SUPPORTING INFORMATION

ent-Pimarane diterpenoids from the aerial parts of *Sigesbeckia pubescens* and their myocardial protective activity

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[1] These authors contributed equally to this work.

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Figure S1. HRESIMS (MeOH) spectrum of compound 1.

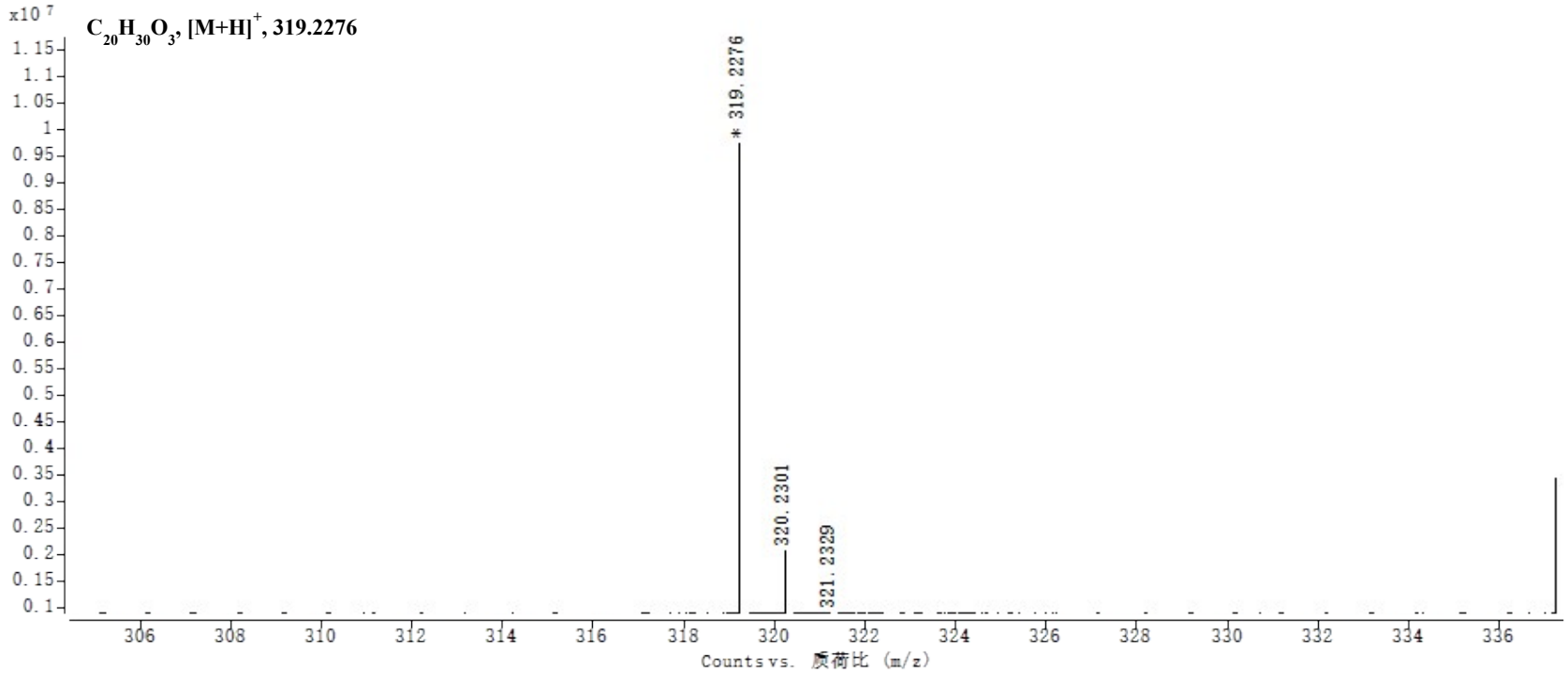


Figure S2. ^{1}H NMR (700 MHz, CD_3OD) spectrum of compound 1.

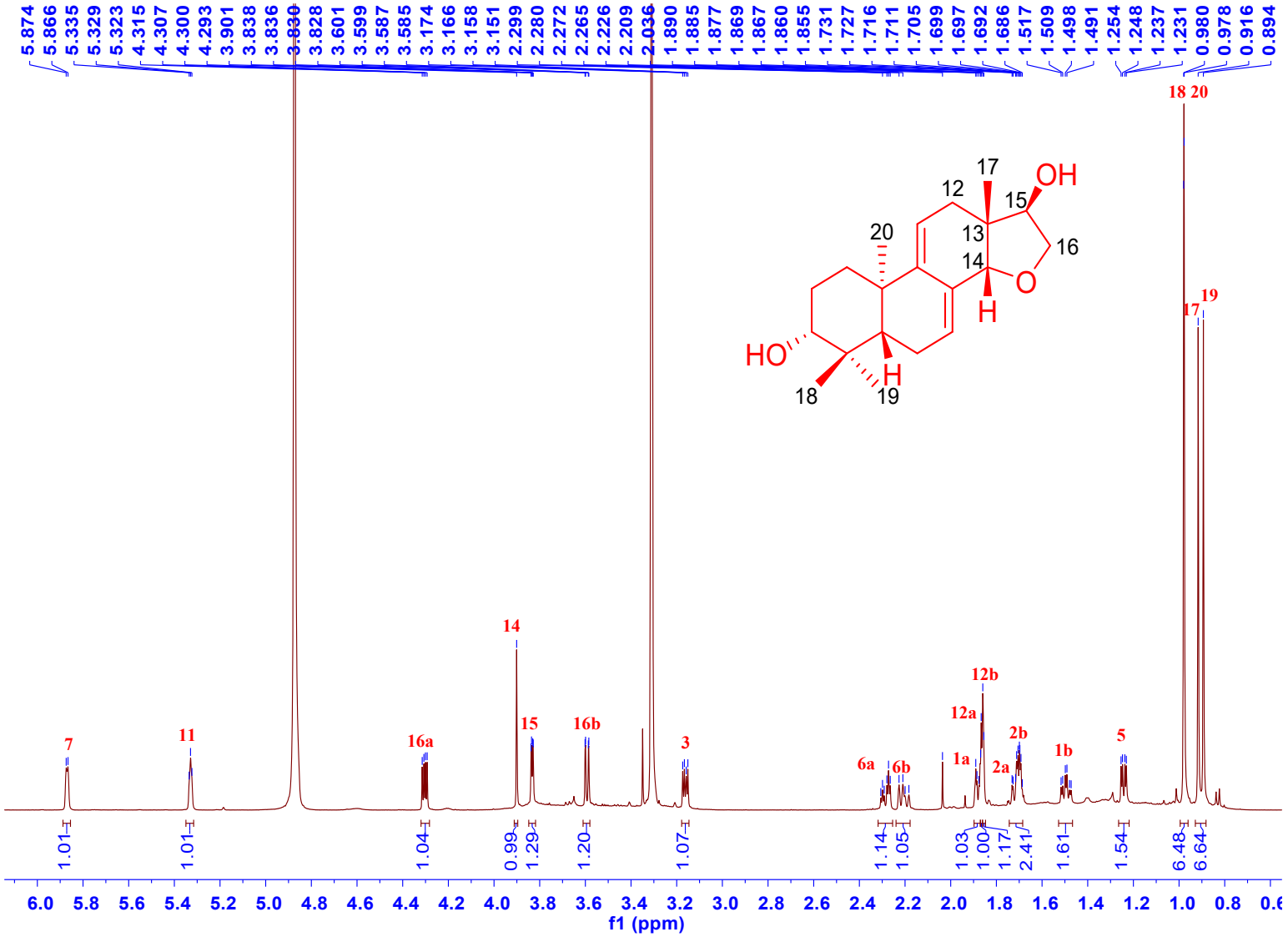


Figure S3. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 1.

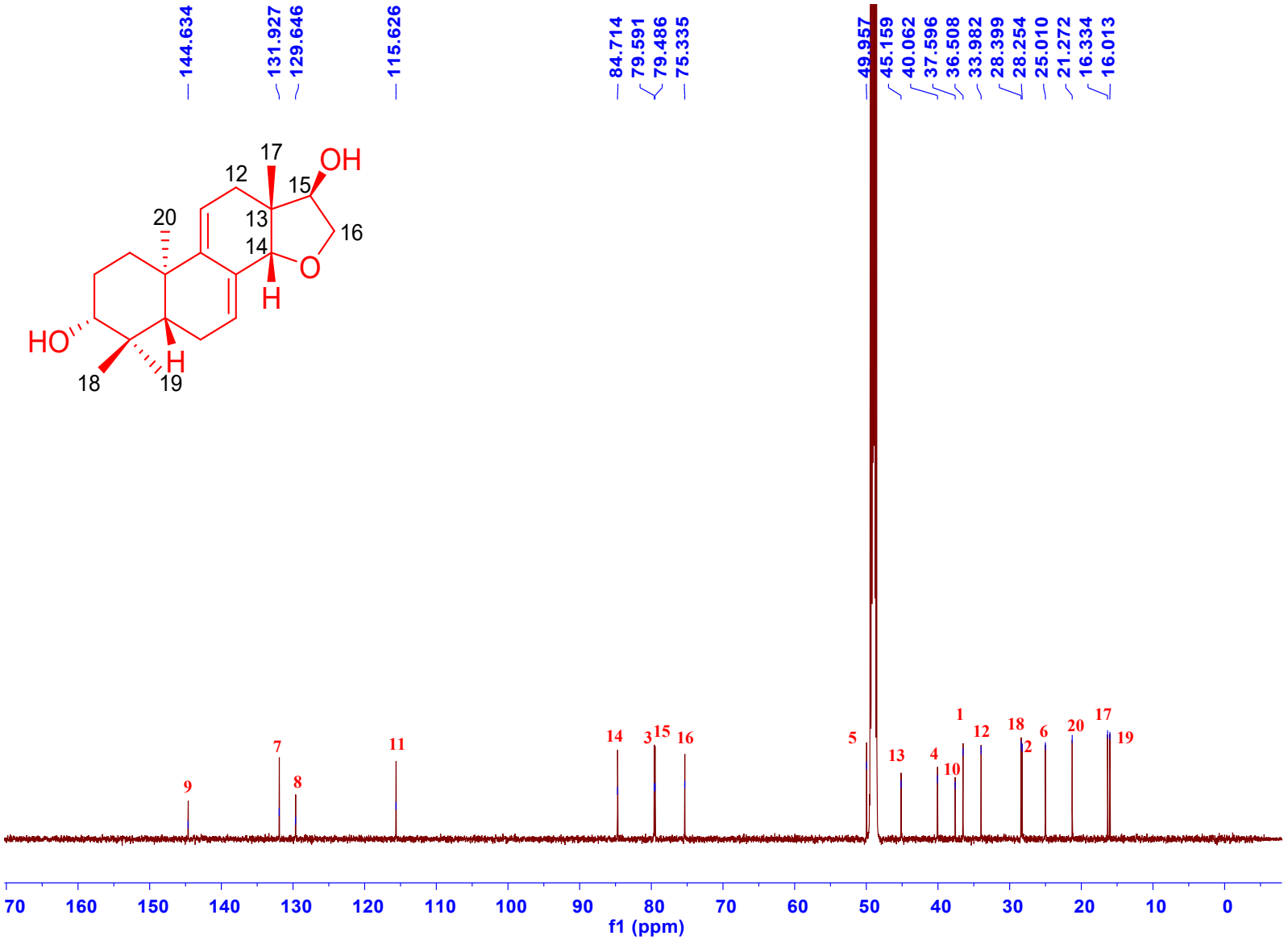


Figure S4. HSQC (CD_3OD) spectrum of compound 1.

Figure S5. HMBC (CD_3OD) spectrum of compound 1.

Figure S6. ^1H-^1H COSY (CD_3OD) spectrum of compound 1.

Figure S7. NOESY (CD_3OD) spectrum of compound 1.

Figure S8. IR spectrum of compound 1.

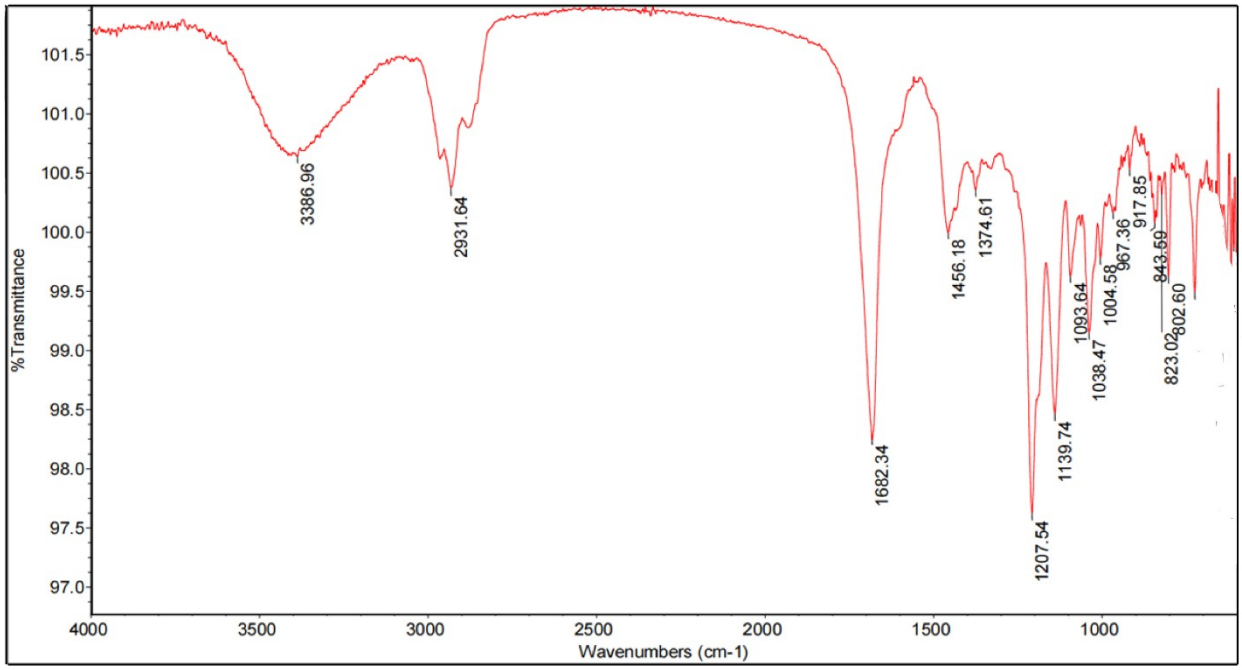


Figure S9. UV spectrum of compound 1.

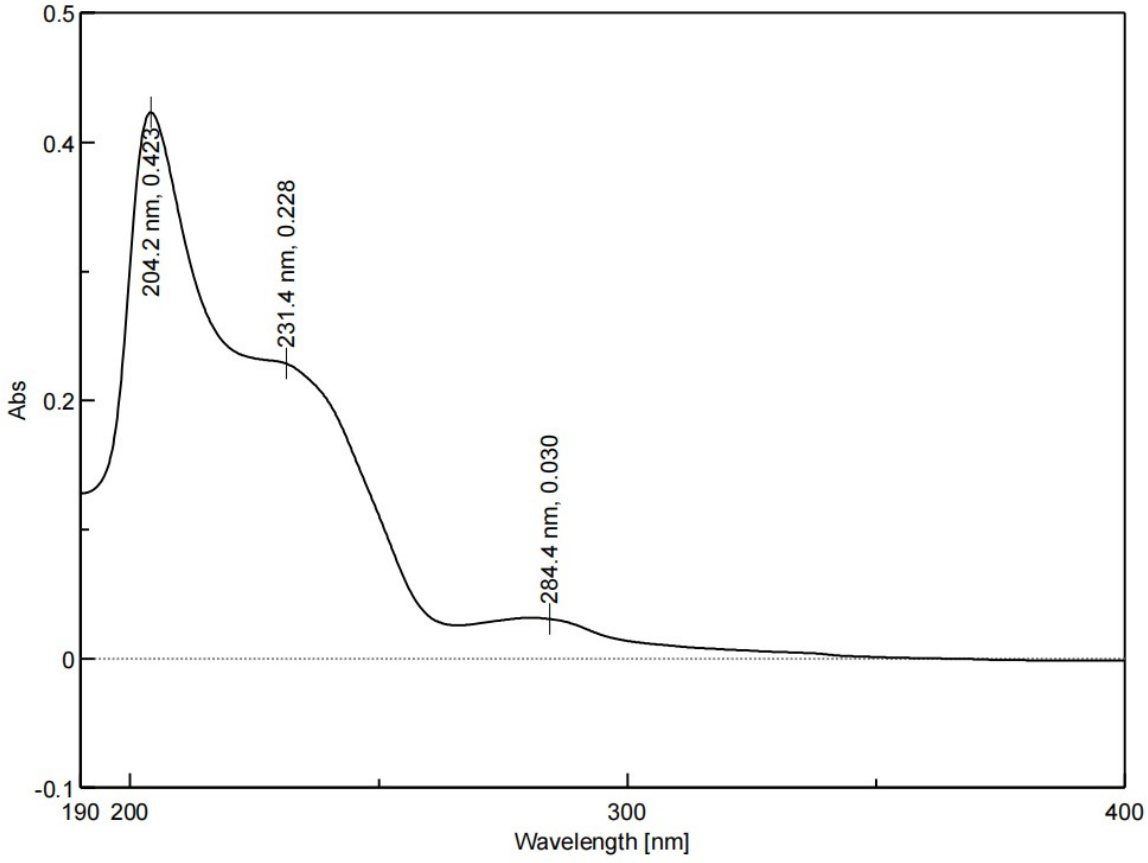


Figure S10. CD spectrum of compound 1.

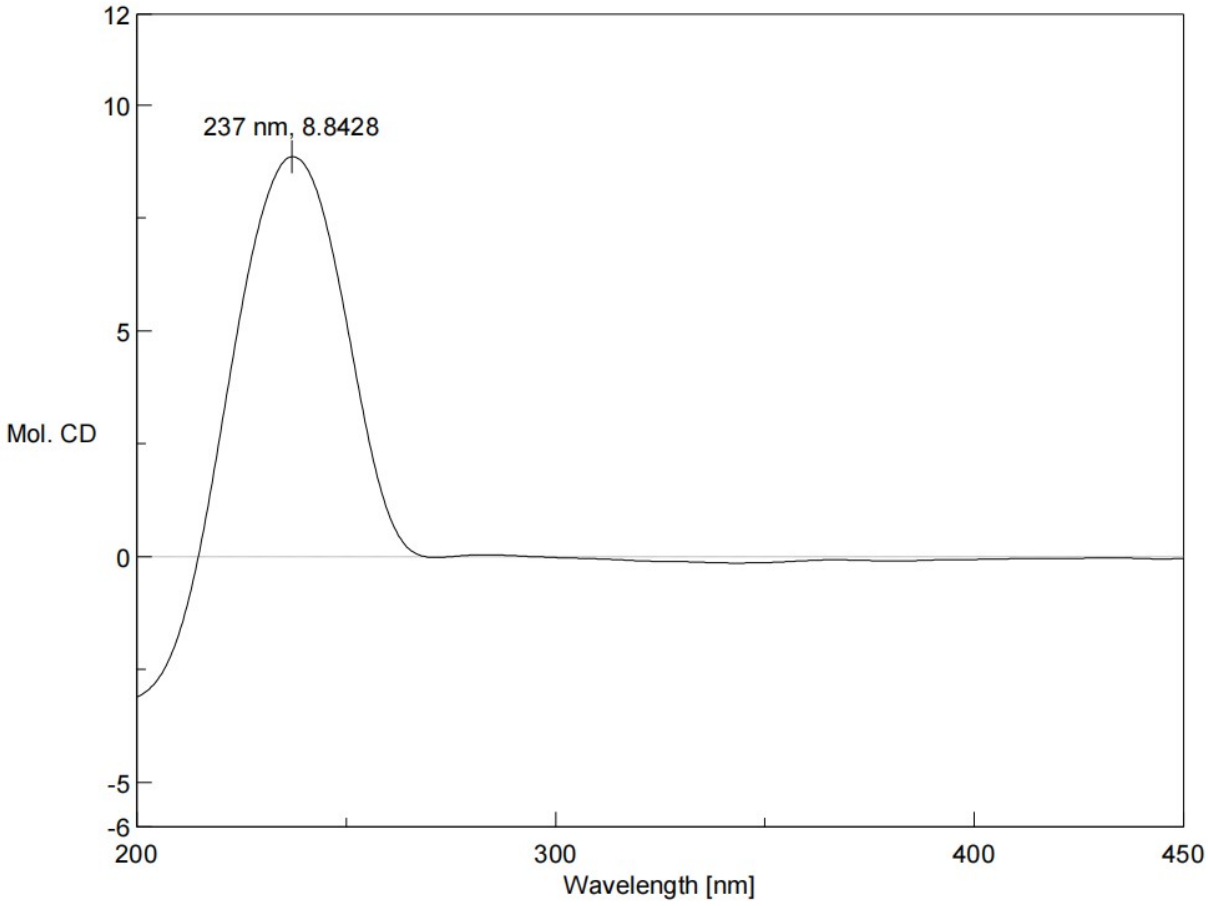


Figure S11. HRESIMS (MeOH) spectrum of compound 2.

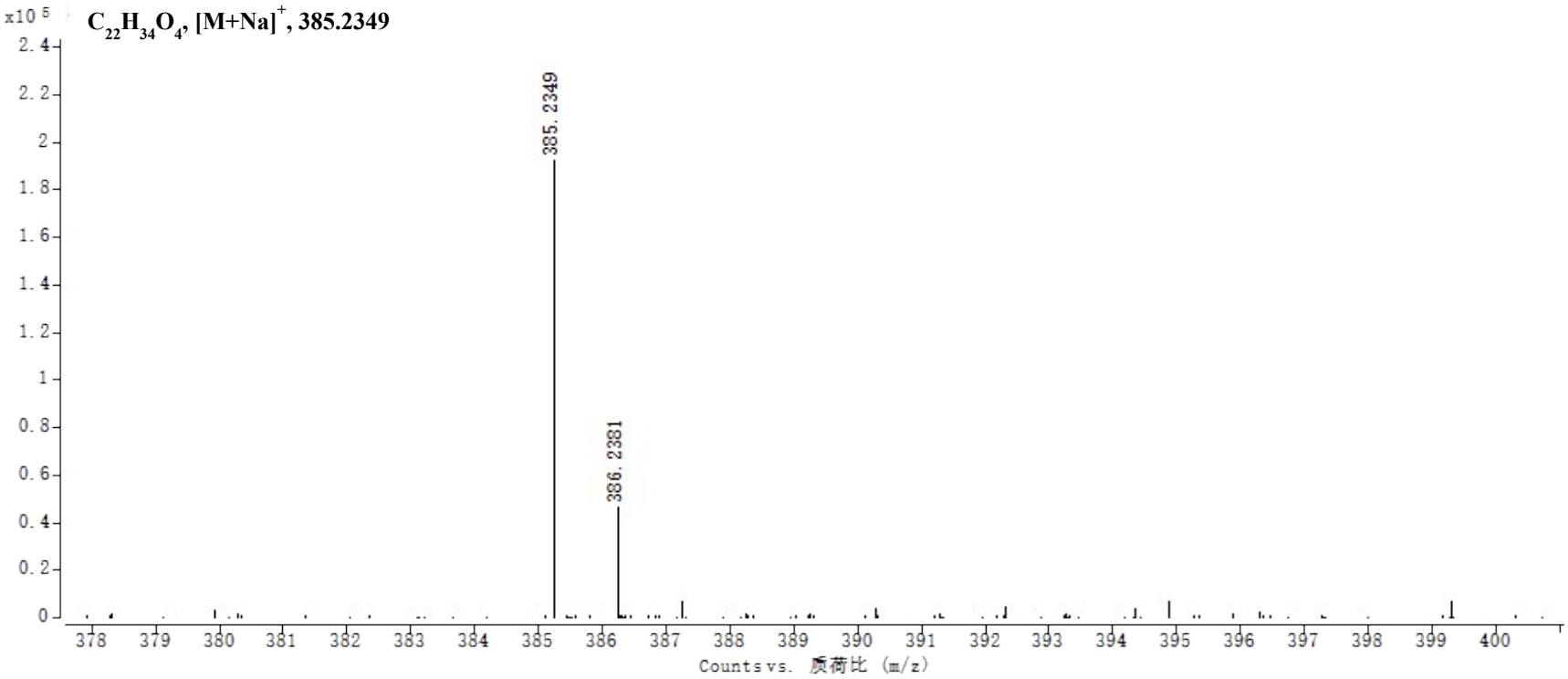


Figure S12. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound 2.

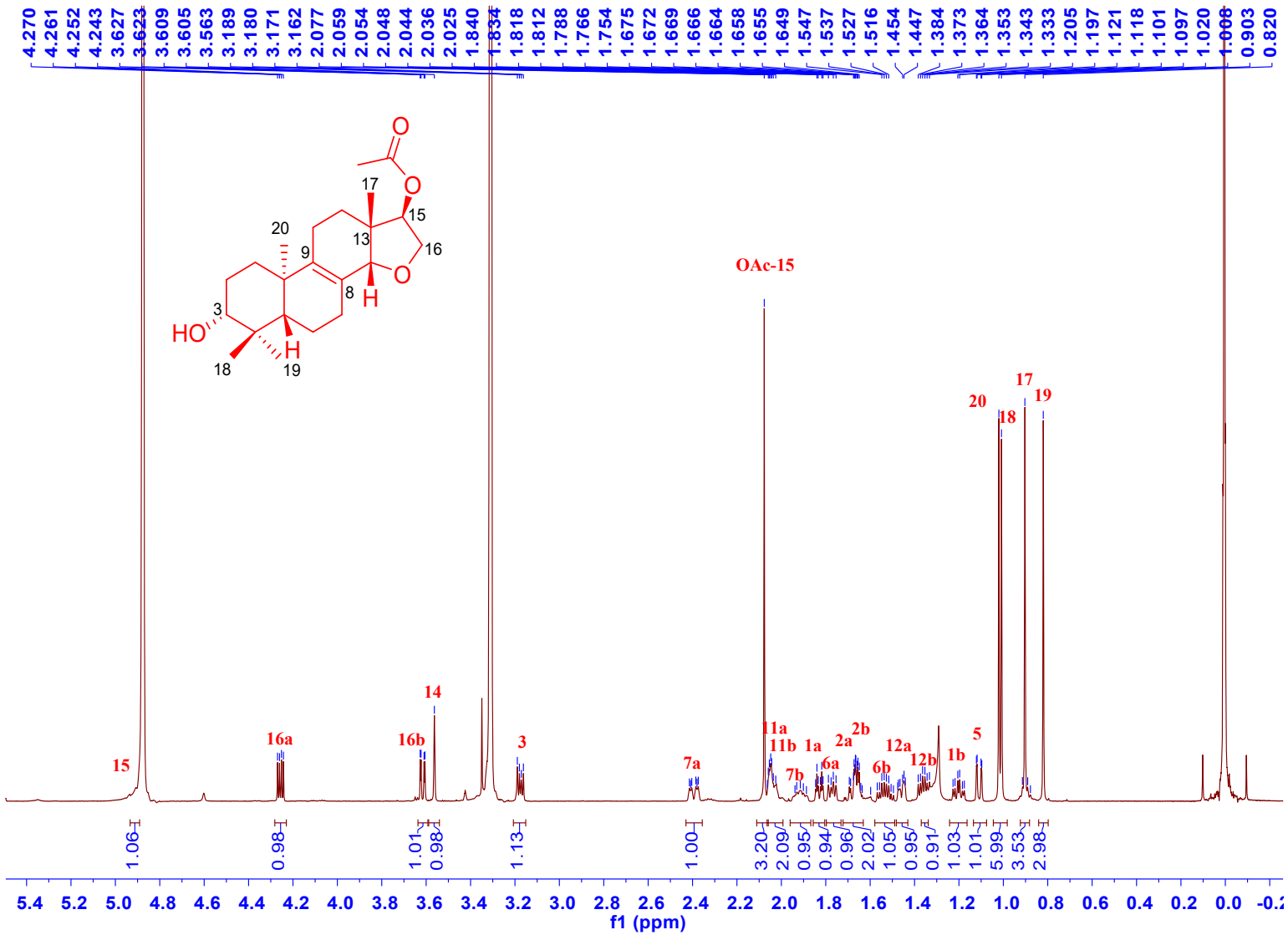


Figure S13. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 2.

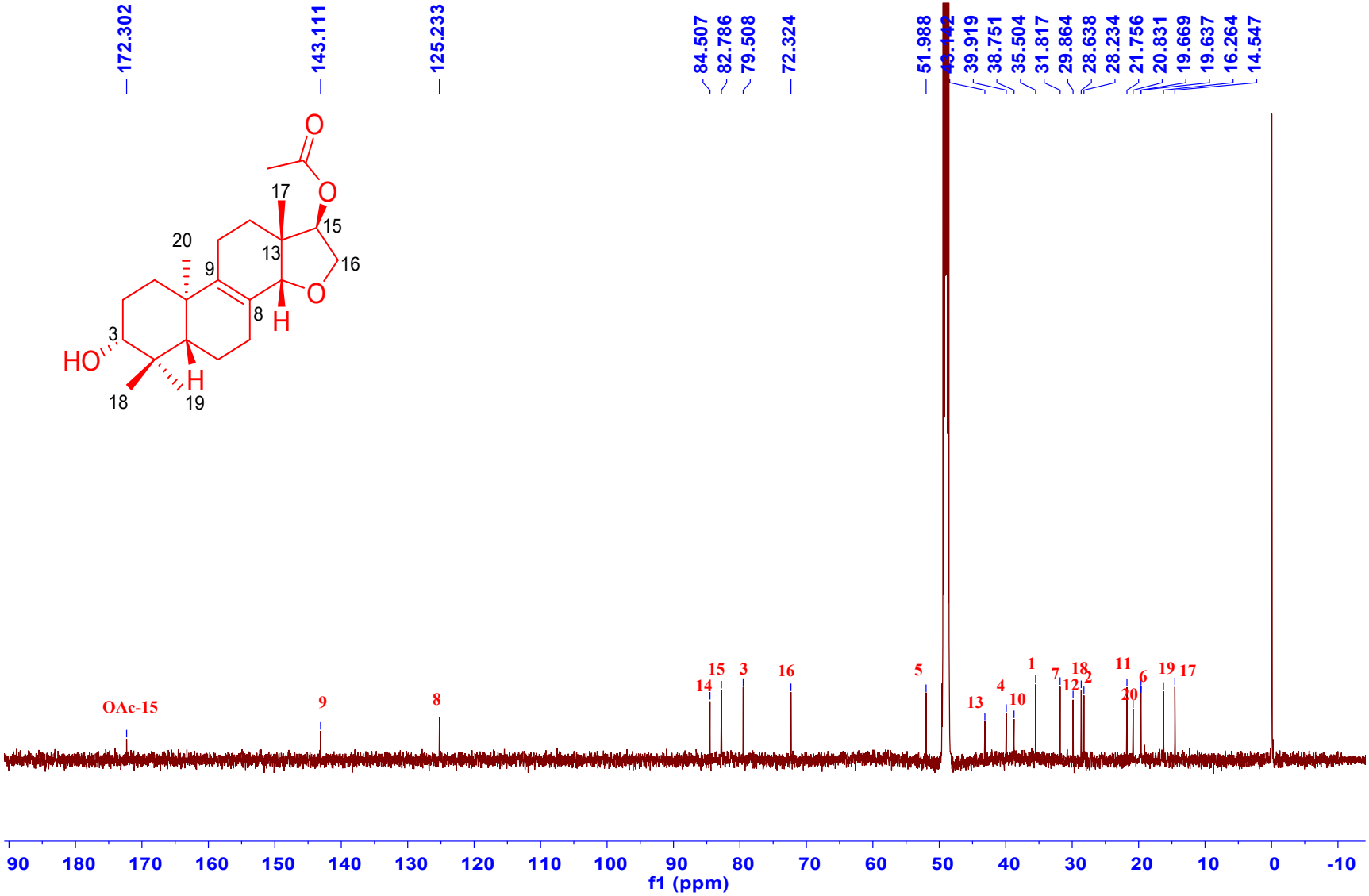


Figure S14. HSQC (CD_3OD) spectrum of compound 2.

Figure S15. HMBC (CD_3OD) spectrum of compound 2.

Figure S16. ^1H-^1H COSY (CD_3OD) spectrum of compound 2.

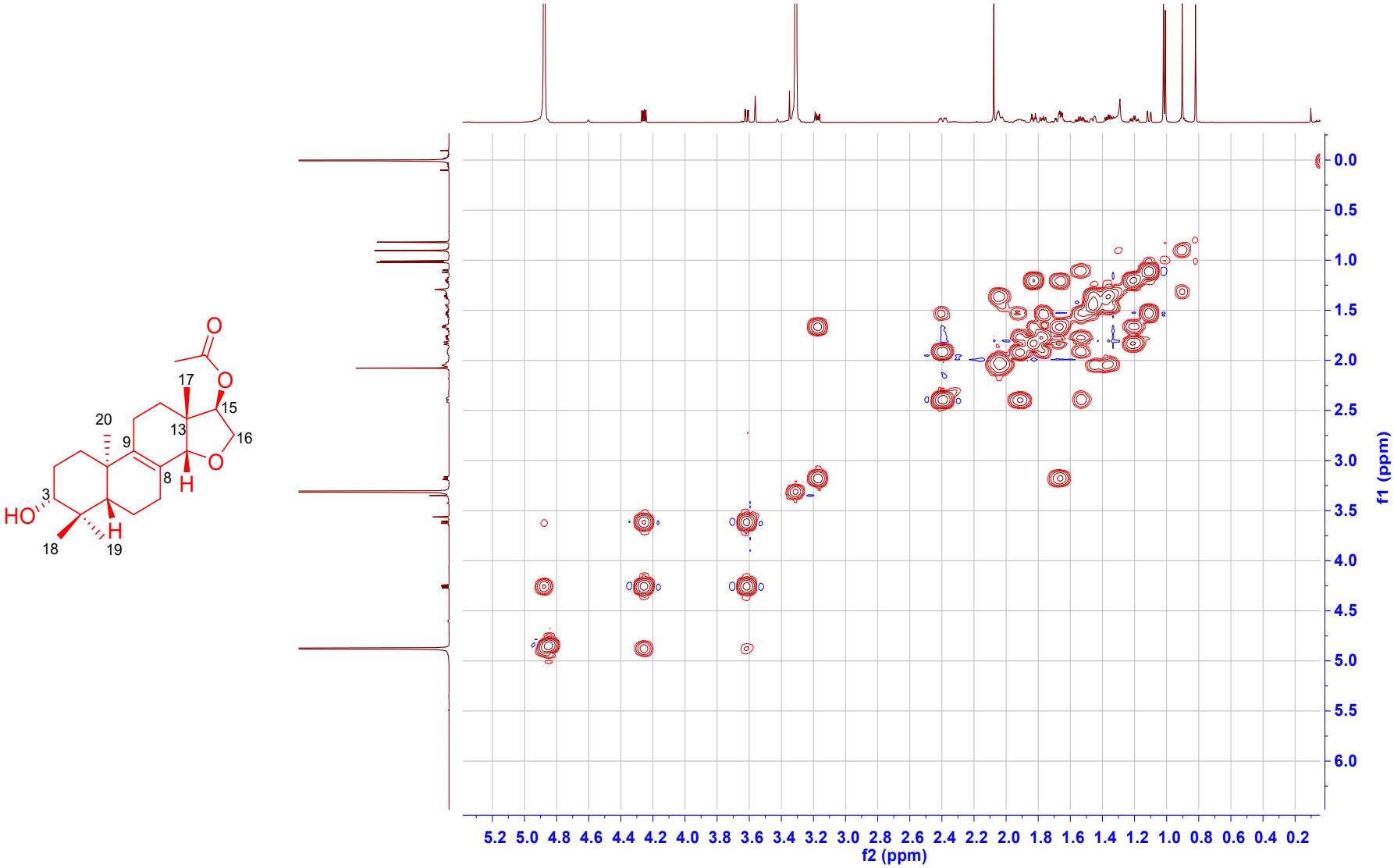
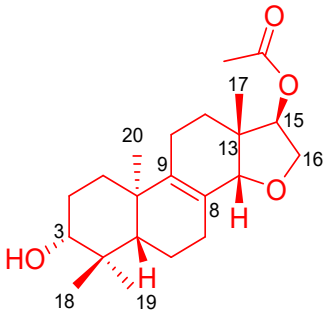


Figure S17. NOESY (CD_3OD) spectrum of compound 2.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O
17
15
16
20
9
13
O
8
H
3
HO
H
18
19

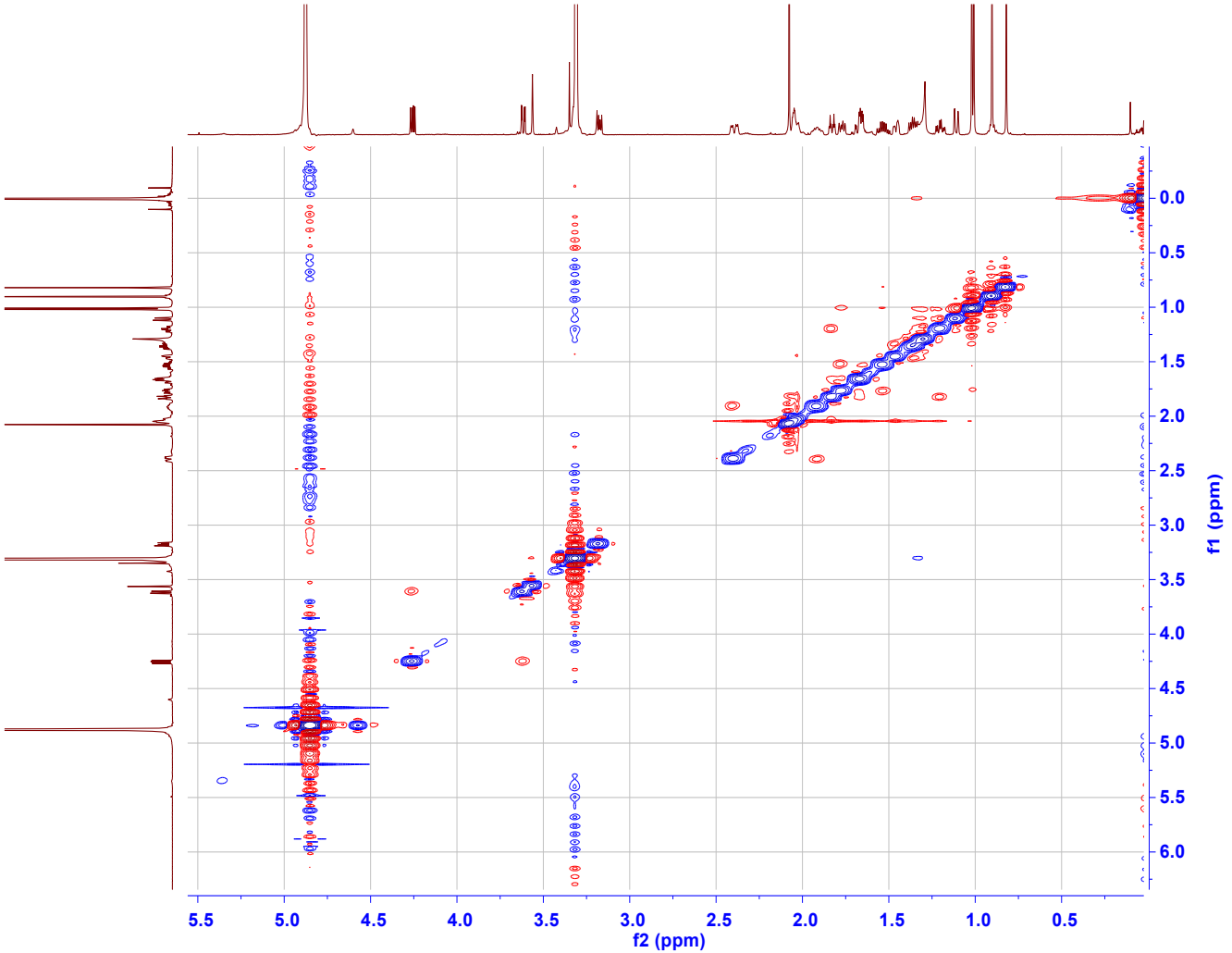

5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
f1 (ppm)

Figure S18. IR spectrum of compound 2.

