

Spongenolactones A–C, Bioactive 5,5,6,6,5-Pentacyclic Spongian Diterpenes from the Red Sea Sponge *Spongia* sp.

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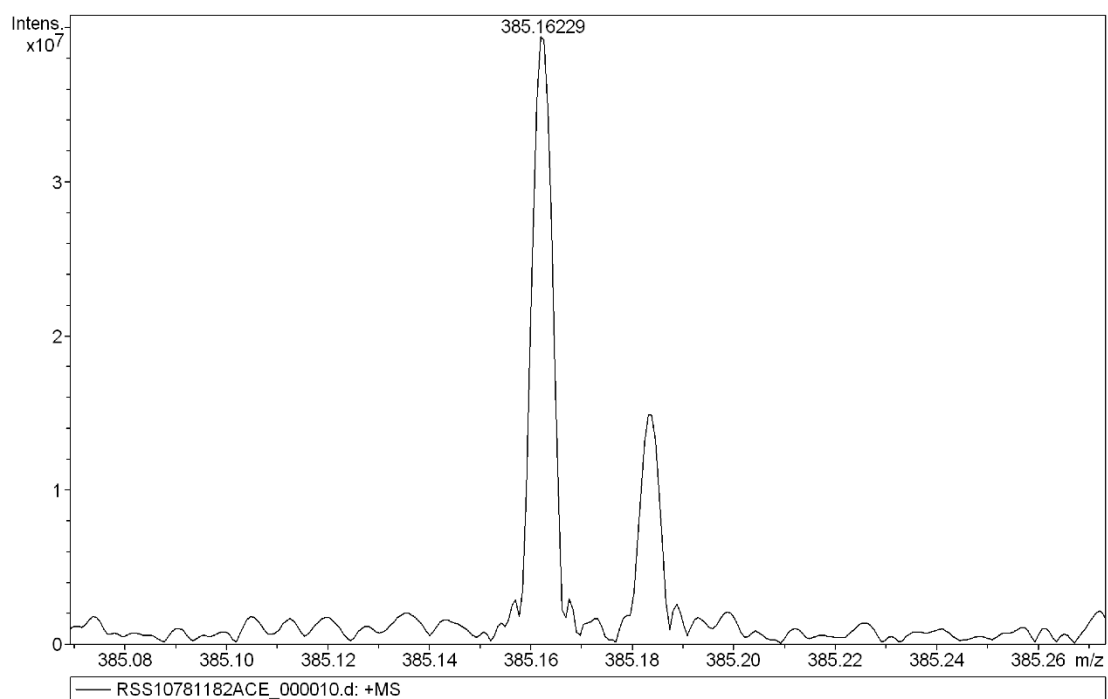
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Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
385.16229	1	C ₂₀ H ₂₆ NaO ₆	100.00	385.16216	-0.13	-0.33	20.9	7.5	even	ok

Figure S1. HRESIMS spectrum of **1**.

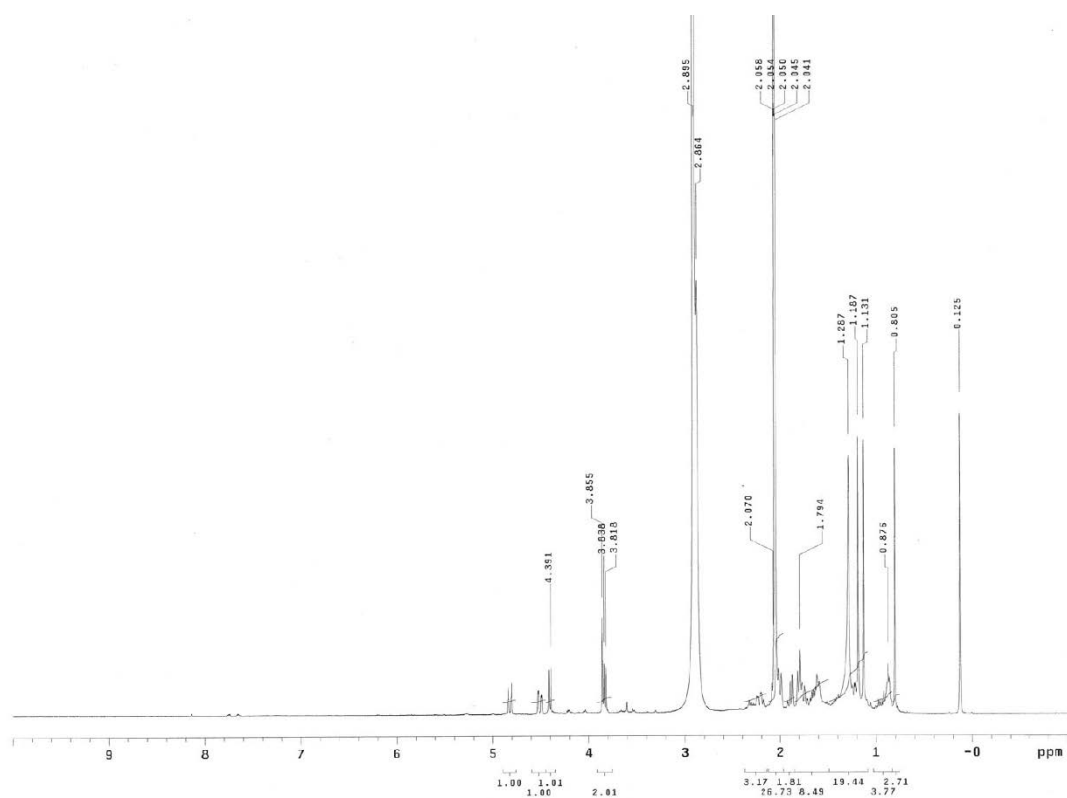


Figure S2. ¹H NMR spectrum of **1**.

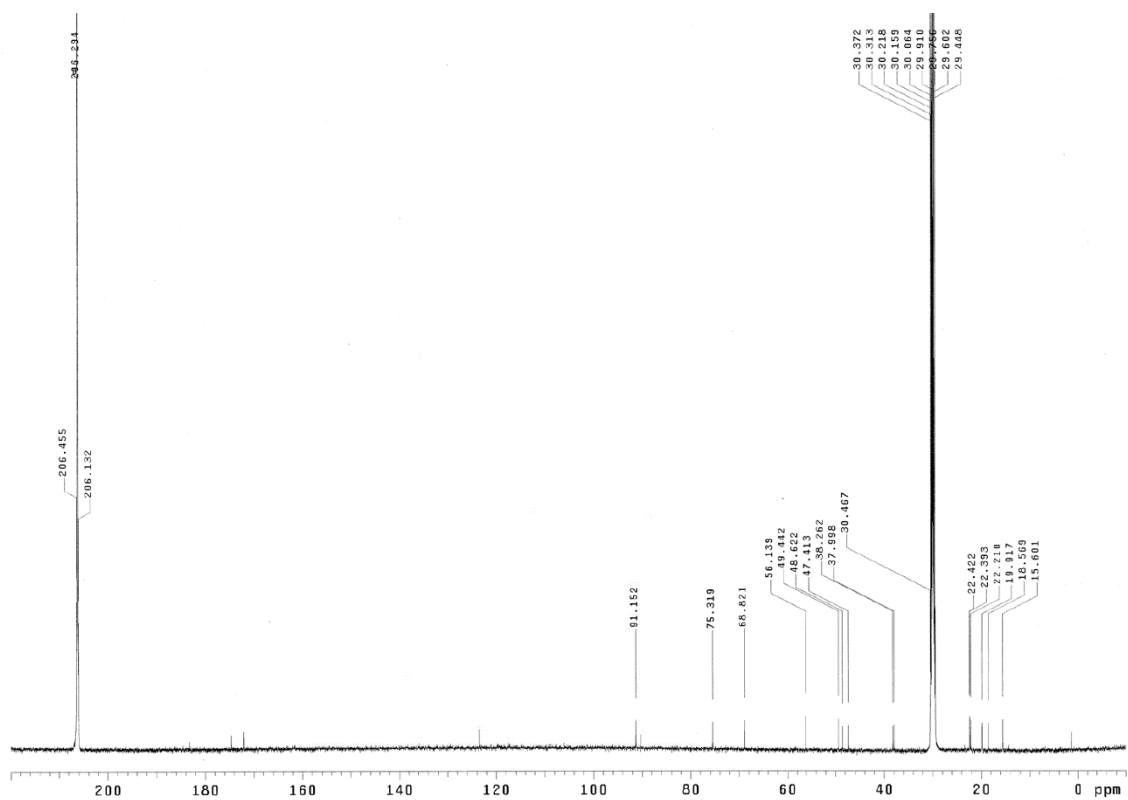


Figure S3. ^{13}C NMR spectrum of **1**.

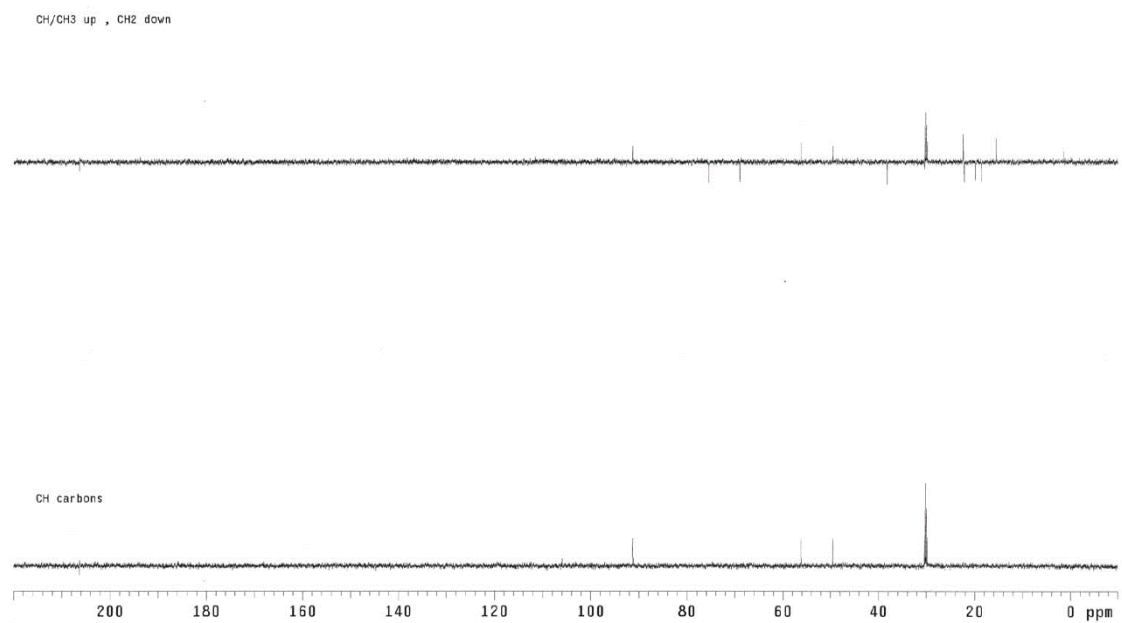


Figure S4. DEPT spectrum of **1**.

