Electronic Supplementary Information for:

Circular Dichroism, Optical Rotation and Absolute Configuration of 2-Cyclohexenone-*cis*-diol Type Phenol Metabolites: Redefining the Role of Substituents and 2-Cyclohexenone Conformation in Electronic Circular Dichroism Spectra

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Total energies (E_{tot}, in Hartree), relative energies (ΔE, ΔG in kcal mol^{-1}), percentage populations, cartesian coordinates and structures as well as UV and CD spectra of individual conformers of keto-*cis*-diols **1a-1e, 2a-2c, 3a-3c** calculated at the various levels of theory are available on request (165 pages) from the authors.

Full version of **Figure 5.**

Experimental details

Table A1. Relative energies and populations of the stable low-energy conformers of **1-4** calculated at various levels of theory.

Table A2. Relative energies and populations of the stable low-energy conformers of **1a**, **1b** and **1e** calculated at PCM(MeCN)/MP2/Aug-cc-pVTZ//PCM(MeCN)/MP2/6-311G(d,p) level of theory.

Table B1. Structural parameters that characterize low-energy conformers of **1-4** calculated at the PCM(MeCN)/B3LYP/6-311++G(2d,2p) level.

Table B2. Values of intraring torsion angles that characterize the low-energy conformers of **1-4** calculated at the PCM(MeCN)/B3LYP/6-311++G(2d,2p) level.

Table B3. Structural parameters that characterize low-energy conformers of **1a**, **1b** and **1c** calculated at the PCM(MeCN)/MP2/6-311G(d,p) level.

Table B4. Values of intra-ring torsion angles that characterize the low-energy conformers of **1a**, **1b** and **1c** calculated at the PCM(MeCN)/MP2/6-311G(d,p) level.

Table C. Specific optical rotations for *cis*-ketodiols **1-4**, measured in methanol solution and calculated at the PCM/B3LYP/Aug-cc-pVTZ level.

Table D. Rotatory strengths and excitation energies calculated at the PCM/B2LYP/6-311++G(2d,2p) level for *P*-type conformers of model compounds **4-23** with varying torsion angles ω and τ.

Table E. Relative energies (ΔE) of **4** with varying torsion angles ω and τ.

Table F. Rotatory strengths *R* calculated at the PCM/B2LYP/6-311++G(2d,2p) level for *P*-type conformers of model compounds **4-23** with planar chromophore relative to **4** and substituent contributions ΔR for Cotton effects I-III.

Table G. Specific optical rotations for enones **6-11**, measured and calculated at the PCM/B3LYP/Aug-cc-pVTZ level.

Figure A. Relative energies of (*P*)-**4** (in kcal mol^{-1}, calculated at the B3LYP/6-311++G(2d,2p) level) as a function of dihedral angles ω and τ.

Figure B. UV spectra of *cis*-ketodiols **1a**-**1e**, experimental (in acetonitrile solutions, solid lines) and ΔE_{MP2} Boltzmann averaged calculated at PCM/B2LYP/Aug-cc-pVTZ level (dashed lines) (left column) and UV spectra of *cis*-ketodiols *ent*-**2a**-**2c** experimental (in acetonitrile solutions, solid lines), ΔE_{MP2} Boltzmann averaged calculated at PCM/B2LYP/Aug-cc-pVTZ level for **2a**-**2c** (dashed lines) and **3a**-**3c** (dash-dot-dot lines) (right column). All calculated spectra were wavelength corrected to match experimental short-wavelength UV λ_{max} at ca. 220 nm.

Figure B1. ECD spectra calculated at the PCM/B2LYP/Aug-cc-pVTZ level for individual conformers of **1a**, optimized at the PCM/MP2/6-311G(d,p) level (red lines) and at the PCM/B3LYP/6-311++G(2d,2p) level (blue lines).

Figure B2. ECD spectra calculated at the PCM/B2LYP/Aug-cc-pVTZ level for individual conformers of **1b**, optimized at the PCM/MP2/6-311G(d,p) level (red lines) and at the PCM/B3LYP/6-311++G(2d,2p) level (blue lines).

Figure B3. ECD spectra calculated at the PCM/B2LYP/Aug-cc-pVTZ level for individual conformers of **1e**, optimized at the PCM/MP2/6-311G(d,p) level (red lines) and at the PCM/B3LYP/6-311++G(2d,2p) level (blue lines).

Figure B4. ECD spectra of *cis*-ketodiols **1a**, **1b** and **1e** calculated at the PCM/B2LYP/Aug-cc-pVTZ level and ΔE_{MP2} Boltzmann averaged. Geometries were optimized at the PCM/MP2/Aug-cc-pVTZ//PCM/MP2/6-311G(d,p) level (red lines) and at the PCM/MP2/Aug-cc-pVTZ//PCM/B3LYP/6-311++G(2d,2p) level. Wavelength not corrected.

Figure C. Efect of percentage populations of the lowest-energy *P* and *M* conformers on averaged ECD spectra of **1e**. ECD spectra were calculated at PCM/B2LYP/Aug-cc-pVTZ level.

Figure D. Effect of methyl and hydroxy substituents on the CD spectra of selected monosubstituted (*P*)-2-cyclohexenones with a planar chromophore (ω = 180º, τ = 0º). All spectra were calculated at the PCM/B2LYP/Aug-cc-pVTZ level for the structures optimized at the PCM/B3LYP/6-311++G(2d,2p) level. Inserts show long wavelength (ca. 300 nm) $n_{C=O}$-$\pi_{C=O}$* Cotton effects. Wavelength not corrected.

Figure E. Effect of non-planarity of the chromophore (ω and τ angles) on the rotatory strengths *R* for the three low-energy electronic transitions, calculated conformers of acrolein. All rotatory strengths were calculated at the PCM/B2LYP/6-311++G(2d,2p) level.

Figure F. Effect of non-planarity of the chromophore (ω and τ angles) on the rotatory strengths *R* for the three low-energy electronic transitions, calculated for *P*-type conformers of **4**. All rotatory strengths were calculated at the PCM/B2LYP/6-311++G(2d,2p) level.

Figure G. Calculated contribution of the C4-C5-C6 chain to the rotatory strengths of 2-cyclohexenone obtained by subtraction of rotatory strengths calculated for acrolein (Figure D) from those obtained for **4** (Figure E). All rotatory strengths were calculated at the PCM/B2LYP/6-311++G(2d,2p) level.

Figure H. Effect of the twist of ω and τ angles on the CD spectra of *P*-type conformer of **5** calculated at PCM/B2LYP/6-311++G(2d,2p) level. Vertical bars represent rotatory strengths. Wavelength not corrected.

Figure I. Effect of deviation from planarity (angles ω and τ) on the rotatory strengths *R* for the three low-energy electronic transitions, calculated for *P*-type conformers of (4*S*)-**7**. All rotatory strengths were calculated at the PCM/B2LYP/6-311++G(2d,2p) level.

Figure J. Effect of methyl and hydroxy substituents on the CD spectra of selected disubstituted 2-cyclohexenone *P*-type conformers with planar chromophore moieties. All spectra were calculated at the PCM/B2LYP/6-311++G(2d,2p) level. Inserts show the long wavelength (> 300 nm) n-π* Cotton effects. Wavelength not corrected.

Figure K. Effect of methods used for calculations of ECD and for Boltzmann averaging on the shapes of the CD spectra of **1a**.

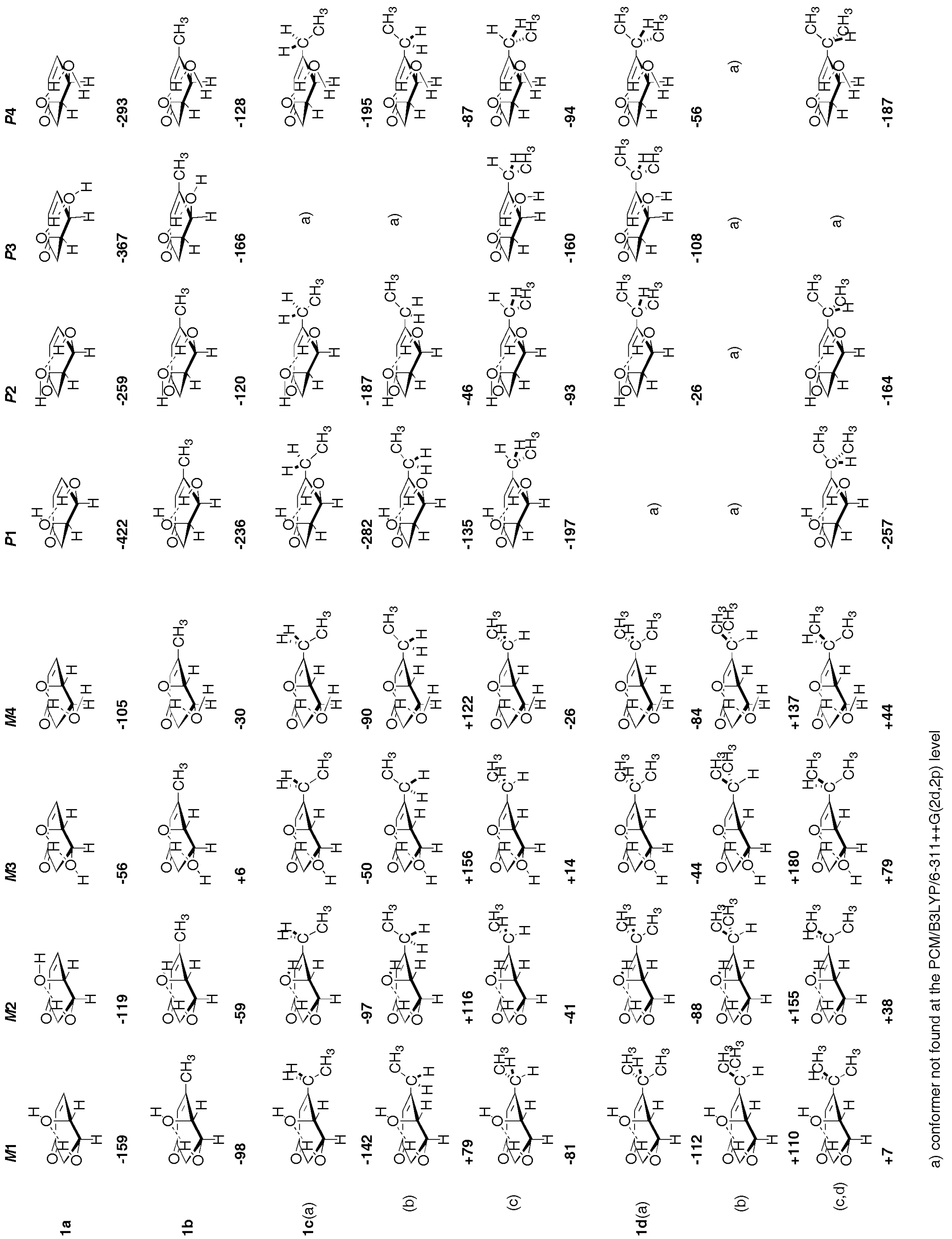

Figure 5 (full version). Effect of rotation of hydroxy, ethyl, and isopropyl substituents on the calculated (PCM/B3LYP/Aug-cc-pVTZ level) optical rotation at 589 nm for low-energy conformers of **1a**-**1d**.

Experimental details

The bacterial biotransformations of the corresponding phenols using *Pseudomonas putida* UV4 to yield the 2-cyclohexenone metabolites **1a-1e** and **2a-2c** and their full characterization is reported elsewhere.[1,2] For optical rotation ($[\alpha]_D$) measurements (*ca* 20 °C, 10^{-1} deg cm ^{2} g^{-1}) a Perkin-Elmer 214 polarimeter and methanol solvent were used.

Computational details

Starting geometries of keto-*cis*-diols **1-3** were obtained by optimisation at the B3LYP/6-311++G(d,p)[3] level of theory. From these geometries, for both *P* and *M* helicity enones, relaxed potential energy surfaces (PES) were obtained by changing the dihedral angles of H-C4-O-H, H-C5-O-H and, if necessary, of C2=C3-CH_2-CH_3 and C2=C3-C$(Me)_2$-H in the range 0 to 360° by 30 degree steps. This allowed us to identify the minimum energy structures which were further optimised *in vacuo* at the B3LYP/6-311++G(2d,2p) level of theory and in the acetonitrile and methanol solutions, using the polarizable continuum model (PCM),[4] at the same level. The structures thus obtained were real minimum energy conformers (no imaginary frequencies have been found). Free energy values were used to obtain the Boltzmann population of conformers at 298.15 K. For all stable conformers, the single point energies were calculated at the MP2/Aug-cc-pVTZ level with or without the use of the PCM solvent model. For both DFT and MP2 calculations, only the results for conformers that differ from the most stable by less than 2 kcal mol^{-1} have been taken into account for further calculations, following a generally accepted protocol.[5] In the case of **1a**, **1b** and **1e** additional calculations at the PCM(MaCN)/MP2/Aug-cc-pVTZ//PCM(MeCN)/MP2/6-311G(d,p) level were performed (results were colected in Tables A2, B3 and B4).
The calculations of optical rotations were carried out for all stable conformers at four different wavelengths (589, 578, 546 and 436 nm), both *in vacuo* and in the solvent, using the DFT/B3LYP/Aug-cc-pVTZ method. London orbitals (which ensure the origin independency of the results) have been used. Since the experimental data were recorded in methanol solution, optical rotations calculated with the use of the PCM model were further taken into account.[6]

For all investigated compounds the ECD spectra were measured in acetonitrile solution and calculated at the (PCM)/TDDFT/6-311++G(2d,2p) and (PCM)/TDDFT/Aug-cc-pVTZ levels for all stable geometries optimised at the (PCM)/B3LYP/6-311++G(2d,2p) or at the PCM/MP2/6-311G(d,p) level. In order to determine which combination of functional/basis sets performs better in ECD calculations we employed several density functionals (B3LYP,[7] mPW1PW91,[3] BHandHLYP,[8] B2LYP and B2PLYP[9,10]) in conjunction with 6-311++G(2d,2p) and Aug-cc-pVTZ basis sets and PCM solvent model. The test calculations were performed for 2-cyclohexenone **1a**, since its absolute configuration has been known. Arbitrarily we selected the combination of PCM/B2LYP/Aug-cc-pVTZ as a method for further calculations of the ECD spectra of keto-*cis*-diols **1-3**. It should be noted that calculation of perturbative correction to excitation energies (B2PLYP functional) did not improve significantly the results for 2-cyclohexenone **1a**, but considerably increased the CPU time.[11] The second best performing was the BHandHLYP/6-311++G(2d,2p) method, due to a similar value of HF-exchange, as in the case of B2LYP functional (50% and 42%, respectively). Interestingly, the most popular hybrid functionals B3LYP and mPW1PW91 did not provide satisfactory results in these studies. The calculated Boltzmann averaged ECD spectra with the use of these functionals correctly reproduced the signs of the long-wavelength $n_{C=O}$-$\pi_{C=O}$* and short wavelength

n_{OH}-$\pi_{C=O}$* Cotton effects, however in the spectral region between 280 and 220 nm two negative Cotton effects appeared, which was in disagreement with the experimental spectrum of 2-cyclohexenone **1a** (see Figure K).

The ECD spectra calculated with the use of B3LYP and mPW1PW91 hybrid functionals are a superposition of at least 10 electronic transitions, contrary to the results obtained with the use of B2(P)LYP and BHandHLYP hybrid functionals, where the first three Cotton effects are due to the single electronic transition at a given wavelength.

Rotatory strengths were calculated using both length and velocity representations. In the present study, the differences between the length and velocity of the calculated values of rotatory strengths were quite small and for this reason only the velocity representations were further used. The CD spectra were simulated by overlapping Gaussian functions[12] for each transition, according to the procedure previously described.[13,14-17]

The geometry/ECD calculations for the model compounds **4-23** were performed similarly to the procedure described above. Note that the geometry optimisations were performed for conformers having fixed given structural parameter. The ECD spectra for **4-23** were calculated at the PCM/B2LYP/6-311++G(2d,2p) level for conformers optimised at the PCM/B3LYP/6-311++G(2d,2p) level.

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Table A1. Relative energies and populations of the stable low-energy conformers of **1-4** calculated at MP2/Aug-cc-pVTZ level of theory with and without the use of PCM model.

Diol	Gas phase		Acetonitrile		Methanol	
	ΔE[a] [kcal mol^{-1}]	Population [%]	ΔE[b] [kcal mol^{-1}]	Population [%]	ΔE[c] [kcal mol^{-1}]	Population [%]
1a(*P*1)	0.00	48	1.96	1	1.72	2
1a(*P*2)	0.52	20	0.47	18	0.29	22
1a(*P*3)	1.45	4	0.34	22	0.42	17
1a(*P*4)	1.16	7	0.00	40	0.00	35
1a(*M*1)	1.20	6	1.80	2	1.56	2
1a(*M*2)	1.57	3	1.39	4	0.90	8
1a(*M*3)	1.02	8	1.19	5	1.04	6
1a(*M*4)	1.5	4	1.02	8	0.86	8
1b(*P*1)	0.00	38	2.32	-	2.13	-
1b(*P*2)	0.44	18	0.91	11	0.83	11
1b(*P*3)	1.59	3	[d]	-	0.68	14
1b(*P*4)	[d]	-	0.00	54	0.00	44
1b(*M*1)	0.82	9	1.77	3	1.64	2
1b(*M*2)	1.54	3	0.99	10	0.89	9
1b(*M*3)	0.36	21	1.08	8	1.02	8
1b(*M*4)	0.92	8	0.79	14	0.76	12
1c(*P*1a)[e]	0.11	19	2.61	-	1.90	1
1c(*P*1b)[e]	0.92	5	3.01	-	2.39	-
1c(*P*1c)[e]	0.00	24	2.13	-	1.53	1
1c(*P*2a)[e]	0.98	4	1.06	5	0.63	5
1c(*P*2b)[e]	1.46	2	1.68	2	1.35	1
1c(*P*2c)[e]	0.53	10	0.86	7	0.39	8
1c(*P*3a)[e]	2.06	-	[d]	-	0.88	3
1c(*P*3b)[e]	2.68	-	[d]	-	[d]	-
1c(*P*4a)[e]	1.71	1	0.94	6	0.24	10
1c(*P*4b)[e]	2.08	-	1.15	4	0.64	5
1c(*P*4c)[e]	1.41	2	0.00	32	0.00	15
1c(*M*1a)[e]	1.04	4	1.77	1	1.12	2
1c(*M*1b)[e]	1.60	1	2.00	1	1.82	1
1c(*M*1c)[e]	1.17	3	1.87	1	1.32	2
1c(*M*2a)[e]	1.76	1	1.01	6	0.43	7

1c(*M*2b)[e]	1.98	1	1.43	3	1.19	2
1c(*M*2c)[e]	1.99	1	1.52	2	0.60	5
1c(*M*3a)[e]	0.61	9	1.15	4	0.60	5
1c(*M*3b)[e]	1.21	3	1.61	2	1.31	2
1c(*M*3c)[e]	0.96	4	1.33	3	0.78	3
1c(*M*4a)[e]	1.15	3	0.79	8	0.24	10
1c(*M*4b)[e]	1.63	1	1.14	5	0.68	5
1c(*M*4c)[e]	1.54	2	0.96	6	0.41	7
1d(*P*1a)[e]	1.09	5	3.41	-	[d]	-
1d(*P*1c)[e]	1.26	4	3.43	-	3.27	-
1d(*P*1d)[e]	0.00	30	2.27	-	1.94	1
1d(*P*2a)[e]	1.76	1	1.66	2	1.52	2
1d(*P*2c)[e]	1.78	1	2.27	-	1.67	1
1d(*P*2d)[e]	0.56	11	0.78	9	0.38	13
1d(*P*3a)[e]	2.85	-	1.67	2	1.45	2
1d(*P*3c)[e]	3.85	-	[d]	-	[d]	-
1d(*P*3d)[e]	2.02	-	[d]	-	[d]	-
1d(*P*4a)[e]	2.37	-	1.27	4	1.18	4
1d(*P*4c)[e]	2.74	-	1.48	3	1.67	1
1d(*P*4d)[e]	1.43	3	0.00	35	0.00	25
1d(*M*1a)[e]	1.00	6	1.70	2	1.43	2
1d(*M*1b)[e]	1.50	2	1.85	1	2.15	-
1d(*M*1c)[e]	1.33	3	1.98	1	1.75	1
1d(*M*2a)[e]	1.86	1	0.91	7	0.79	7
1d(*M*2b)[e]	1.86	1	1.35	3	1.15	4
1d(*M*2c)[e]	1.52	2	1.32	4	1.16	4
1d(*M*3a)[e]	0.44	14	1.10	5	0.81	6
1d(*M*3b)[e]	1.22	4	1.76	2	1.38	2
1d(*M*3c)[e]	1.07	6	1.50	3	1.28	3
1d(*M*4a)[e]	1.35	3	0.72	10	0.55	10
1d(*M*4b)[e]	1.61	2	1.59	2	0.89	6
1d(*M*4c)[e]	1.54	2	1.11	5	0.85	6
1e(*P*1)	0.97	8	3.52	-	3.25	-
1e(*P*2)	1.52	3	1.98	2	1.80	2
1e(*P*4)	2.56	-	1.42	4	1.62	3

1e(*M*1)	0.22	28	[d]	-	0.84	12
1e(*M*2)	[d]	-	0.29	28	0.24	33
1e(*M*3)	0.00	42	0.50	20	[d]	-
1e(*M*4)	0.46	19	0.00	46	0.00	50
2a(*P*1)	0.00	70	1.52	3	1.50	3
2a(*P*2)	[d]	-	0.00	38	0.14	35
2a(*P*3)	1.09	10	0.23	25	0.53	18
2a(*P*4)	0.74	20	0.06	34	0.00	44
2a(*M*1)	2.72	-	4.27	-	4.31	-
2a(*M*2)	2.99	-	3.01	-	2.76	-
2a(*M*3)	2.89	-	2.67	-	2.59	-
2a(*M*4)	2.5	-	2.30	-	2.51	-
2b(*P*1)	0.00	54	1.91	2	1.59	4
2b(*P*2)	0.25	35	0.45	31	0.35	34
2b(*P*3)	1.60	3	[d]	-	[d]	-
2b(*P*4)	1.13	8	0.00	67	0.00	62
2b(*M*1)	2.77	-	4.43	-	4.42	-
2b(*M*2)	3.19	-	3.15	-	2.27	-
2b(*M*3)	2.18	-	2.19	-	2.20	-
2b(*M*4)	2.61	-	2.09	-	2.11	-
2c(*P*1a)[e]	0.00	36	2.47	-	2.25	-
2c(*P*1b)[e]	0.47	16	1.51	3	1.46	4
2c(*P*1c)[e]	0.51	15	1.17	6	1.05	6
2c(*P*2a)[e]	0.52	15	0.74	13	0.00	37
2c(*P*2b)[e]	1.17	5	2.72	-	2.51	-
2c(*P*2c)[e]	1.32	4	3.47	-	3.48	-
2c(*P*3a)[e]	1.60	2	[d]	-	1.23	4
2c(*P*3b)[e]	1.63	2	0.68	14	[d]	-
2c(*P*3c)[e]	1.64	2	[d]	-	[d]	-
2c(*P*4a)[e]	1.81	2	0.83	12	0.78	10
2c(*P*4b)[e]	1.99	1	0.00	46	0.01	37
2c(*P*4c)[e]	2.09	-	2.14	-	2.09	-
2c(*M*1a)[e]	2.30	-	3.48	-	3.56	-
2c(*M*1b)[e]	2.57	-	6.20	-	6.20	-
2c(*M*1c)[e]	2.85	-	[d]	-	[d]	-

2c(*M*2a)[e]	3.14	-	1.87	2	2.10	-
2c(*M*2b)[e]	3.41	-	4.62	-	4.53	-
2c(*M*2c)[e]	4.11	-	[d]	-	[d]	-
2c(*M*3a)[e]	4.59	-	1.94	2	1.93	1
2c(*M*3b)[e]	4.61	-	4.02	-	4.12	-
2c(*M*3c)[e]	5.00	-	4.73	-	4.94	-
2c(*M*4a)[e]	5.09	-	1.94	2	1.99	1
2c(*M*4b)[e]	5.17	-	4.05	-	3.98	-
2c(*M*4c)[e]	5.41	-	4.91	-	4.95	-
3a(*P*1)	0.00	24	1.38	2	1.53	2
3a(*P*2)	0.12	20	0.06	23	0.06	24
3a(*P*3)	1.22	3	0.11	21	0.16	20
3a(*P*4)	0.89	5	0.00	26	0.00	26
3a(*M*1)	0.30	16	0.86	6	0.84	6
3a(*M*2)	0.82	6	0.70	8	0.81	6
3a(*M*3)	0.11	20	1.06	4	0.93	6
3a(*M*4)	0.78	6	0.62	10	0.55	10
3b(*P*1)	0.17	24	1.66	2	1.62	2
3b(*P*2)	0.56	13	0.48	14	0.39	15
3b(*P*3)	1.88	1	0.63	11	[d]	-
3b(*P*4)	1.46	3	0.00	32	0.00	30
3b(*M*1)	0.50	14	0.85	7	0.71	9
3b(*M*2)	1.36	3	0.41	16	0.34	17
3b(*M*3)	0.00	33	[d]	-	0.70	9
3b(*M*4)	0.73	9	0.34	18	0.31	18
3c(*P*1a)[e]	0.00	24	2.02	-	1.72	1
3c(*P*1b)[e]	2.09	-	4.31	-	3.88	-
3c(*P*1c)[e]	0.48	11	2.84	-	1.28	2
3c(*P*2a)[e]	0.38	13	0.81	11	0.05	19
3c(*P*2b)[e]	2.62	-	3.23	-	2.66	-
3c(*P*2c)[e]	1.07	4	1.21	6	0.50	9
3c(*P*3a)[e]	1.79	1	0.98	8	1.15	3
3c(*P*3b)[e]	3.65	-	[d]	-	[d]	-
3c(*P*3c)[e]	2.44	-	1.56	3	0.86	5
3c(*P*4a)[e]	1.36	2	0.00	45	0.00	21

3c(*P*4b)[e]	3.13	-	2.94	-	2.36	-
3c(*P*4c)[e]	2.08	-	0.99	8	0.31	12
3c(*M*1a)[e]	1.19	3	2.41	-	1.81	1
3c(*M*1b)[e]	0.62	8	1.63	3	0.94	5
3c(*M*1c)[e]	2.24	-	3.46	-	2.76	-
3c(*M*2a)[e]	2.12	-	2.05	-	1.78	1
3c(*M*2b)[e]	1.42	2	1.13	6	0.54	9
3c(*M*2c)[e]	1.02	4	3.46	-	1.86	1
3c(*M*3a)[e]	0.12	20	2.55	-	[d]	-
3c(*M*3b)[e]	1.95	1	[d]	-	2.73	-
3c(*M*3c)[e]	3.08	-	3.57	-	2.90	-
3c(*M*4a)[e]	1.59	1	1.91	2	1.35	2
3c(*M*4b)[e]	0.84	6	1.08	7	0.48	9
3c(*M*4c)[e]	2.45	-	2.86	-	2.29	-
4(*P*)=**4**(*M*)	0.00	100	0.00	100	0.00	100

[a] MP2/Aug-cc-pVTZ//B3LYP/6-311++G(2d,2p); [b] PCM(MeCN)/MP2/Aug-cc-pVTZ//PCM(MeCN)/B3LYP/6-311++G(2d,2p); [c] PCM(MeOH)/MP2/Aug-cc-pVTZ//PCM(MeOH)/B3LYP/6-311++G(2d,2p); [d] not found at this level of theory; [e] labels a-d refer to the rotamers due to the Et or *i*-Pr substituents (see Figure 5).

