

Supporting Information

Rec. Nat. Prod. 17:1 (2023) 99-105

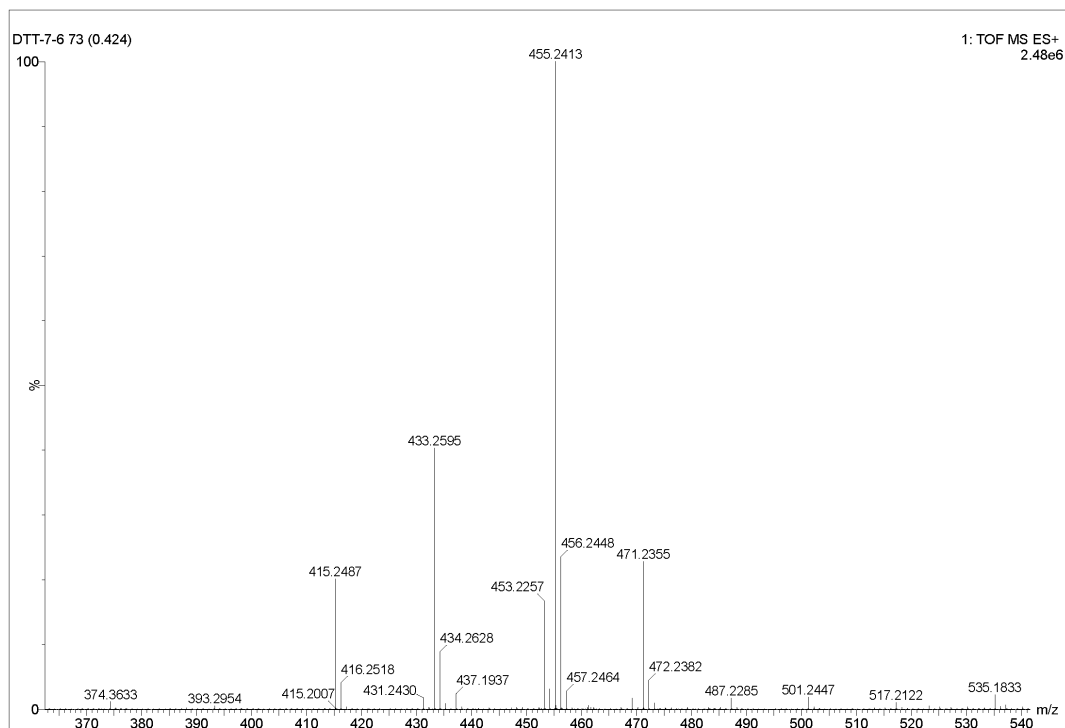
Secondary Metabolites with Antioxidant and Mushroom Tyrosinase Inhibitory Activities from *Ajuga nipponensis*

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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)

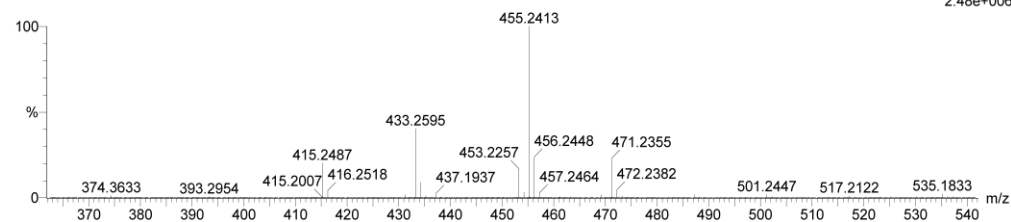
Elements Used:

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+

2.48e+006



Minimum: -1.5
Maximum: 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	C ₂₅ H ₃₆ O ₆ Na

