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Electronic supplementary information

Altereporenes A-E, five epoxy octa-hydronaphthalene polyketides produced by an endophytic fungus *Alternaria* sp. YUD20002

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contents

Table S1. Inhibitory activities of **1-5** on AchE

compound	Inhibitation(%)[a]
1	1.47
2	6.89
3	9.93
4	0.73
5	10.51
tacrine[b]	61.43

[a]Tested at 50 μM; [b]Positive control.

Table S2. Inhibitory activities of **1-5** on NO production

compound	Inhibitation(%)[a]
1	20.30 ± 2.79
2	19.85 ± 2.15
3	6.98 ± 0.83
4	29.22 ± 3.01
5	11.96 ± 2.42
L-NMMA[b]	57.42 ± 1.41

[a]Tested at 50 μM; [b]Positive control.

Table S3. Inhibitory activities of **1-5** was tested at 40 μM against five human cancer cell lines

compound	Inhibitation(%)[a]				
	HL-60	A-549	SMMC-7721	MDA-MB-231	SW480
1	3.82	5.84	18.35	1.93	0.99
2	0.57	2.66	17.67	12.97	8.05
3	3.60	3.18	3.01	8.98	9.91
4	2.64	8.14	25.22	8.97	7.56
5	2.44	0.39	11.46	10.93	6.85
DDP[b]	78.45	71.66	77.57	61.14	57.61

[a]Tested at 40 μM; [b]Positive control.

Table S4. Optimized Cartesian coordinates (in Å), thermal correction to Gibbs Free Energy and thermal correction to Gibbs Free Energy for studied compound **1**-**5** at the B3LYP/6-31g (d, p) level of theory in the methanol

1	B3LYP/6-31G(d, p) (0 imaginary Frequencies, solvent=methanol, thermal correction to Gibbs Free Energy= -1197.222070, thermal correction to Gibbs Free Energy= 0.471830)			
	C	-0.78330000	0.17180000	-0.51210000
	C	-0.99150000	1.73060000	-0.71280000
	C	-2.36010000	2.02390000	-1.29980000
	C	-3.47180000	1.01140000	-1.27580000
	C	-3.27310000	-0.37190000	-0.72060000
	C	-2.01420000	-0.48710000	0.17590000
	C	-4.51890000	-0.82590000	0.07010000
	C	-4.31320000	-2.11390000	0.82710000
	C	-3.08580000	-2.63320000	1.01020000
	C	-1.81620000	-1.97630000	0.55240000
	O	-2.69380000	1.25850000	-2.46590000
	C	0.50700000	-0.15690000	0.22960000
	C	1.57450000	-0.73280000	-0.34660000
	C	2.78660000	-1.02690000	0.38320000
	C	3.88920000	-1.63920000	-0.09360000
	C	5.09260000	-1.83770000	0.81220000
	C	6.33510000	-1.04740000	0.39460000
	C	4.04940000	-2.19320000	-1.48610000
	C	6.11550000	0.45970000	0.38160000
	O	7.35380000	1.09800000	0.09240000
	C	-0.71700000	2.57570000	0.55760000
	C	-1.67160000	2.79910000	1.49000000
	C	0.67070000	3.16880000	0.66810000
	C	-1.57900000	3.64110000	2.72440000
	C	-5.55220000	-2.79040000	1.33590000
	O	-1.35310000	-2.73980000	-0.55300000
	O	-0.05800000	2.16290000	-1.71920000
	H	-0.69740000	-0.27290000	-1.51570000
	H	-2.59780000	3.07970000	-1.33120000
	H	-4.49940000	1.34920000	-1.29850000
	H	-3.16000000	-1.05140000	-1.57800000
	H	-2.21120000	0.05090000	1.11330000
	H	-4.81670000	-0.04640000	0.78370000
	H	-5.35260000	-0.94360000	-0.63410000
	H	-2.96750000	-3.58680000	1.51900000
	H	-1.08470000	-2.06360000	1.36470000

	H	0.53590000	0.10670000	1.28580000
	H	1.53940000	-0.96730000	-1.40660000
	H	2.79290000	-0.69010000	1.42050000
	H	4.84350000	-1.57310000	1.84820000
	H	5.34090000	-2.90650000	0.83410000
	H	7.15440000	-1.28320000	1.08610000
	H	6.68950000	-1.37340000	-0.59120000
	H	3.10990000	-2.25980000	-2.03910000
	H	4.73720000	-1.57050000	-2.06660000
	H	4.45660000	-3.20930000	-1.44300000
	H	5.39350000	0.75150000	-0.38700000
	H	5.76430000	0.81310000	1.35620000
	H	7.17520000	2.05300000	0.04740000
	H	-2.65390000	2.34820000	1.35990000
	H	1.43970000	2.44620000	0.38000000
	H	0.75910000	4.04210000	0.01370000
	H	0.92270000	3.47880000	1.68530000
	H	-0.70490000	4.29470000	2.74650000
	H	-2.46150000	4.28630000	2.78920000
	H	-1.56160000	3.00060000	3.61130000
	H	-6.09250000	-2.12630000	2.01820000
	H	-6.21440000	-3.04820000	0.50320000
	H	-5.32390000	-3.71320000	1.87940000
	H	-0.38700000	-2.63350000	-0.58450000
	H	-0.37140000	1.77710000	-2.55740000
2	B3LYP/6-31g (d, p) (0 imaginary Frequencies, solvent=methanol, thermal correction to Gibbs Free Energy= -1251.402930, thermal correction to Gibbs Free Energy= 0.465585)			
	C	1.04580000	-0.61490000	-0.54820000
	C	2.51460000	-1.20410000	-0.63070000
	C	3.47820000	-0.18200000	-1.20740000
	C	3.14540000	1.28370000	-1.26370000
	C	1.81190000	1.81270000	-0.81240000
	C	1.03650000	0.81120000	0.07840000
	C	1.98120000	3.15170000	-0.06180000
	C	0.72030000	3.63110000	0.61480000
	C	-0.34690000	2.82570000	0.76380000
	C	-0.37890000	1.38490000	0.33770000
	O	3.05150000	0.43710000	-2.42870000
	C	0.07750000	-1.53900000	0.17950000
	C	-0.96460000	-2.14230000	-0.41620000
	C	-1.99500000	-2.96110000	0.30860000
	C	-3.36150000	-2.30990000	0.19970000
	C	-3.66890000	-1.25770000	0.98620000

C	-4.91620000	-0.42490000	0.97380000
C	-4.25630000	-2.88370000	-0.86320000
C	-4.67520000	0.83090000	0.14600000
N	-5.61490000	1.09430000	-0.80740000
C	3.03730000	-1.79570000	0.70500000
C	3.64830000	-1.03050000	1.63870000
C	2.85530000	-3.28740000	0.88000000
C	4.25750000	-1.46490000	2.93500000
C	0.72010000	5.05480000	1.08760000
O	-1.17970000	1.31880000	-0.83450000
O	2.50390000	-2.27730000	-1.59020000
O	-3.71180000	1.58010000	0.29270000
H	1.53920000	0.75820000	1.05400000
H	0.67970000	-0.51580000	-1.58170000
H	1.22100000	2.01410000	-1.71780000
H	4.51350000	-0.49500000	-1.16200000
H	3.94600000	2.01120000	-1.26560000
H	2.76820000	3.05870000	0.69830000
H	2.32340000	3.90980000	-0.77800000
H	-1.25980000	3.20340000	1.21900000
H	-0.86850000	0.80130000	1.12580000
H	0.22860000	-1.66350000	1.24980000
H	-1.12200000	-2.00340000	-1.48410000
H	-2.01730000	-3.97260000	-0.11400000
H	-1.72750000	-3.08330000	1.36610000
H	-2.91500000	-0.91100000	1.69460000
H	-5.77980000	-0.98070000	0.59850000
H	-5.16320000	-0.11490000	1.99530000
H	-3.74560000	-2.87740000	-1.83190000
H	-4.51600000	-3.91840000	-0.61650000
H	-5.18850000	-2.32820000	-0.98900000
H	-5.48160000	1.92130000	-1.39270000
H	-6.41300000	0.48670000	-0.99240000
H	3.74920000	0.03870000	1.46100000
H	1.86700000	-3.61330000	0.54260000
H	3.61040000	-3.82850000	0.30030000
H	2.93220000	-3.60720000	1.92210000
H	4.38880000	-2.54540000	3.01880000
H	5.25020000	-1.01400000	3.03730000
H	3.64080000	-1.11990000	3.77020000
H	1.52620000	5.21330000	1.81110000
H	0.87020000	5.73590000	0.24380000
H	-0.22280000	5.32720000	1.57330000
H	-2.09830000	1.49410000	-0.53470000

	H	2.28150000	-1.86280000	-2.44340000
3	B3LYP/6-31g (d, p) (0 imaginary Frequencies, solvent=methanol, thermal correction to Gibbs Free Energy= -1001.981142, thermal correction to Gibbs Free Energy= 0.363314)			
	C	-0.34610000	0.18350000	-0.61170000
	C	-1.07290000	-1.22150000	-0.52920000
	C	-0.10140000	-2.36360000	-0.74250000
	C	1.38980000	-2.16650000	-0.69960000
	C	2.00500000	-0.81070000	-0.48560000
	C	1.01450000	0.20150000	0.14170000
	C	3.26830000	-0.92210000	0.39570000
	C	3.81350000	0.41150000	0.84030000
	C	3.09590000	1.54200000	0.71300000
	C	1.69150000	1.59390000	0.18760000
	O	0.67410000	-2.27120000	-1.94660000
	C	-1.26030000	1.31750000	-0.15960000
	C	-1.81700000	2.21740000	-0.98950000
	C	-2.74910000	3.32710000	-0.60570000
	O	-3.14230000	3.23010000	0.75290000
	C	-1.92220000	-1.43440000	0.75560000
	C	-3.27420000	-1.48980000	0.72680000
	C	-1.16020000	-1.60950000	2.04710000
	C	-4.22000000	-1.64940000	1.87470000
	C	5.20350000	0.40580000	1.40550000
	O	1.77610000	2.17840000	-1.10510000
	O	-1.96620000	-1.26820000	-1.66370000
	H	0.84260000	-0.09770000	1.18260000
	H	-0.11920000	0.36210000	-1.67440000
	H	2.32000000	-0.43440000	-1.46980000
	H	-0.52090000	-3.33470000	-0.51260000
	H	2.02740000	-3.00180000	-0.44160000
	H	3.05250000	-1.52340000	1.28870000
	H	4.03810000	-1.46320000	-0.16960000
	H	3.52830000	2.49760000	0.99980000
	H	1.11730000	2.26770000	0.83470000
	H	-1.46680000	1.37500000	0.90800000
	H	-1.61170000	2.14940000	-2.05660000
	H	-2.26050000	4.29390000	-0.75810000
	H	-3.64920000	3.29500000	-1.22760000
	H	-3.60000000	2.37570000	0.84140000
	H	-3.78000000	-1.38580000	-0.23340000
	H	-0.93730000	-0.63610000	2.49360000
	H	-1.71370000	-2.20200000	2.78150000
	H	-0.21970000	-2.14570000	1.89110000

	H	-3.74900000	-1.51350000	2.85060000
	H	-5.01510000	-0.90060000	1.79600000
	H	-4.68230000	-2.64040000	1.84240000
	H	5.25160000	-0.24490000	2.28460000
	H	5.91590000	0.03790000	0.66020000
	H	5.52730000	1.40580000	1.71250000
	H	0.91280000	2.58840000	-1.28270000
	H	-1.39690000	-1.40370000	-2.44320000
4	B3LYP/6-31g (d, p) (0 imaginary Frequencies, solvent=methanol, thermal correction to Gibbs Free Energy= -1117.476395, thermal correction to Gibbs Free Energy= 0.394166)			
	C	0.30840000	0.31350000	0.44580000
	C	0.76530000	1.82460000	0.58560000
	C	2.19800000	1.93260000	1.06500000
	C	3.13650000	0.75700000	1.04770000
	C	2.68840000	-0.61120000	0.61570000
	C	1.38840000	-0.58110000	-0.22610000
	C	3.80340000	-1.32980000	-0.17450000
	C	3.34970000	-2.60680000	-0.84050000
	C	2.04660000	-2.92690000	-0.93870000
	C	0.93080000	-2.04270000	-0.45600000
	O	2.49360000	1.19840000	2.26110000
	C	-1.04490000	0.19350000	-0.25240000
	C	-2.13640000	-0.32930000	0.32970000
	C	-3.41330000	-0.42120000	-0.34470000
	C	-4.53720000	-0.96450000	0.15740000
	C	-5.73730000	-0.93540000	-0.72660000
	O	-6.81460000	-1.41790000	-0.39760000
	C	-4.74260000	-1.60240000	1.49670000
	C	0.53740000	2.69150000	-0.68630000
	C	-0.38780000	3.67830000	-0.73010000
	C	1.42590000	2.40140000	-1.87150000
	C	-0.74540000	4.56450000	-1.88080000
	C	4.43570000	-3.49590000	-1.37260000
	O	0.43380000	-2.60390000	0.75320000
	O	-0.03150000	2.38440000	1.65090000
	H	1.62790000	-0.16290000	-1.21090000
	H	0.17520000	-0.07010000	1.46950000
	H	2.50610000	-1.19490000	1.53000000
	H	2.59600000	2.93770000	1.00630000
	H	4.20240000	0.92990000	0.98060000
	H	4.20480000	-0.66110000	-0.94740000
	H	4.63070000	-1.54880000	0.51290000
	H	1.75240000	-3.86380000	-1.40570000

	H	0.12610000	-2.06550000	-1.19940000
	H	-1.10100000	0.56320000	-1.27370000
	H	-2.05850000	-0.69600000	1.34990000
	H	-3.42800000	0.00540000	-1.34770000
	H	-5.60540000	-0.45260000	-1.70960000
	H	-3.83980000	-1.62100000	2.11120000
	H	-5.50900000	-1.06040000	2.06120000
	H	-5.07200000	-2.64010000	1.37660000
	H	-0.99000000	3.86800000	0.15900000
	H	0.99410000	1.60600000	-2.48590000
	H	1.57400000	3.27970000	-2.50660000
	H	2.42900000	2.09600000	-1.56020000
	H	-0.32760000	4.23250000	-2.83370000
	H	-1.83400000	4.58510000	-1.99820000
	H	-0.40560000	5.58580000	-1.68500000
	H	5.03180000	-2.96030000	-2.11840000
	H	5.09740000	-3.81520000	-0.56110000
	H	4.03390000	-4.39580000	-1.84990000
	H	0.25140000	-3.54350000	0.58590000
	H	0.28620000	1.96260000	2.46990000
5	B3LYP/6-31g (d, p) (0 imaginary Frequencies, solvent=methanol, thermal correction to Gibbs Free Energy= -1192.719060, thermal correction to Gibbs Free Energy= 0.399097)			
	O	5.48880000	-0.11570000	1.70140000
	C	5.66340000	-0.55300000	0.44300000
	C	4.42300000	-0.57890000	-0.37720000
	C	3.25280000	-0.17100000	0.15380000
	O	6.76850000	-0.89270000	0.05560000
	C	1.96760000	-0.13430000	-0.51190000
	C	0.84690000	0.27660000	0.10350000
	C	-0.52110000	0.32430000	-0.56970000
	C	4.64530000	-1.08480000	-1.77370000
	C	-1.08630000	1.80110000	-0.69250000
	C	-2.51990000	1.79900000	-1.19130000
	C	-3.37610000	0.56410000	-1.14820000
	C	-2.83900000	-0.75750000	-0.67580000
	C	-1.53070000	-0.62150000	0.14290000
	C	-3.89550000	-1.51520000	0.15650000
	C	-3.35430000	-2.74350000	0.84850000
	C	-2.03250000	-2.98190000	0.93020000
	C	-0.98060000	-2.04520000	0.40410000
	O	-2.75440000	1.01660000	-2.36970000
	O	-0.47190000	-2.60990000	-0.79890000
	C	-4.37490000	-3.68070000	1.42500000

	O	-0.33900000	2.46610000	-1.72700000
	C	-0.93360000	2.64980000	0.59710000
	C	-1.84980000	2.61290000	1.59210000
	C	0.28260000	3.54830000	0.65390000
	C	-1.87370000	3.41460000	2.85600000
	H	-1.77700000	-0.18720000	1.12150000
	H	-0.38980000	-0.05400000	-1.59520000
	H	-2.63540000	-1.35950000	-1.57340000
	H	6.38950000	-0.15960000	2.08360000
	H	3.23480000	0.17710000	1.18680000
	H	1.90510000	-0.45240000	-1.54850000
	H	0.88500000	0.59300000	1.14420000
	H	5.04870000	-2.10310000	-1.74830000
	H	3.73700000	-1.11620000	-2.37900000
	H	5.36080000	-0.44330000	-2.29980000
	H	-2.98640000	2.77560000	-1.16090000
	H	-4.45190000	0.66420000	-1.09400000
	H	-4.32140000	-0.84820000	0.91770000
	H	-4.72070000	-1.80270000	-0.50760000
	H	-1.67370000	-3.88580000	1.41620000
	H	-0.16390000	-1.99900000	1.13310000
	H	-0.18590000	-3.51560000	-0.59490000
	H	-4.98950000	-3.16100000	2.16720000
	H	-5.03010000	-4.06200000	0.63520000
	H	-3.91120000	-4.54100000	1.91890000
	H	-0.57260000	2.01190000	-2.55670000
	H	-2.70520000	1.94640000	1.49790000
	H	0.12340000	4.43580000	0.03270000
	H	0.52110000	3.88060000	1.66720000
	H	1.17780000	3.03350000	0.29270000
	H	-1.17730000	4.25520000	2.85690000
	H	-2.87620000	3.83070000	3.00140000
	H	-1.64740000	2.76950000	3.71020000

