Electronic Supplementary Information (ESI)

Cycloabiesesquine A, a Unique Sesquiterpenoid from *Abies delavayi*

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Isolation Procedures

The aerial parts of *A. delavayi* were collected in Dali city of Yunnan Province, China, and identified by L. S. Xie of Kunming Institute of Botany, Chinese Academy of Sciences. A herbarium specimen is deposited in the School of Pharmacy, Second Military Medical University, China (herbarium No. 2006-07-0101). The air-dried samples (14 kg) were extracted with 85% EtOH. The resin was filtered and the filtrate successively partitioned with $CHCl_3$, EtOAc and *n*-BuOH. The $CHCl_3$-soluble extract and the resin were combined and chromatographed over a silica gel column eluting with a gradient of petroleum ether/$CHCl_3$ (100:0→0:100) to give five fractions (Fr.1–Fr.5). Fr.5 was divided into 16 subfractions (Fr.5.1–Fr.5.16) by RP-MPLC eluting with MeOH-H_2O (5:95–100:0). Fraction Fr.5.2 was subjected repeatedly to CC over Sephadex LH-20 ($CHCl_3$/MeOH, 1:1; MeOH), followed by prep. TLC using $CHCl_3$/MeOH (5:1) to give cycloabiesesquine A (**1**, 7.8 mg).

Computational Methods

Potential energy surface of compound **1** and its C-7 epimer **2** were scanned at AM1 level by rotating about the C8-C7 and C7-C1 bonds. Eight minimum energy points were found for compound **1** and six for compound **2**. All conformers were relocated and confirmed at the B3LYP/6-31G** level (denoted as: **1a**–**1h** and **2a**–**2f**). Excitation energy (in nm) and rotatory strength R (velocity form R^{vel} and length form R^{len} in 10^{-40} erg-esu-cm/Gauss) between different states were calculated by time dependant density functional theory (TDDFT) at both B3LYP/6-31G** and B3LYP/6-311++G** levels in the gas phase and at B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with "COnductor-like continuum Solvent Model" (COSMO) in MeOH. All calculations are performed by the Gaussian03 program package.

The ECD spectra were then simulated by overlapping Gaussian functions for each transition according to

$$\Delta\epsilon\,(E) = \frac{1}{2.297 \times 10^{-39}} \frac{1}{\sqrt{2\pi\sigma}} \sum_{i}^{A} \Delta E_i R_i e^{-[(E-\Delta E_i)/(2\sigma)]^2}$$

where σ is the width of the band at 1/e height and ΔE_i and R_i are the excitation energies and rotatory strengths for transition *i*, respectively, σ = 0.20 eV and R^{len} have been used in this work. Conformational analysis has been carried out and theoretically weighted ECD spectra have been simulated at different levels mentioned above.

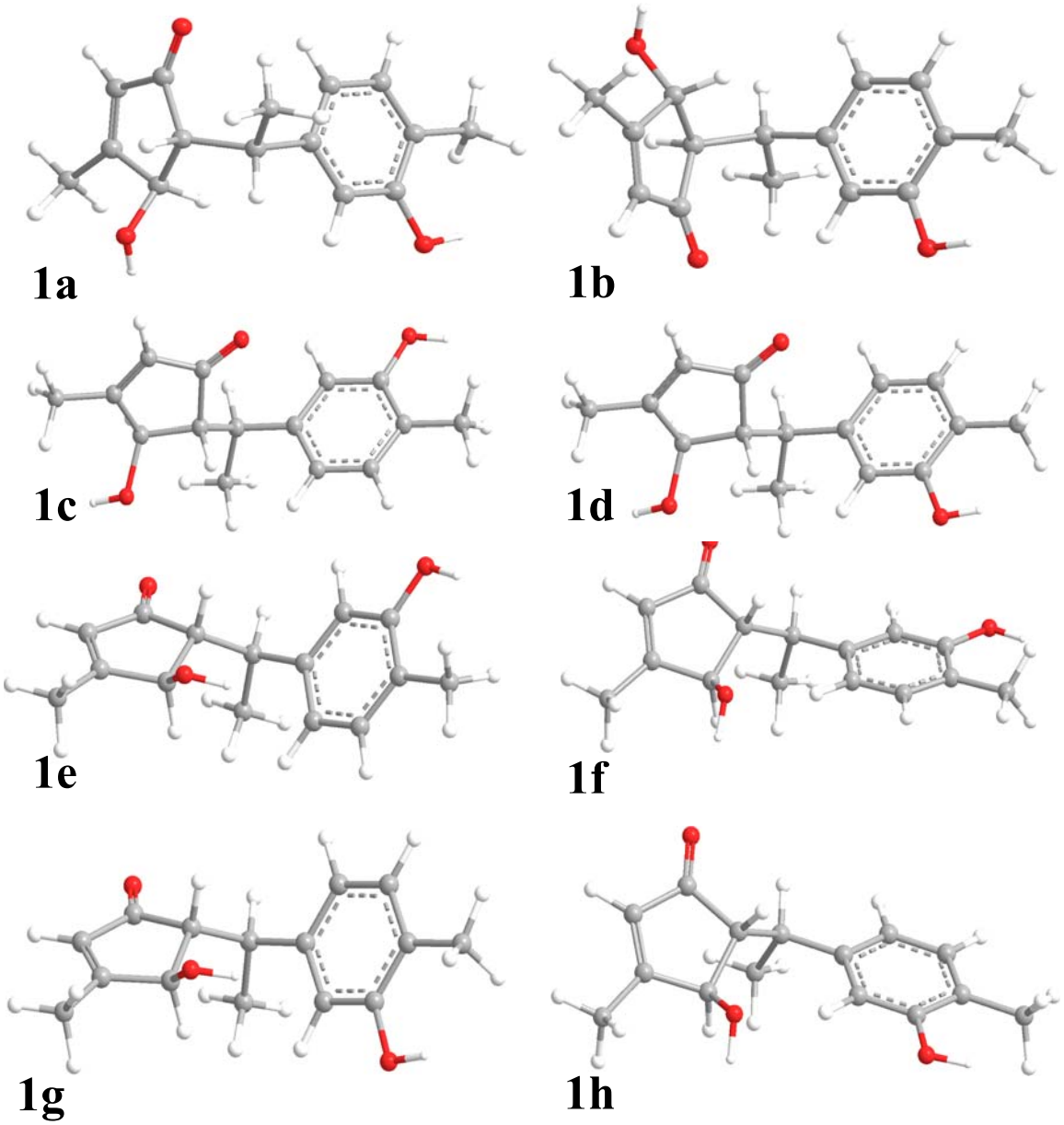


Fig.S1 Optimized geometries of conformers of compound **1** at B3LYP/6-31G** level in the gas phase.

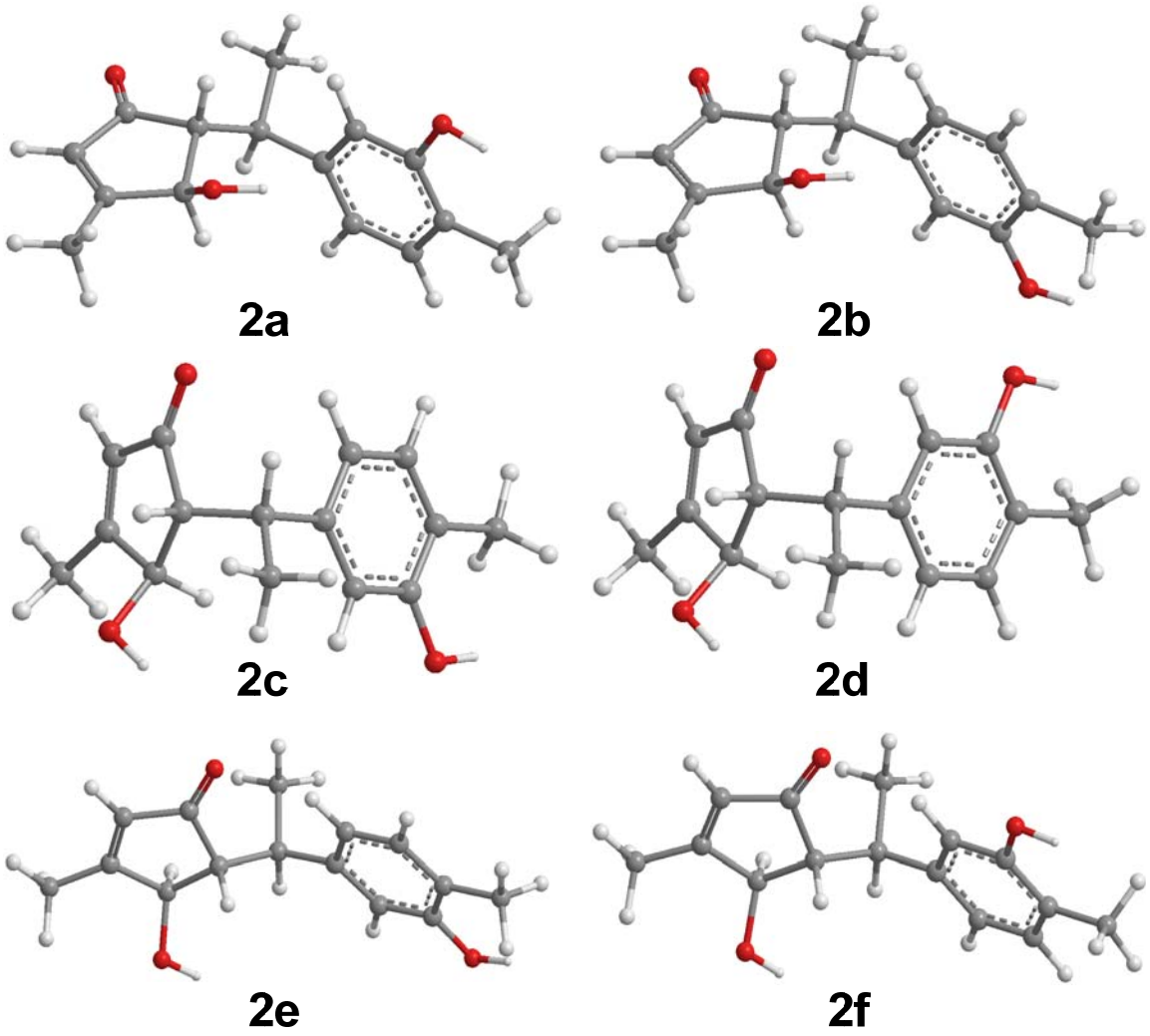


Fig. S2 Optimized geometries of conformers of compound **2** at B3LYP/6-31G** level in the gas phase.