Figure S1: HR-ESI-MS spectrum of 1

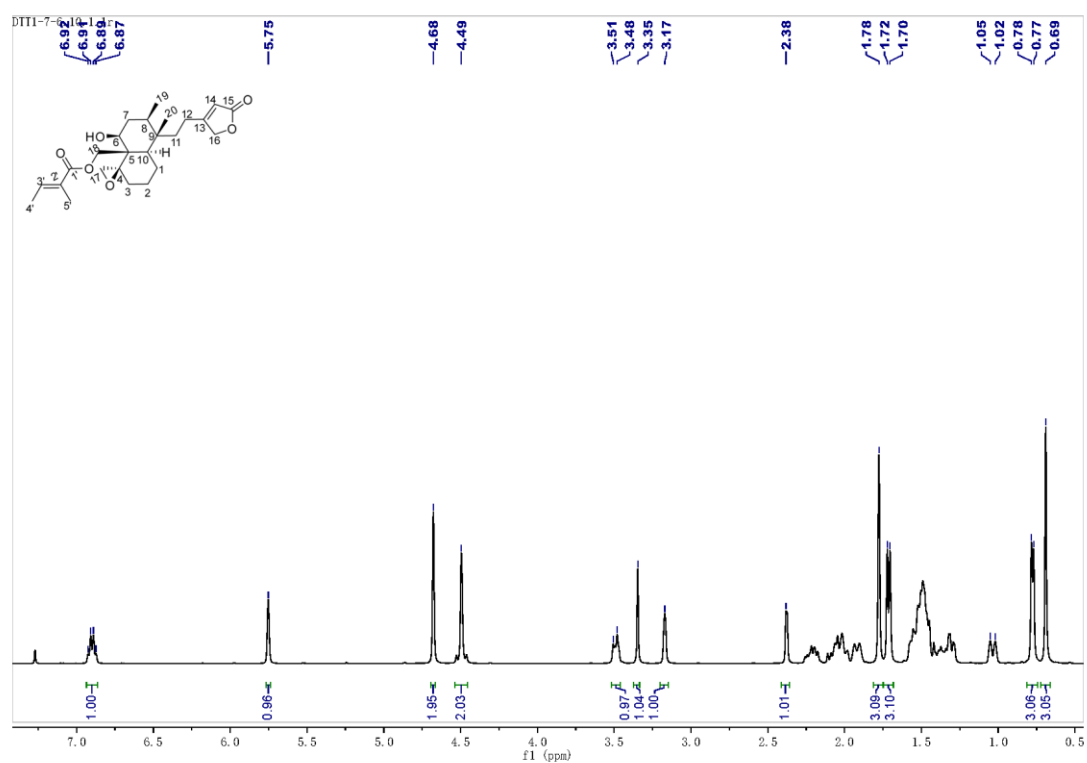


Figure S2: ^1H NMR spectrum (400 MHz) of 1 in CDCl_3

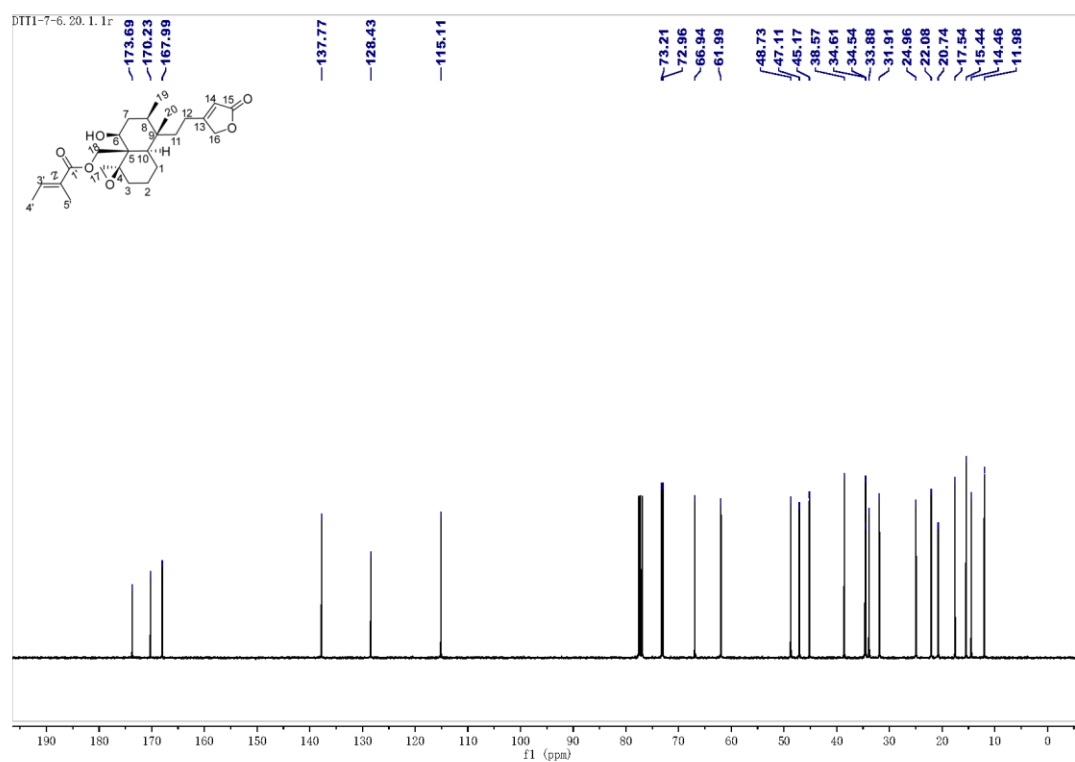


Figure S3: ^{13}C NMR spectrum (100 MHz) of 1 in CDCl_3

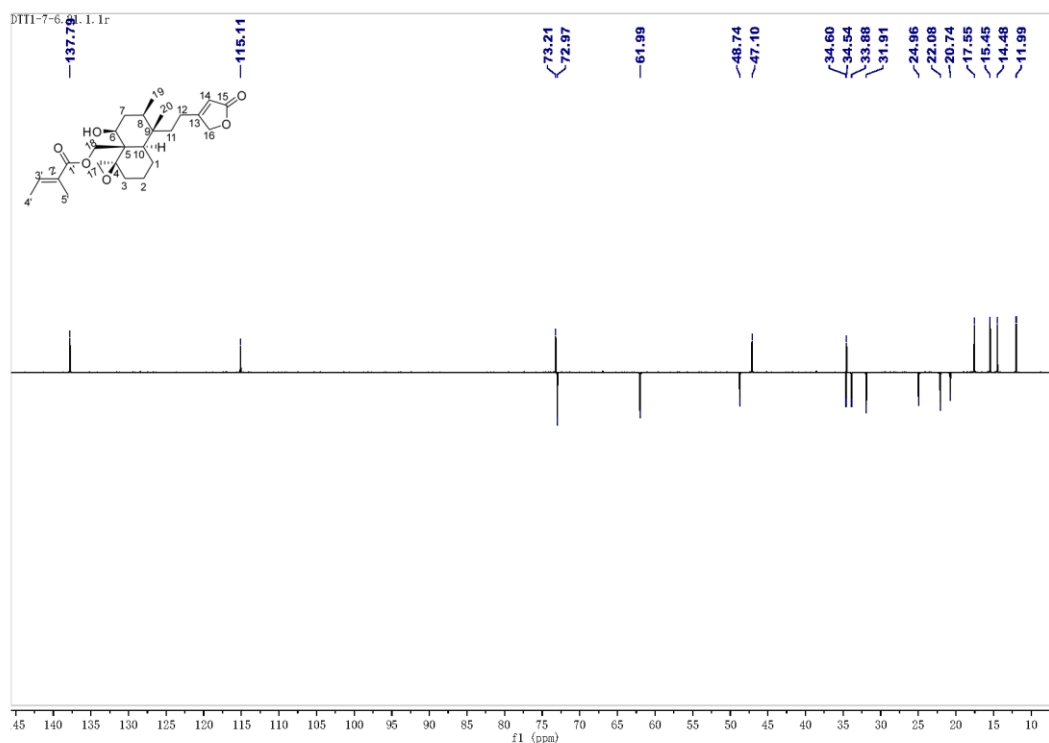


Figure S4: DEPT NMR spectrum (100 MHz) of 1 in CDCl₃

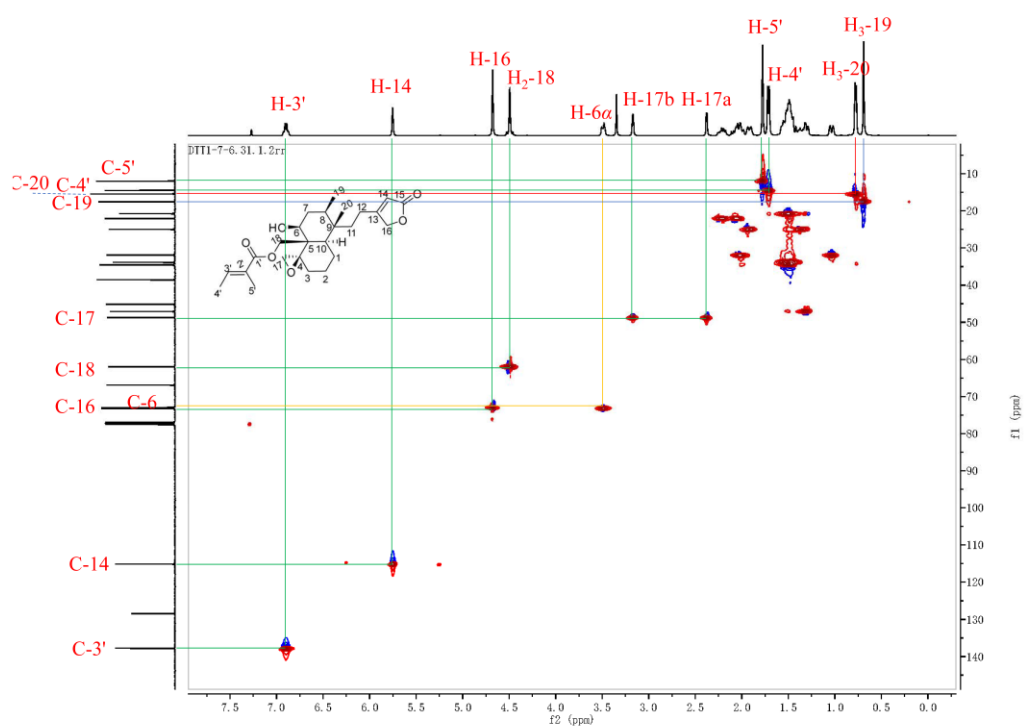


Figure S5: HSQC spectrum of 1 in CDCl₃

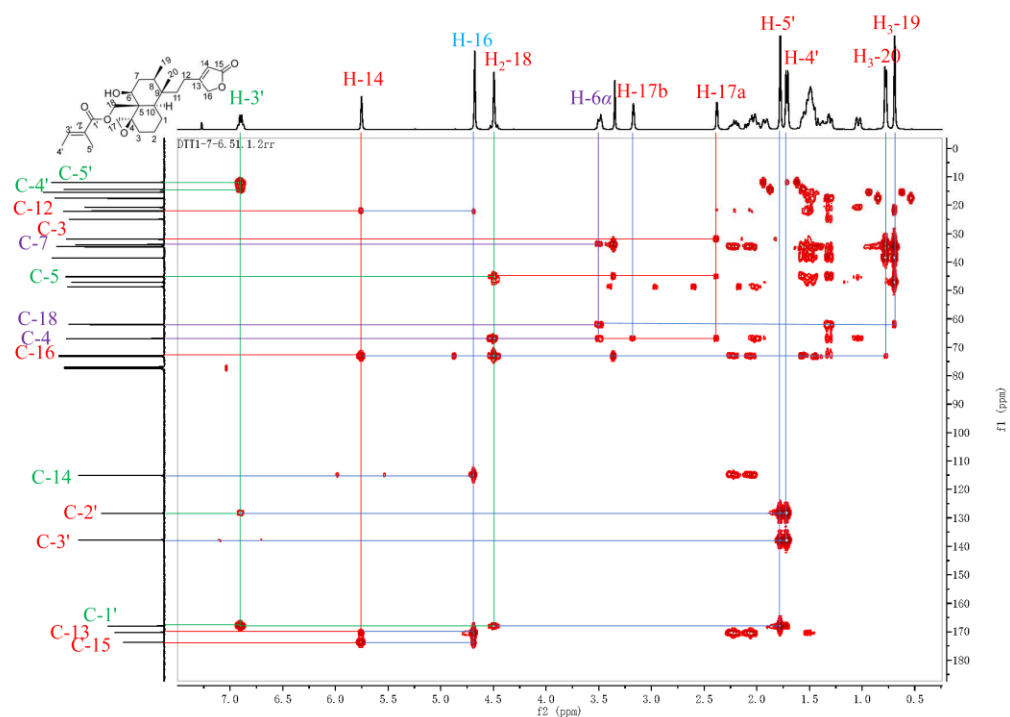


