Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Double helicity induction in chiral bis(triphenylacetamides)

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Table 2 (full). Dihedral angles α, β, γ and ω (in degrees) and selected interatom distances $l_1 - l_5$ (in Å) and helicity of trityl group observed in the crystal structures and calculated at DFT/6-311G(2d,2p) level for individual low-energy conformers of amides **1**, **4**, **5**-**7**.

Amide[a]	α[b]	β_1[c]	β_2[c]	β_3[c]	γ_1[d]	γ_2[d]	γ_3[d]	ω[e]	l_1[f]	l_2[g]	l_3[h]	l_4[i]	l_5[j]	Helicity
1 (X-ray)														
A	2.4	-83.8(3)	156.1(2)	33.9(3)	-26.4(3)	-50.8(3)	-57.6(3)	-117.7(2)	2.438	2.407	2.336	6.913(3)		*MMM*
	-8.5	-99.3(3)	138.6(2)	16.6(3)	-2.1(3)	-54.0(3)	-56.3(3)		2.446	2.473	2.359			*0MM*
B	38.8	-65.9(3)	52.9(3)	173.8(2)	22.3(3)	48.7(3)	64.5(3)	-90.1(2)	2.471	2.260	2.424	6.975(3)		*PPP*
	2.6	-85.1(3)	155.2(2)	33.3(3)	-29.3(3)	-52.1(3)	-58.8(3)		2.420	2.419	2.362			*MMM*
1 (conf. 1)	-35.6	-99.7	139.4	18.5	-23.4	-52.9	-58.8	-72.7	2.551	2.467	2.394	6.472	2.158	*MMM*
	54.7	-103.3	13.6	134.7	-5.3	-55.0	-60.0		2.682	2.415	2.533			*0MM*
1 (conf. 3)	-62.8	85.3	154.1	32.5	-28.9	-54.4	-57.9	-100.1	2.945	2.355	2.310	6.800		*MMM*
	174.5	-48.5	-167.0	70.8	-1.8	57.0	68.8		3.859	2.198	2.386			*0PP*
1 (conf. 4)	-52.3	-83.2	156.4	34.7	-32.2	-55.0	-56.1	-114.9	2.724	2.311	2.326	7.134		*MMM*
	-172.9	-51.3	67.9	-171.9	28.7	50.2	63.5		3.827	2.091	2.296			*PPP*
1 (conf. 5)[k]	21.5	-58.4	59.6	-178.9	-36.2	-36.4	-67.6	-69.5	2.328	2.116	2.297	6.806		*MMM*
1 (conf. 6)	-176.3	-72.3	45.4	167.7	-33.7	-49.6	-60.1	-80.6	3.865	2.121	2.293	7.166		*MMM*
	177.9	-60.9	57.4	177.9	33.2	41.6	67.1		3.849	2.189	2.282			*PPP*
1 (conf. 7)	43.2	-80.6	36.3	158.7	-17.9	-54.2	-60.0	-72.9	2.550	2.279	2.286	6.784		*MMM*
	178.2	59.9	-58.5	-178.8	-32.0	-43.0	-66.9		3.853	2.119	2.284			*MMM*
1 (conf. 8)	-14.3	-141.9	-24.9	94.8	30.7	-42.5	-73.7	-101.4	2.360	2.580	2.531	6.432		*PMM*
	-33.3	-47.9	-165.3	72.0	-22.4	51.9	77.0		2.500	2.392[l]	2.385			*MPP*
4a (X-ray)	-11.7	80.3(2)	-159.2(2)	-35.9(2)	15.3(2)	60.3(2)	61.1(2)	-65.5(2)	2.448	2.423	2.301	5.486(3)		*PPP*

	16.9	61.2(2)	-55.1(2)	-178.2(2)	34.4(2)	50.5(2)	64.2(2)		2.398	2.220	2.311			*PPP*
4a (conf. 1)	-26.3	78.8	-38.4	-161.0	24.8	51.5	59.2	-60.2	2.476	2.242	2.278	6.133	2.164	*PPP*
	45.4	40.4	157.8	-78.6	16.9	-48.0	-81.9		2.541	2.285	2.506			*PMM*
4a (conf. 3)	-17.1	84.2	-155.0	-32.5	21.0	56.2	59.5	-60.0	2.373	2.400	2.310	6.012	2.777	*PPP*
	31.1	48.9	-68.3	169.1	39.2	39.2	68.0		2.367	2.162	2.379			*PPP*
4b (X-ray)	-8.8	-113.0(2)	120.9(1)	3.1(2)	-5.0(2)	-39.2(2)	-69.9(2)	-69.2(2)	2.302	2.824		6.166(2)		*0MM*
	-4.4	-115.4(2)	119.6(2)	1.4(2)	2.6(2)	-46.0(2)	-65.9(2)		2.266	2.866				*0MM*
4b (conf. 1)[k]	173.9	105.0	-128.7	-9.8	1.5	49.3	61.1	-56.8	3.788	2.530		7.201		*0PP*
4b (conf. 5)	175.0	-129.2	-14.7	102.9	15.2	-51.0	-57.7	-58.0	3.791	2.555		6.062		*PMM*
	175.9	106.2	-128.1	-9.3	8.3	47.6	62.2		3.782	2.554				*PPP*
4b (conf. 7)[k]	37.8	121.8	7.1	-110.6	-10.4	53.9	54.2	-56.8	2.231	2.538		7.447		*MPP*
4b (conf. 8)[k]	-174.0	123.1	-110.9	7.1	-3.2	53.0	57.4	-46.1	3.772	2.615		6.707		*0PP*
5 (X-ray)	-171.3	123.0(1)	4.8(2)	-115.8(1)	-5.7(2)	50.3(2)	68.1(2)	87.4(1)	3.785	2.470	2.647	6.868(2)	2.184	*MPP*
	29.4	-123.5(1)	-6.4(2)	112.2(2)	20.6(2)	-42.8(2)	-68.5(1)		2.365	2.416	2.755			*PMM*
5 (conf. 1)[k]	15.5	129.0	11.5	-109.2	-20.6	43.4	72.8	46.2	2.352	2.410	2.571	6.507		*MPP*
5 (conf. 5)	3.0	-29.6	-147.3	89.6	-36.1	36.7	-77.0	48.9	2.383	2.461	2.500	6.356		*MPM*
	5.2	124.0	6.3	-113.1	-14.8	49.5	60.1		2.394	2.489	2.654			*MPP*
5 (conf. 60)	26.0	-126.6	-8.4	111.9	13.2	-49.0	-68.7	87.0	2.349	2.474	2.697	6.713	1.918	*PMM*
	-168.5	148.3	30.5	-89.0	-35.5	37.6	77.3		3.893	2.485	2.442			*MPP*
5 (conf. 61)	32.4	-82.2	35.9	156.0	34.9	39.4	75.7	-58.6	2.521	2.370[l]	2.445	5.535	2.298	*PPP*
	-35.1	-111.9	127.4	6.8	-14.9	-53.3	-61.3		2.418	2.297	2.372			*MMM*
5 (conf. 69)[k]	-159.5	-81.5	158.8	35.8	-35.8	-49.2	-63.1	-44.1	3.866	2.407	2.312	5.459		*MMM*

6 (X-ray)	-9.4	-91.7(2)	25.8(2)	147.8(2)	30.0(2)	43.0(2)	75.7(2)	-104.3(2)	2.364	2.443	2.464	6.691(2)		*PPP*
	39.2	53.3(2)	-63.4(2)	174.1(2)	42.9(2)	48.7(2)	66.7(2)		2.479	2.296	2.345			*PPP*
6 (conf. 1)	-5.1	63.7	-55.0	-175.7	-25.3	-44.5	-70.6	-106.7	2.274	2.148	2.308	6.510		*MMM*
	-11.6	92.8	-145.5	-24.1	18.0	52.6	60.1		2.317	2.453	2.356			*PPP*
6 (conf. 31)	-7.0	-109.3	7.3	128.0	4.3	-55.7	-59.7	-109.4	2.337	2.511	2.500	6.749		*0MM*
	-15.4	60.1	-58.3	-178.6	-33.4	-37.4	-70.0		2.312	2.115	2.300			*MMM*
6 (conf. 32)	-6.8	-126.7	-9.7	110.2	17.6	-49.3	-65.3	-108.2	2.331	2.474[l]	2.753	6.671		*PMM*
	-19.7	61.1	-57.2	-177.5	-33.5	-37.0	-70.3		2.331	2.119	2.302			*MMM*
6 (conf. 37)[k]	-9.1	-102.9	13.6	134.8	-0.3	-55.2	-59.7	-109.0	2.329	2.435	2.441	6.817		*0MM*
6 (conf. 62)	-6.7	66.4	-51.8	-172.5	-29.6	-41.0	-71.9	-112.8	2.291	2.150	2.319	6.658		*MMM*
	-27.6	-71.8	47.7	169.0	9.9	49.5	72.3		2.400	2.308[l]	2.373			*PPP*
6 (conf. 68)[k]	-11.5	88.3	-150.3	-28.7	22.0	53.1	59.6	-104.6	2.292	2.414	2.336	6.338		*PPP*
6 (conf. 70)	-7.5	-104.7	12.0	133.0	0.0	-55.3	-59.7	-108.6	2.325	2.454[l]	2.457	6.815		*0MM*
	-9.1	-95.6	21.0	142.6	-7.5	-56.8	-58.7		2.322	2.413	2.384			*MMM*
6 (conf. 73)	-11.8	-140.1	-22.9	96.7	30.6	-40.0	-74.5	-104.0	2.313	2.487	2.564	6.343		*PMM*
	-20.4	89.4	-149.4	-27.9	24.3	53.1	59.1		2.322	2.404	2.338			*PPP*
6 (conf. 81)	-40.7	58.2	-60.6	178.8	-27.7	-44.5	-67.7	-110.9	2.500	2.118	2.318	6.888		*MMM*
	42.0	53.6	-65.2	174.7	-34.9	-47.0	-62.5		2.540	2.106	2.304			*MMM*
6 (conf. 87)	-4.8	-136.4	-19.4	100.2	26.5	-44.5	-70.3	-111.3	2.329	2.493[l]	2.616	6.621		*PMM*
	-35.3	-74.4	45.0	166.3	12.1	47.9	73.7		2.450	2.395[l]	2.385			*PPP*
6 (conf. 90)[k]	35.2	-62.6	55.6	177.5	-36.9	-39.6	-64.8	-104.9	2.418	2.125	2.301	7.392		*MMM*
7 (conf. 1)	-8.8[m]	-127.2	-9.6	109.7	12.3	-51.4	-62.5	-90.1[n]	2.182[o]	2.572	2.765	6.998	2.341[p]	*PMM*

	-18.8[m]	35.2	152.3	-84.3	20.1	-47.2	-81.9		2.235[o]	2.281	2.418		2.372[p]	*PMM*
7 (conf. 2)	-9.3[m]	86.7	-151.8	-29.7	22.0	53.4	59.4	-92.1[n]	2.139[o]	2.397	2.327	6.882	2.380[p]	*PPP*
	-19.7[m]	34.2	151.3	-85.3	21.8	-45.6	89.2		2.225[o]	2.293	2.430		2.369[p]	*PMP*
7 (conf. 3)[k]	-29.1[m]	52.0	-67.4	170.9	-16.7	-56.3	-64.1	-87.7[n]	2.319[o]	2.111	2.297	6.758	2.464[p]	*MMM*
7 (conf. 4)[k]	-19.1[m]	-100.6	137.6	17.1	-20.2	-53.1	-60.0	-89.3[n]	2.244[o]	2.502	2.442	7.116	2.411[p]	*MMM*
7 (conf. 6)	-3.7[m]	-122.1	-5.5	114.4	13.8	-49.4	-63.8	-100.1[n]	2.152[o]	2.473	2.661	7.430	2.345[p]	*PMM*
	17.8[m]	79.3	-37.8	-158.8	-31.0	-38.0	-75.8		2.157[o]	2.238	2.391		2.428[p]	*MMM*

[a] – conformers are numbered according to their appearance during conformational search; [b] – α = H-C*-N-C(=O); [c] – β = O=C-C-C_{ipso}; [d] – γ = C(=O)-C-C_{ipso}-C_{ortho} (of the two possibilities the absolute values ≤90° has been chosen); [e] – ω = N-C*-C*-N; [f] – l_1 = (C=)O···H(C*) [g] – l_2 = (C=)O···H(C_{ortho}); [h] – l_3 = (N)H···C_{ipso}; [i] – l_4 = Csp^3(trityl)···Csp^3(trityl); [j] – l_5 = (C=)O···HN; [k] – C_2-symmetry conformer; [l] – attractive (C=)O···H(C_{ortho}) interaction between adjacent trityl groups or attractive interaction between oxygen and hydrogen atom connected with adjacent stereogenic center; [m] – α = C3-C2-N-C(=O); [n] – ω = C1-C2-C2'-C1'; [o] – l_1 = (C=)O···H(C6); [p] – l_5 = C2···HN.

Table 3 (full). ECD and UV data for triphenylacetamides **1**-**8** measured in cyclohexane and acetonitrile solution.

	cyclohexane				acetonitrile			
Amide	Δε (nm)		ε (nm)		Δε (nm)		ε (nm)	
1	0.9 (258)	-19.0 (219)	29.2 (196)	160 000 (192)	1.4 (246)	-17.6 (208)	28.2 (195)	162 000 (193)
2	1.1 (258)	31.6 (213)	29.2 (196)	209 400 (189)	1.0 (257)	22.0 (208)	-18.0 (190)	201 900 (189)
3	1.6 (245)	-19.6 (213)	-40.3 (197)	150 600 (192)	1.6 (247)	-18.2 (212)	38.7 (196)	146 900 (192)
4a	1.3 (245)	-18.5 (223)	24.9 (198)	148 600 (194)	2.38 (245)	-23.0 (209)	28.0 (195)	143 700 (193)
4b	45.7 (232)	-97.9 (211)		142 900 (192)	38.3 (232)	-85.5 (208)	30.4 (196)	142 900 (193)
5	-6.5 (239)	-66.5 (208)		208 500 (190)	-8.4 (239)	-76.9 (210)	31.6 (193)	206 000 (191)
6		-126.5 (212)	212.1 (193)	204 300 (189)		-113.7 (210)	153.6 (191)	198 200 (188)
7	-7.7 (287)	7.8 (245)	6.3 (227)	27 200 (256)	-5.6 (285)	-6.0 (272)	7.2 (241)	20 900 (255)
		-30.5 (212)	65.1 (196)	170 900 (194)		-48.9 (208)	45.6 (187)	164 700 (193)
8	-7.7 (341)	-10.3 (311)	35.3 (290)	5 200 (338)	-5.2 (339)	-10.1 (310)	21.8 (289)	3 600 (336)
	-18.5 (265)	-39.7 (247)	-67.6 (219)	5 500 (322)	-15.1 (265)	-42.1 (245)	-86.0 (221)	
			160.0 (201)	19 800 (293)			123.9 (200)	16 800 (292)
				70 100 (253)				59 200 (251)
				159 400 (194)				160 400 (193)

Experimental Section

^{1}H and ^{13}C NMR spectra were recorded on Varian VNMR-S 400 MHz instrument. Chemical shifts (δ) are reported in ppm relative to $SiMe_4$ and coupling constants (*J*) are given in Hz. HR-MS spectra were obtained with a Bruker 320 MS spectrometer. UV and ECD spectra were recorded in spectroscopic grade cyclohexane or acetonitrile using a JASCO J-810 instrument. FTIR spectra were measured on a Bruker FT-IR IFS 66/s in KBr pellets. A PerkinElmer 341 polarimeter was used for optical rotation ($[\alpha]_D$) measurements (ca. 20 °C). Flash column chromatography was performed on Merck Kieselgel type 60 (250 - 400 mesh). Merck Kieselgel type $60F_{254}$ analytical plates were employed for TLC. Melting points were measured on Büchi Melting Point B-545 and uncorrected. All reagents were used as purchased from commercial suppliers. All solvents were provided by a local supplier and were purified by conventional methods prior to use.

General procedure of synthesis diamides 1-8

To a suspension of triphenylacetic acid (1.2-1.5 mmol) in 5 mL of dry toluene, containing one drop of DMF, thionyl chloride (0.5 mL, 6.6 mmol) was added drop wise. The mixture was gently refluxed at 80 °C for 3 hours. After evaporation of an excess of thionyl chloride and the organic solvent under reduced pressure the crude acid chloride was immediately used without further purification for next reaction.

To a solution of respective diamine (0.5 mmol) in CH_2Cl_2 (2 mL) and triethylamine (1 mL) the solution of triphenylacetyl chloride (1.2-1.5 mmol) in CH_2Cl_2 (2 mL) was added drop vise and stirred overnight. The reaction was quenched with water and the mixture was extracted with 10% HCl, H_2O, saturated $NaHCO_3$ and brine. The organic layer was dried over Na_2SO_4 and evaporated to dryness. The crude product was purified by flash chromatography on silica gel.

***N,N'*-((1*R*,2*R*)-cyclopentane-1,2-diyl)bis(2,2,2-triphenylacetamide) 1**: eluent: *n*-hexane:CH_2Cl_2 1:1, white solid, yield 519 mg (83%). M. p. 222-226 ˚C (diethyl ether-hexane); $[\alpha]^{20}_D$ = –36.7 (c = 1.0, $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$, TMS): δ = 1.19-1.32 (m, 2H), 1.55-1.68 (m, 2H), 2.09-2.20 (m, 2H), 3.90-4.03 (m, 2H), 6.14 (d, *J* = 6.2 Hz, 2H, NH), 7.13-7.25 ppm (m, 30H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 20.0, 30.0, 56.6, 67.5, 126.9, 127.9, 130.5, 143.2, 173.7 ppm; EIMS m/z 640.2 $[M]^+$; FT-IR (KBr): *v* = 3420 (N-H), 3056, 2953, 1662 (C=O), 1491, 1445, 742, 699 cm^{-1}.

***N,N'*-((3*R*,4*R*)-1-benzylpyrrolidine-3,4-diyl)bis(2,2,2-triphenylacetamide) 2**: eluent: CH_2Cl_2 to CH_2Cl_2:MeOH (1%), white solid, yield 100 mg (26%). M. p. 192-193 ˚C (diethyl ether); $[\alpha]^{20}_D$ = +43.4 (c = 0.665, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$, TMS): *δ* = 2.26 (dd, *J* = 5.4, 9.7 Hz, 2H), 2.93 (dd, *J* = 6.7, 9.6 Hz, 2H), 3.49 (dd, *J* = 13.1, 22.4 Hz, 2H), 4.16 (dq, *J* = 5.3, 10.5 Hz, 2H), 6.19 (d, *J* = 6.5 Hz, 2H, NH), 7.12-7.14 (m, 2H), 7.16-7.22 (m, 12H), 7.22-7.30 ppm (m, 21H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* = 56.1, 58.4, 59.4, 67.4, 127.0, 127.1, 127.9, 128.3, 128.4, 130.4, 138.0, 143.1, 173.3 ppm; EIMS *m/z* 731.3 $[M]^+$; FT-IR (KBr): *v* = 3480 (N-H), 3408 (N-H), 3058, 2800, 2777, 1681 (C=O), 1669 (C=O), 1490, 1443, 760, 750, 698 cm^{-1}.

***N,N'*-((1*R*,2*R*)-cyclohex-4-ene-1,2-diyl)bis(2,2,2-triphenylacetamide) 3**: eluent *n*-hexane:CH_2Cl_2 1:1 to CH_2Cl_2, white solid, yield 1.09 g (82%) . M. p. 165-166 ˚C (diethyl ether-hexane); $[\alpha]^{20}_D$ = -60.5 (c = 1.08, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 1.79-1.85 (m, 2H), 2.37 (d, *J* = 17.8 Hz, 2H), 4.04-4.09 (m, 2H), 5.47 (d, *J* = 2.1 Hz, 2H), 6.07 (d, *J* = 7.2 Hz, 2H, NH), 7.13-7.16 (m, 12H), 7.19-7.25 ppm (m, 18H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 31.2, 49.1, 67.7, 124.4, 127.0, 127.9, 130.4, 143.1, 173.5 ppm; EIMS *m/z* 652.2 $[M]^+$; FT-IR (KBr): *v* = 3410 (N-H), 3404 (N-H), 3054, 3038, 2966, 1656 (C=O), 1503, 1489, 1445, 1440, 740, 727, 700, 557, 503 cm^{-1}.

***N,N'*-((1*R*,2*R*)-cyclohexane-1,2-diyl)bis(2,2,2-triphenylacetamide) 4a**: eluent: *n*-hexane-CH_2Cl_2 (1:1) white solid, yield 1.01 g (89%). M. p. 188-189 ˚C (dichloromethane-hexane); $[\alpha]^{20}_D$ = -32.7 (c = 0.515, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 1.01-1.33 (m, 4H), 1.65-1.68 (m, 2H), 2.04 (d, *J* = 2.04 Hz, 2H), 3.65-3.76 (m, 2H), 6.11 (d, *J* = 6.7 Hz, 2H), 7-13-7.33 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 24.5, 32.4, 53.5, 127.0, 127.9, 130.5, 143.2, 173.6 ppm; EIMS *m/z* 654.7 $[M]^+$; FT-IR (KBr): *v* = 3579 (N-H), 3401 (N-H), 3055, 2926, 1647 (C=O), 1503, 1489, 1443, 1440, 740, 728, 700, 549 cm^{-1}.

***N,N*'-((1*R*,2*R*)-cyclohexane-1,2-diyl)bis(*N*-methyl-2,2,2-triphenylacetamide) 4b**: eluent: *n*-hexane-CH_2Cl_2 (7:3) white solid, yield 0.32 g (59%). M. p. 261-262 ˚C (dichloromethane-hexane); $[\alpha]^{20}_D$ = -52.2 (c = 0.5, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 1.15 (br, 4H), 7.32-7.19 (m 30 H), 1.65 (br, 4H), 2.40 (s, 6H), 4.74 (br, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 25.0, 28.5, 32.2, 55.1, 126.4, 130.4, 127.6, 143.0, 173.6 ppm; EIMS *m/z* 682.6 $[M]^+$; FT-IR (KBr): *v* = 3056, 2934, 1626 (C=O), 1490, 1443, 1389, 1312, 760, 717, 695, 603 cm^{-1}.

***N,N'*-((1*R*,2*R*)-1,2-diphenylethane-1,2-diyl)bis(2,2,2-triphenylacetamide) 5**: eluent *n*-hexane-AcOEt (9:1 to 4:1), white solid, yield 363 mg (86%). M. p. 215-217 ˚C (diethyl ether-hexane); $[\alpha]^{20}_D$ = –8.7 (c = 1.03, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 5.27-5.32 (m, 2H), 6.42 (d, *J* = 7.1 Hz, 2H, NH), 6.52-6.57 (m, 4H), 6.98-7.14 (m, 18H), 7.14-7.24 ppm (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 57.8, 67.6, 126.9, 127.3, 127.6, 127.9, 128.2, 130.4, 137.4, 143.0, 172.9 ppm; EIMS *m/z* 753.5 $[M+H]^+$; FT-IR (KBr): *v* = 3423 (N-H), 3350 (N-H), 3057, 3030, 2922, 1678 (C=O), 1670 (C=O), 1521 (N-H), 1488, 1448, 746, 696, 507 cm^{-1}.

***N,N*'-((9*S*,10*S*,11*R*,12*R*)-9,10-dihydro-9,10-ethanoanthracene-11,12-diyl)bis(2,2,2-triphenylacetamide) 6**: eluent: *n*-hexane:CH_2Cl_2 1:1 to 100% CH_2Cl_2, white solid, yield 711 mg (86.5%). M. p. 233-235 ˚C (diethyl ether-hexane); $[\alpha]^{20}_D$ = –70 (c = 1.025, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 3.91 (dt, *J* = 2.8, 5.2 Hz, 2H), 4.23 (d, *J* = 2.7 Hz, 2H), 5.56 (d, *J* = 7.9 Hz, 2H), 6.94 (d, *J* = 6.3 Hz, 2H), 7.01 (td, *J* = 1.2, 7.4 Hz, 2H), 7.08 (td, *J* = 1.3, 7.4 Hz, 2H), 7.14-7.23 ppm (m, 32H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 48.8, 57.5, 67.5, 124.8, 125.4, 126.60, 126.63, 126.9, 127.9, 130.3, 138.3, 140.0, 142.9, 172.7 ppm; EIMS *m/z* 776.4 $[M]^+$; FT-IR (KBr): *v* = 3422 (N-H), 3061, 2999, 1661 (C=O), 1491, 769, 698, 564 cm^{-1}.

(*R*)-*N,N'*-(6,6'-dimethylbiphenyl-2,2'-diyl)bis(2,2,2-triphenylacetamide) 7: eluent: *n*-hexane:CH_2Cl_2 1:1 to 100% CH_2Cl_2, white solid, yield 271 mg (62%). M. p. 224-226 ˚C (dichloromethane-hexane); $[\alpha]^{20}_D$ = -2.3 (c = 0.82, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 1.59 (s, 6H), 6.70 (d, *J* = 7.9 Hz, 2H, NH), 6.94 (s, 2H), 7.00-7.04 (m, 12H), 7.08-7.19 (m, 20H), 8.35 ppm (d, *J* = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 19.6, 68.6, 117.7, 123.8, 125.7, 126.9, 128.0, 130.0, 136.0, 136.5, 142.7, 171 ppm; EIMS *m/z* 753.4 $[M+H]^+$; FT-IR (KBr): *v* = 3379 (N-H), 3368 (N-H), 3058, 3003, 2920, 1690 (C=O), 1681 (C=O), 1600 (N-H), 1518 (N-H), 1503, 1497, 1492, 1463, 1448, 1404, 1294, 780, 758, 748, 726, 697, 597, 575, 571 cm^{-1}.

(*R*)-*N,N'*-(1,1'-binaphthyl-2,2'-diyl)bis(2,2,2-triphenylacetamide) 8: eluent *n*-hexane:CH_2Cl_2 1:1 to 100% CH_2Cl_2, colorless oil, yield 306 mg (37%). $[\alpha]^{20}_D$ = –49.4 (c = 1.16, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ = 6.80 (d, *J* = 0.9 Hz, 1H), 6.83 (d, *J* = 0.9 Hz, 1H), 6.84-6.87 (m, 12H), 6.97-7.02 (m, 12H), 7.03-7.07 (m, 6H), 7.14-7.18 (m, 4H), 7.32-7.36 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 2H), 7.75 (d, *J* = 8.1 Hz, 2H), 7.82 (d, *J* = 9.2 Hz, 2H), 8.69 ppm (d, *J* = 9.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 53.4, 68.5, 118.1, 119.9, 124.4, 125.1, 126.8, 127.1, 127.8, 128.1, 129.8, 130.8, 131.8, 135.3, 142.3, 171.4 ppm; EIMS *m/z* 824.5 $[M]^+$; FT-IR (KBr): *v* = 3364 (N-H), 3054, 1685 (C=O), 1592 (N-H), 1489, 1424, 1274, 820, 747, 698 cm^{-1}.

Calculation details

Starting geometries of triphenylacetamides **1**, **4**, **5**-**7** with assumed *R* absolute configuration of all stereogenic elements were obtained by conformational search with the use of a Scigress [1] software and pre-optimization of all conformers at the B3LYP/6-31G(d) level. The conformational searches were done by systematic changes of all rotatable torsion angles with 30° steps. This allowed to identify the minimum energy structures which were further re-optimised with the independent use of six density functionals: B3LYP, [2] M06-2X [3] hybrid functionals with and without dispersion correction [4] and pure B97-D and B97-D3 functionals including empirical long-range correction, [5] all in conjunction with the enhanced 6-311++G(d,p) basis set. [6] The structures thus obtained were the real minimum energy conformers (no imaginary frequencies have been found). The total and free energy values were used to obtain the Boltzmann population of conformers at 298.15 K. For density functional theory calculations, only the results for conformers that differ from the most stable one by less than 2 kcal mol^{-1} were taken into account, following a generally accepted protocol. Relative energies (unit kcal mol^{-1}) discussed in the main text refer to Gibbs free energies ($\Delta G°$) computed at the B3LYP/6-311G(2d,2p) or M06-2X/6-311G(2d,2p) (for **5**) levels.

ECD spectra for all structures optimized at the DFT/6-311G(2d,2p) level were calculated employing B3LYP, [2] CAM-B3LYP, [7] B2LYP, [8] LC-wPBE [9] and M06-2X [3] hybrid functional, all in conjunction with 6-311G(2d,2p) basis set.[6] The calculated ECD spectra were Boltzmann averaged by taking into account conformers of **1**, **4**, **5**-**7** ranging from 0 to 2.0 kcal mol^{-1} in relative energies, following a generally accepted protocol.[10] Rotatory strengths were calculated using both length and velocity representations. In the present study, the differences between the length and velocity calculated values of rotatory strengths were quite small, and for this reason, only the velocity representations were further used. The ECD spectra were simulated by overlapping Gaussian functions for each transition, according to the procedure previously described by Harada and Stephens.[11]

The solvent effect on structure and ECD spectra was not taken into account, since all measurements for amides **1**, **4**, **5**-**7** were done in non-polar cyclohexane.

The best combination of methods for structure/spectra prediction was chosen by comparison of experimental and Boltzmann averaged CD spectra calculated using all possible combinations of methods. The best performed combination for prediction structure and ECD spectra of triphenylacetamides **1**, **4**, **6**-**7** consists of B3LYP/6-311G(2d,2p) method for structure optimization and TD-M06-2X/6-311G(2d,2p) for calculations of rotatory strengths. The amide **5** is an exception, the slightly better results were obtained for combination of M06-2X/6-311G(2d,2p) method for geometry calculations and TD-M06-2X/6-311G(2d,2p) method for calculations of chiroptical properties. For the particular amide **5** the aromatic-aromatic interaction between inductor and acceptor may take a part. In fact in crystals the percentage of molecular surface involved in aromatic/aromatic CH•••π interactions is significantly higher in **5** than in the remaining complexes (33 vs 25%, the latter value being averaged from **5** observations). This might be the reason why the M06-2X functional, originally constructed for better reproduction of aromatic-aromatic stacking interactions, gave better results for 5 than for other compounds under study. Thus, the M06-2X functional originally constructed for better reproduction of aromatic-aromatic stacking interactions, gave the better results. In fact, the differences between results obtained with the use of TD-M06-2X/6-311G(2d,2p)//M06-2X/6-311G(2d,2p) and TD-M06-2X/6-311G(2d,2p)//B3LYP/6-311G(2d,2p) methods were very small and it is permissible to use the results obtained with the use of both combinations of hybrid functionals for further discussion.

The comparison of experimental and calculated with the use of various methods ECD spectra provided some general conclusions. First – the use of functionals that have long-range corrections do not improve the final results, but elongated CPU time. Thus the structure of investigated amides is controlled by intermolecular interactions satisfactorily reproduced by “classical” B3LYP functional. Second, the calculations of ECD spectra with the use of B3LYP hybrid functional statistically gave the worst results regardless the used method for structure optimization, which is in agreement with previous findings.[12]

These studies are a part of the project focused on improving the performance of modern theoretical methods for the prediction of chiroptical properties of organic compounds representing so called “difficult” cases. [13]

Table S1. Selected crystal data and structure refinement details.

	1	4a	4b	5	6
Crystal data					
Chemical formula	$C_{45}H_{40}N_2O_2$	$C_{46}H_{42}N_2O_2{\cdot}CH_2Cl_2$	$C_{48}H_{46}N_2O_2{\cdot}CH_2Cl_2$	$C_{54}H_{44}N_2O_2$	$C_{56}H_{44}N_2O_2$
M_r	640.79	739.74	767.79	752.91	776.93
Crystal system, space group	Monoclinic, $P2_1$	Monoclinic, $P2_1$	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1$	Monoclinic, $P2_1$
Temperature (K)	130	130	295	295	130
a, *b*, *c* (Å)	8.3781 (2), 49.2719 (9), 9.1582 (2)	9.0299 (2), 10.5552 (2), 20.7459 (3)	10.4884 (2), 19.7670 (3), 20.3090 (3)	9.4437 (1), 15.7060 (2), 13.4756 (2)	13.2132 (5), 9.3519 (3), 17.3912 (7)
α, β, γ (°)	90, 115.792 (2), 90	90, 94.859 (2), 90	90, 90, 90	90, 93.428 (1), 90	90, 107.395 (4), 90
V (Å^3)	3403.93 (13)	1970.24 (6)	4210.55 (12)	1995.16 (4)	2050.72 (13)
Z	4	2	4	2	2
D_x (Mg m^{-3})	1.250	1.247	1.211	1.253	1.258
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Mo $K\alpha$
θ range (°) for cell measurement	2.7–76.4	4.2–76.3	2.2–76.3	2.8–76.2	3.1–29.0
μ (mm^{-1})	0.59	1.80	1.70	0.59	0.08
Crystal size (mm)	0.2 × 0.1 × 0.1	0.35 × 0.20 × 0.08	0.60 × 0.25 × 0.20	0.5 × 0.1 × 0.1	0.60 × 0.20 × 0.02
Data collection					
Diffractometer	SuperNova, Atlas diffractometer	SuperNova, Atlas diffractometer	SuperNova, Atlas diffractometer	SuperNova, Atlas diffractometer	Xcalibur, Eos diffractometer
T_{min}, T_{max}	0.911, 1.000	0.791, 1.000	0.874, 1.000	0.527, 1.000	0.948, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27330, 11975, 11561	20573, 6844, 6790	53532, 8783, 8690	40929, 7046, 7002	16281, 7239, 6285
R_{int}	0.044	0.013	0.040	0.019	0.027
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.595	0.595	0.631	0.595	0.595
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.113, 1.06	0.036, 0.107, 1.05	0.045, 0.136, 1.03	0.031, 0.079, 1.05	0.036, 0.073, 1.04
No. of reflections	11975	6844	8783	7046	7239
No. of parameters	883	478	527	523	541
No. of restraints	1	2	12	7	1
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.17, -0.21	0.45, -0.40	0.31, -0.34	0.12, -0.18	0.14, -0.18
Absolute structure parameter	-0.2 (2)	0.017 (12)	0.00 (3)	-0.09 (16)	-1.7 (11)

Data collection used *ω* scans. Refinement was carried out on F^2. H-atom parameters were constrained. The absolute structure was obtained using Flack H D (1983), *Acta Cryst. A39*, 876-881.

Computer programs: *CrysAlis PRO* [14], *SHELXS86* [15], *SHELXL97* [16], *Mercury* [17].

Table S2. Geometry of intramolecular hydrogen bonds in the investigated crystal structures.

	D–H [Å]	H···A [Å]	D···A [Å]	D–H···A [°]
1				
mol1				
C3A–H3A···O1A	1.00	2.43	2.818(3)	102
C32A–H32A···O1A	0.95	2.40	2.828(3)	107
C7A–H7A···O2A	1.00	2.44	2.840(3)	103
C12A–H12A···O2A	0.95	2.71	3.386(3)	129
C62A–H62A···O2A	0.95	2.47	2.844(3)	103
C26A–H26A···Cg(C11A-C16A)	0.95	2.98	3.664(3)	132
C36A–H36A···Cg(C21A-C26A)	0.95	2.96	3.663(3)	133
N1A–H1A···Cg(C21A-C26A)	0.88	2.99	3.641(3)	135
N2A–H2A···Cg(C51A-C56A)	0.88	2.95	3.521(3)	126
mol2				
C3B–H3B···O1B	0.98	2.47	2.736(3)	94
C62B–H62B···O2B	0.93	2.41	2.827(3)	106
C16B–H16B···Cg(C31B-C36B)	0.93	3.01	3.601(3)	123
C26B–H26B···Cg(C11B-C16B)	0.93	3.05	3.719(3)	131
C36B–H36B···Cg(C21B-C26B)	0.93	2.97	3.674(3)	133
C56B–H56B···Cg(C41B-C46B)	0.93	2.95	3.641(3)	132
C66B–H66B···Cg(C51B-C56B)	0.93	2.99	3.686(3)	133
N1B–H1B···Cg(C31B-C36B)	0.86	3.10	3.762(3)	135
N2B–H2B···Cg(C51B-C56B)	0.86	3.02	3.622(3)	129
4a				
C3–H3···O1	1.00	2.45	2.827(3)	102
C32–H32···O1	0.95	2.42	2.830(3)	106
C62–H62···O1	0.95	2.75	3.257(3)	114
C8–H8···O2	1.00	2.40	2.779(3)	102
C52–H52···O2	0.95	2.22	2.843(3)	122
C26–H26···Cg(C11-C16)	0.95	2.97	3.682(3)	133
C46–H46···Cg(C51-C56)	0.95	2.92	3.554(3)	125
C56–H56···Cg(C61-C66)	0.95	3.07	3.763(3)	131
C66–H66···Cg(C41-C46)	0.95	3.00	3.701(3)	132
N1–H1···Cg(C21-C26)	0.88	2.81	3.471(3)	133
N2–H2···Cg(C31-C36)	0.88	2.85	3.579(3)	142
4b				
C3–H3···O1	0.98	2.30	2.728(2)	105
C42–H42···O1	0.93	2.60	3.437(2)	149
C8–H8···O2	0.98	2.27	2.718(2)	107
C12–H12···O2	0.93	2.57	3.420(2)	153
C36–H36···Cg(C21-C26)	0.93	2.99	3.684(2)	133
C9'–H9'C···Cg(C51-C56)	0.96	3.02	3.532(2)	115
C66–H66···Cg(C51-C56)	0.93	3.08	3.750(2)	131
5				
C22-H22···O1	0.93	2.47	2.819(2)	102
C4-H4···O2	0.98	2.36	2.745(2)	102
C52-H52···O2	0.93	2.42	2.826(2)	107
N2-H2···O1	0.86	2.18	2.831(1)	132
C8'-H8'···Cg(C61-C66)	0.93	2.72	3.563(2)	151

C12-H12···Cg(C7'-C12')	0.93	2.60	3.428(2)	149
C42-H42···Cg(C1'-C6')	0.93	3.07	3.668(2)	123
6				
C16'-H16'···O1	1.00	2.36	2.788(2)	105
C12-H12···O1	0.95	2.43	3.107(2)	128
C22-H22···O1	0.95	2.57	2.875(2)	99
C15'-H15'···O2	1.00	2.48	2.719(2)	93
C52-H52···O2	0.95	2.28	2.901(2)	122
C13-H13···Cg(C51-C56)	0.95	2.50	3.396(2)	161
C26-H26···Cg(C11-C16)	0.95	3.00	3.646(2)	128
C36-H36···Cg(C21-C26)	0.95	3.02	3.687(2)	130
C56-H56···Cg(C7'-C12')	0.95	3.06	3.739(2)	131
C66–H66···Cg(C51-C56)	0.95	2.94	3.641(2)	133
N1-H1···Cg(C31-C36)	0.88	3.07	3.704(2)	132
N2-H2···Cg(C61-C66)	0.88	2.91	3.602(2)	139

Table S3. Geometry of intermolecular hydrogen bonds in investigated crystal structures.

	D–H [Å]	H···A [Å]	D···A [Å]	D–H···A [°]	Symmetry operation on A
1					
mol1					
C45A-H45A···O2A	0.95	2.88	3.698(3)	147	1+x, y, 1+z
C34A-H34A···O2B	0.95	2.70	3.625(3)	173	x, y, z
C53A-H53A···Cg(C61A-C66A)	0.95	3.08	3.874(2)	145	-1+x, y, z
C14A-H14A···Cg(C41A-C46A)	0.95	2.87	3.725(2)	154	x, y, -1+z
mol2					
C64B–H64B···O1A	0.95	2.72	3.645(3)	172	1+x, y, z
C35B-H35B···O1B	0.95	2.43	3.245(3)	136	-1+x, y, z
C55B–H55B···O2B	0.95	2.63	3.320(3)	133	x, y, 1+z
C63B-H63B···Cg(C31A-C36A)	0.95	3.06	3.871(2)	146	1+x, y, z
C44B–H44B···Cg(C31B-C36B)	0.95	2.60	3.486(2)	160	1+x, y, 1+z
C5B–H5B2···Cg(C41B-C46B)	0.99	2.93	3.857(2)	160	-1+x, y, z
4a					
C1S-H1S1···O1	0.99	2.26	3.222(3)	163	x, y, z
C1S-H1S2···O2	0.99	2.10	3.052(3)	160	-1+x, y, z
C44-H44···Cl2	0.95	2.95	3.638(3)	130	1+x, -1+y, z
C3-H3···Cl1	1.00	3.06	3.993(3)	147	x, y, z
C7-H7B···Cl1	0.99	3.02	3.900(3)	123	x, y, z
C43-H43···Cl1	0.95	3.06	3.688(3)	125	1-x, -1/2+y, 2-z
C43-H43···Cl2	0.95	3.04	3.992(3)	175	1-x, -1/2+y, 2-z
C4-H4A···Cg(C41-C46)	0.99	3.08	4.002(2)	155	x, 1+y, z
C13-H13···Cg(C61-C66)	0.95	3.00	3.677(2)	129	x, 1+y, z
C54-H54···Cg(C31-C36)	0.95	3.01	3.827(2)	145	1-x, -1/2+y, 1-z
C64-H64···Cg(C41-C46)	0.95	2.87	3.732(2)	151	-1+x, y, z
4b					
C81-H81A···O1	0.97	2.45	3.388(2)	163	1.5-x, -y, 1/2-z
C81-H81B···O2	0.97	2.52	3.395(2)	150	1/2-x, -y, 1/2+z
C55-H55···Cl1	0.93	2.81	3.534(2)	135	x, y, z
C26-H26···Cl2	0.93	2.92	3.546(2)	126	x, y, -1+z
C53-H53···Cg(C11-C16)	0.93	2.85	3.729(2)	158	1/2-x, -y, 1/2+z
C23-H23···Cg(C61-C66)	0.93	3.02	3.871(2)	152	1-x, -1/2+y, 1/2-z
5					
C4'-H4'···O2	0.93	2.78	3.584(2)	145	1-x, 1/2+y, -z
C25-H25···O2	0.93	2.86	3.699(2)	150	x, y, 1+z
C3'-H3'···Cg(C21-C26)	0.93	2.95	3.730(2)	142	1-x, 1/2+y, 1-z
C54-H54···Cg(C31-C36)	0.93	2.91	3.725(2)	147	-1+x, y, -1+z
C15-H15···Cg(C41-C46)	0.93	3.10	4.019(2)	171	1-x, -1/2+y, 1-z
C45-H45···Cg(C1'-C6')	0.93	2.93	3.605(2)	131	-1+x, y, z
C5'-H5'···Cg(C7'-C12')	0.93	2.64	3.442(2)	145	1-x, 1/2+y, -z
6					
C53-H53···O1	0.95	2.71	3.558(2)	153	x, 1+y, z
C55-H55···O1	0.95	2.46	3.366(2)	166	1-x, 1/2+y, 1-z
C10'-H10'···O2	0.95	2.48	3.254(2)	141	x, -1+y, z
C11'-H11'···Cg(C41-C46)	0.95	2.30	3.736(2)	138	x, -1+y, z
C43-H43···Cg(C9'-C14')	0.95	3.04	3.874(2)	150	-x, -1/2+y, -z

Table S4. Relative contributions to the Hirshfeld surface area for the various intermolecular contacts to the amides **1** (two independent molecule **A** and **B**), **4a**, **4b**, **5** and **6**.

	1		**4a**	**4b**	**5**	**6**
	A	**B**				
H···H %	66.6	67.7	68.3	68.3	63.7	64.5
H···C %	27.6	24.6	21.1	22.3	32.6	29.1
H···O %	4.7	6.9	2.7	2.3	3.7	5.5
C···C %	0.1	0.8	0.0	0.4	0.0	0.8
H···N %	0.0	0.0	0.0	0.0	0.0	0.1
C···Cl %	---	---	0.5	0.0	---	---
H···Cl %	---	---	7.4	6.8	---	---

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Table A1. Intra-ring torsion angles φ_1 – φ_5 (in degrees) observed in the crystal structures and calculated at the B3LYP/6-311G(2d,2p) level for individual low-energy conformers of amide **1**.

Conformer[b]	φ_1	φ_2	φ_3	φ_4	φ_5
X-ray	22.8	4.0	-29.3	43.42	-40.8
	-1.8	-24.2	41.2	-42.5	27.2
conf. 1	-21.7	-4.1	28.7	-41.9	39.1
conf. 3	6.5	-29.0	40.7	-36.1	18.2
conf. 4	15.8	-36.0	41.9	-32.1	10.1
conf. 5	-35.4	13.6	13.6	-35.4	43.8
conf. 6	10.0	-30.5	39.3	-32.9	14.1
conf. 7	-36.1	14.2	13.7	-36.3	44.8
conf. 8	19.0	-38.0	42.3	-30.4	7.0

[a] The carbon atoms were numbered in anticlockwise manner; φ_1 – C5-C1*-C2*-C3; φ_2 – C1*-C2*-C3-C4; φ_3 – C2*-C3-C4-C5; φ_4 – C3-C4-C5-C1*; φ_5 – C4-C5-C1*-C2*; [b] – conformers are numbered according to their appearance during conformational search.

Table B1. Total energies (in Hartree), relative energies (ΔE, $\Delta\Delta G°$ in kcal mol^{-1}) and percentage populations calculated for individual conformers of amides **1**, **4**, **5**-**7** at the B97-D/6-311G(2d,2p) level.

Amide[a]	Energy	ΔE	Population	$\Delta\Delta G°$	Population
1 (conf. 1)	-1997.90223	0.65	24.95	0.00	95.7
1 (conf. 6)	-1997.90326	0.00	75.05	1.84	4.3
4a (conf. 1)	-2037.209969	1.78	4.69	0.83	19.7
4a (conf. 3)	-2037.213	0.00	95.31	0.00	80.3
4b (conf. 1)	-2115.76539	1.68	3.97	0.48	19.18
4b (conf. 5)	-2115.76392	2.60		0.81	10.94
4b (conf. 7)	-2115.76205	3.77		1.76	2.18
4b (conf. 8)	-2115.76807	0.00	67.44	0.00	42.91
4b (conf. 11)	-2115.76436	2.32		1.30	4.74
4b (conf. 24)	-2115.76691	0.73	19.81	1.62	2.76
4b (conf. 26)	-2115.76614	1.21	8.79	0.54	17.3
5 (conf. 1)	-2343.094935	0.26	27.88	0.96	14.88
5 (conf. 5)	-2343.095348	0.00	43.17	1.16	10.45
5 (conf. 60)	-2343.09497	0.24	28.94	0.00	74.67
6 (conf. 13)	-2419.269142	0.00		0.00	58.67
6 (conf. 70)	-2419.263811	3.35		1.00	10.85
6 (conf. 73)	-2419.264107	3.16		0.39	30.48
7 (conf. 1)	-2343.11851	0.00	60.14	0.34	36.22
7 (conf. 2)	-2343.11801	0.31	35.69	0.00	63.78
7 (conf. 3)	-2343.11599	1.58	4.17	3.17	

[a] – conformers are numbered according to their appearance during conformational search

Table B2. Total energies (in Hartree), relative energies (ΔE, $\Delta\Delta G°$ in kcal mol^{-1}) and percentage populations calculated for individual conformers of amides **1**, **4**, **5**-**7** at the B97-D3/6-311G(2d,2p) level.

Amide[a]	Energy	ΔE	Population	$\Delta\Delta G°$	Population
1 (conf. 1)	-1998.081797	0.00	64.93	0.00	100
1 (conf. 6)	-1998.081141	0.41	32.41	3.51	
1 (conf. 7)	-1998.07878	1.89	2.65	3.12	
4a (conf. 3)	-2037.397813	0.00	100	0.00	100
4b (conf. 1)	-2115.95095	1.68	2.98	2.38	
4b (conf. 8)	-2115.95354	0.05	46.39	0.00	64.56
4b (conf. 26)	-2115.95362	0.00	50.63	0.36	35.44
5 (conf. 1)	-2343.309679	0.42	18.56	0.00	86.69
5 (conf. 5)	-2343.310309	0.03	36.21	2.28	
5 (conf. 42)	-2343.309	1.12	5.75	3.65	
5 (conf. 60)	-2343.31	0.00	37.82	4.50	
5 (conf. 67)	-2343.307	1.85	1.67	1.11	13.31
6 (conf. 1)	-2419.49417	0.00	48.06	2.72	
6 (conf. 13)	-2419.49353	0.40	24.4	2.38	
6 (conf. 31)	-2419.49356	0.38	25.2	0.00	100
6 (conf. 70)	-2419.49132	1.79	2.34	2.80	
7 (conf. 1)	-2343.33786	0.90	15.8	2.08	
7 (conf. 2)	-2343.33929	0.00	72.03	0.00	100
7 (conf. 3)	-2343.33761	1.05	12.17	2.89	

[a] – conformers are numbered according to their appearance during conformational search

Table B3. Total energies (in Hartree), relative energies (ΔE, $\Delta\Delta G°$ in kcal mol^{-1}) and percentage populations calculated for individual conformers of amides **1**, **4**, **5**-**7** at the B3LYP/6-311G(2d,2p) level.

Amide[a]	Energy	ΔE	Population	$\Delta\Delta G°$	Population
1 (conf. 1)	-1999.337412	0.00	40.46	0.00	56.37
1 (conf. 3)	-1999.335676	1.09	6.42	3.08	
1 (conf. 4)	-1999.337	0.27	25.76	0.67	18.33
1 (conf. 5)	-1999.336238	0.74	11.66	0.69	17.66
1 (conf. 6)	-1999.335284	1.34	4.24	1.50	4.48
1 (conf. 7)	-1999.334336	1.93	1.55	1.71	3.16
1 (conf. 8)	-1999.336085	0.83	9.91	2.1	
4a (conf. 1)	-2038.670358	0.54	28.57	1.19	11.88
4a (conf. 3)	-2038.671223	0.00	71.43	0.00	88.12
4b (conf. 1)	-2117.26568	0.03	43.9	0.08	41.4
4b (conf. 5)	-2117.26427	0.92	9.84	1.05	8.08
4b (conf. 7)	-2117.26226	2.18		1.69	2.75
4b (conf. 8)	-2117.26573	0.00	46.26	0.00	47.77
5 (conf. 61)	-2344.780648	0.00	85.78	0.00	80.73
5 (conf. 67)	-2344.777874	1.74	4.54	4.26	
5 (conf. 99)	-2344.778589	1.29	9.68	0.85	19.27
6 (conf. 1)	-2421.021116	0.04	17.5	1.19	4.27
6 (conf. 31)	-2421.020526	0.41	9.36	1.35	3.21
6 (conf. 32)	-2421.020666	0.32	10.87	1.55	2.3
6 (conf. 37)	-2421.021176	0.00	18.65	1.87	1.33
6 (conf. 62)	-2421.018833	1.47	1.56	2.69	
6 (conf. 68)	-2421.020267	0.57	7.12	0.03	30.22
6 (conf. 70)	-2421.021175	0.00	18.62	0.75	8.85
6 (conf. 73)	-2421.02065	0.33	10.68	0.81	7.99
6 (conf. 81)	-2421.019186	1.25	2.26	0.77	8.6
6 (conf. 87)	-2421.018446	1.71	1.03	1.77	1.59
6 (conf. 90)	-2421.019218	1.23	2.34	0.00	31.63
7 (conf. 1)	-2344.795749	0.50	22.14	0.99	9.84
7 (conf. 2)	-2344.796541	0.00	51.24	0.00	52.28

7 (conf. 3)	-2344.793589	1.85	2.24	2.20	
7 (conf. 4)	-2344.795708	0.52	21.2	0.93	10.81
7 (conf. 6)	-2344.793915	1.65	3.17	0.39	27.07

[a] – conformers are numbered according to their appearance during conformational search

Table B4. Total energies (in Hartree), relative energies (ΔE, $\Delta\Delta G°$ in kcal mol^{-1}) and percentage populations calculated for individual conformers of amides **1**, **4**, **5**-**7** at the B3LYP-GD3BJ/6-311G(2d,2p) level.

Amide[a]	Energy	ΔE	Population	$\Delta\Delta G°$	Population
1 (conf. 1)	-1999.587596	0.00	88.41	0.13	43.13
1 (conf. 5)	-1999.582045	3.48		1.75	2.81
1 (conf. 6)	-1999.585678	1.20	11.59	4.02	
1 (conf. 7)	-1999.584047	2.23		0.00	54.06
4a (conf. 3)	-2038.93343	0	100	0	100
4b (conf. 1)	-2117.54632	1.74	2.88	3.97	
4b (conf. 5)	-2117.54413	3.11		1.08	7.84
4b (conf. 8)	-2117.54909	0.00	54.23	0.00	48.52
4b (conf. 26)	-2117.54886	0.14	42.89	0.06	43.64
5 (conf. 1)	-2345.0814	1.23	6.22	0.01	42.96
5 (conf. 5)	-2345.08286	0.32	29.19	0.00	43.33
5 (conf. 42)	-2345.08179	0.99	9.4	0.68	13.71
5 (conf. 60)	-2345.08337	0.00	49.94	3.10	
5 (conf. 67)	-2345.08124	1.33	5.24	2.37	
6 (conf. 1)	-2421.33028	0.25	28.67	0.13	33.11
6 (conf. 13)	-2421.33012	0.35	24.27	0.00	41.5
6 (conf. 31)	-2421.33067	0.00	43.55	0.57	15.84
6 (conf. 37)	-2421.3283	1.49	3.51	2.99	
6 (conf. 68)	-2421.32551	3.24		1.12	6.29
6 (conf. 73)	-2421.327001	2.30		1.51	3.27
7 (conf. 1)	-2345.108244	1.13	10.69	2.03	
7 (conf. 2)	-2345.110049	0.00	72.35	0.00	100
7 (conf. 3)	-2345.10868	0.86	16.96	2.82	

[a] – conformers are numbered according to their appearance during conformational search

Table B5. Total energies (in Hartree), relative energies (ΔE, $\Delta\Delta G°$ in kcal mol^{-1}) and percentage populations calculated for individual conformers of amides **1**, **4**, **5**-**7** at the M06-2X/6-311G(2d,2p) level.

Amide[a]	Energy	ΔE	Population	$\Delta\Delta G°$	Population
1 (conf. 1)	-1998.547	0.00	69.33	0.00	34.63
1 (conf. 3)	-1998.545874	1.02	12.43	1.08	5.59
1 (conf. 4)	-1998.545237	1.42	6.33	1.17	4.84
1 (conf. 5)	-1998.540124	4.63		0.13	27.63
1 (conf. 6)	-1998.545605	1.19	9.35	0.19	24.99
1 (conf. 8)	-1998.544	1.96	2.55	1.60	2.32
4a (conf. 3)	-2037.86761	0	100	0	100
4b (conf. 1)	-2116.43368	1.80	4.6	0.21	26.37
4b (conf. 5)	-2116.42995	4.14		0.99	7.09
4b (conf. 7)	-2116.42899	4.74		0.46	17.29
4b (conf. 8)	-2116.43654	0.00	95.4	0.00	37.72
4b (conf. 11)	-2116.43046	3.82		1.23	4.7
4b (conf. 24)	-2116.43245	2.57		1.88	1.59
4b (conf. 26)	-2116.43244	2.57		1.17	5.24
5 (conf. 1)	-2343.865626	0.96	10.12	1.41	5.62
5 (conf. 05)	-2343.866888	0.17	38.52	0.52	25.19
5 (conf. 60)	-2343.867159	0.00	51.36	0.00	60.52
5 (conf. 61)	-2343.859347	4.90		1.85	2.65
5 (conf. 69)	-2343.863	2.67		1.37	6.02
6 (conf. 1)	-2420.085349	0.00	85.78	0.00	43.58
6 (conf. 13)	-2420.082486	1.80	4.13	0.53	17.82
6 (conf. 31)	-2420.0827	1.66	5.18	1.26	5.16
6 (conf. 44)	-2420.08265	1.69	4.91	0.25	28.55
6 (conf. 70)	-2420.081951	2.13		1.29	4.9
7 (conf. 1)	-2343.88738	0.91	15.27	0.29	25.6
7 (conf. 2)	-2343.88882	0.00	70.46	0.14	32.67
7 (conf. 3)	-2343.88731	0.95	14.27	0.00	41.73

[a] – conformers are numbered according to their appearance during conformational search

Table B6. Total energies (in Hartree), relative energies (ΔE, $\Delta\Delta G°$ in kcal mol^{-1}) and percentage populations calculated for individual conformers of amides **1**, **4**, **5**-**7** at the M06-2X-D3/6-311G(2d,2p) level.

Amide[a]	Energy	ΔE	Population	$\Delta\Delta G°$	Population
1 (conf. 1)	-1998.56009	0.00	81.86	0.00	100
1 (conf. 3)	-1998.55794	1.35	8.36	2.62	
1 (conf. 4)	-1998.55726	1.78	4.07	2.89	
1 (conf. 6)	-1998.55758	1.58	5.71	2.04	
4a (conf. 3)	-2037.881149	0.00	100	0.00	100
4b (conf. 1)	-2116.44756	2.34		0.79	11.92
4b (conf. 5)	-2116.44395	4.61		1.71	2.52
4b (conf. 7)	-2116.44265	5.42		0.18	33.29
4b (conf. 08)	-2116.45128	0.00	100	0.00	45.17
4b (conf. 24)	-2116.44741	2.43		1.81	2.11
4b (conf. 26)	-2116.44754	2.35		1.30	4.99
5 (conf. 1)	-2343.882429	0.90	11.35	1.08	8.03
5 (conf. 5)	-2343.883859	0.00	51.62	0.18	36.62
5 (conf. 60)	-2343.883545	0.20	37.03	0.00	49.69
5 (conf. 61)	-2343.875503	5.24		1.87	2.13
5 (conf. 69)	-2343.87887	3.13		1.57	3.53
6 (conf. 1)	-2420.10205	0.00	96.33	0.00	57.45
6 (conf. 13)	-2420.09896	1.94	3.67	0.63	19.78
6 (conf. 31)	-2420.09873	2.08		1.73	3.1
6 (conf. 44)	-2420.09867	2.12		0.64	19.66
7 (conf. 1)	-2343.904156	0.87	16.56	0.25	30.37
7 (conf. 2)	-2343.905537	0	71.48	0.42	23.08
7 (conf. 3)	-2343.903849	1.06	11.96	0.00	46.55

[a] – conformers are numbered according to their appearance during conformational search

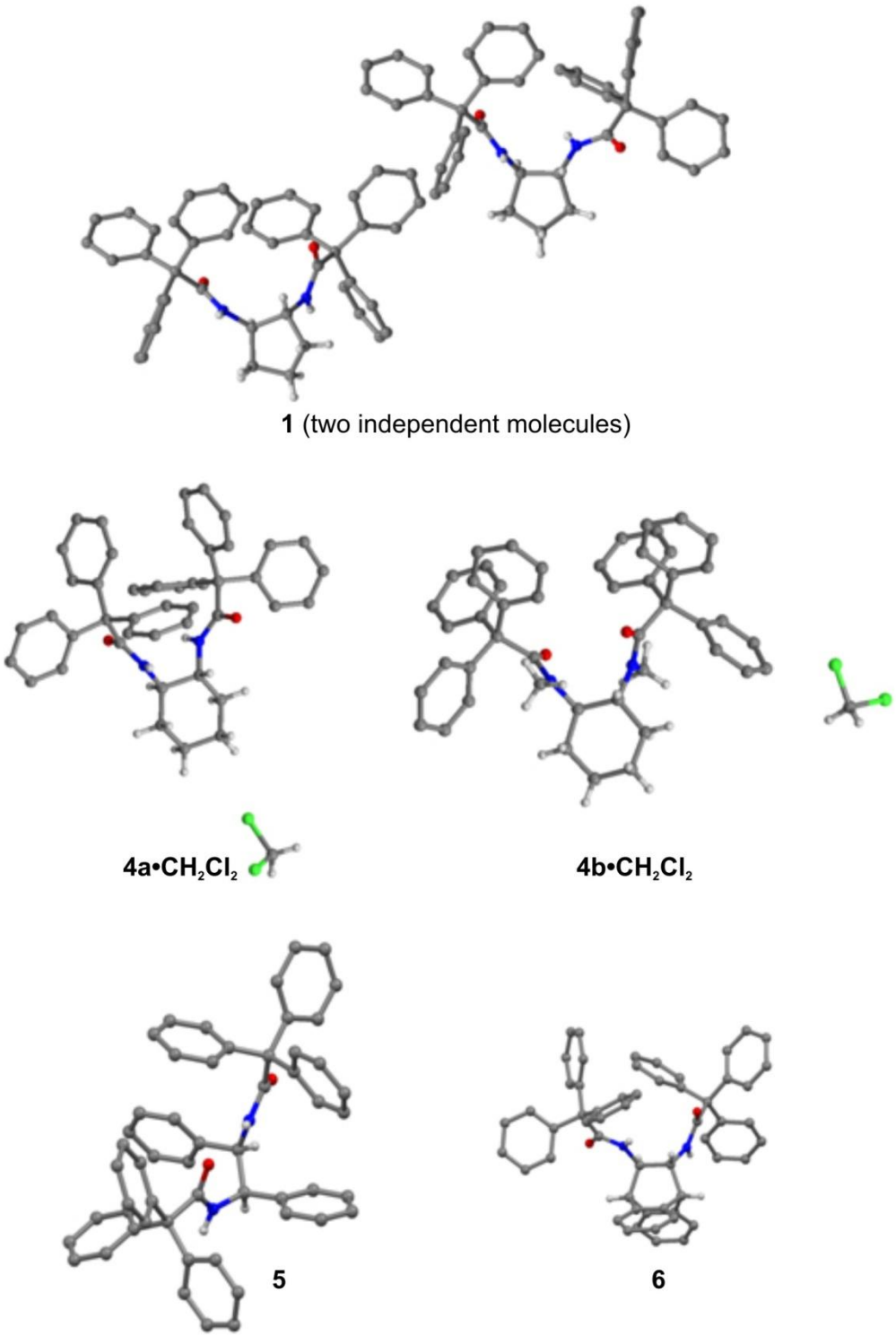
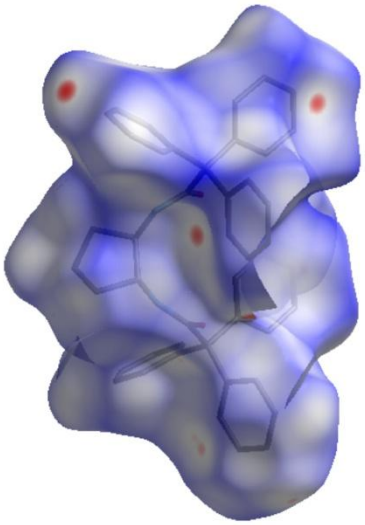
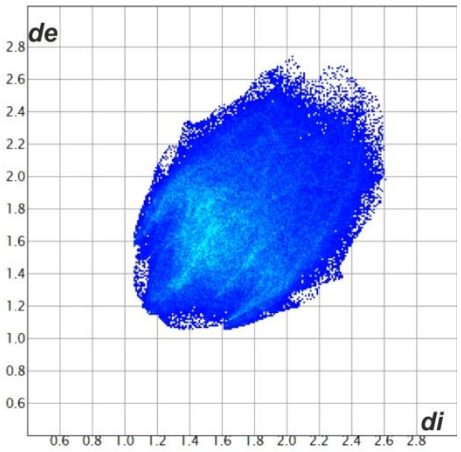
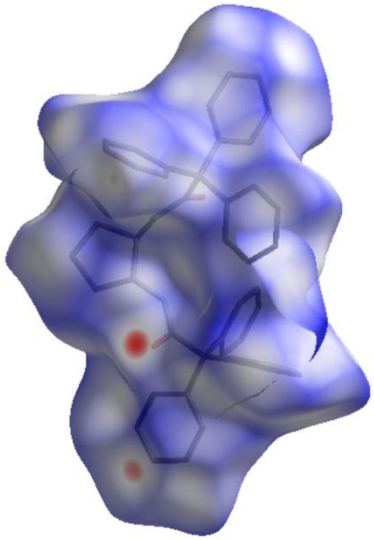


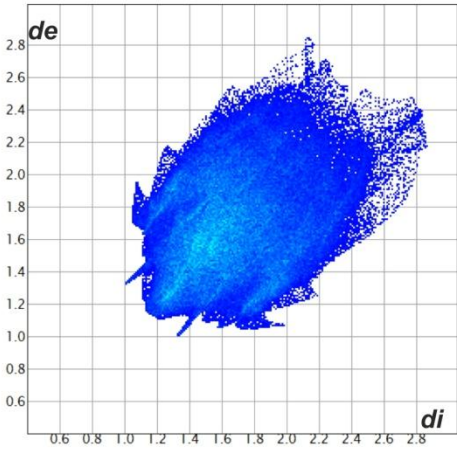
Figure S1. Perspective view of molecules **1** (two independent molecules), **4a**, **4b**, **5** and **6** as present in crystals. Hydrogen atoms in aromatic systems have been omitted for clarity.



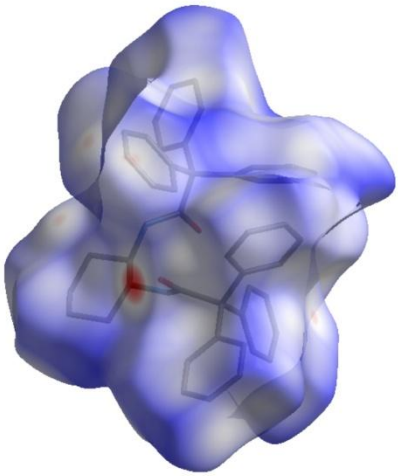

de
di
0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

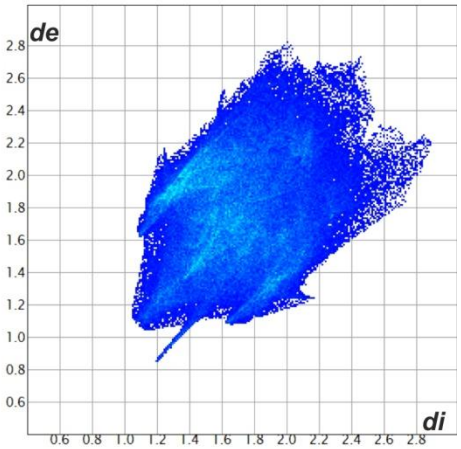
1A




de
di
0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

1B




de
di
0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

4a

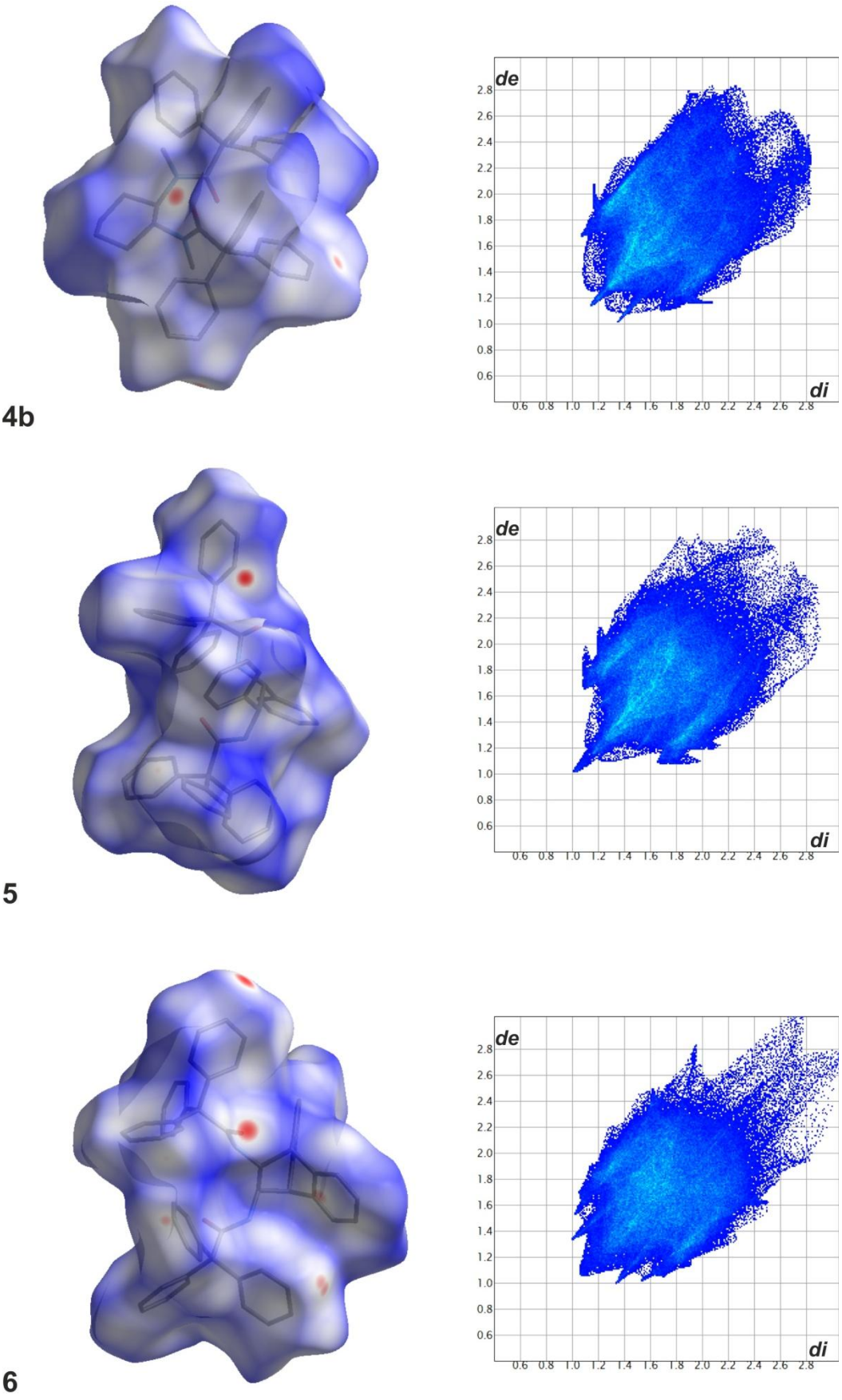


Figure S2. Hirshfeld surface (H-atoms not shown) and fingerprint plot derived from it, calculated with the program Crystal Explorer. [4]

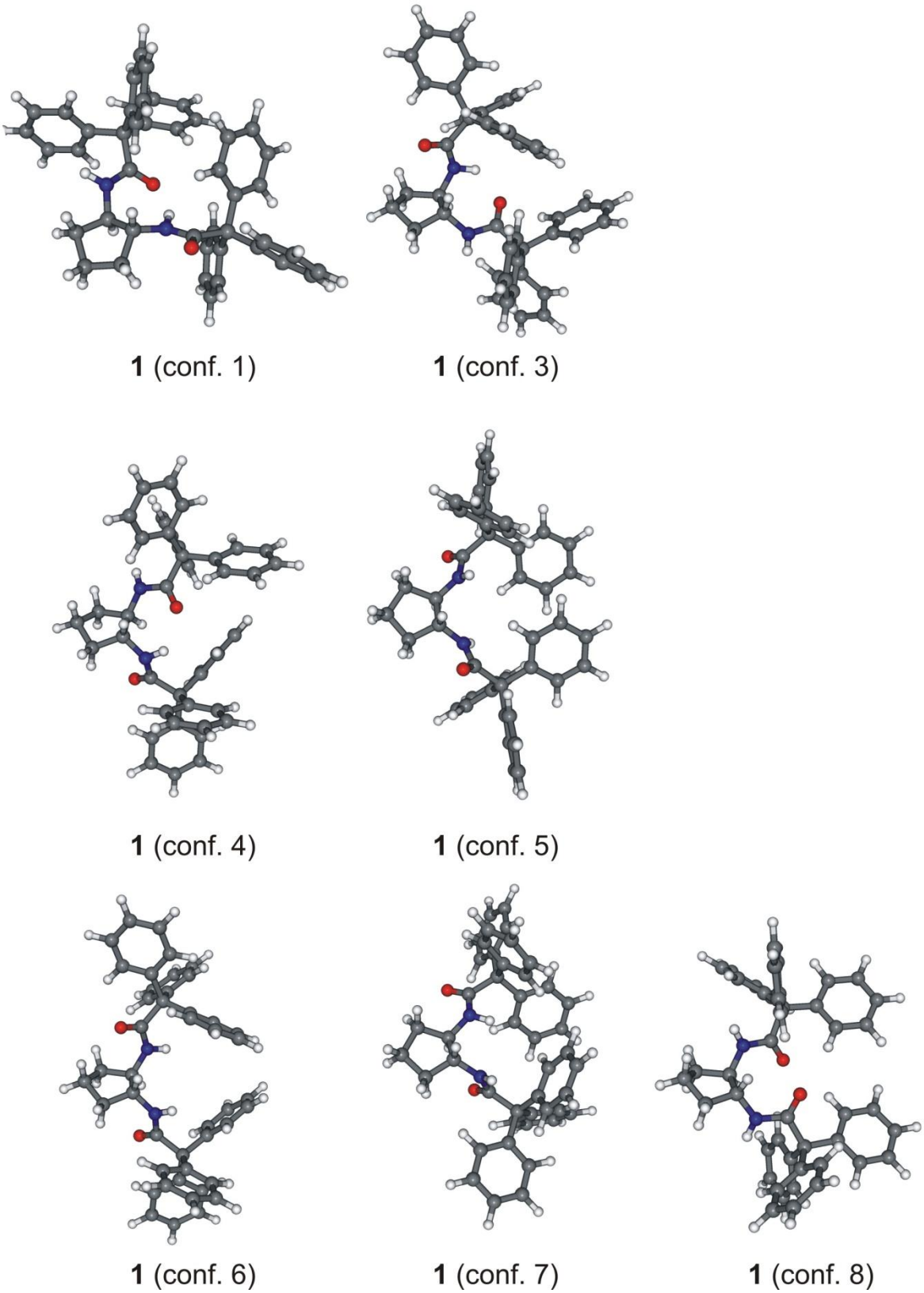


Figure A1. Structures of individual low-energy conformers of triphenylacetamides **1** calculated at the B3LYP/6-311G(2d,2p) level.

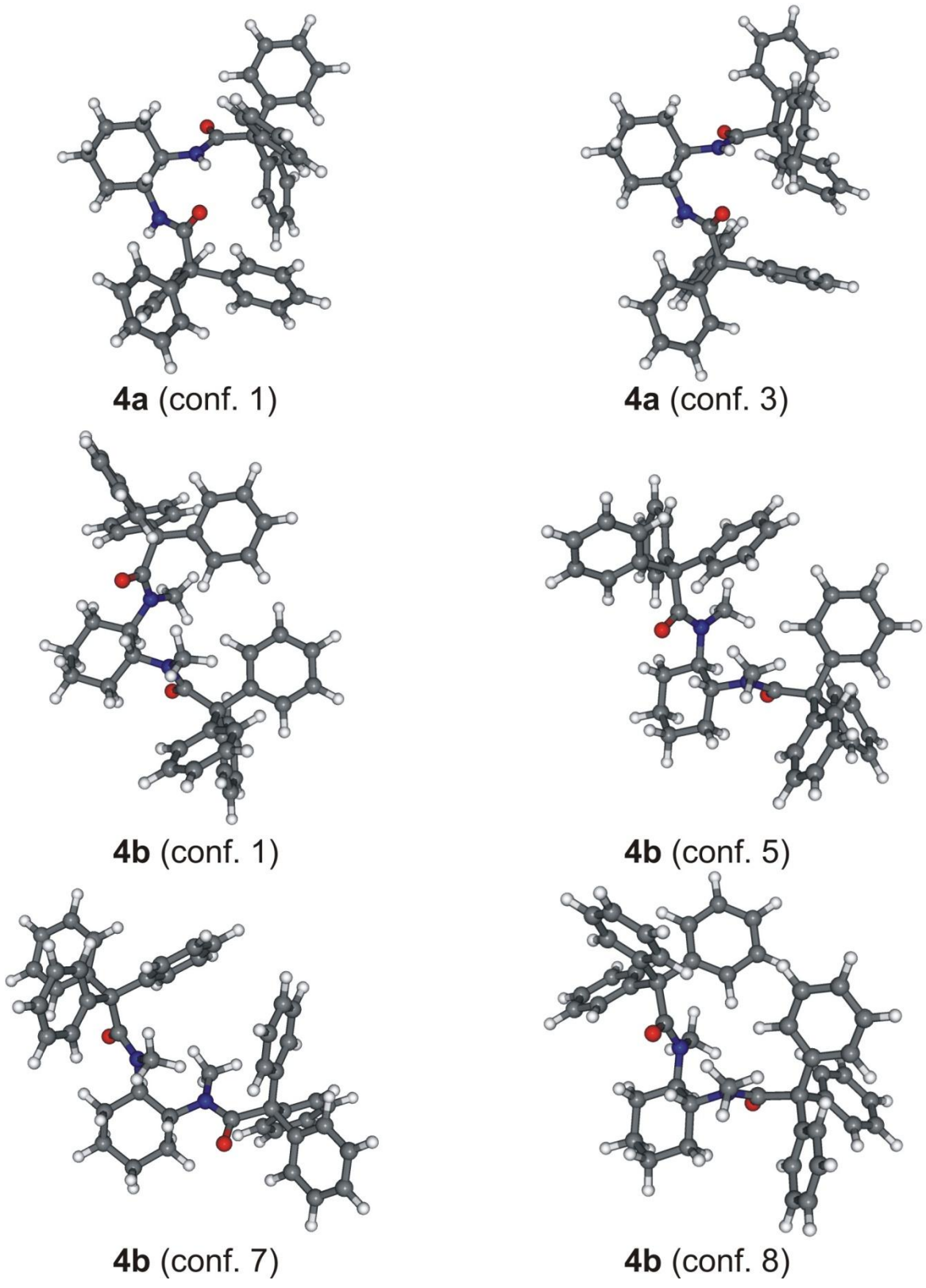


Figure A2. Structures of individual low-energy conformers of triphenylacetamides **4a** and **4b** calculated at the B3LYP/6-311G(2d,2p) level.

