Supporting Information For

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

Jinsheng Li [1,2,3], Xueli Hou [1,2,3], Jinlong Xiao [2,3], Li Zhu [2,3], Yujie Deng [2,3], Ziyi Li [2,3], Zijian Zhao [1,2,3,*], Zhenghong Luo [2,3,*] and Hao Wei [1,2]

[1] Department of Pharmacology, Shaanxi University of Chinese Medicine, Xianyang 712046, China; jsli1006@163.com (J.L.); xlhou199885@163.com (X.H.); weihao217@163.com (H.W.)
[2] School of Chemistry and Materials Science, Huaihua University, Huaihua 418000, China; jlxiao0204@163.com (J.X.); lizzz082803@163.com (L.Z.); dyj20040128@163.com (Y.D.); zyli1202@163.com (Z.L.);
[3] Key Laboratory of Research and Utilization of Ethnomedicinal Plant Resources of Hunan Province, Huaihua University, Huaihua 418000, China
* Correspondence: luozhenghong06@163.com (Z.L.); zzj@hhtc.edu.cn (Z.Z.)

CATALOG

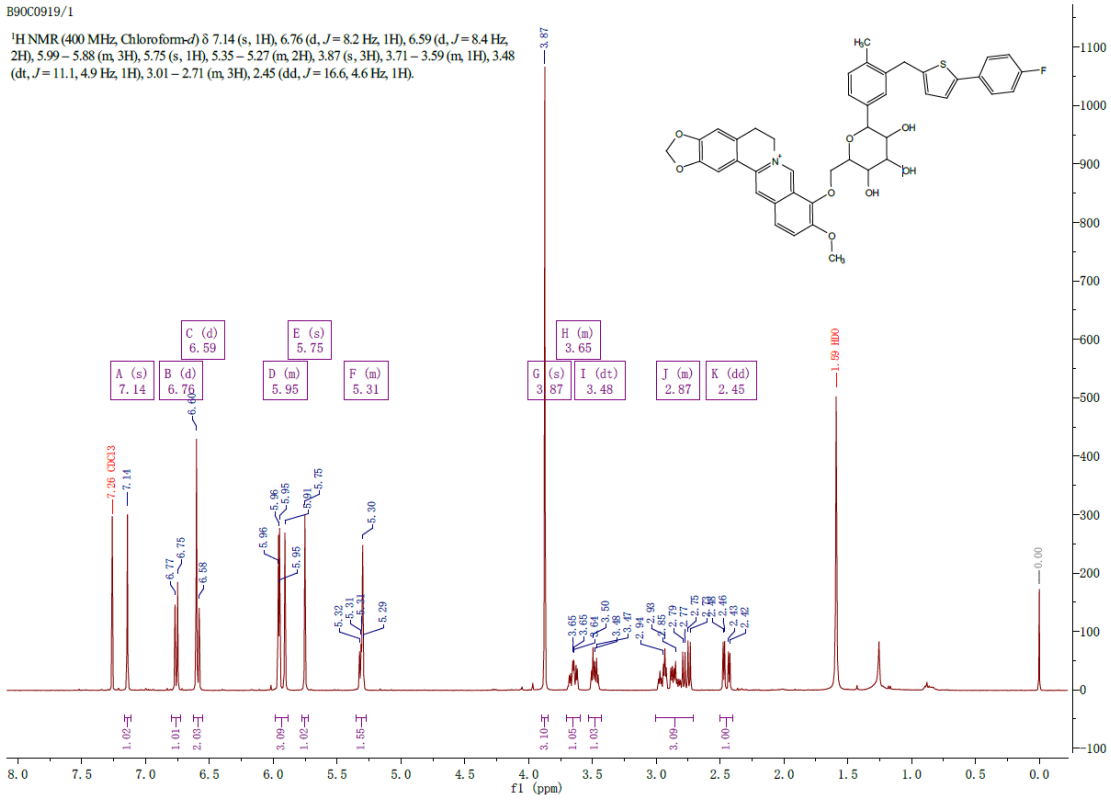


Figure S 1 ¹H NMR spectra of compound **B9OC**

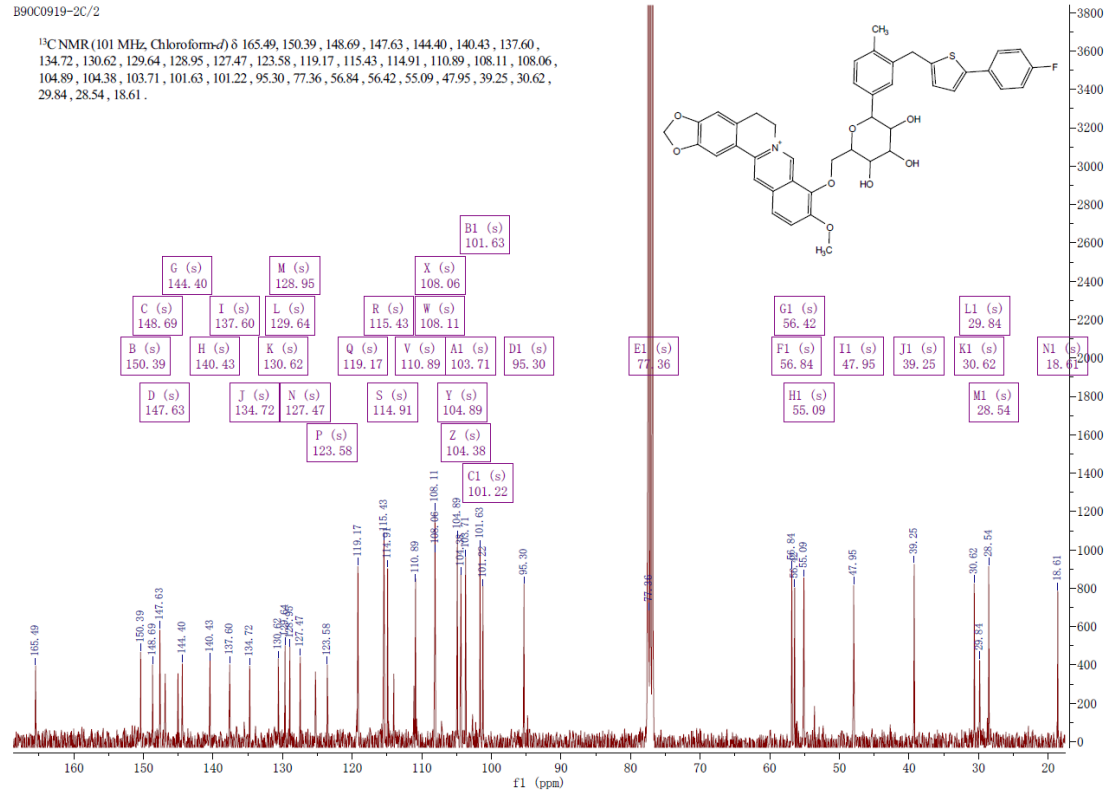


Figure S 2 ¹³C NMR spectra of compound **B9OC**

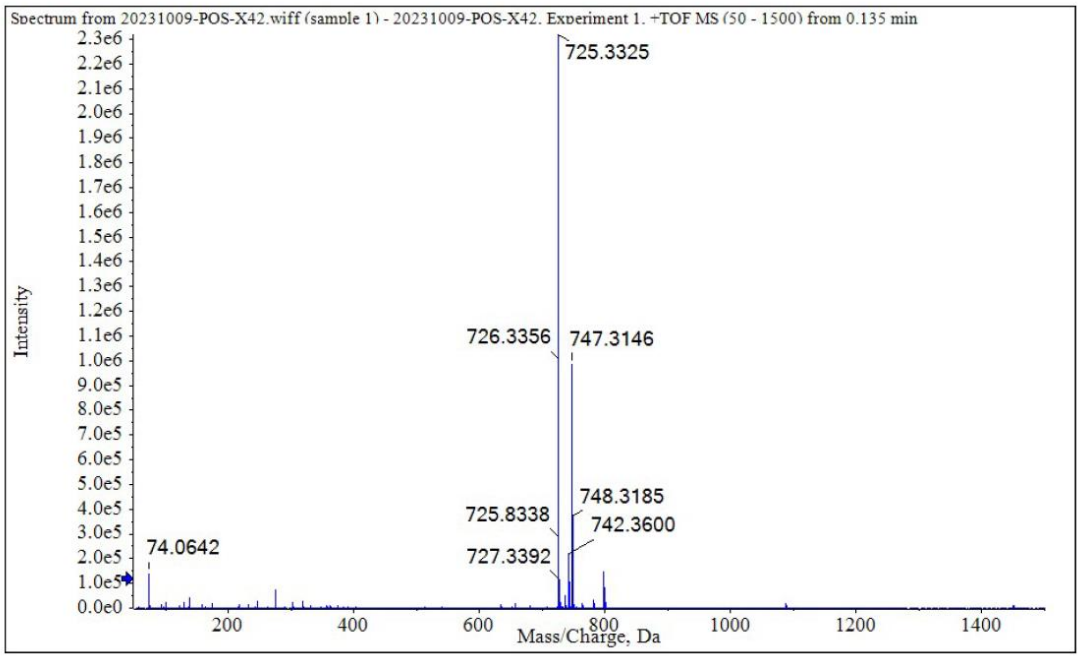


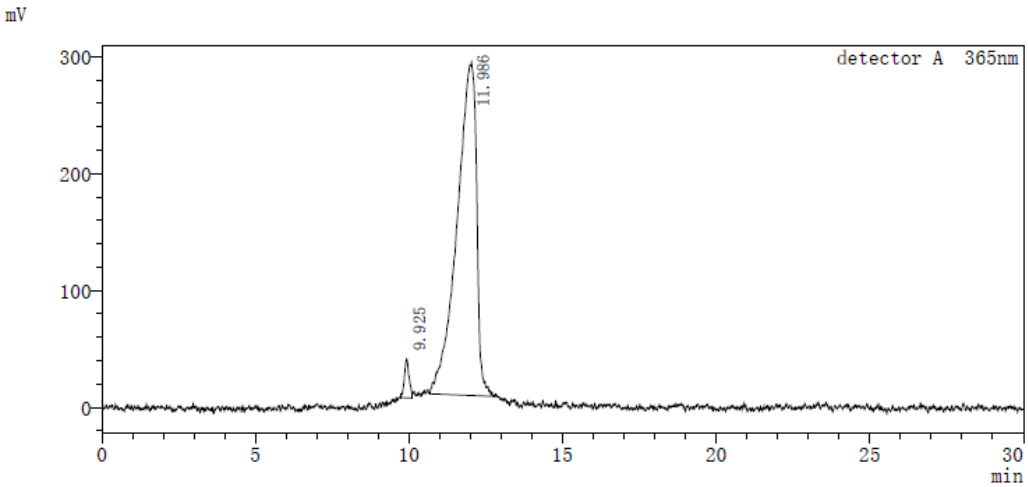
Figure S 3 MS spectra of compound B9OC

