

Supplementary Information

Incarviate A, a structurally unique natural product hybrid with a new carbon skeleton from *Incarvillea delavayi*, and its absolute configuration via calculated electronic circular dichroic spectra†

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Complete citation of reference 19

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Figure S1 The structure of clerindicin F

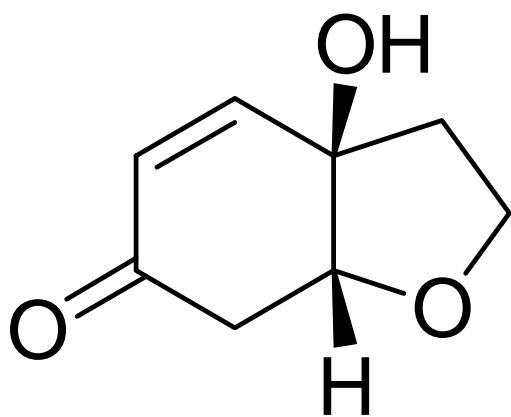
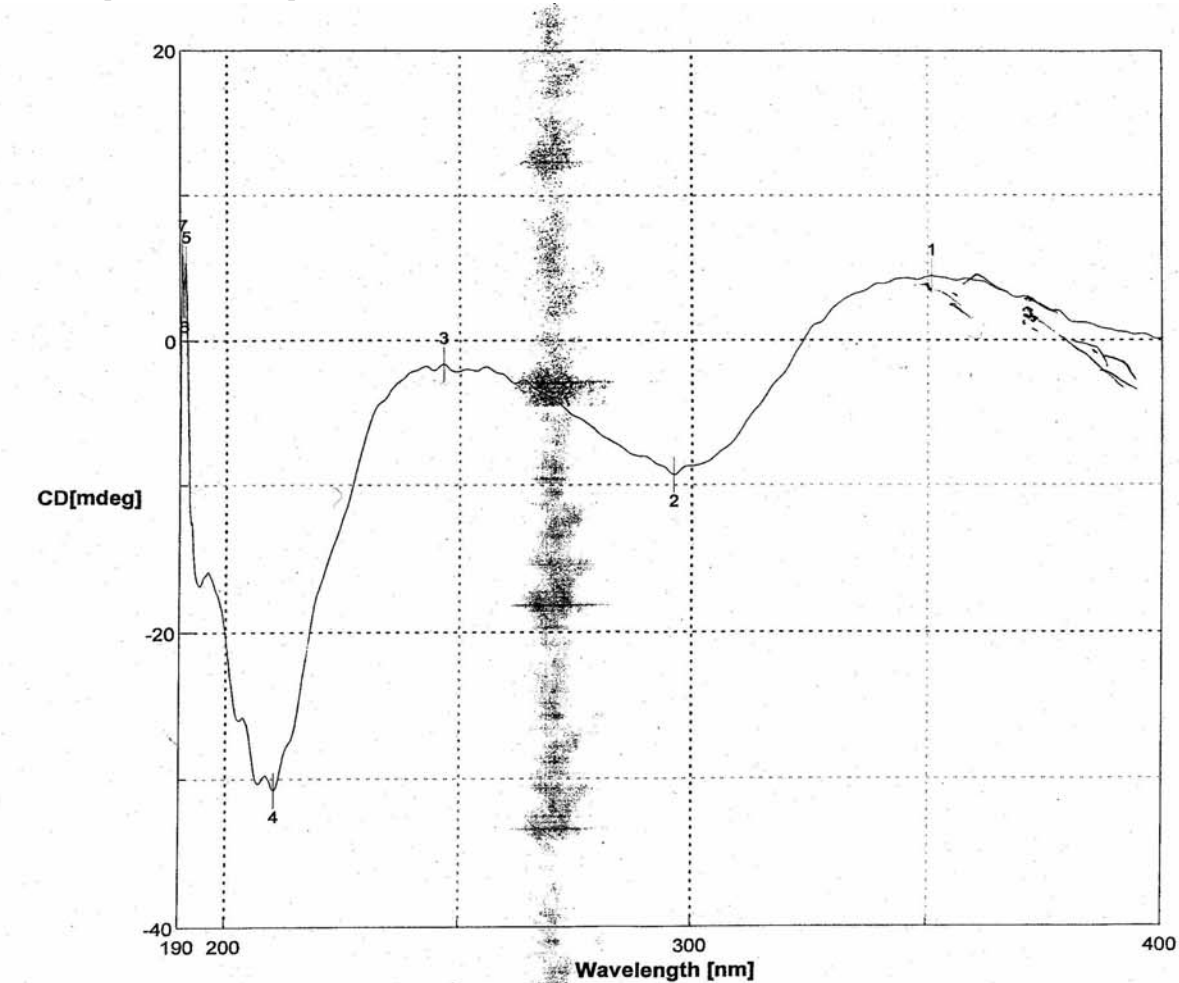


Figure S2 Experimental CD spectrum of incarvatonone A (1)



Date/Time 10/18/07 10:41AM
Operator feng
File Name LID-22 s
Sample Name LID-22
Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	350.9	4.39227	2	296.2	-9.29192	3	246.5	-1.65228
4	210.4	-30.7474	5	191.3	5.31832	6	190.9	2.77369
7	190.6	6.10821						