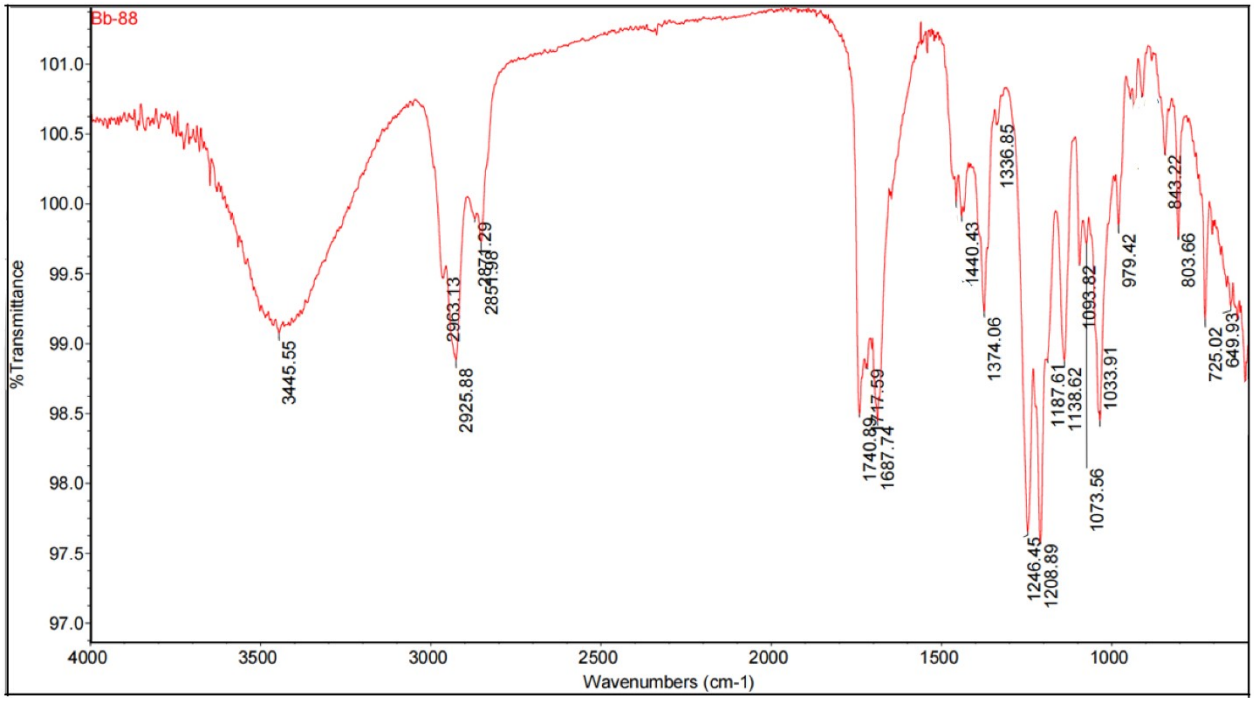


Figure S19. UV spectrum of compound 2.

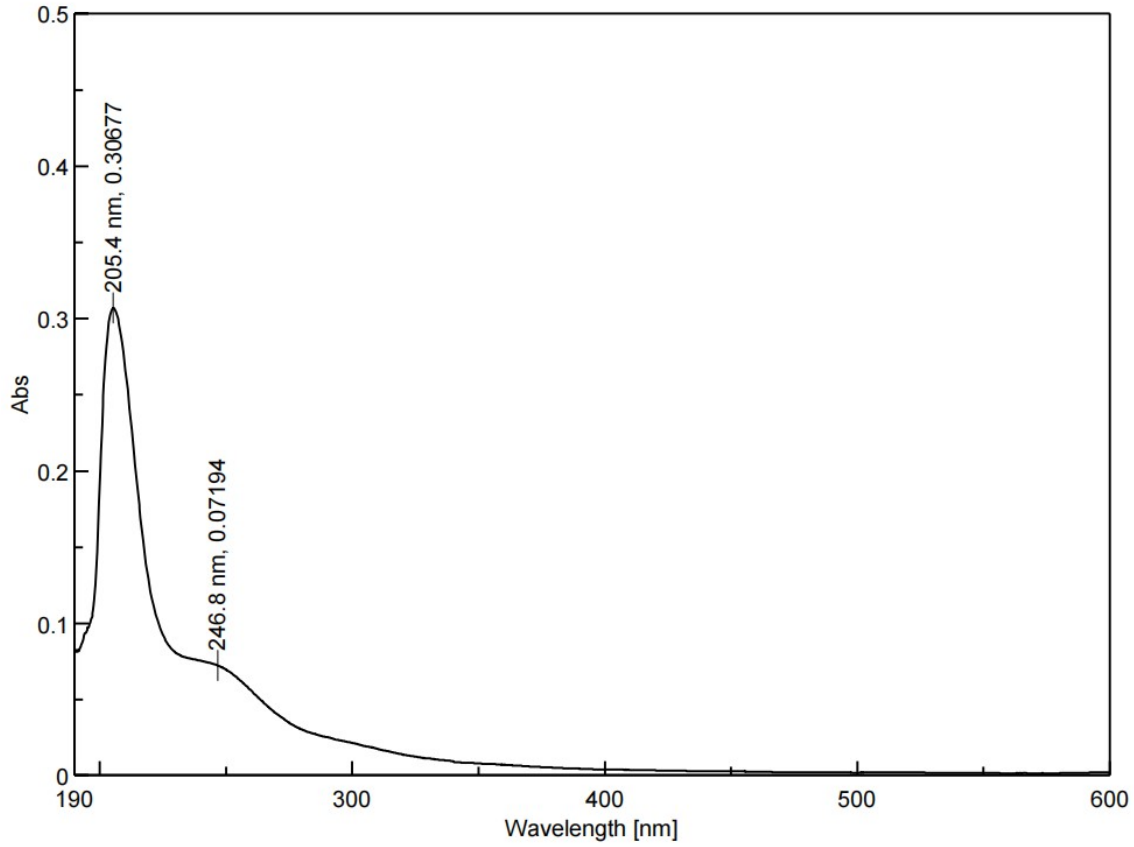


Figure S20. CD spectrum of compound 2.

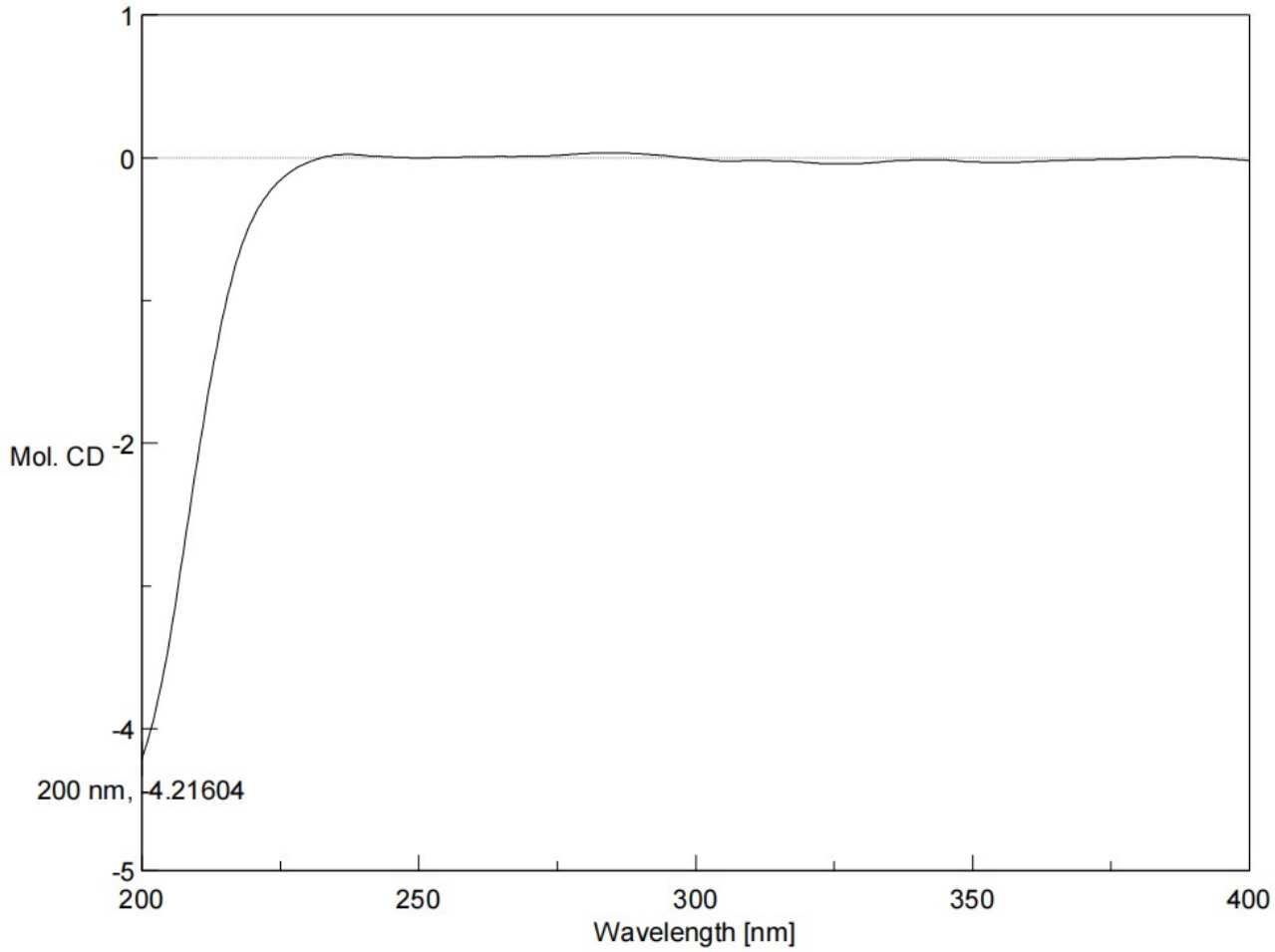


Figure S21. HRESIMS (MeOH) spectrum of compound 3.

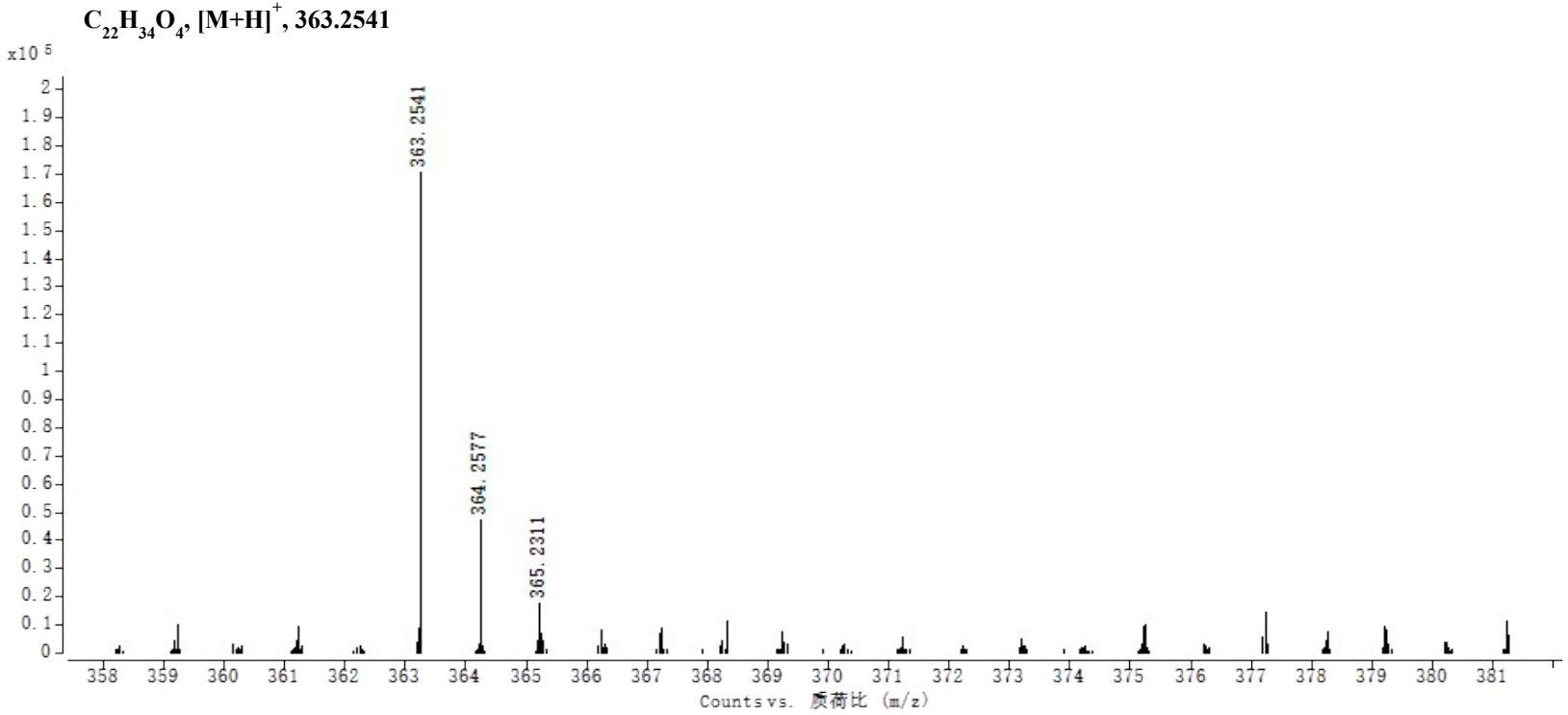


Figure S22. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound 3.

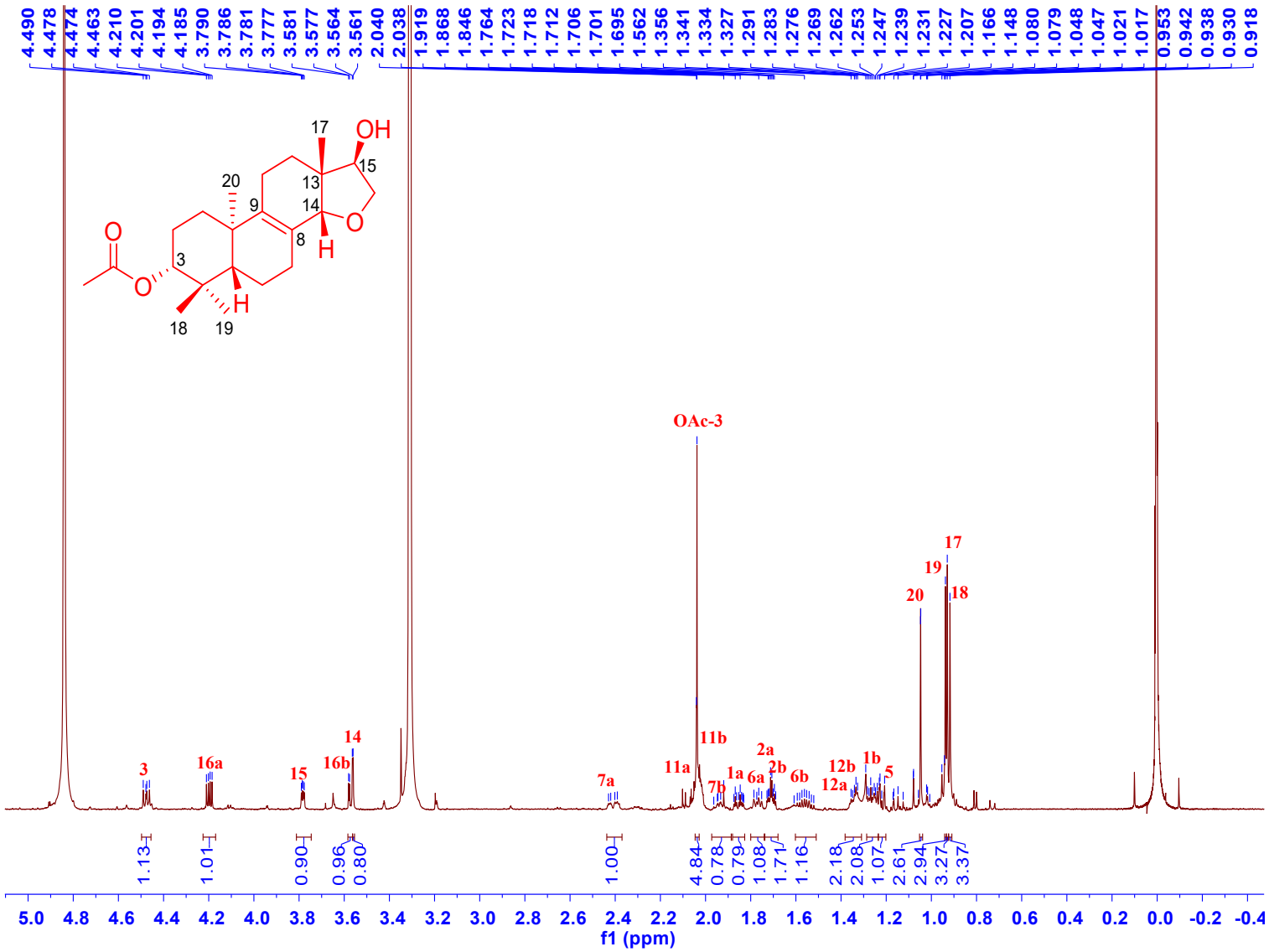


Figure S23. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 3.

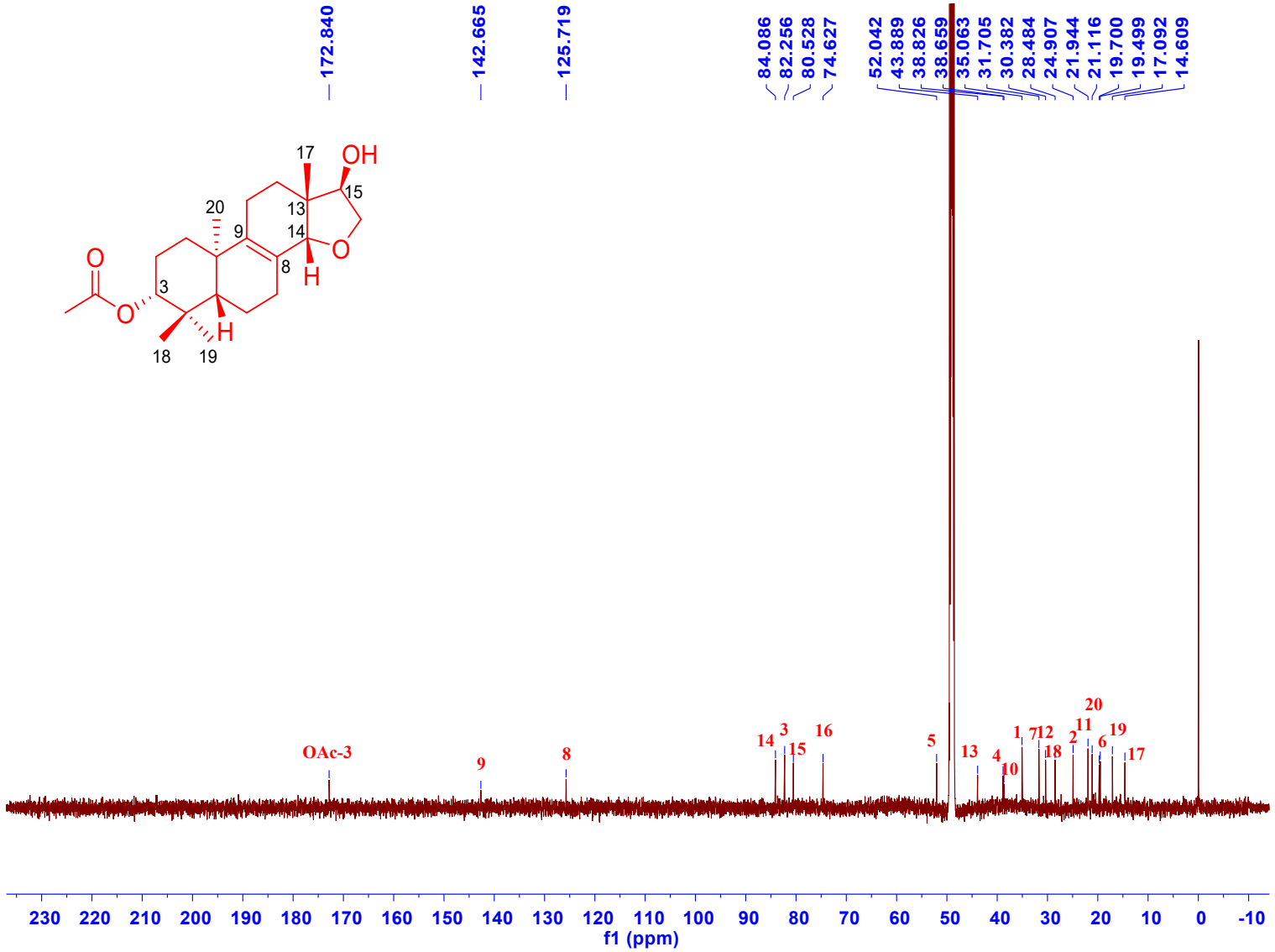


Figure S24. HSQC (CD_3OD) spectrum of compound 3.

Figure S25. HMBC (CD_3OD) spectrum of compound 3.

Figure S26. ^1H-^1H COSY (CD_3OD) spectrum of compound 3.

Figure S27. NOESY (CD_3OD) spectrum of compound 3.

Figure S28. IR spectrum of compound 3.

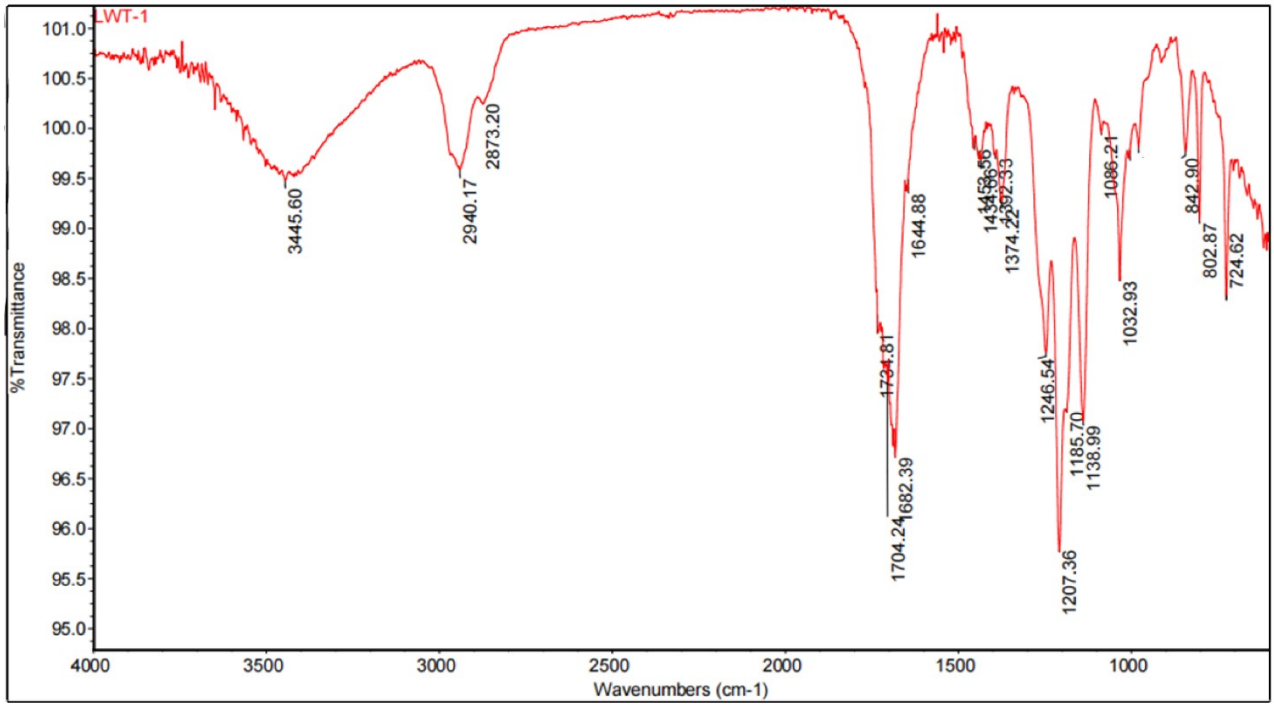


Figure S29. UV spectrum of compound 3.

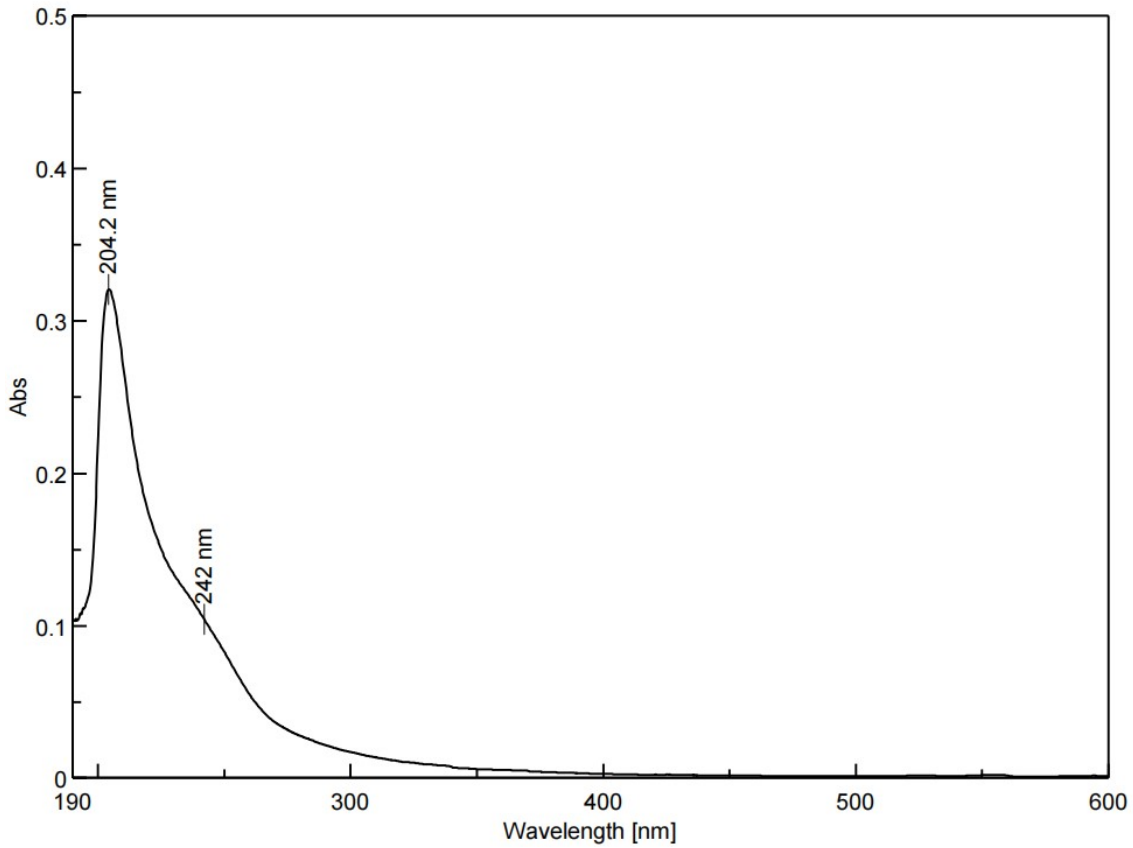


Figure S30. CD spectrum of compound 3.

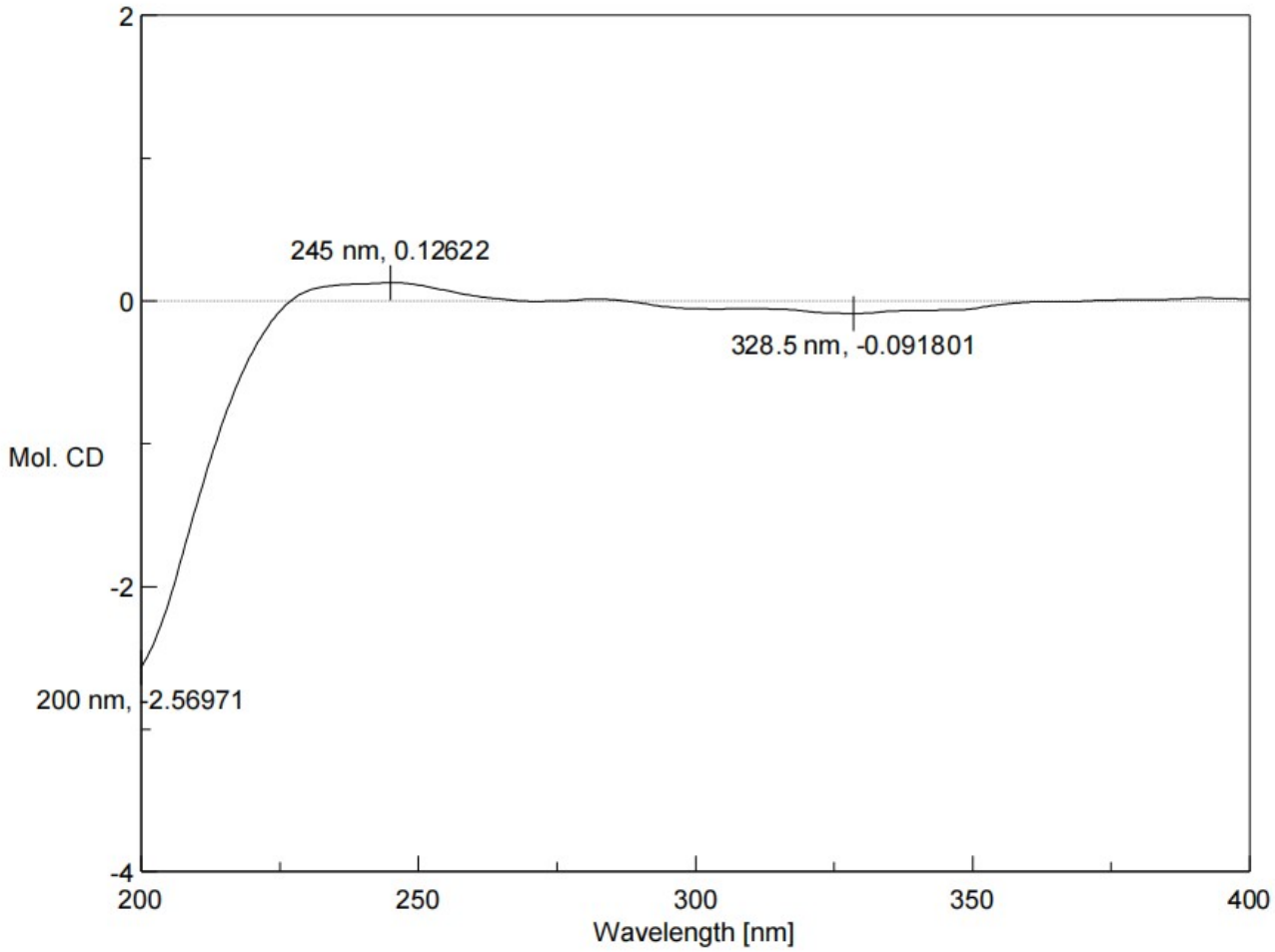


Figure S31. HRESIMS (MeOH) spectrum of compound 4.

