Supporting Information

Amplification of the Chiroptical Response of UV-transparent Amines and Alcohols by *N*-Phthalimide Derivatization Enabling Absolute Configuration Determination through ECD Computational Analysis

Daniele Padula,[a,b] Giuseppe Mazzeo,[a,c] Ernesto Santoro,[a] Patrizia Scafato,[a]

Sandra Belviso,[a] and Stefano Superchi*[,a]

[a]*Dipartimento di Scienze, Università degli Studi della Basilicata, via dell'Ateneo Lucano, 85100 Potenza, Italy.*
[b]*Dipartimento di Biotecnologie, Chimica e Farmacia, Università di Siena, via A. Moro 2, 53100; Siena, Italy.*
[c]*Dipartimento di Medicina Molecolare e Traslazionle, Università di Brescia, Viale Europa 11, 25123 Brescia, Italy.*

* Correspondence to: stefano.superchi@unibas.it

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Table S1: Comparison of Experimental $[\alpha]_D$ and number of computed conformers between phthalimides **2a-l** and their parent amines and alcohols.

Amines/alcohols			Phthalimides		
compound	$[\alpha]_D$ [a]	Number of conformers by MM[b]	compound	$[\alpha]_D$ [a]	Number of conformers by MM[b](DFT)[c]
1a	+18[d]	3	**2a**	+18	1 (1)
1b	+7	9	**2b**	+17	3 (3)
1c	+7	6	**2c**	+25	3 (3)
1d	+4	12	**2d**	+10	4 (4)
1e	-5	7	**2e**	-17	2 (2)
1f	+61	11	**2f**	-58	3 (2)
1g	+10	52	**2g**	+6	5 (5)
1h	+16	19	**2h**	-10	8 (7)
1i	+10	9	**2i**	-16	3 (3)
1j	-42	8	**2j**	+4	5 (5)
1k	-6	4	**2k**	+5	2 (2)
1l	-47	3	**2l**	-6	1(1)

[a]Recorded in $CHCl_3$; c =1.0. [b]Conformers found within 10 kcal/mol by MM computations (MMFF94 force field). [c]Conformers found by DFT/B3LYP/TZVP/gas phase computations. [d]Recorded in methanol.[1]

Table S2: Experimental $[\alpha]_D$ for selected phthalimides **2** in different solvents.

Phthalimide	$CHCl_3$(c)	MeOH(c)	Hexane(c)
2a	+18(0.8)	/	+7(0.9)
2b	+17(1.0)	+17(1.4)	+16(2.0)
2c	+25(1.1)	+21(0.9)	+22(0.9)
2e	-17(1.0)	-22(1.0)	-21(1.0)

[1] M. C. Schopohl, A. Faust, D. Mirk, R. Fröhlich, O. Kataeva, S. R. Waldvogel, *Eur. J. Org. Chem.* 2005, **14**, 2987.

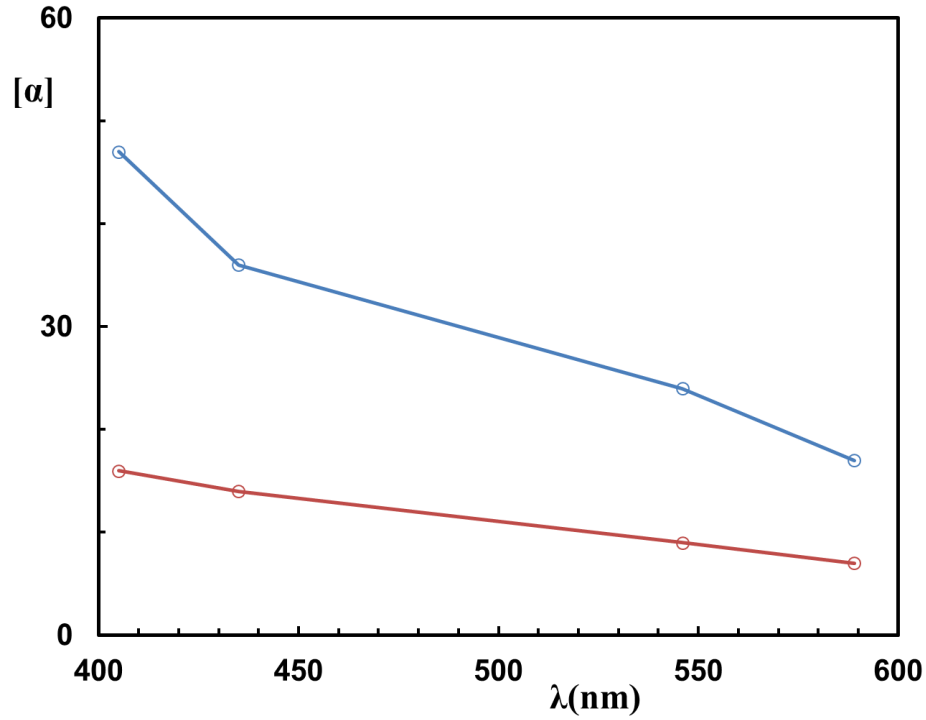


Figure S1: Experimental ($CHCl_3$) ORD curve recorded for amine **1b** (red line) and phthalimide **2b** (blue line).

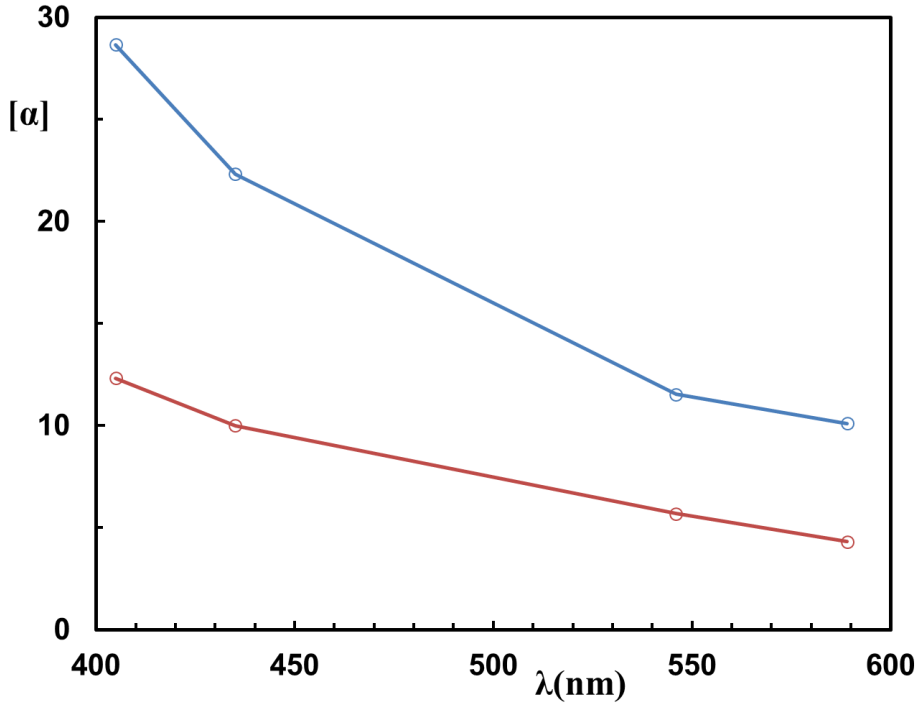


Figure S2: Experimental ($CHCl_3$) ORD curve recorded for amine **1d** (red line) and phthalimide **2d** (blue line).