Figure S3 150 MHz ¹³C and DEPT NMR Spectra of incarviateone A (1) in CDCl₃

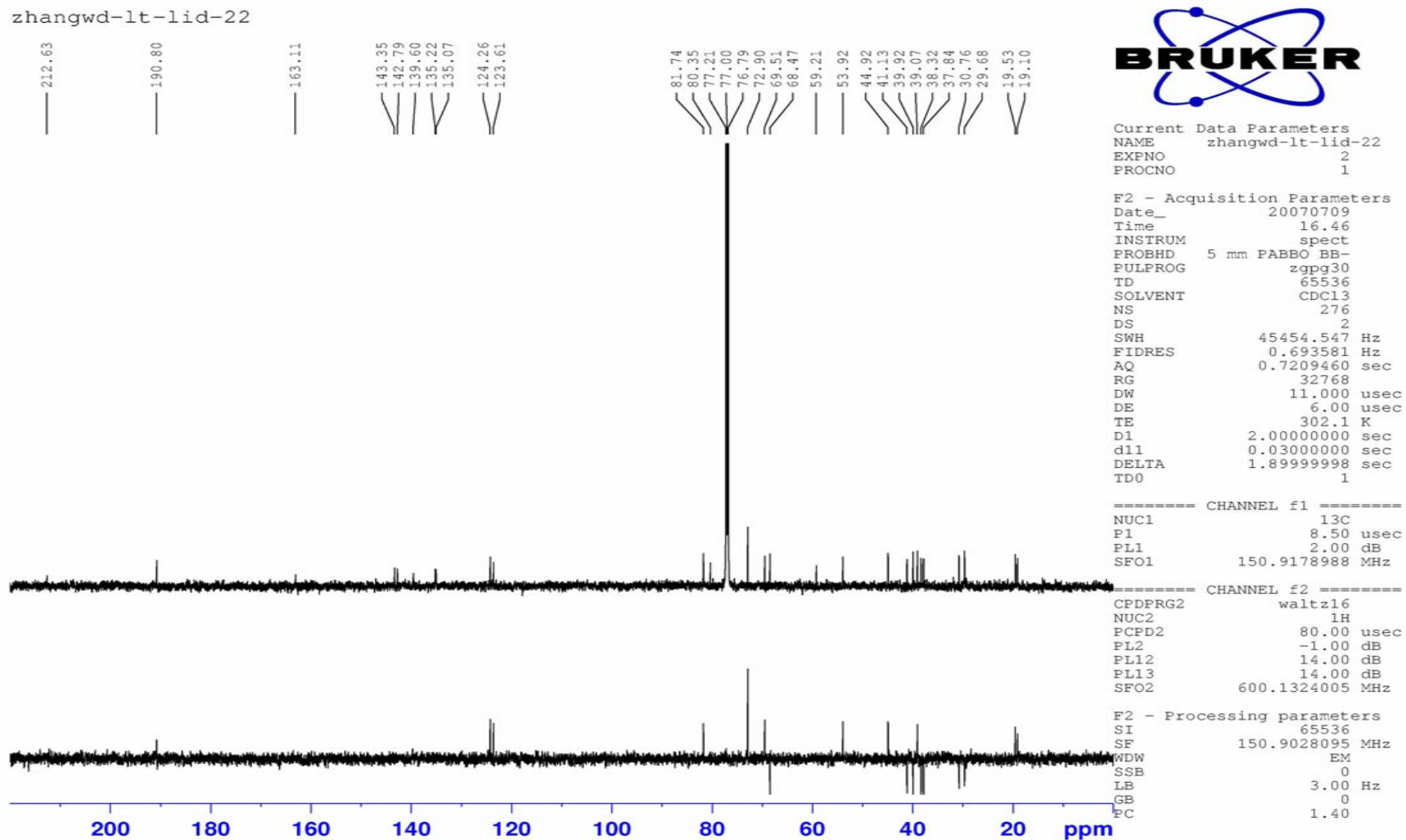


Figure S4 600 MHz ^1H NMR Spectrum