Figure S6: HMBC spectrum of 1 in CDCl₃

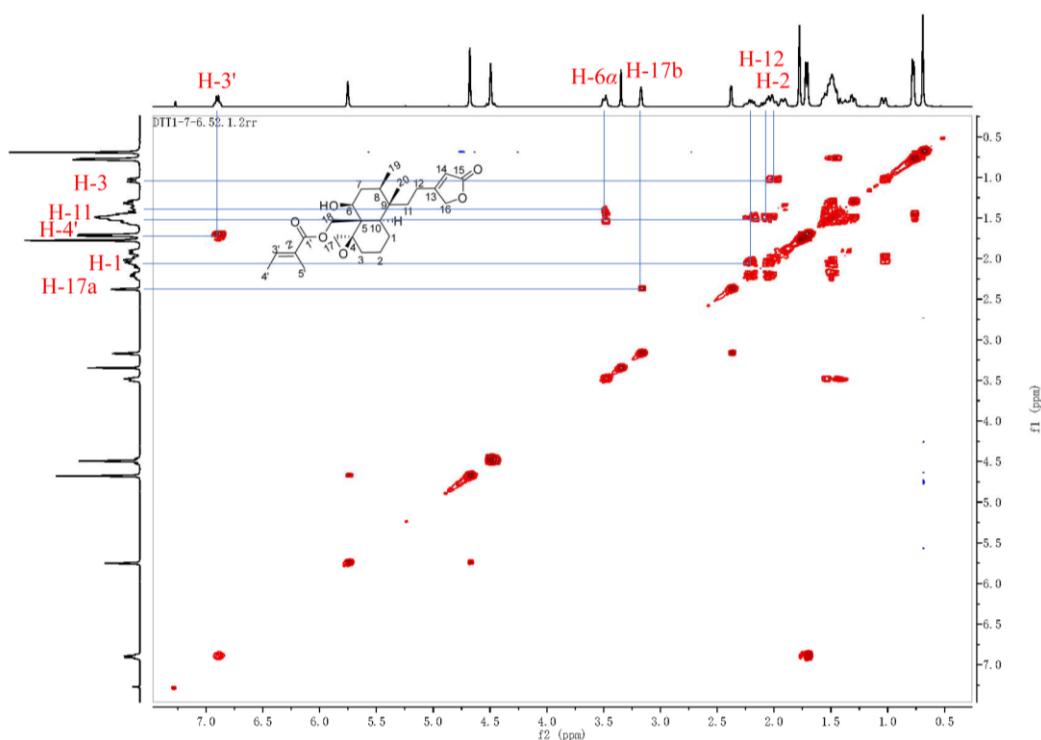


Figure S7: ¹H-¹H COSY spectrum of 1 in CDCl₃

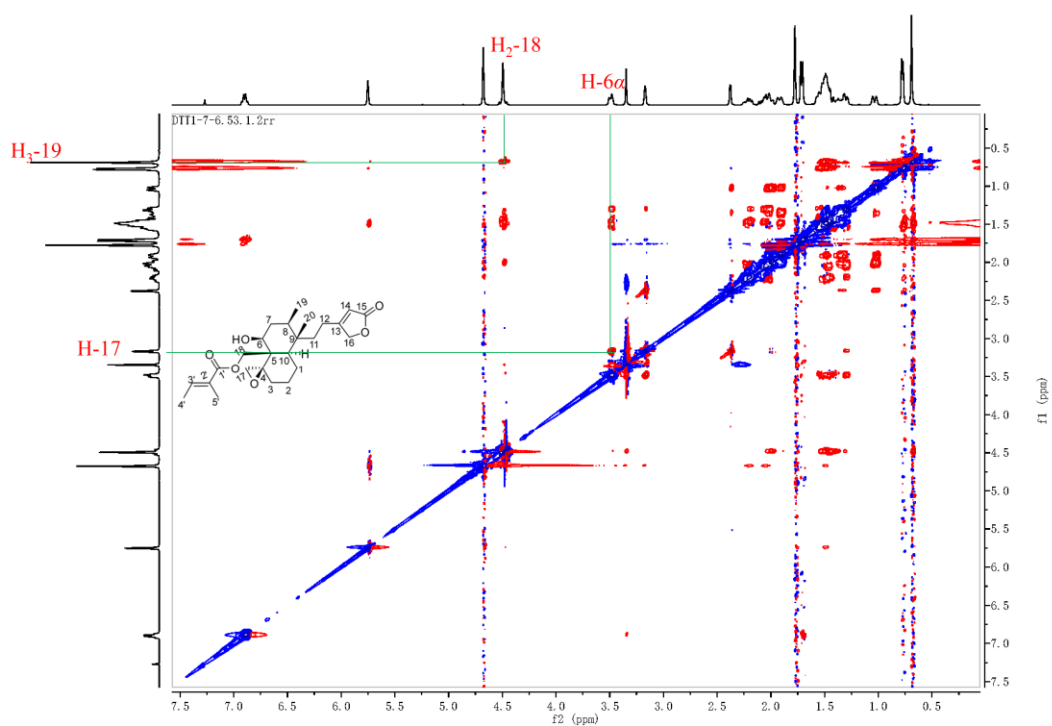


Figure S8: NOESY spectrum of 1 in CDCl_3

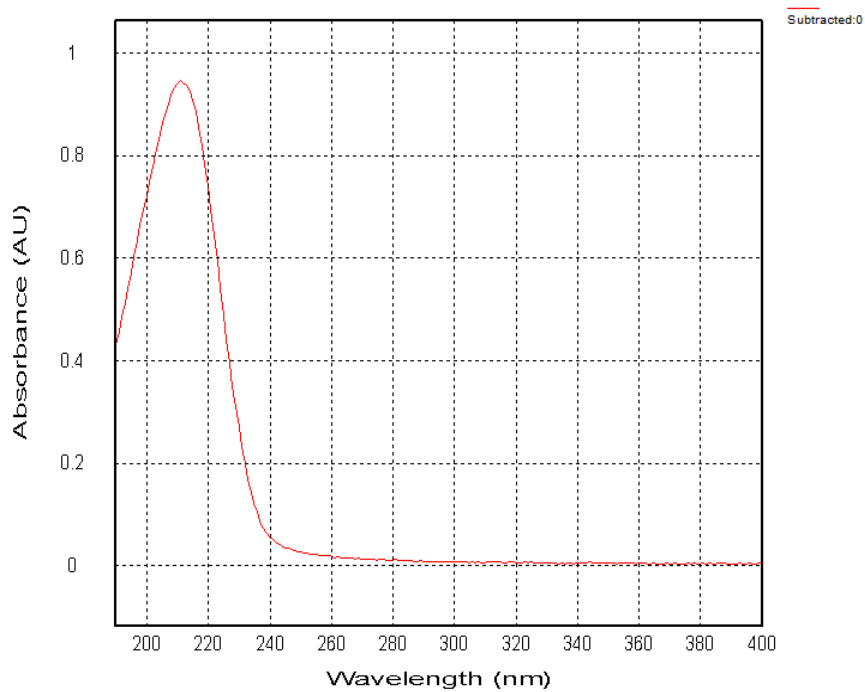


Figure S9: UV spectrum of 1 in CH_3CN

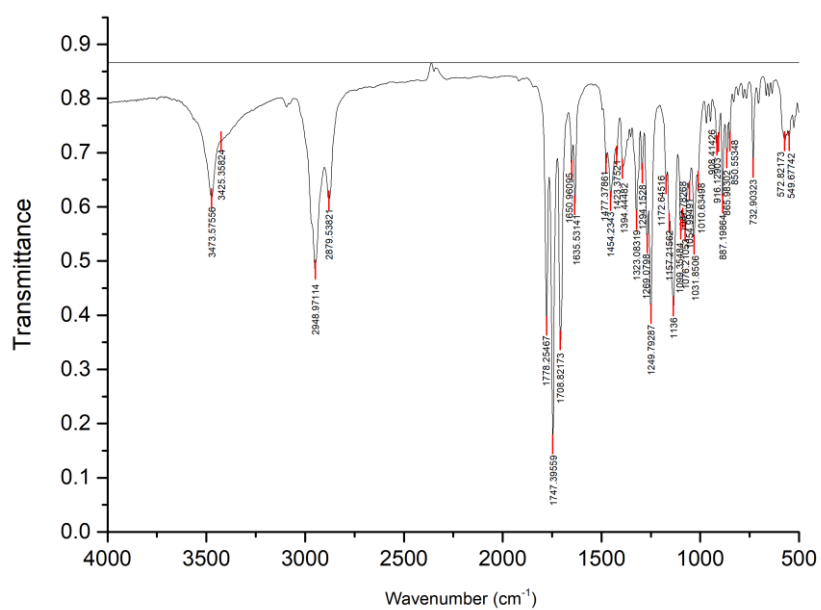


Figure S10: IR spectrum of 1

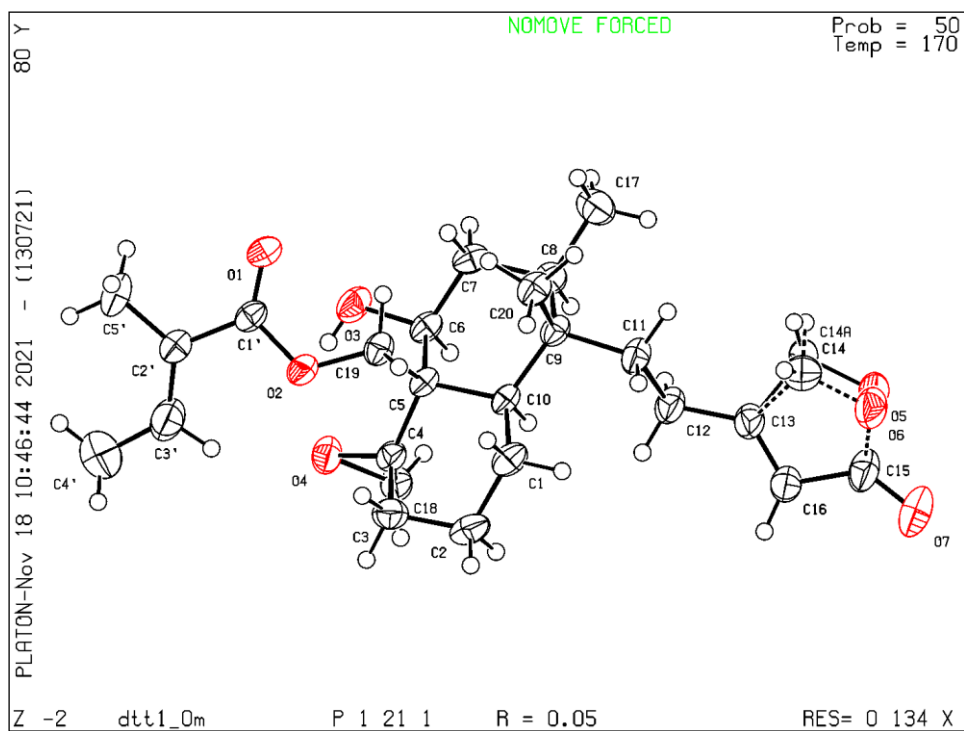


Figure S11: Crystal packing of 1 170 K