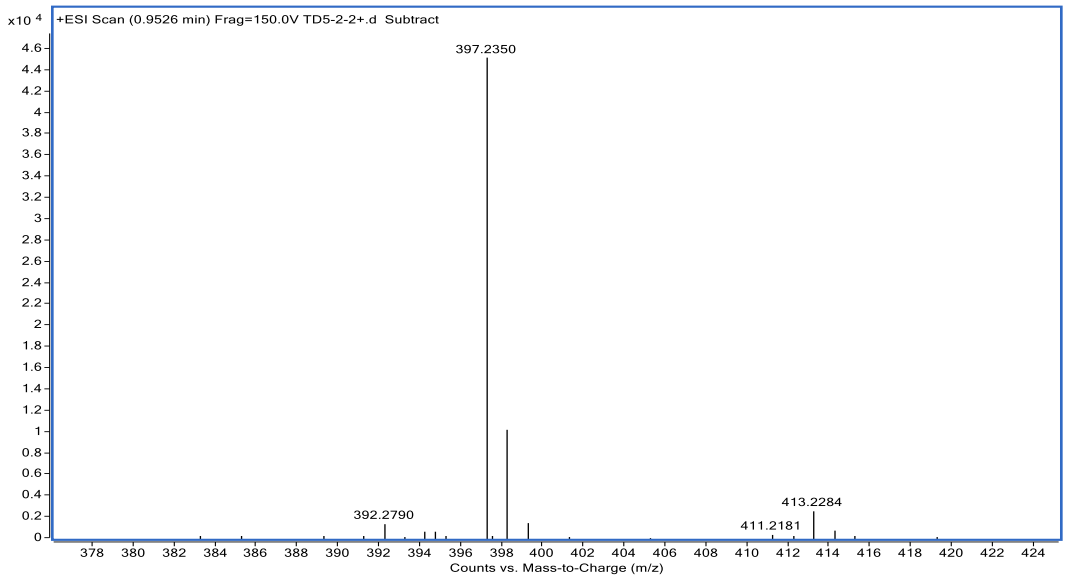

Figure S1. HRESIMS spectrum of compound **1**

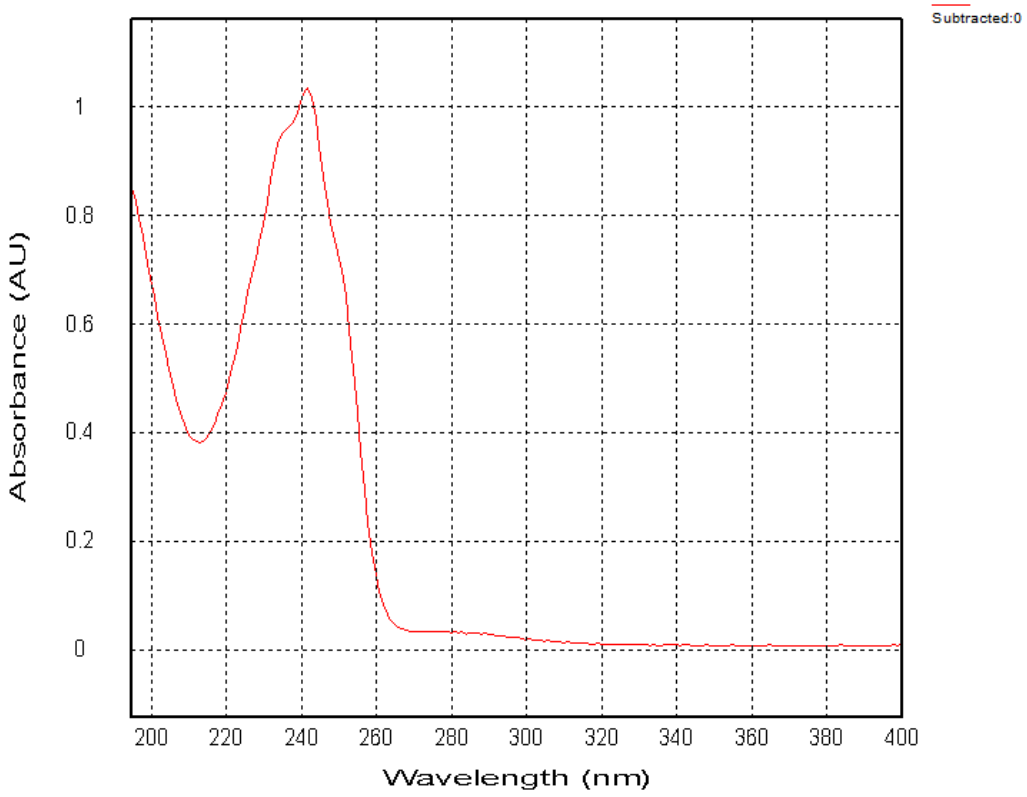

Figure S2. UV-vis spectrum of compound **1** in MeOH

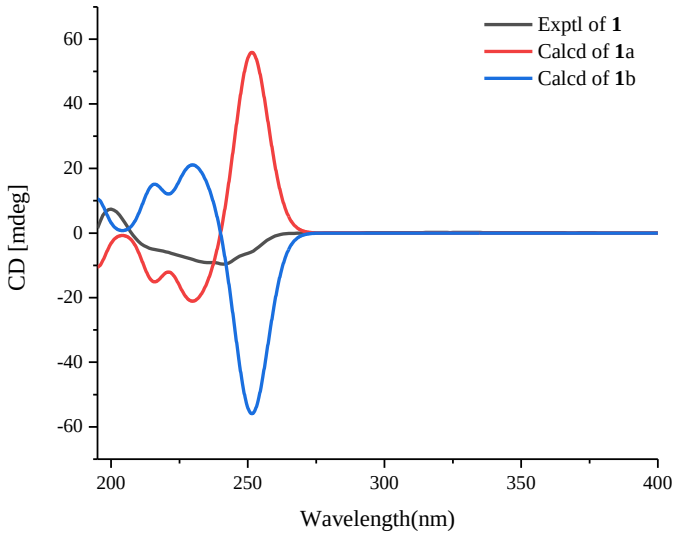

Figure S3. Experimental and calculated ECD spectra of compound **1**

(**1**a: 8*R*,9*S*,10*R*,14*S*,15*R*,16*R*,17*R*; **1**b: 8*S*,9*R*,10*S*,14*R*,15*S*,16*S*,17*S*)

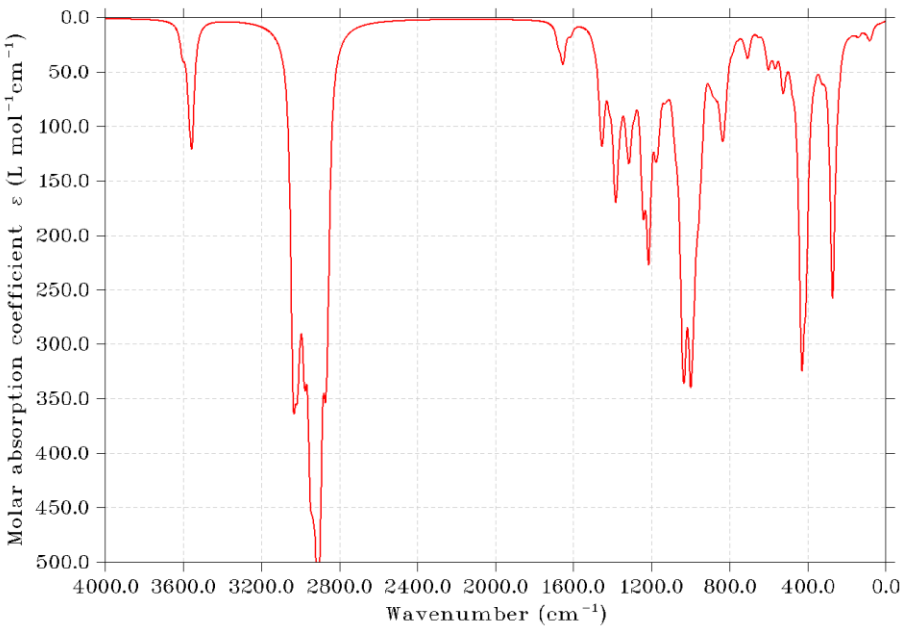

Figure S4. The computed IR spectrum of compound **1** at B3LYP/6-31g (d, p) level in methanol[1]

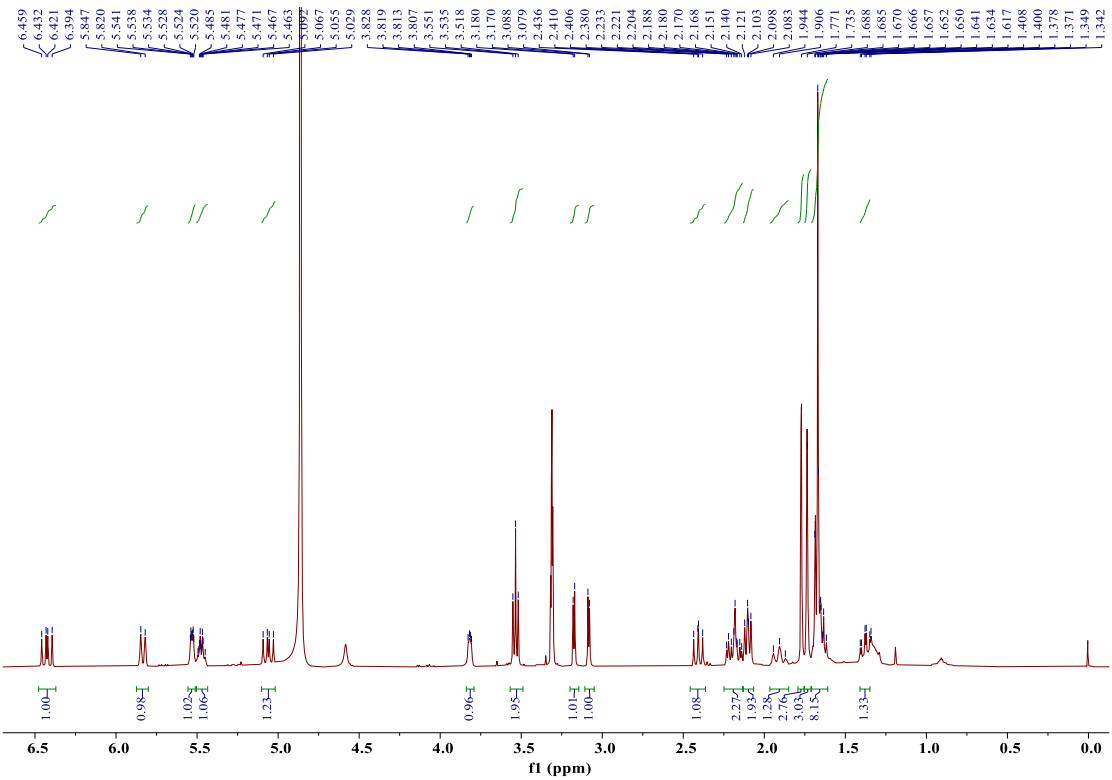

Figure S5. ^{1}H NMR spectrum of compound **1** in methanol-d_4 (400 MHz)

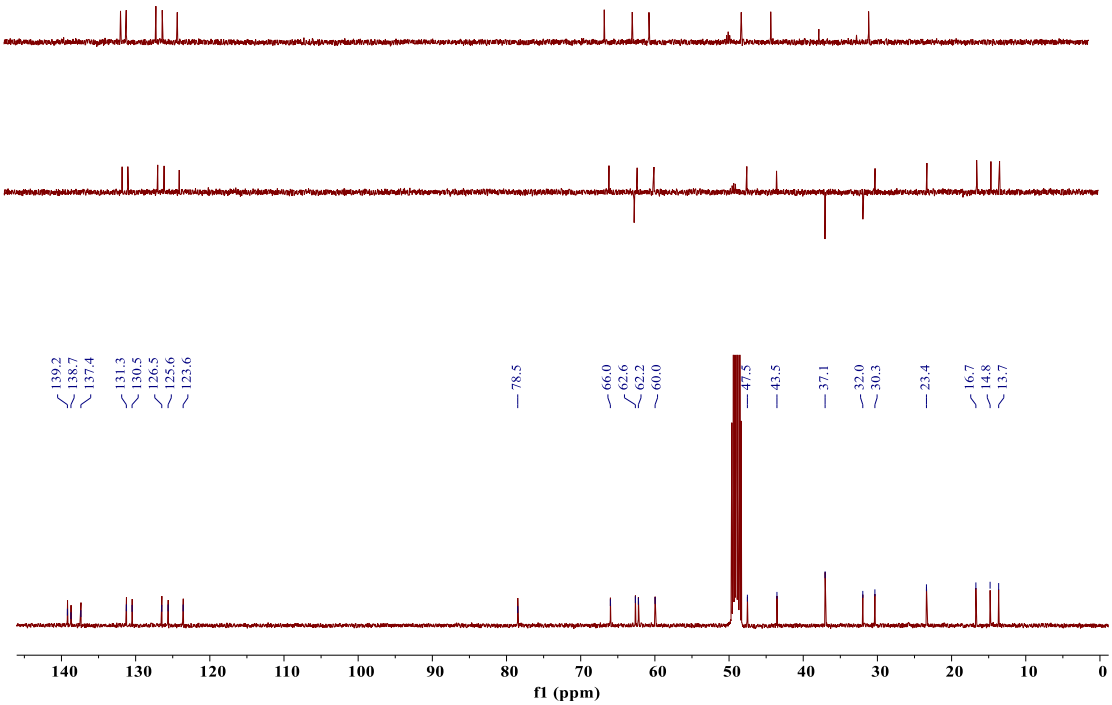

Figure S6. ^{13}C NMR and DEPT spectra of compound **1** in methanol-d_4 (100 MHz)

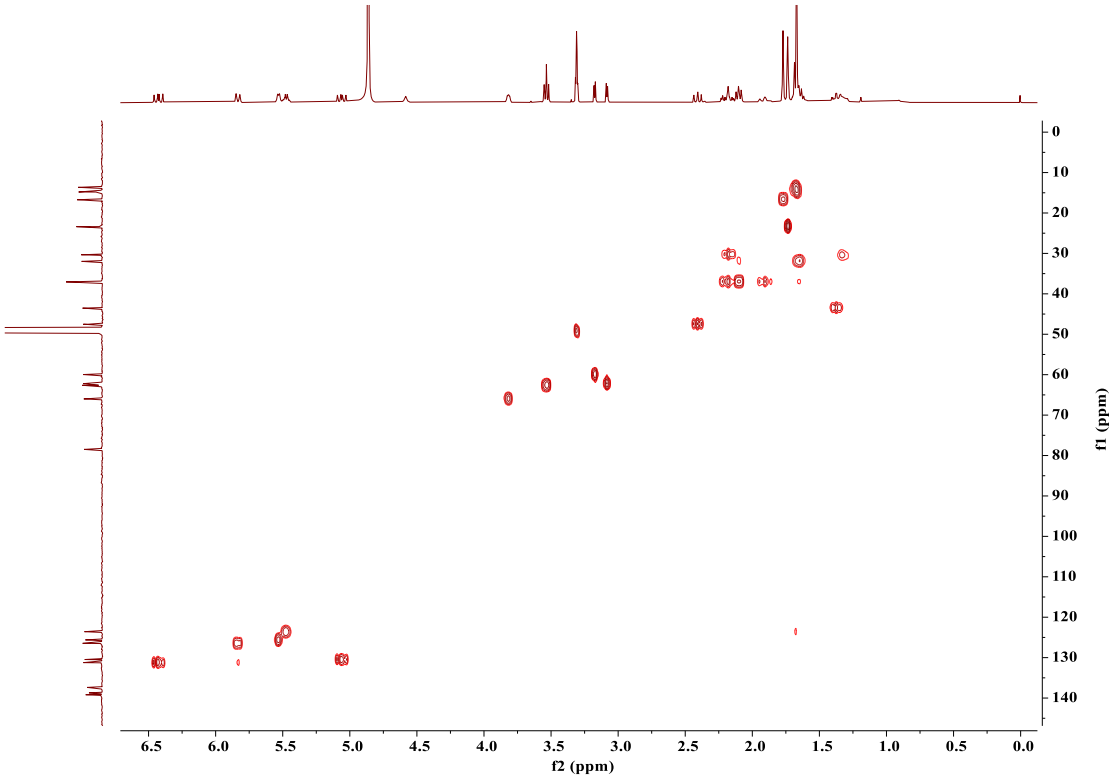

Figure S7. HSQC spectrum of compound **1** in methanol-d_4 (^{1}H-400 MHz)

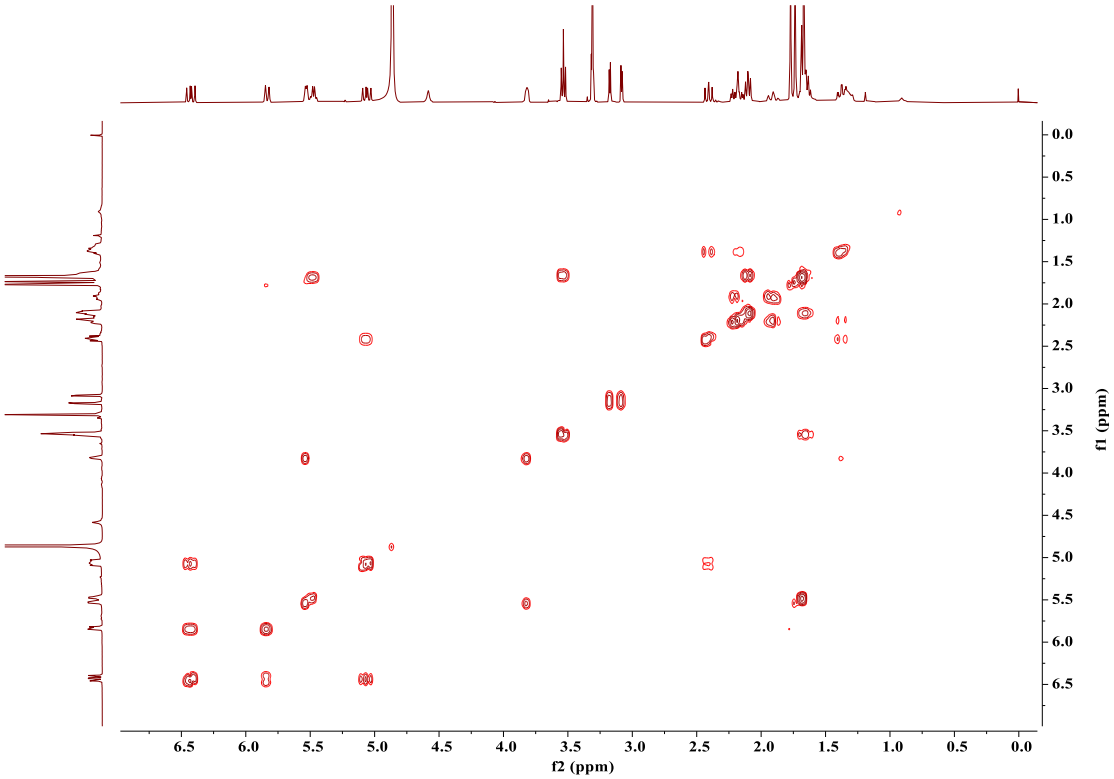

Figure S8. ^{1}H-^{1}H COSY spectrum of compound **1** in methanol-d_4 (400 MHz)

