

Supporting information

**An ingenious method for the determination of the
relative and absolute configurations of compounds
containing aryl-glycerol fragments by ^1H NMR
spectroscopy**

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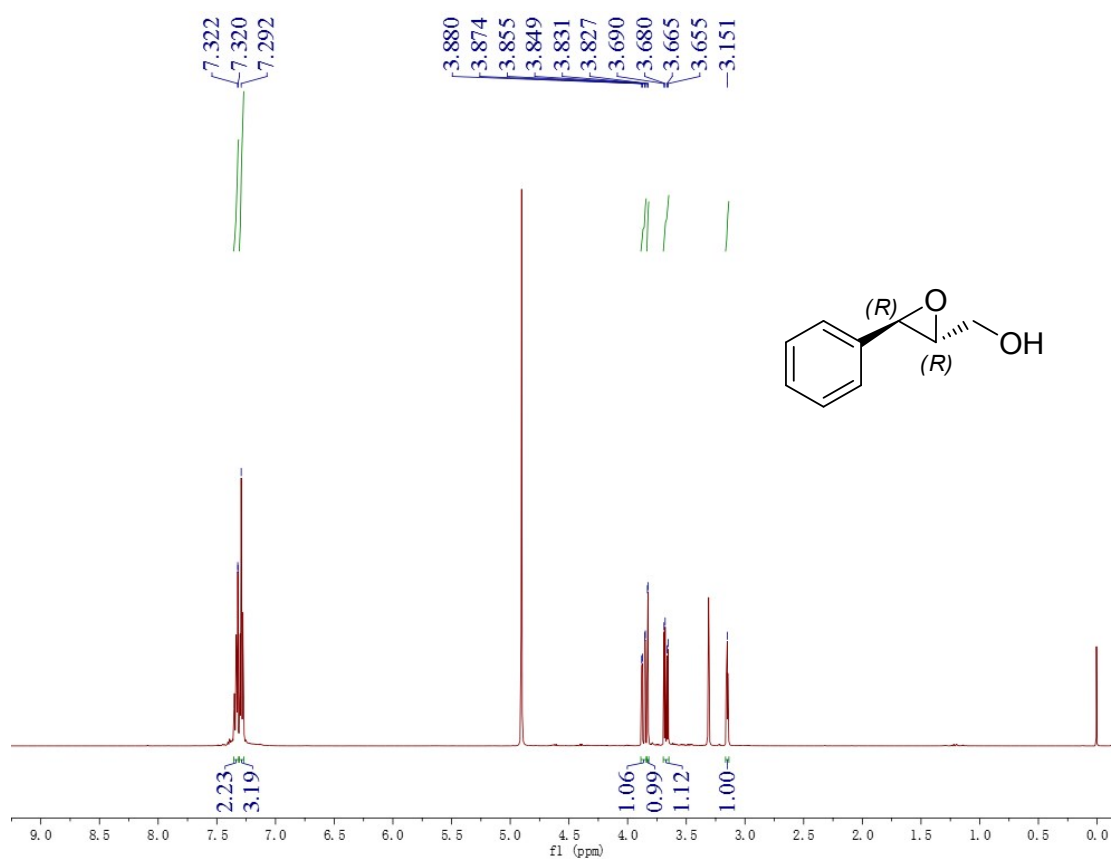


Figure S1. The ¹H NMR spectrum of (2*R*,3*R*)-3-phenyl-2-oxiranemethanol

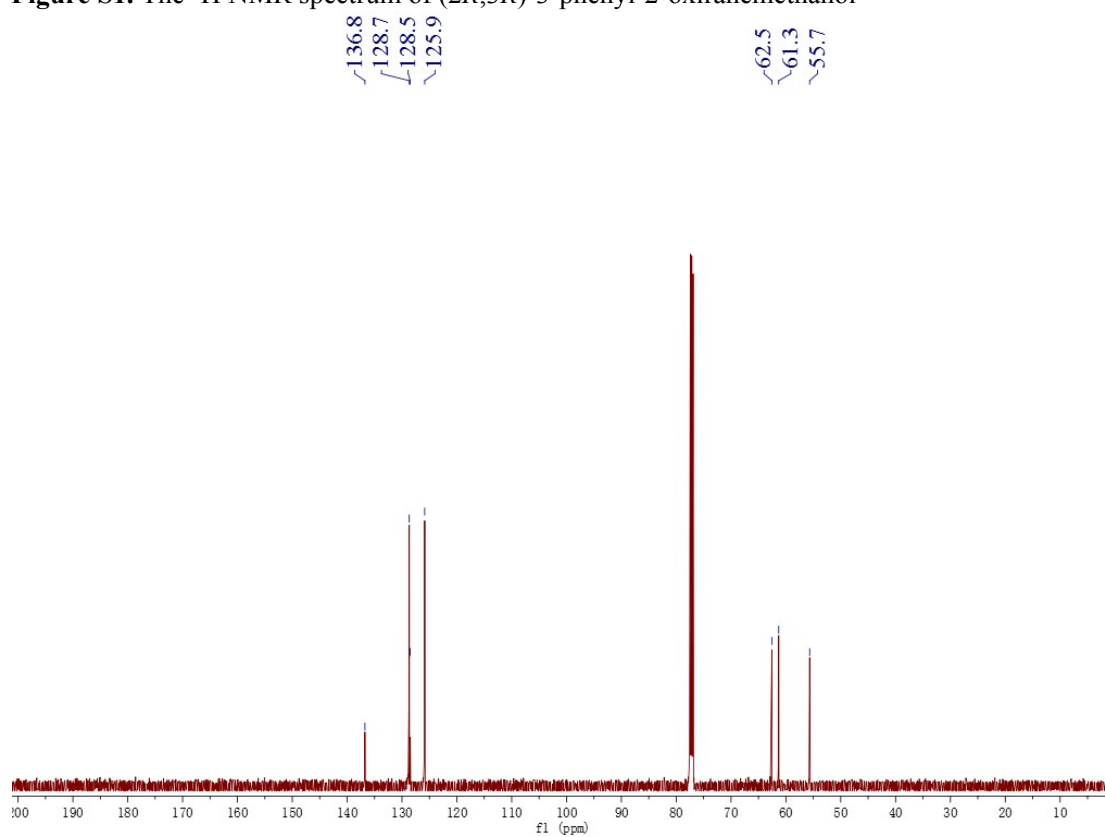
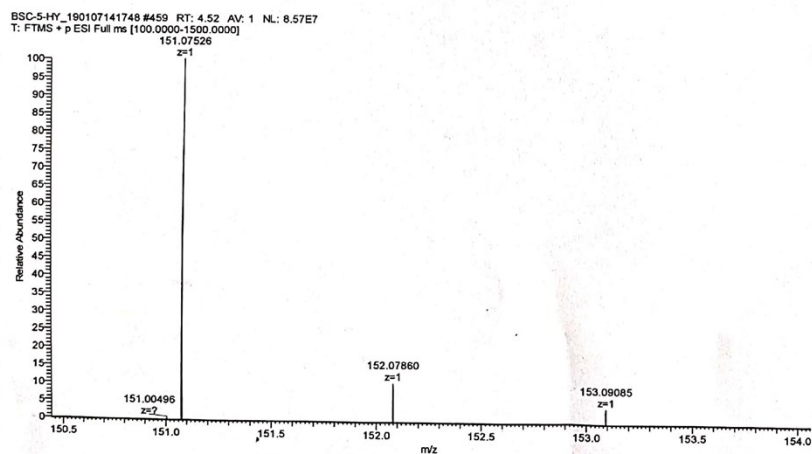
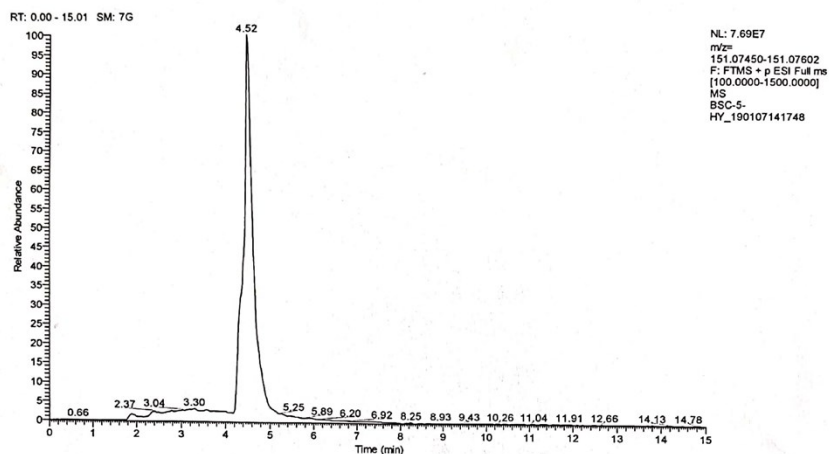


Figure S2. The ¹³C NMR spectrum of compounds (2*R*,3*R*)-3-phenyl-2-oxiranemethanol

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compound NO. : BSC-5-HY
Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
151.07526	151.07536	-0.64	4.5	C9 H11 O2	M+H

Figure S3. The HR-ESI-MS data of compounds (2*R*,3*R*)-3-phenyl-2-oxiranemethanol

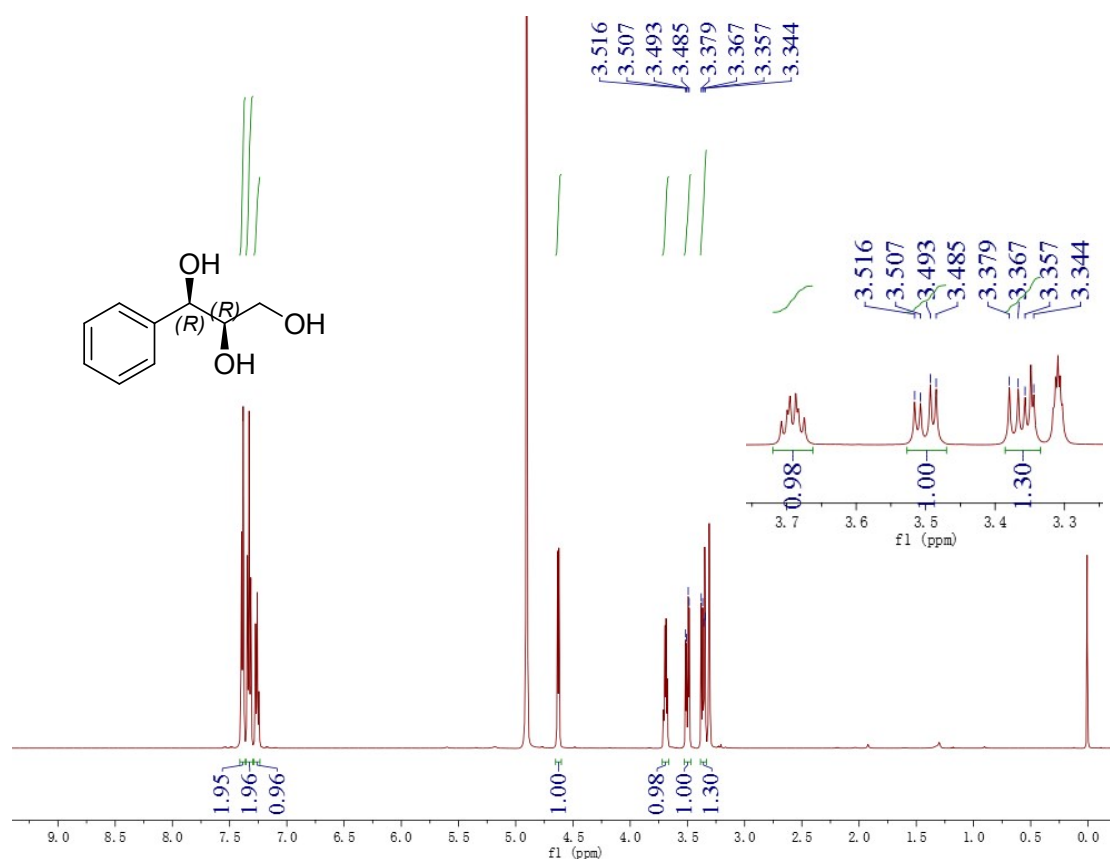


Figure S4. The ¹H NMR spectrum of compound **M1** in methanol-*d*₄

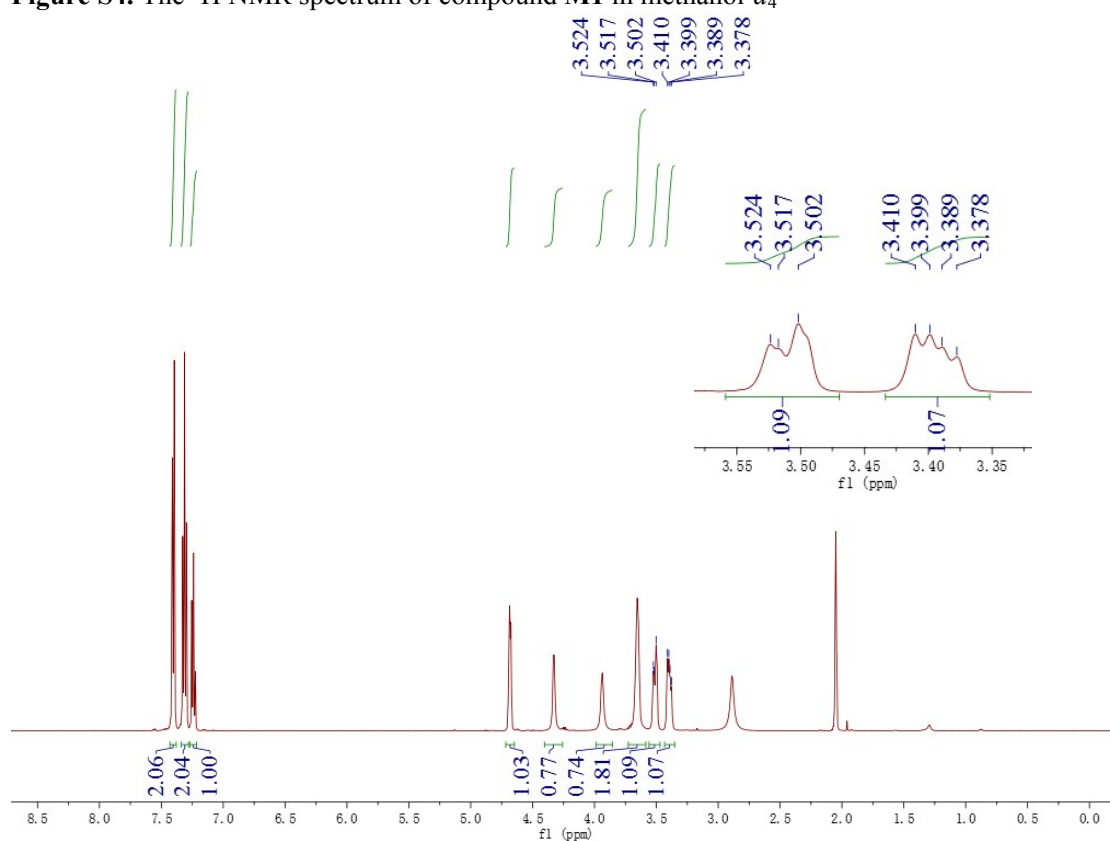


Figure S5. The ¹H NMR spectrum of compound **M1** in acetone-*d*₆

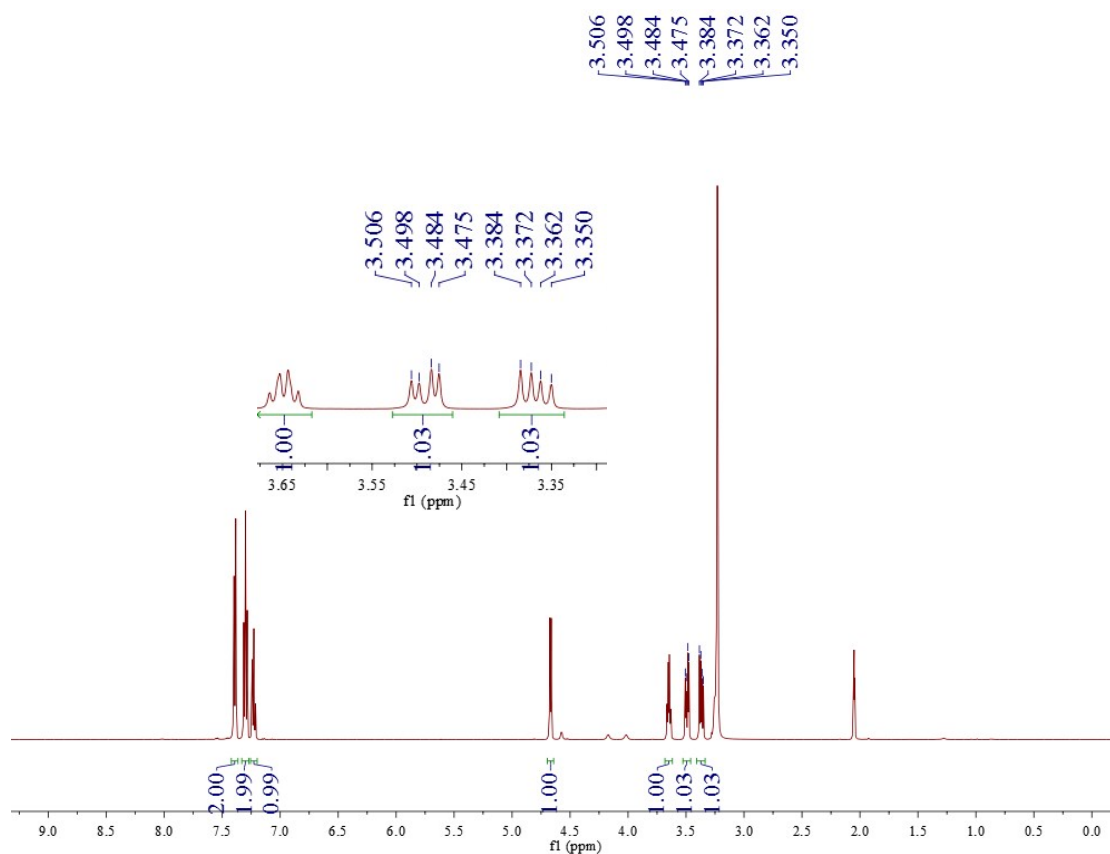


Figure S6. The H-D exchange ^1H NMR spectrum of compound **M1** in acetone- d_6

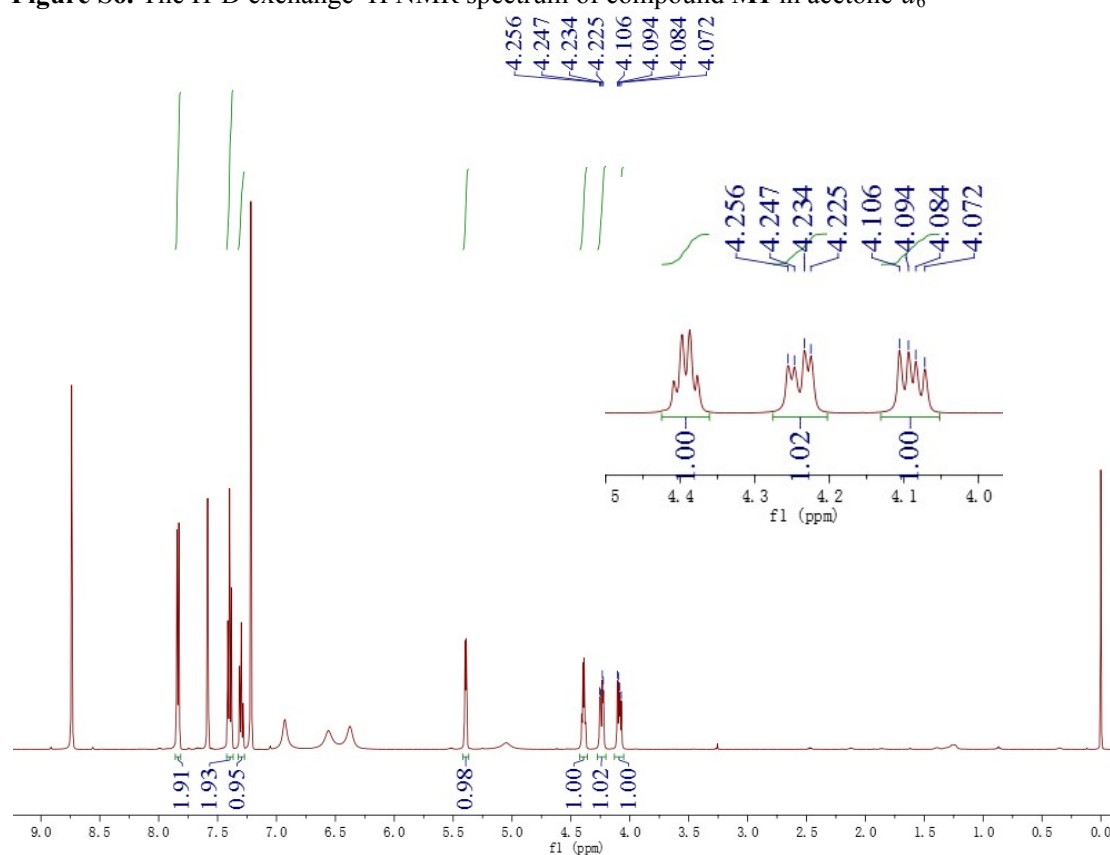


Figure S7. The ^1H NMR spectrum of compound **M1** in pyridine- d_5

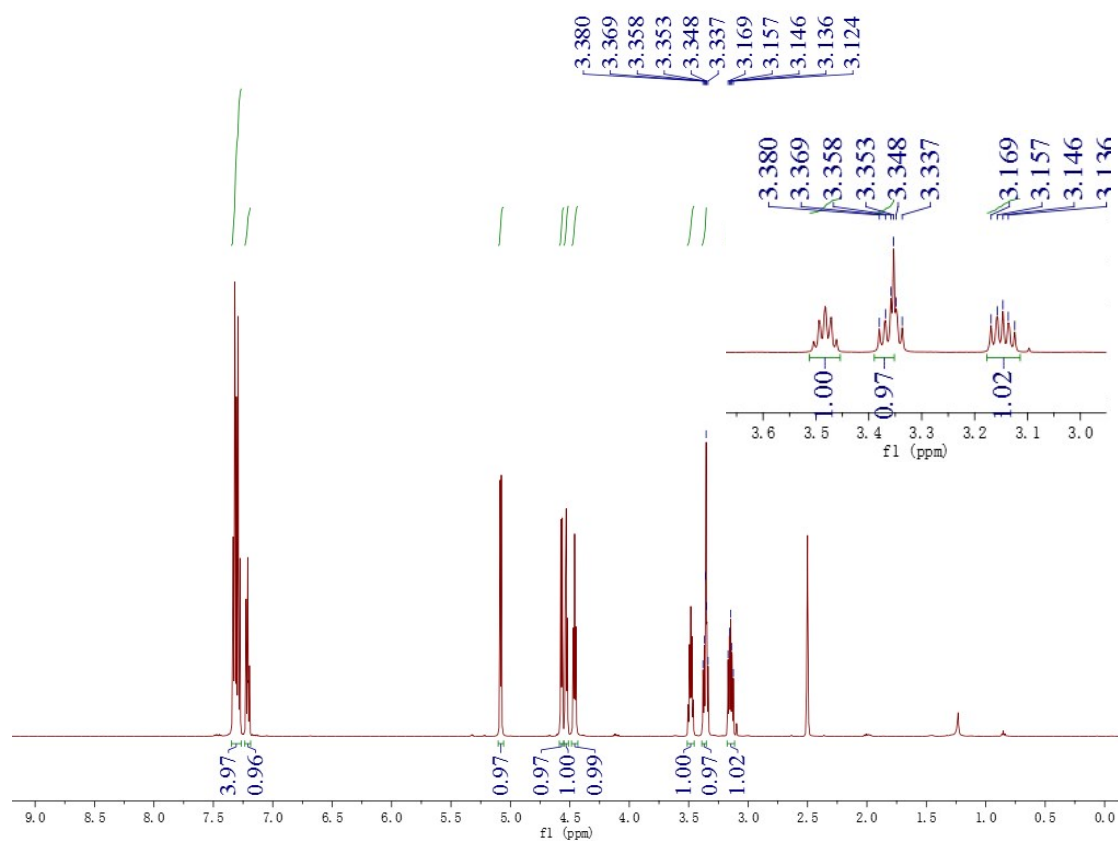


Figure S8. The ^1H NMR spectrum of compound **M1** in $\text{DMSO-}d_6$

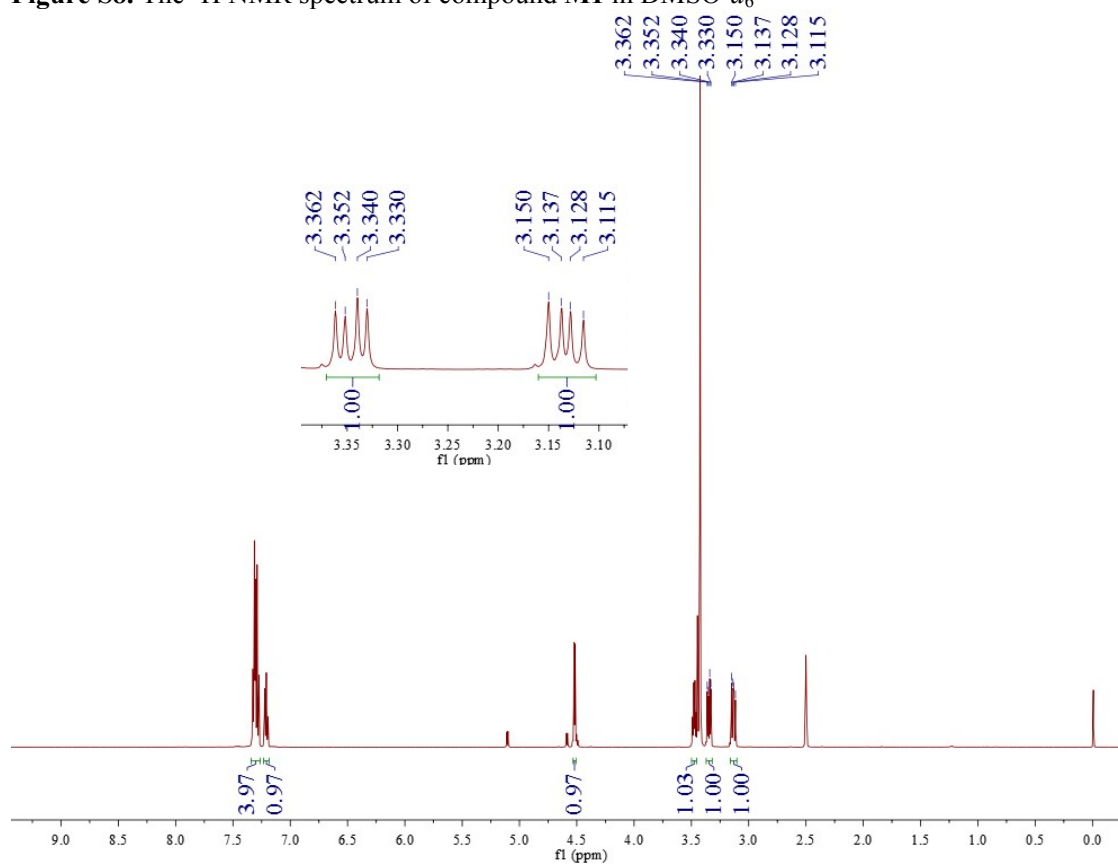


Figure S9. The H-D exchange ^1H NMR spectrum of compound **M1** in $\text{DMSO-}d_6$

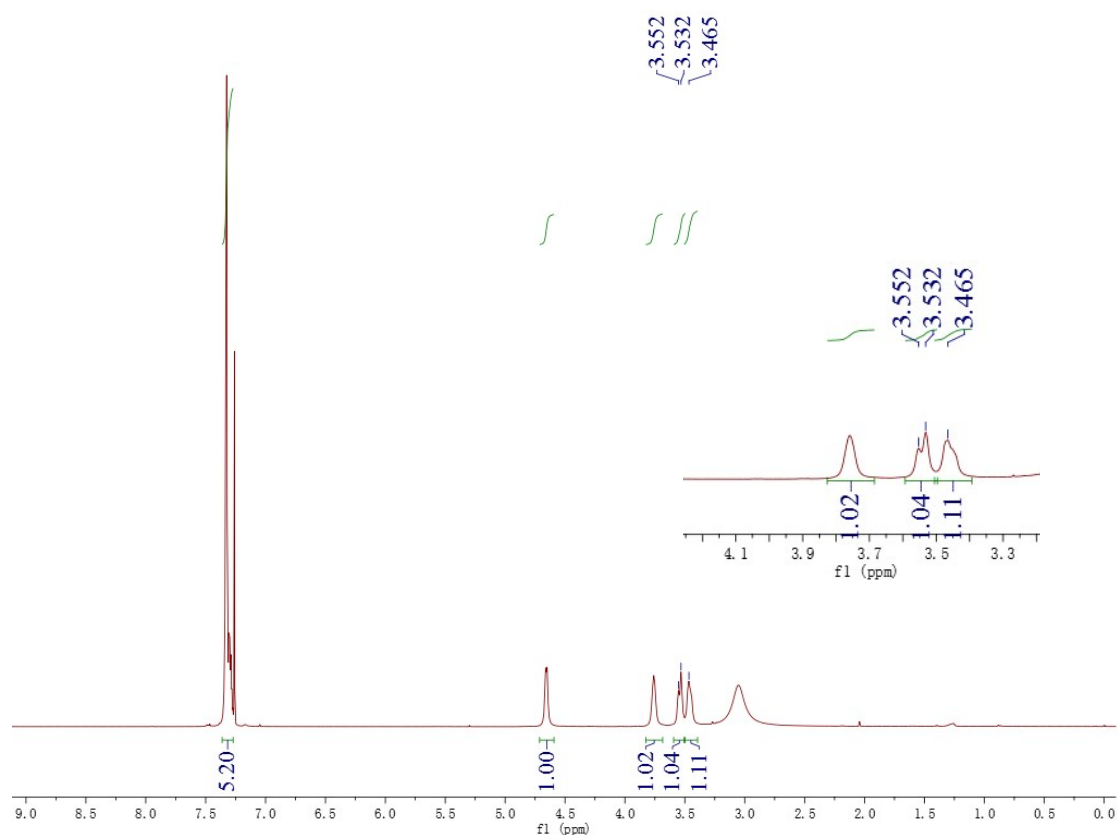


Figure S10. The ¹H NMR spectrum of compound **M1** in CDCl₃

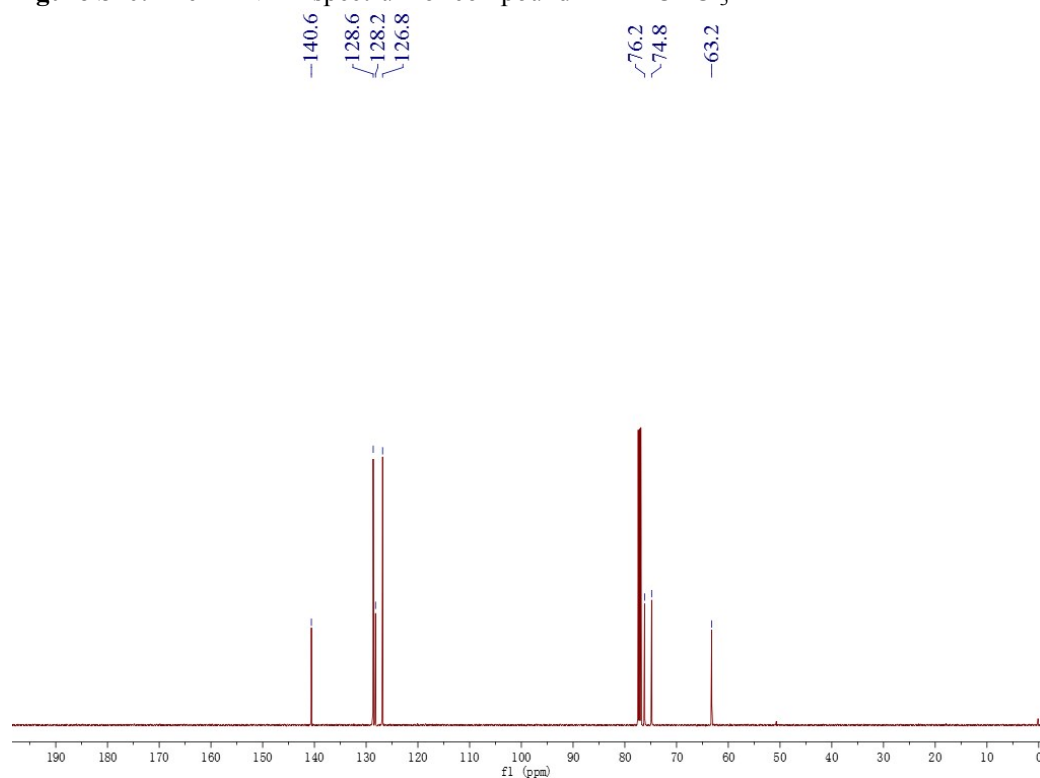


Figure S11. The ¹³C NMR spectrum of compound **M1** in CDCl₃

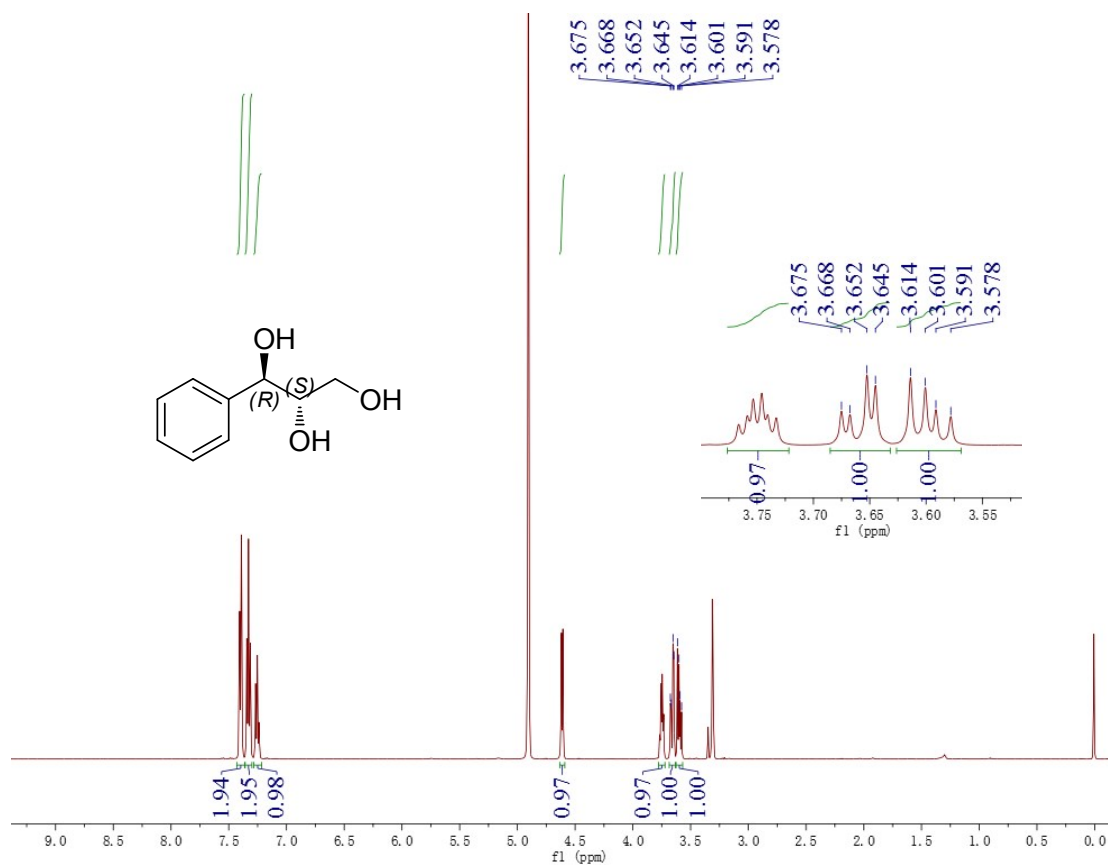


Figure S12. The ^1H NMR spectrum of compound **M3** in methanol- d_4

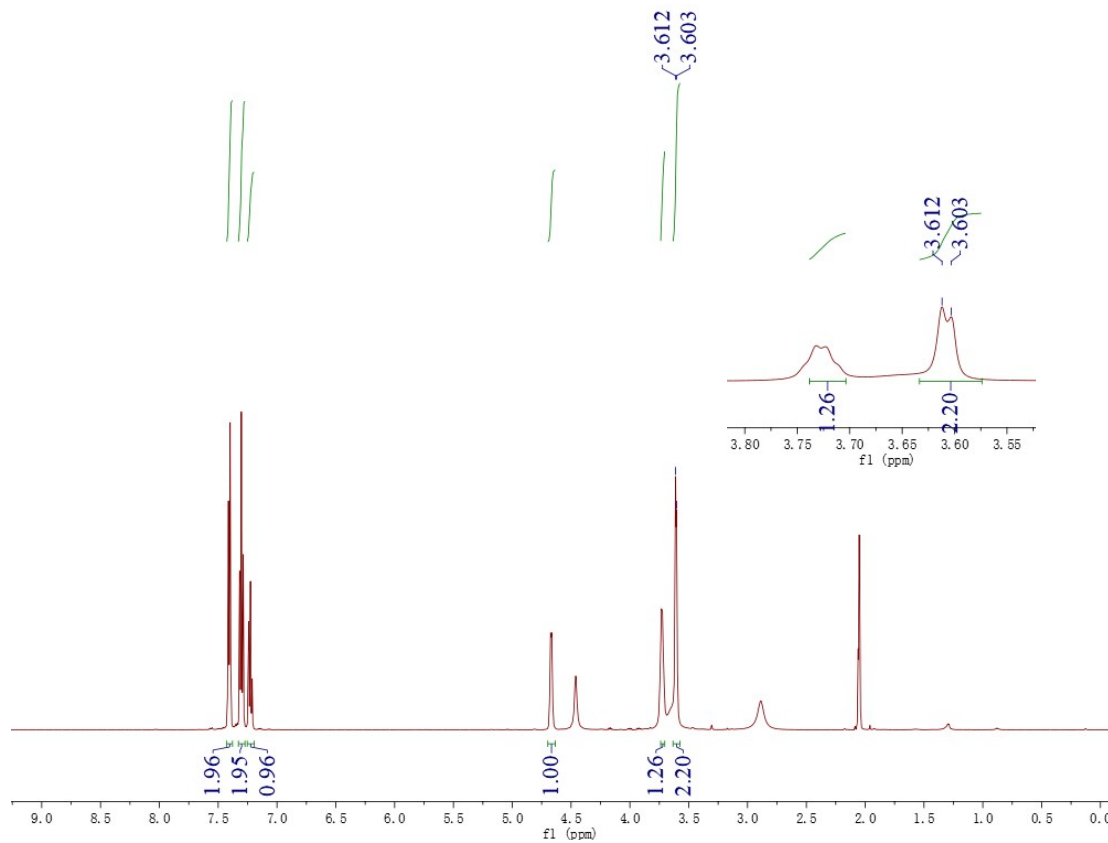


Figure S13. The ^1H NMR spectrum of compound **M3** in acetone- d_6

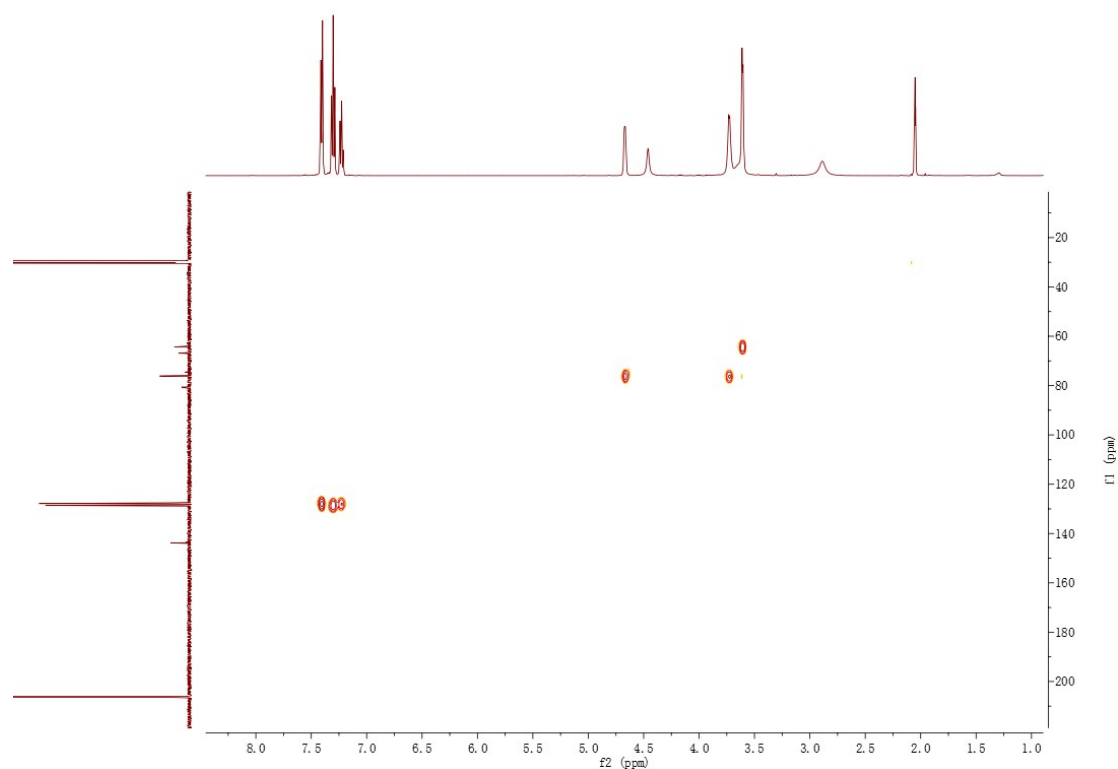


Figure S14. The HSQC spectrum of compound **M3** in acetone- d_6

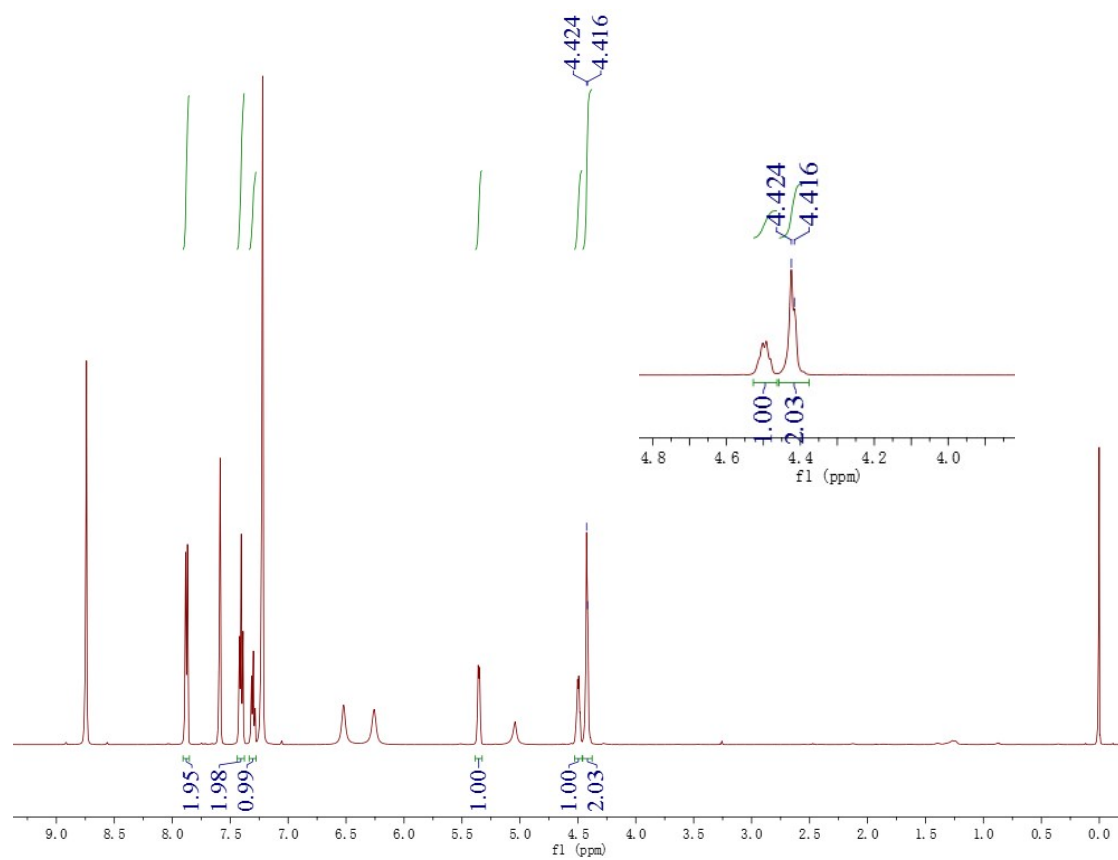


Figure S15. The ^1H NMR spectrum of compound **M3** in pyridine- d_5

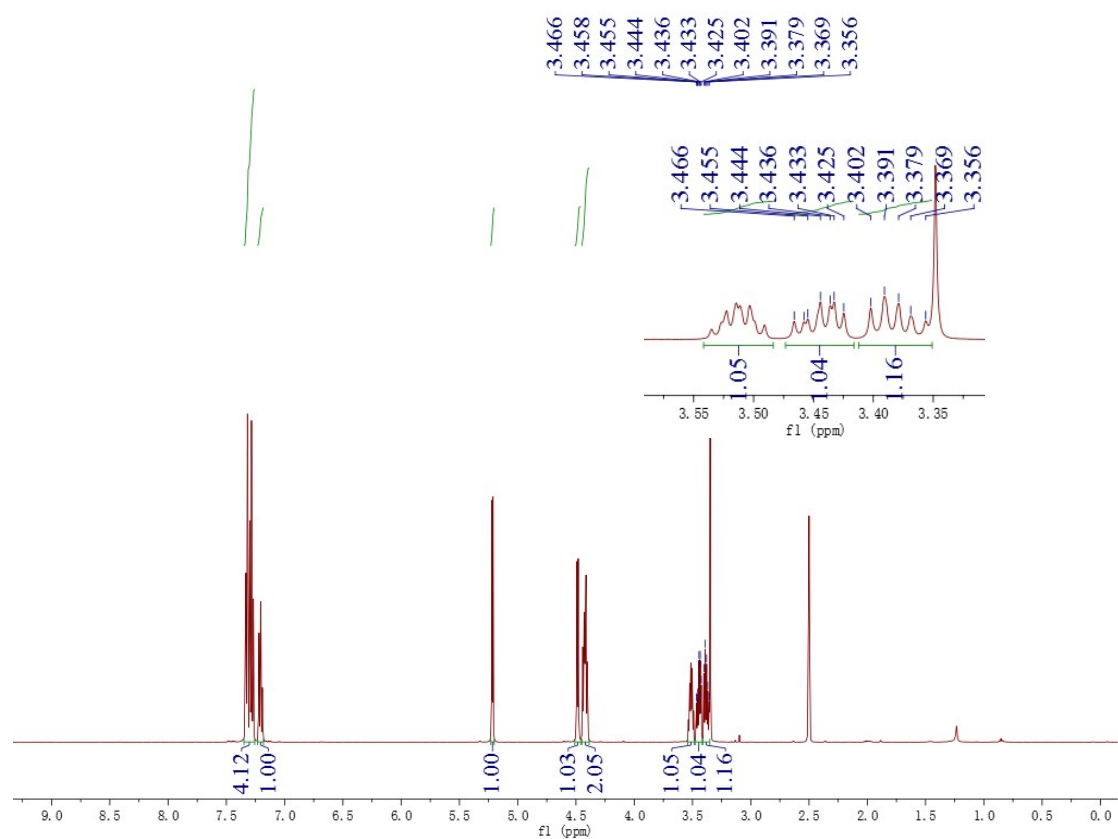


Figure S16. The ^1H NMR spectrum of compound **M3** in $\text{DMSO-}d_6$

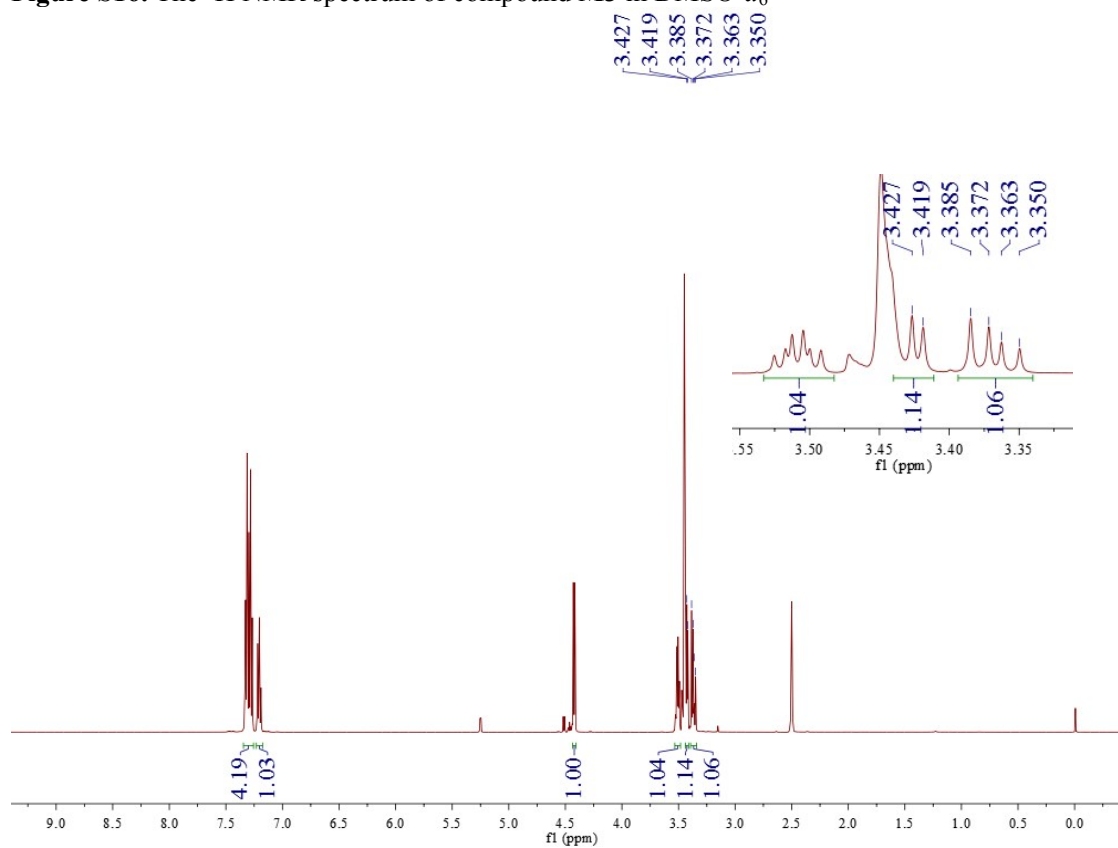


Figure S17. The H-D exchange ^1H NMR spectrum of compound **M3** in $\text{DMSO-}d_6$