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

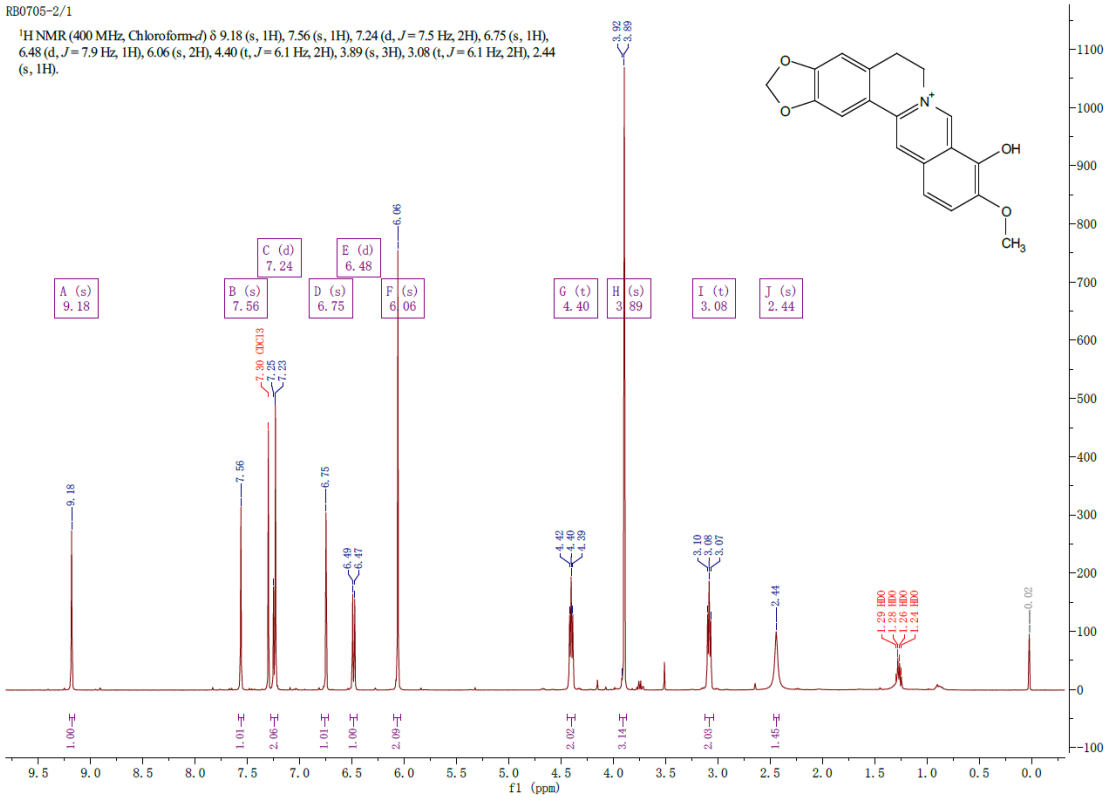


Figure S 5 ¹H NMR spectra of compound **Berberrubine**

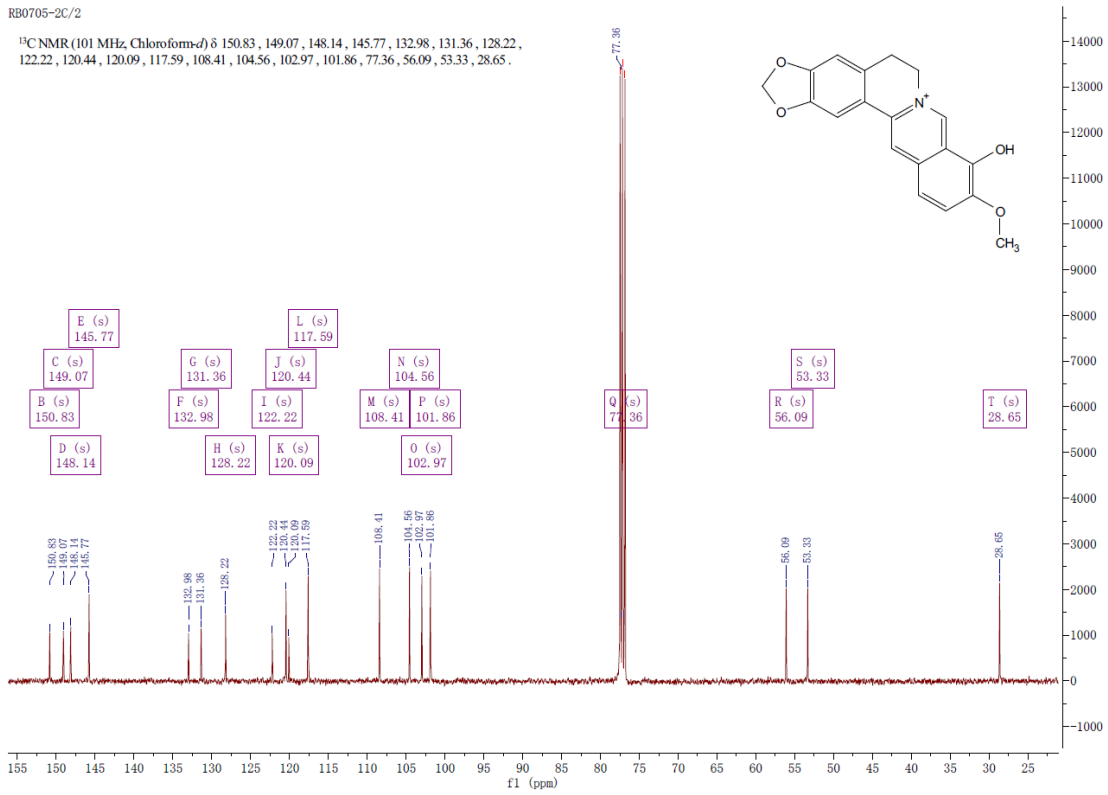


Figure S 6 ¹³C NMR spectra of compound **Berberrubine**

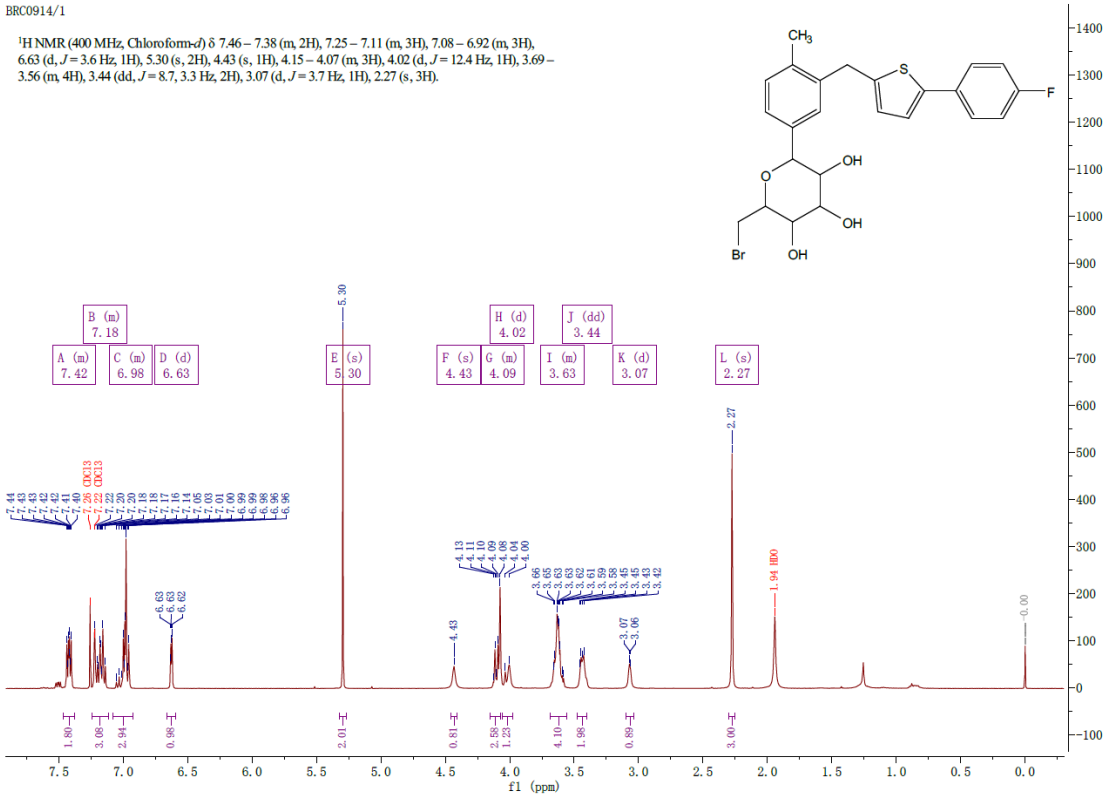


