

Synthesis of new derivatives of berberine canagliflozin and study on their antibacterial activity and mechanism

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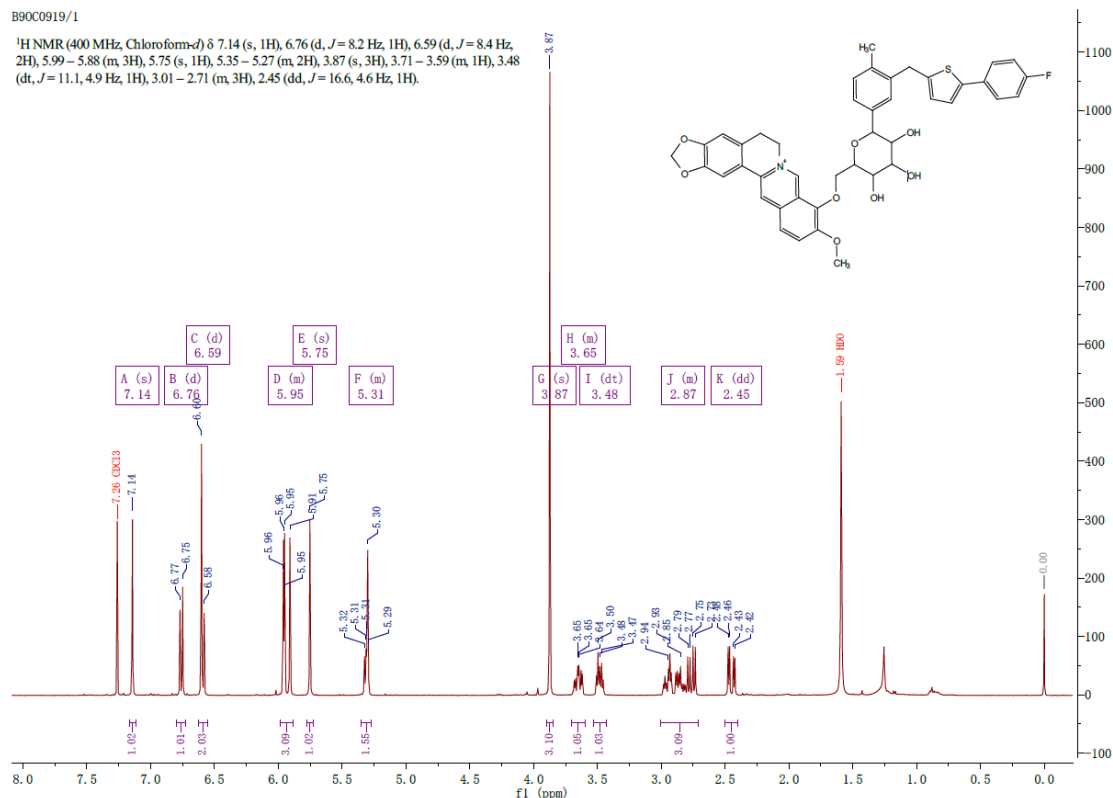


