

Supporting Information

Stereoselective Functionalization of Platensimycin and Platencin by Sulfa-Michael/Aldol Reactions

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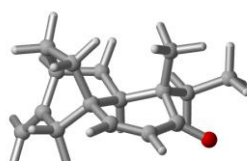
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Computational Data

- M06-2X/6-31+G(d) solution-phase potential energy (E)
- M06-2X/6-31+G(d) solution-phase enthalpy at 298.15 K (H)
- M06-2X/6-31+G(d) solution-phase Gibbs free energy at 298.15 K and 1 mol/L (G)

Compound 12

(M06-2X/6-31+G(d))/CPCM (water)



C	-2.16655600	-1.48580900	-0.60689100
C	-1.49231100	-0.28251700	0.08737700
C	-2.05967700	1.03674400	-0.44332800
C	-1.25945100	2.26048800	-0.20121800
O	-3.13922500	1.11372200	-1.01358300
C	0.04275600	2.20968400	0.11073000
C	0.02075900	-0.28781700	-0.27282400
C	0.83641400	0.94496100	0.19421700
C	2.29289700	-1.21424800	0.31048100
C	2.71439200	-0.32624000	-0.83718900
C	2.05277500	1.03987000	-0.76376700
C	-1.78318900	-0.29115300	1.60172400
C	2.44623100	-0.41200000	1.61360200
C	1.42329400	0.75038500	1.61683100
C	0.79833000	-1.56192400	0.13449000
C	3.54648600	-0.69982200	-1.81087600
H	0.59116800	3.13814000	0.28026700
H	-1.78250500	3.20642600	-0.31765100
H	-1.54873000	-2.37169600	-0.41997800
H	-2.13643400	-1.30931200	-1.68996700
H	0.03991300	-0.24379400	-1.37476300
H	2.89826300	-2.12594000	0.33787500
H	1.73703500	1.37227600	-1.75986800
H	2.75910100	1.78777100	-0.37652100
H	-1.37603800	0.59006100	2.10131300
H	-1.36790000	-1.18676100	2.07678900
H	-2.86302800	-0.29119500	1.77598000
H	3.47051700	-0.03137600	1.69400400

H	2.27636600	-1.07073600	2.47209600
H	0.62445200	0.55289000	2.33391900
H	1.90189400	1.68614900	1.92890700
H	0.68184100	-2.33813400	-0.62757600
H	0.41929200	-1.97256200	1.07992800
H	3.79772500	-0.03243800	-2.63270300
H	4.00491300	-1.68629200	-1.81241900
C	-3.59966900	-1.81919700	-0.18497100
H	-4.25799200	-0.95065200	-0.25964100
H	-3.99880500	-2.60564200	-0.83391700
H	-3.63813300	-2.19540000	0.84226600

0 imaginary frequency

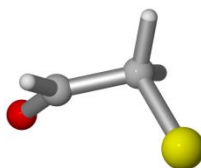
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H = -697.497211

G = -697.554560

CHOCH2S⁻

(M06-2X/6-31+G(d)/CPCM (water))



S	1.48107300	-0.29122500	-0.02914100
C	0.02807400	0.84758200	-0.09358500
C	-1.11448300	0.02992100	0.40498100
O	-2.01332500	-0.41049400	-0.29233700
H	-0.18022400	1.19382400	-1.10950600
H	0.18762300	1.70839600	0.56397000
H	-1.07951000	-0.22367800	1.48210400

0 imaginary frequency

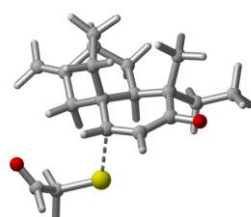
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TS-M1

(M06-2X /6-31+G(d)/CPCM (water))



C	2.97091400	-0.66357100	-1.32669700
C	2.17478300	-0.32002700	-0.03470900
C	1.79249100	-1.62499200	0.69946500
C	0.46032100	-1.85101300	1.11678000
O	2.71949300	-2.43559000	0.96349800
C	-0.62388400	-0.99707300	0.83697900
C	0.90818600	0.44680200	-0.52246100
C	-0.31474900	0.42140100	0.41695500
C	0.25864100	2.89647000	-0.19426200
C	-1.18568300	2.58342000	-0.49198600
C	-1.47717400	1.10374100	-0.33232400
C	3.07847300	0.46383800	0.93451600
C	0.46927400	2.66411200	1.31374500
C	-0.08360100	1.27023800	1.69681300
C	1.15860800	1.91745200	-0.97560400
C	-2.09868000	3.49634400	-0.83278400
C	-3.43957600	-1.54489800	-1.09425900
H	-1.50102700	-1.08087600	1.48019400
S	-1.67874700	-2.05373600	-0.89703200
C	-4.04725600	-1.69250900	0.26346500
O	-4.33504900	-0.76181100	0.99367500
H	2.93361600	0.22318100	-1.97615400
H	2.41791100	-1.45062900	-1.85906600
H	0.27597700	-2.78333200	1.64756200
H	0.57158700	-0.11813300	-1.40401300
H	0.49745500	3.93184200	-0.46142200
H	-1.57713800	0.64260600	-1.32261600
H	-2.42406500	0.93695500	0.19872100
H	2.53876200	0.78279200	1.82932500
H	3.51851200	1.34980500	0.46465200
H	3.89883000	-0.18260800	1.25723600
H	-0.03501100	3.44911400	1.88708300
H	1.54040300	2.73566600	1.53699400
H	0.58162300	0.75098100	2.39169000
H	-1.05041000	1.37302600	2.20764200
H	0.95978700	2.02426300	-2.04846600
H	2.20306800	2.20876100	-0.82451200

H	-3.13885700	3.22463800	-1.00321300
H	-1.83276700	4.54418300	-0.95535100
H	-3.54054100	-0.51694400	-1.45097700
H	-3.91765700	-2.23631600	-1.79600100
H	-4.17019700	-2.73364400	0.61789600
C	4.43418100	-1.08301000	-1.18264300
H	4.53360400	-1.94861500	-0.52451700
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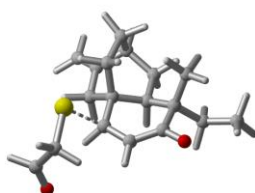
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H = -1248.887563

G = -1248.956601

TS-M2

(M06-2X /6-31+G(d)/CPCM (water))



C	2.83491700	-1.68230100	-1.03427600
C	1.78227100	-1.14976200	-0.01448200
C	0.60790500	-2.15340500	0.02439200
C	-0.69486900	-1.70795100	-0.30194000
O	0.87776600	-3.36360700	0.23924500
C	-1.11119900	-0.36161300	-0.32344100
C	1.30030300	0.21024100	-0.59551700
C	-0.06880500	0.72505900	-0.07200500
C	1.76092500	2.58855700	0.19052800
C	0.57108500	3.09182200	-0.59120300
C	-0.41848000	1.98022500	-0.89816100
C	2.41270000	-1.09371800	1.38613900
C	1.26860400	2.12474600	1.57402800
C	0.03824800	1.20735600	1.39398500
C	2.34702600	1.36095500	-0.52700300
C	0.39947800	4.36466900	-0.95609200
C	-3.89363000	-1.22639900	0.58365600
H	-1.85802600	-0.09583200	-1.07125900
S	-2.72405200	-0.00023100	1.27317100

C	-4.48440000	-0.61196600	-0.64554600
O	-4.20880800	-0.94895700	-1.78246700
H	3.45356700	-0.82808500	-1.34285000
H	2.29159800	-2.00179600	-1.93461800
H	-1.41851300	-2.48955800	-0.52838400
H	1.12122000	-0.00242200	-1.65910700
H	2.51802500	3.37390500	0.29114600
H	-0.38784400	1.73311000	-1.96920300
H	-1.44461600	2.29758000	-0.66861200
H	1.73469900	-0.67682100	2.13364300
H	3.33806400	-0.50693000	1.39658100
H	2.66219400	-2.11128600	1.69969700
H	1.00920200	2.98933800	2.19415900
H	2.08705600	1.59718000	2.07828300
H	0.04830600	0.36340700	2.08837100
H	-0.86816500	1.78084200	1.61936700
H	2.66790000	1.64278000	-1.53645200
H	3.24795300	1.04500000	0.01037800
H	-0.48707300	4.68552900	-1.49990500
H	1.14359600	5.12437500	-0.72654900
H	-3.38564700	-2.16455300	0.33898300
H	-4.67605400	-1.41381900	1.32508500
H	-5.16834000	0.24005100	-0.47058600
C	3.77259200	-2.80354400	-0.58529300
H	3.21170700	-3.67438300	-0.24036600
H	4.41071300	-3.10616900	-1.42323900
H	4.43362000	-2.47506100	0.22386700

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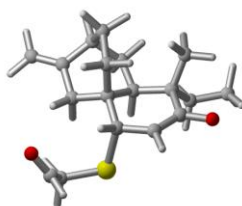
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H = -1248.881191

G = -1248.951732

TS-M1 intermediate

(M06-2X /6-31+G(d)/CPCM (water))



C	3.01419800	-0.52665500	-1.27721500
C	2.14800600	-0.25946500	-0.01144900
C	1.77557400	-1.60295500	0.66180100
C	0.45695300	-1.90828400	0.94068700
O	2.75741400	-2.37072800	0.97701400
C	-0.73008600	-1.10039400	0.56452100
C	0.88588400	0.49157500	-0.54382700
C	-0.39552700	0.37417400	0.30985900
C	0.17123800	2.89966100	-0.07171800
C	-1.24678700	2.59865300	-0.47837300
C	-1.52540800	1.10828700	-0.44211100
C	2.98618300	0.51638100	1.02047000
C	0.29810800	2.54551000	1.42251000
C	-0.24214200	1.11252400	1.65911400
C	1.11474300	1.99479600	-0.89003700
C	-2.15161700	3.52385400	-0.80730300
C	-3.24749200	-1.59072200	-1.04012400
H	-1.52026900	-1.15638300	1.32673600
S	-1.46330100	-2.02122600	-0.92500500
C	-3.88496600	-1.80387900	0.29934800
O	-4.35041400	-0.91180600	0.97904900
H	2.98353700	0.38374400	-1.89494000
H	2.50783600	-1.30652100	-1.86455600
H	0.26548400	-2.86953700	1.41755600
H	0.63486800	-0.02617400	-1.48160500
H	0.40992400	3.95601800	-0.23878600
H	-1.58819200	0.72426400	-1.46938700
H	-2.49082600	0.91031700	0.04325500
H	2.40432800	0.77142100	1.90934700
H	3.41366000	1.43890900	0.61228900
H	3.81462400	-0.11904500	1.34320900
H	-0.26130900	3.27110800	2.02281600
H	1.35056600	2.62614400	1.71725500
H	0.40194300	0.54510800	2.33670700
H	-1.23331300	1.15738500	2.13145700
H	0.93836300	2.17220000	-1.95783400
H	2.14902900	2.29527800	-0.69639500
H	-3.17469300	3.25439100	-1.06325200
H	-1.89519100	4.58093500	-0.83169700
H	-3.42551500	-0.57619900	-1.39875200
H	-3.65847900	-2.31424900	-1.75269900
H	-3.87344500	-2.84508300	0.67310500
C	4.48050900	-0.91464800	-1.08357800
H	4.56689400	-1.80313800	-0.45499900

H	4.94251100	-1.11731000	-2.05689600
H	5.05026300	-0.10417900	-0.61582100

0 imaginary frequency

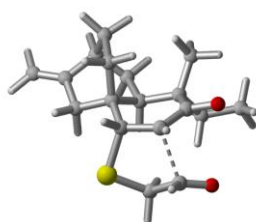
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G = -1248.961303

TS-A1

(M06-2X /6-31+G(d)/CPCM (water))



C	1.50233200	1.74062200	-1.34176900
C	0.68320700	1.39971200	-0.06255500
C	1.57918100	0.64448700	0.94874900
C	1.34788100	-0.71562900	1.26596300
O	2.54449500	1.27438300	1.44704400
C	0.07735700	-1.43326400	0.94515200
C	-0.50884100	0.51526200	-0.56159800
C	-1.05244100	-0.51145400	0.45325100
C	-3.00021100	1.04529200	-0.34699700
C	-3.37434300	-0.40489000	-0.49969600
C	-2.18307400	-1.30489700	-0.24116000
C	0.28882600	2.71306300	0.63894500
C	-2.72100400	1.27118300	1.15114000
C	-1.70932400	0.20933900	1.65288900
C	-1.71286300	1.30812100	-1.15653200
C	-4.60050300	-0.84188900	-0.79701400
S	0.45789700	-2.86451600	-0.23939400
C	1.92069800	-2.15050100	-1.01236800
C	2.91166300	-1.62987200	0.01832000
O	3.83807100	-0.86330400	-0.31629600
H	-0.29273100	-1.97440300	1.82491200
H	1.86980100	-1.04737500	2.16108700
H	0.77720400	2.01694700	-2.12226300
H	1.98771300	0.81773300	-1.68480600
H	-0.09189000	-0.09437400	-1.37647900

H	-3.81066000	1.69807200	-0.69005800
H	-1.81416900	-1.70214100	-1.19413500
H	-2.47134400	-2.17077800	0.37127200
H	-0.31471100	2.54015800	1.53322700
H	-0.25738100	3.39295900	-0.02235200
H	1.20088700	3.21925600	0.96019800
H	-3.65893600	1.20174500	1.71233200
H	-2.33762000	2.28700500	1.29211100
H	-0.94644400	0.65682000	2.29878400
H	-2.22626900	-0.54672300	2.25920900
H	-1.88393600	1.01197000	-2.19832100
H	-1.51492000	2.38337700	-1.17207600
H	-4.82748400	-1.90472000	-0.85629100
H	-5.41512400	-0.14760000	-0.99240600
H	1.67507700	-1.36416600	-1.73170300
H	2.40723800	-2.97012700	-1.55801200
H	3.07350600	-2.34597000	0.84611500
C	2.55420100	2.84566800	-1.24915200
H	3.27966800	2.63695700	-0.45963400
H	3.08864400	2.92520300	-2.20258600
H	2.10054100	3.82169300	-1.04720800

1 imaginary frequency (-184.15)

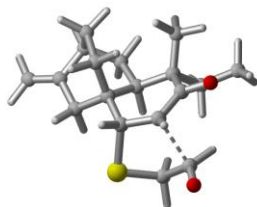
E = -1249.312098

H = -1248.892837

G = -1248.957211

TS-A2

(M06-2X /6-31+G(d)/CPCM (water))



C	1.23424400	2.02221600	-1.37510100
C	0.51553000	1.54508900	-0.07834300
C	1.53996000	0.86410100	0.85954800
C	1.48362000	-0.52758400	1.11801900
O	2.46464000	1.58109700	1.32349000
C	0.28309700	-1.37666500	0.84578600
C	-0.58971100	0.54819300	-0.56421800

C	-0.96355400	-0.57590600	0.42653700
C	-3.11449900	0.76966900	-0.22526500
C	-3.31875000	-0.70709800	-0.43582300
C	-2.02202700	-1.47018700	-0.25463600
C	0.00675500	2.78141600	0.68538900
C	-2.80125400	0.96417800	1.27076100
C	-1.64206700	0.01999800	1.68088800
C	-1.90406800	1.22033500	-1.06923600
C	-4.49362500	-1.27453900	-0.71939400
S	0.77519200	-2.74974300	-0.35262400
C	2.08238500	-1.83125100	-1.20056500
C	3.06161000	-1.19536800	-0.21999700
O	3.84914500	-1.90744700	0.44154800
H	0.01590200	-1.95577200	1.73900400
H	2.12017200	-0.85318600	1.93558400
H	0.44720000	2.25681400	-2.10773100
H	1.78642200	1.16869000	-1.79296600
H	-0.14667300	0.02692200	-1.42461800
H	-4.01045900	1.33378700	-0.50710500
H	-1.64585600	-1.79398000	-1.23238700
H	-2.18495100	-2.38213400	0.33673600
H	-0.56073400	2.51097300	1.57865100
H	-0.61749900	3.42796600	0.06087700
H	0.86962000	3.36469100	1.01251400
H	-3.69754700	0.75027900	1.86262800
H	-2.54434600	2.01404200	1.44703000
H	-0.90658300	0.53770900	2.30616500
H	-2.02979300	-0.81309000	2.28238100
H	-2.08611000	0.95321000	-2.11692200
H	-1.83410000	2.31108600	-1.03935200
H	-4.59436700	-2.35327700	-0.82420200
H	-5.39171400	-0.67596500	-0.85711900
H	1.65455600	-1.07063700	-1.85994700
H	2.62793800	-2.55807200	-1.81418300
H	3.37292100	-0.16839400	-0.49141300
C	2.17577500	3.22170000	-1.27592200
H	2.95062700	3.05588100	-0.52408000
H	2.65652300	3.39270900	-2.24549600
H	1.63499600	4.13663900	-1.01294500

1 imaginary frequency (-222.09)

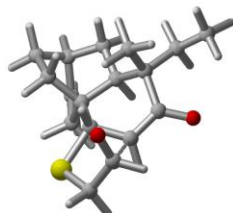
E= -1249.310170

H = -1248.890423

G = -1248.955618

TS-A3

(M06-2X /6-31+G(d)/CPCM (water))



C	-0.67523900	3.13428100	-0.32047500
C	-0.03288800	1.79471700	0.09909900
C	1.14015100	1.42890200	-0.85920300
C	1.56910300	0.08374900	-0.84059900
O	1.57857300	2.29033800	-1.66952900
C	0.90713800	-0.87561700	0.09888800
C	-1.07809100	0.66131100	-0.15708700
C	-0.62626300	-0.79601000	0.18252300
C	-3.20690500	-0.51162500	0.47214500
C	-2.85921000	-1.28449800	-0.78230600
C	-1.39189300	-1.69214600	-0.80927600
C	0.44287300	1.90719600	1.55705700
C	-2.63111300	-1.28513800	1.67016200
C	-1.09086600	-1.19029900	1.60407700
C	-2.49574300	0.86188800	0.41998600
C	-3.73077000	-1.56249700	-1.75450100
S	1.59661900	-2.55036400	-0.21947000
C	3.32540800	-1.95383500	-0.46643800
C	3.56004800	-0.57802300	0.15113400
O	3.50597800	-0.42255600	1.37909400
H	1.26767300	-0.66431100	1.11434500
H	1.98544700	-0.27894900	-1.77824900
H	-1.64056900	3.22629400	0.19333100
H	-0.89534400	3.08668300	-1.39443800
H	-1.19860300	0.67160400	-1.25237600
H	-4.29143500	-0.38748700	0.56222600
H	-0.97790300	-1.59925300	-1.82138800
H	-1.29320600	-2.74710300	-0.51147300
H	0.92950600	1.00270900	1.92557300
H	-0.39776800	2.13746700	2.22506700
H	1.17040800	2.71976300	1.65006900
H	-2.96596700	-2.32860800	1.63553200

H	-3.00682500	-0.85583500	2.60572300
H	-0.72403600	-0.44798500	2.32132800
H	-0.62735800	-2.14736700	1.87677300
H	-3.06532600	1.55717500	-0.20492200
H	-2.46191700	1.28511900	1.43464700
H	-3.43021600	-2.10187800	-2.65079600
H	-4.77407500	-1.26254500	-1.68160900
H	3.55550800	-1.93262000	-1.53382200
H	3.99216400	-2.66993200	0.02468900
H	4.10169900	0.14044800	-0.48424000
C	0.13132500	4.40202900	-0.02522600
H	1.15513900	4.31116400	-0.39441600
H	-0.33556900	5.26447400	-0.51413400
H	0.16387700	4.61823700	1.04778500

1 imaginary frequency (-200.00)

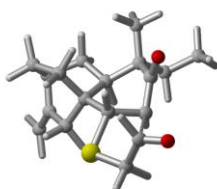
E = -1249.294893

H = -1248.875635

G = -1248.941323

TS-A4

(M06-2X /6-31+G(d)/CPCM (water))



C	1.01642500	2.74199100	1.28718200
C	0.73963100	1.92333300	0.00315800
C	-0.77753600	1.72595500	-0.17885700
C	-1.39335300	0.71548700	0.68388600
O	-1.34184900	2.23704900	-1.15963400
C	-1.05822900	-0.51413300	-0.14317600
C	1.33323200	0.47516200	0.23017800
C	0.49480500	-0.77897100	-0.23497200
C	3.08411300	-1.19801800	-0.48774000
C	2.51063500	-1.95451800	0.68260400
C	0.99200600	-1.92392200	0.67626800
C	1.32607800	2.65824200	-1.20432700

C	2.34013800	-1.64331100	-1.76096900
C	0.87451000	-1.15071700	-1.68415600
C	2.78242900	0.30095300	-0.28366900
C	3.24223400	-2.55820900	1.62227300
S	-1.95317300	-2.08343200	0.37727800
C	-3.60953000	-1.42210400	0.68678100
C	-4.15411900	-0.56309800	-0.42701000
O	-5.09125100	0.19260300	-0.27878300
H	-1.40139300	-0.35188500	-1.17169100
H	-0.81055700	0.62173800	1.61516300
H	2.09718700	2.70644900	1.48757000
H	0.52823900	2.24037800	2.13190400
H	1.38188400	0.36871500	1.32260200
H	4.16179700	-1.37182900	-0.57932200
H	0.60385800	-1.80625300	1.69528200
H	0.61547400	-2.88511100	0.29672300
H	1.27944100	2.04880300	-2.11291200
H	2.37224100	2.93495000	-1.02706700
H	0.75863800	3.57089200	-1.40075900
H	2.38061300	-2.73549300	-1.84947400
H	2.84193600	-1.22909500	-2.64290800
H	0.72316800	-0.27269200	-2.32594000
H	0.18695000	-1.92541900	-2.04837100
H	3.48992200	0.74944500	0.42394400
H	2.92760500	0.79978200	-1.24816400
H	2.77787800	-3.06235800	2.46771400
H	4.32894800	-2.56962800	1.57184400
H	-3.65431800	-0.85818100	1.61994900
H	-4.26716900	-2.29719400	0.77725100
H	-3.69325200	-0.69365200	-1.42456100
C	0.55433000	4.19799900	1.23448700
H	-0.50299700	4.26681400	0.95100600
H	0.66925000	4.67134600	2.21494500
H	1.13342700	4.78445100	0.51450600

1 imaginary frequency (-55.27)

E = -1249.254263

H = -1248.835675

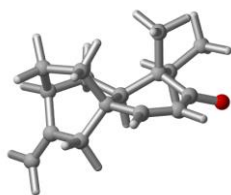
G = -1248.903047

Computational Data

- M06-2X/6-311+G(d,p) solution-phase potential energy (E)
- M06-2X/6-311+G(d,p) solution-phase enthalpy at 298.15 K (H)
- M06-2X/6-311+G(d,p) solution-phase Gibbs free energy at 298.15 K and 1 mol/L (G)

Compound 12

(M06-2X /6-311+G(d,p)/CPCM (water))



C	-2.16561000	-1.48630000	-0.59984000
C	-1.49114000	-0.28210100	0.09016600
C	-2.05415600	1.03482100	-0.44873800
C	-1.25595000	2.25751500	-0.19414000
O	-3.11733700	1.11079200	-1.03591700
C	0.04157200	2.20594300	0.11951700
C	0.02060100	-0.28896000	-0.27011800
C	0.83504800	0.94230200	0.19893300
C	2.29148300	-1.21504500	0.30610900
C	2.70561700	-0.32586400	-0.84178000
C	2.04934900	1.04082500	-0.76023700
C	-1.78184800	-0.28212400	1.60364500
C	2.45130700	-0.41330200	1.60802800
C	1.42263200	0.74298800	1.61953800
C	0.79646100	-1.56267000	0.13746600
C	3.52596600	-0.69793500	-1.82074700
H	0.58902000	3.13117600	0.29431700
H	-1.77798600	3.20164800	-0.30806400
H	-1.55193000	-2.37035800	-0.40698400
H	-2.13237400	-1.31368700	-1.68050600
H	0.04045900	-0.24374900	-1.36897300
H	2.89645100	-2.12340500	0.32753000
H	1.73335200	1.37651500	-1.75180000
H	2.75762600	1.78049300	-0.36855300
H	-1.37797100	0.60188800	2.09499700
H	-1.36595600	-1.17235600	2.08193800
H	-2.85942500	-0.28352600	1.77581800

H	3.47132800	-0.02750800	1.67867700
H	2.29120500	-1.07144900	2.46503000
H	0.62732300	0.53450700	2.33301600
H	1.89601700	1.67651000	1.93592200
H	0.67649700	-2.33803100	-0.62087800
H	0.42198100	-1.96738700	1.08403200
H	3.76939500	-0.02866700	-2.63996300
H	3.97955800	-1.68371400	-1.82721600
C	-3.60004900	-1.81114000	-0.17791000
H	-4.25154800	-0.94098500	-0.25552500
H	-4.00233100	-2.59538000	-0.82298600
H	-3.63968300	-2.18257900	0.84815500

0 imaginary frequency

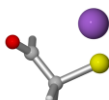
E = -698.03563123

H = -697.671794

G = -697.728974

CHOCH3S⁻Na⁺

(M06-2X /6-311+G(d,p)/CPCM (water))



C	-0.97597300	-0.80657600	0.55029200
C	-1.51843700	0.27349700	-0.32129200
O	-1.57229000	1.44600400	-0.01411400
H	-0.88316600	-0.44895600	1.57555400
H	-1.62571200	-1.68258200	0.51365700
H	-1.82887000	-0.05003700	-1.33219500
S	0.66515800	-1.21873600	-0.18786300
Na	1.93090900	1.21016300	0.08979200

0 imaginary frequency

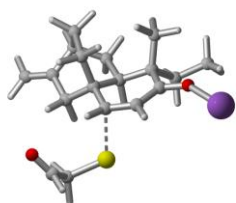
E = -713.75469835

H = -713.698854

G = -713.738640

TS-M1

(M06-2X /6-311+G(d,p)/CPCM (water))