Figure S 7 ¹H NMR spectra of compound **Canagliflozin bromide**

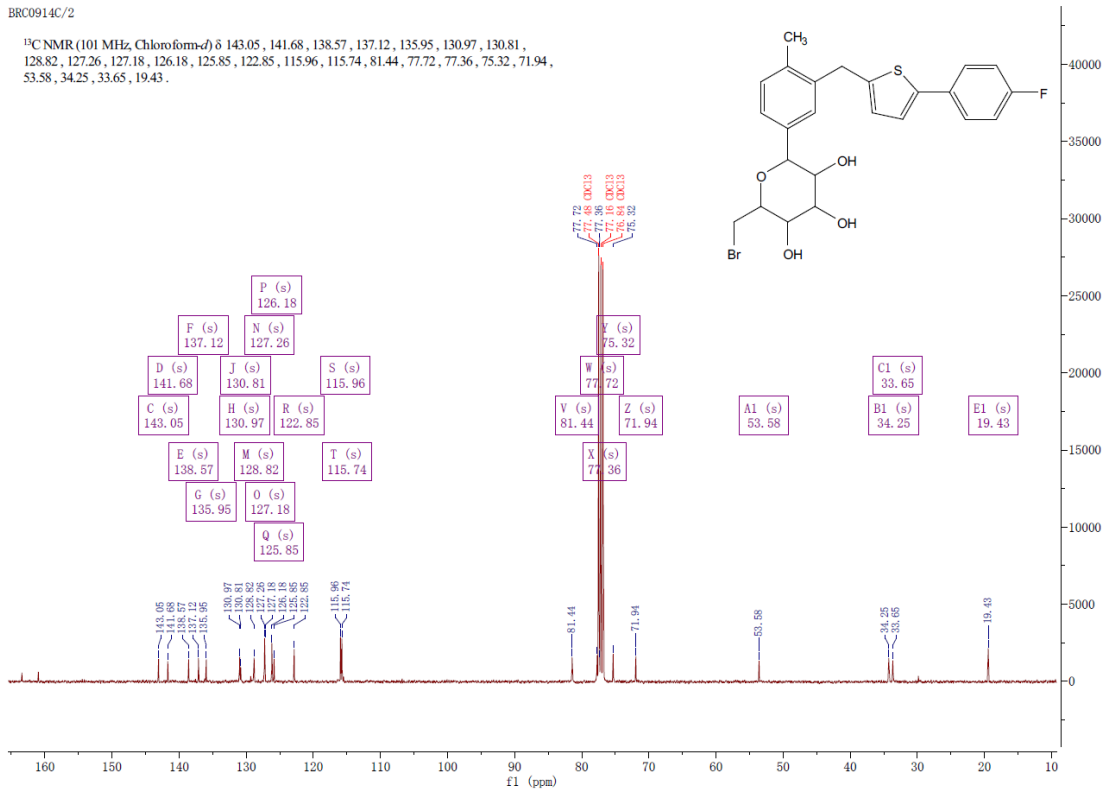


Figure S 8 ¹³C NMR spectra of compound **Canagliflozin bromide**

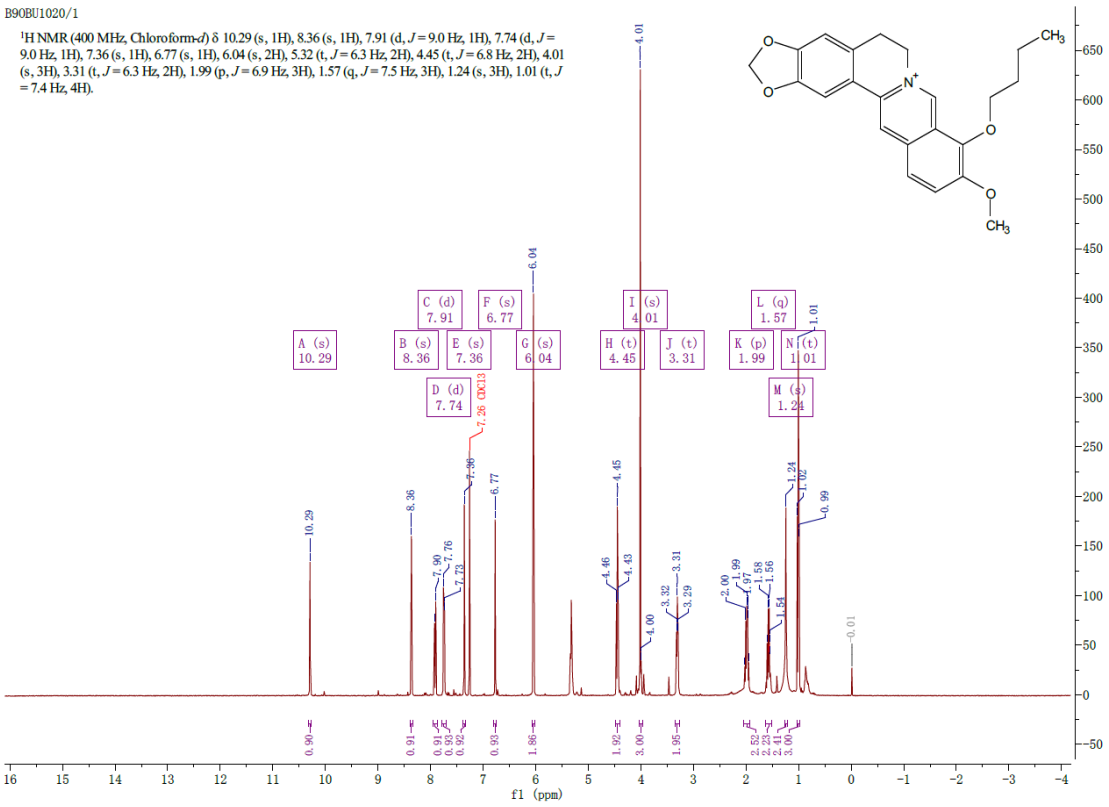


Figure S 9 ¹H NMR spectra of compound **B9OBU**