Figure S 1 ¹H NMR spectra of compound B9OC

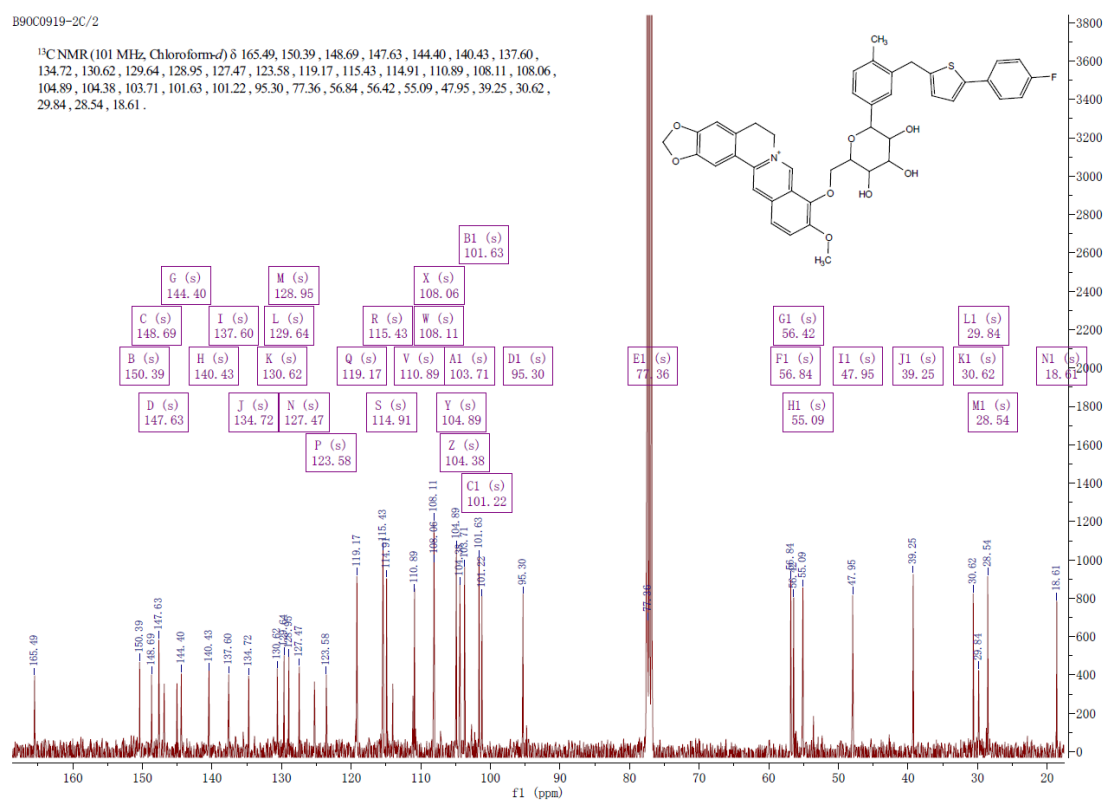


Figure S 2 ¹³C NMR spectra of compound B9OC

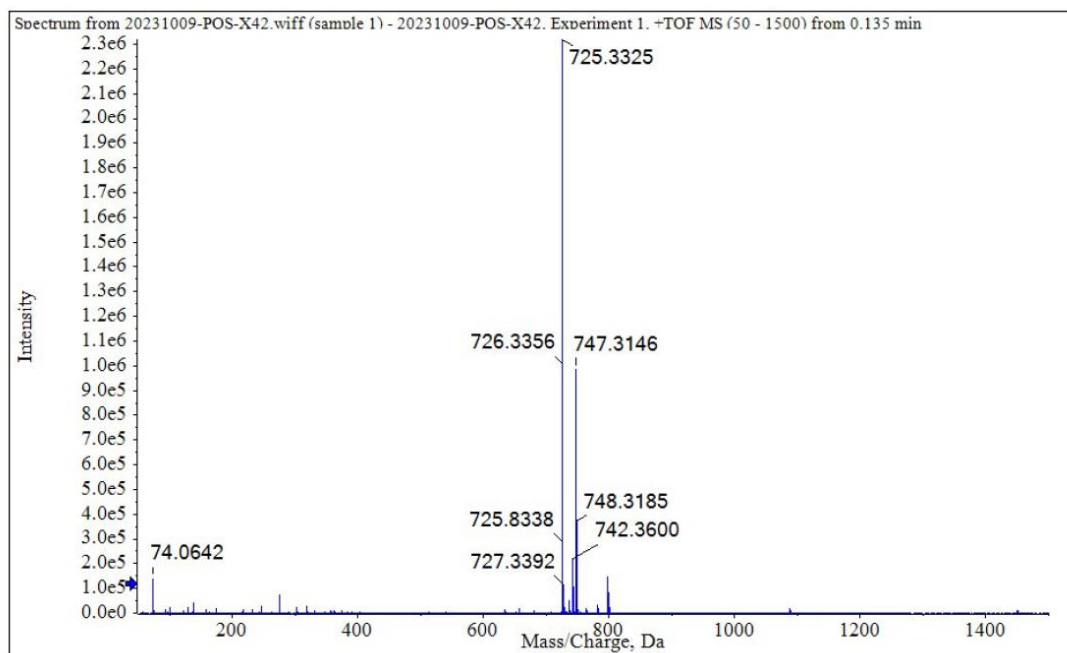


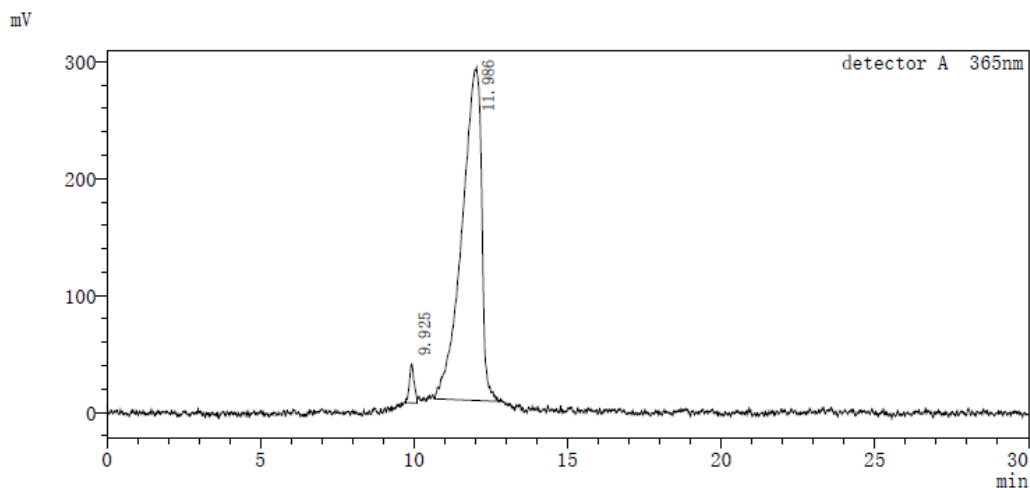
Figure S 3 MS spectra of compound B9OC

SHIMADZU
LabSolutions Analysis report

<Sample Information>

Sample : b9oca365nm
 Sample ID : 01
 Inj. Volume : 10 uL
 Acquisition Date : 2023/9/13 10:37:25