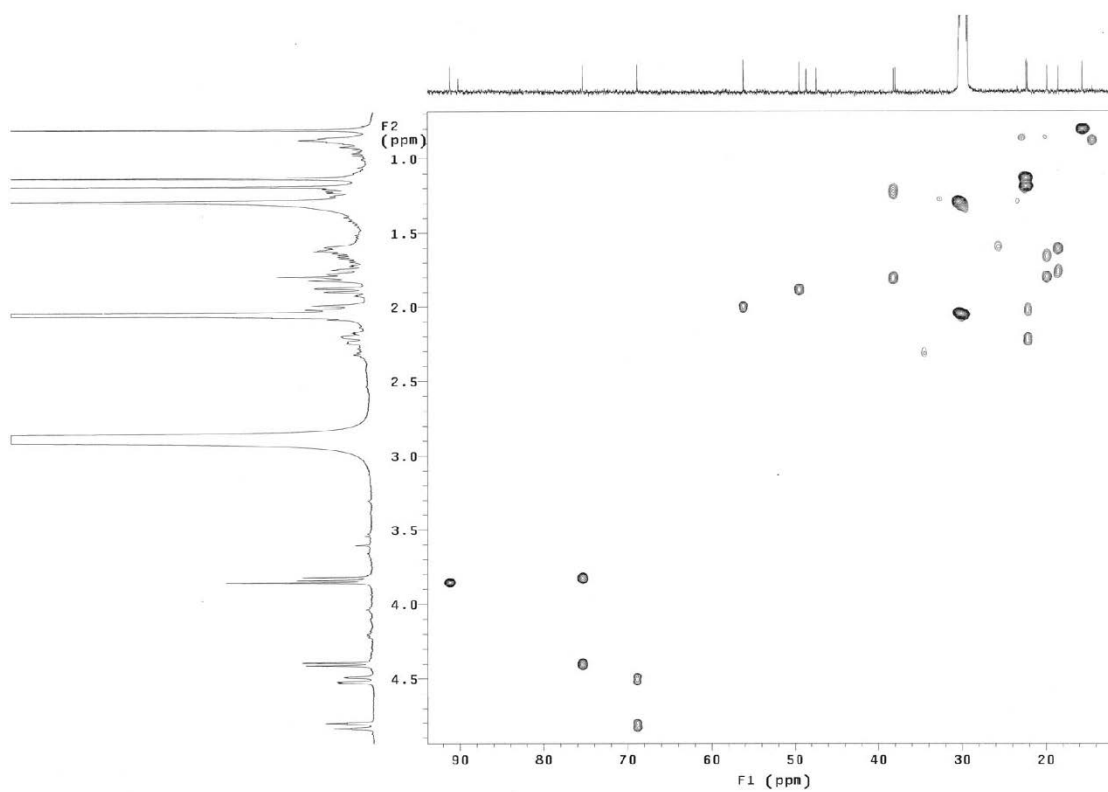


Figure S5. HSQC spectrum of **1**

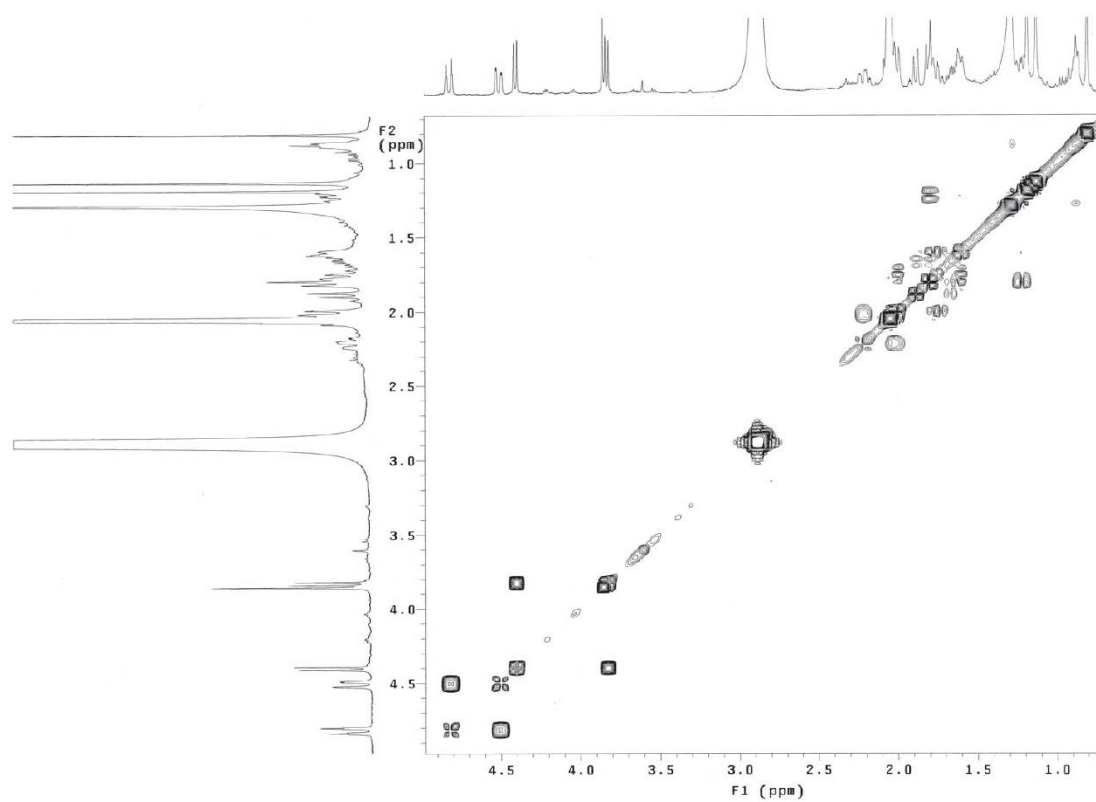


Figure S6. ^1H – ^1H COSY spectrum of **1**.

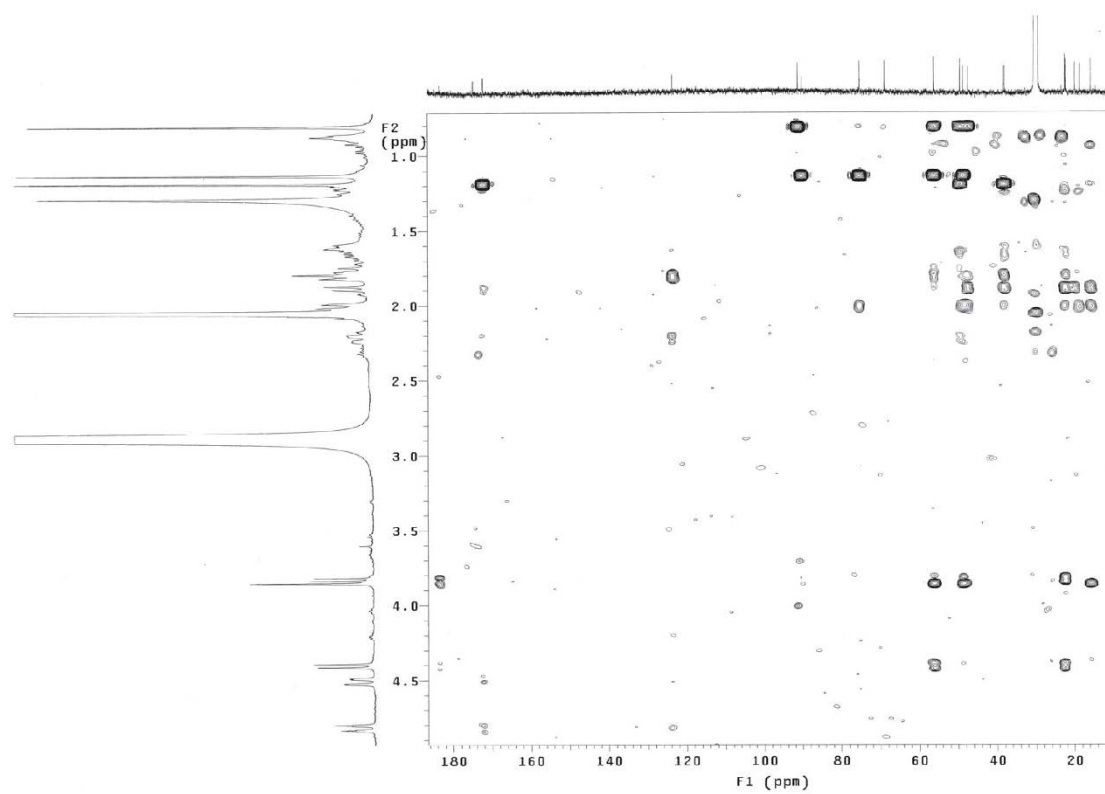


Figure S7. HMBC spectrum of **1**.

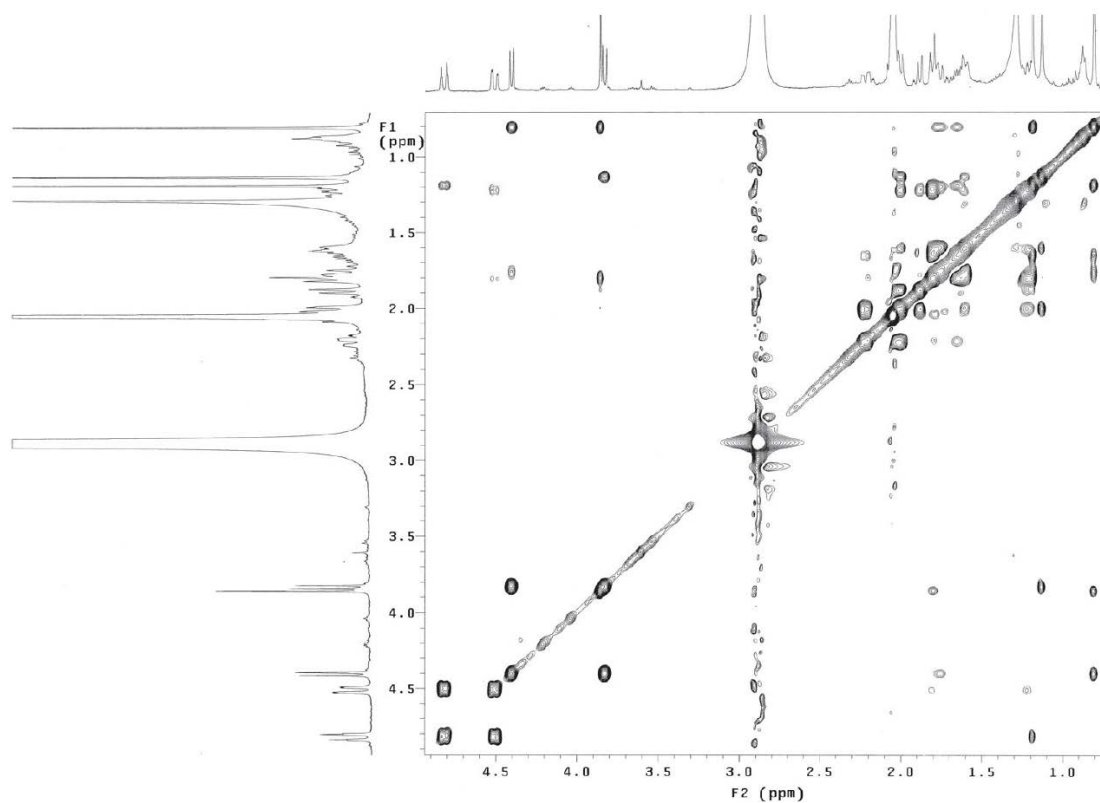


Figure S8. NOESY spectrum of **1**.