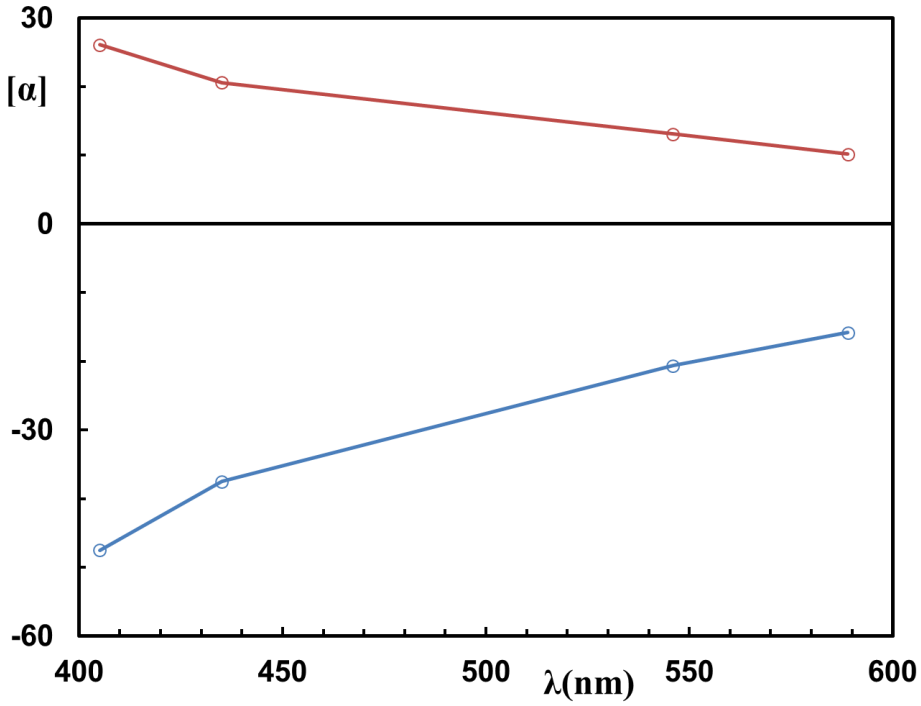


Figure S3: Experimental ($CHCl_3$) ORD curve recorded for carbinol **1i** (red line) and phthalimide **2i** (blue line), corresponding to **ent-2b**.

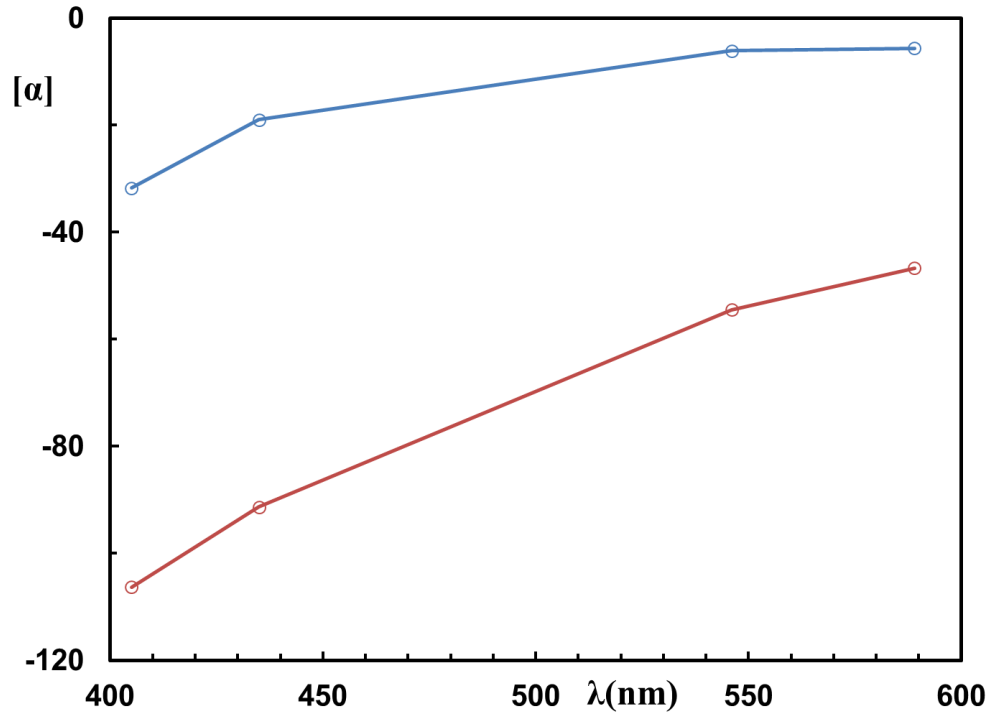


Figure S4: Experimental ($CHCl_3$) ORD curve recorded for carbinol **1l** (red line) and phthalimide **2l** (blue line).

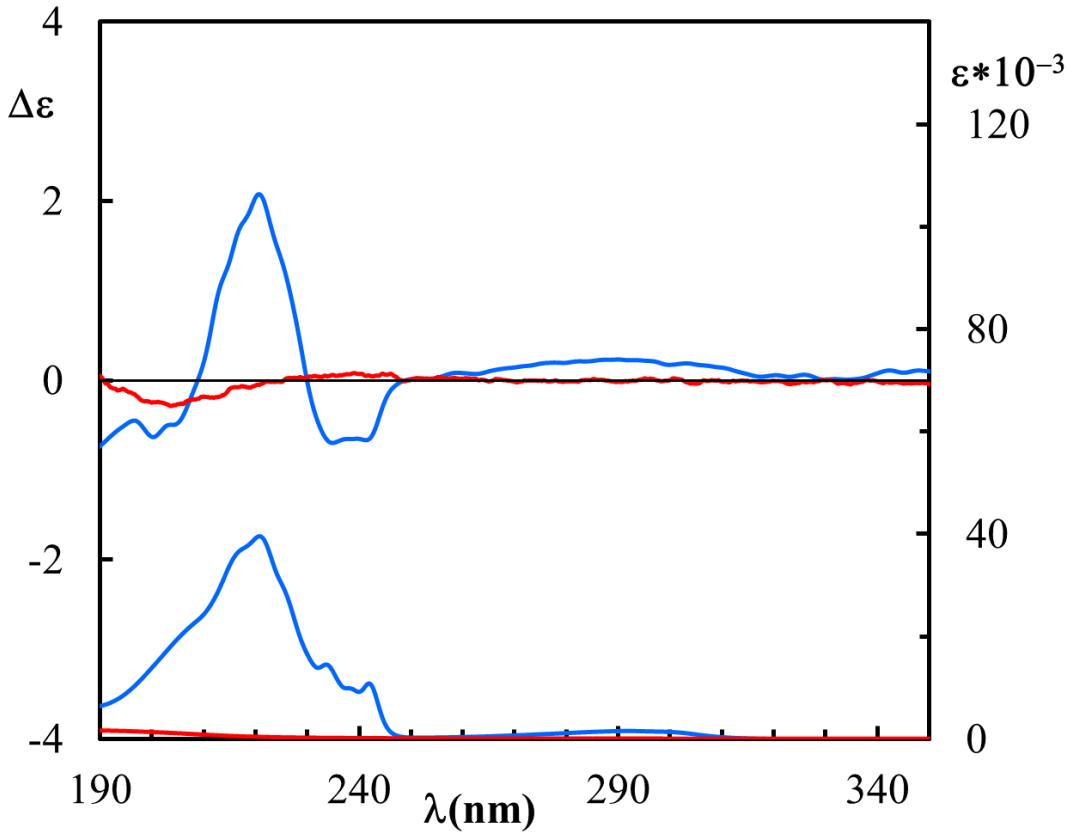


Figure S5: Experimental ECD and UV spectra (in CH_3CN) recorded for amine **1b** (red line) and phthalimide **2b** (blue line).