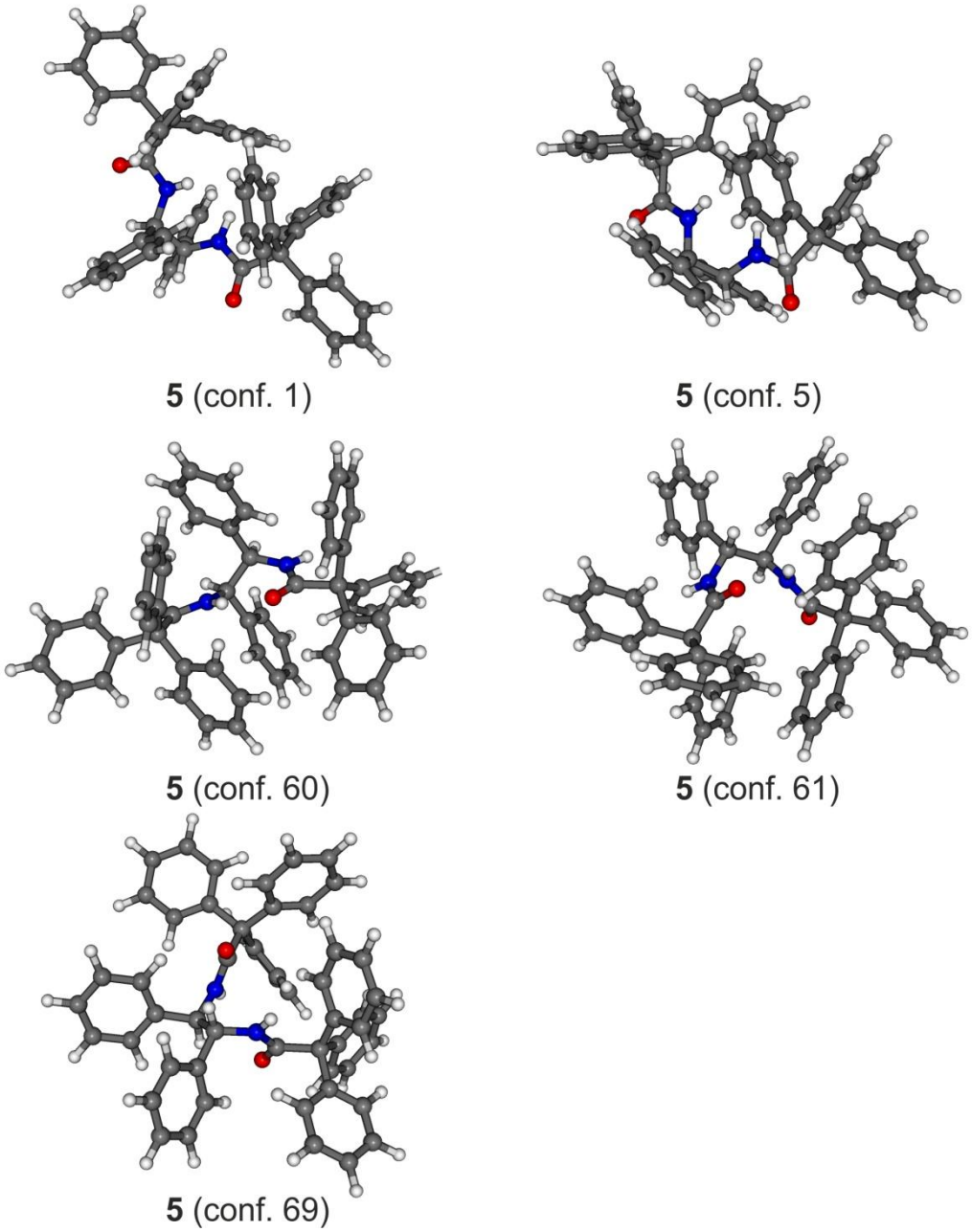


Figure A3. Structures of individual low-energy conformers of triphenylacetamides **5** calculated at the M06-2X/6-311G(2d,2p) level.

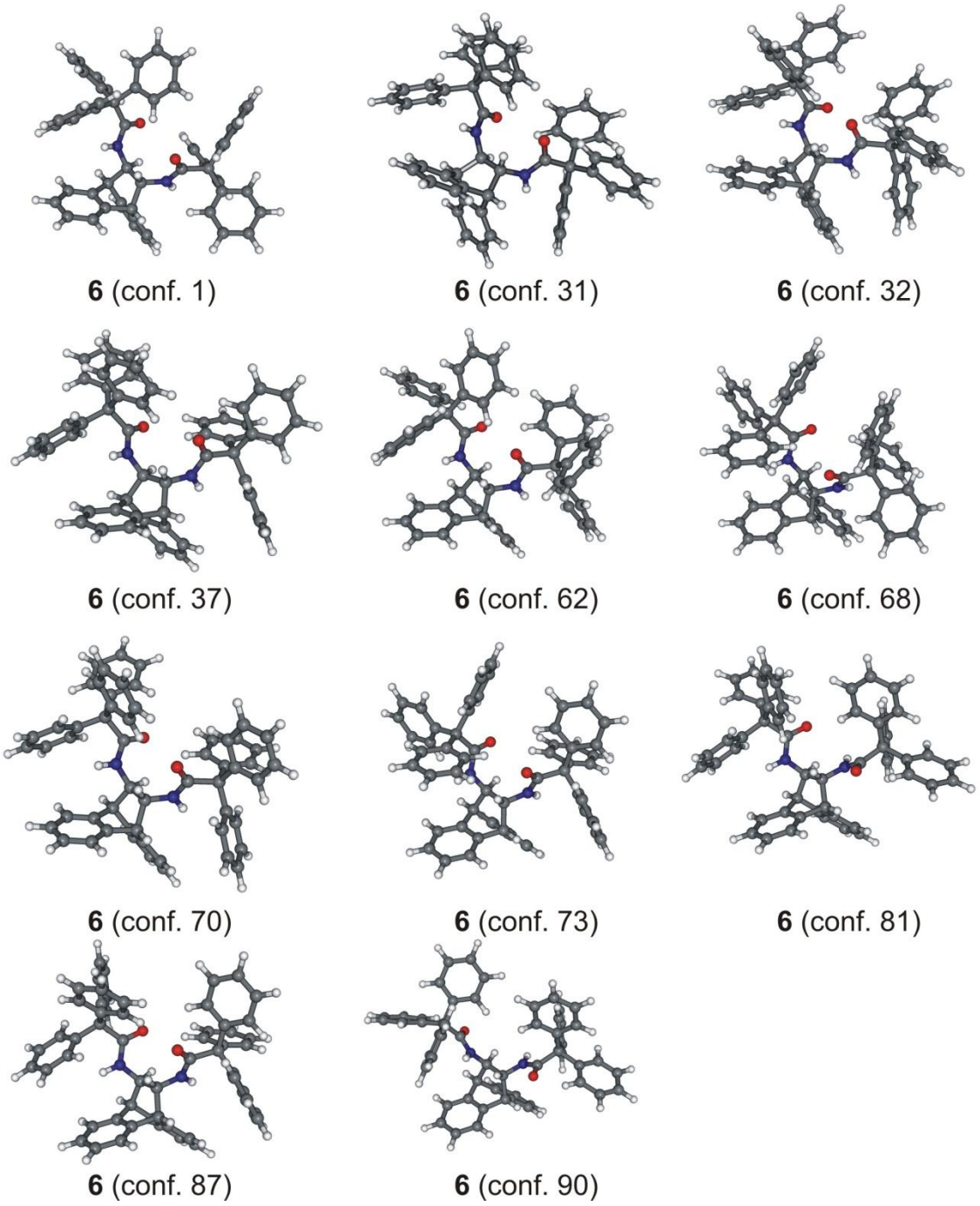


Figure A4. Structures of individual low-energy conformers of triphenylacetamides **6** calculated at the B3LYP/6-311G(2d,2p) level.

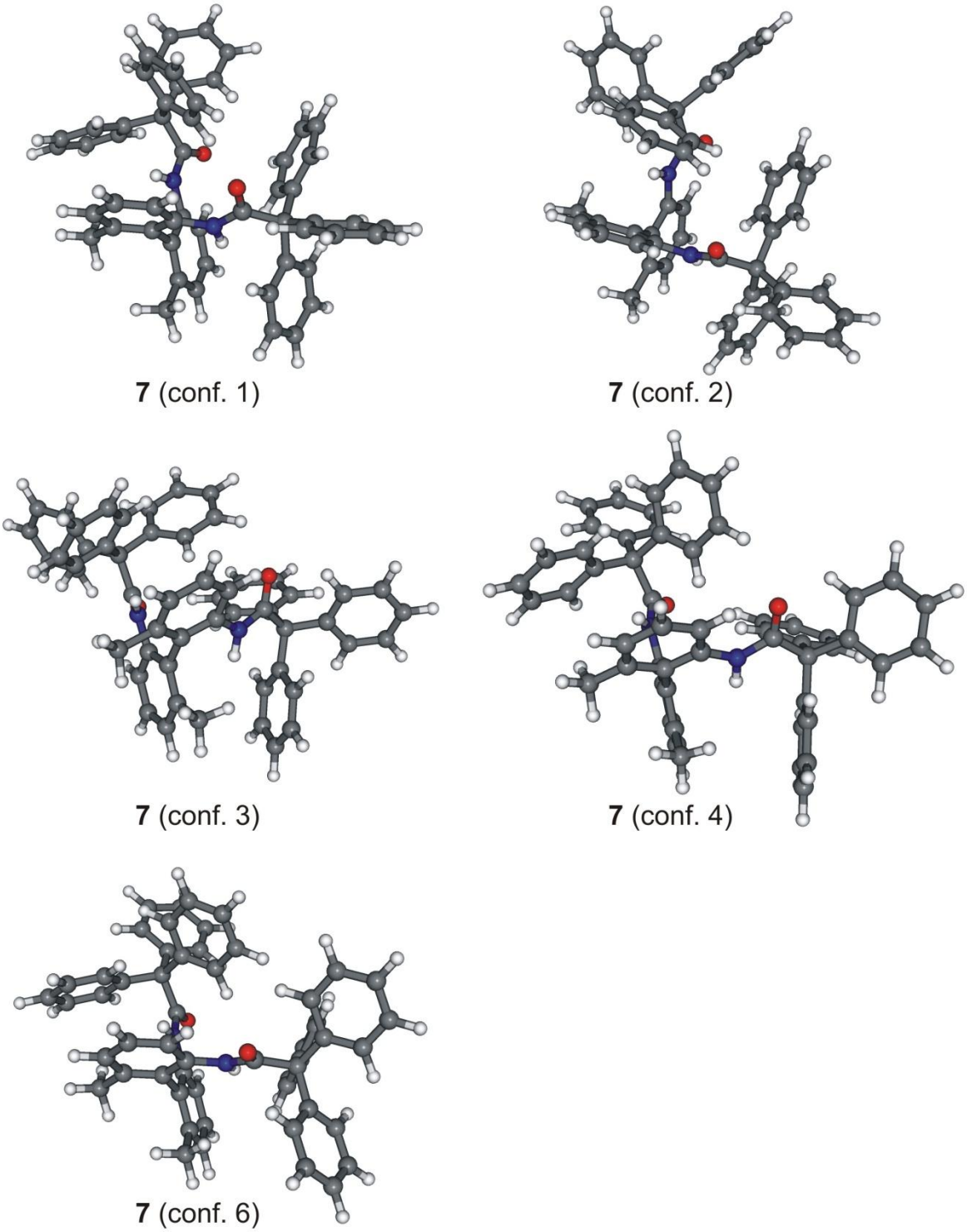


Figure A5. Structures of individual low-energy conformers of triphenylacetamides **7** calculated at the B3LYP/6-311G(2d,2p) level.

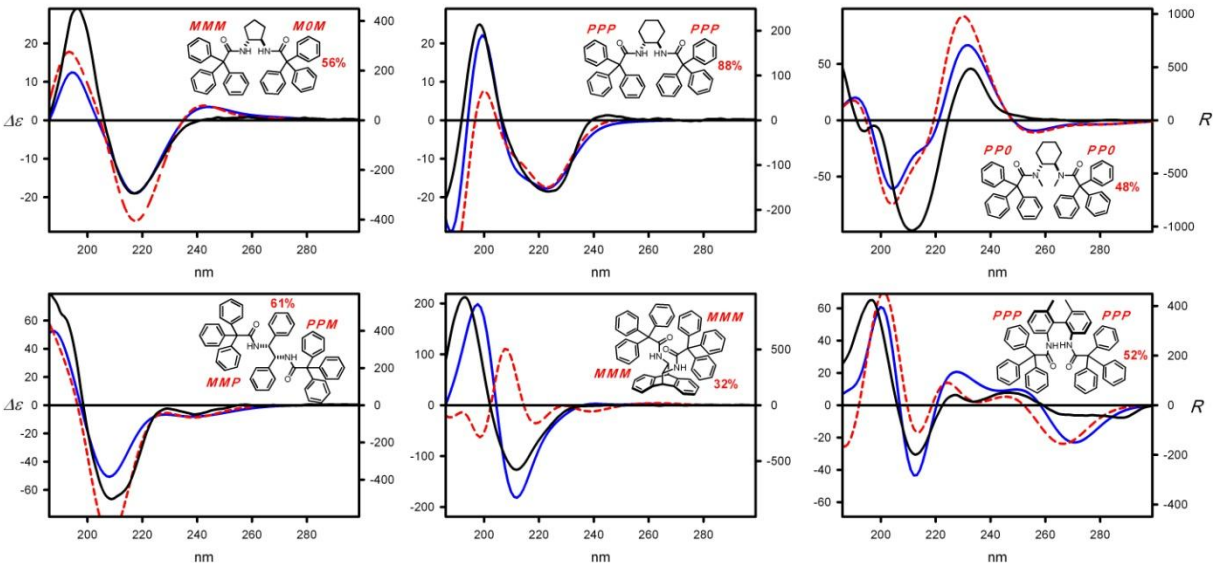


Figure A6. Experimental (solid black lines) and Boltzmann averaged (blue lines) calculated at the TD-M06-2X/6-311G(2d,2p) level for structures optimized at the DFT/6-311G(2d,2p) levels ECD spectra of triphenylacetamides **1**, **4a**, **4b**, **5**, **6** and **7**. Red dashed lines represent ECD spectra calculated for the lowest energy conformers of triphenylacetamides **1**, **4a**, **4b**, **5**, **6** and **7**. Inserts show structures, helicities and populations of respective conformers. All calculated ECD spectra were wavelength corrected.

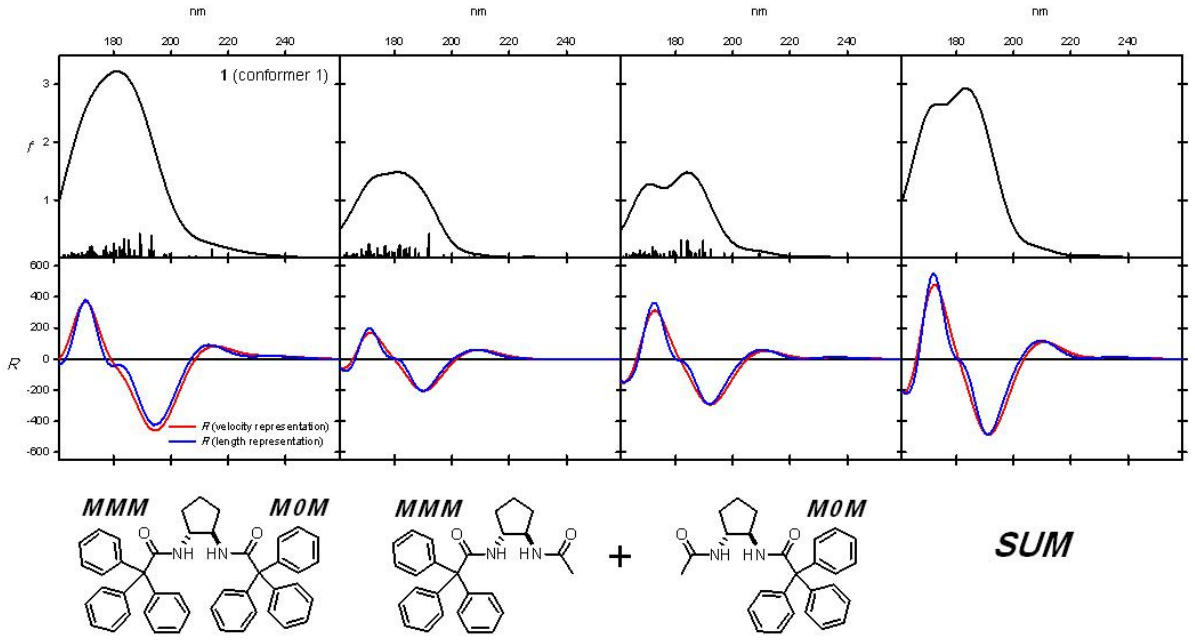


Figure A7. ECD and UV spectra calculated at the TD-M06-2X/6-311G(2d,2p) level for the lowest energy conformer 1 of amide **1** and for model compounds **1**(s1) and **1**(s2). Last column shows effect of summation of UV and CD spectra of **1**(s1) and **1**(s2). Wavelengths were not corrected.

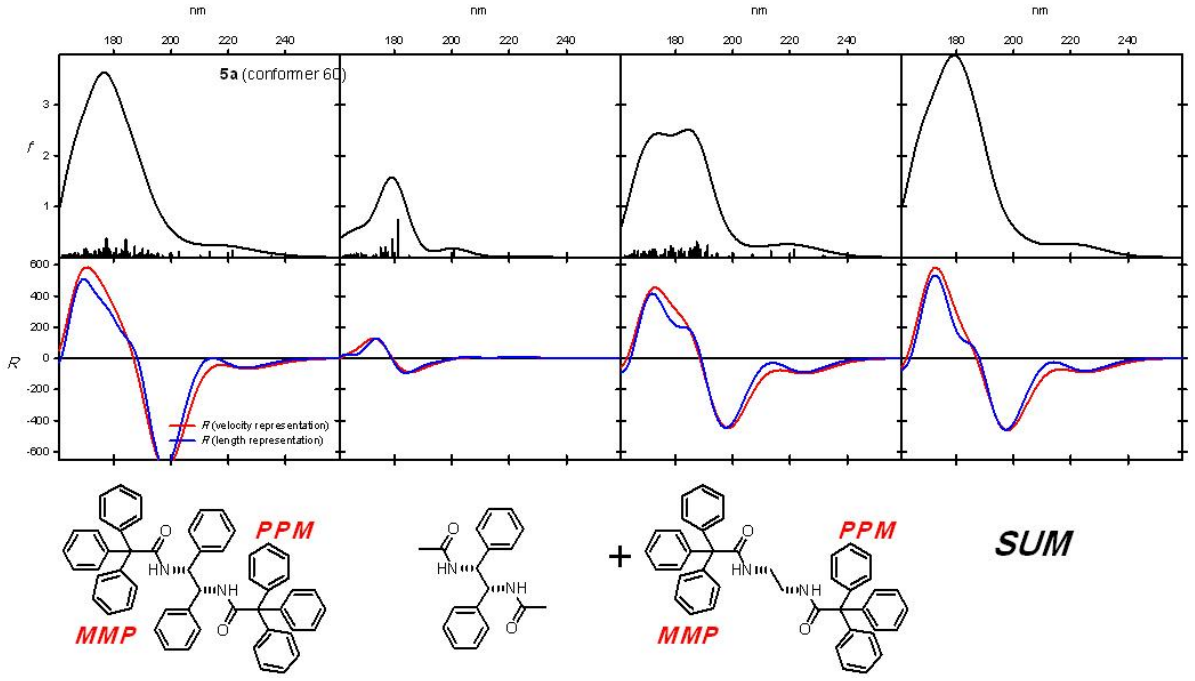


Figure A8. ECD and UV spectra calculated at the TD-M06-2X/6-311G(2d,2p) level for the lowest energy conformer 60 of amide **5** and for model compounds **5**(s1) and **5**(s2). Last column shows effect of summation of UV and CD spectra of **5**(s1) and **5**(s2). Wavelengths were not corrected.

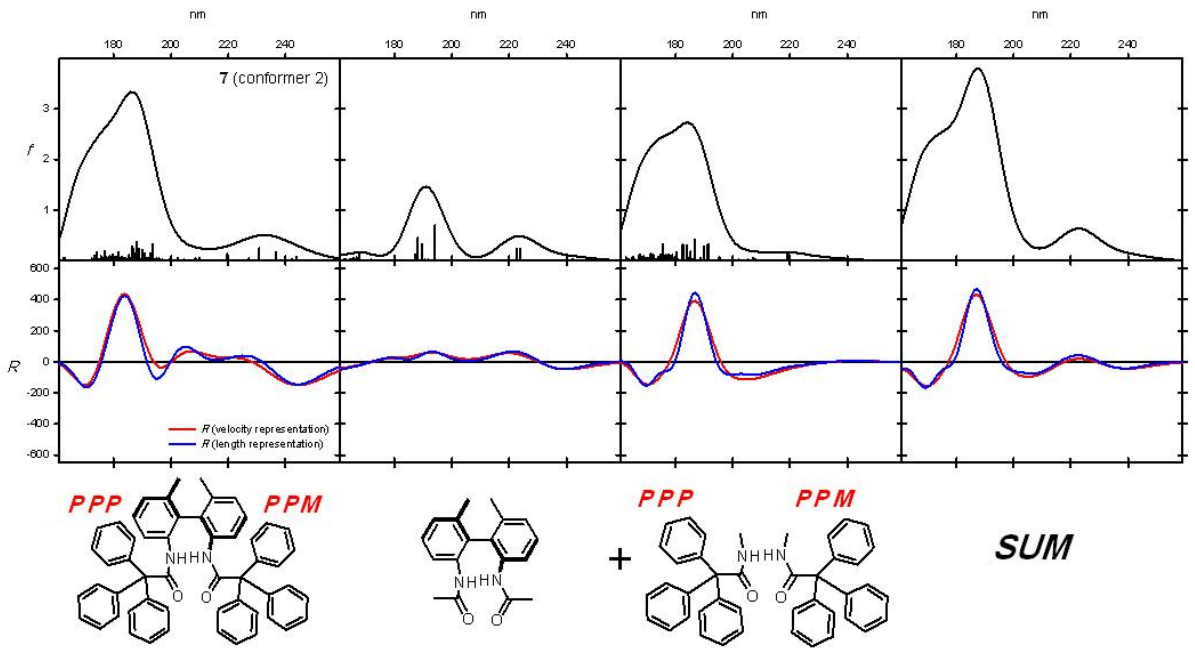
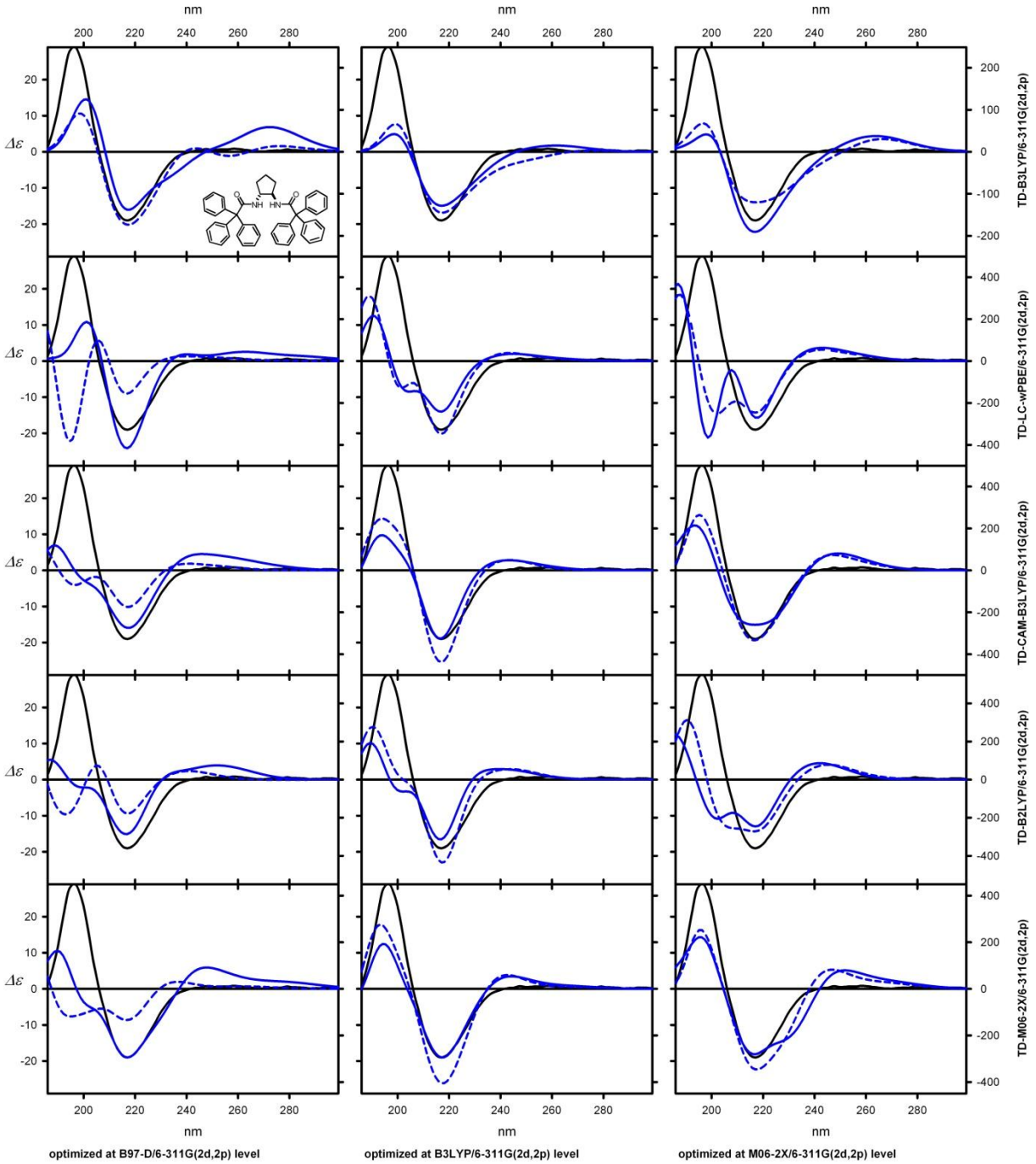


Figure A9. ECD and UV spectra calculated at the TD-M06-2X/6-311G(2d,2p) level for the lowest energy conformer 2 of amide **7** and for model compounds **7**(s1) and **7**(s2). Last column shows effect of summation of UV and CD spectra of **7**(s1) and **7**(s2). Wavelengths were not corrected.


nm
Δε
TD-B3LYP/6-311G(2d,2p)
TD-LC-wPBE/6-311G(2d,2p)
TD-CAM-B3LYP/6-311G(2d,2p)
TD-B2LYP/6-311G(2d,2p)
TD-M06-2X/6-311G(2d,2p)
optimized at B97-D/6-311G(2d,2p) level
optimized at B3LYP/6-311G(2d,2p) level
optimized at M06-2X/6-311G(2d,2p) level

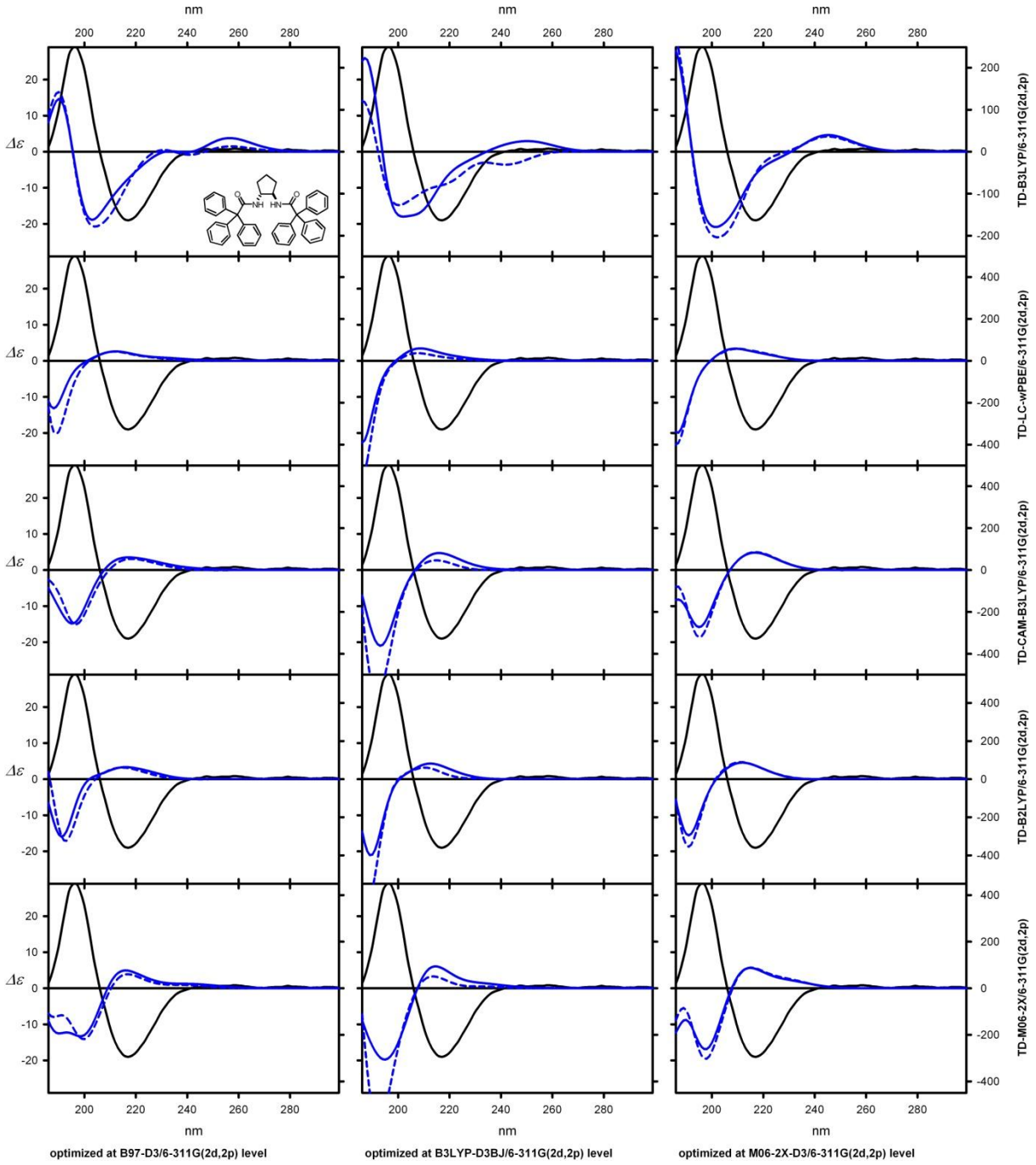
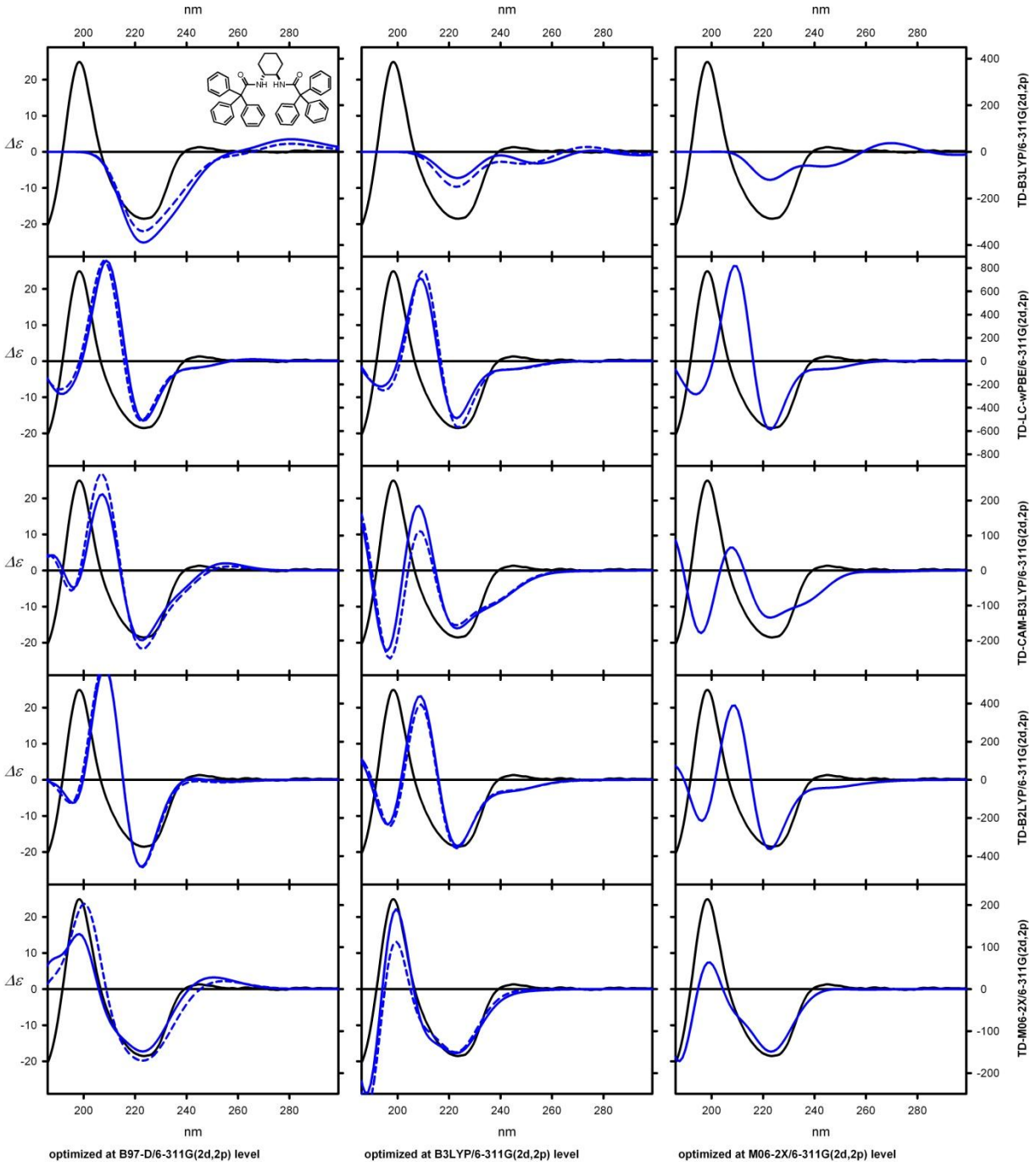


Figure B1. Experimental (solid black lines) and Boltzmann averaged (blue lines) calculated at the TD-DFT/6-311G(2d,2p) level for structures optimized at the DFT/6-311G(2d,2p) levels ECD spectra of triphenylacetamide **1**. All calculated ECD spectra were wavelength corrected.


nm
Δε
TD-B3LYP/6-311G(2d,2p)
TD-LC-wPBE/6-311G(2d,2p)
TD-CAM-B3LYP/6-311G(2d,2p)
TD-B2LYP/6-311G(2d,2p)
TD-M06-2X/6-311G(2d,2p)
optimized at B97-D/6-311G(2d,2p) level
optimized at B3LYP/6-311G(2d,2p) level
optimized at M06-2X/6-311G(2d,2p) level

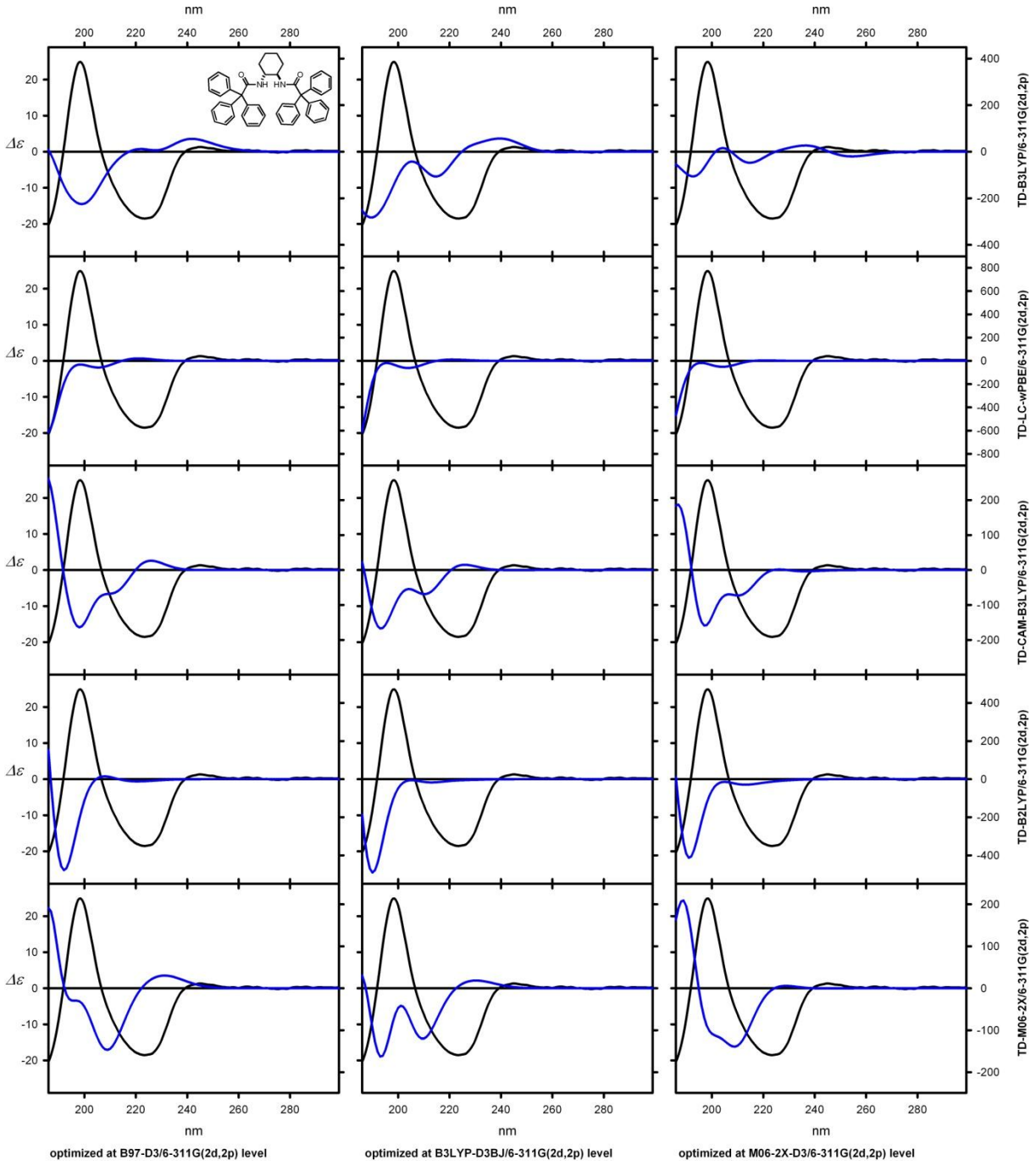
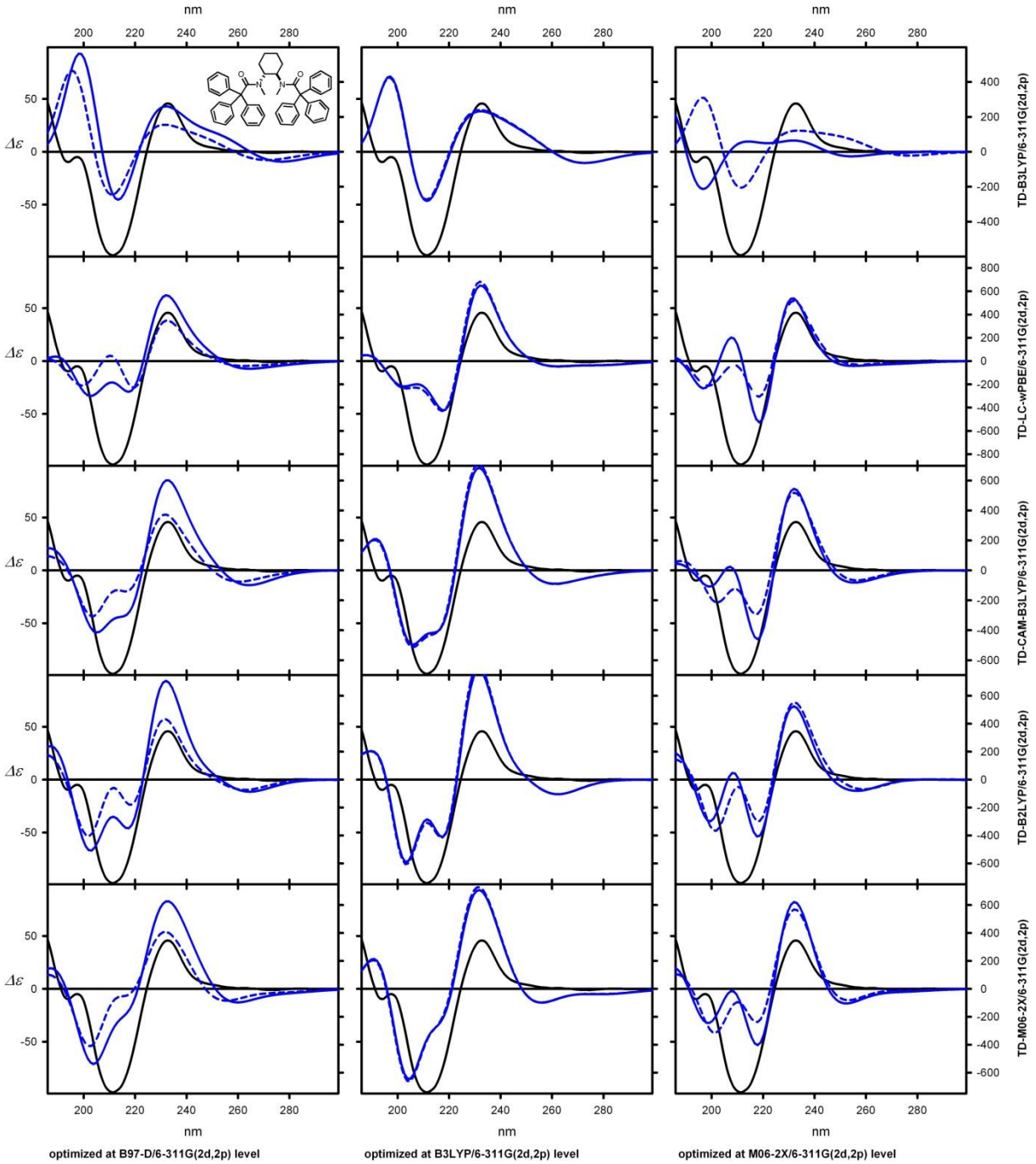


Figure B2. Experimental (solid black lines) and Boltzmann averaged (blue lines) calculated at the TD-DFT/6-311G(2d,2p) level for structures optimized at the DFT/6-311G(2d,2p) levels ECD spectra of triphenylacetamide **4a**. All calculated ECD spectra were wavelength corrected.


nm
Δε
TD-B3LYP/6-311G(2d,2p)
TD-LC-wPBE/6-311G(2d,2p)
TD-CAM-B3LYP/6-311G(2d,2p)
TD-B2LYP/6-311G(2d,2p)
TD-M06-2X/6-311G(2d,2p)
optimized at B97-D/6-311G(2d,2p) level
optimized at B3LYP/6-311G(2d,2p) level
optimized at M06-2X/6-311G(2d,2p) level

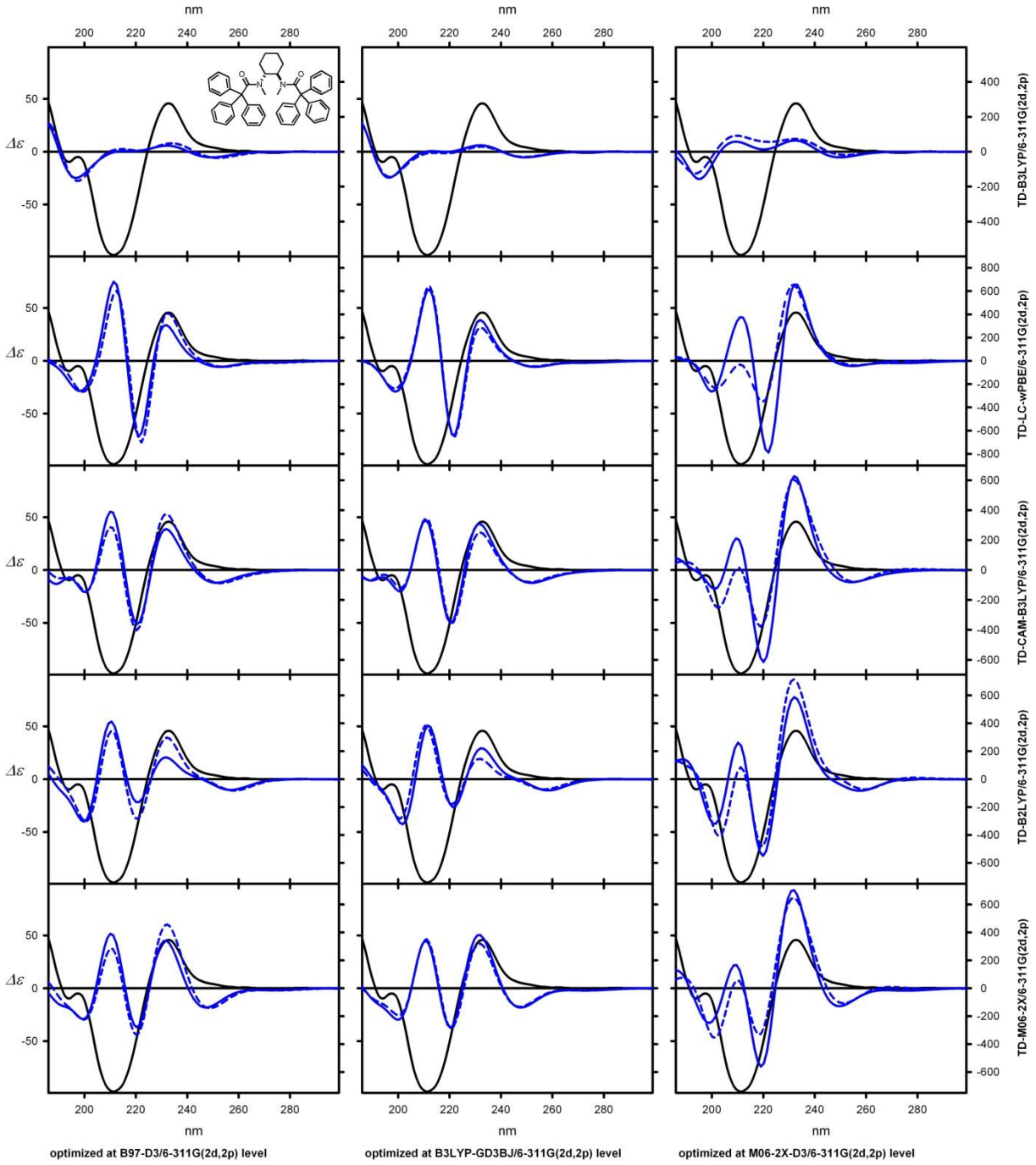
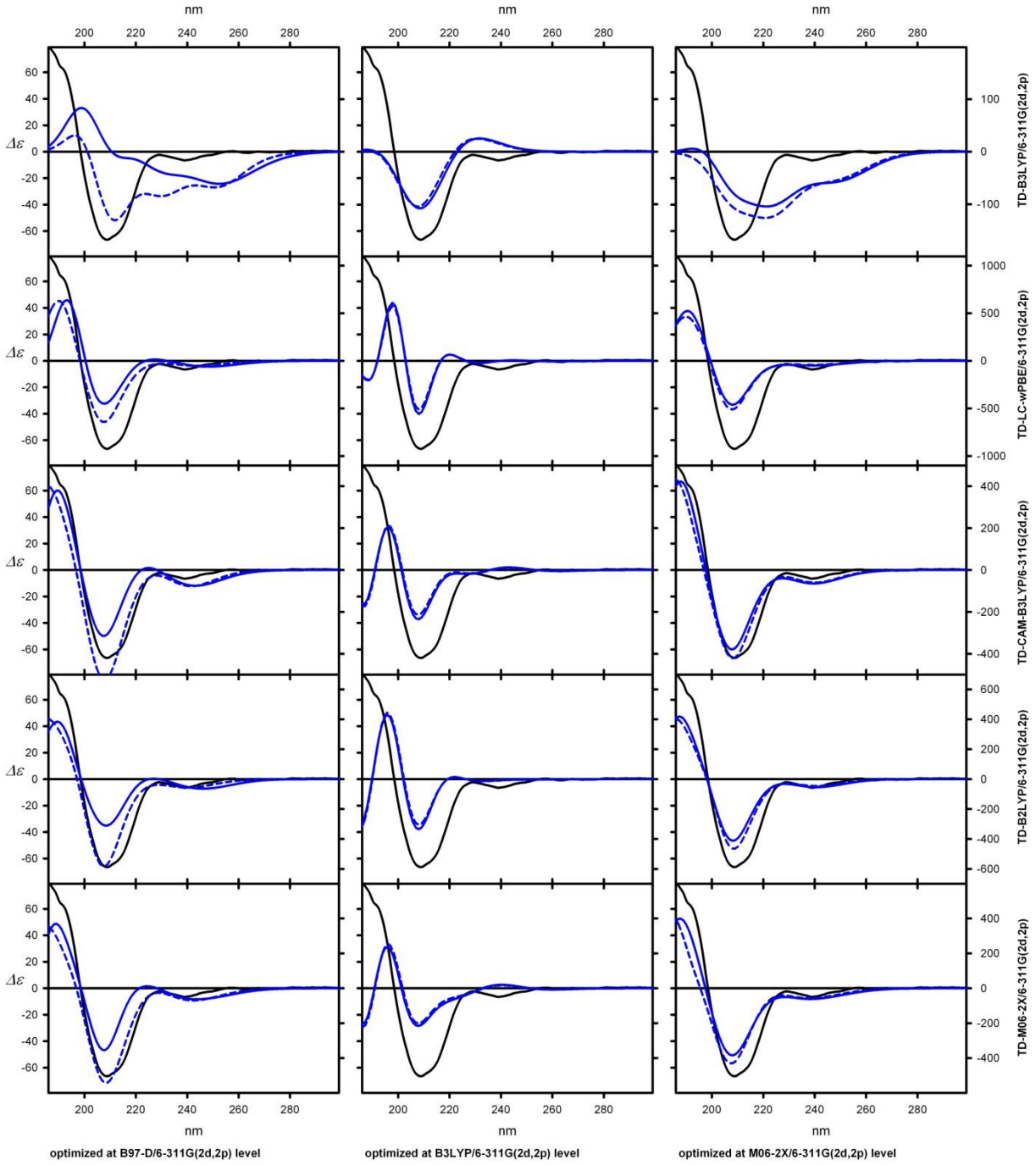


Figure B3. Experimental (solid black lines) and Boltzmann averaged (blue lines) calculated at the TD-DFT/6-311G(2d,2p) level for structures optimized at the DFT/6-311G(2d,2p) levels ECD spectra of triphenylacetamide **4b**. All calculated ECD spectra were wavelength corrected.


nm
200 220 240 260 280
Δε
TD-B3LYP/6-311G(2d,2p)
TD-LC-wPBE/6-311G(2d,2p)
TD-CAM-B3LYP/6-311G(2d,2p)
TD-B2LYP/6-311G(2d,2p)
TD-M06-2X/6-311G(2d,2p)
optimized at B97-D/6-311G(2d,2p) level
optimized at B3LYP/6-311G(2d,2p) level
optimized at M06-2X/6-311G(2d,2p) level

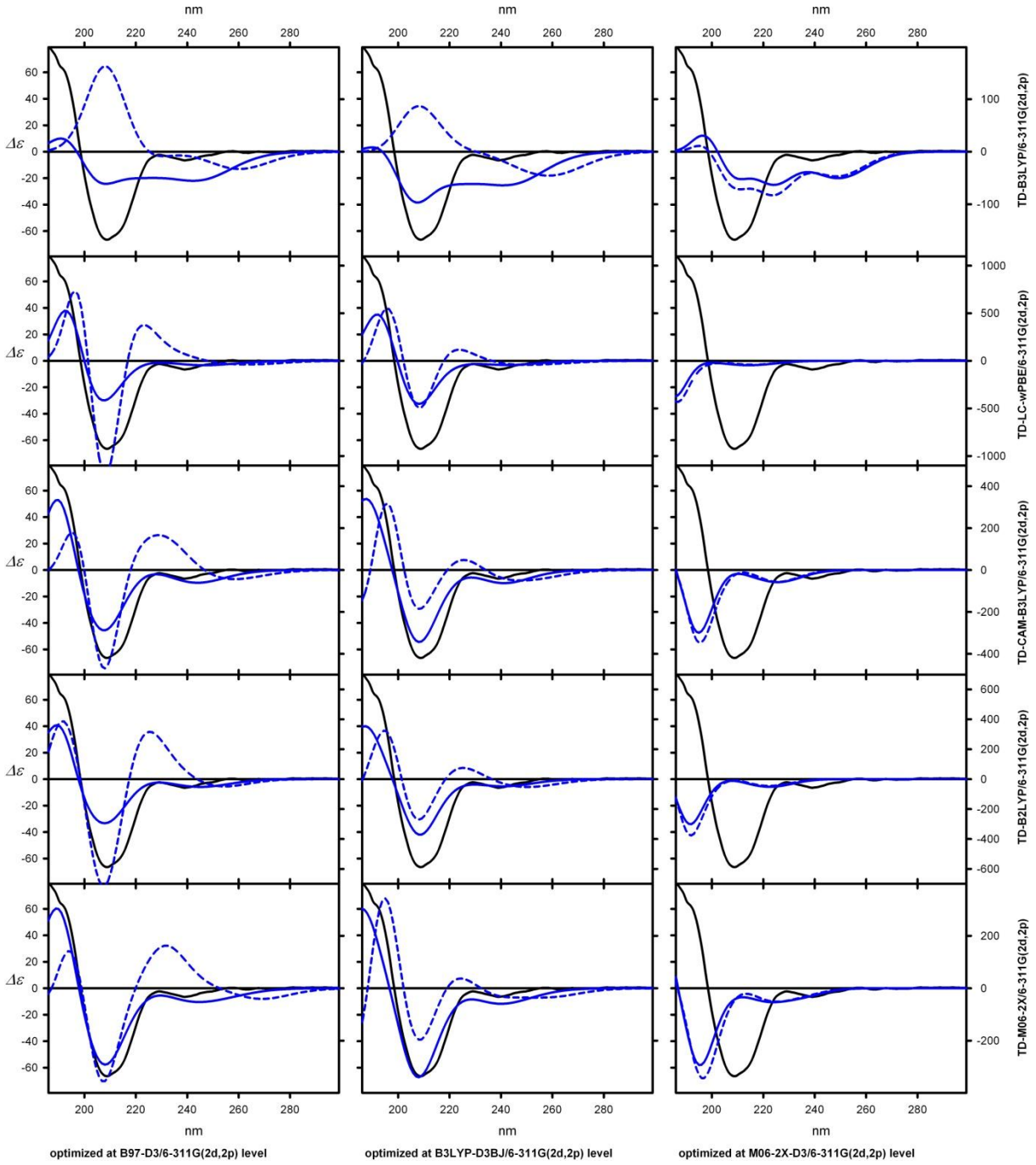
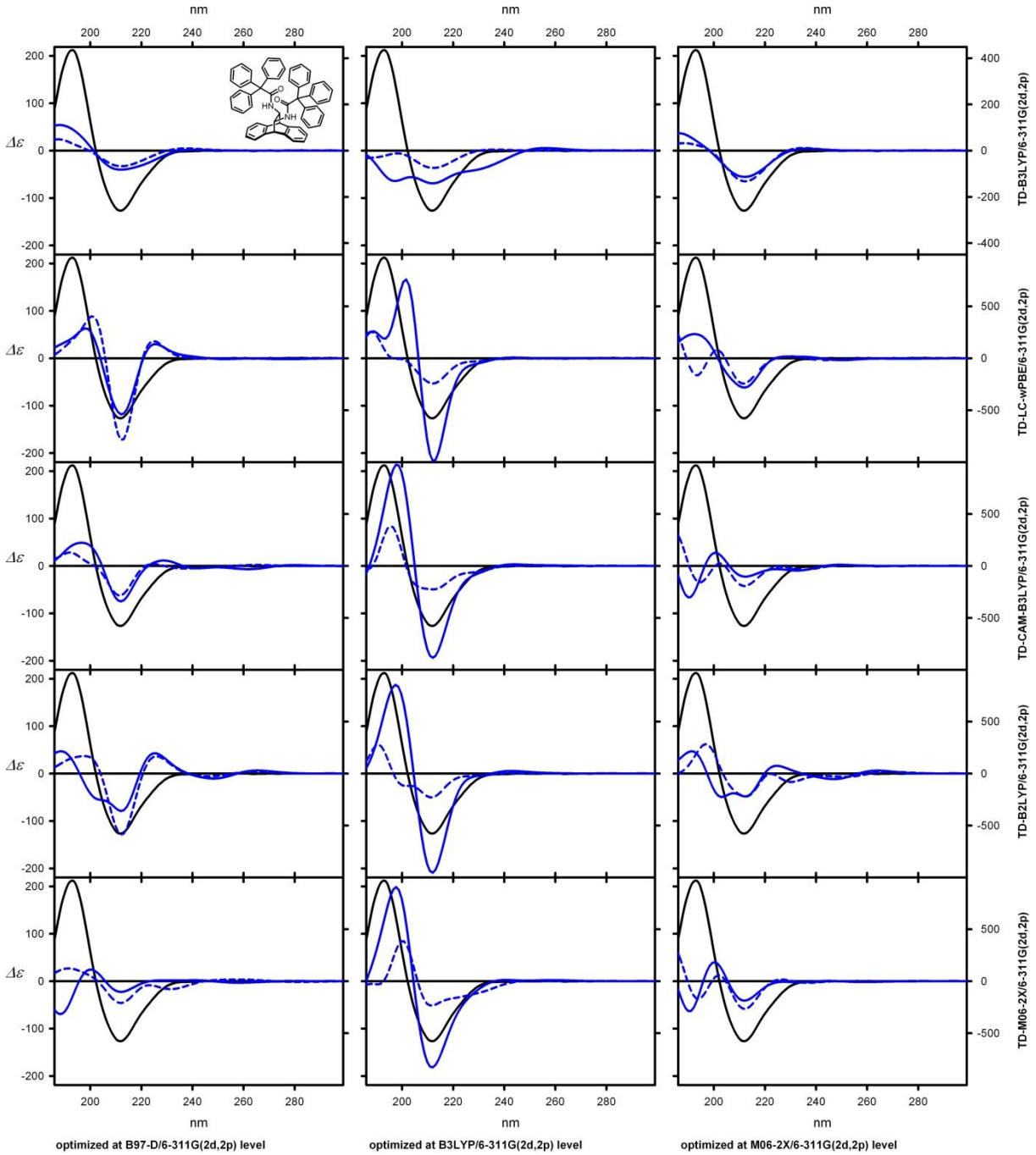


Figure B4. Experimental (solid black lines) and Boltzmann averaged (blue lines) calculated at the TD-DFT/6-311G(2d,2p) level for structures optimized at the DFT/6-311G(2d,2p) levels ECD spectra of triphenylacetamide **5**. All calculated ECD spectra were wavelength corrected.


nm
Δε
TD-B3LYP/6-311G(2d,2p)
TD-LC-wPBE/6-311G(2d,2p)
TD-CAM-B3LYP/6-311G(2d,2p)
TD-B2LYP/6-311G(2d,2p)
TD-M06-2X/6-311G(2d,2p)
optimized at B97-D/6-311G(2d,2p) level
optimized at B3LYP/6-311G(2d,2p) level
optimized at M06-2X/6-311G(2d,2p) level

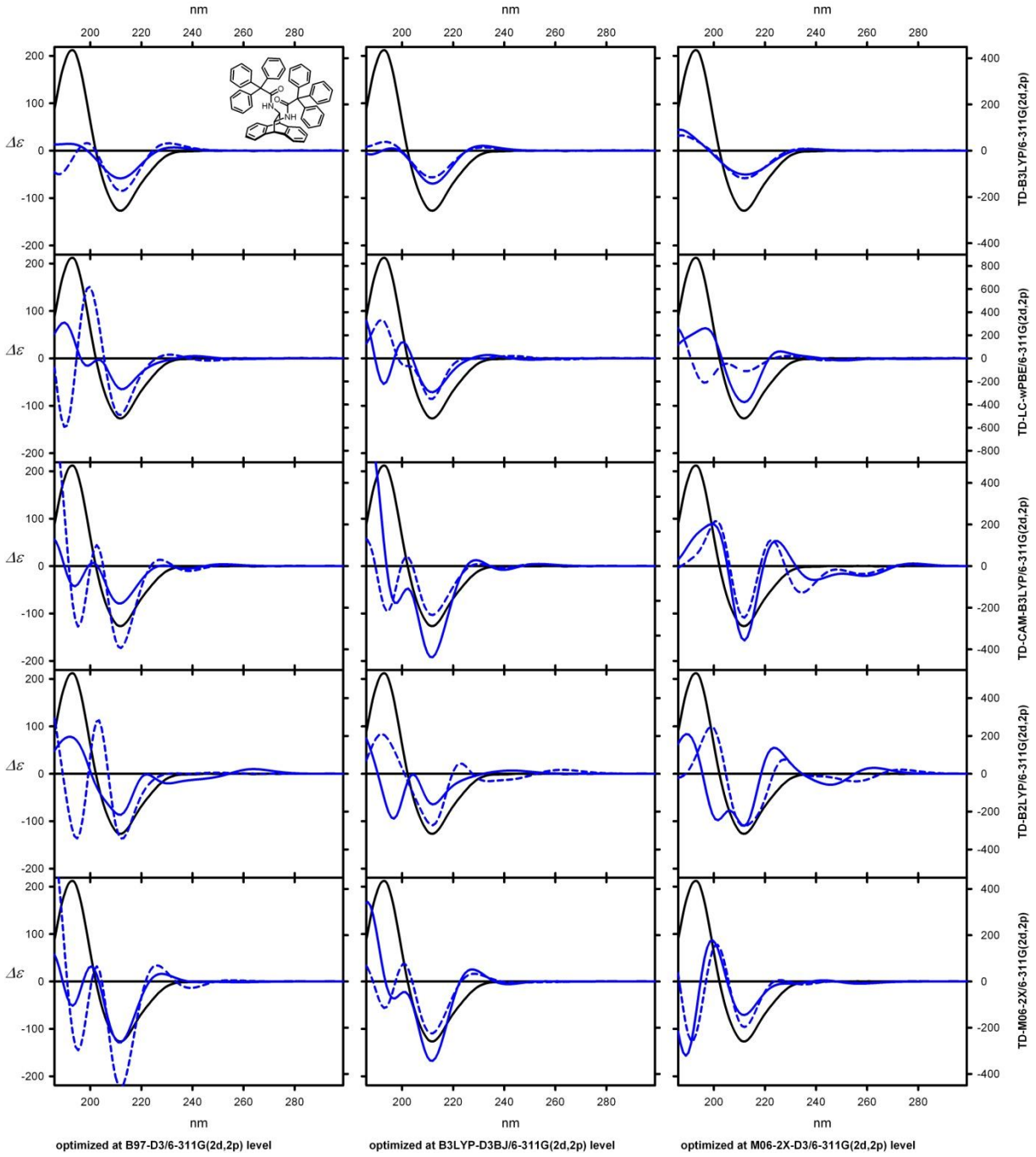
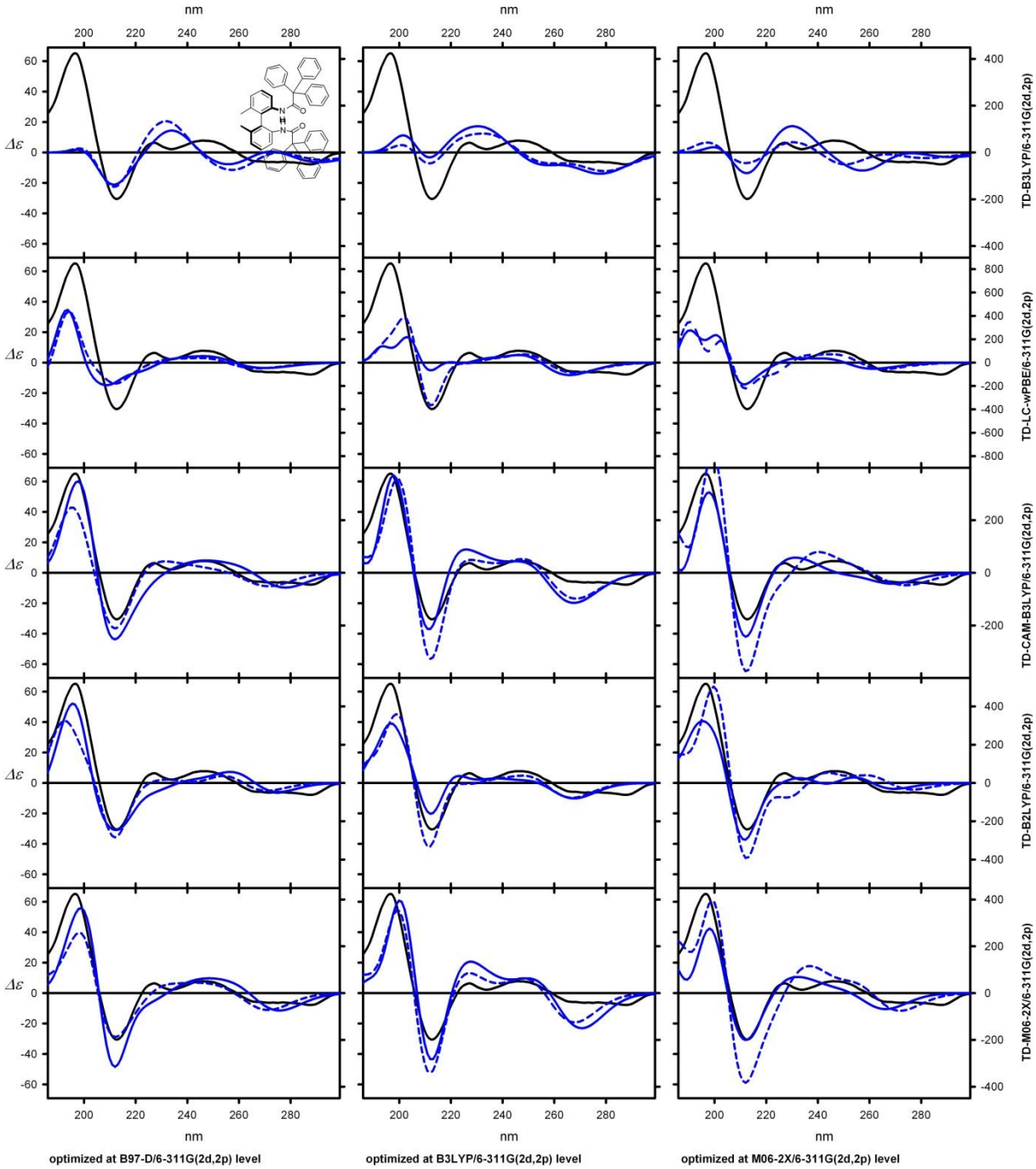


Figure B5. Experimental (solid black lines) and Boltzmann averaged (blue lines) calculated at the TD-DFT/6-311G(2d,2p) level for structures optimized at the DFT/6-311G(2d,2p) levels ECD spectra of triphenylacetamide **6**. All calculated ECD spectra were wavelength corrected.


nm
200 220 240 260 280
Δε
TD-B3LYP/6-311G(2d,2p)
TD-LC-wPBE/6-311G(2d,2p)
TD-CAM-B3LYP/6-311G(2d,2p)
TD-B2LYP/6-311G(2d,2p)
TD-M06-2X/6-311G(2d,2p)
optimized at B97-D/6-311G(2d,2p) level
optimized at B3LYP/6-311G(2d,2p) level
optimized at M06-2X/6-311G(2d,2p) level

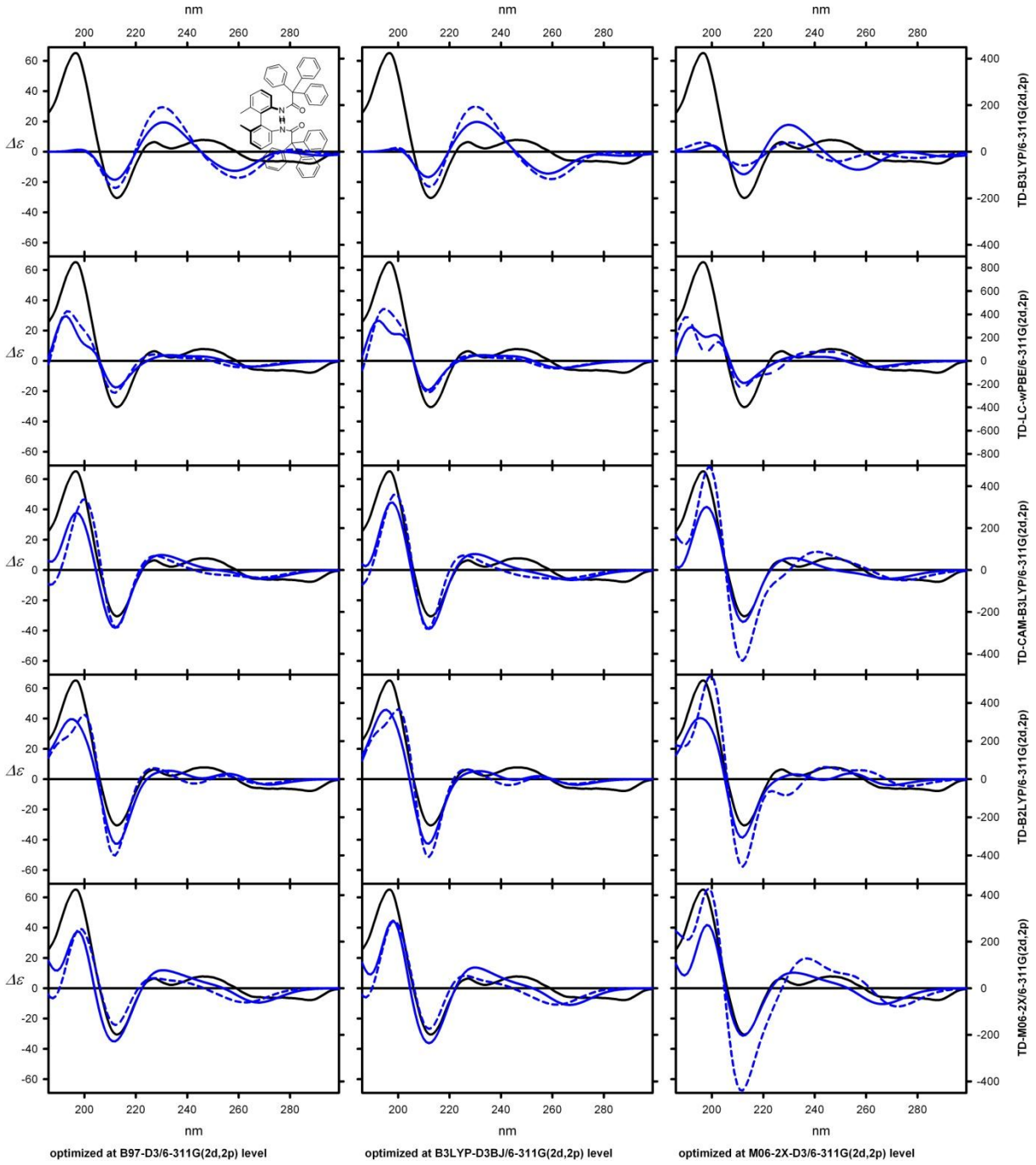
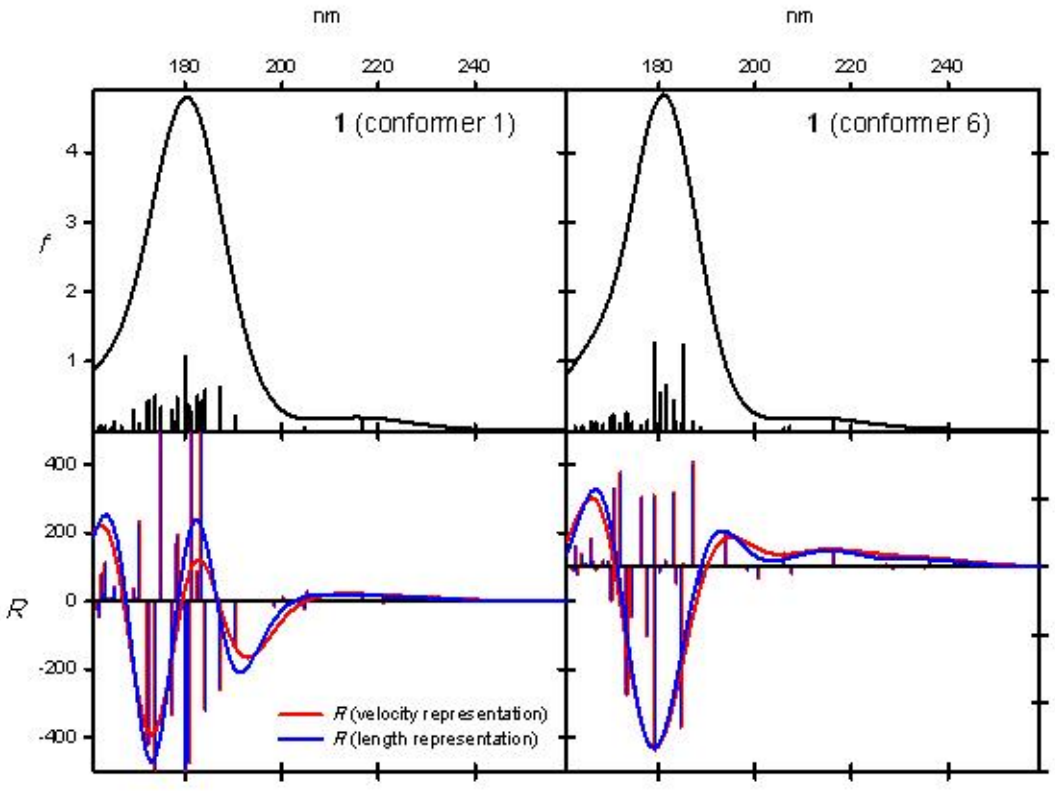
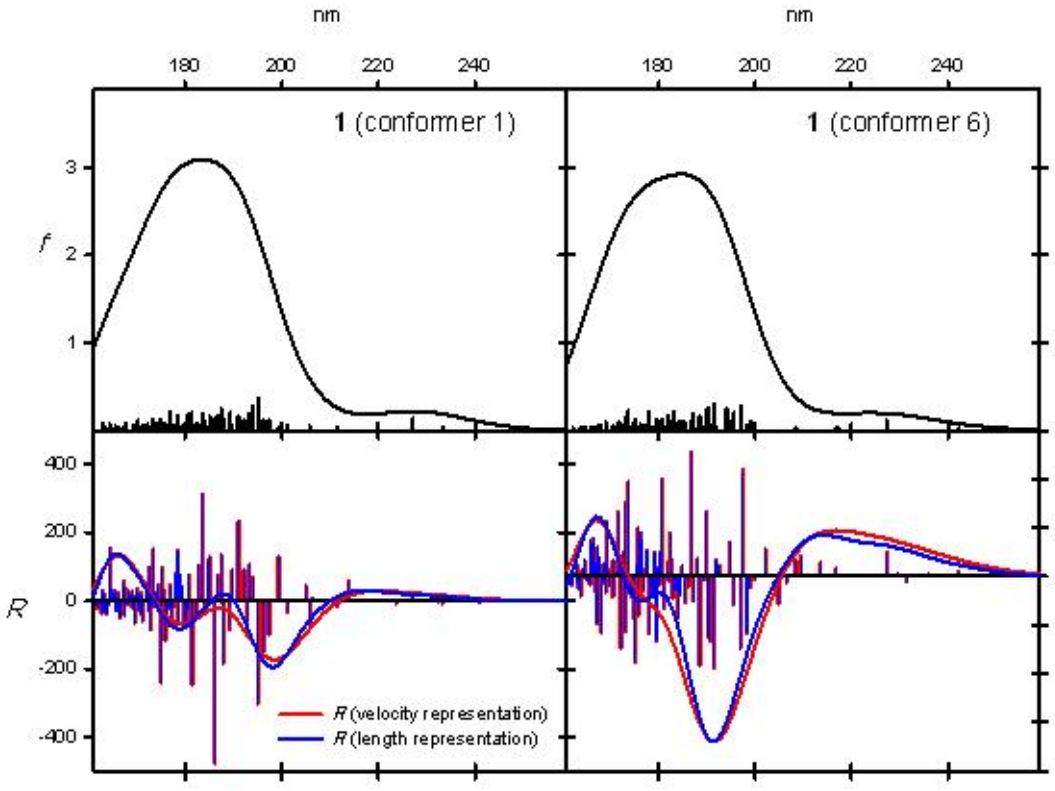


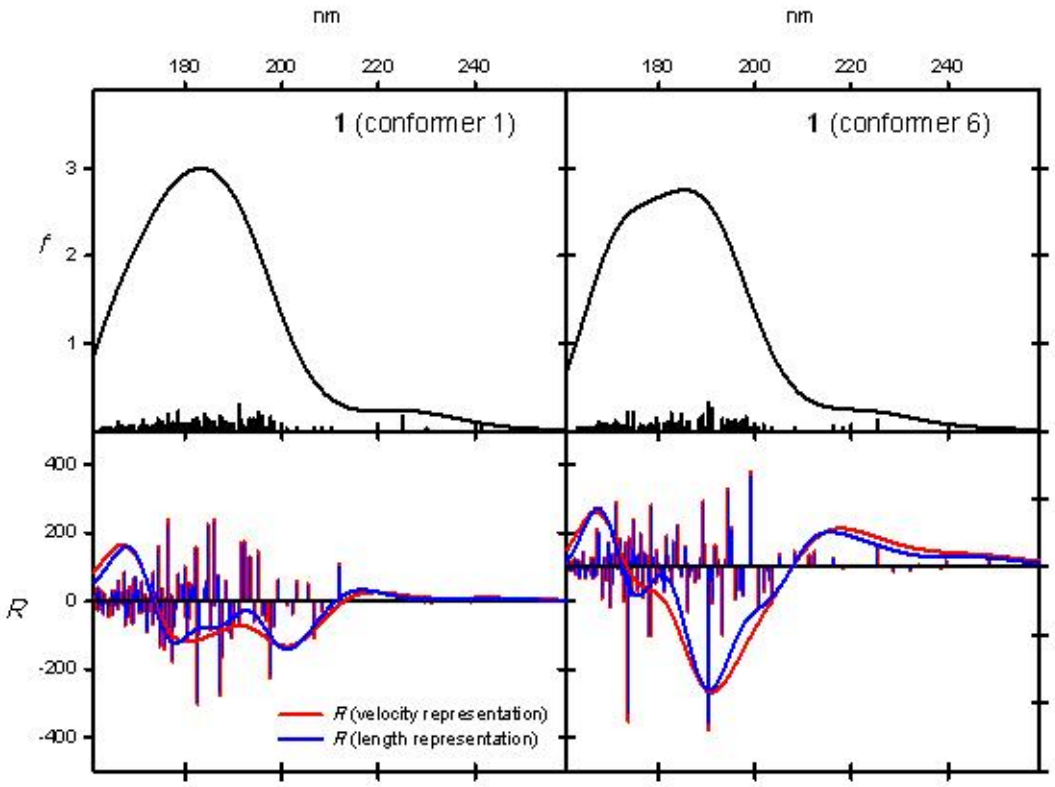
Figure B6. Experimental (solid black lines) and Boltzmann averaged (blue lines) calculated at the TD-DFT/6-311G(2d,2p) level for structures optimized at the DFT/6-311G(2d,2p) levels ECD spectra of triphenylacetamide **7**. All calculated ECD spectra were wavelength corrected.