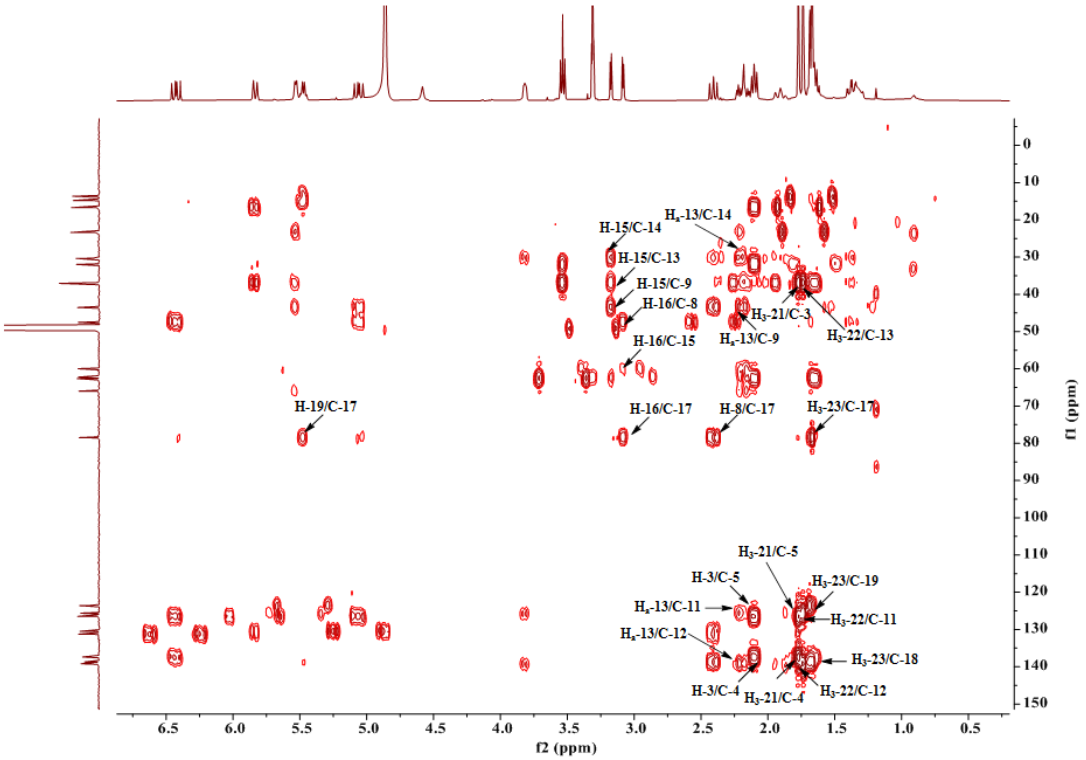

Figure S9. HMBC spectrum of compound **1** in methanol-d_4 (400 MHz)

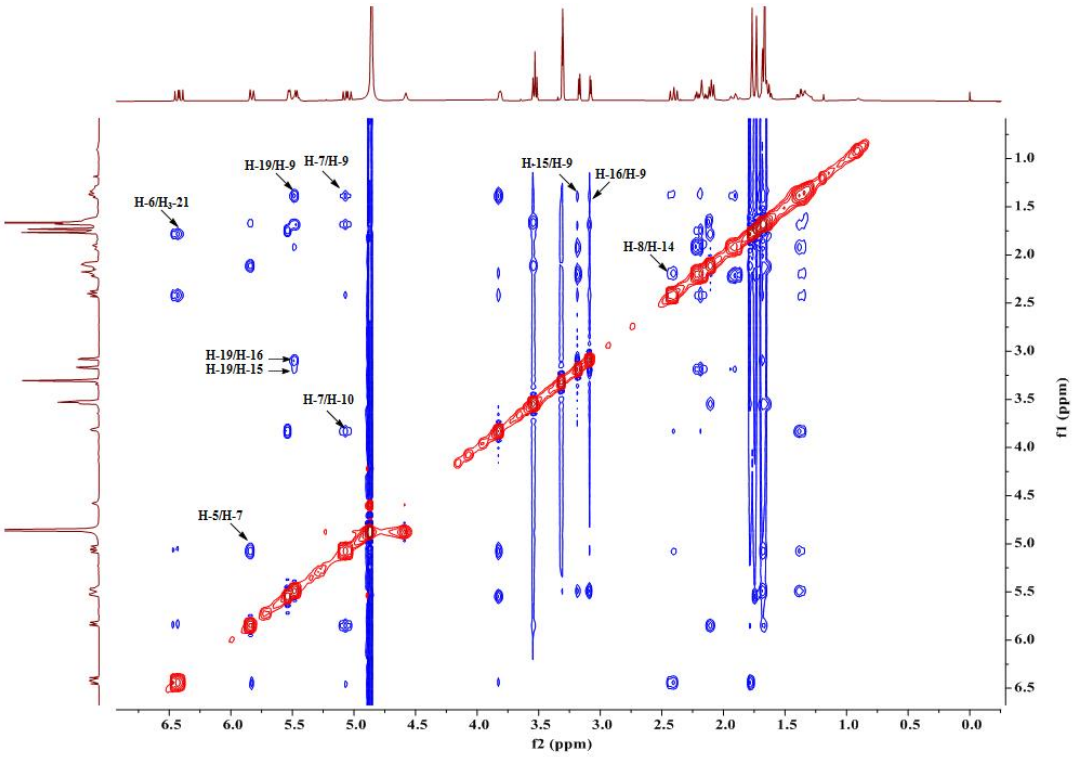

Figure S10. NOESY spectrum of compound **1** in methanol-d_4 (400 MHz)

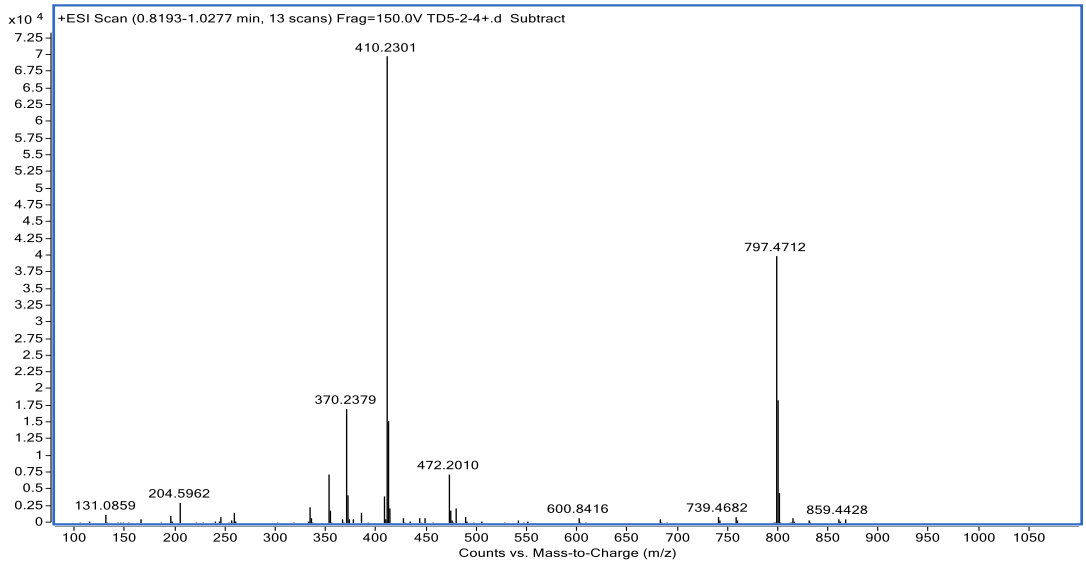

Figure S11. HRESIMS spectrum of compound **2**

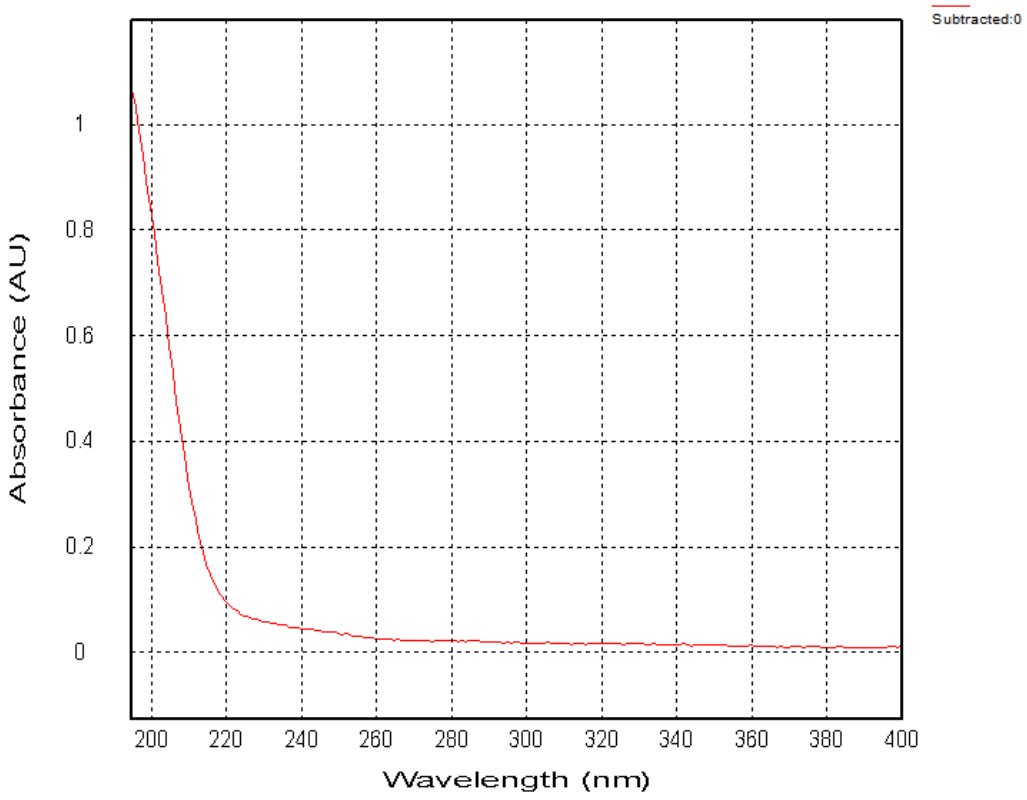

Figure S12. UV-vis spectrum of compound **2** in MeOH

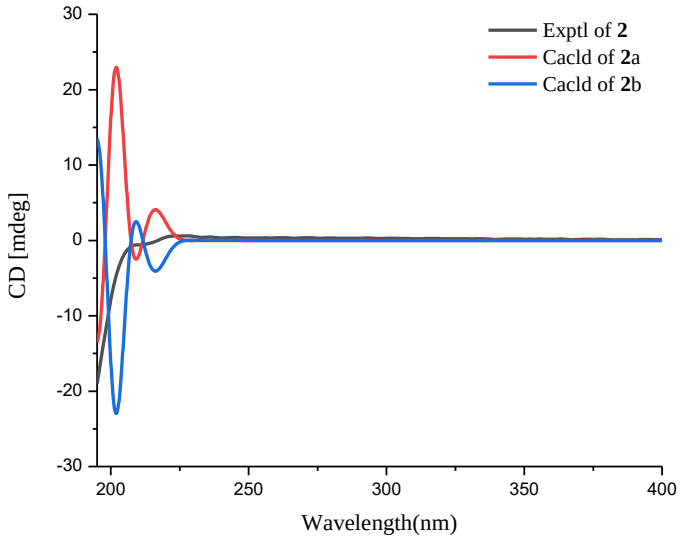

Figure S13. Experimental and calculated ECD spectra of compound **2**

(**2**a: 8*R*,9*S*,10*R*,14*S*,15*R*,16*R*,17*R*; **2**b: 8*S*,9*R*,10*S*,14*R*,15*S*,16*S*,17*S*)

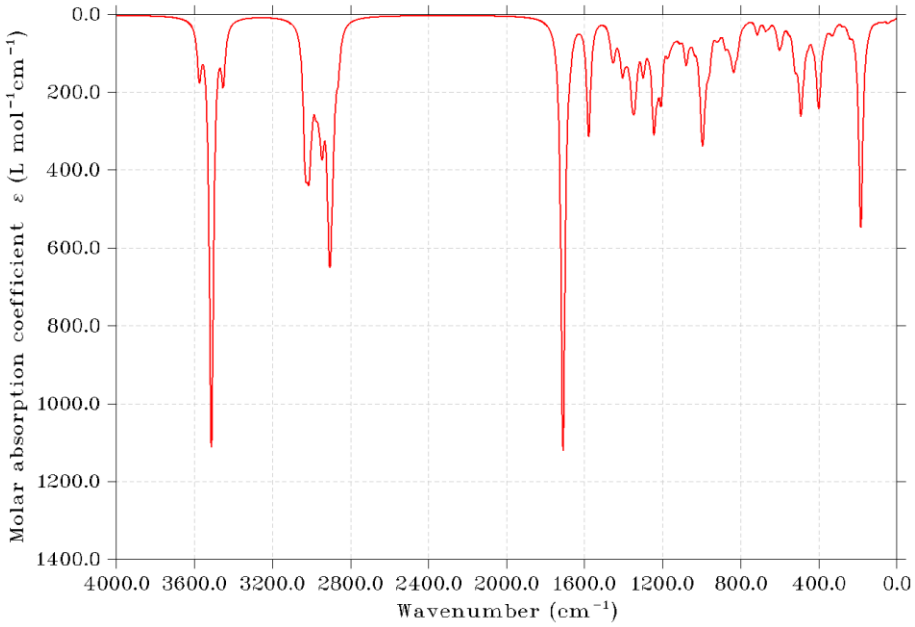

Figure S14. The computed IR spectrum of compound **2** at B3LYP/6-31g (d, p) level in methanol

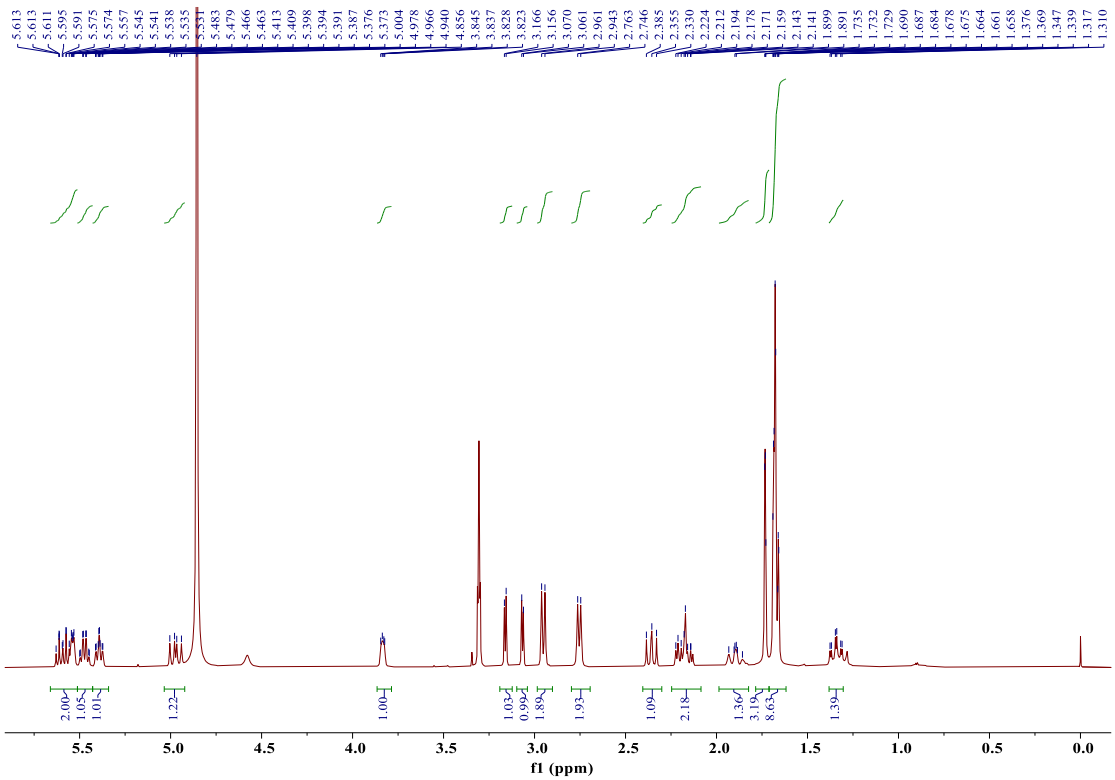

Figure S15. ^{1}H NMR spectrum of compound **2** in methanol-d_4 (400 MHz)

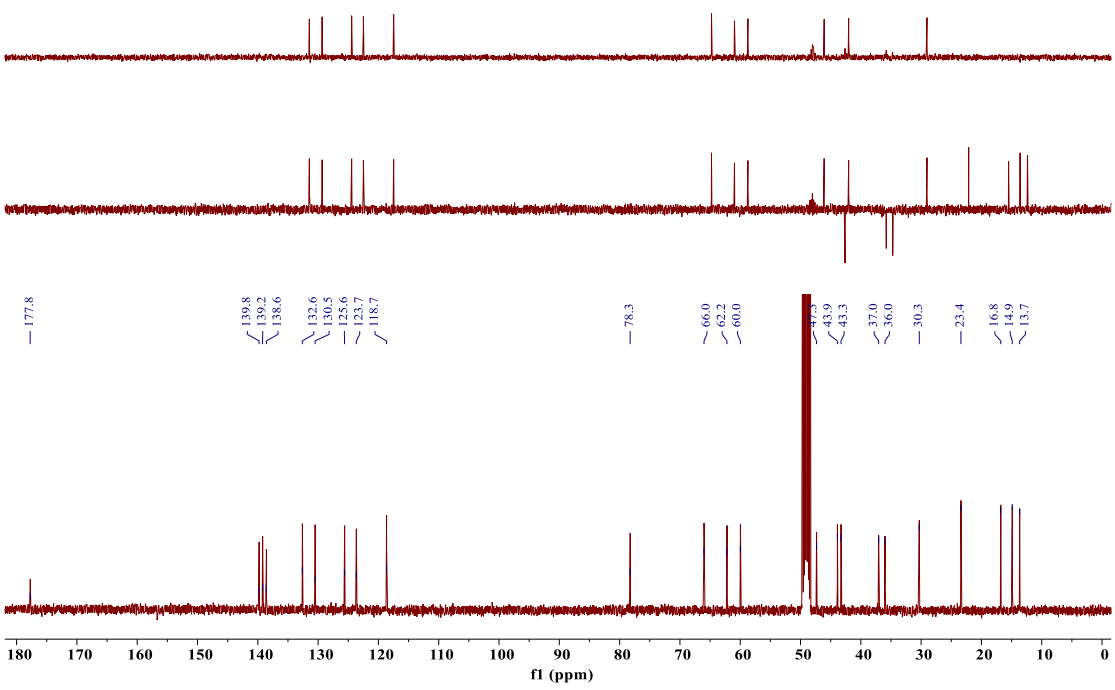

Figure S16. ^{13}C NMR and DEPT spectra of compound **2** in methanol-d_4 (100 MHz)