<Chromatogram>



<Chromatogram peak table>

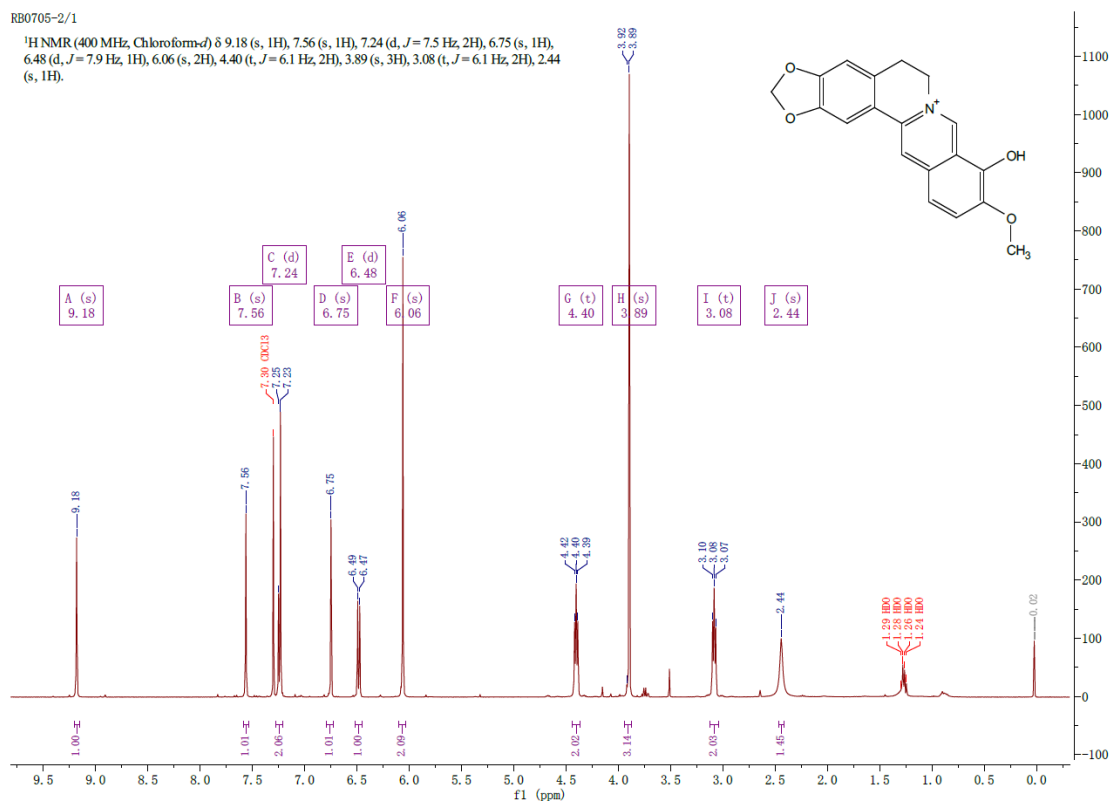
detector A 365nm

number	retention time	peak area	hight	concentration
1	9.925	353117	32886	2.743 %
2	11.986	12519188	282176	97.257 %
总计		12872305	315063	

Figure S 4 The purity of B9OC from HPLC

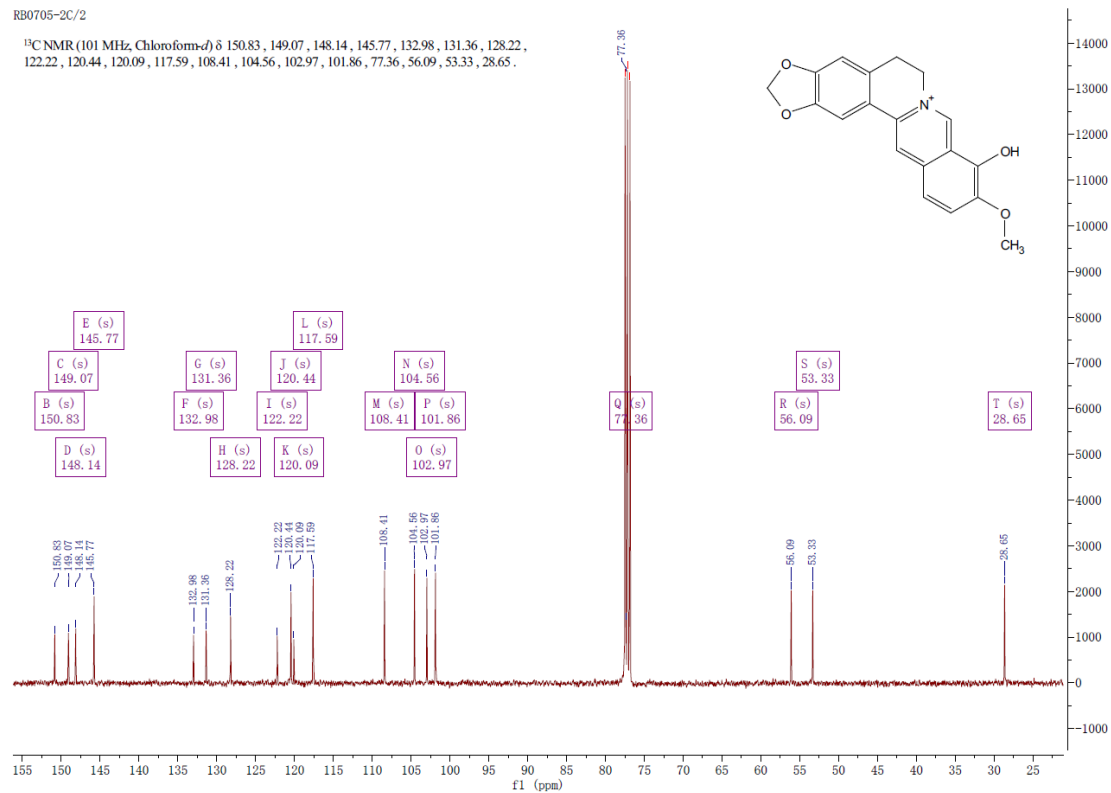
RB0705-2/1

^1H NMR (400 MHz, Chloroform- d) δ 9.18 (s, 1H), 7.56 (s, 1H), 7.24 (d, $J = 7.5$ Hz, 2H), 6.75 (s, 1H), 6.48 (d, $J = 7.9$ Hz, 1H), 6.06 (s, 2H), 4.40 (t, $J = 6.1$ Hz, 2H), 3.89 (s, 3H), 3.08 (t, $J = 6.1$ Hz, 2H), 2.44 (s, 1H).