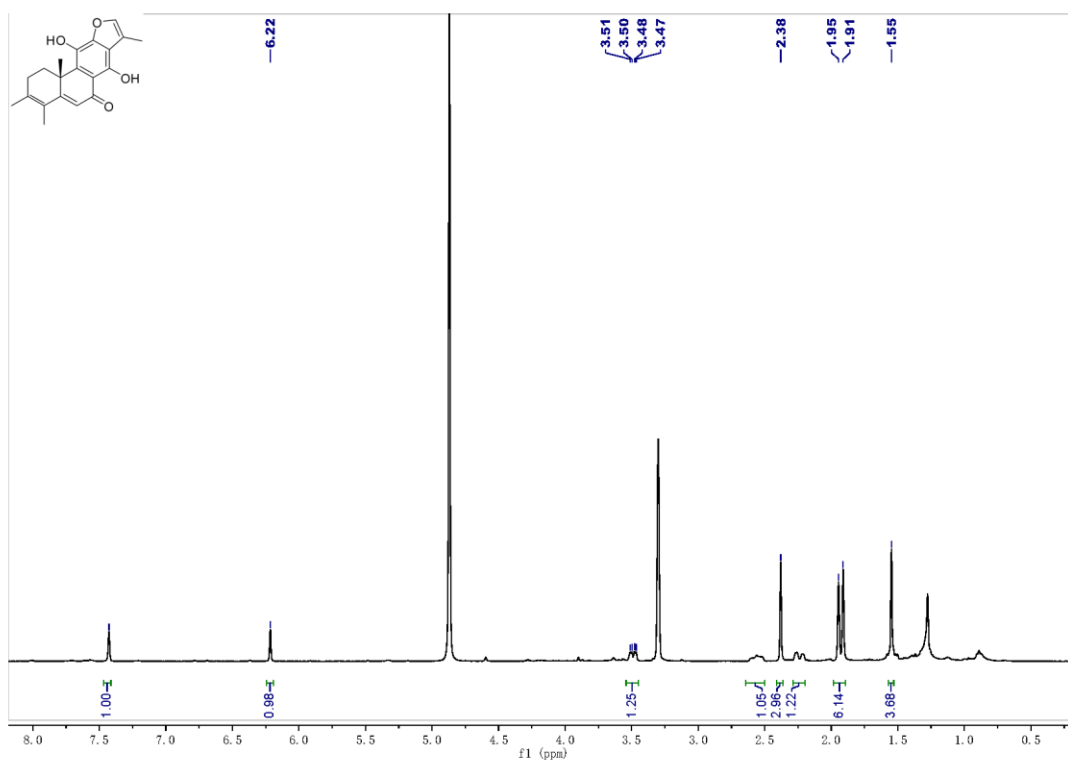


Figure S12: ¹H NMR spectrum (400 MHz) of 2 in CD₃OD

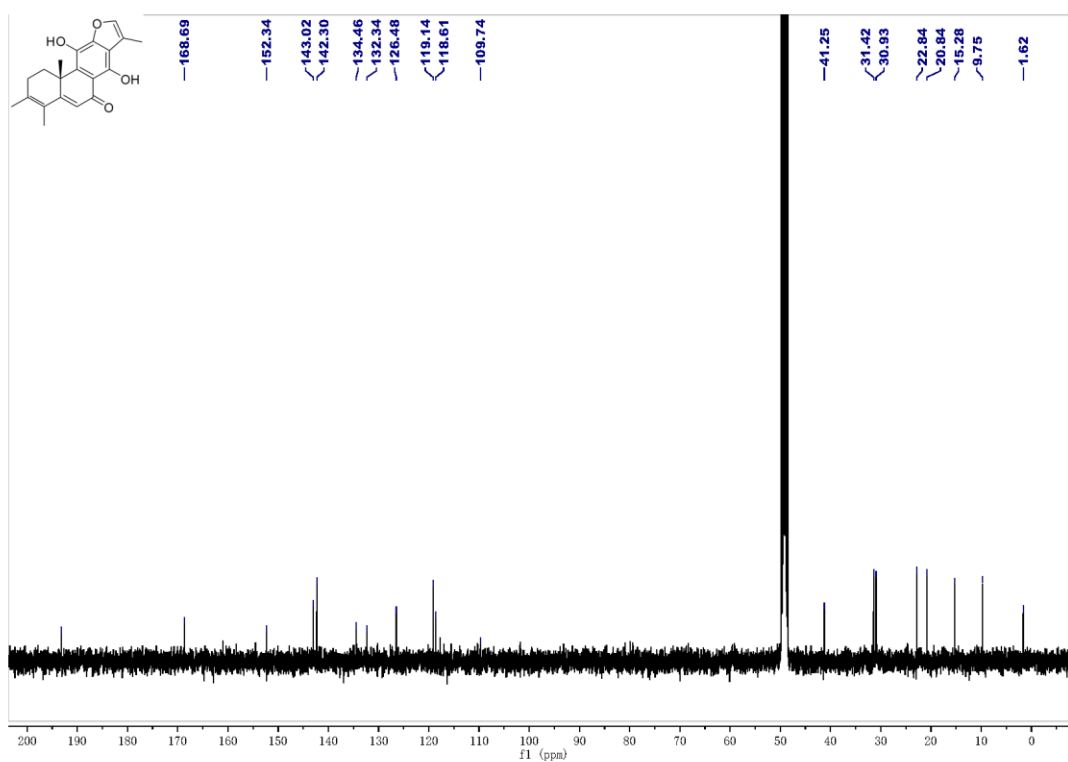


Figure S13: ¹³C NMR spectrum (100 MHz) of 2 in CD₃OD

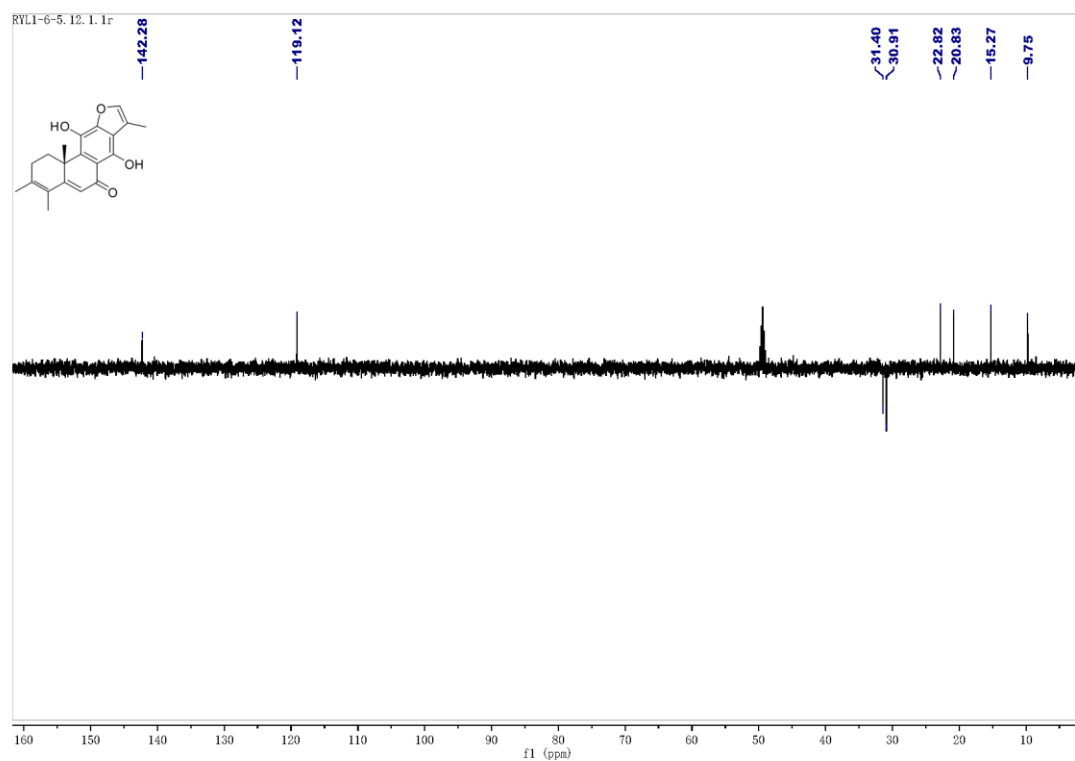


Figure S14: DEPT NMR spectrum (100 MHz) of 2 in CD₃OD

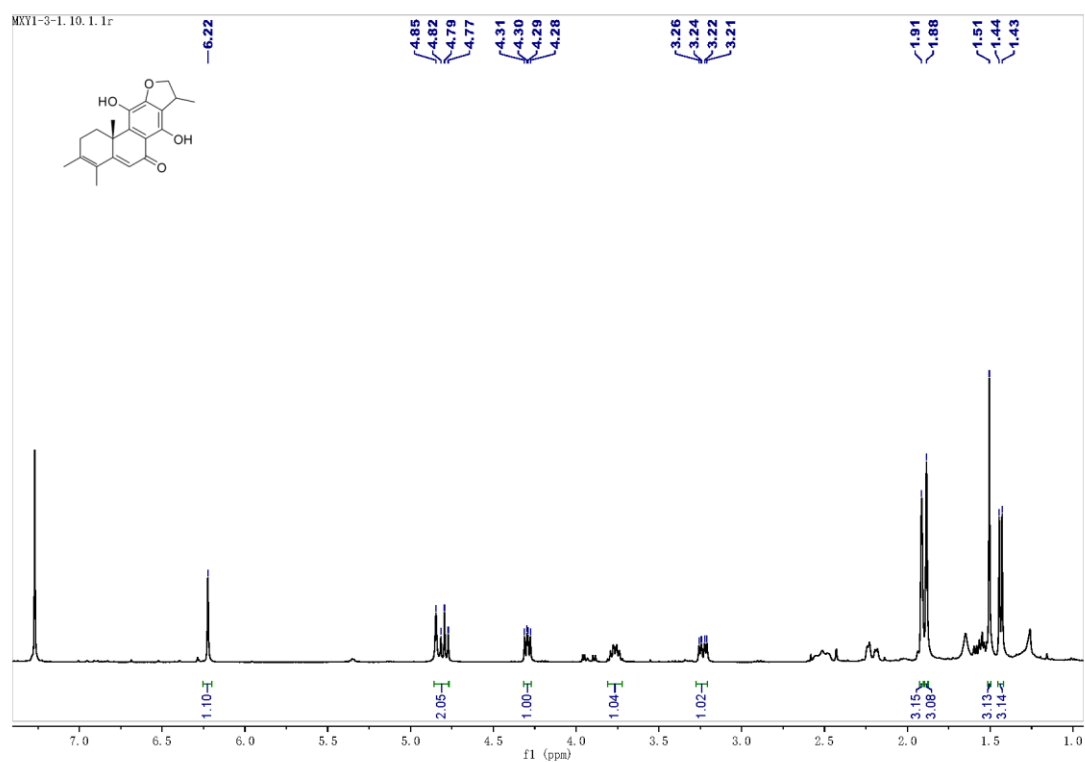


Figure S15: ¹H NMR spectrum (400 MHz) of 3 in CDCl₃

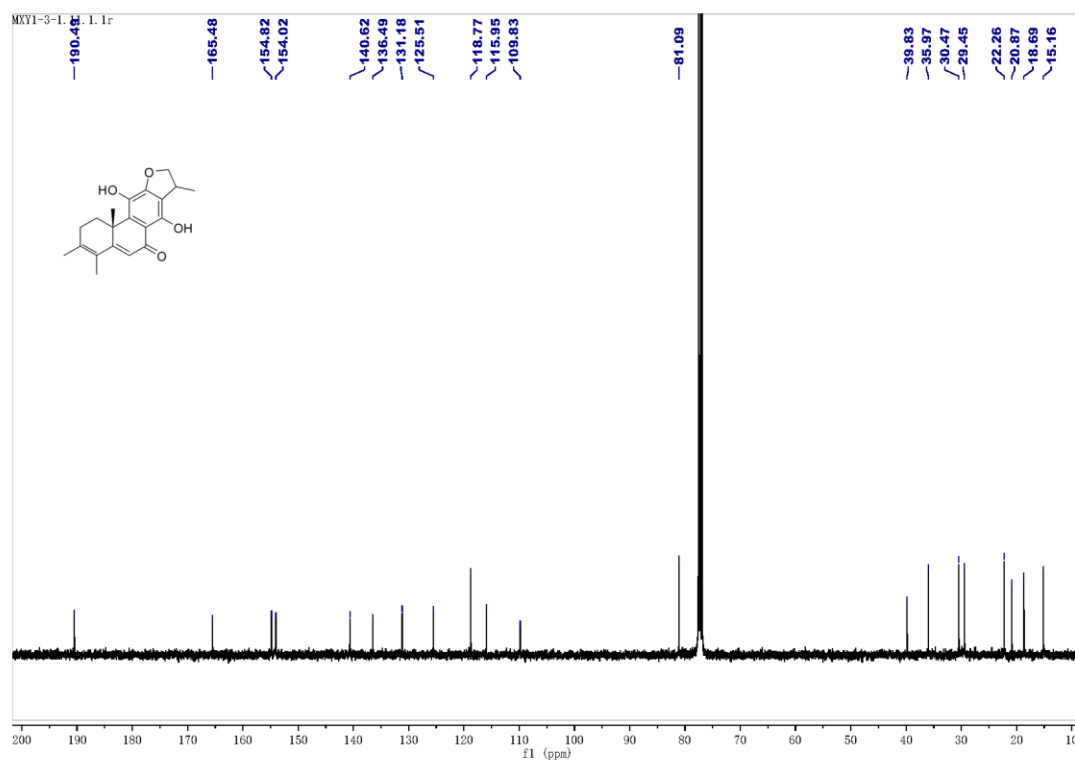


Figure S16: ^{13}C NMR spectrum (100 MHz) of 3 in CDCl_3