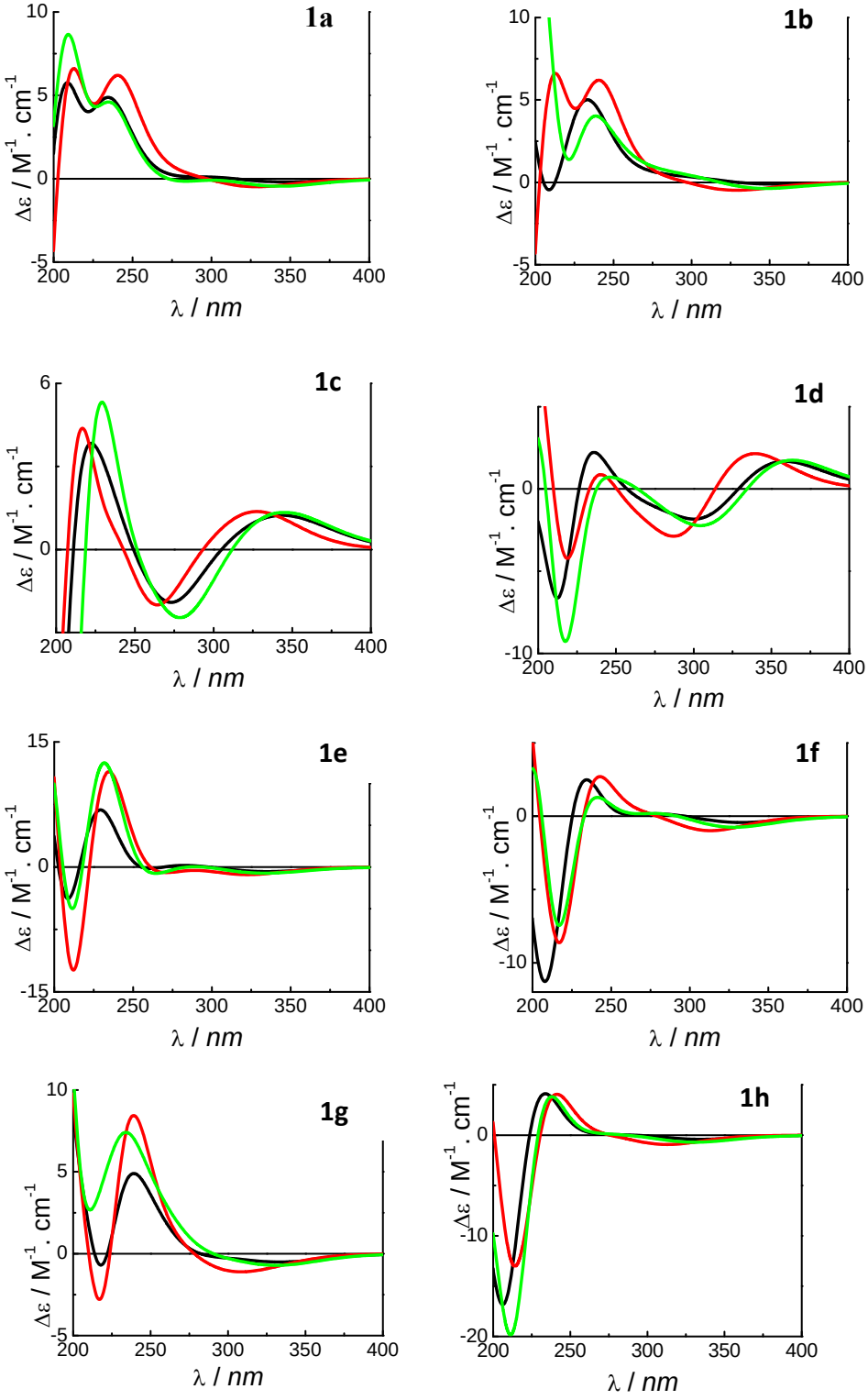


Fig. S3 Calculated ECD spectra of conformers of compound **1** (— at B3LYP/6-31G** level in the gas; — at B3LYP-SCRF/6-31G**// B3LYP/6-31G** level with COSMO model in MeOH; — at B3LYP/6-311++G**//B3LYP/6-31G** level in the gas).

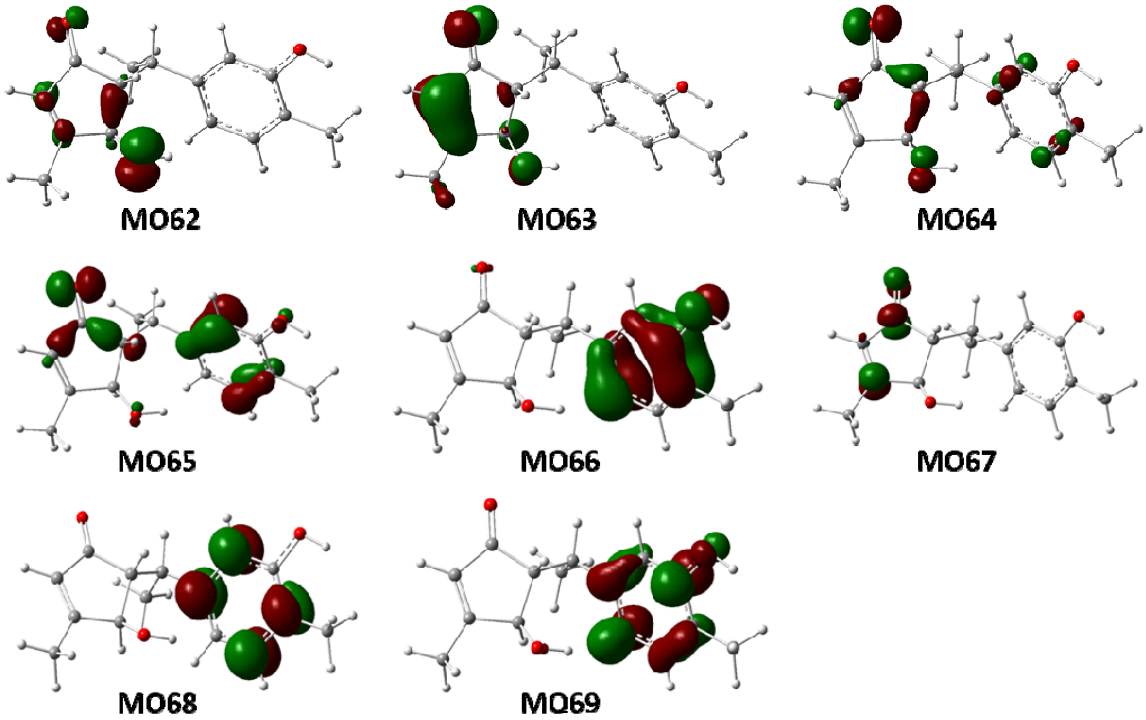


Fig. S4 Some molecular orbitals involved in key transitions in ECD of conformer **1e** of compound **1** at B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with COSMO model in MeOH.

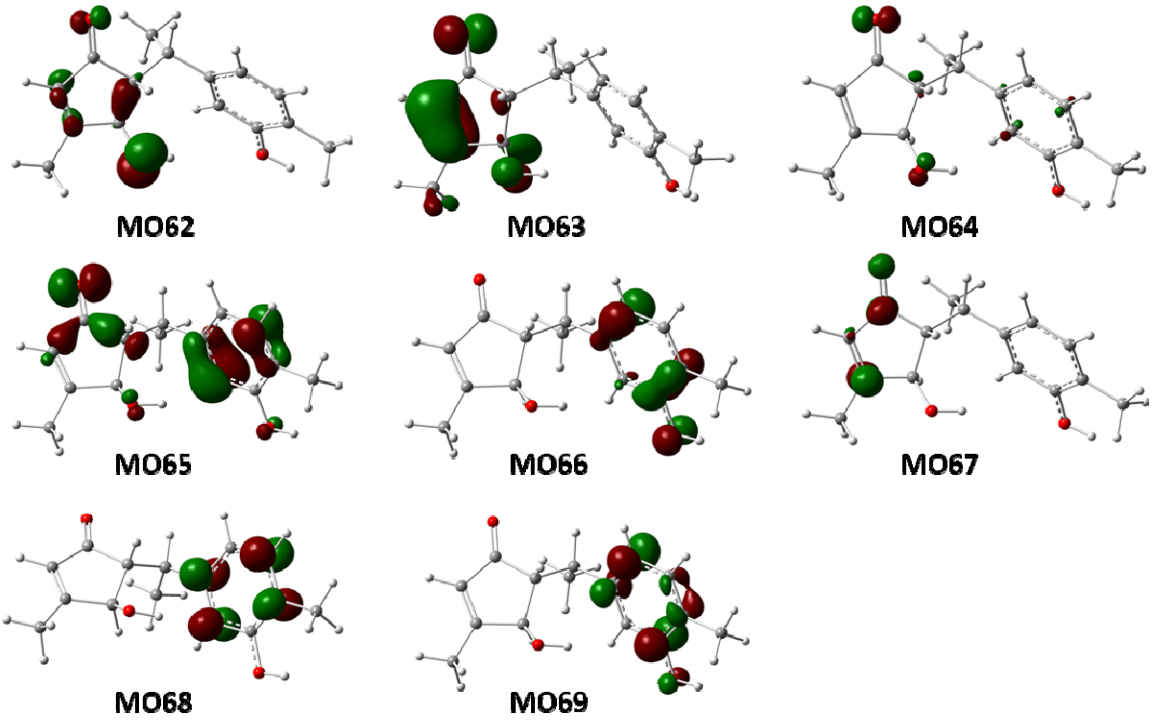


Fig. S5 Some molecular orbitals involved in key transitions in ECD of conformer **1g** of compound **1** at B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with COSMO model in MeOH.

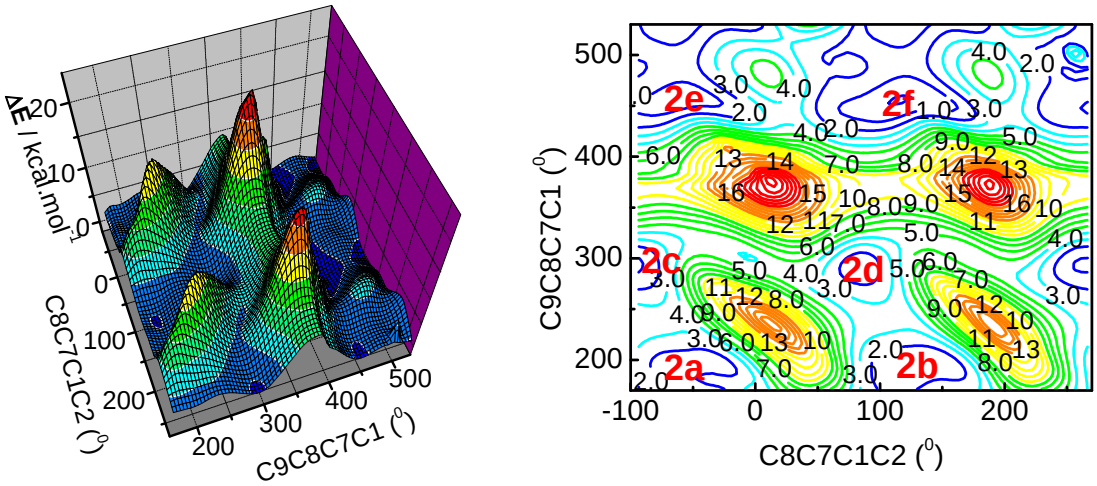


Fig. S6 Potential energy surface of **2** at the AM1 level in the gas phase (left: 3D color map surface; right: contours).

Table S1. Important Dihedral Angles of Optimized **1** at B3LYP/6-31G** Level in the Gas Phase (Degree).

	C9-C8- C7-C1	C8-C7-C1-C2	H-C12-C8-H	H-C8-C7-H
1a	-62	-107	-149	63
1b	-63	73	-148	63
1c	65	-126	-148	-173
1d	65	59	-149	-172
1e	172	-93	-151	-61
1f	154	-152	-143	-78
1g	171	86	-151	-61
1h	157	28	-141	-76

Table S2. Important Thermodynamic Parameters of Compound **1** (au).