Figure S 5 ^1H NMR spectra of compound **Berberrubine**

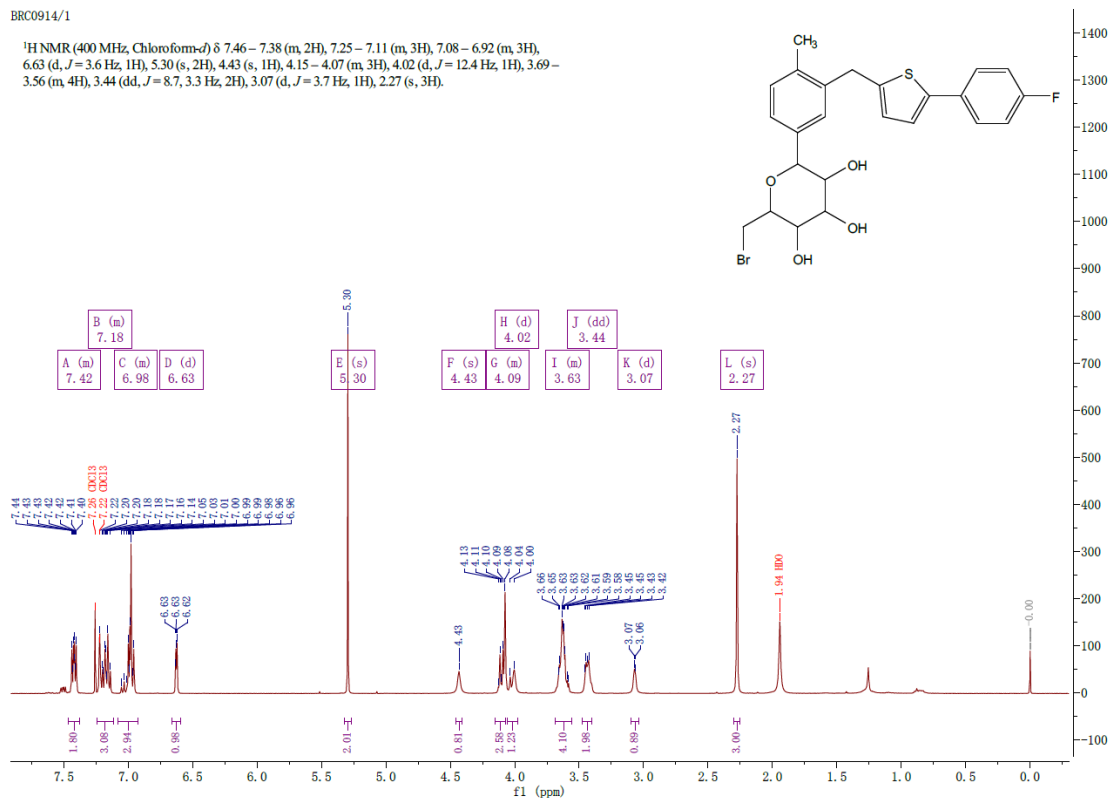
RB0705-2C/2

^{13}C NMR (101 MHz, Chloroform- d) δ 150.83, 149.07, 148.14, 145.77, 132.98, 131.36, 128.22, 122.22, 120.44, 120.09, 117.59, 108.41, 104.56, 102.97, 101.86, 77.36, 56.09, 53.33, 28.65.

