Supporting Information

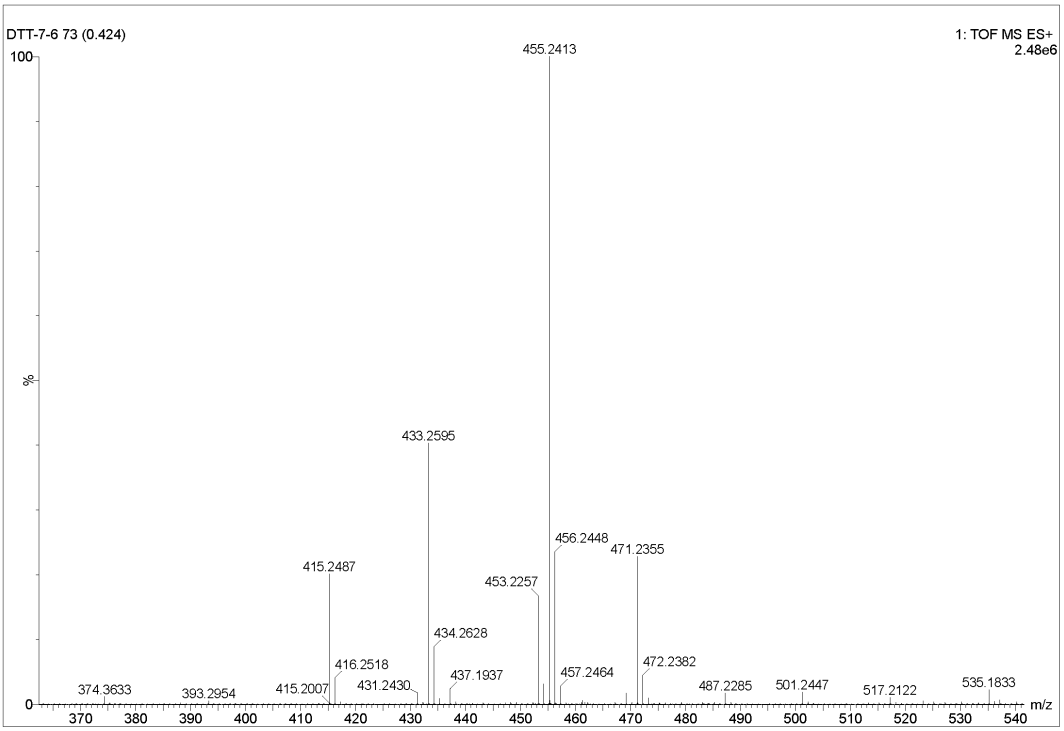
***Rec. Nat. Prod.* X:X (202X) XX-XX**

Secondary Metabolites with Antioxidant and Mushroom Tyrosinase Inhibitory Activities from *Ajuga nipponensis*

Na Sun, Tingting Du, Yifang Zhang, Yiming Luo, Xinyu Ma, Ru Zhang, Xinru Wu, Huanhuan Yang, Miao Zhou, Penghua Shu* and Jihong Huang*

Food and Pharmacy College, Xuchang University, Xuchang, Henan 461000, P. R. China

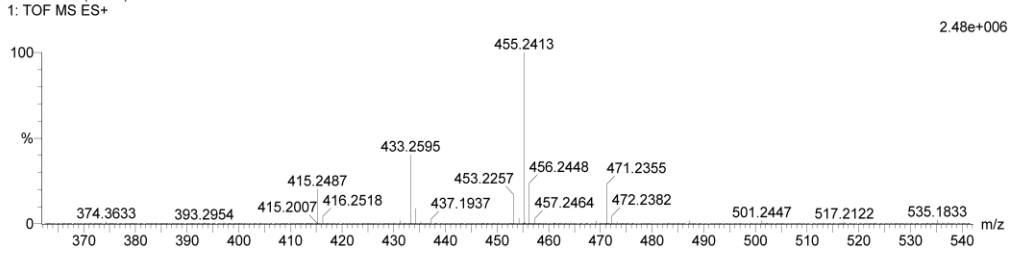
Table of Contents — **Page**



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
210 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 25-25 H: 0-60 N: 0-10 O: 0-9 Na: 0-1
DTT-7-6 73 (0.424)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
455.2413	455.2410	0.3	0.7	7.5	801.1	n/a	n/a	C25 H36 O6 Na

