Supporting Information

Determination of the Absolute Configurations of Bicyclo[3.1.0]hexane Derivatives via Electronic Circular Dichroism, Optical Rotation Dispersion, and Vibrational Circular Dichroism Spectroscopy and Density Functional Theory Calculations

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Completion of reference 19.

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, 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 03, Revision C.02. Gaussian, Inc., Pittsburgh PA, 2003.
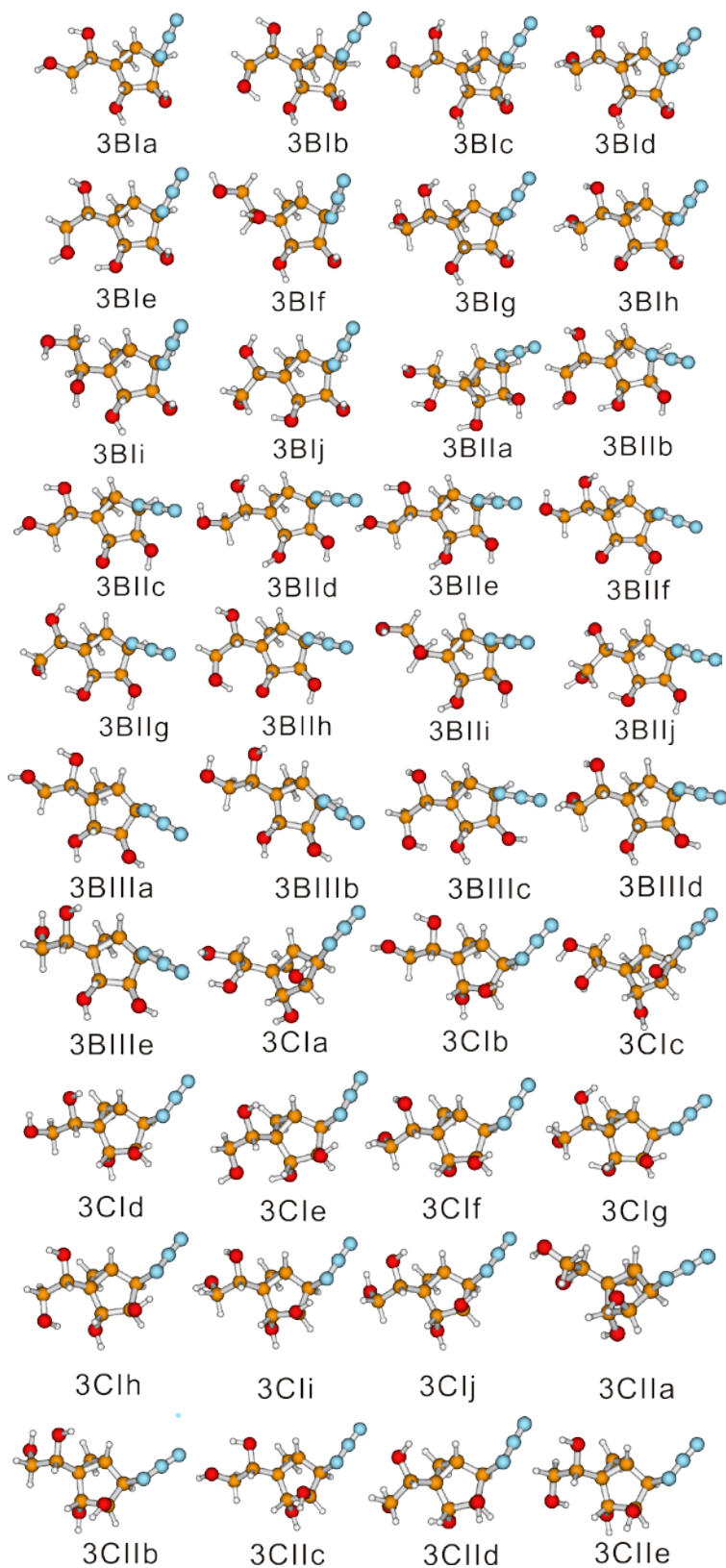
Figure S1. Optimized geometries of the 40 most stable conformers of **3** at the B3LYP/6-311++G** level of theory.