C	2.70294900	1.10879400	-1.28159900
C	1.92842200	0.85729100	0.04454900
C	2.08798200	-0.61518300	0.46086300
C	0.96583100	-1.39983200	0.80704400
C	-0.35480700	-0.95621200	0.73211700
C	0.44161700	1.18737000	-0.27800400
C	-0.61812900	0.52217400	0.62134900
C	-1.02804000	3.09804300	0.55881000
C	-2.27215200	2.33970500	0.17482500
C	-1.99692900	0.85710300	0.01960000
C	2.55637600	1.68869000	1.17862900
C	-0.65127500	2.66042300	1.98564300
C	-0.62855100	1.11528500	2.05643200
C	0.11581700	2.70575000	-0.39707400
C	-3.46970000	2.89779900	0.01099100
C	-2.94866500	-2.09668800	-1.38039500
H	-1.11018000	-1.51194000	1.28129600
S	-1.11403900	-1.96987700	-1.28889500
C	-3.34135400	-2.73657300	-0.09015500
O	-3.85001700	-2.15032600	0.84075200
H	2.30079900	2.03234300	-1.71441900
H	2.43403100	0.30665200	-1.97879500
H	1.16970900	-2.42288800	1.10827100
H	0.27006800	0.73147500	-1.26044700
H	-1.20351000	4.17551100	0.52106500
H	-1.98758300	0.59690200	-1.04294800
H	-2.77749300	0.25460100	0.49625000
H	1.99926100	1.59602300	2.11057200
H	2.62167200	2.74743200	0.91948000
H	3.56987500	1.32902700	1.35952600
H	-1.36966900	3.06510200	2.70181000
H	0.32862300	3.07702500	2.23490800
H	0.22210100	0.75281600	2.63350600
H	-1.52840300	0.74613500	2.55970000
H	-0.17254600	2.95139800	-1.42262700
H	0.98860700	3.31846900	-0.16325500
H	-4.34266300	2.29995100	-0.23375800

H	-3.60989700	3.96918500	0.11344800
H	-3.42388100	-1.12165000	-1.48786300
H	-3.21275300	-2.74466900	-2.21855200
H	-3.07396900	-3.80530600	0.00381800
C	4.22422700	1.23851000	-1.21609100
H	4.67907500	0.34925200	-0.78229500
H	4.62344500	1.37998700	-2.22365600
H	4.52538300	2.10443000	-0.62215700
O	3.25717100	-1.07012000	0.53914000
Na	4.34252100	-2.97436100	0.85618400

1 imaginary frequency (-207.53)

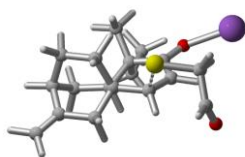
E = -1411.77671341

H = -1411.356520

G = -1411.432306

TS-M2

(M06-2X /6-311+G(d,p)/CPCM (water))



C	0.83278200	3.04130700	1.03036900
C	0.51871300	1.87046000	0.04976200
C	-0.98897600	1.57393500	0.13282100
C	-1.43133900	0.28352500	0.49469900
C	-0.63936200	-0.86980800	0.45214100
C	1.32209300	0.65530600	0.59056300
C	0.84047700	-0.74273800	0.11464200
C	3.41590200	-0.48157800	-0.29856400
C	3.11315400	-1.70283800	0.53410000
C	1.64547900	-1.78435200	0.91760400
C	0.84599400	2.30258600	-1.38804400
C	2.67095800	-0.60796700	-1.63869500
C	1.19948100	-0.99055300	-1.36859900
C	2.86527200	0.76063600	0.42016200
C	4.02215400	-2.61165600	0.88084400
C	-3.22832900	-2.23539400	-0.59607800
H	-0.88092300	-1.65743700	1.15817700
S	-1.50310100	-2.34677300	-1.19015500

C	-3.26694300	-2.93337500	0.72377200
O	-3.37607200	-2.37332700	1.79239400
H	1.90423400	2.99517500	1.25490600
H	0.31692100	2.82981100	1.97399700
H	-2.46776100	0.19974300	0.80664900
H	1.11441500	0.65929000	1.66688700
H	4.49196400	-0.38537600	-0.45986000
H	1.52645500	-1.59126100	1.99038700
H	1.25089200	-2.78681000	0.72027800
H	0.69833100	1.49940100	-2.10829100
H	1.87362300	2.66237200	-1.47825200
H	0.18387900	3.12341800	-1.66753400
H	3.14773900	-1.36206300	-2.26874800
H	2.73852600	0.34823800	-2.16597100
H	0.51067600	-0.46866600	-2.03082300
H	1.06477800	-2.05766700	-1.56399800
H	3.34553800	0.86410400	1.39660800
H	3.13855400	1.64494400	-0.16032100
H	3.75286400	-3.48722900	1.46395100
H	5.06266500	-2.50352400	0.59229500
H	-3.54061300	-1.19493800	-0.49229100
H	-3.87207200	-2.74835100	-1.31269400
H	-3.12366700	-4.02892900	0.68034300
C	0.50616800	4.46461100	0.57943700
H	-0.54735500	4.56610700	0.32338100
H	0.73951800	5.16555600	1.38493600
H	1.10268600	4.75555300	-0.28809800
O	-1.78354900	2.53567200	-0.03015100
Na	-3.96975900	2.65959100	-0.38700000

1 imaginary frequency (-242.46)

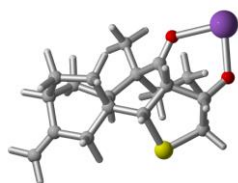
E = -1411.77058161

H = -1411.350524

G = -1411.426028

TS-M1 intermediate

(M06-2X /6-311+G(d,p)/CPCM (water))



C	2.58514900	0.93389700	-1.60461600
C	1.81620600	0.70620200	-0.26973600
C	1.96591500	-0.76150400	0.17835200
C	0.86745200	-1.52735800	0.47565500
C	-0.55355100	-1.12359800	0.30797000
C	0.33178200	1.05681800	-0.60147900
C	-0.74465000	0.39715400	0.28524000
C	-1.06707400	2.99141800	0.30288300
C	-2.34178800	2.29337600	-0.08599800
C	-2.12269100	0.80518100	-0.27456200
C	2.46160000	1.55634400	0.84028400
C	-0.68635700	2.49357500	1.70957800
C	-0.69988600	0.94507500	1.72877000
C	0.03379000	2.58360100	-0.69562200
C	-3.51993200	2.89741400	-0.22545600
C	-2.92516500	-2.23103800	-1.15344100
H	-1.18682500	-1.54670900	1.09559800
S	-1.10602700	-2.01797400	-1.26154700
C	-3.25067300	-2.87154900	0.16037600
O	-3.86568900	-2.32403600	1.04410800
H	2.18593100	1.85043200	-2.05673800
H	2.31142800	0.11758500	-2.28377600
H	1.05023300	-2.55212500	0.79057900
H	0.16497000	0.62648700	-1.59675700
H	-1.20338800	4.07539600	0.30247100
H	-2.16912300	0.56263700	-1.34192200
H	-2.91410500	0.24041800	0.23002100
H	1.91775900	1.47547900	1.78111800
H	2.53563600	2.61288600	0.57270900
H	3.47273900	1.18655100	1.01041300
H	-1.39153400	2.89082300	2.44322500
H	0.30153600	2.88451100	1.96627700
H	0.15899900	0.54136500	2.26557500
H	-1.59444800	0.58486600	2.24913700
H	-0.28986900	2.84674800	-1.70652600
H	0.92887500	3.17367500	-0.49284500
H	-4.41575200	2.33827100	-0.47864500
H	-3.62068400	3.96978900	-0.09144200
H	-3.47573800	-1.30255000	-1.28601400
H	-3.16297600	-2.92762500	-1.96111700
H	-2.84663300	-3.89055900	0.30159100
C	4.10754400	1.05968500	-1.55000700
H	4.55336700	0.18162200	-1.08561700
H	4.50608300	1.16843000	-2.56239400

H	4.41396800	1.94245800	-0.98355700
O	3.17703000	-1.19413100	0.29861200
Na	4.13452100	-2.94133600	1.18539400

0 imaginary frequency

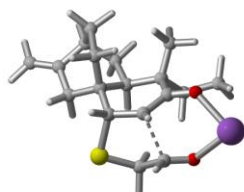
E = -1411.78601054

H = -1411.364883

G = -1411.440361

TS-A1

(M06-2X /6-311+G(d,p)/CPCM (water))



C	-0.67932100	2.04296600	-0.49418100
C	-0.37345400	1.06248800	-1.66504600
C	-1.55488200	0.08940800	-1.84669300
C	-1.41719600	-1.29568300	-1.64063200
O	-2.67059900	0.59065200	-2.14182700
C	-0.10377500	-1.98059100	-1.44865000
C	0.93610300	0.31705400	-1.24706800
C	1.10817100	-1.10708300	-1.81087700
C	3.17679400	0.35002400	-2.47133000
C	3.60886100	-0.93086300	-1.81033600
C	2.42322700	-1.67960500	-1.23913900
C	-0.29504600	1.85820800	-2.98208200
C	2.38333600	-0.04658200	-3.73083100
C	1.28598700	-1.07052400	-3.34493500
C	2.25111700	1.11382100	-1.50225200
C	4.86692100	-1.36286800	-1.75513500
S	-0.03289700	-2.68632900	0.30423600
C	-1.14933300	-1.50779500	1.08727100
C	-2.43658600	-1.36443200	0.29981600
O	-3.20675500	-0.40061300	0.49095400
H	-0.05623600	-2.89173400	-2.05138400
H	-2.21868500	-1.89027200	-2.06525100
H	0.27635000	2.49324500	-0.19835100
H	-1.01525300	1.44639200	0.36048700

H	0.85067800	0.17900500	-0.16233800
H	4.04189700	0.96127000	-2.73850200
H	2.41964800	-1.57429800	-0.15078000
H	2.49699100	-2.75102300	-1.45695200
H	-0.05487400	1.22272700	-3.83380600
H	0.43702400	2.66615700	-2.93390900
H	-1.27050200	2.30318400	-3.17349000
H	3.06216300	-0.47540500	-4.47119100
H	1.95034500	0.85364000	-4.17190900
H	0.33794300	-0.84657600	-3.83806700
H	1.57856900	-2.07428600	-3.67116600
H	2.78201600	1.27336600	-0.55989000
H	2.04529100	2.10295700	-1.91260400
H	5.11859800	-2.31479900	-1.29754200
H	5.68116700	-0.77390700	-2.16505800
H	-0.68722500	-0.53356200	1.24725100
H	-1.39976300	-1.93645600	2.06388500
H	-2.85286200	-2.33477500	-0.01413000
C	-1.68404500	3.16767200	-0.73890500
H	-2.64513600	2.77564800	-1.07007500
H	-1.83654200	3.72901300	0.18641200
H	-1.32398900	3.87146700	-1.49259900
Na	-4.61486900	0.41640400	-1.06629100

1 imaginary frequency (-170.74)

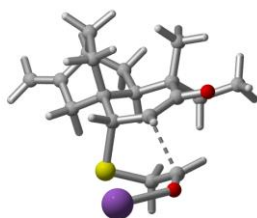
E = -1411.792804

H = -1411.371935

G = -1411.440230

TS-A2

(M06-2X /6-311+G(d,p)/CPCM (water))



C	-0.30264600	2.74072600	-0.88132800
C	-0.46612000	1.72085300	0.28349500
C	0.91044700	1.44064800	0.93334800
C	1.43872600	0.14372600	0.96743900

O	1.53127300	2.43041200	1.41061500
C	0.73411900	-1.08168200	0.52296300
C	-1.07862200	0.44280900	-0.37436600
C	-0.77805200	-0.89578300	0.33098200
C	-3.36492800	-0.60056300	0.08268600
C	-2.91673400	-1.92795500	-0.46780300
C	-1.40593600	-2.02126500	-0.51850600
C	-1.31705000	2.36236300	1.39654600
C	-2.97026500	-0.57717200	1.57073000
C	-1.47705700	-0.96201800	1.70915400
C	-2.60959200	0.52004300	-0.65942700
C	-3.74123800	-2.90450200	-0.84082100
S	1.62107500	-1.79795500	-1.01483500
C	2.22870400	-0.23611900	-1.69809600
C	3.09061400	0.51032300	-0.70409400
H	0.88800900	-1.90358500	1.22888300
H	2.32249900	0.01312600	1.58070000
H	-1.21567900	2.68617800	-1.48765300
H	0.50853000	2.38610300	-1.52838500
H	-0.58237700	0.35963600	-1.34820300
H	-4.44436100	-0.47648900	-0.03191300
H	-1.07064100	-1.92492800	-1.55497600
H	-1.06484800	-2.99996900	-0.16264200
H	-1.49172600	1.67677100	2.22592500
H	-2.28208800	2.71837700	1.02991100
H	-0.77371500	3.21954300	1.79237200
H	-3.59821500	-1.27425300	2.12987200
H	-3.16077100	0.42186400	1.96903600
H	-0.96362200	-0.32481100	2.43123700
H	-1.38726400	-1.98938500	2.07846200
H	-2.79737200	0.42186500	-1.73219700
H	-3.02243000	1.48454400	-0.36111000
H	-3.36430700	-3.85838900	-1.19743400
H	-4.81812500	-2.77521500	-0.80117400
H	1.40619600	0.38685400	-2.04516500
H	2.85300100	-0.50891700	-2.55495700
H	2.92843900	1.59568700	-0.62601300
C	-0.04909500	4.20601400	-0.52836300
H	0.83230000	4.30804100	0.10353700
H	0.10277900	4.78265700	-1.44459200
H	-0.90116000	4.64459600	-0.00416800
O	4.12963200	0.01162900	-0.26207000
Na	4.31058600	-2.22511900	0.17771100

1 imaginary frequency (-117.35)

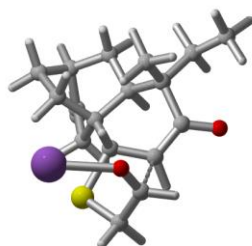
E = -1411.780275

H = -1411.360451

G = -1411.431250

TS-A3

(M06-2X /6-311+G(d,p)/CPCM (water))



C	-0.99662800	3.19291200	-0.62070300
C	-0.31718000	1.87499300	-0.19129100
C	0.70491000	1.41562300	-1.27539800
C	1.11668700	0.06764700	-1.21938800
O	1.03344000	2.20454300	-2.19465400
C	0.58151400	-0.80598500	-0.13227800
C	-1.40235800	0.75238700	-0.20901900
C	-0.92290300	-0.68669100	0.16438800
C	-3.42587100	-0.32978900	0.80708000
C	-3.27500800	-1.18876500	-0.42816500
C	-1.83491700	-1.63260100	-0.63782400
C	0.36210700	2.08640100	1.17076500
C	-2.68885500	-1.03448200	1.95765400
C	-1.17511700	-0.97128800	1.66309400
C	-2.71589300	1.02144300	0.55584900
C	-4.27823000	-1.50768600	-1.24272600
S	1.16891000	-2.53407400	-0.40322500
C	2.82592500	-2.06100200	-1.05022600
C	3.26702400	-0.73517100	-0.46382100
H	1.07696000	-0.52571400	0.80306300
H	1.41614100	-0.36038300	-2.16868600
H	-1.87846000	3.34157200	0.01019600
H	-1.35976600	3.06949000	-1.64553500
H	-1.68126100	0.69078200	-1.27009000
H	-4.48101700	-0.17784800	1.04328500
H	-1.57466900	-1.62138400	-1.70068300
H	-1.71183900	-2.66190600	-0.27778900
H	0.86692200	1.19869800	1.54750200

H	-0.36897000	2.40411000	1.92199700
H	1.11568200	2.87278200	1.09045700
H	-3.03262400	-2.06938000	2.03856600
H	-2.91864500	-0.53947300	2.90433400
H	-0.70622200	-0.18569900	2.26022800
H	-0.68389300	-1.91183000	1.93415600
H	-3.36175300	1.68283400	-0.02473000
H	-2.52570800	1.50818700	1.52010600
H	-4.11356200	-2.10645500	-2.13335500
H	-5.29315400	-1.18077400	-1.04004700
H	2.81301100	-2.02615600	-2.13732400
H	3.52474600	-2.83655800	-0.72627300
H	3.74554500	-0.02398400	-1.14650900
C	-0.14313900	4.46060900	-0.53332700
H	0.81594200	4.32296900	-1.03142000
H	-0.66305200	5.29379400	-1.01325800
H	0.04006900	4.74896800	0.50433100
O	3.35592400	-0.59955800	0.76066200
Na	2.67287500	-2.16749100	2.30207400

1 imaginary frequency (-180.82)

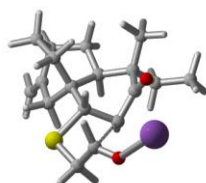
E = -1411.762463

H = -1411.342829

G = -1411.413309

TS-A4

(M06-2X /6-311+G(d,p)/CPCM (water))



C	0.06706500	2.97856300	1.12313600
C	0.26649000	2.02746200	-0.08130300
C	-1.04979000	1.27093400	-0.35660000
C	-1.32656500	0.13390200	0.53016100
O	-1.67600600	1.50761700	-1.39344600
C	-0.45141900	-0.89454200	-0.16459500
C	1.32293600	0.93908000	0.35085000
C	1.08129500	-0.56399400	-0.06173900

C	3.64509700	0.01743000	0.01196700
C	3.23017700	-0.82167000	1.19233700
C	1.82702100	-1.37522400	1.02019900
C	0.67591100	2.83911800	-1.31183400
C	3.30856900	-0.76334700	-1.27178400
C	1.77075900	-0.85449200	-1.41046500
C	2.78634000	1.29924000	0.00549100
C	3.99033400	-1.03863100	2.26373500
S	-0.75793900	-2.67466100	0.35626200
C	-2.56800700	-2.68148600	0.35849000
C	-3.17544000	-2.10718000	-0.88843600
H	-0.68938400	-0.89992400	-1.23180800
H	-0.85480200	0.31556800	1.50666200
H	1.05018200	3.36934100	1.41270500
H	-0.29421200	2.38859300	1.97138600
H	1.26653200	0.92318100	1.44467900
H	4.70915100	0.25908300	0.05972300
H	1.28387900	-1.34922900	1.96928000
H	1.89412000	-2.42574900	0.71130700
H	0.96041700	2.19111100	-2.14412600
H	1.51716500	3.49979300	-1.08367400
H	-0.16044600	3.45043200	-1.64880300
H	3.75394900	-1.76098100	-1.22203200
H	3.74550200	-0.25572600	-2.13540700
H	1.40443800	-0.13844500	-2.15345100
H	1.47290800	-1.84887000	-1.75846300
H	3.17204400	2.03184200	0.72000600
H	2.86436100	1.74229600	-0.99054200
H	3.63091600	-1.62673000	3.10275500
H	4.99599800	-0.63573200	2.32992800
H	-2.97752200	-2.16357200	1.22318000
H	-2.86059100	-3.73715200	0.40218000
H	-2.55368500	-2.13711900	-1.79982700
C	-0.89275400	4.14004700	0.87181700
H	-1.85597600	3.78022000	0.49867300
H	-1.07639000	4.68955300	1.79753500
H	-0.49303700	4.84661900	0.14178500
O	-4.30968500	-1.68524700	-0.93477100
Na	-5.51469600	-0.63055700	-2.62785700

1 imaginary frequency (-73.99)

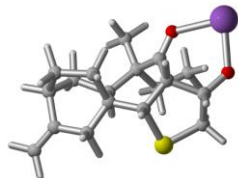
E = -1411.717456

H = -1411.298278

G = -1411.372523

TS-A1 intermediate

(M06-2X /6-311+G(d,p)/CPCM (water))



C	0.87751500	-0.84963700	2.09586400
C	0.27498600	-1.26326300	0.71593500
C	1.24490400	-0.79738000	-0.37961300
C	1.20524100	0.58902100	-0.96815500
O	2.08453700	-1.57733400	-0.80361900
C	-0.06919500	1.36518900	-0.67939400
C	-1.15017700	-0.58879600	0.60707900
C	-1.29853500	0.47365900	-0.51313400
C	-3.47666900	-0.96077400	-0.35828500
C	-3.71492800	0.44098700	0.13069500
C	-2.53569100	1.33526700	-0.18789700
C	0.23243100	-2.79753900	0.67007900
C	-2.99128000	-0.88546200	-1.81754700
C	-1.57322200	-0.26722400	-1.84349200
C	-2.33782300	-1.58532000	0.47008100
C	-4.80557000	0.84009400	0.78063900
S	0.27907100	2.46058100	0.79065100
C	2.06763100	2.11154800	0.81206400
C	2.44507700	1.50633200	-0.56002300
O	3.65679200	0.92975500	-0.58327600
H	-0.26510700	2.04913100	-1.50908500
H	1.30944600	0.43114500	-2.04589300
H	0.23701800	-1.32070600	2.85015700
H	0.74993800	0.22578100	2.22198800
H	-1.29962800	-0.04838700	1.54735300
H	-4.38402400	-1.56276300	-0.27609000
H	-2.33302500	2.00599900	0.65174400
H	-2.76481000	1.96197300	-1.05956500
H	-0.08275800	-3.16668300	-0.30780100
H	-0.45695300	-3.17651700	1.42698600
H	1.22075600	-3.20913300	0.86376400
H	-3.68613500	-0.28135400	-2.40684800
H	-2.97948800	-1.88699000	-2.25374200

H	-0.82236300	-1.05256000	-1.98427200
H	-1.46706200	0.42449000	-2.68432100
H	-2.69628600	-1.87738200	1.45995500
H	-2.03831400	-2.49832200	-0.04564800
H	-4.90883200	1.85919800	1.14016000
H	-5.62739200	0.15678500	0.96885500
H	2.31897100	1.41077900	1.60962000
H	2.60728000	3.04423800	0.97828000
H	2.34108200	2.34457900	-1.28498500
C	2.33570800	-1.23154800	2.34515800
H	2.99955700	-0.78693100	1.59907900
H	2.64528500	-0.86955600	3.32847000
H	2.48801100	-2.31226300	2.33147900
Na	4.19242100	-0.96946700	-1.50865600

0 imaginary frequency

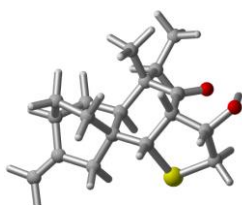
E = -1411.80783161

H = -1411.384670

G = -1411.453313

Product

(M06-2X /6-311+G(d,p)/CPCM (water))



C	0.58906800	2.60675800	-1.19163400
C	0.38809500	1.56330100	-0.07055700
C	1.63500000	0.69171800	0.05171500
C	1.53563400	-0.57170300	0.90421100
O	2.67880400	0.97861500	-0.50012900
C	0.36076600	-1.43626900	0.43668200
C	-0.79388200	0.63901400	-0.49517000
C	-0.96197200	-0.68641900	0.29117200
C	-3.24948200	0.56607600	0.17356900
C	-3.35020900	-0.81564800	-0.42518200
C	-2.00136700	-1.51459600	-0.49494300
C	0.19293900	2.27005500	1.28648000
C	-2.80136400	0.42920000	1.63953600
C	-1.57792300	-0.50747500	1.70103000

C	-2.16845800	1.36371600	-0.57511900
C	-4.48927300	-1.37009000	-0.83210900
S	0.97730300	-2.19205800	-1.14287500
C	2.74154900	-2.04869100	-0.66811500
C	2.76750900	-1.47605000	0.75958300
H	0.21886100	-2.25553900	1.14702100
H	1.40120800	-0.27758900	1.95059500
H	-0.39700500	2.99108200	-1.46825300
H	0.97579200	2.08207700	-2.07032000
H	-0.52963900	0.32604600	-1.51203900
H	-4.20996600	1.08143000	0.10976500
H	-1.68929200	-1.61109200	-1.54085000
H	-2.07103400	-2.52498100	-0.07859800
H	-0.04444300	1.58334500	2.09544500
H	-0.61208400	3.00404400	1.21570000
H	1.10112900	2.80871400	1.56482000
H	-3.61467900	0.03607500	2.25246000
H	-2.55158800	1.42264000	2.02433000
H	-0.84811400	-0.16294100	2.43373100
H	-1.88796300	-1.50267000	2.03513000
H	-2.46151700	1.49706800	-1.61892200
H	-2.11375100	2.36143500	-0.13285500
H	-4.51578200	-2.37752500	-1.23578600
H	-5.42848400	-0.82994100	-0.77324600
H	3.24037900	-1.36838100	-1.35725000
H	3.21869100	-3.02575900	-0.71310700
H	2.64986700	-2.29837300	1.46918800
C	1.49587500	3.79482500	-0.86747300
H	2.47518300	3.47016600	-0.51457500
H	1.64411900	4.39845500	-1.76549600
H	1.05337800	4.44336300	-0.10863400
O	3.99702600	-0.86445500	1.07989600
H	4.07821100	-0.09783300	0.49754700

0 imaginary frequency

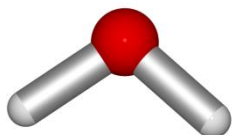
E = -1250.08009264

H = -1249.645732

G = -1249.710890

H₂O

(M06-2X /6-311+G(d,p)/CPCM (water))



O	0.00000000	0.00000000	0.11525900
H	0.00000000	0.76003000	-0.47274100
H	0.00000000	-0.76003000	-0.47274100

0 imaginary frequency

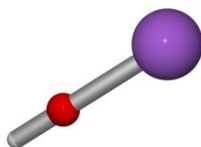
E = -76.42894147

H = -76.403642

G = -76.425063

NaOH

(M06-2X /6-311+G(d,p)/CPCM (water))



O	0.00001300	1.10525900	0.00000000
H	-0.00025400	2.06121300	0.00000000
Na	0.00001300	-0.99120700	0.00000000

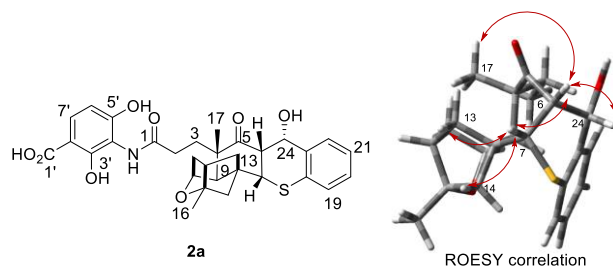
0 imaginary frequency

E = -238.15026851

H = -238.135271

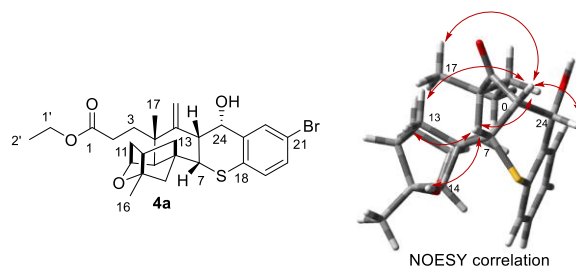
G = -238.156133

Table S1. Summary of ^1H NMR (500 MHz) and ^{13}C NMR (101 MHz) data for compound **2a** in CD_3OD (δ in ppm, J in Hz). Assignments are based on 1D and 2D NMR experiments.