Figure S 6 ^{13}C NMR spectra of compound **Berberrubine**

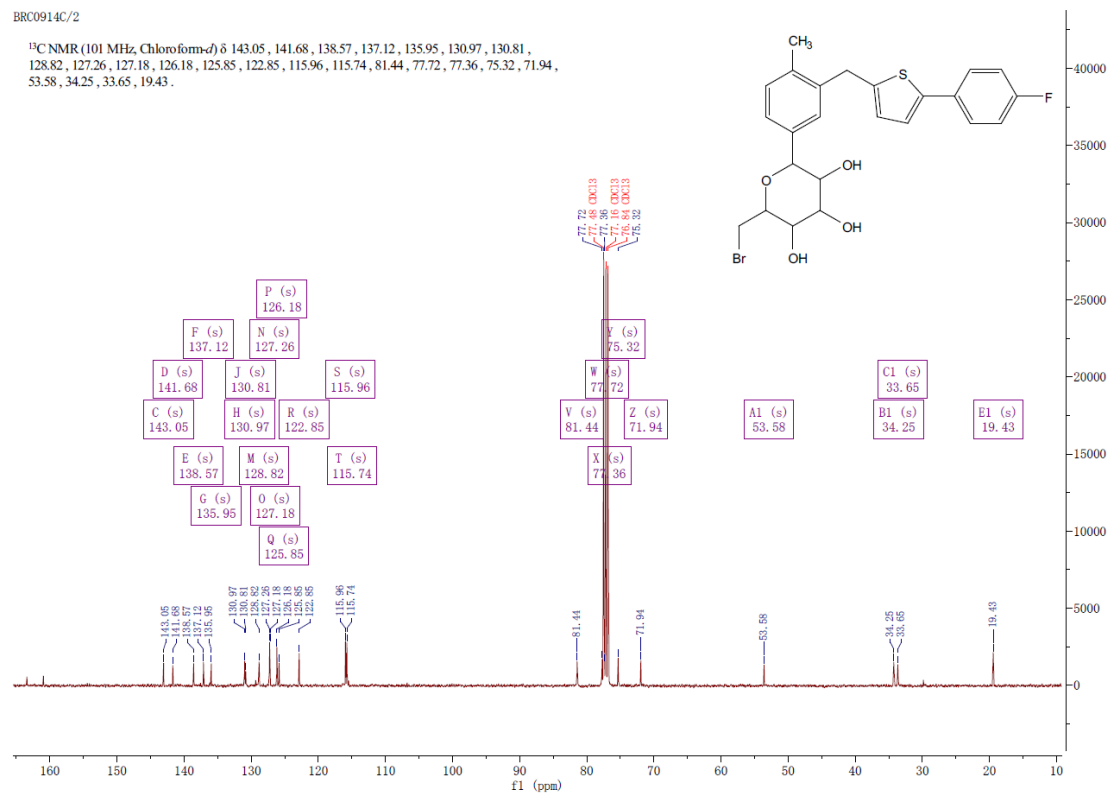
BRC0914/1

^1H NMR (400 MHz, Chloroform- d) δ 7.46–7.38 (m, 2H), 7.25–7.11 (m, 3H), 7.08–6.92 (m, 3H), 6.63 (d, J = 3.6 Hz, 1H), 5.30 (s, 2H), 4.43 (s, 1H), 4.15–4.07 (m, 3H), 4.02 (d, J = 12.4 Hz, 1H), 3.69–3.56 (m, 4H), 3.44 (dd, J = 8.7, 3.3 Hz, 2H), 3.07 (d, J = 3.7 Hz, 1H), 2.27 (s, 3H).

Figure S 7 ^1H NMR spectra of compound Canagliflozin bromide

BRC0914C/2

^{13}C NMR (101 MHz, Chloroform- d) δ 143.05, 141.68, 138.57, 137.12, 135.95, 130.97, 130.81, 128.82, 127.26, 127.18, 126.18, 125.85, 122.85, 115.96, 115.74, 81.44, 77.72, 77.36, 75.32, 71.94, 53.58, 34.25, 33.65, 19.43.

Figure S 8 ^{13}C NMR spectra of compound Canagliflozin bromide

B90BU1020/1

^1H NMR (400 MHz, Chloroform- d) δ 10.29 (s, 1H), 8.36 (s, 1H), 7.91 (d, J = 9.0 Hz, 1H), 7.74 (d, J = 9.0 Hz, 1H), 7.36 (s, 1H), 6.77 (s, 1H), 6.04 (s, 2H), 5.32 (t, J = 6.3 Hz, 2H), 4.45 (t, J = 6.8 Hz, 2H), 4.01 (s, 3H), 3.31 (t, J = 6.3 Hz, 2H), 1.99 (p, J = 6.9 Hz, 3H), 1.57 (q, J = 7.5 Hz, 3H), 1.24 (s, 3H), 1.01 (t, J = 7.4 Hz, 4H).

