Electronic Supporting Information (ESI) for

ent*-Abietane diterpenoids with anti-neuroinflammatory activity from the rare Chloranthaceae plant *Chloranthus oldhamii

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Table of Contents

Quantum Chemical ECD Calculations:

General procedure for the ECD calculation

The structures of the representative low energy conformations (relative Gibbs free energy less than 20 kcal/mol) of **4** and **5** were optimized by applying the DFT method at B3LYP/6-31G(d,p), B3LYP/6-31++G(2d,p) and MPW1PW91/6-31++G(2d,p), respectively, using the PCM solvation model with the dielectric constant representing acetonitrile. The generated structures were then used for the frequency calculations at the corresponding level to verify the true energy minimal and generate the thermodynamic data. The verified structures were then subject to the TDDFT calculations at B3LYP/6-31G(d,p), B3LYP/6-31++G(2d,p) or MPW1PW91/6-31++G(2d,p) computation levels, accordingly. The acquired excitation energies and rotational strengths were then Boltzmann averaged based on the calculated Gibbs free energy at the NIST standard condition and then plotted by using a Gaussian function to generate the simulated ECD spectra which were then superimposed with the corresponding experiment CD spectra for comparison.

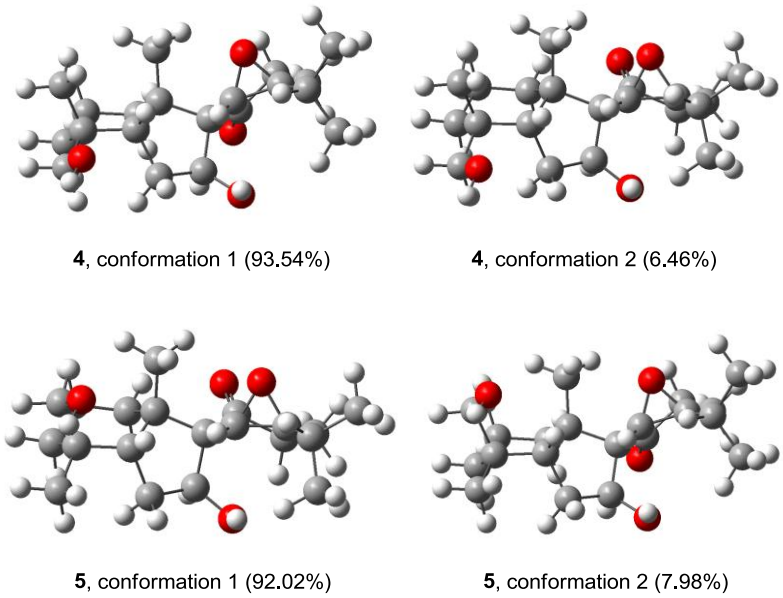


Figure S1-1. Calculated low energy conformations of **4** and **5** with the corresponding Boltzmann populations at MPW1PW91/6-31++G(2d,p) level applying the PCM (acetonitrile) solvation model.

Table S1-1. Calculated thermodynamic data of the low energy conformations of **4** and **5** using different DFT methods applying the PCM solvation model (acetonitrile), with the unit in eV.

Species	Method	E_{total}	E_{zpe}	U_{298K}	H_{298K}	G_{298K}
4, conf. 1	B3LYP/6-31G(d,p)	-1082.3059	-1081.8095	-1081.7850	-1081.7841	-1081.8607
4, conf. 2	B3LYP/6-31G(d,p)	-1082.3029	-1081.8066	-1081.7819	-1081.7810	-1081.8588
4, conf. 1	B3LYP/6-31++G(2d,p)	-1082.3656	-1081.8712	-1081.8467	-1081.8458	-1081.9220
4, conf. 2	B3LYP/6-31++G(2d,p)	-1082.3623	-1081.8682	-1081.8435	-1081.8426	-1081.9192
4, conf. 1	MPW1PW91/6-31++g(2d,p)	-1082.1365	-1081.6380	-1081.6137	-1081.6127	-1081.6887
4, conf. 2	MPW1PW91/6-31++g(2d,p)	-1082.1332	-1081.6350	-1081.6104	-1081.6095	-1081.6861
5, conf. 1	B3LYP/6-31G(d,p)	-1082.3069	-1081.8097	-1081.7854	-1081.7845	-1081.8607
5, conf. 2	B3LYP/6-31G(d,p)	-1082.3038	-1081.8071	-1081.7826	-1081.7816	-1081.8584
5, conf. 1	B3LYP/6-31++G(2d,p)	-1082.3657	-1081.8708	-1081.8465	-1081.8456	-1081.9215
5, conf. 2	B3LYP/6-31++G(2d,p)	-1082.3621	-1081.8680	-1081.8434	-1081.8424	-1081.9195
5, conf. 1	MPW1PW91/6-31++g(2d,p)	-1082.1367	-1081.6378	-1081.6136	-1081.6126	-1081.6884
5, conf. 2	MPW1PW91/6-31++g(2d,p)	-1082.1332	-1081.6349	-1081.6104	-1081.6095	-1081.6860

Table S1-2. Calculated Boltzmann populations of the low energy conformations of **4** and **5** using different DFT methods applying the PCM solvation model (acetonitrile).

Species	Method	E_{total}	E_{zpe}	U_{298K}	H_{298K}	G_{298K}
4, conf. 1	B3LYP/6-31G(d,p)	95.75%	95.57%	96.30%	96.30%	88.07%
4, conf. 2	B3LYP/6-31G(d,p)	4.25%	4.43%	3.70%	3.70%	11.93%
4, conf. 1	B3LYP/6-31++G(2d,p)	97.05%	96.13%	96.80%	96.80%	94.72%
4, conf. 2	B3LYP/6-31++G(2d,p)	2.95%	3.87%	3.20%	3.20%	5.28%
4, conf. 1	MPW1PW91/6-31++g(2d,p)	97.10%	95.98%	96.72%	96.72%	93.54%
4, conf. 2	MPW1PW91/6-31++g(2d,p)	2.90%	4.02%	3.28%	3.28%	6.46%
5, conf. 1	B3LYP/6-31G(d,p)	96.40%	94.18%	95.35%	95.35%	91.67%
5, conf. 2	B3LYP/6-31G(d,p)	3.60%	5.82%	4.65%	4.65%	8.33%
5, conf. 1	B3LYP/6-31++G(2d,p)	96.40%	94.18%	95.35%	95.35%	91.67%
5, conf. 2	B3LYP/6-31++G(2d,p)	3.60%	5.82%	4.65%	4.65%	8.33%
5, conf. 1	MPW1PW91/6-31++g(2d,p)	97.63%	95.37%	96.45%	96.45%	92.02%
5, conf. 2	MPW1PW91/6-31++g(2d,p)	2.37%	4.63%	3.55%	3.55%	7.98%

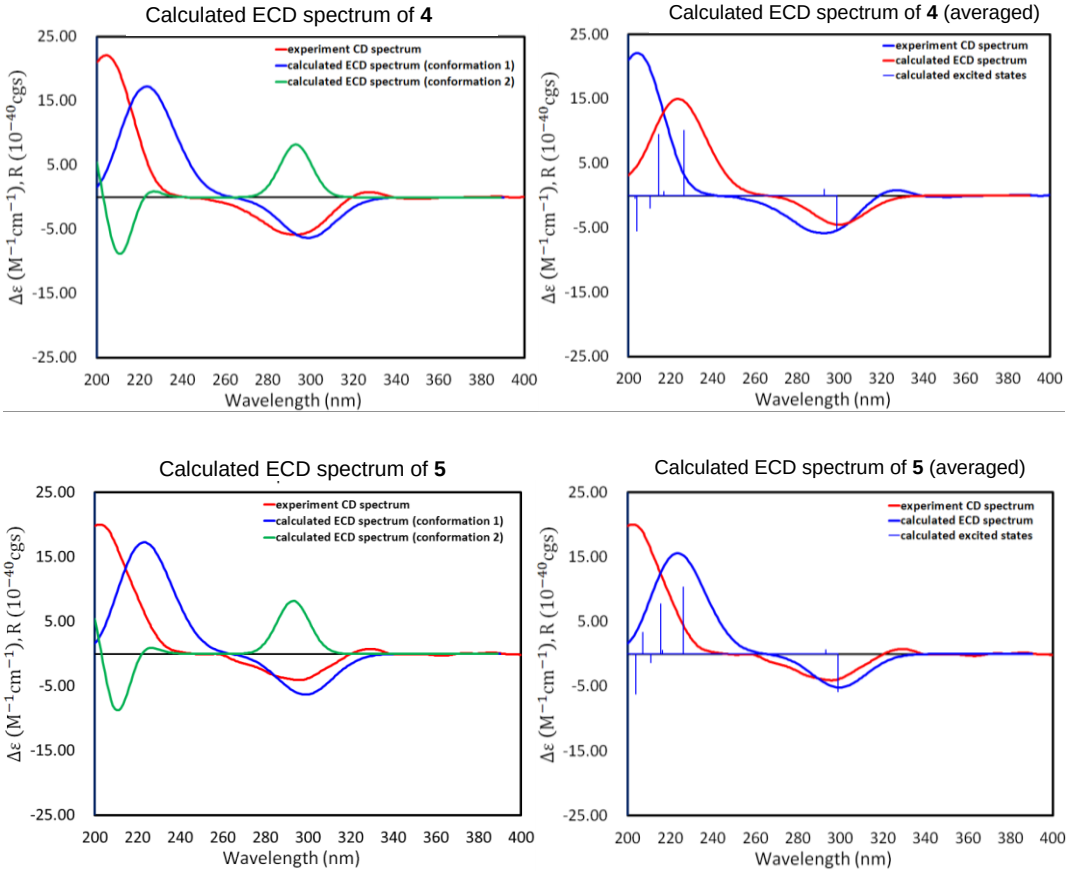


Figure S1-2. Calculated ECD spectra of **4** and **5** at B3LYP/6-31G(d,p) level applying the PCM solvation model (acetonitrile).

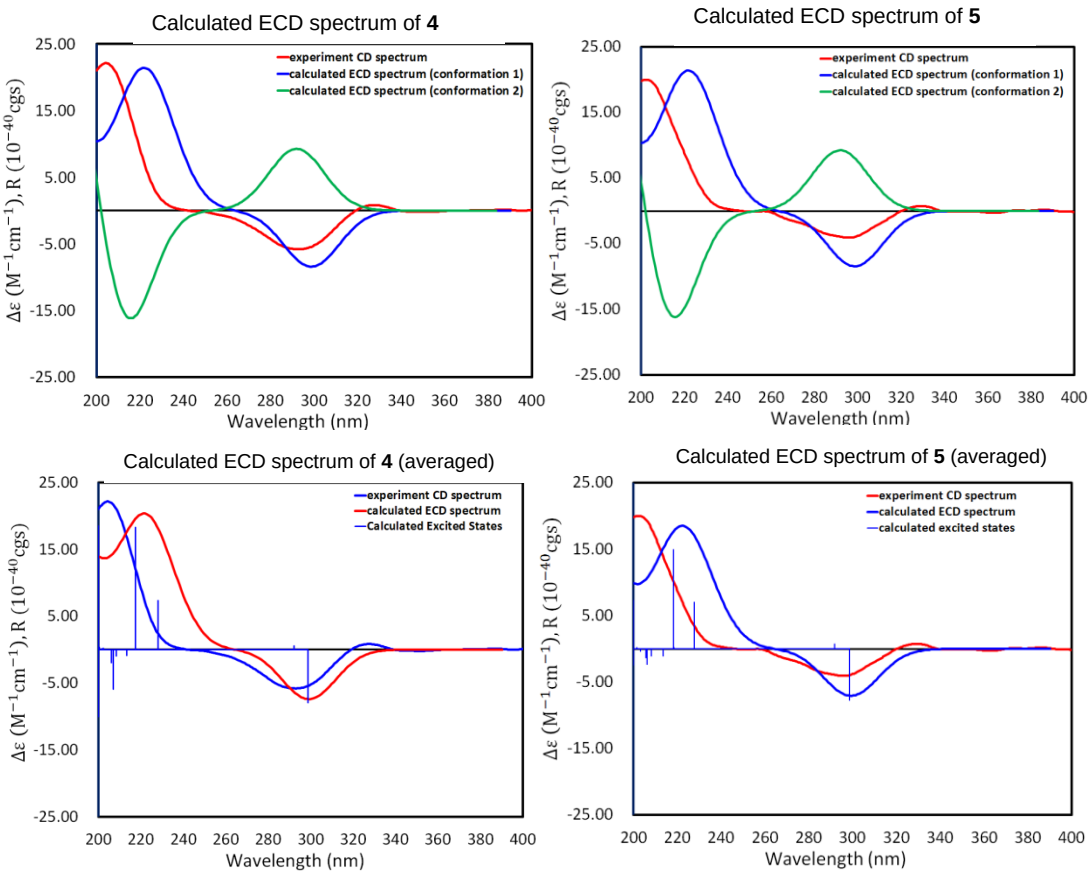


Figure S1-3. Calculated ECD spectra of **4** and **5** at B3LYP/6-31++G(2d,p) level applying the PCM solvation model (acetonitrile).

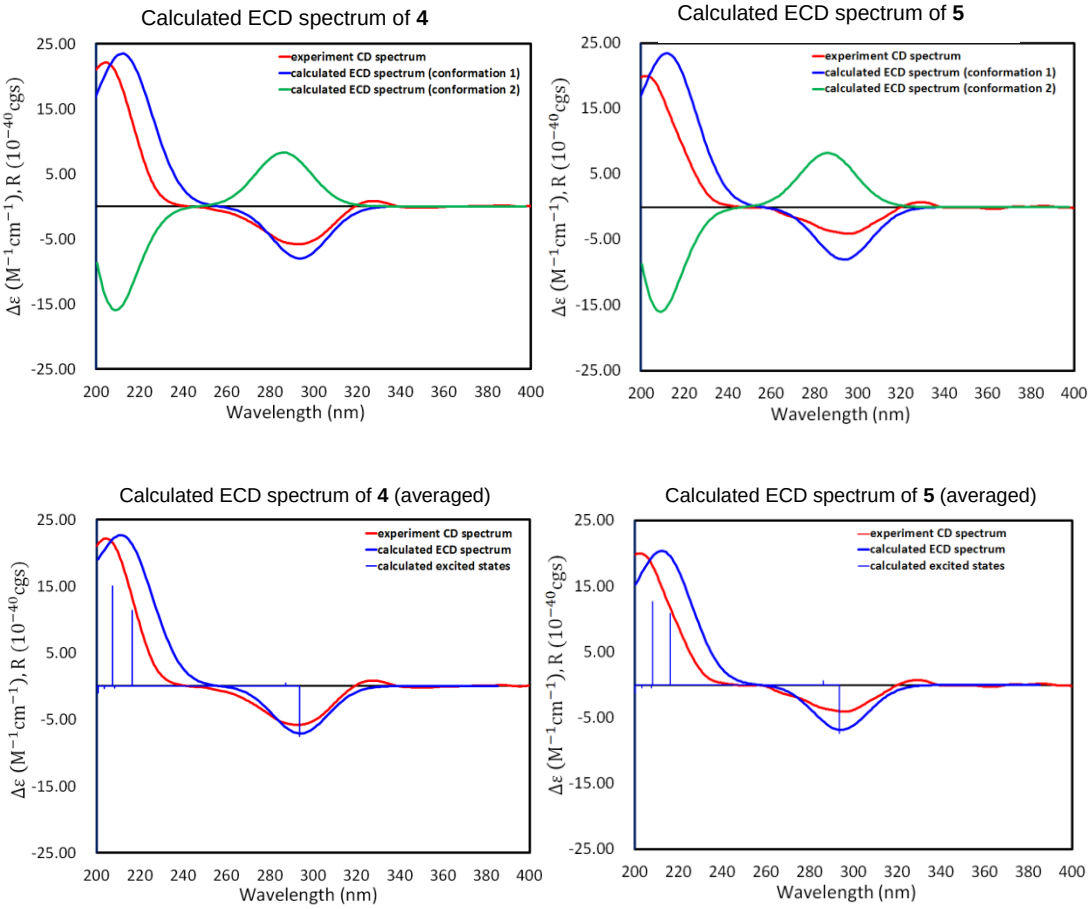


Figure S1-4. The calculated ECD spectra of **4** and **5** at MPW1PW91/6-31++g(2d,p) level applying the PCM solvation model (acetonitrile).

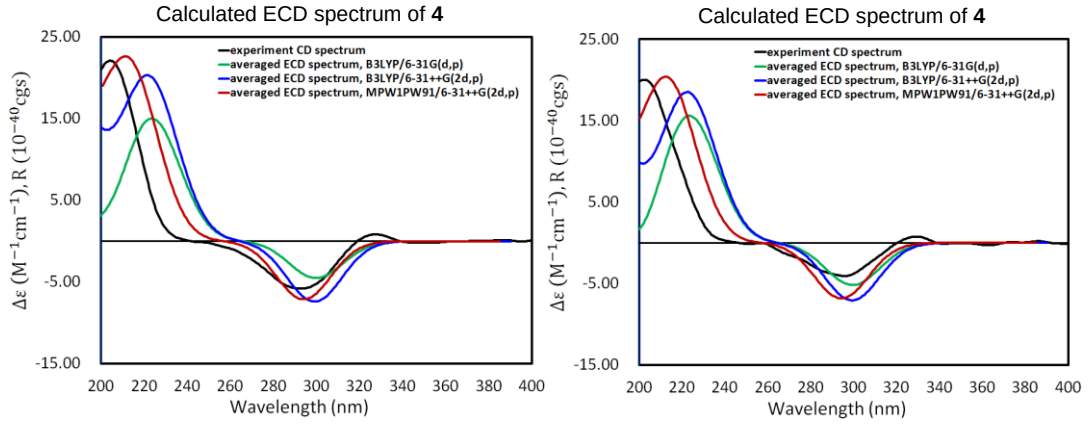


Figure S1-5. Comparison of the averaged ECD spectra of **4** and **5** at different computation level applying the PCM solvation model (acetonitrile).

Table S1-3. Coordinates and absolute energies of the low energy conformations of **4** and **5** at different theoretical levels of optimizations.

B3LYP/6-31G(d,p)/PCM(MeCN)			
Compound **4**, Conf. 1		HF = −1082.30588909 a.u.	
C	3.28522700	1.93071700	-0.38261500
C	3.94571600	0.66417900	0.17506100
C	3.23684400	-0.63217600	-0.28125700
C	1.69790800	-0.53345800	-0.01100900
C	0.97684100	0.78784500	-0.46874300
C	1.80109000	2.01716900	0.00760000
C	1.30017000	-0.69410200	1.48074500
C	0.03744600	0.16078600	1.72300800
C	-0.41807700	0.66524700	0.31160100
C	-1.31961400	-0.41524600	-0.29506800
C	-2.78655500	-0.29602600	-0.41925200
C	-3.42468000	1.03169300	-0.04634800
C	-2.45936900	2.20282300	-0.29077800
C	-1.16173600	2.00349900	0.46504700
C	0.75048000	0.89974500	-1.98912000
H	1.24240100	-1.36179900	-0.56256100
C	3.53334200	-0.91200500	-1.77178500
C	3.83788300	-1.80587800	0.51861800
O	-0.73965600	2.87364700	1.21402000
O	-1.93170500	-0.21134200	-1.58705600
C	-3.65089600	-1.55499900	-0.37231900
C	-4.25240900	-1.78375600	1.02381300
C	-4.73513500	-1.53995400	-1.46153400
O	-0.98621300	-0.48886400	2.47517900
H	3.80453000	2.81479400	0.00543000
H	3.40222200	1.96942000	-1.47175100
H	5.00199300	0.62422400	-0.11948900
H	1.36231800	2.93237300	-0.40362800
H	1.74087500	2.12325400	1.09450200
H	1.11107700	-1.74641100	1.71765500
H	2.09265600	-0.36712800	2.15905500
H	0.28119600	1.04667800	2.31094800
H	-0.92833300	-1.42780300	-0.18752000
H	-4.34102200	1.18712900	-0.62555400
H	-3.71693100	1.00411200	1.00939200
H	-2.23723100	2.26082200	-1.36202600
H	-2.89527900	3.15264500	0.02670600
H	0.38019100	-0.03127500	-2.42282200
H	0.01938300	1.68234800	-2.21327400

H	1.67023100	1.17074000	-2.50951600
H	3.23225700	-0.09586900	-2.42840600
H	4.60971600	-1.06388100	-1.91331700
H	4.91192900	-1.87128400	0.28432600
H	3.75460700	-1.61823300	1.59732700
H	-2.97625900	-2.39245100	-0.59322200
H	-5.01545800	-1.03396400	1.25879100
H	-4.73047900	-2.76682700	1.07530700
H	-3.48653300	-1.73589800	1.80429800
H	-5.25979700	-2.50032600	-1.48903400
H	-5.48440600	-0.76204900	-1.27854000
H	-4.29550100	-1.36533800	-2.44825900
H	-1.04653200	-1.40613800	2.17612200
H	3.93613500	0.71971800	1.27237800
H	3.02312600	-1.82023100	-2.10323100
O	3.17009200	-3.01923100	0.16812800
H	3.56991900	-3.73167100	0.68376500

B3LYP/6-31G(d,p)/PCM(MeCN)			
Compound **4**, Conf.2	HF = −1082.30292892 a.u.		
C	-3.36047600	-1.91072300	-0.19130500
C	-3.96847400	-0.59526500	0.30674000
C	-3.23752500	0.64884200	-0.24921200
C	-1.69456100	0.51612200	-0.02896500
C	-1.01988100	-0.84415500	-0.43984200
C	-1.86423700	-2.01902900	0.14101200
C	-1.24383800	0.73029100	1.44125400
C	0.00734700	-0.14345900	1.68846600
C	0.39178500	-0.71950600	0.27239900
C	1.29931500	0.28395500	-0.44822300
C	2.77951500	0.24544100	-0.39804100
C	3.50164300	-0.87491200	0.33821200
C	2.56039300	-1.84523900	1.08530500
C	1.21722600	-2.01084400	0.39692400
C	-0.84143800	-1.04699800	-1.95703200
H	-1.24022800	1.31059700	-0.62951200
C	-3.57840400	0.85177600	-1.74245800
C	-3.77292300	1.88441800	0.50230400
O	0.84596900	-3.10146000	-0.00735200
O	2.05522400	-0.23082800	-1.56401900
C	3.55756500	1.53534800	-0.66854600
C	3.85260700	2.32845500	0.61344200
C	4.84240400	1.25387400	-1.46444700

O	1.05048600	0.52245200	2.39139400
H	-3.88754500	-2.75483500	0.26924400
H	-3.51905800	-2.01427800	-1.27120400
H	-5.03236500	-0.54118100	0.04295500
H	-1.46476300	-2.96336700	-0.22981800
H	-1.76446000	-2.05670800	1.23278200
H	-1.01420700	1.78450400	1.62722400
H	-2.02233500	0.45579200	2.15779700
H	-0.24670500	-0.98505100	2.33817400
H	0.84668400	1.25487700	-0.65242900
H	4.08791600	-1.42541300	-0.40546300
H	4.21695700	-0.45375300	1.05008300
H	3.01639900	-2.83240500	1.18830700
H	2.36916300	-1.43754900	2.08298100
H	-0.45235700	-0.15124700	-2.44905500
H	-0.14030000	-1.86462500	-2.14108100
H	-1.78175100	-1.31028800	-2.44405500
H	-3.31849700	-0.00772700	-2.36040600
H	-4.65506200	1.02320200	-1.85730400
H	-4.85211600	1.97258600	0.30126800
H	-3.65740600	1.75325100	1.58653900
H	2.90433700	2.14940700	-1.30176200
H	4.49471600	1.76912300	1.30180800
H	4.36881900	3.26196600	0.36827800
H	2.93463300	2.59315300	1.14802600
H	5.32156300	2.19294100	-1.75844500
H	5.56737700	0.68463900	-0.87259600
H	4.62360900	0.68613900	-2.37416700
H	1.18562400	1.39042600	1.98734700
H	-3.92573500	-0.58421300	1.40474600
H	-3.05783100	1.72615700	-2.14196100
O	-3.08052300	3.05441700	0.06308800
H	-3.44258700	3.80688100	0.54889600

B3LYP/6-31++G(2d,p)/PCM(MeCN)			
Compound **4**, Conf. 1	HF = −1082.36559192 a.u.		
C	3.27915700	1.92708300	-0.40035700
C	3.93476900	0.66559200	0.17294700
C	3.22744100	-0.63411600	-0.27414300
C	1.68977100	-0.53619800	-0.00202800
C	0.97065700	0.78055900	-0.47598700
C	1.79265900	2.01857200	-0.02250200
C	1.28561400	-0.68544200	1.49026700

C	0.06378400	0.22216000	1.73143600
C	-0.42104800	0.67266400	0.31653500
C	-1.31803600	-0.43403700	-0.24888700
C	-2.78238300	-0.32030800	-0.41518500
C	-3.42469000	1.02497900	-0.13392000
C	-2.44507600	2.18467800	-0.37801000
C	-1.17696200	2.00707800	0.42601100
C	0.74570100	0.86762200	-1.99730800
H	1.23416200	-1.36558600	-0.55042600
C	3.52315200	-0.91912000	-1.76430400
C	3.84408200	-1.79224400	0.53341000
O	-0.78878300	2.88841800	1.17417400
O	-1.89882600	-0.29978100	-1.56403300
C	-3.65353500	-1.57110400	-0.33115200
C	-4.29711200	-1.74381800	1.05408900
C	-4.71325400	-1.59838700	-1.44483800
O	-0.95101300	-0.35050700	2.55674900
H	3.79437300	2.81284100	-0.01115600
H	3.40709700	1.96054800	-1.48816300
H	4.99139100	0.62242700	-0.11934700
H	1.35730400	2.92341200	-0.45975300
H	1.72936000	2.15117600	1.06085200
H	1.04189400	-1.72746400	1.72164500
H	2.08725400	-0.39906500	2.17490700
H	0.35702100	1.12259400	2.26919300
H	-0.93692500	-1.44100900	-0.08277900
H	-4.30839700	1.15999200	-0.76596400
H	-3.77199200	1.04575400	0.90515100
H	-2.18255700	2.21277900	-1.44125900
H	-2.89336000	3.14271400	-0.10640400
H	0.40069100	-0.07756600	-2.42124400
H	-0.00098600	1.63078700	-2.23595600
H	1.66194400	1.15322300	-2.51582100
H	3.27191000	-0.08145300	-2.41481400
H	4.59179700	-1.12516400	-1.89734100
H	4.91963500	-1.83694900	0.31078800
H	3.73485400	-1.61939500	1.61015100
H	-2.97795300	-2.41958000	-0.49869400
H	-5.04866700	-0.97069400	1.24842000
H	-4.80082100	-2.71407200	1.11383300
H	-3.55476400	-1.70020700	1.85773400
H	-5.23010300	-2.56380500	-1.44855700
H	-5.47195900	-0.82060600	-1.30268700
H	-4.25710400	-1.45558300	-2.42966100

H	-1.07969400	-1.27570800	2.31468100
H	3.92172700	0.73124700	1.26967900
H	2.96912400	-1.79437300	-2.11483300
O	3.22141900	-3.03340600	0.17564300
H	3.63322300	-3.73628800	0.69111900

B3LYP/6-31++G(2d,p)/PCM(MeCN)			
Compound **4**, Conf.2	HF = −1082.36227202 a.u.		
C	-3.35953300	-1.91073500	-0.18408400
C	-3.96282800	-0.59323800	0.31254100
C	-3.22847200	0.64826100	-0.24361600
C	-1.68700200	0.51136500	-0.02328000
C	-1.01742600	-0.84752300	-0.44370600
C	-1.86077400	-2.02312100	0.13423400
C	-1.23350400	0.71286400	1.44694800
C	0.01312600	-0.16627900	1.68321700
C	0.39923300	-0.72849800	0.26259200
C	1.30309000	0.27601200	-0.45885800
C	2.78192200	0.25241000	-0.39842100
C	3.50521700	-0.84890100	0.35792900
C	2.57227600	-1.85974000	1.06207200
C	1.22846900	-2.01813400	0.37955800
C	-0.85218800	-1.03658400	-1.96345700
H	-1.22979800	1.30554800	-0.62072800
C	-3.57314200	0.84933000	-1.73668000
C	-3.77086700	1.87567500	0.51310700
O	0.85467700	-3.10247000	-0.02753400
O	2.07089800	-0.24408300	-1.56569500
C	3.54918000	1.54536500	-0.67582000
C	3.78415000	2.37950200	0.59275300
C	4.86831700	1.26768200	-1.41508900
O	1.05312000	0.49143000	2.40100000
H	-3.88231200	-2.75051400	0.28878100
H	-3.52988800	-2.02302200	-1.26118000
H	-5.02534600	-0.53692500	0.04434900
H	-1.47236100	-2.96609800	-0.25143600
H	-1.75125900	-2.07311500	1.22409700
H	-0.99332800	1.76246800	1.64261900
H	-2.00930900	0.43541600	2.16442300
H	-0.24078500	-1.01320700	2.32366500
H	0.84642700	1.23901400	-0.68131100
H	4.13949400	-1.37522900	-0.36338000
H	4.17664300	-0.40815700	1.09971700

H	3.04085200	-2.84380400	1.12623500
H	2.37615200	-1.50131400	2.07762900
H	-0.47302800	-0.13405500	-2.45146200
H	-0.15172600	-1.85070200	-2.16656700
H	-1.79727200	-1.29659200	-2.44214100
H	-3.38315000	-0.03954200	-2.33850000
H	-4.63702100	1.09276000	-1.84218000
H	-4.85292200	1.94600300	0.33221400
H	-3.62117000	1.76417000	1.59330500
H	2.90946300	2.13110400	-1.34770800
H	4.39212800	1.84414600	1.33003000
H	4.31325000	3.30393400	0.33883000
H	2.84154700	2.66531300	1.07164700
H	5.33334600	2.20993100	-1.72265300
H	5.58523900	0.73795300	-0.77782600
H	4.70022800	0.66502600	-2.31367000
H	1.19831200	1.36797400	2.02461700
H	-3.92360000	-0.58111000	1.41053500
H	-2.99813800	1.67446700	-2.16623600
O	-3.12256100	3.06981500	0.05444700
H	-3.48520000	3.81632100	0.54489300

MPW1PW91/6-31++g(2d,p)			
Compound **4**, Conf. 1		HF = −1082.13652898 a.u.	
C	3.26383700	1.90456600	-0.40517000
C	3.91193600	0.65001500	0.17014400
C	3.20056400	-0.63851100	-0.27079000
C	1.67544600	-0.53217100	0.00477900
C	0.96636300	0.77507500	-0.47270500
C	1.78771600	2.00267000	-0.02208400
C	1.28421600	-0.65980700	1.49214600
C	0.06162200	0.23827600	1.72382400
C	-0.41331900	0.67431200	0.31099100
C	-1.30140500	-0.43197600	-0.24513600
C	-2.76077100	-0.32091500	-0.40718400
C	-3.40018400	1.01734900	-0.12397800
C	-2.42951400	2.16794700	-0.39118900
C	-1.16437200	2.00253600	0.40658200
C	0.74303000	0.85866400	-1.98589300
H	1.21335800	-1.36512900	-0.53325000
C	3.48989700	-0.92662400	-1.75192400
C	3.80452500	-1.79396500	0.53423300
O	-0.77303300	2.88872800	1.13999600

O	-1.88483700	-0.30147500	-1.54580600
C	-3.62591600	-1.56642100	-0.32045600
C	-4.28014400	-1.72323100	1.05199900
C	-4.66925200	-1.60022000	-1.43791900
O	-0.94634400	-0.33100500	2.53941100
H	3.78449600	2.79001300	-0.02634200
H	3.38655600	1.93010100	-1.49310000
H	4.96733200	0.59912000	-0.12161300
H	1.35266700	2.90925000	-0.45387800
H	1.72865300	2.13150700	1.06185300
H	1.05188900	-1.69852800	1.74536100
H	2.08852100	-0.35394300	2.16459000
H	0.34960700	1.14580800	2.25323800
H	-0.91942400	-1.43801300	-0.07402400
H	-4.29335600	1.14620100	-0.74217900
H	-3.73035700	1.04290100	0.91936100
H	-2.17118100	2.17544800	-1.45484000
H	-2.87478500	3.13026400	-0.13504700
H	0.40531300	-0.08896500	-2.40839500
H	-0.00840000	1.61553500	-2.22530600
H	1.65632900	1.15114400	-2.50436400
H	3.23945300	-0.09048700	-2.40362000
H	4.55646900	-1.13573900	-1.88678900
H	4.88005700	-1.84257900	0.31342500
H	3.69710700	-1.61277600	1.60990800
H	-2.94753000	-2.41427300	-0.47443000
H	-5.03388500	-0.94955900	1.22749600
H	-4.78371800	-2.69145400	1.11854400
H	-3.54840100	-1.66885700	1.86261900
H	-5.18823100	-2.56282600	-1.43954700
H	-5.42672700	-0.82093300	-1.30827300
H	-4.20442100	-1.46566900	-2.41821900
H	-1.07894100	-1.24833400	2.28469100
H	3.89951300	0.71923500	1.26595600
H	2.93263700	-1.80022900	-2.09824000
O	3.17612400	-3.01911900	0.18073700
H	3.57846600	-3.72068700	0.69809800

MPW1PW91/6-31++g(2d,p)			
Compound **4**, Conf.2		HF = −1082.13319312 a.u.	
C	-3.33800400	-1.89763600	-0.18340600
C	-3.93943700	-0.58707200	0.30898300
C	-3.20593600	0.64465900	-0.24449800

C	-1.67631700	0.50736300	-0.01948300
C	-1.01277900	-0.84198500	-0.43704200
C	-1.84983100	-2.00696000	0.14482300
C	-1.23563200	0.69706800	1.44594900
C	0.01714000	-0.16384200	1.67511700
C	0.39181900	-0.72241400	0.26145000
C	1.29016700	0.27126600	-0.46441500
C	2.76292200	0.24900100	-0.39163100
C	3.47840400	-0.83017900	0.38818700
C	2.54656200	-1.84436100	1.06886900
C	1.21922000	-2.00348400	0.37067100
C	-0.84705200	-1.03458300	-1.94754400
H	-1.21527600	1.30419300	-0.61116300
C	-3.54362500	0.84359500	-1.72963900
C	-3.74180700	1.86825100	0.50603000
O	0.85402300	-3.08075900	-0.04968900
O	2.06527500	-0.26454600	-1.54302500
C	3.52767800	1.53075200	-0.68574400
C	3.73964000	2.39023600	0.55933300
C	4.85248700	1.23620800	-1.39015300
O	1.05008200	0.50155300	2.37335600
H	-3.86416900	-2.73768200	0.28201100
H	-3.49982600	-2.00734000	-1.26130700
H	-5.00052200	-0.52826900	0.03972900
H	-1.45502400	-2.95221300	-0.22735500
H	-1.74733100	-2.04283400	1.23552100
H	-1.01273400	1.74627800	1.65854300
H	-2.01188100	0.39776600	2.15374600
H	-0.22518200	-1.01153400	2.31935900
H	0.83477100	1.23044600	-0.70592000
H	4.13840400	-1.34989000	-0.31297300
H	4.12420500	-0.37360800	1.14186700
H	3.01689700	-2.82597200	1.13726800
H	2.33050900	-1.49114800	2.08130900
H	-0.48005600	-0.12950500	-2.43840600
H	-0.13632000	-1.83968600	-2.14557700
H	-1.78745500	-1.30986800	-2.42527900
H	-3.34854500	-0.04388800	-2.33054000
H	-4.60668200	1.08364200	-1.83894800
H	-4.82408400	1.93621600	0.32712600
H	-3.59276800	1.75198400	1.58593600
H	2.89727500	2.09620100	-1.38223100
H	4.32792300	1.87086300	1.32164600
H	4.27988100	3.30357300	0.29503000

H	2.79076400	2.69471700	1.01003000
H	5.32327500	2.16845400	-1.71375600
H	5.55640700	0.72476200	-0.72624500
H	4.70134000	0.61023100	-2.27396900
H	1.20276500	1.35936200	1.96757800
H	-3.90155600	-0.57357800	1.40626600
H	-2.96975900	1.66989000	-2.15579500
O	-3.09498300	3.04871000	0.04870300
H	-3.45414000	3.79347900	0.53658800

B3LYP/6-31G(d,p)/PCM(MeCN)			
Compound **5**, Conf. 1		HF = −1082.3069165 a.u.	
C	3.35870600	1.65525200	-0.71181100
C	3.95729300	0.64636800	0.27739700
C	3.23326000	-0.71946000	0.27487100
C	1.68817500	-0.52520500	0.39206800
C	1.02891900	0.56519700	-0.53302500
C	1.85925100	1.87775400	-0.45998600
C	1.20114600	-0.16703700	1.82314400
C	-0.04127900	0.73921000	1.68011400
C	-0.40734500	0.73116500	0.15764400
C	-1.30685500	-0.48364300	-0.09350400
C	-2.76120600	-0.40091300	-0.33827800
C	-3.37872900	0.97961300	-0.48513600
C	-2.36727200	1.98582500	-1.05765200
C	-1.12007900	2.04733000	-0.20045700
C	0.88608200	0.14412000	-2.00884000
H	1.25184800	-1.49184900	0.11917300
C	3.61340200	-1.47850100	-1.02524400
O	2.92728200	-2.71636200	-1.21001200
C	3.75055000	-1.57402400	1.45381300
O	-0.71597700	3.11757300	0.23242600
O	-1.84392200	-0.73361100	-1.41037900
C	-3.66296800	-1.55717200	0.09031200
C	-4.34859500	-1.27693600	1.43741500
C	-4.68208400	-1.91905700	-1.00179900
O	-1.12291600	0.40819900	2.54976000
H	3.87910100	2.61507300	-0.61183600
H	3.53458500	1.33063600	-1.74404900
H	5.02492400	0.49491100	0.07005400
H	1.46511400	2.60032500	-1.18236700
H	1.74697400	2.34888900	0.52073500
H	0.95118600	-1.06897900	2.39304000

H	1.96590300	0.35541100	2.40386400
H	0.20580000	1.76966100	1.93899500
H	-0.95123700	-1.39968200	0.37945100
H	-4.25694000	0.93303000	-1.13770300
H	-3.72948000	1.32075100	0.49522800
H	-2.08558800	1.66861300	-2.06771700
H	-2.79191200	2.99059700	-1.11336400
H	0.52678100	-0.88123400	-2.11211700
H	0.18077900	0.79784700	-2.53015500
H	1.83630100	0.22234500	-2.53981400
H	3.38445900	-0.88957300	-1.91297900
H	4.70238400	-1.63808100	-1.01926100
H	3.24653000	-3.33501000	-0.53970200
H	4.81865500	-1.78622400	1.32847700
H	3.62953100	-1.06748400	2.41425100
H	3.22190000	-2.53186900	1.52357700
H	-3.00123200	-2.42349600	0.21986400
H	-5.10940300	-0.49436400	1.34540100
H	-4.84759900	-2.17883700	1.80510200
H	-3.62760400	-0.95304900	2.19450900
H	-5.23574800	-2.82068900	-0.72093500
H	-5.41464200	-1.11933300	-1.15649500
H	-4.18075700	-2.11192300	-1.95511400
H	-1.20339600	-0.55467800	2.58330600
H	3.90482500	1.07256800	1.28795100

B3LYP/6-31G(d,p)/PCM(MeCN)			
Compound **5**, Conf. 2	HF = −1082.30379283 a.u.		
C	3.42383000	1.70988500	-0.43528400
C	3.97179600	0.58188900	0.44723500
C	3.22115400	-0.75668800	0.26412800
C	1.67775600	-0.54106500	0.34214600
C	1.06679300	0.65046800	-0.48496200
C	1.91774800	1.93076000	-0.22546000
C	1.14433200	-0.31166000	1.78266300
C	-0.08692000	0.61996500	1.69118500
C	-0.38138600	0.76036000	0.14952200
C	-1.27788300	-0.39996300	-0.29895900
C	-2.75724400	-0.32994500	-0.35566100
C	-3.48403800	0.96785800	-0.02908500
C	-2.55686200	2.09713100	0.47142500
C	-1.17381000	2.04251500	-0.15294200
C	0.97236100	0.39929000	-2.00341600

H	1.23938600	-1.46998500	-0.03735300
C	3.63489800	-1.37524400	-1.09911900
O	2.93191000	-2.56841200	-1.44487200
C	3.67421000	-1.74877500	1.35859800
O	-0.74906100	2.96611100	-0.82915200
O	-1.95405500	-0.22903200	-1.56165500
C	-3.55649700	-1.63285200	-0.28080100
C	-3.93035700	-2.01478200	1.15941200
C	-4.79519100	-1.57901300	-1.18944600
O	-1.18513500	0.21103200	2.49842900
H	3.95339400	2.64224200	-0.20551700
H	3.63440000	1.50425100	-1.49149200
H	5.04241400	0.42987100	0.25554600
H	1.56297400	2.73324700	-0.87283400
H	1.77058700	2.28458200	0.80251500
H	0.85739300	-1.25523100	2.25878400
H	1.89477800	0.14329800	2.43462500
H	0.16418500	1.61030800	2.07946700
H	-0.84366600	-1.39332200	-0.17967700
H	-4.00017500	1.28841000	-0.94042200
H	-4.25889600	0.78496200	0.72060000
H	-2.98842800	3.07908000	0.26527800
H	-2.43258700	1.98278500	1.55287100
H	0.61632500	-0.60872300	-2.23140200
H	0.28114500	1.11387500	-2.45624000
H	1.93705800	0.52738000	-2.49811700
H	3.44879900	-0.68506700	-1.92141900
H	4.71970400	-1.56036500	-1.07408000
H	3.20929600	-3.26256700	-0.83240700
H	4.74520400	-1.96000400	1.25884100
H	3.51197300	-1.35427300	2.36454200
H	3.13487100	-2.70123100	1.29376100
H	-2.89054400	-2.41187200	-0.67359700
H	-4.58560600	-1.27046300	1.62396100
H	-4.46150400	-2.97173300	1.16967700
H	-3.04467100	-2.12766300	1.79364800
H	-5.28742800	-2.55605000	-1.22048000
H	-5.52934400	-0.85088200	-0.82794100
H	-4.51939300	-1.30616800	-2.21281800
H	-1.35514500	-0.72670200	2.33378300
H	3.89607900	0.88961800	1.49881300

B3LYP/6-31++G(2d,p)/PCM(MeCN)			
Compound **5**, Conf. 1	HF = −1082.36568893 a.u.		
C	3.35276800	1.64964100	-0.72939500
C	3.94420100	0.65495100	0.27720000
C	3.22650500	-0.71358800	0.28320600
C	1.68118500	-0.52269700	0.39116600
C	1.02271900	0.56193000	-0.54166400
C	1.85233200	1.87439800	-0.48799400
C	1.18556100	-0.16388300	1.82030400
C	-0.01845900	0.78524100	1.66633700
C	-0.41147800	0.73906100	0.15549200
C	-1.30885900	-0.48496500	-0.05910700
C	-2.76077400	-0.41935600	-0.32923900
C	-3.37887600	0.94909700	-0.54384000
C	-2.35926100	1.94984800	-1.11220400
C	-1.13435700	2.04036900	-0.23081900
C	0.87899700	0.12814000	-2.01281900
H	1.24473700	-1.48907500	0.12059500
C	3.62350200	-1.47502900	-1.00814500
O	2.99150200	-2.74920600	-1.16935500
C	3.74500200	-1.55387300	1.47182300
O	-0.75643700	3.11801900	0.19684100
O	-1.82511500	-0.78997600	-1.37260300
C	-3.66661400	-1.56295500	0.11998400
C	-4.38123100	-1.25619700	1.44577700
C	-4.67039500	-1.95598900	-0.97655800
O	-1.09324400	0.53572700	2.57266300
H	3.86983200	2.61161600	-0.63443900
H	3.53749500	1.31450800	-1.75652300
H	5.01428000	0.50541300	0.08267100
H	1.46186200	2.58204200	-1.22704700
H	1.73999600	2.36459300	0.48286600
H	0.89181100	-1.06442000	2.37028300
H	1.95462500	0.32427100	2.42302900
H	0.27424700	1.81061600	1.88773100
H	-0.96035400	-1.38269500	0.45014700
H	-4.23081500	0.87406700	-1.22735400
H	-3.76976400	1.31937300	0.41044400
H	-2.04827200	1.61612400	-2.10831000
H	-2.79422600	2.94761500	-1.20088900
H	0.52853500	-0.90110100	-2.10925200
H	0.16837600	0.77245100	-2.53870200
H	1.82765500	0.21221500	-2.54566200
H	3.35949600	-0.91660000	-1.90442100

H	4.71529900	-1.59888100	-1.01144800
H	3.35522000	-3.36240200	-0.52006600
H	4.80654000	-1.79116900	1.33209300
H	3.65422300	-1.02084800	2.42149300
H	3.19773600	-2.49813400	1.57588100
H	-3.00552300	-2.42355200	0.28306400
H	-5.12163500	-0.45717500	1.32915100
H	-4.91109500	-2.14648500	1.79968800
H	-3.67787000	-0.95033800	2.22709400
H	-5.21456000	-2.85920900	-0.68106700
H	-5.41214000	-1.16844900	-1.15103700
H	-4.16156800	-2.16268400	-1.92349400
H	-1.24106900	-0.41530300	2.64385800
H	3.87848500	1.09223400	1.28222200

B3LYP/6-31++G(2d,p)/PCM(MeCN)

Compound **5**, Conf. 2 HF = −1082.36214917 a.u.