Figure S1: HR-ESI-MS spectrum of **1**

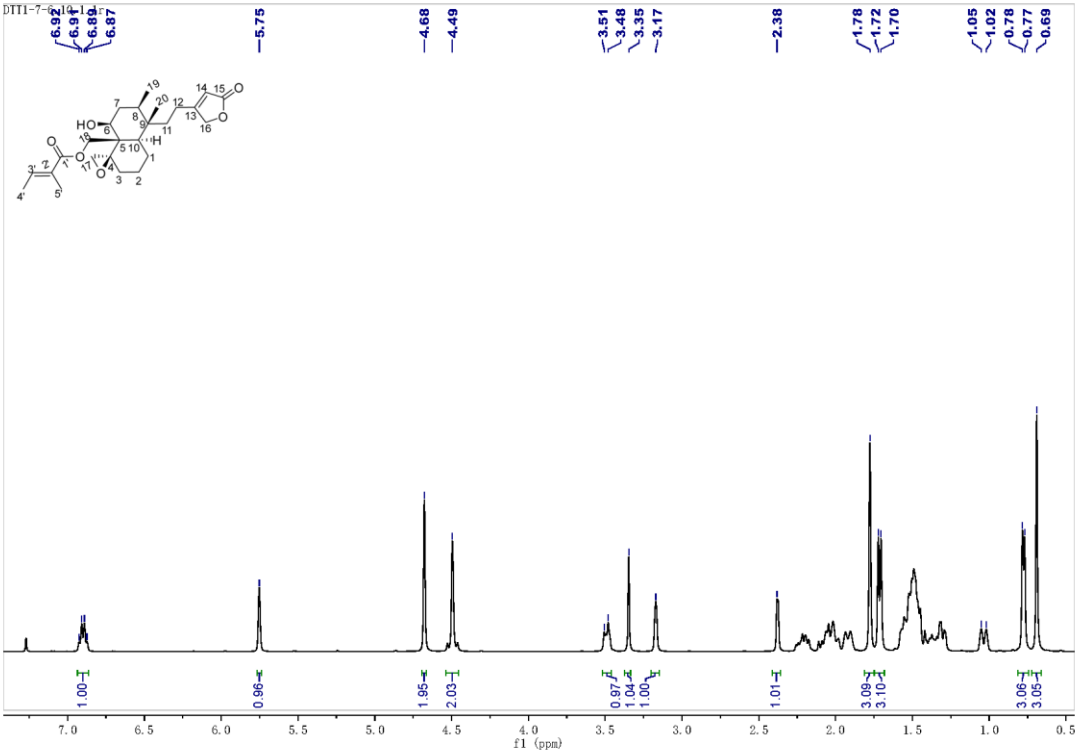


Figure S2: ^{1}H NMR spectrum (400 MHz) of 1 in $CDCl_3$

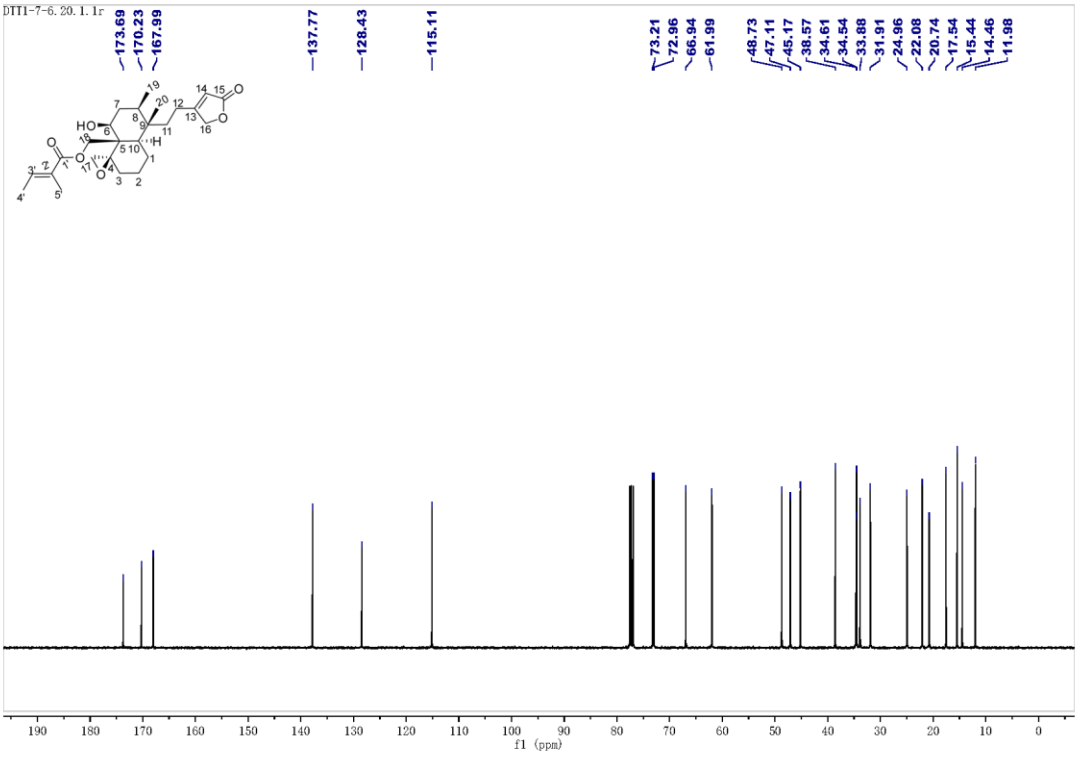


Figure S3: ^{13}C NMR spectrum (100 MHz) of 1 in $CDCl_3$

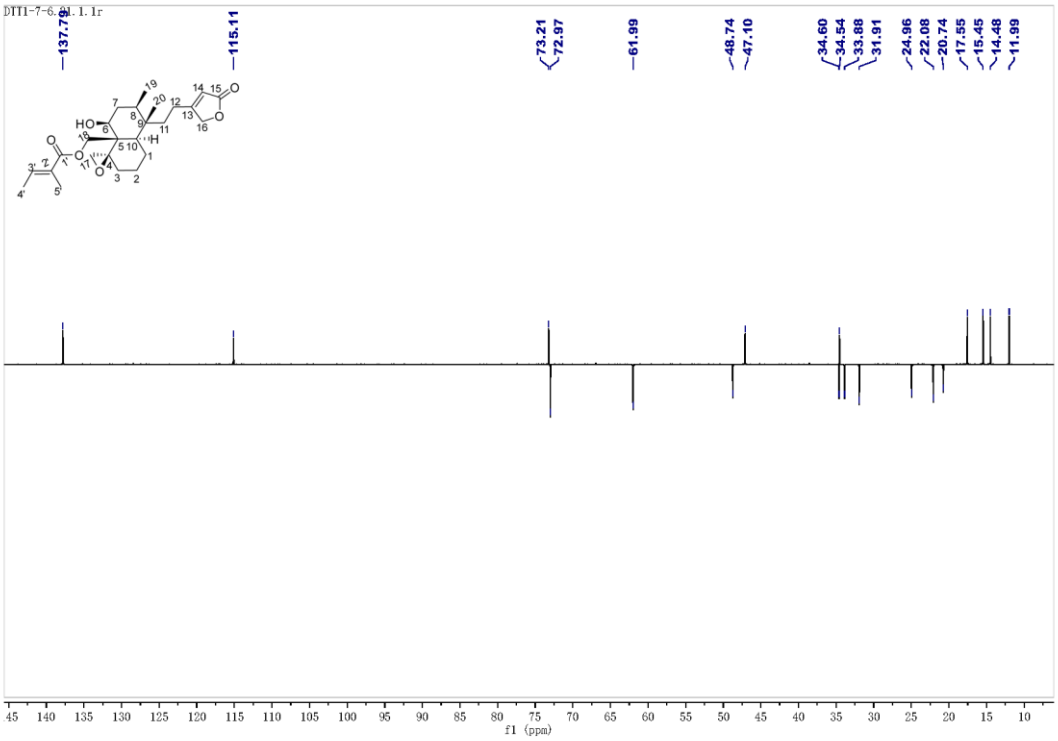


Figure S4: DEPT NMR spectrum (100 MHz) of 1 in $CDCl_3$

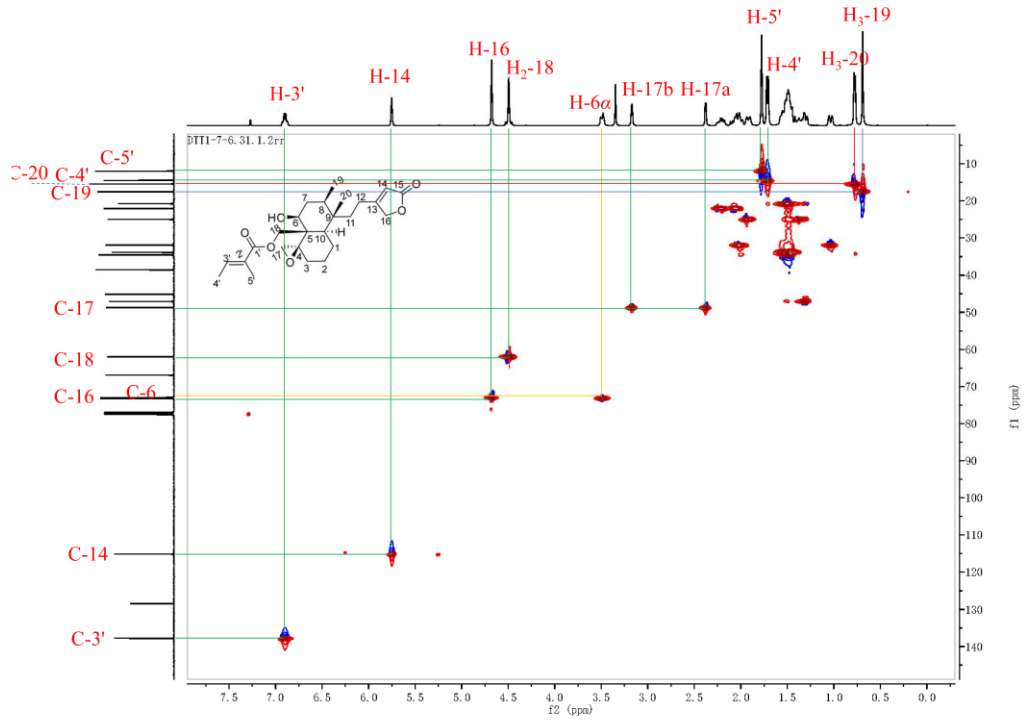


Figure S5: HSQC spectrum of 1 in $CDCl_3$

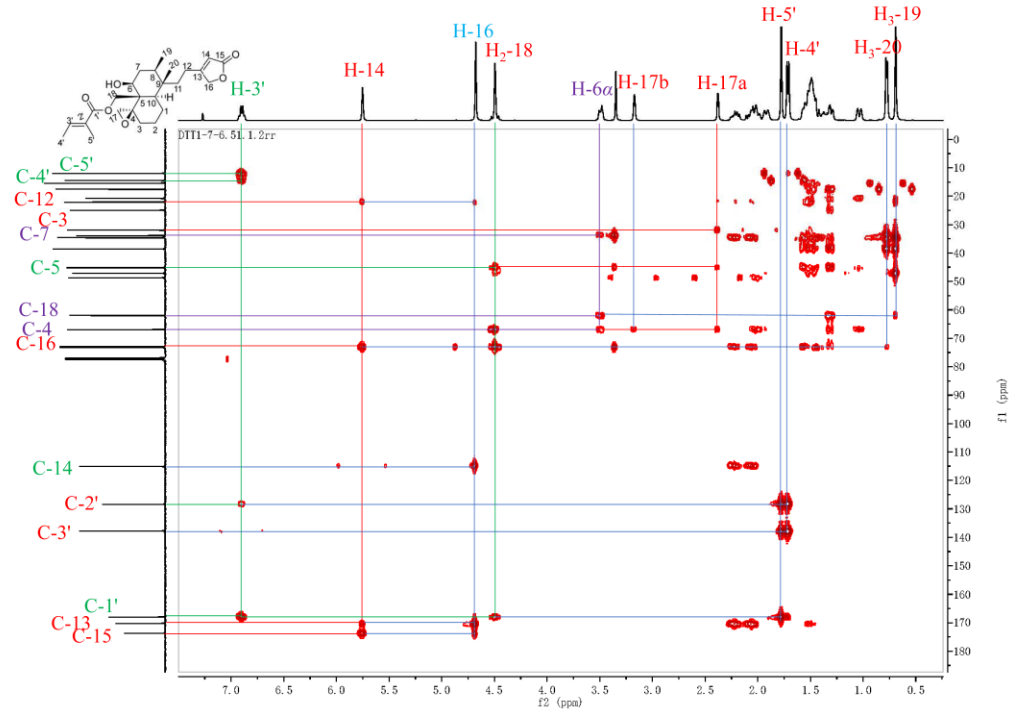


Figure S6: HMBC spectrum of 1 in $CDCl_3$