of incarviateone A (**1**) in CDCl_3

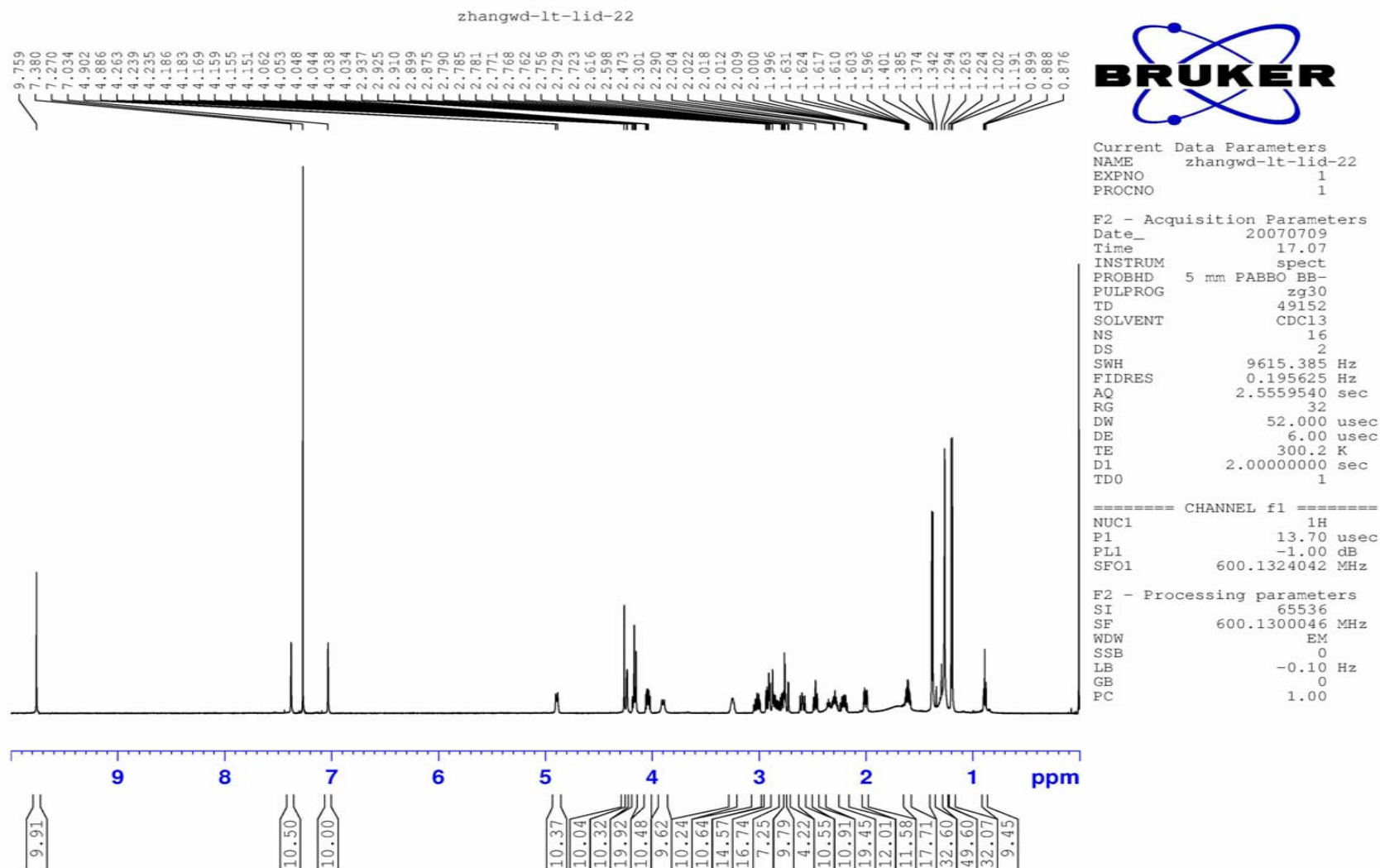


Figure S5 HSQC NMR Spectrum of incarviateone A (1) in CDCl₃