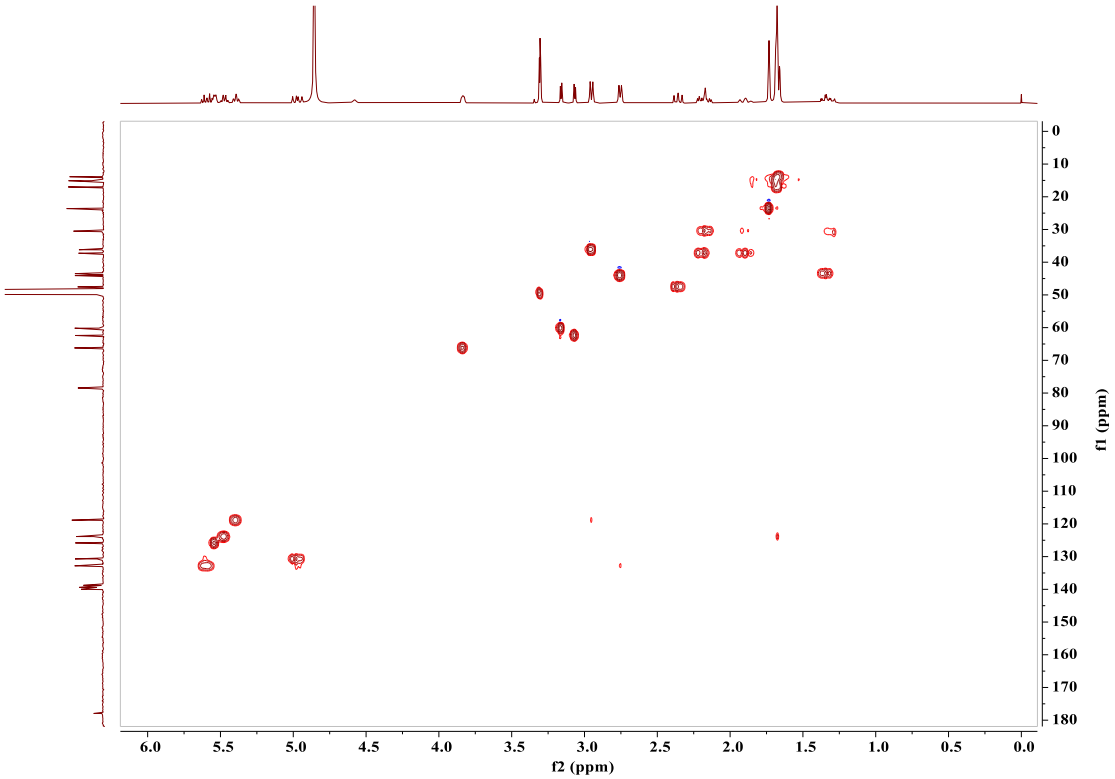

Figure S17. HSQC spectrum of compound **2** in methanol-d_4 (^{1}H-400 MHz)

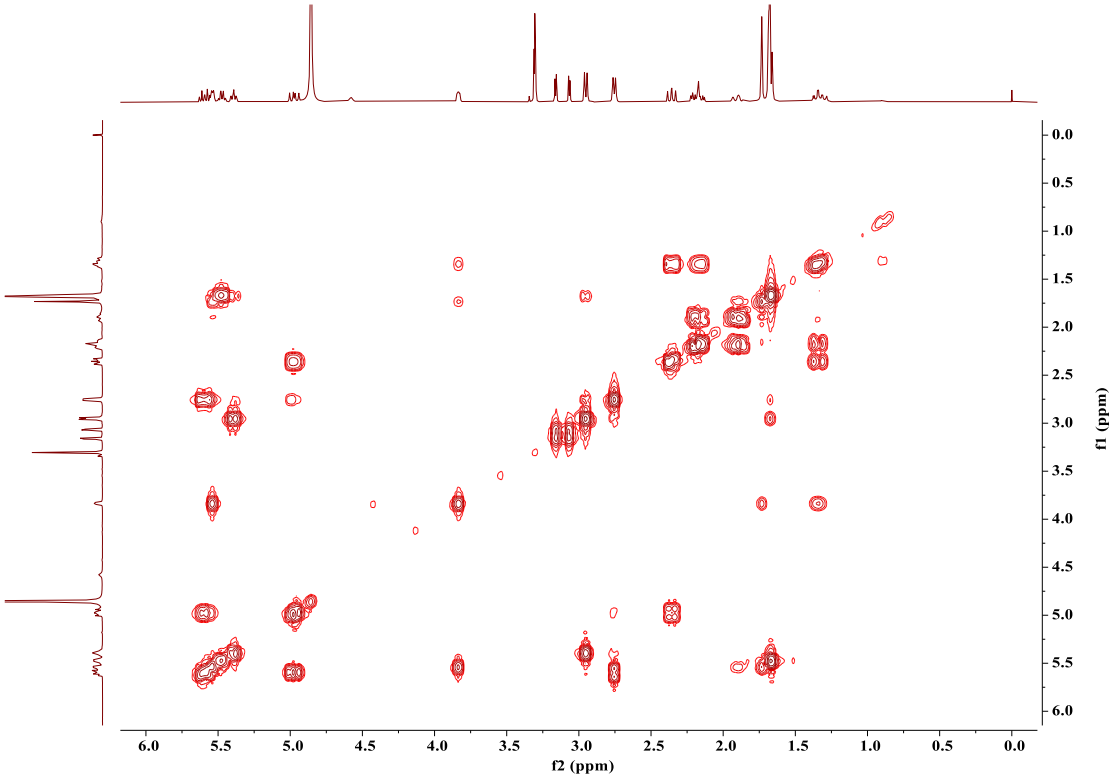

Figure S18. ^{1}H-^{1}H COSY spectrum of compound **2** in methanol-d_4 (400 MHz)

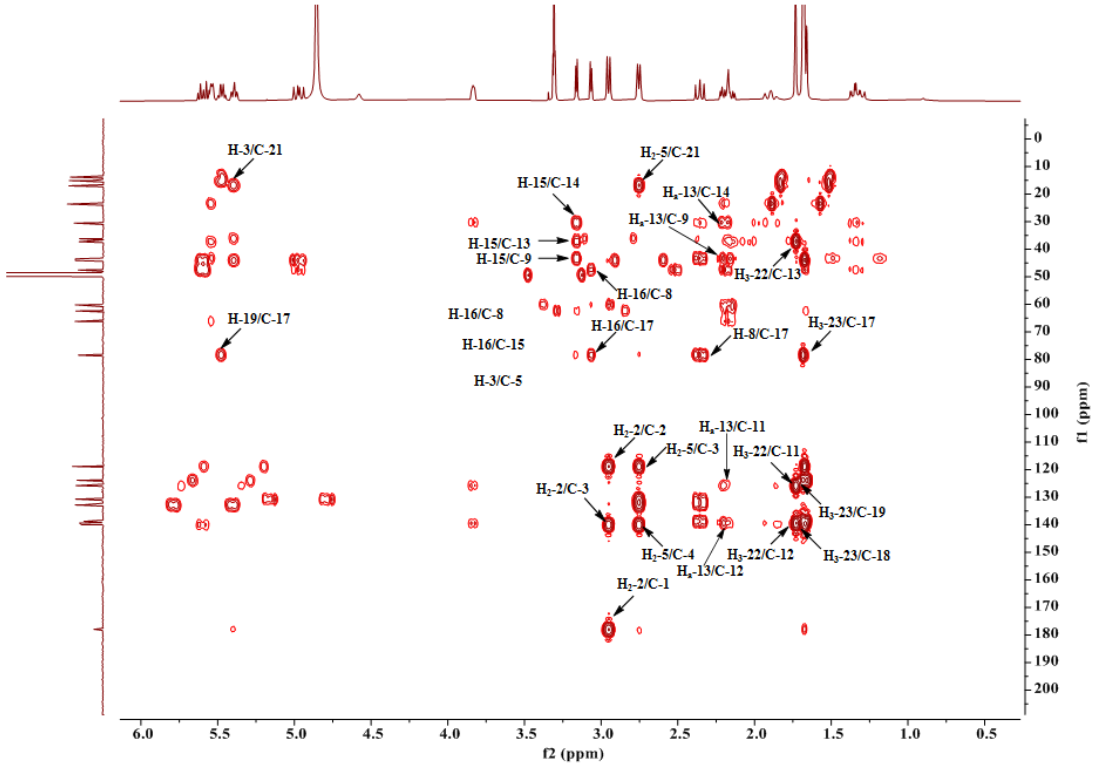

Figure S19. HMBC spectrum of compound **2** in methanol-d_4 (400 MHz)

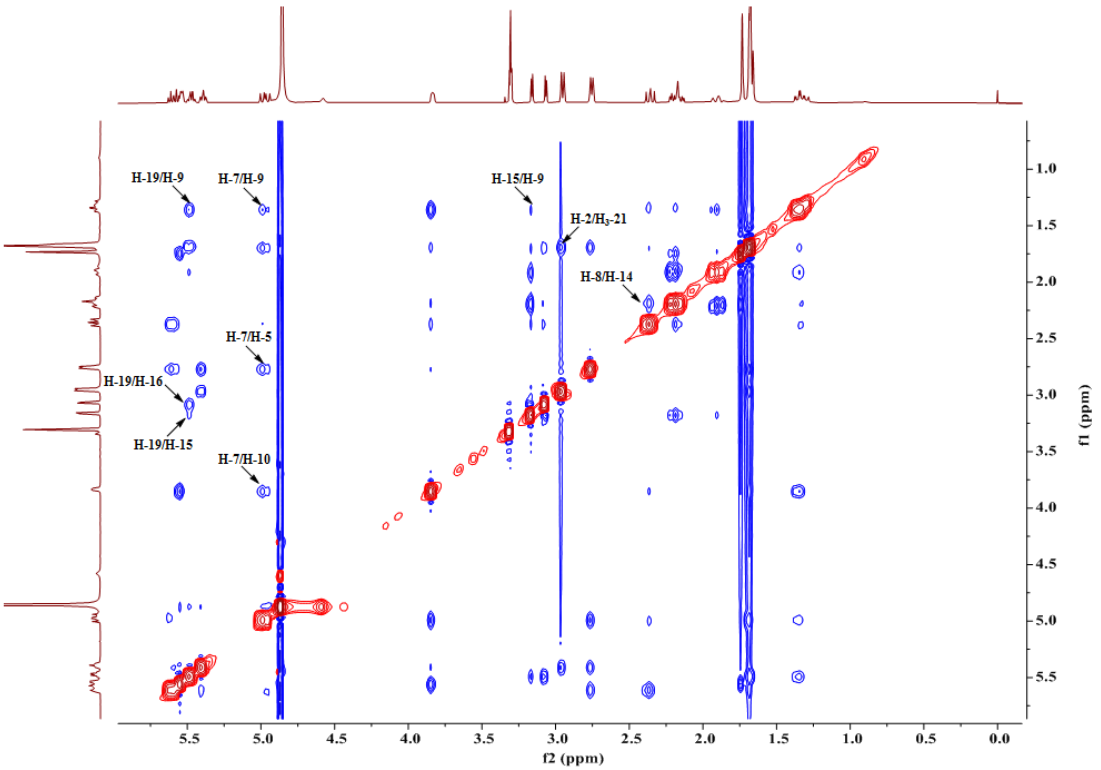

Figure S20. NOESY spectrum of compound **2** in methanol-d_4 (400 MHz)

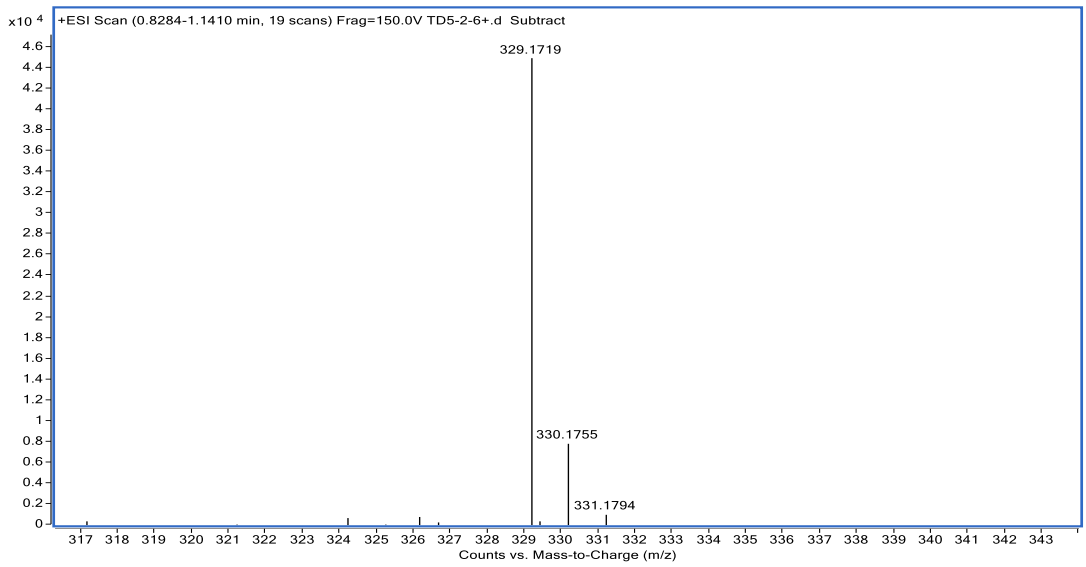

Figure S21. HRESIMS spectrum of compound **3**

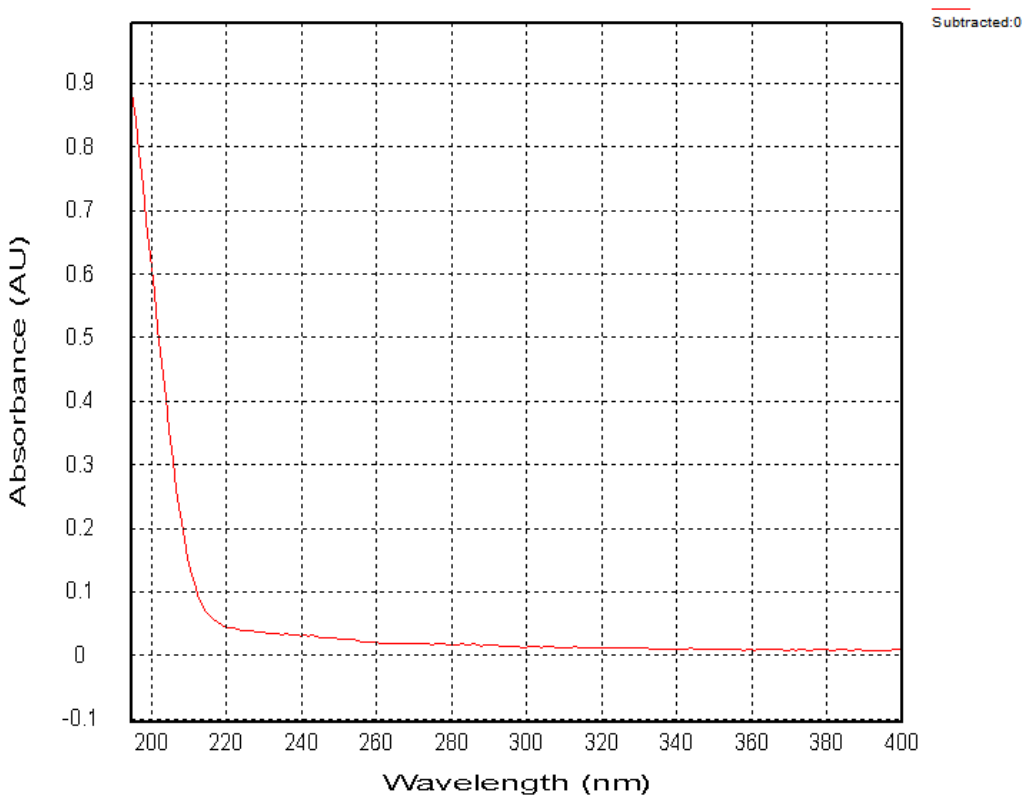

Figure S22. UV-vis spectrum of compound **3** in MeOH

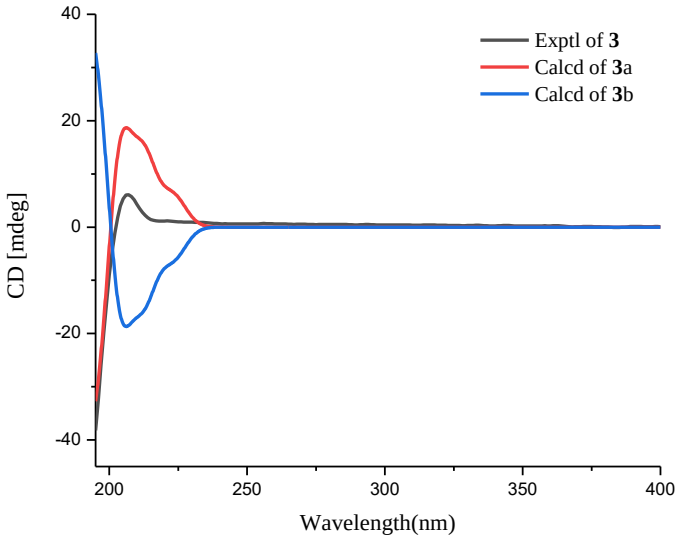

Figure S23. Experimental and calculated ECD spectra of compound **3**

(**3**a: 4*R*,5*S*,6*R*,10*S*,11*R*,12*R*,13*R*; **3**b: 4*S*,5*R*,6*S*,10*R*,11*S*,12*S*,13*S*)