Table A2. Relative energies and populations of the stable low-energy conformers of **1a**, **1b** and **1e** calculated at PCM(MeCN)/MP2/Aug-cc-pVTZ//PCM(MeCN)/MP2/6-311G(d,p) level of theory.

Conformer	**1a**		**1b**		**1e**	
	ΔE [kcal mol^{-1}]	Population [%]	*ΔE* [kcal mol^{-1}]	Population [%]	*ΔE* [kcal mol^{-1}]	Population [%]
(*P*1)	0.55	11	0.39	14	1.33	3
(*P*2)	0.00	27	0.06	24	0.93	5
(*P*3)	0.59	10	-	-	-	-
(*P*4)	0.02	27	0.00	27	1.20	3
(*M*1)	0.78	7	0.66	9	0.00	27
(*M*2)	0.77	7	0.76	7	0.12	22
(*M*3)	1.10	4	0.85	6	0.35	15
(*M*4)	0.8	7	0.55	11	0.04	25

Table B1. Structural parameters that characterize low-energy conformers of **1-4** calculated at the PCM(MeCN)/B3LYP/6-311++G(2d,2p) level.

Diol	OH···O [Å]			Torsion angle [°]		
		α[a]	β[b]	ω[c]	φ[d]	φ'[d]
1a(*P*1)	2.503	-176.3	-168.8	179.1		
1a(*P*2)	2.440	-176.4	-37.7	177.3		
1a(*P*3)	2.472	43.9	54.7	177.3		
1a(*P*4)	2.507	-42.1	60.0	177.8		
1a(*M*1)	2.505	156.9	176.6	-176.4		
1a(*M*2)	2.480	30.6	177.8	-177.8		
1a(*M*3)	2.582	-45.2	-47.6	-177.5		
1a(*M*4)	2.495	-59.6	37.5	-179.1		
1b(*P*1)	2.392	-167.0	-167.6	179.1		
1b(*P*2)	2.365	-168.9	-41.1	177.6		
1b(*P*3)[e]	2.443	16.6	56.7	178.3		
1b(*P*4)	2.402	-42.8	65.9	178.1		
1b(*M*1)	2.522	159.8	177.4	-178.4		
1b(*M*2)	2.618	-26.4	-174.7	-178.9		
1b(*M*3)	2.585	-45.6	-45.7	-179.2		
1b(*M*4)	2.579	-52.4	40.4	178.8		
1c(*P*1a)	2.445	-171.1	-169.3	-179.6	-3.6	
1c(*P*1b)	2.308	-156.3	-163.8	179.0	90.8	
1c(*P*1c)	2.430	-168.4	-169.3	-179.3	-111.5	
1c(*P*2a)	2.376	-170.1	-43.3	177.5	-3.8	
1c(*P*2b)	2.257	-157.3	-39.6	176.7	90.9	
1c(*P*2c)	2.357	-167.9	-39.6	178.2	-112.7	
1c(*P*3a)[e]	2.505	24.2	54.3	178.2	-3.2	
1c(*P*4a)	2.504	-43.0	59.2	178.4	-3.5	
1c(*P*4b)	2.443	-38.8	61.6	176.8	92.0	
1c(*P*4c)	2.442	-41.4	64.9	178.6	-113.3	
1c(*M*1a)	2.508	158.4	176.7	-178.1	4.9	
1c(*M*1b)	2.420	160.2	170.9	-179.6	119.2	
1c(*M*1c)	2.520	158.7	177.5	-178.0	-102.6	
1c(*M*2a)	2.625	-25.0	-174.2	-179.1	4.2	
1c(*M*2b)	2.536	-24.4	179.4	179.9	118.4	

1c(*M*2c)	2.499	18.6	178.0	-179.0	-104.4	
1c(*M*3a)	2.579	-45.6	-46.4	-179.2	4.0	
1c(*M*3b)	2.509	-50.9	-49.0	179.1	119.6	
1c(*M*3c)	2.602	-43.3	-46.9	-178.8	-103.0	
1c(*M*4a)	2.554	-54.4	42.0	179.3	3.2	
1c(*M*4b)	2.498	-57.7	42.0	177.4	119.1	
1c(*M*4c)	2.605	-49.9	42.0	179.6	-103.6	
1d(*P*1a)	2.253	-155.9	-161.4	178.5		-158.8
1d(*P*1c)	2.263	-158.2	-161.3	178.5		-11.2
1d(*P*1d)	2.398	-167.1	-168.4	-179.9		132.5
1d(*P*2a)	2.226	-157.6	-40.3	175.4		-158.8
1d(*P*2c)	2.204	-156.0	-39.2	176.3		-12.8
1d(*P*2d)	2.389	-170.1	-39.7	178.4		133.3
1d(*P*3a)	2.419	22.1	56.8	177.1		-157.9
1d(*P*4a)	2.453	-40.4	60.5	176.6		-156.6
1d(*P*4c)	2.400	-39.7	63.2	177.1		-11.9
1d(*P*4d)	2.442	-43.7	65.0	178.4		131.1
1d(*M*1a)	2.479	160.7	173.4	-177.7		149.0
1d(*M*1b)	2.444	160.4	172.6	179.5		-128.4
1d(*M*1c)	2.516	160.0	177.5	-178.8		8.9
1d(*M*2a)	2.627	-24.8	-174.1	-178.3		144.1
1d(*M*2b)	2.497	-8.3	177.2	177.8		-128.7
1d(*M*2c)	2.641	-25.5	-173.7	180.0		10.2
1d(*M*3a)	2.632	-41.3	-48.3	-178.4		144.1
1d(*M*3b)	2.345	-66.5	-68.7	180.0		-131.0
1d(*M*3c)	2.592	-44.6	-54.8	-179.8		10.5
1d(*M*4a)	2.592	-51.3	42.4	179.8		144.1
1d(*M*4b)	2.385	-66.2	39.7	178.8		-131.0
1d(*M*4c)	2.619	-48.4	42.5	178.2		9.8
1e(*P*1)	2.239	-155.3	-166.1	177.9	-13.2	
1e(*P*2)	2.188	-155.8	-39.2	175.6	-13.4	
1e(*P*4)	2.361	-39.8	64.6	176.0	-13.5	
1e(*M*1)[e]	2.517	158.5	177.8	-179.7	11.7	
1e(*M*2)	2.581	-25.5	-171.0	179.2	10.0	
1e(*M*3)	2.686	-36.9	-50.4	178.4	11.2	

1e(*M*4)	2.605	-50.0	42.9	177.6	10.3
2a(*P*1)	2.513	-176.1	-174.5	175.2	
2a(*P*2)	2.602	174.1	27.5	173.4	
2a(*P*3)	2.508	46.6	51.0	174.3	
2a(*P*4)	2.509	-37.7	57.0	173.5	
2a(*M*1)	2.308	147.3	159.1	-173.1	
2a(*M*2)	2.310	29.6	158.8	-174.0	
2a(*M*3)	2.562	-47.5	-48.8	-175.2	
2a(*M*4)	2.443	-63.1	37.1	-176.6	
2b(*P*1)	2.410	-167.9	-171.4	175.7	
2b(*P*2)	2.408	-171.7	-9.2	174.2	
2b(*P*4)	2.504	-42.8	59.3	174.7	
2b(*M*1)	2.270	159.5	153.7	-174.0	
2b(*M*2)	2.218	7.0	158.5	-178.0	
2b(*M*3)	2.470	-53.0	-45.8	-176.3	
2b(*M*4)	2.453	-61.8	38.4	-178.0	
2c(*P*1a)	2.408	-167.1	-173.4	171.9	78.2[f]
2c(*P*1b)	2.432	-168.1	-174.2	178.9	167.7[f]
2c(*P*2c)	2.240	-155.2	-171.2	178.4	-65.2[f]
2c(*P*2a)	2.375	-170.1	-19.4	169.5	78.6[f]
2c(*P*2b)	2.358	-167.7	-30.9	174.6	167.4[f]
2c(*P*2c)	2.379	-170.3	32.5	178.5	-66.1[f]
2c(*P*3b)	2.489	15.4	51.6	175.1	168.3[f]
2c(*P*4a)	2.469	-42.5	59.1	169.8	78.9[f]
2c(*P*4b)	2.486	-43.3	60.2	175.3	168.4[f]
2c(*P*4c)	2.477	-44.4	59.6	178.7	-63.4[f]
2c(*M*1a)	2.281	157.4	154.5	-170.6	73.6[f]
2c(*M*1b)	2.263	155.4	152.3	-176.2	146.8[f]
2c(*M*2a)	2.288	5.5	158.6	-170.6	70.1[f]
2c(*M*2b)	2.263	4.6	154.2	-174.7	149.8[f]
2c(*M*3a)	2.472	-53.3	-48.8	-172.1	72.1[f]
2c(*M*3b)	2.495	-51.6	-44.1	-175.5	156.9[f]
2c(*M*3c)	2.312	-66.2	-56.1	-177.7	-45.4[f]
2c(*M*4a)	2.416	-65.0	38.5	-173.1	71.2[f]
2c(*M*4b)	2.400	-63.8	35.6	-175.2	157.6[f]

2c(*M*4c)	2.459	-72.4	31.2	-177.5	-46.5[f]
3a(*P*1)	2.456	-174.9	-176.8	179.4	
3a(*P*2)	2.372	-174.1	-45.9	176.3	
3a(*P*3)	2.430	46.7	55.9	176.5	
3a(*P*4)	2.441	-40.6	62.3	176.4	
3a(*M*1)	2.473	162.5	175.6	-174.5	
3a(*M*2)	2.402	35.2	173.9	-175.6	
3a(*M*3)	2.555	-45.4	-17.7	-175.0	
3a(*M*4)	2.562	-51.3	37.8	-177.7	
3b(*P*1)	2.380	-167.7	-172.3	179.8	
3b(*P*2)	2.326	-168.8	-44.6	176.6	
3b(*P*3)	2.447	9.4	54.7	177.1	
3b(*P*4)	2.434	-40.9	61.7	176.9	
3b(*M*1)	2.464	165.8	175.0	-176.2	
3b(*M*2)	2.608	-29.6	-173.2	-176.9	
3b(*M*3)[e]	2.519	-47.5	-12.5	-176.3	
3b(*M*4)	2.523	-53.9	39.0	-179.6	
3c(*P*1a)	2.376	-167.3	-172.6	174.0	-70.4[f]
3c(*P*1b)	2.283	-163.3	-166.5	175.2	57.0[f]
3c(*P*1c)	2.338	-165.2	-168.5	178.4	-168.3[f]
3c(*P*2a)	2.184	-159.8	-52.2	173.2	-70.3[f]
3c(*P*2b)	2.247	-165.6	-44.1	-179.3	60.6[f]
3c(*P*2c)	2.339	-169.5	-42.2	176.6	-169.9[f]
3c(*P*3a)	2.322	35.9	66.5	173.9	-73.2[f]
3c(*P*3c)	2.439	18.2	54.4	177.3	-170.2[f]
3c(*P*4a)	2.381	-40.9	64.8	171.8	-71.0[f]
3c(*P*4b)	2.341	-40.4	65.2	-177.9	62.9[f]
3c(*P*4c)	2.365	-41.2	69.0	177.9	-168.2[f]
3c(*M*1a)	2.384	164.9	170.4	-170.9	-80.0[f]
3c(*M*1b)	2.514	165.8	176.9	180.0	63.0[f]
3c(*M*1c)	2.381	165.2	166.8	-175.0	-145.4[f]
3c(*M*2a)	2.580	-27.9	-174.0	-171.9	-80.2[f]
3c(*M*2b)	2.637	-29.3	-172.5	179.5	69.2[f]
3c(*M*3c)	2.379	14.4	168.9	-177.9	-145.4[f]
3c(*M*3a)	2.533	-46.0	-10.3	-172.1	-80.0[f]

3c(*M*3c)	2.578	-44.5	-12.8	-177.9	-142.8[f]
3c(*M*4a)	2.514	-52.4	37.1	-174.5	-80.5[f]
3c(*M*4b)	2.505	-56.0	39.6	179.2	70.2[f]
3c(*M*4c)	2.516	-55.3	40.7	179.8	-143.9[f]
4(*M*,*P*)				±174.5	

[a] H-C4-O-H; [b] H-C5-O-H; [c] C3-C2-C1=O; [d] φ = C2=C3-C(H$_2$)-C(H$_3$), φ' = C2=C3-C(Me$_2$)-H; [e] found at PCM(MeOH)/B3LYP/6-311++G(2d,2p) level; [f] C1-C6-C(H$_2$)-C(H$_3$)

Table B2. Values of intra-ring torsion angles that characterize the low-energy conformers of **1-4** calculated at the PCM(MeCN)/B3LYP/6-311++G(2d,2p) level.

Compound	Torsion angle[a] [°]					
	C_1	C_2	C_3	C_4	C_5	C_6
1a(*P*1)	-0.3	-23.3	47.9	-51.5	28.7	-2.1
1a(*P*2)	-0.2	-21.5	46.6	-52.6	31.7	-4.8
1a(*P*3)	0.2	-23.8	48.2	-51.5	29.0	-2.6
1a(*P*4)	0.7	-24.3	48.2	-50.8	28.3	-2.5
1a(*M*1)	-0.2	20.6	-46.1	52.8	-33.0	6.6
1a(*M*2)	0.1	22.4	-48.5	54.1	-32.2	4.8
1a(*M*3)	1.7	20.2	-48.5	55.8	-34.0	5.4
1a(*M*4)	1.7	20.5	-47.9	54.3	-32.5	4.4
1b(*P*1)	2.0	-26.2	49.3	-50.4	27.4	-2.4
1b(*P*2)	1.9	-25.7	50.1	-52.7	30.1	-4.1
1b(*P*4)	2.3	-25.9	49.9	-51.7	29.4	-3.9
1b(*M*1)	-0.9	25.3	-50.6	52.5	-28.6	2.5
1b(*M*2)	0.4	24.4	-50.5	53.3	-29.4	2.2
1b(*M*3)	0.1	25.4	-51.8	54.0	-29.1	1.8
1b(*M*4)	0.0	26.8	-52.8	52.9	-26.9	-0.1
1c(*P*1a)	2.6	-28.2	50.8	-49.9	25.8	-1.2
1c(*P*1b)	2.1	-26.1	49.7	-50.8	27.8	-2.7
1c(*P*1c)	2.9	-29.1	51.5	-49.9	24.9	-0.5
1c(*P*2a)	2.2	-26.0	50.2	-52.4	29.8	-4.1
1c(*P*2b)	2.8	-25.4	49.1	-52.0	30.4	-5.3
1c(*P*2c)	1.6	-25.8	50.4	-52.6	29.5	-3.4
1c(*P*4a)	2.6	-27.0	50.9	-52.0	29.1	-3.5
1c(*P*4b)	3.2	-25.9	49.4	-51.7	30.4	-5.3
1c(*P*4c)	1.8	-25.9	50.3	-52.0	29.2	-3.3
1c(*M*1a)	-0.9	25.3	-50.8	52.7	-29.1	2.9
1c(*M*1b)	-2.1	28.6	-52.7	51.5	-25.7	0.5
1c(*M*1c)	-1.2	25.4	-50.7	52.7	-29.0	3.0
1c(*M*2a)	-0.4	25.8	-51.5	53.0	-28.5	1.8
1c(*M*2b)	-1.4	28.6	-53.4	52.4	-26.1	-0.1
1c(*M*2c)	-1.3	27.0	-52.3	53.3	-28.3	1.9
1c(*M*3a)	-0.3	26.2	-52.4	53.9	-28.8	1.7

1c(*M*3b)	-1.6	29.8	-54.7	52.9	-25.3	-0.8
1c(*M*3c)	-0.9	26.3	-52.0	53.5	-28.8	2.2
1c(*M*4a)	-0.3	27.1	-53.0	53.0	-27.1	0.1
1c(*M*4b)	-1.6	30.7	-55.2	51.7	-23.3	-2.6
1c(*M*4c)	-0.9	27.3	-52.8	52.8	-27.1	0.6
1d(*P*1a)	0.8	-23.8	-48.0	-50.8	29.2	-3.4
1d(*P*1c)	1.2	-24.0	47.9	-50.4	28.7	-3.5
1d(*P*1d)	1.7	-27.0	50.2	-49.9	26.1	-1.1
1d(*P*2a)	1.4	-22.8	47.6	-52.5	32.4	-6.3
1d(*P*2c)	1.3	-22.5	47.5	-52.4	32.0	-6.2
1d(*P*2d)	1.6	-26.4	51.2	-52.9	29.4	-3.1
1d(*P*3a)	1.7	-24.2	48.5	-52.0	30.9	-5.0
1d(*P*4a)	1.8	24.2	49.1	-52.7	31.8	-5.7
1d(*P*4c)	2.4	-25.0	49.4	-52.1	30.5	-5.2
1d(*P*4d)	2.4	-27.5	52.0	-52.7	29.1	-3.1
1d(*M*1a)	-2.2	26.2	-50.6	51.9	-28.7	3.5
1d(*M*1b)	-2.7	30.8	-54.7	51.5	-24.2	-0.9
1d(*M*1c)	-3.2	29.6	-53.4	51.8	-26.1	1.3
1d(*M*2a)	-1.2	26.1	-51.3	52.6	-28.7	2.6
1d(*M*2b)	-2.2	31.7	-55.5	51.3	-22.8	-2.6
1d(*M*2c)	-2.5	29.7	-53.9	52.0	-25.5	0.1
1d(*M*3a)	-1.4	27.0	-52.6	53.7	-28.9	2.4
1d(*M*3b)	-0.5	28.1	-54.4	54.1	-27.2	-0.0
1d(*M*3c)	-3.0	306	-55.1	53.2	-26.1	0.5
1d(*M*4a)	-1.3	27.8	-53.0	52.5	-26.9	0.7
1d(*M*4b)	-0.5	28.5	-54.0	52.3	-25.1	-1.5
1d(*M*4c)	-2.7	31.7	-55.7	51.7	-23.5	-1.8
1e(*P*1)	0.4	-22.8	48.1	-51.6	30.3	-4.2
1e(*P*2)	0.7	-21.6	47.8	-53.2	33.1	-6.8
1e(*P*4)	1.3	-22.7	48.5	-52.9	32.7	-6.6
1e(*M*2)	-3.4	32.3	-56.0	51.6	-23.7	-1.2
1e(*M*3)	-3.9	33.7	-57.2	51.6	-22.6	-2.0
1e(*M*4)	-3.4	33.5	-57.2	51.3	-22.1	-2.8
2a(*P*1)	1.6	-24.4	50.1	-54.8	33.2	-6.1
2a(*P*2)	0.2	-21.2	49.1	-57.2	37.2	-8.6

2a(*P*3)	0.8	-22.9	50.3	-56.9	36.0	-7.7
2a(*P*4)	1.6	-23.1	50.1	-56.7	36.2	-8.5
2a(*M*1)	1.3	15.0	-41.8	51.5	-34.9	9.5
2a(*M*2)	0.7	17.8	-44.3	52.0	-33.3	7.8
2a(*M*3)	1.7	17.3	-44.8	52.9	-33.4	7.2
2a(*M*4)	2.2	17.3	-45.0	52.4	-32.5	6.0
2b(*P*1)	2.8	-25.8	50.9	-53.7	31.7	-6.0
2b(*P*3)	2.1	-24.1	51.1	-56.2	35.2	-8.1
2b(*P*4)	2.6	-25.3	52.0	-56.1	34.5	-7.6
2b(*M*1)	1.7	15.6	-42.9	51.5	-34.1	8.5
2b(*M*2)	1.8	18.6	-45.4	51.8	-32.1	5.5
2b(*M*3)	1.6	18.5	-45.9	52.0	-31.7	5.8
2b(*M*4)	1.6	19.5	-46.7	51.4	-30.1	4.2
2c(*P*1a)	2.9	-24.5	50.6	-55.5	34.9	-8.6
2c(*P*1b)	1.6	-27.0	52.8	-53.7	29.4	-3.1
2c(*P*1c)	-0.3	-24.4	51.6	-55.1	31.3	-3.4
2c(*P*2a)	2.2	-22.0	50.1	-58.1	39.0	-11.5
2c(*P*2b)	1.9	-24.1	51.4	-56.5	35.3	-8.1
2c(*P*2c)	0.1	-24.1	52.1	-56.8	33.9	-5.3
2c(*P*3b)	1.9	-24.2	51.0	-55.5	34.4	-7.5
2c(*P*4a)	2.9	-23.0	50.7	-57.9	38.8	-11.5
2c(*P*4b)	2.5	-25.4	52.1	-55.6	33.9	-7.1
2c(*P*4c)	1.8	-26.9	53.7	-56.1	32.4	-4.8
2c(*M*1a)	0.0	16.5	-44.0	53.2	-36.3	11.0
2c(*M*1b)	0.8	18.4	-44.0	48.7	-29.5	5.5
2c(*M*2a)	0.7	16.0	-44.3	54.3	-37.3	11.1
2c(*M*2b)	1.9	16.4	-44.0	51.9	-33.8	7.8
2c(*M*3a)	0.8	17.4	-46.0	54.6	-35.8	9.4
2c(*M*3b)	2.2	17.4	-46.3	53.6	-33.7	6.9
2c(*M*3c)	3.8	14.0	-40.9	48.3	-29.9	5.0
2c(*M*4a)	0.9	17.9	-46.2	54.0	-34.8	8.5
2c(*M*4b)	3.1	15.4	-44.6	53.2	-34.8	7.6
2c(*M*4c)	4.4	1.3	-40.2	47.7	-29.6	4.6
3a(*P*1)	0.4	-24.4	49.0	-51.2	28.0	-2.1
3a(*P*2)	0.8	-22.4	47.7	-52.6	31.8	-5.8

3a(*P*3)	1.1	-22.8	47.9	-52.5	31.7	-5.7
3a(*P*4)	1.7	-23.4	47.9	-52.0	31.3	-5.8
3a(*M*1)	-0.7	21.4	-47.8	53.4	-32.9	7.0
3a(*M*2)	-0.6	22.9	-49.5	54.3	-32.4	5.8
3a(*M*3)	0.5	20.9	-48.5	54.8	-33.8	6.5
3a(*M*4)	0.4	22.9	-50.2	53.9	-30.9	3.9
3b(*P*1)	1.8	-26.2	49.9	-49.9	26.2	-1.8
3b(*P*2)	2.6	-24.9	49.3	-51.8	30.1	-5.5
3b(*P*3)	2.2	-22.4	49.0	-51.5	30.0	-5.1
3b(*P*4)	2.7	-25.0	49.4	-51.5	30.0	-5.4
3b(*M*1)	-0.5	23.0	-49.7	53.2	-31.2	5.2
3b(*M*2)	0.3	22.6	-49.9	53.5	-31.2	4.5
3b(*M*4)	0.1	25.0	-52.0	53.0	-28.5	1.8
3c(*P*1a)	2.2	-23.5	49.3	-53.7	32.9	-7.2
3c(*P*1b)	2.1	-28.0	47.0	-41.0	25.7	-4.4
3c(*P*1c)	2.1	-23.1	48.8	-49.7	27.6	-3.5
3c(*P*2a)	1.9	-21.1	46.9	-53.3	34.4	-9.0
3c(*P*2b)	2.3	-25.6	46.6	-44.7	21.7	-0.4
3c(*P*2c)	2.0	-24.1	49.2	-52.3	30.8	-5.8
3c(*P*3a)	2.8	-23.9	49.6	-53.9	33.3	-7.8
3c(*P*3c)	2.0	-24.2	48.8	-51.3	30.0	-5.2
3c(*P*4a)	3.4	-23.2	48.8	-54.1	35.0	-9.8
3c(*P*4b)	2.7	-26.7	46.7	-42.8	29.3	1.2
3c(*P*4c)	2.0	-24.3	48.9	-51.0	29.6	-4.9
3c(*M*1a)	-1.3	21.2	-48.6	54.7	-35.4	9.3
3c(*M*1b)	0.2	24.7	-51.5	52.9	-28.6	2.1
3c(*M*1c)	-0.0	21.9	-49.6	54.1	-32.7	6.2
3c(*M*2a)	-0.5	21.4	-49.5	55.4	-35.2	8.2
3c(*M*2b)	0.7	24.4	-51.2	52.7	-28.4	1.7
3c(*M*2c)	-0.2	24.1	-51.5	54.1	-30.6	4.0
3c(*M*3a)	-0.5	21.8	-50.1	55.9	-35.2	8.0
3c(*M*3c)	0.6	23.2	-51.4	54.8	-31.5	4.1
3c(*M*4a)	-0.8	24.0	-51.9	55.2	-32.6	5.6
3c(*M*4b)	1.8	24.2	-51.8	534	-28.7	1.4
3c(*M*4c)	0.8	24.4	-52.4	53.9	-29.2	2.1

4(*M*)	3.1	19.4	-46.3	52.6	-31.2	3.0

[a] $C_1 = \tau$; C_2 = C2=C3-C4-C5; C_3 = C3-C4-C5-C6; C_4 = C4-C5-C6-C1; C_5 = C5-C6-C1-C2; C_6 = C6-C1-C2=C3

Table B3. Structural parameters that characterize low-energy conformers of **1a**, **1b** and **1c** calculated at the PCM(MeCN)/MP2/6-311G(d,p) level.