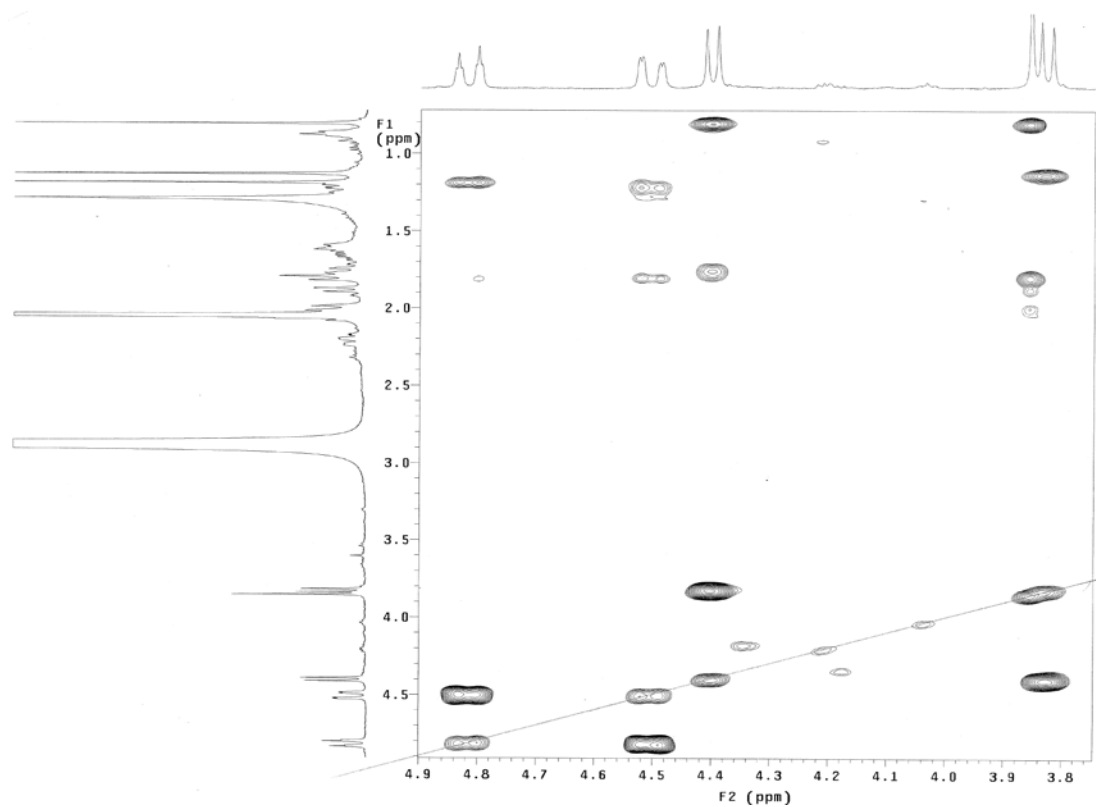
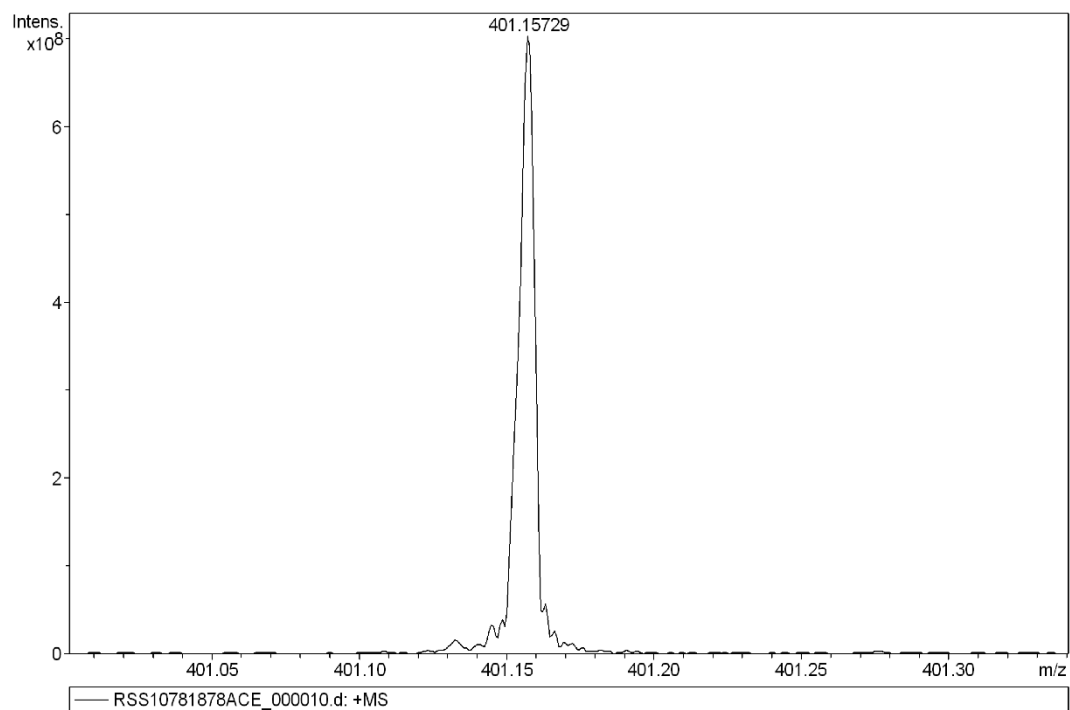


Figure S9. The partial NOESY spectrum of **1**.

Table S1. The cartesian coordinates of conformer **1**.

C	0.70248400	-0.20906500	0.39088000	H	0.70787800	0.89531800	-1.41518100
C	1.08764200	1.07733100	-0.39752400	H	0.56607200	2.55719300	1.12496100
C	0.34766600	2.32798100	0.07582700	H	0.65995800	3.20459500	-0.50263700
C	-1.16613600	2.10892300	-0.13621200	H	-1.34947600	2.04286600	-1.21644500
C	-1.70961500	0.82182500	0.54934800	H	-1.72536000	2.97987400	0.22537700
C	-0.82074900	-0.42075200	0.14823000	H	-0.91410100	-0.46910500	-0.94747700
C	-3.10126100	0.48946300	0.05290500	H	-2.62607300	-2.47184100	-0.99677300
C	-3.56092700	-0.75516100	-0.16189400	H	-3.35962000	-2.75732800	0.56675400
C	-2.78005000	-2.02344400	-0.00535500	H	-1.55539500	-1.70656900	1.75543900
C	-1.42113600	-1.74203200	0.66903700	H	-0.72921200	-2.56452400	0.46997100
C	-4.20689500	1.46648600	-0.24005100	H	-4.50476800	2.06293900	0.62945400
O	-5.32637000	0.65424300	-0.64161300	H	-3.96528700	2.15355200	-1.05846600
C	-4.96198700	-0.66941300	-0.60553300	H	2.13838300	-0.40151900	2.05460700
C	1.07604500	-0.21822200	1.89294700	H	0.54918200	-1.02370700	2.40873900
C	-1.85118700	1.08787500	2.07557200	H	0.82245200	0.71474800	2.39497600
O	-5.74056100	-1.55230600	-0.90624000	H	-2.04009600	0.17181600	2.63918000
C	1.59003100	-1.23133600	-0.36059600	H	-2.69381000	1.76255800	2.25616800
C	2.91957800	-0.47144500	-0.74354200	H	-0.96721900	1.57050500	2.49276000
C	2.62394900	1.05578000	-0.59617800	H	1.12881500	-1.46609700	-1.33156700
C	4.06363000	-0.73607100	0.22841000	H	2.85962600	1.72675800	1.52320300
O	4.28090100	0.31324500	1.03498300	H	4.15276000	2.27366500	0.44069400
C	3.46048500	1.45714200	0.65514900	H	2.37846100	-2.99949100	-0.10258600
O	1.78866500	-2.41481900	0.39439200	H	3.97500100	-1.58902300	-1.92499400
O	3.35282400	-0.85279300	-2.04197200	H	4.14373400	1.77174300	-1.98492900
O	4.73982600	-1.74336600	0.25177300	H	2.86645200	2.94644100	-1.63272300
C	3.07080900	1.88494500	-1.80588100	H	2.54510100	1.57614700	-2.71233700



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
401.15729	1	C ₂₀ H ₂₆ NaO ₇	100.00	401.15707	-0.22	-0.54	11.1	7.5	even		ok

Figure S10. HRESIMS spectrum of **2**.