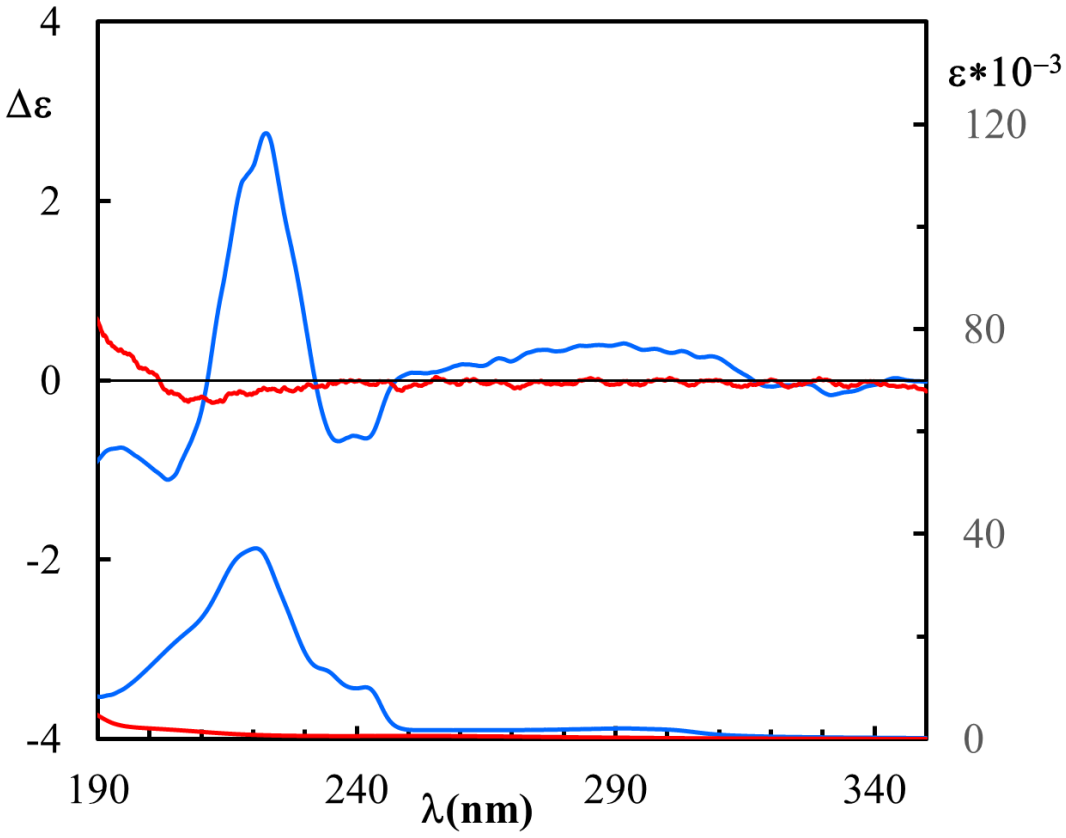
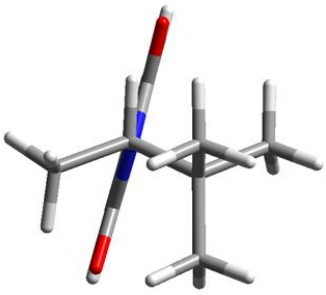
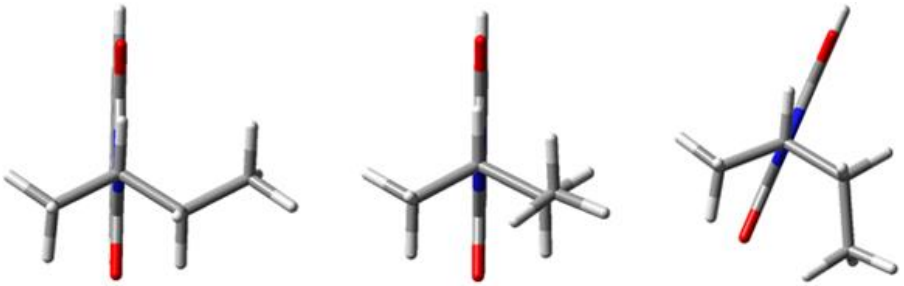


Figure S6: Experimental ECD and UV spectra (in CH_3CN) recorded for amine **1d** (red line) and phthalimide **2d** (blue line).



Conf. 1

Figure S7: structure of the only conformer of compound **2a**.

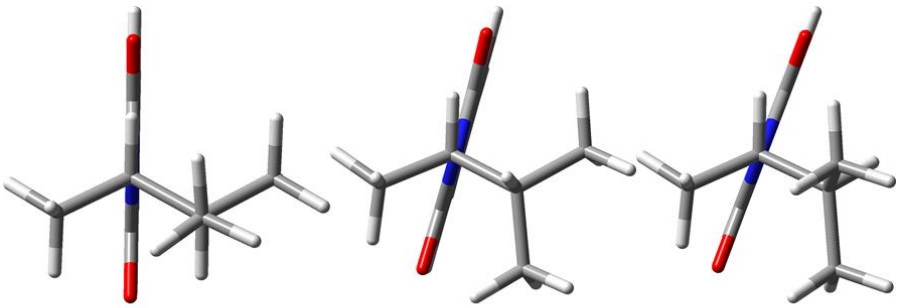


Conf. 1
69.7%

Conf. 2
29.3%

Conf. 3
1%

Figure S8: structures and populations of the three conformers of compound **2b**.



Conf. 1
93.2%

Conf. 2
2.5%

Conf. 3
4.3%

Figure S9: structures and populations of the three conformers of compound **2c**.