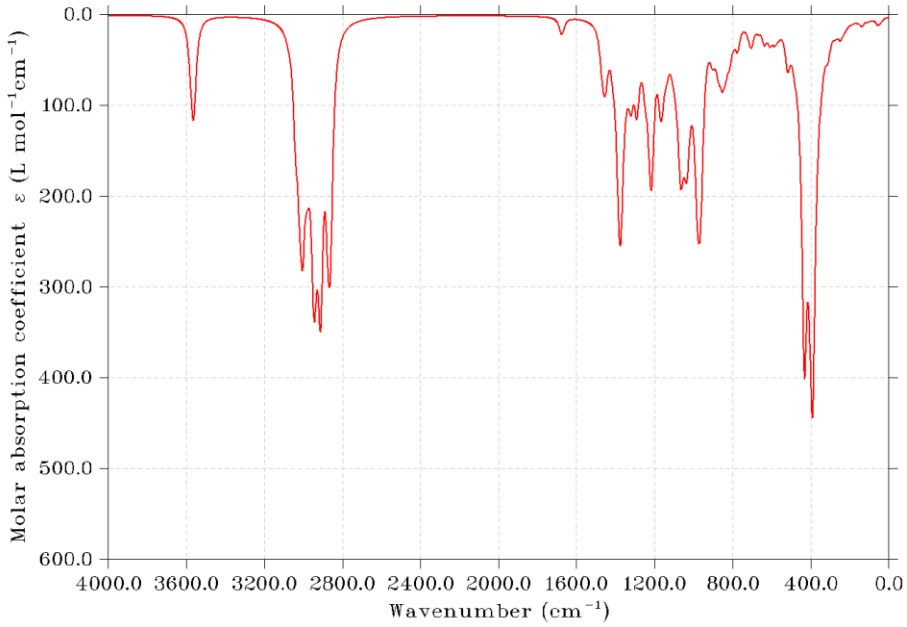

Figure S24. The computed IR spectrum of compound **3** at B3LYP/6-31g (d, p) level in methanol

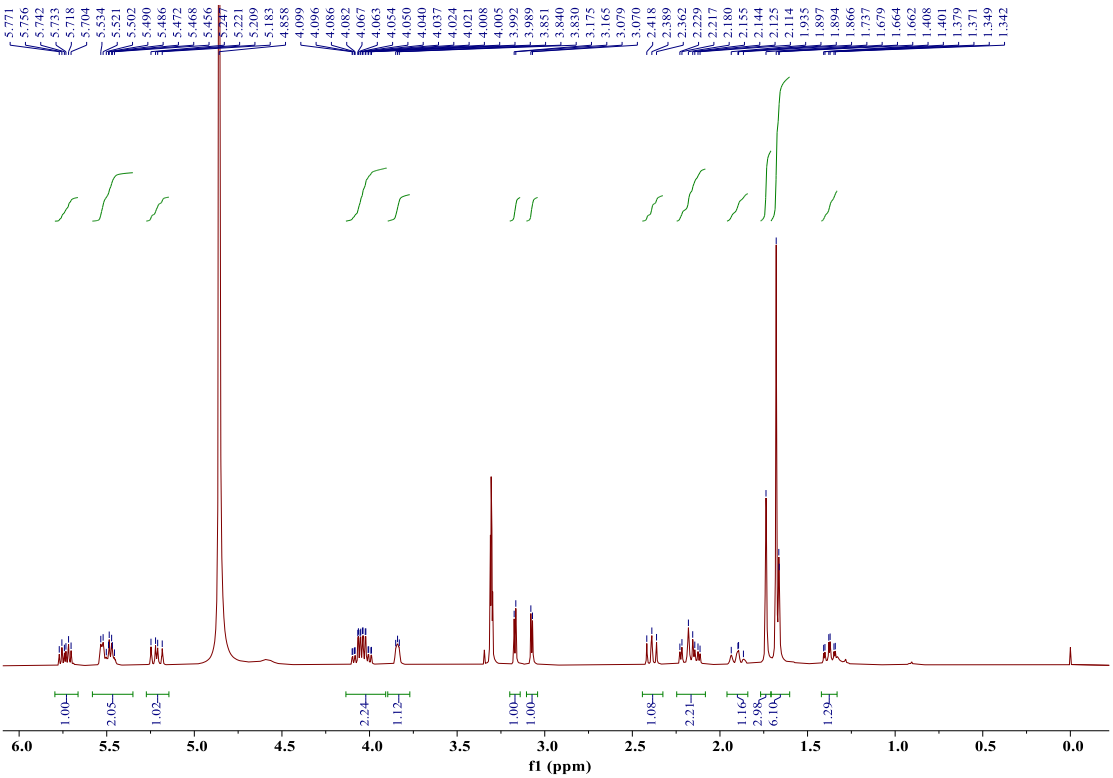

Figure S25. ^{1}H NMR spectrum of compound **3** in methanol-d_4 (400 MHz)

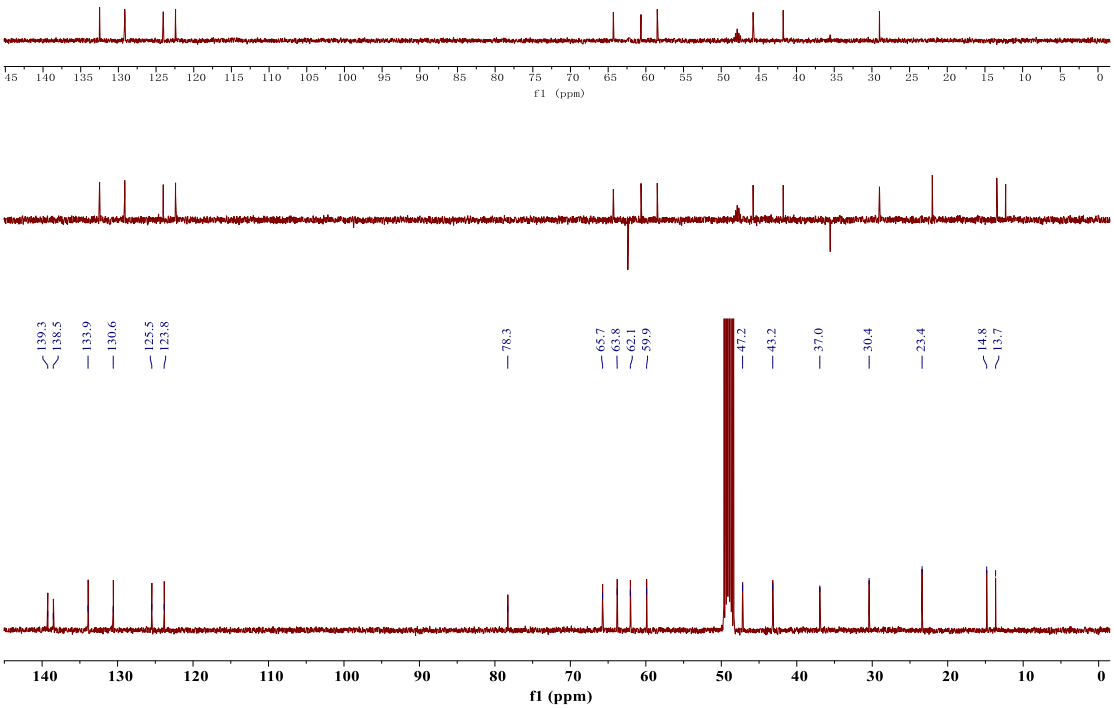

Figure S26. ^{13}C NMR and DEPT spectra of compound **3** in methanol-d_4 (100 MHz)

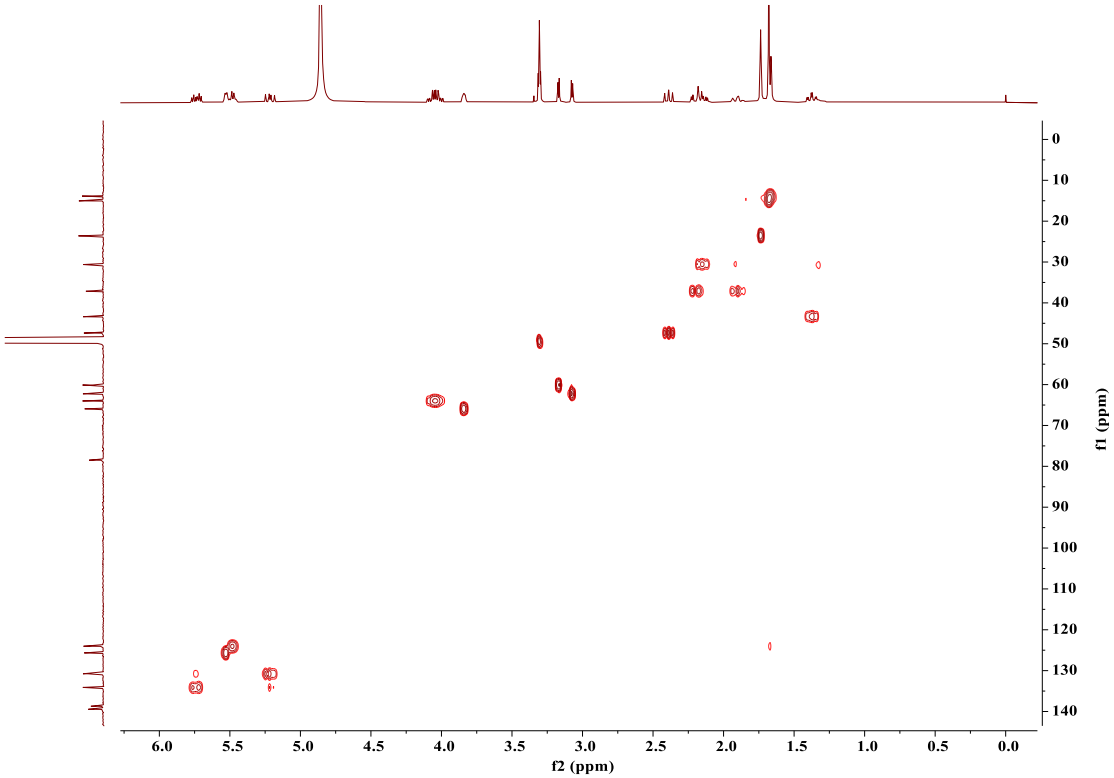

Figure S27. HSQC spectrum of compound **3** in methanol-d_4 (^{1}H-400 MHz)

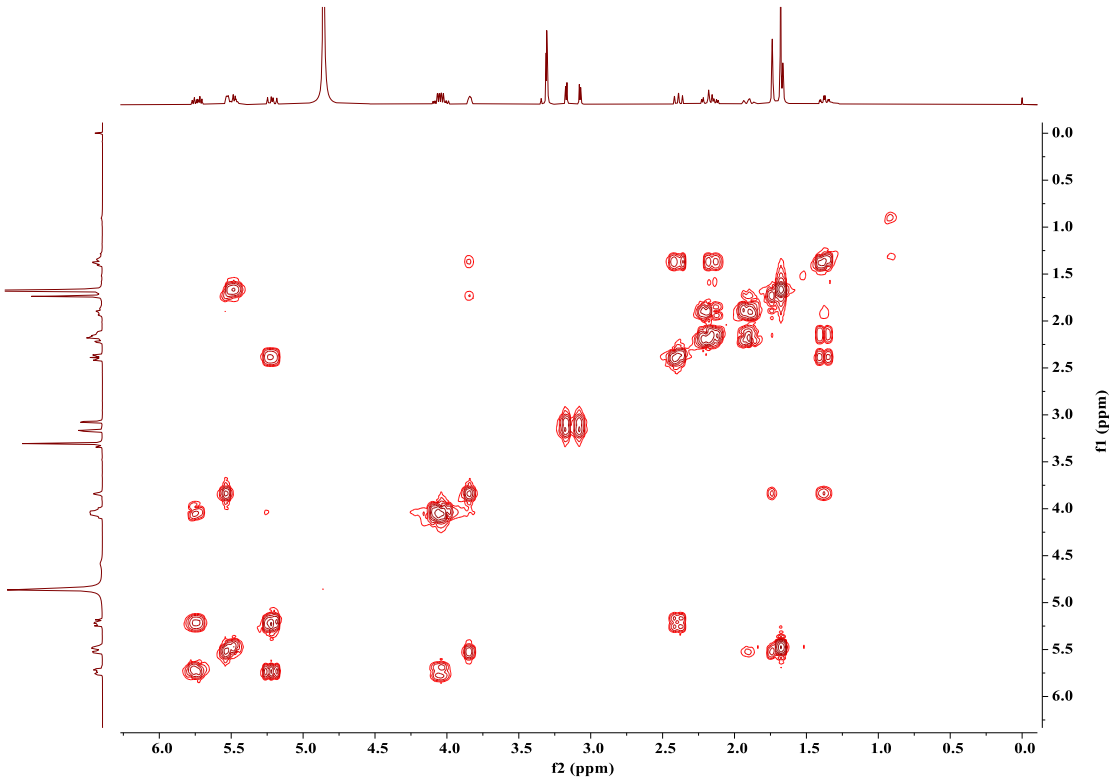

Figure S28. ^{1}H-^{1}H COSY spectrum of compound **3** in methanol-d_4 (400 MHz)

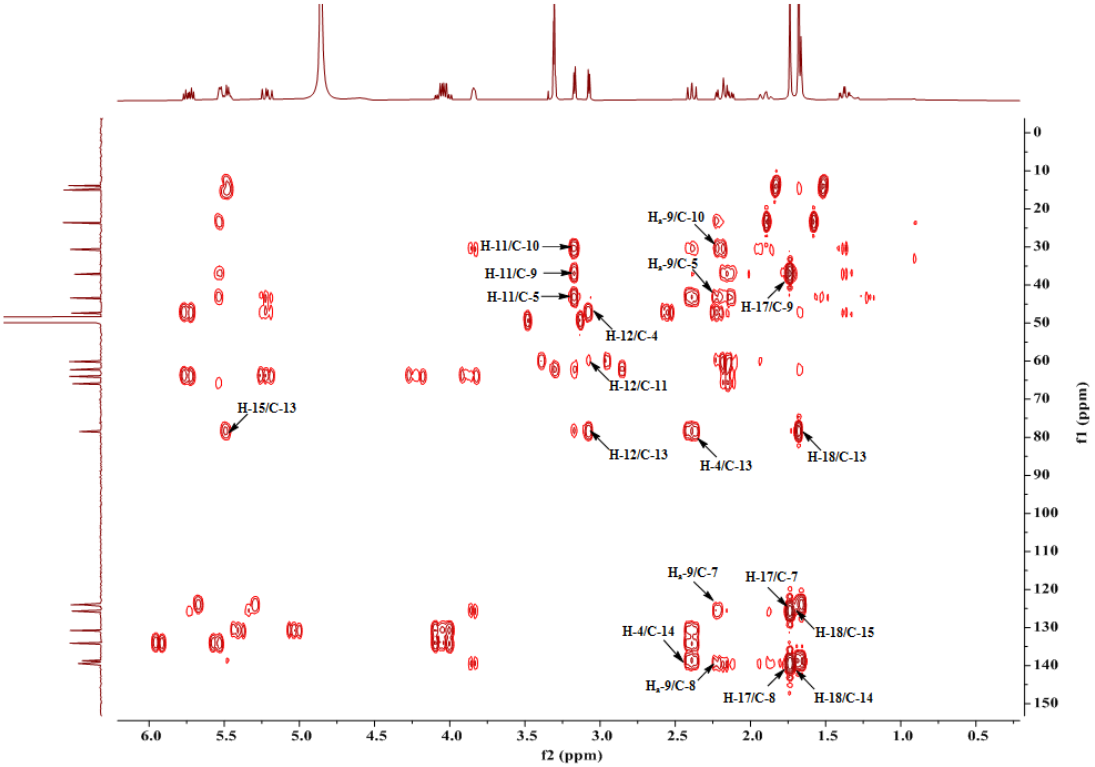

Figure S29. HMBC spectrum of compound **3** in methanol-d_4 (400 MHz)

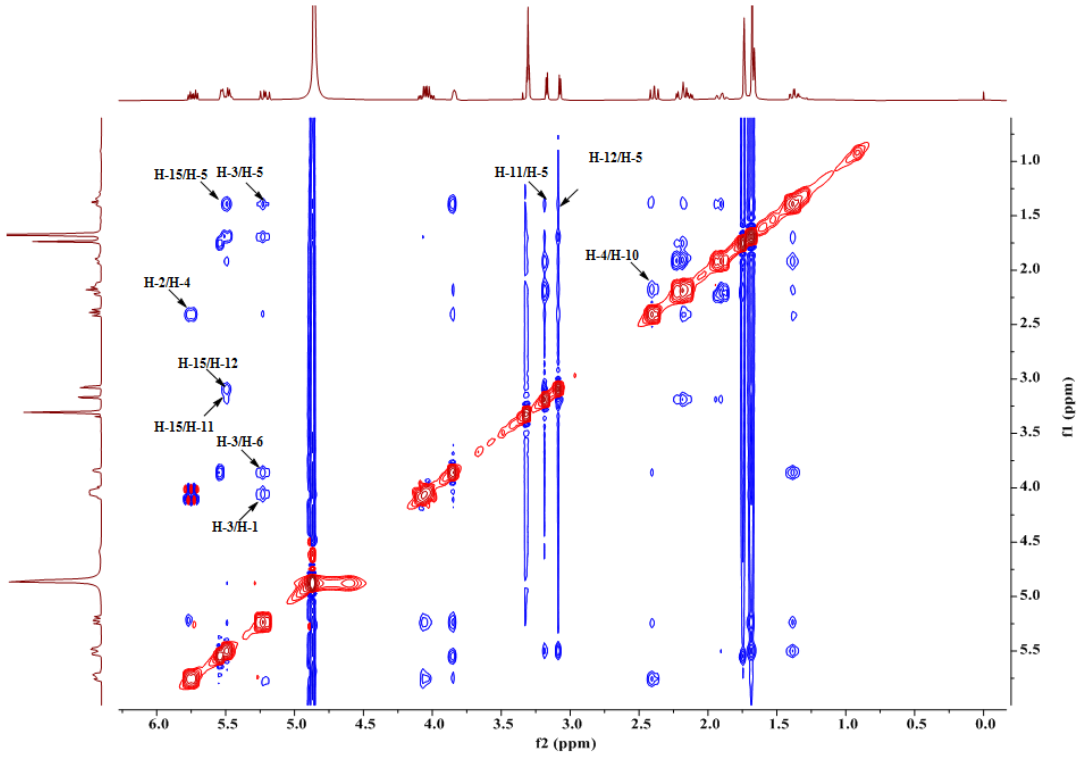

Figure S30. NOESY spectrum of compound **3** in methanol-d_4 (400 MHz)