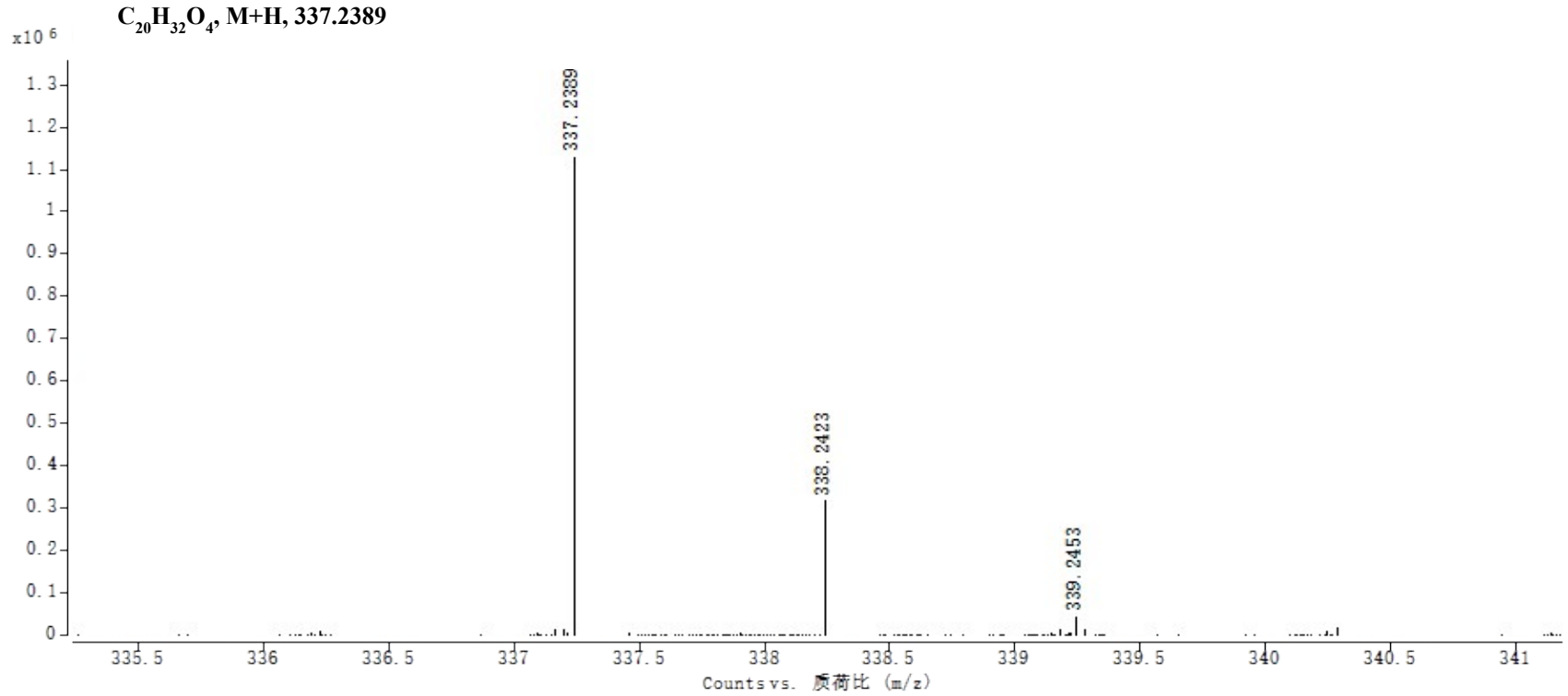


Figure S32. ^{1}H NMR (700 MHz, CD_3OD) spectrum of compound 4.

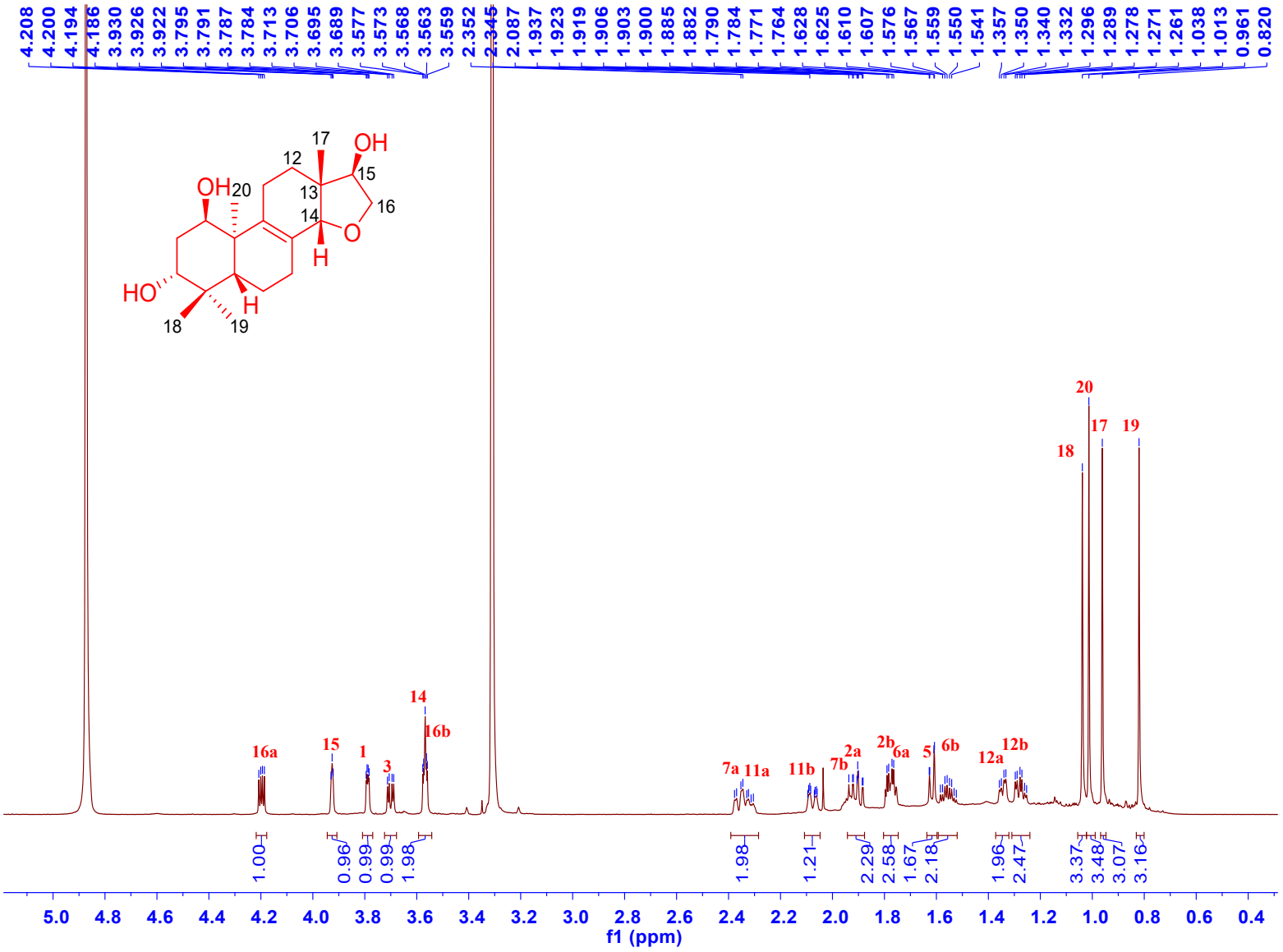


Figure S33. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 4.

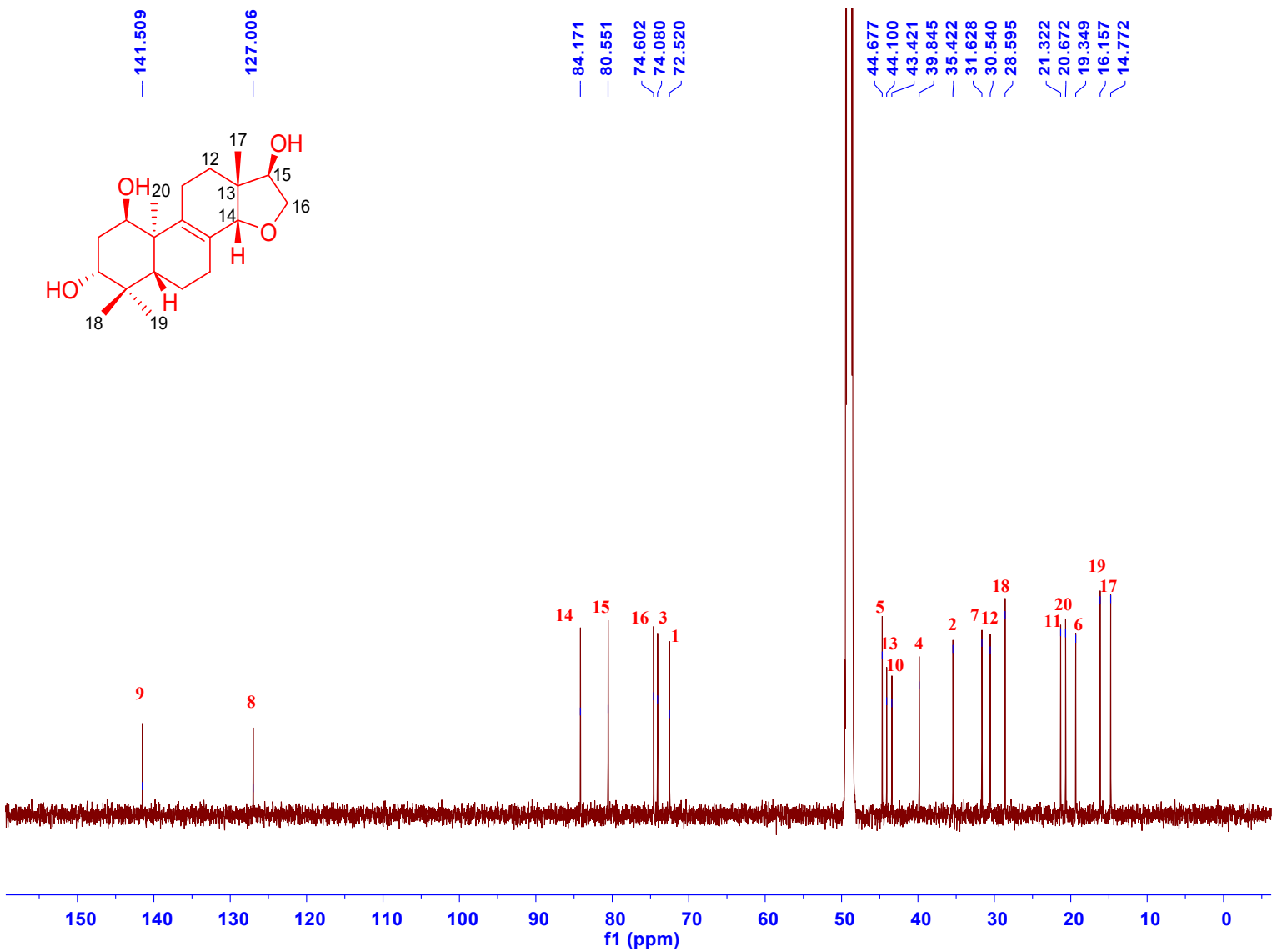


Figure S34. HSQC (CD_3OD) spectrum of compound 4.

Figure S35. HMBC (CD_3OD) spectrum of compound 4.

Figure S36. ^1H-^1H COSY (CD_3OD) spectrum of compound 4.

Figure S37. NOESY (CD_3OD) spectrum of compound 4.

Figure S38. IR spectrum of compound 4.

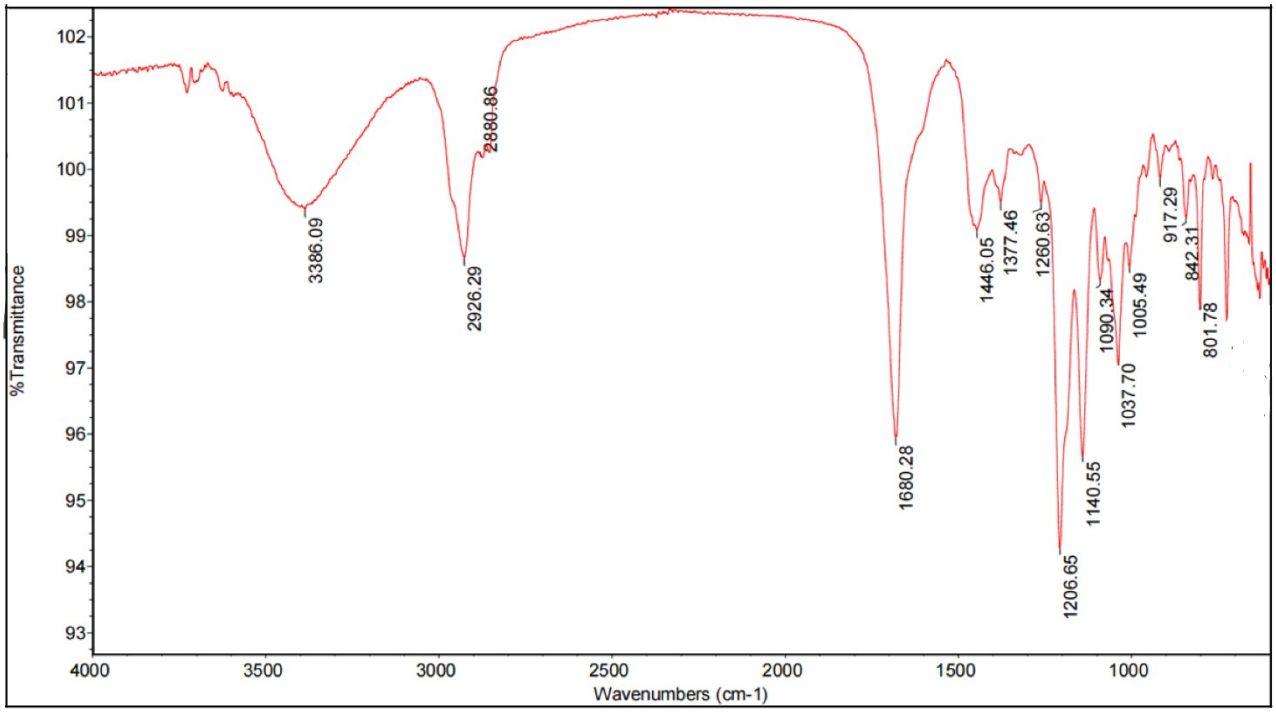


Figure S39. UV spectrum of compound 4.

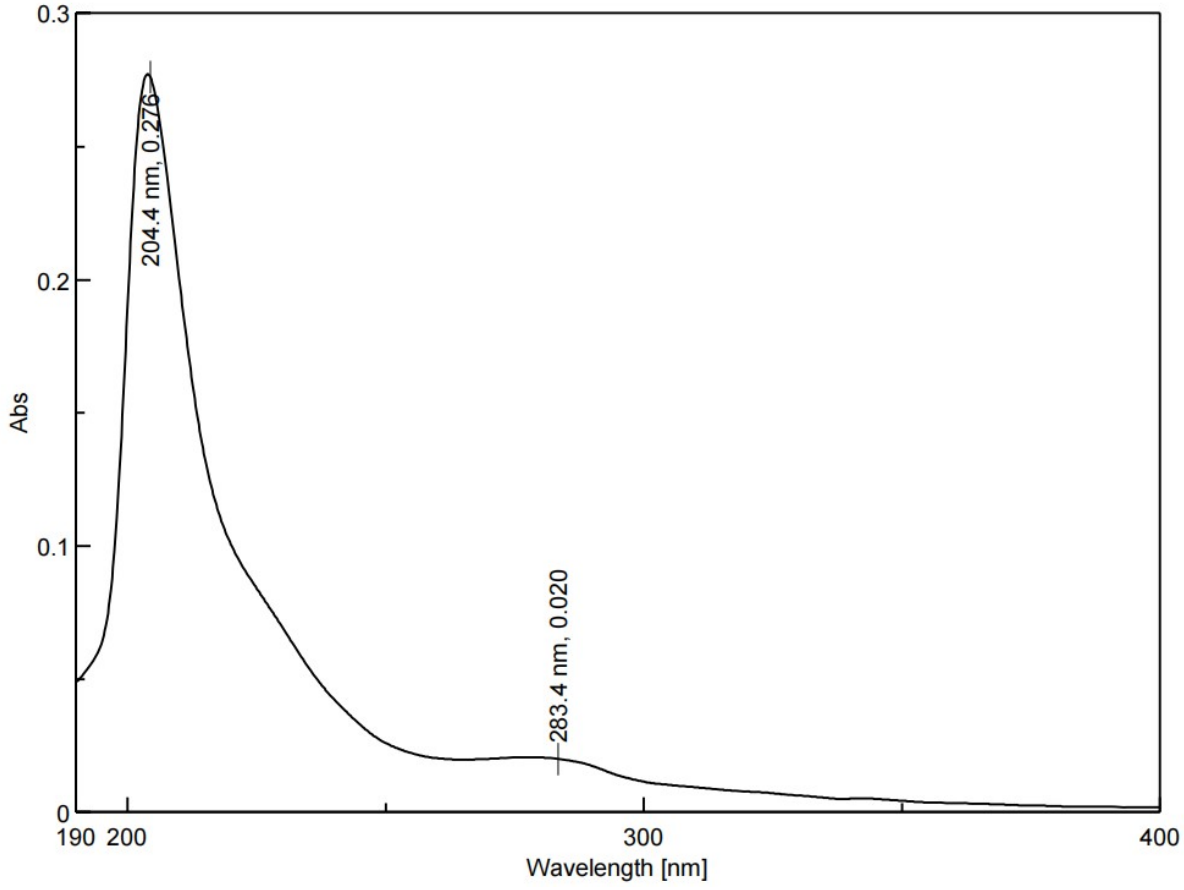


Figure S40. CD spectrum of compound 4.

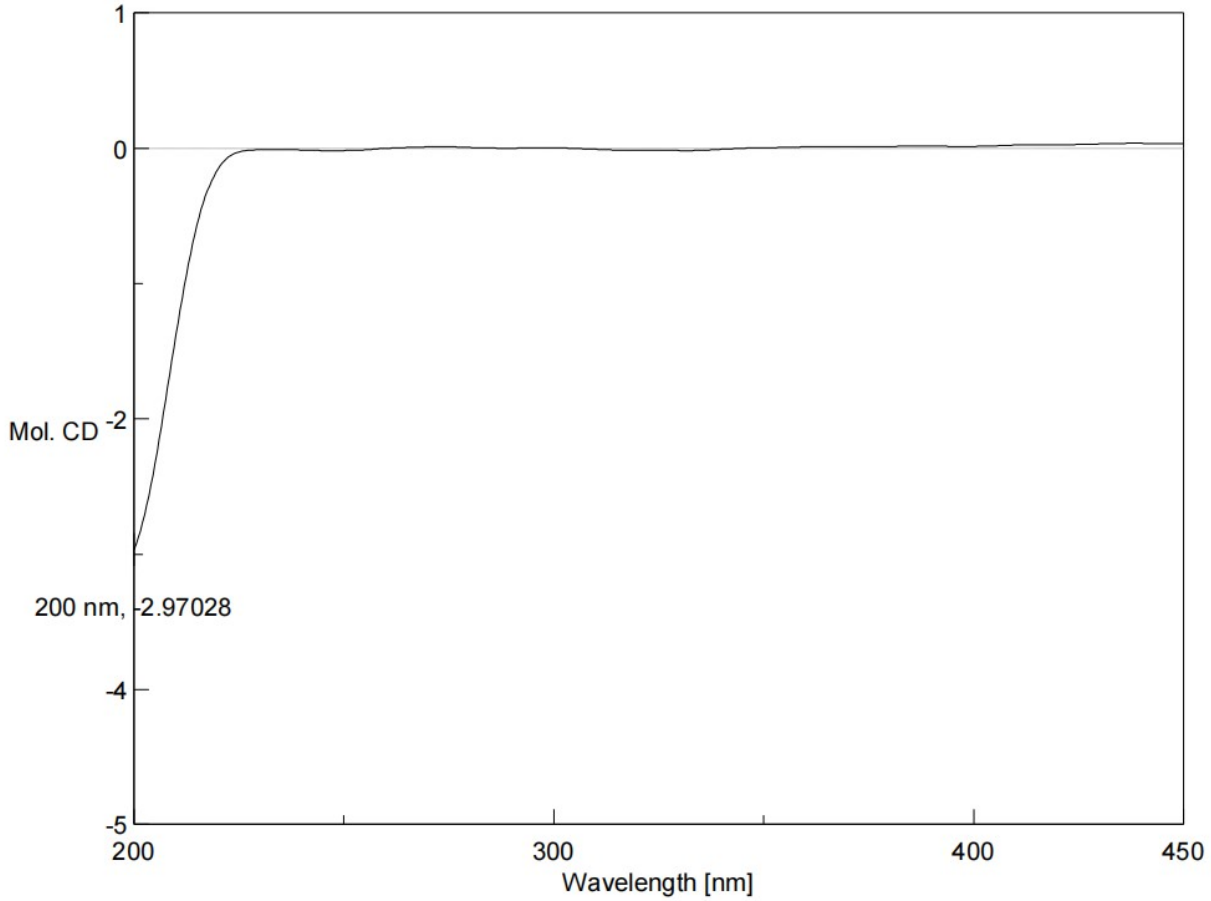


Figure S41. HRESIMS (MeOH) spectrum of compound 5.

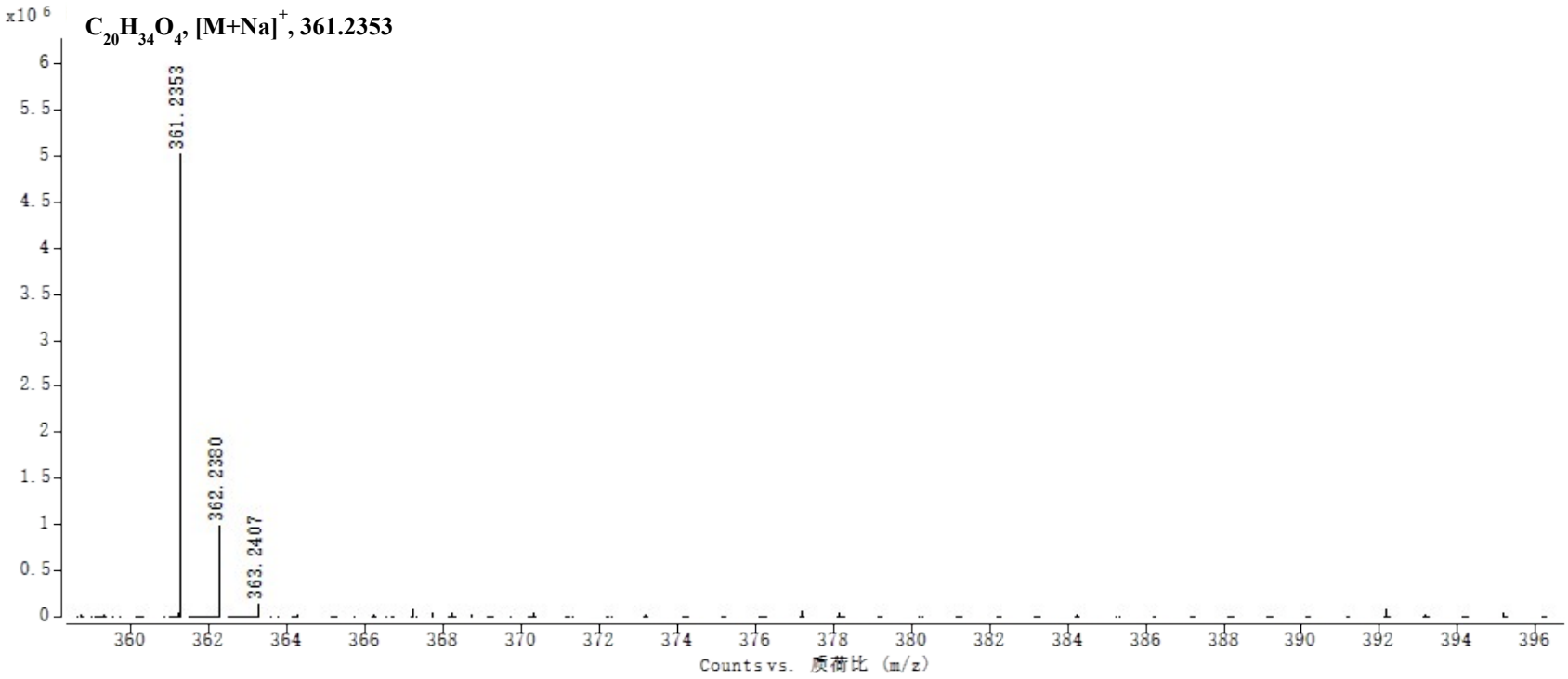


Figure S42. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound 5.

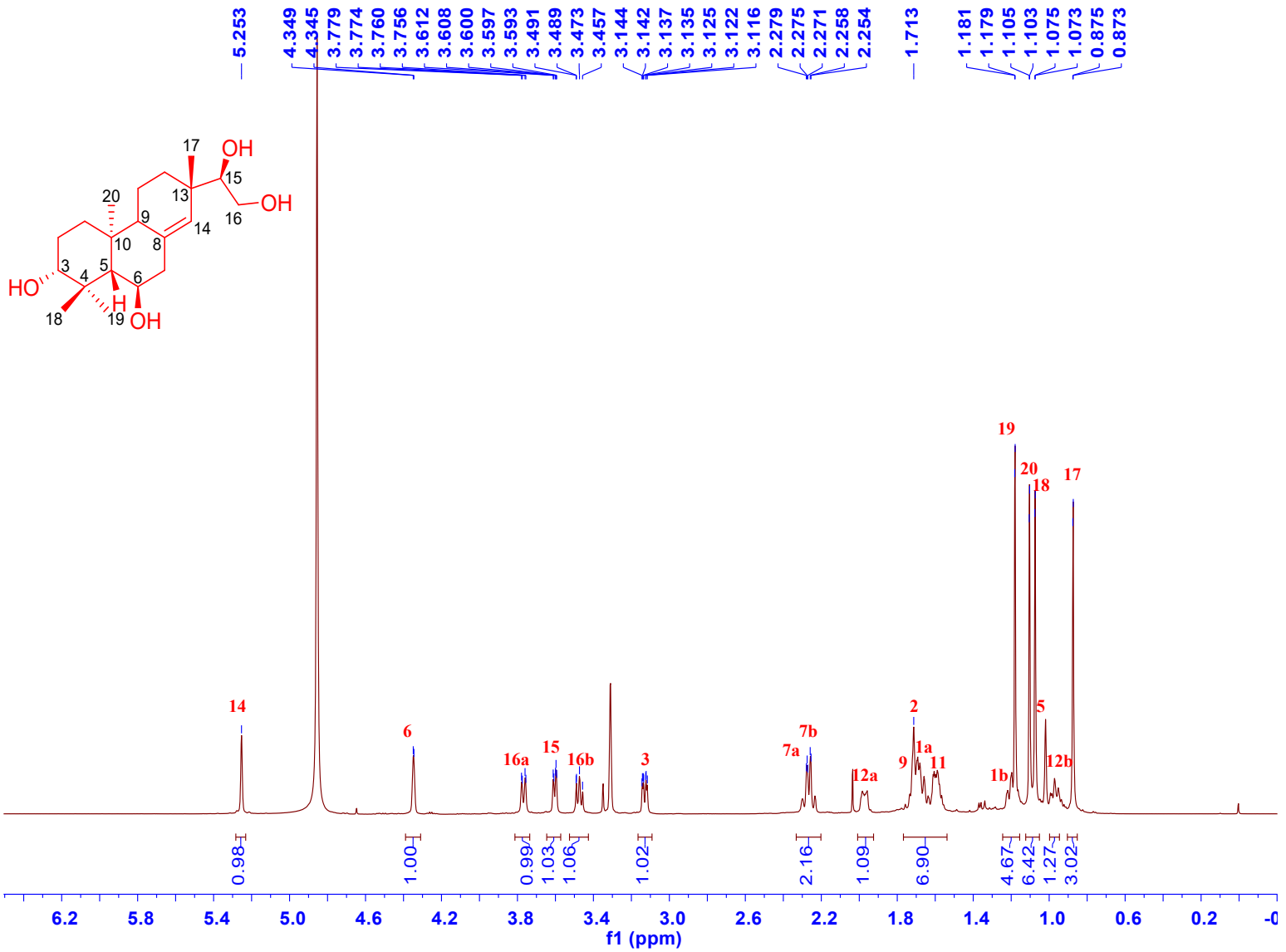


Figure S43. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 5.

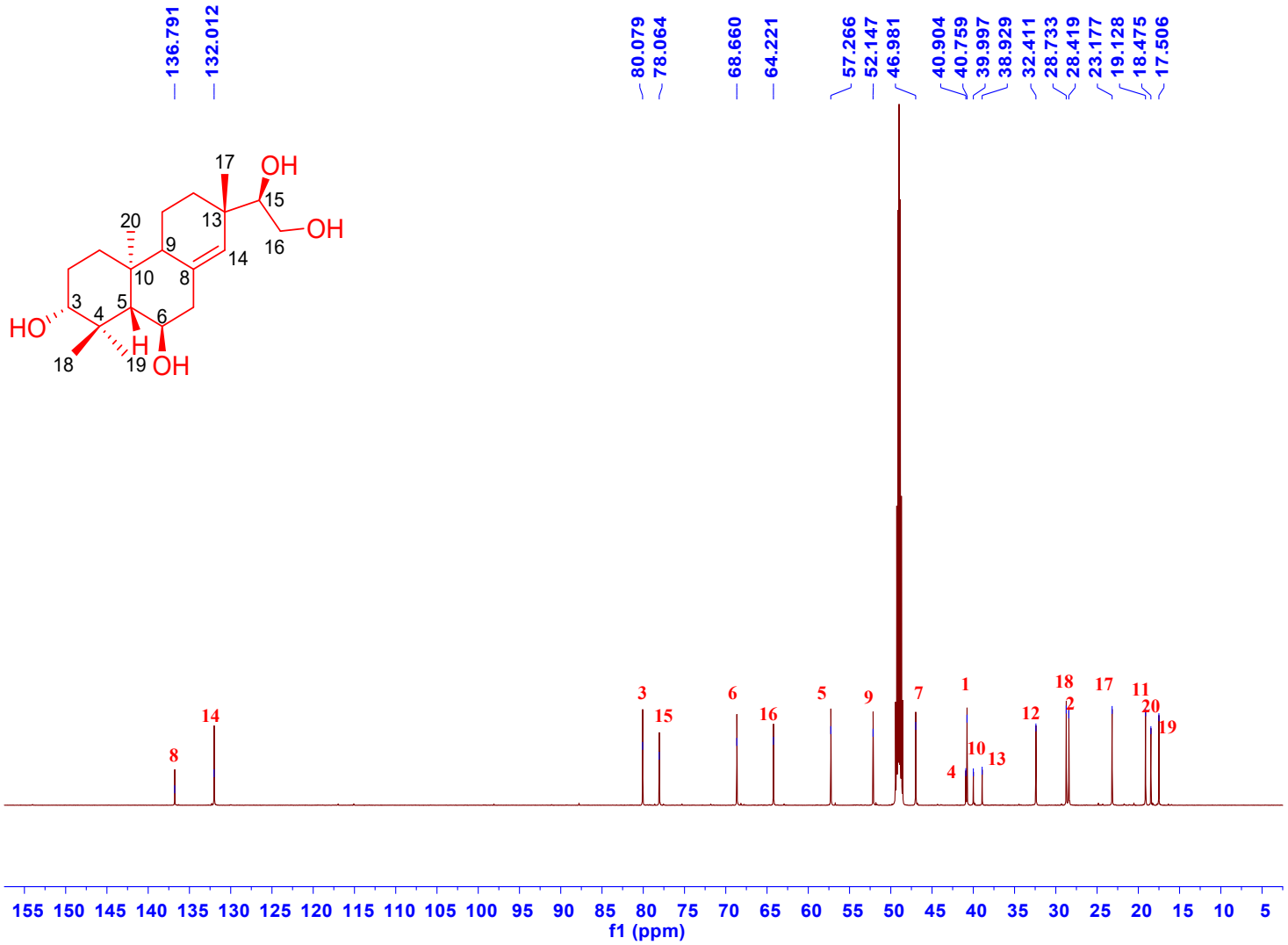


Figure S44. HSQC (CD_3OD) spectrum of compound 5.

Figure S45. HMBC (CD_3OD) spectrum of compound 5.

Figure S46. ^{1}H-^{1}H COSY (CD_3OD) spectrum of compound 5.

Figure S47. NOESY (CD_3OD) spectrum of compound 5.

Figure S48. IR spectrum of compound 5.

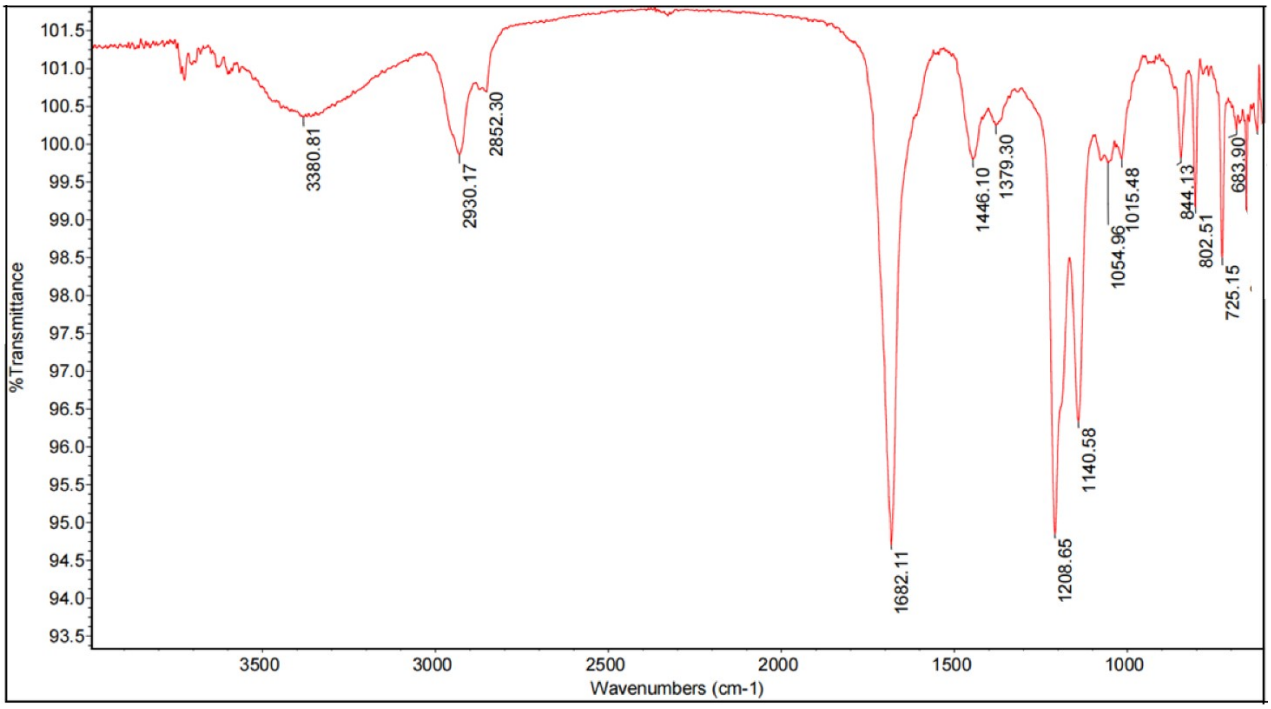


Figure S49. UV spectrum of compound 5.

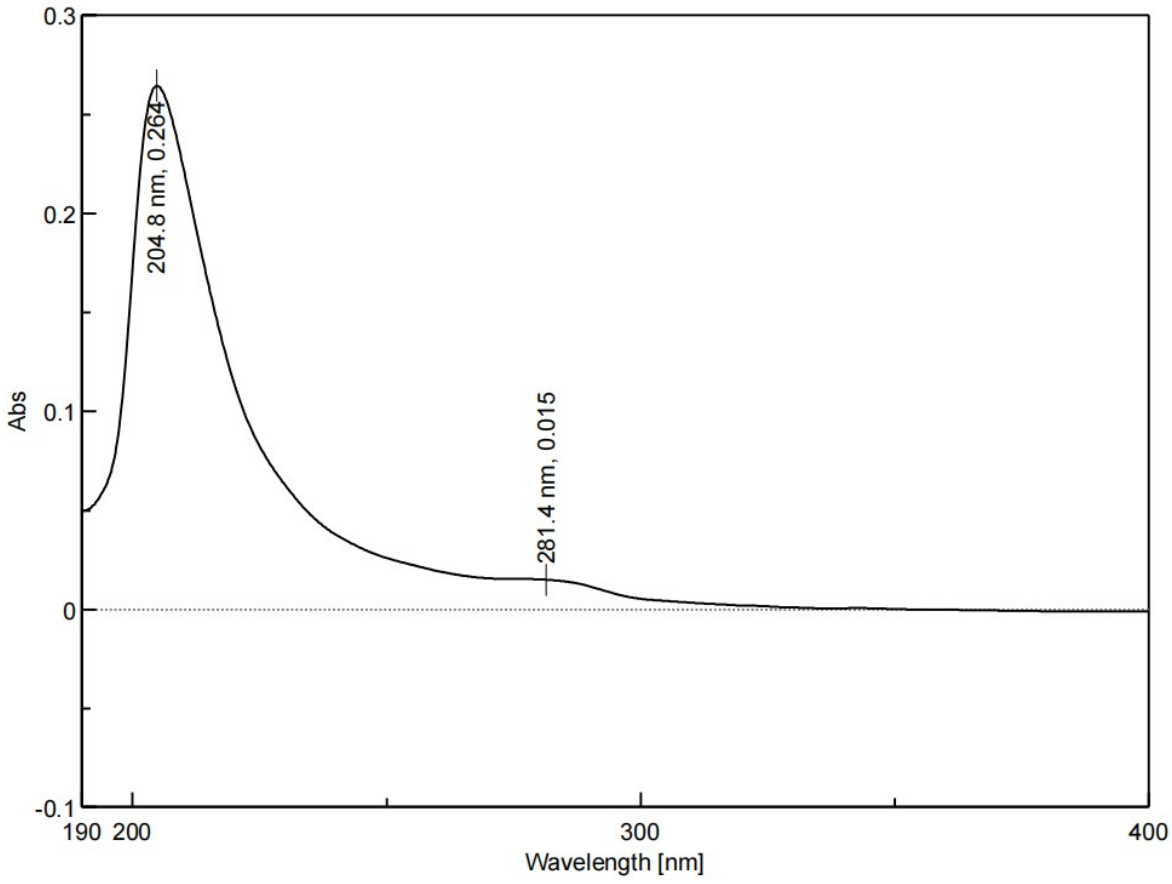


Figure S50. CD spectrum of compound 5.