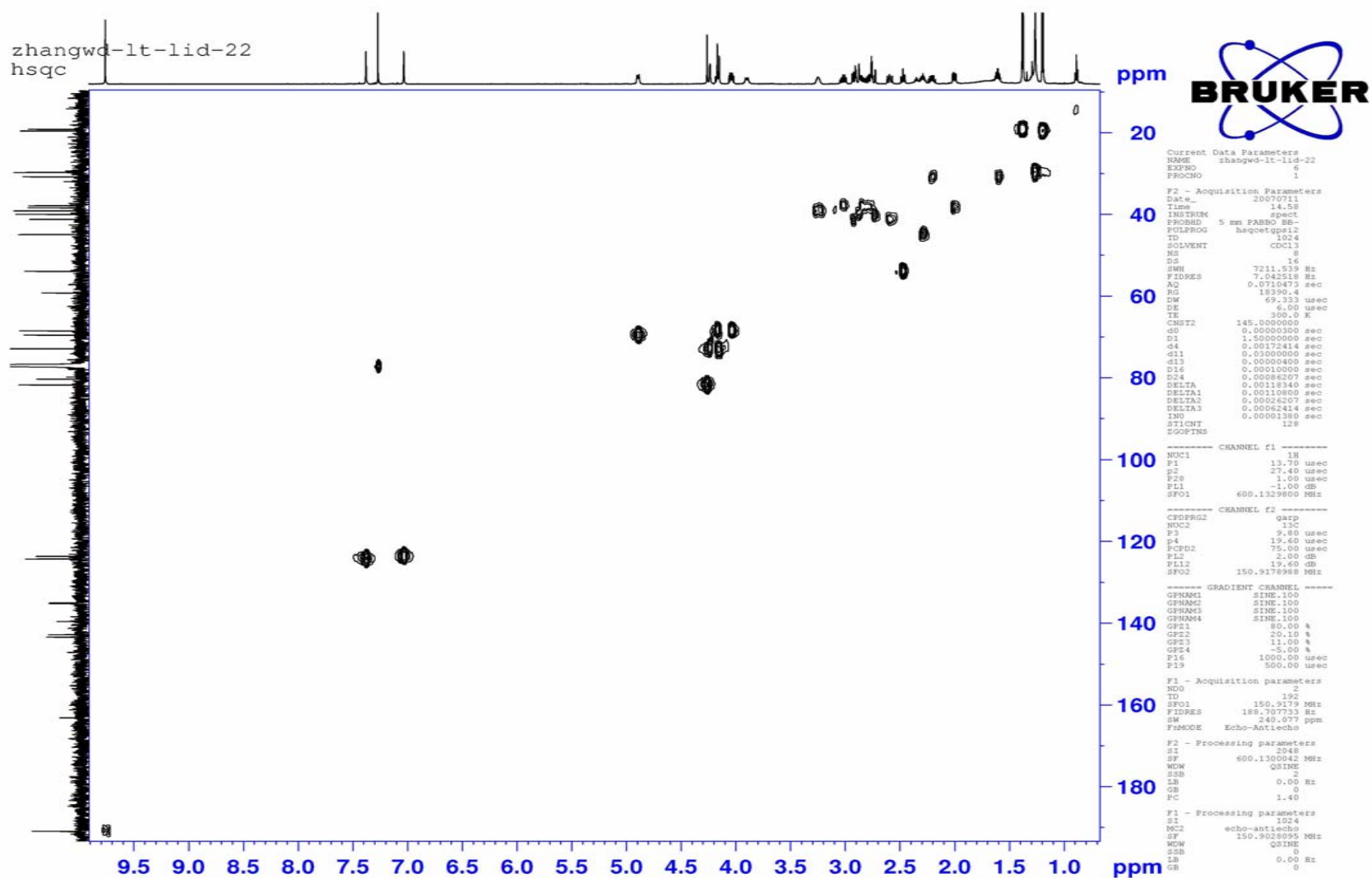


Figure S6 ^1H - ^1H COSY NMR Spectrum of incarviateone A (1) in CDCl_3

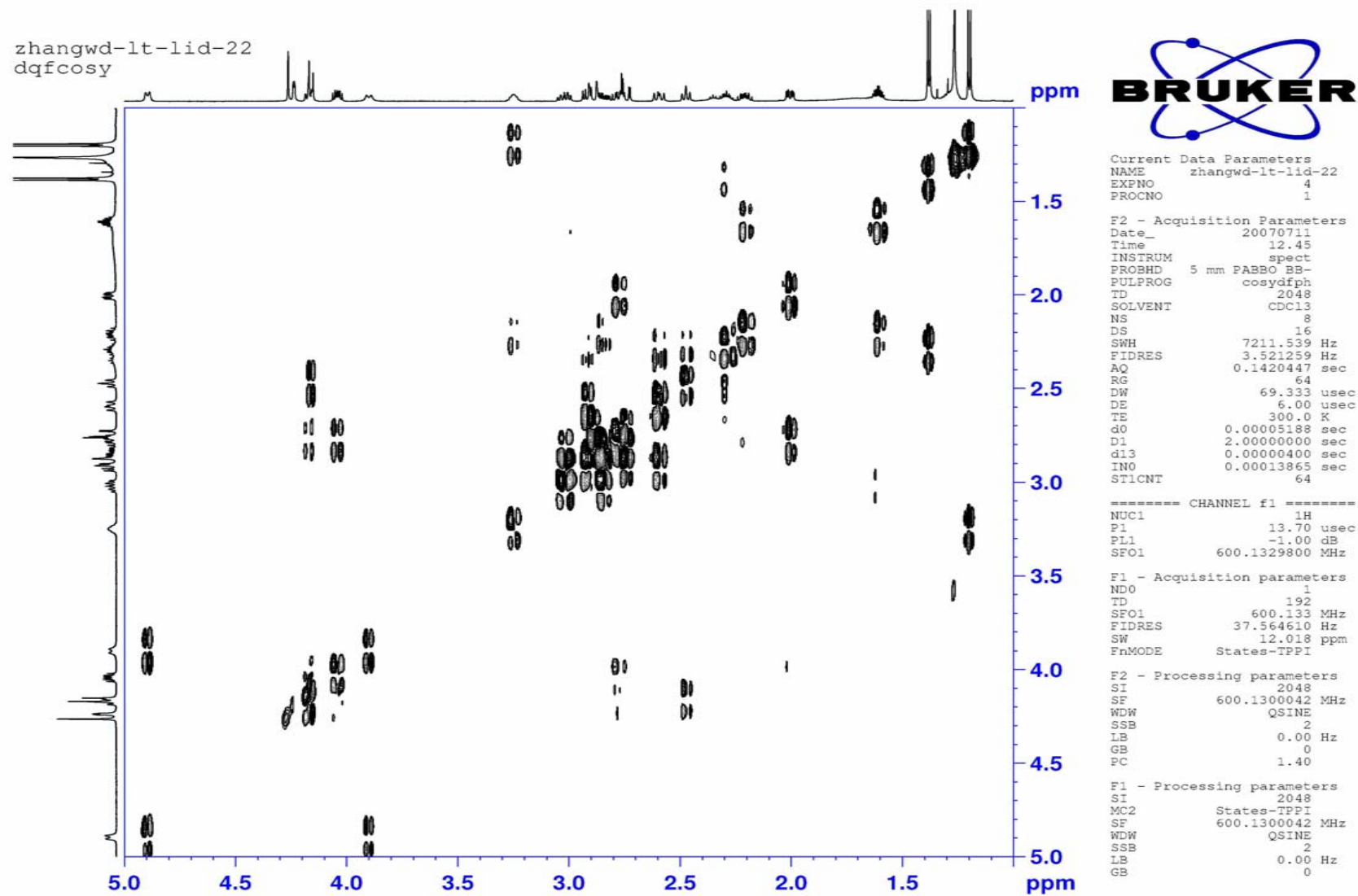