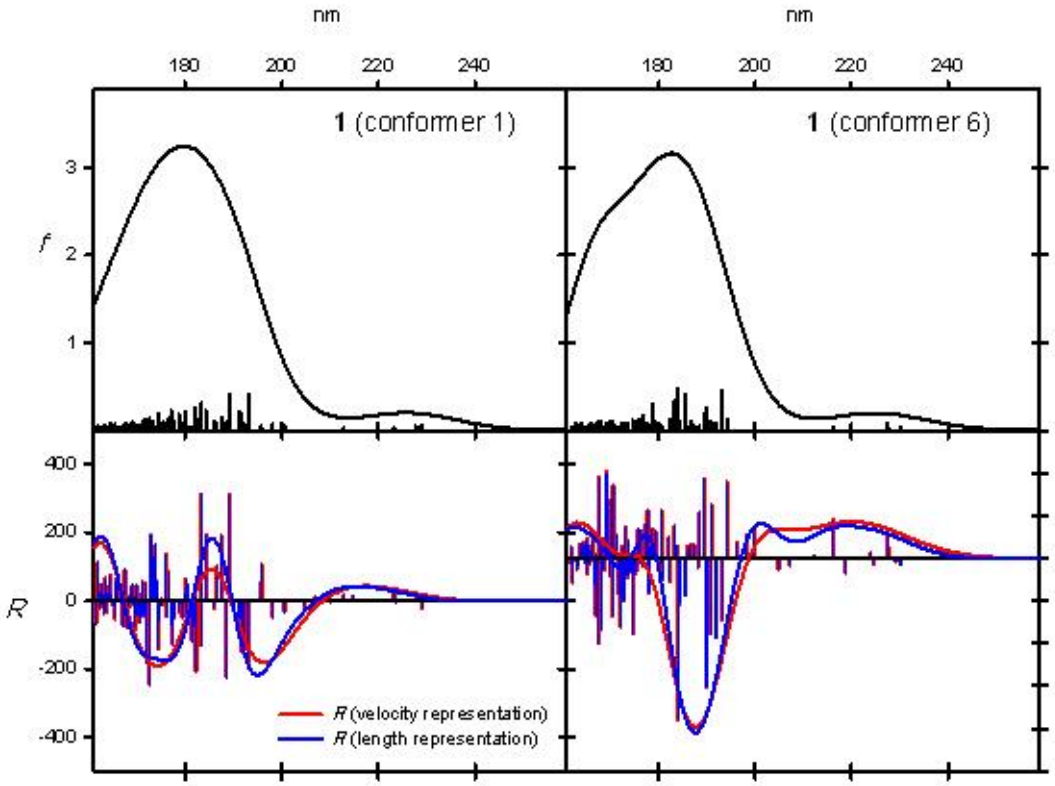
TD-LC-wPBE/6-311G(2d,2p)//B97-D/6-311G(2d,2p)



TD-CAM-B3LYP/6-311G(2d,2p)//B97-D/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B97-D/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B97-D/6-311G(2d,2p)

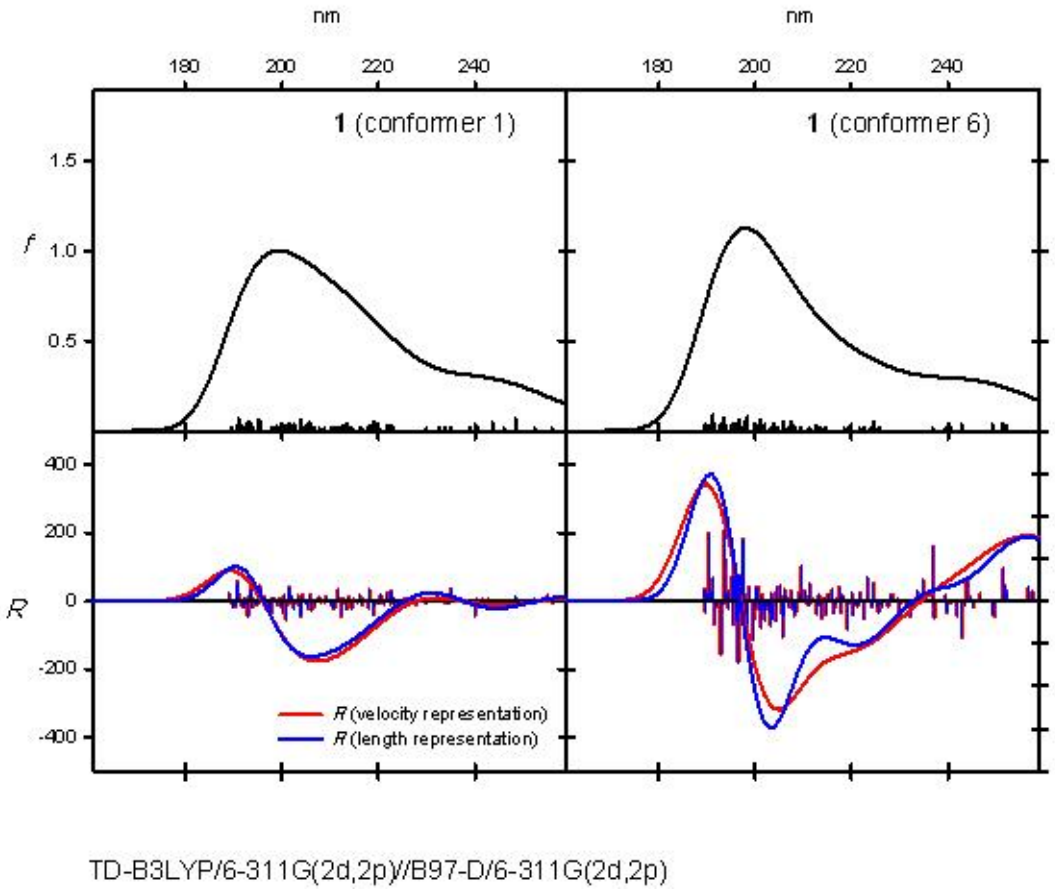
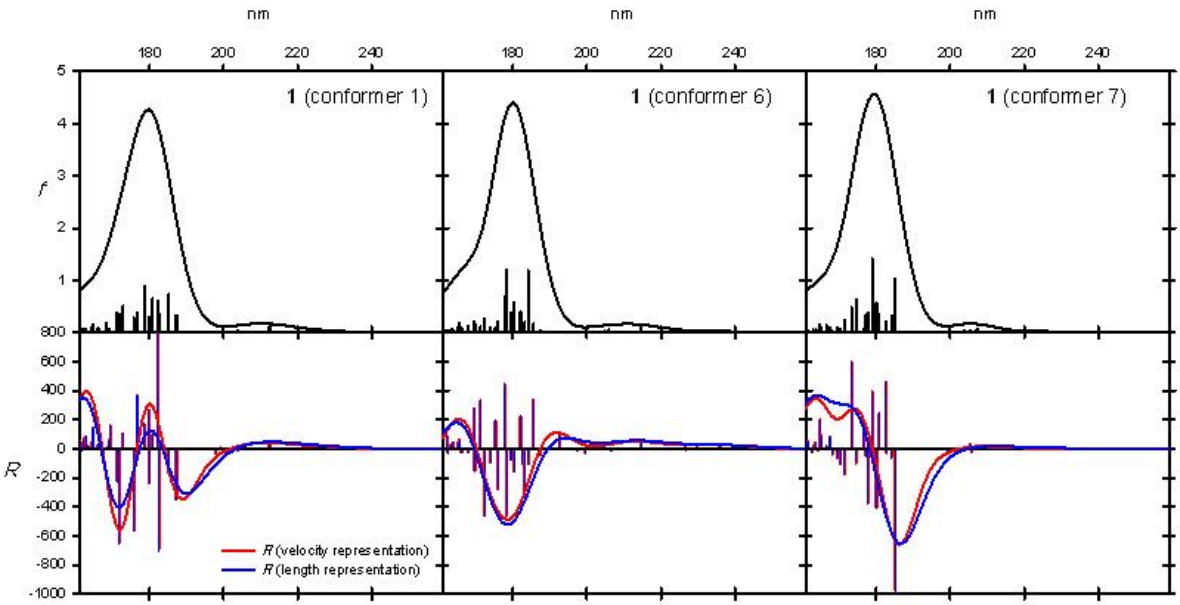
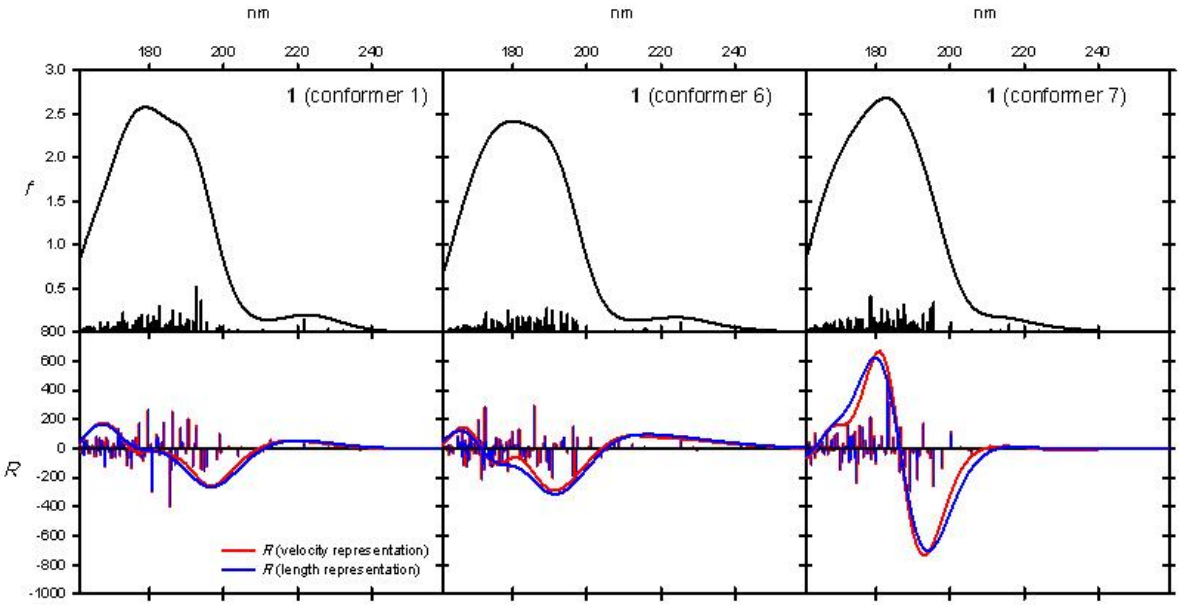


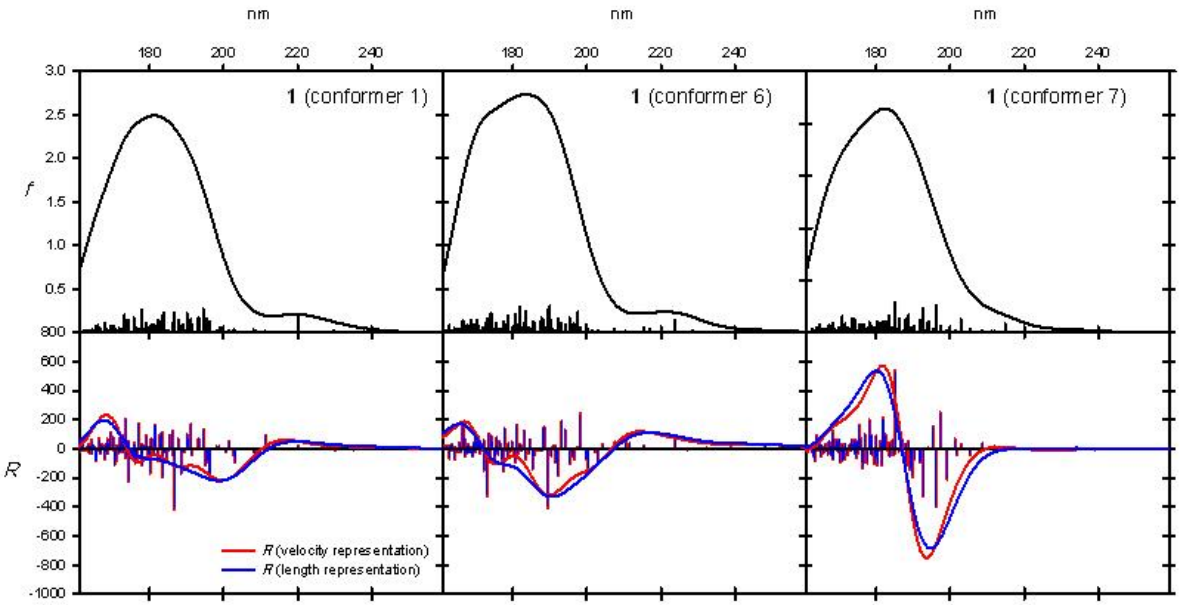
Figure C1. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **1** optimized at the B97-D/6-311G(2d,2p) level. Wavelengths were not corrected.



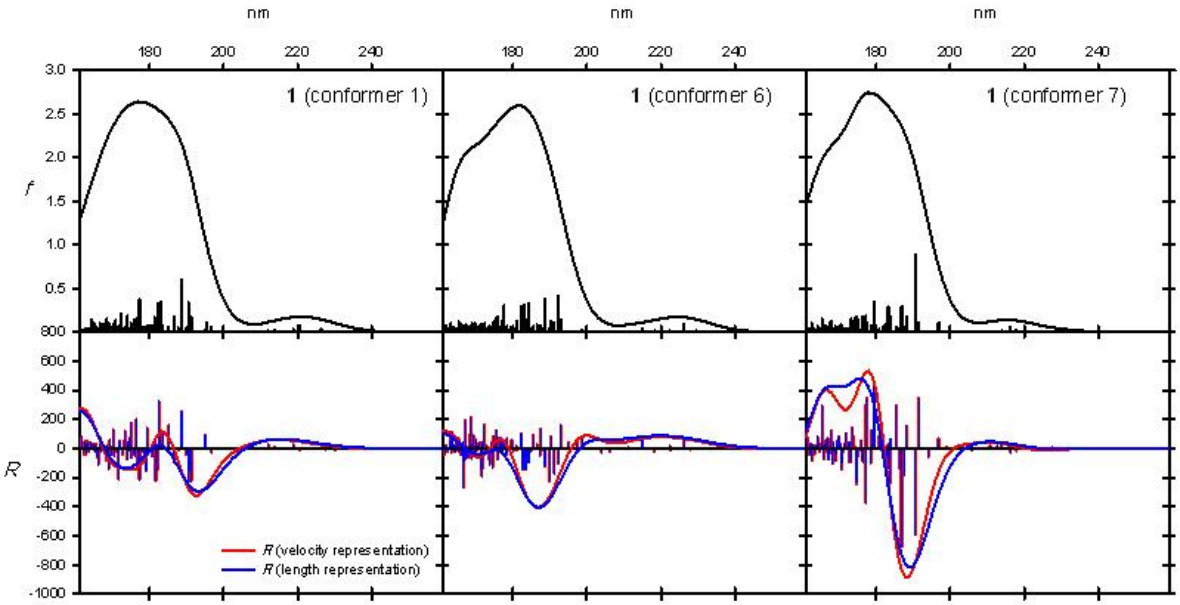
TD-LC-wPBE/6-311G(2d,2p)//B97D3/6-311G(2d,2p)



TD-CAM-B3LYP/6-311G(2d,2p)//B97D3/6-311G(2d,2p)



TD-M062X/6-311G(2d,2p)//B97D3/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B97D3/6-311G(2d,2p)

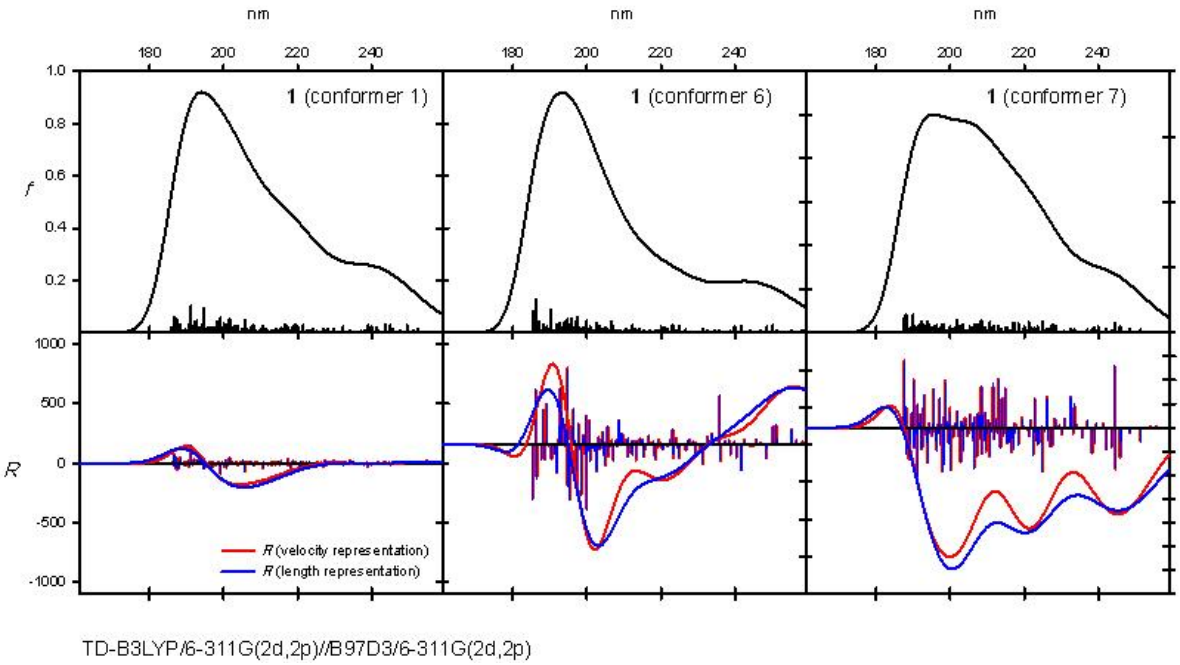
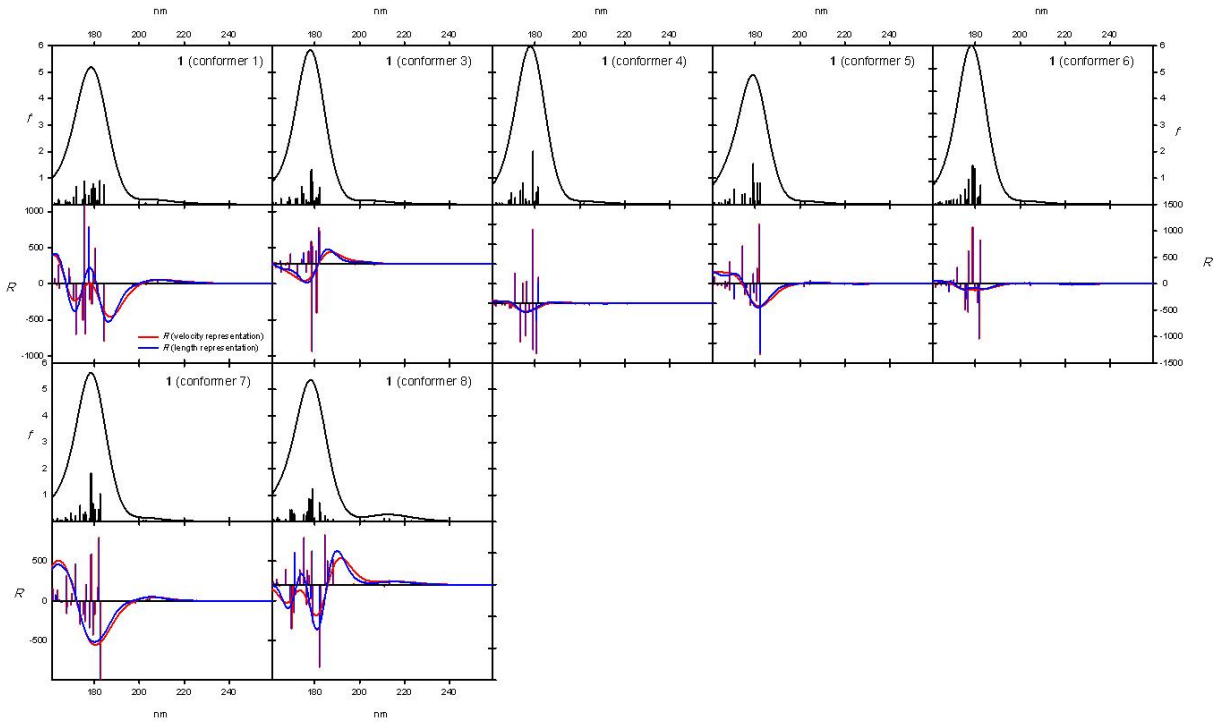
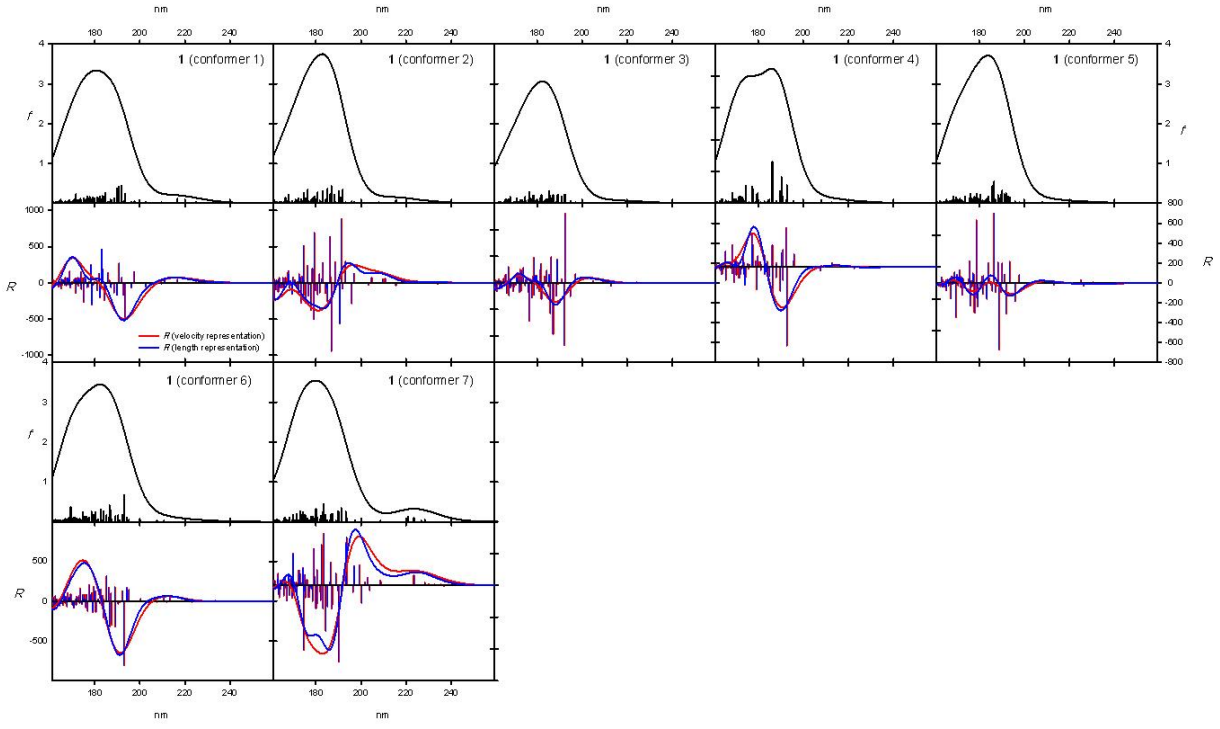


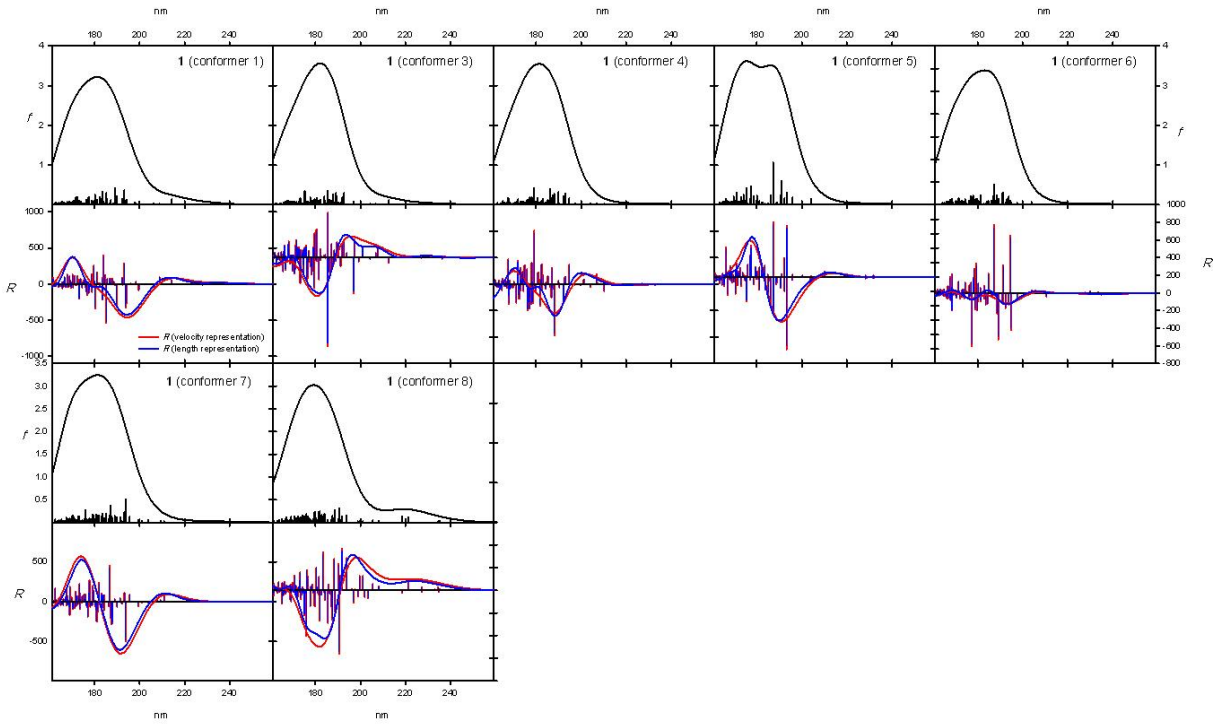
Figure C2. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **1** optimized at the B97-D3/6-311G(2d,2p) level. Wavelengths were not corrected.



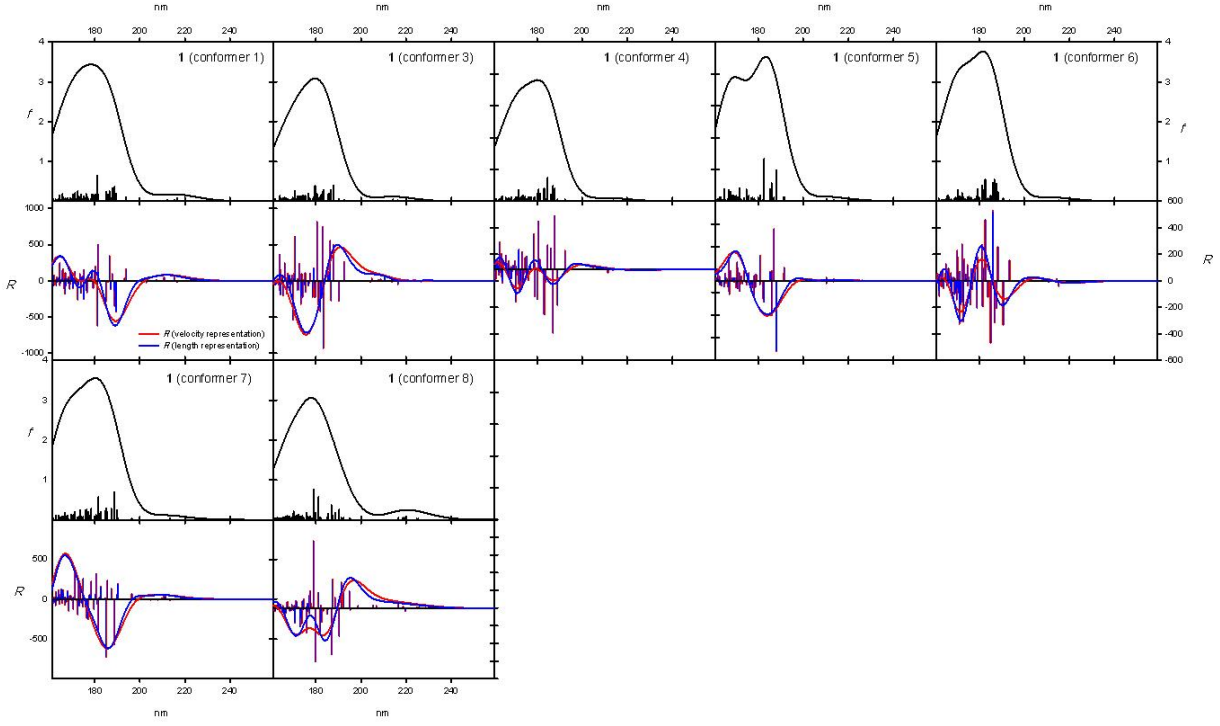
TD-LC-wPBE/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-CAM-B3LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)

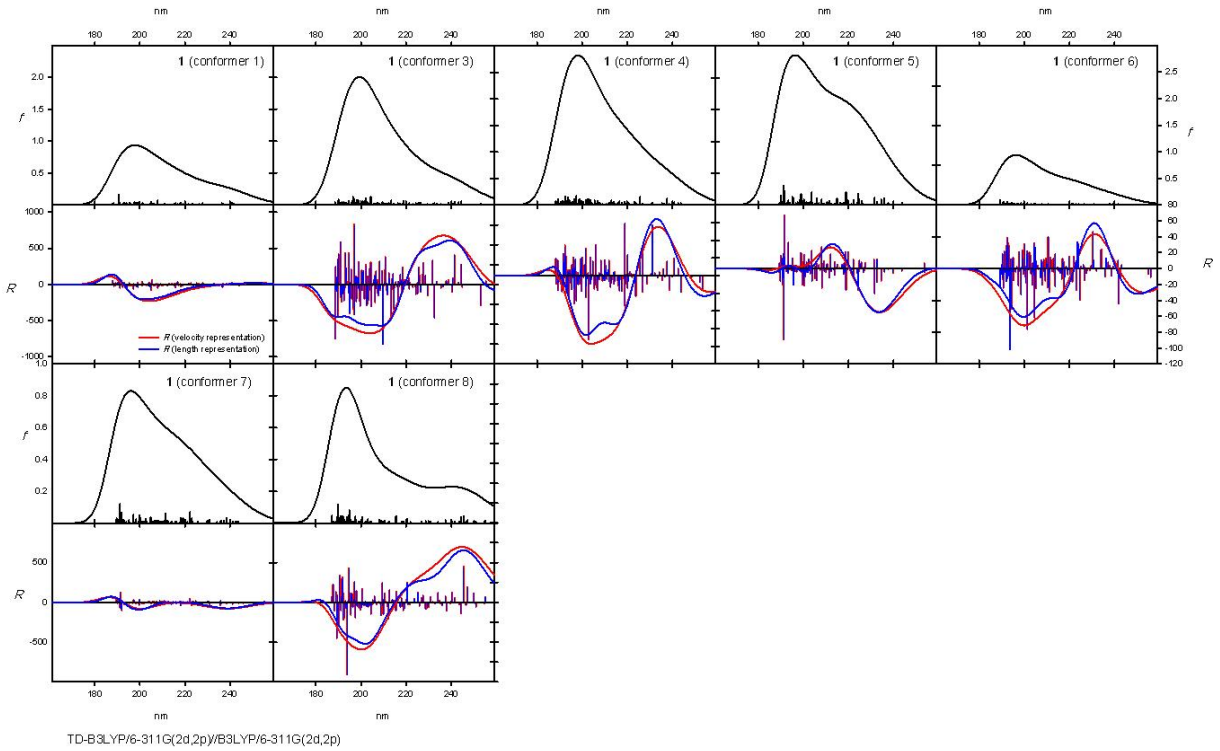
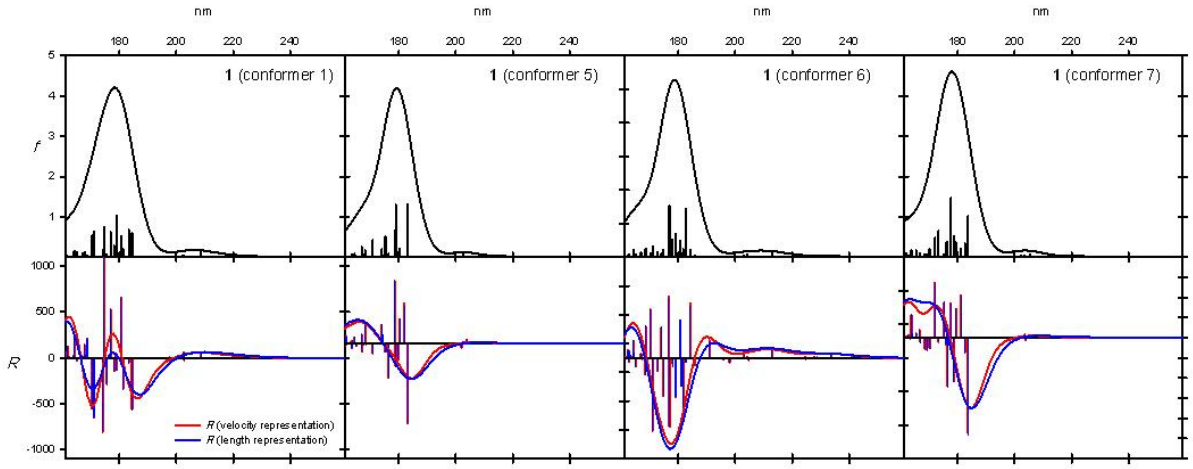
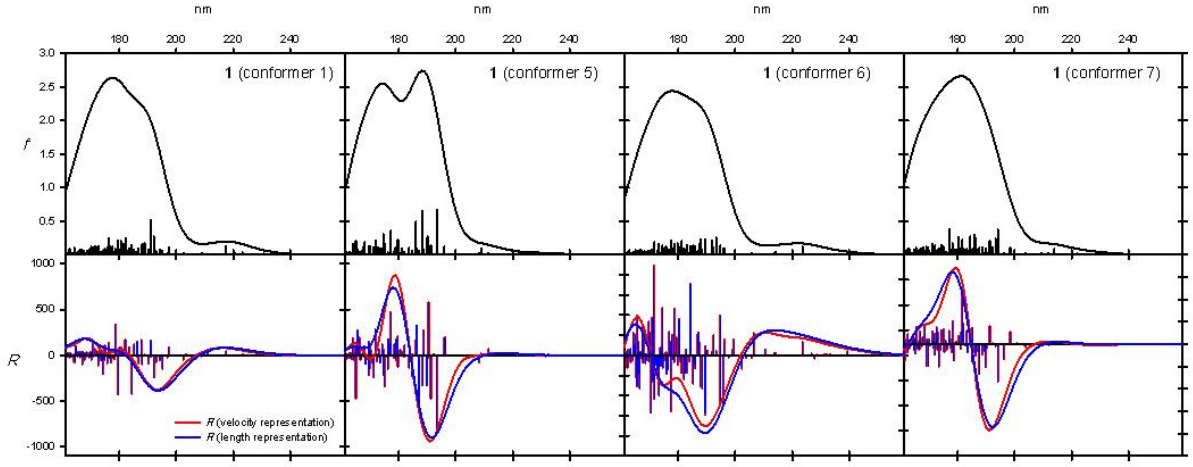


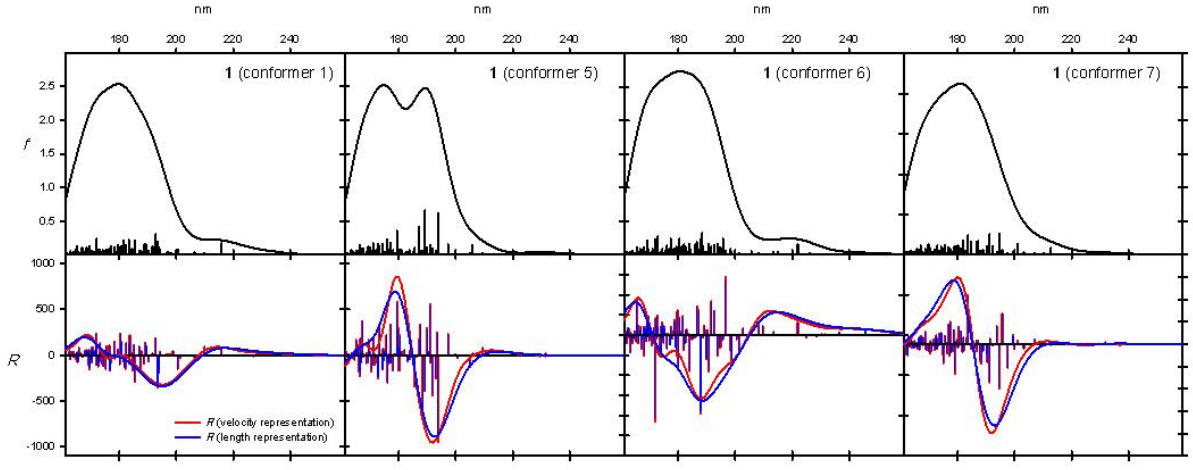
Figure C3. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **1** optimized at the B3LYP/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-LC-wPBE/6-311G(2d,2p)//B3LYP-D3BJ/6-311G(2d,2p)



TD-CAM-B3LYP/6-311G(2d,2p)//B3LYP-D3BJ/6-311G(2d,2p)



TD-M062X/6-311G(2d,2p)//B3LYP-D3BJ/6-311G(2d,2p)

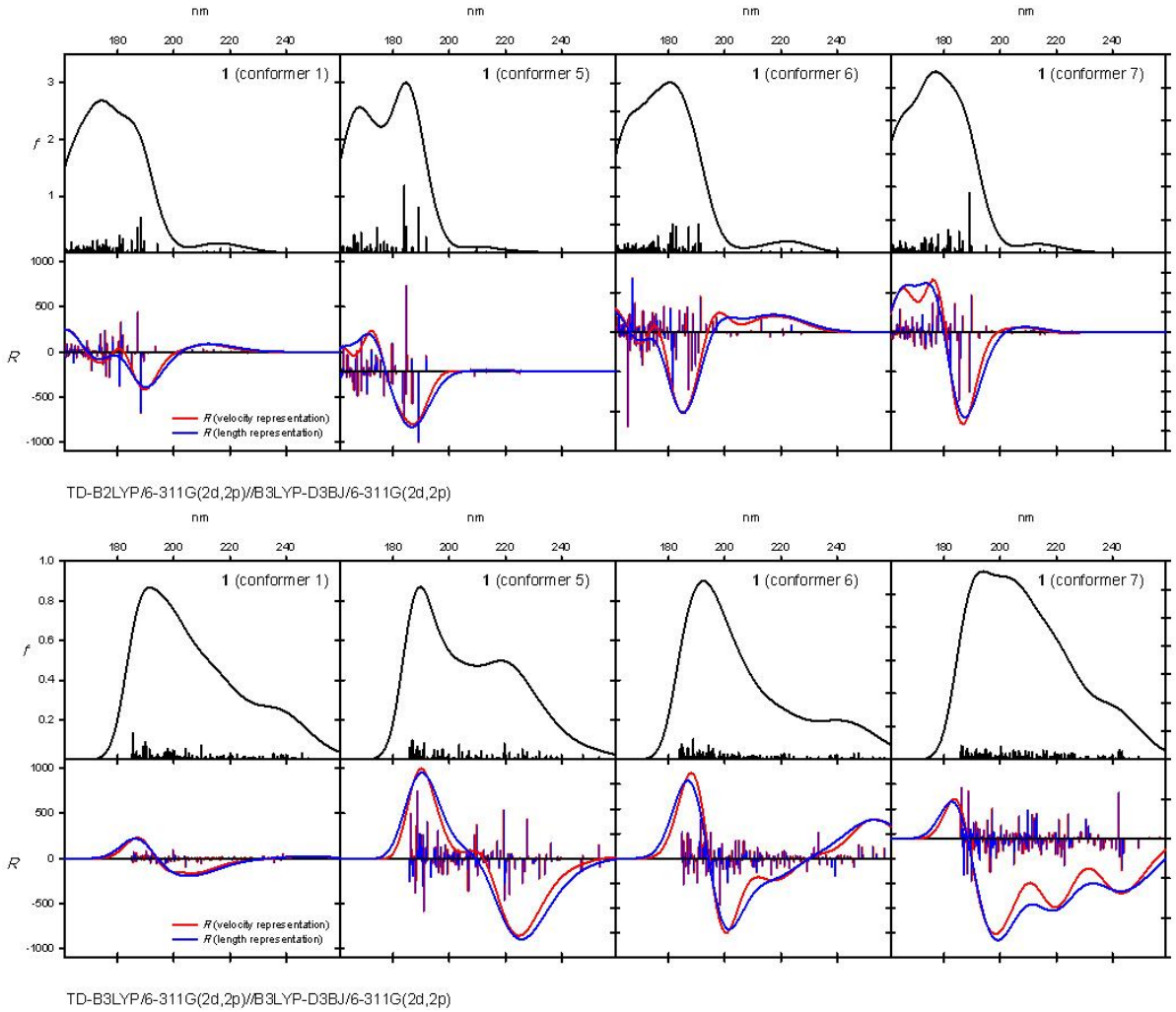
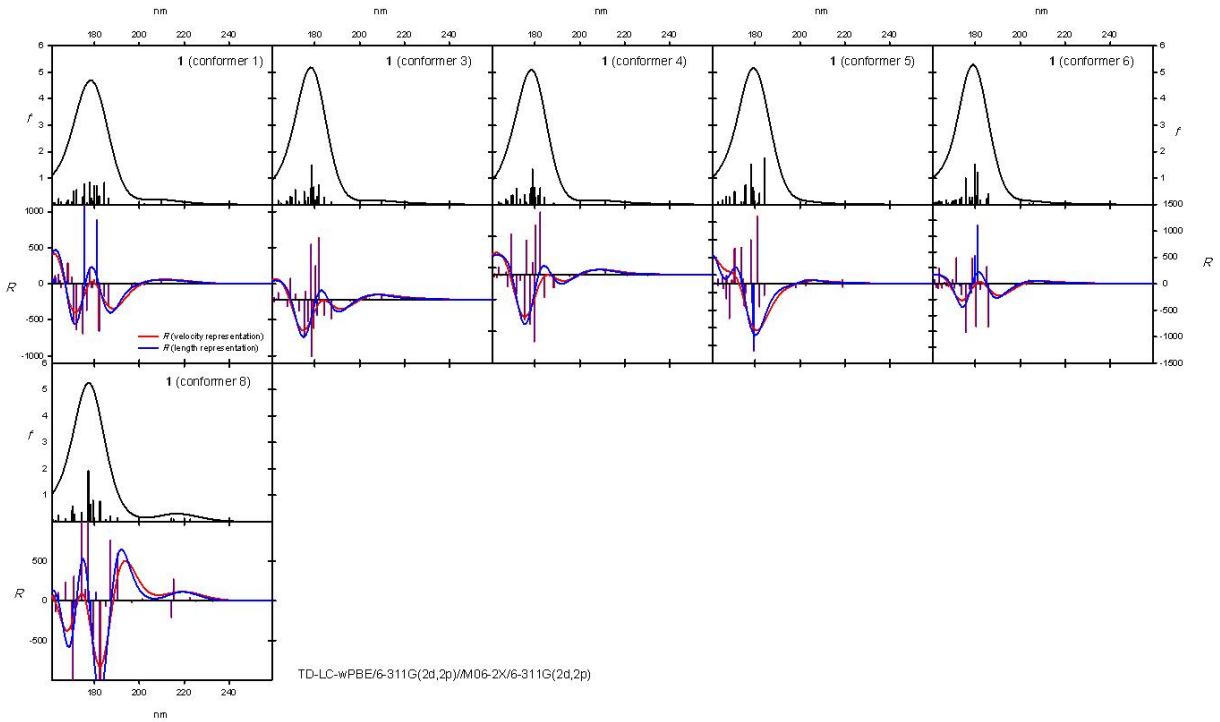
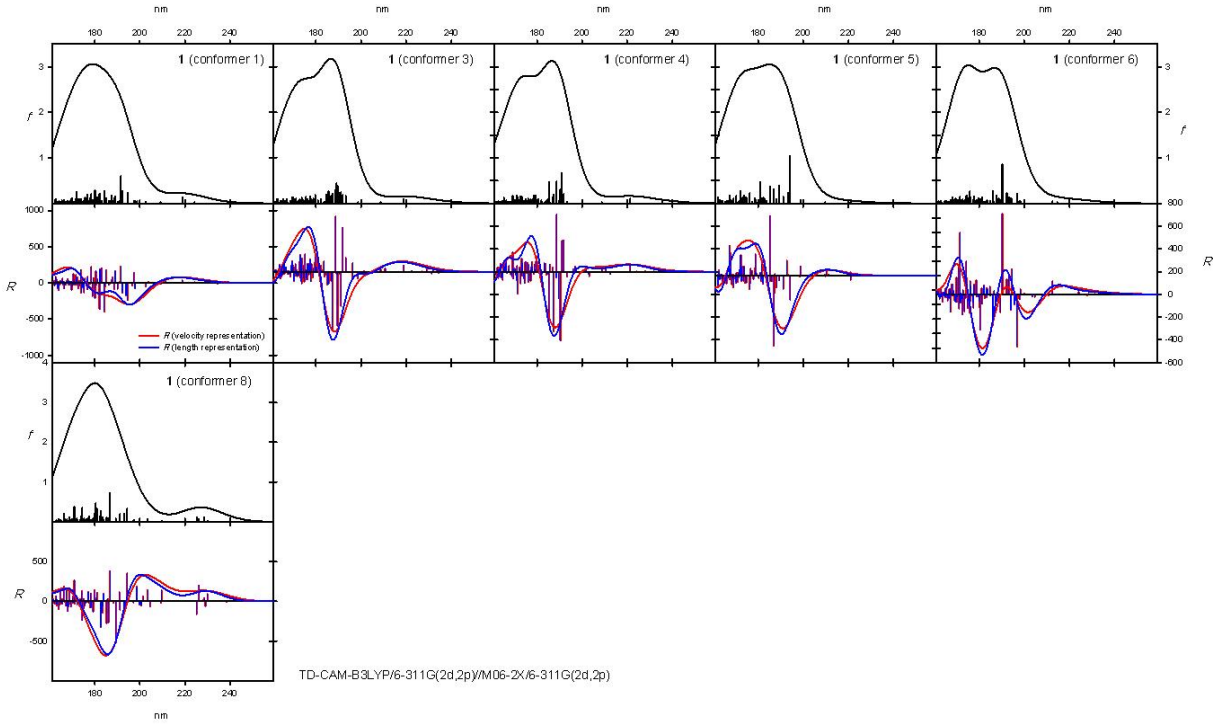
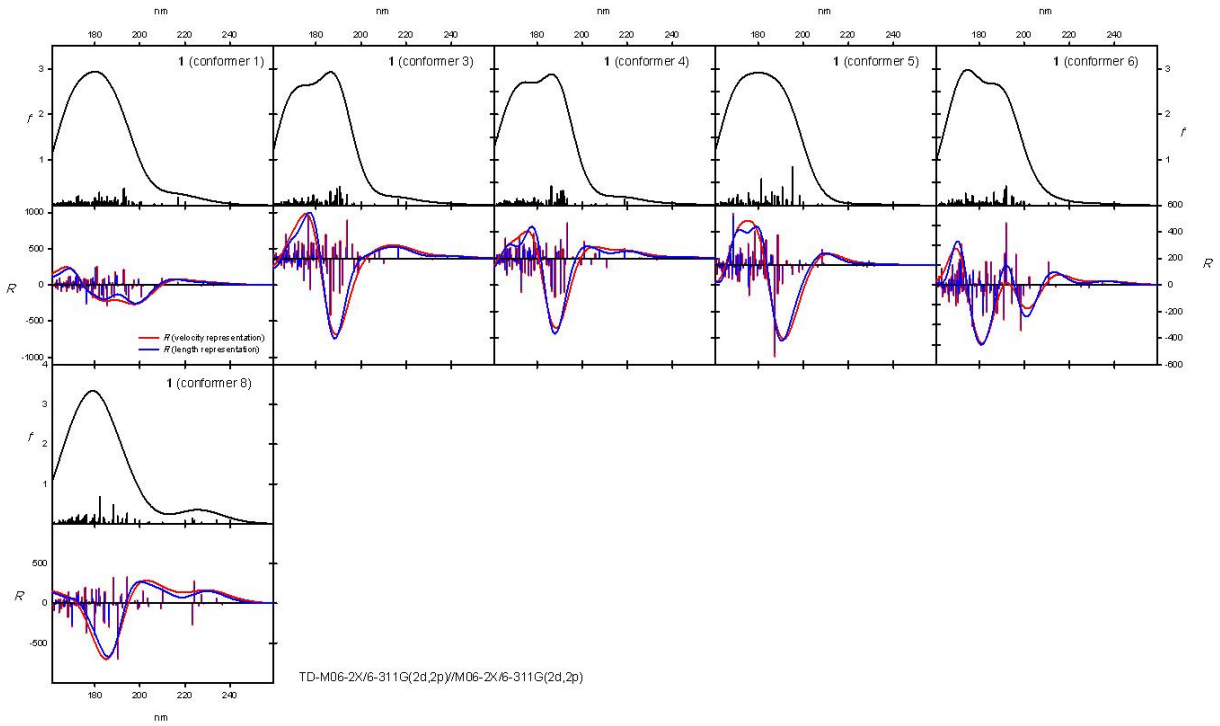
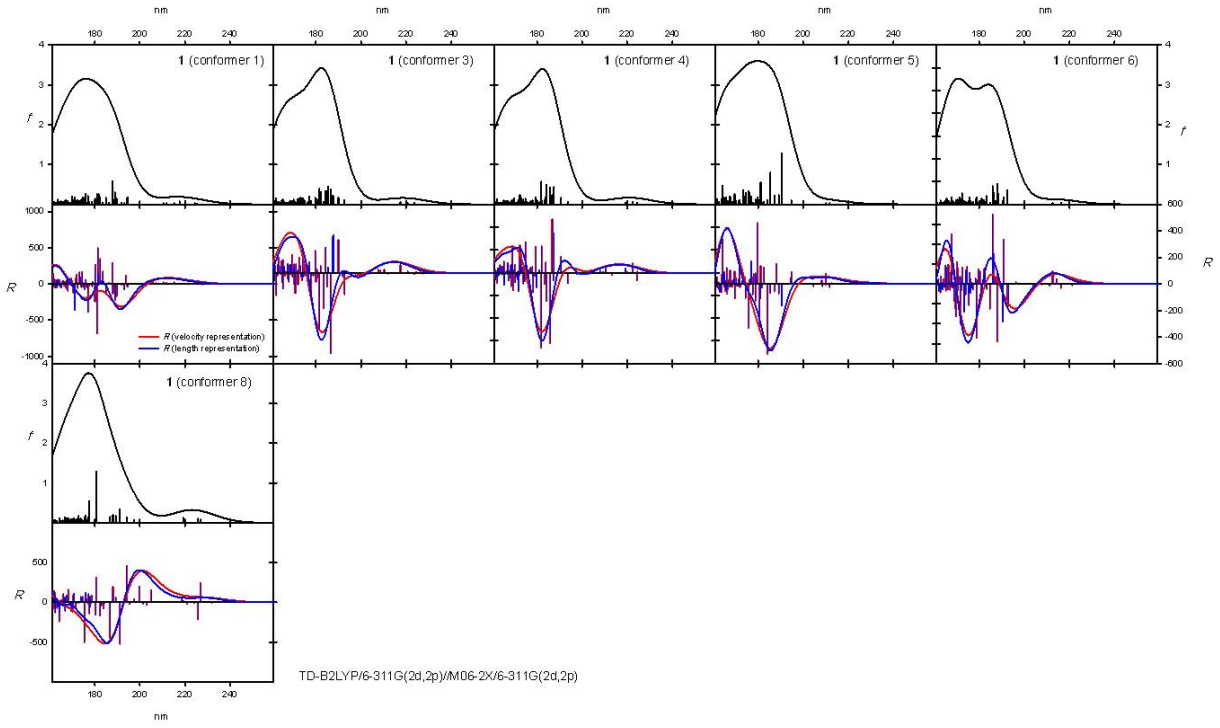


Figure C4. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **1** optimized at the B3LYP-GD3BJ/6-311G(2d,2p) level. Wavelengths were not corrected.


1 (conformer 1)
1 (conformer 3)
1 (conformer 4)
1 (conformer 5)
1 (conformer 6)
1 (conformer 8)
R (velocity representation)
R (length representation)
nm
f
R
TD-LC-wPBE/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)


1 (conformer 1)
1 (conformer 3)
1 (conformer 4)
1 (conformer 5)
1 (conformer 6)
1 (conformer 8)
R (velocity representation)
R (length representation)
nm
f
R
TD-CAM-B3LYP/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)


1 (conformer 1)
1 (conformer 3)
1 (conformer 4)
1 (conformer 5)
1 (conformer 6)
1 (conformer 8)
R (velocity representation)
R (length representation)
nm
f
R
TD-M06-2X/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)


1 (conformer 1)
1 (conformer 3)
1 (conformer 4)
1 (conformer 5)
1 (conformer 6)
1 (conformer 8)
R (velocity representation)
R (length representation)
nm
f
R
TD-B2LYP/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)

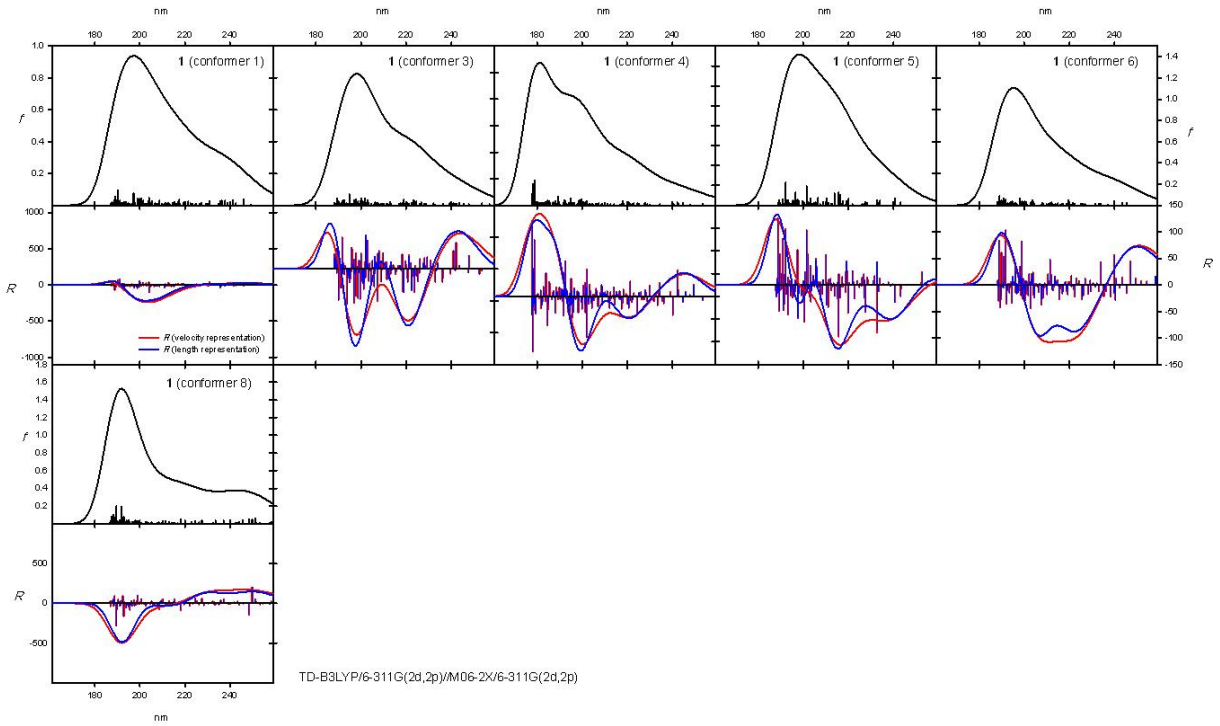
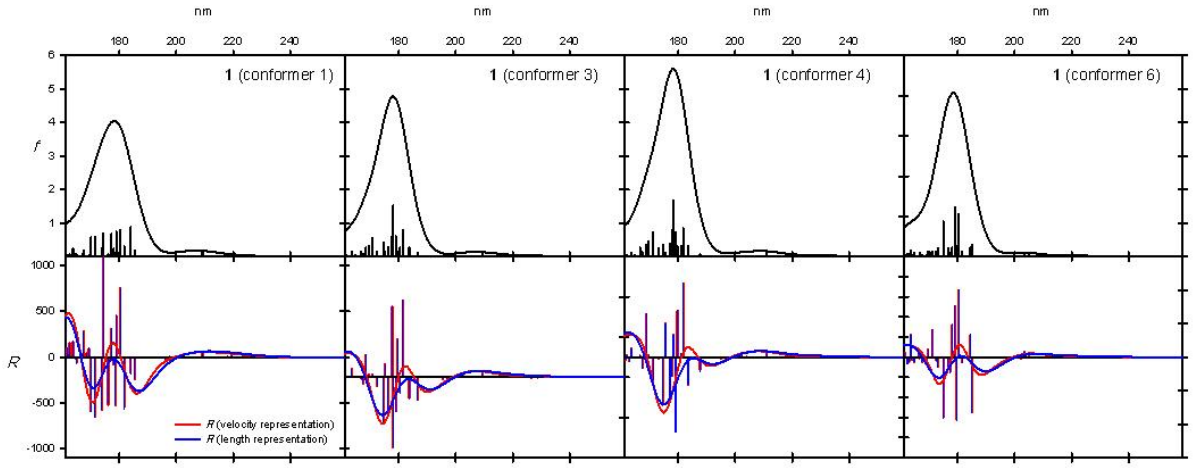
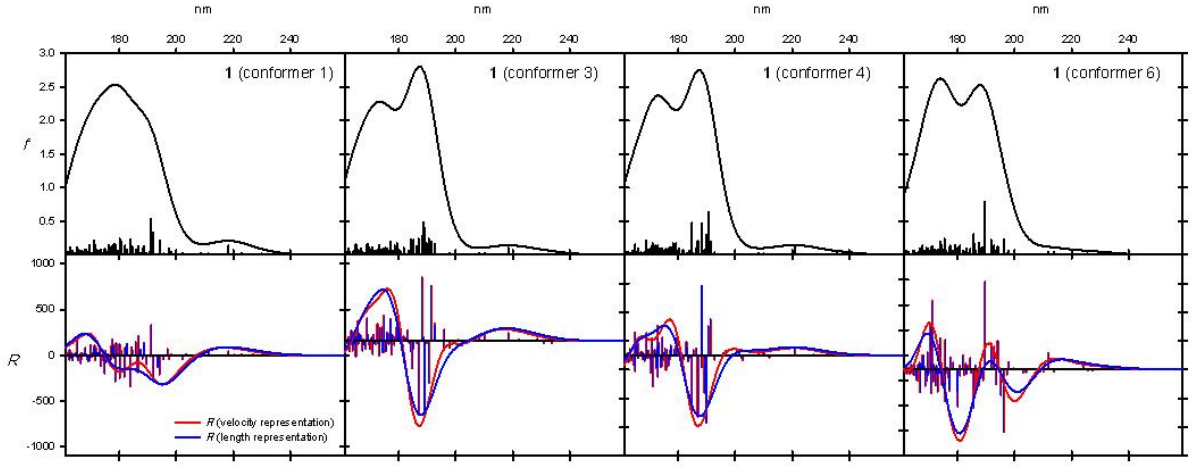


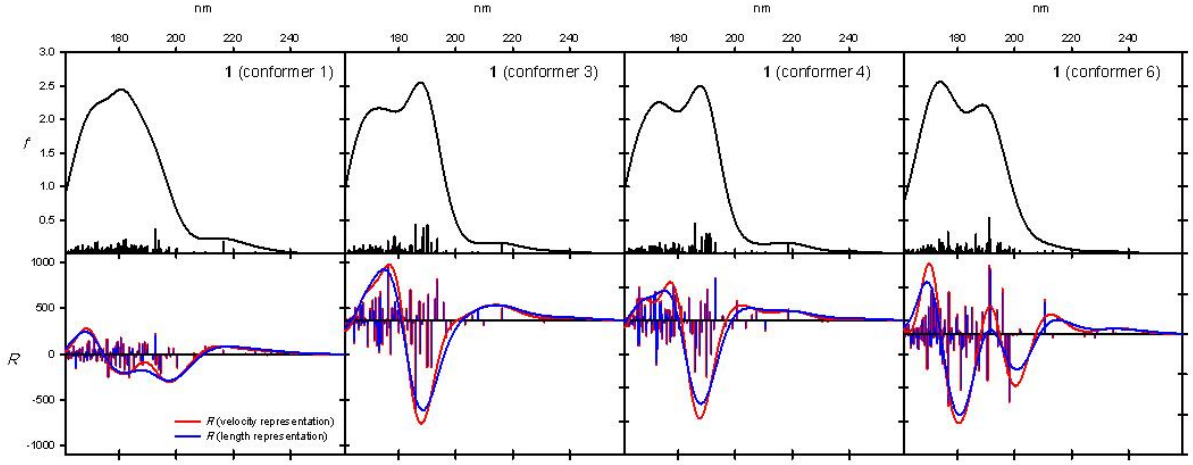
Figure C5. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **1** optimized at the M06-2X/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-LC-wPBE/6-311G(2d,2p)//M062X-D3/6-311G(2d,2p)



TD-CAM-B3LYP/6-311G(2d,2p)//M062X-D3/6-311G(2d,2p)



TD-M062X/6-311G(2d,2p)//M062X-D3/6-311G(2d,2p)

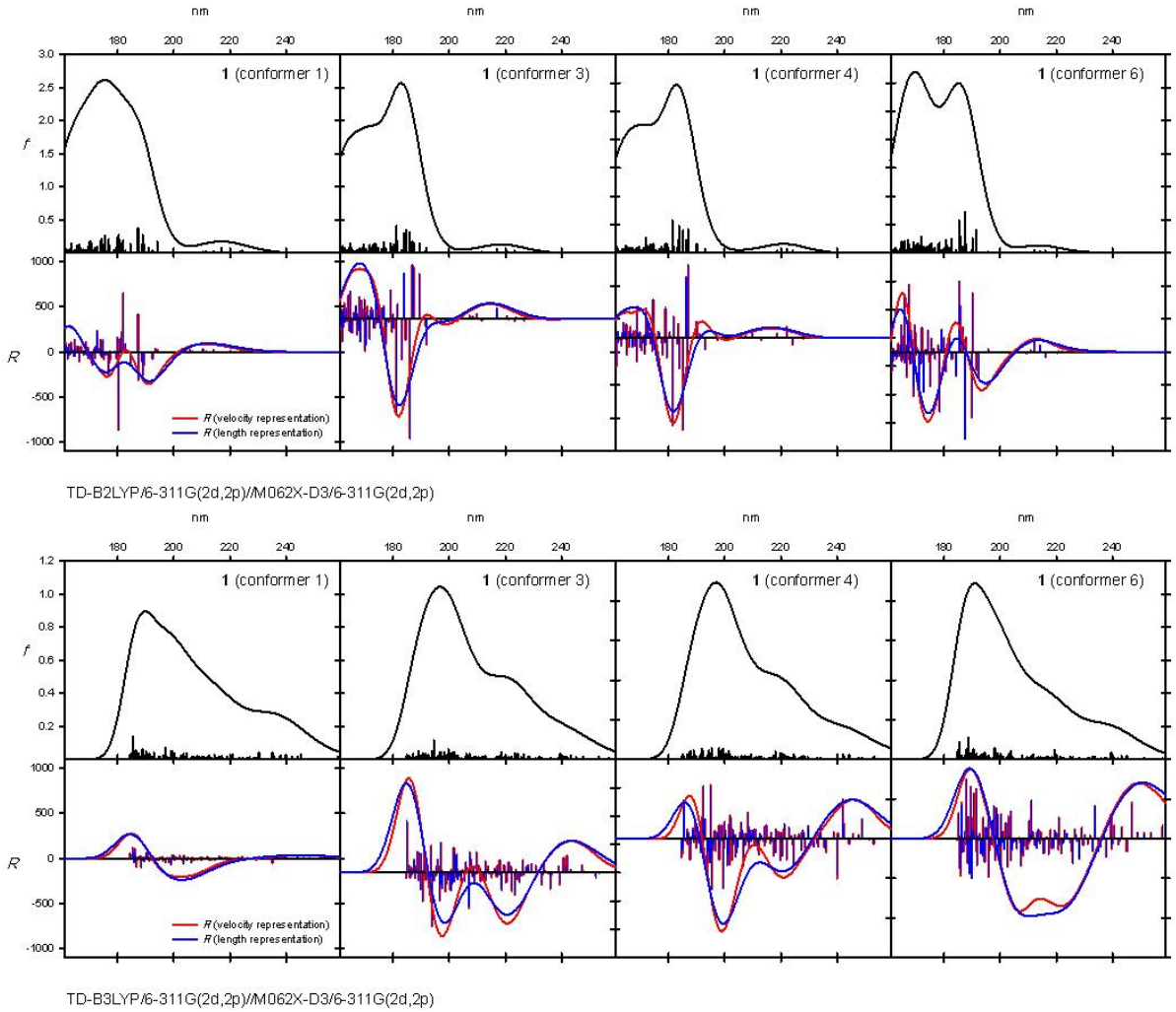
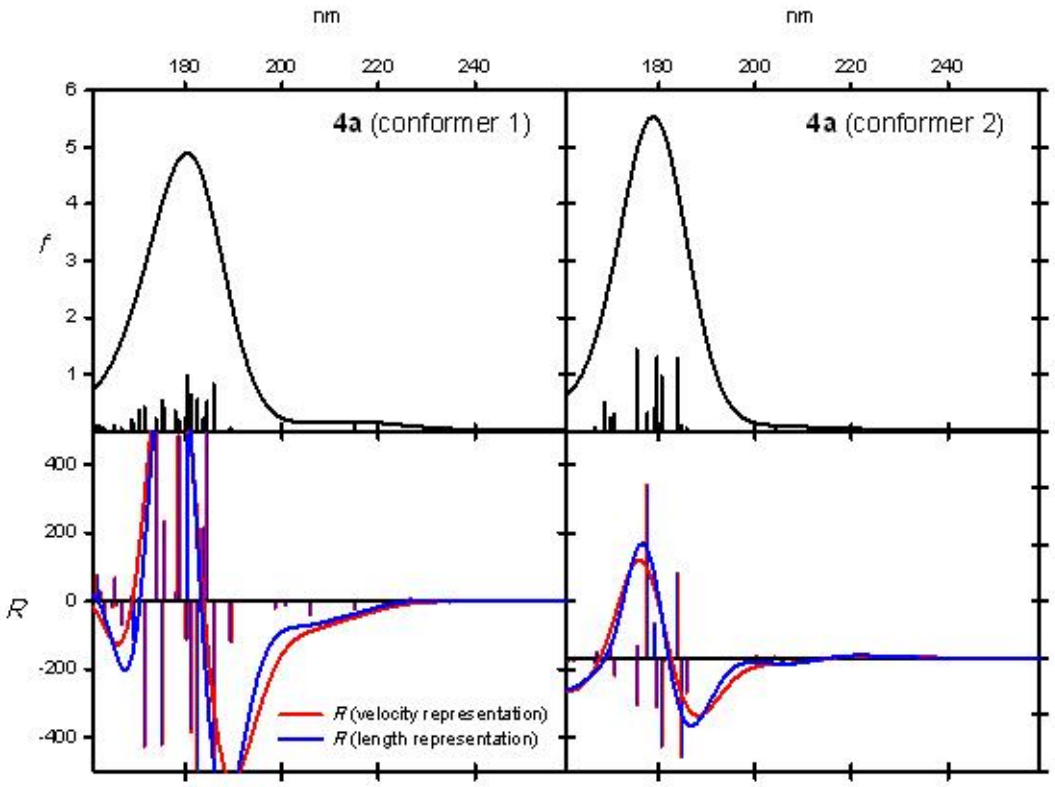
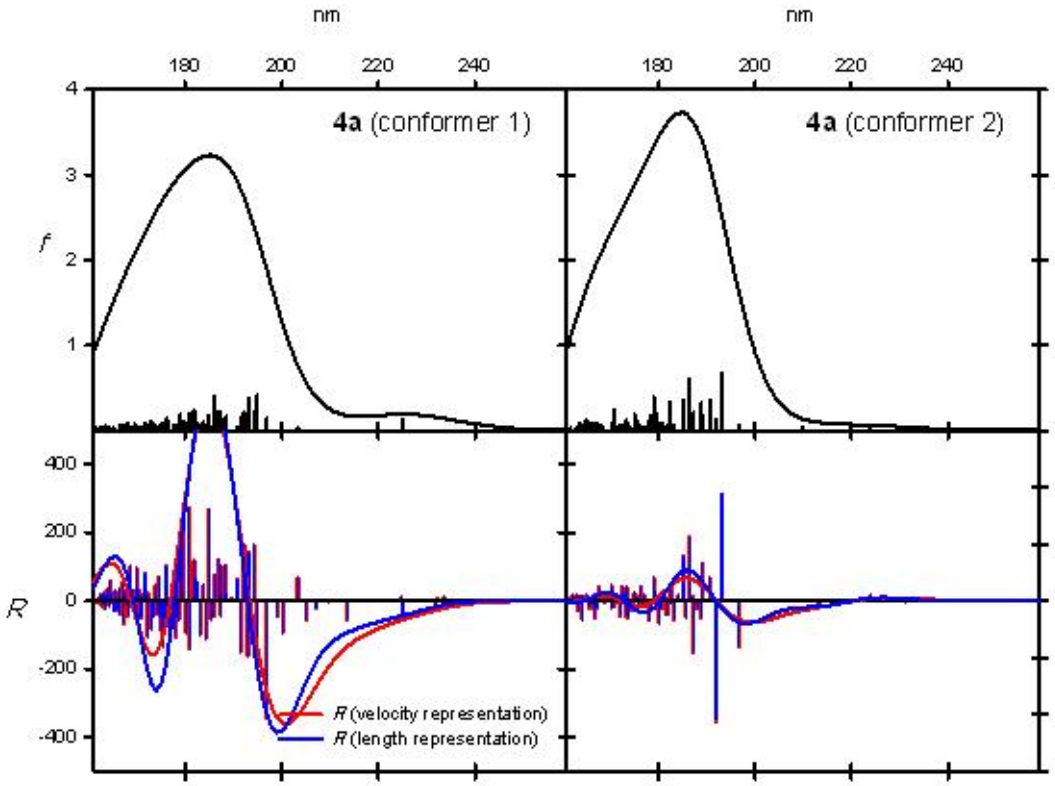


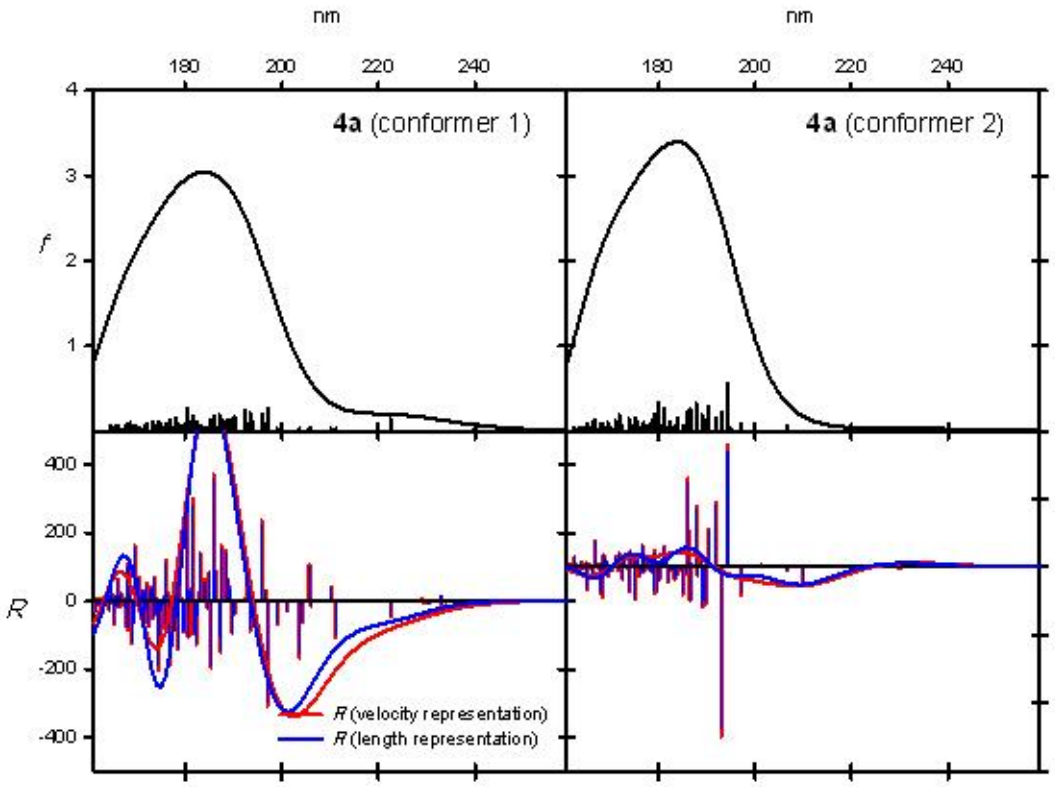
Figure C6. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **1** optimized at the M06-2X-D3/6-311G(2d,2p) level. Wavelengths were not corrected.



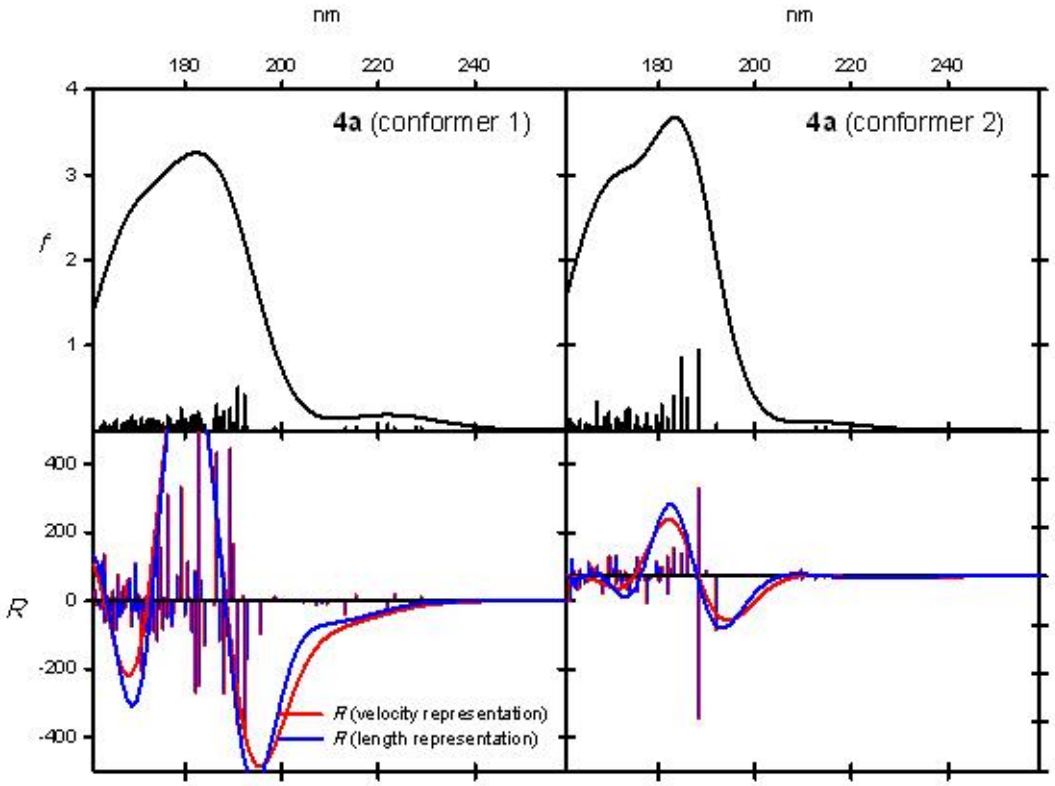
TD-LC-wPBE/6-311G(2d,2p)//B97-D/6-311G(2d,2p)



TD-CAM-B3LYP/6-311G(2d,2p)//B97-D/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B97-D/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B97-D/6-311G(2d,2p)

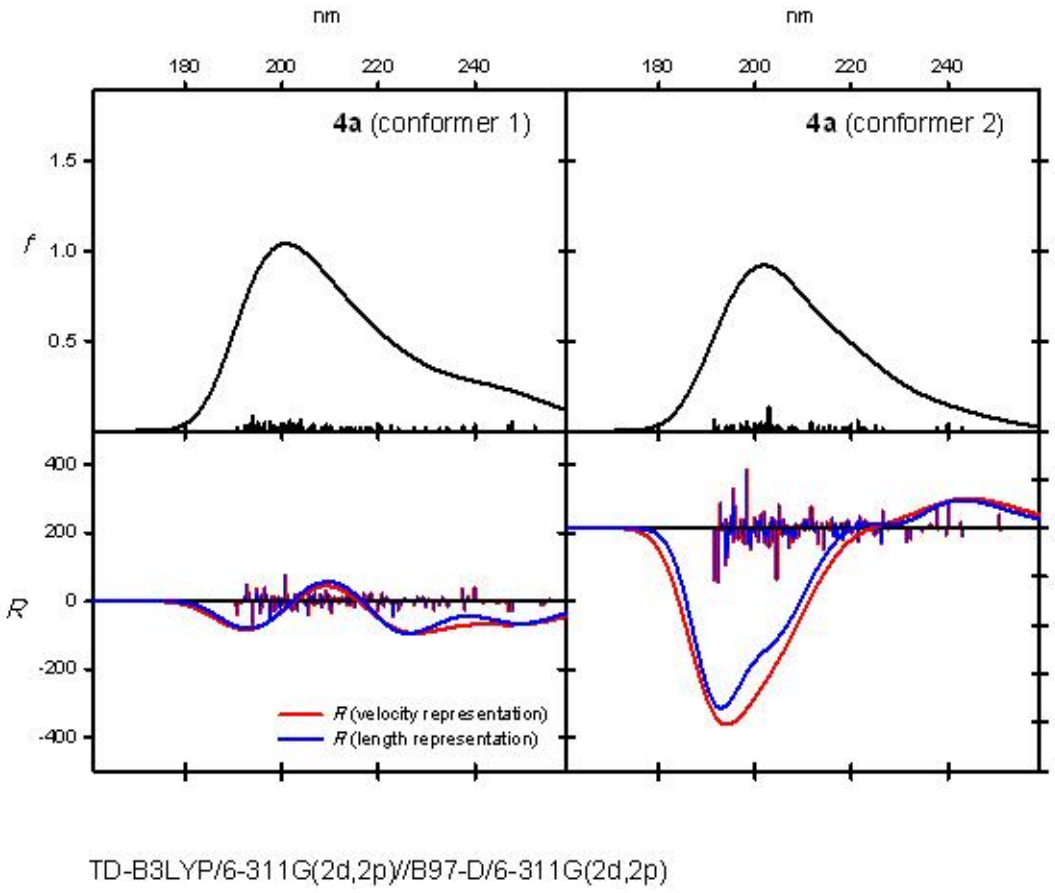


Figure D1. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4a** optimized at the B97-D/6-311G(2d,2p) level. Wavelengths were not corrected.