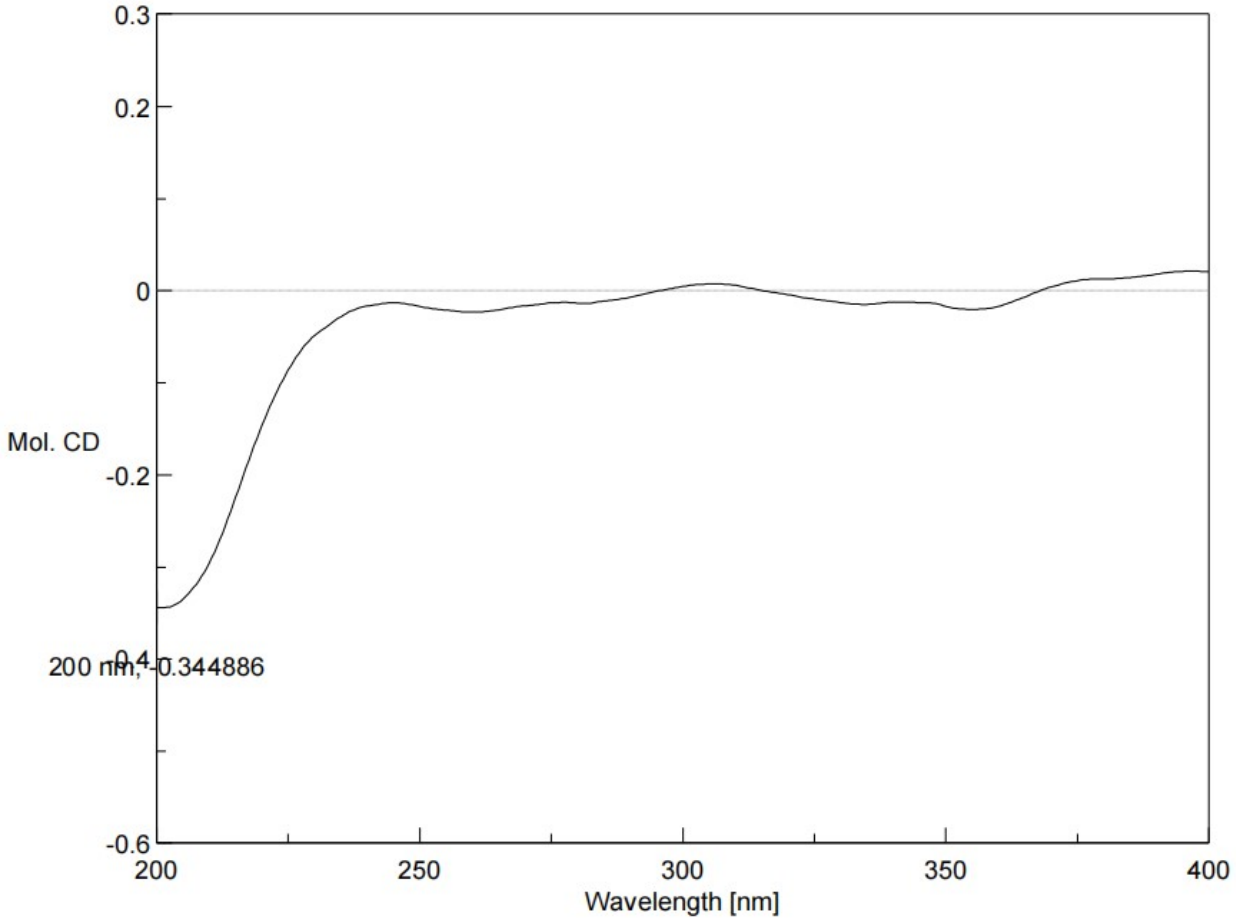


Figure S51. HRESIMS (MeOH) spectrum of compound 6.

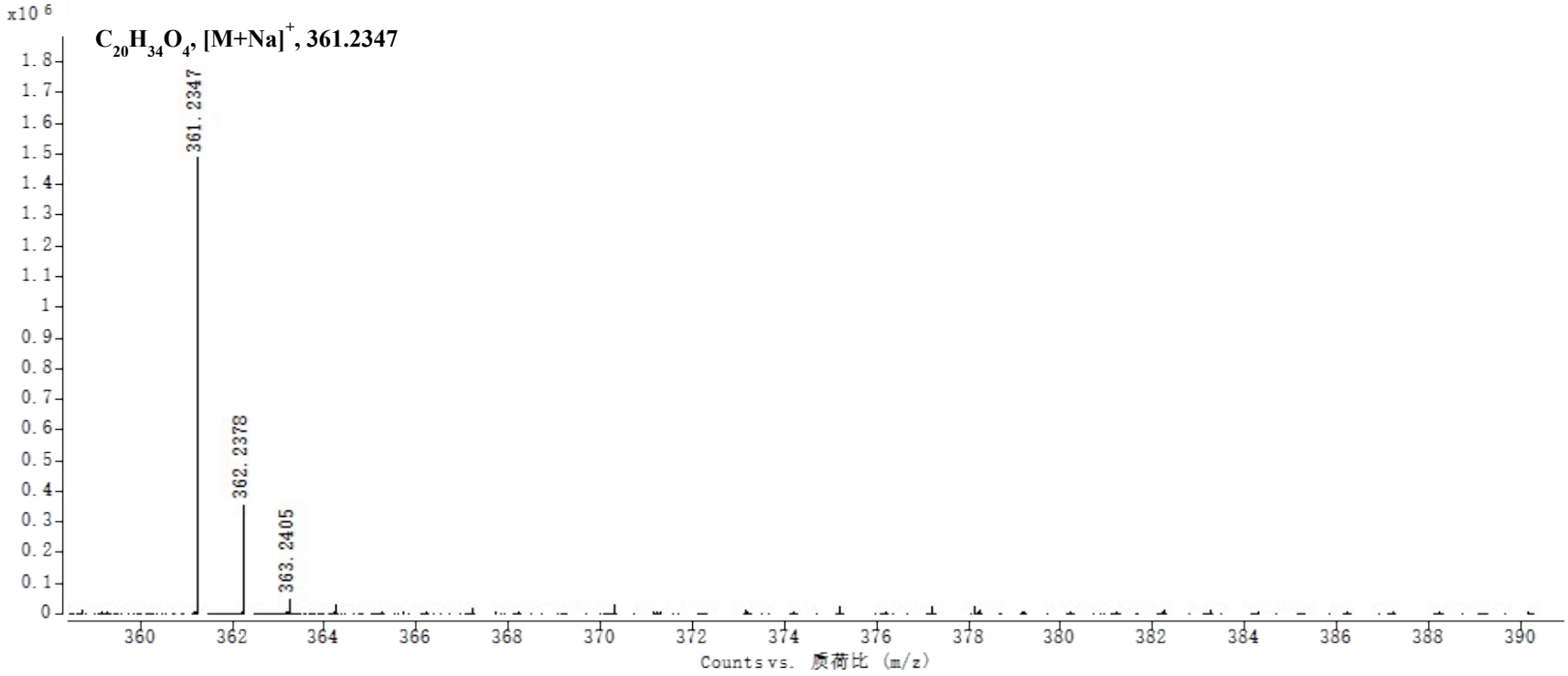


Figure S52. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound 6.

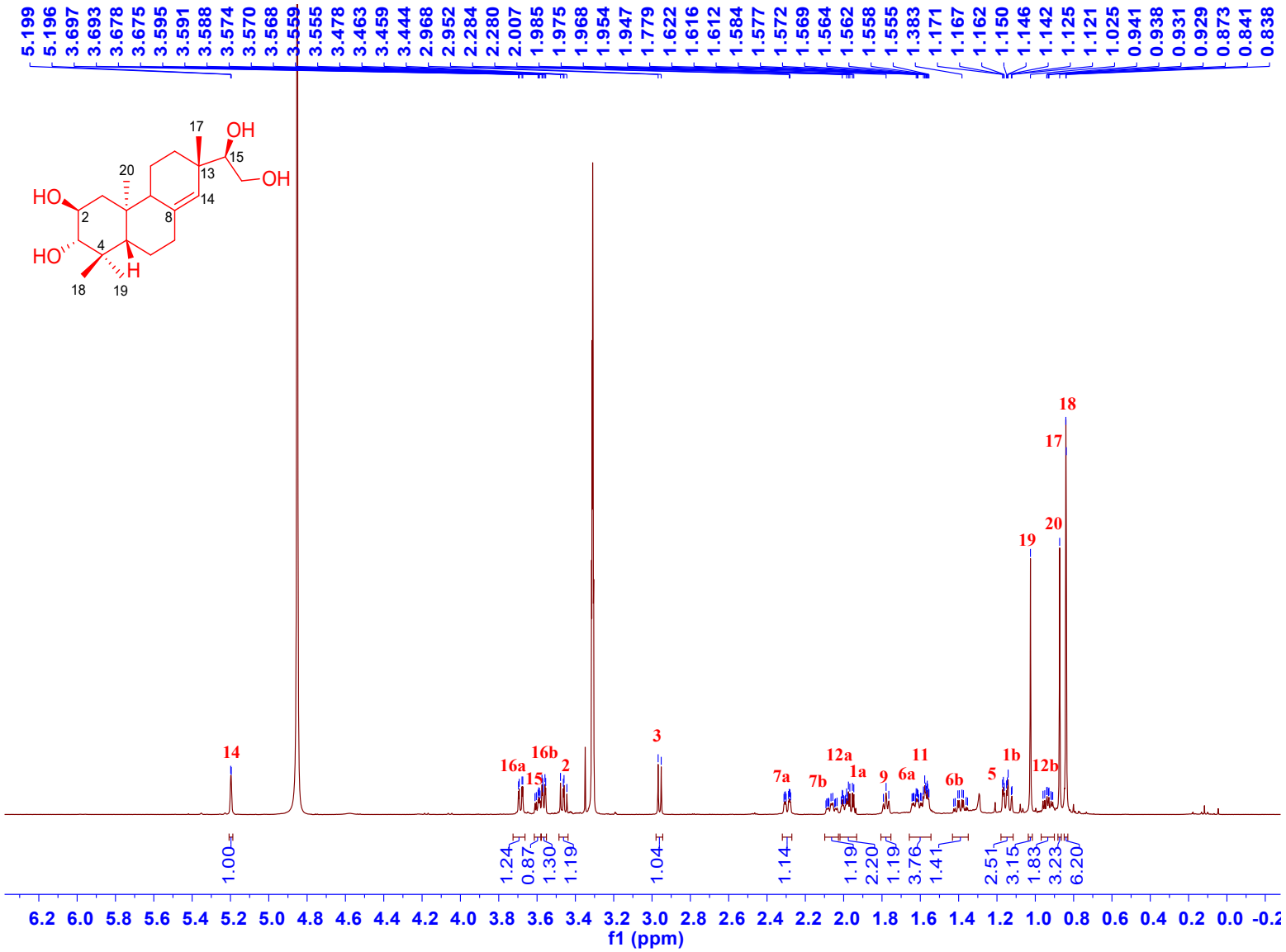


Figure S53. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 6.

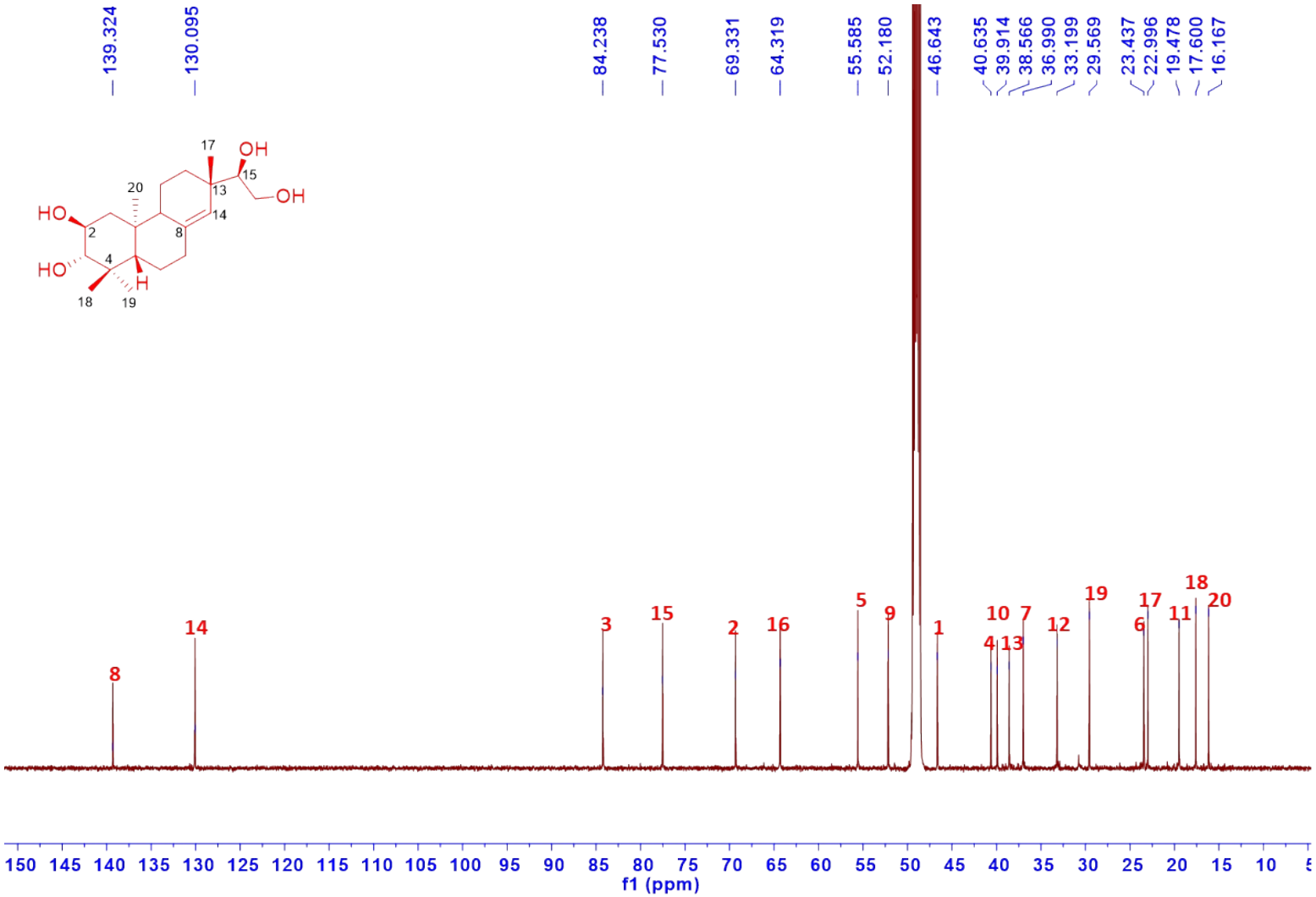


Figure S54. HSQC (CD_3OD) spectrum of compound 6.

Figure S55. HMBC (CD_3OD) spectrum of compound 6.

Figure S56. ^1H-^1H COSY (CD_3OD) spectrum of compound 6.

Figure S57. NOESY (CD_3OD) spectrum of compound 6.

Figure S58. IR spectrum of compound 6.

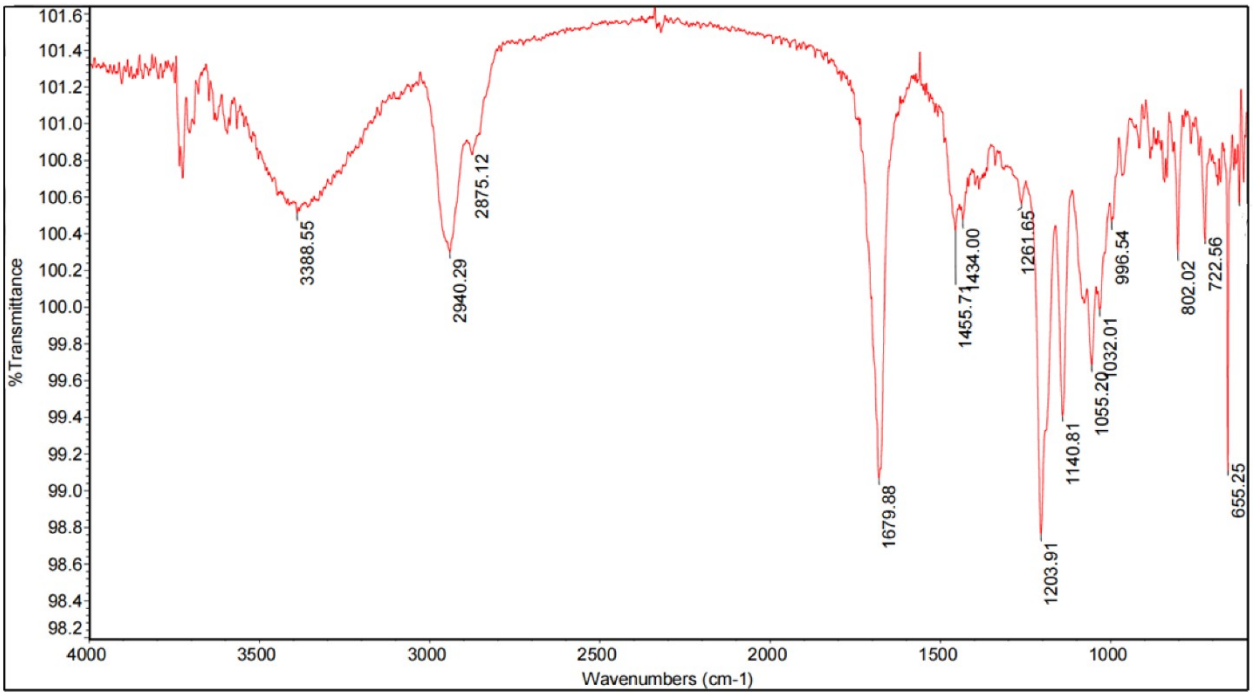


Figure S59. UV spectrum of compound 6.

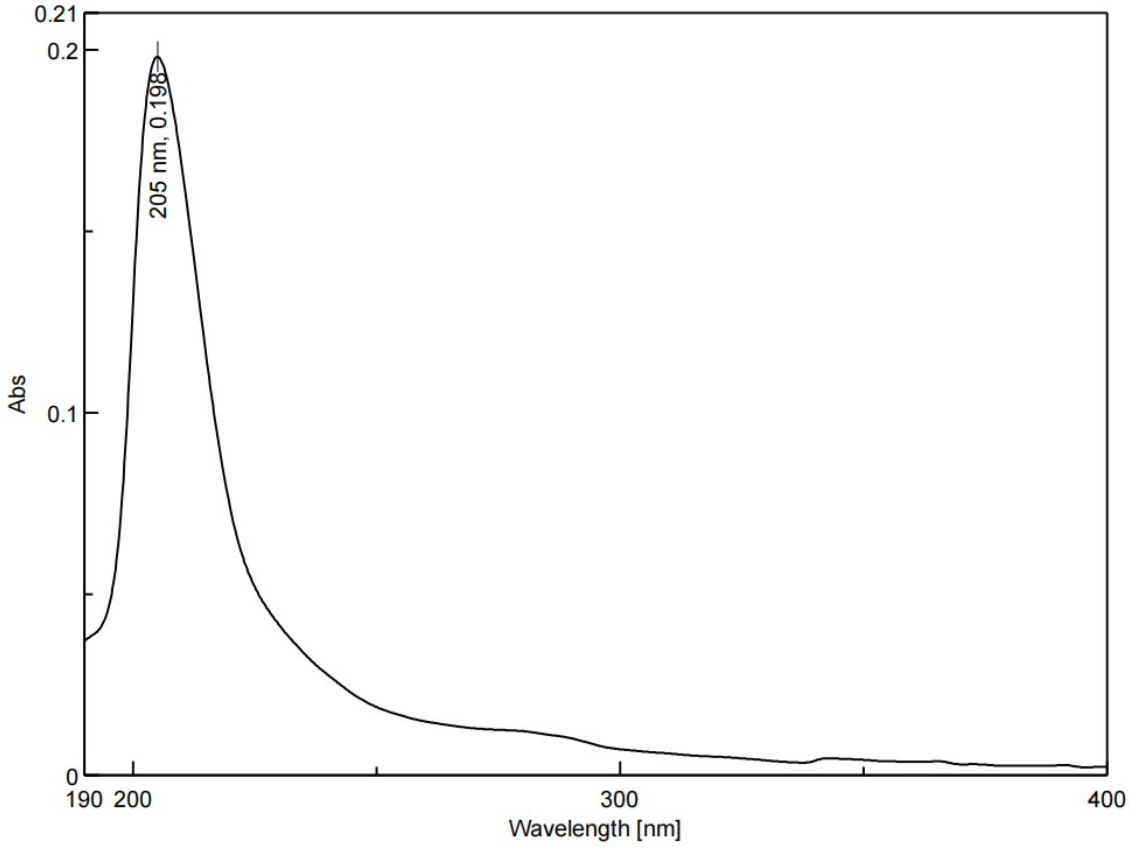


Figure S60. CD spectrum of compound 6.

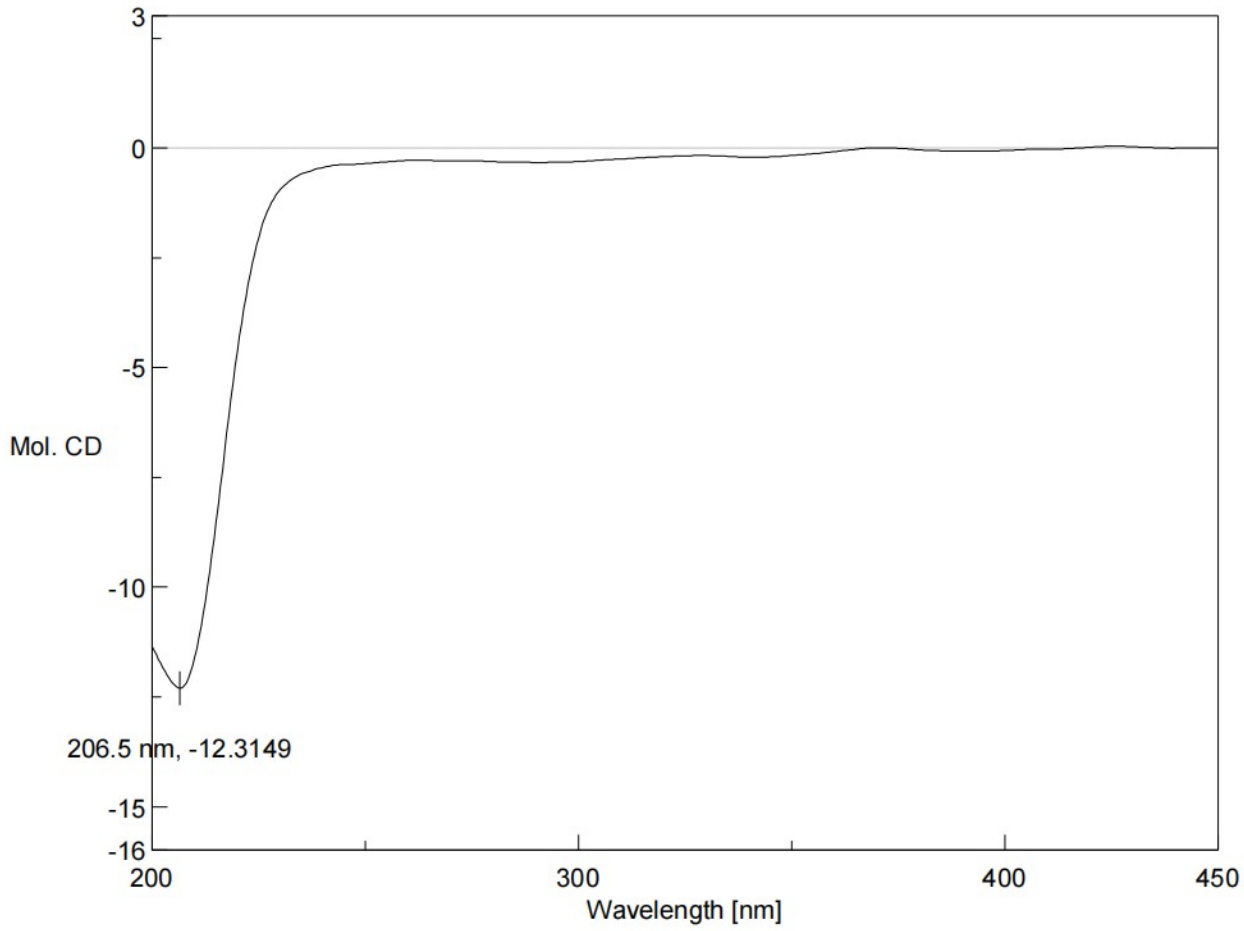


Figure S61. HRESIMS (MeOH) spectrum of compound 7.

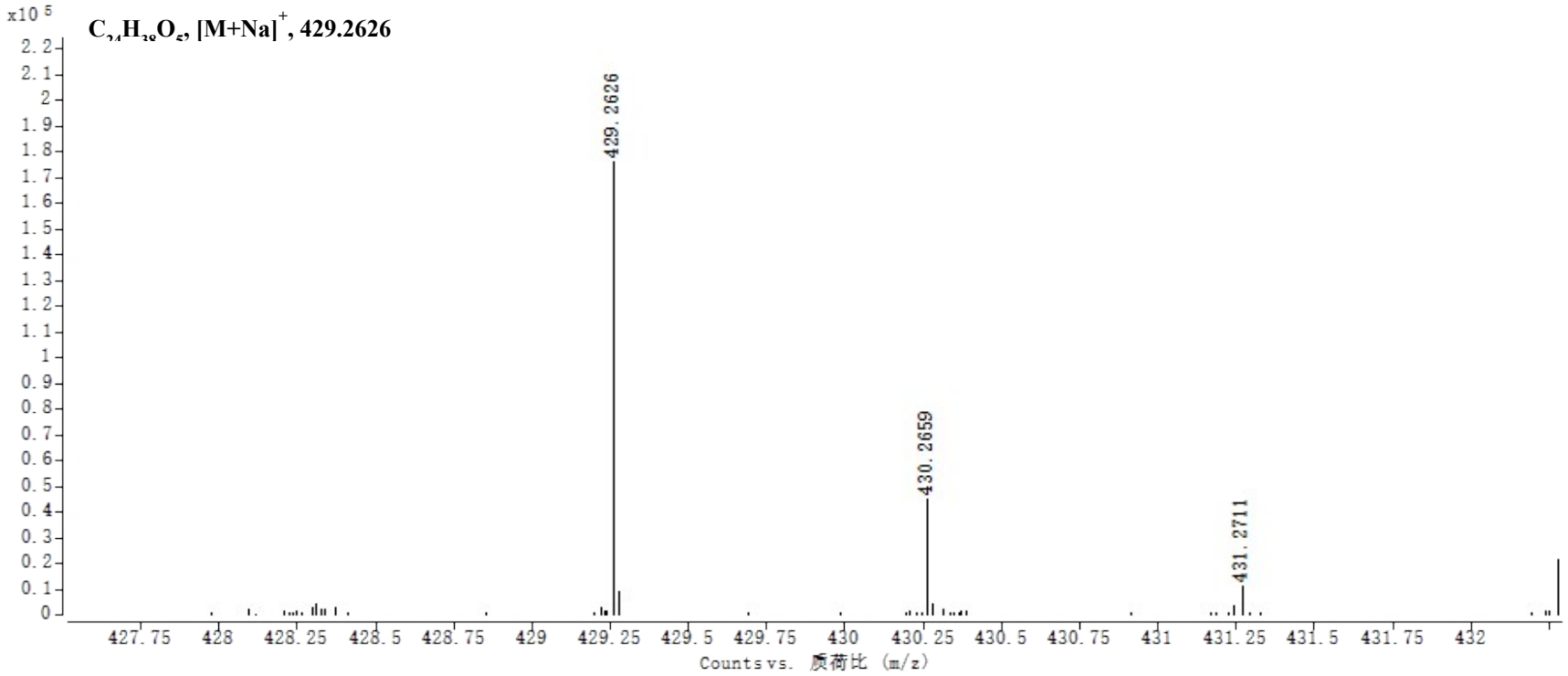


Figure S62. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound 7.

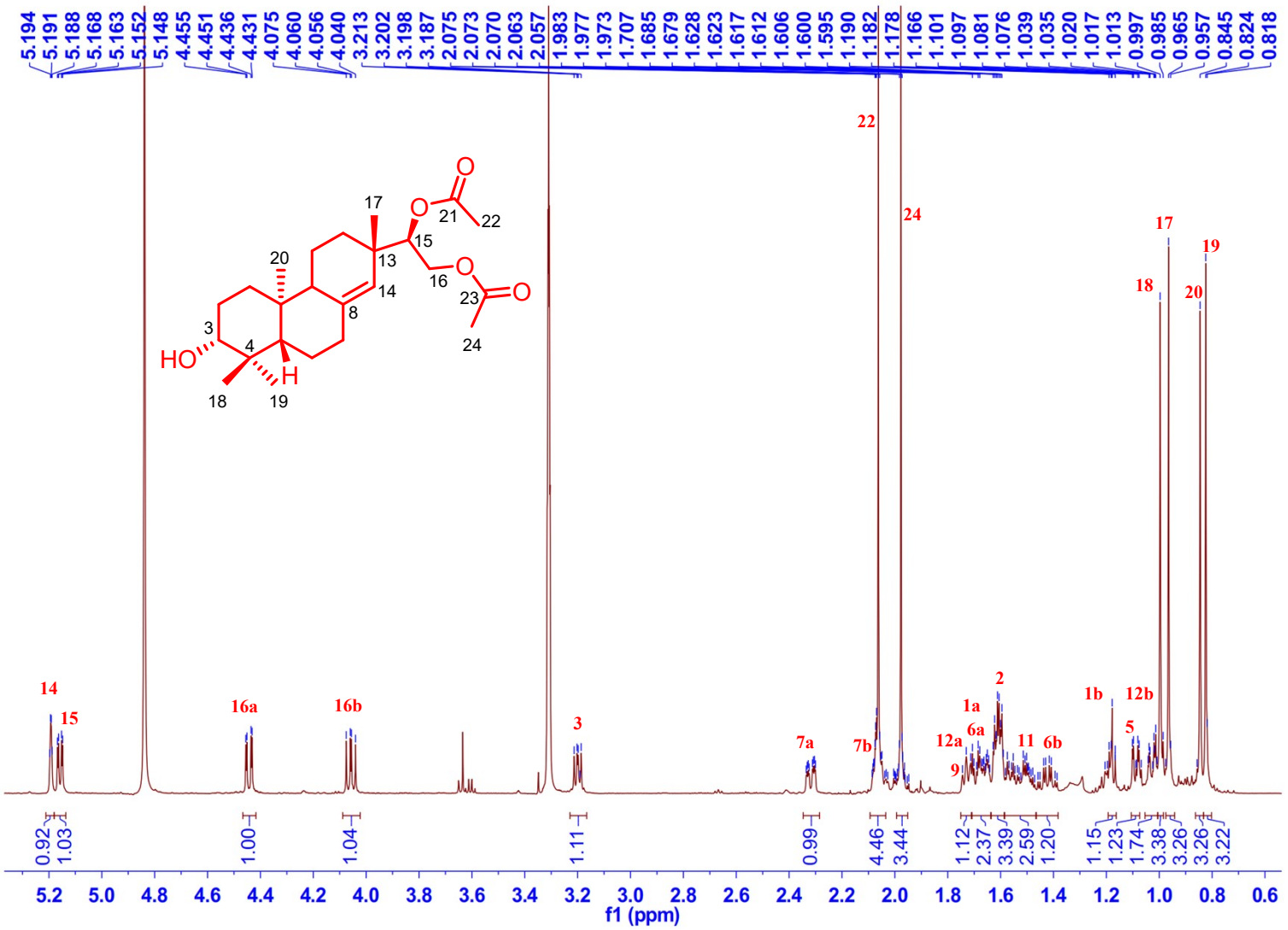


Figure S63. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 7.

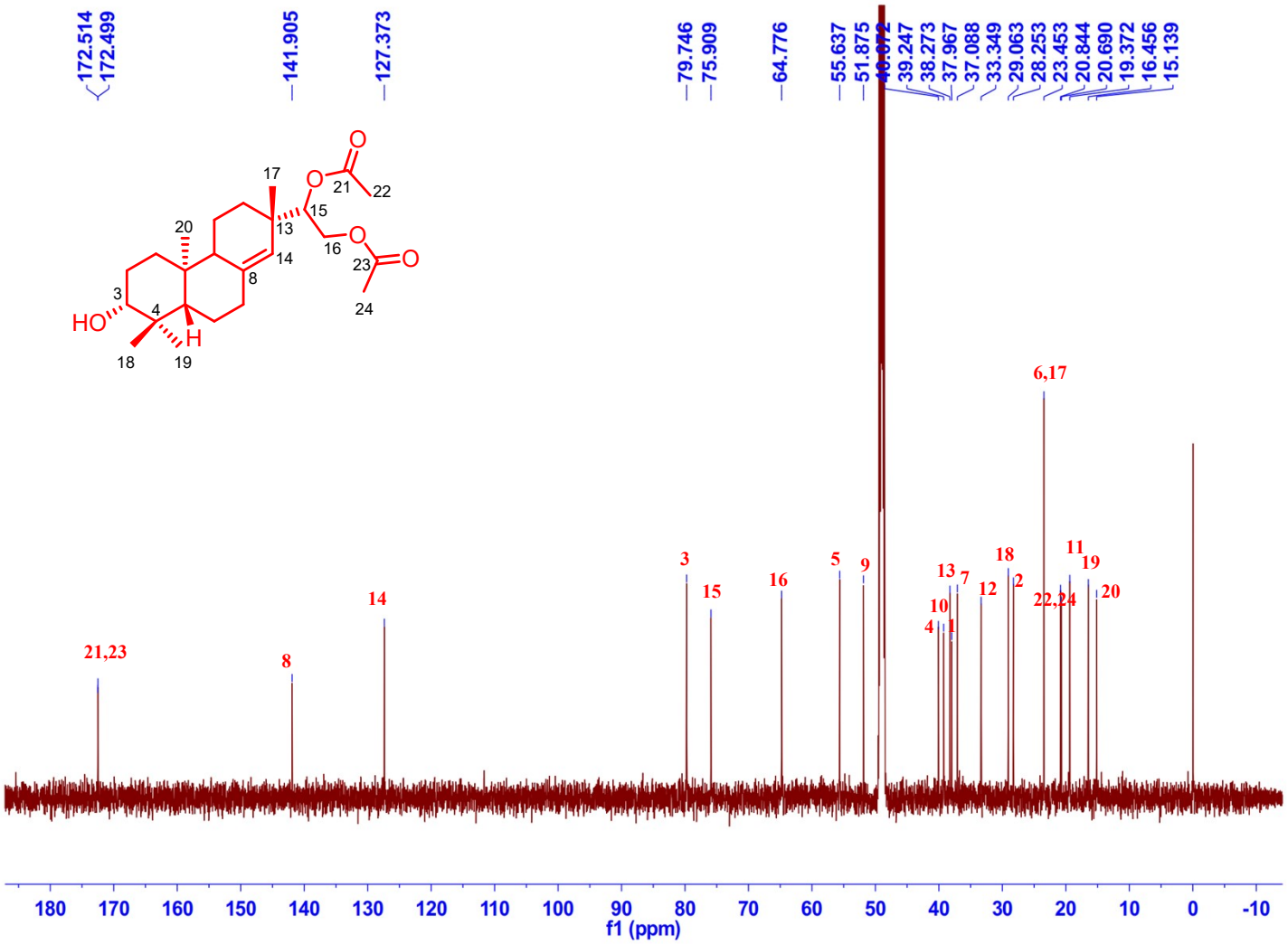


Figure S64. HSQC (CD_3OD) spectrum of compound 7.