C	3.42103200	1.71717600	-0.41706800
C	3.96186500	0.58398900	0.46166400
C	3.21438900	-0.75373100	0.26381700
C	1.67134800	-0.53685400	0.33124400
C	1.06339800	0.66128700	-0.48765700
C	1.91373500	1.93815200	-0.21712600
C	1.13431100	-0.31815400	1.77096100
C	-0.09553600	0.61014100	1.68183600
C	-0.38921400	0.76428900	0.14169000
C	-1.28317700	-0.38663600	-0.33059700
C	-2.76183400	-0.32953800	-0.35507400
C	-3.48998600	0.94212300	0.04387500
C	-2.56502800	2.10118500	0.48023500
C	-1.18537900	2.04768400	-0.14528900
C	0.97817600	0.41968200	-2.00766200
H	1.22954100	-1.46105000	-0.05369400
C	3.65078100	-1.35758900	-1.09659300
O	2.99247000	-2.57904700	-1.44793700
C	3.66049200	-1.74977500	1.35736000
O	-0.76007800	2.97450900	-0.80959100
O	-1.98513500	-0.17246200	-1.57434400
C	-3.54699400	-1.64088700	-0.31598700
C	-3.85928100	-2.10384400	1.11529300
C	-4.82494300	-1.55727700	-1.16651000
O	-1.19194800	0.19222700	2.48990800
H	3.94711700	2.64782000	-0.17340800

H	3.64096500	1.52138800	-1.47310400
H	5.03368400	0.43367200	0.27680300
H	1.56998000	2.74277800	-0.86771200
H	1.75913700	2.29114100	0.80966500
H	0.84891800	-1.26591400	2.23822000
H	1.88022000	0.13564500	2.42775600
H	0.15061500	1.59717800	2.07838900
H	-0.83961700	-1.37885300	-0.26391500
H	-4.09048200	1.25699100	-0.81627100
H	-4.19353000	0.72544100	0.85220000
H	-3.01123300	3.06823500	0.24005700
H	-2.42543700	2.04353800	1.56452600
H	0.61819100	-0.58508000	-2.24555300
H	0.29598600	1.14036500	-2.46550000
H	1.94734400	0.54489800	-2.49387200
H	3.44353300	-0.67970100	-1.92263900
H	4.73793100	-1.51607600	-1.06927300
H	3.30776800	-3.28130800	-0.86718600
H	4.72811900	-1.97595900	1.24912400
H	3.51395600	-1.34740300	2.36287600
H	3.10707700	-2.69479900	1.30239400
H	-2.89104100	-2.39108400	-0.77491100
H	-4.49733300	-1.39031900	1.64780600
H	-4.38769500	-3.06254000	1.09032900
H	-2.94784500	-2.25129500	1.70481900
H	-5.29625900	-2.54307300	-1.23561200
H	-5.55803400	-0.87098500	-0.72812300
H	-4.60411000	-1.21697900	-2.18350800
H	-1.34636800	-0.75162200	2.36002200
H	3.87748800	0.88460600	1.51452100

MPW1PW91/6-31++g(2d,p)			
Compound **5**, Conf. 1		HF = −1082.13671581 a.u.	
C	3.33460200	1.63104900	-0.72649400
C	3.91945300	0.64316900	0.27820200
C	3.20090200	-0.71432700	0.28273600
C	1.66725600	-0.51876300	0.39178600
C	1.01688500	0.55763700	-0.53731600
C	1.84395900	1.86050300	-0.48195900
C	1.18252900	-0.14934900	1.81142800
C	-0.01765200	0.79341900	1.65463300
C	-0.40377900	0.73679900	0.15215500
C	-1.29337800	-0.48348600	-0.05382900

C	-2.74029600	-0.41792600	-0.32085500
C	-3.35427200	0.94511700	-0.53196300
C	-2.34119300	1.92943300	-1.11720400
C	-1.12136500	2.02826400	-0.24217600
C	0.87275900	0.12619500	-2.00030900
H	1.22730900	-1.48555300	0.12622500
C	3.59014600	-1.47219900	-1.00211000
O	2.95901200	-2.73389300	-1.15783200
C	3.71060600	-1.55393900	1.46380500
O	-0.74210900	3.10439200	0.17534900
O	-1.81164600	-0.78727700	-1.35305200
C	-3.64239700	-1.55457600	0.12802000
C	-4.37041600	-1.23512600	1.43336000
C	-4.62719800	-1.95495400	-0.97138300
O	-1.08494800	0.54828900	2.55232600
H	3.85567300	2.58997800	-0.63836000
H	3.51531600	1.29119500	-1.75192900
H	4.98879800	0.48948400	0.08854200
H	1.45240600	2.57140400	-1.21605300
H	1.73492500	2.34649800	0.49121200
H	0.89305000	-1.04288700	2.37334600
H	1.95565700	0.34455700	2.40355100
H	0.27572100	1.82118300	1.86561700
H	-0.94529000	-1.37849000	0.46109200
H	-4.21529200	0.87016600	-1.20242500
H	-3.72935900	1.32097200	0.42517900
H	-2.03252300	1.57607700	-2.10617100
H	-2.77193400	2.92606500	-1.22257400
H	0.53329400	-0.90600900	-2.09595100
H	0.15368900	0.76291500	-2.52187600
H	1.81712600	0.22183800	-2.53737400
H	3.32721700	-0.90934800	-1.89578200
H	4.68196400	-1.59409700	-1.00793600
H	3.31663100	-3.33867400	-0.50290400
H	4.76932800	-1.79888500	1.32474100
H	3.62346500	-1.02072700	2.41278900
H	3.15580800	-2.49247900	1.56875300
H	-2.98065000	-2.41065700	0.30637900
H	-5.11062400	-0.44114100	1.29535100
H	-4.90268000	-2.12030400	1.79188600
H	-3.68005600	-0.91681400	2.21915600
H	-5.17471500	-2.85445500	-0.67620700
H	-5.36615000	-1.16991000	-1.15990800
H	-4.10801600	-2.16838300	-1.90945800

H	-1.23679300	-0.39906100	2.61194800
H	3.85132200	1.08181000	1.28165900

MPW1PW91/6-31++g(2d,p)			
Compound **5**, Conf. 2		HF = −1082.133181 a.u.	
C	3.40207300	1.70882900	-0.38074800
C	3.93392400	0.56827400	0.47985500
C	3.18738500	-0.75555200	0.25742500
C	1.65566300	-0.53679400	0.32335100
C	1.06014100	0.66563700	-0.47616800
C	1.90367800	1.92845200	-0.17733800
C	1.12167900	-0.33082900	1.75576300
C	-0.10775500	0.58752700	1.67078700
C	-0.38260300	0.75902700	0.14034400
C	-1.26903700	-0.37427200	-0.35990900
C	-2.74163200	-0.31958600	-0.35330100
C	-3.46196700	0.91986800	0.12149800
C	-2.54070600	2.09109300	0.49993800
C	-1.17572300	2.03498400	-0.14056100
C	0.98140000	0.45059300	-1.99211800
H	1.21249000	-1.45572000	-0.07395200
C	3.62190300	-1.33330300	-1.10444400
O	2.96514800	-2.53646200	-1.47304100
C	3.62064500	-1.76671500	1.32912000
O	-0.75459500	2.95854400	-0.80406500
O	-1.99400200	-0.10475700	-1.56627900
C	-3.51698300	-1.62868600	-0.35636800
C	-3.74633800	-2.17882400	1.05054400
C	-4.83343300	-1.49862100	-1.12309400
O	-1.20290800	0.15585800	2.45244400
H	3.93124800	2.63341300	-0.12701600
H	3.62093100	1.52577300	-1.43843500
H	5.00536400	0.41639200	0.30003600
H	1.55818000	2.74768700	-0.80782700
H	1.74927300	2.25515100	0.85770200
H	0.84117300	-1.27998100	2.22068300
H	1.86730300	0.12354800	2.41201500
H	0.13186800	1.57015000	2.08236200
H	-0.82181500	-1.36707200	-0.34589100
H	-4.13476100	1.23030500	-0.68363200
H	-4.09612400	0.66815400	0.97493300
H	-2.99525300	3.04873900	0.24385300
H	-2.37533500	2.06869300	1.58139200

H	0.64283900	-0.55668000	-2.24689000
H	0.28529000	1.16513100	-2.43615700
H	1.94675400	0.60475300	-2.47602600
H	3.42008100	-0.63671000	-1.91604500
H	4.70892500	-1.49108200	-1.07721100
H	3.27335700	-3.24207500	-0.89889700
H	4.68597400	-1.99850500	1.22170300
H	3.47265500	-1.37963000	2.33959300
H	3.06019100	-2.70527500	1.25775100
H	-2.88409600	-2.34167700	-0.89782200
H	-4.32577000	-1.48923100	1.67155400
H	-4.30247700	-3.11893900	0.99881800
H	-2.80322500	-2.39188000	1.56286300
H	-5.30131500	-2.48031600	-1.23644200
H	-5.54457800	-0.85438000	-0.59694900
H	-4.67348200	-1.08478900	-2.12263900
H	-1.38273100	-0.76890400	2.26071000
H	3.84403600	0.85288700	1.53594100

Figure S1. ^{1}H NMR (600 MHz, methanol-d_4) spectrum of **1**

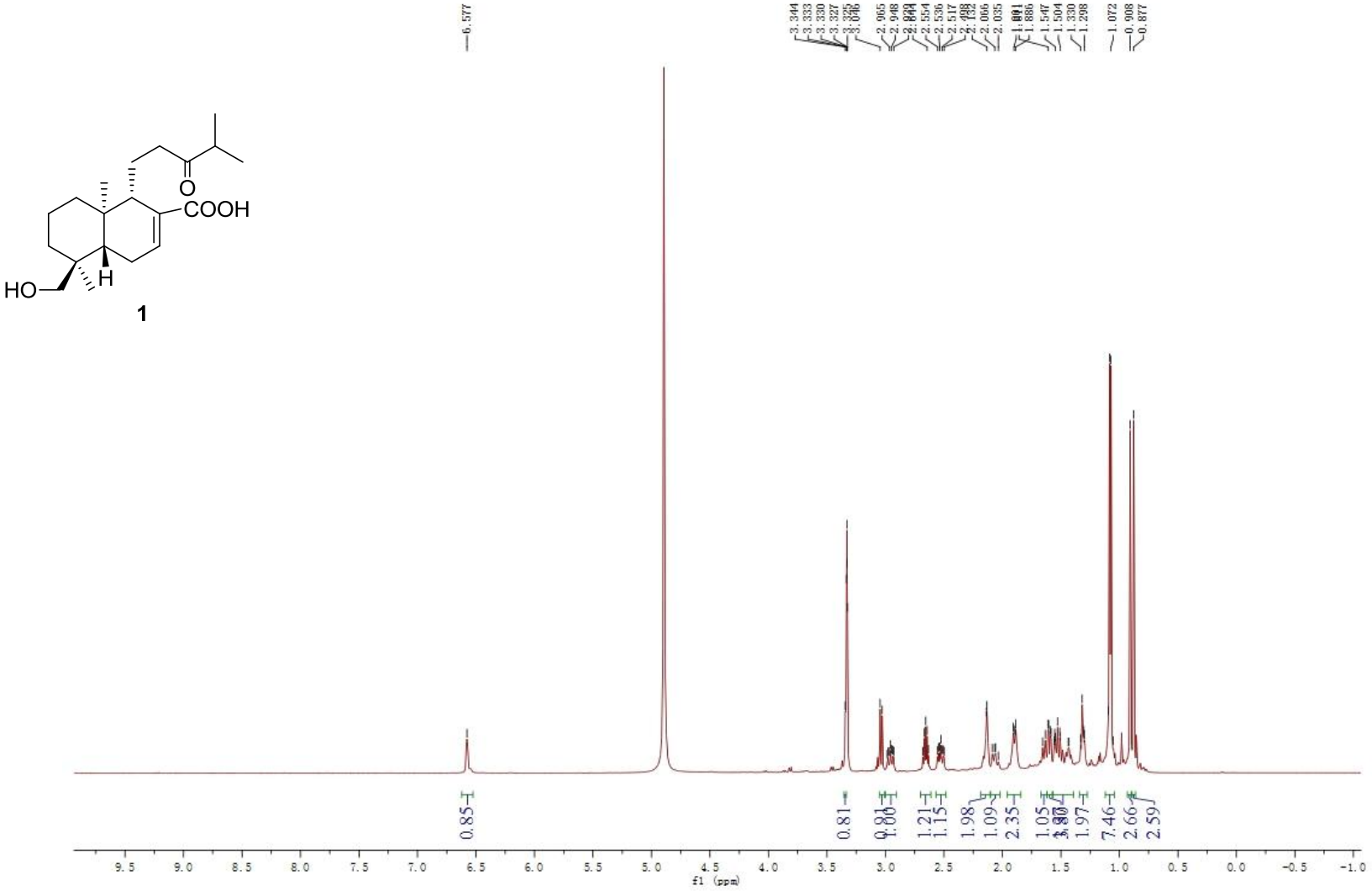


Figure S2. ^{1}H NMR (600 MHz, methanol-d_4) spectrum of **1**-expansion

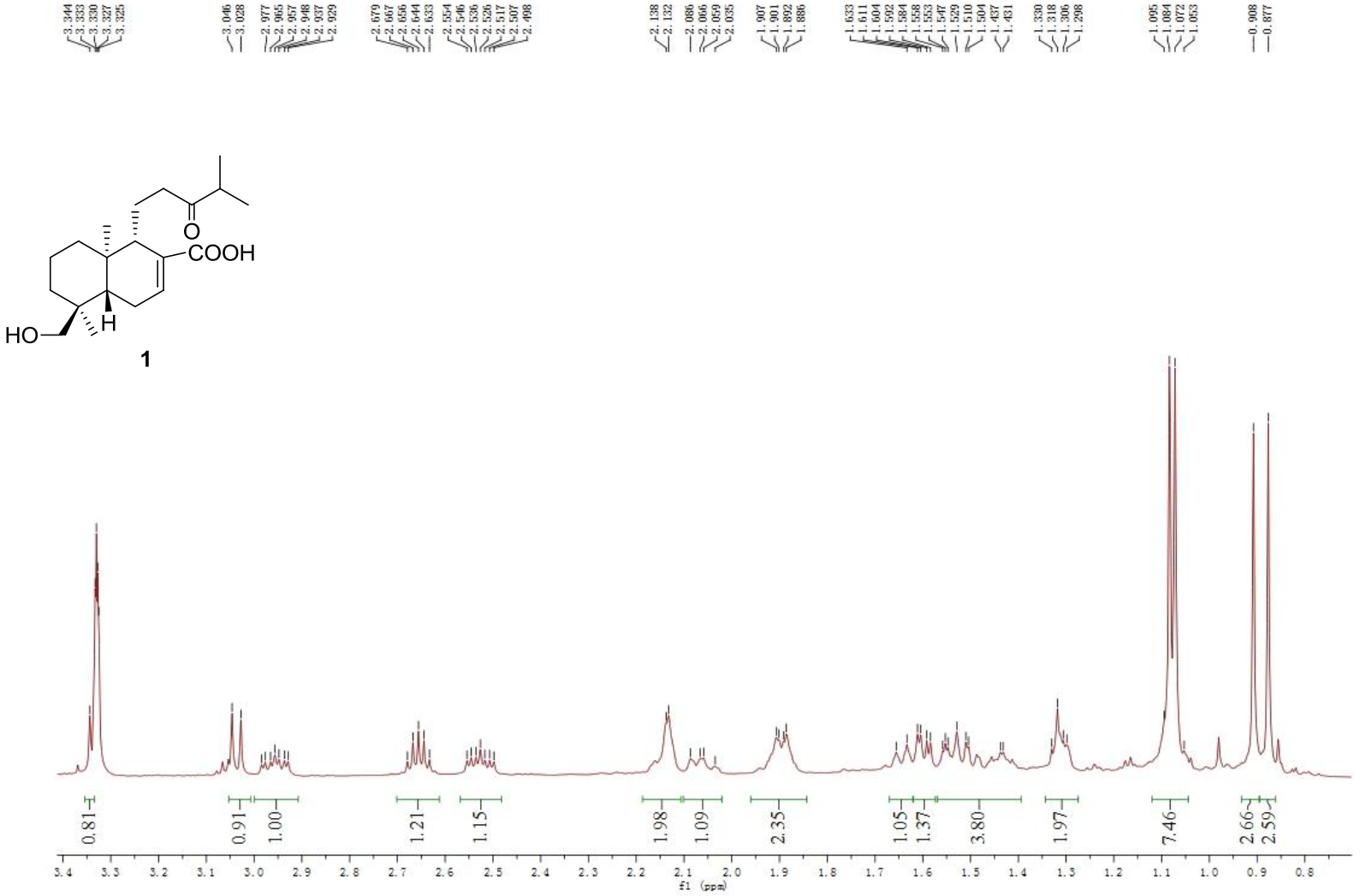


Figure S3. ^{13}C NMR (600 MHz, methanol-d_4) spectrum of **1**

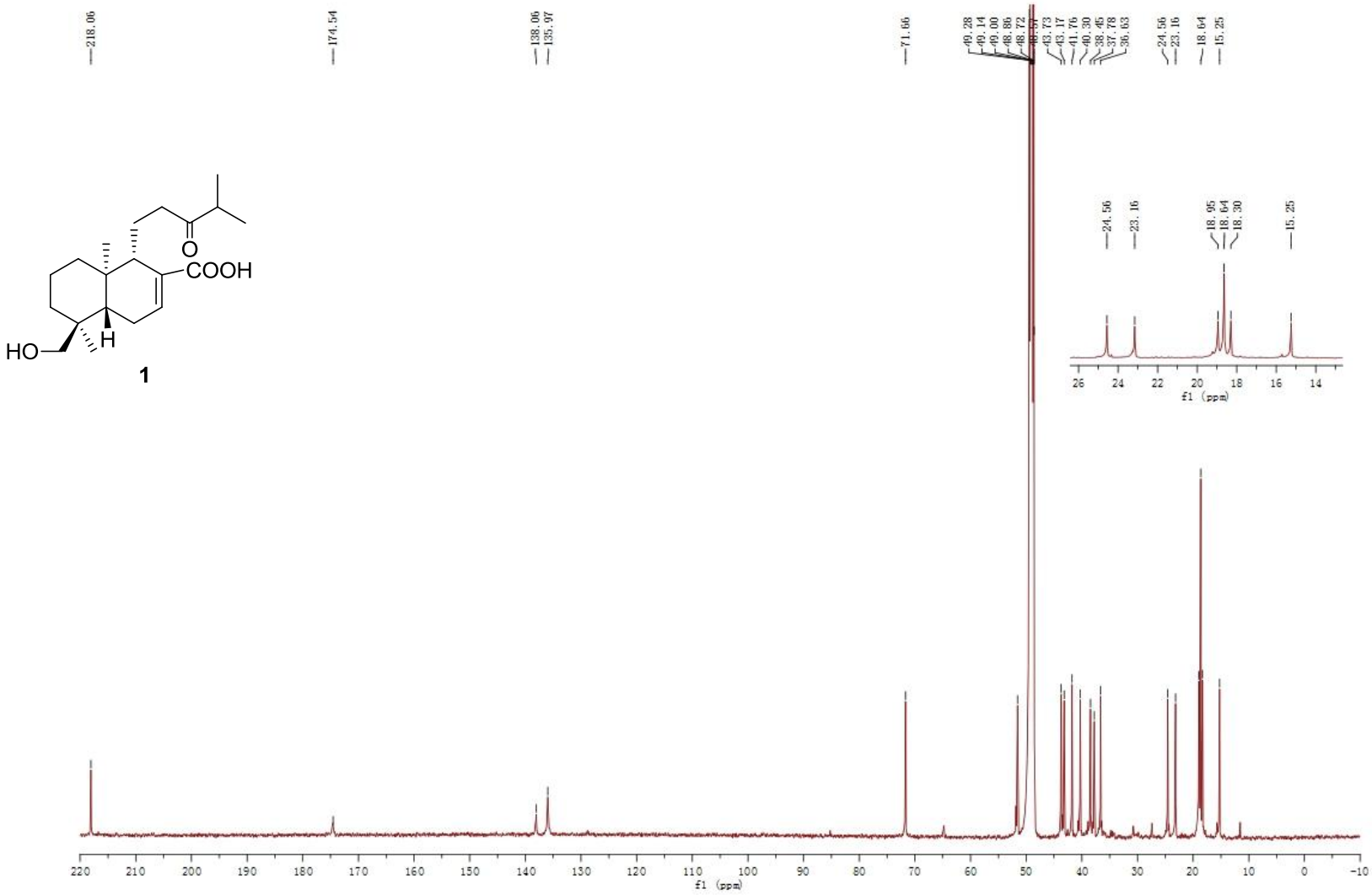


Figure S4. ^{1}H-^{1}H COSY (600 MHz, methanol-d_4) spectrum of **1**

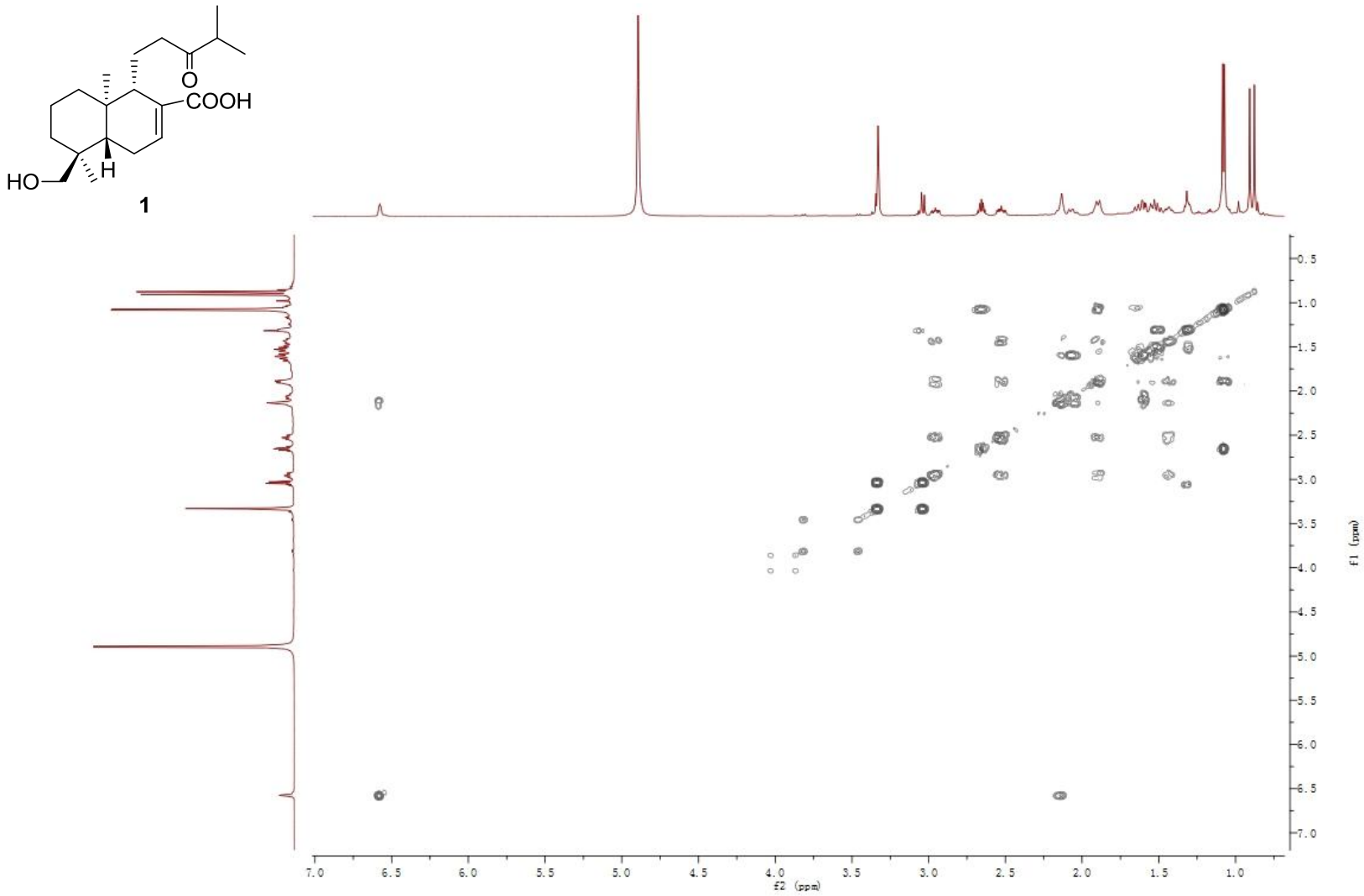


Figure S5. HMBC (600 MHz, methanol-d_4) spectrum of **1**

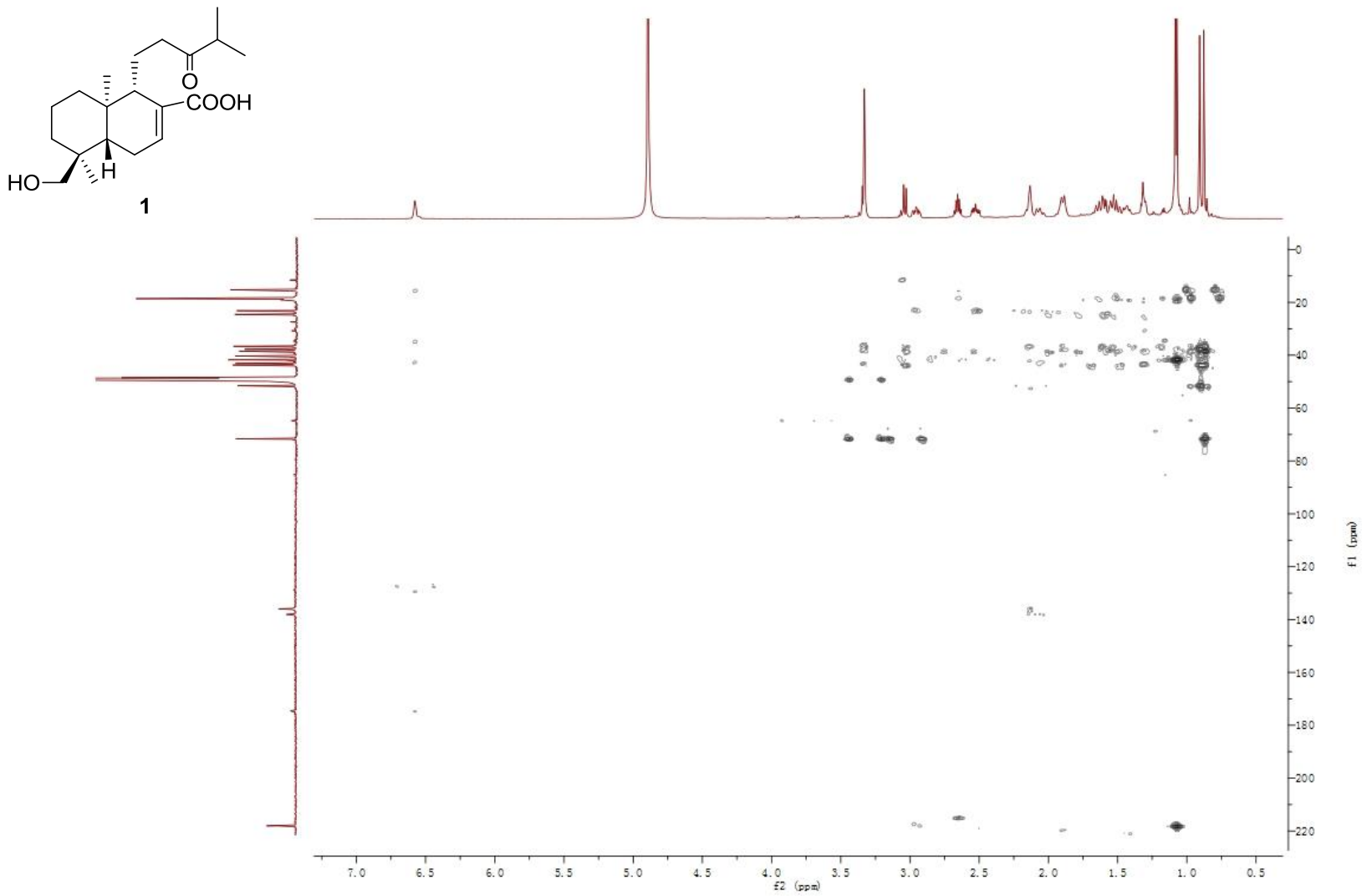


Figure S6. HMBC (600 MHz, methanol-d_4) spectrum of **1**-expansion

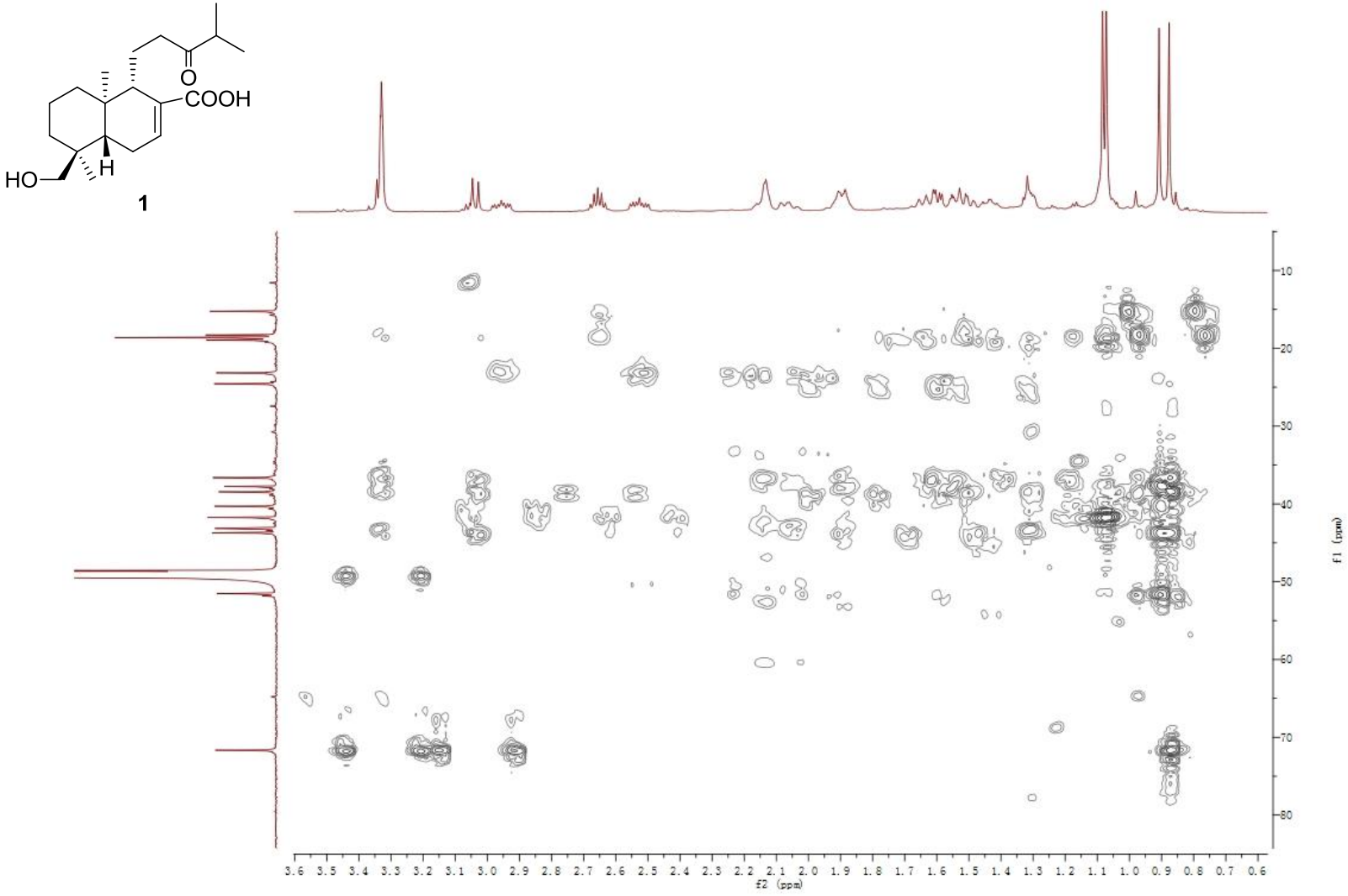


Figure S7. NOESY (400 MHz, methanol-d_4) spectrum of **1**

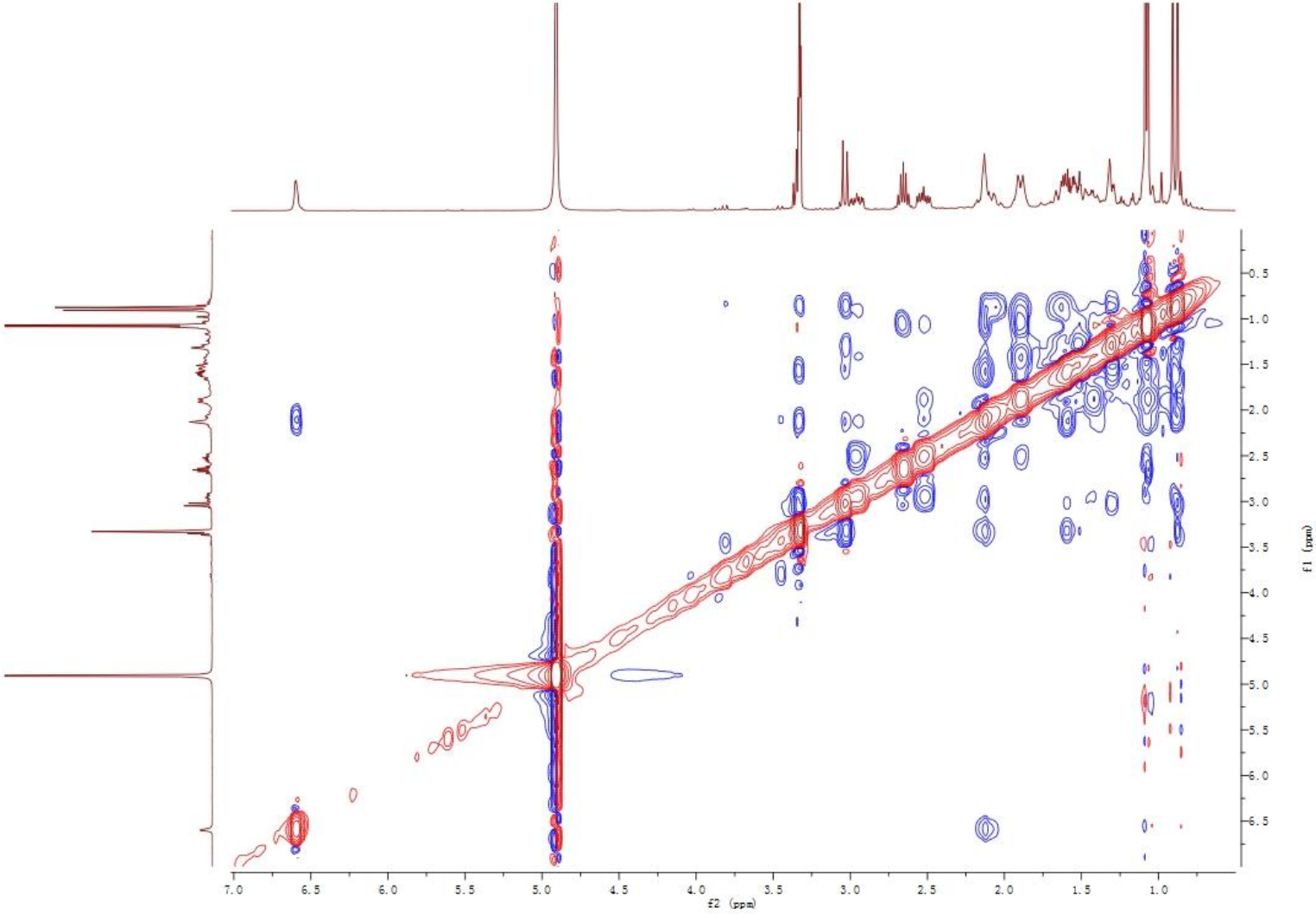
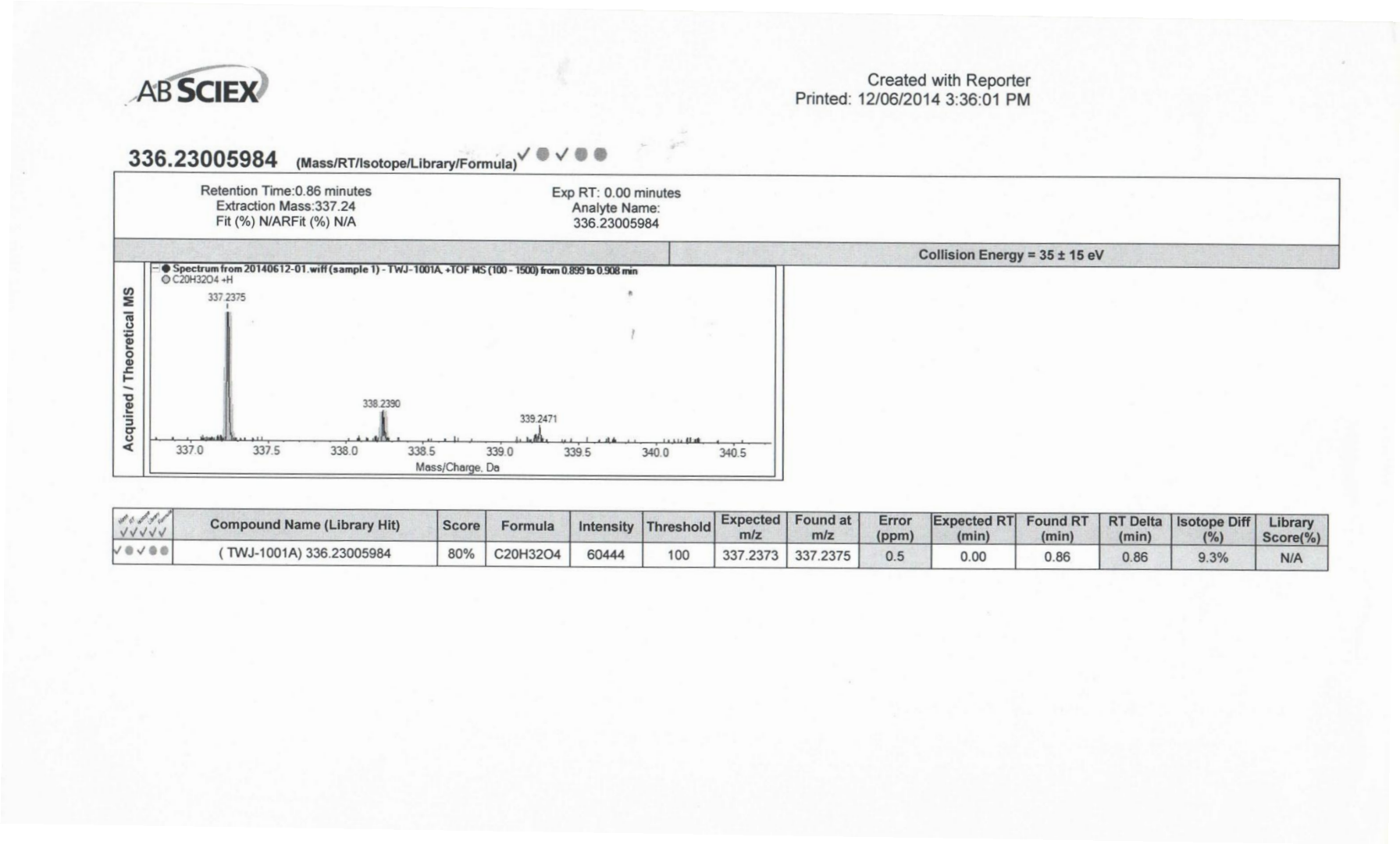


Figure S8. HRESIMS spectrum of **1**



Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
(TWJ-1001A) 336.23005984	80%	C20H32O4	60444	100	337.2373	337.2375	0.5	0.00	0.86	0.86	9.3%	N/A