Species	In Gas Phase					In Methanol
	E	*E′=E+ZPE*	*H*	*G*	E_{lbs}	E_s
1a	-808.1232657	-807.823207	-807.804111	-807.869262	-808.327477	-808.1440688
1b	-808.1226361	-807.822712	-807.803607	-807.868939	-808.3268484	-808.1441376
1c	-808.1188508	-807.819385	-807.800171	-807.866136	-808.3232327	-808.1425228
1d	-808.1190574	-807.819606	-807.800387	-807.866424	-808.3234687	-808.1425794
1e	-808.1263051	-807.825963	-807.807144	-807.871627	-808.3307051	-808.145427
1f	-808.1211424	-807.821156	-807.802043	-807.867665	-808.3247129	-808.1437582
1g	-808.1263628	-807.826179	-807.807267	-807.872237	-808.3309711	-808.1452658
1h	-808.1214755	-807.821668	-807.802456	-807.868487	-808.3249752	-808.1439052

*E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy in the gas phase at B3LYP/6-31G** level;* E_{lbs}*: single point energy in gas at B3LYP/6-311++G**//B3LYP/6-31G** level;* E_s*: single point energy in methanol solution at B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with COSMO model.*

Table S3. Conformational Analysis of Compound **1**.

Species	In Gas Phase								In Methanol	
	ΔE^a	$P_E\%^b$	ΔE^c	$P_E\%^d$	ΔG^e	$P_G\%^f$	$\Delta E_{lbs}{}^g$	$P_{Elbs}\%^h$	ΔEs^i	$P_{Es}\%^j$
1a	1.94	1.9	1.86	2.3	1.87	2.6	2.19	1.4	0.85	8.5
1b	2.34	1.0	2.18	1.4	2.07	1.9	2.59	0.7	0.81	9.1
1c	4.71	0.0	4.26	0.0	3.83	0.1	4.86	0.0	1.82	1.6
1d	4.58	0.0	4.12	0.1	3.65	0.1	4.71	0.0	1.79	1.7
1e	0.04	46.8	0.14	42.3	0.38	32.2	0.17	42.0	0.00	35.7
1f	3.28	0.2	3.15	0.3	2.87	0.5	3.93	0.1	1.05	6.1
1g	0.00	49.8	0.00	53.2	0.00	61.4	0.00	55.7	0.10	30.1
1h	3.07	0.3	2.83	0.4	2.35	1.2	3.76	0.1	0.95	7.1

[a,c,e] Relative energy, relative energy with *ZPE*, and relative Gibbs free energy at B3LYP/6-31G** level in the gas phase, respectively (kcal/mol). [b,d,f] Conformational distribution calculated by using the respective parameters above at B3LYP/6-31G** level in the gas phase. [g,h] Relative energy (kcal/mol) and conformational distribution in the gas phase at B3LYP/6-311++G**//B3LYP/6-31G** level. [i,j] Relative energy (kcal/mol) and conformational distribution in methanol solution at B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with COSMO model, respectively.

Table S4. Key Transitions, Oscillator Strengths, and Rotatory Strengths in the ECD Spectra of Conformers **1e** and **1g** of **1** in the MeOH with COSMO at B3LYP-SCRF/6-31G**//B3LYP/6-31G** Level

Species	Excited State	ΔE^a (eV)	λ^b (nm)	f^c	$R_{vel}{}^d$	$R_{len}{}^e$
	65→67	3.87	321	0.001	-2.5	-6.6
	66→67	4.23	293	0.000	1.7	1.2
	64→67	4.75	261	0.004	-4.4	-5.2
	66→68	5.10	243	0.051	-12.4	-13.1
1e	63→67	5.30	234	0.050	65.2	68.7
	66→69	5.72	217	0.024	53.5	55.9
	62→67	5.87	211	0.328	-168.3	-169.6
	64→68	6.00	207	0.031	38.4	42.4
	64→69	6.18	200	0.069	12.9	14.4
	65→67	3.86	321	0.002	-0.0	-4.3
	66→67	4.20	295	0.002	-3.6	-4.4
	64→67	4.77	260	0.002	5.2	4.4
1g	66→68	5.07	245	0.066	-2.1	-1.5
	62→67	5.30	234	0.047	53.6	56.3
	66→69	5.74	216	0.107	-113.9	-117.7
	63→67	5.86	212	0.180	113.2	122.9
	64→68	5.96	208	0.060	-33.0	-34.1

[a] Excitation energy. [b] Wavelength. [c] Oscillator strength. [d] Rotatory strength in velocity form (10^{-40} cgs). [e] Rotatory strength in length form (10^{-40} cgs).

Table S5. Important Dihedral Angles of Optimized **2** at B3LYP/6-31G** Level in the Gas Phase (Degree).

Species	C8-C7-C1-C2	C9-C8- C7-C1	H-C12-C8-H	H-C8-C7-H
2a	-61	-165	-149	-168
2b	121	-164	-149	-166
2c	-95	291	-147	-70
2d	86	291	-147	-70
2e	-56	451	-149	85
2f	124	450	-149	85

Table S6. Important Thermodynamic Parameters of Compound **2** (au).

Species	*E*	*E′=E+ZPE*	*H*	*G*
2a	-808.1273381	-807.827180	-807.808325	-807.873026
2b	-808.1275304	-807.827336	-807.808487	-807.873189
2c	-808.1239865	-807.823897	-807.804847	-807.870188
2d	-808.1231758	-807.823392	-807.804281	-807.869848
2e	-808.1217947	-807.821857	-807.802842	-807.867893
2f	-808.1223986	-807.822403	-807.803394	-807.868410

*E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy in the gas phase at B3LYP/6-31G** level.*

Table S7. Conformational Analysis of Compound **2**.

Species	ΔE^a	$P_E\%^b$	ΔE^c	$P_E\%^d$	ΔG^e	$P_G\%^f$
2a	0.12	44.0	0.10	44.7	0.10	43.8
2b	0.00	53.9	0.00	52.7	0.00	52.0
2c	2.22	1.3	2.16	1.4	1.88	2.2
2d	2.73	0.5	2.47	0.8	2.10	1.5
2e	3.60	0.1	3.44	0.2	3.32	0.2
2f	3.22	0.2	3.10	0.3	3.00	0.3

[a,c,e] Relative energy, relative energy with *ZPE*, and relative Gibbs free energy at B3LYP/6-31G** level in the gas phase, respectively (kcal/mol). [b,d,f] Conformational distribution calculated by using the respective parameters above at B3LYP/6-31G** level in the gas phase.

Table S8. Optimized Z-Matrixes of **1** in the Gas Phase (Å).

1a				**1b**			
C	0.793300	-0.695600	-0.563600	C	-0.733900	-0.558600	0.861800
C	1.596000	0.291600	-1.145400	C	-1.439700	-0.803300	-0.322600
C	2.777800	0.717600	-0.534100	C	-2.660100	-0.171100	-0.568100
C	3.199800	0.164600	0.686000	C	-3.219900	0.727800	0.359000
C	2.389500	-0.823100	1.256700	C	-2.506700	0.961500	1.537000
C	1.208600	-1.254000	0.655800	C	-1.287500	0.334100	1.791200
C	-0.484900	-1.135100	-1.271100	C	0.596500	-1.240500	1.165400
C	4.480500	0.624200	1.340600	C	-4.541900	1.401400	0.079500
C	-0.539500	-2.656300	-1.507800	C	0.503800	-2.777200	1.109000
C	-1.779300	-0.616400	-0.593200	C	1.778900	-0.706700	0.316400
O	3.491800	1.691500	-1.183800	O	-3.279200	-0.471100	-1.752400
C	-2.079900	-1.063300	0.850600	C	1.727600	-0.896000	-1.212100
C	-2.709400	0.081600	1.536500	C	2.328600	0.307900	-1.818800
C	-2.674500	1.181300	0.762600	C	2.580000	1.240600	-0.882900
C	-1.933700	0.913300	-0.541100	C	2.097600	0.788000	0.489200
O	-1.871400	-2.166600	1.329700	O	1.305700	-1.872300	-1.810500
C	-3.234900	2.533300	1.055700	C	3.219100	2.577700	-1.063000
H	-2.629400	-0.977000	-1.190700	H	2.683900	-1.239700	0.642800
H	1.323800	0.740800	-2.096400	H	-1.056300	-1.483500	-1.074400
H	2.698100	-1.266800	2.200400	H	-2.921100	1.647200	2.272300
H	0.609200	-2.018500	1.135600	H	-0.767300	0.529700	2.725200
H	-0.476700	-0.653000	-2.257600	H	0.853000	-0.968700	2.197900
H	4.648000	0.093700	2.280800	H	-4.824600	2.059700	0.904300
H	5.360000	0.439100	0.708100	H	-4.509000	2.019500	-0.828500
H	4.465200	1.697600	1.575800	H	-5.358400	0.676800	-0.046100
H	-1.410100	-2.913500	-2.121500	H	1.442900	-3.226900	1.450600
H	0.358400	-2.993200	-2.034600	H	-0.300100	-3.134700	1.759400
H	-0.623800	-3.203300	-0.567700	H	0.319000	-3.128500	0.092900
H	4.296300	1.882700	-0.685500	H	-4.115500	0.007500	-1.808800
H	-3.129600	0.002300	2.533500	H	2.523200	0.386600	-2.883100

H	-3.756300	2.563900	2.014900	H	3.530300	2.749100	-2.095700
H	-3.935700	2.823000	0.264100	H	4.098100	2.659400	-0.413100
H	-2.440100	3.291000	1.070200	H	2.531100	3.382500	-0.771600
H	-0.942100	1.387900	-0.487000	H	1.179100	1.340500	0.740600
O	-2.635200	1.379900	-1.695600	O	3.071600	0.967600	1.520100
H	-2.353800	2.284800	-1.877400	H	2.967800	1.855200	1.884600
1c				**1d**			
C	0.026700	0.041400	-0.040000	C	0.055900	0.007200	-0.031100
C	-0.046100	0.085300	-1.432600	C	-0.102300	0.445100	-1.349300
C	-1.277900	0.060900	-2.088900	C	-1.359600	0.453300	-1.953900
C	-2.482400	-0.006900	-1.368200	C	-2.502400	0.013400	-1.262400
C	-2.394600	-0.046300	0.026900	C	-2.327100	-0.427200	0.052200
C	-1.169400	-0.018600	0.688400	C	-1.075300	-0.433600	0.663700
C	1.379400	0.135400	0.658000	C	1.436600	-0.058400	0.613000
C	-3.810800	-0.037400	-2.085500	C	-3.858300	0.025800	-1.926700
C	1.509400	1.504500	1.359300	C	2.296000	-1.127900	-0.094300
C	1.634200	-1.035100	1.635000	C	2.145200	1.314900	0.651800
O	-1.248200	0.109400	-3.458600	O	-1.419000	0.902400	-3.248300
C	1.734600	-2.427700	0.975600	C	1.462800	2.375300	1.542700
C	2.765500	-3.186700	1.716200	C	2.538100	3.176700	2.166300
C	3.412200	-2.390300	2.583600	C	3.740100	2.624300	1.931400
C	2.916500	-0.951800	2.484400	C	3.603600	1.323900	1.147000
O	1.089200	-2.824900	0.024200	O	0.266200	2.519400	1.707400
C	4.499600	-2.756400	3.539600	C	5.083400	3.119200	2.357100
H	0.808800	-1.091900	2.357500	H	2.178300	1.735500	-0.362500
H	0.854800	0.124400	-2.037100	H	0.741800	0.790100	-1.938900
H	-3.313800	-0.097900	0.605600	H	-3.196800	-0.767800	0.609000
H	-1.152700	-0.043700	1.774100	H	-0.979100	-0.770600	1.691600
H	2.152200	0.083700	-0.120700	H	1.292400	-0.380100	1.653200
H	-4.636700	-0.081100	-1.371600	H	-4.626100	-0.352600	-1.247600
H	-3.969100	0.856200	-2.705300	H	-4.165800	1.038000	-2.224500
H	-3.908800	-0.914000	-2.741200	H	-3.886600	-0.604600	-2.826600