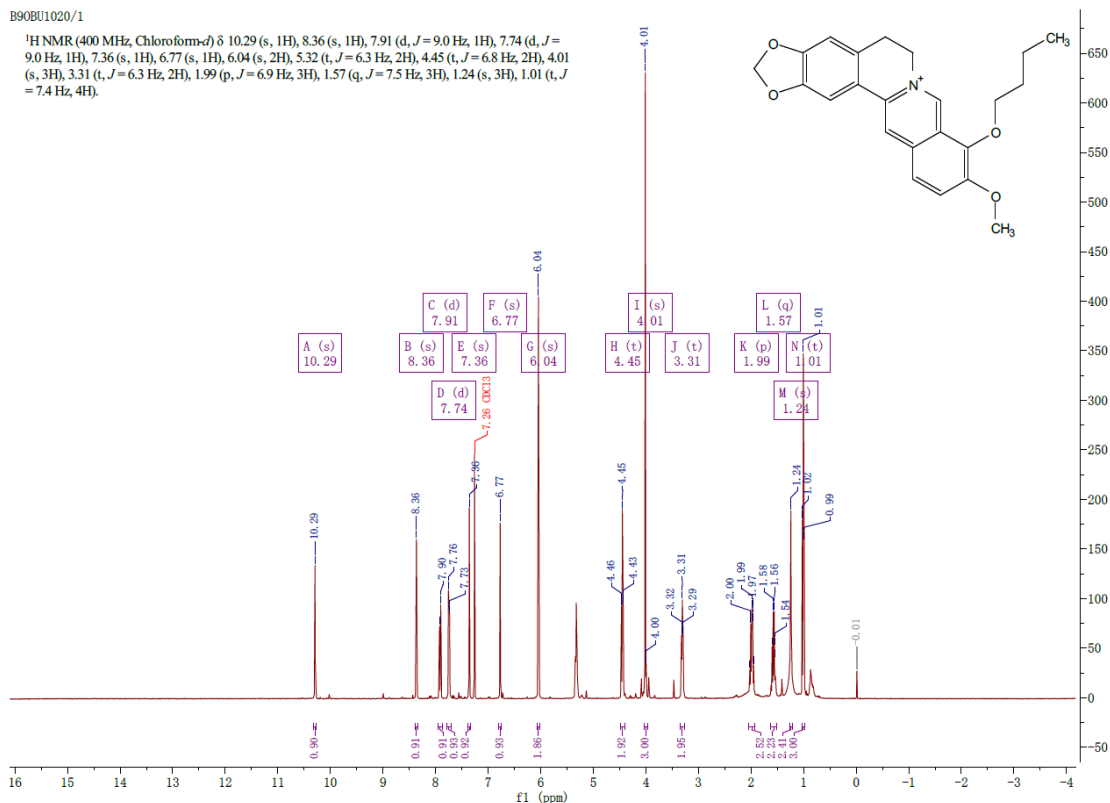


Figure S 9 ^1H NMR spectra of compound B90BU

B90BU1020C/2

^{13}C NMR (101 MHz, Chloroform- d) δ 150.75, 148.39, 146.76, 137.68, 133.48, 130.62, 126.11, 123.02, 122.49, 120.38, 119.85, 108.61, 105.42, 102.22, 77.36, 75.46, 57.09, 56.21, 32.33, 29.83, 27.79, 19.22, 14.09.