Figure S9. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2**

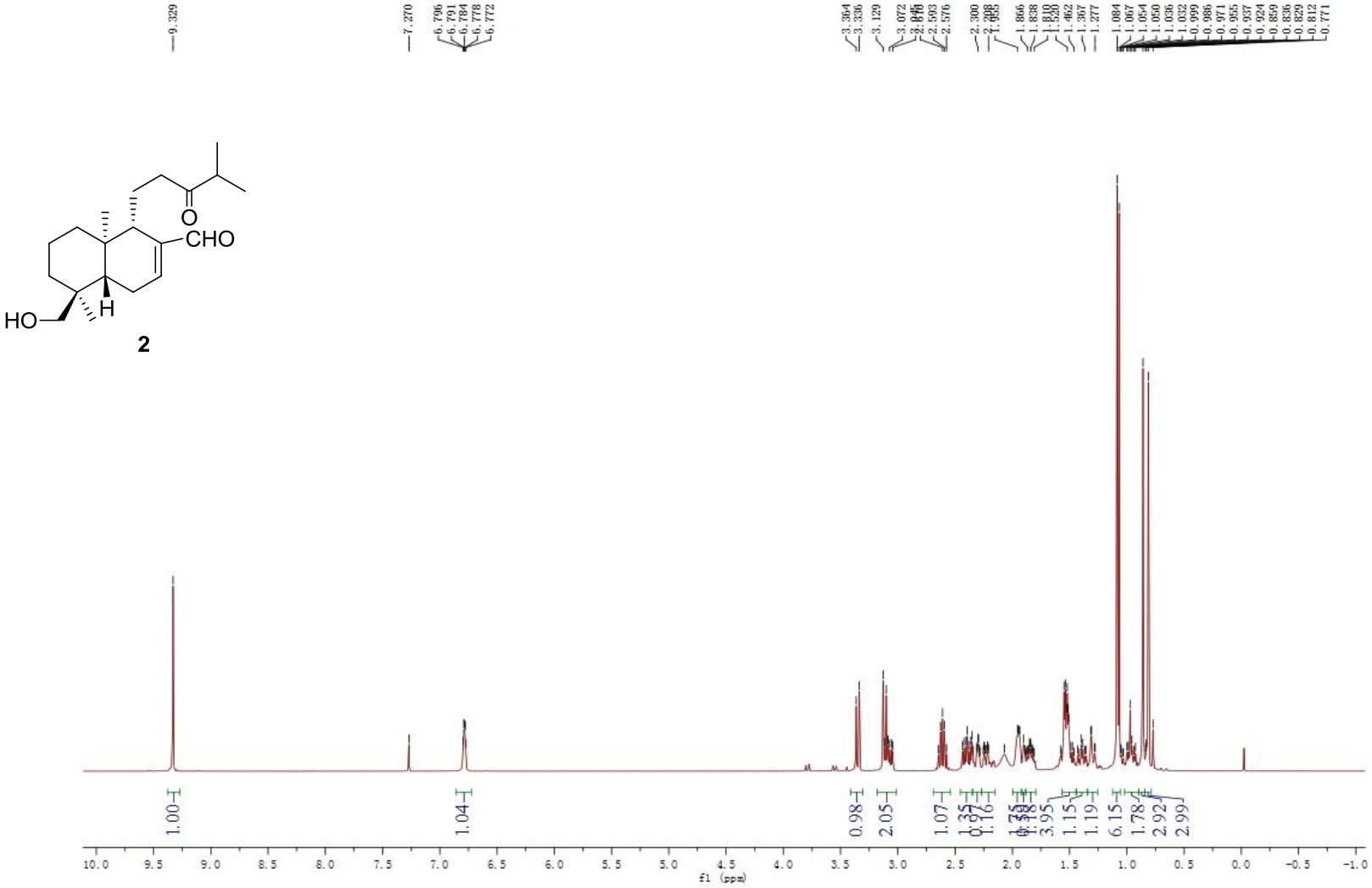


Figure S10. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2**-expansion

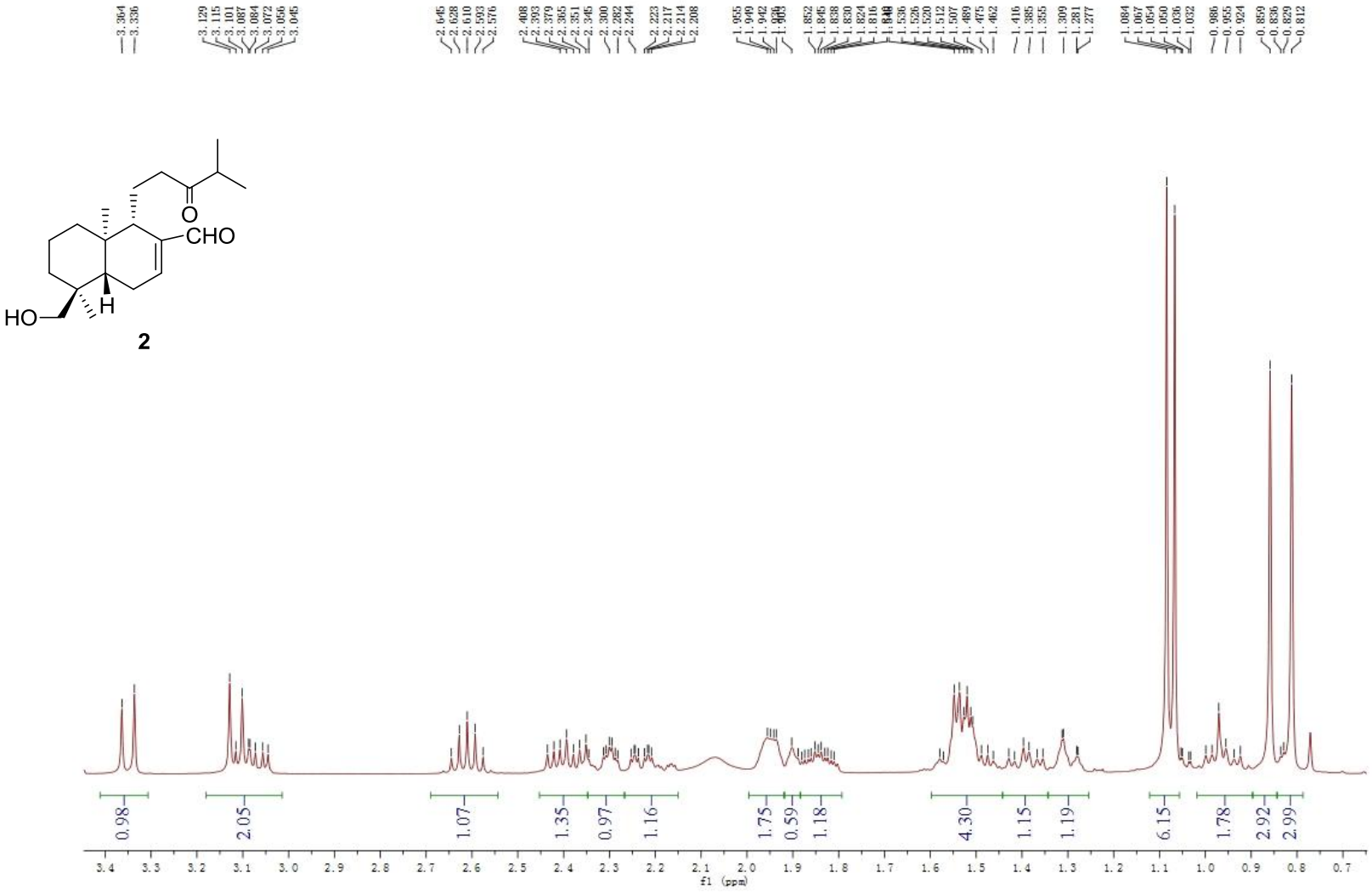


Figure S11. ^{13}C NMR (400 MHz, $CDCl_3$) spectrum of **2**

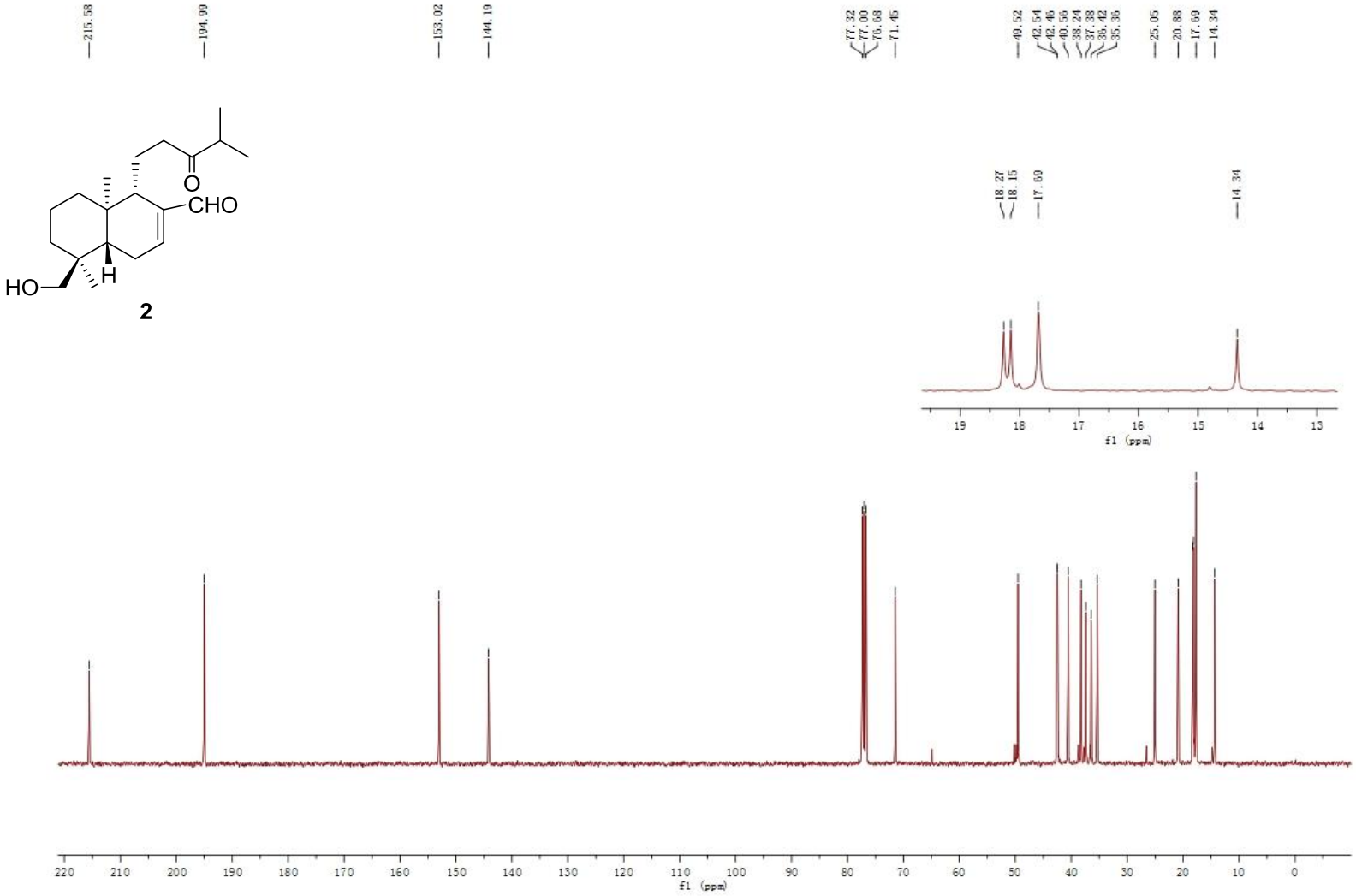


Figure S12. HSQC (400 MHz, $CDCl_3$) spectrum of **2**

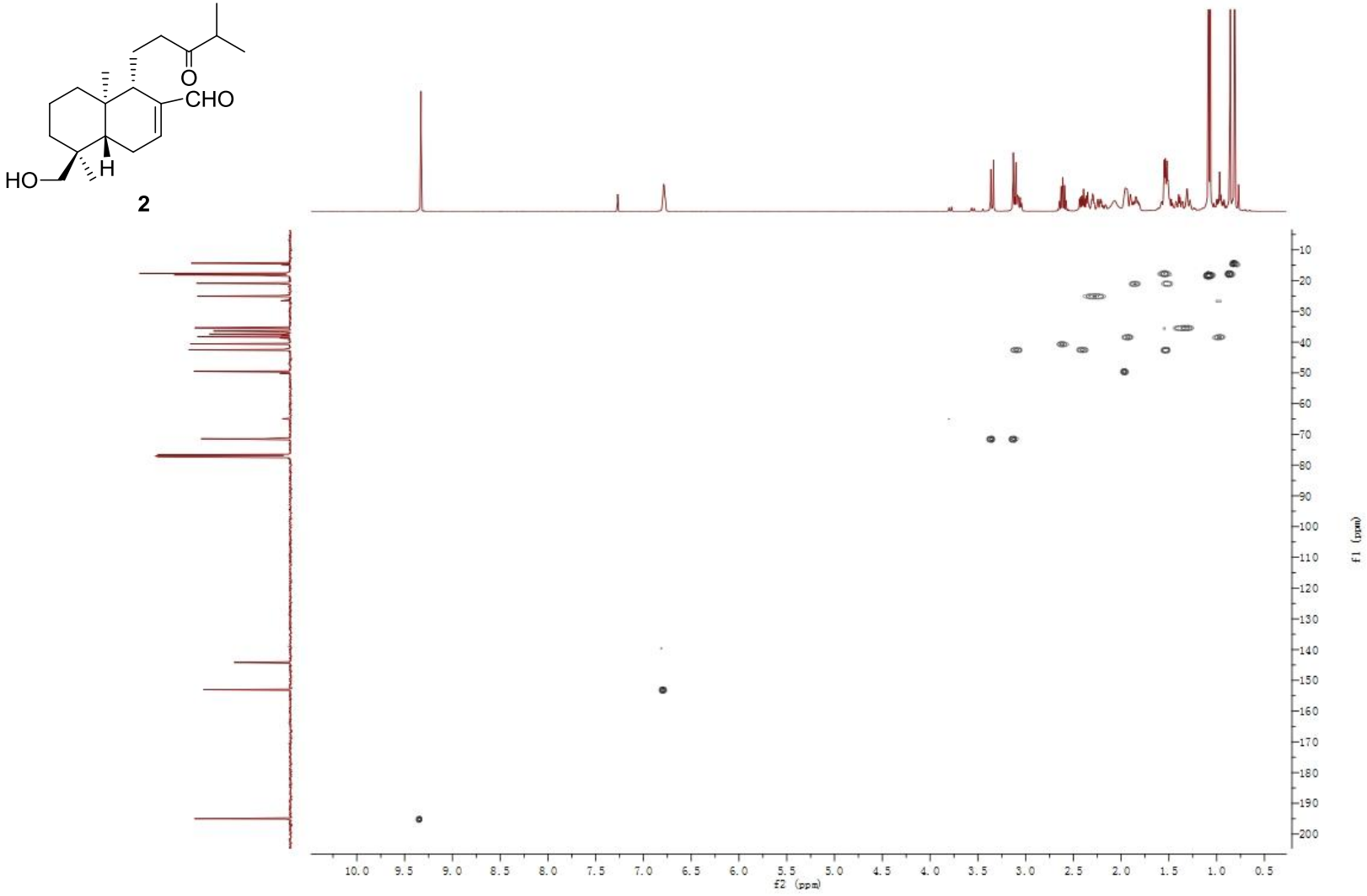


Figure S13. HMBC (400 MHz, $CDCl_3$) spectrum of **2**

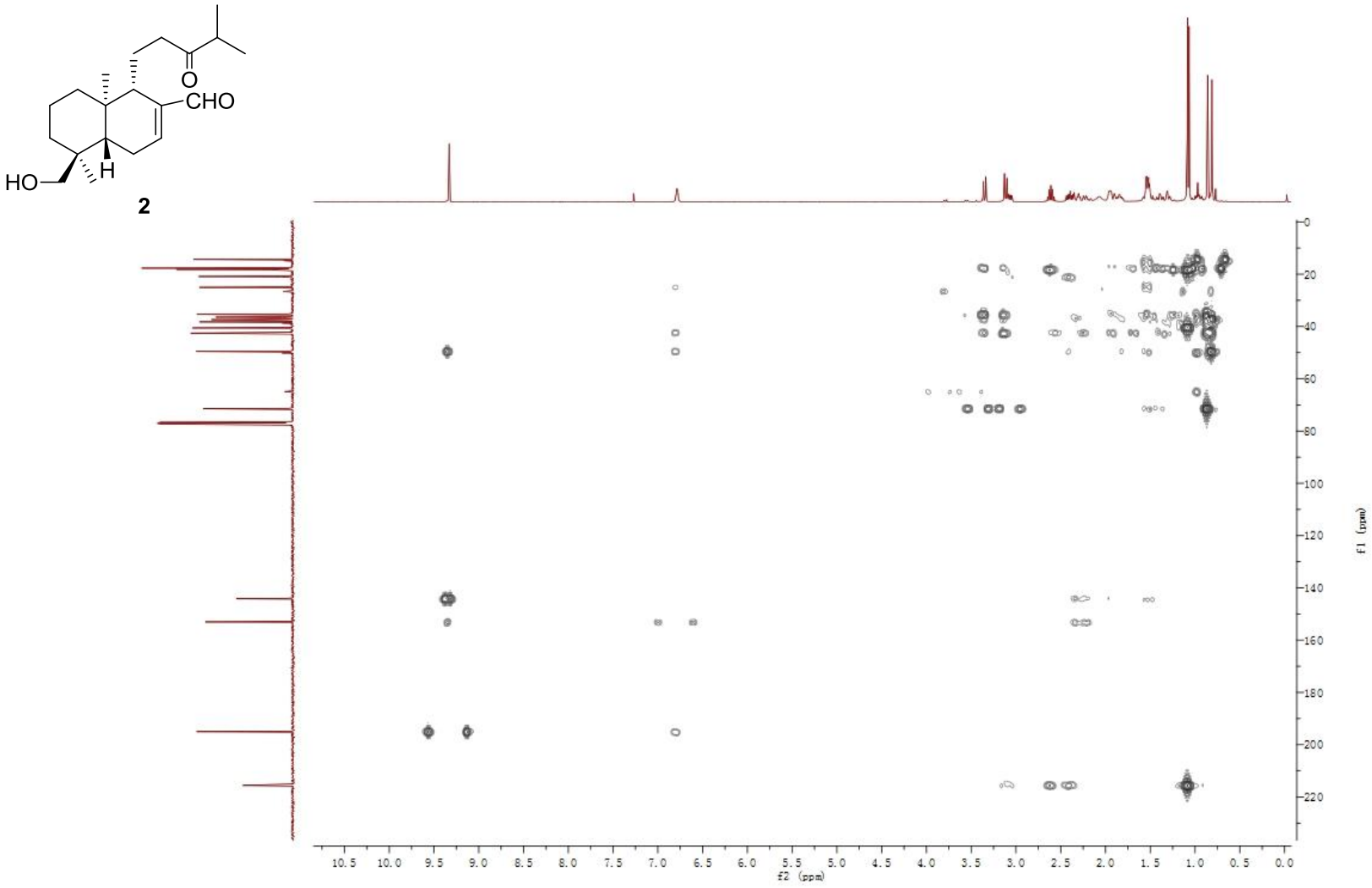


Figure S14. HMBC (400 MHz, $CDCl_3$) spectrum of **2**-expansion

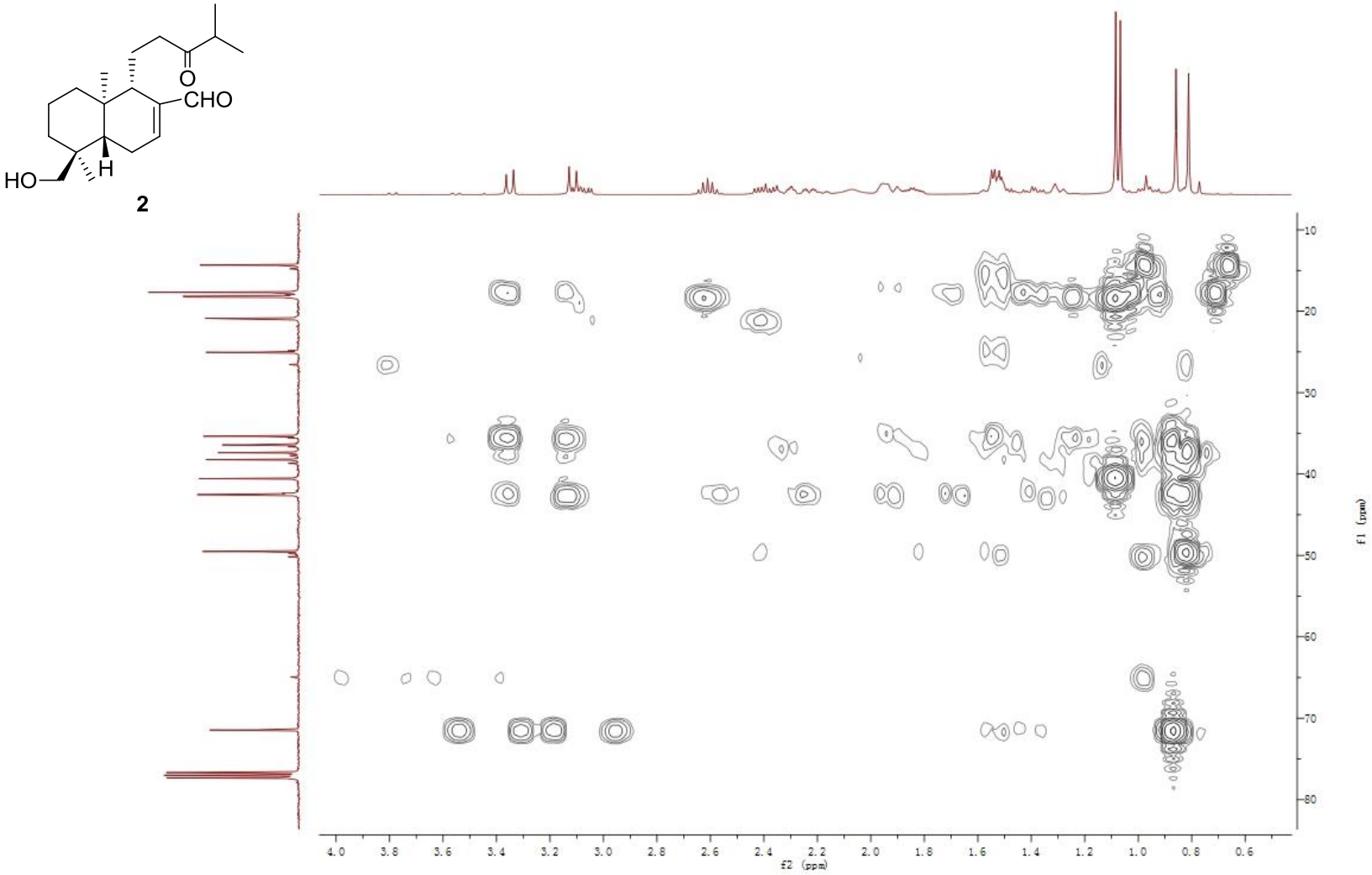


Figure S15. NOESY (400 MHz, $CDCl_3$) spectrum of **2**

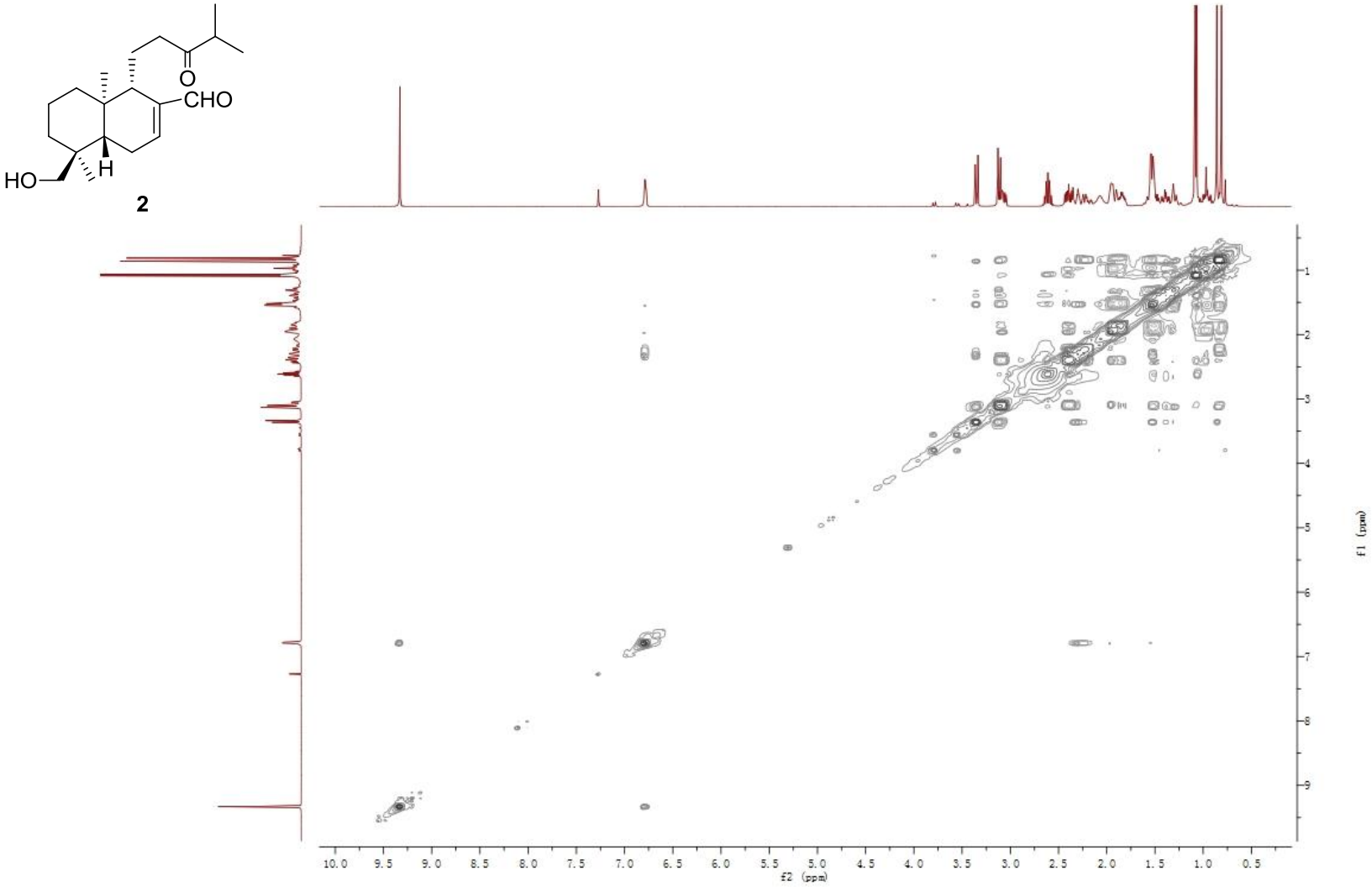


Figure S16. NOESY (400 MHz, $CDCl_3$) spectrum of **2**-expansion

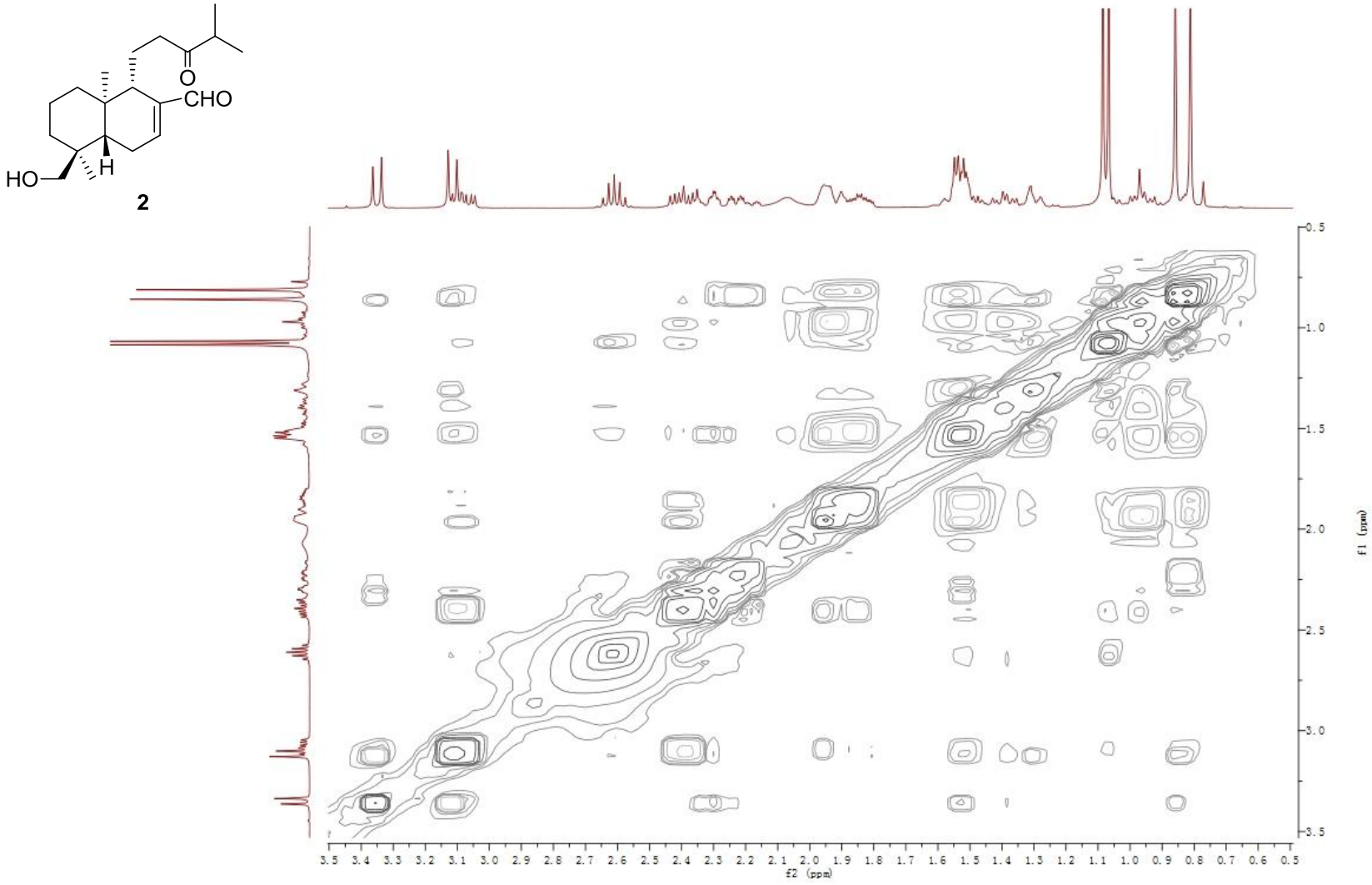
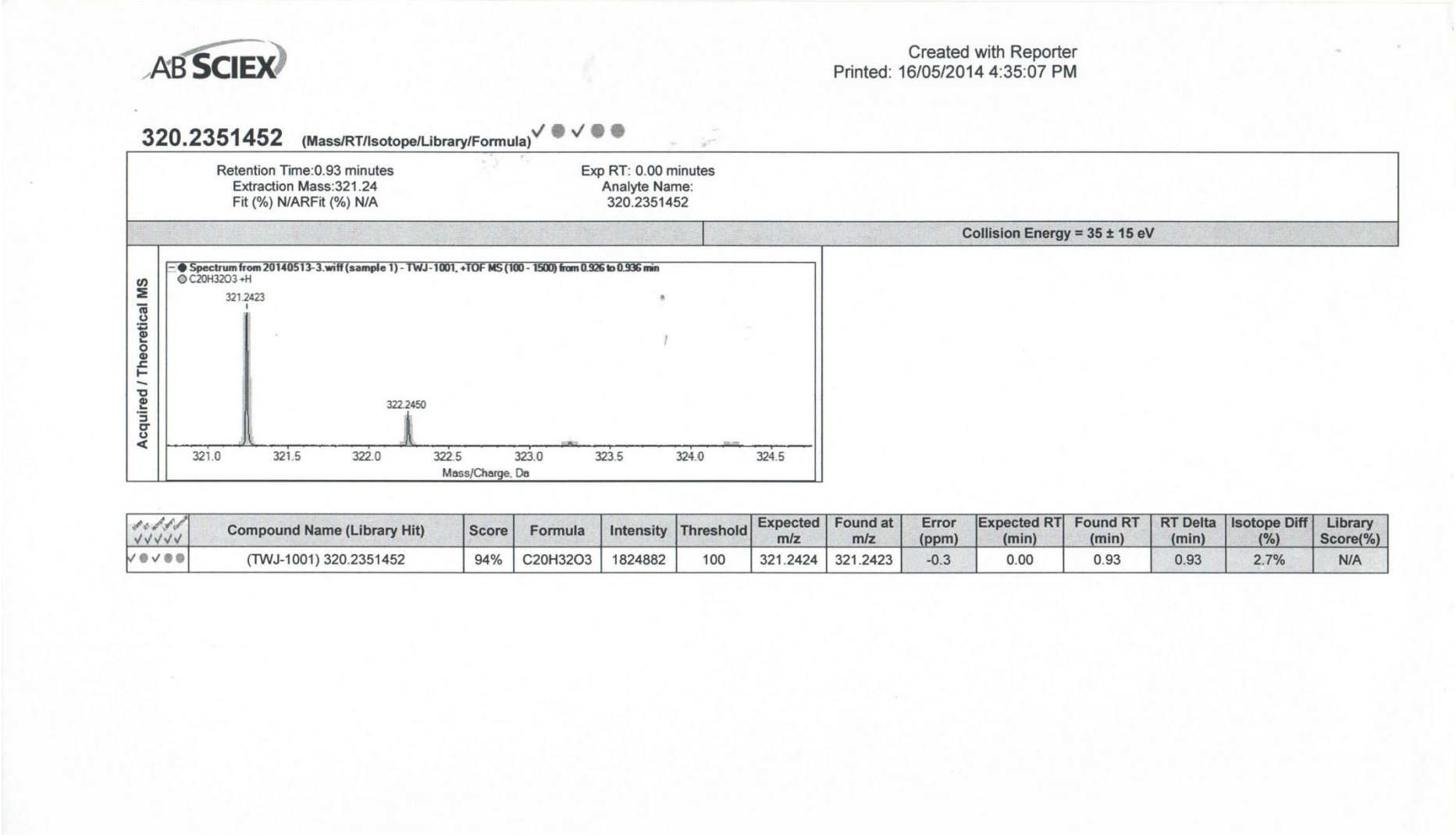


Figure S17. HRESIMS spectrum of **2**



	Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
✓●✓●●	(TWJ-1001) 320.2351452	94%	C20H32O3	1824882	100	321.2424	321.2423	-0.3	0.00	0.93	0.93	2.7%	N/A

Figure S18. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3**

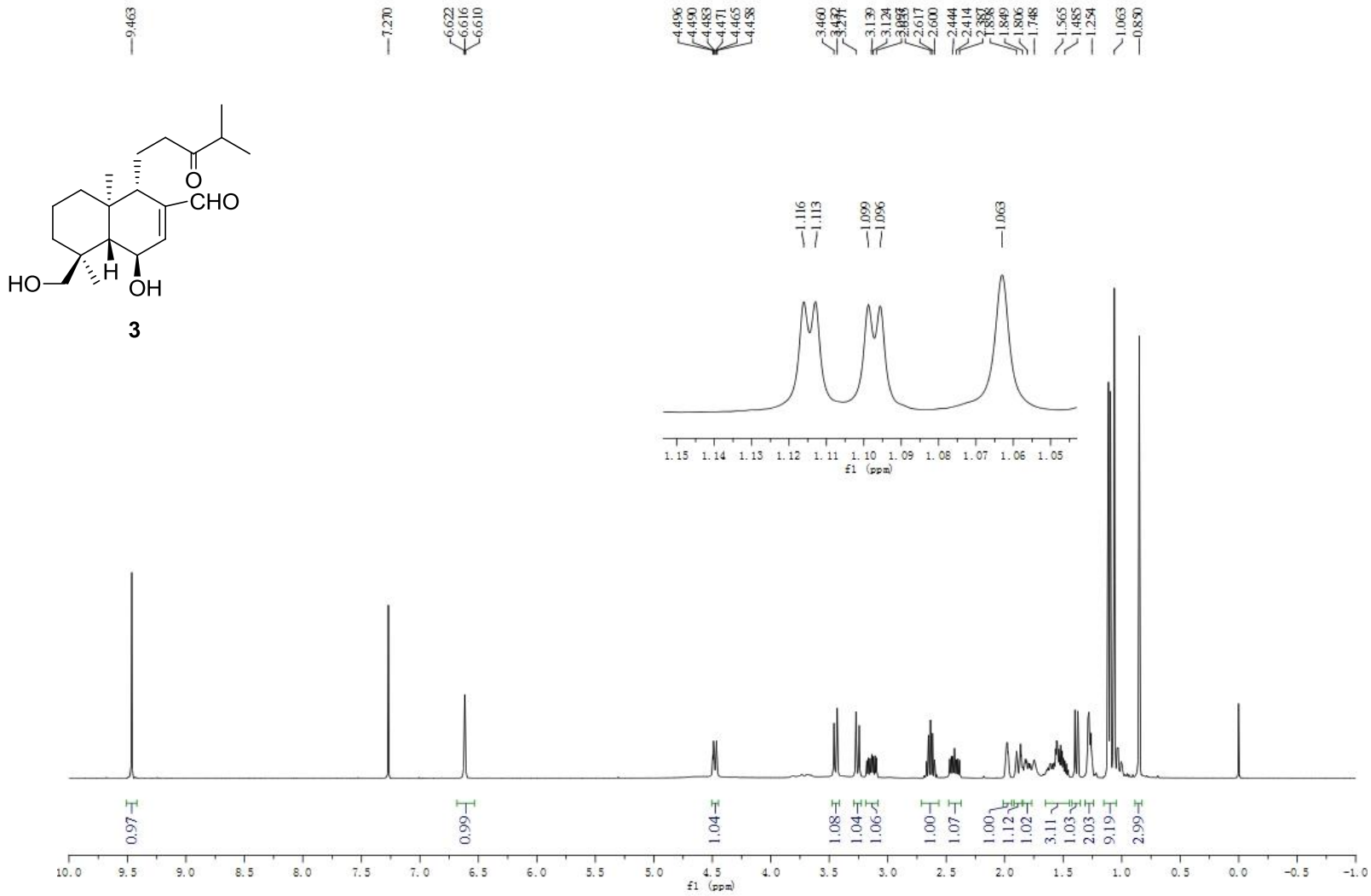
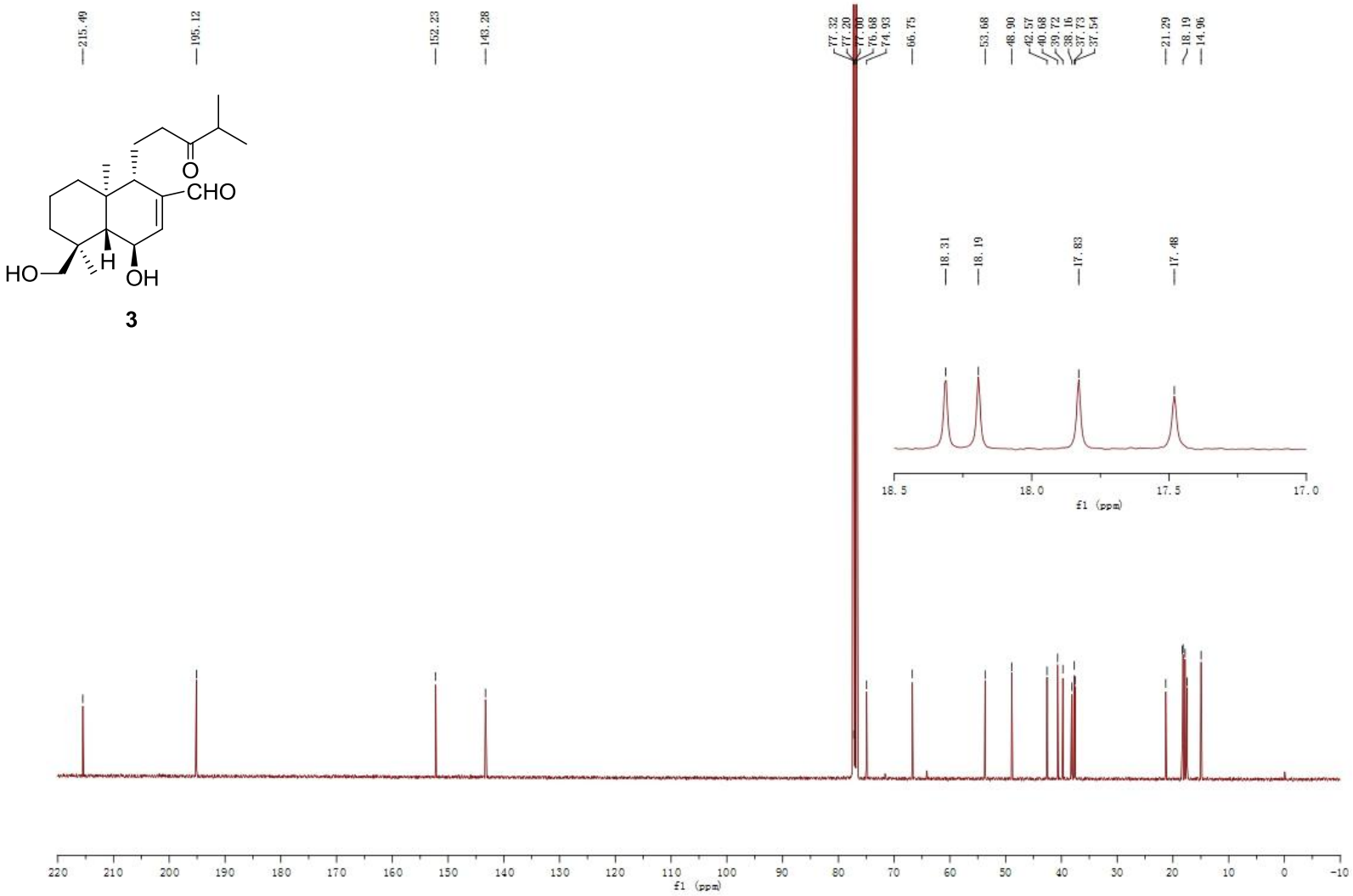
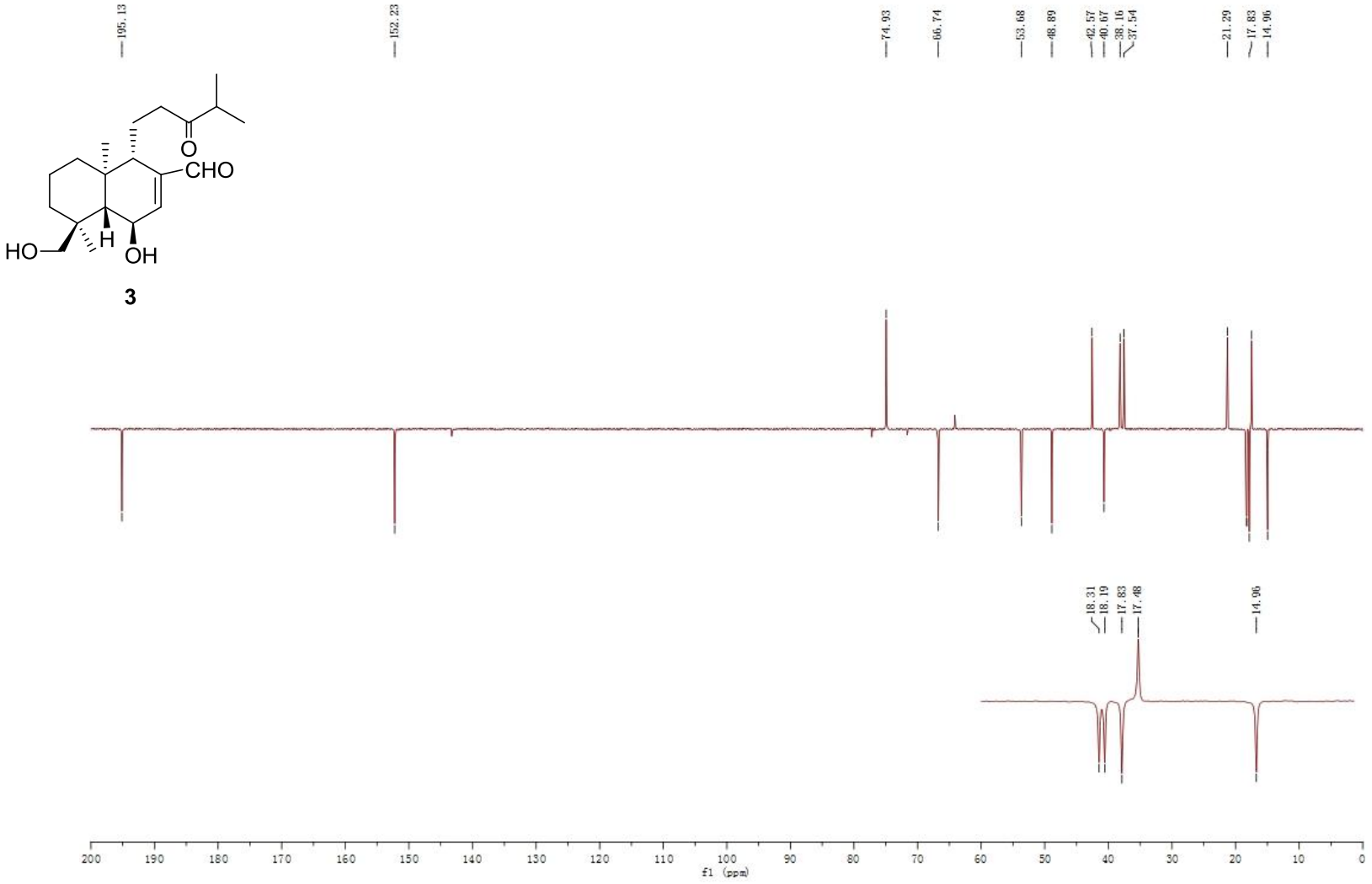


Figure S19. ^{13}C NMR (400 MHz, $CDCl_3$) spectrum of **3**



3

Figure S20. DEPT-135 (400 MHz, $CDCl_3$) spectrum of **3**



3

Figure S21. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of **3**

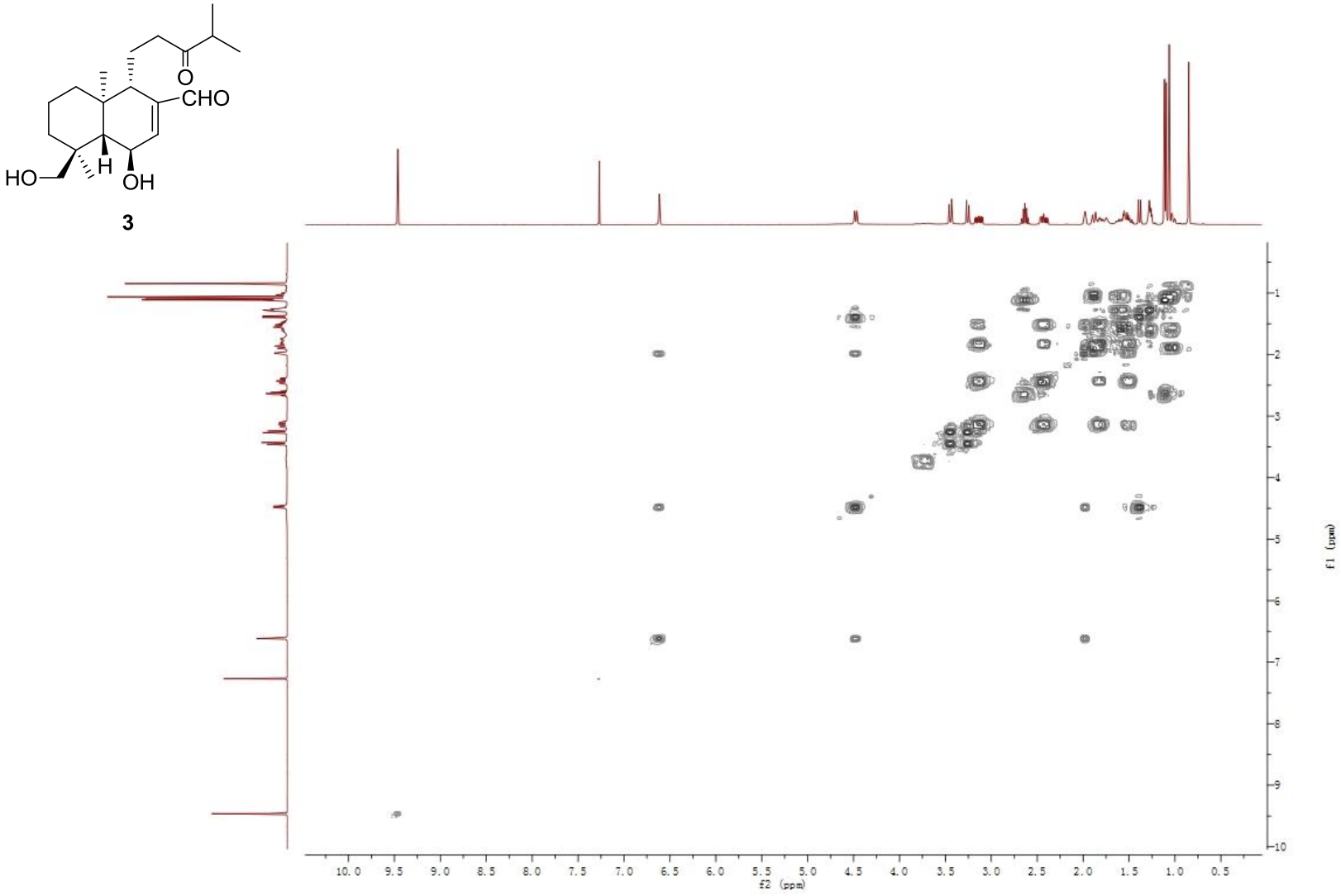


Figure S22. HSQC (400 MHz, $CDCl_3$) spectrum of **3**

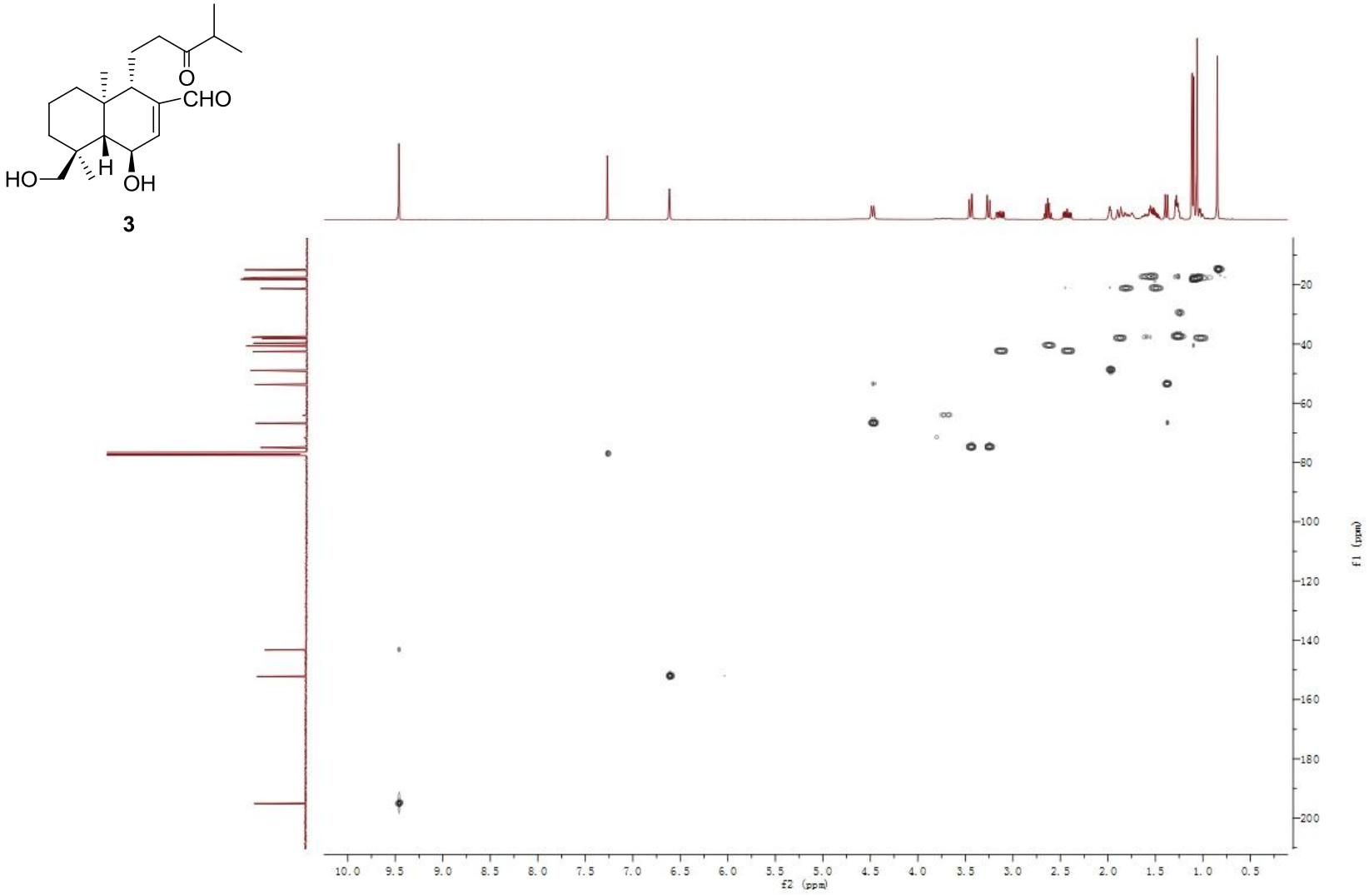


Figure S23. HMBC (400 MHz, $CDCl_3$) spectrum of **3**

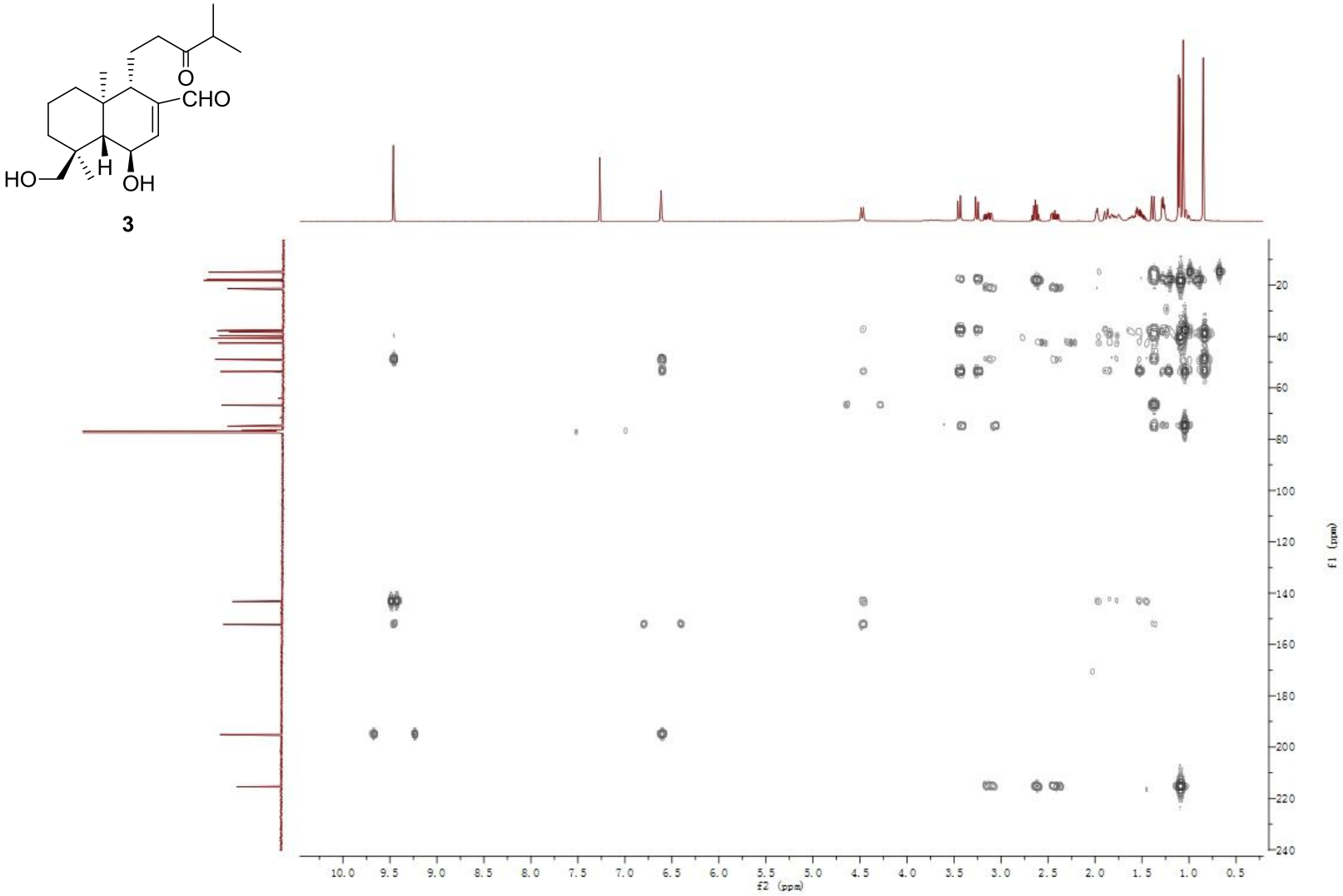


Figure S24. HMBC (400 MHz, $CDCl_3$) spectrum of **3**-expansion

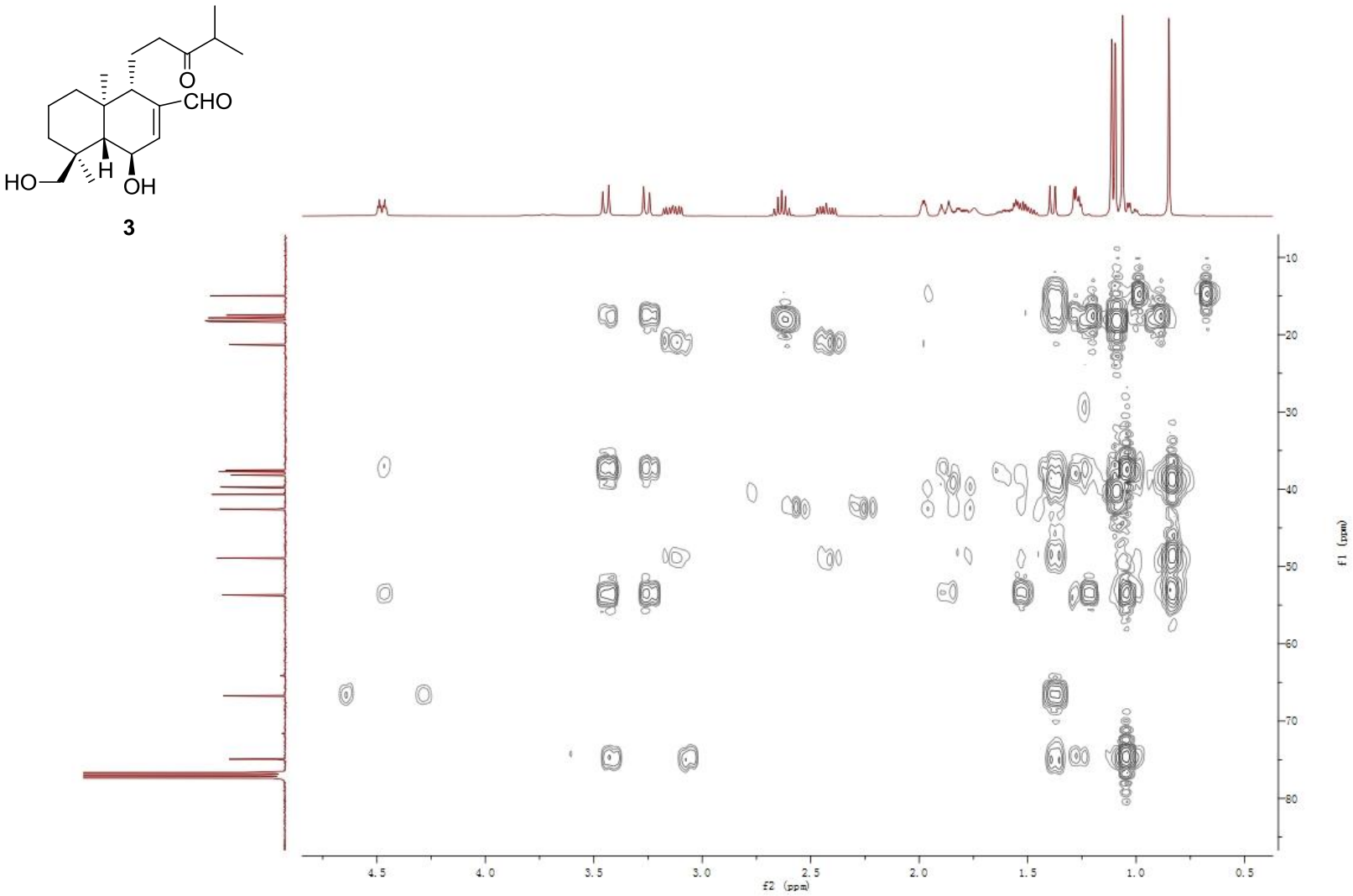


Figure S25. NOESY (400 MHz, $CDCl_3$) spectrum of **3**

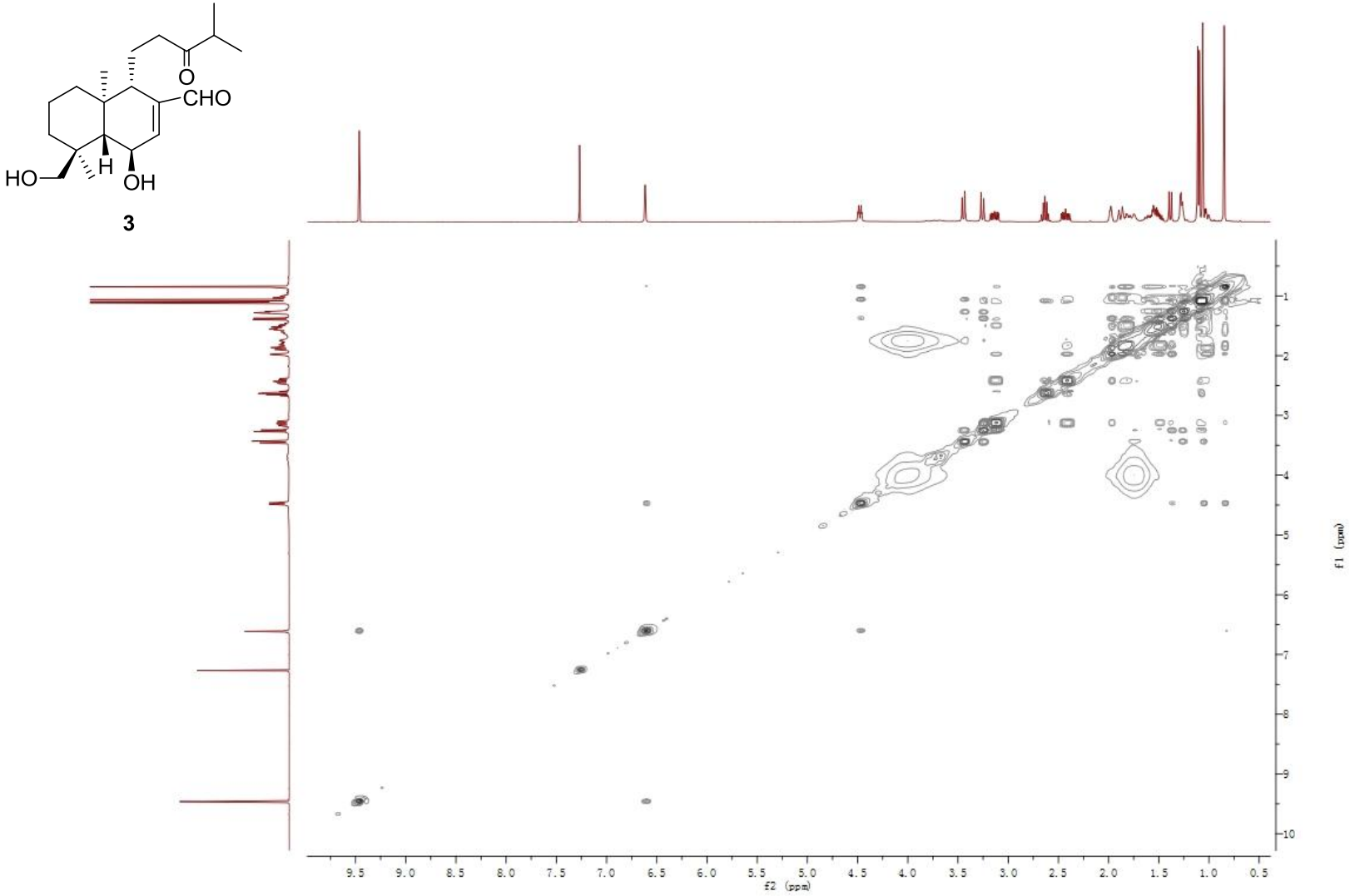
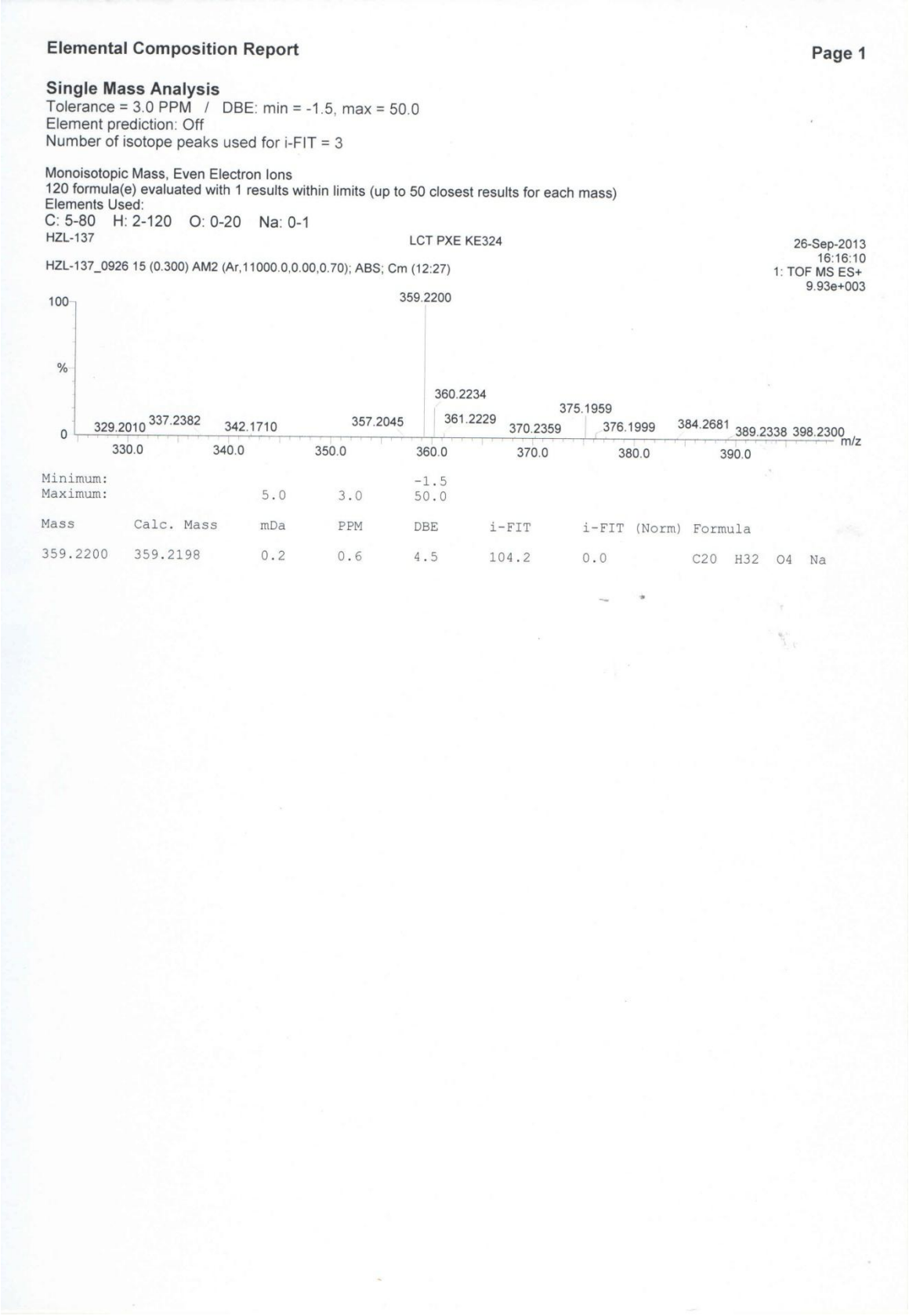


Figure S26. HRESIMS spectrum of **3**



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
120 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1

HZL-137 LCT PXE KE324 26-Sep-2013 16:16:10

HZL-137_0926 15 (0.300) AM2 (Ar,11000.0,0.00,0.70); ABS; Cm (12:27) 1: TOF MS ES+ 9.93e+003

Minimum:				-1.5			
Maximum:		5.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
359.2200	359.2198	0.2	0.6	4.5	104.2	0.0	C20 H32 O4 Na