H	2.503800	1.650100	1.791900	H	3.257300	-1.276500	0.406700
H	1.328400	2.310300	0.641900	H	1.766300	-2.085000	-0.105400
H	0.780800	1.603000	2.169400	H	2.505900	-0.845400	-1.130000
H	-2.149500	0.049200	-3.798700	H	-2.335500	0.880500	-3.550300
H	2.951600	-4.240600	1.538600	H	2.336400	4.072600	2.743900
H	4.732700	-3.822800	3.506100	H	5.018400	4.064500	2.900100
H	4.201000	-2.496600	4.562100	H	5.723400	3.264800	1.478900
H	5.419500	-2.196500	3.323300	H	5.587200	2.386200	3.001600
H	3.680700	-0.353400	1.960600	H	3.775500	0.480200	1.836600
O	2.628700	-0.368000	3.755400	O	4.501500	1.238200	0.040400
H	3.452500	-0.036400	4.134500	H	5.358000	0.931600	0.363700
1e				**1f**			
C	0.011700	-0.003800	-0.038700	C	0.109100	-0.156200	-0.083500
C	-0.006300	-1.397100	-0.144800	C	-0.112000	0.072600	-1.447100
C	-1.201900	-2.114200	-0.059200	C	-1.402900	0.198700	-1.958300
C	-2.430100	-1.457600	0.140800	C	-2.527000	0.095000	-1.118500
C	-2.402000	-0.064200	0.242300	C	-2.292400	-0.140100	0.238100
C	-1.211500	0.659900	0.154400	C	-1.003800	-0.263400	0.760400
C	1.344100	0.736600	-0.081400	C	1.551400	-0.239000	0.404300
C	-3.718300	-2.239800	0.232500	C	-3.923300	0.225300	-1.678500
C	1.307900	2.021400	-0.926400	C	2.166000	1.171300	0.534200
C	1.881000	0.964200	1.351800	C	1.791900	-1.112800	1.659000
O	-1.113300	-3.473200	-0.179100	O	-1.516800	0.420500	-3.306300
C	3.315300	1.520700	1.411800	C	3.243500	-1.644600	1.686200
C	3.388200	2.393500	2.598600	C	3.704600	-1.628600	3.085900
C	2.165800	2.573200	3.134200	C	2.797100	-1.028700	3.874700
C	1.091900	1.887600	2.306000	C	1.596500	-0.530700	3.075400
O	4.205900	1.266700	0.619000	O	3.877100	-2.002600	0.709800
C	1.796200	3.351000	4.352300	C	2.858800	-0.822100	5.352500
H	1.921600	-0.009800	1.859300	H	1.147000	-1.999600	1.599100
H	0.913300	-1.953700	-0.299100	H	0.720800	0.149000	-2.140600
H	-3.339800	0.467100	0.386100	H	-3.147100	-0.232500	0.904500

H	-1.246600	1.743400	0.211000	H	-0.872200	-0.463800	1.818000
H	2.076200	0.071300	-0.554000	H	2.120900	-0.755000	-0.379000
H	-4.569000	-1.571300	0.383500	H	-4.669700	0.120400	-0.887500
H	-3.920400	-2.813900	-0.682200	H	-4.091600	1.202600	-2.151900
H	-3.713900	-2.948300	1.072200	H	-4.143400	-0.545800	-2.430200
H	2.312600	2.443900	-1.007800	H	3.211500	1.121200	0.858100
H	0.948300	1.803100	-1.936200	H	2.139900	1.685400	-0.430200
H	0.652100	2.790400	-0.504900	H	1.610200	1.793300	1.244100
H	-1.994600	-3.861700	-0.112000	H	-2.451300	0.463000	-3.544400
H	4.317400	2.826000	2.953200	H	4.658000	-2.044500	3.393300
H	2.671200	3.785600	4.840800	H	3.766900	-1.244200	5.788000
H	1.271700	2.700200	5.059900	H	1.991200	-1.291300	5.830600
H	1.097100	4.157800	4.098900	H	2.821800	0.247000	5.601000
H	0.566200	2.670500	1.732700	H	1.613000	0.568100	3.054600
O	0.175500	1.224100	3.165200	O	0.363400	-0.982300	3.652000
H	-0.512100	0.841000	2.600600	H	0.070400	-0.325700	4.296000
1g				**1h**			
C	0.931000	0.883800	-0.236600	C	-0.034900	0.184600	-0.069500
C	1.538000	-0.211700	-0.864900	C	-0.117300	0.389700	-1.448600
C	2.817400	-0.636700	-0.492200	C	-1.339600	0.265000	-2.116100
C	3.535000	0.018200	0.524400	C	-2.519100	-0.067000	-1.430400
C	2.918600	1.111400	1.140500	C	-2.422400	-0.262300	-0.048100
C	1.644700	1.541500	0.774500	C	-1.210900	-0.140200	0.625300
C	-0.481600	1.337900	-0.588200	C	1.273600	0.255300	0.709500
C	4.917300	-0.446500	0.915300	C	-3.832300	-0.196300	-2.164700
C	-0.778800	1.331100	-2.096900	C	1.804900	-1.163900	1.008000
C	-1.524000	0.550700	0.241300	C	2.364100	1.187200	0.128800
O	3.326000	-1.712400	-1.168900	O	-1.321100	0.482400	-3.470800
C	-2.964700	1.078200	0.113800	C	3.354400	1.618200	1.234500
C	-3.860200	-0.089600	0.211800	C	4.707300	1.630400	0.650600
C	-3.153100	-1.235600	0.196500	C	4.686700	1.139800	-0.600400
C	-1.669300	-0.969200	0.006300	C	3.284200	0.703900	-1.013300

O	-3.278900	2.247200	-0.032500	O	3.048400	1.887500	2.382400
C	-3.659000	-2.634400	0.308600	C	5.829700	1.002000	-1.551300
H	-1.263900	0.655100	1.303900	H	1.886200	2.108900	-0.228500
H	1.050800	-0.742000	-1.676500	H	0.752500	0.673600	-2.030400
H	3.456100	1.638500	1.925000	H	-3.323200	-0.509800	0.508600
H	1.200600	2.397400	1.274900	H	-1.176700	-0.291200	1.701000
H	-0.582900	2.377100	-0.253200	H	1.039900	0.708800	1.681100
H	5.321200	0.171800	1.720200	H	-4.637200	-0.464900	-1.476500
H	4.919600	-1.484300	1.276200	H	-4.130100	0.741900	-2.653900
H	5.626800	-0.386700	0.078500	H	-3.799900	-0.974700	-2.939800
H	-1.759600	1.774300	-2.287200	H	2.726500	-1.127000	1.599100
H	-0.030000	1.918700	-2.636000	H	1.065900	-1.732800	1.578700
H	-0.775500	0.324200	-2.527200	H	2.001500	-1.726800	0.089200
H	4.211800	-1.910800	-0.839900	H	-2.218300	0.403100	-3.817900
H	-4.939300	0.001100	0.271500	H	5.576000	1.986500	1.193600
H	-4.742800	-2.668000	0.440800	H	6.764400	1.373800	-1.126200
H	-3.174700	-3.134800	1.153800	H	5.616000	1.559400	-2.470500
H	-3.394700	-3.213600	-0.585100	H	5.974700	-0.047400	-1.840600
H	-1.416500	-1.221400	-1.037700	H	3.259400	-0.391000	-1.102500
O	-0.919300	-1.788100	0.892500	O	2.908000	1.298300	-2.263200
H	0.015600	-1.639100	0.689600	H	3.126500	0.684000	-2.974600

Table S9. Frequencies of Compound **1** at B3LYP/6-31G** Level in the Gas Phase.

Species	**Frequencies**(cm^{-1})
1a	30 37 53 81 136 143 145 164 177 186 201 216 238 252 254 281 298 309 324 359 403 437 443 484 526 558 574 582 591 636 671 706 712 735 772 835 846 883 892 909 929 959 965 1000 1011 1023 1051 1059 1061 1083 1110 1118 1152 1179 1182 1193 1206 1232 1247 1258 1283 1306 1323 1334 1341 1350 1361 1399 1414 1422 1424 1426 1482 1490 1497 1502 1507 1518 1523 1551 1626 1680 1694 1794 3005 3011 3026 3031 3032 3048 3056 3088 3113 3128 3139 3159 3175 3190 3217 3227 3833 3834
1b	26 34 54 79 133 144 149 164 175 177 203 220 243 253 259 277 300 305 326 359 401 438 470 486 523 537 572 580 589 638 671 705 714 737 768 823 839 887 911 915 932 940 962 1002 1012 1024 1052 1059 1061 1082 1111 1115 1150 1176 1181 1195 1200 1234 1243 1253 1282 1303 1315 1331 1341 1357 1362 1403 1415 1422 1425 1426 1480 1490 1498 1502 1508 1518 1524 1549 1624 1679 1694 1794 3001 3012 3025 3030 3032 3048 3058 3087 3113 3127 3139 3158 3166 3185 3218 3223 3831 3834
1c	21 31 49 76 132 139 143 161 181 184 219 220 231 256 260 267 290 302 320 364 387 410 460 471 535 559 571 583 608 618 662 693 723 746 770 819 836 882 892 911 922 939 960 1000 1009 1042 1048 1059 1064 1074 1097 1127 1149 1176 1181 1188 1201 1211 1247 1256 1280 1305 1316 1324 1334 1343 1369 1390 1413 1423 1425 1429 1481 1491 1500 1502 1504 1513 1520 1552 1630 1683 1699 1813 2976 3010 3026 3029 3049 3051 3056 3085 3121 3126 3129 3139 3169 3189 3198 3218 3823 3834
1d	18 34 48 75 132 135 149 150 171 184 218 222 231 255 264 271 299 302 323 364 387 410 469 485 527 557 566 584 597 616 662 691 724 745 770 819 836 882 893 912 924 939 955 1001 1009 1045 1049 1060 1066 1075 1096 1131 1150 1175 1179 1191 1202 1210 1242 1256 1280 1302 1313 1322 1339 1348 1368 1394 1413 1422 1423 1425 1481 1490 1498 1501 1502 1512 1520 1552 1631 1683 1699 1812 2974 3010 3026 3029 3049 3050 3055 3085 3121 3127 3128 3139 3171 3192 3194 3218 3825 3836
1e	27 49 55 71 139 142 158 172 177 190 204 230 239 255 278 302 310 329 361 383 408 443 472 490 524 553 569 576 611 626 672 702 728 745 770 826 838 874 891 909 937 944 958 988 1010 1020 1052 1057 1060 1100 1110 1143 1149 1175 1179 1192 1198 1235 1237 1255 1284 1307 1319 1330 1336 1357 1373 1394 1422 1422 1427 1429 1479 1486 1493 1502 1512 1518 1520 1549 1623 1678 1689 1801 2968 3015 3035 3040 3049 3057 3061 3100 3115 3129 3136 3141 3173 3195 3199 3222 3775 3832
1f	19 37 60 81 116 142 149 171 177 187 197 212 224 260 266 276 295 302 341 352 382 441 475 503 532 546 574 578 615 641 653 693 724 754 771 838 845 878 889 912 927 955 965 978 1011 1015 1044 1059 1060 1073 1095 1132 1158 1175 1181 1191 1208 1221 1239 1259 1288 1307 1320 1335 1336 1351 1366 1393 1415 1419 1425 1426 1482 1490 1499 1502