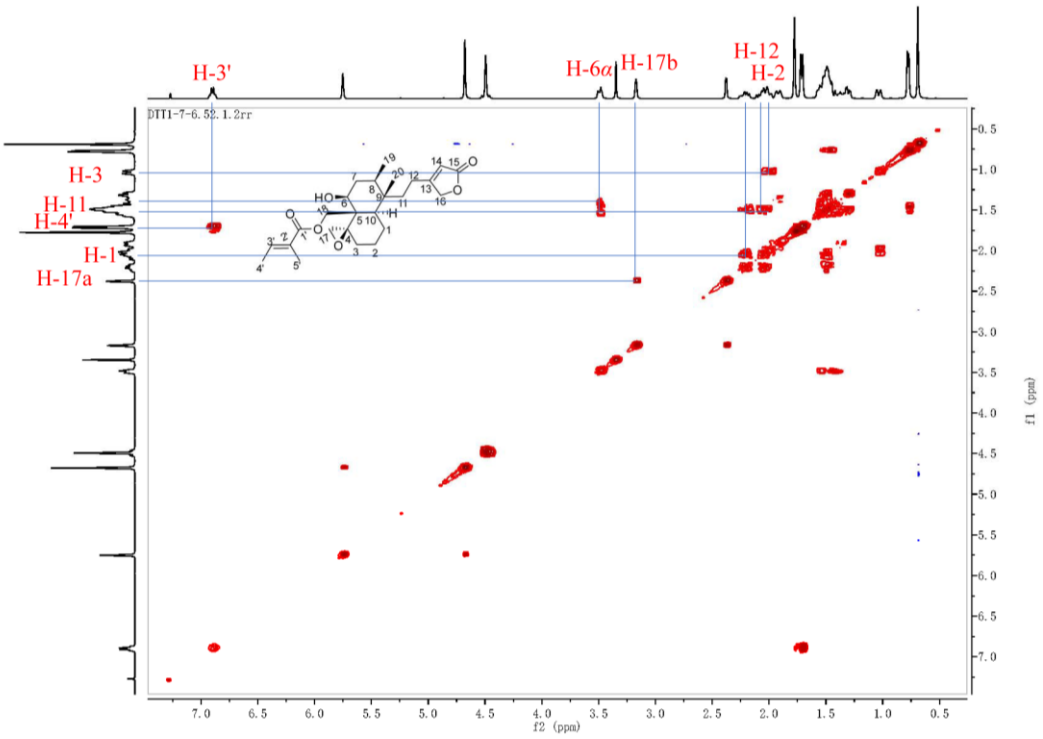


Figure S7: ^{1}H-^{1}H COSY spectrum of 1 in $CDCl_3$

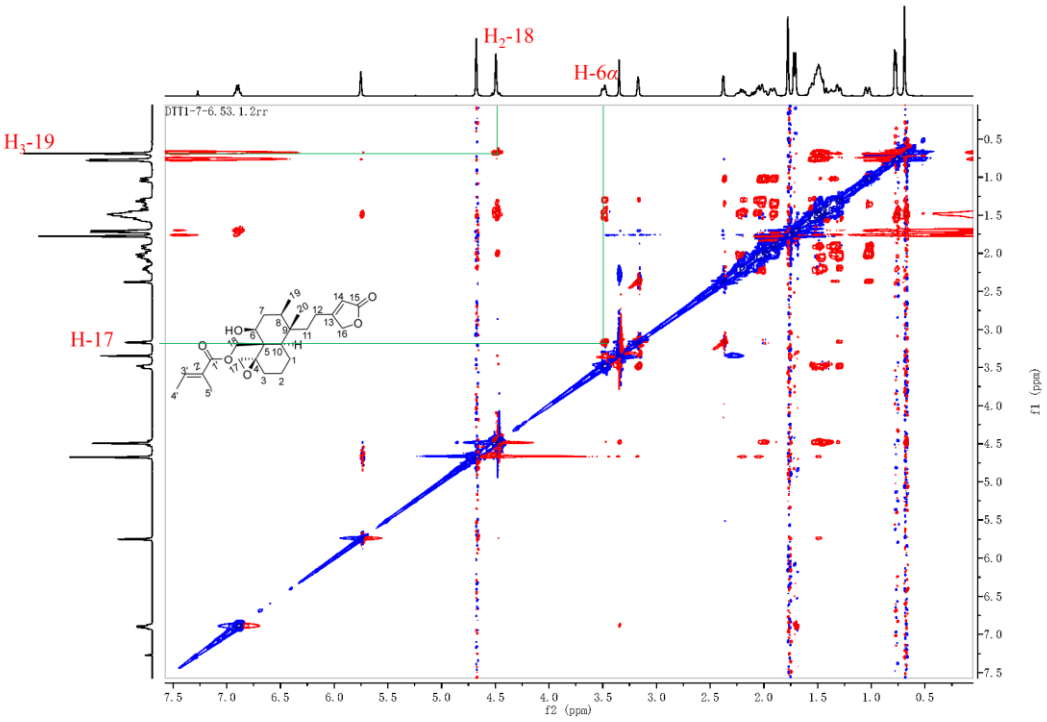


Figure S8: NOESY spectrum of 1 in $CDCl_3$

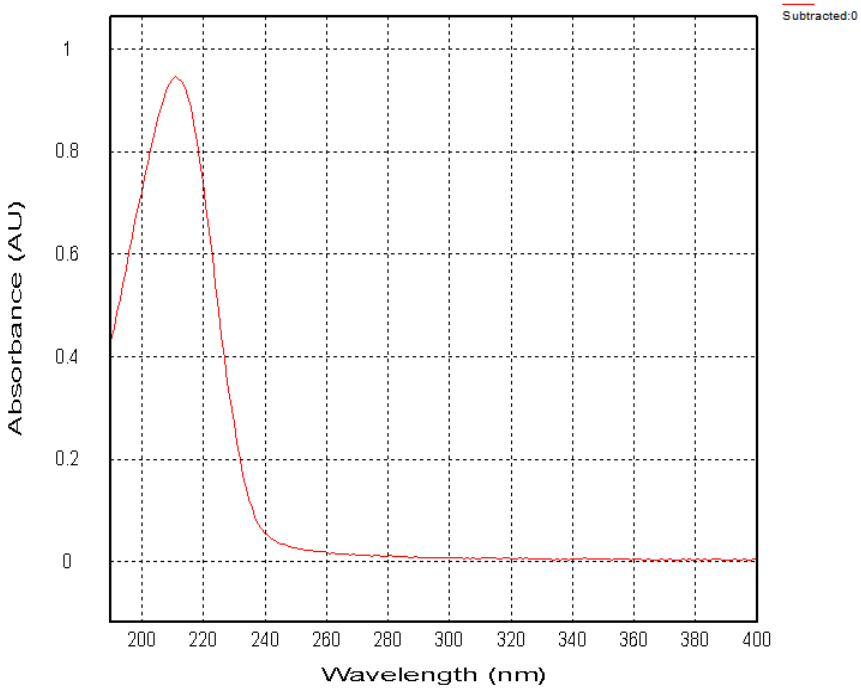


Figure S9: UV spectrum of 1 in CH_3CN

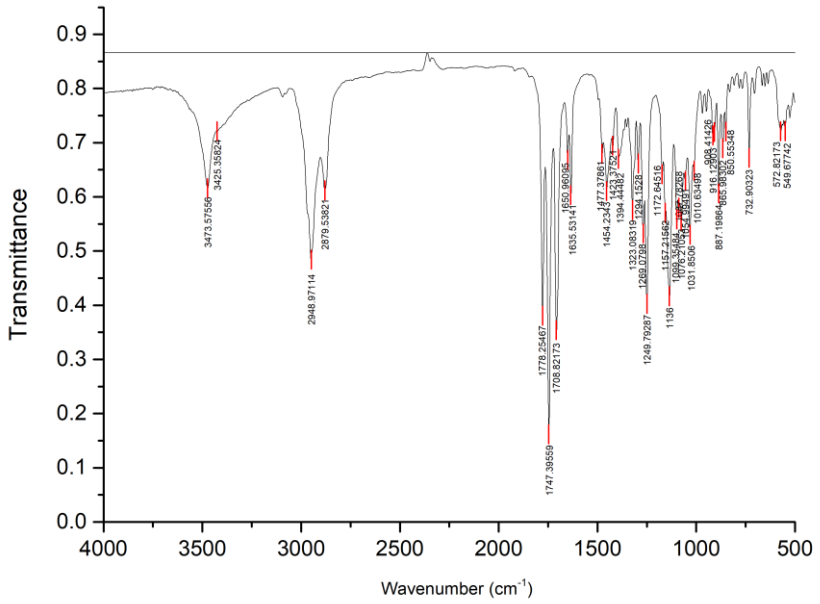


Figure S10: IR spectrum of 1

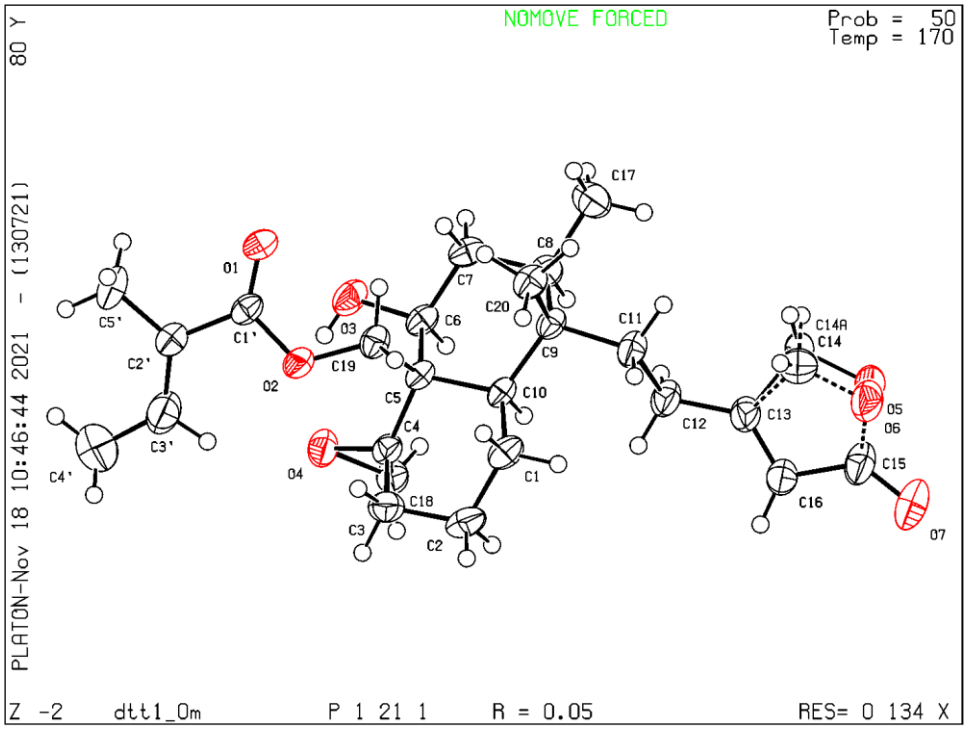


Figure S11: Crystal packing of 1 170 K

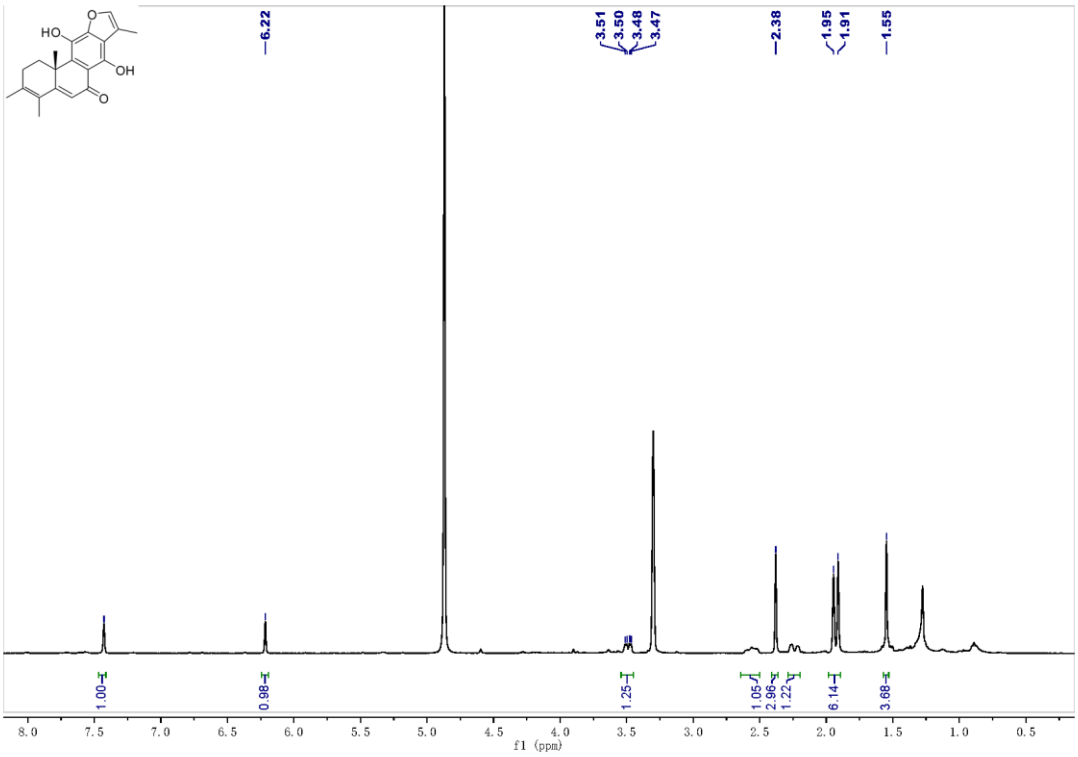


Figure S12: ^{1}H NMR spectrum (400 MHz) of 2 in CD_3OD

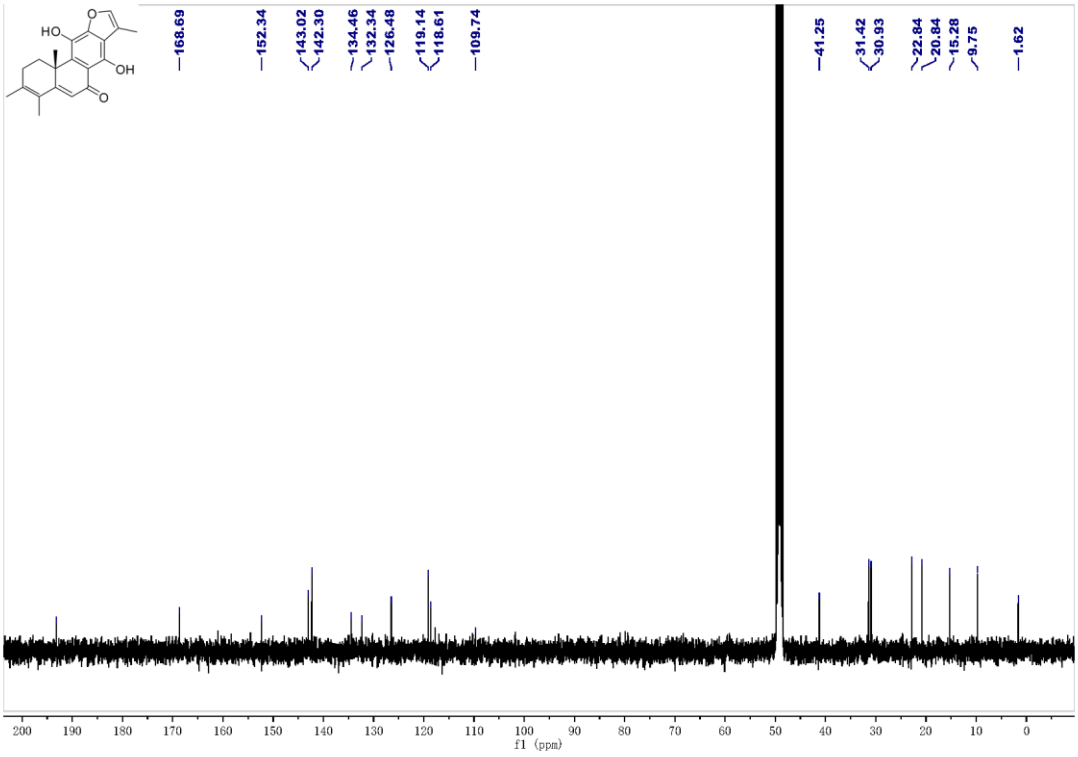