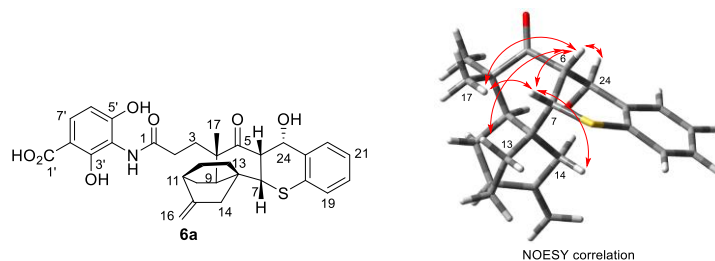
No.	δ_{C}	δ_{H} (J in Hz)
1	172.14	
2	31.05	2.55 (m, 1H), 2.36 (m, 1H)
3	32.57	2.11 (dd, $J = 15.2, 5.0$ Hz, 1H), 1.86 (dd, $J = 17.5, 7.5$ Hz, 1H)
4	48.86	
5	211.20	
6	48.48	3.57 (br, s, 1H)
7	45.25	3.76 (d, $J = 2.6$ Hz, 1H)
8	48.48	
9	45.07	2.69 (br, s, 1H)
10	77.08	4.50 (br, s, 1H)
11	40.39	2.25 (d, $J = 11.7$ Hz, 1H), 2.07 (m, 1H)
12	44.71	2.47 (d, $J = 6.6$ Hz, 1H)
13	42.68	2.44 (m, 1H), 1.76 (dd, $J = 10.7, 7.2$ Hz, 1H)
14	51.79	2.05 (d, $J = 7.9$ Hz, 1H), 1.64 (d, $J = 11.3$ Hz, 1H)
15	86.88	
16	21.88	1.46 (s, 3H)
17	26.02	1.32 (s, 3H)
18	131.20	
19	131.57	7.40 (d, $J = 8.1$ Hz, 1H)
20	127.55	7.16 – 7.11 (m, 1H)
21	126.30	7.08(d, $J = 8.4$ Hz, 1H)
22	124.49	7.16 – 7.11 (m, 1H)
23	132.92	
24	66.05	5.06 (d, $J = 1.8$ Hz, 1H)
1'	174.76	
2'	104.63	
3'	157.97	
4'	112.53	
5'	154.67	
6'	108.17	6.40(d, $J = 8.7$ Hz, 1H)
7'	129.05	7.65 (d, $J = 8.8$ Hz, 1H)

Table S2. Summary of ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) data for compounds **4a** in CDCl_3 (δ in ppm, J in Hz). Assignments are based on 1D and 2D NMR experiments.



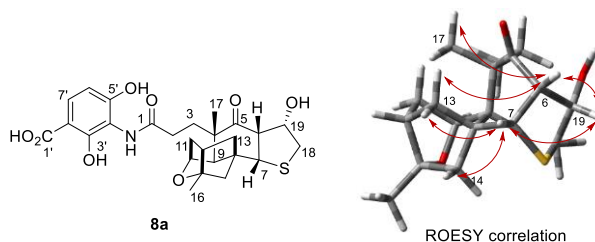
No.	δ_C	δ_H (J in Hz)
1	173.68	
2	29.38	2.37 (dd, $J = 11.2, 5.2$ Hz, 1H); 2.17 (dd, $J = 11.0, 5.4$ Hz, 1H)
3	31.64	2.03 (d, $J = 5.6$ Hz, 1H), 1.68 (m, 1H)
4	46.87	
5	210.01	
6	47.49	3.46 (d, $J = 3.1$ Hz, 1H)
7	45.51	3.68 (d, $J = 3.2$ Hz, 1H)
8	48.83	
9	44.99	2.57 (s, 1H)
10	76.79	4.38 (s, 1H)
11	40.83	2.13 (d, $J = 3.7$ Hz, 1H), 2.09 (d, $J = 5.6$ Hz, 1H)
12	44.44	2.45 (t, $J = 6.3$ Hz, 1H)
13	43.40	2.32 (dd, $J = 10.8, 4.7$ Hz, 1H), 1.73 (m, 1H)
14	52.11	2.07 (d, $J = 2.5$ Hz, 1H), 1.56 (d, $J = 11.2$ Hz, 1H)
15	86.53	
16	23.05	1.47 (s, 3H)
17	26.76	1.27 (s, 3H)
18	130.60	
19	128.43	6.98 (d, $J = 8.5$ Hz, 1H)
20	131.33	7.29 (m, 1H)
21	130.60	
22	133.76	7.51 (d, $J = 2.1$ Hz, 1H)
23	134.51	
24	66.52	5.04 (d, $J = 2.9$ Hz, 1H)
1'	60.37	4.07 (m, 2H)
2'	14.22	1.21 (t, $J = 7.1$ Hz, 3H)

Table S3. Summary of ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) data for compounds **6a** in CD_3OD (δ in ppm, J in Hz). Assignments are based on 1D and 2D NMR experiments.



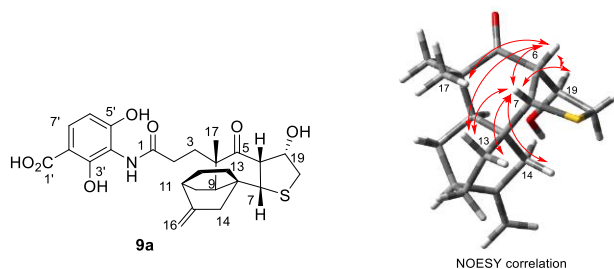
No.	δ_C	δ_H (J in Hz)
1	174.74	
2	31.06	2.47 (dd, $J = 14.3, 5.2$ Hz, 1H), 2.35 (m, 1H)
3	32.08	1.97 (m, 1H), 1.67 (m, 1H);
4	50.54	
5	212.50	
6	46.10	3.76 (dd, $J = 5.0, 3.1$ Hz, 1H)
7	69.27	3.67 (d, $J = 2.3$ Hz, 1H)
8	36.53	
9	38.55	2.58 (m, 1H)
10	27.53	1.79 (d, $J = 7.4$ Hz, 1H), 1.73 (m, 1H);
11	35.49	2.41 (dd, $J = 11.7, 5.6$ Hz, 1H)
12	26.49	1.87 (s, 1H), 1.85 (s, 1H)
13	27.64	2.53 (d, $J = 12.1$ Hz, 1H), 1.49 (dd, $J = 21.9, 8.1$ Hz, 1H);
14	42.51	2.67 (d, $J = 18.1$ Hz, 1H), 2.26 (m, 1H);
15	149.66	
16	105.67	4.90 (d, $J = 1.6$ Hz, 1H), 4.75 (d, $J = 1.6$ Hz, 1H)
17	21.86	1.32 (s, 3H)
18	131.38	
19	131.41	7.41 (m, 1H)
20	124.44	7.13 (m, 1H)
21	127.49	7.13 (m, 1H)
22	126.34	7.13 (m, 1H)
23	132.80	
24	66.22	5.08 (d, $J = 2.5$ Hz, 1H)
1'	missing	
2'	105.67	
3'	156.90	
4'	112.41	
5'	154.53	
6'	106.67	6.30 (d, $J = 8.7$ Hz, 1H)
7'	128.67	7.61 (d, $J = 8.7$ Hz, 1H)

Table S4. Summary of ^1H NMR (500 MHz) and ^{13}C NMR (126 MHz) data for compounds **8a** in CD_3OD (δ in ppm, J in Hz). Assignments are based on 1D and 2D NMR experiments.



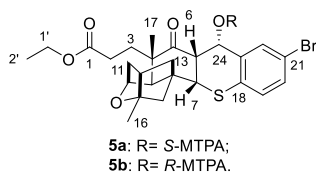
No.	δ_C	δ_H (J in Hz)
1	173.68	
2	30.94	2.55 (m, 1H), 2.44 (d, $J = 6.6$ Hz, 1H)
3	32.31	2.18 (m, 1H); 1.85 (m, 1H)
4	48.65	
5	211.77	
6	56.78	3.18 (d, $J = 4.1$ Hz, 1H)
7	55.52	3.80 (d, $J = 4.3$ Hz, 1H)
8	48.48	
9	43.18	2.64 (br, s, 1H),
10	76.89	4.50 (br, s, 1H),
11	40.25	2.23 (d, $J = 11.6$ Hz, 1H), 2.05 (m, 1H)
12	45.19	2.46 (br, s, 1H)
13	44.33	2.31 (m, 1H), 1.74 (br, s, 1H)
14	55.00	1.77 (d, $J = 3.6$ Hz, 1H), 1.69 (d, $J = 11.2$ Hz, 1H)
15	86.82	
16	21.74	1.42 (s, 3H)
17	25.13	1.31 (s, 3H)
18	36.95	3.11 (dd, $J = 11.5, 4.8$ Hz, 1H), 2.75 (d, $J = 11.5$ Hz, 1H)
19	73.82	5.03 (d, $J = 4.5$ Hz, 1H)
1'	174.73	
2'	107.63	
3'	157.52	
4'	112.51	
5'	156.77	
6'	107.63	6.41 (d, $J = 8.6$ Hz, 1H)
7'	129.08	7.67 (d, $J = 8.6$ Hz, 1H)

Table S5. Summary of ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) data for compounds **9a** in CD_3OD (δ in ppm, J in Hz). Assignments are based on 1D and 2D NMR experiments.



No.	δ_C	δ_H (J in Hz)
1	175.08	
2	31.04	2.51 (m, 1H), 2.43 (dt, $J = 9.6, 4.2$ Hz, 1H)
3	31.73	2.04 (m, 1H), 1.57 (dd, $J = 21.7, 9.5$ Hz, 1H)
4	50.37	
5	213.06	
6	55.66	3.30 (d, $J = 3.9$ Hz, 1H)
7	57.19	3.83 (d, $J = 4.4$ Hz, 1H)
8	34.19	
9	36.76	2.51 (m, 1H)
10	27.48	1.67 (m, 2H)
11	35.75	2.38 (d, $J = 9.6$ Hz, 1H)
12	26.76	1.81 (d, $J = 1.3$ Hz, 1H), 1.78 (m, 1H)
13	30.03	2.34(m. 1H), 1.49 (d, $J = 13.7$ Hz, 1H)
14	45.96	2.29 (s, 2H)
15	150.01	
16	105.55	4.84 (m, 1H), 4.67 (d, $J = 1.5$ Hz, 1H)
17	20.39	1.27 (s, 3H)
18	36.69	3.11 (dd, $J = 11.5, 4.8$ Hz, 1H), 2.77 (dd, $J = 24.4, 11.1$ Hz, 1H)
19	73.89	5.05 (d, $J = 4.2$ Hz, 1H)
1'	172.17	
2'	104.73	
3'	157.59	
4'	112.72	
5'	157.56	
6'	108.49	6.35 (d, $J = 8.7$ Hz, 1H)
7'	129.08	7.63 (d, $J = 8.7$ Hz, 1H)

Table S6. ^1H NMR spectroscopic data in CDCl_3 (δ in ppm, J in Hz) for MTPA-esters **5a** and **5b** and their corresponding $\Delta\delta_{\text{S-R}}$.



Position	δ_{H} for 5a (<i>S</i> -MTPA)	δ_{H} for 5b (<i>R</i> -MTPA)	$\Delta\delta_{\text{S-R}}$
2a	2.3530	2.3899	-0.0369
2b	2.2241	2.1970	+0.0271
3a	2.0676	2.0733	-0.0057
3b	1.7480	1.7516	-0.0036
6	3.4227	3.5630	-0.1403
7	3.4014	3.5447	-0.1433
9	2.5487	2.5809	-0.0322
10	4.4035	4.4241	-0.0206
11a	2.1172	2.1427	-0.0255
11b	2.1086	2.1153	-0.0067
12	2.4159	2.4637	-0.0478
13a	2.1628	2.2565	-0.0937
13b	1.4361	1.6011	-0.1650
14a	2.0111	2.0340	-0.0229
14b	1.4652	1.5335	-0.0683
16	1.4499	1.4725	-0.0226
17	1.2924	1.3137	-0.0213
19	7.0010	6.9610	+0.0400
20	7.3304	7.4177	-0.0873
22	7.4100	7.4289	-0.0189
24	6.5549	6.5164	+0.0385
1'	4.0906	4.0921	-0.0015
2'	1.2268	1.2277	-0.0009

Figure S1. Structures of bioactive thiochromanes and tetra-hydrothiophenes (A).

Structures of adamantane derivatives (B).

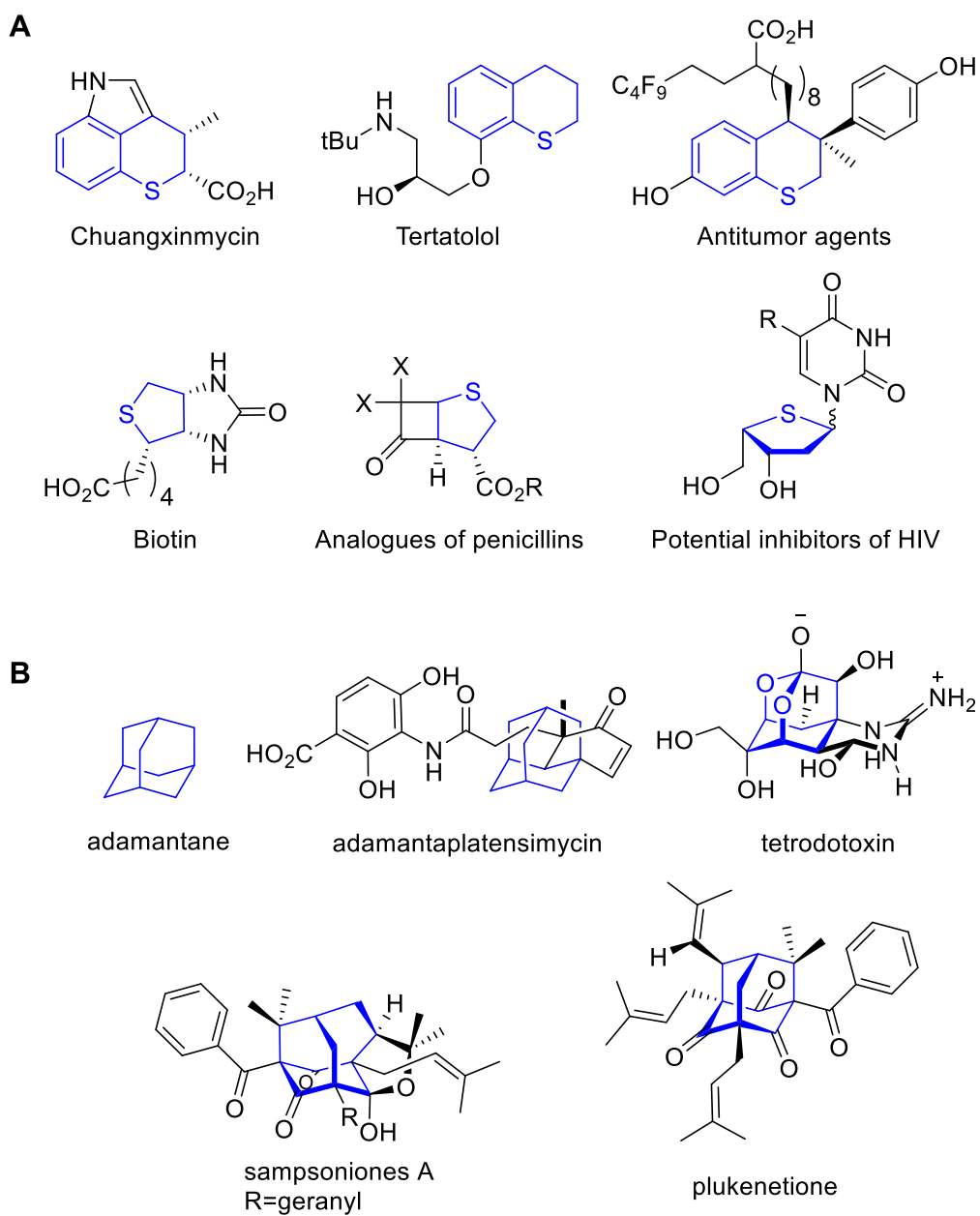


Figure S2. ^1H NMR (500 MHz) and ^{13}C NMR (101 MHz) spectrum of **2a** in CD_3OD .

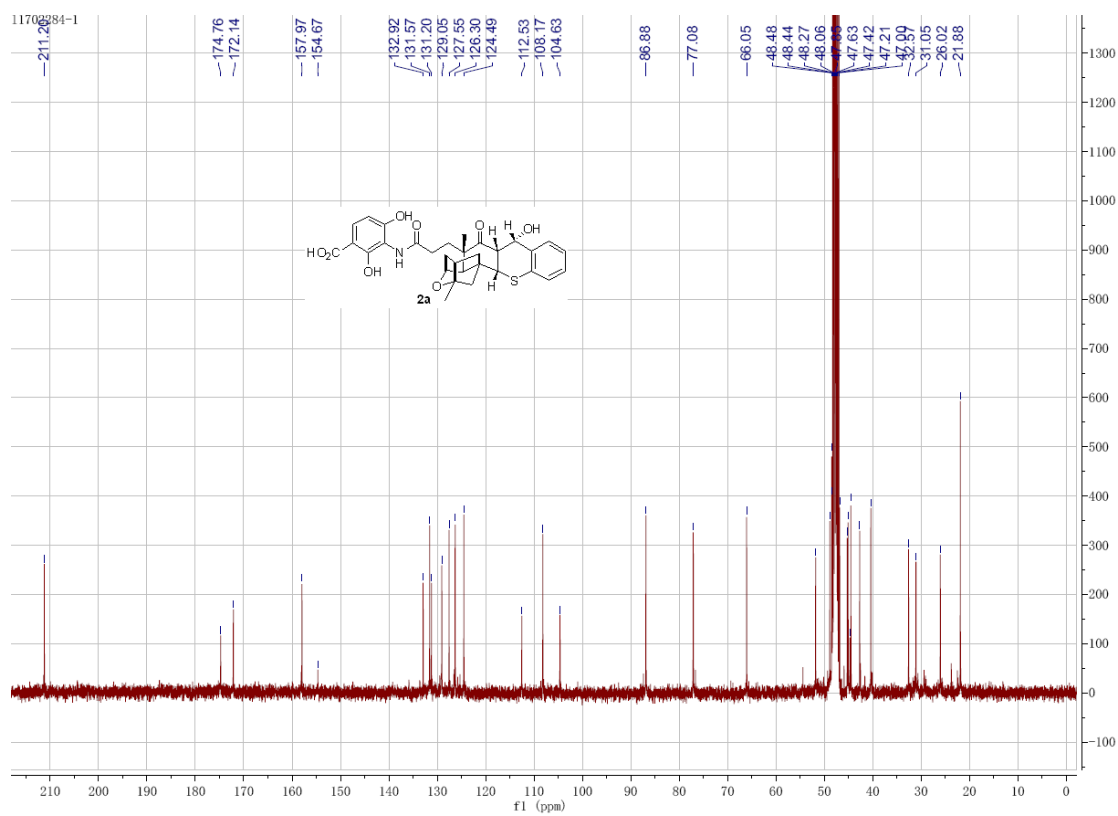
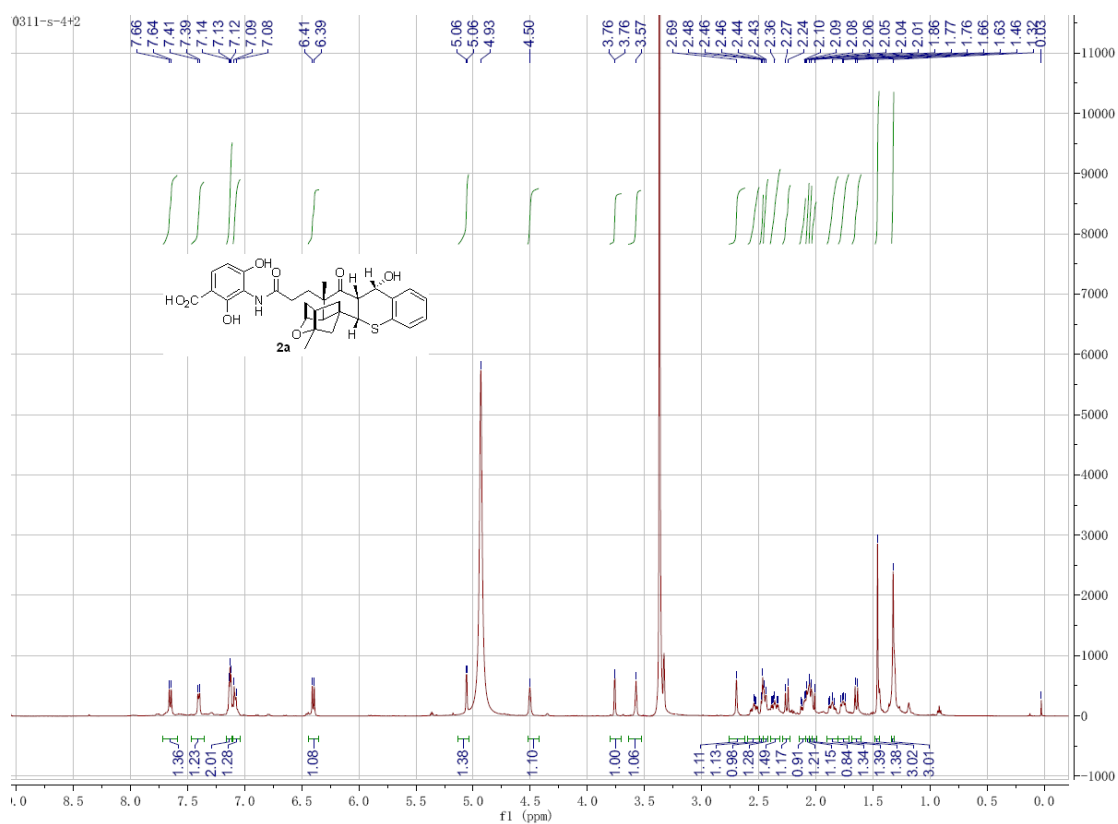


Figure S3. ^1H - ^1H COSY spectrum of **2a** in CD_3OD .

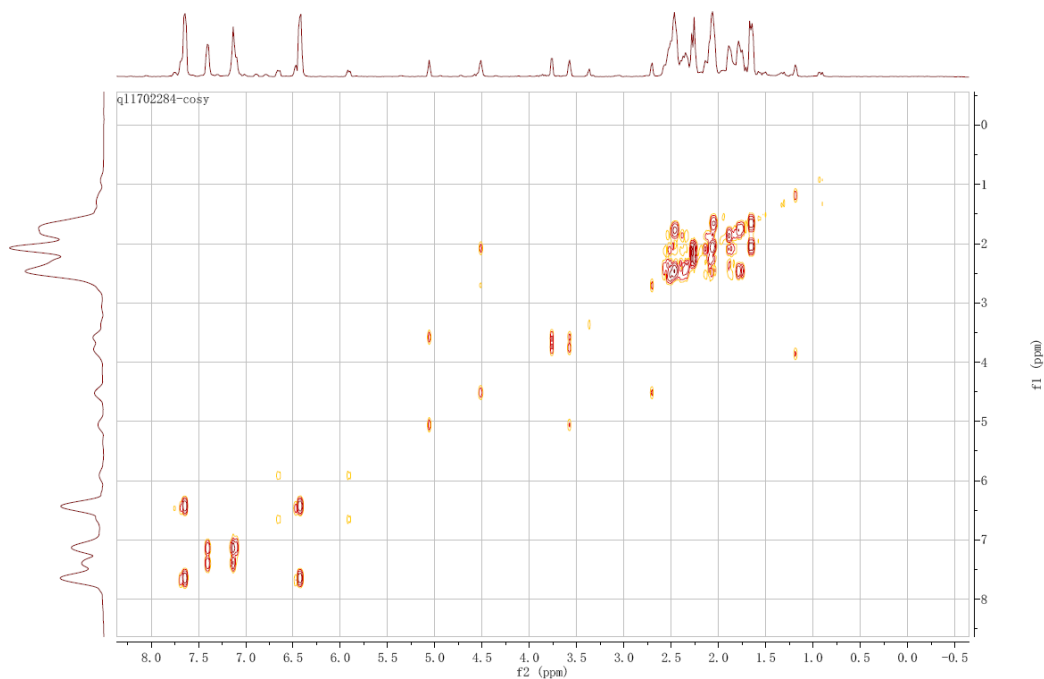


Figure S4. ^1H - ^{13}C HSQC spectrum of **2a** in CD_3OD .