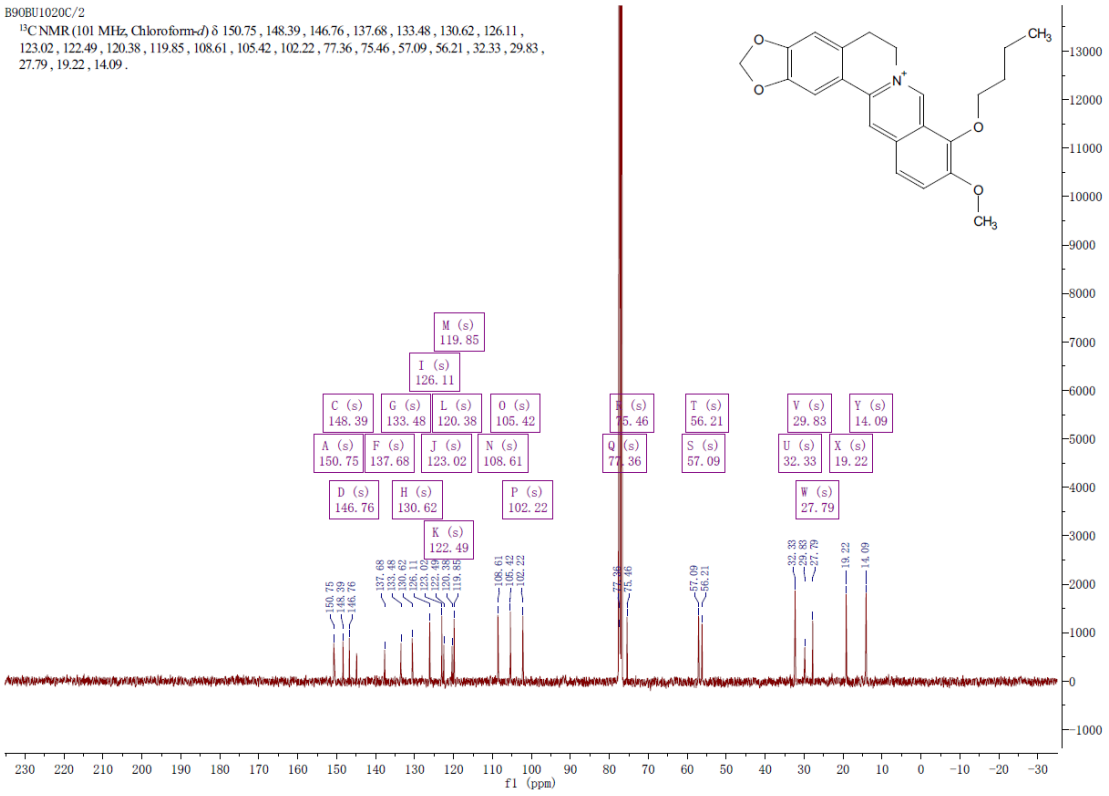


Figure S 10 ¹³C NMR spectra of compound **B9OBU**

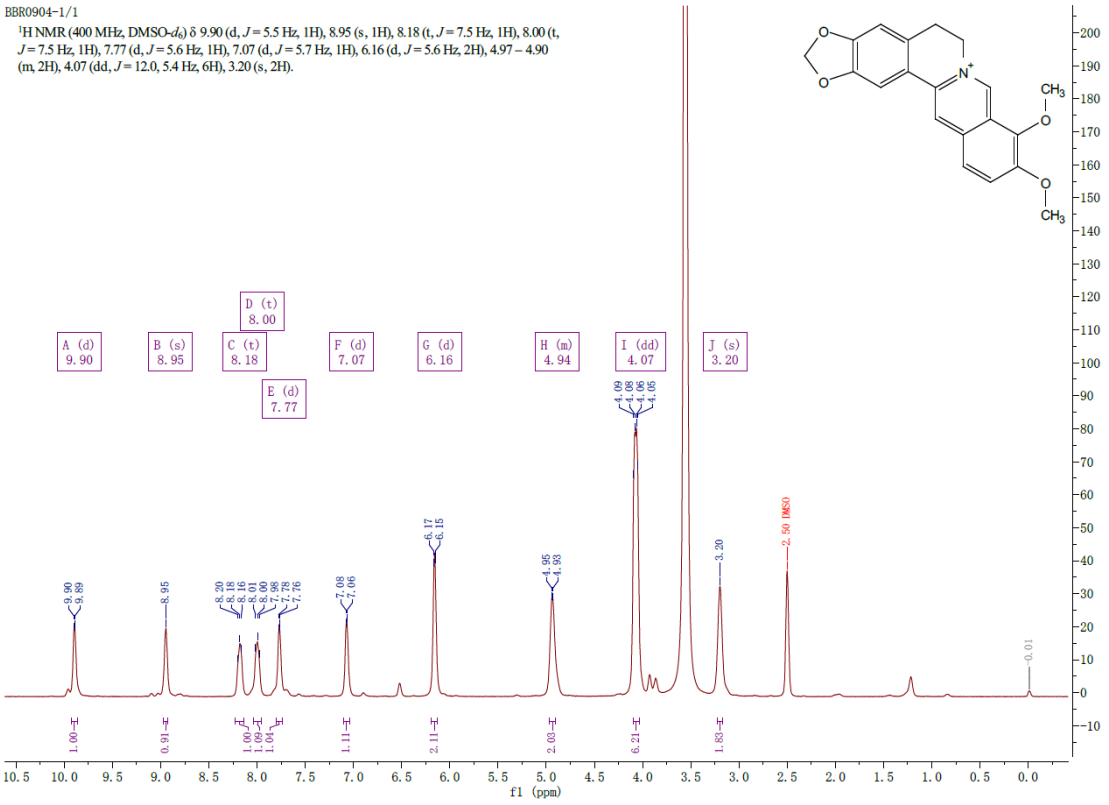


Figure S 11 ¹H NMR spectra of compound **BBR**

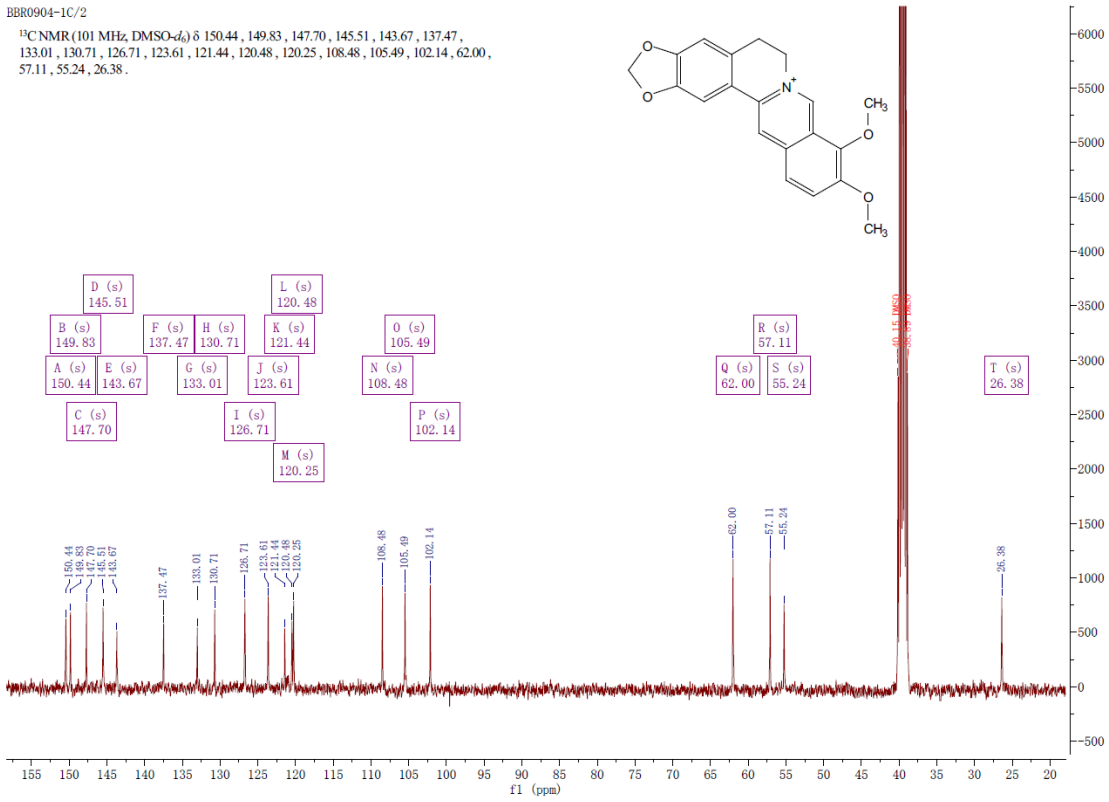


Figure S 12 ¹³C NMR spectra of compound **BBR**