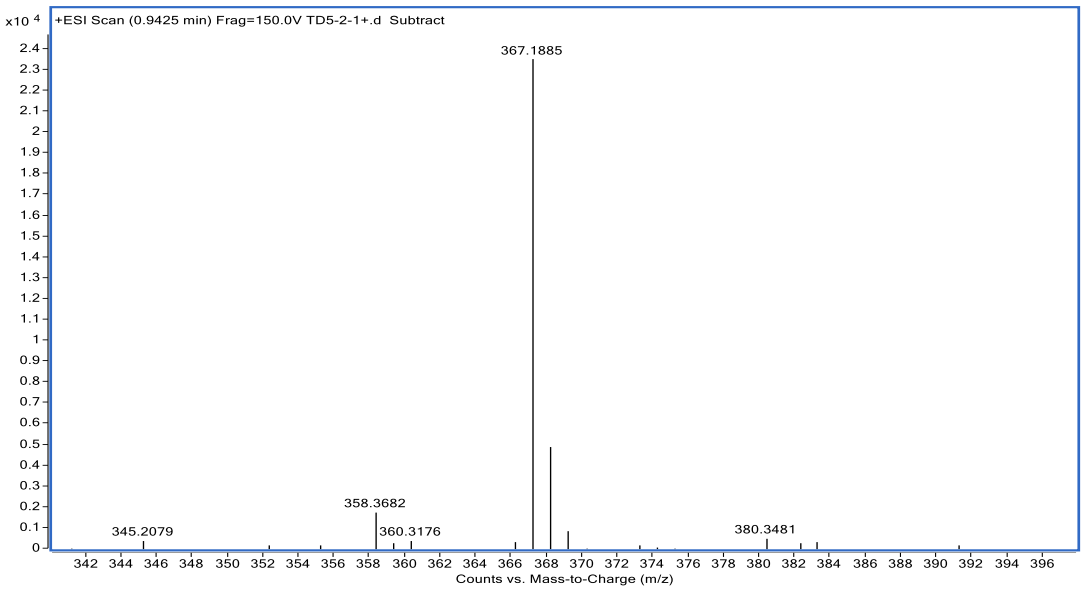

Figure S31. HRESIMS spectrum of compound **4**

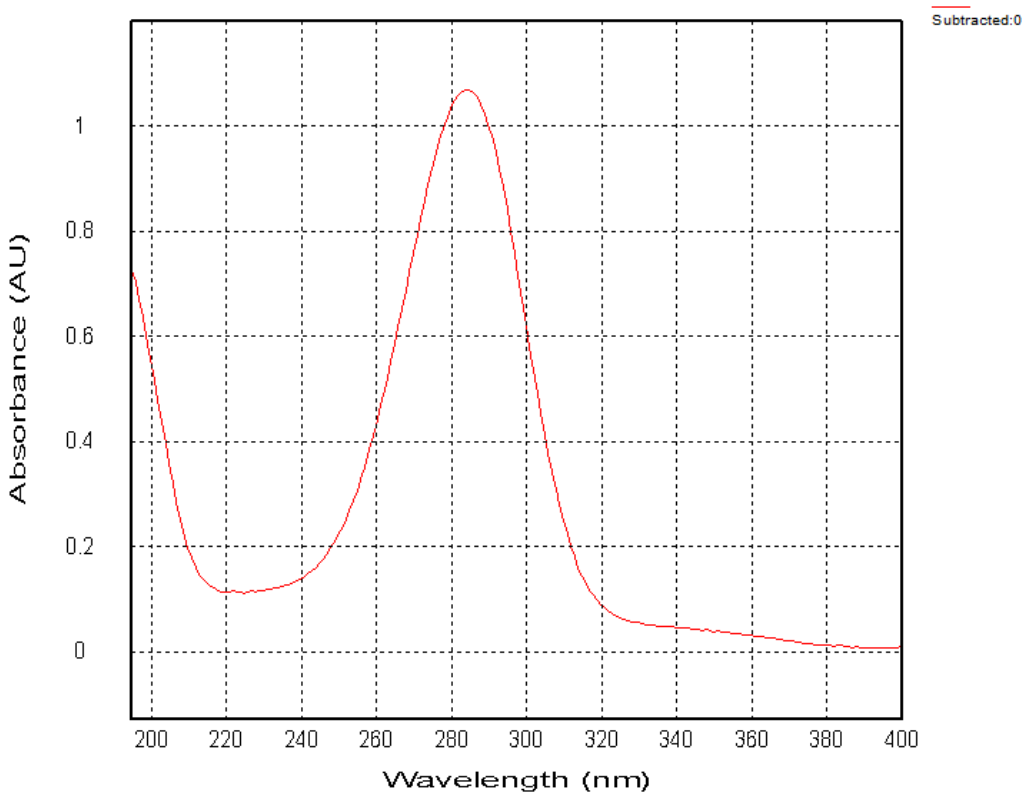

Figure S32. UV-vis spectrum of compound **4** in MeOH

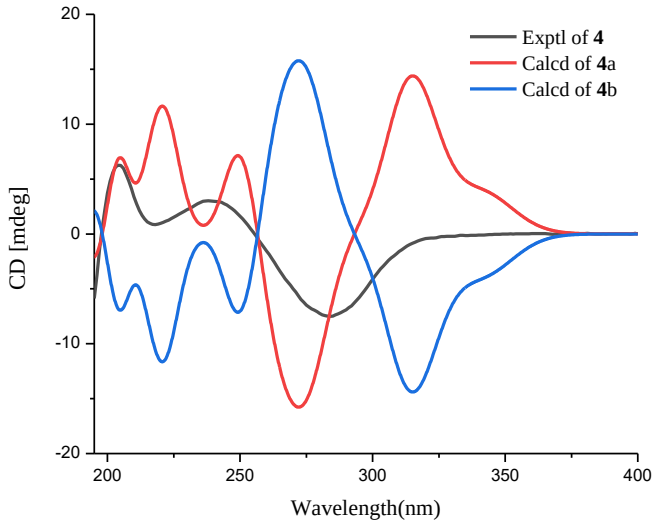

Figure S33. Experimental and calculated ECD spectra of compound **4**

(**4**a: 6*R*,7*S*,8*R*,12*S*,13*R*,14*R*,15*R*; **4**b: 6*S*,7*R*,8*S*,12*R*,13*S*,14*S*,15*S*)

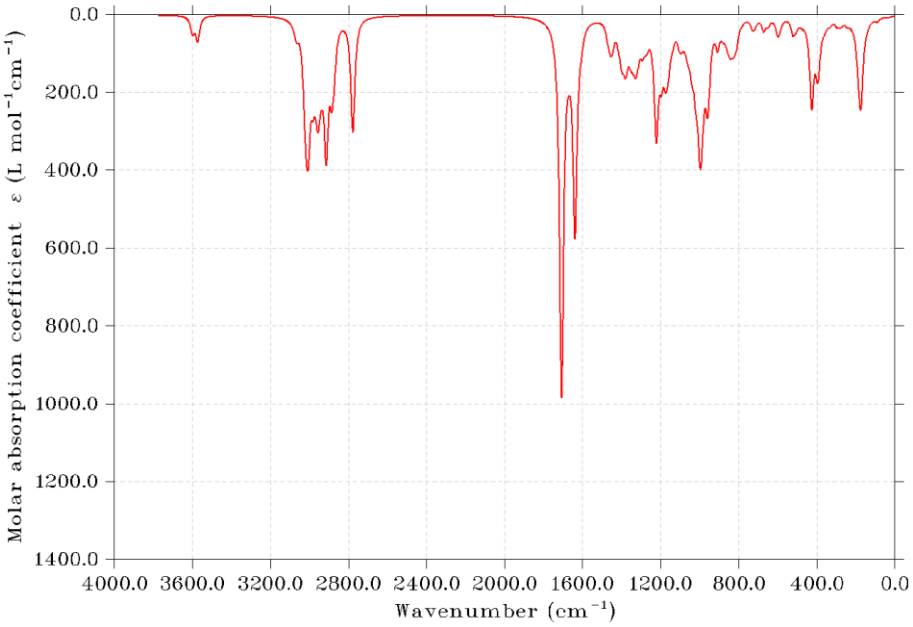

Figure S34. The computed IR spectrum of compound **4** at B3LYP/6-31g (d, p) level in methanol

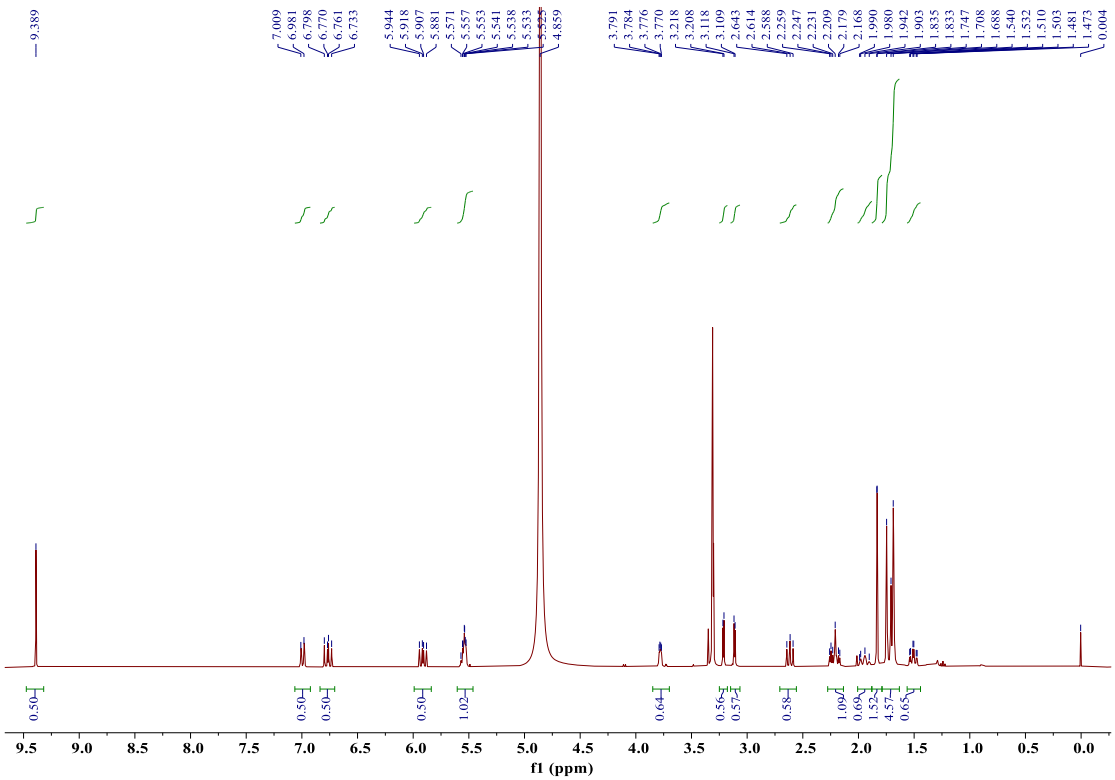

Figure S35. ^{1}H NMR spectrum of compound **4** in methanol-d_4 (400 MHz)

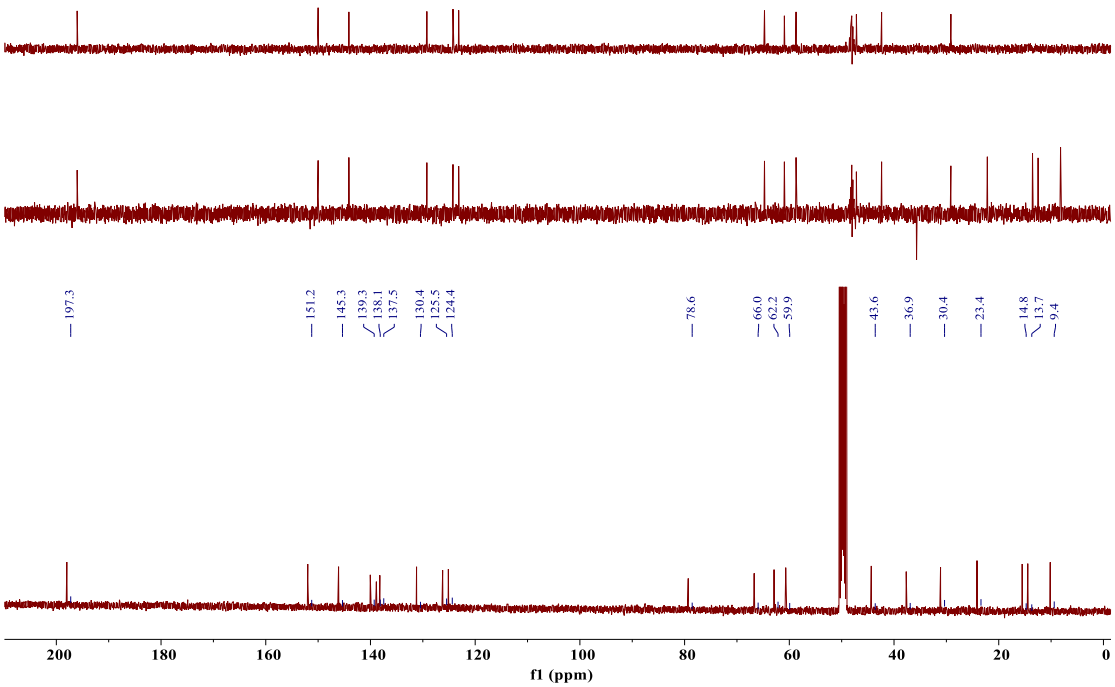

Figure S36. ^{13}C NMR and DEPT spectra of compound **4** in methanol-d_4 (100 MHz)

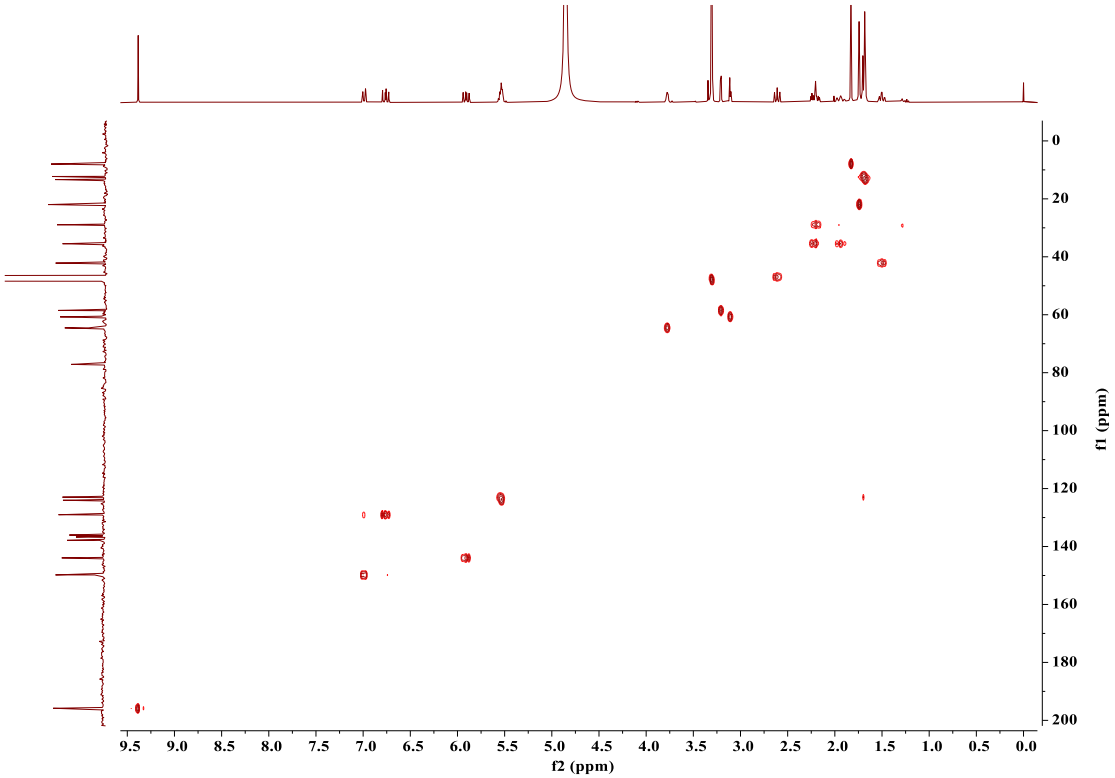

Figure S37. HSQC spectrum of compound **4** in methanol-d_4 (^{1}H-400 MHz)

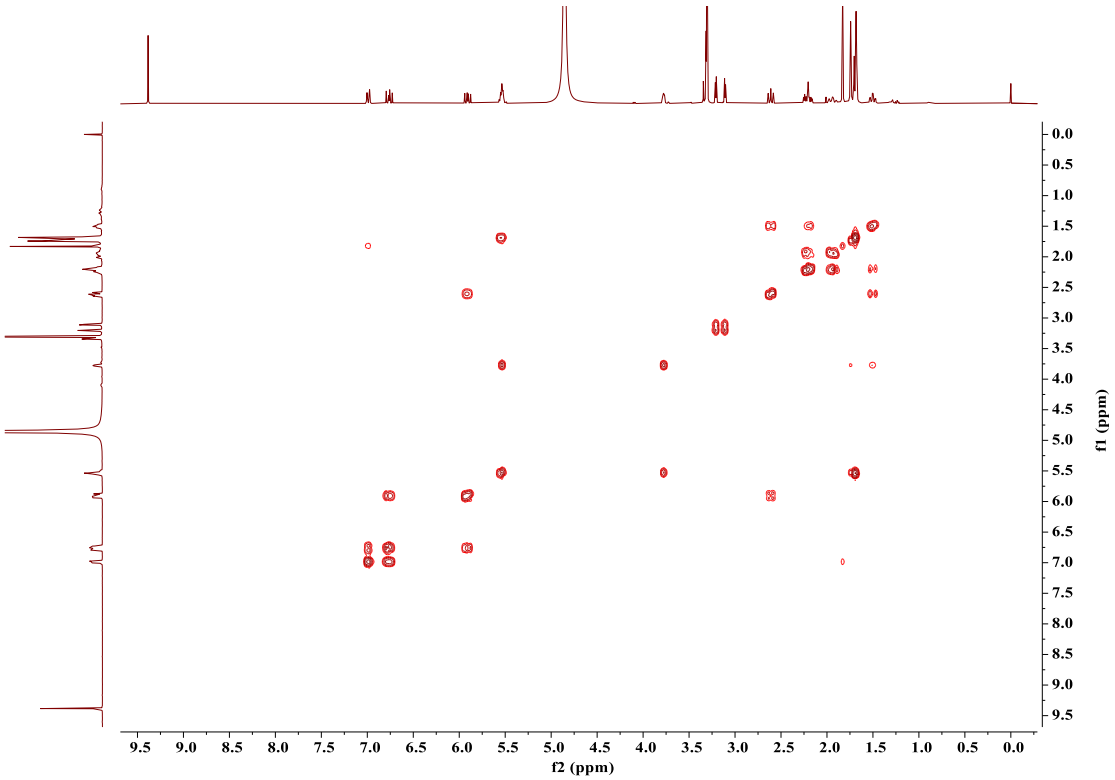

Figure S38. ^{1}H-^{1}H COSY spectrum of compound **4** in methanol-d_4 (400 MHz)