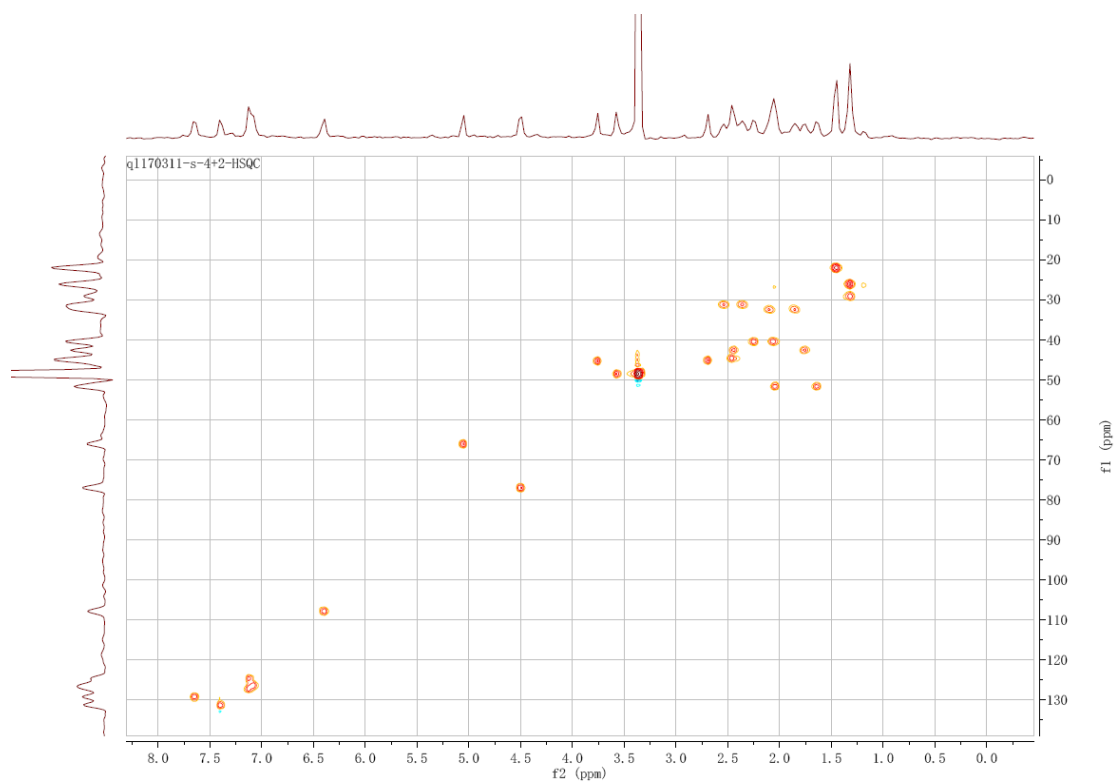


Figure S5. ^1H - ^{13}C HMBC spectrum of **2a** in CD_3OD .

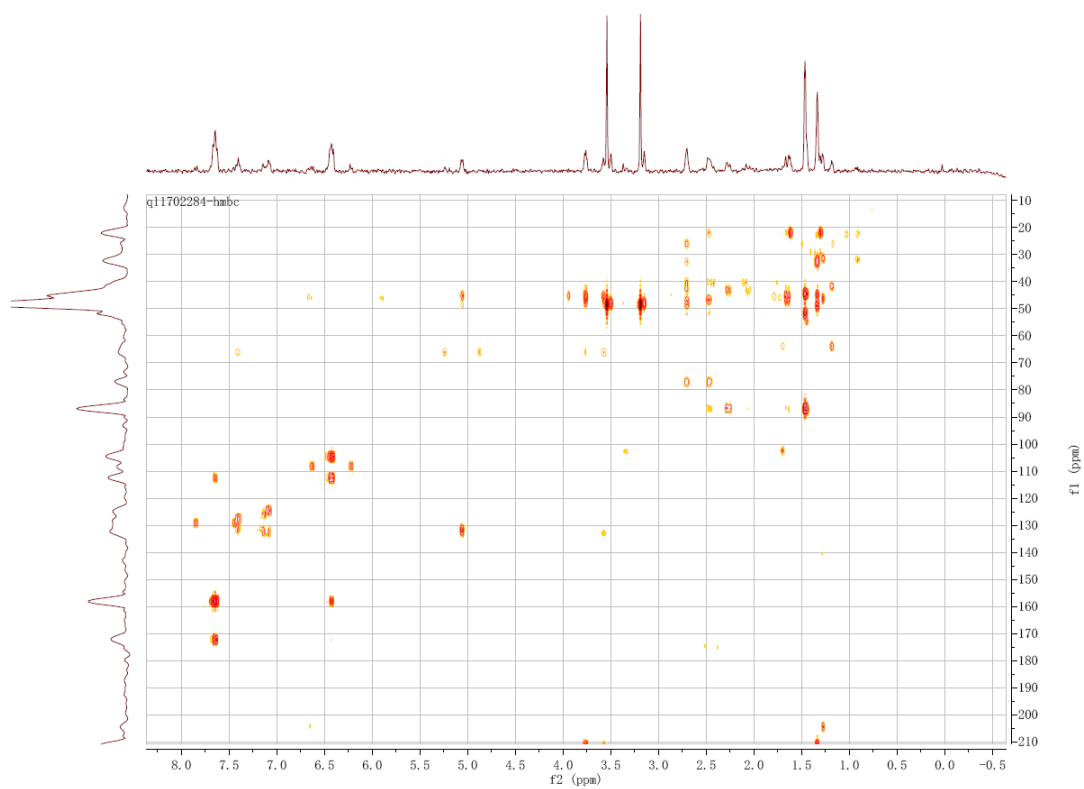


Figure S6. ^1H - ^1H ROESY spectrum of **2a** in CD_3OD .

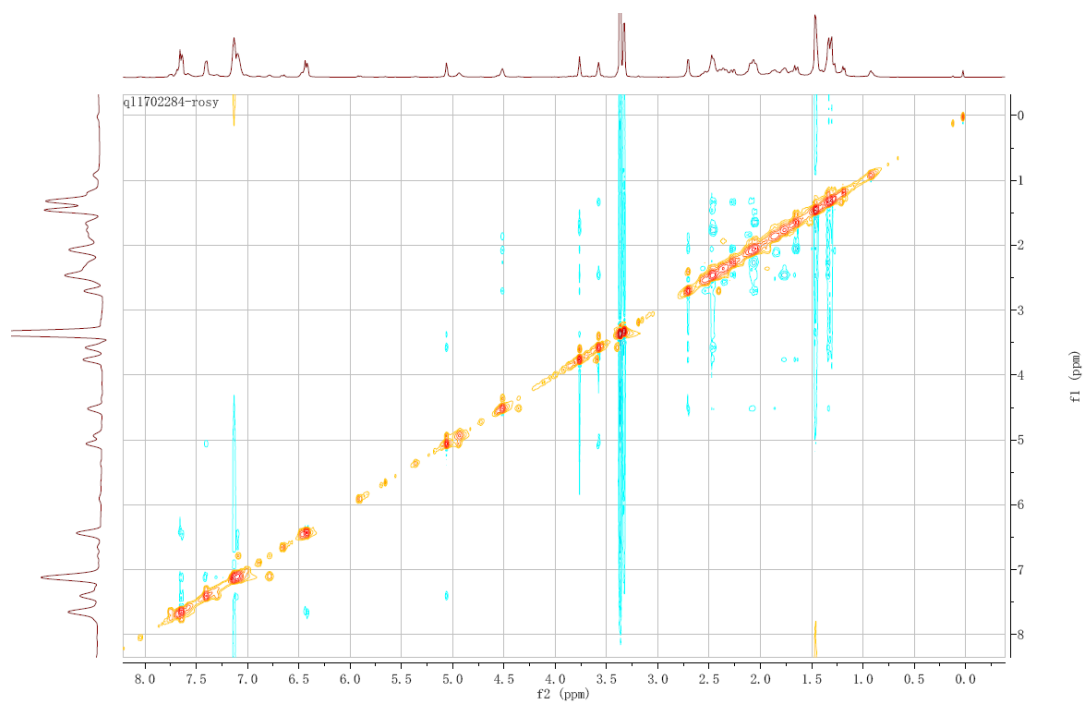


Figure S7. Zoomed in ^1H - ^1H ROESY spectrum of **2a** in CD_3OD (3.0 – 5.5 ppm).

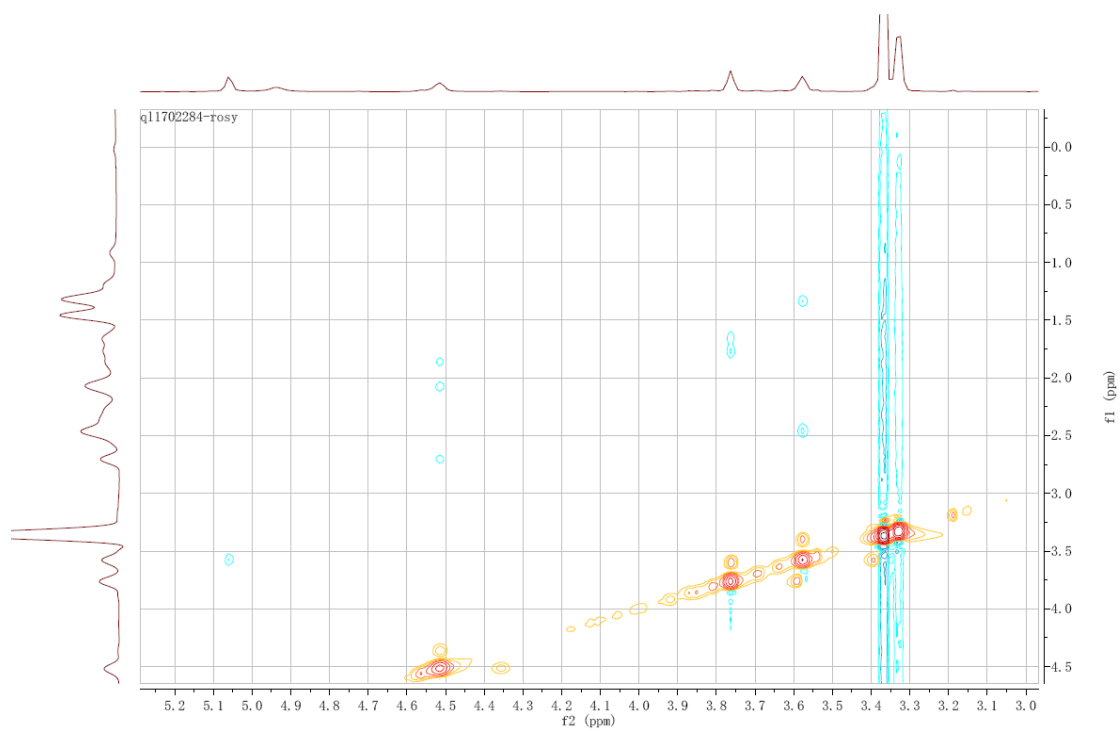


Figure S8. ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectrum of **4a** in CDCl_3 .

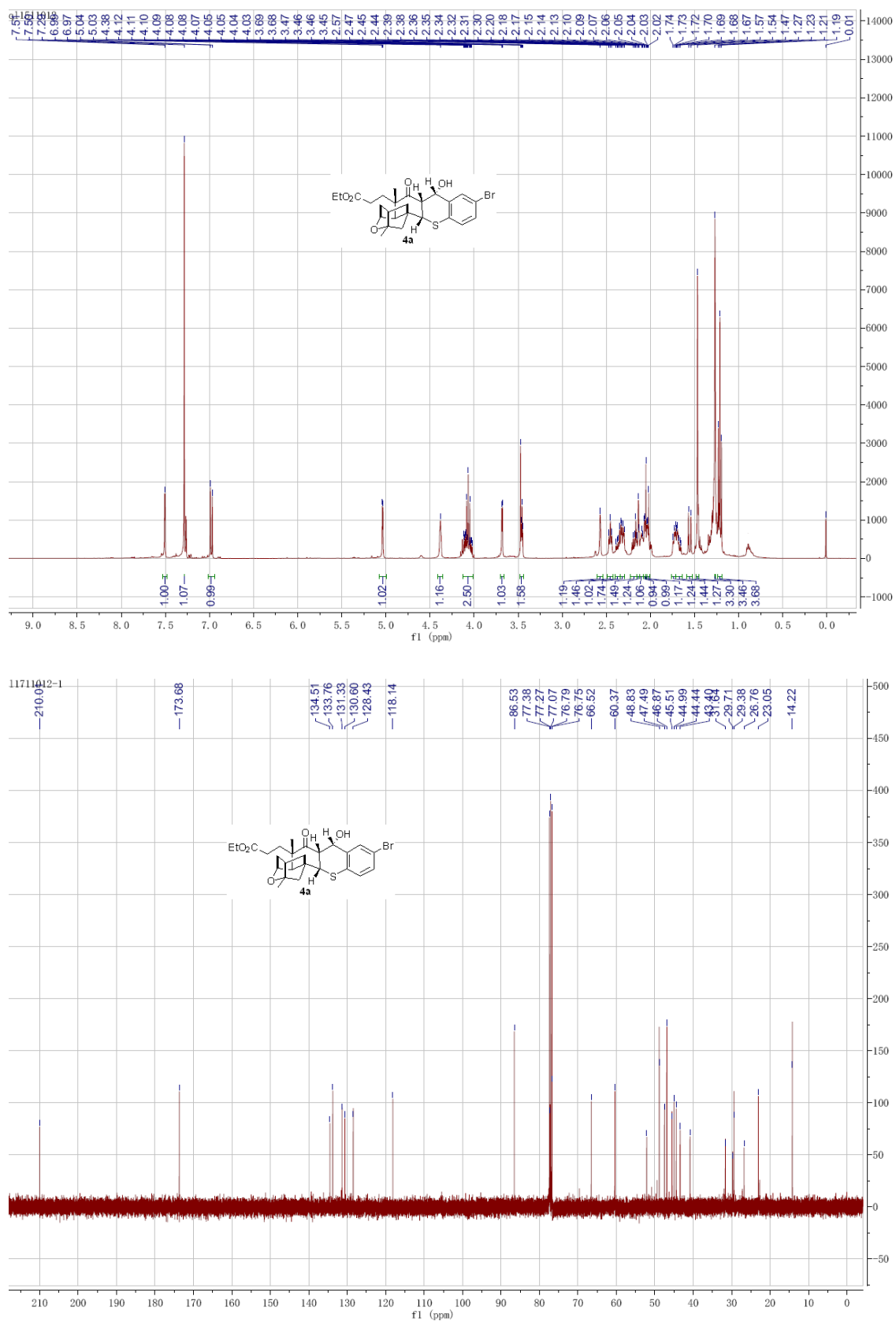


Figure S9. ^1H - ^1H COSY spectrum of **4a** in CDCl_3 .

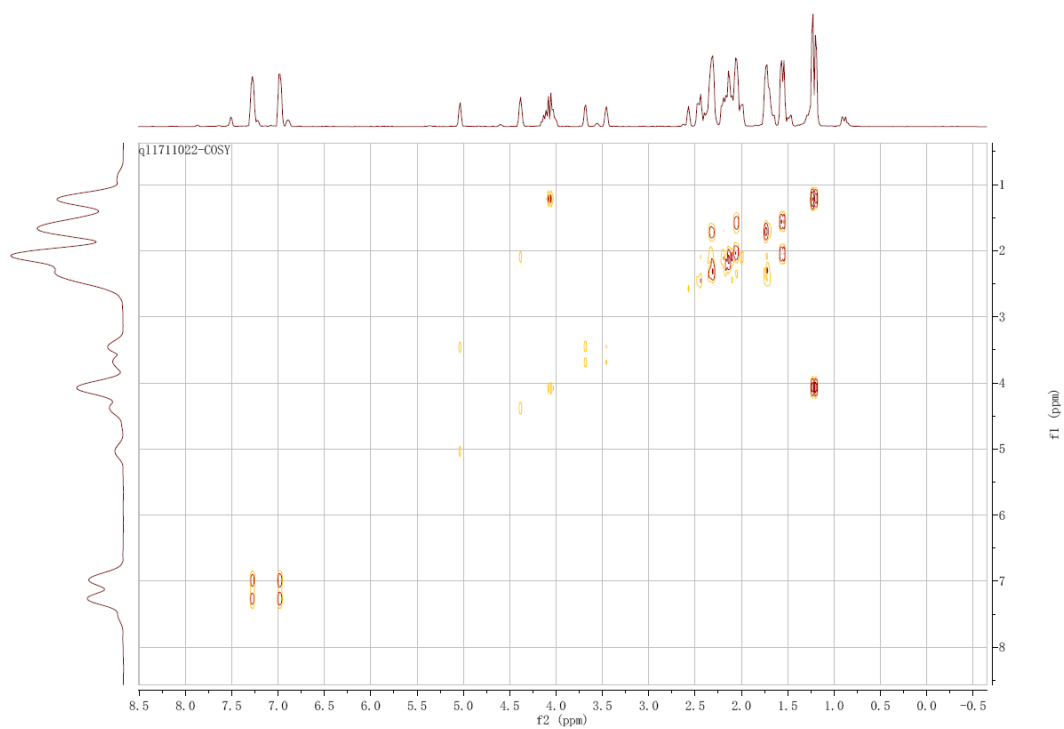


Figure S10. ^1H - ^{13}C HSQC spectrum of **4a** in CDCl_3 .

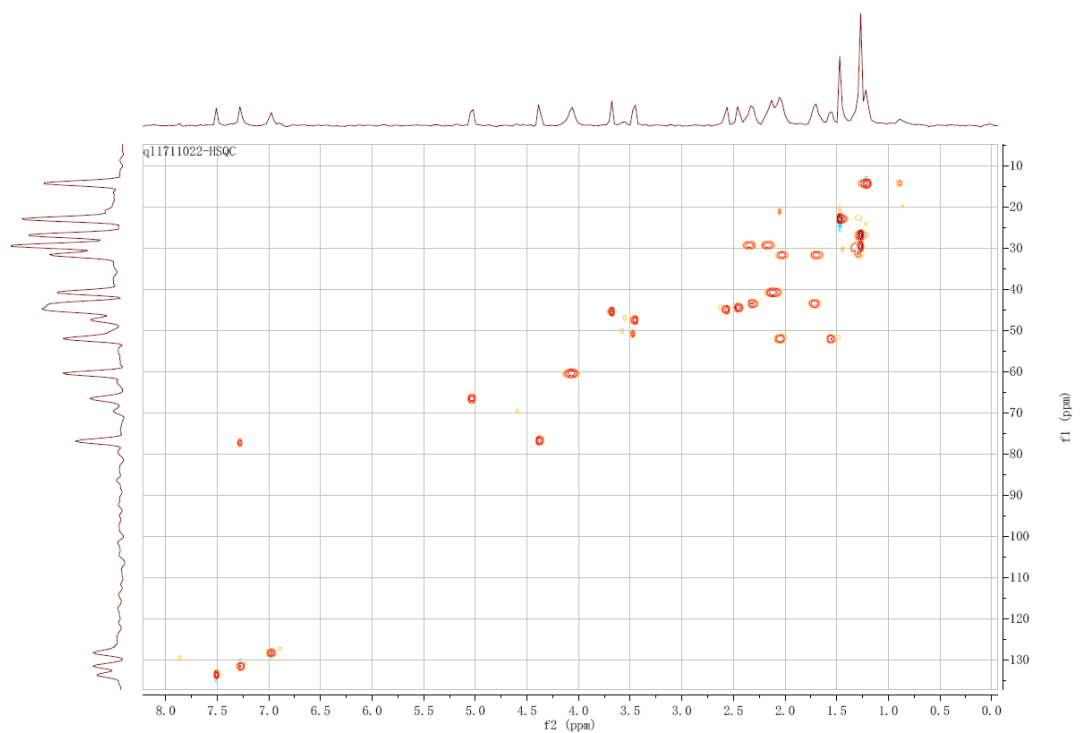


Figure S11. ^1H - ^{13}C HMBC spectrum of **4a** in CDCl_3 .

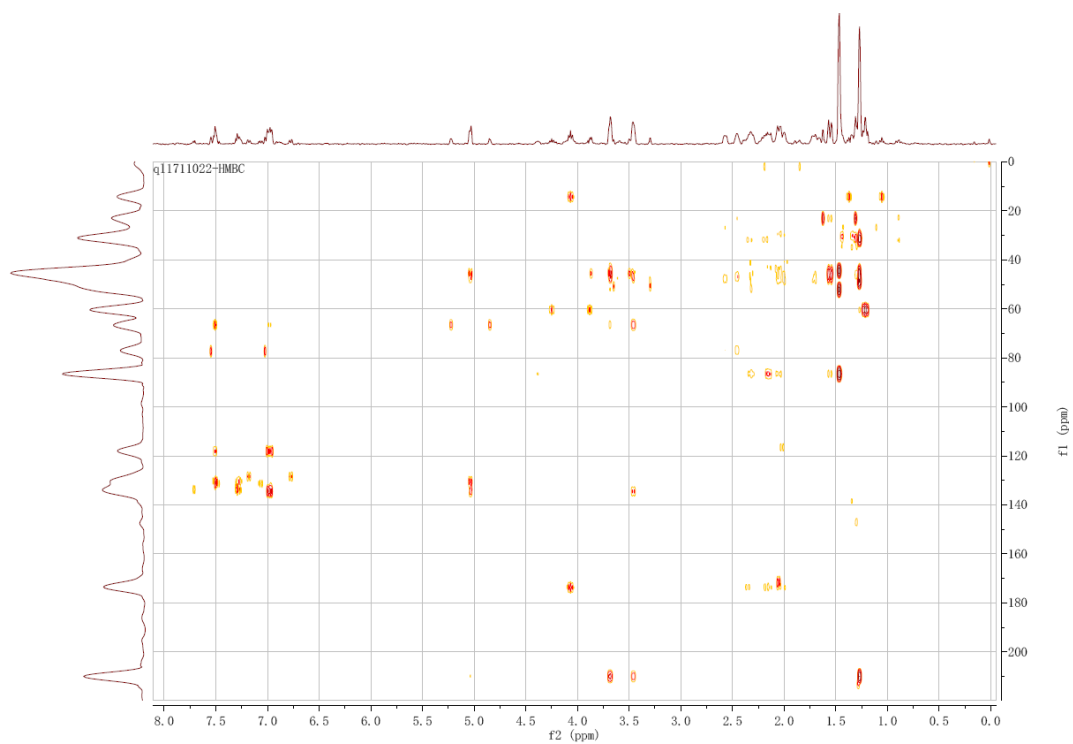


Figure S12. ^1H - ^1H NOESY spectrum of **4a** in CDCl_3 .

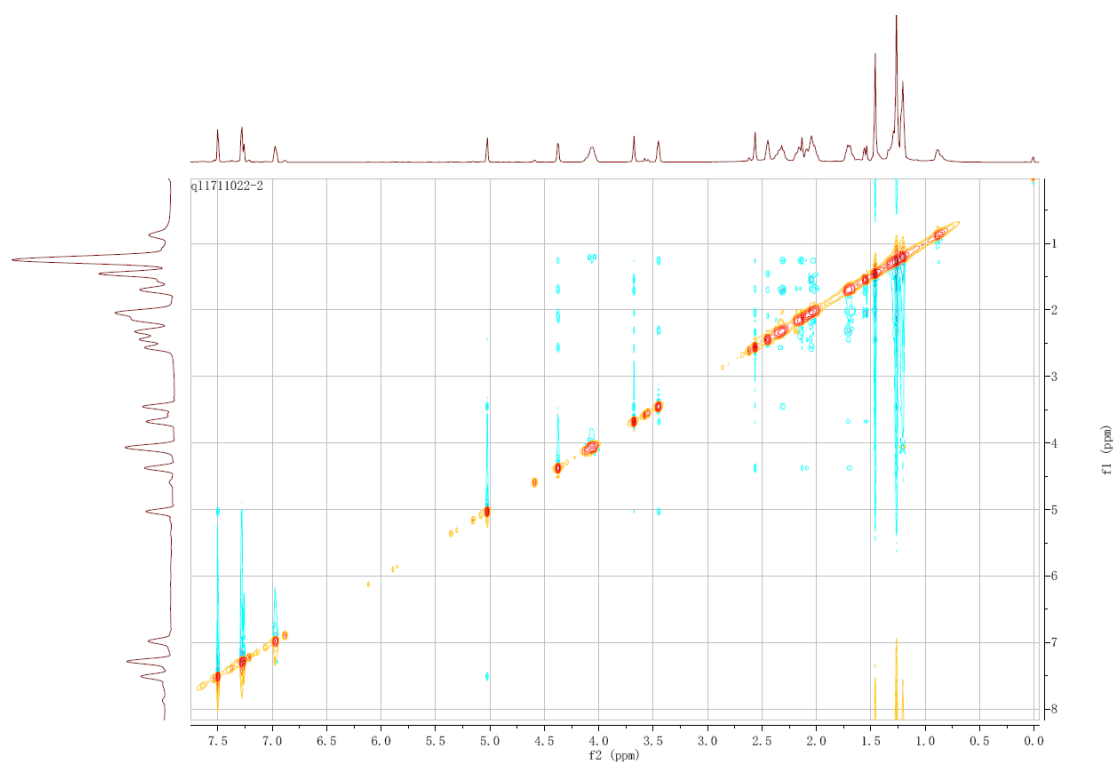


Figure S13. Zoomed in ^1H - ^1H NOESY spectrum of **4a** in CDCl_3 (3.0 – 5.5 ppm).