Figure S65. HMBC (CD_3OD) spectrum of compound 7.

Figure S66. ^1H-^1H COSY (CD_3OD) spectrum of compound 7.

Figure S67. NOESY (CD_3OD) spectrum of compound 7.

Figure S68. IR spectrum of compound 7.

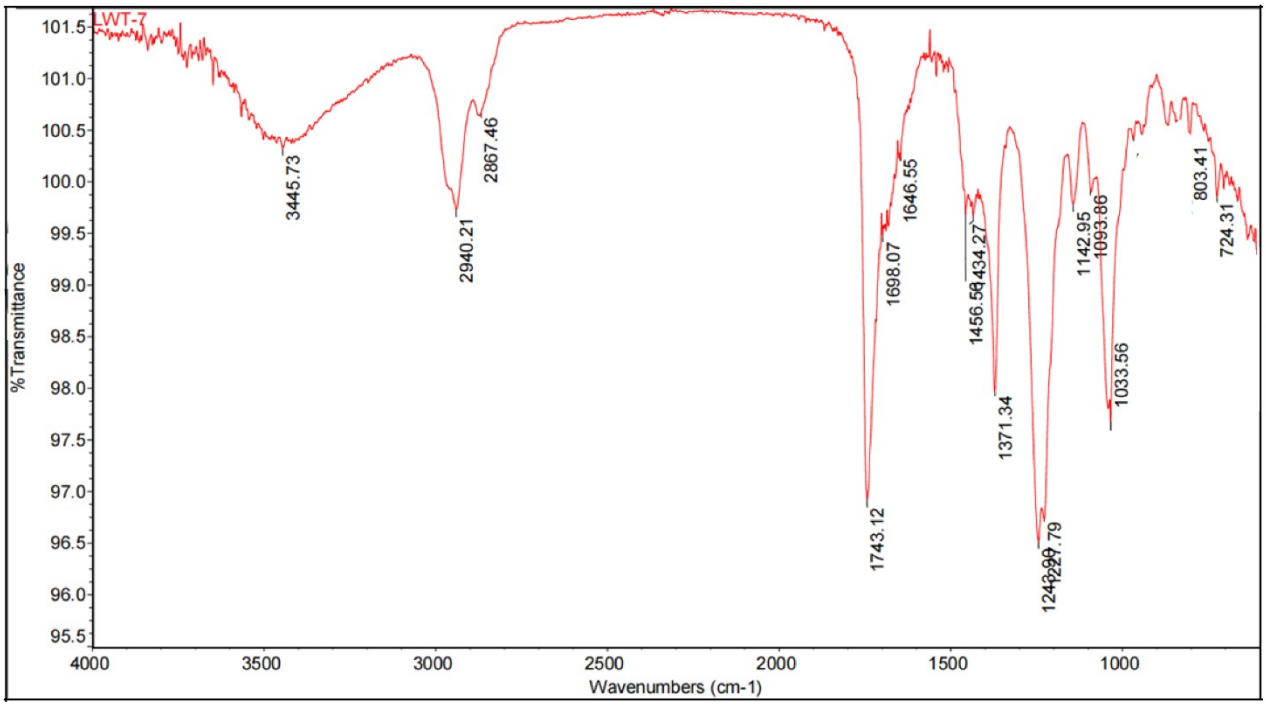


Figure S69. UV spectrum of compound 7.

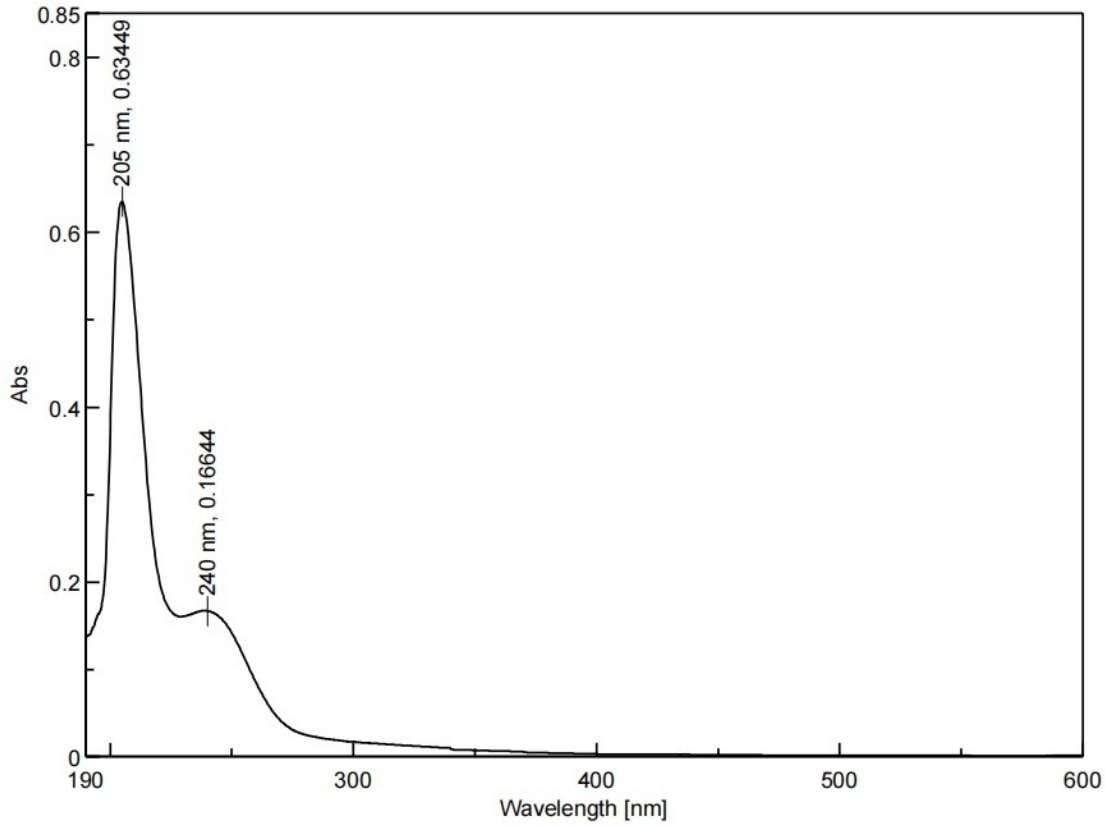


Figure S70. CD spectrum of compound 7.

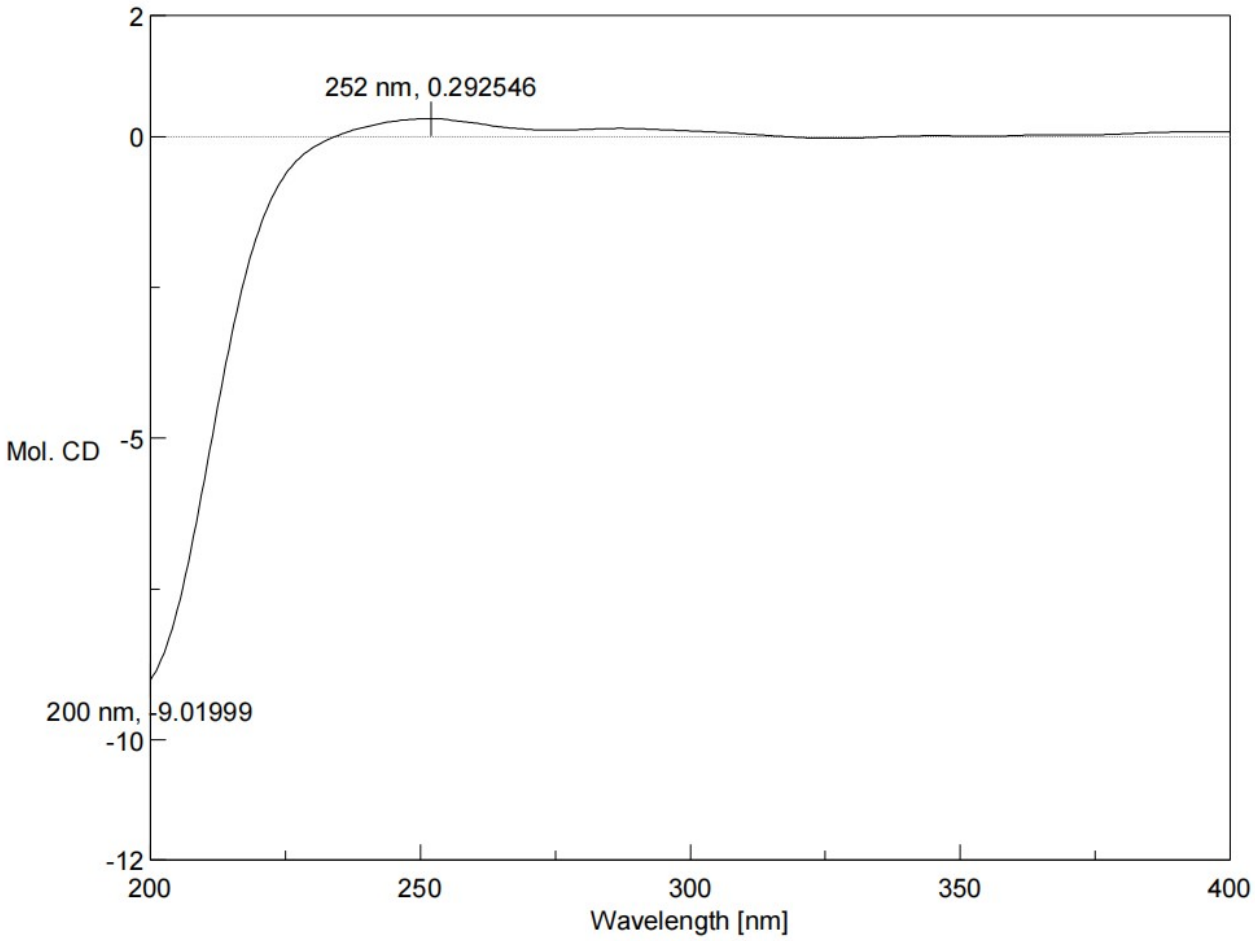


Figure S71. HRESIMS (MeOH) spectrum of compound 8.

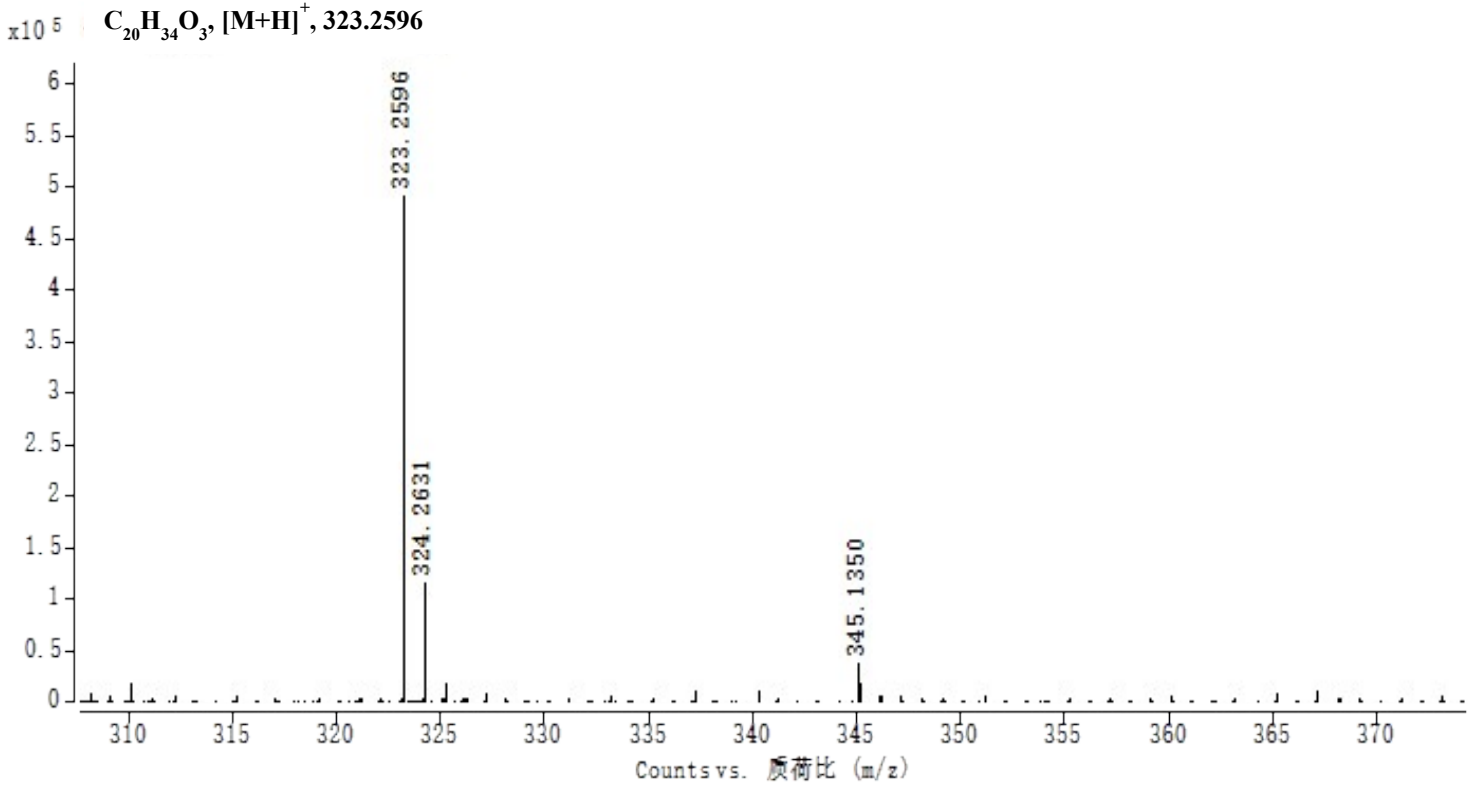


Figure S72. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound 8.

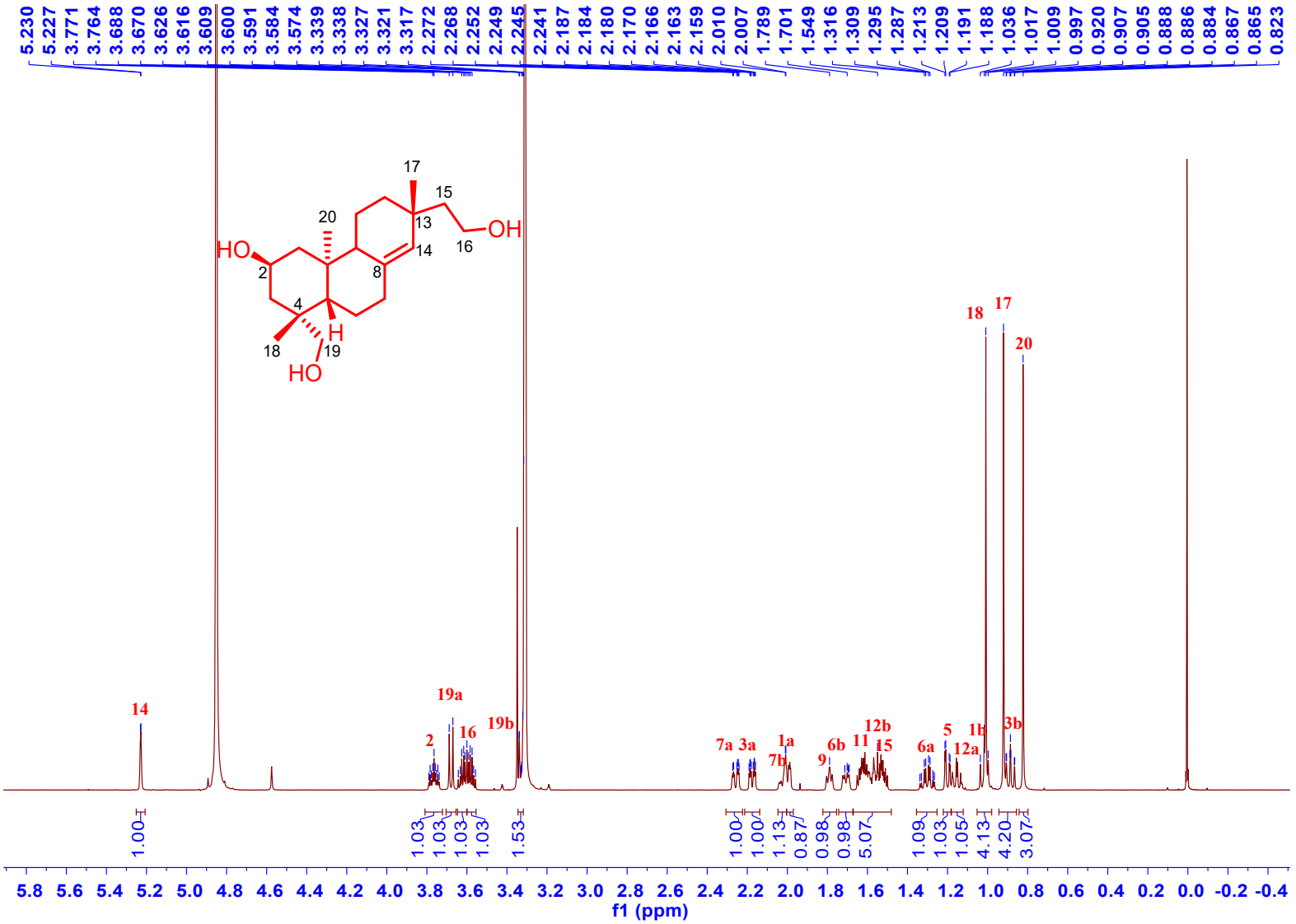


Figure S73. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 8.

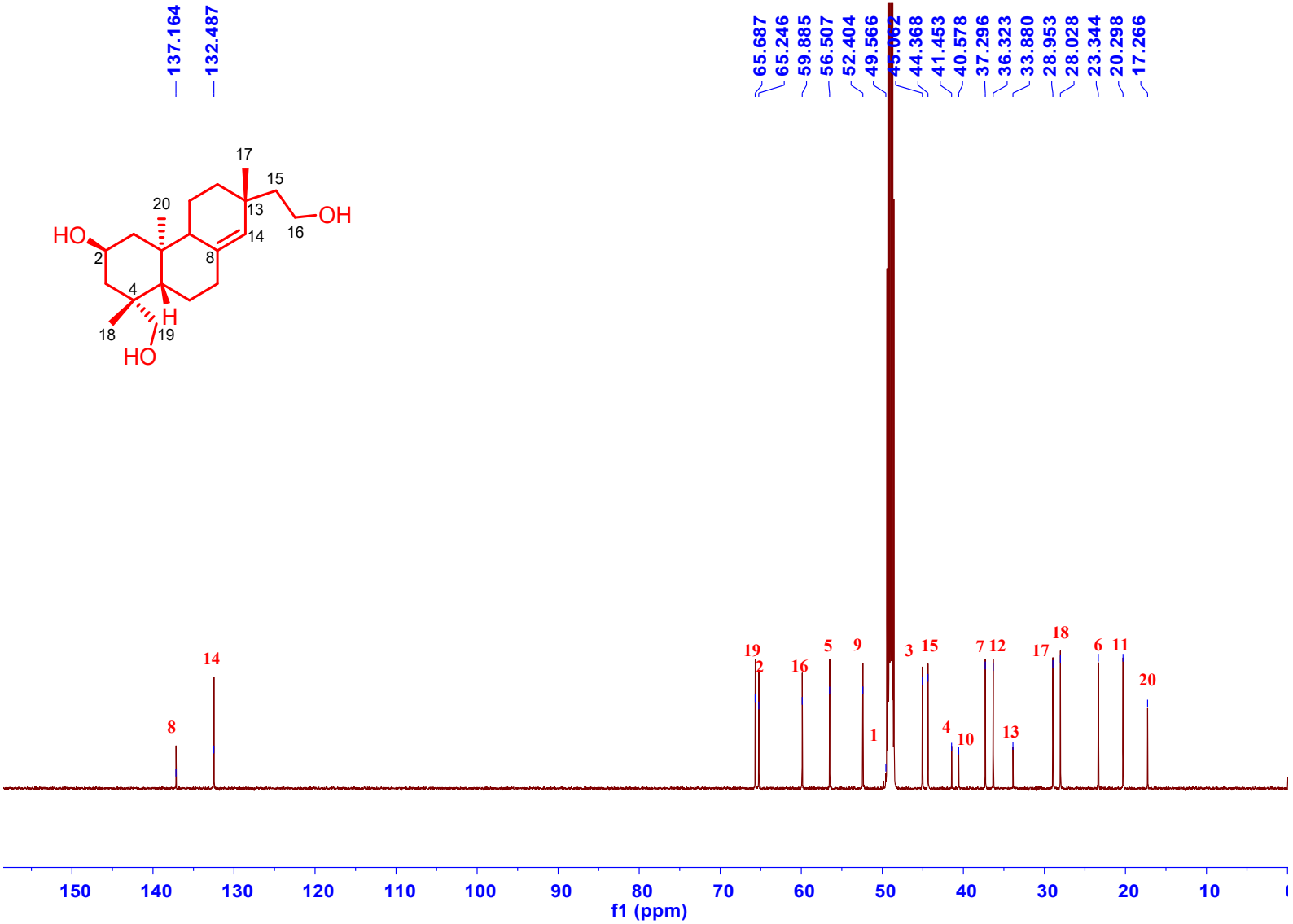


Figure S74. HSQC (CD3OD) spectrum of compound 8.

Figure S75. HMBC (CD_3OD) spectrum of compound 8.

Figure S76. ^1H-^1H COSY (CD_3OD) spectrum of compound 8.

Figure S77. NOESY (CD_3OD) spectrum of compound 8.

Figure S78. IR spectrum of compound 8.

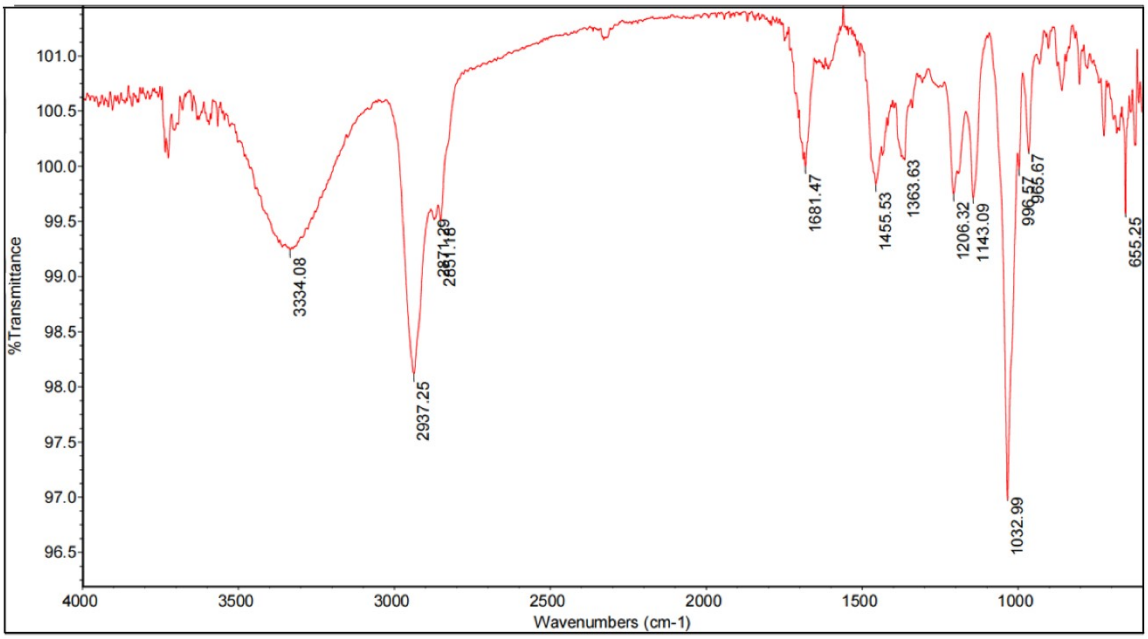


Figure S79. UV spectrum of compound 8.

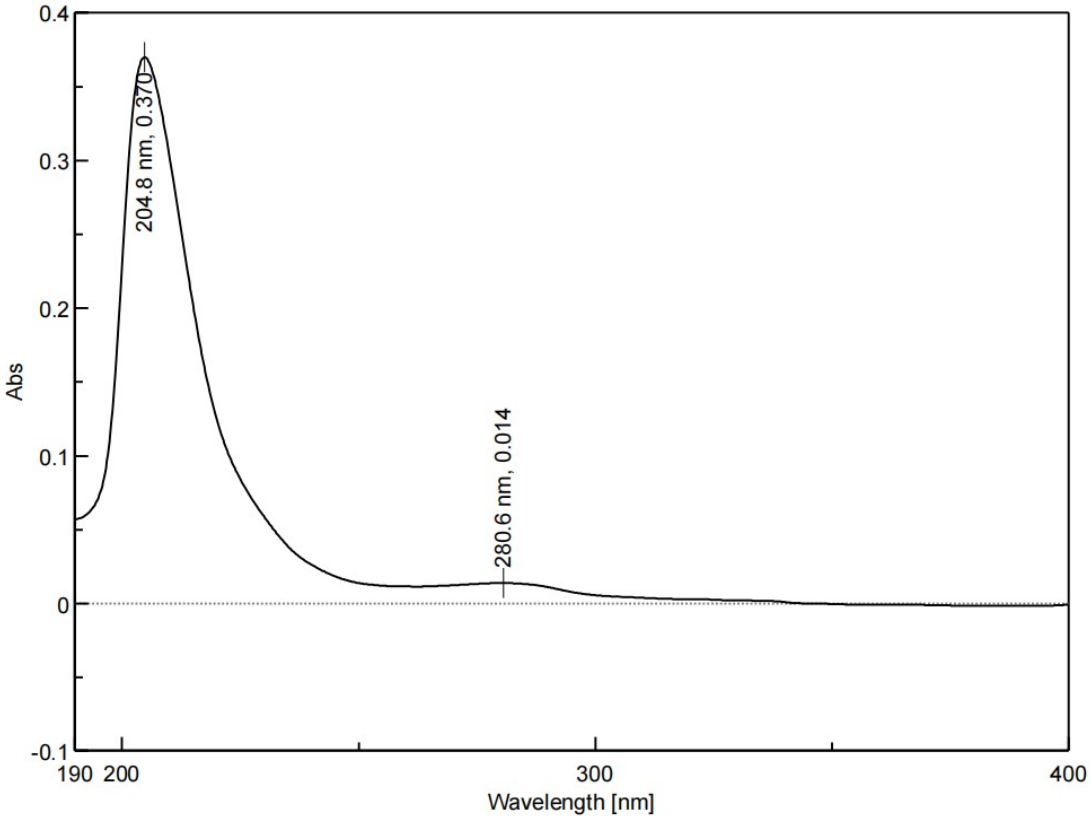


Figure S80. CD spectrum of compound 8.

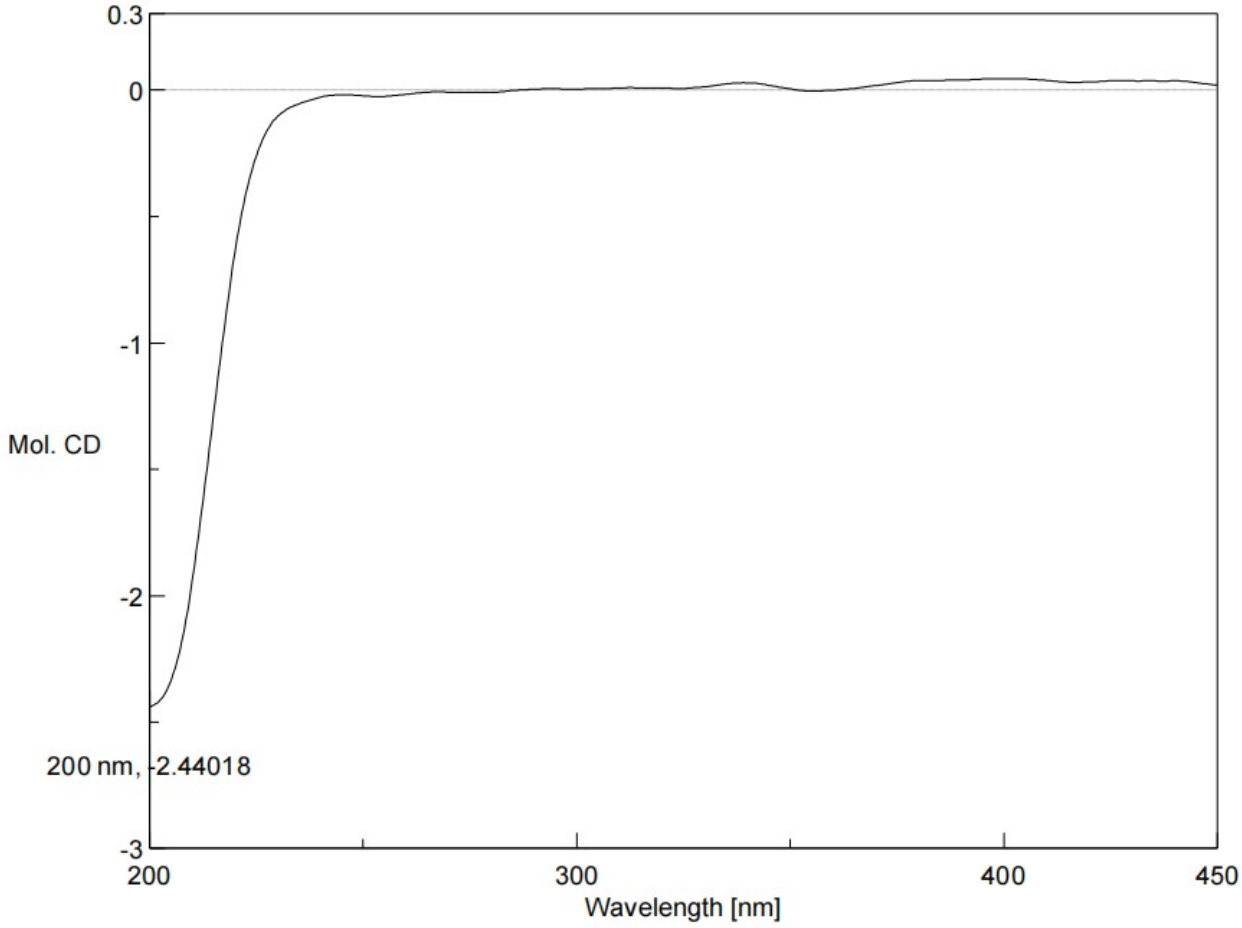


Figure S81. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound 9.

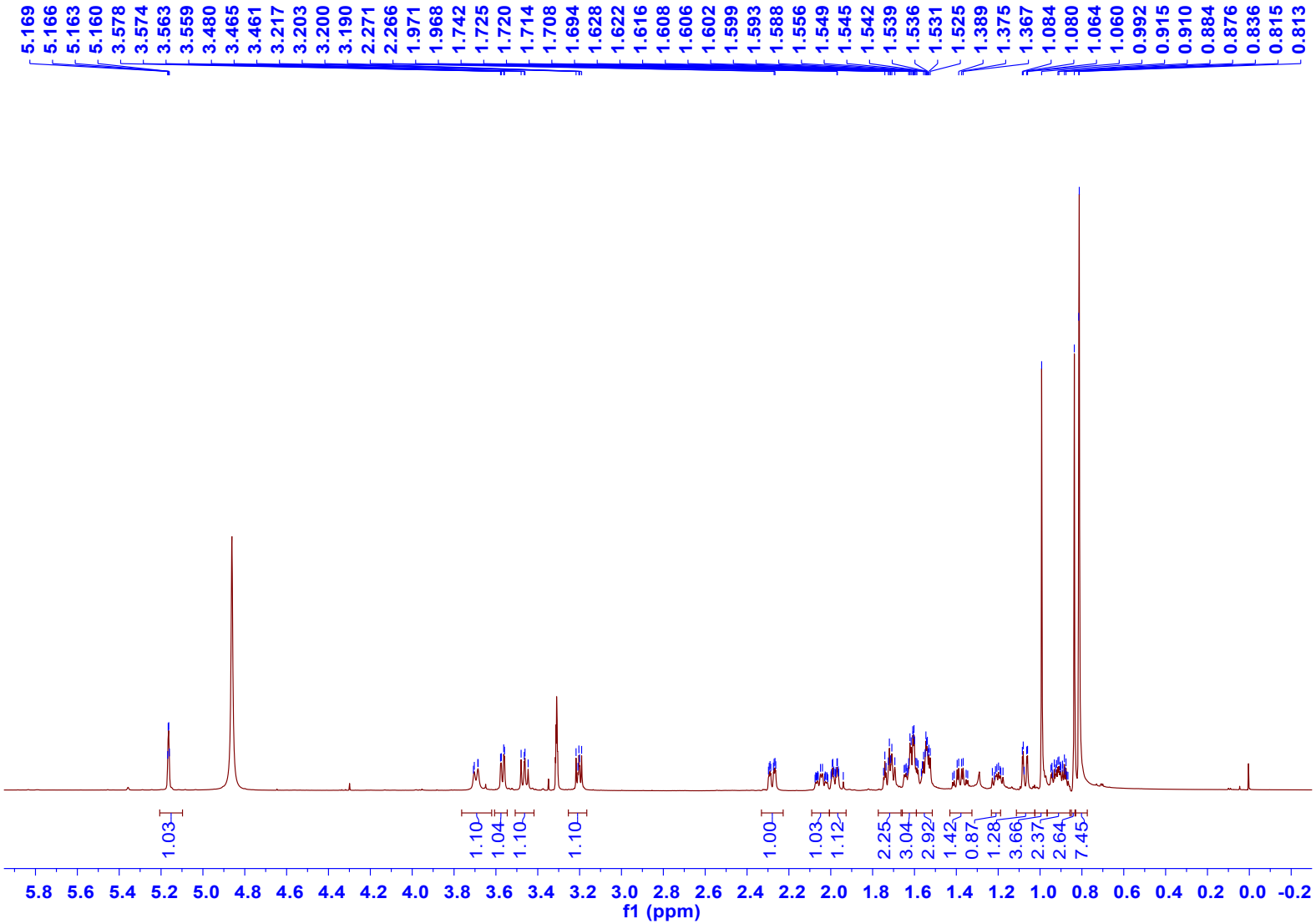


Figure S82. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 9.

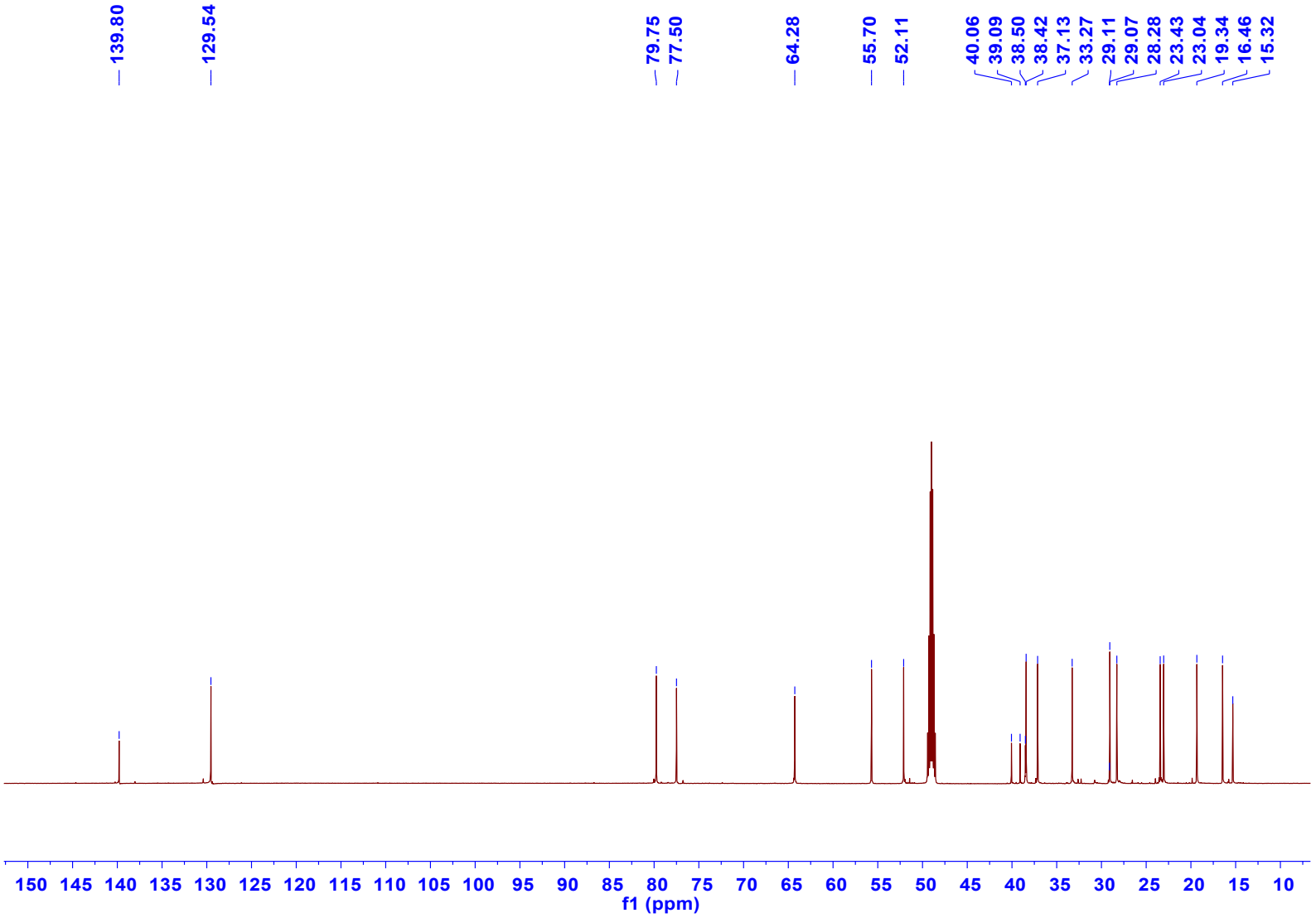


Figure S83. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound 10.