	1506 1517 1522 1554 1627 1683 1698 1807 3011 3023 3031 3040 3046 3052 3056 3088 3110 3126 3127 3140 3168 3190 3212 3221 3831 3835
1g	26 40 51 70 135 136 140 168 176 186 207 234 242 253 283 299 318 328 359 381 395 459 474 492 522 546 559 576 604 624 670 701 729 743 770 828 837 875 887 911 935 950 955 988 1010 1017 1053 1060 1062 1099 1110 1144 1153 1173 1176 1192 1200 1231 1235 1250 1282 1299 1313 1332 1343 1356 1368 1396 1419 1423 1428 1430 1479 1484 1492 1501 1513 1517 1520 1549 1625 1677 1688 1801 2972 3014 3035 3040 3051 3055 3060 3100 3117 3130 3136 3140 3173 3193 3205 3221 3781 3832
1h	20 31 57 78 112 138 145 166 171 172 199 206 235 251 263 268 302 303 340 350 383 455 474 500 525 557 560 579 605 642 654 694 727 756 772 824 838 882 912 921 936 946 948 990 1009 1014 1047 1058 1060 1074 1092 1134 1148 1175 1186 1192 1208 1222 1241 1252 1284 1305 1318 1327 1338 1360 1364 1391 1414 1420 1423 1424 1479 1489 1498 1502 1505 1517 1519 1554 1627 1682 1698 1806 3010 3023 3032 3040 3046 3052 3055 3089 3110 3125 3126 3140 3168 3187 3215 3220 3833 3835

Table S10. Optimized Z-Matrixes of **2** in the Gas Phase (Å).

2a				**2b**			
C	0.013161	0.065653	0.007786	C	0.004824	-0.068304	-0.007905
C	0.027529	0.067377	1.410322	C	0.049113	-0.137528	1.386060
C	1.232965	0.044096	2.116539	C	1.263898	-0.073782	2.075478
C	2.469951	0.012365	1.444425	C	2.481802	0.070677	1.388299
C	2.440720	0.009967	0.048125	C	2.426285	0.140774	-0.007730
C	1.241056	0.033994	-0.664383	C	1.218861	0.072584	-0.703281
C	-1.300220	0.109736	-0.766523	C	-1.330693	-0.152473	-0.739507
C	3.766036	-0.013158	2.218490	C	3.788889	0.143413	2.140643
C	-2.188845	-1.122556	-0.465558	C	-1.602049	1.110766	-1.594062
O	1.145309	0.052923	3.481554	O	1.199453	-0.152538	3.439071
C	-3.355906	-1.340565	-1.454844	C	-3.067601	1.278953	-2.052576
C	-3.493924	-2.795508	-1.649031	C	-3.375692	2.719808	-2.002079
C	-2.478270	-3.457809	-1.066119	C	-2.376327	3.405822	-1.418376
C	-1.476313	-2.497741	-0.452626	C	-1.280517	2.474639	-0.933687
O	-4.031993	-0.472465	-1.981587	O	-3.828675	0.386174	-2.387107
C	-2.250445	-4.930630	-1.002674	C	-2.272009	4.876577	-1.192918
H	-2.646038	-1.009743	0.527914	H	-0.997097	1.070183	-2.511104
H	-0.893529	0.108702	1.983849	H	-0.862051	-0.248616	1.966280
H	3.383354	-0.012618	-0.493163	H	3.356162	0.246438	-0.561277
H	1.259916	0.035351	-1.750527	H	1.226022	0.111619	-1.788522
H	4.622634	-0.036984	1.541089	H	4.628621	0.256138	1.451134
H	3.885494	0.874473	2.854888	H	3.822912	0.997594	2.830773
H	3.844326	-0.896706	2.866817	H	3.978176	-0.764396	2.729856
H	2.032420	0.045354	3.862510	H	2.090683	-0.108673	3.807907
H	-4.310581	-3.231454	-2.213960	H	-4.307684	3.128334	-2.377096
H	-3.051610	-5.489473	-1.491617	H	-3.134232	5.414065	-1.594058
H	-2.173194	-5.247008	0.042848	H	-1.357632	5.256852	-1.660210
H	-1.296483	-5.194782	-1.476153	H	-2.185735	5.097544	-0.121639
H	-0.591154	-2.460544	-1.111743	H	-1.369377	2.383479	0.162939
O	-1.101487	-2.970746	0.833001	O	-0.014442	3.023655	-1.271087

H	-0.427481	-2.363790	1.172408	H	0.656851	2.443226	-0.882781
H	-1.043595	0.071743	-1.833519	H	-2.115840	-0.200721	0.026301
C	-2.054880	1.429257	-0.514326	C	-1.425217	-1.437589	-1.585025
H	-2.966622	1.460475	-1.112601	H	-2.403100	-1.498774	-2.065226
H	-2.332300	1.524385	0.541424	H	-0.655853	-1.448932	-2.365290
H	-1.424298	2.286126	-0.770885	H	-1.275498	-2.321443	-0.957307
2c				**2d**			
C	0.044138	0.061534	0.007385	C	0.052263	-0.008793	-0.045292
C	0.061602	0.046685	1.406774	C	0.016539	0.092740	1.350200
C	1.267658	0.067841	2.111582	C	1.193353	0.091030	2.101108
C	2.501592	0.110013	1.441977	C	2.452693	-0.011887	1.482146
C	2.470597	0.128873	0.043940	C	2.475418	-0.114915	0.089263
C	1.273761	0.106716	-0.668007	C	1.304607	-0.115934	-0.668908
C	-1.257993	0.025516	-0.791071	C	-1.258552	0.004924	-0.830221
C	3.798878	0.140976	2.214448	C	3.718804	-0.018233	2.304400
C	-1.659399	-1.403304	-1.237358	C	-1.761545	1.434731	-1.156302
O	1.179434	0.048882	3.479852	O	1.056167	0.188893	3.459456
C	-0.725199	-2.003369	-2.306429	C	-2.235794	2.223451	0.080335
C	-0.596050	-3.441237	-2.019825	C	-1.844670	3.629030	-0.120323
C	-1.200529	-3.752753	-0.858368	C	-1.086949	3.760736	-1.224855
C	-1.770264	-2.520385	-0.175131	C	-0.816884	2.417431	-1.881997
O	-0.212677	-1.382243	-3.222455	O	-2.839553	1.749463	1.027573
C	-1.328640	-5.094042	-0.218154	C	-0.512308	5.009989	-1.803685
H	-2.647816	-1.343134	-1.714477	H	-2.649569	1.341229	-1.797795
H	-0.852416	0.035483	1.990921	H	-0.930080	0.180616	1.872494
H	3.412321	0.167993	-0.497958	H	3.436525	-0.203178	-0.411815
H	1.286231	0.118457	-1.752391	H	1.377128	-0.219352	-1.746454
H	4.654391	0.169996	1.535813	H	4.599027	-0.102733	1.662815
H	3.874853	1.024617	2.863025	H	3.836466	0.903032	2.891697
H	3.924776	-0.745644	2.851093	H	3.752087	-0.862216	3.007297
H	2.068255	0.077969	3.855264	H	1.927888	0.169821	3.873631
H	-0.067098	-4.124399	-2.674850	H	-2.139098	4.422298	0.557834

H	-0.875392	-5.881599	-0.824255	H	-0.791699	5.893914	-1.225956
H	-2.385703	-5.327084	-0.053847	H	-0.853570	5.130361	-2.837192
H	-0.854056	-5.094951	0.771055	H	0.582573	4.948150	-1.843712
H	-1.135258	-2.285757	0.693350	H	0.234320	2.148631	-1.693391
O	-3.099596	-2.810536	0.256526	O	-1.042925	2.542269	-3.287045
H	-3.369006	-2.118076	0.872577	H	-0.684727	1.754634	-3.714837
H	-1.062744	0.560032	-1.728136	H	-2.026330	-0.410343	-0.166547
C	-2.426367	0.738310	-0.091261	C	-1.220492	-0.870395	-2.093916
H	-3.293718	0.792772	-0.756638	H	-2.213308	-0.921629	-2.552261
H	-2.750285	0.224015	0.821298	H	-0.530960	-0.484905	-2.854618
H	-2.150795	1.757400	0.194808	H	-0.900641	-1.889423	-1.857157
2e				**2f**			
C	0.064788	-0.021770	0.003859	C	0.037146	0.105133	0.148889
C	0.037113	0.001903	1.402041	C	0.207597	-0.180930	1.506498
C	1.227076	0.017701	2.132352	C	1.481309	-0.240212	2.075786
C	2.480884	0.013683	1.493179	C	2.630005	-0.012362	1.300034
C	2.490106	-0.007025	0.096189	C	2.442646	0.273007	-0.056789
C	1.308303	-0.025878	-0.642442	C	1.176744	0.332966	-0.636207
C	-1.213635	-0.015623	-0.827102	C	-1.371805	0.132653	-0.433560
C	3.758044	0.029393	2.298681	C	4.005328	-0.074992	1.920794
C	-2.200695	-1.166258	-0.483391	C	-1.736487	1.466553	-1.144367
O	1.110107	0.036006	3.497208	O	1.546282	-0.525641	3.415677
C	-3.273682	-0.910281	0.596011	C	-1.440752	1.596673	-2.653779
C	-4.508718	-1.582151	0.151068	C	-2.557046	2.350589	-3.253388
C	-4.379099	-2.052909	-1.102434	C	-3.547310	2.539892	-2.362686
C	-3.030441	-1.678390	-1.685670	C	-3.232215	1.853864	-1.047675
O	-3.132958	-0.280858	1.632170	O	-0.463527	1.170195	-3.248544
C	-5.372059	-2.817175	-1.911942	C	-4.832316	3.274323	-2.548586
H	-1.626087	-2.032882	-0.130315	H	-1.187285	2.286572	-0.662881
H	-0.907072	0.007058	1.936786	H	-0.646601	-0.366311	2.151930
H	3.446630	-0.011675	-0.421059	H	3.318854	0.453806	-0.675103
H	1.355093	-0.041959	-1.728392	H	1.065243	0.558555	-1.691257