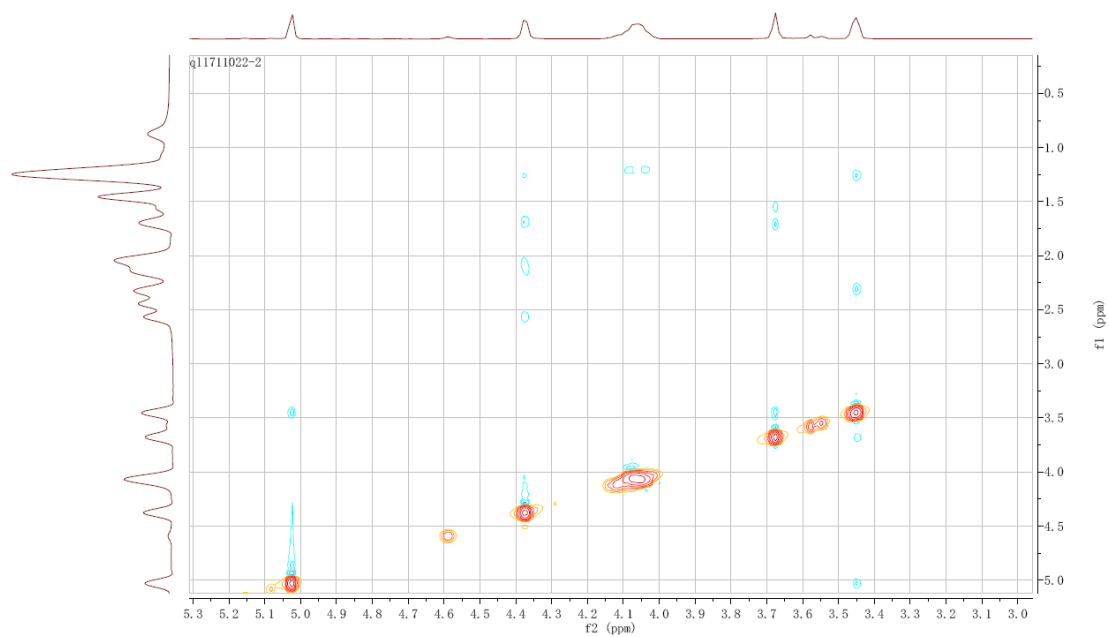


Figure S14. ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectrum of **5a** in CDCl_3 .

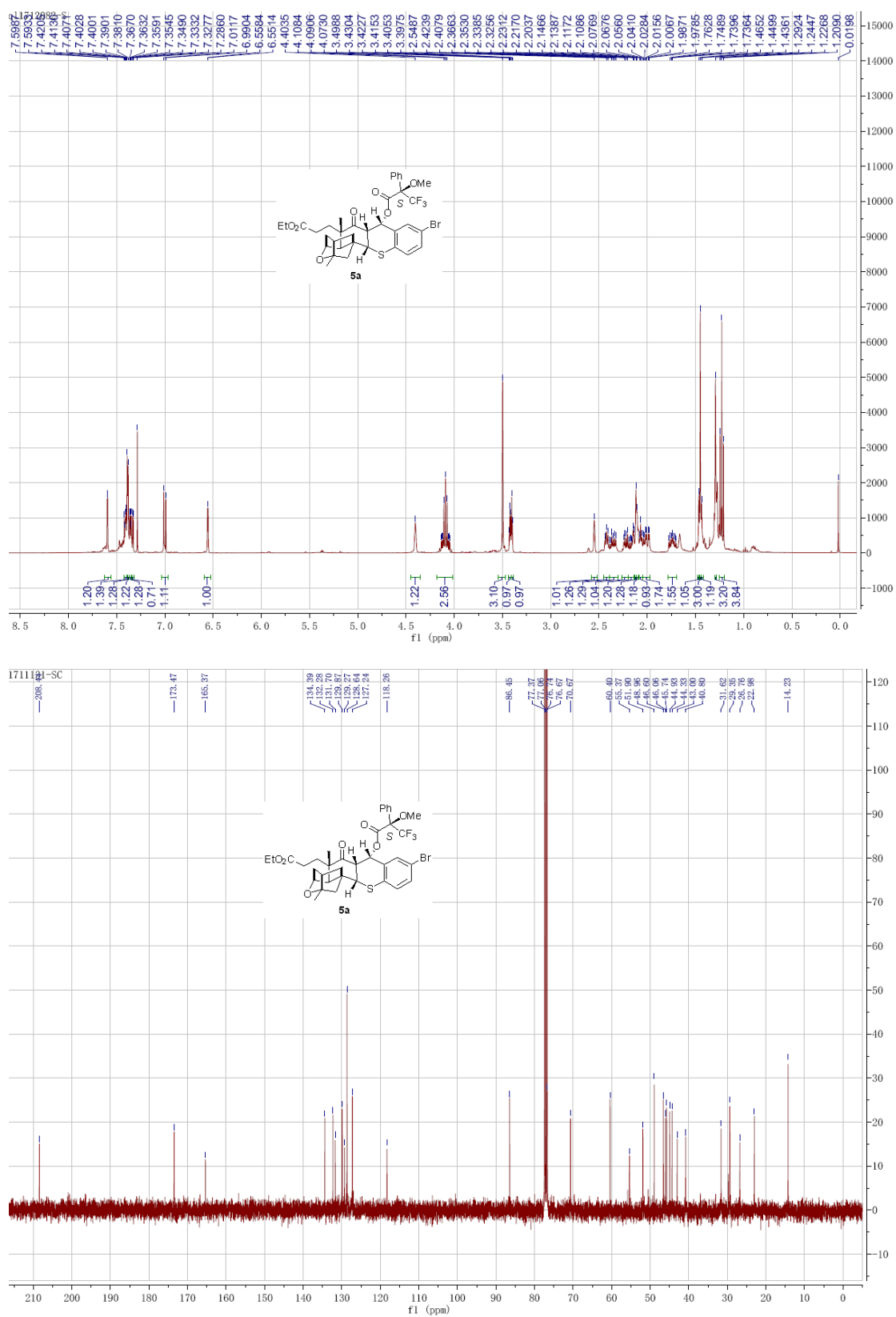


Figure S15. ^1H - ^1H COSY spectrum of **5a** in CDCl_3 .

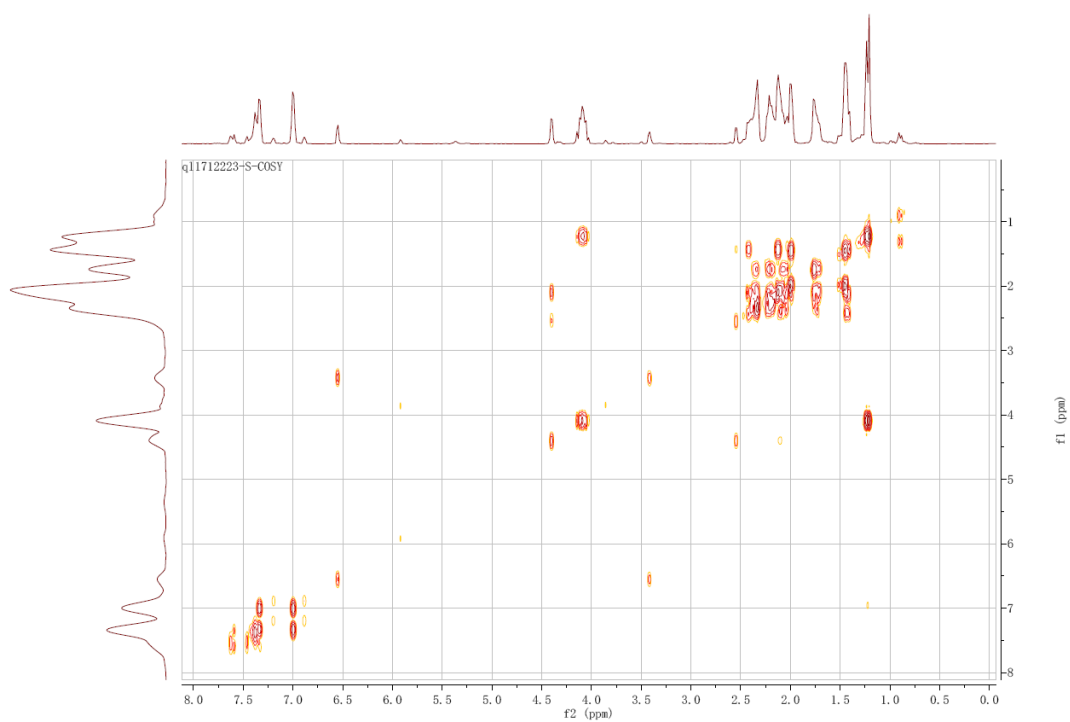


Figure S16. ^1H - ^{13}C HSQC spectrum of **5a** in CDCl_3 .

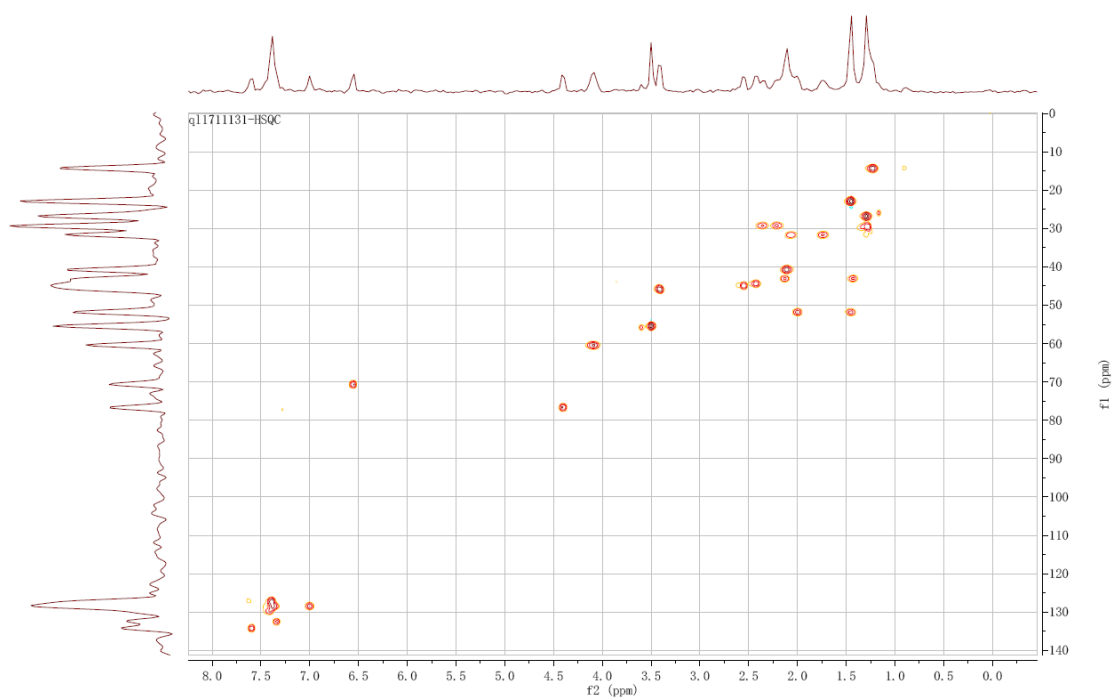


Figure S17. ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectrum of **5b** in CDCl_3 .

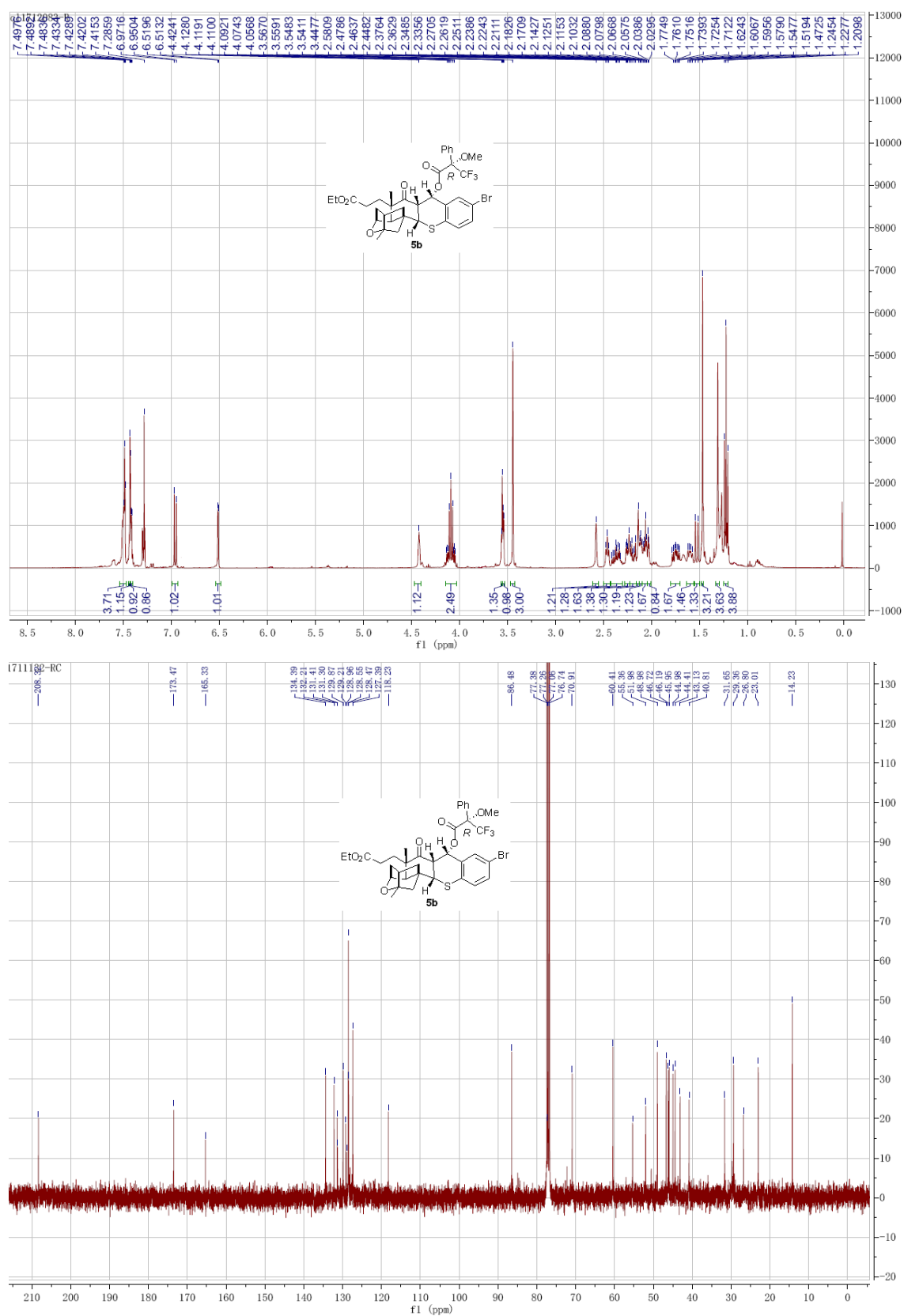


Figure S18. ^1H - ^1H COSY spectrum of **5b** in CDCl_3 .

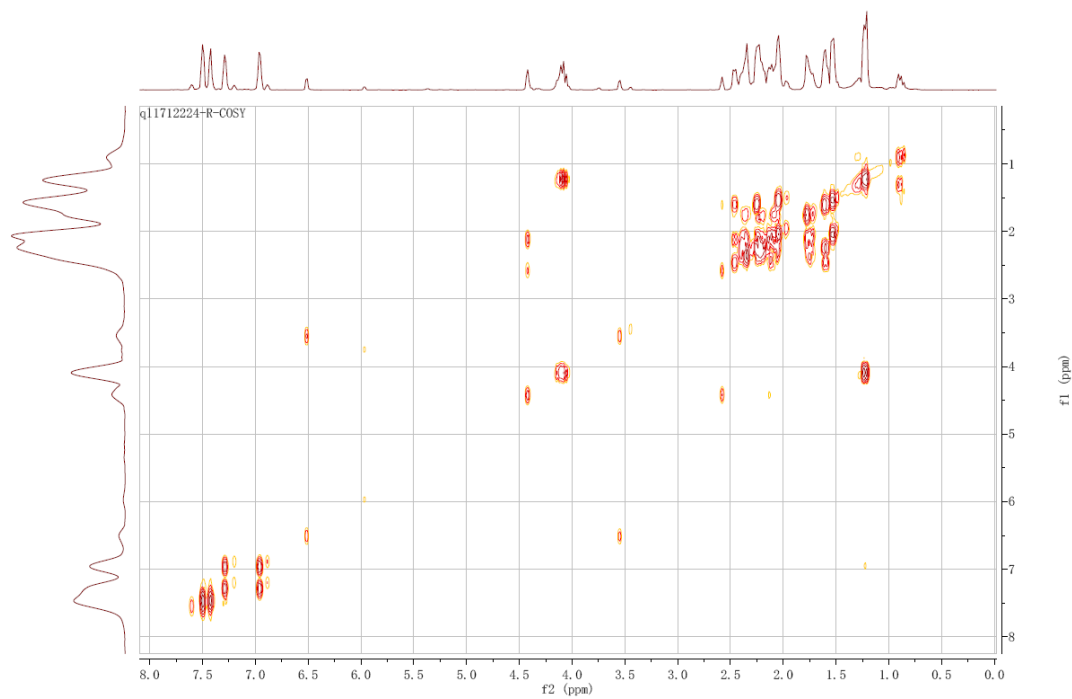


Figure S19. ^1H - ^{13}C HSQC spectrum of **5b** in CDCl_3 .

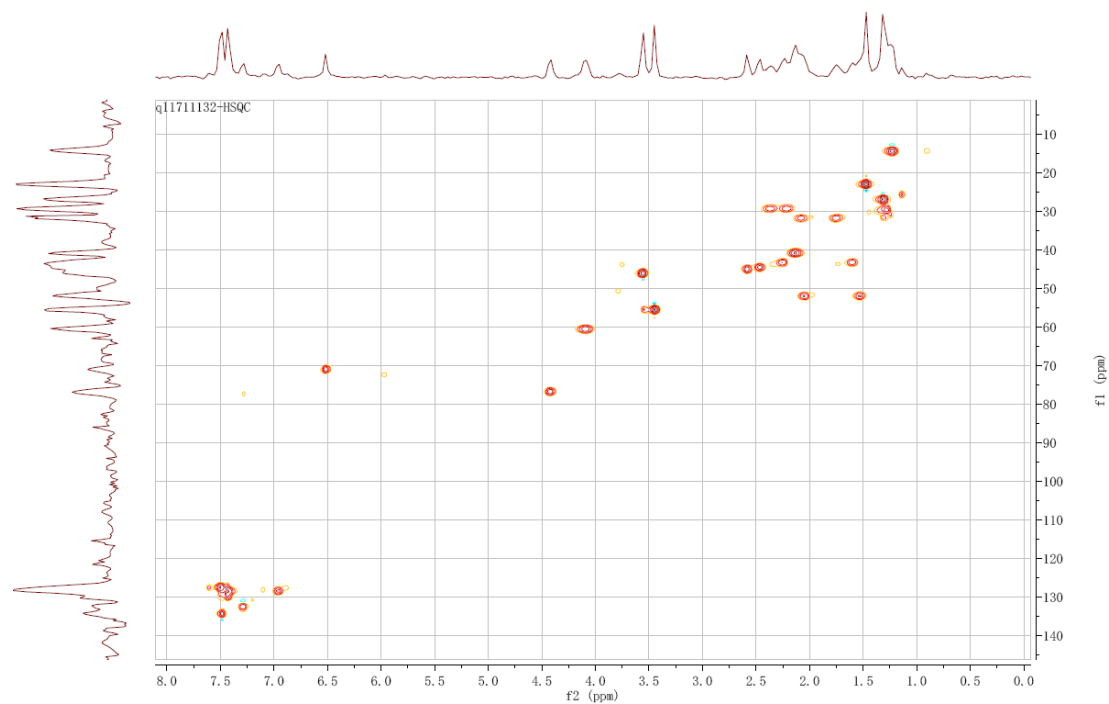


Figure S20. ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectrum of **6a** in CD_3OD .

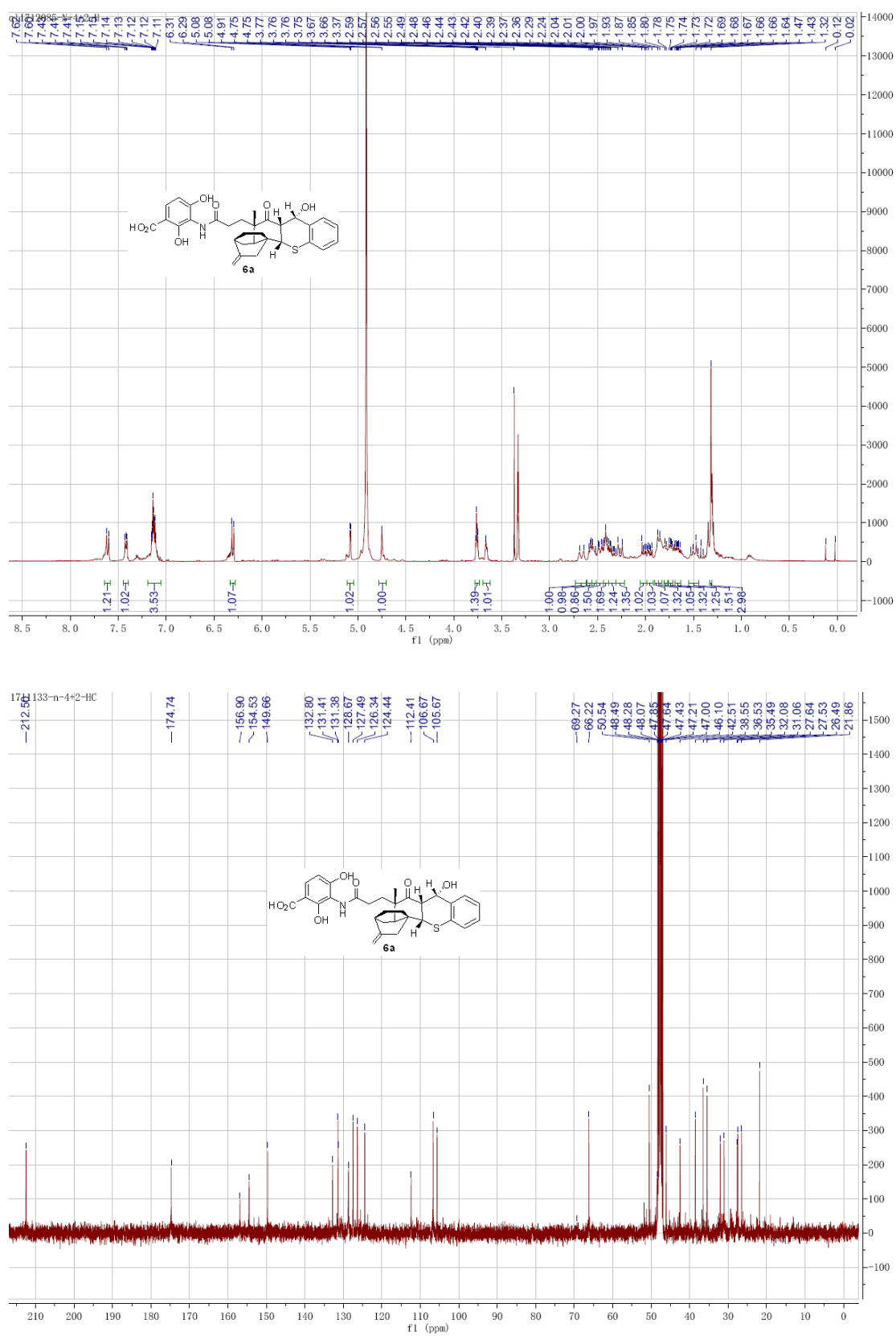


Figure S21. ^1H - ^1H COSY spectrum of **6a** in CD_3OD .

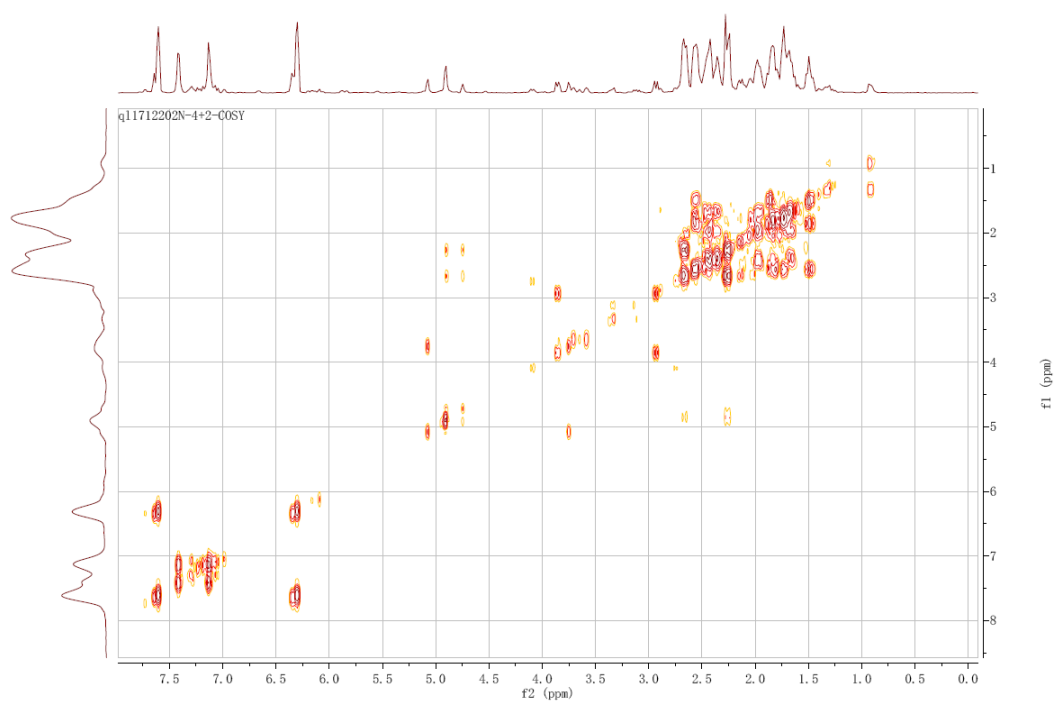


Figure S22. ^1H - ^{13}C HSQC spectrum of **6a** in CD_3OD .