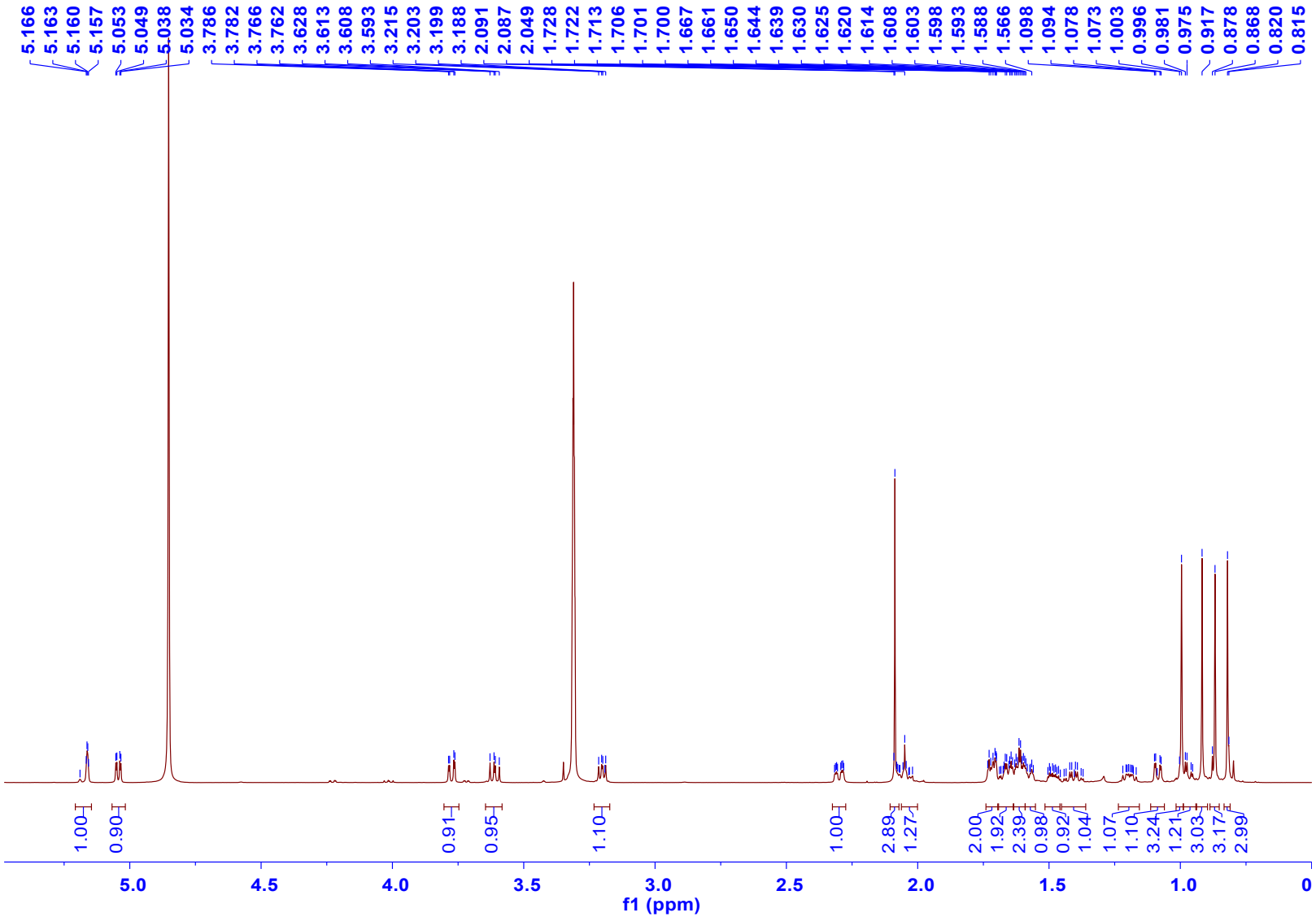


Figure S84. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 10.

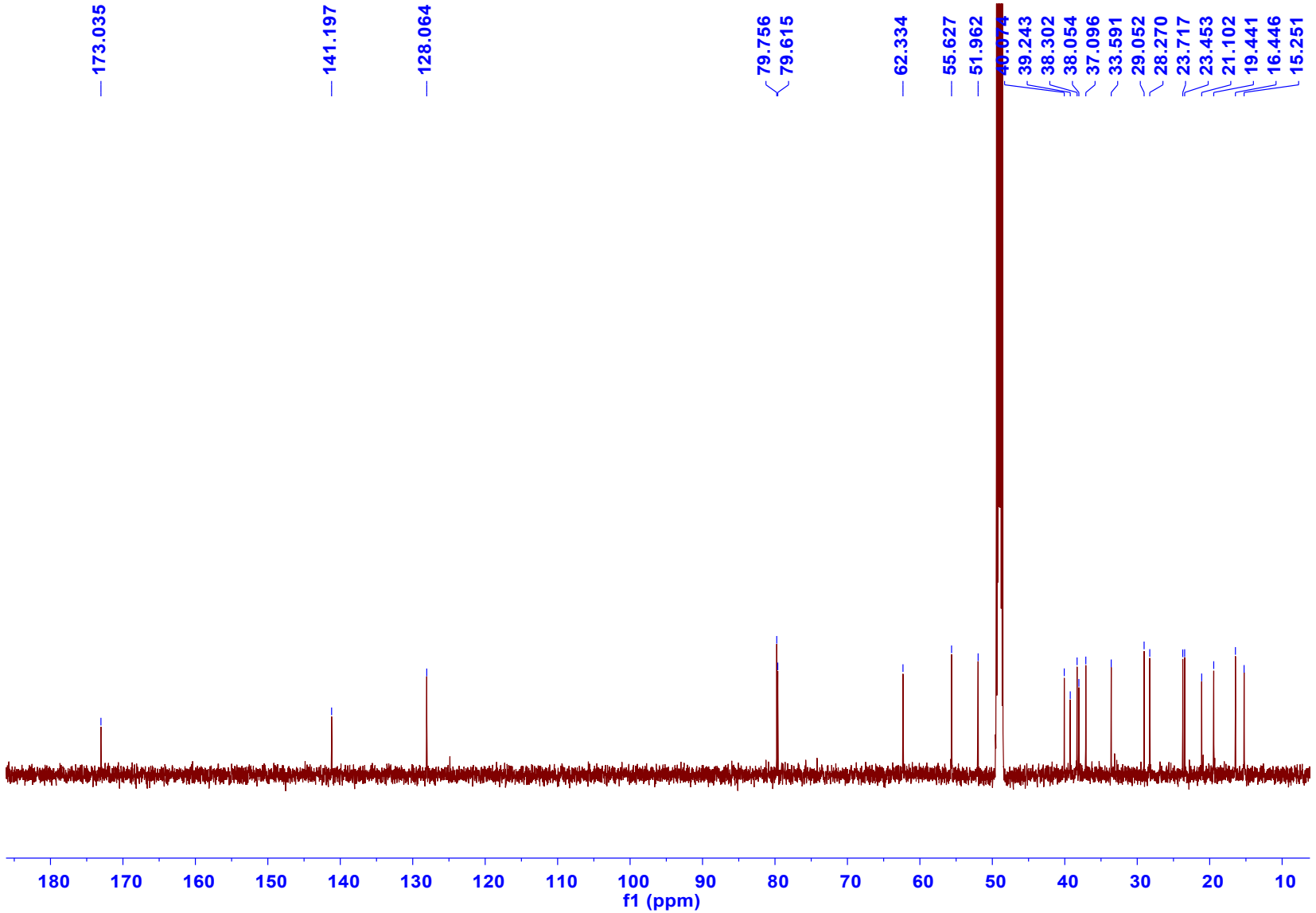


Figure S85. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound 11.

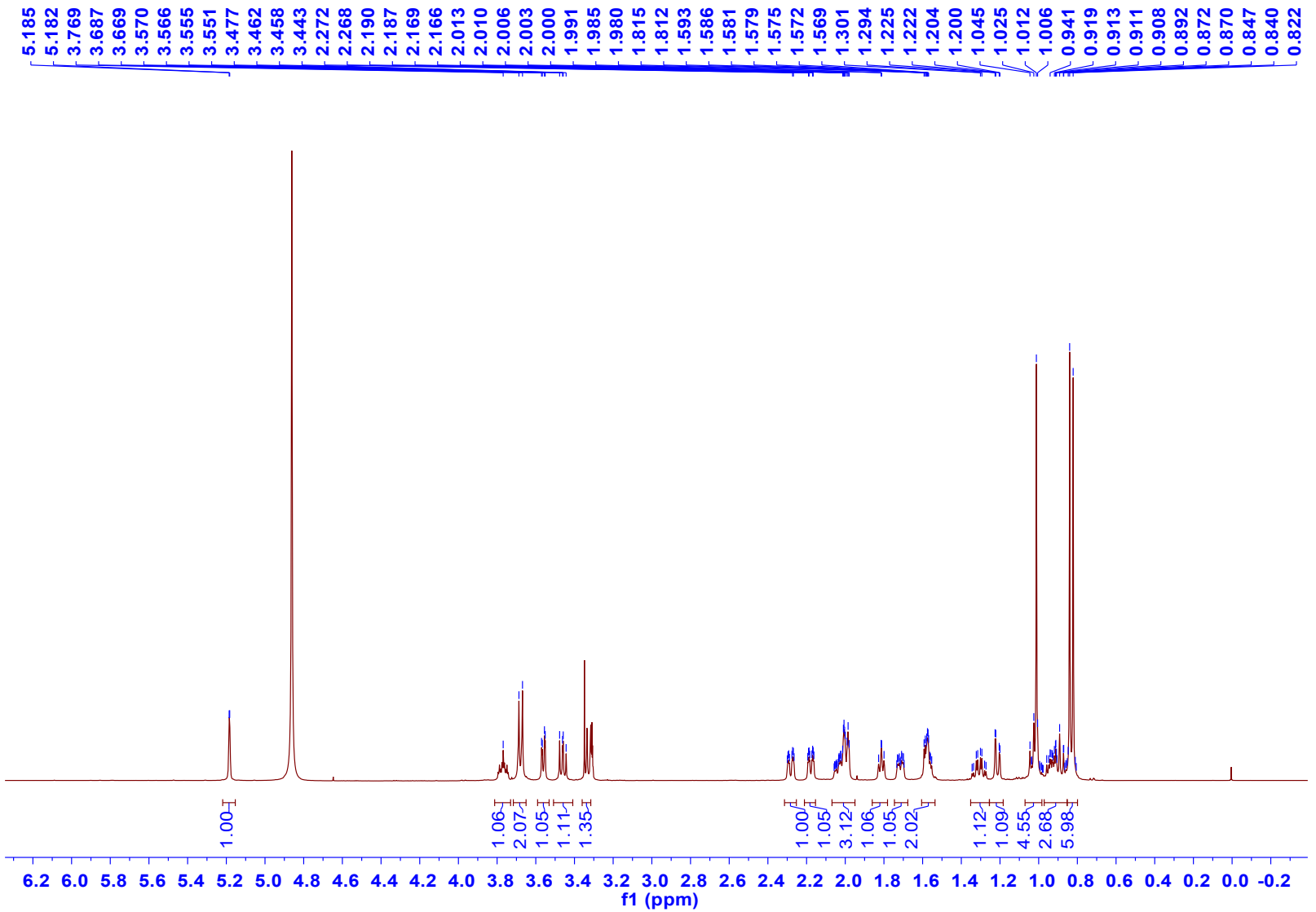
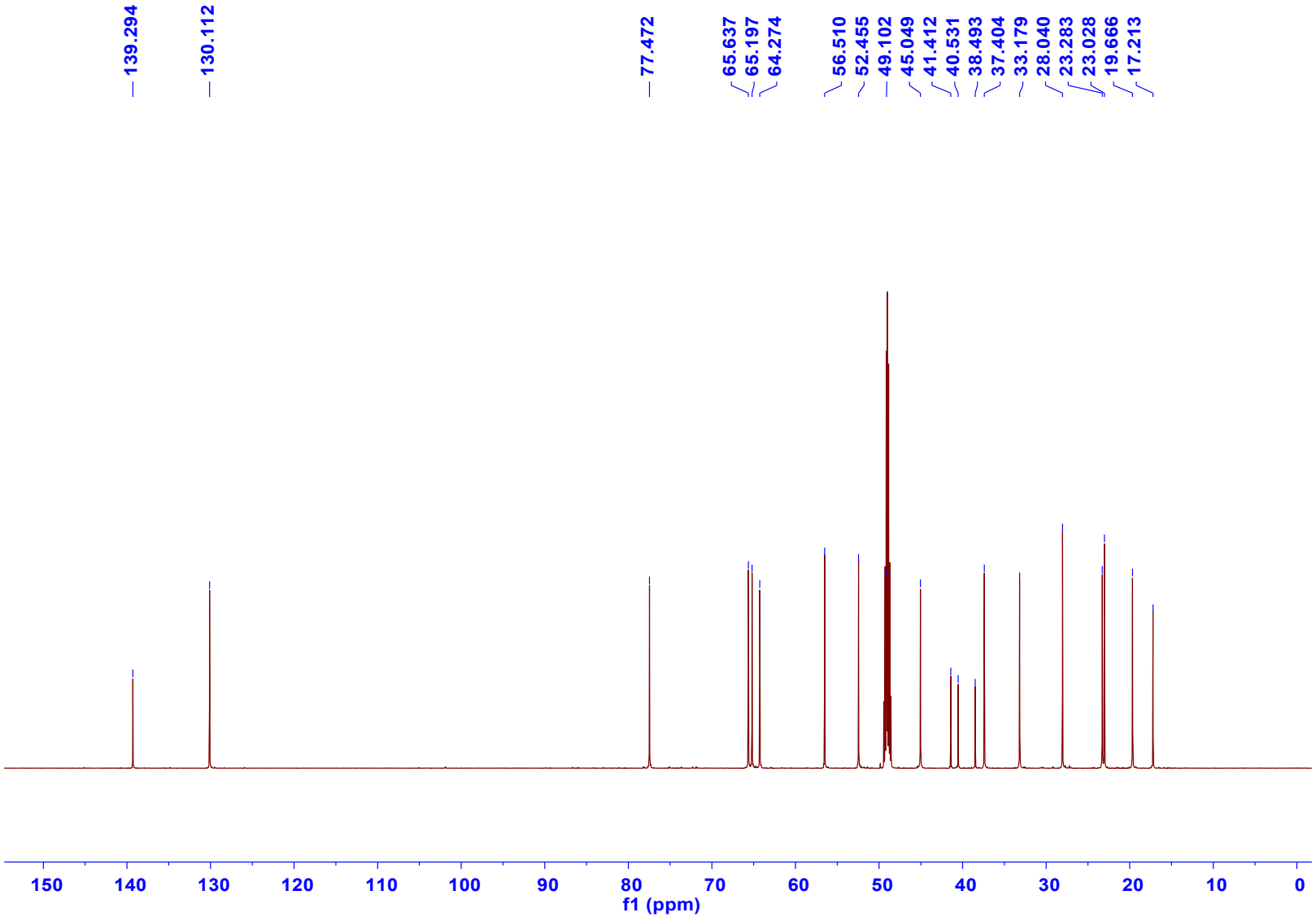


Figure S86. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 11.



2. X-ray Crystallographic Data of Compounds 1, 5 and 8

Crystallographic data for the structures of **1**, **5** and **8** have been deposited with the Cambridge Crystallographic Data Centre (CCDC 2453116 for **1**; CCDC 2453118 for **5**; CCDC 2453134 for **8**). Copies of these data can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, U,K.; fax (+44)1223-336-033; or deposit@ccdc.cam.uk).

Table S1. Crystal data and structure refinement for 1.

Identification code	**1**
Empirical formula	$C_{20}H_{32}O_4$
Formula weight	336.45
Temperature/K	169.99(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	6.84365(12)
b/Å	11.17471(20)
c/Å	11.9856(2)
α/°	90
β/°	92.9687(16)
γ/°	90
Volume/Å^3	915.38(3)
Z	2
ρ_{calc}g/cm^3	1.221
μ/mm^{-1}	0.663
F(000)	368.0
Crystal size/mm^3	0.15 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.386 to 148.144
Index ranges	$-8 \leq h \leq 8$, $-13 \leq k \leq 13$, $-14 \leq l \leq 9$
Reflections collected	6787
Independent reflections	3579 [R_{int} = 0.0210, R_{sigma} = 0.0247]
Data/restraints/parameters	3579/1/231
Goodness-of-fit on F^2	1.003
Final R indexes [I>=2σ (I)]	R_1 = 0.0299, wR_2 = 0.0837
Final R indexes [all data]	R_1 = 0.0305, wR_2 = 0.0843
Largest diff. peak/hole / e Å^{-3}	0.21/-0.13
Flack/Hooft parameter	0.10(9)/0.12(6)

Table S2. Crystal data and structure refinement for 5.

Identification code	**5**
Empirical formula	$C_{20}H_{34}O_4$
Formula weight	338.47
Temperature/K	149.99(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.3800(4)
b/Å	12.1066(4)
c/Å	20.3919(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1821.95(15)
Z	4
ρ_{calc}g/cm^3	1.234
μ/mm^{-1}	0.667
F(000)	744.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.494 to 148.322
Index ranges	$-7 \leq h \leq 9$, $-14 \leq k \leq 14$, $-25 \leq l \leq 25$
Reflections collected	20517
Independent reflections	3654 [R_{int} = 0.1125, R_{sigma} = 0.0672]
Data/restraints/parameters	3654/255/225
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0765, wR_2 = 0.2042
Final R indexes [all data]	R_1 = 0.0822, wR_2 = 0.2114
Largest diff. peak/hole / e Å^{-3}	0.46/-0.41
Flack/Hooft parameter	0.03(17)/0.09(15)

Table S3. Crystal data and structure refinement for 8.

Identification code	**8**
Empirical formula	$C_{20}H_{34}O_3$
Formula weight	322.47
Temperature/K	170.00(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	11.2450(3)
b/Å	7.2402(2)
c/Å	11.5790(3)
α/°	90
β/°	99.615(3)
γ/°	90
Volume/Å^3	929.48(5)
Z	2
ρ_{calc}g/cm^3	1.152
μ/mm^{-1}	0.588
F(000)	356.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.744 to 147.56
Index ranges	$-13 \leq h \leq 14$, $-8 \leq k \leq 8$, $-13 \leq l \leq 14$
Reflections collected	7872
Independent reflections	3472 [R_{int} = 0.0258, R_{sigma} = 0.0273]
Data/restraints/parameters	3472/1/220
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0338, wR_2 = 0.0849
Final R indexes [all data]	R_1 = 0.0346, wR_2 = 0.0859
Largest diff. peak/hole / e Å^{-3}	0.14/-0.18
Flack/Hooft parameter	-0.01(10)/0.03(9)

3. *In silico* prediction ECD spectrum.

All calculations were performed using Gaussian 16.1. Conformation search using molecular mechanics calculations was performed in DS (Discovery Studio) 2018 with MMFF94s force field with 20 kcal mol^{-1} upper energy limit at best level. The conformers performed with the DS 2018 software package were further optimized by using the TDDFT method at the B3LYP/6-31G(d, p) level, and the frequency was calculated at the same level of theory. For all optimized structures, vibrational spectra were calculated to ensure that no imaginary frequencies for energy minimum were obtained. The average values were obtained by the Boltzmann distributions, using the relative Gibbs free energies as weighting factors. The stable conformers were subjected to ECD calculation by the TDDFT method at the B3LYP/6-311G+(d,p) level with the CPCM model in MeOH. ECD spectra of different conformers were simulated using SpecDis 1.71 with a half-bandwidth of 0.3 eV, and the final calculated ECD spectra were obtained according to the Boltzmann-calculated contribution of each con-former. The calculated ECD spectra were compared with the experimental data. Additional details are provided in Supporting Information (pages 86-117).

Reference

(1) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16, Revision A. 03, Gaussian. *Inc., Wallingford CT*, 2016, 3.

(2) T. Bruhn, A. Schaumlöffel, Y. Hemberger and G. Pescitelli, *SpecDis version 1.71*, Berlin, Germany, 2017, http:/specdis-software.jimdo.com

Table S4. Cartesian coordinates and equilibrium populations of low-energy conformers (>1%) of 1 in MeOH.

Conformer 1 P (%) = 31.34%				Conformer 2 P (%) = 20.80%			
C	-3.331152	-1.824941	0.14774	C	-3.32696	1.836376	-0.111861
C	-3.859131	-0.686768	-0.720142	C	-3.869995	0.685693	0.729816
C	-3.342022	0.69789	-0.270478	C	-3.340659	-0.698614	0.26629
C	-1.778889	0.631948	-0.206159	C	-1.777849	-0.633217	0.205546
C	-1.131257	-0.577966	0.55179	C	-1.129332	0.583518	-0.538286
C	-1.805363	-1.884295	0.086687	C	-1.800548	1.884415	-0.054251
C	-1.144339	1.95467	0.249117	C	-1.141306	-1.953238	-0.256197
C	0.351705	1.885303	0.260895	C	0.354599	-1.883822	-0.266905
C	1.040317	0.732571	0.231375	C	1.041959	-0.730825	-0.228793
C	0.364865	-0.573074	0.209264	C	0.367491	0.574641	-0.197852
C	2.540982	0.74976	0.190844	C	2.542773	-0.745175	-0.189887
C	3.162943	-0.355325	-0.67968	C	3.169502	0.348016	0.691811
C	2.557137	-1.717104	-0.27882	C	2.560115	1.713266	0.303936
C	1.072185	-1.687887	-0.047763	C	1.076414	1.686342	0.067127
O	3.092143	0.492574	1.49085	O	3.092748	-0.492424	-1.490267
C	4.458084	0.116145	1.297725	C	4.444453	-0.05498	-1.311816
C	4.626273	-0.295192	-0.181277	C	4.631736	0.292888	0.18723
O	5.400234	0.722342	-0.812699	O	5.446285	-0.653898	0.869137
O	-5.287339	-0.64686	-0.726225	O	-5.295645	0.726077	0.814213
C	-4.024951	1.122996	1.044216	C	-4.021184	-1.110086	-1.054678
C	-3.752975	1.718215	-1.354745	C	-3.756708	-1.730974	1.335195
C	-1.216596	-0.47326	2.093666	C	-1.219596	0.493531	-2.080377
C	2.99106	-0.095092	-2.173742	C	3.005712	0.079608	2.184564
H	2.889741	1.731053	-0.166428	H	2.875229	-1.740119	0.16142
H	-1.461989	0.489895	-1.251128	H	-1.466924	-0.499654	1.253318
H	-3.748192	-2.776877	-0.211503	H	-3.748811	2.774473	0.266263
H	-3.688202	-1.699484	1.175705	H	-3.671326	1.735515	-1.150467
H	-3.492435	-0.850312	-1.74978	H	-3.536394	0.83444	1.765246
H	-1.503232	-2.087526	-0.949666	H	-1.497391	2.071814	0.984489
H	-1.444678	-2.725662	0.689362	H	-1.437576	2.73353	-0.644715
H	-1.502452	2.232979	1.250703	H	-1.496504	-2.226525	-1.260431
H	-1.460791	2.770979	-0.410344	H	-1.45897	-2.77308	0.39837
H	0.898173	2.826666	0.292148	H	0.900551	-2.825408	-0.305063
H	2.802047	-2.459786	-1.050813	H	2.80058	2.443124	1.088705
H	3.037981	-2.082519	0.640803	H	3.042475	2.096157	-0.60776
H	0.57924	-2.655388	-0.047857	H	0.584349	2.654165	0.075012
H	4.685143	-0.697194	1.994151	H	4.614667	0.79993	-1.975017

H	5.130949	0.958751	1.502661	H	5.151406	-0.849706	-1.58956
H	5.126483	-1.269773	-0.286244	H	5.144321	1.248424	0.329765
H	5.510277	0.471653	-1.742862	H	5.054212	-1.532666	0.739934
H	-5.598278	-1.517082	-1.018176	H	-5.635284	0.751496	-0.093929
H	-5.102044	1.207823	0.882138	H	-3.921215	-0.365629	-1.848293
H	-3.873249	0.41237	1.858311	H	-3.616075	-2.050901	-1.43739
H	-3.657226	2.097097	1.380506	H	-5.090356	-1.27407	-0.881225
H	-3.539984	2.746822	-1.04721	H	-3.210481	-1.571228	2.272736
H	-3.223016	1.529669	-2.296591	H	-4.824927	-1.628231	1.545241
H	-4.826117	1.639627	-1.546952	H	-3.572633	-2.759194	1.00737
H	-0.672126	-1.313176	2.537601	H	-0.683019	1.341078	-2.519277
H	-0.752232	0.444811	2.462249	H	-0.750931	-0.418311	-2.459416
H	-2.244164	-0.506826	2.459499	H	-2.248909	0.523641	-2.442627
H	3.535316	-0.836763	-2.772855	H	1.948015	0.131851	2.463603
H	1.933719	-0.16108	-2.449579	H	3.386421	-0.907821	2.460287
H	3.347776	0.90324	-2.44633	H	3.554701	0.82068	2.775075

Conformer 3 P (%) = 18.95%				**Conformer 4 P (%) = 15.31%**			
C	-3.334354	1.829848	-0.14841	C	-3.330137	-1.825795	0.139719
C	-3.858993	0.697406	0.71961	C	-3.859326	-0.682493	-0.720641
C	-3.341852	-0.695141	0.262834	C	-3.341417	0.699556	-0.263792
C	-1.7786	-0.63557	0.199802	C	-1.778245	0.63296	-0.202006
C	-1.131263	0.581349	-0.549819	C	-1.129479	-0.581804	0.547399
C	-1.80893	1.885372	-0.083894	C	-1.804494	-1.885159	0.075415
C	-1.144432	-1.953347	-0.273072	C	-1.143341	1.952702	0.261484
C	0.351937	-1.883579	-0.285077	C	0.352595	1.883261	0.270598
C	1.040043	-0.731119	-0.239686	C	1.040325	0.730446	0.2304
C	0.363705	0.573557	-0.203019	C	0.365695	-0.575121	0.201253
C	2.540764	-0.748493	-0.196863	C	2.540901	0.744524	0.187736
C	3.160983	0.348033	0.685699	C	3.16521	-0.349506	-0.694784
C	2.554602	1.71351	0.298666	C	2.556852	-1.714475	-0.30402
C	1.069743	1.686013	0.067091	C	1.073506	-1.687226	-0.064651
O	3.093279	-0.478433	-1.493473	O	3.094768	0.492269	1.486806
C	4.458652	-0.102313	-1.29511	C	4.446205	0.056399	1.304461
C	4.624928	0.293791	0.188161	C	4.628854	-0.294045	-0.194553
O	5.398698	-0.729862	0.809945	O	5.441817	0.65153	-0.880478
O	-5.283267	0.794248	0.718357	O	-5.287424	-0.642035	-0.723988
C	-4.021708	-1.114917	-1.052865	C	-4.022333	1.117244	1.054278
C	-3.748282	-1.723078	1.341389	C	-3.753585	1.725921	-1.341854
C	-1.208841	0.489069	-2.093597	C	-1.212048	-0.486787	2.090021
C	2.987969	0.072277	2.176836	C	2.99714	-0.082429	-2.187288
H	2.889122	-1.733285	0.151154	H	2.872914	1.739139	-0.164955

H	-1.458585	-0.503475	1.245445	H	-1.462598	0.497888	-1.248193
H	-3.763002	2.771249	0.21241	H	-3.747876	-2.775487	-0.224406
H	-3.688622	1.701374	-1.177277	H	-3.68541	-1.706362	1.169015
H	-3.482395	0.861402	1.745217	H	-3.49431	-0.840044	-1.751763
H	-1.50903	2.089183	0.952975	H	-1.504345	-2.081991	-0.962691
H	-1.44635	2.726656	-0.685697	H	-1.442771	-2.730242	0.672229
H	-1.506279	-2.21831	-1.277001	H	-1.499949	2.223976	1.265489
H	-1.455966	-2.780085	0.375802	H	-1.46057	2.773492	-0.391947
H	0.89834	-2.824498	-0.32772	H	0.898662	2.824827	0.308347
H	2.799262	2.448611	1.077903	H	2.796536	-2.445235	-1.088235
H	3.034991	2.088339	-0.617428	H	3.04106	-2.095594	0.607456
H	0.575687	2.652823	0.077245	H	0.581088	-2.654968	-0.069651
H	4.685296	0.718466	-1.982848	H	4.619968	-0.797016	1.968666
H	5.132601	-0.941996	-1.50823	H	5.153243	0.852527	1.578167
H	5.124514	1.267451	0.303678	H	5.140874	-1.249885	-0.337118
H	5.509561	-0.48757	1.742234	H	5.051222	1.530728	-0.749787
H	-5.623818	0.178953	1.384683	H	-5.599377	-1.509479	-1.023034
H	-3.729209	-2.128796	-1.343033	H	-3.656352	2.090818	1.394106
H	-5.106919	-1.100225	-0.921396	H	-5.099927	1.200223	0.894823
H	-3.788881	-0.450997	-1.885835	H	-3.867234	0.403427	1.864928
H	-3.293089	-1.48682	2.311046	H	-4.827117	1.649108	-1.532472
H	-4.837335	-1.744548	1.471746	H	-3.539419	2.752826	-1.029404
H	-3.453943	-2.740741	1.069514	H	-3.225619	1.541879	-2.285686
H	-2.232337	0.556901	-2.466165	H	-0.74787	0.429245	2.463988
H	-0.639632	1.31862	-2.525478	H	-2.23896	-0.523377	2.457292
H	-0.766851	-0.436983	-2.469421	H	-0.666497	-1.329256	2.52773
H	3.531053	0.808233	2.783969	H	3.544172	-0.824294	-2.778656
H	1.93034	0.134904	2.452369	H	1.938565	-0.134605	-2.462926
H	3.34538	-0.928475	2.439442	H	3.377347	0.904586	-2.46508

Conformer 5 P (%) = 13.60%			
C	-3.325072	1.836222	-0.104197
C	-3.86961	0.680577	0.729615
C	-3.339076	-0.700913	0.259545
C	-1.776015	-0.635149	0.201884
C	-1.126275	0.586187	-0.53346
C	-1.798798	1.883982	-0.043226
C	-1.138242	-1.952087	-0.266724
C	0.357795	-1.882354	-0.274263
C	1.045619	-0.729791	-0.229585
C	0.370002	0.574865	-0.190585
C	2.546157	-0.748728	-0.188168

C	3.169194	0.342951	0.699336
C	2.560284	1.712807	0.325605
C	1.076997	1.685006	0.085755
O	3.0938	-0.47925	-1.492134
C	4.430855	-0.013044	-1.312202
C	4.622003	0.290892	0.193899
O	5.297018	-0.765685	0.872632
O	-5.295848	0.720636	0.810866
C	-4.017068	-1.105164	-1.064977
C	-3.756757	-1.739346	1.321915
C	-1.21356	0.50518	-2.076258
C	3.002622	0.059005	2.190011
H	2.893063	-1.7345	0.153948
H	-1.466878	-0.507835	1.250928
H	-3.747995	2.771996	0.278575
H	-3.667373	1.741354	-1.14404
H	-3.538648	0.823598	1.766671
H	-1.497886	2.065161	0.997257
H	-1.434658	2.736732	-0.627768
H	-1.491871	-2.218864	-1.273346
H	-1.457244	-2.776012	0.38207
H	0.904471	-2.823179	-0.314921
H	2.796494	2.434208	1.119548
H	3.042446	2.109283	-0.580301
H	0.583997	2.652273	0.101687
H	4.574528	0.873328	-1.941768
H	5.151846	-0.780947	-1.631443
H	5.14667	1.244421	0.357538
H	6.16578	-0.876229	0.457631
H	-5.632879	0.746611	-0.098214
H	-5.086474	-1.271119	-0.894609
H	-3.916031	-0.355887	-1.853894
H	-3.610231	-2.043242	-1.452361
H	-3.212166	-1.584606	2.261201
H	-4.825433	-1.638386	1.530662
H	-3.571313	-2.765522	0.988672
H	-2.242111	0.536931	-2.440699
H	-0.676398	1.355584	-2.508927
H	-0.743303	-0.404131	-2.459217
H	3.387537	-0.929941	2.44812
H	3.543177	0.799051	2.790427
H	1.942795	0.10768	2.462159

Table S5. Cartesian coordinates and equilibrium populations of low-energy conformers (>1%) of 2 in MeOH.