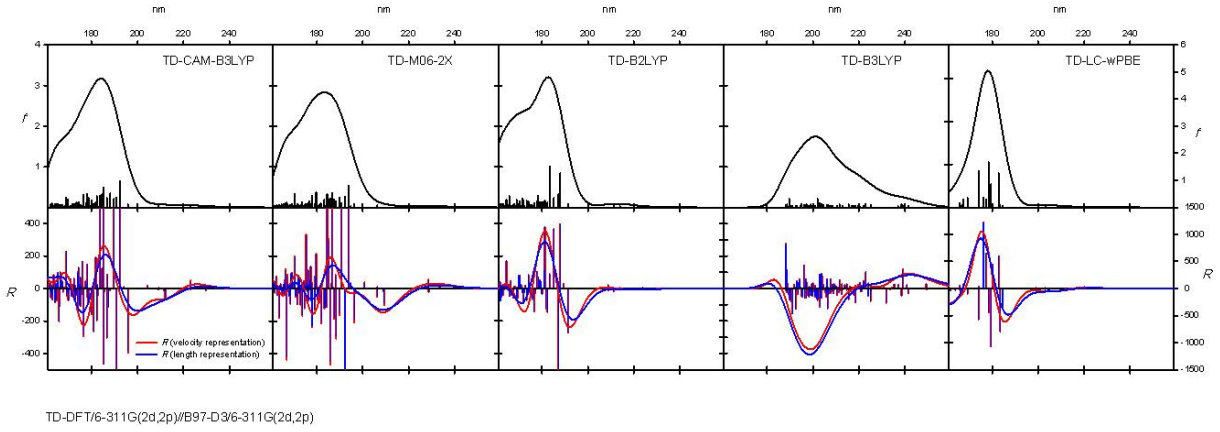
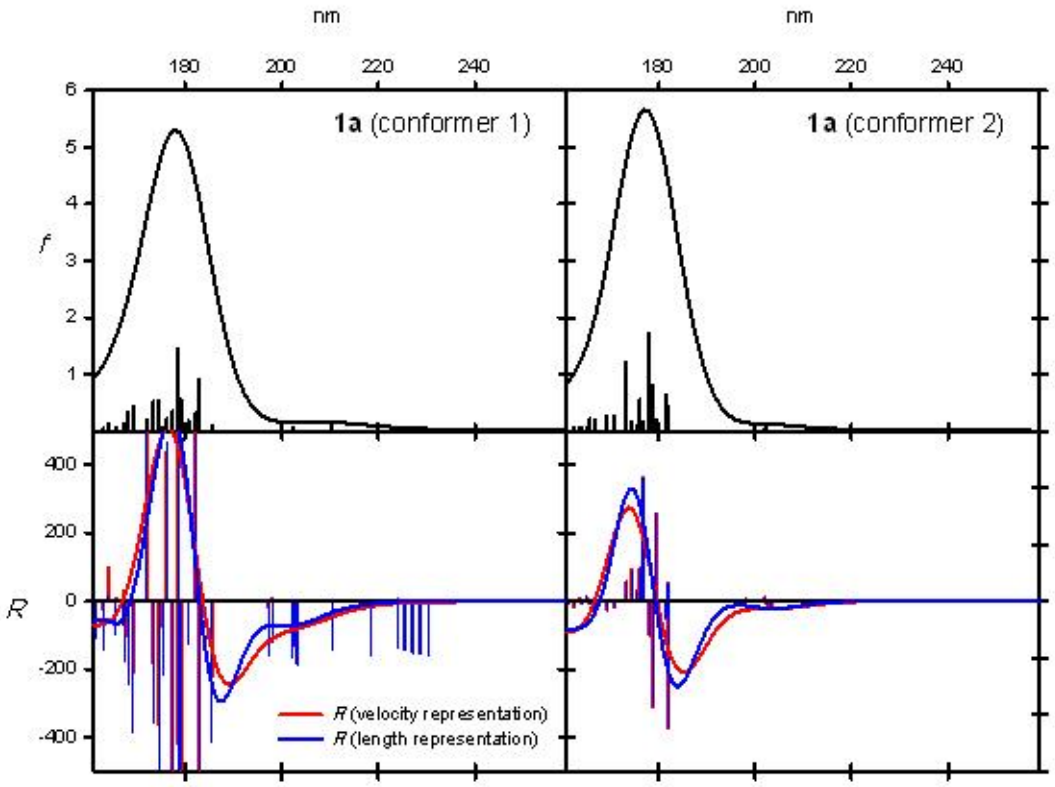
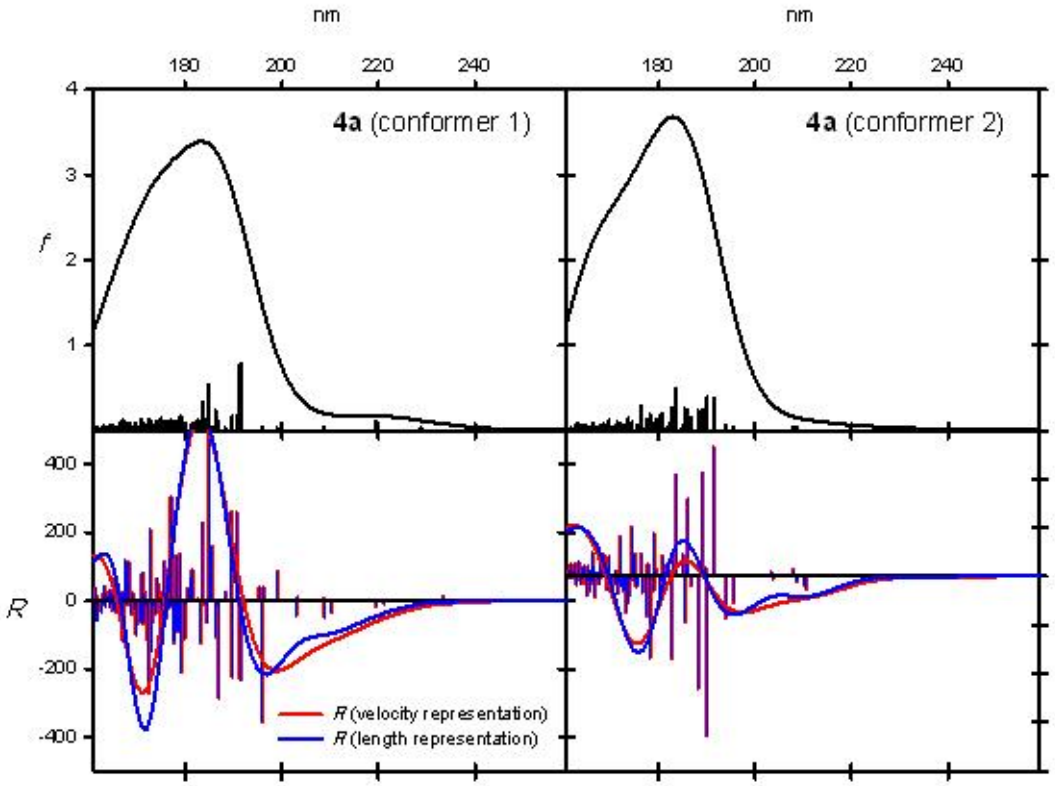


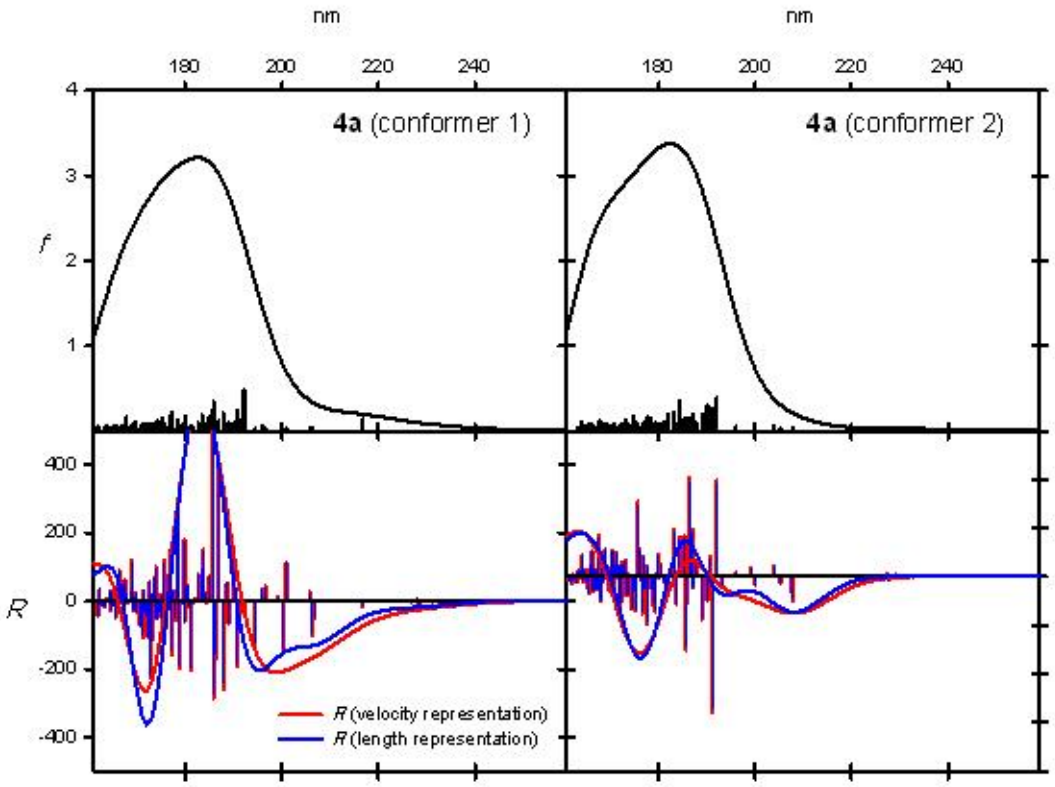
Figure D2. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4a** optimized at the B97-D3/6-311G(2d,2p) level. Wavelengths were not corrected.



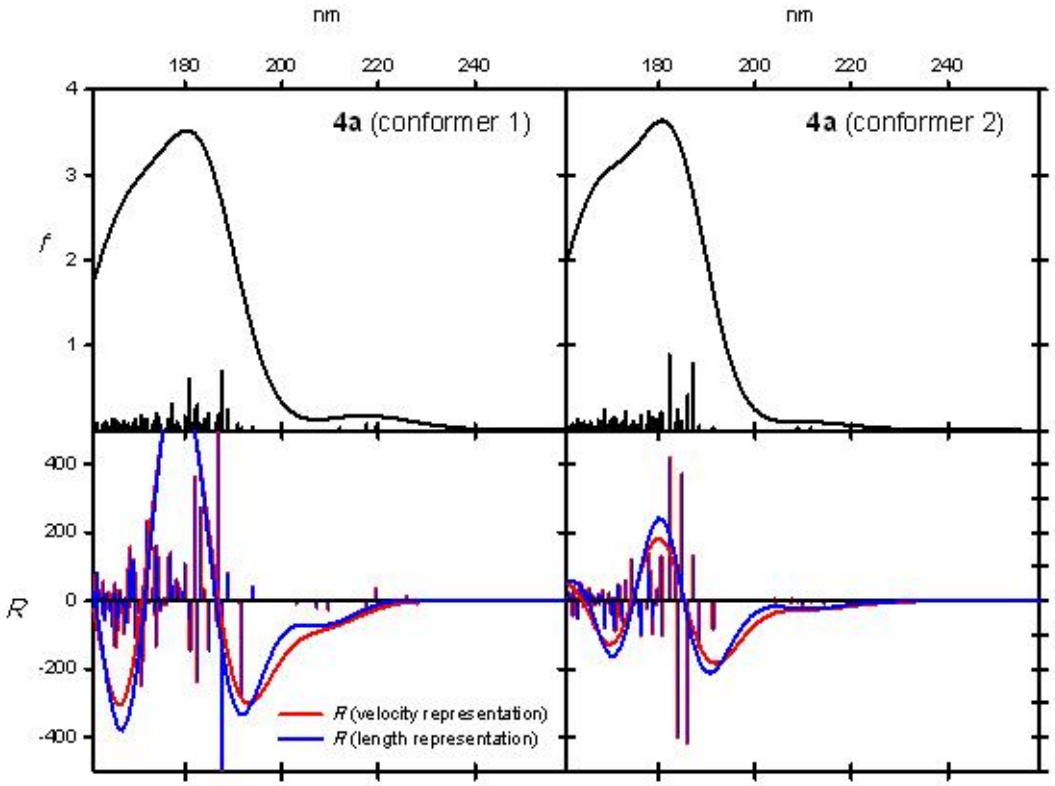
TD-LC-wPBE/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-CAM-B3LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)

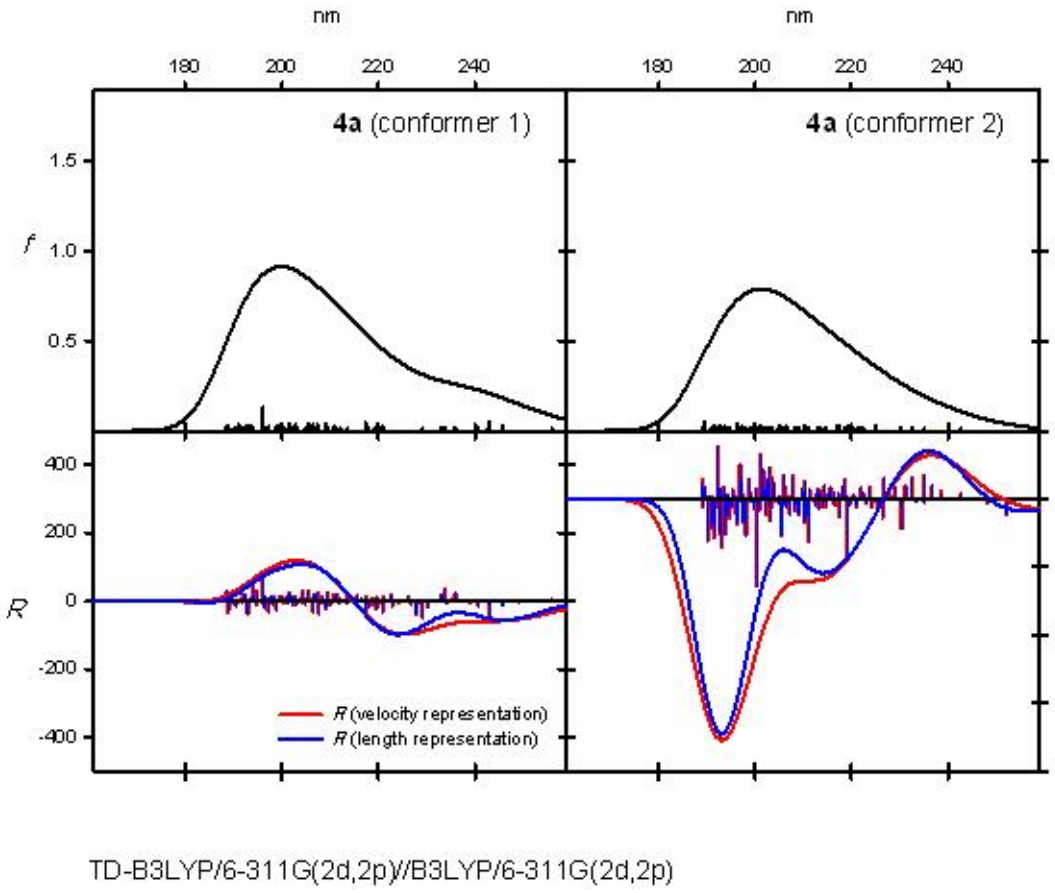


Figure D3. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4a** optimized at the B3LYP/6-311G(2d,2p) level. Wavelengths were not corrected.

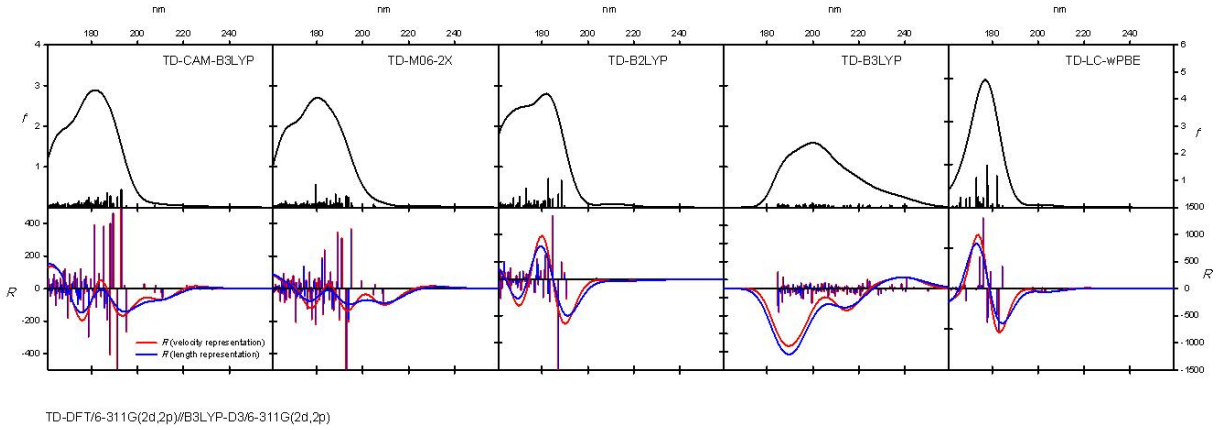


Figure D4. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4a** optimized at the B3LYP-GD3BJ/6-311G(2d,2p) level. Wavelengths were not corrected.

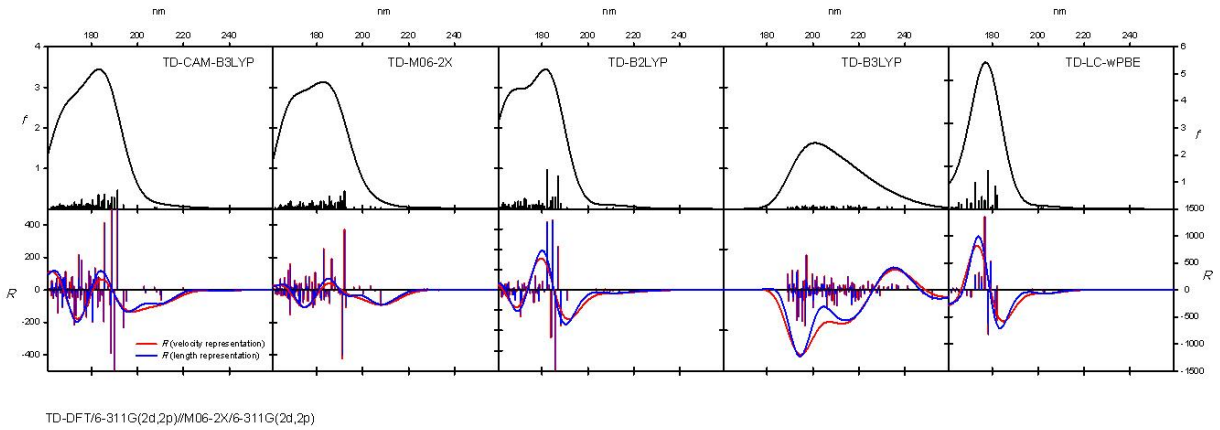


Figure D5. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4a** optimized at the M06-2X/6-311G(2d,2p) level. Wavelengths were not corrected.

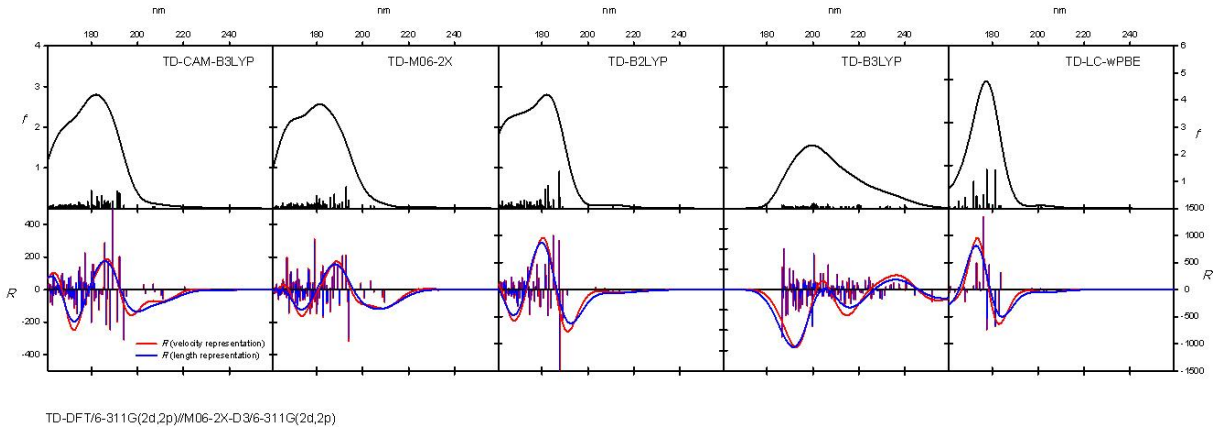
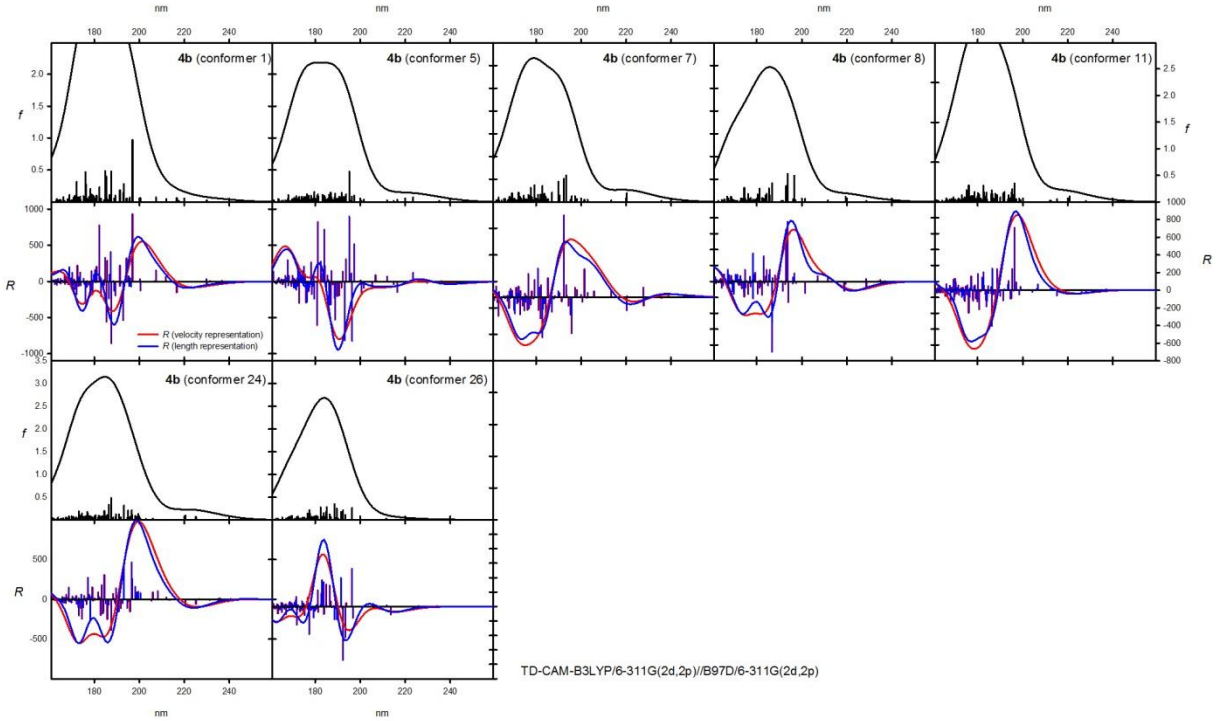
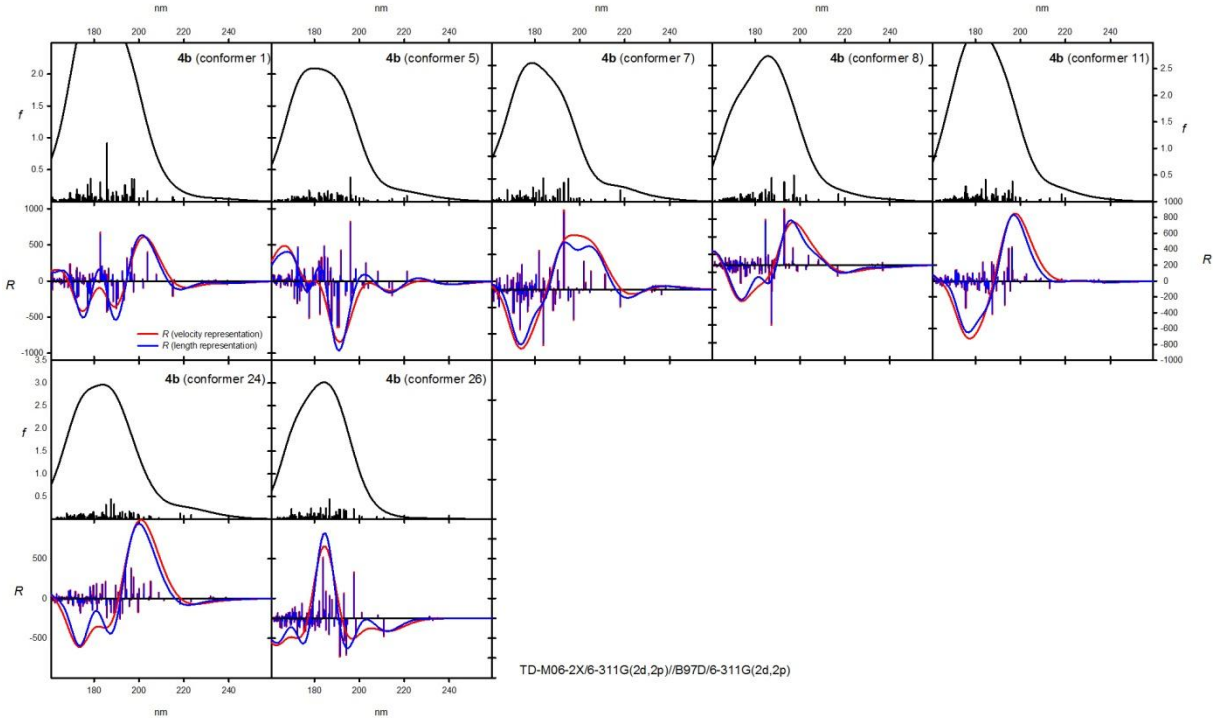
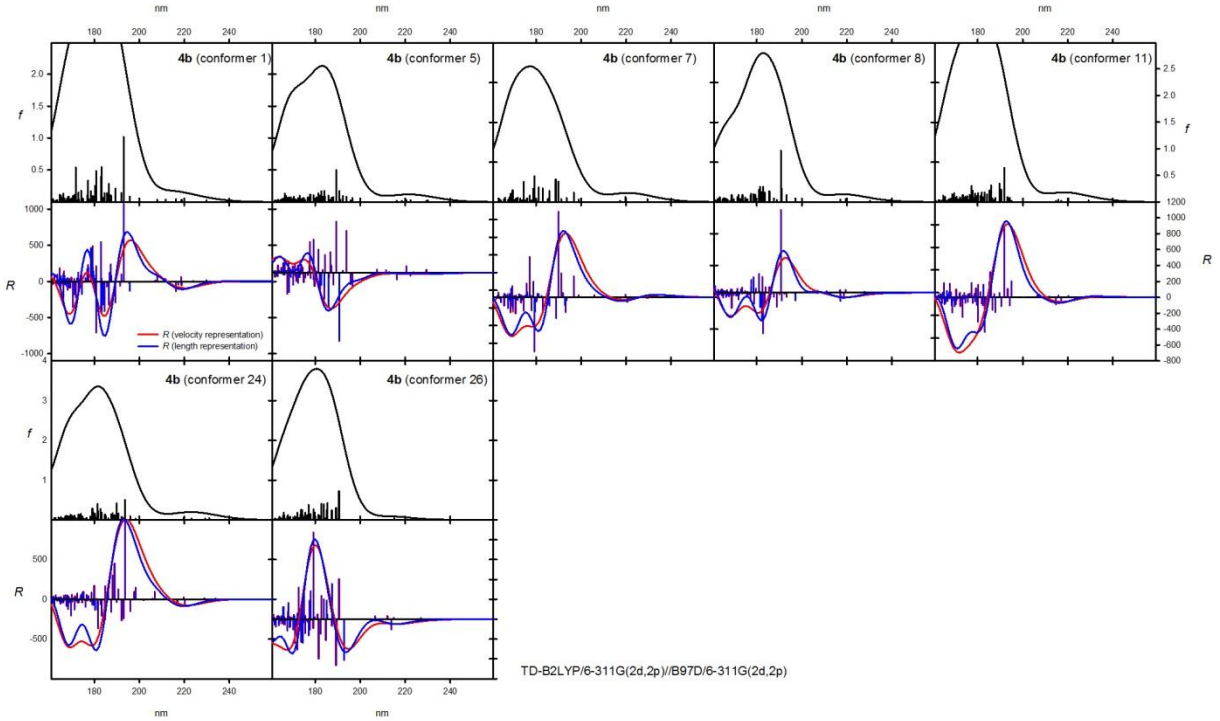
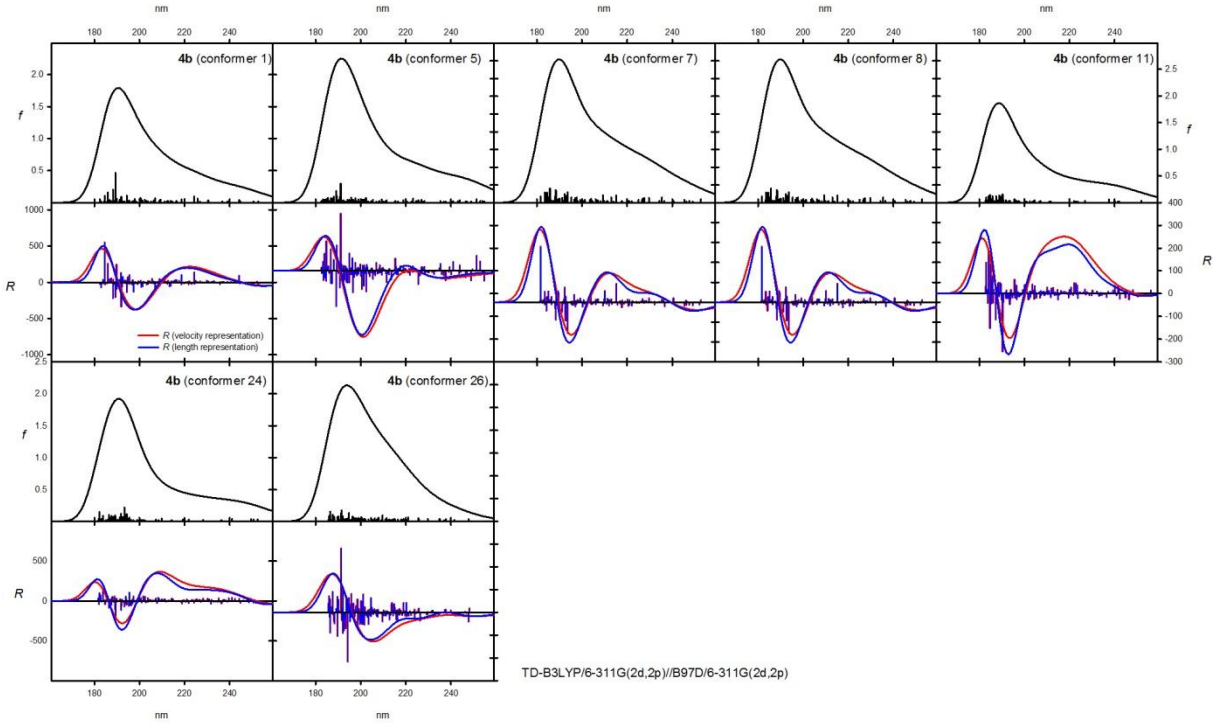


Figure D6. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4a** optimized at the M06-2X-D3/6-311G(2d,2p) level. Wavelengths were not corrected.


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 11)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-CAM-B3LYP/6-311G(2d,2p)//B97D/6-311G(2d,2p)


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 11)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-M06-2X/6-311G(2d,2p)//B97D/6-311G(2d,2p)


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 11)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-B2LYP/6-311G(2d,2p)//B97D/6-311G(2d,2p)


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 11)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-B3LYP/6-311G(2d,2p)//B97D/6-311G(2d,2p)

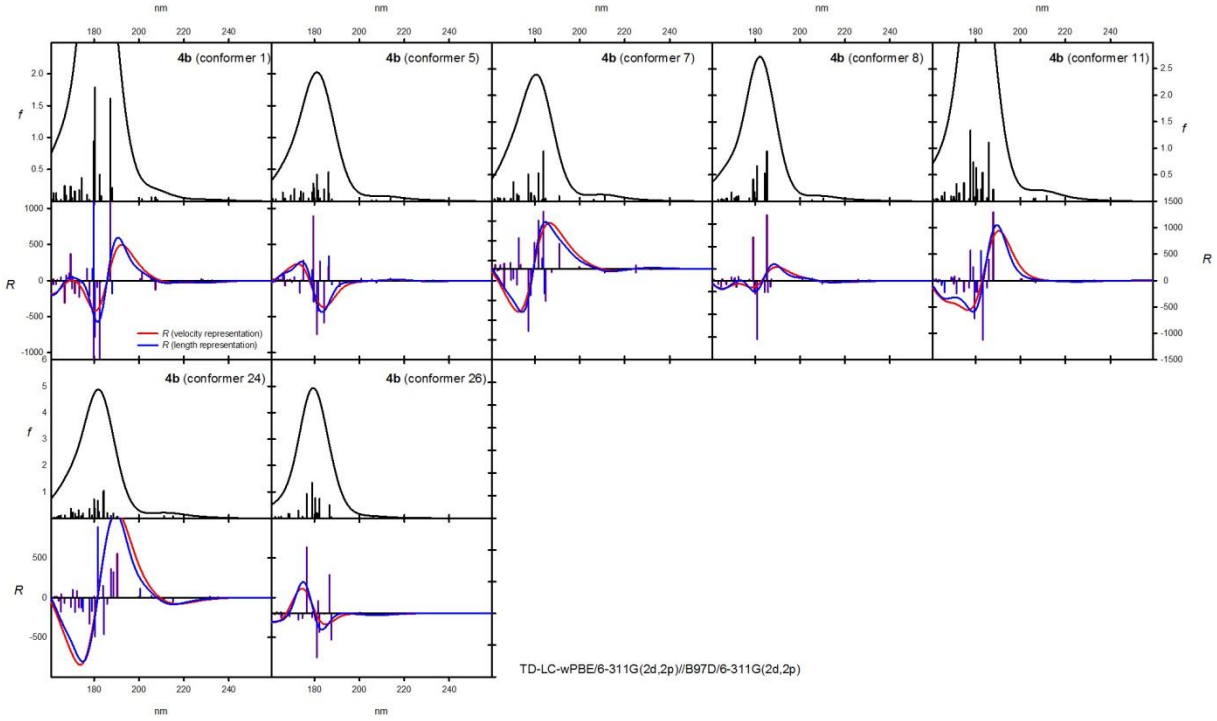
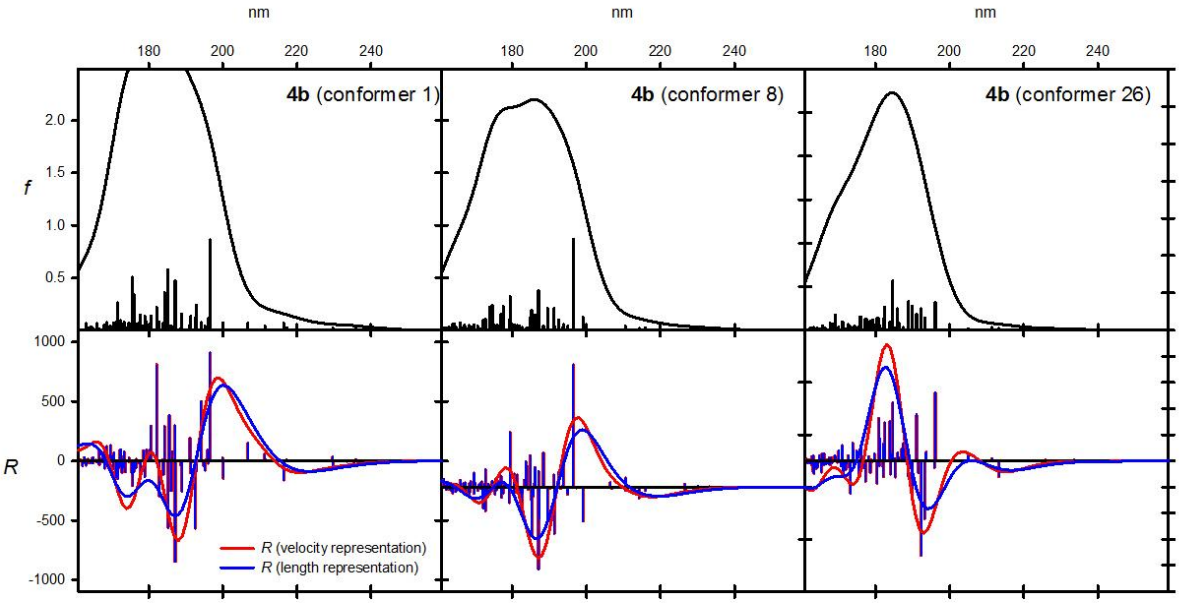
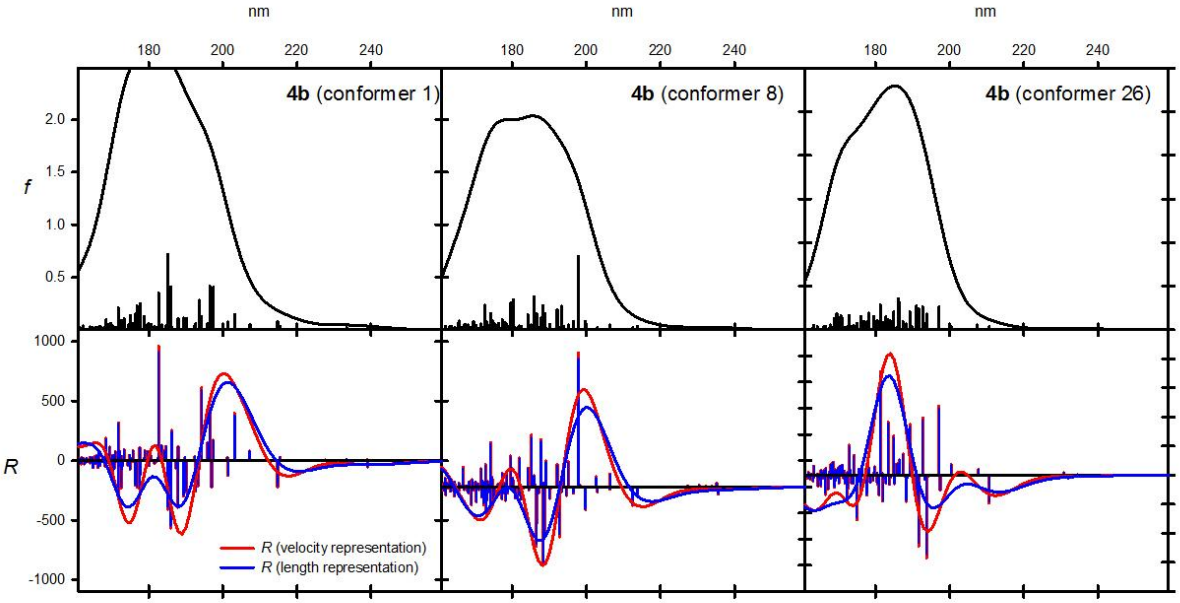


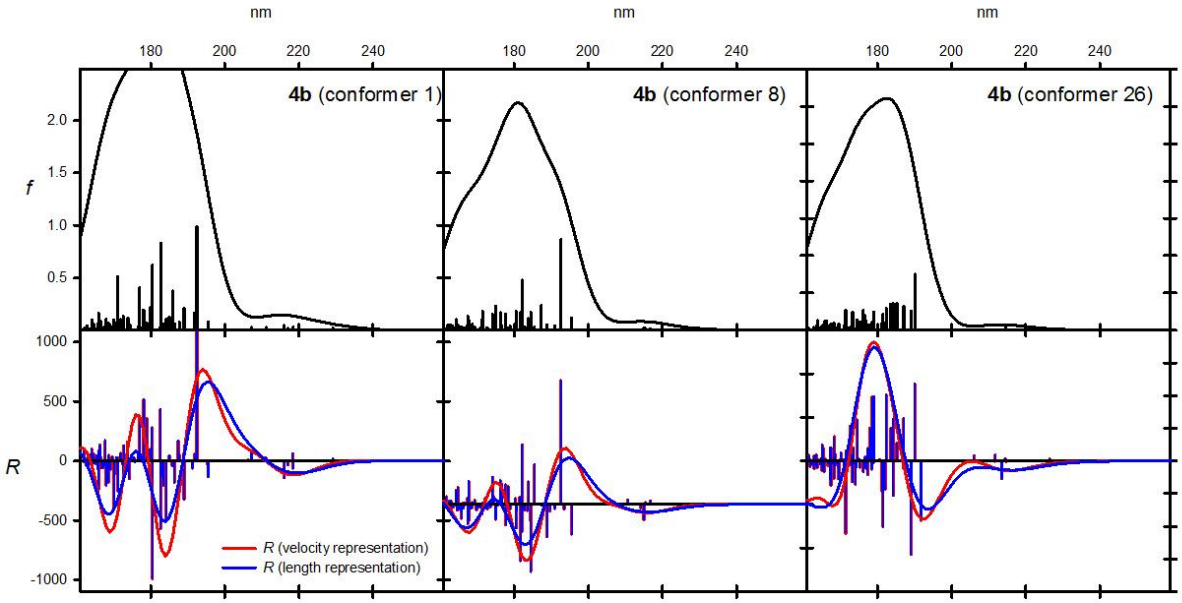
Figure E1. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4b** optimized at the B97-D/6-311G(2d,2p) level. Wavelengths were not corrected.



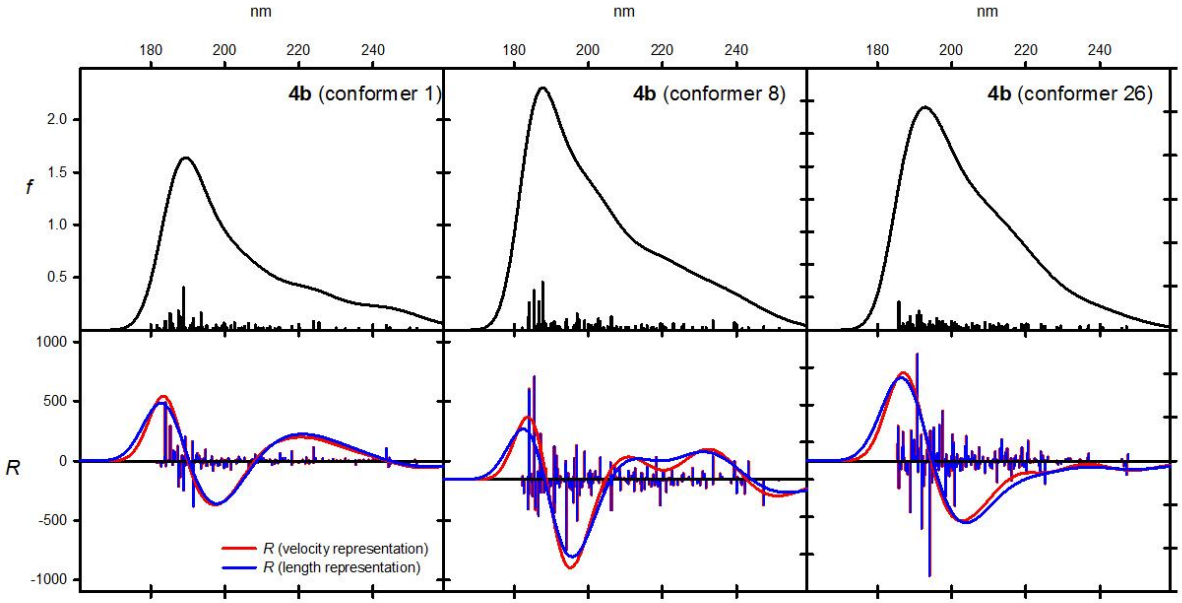
TD-CAM-B3LYP/6-311G(2d,2p)//B97-D3/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B97-D3/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B97-D3/6-311G(2d,2p)



TD-B3LYP/6-311G(2d,2p)//B97-D3/6-311G(2d,2p)

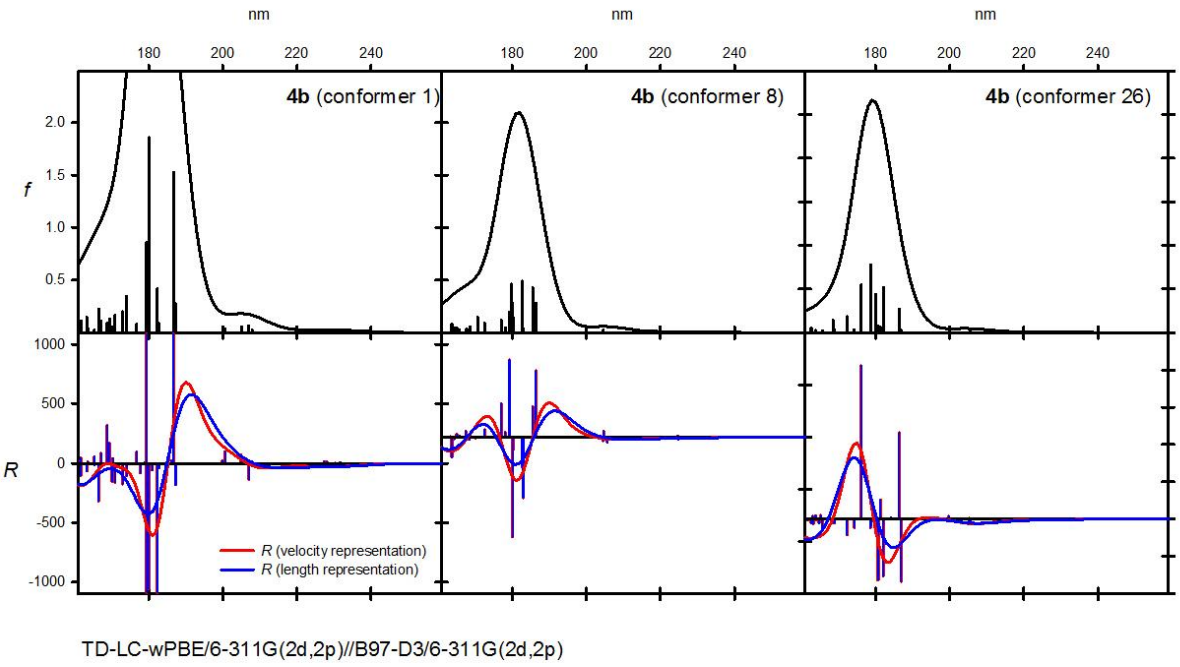
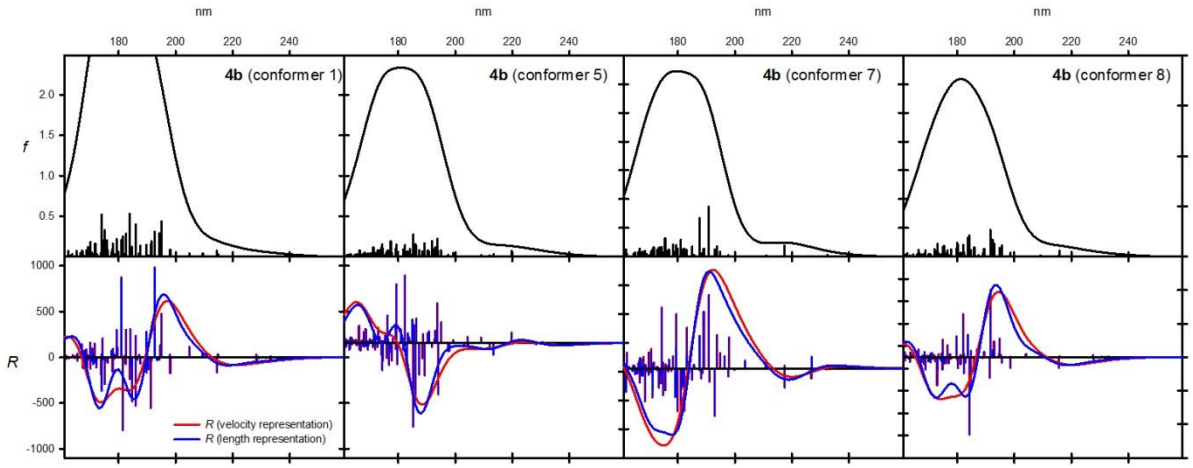
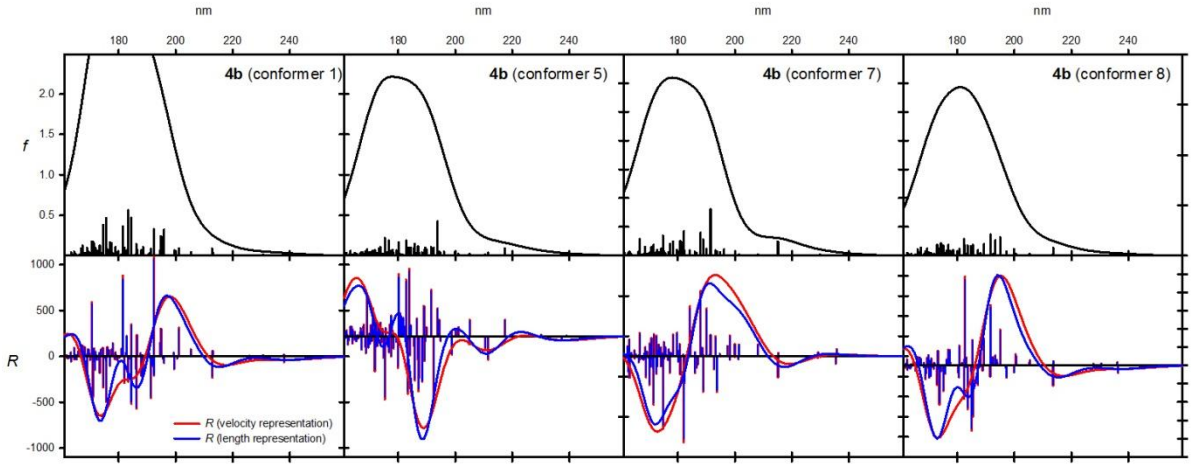


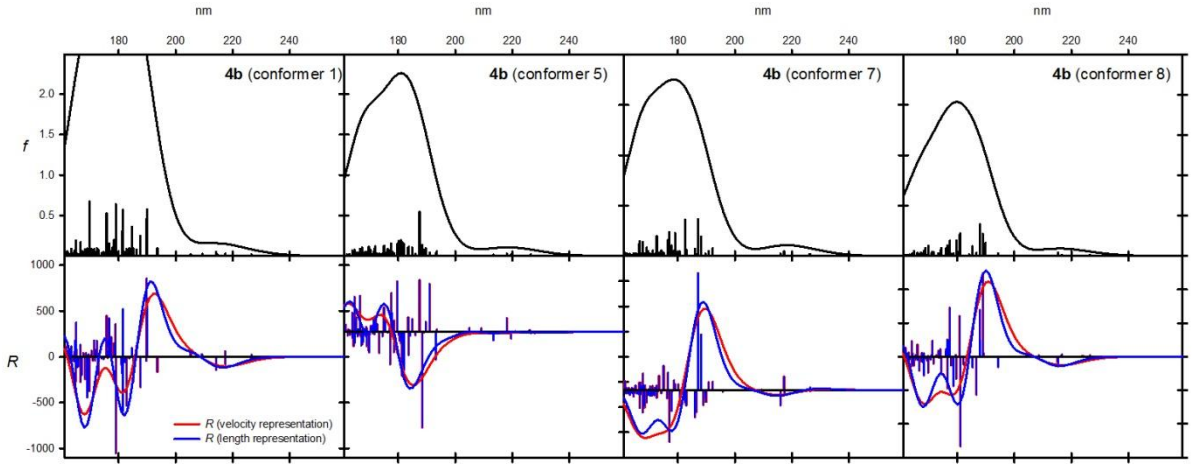
Figure E2. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4b** optimized at the B97-D3/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



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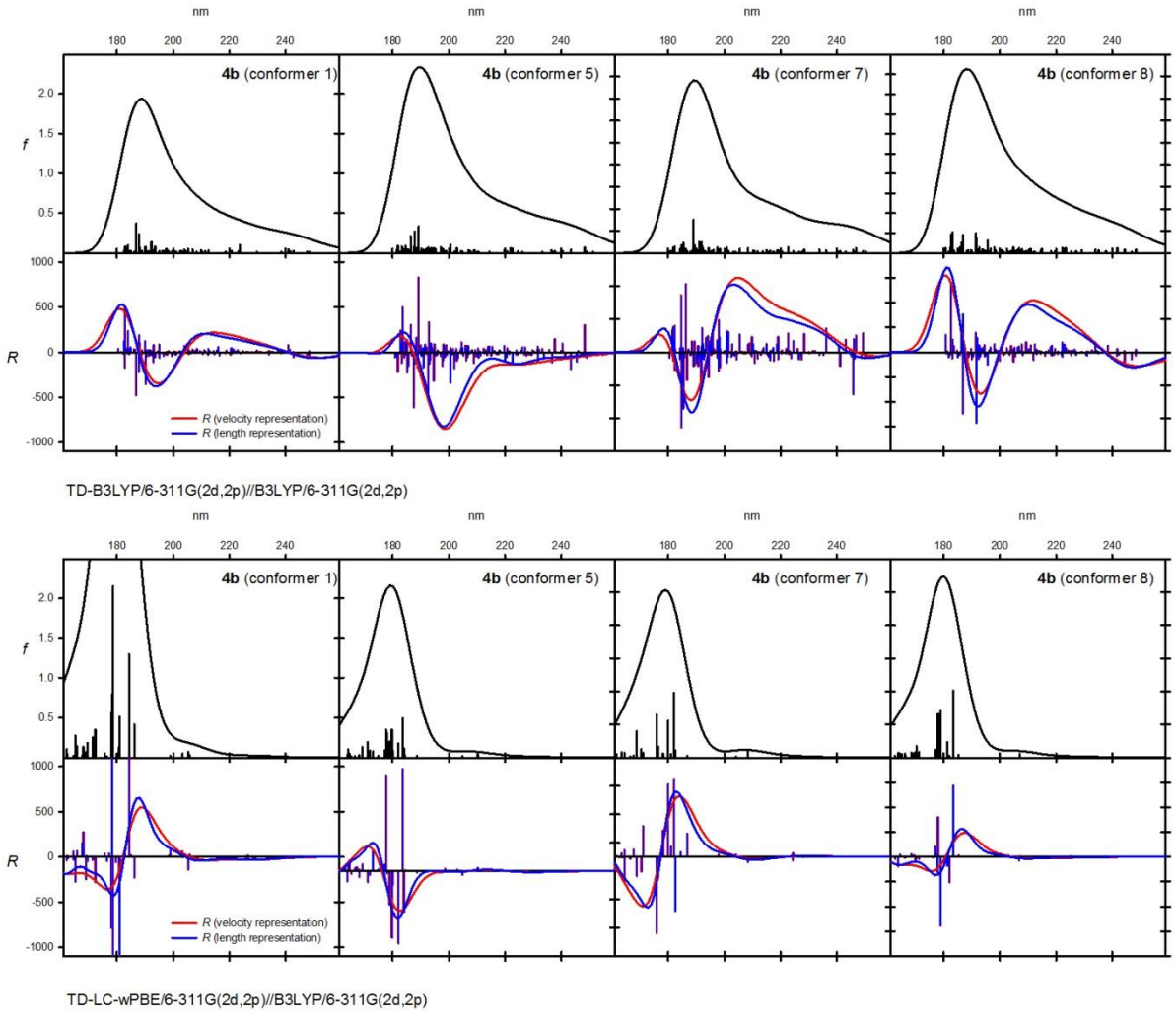
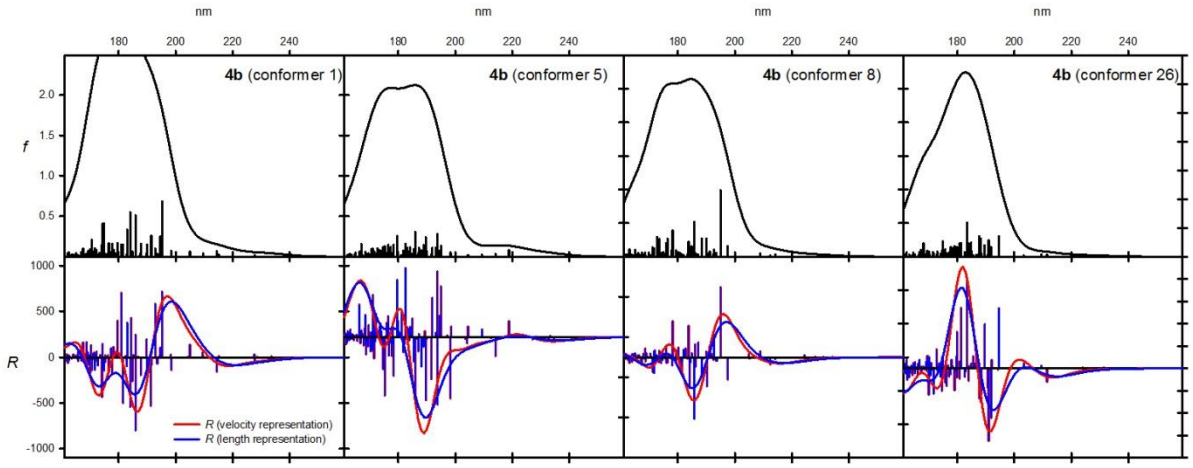
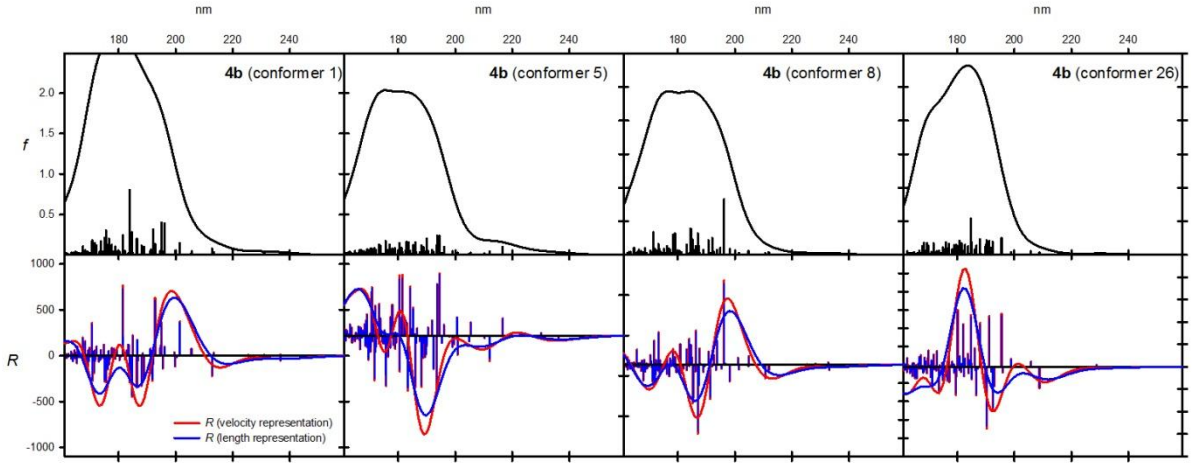


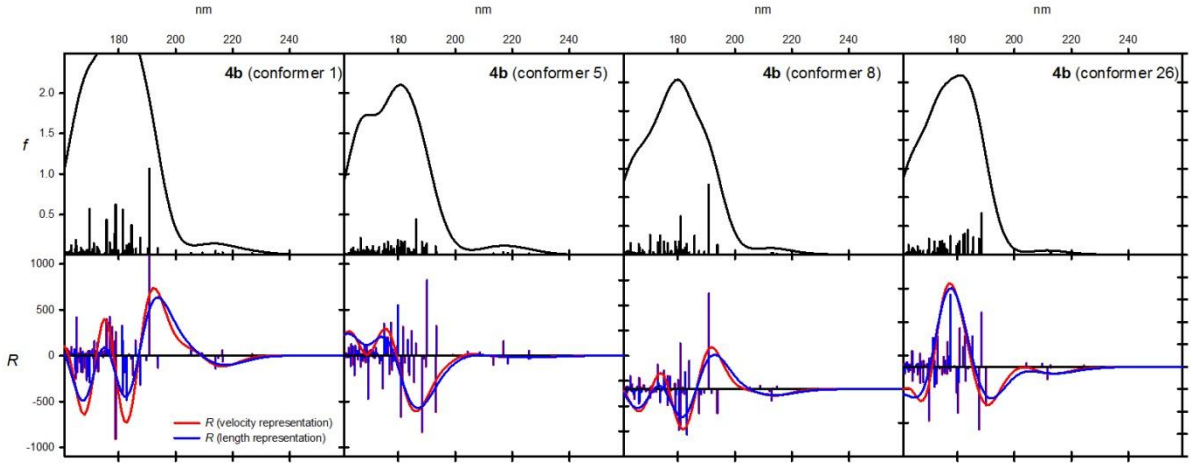
Figure E3. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4b** optimized at the B3LYP/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311G(2d,2p)//B3LYP-GD3BJ/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B3LYP-GD3BJ/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B3LYP-GD3BJ/6-311G(2d,2p)

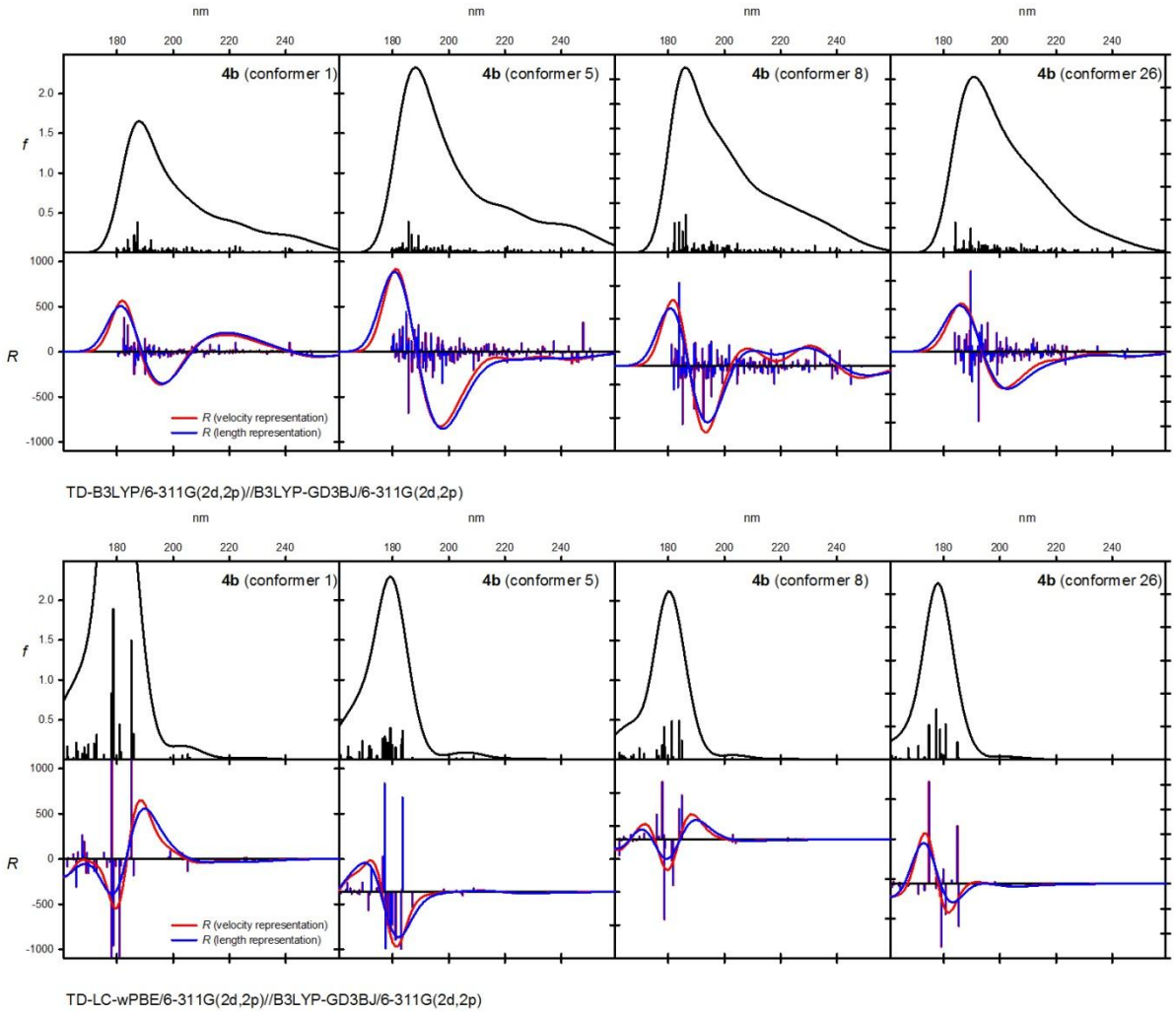
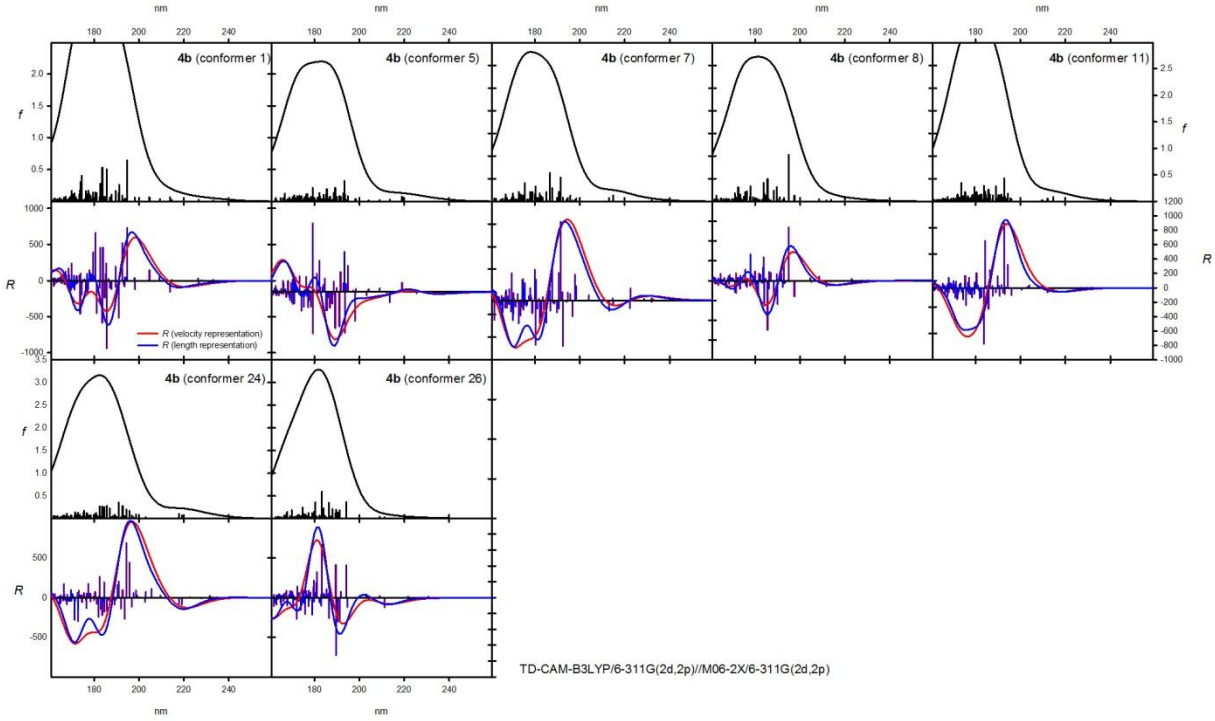
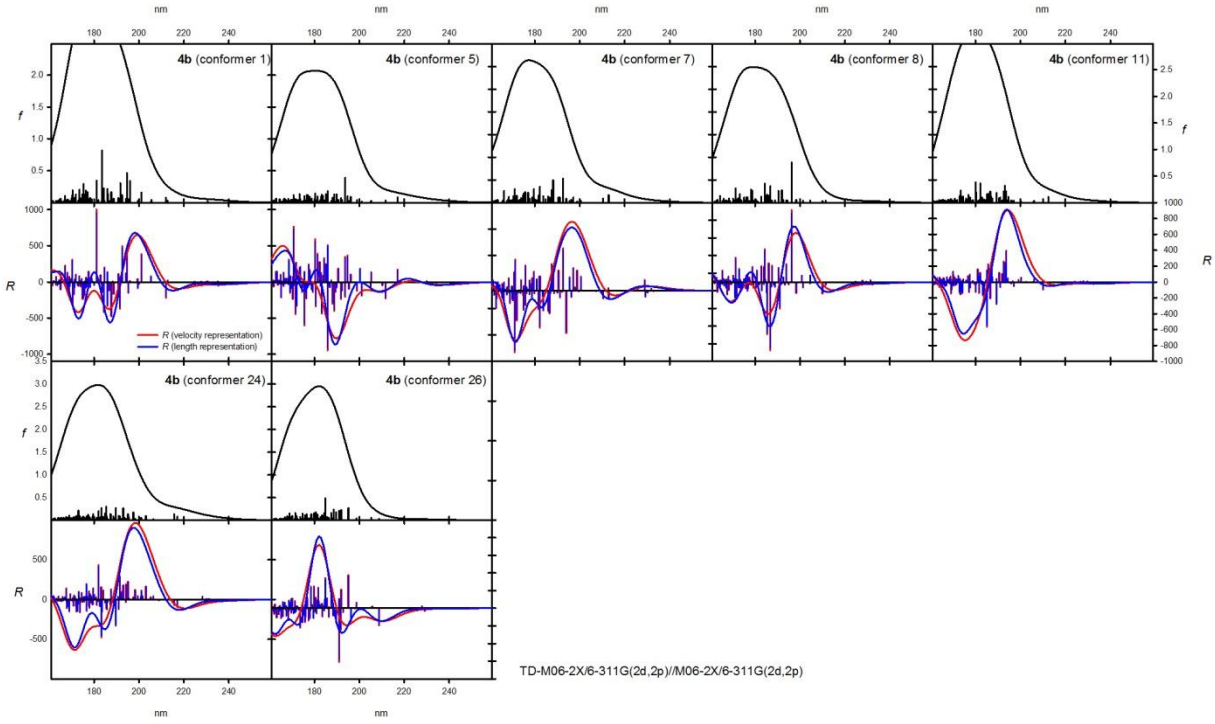
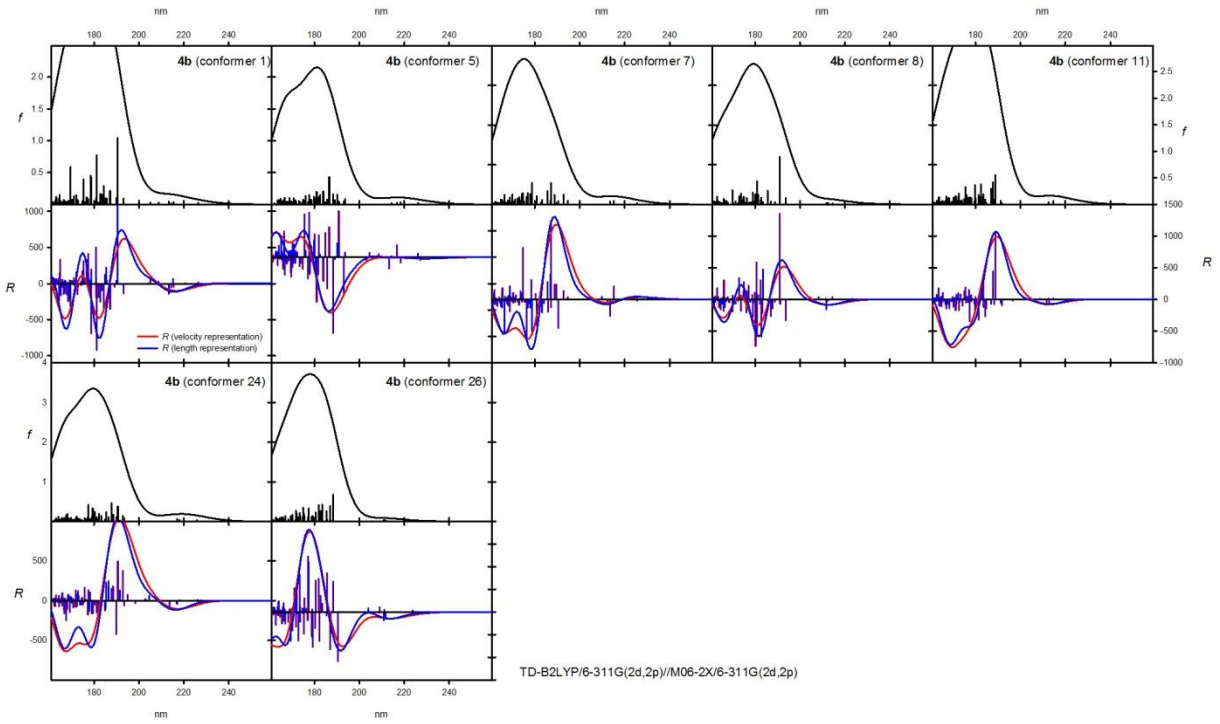
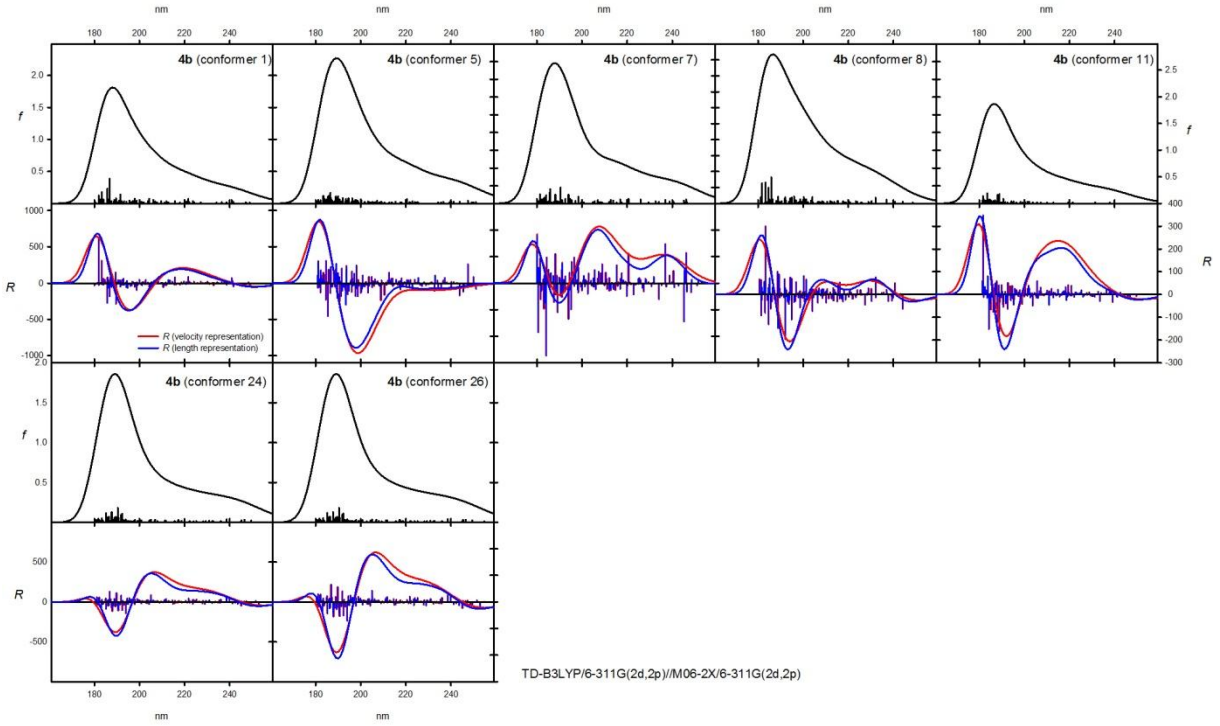


Figure E4. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4b** optimized at the B3LYP-GD3BJ/6-311G(2d,2p) level. Wavelengths were not corrected.


