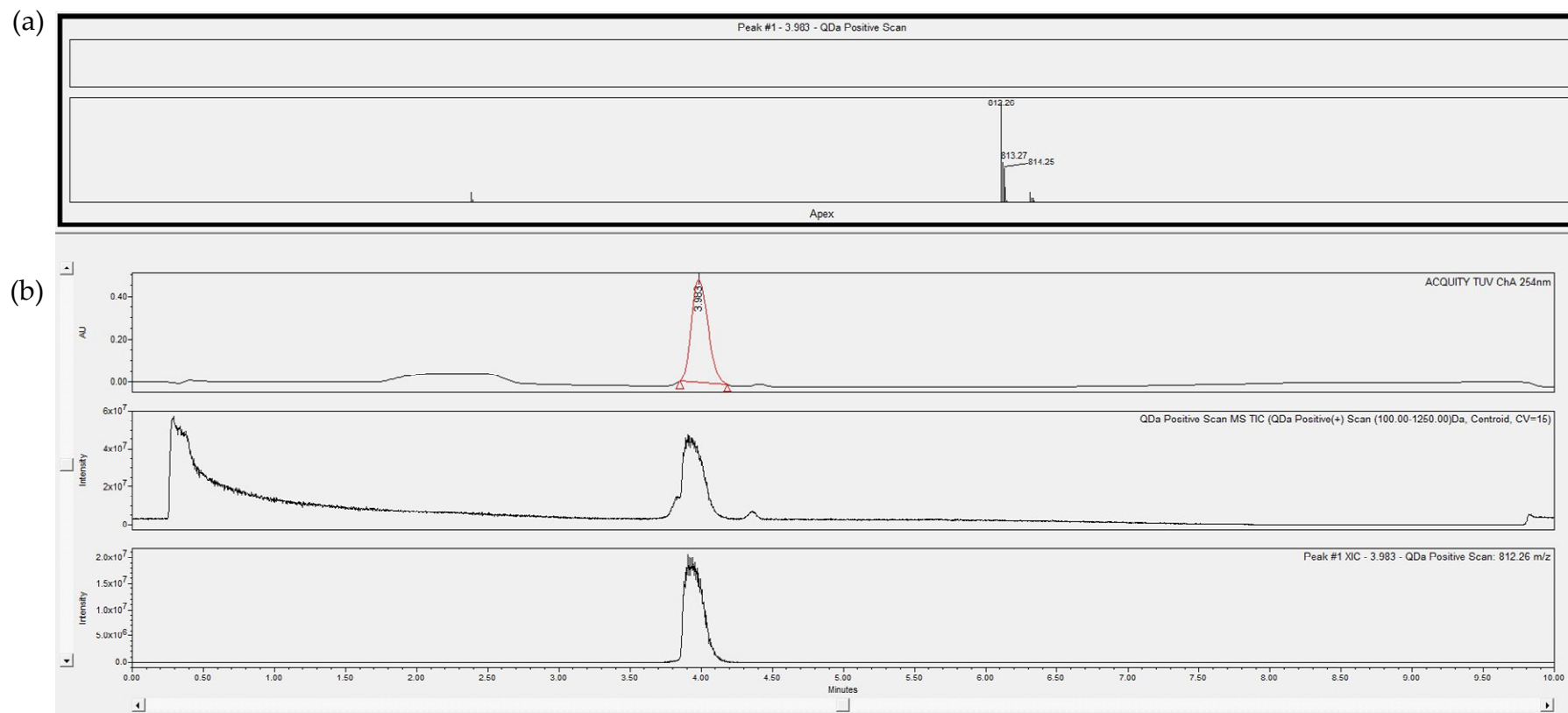
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 (d,  $J$  = 9.6 Hz, 1H), 7.95 (s, 1H), 7.87 (d,  $J$  = 8.2 Hz, 1H), 7.56 (d,  $J$  = 8.7 Hz, 1H), 7.48 (d,  $J$  = 11.1 Hz, 1H), 7.38 (d,  $J$  = 7.3 Hz, 1H), 7.01 (s, 1H), 6.98 (d,  $J$  = 9.6 Hz, 1H), 6.86 (dd,  $J$  = 8.7, 2.4 Hz, 1H), 4.94 (dd,  $J$  = 12.3, 5.3 Hz, 1H), 4.52 (d,  $J$  = 13.2 Hz, 2H), 4.38 – 4.29 (m, 1H), 4.10 – 4.00 (m, 1H), 3.34 – 3.24 (m, 4H), 3.12 – 3.00 (m, 2H), 2.95 – 2.69 (m, 3H), 2.65 – 2.58 (m, 4H), 2.30 (d,  $J$  = 6.9 Hz, 2H), 2.24 – 2.09 (m, 5H), 2.00 – 1.93 (m, 2H), 1.92 – 1.85 (m, 1H), 1.75 – 1.64 (m, 2H), 1.51 – 1.42 (m, 2H), 1.32 – 1.25 (m, 2H).



**Figure S1.**  $^1\text{H}$ -NMR (400 MHz,  $\text{CDCl}_3$ ) spectra of ARV-110

## ARV-110: Mass

HPLC-QDa/ESI-MS (Waters) equipped with Empower 3.0 software  
 $m/z$  812.26  $[M+H]^+$ .



**Figure S2.** QDa-MS profile of ARV-110 (a) and high-performance liquid chromatography-single quadrupole mass spectrometry (HPLC-UV-QDa) chromatograms for ARV-110 (b).