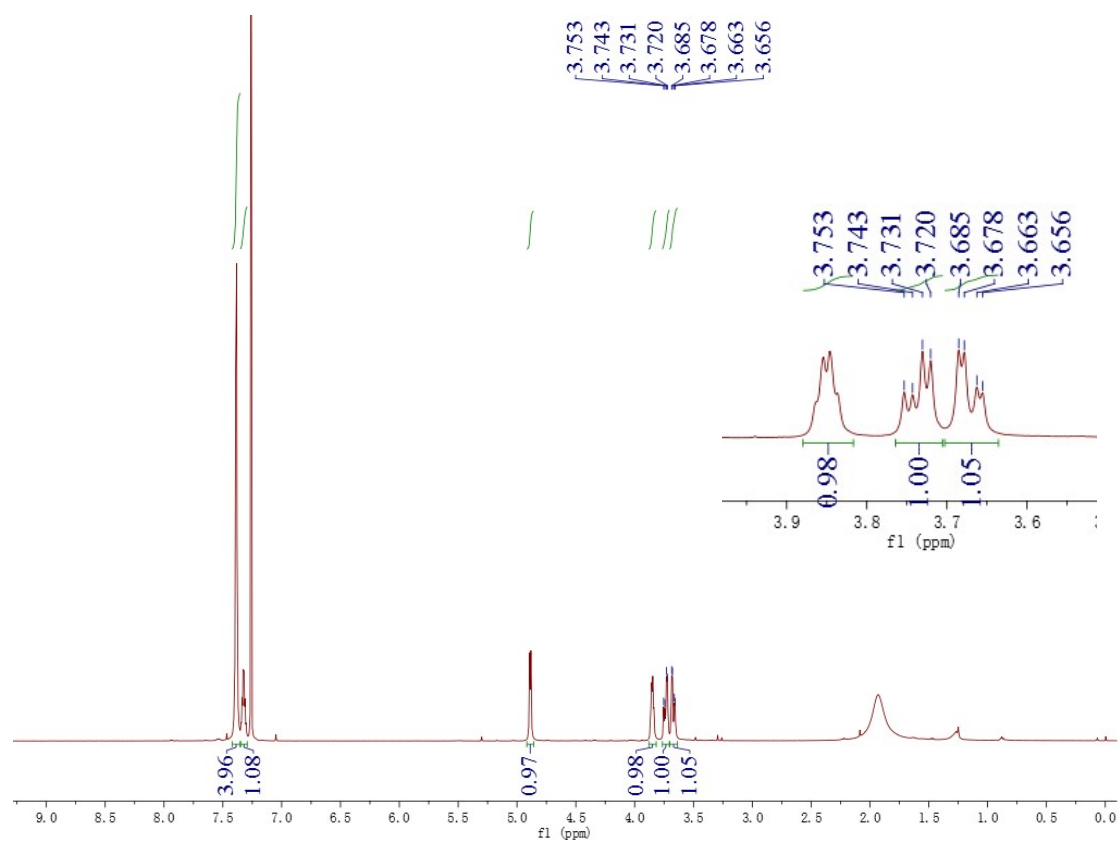


Figure S18. The ^1H NMR spectrum of compound **M3** in CDCl_3

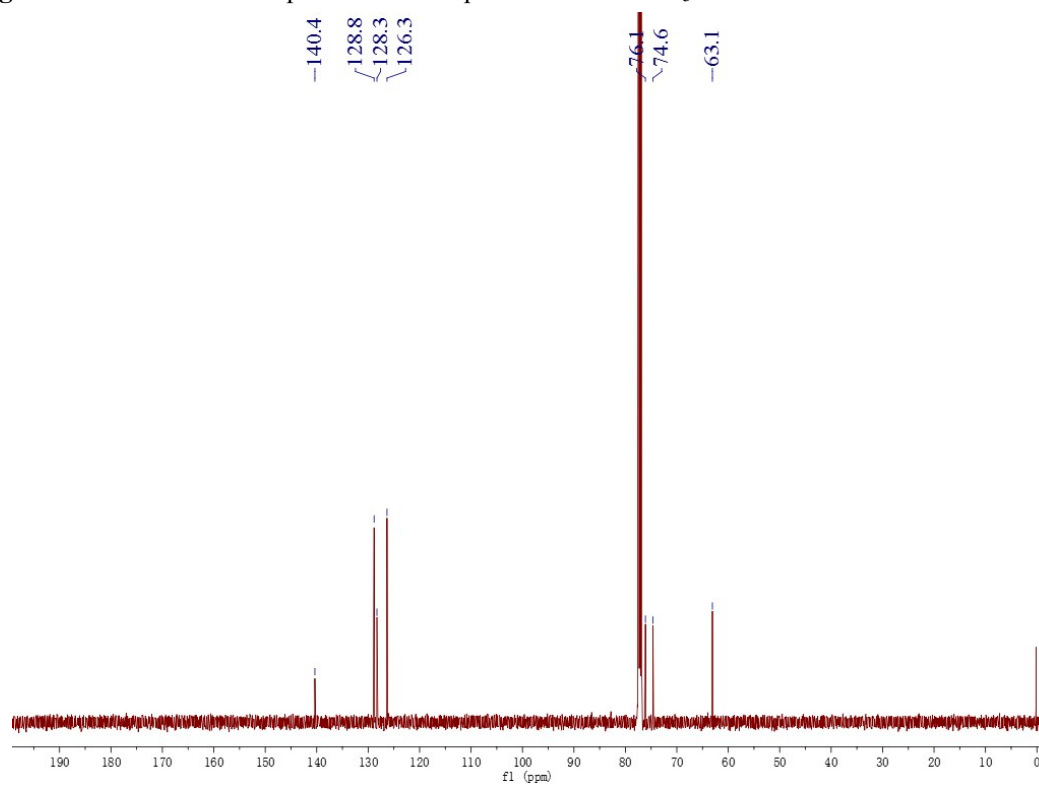
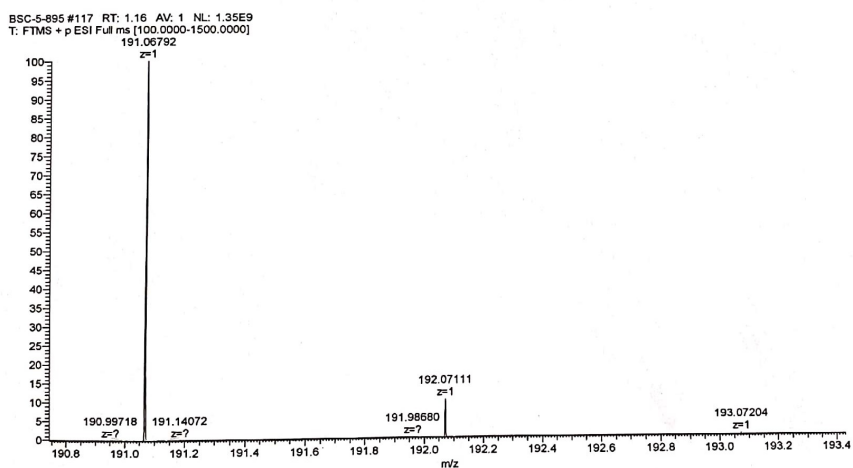
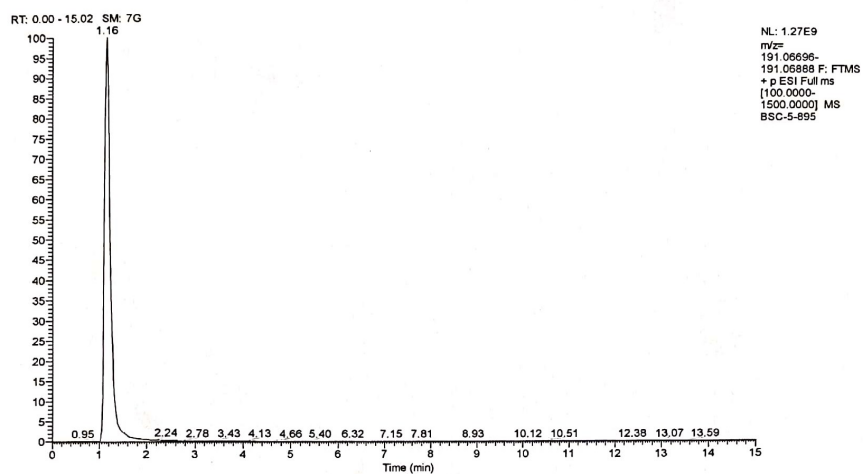


Figure S19. The ^{13}C NMR spectrum of compound **M3** in CDCl_3

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compound NO. : BSC-5-8.95

Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
191.06792	191.06787	0.29	3.5	C9 H12 O3 Na	M+Na