Diol	OH···O [Å]	Torsion angle [°]			
		α^a	β^b	ω^c	φ^d
1a(*P*1)	2.179	-160.0	-175.3	178.5	
1a(*P*2)	2.110	-161.9	-40.0	172.9	
1a(*P*3)	2.124	62.6	76.1	172.5	
1a(*P*4)	2.153	-42.9	79.1	172.2	
1a(*M*1)	2.180	159.1	161.7	-172.9	
1a(*M*2)	2.150	43.0	163.2	-174.1	
1a(*M*3)	2.168	-71.2	-72.7	-174.9	
1a(*M*4)	2.187	-74.3	43.3	-175.4	
1b(*P*1)	2.181	-160.2	-175.5	178.5	
1b(*P*2)	2.111	-161.7	-41.2	173.0	
1b(*P*4)	2.156	-41.6	77.8	172.3	
1b(*M*1)	2.201	160.6	162.5	-174.1	
1b(*M*2)	2.167	29.9	164.1	-174.9	
1b(*M*3)	2.175	-71.0	-72.9	-175.7	
1b(*M*4)	2.193	-74.4	43.6	-176.0	
1e(*P*1)	2.133	-157.5	-177.3	177.5	-14.5
1e(*P*2)	2.067	-159.2	-40.8	171.9	-17.0
1e(*P*4)	2.135	-47.7	76.9	171.1	-17.4
1e(*M*1)	2.229	154.9	165.9	-175.9	11.1
1e(*M*2)	2.202	37.5	166.2	-176.6	12.5
1e(*M*3)	2.195	-69.0	-75.0	-177.8	11.5
1e(*M*4)	2.211	-71.8	45.5	-178.1	11.6

[a] H-C4-O-H; [b] H-C5-O-H; [c] C3-C2-C1=O; [d] φ = C2=C3-C-C(H_3).

Table B4. Values of intra-ring torsion angles that characterize the low-energy conformers of **1a**, **1b** and **1c** calculated at the PCM(MeCN)/MP2/6-311G(d,p) level.

Diol	Torsion angle[a] [°]					
	C_1	C_2	C_3	C_4	C_5	C_6

1a(*P*1)	-0.1	-25.0	51.7	-55.8	30.8	-2.6
1a(*P*2)	0.0	-20.7	49.2	-58.5	37.6	-8.6
1a(*P*3)	0.4	-20.9	49.2	-58.5	38.4	-9.3
1a(*P*4)	0.9	-21.6	49.0	-58.0	38.2	-9.7
1a(*M*1)	-1.2	22.5	-49.7	57.0	-36.1	8.2
1a(*M*2)	-0.6	23.6	-51.5	58.4	-36.0	7.0
1a(*M*3)	0.2	23.0	-51.8	59.1	-36.0	6.5
1a(*M*4)	0.2	23.0	-51.5	58.2	-35.3	6.1
1b(*P*1)	0.9	-26.1	52.6	-55.2	30.1	-2.7
1b(*P*2)	1.5	-22.3	49.9	-57.4	36.5	-8.8
1b(*P*4)	1.8	-22.0	49.5	-57.2	37.5	-9.9
1b(*M*1)	-1.5	24.1	-50.9	56.2	-34.5	7.0
1b(*M*2)	-0.4	24.1	-52.0	57.8	-35.2	6.3
1b(*M*3)	0.0	23.8	-52.4	58.2	-34.9	5.9
1b(*M*4)	0.1	23.5	-51.9	57.5	-34.6	5.6
1e(*P*1)	0.0	-24.0	52.2	-56.1	31.9	-4.1
1e(*P*2)	0.3	-19.6	49.0	-58.3	38.6	-10.4
1e(*P*4)	0.8	-19.5	48.8	-58.3	38.6	-11.5
1e(*M*1)	-3.8	29.7	-55.0	54.8	-29.9	4.0
1e(*M*2)	-2.6	29.2	-55.6	56.3	-30.9	3.6
1e(*M*3)	-2.3	29.6	-56.5	56.4	-29.9	2.6
1e(*M*4)	-2.1	293.1	-55.8	5.7	-29.5	2.3

[a] C_1 = τ; C_2 = C2=C3-C4-C5; C_3 = C3-C4-C5-C6; C_4 = C4-C5-C6-C1; C_5 = C5-C6-C1-C2; C_6 = C6-C1-C2=C3

Table C. Specific optical rotations for *cis*-ketodiols **1-4**, calculated at the IEFPCM/B3LYP/Aug-cc-pVTZ level and measured in methanol solution.

Diol	Conformer	Calculated opical rotations				Measured optical rotations			
		589 nm	578 nm	546 nm	436 nm	589 nm	578 nm	546 nm	436 nm
1a	(*P*1)	-422	-544	-637	-1269				
	(*P*2)	-259	-365	-432	-930				
	(*P*3)	-367	-462	-534	-980				
	(*P*4)	-293	-391	-455	-857				
	(*M*1)	-159	-107	-111	-11				
	(*M*2)	-119	-98	-105	-63				
	(*M*3)	-56	-41	-39	+66				
	(*M*4)	-105	-131	-148	-234				
***ΔE*[a] Boltzmann averaged**		-255	-329	-383	-716	-217	-227	-261	-465
1b	(*P*1)	-236	-288	-335	-635				
	(*P*2)	-120	-174	-206	-444				
	(*P*3)	-166	-225	-261	-475				
	(*P*4)	-128	-178	-206	-380				
	(*M*1)	-98	-58	-60	+1				
	(*M*2)	-59	-44	-46	-3				
	(*M*3)	+6	+13	+20	+121				
	(*M*4)	-30	-58	-67	-114				
***ΔE* Boltzmann averaged**		-103	-140	-162	-287	-119	-124	-141	-237
1c	(*P*1a)	-197	-241	-280	-523				
	(*P*1b)	-135	-251	-292	-567				
	(*P*1c)	-282	-259	-299	-531				
	(*P*2a)	-93	-138	-163	-345				
	(*P*2b)	-46	-158	-189	-437				
	(*P*2c)	-187	-163	-190	-377				
	(*P*3a)	-160	-210	-241	-419				
	(*P*4a)	-94	-143	-167	-317				
	(*P*4b)	-87	-202	-237	-469				
	(*P*4c)	-195	-176	-203	-350				
	(*M*1a)	-81	-36	-35	+37				
	(*M*1b)	+79	+56	+68	+184				
	(*M*1c)	-142	-44	-44	+40				

	(*M*2a)	-41	-22	-21	+30				
	(*M*2b)	+116	+72	+85	+191				
	(*M*2c)	-97	-19	-16	+61				
	(*M*3a)	+14	+25	+33	+131				
	(*M*3b)	+156	+103	+120	+245				
	(*M*3c)	-50	+21	+30	+150				
	(*M*4a)	-26	-47	-54	-93				
	(*M*4b)	+122	+35	+38	+20				
	(*M*4c)	-90	-50	-57	-80				
ΔE Boltzmann averaged		-82	-88	-101	-168	-103	-107	-123	-201
1d	(*P*1c)	-167	-225	-264	-525				
	(*P*1d)	-257	-230	-264	-451				
	(*P*2a)	-26	-118	-142	-349				
	(*P*2c)	-77	-131	-158	-389				
	(*P*2d)	-164	-134	-156	-304				
	(*P*3a)	-108	-208	-242	-473				
	(*P*4a)	-56	-162	-191	-401				
	(*P*4c)	-111	-172	-202	-417				
	(*P*4d)	-187	-163	-186	-306				
	(*M*1a)	-112	-18	-14	+85				
	(*M*1b)	+110	+80	+95	+216				
	(*M*1c)	+7	+49	+61	+195				
	(*M*2a)	-88	-12	-9	+65				
	(*M*2b)	+155	+120	+140	+284				
	(*M*2c)	+38	+68	+82	+214				
	(*M*3a)	-44	+22	+30	+136				
	(*M*3b)	+180	+120	+136	+224				
	(*M*3c)	+79	+96	+114	+263				
	(*M*4a)	-84	-45	-51	-74				
	(*M*4b)	+137	+61	+67	+75				
	(*M*4c)	+44	+32	+36	+56				
ΔE Boltzmann averaged		-72	-62	-71	-112	-79	-82	-94	-150
1e	(*P*1)	-119	-173	-203	-412				
	(*P*2)	-43	-92	-113	-300				
	(*P*4)	-78	-133	-158	-345				

	(*M*1)	+30	+71	+86	+228				
	(*M*2)	+63	+94	+111	+249				
	(*M*4)	+58	+49	+56	+83				
***ΔE* Boltzmann averaged**		+51	+63	+74	+151	-9	-9	-10	-17
2a	(*P*1)	-321	-408	-480	-999				
	(*P*2)	-300	-382	-450	-943				
	(*P*3)	-296	-364	-424	-827				
	(*P*4)	-220	-292	-343	-693				
	(*M*1)	-109	+6	+17	+196				
	(*M*2)	-171	-73	-74	+25				
	(*M*3)	-36	+40	+53	+207				
	(*M*4)	-87	-48	-53	-66				
***ΔE* Boltzmann averaged**		-264	-340	-399	-814	+223[b]	+234[b]	+273[b]	+540[b]
2b	(*P*1)	-183	-210	-246	-498				
	(*P*2)	-127	-155	-185	-425				
	(*P*4)	-88	-120	-142	-303				
	(*M*1)	-75	+33	+46	+210				
	(*M*2)	-101	-19	-15	+88				
	(*M*3)	+18	+93	+113	+298				
	(*M*4)	-34	+4	+6	+41				
***ΔE* Boltzmann averaged**		-105	-135	-161	-352	+94[b]	+98[b]	+116[b]	+237[b]
2c	(*P*1a)	-159	-224	-267	-607				
	(*P*1b)	-183	-223	-259	-482				
	(*P*2c)	-192	-174	-201	-360				
	(*P*2a)	-99	-161	-196	-507				
	(*P*2b)	-163	-202	-236	-479				
	(*P*2c)	-161	-141	-165	-328				
	(*P*3b)	-91	-142	-166	-328				
	(*P*3c)	-110	-97	-112	-189				
	(*P*4a)	-60	-152	-153	-394				
	(*P*4b)	-93	-141	-164	-318				
	(*P*4c)	-110	-97	-112	-190				
	(*M*1a)	-56	+104	+133	+449				
	(*M*1b)	-6	+52	+65	+202				
	(*M*2a)	-84	+48	+66	+307				

	(*M*2b)	-56	-14	-11	+79				
	(*M*2c)	-65	-27	-32	-55				
	(*M*3a)	+32	+160	+195	+518				
	(*M*3b)	+31	+54	+67	+203				
	(*M*3c)	-65	-28	-33	-58				
	(*M*4a)	-15	+83	+103	+307				
	(*M*4b)	-20	-23	-24	-8				
	(*M*4c)	-105	-99	-117	-257				
ΔE Boltzmann averaged		-96	-144	-168	-377	+104[b]	+109[b]	+128[b]	+259[b]
3a	(*P*1)	-364	-506	-588	-1108				
	(*P*2)	-221	-352	-412	-829				
	(*P*3)	-329	-445	-512	-897				
	(*P*4)	-263	-391	-451	-811				
	(*M*1)	-190	-184	-200	-170				
	(*M*2)	-224	-229	-252	-271				
	(*M*3)	-115	-134	-144	-111				
	(*M*4)	-130	-187	-211	-326				
ΔE Boltzmann averaged		-239	-337	-387	-677				
3b	(*P*1)	-225	-319	-368	-656				
	(*P*2)	-140	-233	-272	-535				
	(*P*4)	-139	-239	-276	-491				
	(*M*1)	-158	-162	-179	-200				
	(*M*2)	-103	-129	-142	-162				
	(*M*3)	-74	-100	-108	-88				
	(*M*4)	-87	-148	-167	-271				
ΔE Boltzmann averaged		-121	-185	-211	-343				
3c	(*P*1a)	-169	-321	-374	-745				
	(*P*1b)	-166	-192	-214	-263				
	(*P*1c)	-212	-271	-312	-542				
	(*P*2a)	-112	-271	-321	-707				
	(*P*2b)	-95	-127	-143	-198				
	(*P*2c)	-126	-183	-213	-418				
	(*P*3a)	-170	-325	-378	-745				
	(*P*3c)	-161	-220	-253	-440				
	(*P*4a)	-116	-286	-336	-698				

	(*P*4b)	-88	-138	-153	-167
	(*P*4c)	-132	-186	-214	-363
	(*M*1a)	-183	-150	-160	-101
	(*M*1b)	-121	-174	-197	-297
	(*M*1c)	-101	-73	-79	-55
	(*M*2a)	-196	-177	-192	-163
	(*M*2b)	-72	-142	-162	-262
	(*M*3c)	-89	-75	-81	-61
	(*M*3a)	-105	-102	-107	-41
	(*M*3c)	-18	-18	-16	+42
	(*M*4b)	-54	-151	-175	-337
	(*M*4c)	-30	-59	-68	-118
***ΔE* Boltzmann averaged**		-108	-151	-171	-248
4	(*P*,*M*)	±53	±75	±87	±173

[a] relative energies calculated at PCM/MP2/Aug-cc-pVTZ level for structures optimized at PCM/B3LYP/6-311++G(2d,2p) level; [b] measured for enantiomer

Table D. Rotatory strengths and excitation energies calculated at the PCM/B2LYP/6-311++G(2d,2p) level for *P*-type conformers of model compounds **4-23** with varying torsion angles ω and τ.

Compound	Angle [º]		1st transition (n-π*)		2nd transition (π-π*)		3rd transition (π-σ*)	
	ω	τ	R^a	λ [nm]	R^a	λ [nm]	R^a	λ [nm]
4	-175	-5	-2.3036	282.77	38.4577	210.52	-4.7642	176.63
4	-175	-4	-0.7182	282.74	27.7952	210.2	-7.2085	176.51
4	-175	-3	0.8917	282.72	16.8432	209.96	-9.8075	176.43
4	-175	-2	2.5156	282.7	6.2868	209.81	-12.4814	176.4
4	-175	-1	4.1376	282.68	-4.3035	209.75	-15.0086	176.42
4	-175	0	5.8482	282.66	-14.5094	209.78	-17.3719	176.49
4	-175	1	7.5914	282.63	-24.2454	209.9	-19.2077	176.62
4	-175	2	9.3639	282.57	-33.3122	210.14	-20.1758	176.82
4	-175	3	11.1847	282.51	-41.4683	210.5	-19.3049	177.09
4	-175	4	13.0399	282.43	-48.2944	211.02	-4.4607	177.47
4	-175	5	14.9507	282.33	-53.7894	211.74	-51.0585	180.54
4	-176	-5	-2.5053	283.02	40.6438	210.57	-5.2391	176.64
4	-176	-4	-0.9701	282.98	29.8247	210.23	-7.7166	176.52
4	-176	-3	0.625	282.95	18.8124	209.97	-10.305	176.43
4	-176	-2	2.236	282.93	7.9943	209.8	-13.0334	176.4
4	-176	-1	3.8418	282.91	-2.536	209.72	-15.6798	176.41
4	-176	0	5.4865	282.89	-13.0424	209.72	-18.0846	176.47
4	-176	1	7.2265	282.85	-23.1559	209.81	-20.1579	176.59
4	-176	2	8.9675	282.82	-32.6747	210.01	-21.5224	176.77
4	-176	3	10.7693	282.76	-41.4475	210.31	-21.8347	177.02
4	-176	4	12.5915	282.68	-49.1018	210.75	-19.559	177.34
4	-176	5	14.4867	282.59	-55.4533	211.35	9.4042	177.9
4	-177	-5	-2.6919	283.26	42.8848	210.64	-5.7667	176.66
4	-177	-4	-1.184	283.21	32.0139	210.27	-8.2408	176.53
4	-177	-3	0.3531	283.18	21.03	210	-10.8929	176.45
4	-177	-2	1.943	283.15	9.8518	209.81	-13.5857	176.41
4	-177	-1	3.5657	283.13	-0.8924	209.7	-16.3119	176.41
4	-177	0	5.1679	283.1	-11.4967	209.68	-18.7971	176.47
4	-177	1	6.8351	283.07	-21.7756	209.75	-20.9405	176.58
4	-177	2	8.6015	283.03	-31.7116	209.91	-22.6009	176.75
4	-177	3	10.369	282.98	-40.9794	210.17	-23.4336	176.98

4	-177	4	12.1666	282.91	-49.315	210.55	-22.9604	177.27
4	-177	5	14.0096	282.82	-56.5242	211.05	-18.6965	177.64
4	-178	-5	-2.8839	283.5	45.1557	210.71	-6.3333	176.69
4	-178	-4	-1.3924	283.44	34.2812	210.33	-8.8077	176.56
4	-178	-3	0.1164	283.39	23.2281	210.04	-11.4578	176.47
4	-178	-2	1.6664	283.36	12.1239	209.83	-14.1971	176.42
4	-178	-1	3.265	283.33	0.8917	209.71	-16.9147	176.42
4	-178	0	4.8559	283.3	-9.8408	209.67	-19.4636	176.48
4	-178	1	6.503	283.27	-20.2842	209.72	-21.7131	176.58
4	-178	2	8.1999	283.24	-30.4406	209.85	-23.4631	176.74
4	-178	3	9.983	283.18	-40.1561	210.07	-24.6211	176.95
4	-178	4	11.7543	283.13	-49.0905	210.4	-24.8562	177.22
4	-178	5	13.5833	283.05	-57.0428	210.84	-23.5809	177.56
4	-179	-5	-3.0607	283.74	47.5089	210.81	-6.9929	176.72
4	-179	-4	-1.5995	283.66	36.6167	210.4	-9.4398	176.58
4	-179	-3	-0.1087	283.6	25.5034	210.09	-12.0679	176.49
4	-179	-2	1.4141	283.56	14.3265	209.87	-14.8285	176.45
4	-179	-1	2.9787	283.52	3.164	209.73	-17.5663	176.45
4	-179	0	4.558	283.49	-7.9785	209.67	-20.1147	176.49
4	-179	1	6.1855	283.46	-18.677	209.7	-22.4159	176.59
4	-179	2	7.8382	283.42	-28.9747	209.81	-24.2587	176.74
4	-179	3	9.5985	283.38	-39.0774	210	-25.5995	176.94
4	-179	4	11.3672	283.31	-48.4256	210.29	-26.2	177.2
4	-179	5	13.1604	283.24	-56.9984	210.68	-25.8417	177.51
4	180	-5	1.7689	283.25	16.9983	209.46	-10.3599	176.48
4	180	-4	2.2269	283.32	12.7164	209.48	-12.4457	176.48
4	180	-3	2.7285	283.4	8.1994	209.5	-14.5832	176.47
4	180	-2	3.2206	283.49	3.6946	209.54	-16.6503	176.48
4	180	-1	3.7474	283.57	-0.9521	209.61	-18.7606	176.5
4	180	0	4.2643	283.67	-5.5887	209.69	-20.8189	176.52
4	180	1	4.7981	283.78	-10.2901	209.79	-22.8532	176.55
4	180	2	5.3404	283.89	-15.0576	209.9	-24.8285	176.58
4	180	3	5.8679	284.03	-19.7705	210.05	-26.6253	176.62
4	180	4	6.4689	284.16	-24.6474	210.2	-28.4204	176.67
4	180	5	7.0523	284.31	-29.5453	210.37	-30.0056	176.73

4	179	-5	-3.3927	284.2	52.3542	211.03	-8.6764	176.79
4	179	-4	-2.0029	284.09	41.4425	210.58	-10.8955	176.66
4	179	-3	-0.5656	284.01	30.2921	210.24	-13.4308	176.56
4	179	-2	0.9195	283.94	19.0334	209.98	-16.1542	176.51
4	179	-1	2.4364	283.88	7.6406	209.81	-18.8677	176.51
4	179	0	3.9909	283.83	-3.6198	209.72	-21.4746	176.55
4	179	1	5.6262	283.79	-14.9579	209.71	-23.7701	176.64
4	179	2	7.185	283.75	-25.6331	209.79	-25.6942	176.78
4	179	3	8.8724	283.7	-35.9905	209.94	-27.199	176.96
4	179	4	10.5839	283.65	-45.9462	210.17	-28.138	177.2
4	179	5	12.3618	283.59	-55.6035	210.49	-28.5199	177.48
4	178	-5	-3.5544	284.43	54.7388	211.16	-9.8321	176.84
4	178	-4	-2.1913	284.3	43.9942	210.69	-11.8102	176.7
4	178	-3	-0.7834	284.2	32.8205	210.32	-14.2327	176.61
4	178	-2	0.6688	284.12	21.49	210.05	-16.867	176.55
4	178	-1	2.1751	284.05	10.1126	209.86	-19.5711	176.55
4	178	0	3.7055	283.99	-1.3043	209.76	-22.1357	176.59
4	178	1	5.3212	283.94	-12.7945	209.74	-24.4319	176.67
4	178	2	6.8612	283.89	-23.6157	209.8	-26.3598	176.81
4	178	3	8.5138	283.84	-34.2928	209.93	-27.8686	176.99
4	178	4	10.2222	283.79	-44.4472	210.14	-28.9304	177.21
4	178	5	11.9621	283.73	-54.1853	210.44	-29.4393	177.49
4	177	-5	-3.7061	284.66	57.1868	211.31	-11.6419	176.89
4	177	-4	-2.3705	284.52	46.512	210.81	-12.895	176.75
4	177	-3	-0.9989	284.4	35.4283	210.42	-15.1496	176.65
4	177	-2	0.4346	284.3	24.0795	210.13	-17.6747	176.6
4	177	-1	1.9052	284.22	12.6098	209.93	-20.2817	176.59
4	177	0	3.4177	284.14	1.1512	209.81	-22.8153	176.63
4	177	1	5.0006	284.08	-10.4864	209.77	-25.0883	176.71
4	177	2	6.6034	284.03	-21.5952	209.82	-27.0242	176.84
4	177	3	8.1778	283.97	-32.2932	209.94	-28.5313	177.02
4	177	4	9.8657	283.92	-42.7555	210.14	-29.6436	177.24
4	177	5	11.587	283.86	-52.6927	210.41	-30.2587	177.51
4	176	-5	-3.857	284.88	59.5697	211.47	-17.4488	176.99
4	176	-4	-2.5602	284.73	49.0833	210.95	-14.3918	176.81