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 11)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-CAM-B3LYP/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 11)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-M06-2X/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 11)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-B2LYP/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 11)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-B3LYP/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)

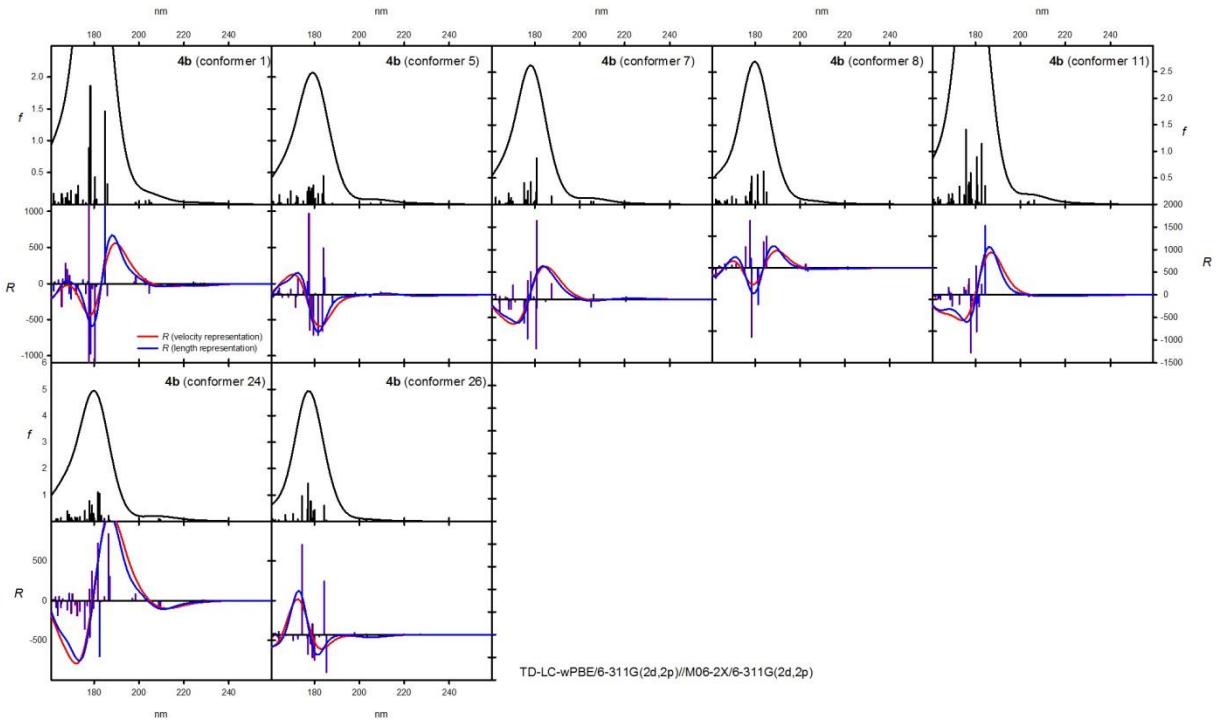
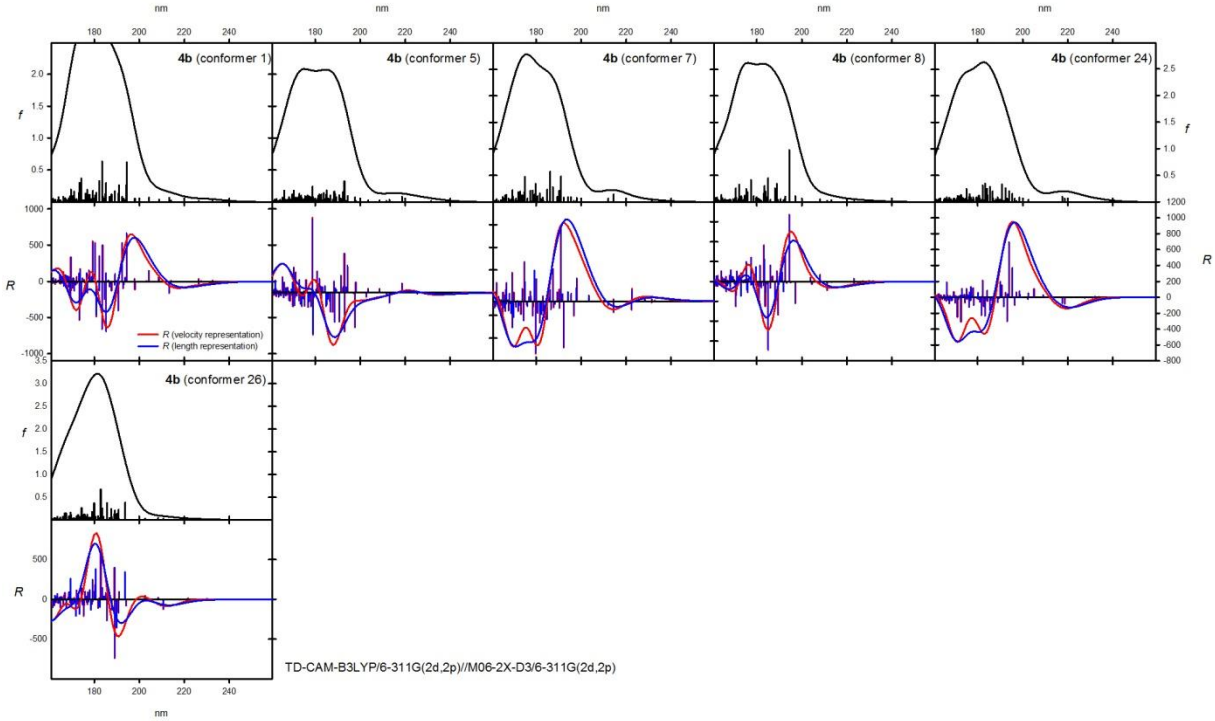
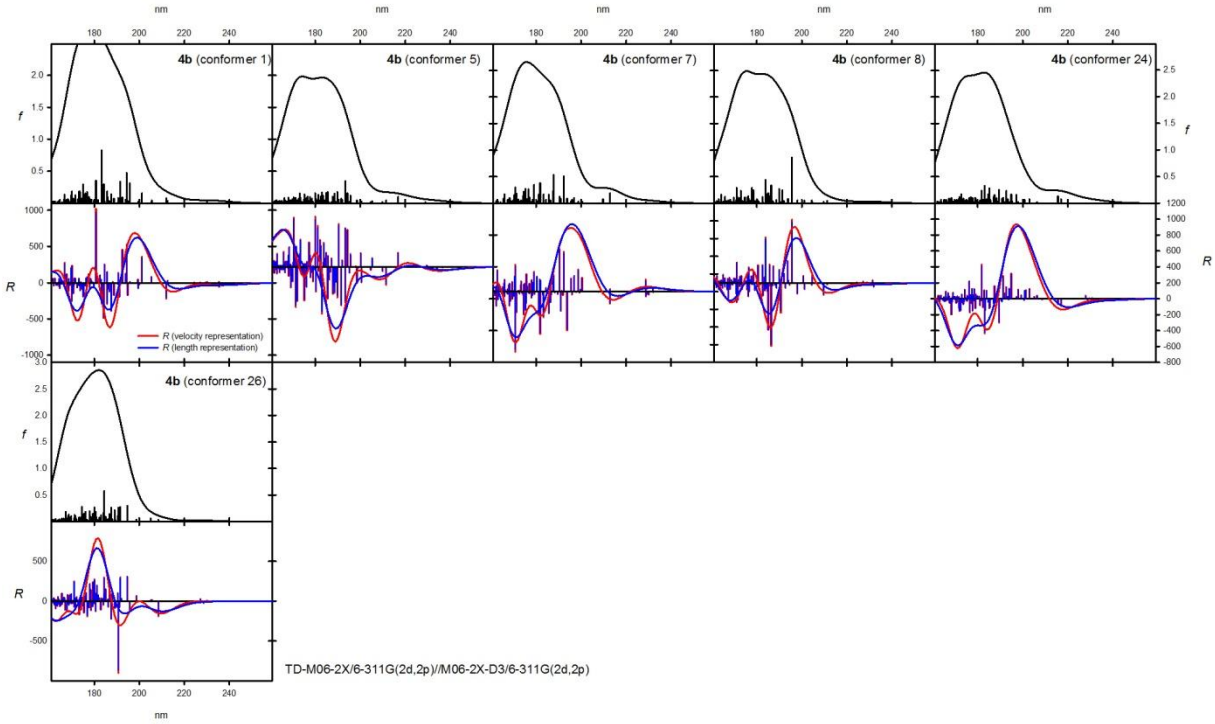
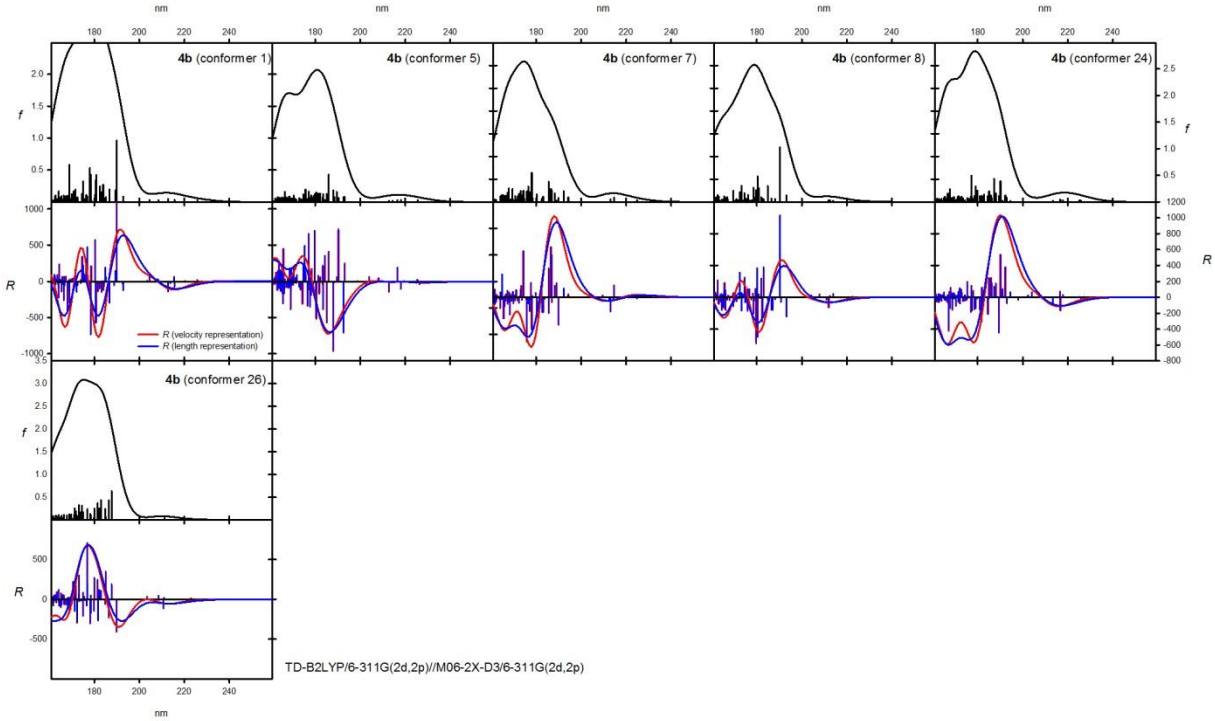
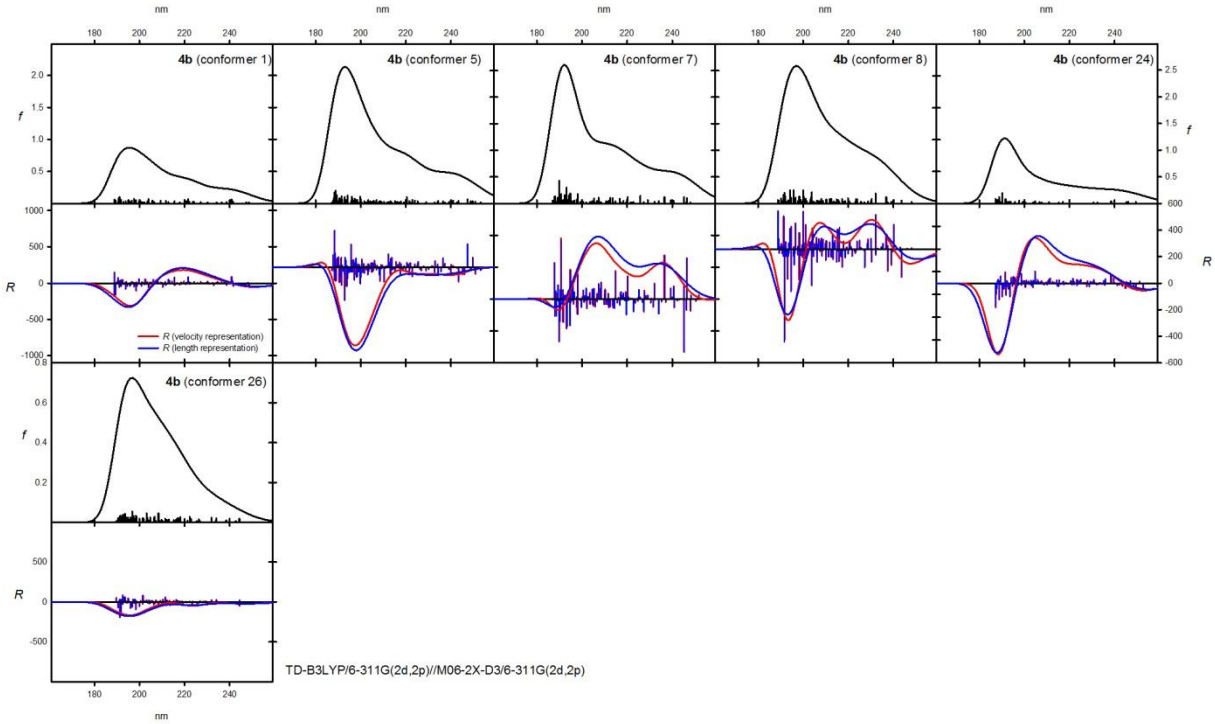


Figure E5. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4b** optimized at the M06-2X/6-311G(2d,2p) level. Wavelengths were not corrected.


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-CAM-B3LYP/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-M06-2X/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-B2LYP/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)


4b (conformer 1)
4b (conformer 5)
4b (conformer 7)
4b (conformer 8)
4b (conformer 24)
4b (conformer 26)
f
R
nm
R (velocity representation)
R (length representation)
TD-B3LYP/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)

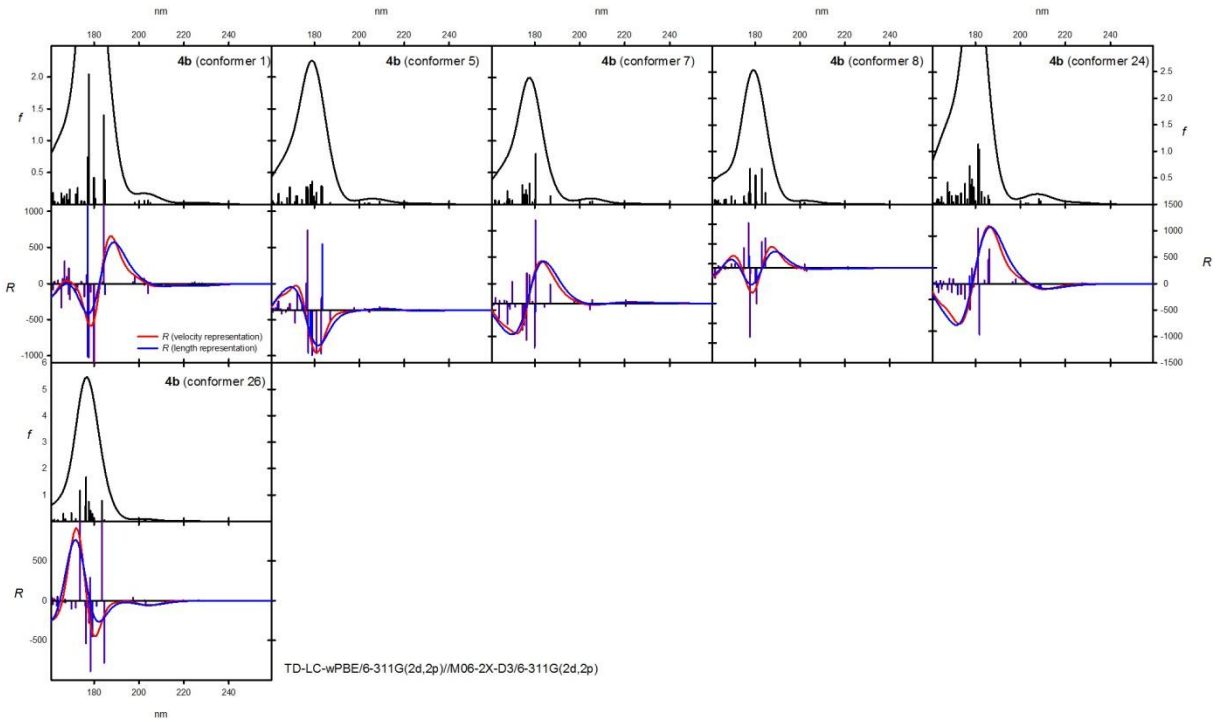
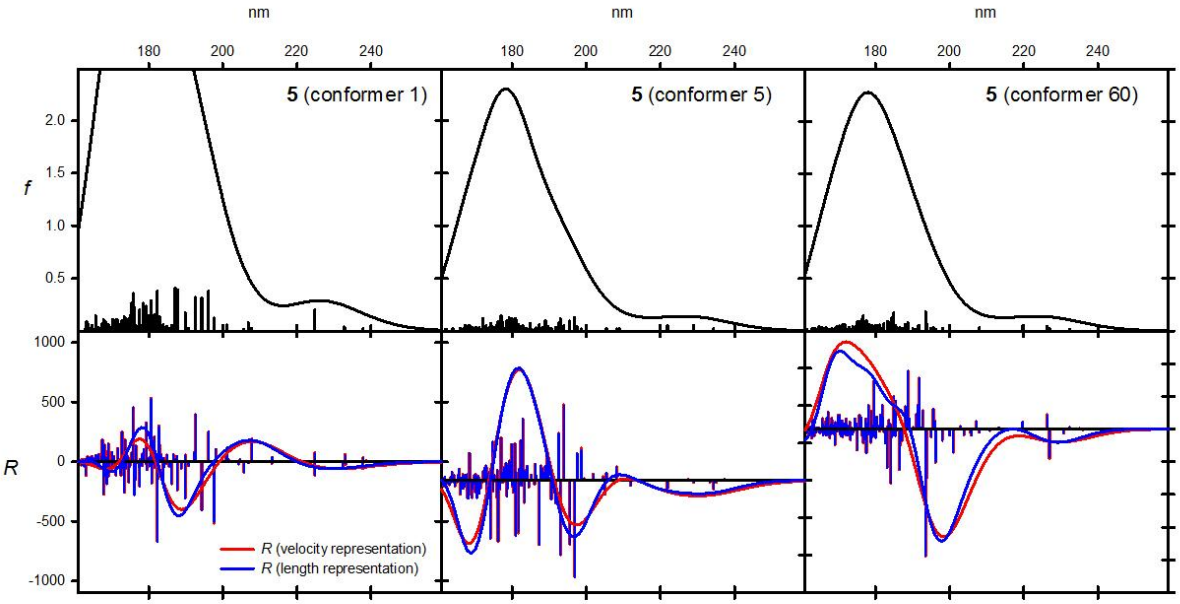
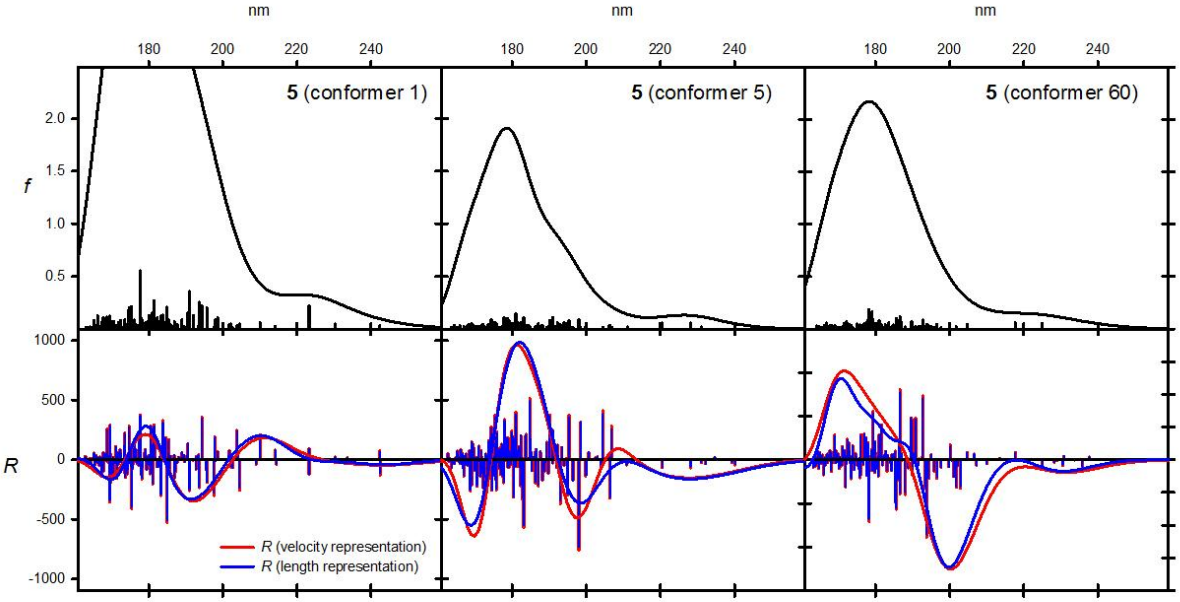


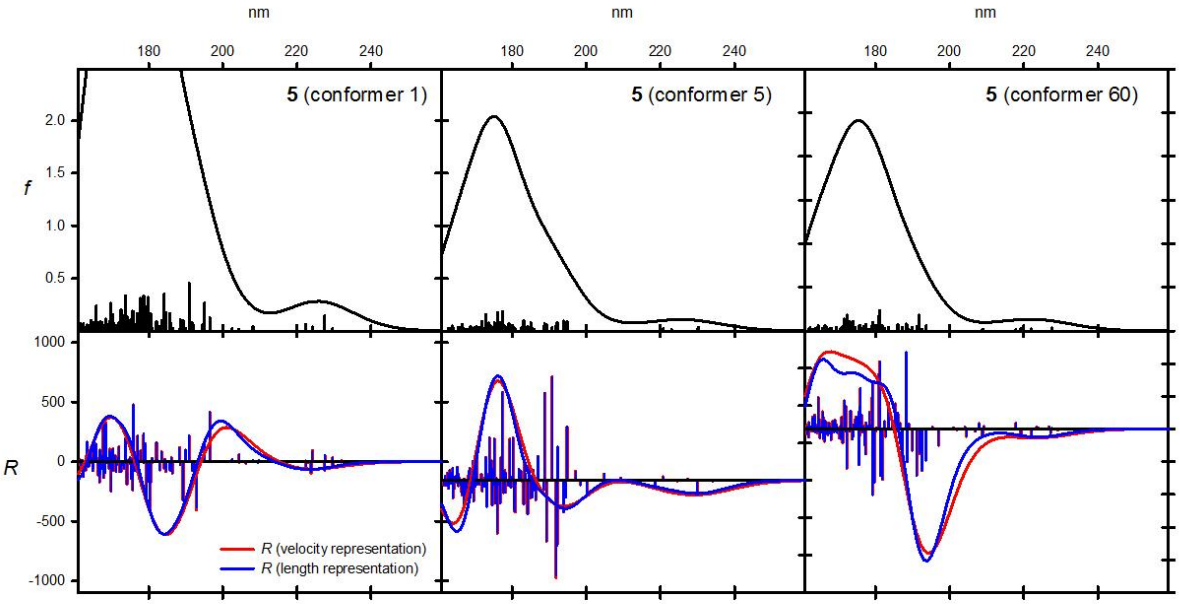
Figure E6. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **4b** optimized at the M06-2X-D3/6-311G(2d,2p) level. Wavelengths were not corrected.



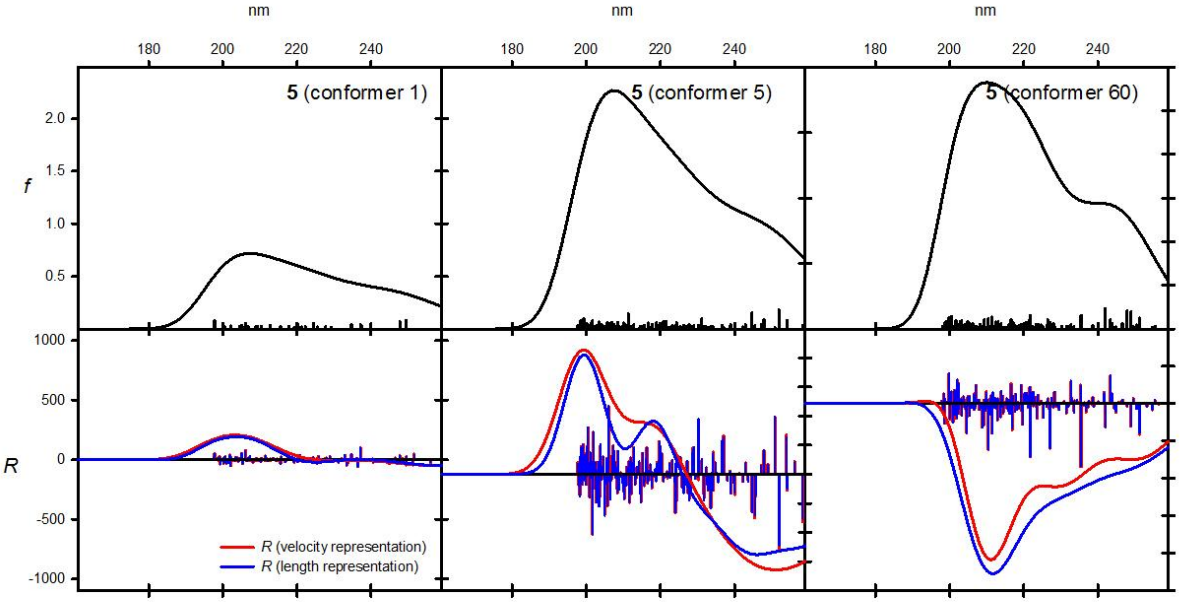
TD-CAM-B3LYP/6-311G(2d,2p)//B97D/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B97D/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B97D/6-311G(2d,2p)



TD-B3LYP/6-311G(2d,2p)//B97D/6-311G(2d,2p)

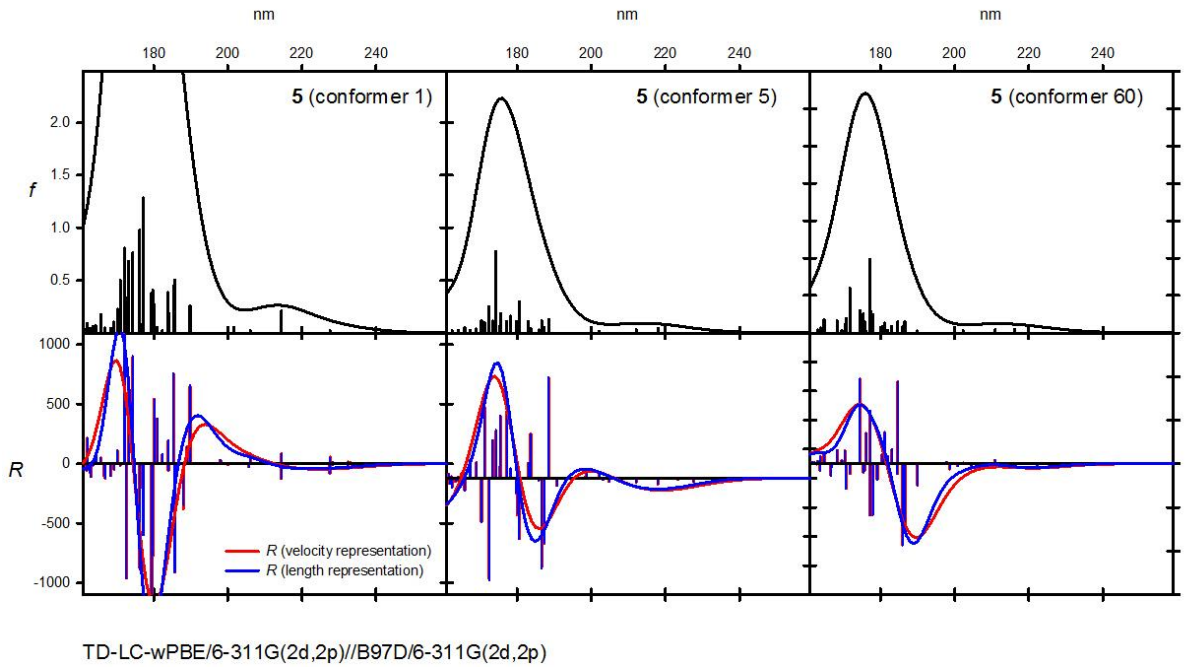
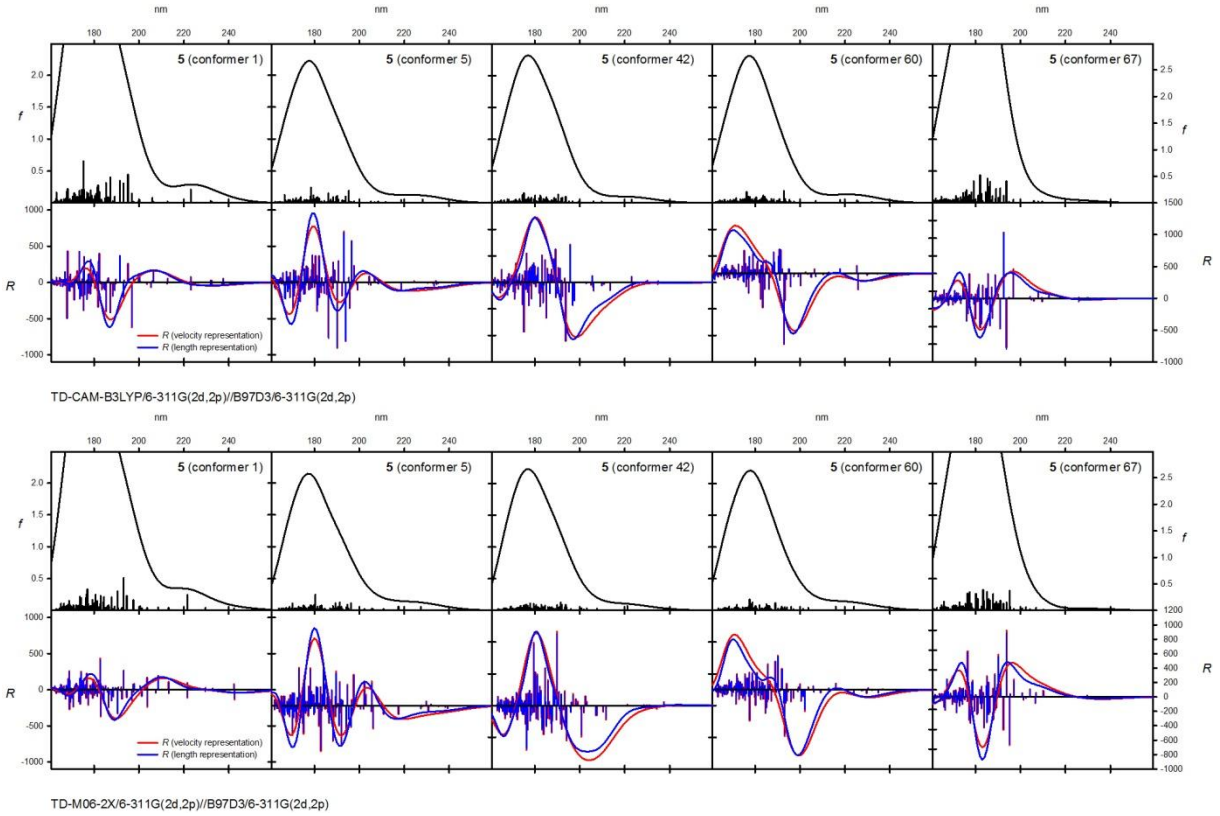


Figure F1. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **5** optimized at the B97-D/6-311G(2d,2p) level. Wavelengths were not corrected.



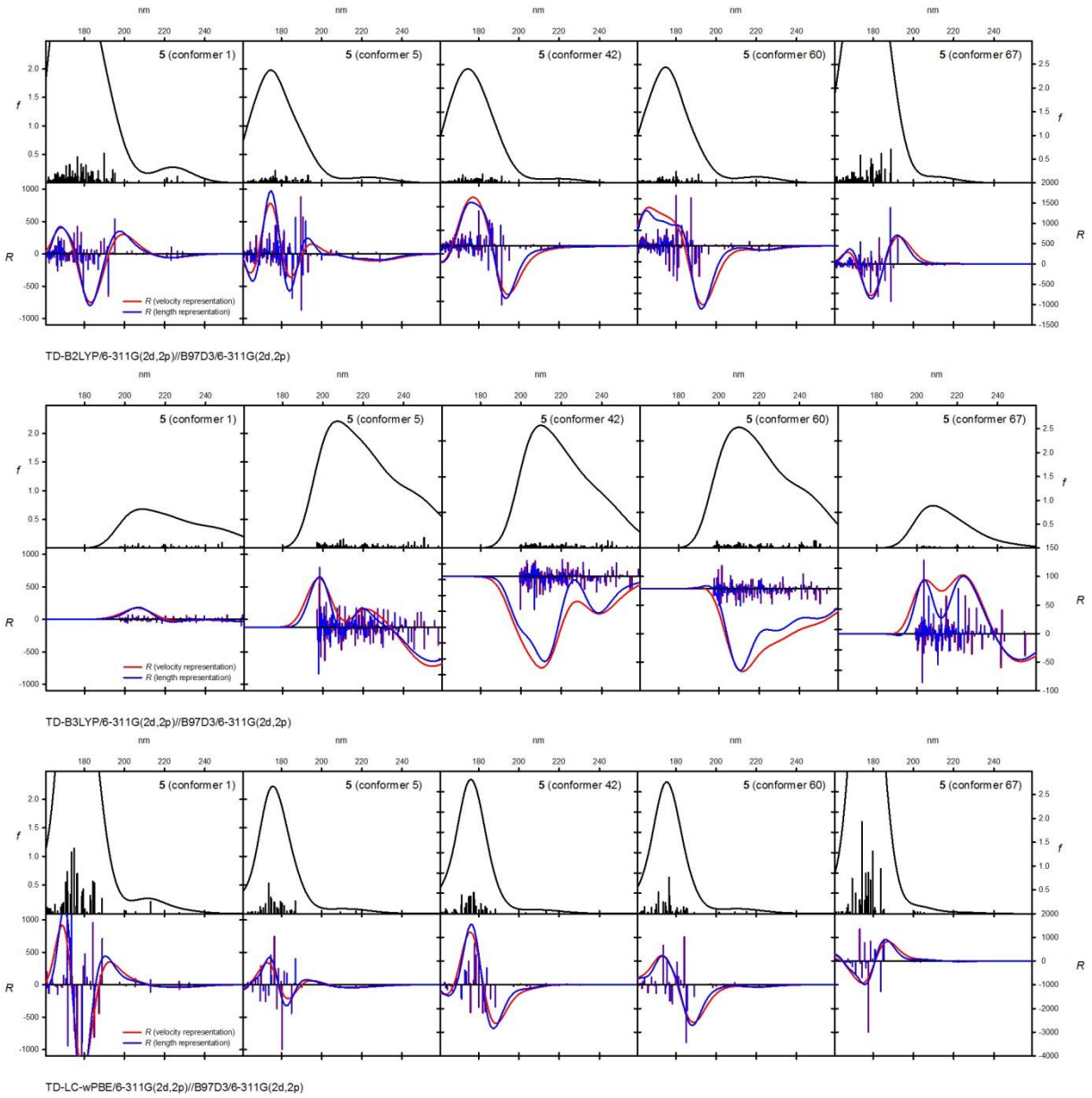
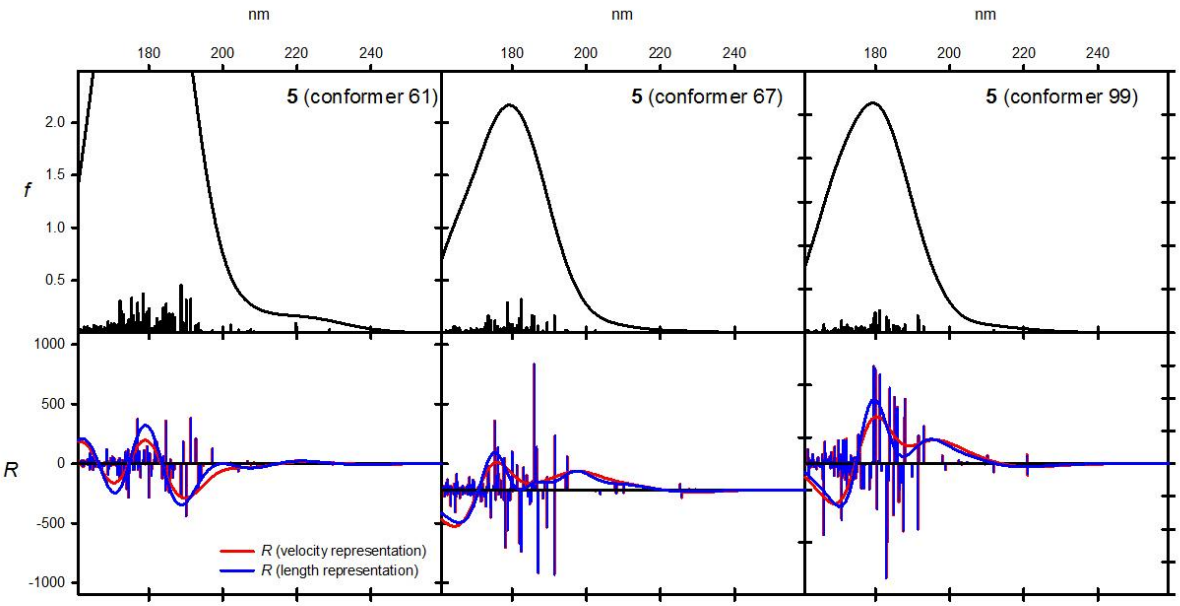
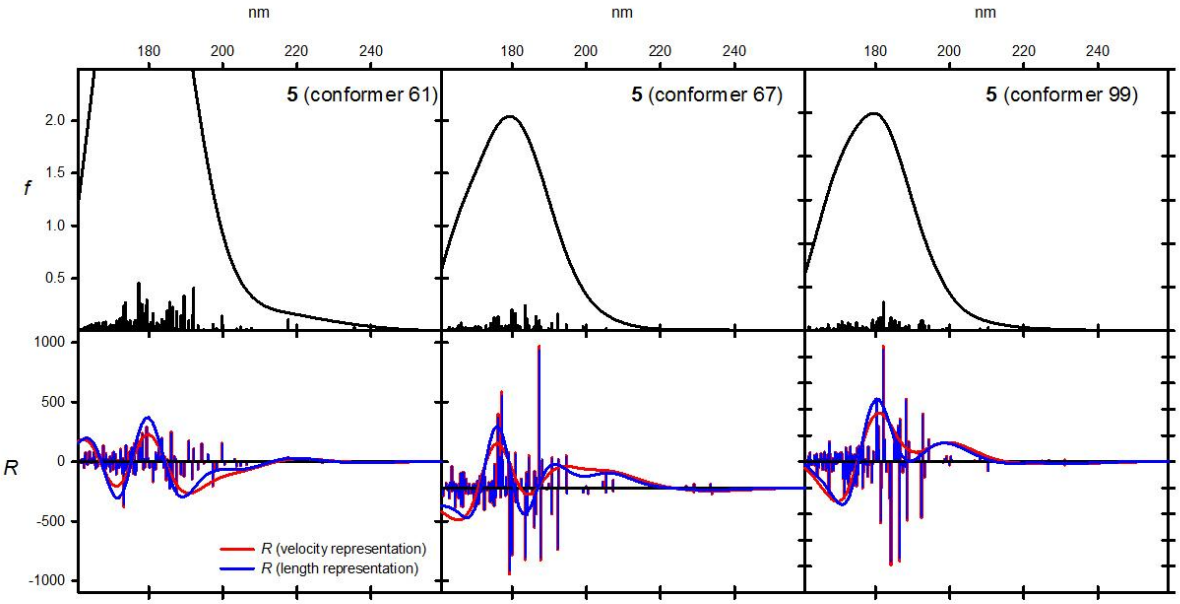


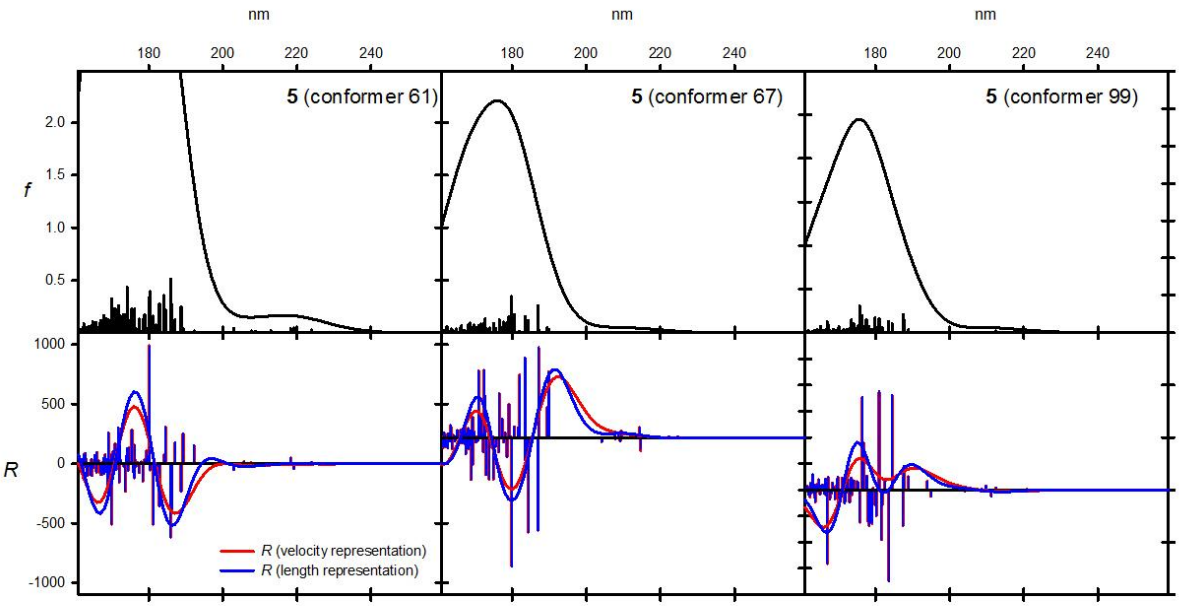
Figure F2. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **5** optimized at the B97-D3/6-311G(2d,2p) level. Wavelengths were not corrected.



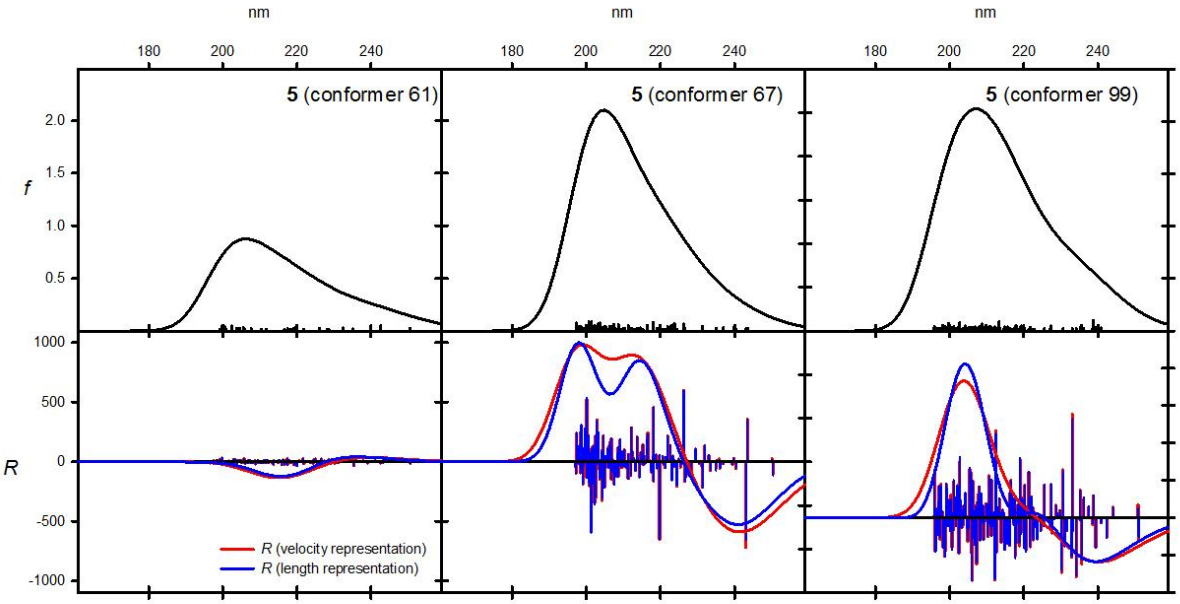
TD-CAM-B3LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)



TD-B3LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)

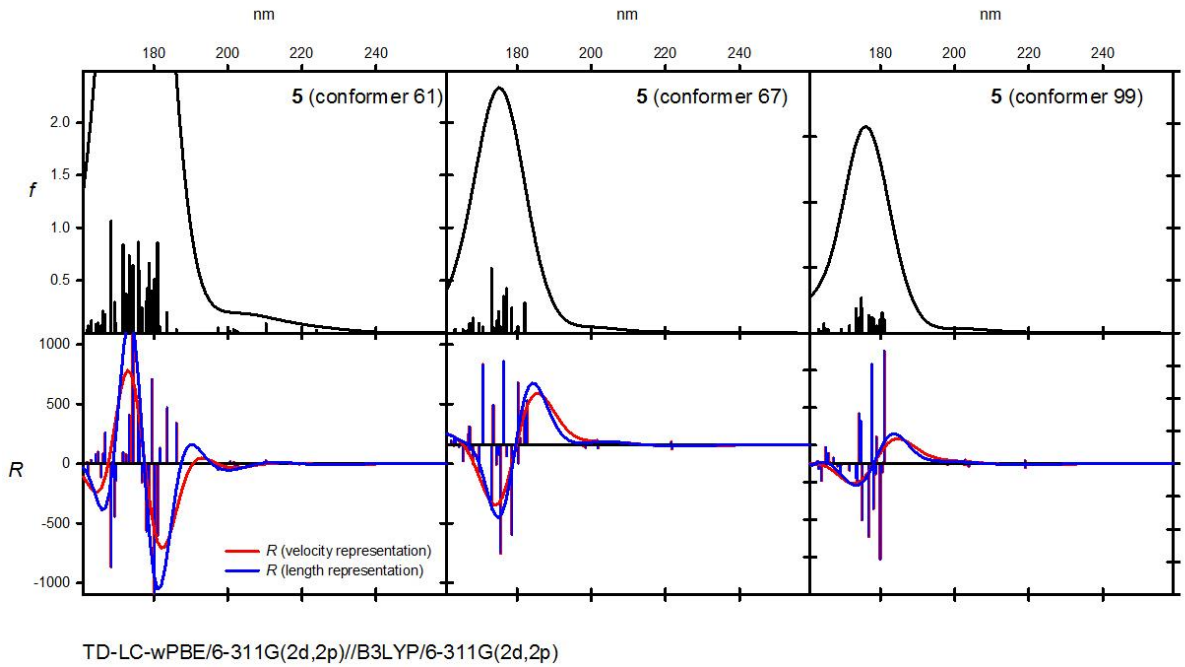
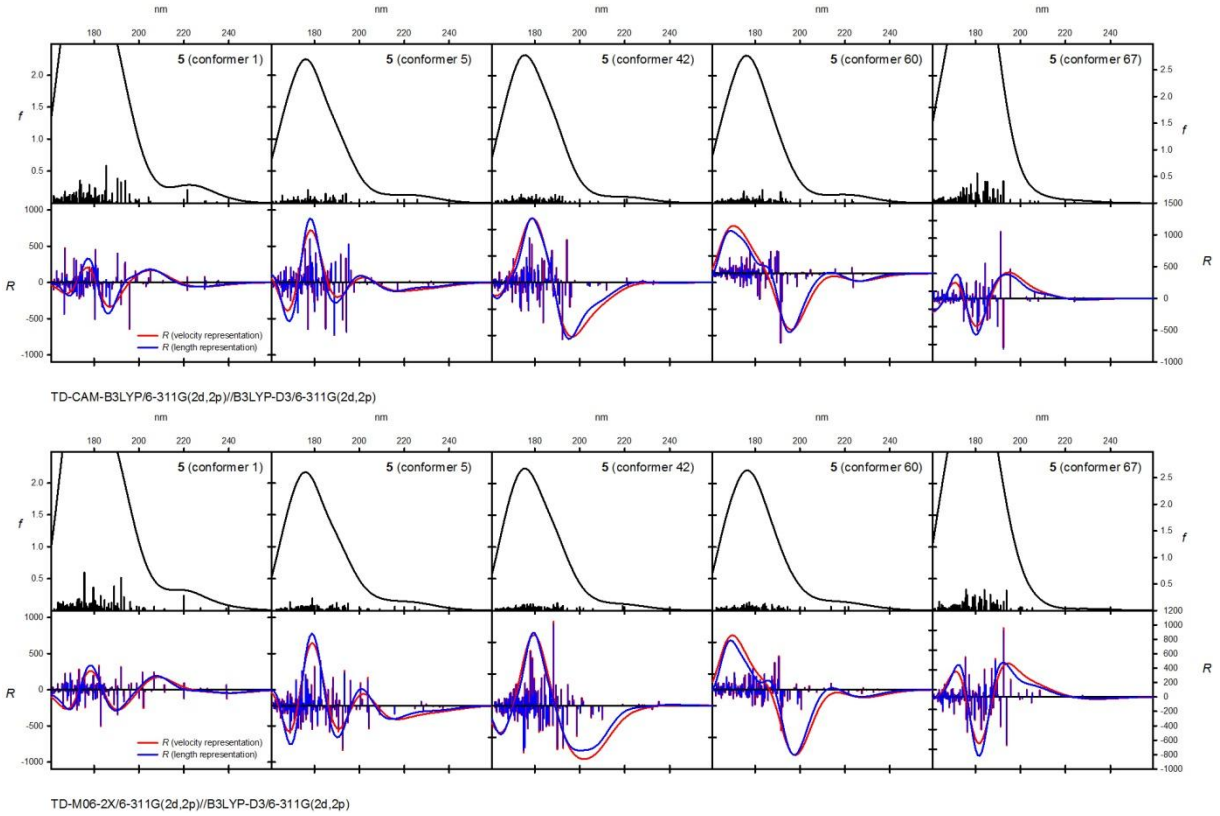


Figure F3. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **5** optimized at the B3LYP/6-311G(2d,2p) level. Wavelengths were not corrected.



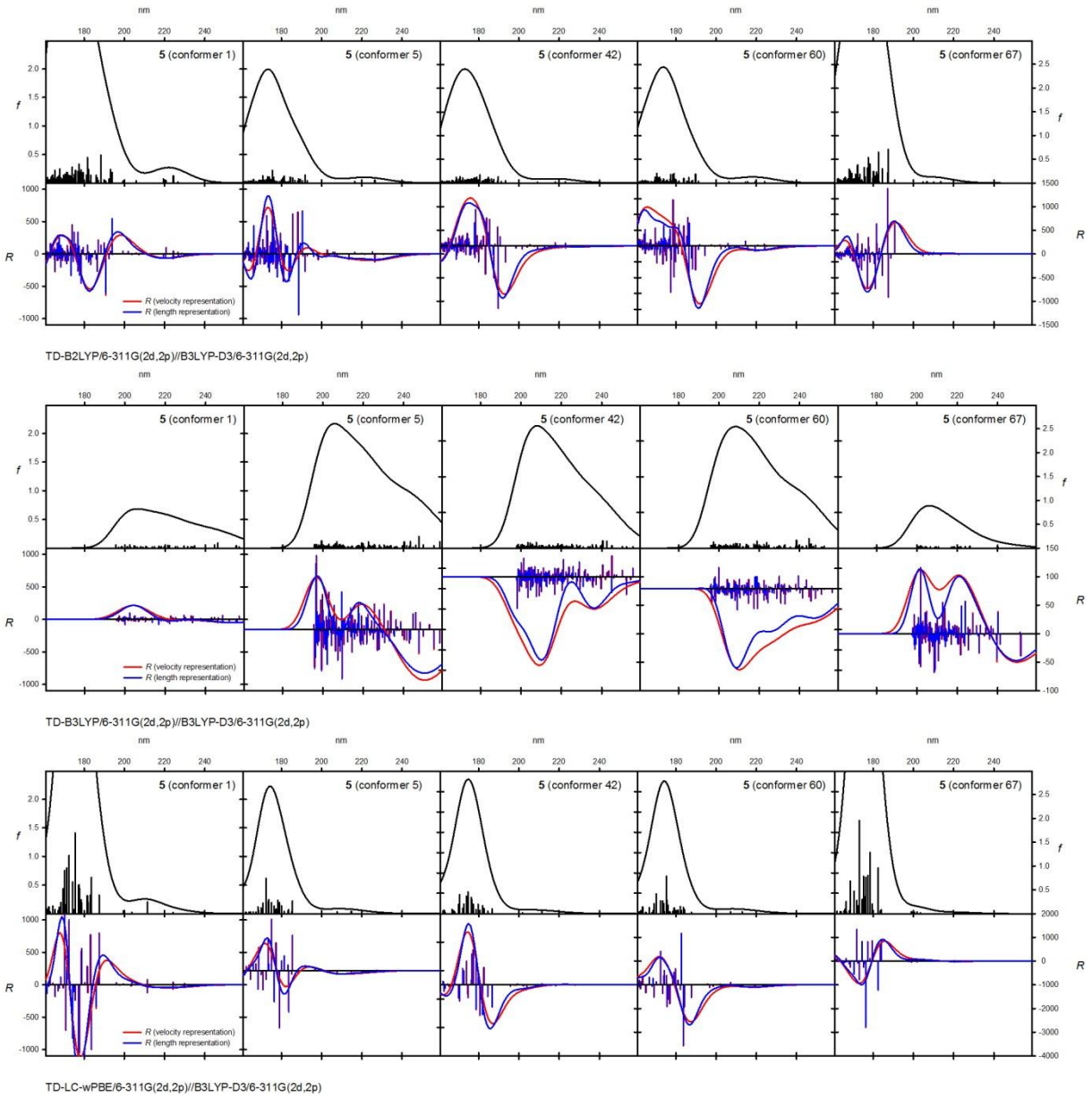
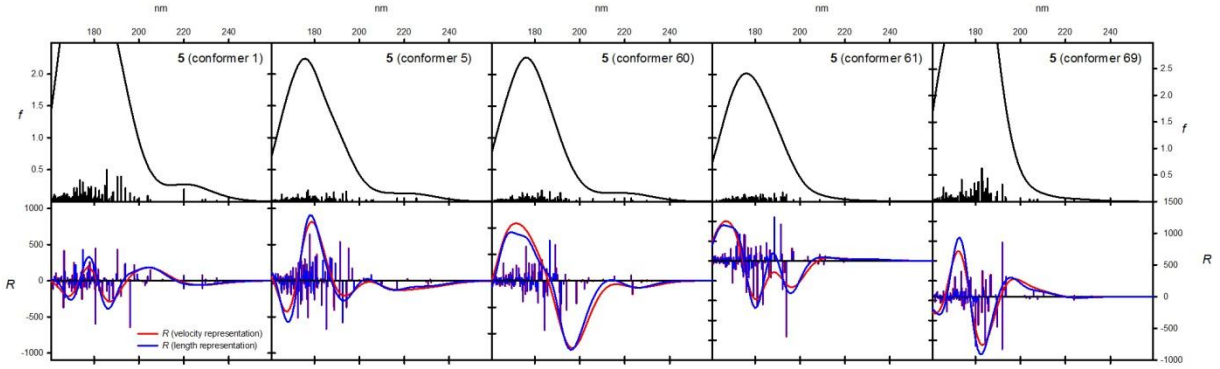
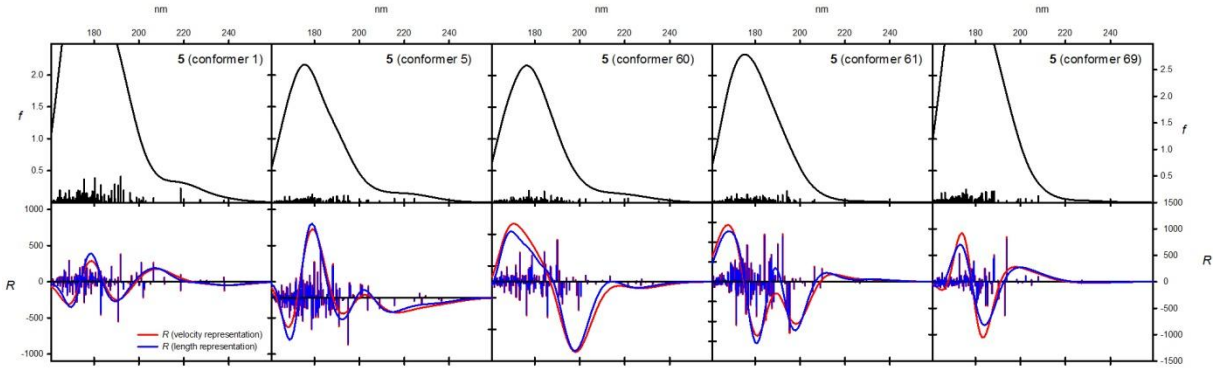


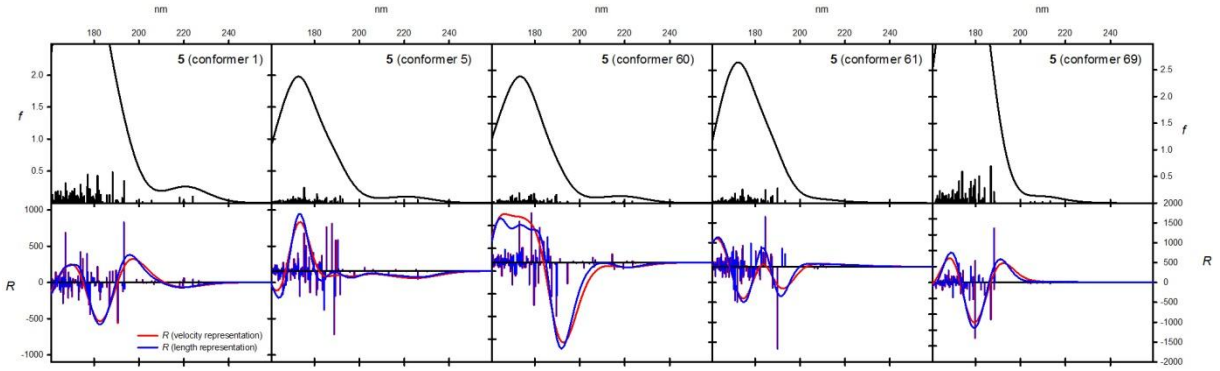
Figure F4. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **5** optimized at the B3LYP-GD3BJ/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)

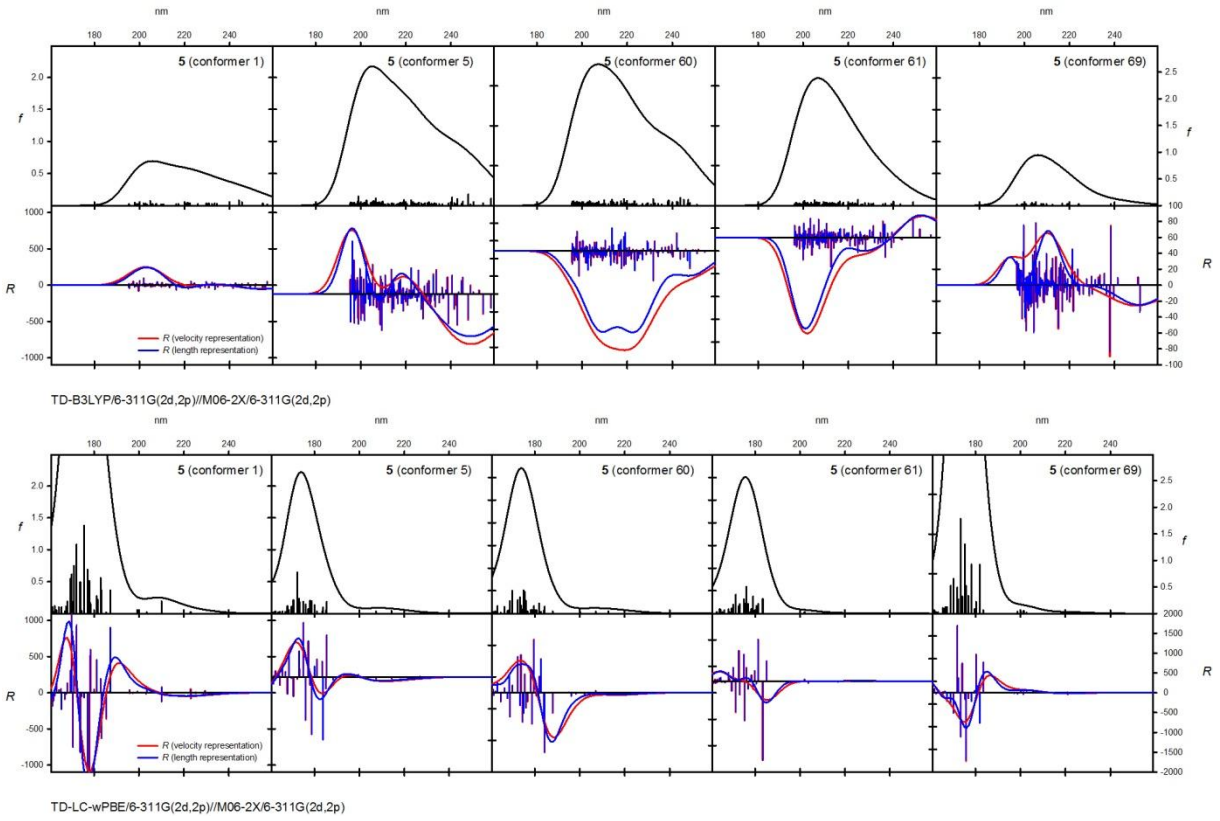
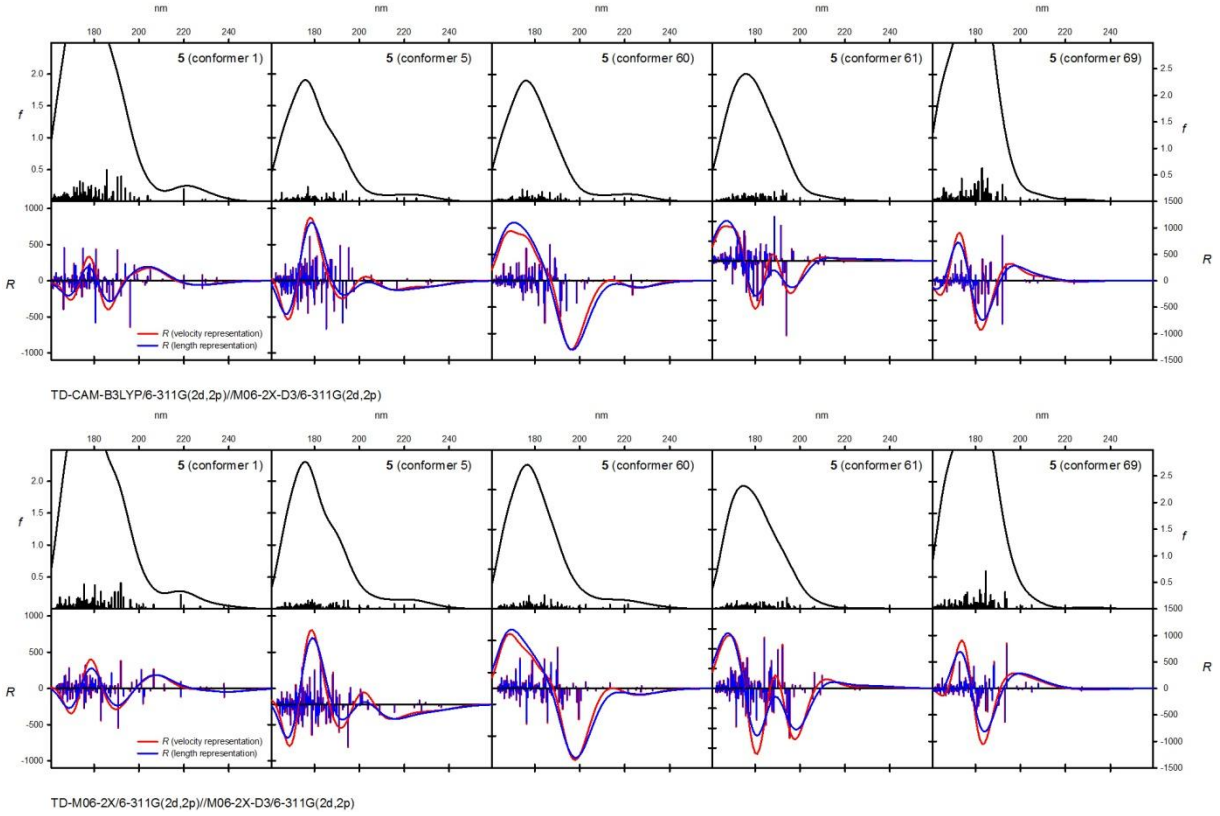


Figure F5. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **5** optimized at the M06-2X/6-311G(2d,2p) level. Wavelengths were not corrected.



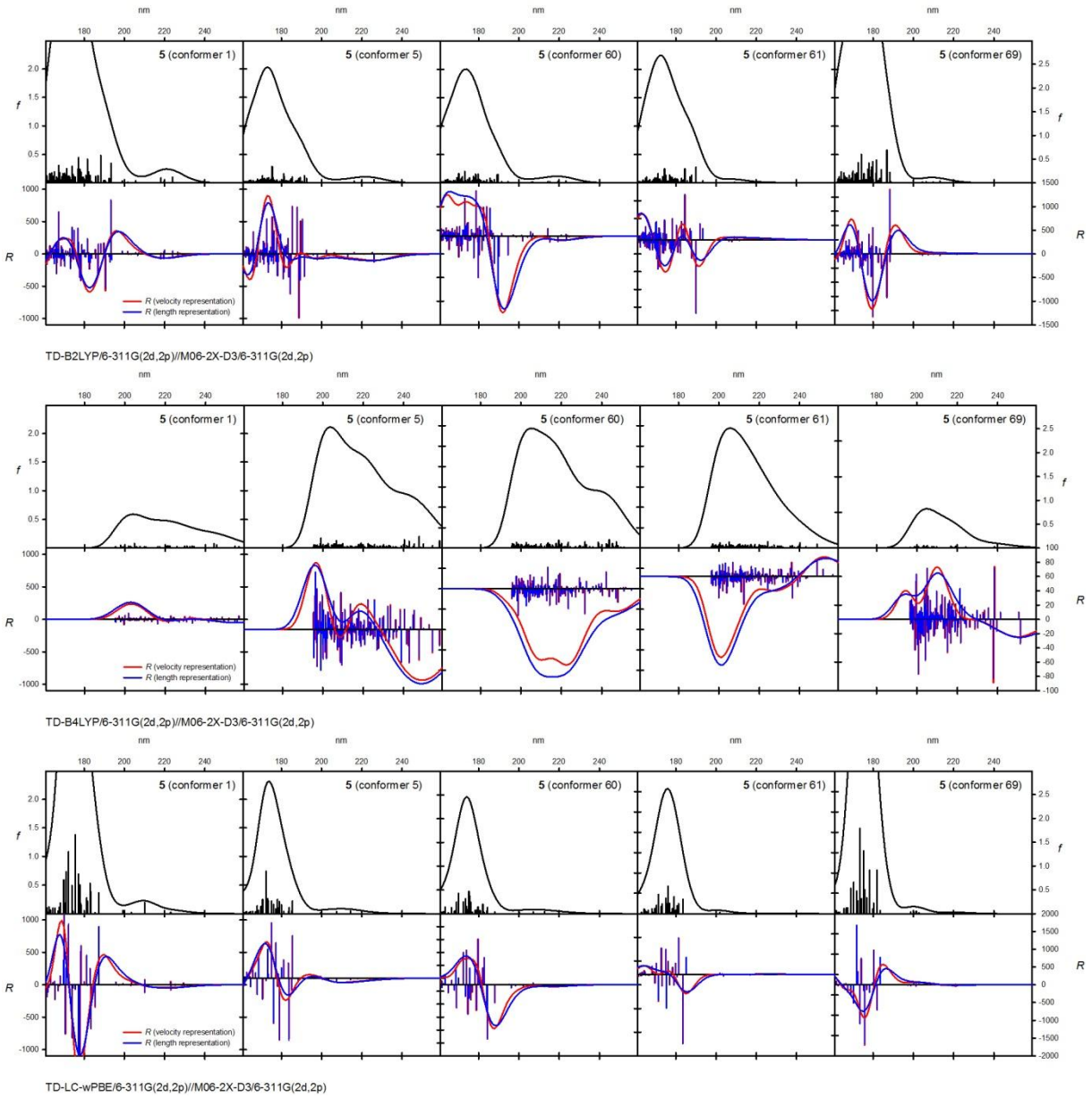
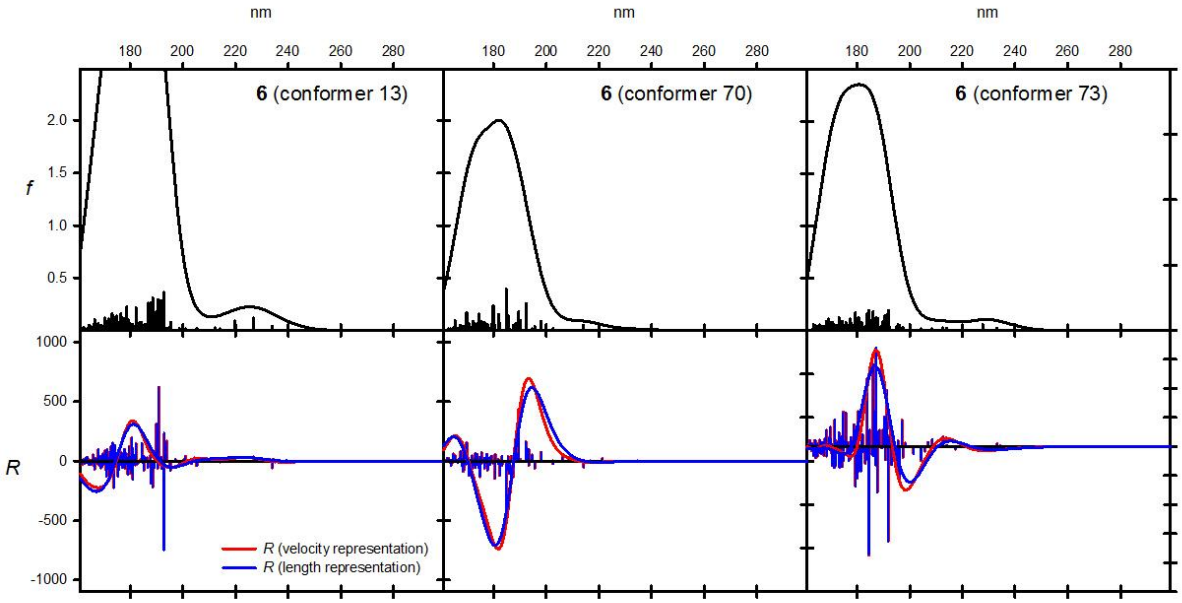
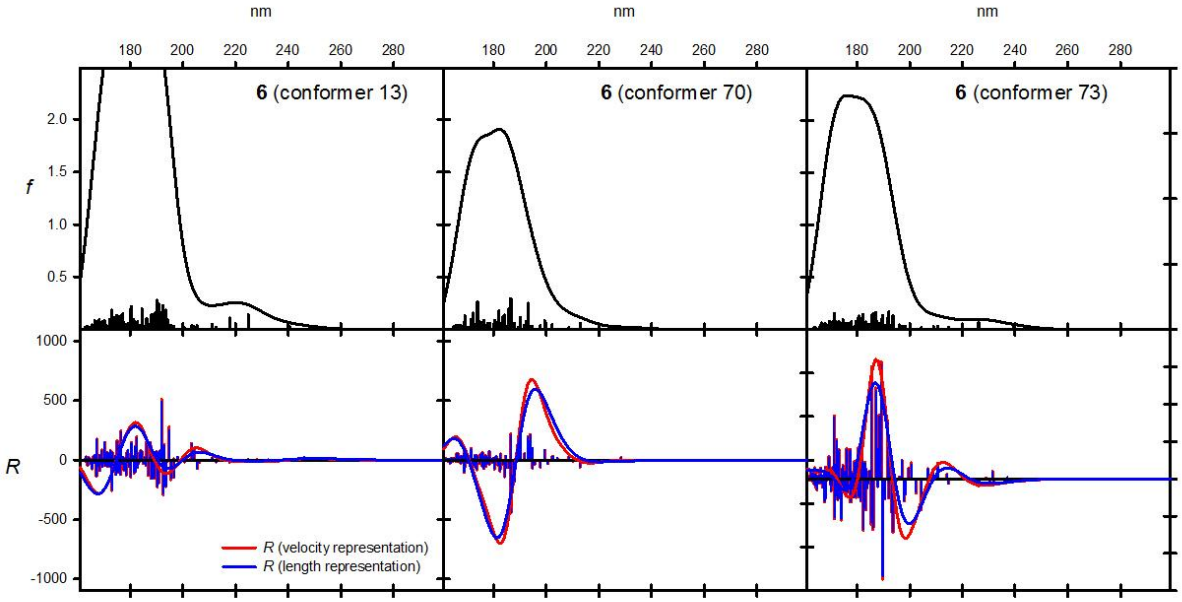


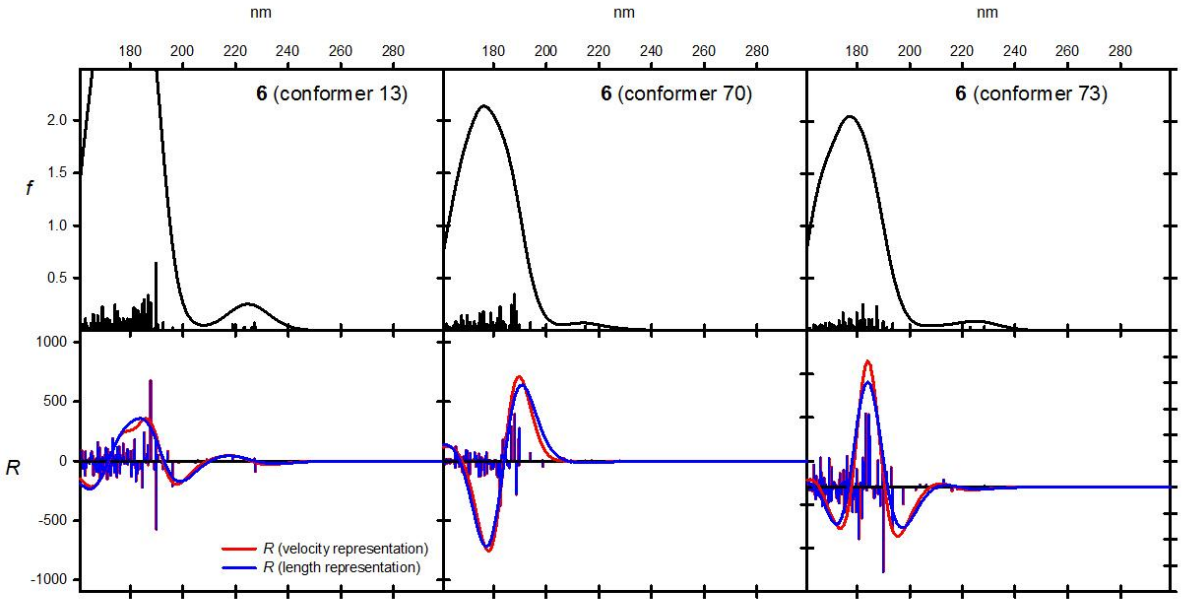
Figure F6. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **5** optimized at the M06-2X-D3/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311G(2d,2p)//B97D3/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B97D3/6-311G(2d,2p)



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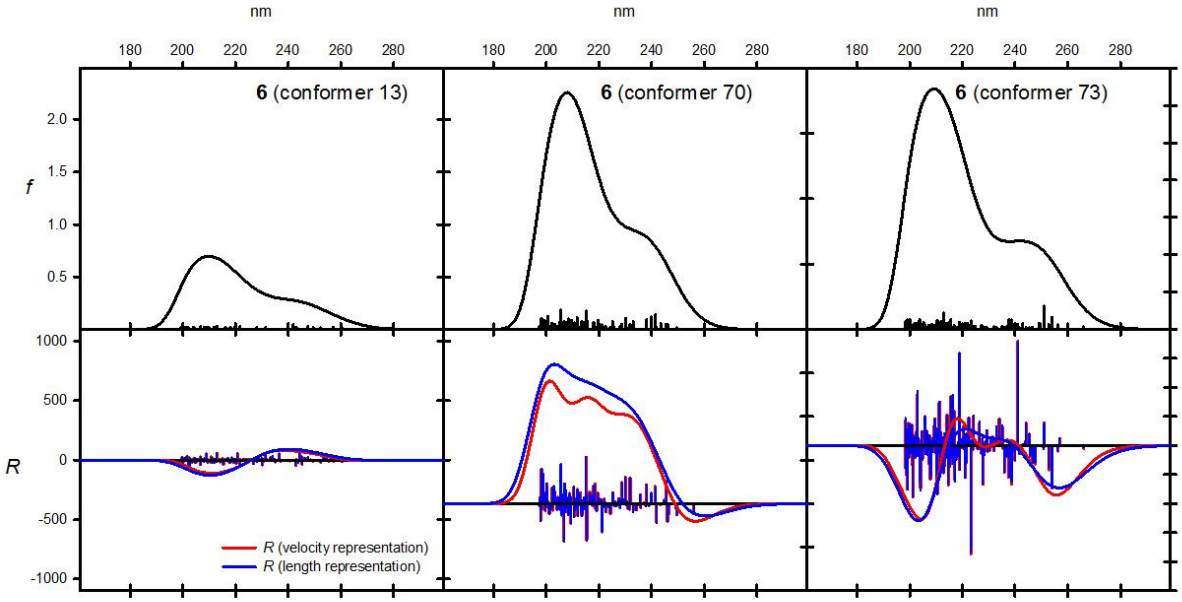

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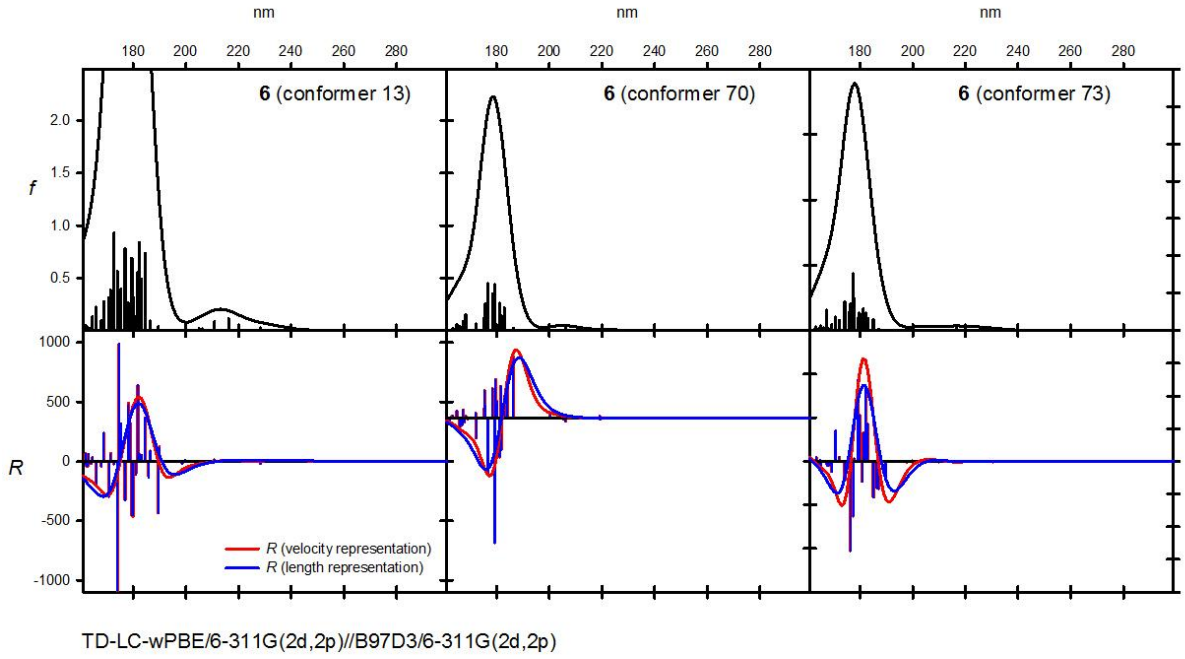
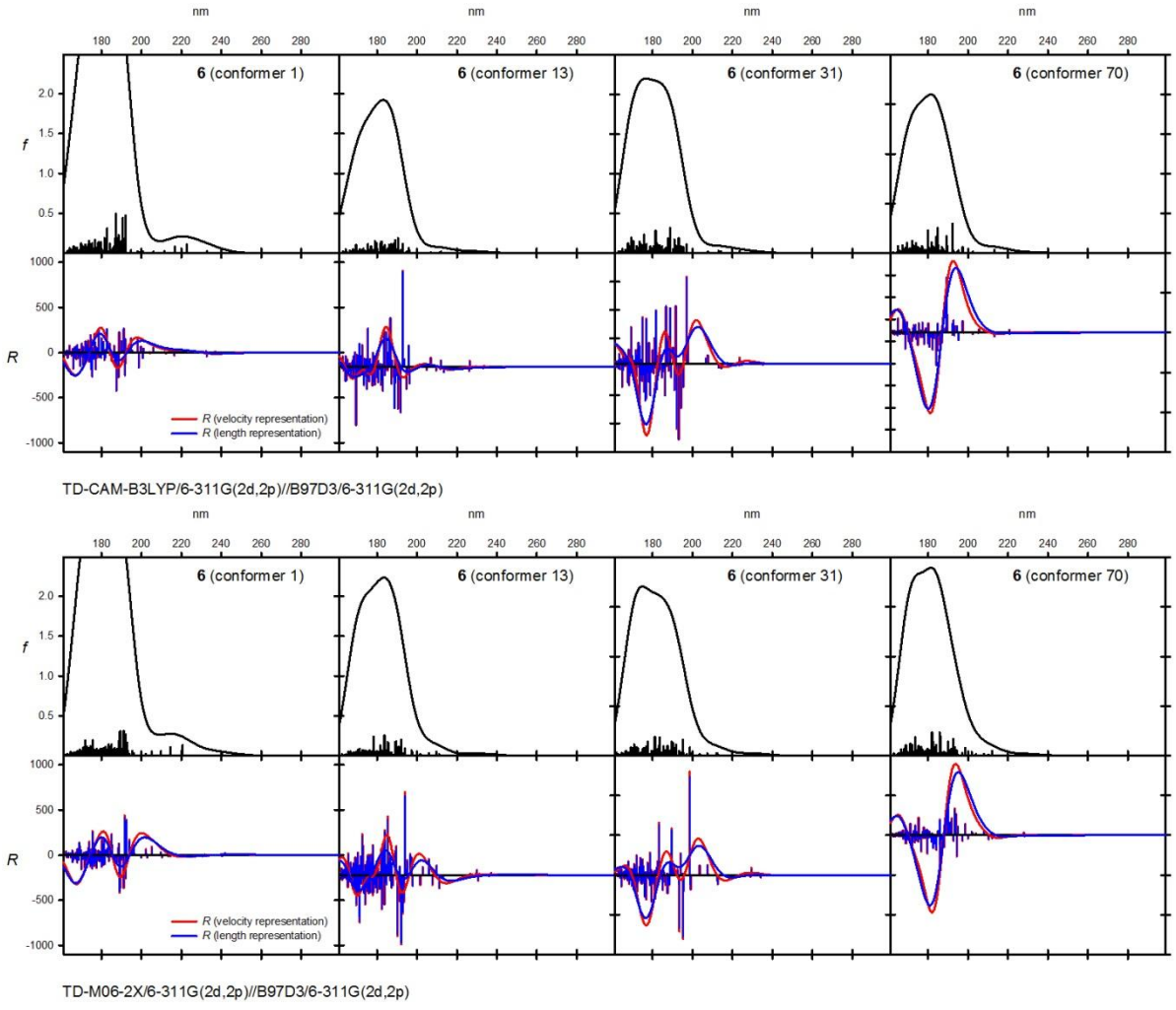


Figure G1. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **6** optimized at the B97-D/6-311G(2d,2p) level. Wavelengths were not corrected.