Figure S20. The HR-ESI-MS data of compound **M3**

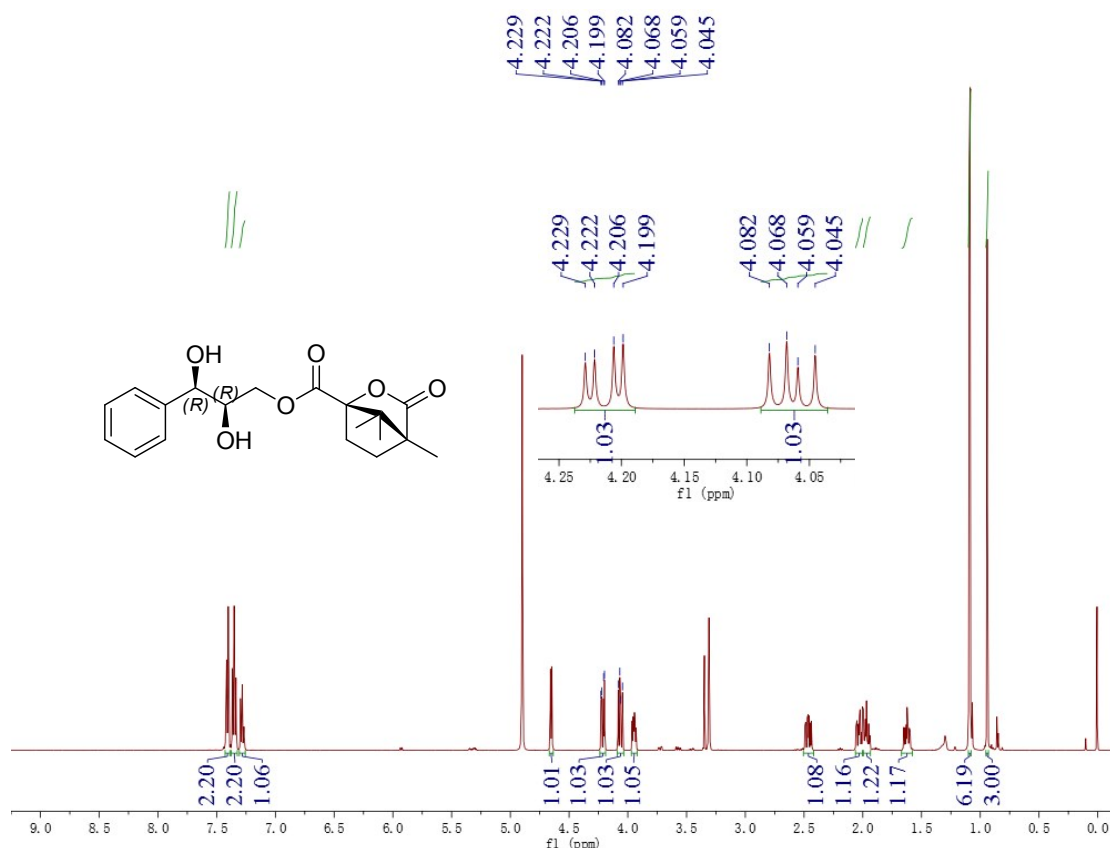


Figure S21. The ^1H NMR spectrum of compound **M1a** in methanol- d_4

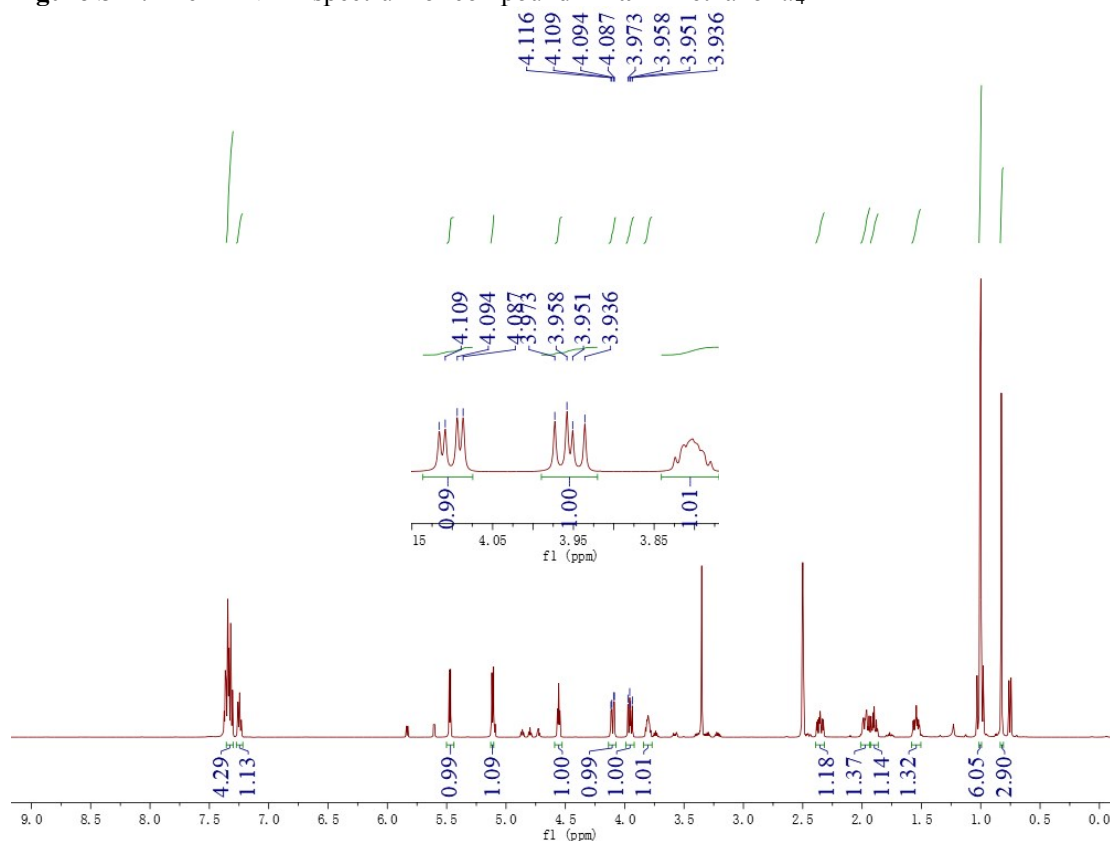


Figure S22. The ^1H NMR spectrum of compound **M1a** in DMSO- d_6

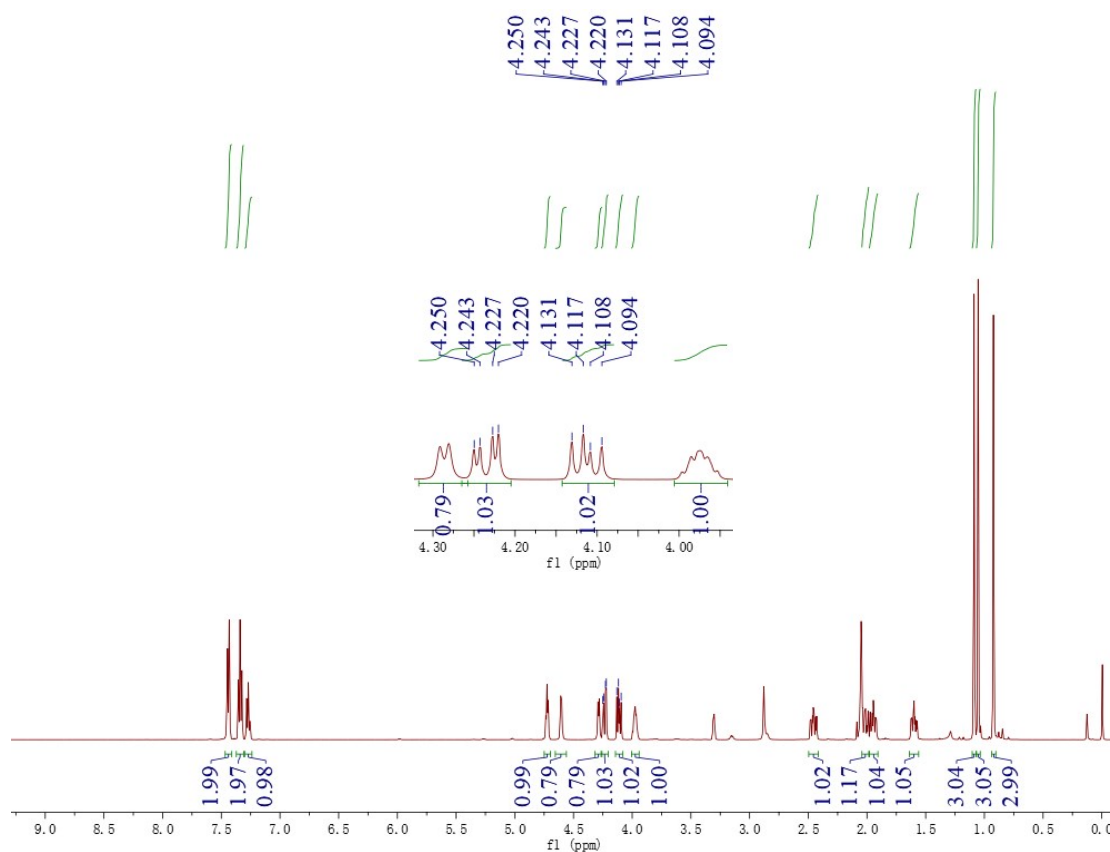


Figure S23. The ^1H NMR spectrum of compound **M1a** in acetone- d_6

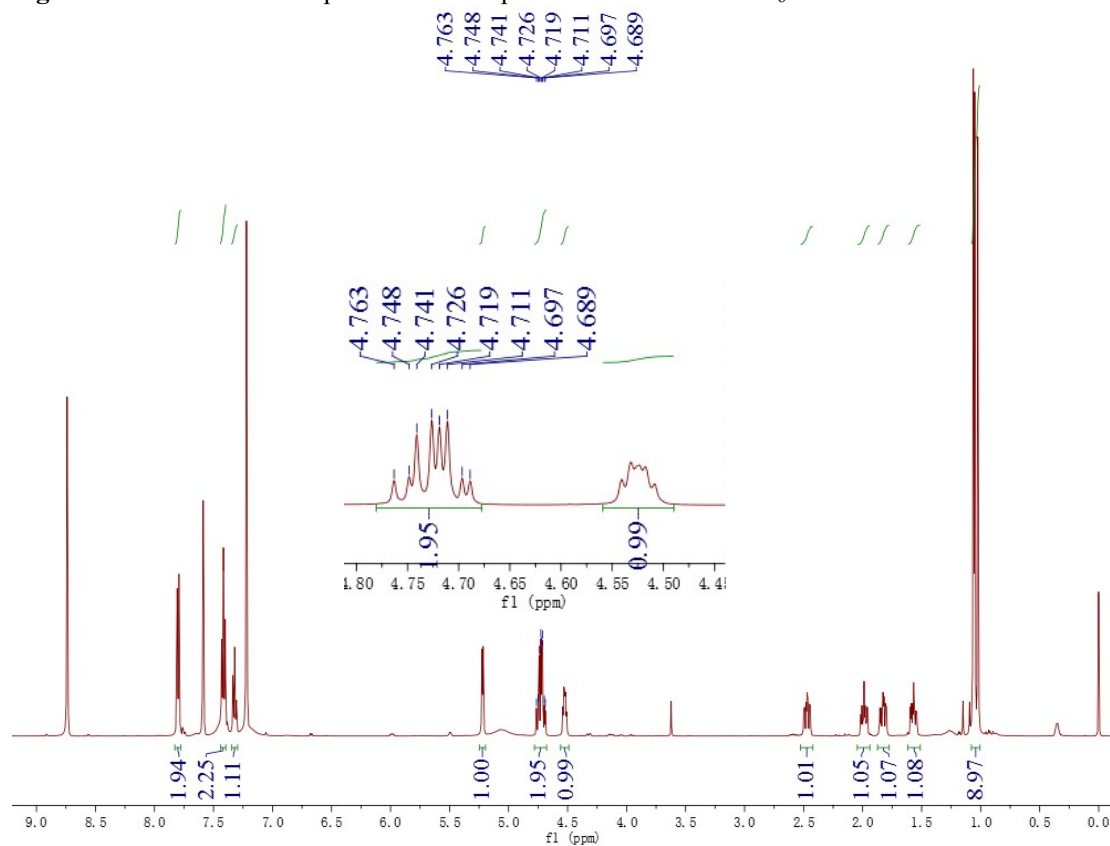


Figure S24. The ^1H NMR spectrum of compound **M1a** in pyridine- d_5

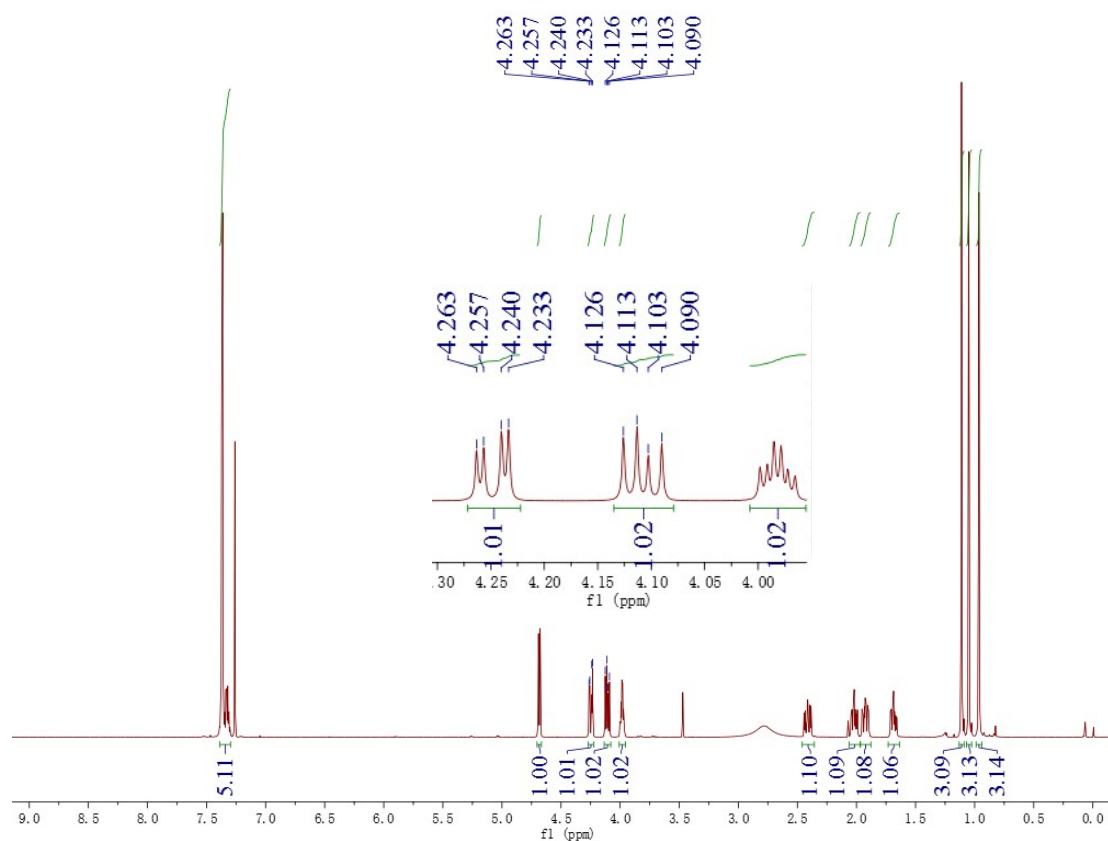


Figure S25. The ^1H NMR spectrum of compound **M1a** in CDCl_3

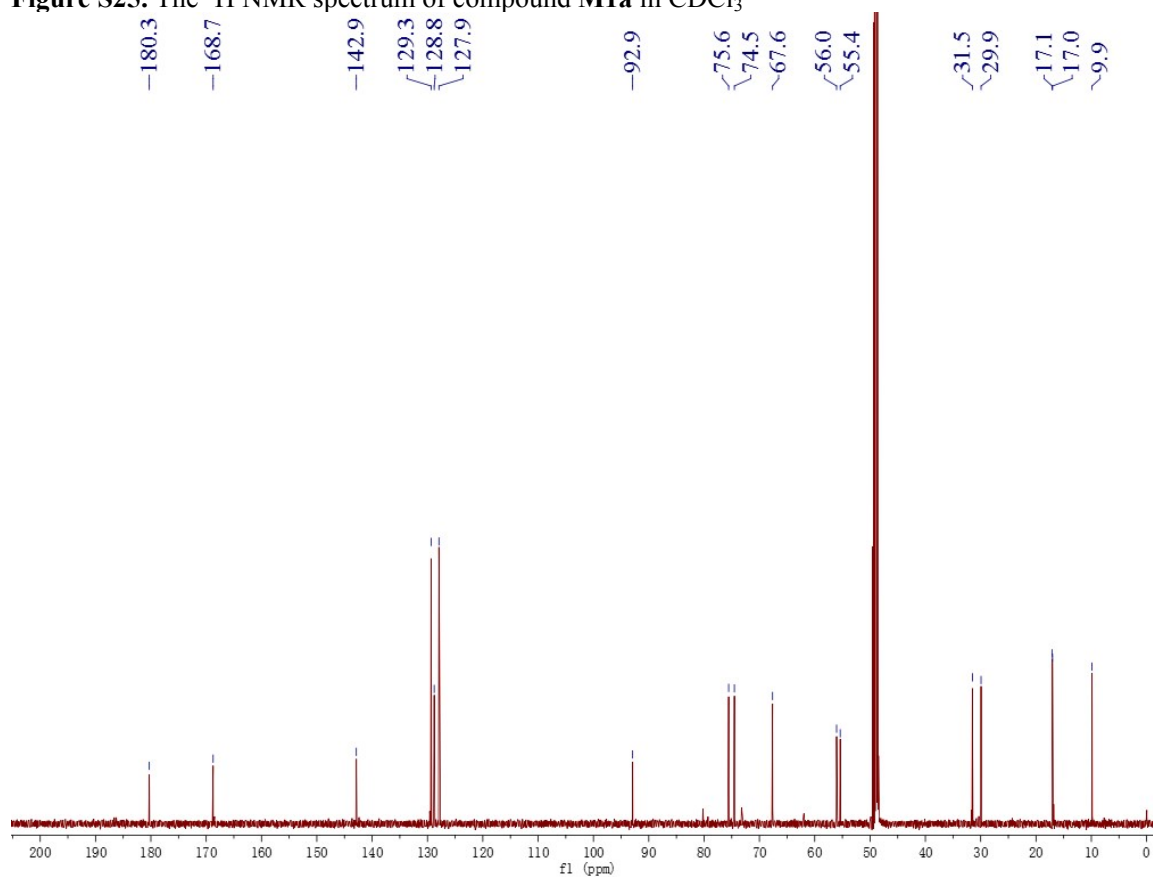


Figure S26. The ^{13}C NMR spectrum of compound **M1a** in $\text{methanol-}d_4$

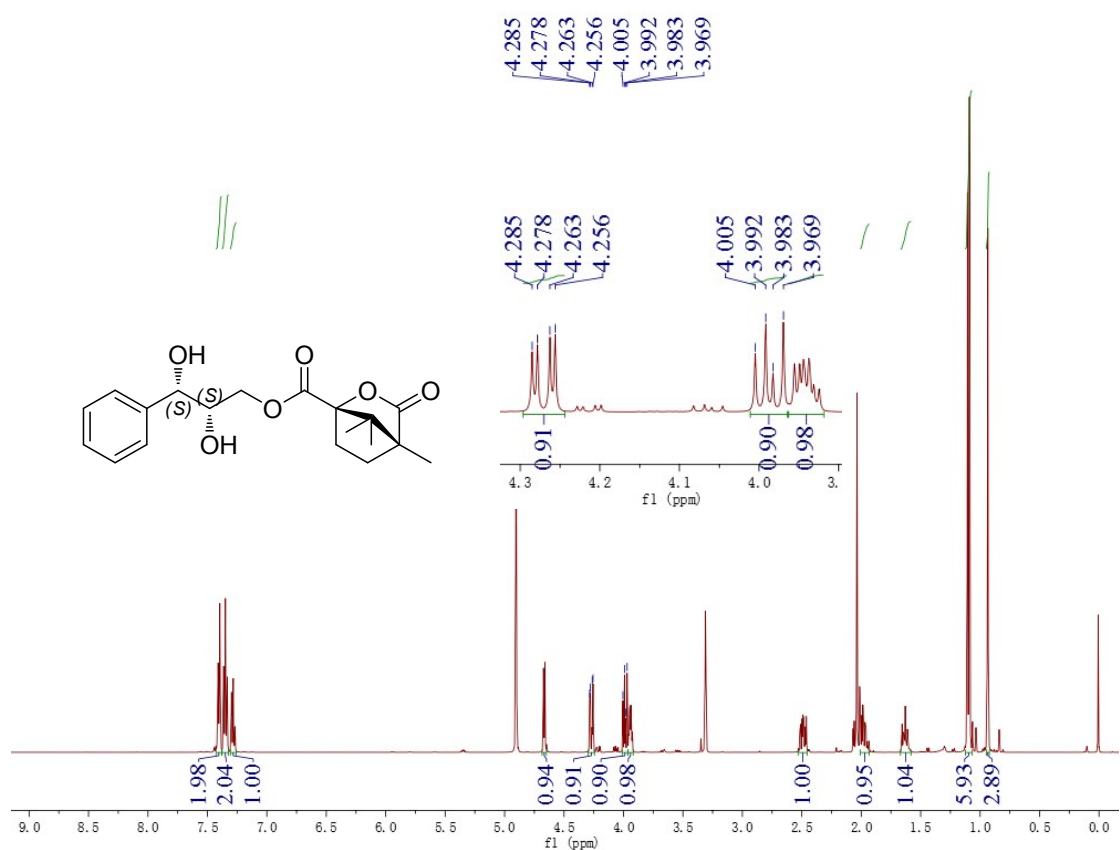


Figure S27. The ¹H NMR spectrum of compound **M2a** in methanol-*d*₄

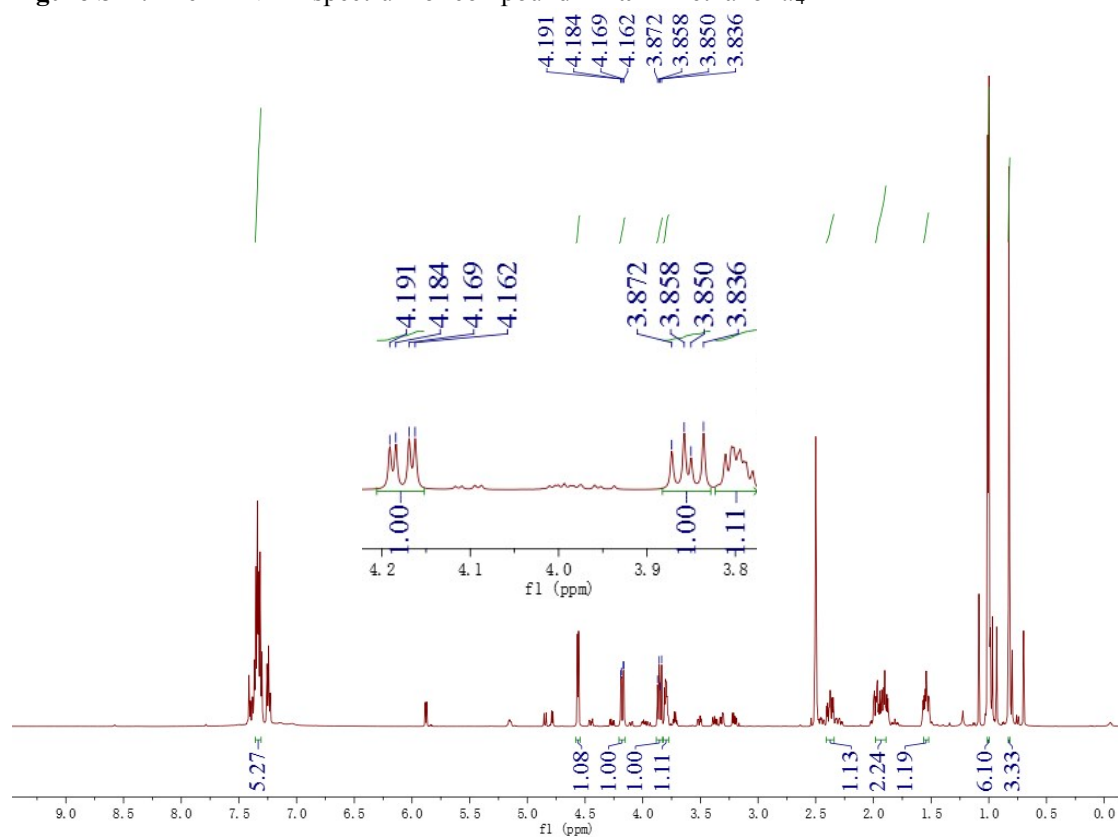


Figure S28. The ¹H NMR spectrum of compound **M2a** in DMSO-*d*₆

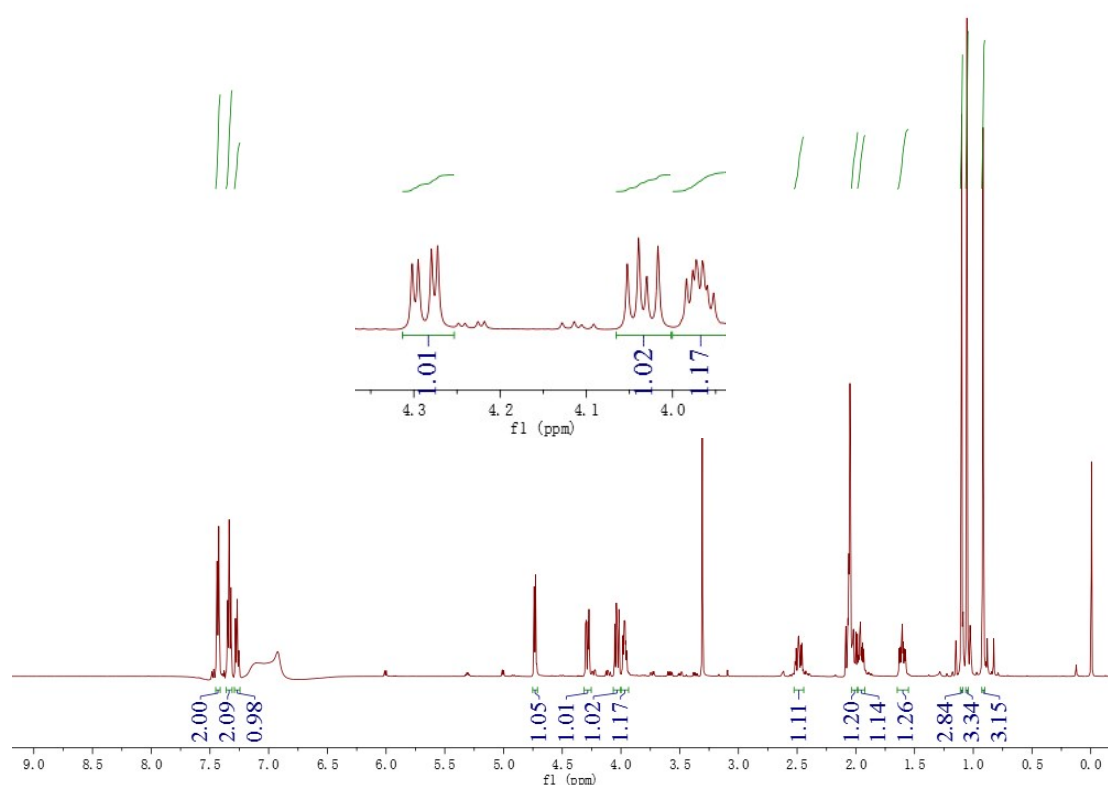


Figure S29. The ^1H NMR spectrum of compound **M2a** in acetone- d_6

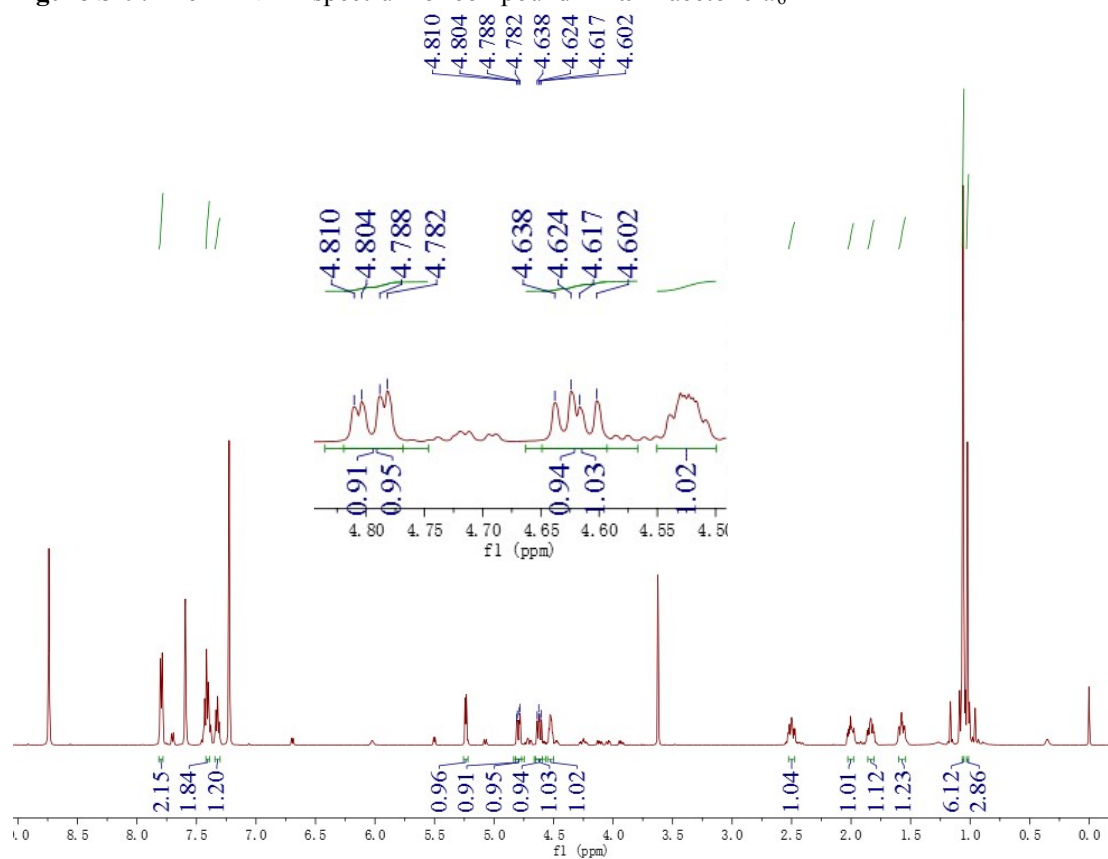


Figure S30. The ^1H NMR spectrum of compound **M2a** in pyridine- d_5

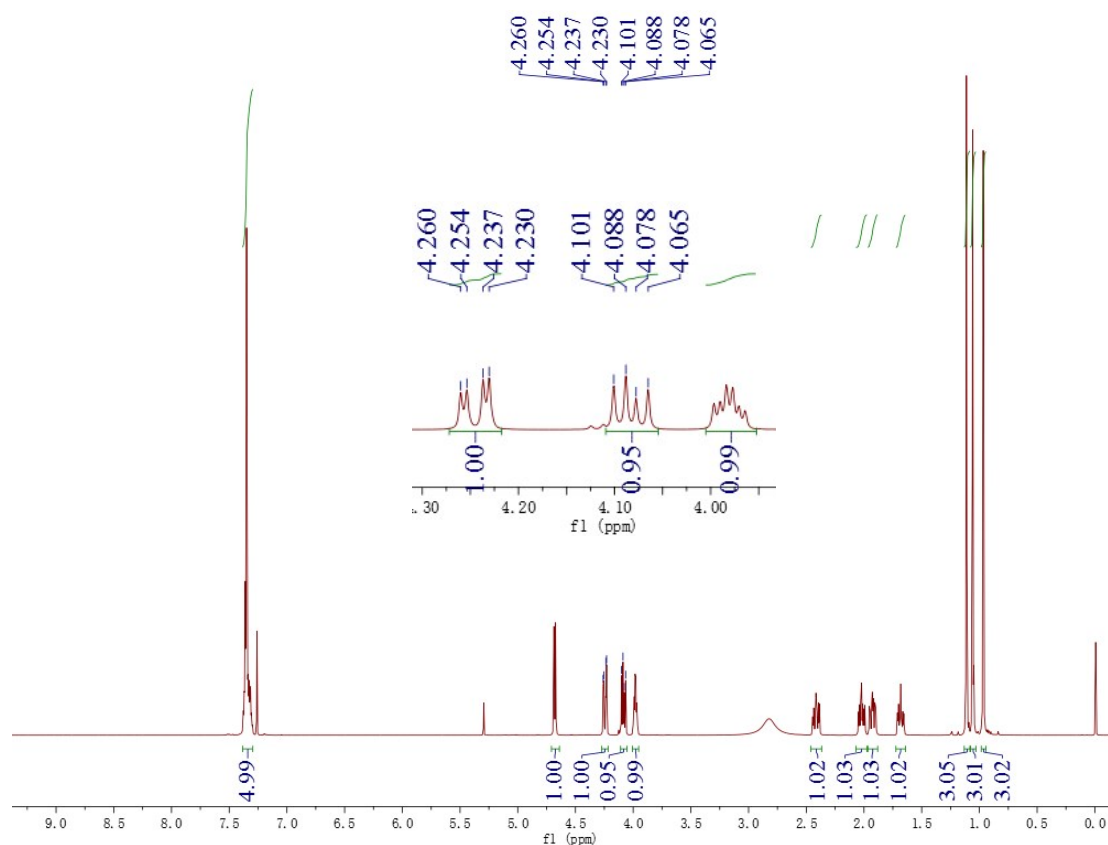


Figure S31. The ^1H NMR spectrum of compound **M2a** in CDCl_3

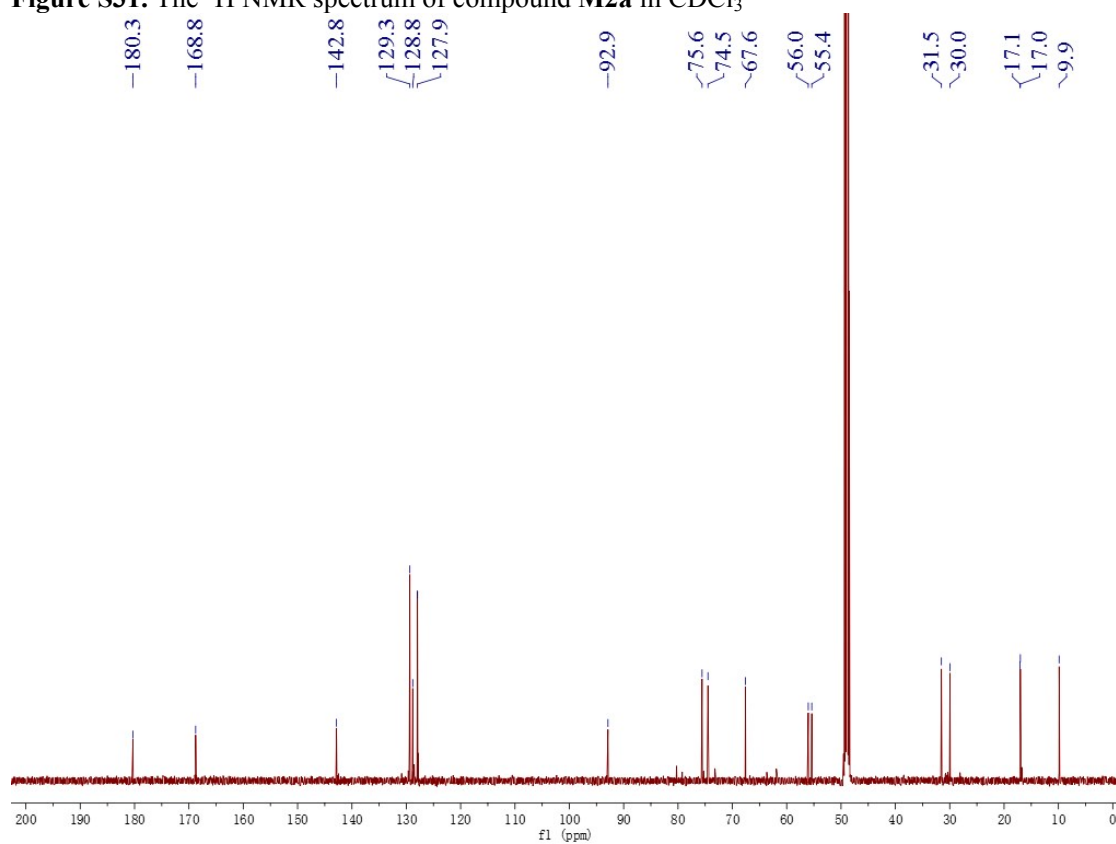


Figure S32. The ^{13}C NMR spectrum of compound **M2a** in methanol- d_4

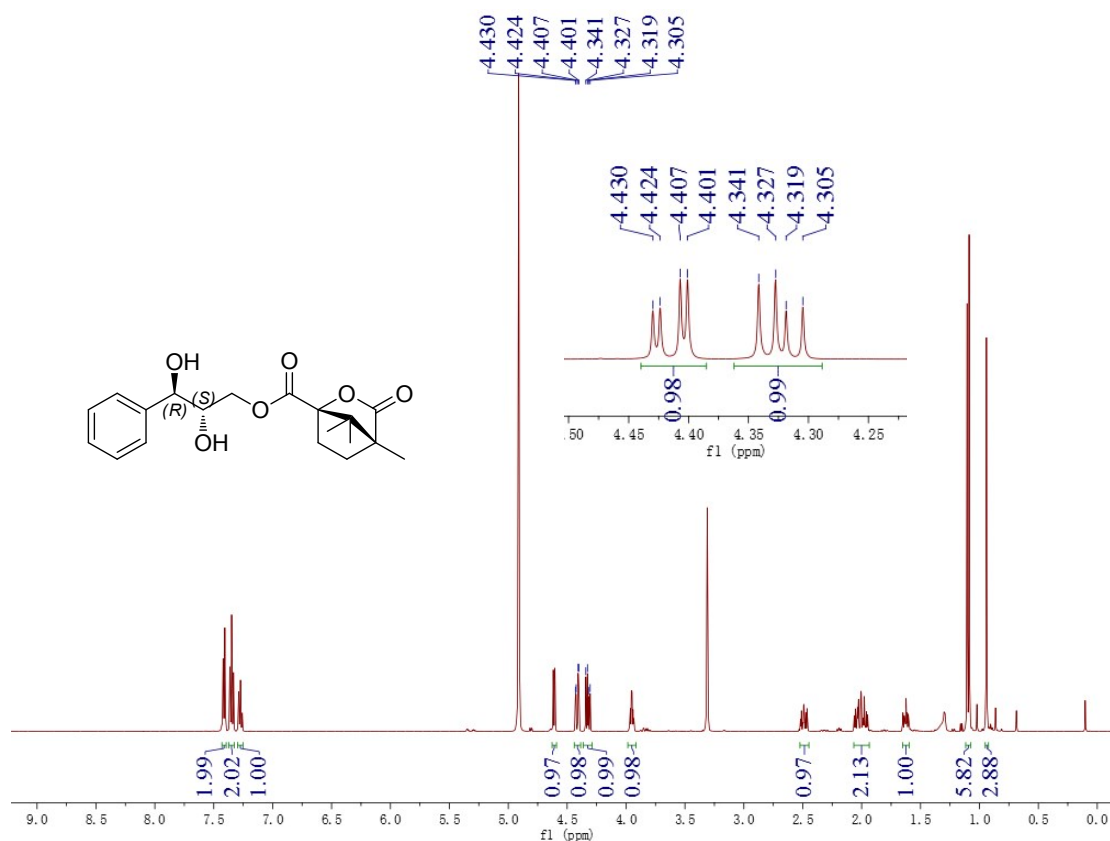


Figure S33. The ^1H NMR spectrum of compound **M3a** in methanol- d_4

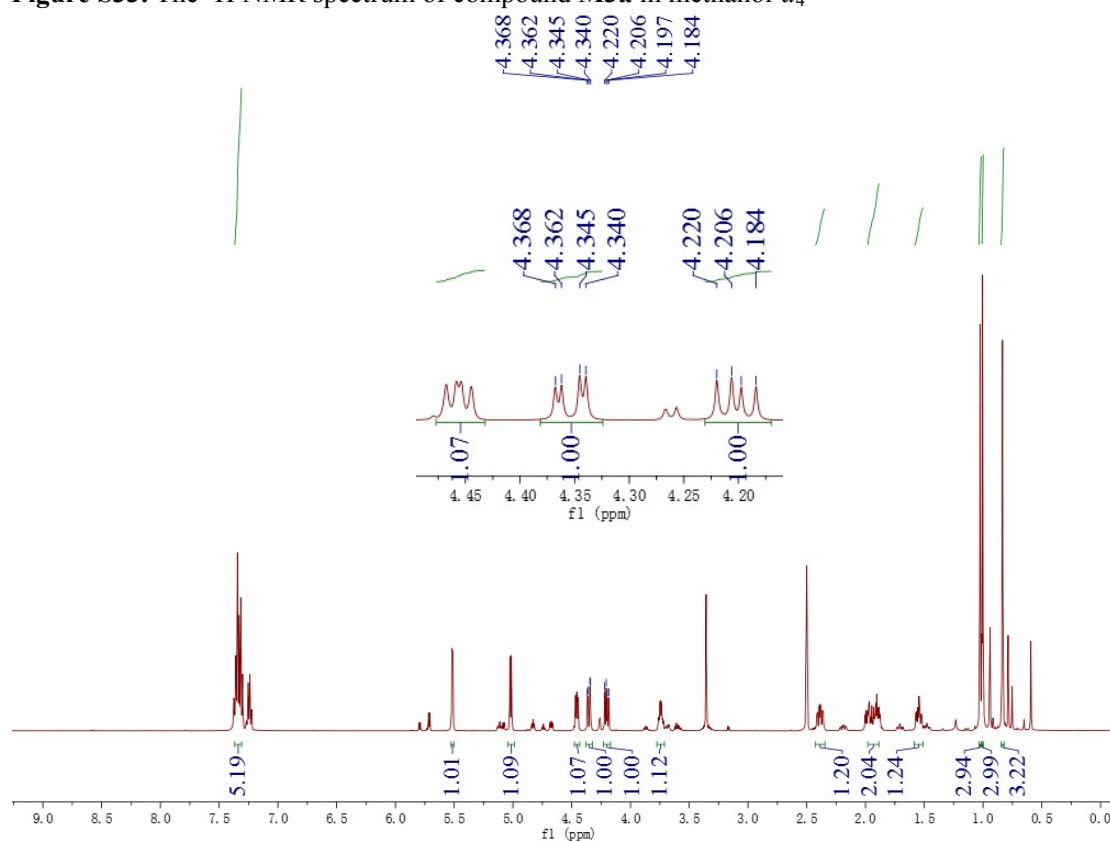


Figure S34. The ^1H NMR spectrum of compound **M3a** in DMSO- d_6

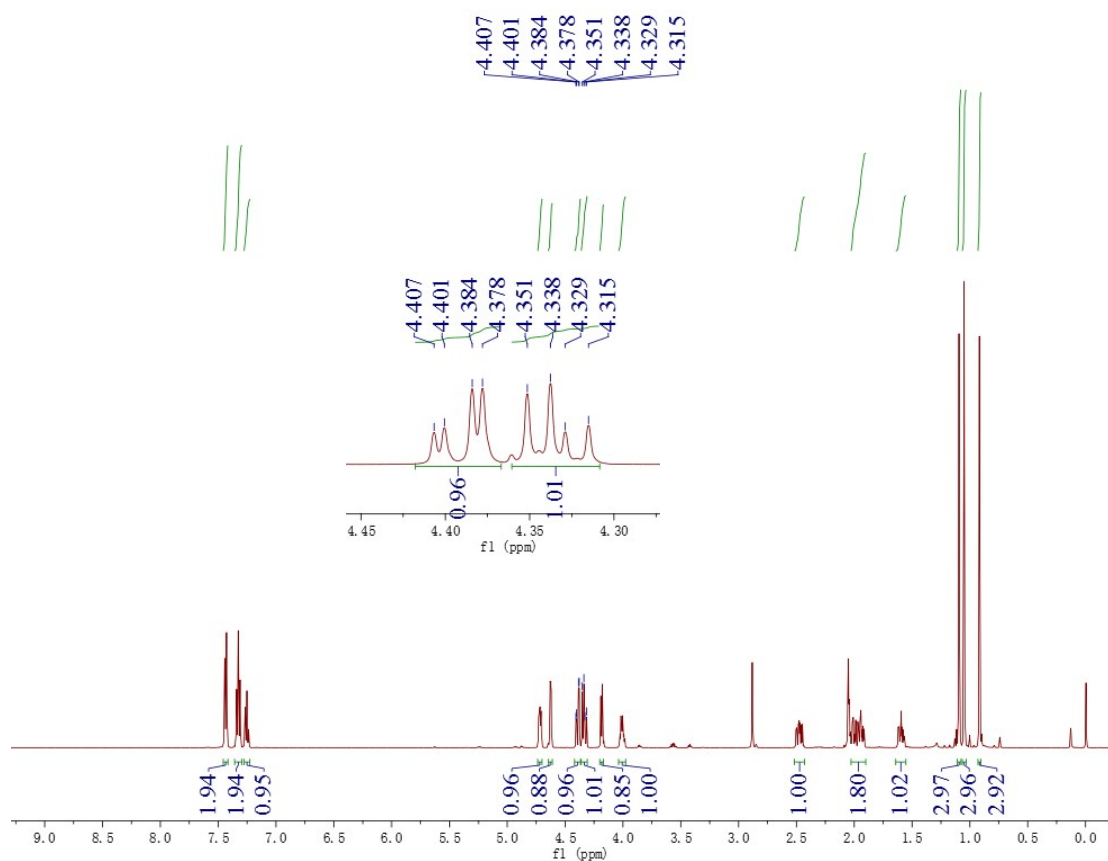


Figure S35. The ^1H NMR spectrum of compound **M3a** in acetone- d_6

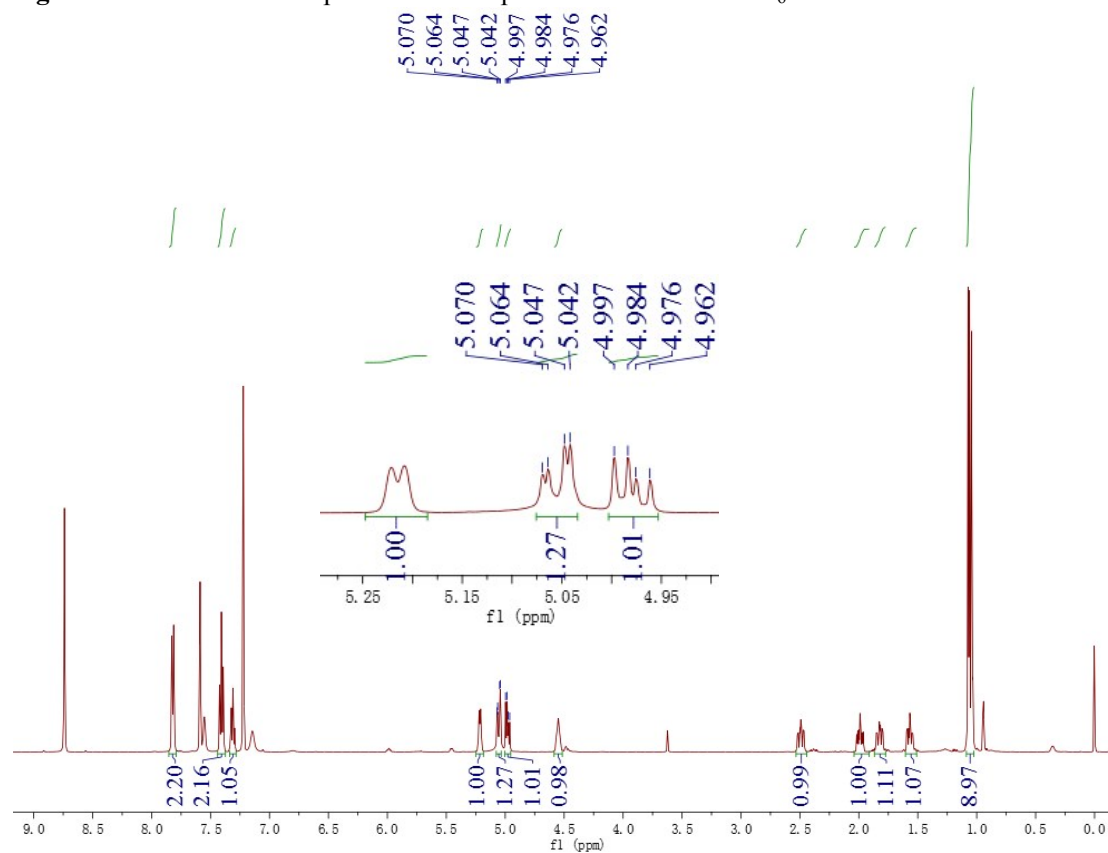


Figure S36. The ^1H NMR spectrum of compound **M3a** in pyridine- d_5

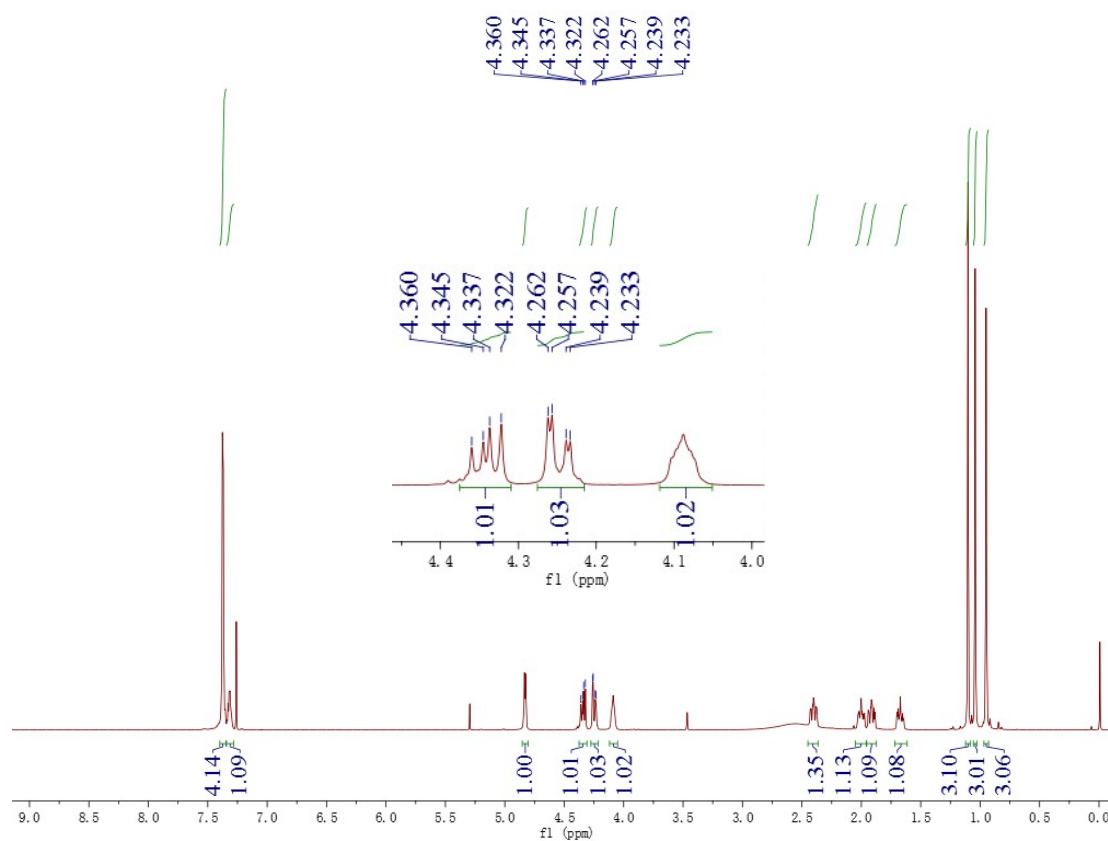


Figure S37. The ^1H NMR spectrum of compound **M3a** in CDCl_3

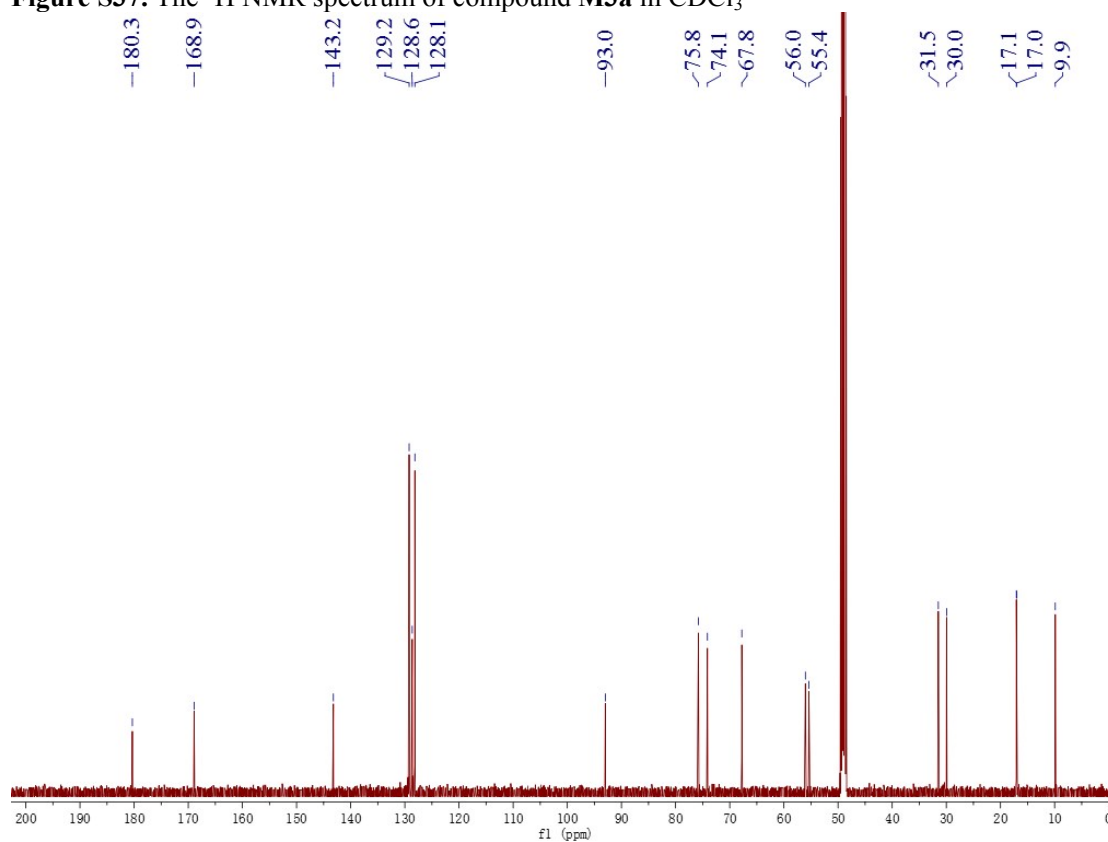


Figure S38. The ^{13}C NMR spectrum of compound **M3a** in methanol- d_4

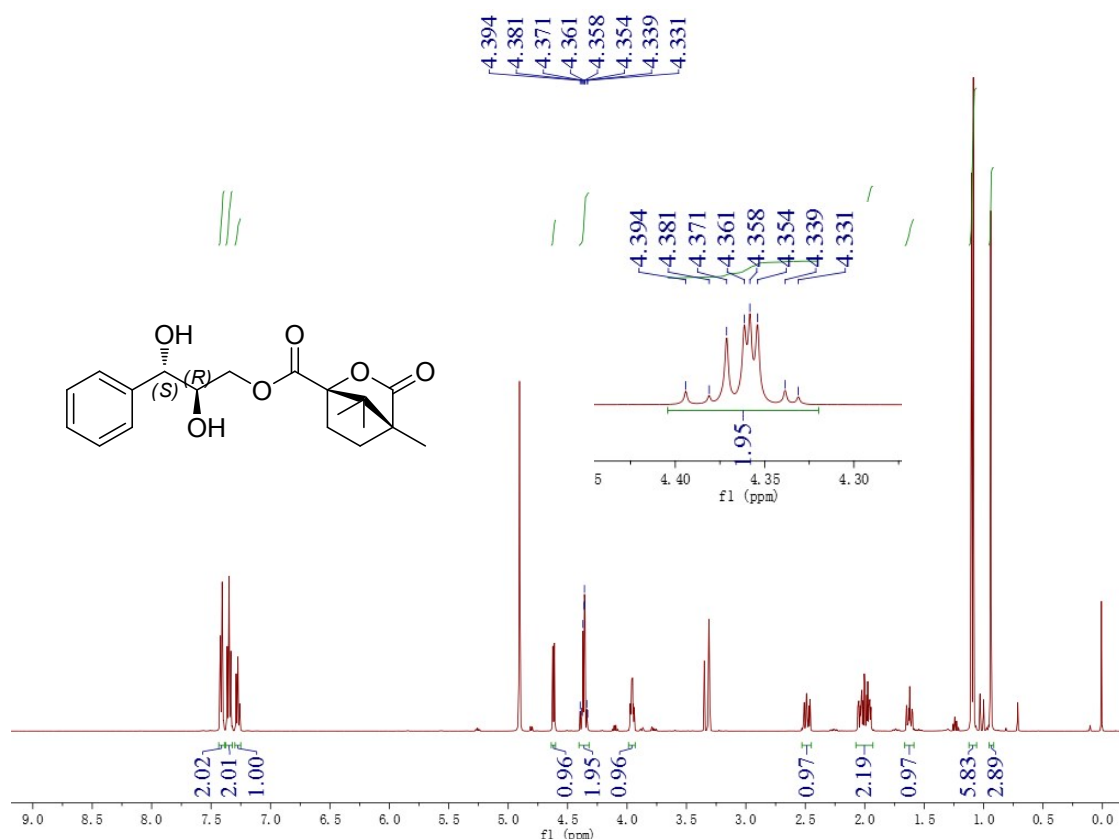


Figure S39. The ¹H NMR spectrum of compound **M4a** in methanol-*d*₄

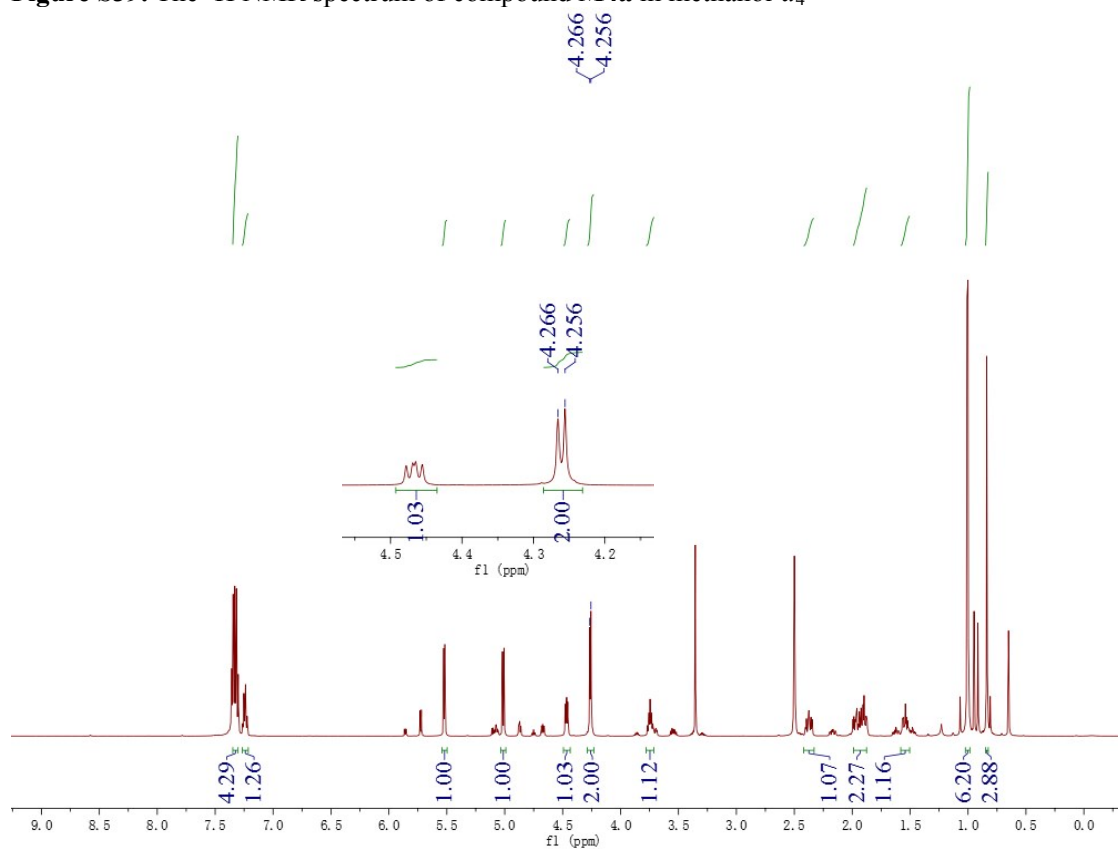


Figure S40. The ¹H NMR spectrum of compound **M4a** in DMSO-*d*₆

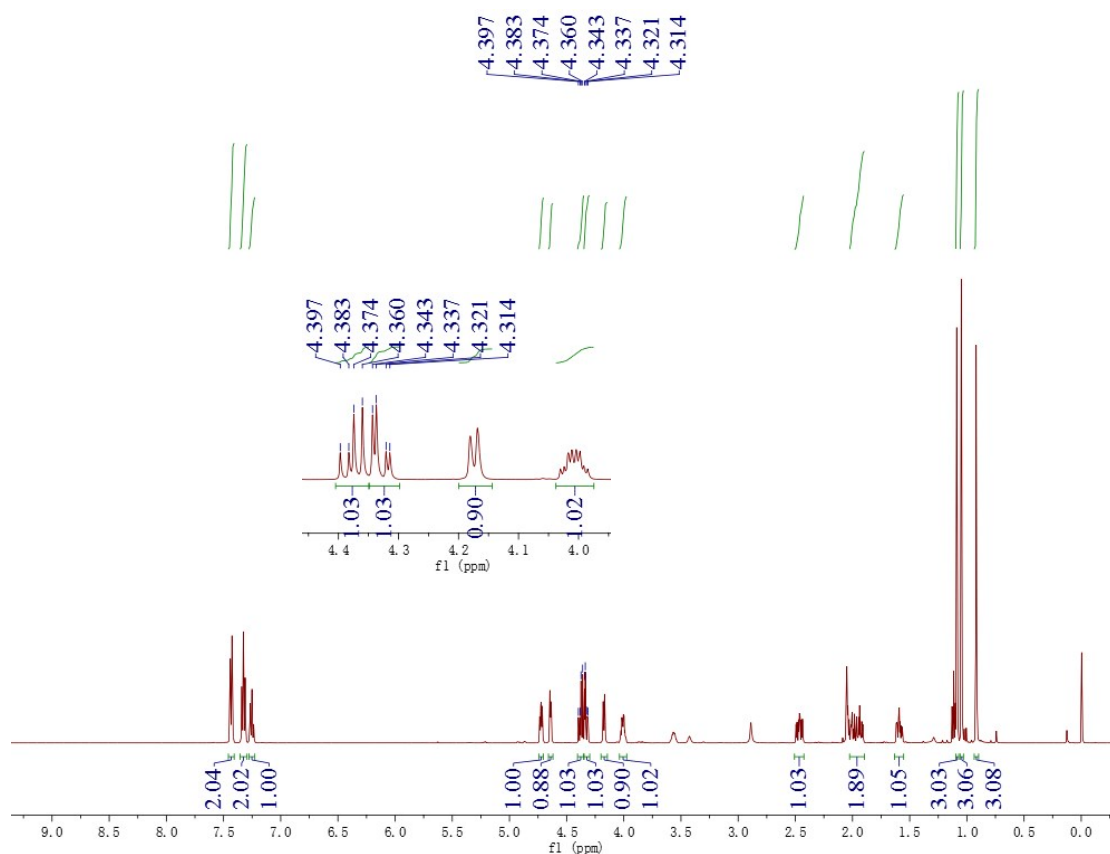


Figure S41. The ^1H NMR spectrum of compound **M4a** in acetone- d_6

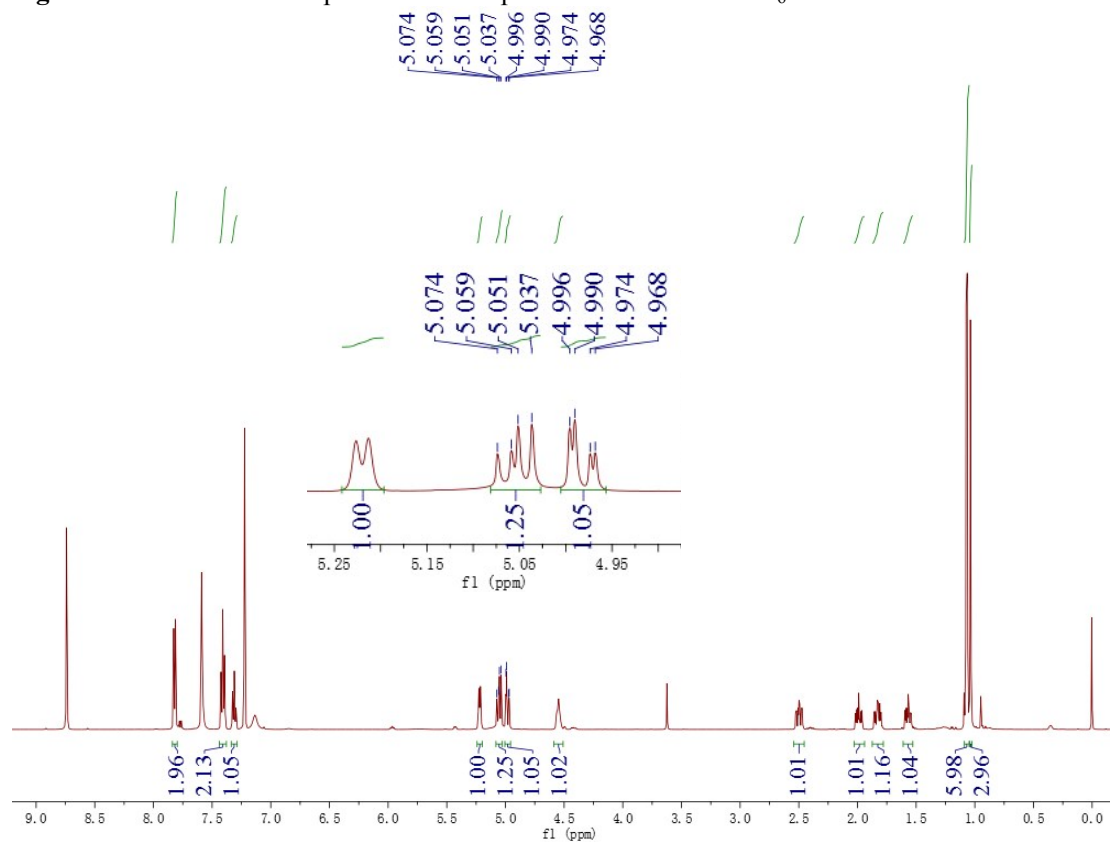


Figure S42. The ^1H NMR spectrum of compound **M4a** in pyridine- d_5

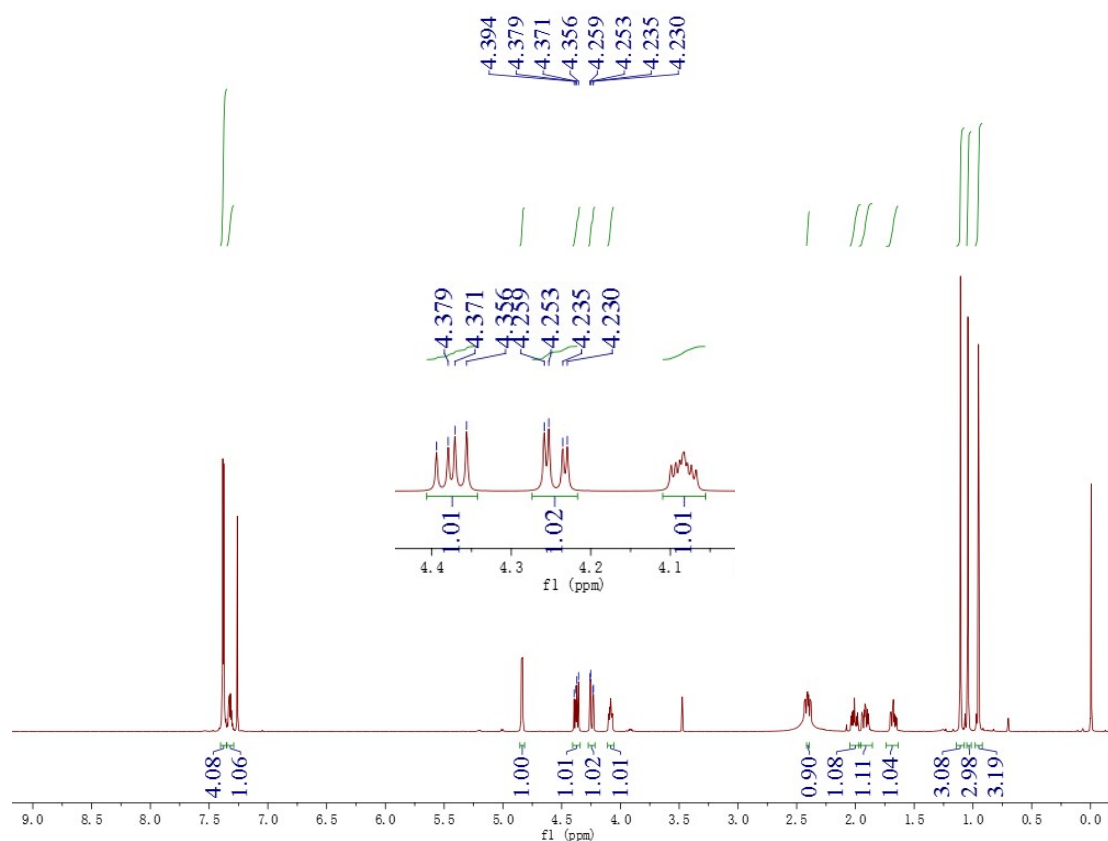


Figure S43. The ^1H NMR spectrum of compound **M4a** in CDCl_3

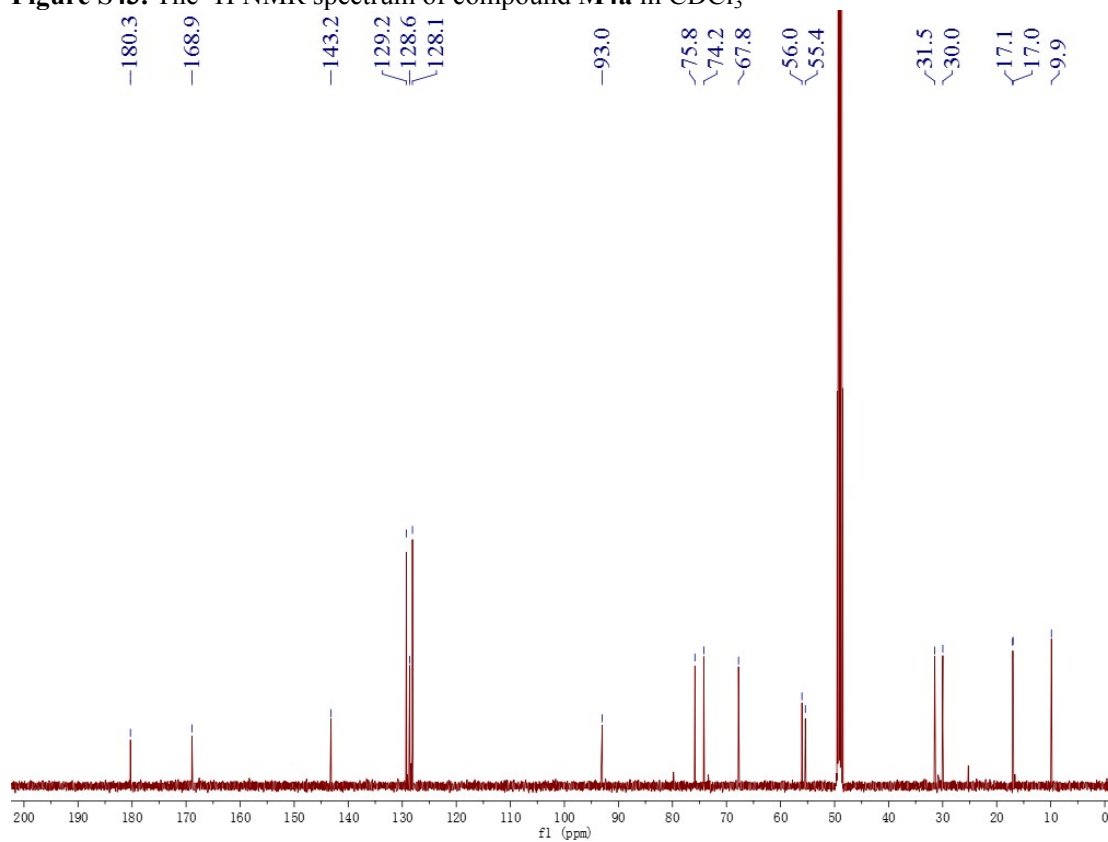
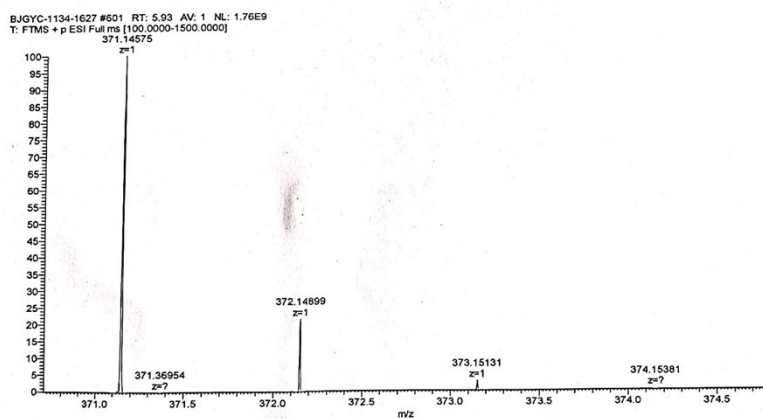
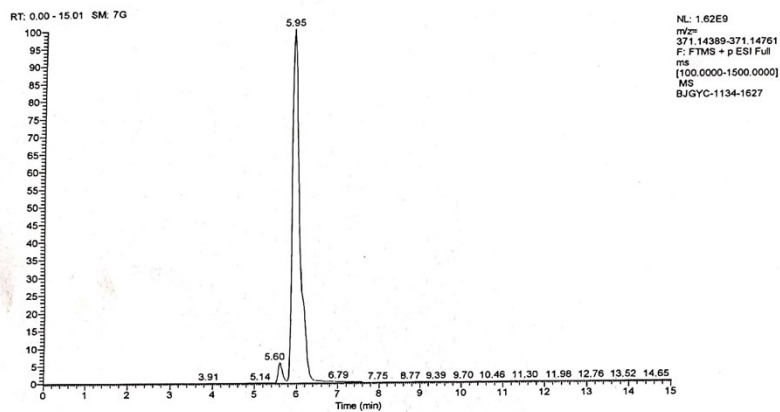


Figure S44. The ^{13}C NMR spectrum of compound **M4a** in $\text{methanol-}d_4$

Thermo Qexactive Focus Report

compound NO. : BJGYC-1134-1627
Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
371.14575	371.14651	-2.05	7.5	C19 H24 O6 Na	M+Na

Figure S45. The HR-ESI-MS data of **M1a**

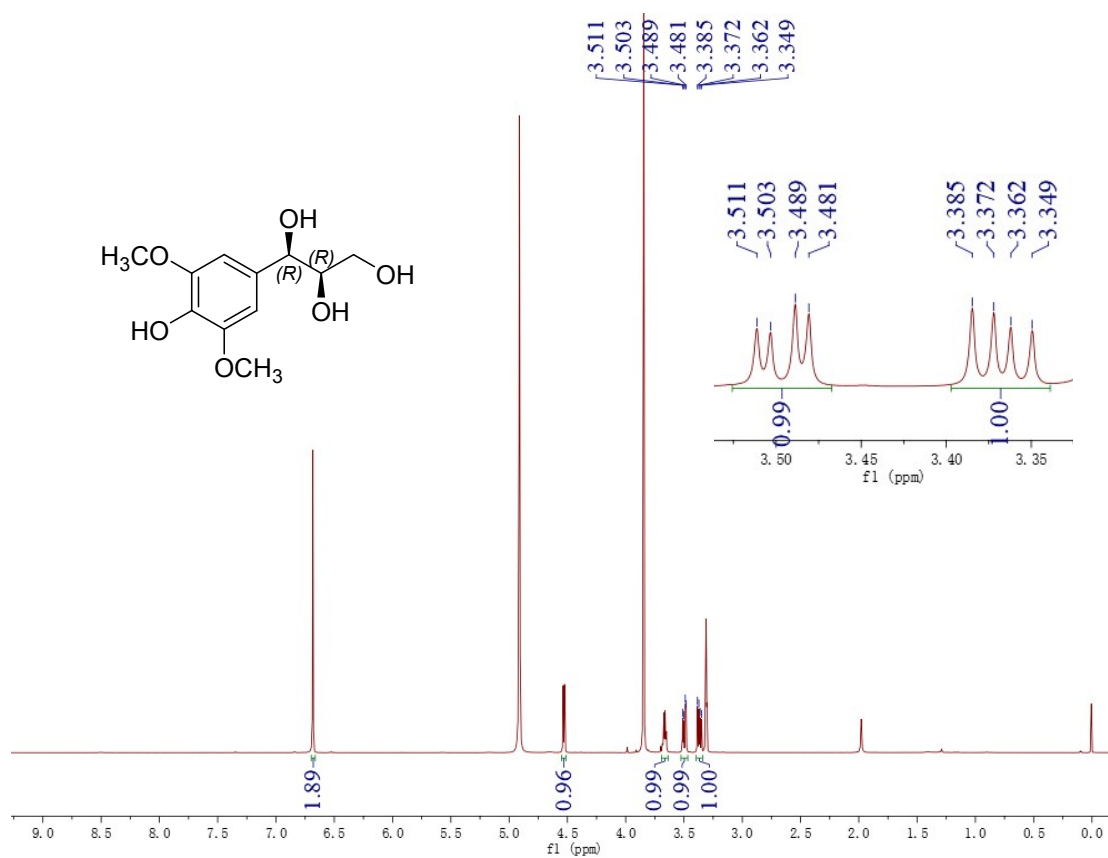


Figure S46. The ¹H NMR spectrum of compound **1** in methanol-*d*₄

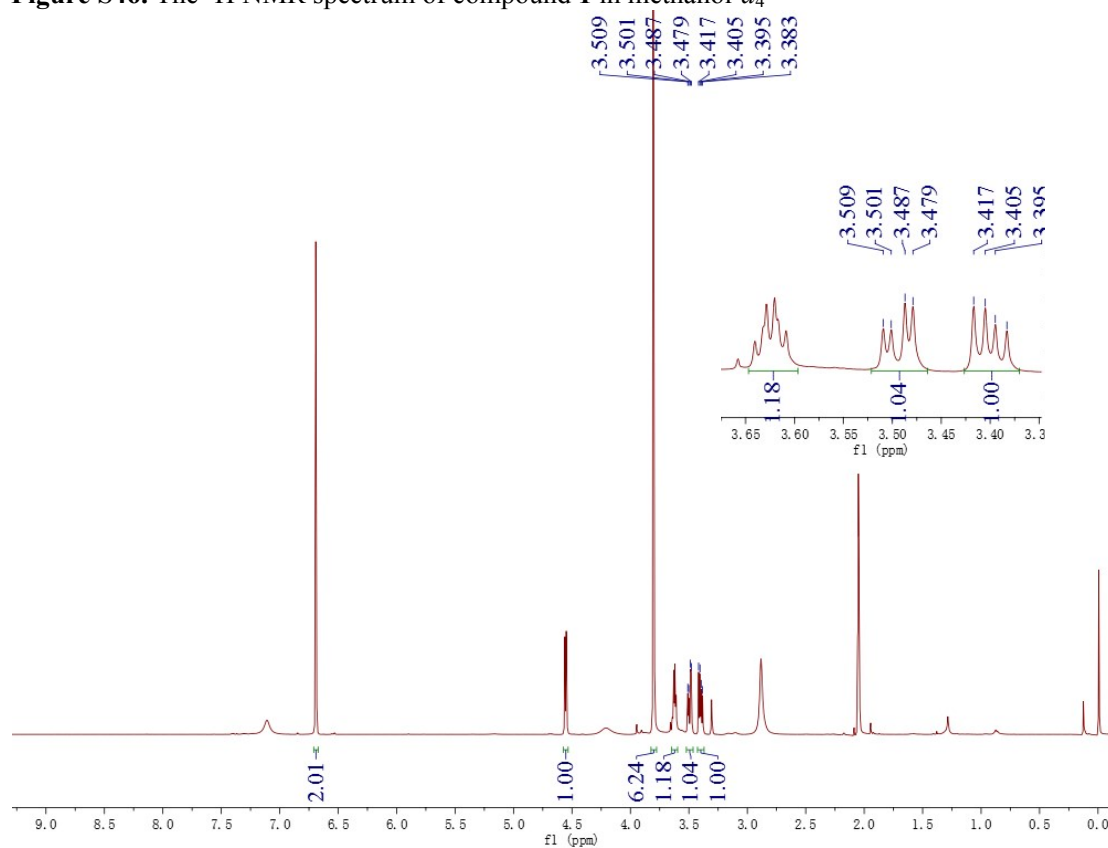


Figure S47. The ¹H NMR spectrum of compound **1** in acetone-*d*₆

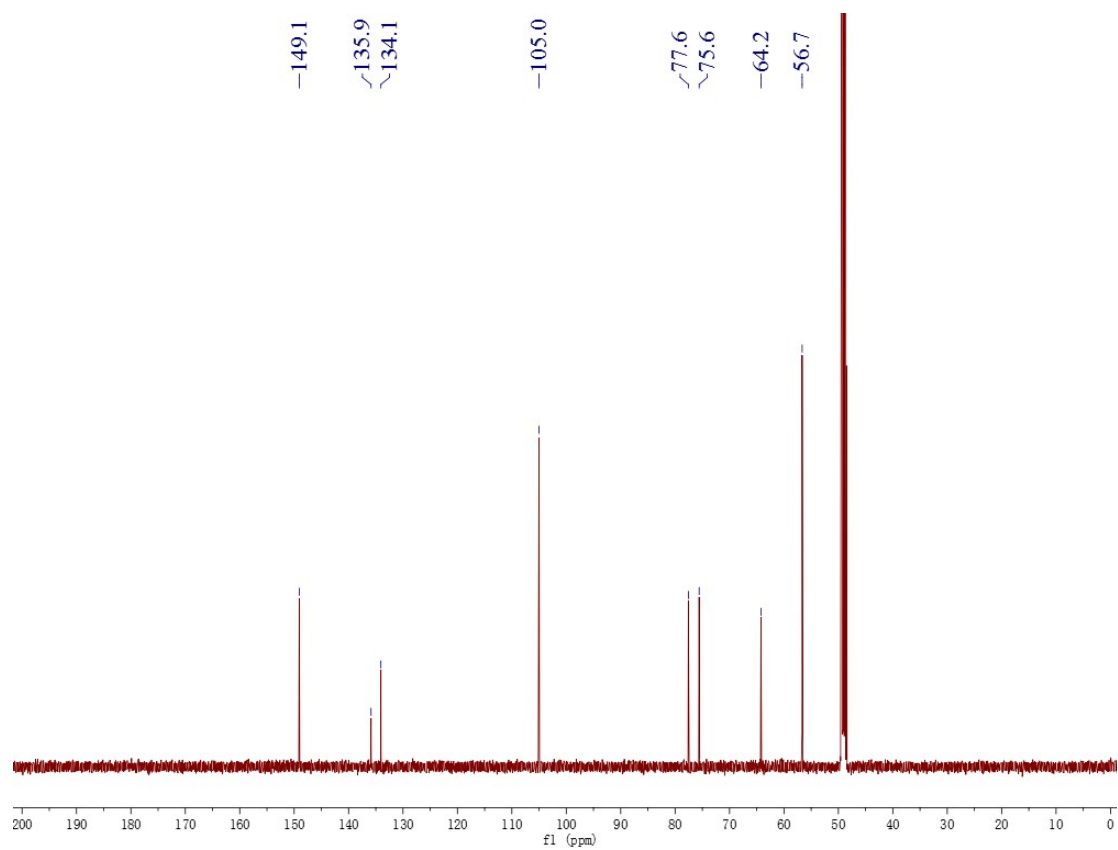
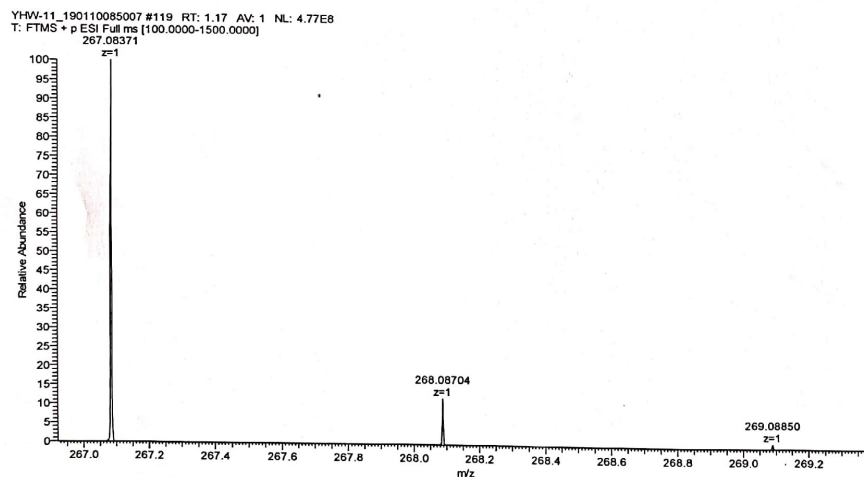
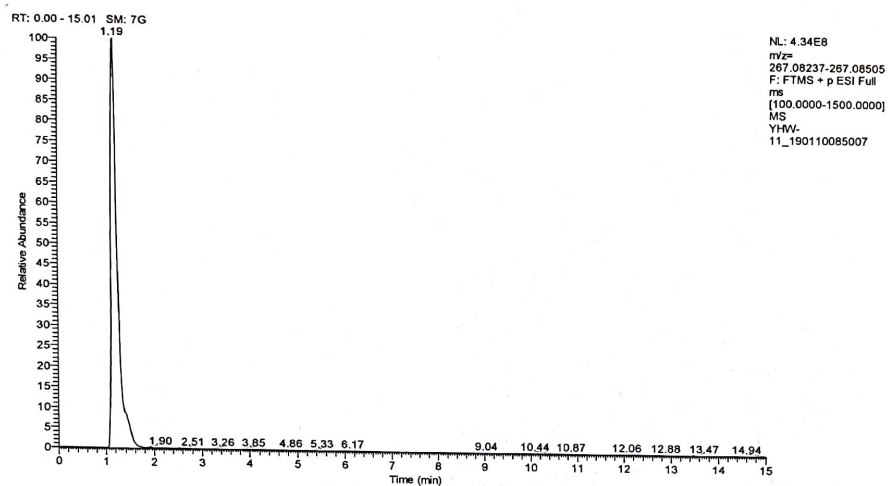


Figure S48. The ^{13}C NMR spectrum of compound **1** in methanol- d_4

Thermo Qexactive Focus Report

compound NO. : YHW-11

Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
267.08371	267.08391	-0.75	3.5	C11 H16 O6 Na	M+Na

Figure S49. The HR-ESI-MS data of **1**

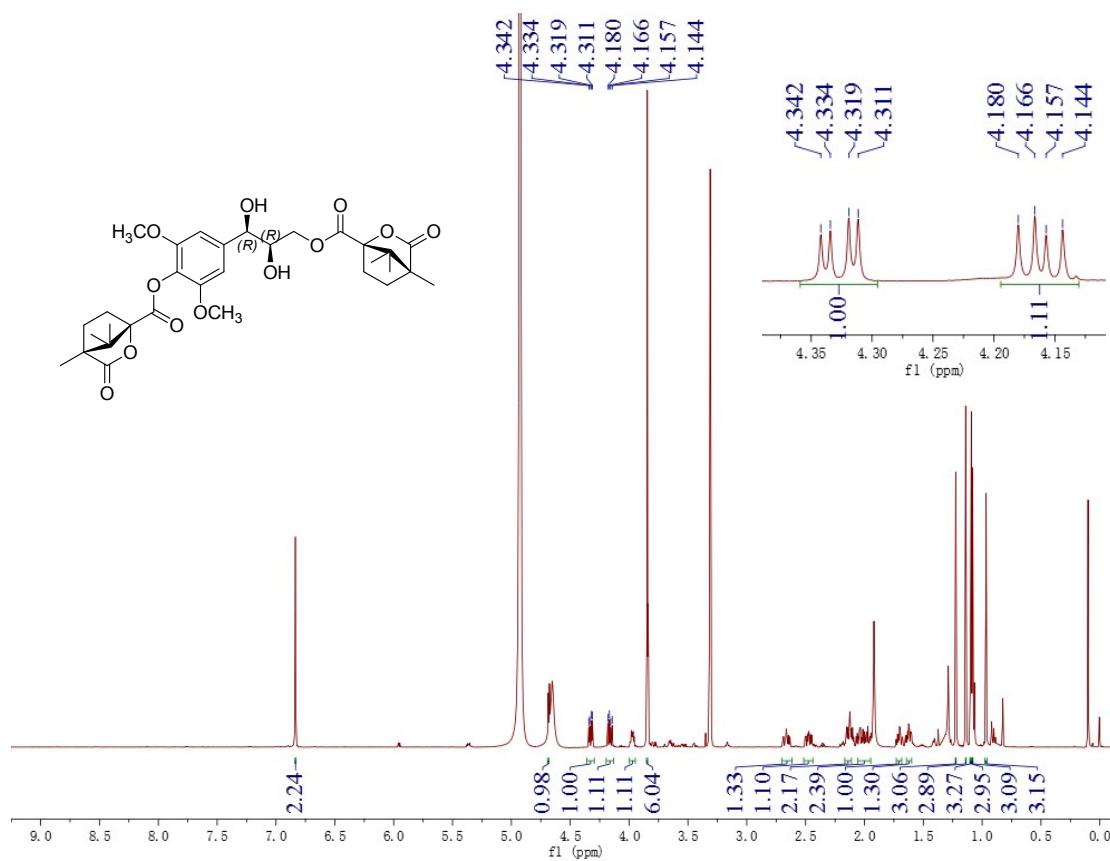


Figure S50. The ¹H NMR spectrum of compound **1a** in methanol-*d*₄

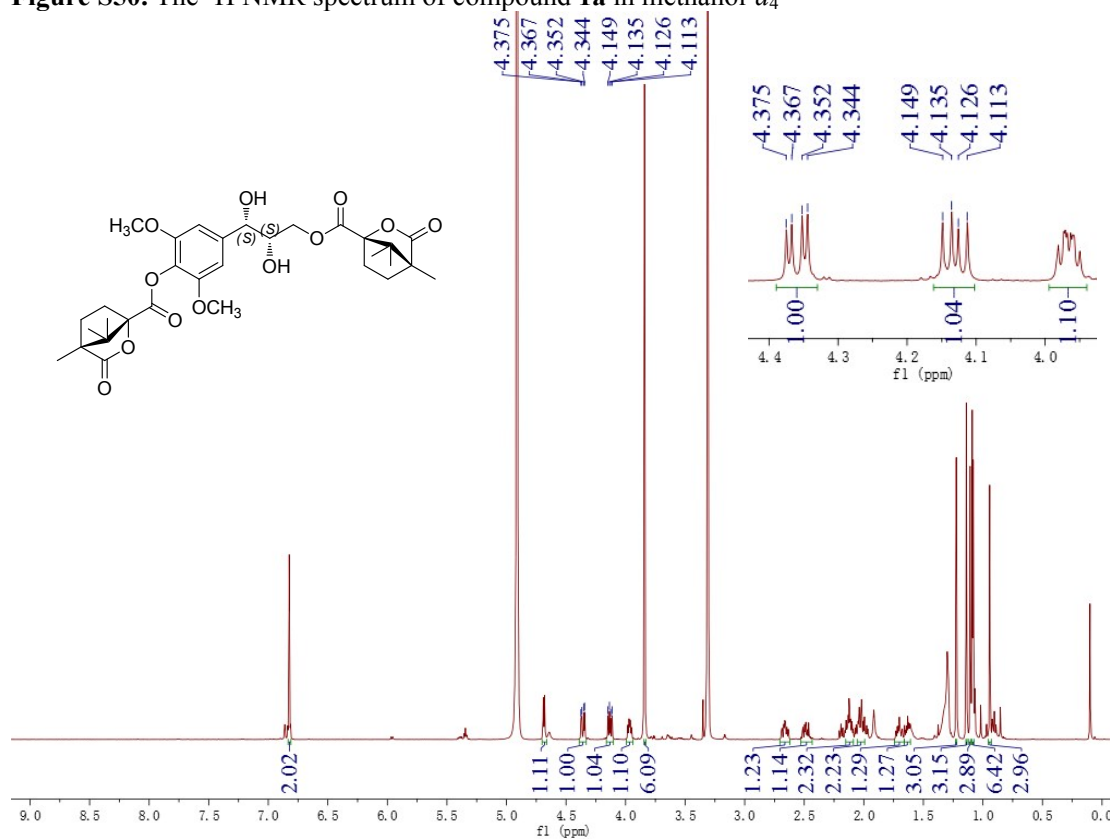
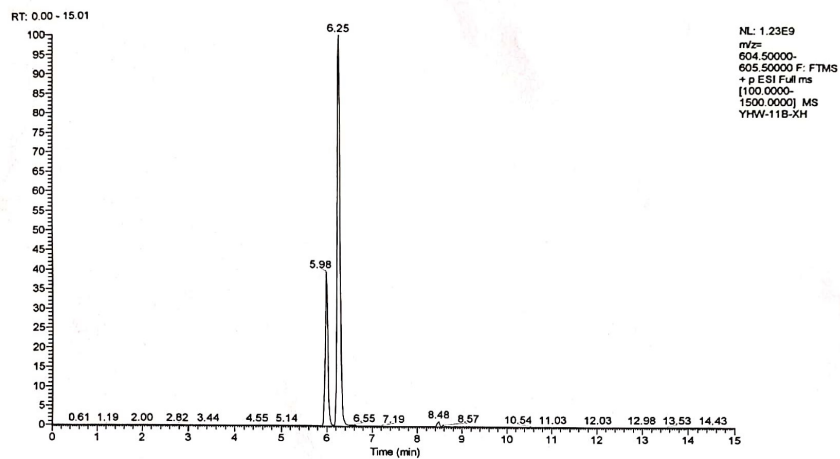


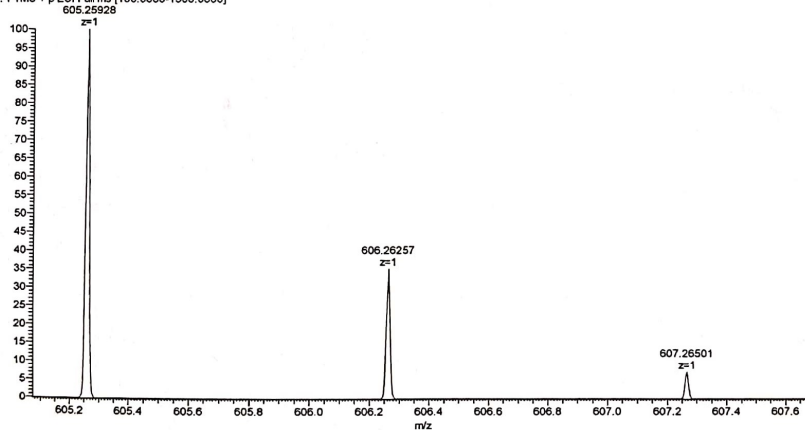
Figure S51. The ¹H NMR spectrum of compound **2a** in methanol-*d*₄

Thermo Qexactive Focus Report

compound NO. : YHW-11B-XH
Method : LCMS(compound)-low



YHW-11B-XH #603 RT: 5.98 AV: 1 NL: 4.87E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

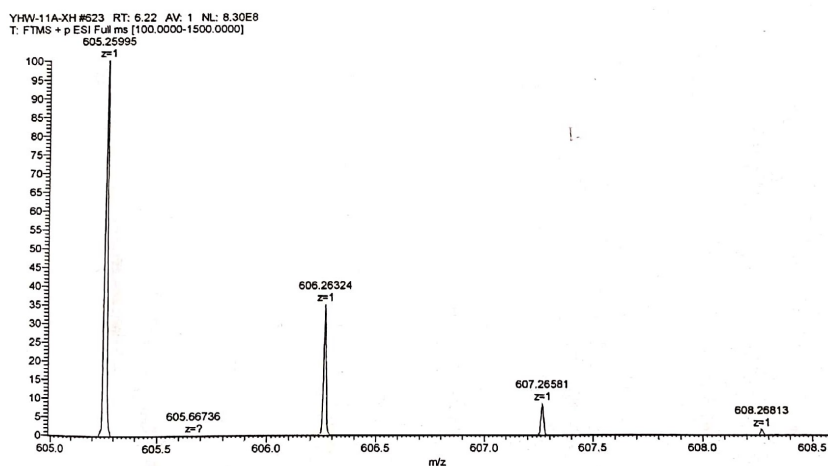
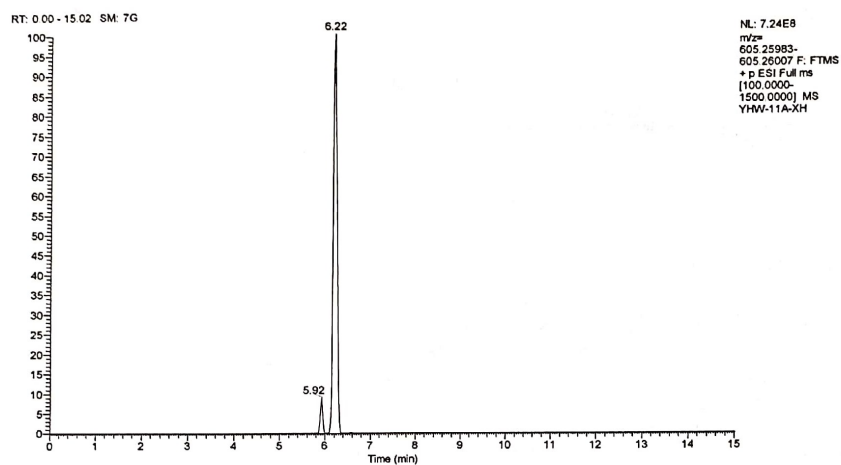


m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
605.25928	605.25925	0.04	11.5	C31 H41 O12	M+H

Figure S52. The HR-ESI-MS data of 1a

Thermo Qexactive Focus Report

compound NO. : YHW-11A-XH
Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
605.25995	605.25925	1.15	11.5	C31 H41 O12	M+H

Figure S53. The HR-ESI-MS data of **2a**

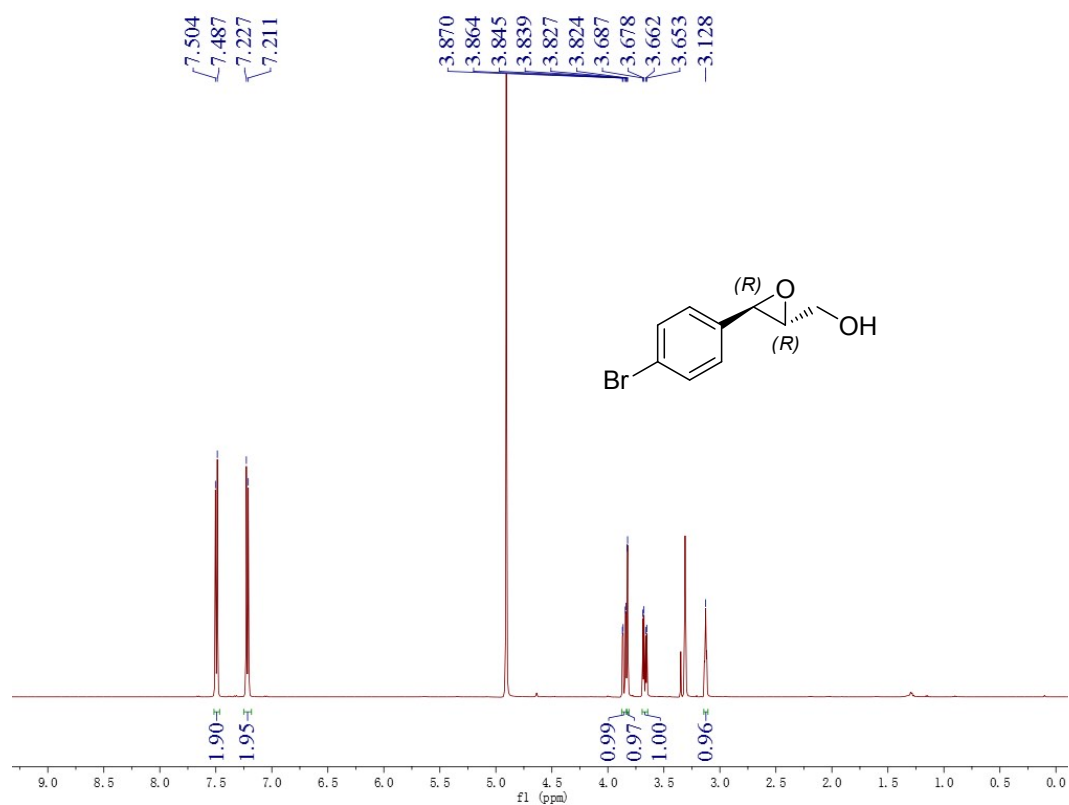


Figure S54. The ^1H NMR spectrum of ((2*R*,3*R*)-3-(4-bromophenyl)oxiran-2-yl)methanol