4	176	-3	-1.2065	284.59	38.0751	210.54	-16.1842	176.71
4	176	-2	0.188	284.47	26.7556	210.22	-18.5575	176.65
4	176	-1	1.6455	284.37	15.2685	210	-21.0613	176.64
4	176	0	3.1363	284.29	3.7367	209.87	-23.5348	176.68
4	176	1	4.6959	284.22	-8.0086	209.82	-25.758	176.76
4	176	2	6.2742	284.16	-19.2701	209.85	-27.671	176.89
4	176	3	7.8978	284.09	-30.2785	209.96	-29.1735	177.06
4	176	4	9.5103	284.03	-40.8394	210.14	-30.3094	177.27
4	176	5	11.214	283.97	-51.0072	210.4	-30.9875	177.53
4	175	-5	-4.0113	285.1	61.2258	211.65	-24.9326	177.83
4	175	-4	-2.7461	284.93	51.6471	211.1	-17.3871	176.89
4	175	-3	-1.4271	284.77	40.7877	210.66	-17.4796	176.77
4	175	-2	-0.0497	284.64	29.5503	210.33	-19.5661	176.71
4	175	-1	1.3813	284.53	18.0139	210.09	-21.9215	176.7
4	175	0	2.8579	284.43	6.3945	209.94	-24.228	176.73
4	175	1	4.3832	284.34	-5.4163	209.88	-26.4378	176.81
4	175	2	5.9465	284.27	-16.7389	209.9	-28.3013	176.93
4	175	3	7.5252	284.2	-27.6654	209.99	-29.835	177.1
4	175	4	9.1573	284.14	-38.6547	210.16	-30.939	177.31
4	175	5	10.8486	284.08	-49.0721	210.4	-31.6577	177.57
5	-175	0	10.2661	277.04	-42.1523	214.34	-7.6321	182.87
5	-175	5	22.2241	278.31	-125.635	215.91	72.7419	186.23
5	180	-5	-7.3694	275.97	58.8142	215.7	-13.2294	184.11
5	180	0	5.1765	276.58	-5.2952	213.95	-10.4907	182.89
5	180	5	17.3777	277.58	-78.2184	214.39	-6.9882	183.31
5	175	-5	-13.8362	275.39	69.6804	218.75	-14.3524	187.07
5	175	0	-0.3946	275.83	19.7117	215.02	-12.4079	184.11
5	175	5	12.2952	276.64	-44.4255	214.19	-9.5298	183.5
(4*S*)-**6**	-175	-5	-9.4679	283.81	36.133	214.56	18.4461	177.21
(4*S*)-**6**	-175	0	1.4299	284.42	-23.4174	211.7	16.916	177.18
(4*S*)-**6**	-175	5	11.9497	285.46	-99.9001	211.85	49.7272	184.28
(4*S*)-**6**	180	-5	-14.8516	283.43	36.1332	218.85	12.5998	180.62
(4*S*)-**6**	180	0	4.5925	284.13	-38.909	210.77	-18.7152	175.18
(4*S*)-**6**	180	5	7.3213	284.86	-60.3205	211.53	-17.8685	175.64
(4*S*)-**6**	175	-5	-21.7914	282.51	2.9522	232.34	2.592	191.69

(4*S*)-**6**	175	0	-8.56	283.01	-3.7455	219.24	1.801	181.36
(4*S*)-**6**	175	5	2.6224	283.78	-40.3535	213.66	-13.492	177.13
(4*R*)-**6**	-175	-5	-4.2624	284.74	77.1275	214.65	-3.9704	177.05
(4*R*)-**6**	-175	0	5.62	285.26	11.9874	212.61	10.5413	184.13
(4*R*)-**6**	-175	5	15.8173	286.3	-79.6847	213.04	58.3572	193.94
(4*R*)-**6**	180	-5	-7.4293	284.58	97.4792	216.21	-2.84	177.06
(4*R*)-**6**	180	0	2.1134	284.86	44.8022	212.87	-20.49	175.86
(4*R*)-**6**	180	5	11.8174	285.57	-24.0679	212.17	35.0631	181.07
(4*R*)-**6**	175	-5	-11.0286	284.27	103.4973	222.37	18.5646	185.08
(4*R*)-**6**	175	0	-1.2953	284.29	65.7241	215.31	-22.0578	176.9
(4*R*)-**6**	175	5	8.2756	284.71	7.3405	212.79	-42.5315	176.43
(4*S*)-**7**	-175	-5	-2.747	285.76	-20.4479	209.2	52.2155	190.05
(4*S*)-**7**	-175	-4	-0.7389	285.73	-34.8596	209.05	57.8486	189.72
(4*S*)-**7**	-175	-3	1.2802	285.72	-48.6588	208.94	62.8802	189.41
(4*S*)-**7**	-175	-2	3.3129	285.69	-61.9209	208.89	67.1842	189.13
(4*S*)-**7**	-175	-1	5.3742	285.65	-74.5888	208.87	70.6511	188.86
(4*S*)-**7**	-175	0	7.4127	285.6	-86.5227	208.9	73.2104	188.64
(4*S*)-**7**	-175	1	9.4971	285.61	-97.7963	208.97	74.4749	188.46
(4*S*)-**7**	-175	2	11.5656	285.53	-108.223	209.07	74.4375	188.33
(4*S*)-**7**	-175	3	13.5947	285.44	-117.466	209.2	71.9972	188.31
(4*S*)-**7**	-175	4	15.6714	285.33	-126.352	209.37	65.6202	188.51
(4*S*)-**7**	-175	5	17.6799	285.19	-134.246	209.59	52.6871	189.15
(4*S*)-**7**	180	-5	-5.6548	286.94	-4.9399	209.9	60.7009	190.8
(4*S*)-**7**	180	-4	-3.7253	286.88	-19.6322	209.78	66.9893	190.34
(4*S*)-**7**	180	-3	-1.7487	286.83	-33.9215	209.72	72.7087	189.92
(4*S*)-**7**	180	-2	0.2094	286.79	-47.6509	209.71	77.8014	189.52
(4*S*)-**7**	180	-1	2.2033	286.76	-60.9534	209.74	82.2228	189.15
(4*S*)-**7**	180	0	4.2292	286.72	-73.4198	209.82	85.8777	188.8
(4*S*)-**7**	180	1	6.2767	286.69	-85.2198	209.92	88.7647	188.47
(4*S*)-**7**	180	2	8.3462	286.65	-96.3937	210.06	90.8884	188.18
(4*S*)-**7**	180	3	10.4317	286.6	-106.923	210.24	92.151	187.92
(4*S*)-**7**	180	4	12.5016	286.53	-116.953	210.44	92.482	187.7
(4*S*)-**7**	180	5	14.614	286.44	-126.36	210.67	91.6528	187.53
(4*S*)-**7**	175	-5	-8.6196	287.84	15.7699	210.55	61.3159	191.72
(4*S*)-**7**	175	-4	-6.7564	287.71	0.7895	210.44	68.3534	191.03

(4*S*)-**7**	175	-3	-4.9207	287.57	-13.6606	210.39	74.3608	190.39
(4*S*)-**7**	175	-2	-3.004	287.48	-27.4865	210.41	80.0941	189.84
(4*S*)-**7**	175	-1	-1.0603	287.41	-41.0893	210.48	85.1297	189.33
(4*S*)-**7**	175	0	0.873	287.37	-53.8732	210.6	89.472	188.87
(4*S*)-**7**	175	1	2.8811	287.31	-66.0937	210.75	93.0756	188.44
(4*S*)-**7**	175	2	4.9248	287.26	-77.7747	210.93	96.0055	188.04
(4*S*)-**7**	175	3	6.9927	287.2	-89.1473	211.14	98.242	187.68
(4*S*)-**7**	175	4	9.0873	287.15	-99.7792	211.39	99.8036	187.36
(4*S*)-**7**	175	5	11.198	287.09	-109.656	211.66	100.5868	187.06
(4*S*)-**7**[b]	180	-2	5.5024	285.26	-61.3092	211.25	105.9901	182.18
(4*S*)-**7**[b]	180	-1	5.9512	285.3	-64.7207	211.41	107.3148	182.1
(4*S*)-**7**[b]	180	0	4.6029	285.81	-61.4557	212.43	108.5535	183.41
(4*S*)-**7**[b]	180	1	6.902	285.42	-71.4999	211.78	109.8861	181.98
(4*S*)-**7**[b]	180	2	7.4094	285.5	-74.8818	211.99	111.1203	181.94
(4*S*)-**7**[b]	179	-2	4.8103	285.2	-59.3379	211.19	106.0749	182.13
(4*S*)-**7**[b]	179	-1	5.2452	285.24	-62.8025	211.34	107.4137	182.06
(4*S*)-**7**[b]	179	0	5.729	285.25	-66.2731	211.51	108.7152	181.98
(4*S*)-**7**[b]	179	1	6.1904	285.31	-69.6594	211.68	109.9751	181.92
(4*S*)-**7**[b]	179	2	6.7045	285.36	-73.0166	211.89	111.2618	181.86
(4*S*)-**7**[b]	178	-2	4.1496	285.13	-57.4367	211.13	106.023	182.07
(4*S*)-**7**[b]	178	-1	4.6033	285.14	-60.9351	211.28	107.4614	181.99
(4*S*)-**7**[b]	178	0	5.0516	285.17	-64.3732	211.44	108.7958	181.92
(4*S*)-**7**[b]	178	1	5.5018	285.22	-67.8289	211.61	110.1375	181.87
(4*S*)-**7**[b]	178	2	5.9832	285.27	-71.1849	211.8	111.426	181.81
(4*S*)-**7**[b]	177	-2	3.4914	285.04	-55.5807	211.06	106.0226	182.01
(4*S*)-**7**[b]	177	-1	3.9551	285.06	-59.0778	211.21	107.4887	181.92
(4*S*)-**7**[b]	177	0	4.4032	285.08	-62.5137	211.37	108.8451	181.84
(4*S*)-**7**[b]	177	1	4.8605	285.1	-65.9275	211.54	110.1516	181.78
(4*S*)-**7**[b]	177	2	5.3063	285.14	-69.402	211.71	111.4981	181.73
(4*R*)-**7**	-175	-5	-6.6112	291.08	74.4017	213.26	-62.8953	192.38
(4*R*)-**7**	-175	-4	-5.132	290.95	68.0391	212.44	-64.6742	192.65
(4*R*)-**7**	-175	-3	-3.6416	290.82	62.0916	211.68	-65.5344	192.94
(4*R*)-**7**	-175	-2	-2.1984	290.61	55.8493	211.06	-66.3422	193.37
(4*R*)-**7**	-175	-1	-0.7183	290.46	48.7437	210.39	-66.1078	193.68
(4*R*)-**7**	-175	0	2.8584	291.83	38.6997	209.6	-63.7148	199.97

(4*R*)-**7**	-175	1	2.3152	290.15	32.9903	209.18	-62.2701	194.26
(4*R*)-**7**	-175	2	3.6453	289.9	24.1667	208.72	-59.0408	194.67
(4*R*)-**7**	-175	3	5.1781	289.66	14.6205	208.27	-53.6778	195.08
(4*R*)-**7**	-175	4	6.6511	289.4	4.6177	207.87	-45.5589	195.58
(4*R*)-**7**	-175	5	8.0477	289.11	-5.8812	207.54	-33.2989	196.28
(4*R*)-**7**	180	-5	-7.9366	292.33	83.4663	213.65	-54.0962	192.92
(4*R*)-**7**	180	-4	-6.3779	292.18	77.089	212.82	-56.4774	193.23
(4*R*)-**7**	180	-3	-4.8581	292.03	70.2995	212.03	-58.2896	193.51
(4*R*)-**7**	180	-2	-3.3658	291.88	63.0401	211.3	-59.2628	193.82
(4*R*)-**7**	180	-1	-1.8675	291.75	55.3136	210.63	-59.4624	194.14
(4*R*)-**7**	180	0	-0.4325	291.55	47.6424	210.1	-59.5388	194.6
(4*R*)-**7**	180	1	1.0682	291.41	38.9889	209.53	-57.9159	194.92
(4*R*)-**7**	180	2	2.4835	291.27	29.3993	209	-55.2338	195.18
(4*R*)-**7**	180	3	3.9346	291.1	19.0424	208.56	-51.6331	195.48
(4*R*)-**7**	180	4	5.3592	290.92	7.902	208.17	-46.8189	195.78
(4*R*)-**7**	180	5	6.7833	290.67	-3.5429	207.89	-41.31	196.15
(4*R*)-**7**	175	-5	-9.5073	293.27	93.193	213.96	-42.9965	193.11
(4*R*)-**7**	175	-4	-7.9669	293.07	86.8096	213.1	-46.4594	193.38
(4*R*)-**7**	175	-3	-6.4409	292.88	79.8918	212.3	-48.8993	193.67
(4*R*)-**7**	175	-2	-4.9073	292.7	72.4461	211.57	-50.4976	194
(4*R*)-**7**	175	-1	-3.3883	292.54	64.2819	210.89	-50.9997	194.31
(4*R*)-**7**	175	0	-2.8569	291.26	52.2065	211.51	-38.6748	197.44
(4*R*)-**7**	175	1	-0.7731	292.23	46.3572	209.72	-49.264	194.95
(4*R*)-**7**	175	2	1.0727	292.09	35.8207	209.23	-46.7535	195.27
(4*R*)-**7**	175	3	2.5146	291.87	25.4909	208.87	-44.0925	195.73
(4*R*)-**7**	175	4	4.0016	291.72	13.5532	208.51	-39.4964	196.01
(4*R*)-**7**	175	5	5.4841	291.56	0.2787	208.2	-33.4383	196.24
(5*R*)-**8**	-175	-5	-13.8905	285.64	69.251	216.36	11.6424	178.95
(5*R*)-**8**	-175	0	-3.3227	286.36	25.5927	213.34	-3.5597	177
(5*R*)-**8**	-175	5	6.7449	287.4	-41.2302	212.78	24.2977	183.55
(5*R*)-**8**	180	-5	-19.4573	285.17	51.9663	221.13	14.5916	182.26
(5*R*)-**8**	180	0	-0.6028	286.17	10.0251	212.21	-1.5029	176.22
(5*R*)-**8**	180	5	2.0535	286.77	-9.0322	213.43	-11.903	176.64
(5*R*)-**8**	175	-5	-26.3351	283.7	-8.388	235.9	17.4968	193.37
(5*R*)-**8**	175	0	-13.6605	284.59	10.1324	222.34	8.4294	183.32

(5*R*)-**8**	175	5	-2.7203	285.59	-4.3427	216.41	-3.8707	178.85
(5*S*)-**8**	-175	-5	-3.0954	283.69	25.3386	210.65	13.2595	176.73
(5*S*)-**8**	-175	0	6.5429	284.32	-44.0078	209.94	35.5624	182.72
(5*S*)-**8**	-175	5	16.4739	285.32	-126.965	212.17	73.0378	190.79
(5*S*)-**8**	180	-5	-7.3038	283.66	47.6576	211.8	2.4529	177.38
(5*S*)-**8**	180	0	2.4934	284.15	-10.8928	209.3	-21.976	175.9
(5*S*)-**8**	180	5	12.2286	284.96	-73.8303	210.26	54.7665	179.46
(5*S*)-**8**	175	-5	-11.6115	283.16	50.9367	216.23	1.5321	180.6
(5*S*)-**8**	175	0	-1.6878	283.54	13.2345	211.51	-14.0562	177.46
(5*S*)-**8**	175	5	8.1085	284.23	-41.8657	210.34	-36.026	177.00
(5*R*)-**9**	-175	-5	-5.8837	286.2	15.9721	210.83	5.4624	187.02
(5*R*)-**9**	-175	-4	-4.0369	285.98	4.0142	210.5	9.4798	186.42
(5*R*)-**9**	-175	-3	-2.193	285.79	-7.7377	210.22	12.3755	186.03
(5*R*)-**9**	-175	-2	-0.3102	285.62	-18.6575	209.99	13.925	185.88
(5*R*)-**9**	-175	-1	1.5663	285.45	-29.4181	209.81	13.9739	186.04
(5*R*)-**9**	-175	0	3.5215	285.25	-39.4255	209.67	12.2486	186.57
(5*R*)-**9**	-175	1	5.4845	285.08	-48.8145	209.58	8.9373	187.54
(5*R*)-**9**	-175	2	7.4716	284.9	-57.4706	209.52	4.5769	189.09
(5*R*)-**9**	-175	3	9.4634	284.7	-65.4153	209.52	-0.4864	191.31
(5*R*)-**9**	-175	4	11.47	284.5	-71.9836	209.55	-5.9003	194.29
(5*R*)-**9**	-175	5	13.4342	284.28	-75.8523	209.62	-12.7169	198.07
(5*R*)-**9**	180	-5	-7.5021	288.15	27.4111	211.36	4.1716	189.96
(5*R*)-**9**	180	-4	-5.8162	287.85	13.51	211.01	10.6479	188.69
(5*R*)-**9**	180	-3	-4.0653	287.58	0.7411	210.74	16.7668	187.61
(5*R*)-**9**	180	-2	-2.2676	287.32	-11.0577	210.52	22.1809	186.72
(5*R*)-**9**	180	-1	-0.4333	287.08	-22.9351	210.36	26.5114	186.01
(5*R*)-**9**	180	0	1.4418	286.86	-34.3006	210.23	29.4132	185.5
(5*R*)-**9**	180	1	3.3329	286.66	-45.1314	210.15	30.5231	185.23
(5*R*)-**9**	180	2	5.2591	286.46	-55.4409	210.11	29.525	185.26
(5*R*)-**9**	180	3	7.1553	286.27	-65.1366	210.11	26.312	185.62
(5*R*)-**9**	180	4	9.134	286.11	-74.2582	210.17	21.1061	186.43
(5*R*)-**9**	180	5	11.1328	285.87	-82.7265	210.24	14.5089	187.83
(5*R*)-**9**	175	-5	-9.1811	290.31	45.0117	211.92	-5.154	194.96
(5*R*)-**9**	175	-4	-7.601	289.89	30.1036	211.54	1.6947	193.09
(5*R*)-**9**	175	-3	-5.9292	289.41	16.4957	211.28	9.0591	191.5

(5*R*)-**9**	175	-2	-4.2466	289.08	2.8491	211.05	16.0455	189.92
(5*R*)-**9**	175	-1	-2.5395	288.71	-10.3231	210.9	22.8941	188.58
(5*R*)-**9**	175	0	-0.7557	288.4	-22.8715	210.79	29.1731	187.38
(5*R*)-**9**	175	1	1.0625	288.11	-34.8146	210.73	34.5928	186.38
(5*R*)-**9**	175	2	2.928	287.84	-46.2112	210.72	38.7722	185.57
(5*R*)-**9**	175	3	4.8472	287.58	-57.0946	210.75	41.3002	184.98
(5*R*)-**9**	175	4	6.7937	287.39	-67.4426	210.83	41.7781	184.61
(5*R*)-**9**	175	5	8.6442	287.13	-76.9865	210.92	39.5979	184.54
(5*R*)-**9**[c]	180	-2	1.261	283.23	-5.9483	208.95	1.8694	181.95
(5*R*)-**9**[c]	180	-1	1.8212	283.32	-10.8605	209.02	4.8279	181.98
(5*R*)-**9**[c]	180	0	1.5275	286.84	-38.5513	209.86	30.29	185.5
(5*R*)-**9**[c]	180	1	2.9319	283.53	-20.6491	209.23	10.8128	182.06
(5*R*)-**9**[c]	180	2	3.4938	283.66	-25.6696	209.35	13.8668	182.1
(5*R*)-**9**[c]	179	-2	0.6051	283.14	-4.0255	208.89	2.3649	181.89
(5*R*)-**9**[c]	179	-1	1.1934	283.22	-9.024	208.96	5.3974	181.92
(5*R*)-**9**[c]	179	0	1.7082	283.29	-13.6879	209.02	8.1247	181.94
(5*R*)-**9**[c]	179	1	2.2774	283.39	-18.7409	209.12	11.2199	181.98
(5*R*)-**9**[c]	179	2	2.8297	283.5	-23.6444	209.25	14.2781	182.03
(5*R*)-**9**[c]	178	-2	-0.065	283.03	-2.0828	208.82	2.7196	181.84
(5*R*)-**9**[c]	178	-1	0.5176	283.1	-7.0103	208.88	5.719	181.85
(5*R*)-**9**[c]	178	0	1.0764	283.17	-11.8968	208.95	8.714	181.88
(5*R*)-**9**[c]	178	1	1.6377	283.26	-16.8405	209.04	11.717	181.91
(5*R*)-**9**[c]	178	2	2.1586	283.33	-21.5636	209.14	14.5689	181.94
(5*R*)-**9**[c]	177	-2	-0.7599	282.93	-0.0778	208.76	3.1021	181.79
(5*R*)-**9**[c]	177	-1	-0.1812	282.98	-4.9272	208.8	6.0022	181.8
(5*R*)-**9**[c]	177	0	0.3877	283.05	-9.774	208.87	8.9413	181.81
(5*R*)-**9**[c]	177	1	1.0069	283.12	-14.9764	208.96	12.2251	181.84
(5*R*)-**9**[c]	177	2	1.4565	283.19	-19.3384	209.04	14.7764	181.87
(5*S*)-**9**	-175	-5	-8.1418	281.73	40.5743	210.08	-7.8288	186.26
(5*S*)-**9**	-175	0	-0.9525	281.91	-25.4731	209.29	21.2408	192.78
(5*S*)-**9**	-175	5	6.6494	282.33	-103.981	212.8	59.0074	199.22
(5*S*)-**9**	180	-5	-8.7155	282.04	52.3961	211.47	-7.5557	178.54
(5*S*)-**9**	180	0	-2.0047	282.11	3.7925	208.77	0.1491	182.66
(5*S*)-**9**	180	5	5.2362	282.42	-54.1601	209.59	21.9117	189.08
(5*S*)-**9**	175	-5	-8.4422	281.92	45.4208	215.53	54.3787	178.26

(5*S*)-**9**	175	0	-2.2974	281.86	16.2851	211.17	12.4415	176.2
(5*S*)-**9**	175	5	4.3002	282.07	-28.3469	209.87	8.0705	179.74
(6*R*)-**10**	-175	-5	-9.3016	286.05	73.6783	213.14	9.0447	178.85
(6*R*)-**10**	-175	0	0.0885	286.8	17.3815	210.59	-5.9235	176.99
(6*R*)-**10**	-175	5	9.5245	287.96	-56.9549	210.62	41.2633	181.97
(6*R*)-**10**	180	-5	-13.021	285.51	78.5866	216.7	3.3512	181.84
(6*R*)-**10**	180	0	3.2208	286.19	3.3814	209.1	-20.1435	176.73
(6*R*)-**10**	180	5	5.6236	287.1	-15.6865	210.23	-30.5016	177.31
(6*R*)-**10**	175	-5	-15.9665	284.42	46.8842	227.92	-10.5235	191.33
(6*R*)-**10**	175	0	-6.8013	285.03	42.2143	216.87	-7.1657	182.61
(6*R*)-**10**	175	5	2.2048	285.88	6.1251	212.09	-19.5154	178.94
(6*S*)-**10**	-175	-5	-3.4099	285.92	15.7119	210.95	13.1915	176.14
(6*S*)-**10**	-175	0	6.3924	286.4	-49.0821	209.96	25.4155	180.33
(6*S*)-**10**	-175	5	16.0833	287.23	-127.552	211.57	62.3496	187.92
(6*S*)-**10**	180	-5	-7.4036	285.37	29.7656	212.08	10.8316	177.41
(6*S*)-**10**	180	0	2.7152	285.81	-22.7426	209.33	-4.9236	175.26
(6*S*)-**10**	180	5	12.16	286.59	-80.8042	210.07	41.9403	177.73
(6*S*)-**10**	175	-5	-11.6251	284.28	18.1949	216.42	4.8495	181.09
(6*S*)-**10**	175	0	-1.4194	284.71	-9.905	211.57	-2.2338	177.31
(6*S*)-**10**	175	5	8.4328	285.43	-56.8802	210.22	-23.1704	176.1
(6*R*)-**11**	-175	-5	-15.5683	279.27	91.2692	215.91	-51.9393	183.57
(6*R*)-**11**	-175	0	-3.5629	279.74	40.9887	213.55	-67.6012	184.91
(6*R*)-**11**	-175	5	8.2281	280.51	-23.9851	213.33	-68.4968	187.05
(6*R*)-**11**	180	-5	-20.9924	278.79	95.9622	218.93	-33.8914	182.84
(6*R*)-**11**	180	0	-0.2057	278.17	29.6749	212.23	-67.386	183.7
(6*R*)-**11**	180	5	2.9998	279.92	11.2896	213.25	-67.0208	184.75
(6*R*)-**11**	175	-5	-26.4958	277.65	63.0892	228.33	-14.5214	186.38
(6*R*)-**11**	175	0	-13.5834	278.17	60.6364	218.68	-33.2403	182.87
(6*R*)-**11**	175	5	-1.7781	278.86	28.3068	214.72	-49.6235	183.51
(6*S*)-**11**	-175	-5	-1.8874	299.52	35.1803	214.52	-1.2623	183.17
(6*S*)-**11**	-175	0	5.9209	300.16	-27.4383	213.53	12.4677	186.37
(6*S*)-**11**	-175	5	13.6666	301.23	-93.8146	215.81	42.4366	190.91
(6*S*)-**11**	180	-5	-3.3917	298.62	41.4512	214.92	-2.8919	182.38
(6*S*)-**11**	180	0	4.1634	299.29	-6.3699	212.82	2.2906	183.64
(6*S*)-**11**	180	5	11.4968	300.33	-58.0072	213.89	6.6342	185.19