Figure S27. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4**

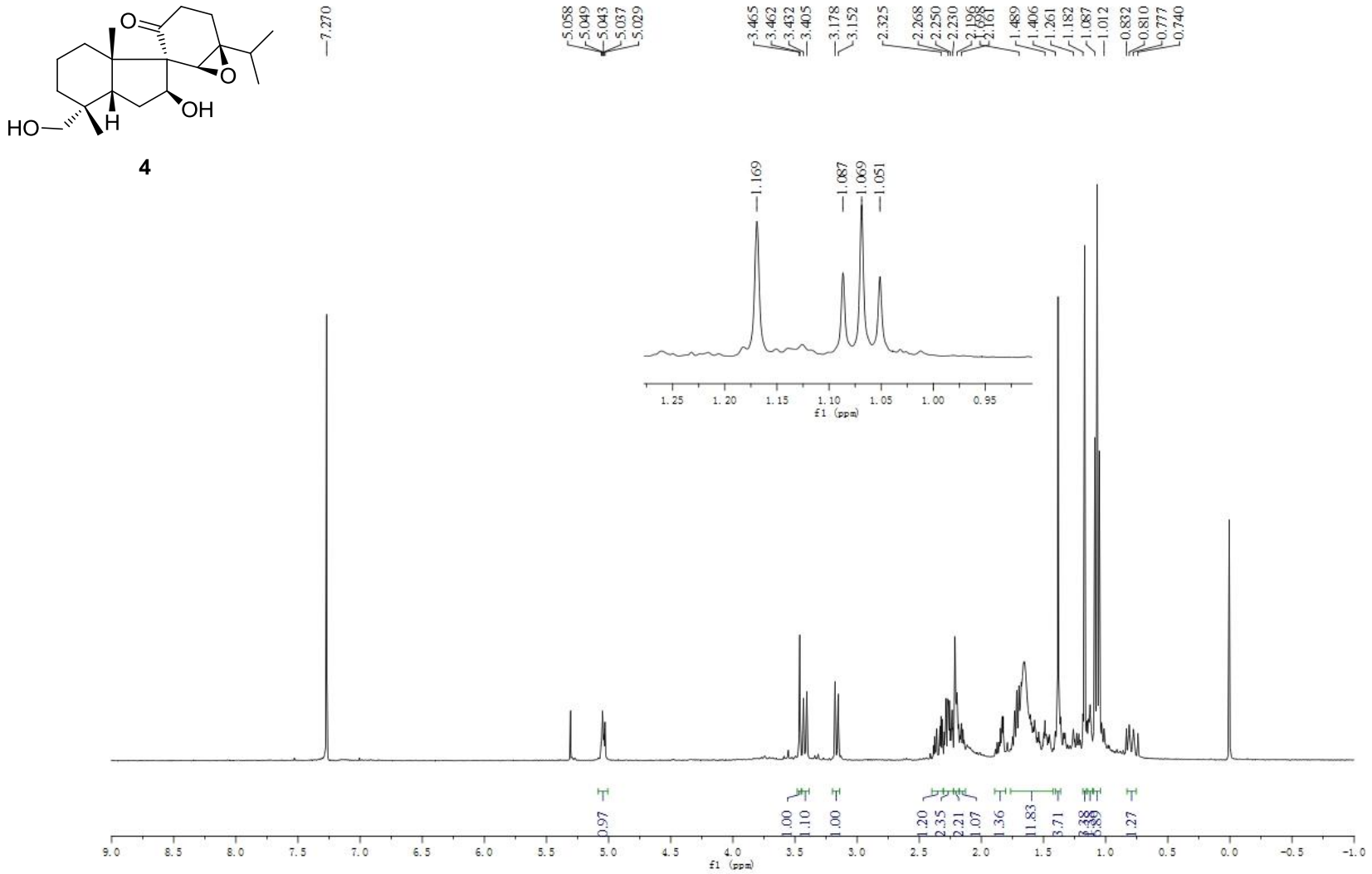
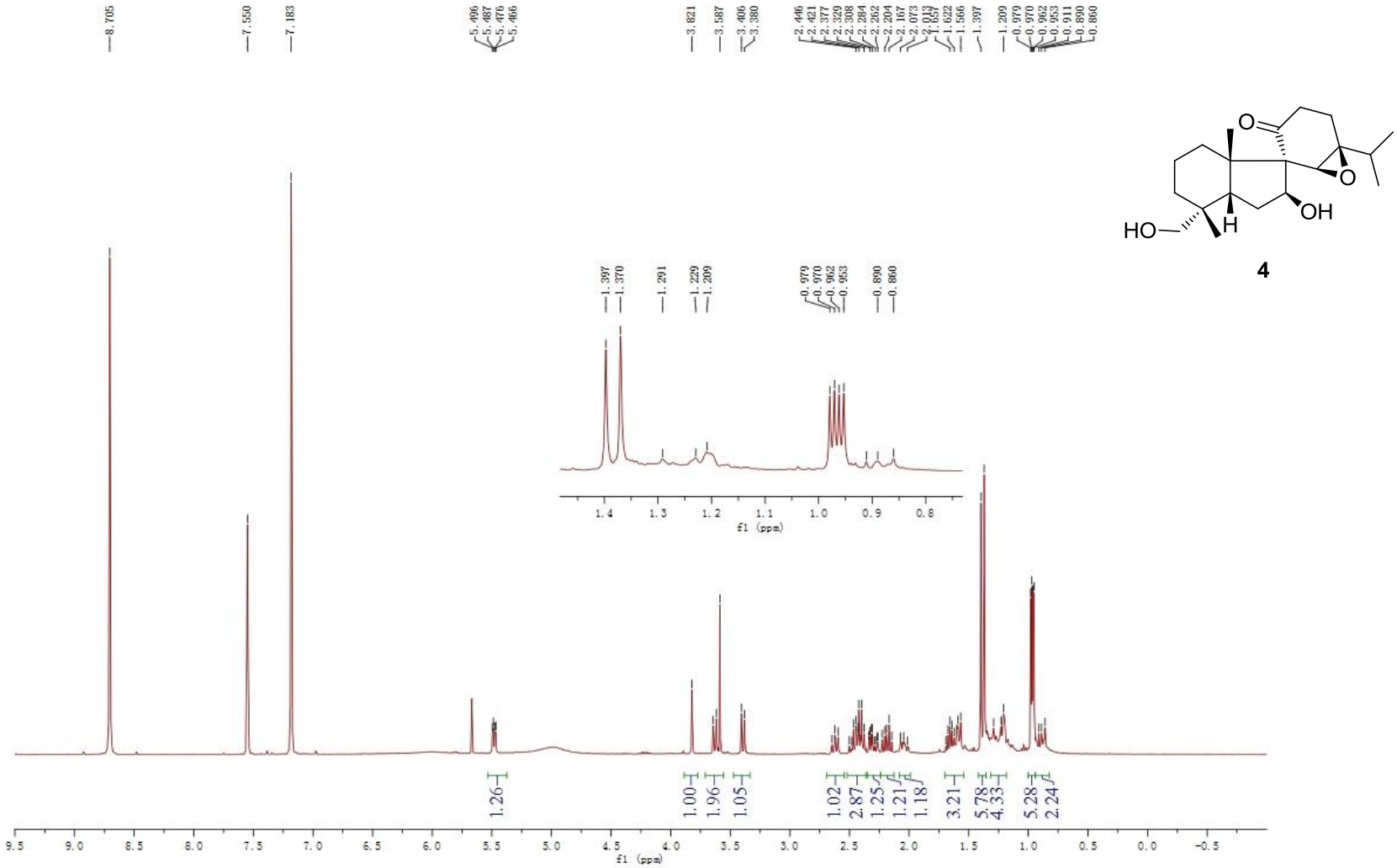
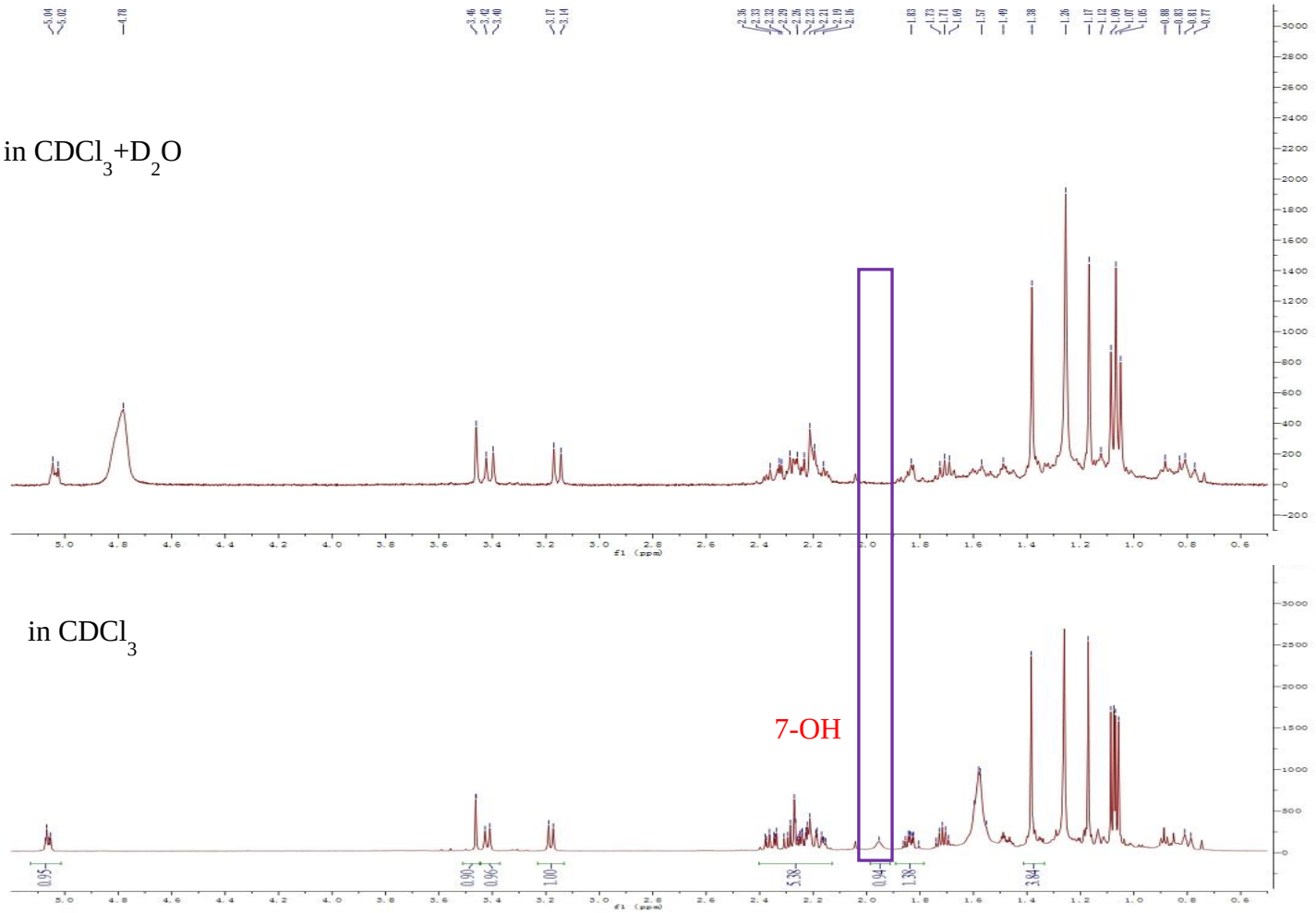


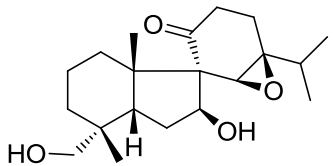
Figure S28. ^{1}H NMR (400 MHz, pyridine-d_5) spectrum of **4**



4

Figure S29. ^{1}H NMR (400 MHz, $CDCl_3$+D_2O) spectrum of **4**





4

Figure S30. ^{13}C NMR (400 MHz, $CDCl_3$) spectrum of **4**

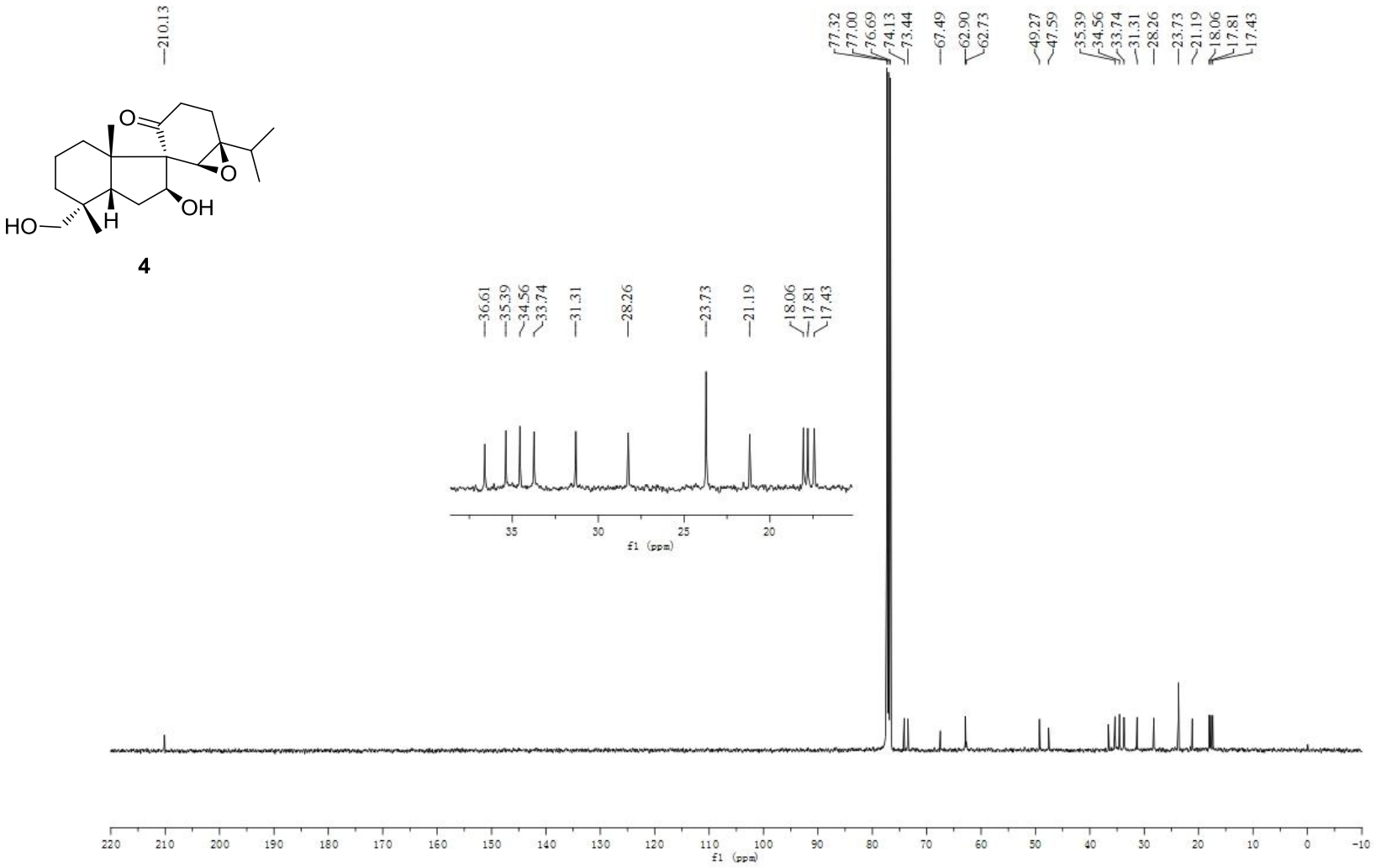


Figure S31. ^{13}C NMR (400 MHz, pyridine-d_5) spectrum of **4**

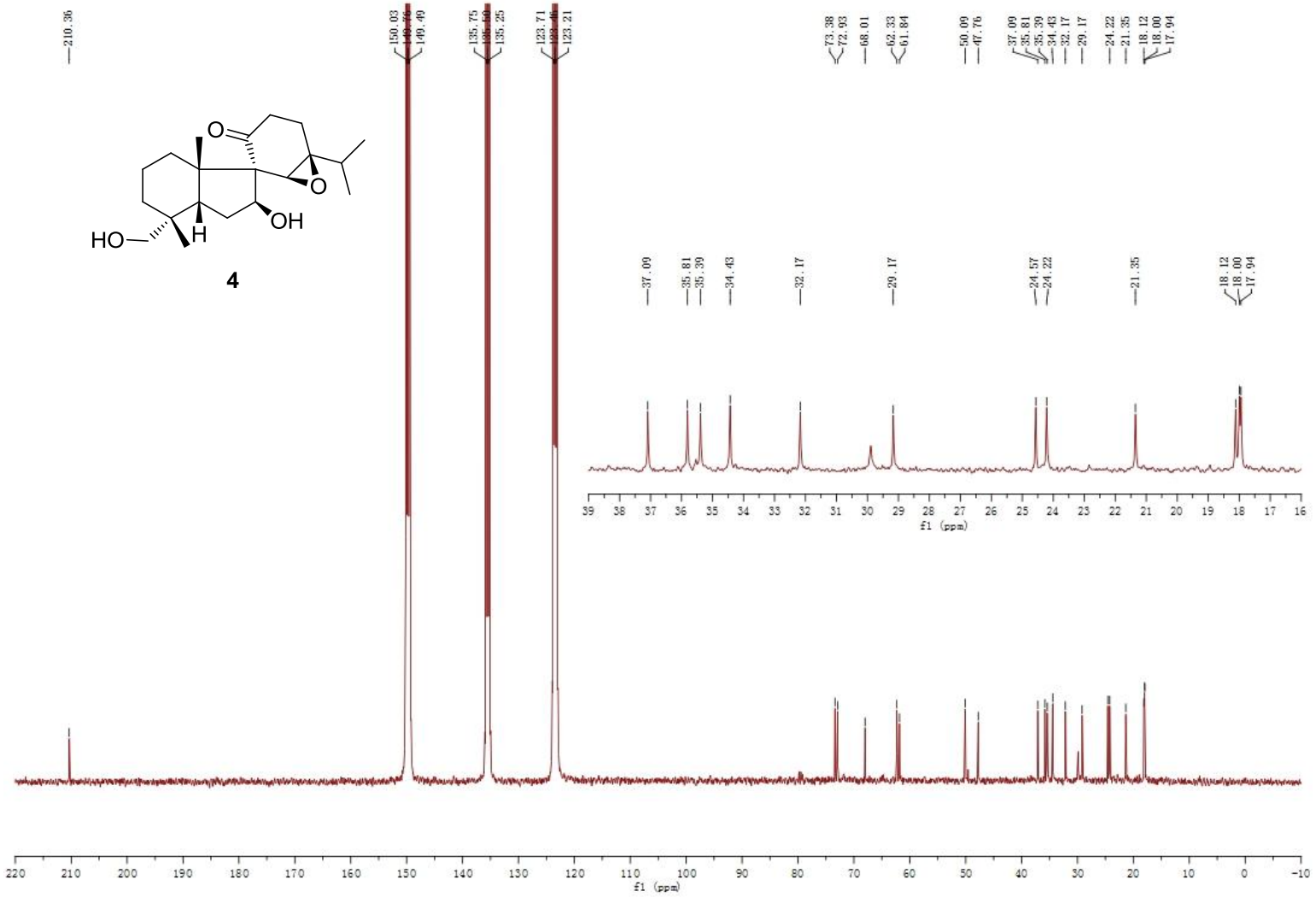


Figure S32. ^{1}H-^{1}H COSY (400 MHz, pyridine-d_5) spectrum of **4**

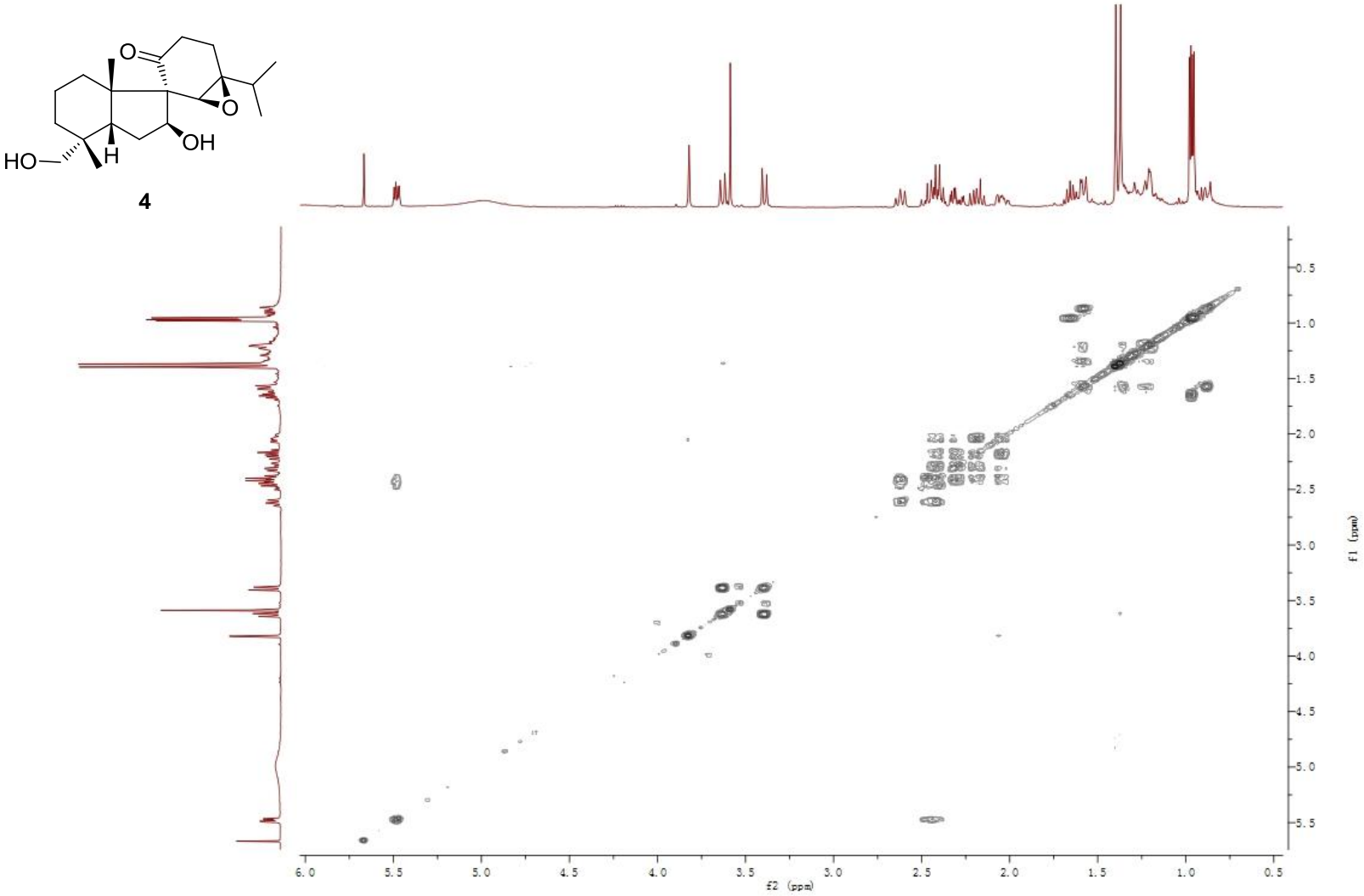


Figure S33. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **4**

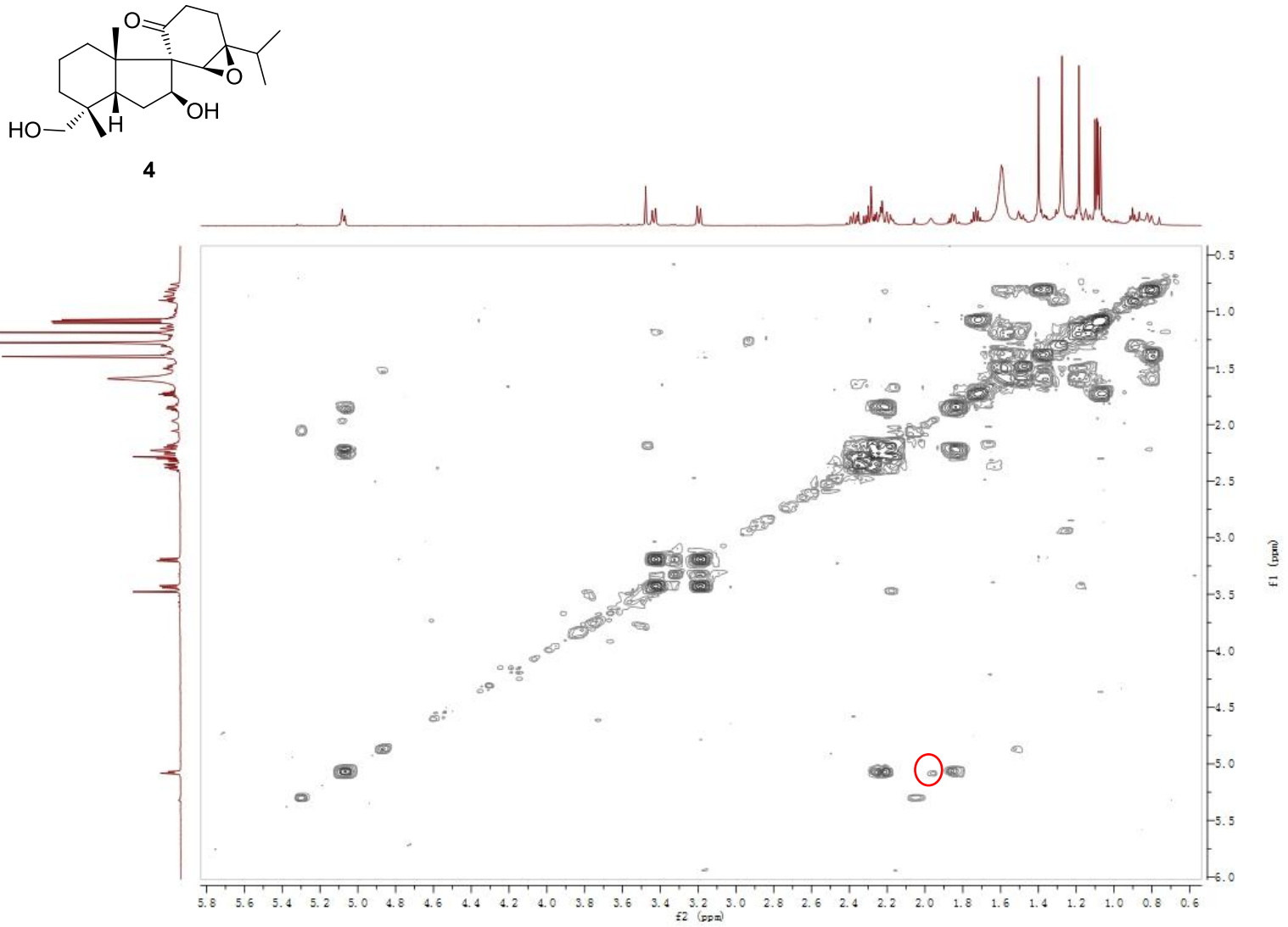


Figure S34. HSQC (400 MHz, $CDCl_3$) spectrum of **4**

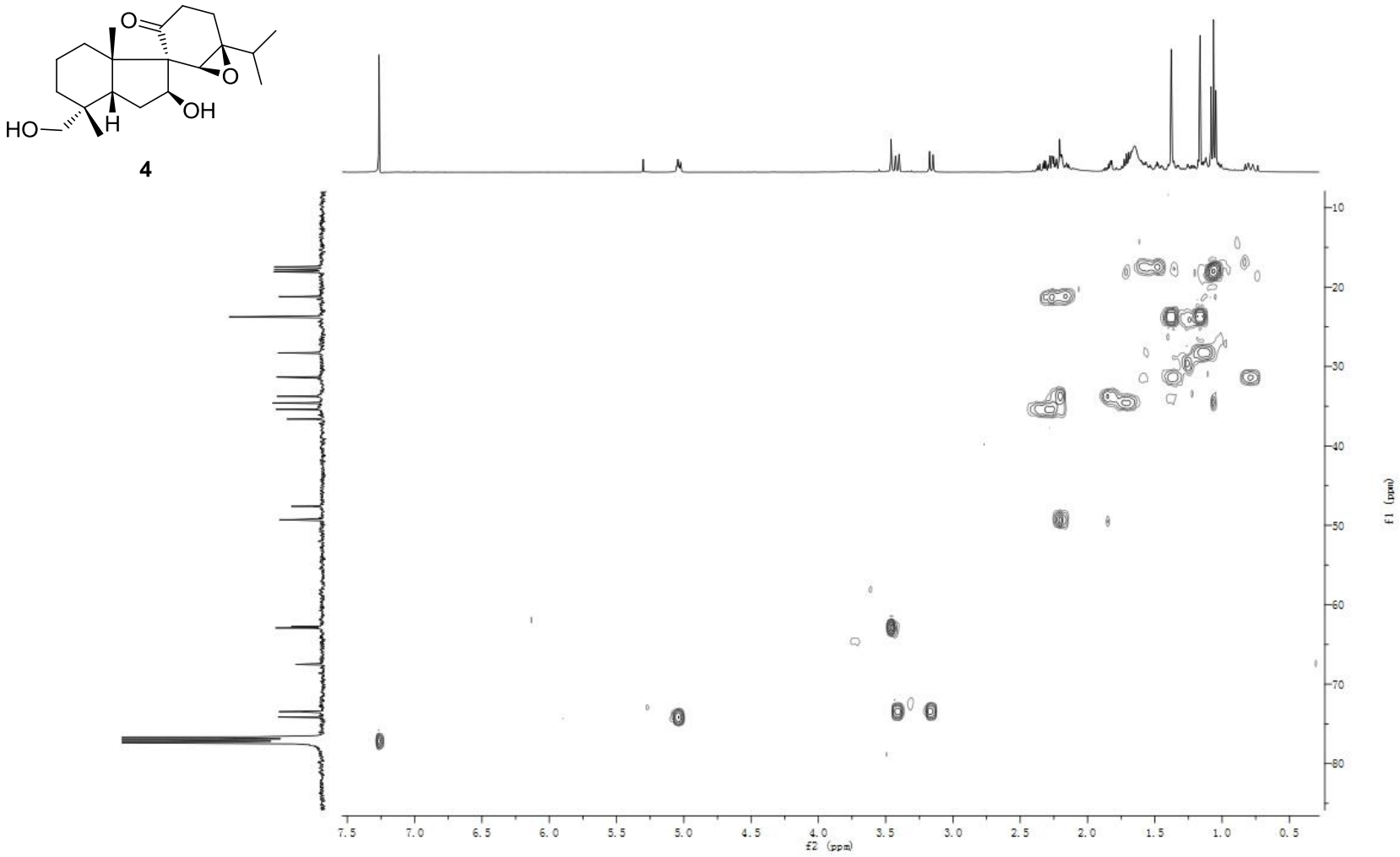


Figure S35. HMBC (400 MHz, pyridine-d_5) spectrum of **4**

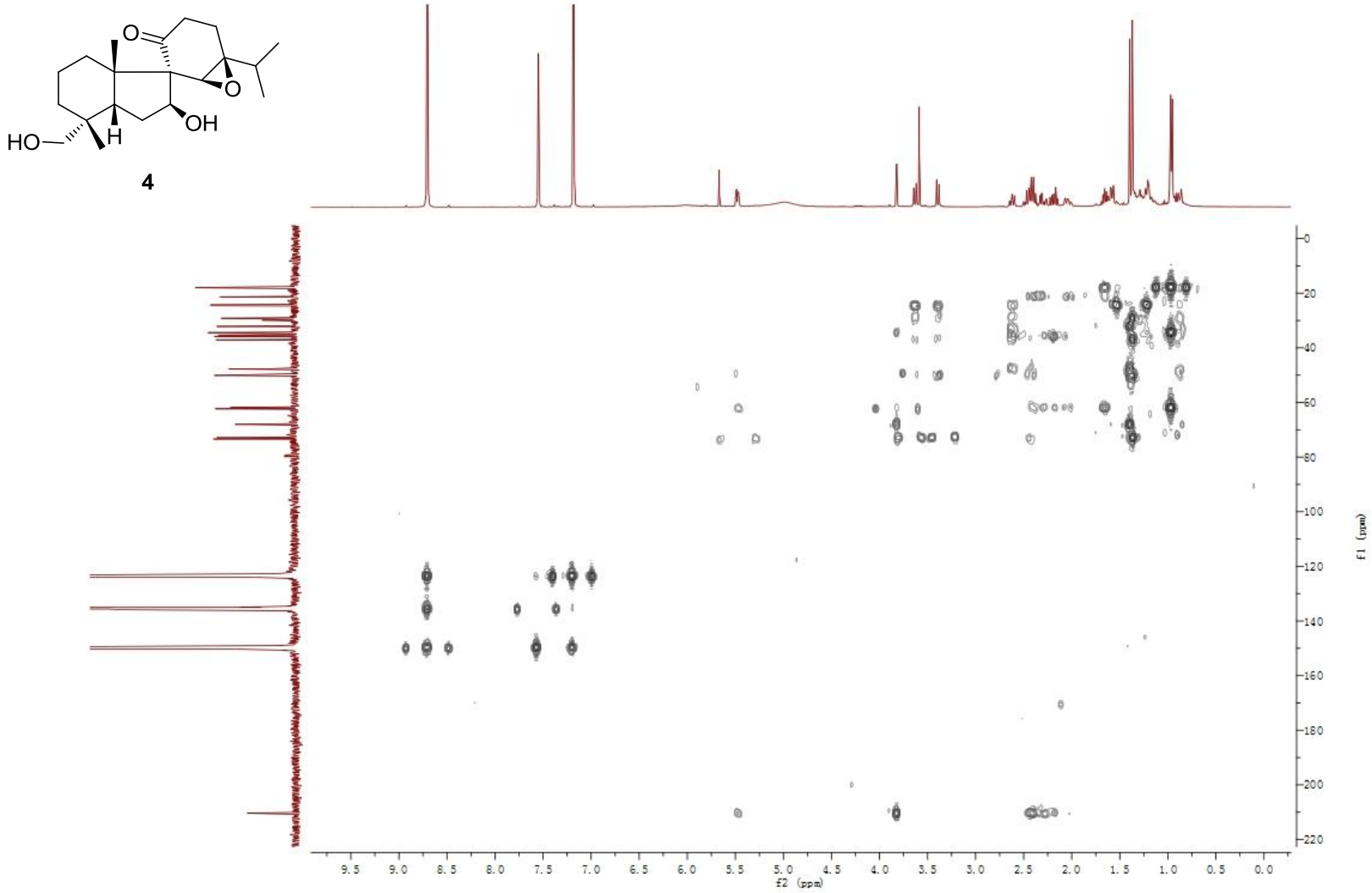


Figure S36. HMBC (400 MHz, pyridine-d_5) spectrum of **4**-expansion

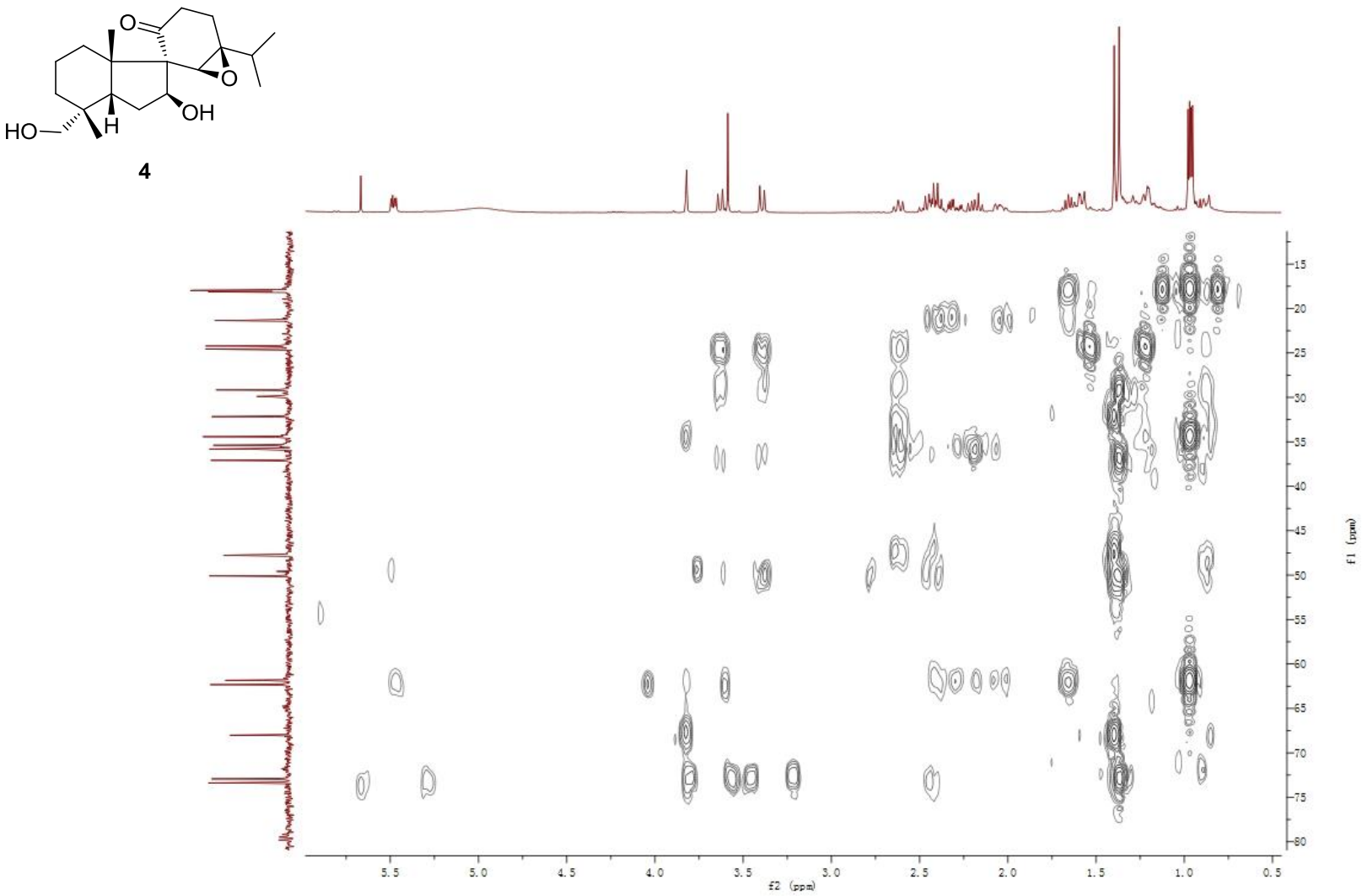


Figure S37. NOESY (400 MHz, $CDCl_3$) spectrum of **4**

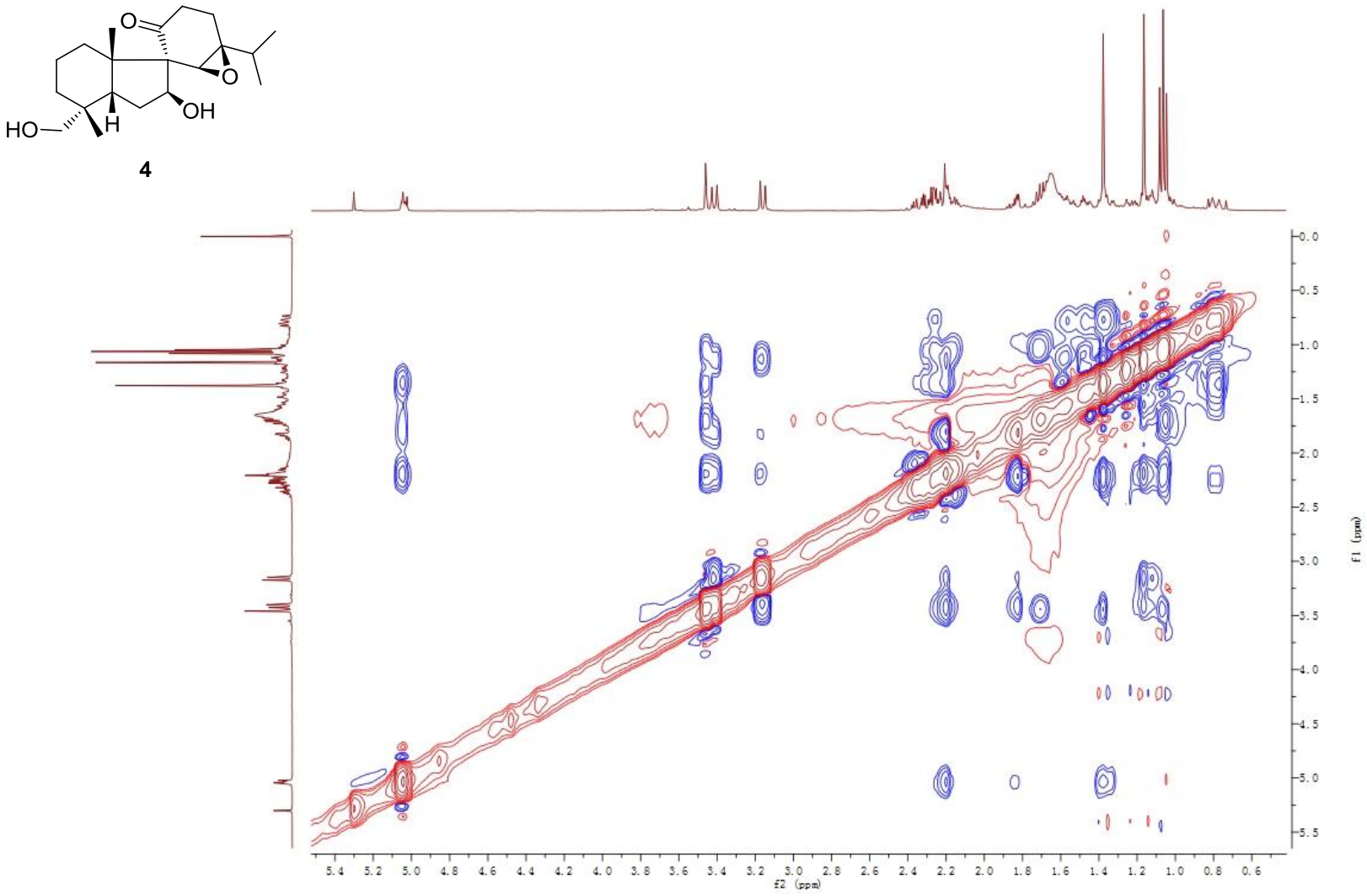
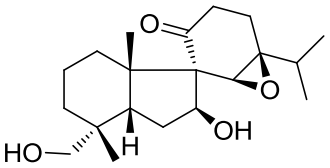
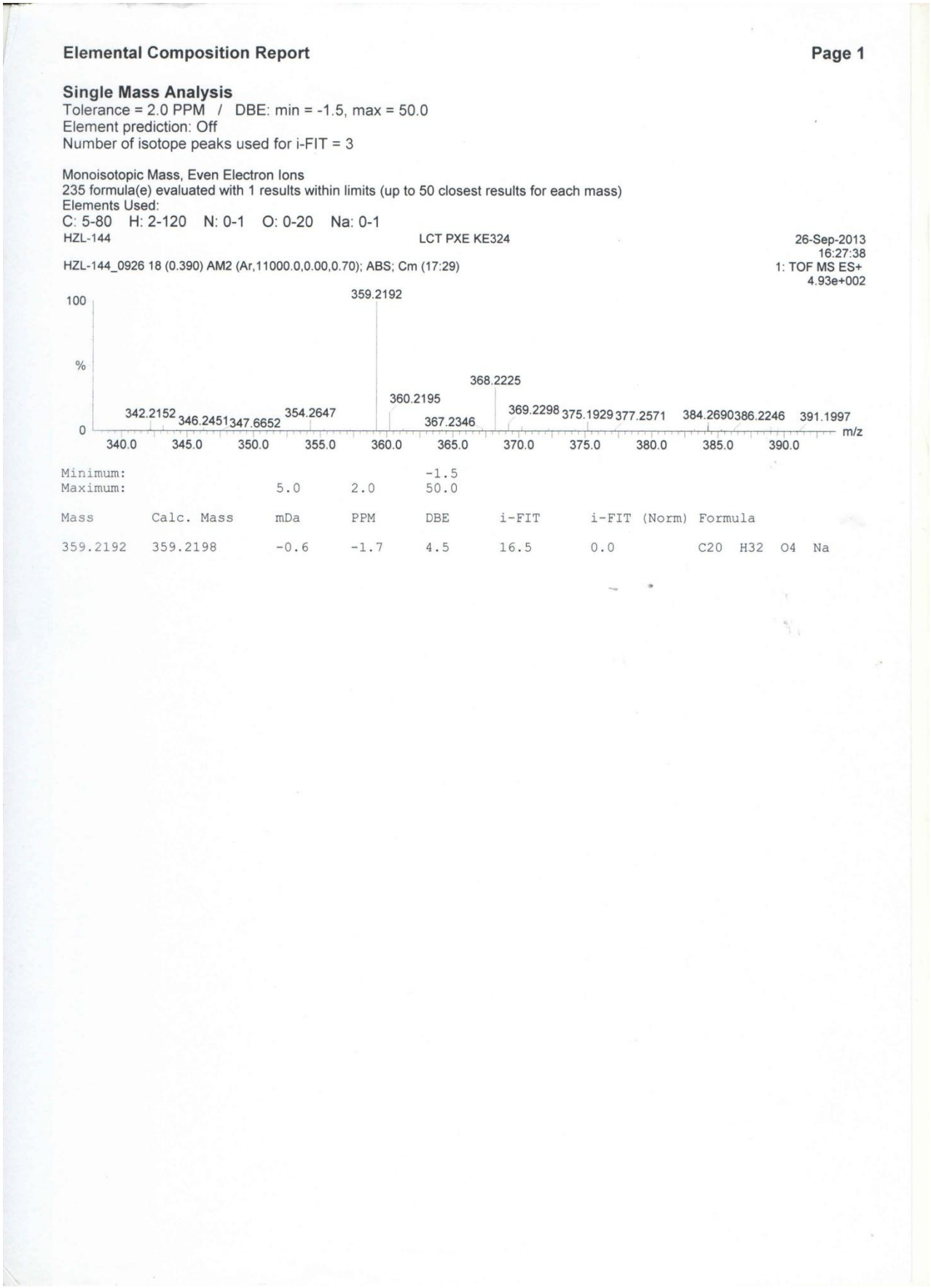


Figure S38. NOESY (400 MHz, pyridine-d_5) spectrum of **4**



4

Figure S39. HRESIMS spectrum of **4**



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
235 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 N: 0-1 O: 0-20 Na: 0-1

HZL-144 LCT PXE KE324 26-Sep-2013 16:27:38

HZL-144_0926 18 (0.390) AM2 (Ar,11000.0,0.00,0.70); ABS; Cm (17:29) 1: TOF MS ES+ 4.93e+002

Minimum:				-1.5			
Maximum:		5.0	2.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
359.2192	359.2198	-0.6	-1.7	4.5	16.5	0.0	C20 H32 O4 Na

Figure S40. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5**

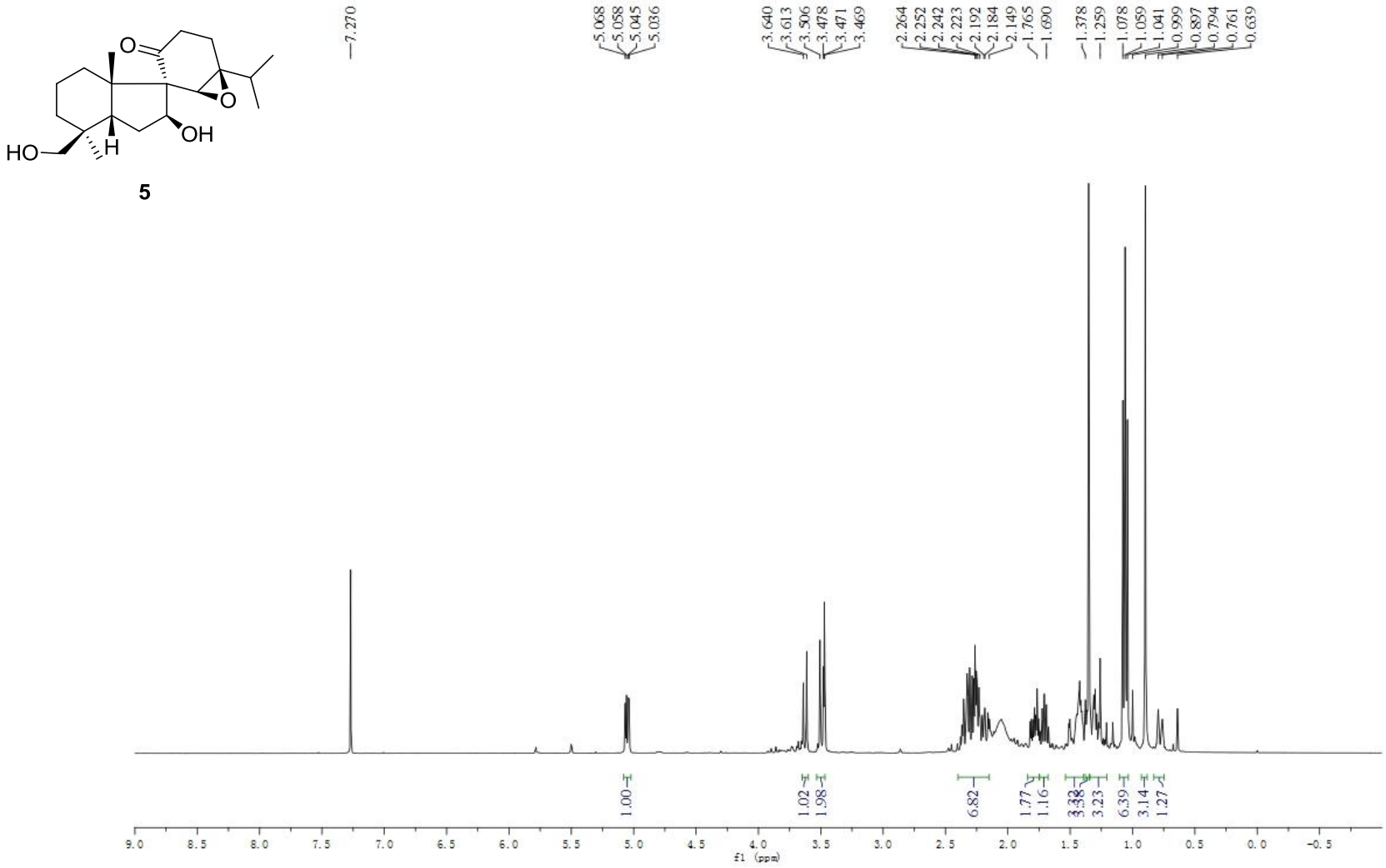


Figure S41. ^{13}C NMR (400 MHz, $CDCl_3$) spectrum of **5**

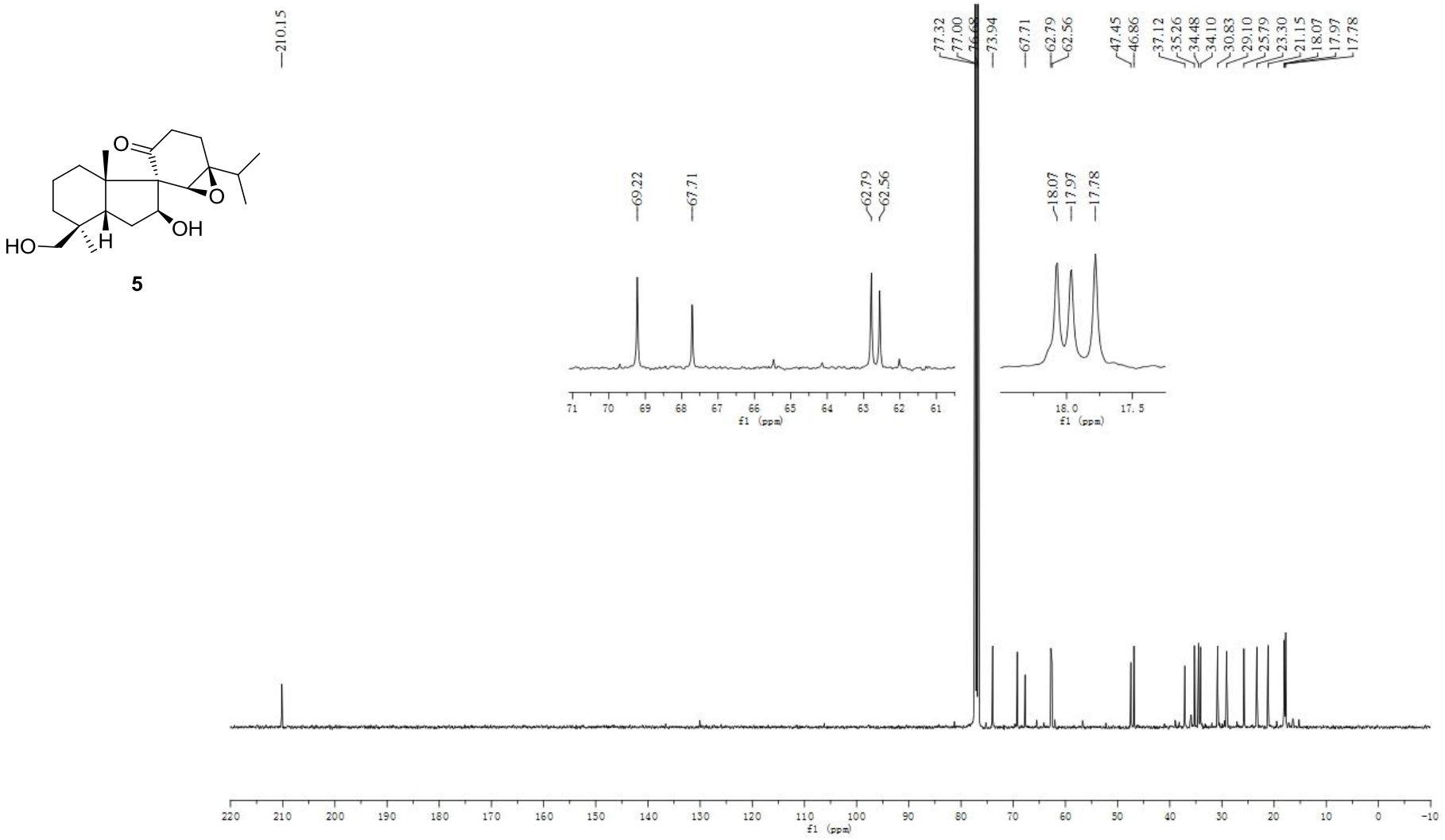
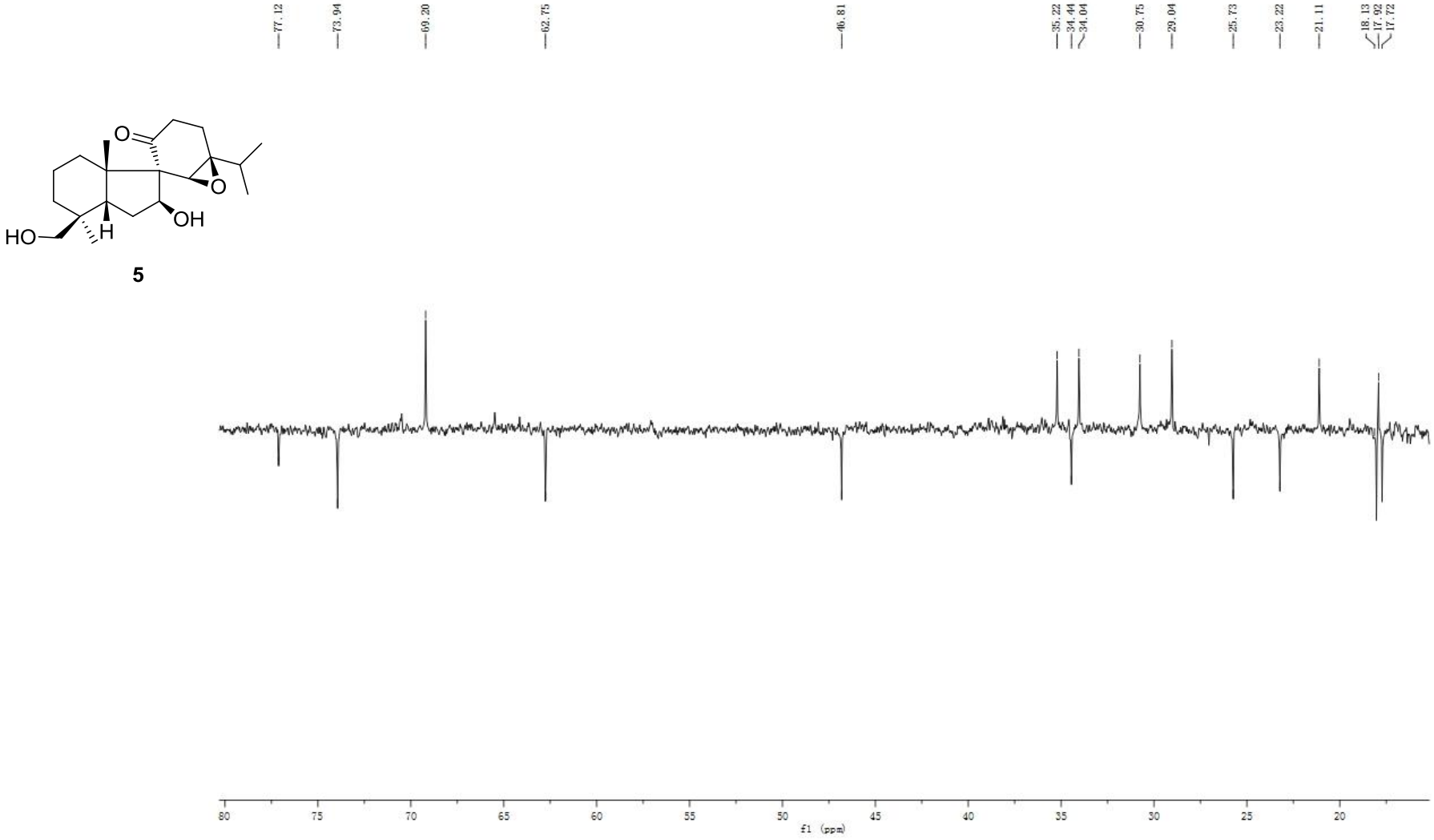