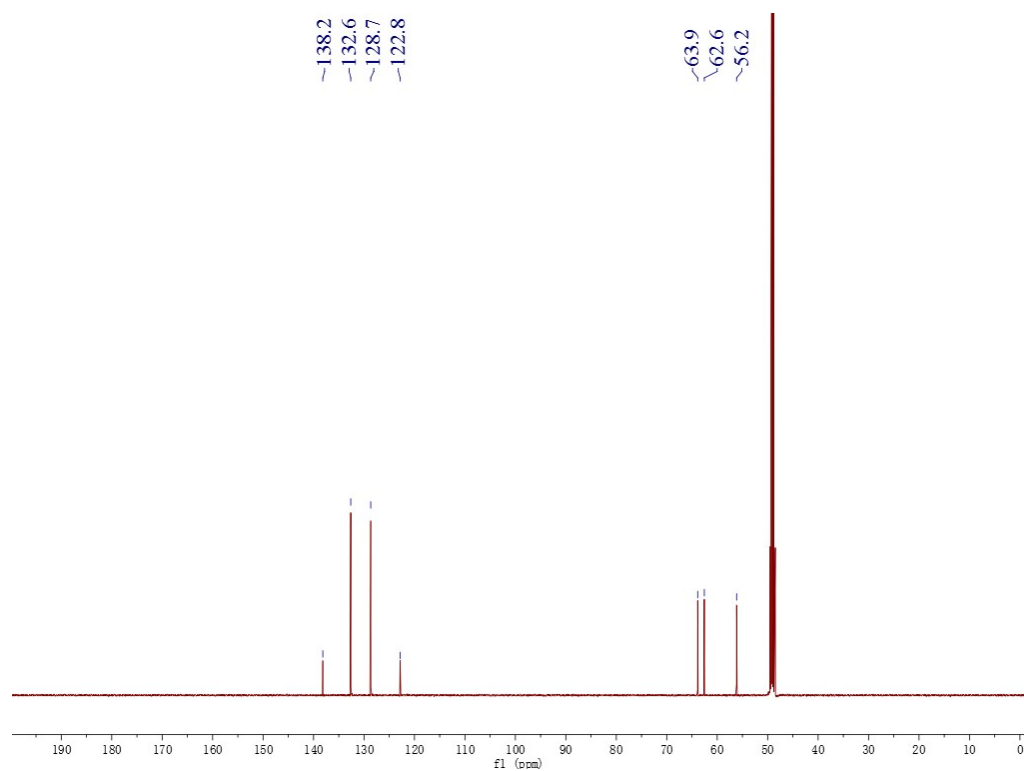
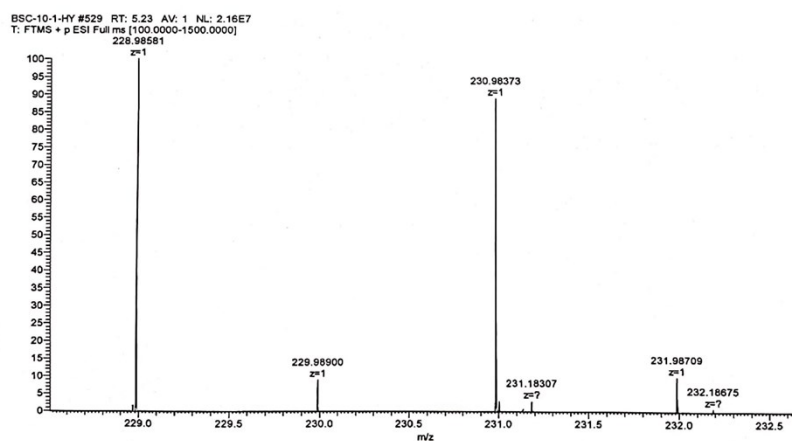
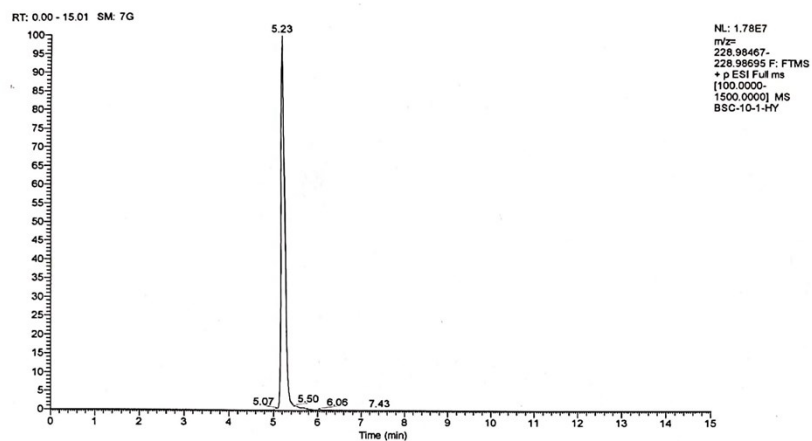


Figure S55. The ^{13}C NMR spectrum of ((2*R*,3*R*)-3-(4-bromophenyl)oxiran-2-yl)methanol

Thermo Qexactive Focus Report

compound NO. : BSC-10-1-HY
Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
228.98581	228.98587	-0.26	4.5	C9 H10 O2 Br	M+H

Figure S56. The HR-ESI-MS data of ((2*R*,3*R*)-3-(4-bromophenyl)oxiran-2-yl)methanol

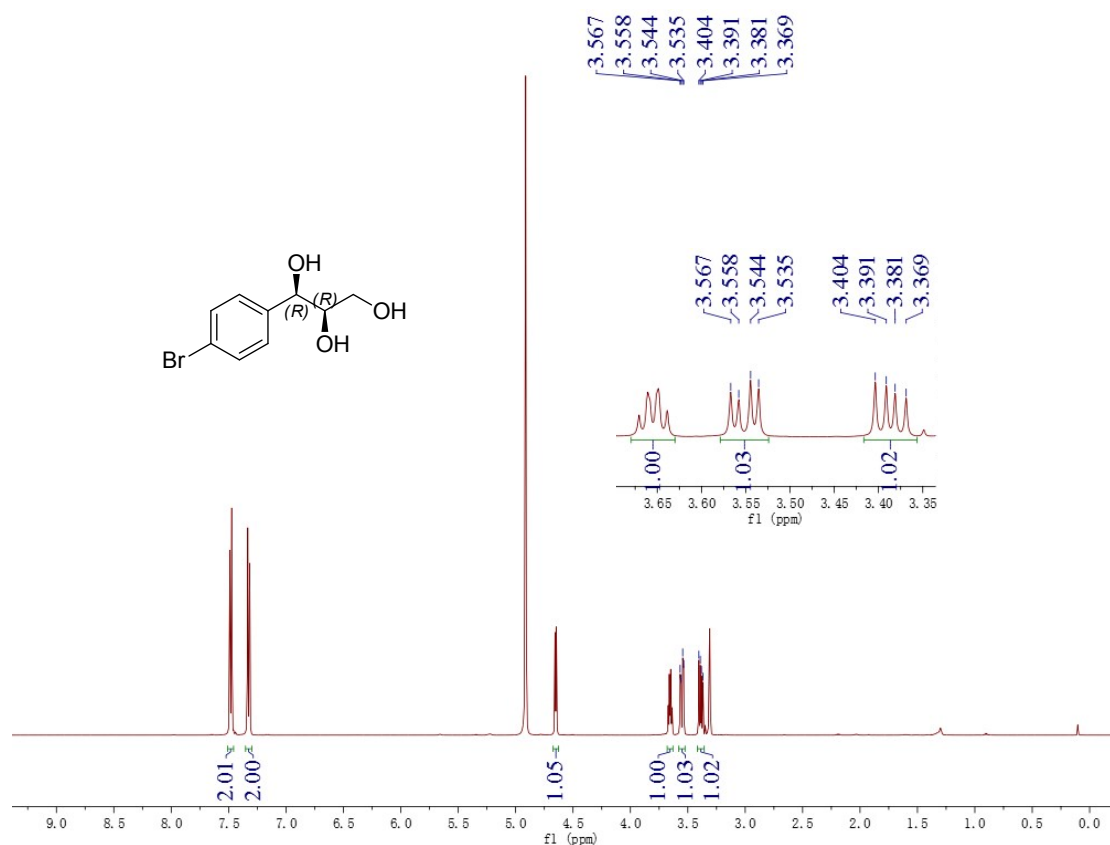


Figure S57. The ¹H NMR spectrum of compound **3** in methanol-*d*₄

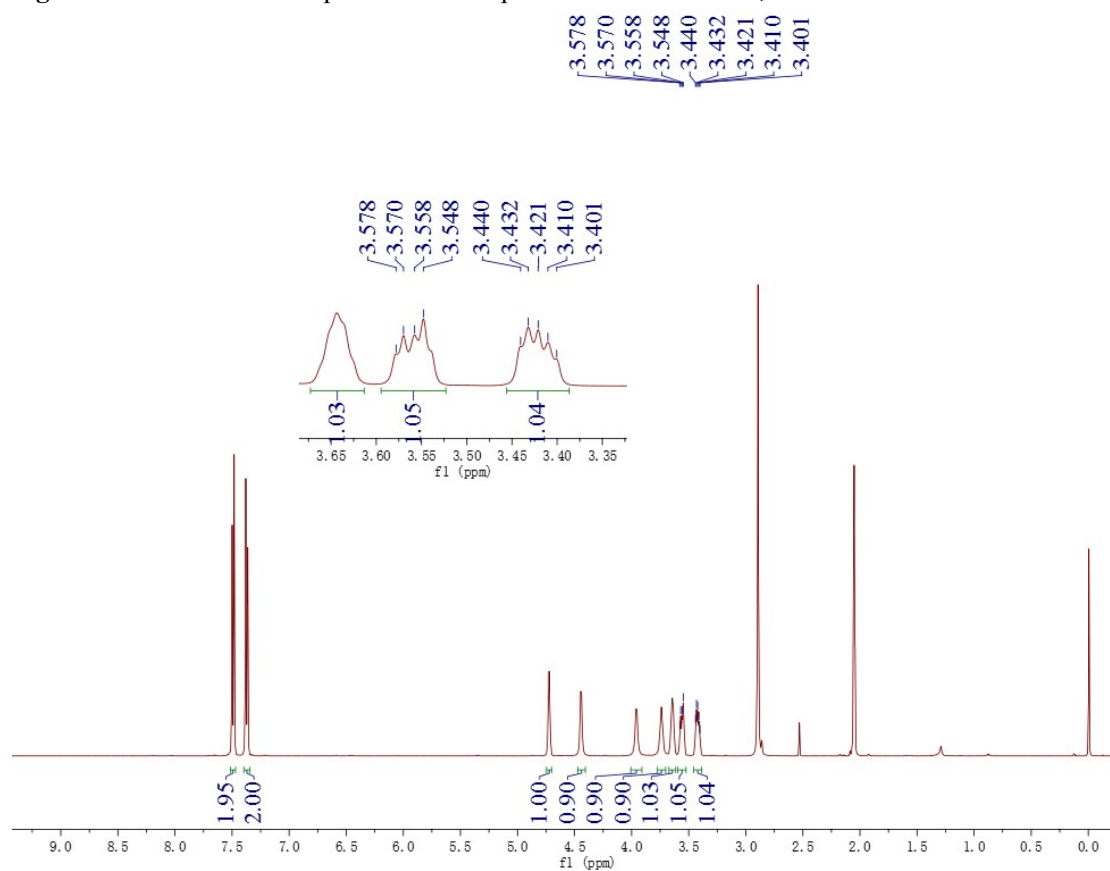


Figure S58. The ¹H NMR spectrum of compound **3** in acetone-*d*₆

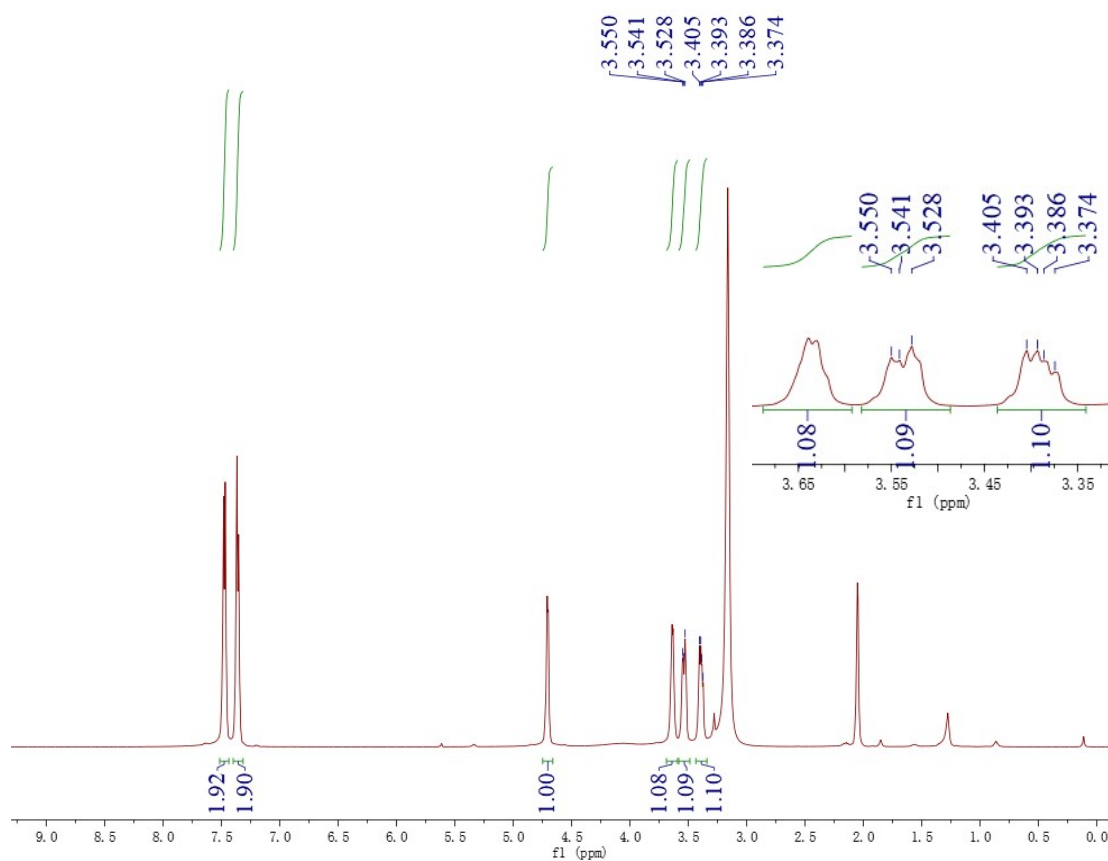


Figure S59. The H-D exchange ^1H NMR spectrum of compound **3** in acetone- d_6

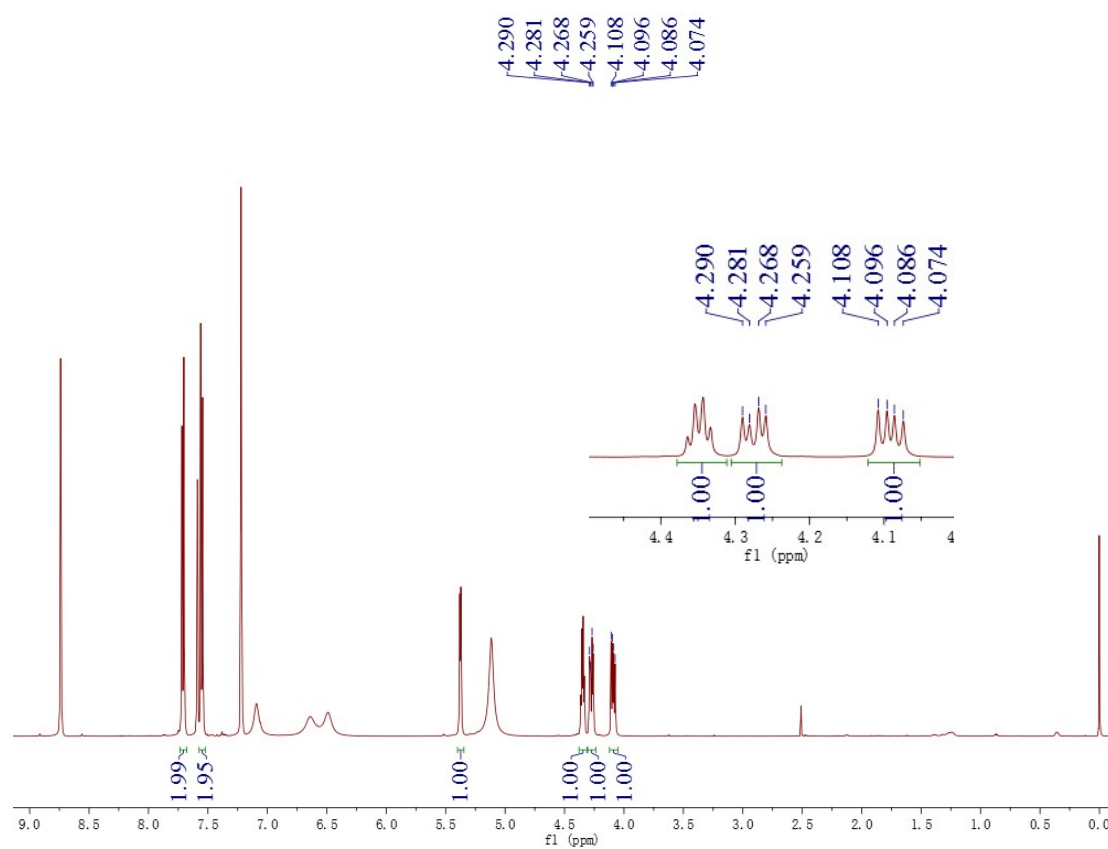


Figure S60. The ^1H NMR spectrum of compound **3** in pyridine- d_5

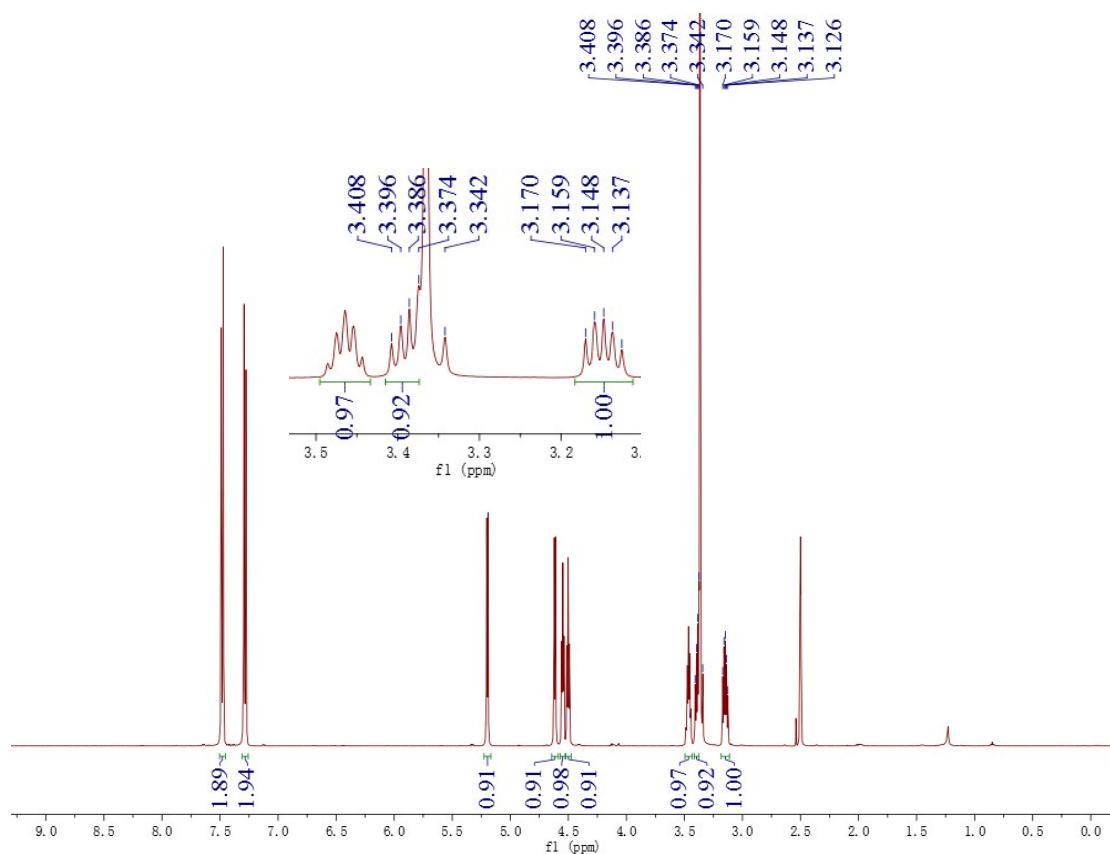


Figure S61. The ^1H NMR spectrum of compound **3** in $\text{DMSO-}d_6$

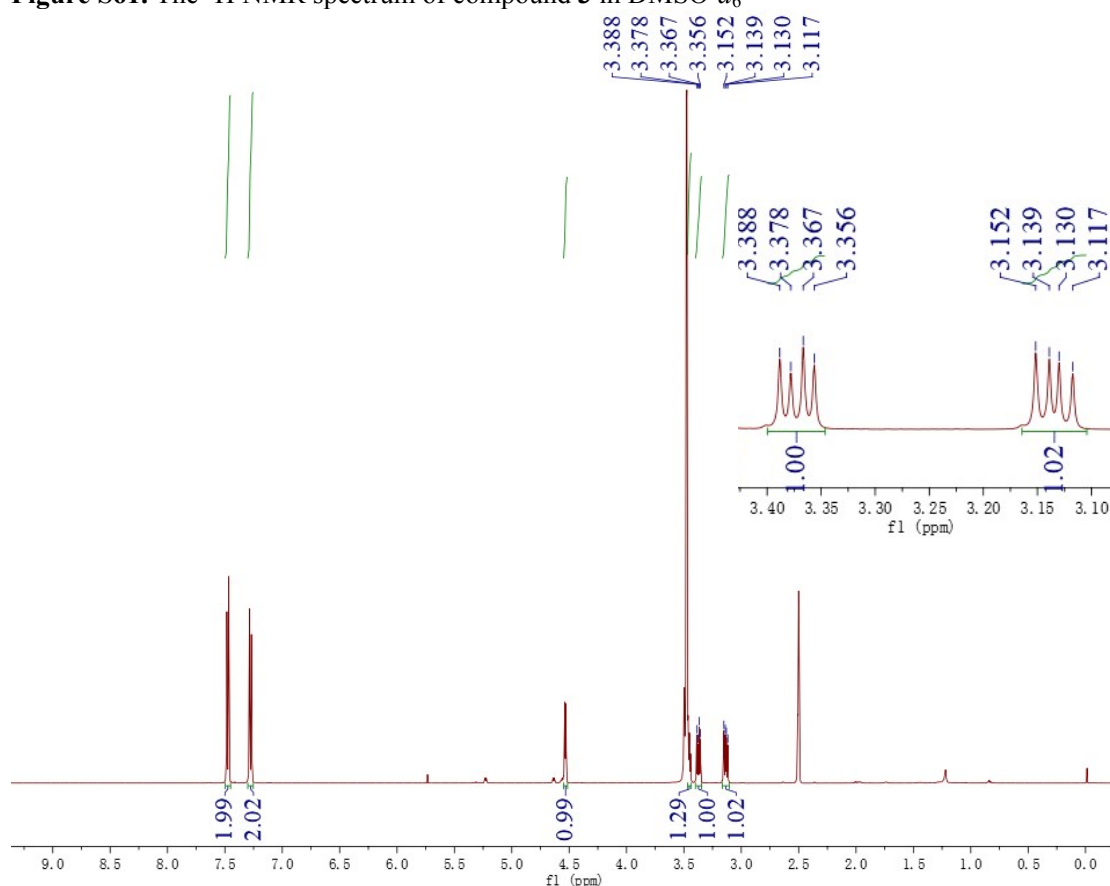


Figure S62. The H-D exchange ^1H NMR spectrum of compound **3** in $\text{DMSO-}d_6$

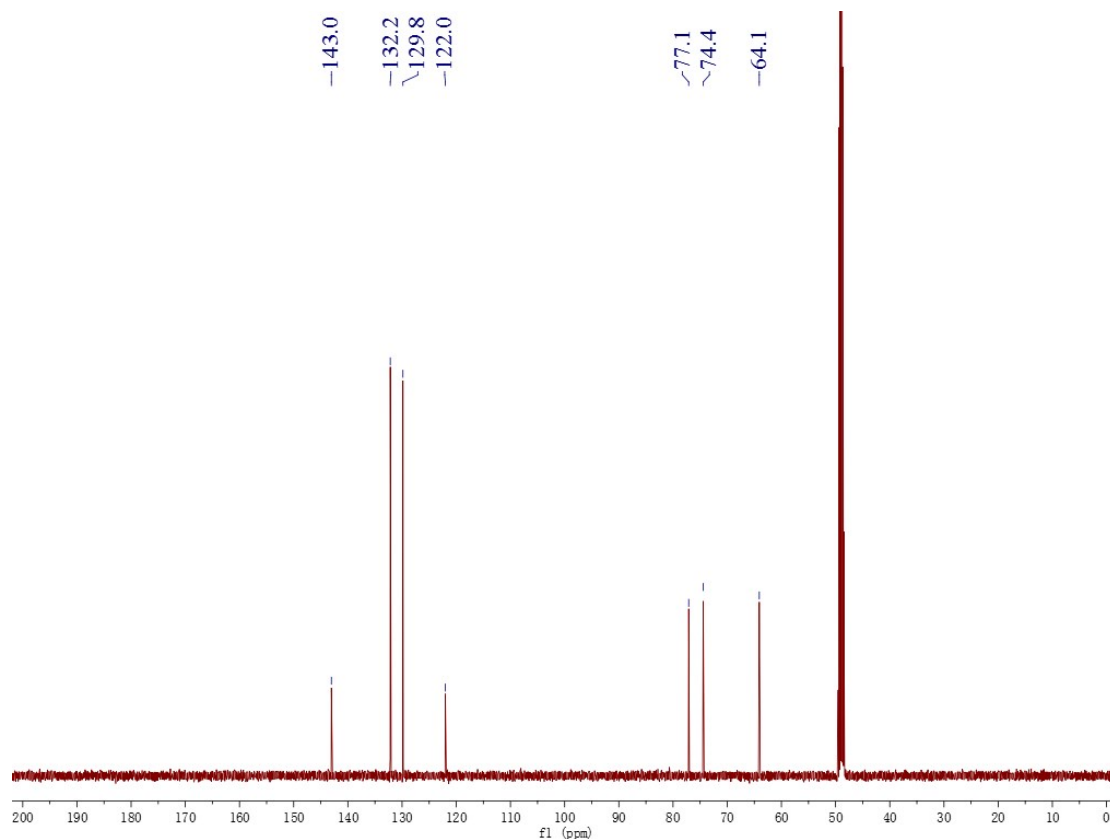


Figure S63. The ¹³C NMR spectrum of compound **3** in methanol-*d*₄

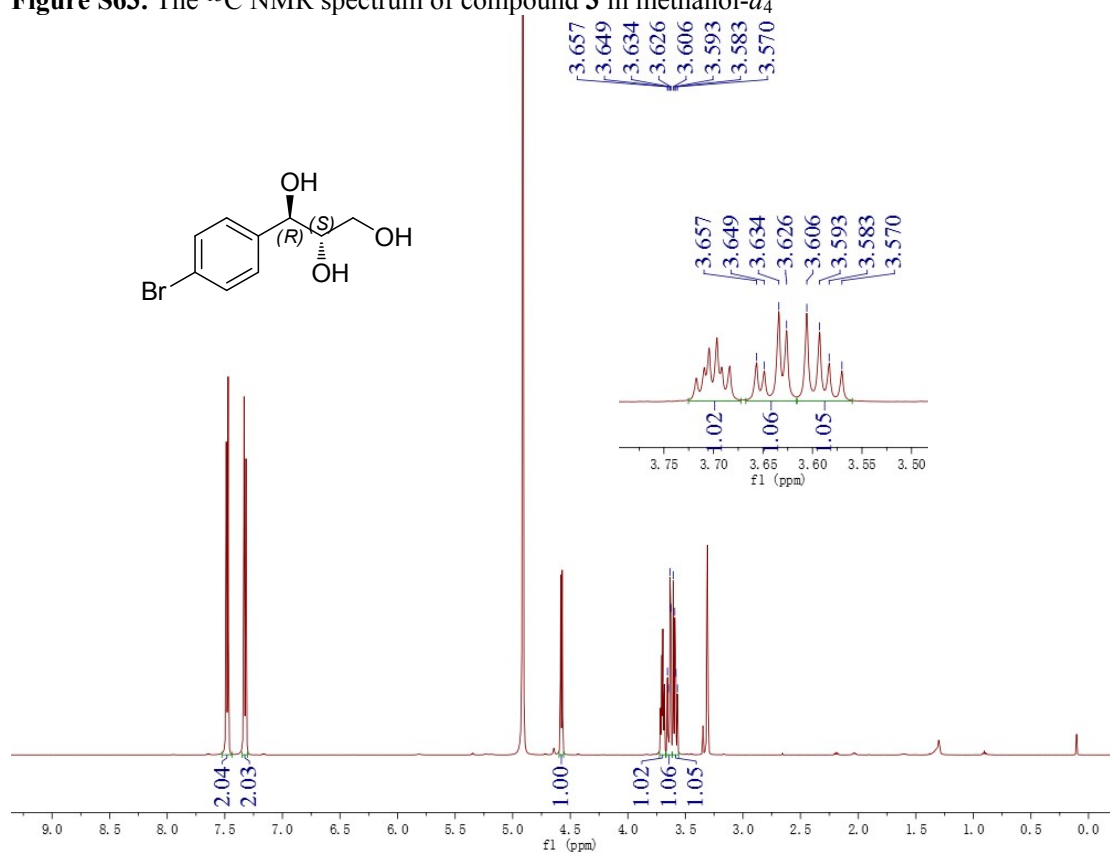


Figure S64. The ¹H NMR spectrum of compound **5** in methanol-*d*₄

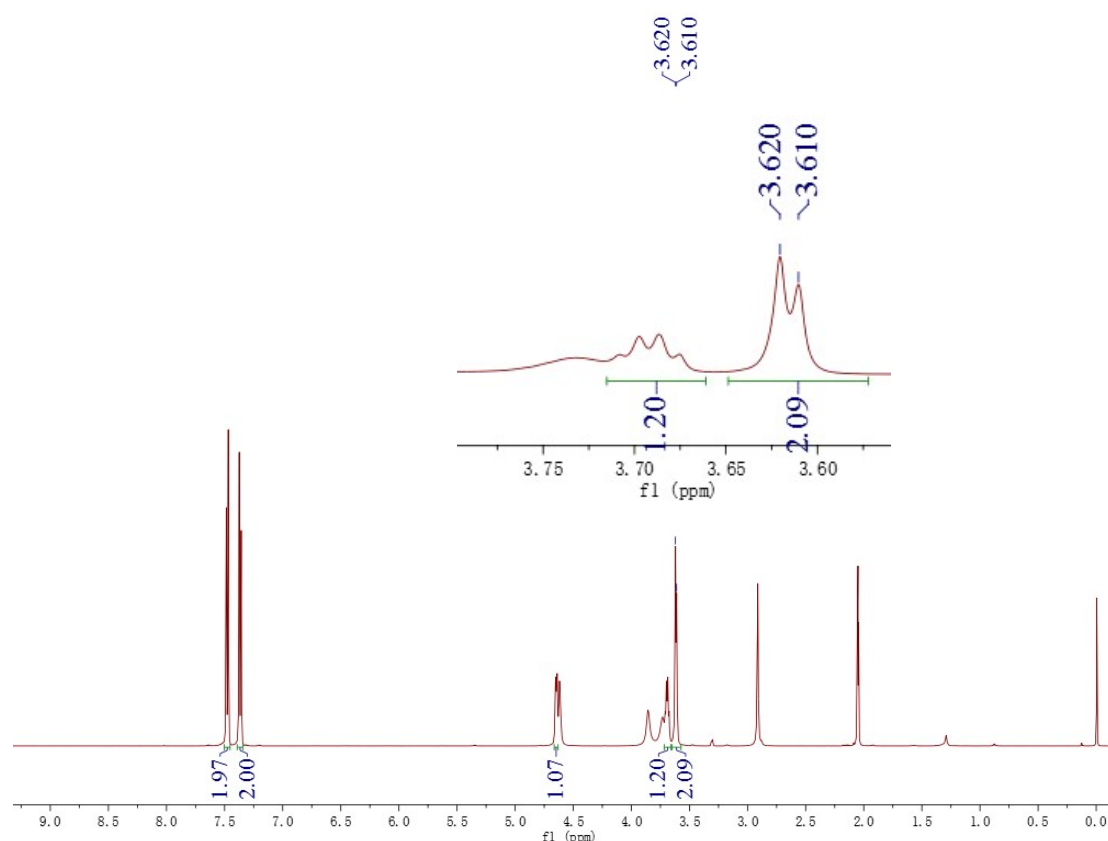


Figure S65. The ^1H NMR spectrum of compound **5** in $\text{acetone-}d_6$

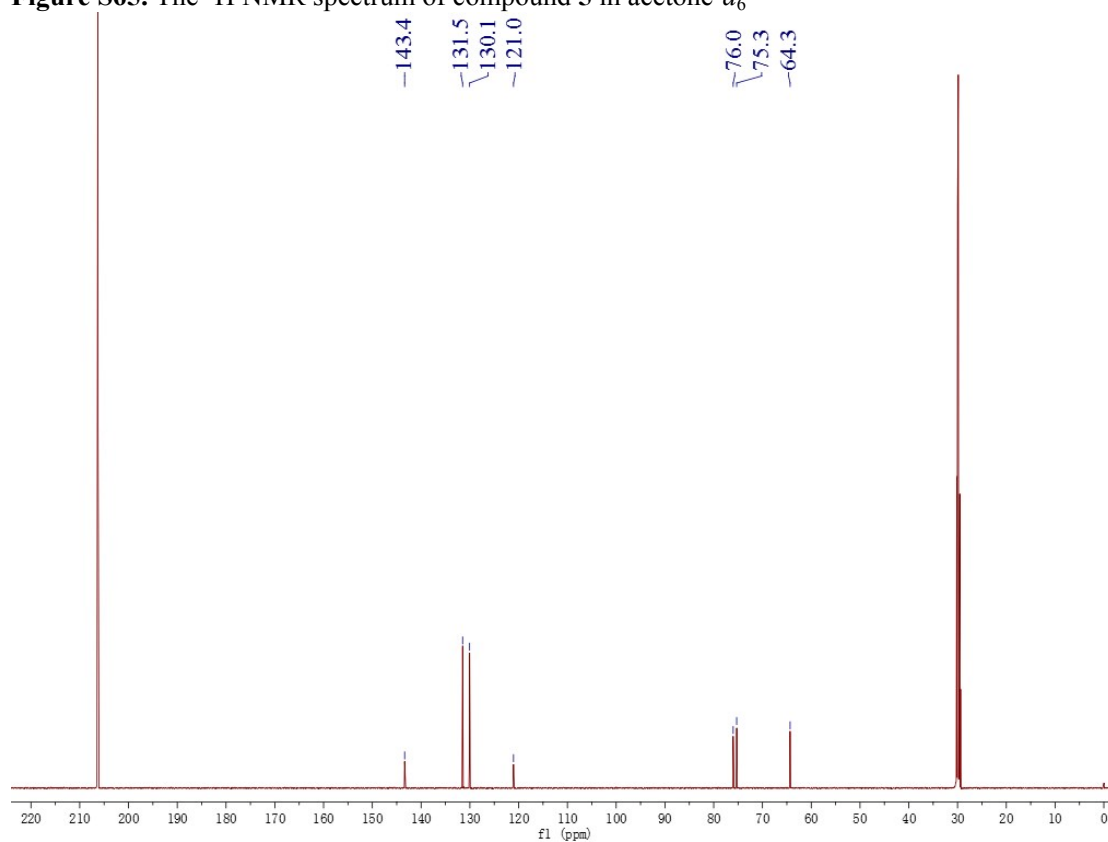


Figure S66. The ^{13}C NMR spectrum of compound **5** in $\text{acetone-}d_6$

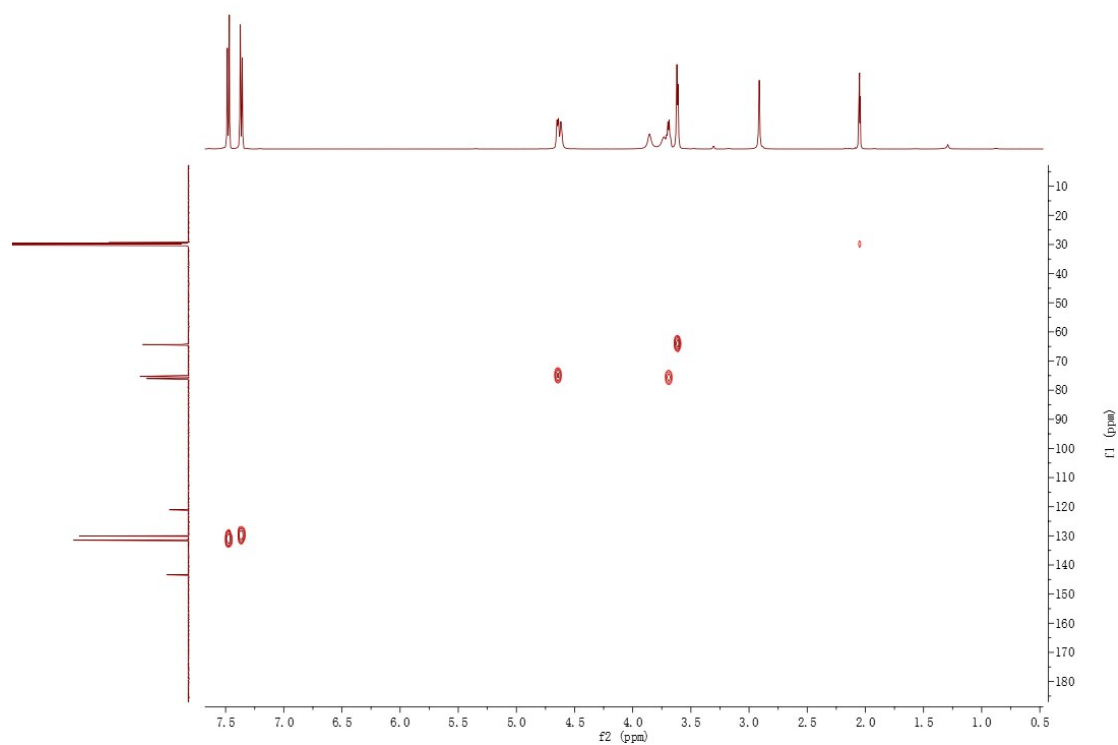


Figure S67. The HSQC spectrum of compound **5** in acetone- d_6

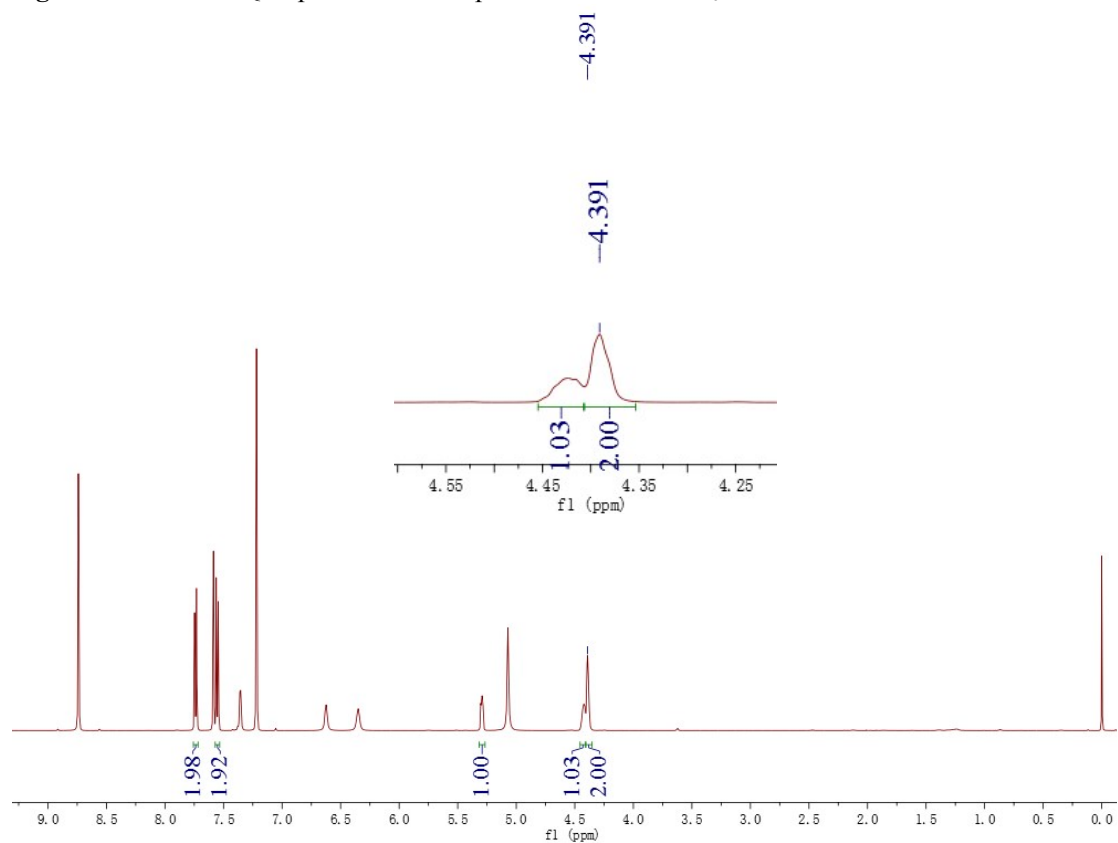


Figure S68. The ^1H NMR spectrum of compound **5** in pyridine- d_5

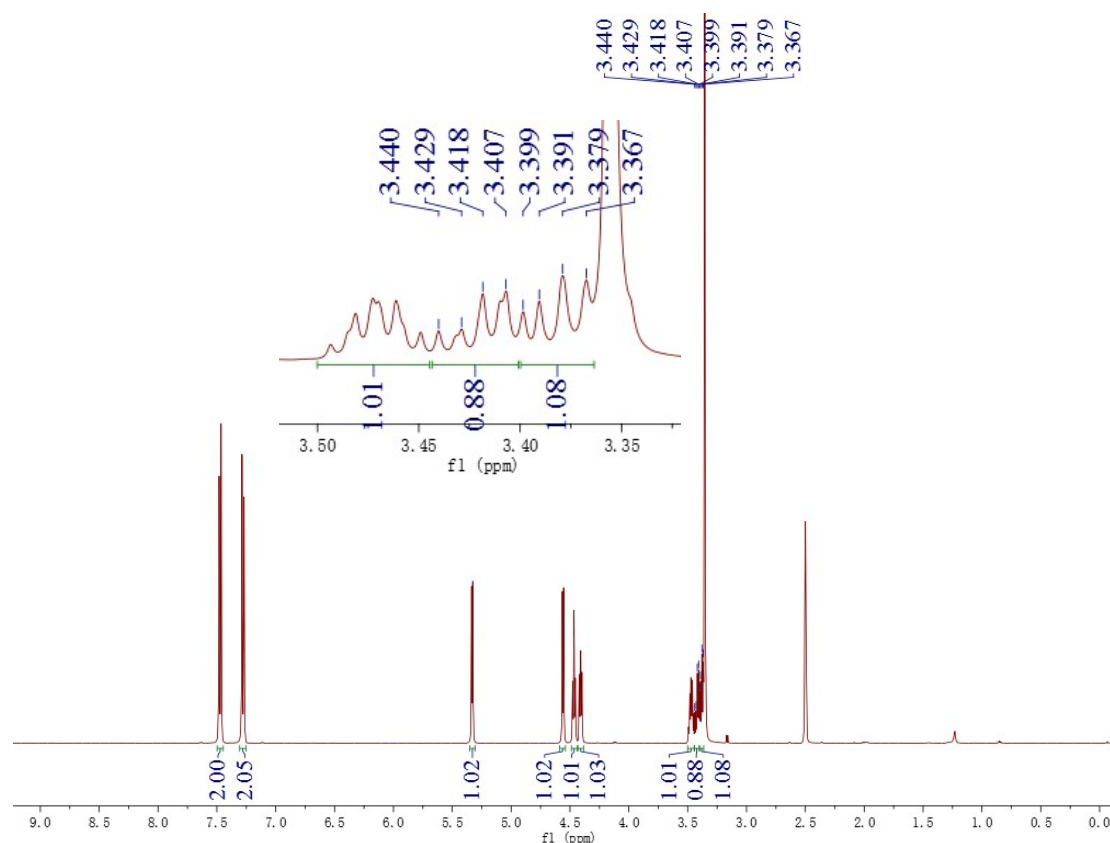


Figure S69. The ^1H NMR spectrum of compound **5** in $\text{DMSO}-d_6$

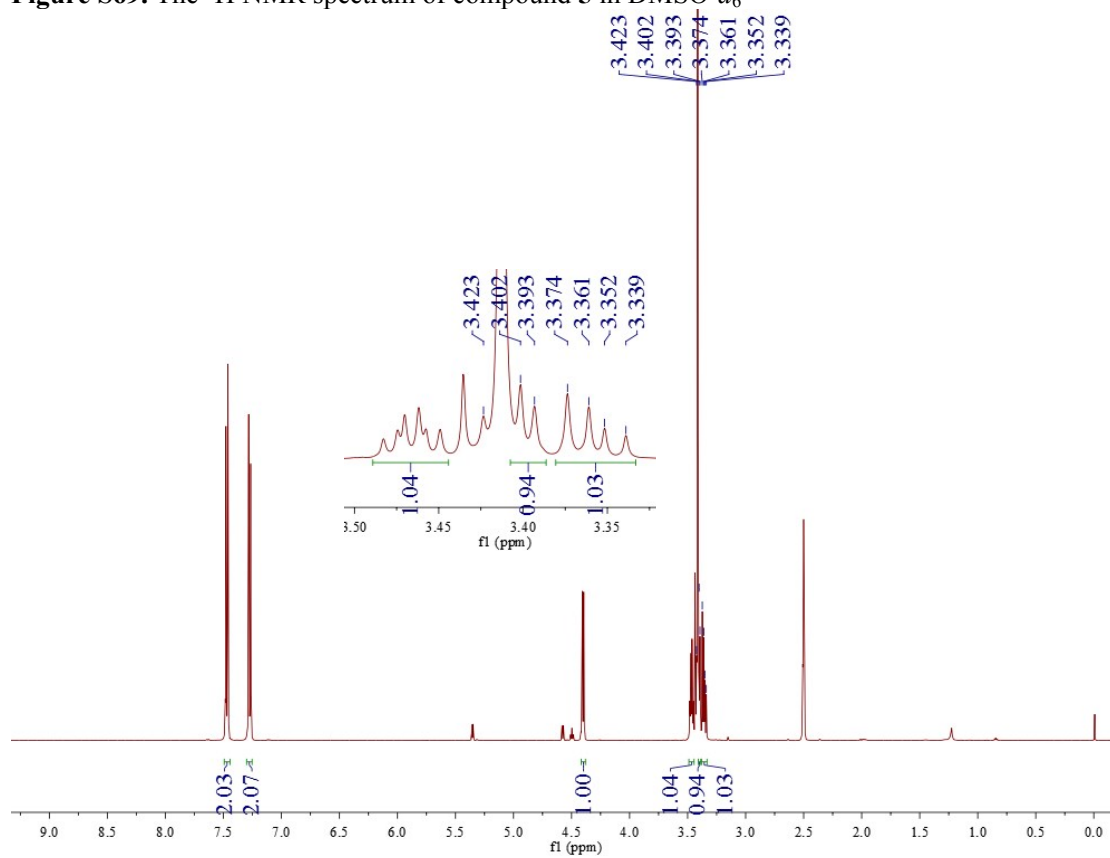


Figure S70. The H-D exchange ^1H NMR spectrum of compound **5** in $\text{DMSO}-d_6$

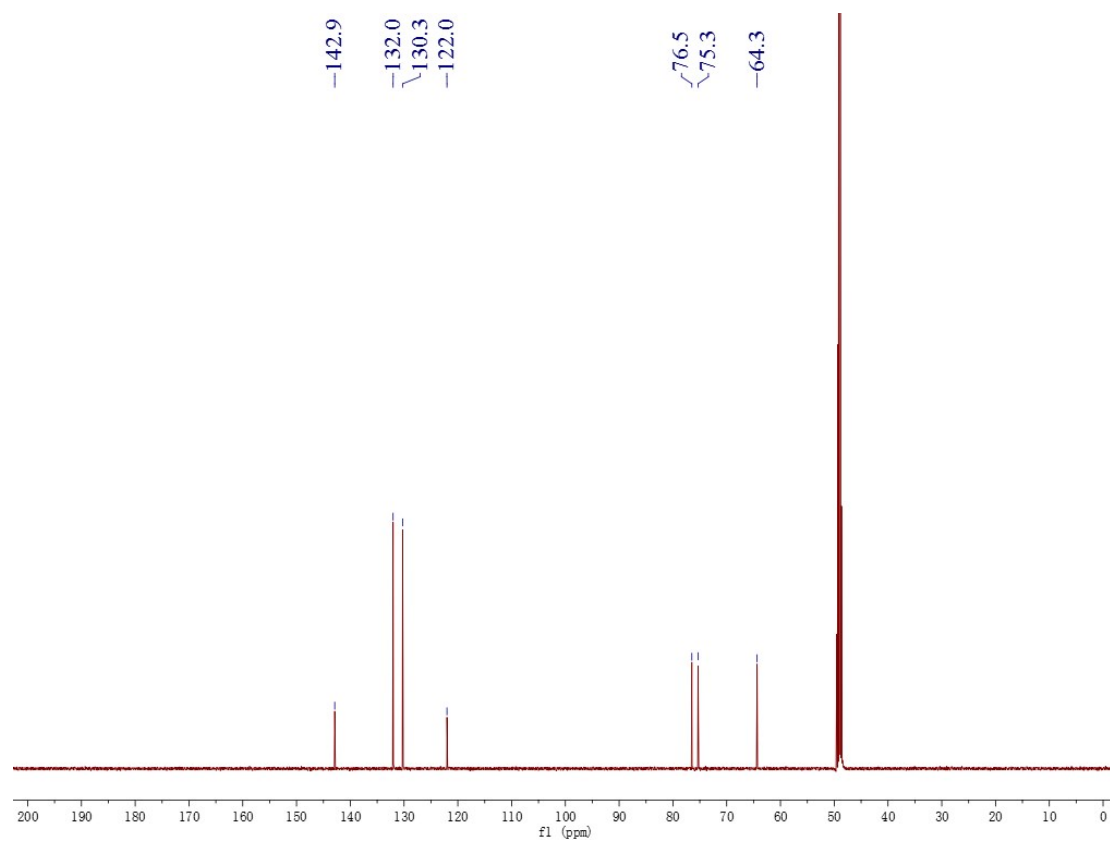
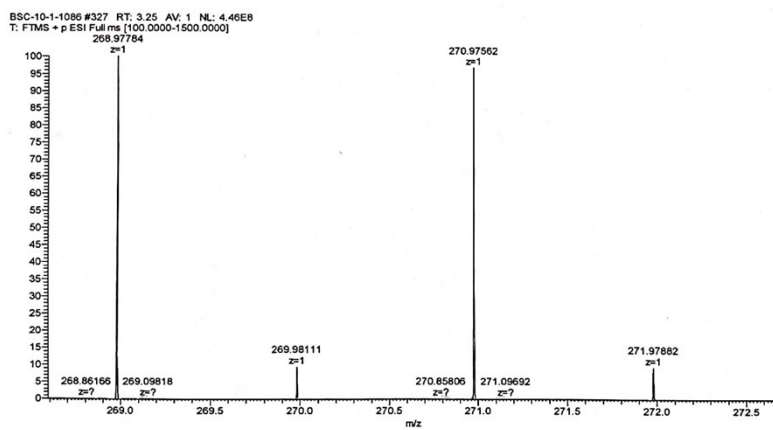
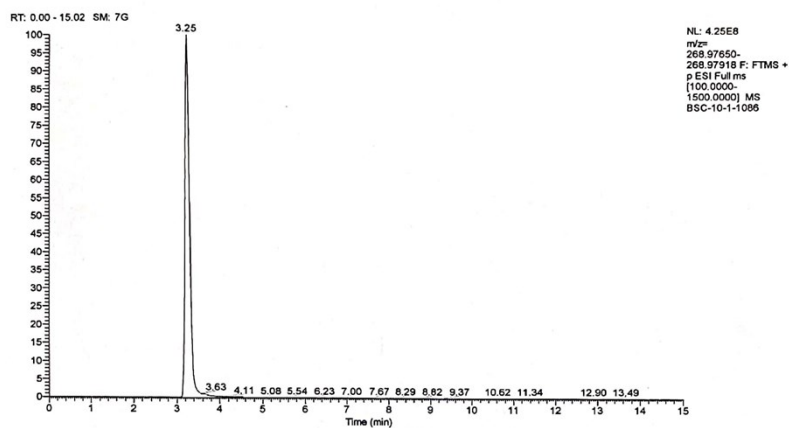


Figure S71. The ^{13}C NMR spectrum of compound **5** in methanol- d_4

Thermo Qexactive Focus Report

compound NO. : BSC-10-1-1086

Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
268.97784	268.97838	-2	3.5	C9 H11 O3 Br Na	M+Na