Conformer 1 P (%) = 57.00%				Conformer 2 P (%) =42.98%			
C	-3.927	-1.621	0.169	C	-3.648	-1.786	0.049
C	-4.545	-0.313	-0.356	C	-4.346	-0.544	-0.526
C	-3.904	0.965	0.264	C	-3.87	0.792	0.127
C	-2.346	0.857	0.118	C	-2.299	0.825	0.116
C	-1.675	-0.465	0.617	C	-1.544	-0.441	0.641
C	-2.409	-1.656	-0.046	C	-2.125	-1.683	-0.077
C	-1.557	2.074	0.632	C	-1.673	2.091	0.728
C	-0.129	2.046	0.084	C	-0.203	2.215	0.316
C	0.517	0.674	0.045	C	0.561	0.907	0.228
C	-0.185	-0.47	0.249	C	-0.044	-0.302	0.354
C	2.008	0.663	-0.248	C	2.053	1.039	-0.028
C	2.68	-0.693	-0.526	C	2.858	-0.244	-0.305
C	2.023	-1.759	0.366	C	2.263	-1.391	0.527
C	0.509	-1.815	0.128	C	0.774	-1.576	0.221
O	2.728	1.133	0.866	O	2.711	1.582	1.089
C	4.097	0.889	0.679	C	4.098	1.475	0.906
C	4.137	-0.469	-0.033	C	4.266	0.09	0.279
O	5.06	-0.434	-1.128	O	5.291	0.146	-0.719
O	-5.946	-0.339	-0.126	O	-5.746	-0.746	-0.385
C	-4.359	1.181	1.729	C	-4.389	1.97	-0.738
C	-4.399	2.187	-0.55	C	-4.462	0.973	1.546
C	-1.696	-0.637	2.157	C	-1.634	-0.641	2.174
C	2.588	-1.047	-2.018	C	2.818	-0.533	-1.815
H	2.213	1.348	-1.061	H	2.201	1.745	-0.836
H	-2.188	0.856	-0.963	H	-2.052	0.871	-0.948
C	6.364	-0.317	-0.834	C	5.788	-1.02	-1.163
O	6.796	-0.258	0.296	O	5.445	-2.101	-0.739
C	7.343	-0.261	-1.978	C	6.831	-0.981	-2.248
H	-4.159	-1.76	1.225	H	-3.983	-2.679	-0.481
H	-4.372	-2.473	-0.346	H	-3.926	-1.937	1.093
H	-4.404	-0.286	-1.438	H	-4.136	-0.514	-1.597
H	-2.21	-1.655	-1.119	H	-1.69	-2.602	0.313
H	-2.033	-2.607	0.331	H	-1.865	-1.649	-1.137
H	-2.017	3.013	0.331	H	-1.754	2.076	1.814
H	-1.536	2.092	1.721	H	-2.185	2.996	0.411
H	-0.14	2.433	-0.936	H	-0.159	2.687	-0.667
H	0.493	2.732	0.658	H	0.307	2.896	0.998

H	2.206	-1.54	1.42	H	2.803	-2.319	0.333
H	2.466	-2.738	0.177	H	2.378	-1.186	1.593
H	0.087	-2.517	0.846	H	0.389	-2.335	0.901
H	0.301	-2.232	-0.857	H	0.644	-1.976	-0.785
H	4.492	1.675	0.051	H	4.616	1.594	1.846
H	4.615	0.9	1.627	H	4.411	2.257	0.227
H	4.442	-1.256	0.646	H	4.568	-0.603	1.055
H	-6.322	-1.101	-0.595	H	-6.216	-0.053	-0.874
H	-5.367	1.594	1.767	H	-3.976	1.938	-1.747
H	-3.715	1.88	2.261	H	-4.141	2.939	-0.31
H	-4.407	0.258	2.3	H	-5.474	1.962	-0.833
H	-5.488	2.226	-0.591	H	-3.977	1.78	2.094
H	-4.04	2.157	-1.578	H	-4.41	0.071	2.148
H	-4.079	3.132	-0.113	H	-5.522	1.226	1.494
H	-1.141	-1.524	2.463	H	-1.247	0.212	2.73
H	-2.692	-0.775	2.561	H	-1.05	-1.505	2.49
H	-1.243	0.205	2.678	H	-2.641	-0.832	2.525
H	3.08	-0.296	-2.637	H	3.335	0.241	-2.383
H	1.554	-1.11	-2.355	H	1.794	-0.572	-2.188
H	3.063	-2.006	-2.221	H	3.281	-1.49	-2.053
H	8.369	-0.218	-1.612	H	6.459	-1.468	-3.15
H	7.239	-1.144	-2.608	H	7.737	-1.495	-1.926
H	7.159	0.623	-2.589	H	7.091	0.048	-2.497

Conformer 3 P (%) = 0.02%			
C	-3.921	-1.609	0.202
C	-4.525	-0.322	-0.382
C	-3.887	0.98	0.201
C	-2.324	0.857	0.111
C	-1.67	-0.457	0.655
C	-2.402	-1.659	0.009
C	-1.543	2.078	0.632
C	-0.095	2.038	0.137
C	0.54	0.661	0.109
C	-0.175	-0.477	0.308
C	2.034	0.638	-0.167
C	2.67	-0.712	-0.522
C	2.033	-1.792	0.371
C	0.509	-1.83	0.198
O	2.746	1.009	0.987
C	4.112	0.728	0.817
C	4.15	-0.512	-0.09

O	4.994	-0.28	-1.228
O	-5.929	-0.379	-0.166
C	-4.335	2.18	-0.676
C	-4.384	1.258	1.641
C	-1.719	-0.595	2.198
C	2.503	-1.025	-2.017
H	2.27	1.368	-0.931
H	-2.131	0.835	-0.965
C	6.332	-0.226	-1.061
O	7.074	-0.046	-2.001
C	6.987	-0.39	0.294
H	-4.364	-2.48	-0.285
H	-4.167	-1.705	1.26
H	-4.369	-0.347	-1.463
H	-2.036	-2.602	0.414
H	-2.187	-1.685	-1.06
H	-1.564	2.114	1.72
H	-1.983	3.016	0.301
H	-0.065	2.434	-0.878
H	0.513	2.713	0.741
H	2.455	-2.771	0.142
H	2.264	-1.602	1.421
H	0.105	-2.507	0.95
H	0.26	-2.269	-0.767
H	4.573	0.573	1.781
H	4.571	1.582	0.34
H	4.505	-1.389	0.432
H	-6.354	0.34	-0.659
H	-3.972	2.085	-1.7
H	-3.98	3.132	-0.286
H	-5.419	2.272	-0.724
H	-3.788	2.022	2.139
H	-4.395	0.372	2.267
H	-5.412	1.621	1.632
H	-1.251	0.245	2.708
H	-1.186	-1.488	2.527
H	-2.722	-0.703	2.592
H	2.962	-0.257	-2.64
H	1.453	-1.079	-2.302
H	2.966	-1.978	-2.27
H	6.759	0.458	0.939
H	8.071	-0.445	0.191
H	6.659	-1.307	0.783

Table S6. Cartesian coordinates and equilibrium populations of low-energy conformers (>1%) of 3 in MeOH.

Conformer 1 P (%) = 99.27%				Conformer 2 P (%) =0.73%			
C	-2.573	1.142	1.1	C	-2.432	1.176	1.259
C	-2.419	2.192	-0.016	C	-2.401	2.149	0.069
C	-0.945	2.614	-0.251	C	-0.965	2.606	-0.286
C	-0.063	1.331	-0.413	C	-0.048	1.347	-0.447
C	-0.205	0.227	0.684	C	-0.081	0.278	0.697
C	-1.711	-0.1	0.837	C	-1.561	-0.06	1.005
C	1.424	1.601	-0.699	C	1.406	1.665	-0.834
C	2.097	0.333	-1.232	C	2.107	0.408	-1.355
C	1.651	-0.959	-0.573	C	1.73	-0.879	-0.649
C	0.589	-1.02	0.272	C	0.721	-0.957	0.256
C	2.471	-2.188	-0.929	C	2.553	-2.1	-1.021
C	1.953	-3.566	-0.471	C	1.901	-3.501	-0.839
C	1.286	-3.397	0.905	C	0.496	-3.423	-0.219
C	0.163	-2.356	0.855	C	0.407	-2.321	0.844
C	4.397	-3.355	-0.479	C	4.181	-3.45	-0.099
C	3.274	-4.374	-0.259	C	2.881	-4.205	0.142
O	-3.19	3.361	0.292	O	-3.204	3.303	0.352
C	-0.46	3.555	0.878	C	-0.436	3.617	0.758
C	-0.908	3.432	-1.564	C	-1.048	3.357	-1.638
C	0.38	0.627	2.062	C	0.61	0.728	2.007
C	0.972	-4.12	-1.52	C	1.84	-4.176	-2.223
H	-0.448	0.869	-1.326	H	-0.469	0.834	-1.316
O	3.745	-2.121	-0.334	O	3.71	-2.133	-0.215
C	-4.528	3.278	0.224	C	-4.538	3.157	0.373
C	-5.325	4.495	0.618	C	-5.376	4.354	0.74
O	-5.126	2.289	-0.138	O	-5.108	2.121	0.111
O	3.434	-5.455	-1.164	O	3.035	-5.593	-0.108
H	2.635	-2.198	-1.999	H	2.91	-1.981	-2.035
H	-2.322	1.578	2.066	H	-2.113	1.683	2.169
H	-3.613	0.83	1.181	H	-3.453	0.847	1.45
H	-2.799	1.763	-0.946	H	-2.82	1.643	-0.804
H	-2.072	-0.588	-0.07	H	-1.989	-0.625	0.176
H	-1.876	-0.809	1.648	H	-1.64	-0.693	1.889
H	1.558	2.391	-1.435	H	1.462	2.426	-1.609
H	1.934	1.944	0.199	H	1.952	2.072	0.015
H	1.883	0.249	-2.297	H	1.862	0.287	-2.411
H	3.179	0.437	-1.151	H	3.187	0.547	-1.311

H	2.021	-3.082	1.648	H	-0.241	-3.211	-0.995
H	0.892	-4.353	1.253	H	0.216	-4.388	0.207
H	-0.206	-2.215	1.87	H	-0.588	-2.359	1.277
H	-0.68	-2.739	0.28	H	1.095	-2.518	1.666
H	4.81	-3.392	-1.479	H	4.889	-3.529	0.713
H	5.203	-3.436	0.235	H	4.661	-3.735	-1.026
H	3.34	-4.784	0.74	H	2.572	-4.085	1.172
H	-0.765	3.229	1.867	H	0.626	3.822	0.627
H	-0.888	4.551	0.762	H	-0.595	3.299	1.783
H	0.622	3.677	0.875	H	-0.954	4.573	0.668
H	-1.16	2.816	-2.428	H	-1.333	2.688	-2.45
H	0.07	3.876	-1.748	H	-0.104	3.826	-1.91
H	-1.621	4.257	-1.539	H	-1.791	4.155	-1.603
H	0.341	-0.208	2.762	H	0.63	-0.088	2.732
H	-0.168	1.426	2.546	H	0.099	1.543	2.507
H	1.424	0.929	2.001	H	1.646	1.03	1.855
H	0.565	-5.081	-1.206	H	1.245	-3.585	-2.921
H	1.459	-4.264	-2.486	H	1.383	-5.164	-2.166
H	0.134	-3.445	-1.687	H	2.834	-4.294	-2.658
H	-6.391	4.336	0.448	H	-5.919	4.167	1.667
H	-5.175	4.719	1.674	H	-6.098	4.569	-0.047
H	-5.009	5.359	0.035	H	-4.749	5.235	0.881
H	2.744	-6.11	-0.976	H	3.677	-5.944	0.529

Table S7. Cartesian coordinates and equilibrium populations of low-energy conformers (>1%) of 4 in MeOH.

Conformer 1 P (%) = 33.91%				Conformer 2 P (%) = 29.23%			
C	-3.212431	-1.705278	0.346447	C	-3.210924	-1.712977	0.339895
C	-3.801252	-0.666332	-0.608396	C	-3.805902	-0.674665	-0.611525
C	-3.321476	0.773405	-0.317124	C	-3.319018	0.770873	-0.322441
C	-1.762061	0.746699	-0.247558	C	-1.760404	0.746818	-0.248871
C	-1.109123	-0.307326	0.70139	C	-1.108661	-0.309036	0.698225
C	-1.681187	-1.699454	0.339723	C	-1.679871	-1.700454	0.330945
C	-1.111552	2.115175	-0.019905	C	-1.110018	2.115447	-0.020967
C	0.358984	2.052892	-0.43318	C	0.360947	2.053118	-0.432943
C	1.045948	0.770367	-0.034114	C	1.04715	0.770152	-0.0339
C	0.413935	-0.293982	0.488252	C	0.414642	-0.294747	0.486649
C	2.527454	0.768701	-0.302255	C	2.529137	0.768942	-0.29986
C	3.228385	-0.594781	-0.224985	C	3.22945	-0.594873	-0.224996
C	2.68667	-1.312781	1.019214	C	2.686385	-1.31591	1.016877
C	1.175999	-1.529616	0.924958	C	1.175697	-1.531911	0.920671
O	3.196698	1.571505	0.685473	O	3.195947	1.569097	0.69167
C	4.581339	1.248638	0.612925	C	4.580615	1.243475	0.626111
C	4.704595	-0.170507	0.013975	C	4.705109	-0.170942	0.01667
O	5.481935	-0.045068	-1.175437	O	5.481108	-0.035632	-1.172447
O	-5.230842	-0.68056	-0.553245	O	-5.229665	-0.783577	-0.654417
C	-4.01273	1.348062	0.934211	C	-4.010195	1.346769	0.929438
C	-3.752102	1.641774	-1.519951	C	-3.753168	1.6378	-1.523154
C	-1.347629	-0.061722	2.211484	C	-1.347994	-0.065386	2.208269
C	3.027324	-1.424808	-1.493095	C	3.029926	-1.422102	-1.495189
H	2.708284	1.210302	-1.298885	H	2.711794	1.213158	-1.294908
H	-1.449361	0.422874	-1.249657	H	-1.448592	0.423112	-1.25101
O	-1.186097	-2.044785	-0.963505	O	-1.187996	-2.035083	-0.974861
H	-3.594934	-1.535202	1.357645	H	-3.578443	-1.549468	1.360677
H	-3.565907	-2.707695	0.05545	H	-3.574656	-2.707034	0.045741
H	-3.46711	-0.916077	-1.626792	H	-3.485385	-0.927788	-1.627201
H	-1.319619	-2.436046	1.072202	H	-1.314749	-2.440866	1.058029
H	-1.192908	2.412122	1.031047	H	-1.191313	2.412688	1.030214
H	-1.618475	2.892771	-0.598235	H	-1.616843	2.892796	-0.600078
H	0.438448	2.163656	-1.526577	H	0.441014	2.164234	-1.52618
H	0.921443	2.895621	-0.010105	H	0.923158	2.895615	-0.009158
H	2.907331	-0.698121	1.899787	H	2.906522	-0.703884	1.899427
H	3.198715	-2.274483	1.155358	H	3.197689	-2.278251	1.150751
H	0.808068	-1.865117	1.903057	H	0.806849	-1.870326	1.89744

H	0.94932	-2.346637	0.229154	H	0.949004	-2.346725	0.222301
H	4.995774	1.331813	1.621881	H	4.988015	1.317052	1.638718
H	5.118123	1.940595	-0.051309	H	5.123497	1.93997	-0.028186
H	5.197837	-0.868289	0.70693	H	5.199606	-0.873285	0.704102
H	5.594879	-0.933677	-1.546457	H	5.595019	-0.921239	-1.550305
H	-5.525378	-1.554051	-0.852238	H	-5.557882	-0.617829	0.243425
H	-5.069615	1.52847	0.7222	H	-5.061897	1.564392	0.712016
H	-3.969395	0.682553	1.797648	H	-3.980638	0.678498	1.793729
H	-3.555188	2.300332	1.220867	H	-3.543385	2.288902	1.231509
H	-3.61294	2.708792	-1.321996	H	-3.629006	2.706714	-1.324283
H	-3.178401	1.38618	-2.419181	H	-3.172671	1.389866	-2.419688
H	-4.81231	1.475736	-1.729412	H	-4.809667	1.45517	-1.739923
H	-2.379654	-0.236519	2.517672	H	-0.72094	-0.73737	2.802736
H	-0.717152	-0.730444	2.806185	H	-1.079841	0.955252	2.488555
H	-1.082956	0.960389	2.489265	H	-2.380746	-0.238244	2.514729
H	3.442083	-0.908857	-2.363949	H	1.965856	-1.592962	-1.684191
H	3.51098	-2.407411	-1.407794	H	3.444513	-0.903715	-2.364675
H	1.962859	-1.594726	-1.68081	H	3.514561	-2.404332	-1.411789
H	-1.570937	-2.902349	-1.201337	H	-1.613023	-2.864909	-1.241504

Conformer 3 P (%) = 19.63%				**Conformer 4 P (%) = 9.35%**			
C	-3.215624	-1.703647	0.32797	C	-3.208466	-1.727289	0.273758
C	-3.811462	-0.646751	-0.602053	C	-3.81293	-0.635396	-0.609915
C	-3.307852	0.790001	-0.298346	C	-3.324008	0.789493	-0.26163
C	-1.748586	0.751242	-0.2413	C	-1.764234	0.751184	-0.227003
C	-1.096942	-0.324096	0.683502	C	-1.106489	-0.337738	0.676445
C	-1.68457	-1.704621	0.301675	C	-1.681189	-1.715566	0.250024
C	-1.083936	2.11042	0.000392	C	-1.081317	2.101037	0.009955
C	0.383484	2.041769	-0.42344	C	0.370311	2.017269	-0.463266
C	1.062927	0.747373	-0.050209	C	1.052645	0.722694	-0.09378
C	0.424408	-0.320093	0.457385	C	0.417187	-0.333801	0.445918
C	2.542705	0.742067	-0.335128	C	2.534705	0.72189	-0.376438
C	3.236558	-0.624424	-0.256633	C	3.249948	-0.629099	-0.231381
C	2.686924	-1.359787	0.976107	C	2.6891	-1.329617	1.016849
C	1.177163	-1.571746	0.861865	C	1.184222	-1.568834	0.891968
O	3.218546	1.577661	0.633937	O	3.185373	1.612548	0.557657
C	4.526985	1.065224	0.86257	C	4.489065	1.119614	0.851916
C	4.694437	-0.190739	-0.01098	C	4.695621	-0.16007	0.02559
O	5.292252	0.116849	-1.269635	O	5.306678	0.116634	-1.233227
O	-5.236776	-0.741365	-0.629779	O	-5.241528	-0.64595	-0.52026
C	-3.980301	1.354853	0.968636	C	-3.986833	1.311553	1.027537
C	-3.746612	1.677522	-1.482253	C	-3.772771	1.714385	-1.414576

C	-1.318625	-0.10081	2.199508	C	-1.333453	-0.142835	2.19367
C	3.045159	-1.450244	-1.530661	C	3.111316	-1.506375	-1.477208
H	2.71176	1.172698	-1.335122	H	2.701213	1.110197	-1.393967
H	-1.449453	0.439629	-1.25102	H	-1.486738	0.454113	-1.248821
O	-1.210616	-2.022936	-1.014196	O	-1.288815	-2.065612	-1.083841
H	-3.570506	-1.551195	1.355037	H	-3.576655	-1.620681	1.298847
H	-3.591524	-2.690113	0.023819	H	-3.547609	-2.708641	-0.083715
H	-3.50506	-0.888625	-1.624741	H	-3.505295	-0.837337	-1.645956
H	-1.318189	-2.459181	1.013418	H	-1.310988	-2.485212	0.943348
H	-1.154816	2.393761	1.056192	H	-1.113101	2.371407	1.070868
H	-1.588548	2.900041	-0.563948	H	-1.593652	2.902761	-0.528844
H	0.457066	2.168677	-1.515404	H	0.410987	2.133635	-1.558121
H	0.955182	2.873443	0.008888	H	0.965836	2.844588	-0.056602
H	2.892881	-0.768809	1.876126	H	2.869195	-0.704	1.898589
H	3.19563	-2.324647	1.096295	H	3.209806	-2.281137	1.180817
H	0.801433	-1.936451	1.826392	H	0.801047	-1.90659	1.861721
H	0.954359	-2.365877	0.139296	H	0.989138	-2.404532	0.206341
H	4.640817	0.83337	1.930484	H	4.565786	0.921879	1.929866
H	5.280912	1.822654	0.600497	H	5.243228	1.877059	0.59368
H	5.271881	-0.974011	0.504003	H	5.27723	-0.915136	0.576346
H	6.145972	0.5398	-1.092708	H	6.156976	0.547692	-1.059376
H	-5.552399	-0.58715	0.2746	H	-5.542692	-1.50678	-0.848251
H	-3.946478	0.674881	1.823614	H	-5.039984	1.532206	0.836081
H	-3.502324	2.289055	1.2778	H	-3.957644	0.595766	1.850171
H	-5.032576	1.583846	0.766016	H	-3.501796	2.233641	1.364629
H	-3.609463	2.742404	-1.27038	H	-3.630322	2.77153	-1.169542
H	-3.178639	1.436165	-2.38851	H	-3.216522	1.501042	-2.335629
H	-4.80723	1.508237	-1.689631	H	-4.836271	1.55653	-1.612713
H	-0.6908	-0.786795	2.777125	H	-0.694115	-0.822182	2.765682
H	-1.039032	0.913318	2.492026	H	-1.081736	0.874186	2.502762
H	-2.349477	-0.269777	2.514472	H	-2.361288	-0.341191	2.496712
H	3.499295	-0.949156	-2.387348	H	3.5643	-1.022761	-2.344102
H	3.512289	-2.43693	-1.428529	H	3.605279	-2.473537	-1.330345
H	1.980287	-1.595948	-1.737535	H	2.057581	-1.699497	-1.703725
H	-1.637944	-2.850044	-1.285489	H	-0.449453	-1.614979	-1.269992

Conformer 5 P (%) = 7.88%			
C	-3.208176	-1.737546	0.26087
C	-3.823887	-0.642897	-0.611313
C	-3.321759	0.787199	-0.266899
C	-1.763047	0.750759	-0.23118
C	-1.106488	-0.341239	0.668587

C	-1.680523	-1.716903	0.232933
C	-1.079798	2.100321	0.007701
C	0.3724	2.017146	-0.463788
C	1.054064	0.722077	-0.094758
C	0.417632	-0.33596	0.440645
C	2.537011	0.722985	-0.373158
C	3.252786	-0.627884	-0.230111
C	2.688204	-1.3333	1.013682
C	1.183912	-1.572835	0.882955
O	3.183655	1.611315	0.56602
C	4.486228	1.117628	0.86459
C	4.697119	-0.15847	0.033778
O	5.312008	0.124063	-1.22164
O	-5.250312	-0.732847	-0.608197
C	-3.981702	1.312188	1.023427
C	-3.776058	1.70987	-1.417494
C	-1.334543	-0.151604	2.186236
C	3.119316	-1.500916	-1.479512
H	2.70634	1.114695	-1.388855
H	-1.487525	0.455047	-1.253612
O	-1.293452	-2.050721	-1.105085
H	-3.558218	-1.64352	1.2969
H	-3.556661	-2.709714	-0.102926
H	-3.540569	-0.848512	-1.64763
H	-1.305541	-2.491837	0.917985
H	-1.111814	2.369601	1.069175
H	-1.591922	2.902565	-0.53089
H	0.414133	2.134374	-1.558436
H	0.967364	2.84414	-0.05574
H	2.865089	-0.711018	1.89843
H	3.208732	-2.285209	1.175694
H	0.798033	-1.916511	1.849571
H	0.991943	-2.405148	0.19228
H	4.557849	0.915311	1.942048
H	5.241158	1.876498	0.613138
H	5.277456	-0.915203	0.583573
H	6.163108	0.551731	-1.043407
H	-5.540624	-0.658126	0.314489
H	-3.956942	0.598143	1.850445
H	-3.491567	2.227569	1.369017
H	-5.031216	1.560007	0.831444
H	-3.644665	2.76895	-1.173644
H	-3.217303	1.500824	-2.337587

H	-4.837401	1.538514	-1.618628
H	-1.085774	0.865185	2.498847
H	-2.361501	-0.355174	2.490223
H	-0.693787	-0.830664	2.756822
H	3.575683	-1.014229	-2.342884
H	3.612898	-2.468452	-1.334024
H	2.066584	-1.693492	-1.711111
H	-0.444664	-1.614527	-1.28261

Table S8. Cartesian coordinates and equilibrium populations of low-energy conformers (>1%) of 5 in MeOH.

Conformer 1 P (%) = 32.27%				**Conformer 2 P (%) = 19.16%**			
C	-2.80953	-2.28951	-0.4433	C	-2.81417	-2.2948	-0.44121
C	-3.85405	-1.18637	-0.57851	C	-3.86855	-1.20103	-0.57043
C	-3.51518	0.116904	0.199833	C	-3.52313	0.12929	0.177741
C	-2.04099	0.557531	-0.16845	C	-2.04301	0.563086	-0.17981
C	-0.92417	-0.56791	-0.18952	C	-0.93126	-0.56726	-0.19451
C	-1.45385	-1.80342	-0.95471	C	-1.46463	-1.80021	-0.96025
C	-1.50045	1.771397	0.633909	C	-1.49689	1.76284	0.62867
C	-0.20039	2.30407	0.005673	C	-0.20026	2.298031	-0.00291
C	0.845543	1.265785	-0.3214	C	0.846559	1.259939	-0.32579
C	0.31516	0.006335	-0.98185	C	0.314322	-0.00059	-0.98282
C	2.151821	1.51262	-0.13138	C	2.153002	1.505999	-0.13595
C	3.296428	0.64099	-0.61701	C	3.2975	0.633346	-0.61986
C	2.746117	-0.34721	-1.67302	C	2.745801	-0.36318	-1.66728
C	1.432292	-1.0235	-1.26031	C	1.430757	-1.03426	-1.24961
C	5.087284	-1.03182	0.354431	C	5.098797	-1.02412	0.358983
C	3.959158	-0.03505	0.626715	C	3.965031	-0.03252	0.626609
O	3.027307	-0.77678	1.424139	O	3.037561	-0.77495	1.428418
C	-4.53588	1.17394	-0.30212	C	-4.53629	1.171084	-0.36321
C	-3.75964	-0.06765	1.713379	C	-3.77891	-0.01565	1.693987
C	-0.47963	-1.00931	1.225289	C	-0.49276	-1.01318	1.22137
C	4.346692	1.559831	-1.2843	C	4.343838	1.54987	-1.29651
O	5.644478	-1.49497	1.573592	O	5.658046	-1.47873	1.58053
O	-5.14071	-1.63388	-0.14308	O	-5.16626	-1.69401	-0.2277
O	-2.40984	2.86191	0.784686	O	-2.45418	2.825003	0.667856
H	-3.13128	-3.1636	-1.02864	H	-3.14705	-3.16723	-1.01602
H	-2.75198	-2.62256	0.59938	H	-2.73154	-2.62565	0.604098
H	-3.90759	-0.91231	-1.64855	H	-3.9568	-0.95353	-1.63682
H	-2.11096	0.89122	-1.2187	H	-2.10712	0.906141	-1.22449
H	-1.55114	-1.5475	-2.02106	H	-1.57366	-1.5407	-2.02433
H	-0.72133	-2.61652	-0.89858	H	-0.72867	-2.61087	-0.91427

H	-1.30844	1.464222	1.665056	H	-1.29596	1.43608	1.658363
H	-0.49243	2.791948	-0.94156	H	-0.50784	2.787902	-0.94
H	0.209588	3.094845	0.643781	H	0.226292	3.085733	0.634483
H	-0.08836	0.318137	-1.9615	H	-0.08303	0.3082	-1.96546
H	2.439361	2.450409	0.349622	H	2.441975	2.444892	0.342518
H	3.49702	-1.1087	-1.91363	H	3.495844	-1.12757	-1.90104
H	2.579694	0.219753	-2.60003	H	2.580142	0.195797	-2.59917
H	1.622731	-1.63771	-0.37768	H	1.618902	-1.6407	-0.36098
H	1.11227	-1.70093	-2.06013	H	1.111338	-1.71835	-2.04371
H	4.701715	-1.87102	-0.24547	H	4.718529	-1.86799	-0.23764
H	5.900151	-0.55884	-0.20341	H	5.909412	-0.54876	-0.20006
H	4.387882	0.773378	1.242291	H	4.389804	0.781575	1.237713
H	2.296297	-0.17682	1.645576	H	2.297961	-0.18076	1.636365
H	-4.31376	1.48525	-1.33247	H	-4.31567	1.428199	-1.40685
H	-5.5369	0.733492	-0.29868	H	-5.54004	0.735922	-0.32997
H	-4.54537	2.059001	0.334328	H	-4.52321	2.093181	0.215697
H	-4.81839	-0.27469	1.888709	H	-4.84762	-0.17395	1.875195
H	-3.19567	-0.89658	2.148308	H	-3.23625	-0.84586	2.157771
H	-3.49919	0.846437	2.254714	H	-3.50157	0.902742	2.218594
H	-0.03217	-0.19026	1.796785	H	-0.00754	-0.20775	1.781475
H	-1.31103	-1.39357	1.817446	H	-1.33392	-1.35719	1.824994
H	0.266251	-1.80717	1.164121	H	0.219269	-1.8417	1.161906
H	4.797715	2.247677	-0.55849	H	4.797611	2.241949	-0.57637
H	5.154299	0.980326	-1.74527	H	5.149818	0.968531	-1.75794
H	3.879313	2.162968	-2.07008	H	3.872411	2.148212	-2.08348
H	4.881062	-1.74384	2.121865	H	4.896237	-1.7337	2.128141
H	-5.37414	-2.40717	-0.67914	H	-5.11097	-2.05167	0.672417
H	-2.64561	3.174414	-0.1038	H	-2.05292	3.550247	1.172622

Conformer 3 P (%) = 12.52%				**Conformer 4 P (%) = 12.04%**			
C	-2.80867	-2.29518	-0.41114	C	-2.80487	-2.30426	-0.40638
C	-3.85858	-1.19965	-0.56078	C	-3.85381	-1.21641	-0.56672
C	-3.52471	0.125826	0.183427	C	-3.52328	0.11741	0.182744
C	-2.04582	0.561274	-0.17947	C	-2.04642	0.561704	-0.17712
C	-0.9302	-0.56685	-0.1864	C	-0.92922	-0.56598	-0.18228
C	-1.46044	-1.80834	-0.94016	C	-1.45728	-1.81189	-0.93046
C	-1.50277	1.765417	0.62434	C	-1.50425	1.765288	0.629709
C	-0.20199	2.296429	-0.00399	C	-0.20289	2.29741	0.003628
C	0.845193	1.258727	-0.32638	C	0.844288	1.260594	-0.32249
C	0.31259	-0.00276	-0.98063	C	0.311133	0.000362	-0.97854
C	2.151764	1.505337	-0.13836	C	2.150878	1.507527	-0.13544
C	3.295891	0.632464	-0.62285	C	3.294401	0.63561	-0.62308

C	2.743207	-0.36592	-1.668	C	2.740695	-0.35965	-1.67073
C	1.428697	-1.03662	-1.24794	C	1.427048	-1.03226	-1.25118
C	5.101272	-1.02073	0.355894	C	5.09839	-1.02242	0.349963
C	3.965567	-0.0313	0.62352	C	3.964492	-0.03187	0.621229
O	3.040341	-0.7753	1.426194	O	3.039246	-0.77626	1.423451
C	-4.5386	1.166084	-0.36302	C	-4.52912	1.164919	-0.36372
C	-3.78018	-0.0185	1.69937	C	-3.77931	-0.02673	1.696927
C	-0.48711	-1.00083	1.231911	C	-0.48174	-0.99672	1.23585
C	4.340859	1.548285	-1.30254	C	4.339362	1.552885	-1.30076
O	5.660937	-1.47473	1.577505	O	5.659966	-1.47876	1.569772
O	-5.13978	-1.6455	-0.10625	O	-5.09817	-1.78633	-0.15864
O	-2.45609	2.8319	0.64967	O	-2.45603	2.835057	0.658086
H	-3.1292	-3.18129	-0.97884	H	-3.13311	-3.18665	-0.96783
H	-2.74196	-2.6093	0.636902	H	-2.74058	-2.61303	0.643624
H	-3.9214	-0.95033	-1.63582	H	-3.90389	-0.97044	-1.64292
H	-2.10888	0.899157	-1.22605	H	-2.10748	0.900557	-1.22371
H	-1.5691	-1.55945	-2.00707	H	-1.56152	-1.56981	-1.99931
H	-0.72354	-2.61749	-0.88545	H	-0.71805	-2.61843	-0.86824
H	-1.31041	1.44495	1.657217	H	-1.3149	1.442916	1.662236
H	-0.50728	2.786495	-0.94172	H	-0.50779	2.79096	-0.93246
H	0.223805	3.08421	0.63372	H	0.223063	3.082877	0.644155
H	-0.08719	0.303933	-1.96298	H	-0.09106	0.30856	-1.95945
H	2.441148	2.444591	0.339133	H	2.440687	2.44557	0.344217
H	3.493237	-1.13051	-1.90134	H	3.49069	-1.12322	-1.90734
H	2.576417	0.191619	-2.60059	H	2.572738	0.200778	-2.60138
H	1.618005	-1.64249	-0.35919	H	1.618016	-1.64143	-0.36512
H	1.108233	-1.72146	-2.04111	H	1.105104	-1.71423	-2.04608
H	4.722709	-1.86518	-0.24105	H	4.717459	-1.86548	-0.24736
H	5.911209	-0.54377	-0.2028	H	5.907865	-0.54577	-0.20965
H	4.389019	0.784111	1.233831	H	4.389941	0.78159	1.23276
H	2.298879	-0.18337	1.634119	H	2.298624	-0.18413	1.633633
H	-4.33051	1.402998	-1.41439	H	-4.37754	1.337444	-1.43684
H	-5.5462	0.743942	-0.30513	H	-5.56073	0.81361	-0.22446
H	-4.50617	2.097126	0.19993	H	-4.43706	2.121084	0.147034
H	-4.83697	-0.23694	1.871598	H	-4.82455	-0.29736	1.870201
H	-3.20623	-0.82421	2.165089	H	-3.17149	-0.80286	2.168261
H	-3.53958	0.916528	2.213842	H	-3.58481	0.92057	2.208752
H	-0.00974	-0.18747	1.78721	H	-1.31366	-1.36522	1.837166
H	-1.32476	-1.34976	1.836965	H	0.252157	-1.80586	1.176988
H	0.233397	-1.8223	1.176096	H	-0.01845	-0.17905	1.796646
H	4.795825	2.241322	-0.58407	H	4.794517	2.24427	-0.58082
H	5.146114	0.966546	-1.7648	H	5.144479	0.972036	-1.76433
H	3.867799	2.145655	-2.08928	H	3.866373	2.151972	-2.08626

H	4.899101	-1.7289	2.125509	H	4.89923	-1.73558	2.118048
H	-5.38073	-2.4188	-0.63889	H	-5.80514	-1.17174	-0.40624
H	-2.06415	3.549893	1.171695	H	-2.06008	3.552547	1.177758

Conformer 5 P (%) = 11.28%				**Conformer 6 P (%) = 6.44%**			
C	-2.98983	-2.24617	0.146844	C	-2.99178	-2.25042	0.15457
C	-3.97472	-1.13705	-0.20702	C	-3.98869	-1.15112	-0.19377
C	-3.51584	0.284755	0.222117	C	-3.52414	0.291359	0.19325
C	-2.03686	0.519058	-0.29536	C	-2.03853	0.521662	-0.30967
C	-0.99521	-0.65912	-0.09666	C	-1.00193	-0.65886	-0.10138
C	-1.64601	-1.99176	-0.53385	C	-1.65556	-1.98927	-0.53833
C	-1.37481	1.840121	0.177974	C	-1.37211	1.829076	0.174775
C	-0.10037	2.121311	-0.63516	C	-0.10181	2.114451	-0.6424
C	0.867423	0.96763	-0.72414	C	0.867977	0.962054	-0.72583
C	0.236658	-0.37555	-1.04267	C	0.236353	-0.3819	-1.04069
C	2.188214	1.158306	-0.59335	C	2.188752	1.152351	-0.59407
C	3.25865	0.112281	-0.83869	C	3.259368	0.105932	-0.83716
C	2.630625	-1.0531	-1.64243	C	2.629995	-1.06482	-1.63178
C	1.282413	-1.51201	-1.07528	C	1.281951	-1.51856	-1.06012
C	4.357337	0.636402	1.466386	C	4.370418	0.642912	1.459424
C	3.812373	-0.42753	0.512117	C	3.818314	-0.4259	0.514752
O	4.841775	-1.37261	0.238845	O	4.844771	-1.3743	0.243024
C	-4.491	1.266666	-0.48171	C	-4.49359	1.244859	-0.5515
C	-3.69402	0.481151	1.743501	C	-3.71397	0.533709	1.707034
C	-0.49881	-0.79104	1.365433	C	-0.51422	-0.79376	1.364279
C	4.397832	0.739666	-1.6719	C	4.395151	0.729777	-1.67776
O	4.853914	-0.08825	2.599784	O	4.866144	-0.07432	2.59792
O	-5.26027	-1.37593	0.373436	O	-5.29179	-1.45405	0.312585
O	-2.21021	2.998581	0.131109	O	-2.26588	2.938551	0.037581
H	-3.39844	-3.21114	-0.18847	H	-3.40947	-3.21242	-0.16576
H	-2.88047	-2.31805	1.235301	H	-2.85585	-2.31575	1.243999
H	-4.07091	-1.12241	-1.3087	H	-4.12376	-1.16383	-1.28364
H	-2.14403	0.606553	-1.39095	H	-2.1367	0.619033	-1.40255
H	-1.80023	-1.97543	-1.62395	H	-1.82283	-1.96924	-1.62615
H	-0.96047	-2.82217	-0.33152	H	-0.96619	-2.81915	-0.34685
H	-1.11977	1.75686	1.237941	H	-1.1065	1.722052	1.236112
H	-0.4328	2.372409	-1.65881	H	-0.44689	2.37224	-1.65608
H	0.387364	3.01878	-0.23876	H	0.401889	3.007778	-0.24598
H	-0.18843	-0.29119	-2.05851	H	-0.18201	-0.3022	-2.05926
H	2.541081	2.165957	-0.3656	H	2.542651	2.1606	-0.36947
H	3.331872	-1.89318	-1.67401	H	3.330943	-1.90527	-1.65799
H	2.48774	-0.71233	-2.67712	H	2.486084	-0.73171	-2.66876

H	1.438315	-1.9139	-0.06855	H	1.436944	-1.90997	-0.04893
H	0.90307	-2.34496	-1.67787	H	0.903264	-2.35739	-1.65459
H	5.168294	1.202068	0.988335	H	5.182761	1.20069	0.974653
H	3.56342	1.334651	1.763844	H	3.580691	1.34763	1.753271
H	2.987075	-0.92464	1.047417	H	2.994398	-0.91794	1.056925
H	5.266802	-1.53516	1.099165	H	5.270717	-1.53541	1.103128
H	-4.30222	1.309324	-1.56349	H	-4.30998	1.224028	-1.63311
H	-5.51721	0.916578	-0.33833	H	-5.52113	0.909124	-0.37932
H	-4.40856	2.274602	-0.07422	H	-4.38939	2.275855	-0.21654
H	-4.75642	0.431369	1.996135	H	-4.78184	0.527555	1.952138
H	-3.19	-0.28143	2.342622	H	-3.2252	-0.21498	2.339679
H	-3.31904	1.462806	2.046336	H	-3.32926	1.517654	1.987828
H	-1.31554	-0.77608	2.087692	H	-1.33158	-0.73622	2.084525
H	0.033414	-1.73784	1.506404	H	-0.022	-1.75998	1.518705
H	0.196685	0.009069	1.636109	H	0.211999	-0.01904	1.628292
H	4.826899	1.621864	-1.18203	H	4.825629	1.614954	-1.19436
H	5.201114	0.01429	-1.82823	H	5.198335	0.004062	-1.83309
H	4.018365	1.061389	-2.64799	H	4.012031	1.045754	-2.65424
H	5.402943	0.509235	3.127947	H	5.432178	0.520261	3.111161
H	-5.56418	-2.23927	0.053819	H	-5.20701	-1.5755	1.271342
H	-2.47176	3.132849	-0.79426	H	-1.78067	3.728482	0.324305

Conformer 7 P (%) = 6.28%			
C	-2.9845	-2.2522	0.152953
C	-3.9825	-1.15469	-0.1984
C	-3.52083	0.288838	0.188218
C	-2.03463	0.521488	-0.31206
C	-0.99713	-0.6578	-0.10212
C	-1.64808	-1.98967	-0.53885
C	-1.3703	1.829373	0.174594
C	-0.09915	2.11732	-0.64092
C	0.871791	0.966115	-0.72624
C	0.240373	-0.37787	-1.04126
C	2.192719	1.157862	-0.59602
C	3.265916	0.113183	-0.8334
C	2.631471	-1.05076	-1.63324
C	1.286761	-1.51367	-1.06004
C	4.376077	0.657321	1.478573
C	3.818793	-0.40844	0.532085
O	4.908909	-1.33365	0.359291
C	-4.48985	1.240322	-0.55964
C	-3.71385	0.5321	1.701495

C	-0.51047	-0.7904	1.364155
C	4.406704	0.734236	-1.66802
O	4.808622	0.063066	2.690677
O	-5.28566	-1.45967	0.305169
O	-2.2652	2.936981	0.036041
H	-3.4002	-3.21515	-0.16688
H	-2.84962	-2.31606	1.242514
H	-4.11513	-1.16877	-1.28859
H	-2.13116	0.619299	-1.40508
H	-1.81434	-1.97111	-1.6269
H	-0.95811	-2.81893	-0.34532
H	-1.10604	1.721942	1.236066
H	-0.4436	2.376789	-1.65434
H	0.403758	3.009757	-0.24247
H	-0.17718	-0.30052	-2.06017
H	2.546789	2.164475	-0.36787
H	3.331418	-1.89542	-1.69389
H	2.483131	-0.71185	-2.66716
H	1.438722	-1.90194	-0.04649
H	0.909891	-2.35366	-1.6538
H	5.200132	1.200406	0.990493
H	3.596048	1.378814	1.736189
H	3.004781	-0.91007	1.07394
H	4.543553	-2.1938	0.106569
H	-4.30463	1.217894	-1.64096
H	-5.51731	0.903945	-0.38857
H	-4.38698	2.271859	-0.22611
H	-4.78219	0.526217	1.944314
H	-3.2266	-0.21618	2.335915
H	-3.33	1.516119	1.982916
H	-1.32848	-0.72797	2.083033
H	-0.02302	-1.7586	1.523087
H	0.217612	-0.01745	1.627894
H	4.824865	1.62592	-1.18804
H	5.219221	0.013814	-1.80379
H	4.035921	1.034579	-2.65421
H	5.362392	-0.68652	2.412349
H	-5.2049	-1.5734	1.265238
H	-1.78811	3.725642	0.339444

Table S9. Cartesian coordinates and equilibrium populations of low-energy conformers (>1%) of 6 in MeOH.