Figure S13: ^{13}C NMR spectrum (100 MHz) of 2 in CD_3OD

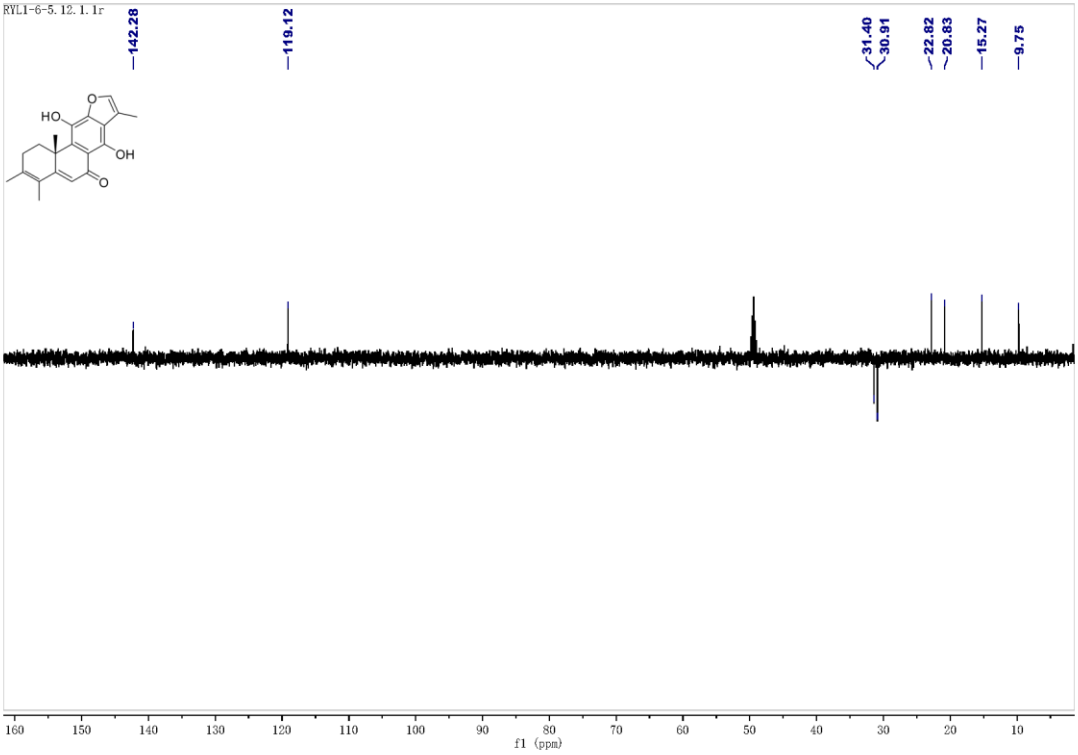


Figure S14: DEPT NMR spectrum (100 MHz) of 2 in CD_3OD

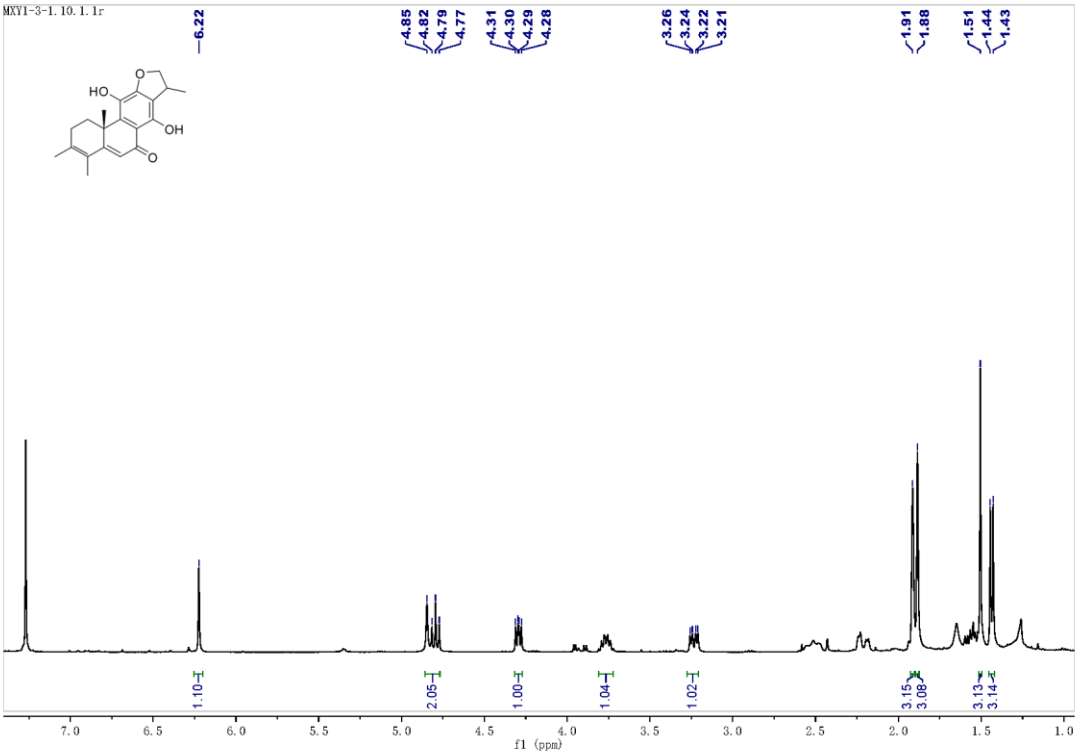


Figure S15: ^1H NMR spectrum (400 MHz) of 3 in $CDCl_3$

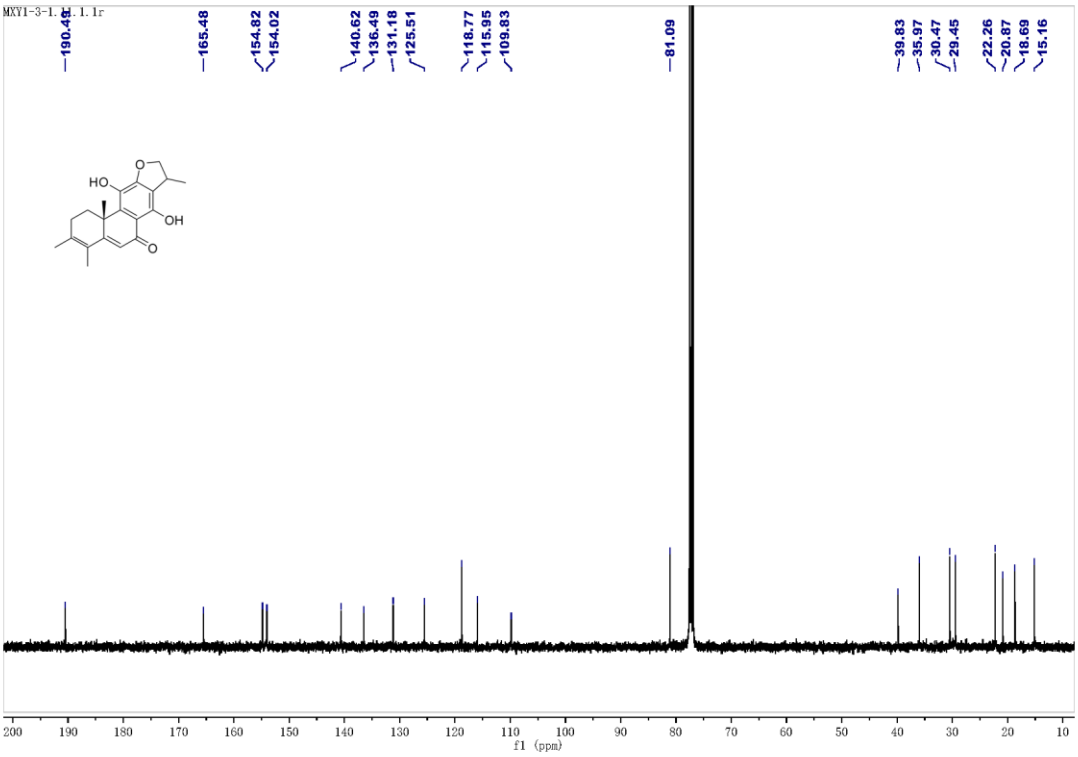


Figure S16: ^{13}C NMR spectrum (100 MHz) of 3 in $CDCl_3$

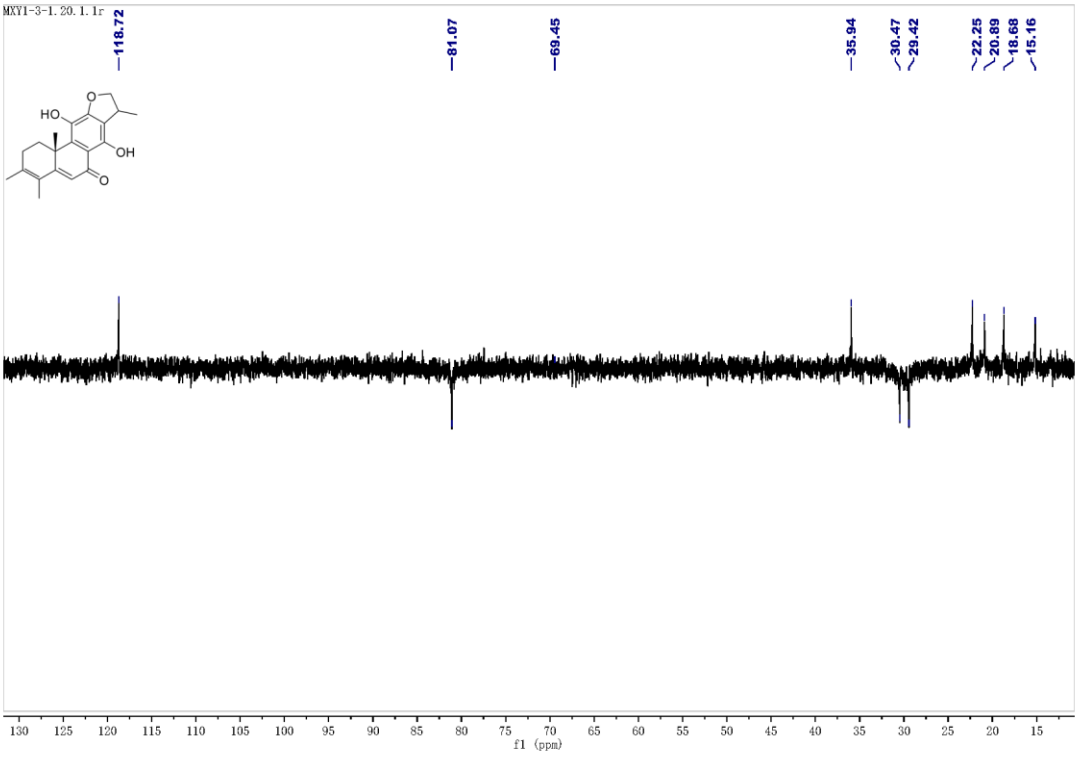


Figure S17: DEPT NMR spectrum (100 MHz) of 3 in $CDCl_3$

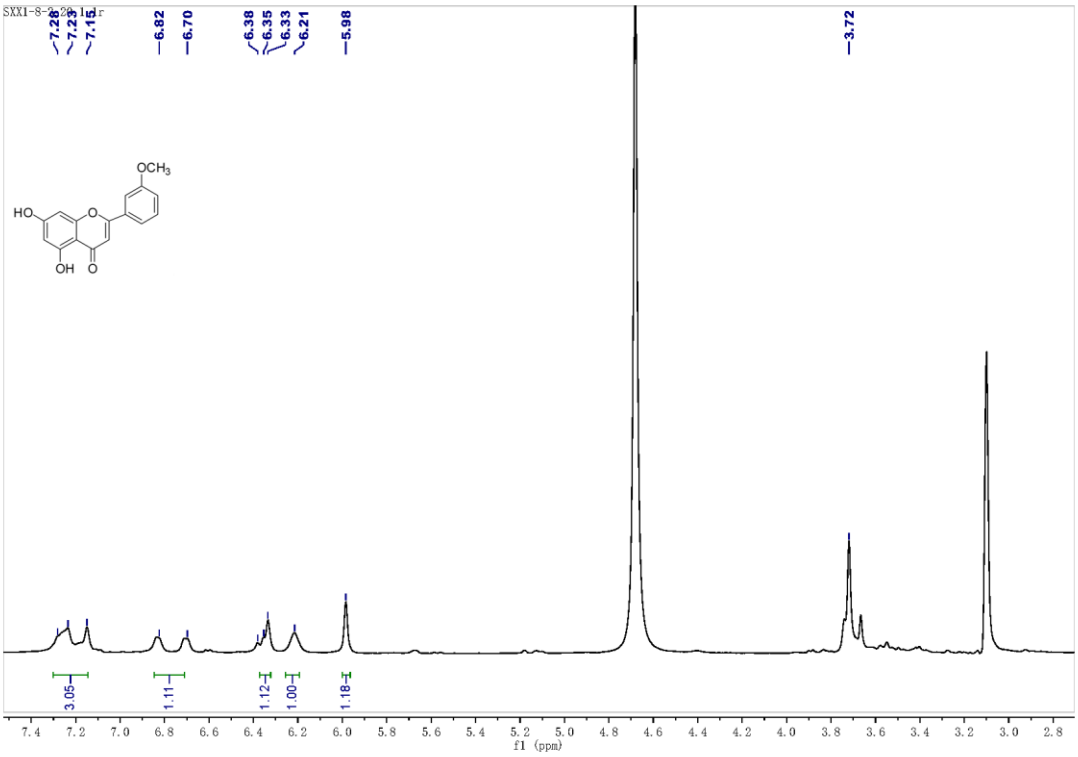