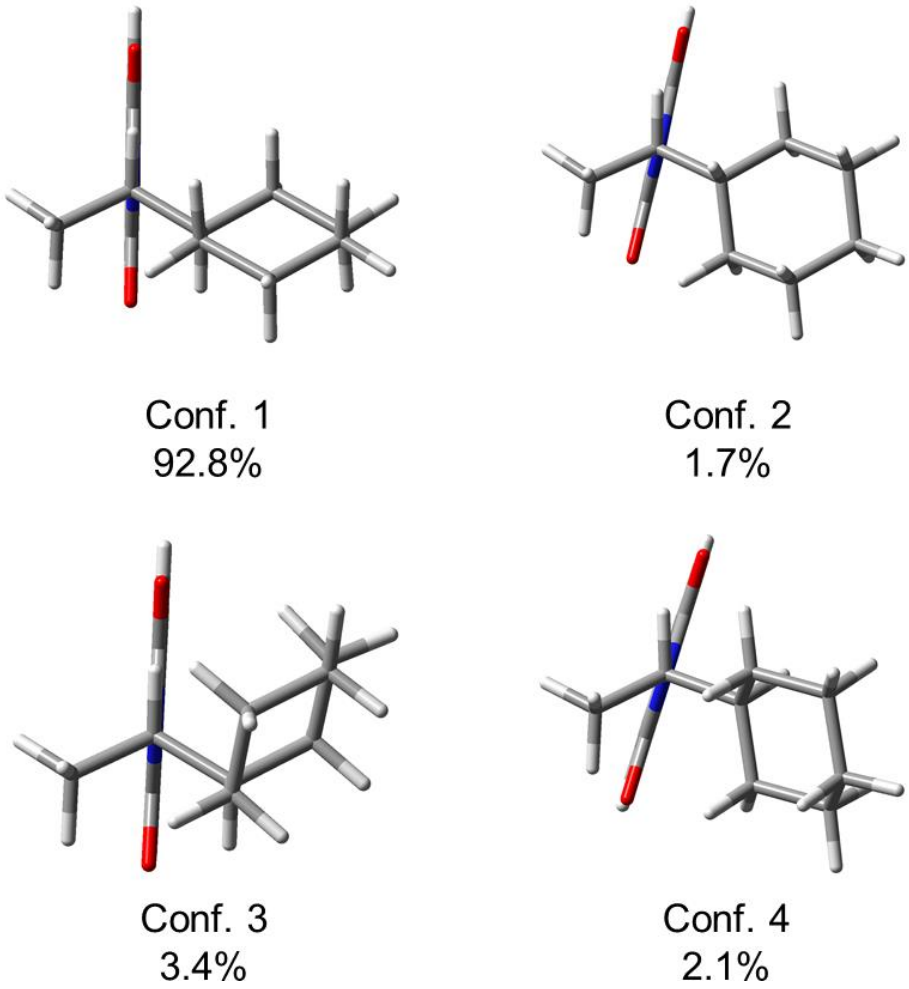


Figure S10: structures and populations of the four conformers of compound **2d**.

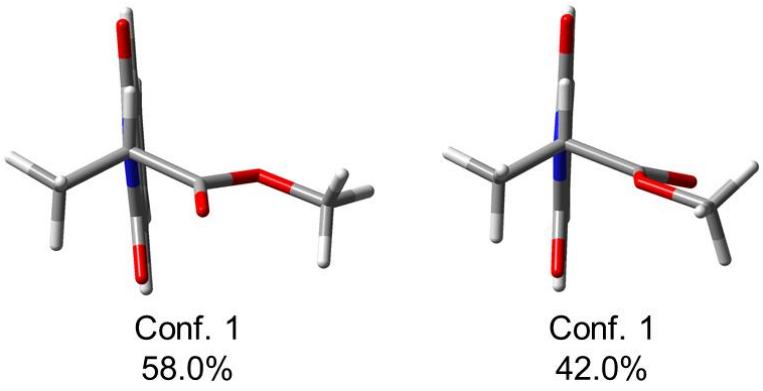


Figure S11: structures and populations of the two conformers of compound **2e**.

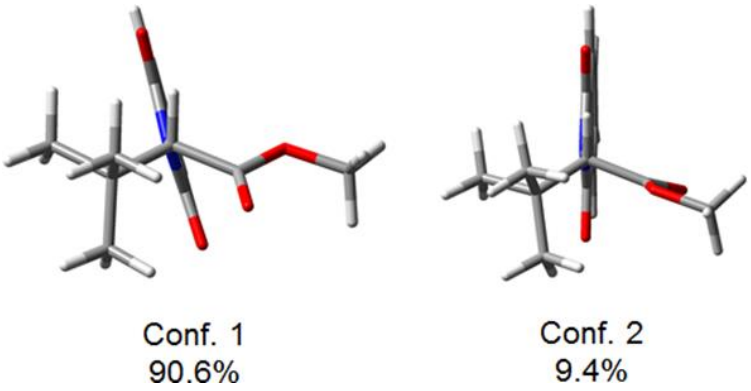


Figure S12: structures and populations of the two conformers of compound **2f**.

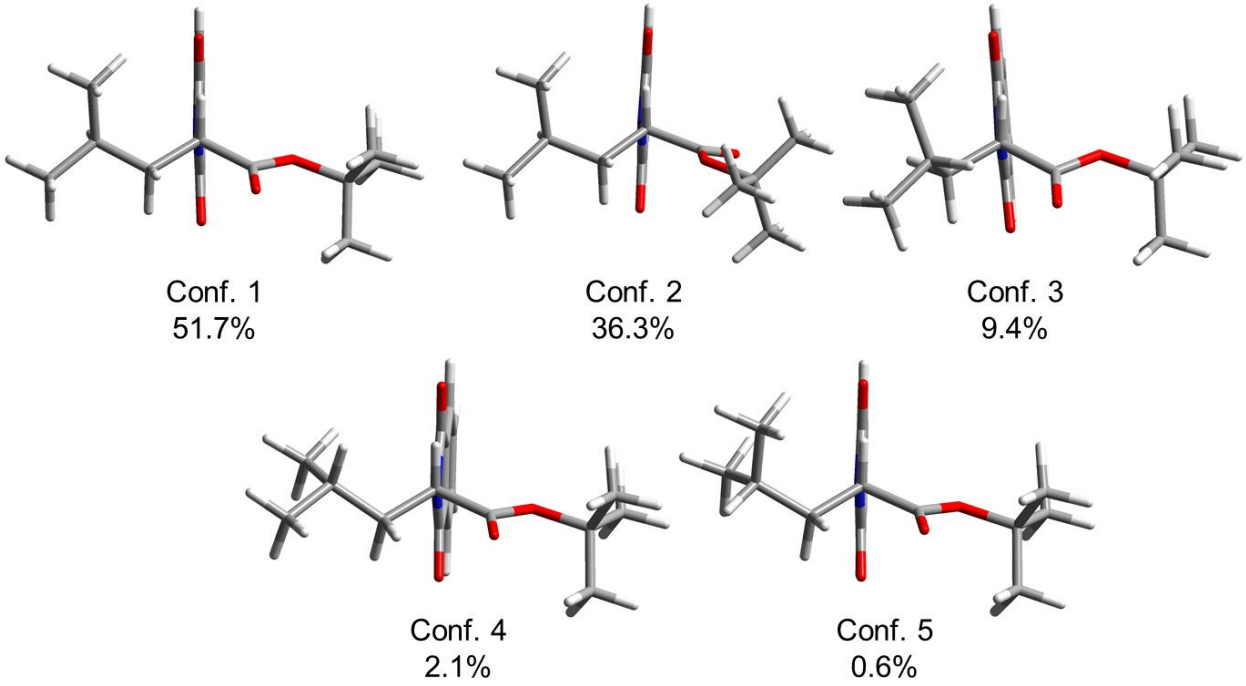


Figure S13: structures and populations of the five conformers of compound **2g**.