Figure S72. The HR-ESI-MS data of **3**

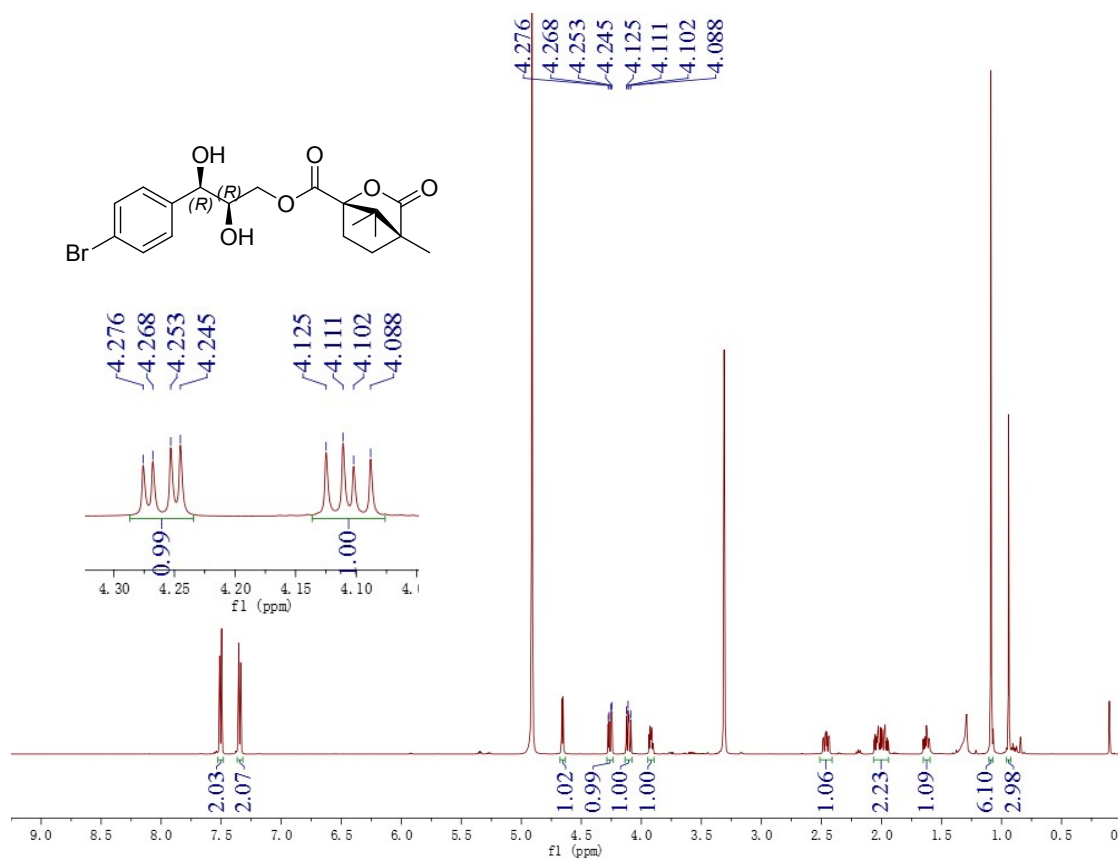


Figure S73. The ^1H NMR spectrum of compound **3a** in $\text{methanol-}d_4$

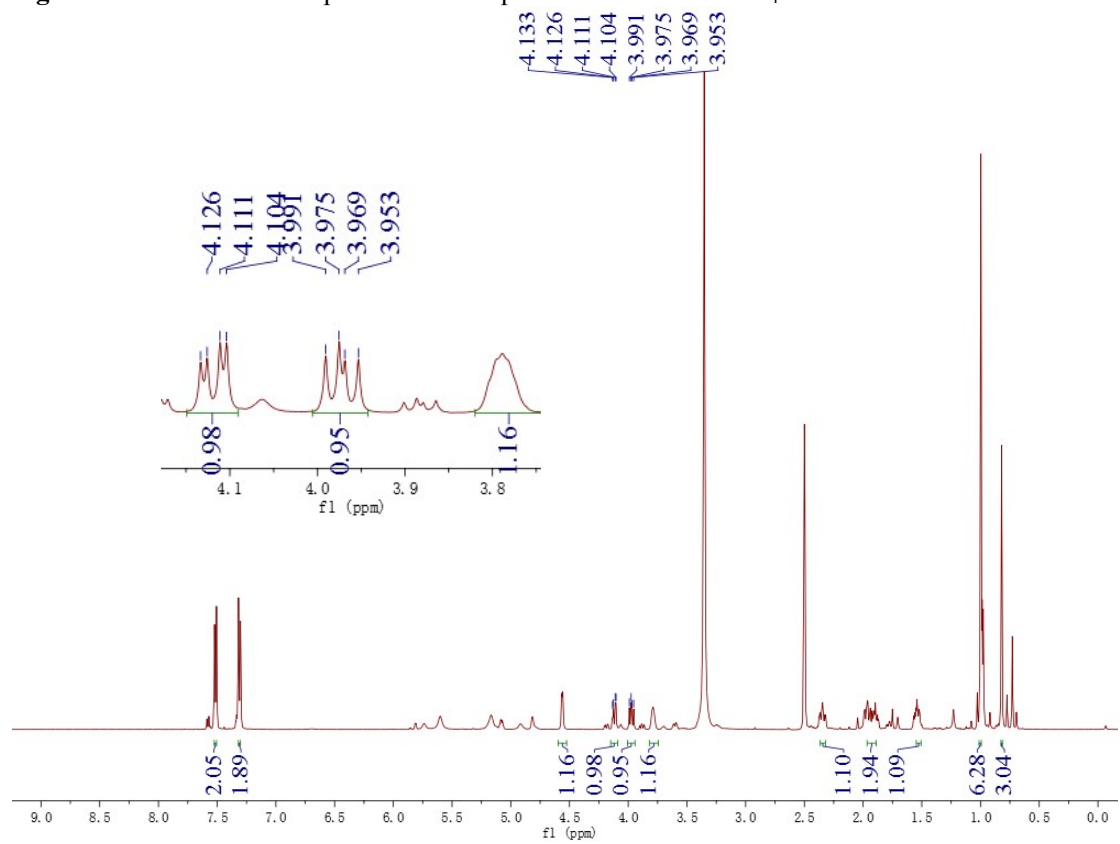


Figure S74. The ^1H NMR spectrum of compound **3a** in $\text{DMSO-}d_6$

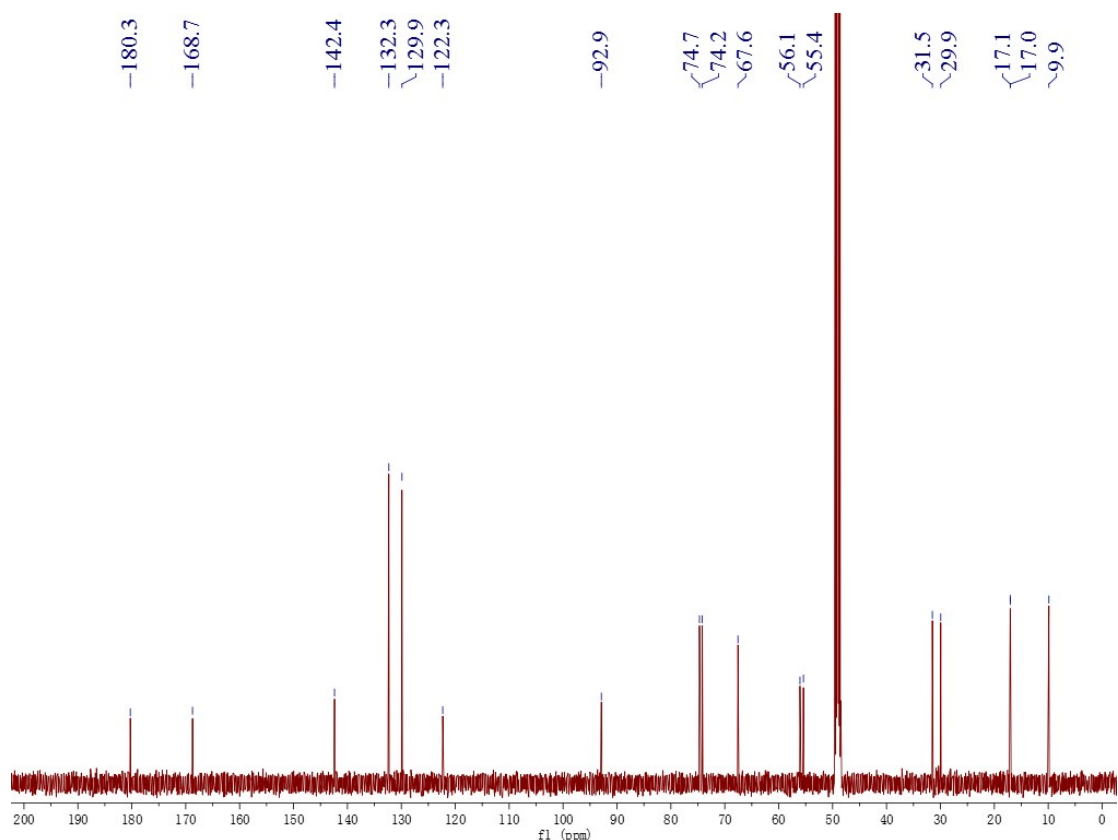


Figure S75. The ^{13}C NMR spectrum of compound **3a** in methanol- d_4

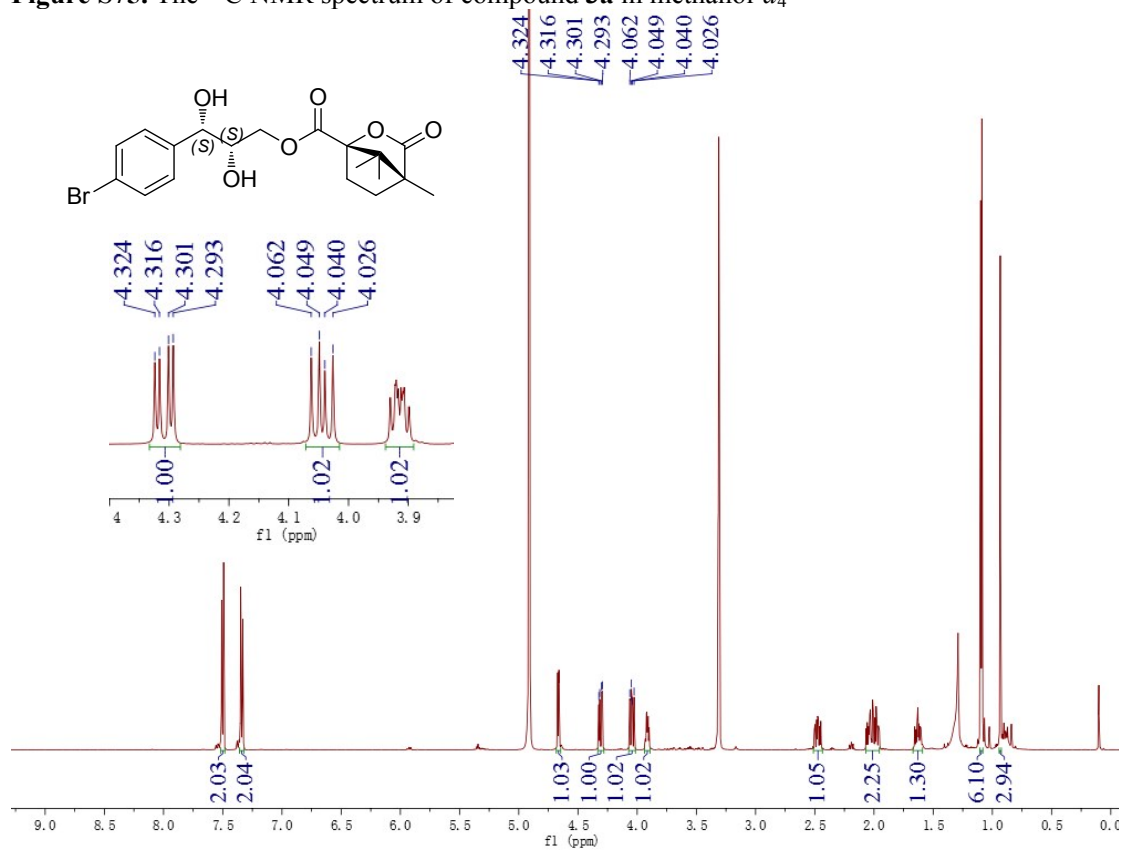
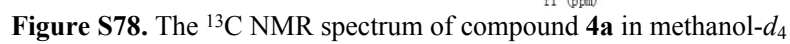
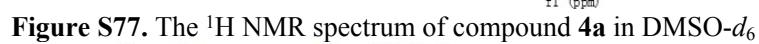


Figure S76. The ^1H NMR spectrum of compound **4a** in methanol- d_4



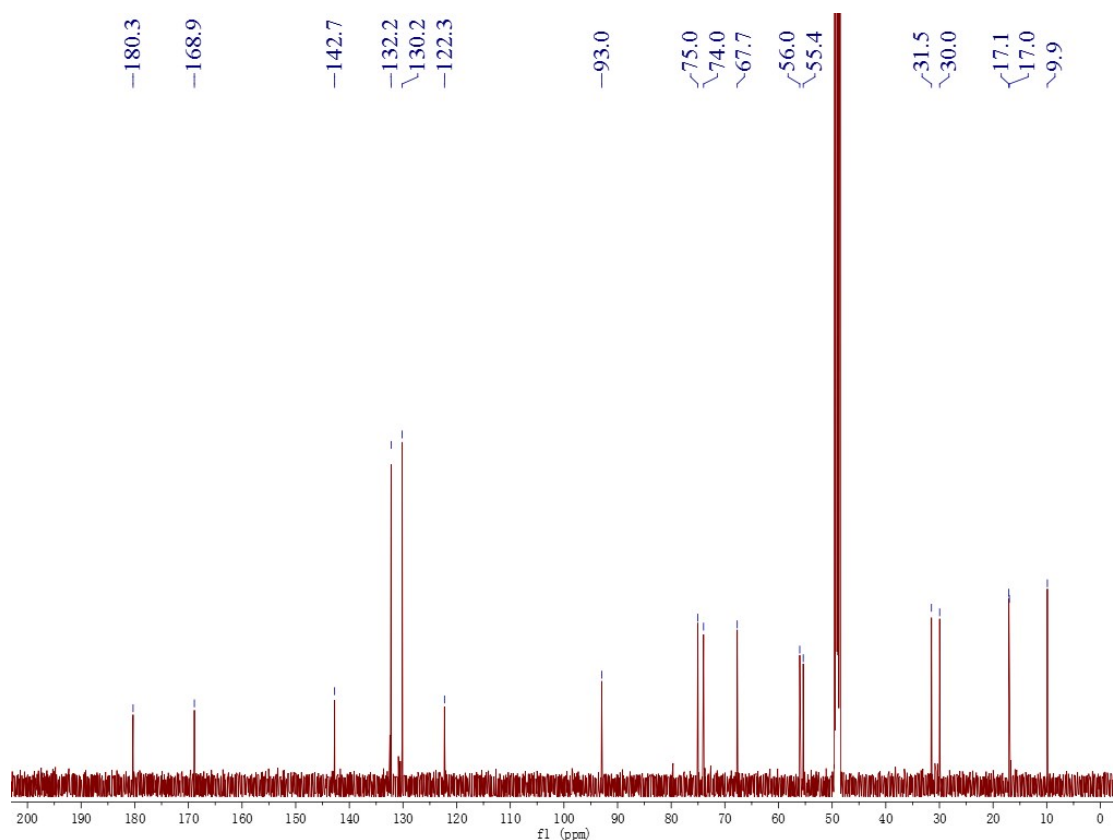


Figure S81. The ^{13}C NMR spectrum of compound **5a** in methanol- d_4

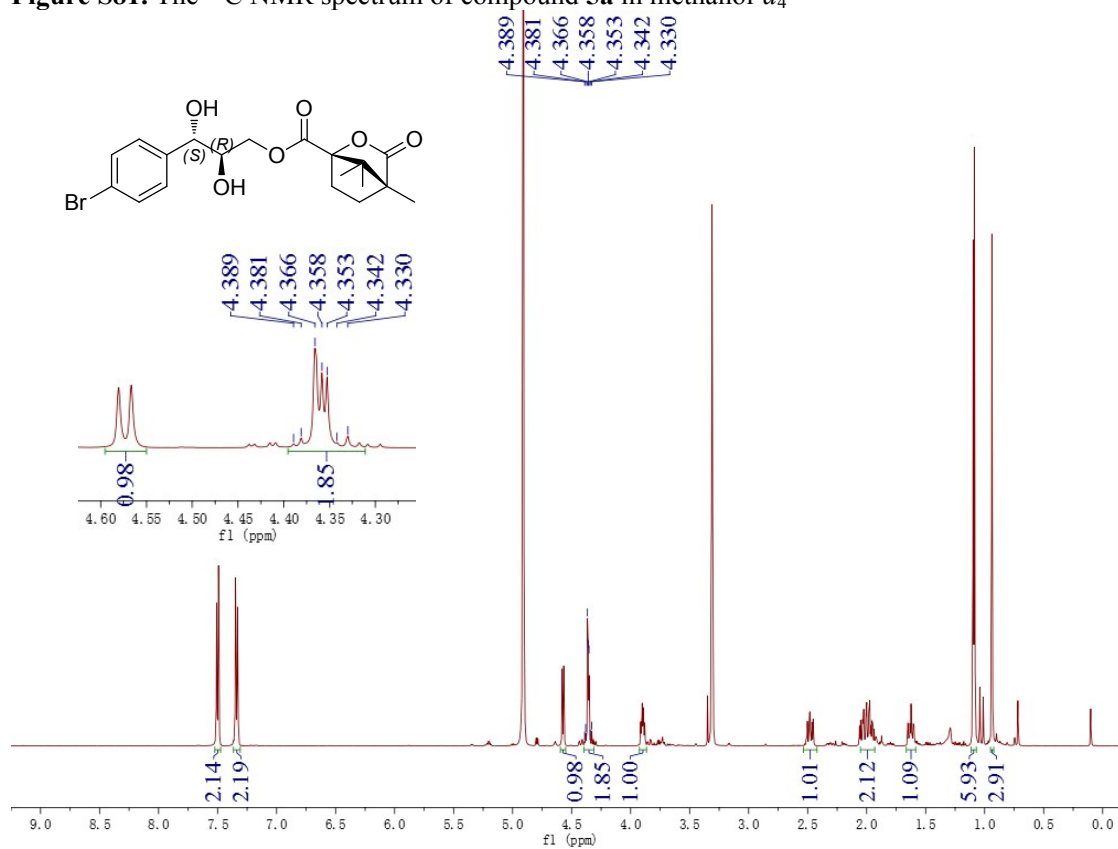


Figure S82. The ^1H NMR spectrum of compound **6a** in methanol- d_4

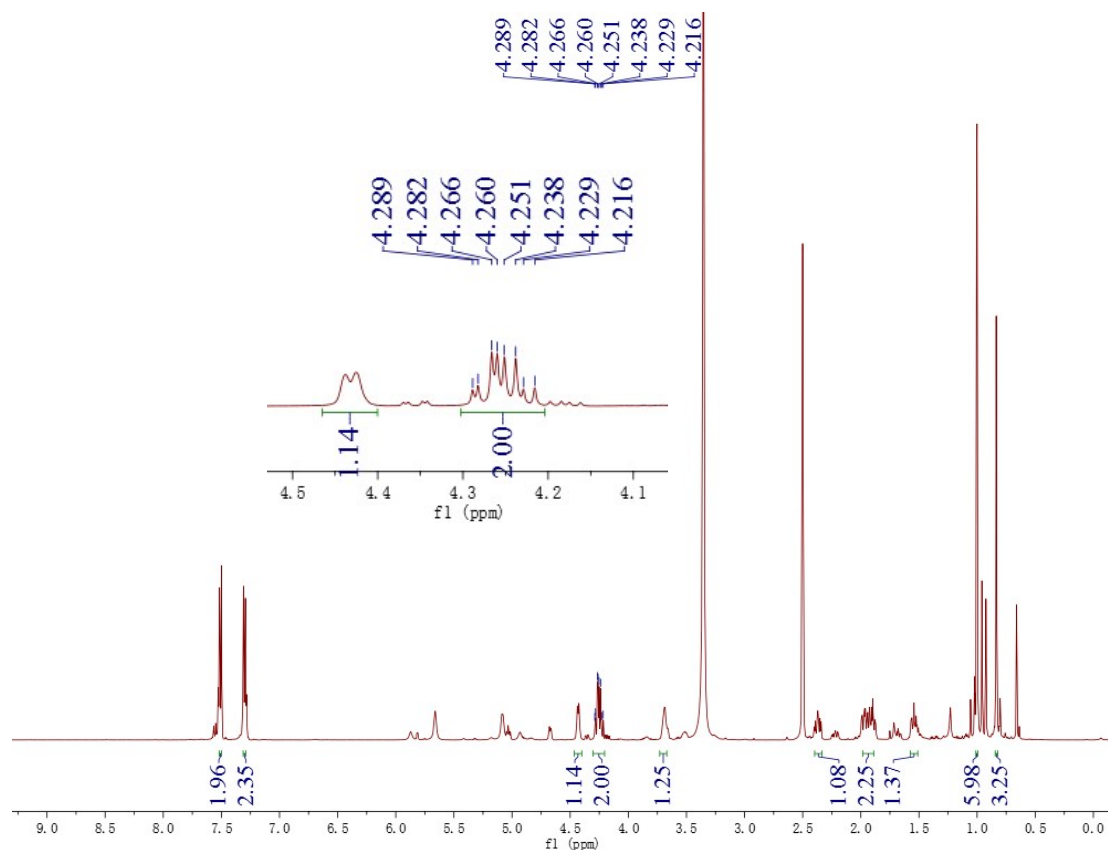


Figure S83. The ^1H NMR spectrum of compound **6a** in $\text{DMSO-}d_6$

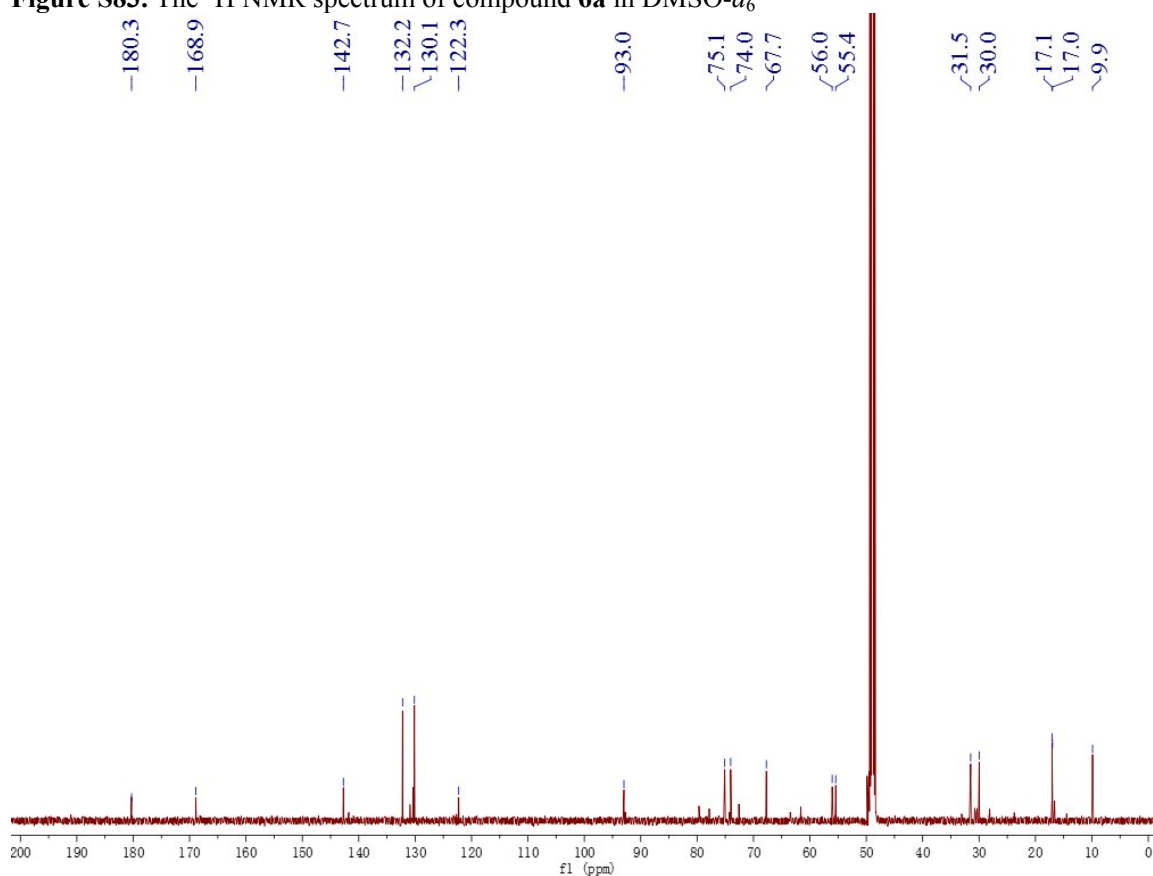
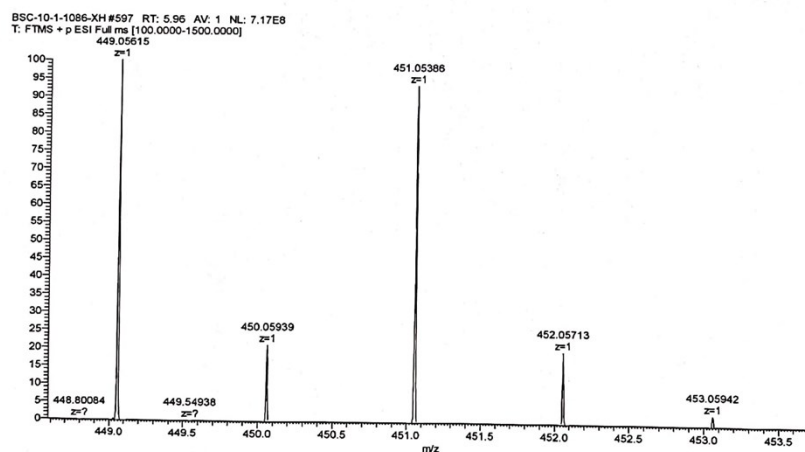
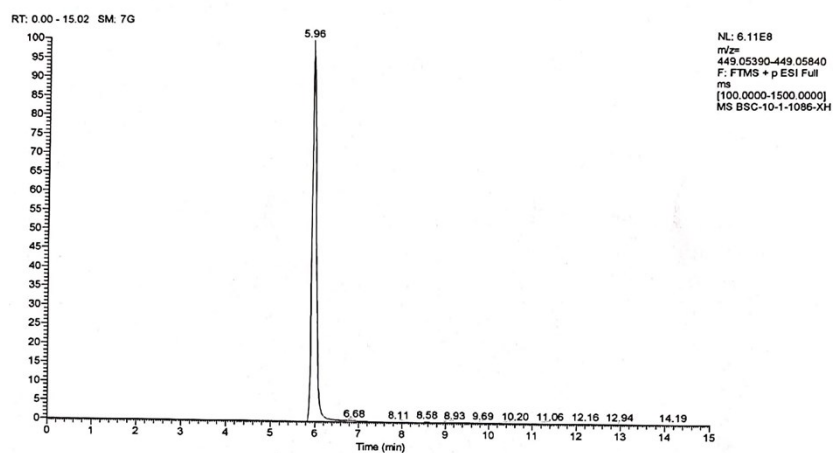


Figure S84. The ^{13}C NMR spectrum of compound **6a** in $\text{methanol-}d_4$

Thermo Qexactive Focus Report

compound NO. : BSC-10-1-10.86-XH

Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
449.05615	449.05702	-1.94	7.5	C19 H23 O6 Br Na	M+Na

Figure S85. The HR-ESI-MS data of **3a**

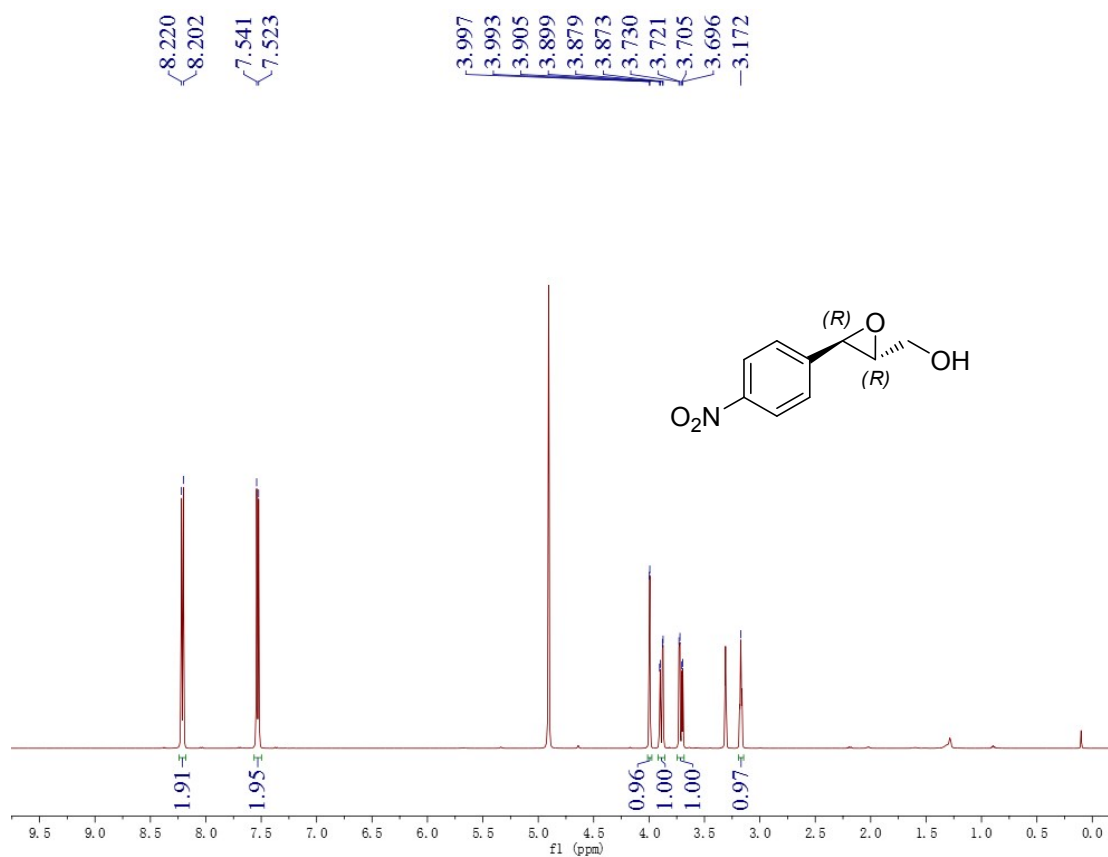


Figure S86. The ¹H NMR spectrum of ((2*R*,3*R*)-3-(4-nitrophenyl)oxiran-2-yl)methanol

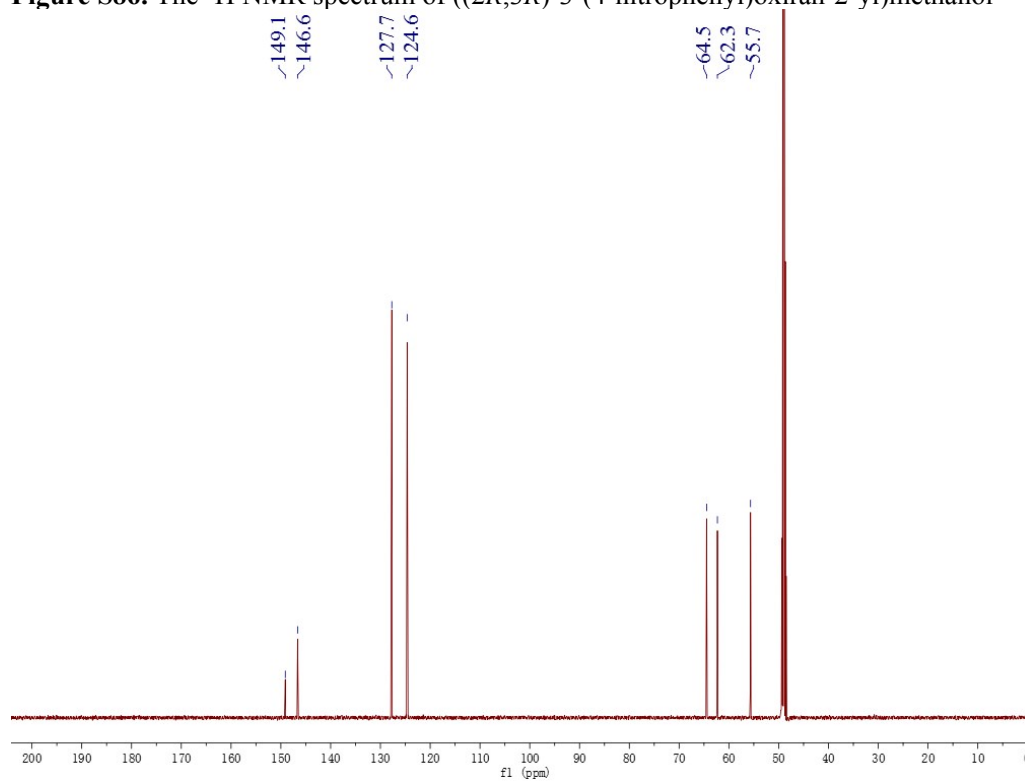
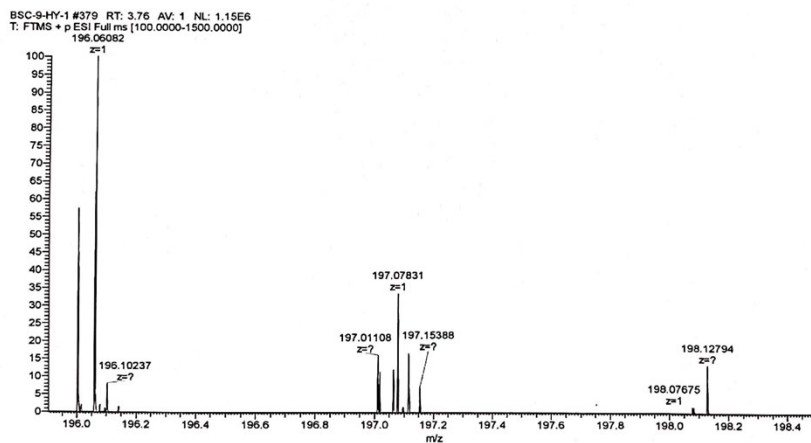
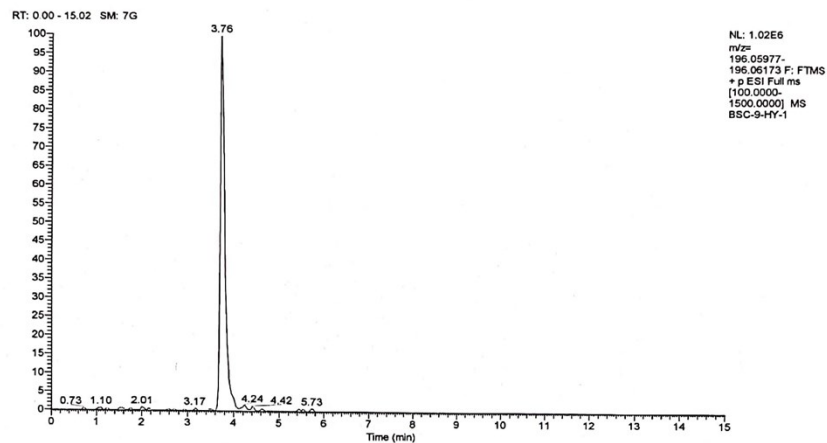


Figure S87. The ¹³C NMR spectrum of ((2*R*,3*R*)-3-(4-nitrophenyl)oxiran-2-yl)methanol

Thermo Qexactive Focus Report

compound NO. : BSC-9-HY-1
Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
196.06082	196.06043	1.97	5.5	C9 H10 O4 N	M+H

Figure S88. The HR-ESI-MS data of ((2*R*,3*R*)-3-(4-nitrophenyl)oxiran-2-yl)methanol

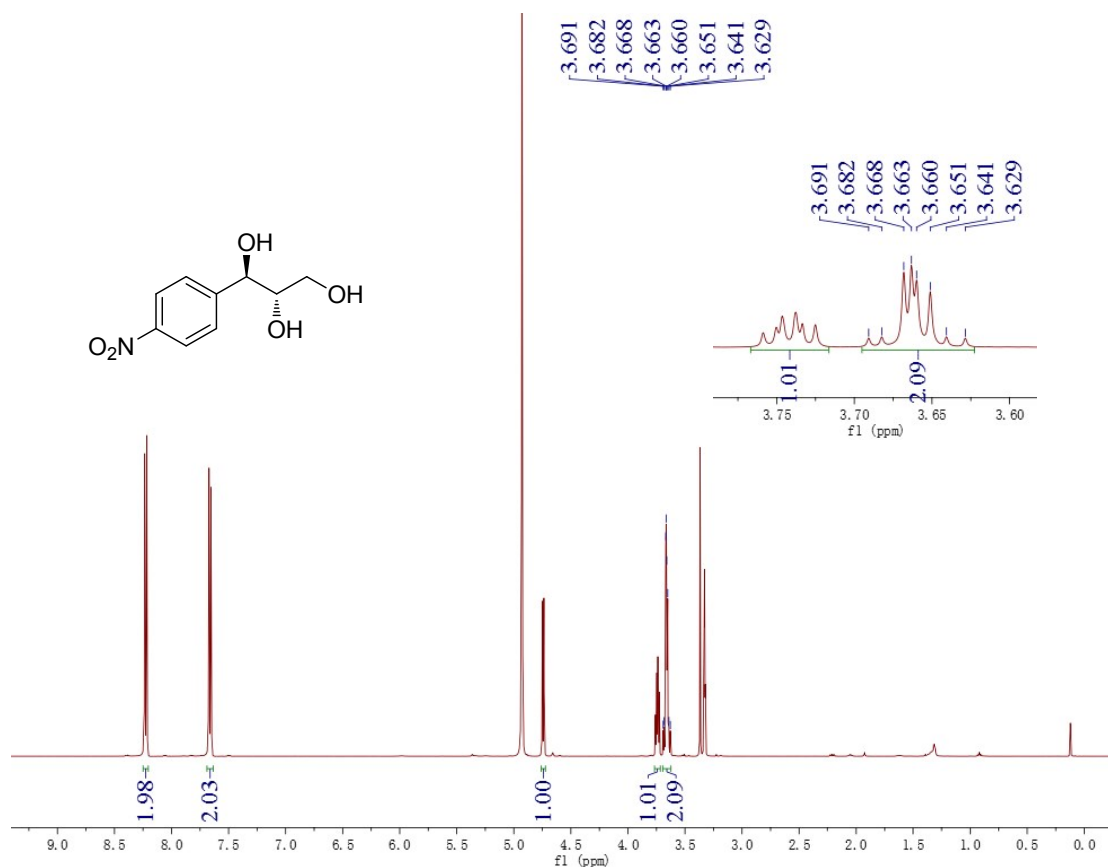


Figure S89. The ¹H NMR spectrum of compound 7 in methanol-*d*₄

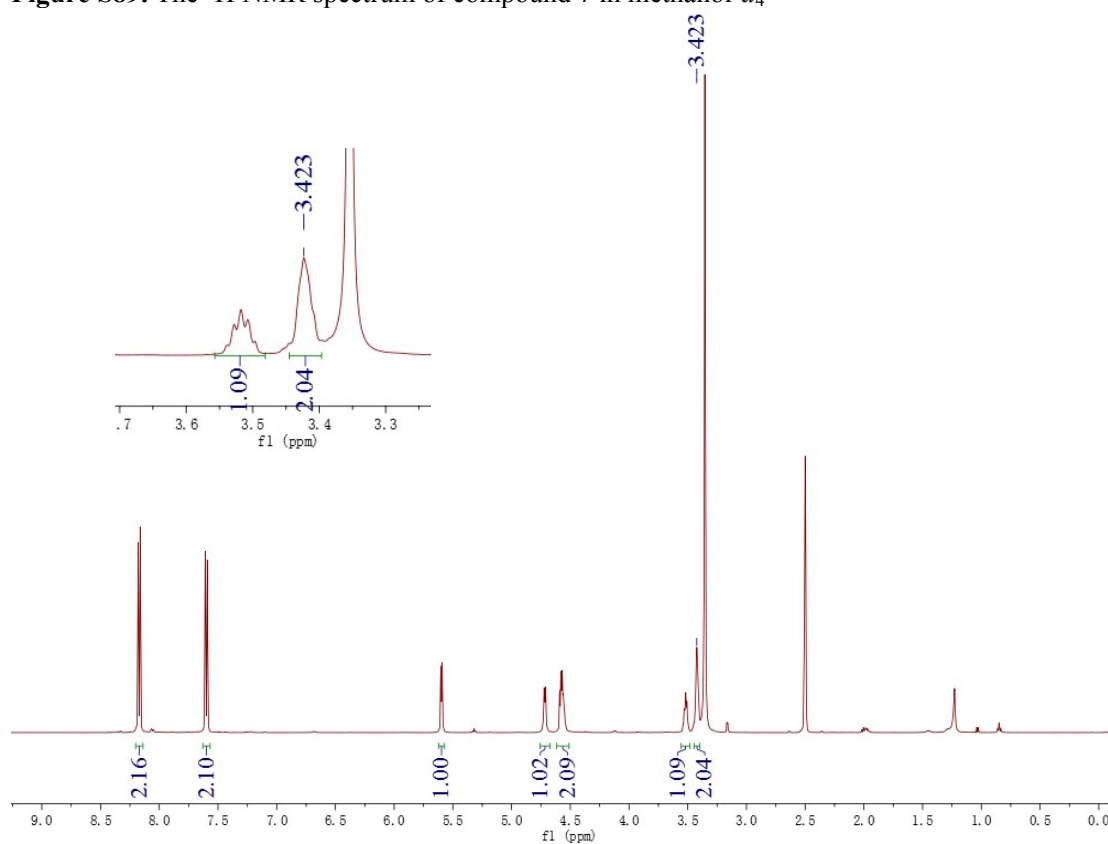


Figure S90. The ¹H NMR spectrum of compound 7 in DMSO-*d*₆

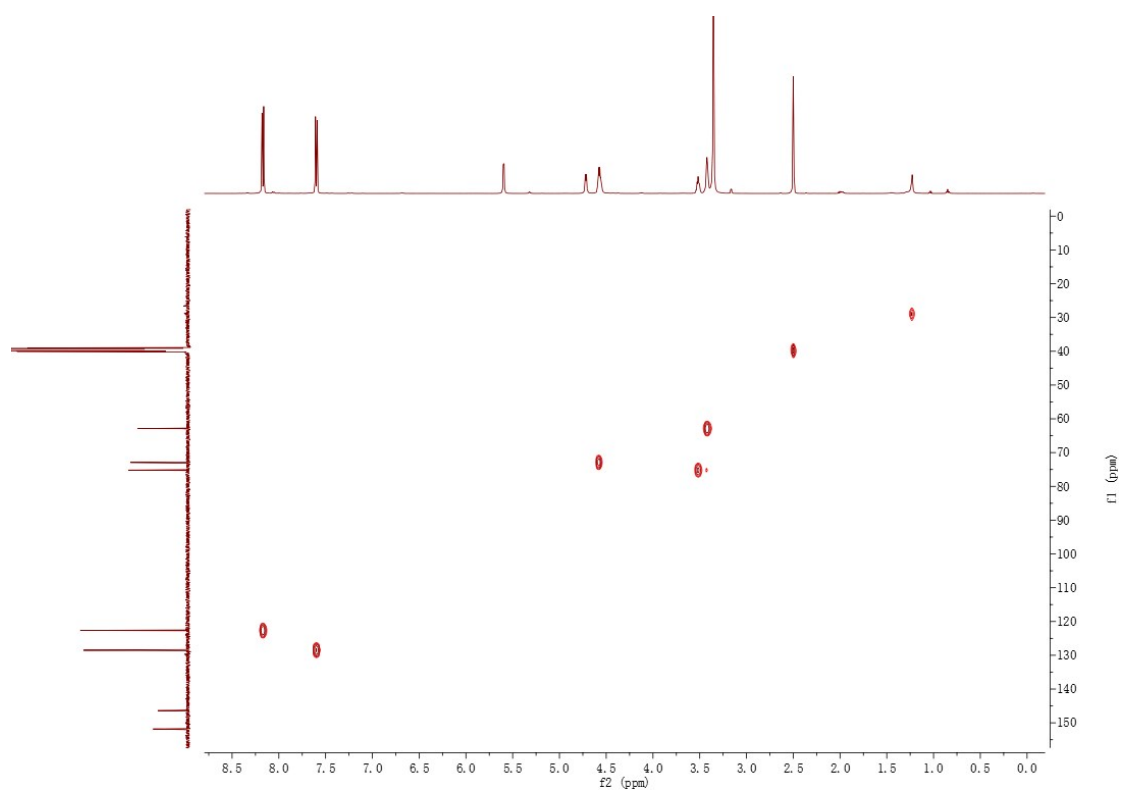


Figure S91. The HSQC spectrum of compound **7** in DMSO- d_6

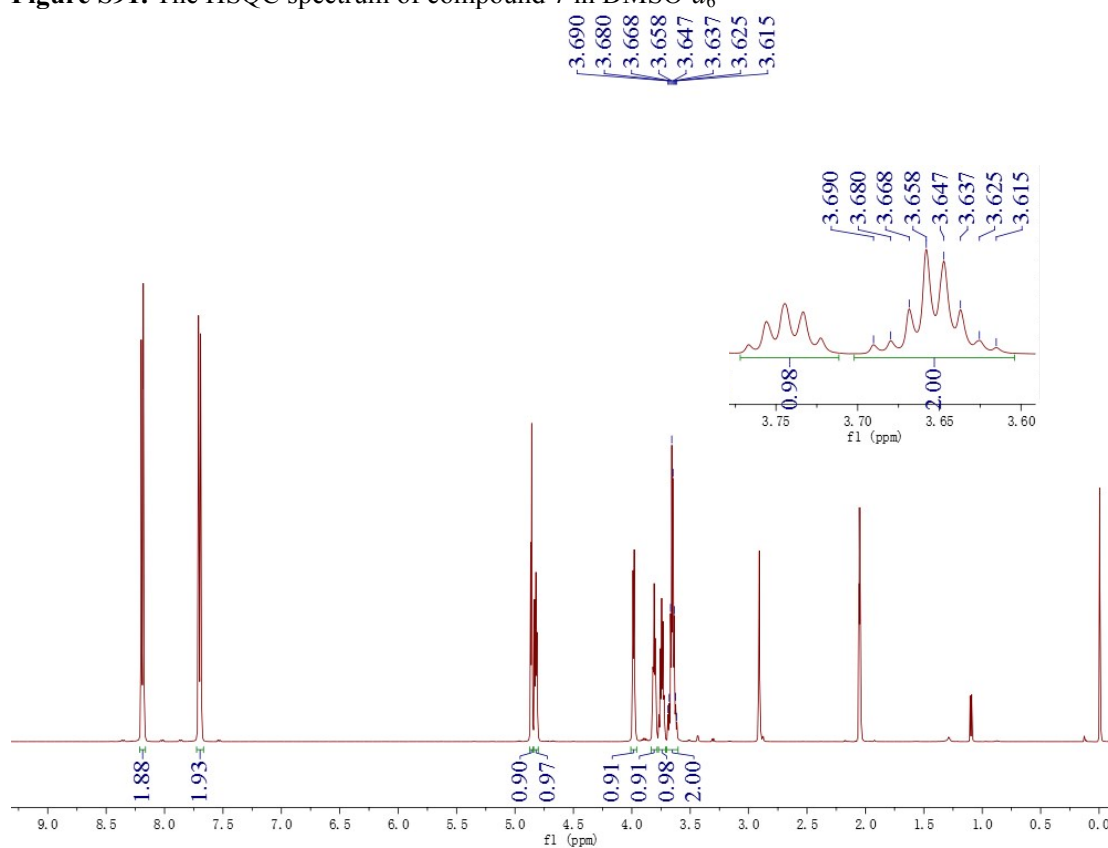


Figure S92. The ^1H NMR spectrum of compound **7** in acetone- d_6

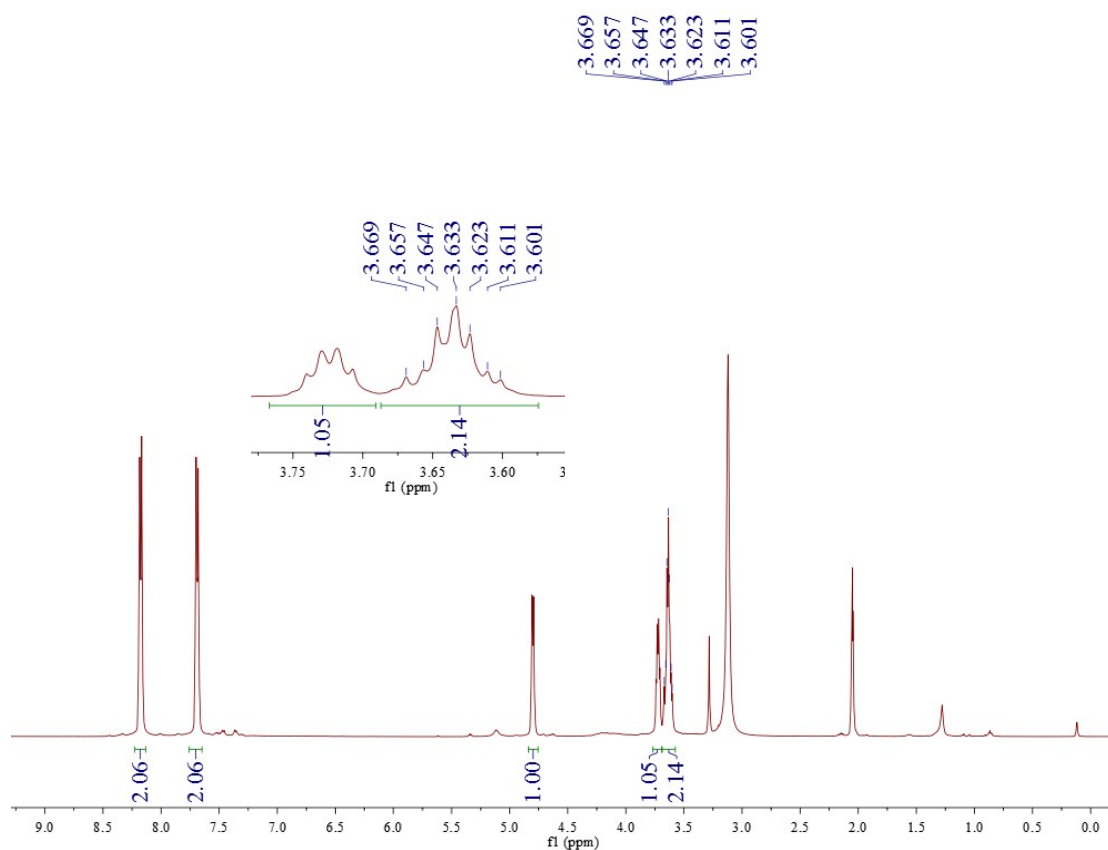


Figure S93. The H-D exchange ^1H NMR spectrum of compound **7** in acetone- d_6

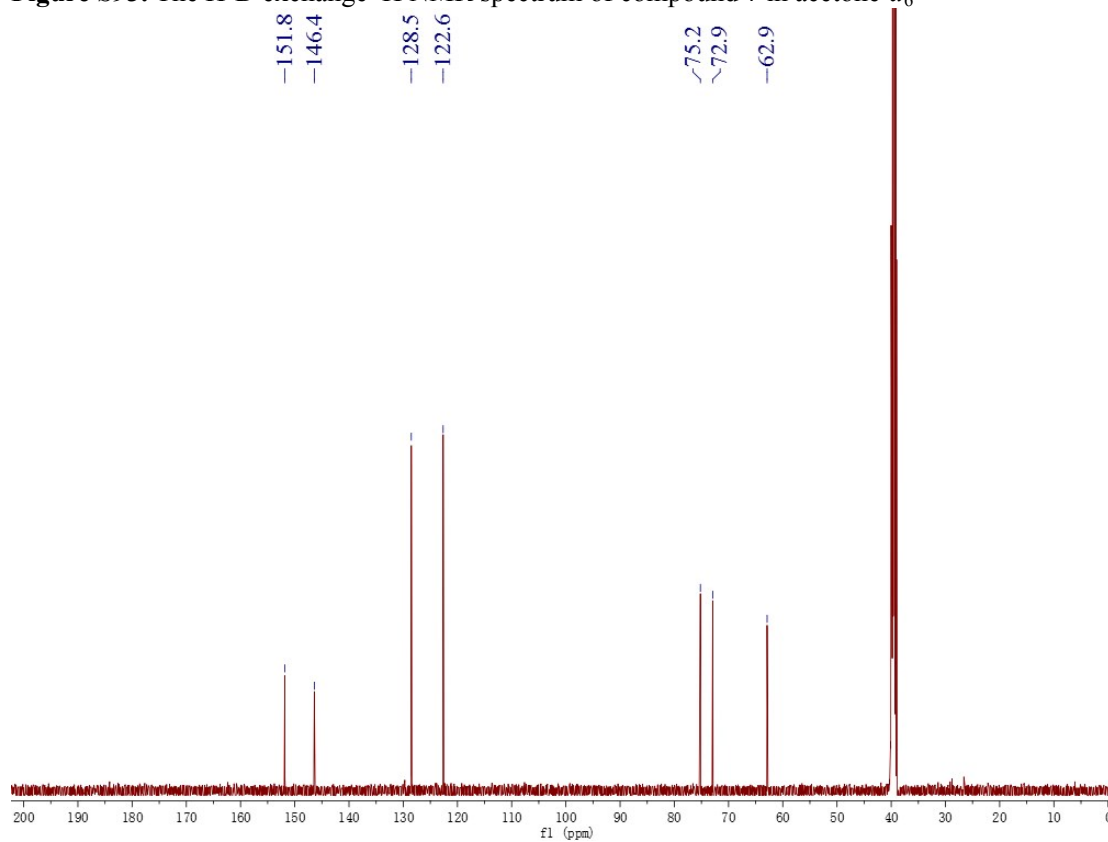
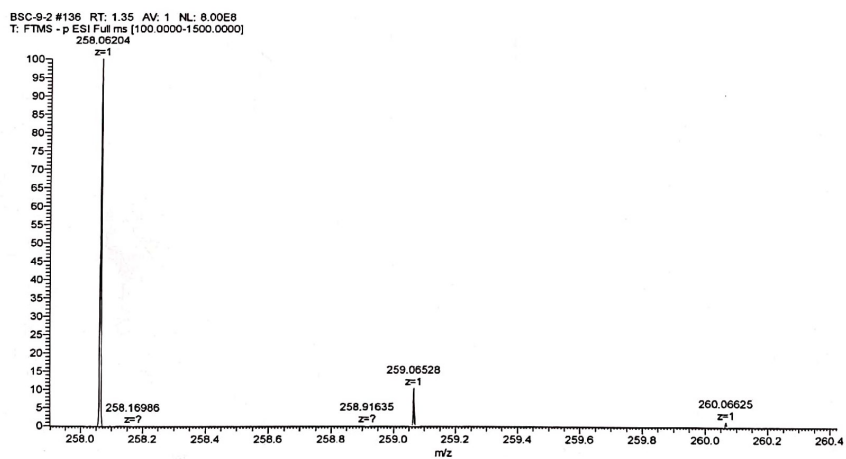
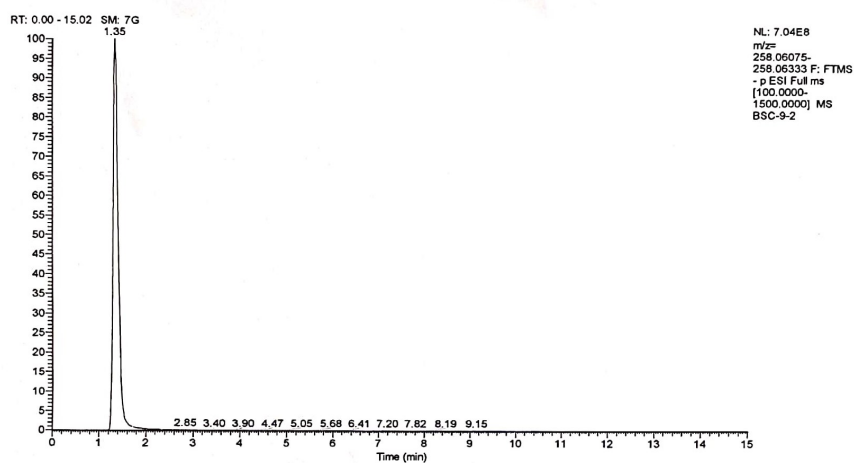


Figure S94. The ^{13}C NMR spectrum of compound **7** in DMSO- d_6

Thermo Qexactive Focus Report

compound NO. : BSC-9-2

Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
258.06204	258.06192	0.45	5.5	C10 H12 O7 N	M+HCOO