Table S1. The calculated dihedral angles and the pseudorotational phase angles for the six most stable conformers. Both are in units of degrees.

Conformers	Dihedral angle[a]		pseudorotational phase angle[b]
3BIa	C(2)-C(3)-C(4)-C(5)	-30.6939	342
	C(1)-C(2)-C(3)-C(4)	19.3696	
	C(5)-C(1)-C(2)-C(3)	-0.2169	
	C(4)-C(5)-C(1)-C(2)	-19.1715	
	C(3)-C(4)-C(5)-C(1)	31.1049	
3BIb	C(2)-C(3)-C(4)-C(5)	-30.7117	343
	C(6)-C(2)-C(3)-C(4)	19.7542	
	C(5)-C(6)-C(2)-C(3)	-0.7663	
	C(4)-C(5)-C(6)-C(2)	-18.7045	
	C(3)-C(4)-C(5)-C(6)	30.9156	
3BIc	C(2)-C(3)-C(4)-C(5)	-30.5864	343
	C(1)-C(2)-C(3)-C(4)	19.5848	
	C(5)-C(1)-C(2)-C(3)	-0.7007	
	C(4)-C(5)-C(1)-C(2)	-18.6161	
	C(3)-C(4)-C(5)-C(1)	30.7324	
3BId	C(6)-C(5)-C(4)-C(3)	-30.9107	342
	C(2)-C(6)-C(5)-C(4)	19.5087	
	C(3)-C(2)-C(6)-C(5)	-0.2177	
	C(4)-C(3)-C(2)-C(6)	-19.3359	
	C(5)-C(4)-C(3)-C(2)	31.402	
3BIIa	C(1)-C(5)-C(4)-C(3)	-32.183	348
	C(2)-C(1)-C(5)-C(4)	21.1698	
	C(3)-C(2)-C(1)-C(5)	-2.0237	
	C(4)-C(3)-C(2)-C(1)	-18.158	
	C(5)-C(4)-C(3)-C(2)	31.4292	
3BIIb	C(1)-C(5)-C(4)-C(3)	-32.183	345
	C(2)-C(1)-C(5)-C(4)	21.1698	
	C(3)-C(2)-C(1)-C(5)	-2.0237	
	C(4)-C(3)-C(2)-C(1)	-18.158	
	C(5)-C(4)-C(3)-C(2)	31.4292	

[a] See Chart 1 for atom labelling. [b] Calculated using the Altona-Sundaralingam system (Ref. 11). The Cremer-Pople (D. Cremer and J. A. Pople, J. Am. Chem. Soc., 97, 1354-1358, 1975) phase angle values can be obtained by simply subtracting 90º from these values.

Table S2. Calculated excitation energies, oscillator strengths and rotational strengths for conformer **3BIa** in the gas phase at the B3LYP/ 6-311++G** level.

Compound **3BIa**

#	Gas				
	eV	λ^a	f^b	$R_{velocity}{}^c$	$R_{length}{}^c$
1	4.4297	279.89	0.0001	-1.1470	-1.3541
2	5.3798	230.46	0.0004	-0.9580	-0.9255
3	5.6294	220.24	0.0005	-0.4293	-0.4620
4	5.7666	215.00	0.0006	1.1891	1.6772
5	6.1576	201.35	0.0068	-4.1269	-4.2489
6	6.2555	198.20	0.0084	12.6665	12.9337
7	6.3088	196.53	0.0023	-2.0999	-2.3854
8	6.3274	195.95	0.0104	8.7879	8.7672
9	6.3616	194.89	0.0080	0.2124	0.1439
10	6.4436	192.41	0.0091	-1.9839	-2.2874
11	6.4748	191.49	0.0065	-5.7102	-6.2725
12	6.4962	190.86	0.0066	-8.1989	-8.4517
13	6.5755	188.56	0.0004	3.2103	2.9539
14	6.6035	187.76	0.0027	6.3338	6.0407
15	6.6594	186.18	0.0067	-5.5356	-5.2096
16	6.6862	185.43	0.0014	3.1802	3.1965
17	6.7530	183.60	0.0208	-30.6343	-31.7770
18	6.7668	183.22	0.0111	14.6190	15.2348
19	6.7892	182.62	0.0118	2.1928	1.9343
20	6.8009	182.30	0.0029	0.1101	0.3237
21	6.8653	180.60	0.0035	10.6316	10.8839
22	6.9534	178.31	0.0078	6.9483	7.0019
23	6.9714	177.85	0.0077	-16.8196	-17.5119
24	6.9888	177.40	0.0012	0.7252	0.5763
25	7.0924	174.81	0.0124	4.7283	4.3936
26	7.1273	173.96	0.0089	10.1625	10.2818
27	7.1355	173.76	0.0021	-1.6973	-1.3238
28	7.1597	173.17	0.0078	14.4850	-14.1042
29	7.2038	172.11	0.0046	-1.2100	-2.0217
30	7.2647	170.67	0.0082	4.2070	4.7662