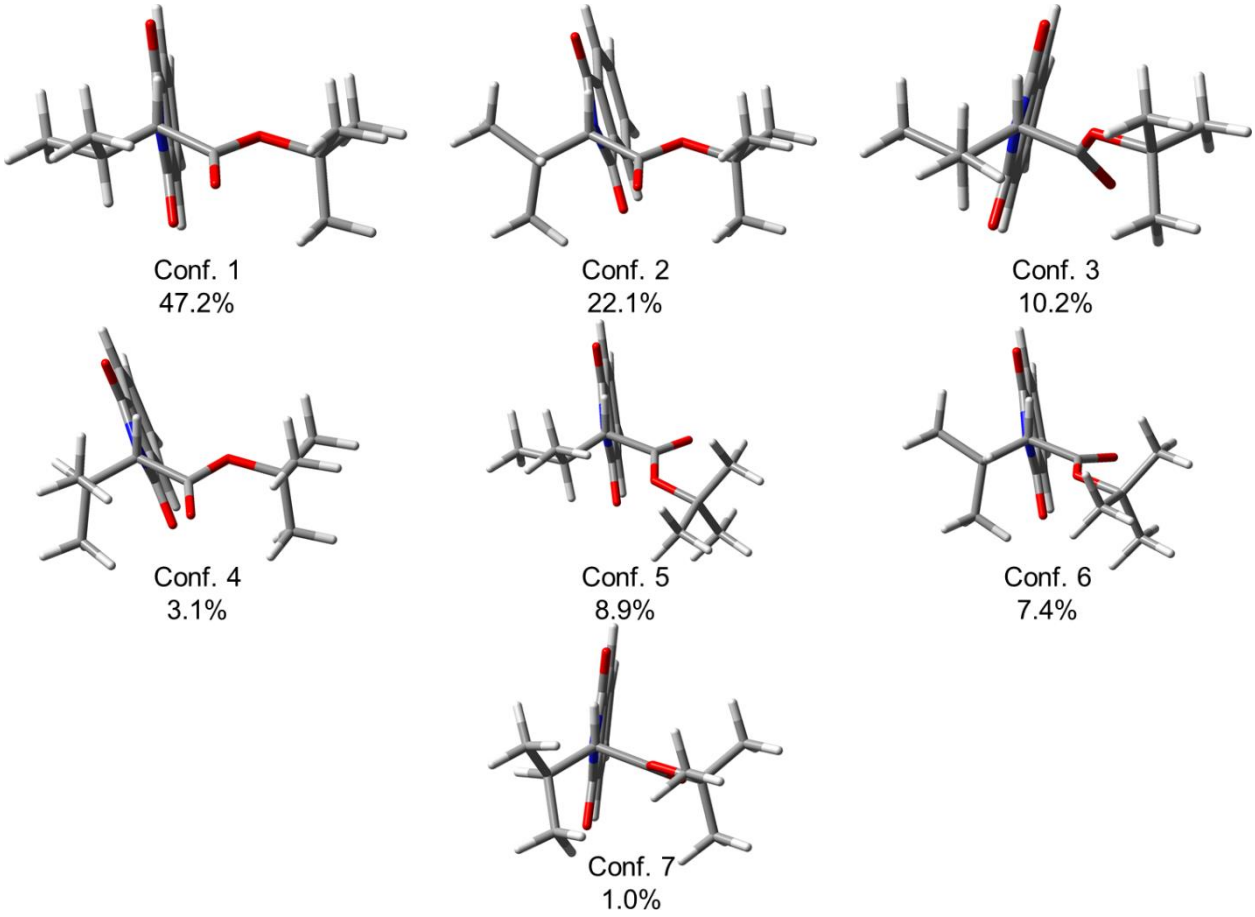


Figure S14: structures and populations of the seven conformers of compound **2h**.

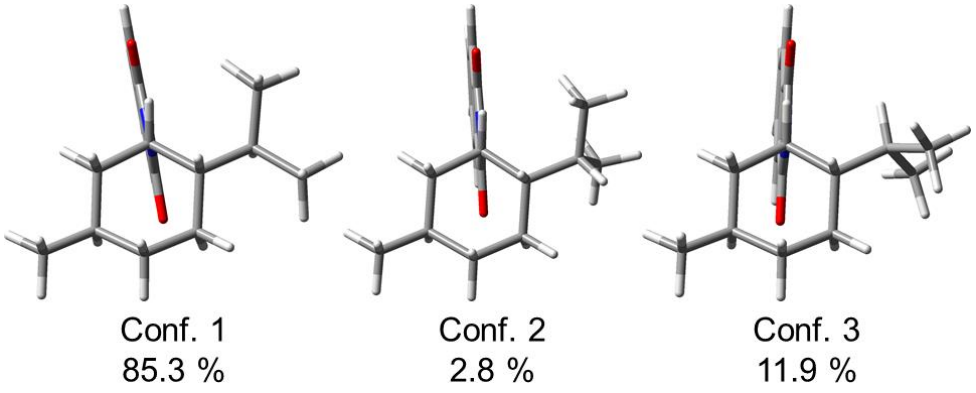


Figure S15: structures and populations of the three conformers of compound **2j**.

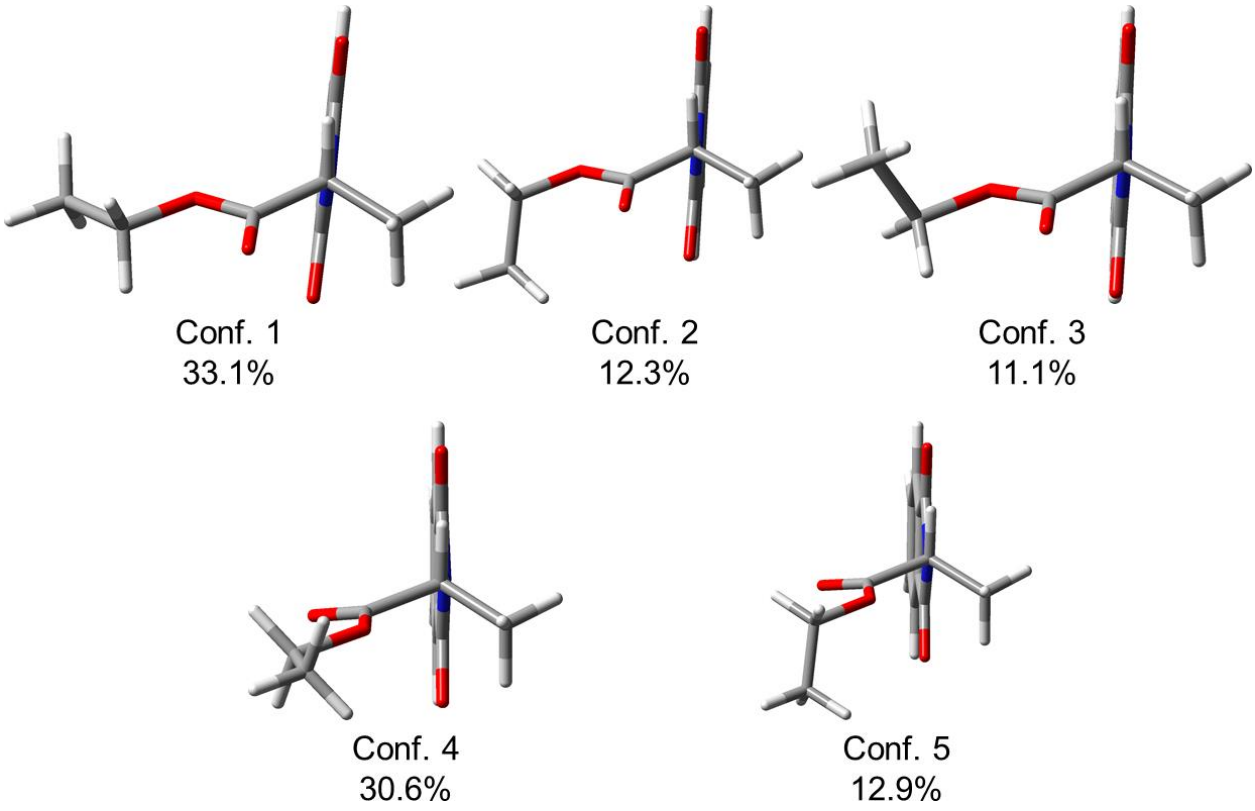


Figure S16: structures and populations of the five conformers of compound **2k**.