Figure S18: ^{1}H NMR spectrum (400 MHz) of 4 in CD_3OD

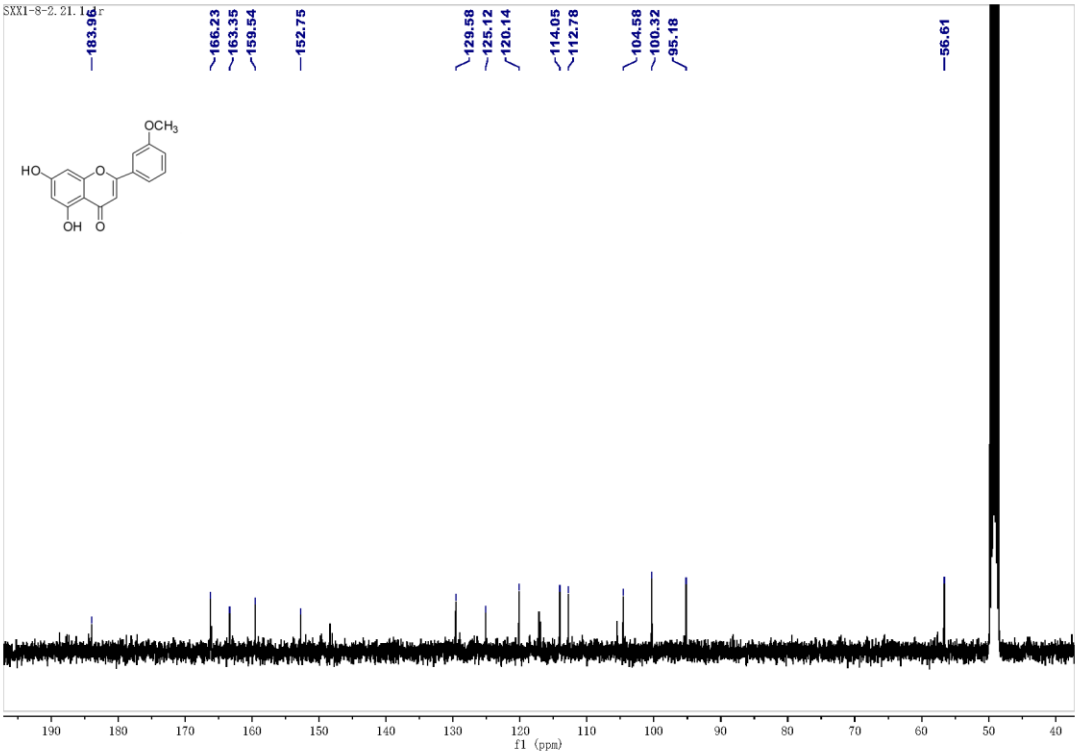


Figure S19: ^{13}C NMR spectrum (100 MHz) of 4 in CD_3OD

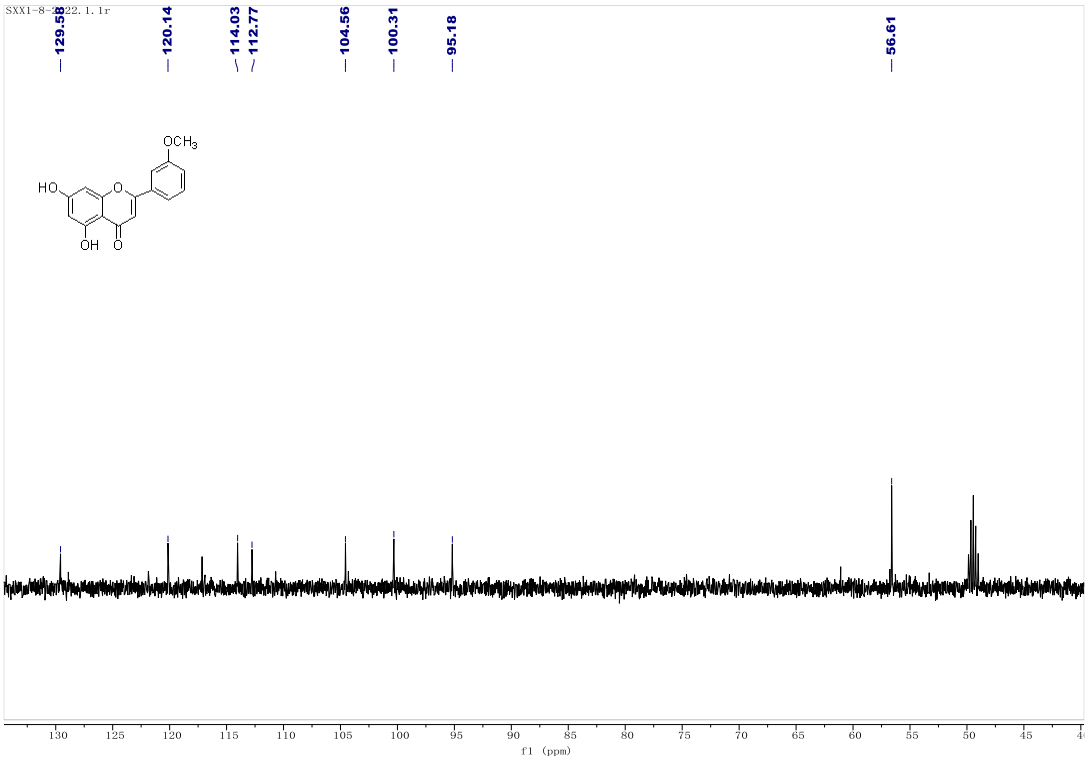


Figure S20: DEPT NMR spectrum (100 MHz) of 4 in CD_3OD

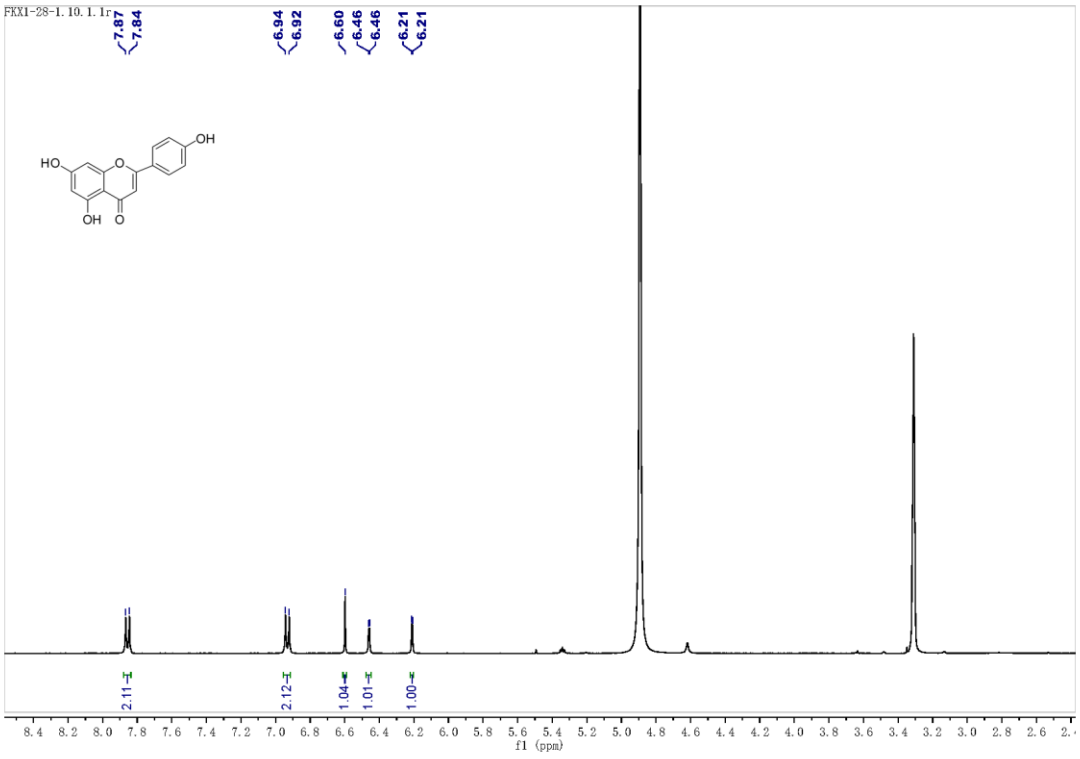


Figure S21: ^1H NMR spectrum (400 MHz) of 5 in CD_3OD

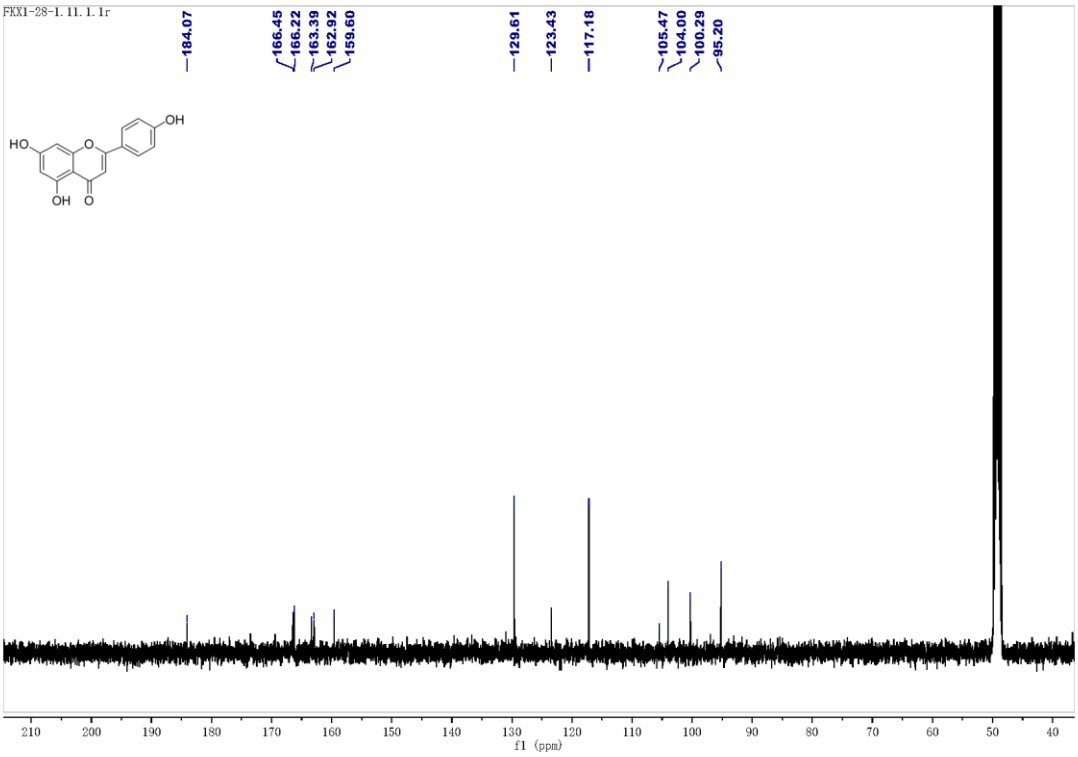


Figure S22: ^{13}C NMR spectrum (100 MHz) of 9 in CD_3OD

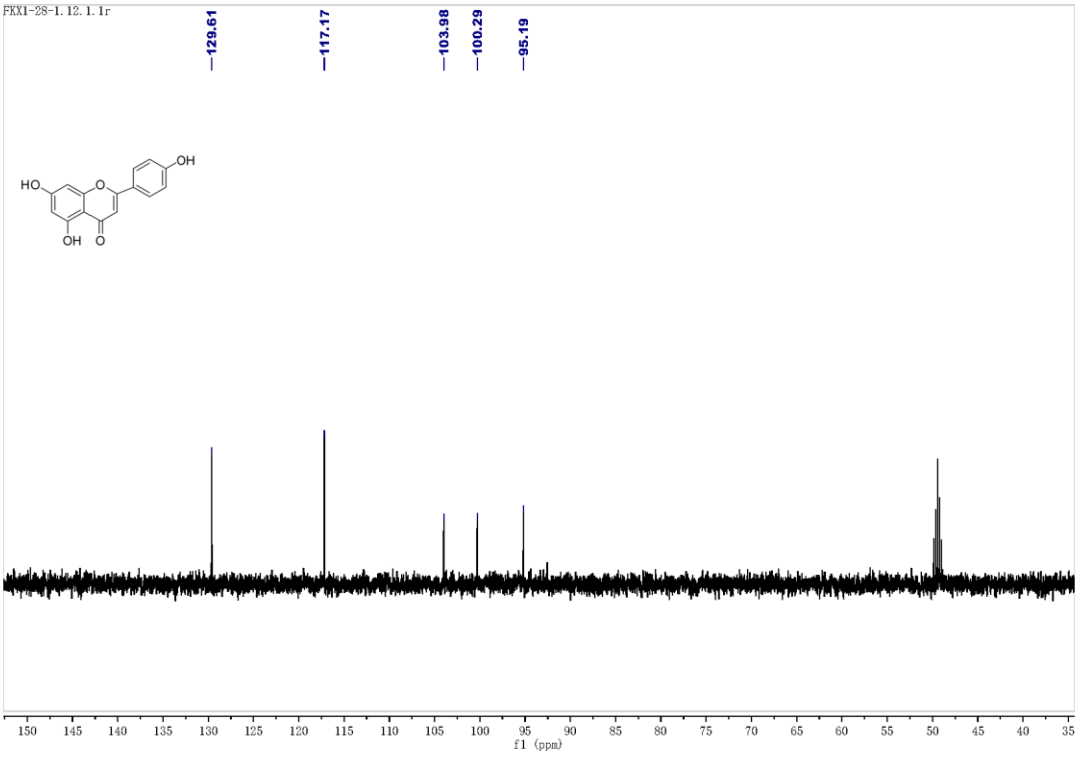


Figure S23: DEPT NMR spectrum (100 MHz) of 5 in CD_3OD