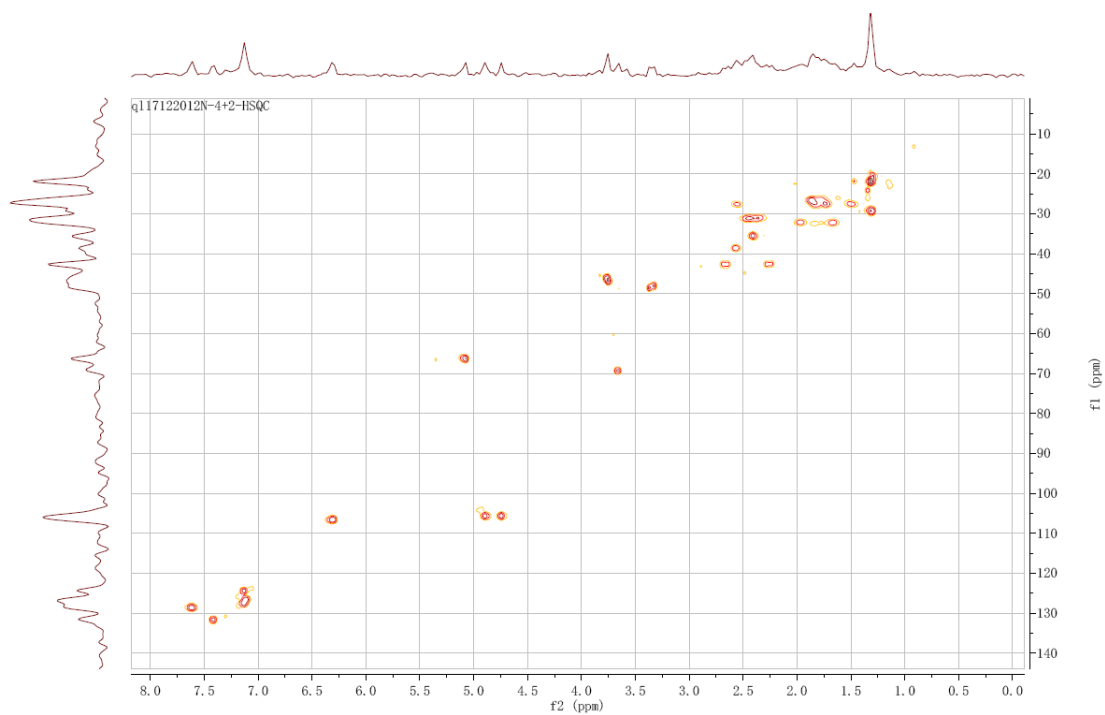


Figure S23. ^1H - ^{13}C HMBC spectrum of **6a** in CD_3OD .

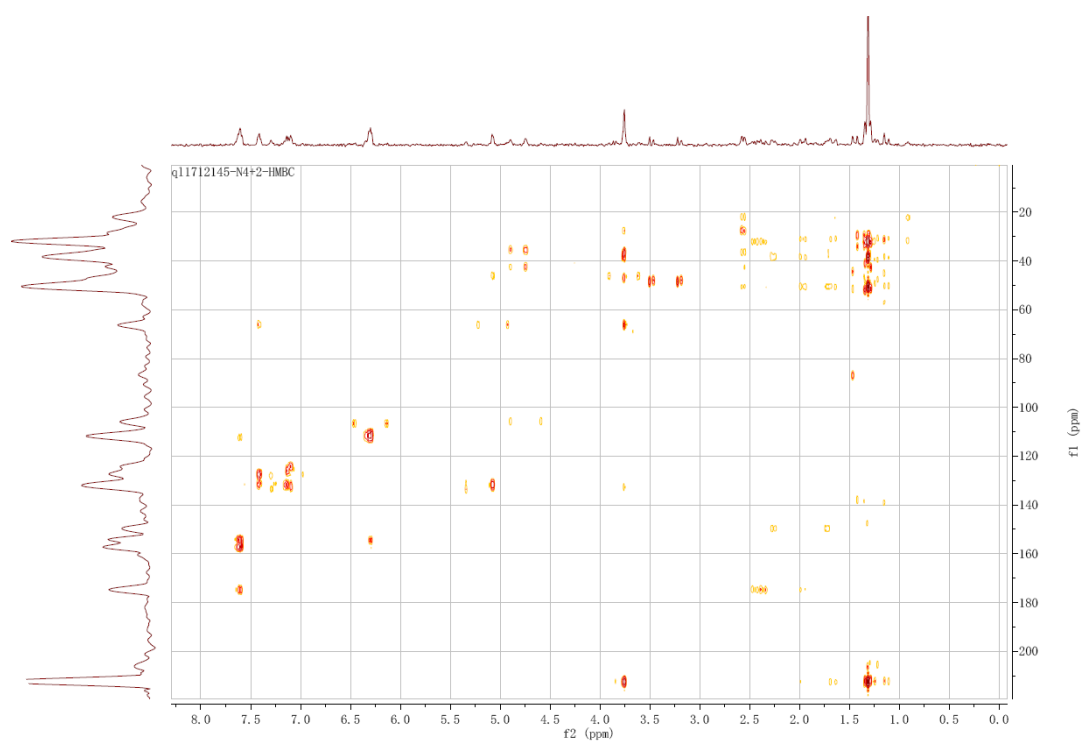


Figure S24. ^1H - ^1H NOESY spectrum of **6a** in CD_3OD .

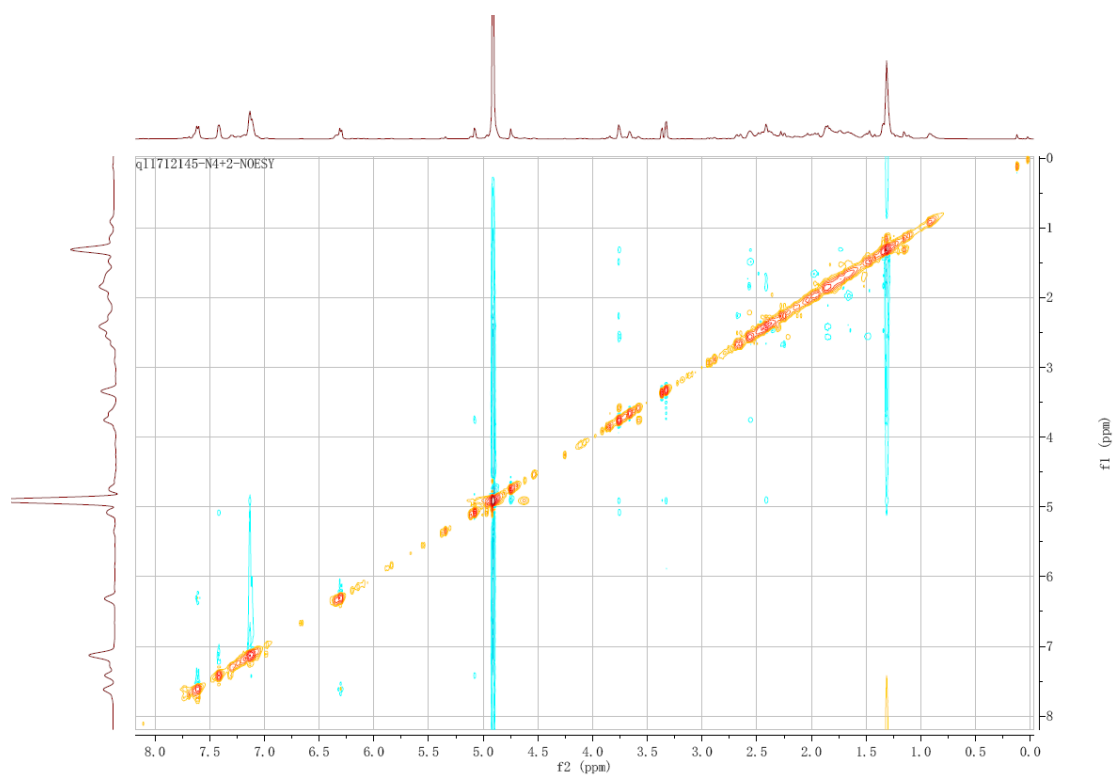


Figure S25. Zoomed in ^1H - ^1H NOESY spectrum of **6a** in CDCl_3 (3.0 – 5.5 ppm).

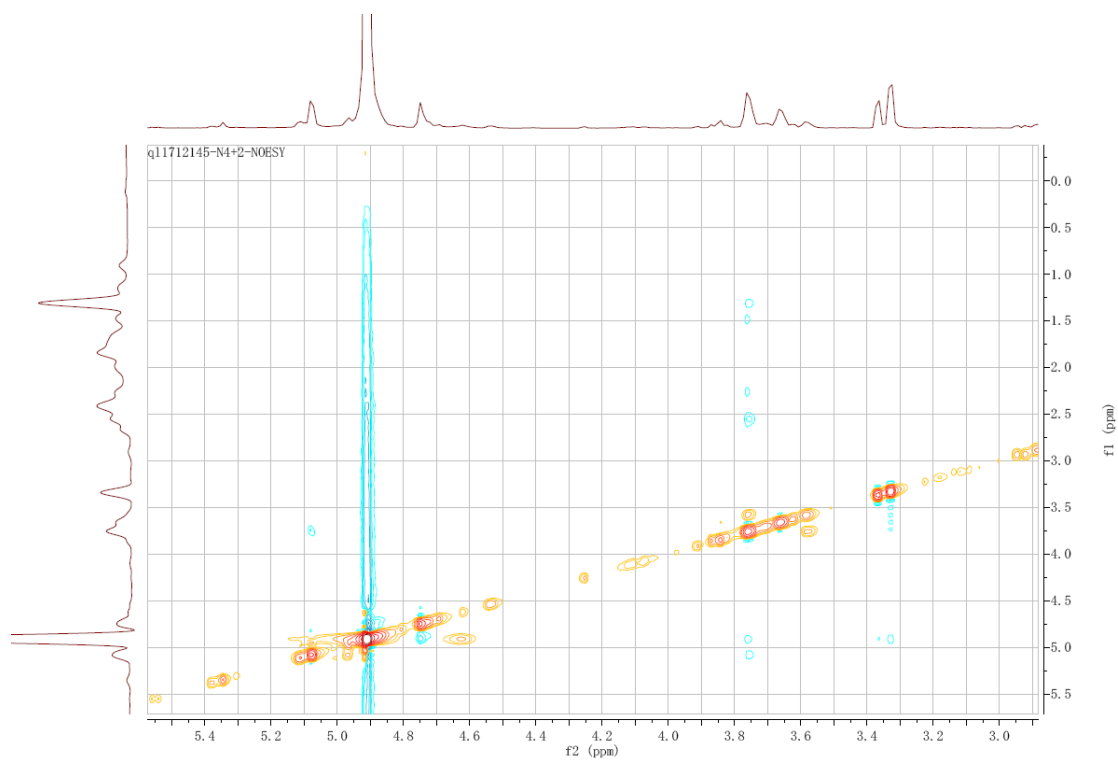


Figure S26. ^1H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectrum of **8a** in CD_3OD .

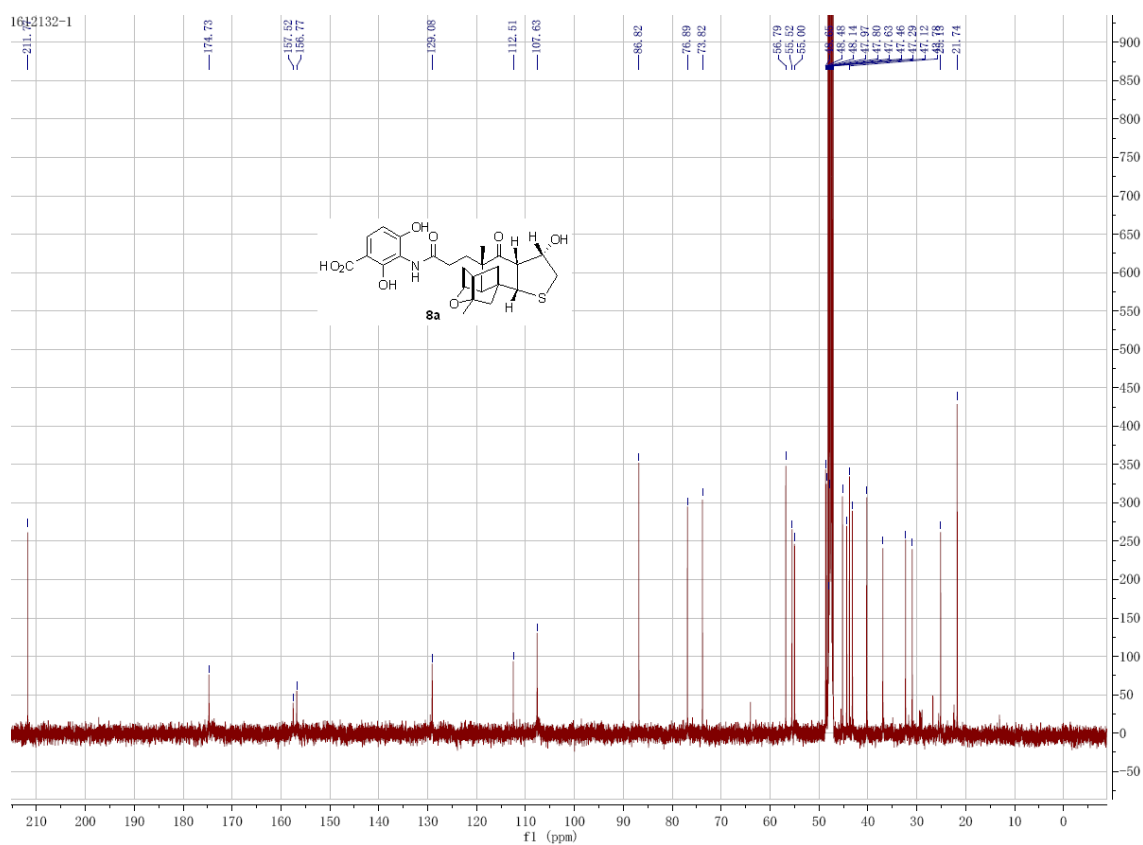
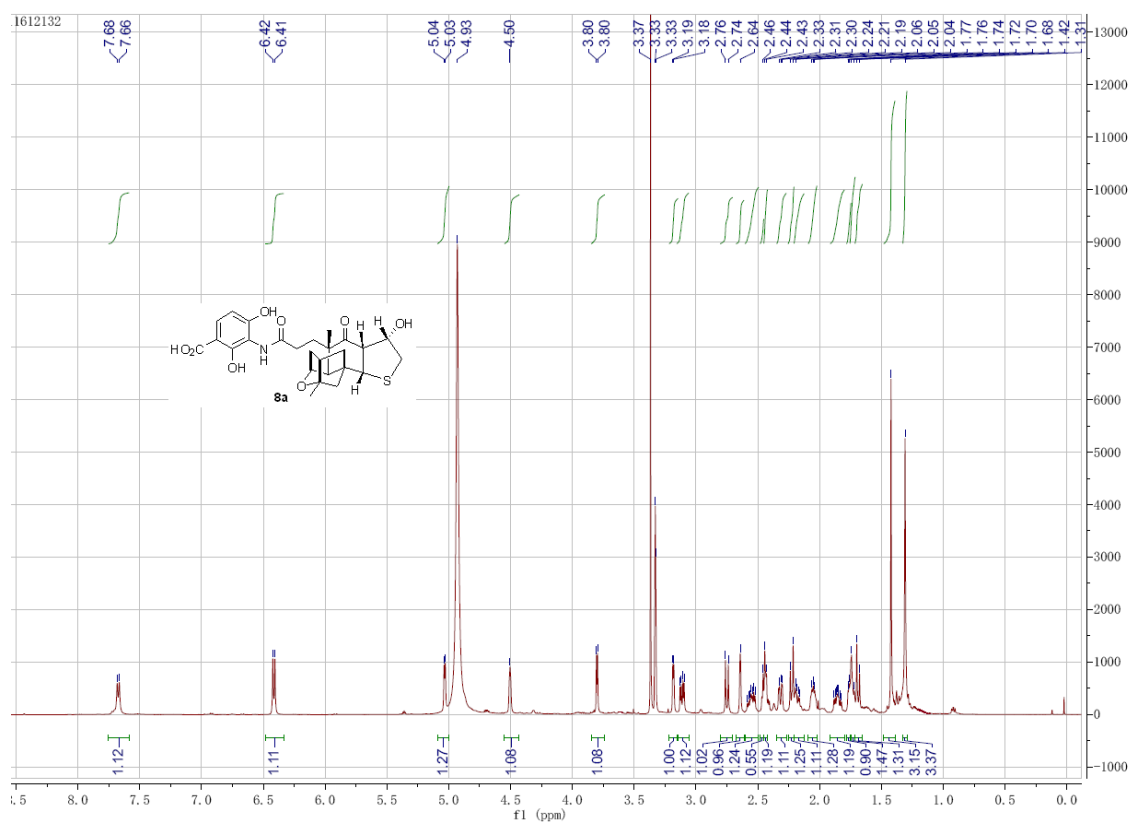


Figure S27. ^1H - ^1H COSY spectrum of **8a** in CD_3OD .

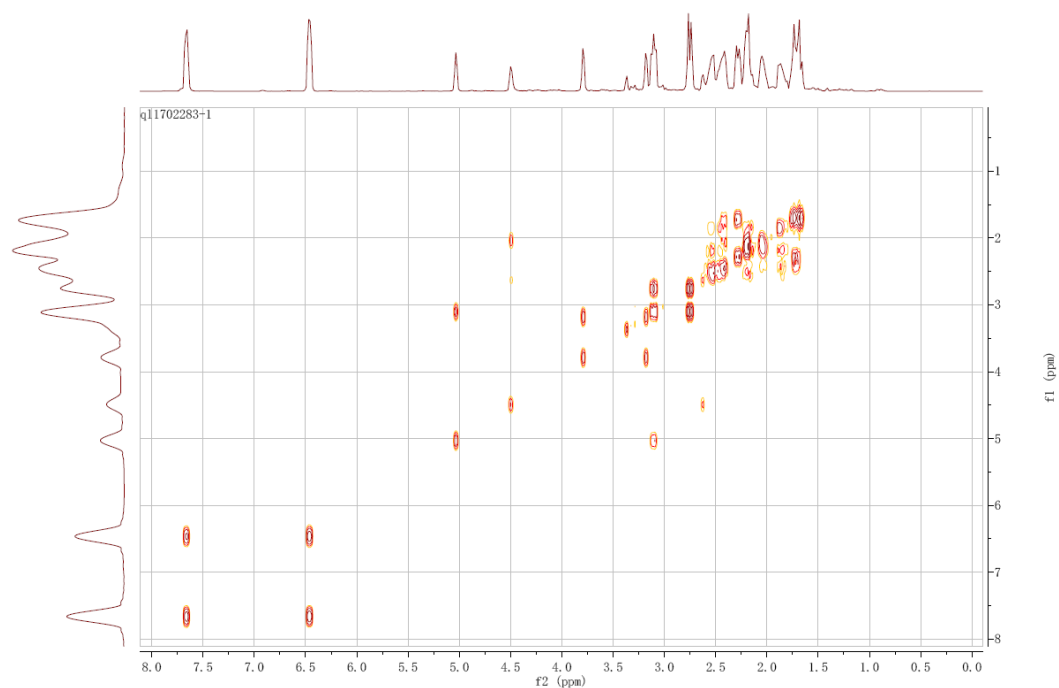


Figure S28. ^1H - ^{13}C HSQC spectrum of **8a** in CD_3OD .

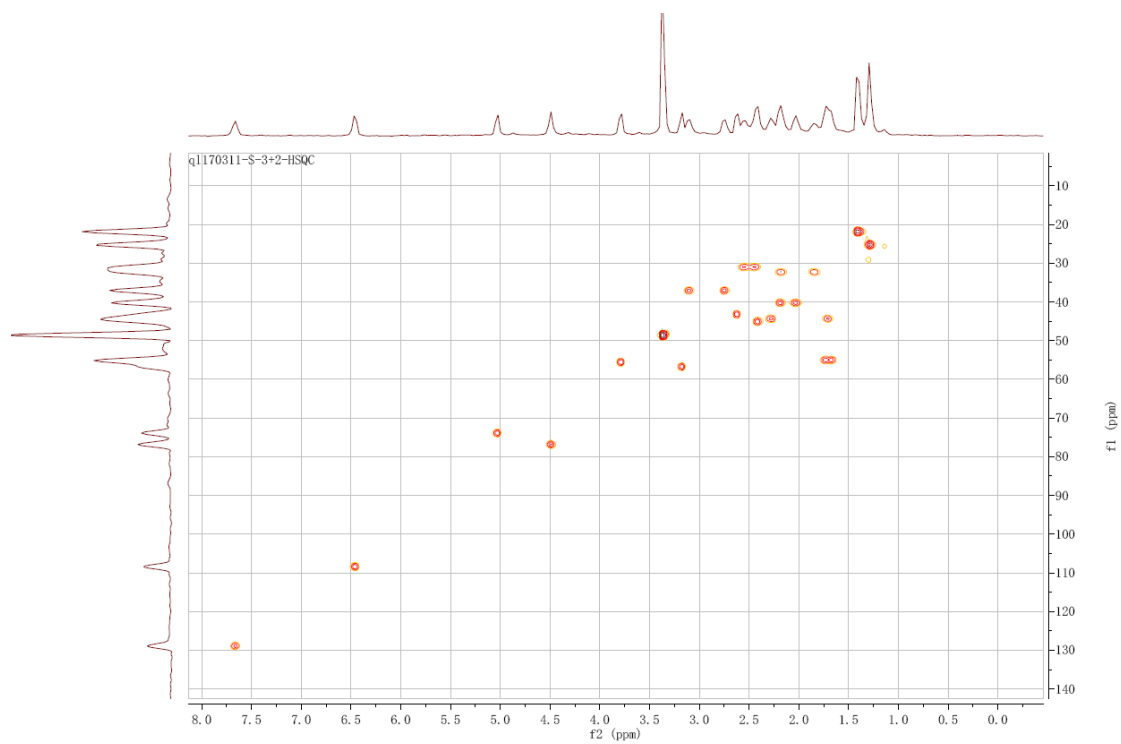


Figure S29. ^1H - ^{13}C HMBC spectrum of **8a** in CD_3OD .

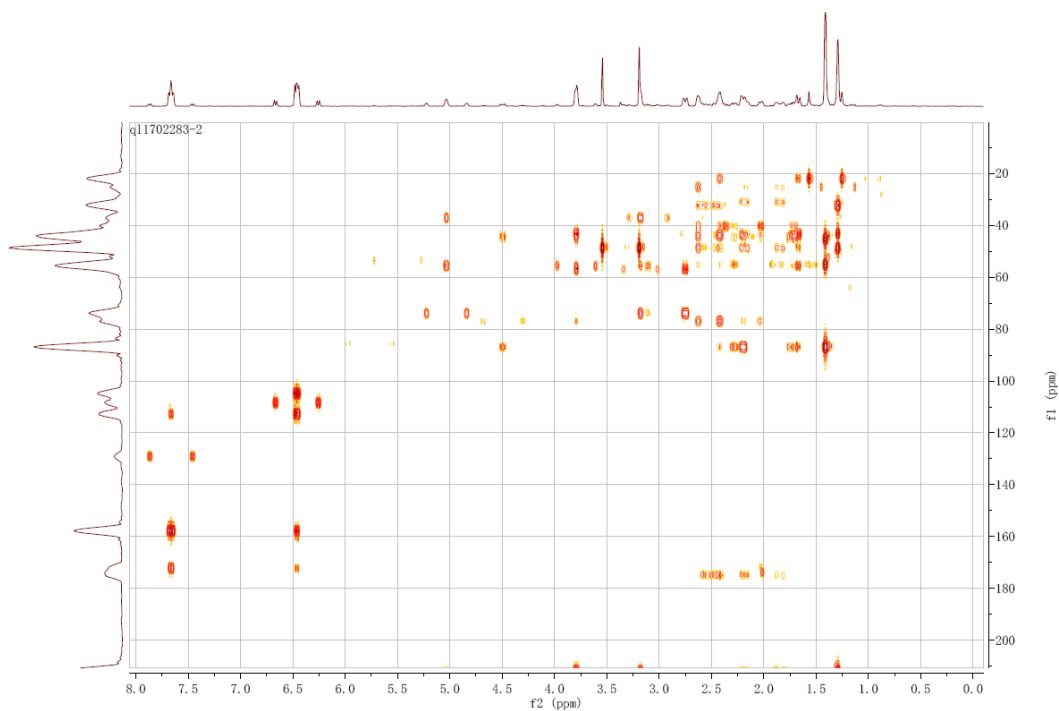


Figure S30. ^1H - ^1H ROESY spectrum of **8a** in CD_3OD .

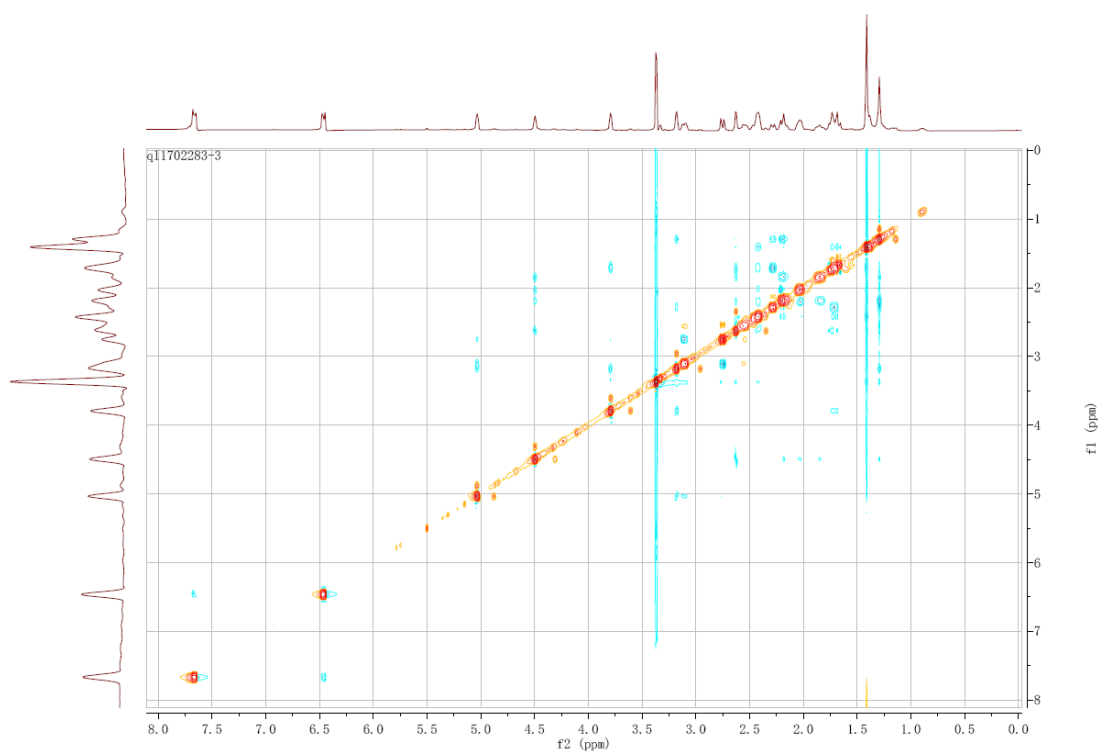


Figure S31. Zoomed in ^1H - ^1H ROESY spectrum of **8a** in CDCl_3 (3.0 – 5.5 ppm).