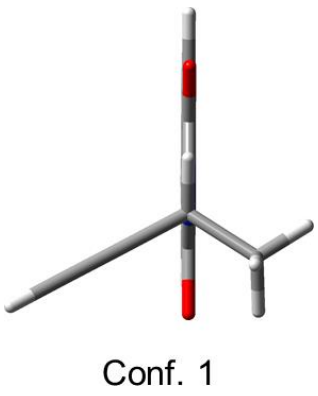


Figure S17: structures and populations of the only conformer of compound **2l**.

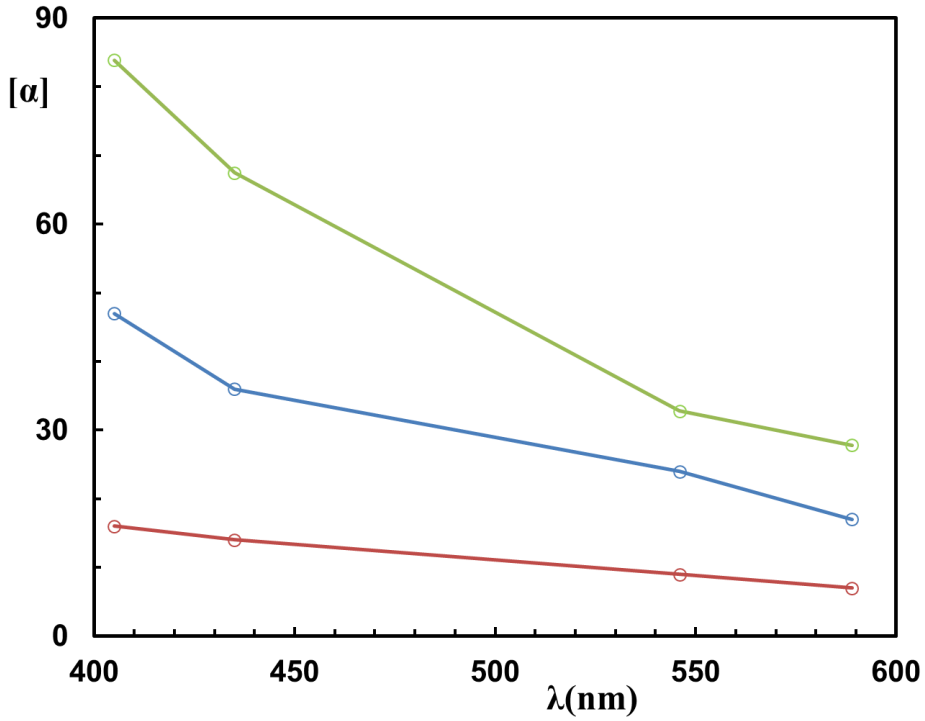


Figure S18: Experimental ($CHCl_3$) ORD curve recorded for amine **1b** (red line), its phthalimide **2b** (blue line), and its napthimide **3b** (green line).

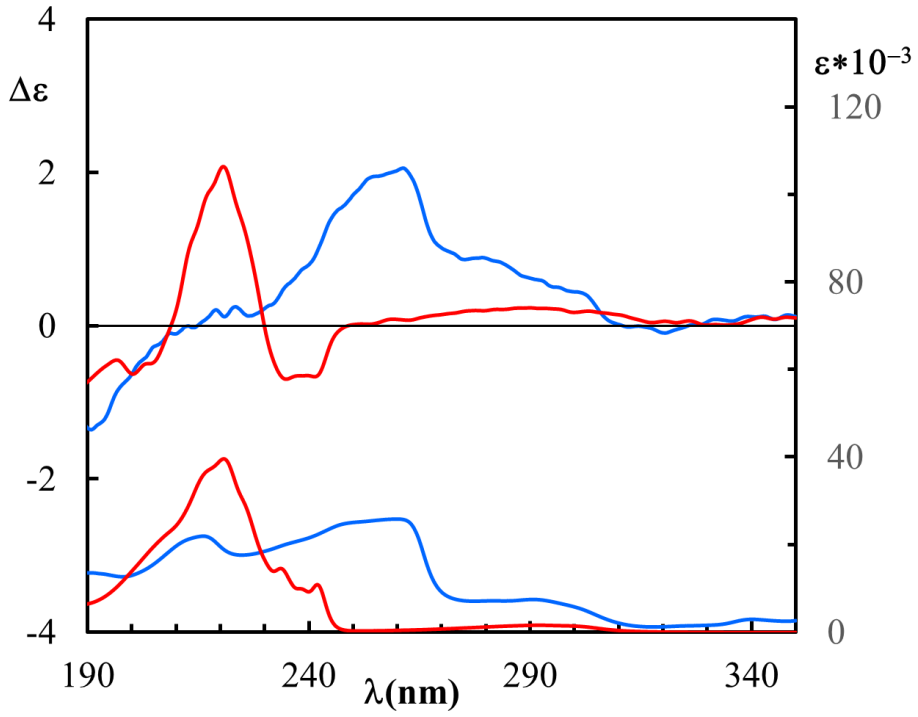


Figure S19: Experimental (CH_3CN) ECD and UV spectra recorded for phthalimide **2b** (red line) and napthimide **3b** (blue line) derived from amine **1b**.

