Supporting Information.

Barettin Suppresses Pancreatic Ductal Adenocarcinoma Proliferation via Topoisomerase IIα Inhibition

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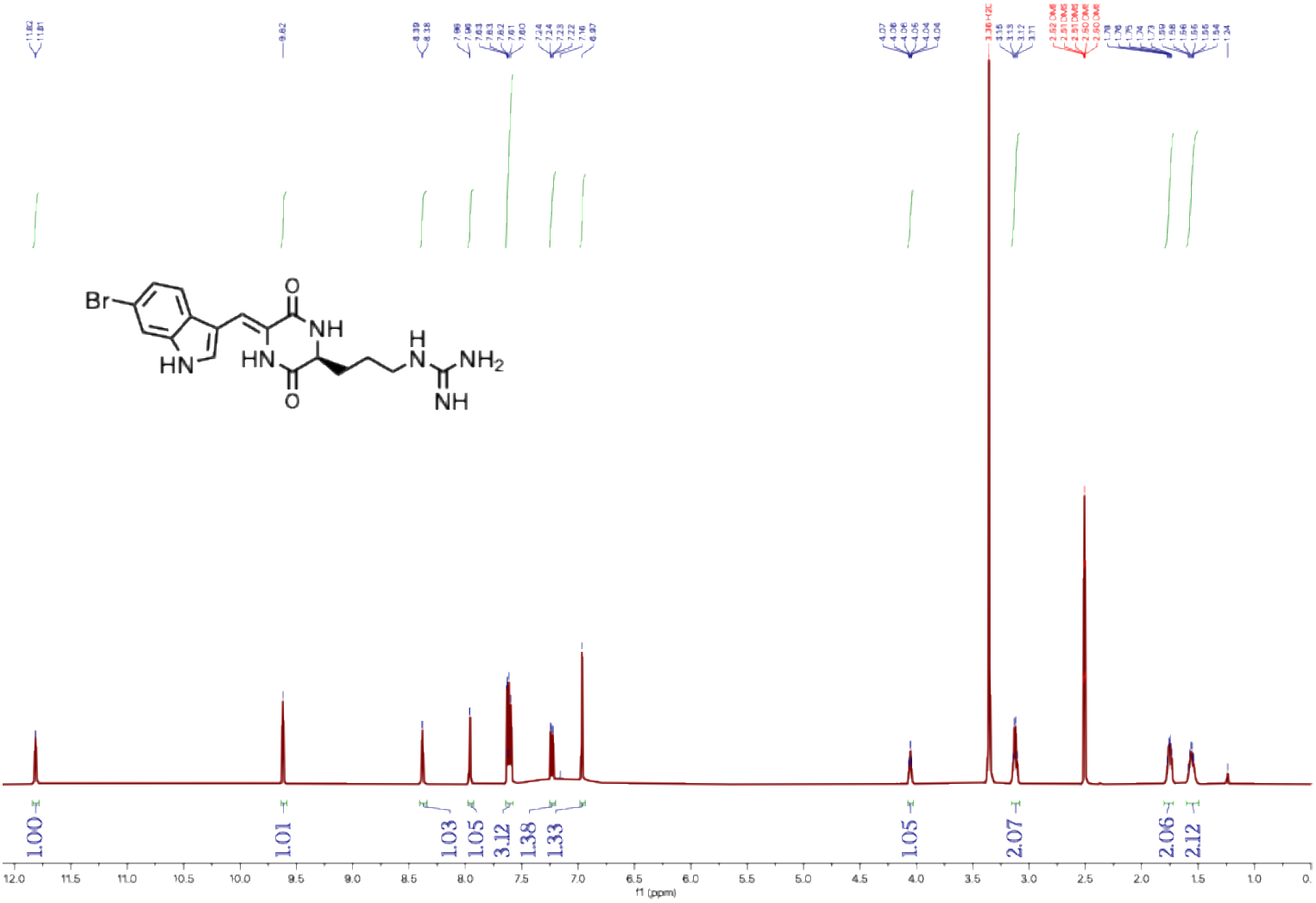