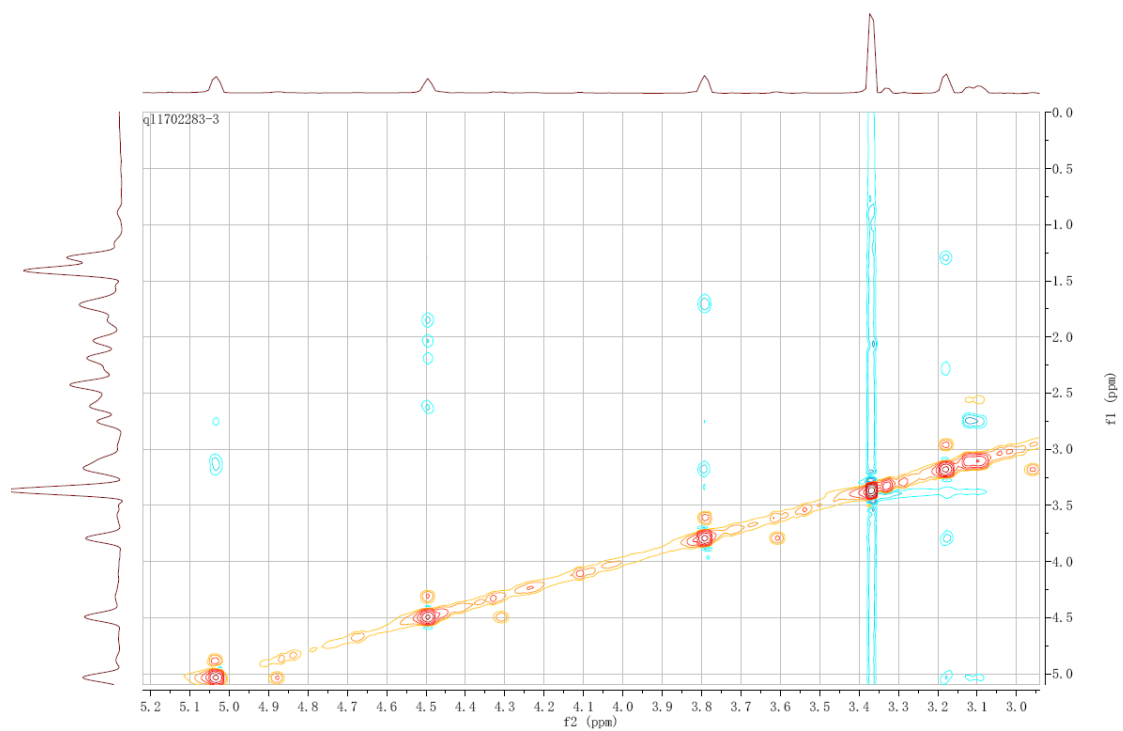


Figure S32. ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectrum of **9a** in CD_3OD .

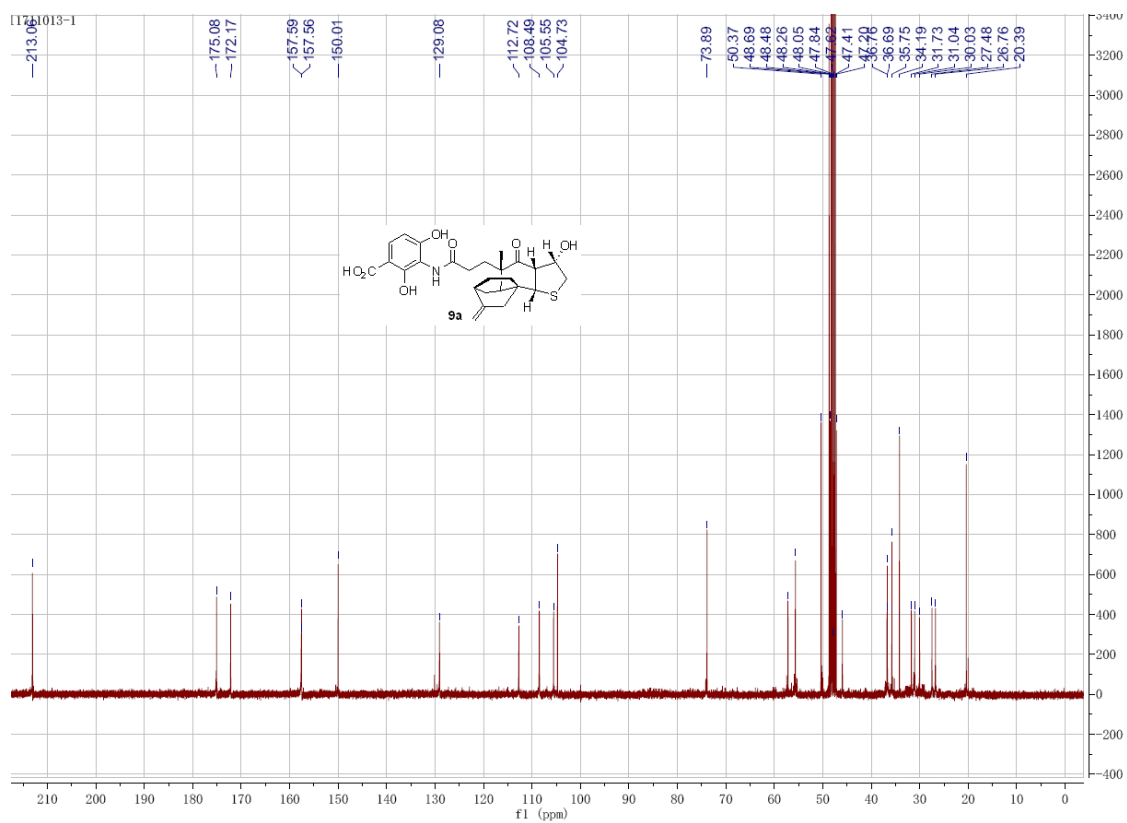
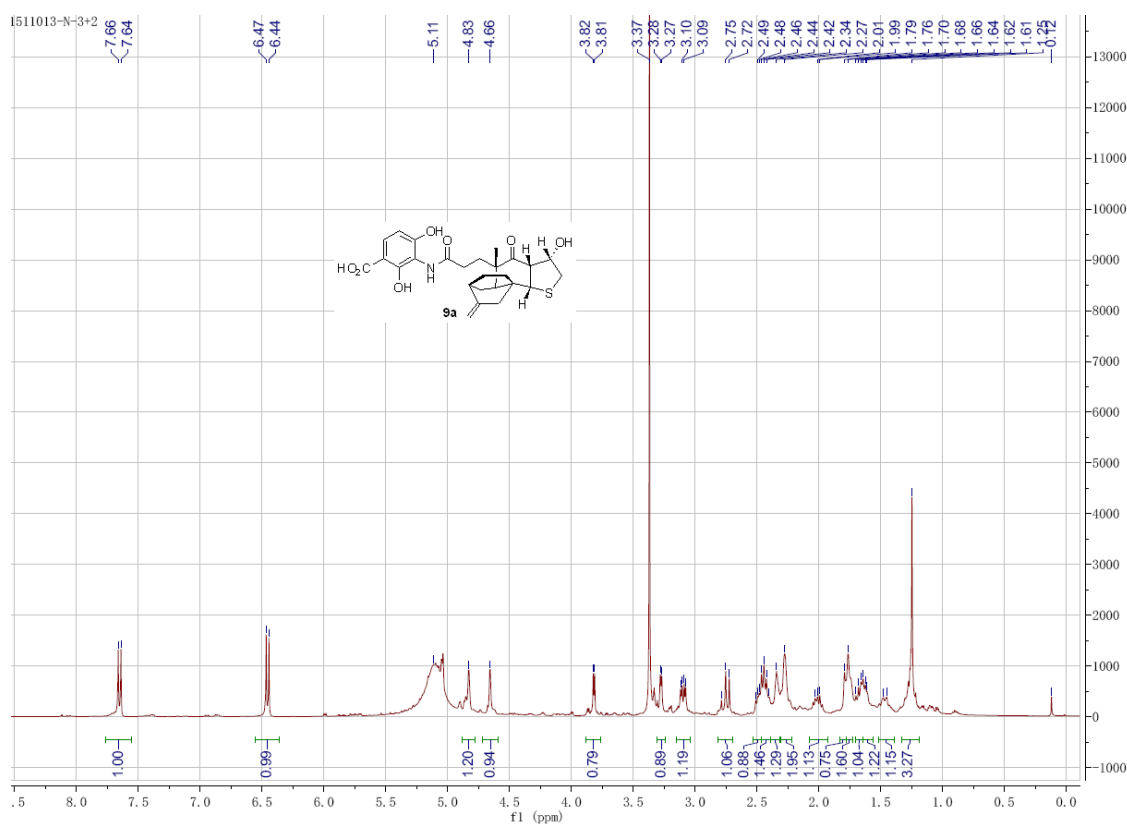


Figure S33. ^1H - ^1H COSY spectrum of **9a** in CD_3OD .

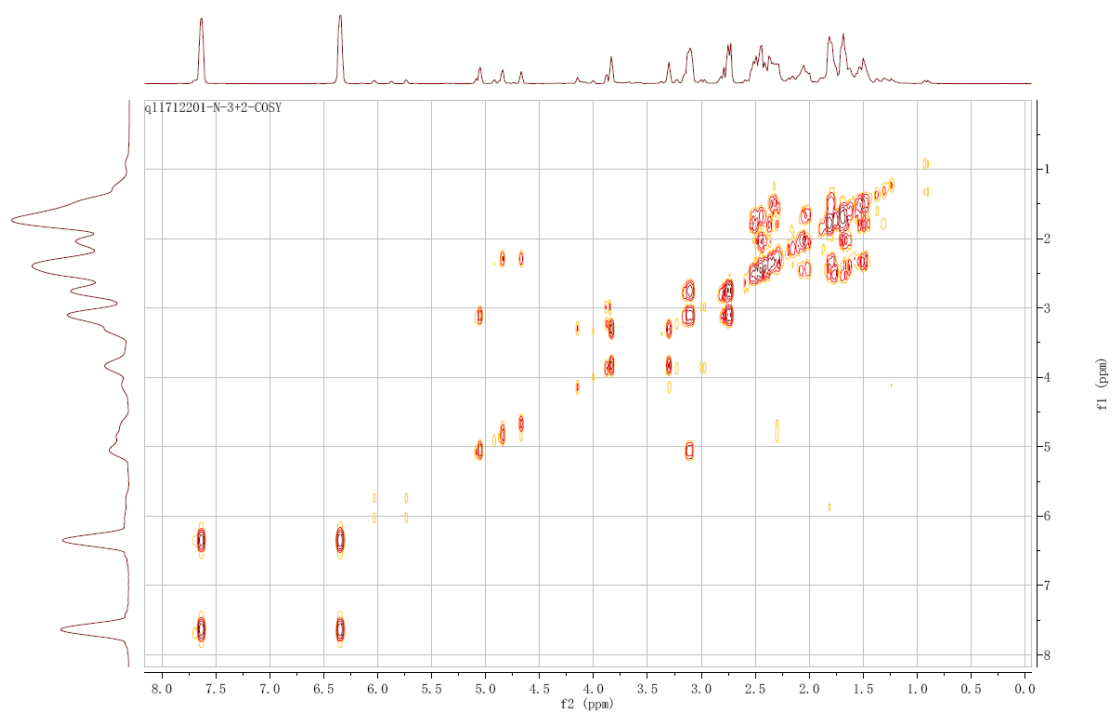


Figure S34. ^1H - ^{13}C HSQC spectrum of **9a** in CD_3OD .

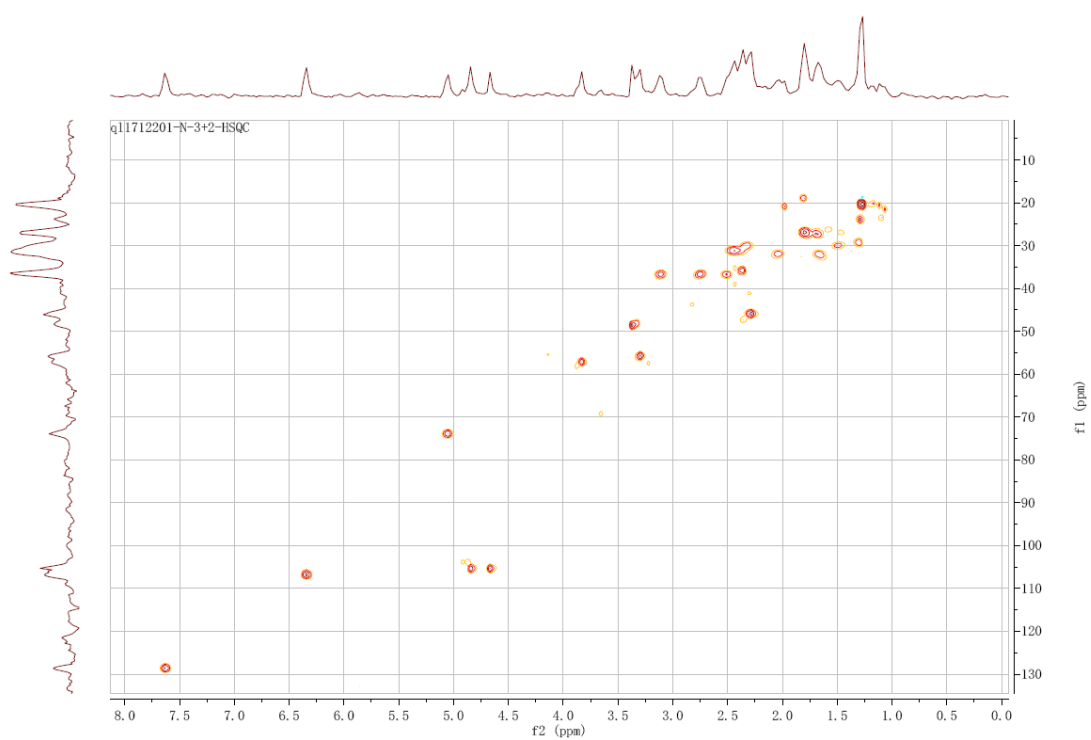


Figure S35. ^1H - ^{13}C HMBC spectrum of **9a** in CD_3OD .

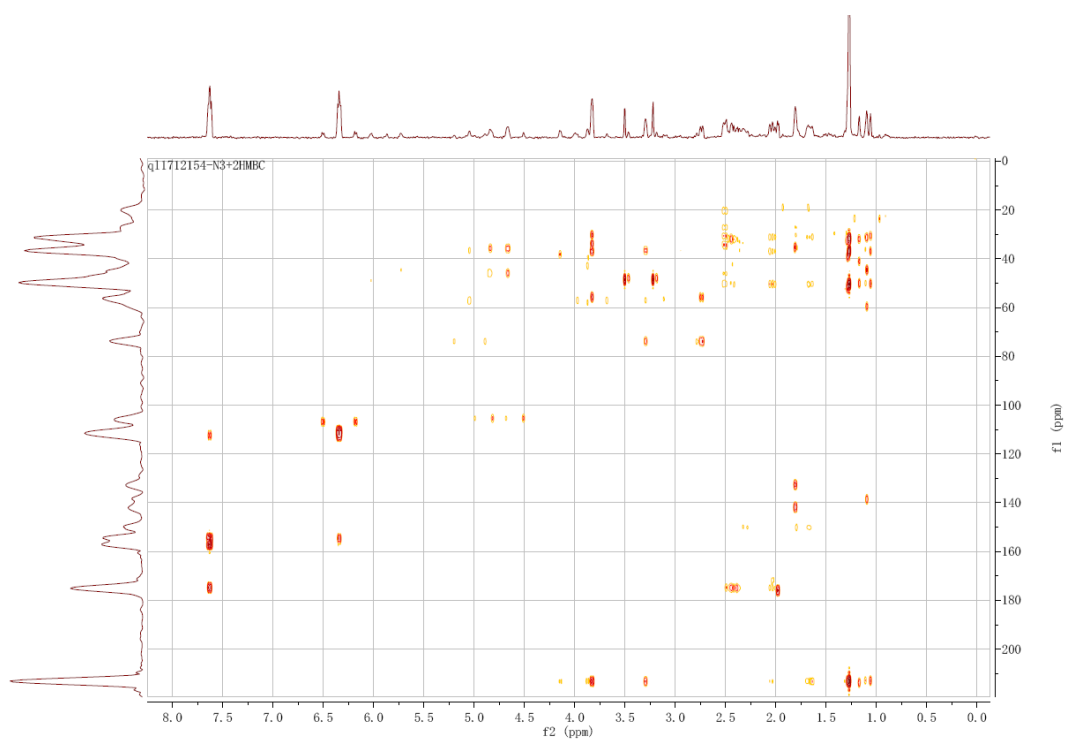


Figure S36. ^1H - ^1H NOESY spectrum of **9a** in CD_3OD .

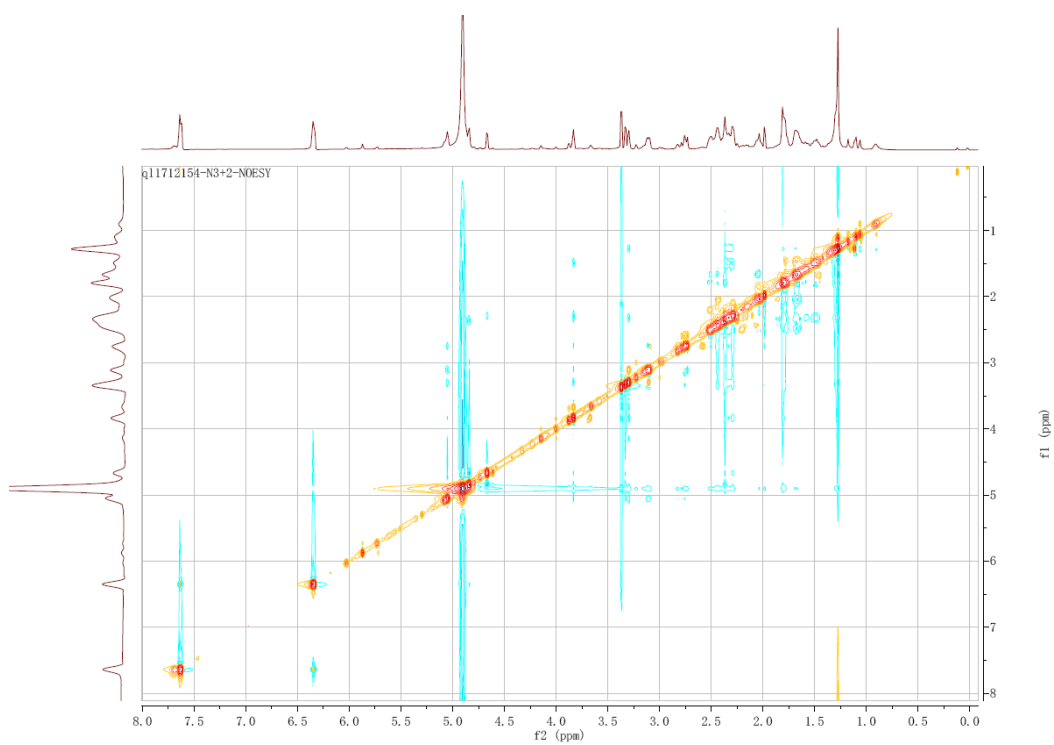


Figure S37. Zoomed in ^1H - ^1H NOESY spectrum of **9a** in CD_3OD (3.0 – 5.5 ppm).

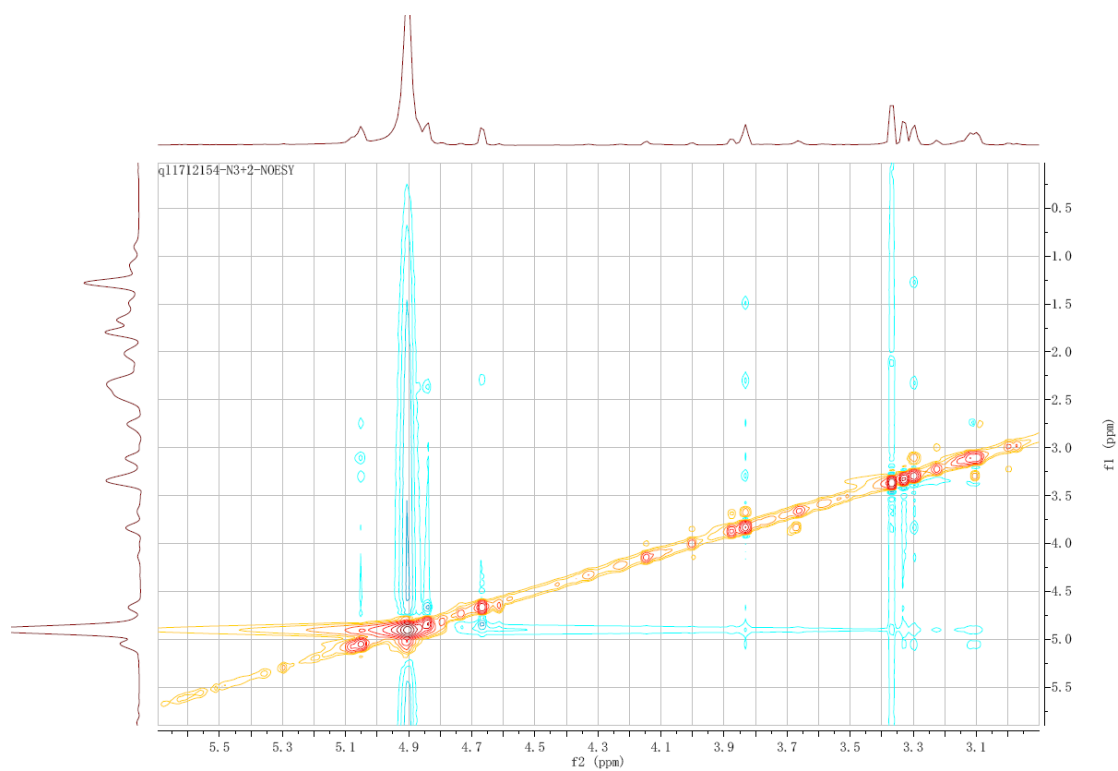


Figure S38. ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectrum of **2b** in CD_3OD .