Figure S95. The HR-ESI-MS data of **7**

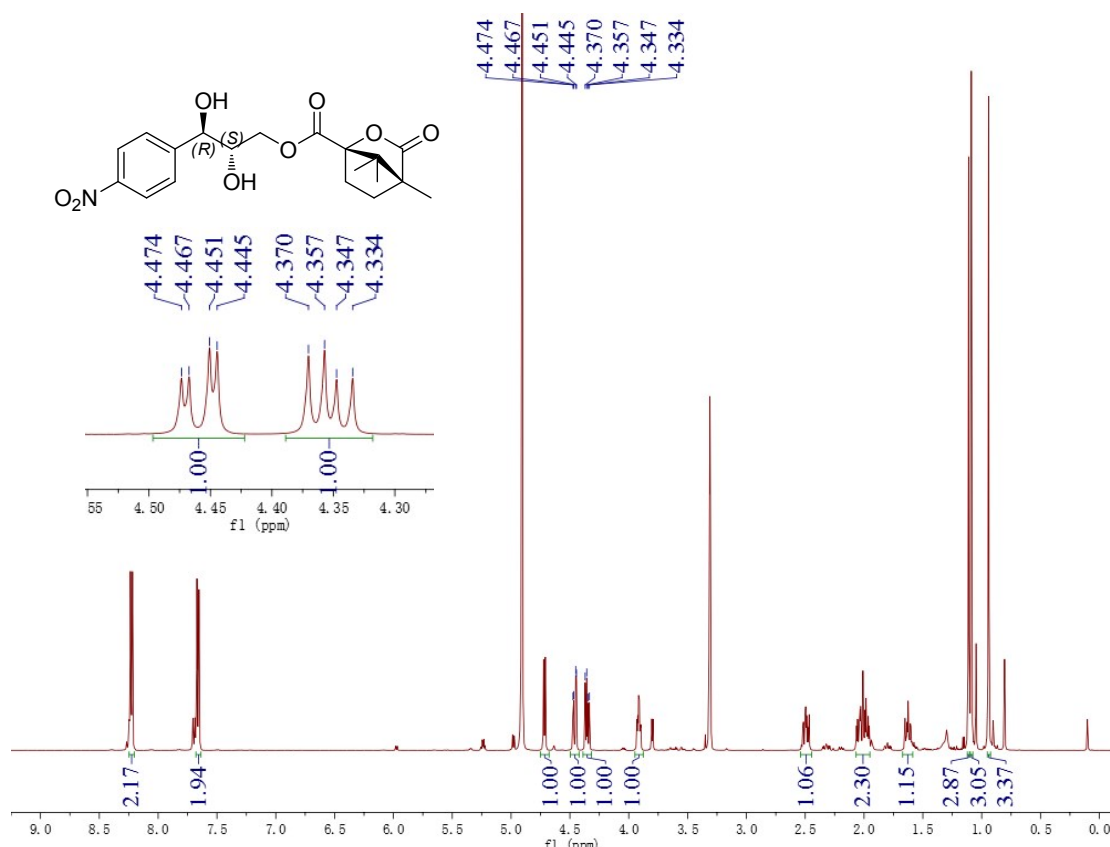


Figure S96. The ¹H NMR spectrum of compound **7a** in methanol-*d*₄

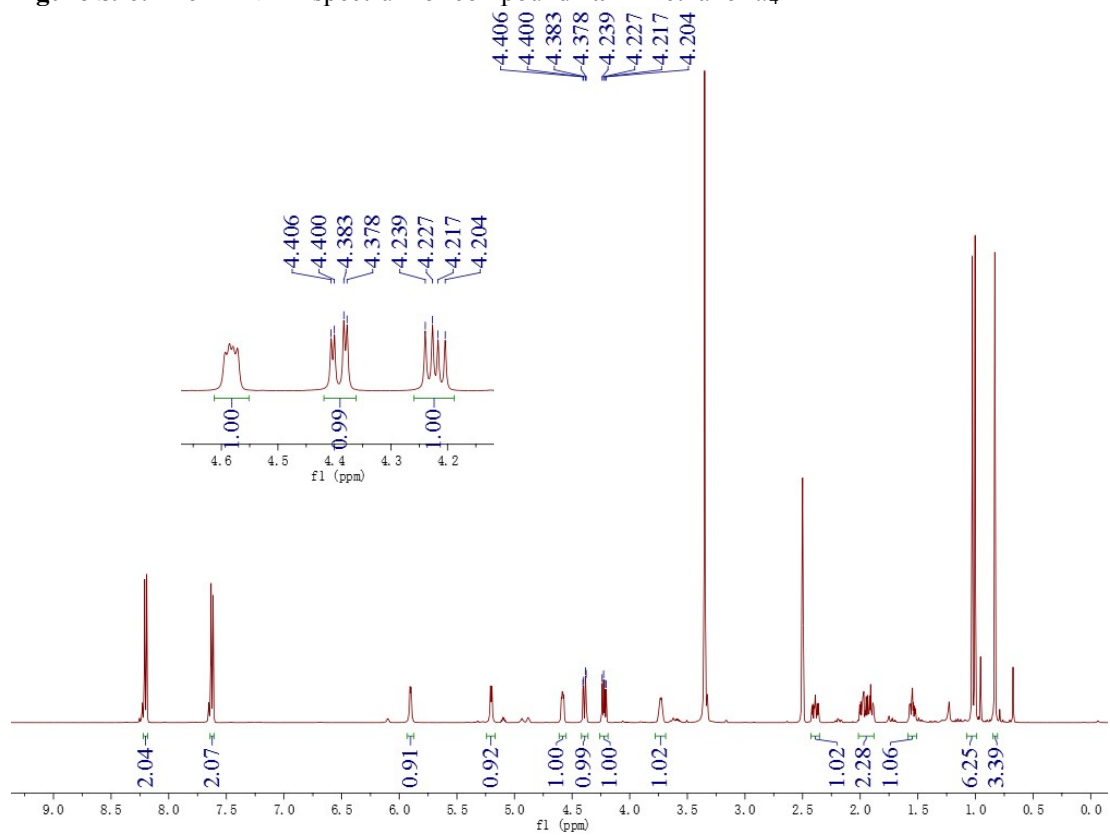


Figure S97. The ¹H NMR spectrum of compound **7a** in DMSO-*d*₆

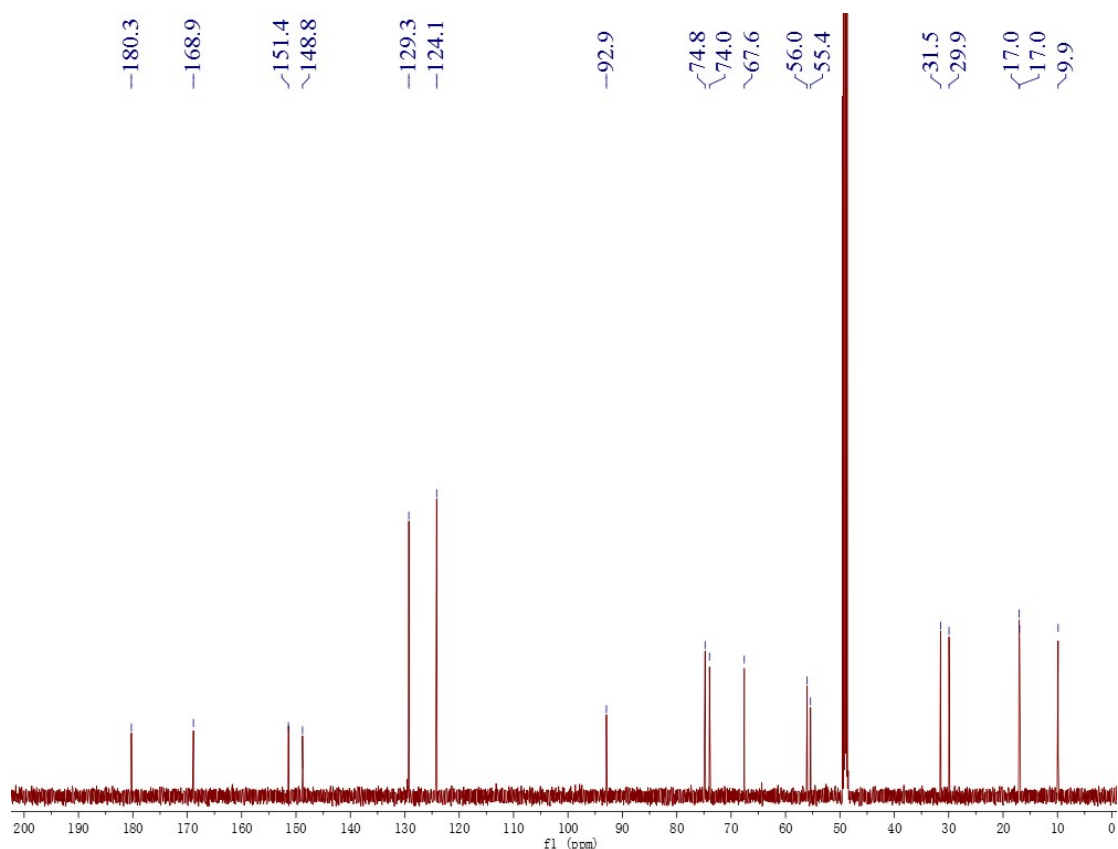


Figure S98. The ^{13}C NMR spectrum of compound **7a** in methanol- d_4

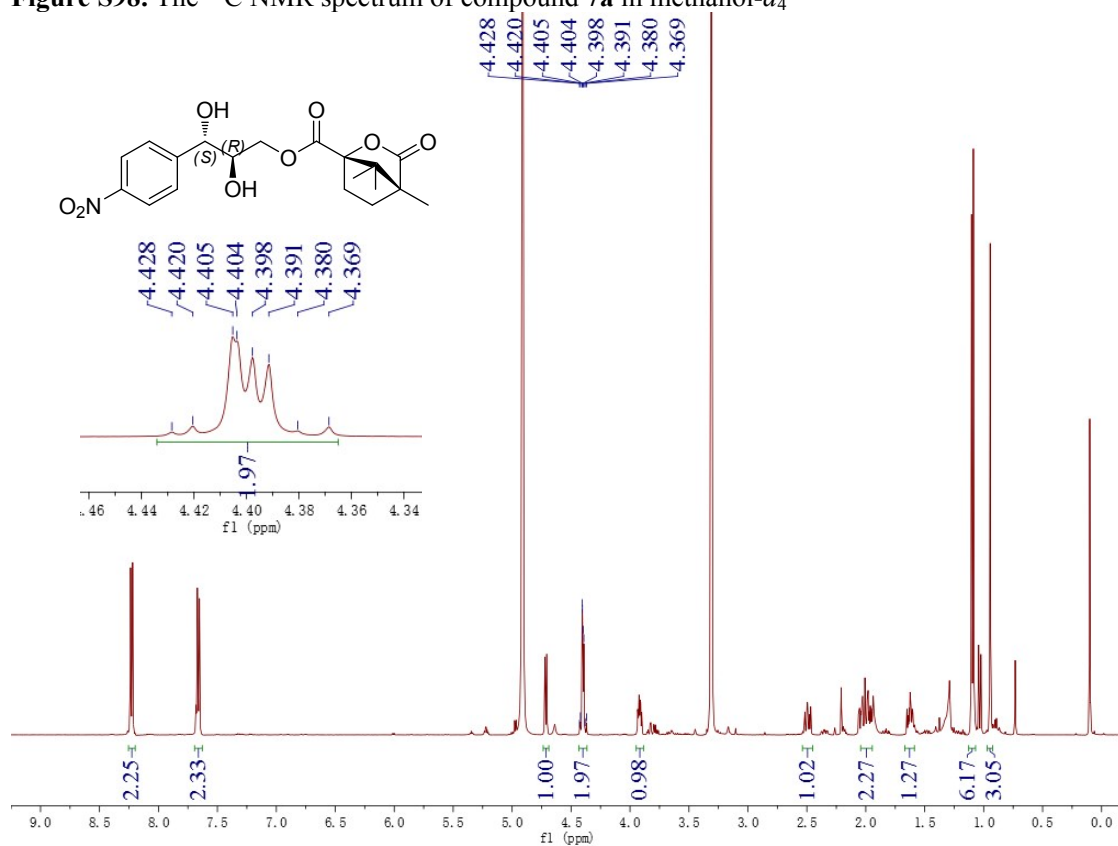


Figure S99. The ^1H NMR spectrum of compound **8a** in methanol- d_4

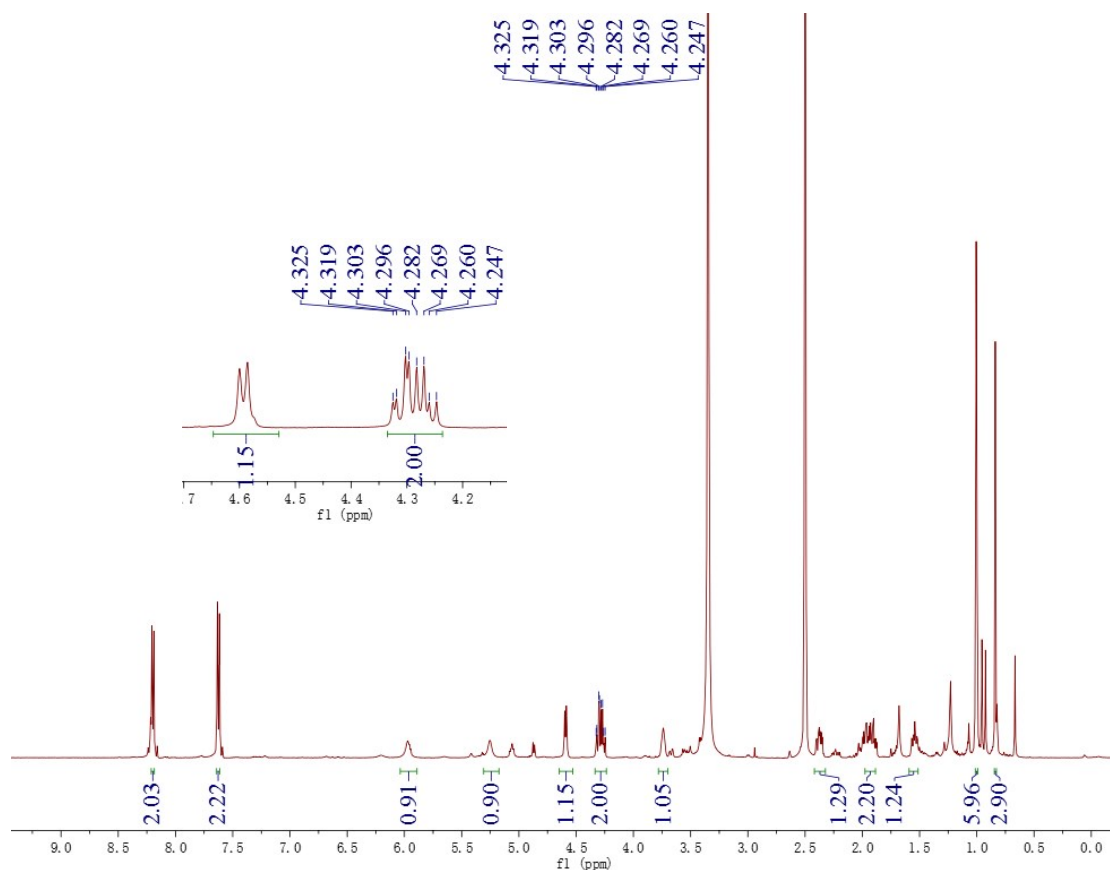


Figure S100. The ^1H NMR spectrum of compound **8a** in $\text{DMSO}-d_6$

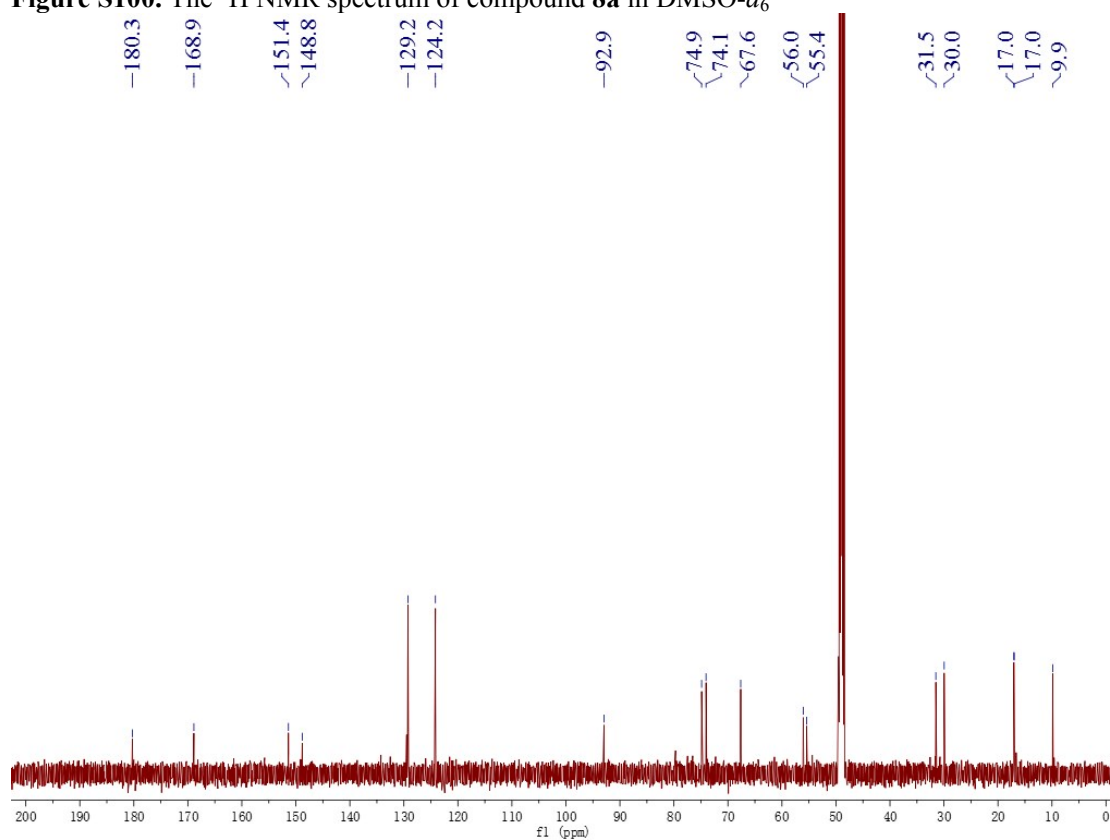
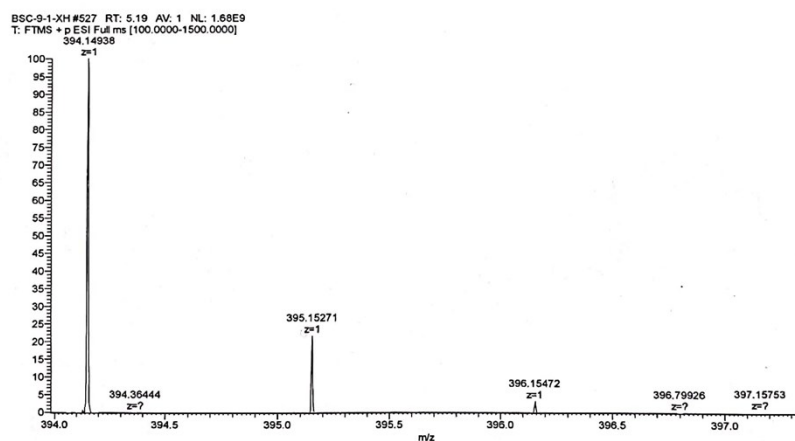
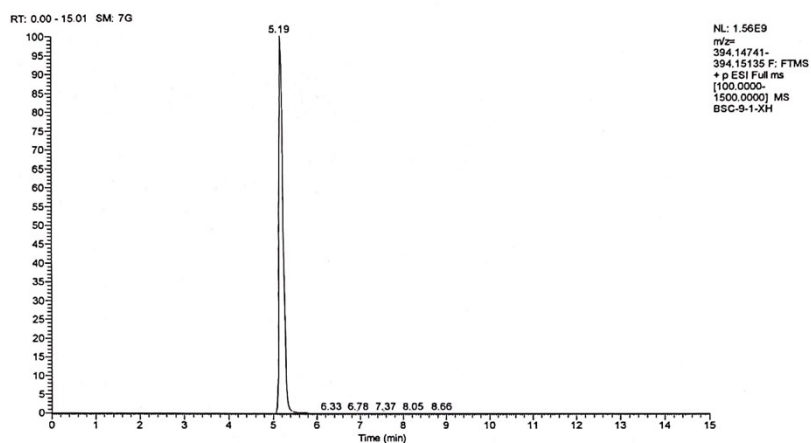


Figure S101. The ^{13}C NMR spectrum of compound **8a** in $\text{methanol}-d_4$

Thermo Qexactive Focus Report

compound NO. : BSC-9-1-XH
Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
394.14938	394.14964	-0.67	8.5	C19 H24 O8 N	M+H

Figure S102. The HR-ESI-MS data of **7a**

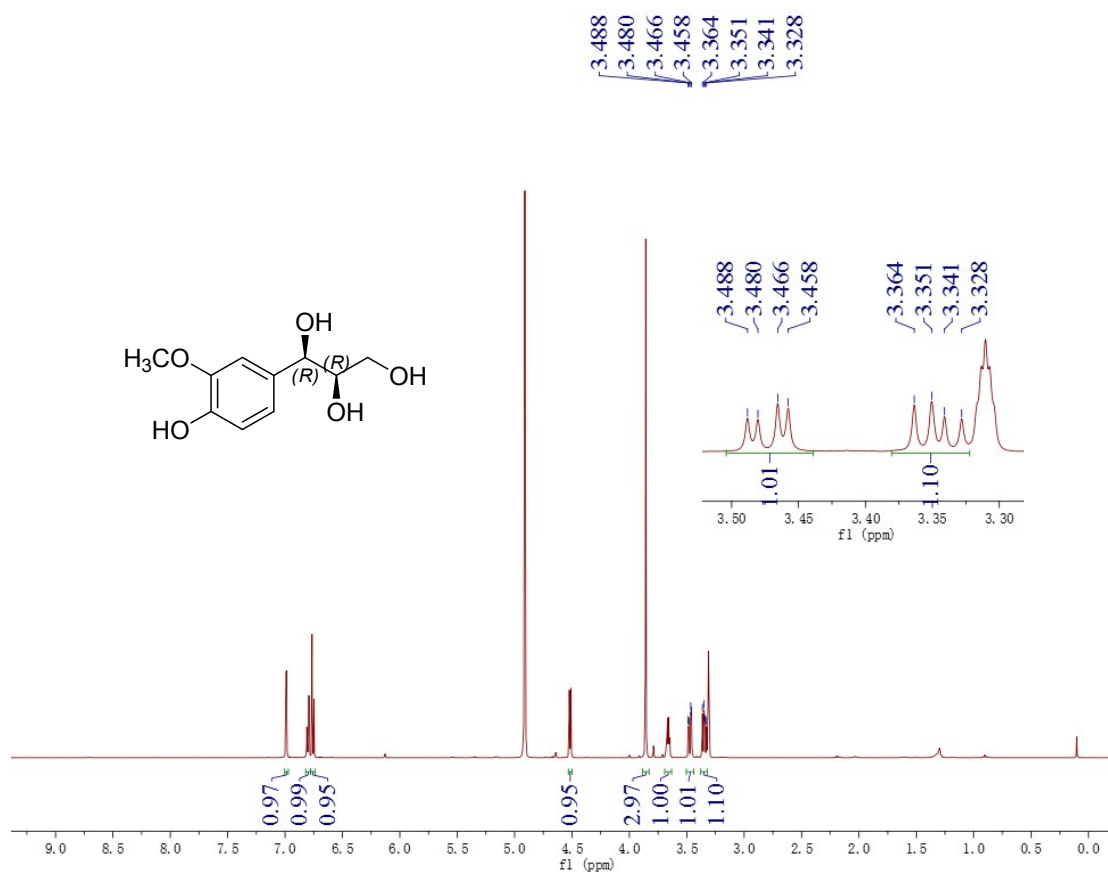


Figure S103. The ¹H NMR spectrum of compound **9** in methanol-*d*₄

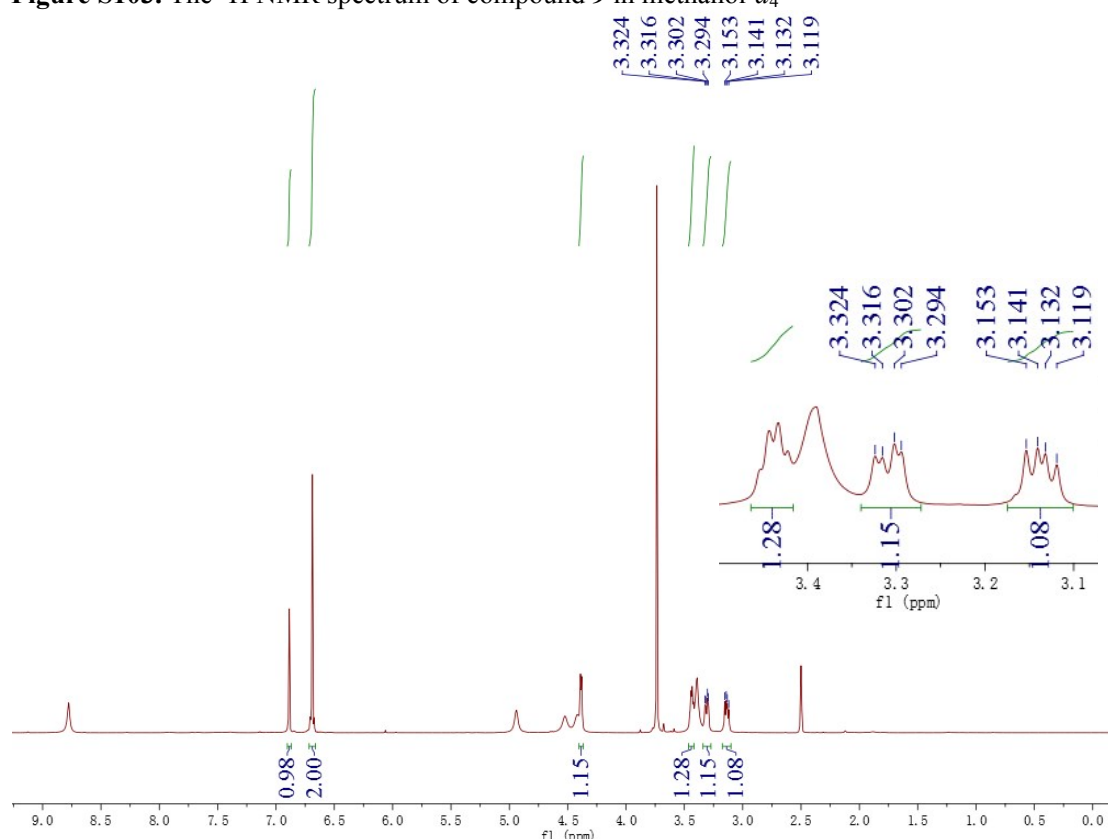


Figure S104. The ¹H NMR spectrum of compound **9** in DMSO-*d*₆

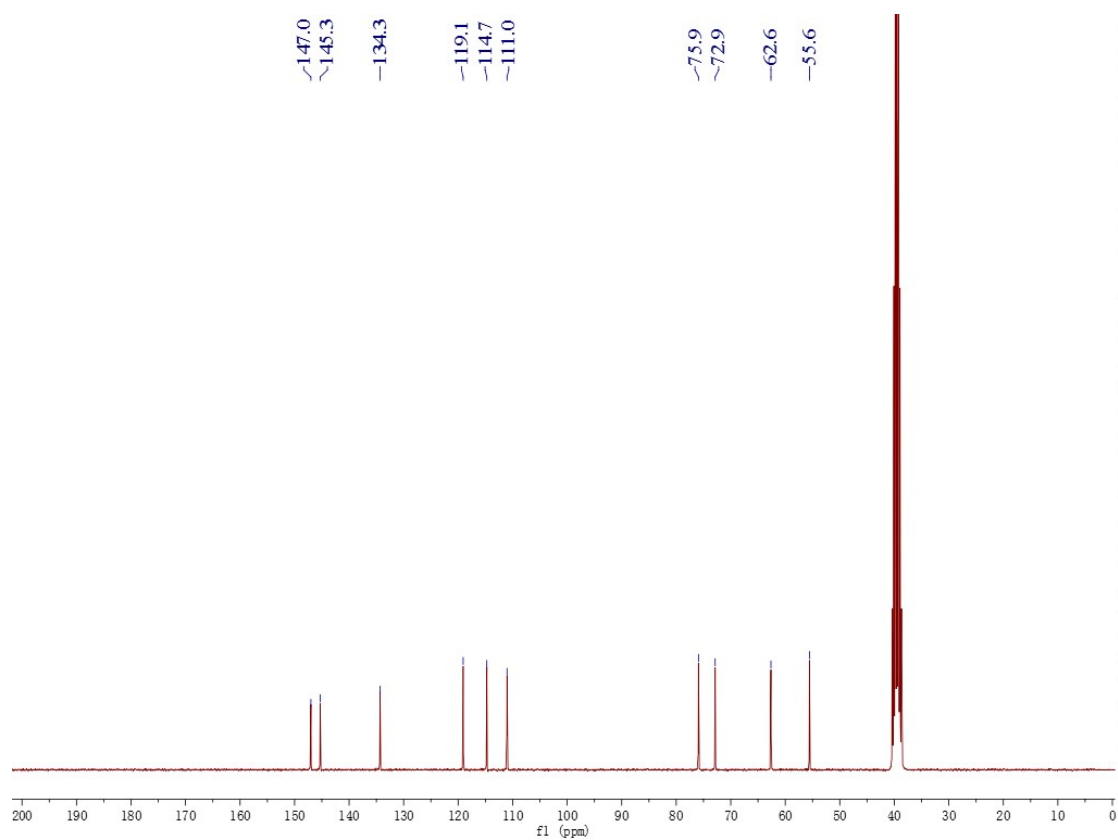


Figure S105. The ¹³C NMR spectrum of compound **9** in DMSO-*d*₆

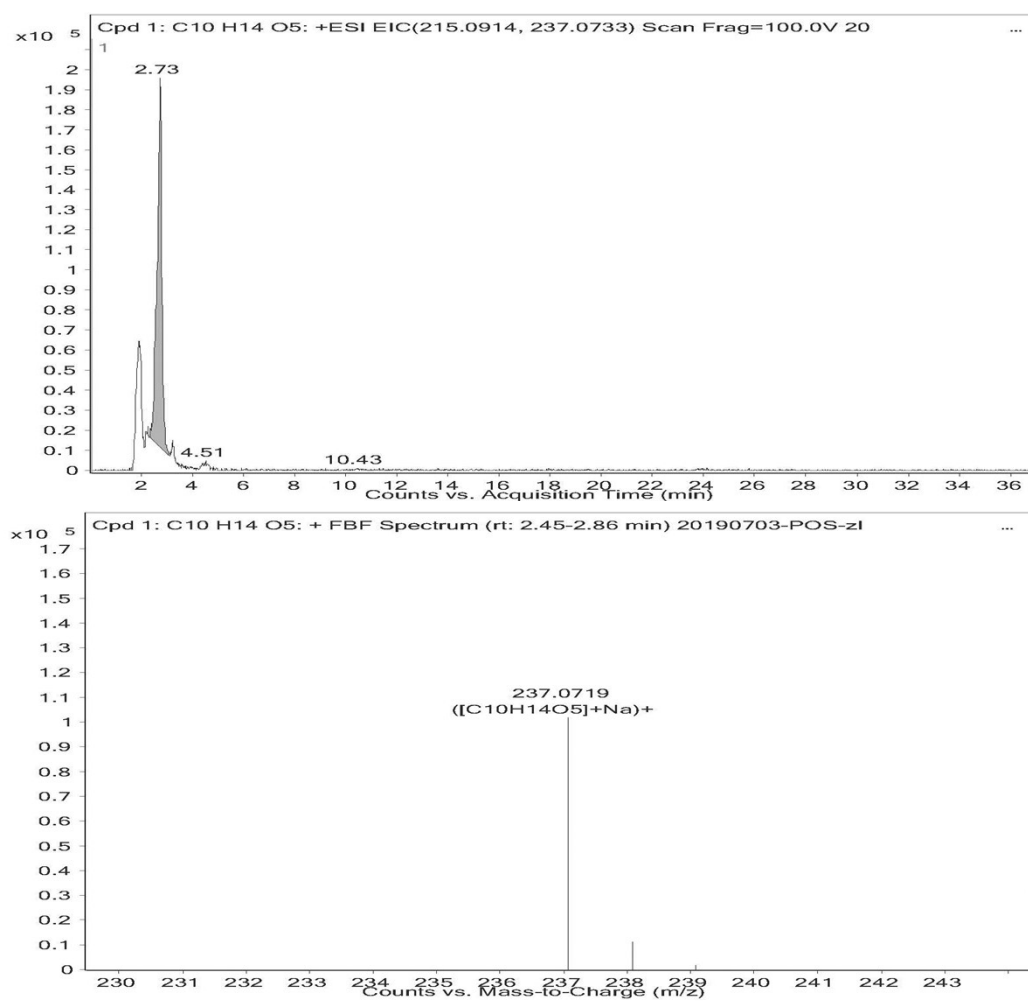


Figure S106. The HR-ESI-MS data of **9**

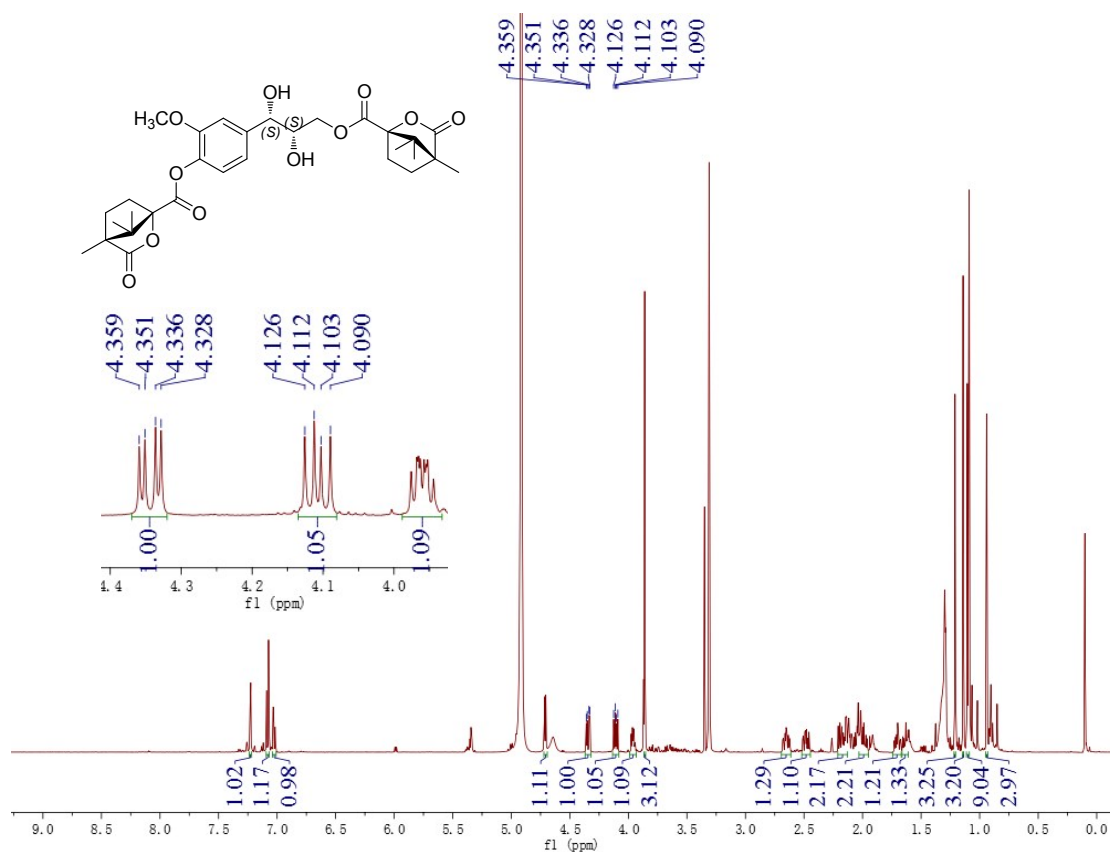
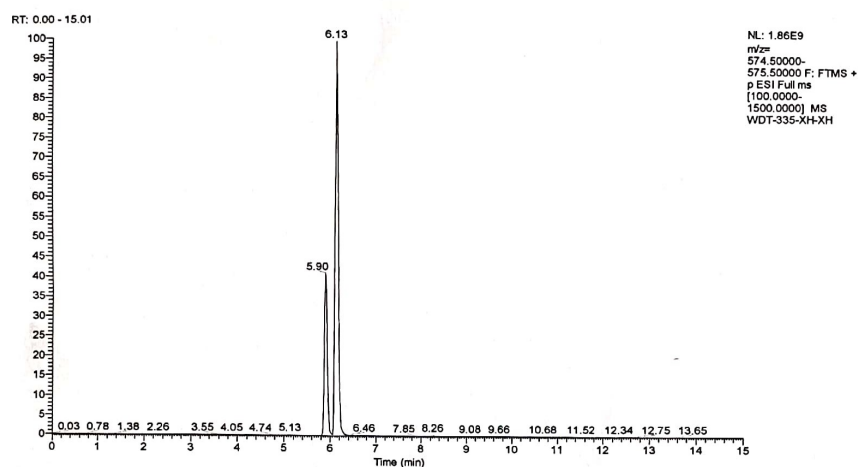


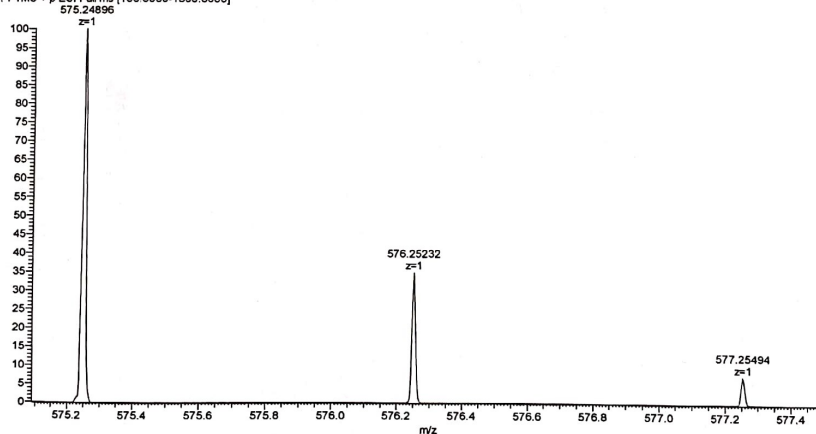
Figure S107. The ^1H NMR spectrum of compound **10a** in methanol- d_4

Thermo Qexactive Focus Report

compound NO. : WDT-335-XH-XH
Method : LCMS(compound)-low



WDT-335-XH-XH #617 RT: 6.11 AV: 1 NL: 1.53E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
575.24896	575.24869	0.47	11.5	C30 H39 O11	M+H

Figure S108. The HR-ESI-MS data of 10a

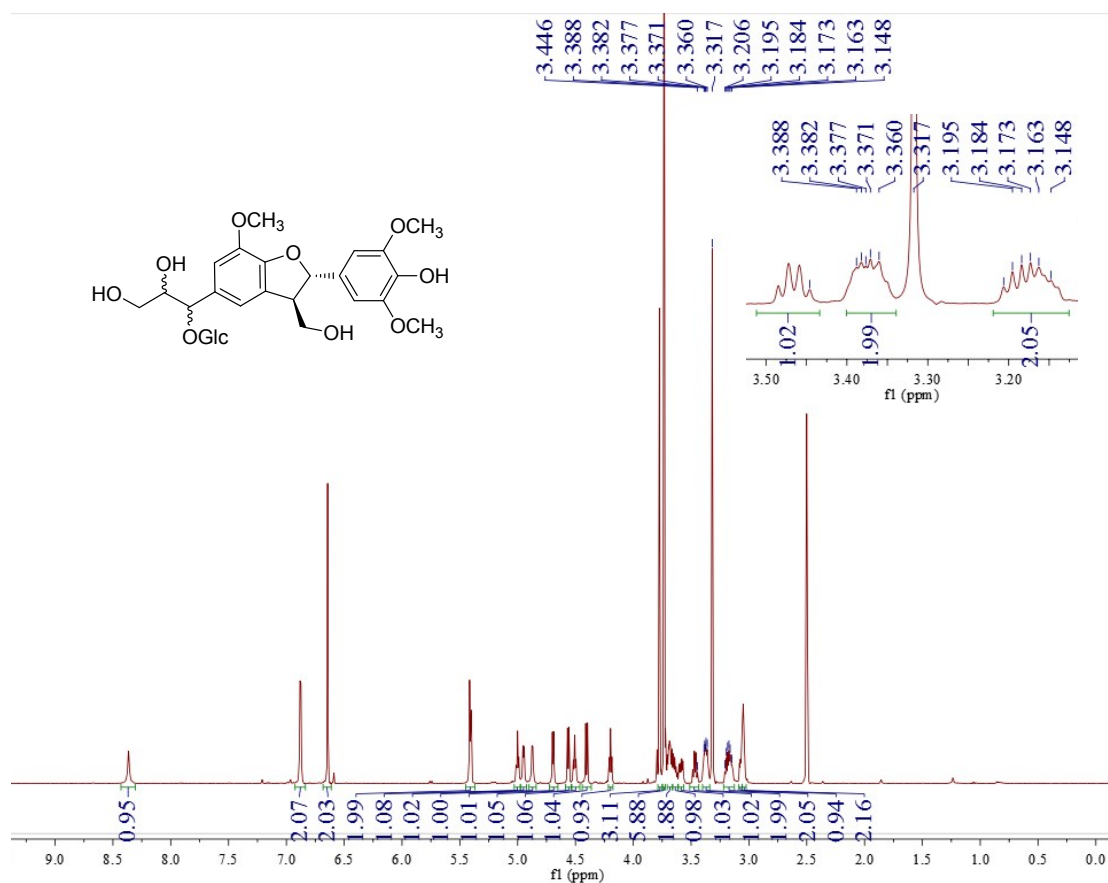


Figure S109. The ¹H NMR spectrum of compound 11 in DMSO-*d*₆

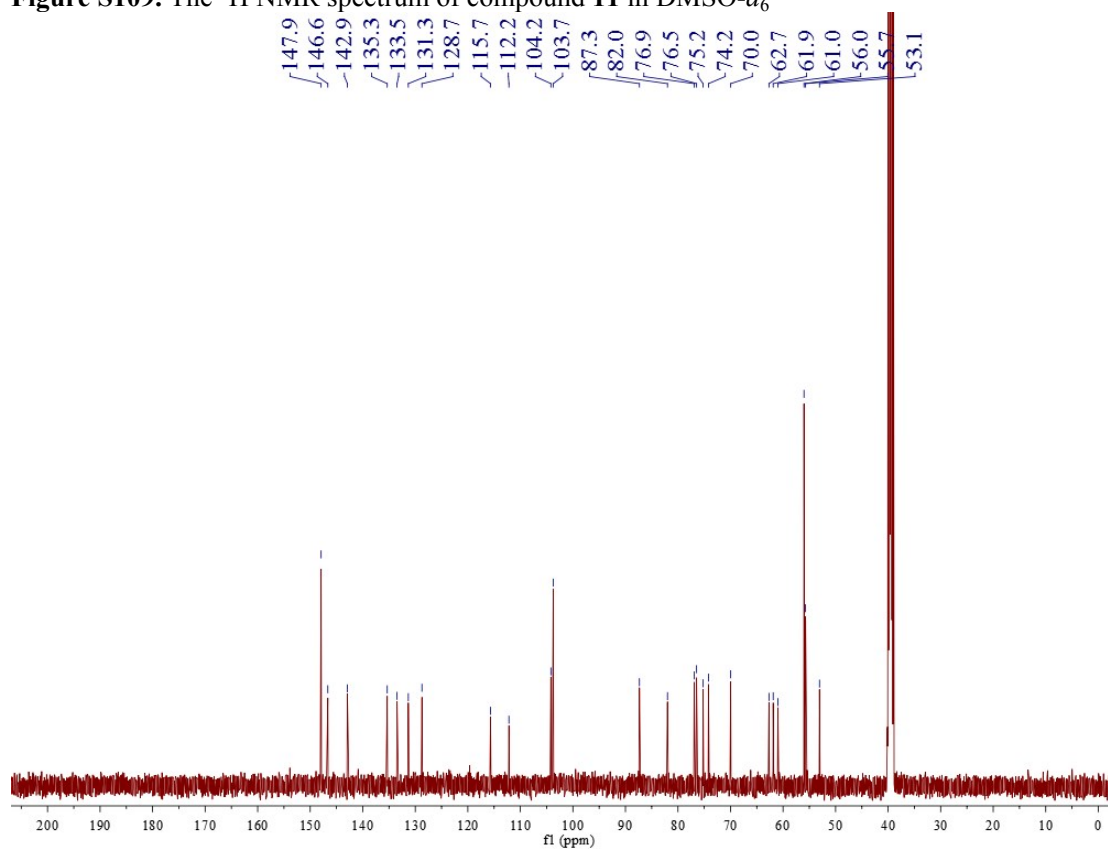


Figure S110. The ¹³C NMR spectrum of compound 11 in DMSO-*d*₆

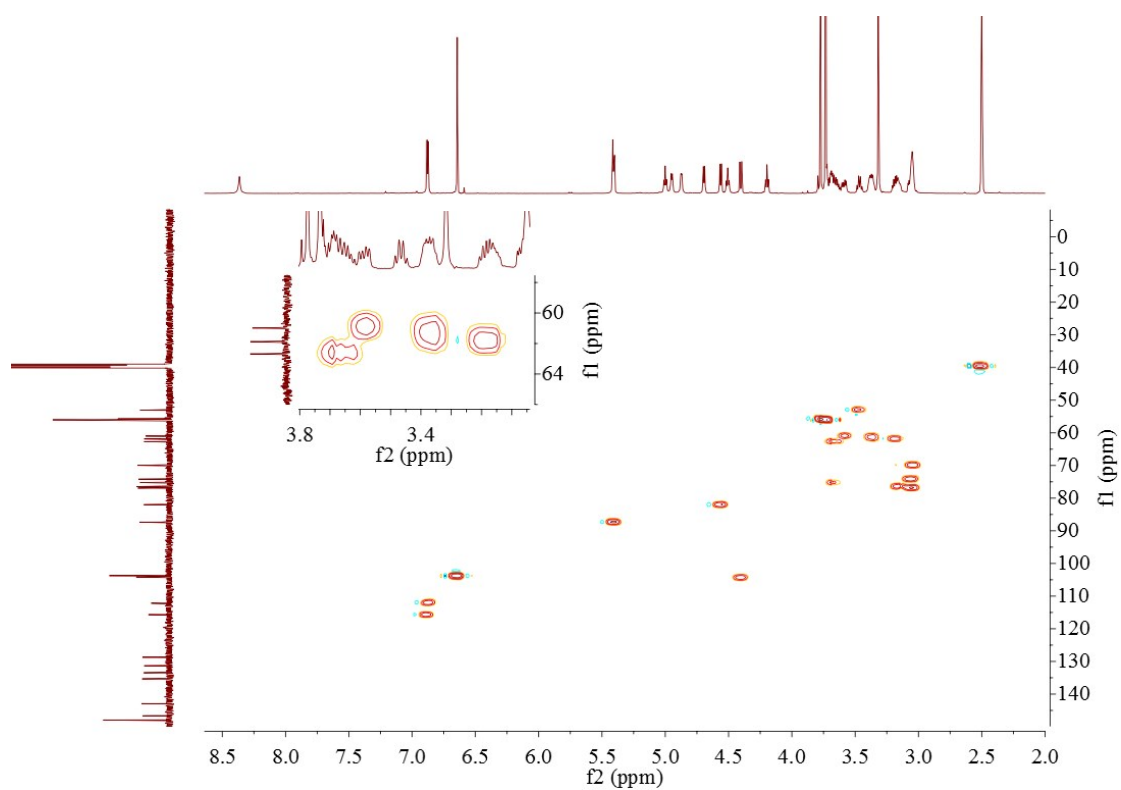


Figure S111. The HSQC spectrum of compound **11** in DMSO- d_6

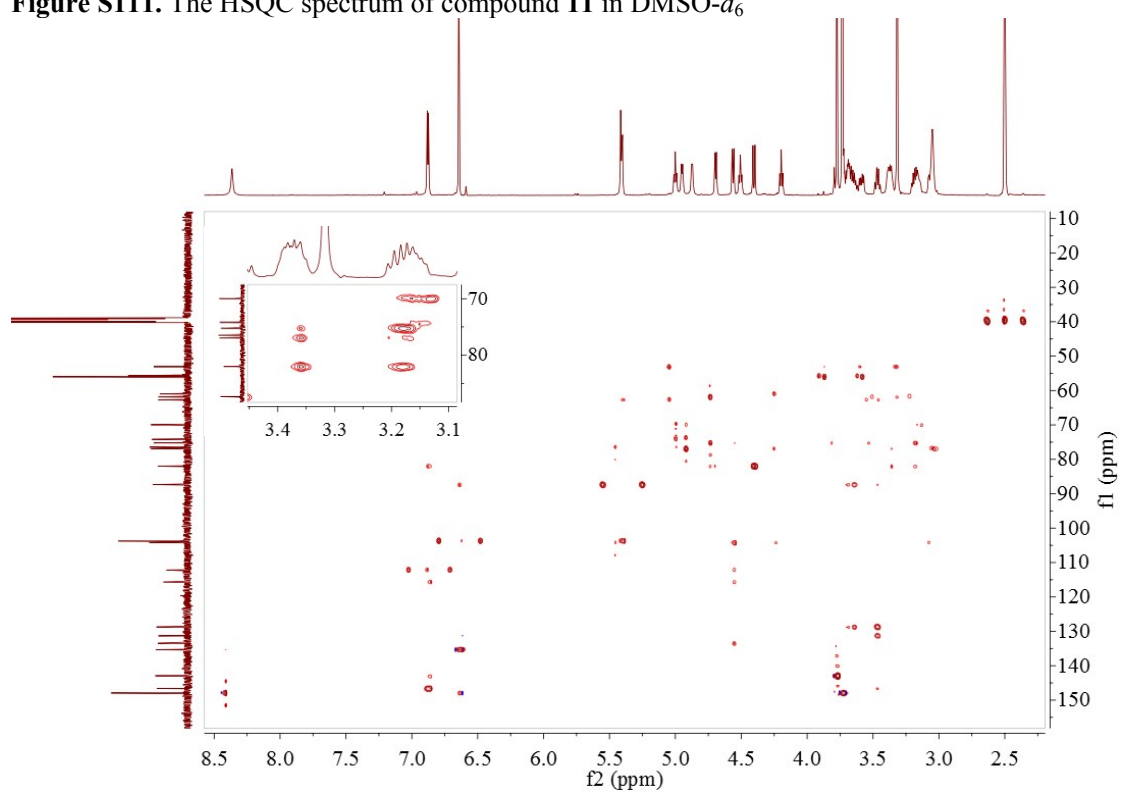


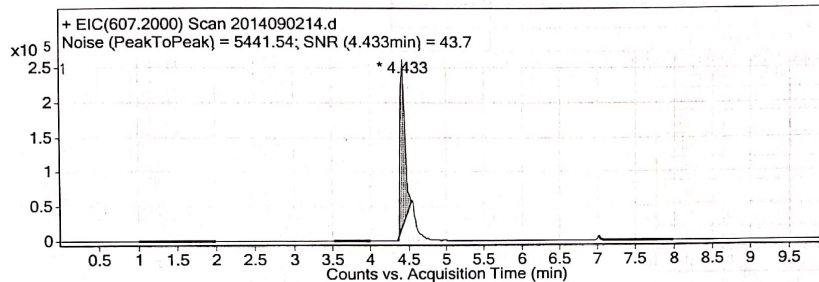
Figure S112. The HMBC spectrum of compound **11** in DMSO- d_6

Qualitative Analysis Report

Data Filename	2014090214.d	Sample Name	DGP-35
Sample Type	Sample	Position	P1-C8
Instrument Name	Instrument 1	User Name	
Acq Method	TEST LCMS.m	IRM Calibration Status	Success
DA Method	TEST LCMS.m	Comment	

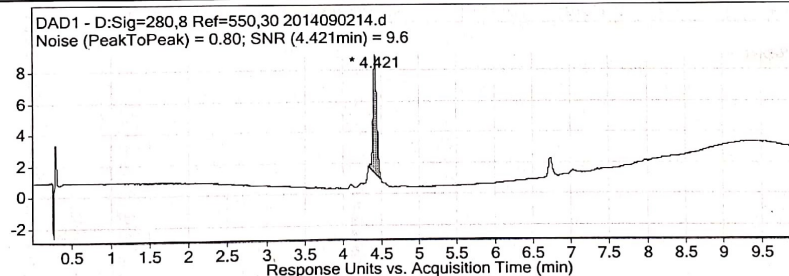
User Chromatograms

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	4.352	4.433	4.546	237708	1176995	100	43.7



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	4.335	4.421	4.498	7.72	25.57	100	9.6

User Spectra

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI

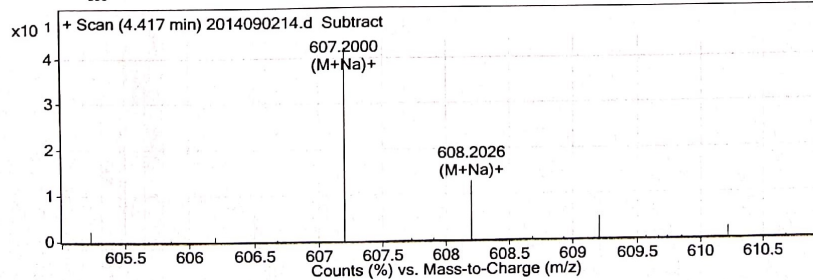


Figure S113. The HR-ESI-MS data of 11

Synthesis procedures

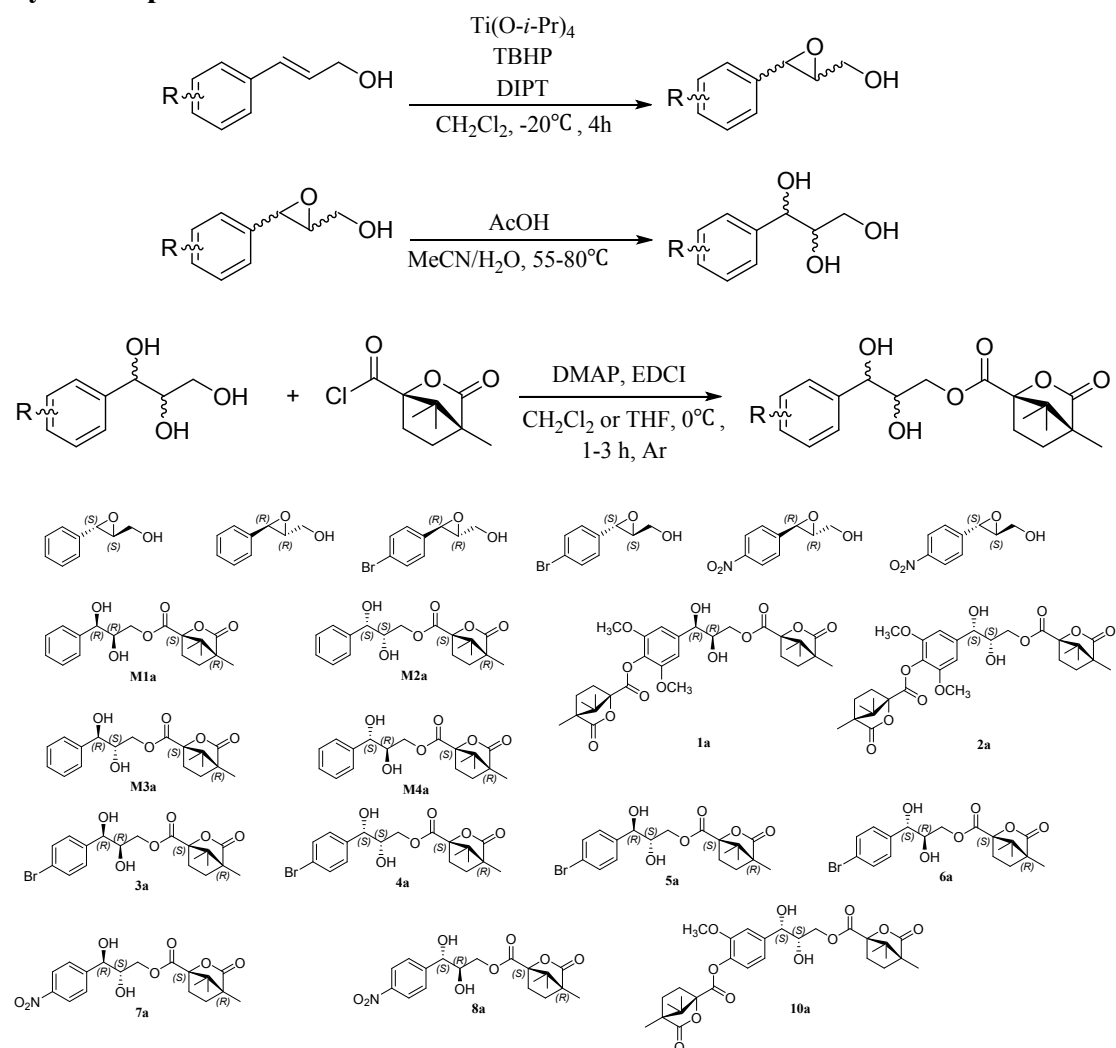


Figure S114. Structures of epoxides and compounds **M1a-M4a**, **1a-8a**, and **10a**.