Figure S7 HMBC NMR Spectrum of incarviateone A (1) in CDCl₃

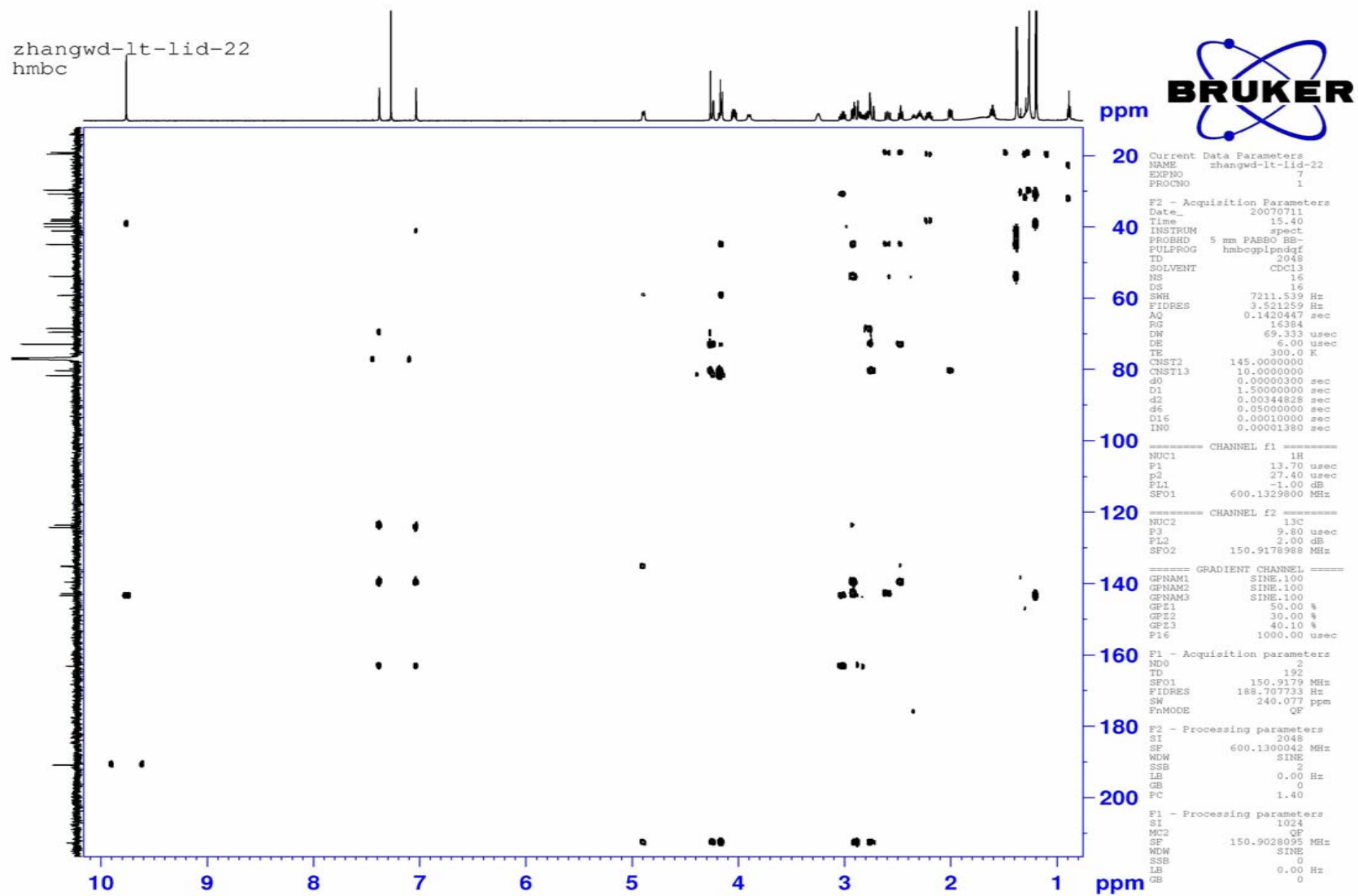
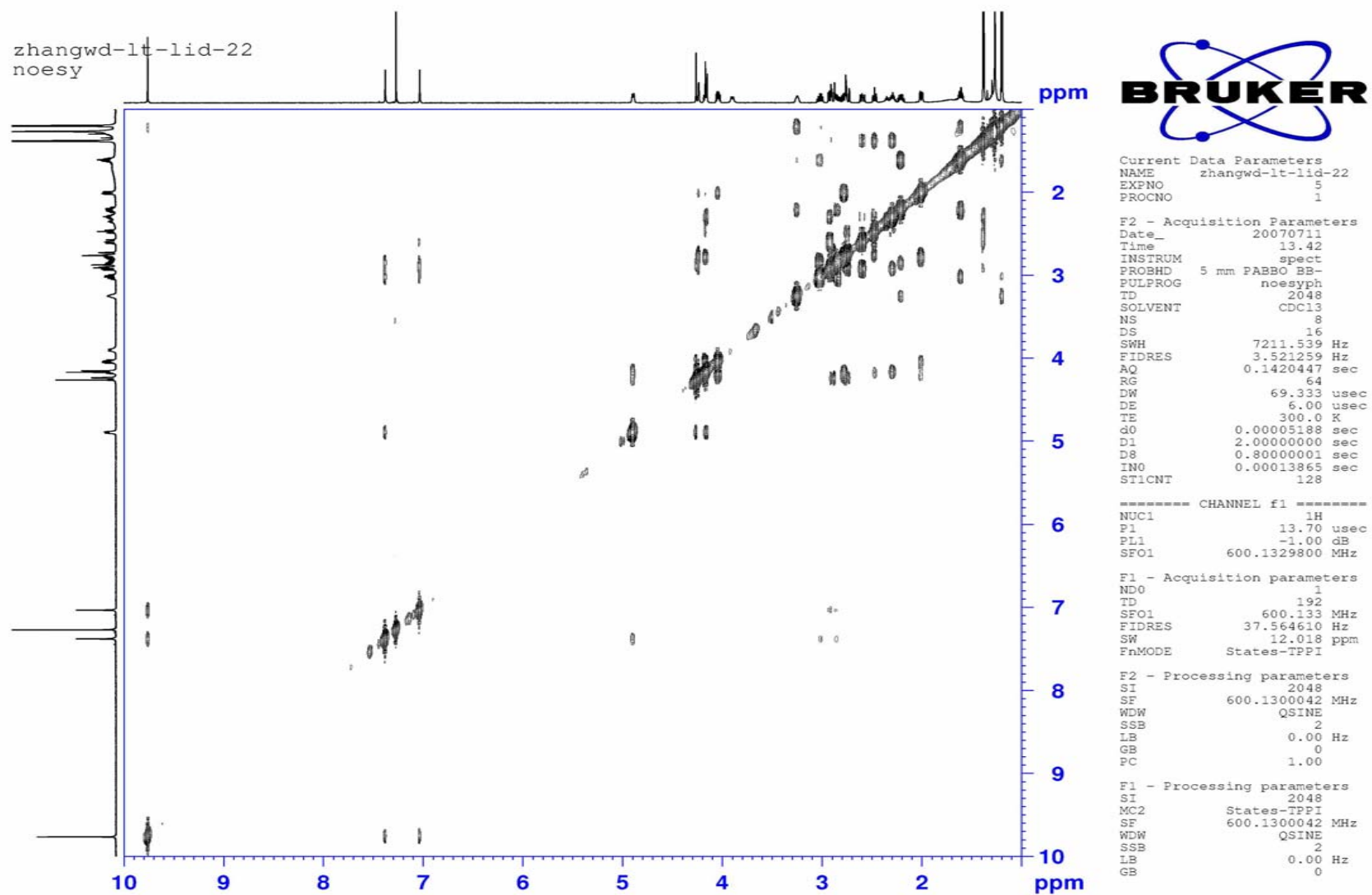