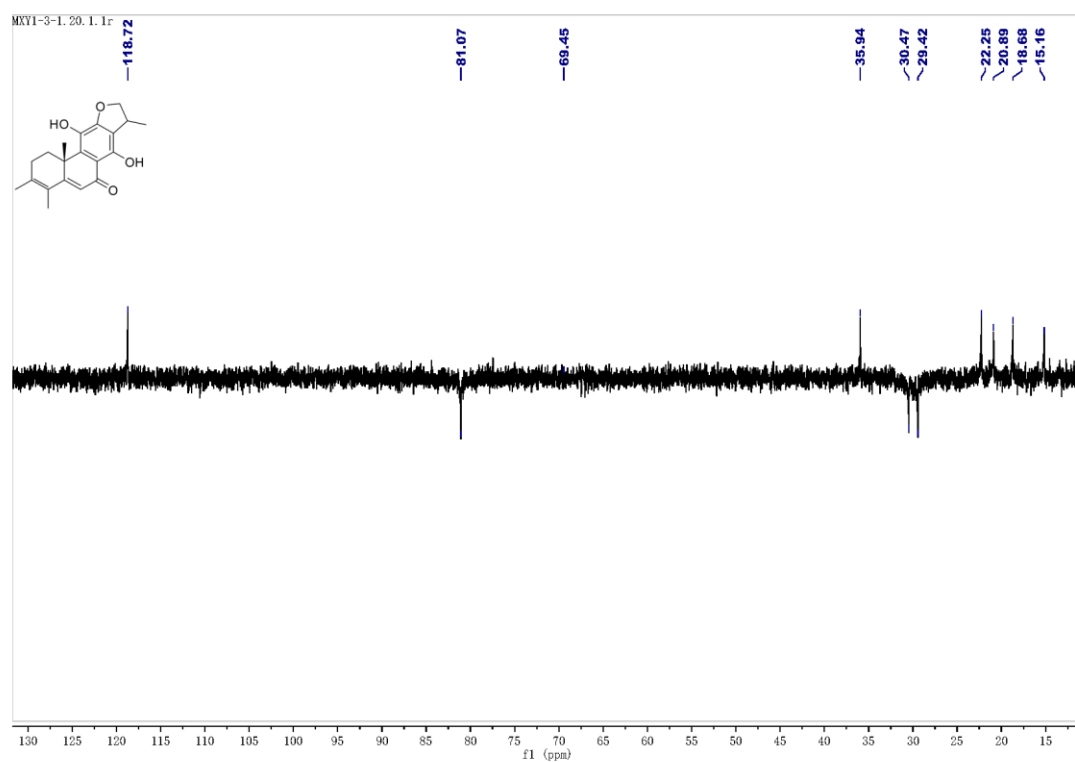


Figure S17: DEPT NMR spectrum (100 MHz) of 3 in CDCl_3

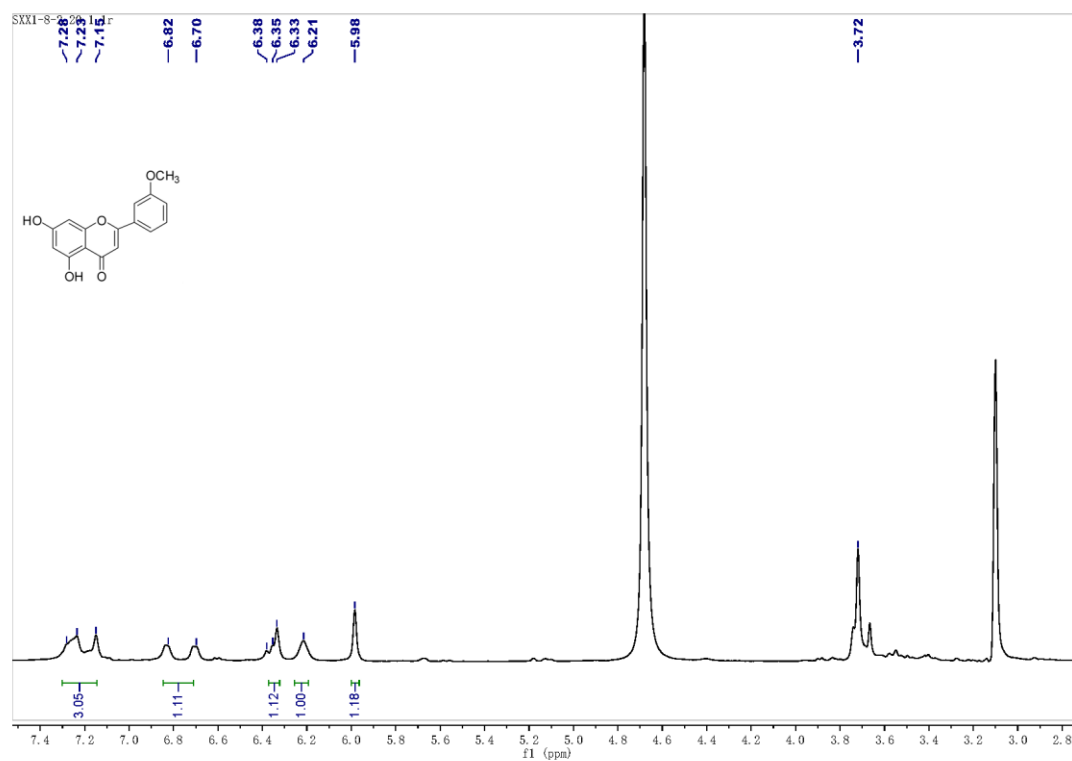


Figure S18: ¹H NMR spectrum (400 MHz) of 4 in CD₃OD

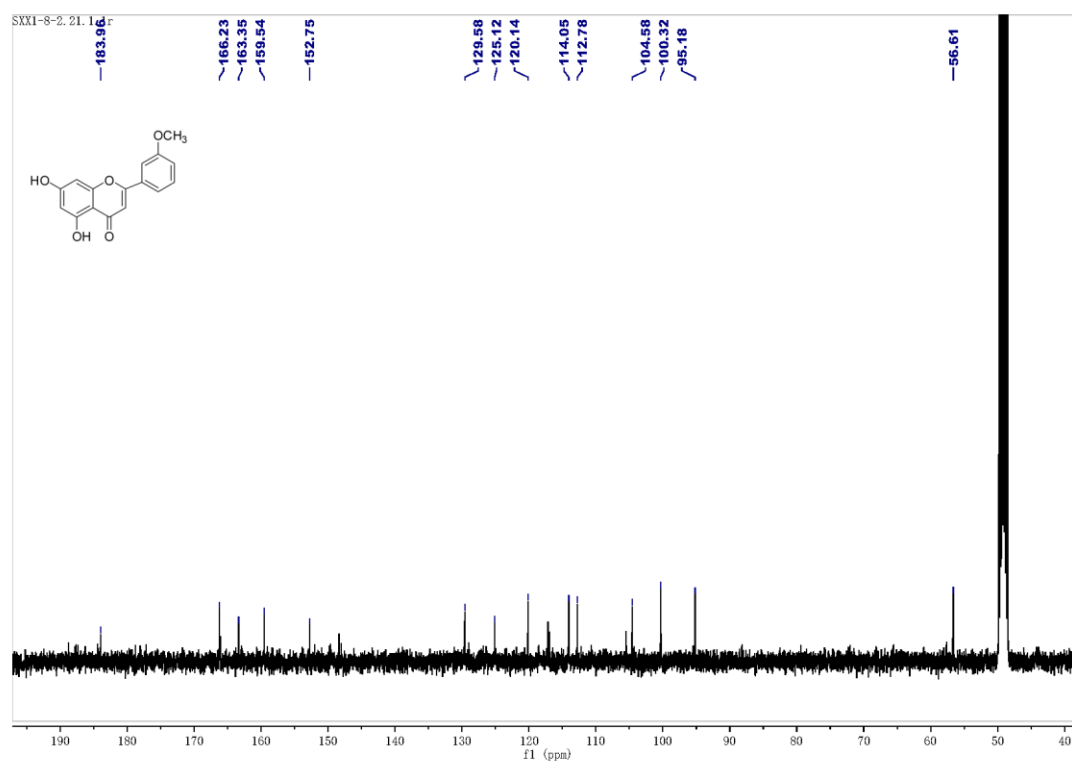


Figure S19: ¹³C NMR spectrum (100 MHz) of 4 in CD₃OD

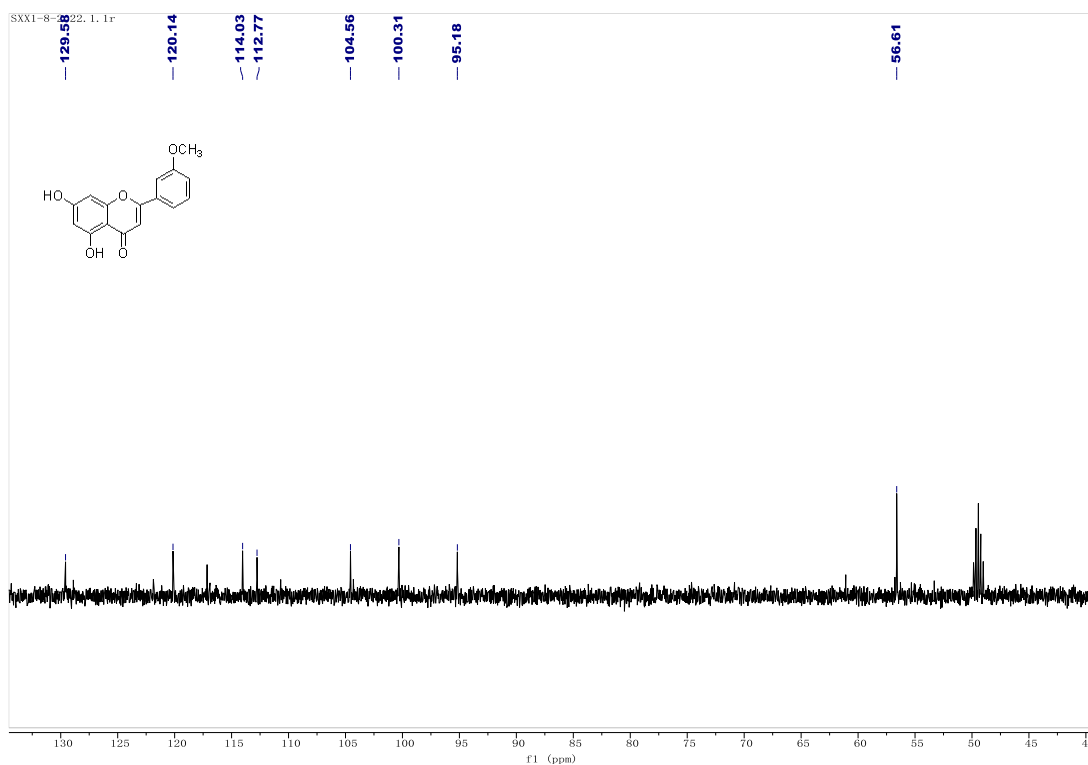


Figure S20: DEPT NMR spectrum (100 MHz) of 4 in CD₃OD

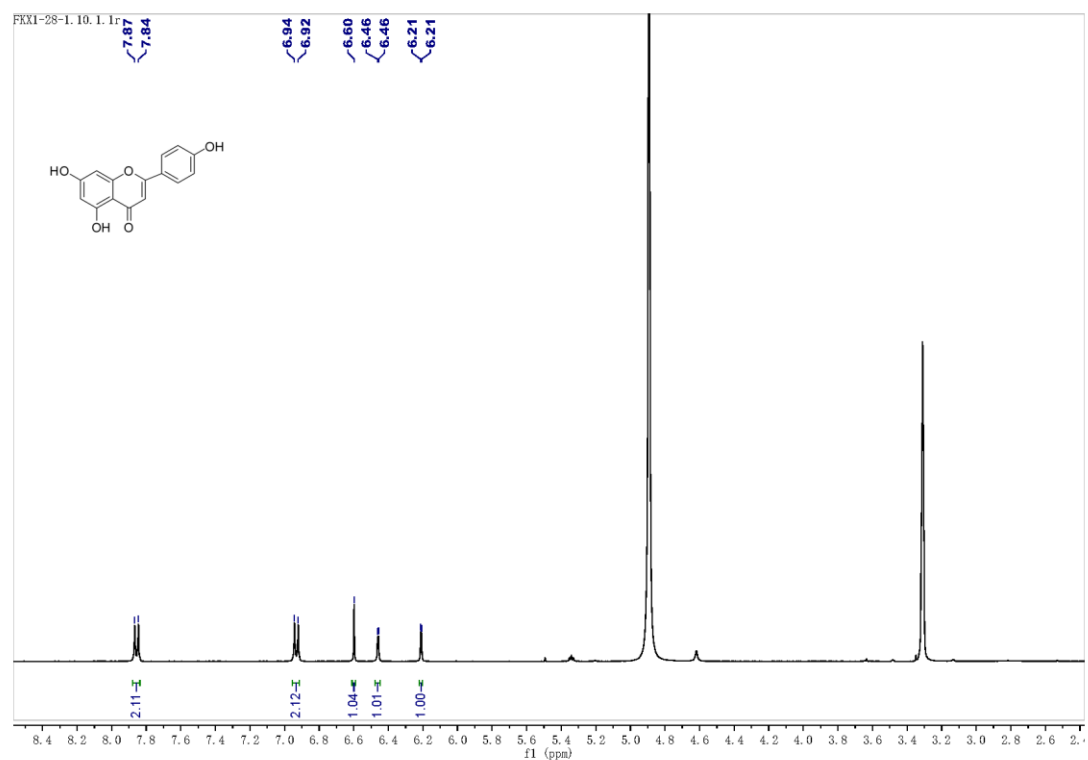