Figure S1: ^{1}H NMR of Barettin

^{1}H NMR (500 MHz, DMSO) δ 11.82 (s, 1H), 9.65 (s, 1H), 8.40 (d, *J* = 2.7 Hz, 1H), 7.96 (d, *J* = 2.7 Hz, 1H), 7.65 – 7.56 (m, 3H), 7.23 (d, *J* = 8.5 Hz, 1H), 6.96 (s, 1H), 4.05 (td, *J* = 5.7, 2.6 Hz, 1H), 3.12 (q, *J* = 6.7 Hz, 2H), 1.74 (dd, *J* = 9.5, 5.6 Hz, 2H), 1.55 (h, *J* = 6.5 Hz, 2H).

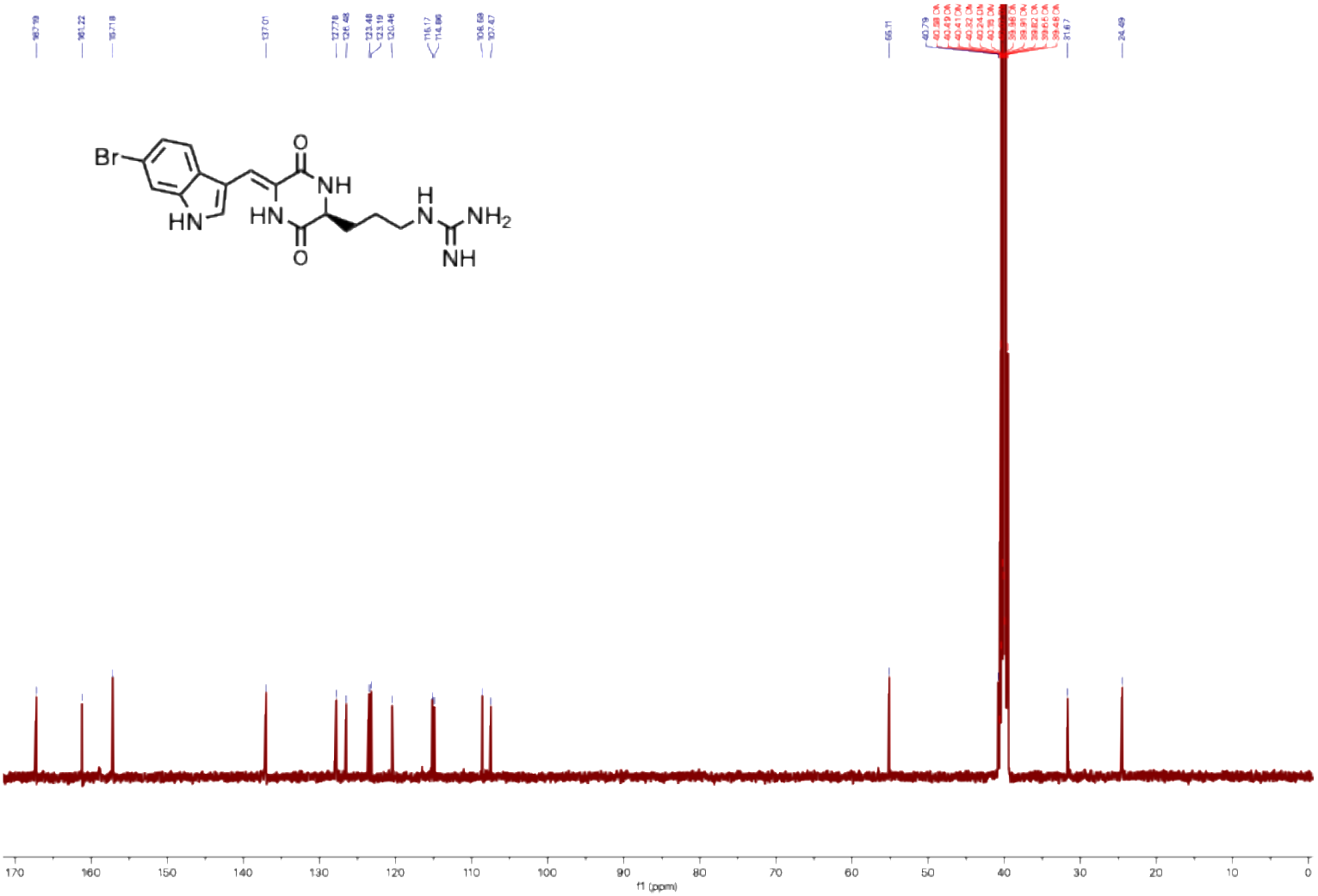

Figure S2: ^{13}C NMR of Barettin.