Figure S42. DEPT-135 (400 MHz, $CDCl_3$) spectrum of **5**



5

Figure S43. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of **5**

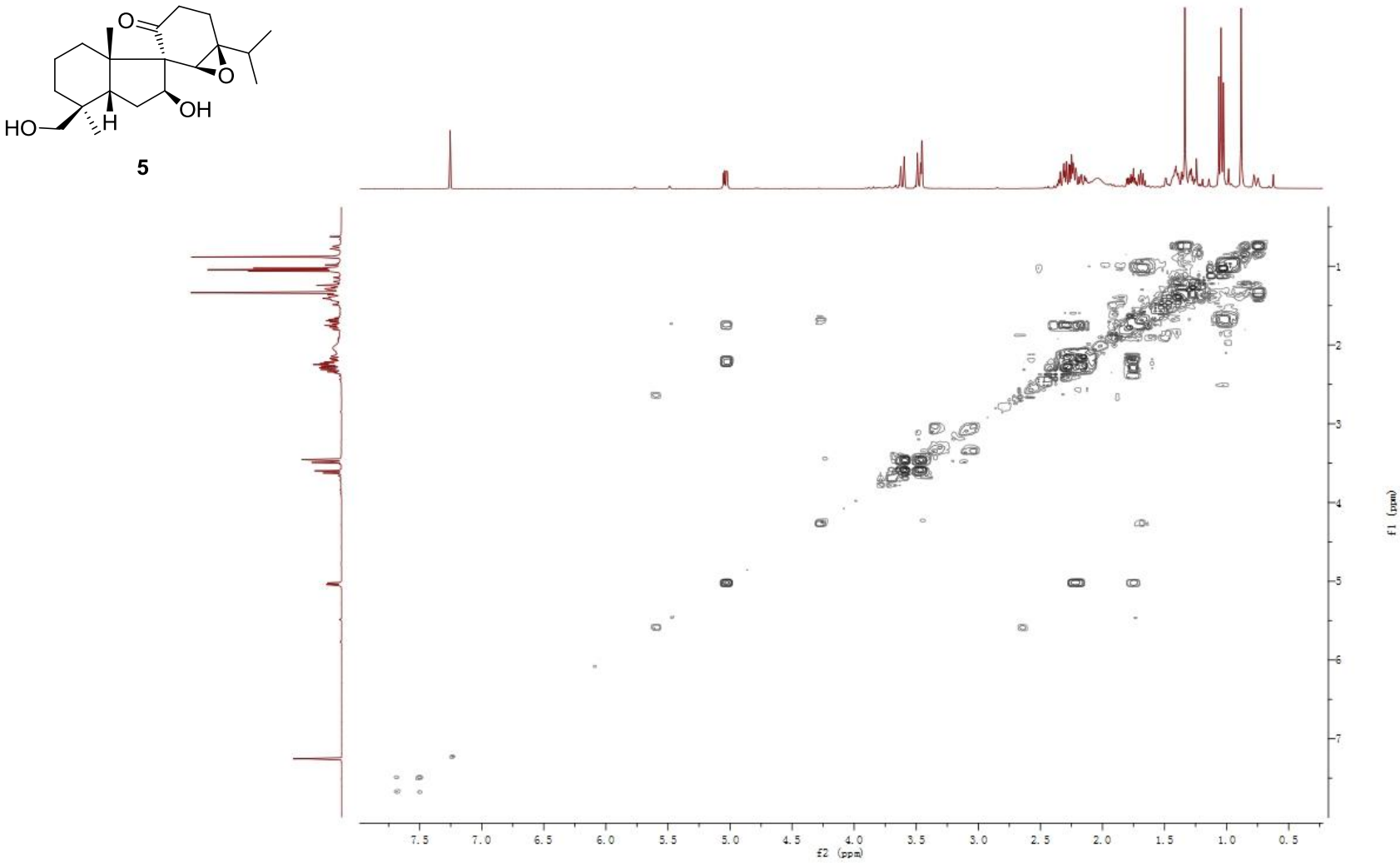
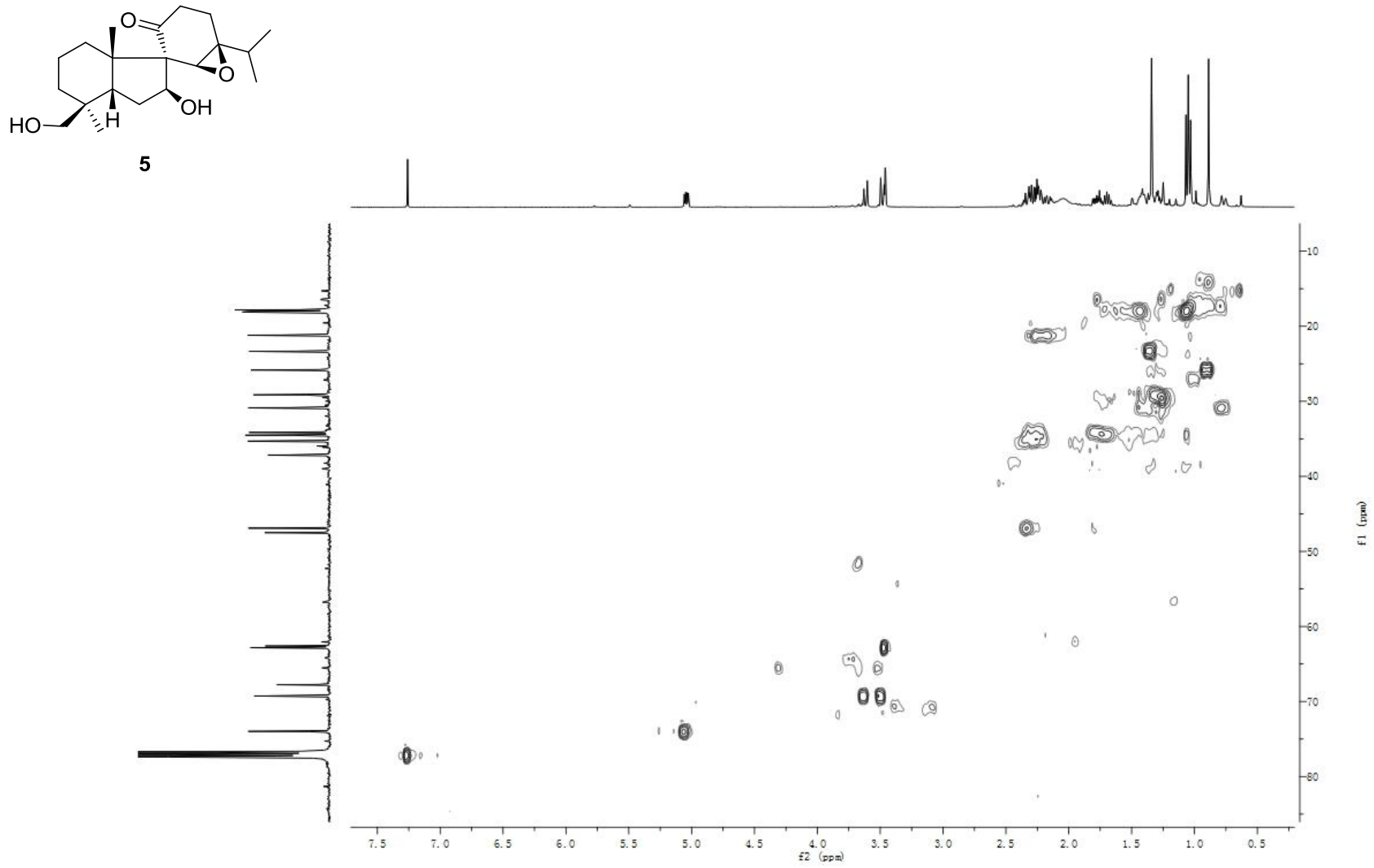


Figure S44. HSQC (400 MHz, $CDCl_3$) spectrum of **5**



5

Figure S45. HMBC (400 MHz, $CDCl_3$) spectrum of **5**

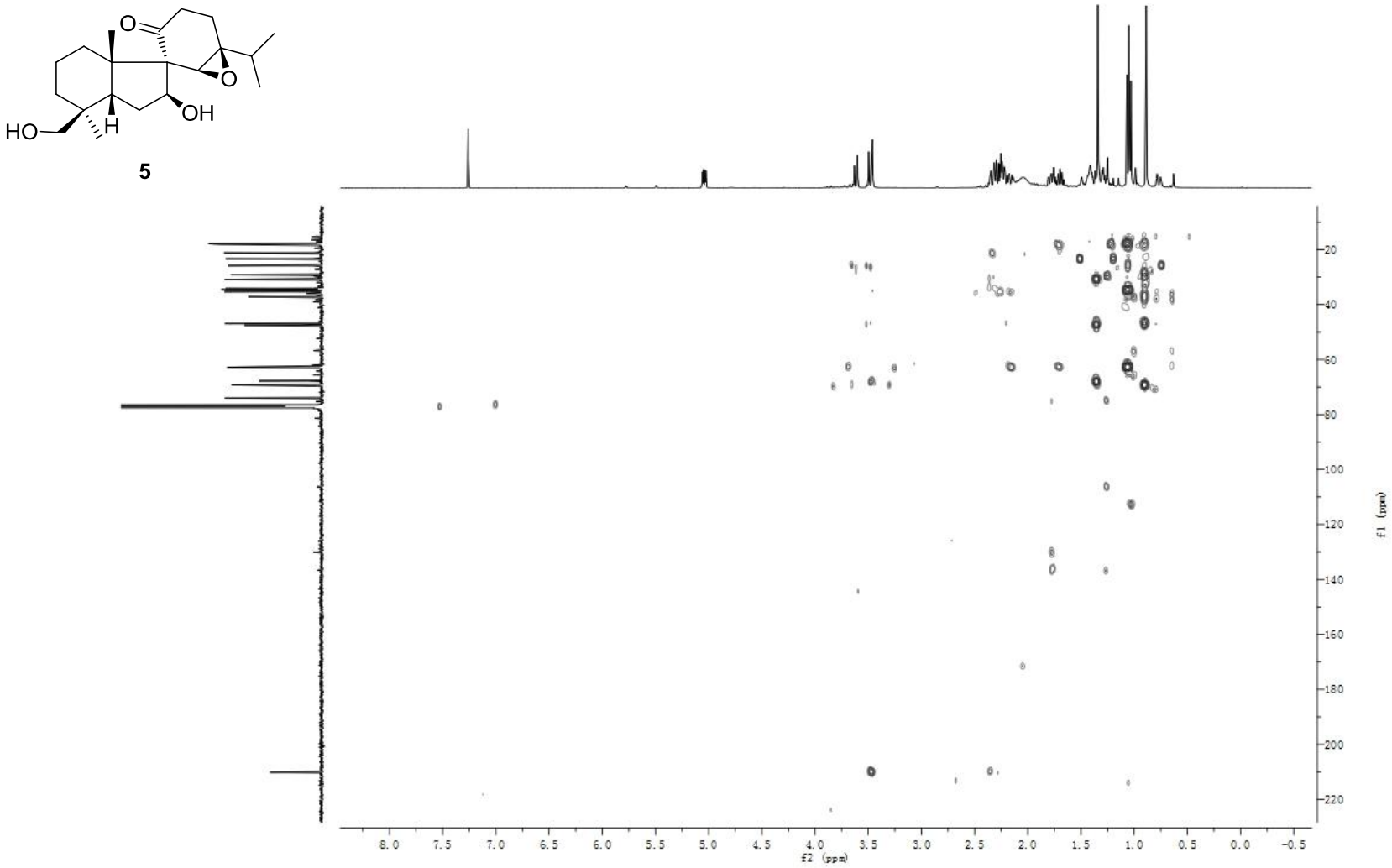
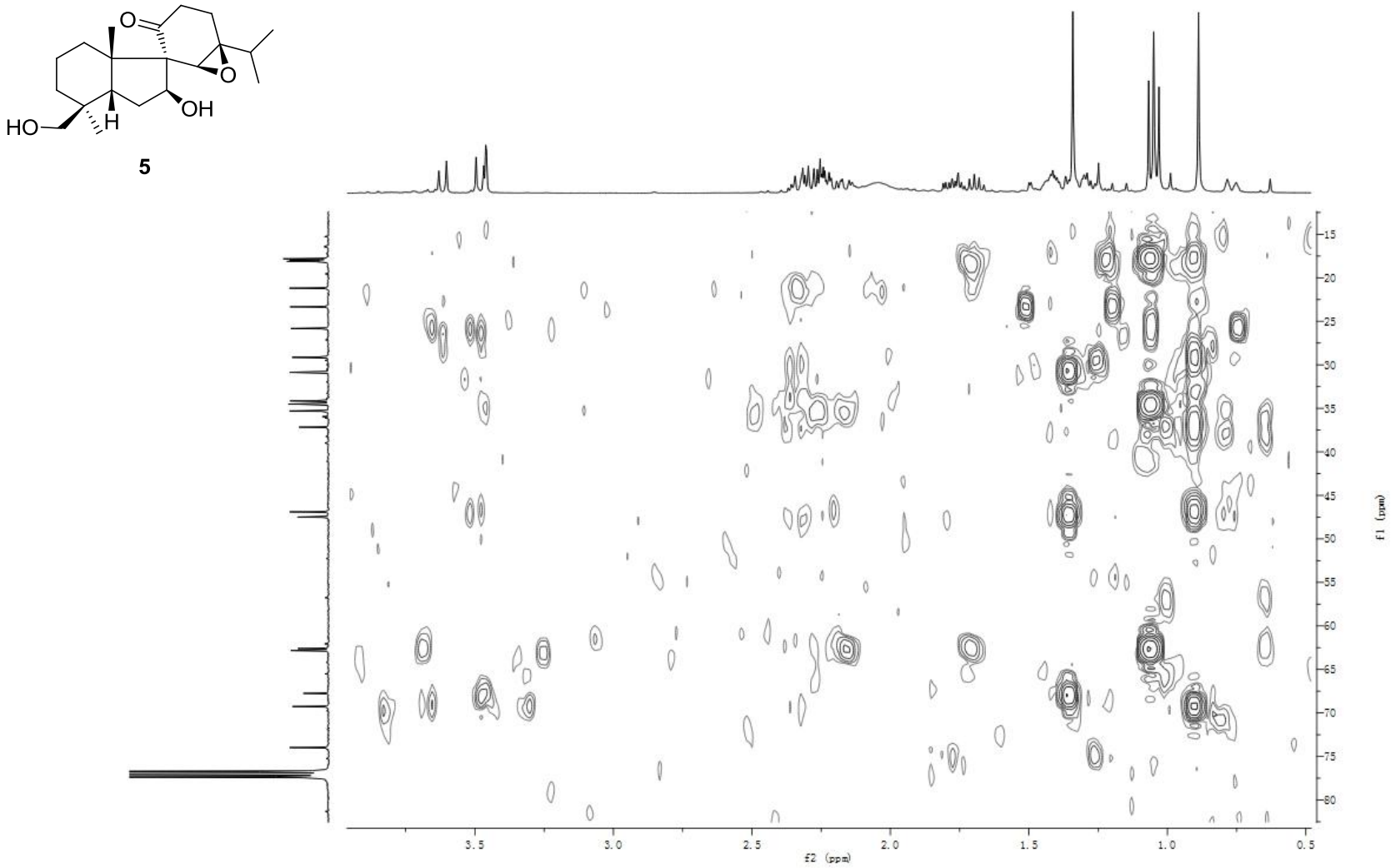


Figure S46. HMBC (400 MHz, $CDCl_3$) spectrum of **5**-expansion



5

Figure S47. NOESY (400 MHz, $CDCl_3$) spectrum of **5**

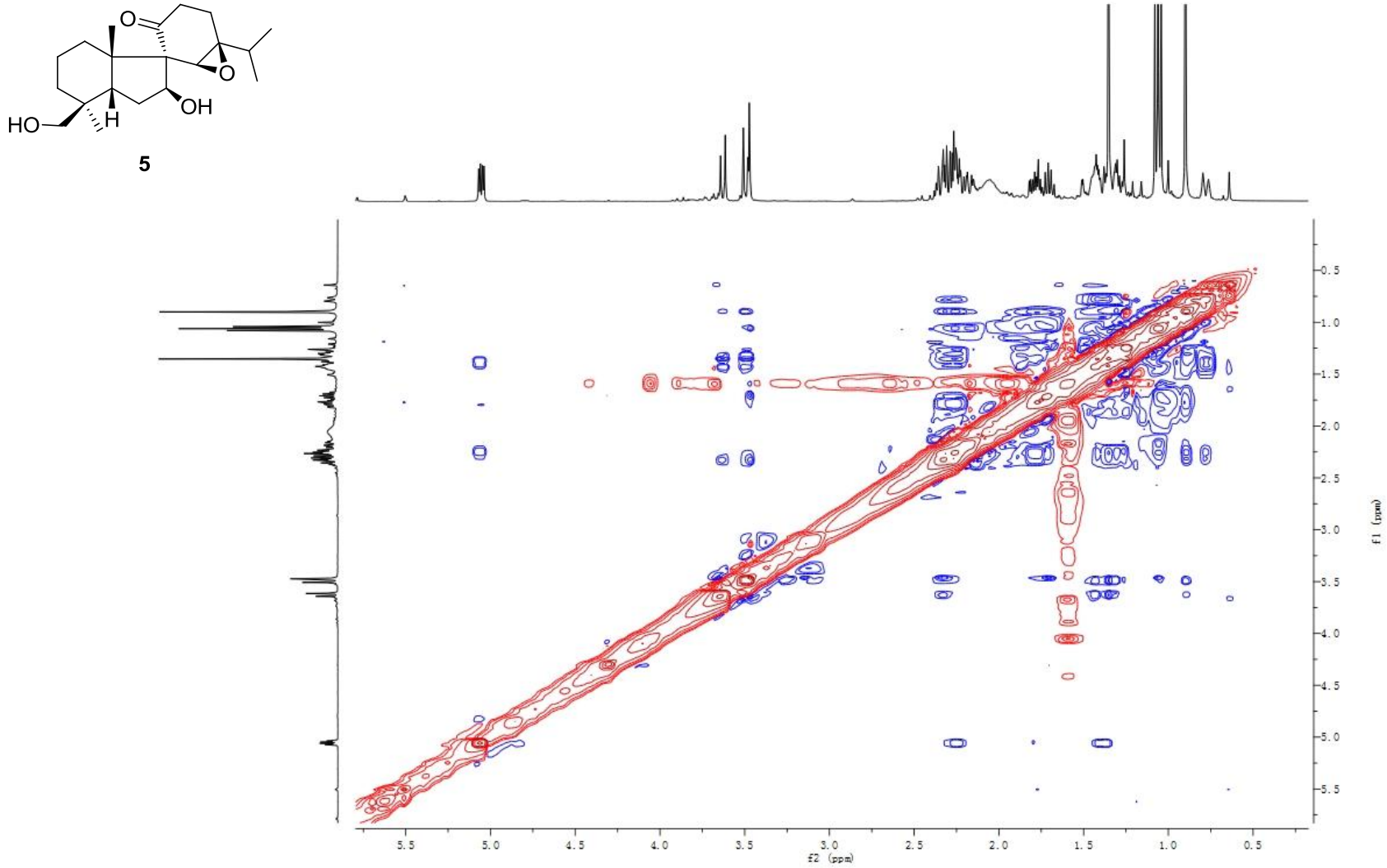
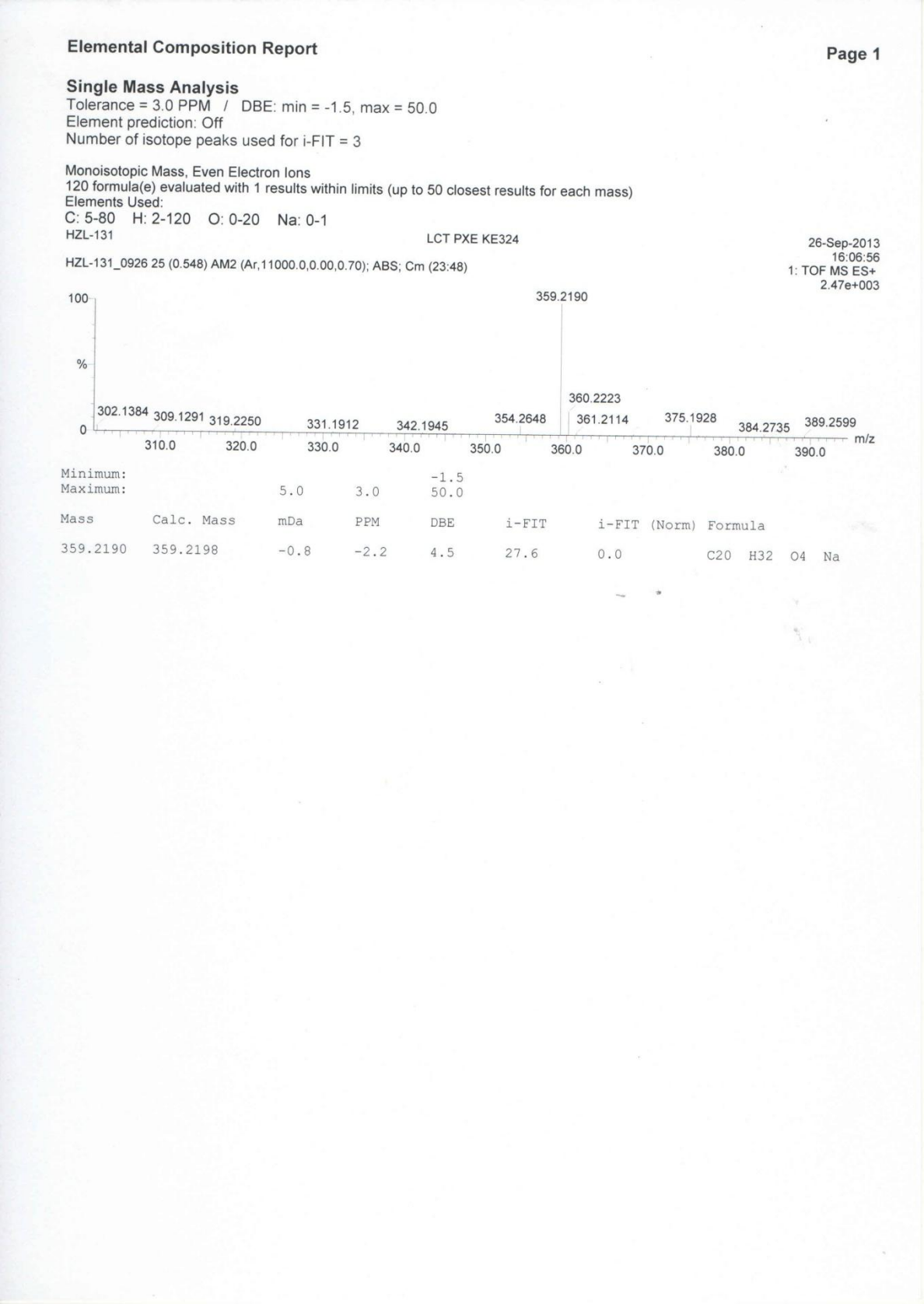


Figure S48. HRESIMS spectrum of **5**



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
120 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1

HZL-131 LCT PXE KE324 26-Sep-2013 16:06:56

HZL-131_0926 25 (0.548) AM2 (Ar,11000.0,0.00,0.70); ABS; Cm (23:48) 1: TOF MS ES+ 2.47e+003

Minimum:				-1.5			
Maximum:		5.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
359.2190	359.2198	-0.8	-2.2	4.5	27.6	0.0	C20 H32 O4 Na

Figure S49. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **5a**

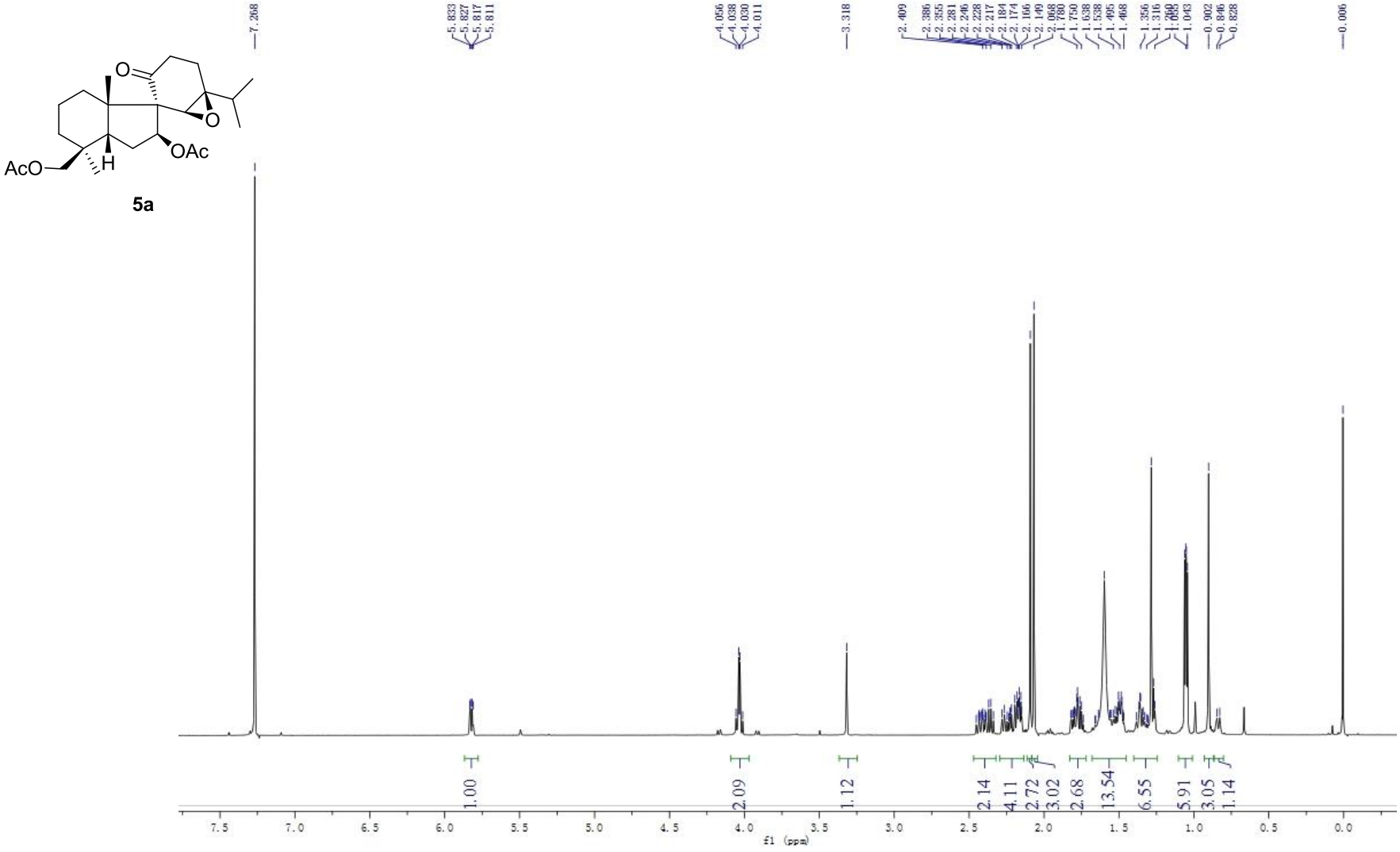


Figure S50. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **5a**

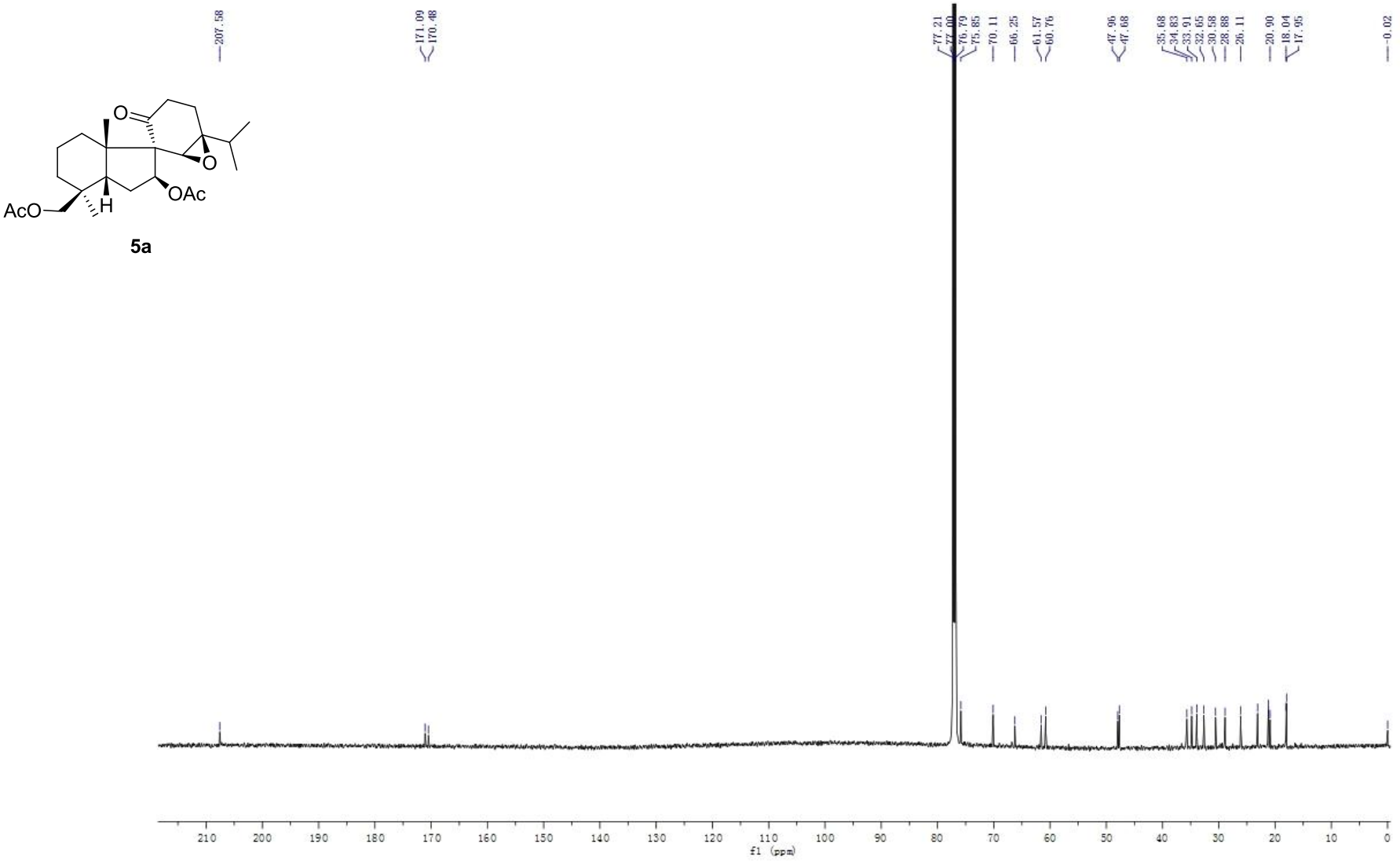


Figure S51. ^{1}H-^{1}H COSY (600 MHz, $CDCl_3$) spectrum of **5a**

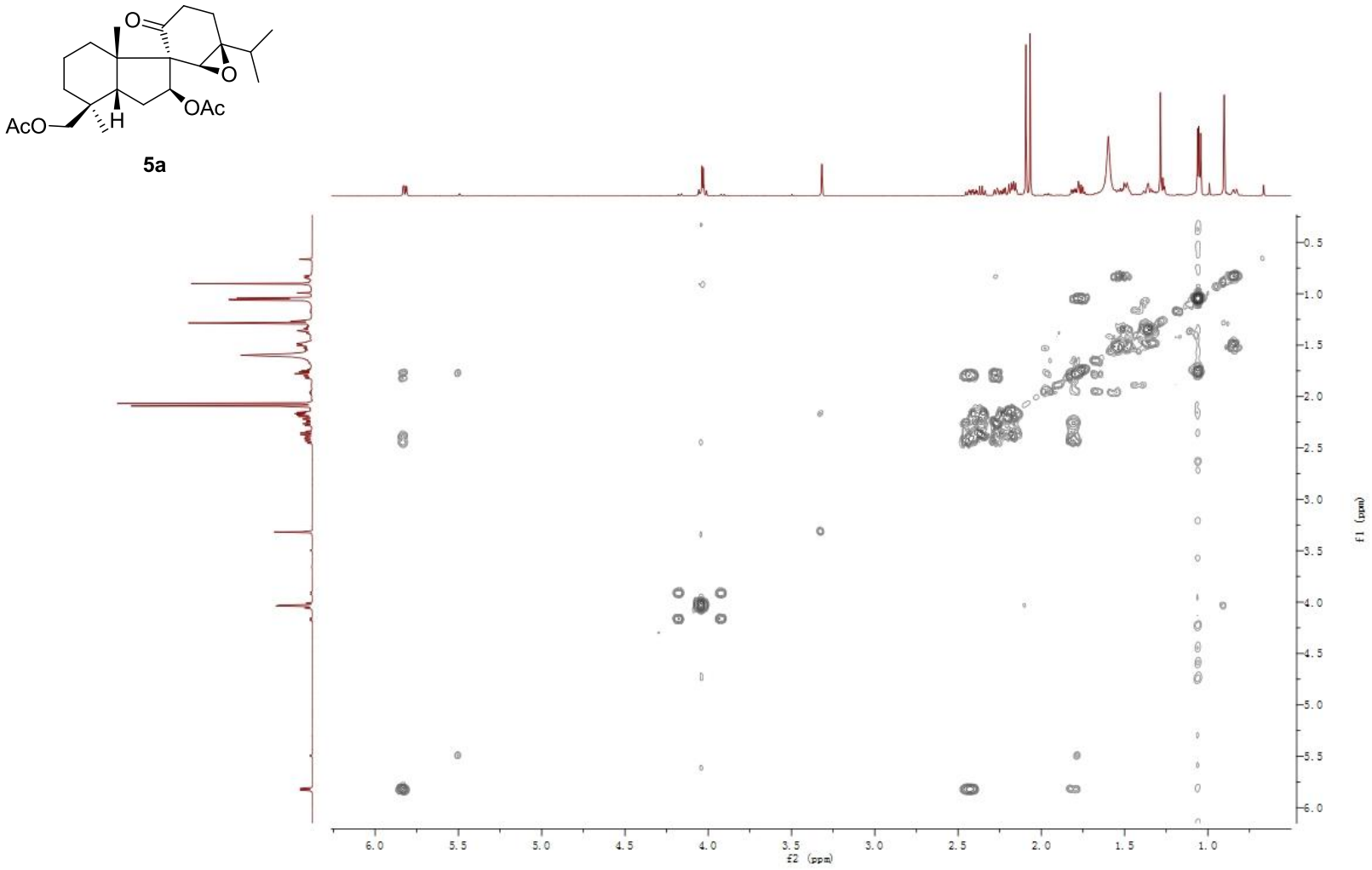
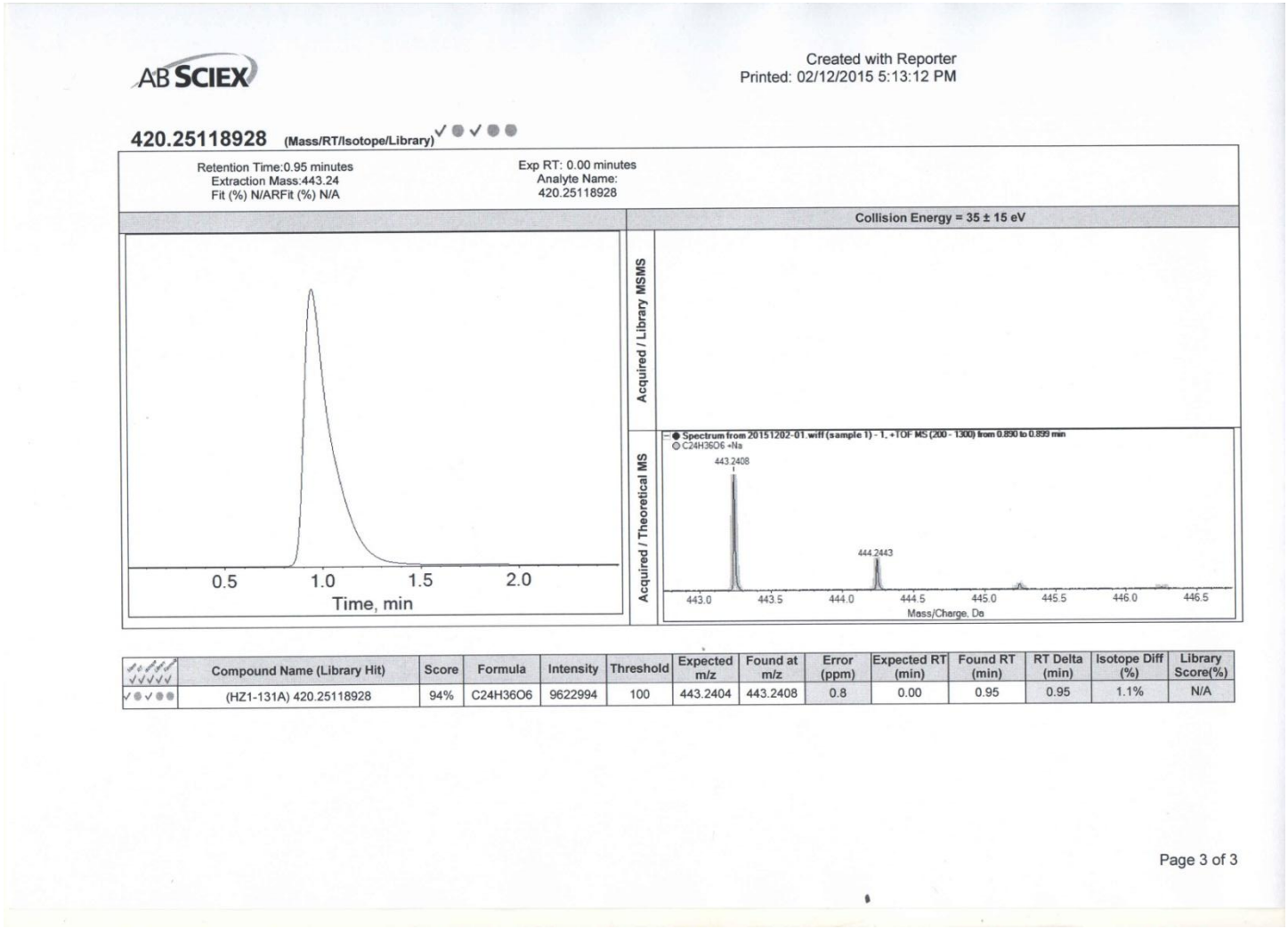


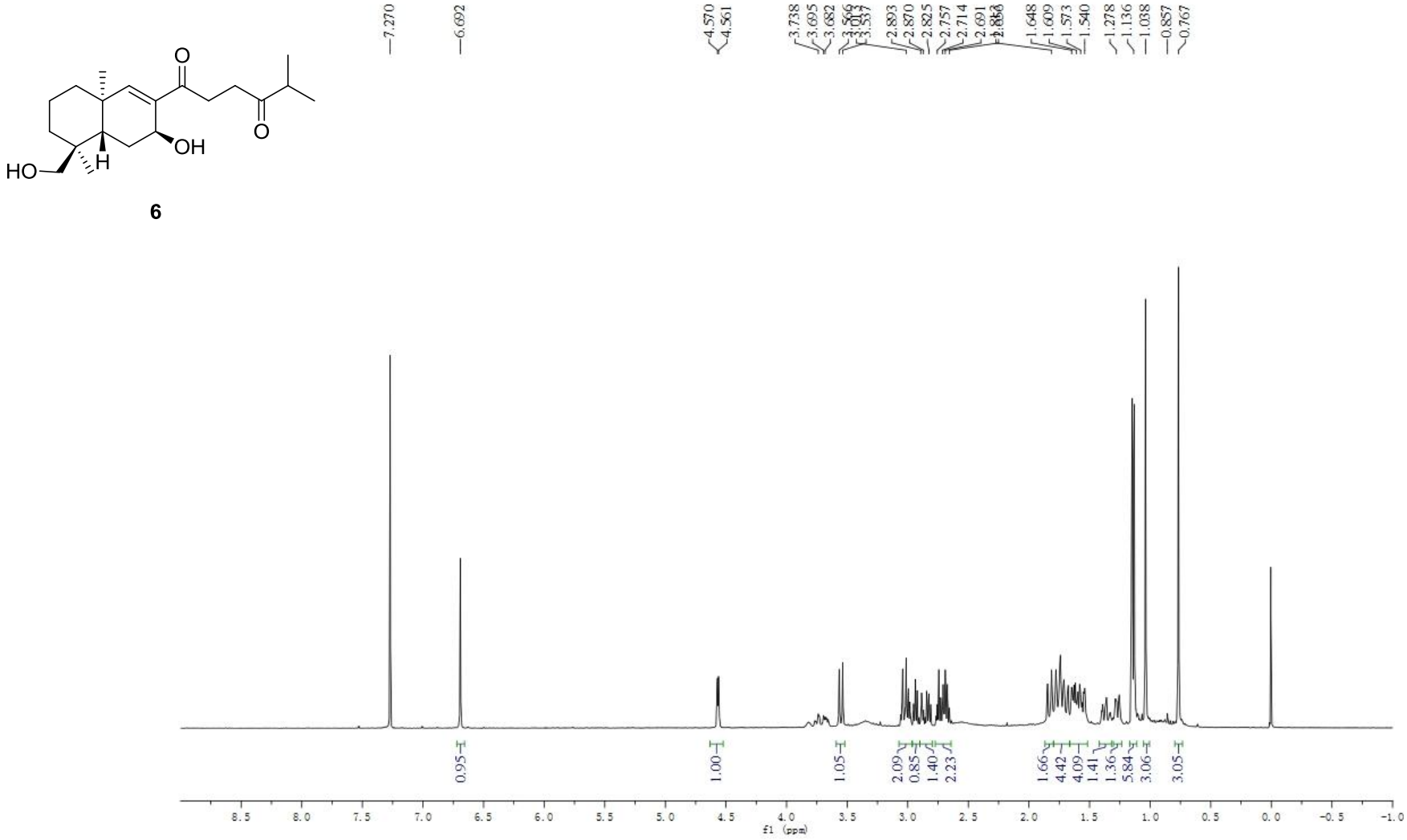
Figure S52. HRESIMS spectrum of **5a**



Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
(HZ1-131A) 420.25118928	94%	C24H36O6	9622994	100	443.2404	443.2408	0.8	0.00	0.95	0.95	1.1%	N/A

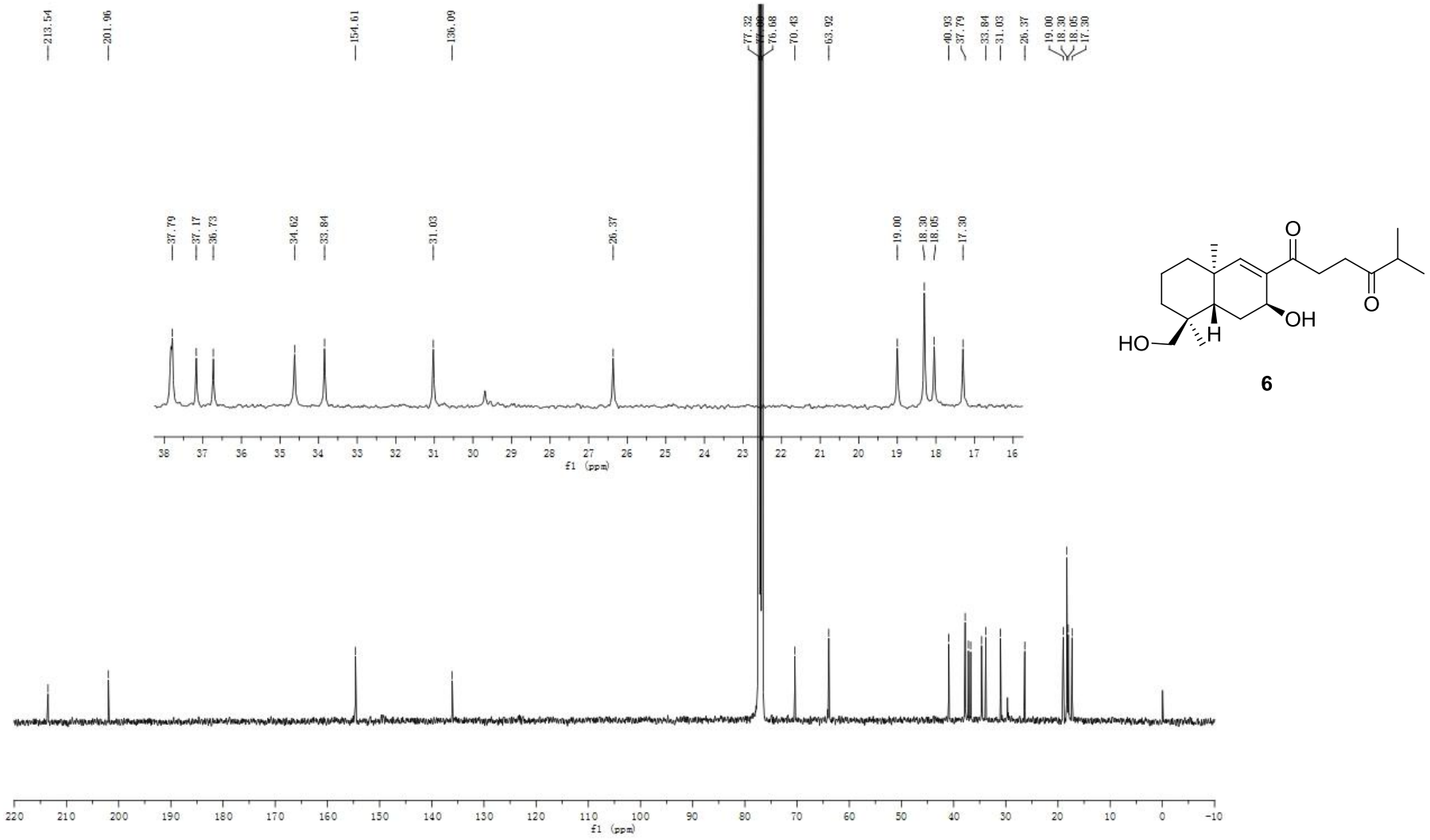
Page 3 of 3

Figure S53. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6**



6

Figure S54. ^{13}C NMR (400 MHz, $CDCl_3$) spectrum of **6**



6

Figure S55. DEPT-135 (400 MHz, $CDCl_3$) spectrum of **6**

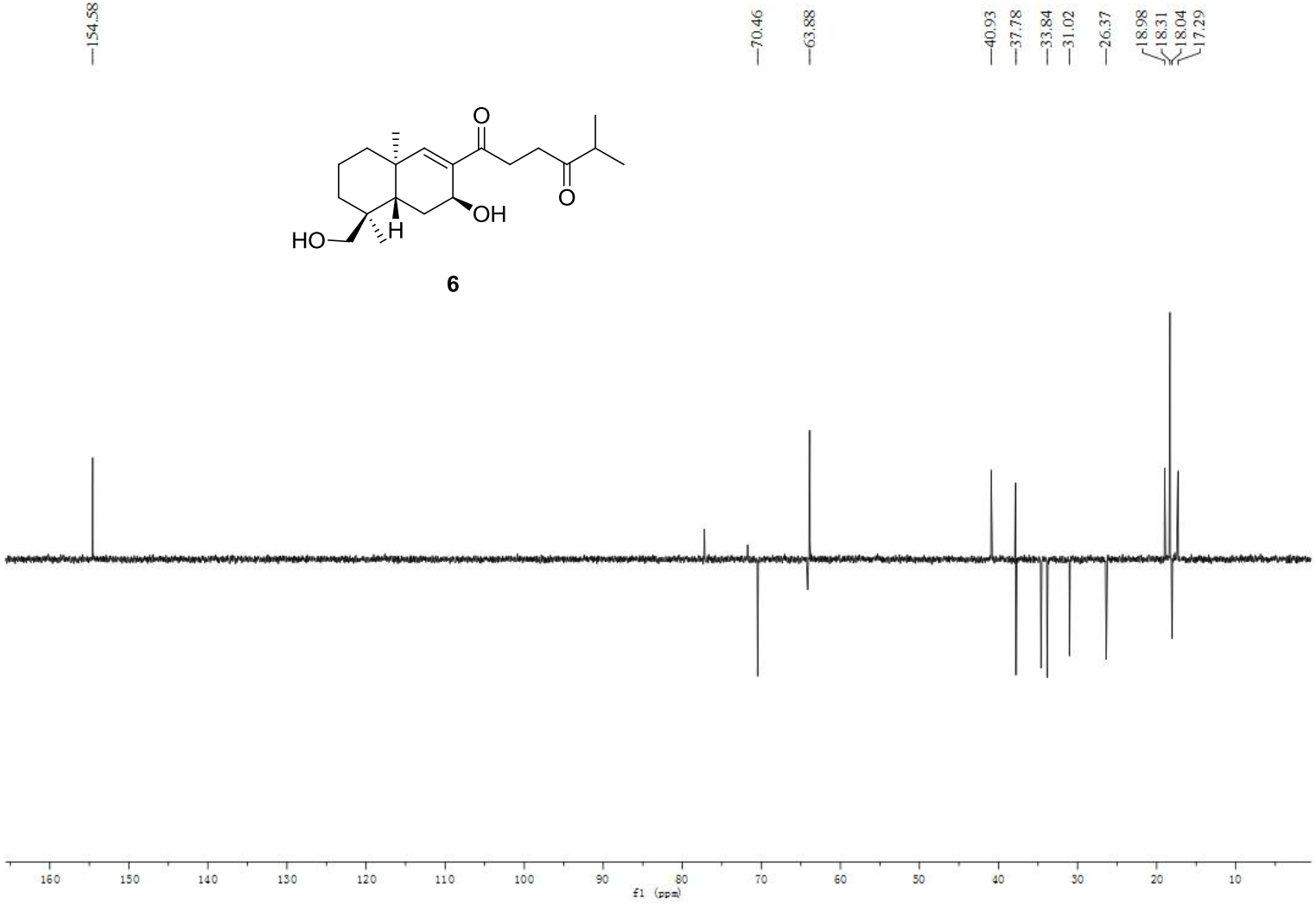
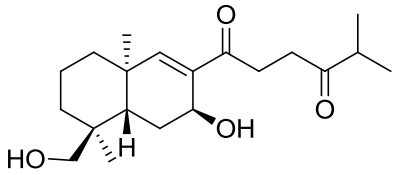