Figure S8 NOESY NMR Spectrum of incarviateone A (1) in CDCl₃



Complete citation of reference 19

Gaussian 03, Revision D.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

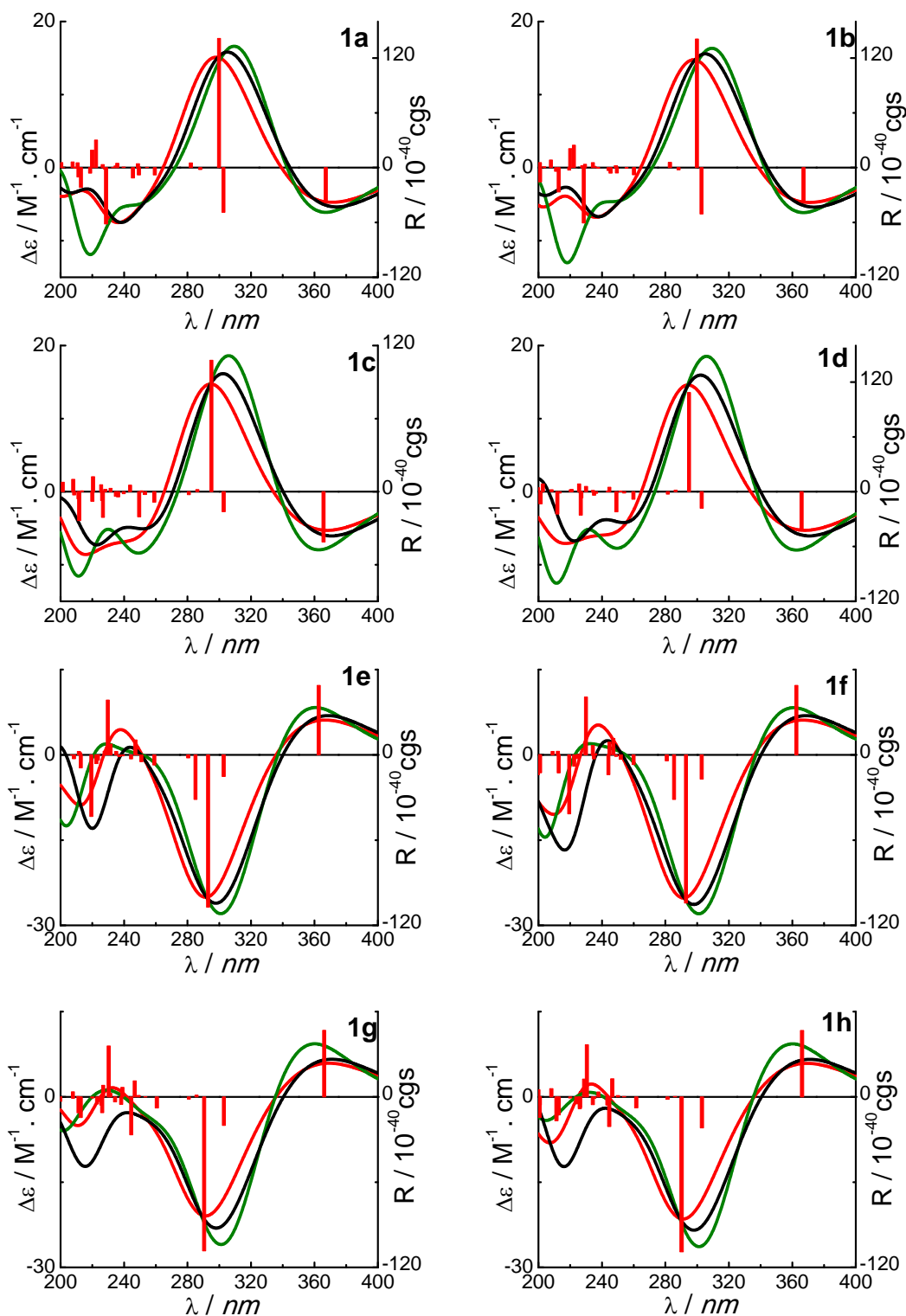


Figure S9 Calculated ECD spectra of individual conformer of **1a-1h** (red —, at the B3LYP/6-31G** level in the gas phase; black —, at the B3LYP/6-311++G**//B3LYP/6-31G** level in the gas phase; olive —, at the B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with the COSMO model in MeOH)