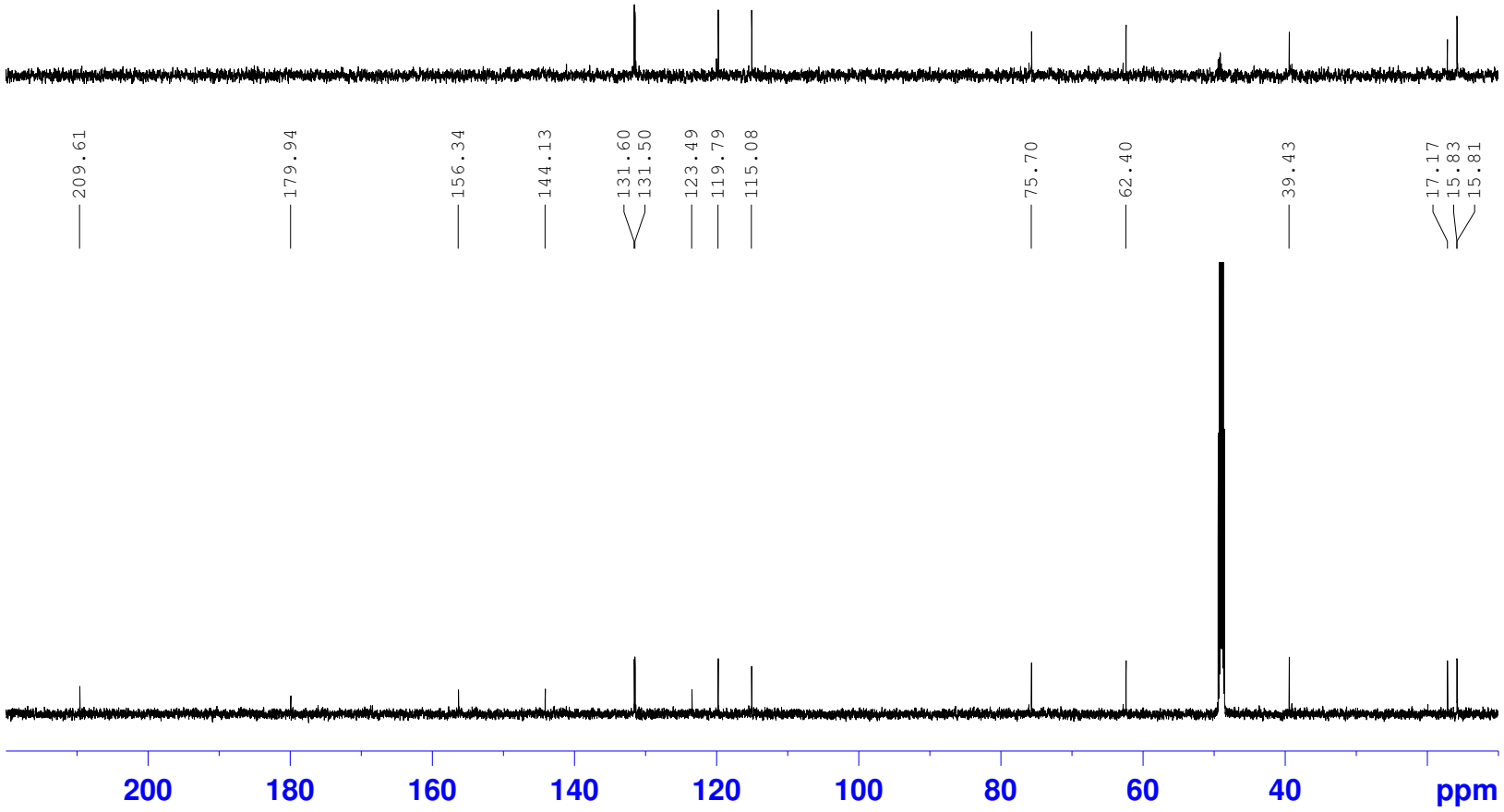
H	4.631773	0.022295	1.642675	H	4.776717	0.131302	1.175209
H	3.838998	0.924759	2.930746	H	4.132481	0.662304	2.725847
H	3.844067	-0.846108	2.957274	H	4.225533	-1.064906	2.344348
H	1.989821	0.051615	3.894142	H	2.470948	-0.540882	3.692580
H	-5.389419	-1.651990	0.780043	H	-2.546016	2.677988	-4.287235
H	-6.291364	-3.009158	-1.354162	H	-4.910070	3.714044	-3.545403
H	-4.936017	-3.770218	-2.229318	H	-4.918679	4.065418	-1.796348
H	-5.625107	-2.271601	-2.829778	H	-5.686982	2.604095	-2.392267
H	-3.185082	-0.857176	-2.408312	H	-3.849256	0.939948	-0.981175
O	-2.480218	-2.807795	-2.355464	O	-3.556162	2.730059	0.026163
H	-1.671282	-2.524328	-2.800970	H	-3.445394	2.242501	0.852753
H	-0.891778	-0.211025	-1.861038	H	-2.050482	0.071152	0.430095
C	-1.889187	1.370572	-0.825602	C	-1.651460	-1.104713	-1.310141
H	-2.775800	1.381351	-1.471268	H	-2.684859	-1.105565	-1.677729
H	-2.201301	1.651260	0.182365	H	-0.985273	-1.128333	-2.174896
H	-1.195060	2.130414	-1.195750	H	-1.499898	-2.020785	-0.732324

Table S11. Frequencies of Compound **2** at B3LYP/6-31G** Level in the Gas Phase.

Species	**Frequencies**(cm^{-1})
2a	34 39 55 59 136 140 153 162 171 194 212 247 259 268 286 298 307 321 365 390 405 428 474 480 515 555 573 584 596 622 660 695 728 749 769 827 840 885 889 913 935 948 960 1001 1012 1026 1055 1060 1064 1107 1117 1129 1150 1173 1184 1193 1199 1225 1239 1246 1261 1303 1313 1328 1343 1353 1365 1392 1419 1421 1427 1430 1479 1485 1493 1503 1507 1519 1527 1549 1626 1677 1695 1796 2962 3015 3027 3039 3041 3048 3062 3101 3113 3131 3141 3160 3174 3193 3199 3223 3775 3834
2b	30 38 60 63 139 141 151 163 177 191 214 246 256 265 283 297 302 320 365 395 409 427 448 477 534 561 575 583 602 624 662 695 726 748 770 827 840 885 891 913 938 945 960 997 1011 1025 1055 1059 1060 1106 1116 1126 1150 1175 1185 1192 1201 1232 1241 1254 1261 1308 1319 1329 1336 1356 1367 1390 1415 1420 1425 1435 1480 1485 1493 1502 1507 1519 1525 1549 1624 1677 1695 1796 2967 3015 3029 3040 3041 3048 3062 3101 3113 3130 3141 3157 3174 3195 3197 3223 3770 3833
2c	25 35 51 76 135 139 142 150 174 187 220 231 254 265 275 282 303 309 328 359 400 443 464 491 537 541 559 579 602 614 674 707 717 736 772 837 848 884 886 909 930 961 964 987 1012 1016 1056 1059 1066 1091 1103 1130 1157 1173 1184 1199 1207 1228 1236 1250 1265 1304 1319 1331 1345 1351 1360 1404 1419 1422 1426 1430 1481 1485 1493 1502 1508 1518 1521 1552 1627 1681 1693 1799 3004 3014 3033 3040 3042 3056 3060 3102 3102 3126 3130 3142 3176 3205 3216 3225 3829 3836
2d	23 34 53 74 135 136 141 144 175 190 215 238 250 260 271 274 298 305 325 360 401 435 456 488 532 555 566 580 606 614 673 707 717 736 770 824 843 884 908 910 927 942 963 987 1009 1015 1054 1059 1063 1089 1101 1128 1152 1173 1184 1196 1204 1226 1234 1251 1266 1308 1326 1331 1344 1346 1361 1399 1419 1421 1424 1428 1480 1485 1493 1502 1507 1515 1517 1551 1625 1680 1693 1801 2999 3013 3030 3035 3040 3054 3059 3099 3100 3123 3128 3141 3172 3203 3216 3224 3830 3834
2e	29 37 57 82 133 141 151 159 174 181 205 234 254 267 267 273 298 305 339 357 388 438 473 495 532 539 572 576 600 647 676 706 730 745 770 819 831 871 908 916 932 951 958 1007 1012 1038 1050 1059 1072 1082 1113 1128 1150 1175 1186 1193 1206 1220 1230 1250 1275 1305 1318 1331 1351 1354 1365 1397 1421 1424 1425 1429 1481 1485 1493 1502 1509 1520 1521 1551 1626 1680 1696 1793 2957 2995 3012 3040 3041 3049 3057 3101 3111 3127 3142 3150 3166 3184 3211 3224 3819 3834
2f	28 40 56 84 138 143 148 161 175 184 207 223 252 263 270 272 299 305 338 356 387 432 471 484 526 555 572 576 610 646 677 707 729 743 773 830 856 868 883 907 914 961 982 1004 1011 1035 1049 1059 1069 1085 1114 1128 1150 1175 1185 1191 1206 1220 1229 1253 1275 1306 1325 1332 1340 1351 1365 1393 1421 1423 1424 1429 1484 1485 1493 1502

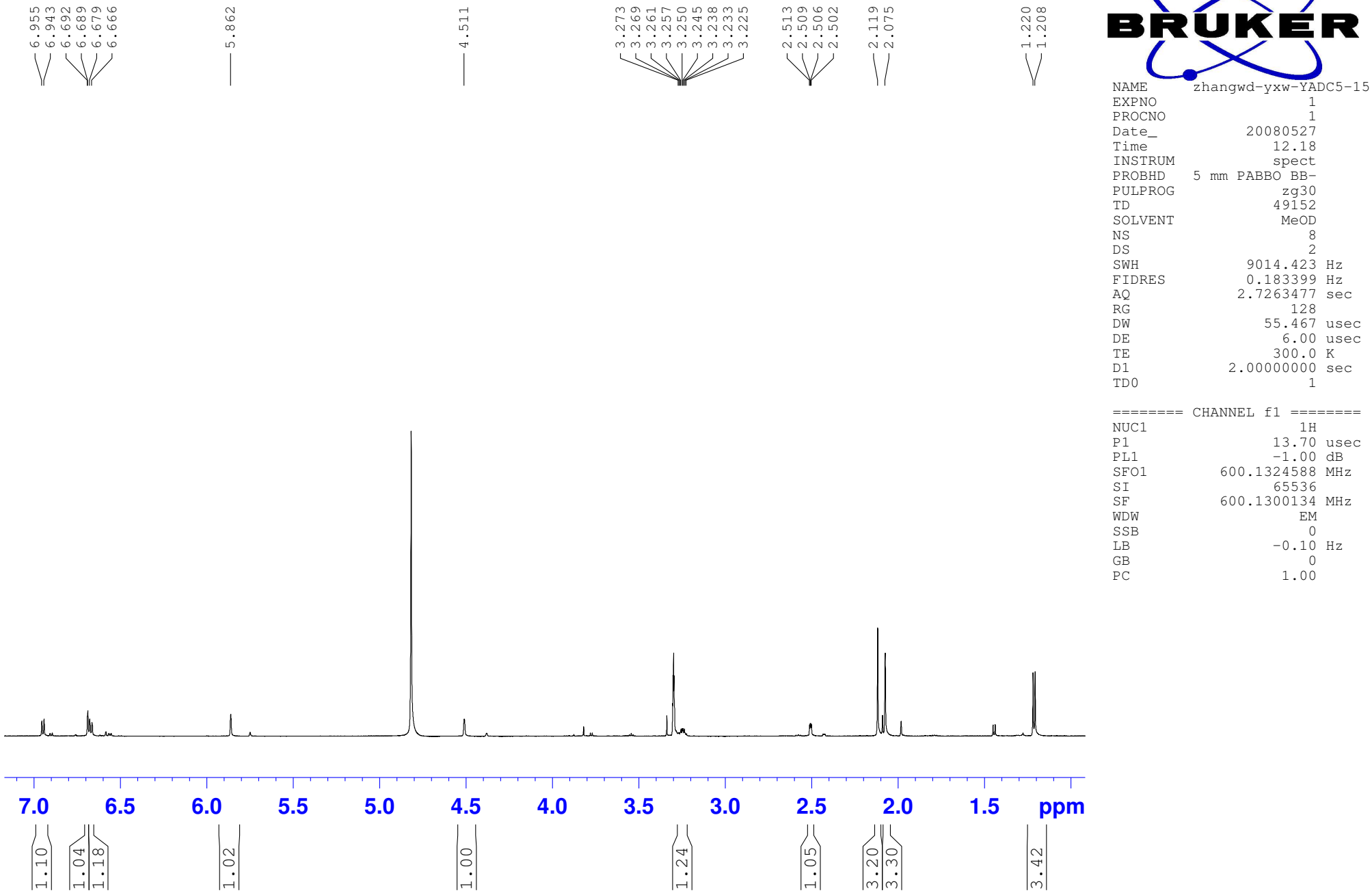
	1510 1519 1522 1552 1629 1682 1696 1790 2957 2997 3011 3040 3042 3048 3056 3101 3112 3128 3142 3150 3173 3187 3214 3224 3819 3834