Figure S56. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of **6**



6

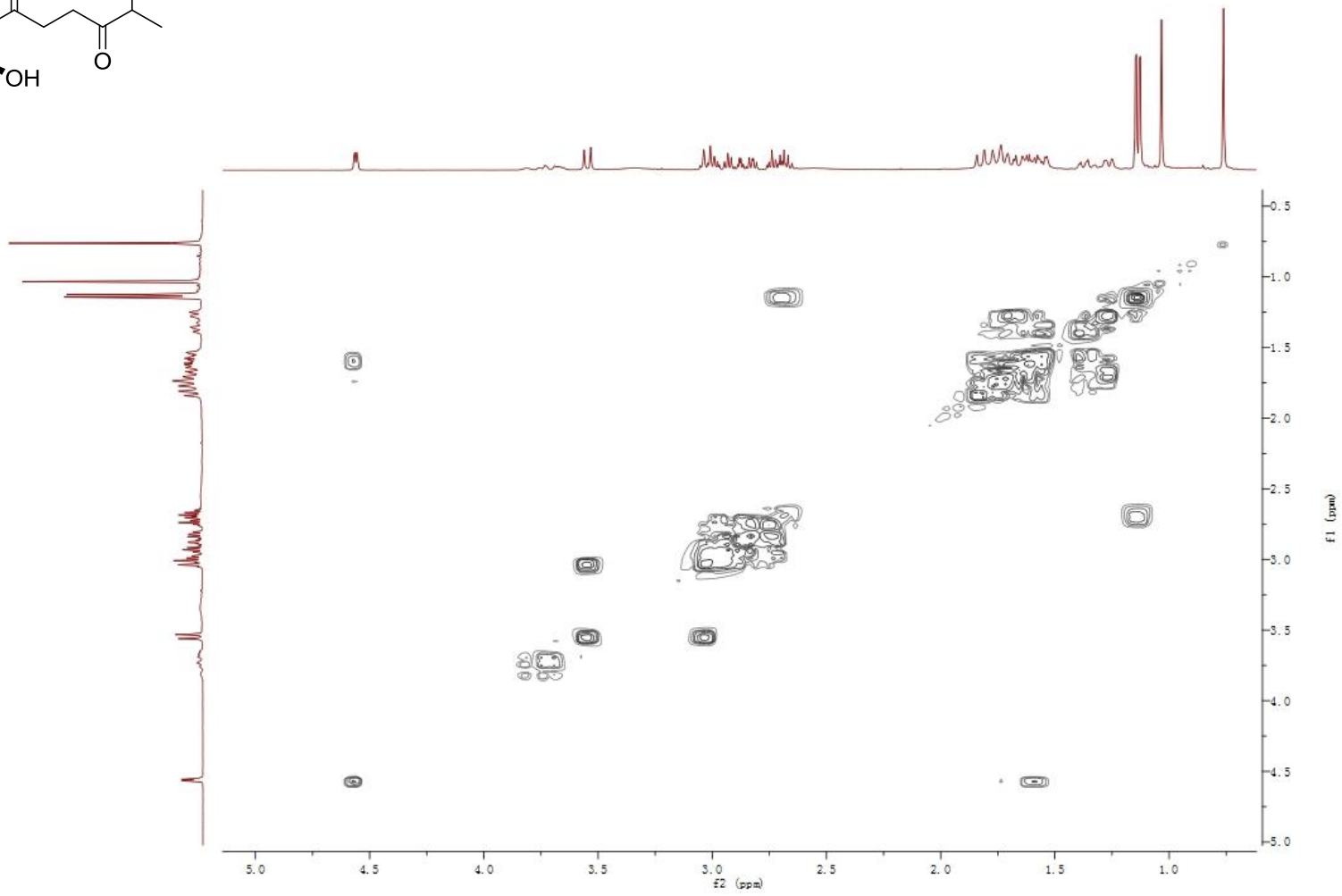
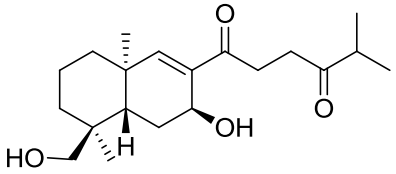


Figure S57. HSQC (400 MHz, $CDCl_3$) spectrum of **6**



6

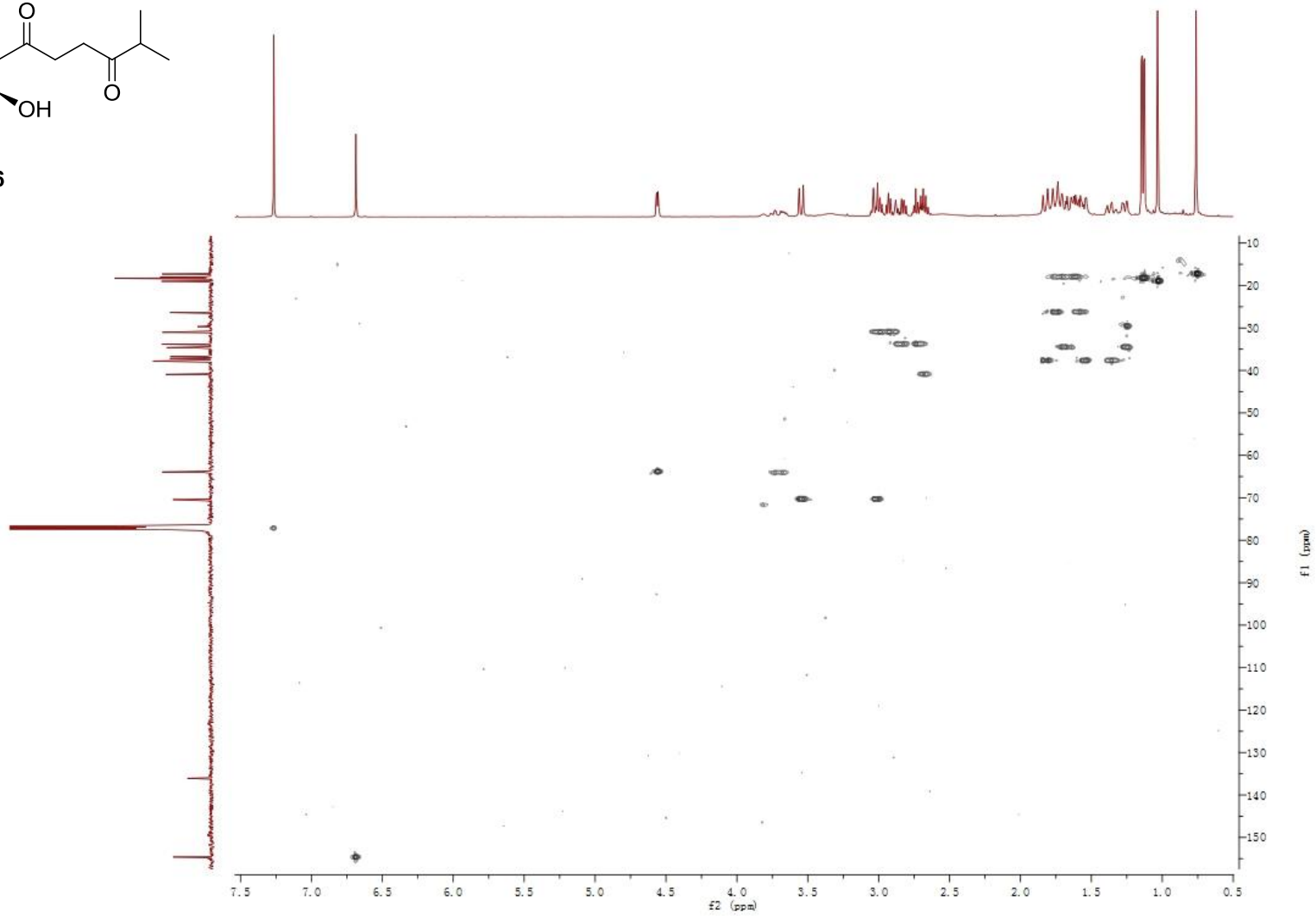


Figure S58. HMBC (400 MHz, $CDCl_3$) spectrum of **6**

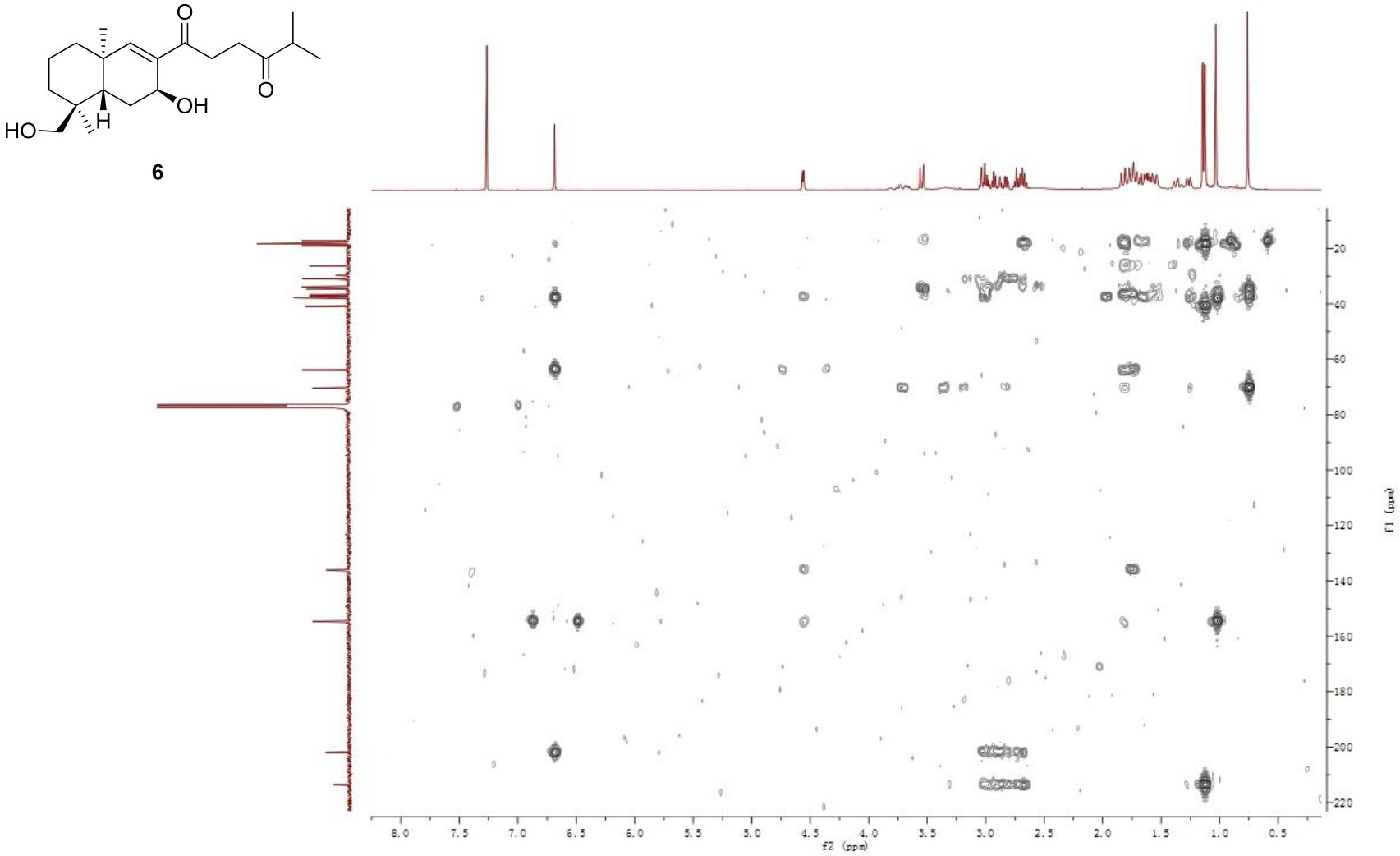
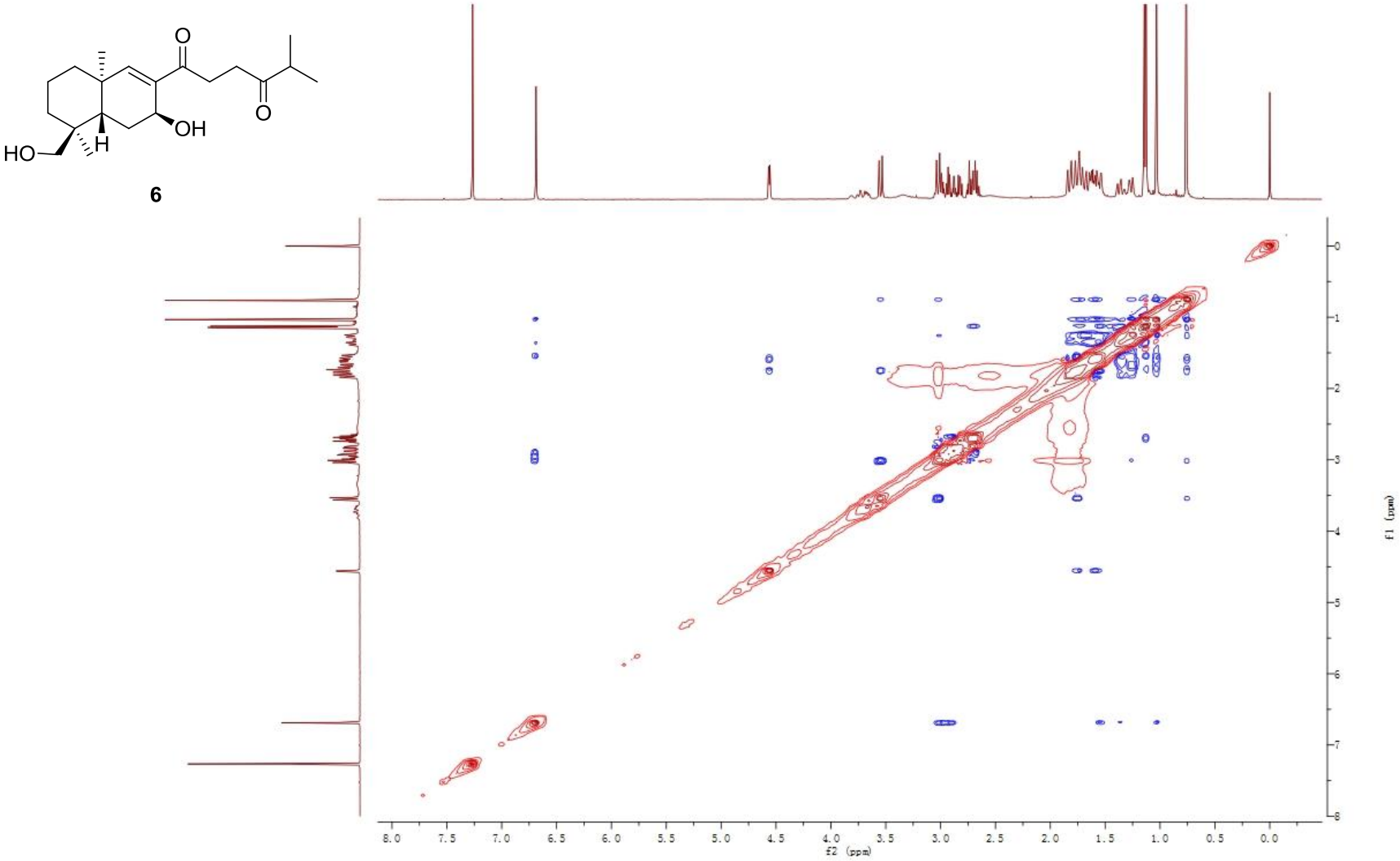
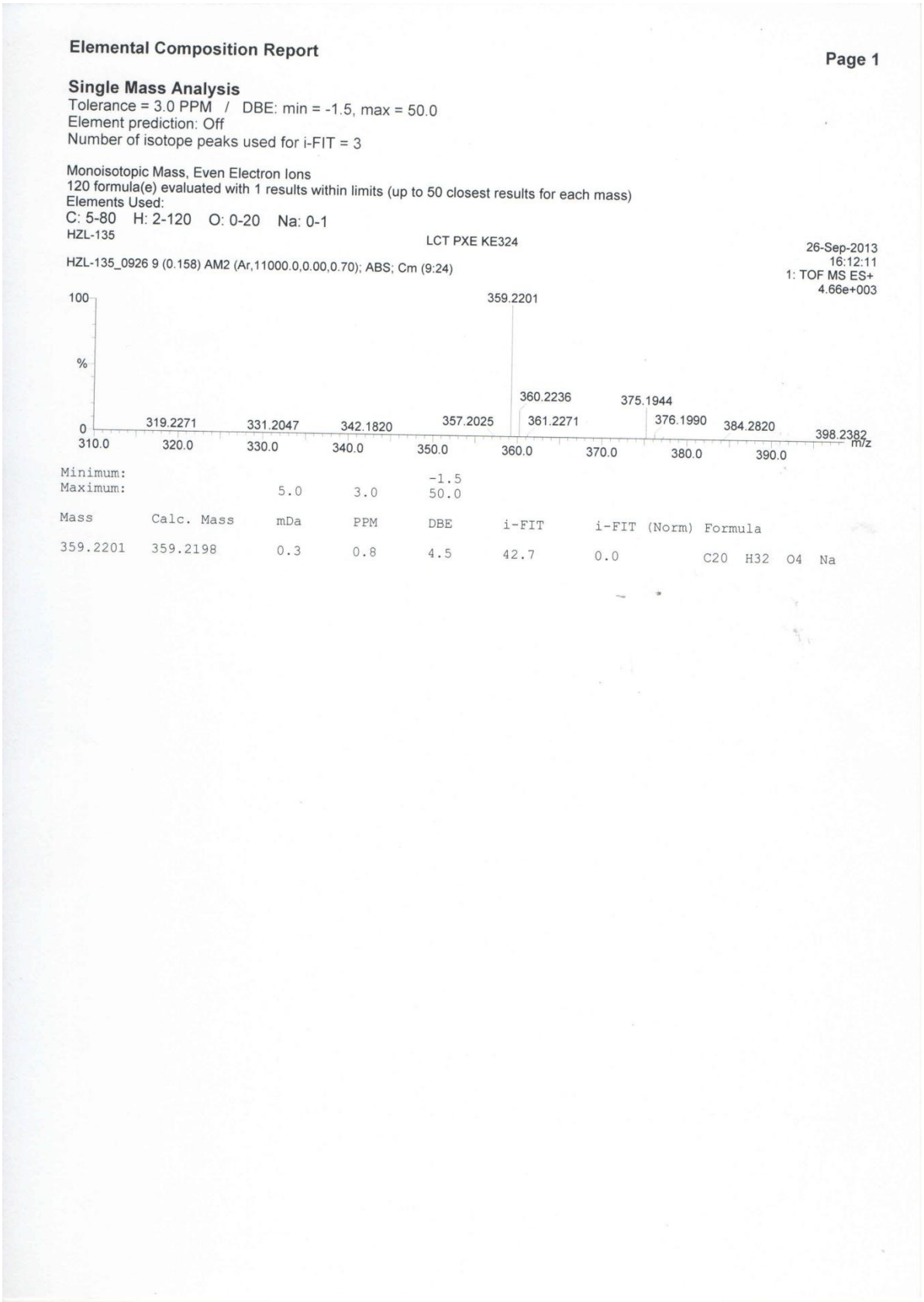


Figure S59. NOESY (400 MHz, $CDCl_3$) spectrum of **6**



6

Figure S60. HRESIMS spectrum of **6**



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
120 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1
HZL-135

LCT PXE KE324

HZL-135_0926 9 (0.158) AM2 (Ar,11000.0,0.00,0.70); ABS; Cm (9:24)

26-Sep-2013
16:12:11
1: TOF MS ES+
4.66e+003

Minimum:				-1.5			
Maximum:		5.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
359.2201	359.2198	0.3	0.8	4.5	42.7	0.0	C20 H32 O4 Na

Figure S61. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **7**

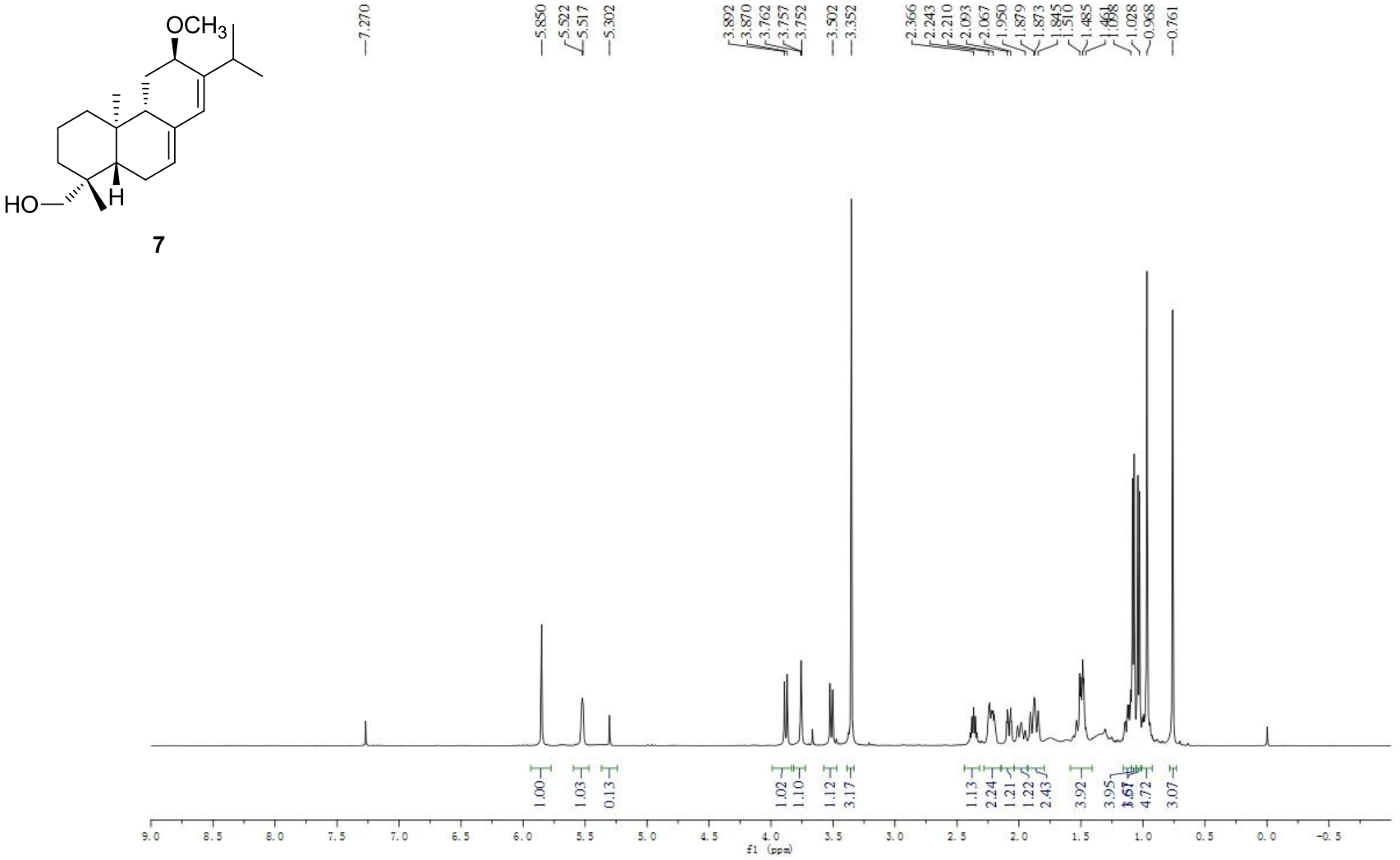


Figure S62. ^{13}C NMR (500 MHz, $CDCl_3$) spectrum of **7**

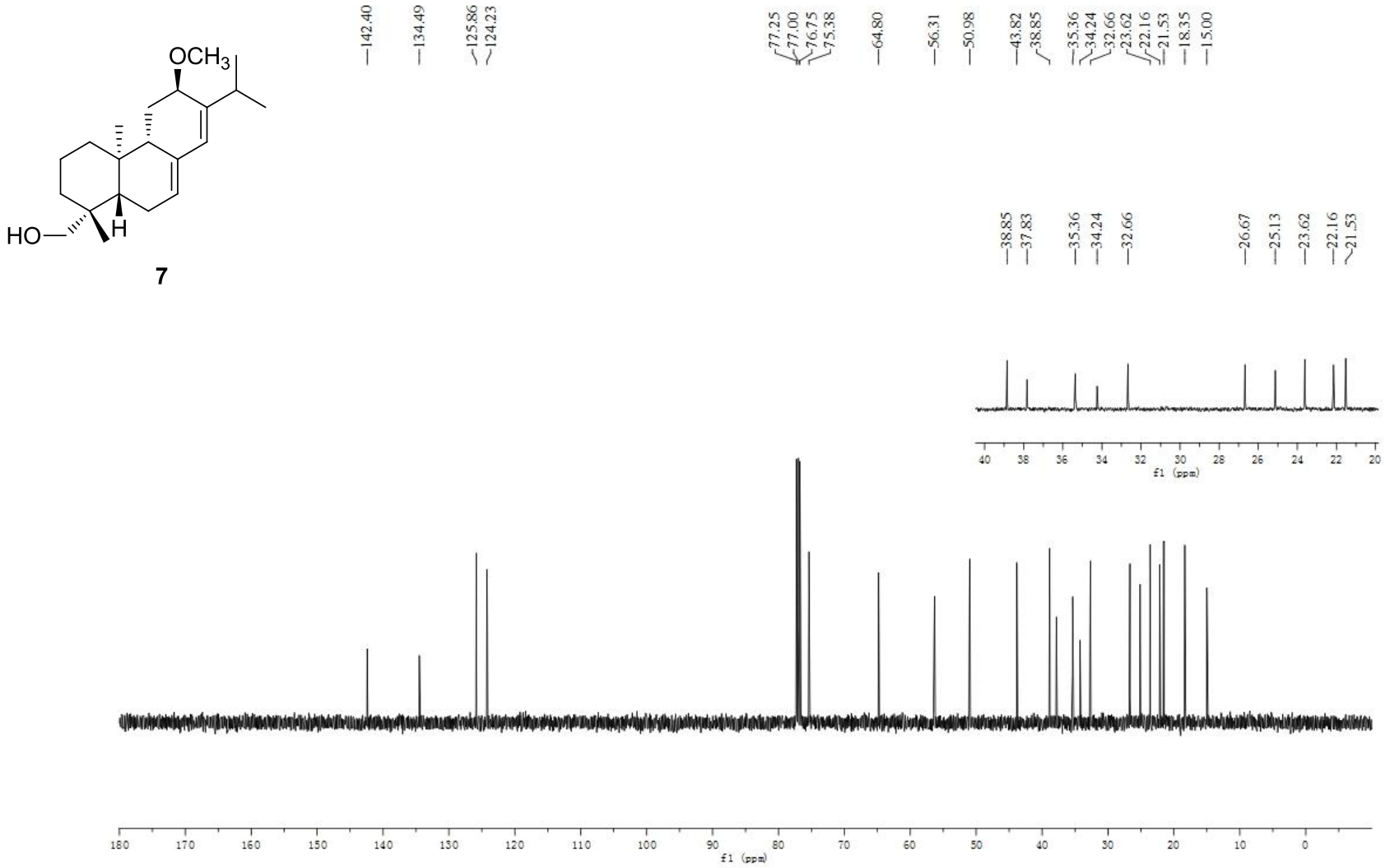


Figure S63. DEPT-135 (500 MHz, $CDCl_3$) spectrum of **7**

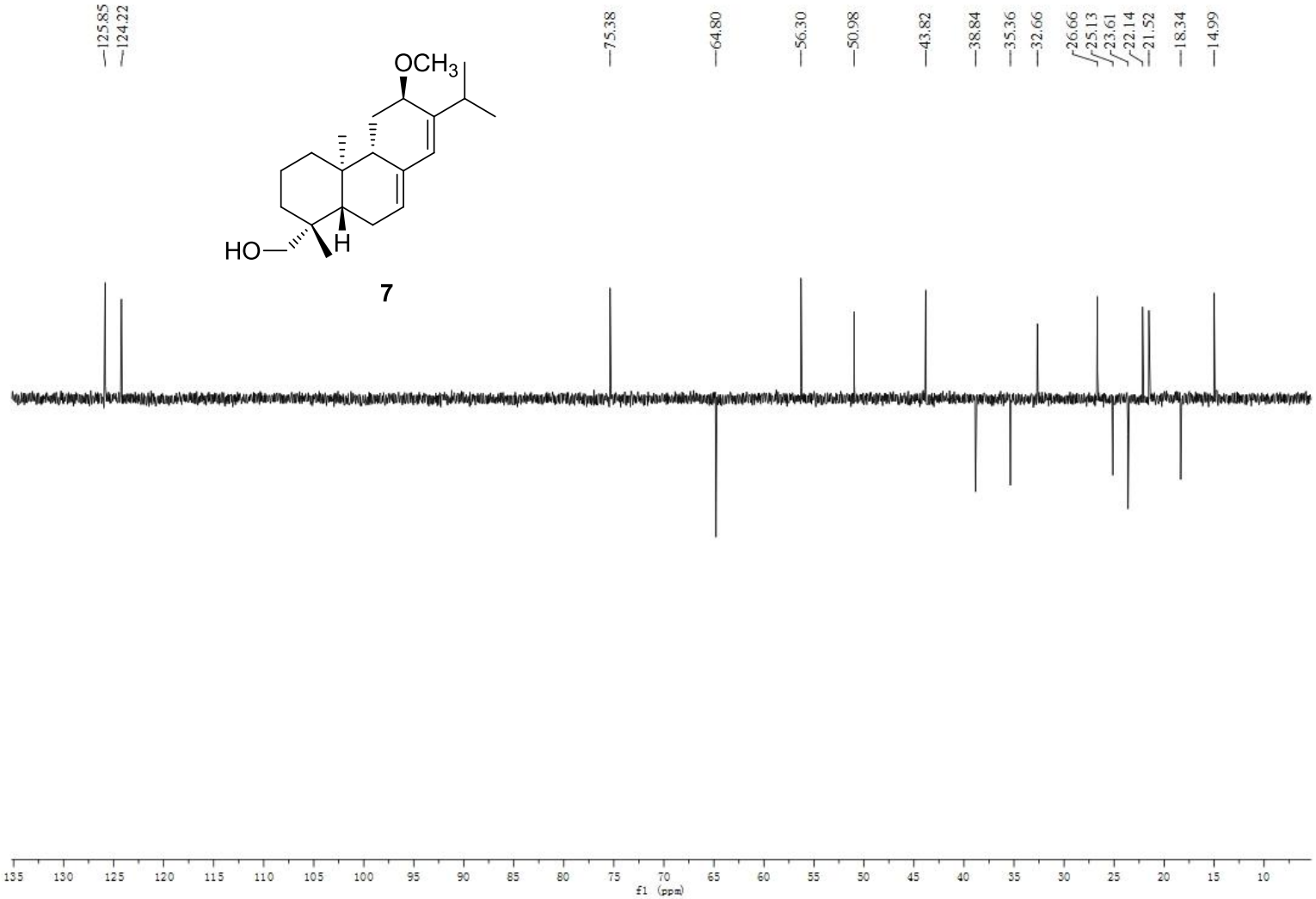


Figure S64. ^{1}H-^{1}H COSY (500 MHz, $CDCl_3$) spectrum of **7**

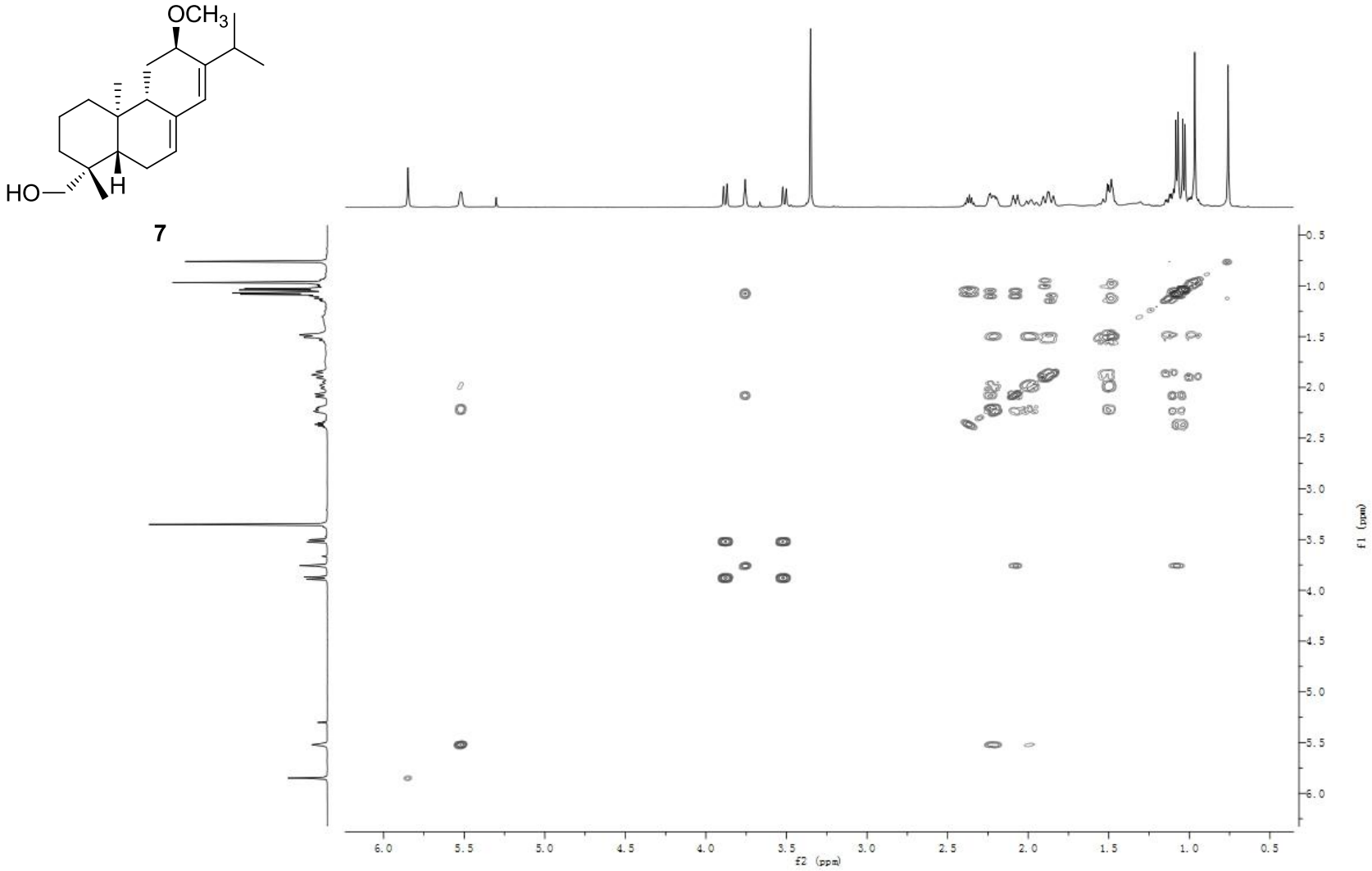


Figure S65. HMBC (500 MHz, $CDCl_3$) spectrum of **7**

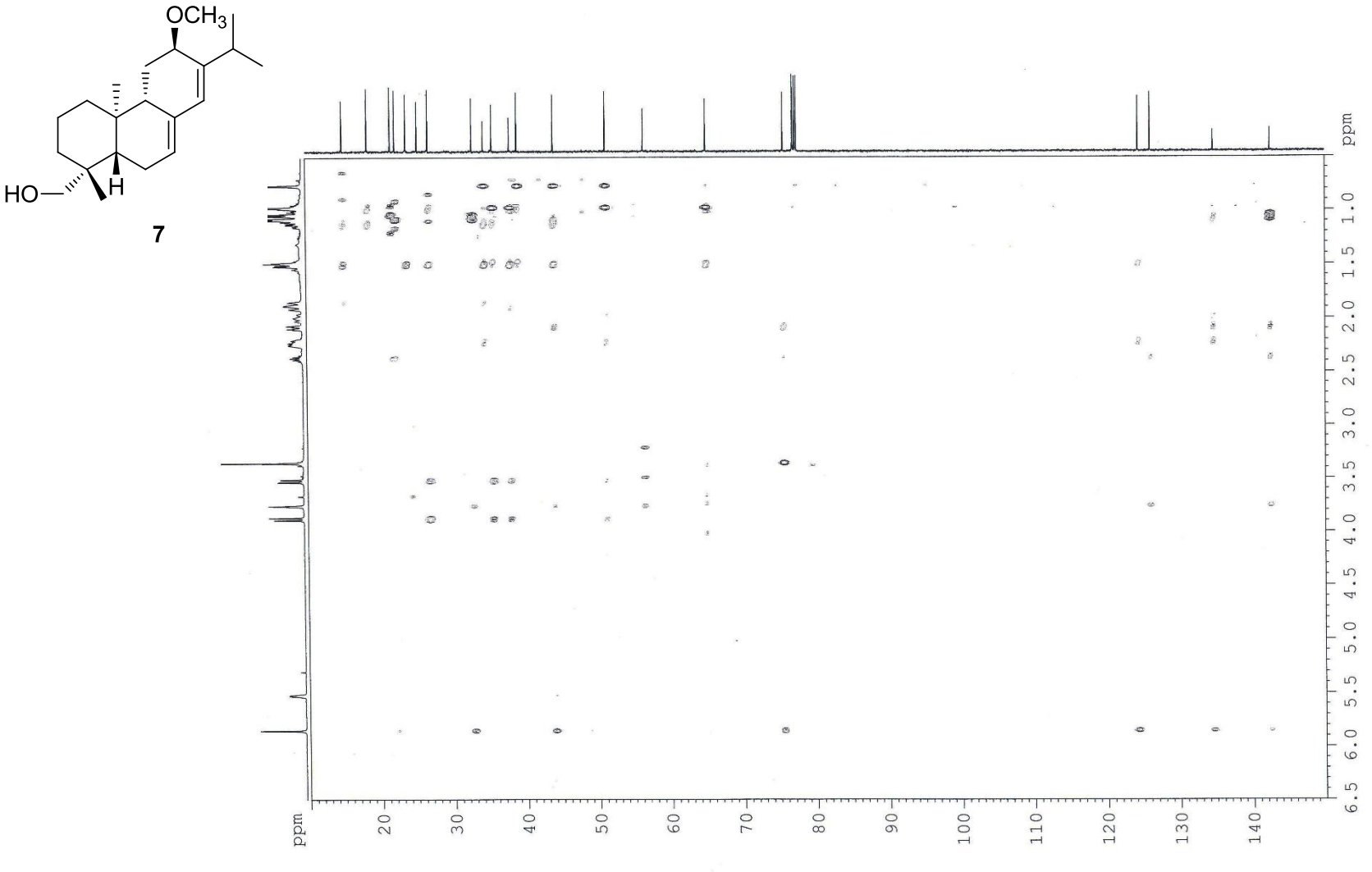


Figure S66. HMBC (500 MHz, $CDCl_3$) spectrum of **7**-expansion

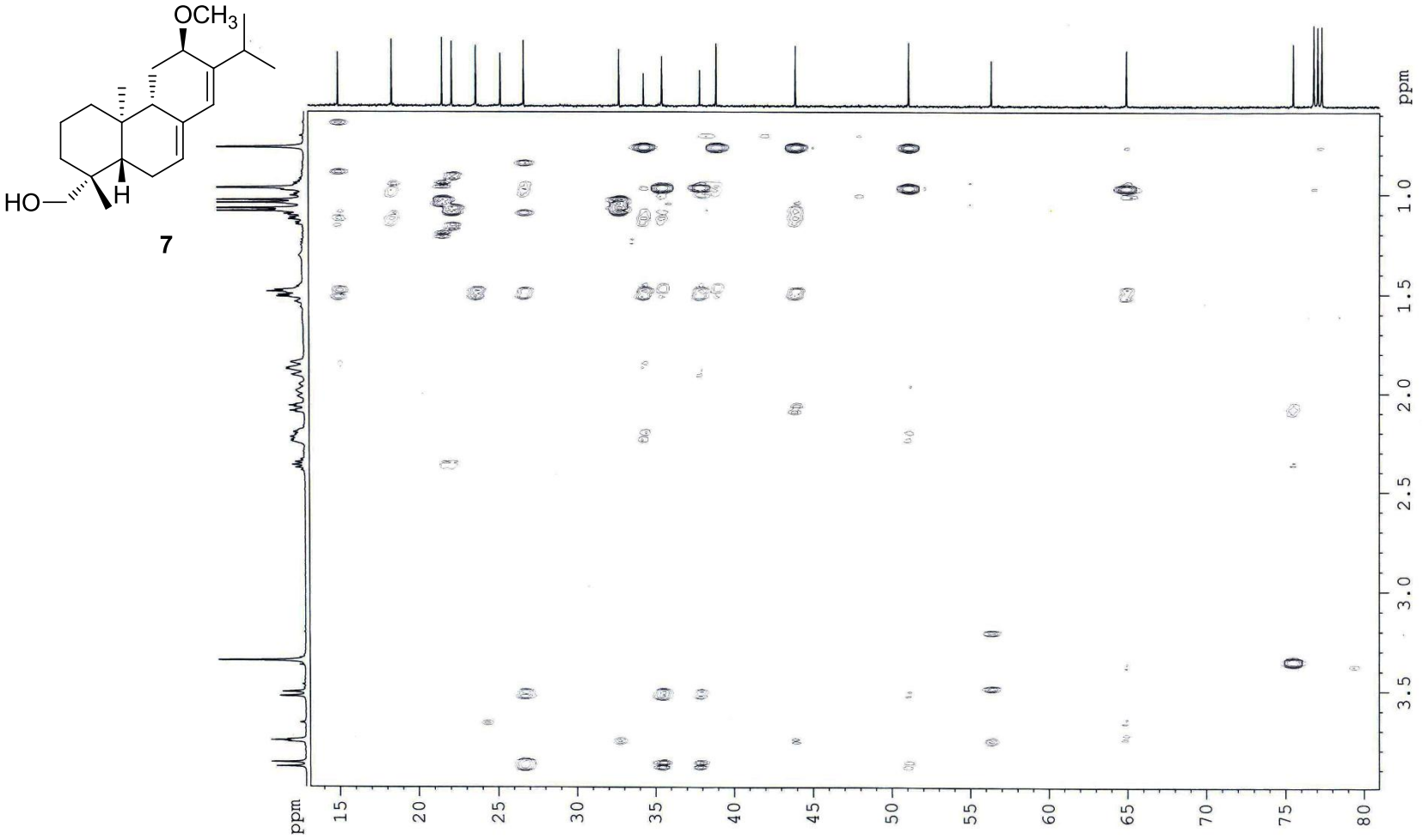


Figure S67. NOESY (500 MHz, $CDCl_3$) spectrum of **7**

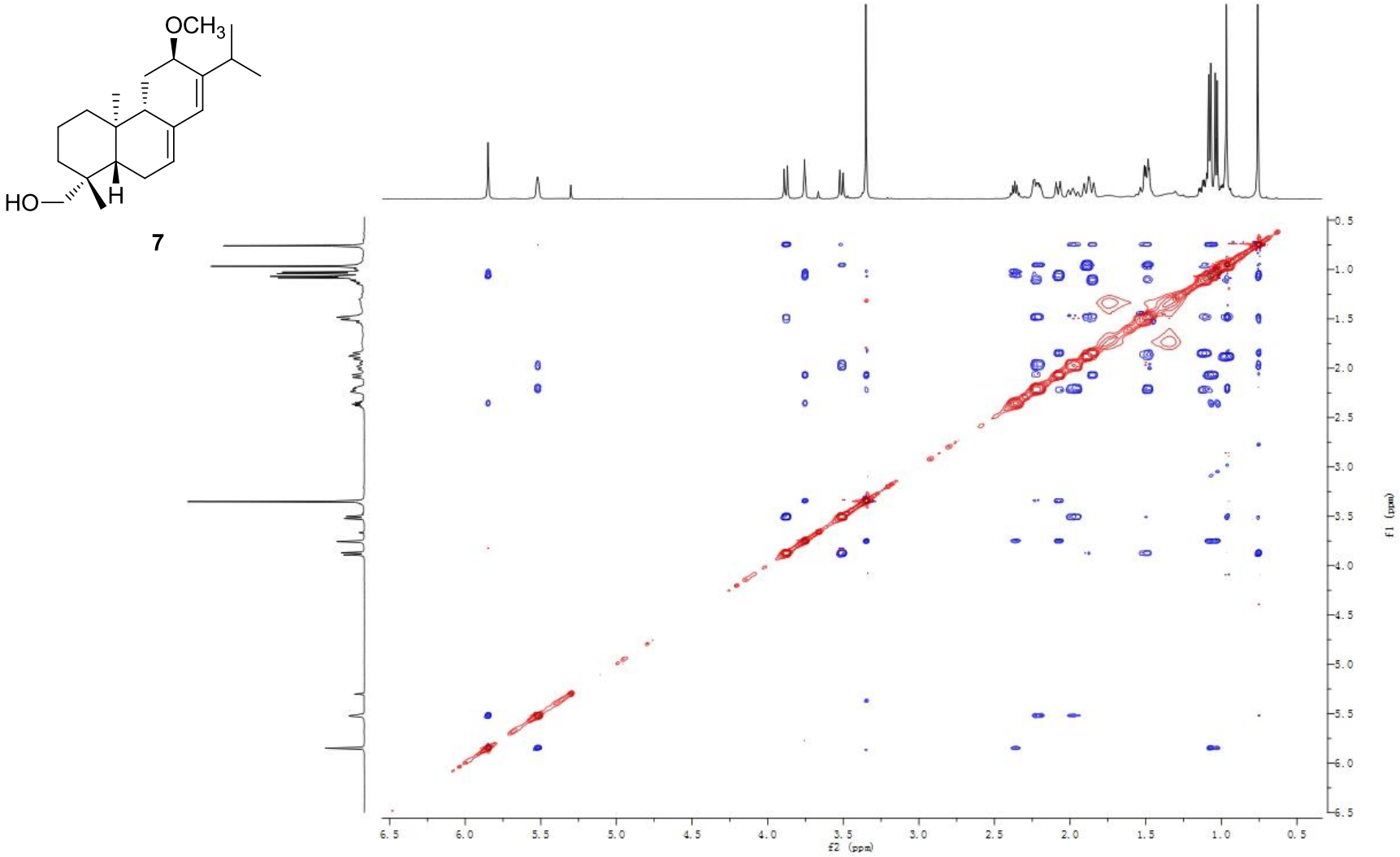


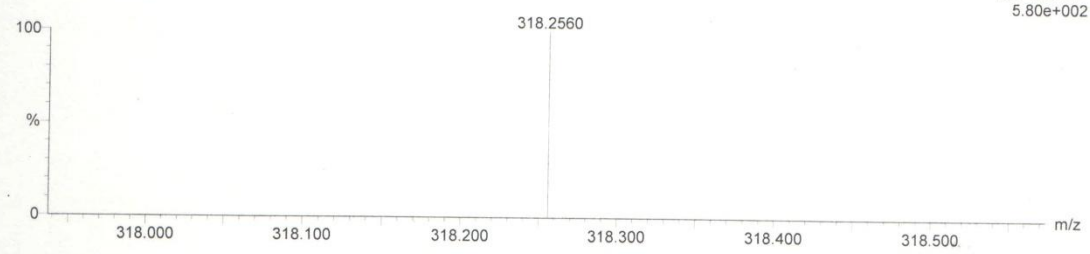
Figure S68. HREIMS spectrum of **7**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-21 H: 0-35 O: 0-2
HZL-125
20120709008 222 (3.700)

TOF MS EI+
5.80e+002



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
318.2560	318.2559	0.1	0.3	5.0	5546302.5	C21 H34 O2

Figure S69. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8**

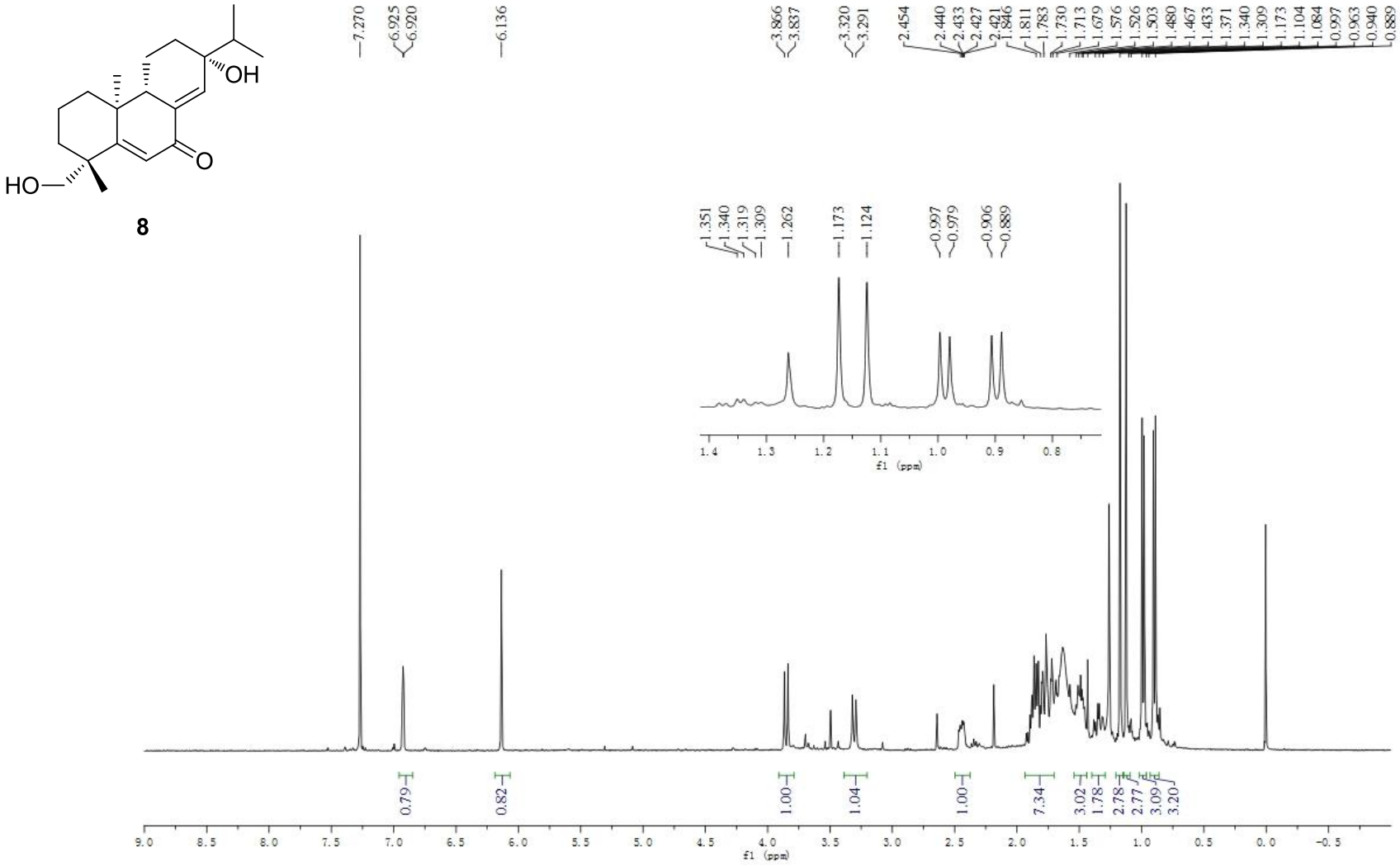
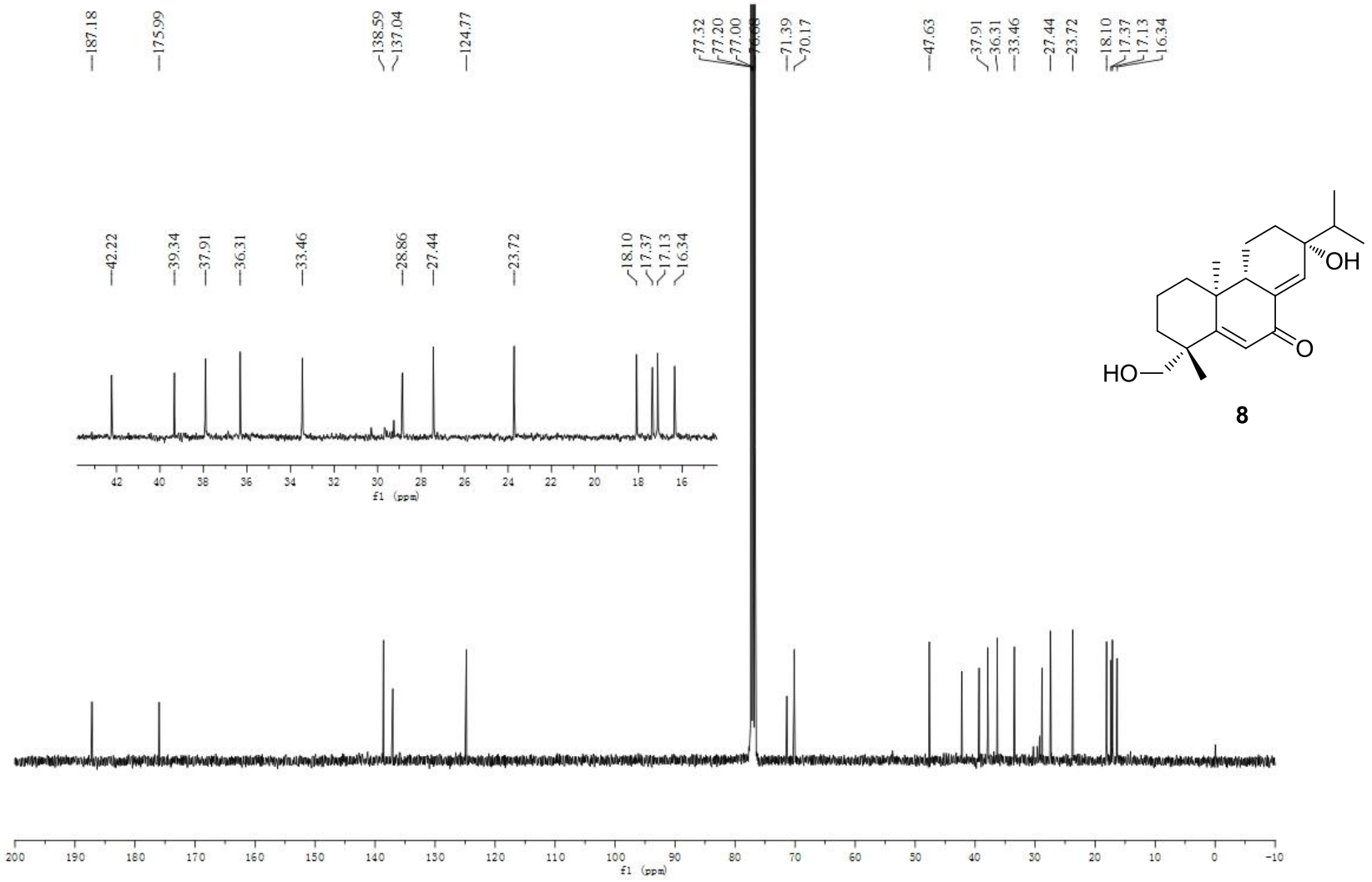