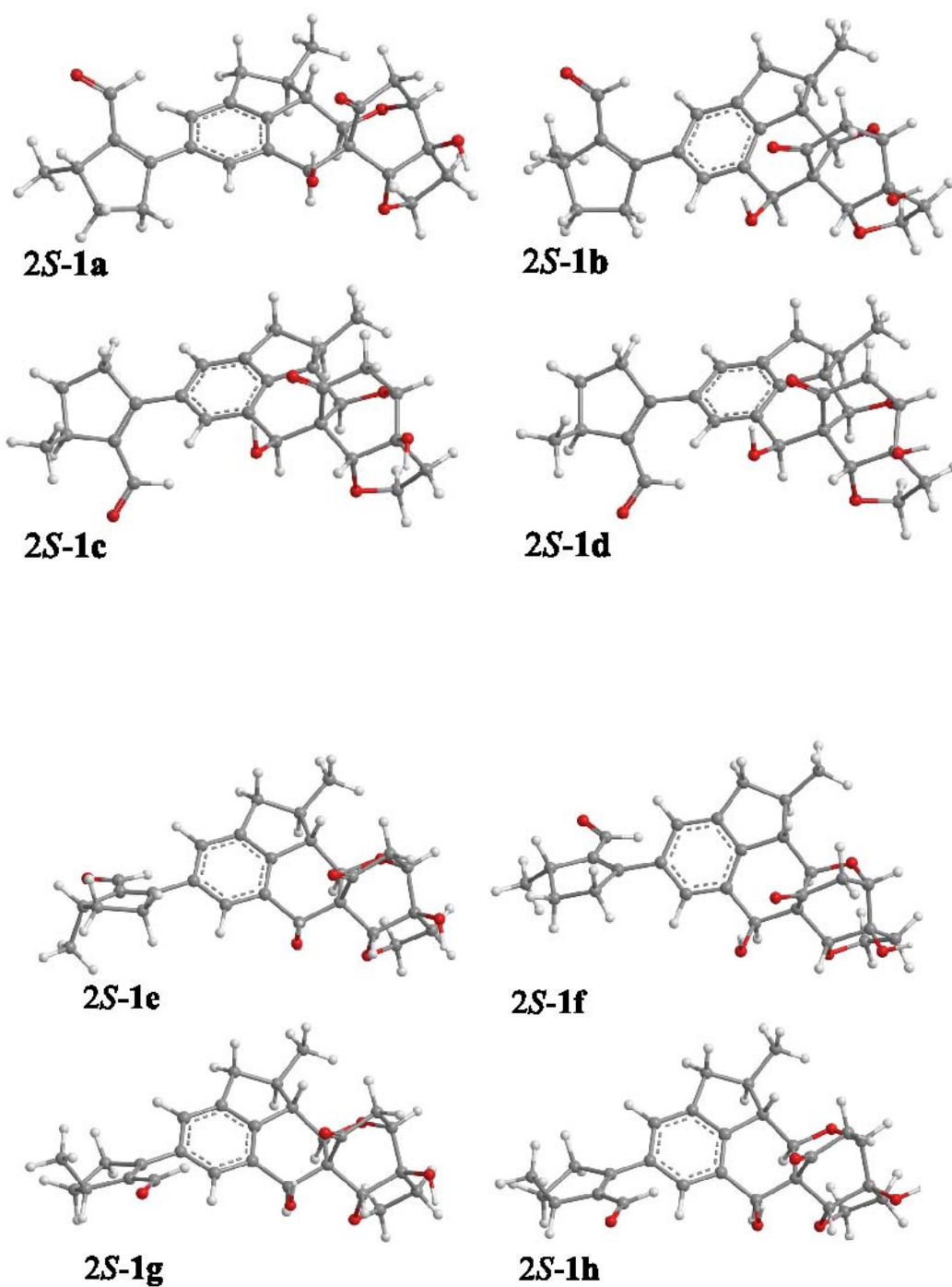


Figure S10 Optimized geometries of predominant conformers of 2S-1 in the gas phase at the B3LYP/6-31G** level.

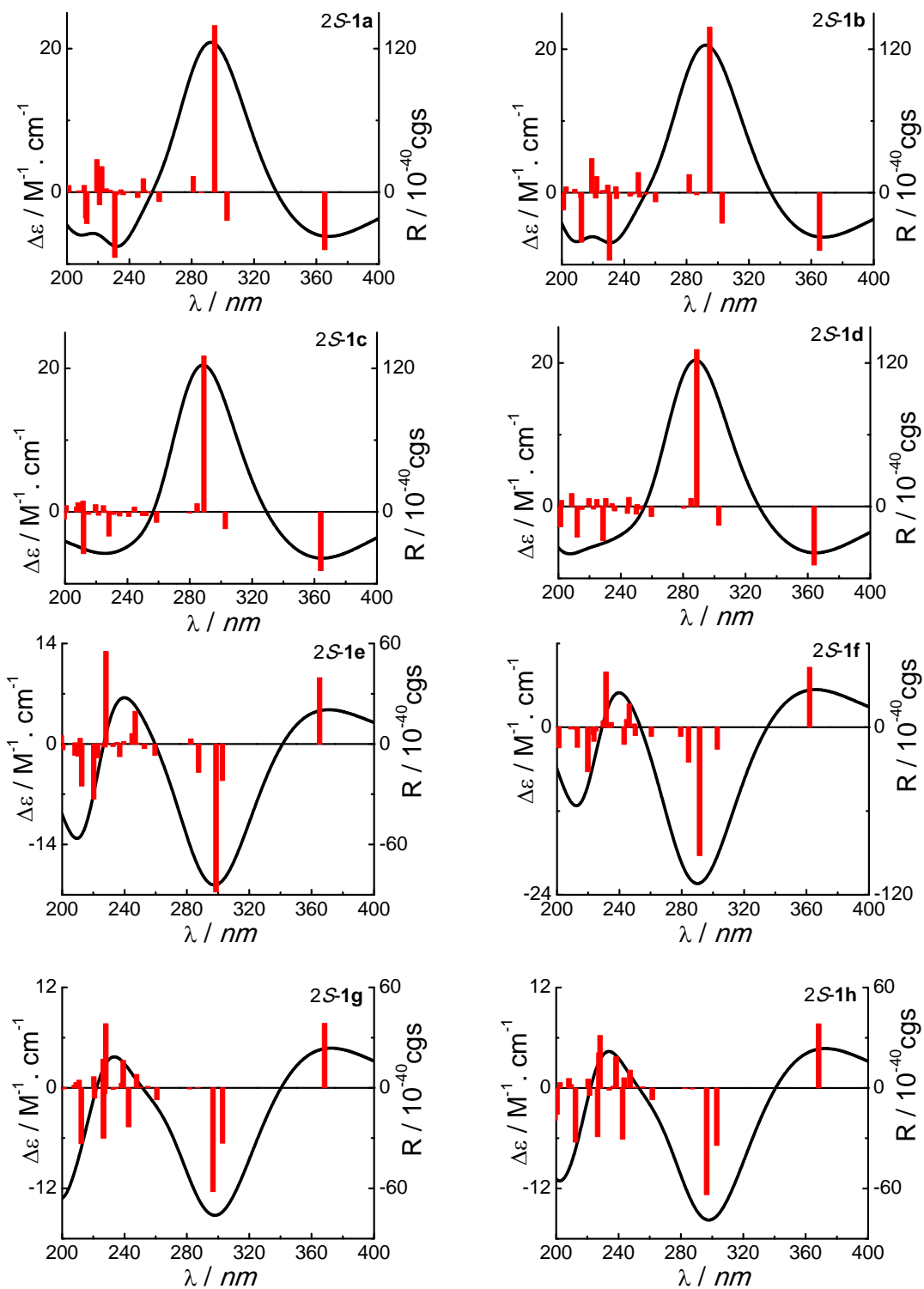


Figure S11 Calculated ECD spectra of individual conformer of 2S-1 at the B3LYP/6-31G** level in the gas phase.