Fig. S7



NAME	zhangwd-yxw-YADC5-15
EXPNO	2
PROCNO	1
Date_	20080527
Time	12.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	262
DS	2
SWH	45454.547 Hz
FIDRES	0.693581 Hz
AQ	0.7209460 sec
RG	32768
DW	11.000 usec
DE	6.00 usec
TE	300.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	2.00 dB
SFO1	150.9178990 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	14.00 dB
PL13	14.00 dB
SFO2	600.1324005 MHz
SI	65536
SF	150.9025976 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40

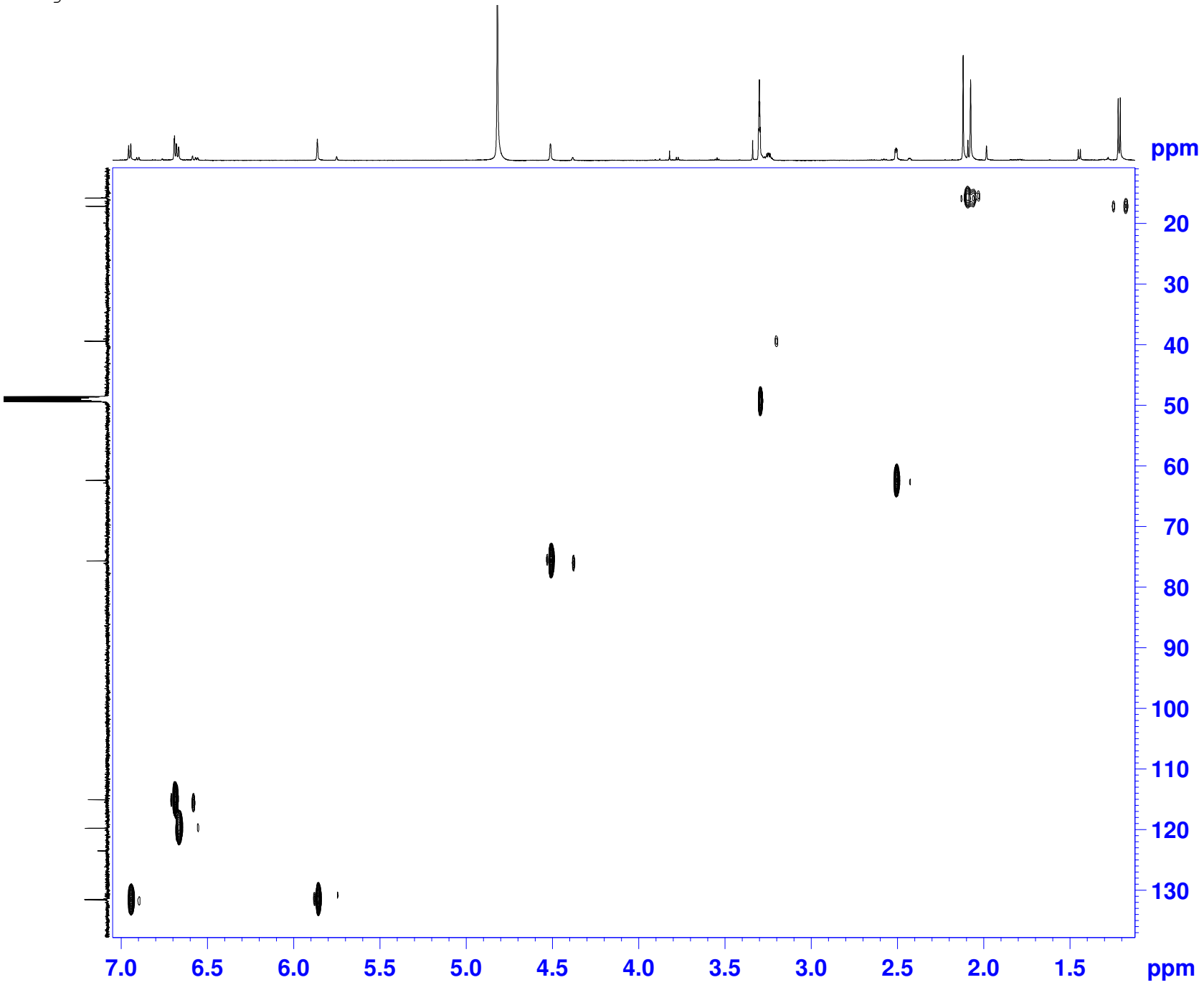
Fig. S8



BRUKER

NAME	zhangwd-yxw-YADC5-15
EXPNO	1
PROCNO	1
Date_	20080527
Time	12.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	49152
SOLVENT	MeOD
NS	8
DS	2
SWH	9014.423 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	128
DW	55.467 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.70 usec
PL1	-1.00 dB
SFO1	600.1324588 MHz
SI	65536
SF	600.1300134 MHz
WDW	EM
SSB	0
LB	-0.10 Hz
GB	0
PC	1.00