Figure S70. ^{13}C NMR (400 MHz, $CDCl_3$) spectrum of **8**



8

Figure S71. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of **8**

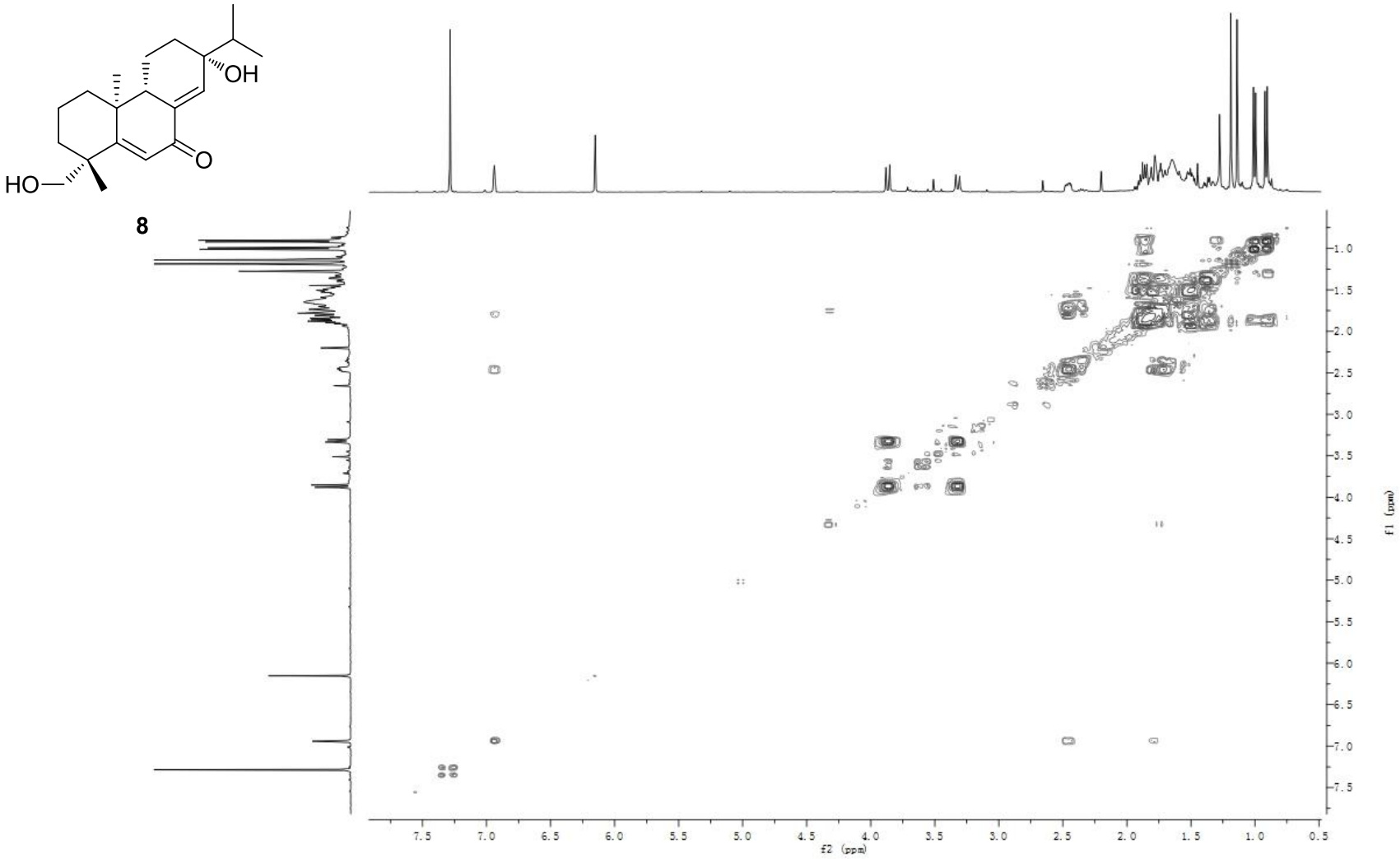


Figure S72. HSQC (400 MHz, $CDCl_3$) spectrum of **8**

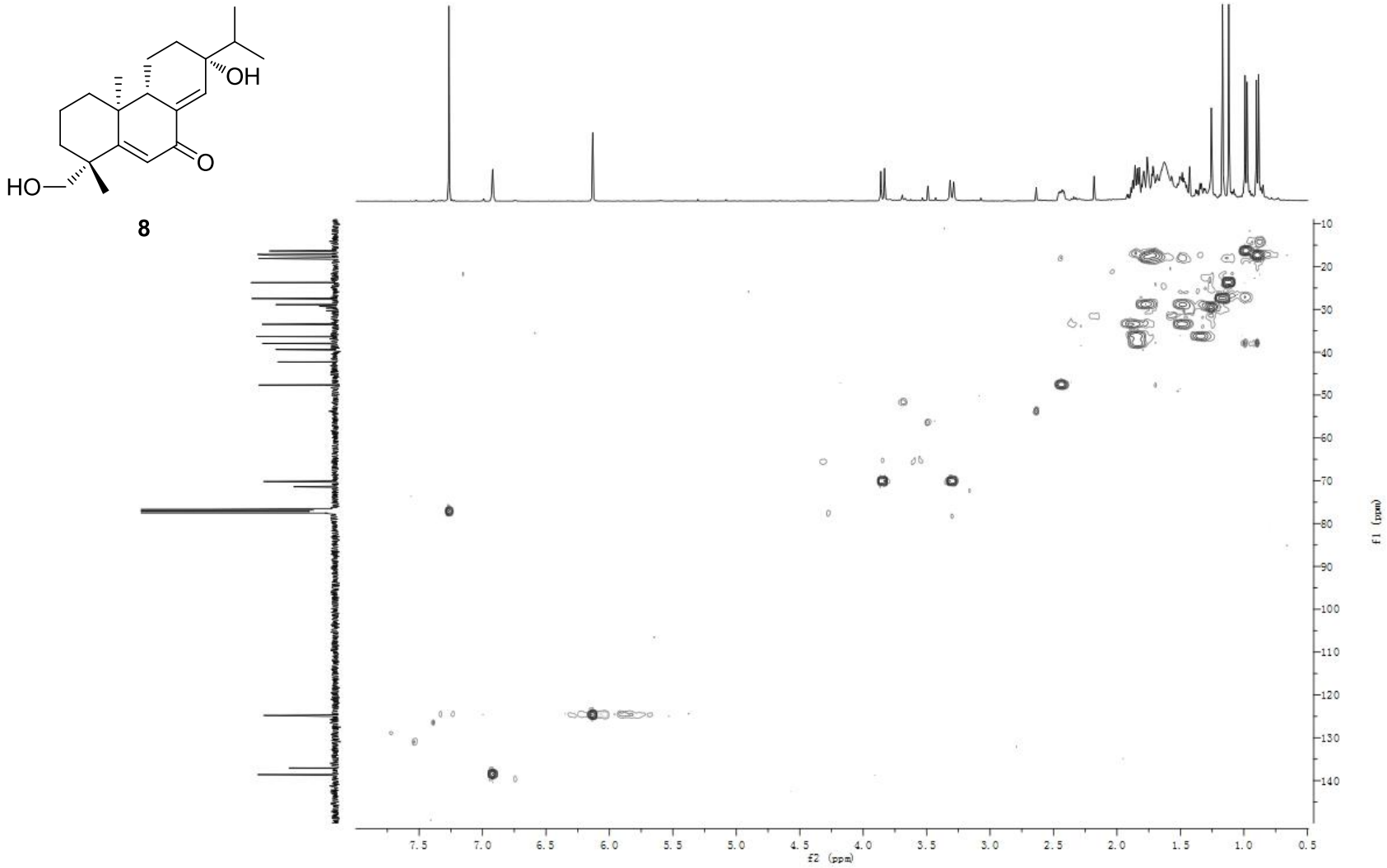


Figure S73. HMBC (400 MHz, $CDCl_3$) spectrum of **8**

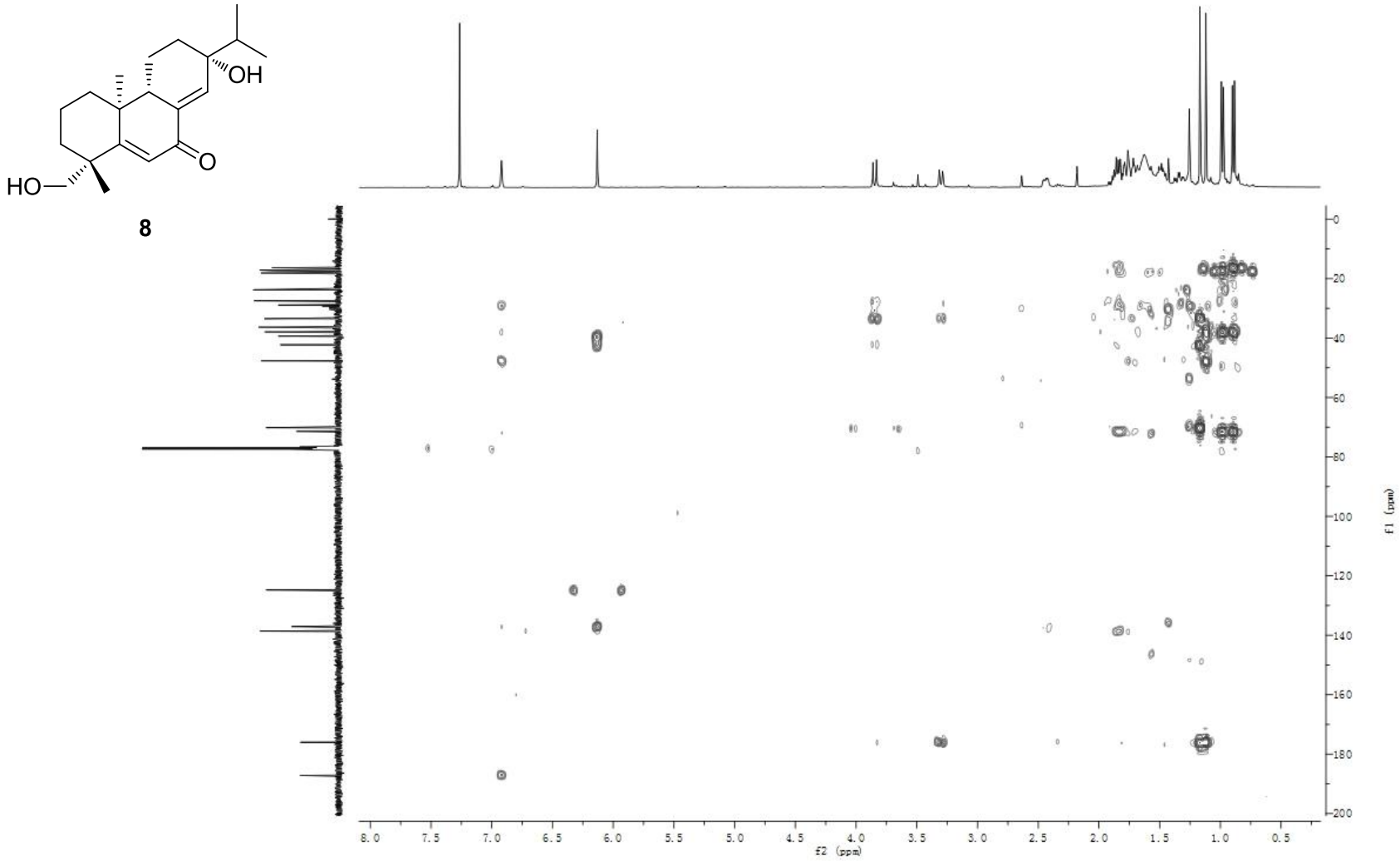


Figure S74. HMBC (500 MHz, $CDCl_3$) spectrum of **8**-expansion

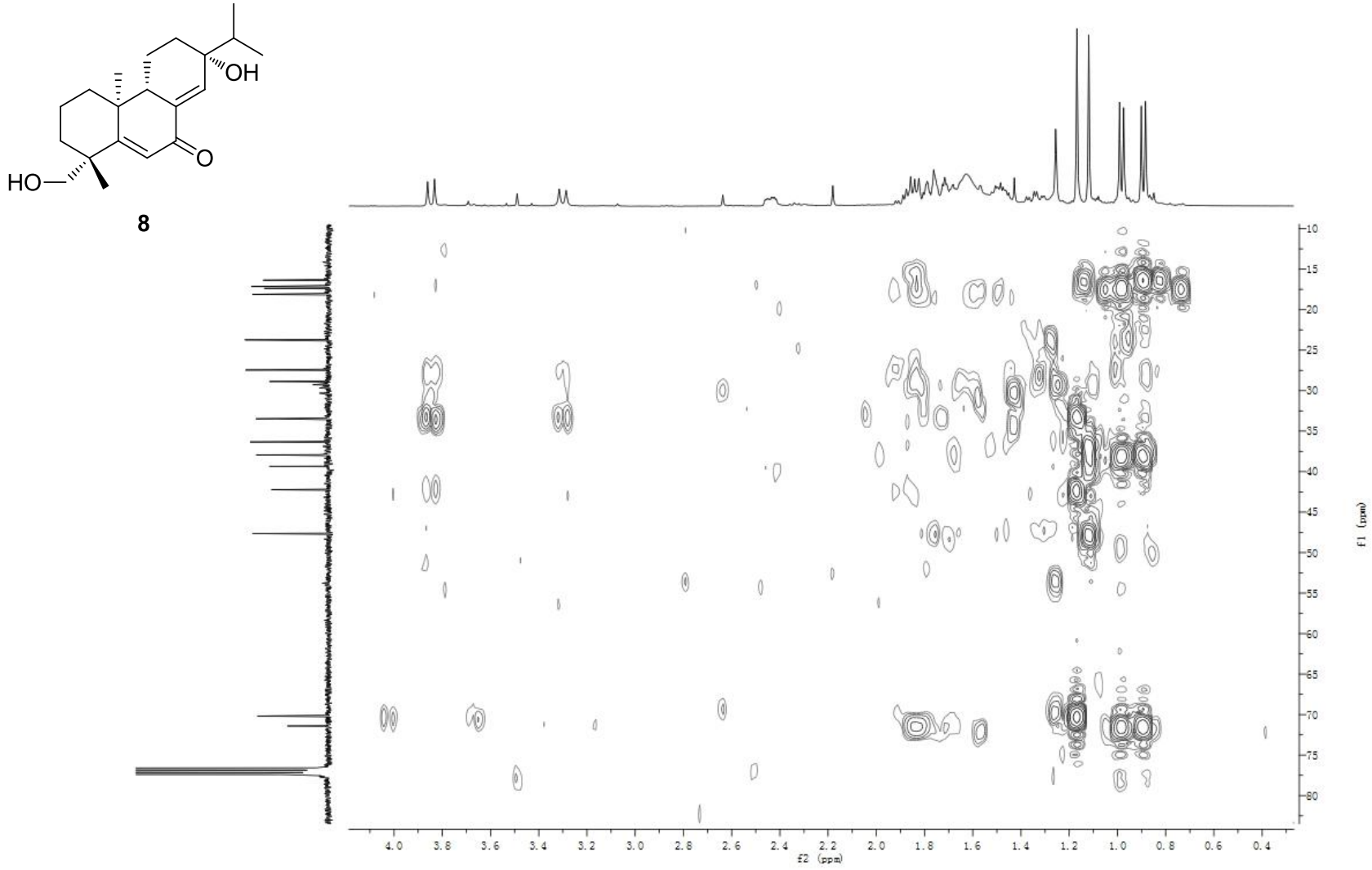


Figure S75. NOESY (400 MHz, $CDCl_3$) spectrum of **8**

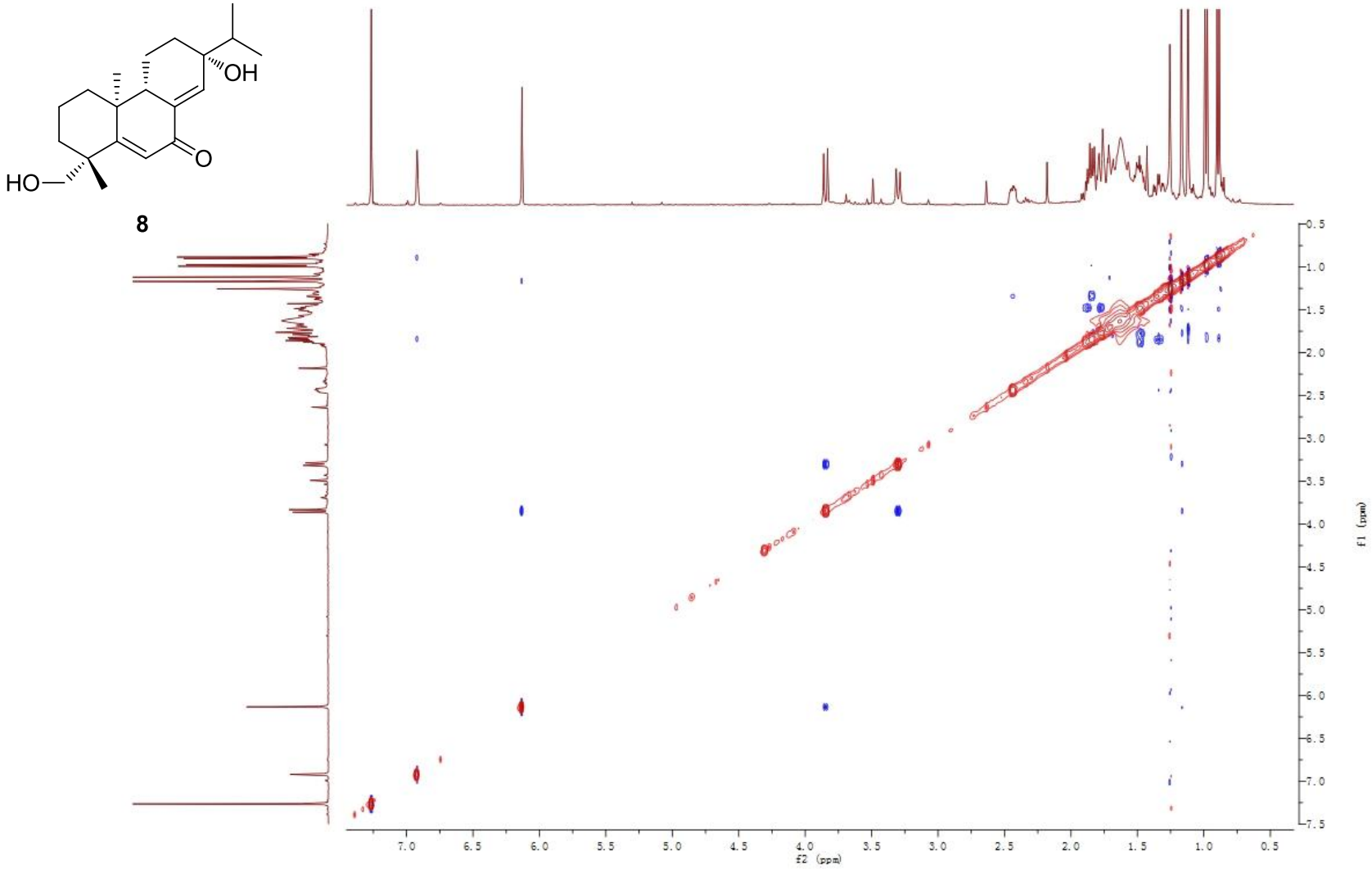
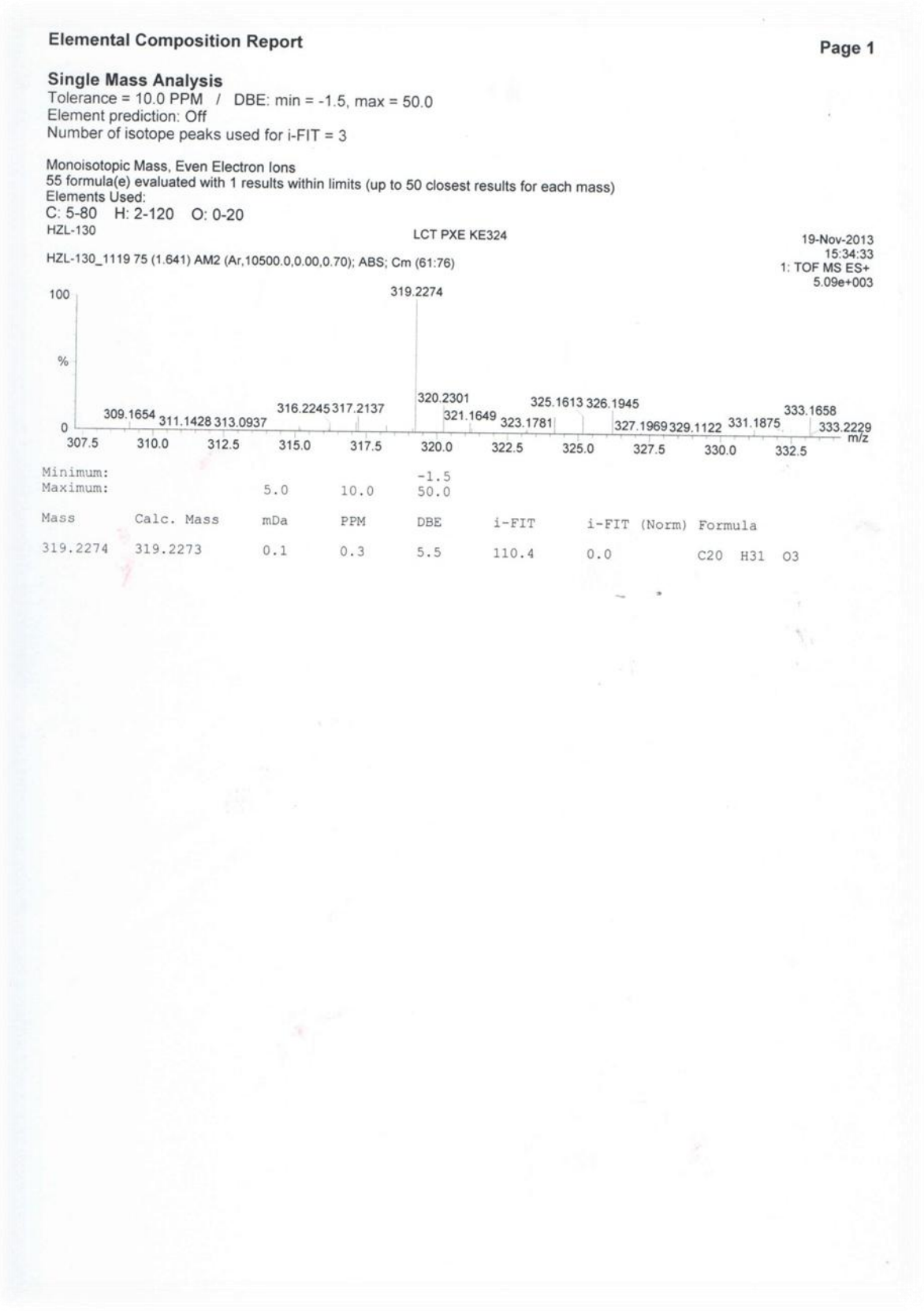


Figure S76. HRESIMS spectrum of **8**



Elemental Composition Report Page 1

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

Monoisotopic Mass, Even Electron Ions
55 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20
HZL-130

LCT PXE KE324

19-Nov-2013
15:34:33
1: TOF MS ES+
5.09e+003

HZL-130_1119 75 (1.641) AM2 (Ar,10500.0,0.00,0.70); ABS; Cm (61:76)

Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
319.2274	319.2273	0.1	0.3	5.5	110.4	0.0	C20 H31 O3

Figure S77. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **9**

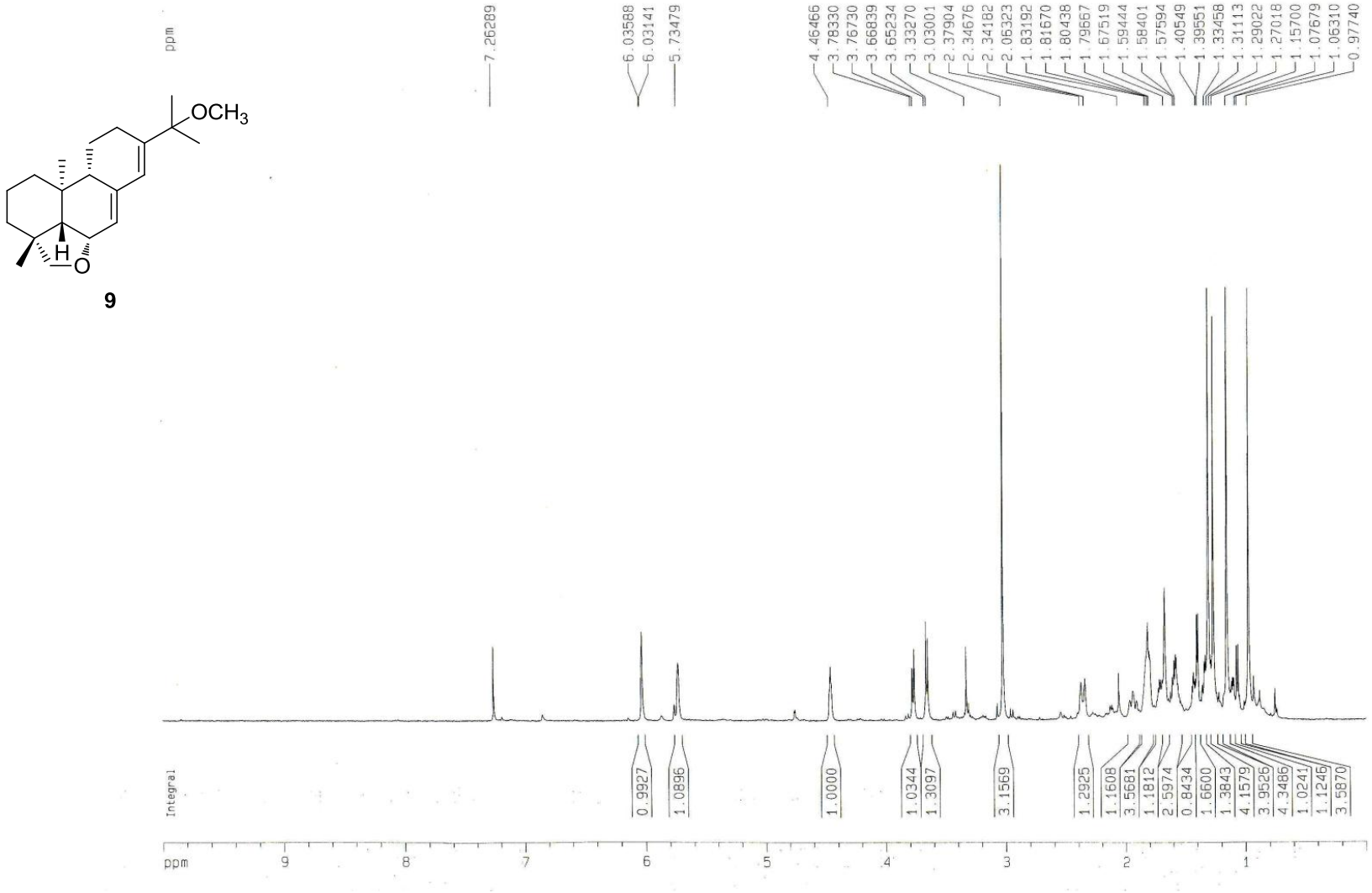


Figure S78. ^{13}C NMR (500 MHz, $CDCl_3$) spectrum of **9**

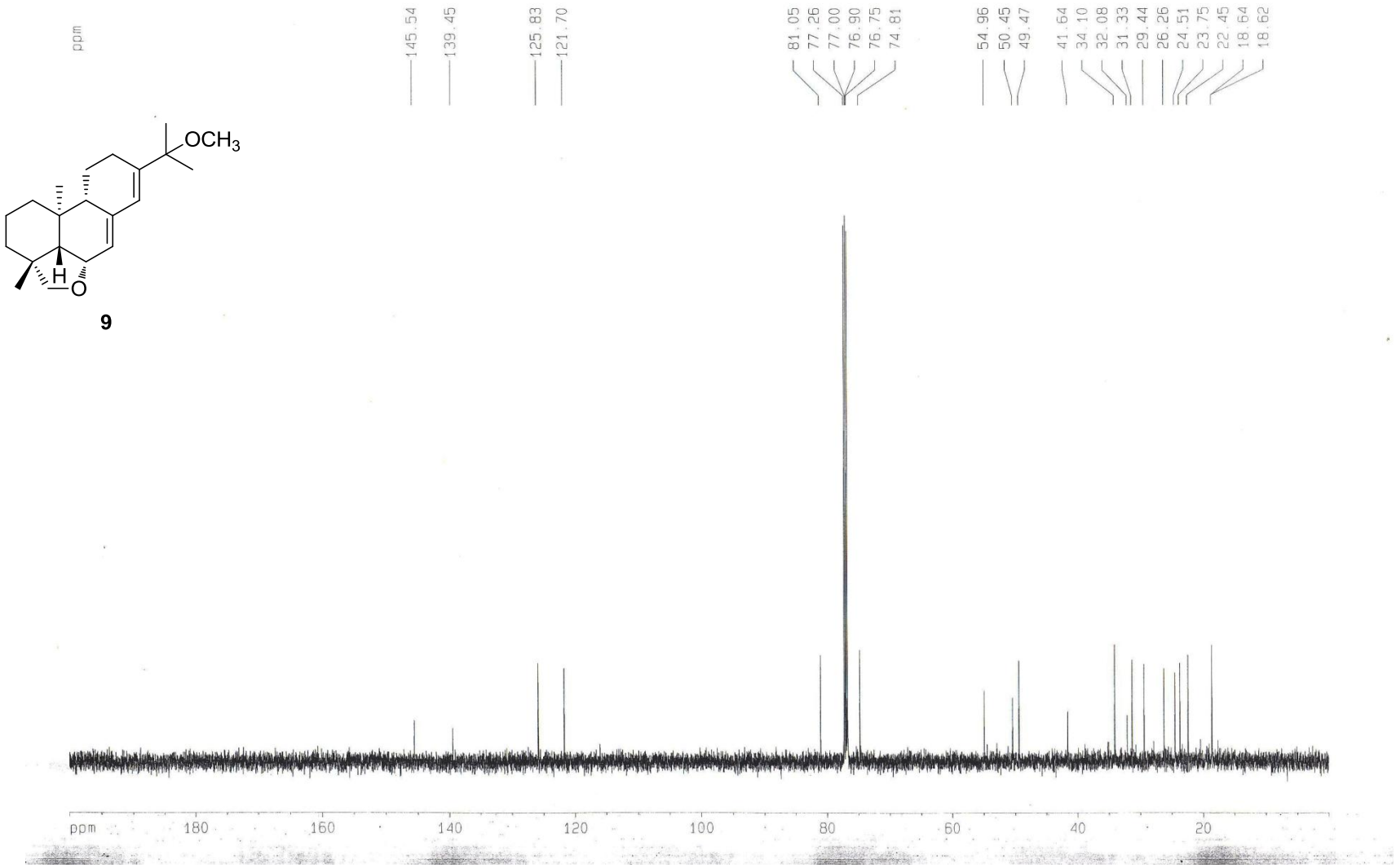


Figure S79. DEPT-135 (500 MHz, $CDCl_3$) spectrum of **9**

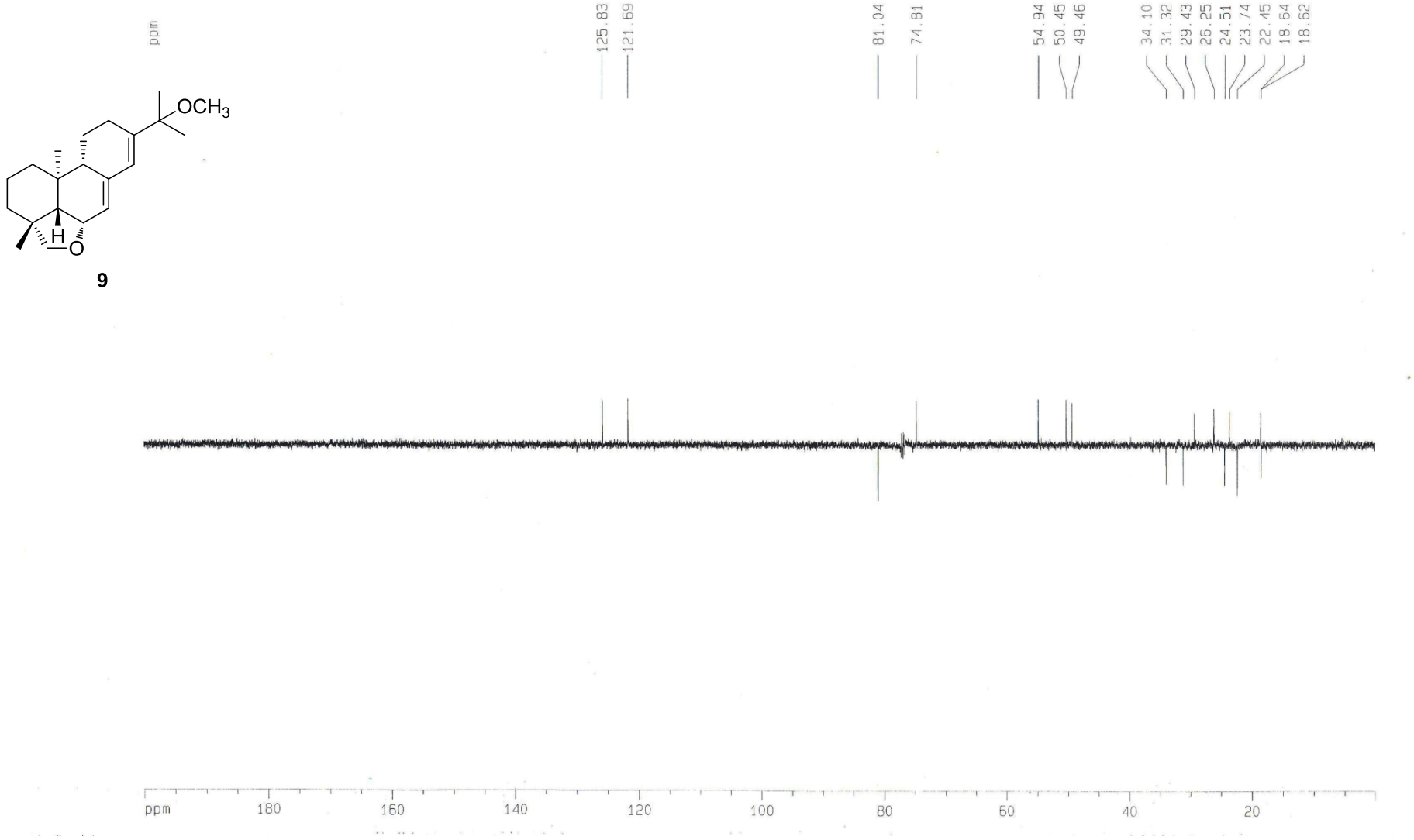


Figure S80. HMBC (500 MHz, $CDCl_3$) spectrum of **9**

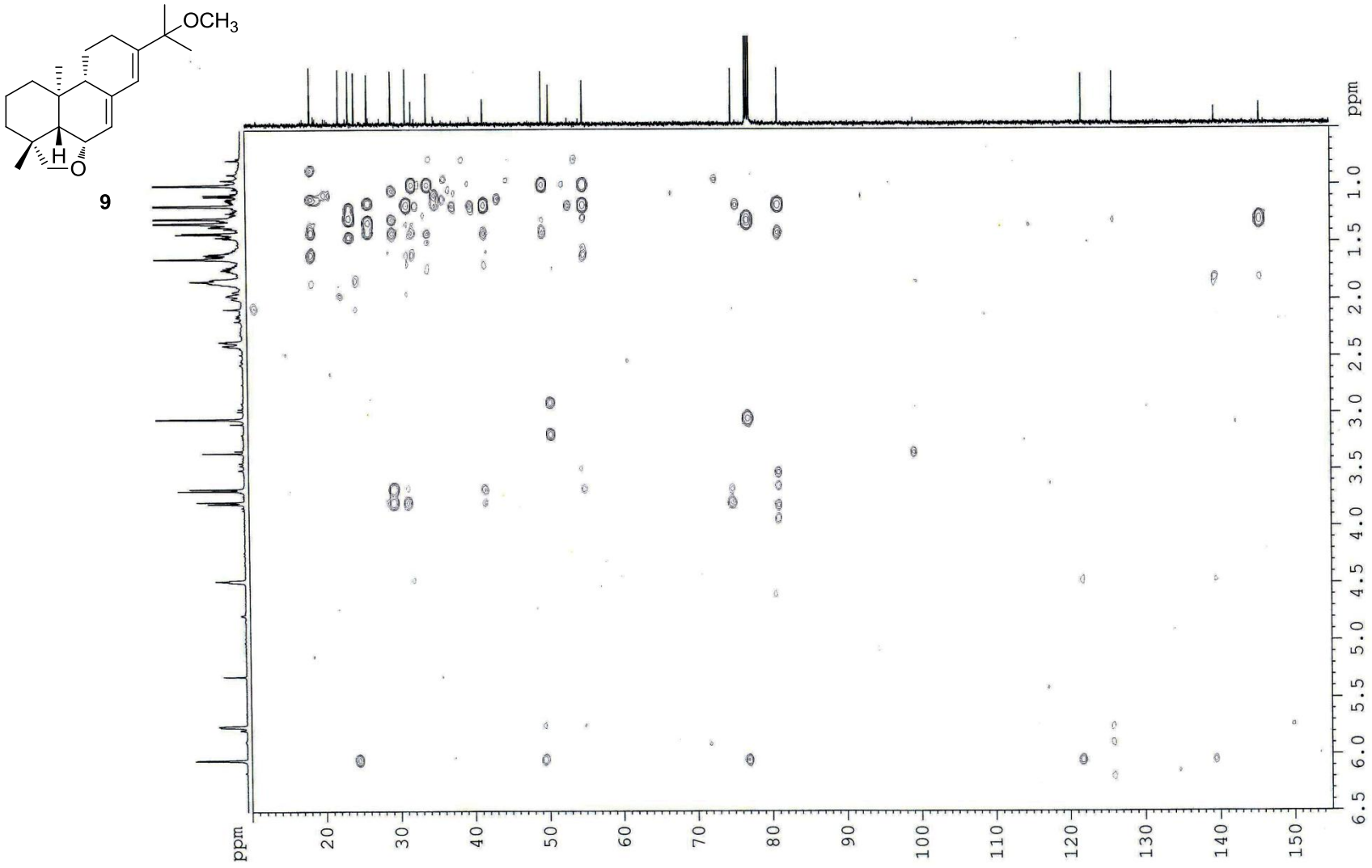
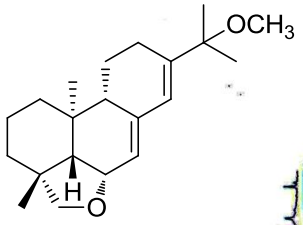


Figure S81. HMBC (500 MHz, $CDCl_3$) spectrum of **9**-expansion



9

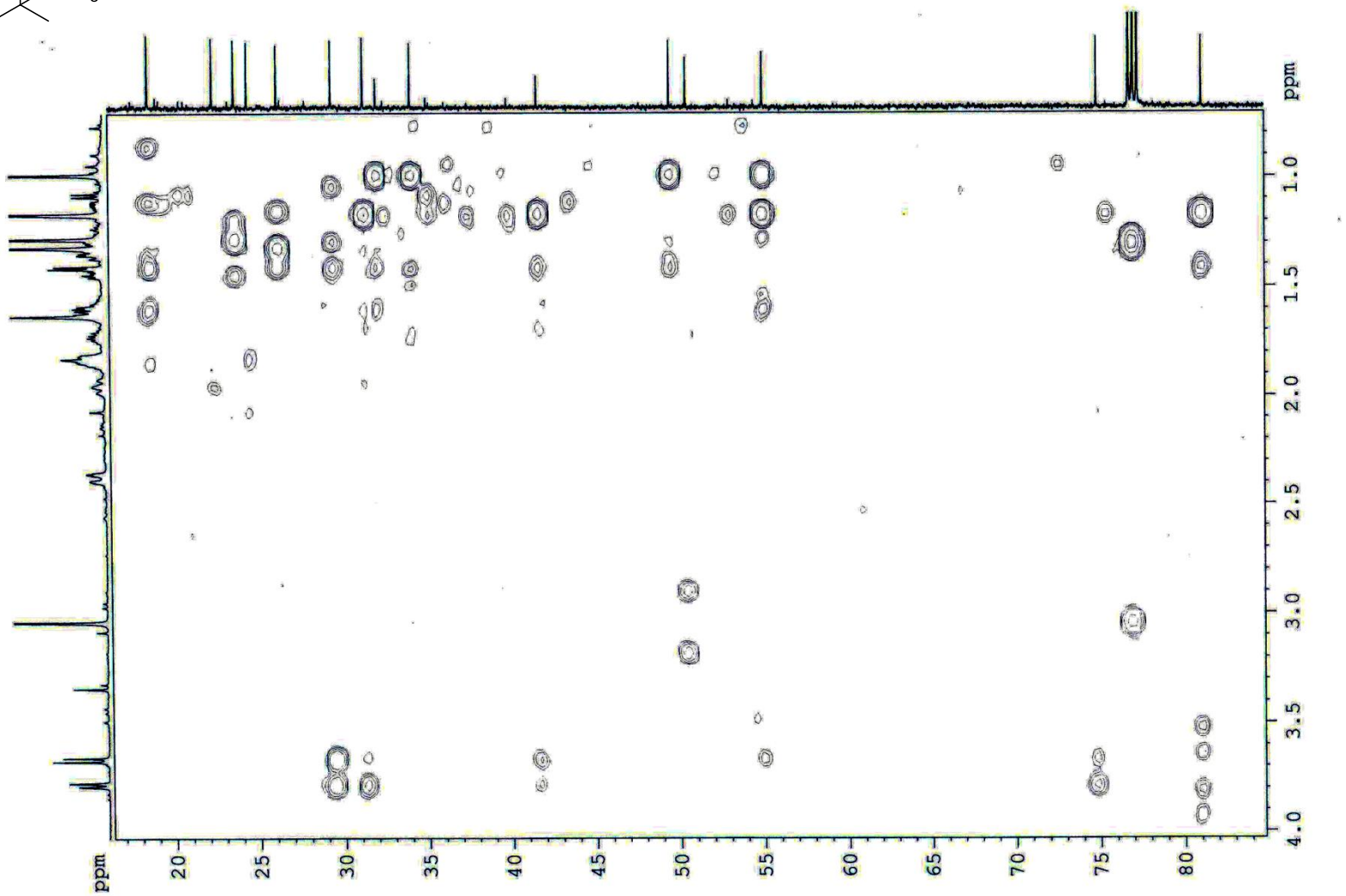
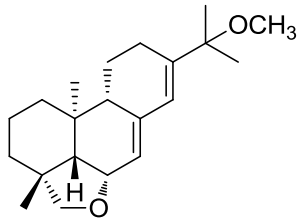


Figure S82. NOESY (500 MHz, $CDCl_3$) spectrum of **9**



9

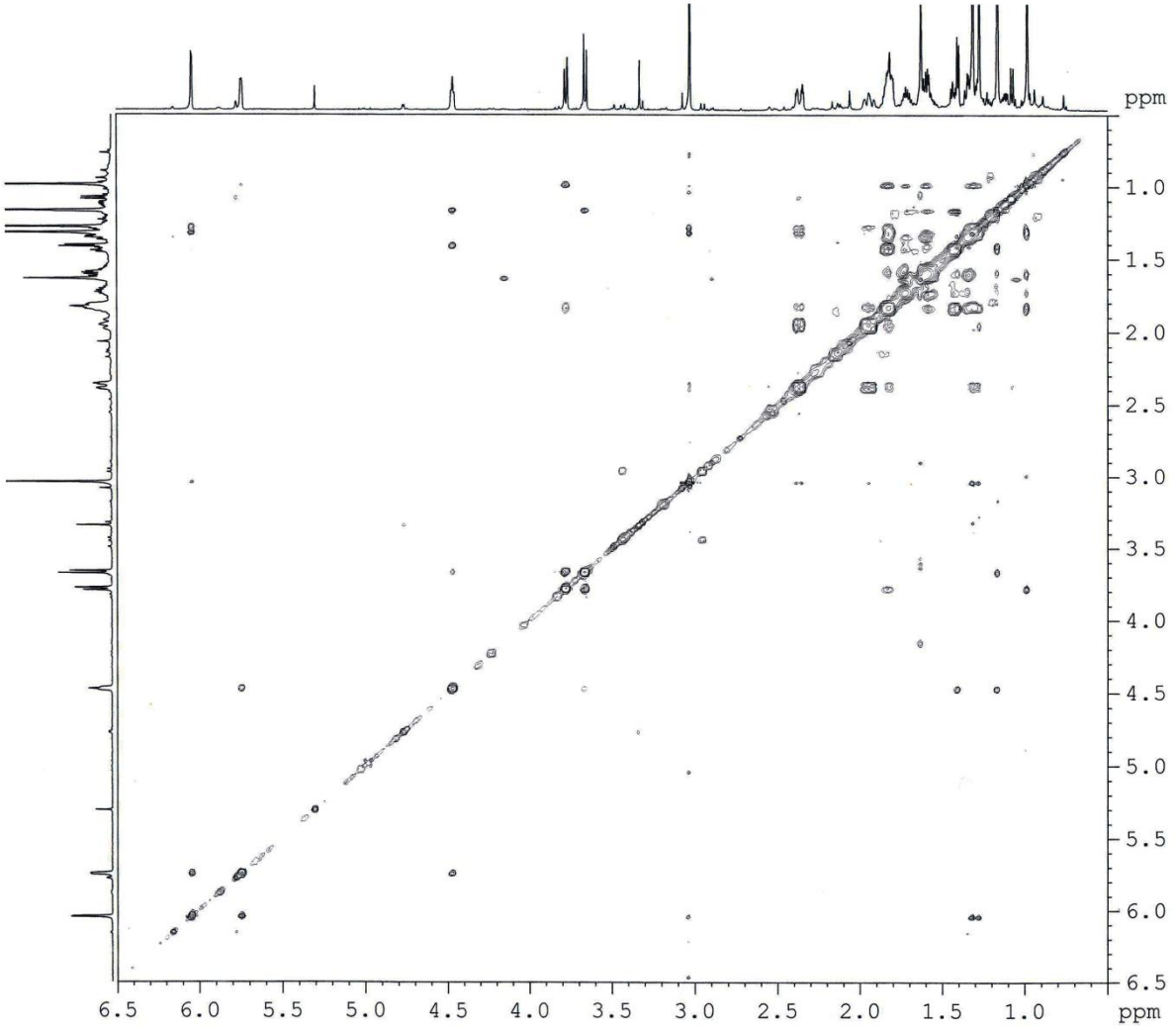


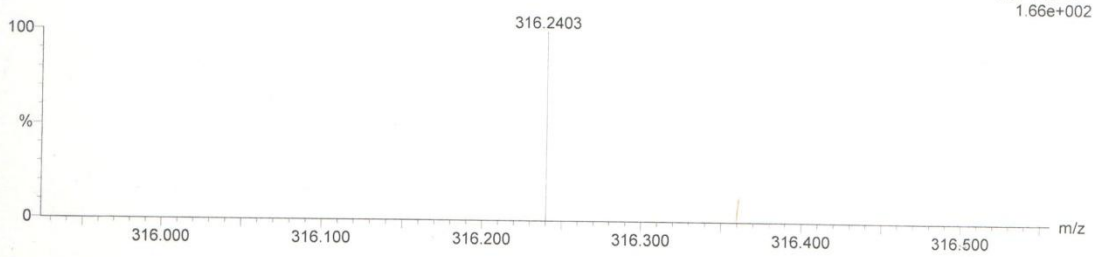
Figure S83. HREIMS spectrum of **9**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-21 H: 0-35 O: 0-2
HZL-114
20120709007 66 (1.100)

TOF MS EI+
1.66e+002



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
316.2403	316.2402	0.1	0.3	6.0	5546096.5	C21 H32 O2