Table S1 Important dihedral angles of optimized conformers of **1** in the gas phase at the B3LYP/6-31G** level

Species	1a	1b	1c	1d	1e	1f	1g	1h
O-C-26-C-1-C-5	178	178	179	180	-175	-175	-176	-176
C-1-C-5-C-6-C-7	143	143	-44	-44	-138	-138	43	43
HO-C-19-C-18	176	-69	176	-70	177	-69	176	-69

Table S2 Conformational analysis of **1**

Species	Gas phase								MeOH	
	E ^a	P _E % ^b	E ^c	P _E % ^d	G ^e	P _G % ^f	E ^g	P _E % ^h	E _s ⁱ	P _{Es} % ^j
1a	0.12	22.8	0.24	19.9	0.44	16.1	0.22	23.5	0.40	9.8
1b	0.79	7.4	0.89	6.6	1.08	5.4	1.16	4.8	0.11	15.8
1c	0.66	9.2	0.66	9.8	0.69	10.6	0.75	9.6	0.72	5.7
1d	1.38	2.7	1.36	3.0	1.35	3.5	1.78	1.7	0.51	8.1
Subtotal		42.1		39.3		35.6		39.6		39.4
1e	0.00	27.9	0.00	29.7	0.00	33.9	0.00	33.9	0.28	11.9
1f	0.67	9.0	0.68	9.5	0.67	10.9	0.94	7.0	0.06	17.5
1g	0.32	16.2	0.34	16.6	0.48	15.0	0.43	16.5	0.28	11.9
1h	1.05	4.8	1.06	5.0	1.19	4.6	1.43	3.1	0.00	19.2
Subtotal		57.9		60.8		64.4		60.5		60.5

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

Table S3. Important Thermodynamic Parameters of **1** (au)

Species	In the Gas					In MeOH
	E	E'=E+ZPE	H	G	E''	E _s
1a	-1498.296535	-1497.768721	-1497.739677	-1497.825833	-1498.657828	-1498.322158
1b	-1498.295473	-1497.767680	-1497.738616	-1497.824807	-1498.656329	-1498.322607
1c	-1498.295684	-1497.768050	-1497.738953	-1497.825438	-1498.65698	-1498.321643
1d	-1498.294522	-1497.766938	-1497.737807	-1497.824379	-1498.655341	-1498.32197
1e	-1498.296728	-1497.769099	-1497.739972	-1497.826534	-1498.658175	-1498.322339
1f	-1498.295656	-1497.768020	-1497.738884	-1497.825467	-1498.656678	-1498.322700
1g	-1498.296214	-1497.768553	-1497.739463	-1497.825762	-1498.657495	-1498.322340
1h	-1498.295056	-1497.767409	-1497.738304	-1497.824639	-1498.655903	-1498.322788

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

Table S4 Key transitions and their related rotatory and oscillator strengths of conformer **1e** at the B3LYP/6-31G** level in the gas phase

Transition	ΔE (eV)	λ (nm)	f	R^{vel}	R^{len}
119→121	3.42	363	0.012	45.3	48.9
117→122	4.09	303	0.001	-15.9	-15.2
120→121	4.23	293	0.348	-102.2	-107.2
120→122	4.35	285	0.041	-30.5	-31.3
120→123	5.02	247	0.034	12.3	10.5
119→123	5.40	230	0.033	36.3	38.6
119→124	5.65	219	0.041	-39.6	-43.3

E: excited energy; λ : wavelength; f : oscillator strength; R^{vel} : rotatory strength in velocity form(10^{-40} cgs); R^{len} : rotatory strength in length form(10^{-40} cgs).

Table S5 Conformational analysis of 2S-1

Species	In the Gas						In MeOH	
	E ^a	P _E % ^b	E ^c	P _E '% ^d	G ^e	P _G % ^f	E _s ^g	P _{Es} % ^h
2S-1a	0.00	30.6	0.00	29.9	0.00	30.7	0.29	14.7
2S-1b	0.67	9.9	0.66	9.8	0.65	10.3	0.00	24.1
2S-1c	0.48	13.6	0.41	15.0	0.38	16.0	0.56	9.4
2S-1d	1.21	4.0	1.15	4.3	1.09	4.9	0.32	14.1
subtotal		58.1		59.0		61.9		62.3
2S-1e	0.28	18.9	0.33	17.1	0.39	15.9	0.69	7.5
2S-1f	1.17	4.3	1.10	4.7	1.05	5.2	0.78	6.4
2S-1g	0.45	14.4	0.41	14.8	0.51	13.0	0.55	9.5
2S-1h	1.17	4.3	1.13	4.4	1.21	4.0	0.32	14.1
subtotal		41.9		41.0		38.1		37.5

^{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 methanol solution at B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with COSMO model, respectively.

Table S6. Important Thermodynamic Parameters of 2S-1 (au)

Species	In the Gas					In MeOH
	E	E'=E+ZPE	H	G	E''	E _s
2S-1a	-1498.296535	-1497.768721	-1497.739677	-1497.825833	-1498.657828	-1498.322158
2S-1b	-1498.295473	-1497.767680	-1497.738616	-1497.824807	-1498.656329	-1498.322607
2S-1c	-1498.295684	-1497.768050	-1497.738953	-1497.825438	-1498.65698	-1498.321643
2S-1d	-1498.294522	-1497.766938	-1497.737807	-1497.824379	-1498.655341	-1498.32197
2S-1e	-1498.296728	-1497.769099	-1497.739972	-1497.826534	-1498.658175	-1498.322339
2S-1f	-1498.295656	-1497.768020	-1497.738884	-1497.825467	-1498.656678	-1498.322700
2S-1g	-1498.296214	-1497.768553	-1497.739463	-1497.825762	-1498.657495	-1498.322340
2S-1h	-1498.295056	-1497.767409	-1497.738304	-1497.824639	-1498.655903	-1498.322788

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

Table S7 Important dihedral angles of optimized conformers of 2S-1 in the gas phase at B3LYP/6-31G** level

species	2S-1a	2S-1b	2S-1c	2S-1d	2S-1e	2S-1f	2S-1g	2S-1h
O-C-26-C-1-C-5	175	175	176	176	-178	-168	-179	-179
C-1-C-5-C-6-C-7	143	143	-43	-44	-138	-136	43	43
HO-C-19-C-18	177	-69	177	-70	177	-69	176	-69