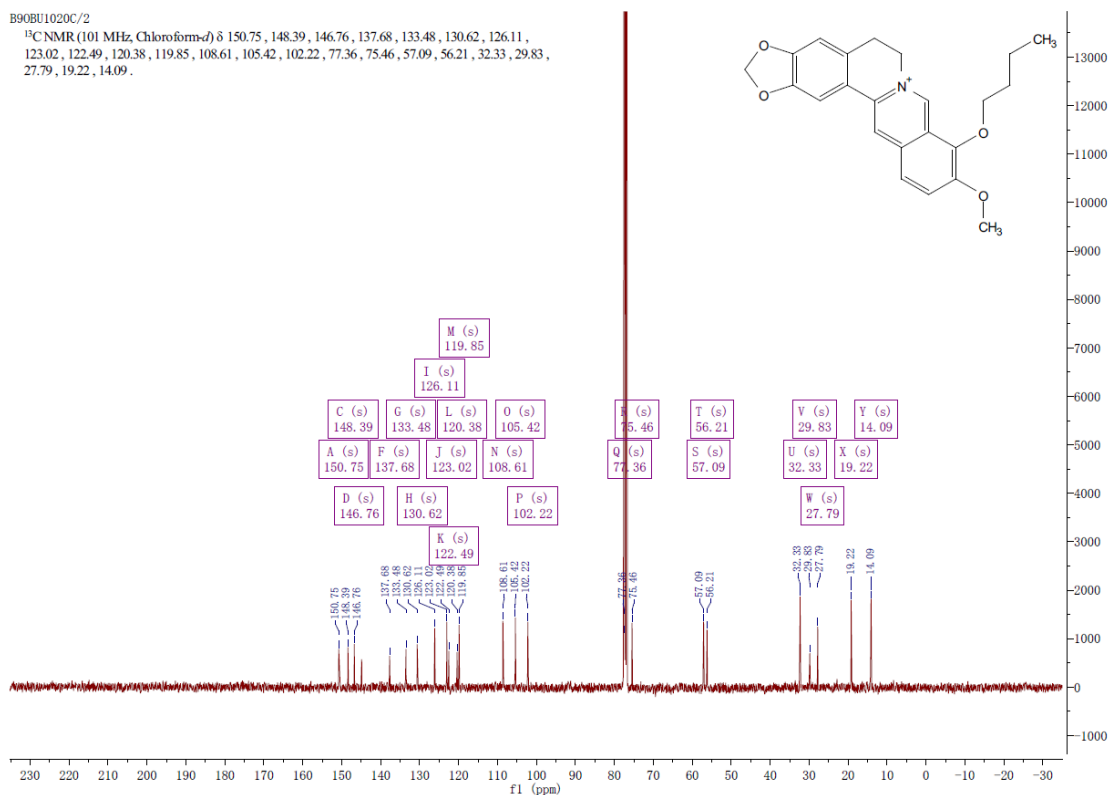


Figure S 10 ^{13}C NMR spectra of compound B90BU

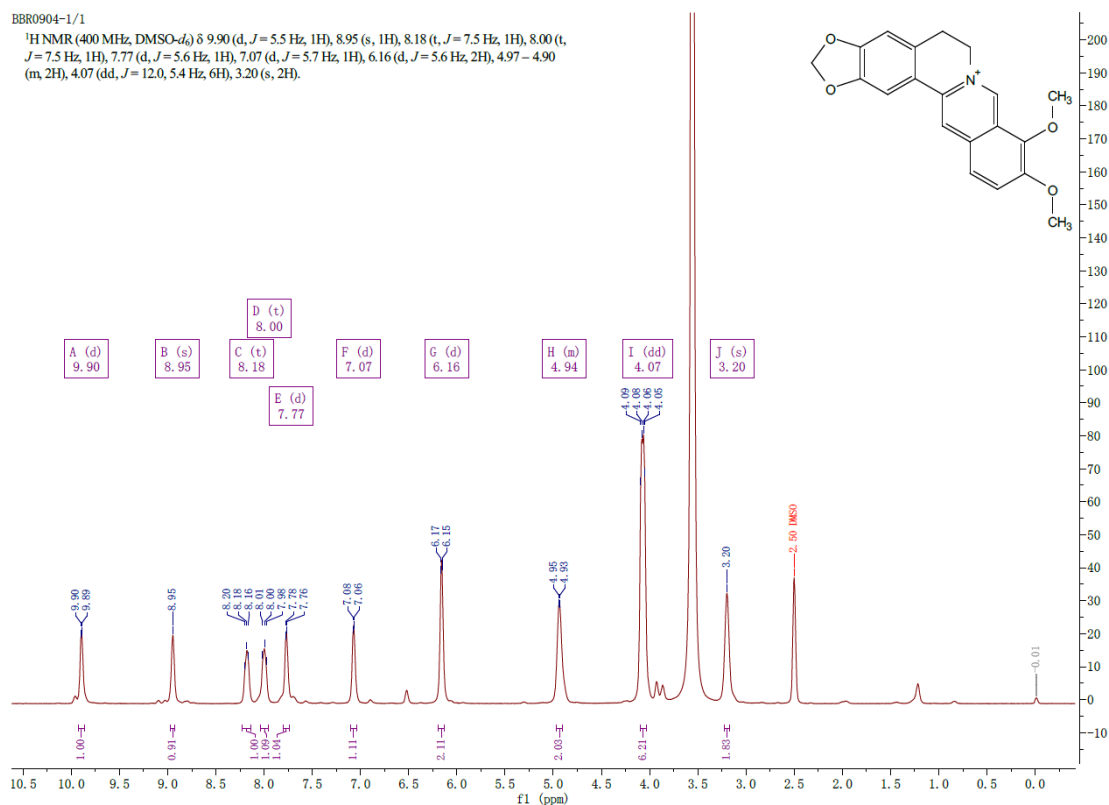


Figure S 11 ^1H NMR spectra of compound BBR

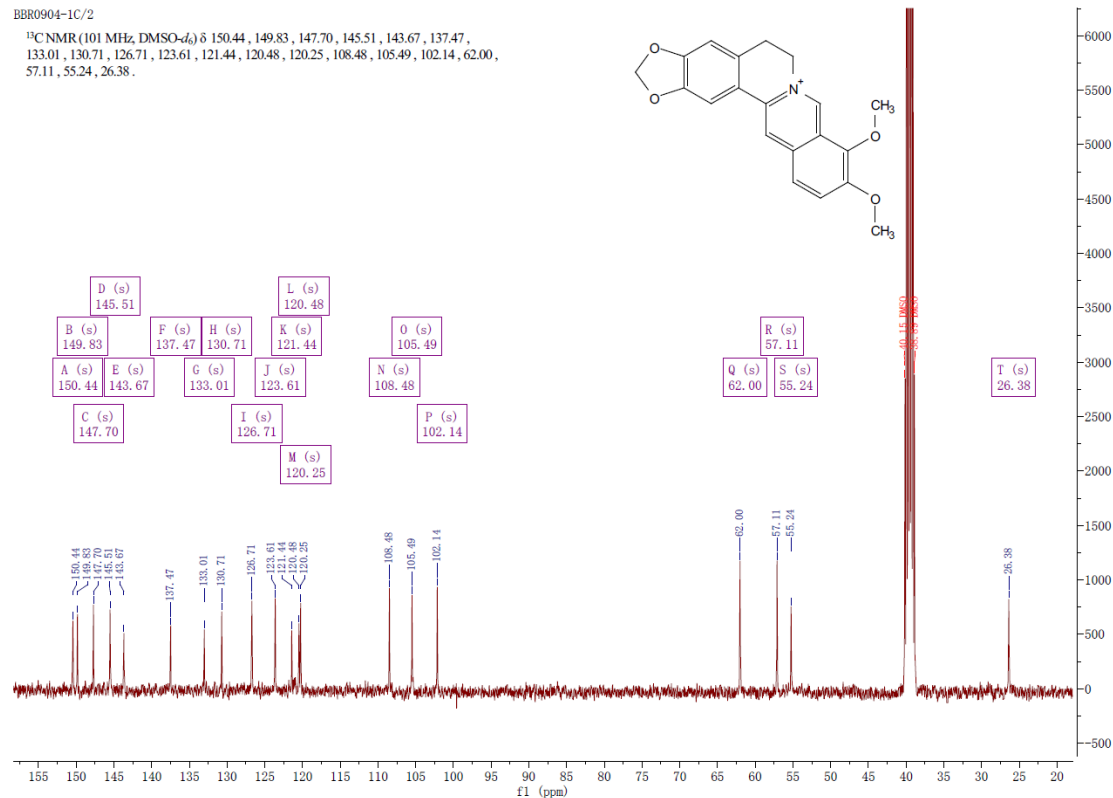


Figure S 12 ^{13}C NMR spectra of compound BBR