Figure S21: ¹H NMR spectrum (400 MHz) of 5 in CD₃OD

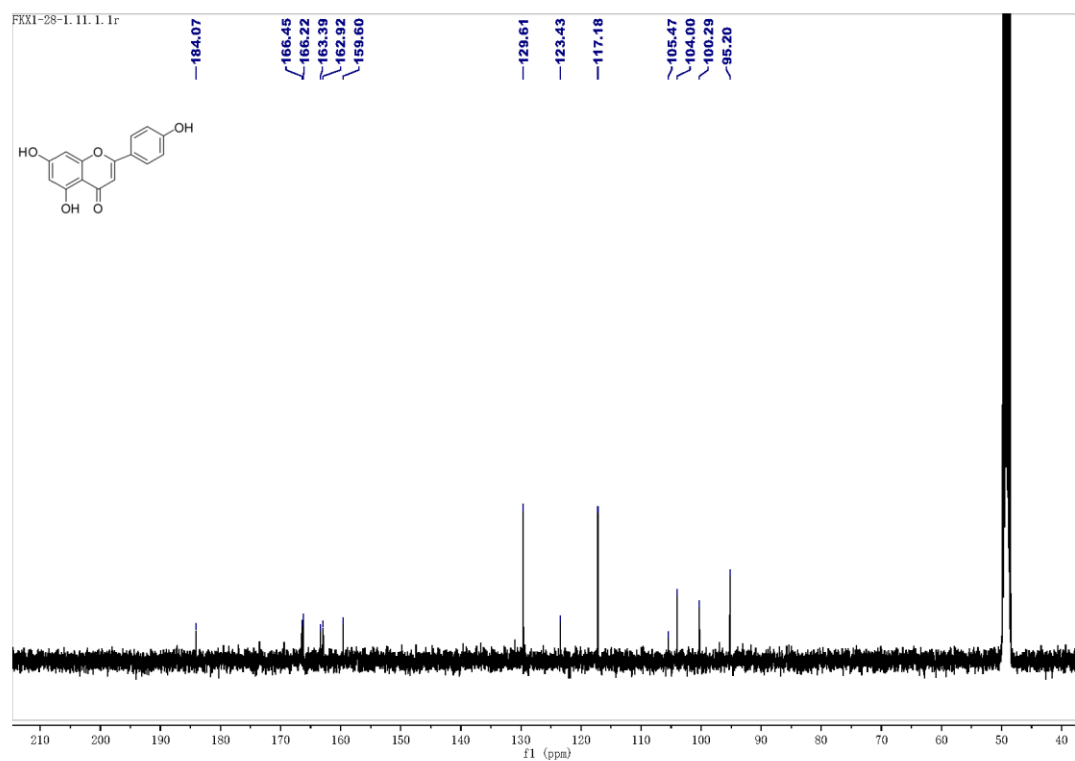


Figure S22: ^{13}C NMR spectrum (100 MHz) of 9 in CD_3OD

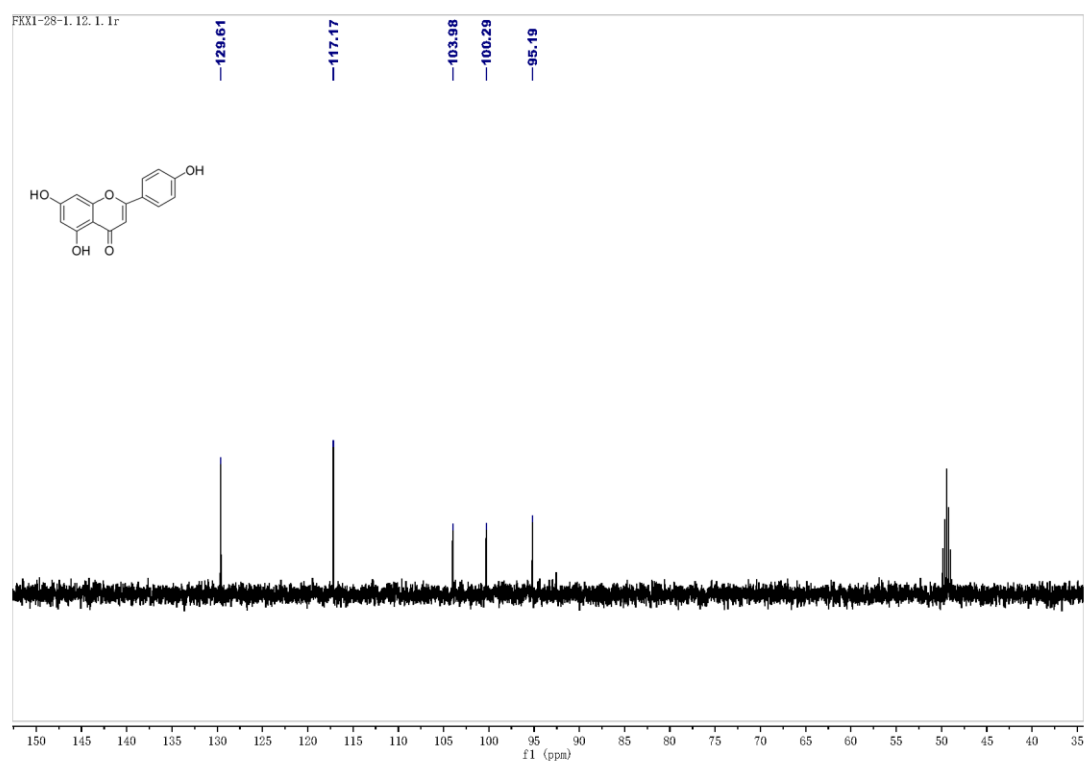


Figure S23: DEPT NMR spectrum (100 MHz) of 5 in CD_3OD

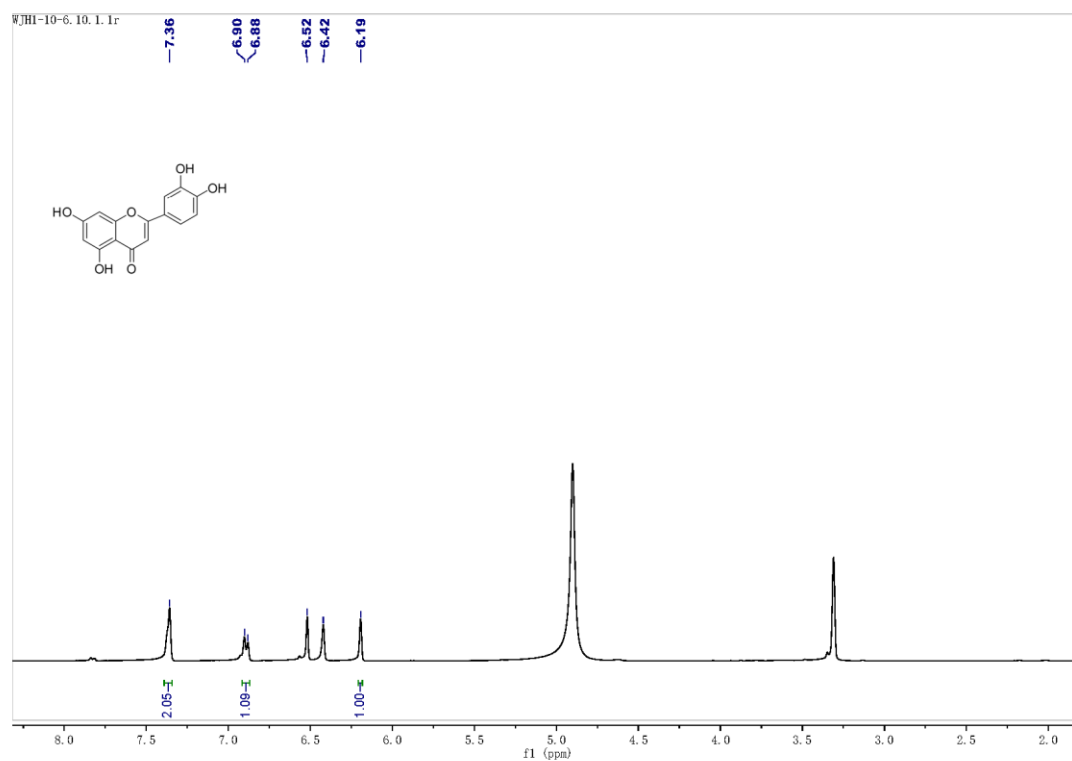


Figure S24: ^1H NMR spectrum (400 MHz) of 6 in CD_3OD

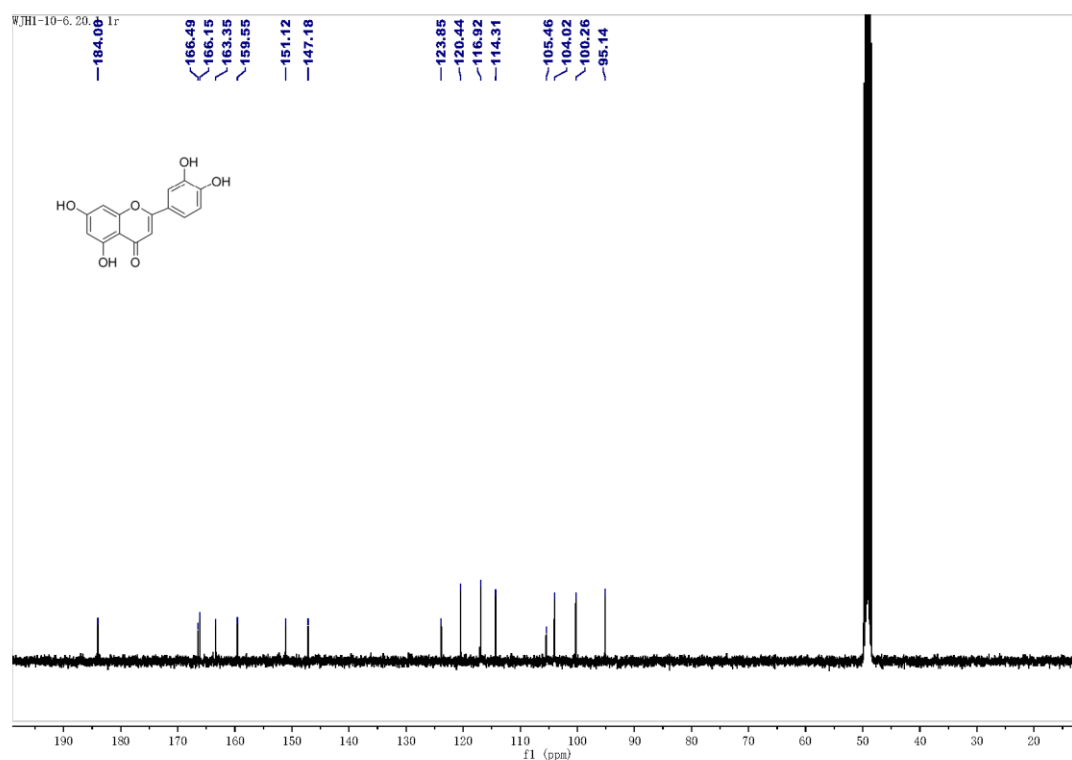
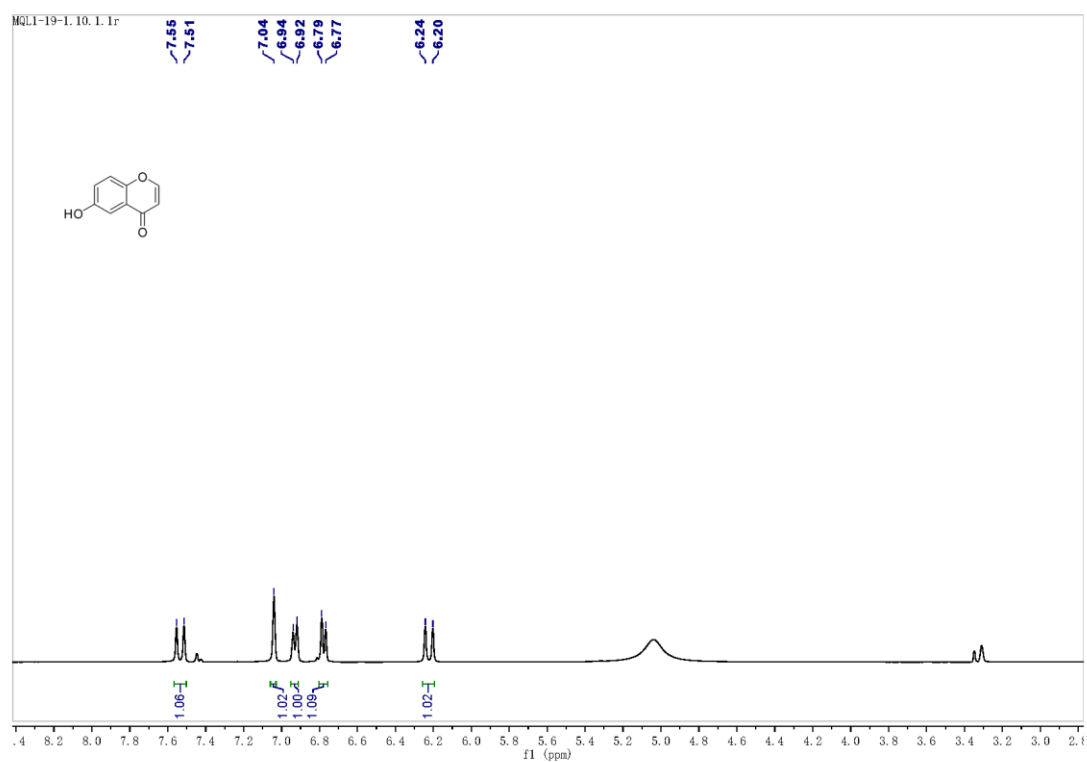
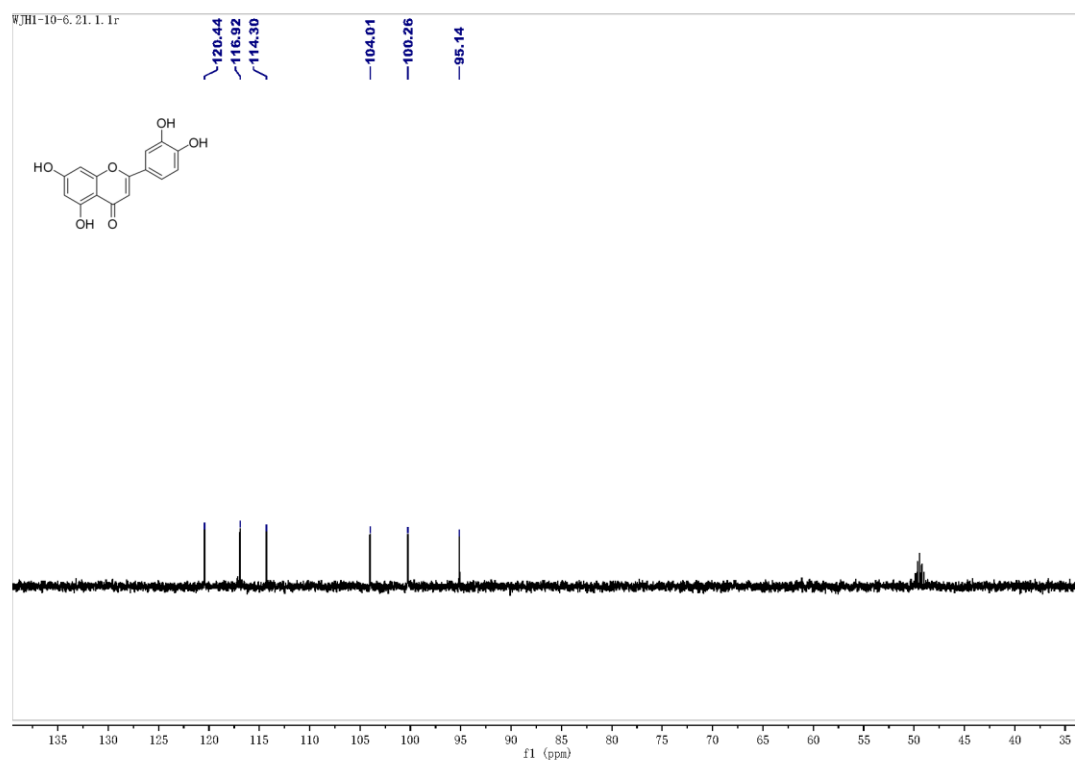