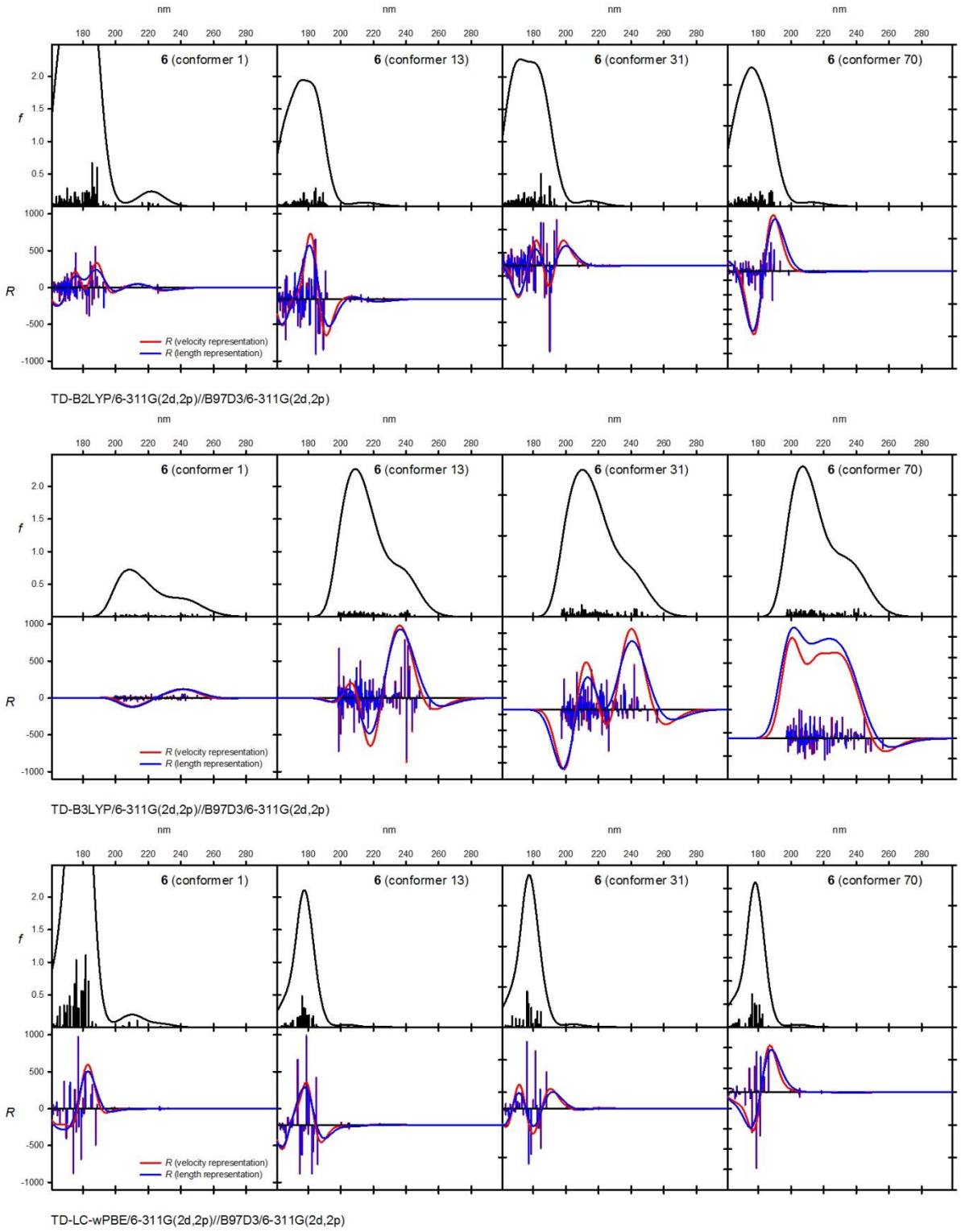
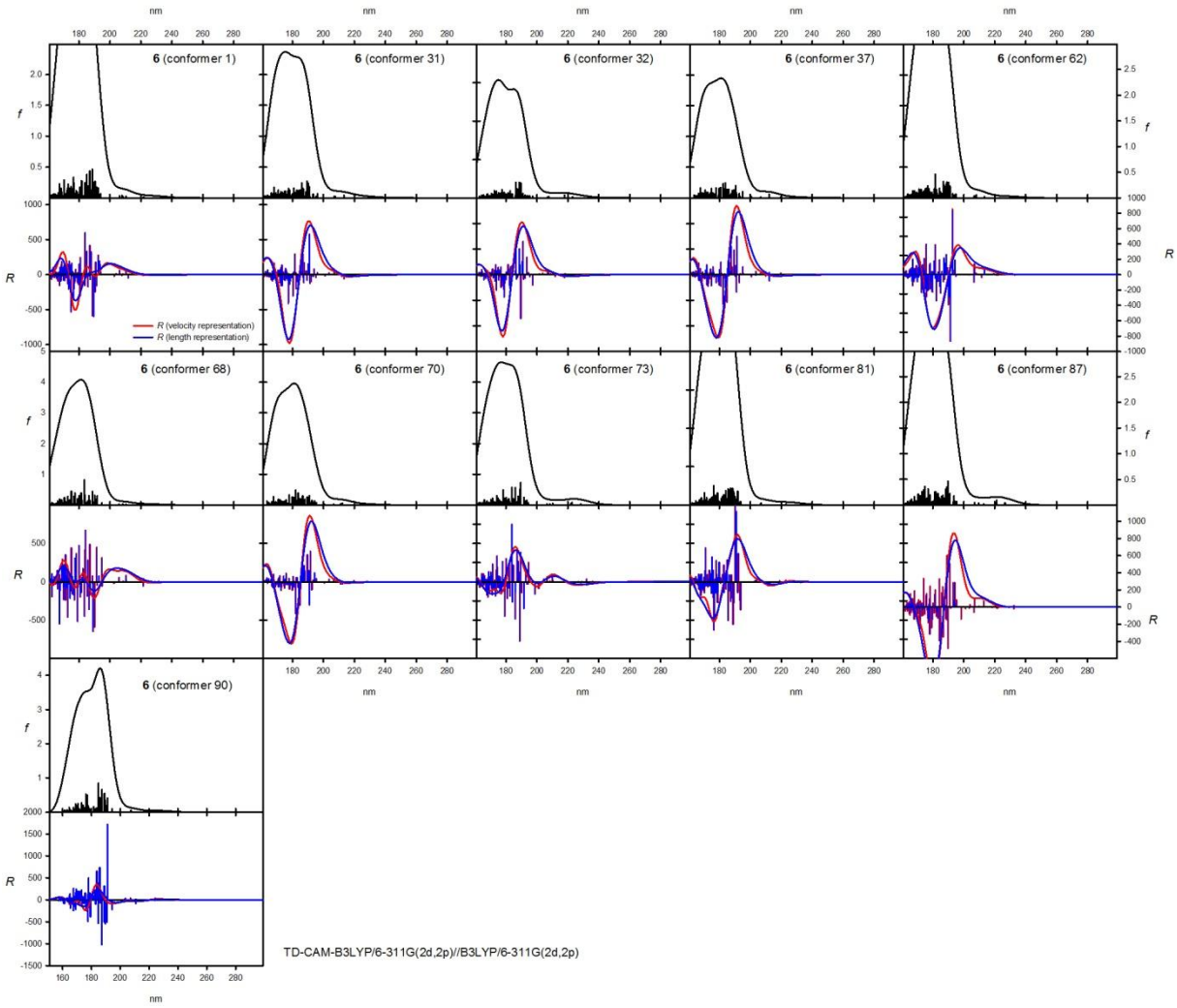


Figure G2. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **6** optimized at the B97-D3/6-311G(2d,2p) level. Wavelengths were not corrected.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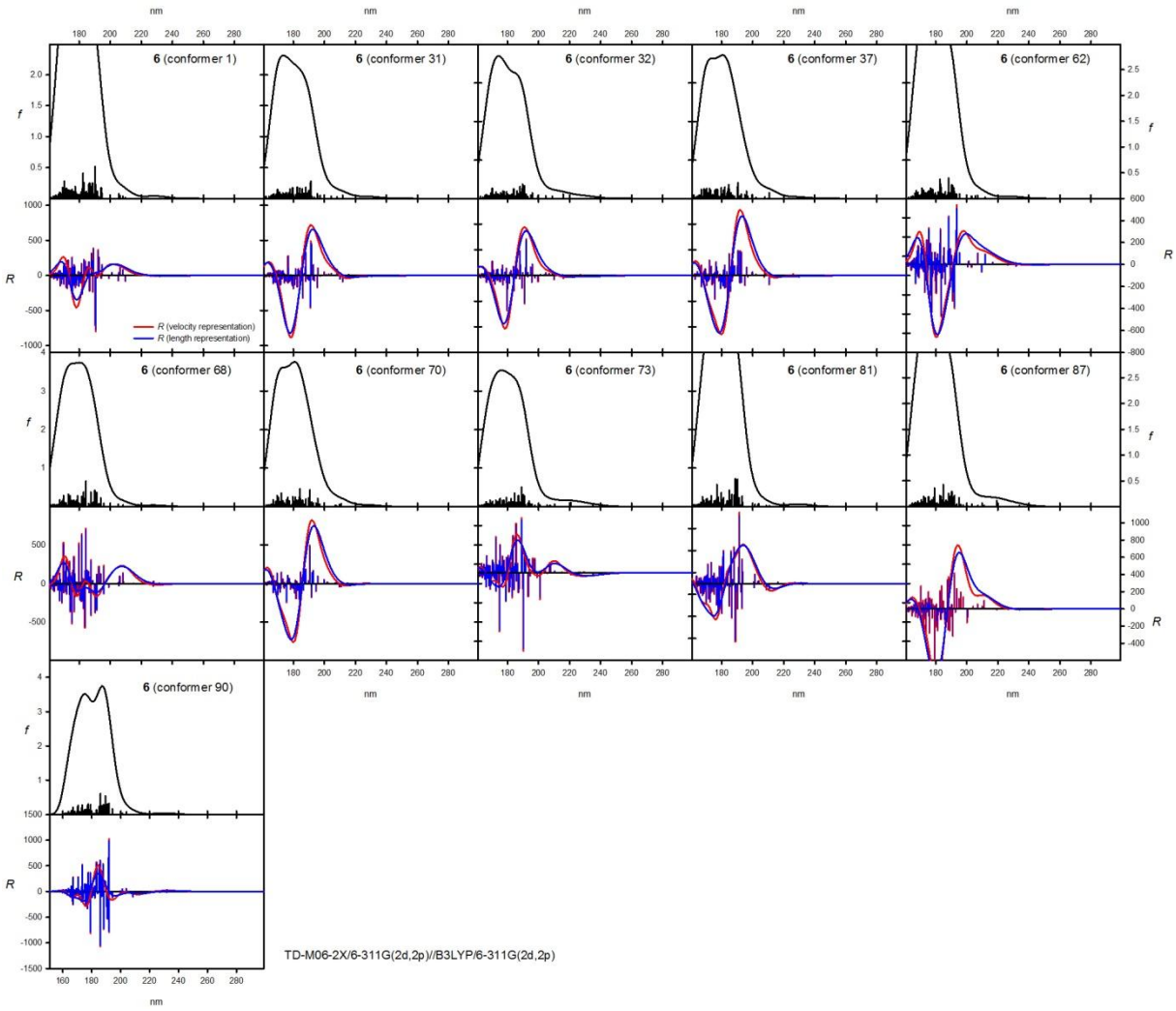
6 (conformer 31)
6 (conformer 32)
6 (conformer 37)
6 (conformer 62)
6 (conformer 68)
6 (conformer 70)
6 (conformer 73)
6 (conformer 81)
6 (conformer 87)
6 (conformer 90)
R (velocity representation)
R (length representation)
f
R
nm
TD-CAM-B3LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)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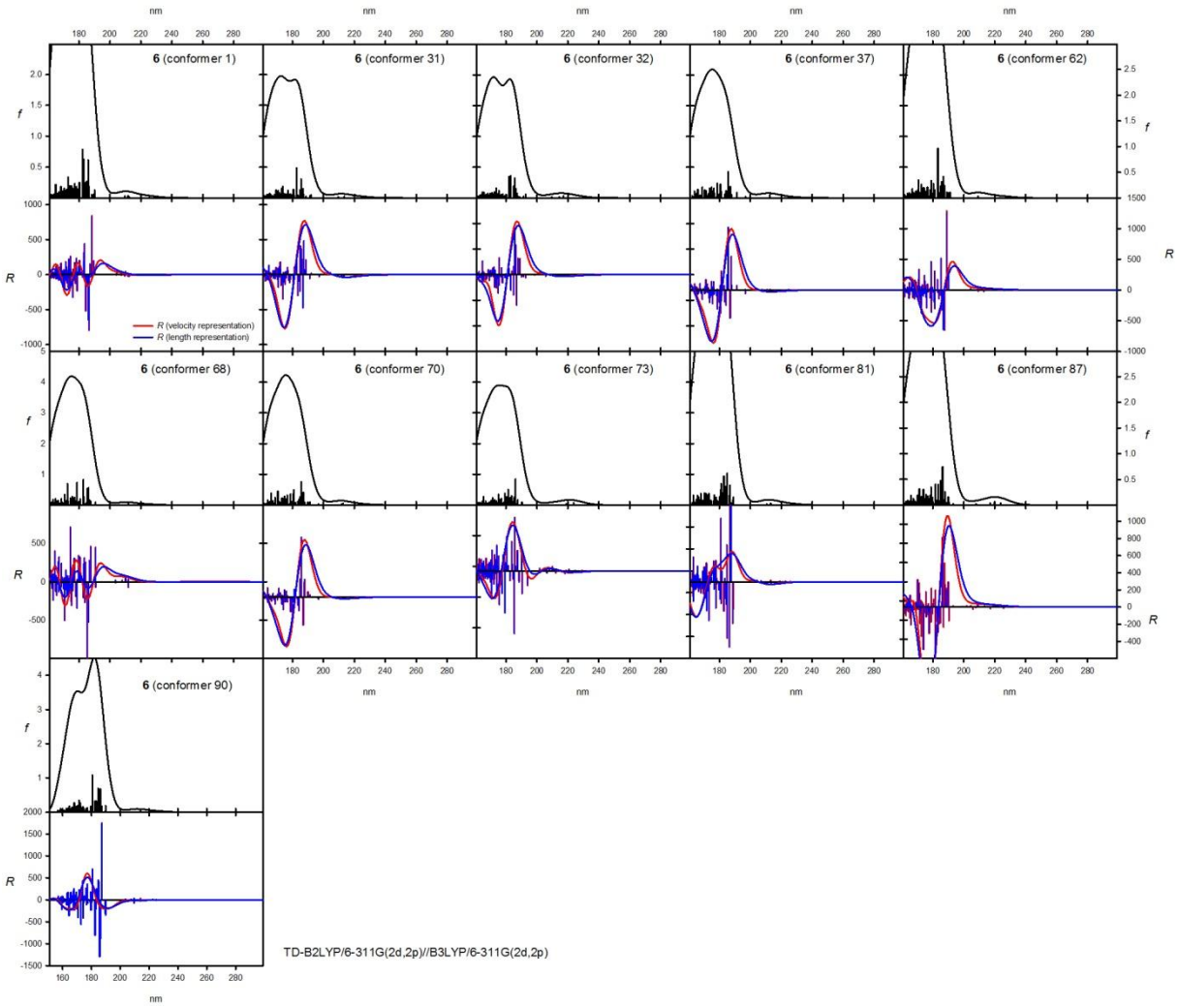
6 (conformer 32)
6 (conformer 37)
6 (conformer 62)
6 (conformer 68)
6 (conformer 70)
6 (conformer 73)
6 (conformer 81)
6 (conformer 87)
6 (conformer 90)
R (velocity representation)
R (length representation)
f
R
nm
TD-M06-2X/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)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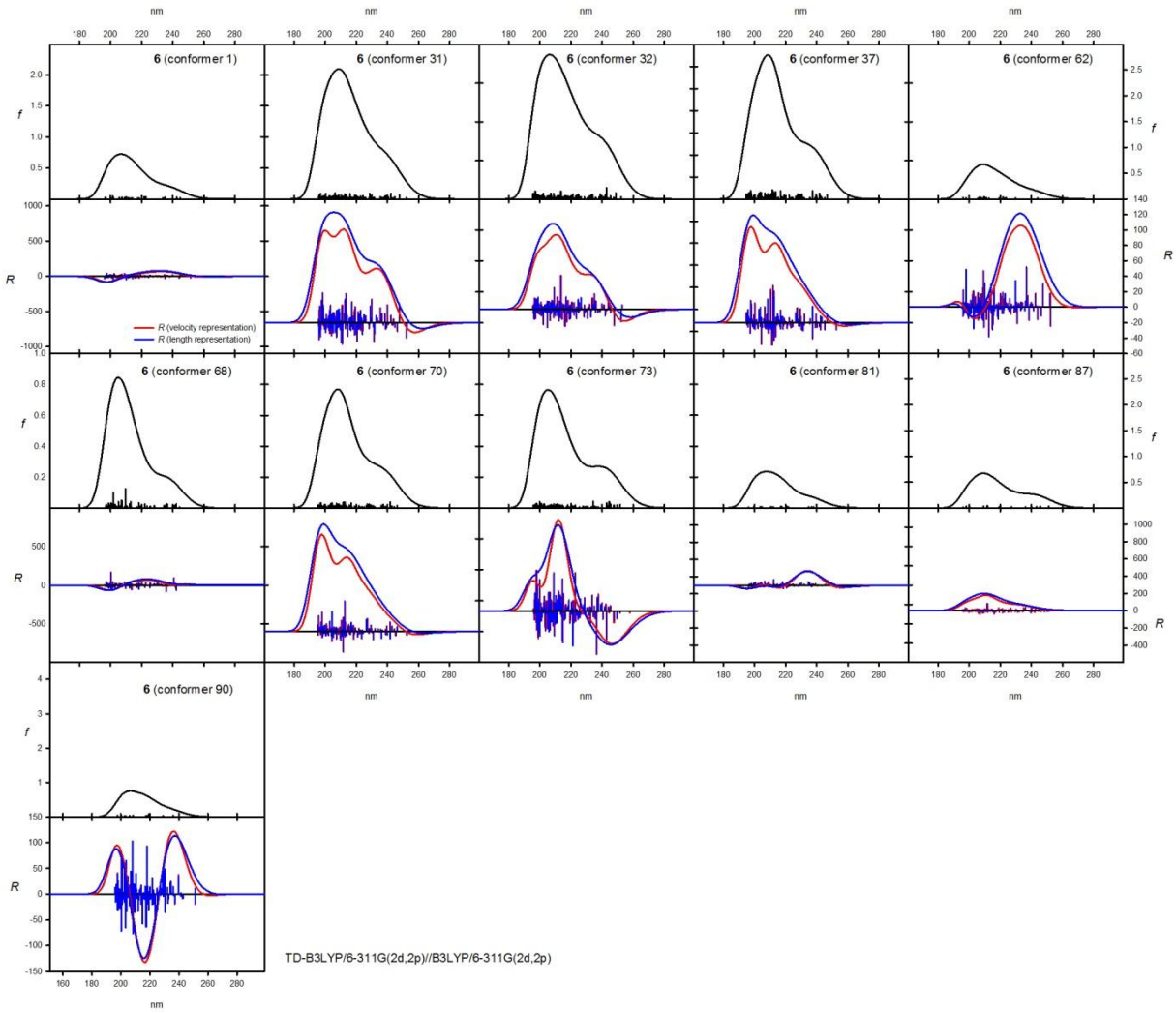
6 (conformer 62)
6 (conformer 68)
6 (conformer 70)
6 (conformer 73)
6 (conformer 81)
6 (conformer 87)
6 (conformer 90)
f
R
nm
R (velocity representation)
R (length representation)
TD-B2LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)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6 (conformer 68)
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6 (conformer 73)
6 (conformer 81)
6 (conformer 87)
6 (conformer 90)
f
R
nm
R (velocity representation)
R (length representation)
TD-B3LYP/6-311G(2d,2p)//B3LYP/6-311G(2d,2p)

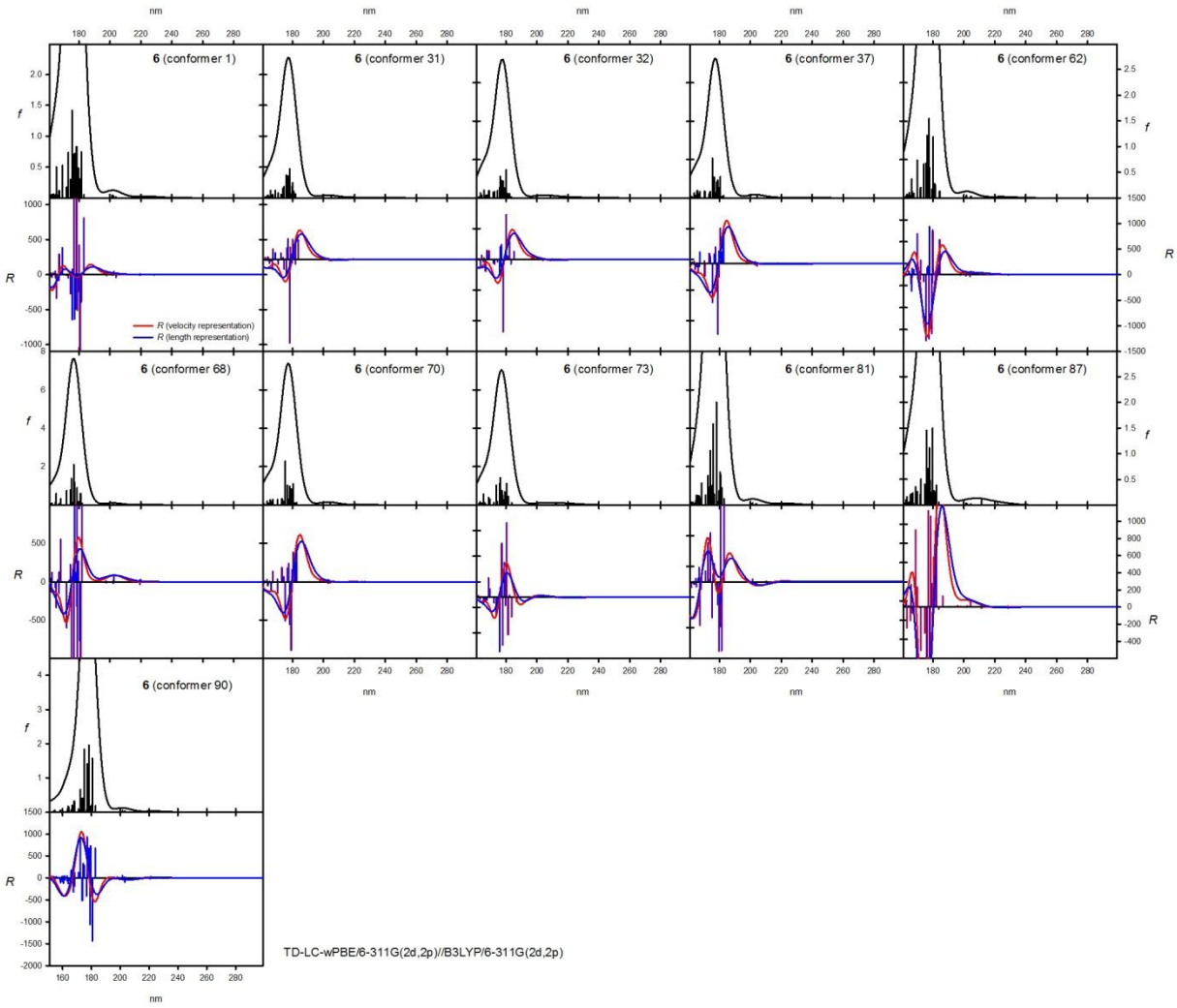
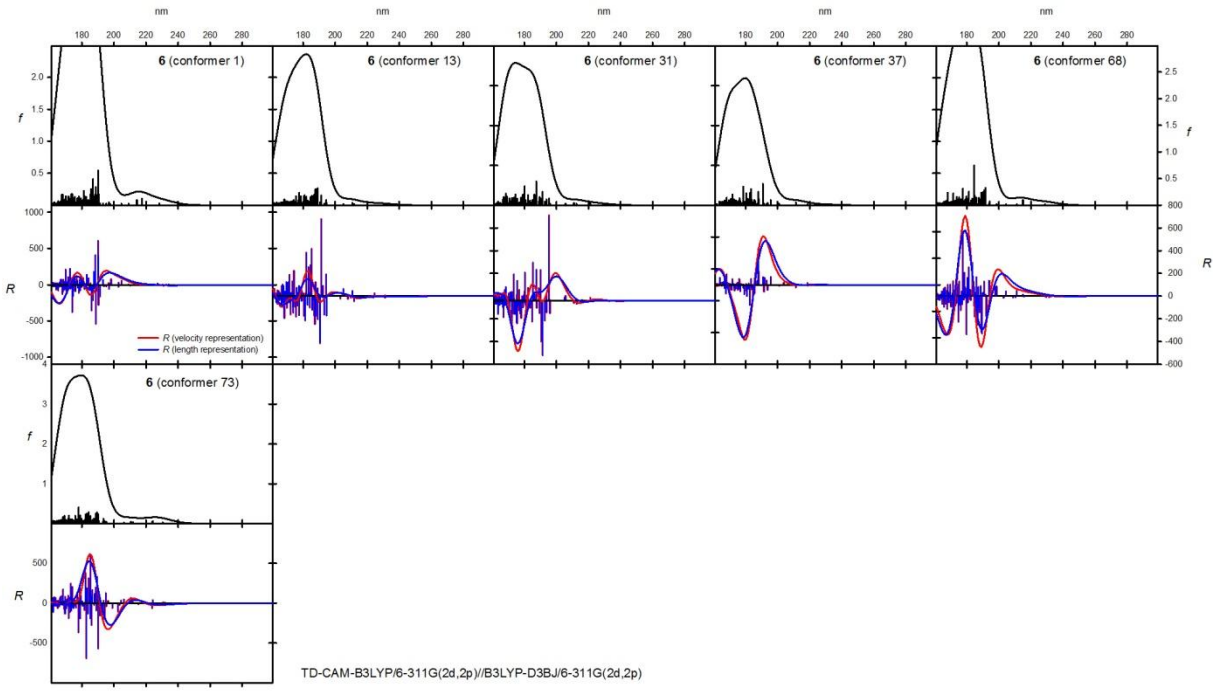
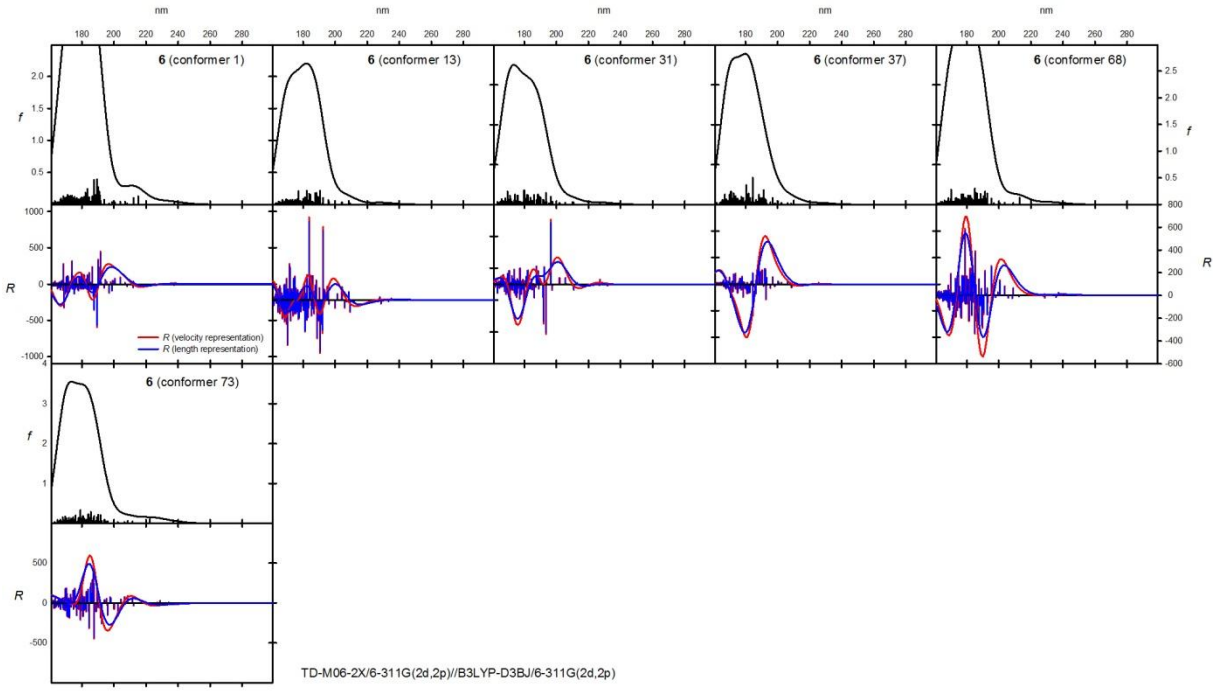


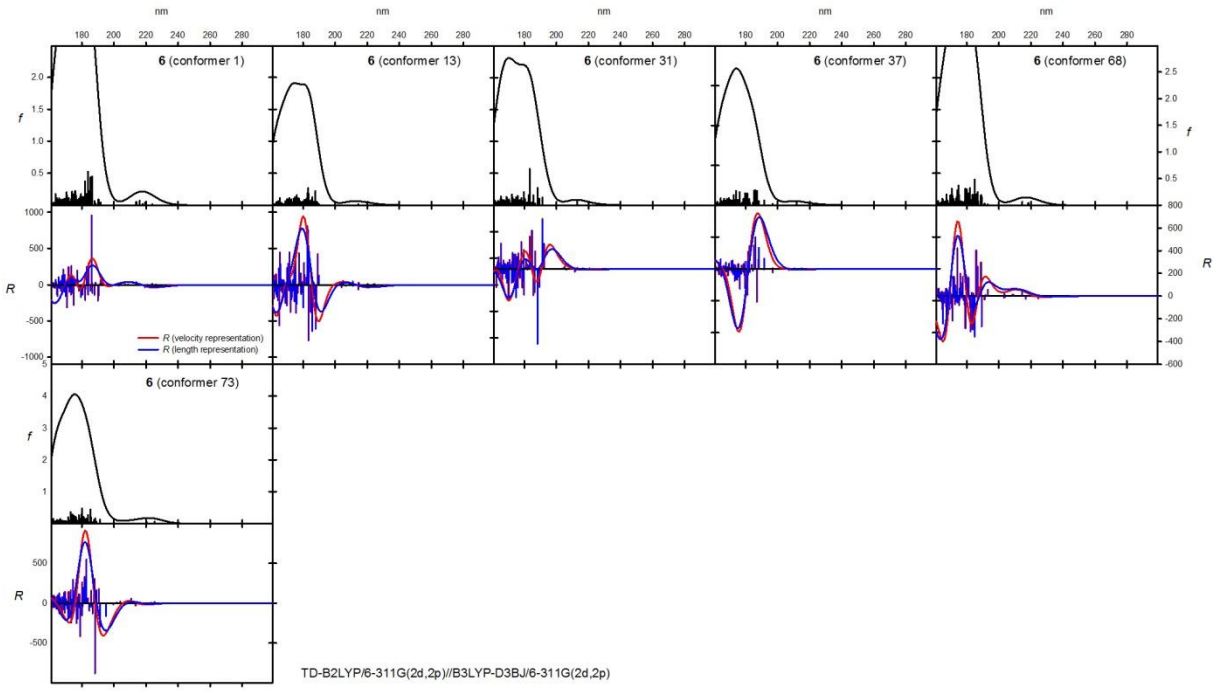
Figure G3. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **6** optimized at the B3LYP/6-311G(2d,2p) level. Wavelengths were not corrected.



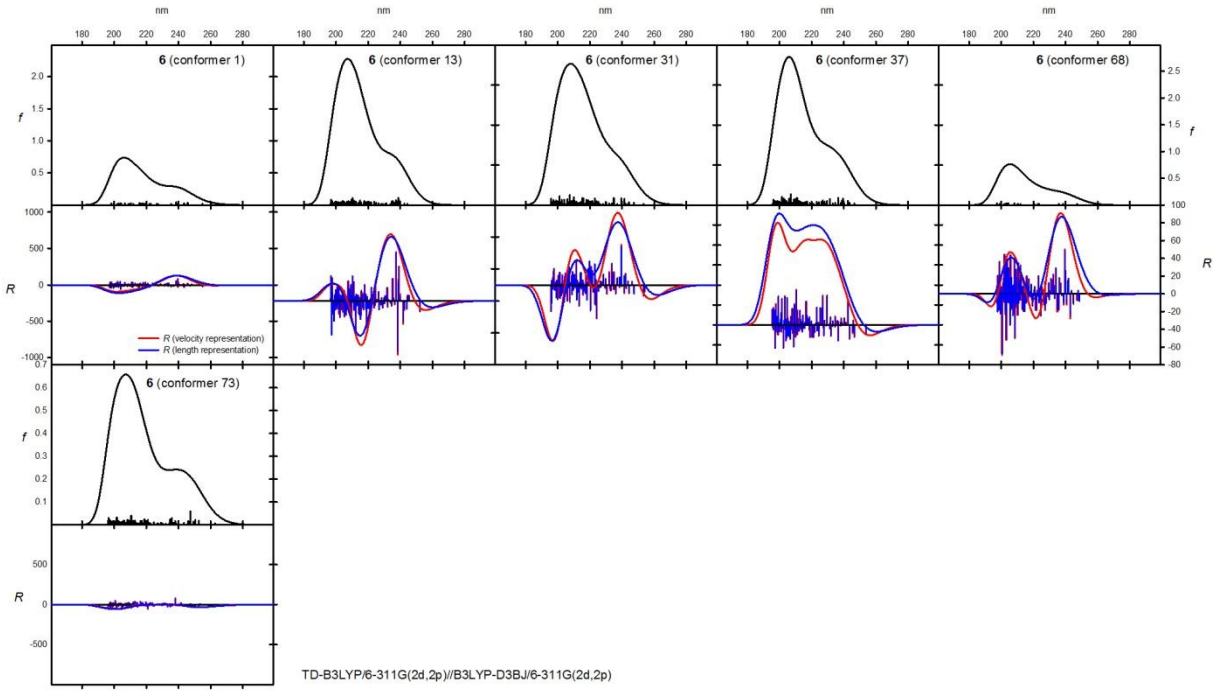
TD-CAM-B3LYP/6-311G(2d,2p)//B3LYP-D3BJ/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B3LYP-D3BJ/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//B3LYP-D3BJ/6-311G(2d,2p)



TD-B3LYP/6-311G(2d,2p)//B3LYP-D3BJ/6-311G(2d,2p)

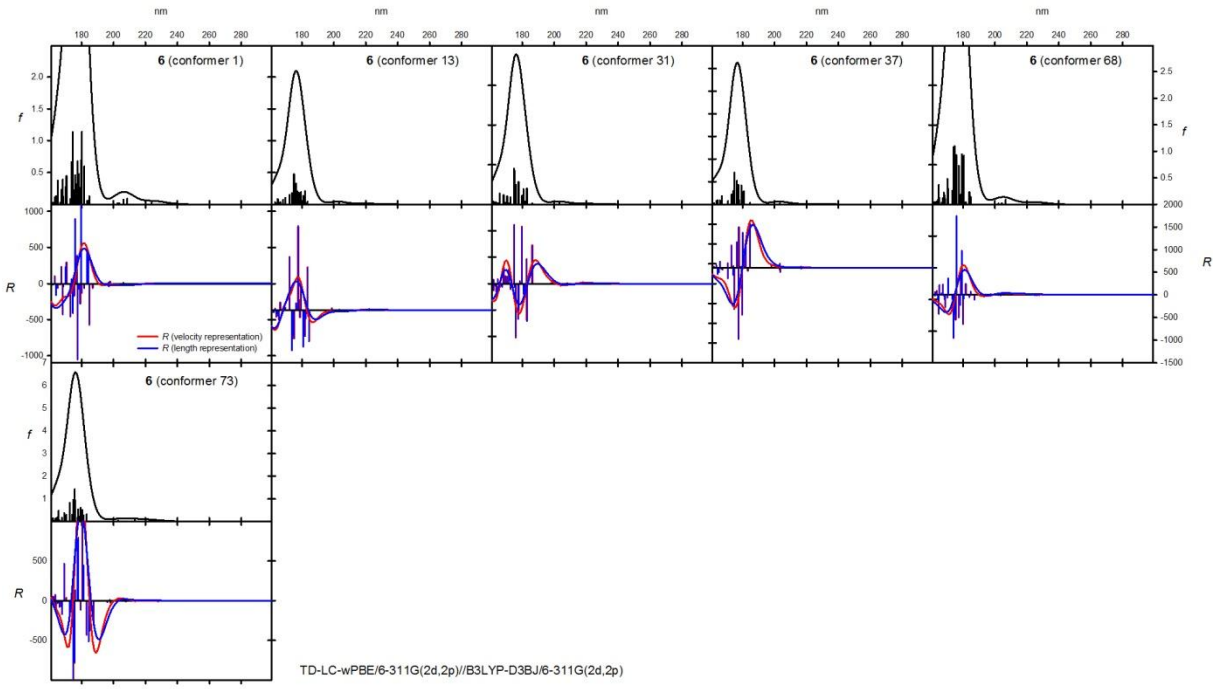
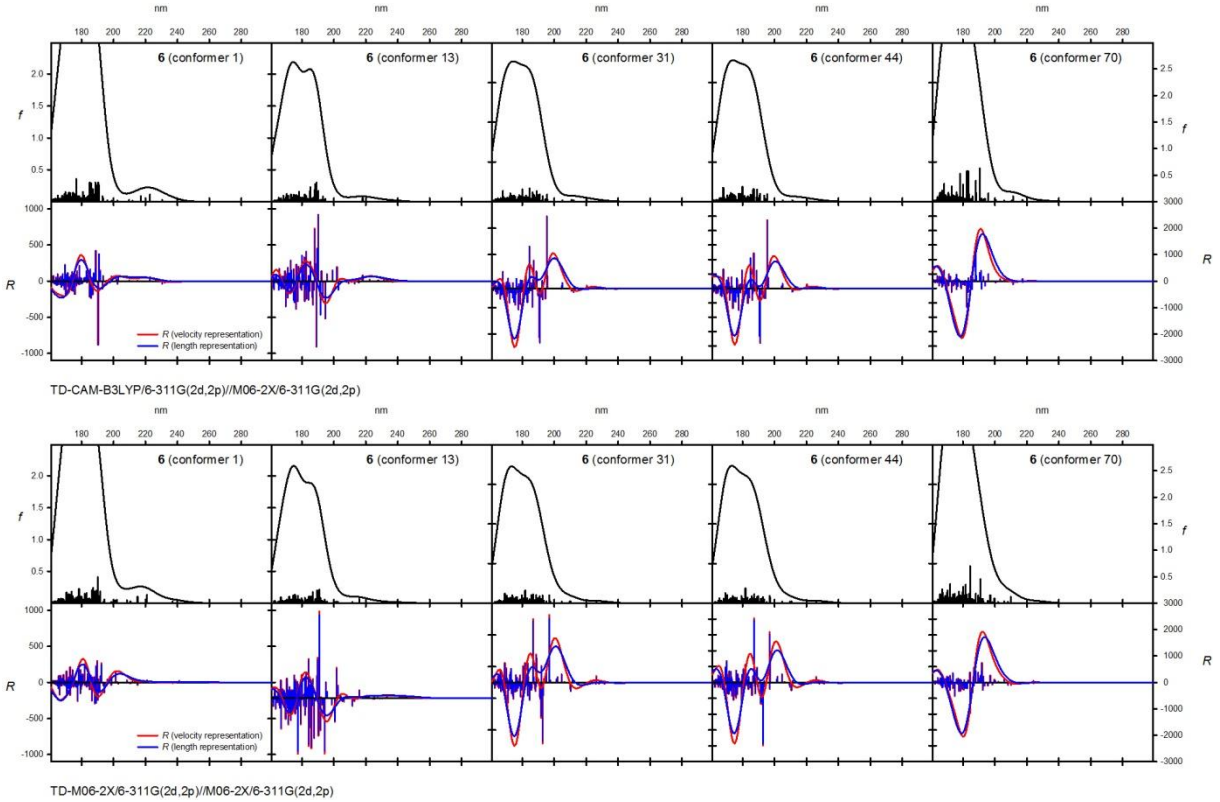


Figure G4. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **6** optimized at the B3LYP-GD3BJ/6-311G(2d,2p) level. Wavelengths were not corrected.



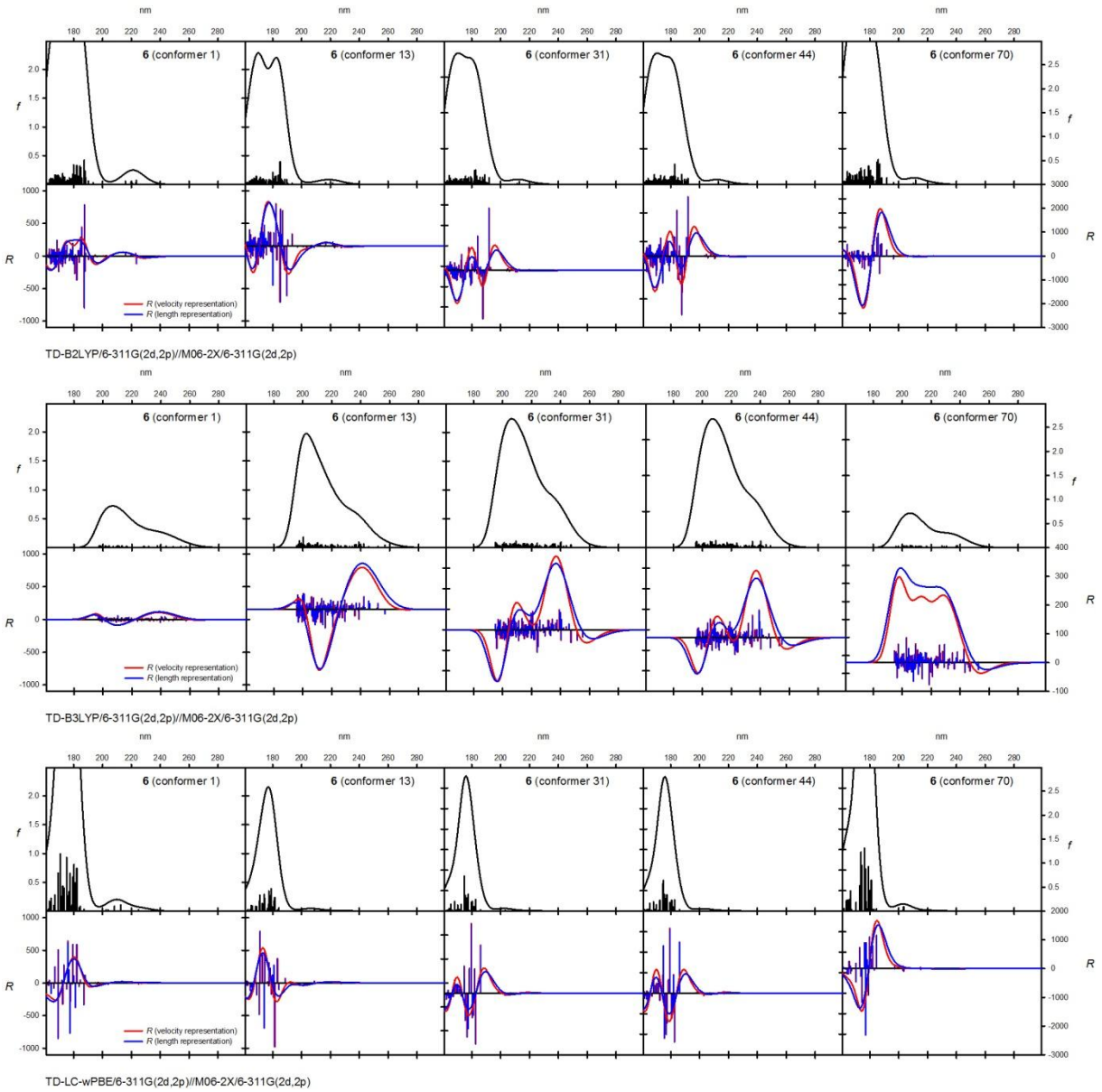
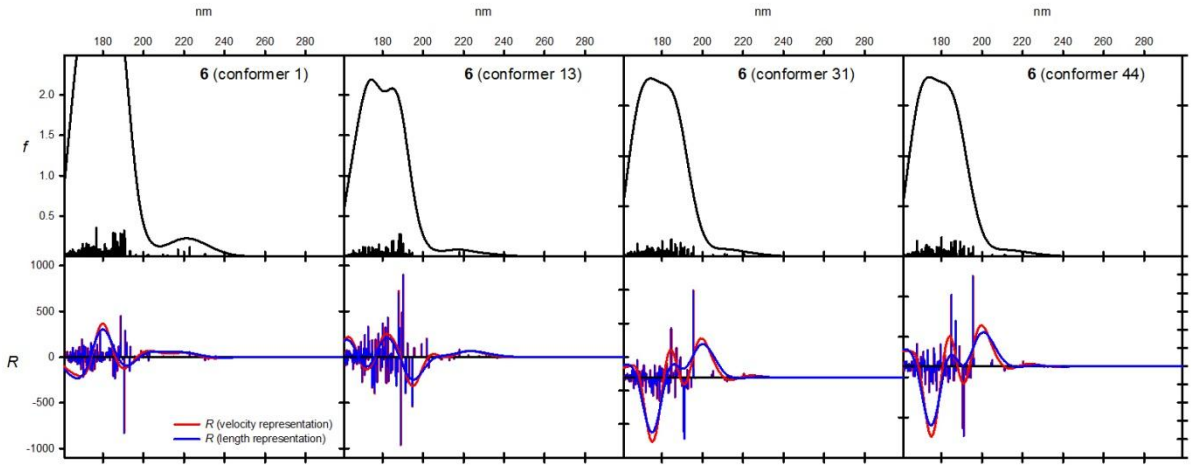
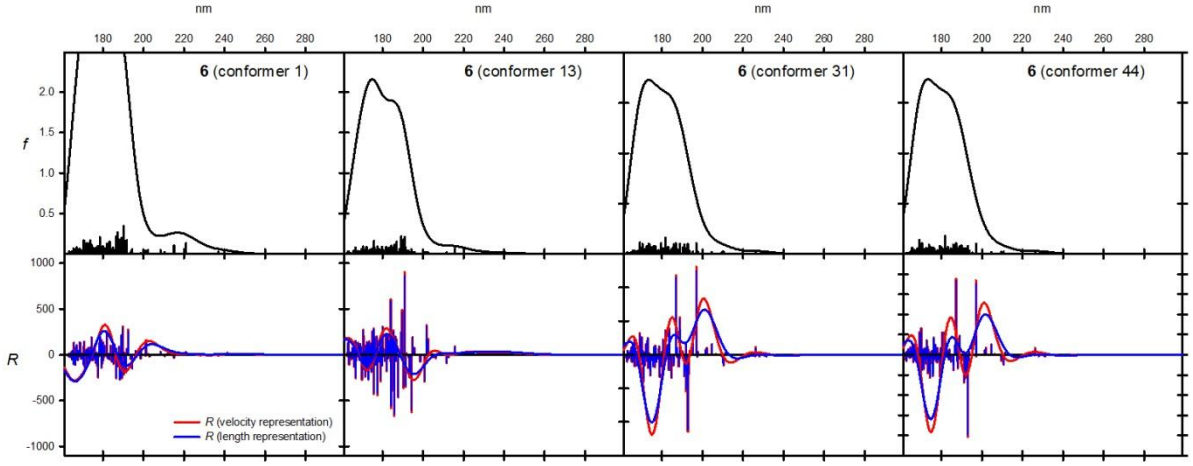


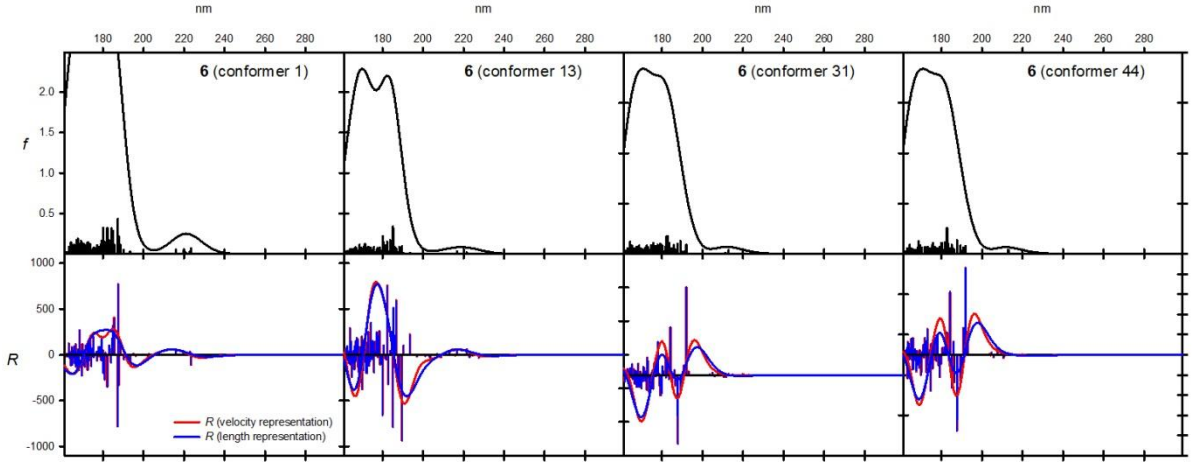
Figure G5. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **6** optimized at the M06-2X/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)

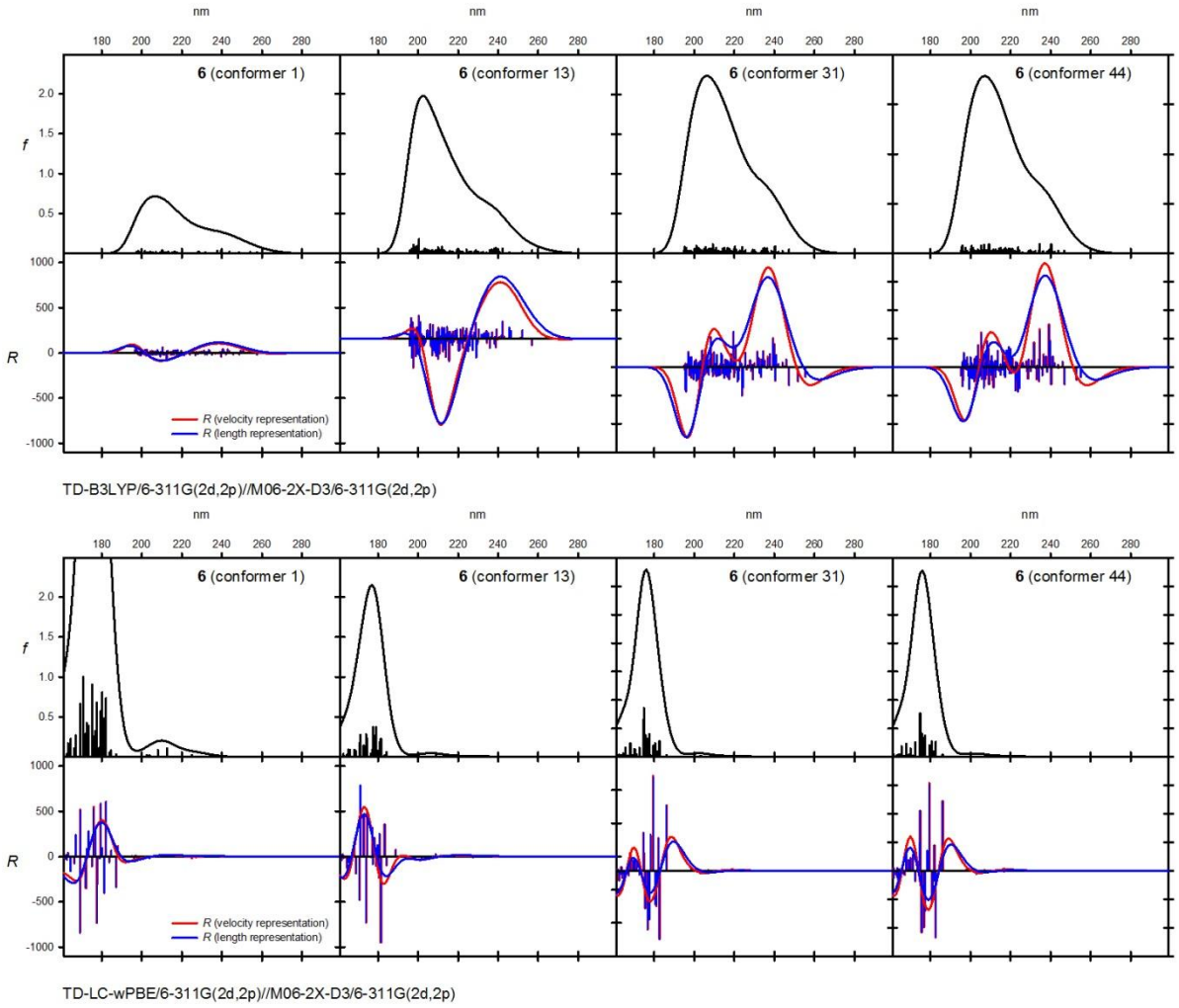
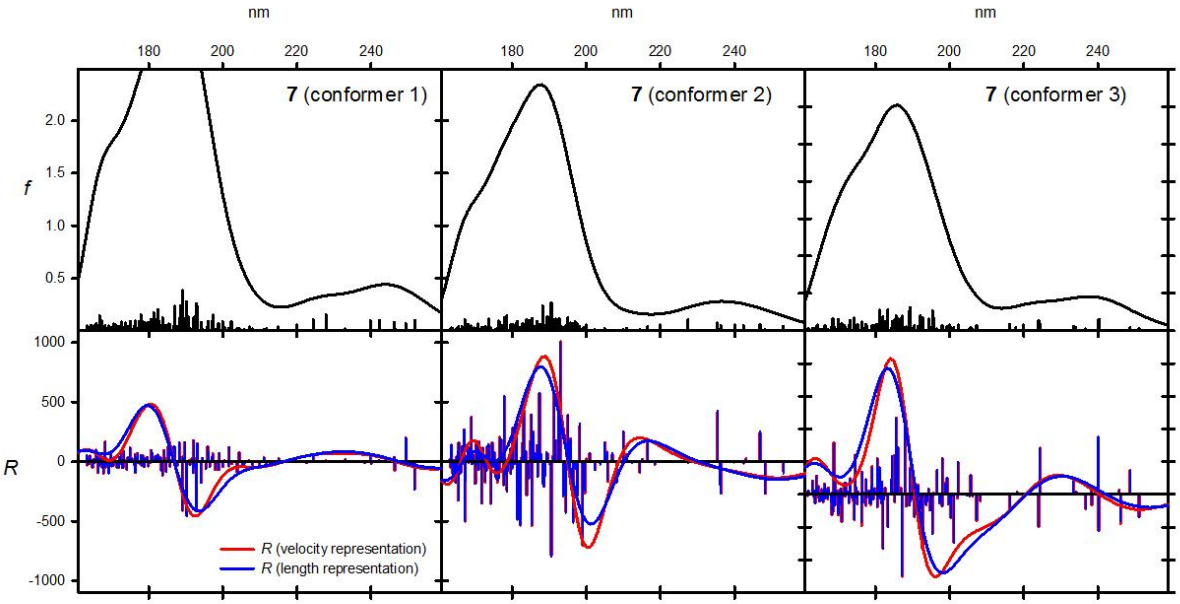
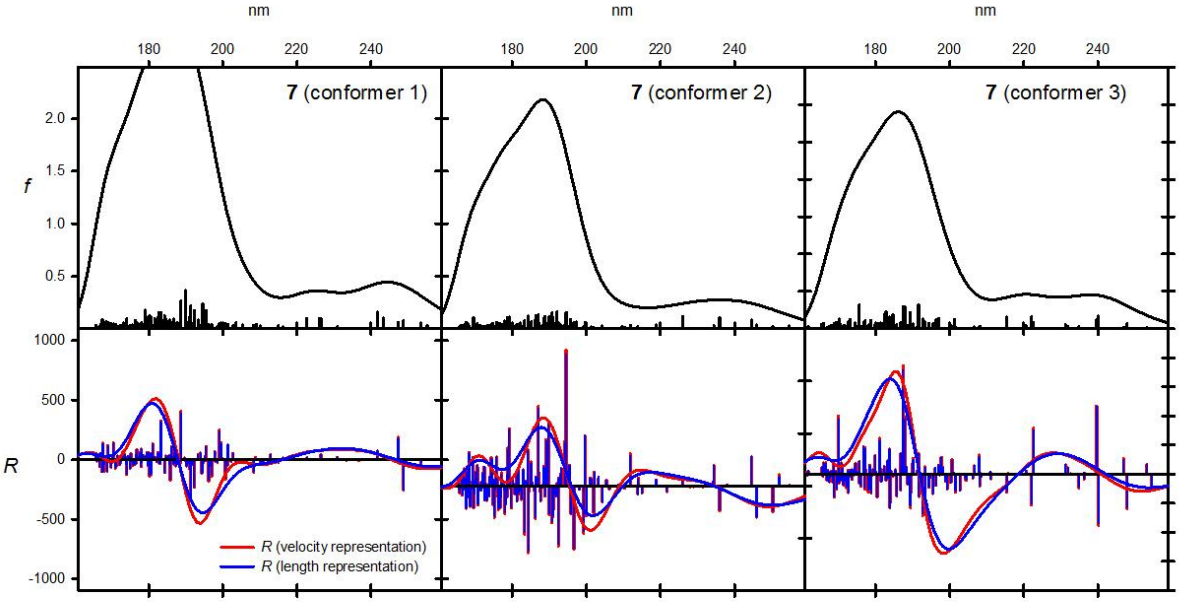


Figure G6. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **6** optimized at the M06-2X-D3/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311G(2d,2p)//B97-D/6-311G(2d,2p)



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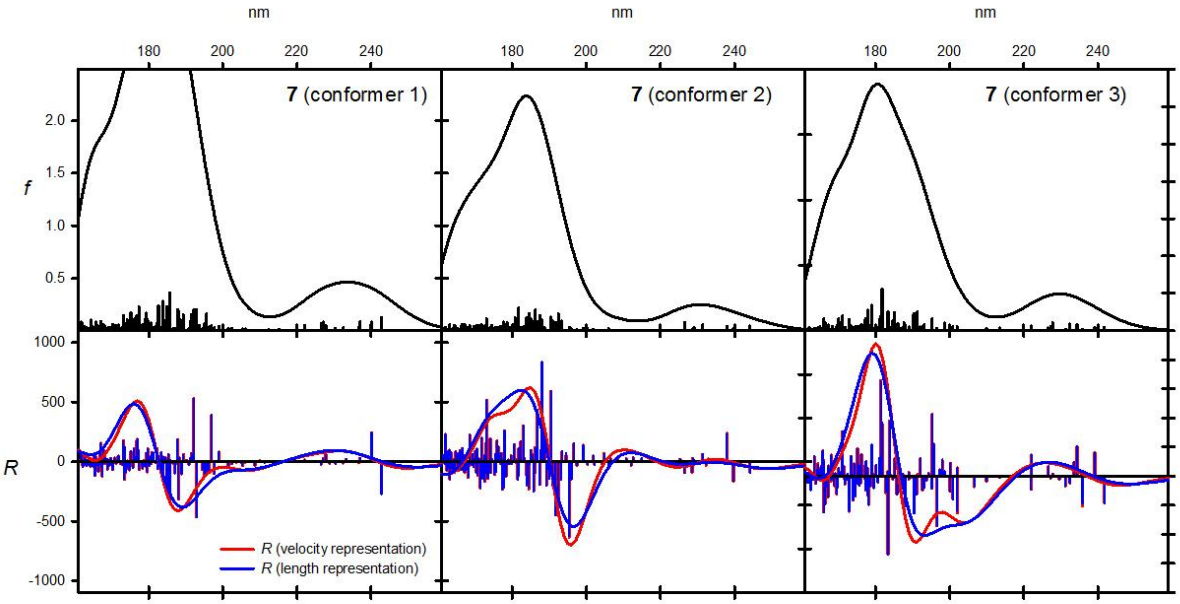

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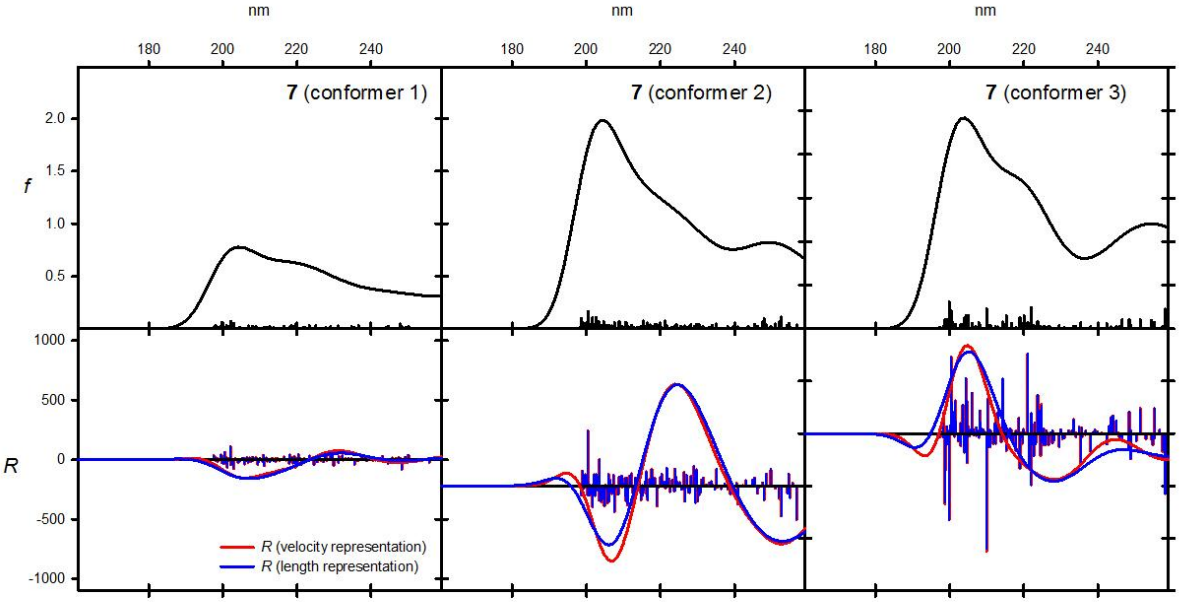


TD-B3LYP/6-311G(2d,2p)//B97-D/6-311G(2d,2p)

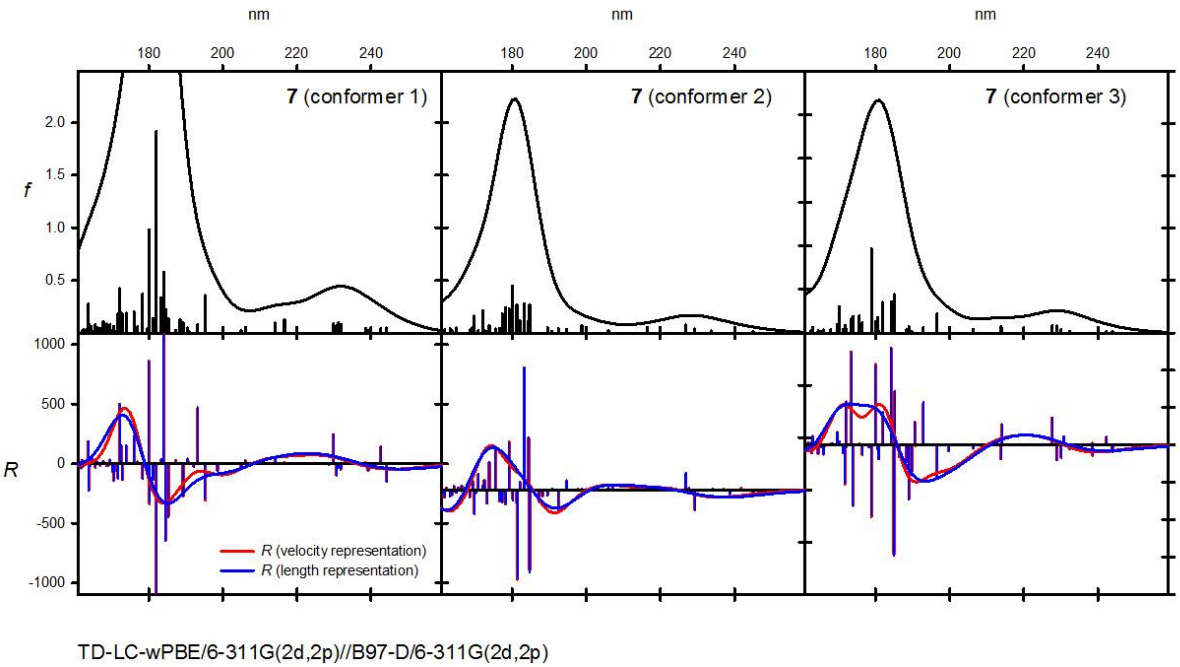
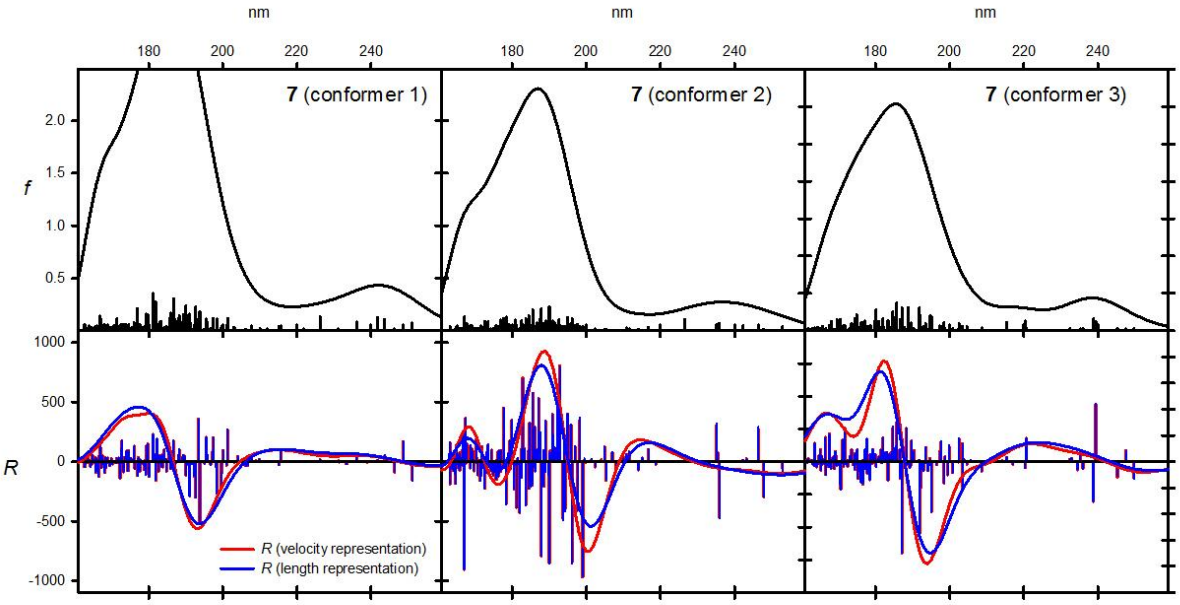
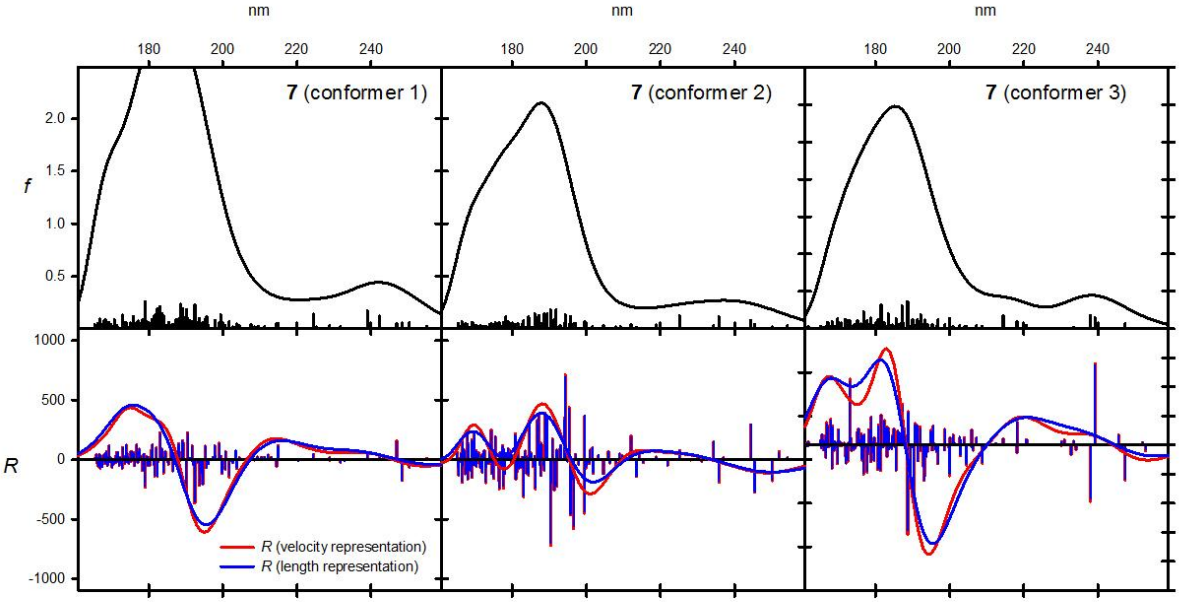


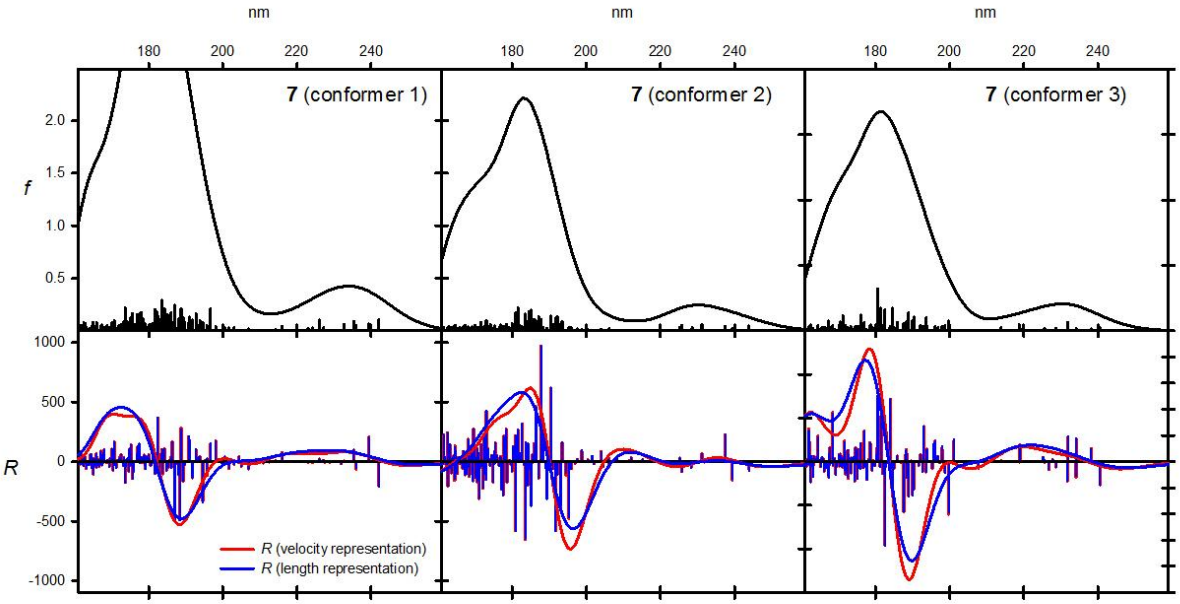
Figure H1. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **7** optimized at the B97-D/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311G(2d,2p)//B97-D3/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//B97-D3/6-311G(2d,2p)



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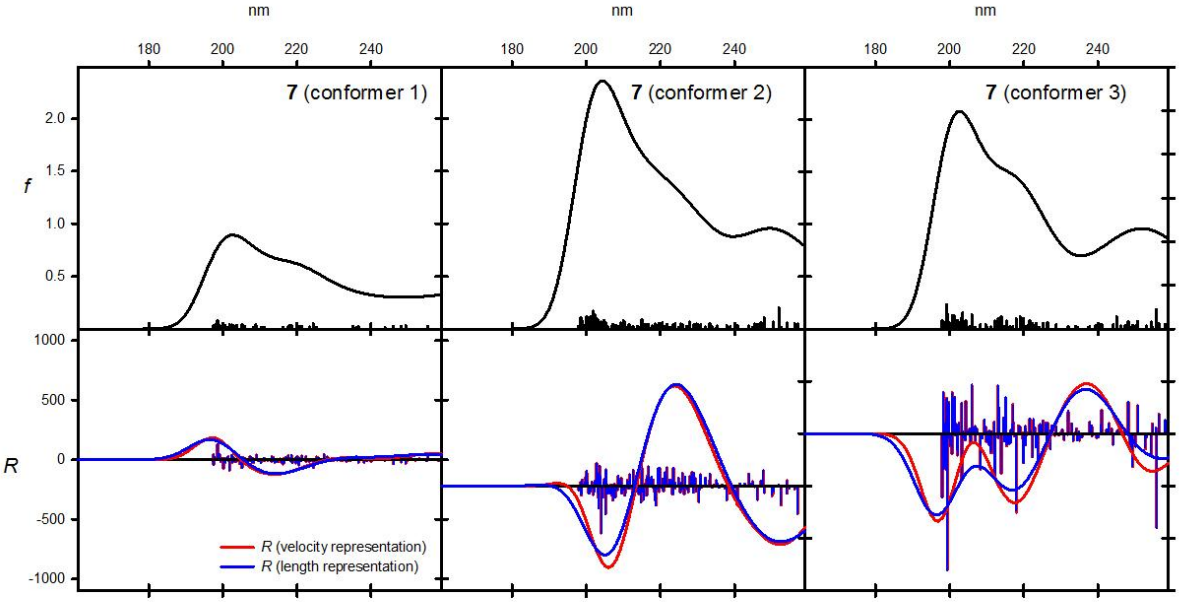

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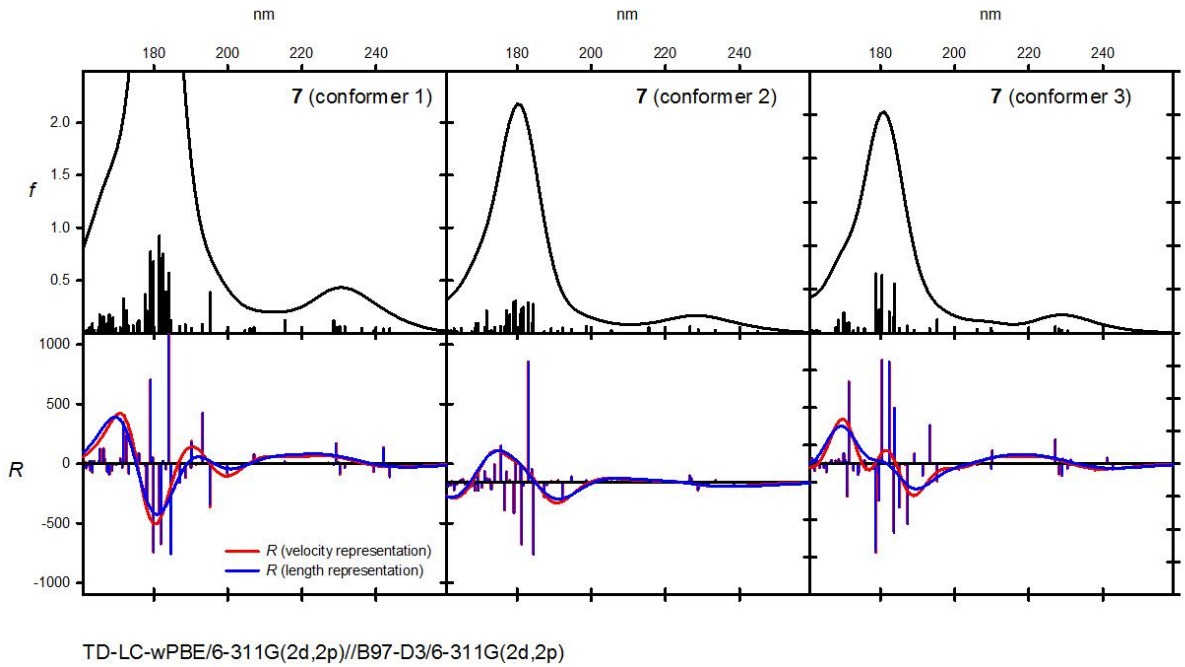
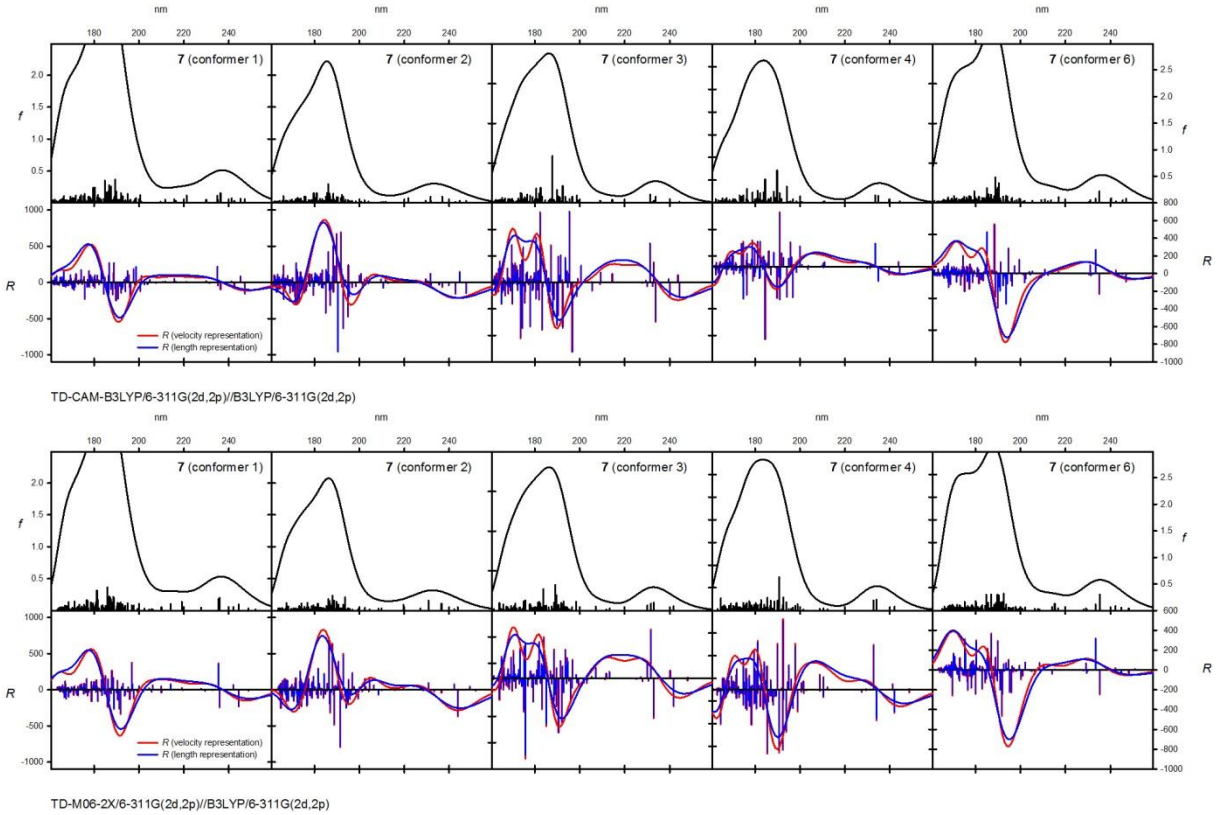


Figure H2. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **7** optimized at the B97-D3/6-311G(2d,2p) level. Wavelengths were not corrected.