Conformer 1 P (%) = 46.57%				Conformer 2 P (%) = 24.59%			
C	-2.865156	-1.737685	-0.141729	C	-2.932892	-1.739771	-0.236646
C	-3.783488	-0.556454	-0.422721	C	-3.854469	-0.53173	-0.377397
C	-3.312508	0.751848	0.246578	C	-3.350058	0.714074	0.38155
C	-1.825777	0.999599	-0.175235	C	-1.879831	0.989064	-0.080624
C	-0.824988	-0.198392	-0.035458	C	-0.883089	-0.222096	-0.082355
C	-1.457179	-1.462628	-0.654531	C	-1.545286	-1.429985	-0.779861
C	-1.22115	2.274069	0.43074	C	-1.241139	2.204917	0.605671
C	0.108175	2.631896	-0.249581	C	0.063586	2.613235	-0.093562
C	1.067416	1.471455	-0.383551	C	1.00794	1.463869	-0.361198
C	0.448976	0.176887	-0.877828	C	0.360898	0.218973	-0.938073
C	2.385468	1.629515	-0.186678	C	2.333391	1.601364	-0.208714
C	3.446479	0.590034	-0.488562	C	3.373337	0.588709	-0.642272
C	2.851413	-0.466481	-1.44384	C	2.726426	-0.36945	-1.66531
C	1.472797	-0.966365	-1.011029	C	1.37022	-0.91327	-1.211528
C	4.894921	-1.196677	0.796225	C	4.887359	-1.275621	0.414198
C	3.970285	0.025369	0.871559	C	3.929058	-0.108868	0.635309
O	2.916134	-0.379006	1.747974	O	2.898345	-0.655859	1.464675
C	-4.19376	1.885343	-0.323606	C	-4.245654	1.89614	-0.050062
C	-3.553996	0.707536	1.767735	C	-3.528732	0.537012	1.901478
C	-0.422389	-0.486543	1.42497	C	-0.429192	-0.638985	1.33049
C	4.623112	1.291486	-1.196388	C	4.531768	1.343551	-1.325126
H	-1.884303	1.176003	-1.261653	H	-1.982763	1.256512	-1.145096
O	4.177679	-2.393238	0.545895	O	5.371901	-1.759113	1.655702
O	-5.10798	-0.857502	-0.006683	O	-5.164064	-0.868735	0.05045
O	-3.469975	-2.850113	-0.821674	O	-3.533769	-2.872709	-0.885453
H	0.068542	0.392107	-1.890653	H	-0.056591	0.522942	-1.913346
H	-2.861759	-1.936894	0.938156	H	-2.885708	-2.037968	0.814017
H	-3.764641	-0.400669	-1.516935	H	-3.87243	-0.272123	-1.456066
H	-1.520313	-1.348823	-1.745165	H	-1.64078	-1.210808	-1.855857
H	-0.818749	-2.334708	-0.465524	H	-0.916079	-2.321508	-0.692617
H	-1.069035	2.15212	1.508136	H	-1.0468	1.990511	1.661363
H	-1.911949	3.114184	0.31316	H	-1.92902	3.055345	0.587958
H	0.594932	3.471257	0.260563	H	0.575903	3.403787	0.466954
H	-0.124262	2.980844	-1.268613	H	-0.204904	3.049422	-1.069209
H	2.74749	2.596963	0.167037	H	2.71793	2.535018	0.206438
H	3.53297	-1.315052	-1.538893	H	3.405197	-1.197267	-1.897784
H	2.765405	-0.000084	-2.434987	H	2.593617	0.191448	-2.600633
H	1.582705	-1.503495	-0.067741	H	1.523421	-1.520505	-0.318516

H	1.107038	-1.694771	-1.742556	H	0.967906	-1.576136	-1.985309
H	5.629824	-1.083051	-0.005555	H	4.372812	-2.07228	-0.144805
H	5.446376	-1.268454	1.747057	H	5.758815	-0.959008	-0.165103
H	4.538534	0.842941	1.345893	H	4.476902	0.656475	1.209278
H	2.189354	0.255436	1.624366	H	2.238746	0.044595	1.599912
H	-3.990832	2.04672	-1.389359	H	-4.088539	2.1474	-1.106259
H	-5.248431	1.618809	-0.216007	H	-5.297019	1.627153	0.082605
H	-4.030259	2.832143	0.200525	H	-4.050818	2.793667	0.545131
H	-4.625706	0.623376	1.961694	H	-4.59232	0.44268	2.131971
H	-3.070474	-0.137885	2.260323	H	-3.033467	-0.350948	2.297618
H	-3.191467	1.623837	2.244456	H	-3.137585	1.405521	2.440749
H	-1.262924	-0.842907	2.020547	H	-1.25105	-1.039746	1.923897
H	0.351608	-1.256205	1.471207	H	0.337651	-1.415005	1.281563
H	-0.030369	0.402087	1.927486	H	-0.01056	0.201437	1.891062
H	5.092054	2.041704	-0.548567	H	5.044511	2.009562	-0.621201
H	5.392578	0.57163	-1.49589	H	5.273265	0.65035	-1.736774
H	4.272176	1.799704	-2.100229	H	4.151382	1.954711	-2.15024
H	3.404857	-2.336967	1.134407	H	4.581276	-1.853369	2.213579
H	-5.263658	-1.766347	-0.315701	H	-5.28476	-1.793225	-0.230961
H	-3.026076	-3.659547	-0.527509	H	-3.479283	-2.714097	-1.843123

Conformer 3 P (%) = 12.17%				**Conformer 4 P (%) = 10.19%**			
C	-2.928299	-1.75239	-0.275474	C	-2.92612	-1.75698	-0.247602
C	-3.851386	-0.541078	-0.377221	C	-3.844033	-0.548895	-0.380903
C	-3.343876	0.708254	0.381841	C	-3.347052	0.704073	0.381496
C	-1.873756	0.984083	-0.083885	C	-1.876776	0.986451	-0.077326
C	-0.881173	-0.228457	-0.095282	C	-0.881874	-0.226008	-0.081617
C	-1.544824	-1.420038	-0.813775	C	-1.542509	-1.426896	-0.786615
C	-1.234739	2.200476	0.602257	C	-1.239514	2.199969	0.615837
C	0.066128	2.611736	-0.10181	C	0.065378	2.611299	-0.081497
C	1.011583	1.462797	-0.365343	C	1.009319	1.46303	-0.354796
C	0.365922	0.218601	-0.944555	C	0.361817	0.220531	-0.935769
C	2.336389	1.601553	-0.208183	C	2.334746	1.60164	-0.203182
C	3.37759	0.588436	-0.637566	C	3.374728	0.591336	-0.641849
C	2.734373	-0.367734	-1.664845	C	2.726869	-0.363927	-1.667146
C	1.376192	-0.912835	-1.218568	C	1.371182	-0.910211	-1.21471
C	4.881941	-1.280204	0.424894	C	4.891943	-1.274694	0.406795
C	3.92634	-0.110613	0.642294	C	3.933297	-0.109187	0.632923
O	2.890785	-0.654172	1.467954	O	2.904954	-0.658659	1.463172
C	-4.239719	1.892415	-0.040972	C	-4.239326	1.887705	-0.052713
C	-3.507193	0.535652	1.906532	C	-3.525989	0.53309	1.901466
C	-0.432459	-0.654476	1.316422	C	-0.424849	-0.645317	1.329888

C	4.540164	1.34289	-1.313716	C	4.531369	1.349665	-1.323901
H	-1.98458	1.253594	-1.146636	H	-1.977658	1.257383	-1.141272
O	5.359252	-1.765733	1.668666	O	5.3784	-1.761657	1.646422
O	-5.185627	-0.929119	-0.012138	O	-5.137985	-0.996843	0.052288
O	-3.462006	-2.826665	-1.036579	O	-3.445984	-2.844589	-1.000858
H	-0.049458	0.523882	-1.920104	H	-0.056319	0.527166	-1.909763
H	-2.855494	-2.054835	0.783956	H	-2.868302	-2.038994	0.814682
H	-3.933882	-0.288946	-1.441469	H	-3.888368	-0.305212	-1.45476
H	-1.655769	-1.191464	-1.882716	H	-1.648875	-1.214357	-1.859441
H	-0.91529	-2.313073	-0.747831	H	-0.9122	-2.318007	-0.704998
H	-1.030306	1.983502	1.65578	H	-1.045185	1.979135	1.670173
H	-1.923911	3.050359	0.591583	H	-1.924298	3.053386	0.6037
H	0.576462	3.405617	0.455776	H	0.57721	3.399196	0.483258
H	-0.205897	3.043741	-1.078252	H	-0.203395	3.052409	-1.054882
H	2.719144	2.53587	0.20726	H	2.71907	2.533934	0.215429
H	3.414071	-1.195083	-1.896215	H	3.40589	-1.190542	-1.903156
H	2.605756	0.194973	-2.599632	H	2.593241	0.200013	-2.600556
H	1.525494	-1.523731	-0.327373	H	1.525083	-1.52135	-0.324521
H	0.976148	-1.572069	-1.995951	H	0.967529	-1.569534	-1.990196
H	4.367496	-2.074955	-0.136677	H	4.377042	-2.069835	-0.153818
H	5.757206	-0.966118	-0.150017	H	5.762525	-0.95577	-0.172597
H	4.474244	0.653229	1.218366	H	4.482021	0.655187	1.207579
H	2.227661	0.045259	1.590687	H	2.24001	0.037767	1.593117
H	-4.068339	2.162691	-1.089641	H	-4.124865	2.105546	-1.121578
H	-5.291929	1.613836	0.067695	H	-5.295308	1.663738	0.139925
H	-4.06074	2.780964	0.572411	H	-4.009726	2.800008	0.505072
H	-4.570184	0.542078	2.176001	H	-4.586102	0.39957	2.132611
H	-3.068482	-0.386383	2.293758	H	-2.999483	-0.332617	2.304087
H	-3.046588	1.36885	2.444454	H	-3.17048	1.419969	2.435471
H	-1.257686	-1.0545	1.906248	H	-1.24204	-1.062064	1.918658
H	0.328294	-1.436132	1.265153	H	0.348831	-1.413972	1.274748
H	-0.007739	0.179581	1.882784	H	-0.013389	0.19381	1.898268
H	5.049714	2.008236	-0.606777	H	5.044552	2.014112	-0.618721
H	5.283187	0.649177	-1.721673	H	5.272912	0.658493	-1.738858
H	4.164694	1.954507	-2.140734	H	4.14915	1.96282	-2.146705
H	4.565312	-1.8603	2.2217	H	4.588037	-1.860177	2.203921
H	-5.17893	-1.119988	0.940144	H	-5.806837	-0.413525	-0.333792
H	-4.424081	-2.78125	-0.893546	H	-4.391002	-2.873746	-0.771962

Conformer 5 P (%) = 6.48%			
C	-3.082722	-1.676676	0.165977

C	-3.953354	-0.447761	-0.055996
C	-3.272542	0.866007	0.381585
C	-1.869319	0.936683	-0.310571
C	-0.945435	-0.328006	-0.203978
C	-1.775628	-1.563431	-0.609007
C	-1.088927	2.219575	0.01373
C	0.090357	2.401559	-0.95788
C	0.955205	1.169442	-0.985883
C	0.208582	-0.118641	-1.257261
C	2.276478	1.222703	-0.775293
C	3.225619	0.042666	-0.718496
C	2.426668	-1.270162	-0.589183
C	1.18197	-1.295298	-1.481636
C	5.131961	-0.835812	0.842879
C	4.118966	0.261813	0.532407
O	3.331045	0.362064	1.726545
C	-4.151993	2.020068	-0.150019
C	-3.252644	0.984013	1.91893
C	-0.339566	-0.545554	1.195252
C	4.10334	0.04648	-1.986926
H	-2.112634	0.996568	-1.383937
O	5.87689	-0.507426	2.003648
O	-5.190537	-0.594486	0.626284

O	-3.877739	-2.784109	-0.28851
H	-0.322926	0.030679	-2.210315
H	-2.89133	-1.788826	1.241562
H	-4.134481	-0.387793	-1.144707
H	-2.023707	-1.512345	-1.677849
H	-1.19263	-2.481166	-0.463658
H	-0.712175	2.189049	1.042617
H	-1.744022	3.093097	-0.053572
H	0.682399	3.284437	-0.69026
H	-0.31939	2.581998	-1.963753
H	2.739917	2.203447	-0.639397
H	2.143958	-1.393625	0.458769
H	3.069341	-2.120108	-0.84829
H	0.665704	-2.252782	-1.362802
H	1.503436	-1.261814	-2.530114
H	4.608055	-1.795981	0.965699
H	5.849941	-0.940246	0.025218
H	4.68035	1.200202	0.389685
H	2.659776	1.046391	1.571504
H	-4.102339	2.087161	-1.243696
H	-5.193026	1.844163	0.133598
H	-3.850184	2.98687	0.26436
H	-4.273421	1.115942	2.285331

H	-2.850649	0.100443	2.418315
H	-2.661945	1.84932	2.235851
H	-1.089907	-0.540244	1.985018
H	0.168189	-1.514138	1.237962
H	0.404623	0.215787	1.440221
H	4.67325	0.979357	-2.070367
H	4.814048	-0.787094	-1.986488
H	3.481053	-0.040602	-2.882697
H	5.213135	-0.226616	2.656213
H	-5.471101	-1.506088	0.436816
H	-3.450674	-3.601811	0.00763

Table S10. Cartesian coordinates and equilibrium populations of low-energy conformers (>1%) of 7 in MeOH.

Conformer 1 P (%) = 41.59%				**Conformer 2 P (%) = 31.94%**			
C	3.66905	1.904864	-0.98055	C	3.667379	1.92697	-0.9347
C	4.758023	0.975125	-0.44416	C	4.755696	0.979015	-0.4298
C	4.251895	-0.00039	0.660289	C	4.261166	-0.00315	0.662798
C	2.961154	-0.72897	0.126856	C	2.968581	-0.72411	0.120776
C	1.836003	0.15692	-0.52226	C	1.840641	0.171296	-0.51197
C	2.489408	1.109664	-1.55068	C	2.489899	1.143884	-1.52434
C	2.352362	-1.72701	1.129314	C	2.360833	-1.73386	1.11169
C	1.329823	-2.64613	0.437727	C	1.336676	-2.64298	0.409241
C	0.300099	-1.88851	-0.36929	C	0.306797	-1.87612	-0.38902
C	0.871754	-0.8273	-1.29712	C	0.877109	-0.80127	-1.30192
C	-1.00332	-2.19388	-0.30054	C	-0.99613	-2.1848	-0.3258
C	-2.08809	-1.57413	-1.16732	C	-2.08142	-1.55819	-1.18682
C	-1.40671	-1.02188	-2.44274	C	-1.39957	-0.98361	-2.45207
C	-0.21389	-0.11067	-2.1343	C	-0.21059	-0.0733	-2.12642
C	5.367013	-1.05163	0.878762	C	5.375363	-1.06154	0.859964
C	4.071497	0.748525	2.0007	C	4.08622	0.727208	2.013334
O	5.916417	1.708706	-0.03576	O	5.875813	1.697754	0.095263

C	1.024542	0.973185	0.509624	C	1.028274	0.96883	0.533968
C	-2.76919	-0.43635	-0.35188	C	-2.7721	-0.43587	-0.35803
C	-3.11279	-2.65954	-1.55827	C	-3.0988	-2.64385	-1.59611
C	-3.90176	0.312996	-1.05198	C	-3.91082	0.31177	-1.05004
O	-3.32754	-1.02945	0.853742	O	-3.32565	-1.0477	0.840349
O	-4.35561	1.407976	-0.23039	O	-4.37345	1.39414	-0.21688
C	-3.57649	2.520577	-0.23976	C	-3.604	2.513618	-0.21578
C	-4.04676	3.511987	0.792637	C	-4.07979	3.489015	0.829216
O	-2.61883	2.662532	-0.97025	O	-2.64979	2.672011	-0.94734
C	-3.11075	-0.40668	2.035786	C	-3.11594	-0.43511	2.029205
O	-2.47513	0.616905	2.173104	O	-2.49202	0.594013	2.177371
C	-3.77668	-1.16917	3.157943	C	-3.77311	-1.21698	3.14315
H	4.109539	2.540655	-1.75798	H	4.095011	2.584033	-1.70694
H	3.326667	2.582478	-0.18489	H	3.341372	2.583887	-0.11972
H	5.117776	0.361481	-1.28128	H	5.087369	0.365664	-1.28795
H	3.341925	-1.33751	-0.71111	H	3.344956	-1.32248	-0.72651
H	2.853944	0.516199	-2.40338	H	2.853431	0.56663	-2.3888
H	1.738725	1.799389	-1.95317	H	1.73758	1.840159	-1.91176
H	1.866158	-1.19506	1.95515	H	1.877859	-1.21248	1.945775
H	3.135479	-2.34779	1.577359	H	3.143581	-2.36187	1.549896
H	0.836977	-3.29802	1.169245	H	0.84342	-3.30326	1.132939
H	1.883573	-3.30876	-0.24774	H	1.889404	-3.29802	-0.2844
H	1.522991	-1.3663	-2.00727	H	1.52775	-1.32883	-2.02126
H	-1.32642	-2.96727	0.396263	H	-1.31846	-2.96737	0.361041
H	-2.12726	-0.49286	-3.07806	H	-2.12078	-0.44689	-3.08022
H	-1.06507	-1.88822	-3.02515	H	-1.05371	-1.83937	-3.04757
H	-0.57651	0.789132	-1.62817	H	-0.5771	0.815411	-1.60359
H	0.224021	0.234932	-3.0776	H	0.226137	0.291313	-3.06316
H	5.464697	-1.71673	0.011453	H	5.480554	-1.70213	-0.02511
H	6.324631	-0.54177	1.021194	H	6.33207	-0.55981	1.030679
H	5.182558	-1.67388	1.760887	H	5.178646	-1.7078	1.721622
H	5.051407	1.030852	2.402212	H	5.064406	1.034815	2.392552
H	3.473646	1.660716	1.91739	H	3.474658	1.629284	1.943012
H	3.591031	0.111748	2.749938	H	3.627756	0.06799	2.757841
H	5.624206	2.375651	0.605411	H	6.188793	2.293864	-0.60234
H	1.664909	1.582195	1.148802	H	1.668279	1.56577	1.184228
H	0.335284	1.661317	0.009822	H	0.338795	1.664664	0.045234
H	0.420789	0.337766	1.163571	H	0.424329	0.321219	1.175612
H	-2.01533	0.285201	-0.04256	H	-2.02436	0.288378	-0.04004
H	-3.64379	-3.03938	-0.67969	H	-3.6308	-3.03829	-0.72456
H	-3.85628	-2.27691	-2.26826	H	-3.84188	-2.25588	-2.30365
H	-2.60265	-3.50195	-2.03816	H	-2.58222	-3.47697	-2.08523
H	-3.57544	0.699969	-2.0187	H	-3.58775	0.711586	-2.0126

H	-4.7797	-0.32237	-1.17935	H	-4.78352	-0.32945	-1.18407
H	-5.1383	3.563566	0.82393	H	-3.72223	3.137655	1.804027
H	-3.69466	3.169322	1.772519	H	-3.66224	4.476338	0.627197
H	-3.62057	4.493391	0.580094	H	-5.17164	3.531139	0.863892
H	-3.55146	-0.68753	4.109977	H	-3.55372	-0.74247	4.100111
H	-4.86035	-1.18967	3.000504	H	-4.85644	-1.24874	2.985199
H	-3.42869	-2.20693	3.17054	H	-3.41271	-2.25057	3.145278

Conformer 3 P (%) = 22.25%				**Conformer 4 P (%) = 4.22%**			
C	3.663293	1.936382	-0.93258	C	-4.28643	1.764643	0.88492
C	4.754058	0.994161	-0.43769	C	-5.26185	0.68131	0.442175
C	4.261917	0.000931	0.659298	C	-4.69881	-0.21917	-0.69881
C	2.969254	-0.72479	0.121987	C	-3.28431	-0.75688	-0.2557
C	1.840213	0.171685	-0.50852	C	-2.26013	0.275414	0.339998
C	2.487271	1.148926	-1.51744	C	-2.98363	1.144967	1.395937
C	2.359745	-1.73392	1.113804	C	-2.58801	-1.63006	-1.31564
C	1.335096	-2.64272	0.411401	C	-1.43106	-2.4203	-0.68649
C	0.306148	-1.87598	-0.38794	C	-0.48373	-1.5753	0.138624
C	0.877605	-0.80102	-1.29981	C	-1.12943	-0.55686	1.065972
C	-0.99669	-2.18498	-0.32549	C	0.836272	-1.80991	0.110079
C	-2.08124	-1.55819	-1.18719	C	1.872102	-1.23722	1.056629
C	-1.39821	-0.98323	-2.4517	C	1.161757	-0.47029	2.203024
C	-0.20933	-0.07299	-2.12528	C	-0.07324	0.324197	1.761909
C	5.370268	-1.06437	0.851737	C	-5.64932	-1.4332	-0.84666
C	4.090988	0.726695	2.011051	C	-4.72061	0.540586	-2.04266
O	5.84011	1.814759	-0.00121	O	-6.47726	1.342256	0.084132
C	1.025567	0.96505	0.538941	C	-1.61912	1.183075	-0.73906
C	-2.77244	-0.43627	-0.35832	C	2.926465	-0.33909	0.342382
C	-3.09831	-2.64373	-1.59756	C	2.649482	-2.4221	1.69014
C	-3.91061	0.311827	-1.05074	C	3.522956	-0.94571	-0.92943
O	-3.32722	-1.04867	0.83933	O	2.32832	0.925731	-0.04841
O	-4.37316	1.394252	-0.21771	O	4.556434	-0.09373	-1.45729
C	-3.60262	2.513217	-0.21632	C	5.785366	-0.2254	-0.88812
C	-4.07889	3.489946	0.827161	C	6.722885	0.840788	-1.39296
O	-2.64727	2.66989	-0.94664	O	6.0547	-1.07696	-0.07023
C	-3.11824	-0.4369	2.028737	C	3.048372	2.058224	0.147493
O	-2.49199	0.590556	2.17852	O	4.13323	2.102176	0.686369
C	-3.77996	-1.21716	3.141165	C	2.30124	3.255893	-0.39159
H	4.097284	2.594101	-1.69479	H	-4.76349	2.356333	1.674821
H	3.337115	2.588809	-0.11385	H	-4.09618	2.454773	0.054039
H	5.081968	0.38627	-1.30073	H	-5.44642	0.025696	1.312774
H	3.343704	-1.32332	-0.72635	H	-3.51475	-1.42806	0.589705

H	2.848687	0.575786	-2.38555	H	-3.21293	0.521401	2.273714
H	1.731715	1.844396	-1.89998	H	-2.31481	1.937554	1.75054
H	1.877243	-1.21044	1.946793	H	-2.21204	-1.00746	-2.13548
H	3.138432	-2.36524	1.554811	H	-3.29131	-2.33908	-1.76501
H	0.841471	-3.30208	1.135688	H	-0.87475	-2.97356	-1.45318
H	1.888025	-3.29872	-0.28124	H	-1.87183	-3.18016	-0.01983
H	1.528999	-1.328	-2.01892	H	-1.65121	-1.13575	1.848849
H	-1.31951	-2.96735	0.361378	H	1.201076	-2.57459	-0.57872
H	-2.11889	-0.44626	-3.08018	H	1.877165	0.19548	2.703465
H	-1.05217	-1.83891	-3.04725	H	0.853854	-1.20942	2.955001
H	-0.57617	0.815954	-1.60319	H	0.246317	1.119161	1.086721
H	0.228387	0.291303	-3.06157	H	-0.51564	0.806673	2.641154
H	5.521571	-1.65955	-0.05766	H	-5.65863	-2.05292	0.058844
H	6.327172	-0.5922	1.109082	H	-6.67844	-1.10398	-1.03957
H	5.142666	-1.75284	1.671176	H	-5.37401	-2.07402	-1.68989
H	5.064977	1.068242	2.373823	H	-5.7551	0.722207	-2.34845
H	3.454084	1.610782	1.947835	H	-4.23688	1.518609	-1.99384
H	3.66574	0.058016	2.76683	H	-4.2336	-0.03905	-2.83368
H	6.604203	1.240987	0.159615	H	-7.1624	0.66782	-0.03715
H	1.662552	1.569323	1.185249	H	-2.35329	1.58578	-1.43773
H	0.330967	1.655344	0.049885	H	-1.11944	2.040217	-0.27553
H	0.426667	0.315756	1.183593	H	-0.86173	0.650071	-1.32245
H	-2.02485	0.287658	-0.03931	H	3.731936	-0.11857	1.046254
H	-2.58147	-3.47666	-2.08676	H	3.174061	-3.02886	0.945233
H	-3.63094	-3.03851	-0.72655	H	3.393631	-2.06225	2.410497
H	-3.84086	-2.25541	-2.30543	H	1.952256	-3.08039	2.218481
H	-3.58699	0.711556	-2.01316	H	3.935104	-1.93749	-0.73866
H	-4.78343	-0.32915	-1.18518	H	2.768812	-0.99474	-1.71661
H	-3.66001	4.47662	0.624777	H	6.605365	0.992257	-2.46944
H	-5.17075	3.533178	0.860279	H	6.469664	1.780645	-0.88912
H	-3.72302	3.139238	1.802832	H	7.751417	0.56795	-1.15311
H	-3.5573	-0.74617	4.099119	H	2.103866	3.122944	-1.46016
H	-4.86356	-1.24106	2.983509	H	2.894963	4.156435	-0.23122
H	-3.42673	-2.2532	3.140797	H	1.332625	3.356888	0.109207

Table S11. Cartesian coordinates and equilibrium populations of low-energy conformers (>1%) of 8 in MeOH.

Conformer 1 P (%) = 59.18%				**Conformer 2 P (%) = 37.84%**			
C	3.385	1.102	0.22	C	3.331	1.114	0.072
C	3.891	0.061	-0.79	C	3.783	-0.118	-0.725

C	3.108	-1.272	-0.723	C	2.9	-1.365	-0.472
C	1.565	-0.964	-0.82	C	1.394	-0.975	-0.695
C	0.976	0.199	0.056	C	0.874	0.362	-0.055
C	1.905	1.435	-0.038	C	1.892	1.5	-0.307
C	0.668	-2.212	-0.701	C	0.395	-2.124	-0.43
C	-0.769	-1.94	-1.164	C	-1.004	-1.809	-0.981
C	-1.368	-0.629	-0.686	C	-1.491	-0.41	-0.666
C	-0.437	0.569	-0.518	C	-0.471	0.719	-0.767
C	-2.702	-0.561	-0.455	C	-2.784	-0.204	-0.333
C	-3.448	0.702	-0.042	C	-3.37	1.162	-0.029
C	-2.563	1.943	-0.297	C	-2.519	2.243	-0.737
C	-1.133	1.741	0.214	C	-1.031	2.114	-0.402
C	-4.656	1.736	2.037	C	-4.225	0.443	2.365
C	-3.846	0.556	1.453	C	-3.392	1.419	1.504
C	3.519	-2.101	-1.97	C	3.295	-2.419	-1.538
C	3.489	-2.077	0.561	C	3.155	-1.975	0.941
C	0.817	-0.198	1.546	C	0.621	0.243	1.473
C	-4.718	0.8	-0.914	C	-4.801	1.235	-0.602
H	1.438	-0.615	-1.847	H	1.338	-0.796	-1.772
O	-5.051	1.448	3.365	O	-3.609	-0.827	2.467
O	4.807	-2.601	0.518	O	4.461	-2.509	1.086
O	4.168	2.281	0.122	O	4.205	2.2	-0.195
H	-0.267	0.931	-1.533	H	-0.252	0.791	-1.833
H	3.516	0.736	1.237	H	3.403	0.918	1.141
H	4.96	-0.11	-0.654	H	4.83	-0.339	-0.52
H	3.793	0.478	-1.795	H	3.744	0.129	-1.788
H	1.577	2.205	0.662	H	1.595	2.396	0.241
H	1.812	1.875	-1.032	H	1.867	1.77	-1.364
H	0.657	-2.576	0.326	H	0.329	-2.335	0.636
H	1.064	-3.035	-1.295	H	0.737	-3.05	-0.889
H	-1.4	-2.778	-0.863	H	-1.709	-2.556	-0.612
H	-0.786	-1.932	-2.254	H	-0.985	-1.921	-2.065
H	-3.285	-1.463	-0.575	H	-3.442	-1.061	-0.283
H	-3.002	2.835	0.149	H	-2.873	3.239	-0.469
H	-2.516	2.148	-1.368	H	-2.637	2.162	-1.819
H	-1.173	1.574	1.288	H	-0.892	2.347	0.65
H	-0.568	2.662	0.069	H	-0.473	2.883	-0.937
H	-5.566	1.915	1.466	H	-5.232	0.308	1.972
H	-4.08	2.662	2.048	H	-4.332	0.838	3.377
H	-2.951	0.407	2.057	H	-3.788	2.421	1.672
H	-4.432	-0.357	1.57	H	-2.377	1.444	1.902
H	3.167	-1.641	-2.894	H	3.031	-2.09	-2.544
H	3.124	-3.116	-1.936	H	2.814	-3.38	-1.367

H	4.602	-2.186	-2.058	H	4.371	-2.6	-1.543
H	2.83	-2.934	0.695	H	2.468	-2.799	1.136
H	3.437	-1.48	1.466	H	3.032	-1.255	1.742
H	0.054	-0.962	1.69	H	-0.129	-0.509	1.716
H	0.528	0.655	2.158	H	0.269	1.179	1.902
H	1.733	-0.567	1.991	H	1.516	0.006	2.034
H	-5.401	-0.029	-0.723	H	-5.438	0.441	-0.214
H	-4.474	0.785	-1.977	H	-4.798	1.137	-1.688
H	-5.264	1.725	-0.728	H	-5.273	2.187	-0.361
H	-4.253	1.391	3.914	H	-2.748	-0.711	2.902
H	5.436	-1.863	0.546	H	5.096	-1.776	1.089
H	4.082	2.642	-0.775	H	4.166	2.409	-1.143

Conformer 3 P (%) = 2.97%			
C	3.57	1.178	-0.33
C	3.964	-0.123	-1.046
C	3.103	-1.331	-0.615
C	1.585	-0.945	-0.786
C	1.1	0.432	-0.199
C	2.105	1.537	-0.619
C	0.578	-2.075	-0.473
C	-0.807	-1.767	-1.047
C	-1.286	-0.407	-0.598
C	-0.313	0.747	-0.81
C	-2.509	-0.271	-0.039
C	-3.083	1.05	0.442
C	-1.934	2.039	0.727
C	-0.924	2.119	-0.425
C	-5.132	-0.043	1.661
C	-3.878	0.852	1.759
C	3.455	-2.484	-1.588
C	3.561	-1.764	0.81
C	0.981	0.418	1.343
C	-4.005	1.612	-0.661
H	1.498	-0.808	-1.866
O	-5.73	-0.141	2.939
O	2.816	-2.854	1.315
O	4.393	2.237	-0.789
H	-0.156	0.805	-1.888
H	3.729	1.093	0.745
H	5.02	-0.34	-0.876
H	3.862	0.027	-2.123

H	1.877	2.476	-0.114
H	1.991	1.733	-1.687
H	0.484	-2.223	0.602
H	0.91	-3.025	-0.885
H	-0.768	-1.784	-2.137
H	-1.509	-2.548	-0.751
H	-3.112	-1.161	0.069
H	-2.338	3.033	0.924
H	-1.419	1.746	1.641
H	-0.162	2.854	-0.18
H	-1.429	2.532	-1.298
H	-4.889	-1.05	1.324
H	-5.869	0.378	0.977
H	-4.181	1.832	2.133
H	-3.208	0.442	2.518
H	2.972	-3.422	-1.318
H	4.53	-2.677	-1.597
H	3.163	-2.248	-2.612
H	3.532	-0.957	1.535
H	4.604	-2.082	0.777
H	1.911	0.175	1.843
H	0.227	-0.287	1.694
H	0.704	1.403	1.718
H	-4.817	0.925	-0.9
H	-4.453	2.558	-0.355
H	-3.467	1.791	-1.592
H	-6.516	-0.707	2.858
H	3.164	-3.074	2.195
H	5.313	2.032	-0.557

4. Bioactivity Assay

Figure S87. The cytotoxicity of Pubescens B (2) and pubescens H (8).