Figure S25: ^{13}C NMR spectrum (100 MHz) of 6 in CD_3OD



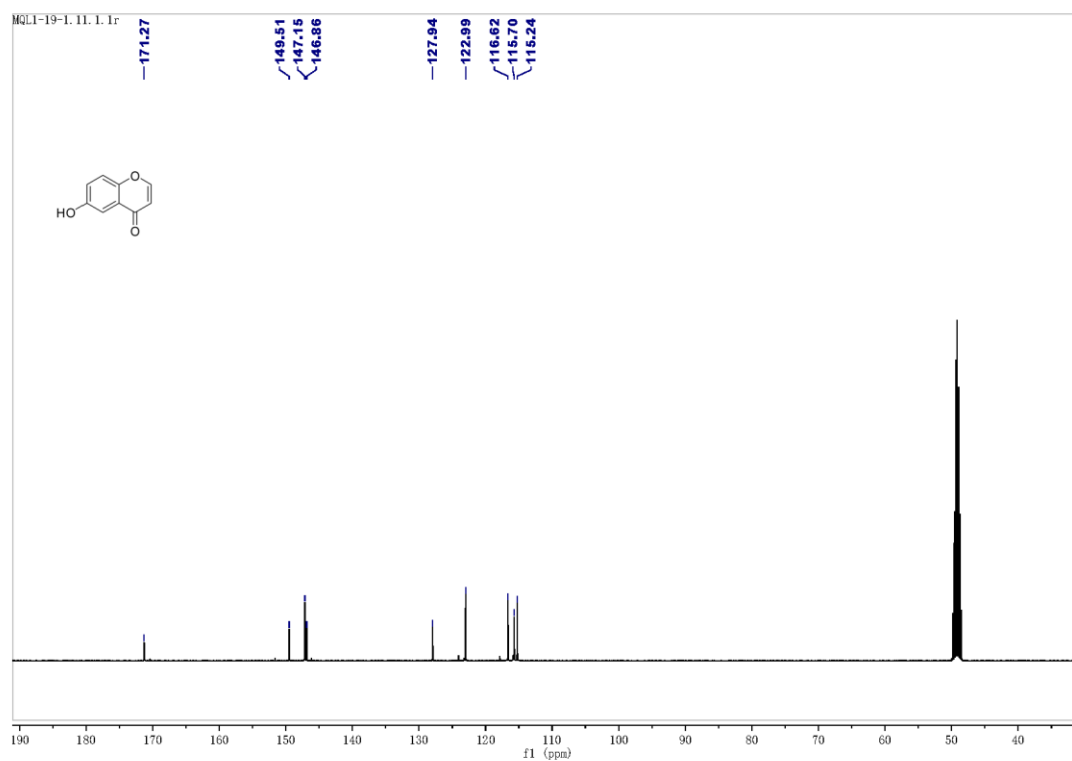


Figure S28: ^{13}C NMR spectrum (100 MHz) of 7 in CD_3OD

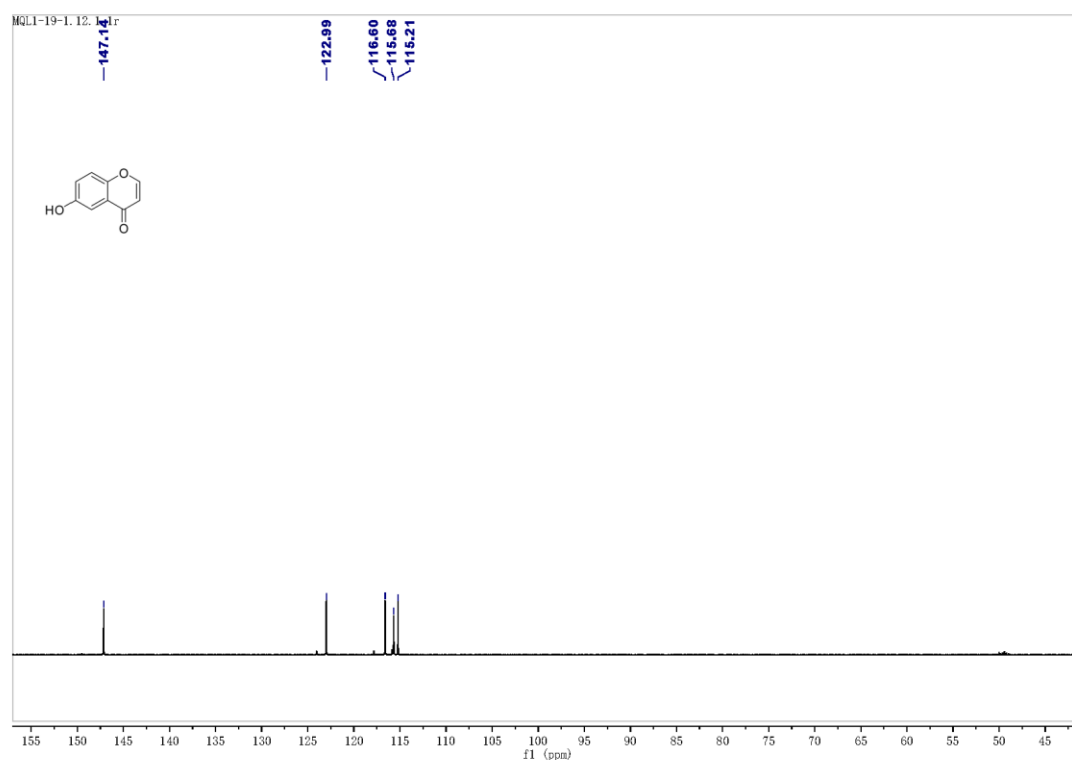


Figure S29: DEPT NMR spectrum (100 MHz) of 7 in CD_3OD

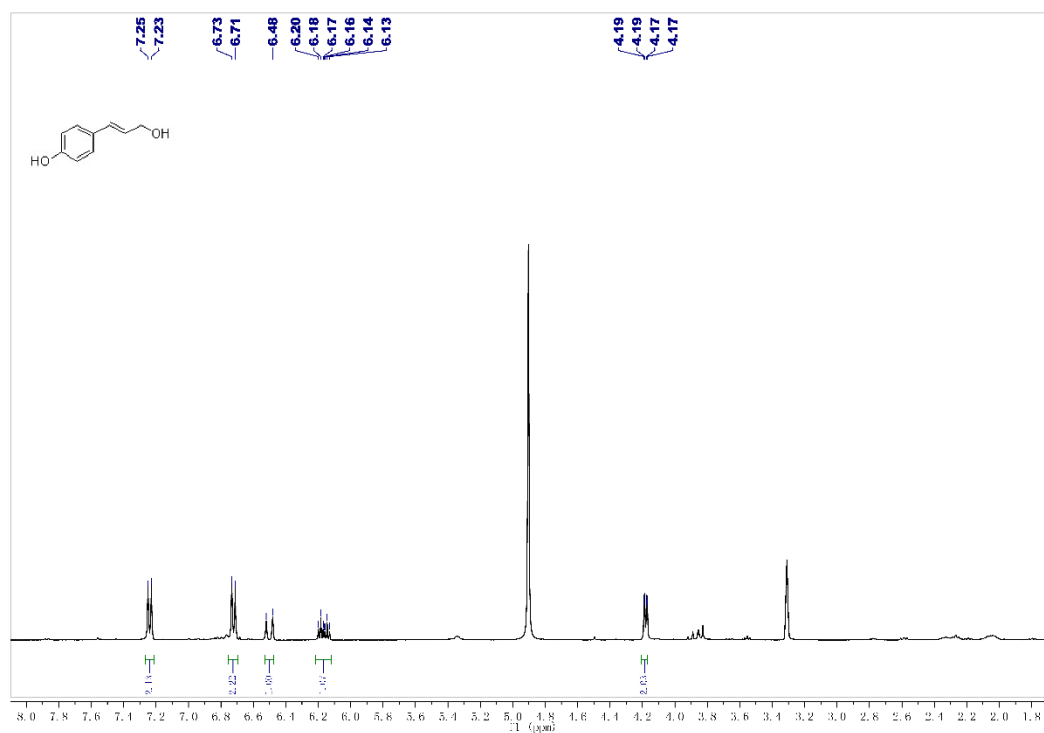


Figure S30: ¹H NMR spectrum (400 MHz) of 8 in CD₃OD

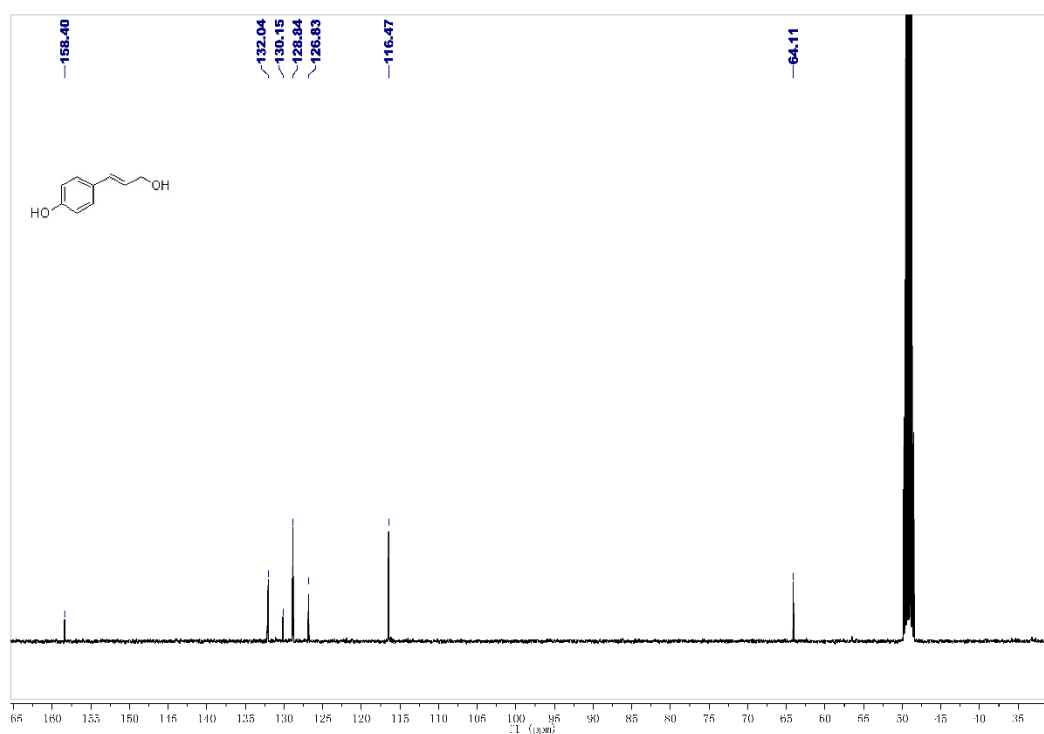


Figure S31: ¹³C NMR spectrum (100 MHz) of 8 in CD₃OD

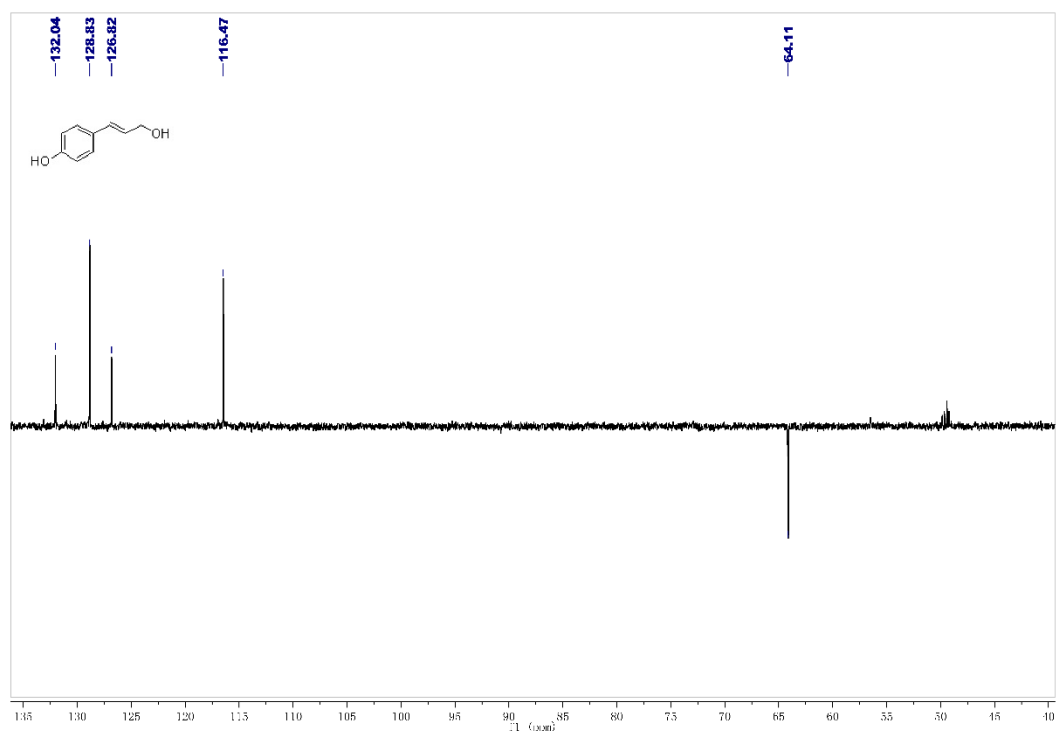