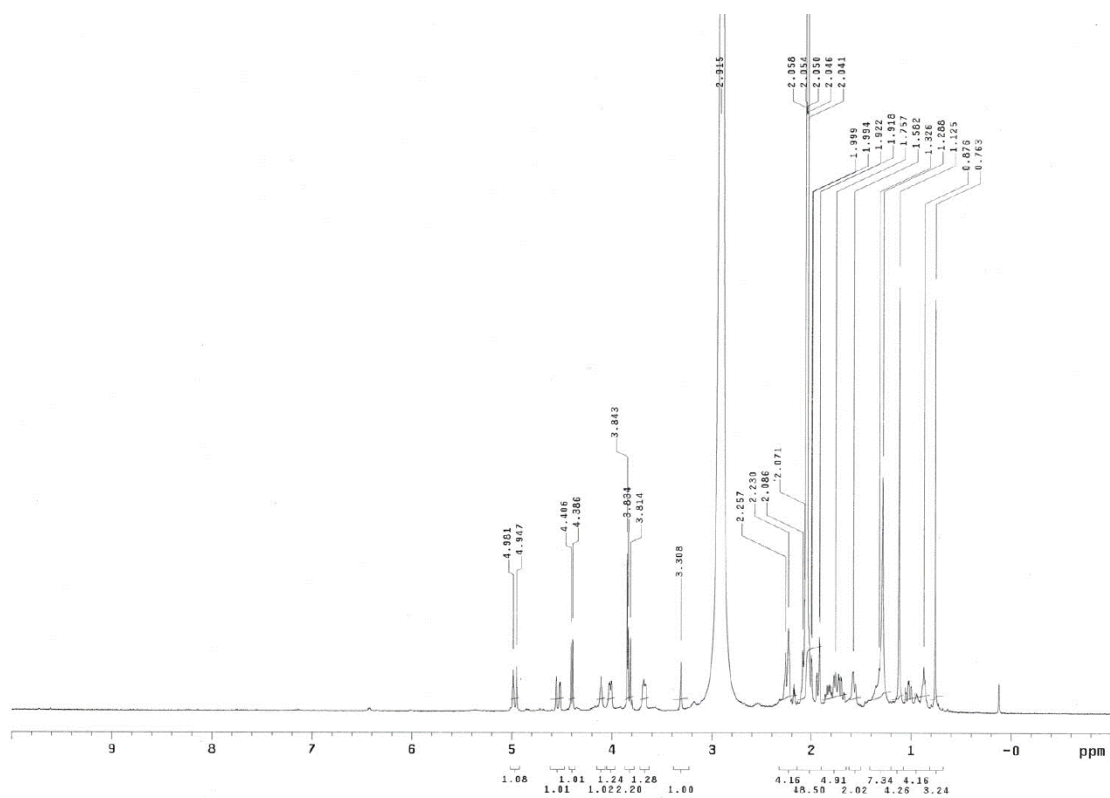


Figure S11. ¹H NMR spectrum of **2**.

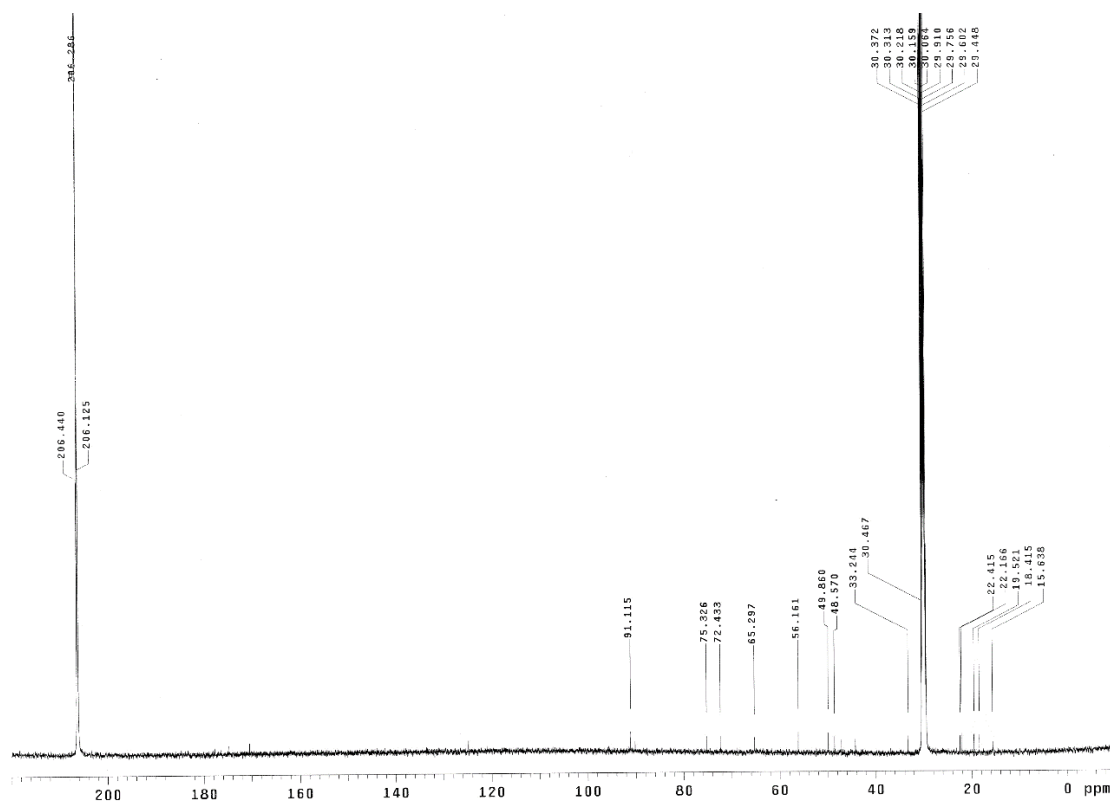


Figure S12. ¹³C NMR spectrum of 2.

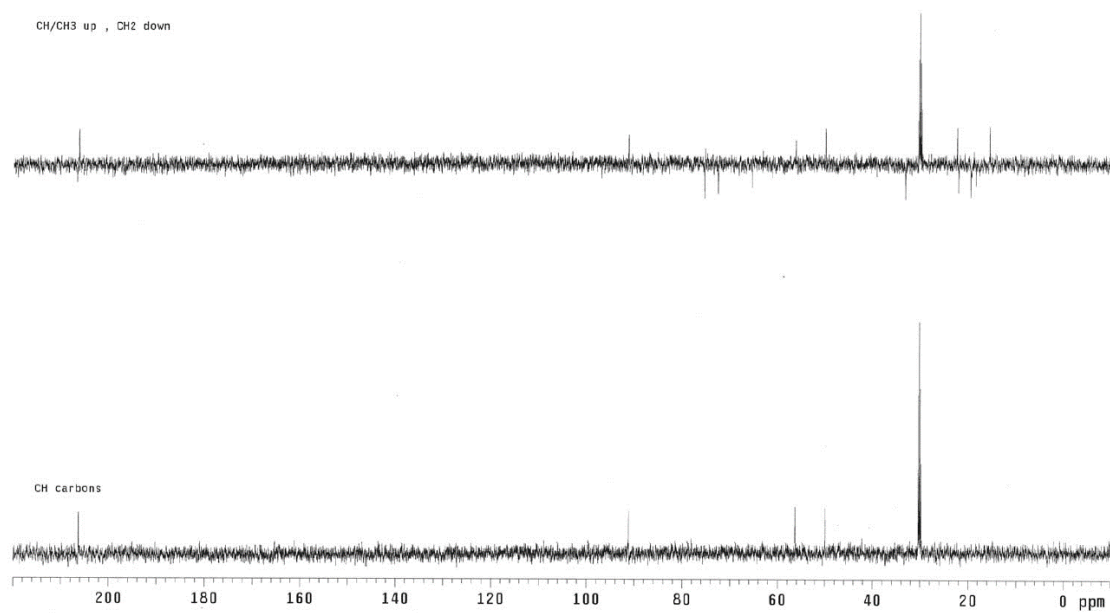


Figure S13. DEPT spectrum of 2.

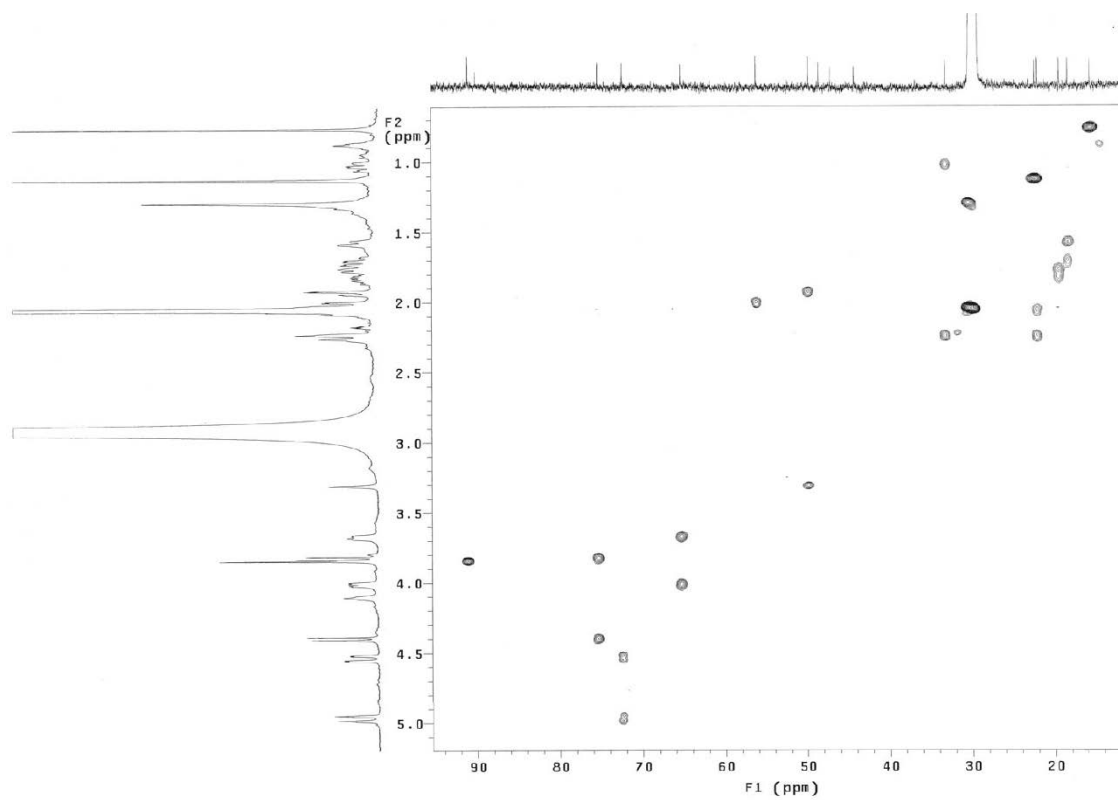


Figure S14. HSQC spectrum of **2**.