^{13}C NMR (126 MHz, DMSO) δ 167.2 (CO), 161.2 (CO), 157.2 ($C(NH)_2NH_2$,) 137.0 (C), 127.8 (CH), 126.5 (C), 123.5 (CH), 123.2 (CH), 120.5 (CH), 115.2 (C), 114.9 (CBr), 108.6 (CH), 107.5 (C), 55.1 (CH), 40.5 (CH_2), 31.7 (CH2), 24.5 (CH_2).

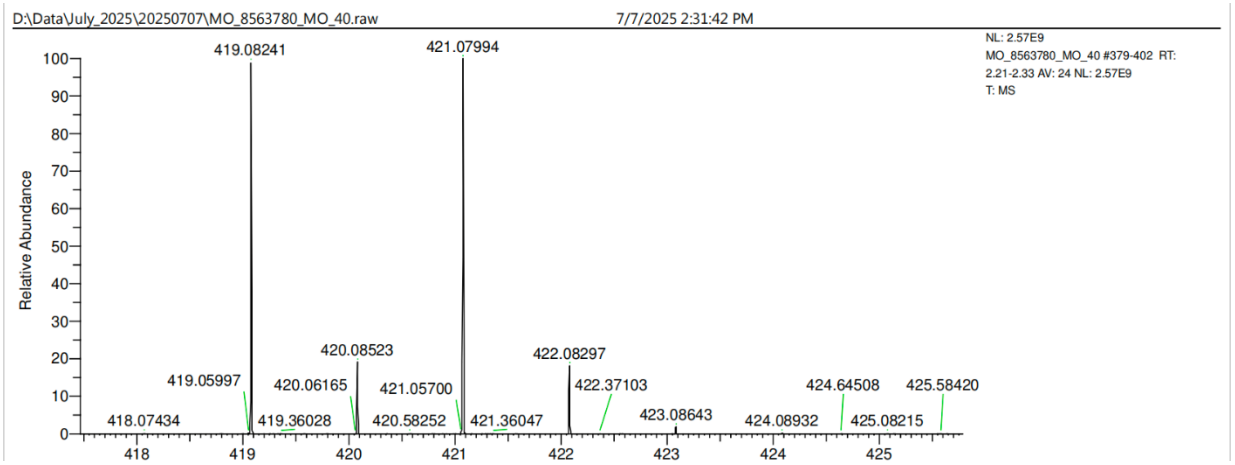

***Figure S3*:** LC and HRMS traces

MS (ESI) *m/z*, 419 (100) [M (^{79}Br) +H]$^+$, 421 (100) [M(^{81}Br) + H] $^+$; **HRMS (FTMS + p ESI):** m/z calculated for: $C_{17}H_{20}BrN_6O$ [M (^{79}Br) + H]$^+$: 419.0826; found: 419.0824.