(6*S*)-**11**	175	-5	-4.3786	297.06	21.1488	217.94	13.521	182.04
(6*S*)-**11**	175	0	2.9112	297.88	-4.8452	213.63	12.8499	182.68
(6*S*)-**11**	175	5	9.9609	298.96	-43.1716	213.46	9.1104	183.15
(4*S*)-**12**	-175	-5	-1.856	276.1	14.7996	215.94	-7.1127	182.72
(4*S*)-**12**	-175	0	10.6543	276.95	-61.2605	215.37	33.1362	183.12
(4*S*)-**12**	-175	5	23.2147	278.26	-147.394	217.32	71.2118	191.58
(4*S*)-**12**	180	-5	-7.5893	275.84	37.8076	216.79	-7.7797	183.48
(4*S*)-**12**	180	0	5.291	276.46	-24.9037	214.98	-8.8407	182.22
(4*S*)-**12**	180	5	17.8999	277.49	-97.7969	215.53	-8.9082	182.72
(4*S*)-**12**	175	-5	-14.0044	275.27	41.6955	220.41	-7.6755	186.44
(4*S*)-**12**	175	0	-0.3192	275.71	-4.005	216.22	-9.2042	183.29
(4*S*)-**12**	175	5	12.6341	276.52	-65.5123	215.33	-9.8803	182.68
(4*R*)-**12**	-175	-5	-5.5943	276.79	79.6377	218.46	-4.7992	182.67
(4*R*)-**12**	-175	0	4.9788	276.56	25.8025	216.85	-5.591	181.91
(4*R*)-**12**	-175	5	16.063	276.03	-18.1208	217.32	-8.0223	182.34
(4*R*)-**12**	180	-5	-7.1989	277.91	91.7671	218.77	-5.7257	182.91
(4*R*)-**12**	180	0	3.4618	277.55	33.4739	216.73	-6.6845	181.86
(4*R*)-**12**	180	5	13.5277	277.04	-19.5957	216.64	-7.7516	182.18
(4*R*)-**12**	175	-5	-8.7014	278.91	104.2687	219.35	-6.8754	183.25
(4*R*)-**12**	175	0	0.972	278.18	47.1188	217.07	-6.7533	182.32
(4*R*)-**12**	175	5	11.3311	277.69	-12.1531	216.58	-7.7548	182.36
(4*S*)-**13**	-175	-5	-0.123	279.25	-20.8298	215.12	54.616	190.46
(4*S*)-**13**	-175	0	12.3063	279.84	-115.018	216.35	108.1051	193.78
(4*S*)-**13**	-175	5	25.5242	280.92	-173.144	222.39	113.4896	196.64
(4*S*)-**13**	180	-5	-6.5619	279.01	20.8394	215.22	26.9613	184.99
(4*S*)-**13**	180	0	6.1262	279.37	-59.8846	213.93	73.707	187.51
(4*S*)-**13**	180	5	18.551	280.18	-140.601	216.39	112.4148	190.58
(4*S*)-**13**	175	-5	-13.143	278.52	34.7366	218.19	43.6285	182.07
(4*S*)-**13**	175	0	-0.0258	278.63	-22.1305	214.2	51.0254	182.74
(4*S*)-**13**	175	5	12.5108	279.21	-97.2916	214.17	91.5551	184.93
(4*R*)-**13**	-175	-5	-7.3103	283.79	73.1529	217.18	-57.9758	192.63
(4*R*)-**13**	-175	0	1.6132	283.08	21.6117	214.2	-40.9085	193.36
(4*R*)-**13**	-175	5	10.0512	282.01	-35.1522	212.74	-4.0459	194.6
(4*R*)-**13**	180	-5	-8.6567	284.96	83.8807	217.61	-52.7996	193.05
(4*R*)-**13**	180	0	0.2747	284.24	29.3862	214.52	-36.7536	193.83

(4*R*)-**13**	180	5	8.9587	283.42	-32.826	213	-6.78	194.49
(4*R*)-**13**	175	-5	-10.1116	285.9	96.1595	218.07	-46.8234	193.12
(4*R*)-**13**	175	0	-1.3626	285.03	40.3541	214.87	-31.931	193.87
(4*R*)-**13**	175	5	7.3861	284.19	-25.5605	213.36	-2.968	194.64
(5*R*)-**14**	-175	-5	-7.387	278.13	36.241	216.96	-11.8783	182.98
(5*R*)-**14**	-175	0	5.2061	278.82	-29.8636	215.86	-8.0034	182.16
(5*R*)-**14**	-175	5	17.143	279.87	-112.955	216.89	55.3638	189.67
(5*R*)-**14**	180	-5	-13.3943	277.99	49.129	218.43	-10.6741	183.95
(5*R*)-**14**	180	0	-0.2805	278.62	-4.2043	216.39	-8.5421	182.38
(5*R*)-**14**	180	5	12.2982	279.54	-70.3113	216.42	-5.1123	182.3
(5*R*)-**14**	175	-5	-20.386	277.27	39.0158	222.42	-5.697	186.84
(5*R*)-**14**	175	0	-6.3979	277.86	6.0632	218.26	-6.6863	183.73
(5*R*)-**14**	175	5	6.8584	278.71	-46.5387	217.14	-4.8314	182.7
(5*S*)-**14**	-175	-5	-3.6563	276.57	27.3229	214.69	-6.9945	182.92
(5*S*)-**14**	-175	0	7.9822	277.14	-46.747	214.16	-2.8597	182.69
(5*S*)-**14**	-175	5	19.6242	278.15	-129.220	216.05	75.5002	189.23
(5*S*)-**14**	180	-5	-8.4641	276.59	54.5945	215.25	-9.3449	183.34
(5*S*)-**14**	180	0	3.251	277.01	-9.328	213.65	-6.0983	182.41
(5*S*)-**14**	180	5	14.933	277.77	-81.5984	214.25	-1.886	182.99
(5*S*)-**14**	175	-5	-14.187	276.24	67.7201	217.99	-10.7971	185.4
(5*S*)-**14**	175	0	-1.7932	276.52	16.3892	214.53	-8.3786	183.11
(5*S*)-**14**	175	5	10.0194	277.13	-47.0584	213.89	-4.9709	182.87
(5*R*)-**15**	-175	-5	-5.4594	279.18	12.7941	215.2	10.0805	185.11
(5*R*)-**15**	-175	0	5.7007	279.98	-51.6134	214.16	26.6354	189.28
(5*R*)-**15**	-175	5	16.4659	281.03	-137.981	215.39	67.4689	196.5
(5*R*)-**15**	180	-5	-9.91	279.22	17.3732	216.22	43.2932	182.68
(5*R*)-**15**	180	0	1.3785	279.8	-28.9656	214.21	27.0364	182.24
(5*R*)-**15**	180	5	12.5691	280.78	-89.7062	214.38	38.9712	185.74
(5*R*)-**15**	175	-5	-14.5261	278.49	-12.2609	220.62	110.1588	188.09
(5*R*)-**15**	175	0	-3.037	279.04	-30.1232	215.91	70.638	182.07
(5*R*)-**15**	175	5	8.1597	279.89	-72.5529	214.71	49.1375	180.34
(5*S*)-**15**	-175	-5	-10.0392	275.05	45.116	214.17	-8.5617	184.07
(5*S*)-**15**	-175	0	-0.9973	275.24	-21.7613	213.44	17.9014	190.18
(5*S*)-**15**	-175	5	8.358	275.7	-100.978	215.75	52.5561	197.28
(5*S*)-**15**	180	-5	-11.0886	275.33	61.361	215.07	-9.5826	181.05

(5*S*)-**15**	180	0	-2.2924	275.38	7.6518	213.19	1.3803	180.81
(5*S*)-**15**	180	5	6.5581	275.72	-56.4012	213.57	22.9262	186.73
(5*S*)-**15**	175	-5	-11.9831	275.32	63.8722	217.77	-11.4109	182.77
(5*S*)-**15**	175	0	-3.6088	275.22	22.4391	214.35	-9.1546	180.8
(5*S*)-**15**	175	5	5.2422	275.4	-30.6684	213.48	-6.123	180.3
(6*R*)-**16**	-175	-5	-2.8219	278.71	39.8768	214.58	-9.9667	183.75
(6*R*)-**16**	-175	0	7.9866	279.62	-33.3535	214.01	-7.7965	183.42
(6*R*)-**16**	-175	5	18.7899	281.01	-116.023	215.67	64.2121	187.58
(6*R*)-**16**	180	-5	-7.0865	278.29	64.133	215.09	-11.9956	184.43
(6*R*)-**16**	180	0	3.8486	278.99	2.6426	213.48	-9.4711	183.3
(6*R*)-**16**	180	5	14.6103	280.08	-67.7427	214.02	-7.0984	183.84
(6*R*)-**16**	175	-5	-11.4637	277.58	73.8465	217.88	-13.973	186.91
(6*R*)-**16**	175	0	-0.2252	278.08	25.7372	214.35	-11.3706	184.3
(6*R*)-**16**	175	5	10.6712	278.96	-35.6115	213.69	-8.818	183.87
(6*S*)-**16**	-175	-5	-6.1101	278.58	26.5943	215.13	-5.7342	182.5
(6*S*)-**16**	-175	0	5.3352	279.04	-43.5996	214.43	-2.4864	181.88
(6*S*)-**16**	-175	5	16.975	279.83	-123.529	215.99	68.6528	185.91
(6*S*)-**16**	180	-5	-10.1175	278.21	45.0151	215.47	-6.4113	183.04
(6*S*)-**16**	180	0	2.3788	278.74	-16.1954	213.93	-4.0262	181.69
(6*S*)-**16**	180	5	12.8247	279.23	-80.8529	214.3	-1.315	181.96
(6*S*)-**16**	175	-5	-15.0202	277.37	44.1662	217.99	-6.1653	185.29
(6*S*)-**16**	175	0	-2.5435	277.65	1.3208	214.55	-4.968	182.65
(6*S*)-**16**	175	5	9.0244	278.27	-55.2782	213.87	-2.8407	181.97
(6*R*)-**17**	-175	-5	-9.7118	271.35	60.2877	217.39	-70.1308	180.12
(6*R*)-**17**	-175	0	4.46	271.97	-5.2639	216.86	-77.3939	182.63
(6*R*)-**17**	-175	5	18.5529	273.03	-81.3602	218.08	-44.6556	186.85
(6*R*)-**17**	180	-5	-15.5067	271.08	83.72	217.69	-13.536	180.57
(6*R*)-**17**	180	0	-1.197	271.53	26.1133	216.44	-66.7571	179.9
(6*R*)-**17**	180	5	12.9167	272.35	-38.8834	216.99	-77.4361	182.03
(6*R*)-**17**	175	-5	-21.3556	270.45	92.1933	219.64	-16.5442	182.64
(6*R*)-**17**	175	0	-6.7008	270.8	46.49	216.92	-13.1556	180.26
(6*R*)-**17**	175	5	7.4309	271.47	-10.584	216.64	-36.9823	179.81
(6*S*)-**17**	-175	-5	-3.3348	291.88	39.9552	218.81	-15.6061	180.36
(6*S*)-**17**	-175	0	5.7054	292.65	-22.71	218.5	27.1529	182.79
(6*S*)-**17**	-175	5	14.9446	293.52	-94.3576	220.22	54.336	188.24

(6*S*)-**17**	180	-5	-5.2372	291.03	53.1706	218.58	-16.2087	180.9
(6*S*)-**17**	180	0	3.5984	291.81	1.3431	217.41	-6.7853	179.68
(6*S*)-**17**	180	5	12.4917	292.68	-59.3342	218.25	17.3069	181.73
(6*S*)-**17**	175	-5	-6.7637	289.69	45.5417	220.06	-11.1961	182.85
(6*S*)-**17**	175	0	1.8022	290.49	9.8075	217.45	-10.7488	180.35
(6*S*)-**17**	175	5	10.4238	291.39	-40.3551	217.26	2.0004	180.04
(4*S*,5*R*)-**18**	-175	-5	-2.3582	284.58	-7.2784	212.48	9.8217	179.59
(4*S*,5*R*)-**18**	-175	0	7.9126	285.25	-77.2129	211.75	32.3366	187.39
(4*S*,5*R*)-**18**	-175	5	18.3209	286.28	-156.431	214.5	60.327	196.9
(4*S*,5*R*)-**18**	180	-5	-6.5604	284.65	12.0587	213.75	16.5488	176.22
(4*S*,5*R*)-**18**	180	0	3.7455	285.12	-42.8117	211.61	36.5606	176.8
(4*S*,5*R*)-**18**	180	5	14.0275	285.98	-107.221	212.14	41.8616	183.71
(4*S*,5*R*)-**18**	175	-5	-11.0435	284.17	12.7041	218.52	10.1652	179.18
(4*S*,5*R*)-**18**	175	0	-0.4567	284.59	-24.7546	213.39	-9.1166	176.07
(4*S*,5*R*)-**18**	175	5	9.8969	285.33	-77.9103	212.19	-39.7191	175.84
(4*S*,5*S*)-**18**	-175	-5	-5.8594	285.91	21.6021	213.63	-17.971	179.47
(4*S*,5*S*)-**18**	-175	0	4.1119	286.81	-37.5736	212.47	7.0640	187.78
(4*S*,5*S*)-**18**	-175	5	14.0525	288.06	-130.999	214.12	59.793	198.53
(4*S*,5*S*)-**18**	180	-5	-10.4129	285.71	23.9415	215.97	25.5969	177.2
(4*S*,5*S*)-**18**	180	0	-0.0993	286.48	-12.5944	213.31	6.0908	176.66
(4*S*,5*S*)-**18**	180	5	9.8324	287.54	-68.0225	213.35	19.8283	184.3
(4*S*,5*S*)-**18**	175	-5	-15.5773	284.91	-9.7189	223.01	74.3378	182.45
(4*S*,5*S*)-**18**	175	0	-4.5509	285.64	-15.4697	216.33	9.5227	177.12
(4*S*,5*S*)-**18**	175	5	5.6763	286.61	-48.7063	214.41	-10.1332	175.67
(4*R*,5*S*)-**18**	-175	-5	-8.7096	287	103.273	216.95	-22.3926	179.77
(4*R*,5*S*)-**18**	-175	0	1.0669	287.61	52.4278	214.76	-13.4501	187.45
(4*R*,5*S*)-**18**	-175	5	11.0376	288.63	-34.5819	214.65	33.4089	198.36
(4*R*,5*S*)-**18**	180	-5	-11.9765	286.9	107.2516	219.12	54.2542	178.76
(4*R*,5*S*)-**18**	180	0	-2.5914	287.27	70.7958	215.66	12.5346	176.81
(4*R*,5*S*)-**18**	180	5	7.1454	288.02	14.5268	214.64	13.833	183.73
(4*R*,5*S*)-**18**	175	-5	-15.6056	286.42	77.9835	227.48	57.0222	192.27
(4*R*,5*S*)-**18**	175	0	-6.0413	286.63	71.683	218.85	45.9568	180.15
(4*R*,5*S*)-**18**	175	5	3.3037	287.16	31.6605	215.91	-18.1717	175.93
(4*R*,5*R*)-**18**	-175	-5	-5.691	284.55	65.745	213.47	-10.9062	179.53
(4*R*,5*R*)-**18**	-175	0	4.2168	284.82	3.5028	211.55	14.534	186.64

(4*R*,5*R*)-**18**	-175	5	14.4808	285.59	-87.49	212.52	64.2811	195.94
(4*R*,5*R*)-**18**	180	-5	-9.8502	284.46	80.4373	215.29	10.861	177.03
(4*R*,5*R*)-**18**	180	0	0.0429	284.67	32.4847	211.92	16.8148	176.87
(4*R*,5*R*)-**18**	180	5	9.9443	285.13	-32.0847	211.24	36.7224	183.1
(4*R*,5*R*)-**18**	175	-5	-13.8575	283.76	71.6864	221.87	57.9666	183.34
(4*R*,5*R*)-**18**	175	0	-3.8201	283.97	46.3544	214.45	-10.6432	176.78
(4*R*,5*R*)-**18**	175	5	5.9847	284.39	-4.2077	211.82	-37.7547	176.11
(4*R*,5*R*)-**19**	-175	-5	-8.6086	285.41	-31.763	211.8	73.8161	197.47
(4*R*,5*R*)-**19**	-175	0	-1.2791	285.32	-72.059	216.93	75.4457	197.59
(4*R*,5*R*)-**19**	-175	5	7.0063	285.55	-80.406	227.28	36.7354	197.27
(4*R*,5*R*)-**19**	180	-5	-9.5481	285.72	6.8485	210.84	43.5546	191.47
(4*R*,5*R*)-**19**	180	0	-2.6478	285.57	-54.5739	210.61	70.4302	193.17
(4*R*,5*R*)-**19**	180	5	4.6592	285.72	-90.055	215.91	65.4195	194.36
(4*R*,5*R*)-**19**	175	-5	-9.9567	285.63	10.4633	214.48	54.1847	188.19
(4*R*,5*R*)-**19**	175	0	-3.6977	285.31	-28.041	210.3	54.7947	187.79
(4*R*,5*R*)-**19**	175	5	3.1392	285.33	-77.680	211.06	67.7127	189.49
(4*R*,5*S*)-**19**	-175	-5	-3.3049	289.86	-96.3109	211.59	118.0886	197.74
(4*R*,5*S*)-**19**	-175	0	5.7065	290.4	-147.664	215.48	132.8048	198.8
(4*R*,5*S*)-**19**	-175	5	15.3467	291.31	-145.90	225.3	86.4856	199.4
(4*R*,5*S*)-**19**	180	-5	-7.5549	289.68	-43.044	211.55	82.0928	191.56
(4*R*,5*S*)-**19**	180	0	1.181	290.09	-108.341	210.38	113.5629	193
(4*R*,5*S*)-**19**	180	5	10.0138	290.98	-157.881	214.41	126.8853	195.17
(4*R*,5*S*)-**19**	175	-5	-11.1619	289.02	-49.2127	216.8	123.3321	189.98
(4*R*,5*S*)-**19**	175	0	-2.6848	289.27	-72.348	211.02	94.3169	187.56
(4*R*,5*S*)-**19**	175	5	5.9122	290	-123.033	210.88	113.0348	189.05
(4*S*,5*S*)-**19**	-175	-5	-10.1897	295.08	112.1418	217.37	-78.8761	202.43
(4*S*,5*S*)-**19**	-175	0	-1.811	295.2	86.5739	216.55	-95.2261	205.05
(4*S*,5*S*)-**19**	-175	5	6.9083	295.63	26.9018	222.45	-78.5222	208.04
(4*S*,5*S*)-**19**	180	-5	-12.3068	295.45	111.4583	217.4	-60.1419	202.42
(4*S*,5*S*)-**19**	180	0	-4.6919	294.88	105.2849	213.43	-99.1936	201.15
(4*S*,5*S*)-**19**	180	5	3.3249	295.11	93.2022	212.46	-128.034	204.73
(4*S*,5*S*)-**19**	175	-5	-13.4088	295.38	47.7383	224.8	23.1961	209.21
(4*S*,5*S*)-**19**	175	0	-6.6868	294.8	96.3221	214.38	-71.6178	203.17
(4*S*,5*S*)-**19**	175	5	0.6083	294.7	84.8028	210.76	-104.734	201.44
(4*S*,5*R*)-**19**	-175	-5	-12.0372	289.37	93.3918	211.48	-36.1322	200.98

(4*S*,5*R*)-**19**	-175	0	-4.1682	288.87	39.5095	210.57	-18.2231	206.88
(4*S*,5*R*)-**19**	-175	5	-1.2069	288.74	27.7899	206.75	-23.3665	197.05
(4*S*,5*R*)-**19**	180	-5	-14.1573	290.05	101.9244	211.66	-35.5228	196.33
(4*S*,5*R*)-**19**	180	0	-6.5099	289.23	71.0431	208.26	-40.6199	198.44
(4*S*,5*R*)-**19**	180	5	1.2102	288.91	-14.6365	206.75	8.3735	205.68
(4*S*,5*R*)-**19**	175	-5	-16.2889	290.51	98.349	213.71	-13.985	204.07
(4*S*,5*R*)-**19**	175	0	-8.6934	289.37	80.1008	208.73	-38.3627	196.54
(4*S*,5*R*)-**19**	175	5	-1.2069	288.74	27.7899	206.75	-23.3665	197.05
(4*S*,6*S*)-**20**	-175	-5	-3.6019	286.35	-16.7046	211.45	4.6285	177.81
(4*S*,6*S*)-**20**	-175	0	6.1258	286.84	-83.3465	210.66	27.885	184.94
(4*S*,6*S*)-**20**	-175	5	15.9935	287.65	-161.688	212.89	60.3521	193.73
(4*S*,6*S*)-**20**	180	-5	-7.0838	285.98	-6.6578	212.63	29.6503	175.78
(4*S*,6*S*)-**20**	180	0	2.8058	286.38	-56.0608	210.45	27.4669	175.16
(4*S*,6*S*)-**20**	180	5	12.4361	287.09	-116.426	210.91	35.03	181.95
(4*S*,6*S*)-**20**	175	-5	-11.2567	284.89	-22.7899	217.54	15.8516	179.18
(4*S*,6*S*)-**20**	175	0	-0.7092	285.32	-50.8997	212.27	11.1213	175.47
(4*S*,6*S*)-**20**	175	5	9.1006	286.04	-95.7375	211	-21.0113	174.52
(4*S*,6*R*)-**20**	-175	-5	-3.3278	285.64	20.1787	211.19	19.0811	176.26
(4*S*,6*R*)-**20**	-175	0	5.0814	286.19	-31.69	210.9	-23.0759	175.87
(4*S*,6*R*)-**20**	-175	5	14.2433	286.35	-58.0177	213.56	-75.748	184.68
(4*S*,6*R*)-**20**	180	-5	-4.1083	286.13	30.1666	211.38	-13.4919	181.65
(4*S*,6*R*)-**20**	180	0	3.6525	286.61	-26.9045	210.58	-10.8938	176.04
(4*S*,6*R*)-**20**	180	5	12.1826	287.04	-73.7369	211.9	-24.1303	177.18
(4*S*,6*R*)-**20**	175	-5	-4.6286	286.43	40.9511	212.02	-10.2687	189.72
(4*S*,6*R*)-**20**	175	0	2.5726	286.62	-15.4173	210.61	0.3002	179.71
(4*S*,6*R*)-**20**	175	5	10.5378	287.09	-70.9037	211.49	-29.8282	177.22
(4*R*,6*R*)-**20**	-175	-5	-4.9585	287.44	90.506	214.6	-8.5827	178.41
(4*R*,6*R*)-**20**	-175	0	4.2708	288.14	28.9357	212.63	4.9391	185.92
(4*R*,6*R*)-**20**	-175	5	13.5983	289.4	-63.7667	213.15	53.3203	195.74
(4*R*,6*R*)-**20**	180	-5	-7.3137	287.07	109.6827	216.06	-0.2447	177.51
(4*R*,6*R*)-**20**	180	0	1.113	287.49	59.7178	212.88	-16.3104	176.35
(4*R*,6*R*)-**20**	180	5	10.1958	288.33	-6.7096	212.11	21.168	182.64
(4*R*,6*R*)-**20**	175	-5	-9.1006	286.6	112.7711	222	15.7158	185.14
(4*R*,6*R*)-**20**	175	0	-1.0563	286.69	79.1014	215.1	-21.8587	177.19
(4*R*,6*R*)-**20**	175	5	7.3869	287.23	23.9015	212.66	-42.5525	176.84