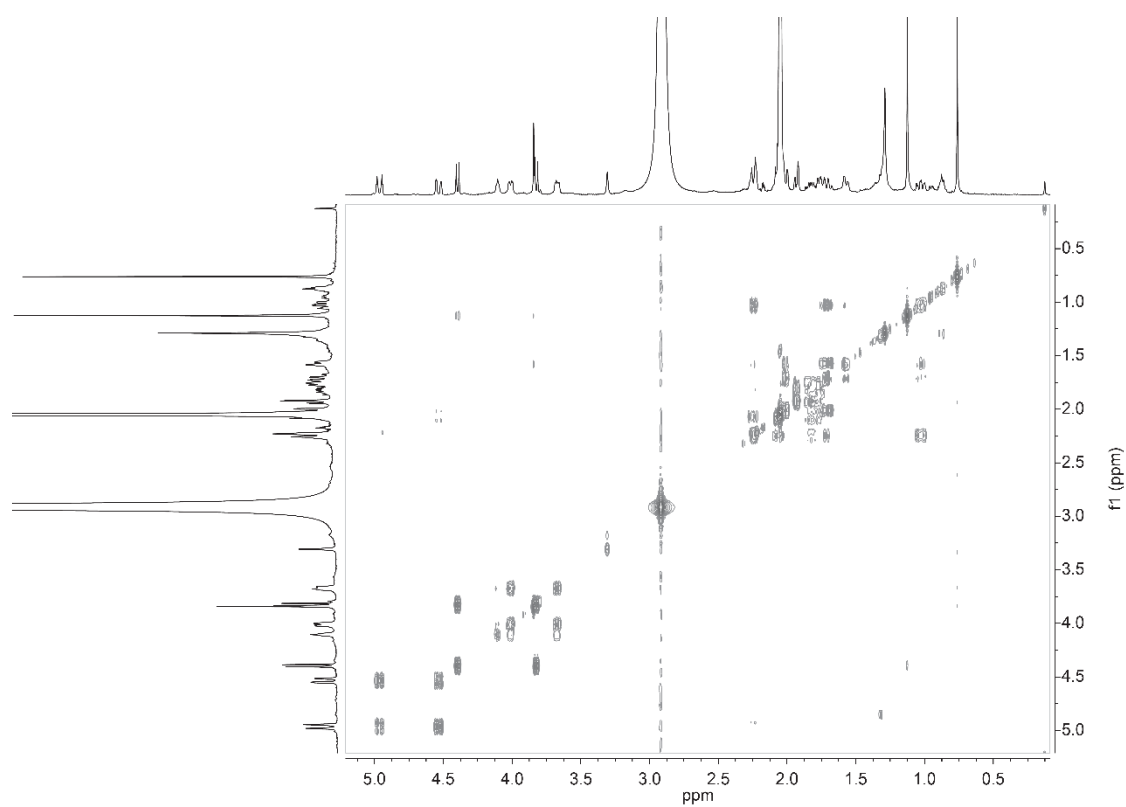


Figure S15. ^1H - ^1H COSY spectrum of **2**.

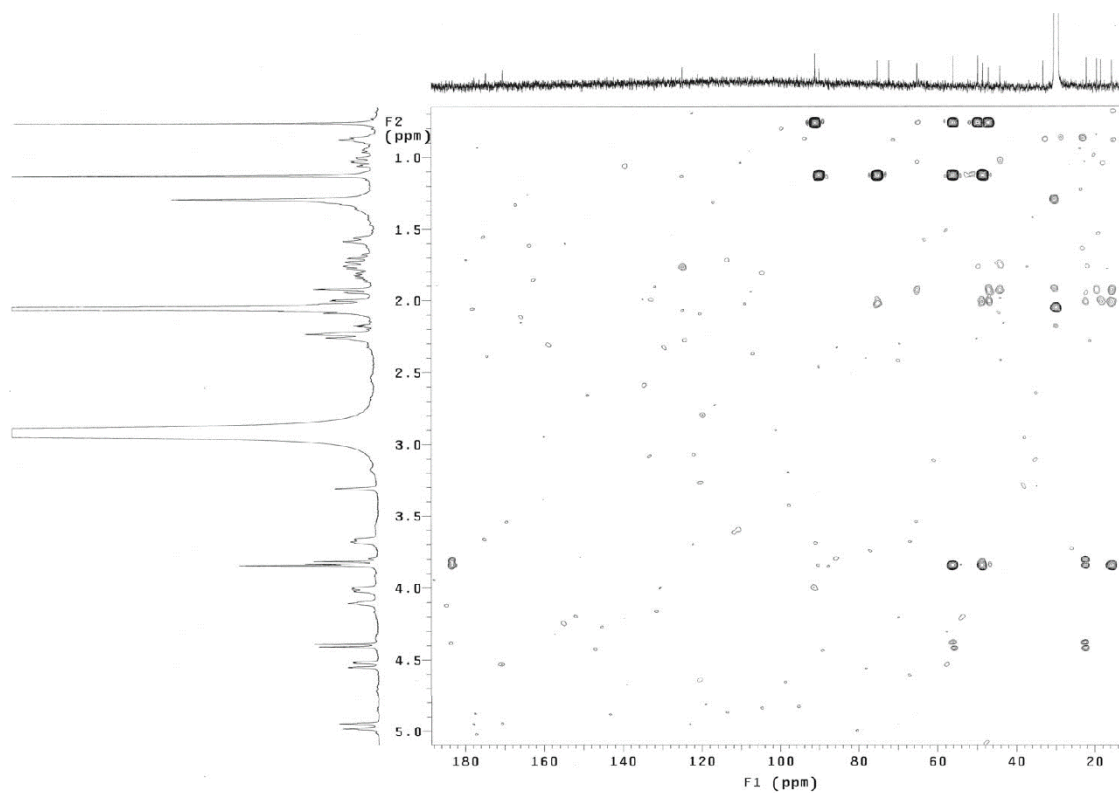


Figure S16. HMBC spectrum of **2**.

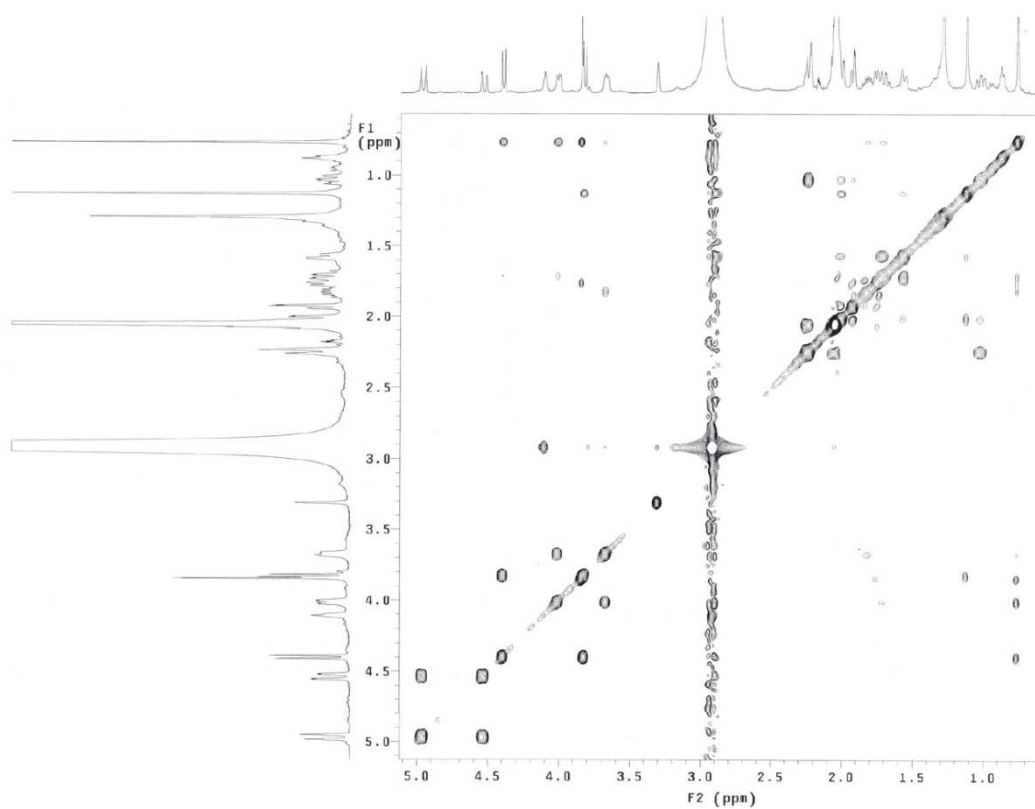


Figure S17. NOESY spectrum of **2**.

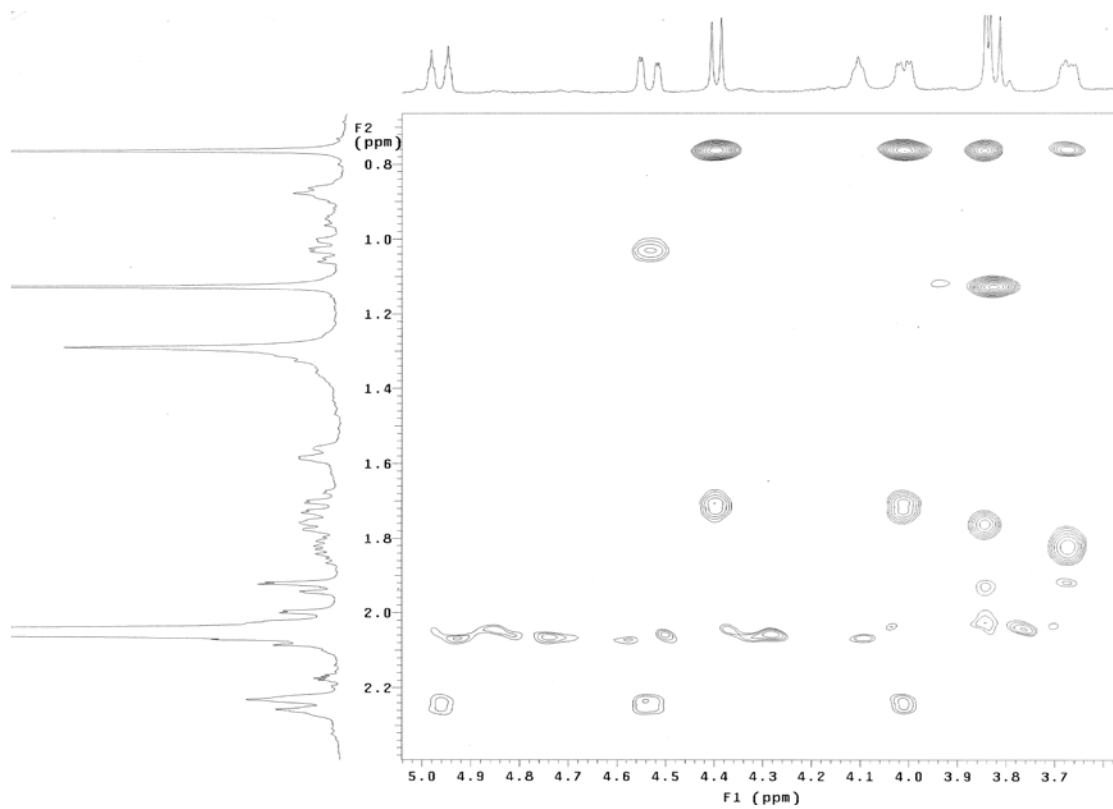


Figure S18. The partial NOESY spectrum of **2**.