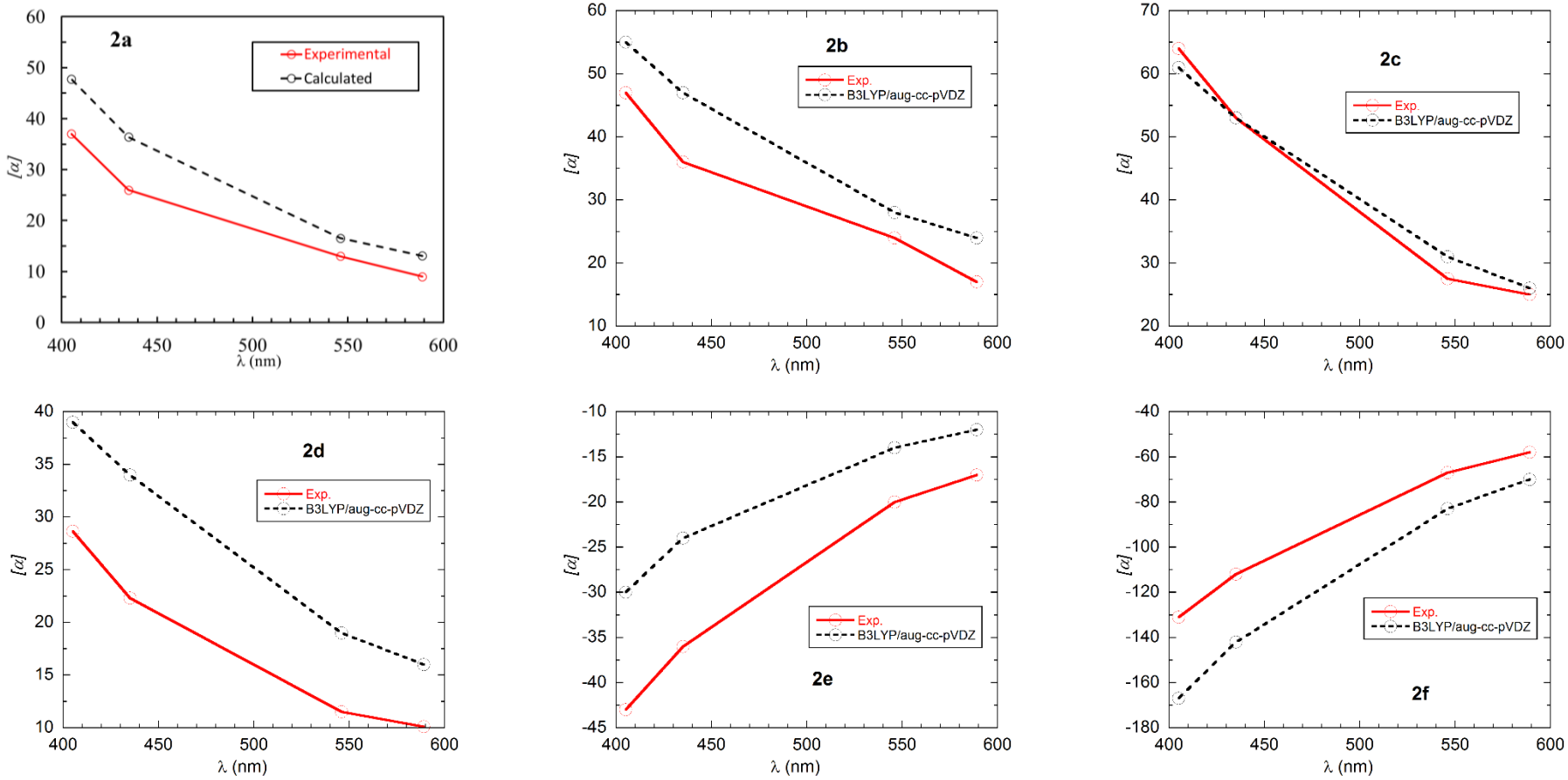


Figure S20: Experimental and calculated (TDDFT/B3LYP/aug-cc-pVDZ) ORD curves for compounds **2a-f**.

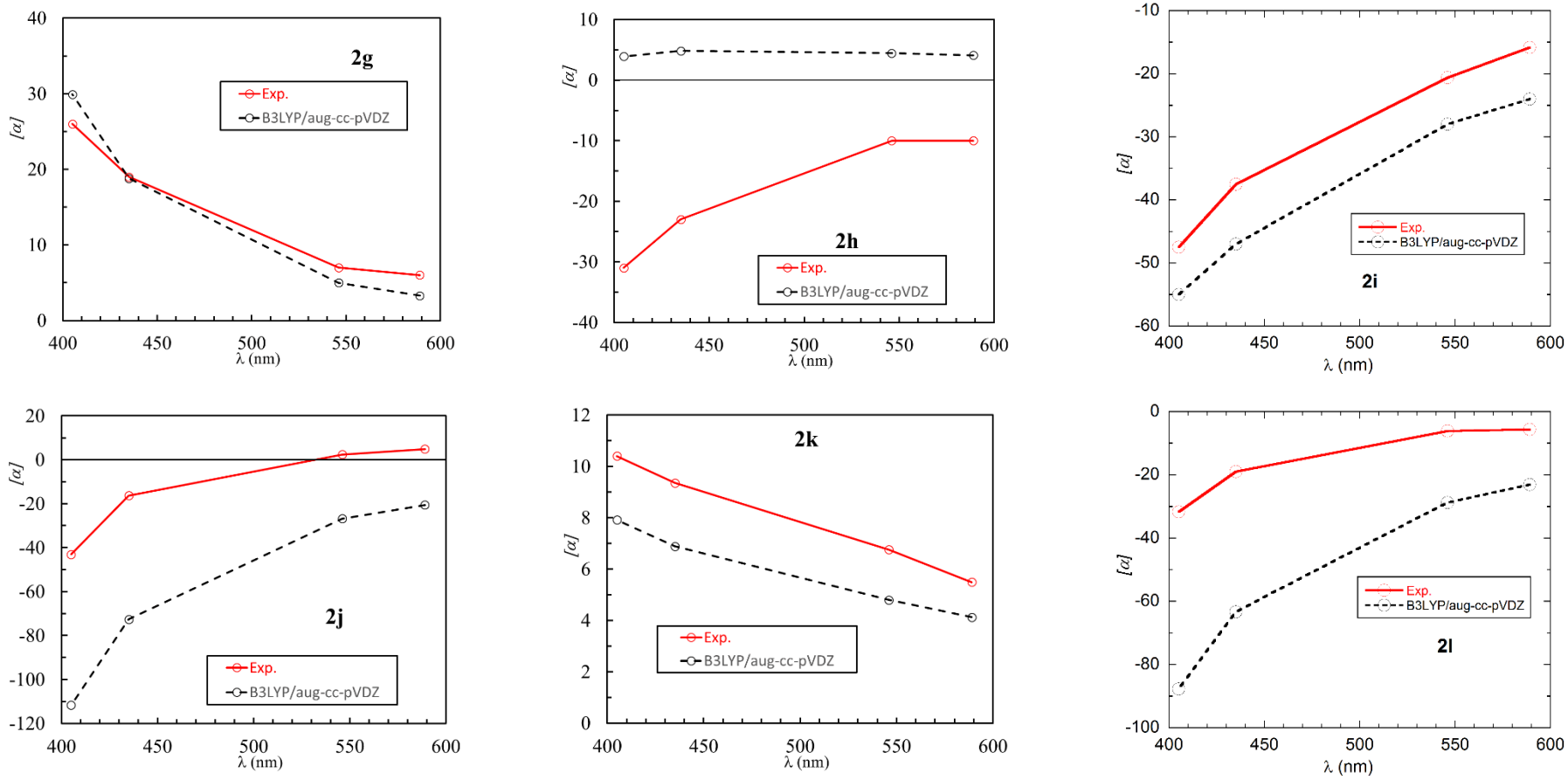


Figure S21: Experimental and calculated (TDDFT/B3LYP/aug-cc-pVDZ) ORD curves for compounds **2g-l**.