(4*R*,6*S*)-**20**	-175	-5	-3.9852	284.19	71.9499	212.9	-21.9205	176.91
(4*R*,6*S*)-**20**	-175	0	3.5437	283.1	22.0678	211.51	-2.673	175.48
(4*R*,6*S*)-**20**	-175	5	11.9042	281.9	-18.0754	214.14	-25.8541	192.76
(4*R*,6*S*)-**20**	180	-5	-4.7757	285.9	82.0978	213.54	-21.1038	180.99
(4*R*,6*S*)-**20**	180	0	2.1794	284.73	31.7649	211.33	4.2752	176.25
(4*R*,6*S*)-**20**	180	5	9.8797	283.59	-21.5193	211.62	-38.7364	175.8
(4*R*,6*S*)-**20**	175	-5	-5.5346	287.43	89.7313	214.5	-8.8883	186.72
(4*R*,6*S*)-**20**	175	0	1.0144	286.07	42.7727	211.61	-12.7908	179.14
(4*R*,6*S*)-**20**	175	5	8.4192	284.85	-13.8435	211.25	12.5742	175.97
(4*S*,6*S*)-**21**	-175	-5	-1.9092	302.29	-30.5574	213.69	69.2102	194.59
(4*S*,6*S*)-**21**	-175	0	5.9067	302.67	-96.4202	216.9	99.1075	196.23
(4*S*,6*S*)-**21**	-175	5	14.5521	303.26	-125.062	224.8	79.66	197.05
(4*S*,6*S*)-**21**	180	-5	-4.5299	301.8	3.4959	212.89	38.1697	189.41
(4*S*,6*S*)-**21**	180	0	2.9348	302.11	-61.2146	212.62	79.8667	191.52
(4*S*,6*S*)-**21**	180	5	10.5405	302.77	-111.583	216.94	89.9994	193.35
(4*S*,6*S*)-**21**	175	-5	-6.5254	300.78	-0.2343	215.83	26.2585	185.99
(4*S*,6*S*)-**21**	175	0	0.4548	301.17	-37.9916	212.03	57.367	186.97
(4*S*,6*S*)-**21**	175	5	7.797	301.71	-90.3161	213.07	84.5599	188.78
(4*S*,6*R*)-**21**	-175	-5	-5.7496	279.29	4.0797	210.35	-0.5257	192.83
(4*S*,6*R*)-**21**	-175	0	5.3197	280.19	-45.1418	209.87	-9.762	193.26
(4*S*,6*R*)-**21**	-175	5	15.704	280.52	-30.0885	211.36	-91.3134	202.62
(4*S*,6*R*)-**21**	180	-5	-8.0257	279.02	5.4148	210.53	19.8347	194.91
(4*S*,6*R*)-**21**	180	0	3.0585	280.17	-55.1705	210.04	36.8944	191.86
(4*S*,6*R*)-**21**	180	5	13.6735	280.98	-96.2581	210.73	15.8813	193.71
(4*S*,6*R*)-**21**	175	-5	-10.2579	278.43	12.4053	210.79	27.3354	199.34
(4*S*,6*R*)-**21**	175	0	0.6784	279.46	-52.0819	210.4	52.2646	192.87
(4*S*,6*R*)-**21**	175	5	11.4845	280.59	-101.398	211.12	61.2603	190.79
(4*R*,6*R*)-**21**	-175	-5	-6.6397	297.21	86.7575	214.45	-48.4044	194.5
(4*R*,6*R*)-**21**	-175	0	1.7244	297.16	52.863	211.31	-57.8465	199.54
(4*R*,6*R*)-**21**	-175	5	10.7212	297.66	3.4328	210.1	-57.9859	208.39
(4*R*,6*R*)-**21**	180	-5	-8.8214	297.67	86.0506	215.69	-36.6426	193.84
(4*R*,6*R*)-**21**	180	0	-1.1395	297.2	59.5502	211.73	-65.1701	192.54
(4*R*,6*R*)-**21**	180	5	7.0391	297.38	9.2823	210.07	-52.8184	196.98
(4*R*,6*R*)-**21**	175	-5	-9.9077	297.85	44.4804	221.12	43.0529	203.84
(4*R*,6*R*)-**21**	175	0	-3.2565	297.12	60.9628	213.11	-44.3474	194.95

(4*R*,6*R*)-**21**	175	5	4.2624	296.96	21.324	210.41	-42.0952	192.71
(4*R*,6*S*)-**21**	-175	-5	-2.7597	308.06	48.1735	214.65	12.4833	200.6
(4*R*,6*S*)-**21**	-175	0	0.6282	304.9	42.3558	211.83	-43.1836	193.83
(4*R*,6*S*)-**21**	-175	5	4.6177	304.81	18.7314	211.8	-30.2327	205.7
(4*R*,6*S*)-**21**	180	-5	-2.8239	306.64	67.1953	215.53	-11.4977	194.62
(4*R*,6*S*)-**21**	180	0	1.1765	305.64	46.5955	211.89	-51.4754	194.54
(4*R*,6*S*)-**21**	180	5	5.0977	304.91	4.1667	210.54	-32.4622	195.67
(4*R*,6*S*)-**21**	175	-5	-2.3463	308.06	58.1562	216.55	34.752	197.34
(4*R*,6*S*)-**21**	175	0	1.6771	306.51	47.697	212.22	-42.6387	195.33
(4*R*,6*S*)-**21**	175	5	5.5724	305.36	6.8467	210.31	-33.8524	196.16
(5*S*,6*R*)-**22**	-175	-5	-2.9162	286.68	33.9784	210.54	14.8984	178.87
(5*S*,6*R*)-**22**	-175	0	6.0834	287.6	-35.1433	210.05	37.0877	185.26
(5*S*,6*R*)-**22**	-175	5	15.3844	288.85	-120.233	212.58	76.2763	192.92
(5*S*,6*R*)-**22**	180	-5	-6.0876	286.48	53.988	211.62	7.9223	177.75
(5*S*,6*R*)-**22**	180	0	2.4216	287.03	1.256	209.69	-16.4844	176.62
(5*S*,6*R*)-**22**	180	5	11.4386	288.14	-64.1203	210.41	50.4039	181.9
(5*S*,6*R*)-**22**	175	-5	-8.3182	285.75	51.9292	216.01	4.7051	180.74
(5*S*,6*R*)-**22**	175	0	-0.4036	286.27	19.3469	211.37	-11.9081	177.81
(5*S*,6*R*)-**22**	175	5	8.2527	287.02	-32.3234	210.35	-35.226	177.54
(5*S*,6*S*)-**22**	-175	-5	-2.06	286.7	5.7022	210.35	3.6182	177.01
(5*S*,6*S*)-**22**	-175	0	7.0714	287.09	-62.0103	209.55	28.0654	183.06
(5*S*,6*S*)-**22**	-175	5	15.2064	287.38	-138.988	211.58	64.2722	190.94
(5*S*,6*S*)-**22**	180	-5	-5.8621	286.58	25.6326	211.51	15.6311	176.2
(5*S*,6*S*)-**22**	180	0	3.4134	286.89	-28.6933	209.38	-9.2739	175.04
(5*S*,6*S*)-**22**	180	5	12.7116	287.63	-91.235	209.8	42.7037	179.8
(5*S*,6*S*)-**22**	175	-5	-9.8056	285.97	27.8016	215.89	10.7245	179.02
(5*S*,6*S*)-**22**	175	0	-0.2293	286.31	-9.4623	211.18	-5.92	176.04
(5*S*,6*S*)-**22**	175	5	8.9802	286.86	-62.5434	209.94	-34.0708	175.8
(5*R*,6*S*)-**22**	-175	-5	-7.2929	288.27	22.1391	212.97	-22.2589	176.98
(5*R*,6*S*)-**22**	-175	0	2.0185	288.69	-31.1394	211.64	-5.3546	183.73
(5*R*,6*S*)-**22**	-175	5	11.5053	289.5	-110.603	212.65	41.4738	192.44
(5*R*,6*S*)-**22**	180	-5	-11.1214	287.76	20.2084	214.75	19.5076	177.24
(5*R*,6*S*)-**22**	180	0	-1.3695	288.33	-13.9732	212.26	5.1489	175.37
(5*R*,6*S*)-**22**	180	5	8.0888	289.08	-65.5933	212.14	10.386	180.65
(5*R*,6*S*)-**22**	175	-5	-15.4398	286.56	-15.4565	220.34	92.873	181.52

(5*R*,6*S*)-**22**	175	0	-5.2088	287.16	-21.9803	214.81	9.0567	177.09
(5*R*,6*S*)-**22**	175	5	4.4499	288.03	-53.4408	213.07	-8.8318	175.65
(5*R*,6*R*)-**22**	-175	-5	-5.4034	287.65	29.5998	213.04	11.802	178.44
(5*R*,6*R*)-**22**	-175	0	4.2157	288.54	-33.0145	211.55	21.849	185.18
(5*R*,6*R*)-**22**	-175	5	13.6576	289.85	-122.637	212.93	72.1875	193.92
(5*R*,6*R*)-**22**	180	-5	-9.2995	287.49	35.4464	215.88	17.4788	179.29
(5*R*,6*R*)-**22**	180	0	0.2335	288.22	-3.4026	212.71	3.4246	177.19
(5*R*,6*R*)-**22**	180	5	9.7709	289.32	-61.6822	212.27	34.0412	181.57
(5*R*,6*R*)-**22**	175	-5	-13.0656	286.52	14.8233	223.53	20.3772	184.09
(5*R*,6*R*)-**22**	175	0	-3.6504	287.26	2.66	216.52	7.2955	179.56
(5*R*,6*R*)-**22**	175	5	5.7389	288.32	-35.8402	213.98	-12.2826	177.91
(5*S*,6*R*)-**23**	-175	-5	-13.0937	275.85	72.5857	212.86	-57.1526	193.51
(5*S*,6*R*)-**23**	-175	0	-3.913	275.88	15.1118	211.78	-39.2274	198.4
(5*S*,6*R*)-**23**	-175	5	6.4933	276.17	-87.746	213.64	25.5138	203.94
(5*S*,6*R*)-**23**	180	-5	-13.9703	276.07	80.4128	214.06	-55.0165	188.45
(5*S*,6*R*)-**23**	180	0	-5.4062	276.03	41.9705	212.12	-58.4326	191.65
(5*S*,6*R*)-**23**	180	5	3.6283	276.27	-13.2573	212.2	-43.5569	196.29
(5*S*,6*R*)-**23**	175	-5	-13.0414	275.86	69.683	217.1	-45.3932	185.5
(5*S*,6*R*)-**23**	175	0	-5.8227	275.8	45.9786	213.61	-53.6853	187.3
(5*S*,6*R*)-**23**	175	5	2.2869	275.96	7.7737	212.7	-57.4019	190.23
(5*S*,6*S*)-**23**	-175	-5	-8.6218	298.03	41.9634	213.31	-7.1423	192.86
(5*S*,6*S*)-**23**	-175	0	-3.0774	297.98	-18.6811	212.53	11.2746	197.69
(5*S*,6*S*)-**23**	-175	5	2.945	297.99	-92.49	215.59	42.8705	202.05
(5*S*,6*S*)-**23**	180	-5	-7.3227	298.06	48.1105	214.15	-4.1861	186.61
(5*S*,6*S*)-**23**	180	0	-2.2721	297.99	6.9322	212.06	-4.9265	190.29
(5*S*,6*S*)-**23**	180	5	2.9276	298.03	-49.1741	212.4	7.6916	195.04
(5*S*,6*S*)-**23**	175	-5	-5.3436	297.59	35.1118	217.1	-0.6289	182.74
(5*S*,6*S*)-**23**	175	0	-1.0685	297.52	8.5828	213.37	-0.2392	184.79
(5*S*,6*S*)-**23**	175	5	3.8244	297.55	-31.1707	212.28	-3.1215	188.24
(5*R*,6*S*)-**23**	-175	-5	-4.5958	304.86	2.4424	216.09	28.9301	199.33
(5*R*,6*S*)-**23**	-175	0	2.6681	305.37	-54.9579	214.94	40.2002	201.53
(5*R*,6*S*)-**23**	-175	5	10.0709	305.99	-130.091	216.86	67.0131	205.24
(5*R*,6*S*)-**23**	180	-5	-7.026	304.37	3.4426	217.82	27.9894	197.24
(5*R*,6*S*)-**23**	180	0	0.6847	304.78	-30.5422	215.00	21.1321	197.54
(5*R*,6*S*)-**23**	180	5	7.789	305.49	-82.3365	214.88	28.375	199.28

(5*R*,6*S*)-**23**	175	-5	-10.1159	303.18	-28.5448	225.52	60.8094	197.75
(5*R*,6*S*)-**23**	175	0	-2.1433	303.69	-35.3436	218.12	22.2566	196.12
(5*R*,6*S*)-**23**	175	5	5.6775	304.22	-66.5922	215.68	13.9464	196.2
(5*R*,6*R*)-**23**	-175	-5	-7.9505	283.61	31.5406	213.11	-26.4497	189.49
(5*R*,6*R*)-**23**	-175	0	1.6802	284.04	-15.3417	211.93	-26.1836	191.43
(5*R*,6*R*)-**23**	-175	5	11.244	284.82	-87.6442	212.82	12.4595	196.15
(5*R*,6*R*)-**23**	180	-5	-11.0408	283.45	20.1743	214.81	13.2285	188.99
(5*R*,6*R*)-**23**	180	0	-1.5026	283.92	-5.3384	212.28	-21.0915	188.4
(5*R*,6*R*)-**23**	180	5	7.8523	284.6	-48.8792	212.18	-28.0421	189.67
(5*R*,6*R*)-**23**	175	-5	-13.0452	282.72	-30.1118	221.92	114.5268	192.02
(5*R*,6*R*)-**23**	175	0	-4.1579	283.15	-26.6546	215.09	37.009	188.53
(5*R*,6*R*)-**23**	175	5	4.9764	283.8	-47.6624	213.02	-8.4924	187.69

[a] $\times 10^{-40}$ erg esu cm Gauss^{-1}; [b] α = 40º; [c] β = 178º

Table E. Relative energies (Δ*E*) of **4** with varying torsion angles ω and τ.

	ω	τ	Energy [Hartree]	Δ*E* [kcal mol^{-1}]
4	-175	-5	-308.111566373	1.39
4	-175	-4	-308.112628255	0.72
4	-175	-3	-308.112853555	0.58
4	-175	-2	-308.112208187	0.99
4	-175	-1	-308.110669596	1.95
4	-175	0	-308.108215133	3.49
4	-175	1	-308.104839089	5.61
4	-175	2	-308.100544590	8.31
4	-175	3	-308.095334679	11.57
4	-175	4	-308.089234085	15.40
4	-175	5	-308.082271769	19.77
4	-176	-5	-308.110757224	1.90
4	-176	-4	-308.112328904	0.91
4	-176	-3	-308.113090060	0.43
4	-176	-2	-308.113006199	0.49
4	-176	-1	-308.112044599	1.09
4	-176	0	-308.110185739	2.26
4	-176	1	-308.107412304	4.00
4	-176	2	-308.103725441	6.31
4	-176	3	-308.099126091	9.20
4	-176	4	-308.093629457	12.64
4	-176	5	-308.087255995	16.64
4	-177	-5	-308.109565128	2.65
4	-177	-4	-308.111629309	1.35
4	-177	-3	-308.112913769	0.54
4	-177	-2	-308.113376623	0.25
4	-177	-1	-308.112986017	0.50
4	-177	0	-308.111714605	1.30
4	-177	1	-308.109543716	2.66
4	-177	2	-308.106461713	4.59
4	-177	3	-308.102473918	7.09
4	-177	4	-308.097586438	10.16
4	-177	5	-308.091817402	13.78

4	-178	-5	-308.108001912	3.63
4	-178	-4	-308.110540154	2.03
4	-178	-3	-308.112329586	0.91
4	-178	-2	-308.113326806	0.28
4	-178	-1	-308.113394411	0.24
4	-178	0	-308.112801086	0.61
4	-178	1	-308.111225202	1.60
4	-178	2	-308.108750948	3.16
4	-178	3	-308.105374461	5.27
4	-178	4	-308.101097161	7.96
4	-178	5	-308.095939445	11.20
4	-179	-5	-308.106079756	4.83
4	-179	-4	-308.109073153	2.95
4	-179	-3	-308.111348331	1.53
4	-179	-2	-308.112862906	0.58
4	-179	-1	-308.113574818	0.13
4	-179	0	-308.113449429	0.21
4	-179	1	-308.112459881	0.83
4	-179	2	-308.110587262	2.00
4	-179	3	-308.107819063	3.74
4	-179	4	-308.104161700	6.04
4	-179	5	-308.099614816	8.89
4	180	-5	-308.113743585	0.02
4	180	-4	-308.113773745	0.01
4	180	-3	-308.113781143	0.00
4	180	-2	-308.113766593	0.01
4	180	-1	-308.113725769	0.03
4	180	0	-308.113664444	0.07
4	180	1	-308.113582175	0.12
4	180	2	-308.113477333	0.19
4	180	3	-308.113350013	0.27
4	180	4	-308.113200491	0.36
4	180	5	-308.113028071	0.47
4	179	-5	-308.101221770	7.88
4	179	-4	-308.105056732	5.47

4	179	-3	-308.108244292	3.47
4	179	-2	-308.110736082	1.91
4	179	-1	-308.112486360	0.81
4	179	0	-308.113453172	0.21
4	179	1	-308.113602707	0.11
4	179	2	-308.112907375	0.55
4	179	3	-308.111347239	1.53
4	179	4	-308.108911909	3.05
4	179	5	-308.105594966	5.14
4	178	-5	-308.098377855	9.67
4	178	-4	-308.102539268	7.05
4	178	-3	-308.106149098	4.79
4	178	-2	-308.109097157	2.94
4	178	-1	-308.111336021	1.53
4	178	0	-308.112824491	0.60
4	178	1	-308.113521268	0.16
4	178	2	-308.113396592	0.24
4	178	3	-308.112426762	0.85
4	178	4	-308.110594779	2.00
4	178	5	-308.107893390	3.69
4	177	-5	-308.095118691	11.71
4	177	-4	-308.099701637	8.83
4	177	-3	-308.103709547	6.32
4	177	-2	-308.107091784	4.20
4	177	-1	-308.109800979	2.50
4	177	0	-308.111788429	1.25
4	177	1	-308.113015282	0.48
4	177	2	-308.113447111	0.21
4	177	3	-308.113054955	0.46
4	177	4	-308.111818312	1.23
4	177	5	-308.109724128	2.55
4	176	-5	-308.091649934	13.89
4	176	-4	-308.096565269	10.80
4	176	-3	-308.100947153	8.05
4	176	-2	-308.104740733	5.67

4	176	-1	-308.107892995	3.69
4	176	0	-308.110358177	2.15
4	176	1	-308.112094385	1.06
4	176	2	-308.113062965	0.45
4	176	3	-308.113237722	0.34
4	176	4	-308.112583976	0.75
4	176	5	-308.111089634	1.69
4	175	-5	-308.087926354	16.22
4	175	-4	-308.093147343	12.95
4	175	-3	-308.097880142	9.98
4	175	-2	-308.102057192	7.36
4	175	-1	-308.105630120	5.11
4	175	0	-308.108551836	3.28
4	175	1	-308.110777489	1.88
4	175	2	-308.112265282	0.95
4	175	3	-308.112982242	0.50
4	175	4	-308.112898344	0.55
4	175	5	-308.111990221	1.12

Table F. Rotatory strengths *R* calculated at the PCM/B2LYP/6-311++G(2d,2p) level for *P*-type conformers of model compounds **4-23** with planar chromophore relative to **4** and substituent contributions *ΔR* for Cotton effects I-III.

		Relative *R*			*ΔR*[a]			*ΔR*[b]		
Enone	Substituent	I	II	III	I	II	III	I	II	III
4		1.00	1.00	1.00	4[c]	-5.5[c]	-21[c]			
5	3-Me	1.21	0.95	0.50	1	ca 0	10			
(4*S*)-**6**	4-Me_{eq}	1.08	6.96	0.90	ca 0	-33	ca 0			
(4*R*)-**6**	4-Me_{ax}	0.50	-8.02	0.98	-2	50	ca 0			
(4*S*)-**7**	4-OH_{eq}	0.99	13.14	-4.13	ca 0	-68	-39			
(4*R*)-**7**	4-OH_{ax}	-0.10	-8.52	2.86	-5	53	38			
(5*R*)-**8**	5-Me_{ax}	-0.14	-1.79	0.07	-5	16	19			
(5*S*)-**8**	5-Me_{eq}	0.58	1.95	1.06	-2	-5	-1			
(5*R*)-**9**	5-OH_{ax}	0.36	6.90	-1.45	-3	-33	51			
(5*S*)-**9**	5-OH_{eq}	-0.47	-0.68	-0.01	-6	9	21			
(6*R*)-**10**	6-Me_{eq}	0.76	-0.61	0.97	-1	9	ca 0			
(6*S*)-**10**	6-Me_{ax}	0.64	4.07	0.24	-1.5	-17	16			
(6*R*)-**11**	6-OH_{eq}	-0.05	-5.31	3.24	-4	35	-46			
(6*S*)-**11**	6-OH_{ax}	0.98	1.14	-0.11	0	-1	23			
(4*S*)-**12**	3-Me,4-Me_{eq}	1.24	4.46	0.42	1	-16	12	1	-33	10
(4*R*)-**12**	3-Me,4-Me_{ax}	0.81	-5.99	0.32	-1	39	14	-1	50	10
(4*S*)-**13**	3-Me,4-OH_{eq}	1.44	10.72	-3.54	2	-54	94	1	-68	-29
(4*R*)-**13**	3-Me,4-OH_{ax}	0.06	-5.26	1.77	-4	35	-16	-4	53	48
(5*R*)-**14**	3-Me,5-Me_{ax}	-0.07	0.75	0.41	-4	1	12	-4	-16	29
(5*S*)-**14**	3-Me,5-Me_{eq}	0.76	1.67	0.29	-1	-4	15	-1	-5	9
(5*R*)-**15**	3-Me,5-OH_{ax}	0.32	5.18	-1.30	-3	-23	48	-2	-33	61
(5*S*)-**15**	3-Me,5-OH_{eq}	-0.54	-1.37	-0.07	-6	13	22	-5	9	31
(6*R*)-**16**	3-Me,6-Me_{eq}	0.90	-0.47	0.45	ca 0	8	11	0	9	10
(6*S*)-**16**	3-Me,6-Me_{ax}	0.56	2.90	0.19	-2	-10	-17	-0.5	-17	26
(6*R*)-**17**	3-Me,4-OH_{eq}	-0.28	-4.67	3.21	-5	31	-46	-3	35	-36
(6*S*)-**17**	3-Me,4-OH_{ax}	0.84	-0.24	0.33	-0.5	7	14	1	-1	33

(4*S*,5*R*)-**18**	4-Me_{eq},5-Me_{eq}	0.88	7.66	-1.76	-0.5	-37	57	-2	-38	-1
(4*S*,5*S*)-**18**	4-Me_{eq},5-Me_{ax}	-0.02	2.25	-0.29	-4	-7	27	-5	-17	19
(4*R*,5*S*)-**18**	4-Me_{ax},5-Me_{ax}	-0.61	-12.67	-0.60	-7	76	33	-7	66	19
(4*R*,5*R*)-**18**	4-Me_{ax},5-Me_{eq}	0.01	-5.81	-0.81	-4	38	37	-8	45	-1
(4*R*,5*R*)-**19**	4-OH_{eq},5-OH_{eq}	-0.62	9.77	-3.38	-7	-49	91	-6	-59	-18
(4*R*,5*S*)-**19**	4-OH_{eq},5-OH_{ax}	0.28	19.39	-5.45	-3	-103	134	-3	-101	12
(4*S*,5*S*)-**19**	4-OH_{ax},5-OH_{ax}	-1.10	-18.84	4.76	-9	111	-78	-8	20	89
(4*S*,5*R*)-**19**	4-OH_{ax},5-OH_{eq}	-1.53	-12.71	1.95	-11	76	-20	-11	62	59
(4*S*,6*S*)-**20**	4-Me_{eq},6-Me_{ax}	0.66	10.03	-1.32	-1.5	-50	48	-1.5	-50	16
(4*S*,6*R*)-**20**	4-Me_{eq},6-Me_{eq}	0.86	4.81	0.52	-1	-21	10	-1	-24	ca 0
(4*R*,6*R*)-**20**	4-Me_{ax},6-Me_{eq}	0.26	-10.69	0.78	-3	65	4	-3	33	16
(4*R*,6*S*)-**20**	4-Me_{ax},6-Me_{ax}	0.51	-5.68	-0.21	-2	37	25	-3	59	ca 0
(4*S*,6*S*)-**21**	4-OH_{eq},6-OH_{ax}	0.69	10.95	-3.84	-1	-55	100	ca 0	-69	-16
(4*S*,6*R*)-**21**	4-OH_{eq},6-OH_{eq}	0.72	9.87	-1.77	-1	-50	61	-4	-33	-85
(4*R*,6*R*)-**21**	4-OH_{ax},6-OH_{eq}	-0.27	-10.66	3.13	-5	65	-44	-5	52	61
(4*R*,6*S*)-**21**	4-OH_{ax},6-OH_{ax}	0.28	-8.34	2.47	-3	52	-31	-9	88	-8
(5*S*,6*R*)-**22**	5-Me_{eq},6-Me_{eq}	0.57	-0.22	0.79	-2	7	4	-6	-1	35
(5*S*,6*S*)-**22**	5-Me_{eq},6-Me_{ax}	0.80	5.13	0.45	-1	-23	11	-6	25	19
(5*R*,6*S*)-**22**	5-Me_{ax},6-Me_{ax}	-0.32	2.50	-0.25	-5	-8	26	-3	4	-1
(5*R*,6*R*)-**22**	5-Me_{ax},6-Me_{eq}	0.05	0.61	-0.16	-4	2	24	-3.5	-1	35
(5*S*,6*R*)-**23**	5-OH_{eq},6-OH_{eq}	-1.27	-7.51	2.81	-10	47	-38	-3	-34	74
(5*S*,6*S*)-**23**	5-OH_{eq},6-OH_{ax}	-0.53	-1.24	0.24	-6	12	-16	-7	2	5
(5*R*,6*S*)-**23**	5-OH_{ax},6-OH_{ax}	0.16	5.47	-1.01	-3.5	-25	42	-10	44	-25
(5*R*,6*R*)-**23**	5-OH_{ax},6-OH_{eq}	-0.35	0.96	1.01	-6	ca 0	ca 0	-6	8	44

[a] obtained by subtraction of *R* for **4** from that for molecules **5-23**; [b] obtained by adding contributions ΔR^a for individual substituents; [c] actual calculated *R* for **4**.