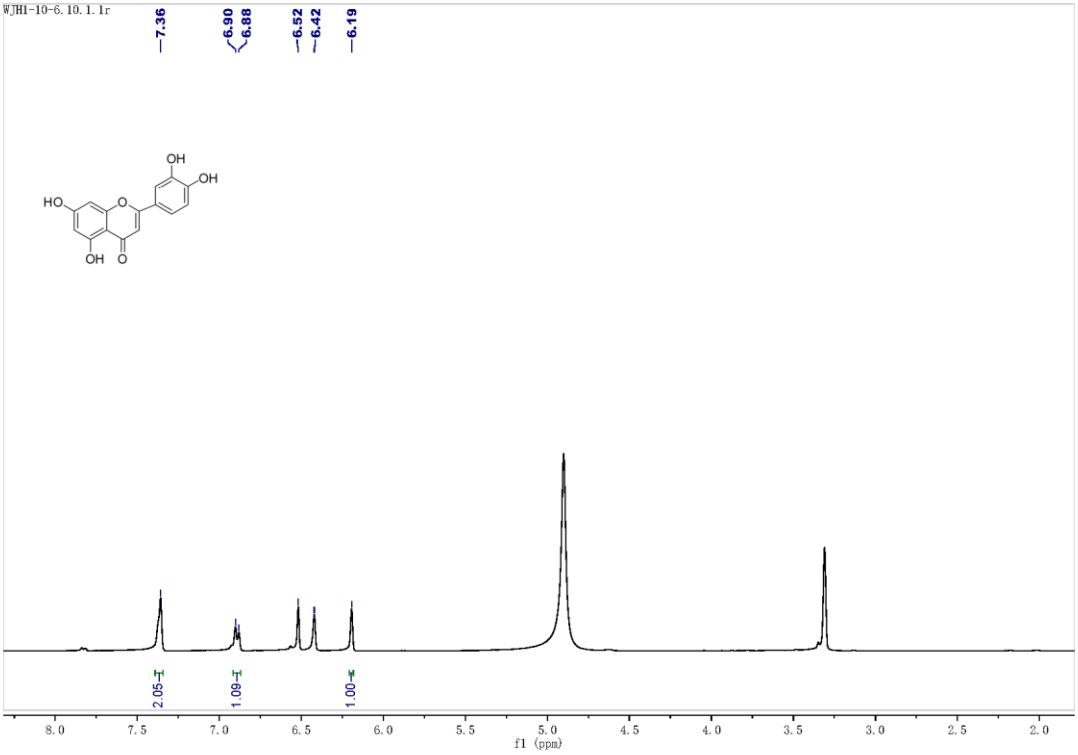


Figure S24: ^{1}H NMR spectrum (400 MHz) of 6 in CD_3OD

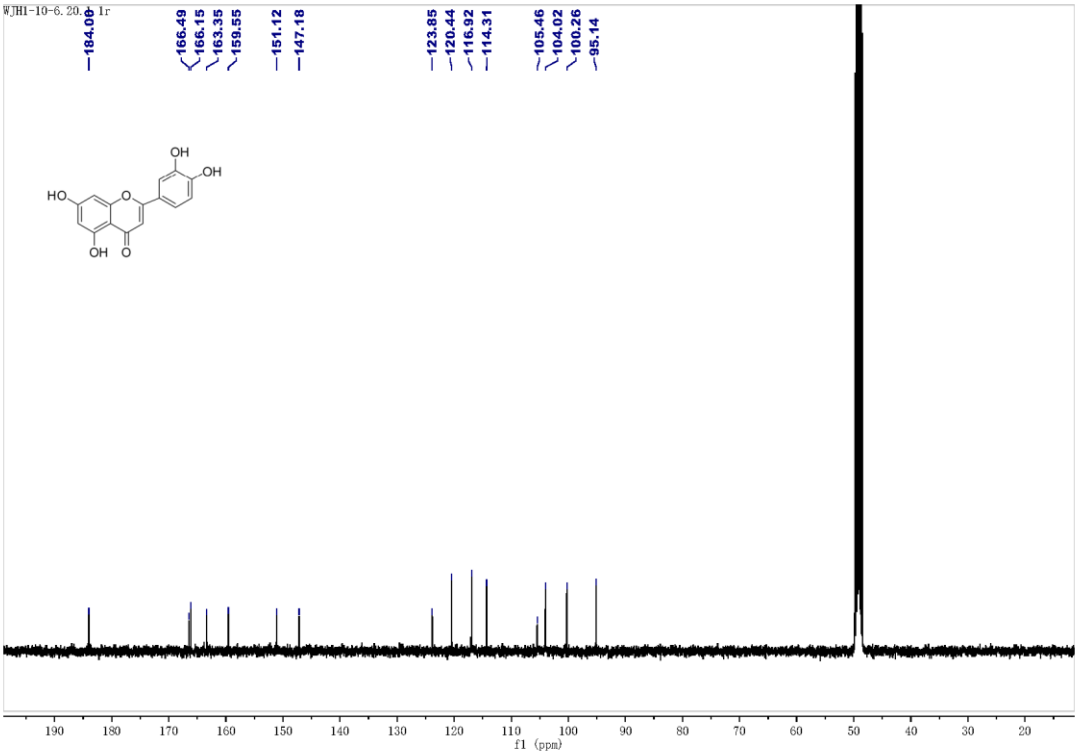


Figure S25: ^{13}C NMR spectrum (100 MHz) of 6 in CD_3OD

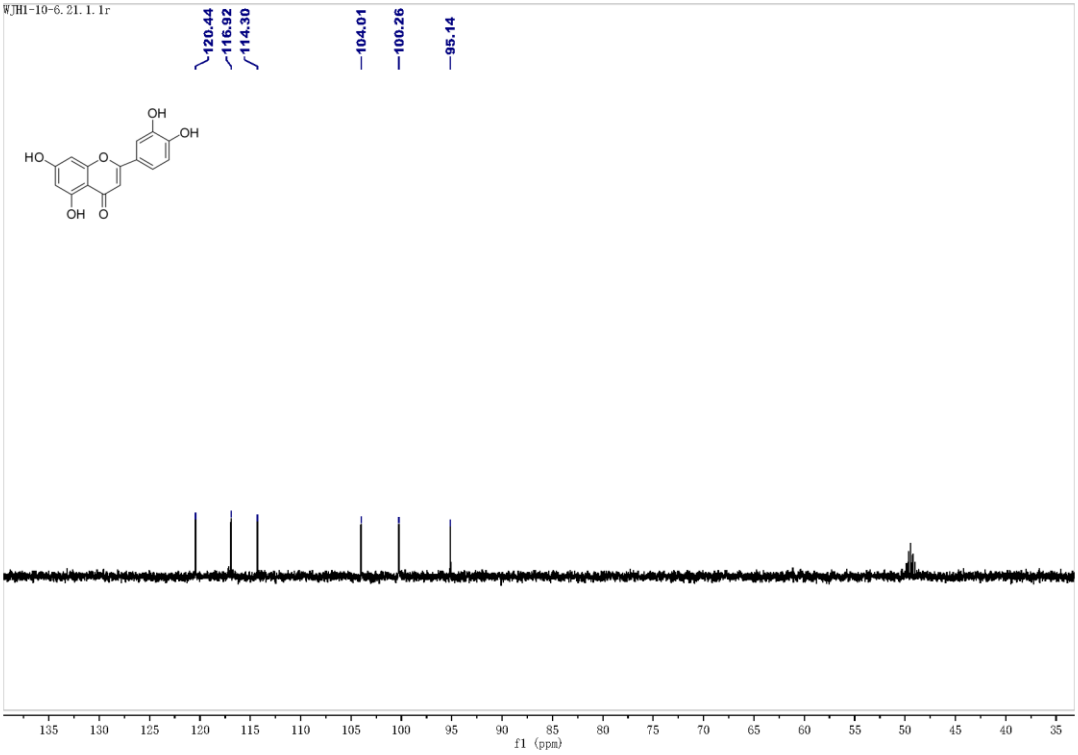


Figure S26: DEPT NMR spectrum (100 MHz) of 6 in CD_3OD

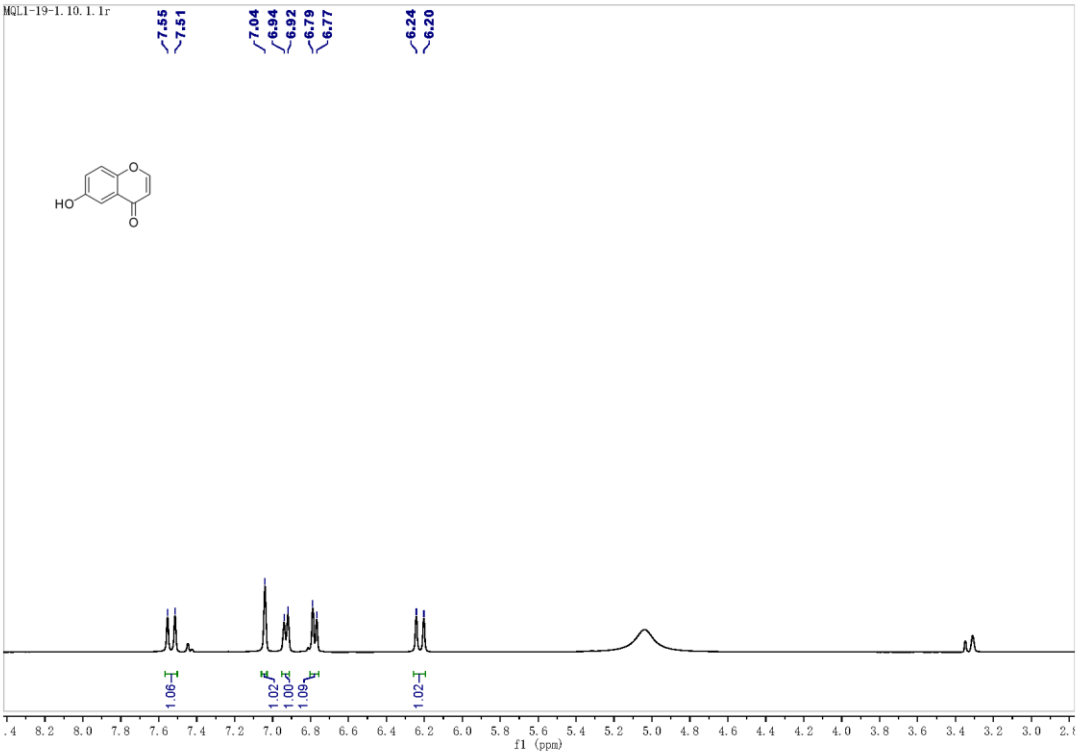


Figure S27: ^1H NMR spectrum (400 MHz) of 7 in CD_3OD

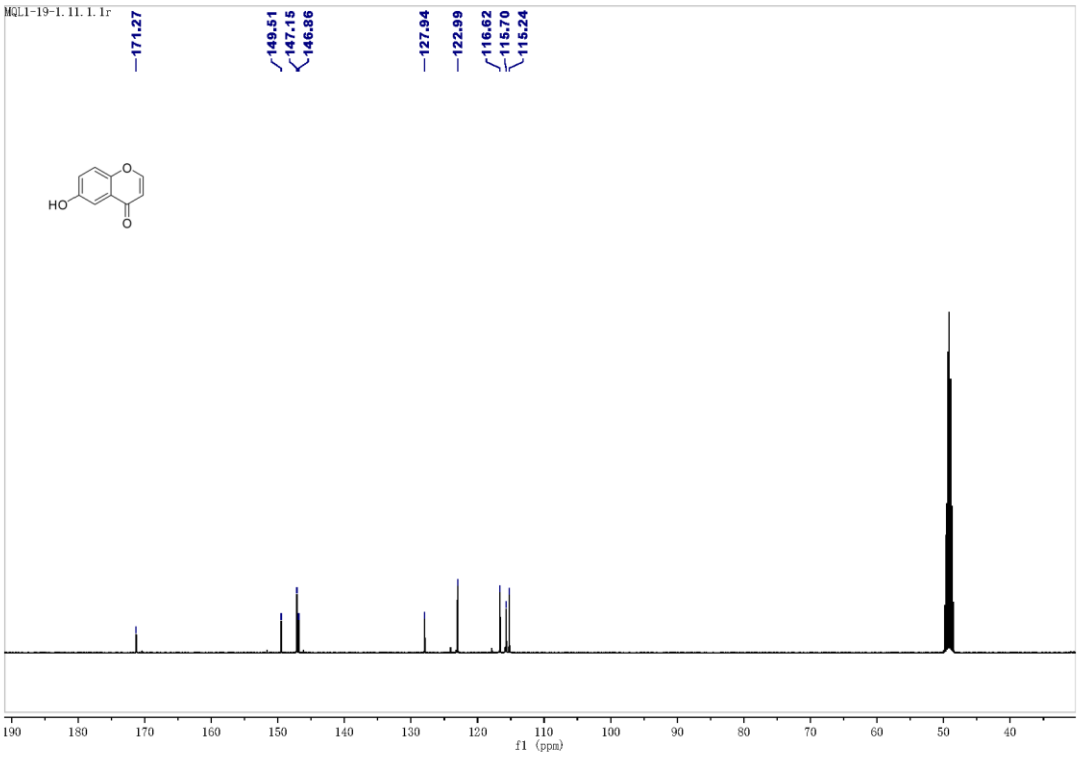


Figure S28: ^{13}C NMR spectrum (100 MHz) of 7 in CD_3OD

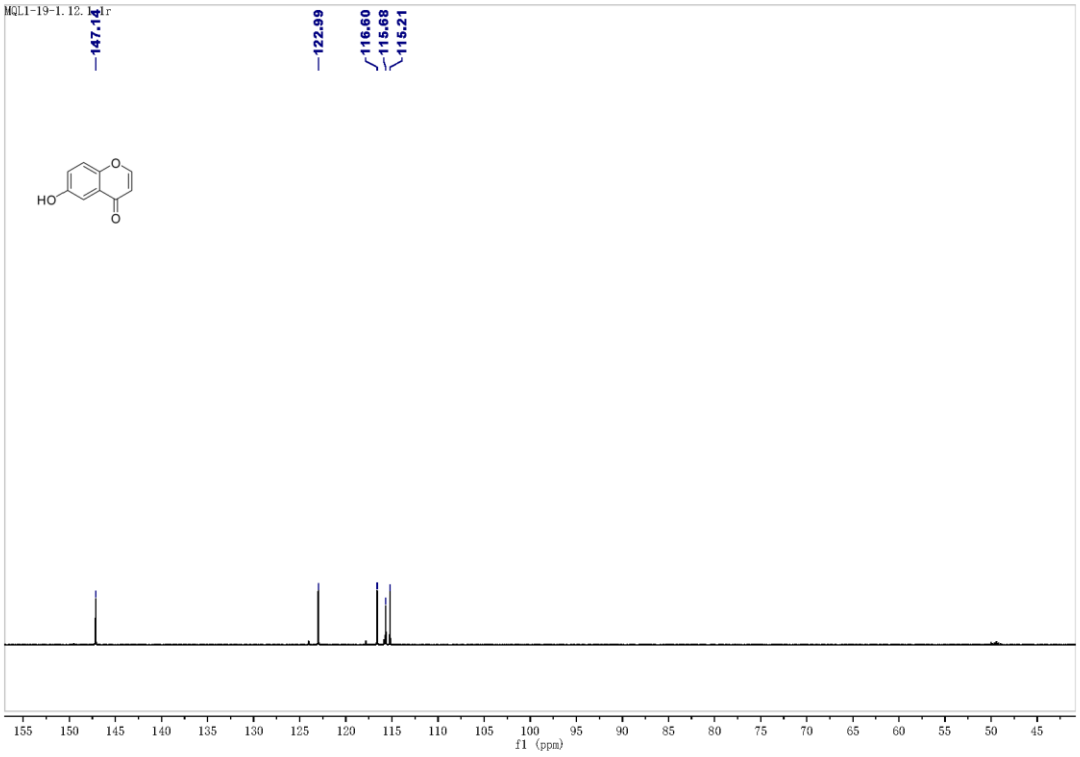