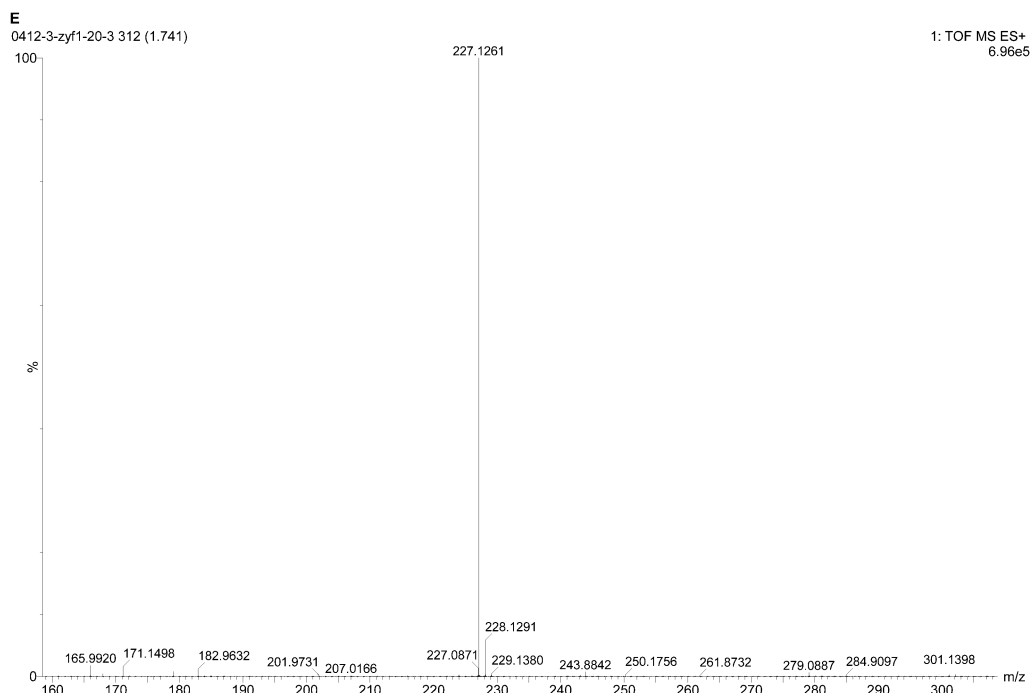


Figure S32: DEPT NMR spectrum (100 MHz) of 8 in CD₃OD



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

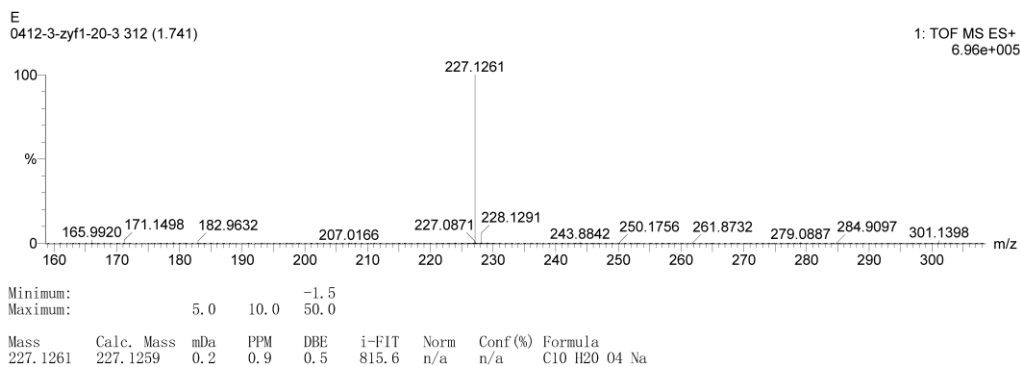


Figure S33: (+)-HR-ESI-MS spectrum of 9

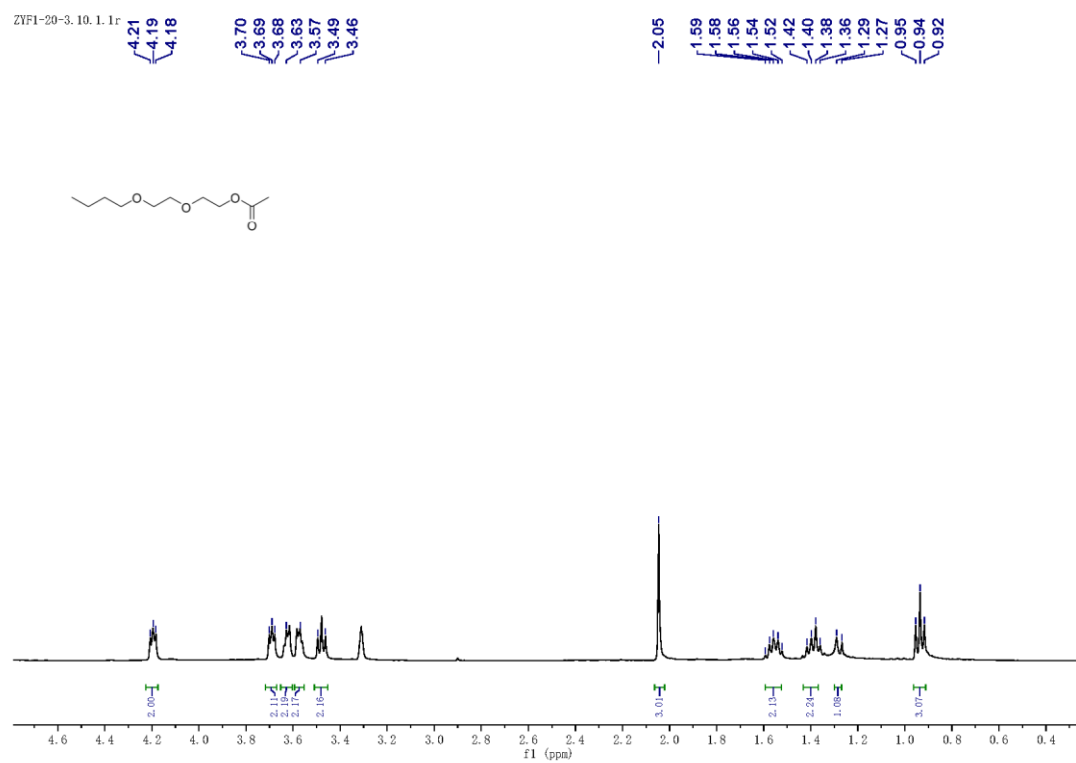


Figure S34: ^1H NMR spectrum (400 MHz) of 9 in CD_3OD

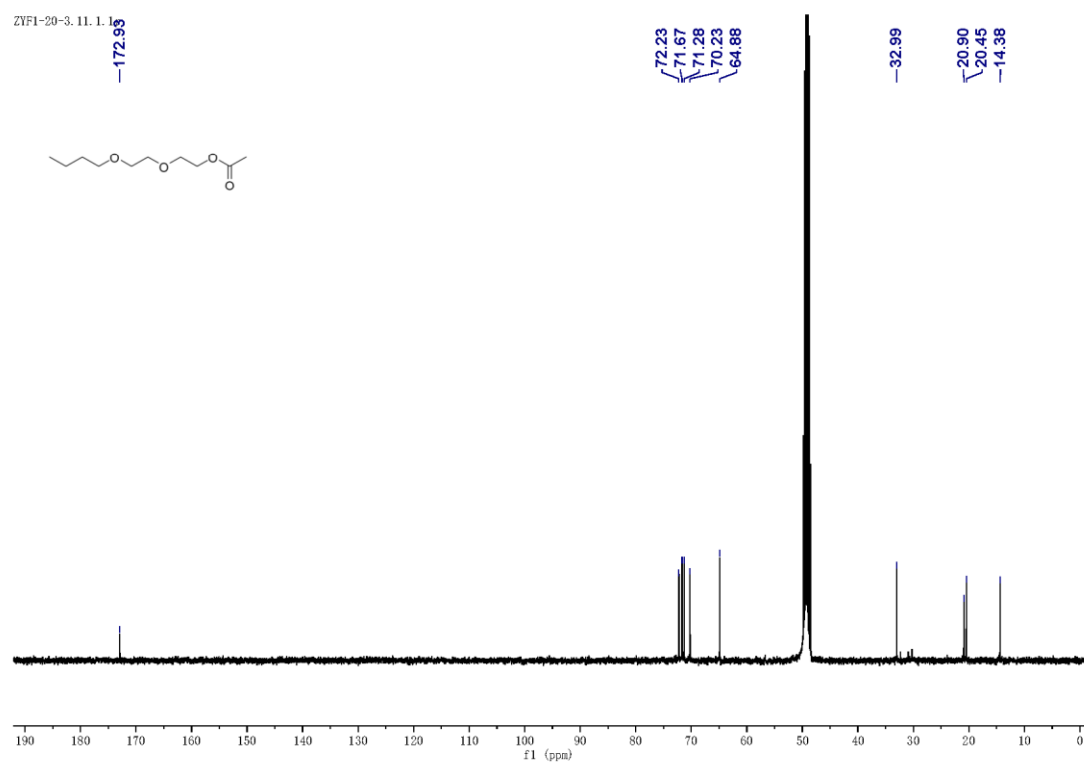


Figure S35: ^{13}C NMR spectrum (100 MHz) of 9 in CD_3OD

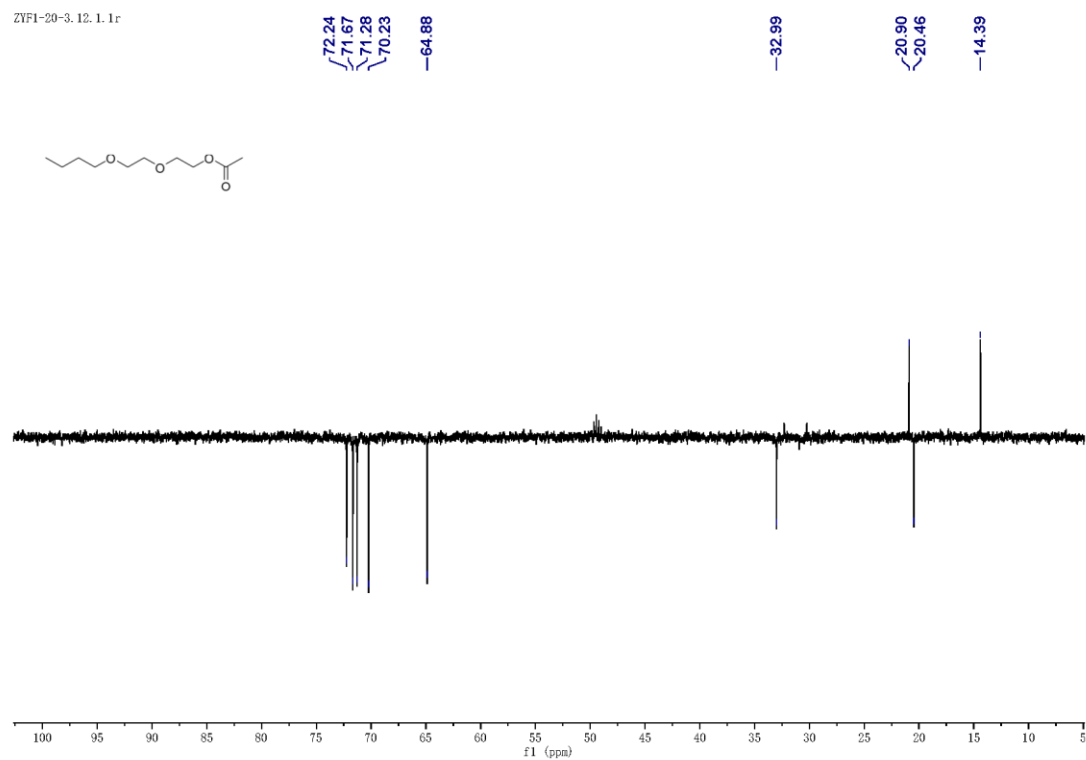


Figure S36: DEPT NMR spectrum (100 MHz) of 9 in CD_3OD