[a] λ in nm. [b] Oscillator Strengths. [c] R values (in 10^{-40} esu^{2}cm^2) using the velocity-gauge representation and length-gauge representation of the electric dipole operator.
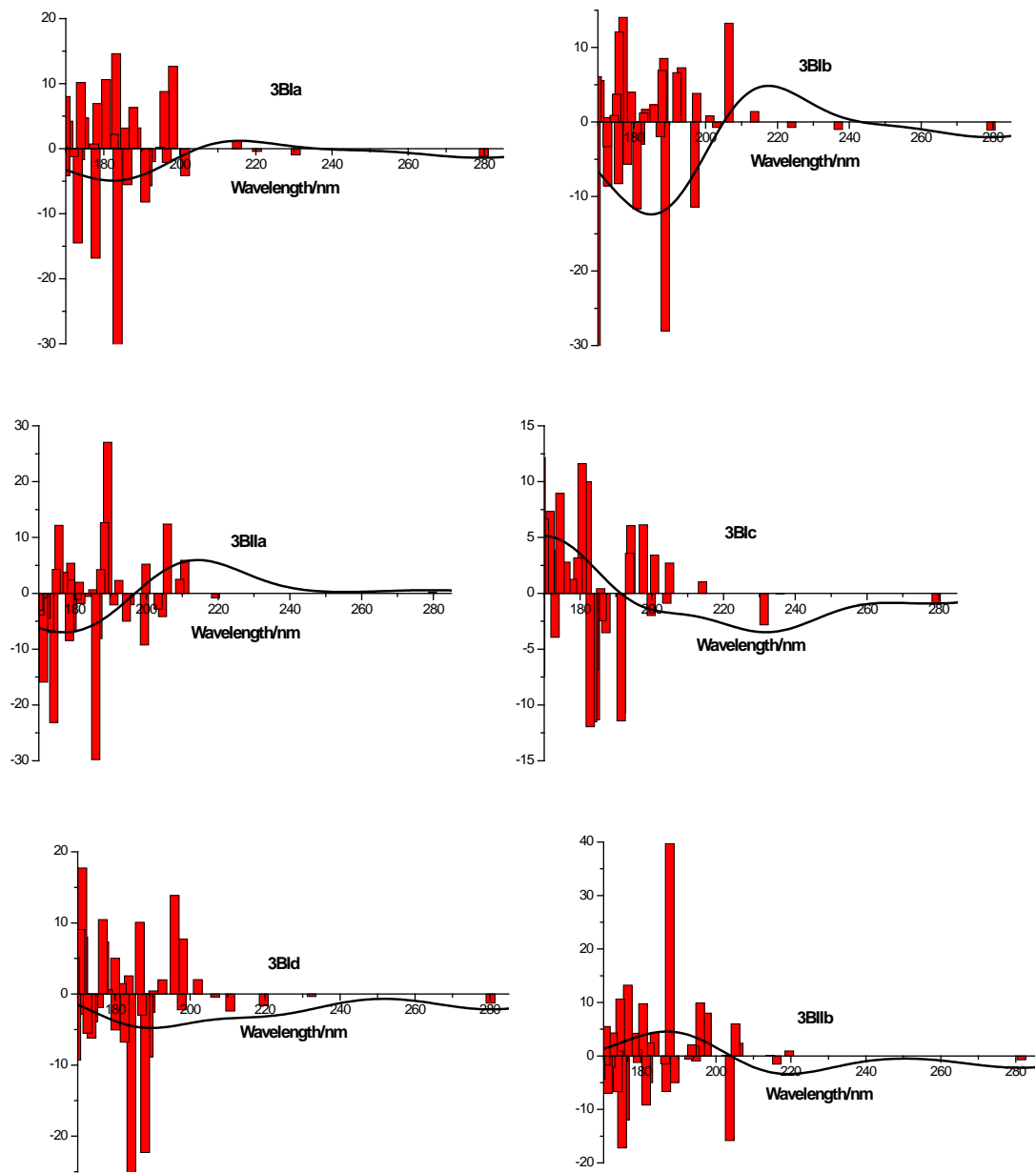
Figure S2. Calculated ECD spectra in the gas phase for the six most stable conformers of