Table S2. The cartesian coordinates of conformer **2**.

C	-0.76119200	0.23711000	0.30999000	H	-0.70752100	-0.48368400	-1.67678900
C	-1.12793200	-0.86204000	-0.73168100	H	-0.71223200	-2.92879600	-1.24964800
C	-0.41889900	-2.19300700	-0.48959400	H	-0.66863400	-2.61312300	0.48718400
C	1.10726000	-1.96637100	-0.59624900	H	1.63751100	-2.89825700	-0.36855300
C	1.65734700	-0.81830500	0.30351100	H	1.33535700	-1.71912400	-1.64176600
C	0.76313400	0.48385200	0.14825800	H	0.88333000	0.74808200	-0.91431500
C	3.03470700	-0.37787000	-0.15905600	H	3.30308500	2.66345100	1.07921900
C	3.49152900	0.88463600	-0.10006500	H	2.57955600	2.75594700	-0.51248900
C	2.72052800	2.08764400	0.34931400	H	0.65964300	2.52148500	0.88132500
C	1.35116100	1.67592700	0.93120200	H	1.46007500	1.43238000	1.99413500
C	4.12501500	-1.25840400	-0.70936800	H	4.45578100	-2.03835600	-0.01436900
O	5.23211400	-0.37113000	-0.95431200	H	3.85227600	-1.73818300	-1.65581200
C	4.87587300	0.90744600	-0.60535600	H	-0.57986700	-0.88317000	2.18543100
C	-1.13998500	-0.04151900	1.77752900	H	-0.92463300	0.84532200	2.38345100
C	1.91274700	-1.34049300	1.75756400	H	-2.19979600	-0.26681200	1.91731200
O	5.64477300	1.83966900	-0.72651500	H	2.91690600	-1.78490300	1.78907100
C	-1.64352300	1.38176800	-0.26730700	H	1.91625700	-0.49900600	2.46112800
C	-2.98978300	0.69691300	-0.65779200	H	-1.20107800	1.70882600	-1.21722600
C	-2.66424800	-0.78987700	-0.98914800	H	-4.27257400	-2.23149900	-0.49487100
C	-3.97912700	0.62211700	0.51155400	H	-2.96915800	-2.19741900	0.71154600
O	-4.31123500	-0.64165800	0.80247600	H	-2.55168900	2.44099100	1.11350300
C	-3.54583500	-1.59188400	0.00987400	H	-3.76496000	2.29942400	-1.42104200
O	-1.80863300	2.56662200	0.49579700	H	-2.46992600	-0.58006600	-3.15288800
O	-3.64293200	1.38076200	-1.72009700	H	-2.74051100	-2.24344000	-2.59796100
O	-4.44615200	1.57506500	1.10815700	H	-4.08229700	-1.08426700	-2.62412200
C	-3.01131800	-1.19510800	-2.42852900	H	1.21019300	-2.61072500	3.05454300
O	0.96833400	-2.33311500	2.15650900				

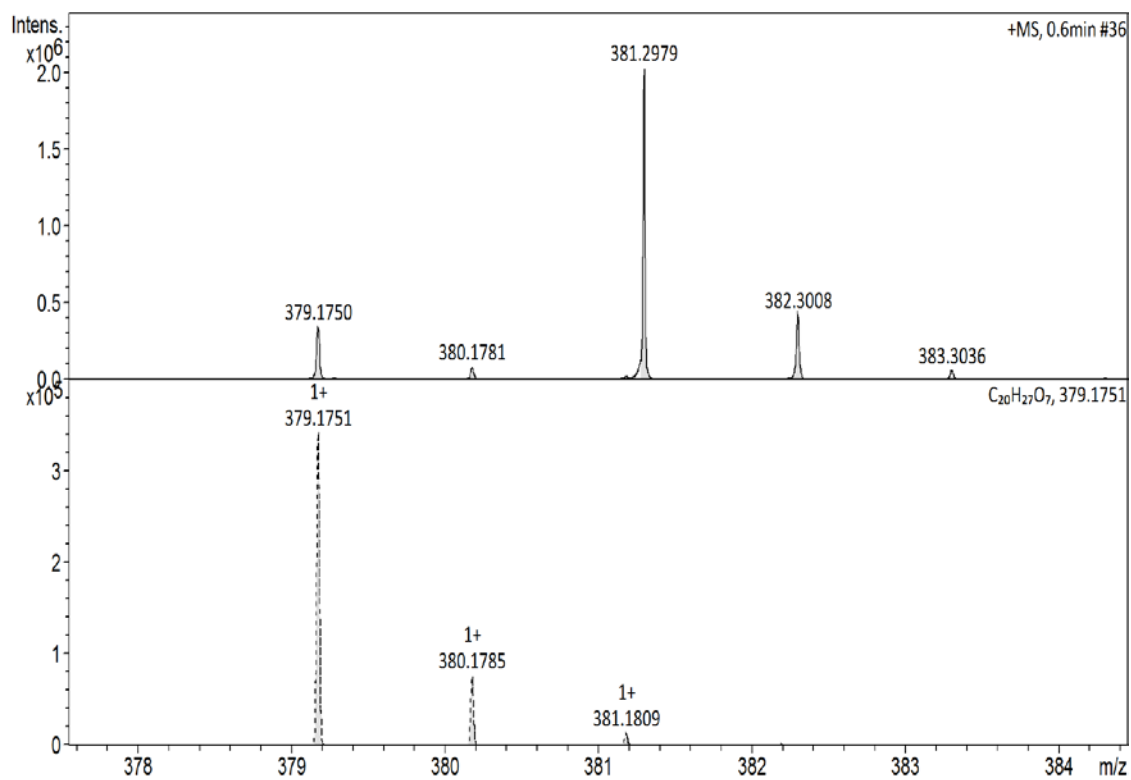


Figure S19. HRESIMS spectrum of **3**.

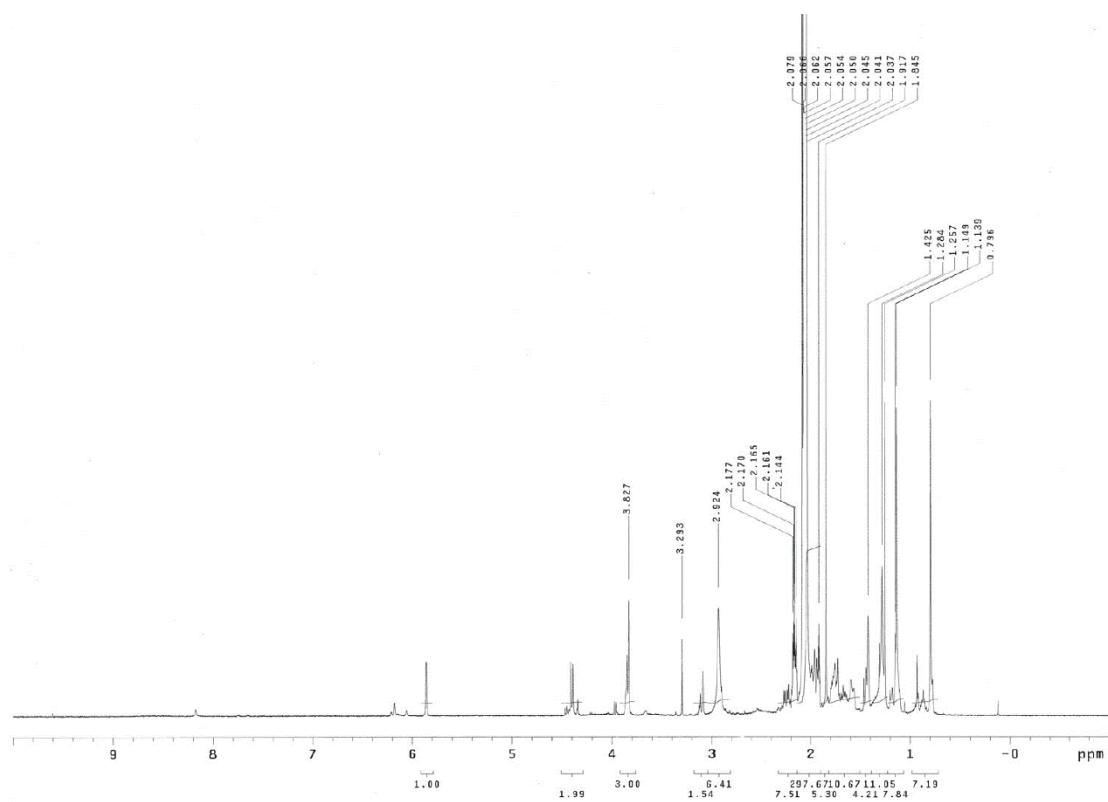


Figure S20. ^1H NMR spectrum of **3**.

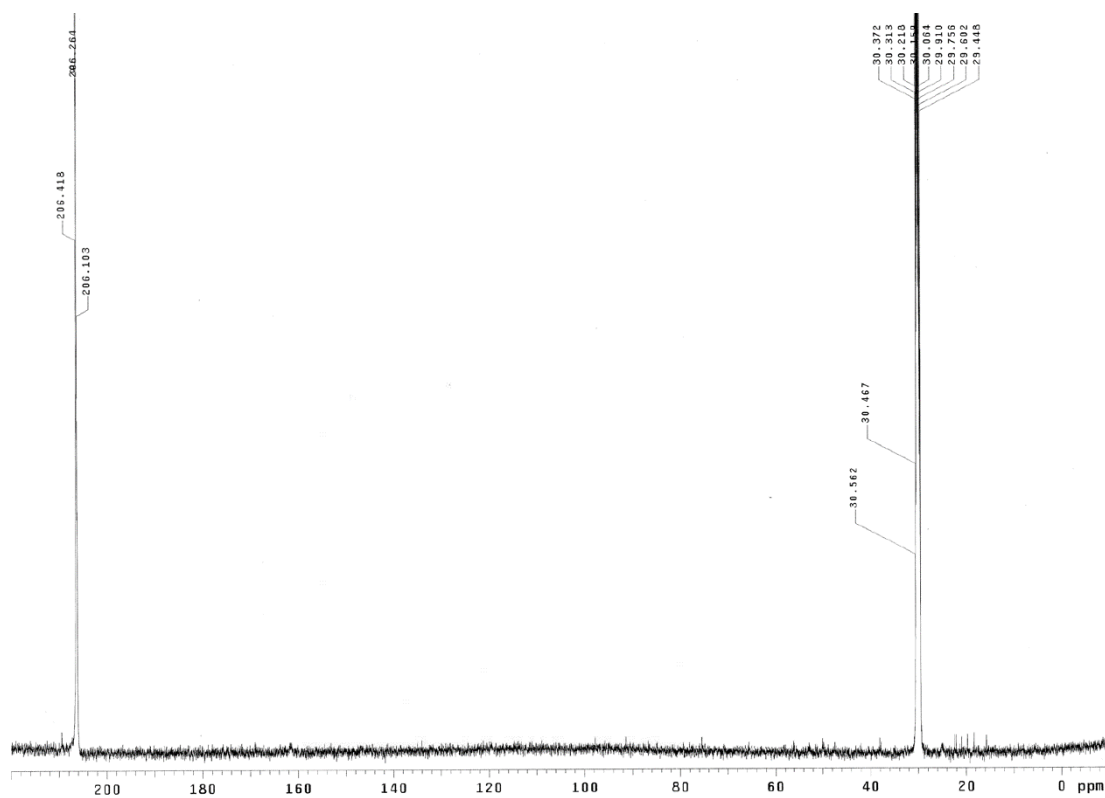


Figure S21. ^{13}C NMR spectrum of **3**.