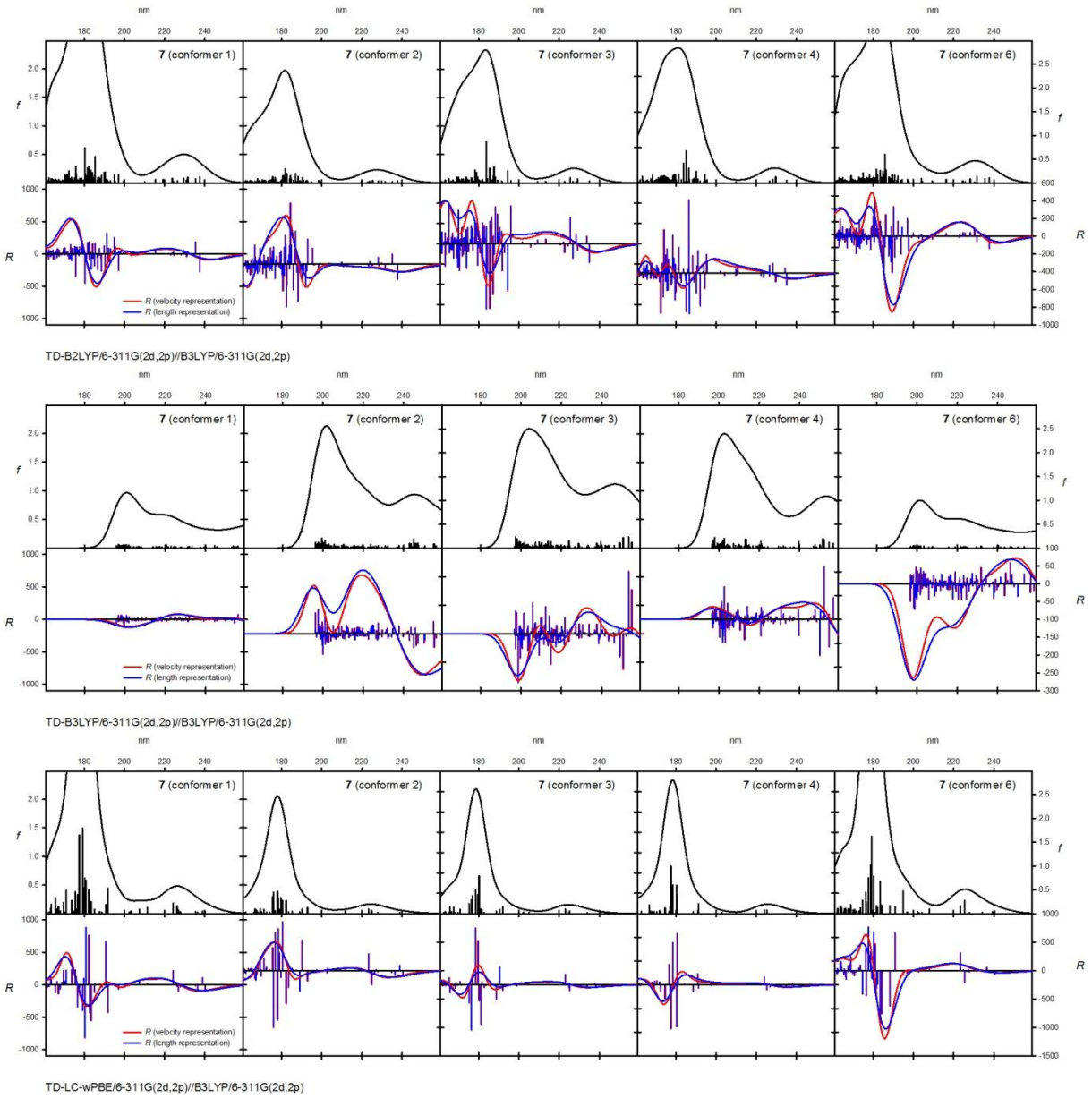
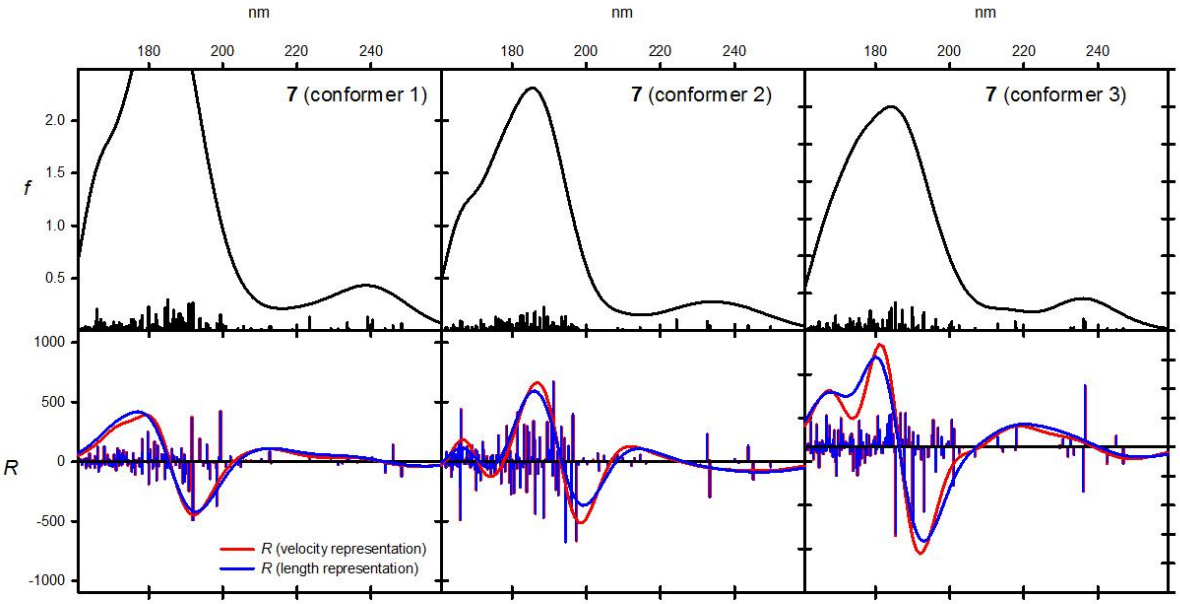
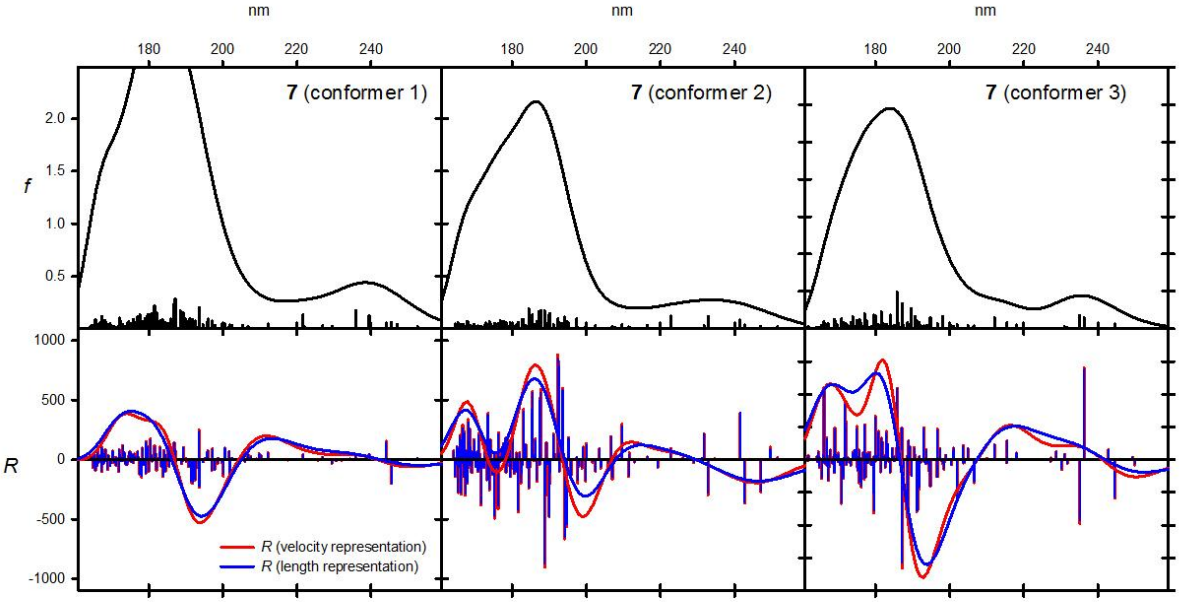


Figure H3. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **7** optimized at the B3LYP/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311G(2d,2p)//B3LYP-D3BJ/6-311G(2d,2p)



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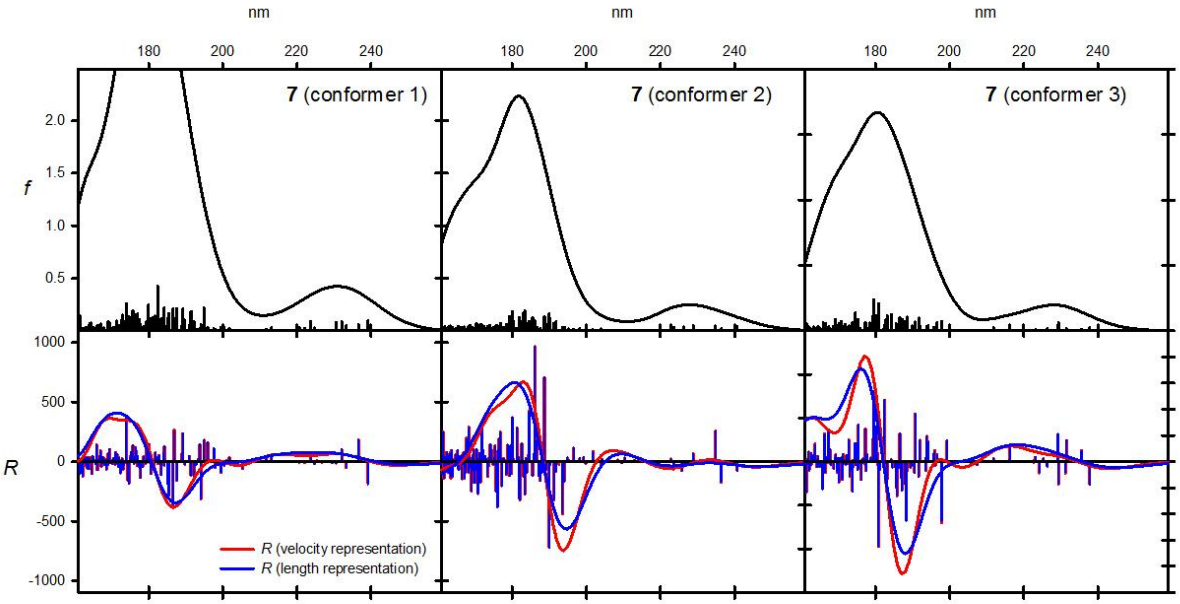

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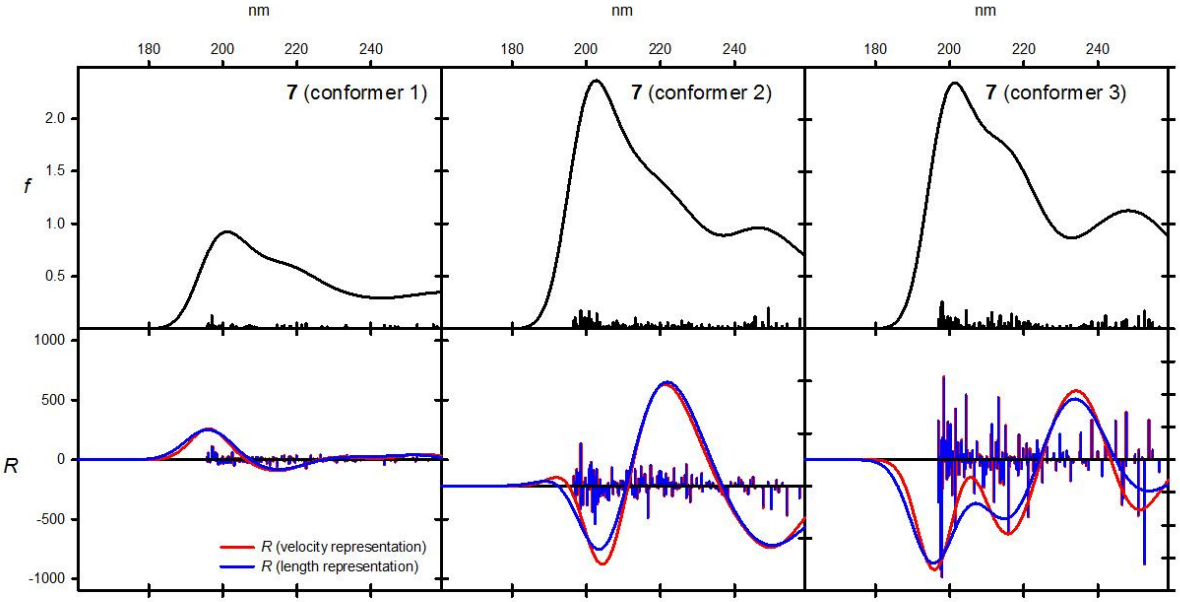

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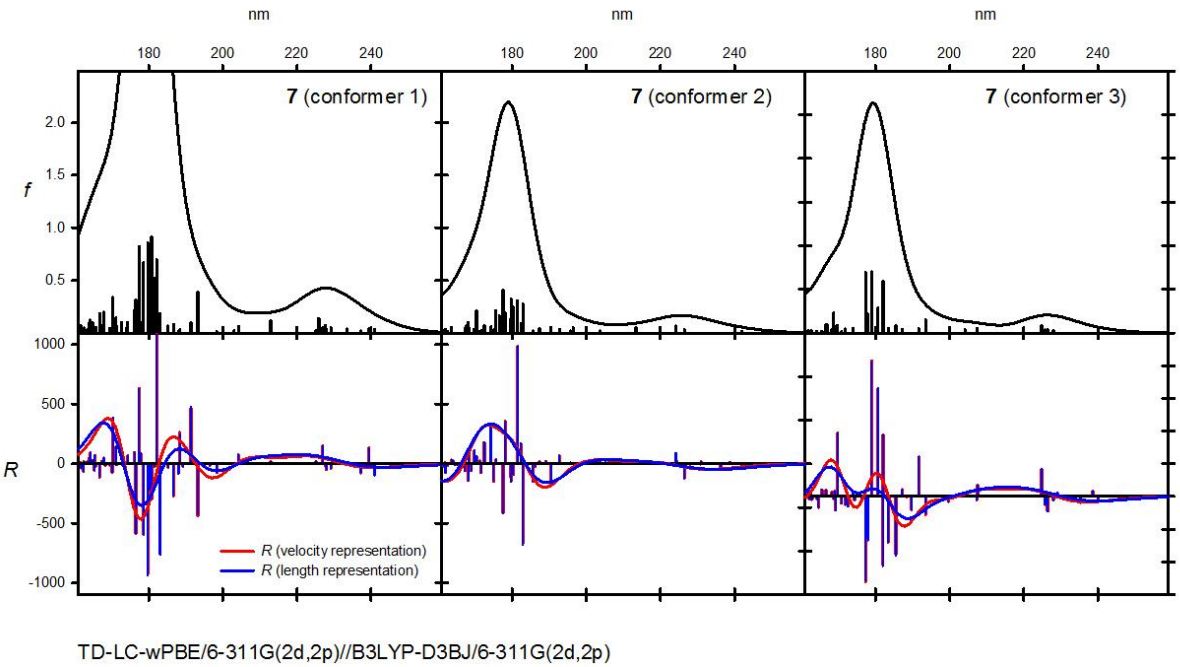
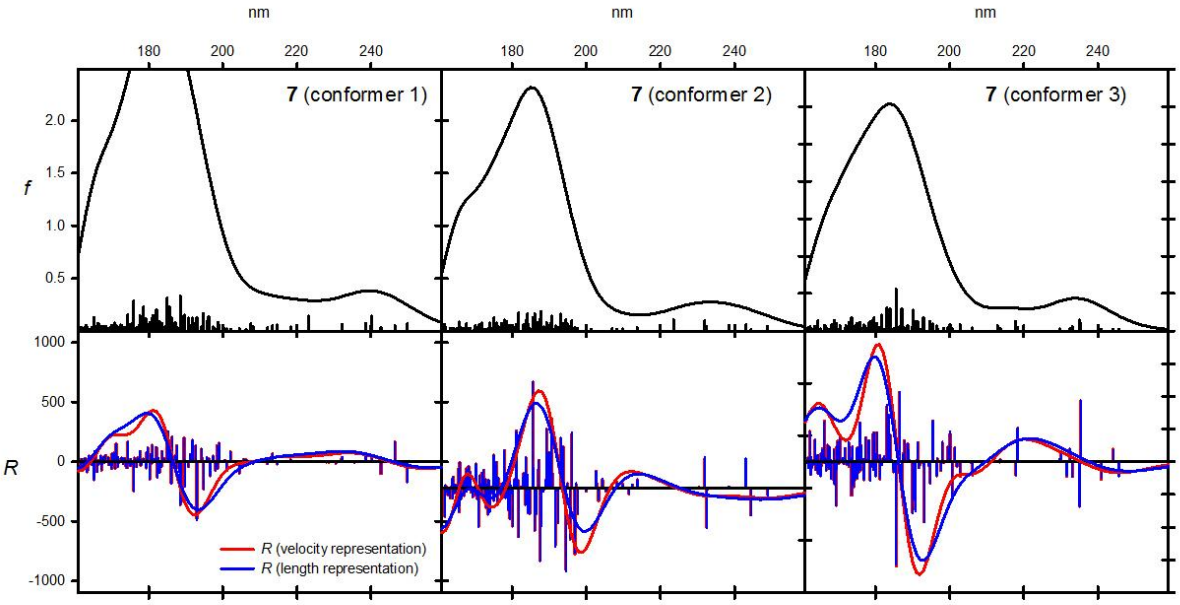
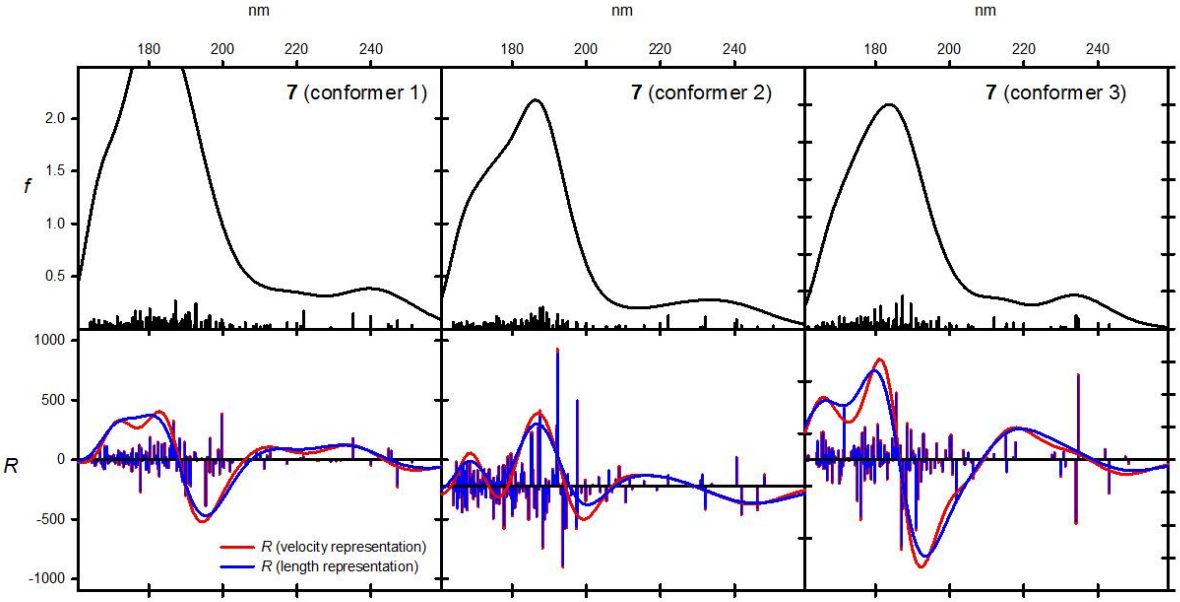


Figure H4. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **7** optimized at the B3LYP-GD3BJ/6-311G(2d,2p) level. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)



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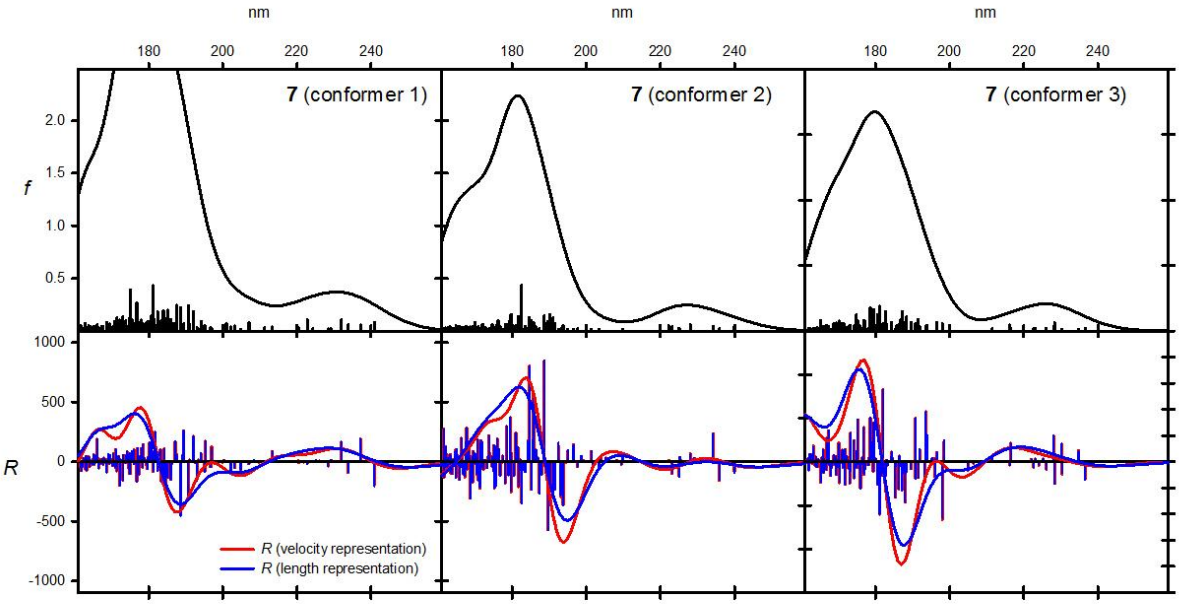

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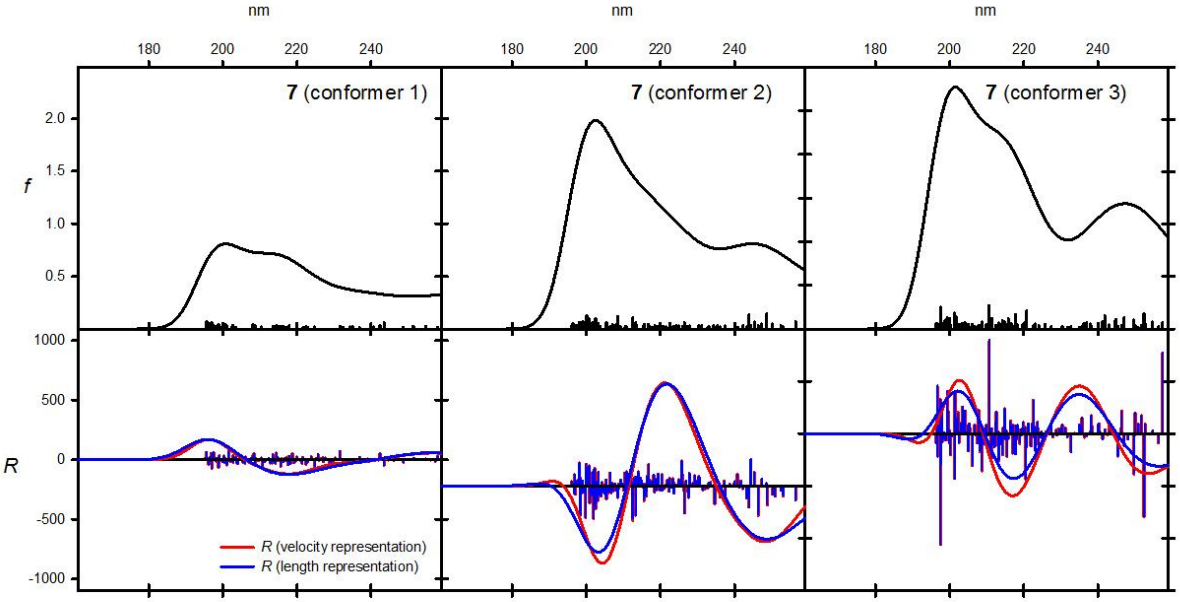
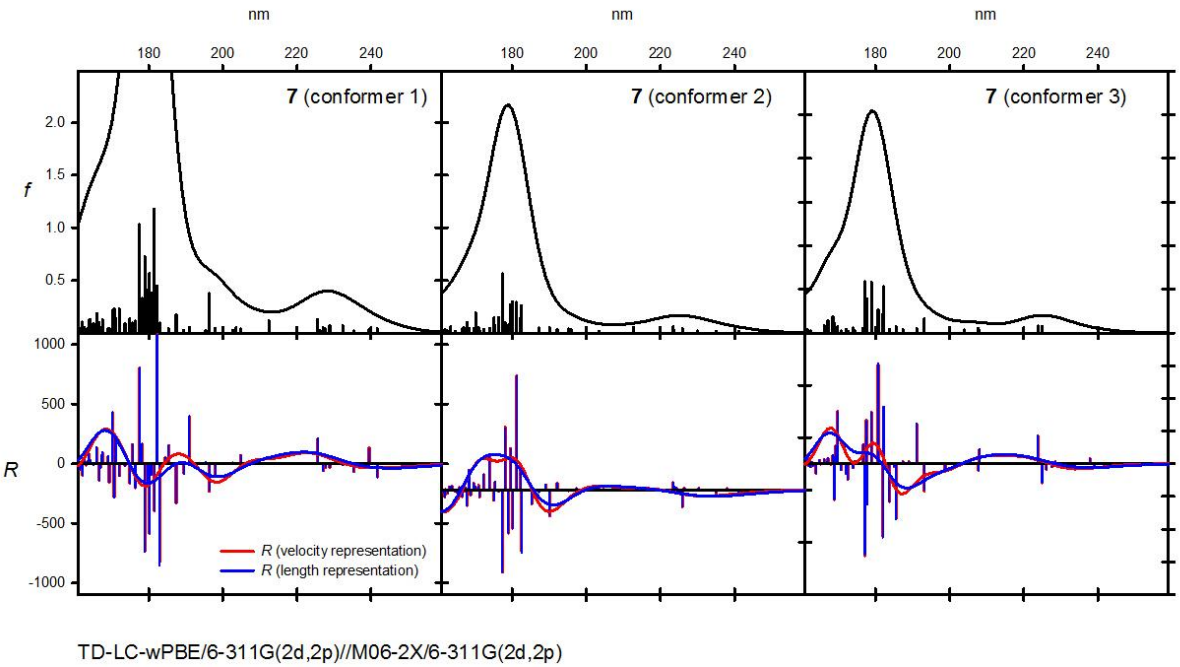
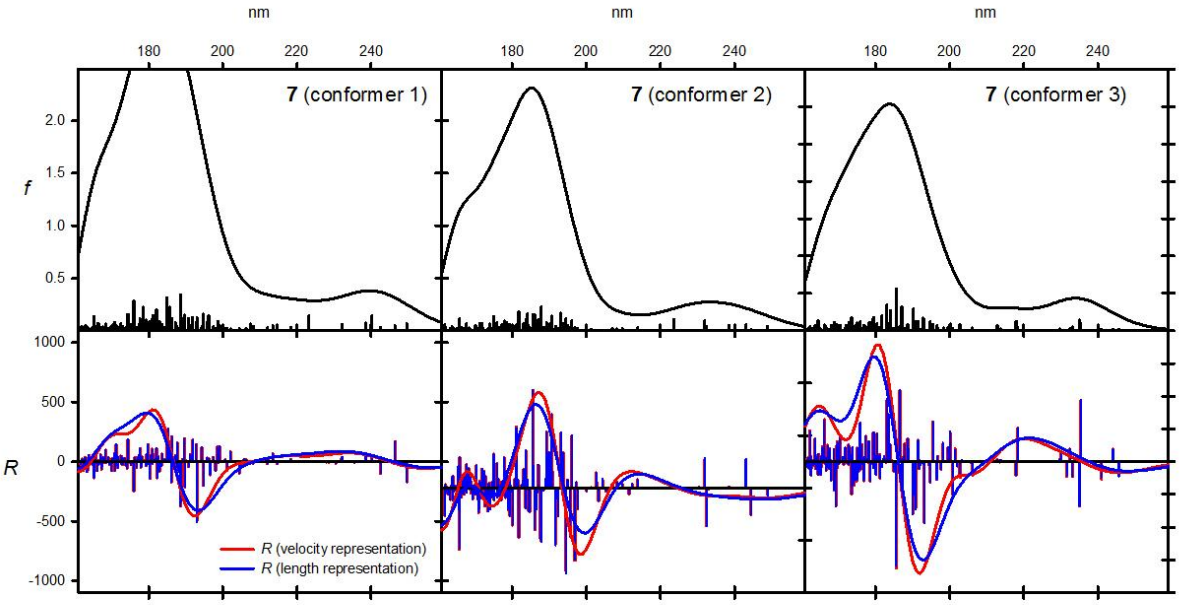


TD-B3LYP/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)

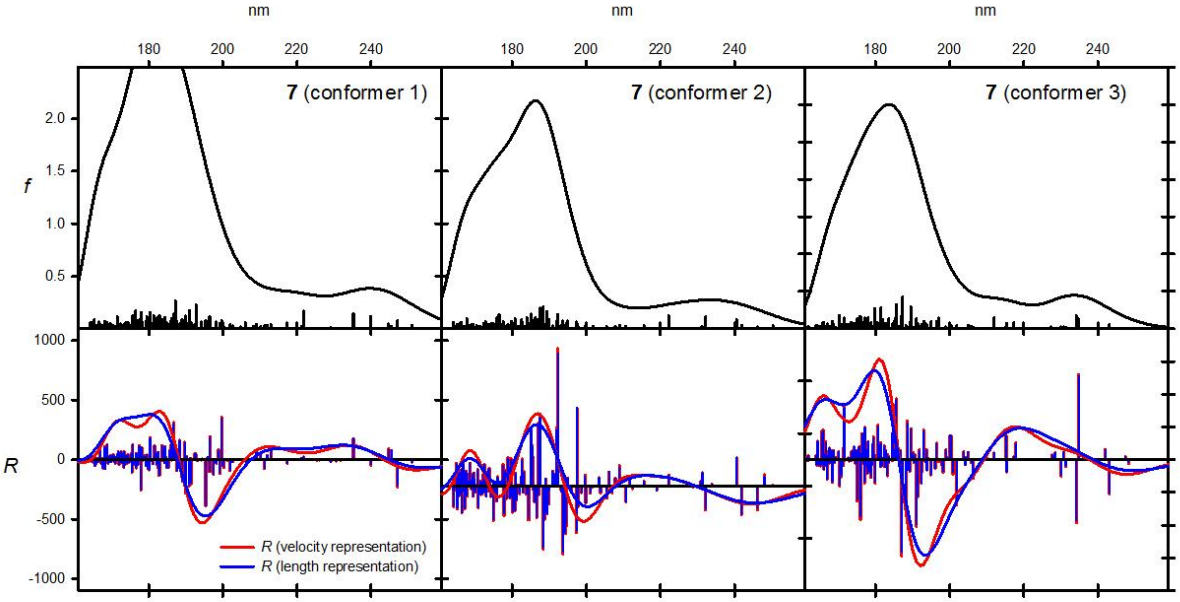


TD-LC-wPBE/6-311G(2d,2p)//M06-2X/6-311G(2d,2p)

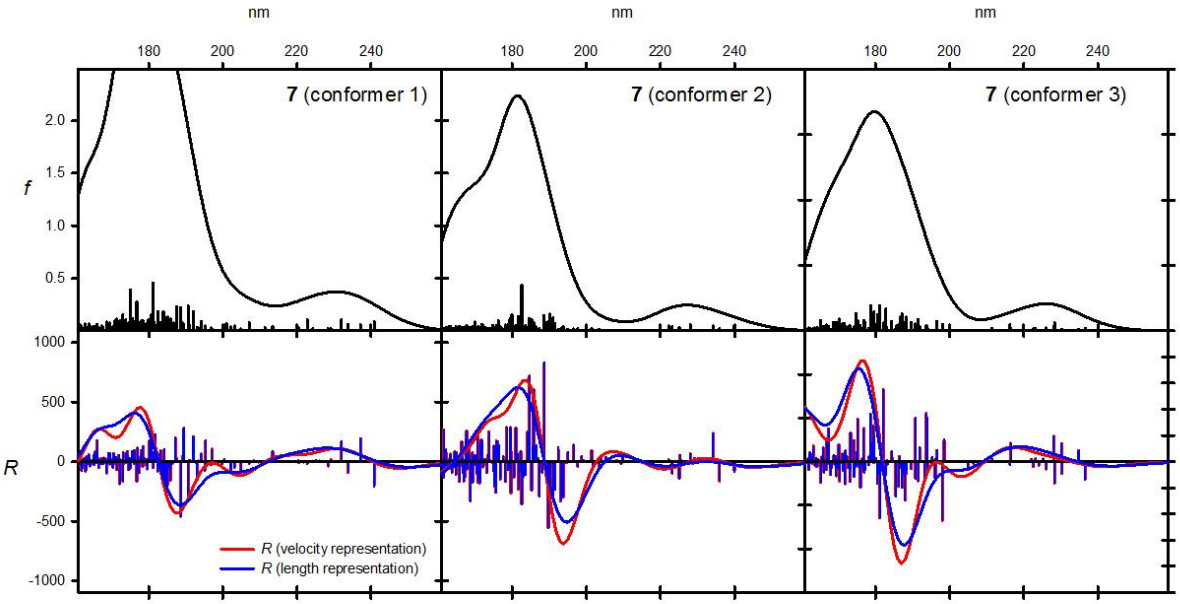
Figure H5. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **7** optimized at the M06-2X/6-311G(2d,2p) level. Wavelengths were not corrected.



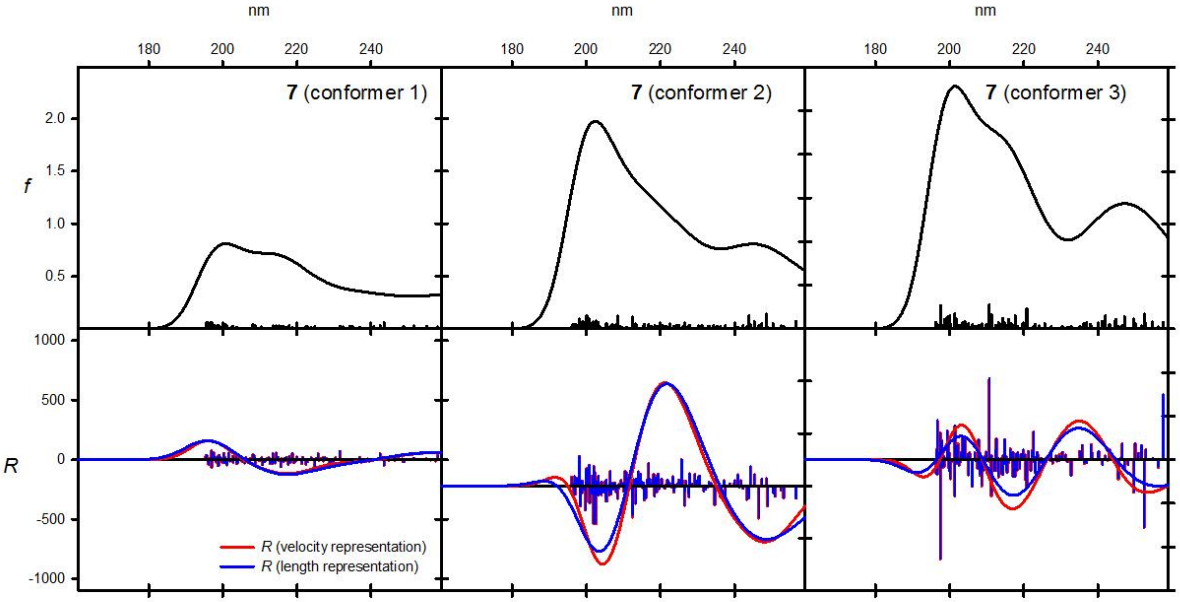
TD-CAM-B3LYP/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)



TD-M06-2X/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)



TD-B2LYP/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)



TD-B3LYP/6-311G(2d,2p)//M06-2X-D3/6-311G(2d,2p)

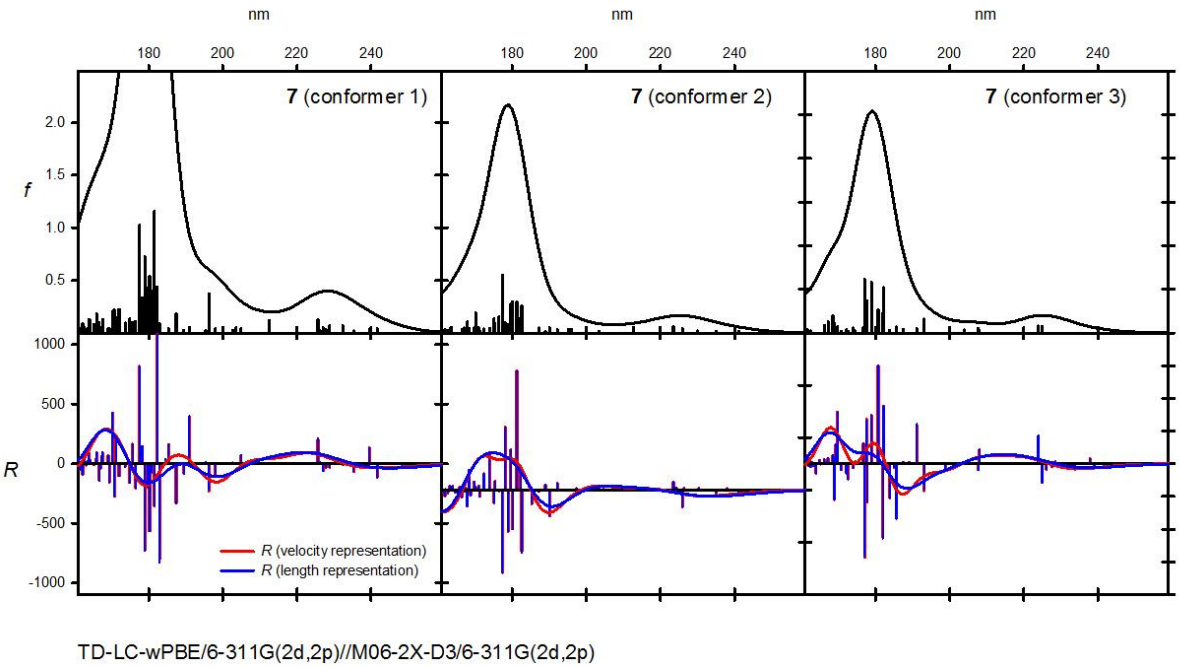
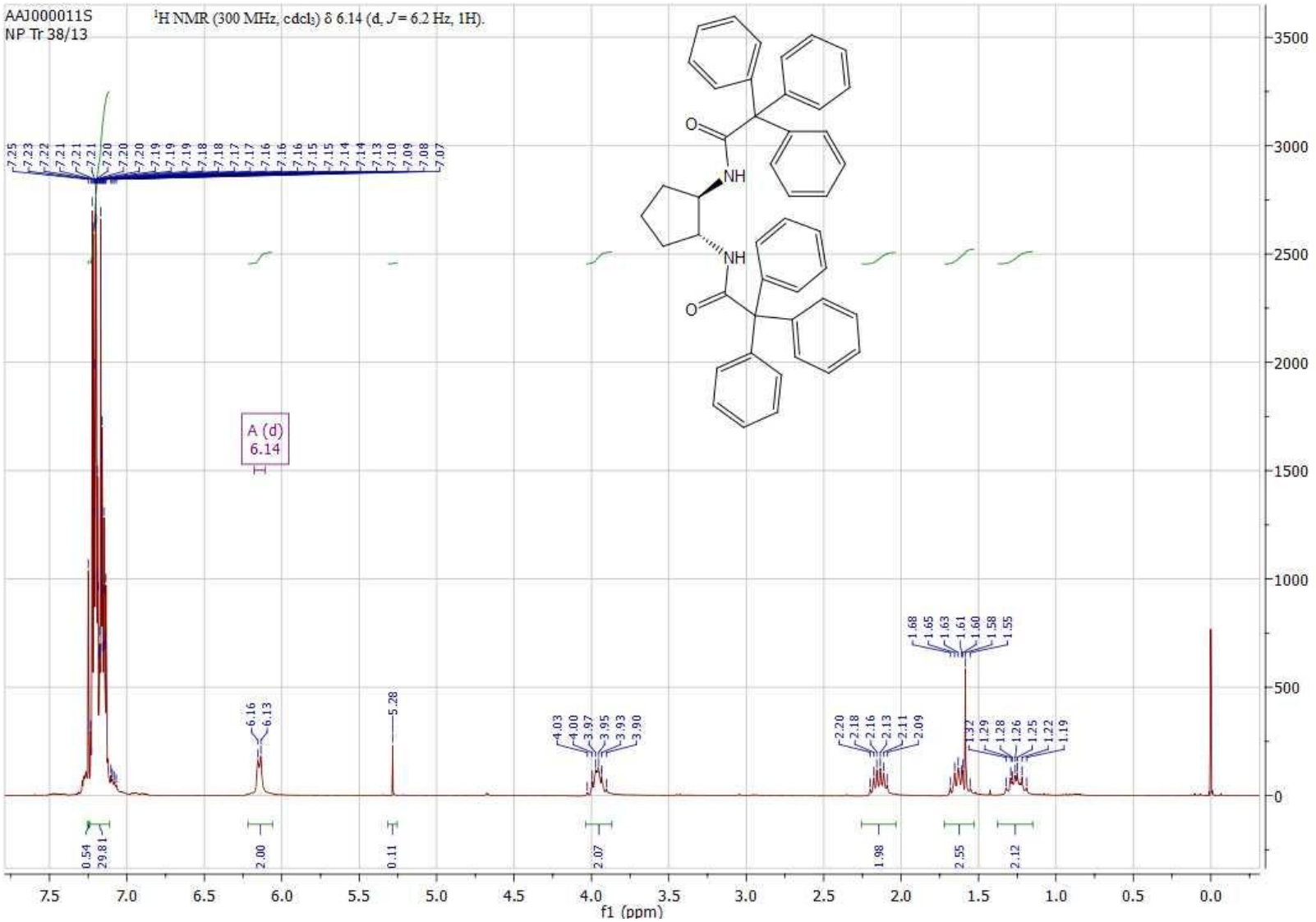
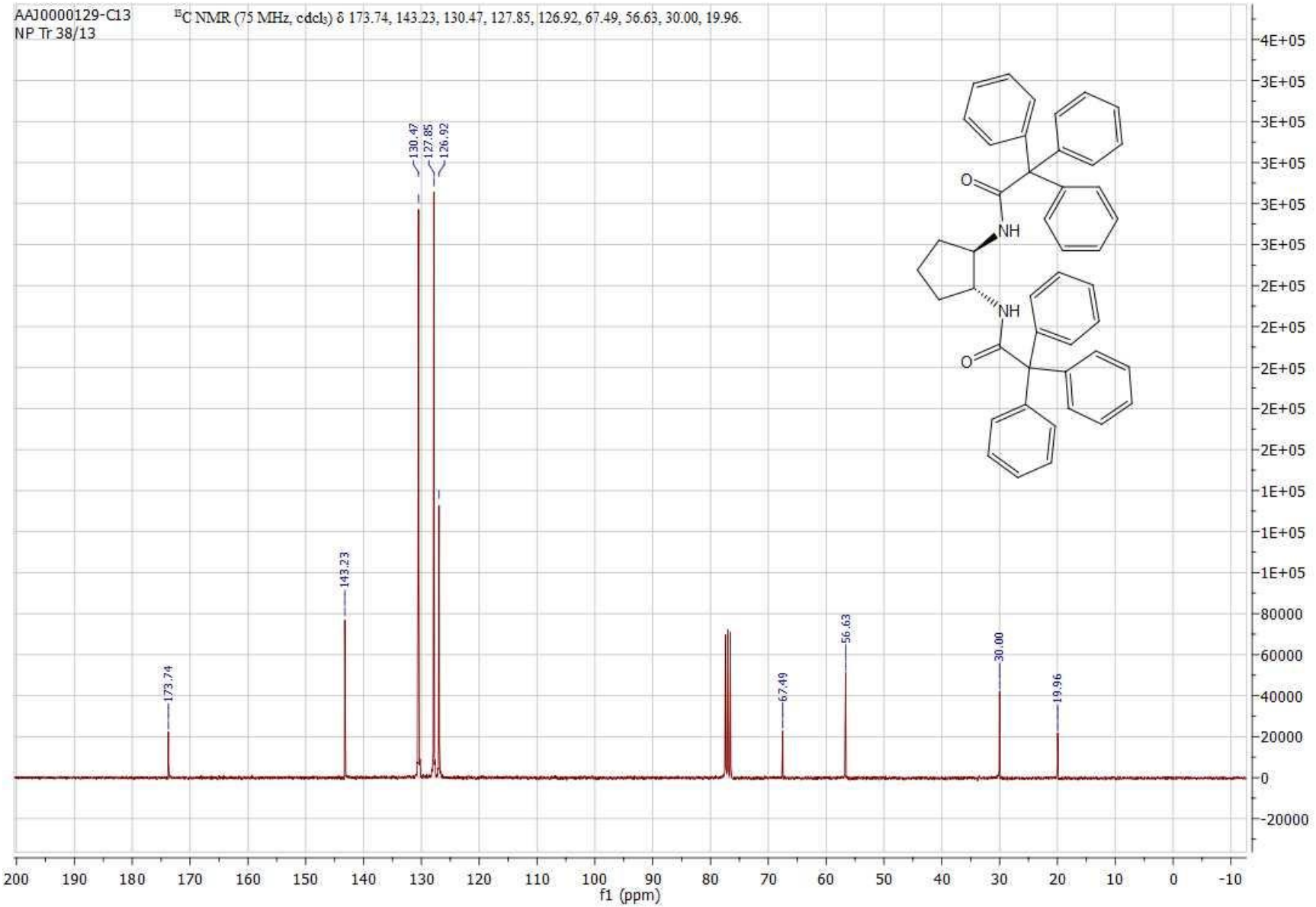
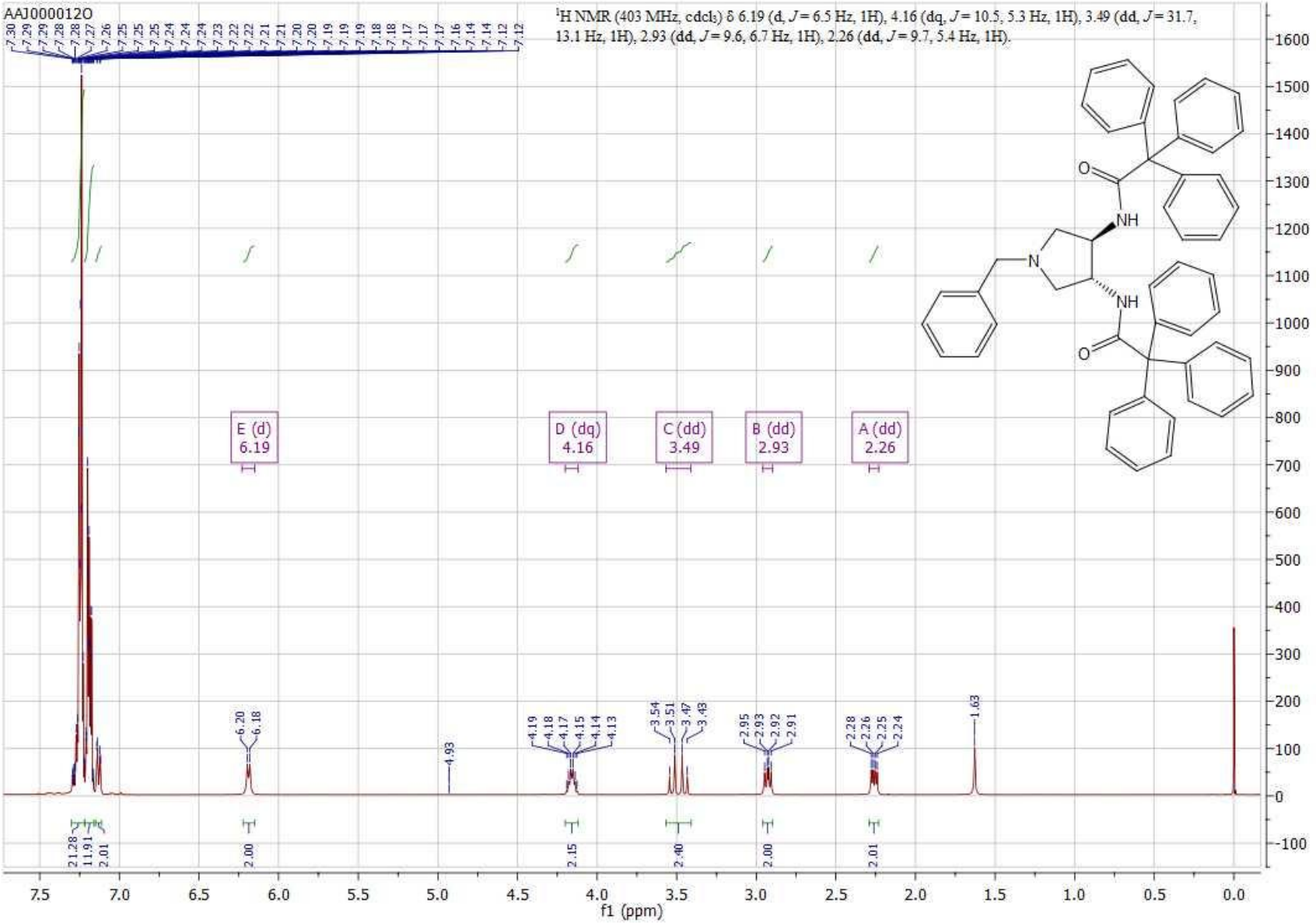


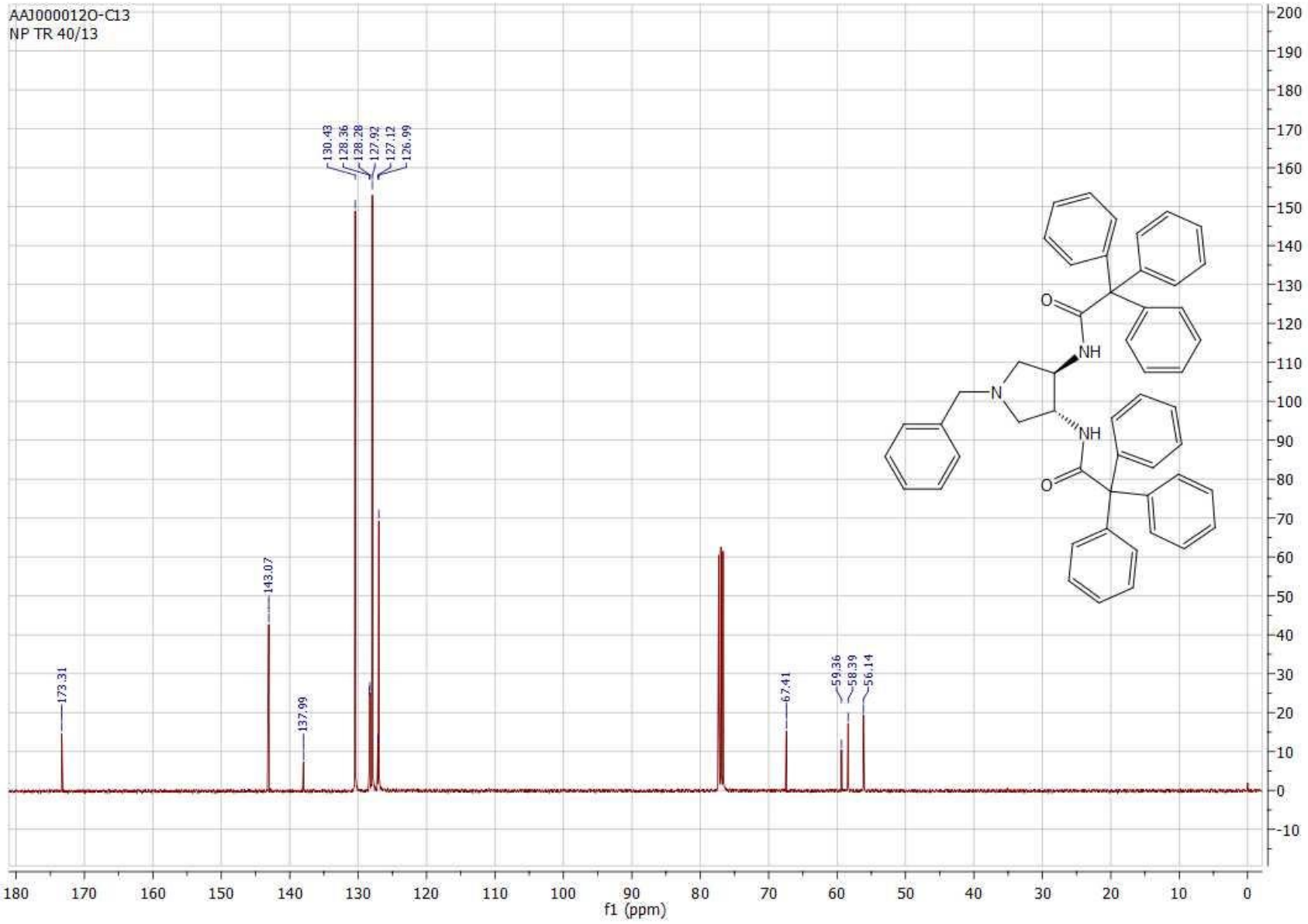
Figure H6. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual low-energy conformers of triphenylacetamide **7** optimized at the M06-2X-D3/6-311G(2d,2p) level. Wavelengths were not corrected.

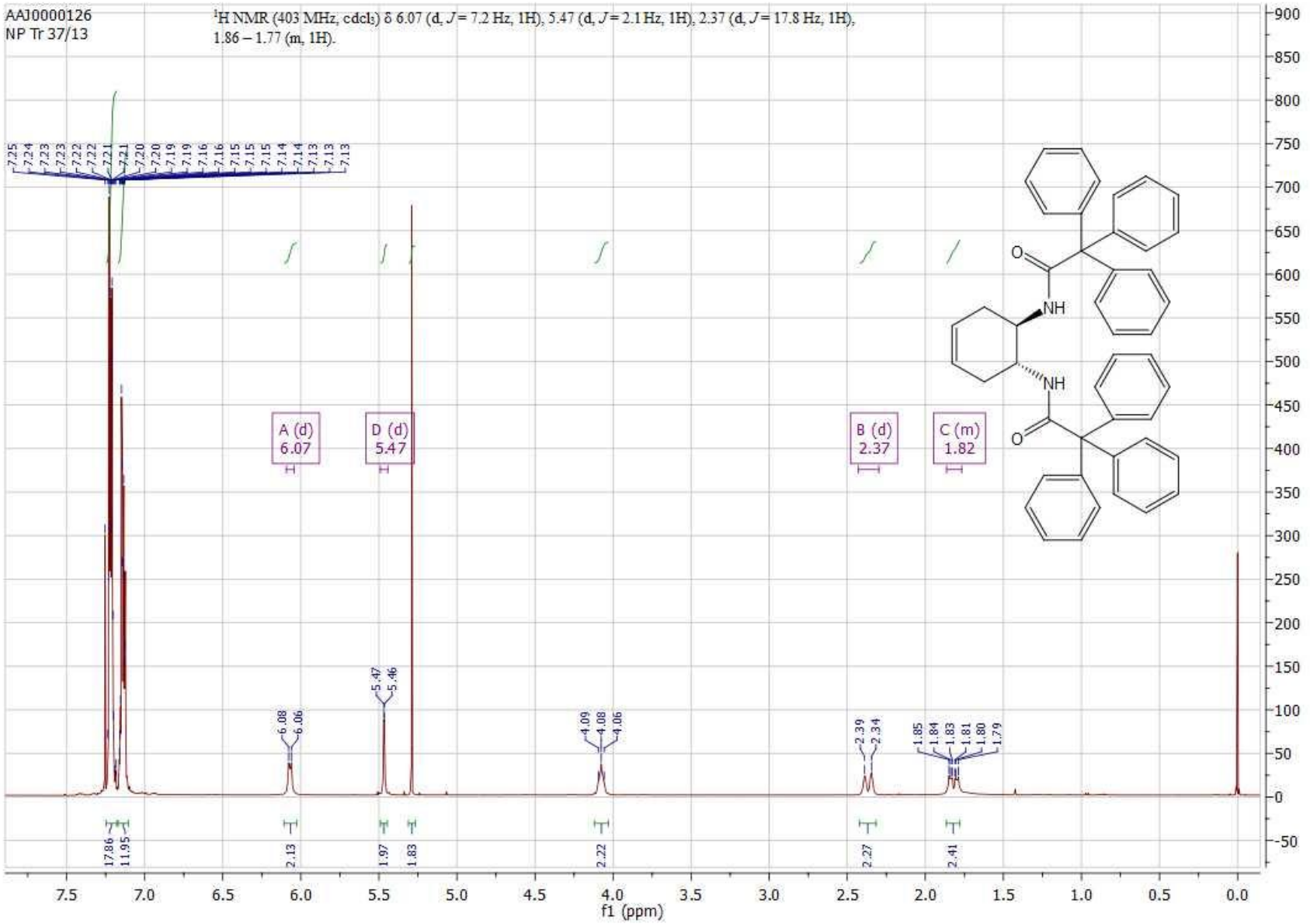
Copies of ^{1}H and ^{13}C NMR spectra

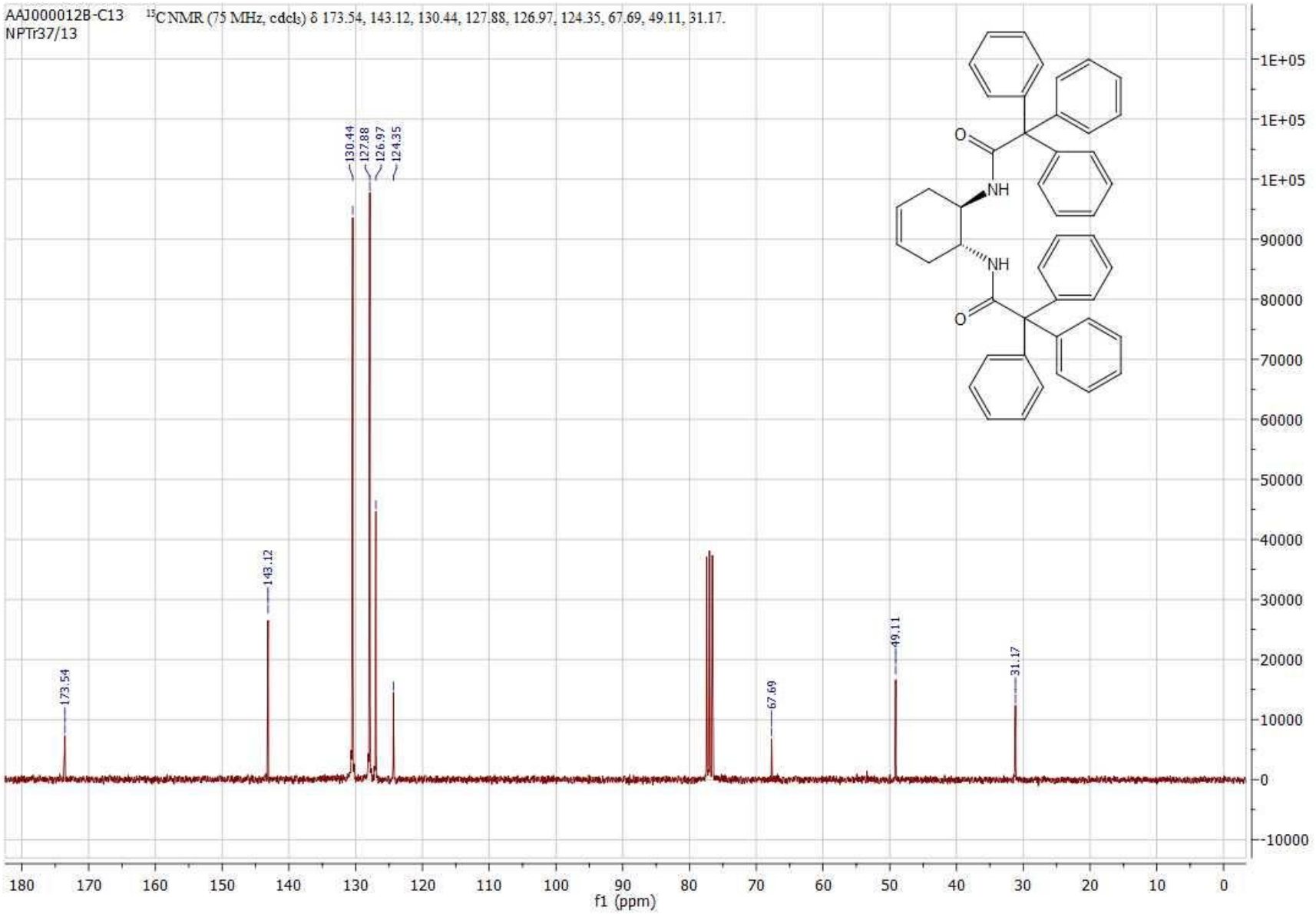


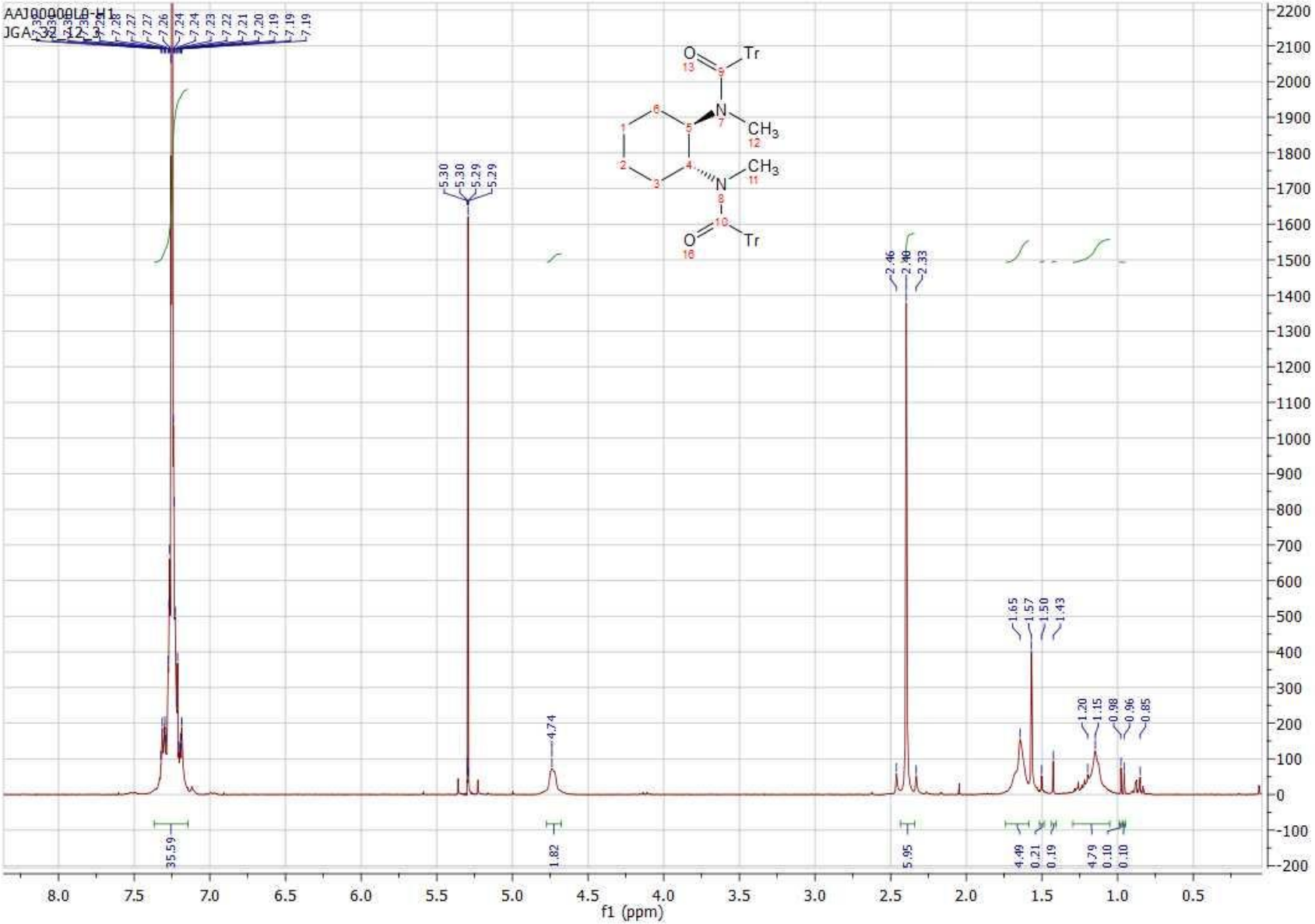

AAJ0000129-C13
NP Tr 38/13
13C NMR (75 MHz, cdcl3) δ 173.74, 143.23, 130.47, 127.85, 126.92, 67.49, 56.63, 30.00, 19.96.
130.47
127.85
126.92
143.23
173.74
67.49
56.63
30.00
19.96
O
NH
NH
O
4E+05
3E+05
3E+05
3E+05
3E+05
3E+05
2E+05
2E+05
2E+05
2E+05
2E+05
2E+05
1E+05
1E+05
1E+05
80000
60000
40000
20000
0
-20000
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