Table 1. $\Delta\delta_{\text{H3a-H3b}}$ values (ppm) of **1a–8a**, and **10a** in different solvents (^1H NMR 500 MHz).

No.	δ_{H3a}	δ_{H3b}	$\Delta\delta_{\text{H3a-H3b}}$	Solvent	Absolute Conf.
1a	4.33	4.16	0.17	methanol- d_4	1 <i>R</i> ,2 <i>R</i>
2a	4.36	4.13	0.23	methanol- d_4	1 <i>S</i> ,2 <i>S</i>
3a	4.26	4.11	0.15	methanol- d_4	1 <i>R</i> ,2 <i>R</i>
	4.12	3.97	0.15	DMSO- d_6	
4a	4.31	4.04	0.27	methanol- d_4	1 <i>S</i> ,2 <i>S</i>
	4.19	3.88	0.31	DMSO- d_6	
5a	4.42	4.31	0.11	methanol- d_4	1 <i>R</i> ,2 <i>S</i>
	4.36	4.18	0.18	DMSO- d_6	
6a	4.37	4.35	0.02	methanol- d_4	1 <i>S</i> ,2 <i>R</i>
	4.28	4.23	0.05	DMSO- d_6	
7a	4.46	4.35	0.11	methanol- d_4	1 <i>R</i> ,2 <i>S</i>
	4.39	4.22	0.17	DMSO- d_6	
8a	4.42	4.39	0.03	methanol- d_4	1 <i>S</i> ,2 <i>R</i>
	4.31	4.26	0.05	DMSO- d_6	
10a	4.34	4.11	0.23	methanol- d_4	1 <i>S</i> ,2 <i>S</i>

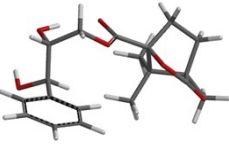
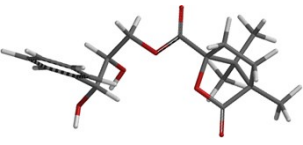
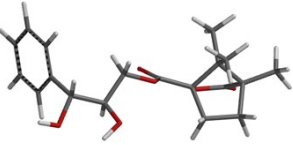
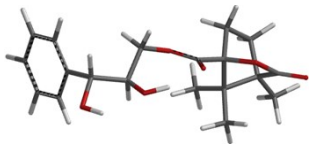
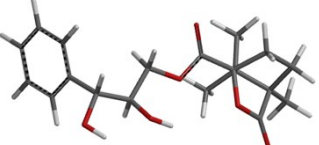
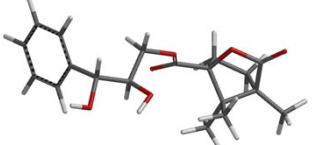
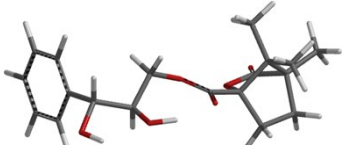
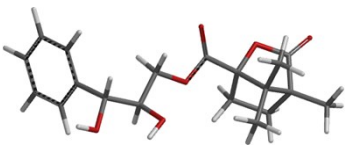
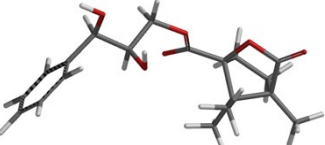
General conformational analyses procedures

The conformational analyses of compounds **M1a-M4a** were performed in the Discovery Studio (version 16.1.0.15350) by using MMFF94s molecular mechanics force field. Conformers with Boltzmann distribution over 1% were chosen for further optimization at the B3LYP/6-311g(d,p) level in SMD solvation model of DMSO by the Gaussian 09 program (Gaussian Inc., Wallingford, CT, USA).

1D NMR calculation for M1a-M4a

Gauge-Independent Atomic Orbital (GIAO) calculations of the optimized conformer's ^1H NMR chemical shifts were completed by density functional theory (DFT) at the B3LYP/6-31g(d,p) level in SMD solvation model of DMSO. The calculated NMR data of the low-energy conformers were averaged according to the Boltzmann distribution theory. The 1D NMR chemical shifts for TMS were calculated by the same protocol and used as the reference.

Table 2. B3LYP/6-311g(d,p) optimized low-energy conformers for M1a

 M1aC1 (18.3%)	 M1aC2 (16.8%)	 M1aC3 (2.3%)
 M1aC4 (7.5%)	 M1aC5 (13.8%)	 M1aC6 (2.6%)
 M1aC7 (8.4%)	 M1aC8 (9.7%)	 M1aC9 (2.5%)
 M1aC10 (1.7%)		

Cartesian coordinates of the low-energy conformers M1aC1

C	-5.54791000	1.36429900	0.02708400
C	-4.93405600	2.58271500	-0.26461900
C	-3.54412800	2.68079700	-0.22097800
C	-2.77366500	1.56716200	0.11232500
C	-3.38108200	0.34024100	0.39886200
C	-4.77717700	0.25084600	0.35553700
C	-2.54333800	-0.87653700	0.73070900
C	-2.31651700	-1.80290900	-0.49388700
C	-1.47519400	-1.19910800	-1.61005900
O	-0.27418300	-0.47739900	-1.17858200
O	-3.19588100	-1.64382600	1.74067300
O	-1.81743900	-3.06303600	-0.03349100
O	1.77924700	1.07377100	-0.91181800
C	2.78799200	1.78937800	-0.32684500
C	3.71082000	0.79166300	0.35698500
C	2.03476500	-0.33209100	-0.60901800
C	4.38950000	0.05948800	-0.84982600
C	3.22780500	-0.73808500	-1.50184800
O	2.85977700	2.98464600	-0.42502900
C	0.79246700	-1.16806300	-0.79900100
O	0.81143800	-2.37245000	-0.61762000
C	2.64348400	-0.25802100	0.83372800
C	1.66018800	0.29366000	1.87646200
C	3.23181300	-1.56856400	1.36105700
C	4.65864800	1.39821300	1.37020200
H	-6.62930600	1.28181800	0.00232900
H	-5.53455300	3.44971800	-0.51758600
H	-3.05772500	3.62567900	-0.43811100
H	-1.69286500	1.65272800	0.14874200
H	-5.25541500	-0.69045900	0.59796100
H	-1.56489000	-0.54378700	1.10030700
H	-3.29505400	-2.01212200	-0.93972400
H	-1.17792000	-1.97656300	-2.31602200
H	-2.04356000	-0.43725100	-2.13836200
H	-2.79951300	-2.52508100	1.66742000
H	-0.84871900	-3.03730000	-0.11380200
H	5.17794600	-0.59807700	-0.48158100
H	4.84713800	0.77319100	-1.53718100
H	3.38925200	-1.81463400	-1.47471200
H	3.03134600	-0.44648300	-2.53429000
H	0.87140600	-0.43611600	2.08070200
H	2.18290100	0.47748700	2.81832100
H	1.18254100	1.22747700	1.57388300
H	2.43449200	-2.28679100	1.56356100
H	3.74979700	-1.37623400	2.30461400
H	3.94067300	-2.03995200	0.68140600
H	4.11846700	1.89573700	2.17937800
H	5.30245600	0.63059000	1.80667900
H	5.30094600	2.14226400	0.89178400

Cartesian coordinates of the low-energy conformers M1aC2

C	-3.78568000	-2.55295100	0.04802200
C	-5.12120200	-2.35414300	0.39479200
C	-5.67114100	-1.07379400	0.31943500
C	-4.88891900	0.00161400	-0.09578200
C	-3.54588600	-0.18887600	-0.44211900
C	-3.00412500	-1.47626800	-0.36992100
C	-2.68480300	0.97980800	-0.87645900
C	-2.23457500	1.88657100	0.28626000
C	-1.35640400	1.20811100	1.31565700
O	-0.23220200	0.58874800	0.63830500
O	-3.39069600	1.87873900	-1.75200800
O	-1.52836700	3.00973500	-0.23138900
O	1.50395900	-0.79985900	-0.74323700
C	2.64141600	-0.85536900	-1.49910700
C	3.80838100	-0.50376200	-0.58705500
C	1.91728000	-0.42486800	0.60958100
C	3.89940500	-1.75128800	0.35539700
C	2.59506100	-1.67701200	1.19487700
O	2.62178400	-1.17388100	-2.65789700
C	0.76063200	0.13804600	1.40560300
O	0.78047500	0.20198200	2.61413100
C	3.10583200	0.56063200	0.32772600
C	2.67828600	1.83007600	-0.42343200
C	3.90016200	0.96931000	1.57061000
C	5.08571400	-0.13080300	-1.30965900
H	-3.35344700	-3.54655500	0.09543400
H	-5.73160400	-3.19129200	0.71529900
H	-6.71127600	-0.91323800	0.58199600
H	-5.32345600	0.99170100	-0.17033100
H	-1.96710400	-1.63584100	-0.64608100
H	-1.78912200	0.60469300	-1.38005300
H	-3.13653900	2.21916300	0.82220900
H	-0.98563500	1.94861500	2.02487300
H	-1.90788300	0.44291100	1.86373600
H	-3.50586600	1.43731600	-2.60247500
H	-2.02143900	3.27652000	-1.01928500
H	4.79137400	-1.67393400	0.97833600
H	3.97767200	-2.67487700	-0.22145900
H	2.78522100	-1.55614300	2.25984300
H	1.94925200	-2.54570100	1.06058400
H	2.09029400	2.48172900	0.22846100
H	3.56321700	2.39089800	-0.73471700
H	2.07958300	1.62731500	-1.31369000
H	3.28008300	1.58417100	2.22800600
H	4.76058600	1.57438200	1.27263000
H	4.27145000	0.12737500	2.15414500
H	4.94000100	0.73442300	-1.96101100
H	5.87846300	0.10409100	-0.59493900
H	5.42995000	-0.96165100	-1.93130400

Cartesian coordinates of the low-energy conformers M1aC3

C	4.98397400	-1.89916500	-1.16527300
C	5.27388800	-2.56502600	0.02632000
C	5.04583200	-1.92917300	1.24561100
C	4.52721900	-0.63478000	1.27235300
C	4.22572700	0.03638100	0.08311700
C	4.46281000	-0.60773900	-1.13728000
C	3.64257100	1.43475100	0.11608000
C	2.13062000	1.49546800	-0.19214400
C	1.30471000	0.83524900	0.89643900
O	-0.10402500	0.85882800	0.54844300
O	4.22745100	2.28433900	-0.88615400
O	1.72119400	2.85510700	-0.28985100
O	-2.58007800	-1.10544100	-1.13987000
C	-3.93741100	-1.14970900	-1.00375400
C	-4.33108000	-0.03911600	-0.04148100
C	-2.10589300	-0.01275700	-0.29264800
C	-4.05573700	1.25807900	-0.87503000
C	-2.50967700	1.28188300	-1.02589200
O	-4.61446000	-1.93898900	-1.60740200
C	-0.63309400	-0.23892300	-0.01695800
O	-0.03348800	-1.25897500	-0.24756500
C	-3.09327900	-0.08870400	0.92449600
C	-2.97816600	-1.40213500	1.71118200
C	-3.00566400	1.08193900	1.90690000
C	-5.72632600	-0.16341400	0.53231300
H	5.16456300	-2.38664500	-2.11730100
H	5.67966800	-3.57045400	0.00352500
H	5.27720400	-2.43700500	2.17564000
H	4.35988500	-0.13909500	2.22339700
H	4.25343500	-0.08702300	-2.06446100
H	3.80271800	1.87202000	1.10869000
H	1.95510000	0.97593700	-1.14509900
H	1.61684500	-0.19381000	1.06145500
H	1.37762900	1.40320500	1.82356700
H	5.13713100	2.47331700	-0.62483600
H	2.41873600	3.29065700	-0.79896200
H	-4.42547800	2.12720800	-0.32965400
H	-4.57333500	1.22581700	-1.83578000
H	-2.05474400	2.15560200	-0.56254300
H	-2.17988100	1.23653400	-2.06477100
H	-2.04685200	-1.42392800	2.28447700
H	-3.80167900	-1.48110200	2.42540200
H	-2.99886900	-2.29049400	1.07694600
H	-2.06011200	1.04869700	2.45261700
H	-3.81124000	1.00013500	2.64196300
H	-3.08434400	2.06064400	1.43474500
H	-5.85095800	-1.09569600	1.08871300
H	-5.94418500	0.67034300	1.20434500
H	-6.47014300	-0.15245900	-0.26898900

Cartesian coordinates of the low-energy conformers M1aC4

C	4.93954300	1.98986900	1.11860700
C	5.41210600	2.49530100	-0.09346300
C	5.28843700	1.73263300	-1.25318300
C	4.69310300	0.47194100	-1.19998100
C	4.20744800	-0.03761200	0.00766600
C	4.34143000	0.73278700	1.16902000
C	3.54295900	-1.39690200	0.06047500
C	2.00069400	-1.31996500	0.18354500
C	1.35344900	-0.82290600	-1.10434600
O	0.03906700	-0.20957300	-0.90599200
O	4.04868400	-2.11339900	1.18648500
O	1.58781900	-2.64549100	0.52550800
O	-3.40693000	-1.12167500	-0.58733000
C	-4.48135000	-0.44503600	-0.08096500
C	-4.01587700	0.96874400	0.23314700
C	-2.28722600	-0.18508600	-0.59785800
C	-3.79442500	1.58316700	-1.18980000
C	-2.57914000	0.79523000	-1.75134100
O	-5.56507500	-0.95426600	0.01867200
C	-1.00958100	-0.99220700	-0.65191500
O	-0.95041000	-2.18929100	-0.46285000
C	-2.54842600	0.65823800	0.70169600
C	-2.47657300	-0.17893600	1.98632100
C	-1.65902600	1.89233000	0.86919500
C	-4.93414100	1.75015000	1.14906800
H	5.03960500	2.57519600	2.02633500
H	5.87862200	3.47360100	-0.13117400
H	5.66135700	2.11294500	-2.19796900
H	4.61082700	-0.12337900	-2.10356700
H	3.99060500	0.33566400	2.11411700
H	3.77551800	-1.94425900	-0.86393300
H	1.75161200	-0.62652200	0.99791400
H	1.93303000	-0.01446300	-1.54344600
H	1.25767100	-1.63392600	-1.82882500
H	3.41555200	-2.82969700	1.33558300
H	0.65738400	-2.73970200	0.26468000
H	-3.58146300	2.64898200	-1.09949500
H	-4.68787100	1.47537500	-1.80736700
H	-1.72365500	1.43695900	-1.95389800
H	-2.81164500	0.23782500	-2.65961100
H	-1.44204300	-0.46250900	2.20037900
H	-2.83414700	0.41126500	2.83370800
H	-3.07052300	-1.09412900	1.94228900
H	-0.63240600	1.59367200	1.09304900
H	-2.01891200	2.48279800	1.71612400
H	-1.63327100	2.54361600	-0.00403400
H	-5.05699800	1.25280100	2.11429700
H	-4.53962400	2.75392900	1.32516300
H	-5.92490000	1.85306900	0.69840300

Cartesian coordinates of the low-energy conformers M1aC5

C	-5.33619900	-1.98065700	-0.58502800
C	-5.64419800	-2.21475700	0.75400000
C	-5.29811000	-1.26687700	1.71807600
C	-4.64260500	-0.09537700	1.34580000
C	-4.32393400	0.14387900	0.00413600
C	-4.68340400	-0.80531900	-0.95681800
C	-3.59150300	1.40576300	-0.39920500
C	-2.08501600	1.35362800	-0.08211000
C	-1.32755600	0.31580500	-0.89000700
O	0.06603500	0.46986700	-0.50217500
O	-4.15836100	2.51685200	0.29533300
O	-1.59571200	2.66859700	-0.37785500
O	2.49607700	1.20215000	0.06689300
C	3.64606300	1.12141100	0.80155000
C	4.27666500	-0.23258200	0.50754800
C	2.38164900	-0.05471900	-0.67177400
C	4.76157600	-0.07680600	-0.97279800
C	3.44273000	0.02301200	-1.78576600
O	4.02189200	2.02723400	1.49621300
C	0.96274600	-0.29071200	-1.13813600
O	0.68751200	-1.10889300	-1.98468000
C	2.97113100	-1.09163200	0.34843600
C	2.15418100	-1.20915100	1.64331500
C	3.18735900	-2.49548700	-0.22125500
C	5.33574600	-0.66782200	1.49835800
H	-5.61078200	-2.70727800	-1.34192200
H	-6.15643000	-3.12545800	1.04459700
H	-5.54148400	-1.43977700	2.76092300
H	-4.38810600	0.64673100	2.09298700
H	-4.45518200	-0.62157400	-2.00185300
H	-3.70033700	1.54932400	-1.48289600
H	-1.96053900	1.14269500	0.98732500
H	-1.65340100	-0.69984100	-0.66424200
H	-1.41900000	0.50069600	-1.96157900
H	-3.49918400	3.22173700	0.22709900
H	-0.67701000	2.71143400	-0.08509600
H	5.35323600	-0.94830300	-1.25648900
H	5.39515600	0.80481700	-1.08744700
H	3.32315800	-0.79250000	-2.49711800
H	3.34196300	0.96528400	-2.32602800
H	1.20277700	-1.71352300	1.45185300
H	2.70191400	-1.81424200	2.37022900
H	1.93582200	-0.24592400	2.10859100
H	2.22497600	-2.97612000	-0.41399400
H	3.71625800	-3.10785300	0.51412800
H	3.76129900	-2.51606500	-1.14733200
H	4.93755700	-0.73415200	2.51384300
H	5.74194300	-1.64424600	1.22299400
H	6.16192100	0.04809200	1.51166700

Cartesian coordinates of the low-energy conformers M1aC6

C	-5.05928900	-1.58431200	1.25825300
C	-5.61567000	-2.14545600	0.10805400
C	-5.44979200	-1.50828300	-1.12060400
C	-4.72852800	-0.31716500	-1.19806700
C	-4.16132000	0.24787800	-0.05146000
C	-4.33683800	-0.39609600	1.17932600
C	-3.35959800	1.53066300	-0.14288700
C	-1.83362700	1.32919000	-0.03211000
C	-1.28035500	0.54564400	-1.21017000
O	0.15889100	0.37411800	-1.11461300
O	-3.65927200	2.43170000	0.93768900
O	-1.19089100	2.59989500	-0.00552400
O	2.73106600	-0.05996700	-1.46440500
C	4.02516700	0.22239700	-1.12943300
C	4.23308600	-0.23620300	0.30767500
C	2.12204700	-0.68380600	-0.28945900
C	4.19579200	-1.79579700	0.18523000
C	2.72623900	-2.09832300	-0.21414600
O	4.79520500	0.71051500	-1.91299000
C	0.61064200	-0.62004000	-0.34785100
O	-0.08819600	-1.38646200	0.27689600
C	2.81133400	0.09335900	0.88703500
C	2.49205000	1.59540900	0.89946400
C	2.53178200	-0.47951300	2.27818200
C	5.46006300	0.33799700	0.98398700
H	-5.18952600	-2.07269400	2.21799500
H	-6.17949000	-3.06970700	0.17099400
H	-5.88668400	-1.93358900	-2.01759200
H	-4.60781100	0.18074900	-2.15492000
H	-3.91989200	0.04582100	2.07682500
H	-3.56694500	2.02245400	-1.10062300
H	-1.63335600	0.78225500	0.89794800
H	-1.75259100	-0.43260900	-1.28497500
H	-1.42310200	1.10059300	-2.13663600
H	-4.55024200	2.77679600	0.80117100
H	-1.72009600	3.13545400	0.60155200
H	4.45951500	-2.24262400	1.14475200
H	4.91681200	-2.15114700	-0.55337500
H	2.20544600	-2.70640200	0.52327800
H	2.63829400	-2.58950100	-1.18432800
H	1.44069400	1.76718200	1.14308000
H	3.09501500	2.09234400	1.66375600
H	2.69042300	2.08836900	-0.05414300
H	1.48931500	-0.30207700	2.55591800
H	3.15665800	0.03250400	3.01502800
H	2.72325600	-1.54868700	2.36421500
H	5.43310400	1.43021900	1.01011300
H	5.54245100	-0.02998600	2.00985400
H	6.36520700	0.04063100	0.44757000

Cartesian coordinates of the low-energy conformers M1aC7

C	-5.12346100	2.07666500	1.19701900
C	-5.43365800	2.61438700	-0.05052000
C	-5.17778100	1.87259000	-1.20485900
C	-4.60916200	0.60452900	-1.11156500
C	-4.28852800	0.05911300	0.13742200
C	-4.55823300	0.80426200	1.28872500
C	-3.65844200	-1.31430000	0.23566000
C	-2.16387500	-1.33134200	-0.17169300
C	-1.28704200	-0.64519000	0.87074200
O	-0.03610600	-0.10786300	0.33161900
O	-4.37030200	-2.20950600	-0.61792000
O	-1.83768500	-2.71410400	-0.32925700
O	2.03240800	1.16289400	-0.60448800
C	3.25707100	1.75851200	-0.47813600
C	4.26028400	0.66403300	-0.14625900
C	2.23436100	-0.26243200	-0.36134300
C	4.34963000	-0.14362400	-1.48485200
C	2.94903000	-0.80179500	-1.61552400
O	3.41247000	2.93692200	-0.65301400
C	0.93736100	-0.94492100	0.00140300
O	0.84419700	-2.15962400	0.00316000
C	3.34995300	-0.25505800	0.74494100
C	2.89936600	0.40985800	2.05379500
C	3.94190500	-1.62826000	1.06979000
C	5.57714900	1.16346500	0.40995000
H	-5.32757900	2.64220800	2.09972400
H	-5.87670100	3.60154900	-0.12422700
H	-5.42351500	2.28229300	-2.17872300
H	-4.42539400	0.02437500	-2.00812900
H	-4.32951900	0.38465900	2.26309100
H	-3.72302300	-1.66196200	1.27622100
H	-2.05667000	-0.80478400	-1.12972800
H	-1.77394800	0.24263400	1.26716100
H	-1.05486300	-1.32802000	1.69016300
H	-3.77635900	-2.96262000	-0.74582400
H	-0.87144300	-2.79252800	-0.27414300
H	5.14426600	-0.88714100	-1.41214300
H	4.58623000	0.51290800	-2.32423100
H	2.99206500	-1.88964700	-1.60463500
H	2.40979600	-0.48984400	-2.51097900
H	2.19473600	-0.23387000	2.58797500
H	3.76266200	0.55863800	2.70710100
H	2.42040600	1.37967500	1.90558300
H	3.19020400	-2.25865400	1.55099000
H	4.76887000	-1.50852100	1.77481100
H	4.31964200	-2.16358100	0.19944900
H	5.43223500	1.74347500	1.32468800
H	6.24476200	0.32786800	0.63403800
H	6.07772800	1.80821000	-0.31720000

Cartesian coordinates of the low-energy conformers M1aC8

C	-5.50515700	-1.92128000	-0.73048400
C	-5.88561000	-2.13306100	0.59351700
C	-5.51950800	-1.21003000	1.57427200
C	-4.77201500	-0.08512700	1.23371500
C	-4.37999500	0.13178800	-0.09303500
C	-4.75861200	-0.79346300	-1.07060900
C	-3.55264000	1.34505200	-0.46589600
C	-2.08291500	1.27676600	-0.00168200
C	-1.31535600	0.16737500	-0.68701200
O	-0.01176700	0.09305500	-0.05453000
O	-4.04509200	2.54493800	0.15744300
O	-1.43845800	2.51006200	-0.30346900
O	3.09872600	-1.65684000	-0.40191500
C	4.38057400	-1.26435400	-0.14422900
C	4.30920400	0.09742300	0.53052200
C	2.22543800	-0.58778100	0.07916400
C	3.70699300	-0.24342800	1.93517000
C	2.25427700	-0.69391500	1.61732300
O	5.32672900	-1.95709700	-0.41002500
C	0.88954100	-0.71975400	-0.62366900
O	0.66973900	-1.42475000	-1.57699700
C	3.07301100	0.69585800	-0.23203500
C	3.31775400	0.90615900	-1.73319200
C	2.52426000	1.99603200	0.36217900
C	5.61267400	0.86750600	0.54724700
H	-5.79421300	-2.62896500	-1.49981400
H	-6.46920000	-3.00759100	0.85952600
H	-5.81826500	-1.36648200	2.60518300
H	-4.50355700	0.63812700	1.99500200
H	-4.47007100	-0.62726300	-2.10369600
H	-3.55871500	1.46798900	-1.55514500
H	-2.07662300	1.09838400	1.08300100
H	-1.81565200	-0.79469400	-0.57312800
H	-1.18662100	0.38372000	-1.74886500
H	-4.88412900	2.77550000	-0.26006200
H	-2.07031300	3.19521000	-0.04510400
H	3.73009900	0.64391600	2.56907700
H	4.28967900	-1.02021300	2.43412900
H	1.50756600	-0.04607900	2.07294200
H	2.04781300	-1.72058100	1.92254300
H	2.39553100	1.22272200	-2.22891800
H	4.05459100	1.69935200	-1.88255700
H	3.68059800	0.01189200	-2.24368500
H	1.57214300	2.25569200	-0.10533100
H	3.22722200	2.80954700	0.16292100
H	2.36087200	1.95410400	1.43881700
H	5.99027200	1.04131700	-0.46348500
H	5.48255100	1.83559800	1.03762000
H	6.37789800	0.31325700	1.09736100

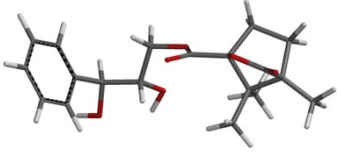
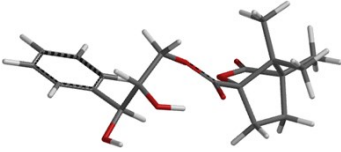
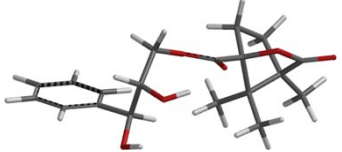
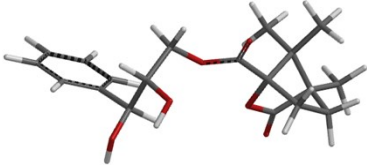
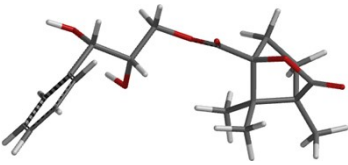
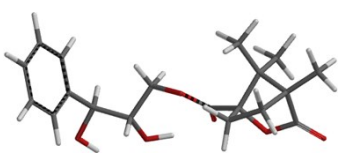
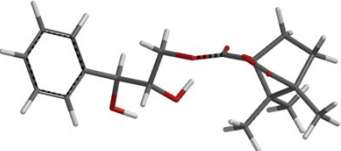
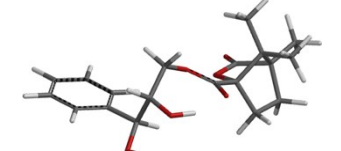
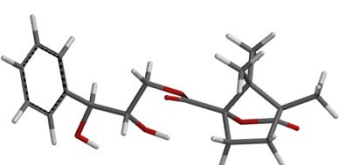
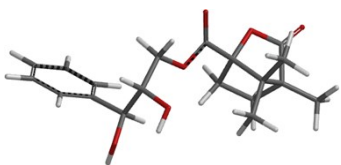
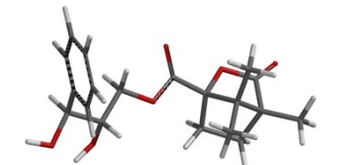
Cartesian coordinates of the low-energy conformers M1aC9

C	-5.64063700	1.75485400	0.91610100
C	-6.22327500	1.89561600	-0.34367200
C	-5.87932600	1.01052000	-1.36440600
C	-4.95358000	-0.00611100	-1.13105500
C	-4.36450100	-0.15280200	0.12858600
C	-4.72067100	0.73482400	1.14984000
C	-3.33036800	-1.22927100	0.40117600
C	-1.89166800	-0.75969600	0.09076500
C	-0.89186200	-1.76572200	0.66697600
O	0.48333500	-1.42102400	0.35663700
O	-3.51504400	-2.39747800	-0.40892200
O	-1.70761000	-0.56802400	-1.30503600
O	3.07902900	-1.30991800	-0.04002000
C	4.15765600	-0.81167300	-0.71479300
C	4.24793800	0.67406600	-0.39331100
C	2.49172800	-0.18950800	0.69482800
C	4.69015600	0.68121700	1.10785100
C	3.46290600	0.09468600	1.85597200
O	4.86837500	-1.51097300	-1.38663800
C	1.06207500	-0.47697500	1.09989600
O	0.51959800	0.12761400	1.99842100
C	2.71583600	1.00504000	-0.29734100
C	1.97234800	0.83984500	-1.63046600
C	2.38736200	2.38308000	0.28079600
C	5.12027600	1.47448000	-1.33714500
H	-5.90876900	2.43360100	1.71850500
H	-6.94332600	2.68580000	-0.52604000
H	-6.33030700	1.11147100	-2.34578500
H	-4.69387400	-0.69244500	-1.92762000
H	-4.27764600	0.62247600	2.13463900
H	-3.37873000	-1.49444900	1.46411900
H	-1.73387200	0.21200300	0.55871200
H	-1.00832400	-1.83629600	1.74947300
H	-1.03004400	-2.74854100	0.21954400
H	-4.43008400	-2.69032500	-0.31693800
H	-2.03698000	-1.36941500	-1.73500000
H	4.90721800	1.70394500	1.41915100
H	5.59710700	0.09171200	1.25490100
H	3.02708200	0.79530000	2.56605200
H	3.68584800	-0.83297200	2.38522700
H	0.89164700	0.90006700	-1.48109400
H	2.25764800	1.64474500	-2.31277900
H	2.18168900	-0.10904000	-2.12879300
H	1.30721700	2.49102300	0.41001900
H	2.71055500	3.15776200	-0.41981700
H	2.85910100	2.58425100	1.24241800
H	4.76803700	1.40419700	-2.36928800
H	5.13363000	2.52858000	-1.04851600
H	6.14933400	1.10616800	-1.31021400

Cartesian coordinates of the low-energy conformers M1aC10

C	-5.76944900	1.54440400	-1.11012700
C	-6.00151600	2.25728900	0.06692500
C	-5.45203300	1.80586100	1.26575300
C	-4.67356800	0.64880400	1.28560000
C	-4.42810000	-0.06570500	0.10922700
C	-4.98837200	0.39106500	-1.08950400
C	-3.55446100	-1.30095900	0.12851800
C	-2.12195200	-1.04228000	-0.40946000
C	-1.32096400	-0.14594100	0.52272200
O	0.02195200	0.08771800	0.01303200
O	-4.15214300	-2.31317300	-0.67898000
O	-1.48086100	-2.30518400	-0.63192400
O	2.28437600	0.62190800	-1.17010600
C	3.52148300	1.20113000	-1.23005200
C	4.39227800	0.51931600	-0.18424100
C	2.35036900	-0.39488900	-0.12361300
C	4.59866500	-0.91366300	-0.78019000
C	3.18263000	-1.54741900	-0.71832400
O	3.78277800	2.06300100	-2.02566400
C	0.97363600	-0.77525900	0.36725500
O	0.79418900	-1.76569000	1.04687600
C	3.30886400	0.27300800	0.92573000
C	2.74478600	1.56898600	1.52696900
C	3.75148100	-0.64506100	2.06702200
C	5.65754500	1.27135700	0.17031200
H	-6.19973000	1.88642300	-2.04530200
H	-6.61109700	3.15415000	0.04994800
H	-5.63514800	2.34821000	2.18704800
H	-4.25672200	0.29455800	2.22296000
H	-4.82258700	-0.17014900	-2.00136400
H	-3.46422400	-1.65670700	1.16510300
H	-2.19882300	-0.57412400	-1.39482300
H	-1.76875700	0.84395600	0.57793100
H	-1.25551200	-0.57022500	1.52605100
H	-3.43378100	-2.93505900	-0.86738100
H	-0.99182500	-2.54327500	0.16882500
H	5.31785500	-1.46243700	-0.17082400
H	4.99446300	-0.86367500	-1.79639000
H	3.14194500	-2.42839400	-0.07998100
H	2.78855600	-1.81763800	-1.69899600
H	1.91735500	1.34872500	2.20728100
H	3.52020900	2.07204300	2.11005500
H	2.38237400	2.27384300	0.77615600
H	2.90456300	-0.87219200	2.71941300
H	4.50406100	-0.13303500	2.67282500
H	4.17810600	-1.59069700	1.73435900
H	5.43708800	2.27298600	0.54766100
H	6.22720400	0.73323500	0.93207000
H	6.29416700	1.38056800	-0.71163200

Table 3. B3LYP/6-311g(d,p) optimized low-energy conformers for M2a

 M2aC1 (2.4%)	 M2aC2 (27.0%)	 M2aC3 (3.4%)
 M2aC4 (4.3%)	 M2aC5 (2.5%)	 M2aC6 (4.5%)
 M2aC7 (14.6%)	 M2aC8 (27.0%)	 M2aC9 (5.5%)
 M2aC10 (2.0%)	 M2aC11 (4.2%)	 M2aC12 (1.9%)

Cartesian coordinates of the low-energy conformers M2aC1

C	-5.33231900	-1.72142900	0.94870300
C	-5.39357200	-2.35663900	-0.29062900
C	-4.82570000	-1.74525200	-1.40918900
C	-4.19564100	-0.50896300	-1.28778000
C	-4.12500200	0.13334400	-0.04567500
C	-4.70413700	-0.48201800	1.06851300
C	-3.42470600	1.47016400	0.09205600
C	-1.88381900	1.37881300	0.06282900
C	-1.33363100	0.65936700	1.28169200
O	0.11245100	0.55755700	1.21481000
O	-3.73105300	2.35199300	-1.00226400
O	-1.33386100	2.69231700	0.04158500
C	2.14498100	-0.40643600	0.56616100
O	2.69212100	-1.71183900	0.20309800
C	3.94782700	-1.49003700	-0.28457200
O	4.66217000	-2.38958800	-0.63982700
C	4.19969700	0.00953300	-0.22125400
C	4.32086800	0.27502800	1.31668800
C	2.88773000	0.00621600	1.85315000
C	2.75081800	0.52533100	-0.54192200
C	2.27391400	0.16994100	-1.95754600
C	2.53559300	2.02380100	-0.31328600
C	5.36304100	0.49412100	-1.06044800
C	0.63575800	-0.52625900	0.61851500
O	-0.00285200	-1.44687900	0.17302100
H	-5.77953700	-2.18576400	1.82088900
H	-5.88591600	-3.31813900	-0.38665700
H	-4.87539800	-2.23163900	-2.37741300
H	-3.77060100	-0.02887000	-2.16158500
H	-4.66701400	0.01451900	2.03291900
H	-3.71940900	1.93969300	1.03784200
H	-1.59536400	0.83139900	-0.84486500
H	-1.52989600	1.23787200	2.18382300
H	-1.75870500	-0.33793000	1.37700300
H	-4.65194300	2.62790200	-0.91610700
H	-1.87652700	3.18153600	-0.59248200
H	5.07096700	-0.37624000	1.76957600
H	4.63301700	1.30628100	1.48634100
H	2.43901300	0.88935200	2.30416400
H	2.84824400	-0.80644100	2.57987400
H	1.23087200	0.46819800	-2.09532100
H	2.34966200	-0.89513300	-2.18563000
H	2.86765000	0.71416400	-2.69633200
H	2.89130200	2.37754500	0.65442100
H	1.47348700	2.26956800	-0.38634700
H	3.06195300	2.58734300	-1.08861600
H	5.22527600	0.25587700	-2.11800100
H	5.48365000	1.57611200	-0.96480800
H	6.29319000	0.02254300	-0.73210900

Cartesian coordinates of the low-energy conformers M2aC2

C	-3.44727900	2.72807100	0.15872400
C	-4.81106800	2.69644000	0.44620700
C	-5.51068100	1.49424500	0.33681000
C	-4.84975100	0.33084900	-0.05201000
C	-3.47965300	0.35333400	-0.33734300
C	-2.78705300	1.56416800	-0.23446800
C	-2.75688300	-0.91833900	-0.72817100
C	-2.38739000	-1.79870100	0.49612200
C	-1.36836700	-1.17995900	1.44740100
O	-0.25527900	-0.47699800	0.80554600
O	-3.58950800	-1.69515300	-1.58719600
O	-2.00931200	-3.10025500	0.03570400
C	1.85766400	-0.33794700	-0.27487800
O	1.49077500	1.07346400	-0.34375400
C	2.66077900	1.78396900	-0.34008100
O	2.67675100	2.98218700	-0.42117900
C	3.79866900	0.77560300	-0.27063800
C	3.74925400	0.09746800	-1.68155200
C	2.41244600	-0.69256300	-1.66734100
C	3.12666600	-0.30587700	0.64972200
C	2.83202000	0.19532500	2.07067500
C	3.88455900	-1.63195200	0.74424800
C	5.13758100	1.35861600	0.12945400
C	0.69496500	-1.17688400	0.20005300
O	0.67604900	-2.38408900	0.04252700
H	-2.89697000	3.65981300	0.23304100
H	-5.32649100	3.60195400	0.74733200
H	-6.57353700	1.46344100	0.55185500
H	-5.39655000	-0.59895900	-0.15241500
H	-1.72636000	1.59635200	-0.45901400
H	-1.83361400	-0.65270700	-1.25935900
H	-3.29764200	-1.94654300	1.08657700
H	-1.83808300	-0.40163200	2.04402600
H	-0.96410600	-1.94532700	2.11191000
H	-3.22825800	-2.59230400	-1.52755500
H	-1.04430600	-3.09226700	-0.08034700
H	3.78934300	0.84299000	-2.47781500
H	4.61098800	-0.56002400	-1.80125500
H	2.55668700	-1.76683600	-1.76880300
H	1.71292100	-0.36744000	-2.43853000
H	2.26344700	-0.55308900	2.62996500
H	2.26980500	1.13101100	2.09585800
H	3.77135200	0.35471900	2.60606700
H	4.15183900	-2.05820900	-0.22204800
H	3.28711400	-2.37150000	1.28346000
H	4.80741800	-1.48156800	1.31073000
H	5.09322200	1.83350800	1.11257200
H	5.90374500	0.57985000	0.15549900
H	5.45335800	2.11631800	-0.59252800

Cartesian coordinates of the low-energy conformers M2aC3

C	3.91658800	2.56777100	-0.36637100
C	5.28061500	2.30452500	-0.47975700
C	5.76662800	1.03603700	-0.16019000
C	4.89316700	0.03638700	0.26219900
C	3.52079100	0.29021300	0.37267300
C	3.04361300	1.56717800	0.06111500
C	2.57094100	-0.80869200	0.79916800
C	2.25013700	-1.79805700	-0.35365600
C	1.43794100	-1.21344800	-1.49955000
O	0.24472000	-0.45375400	-1.11280900
O	3.15869800	-1.55665900	1.86250300
O	1.67052100	-2.98204400	0.20428700
C	-2.04577100	-0.18763200	-0.63298200
O	-3.25914100	-0.99038700	-0.75751300
C	-4.26805000	-0.26785300	-0.18250200
O	-5.40261000	-0.66250800	-0.16468300
C	-3.66110200	1.03290500	0.32061400
C	-3.33288600	1.80081500	-1.00333900
C	-2.20048100	0.95854800	-1.65129200
C	-2.25068100	0.50227400	0.76377900
C	-2.30963100	-0.49120300	1.93272500
C	-1.23076300	1.59274500	1.09744600
C	-4.51526300	1.78682300	1.31825000
C	-0.86029600	-1.11786800	-0.77095000
O	-0.90953000	-2.31353500	-0.56914800
H	3.53119600	3.55371400	-0.60281500
H	5.96101900	3.08271700	-0.80788000
H	6.82807300	0.82602600	-0.23765700
H	5.27362300	-0.94321700	0.52548500
H	1.98498300	1.78342000	0.15869300
H	1.63281400	-0.35583400	1.14519300
H	3.20264300	-2.10595800	-0.80010200
H	2.03285500	-0.48441900	-2.04499900
H	1.13300100	-2.00681900	-2.18417400
H	2.68070200	-2.39968300	1.85695600
H	0.71015700	-2.93910800	0.05991300
H	-4.21610000	1.88282500	-1.63955700
H	-3.00121700	2.81197000	-0.76394000
H	-1.27509100	1.52008900	-1.76176900
H	-2.47129100	0.55196600	-2.62659400
H	-1.31979400	-0.91102200	2.13037200
H	-2.99684800	-1.32224500	1.76295400
H	-2.62932100	0.02771900	2.83994100
H	-1.11225100	2.34286900	0.31610200
H	-0.25161300	1.14680800	1.28939600
H	-1.53764800	2.10744800	2.01195200
H	-4.73576700	1.18062500	2.20012200
H	-4.01084800	2.69993800	1.64373300
H	-5.46753900	2.07245800	0.86329700

Cartesian coordinates of the low-energy conformers M2aC4

C	-3.75674100	2.62182800	0.49720400
C	-5.10258600	2.41379300	0.79527800
C	-5.68606700	1.17488500	0.52702500
C	-4.92632400	0.14813500	-0.02935800
C	-3.57276900	0.34699700	-0.32661700
C	-2.99801100	1.59447900	-0.06311700
C	-2.73584100	-0.77364300	-0.90931900
C	-2.31835700	-1.83966900	0.12462300
C	-1.40011400	-1.32401900	1.21720800
O	-0.23468200	-0.68852000	0.63121100
O	-3.45323200	-1.52573900	-1.90565200
O	-1.65597800	-2.90984300	-0.53894900
C	2.06172100	-0.56170700	0.02643800
O	1.53006300	0.41107300	-0.92918200
C	2.54874500	1.27390400	-1.21839000
O	2.42022100	2.17029400	-2.00908600
C	3.76285000	0.82665600	-0.41648800
C	4.16854300	-0.51111500	-1.12214000
C	2.99530900	-1.47322000	-0.79472300
C	3.03849500	0.31831700	0.88136700
C	2.32495600	1.43045600	1.66295400
C	3.92881400	-0.46534300	1.84883100
C	4.86170300	1.86166200	-0.29900000
C	0.95676200	-1.27563300	0.77412800
O	1.18333400	-2.25272000	1.44933800
H	-3.29821300	3.58491100	0.69361400
H	-5.69500500	3.21276200	1.22749100
H	-6.73446900	1.00878300	0.75029300
H	-5.38633900	-0.80766700	-0.25159300
H	-1.95304700	1.76261100	-0.30224200
H	-1.82489100	-0.35753600	-1.34943100
H	-3.22833600	-2.20302300	0.62659300
H	-1.89634100	-0.56492300	1.82050700
H	-1.08266300	-2.14721000	1.85442500
H	-3.54506100	-0.97028200	-2.68952000
H	-2.14485500	-3.03652800	-1.36387100
H	4.30700000	-0.36351400	-2.19492300
H	5.11494900	-0.86824300	-0.71374200
H	3.30877500	-2.33703800	-0.21108300
H	2.47288200	-1.83233200	-1.68243500
H	1.74852000	1.00606500	2.48988000
H	1.64508300	2.02527900	1.04997500
H	3.06277000	2.11034800	2.09633900
H	4.49473700	-1.26742400	1.37618900
H	3.32345200	-0.90692900	2.64406800
H	4.64311200	0.21686400	2.31803100
H	4.50817400	2.77303700	0.18926500
H	5.70348900	1.46675100	0.27507300
H	5.23194200	2.13830700	-1.28976500

Cartesian coordinates of the low-energy conformers M2aC5

C	-5.88643900	1.23217700	1.13364500
C	-6.12677600	2.08614200	0.05825900
C	-5.47534400	1.86592400	-1.15563800
C	-4.59114400	0.79749200	-1.28987700
C	-4.34020100	-0.06066700	-0.21343200
C	-4.99651300	0.16685200	1.00000100
C	-3.34829100	-1.19776800	-0.37720600
C	-1.90438100	-0.78214500	-0.02083200
C	-0.93106500	-1.87772700	-0.45979200
O	0.44038300	-1.54216900	-0.13147700
O	-3.62950200	-2.30979800	0.48242600
O	-1.78336500	-0.49300300	1.36622800
C	2.50115000	-0.47912200	-0.44393900
O	3.30435200	0.10741000	-1.51546800
C	4.34540300	0.75583600	-0.91567300
O	5.19891600	1.31650200	-1.55043700
C	4.19253700	0.56688900	0.58581700
C	4.51141400	-0.95322100	0.77891300
C	3.32493200	-1.67245100	0.08163500
C	2.62516300	0.60072200	0.68736900
C	2.01617500	1.95643800	0.30049800
C	2.05934900	0.18078700	2.04644100
C	5.01303100	1.51825400	1.43078300
C	1.11601900	-0.76138500	-0.98903000
O	0.67716700	-0.33733100	-2.02942800
H	-6.39163300	1.39482500	2.07971000
H	-6.81996800	2.91361300	0.16271500
H	-5.66237400	2.52042700	-2.00010400
H	-4.09527400	0.62344900	-2.23995700
H	-4.81832700	-0.49560400	1.83801800
H	-3.35824600	-1.51748700	-1.42614100
H	-1.66833100	0.14191700	-0.55019600
H	-1.12281300	-2.80457500	0.07837100
H	-1.01249700	-2.05339800	-1.53302000
H	-4.55176500	-2.56563600	0.35775700
H	-2.17226600	-1.24431800	1.83522300
H	5.47784300	-1.21021200	0.34081600
H	4.55919600	-1.18315400	1.84414100
H	2.74271600	-2.28043200	0.77145000
H	3.63511000	-2.30368000	-0.75228300
H	0.92411500	1.89919400	0.29678800
H	2.33543400	2.31195200	-0.68151700
H	2.29877000	2.71166400	1.03825000
H	2.46633600	-0.75777700	2.42293800
H	0.97384100	0.07355900	1.98598800
H	2.27664800	0.95849600	2.78382100
H	4.76735500	2.56153900	1.21776000
H	4.84295700	1.33390800	2.49444600
H	6.07944800	1.38067900	1.23262700

Cartesian coordinates of the low-energy conformers M2aC6

C	-5.38353300	-1.53234800	-1.46034100
C	-5.66651400	-2.42094200	-0.42178000
C	-5.30281900	-2.09406300	0.88313700
C	-4.65753400	-0.88544200	1.14692500
C	-4.36214300	0.00624400	0.11163200
C	-4.73649200	-0.32768300	-1.19554500
C	-3.64462700	1.30839100	0.39504300
C	-2.16283900	1.29964200	-0.06095400
C	-1.31003000	0.40880600	0.83076900
O	-0.05466900	-0.00503500	0.20207800
O	-4.31943700	2.36475000	-0.28714800
O	-1.74430400	2.66704900	-0.03469500
C	2.23269200	0.16985600	-0.28865500
O	3.20910700	1.20239600	-0.62126700
C	4.43806400	0.60448600	-0.59101600
O	5.44484600	1.20610700	-0.85211600
C	4.22003400	-0.85779300	-0.23207700
C	3.52924800	-1.43381700	-1.51335000
C	2.14381800	-0.73166600	-1.53709800
C	3.01386400	-0.69768300	0.76191800
C	3.36931900	0.07675600	2.03923700
C	2.33082100	-2.00886500	1.15524500
C	5.46499800	-1.59049000	0.22225400
C	0.96781100	0.85165100	0.17992800
O	0.89863100	2.01681700	0.51131000
H	-5.66974500	-1.77785300	-2.47744400
H	-6.17208200	-3.35792200	-0.62858800
H	-5.52671000	-2.77426900	1.69773700
H	-4.38651000	-0.63034800	2.16641700
H	-4.53301100	0.36748700	-2.00147100
H	-3.65954000	1.49643500	1.47770900
H	-2.11589200	0.91888400	-1.08979300
H	-1.08593000	0.89926300	1.78022600
H	-1.81190400	-0.53669000	1.02264200
H	-3.69348000	3.10270300	-0.29006100
H	-0.80123700	2.68988100	0.19405300
H	4.12228900	-1.22801900	-2.40650800
H	3.43461300	-2.51630000	-1.41950000
H	1.31683900	-1.43538700	-1.46317100
H	1.98999000	-0.11654600	-2.42457000
H	2.46927300	0.27712200	2.62733700
H	3.86116700	1.03218600	1.84637200
H	4.03767900	-0.52367300	2.66122300
H	2.03277000	-2.62431400	0.30715800
H	1.43930700	-1.80745900	1.75402800
H	3.01140800	-2.59982100	1.77404400
H	5.90154300	-1.13317800	1.11362000
H	5.23813800	-2.63558200	0.44717800
H	6.22280000	-1.57352000	-0.56557000

Cartesian coordinates of the low-energy conformers M2aC7

C	-5.73131200	1.35058700	1.33243000
C	-6.20388000	1.96432300	0.17158000
C	-5.76745500	1.51338700	-1.07299000
C	-4.86217500	0.45532000	-1.15512900
C	-4.37688900	-0.15894000	0.00329500
C	-4.82387800	0.29697900	1.24913800
C	-3.37732500	-1.29158500	-0.08510000
C	-1.92361600	-0.85204400	0.23905800
C	-1.34583500	0.03892200	-0.85166800
O	0.03382100	0.41196900	-0.57115500
O	-3.74477000	-2.31230400	0.84047300
O	-1.13171700	-2.02903200	0.45409300
C	2.38915900	0.07397800	-0.70743700
O	2.41740800	1.50448500	-0.41626900
C	3.58453400	1.74194000	0.25667200
O	3.90526800	2.84638200	0.60465100
C	4.30994800	0.40958600	0.39053000
C	4.75881800	0.10470400	-1.07736300
C	3.42341100	-0.14454800	-1.82870200
C	3.07039100	-0.53762100	0.56907400
C	2.28365400	-0.28222600	1.86264500
C	3.37944400	-2.03349800	0.47207900
C	5.41270600	0.39003200	1.42796800
C	0.98996300	-0.40618700	-1.00842400
O	0.79135600	-1.46520200	-1.57090600
H	-6.07259600	1.69162300	2.30399600
H	-6.91215300	2.78300800	0.23740500
H	-6.13708300	1.97807700	-1.98062600
H	-4.53540800	0.09940500	-2.12700600
H	-4.47133800	-0.19010600	2.15039500
H	-3.38639000	-1.69554000	-1.10757400
H	-1.92612700	-0.31759500	1.19304000
H	-1.38886500	-0.44767800	-1.82732100
H	-1.88154200	0.98467200	-0.89515100
H	-2.94087200	-2.84011300	0.95681800
H	-0.69995300	-2.26218500	-0.38112700
H	5.32954900	0.93555900	-1.49602800
H	5.40279100	-0.77554700	-1.08561800
H	3.35077900	-1.15126900	-2.23651000
H	3.24727800	0.56574900	-2.63766900
H	1.35678200	-0.86180000	1.86657500
H	2.02351300	0.76722800	2.01375600
H	2.87502300	-0.60604400	2.72281500
H	3.92477800	-2.31707300	-0.42752700
H	2.45234200	-2.61167300	0.49732500
H	3.97610800	-2.33746900	1.33641700
H	5.03700700	0.64368700	2.42218200
H	5.87700100	-0.59805400	1.47749100
H	6.19046600	1.11411400	1.17091000