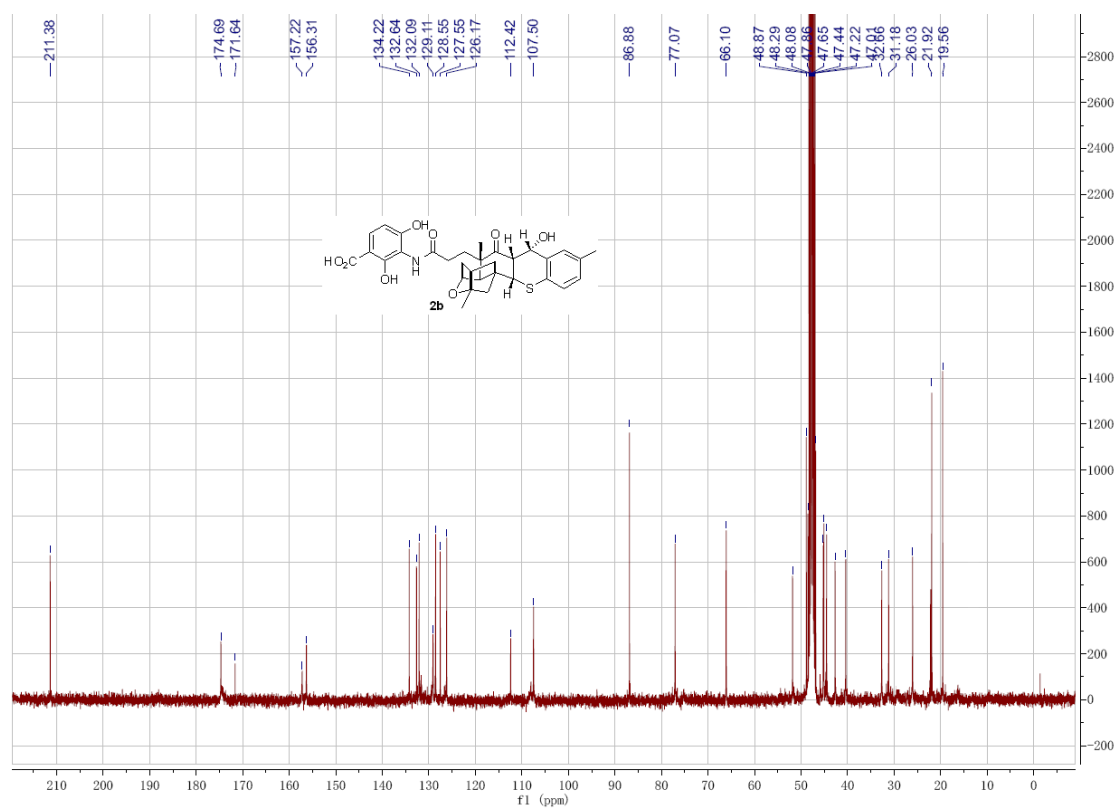
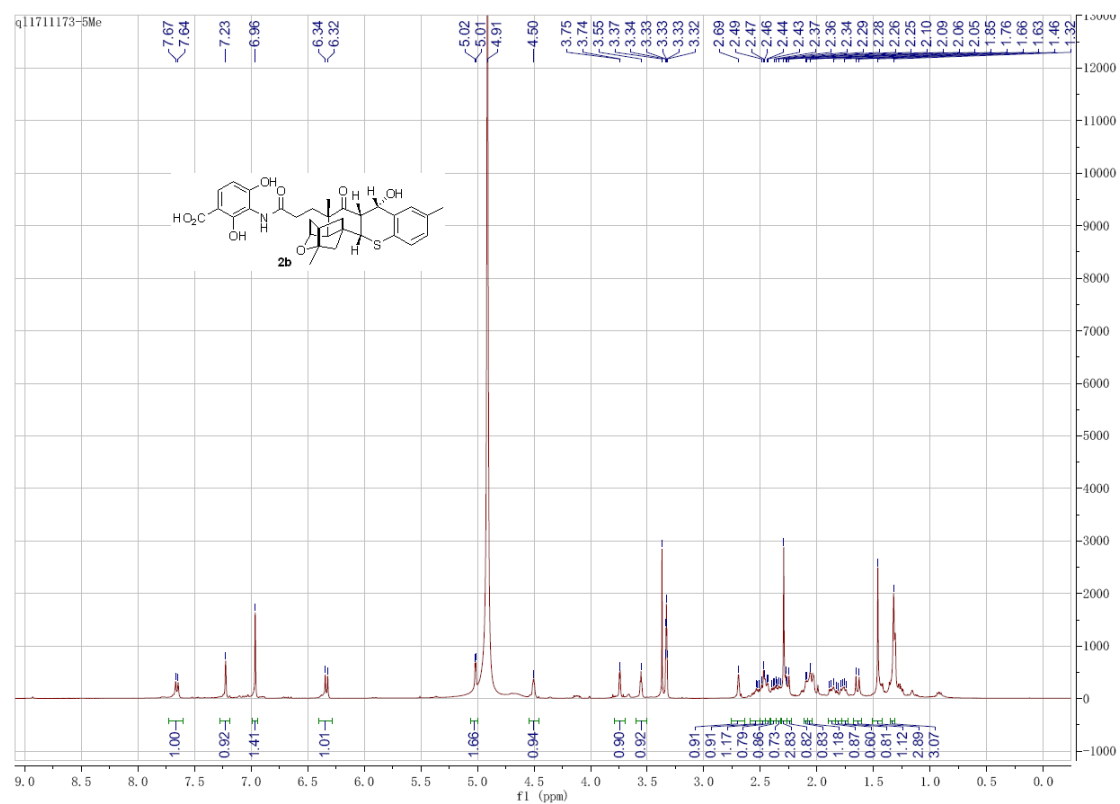


Figure S39. ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectrum of **2c** in CD_3OD .

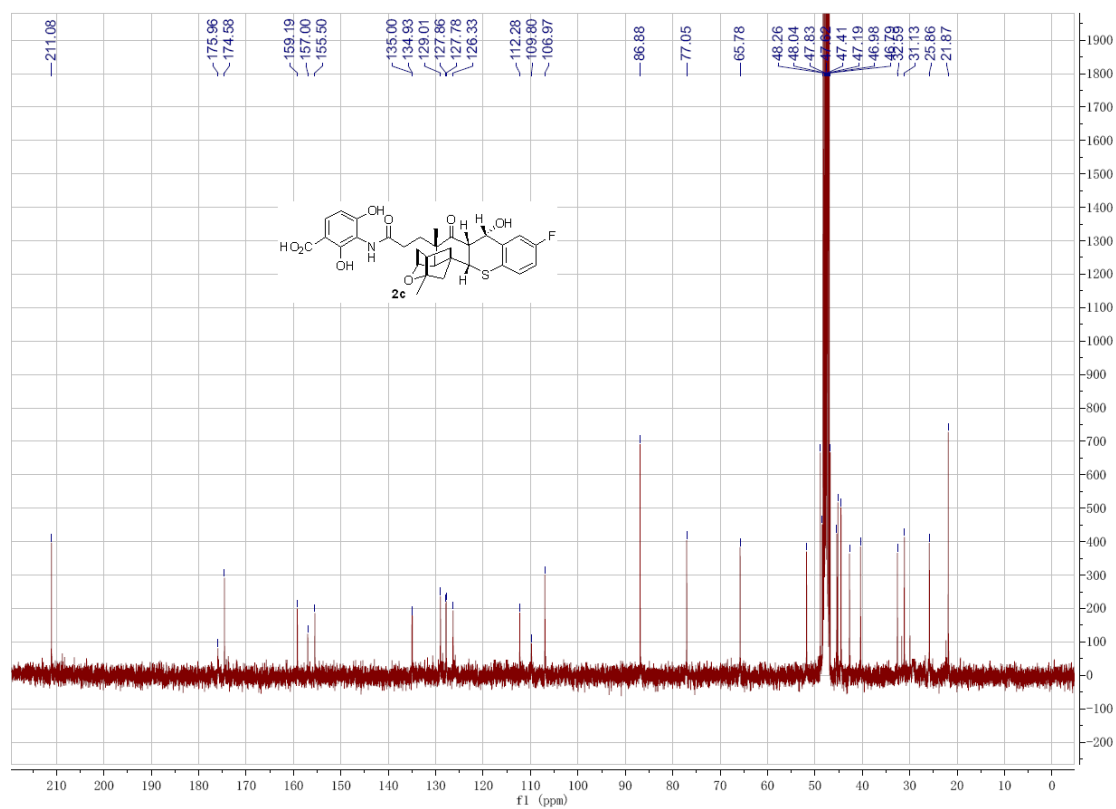
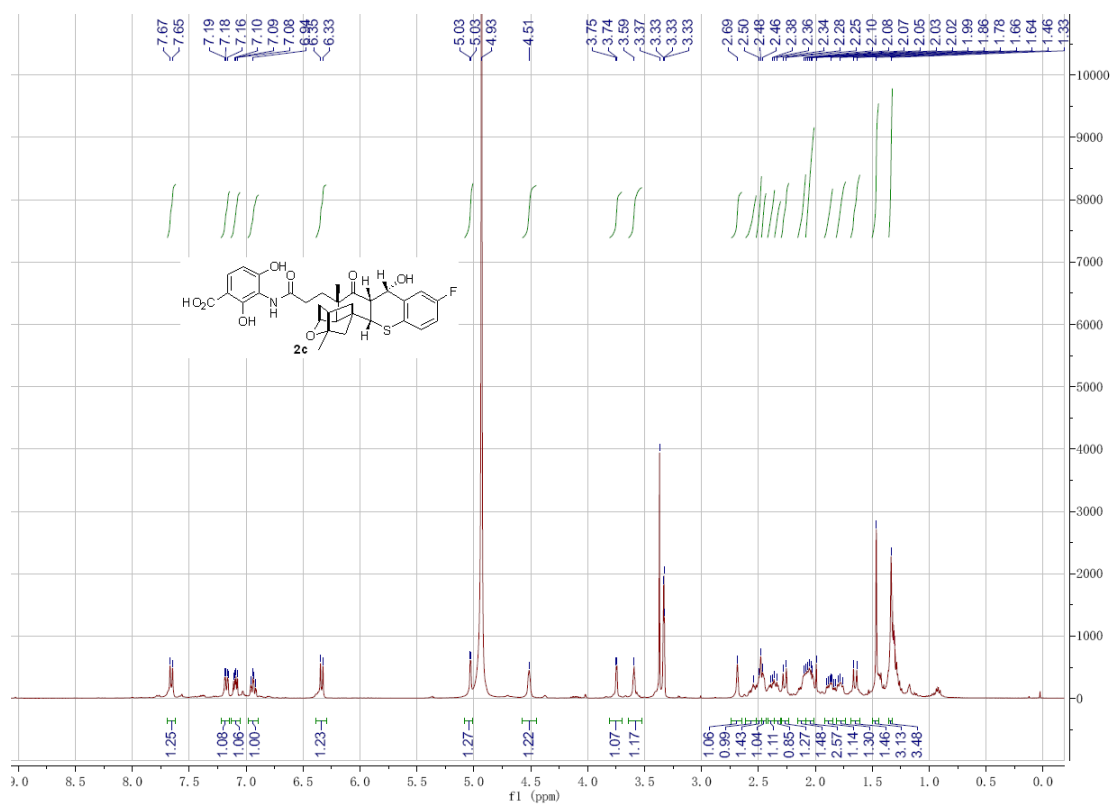


Figure S40. ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectrum of **2d** in CD_3OD .

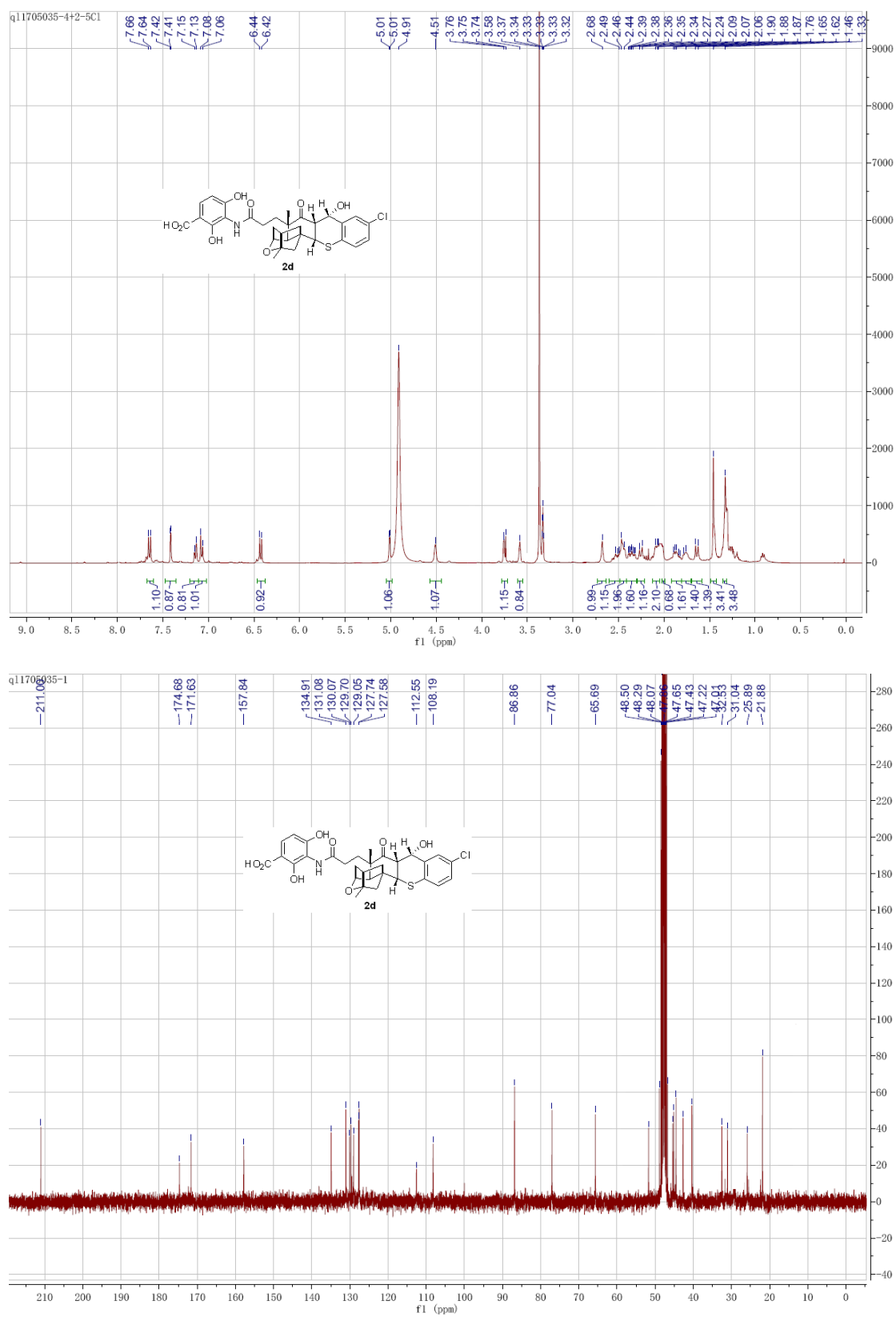


Figure S41. ^1H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectrum of **2e** in CD_3OD .

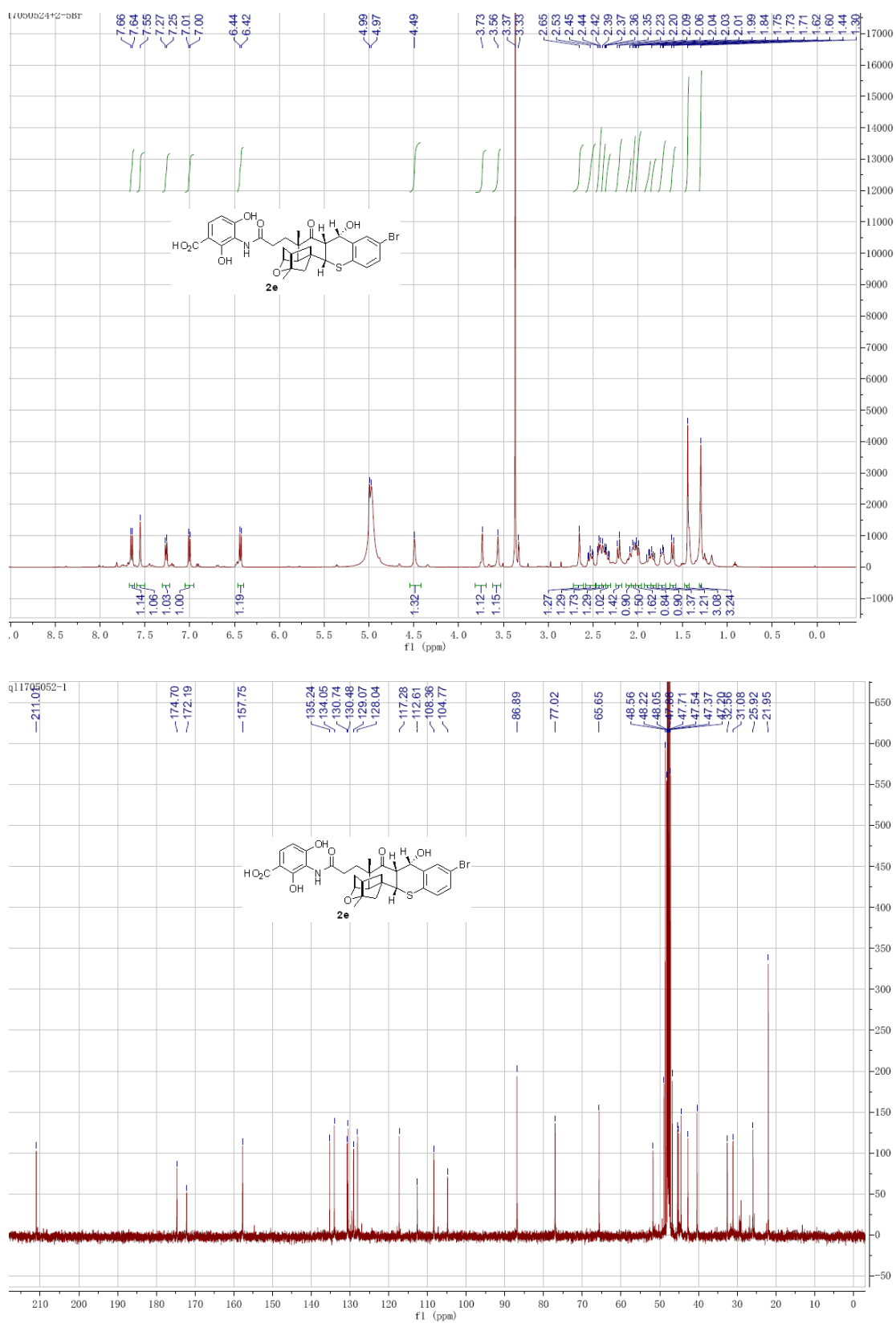


Figure S42. ^1H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectrum of **2f** in CD_3OD .

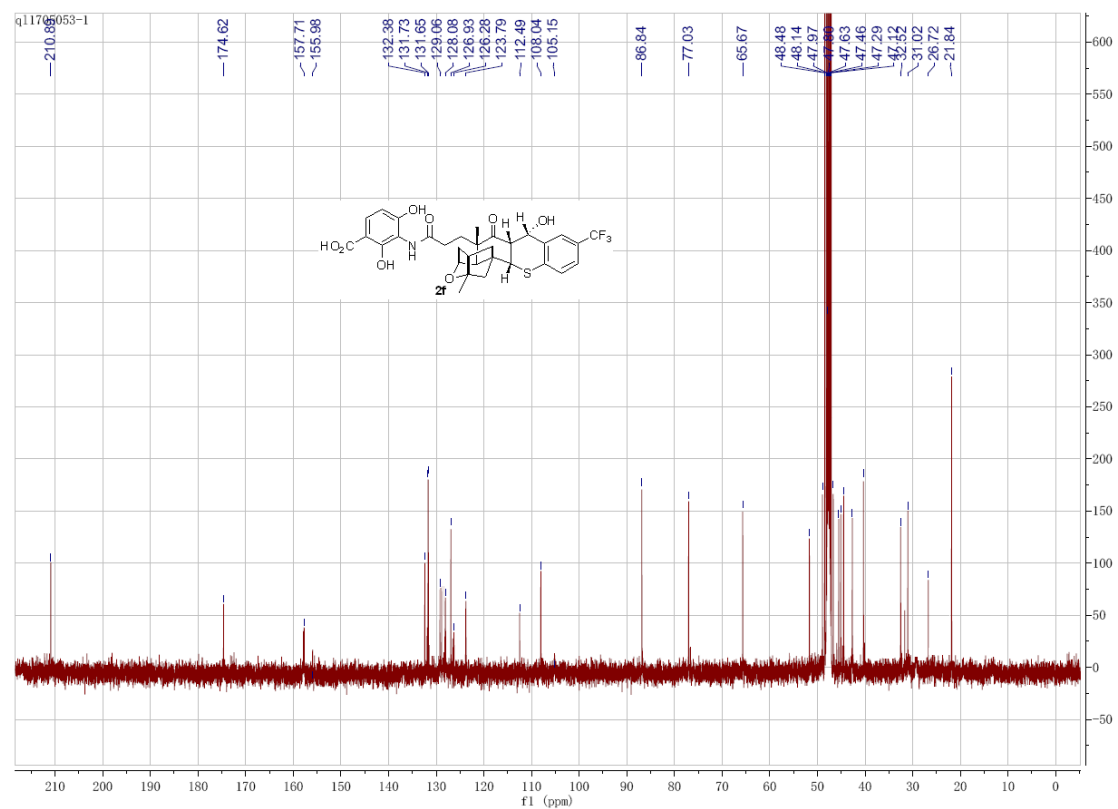
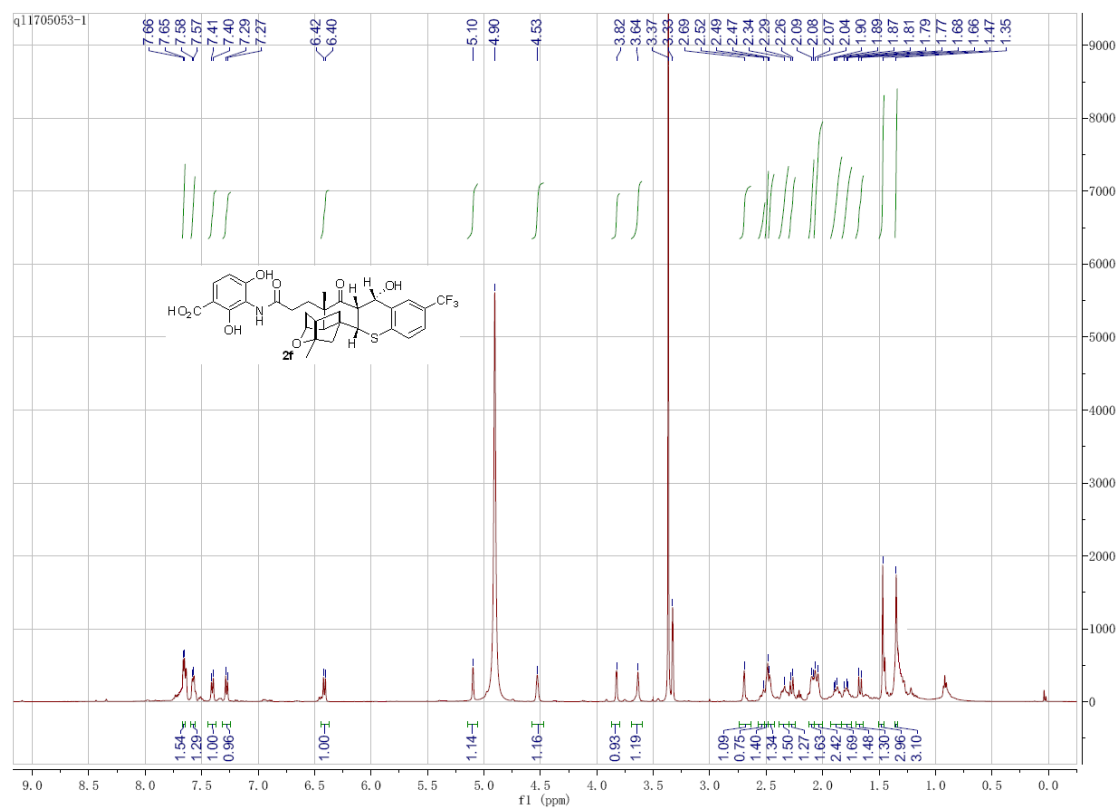


Figure S43. ^1H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectrum of **10a** in CDCl_3 .

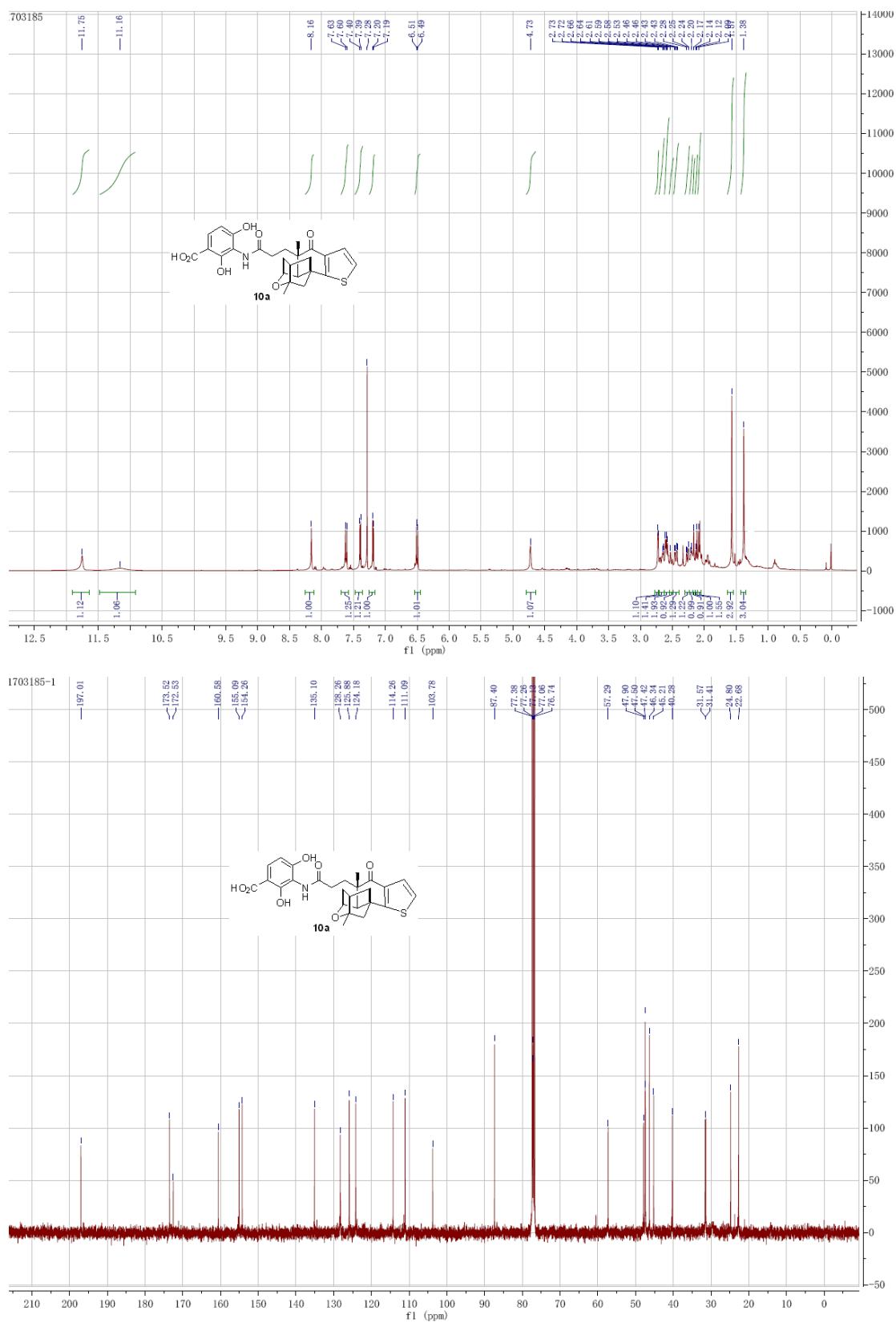


Figure S44. ^1H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectrum of **11a** in CD_3OD .