compound **3** at the B3LYP/ 6-311++G** level.
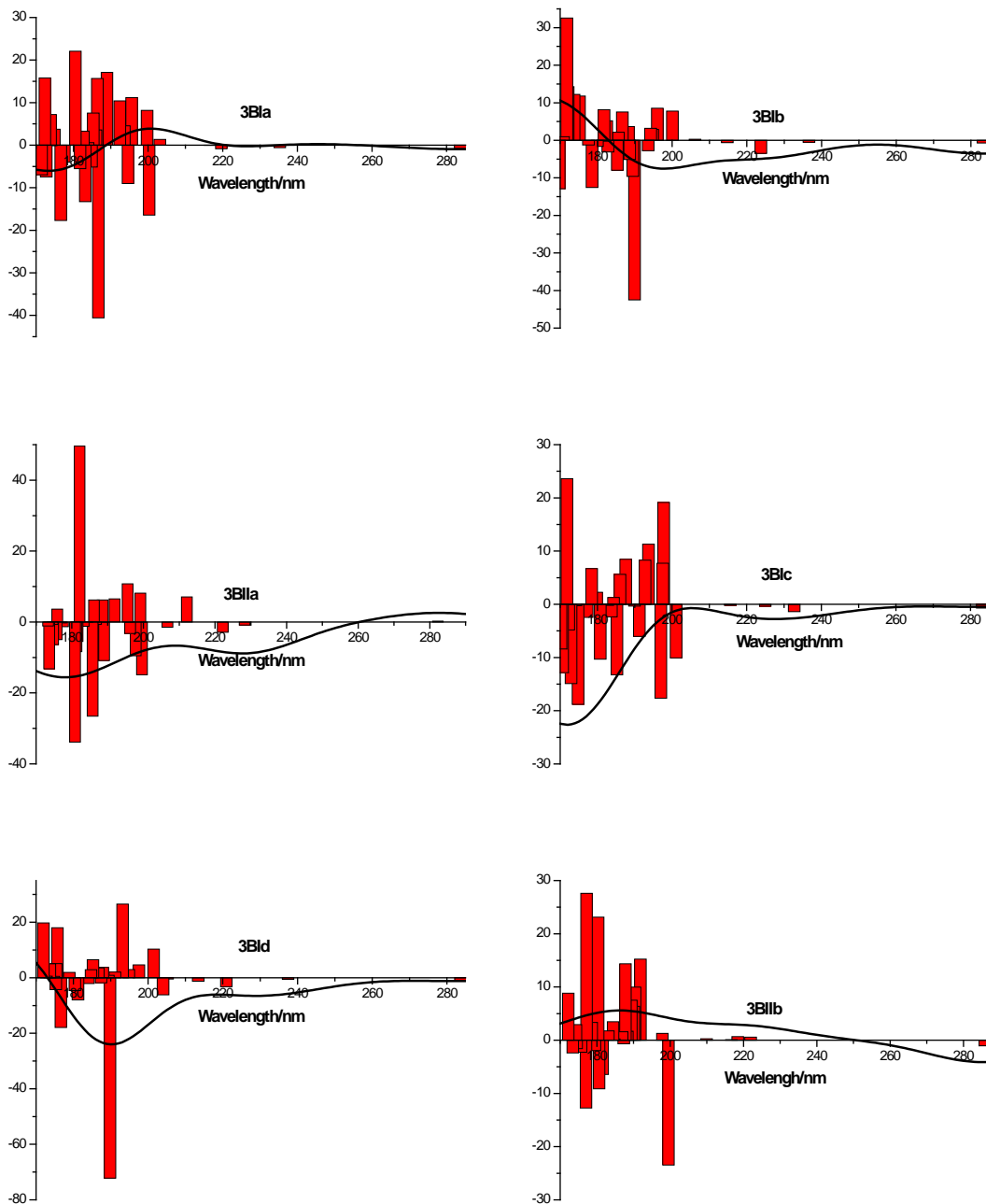
Figure S3. Calculated ECD spectra for the six most stable conformers of compound **3** in acetonitrile with IPCM for solvation at the B3LYP/ 6-311++G** level.
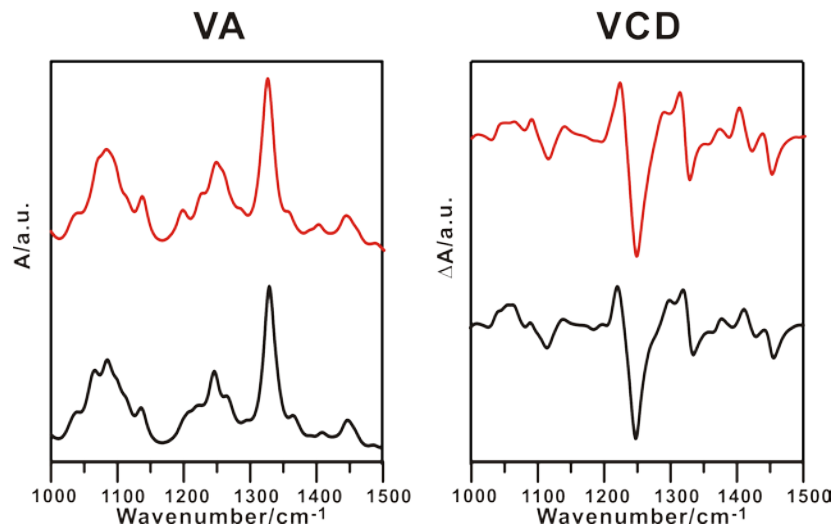