Table G. Specific optical rotations for enones **6-11**, measured and calculated at the PCM/B3LYP/Aug-cc-pVTZ level.

Enone	Conformer	Calculated optical rotations				Measured optical rotations			
		589 nm	578 nm	546 nm	436 nm	589 nm	578 nm	546 nm	436 nm
(4*S*)-**6**	(*P*)	-90	-191	-218	-359				
	(*M*)	-322	-430	-497	-911				
ΔE[a] **Boltzmann averaged**		-148	-251	-288	-497	123[b]			
(4*S*)-**7**	(*P*1)	-191	-244	-282	-512				
	(*P*2)	-199	-237	-269	-432				
	(*P*3)	-71	-78	-86	-84				
	(*M*1)	-221	-204	-277	-286				
	(*M*2)	-36	-5	+4	+190				
	(*M*3)	-186	-236	-272	-490				
ΔE[a] **Boltzmann averaged**		-153	-182	-209	-326	-110[c]			
(5*R*)-**8**	(*P*)	-51	-147	-175	-403				
	(*M*)	-87	-53	-60	-104				
ΔE[a] **Boltzmann averaged**		-148	-251	-288	-497	-95[d]			
(5*R*)-**9**	(*P*1)	-201	-291	-344	-753				
	(*P*2)	-182	-245	-285	-553				
	(*P*3)	-6	-87	-109	-331				
	(*M*1)	-33	+49	+64	+231				
	(*M*2)	-72	-57	-65	-122				
	(*M*3)	+21	+90	+110	+305				
ΔE[a] **Boltzmann averaged**		-50	-40	-45	-66	-48[e]			
(6*R*)-**10**	(*P*)	159	159	181	286				
	(*M*)	-137	-64	-78	-219				
ΔE[a] **Boltzmann averaged**		52	78	88	104	91[f]			
(6*R*)-**11**	(*P*1)	196	151	169	221				
	(*P*2)	104	59	64	52				
	(*M*1)	-64	-29	-38	-140				
ΔE[a] **Boltzmann averaged**		182	140	156	200	n.a			

[a] optimized at PCM/MP2/Aug-cc-pVTZ//PCM/B3LYP/6-311++G(2d,2p) level; [b] measured for (4*R*)-**6** in ethanol, K. Mori, T. Shozo, *Tetrahedron*, **1985**, *41*, 3049; [c] in $CHCl_3$, J. E. Audia, L. Boisvert, A. D. Patten, A. Villalobos, S. J. Danishefsky, J. Org. Chem. **1989**, *54*, 3738; [d] in $CHCl_3$, D. A. Lightner, T. D. Bouman, J. K. Gawroński, K. Gawrońska, J. L. Chappuis, B. V. Crist, A. E. Hansen, *J. Am. Chem. Soc.* **1981**, *103*, 5314; [e] in $CHCl_3$, P. Bolze, G. Dickmeiss, K. A. Jørgensen, *Org. Lett.* **2008**, *10*, 3753. [f] in methanol, H. Iio, M. Monden, K. Okada, T. Tokoroyama, *Chem. Commun.* **1987**, 358.

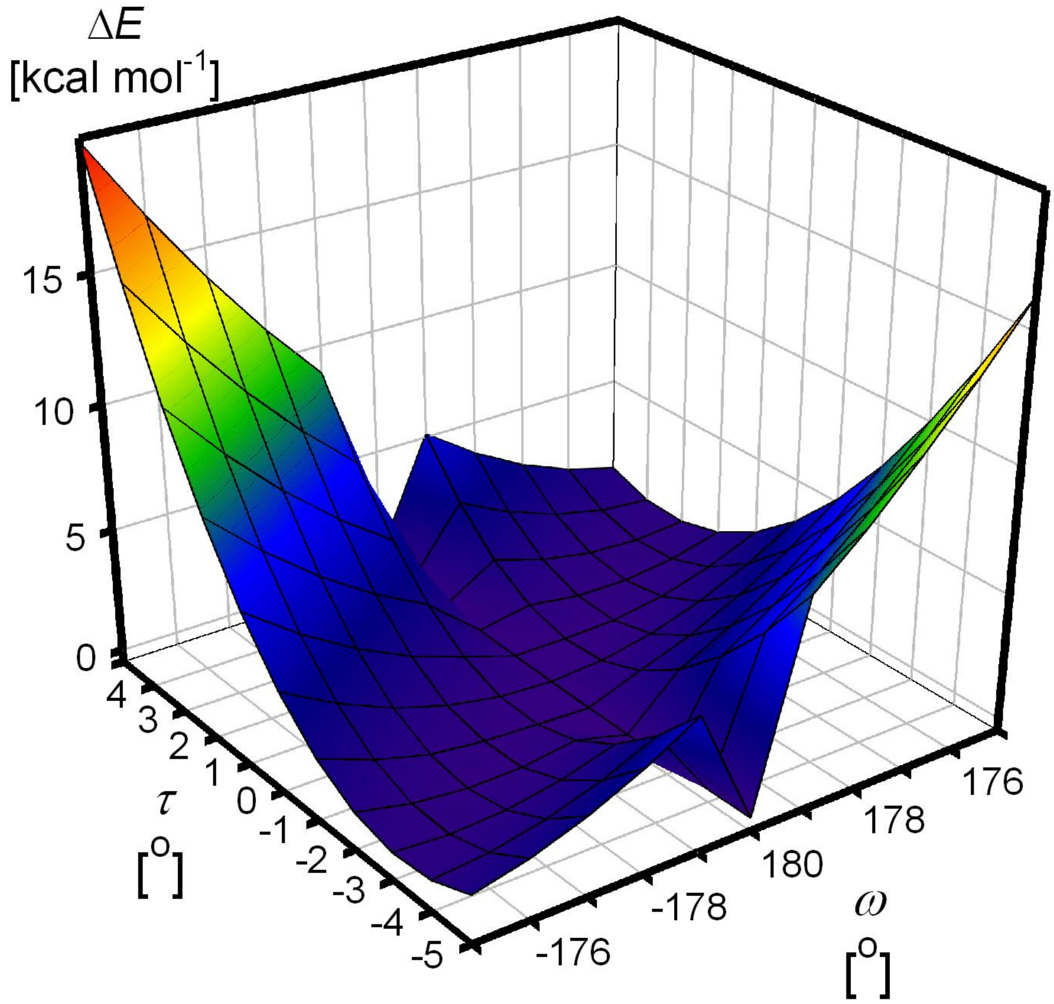

Figure A. Relative energies of (*P*)-**4** (in kcal mol^{-1}, calculated at the B3LYP/6-311++G(2d,2p) level) as a function of dihedral angles ω and τ.

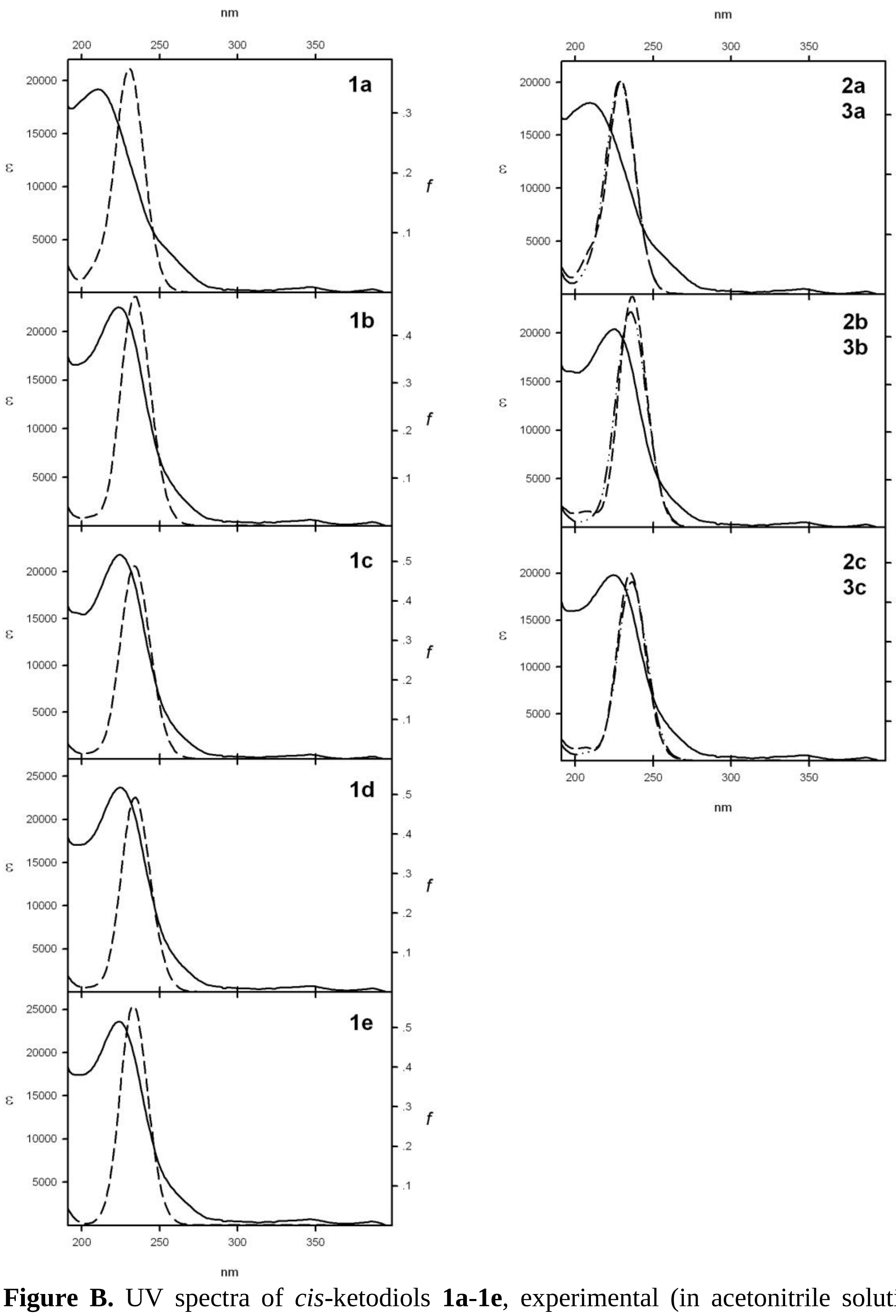

Figure B. UV spectra of *cis*-ketodiols **1a**-**1e**, experimental (in acetonitrile solutions, solid lines) and ΔE_{MP2} Boltzmann averaged calculated at PCM/B2LYP/Aug-cc-pVTZ level (dashed lines) (left column) and UV spectra of *cis*-ketodiols *ent*-**2a**-**2c** experimental (in acetonitrile solutions, solid lines), ΔE_{MP2} Boltzmann averaged calculated at PCM/B2LYP/Aug-cc-pVTZ level for **2a**-**2c** (dashed lines) and **3a**-**3c** (dash-dot-dot lines) (right column). All calculated spectra were wavelength corrected to match experimental short-wavelength UV λ_{max} at ca. 220 nm.

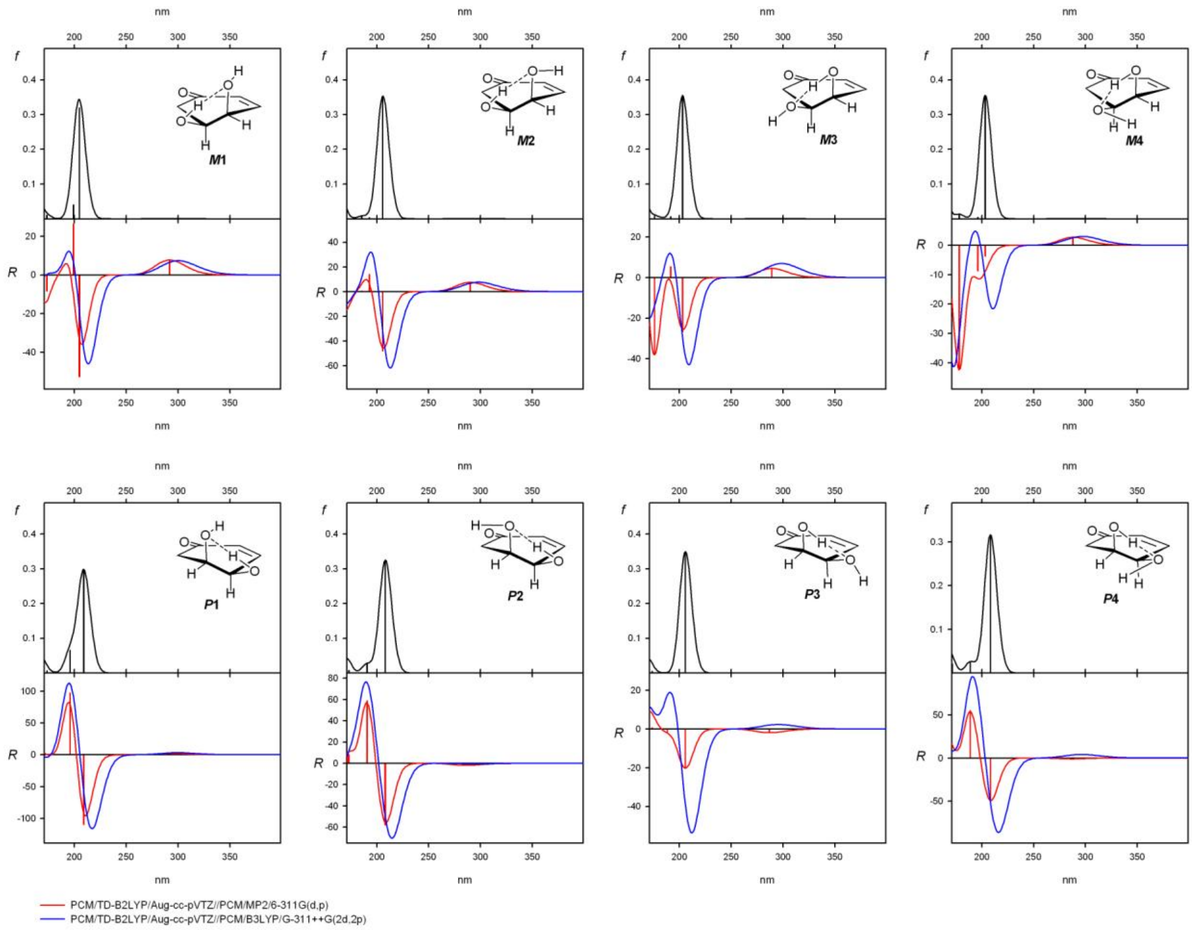

Figure B1. ECD spectra calculated at the PCM/B2LYP/Aug-cc-pVTZ level for individual conformers of **1a**, optimized at the PCM/MP2/6-311G(d,p) level (red lines) and at the PCM/B3LYP/6-311++G(2d,2p) level (blue lines).

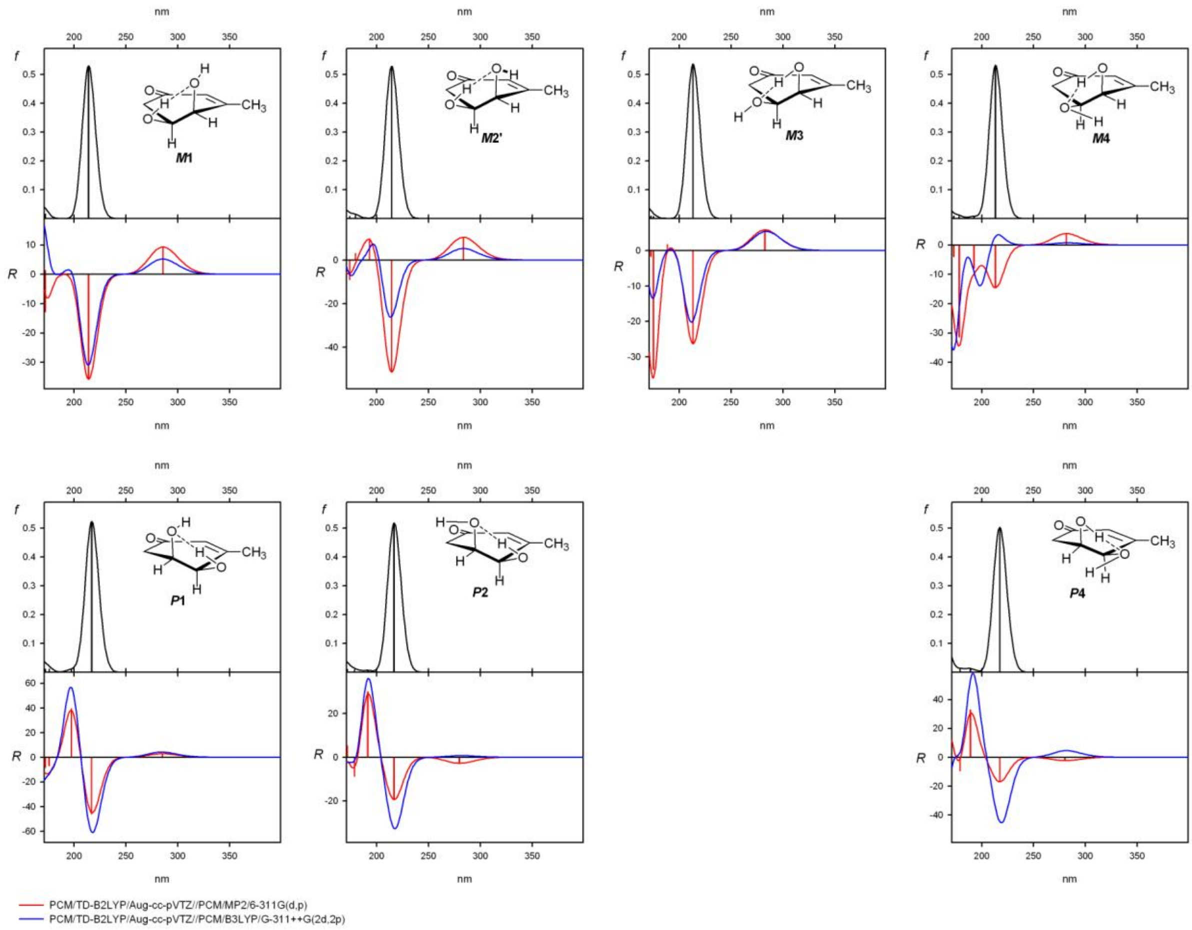

Figure B2. ECD spectra calculated at the PCM/B2LYP/Aug-cc-pVTZ level for individual conformers of **1b**, optimized at the PCM/MP2/6-311G(d,p) level (red lines) and at the PCM/B3LYP/6-311++G(2d,2p) level (blue lines).

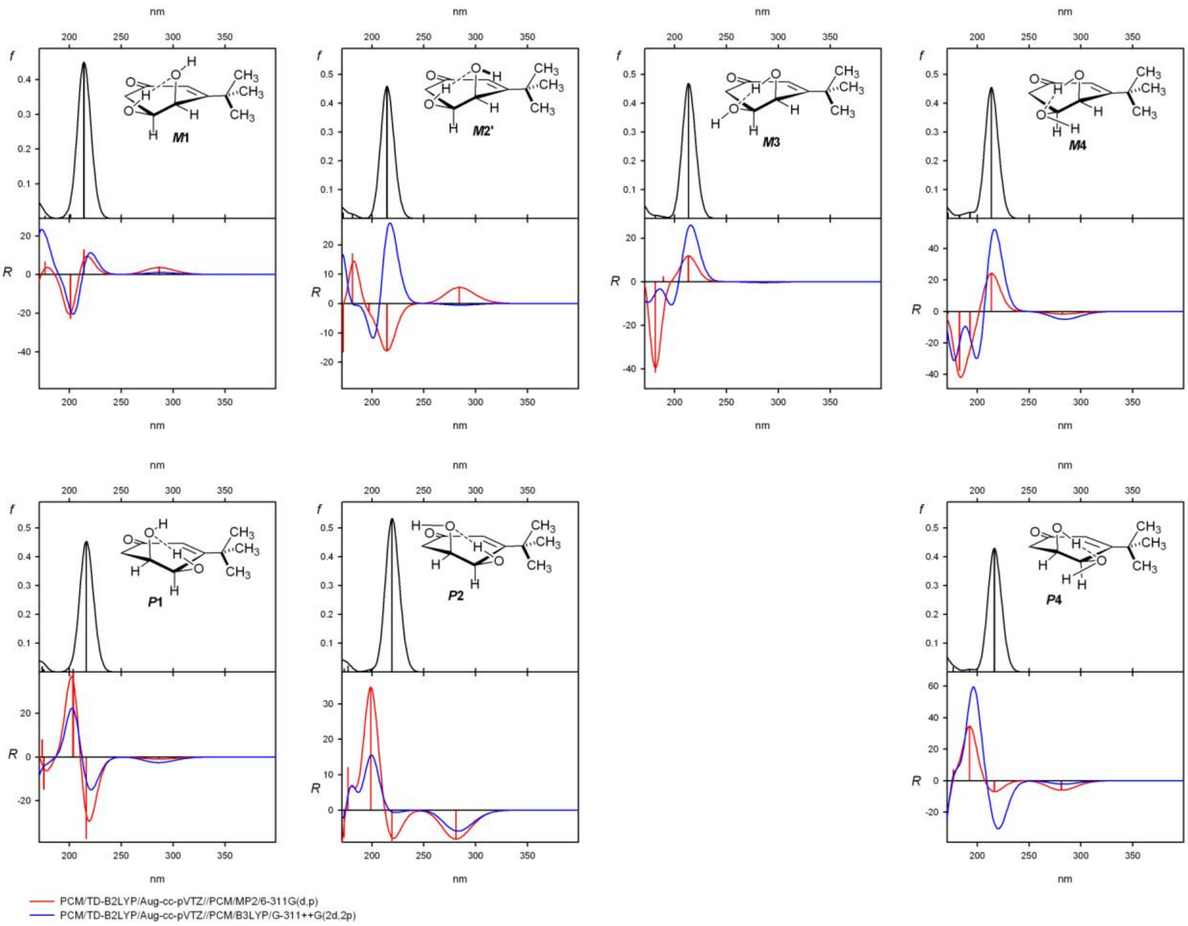

Figure B3. ECD spectra calculated at the PCM/B2LYP/Aug-cc-pVTZ level for individual conformers of **1c**, optimized at the PCM/MP2/6-311G(d,p) level (red lines) and at the PCM/B3LYP/6-311++G(2d,2p) level (blue lines).

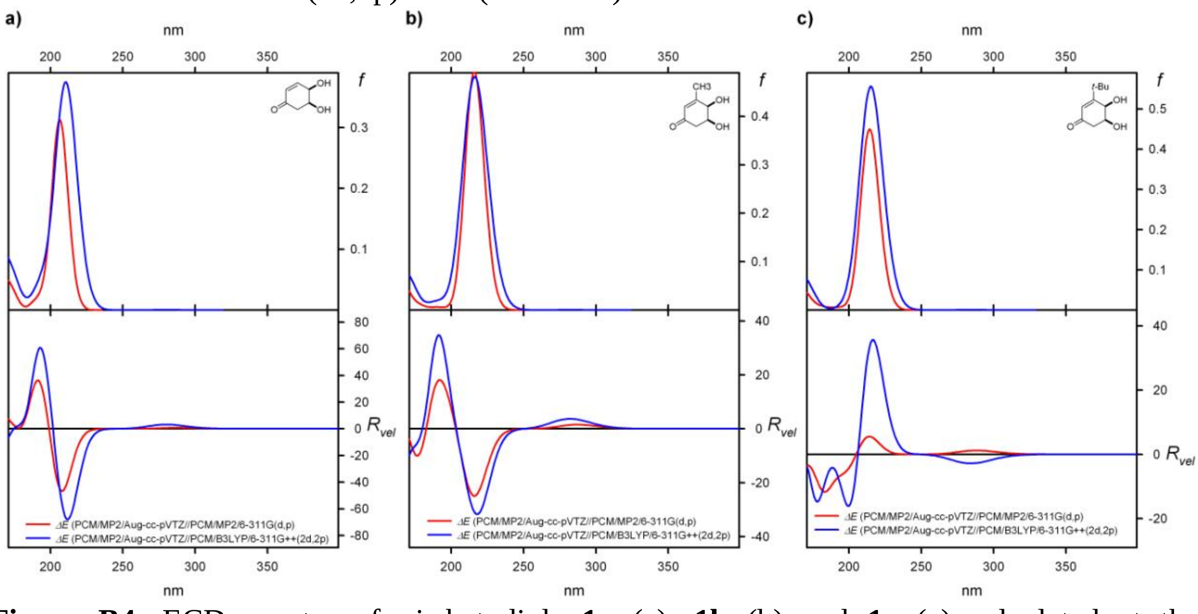

Figure B4. ECD spectra of *cis*-ketodiols **1a** (a), **1b** (b) and **1e** (c) calculated at the PCM/B2LYP/Aug-cc-pVTZ level and ΔE_{MP2} Boltzmann averaged. Geometries were optimized at the PCM/MP2/Aug-cc-pVTZ//PCM/MP2/6-311G(d,p) level (red lines) and at the PCM/MP2/Aug-cc-pVTZ//PCM/B3LYP/6-311++G(2d,2p) level (blue lines). Wavelength not corrected.