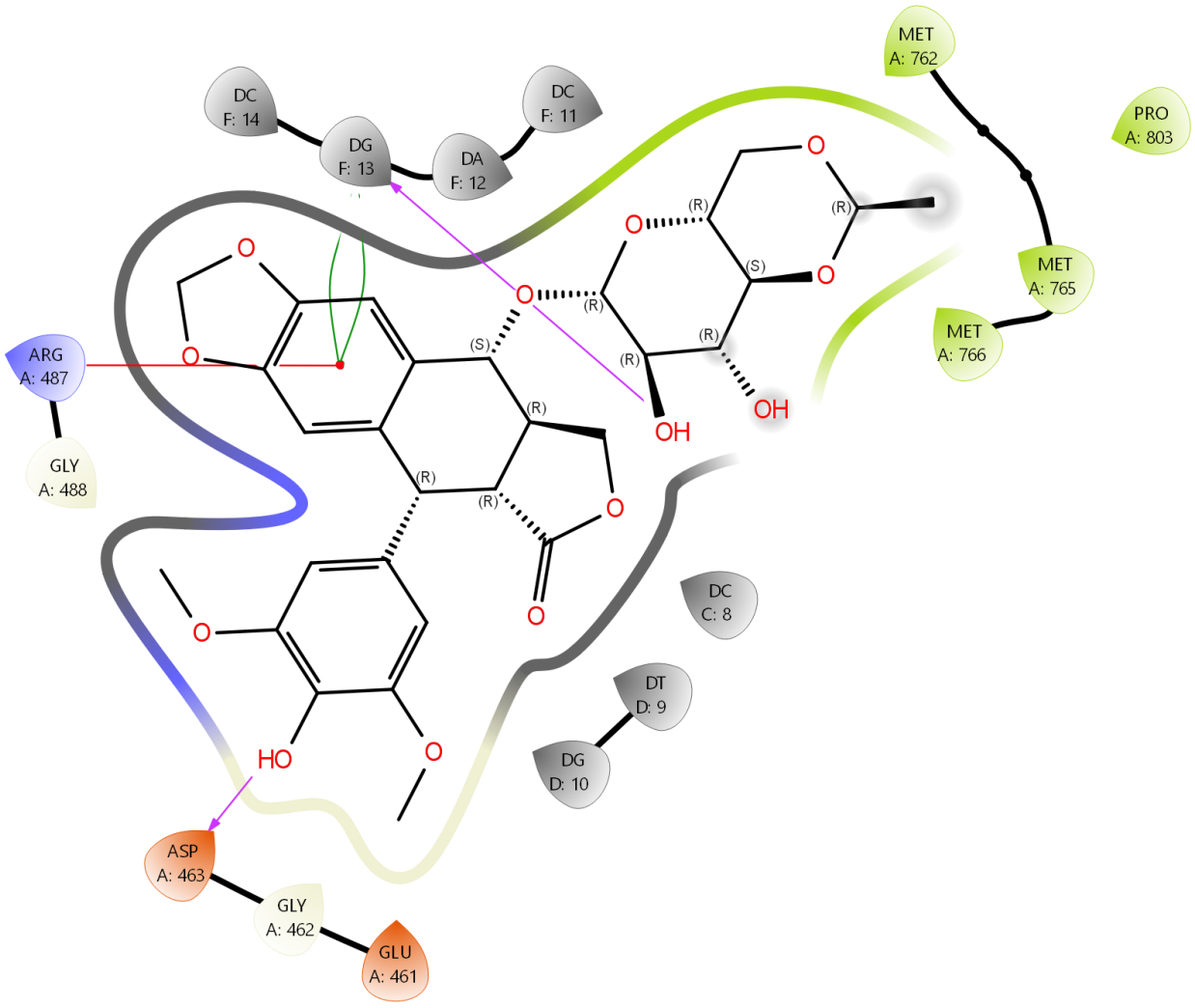

Figure S4: 2D Ligand interaction diagram of etoposide in human TOP2A (PDB:5GWK)