Figure S4. Comparison of the calculated gas phase VA and VCD spectra of conformer **3BIa** at the B3LYP/6-311++G** (bottom) and the B3LYP/aug-cc-pVDZ level (top).
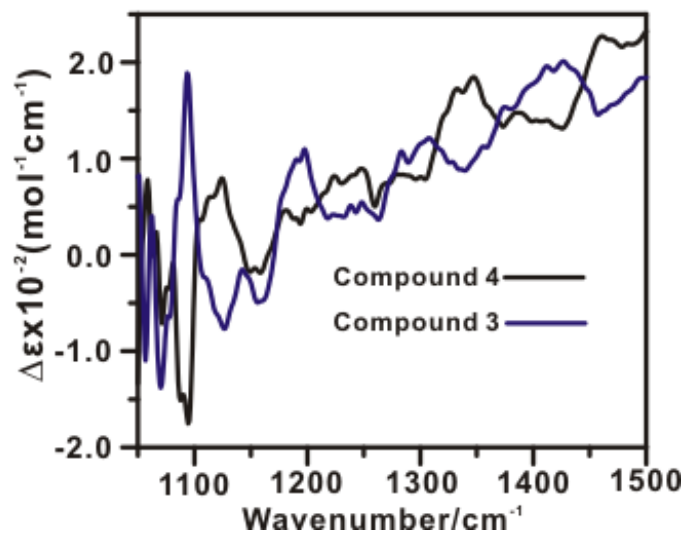

Figure S5. Raw experimental VCD spectra of compound **3** and **4** studied in this paper. The solvent baselines are not corrected.