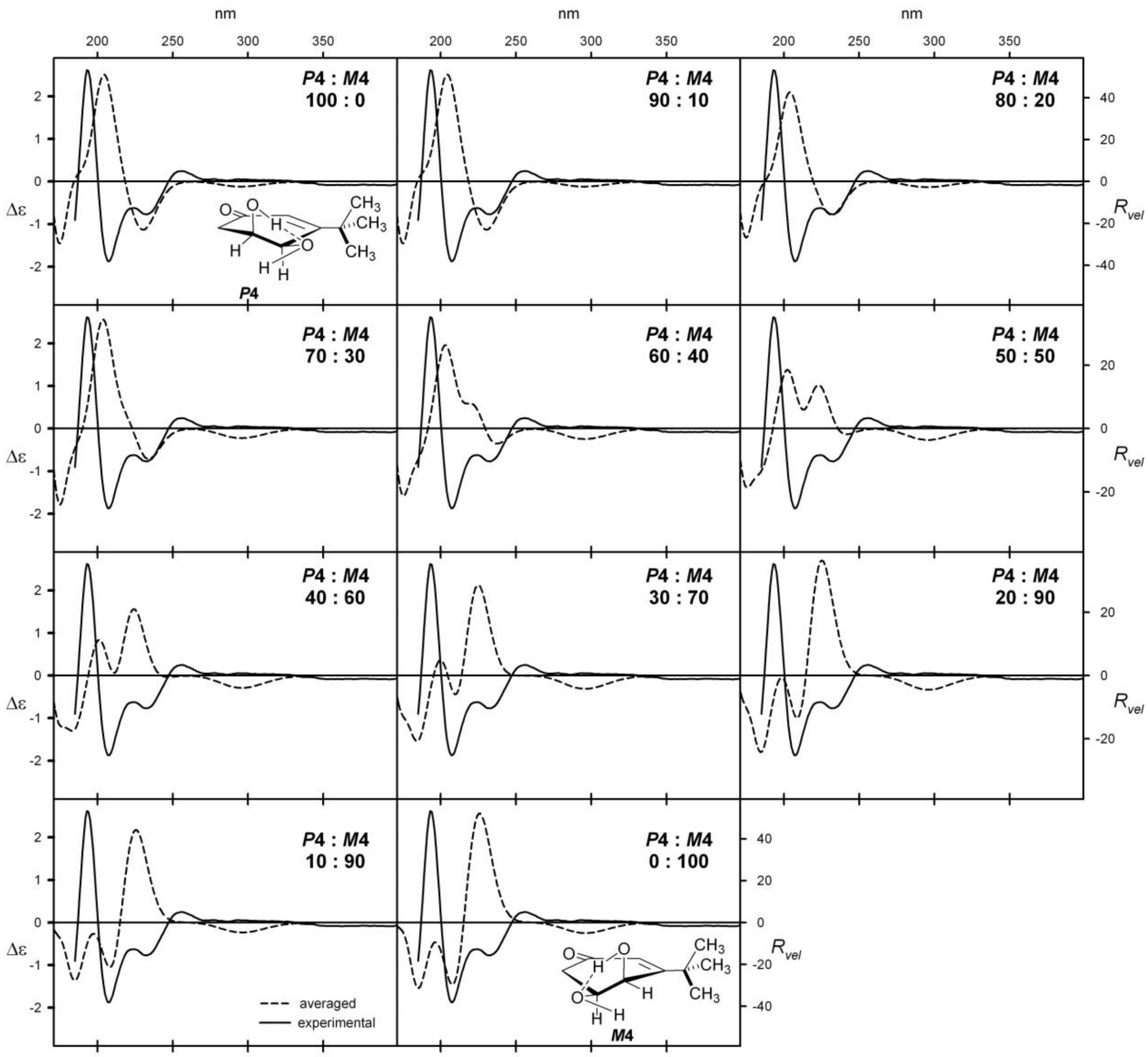

Figure C. Efect of percentage populations of the lowest-energy *P* and *M* conformers on averaged ECD spectra of **1e**. ECD spectra were calculated at PCM/B2LYP/Aug-cc-pVTZ level.

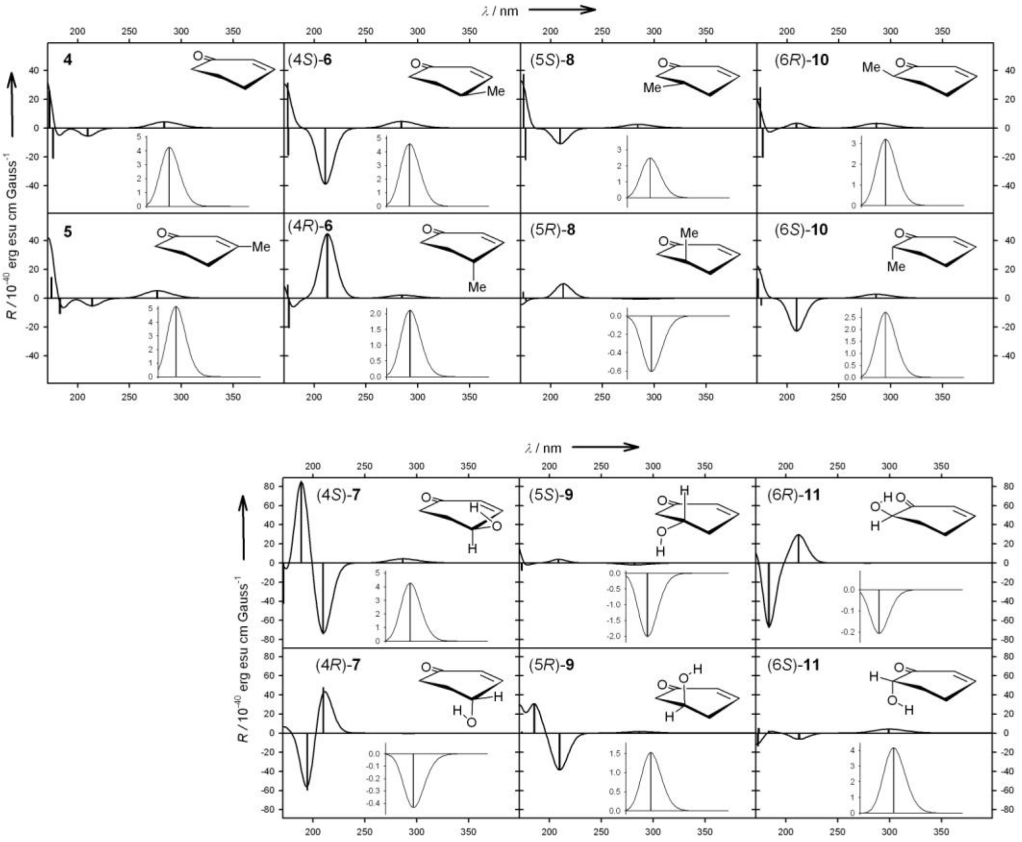

Figure D. Effect of methyl and hydroxy substituents on the ECD spectra of selected monosubstituted (*P*)-2-cyclohexenones with a planar chromophore (ω = 180º, τ = 0º). All spectra were calculated at the PCM/B2LYP/Aug-cc-pVTZ level for the structures optimized at the PCM/B3LYP/6-311++G(2d,2p) level. Inserts show long wavelength (ca. 300 nm) $n_{C=O}$-$\pi_{C=O}$* Cotton effects. Wavelength not corrected.

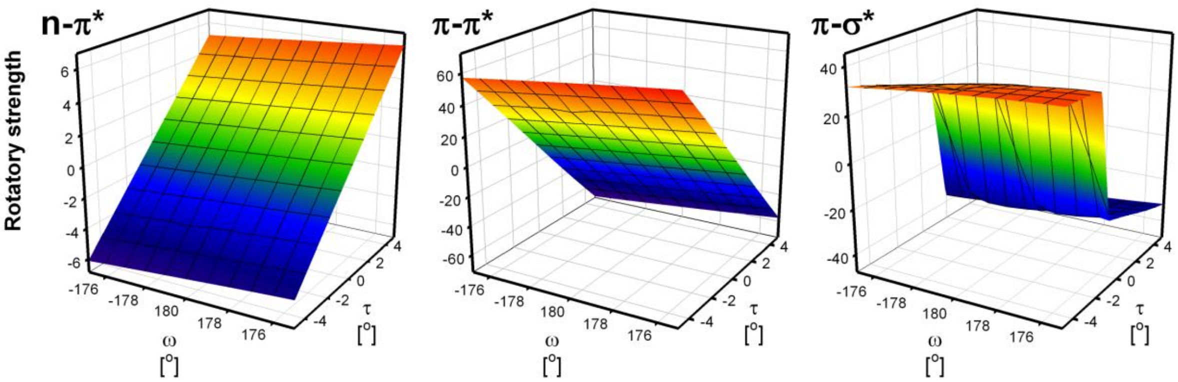

Figure E. Effect of non-planarity of the chromophore (ω and τ angles) on the rotatory strengths *R* for the three low-energy electronic transitions, calculated conformers of acrolein. All rotatory strengths were calculated at the PCM/B2LYP/6-311++G(2d,2p) level.

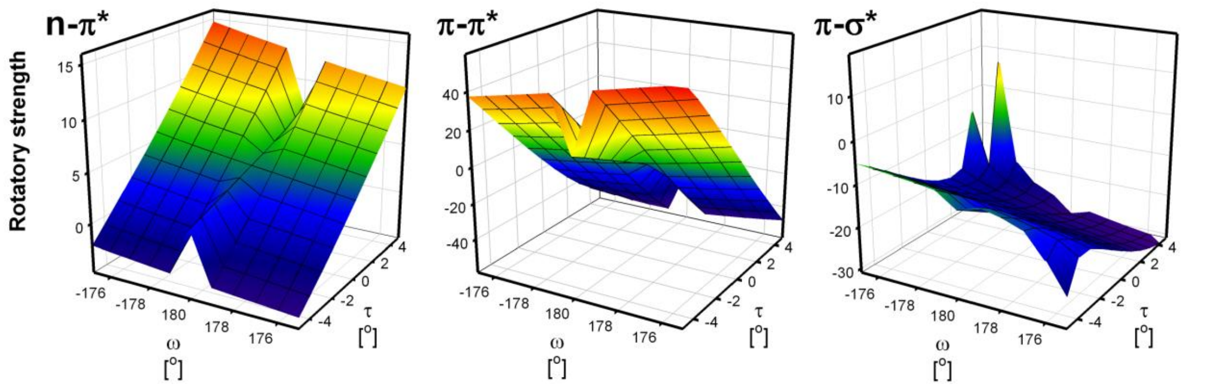

Figure F. Effect of non-planarity of the chromophore (ω and τ angles) on the rotatory strengths *R* for the three low-energy electronic transitions, calculated for *P*-type conformers of **4**. All rotatory strengths were calculated at the PCM/B2LYP/6-311++G(2d,2p) level.

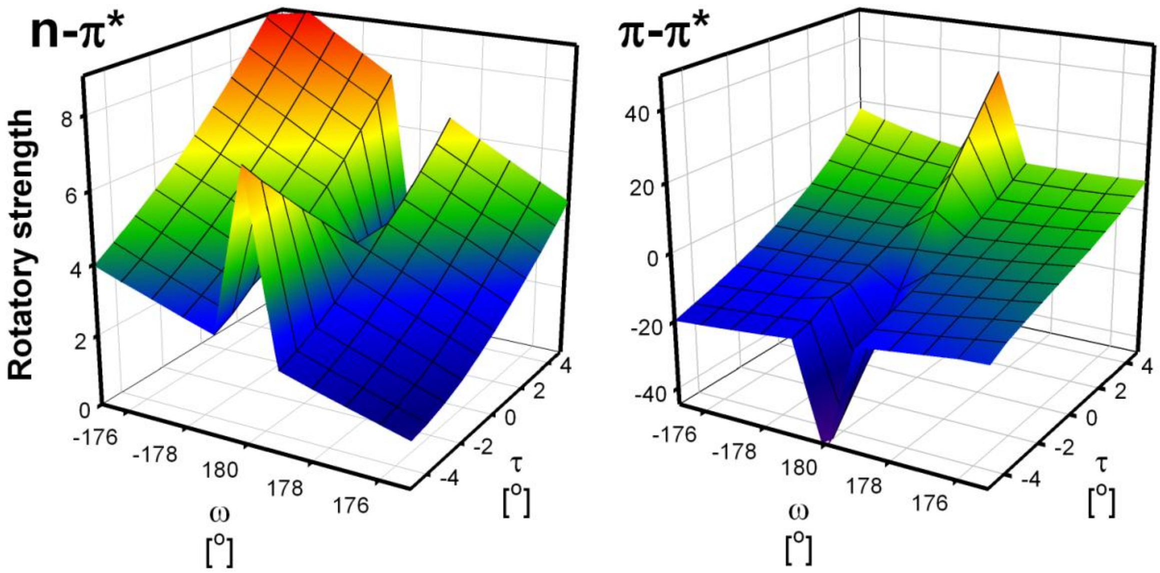

Figure G. Calculated contribution of the C4-C5-C6 chain to the rotatory strengths of 2-cyclohexenone obtained by subtraction of rotatory strengths calculated for acrolein (Figure D) from those obtained for **4** (Figure E). All rotatory strengths were calculated at the PCM/B2LYP/6-311++G(2d,2p) level.

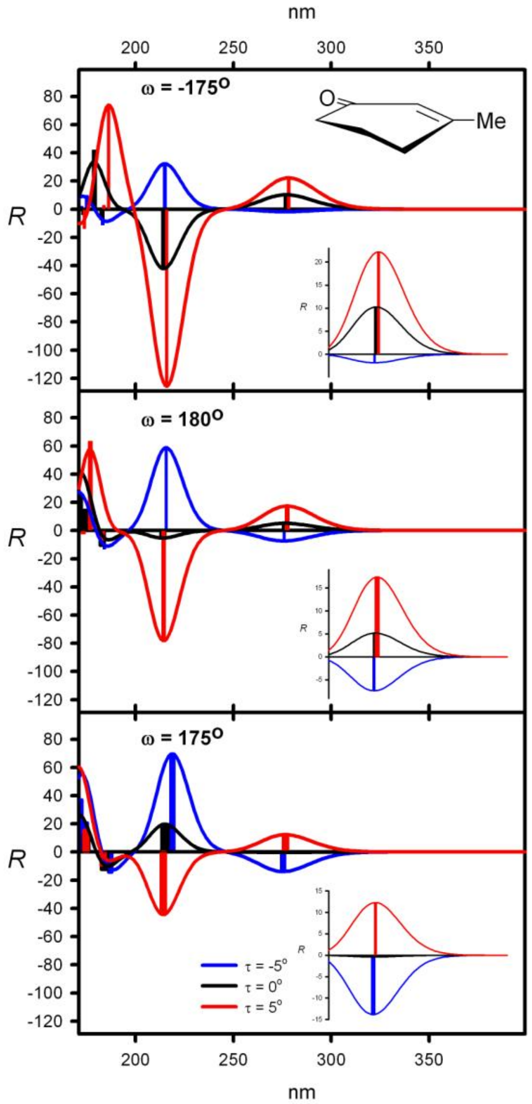

Figure H. Effect of the twist of ω and τ angles on the ECD spectra of *P*-type conformer of **5** calculated at PCM/B2LYP/6-311++G(2d,2p) level. Vertical bars represent rotatory strengths. Wavelength not corrected.

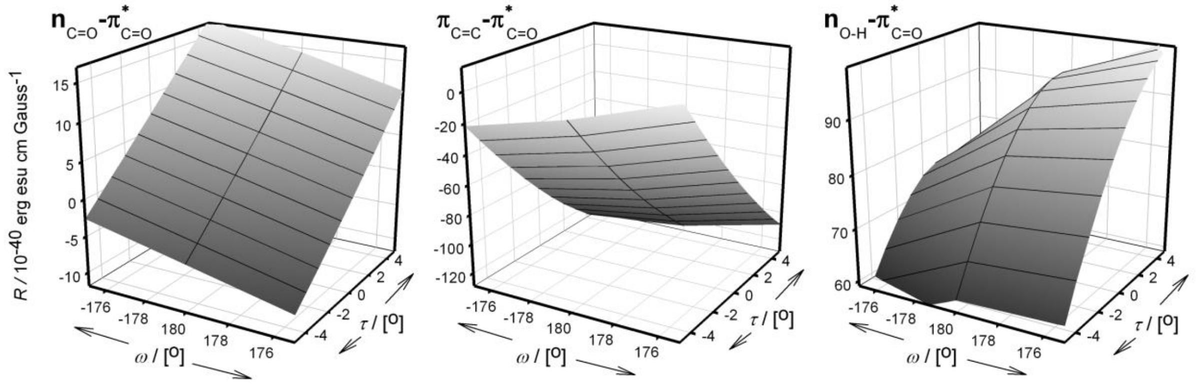

Figure I. Effect of deviation from planarity (angles ω and τ) on the rotatory strengths *R* for the three low-energy electronic transitions, calculated for *P*-type conformers of (4*S*)-**7**. All rotatory strengths were calculated at the PCM/B2LYP/6-311++G(2d,2p) level.

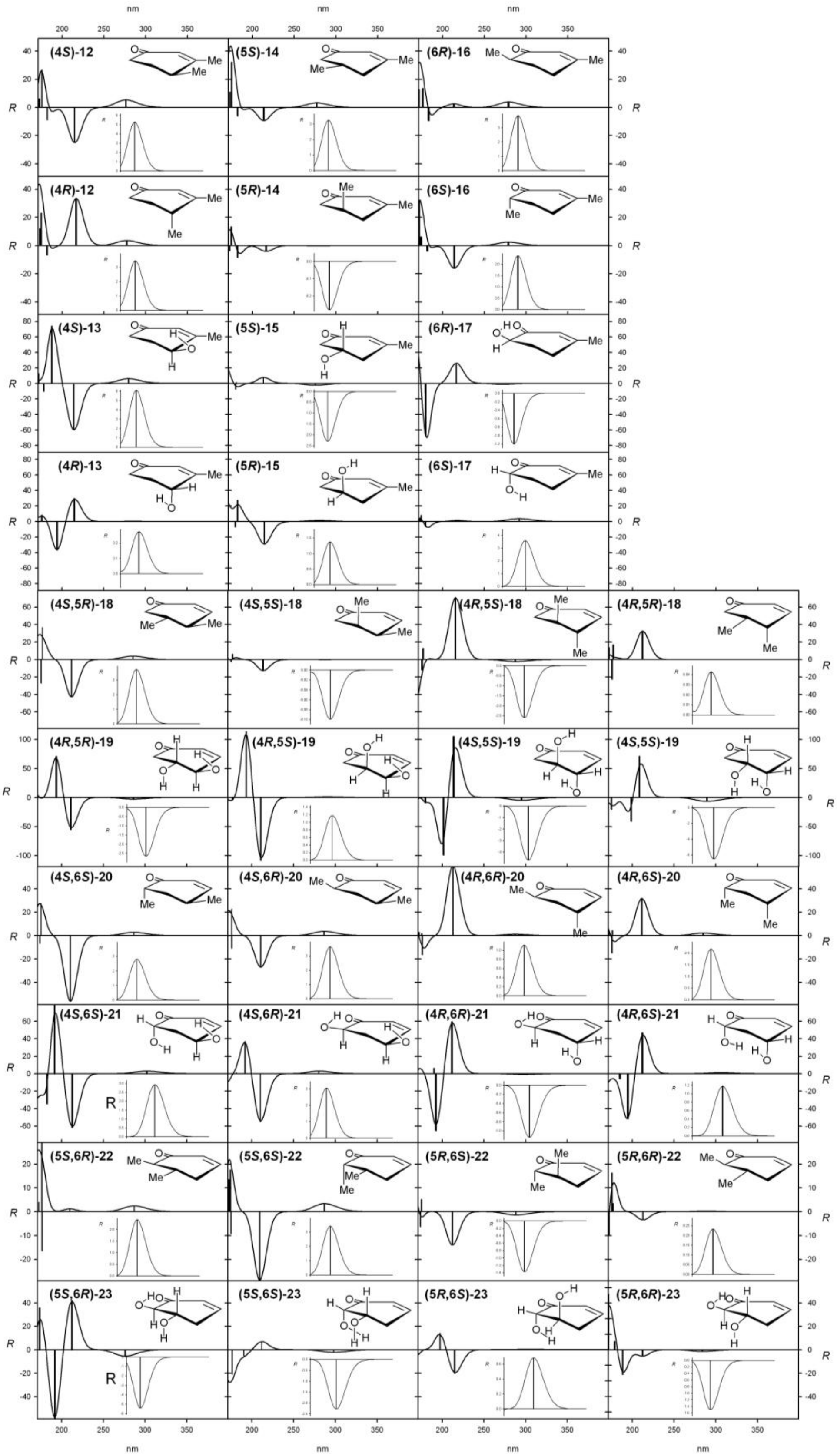

Figure J. Effect of methyl and hydroxy substituents on the ECD spectra of selected disubstituted 2-cyclohexenone *P*-type conformers with planar chromophore moieties. All spectra were calculated at the PCM/B2LYP/6-311++G(2d,2p) level. Inserts show the long wavelength (ca. 300 nm) n-π* Cotton effects. Wavelength not corrected.

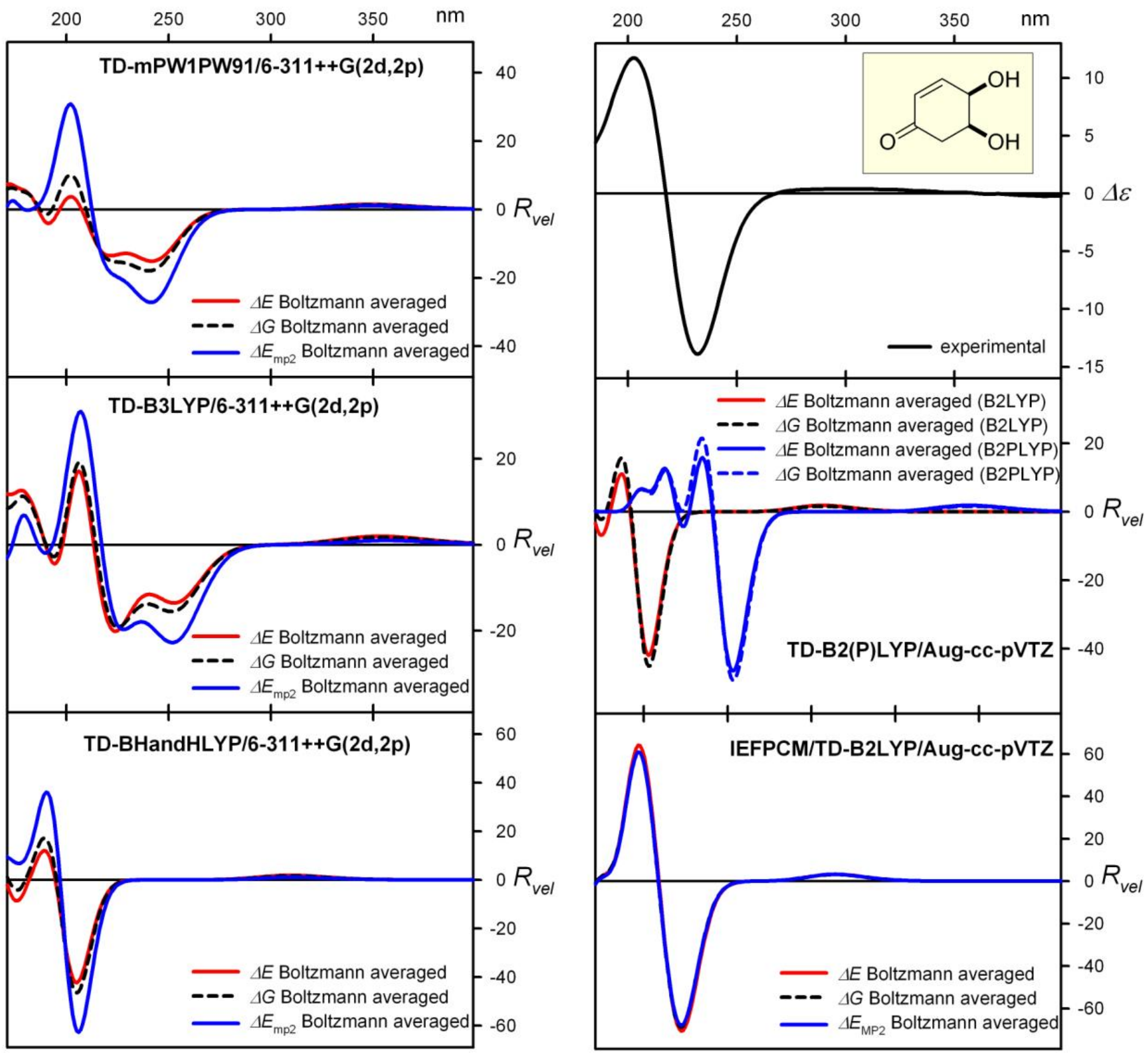

Figure K. Effect of methods used for calculations of ECD and for Boltzmann averaging on the shapes of the ECD spectra of **1a**.