Figure S29: DEPT NMR spectrum (100 MHz) of 7 in CD_3OD

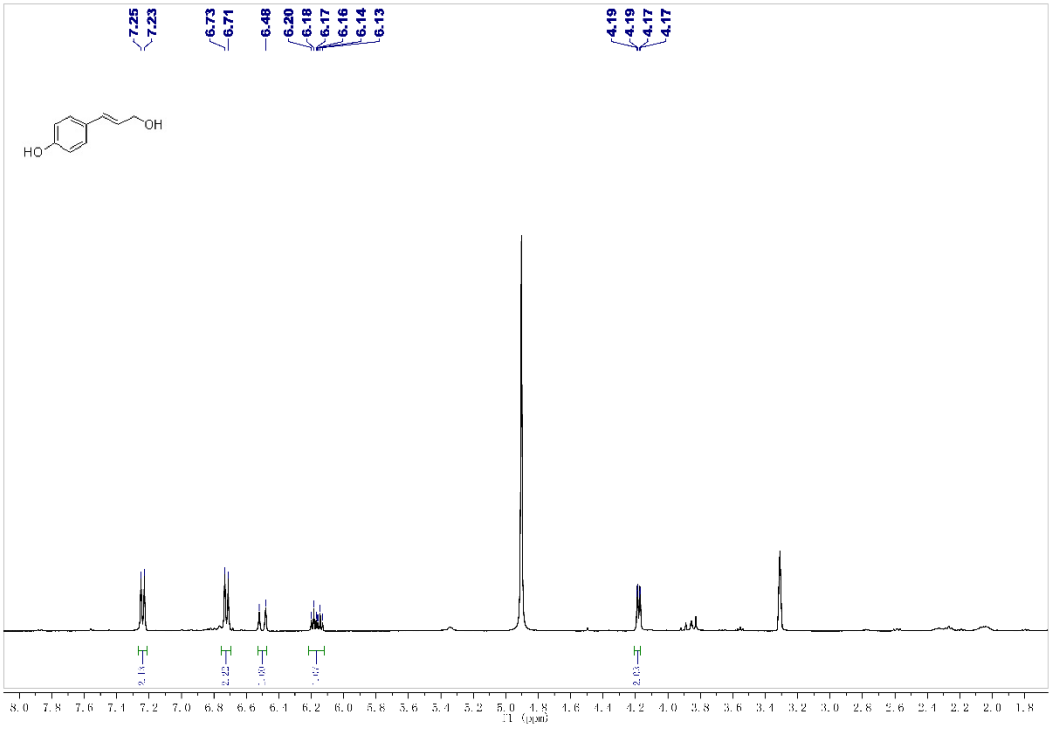


Figure S30: ^{1}H NMR spectrum (400 MHz) of 8 in CD_3OD

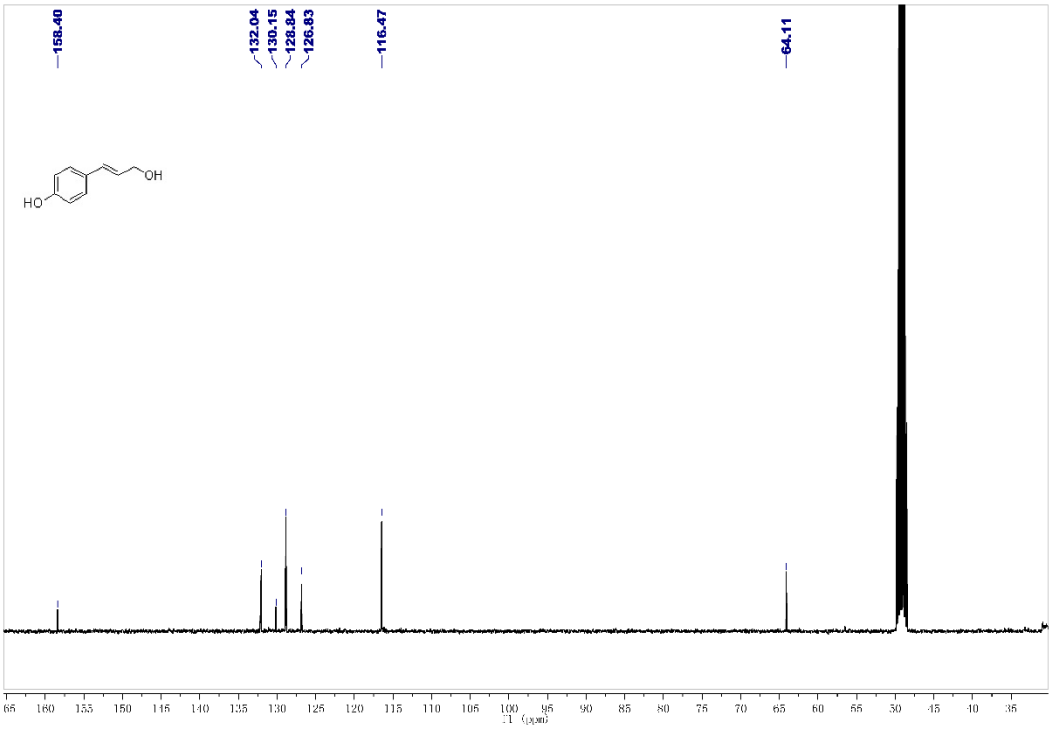


Figure S31: ^{13}C NMR spectrum (100 MHz) of 8 in CD_3OD

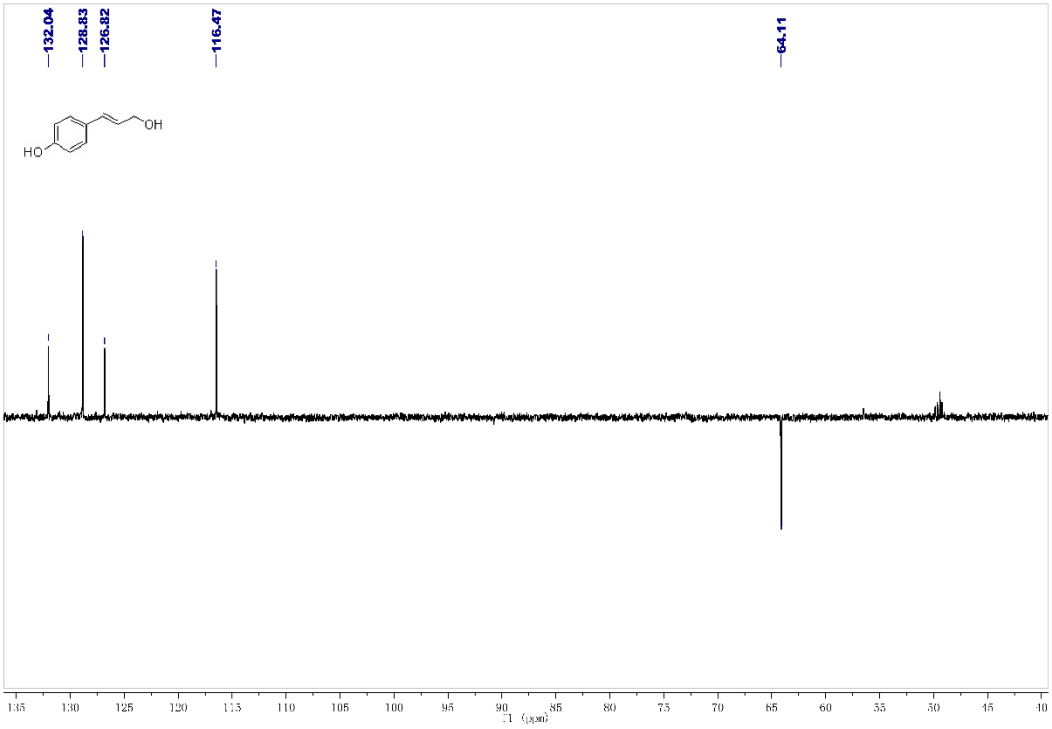
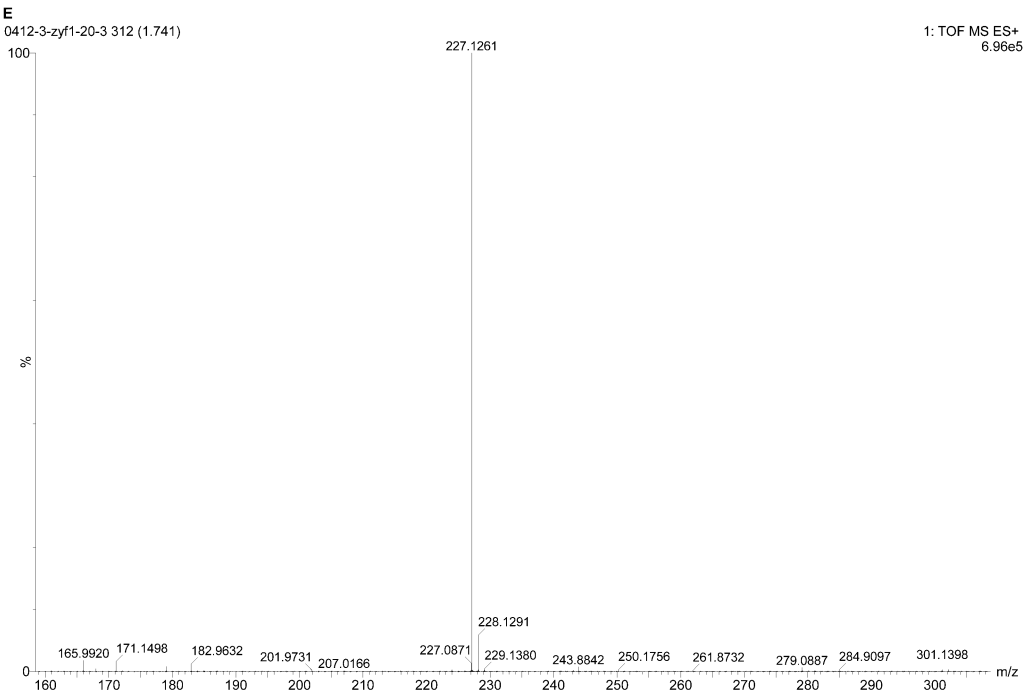


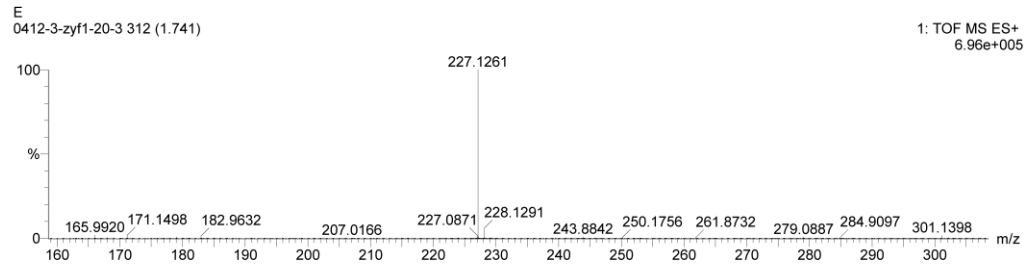
Figure S32: DEPT NMR spectrum (100 MHz) of 8 in CD_3OD



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