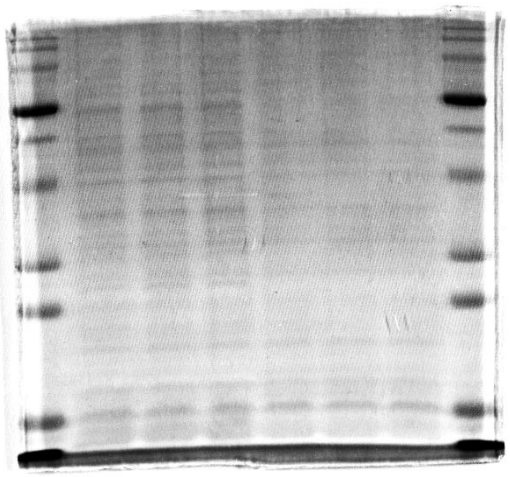


Figure S 13 **Western blot images for PBS-B9OC**

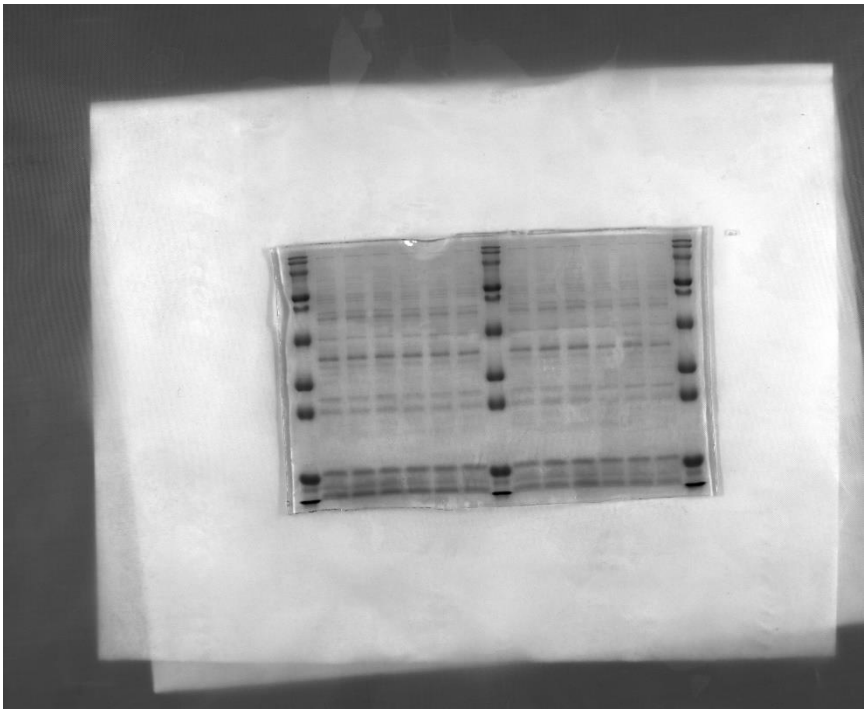


Figure S 14 **Western blot images for PBS-BBR-CAN-BBR+CAN**

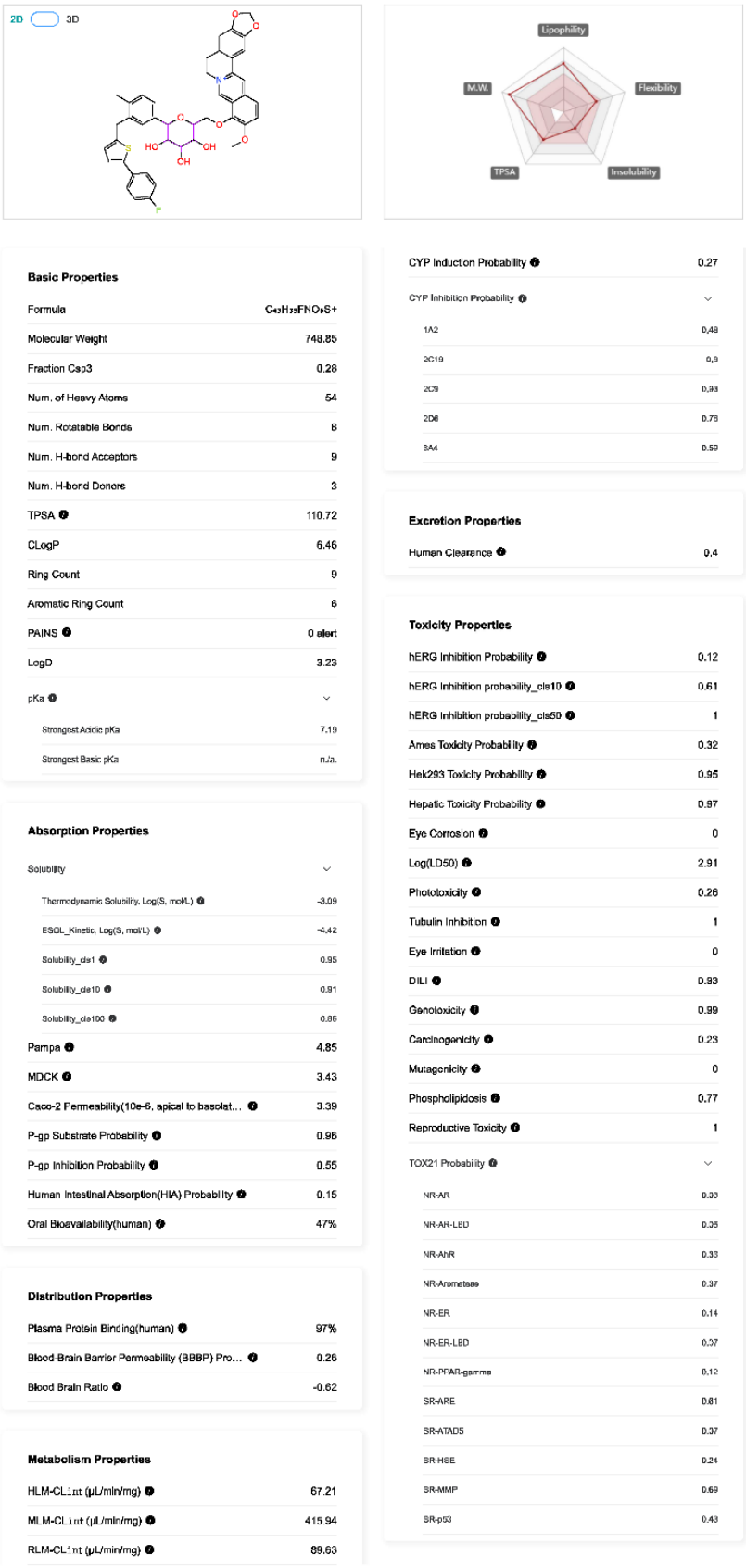


Figure S 15 ADMET Prediction of B9OC Based on Computer Aided