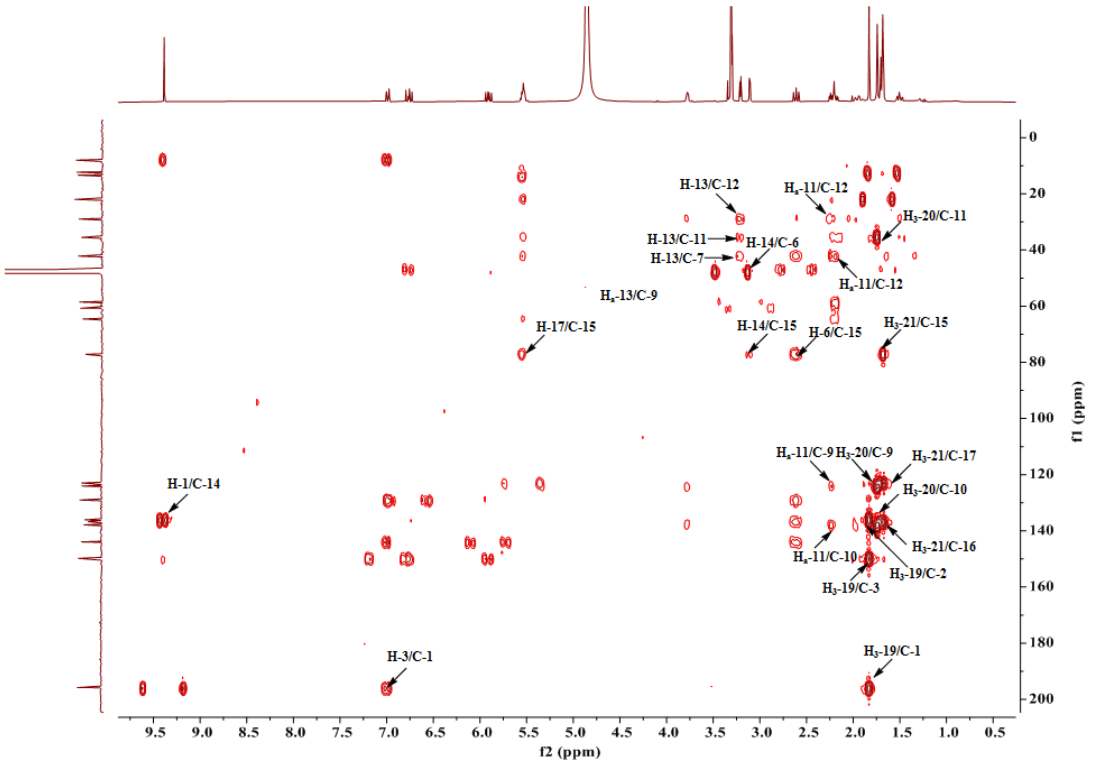

Figure S39. HMBC spectrum of compound **4** in methanol-d_4 (400 MHz)

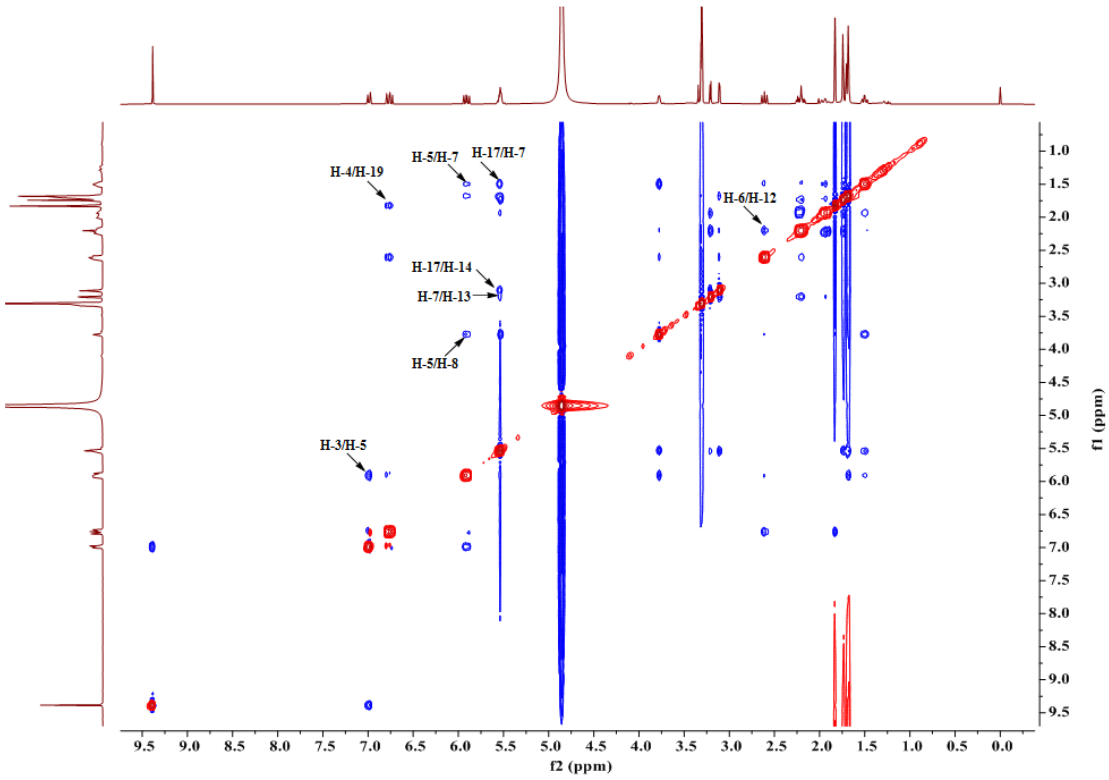

Figure S40. NOESY spectrum of compound **4** in methanol-d_4 (400 MHz)

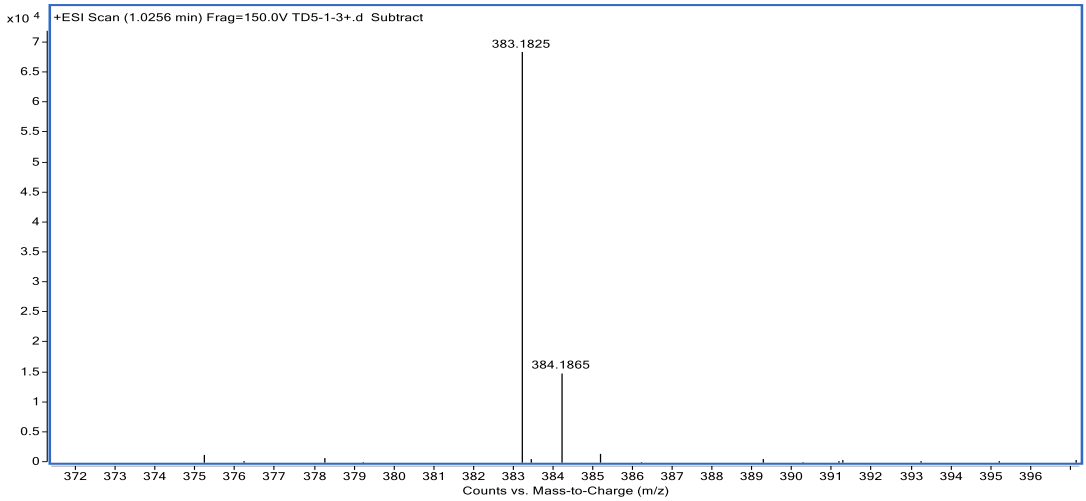

Figure S41. HRESIMS spectrum of compound **5**

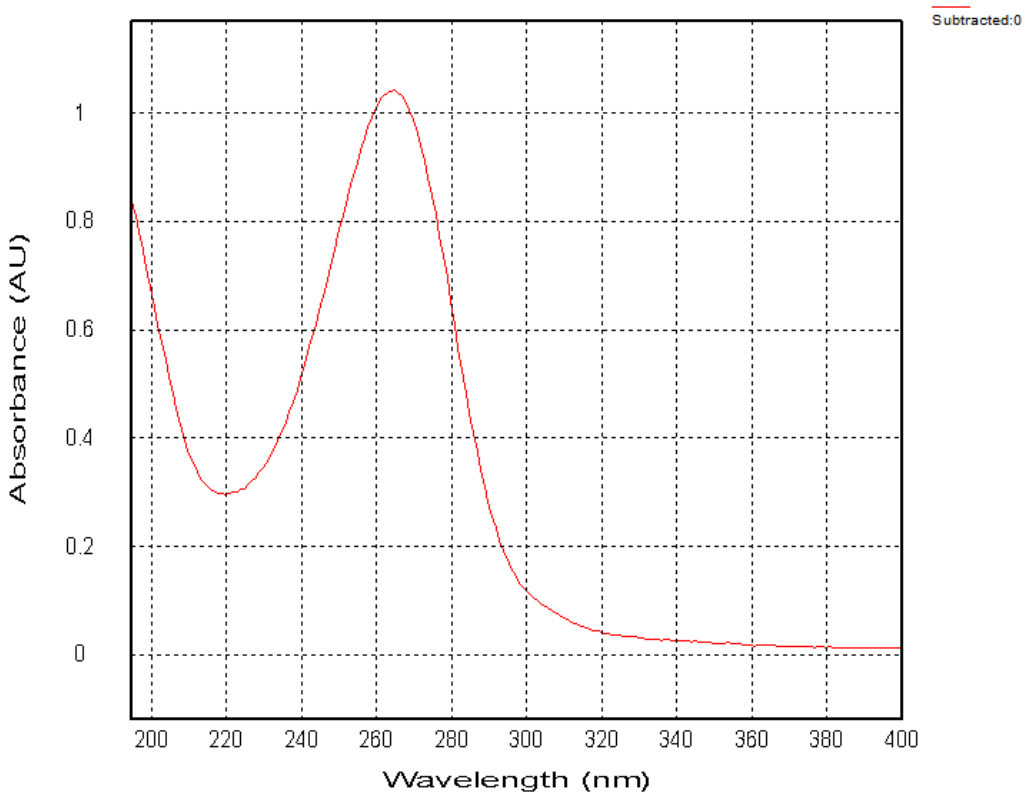

Figure S42. UV-vis spectrum of compound **5** in MeOH

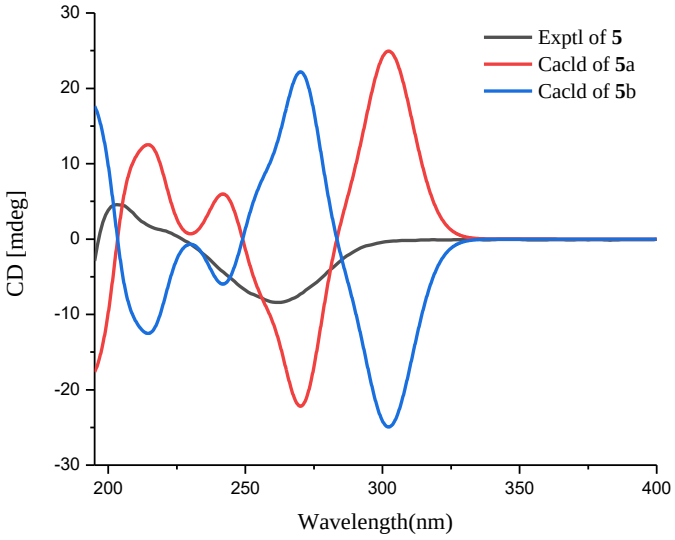

Figure S43. Experimental and calculated ECD spectra of compound **5**

(**5**a: 6*R*,7*S*,8*R*,12*S*,13*R*,14*R*,15*R*; **5**b: 6*S*,7*R*,8*S*,12*R*,13*S*,14*S*,15*S*)

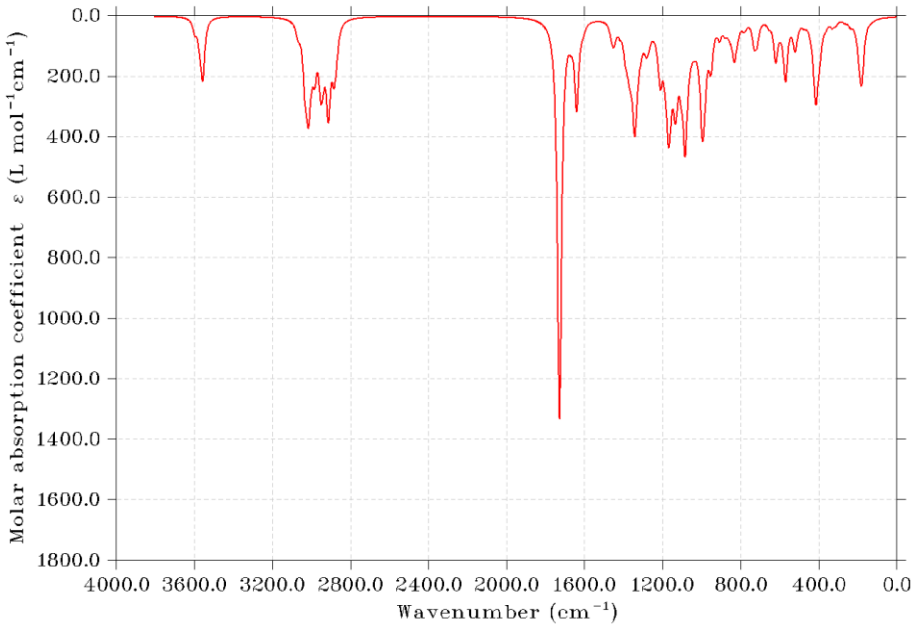

Figure S44. The computed IR spectrum of compound **5** at B3LYP/6-31g (d, p) level in methanol

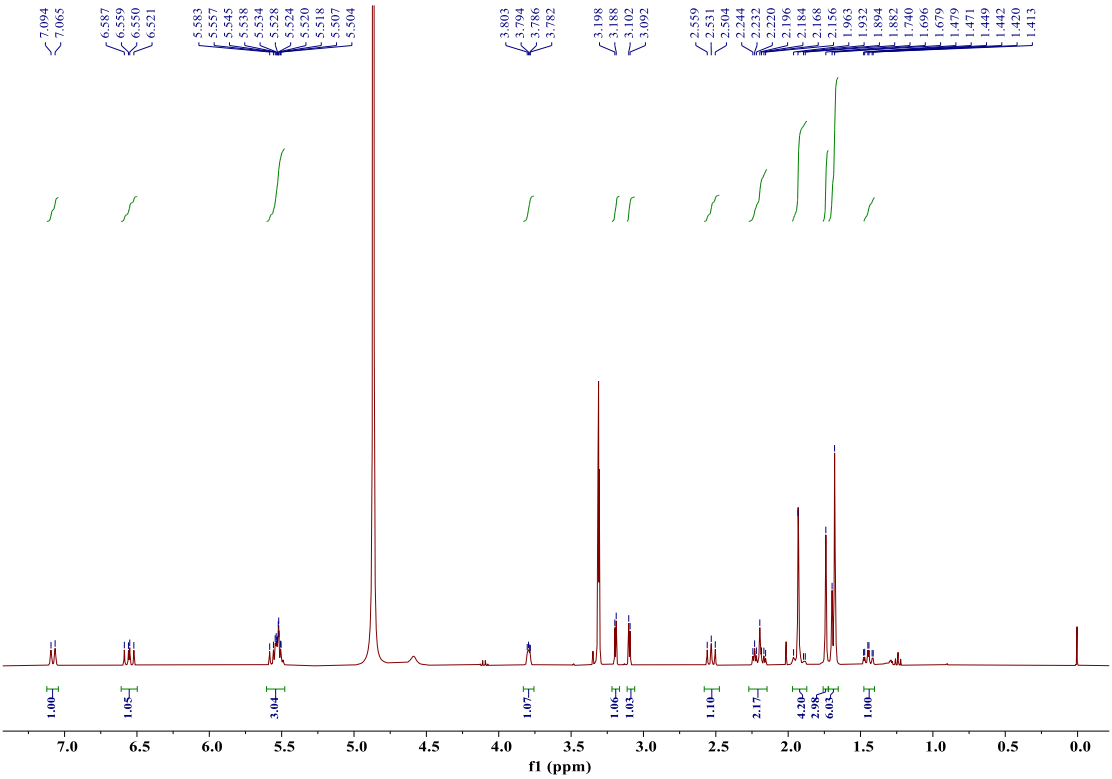

Figure S45. ^{1}H NMR spectrum of compound **5** in methanol-d_4 (400 MHz)

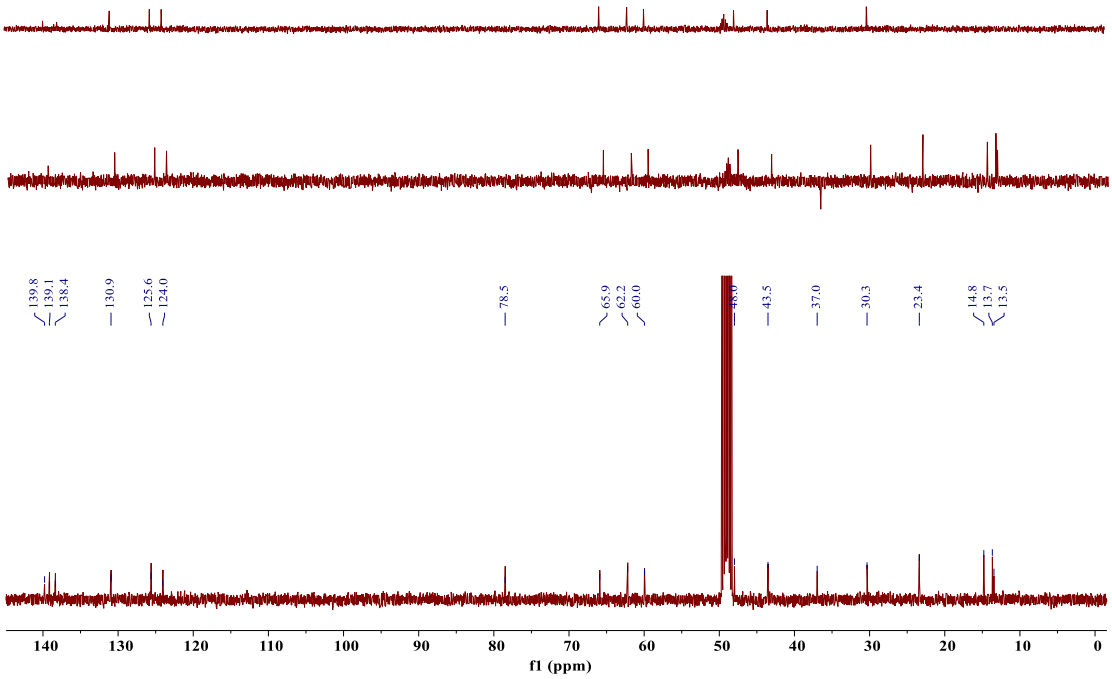

Figure S46. ^{13}C NMR and DEPT spectra of compound **5** in methanol-d_4 (100 MHz)