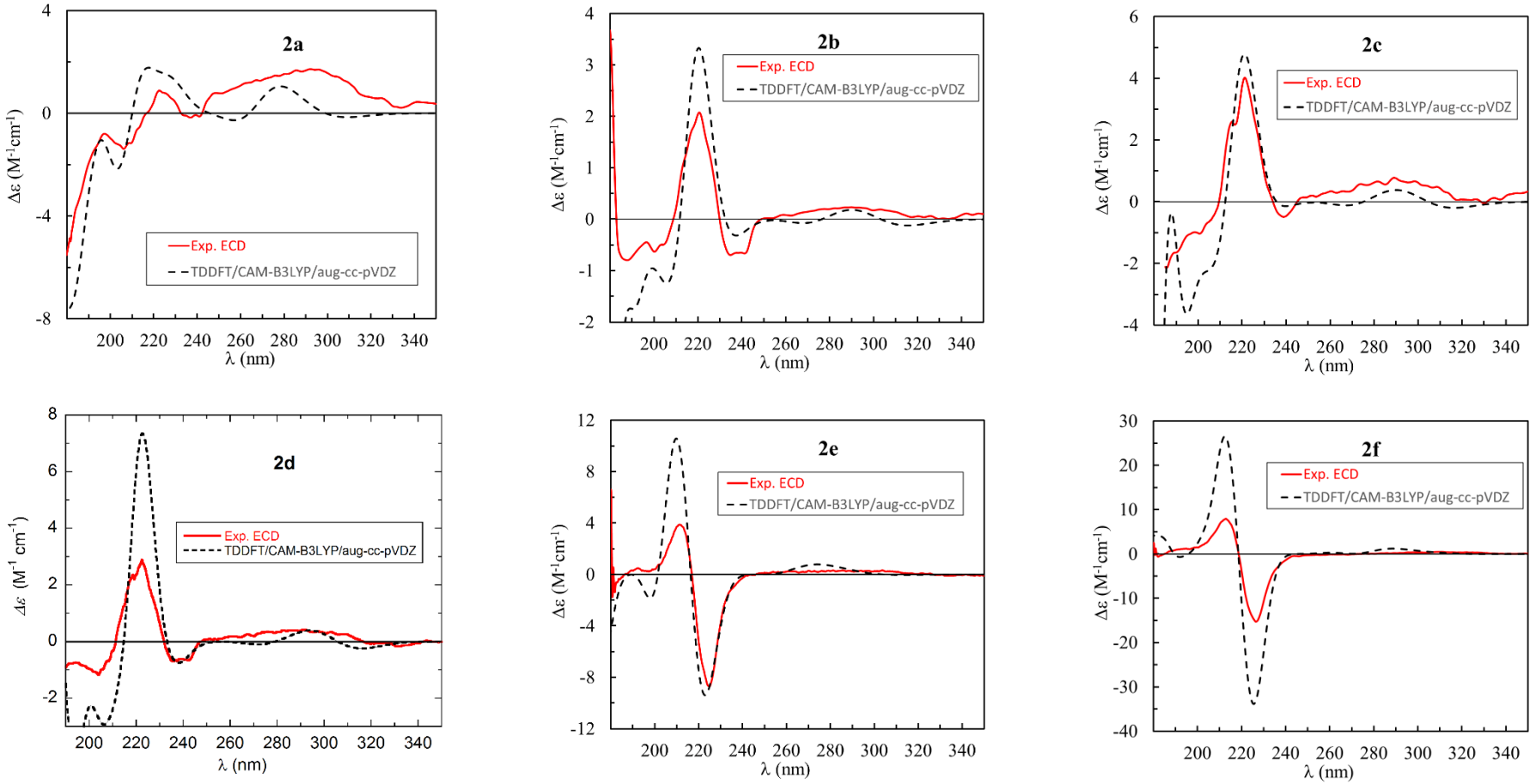


Figure S22: Experimental and calculated (TDDFT/CAM-B3LYP/aug-cc-pVDZ) ECD spectra for compounds **2a-f**.

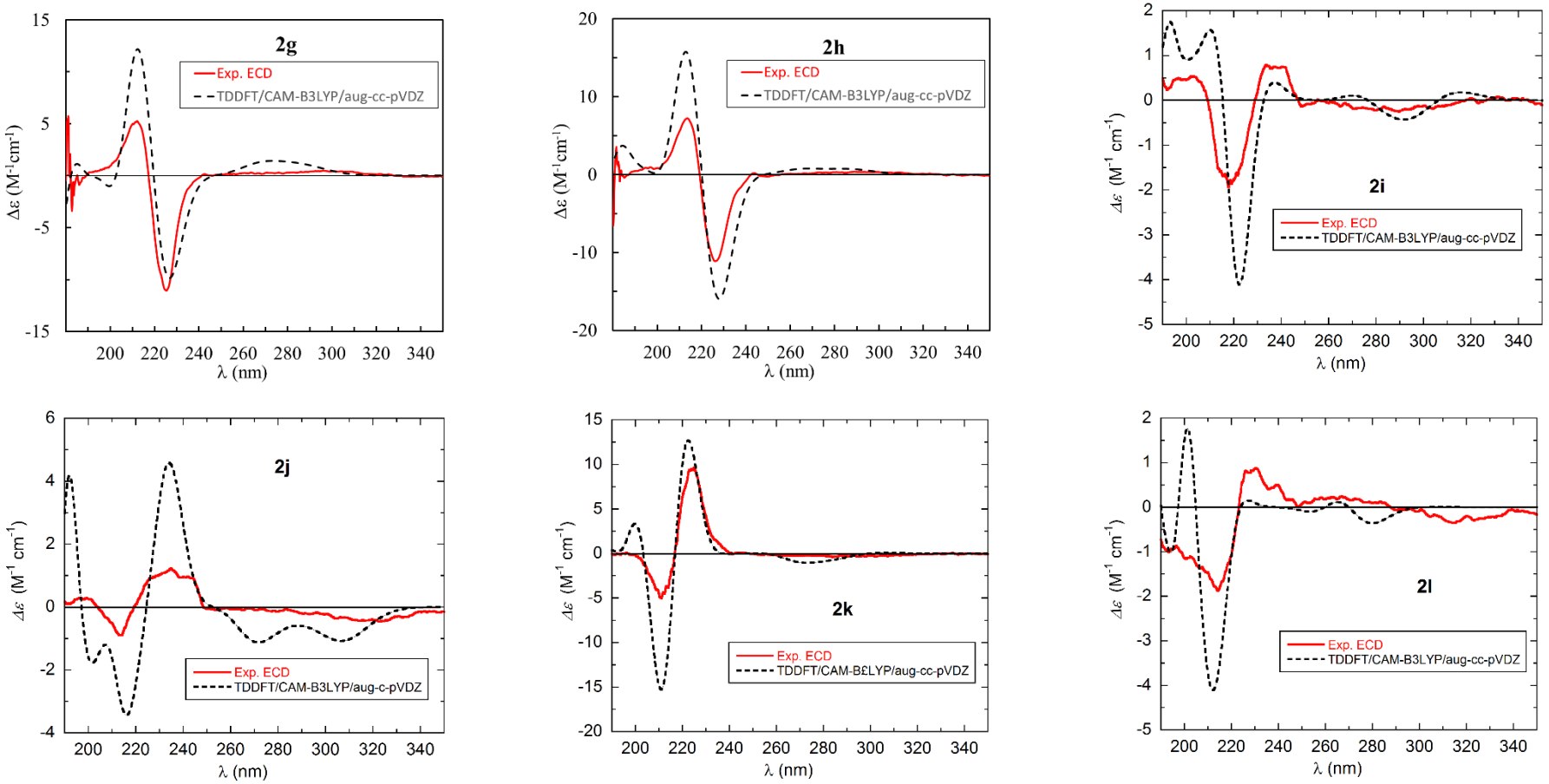


Figure S23: experimental and calculated (TDDFT/CAM-B3LYP/aug-cc-pVDZ) ECD spectra for compounds **2g-l**.