Cartesian coordinates of the low-energy conformers M2aC8

C	5.51097100	1.49398400	-0.33726500
C	4.81149500	2.69631800	-0.44610400
C	3.44782900	2.72808100	-0.15808300
C	2.78759300	1.56417300	0.23509300
C	3.48003300	0.35321600	0.33739600
C	4.85002000	0.33059500	0.05151700
C	2.75721600	-0.91844900	0.72814100
C	2.38736900	-1.79849400	-0.49625000
C	1.36827600	-1.17931300	-1.44715900
O	0.25525700	-0.47654200	-0.80504000
O	3.58996200	-1.69551200	1.58684200
O	2.00921000	-3.10008600	-0.03605800
C	-1.85784700	-0.33779500	0.27513400
O	-1.49121800	1.07368300	0.34404700
C	-2.66135700	1.78395600	0.34007100
O	-2.67755100	2.98217000	0.42112400
C	-3.79904800	0.77539900	0.27032200
C	-3.74986600	0.09736700	1.68129500
C	-2.41294000	-0.69249100	1.66743600
C	-3.12661400	-0.30601300	-0.64979900
C	-2.83163800	0.19512700	-2.07071200
C	-3.88429700	-1.63222400	-0.74446200
C	-5.13796800	1.35814700	-0.13013700
C	-0.69491700	-1.17652500	-0.19956000
O	-0.67588100	-2.38371700	-0.04196400
H	6.57373900	1.46307200	-0.55272800
H	5.32693900	3.60182700	-0.74720700
H	2.89761500	3.65991400	-0.23196200
H	1.72700400	1.59648300	0.46009100
H	5.39673600	-0.59931000	0.15147600
H	1.83407800	-0.65281200	1.25956300
H	3.29744200	-1.94630400	-1.08698800
H	1.83802100	-0.40078800	-2.04351200
H	0.96395100	-1.94438600	-2.11197900
H	3.22879500	-2.59267200	1.52684700
H	1.04422200	-3.09197400	0.08021200
H	-3.79021400	0.84296300	2.47747700
H	-4.61155600	-0.56019800	1.80087500
H	-2.55708900	-1.76678500	1.76885300
H	-1.71368500	-0.36729400	2.43883300
H	-2.26289900	-0.55332200	-2.62979000
H	-2.26941200	1.13080400	-2.09578000
H	-3.77081500	0.35449500	-2.60638800
H	-4.15199000	-2.05833500	0.22178400
H	-3.28652200	-2.37178700	-1.28327900
H	-4.80692700	-1.48200500	-1.31135800
H	-5.09349000	1.83289100	-1.11332500
H	-5.90402000	0.57927200	-0.15622800
H	-5.45401400	2.11592200	0.59165200

Cartesian coordinates of the low-energy conformers M2aC9

C	5.84182200	-0.52596600	1.61324000
C	6.14280400	-1.67727800	0.88455600
C	5.57291500	-1.86541100	-0.37353200
C	4.70560400	-0.90754200	-0.89816100
C	4.39024000	0.24317800	-0.16929100
C	4.97120700	0.42788300	1.09026700
C	3.42703200	1.26643700	-0.73133800
C	2.00785800	1.14552300	-0.14487400
C	1.31807900	-0.15977900	-0.49815200
O	-0.02657000	-0.05005000	0.04459000
O	3.91994800	2.57656700	-0.45312200
O	1.28570300	2.25754600	-0.69242300
C	-2.29396100	-0.75515400	0.20955000
O	-2.30927800	0.20533500	1.31230600
C	-3.57833200	0.71114500	1.37097900
O	-3.90942000	1.50708400	2.20831000
C	-4.38347400	0.04656100	0.26216800
C	-4.52763100	-1.42759600	0.76877000
C	-3.07701500	-1.97999500	0.71519700
C	-3.25983700	-0.07893300	-0.82710900
C	-2.74921500	1.27582300	-1.34085600
C	-3.61806200	-0.95444100	-2.03038800
C	-5.67541900	0.75319400	-0.09004500
C	-0.88777900	-1.02056900	-0.27757900
O	-0.60375700	-1.99530100	-0.93409400
H	6.28805100	-0.36977000	2.58957300
H	6.82186500	-2.41838400	1.29182500
H	5.80896300	-2.75244900	-0.95134800
H	4.27452600	-1.05253300	-1.88367700
H	4.75076200	1.32860900	1.65055800
H	3.34866400	1.12103600	-1.81736700
H	2.06851100	1.24259800	0.94619800
H	1.25411300	-0.29821700	-1.57853000
H	1.81588900	-1.01943400	-0.04842900
H	3.16403000	3.16531800	-0.58654700
H	0.43593100	2.30904000	-0.23815600
H	-4.95467500	-1.45952300	1.77285500
H	-5.19885400	-1.97622800	0.10697000
H	-2.97066200	-2.82025600	0.03114700
H	-2.69726000	-2.28463600	1.69136900
H	-1.87616600	1.13832000	-1.98434700
H	-2.47052000	1.96622600	-0.54241900
H	-3.52354500	1.75824600	-1.94272600
H	-3.98120300	-1.94664400	-1.76474700
H	-2.74523800	-1.07957000	-2.67642600
H	-4.39417000	-0.46031700	-2.62096000
H	-5.49447300	1.78241400	-0.40961300
H	-6.19582600	0.22897300	-0.89553800
H	-6.34274500	0.78524700	0.77538200

Cartesian coordinates of the low-energy conformers M2aC10

C	5.28281800	-1.81790900	-1.07914900
C	5.65254700	-2.24066100	0.19658200
C	5.35266800	-1.44344300	1.30195000
C	4.68155800	-0.23417900	1.13376100
C	4.30205000	0.19425600	-0.14327000
C	4.61571400	-0.60458500	-1.24679300
C	3.55484800	1.49754400	-0.32803200
C	2.05680900	1.38640500	0.01182500
C	1.28925500	0.47267300	-0.93247900
O	-0.12944400	0.56603900	-0.61730500
O	4.13724400	2.49296200	0.51348500
O	1.55860200	2.72801900	-0.07468800
C	-2.14339400	-0.17449300	0.41144000
O	-2.54608700	1.19607900	0.09974900
C	-3.90207200	1.17610200	-0.07385000
O	-4.52803900	2.17253300	-0.31787200
C	-4.36442500	-0.25745100	0.14420600
C	-4.15708200	-0.46016000	1.68318000
C	-2.61424700	-0.42427500	1.85687500
C	-3.13358100	-1.01803300	-0.46647400
C	-2.95375000	-0.78883100	-1.97417900
C	-3.10625000	-2.52409300	-0.19578300
C	-5.75482200	-0.55794300	-0.37337200
C	-0.66857400	-0.38779200	0.15486700
O	-0.07551300	-1.34851500	0.58668100
H	5.52036300	-2.42634800	-1.94503000
H	6.17654700	-3.18092600	0.32894600
H	5.64431200	-1.76340800	2.29655900
H	4.46257800	0.39084400	1.99126700
H	4.33965000	-0.27320600	-2.24275500
H	3.63284500	1.80617700	-1.37938200
H	1.95745500	1.01860700	1.04086600
H	1.37064900	0.82014000	-1.96201300
H	1.61426700	-0.56242300	-0.85412900
H	3.47838500	3.19921200	0.56703100
H	0.63494300	2.72047900	0.20535900
H	-4.66413500	0.32022000	2.25389500
H	-4.58004600	-1.41894900	1.98541100
H	-2.21274400	-1.35956900	2.24299400
H	-2.27350400	0.38648900	2.50221400
H	-2.02569200	-1.25155700	-2.32166800
H	-2.92864400	0.26600400	-2.25404700
H	-3.77595100	-1.25989100	-2.51892800
H	-3.24284600	-2.78913400	0.85208900
H	-2.15497500	-2.94811900	-0.52670000
H	-3.89948100	-3.01059000	-0.77001000
H	-5.83814600	-0.36401400	-1.44556300
H	-6.01707800	-1.60297100	-0.19043200
H	-6.49327800	0.06720900	0.13579700

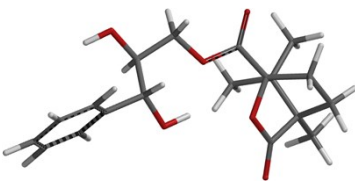
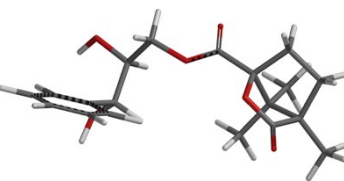
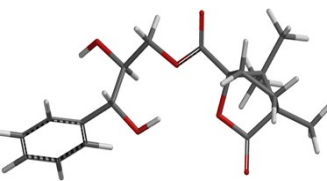
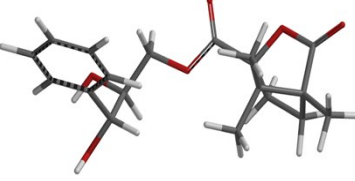
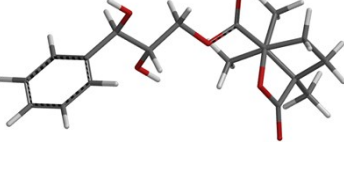
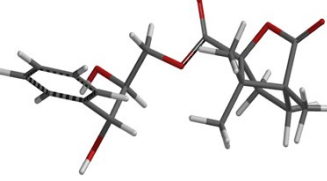
Cartesian coordinates of the low-energy conformers M2aC11

C	5.89360900	-0.99978000	0.13101200
C	5.42693300	-2.29965000	-0.06798000
C	4.10794500	-2.50488200	-0.46959800
C	3.25944900	-1.41573300	-0.66719800
C	3.71602600	-0.11020600	-0.45991300
C	5.04408300	0.08717900	-0.06265000
C	2.78348100	1.07102300	-0.64365700
C	2.25537100	1.64901400	0.68629800
C	1.36850600	0.71221700	1.47937300
O	0.24390900	0.31690100	0.65287800
O	3.44442400	2.19066900	-1.26042700
O	1.52765500	2.84741600	0.43755900
C	-1.92482100	-0.49350600	0.29167500
O	-2.89377700	-1.39105700	0.91722900
C	-4.07729300	-1.21285900	0.26033300
O	-5.06231900	-1.84434100	0.53679100
C	-3.84029900	-0.17087300	-0.82262700
C	-2.93026600	-0.93626100	-1.84123100
C	-1.59449400	-1.13068400	-1.07211500
C	-2.81251000	0.74852400	-0.07119000
C	-3.40094100	1.44912600	1.16137200
C	-2.12597800	1.79796200	-0.94999400
C	-5.09885900	0.44089100	-1.40079800
C	-0.79193500	-0.26859800	1.27194800
O	-0.82219100	-0.54389800	2.44542200
H	6.92099100	-0.83241800	0.43610600
H	6.08889000	-3.14532900	0.08274500
H	3.74019000	-3.51158000	-0.63590500
H	2.23778200	-1.58264400	-0.99196500
H	5.41333300	1.09638300	0.07767100
H	1.92701900	0.77049500	-1.25458200
H	3.12572200	1.86221600	1.32503500
H	1.91487700	-0.17886700	1.79228700
H	0.99639800	1.22465100	2.36695100
H	3.61898200	1.96483000	-2.18235500
H	2.02319200	3.30589000	-0.25511100
H	-3.38594100	-1.88191000	-2.14097300
H	-2.80021800	-0.33299400	-2.74053300
H	-0.76032400	-0.62447000	-1.55425200
H	-1.32613600	-2.17926500	-0.93659200
H	-2.61630300	1.97638600	1.71146000
H	-3.89296300	0.76482000	1.85553700
H	-4.13594300	2.19455600	0.84743400
H	-1.73281400	1.40092800	-1.88589300
H	-1.29488900	2.25992600	-0.41205500
H	-2.84217700	2.58637400	-1.19641000
H	-5.69120800	0.94456700	-0.63292100
H	-4.85144200	1.16747600	-2.17883600
H	-5.72667600	-0.33295600	-1.85083800

Cartesian coordinates of the low-energy conformers M2aC12

C	5.07758600	-1.79301700	1.36960800
C	5.39049000	-2.54715100	0.23773300
C	5.15823100	-2.01744500	-1.03053300
C	4.61210100	-0.74127600	-1.16479900
C	4.28732100	0.01745200	-0.03602700
C	4.52940400	-0.51955600	1.23420900
C	3.67619500	1.39475200	-0.19161400
C	2.17233000	1.46551500	0.14708700
C	1.33332500	0.64863600	-0.81178200
O	-0.03615600	0.69999100	-0.33653900
O	4.26754300	2.35264600	0.70471700
O	1.73804700	2.81926500	0.07429500
C	-2.33146500	0.24667700	-0.46741700
O	-3.32915300	-0.09889200	-1.47848900
C	-4.48572800	-0.37893000	-0.80963200
O	-5.50340400	-0.66002900	-1.38507800
C	-4.20215100	-0.20948900	0.67555400
C	-4.03481000	1.34076100	0.82255700
C	-2.72869800	1.64721700	0.03974200
C	-2.71491600	-0.71417900	0.71175800
C	-2.56130500	-2.19956800	0.35549900
C	-1.98460500	-0.44728500	2.02984500
C	-5.22428100	-0.84785200	1.59201900
C	-0.95909800	0.08597500	-1.08961500
O	-0.72233700	-0.51611100	-2.10749400
H	5.26199800	-2.19733700	2.35906300
H	5.81859000	-3.53781000	0.34463400
H	5.40761700	-2.59312400	-1.91526500
H	4.44115100	-0.32732700	-2.15349800
H	4.30309300	0.06952000	2.11540400
H	3.80437300	1.73184100	-1.22681000
H	2.03358000	1.07494800	1.16546900
H	1.37536300	1.06695800	-1.81914100
H	1.66006000	-0.39102900	-0.83960300
H	5.16681700	2.52950500	0.40227900
H	2.43638000	3.32913200	0.50742000
H	-4.90227000	1.86922500	0.42248000
H	-3.94722400	1.59922000	1.87876200
H	-1.95048300	2.07457400	0.66918200
H	-2.88340400	2.31527600	-0.80882900
H	-1.50347000	-2.46819300	0.28527200
H	-3.03797100	-2.46982400	-0.58889300
H	-3.00276100	-2.81628800	1.14251700
H	-2.03416200	0.58929200	2.36200500
H	-0.93045800	-0.72018700	1.94087600
H	-2.41789200	-1.07102200	2.81654500
H	-5.30983900	-1.92253900	1.41315800
H	-4.95425800	-0.69249800	2.63959400
H	-6.21069700	-0.40469200	1.43091600

Table 4. B3LYP/6-311g(d,p) optimized low-energy conformers for M3a

 M3aC1 (16.6%)	 M3aC2 (4.2%)	 M3aC3 (16.6%)
 M3aC4 (4.9%)	 M3aC5 (52.1%)	 M3aC6 (4.9%)

Cartesian coordinates of the low-energy conformers M3aC1

C	6.34226400	-0.39723000	-0.90334300
C	6.63045000	-1.22763100	0.18340200
C	5.60371000	-1.61225600	1.05314400
C	4.29730700	-1.16630300	0.83828800
C	3.99853200	-0.33195700	-0.25117400
C	5.03289000	0.04565100	-1.11856500
C	2.58401000	0.16769200	-0.47390300
C	2.18935000	1.24787600	0.57581700
C	0.92516100	2.02667000	0.21254700
O	-0.15021800	1.07168200	0.03053300
O	1.70546800	-0.96197900	-0.39639700
O	3.17861700	2.27131200	0.68008600
O	-1.75831600	-0.84804000	-0.58070800
C	-2.72282300	-1.77614700	-0.29659000
C	-4.01010100	-1.01878600	-0.00130900
C	-2.39781900	0.46745900	-0.47126100
C	-4.40978800	-0.44818800	-1.40765300
C	-3.29835200	0.59403100	-1.71709800
O	-2.49358100	-2.96513300	-0.33792100
C	-1.35877000	1.55143000	-0.29547000
O	-1.61733600	2.73392800	-0.41176100
C	-3.40176400	0.24440300	0.71560400
C	-2.70540800	-0.07549900	2.05011100
C	-4.38997000	1.39554400	0.94322400
C	-5.08203700	-1.82816300	0.70511100
H	7.13185700	-0.09823600	-1.58654600
H	7.64561800	-1.57573300	0.35032300
H	5.81994500	-2.26019500	1.89769900
H	3.50288500	-1.47732500	1.50988800
H	4.81286800	0.68512900	-1.96943500
H	2.52698100	0.62634400	-1.47168800
H	2.04755600	0.74385400	1.54216500
H	1.06871600	2.58333900	-0.71782500
H	0.65951400	2.72200200	1.01143000
H	0.78820500	-0.64827900	-0.45096800
H	4.00549700	1.87385600	0.98910000
H	-5.39905500	0.01137600	-1.34558600
H	-4.46522000	-1.24227700	-2.15671400
H	-3.68386700	1.60966700	-1.81642000
H	-2.72518800	0.35744900	-2.61658000
H	-2.21477400	0.81828900	2.44887900
H	-3.44793800	-0.39480700	2.78733400
H	-1.95158200	-0.86286500	1.96895400
H	-4.95057000	1.68154800	0.05245100
H	-5.11010500	1.10774300	1.71532800
H	-3.85864800	2.28182900	1.30272400
H	-4.72911700	-2.21666000	1.66476500
H	-5.38443800	-2.68038900	0.08898800
H	-5.96725900	-1.21139300	0.88578700

Cartesian coordinates of the low-energy conformers M3aC2

C	3.79452600	2.58481100	0.50017000
C	5.16134700	2.32303900	0.63409600
C	5.67268800	1.08955300	0.21686200
C	4.82280900	0.12061200	-0.32398800
C	3.44820900	0.37150600	-0.45611700
C	2.94705700	1.61633200	-0.04608400
C	2.49680500	-0.66382300	-1.03152500
C	2.04383700	-1.77000900	-0.05012100
C	1.40874200	-1.25655800	1.23989100
O	0.20609500	-0.49895400	0.95186800
O	3.07887700	-1.40218800	-2.11893000
O	3.13616900	-2.58494300	0.36612500
O	-1.77163200	1.15184000	0.62494900
C	-2.77453100	1.79028100	-0.04590000
C	-3.83397100	0.75089900	-0.38314700
C	-2.16190600	-0.25757000	0.72216800
C	-4.44921500	0.41577900	1.02093700
C	-3.29234400	-0.29869500	1.77411000
O	-2.74434700	2.98517000	-0.25175000
C	-0.96870400	-1.13943900	1.02015500
O	-1.10277200	-2.32136500	1.28223500
C	-2.89796000	-0.48781300	-0.64598900
C	-1.97732800	-0.31962000	-1.86774800
C	-3.63014400	-1.83041900	-0.76840400
C	-4.82776900	1.17241200	-1.44984700
H	3.38881900	3.54331800	0.81073900
H	5.82353700	3.07546600	1.05241800
H	6.73461400	0.88104500	0.31079200
H	5.23122900	-0.82900000	-0.65310100
H	1.88734000	1.83073200	-0.15778800
H	1.59031300	-0.15033600	-1.37634200
H	1.30743200	-2.38242200	-0.58976100
H	2.06974800	-0.56158300	1.75893500
H	1.16761000	-2.09876000	1.88892000
H	3.43682700	-0.77999200	-2.76752500
H	3.60813000	-2.86106000	-0.43432500
H	-5.31832800	-0.23372100	0.89145600
H	-4.79079600	1.32030700	1.53087900
H	-3.53374000	-1.32747700	2.04520600
H	-2.97802300	0.22801400	2.67820600
H	-1.27757700	-1.15867300	-1.93619800
H	-2.57394900	-0.31901700	-2.78480000
H	-1.39315100	0.60396500	-1.84643800
H	-4.32051400	-2.03525600	0.05075800
H	-4.20259900	-1.84652100	-1.70118500
H	-2.90740600	-2.65031100	-0.80882500
H	-4.32984800	1.41281800	-2.39368600
H	-5.37933300	2.06048600	-1.12652400
H	-5.55233900	0.37383700	-1.63491400

Cartesian coordinates of the low-energy conformers M3aC3

C	6.34210900	-0.39761300	-0.90364300
C	6.63040900	-1.22768900	0.18331900
C	5.60378600	-1.61192700	1.05337300
C	4.29738700	-1.16592400	0.83860200
C	3.99849000	-0.33192000	-0.25109300
C	5.03273500	0.04530900	-1.11878300
C	2.58396700	0.16771400	-0.47380900
C	2.18931800	1.24798500	0.57582300
C	0.92512600	2.02674300	0.21248000
O	-0.15023900	1.07172900	0.03048700
O	1.70543500	-0.96196400	-0.39617700
O	3.17857200	2.27142200	0.68001900
O	-1.75828400	-0.84802400	-0.58077800
C	-2.72274800	-1.77616000	-0.29661100
C	-4.01003700	-1.01884100	-0.00127000
C	-2.39781900	0.46745500	-0.47130200
C	-4.40980700	-0.44825500	-1.40759900
C	-3.29841500	0.59399900	-1.71709100
O	-2.49346600	-2.96513700	-0.33794100
C	-1.35879700	1.55144900	-0.29554000
O	-1.61737000	2.73394000	-0.41189200
C	-3.40172000	0.24437100	0.71561500
C	-2.70531400	-0.07550400	2.05010600
C	-4.38994900	1.39548500	0.94325000
C	-5.08191600	-1.82826000	0.70519000
H	7.13160700	-0.09890800	-1.58708200
H	7.64557400	-1.57583000	0.35017700
H	5.82010800	-2.25960000	1.89811000
H	3.50307200	-1.47664100	1.51047300
H	4.81262300	0.68453100	-1.96982300
H	2.52691200	0.62628000	-1.47163300
H	2.04749700	0.74403700	1.54220900
H	1.06869200	2.58336100	-0.71791800
H	0.65945100	2.72211000	1.01132300
H	0.78817500	-0.64828000	-0.45090000
H	4.00552600	1.87396600	0.98883200
H	-5.39908500	0.01127600	-1.34548700
H	-4.46523800	-1.24234900	-2.15665500
H	-3.68396400	1.60962200	-1.81639600
H	-2.72528800	0.35743400	-2.61660200
H	-2.21477400	0.81832500	2.44889600
H	-3.44781100	-0.39491200	2.78731900
H	-1.95140600	-0.86278600	1.96891400
H	-4.95067300	1.68137000	0.05251500
H	-5.10997800	1.10772200	1.71546700
H	-3.85862400	2.28182700	1.30260300
H	-4.72893700	-2.21676100	1.66482300
H	-5.38431300	-2.68049000	0.08907100
H	-5.96715000	-1.21152300	0.88591600

Cartesian coordinates of the low-energy conformers M3aC4

C	-5.55379800	1.35024900	-0.45703800
C	-4.88338600	2.56942300	-0.60319800
C	-3.54841600	2.67441200	-0.20285000
C	-2.89027500	1.56459000	0.33585300
C	-3.54812000	0.33289000	0.47224500
C	-4.89211400	0.24090300	0.07609600
C	-2.80109600	-0.85987400	1.04599100
C	-2.29873300	-1.89198000	0.00951800
C	-1.37084000	-1.32806300	-1.05903800
O	-0.08343700	-1.08687800	-0.43420100
O	-3.62059700	-1.64545000	1.92807300
O	-3.38044800	-2.49247300	-0.69845400
O	3.24018100	-0.16784100	-1.44904700
C	4.28832400	0.35393800	-0.74946800
C	3.89718600	0.36002300	0.72023200
C	2.19605100	-0.48899500	-0.47289800
C	3.89597500	-1.16609500	1.08507700
C	2.70459000	-1.74469900	0.27045500
O	5.31801700	0.68784000	-1.29671500
C	0.88822500	-0.61754300	-1.23244800
O	0.73282200	-0.34038800	-2.40524500
C	2.36016000	0.67273400	0.57124900
C	2.06611400	2.06300300	-0.01856600
C	1.55527400	0.50946700	1.86723000
C	4.75416200	1.24255600	1.60921400
H	-6.59398400	1.26211200	-0.75735200
H	-5.39971700	3.43083700	-1.01663500
H	-3.02132000	3.61915300	-0.29915900
H	-1.85770900	1.66303300	0.65994700
H	-5.42669800	-0.69562400	0.19357400
H	-1.91943500	-0.49415100	1.58844700
H	-1.75120400	-2.65974700	0.57459100
H	-1.74707700	-0.39832900	-1.49116600
H	-1.24463000	-2.06569800	-1.85480400
H	-4.02959100	-1.06210200	2.58270800
H	-4.02026200	-2.79623300	-0.03692100
H	3.75230900	-1.28218300	2.16198400
H	4.84981900	-1.63546600	0.83065000
H	1.92509100	-2.16954600	0.90409300
H	3.00806600	-2.50617300	-0.45179700
H	0.99344200	2.18125800	-0.20208200
H	2.36211000	2.83891500	0.69367200
H	2.58856200	2.25335500	-0.95966400
H	1.68844300	-0.45722400	2.35483000
H	1.85330300	1.28707900	2.57747400
H	0.48804600	0.63838700	1.66928700
H	4.72368700	2.28883700	1.29143700
H	5.79731700	0.91351300	1.57850800
H	4.41341400	1.18587500	2.64715900

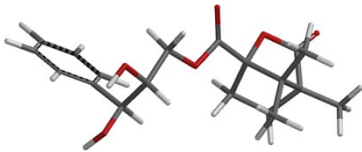
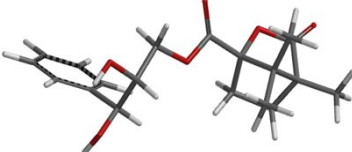
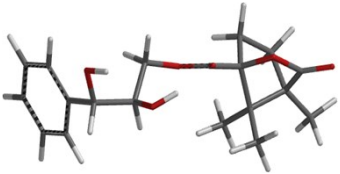
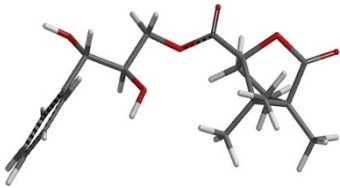
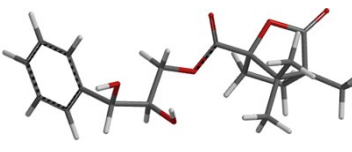
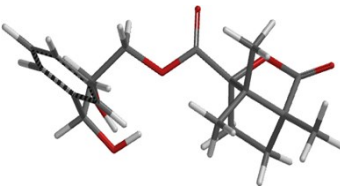
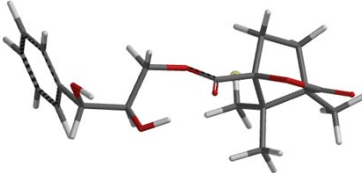
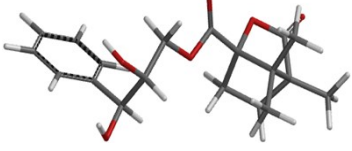
Cartesian coordinates of the low-energy conformers M3aC5

C	-6.40820200	1.04144900	1.22125600
C	-6.77242300	1.65464000	0.01937700
C	-6.05623400	1.36961700	-1.14945600
C	-4.98022600	0.48008900	-1.11388200
C	-4.60459300	-0.13615700	0.09020900
C	-5.33193600	0.14821800	1.25299800
C	-3.44170800	-1.11209100	0.13346600
C	-2.08094300	-0.43651100	-0.11469500
C	-0.94833700	-1.45560500	-0.08416900
O	0.27533400	-0.69854200	-0.30599600
O	-3.55559500	-2.13028700	-0.87270000
O	-1.91021100	0.54095400	0.91065000
O	2.30510900	0.78628400	-1.01088000
C	3.34302700	1.63171100	-0.74011100
C	4.38126100	0.84421600	0.04680000
C	2.65474600	-0.50969800	-0.42143200
C	4.95077500	-0.14852500	-1.02725700
C	3.75428100	-1.09319300	-1.33237500
O	3.35180900	2.77791300	-1.13607800
C	1.42641700	-1.37354300	-0.23368100
O	1.50987300	-2.56688800	-0.00183700
C	3.41822200	-0.07851100	0.88236100
C	2.53410700	0.69194000	1.87902300
C	4.11210200	-1.22554700	1.62820900
C	5.41250100	1.68980100	0.77185200
H	-6.96209800	1.25217300	2.13152500
H	-7.60977900	2.34580000	-0.00930200
H	-6.33697600	1.83953500	-2.08770900
H	-4.43479700	0.25720300	-2.02657800
H	-5.05530400	-0.33015600	2.18908300
H	-3.40858400	-1.57391000	1.13015500
H	-2.09849200	0.04759500	-1.10115300
H	-1.05430500	-2.20128200	-0.87285900
H	-0.88521500	-1.95098000	0.88852600
H	-4.41370400	-2.56516100	-0.76948600
H	-1.06029800	0.98115500	0.76648300
H	5.80391400	-0.68717500	-0.60778400
H	5.30550000	0.38521400	-1.91282400
H	3.95912900	-2.13360800	-1.07706000
H	3.43209000	-1.05503400	-2.37563300
H	1.81473700	0.01669900	2.35337000
H	3.15479600	1.11666200	2.67364600
H	1.97257600	1.50843400	1.41784900
H	4.78624000	-1.81524900	1.00576800
H	4.69454700	-0.81726400	2.46001300
H	3.36631500	-1.90574100	2.04998800
H	4.94360100	2.36743400	1.49122400
H	5.97766700	2.29674300	0.05801700
H	6.12087200	1.05165300	1.30850600

Cartesian coordinates of the low-energy conformers M3aC6

C	3.53653600	2.65954000	0.31694300
C	4.87822100	2.55309900	0.69390200
C	5.55924700	1.34854400	0.48821400
C	4.90181500	0.25497600	-0.08166400
C	3.55181400	0.34850300	-0.45600100
C	2.88284200	1.56583100	-0.25864000
C	2.81044900	-0.82713600	-1.07134700
C	2.31134000	-1.89567800	-0.07108600
C	1.36713000	-1.37709300	1.00615900
O	0.09403600	-1.09794600	0.36849700
O	3.63479800	-1.57908400	-1.97766800
O	3.39306800	-2.50645700	0.62777600
O	-3.30121500	-0.46109500	1.34499300
C	-4.33717700	0.14860600	0.69950400
C	-3.87260700	0.46232200	-0.71471400
C	-2.19640100	-0.54425300	0.38701300
C	-3.77897200	-0.95912400	-1.37315400
C	-2.60686400	-1.64539300	-0.61571700
O	-5.40864900	0.32722900	1.23895700
C	-0.92018600	-0.75887200	1.17952400
O	-0.81926100	-0.63703200	2.38425900
C	-2.36239900	0.79550300	-0.41663100
C	-2.16376900	2.05156300	0.44955700
C	-1.48289200	0.91794800	-1.66696100
C	-4.72533200	1.47338200	-1.45926200
H	3.00075200	3.59342100	0.45987700
H	5.39125200	3.40246600	1.13539700
H	6.60443200	1.25953000	0.77033900
H	5.44450300	-0.66987600	-0.24561100
H	1.84464500	1.66602800	-0.56352200
H	1.92805100	-0.44729300	-1.60275300
H	1.77693100	-2.65094500	-0.66476300
H	1.73982000	-0.46932900	1.48639500
H	1.22375700	-2.14923400	1.76496400
H	4.03895000	-0.97280400	-2.61417600
H	4.03989100	-2.78777200	-0.03676400
H	-3.57190900	-0.85230200	-2.44077000
H	-4.72162800	-1.50419300	-1.27685800
H	-1.77758800	-1.91057800	-1.27253200
H	-2.91353200	-2.54381000	-0.07510800
H	-1.10934800	2.16570500	0.72090100
H	-2.45302900	2.94210500	-0.11635100
H	-2.74658000	2.03652100	1.37415900
H	-1.54279800	0.06078900	-2.33879900
H	-1.77701800	1.80815500	-2.23180800
H	-0.43547300	1.04377300	-1.38086000
H	-4.77132300	2.43032000	-0.93129200
H	-5.74863400	1.10114100	-1.56721400
H	-4.32310200	1.64966300	-2.46120600

Table 5. B3LYP/6-311g(d,p) optimized low-energy conformers for M4a

 M4aC1 (1.3%)	 M4aC2 (1.3%)	 M4aC3 (36.8%)
 M4aC4 (2.6%)	 M4aC5 (15.0%)	 M4aC6 (3.8%)
 M4aC7 (36.8%)	 M4aC8 (1.1%)	

Cartesian coordinates of the low-energy conformers M4aC1

C	5.61326300	1.32651600	-0.27993300
C	4.98685700	2.56595100	-0.14945900
C	3.68307400	2.63049600	0.33953500
C	3.01071300	1.46078600	0.69106500
C	3.62608700	0.21141500	0.55290700
C	4.93889700	0.15774200	0.06780200
C	2.86502800	-1.04885600	0.91921900
C	2.26554900	-1.82311600	-0.27624700
C	1.36922800	-1.01064000	-1.19370500
O	0.19536500	-0.62270400	-0.43840800
O	3.70515800	-2.02915700	1.55037800
O	3.29204800	-2.34431000	-1.11276300
O	-2.76847600	1.33725200	-0.89660700
C	-4.01702800	1.25250600	-0.35057400
C	-3.97444500	0.15901000	0.70666300
C	-1.94553900	0.33141100	-0.22742100
C	-3.08916600	0.79476100	1.83080800
C	-1.67970400	0.89047200	1.18410200
O	-4.91195800	1.97994500	-0.68987000
C	-0.75593000	0.04034600	-1.11921300
O	-0.67227100	0.33631200	-2.28413200
C	-2.97436200	-0.83124000	0.00751300
C	-3.51684800	-1.43218200	-1.29743500
C	-2.47385400	-1.96964000	0.90003800
C	-5.33101200	-0.34813200	1.14870000
H	6.63045200	1.26935400	-0.65232800
H	5.51410500	3.47437000	-0.41957700
H	3.19157100	3.59039500	0.45546500
H	2.00168100	1.52020200	1.08546200
H	5.43810900	-0.79796700	-0.02893600
H	2.03963700	-0.77794600	1.58649300
H	1.67459800	-2.64394800	0.15266500
H	1.06761800	-1.62574800	-2.04270000
H	1.87281200	-0.11802300	-1.56732700
H	4.20827500	-1.58979000	2.24701800
H	3.92802400	-2.76110700	-0.51620000
H	-3.09245800	0.14625400	2.70785400
H	-3.47978200	1.76671500	2.13805000
H	-0.93819300	0.29516800	1.71359900
H	-1.30860700	1.91378600	1.11320100
H	-2.74042500	-2.01446200	-1.80150600
H	-4.34361500	-2.11207100	-1.07672000
H	-3.88105900	-0.68175900	-2.00182000
H	-1.70307100	-2.54611500	0.38283600
H	-2.05904300	-1.63815300	1.85129400
H	-3.30113100	-2.65118300	1.11654200
H	-5.91591900	0.46272600	1.59107100
H	-5.90284400	-0.75151600	0.30937400
H	-5.22452000	-1.13352500	1.90122200

Cartesian coordinates of the low-energy conformers M4aC2

C	5.61279500	1.32676100	-0.28081700
C	4.98644300	2.56619300	-0.14997600
C	3.68289500	2.63069400	0.33962500
C	3.01071500	1.46095000	0.69141200
C	3.62601600	0.21159000	0.55289000
C	4.93860700	0.15795900	0.06714900
C	2.86507900	-1.04864800	0.91949400
C	2.26571600	-1.82328500	-0.27579100
C	1.36933900	-1.01114000	-1.19347400
O	0.19552200	-0.62291000	-0.43823000
O	3.70522600	-2.02871200	1.55103900
O	3.29227100	-2.34459900	-1.11214300
O	-2.76805900	1.33724700	-0.89659300
C	-4.01668200	1.25276700	-0.35063700
C	-3.97441800	0.15927100	0.70656300
C	-1.94541400	0.33115100	-0.22744100
C	-3.08903900	0.79479600	1.83074400
C	-1.67947300	0.89001700	1.18415300
O	-4.91139400	1.98047800	-0.68991700
C	-0.75592100	0.03972900	-1.11921900
O	-0.67247400	0.33508300	-2.28432000
C	-2.97457200	-0.83120800	0.00742400
C	-3.51715100	-1.43198100	-1.29757000
C	-2.47437500	-1.96976900	0.89993500
C	-5.33112200	-0.34757900	1.14858000
H	6.62981400	1.26963100	-0.65368900
H	5.51356900	3.47462700	-0.42029600
H	3.19140500	3.59057100	0.45584100
H	2.00185600	1.52034400	1.08625800
H	5.43781900	-0.79772000	-0.02997400
H	2.03962100	-0.77764200	1.58664200
H	1.67484400	-2.64407400	0.15333100
H	1.06766200	-1.62648900	-2.04225900
H	1.87293900	-0.11865000	-1.56738700
H	4.20992900	-1.58860600	2.24606300
H	3.92811800	-2.76140900	-0.51544500
H	-3.09262700	0.14640500	2.70787100
H	-3.47934000	1.76693400	2.13782200
H	-0.93824800	0.29435500	1.71364100
H	-1.30798700	1.91319700	1.11340400
H	-2.74093500	-2.01472000	-1.80143700
H	-4.34429500	-2.11142500	-1.07693500
H	-3.88080100	-0.68140600	-2.00208700
H	-1.70336200	-2.54610600	0.38293900
H	-2.05998700	-1.63841500	1.85143600
H	-3.30174000	-2.65134200	1.11597100
H	-5.91582900	0.46339500	1.59100800
H	-5.90306900	-0.75077000	0.30924300
H	-5.22471100	-1.13299200	1.90107900

Cartesian coordinates of the low-energy conformers M4aC3

C	4.92712900	2.24900100	0.85413300
C	5.58484200	2.38130600	-0.36949900
C	5.58028100	1.31823300	-1.27031700
C	4.91850200	0.13053600	-0.95570400
C	4.25369600	-0.00699600	0.26590500
C	4.27031200	1.06223900	1.17003500
C	3.52263500	-1.27921300	0.63528000
C	1.98221400	-1.14465000	0.63969900
C	1.42251600	-0.78074400	-0.73344100
O	0.08707200	-0.18238600	-0.66862600
O	3.89969600	-2.33624000	-0.24170000
O	1.51499700	-2.41767500	1.09844500
O	-3.35781400	-1.15157700	-0.64329800
C	-4.48866300	-0.48538900	-0.26195100
C	-4.08042400	0.94281400	0.06565800
C	-2.25863400	-0.19368600	-0.56637100
C	-3.72841300	1.53522200	-1.34055800
C	-2.45191900	0.75732200	-1.76376600
O	-5.56780700	-1.01360700	-0.25848400
C	-0.96748200	-0.97595200	-0.48000600
O	-0.90345000	-2.16475800	-0.24458700
C	-2.66158400	0.66946100	0.68305000
C	-2.70162000	-0.14233000	1.98568300
C	-1.81832200	1.92590600	0.91443000
C	-5.09871100	1.72680200	0.86633100
H	4.93234200	3.06709500	1.56627600
H	6.10151600	3.30288400	-0.61412900
H	6.09545200	1.40966700	-2.22057100
H	4.92312200	-0.69699900	-1.65361000
H	3.77435700	0.96142200	2.13026600
H	3.79264000	-1.54121400	1.66749200
H	1.70374800	-0.35422800	1.34763300
H	1.38479400	-1.64678600	-1.39478500
H	2.01878600	0.00154100	-1.19652300
H	3.29872000	-3.06289700	-0.02516200
H	0.63656700	-2.56342500	0.71182700
H	-3.54070000	2.60571600	-1.24821300
H	-4.55416000	1.40472600	-2.04228700
H	-1.58958100	1.40833200	-1.89557200
H	-2.58507500	0.17800800	-2.67834900
H	-1.68836400	-0.40331000	2.30442800
H	-3.14815900	0.45742600	2.78241900
H	-3.27293800	-1.06872800	1.90315300
H	-0.81510500	1.65493700	1.25127800
H	-1.71682800	2.56096700	0.03502600
H	-2.27790100	2.52292700	1.70683400
H	-6.04137900	1.79549600	0.31670200
H	-5.30834700	1.25367200	1.82879700
H	-4.74318200	2.74342400	1.05152900

Cartesian coordinates of the low-energy conformers M4aC4

C	-5.92913000	1.32464700	1.17229700
C	-6.38389300	1.87401900	-0.02692200
C	-5.88522100	1.39634800	-1.23793400
C	-4.93614500	0.37438600	-1.24885600
C	-4.47183800	-0.17908100	-0.05074900
C	-4.97803400	0.30649300	1.16087400
C	-3.41123400	-1.26703700	-0.06614000
C	-1.99129400	-0.68147100	0.11737500
C	-0.94068300	-1.76573300	-0.02879600
O	0.33810100	-1.22677400	0.39583300
O	-3.58011500	-2.20739000	0.99754100
O	-1.70728000	0.30704600	-0.86887800
O	3.79564600	-1.10278800	-0.51716800
C	4.73686800	-0.12317200	-0.38108200
C	4.09296300	1.01934200	0.39124200
C	2.58431800	-0.61758300	0.14277000
C	3.93891500	0.42206700	1.83002900
C	2.88089500	-0.70182900	1.65330100
O	5.85744300	-0.25254900	-0.79771000
C	1.40274200	-1.39285200	-0.40454000
O	1.41501100	-2.03861000	-1.42255900
C	2.63138900	0.91781800	-0.17485000
C	2.53301900	1.22906900	-1.67602600
C	1.59243700	1.76262300	0.56748400
C	4.83070500	2.33870500	0.30512600
H	-6.31637800	1.68889200	2.11775600
H	-7.12525500	2.66552800	-0.01707300
H	-6.23944600	1.81295500	-2.17458400
H	-4.55969500	-0.00328700	-2.19371300
H	-4.63357400	-0.12610100	2.09296400
H	-3.44452600	-1.77572000	-1.03811700
H	-1.93092800	-0.25524200	1.12662800
H	-0.86874300	-2.09754800	-1.06396400
H	-1.16980400	-2.61218900	0.61635700
H	-4.44651900	-2.61941800	0.89017400
H	-2.26331400	1.07595200	-0.69155300
H	3.59514500	1.20026300	2.51276600
H	4.89331200	0.04909500	2.20671100
H	1.98415300	-0.52695300	2.24443100
H	3.26421200	-1.69322800	1.89893900
H	1.51763700	1.04624700	-2.03738000
H	2.75764800	2.28441000	-1.85015900
H	3.21554200	0.63542700	-2.28711400
H	0.58999800	1.52606700	0.20307600
H	1.59899600	1.62208200	1.64816000
H	1.77743600	2.82167100	0.36723400
H	5.84510900	2.23446500	0.69948000
H	4.90901500	2.68909700	-0.72707700
H	4.31886400	3.10550600	0.89196300

Cartesian coordinates of the low-energy conformers M4aC5

C	-5.60968500	-1.34799500	1.54390600
C	-6.00538400	-2.05577100	0.40813300
C	-5.60429600	-1.61472100	-0.85153800
C	-4.80713400	-0.47674500	-0.97722800
C	-4.40445500	0.23543300	0.15577800
C	-4.81873600	-0.20847900	1.41716200
C	-3.52646100	1.47170500	0.05045600
C	-2.04711300	1.23366000	0.41574200
C	-1.37424000	0.22767500	-0.50951000
O	-0.05326700	-0.03414100	0.03039300
O	-3.49936100	2.03710400	-1.26588400
O	-1.35534800	2.48030800	0.40741500
O	3.11590300	-1.37070100	-0.97677200
C	4.38665500	-1.07643300	-0.57477600
C	4.27832400	-0.10142800	0.58752000
C	2.21305300	-0.60939900	-0.11471100
C	3.69340300	-0.99507700	1.73322500
C	2.25267500	-1.32073200	1.25201100
O	5.35105800	-1.58099000	-1.08591300
C	0.87591300	-0.49634500	-0.81872800
O	0.67810800	-0.75813200	-1.97919700
C	3.02024700	0.71543900	0.11854100
C	3.25045300	1.51532100	-1.17187000
C	2.43508100	1.65222700	1.17871800
C	5.55910200	0.63385000	0.92174200
H	-5.92409300	-1.67905300	2.52777300
H	-6.62522200	-2.94027000	0.50529100
H	-5.91121800	-2.15569400	-1.74022400
H	-4.49895500	-0.13503400	-1.95791300
H	-4.52619500	0.34532000	2.30390600
H	-3.89120100	2.21950100	0.76367600
H	-2.00076700	0.86300700	1.44171000
H	-1.27892100	0.62008000	-1.52135400
H	-1.92065600	-0.71641400	-0.54505700
H	-4.35503200	2.44991500	-1.43617100
H	-1.58629100	2.90395300	-0.43111500
H	3.69542100	-0.43669800	2.67009200
H	4.30052900	-1.89031400	1.88103200
H	1.49026900	-0.92882300	1.92271100
H	2.07507400	-2.38885300	1.11975200
H	2.31510200	1.97066200	-1.50965400
H	3.95730700	2.32781800	-0.98484800
H	3.64305000	0.91155300	-1.99263500
H	1.47726300	2.05556400	0.84227100
H	2.27273000	1.17521600	2.14512900
H	3.11720100	2.49284500	1.33230800
H	6.34408900	-0.07429700	1.20030400
H	5.92329500	1.21577000	0.07147000
H	5.40608200	1.31352700	1.76378100

Cartesian coordinates of the low-energy conformers M4aC6

C	-3.69450300	-2.59935700	-0.01096800
C	-4.87139900	-2.44945600	0.71807800
C	-5.43396500	-1.17993500	0.86017800
C	-4.81801100	-0.07274900	0.28309800
C	-3.62688100	-0.21259500	-0.44220800
C	-3.07758300	-1.48835500	-0.58926400
C	-2.97641300	1.01918300	-1.05518900
C	-2.50132500	2.05396800	-0.00566300
C	-1.51902200	1.53578300	1.03890600
O	-0.30535100	1.07468300	0.36995700
O	-1.91495300	0.72142300	-1.96606500
O	-1.98266800	3.19916800	-0.67455200
O	3.21477200	0.84796200	1.03216800
C	4.19569400	0.04394400	0.52448100
C	3.56850500	-0.78776400	-0.58448800
C	1.99591600	0.55111700	0.28206700
C	3.30639000	0.26881100	-1.70898300
C	2.20768500	1.18695000	-1.10734200
O	5.32806200	0.08850500	0.92468800
C	0.82026900	1.02236000	1.11419600
O	0.86847900	1.29991000	2.28399000
C	2.13639800	-0.99113100	0.02842800
C	2.13360800	-1.82123900	1.32043100
C	1.10810000	-1.58594500	-0.93641800
C	4.37428600	-1.99973400	-1.00093100
H	-3.25373700	-3.58247100	-0.13660400
H	-5.35139300	-3.31253400	1.16600500
H	-6.35649000	-1.05297800	1.41632400
H	-5.27056400	0.90775000	0.39073900
H	-2.17266300	-1.62394500	-1.16883200
H	-3.72372100	1.53445300	-1.66436600
H	-3.37698900	2.39066200	0.55593700
H	-1.93774000	0.70689000	1.61237300
H	-1.25373000	2.34253100	1.71995300
H	-1.16941600	0.38085500	-1.45448100
H	-1.42087700	2.86181500	-1.38524800
H	2.96296000	-0.23947900	-2.61075600
H	4.21866400	0.81182300	-1.96220500
H	1.29442400	1.18081300	-1.69927500
H	2.52865100	2.22299100	-0.99249400
H	1.13785800	-1.82010000	1.77216700
H	2.38676900	-2.85978000	1.09247900
H	2.84063500	-1.46074700	2.06983200
H	0.12663300	-1.63496300	-0.45871200
H	1.00611100	-1.03514200	-1.87150400
H	1.39453000	-2.61150100	-1.18499700
H	5.35976800	-1.69514200	-1.36357200
H	4.52532200	-2.68920500	-0.16681900
H	3.87176900	-2.53894600	-1.80788200

Cartesian coordinates of the low-energy conformers M4aC7

C	-5.57984700	-1.31858600	-1.27035400
C	-5.58449200	-2.38155000	-0.36940900
C	-4.92696500	-2.24907600	0.85430600
C	-4.27025600	-1.06225000	1.17017000
C	-4.25355400	0.00688000	0.26591400
C	-4.91814600	-0.13083200	-0.95578900
C	-3.52270200	1.27918100	0.63526700
C	-1.98220800	1.14495100	0.63953400
C	-1.42260200	0.78100300	-0.73364700
O	-0.08706500	0.18260700	-0.66892600
O	-3.90008300	2.33615100	-0.24162700
O	-1.51530000	2.41809900	1.09800600
O	3.35786000	1.15157300	-0.64327200
C	4.48866900	0.48534100	-0.26192000
C	4.08036300	-0.94288200	0.06568600
C	2.25861300	0.19369000	-0.56634200
C	3.72828200	-1.53531900	-1.34047800
C	2.45186600	-0.75731900	-1.76371300
O	5.56783800	1.01351500	-0.25846900
C	0.96749000	0.97606000	-0.47996100
O	0.90353800	2.16479400	-0.24419200
C	2.66151900	-0.66940300	0.68306700
C	2.70159000	0.14237900	1.98568900
C	1.81815900	-1.92580400	0.91450300
C	5.09861200	-1.72694700	0.86631900
H	-6.09488500	-1.41014900	-2.22068100
H	-6.10110100	-3.30318800	-0.61400300
H	-4.93226000	-3.06709600	1.56655200
H	-3.77447000	-0.96128000	2.13048600
H	-4.92273300	0.69664800	-1.65378900
H	-3.79255300	1.54105700	1.66755700
H	-1.70358300	0.35461200	1.34750000
H	-1.38486100	1.64703100	-1.39500300
H	-2.01880900	-0.00134100	-1.19669700
H	-3.29911700	3.06287800	-0.02530000
H	-0.63657900	2.56364000	0.71197100
H	3.54044700	-2.60578800	-1.24805100
H	4.55402000	-1.40499500	-2.04224800
H	1.58947800	-1.40824200	-1.89561000
H	2.58509300	-0.17800300	-2.67829300
H	1.68833900	0.40332500	2.30448900
H	3.14817900	-0.45737600	2.78239500
H	3.27286600	1.06880500	1.90316300
H	0.81503700	-1.65471400	1.25155100
H	1.71642500	-2.56080800	0.03508600
H	2.27783700	-2.52288600	1.70680300
H	6.04127000	-1.79560900	0.31667000
H	5.30826300	-1.25395400	1.82884600
H	4.74304200	-2.74358100	1.05138100

Cartesian coordinates of the low-energy conformers M4aC8

C	-3.58323000	-2.59796300	0.17920400
C	-4.95032900	-2.57237400	-0.09602800
C	-5.64243700	-1.36460200	-0.02790800
C	-4.97243400	-0.18804400	0.30792500
C	-3.59865000	-0.20094900	0.57504300
C	-2.91473800	-1.42134600	0.51203700
C	-2.84604000	1.08042200	0.90982000
C	-2.29312300	1.81361100	-0.33766000
C	-1.36480100	1.01295100	-1.23950500
O	-0.19841300	0.64318400	-0.46236900
O	-3.65126600	2.00969800	1.63364400
O	-3.37789400	2.33218100	-1.11468700
O	2.74495000	-1.36905600	-0.83369400
C	3.99507700	-1.27174600	-0.29262300
C	3.96209200	-0.13537400	0.71832600
C	1.93134800	-0.32888100	-0.20666200
C	3.07219900	-0.71687200	1.86829300
C	1.66114000	-0.82656600	1.22684400
O	4.88368000	-2.01943200	-0.60280000
C	0.74571200	-0.06383500	-1.11086100
O	0.65785000	-0.41065700	-2.26105200
C	2.97044000	0.83315900	-0.02108900
C	3.51648700	1.37391000	-1.35093400
C	2.48170600	2.01255800	0.82339200
C	5.32352600	0.37734800	1.13853400
H	-3.03806400	-3.53491700	0.14252000
H	-5.47307100	-3.48754400	-0.35145800
H	-6.70795200	-1.33693900	-0.22903200
H	-5.53208400	0.73639400	0.38952700
H	-1.85367600	-1.45463100	0.73670200
H	-2.00419800	0.83092800	1.55876600
H	-1.75862700	2.69417500	0.02620900
H	-1.05705100	1.63040500	-2.08480800
H	-1.84567300	0.11009500	-1.62206500
H	-4.13937800	2.51610400	0.96975200
H	-3.85582600	1.58455800	-1.50215800
H	3.08191400	-0.03258500	2.71761100
H	3.45409500	-1.67899100	2.21493200
H	0.92545000	-0.20348600	1.73182800
H	1.28122800	-1.84858600	1.19848000
H	2.74726600	1.94897200	-1.87398000
H	4.35505300	2.04846400	-1.16051300
H	3.86440900	0.59126700	-2.02789100
H	1.71153500	2.57113300	0.28598200
H	2.07114400	1.72547500	1.79088100
H	3.31469400	2.69718600	1.00513800
H	5.90351800	-0.42231800	1.60710600
H	5.89563800	0.74601400	0.28362000
H	5.22472900	1.18904000	1.86362200

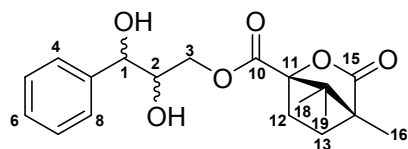


Table 6. Experimental and calculated ^1H NMR data for **M1a** and **M2a** (δ in ppm).

No.	M1a		M2a	
	δ_{H} , exptl	δ_{H} , calcd	δ_{H} , exptl	δ_{H} , calcd
1	4.55	4.55	4.56	4.45
2	3.80	3.77	3.80	3.52
3	4.10; 3.95	4.17; 4.09	4.17; 3.85	4.40; 4.04
4	7.34	7.63	7.35	7.49
5	7.34	7.62	7.35	7.51
6	7.24	7.56	7.24	7.53
7	7.34	7.56	7.35	7.57
8	7.34	7.54	7.35	7.69
12	2.35; 1.97	2.48; 2.11	2.37; 1.97	2.54; 2.08
13	1.90; 1.54	1.91; 1.51	1.90; 1.54	1.94; 1.48
16	1.00	1.00	1.00	0.96
18	1.00	1.00	1.01	0.96
19	0.83	0.89	0.83	0.84

Table 7. Experimental and calculated ^1H NMR data for **M3a** and **M4a** (δ in ppm).

No.	M3a		M4a	
	δ_{H} , exptl	δ_{H} , calcd	δ_{H} , exptl	δ_{H} , calcd
1	4.45	5.09	4.47	4.59
2	3.74	4.08	3.74	4.21
3	4.35; 4.20	4.65; 3.93	4.26; 4.26	4.31; 4.25
4	7.33	7.51	7.33	7.89
5	7.33	7.59	7.33	7.66
6	7.24	7.60	7.24	7.58
7	7.33	7.63	7.33	7.55
8	7.33	7.64	7.33	7.47
12	2.38; 1.97	2.38; 2.12	2.37; 1.97	2.57; 2.15
13	1.90; 1.54	1.86; 1.49	1.90; 1.54	1.95; 1.54
16	1.02	1.00	1.01	1.02
18	1.00	0.98	1.01	1.00
19	0.83	0.90	0.84	0.88