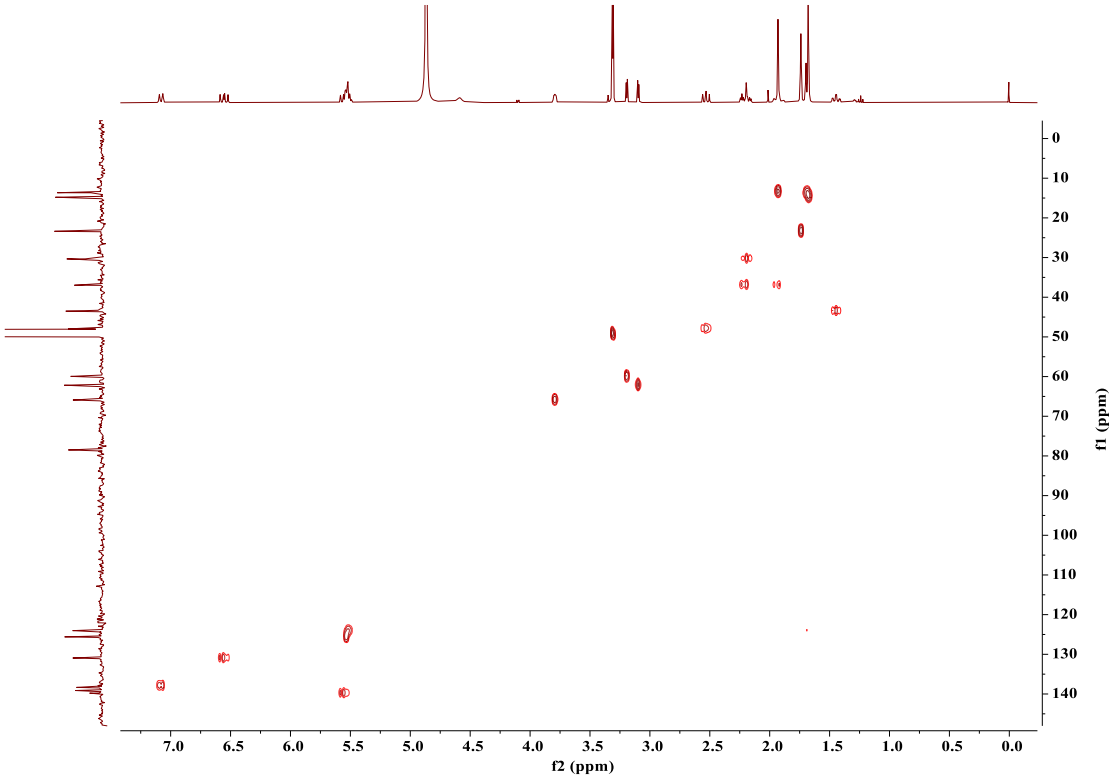

Figure S47. HSQC spectrum of compound **5** in methanol-d_4 (^{1}H-400 MHz)

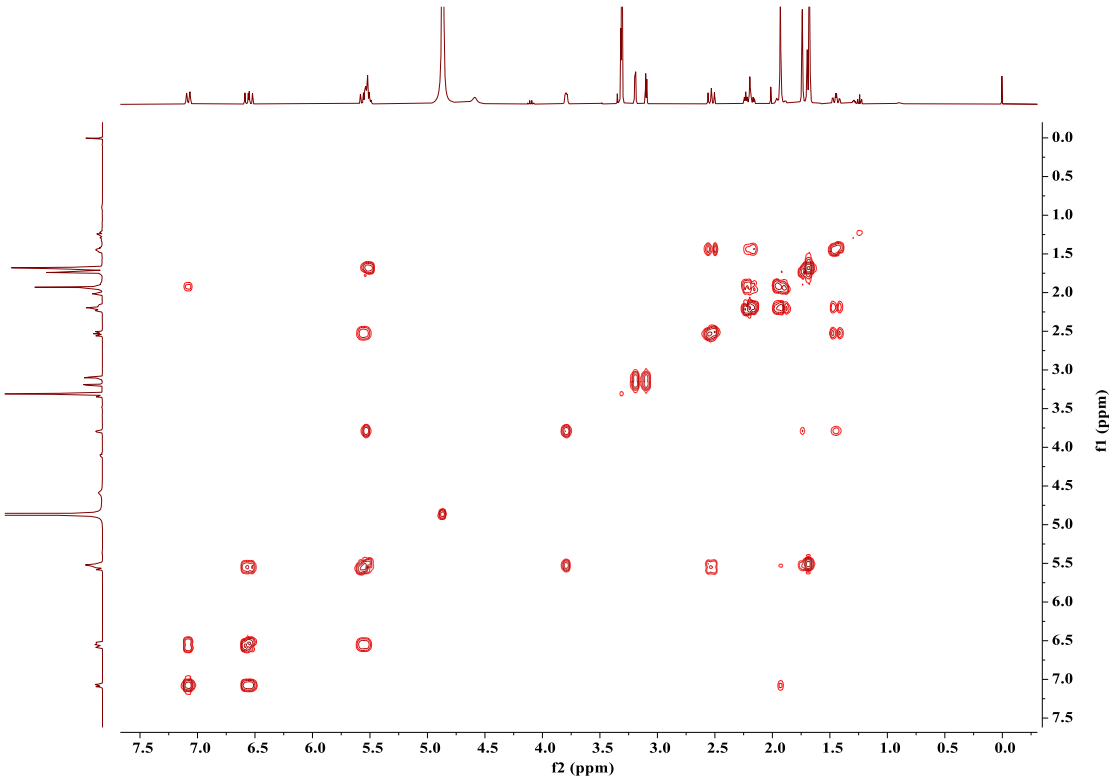

Figure S48. ^{1}H-^{1}H COSY spectrum of compound **5** in methanol-d_4 (400 MHz)

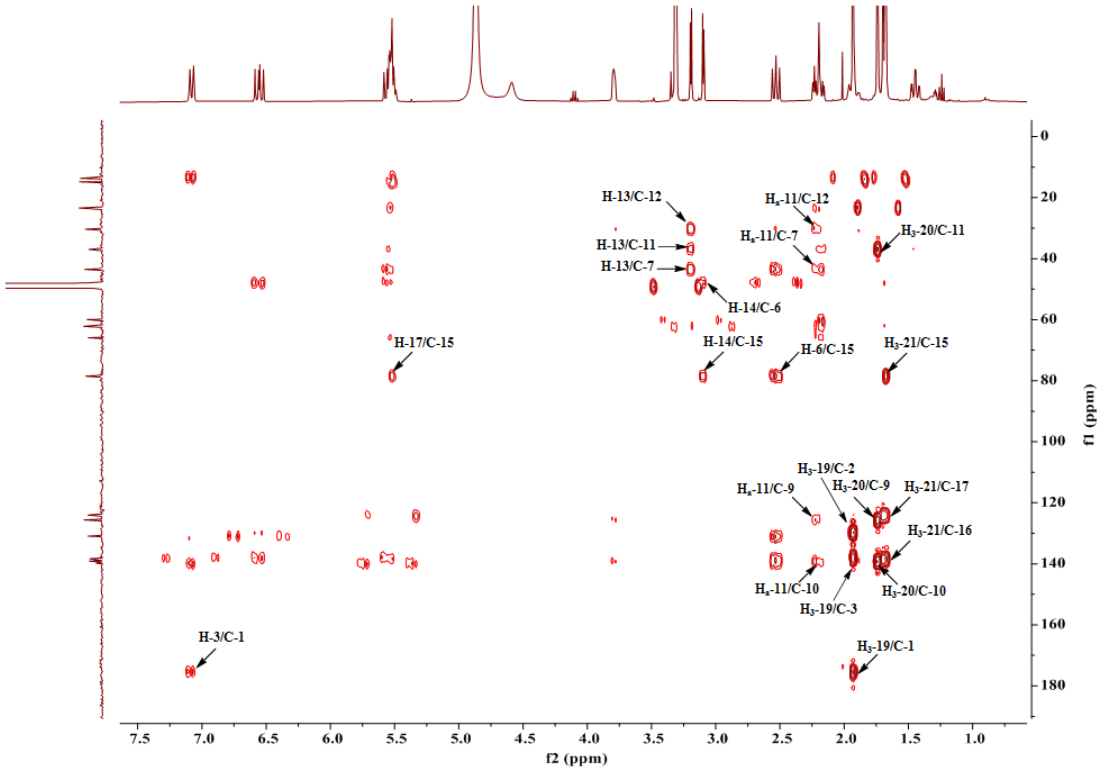

Figure S49. HMBC spectrum of compound **5** in methanol-d_4 (400 MHz)

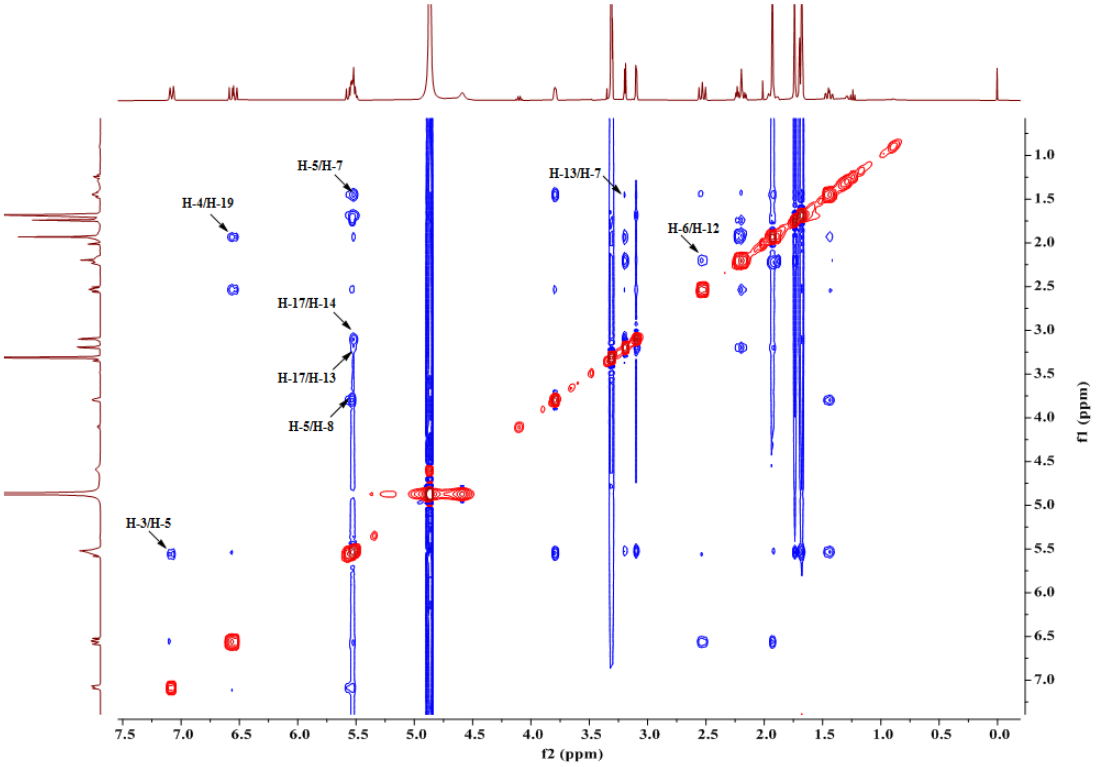

Figure S50. NOESY spectrum of compound **5** in methanol-d_4 (400 MHz)

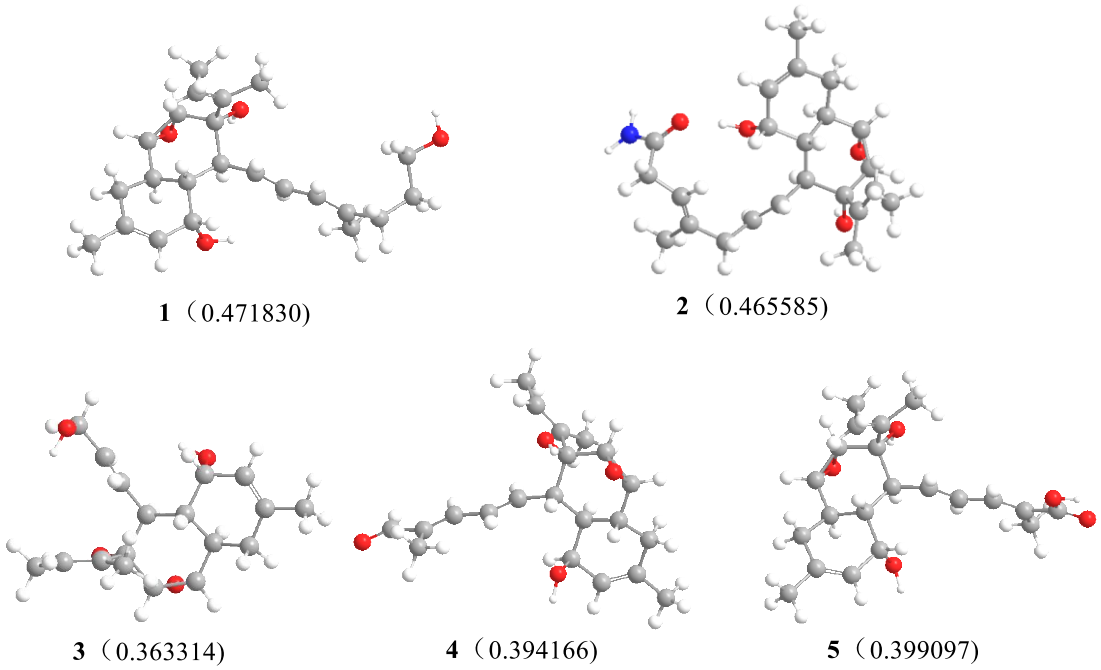

Figure S51. The optimized conformation and Gibbs free energy of compound **1-5** at B3LYP/6-31g (d, p) level in methanol

1

Zero-point correction=	0.533326 (Hartree/Particle)
Thermal correction to Energy=	0.562785
Thermal correction to Enthalpy=	0.563729
Thermal correction to Gibbs Free Energy=	0.471830
Sum of electronic and zero-point Energies=	-1197.160574
Sum of electronic and thermal Energies=	-1197.131115
Sum of electronic and thermal Enthalpies=	-1197.130171
Sum of electronic and thermal Free Energies=	-1197.222070

2

Zero-point correction=	0.527048 (Hartree/Particle)
Thermal correction to Energy=	0.557136
Thermal correction to Enthalpy=	0.558080
Thermal correction to Gibbs Free Energy=	0.465585
Sum of electronic and zero-point Energies=	-1251.341467
Sum of electronic and thermal Energies=	-1251.311380
Sum of electronic and thermal Enthalpies=	-1251.310436
Sum of electronic and thermal Free Energies=	-1251.402930

3

Zero-point correction=	0.414659 (Hartree/Particle)
Thermal correction to Energy=	0.437473
Thermal correction to Enthalpy=	0.438417
Thermal correction to Gibbs Free Energy=	0.363314
Sum of electronic and zero-point Energies=	-1001.929796
Sum of electronic and thermal Energies=	-1001.906983
Sum of electronic and thermal Enthalpies=	-1001.906038
Sum of electronic and thermal Free Energies=	-1001.981142

4

Zero-point correction=	0.451957 (Hartree/Particle)
Thermal correction to Energy=	0.478542
Thermal correction to Enthalpy=	0.479486
Thermal correction to Gibbs Free Energy=	0.394166
Sum of electronic and zero-point Energies=	-1117.418603
Sum of electronic and thermal Energies=	-1117.392019
Sum of electronic and thermal Enthalpies=	-1117.391074
Sum of electronic and thermal Free Energies=	-1117.476395

5

Zero-point correction=	0.457521 (Hartree/Particle)
Thermal correction to Energy=	0.484896
Thermal correction to Enthalpy=	0.485841
Thermal correction to Gibbs Free Energy=	0.399097
Sum of electronic and zero-point Energies=	-1192.660636
Sum of electronic and thermal Energies=	-1192.633261
Sum of electronic and thermal Enthalpies=	-1192.632316
Sum of electronic and thermal Free Energies=	-1192.719060

Figure S52. The thermodynamic date of optimized conformation of compound **1-5** at B3LYP/6-31g (d, p) level in methanol

1a：Molar Mass = 374.5192 grams/mole, [Alpha] (5890.0 A) = 223.67 deg.

1b：Molar Mass = 374.5192 grams/mole, [Alpha] (5890.0 A) = -223.67 deg.

2a：Molar Mass = 387.5180 grams/mole, [Alpha] (5890.0 A) = 124.04 deg.

2b：Molar Mass = 387.5180 grams/mole, [Alpha] (5890.0 A) = -124.04 deg.

3a：Molar Mass = 306.4010 grams/mole, [Alpha] (5890.0 A) = 111.49 deg.

3b：Molar Mass = 306.4010 grams/mole, [Alpha] (5890.0 A) = -111.49 deg.

4a：Molar Mass = 344.4498 grams/mole, [Alpha] (5890.0 A) = 20.11 deg.

4b：Molar Mass = 344.4498 grams/mole, [Alpha] (5890.0 A) = -20.11 deg.

5a：Molar Mass = 360.4492 grams/mole, [Alpha] (5890.0 A) = 225.47 deg.

5b：Molar Mass = 360.4492 grams/mole, [Alpha] (5890.0 A) = -225.47 deg.

Figure S53. Calculated values of optical rotations of compounds **1**-**5**

(**1**a-**2**a: 8*R*,9*S*,10*R*,14*S*,15*R*,16*R*,17*R*; **1**b-**2**b: 8*S*,9*R*,10*S*,14*R*,15*S*,16*S*,17*S*; **3**a: 4*R*,5*S*,6*R*,10*S*,11*R*,12*R*,13*R*; **3**b: 4*S*,5*R*,6*S*,10*R*,11*S*,12*S*,13*S*; **4**a-**5**a: 6*R*,7*S*,8*R*,12*S*,13*R*,14*R*,15*R*; **4**b-**5**b: 6*S*,7*R*,8*S*,12*R*,13*S*,14*S*,15*S*)

1 T. Lu and F. Chen, J Comput Chem, 2012, 33, 580-592.