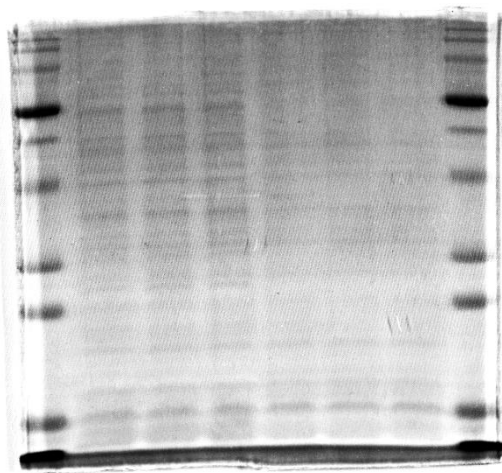


Figure S 13 Western blot images for PBS-B9OC

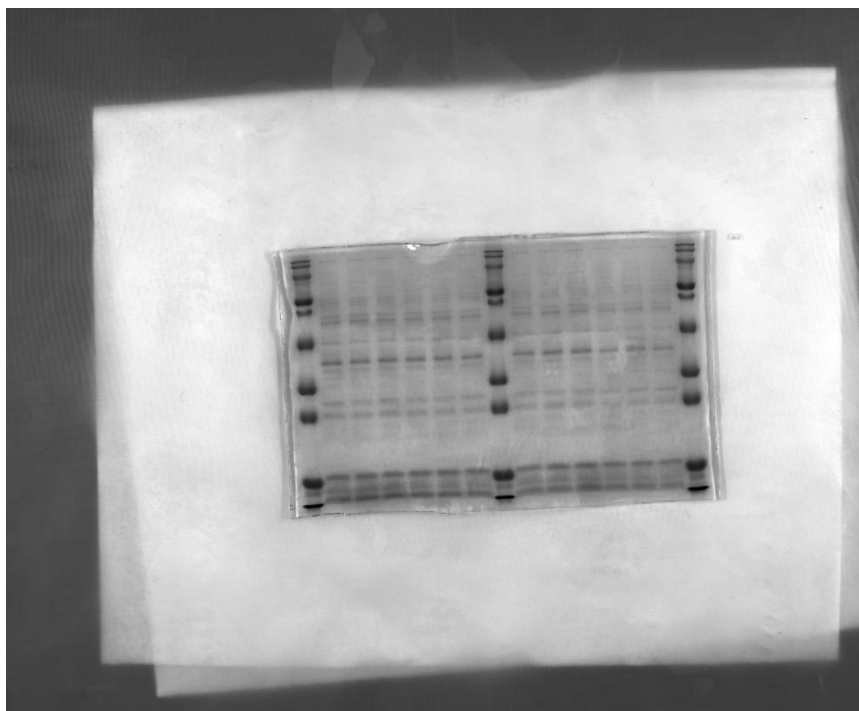


Figure S 14 Western blot images for PBS-BBR-CAN-BBR+CAN

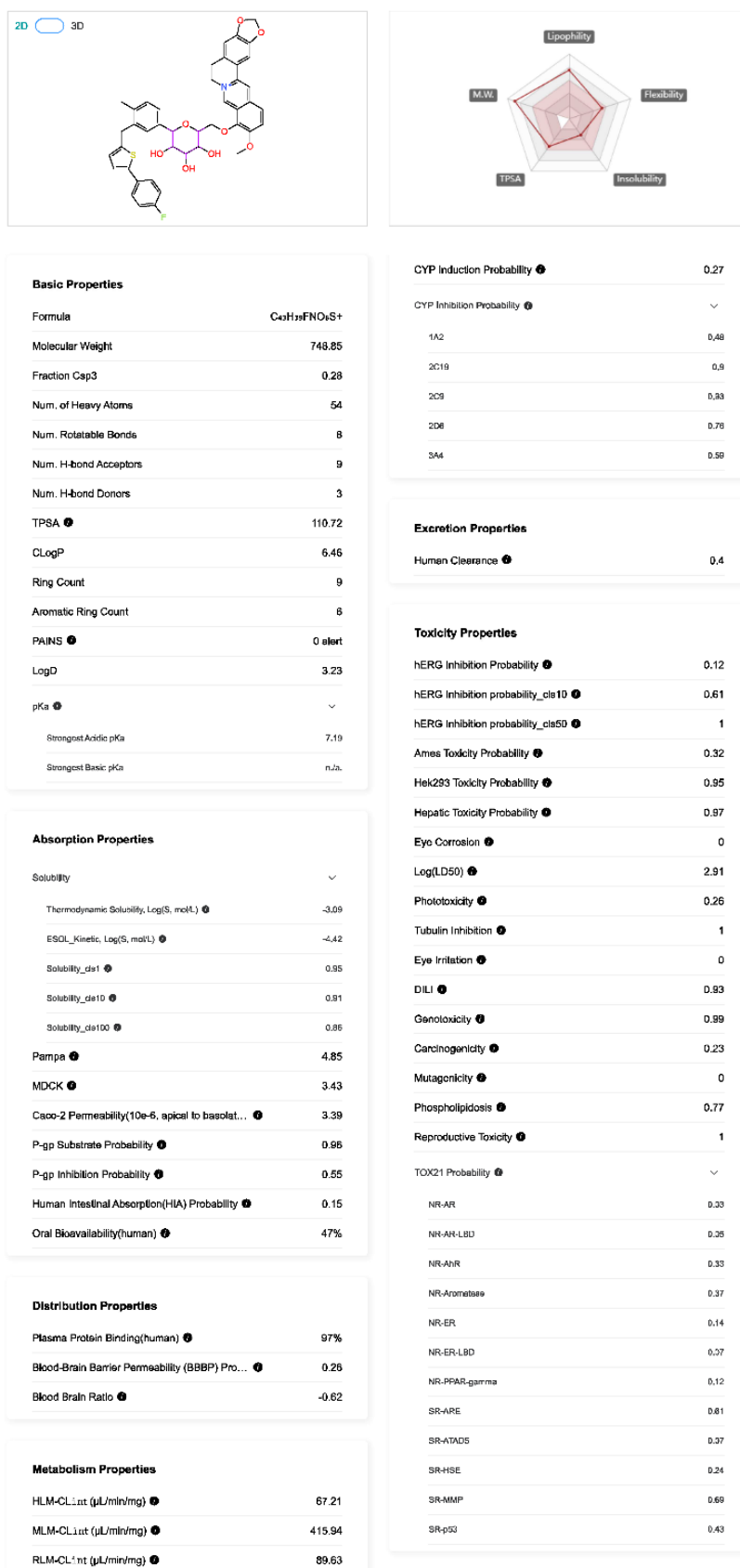


Figure S 15 ADMET Prediction of B9OC Based on Computer Aided