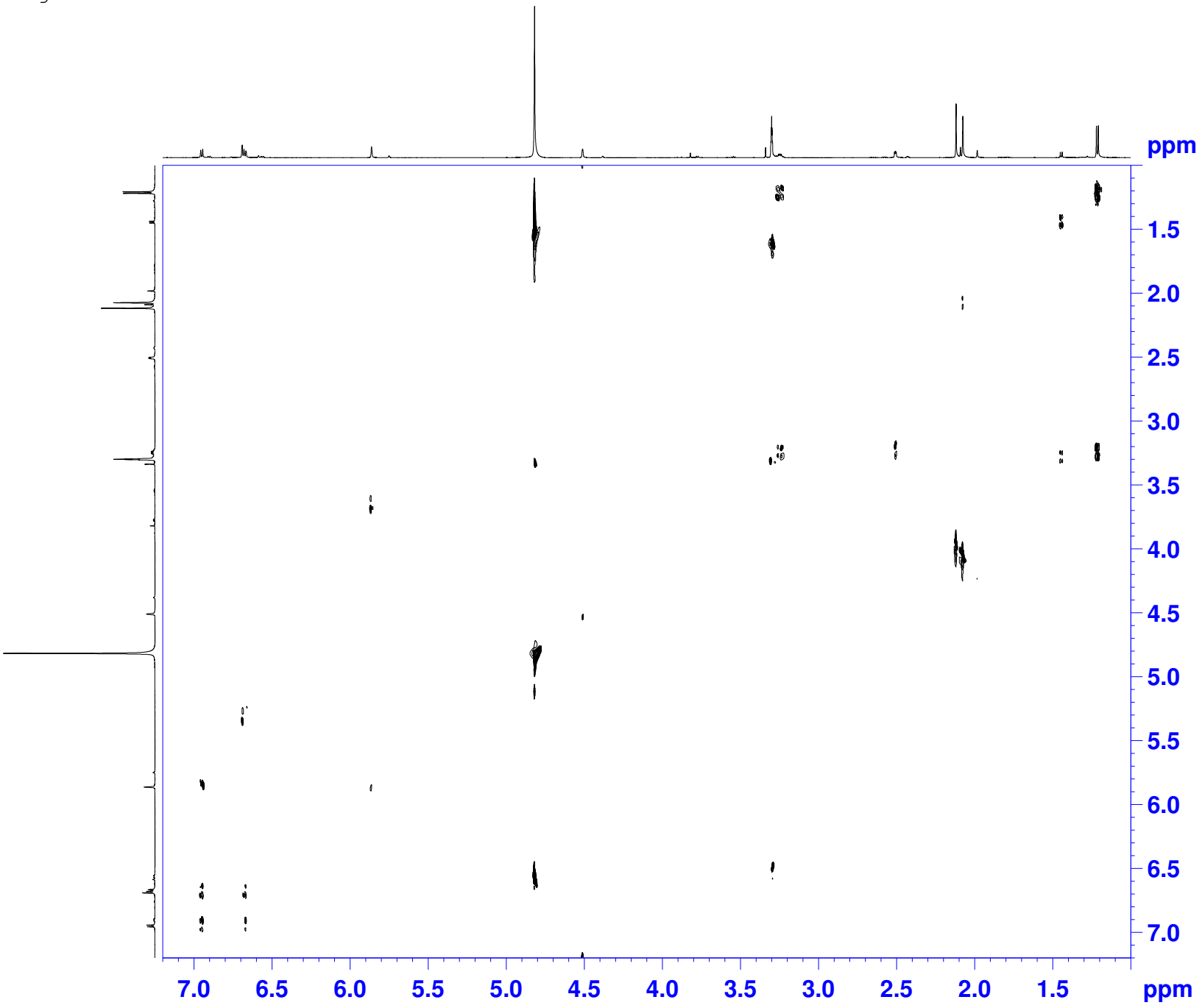
Fig. S9



BRUKER

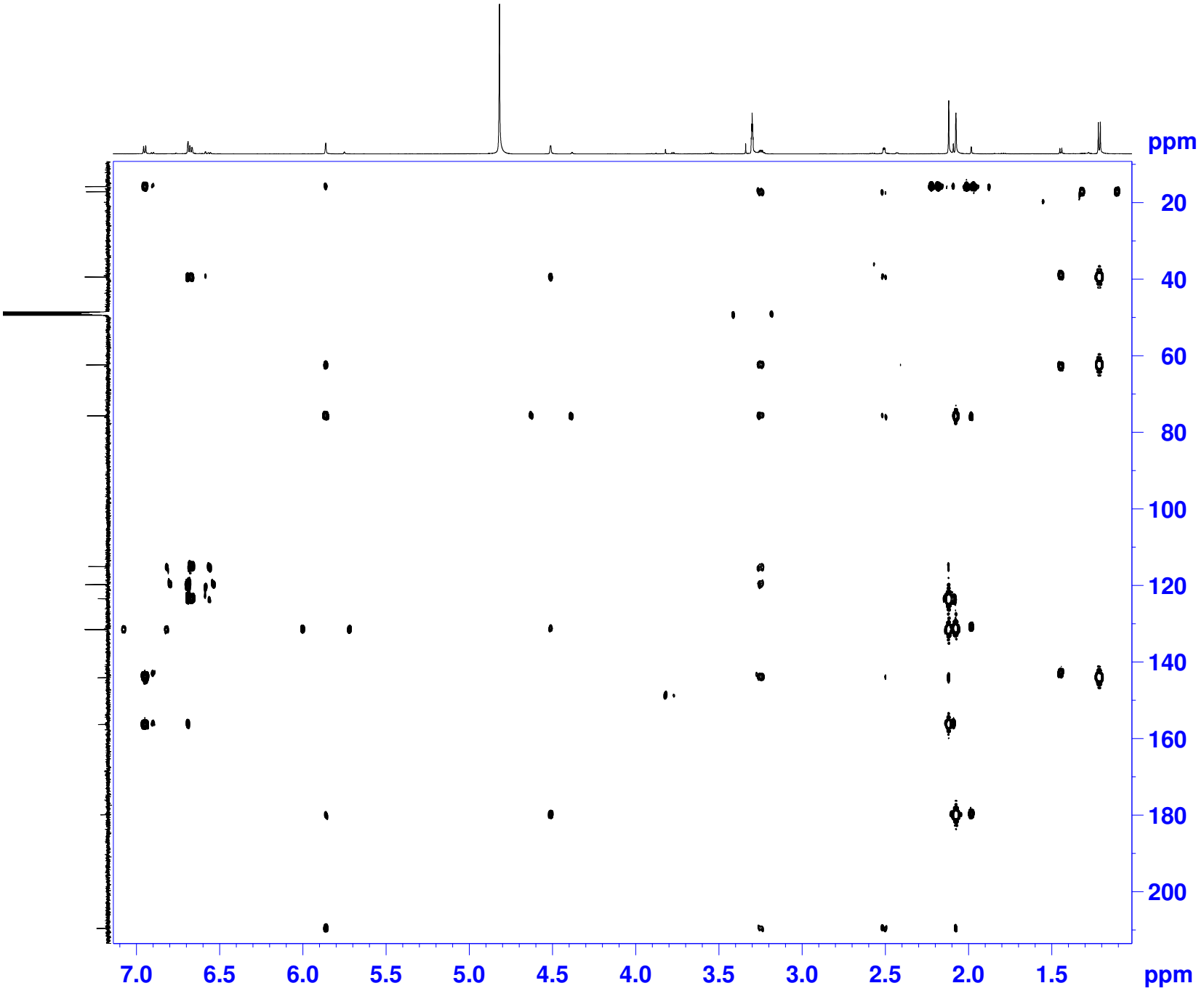
NAME	zhangwd-yxw-YADC5-15
EXPNO	5
PROCNO	1
Date_	20080527
Time	12.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	hsqcetgpsi2
TD	1024
SOLVENT	MeOD
NS	8
DS	16
SWH	4795.396 Hz
FIDRES	4.683004 Hz
AQ	0.1068191 sec
RG	2050
DW	104.267 usec
DE	6.00 usec
TE	300.0 K
CNST2	145.0000000
d0	0.00000300 sec
D1	1.50000000 sec
d4	0.00172414 sec
d11	0.03000000 sec
d13	0.00000400 sec
D16	0.00010000 sec
D24	0.00086207 sec
DELTA	0.00118340 sec
DELTA1	0.00110800 sec
DELTA2	0.00026207 sec
DELTA3	0.00062414 sec
IN0	0.00001380 sec
ST1CNT	0
ZGOPTNS	
======== CHANNEL f1 ========	
NUC1	1H
P1	13.70 usec
p2	27.40 usec
P28	1.00 usec
PL1	-1.00 dB
SFO1	600.1324588 MHz
======== CHANNEL f2 ========	
CPDPRG2	garp
NUC2	13C
P3	9.80 usec
p4	19.60 usec
PCPD2	75.00 usec
PL2	2.00 dB
PL12	19.60 dB
SFO2	150.9178990 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPNAM3	SINE.100
GPNAM4	SINE.100
GPZ1	80.00 %
GPZ2	20.10 %
GPZ3	11.00 %
GPZ4	-5.00 %
P16	1000.00 usec
P19	500.00 usec
ND0	2
TD	128
SFO1	150.9179 MHz
FIDRES	283.061584 Hz
SW	240.077 ppm
FnMODE	Echo-Antiecho
SI	2048
SF	600.1300134 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	150.9025976 MHz
WDW	QSINE
SSB	0
LB	0.00 Hz
GB	0

Fig. S10



NAME	zhangwd-yxw-YADC5-15
EXPNO	4
PROCNO	1
Date_	20080527
Time	12.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	cosygpmfph
TD	2048
SOLVENT	MeOD
NS	1
DS	16
SWH	4795.396 Hz
FIDRES	2.341502 Hz
AQ	0.2135881 sec
RG	2050
DW	104.267 usec
DE	6.00 usec
TE	299.9 K
d0	0.00008683 sec
D1	2.00000000 sec
d13	0.00000400 sec
D16	0.00010000 sec
d20	0.00110400 sec
IN0	0.00020855 sec
ST1CNT	0
======== CHANNEL f1 ========	
NUC1	1H
P1	13.70 usec
p2	27.40 usec
PL1	-1.00 dB
SFO1	600.1324588 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	10.00 %
GPZ2	20.00 %
P16	1000.00 usec
ND0	1
TD	128
SFO1	600.1325 MHz
FIDRES	37.461040 Hz
SW	7.990 ppm
FnMODE	States-TPPI
SI	2048
SF	600.1300134 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	2048
MC2	States-TPPI
SF	600.1300134 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

Fig. S11



BRUKER

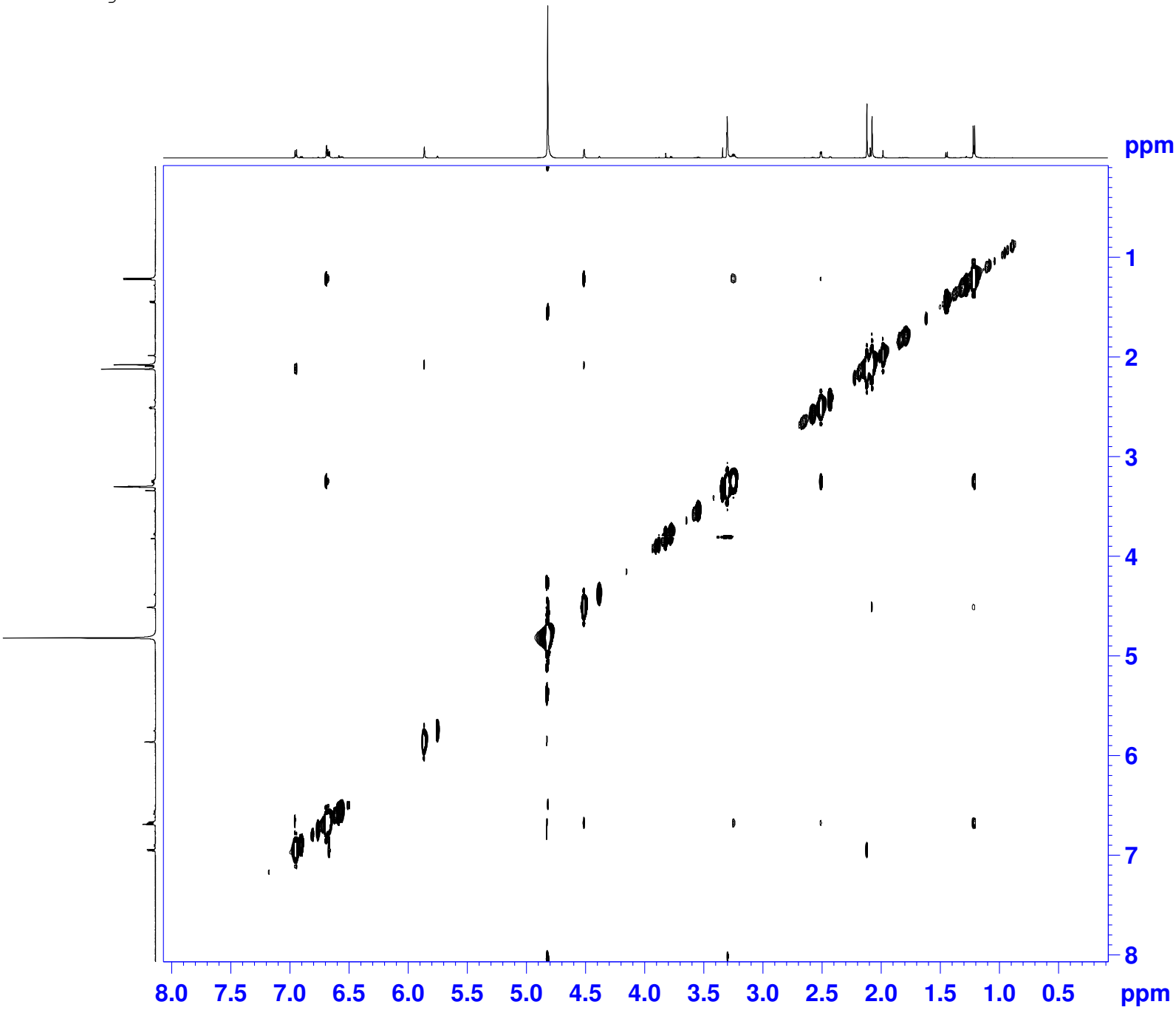
```
NAME          zhangwd-yxw-YADC5-15
EXPNO                            6
PROCNO                           1
Date_                     20080527
Time                         13.18
INSTRUM                      spect
PROBHD    5 mm PABBO BB-
PULPROG     hmbcgplpndqf
TD                            2048
SOLVENT                       MeOD
NS                              16
DS                              16
SWH                     4795.396 Hz
FIDRES                  2.341502 Hz
AQ                     0.2135881 sec
RG                           2050
DW                        104.267 usec
DE                          6.00 usec
TE                         300.0 K
CNST2                145.0000000
CNST13                 8.0000000
d0                    0.00000300 sec
D1                    1.50000000 sec
d2                    0.00344828 sec
d6                    0.06250000 sec
D16                   0.00010000 sec
IN0                   0.00001380 sec

======== CHANNEL f1 ========
NUC1                          1H
P1                         13.70 usec
p2                         27.40 usec
PL1                        -1.00 dB
SFO1                600.1324588 MHz

======== CHANNEL f2 ========
NUC2                         13C
P3                          9.80 usec
PL2                         2.00 dB
SFO2                150.9178990 MHz

====== GRADIENT CHANNEL =====
GPNAM1                  SINE.100
GPNAM2                  SINE.100
GPNAM3                  SINE.100
GPZ1                       50.00 %
GPZ2                       30.00 %
GPZ3                       40.10 %
P16                      1000.00 usec
ND0                            2
TD                           128
SFO1                 150.9179 MHz
FIDRES               283.061584 Hz
SW                      240.077 ppm
FnMODE                       QF
SI                         2048
SF                  600.1300134 MHz
WDW                        SINE
SSB                           2
LB                         0.00 Hz
GB                            0
PC                         1.40
SI                         1024
MC2                          QF
SF                  150.9025976 MHz
WDW                        SINE
SSB                           0
LB                         0.00 Hz
GB                            0
```

Fig. S12



NAME	zhangwd-yxw-YADC5-15
EXPNO	7
PROCNO	1
Date_	20080527
Time	14.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	noesyph
TD	2048
SOLVENT	MeOD
NS	8
DS	16
SWH	4795.396 Hz
FIDRES	2.341502 Hz
AQ	0.2135881 sec
RG	322
DW	104.267 usec
DE	6.00 usec
TE	300.0 K
d0	0.00008683 sec
D1	2.00000000 sec
D8	0.80000001 sec
IN0	0.00020855 sec
ST1CNT	0
======== CHANNEL f1 ========	
NUC1	1H
P1	13.70 usec
PL1	-1.00 dB
SFO1	600.1324588 MHz
ND0	1
TD	128
SFO1	600.1325 MHz
FIDRES	37.461040 Hz
SW	7.990 ppm
FnMODE	States-TPPI
SI	2048
SF	600.1300134 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	2048
MC2	States-TPPI
SF	600.1300134 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0