Figure S84. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **10**

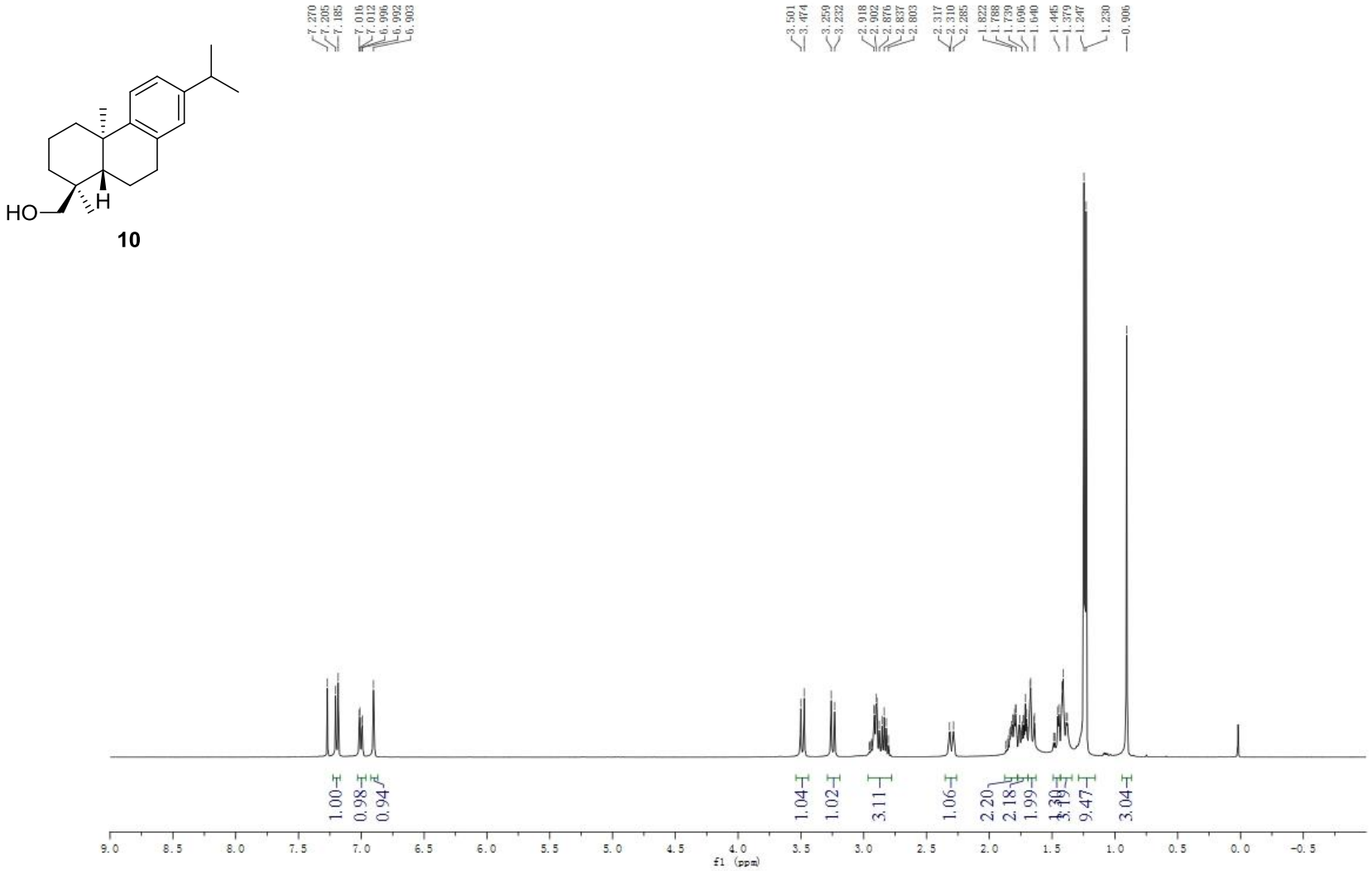


Figure S85. ^{13}C NMR (400 MHz, $CDCl_3$) spectrum of **10**

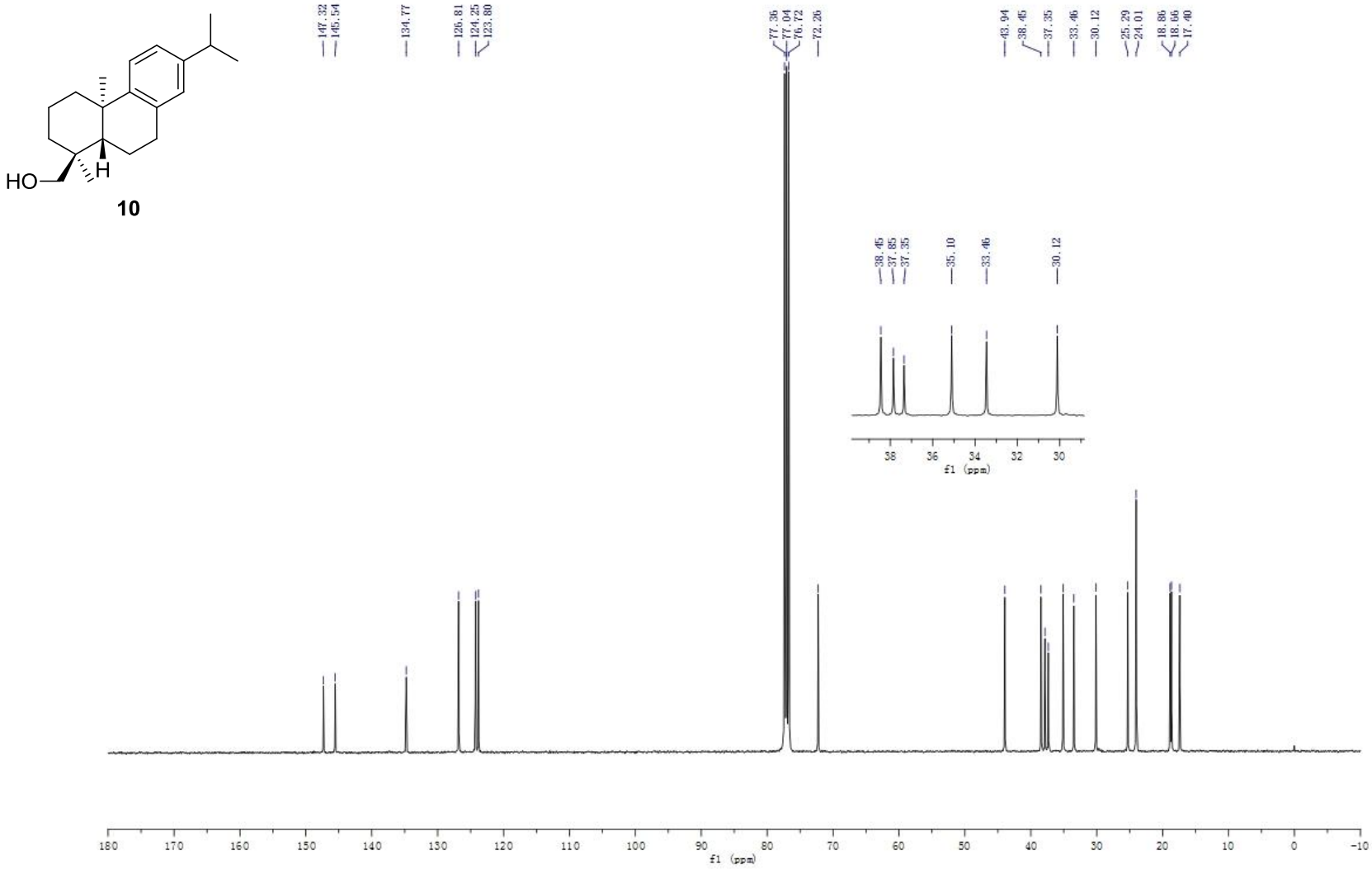


Figure S86. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of **10**

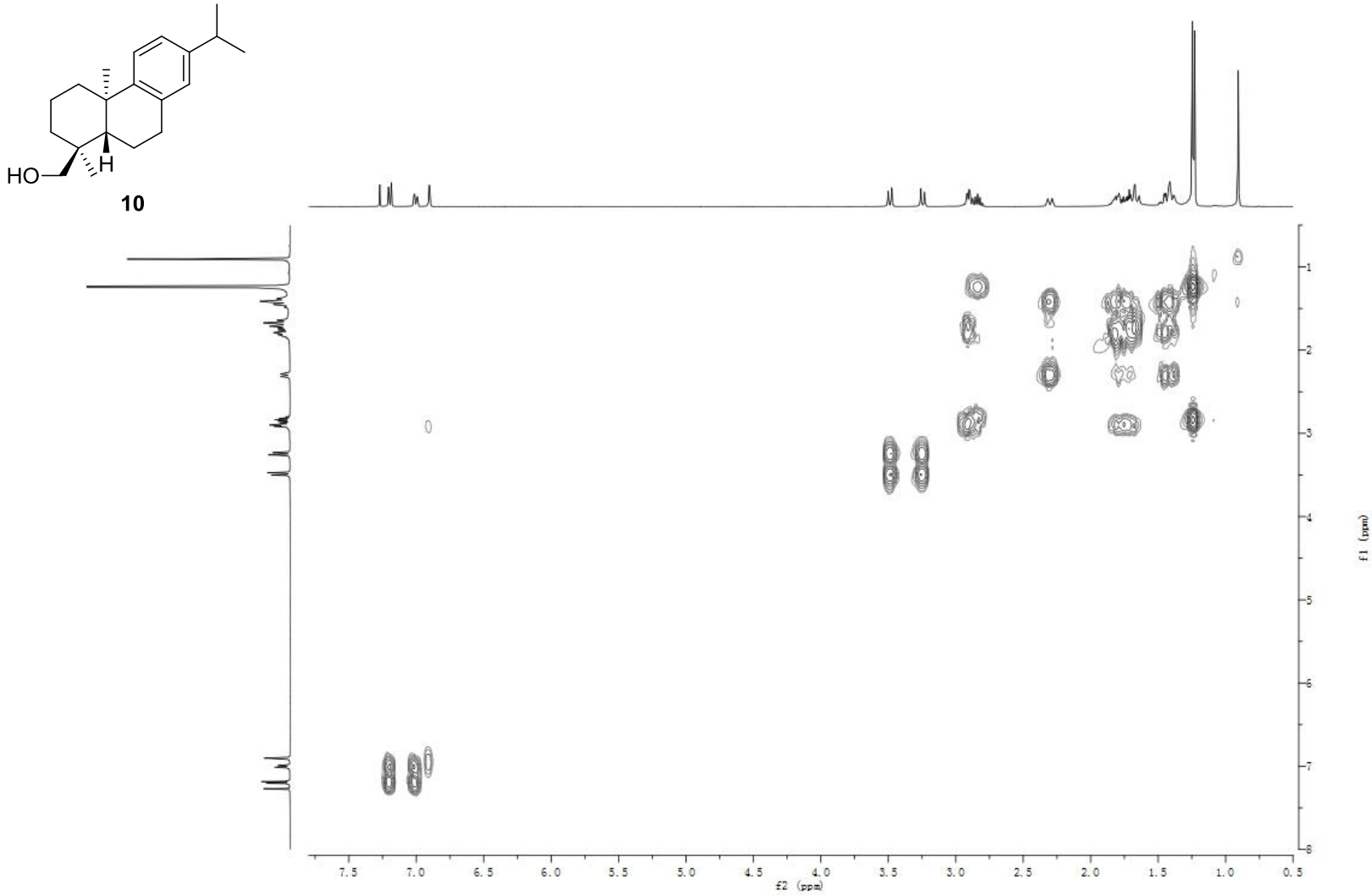


Figure S87. NOESY (400 MHz, $CDCl_3$) spectrum of **10**

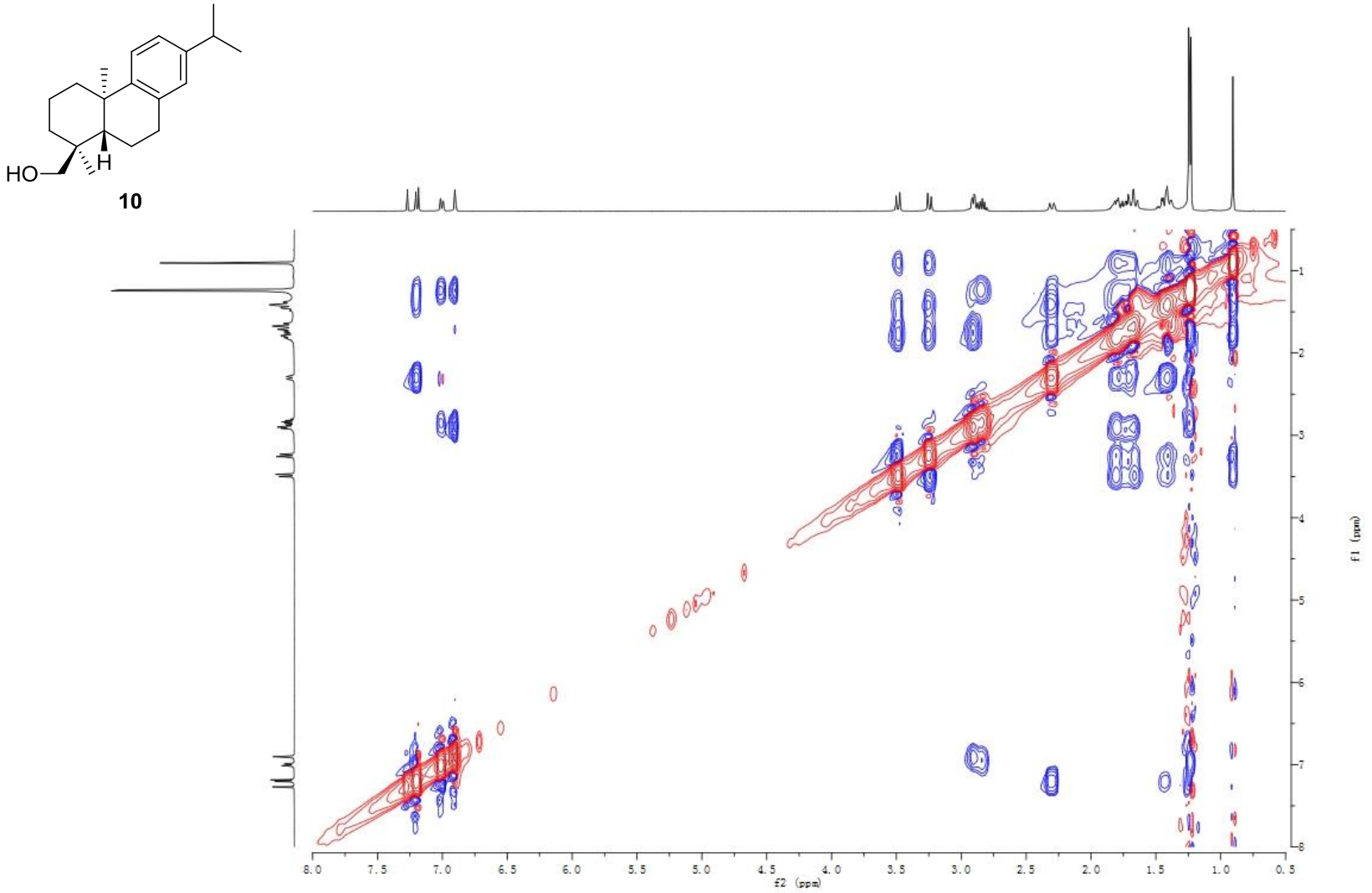
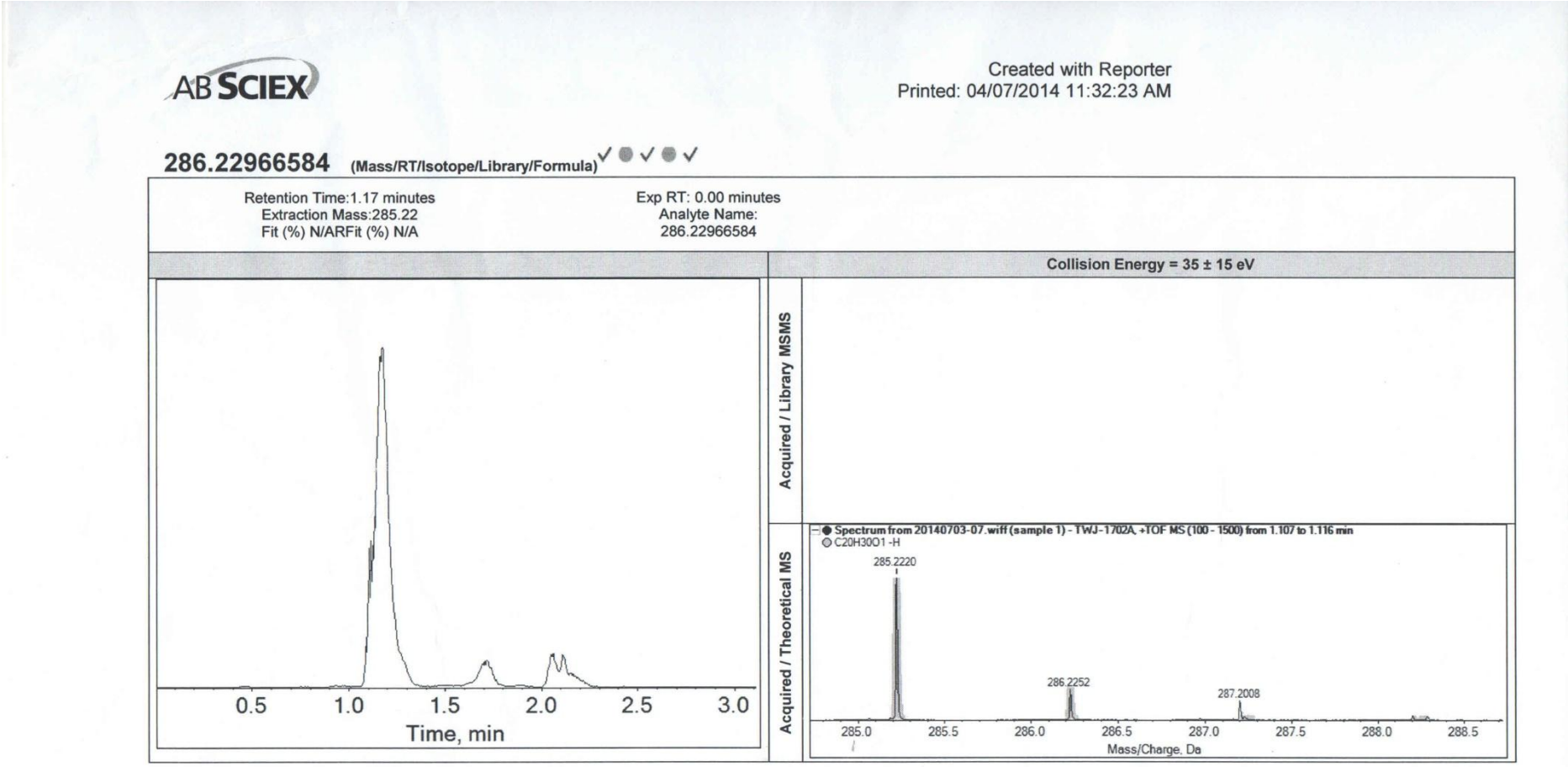


Figure S88. HRESIMS spectrum of **10**



	Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
✓●✓●✓	(TWJ-1702A) 286.22966584	90%	C20H30O1	117061	100	285.2224	285.2220	-1.4	0.00	1.17	1.17	1.4%	N/A

Figure S89. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **11**

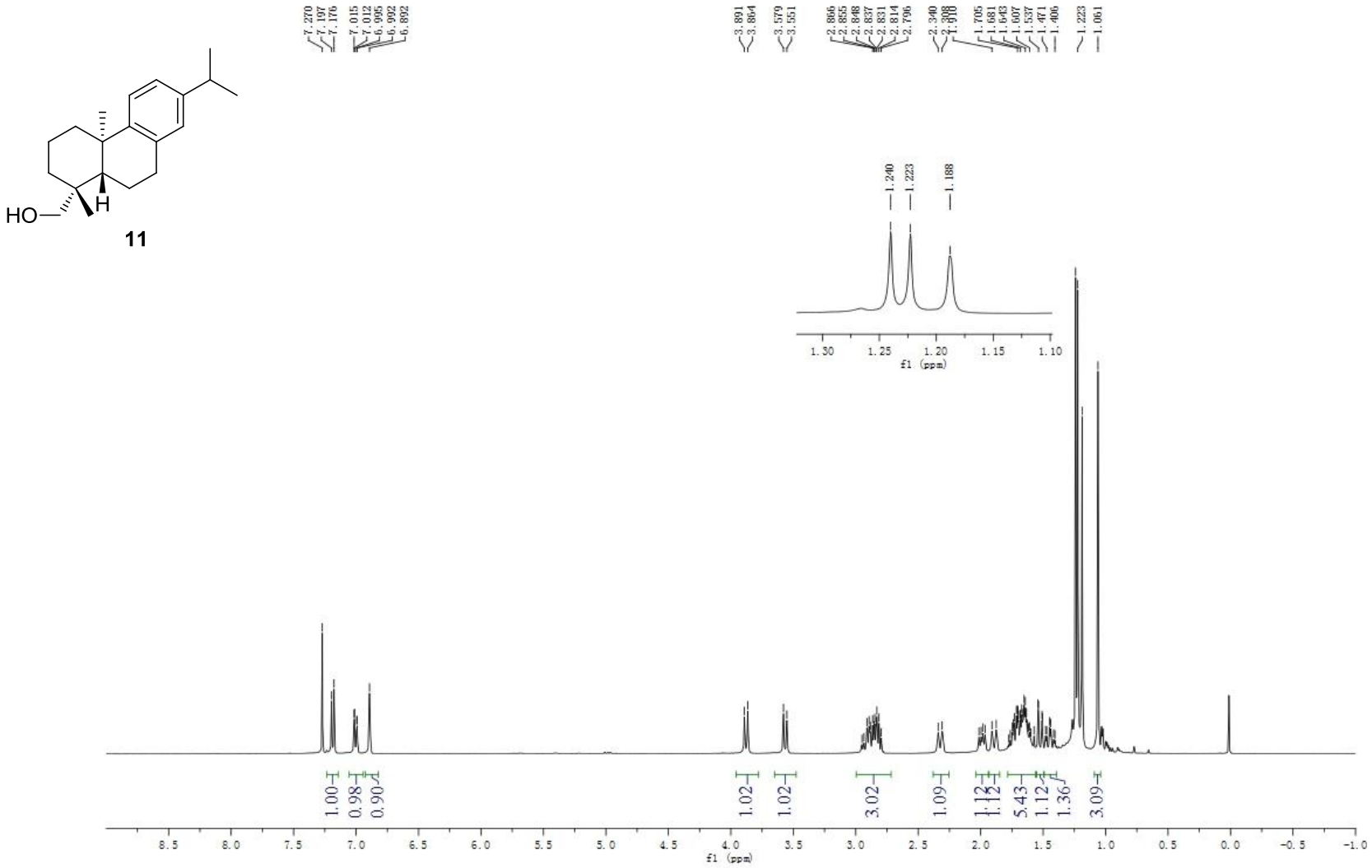


Figure S90. ^{13}C NMR (400 MHz, $CDCl_3$) spectrum of **11**

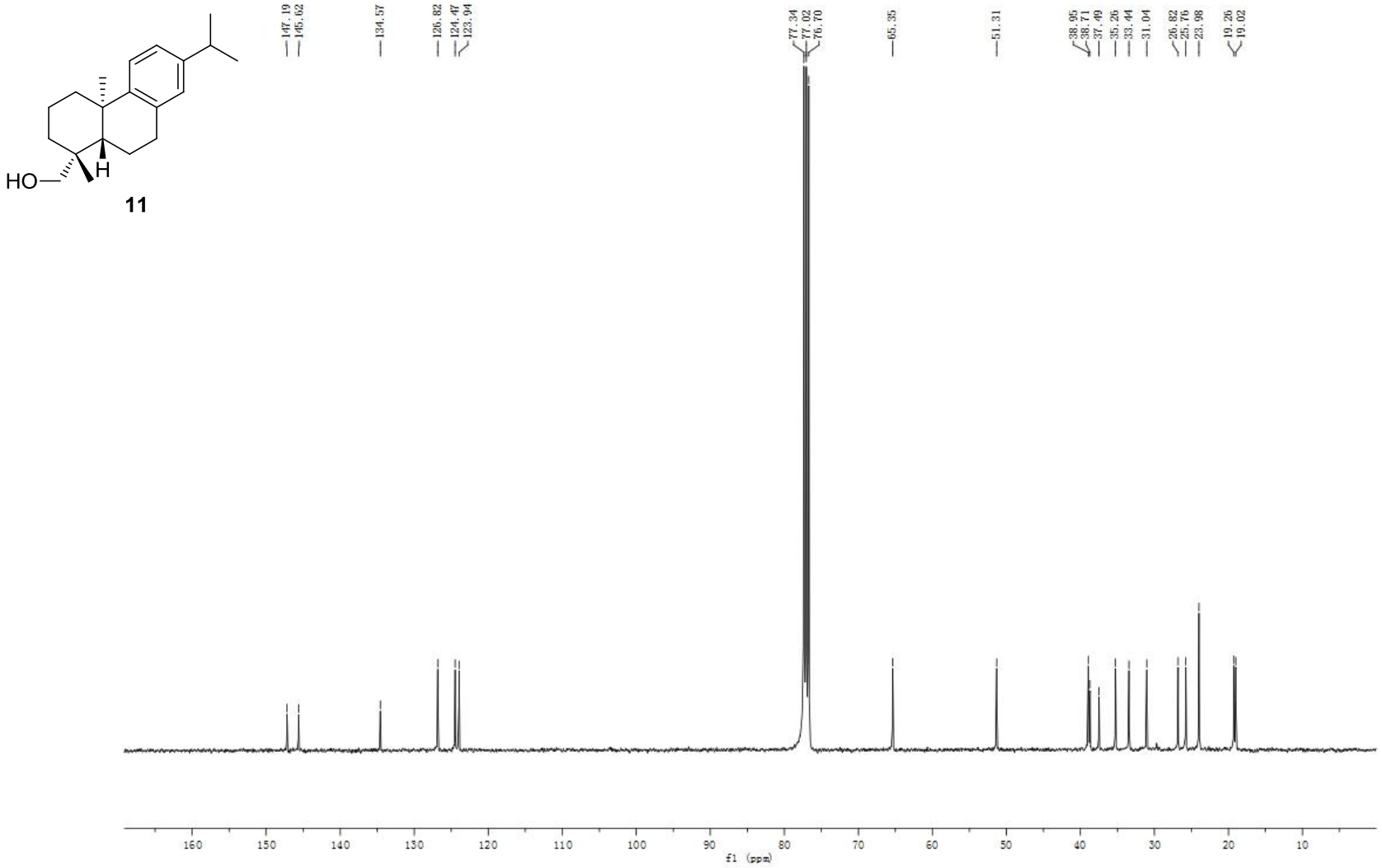


Figure S91. NOESY (400 MHz, $CDCl_3$) spectrum of **11**

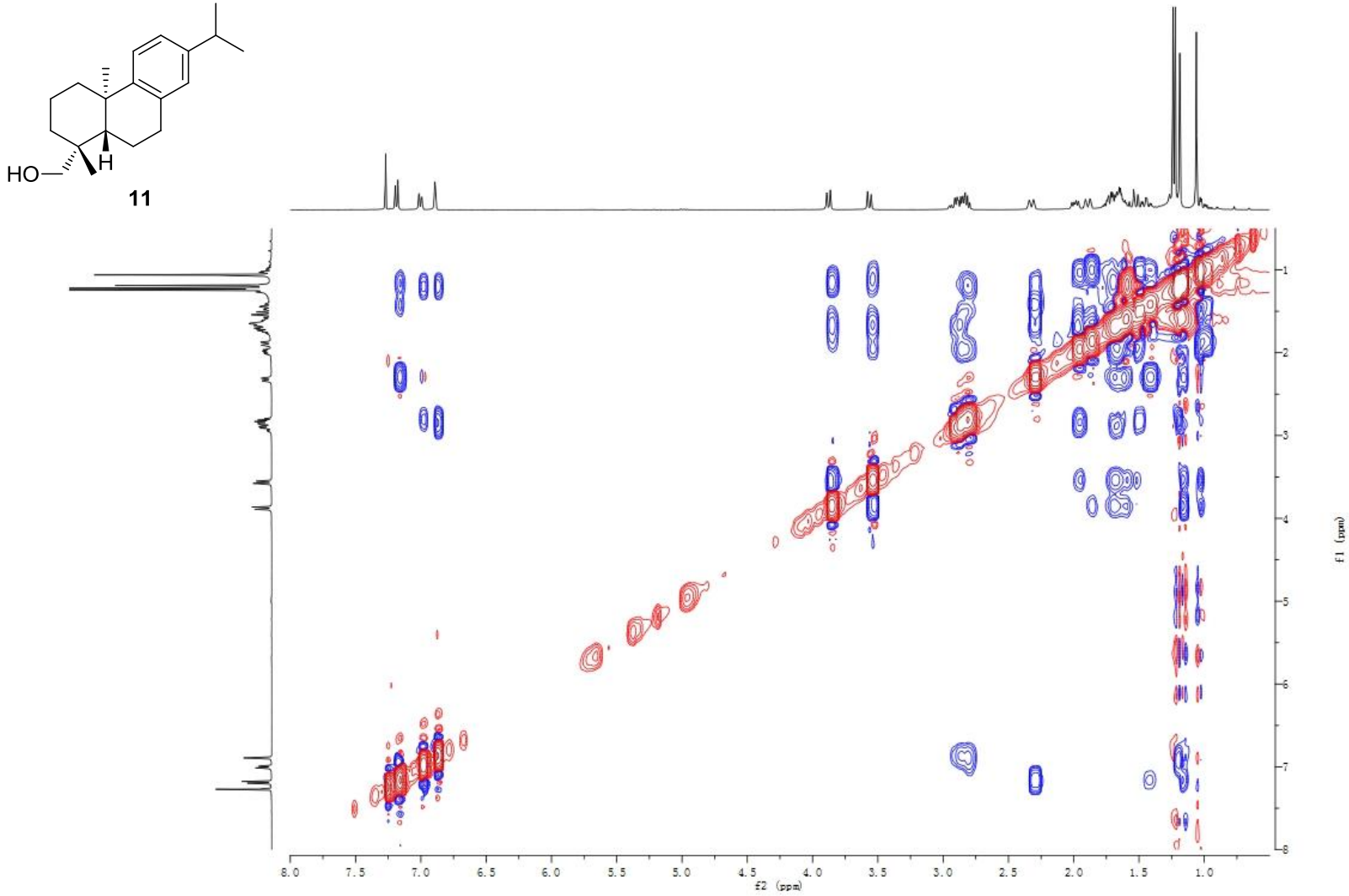
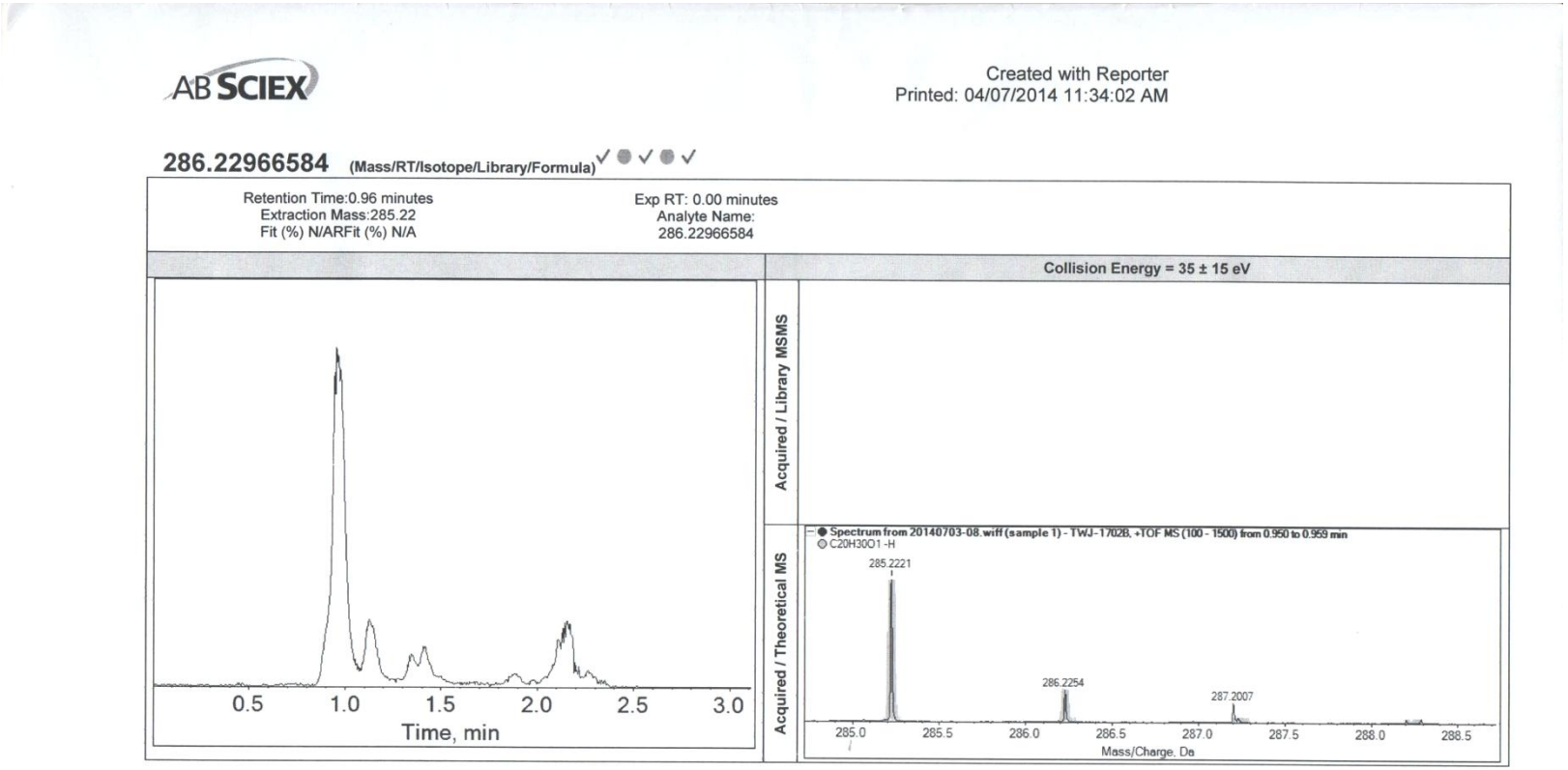


Figure S92. HRESIMS spectrum of **11**



Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
(TWJ-1702B) 286.22966584	91%	C20H30O1	40784	100	285.2224	285.2221	-1.0	0.00	0.96	0.96	0.1%	N/A

Figure S93. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **12**

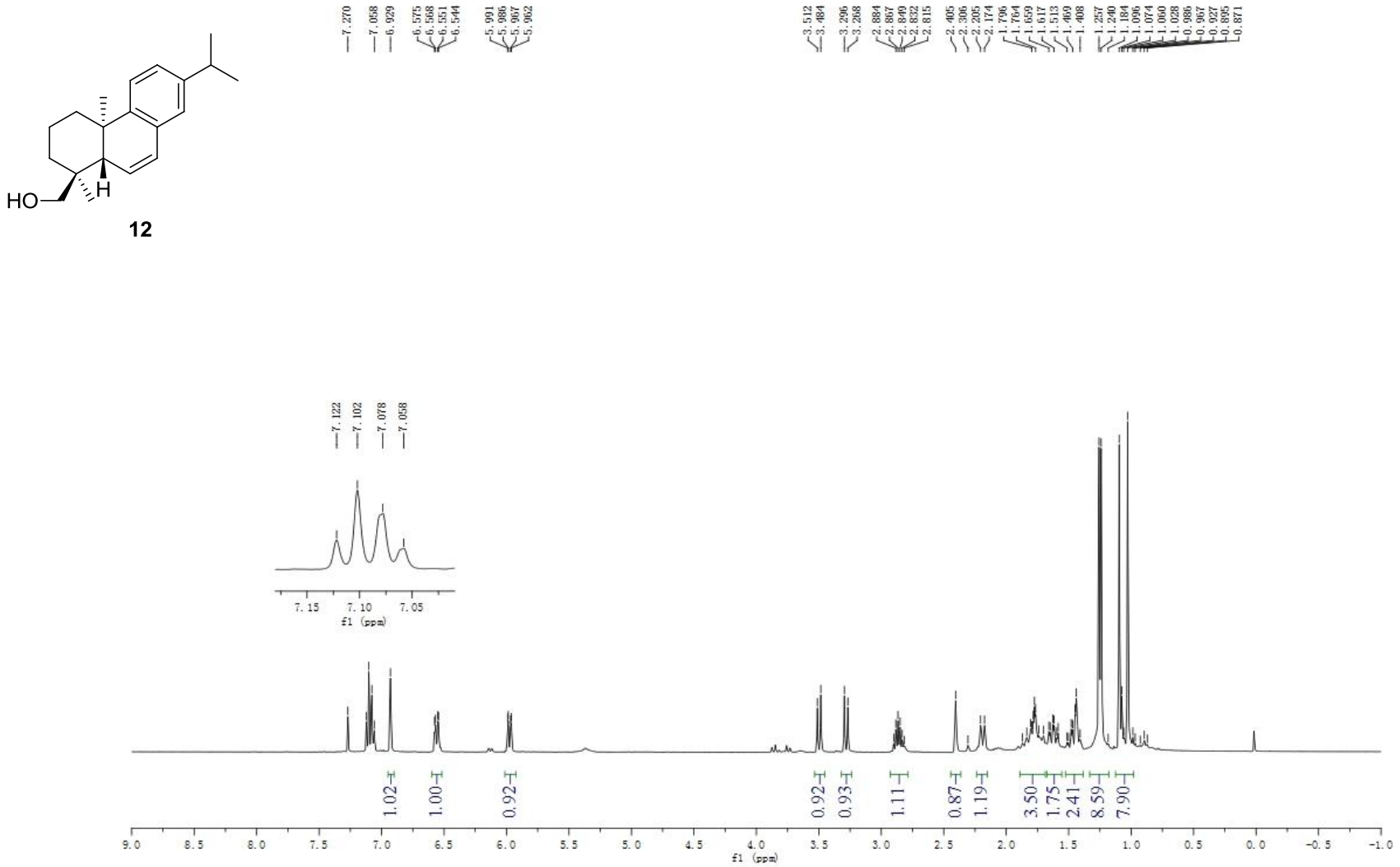


Figure S94. ^{13}C NMR (400 MHz, $CDCl_3$) spectrum of **12**

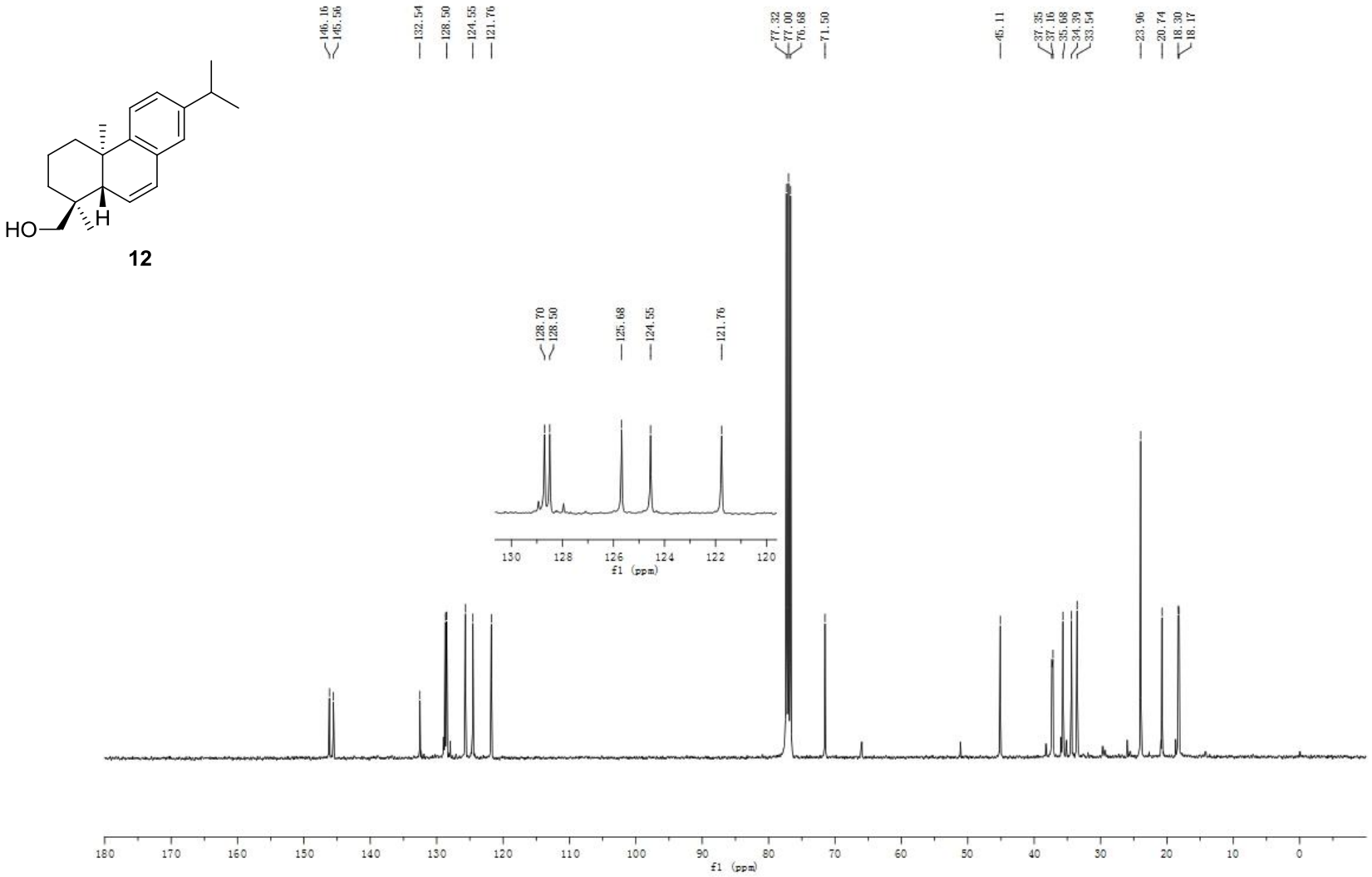


Figure S95. DEPT-135 (400 MHz, $CDCl_3$) spectrum of **12**

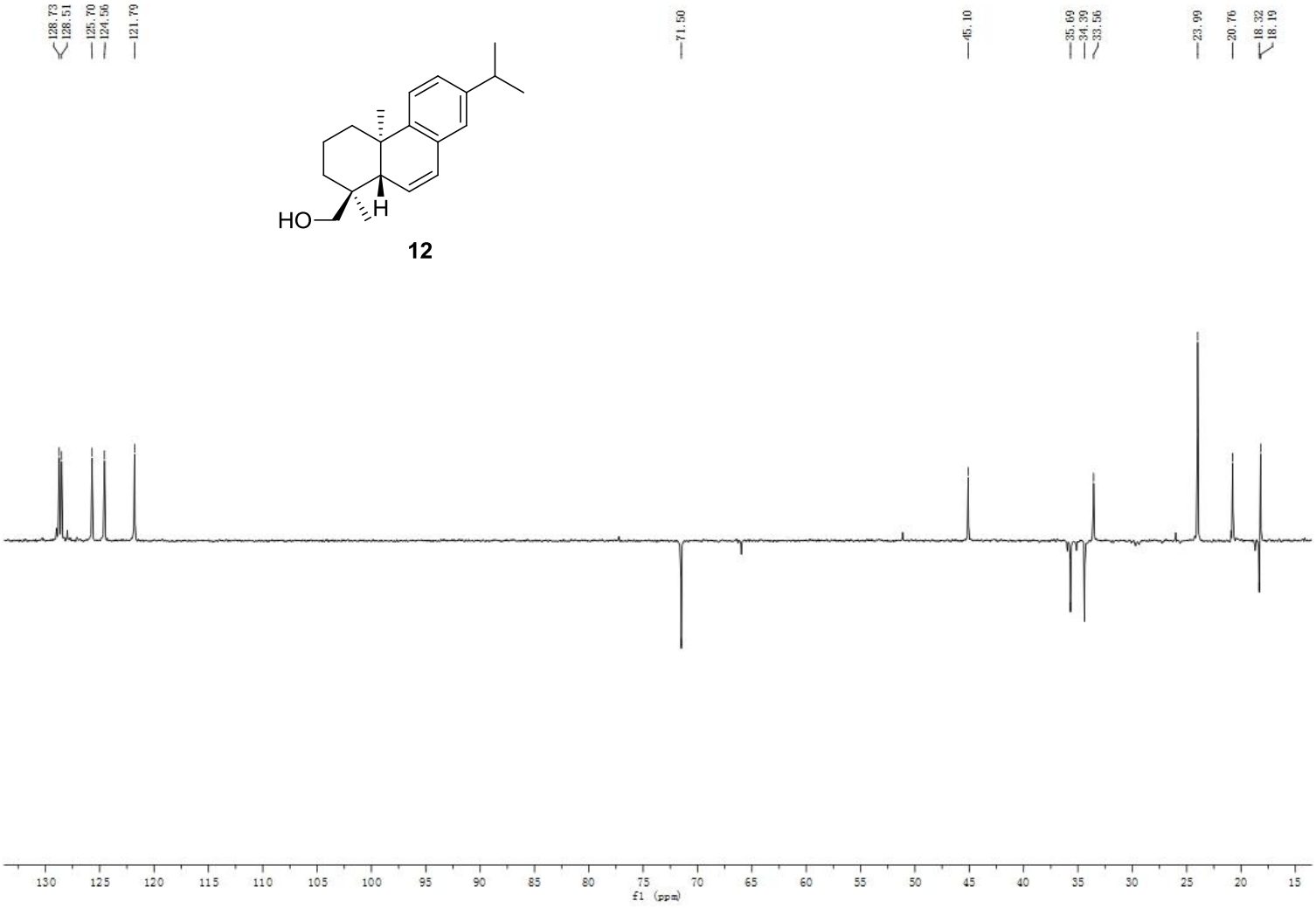


Figure S96. NOESY (400 MHz, $CDCl_3$) spectrum of **12**

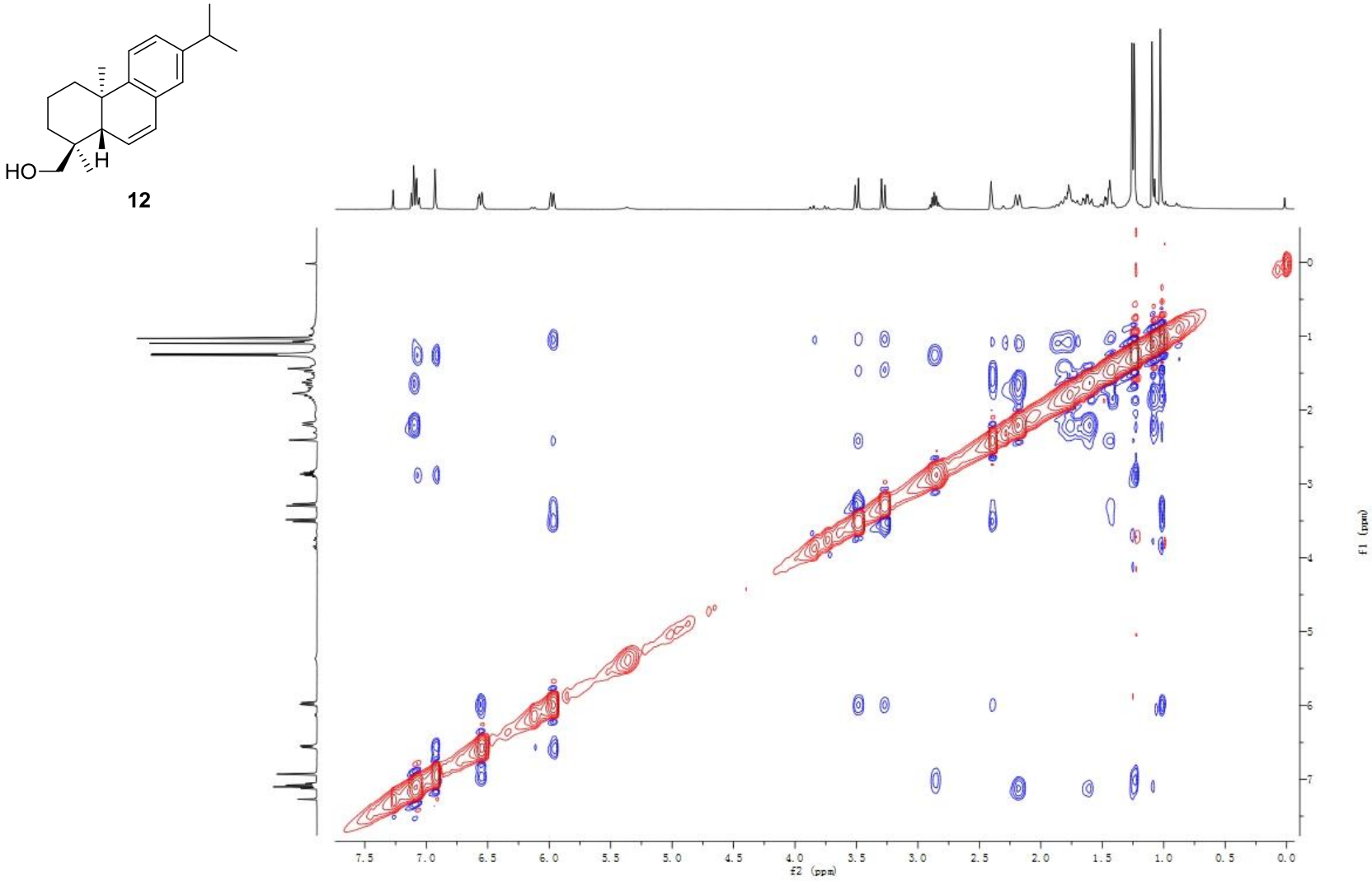
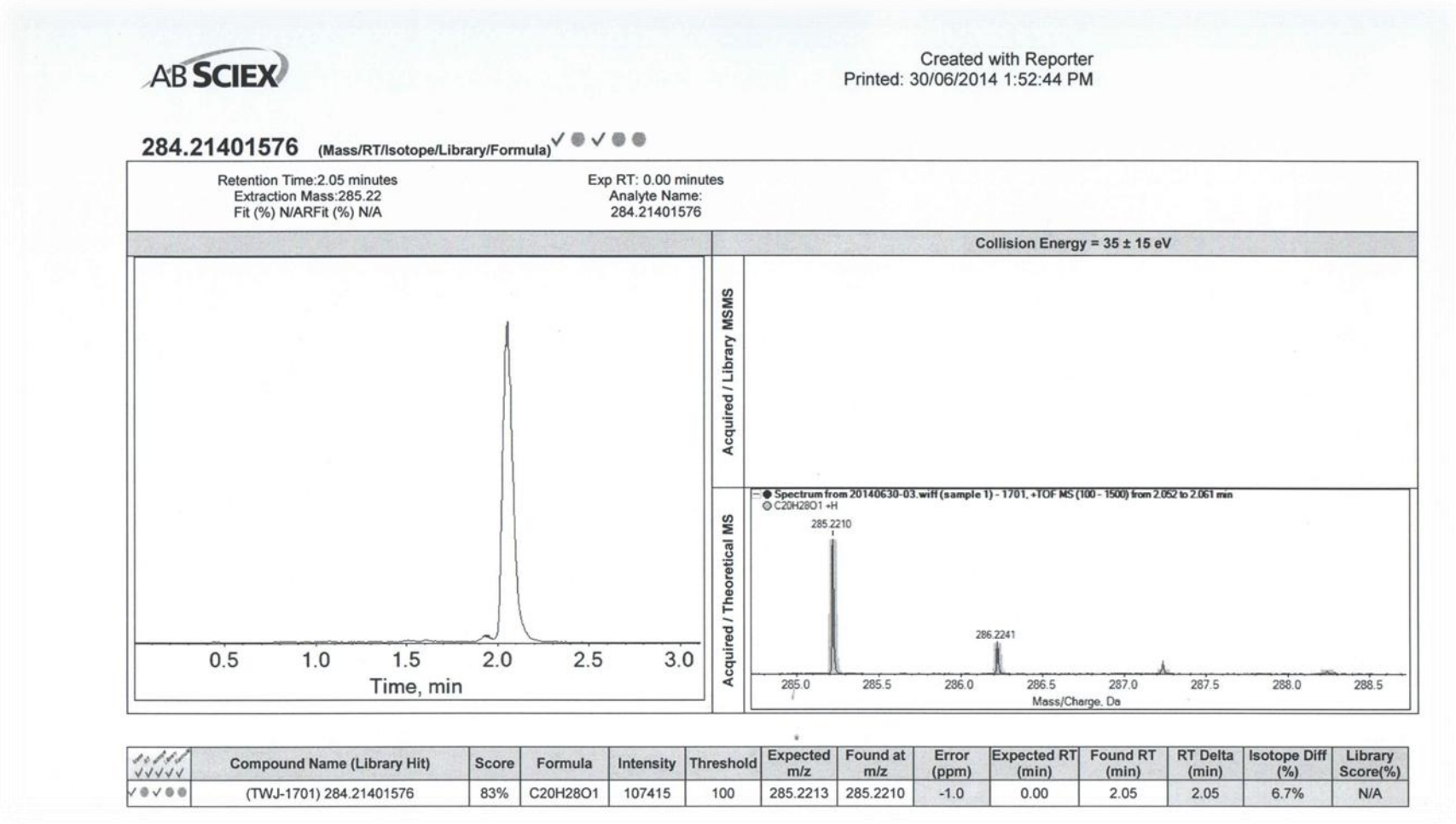


Figure S97. HRESIMS spectrum of **12**



Compound Name (Library Hit)	Score	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)	Expected RT (min)	Found RT (min)	RT Delta (min)	Isotope Diff (%)	Library Score(%)
(TWJ-1701) 284.21401576	83%	C20H28O1	107415	100	285.2213	285.2210	-1.0	0.00	2.05	2.05	6.7%	N/A