105 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-10 H: 0-100 N: 0-20 O: 0-20 Na: 1-1



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
227.1261	227.1259	0.2	0.9	0.5	815.6	n/a	n/a	C10 H20 O4 Na

Figure S33: (+)-HR-ESI-MS spectrum of 9

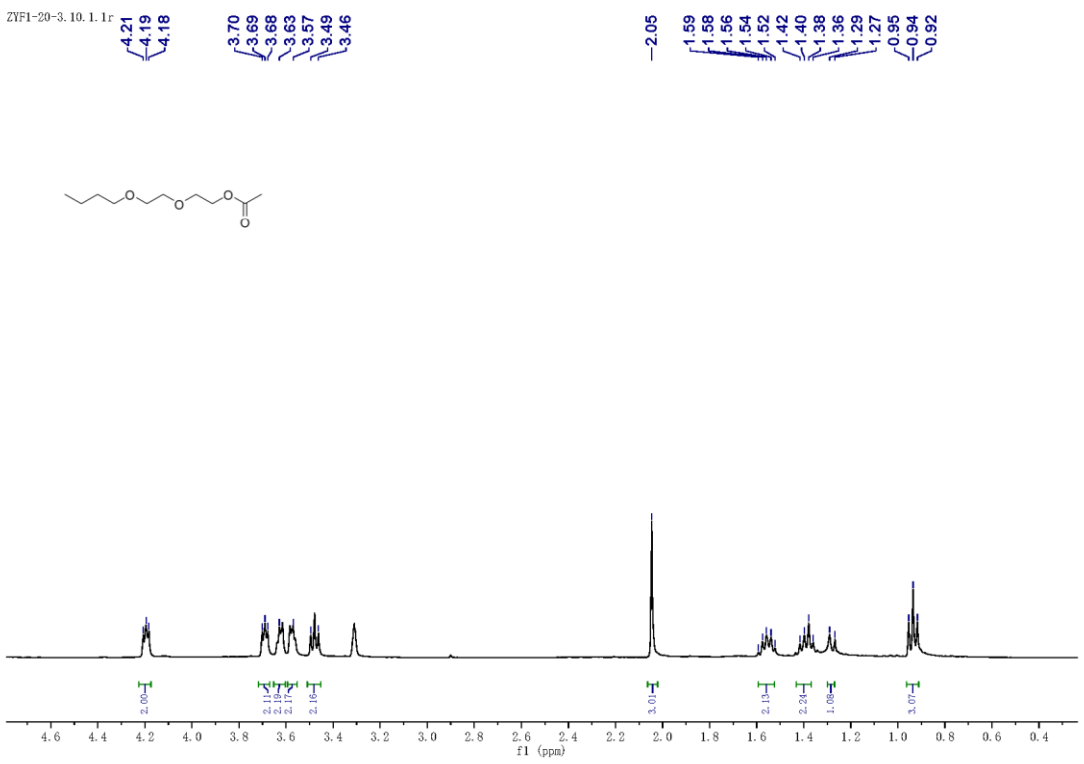


Figure S34: ^{1}H NMR spectrum (400 MHz) of 9 in CD_3OD

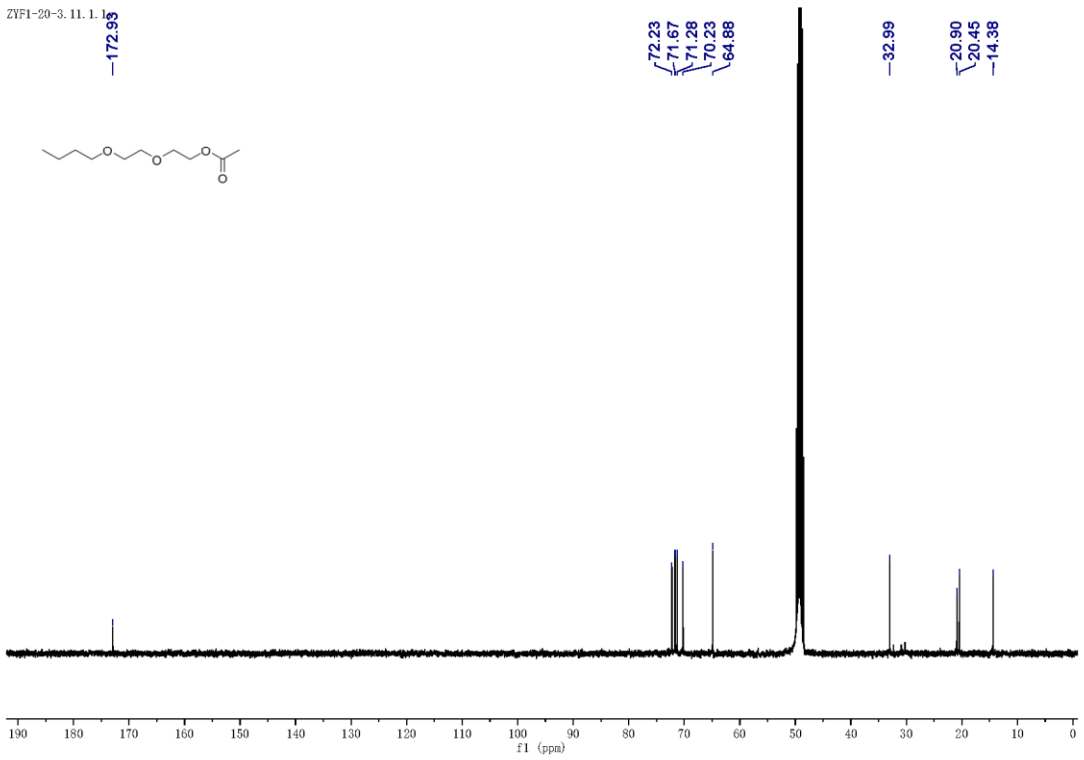


Figure S35: ^{13}C NMR spectrum (100 MHz) of 9 in CD_3OD

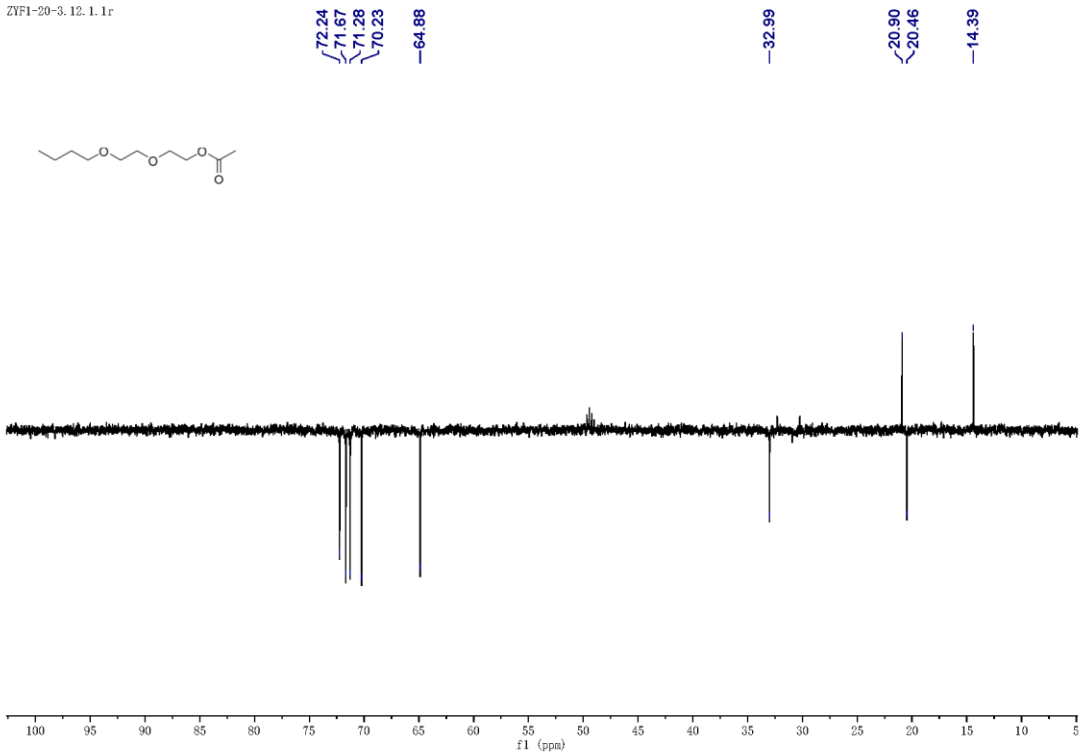


Figure S36: DEPT NMR spectrum (100 MHz) of 9 in CD_3OD