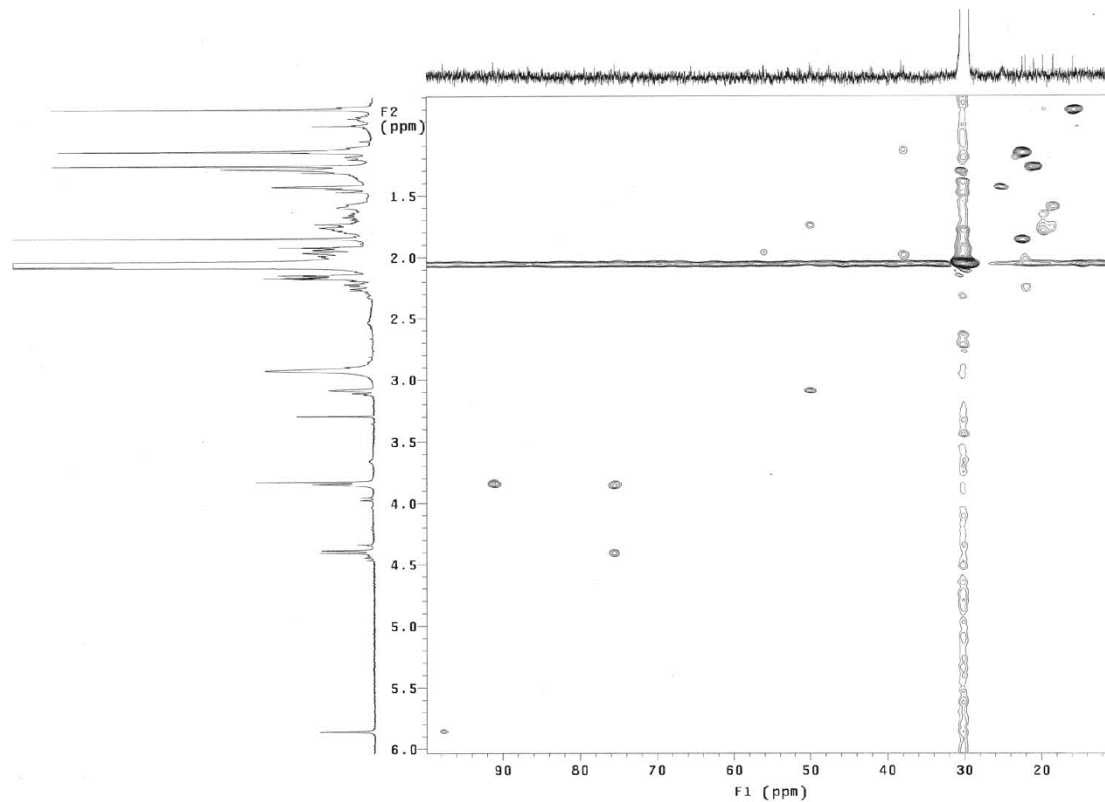


Figure S22. HSQC spectrum of **3**.

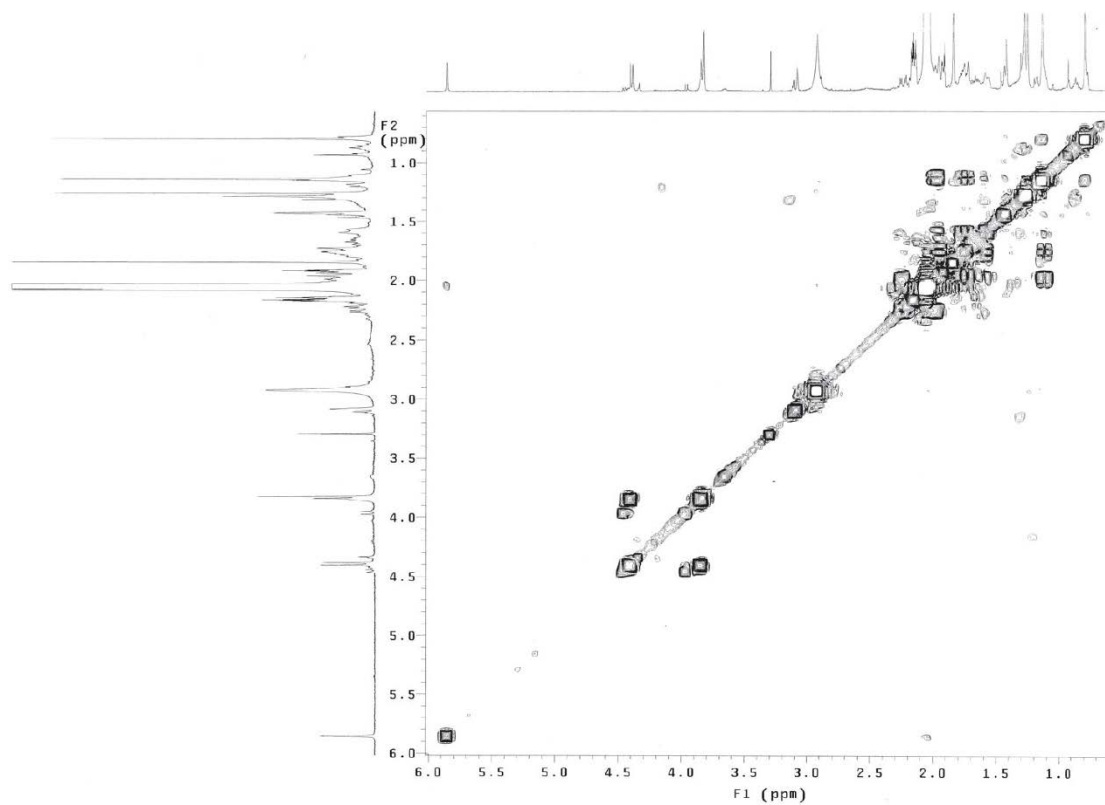


Figure S23. ^1H – ^1H COSY spectrum of **3**.

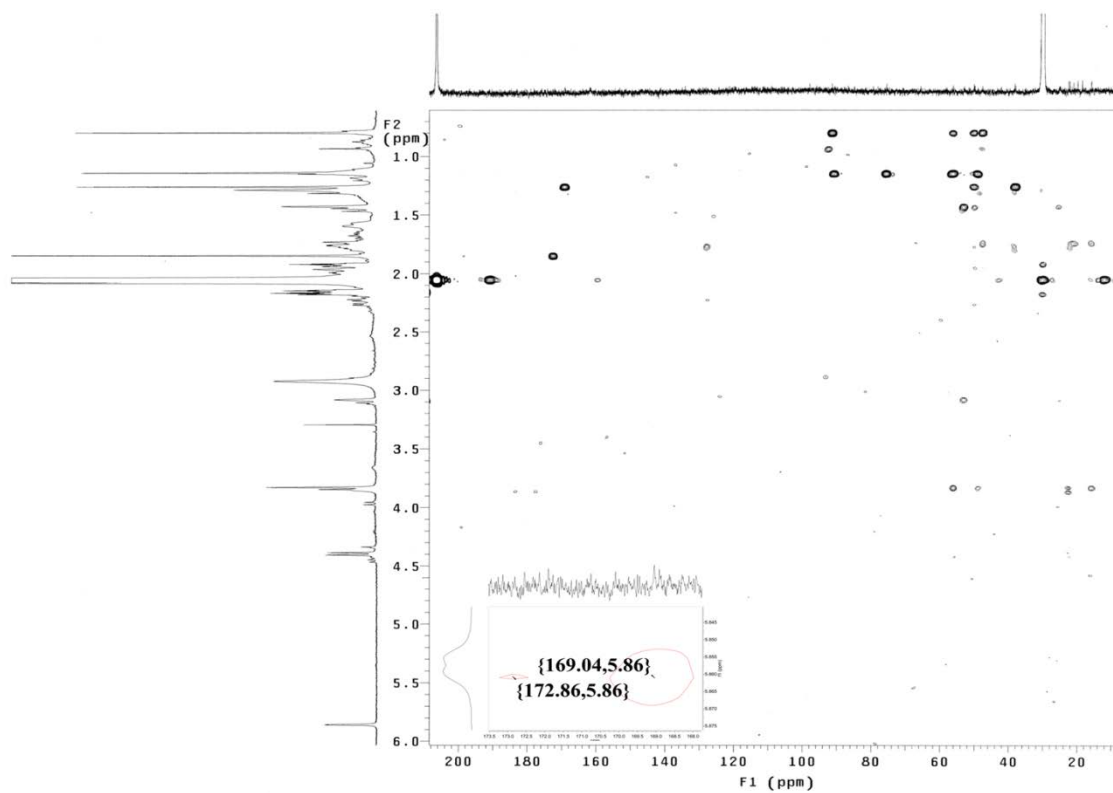


Figure S24. HMBC spectrum of **3**.

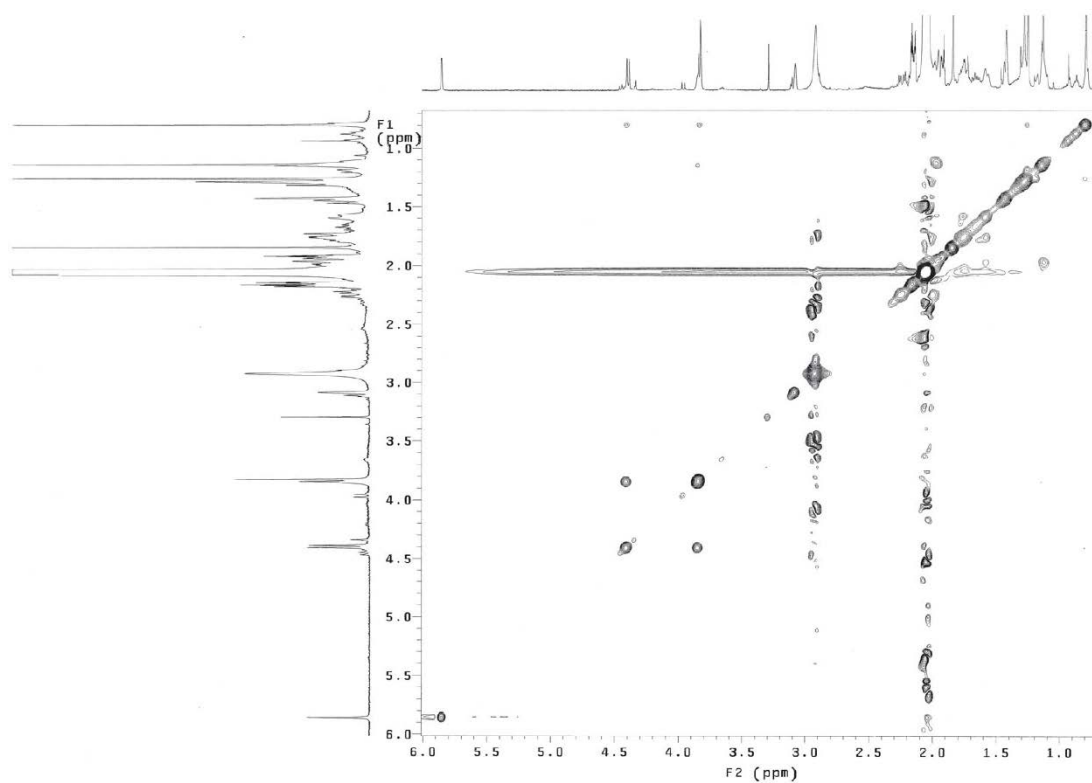


Figure S25. NOESY spectrum of **3**.

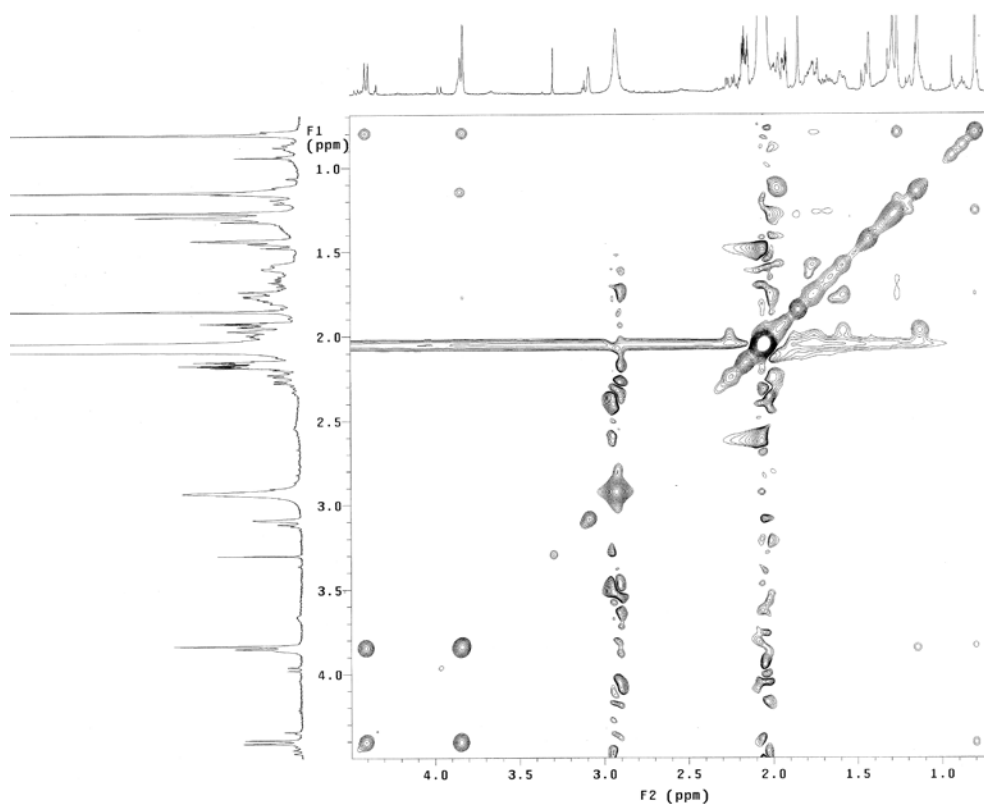


Figure S26. The partial NOESY spectrum of **3**.

Table S3. The cartesian coordinates of conformer **3**.

C -0.89718400 0.24914900 0.36747300	H -0.85292400 -0.79890800 -1.47178300
C -1.22144500 -1.02986700 -0.45948300	H -0.62406200 -2.52751400 1.01853200
C -0.42117000 -2.25762100 -0.02477500	H -0.69300900 -3.13190200 -0.62864700
C 1.07952800 -1.95976800 -0.23612900	H 1.25052100 -1.85337300 -1.31628900
C 1.56492100 -0.66878600 0.48609600	H 1.68597300 -2.81018000 0.09730900
C 0.61294500 0.54241300 0.13053200	H 0.70099000 0.63961200 -0.96318400
C 2.93302600 -0.24935300 -0.01241700	H 2.33108100 2.74566000 -0.90478400
C 3.32932000 1.02219300 -0.17233400	H 3.04374000 2.96566000 0.67933800
C 2.49619700 2.24442800 0.06003000	H 1.27116900 1.79973900 1.79310100
C 1.14598300 1.86993700 0.70704300	H 0.42018500 2.66930600 0.53079000
C 4.06713900 -1.16750700 -0.41334100	H 3.83685900 -1.75342600 -1.31080300
O 5.14343400 -0.27042800 -0.79423400	H -2.34383000 0.28952700 2.03497900
C 4.72363900 1.02780600 -0.66048700	H -0.80844400 1.03013100 2.40159700
C -1.26938900 0.19604800 1.86706200	H -0.94469800 -0.72610600 2.34956200
C 1.72880000 -0.97513200 2.00342500	H 1.86300600 -0.06597200 2.59582900
O 5.44175900 1.96610500 -0.93356600	H 2.61309300 -1.60077500 2.15007400
C -1.83999900 1.24964100 -0.35641400	H 0.87296200 -1.52071800 2.40493000
C -3.13610000 0.43381600 -0.71230100	H -1.40287200 1.50477300 -1.33403400
C -2.75878800 -1.07946400 -0.65898900	H -2.96139800 -1.89636600 1.41078000
C -4.23549100 0.59627000 0.33137700	H -4.22775400 -2.43988200 0.29189000
O -4.45237700 -0.53188800 1.01241800	H -3.02301300 2.66016100 0.34209400
C -3.57567400 -1.60601500 0.55799200	H -4.15808600 1.65952700 -1.82677300
O -2.07462000 2.44343800 0.37753900	H -4.23416600 -1.80855600 -2.09344800
O -3.67011800 0.82894400 -1.96977000	H -2.87613800 -2.91236900 -1.81321100
O -4.86765400 1.62085500 0.51413300	H -2.65281700 -1.45828900 -2.80599500
C -3.15466500 -1.85803500 -1.92062600	H 5.04276400 -2.68252400 0.28872600
O 4.45974000 -1.98929700 0.64060700	

Table S4. The cartesian coordinates of conformer **3c**.

C 0.89862700 -0.32488400 0.33256800	H 0.80085700 1.01490800 -1.30136600
C 1.21724500 1.06925100 -0.28340700	H 0.69338400 2.29455900 1.45151800
C 0.45656700 2.21372800 0.38356300	H 0.72895000 3.17602800 -0.06774500
C -1.05450400 1.98111800 0.16311000	H -1.25876200 2.06645700 -0.91058900
C -1.55039800 0.59505100 0.67184700	H -1.63095900 2.77549100 0.65099800
C -0.62496900 -0.55925500 0.10277000	H -0.74940900 -0.48237300 -0.98939400
C -2.94667800 0.26396300 0.17121600	H -2.39307700 -2.53065300 -1.22258900
C -3.36361600 -0.97266000 -0.15237200	H -3.05538200 -3.03643900 0.31998600
C -2.52700500 -2.21375500 -0.17779700	H -1.25266100 -2.05911100 1.56818700
C -1.15723100 -1.95671500 0.48129400	H -0.44709600 -2.72329700 0.15864000
C -4.12369600 1.21482500 0.06287100	H -4.41613000 1.66471900 1.01725000
O -5.23980900 0.36631600 -0.33175300	H 2.39540800 -0.58132900 1.94865500
C -4.80110200 -0.92019400 -0.48233900	H 0.91525200 -1.48353000 2.17786000
C 1.31324300 -0.53463400 1.80579900	H 0.95021000 0.25444300 2.46378200
C -1.67559600 0.65765600 2.22463600	H -1.81241900 -0.33049000 2.67199000
O -5.55238000 -1.81724200 -0.81648200	H -2.54335500 1.26669600 2.50241900
C 1.80658700 -1.18184200 -0.59779200	H -0.80580600 1.12814600 2.68671100
C 3.12524400 -0.35421500 -0.77030500	H 1.34930200 -1.20194600 -1.59443500
C 2.74955000 1.14387800 -0.54234800	H 3.01801300 1.78827600 1.57664000
C 4.18375100 -0.65034800 0.30295700	H 4.27102800 2.39672200 0.47215100
O 4.46658200 0.43270300 1.03299700	H 2.76733300 -2.63418400 0.34922200
C 3.60626200 1.55841000 0.68682700	H 3.91323600 -1.54274100 -2.11220000
O 2.01655200 -2.54860000 -0.26473200	H 4.15005700 2.06341400 -1.94777100
O 3.72938100 -0.58916400 -2.03821900	H 2.77456200 3.08750500 -1.50149100
O 4.73730300 -1.72175200 0.47934200	H 2.54872000 1.74100400 -2.63473300
C 3.07697000 2.05912600 -1.73134300	H -4.59511700 2.86901700 -0.84276100
O -3.90408600 2.18870000 -0.91133600	

Table S5. Cytotoxicity (ED₅₀ µg/mL) of compounds **1–3**.

Compound	ED₅₀ (µg/mL)
	HCC Huh7 cell
1	> 20 µg/mL
2	> 20 µg/mL
3	> 20 µg/mL

Results are presented as mean ± SD. (n = 3).