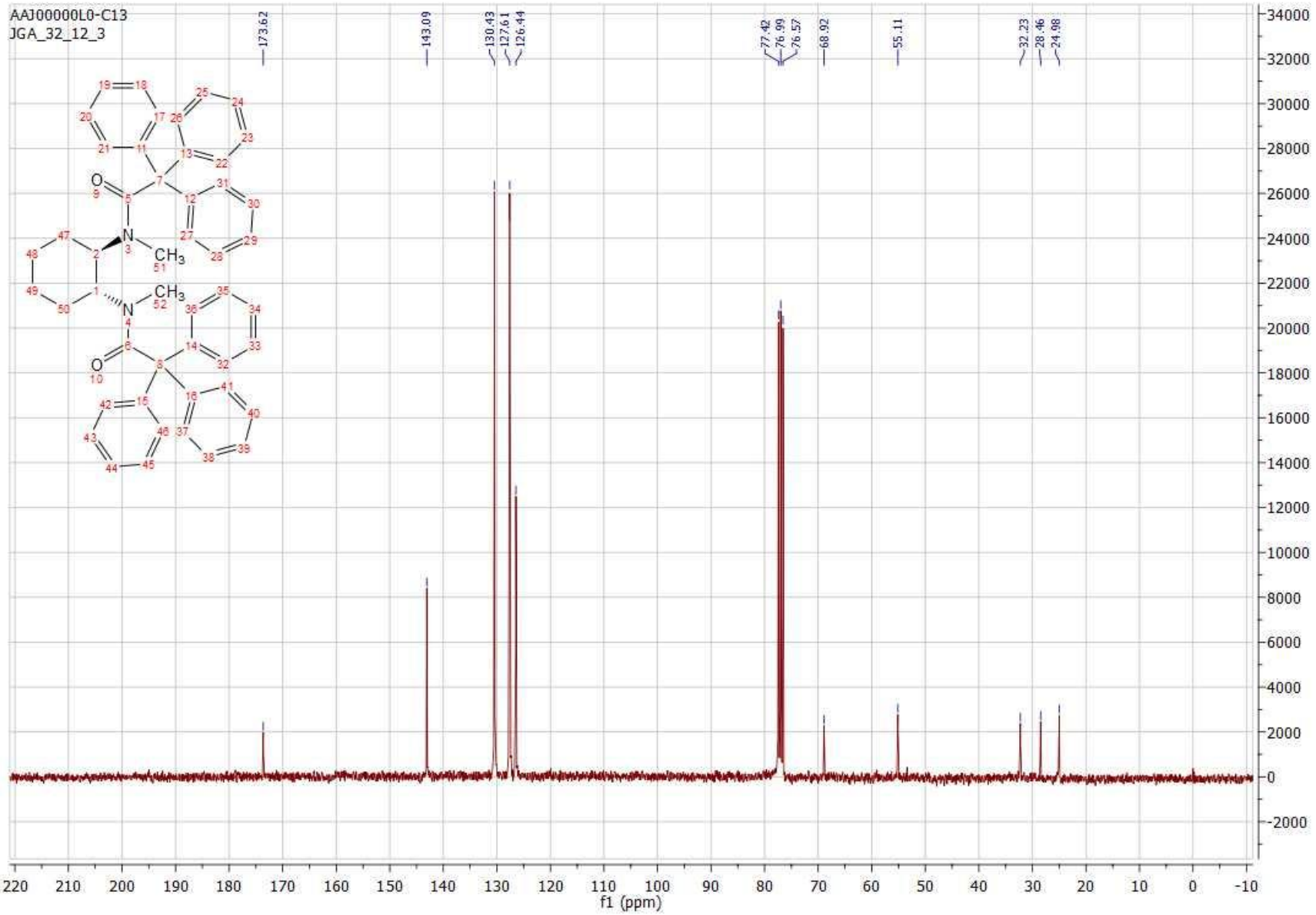

AAJ0000120
^{1}H NMR (403 MHz, cdcl$_3$) δ 6.19 (d, J = 6.5 Hz, 1H), 4.16 (dq, J = 10.5, 5.3 Hz, 1H), 3.49 (dd, J = 31.7, 13.1 Hz, 1H), 2.93 (dd, J = 9.6, 6.7 Hz, 1H), 2.26 (dd, J = 9.7, 5.4 Hz, 1H).
E (d) 6.19
D (dq) 4.16
C (dd) 3.49
B (dd) 2.93
A (dd) 2.26
NH
NH
O
O
N
f1 (ppm)

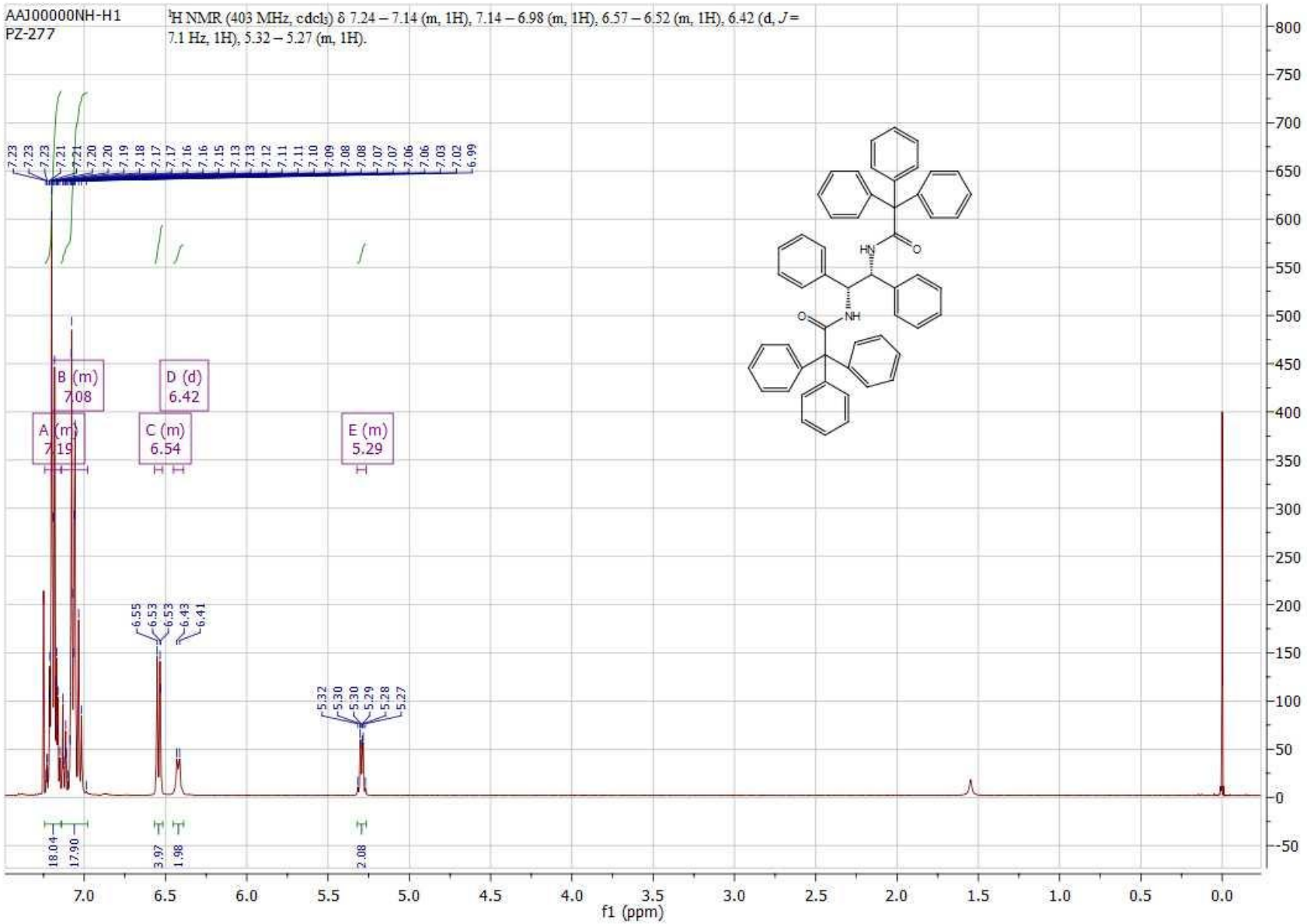

AAJ0000120-C13
NP TR 40/13
130.43
128.36
128.28
127.92
127.12
126.99
143.07
137.99
173.31
67.41
59.36
58.39
56.14
O
NH
N
NH
O
f1 (ppm)

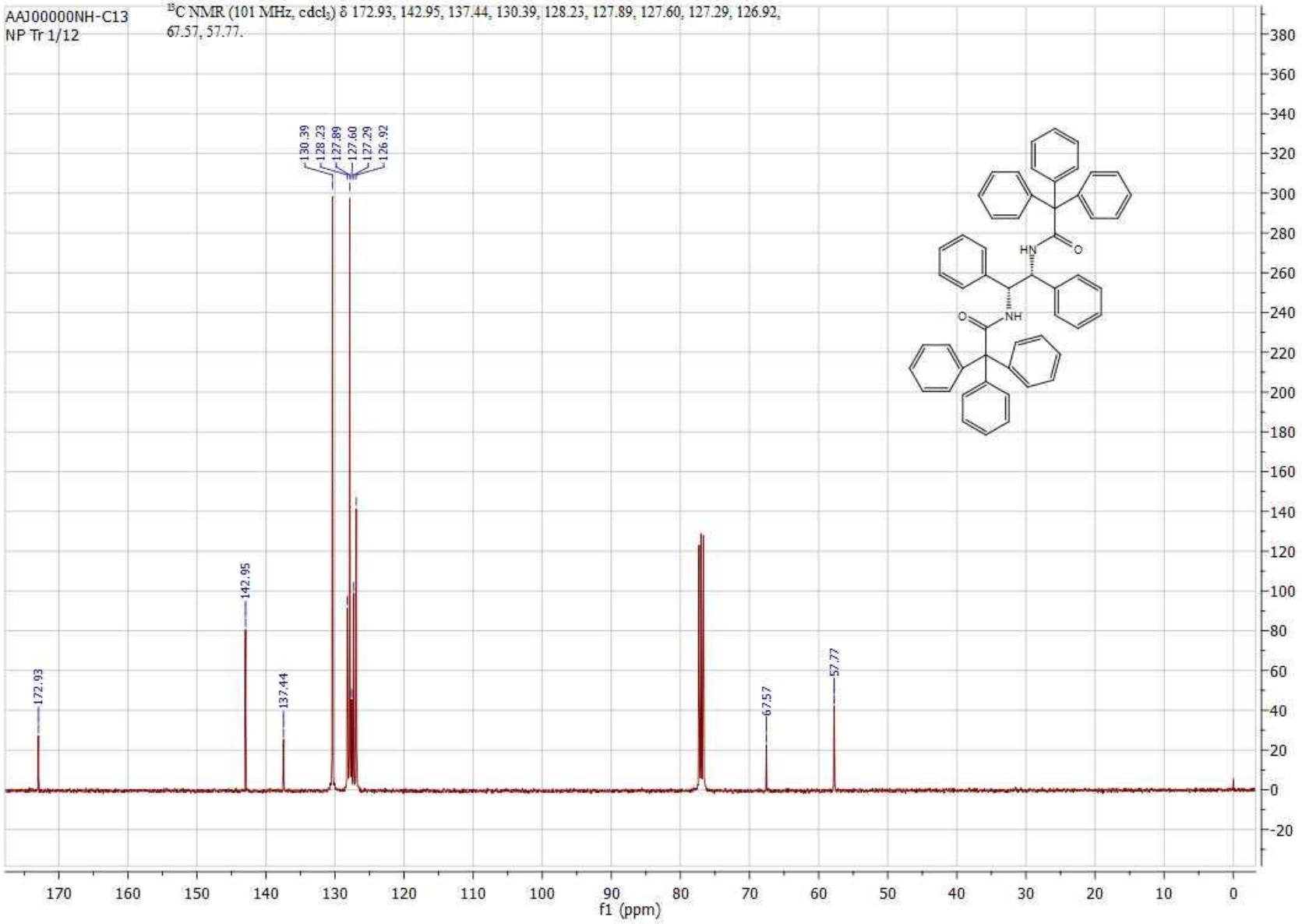

AAJ0000126
NP Tr 37/13
¹H NMR (403 MHz, cdcl₃) δ 6.07 (d, J = 7.2 Hz, 1H), 5.47 (d, J = 2.1 Hz, 1H), 2.37 (d, J = 17.8 Hz, 1H), 1.86 – 1.77 (m, 1H).
A (d) 6.07
D (d) 5.47
B (d) 2.37
C (m) 1.82
NH
NH
O
O
f1 (ppm)

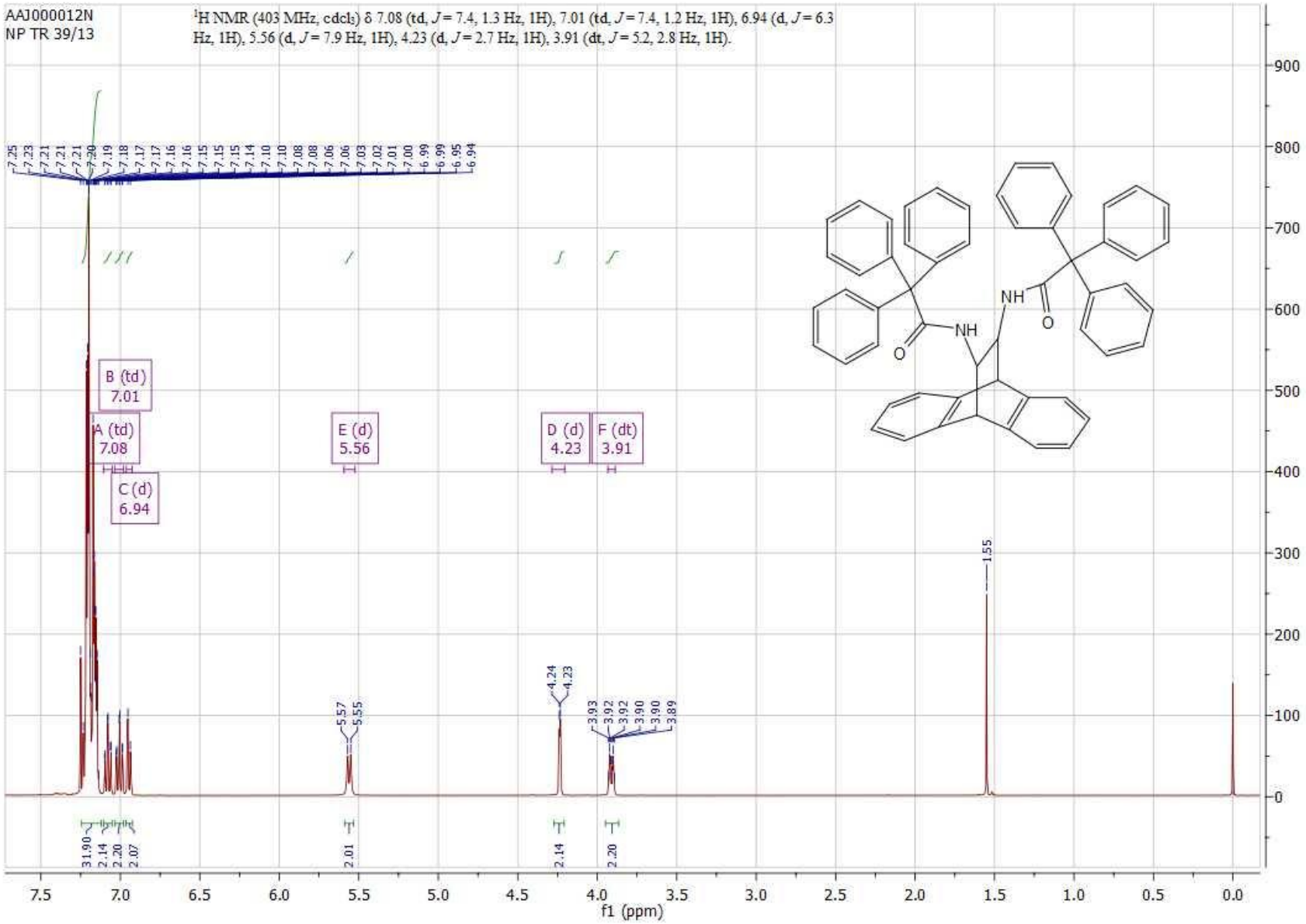

AAJ000012B-C13
NPTr37/13
13C NMR (75 MHz, cdcl3) δ 173.54, 143.12, 130.44, 127.88, 126.97, 124.35, 67.69, 49.11, 31.17.
130.44
127.88
126.97
124.35
143.12
173.54
67.69
49.11
31.17
O
NH
NH
O
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

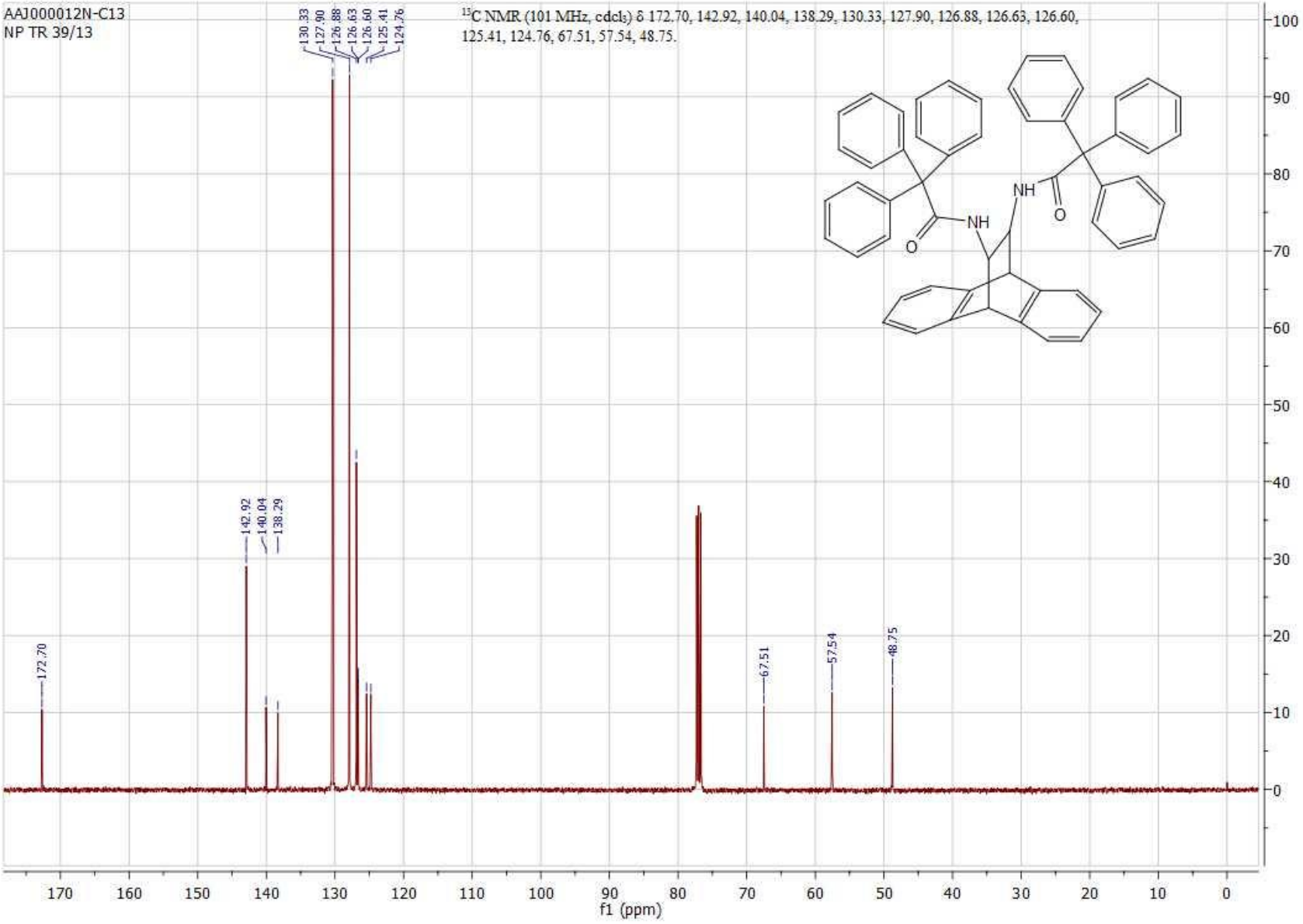

AAJ00000L0-H1
JGA-3-12
Tr
Tr
CH3
CH3
5.30
5.30
5.29
5.29
4.74
2.46
2.40
2.33
1.65
1.57
1.50
1.43
1.20
1.15
0.98
0.96
0.85
35.59
1.82
5.95
4.49
0.21
0.19
4.79
0.10
0.10
f1 (ppm)

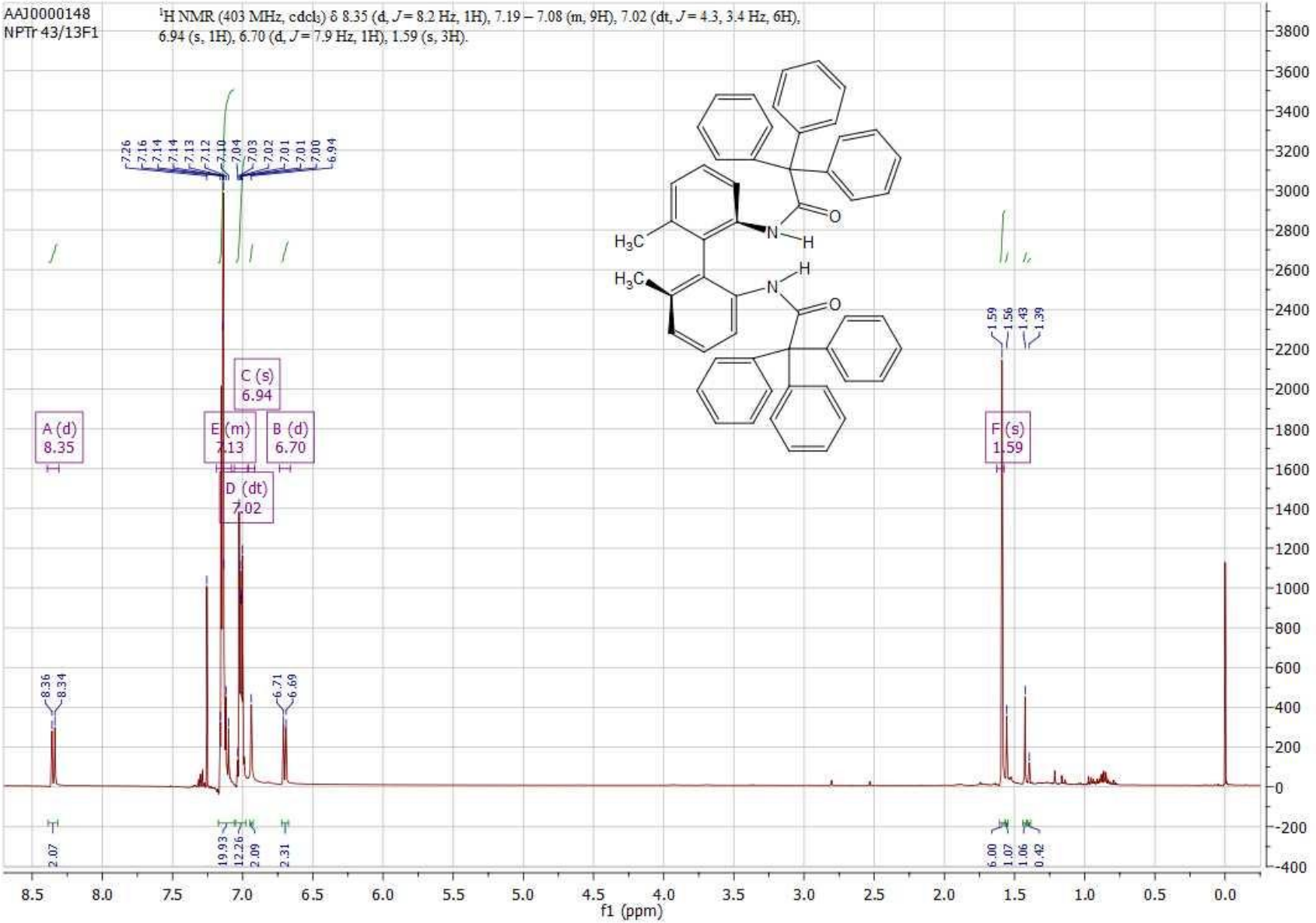

AAJ00000L0-C13
JGA_32_12_3
173.62
143.09
130.43
127.61
126.44
77.42
76.99
76.57
68.92
55.11
32.23
28.46
24.98
f1 (ppm)

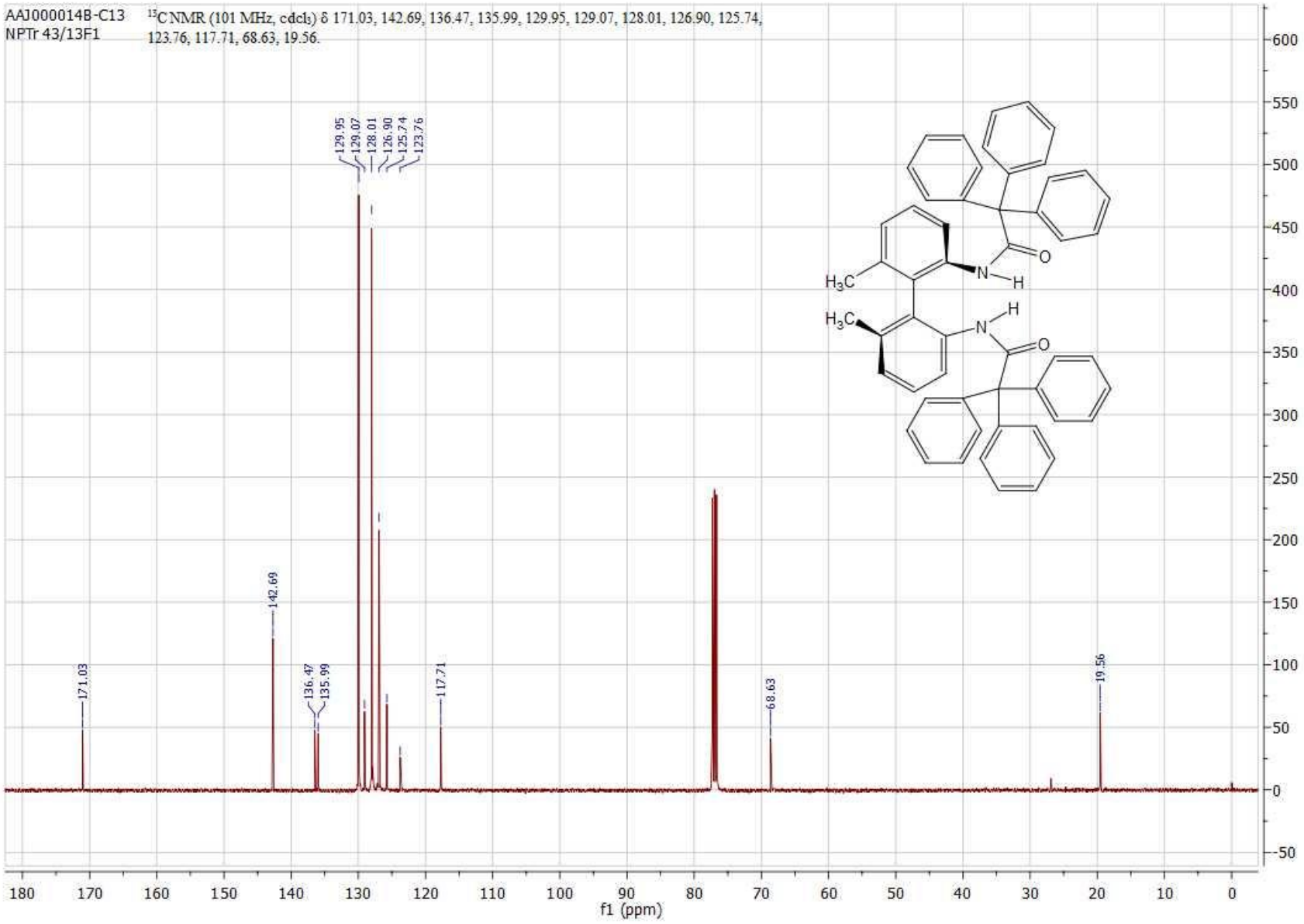

AAJ00000NH-H1
PZ-277
^{1}H NMR (403 MHz, cdcl$_3$) δ 7.24 – 7.14 (m, 1H), 7.14 – 6.98 (m, 1H), 6.57 – 6.52 (m, 1H), 6.42 (d, J = 7.1 Hz, 1H), 5.32 – 5.27 (m, 1H).
B (m) 7.08
D (d) 6.42
A (m) 7.19
C (m) 6.54
E (m) 5.29
HN
O
NH
O
18.04
17.90
3.97
1.98
2.08
f1 (ppm)

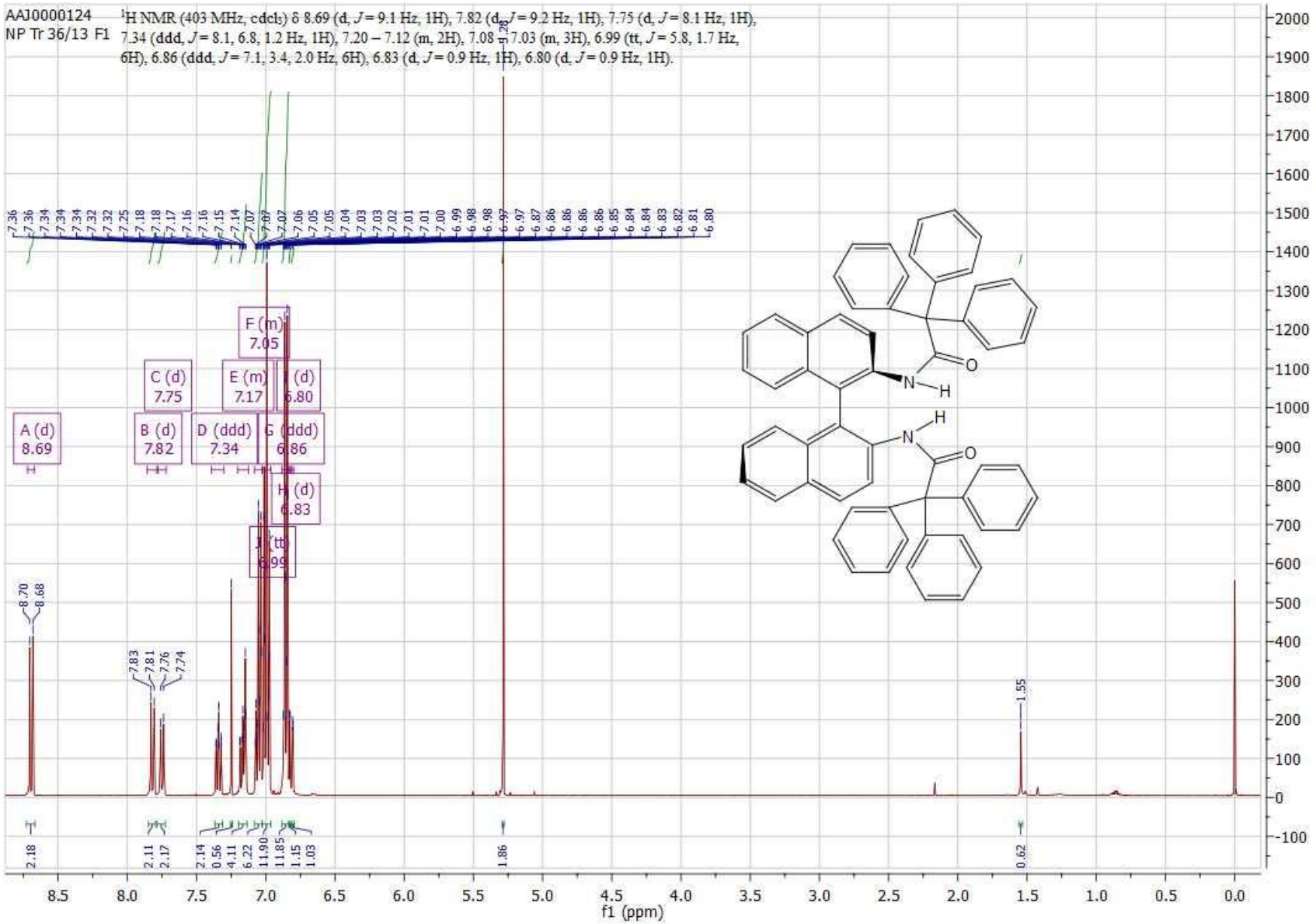

AAJ00000NH-C13
NP Tr 1/12
^{13}C NMR (101 MHz, cdcl$_3$) δ 172.93, 142.95, 137.44, 130.39, 128.23, 127.89, 127.60, 127.29, 126.92, 67.57, 57.77.
130.39
128.23
127.89
127.60
127.29
126.92
142.95
137.44
172.93
67.57
57.77
HN
O
NH
O
f1 (ppm)

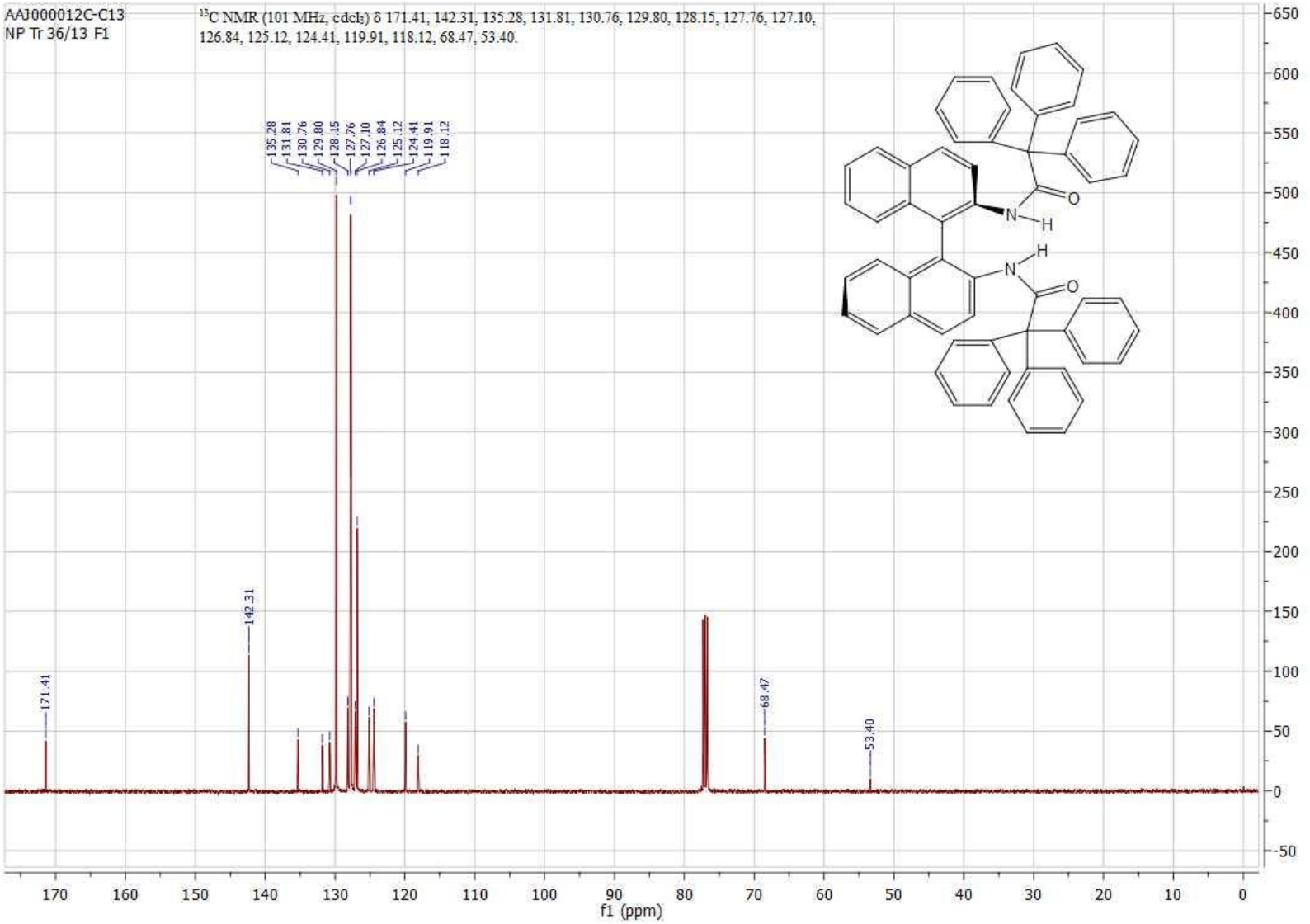

AAJ000012N
NP TR 39/13
^{1}H NMR (403 MHz, cdcl$_3$) δ 7.08 (td, J = 7.4, 1.3 Hz, 1H), 7.01 (td, J = 7.4, 1.2 Hz, 1H), 6.94 (d, J = 6.3 Hz, 1H), 5.56 (d, J = 7.9 Hz, 1H), 4.23 (d, J = 2.7 Hz, 1H), 3.91 (dt, J = 5.2, 2.8 Hz, 1H).
B (td) 7.01
A (td) 7.08
C (d) 6.94
E (d) 5.56
D (d) 4.23
F (dt) 3.91
NH
NH
O
O
1.55
f1 (ppm)


AAJ000012N-C13
NP TR 39/13
^{13}C NMR (101 MHz, cdcl$_3$) δ 172.70, 142.92, 140.04, 138.29, 130.33, 127.90, 126.88, 126.63, 126.60, 125.41, 124.76, 67.51, 57.54, 48.75.
130.33
127.90
126.88
126.63
126.60
125.41
124.76
142.92
140.04
138.29
172.70
67.51
57.54
48.75
NH
O
NH
O
f1 (ppm)


AAJ0000148
NPTr 43/13F1
¹H NMR (403 MHz, cdcl₃) δ 8.35 (d, J = 8.2 Hz, 1H), 7.19 – 7.08 (m, 9H), 7.02 (dt, J = 4.3, 3.4 Hz, 6H), 6.94 (s, 1H), 6.70 (d, J = 7.9 Hz, 1H), 1.59 (s, 3H).
A (d) 8.35
E (m) 7.13
B (d) 6.70
C (s) 6.94
D (dt) 7.02
F (s) 1.59
f1 (ppm)


AAJ000014B-C13
NPTr 43/13F1
13C NMR (101 MHz, cdcl3) δ 171.03, 142.69, 136.47, 135.99, 129.95, 129.07, 128.01, 126.90, 125.74, 123.76, 117.71, 68.63, 19.56.
129.95
129.07
128.01
126.90
125.74
123.76
171.03
142.69
136.47
135.99
117.71
68.63
19.56
H3C
N
H
O
f1 (ppm)


AAJ0000124
NP Tr 36/13 F1
¹H NMR (403 MHz, cdcl₃) δ 8.69 (d, J = 9.1 Hz, 1H), 7.82 (d, J = 9.2 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.34 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H), 7.20 – 7.12 (m, 2H), 7.08 – 7.03 (m, 3H), 6.99 (tt, J = 5.8, 1.7 Hz, 6H), 6.86 (ddd, J = 7.1, 3.4, 2.0 Hz, 6H), 6.83 (d, J = 0.9 Hz, 1H), 6.80 (d, J = 0.9 Hz, 1H).
A (d) 8.69
B (d) 7.82
C (d) 7.75
D (ddd) 7.34
E (m) 7.17
F (m) 7.05
G (ddd) 6.86
H (d) 6.83
I (d) 6.80
J (tt) 6.99
f1 (ppm)


AAJ000012C-C13
NP Tr 36/13 F1
13C NMR (101 MHz, cdcl3) δ 171.41, 142.31, 135.28, 131.81, 130.76, 129.80, 128.15, 127.76, 127.10, 126.84, 125.12, 124.41, 119.91, 118.12, 68.47, 53.40.
135.28
131.81
130.76
129.80
128.15
127.76
127.10
126.84
125.12
124.41
119.91
118.12
142.31
171.41
68.47
53.40
O
N
H
H
N
O
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Cartesian coordinates for low-energy structures optimized at the B3LYP/6-311G(2d,2p) or M06-2X/6-311G(2d,2p) levels

1 (conf. 1)

1	6	0	1.270072	3.874571	-0.999967
2	6	0	0.598923	2.489284	-1.065855
3	6	0	-0.746966	2.750387	-0.359711
4	6	0	-1.190641	4.116129	-0.914701
5	6	0	0.120622	4.878688	-1.250990
6	1	0	2.089693	3.958051	-1.710813
7	1	0	1.687624	4.005756	0.003096
8	7	0	1.354083	1.415329	-0.435492
9	1	0	0.409927	2.233903	-2.116956
10	1	0	-0.541609	2.828134	0.713794
11	7	0	-1.783707	1.735399	-0.534389
12	1	0	-1.827232	4.647399	-0.204953
13	1	0	-1.784051	3.963147	-1.822802
14	1	0	0.235844	5.774606	-0.638414
15	1	0	0.109887	5.209458	-2.291798
16	6	0	2.572118	1.033776	-0.900603
17	6	0	3.317457	-0.042514	-0.016230
18	6	0	2.560316	-1.392143	0.014620
19	6	0	1.508497	-1.690603	-0.855134
20	6	0	0.911255	-2.952505	-0.860281
21	6	0	1.356244	-3.943736	0.006564
22	6	0	2.413402	-3.665462	0.872599
23	6	0	3.010050	-2.410504	0.869006
24	6	0	4.706963	-0.374476	-0.614642
25	6	0	4.836739	-0.667015	-1.979474
26	6	0	6.057329	-1.064487	-2.513575
27	6	0	7.179216	-1.194767	-1.696808
28	6	0	7.061125	-0.926588	-0.338155
29	6	0	5.837379	-0.521828	0.195483
30	6	0	3.422577	0.642587	1.368679
31	6	0	2.666249	0.253010	2.477019
32	6	0	2.733683	0.963970	3.676820
33	6	0	3.552377	2.081514	3.789275
34	6	0	4.298271	2.492864	2.684504
35	6	0	4.229420	1.785266	1.490133
36	6	0	-1.863381	0.628574	0.253987
37	6	0	-3.158345	-0.255589	0.062112
38	6	0	-2.988554	-1.167758	-1.185558
39	6	0	-2.106810	-0.882921	-2.233383
40	6	0	-2.021254	-1.714932	-3.350892
41	6	0	-2.821195	-2.847829	-3.449299

42	6	0	-3.705968	-3.144204	-2.414071
43	6	0	-3.783774	-2.318056	-1.297535
44	6	0	-4.359016	0.705769	-0.109563
45	6	0	-4.578367	1.697906	0.861905
46	6	0	-5.636831	2.591301	0.754551
47	6	0	-6.506538	2.520466	-0.334770
48	6	0	-6.299412	1.550014	-1.306935
49	6	0	-5.234488	0.651846	-1.196650
50	6	0	-3.329566	-1.164945	1.305881
51	6	0	-2.300586	-2.054638	1.652193
52	6	0	-2.435495	-2.916416	2.733868
53	6	0	-3.606565	-2.924217	3.491119
54	6	0	-4.641707	-2.064803	3.145826
55	6	0	-4.504242	-1.194603	2.062081
56	8	0	3.069062	1.540126	-1.894130
57	8	0	-0.972734	0.342848	1.039917
58	1	0	0.927439	0.950782	0.358066
59	1	0	-2.595539	1.989115	-1.077000
60	1	0	1.141604	-0.941093	-1.543847
61	1	0	0.093861	-3.149615	-1.544399
62	1	0	0.892343	-4.923685	0.003690
63	1	0	2.782485	-4.431276	1.546058
64	1	0	3.846139	-2.221818	1.531094
65	1	0	3.981270	-0.573252	-2.632135
66	1	0	6.130506	-1.275100	-3.575000
67	1	0	8.130112	-1.505562	-2.115302
68	1	0	7.919807	-1.030533	0.316291
69	1	0	5.772895	-0.319003	1.256514
70	1	0	2.005431	-0.601063	2.411428
71	1	0	2.135648	0.638449	4.520783
72	1	0	3.606072	2.631335	4.722279
73	1	0	4.933886	3.369081	2.751907
74	1	0	4.805377	2.121523	0.635814
75	1	0	-1.471144	-0.009599	-2.188611
76	1	0	-1.321757	-1.470724	-4.142747
77	1	0	-2.754451	-3.493953	-4.317225
78	1	0	-4.467724	-2.573476	-0.498107
79	1	0	-3.914131	1.763838	1.716921
80	1	0	-5.783938	3.343546	1.521537
81	1	0	-7.332989	3.216654	-0.421269
82	1	0	-6.964193	1.483936	-2.160996
83	1	0	-5.093272	-0.092749	-1.968495
84	1	0	-1.387841	-2.073663	1.074317
85	1	0	-1.620782	-3.587420	2.982485
86	1	0	-3.710544	-3.598497	4.333989

87	1	0	-5.565884	-2.065802	3.713307
88	1	0	-5.332362	-0.546432	1.810178
89	1	0	-4.335166	-4.025570	-2.470472

1 (conf. 3)

1	6	0	-1.042815	-3.229150	-2.139154
2	6	0	-0.508438	-1.900447	-1.529708
3	6	0	0.372056	-2.324723	-0.305913
4	6	0	0.555212	-3.846357	-0.440247
5	6	0	-0.741549	-4.325852	-1.104235
6	1	0	-0.497043	-3.430038	-3.066758
7	1	0	-2.100543	-3.163576	-2.388107
8	7	0	-1.539592	-0.915008	-1.199581
9	1	0	0.128868	-1.397517	-2.256813
10	1	0	-0.190162	-2.098443	0.604141
11	7	0	1.679427	-1.660118	-0.240224
12	1	0	0.756627	-4.325249	0.521273
13	1	0	1.409291	-4.048669	-1.099275
14	1	0	-1.547440	-4.359770	-0.370487
15	1	0	-0.638019	-5.316201	-1.553772
16	6	0	-2.605664	-1.176661	-0.402377
17	6	0	-3.460936	0.057317	0.069174
18	6	0	-3.190183	1.334580	-0.766457
19	6	0	-3.378087	1.282235	-2.157841
20	6	0	-3.220503	2.411691	-2.951655
21	6	0	-2.886565	3.635865	-2.372842
22	6	0	-2.720398	3.710364	-0.995260
23	6	0	-2.871435	2.572420	-0.200756
24	6	0	-4.983704	-0.209702	-0.073344
25	6	0	-5.537375	-1.383510	-0.592454
26	6	0	-6.919983	-1.519508	-0.735354
27	6	0	-7.778093	-0.494949	-0.355369
28	6	0	-7.239576	0.679070	0.169537
29	6	0	-5.863338	0.818460	0.301129
30	6	0	-3.034250	0.181388	1.556013
31	6	0	-1.730754	0.590245	1.879665
32	6	0	-1.304998	0.642502	3.204274
33	6	0	-2.164298	0.270032	4.236143
34	6	0	-3.448034	-0.165050	3.925166
35	6	0	-3.876170	-0.213987	2.598948
36	6	0	1.849284	-0.315276	-0.186286
37	6	0	3.337868	0.190555	0.016892
38	6	0	3.962632	0.412587	-1.388429
39	6	0	3.561923	-0.320350	-2.510715
40	6	0	4.173425	-0.133835	-3.749911

41	6	0	5.208246	0.784379	-3.892945
42	6	0	5.623799	1.516003	-2.782909
43	6	0	5.005716	1.334964	-1.548898
44	6	0	4.137547	-0.867732	0.812716
45	6	0	3.647992	-1.313465	2.053696
46	6	0	4.335423	-2.260213	2.804153
47	6	0	5.536870	-2.790829	2.333256
48	6	0	6.033731	-2.362699	1.108348
49	6	0	5.340606	-1.412316	0.355308
50	6	0	3.303497	1.549696	0.767541
51	6	0	2.593754	2.628889	0.215848
52	6	0	2.575545	3.869555	0.842488
53	6	0	3.278317	4.075047	2.028999
54	6	0	4.006865	3.024668	2.572476
55	6	0	4.020652	1.776635	1.946214
56	8	0	-2.872479	-2.303969	-0.007505
57	8	0	0.916814	0.459173	-0.348069
58	1	0	-1.253434	0.047378	-1.300825
59	1	0	2.470438	-2.240794	-0.006661
60	1	0	-3.661230	0.345128	-2.622274
61	1	0	-3.368239	2.338023	-4.023483
62	1	0	-2.766238	4.519289	-2.989741
63	1	0	-2.473350	4.656537	-0.526437
64	1	0	-2.743508	2.660868	0.869311
65	1	0	-4.896260	-2.209140	-0.860385
66	1	0	-7.320622	-2.441341	-1.143149
67	1	0	-8.851161	-0.605857	-0.465217
68	1	0	-7.891277	1.492001	0.470730
69	1	0	-5.464512	1.745202	0.696171
70	1	0	-1.031331	0.865496	1.099968
71	1	0	-0.297009	0.976844	3.424642
72	1	0	-1.833451	0.311775	5.268045
73	1	0	-4.124615	-0.474873	4.714162
74	1	0	-4.872938	-0.570378	2.379667
75	1	0	2.768799	-1.051452	-2.426560
76	1	0	3.834307	-0.709952	-4.603795
77	1	0	5.683098	0.931151	-4.856418
78	1	0	5.337002	1.920843	-0.701044
79	1	0	2.718034	-0.909367	2.438234
80	1	0	3.932934	-2.583047	3.757813
81	1	0	6.074551	-3.529717	2.916446
82	1	0	6.965172	-2.766425	0.727306
83	1	0	5.748067	-1.097459	-0.595760
84	1	0	2.048829	2.492866	-0.705812
85	1	0	2.011529	4.681406	0.396569

86	1	0	3.264509	5.044321	2.514917
87	1	0	4.574711	3.167203	3.485360
88	1	0	4.610388	0.985347	2.387223
89	1	0	6.428817	2.236631	-2.875526

1 (conf. 4)

1	6	0	-0.349537	-3.524709	-0.937690
2	6	0	-0.333288	-2.043088	-0.519597
3	6	0	0.473869	-2.006350	0.829139
4	6	0	0.852833	-3.476602	1.140173
5	6	0	-0.184304	-4.309677	0.374471
6	1	0	0.516405	-3.701440	-1.577963
7	1	0	-1.244665	-3.793913	-1.506401
8	7	0	-1.707419	-1.548719	-0.342745
9	1	0	0.163961	-1.421928	-1.263244
10	1	0	-0.199206	-1.637376	1.602401
11	7	0	1.603991	-1.081273	0.839332
12	1	0	0.862457	-3.671274	2.215210
13	1	0	1.849598	-3.679884	0.747410
14	1	0	-1.133005	-4.348447	0.922573
15	1	0	0.137726	-5.340664	0.212241
16	6	0	-1.967177	-0.243816	-0.074901
17	6	0	-3.493815	0.179229	-0.021932
18	6	0	-3.953589	0.084968	1.459264
19	6	0	-3.423288	-0.863025	2.341909
20	6	0	-3.884642	-0.966187	3.653193
21	6	0	-4.896825	-0.128357	4.110736
22	6	0	-5.441668	0.813083	3.241424
23	6	0	-4.973424	0.919720	1.934279
24	6	0	-3.624591	1.652103	-0.498271
25	6	0	-2.888775	2.661613	0.144074
26	6	0	-3.020424	3.993712	-0.231529
27	6	0	-3.902752	4.360924	-1.246388
28	6	0	-4.657300	3.377029	-1.872620
29	6	0	-4.520619	2.038340	-1.500281
30	6	0	-4.328714	-0.768875	-0.914051
31	6	0	-5.437650	-1.475888	-0.441113
32	6	0	-6.169859	-2.315081	-1.283824
33	6	0	-5.807246	-2.466850	-2.616674
34	6	0	-4.702345	-1.769526	-3.105899
35	6	0	-3.975962	-0.933347	-2.265717
36	6	0	2.598357	-1.118732	-0.081535
37	6	0	3.639488	0.067157	-0.057770
38	6	0	3.486084	0.914301	1.231177
39	6	0	3.737124	0.307929	2.474790

40	6	0	3.635050	1.023667	3.661284
41	6	0	3.289184	2.375357	3.637682
42	6	0	3.050888	2.992990	2.416217
43	6	0	3.148133	2.269853	1.224808
44	6	0	3.300295	0.891605	-1.331056
45	6	0	4.278276	1.277889	-2.250236
46	6	0	3.945943	2.032287	-3.376293
47	6	0	2.628786	2.412348	-3.607032
48	6	0	1.642292	2.029948	-2.699555
49	6	0	1.972944	1.278170	-1.576357
50	6	0	5.103336	-0.459274	-0.119537
51	6	0	5.465025	-1.660173	-0.744533
52	6	0	6.799667	-2.058618	-0.812108
53	6	0	7.809305	-1.263699	-0.279811
54	6	0	7.468101	-0.056285	0.323140
55	6	0	6.134829	0.336627	0.402821
56	8	0	-1.063140	0.541277	0.172380
57	8	0	2.642292	-1.995488	-0.935886
58	1	0	-2.465163	-2.137015	-0.652674
59	1	0	1.526921	-0.267248	1.427397
60	1	0	-2.646384	-1.538480	2.008242
61	1	0	-3.447713	-1.705160	4.315880
62	1	0	-5.255309	-0.206495	5.130892
63	1	0	-6.232279	1.473705	3.579775
64	1	0	-5.405917	1.663867	1.278116
65	1	0	-2.205478	2.398886	0.936672
66	1	0	-2.432437	4.749381	0.277827
67	1	0	-4.005582	5.400878	-1.535831
68	1	0	-5.361560	3.641857	-2.653675
69	1	0	-5.133771	1.300740	-1.998663
70	1	0	-5.740096	-1.375520	0.592425
71	1	0	-7.026046	-2.850101	-0.888257
72	1	0	-6.375259	-3.119677	-3.269676
73	1	0	-4.406454	-1.874741	-4.143727
74	1	0	-3.125626	-0.392409	-2.665729
75	1	0	4.024678	-0.736486	2.508010
76	1	0	3.832858	0.528066	4.605394
77	1	0	3.211870	2.936950	4.561867
78	1	0	2.963150	2.775279	0.287164
79	1	0	5.308689	0.987701	-2.098105
80	1	0	4.725705	2.316852	-4.074391
81	1	0	2.371316	2.996906	-4.483370
82	1	0	0.608752	2.316442	-2.859740
83	1	0	1.180751	1.002346	-0.889239
84	1	0	4.698903	-2.277978	-1.186556

85	1	0	7.045466	-2.998931	-1.293917
86	1	0	8.846094	-1.576303	-0.337782
87	1	0	8.238296	0.585092	0.737666
88	1	0	5.899424	1.279745	0.878603
89	1	0	2.787613	4.044267	2.379487

1 (conf. 5)

1	6	0	0.070655	1.235839	4.093955
2	6	0	-0.294929	0.711428	2.689585
3	6	0	0.294929	-0.711428	2.689585
4	6	0	-0.070655	-1.235839	4.093955
5	6	0	0.000000	0.000000	5.028860
6	1	0	-0.587323	2.050127	4.401147
7	1	0	1.089009	1.636125	4.064614
8	7	0	0.173314	1.553159	1.601263
9	1	0	-1.382033	0.660869	2.586957
10	1	0	1.382033	-0.660869	2.586957
11	7	0	-0.173314	-1.553159	1.601263
12	1	0	0.587323	-2.050127	4.401147
13	1	0	-1.089009	-1.636125	4.064614
14	1	0	0.874775	-0.042492	5.680643
15	1	0	-0.874775	0.042492	5.680643
16	6	0	-0.646951	2.440733	0.972199
17	6	0	0.000000	3.403177	-0.101434
18	6	0	-0.711446	3.087286	-1.443263
19	6	0	-1.086370	1.774978	-1.757851
20	6	0	-1.666074	1.466190	-2.984861
21	6	0	-1.886646	2.466213	-3.929083
22	6	0	-1.522436	3.774706	-3.628626
23	6	0	-0.942607	4.081532	-2.398262
24	6	0	-0.273083	4.886916	0.295512
25	6	0	-1.477713	5.289406	0.889106
26	6	0	-1.722496	6.630974	1.174163
27	6	0	-0.785551	7.609664	0.855756
28	6	0	0.402541	7.229338	0.240281
29	6	0	0.653570	5.886638	-0.035463
30	6	0	1.525236	3.162724	-0.214980
31	6	0	2.124206	2.613689	-1.352298
32	6	0	3.502198	2.393851	-1.407688
33	6	0	4.313147	2.717320	-0.326592
34	6	0	3.734831	3.273716	0.813969
35	6	0	2.363038	3.496839	0.865146
36	6	0	0.646951	-2.440733	0.972199
37	6	0	0.000000	-3.403177	-0.101434
38	6	0	0.711446	-3.087286	-1.443263

39	6	0	1.086370	-1.774978	-1.757851
40	6	0	1.666074	-1.466190	-2.984861
41	6	0	1.886646	-2.466213	-3.929083
42	6	0	1.522436	-3.774706	-3.628626
43	6	0	0.942607	-4.081532	-2.398262
44	6	0	-1.525236	-3.162724	-0.214980
45	6	0	-2.363038	-3.496839	0.865146
46	6	0	-3.734831	-3.273716	0.813969
47	6	0	-4.313147	-2.717320	-0.326592
48	6	0	-3.502198	-2.393851	-1.407688
49	6	0	-2.124206	-2.613689	-1.352298
50	6	0	0.273083	-4.886916	0.295512
51	6	0	1.477713	-5.289406	0.889106
52	6	0	1.722496	-6.630974	1.174163
53	6	0	0.785551	-7.609664	0.855756
54	6	0	-0.402541	-7.229338	0.240281
55	6	0	-0.653570	-5.886638	-0.035463
56	8	0	-1.847774	2.465735	1.191454
57	8	0	1.847774	-2.465735	1.191454
58	1	0	1.164449	1.586918	1.416669
59	1	0	-1.164449	-1.586918	1.416669
60	1	0	-0.932112	0.979259	-1.039130
61	1	0	-1.945948	0.441007	-3.198663
62	1	0	-2.341683	2.228148	-4.883995
63	1	0	-1.693742	4.567059	-4.348983
64	1	0	-0.677532	5.108272	-2.183948
65	1	0	-2.225988	4.546788	1.121743
66	1	0	-2.660311	6.908436	1.643155
67	1	0	-0.981349	8.653020	1.076853
68	1	0	1.142202	7.975252	-0.029579
69	1	0	1.584330	5.623707	-0.520074
70	1	0	1.516270	2.359444	-2.209794
71	1	0	3.937120	1.966832	-2.304373
72	1	0	5.382169	2.543619	-0.370045
73	1	0	4.353429	3.542441	1.663127
74	1	0	1.934255	3.951262	1.750984
75	1	0	0.932112	-0.979259	-1.039130
76	1	0	1.945948	-0.441007	-3.198663
77	1	0	2.341683	-2.228148	-4.883995
78	1	0	0.677532	-5.108272	-2.183948
79	1	0	-1.934255	-3.951262	1.750984
80	1	0	-4.353429	-3.542441	1.663127
81	1	0	-5.382169	-2.543619	-0.370045
82	1	0	-3.937120	-1.966832	-2.304373
83	1	0	-1.516270	-2.359444	-2.209794

84	1	0	2.225988	-4.546788	1.121743
85	1	0	2.660311	-6.908436	1.643155
86	1	0	0.981349	-8.653020	1.076853
87	1	0	-1.142202	-7.975252	-0.029579
88	1	0	-1.584330	-5.623707	-0.520074
89	1	0	1.693742	-4.567059	-4.348983

1 (conf. 6)

1	6	0	0.947351	3.186005	-1.950140
2	6	0	0.445714	1.840490	-1.346627
3	6	0	-0.414729	2.238791	-0.110461
4	6	0	-0.873094	3.676166	-0.411501
5	6	0	0.377934	4.301177	-1.046886
6	1	0	0.562526	3.282685	-2.968626
7	1	0	2.034990	3.218333	-2.002957
8	7	0	1.491025	0.858941	-1.043495
9	1	0	-0.211383	1.352403	-2.062962
10	1	0	0.249313	2.267501	0.753729
11	7	0	-1.471954	1.282188	0.227330
12	1	0	-1.202986	4.195724	0.491724
13	1	0	-1.701624	3.655876	-1.122957
14	1	0	1.105377	4.544632	-0.268541
15	1	0	0.156792	5.217219	-1.598835
16	6	0	2.534877	1.100722	-0.213434
17	6	0	3.598447	-0.052126	-0.011357
18	6	0	3.235441	-1.303815	-0.848673
19	6	0	3.288526	-1.234810	-2.253337
20	6	0	2.950259	-2.326495	-3.045481
21	6	0	2.560854	-3.528425	-2.454810
22	6	0	2.520064	-3.619498	-1.068747
23	6	0	2.852897	-2.519772	-0.274798
24	6	0	5.012405	0.455855	-0.425802
25	6	0	5.414016	1.786896	-0.248967
26	6	0	6.706382	2.193967	-0.575426
27	6	0	7.637368	1.283754	-1.066186
28	6	0	7.261084	-0.046684	-1.223288
29	6	0	5.966465	-0.452877	-0.907420
30	6	0	3.574114	-0.369445	1.506886
31	6	0	2.351598	-0.428856	2.190105
32	6	0	2.294116	-0.748508	3.542552
33	6	0	3.464879	-1.021015	4.248012
34	6	0	4.684792	-0.968243	3.583007
35	6	0	4.738851	-0.643612	2.227066
36	6	0	-2.466203	0.903345	-0.617394
37	6	0	-3.567950	-0.076592	-0.031201

38	6	0	-4.827653	0.795406	0.222197
39	6	0	-4.716696	2.132974	0.620221
40	6	0	-5.847178	2.898748	0.895033
41	6	0	-7.117601	2.340256	0.786154
42	6	0	-7.242832	1.009078	0.398773
43	6	0	-6.110869	0.247143	0.116931
44	6	0	-3.077888	-0.722354	1.285738
45	6	0	-1.911782	-1.509517	1.280457
46	6	0	-1.438325	-2.109856	2.441946
47	6	0	-2.122069	-1.942738	3.646895
48	6	0	-3.277379	-1.170743	3.669391
49	6	0	-3.749372	-0.566895	2.501840
50	6	0	-3.910168	-1.173558	-1.082269
51	6	0	-4.214177	-0.824002	-2.408123
52	6	0	-4.579688	-1.791569	-3.338759
53	6	0	-4.676410	-3.131998	-2.971653
54	6	0	-4.409002	-3.489878	-1.655829
55	6	0	-4.032807	-2.521919	-0.723750
56	8	0	2.635613	2.155195	0.400307
57	8	0	-2.545066	1.346739	-1.753244
58	1	0	1.450295	-0.028664	-1.516640
59	1	0	-1.453629	0.875156	1.147856
60	1	0	3.610867	-0.316089	-2.729754
61	1	0	2.998563	-2.239984	-4.125261
62	1	0	2.299823	-4.381925	-3.069971
63	1	0	2.230738	-4.550131	-0.593208
64	1	0	2.820543	-2.620467	0.801313
65	1	0	4.713929	2.502297	0.155626
66	1	0	6.983502	3.233307	-0.436297
67	1	0	8.642350	1.604430	-1.317077
68	1	0	7.972794	-0.776430	-1.593702
69	1	0	5.703876	-1.494597	-1.036697
70	1	0	1.427887	-0.225101	1.660715
71	1	0	1.333112	-0.777988	4.044049
72	1	0	3.424790	-1.265204	5.303616
73	1	0	5.605759	-1.171919	4.118140
74	1	0	5.701196	-0.597075	1.735386
75	1	0	-3.740362	2.590556	0.720235
76	1	0	-5.730792	3.935227	1.191875
77	1	0	-7.998612	2.935944	0.996936
78	1	0	-6.231112	-0.783000	-0.192182
79	1	0	-1.374575	-1.661937	0.351440
80	1	0	-0.536520	-2.710420	2.404950
81	1	0	-1.757110	-2.412782	4.553109
82	1	0	-3.822099	-1.032505	4.596713

83	1	0	-4.652528	0.026324	2.545839
84	1	0	-4.152863	0.209841	-2.709341
85	1	0	-4.798630	-1.489709	-4.357279
86	1	0	-4.965923	-3.882810	-3.698565
87	1	0	-4.493486	-4.524606	-1.341919
88	1	0	-3.845059	-2.835777	0.293513
89	1	0	-8.224986	0.558447	0.307347

1 (conf. 7)

1	6	0	-0.951120	-3.467890	-1.949021
2	6	0	-0.485839	-2.177525	-1.256262
3	6	0	0.685182	-2.663734	-0.372215
4	6	0	1.354227	-3.813368	-1.181080
5	6	0	0.372318	-4.150033	-2.333178
6	1	0	-1.601546	-3.259209	-2.798700
7	1	0	-1.514282	-4.080710	-1.234485
8	7	0	-1.499635	-1.475246	-0.480973
9	1	0	-0.106832	-1.490062	-2.013105
10	1	0	0.250487	-3.088843	0.539290
11	7	0	1.590850	-1.616642	0.100471
12	1	0	1.526177	-4.673626	-0.529577
13	1	0	2.317713	-3.490817	-1.570767
14	1	0	0.259858	-5.225039	-2.486965
15	1	0	0.745719	-3.725253	-3.268142
16	6	0	-2.438493	-0.687530	-1.075592
17	6	0	-3.440914	0.053661	-0.098169
18	6	0	-2.874560	1.476833	0.152894
19	6	0	-1.543698	1.816692	-0.107763
20	6	0	-1.064183	3.101864	0.150122
21	6	0	-1.906828	4.070531	0.684998
22	6	0	-3.236044	3.746169	0.950701
23	6	0	-3.713898	2.467718	0.680886
24	6	0	-4.826518	0.207907	-0.785002
25	6	0	-4.913520	0.819382	-2.046099
26	6	0	-6.144528	1.022416	-2.659705
27	6	0	-7.325864	0.642156	-2.025464
28	6	0	-7.257885	0.063281	-0.764382
29	6	0	-6.021860	-0.148609	-0.150916
30	6	0	-3.549068	-0.747264	1.219366
31	6	0	-3.172530	-0.229148	2.461798
32	6	0	-3.263044	-1.000995	3.622815
33	6	0	-3.728109	-2.309181	3.565442
34	6	0	-4.101392	-2.845577	2.332433
35	6	0	-4.010095	-2.075619	1.178684
36	6	0	2.363674	-0.858767	-0.720846

37	6	0	3.341348	0.184365	-0.044444
38	6	0	4.763787	-0.262051	-0.475037
39	6	0	5.105041	-1.621736	-0.455782
40	6	0	6.383701	-2.049874	-0.796241
41	6	0	7.357436	-1.123676	-1.165696
42	6	0	7.032927	0.227961	-1.189858
43	6	0	5.748673	0.654245	-0.849599
44	6	0	3.197309	0.175840	1.498519
45	6	0	1.997541	0.622928	2.082824
46	6	0	1.819547	0.620113	3.462148
47	6	0	2.843684	0.181949	4.301544
48	6	0	4.041321	-0.246475	3.741594
49	6	0	4.216050	-0.249716	2.356096
50	6	0	3.045017	1.617344	-0.579155
51	6	0	2.586245	1.855938	-1.881913
52	6	0	2.387436	3.156117	-2.343975
53	6	0	2.661509	4.250963	-1.529843
54	6	0	3.142171	4.030413	-0.242066
55	6	0	3.329416	2.731356	0.225192
56	8	0	-2.445978	-0.509990	-2.280397
57	8	0	2.350240	-1.009781	-1.933181
58	1	0	-1.587613	-1.676840	0.502564
59	1	0	1.654626	-1.458643	1.092640
60	1	0	-0.865383	1.087272	-0.530686
61	1	0	-0.032021	3.339997	-0.080505
62	1	0	-1.535853	5.069885	0.883089
63	1	0	-3.908589	4.492704	1.358890
64	1	0	-4.754768	2.238896	0.874643
65	1	0	-4.010303	1.125943	-2.550300
66	1	0	-6.178486	1.487572	-3.638844
67	1	0	-8.284695	0.804871	-2.505182
68	1	0	-8.165348	-0.225220	-0.245088
69	1	0	-6.006734	-0.588941	0.836515
70	1	0	-2.806543	0.786179	2.531626
71	1	0	-2.967758	-0.569482	4.572867
72	1	0	-3.800253	-2.906964	4.467007
73	1	0	-4.465801	-3.864976	2.269337
74	1	0	-4.305365	-2.506920	0.228879
75	1	0	4.364676	-2.359745	-0.168538
76	1	0	6.616898	-3.108760	-0.777781
77	1	0	8.353748	-1.454395	-1.436589
78	1	0	5.518583	1.710383	-0.886333
79	1	0	1.198159	0.991564	1.450703
80	1	0	0.882610	0.971326	3.879793
81	1	0	2.709432	0.184221	5.377310

82	1	0	4.852432	-0.579176	4.379798
83	1	0	5.160663	-0.580884	1.947446
84	1	0	2.394600	1.020778	-2.538557
85	1	0	2.019449	3.306902	-3.352787
86	1	0	2.508865	5.260525	-1.894807
87	1	0	3.374082	4.868297	0.406369
88	1	0	3.706536	2.591109	1.229728
89	1	0	7.776836	0.961256	-1.481139

1 (conf. 8)

1	6	0	-1.077812	-4.059035	-0.614969
2	6	0	-0.616971	-2.579531	-0.493907
3	6	0	0.612229	-2.609430	0.485839
4	6	0	0.976959	-4.095037	0.639138
5	6	0	-0.374371	-4.811195	0.530066
6	1	0	-0.745405	-4.461925	-1.576097
7	1	0	-2.165608	-4.145155	-0.594166
8	7	0	-1.682239	-1.700682	-0.038437
9	1	0	-0.303073	-2.177465	-1.456063
10	1	0	0.280346	-2.209217	1.446716
11	7	0	1.750548	-1.805595	0.069273
12	1	0	1.512565	-4.294590	1.569583
13	1	0	1.625828	-4.406983	-0.189565
14	1	0	-0.931783	-4.697262	1.466797
15	1	0	-0.277643	-5.882306	0.341200
16	6	0	-1.932745	-0.481406	-0.588518
17	6	0	-3.215258	0.241887	-0.031758
18	6	0	-3.338005	0.171673	1.509775
19	6	0	-2.196728	0.124327	2.323813
20	6	0	-2.306681	0.185122	3.712843
21	6	0	-3.552581	0.306016	4.319808
22	6	0	-4.691320	0.386653	3.521385
23	6	0	-4.582997	0.327920	2.135232
24	6	0	-3.174136	1.755135	-0.344650
25	6	0	-1.986710	2.480328	-0.187741
26	6	0	-1.967701	3.861862	-0.354013
27	6	0	-3.135391	4.552683	-0.672122
28	6	0	-4.324740	3.845464	-0.813153
29	6	0	-4.342611	2.461407	-0.647169
30	6	0	-4.328459	-0.505703	-0.809856
31	6	0	-5.070850	-1.553993	-0.253963
32	6	0	-5.986771	-2.274168	-1.020339
33	6	0	-6.170232	-1.971735	-2.365712
34	6	0	-5.418106	-0.949209	-2.940051
35	6	0	-4.505814	-0.230512	-2.173901

36	6	0	1.856514	-0.479580	0.344125
37	6	0	3.216621	0.213338	-0.030162
38	6	0	4.046302	-0.556510	-1.088959
39	6	0	3.433064	-0.938785	-2.294515
40	6	0	4.155956	-1.556726	-3.309876
41	6	0	5.521487	-1.790492	-3.158593
42	6	0	6.150860	-1.386631	-1.986280
43	6	0	5.422913	-0.775308	-0.965472
44	6	0	3.879740	0.290656	1.369015
45	6	0	3.774087	1.441168	2.157247
46	6	0	4.273142	1.469246	3.457847
47	6	0	4.873211	0.340982	4.008283
48	6	0	4.954618	-0.823225	3.248412
49	6	0	4.455589	-0.848900	1.949026
50	6	0	2.972818	1.600048	-0.669976
51	6	0	1.763623	1.942742	-1.282771
52	6	0	1.625999	3.160586	-1.950317
53	6	0	2.688046	4.056396	-2.017062
54	6	0	3.901194	3.719433	-1.419507
55	6	0	4.041609	2.501765	-0.762350
56	8	0	-1.291405	-0.035108	-1.524777
57	8	0	0.993910	0.135360	0.951164
58	1	0	-2.216120	-1.974699	0.772216
59	1	0	2.464382	-2.240303	-0.495040
60	1	0	-1.207536	0.067281	1.884577
61	1	0	-1.406131	0.149921	4.316014
62	1	0	-3.635733	0.353742	5.399829
63	1	0	-5.668616	0.506202	3.976227
64	1	0	-5.479076	0.421162	1.534745
65	1	0	-1.068448	1.971232	0.071438
66	1	0	-1.032811	4.397120	-0.230742
67	1	0	-3.118231	5.629229	-0.801362
68	1	0	-5.245768	4.366816	-1.050467
69	1	0	-5.280805	1.932560	-0.759214
70	1	0	-4.943560	-1.817249	0.787983
71	1	0	-6.555644	-3.074029	-0.558834
72	1	0	-6.884213	-2.529369	-2.961379
73	1	0	-5.536289	-0.710642	-3.991292
74	1	0	-3.911262	0.544996	-2.639312
75	1	0	2.382149	-0.726409	-2.452647
76	1	0	3.652229	-1.840210	-4.227345
77	1	0	6.087801	-2.266878	-3.950749
78	1	0	5.942246	-0.458831	-0.071191
79	1	0	3.287298	2.319681	1.757750
80	1	0	4.181171	2.377394	4.043245

81	1	0	5.262053	0.363687	5.020120
82	1	0	5.402461	-1.717846	3.667147
83	1	0	4.512992	-1.772065	1.385896
84	1	0	0.914576	1.273021	-1.250875
85	1	0	0.676560	3.400252	-2.415361
86	1	0	2.576090	5.003116	-2.533806
87	1	0	4.743363	4.400884	-1.470824
88	1	0	4.997008	2.249409	-0.317290
89	1	0	7.216878	-1.540699	-1.859935

4a (conf. 1)

1	6	0	0.769666	2.814517	-0.149047
2	1	0	0.709505	2.761345	-1.241795
3	6	0	1.468686	4.122757	0.263077
4	1	0	2.470800	4.140231	-0.175871
5	1	0	1.601217	4.120735	1.353539
6	6	0	0.679650	5.371988	-0.144316
7	1	0	1.199404	6.266577	0.211833
8	1	0	0.649905	5.441648	-1.238744
9	6	0	-0.750782	5.317728	0.400742
10	1	0	-1.324018	6.183858	0.056882
11	1	0	-0.728486	5.374292	1.496212
12	6	0	-1.447985	4.024141	-0.029668
13	1	0	-2.449814	3.965299	0.396845
14	1	0	-1.553648	4.005577	-1.121821
15	6	0	-0.668713	2.765174	0.405997
16	1	0	-0.628699	2.746157	1.501140
17	6	0	1.747725	0.550750	-0.445865
18	6	0	-2.501196	1.149557	0.579532
19	6	0	2.968708	-0.375933	-0.062031
20	6	0	4.118384	-0.030235	-1.051072
21	6	0	5.133467	-0.965876	-1.291313
22	1	0	5.087229	-1.939388	-0.820183
23	6	0	6.201425	-0.669624	-2.133344
24	1	0	6.971508	-1.414618	-2.300299
25	6	0	6.277000	0.568909	-2.766196
26	1	0	7.103550	0.797088	-3.429525
27	6	0	5.273965	1.505916	-2.542376
28	1	0	5.311580	2.472462	-3.032560
29	6	0	4.210093	1.210117	-1.691201
30	1	0	3.447306	1.961907	-1.538119
31	6	0	3.390397	-0.092865	1.399553
32	6	0	4.666903	0.356716	1.748856
33	1	0	5.412260	0.513329	0.980925
34	6	0	5.000913	0.607353	3.081714

35	1	0	5.999706	0.953259	3.323751
36	6	0	4.064204	0.417210	4.090661
37	1	0	4.324274	0.612583	5.124844
38	6	0	2.783812	-0.026388	3.758423
39	1	0	2.039316	-0.178263	4.531787
40	6	0	2.453070	-0.277966	2.431751
41	1	0	1.452633	-0.622369	2.195186
42	6	0	2.599559	-1.872798	-0.256622
43	6	0	2.906446	-2.838431	0.709596
44	1	0	3.359693	-2.546245	1.646704
45	6	0	2.650937	-4.192580	0.486904
46	1	0	2.903829	-4.914721	1.255572
47	6	0	2.081606	-4.612447	-0.709509
48	1	0	1.878931	-5.663372	-0.883164
49	6	0	1.787399	-3.664401	-1.687317
50	1	0	1.355070	-3.973689	-2.632516
51	6	0	2.052787	-2.315738	-1.471644
52	1	0	1.826982	-1.598944	-2.245716
53	6	0	-3.159948	-0.189816	0.086358
54	6	0	-4.709324	-0.109333	0.112827
55	6	0	-5.434709	-1.297654	-0.056083
56	1	0	-4.906215	-2.240399	-0.132281
57	6	0	-6.822619	-1.294858	-0.131366
58	1	0	-7.353931	-2.231737	-0.258822
59	6	0	-7.526093	-0.094345	-0.050253
60	1	0	-8.608729	-0.086949	-0.110455
61	6	0	-6.820188	1.092417	0.109264
62	1	0	-7.351151	2.035795	0.177712
63	6	0	-5.427029	1.087415	0.192212
64	1	0	-4.908318	2.020824	0.349337
65	6	0	-2.822407	-0.539005	-1.383858
66	6	0	-2.530214	-1.838957	-1.809882
67	1	0	-2.450658	-2.640888	-1.088570
68	6	0	-2.342873	-2.130073	-3.160597
69	1	0	-2.114896	-3.147801	-3.457886
70	6	0	-2.449825	-1.129417	-4.119978
71	1	0	-2.300555	-1.355534	-5.169733
72	6	0	-2.763543	0.166182	-3.715233
73	1	0	-2.868283	0.956536	-4.450370
74	6	0	-2.955037	0.452400	-2.368176
75	1	0	-3.226811	1.460655	-2.079804
76	6	0	-2.619500	-1.193787	1.134769
77	6	0	-1.338931	-1.750111	1.015407
78	1	0	-0.731324	-1.537922	0.144689
79	6	0	-0.826242	-2.589347	2.003130

80	1	0	0.156120	-3.026871	1.867884
81	6	0	-1.571804	-2.867162	3.146379
82	1	0	-1.174935	-3.523097	3.913447
83	6	0	-2.828564	-2.287858	3.295603
84	1	0	-3.414463	-2.477771	4.188274
85	6	0	-3.343687	-1.457285	2.303295
86	1	0	-4.315893	-1.004621	2.442477
87	7	0	1.612963	1.692823	0.274633
88	7	0	-1.356535	1.549067	-0.033035
89	8	0	1.011518	0.308017	-1.393396
90	8	0	-2.969983	1.759801	1.530071
91	1	0	2.213016	1.830432	1.073569
92	1	0	-0.943822	1.007086	-0.783581

4a (conf. 3)

1	6	0	-0.649327	2.797004	0.284917
2	1	0	-0.623650	2.743395	1.376928
3	6	0	-1.474419	4.034554	-0.122720
4	1	0	-2.470205	3.939620	0.317074
5	1	0	-1.600331	4.029227	-1.212916
6	6	0	-0.813508	5.345586	0.315635
7	1	0	-1.412250	6.197049	-0.021499
8	1	0	-0.791403	5.394108	1.411455
9	6	0	0.615081	5.445030	-0.228686
10	1	0	1.101520	6.358578	0.126298
11	1	0	0.584213	5.511848	-1.323316
12	6	0	1.446250	4.223863	0.181966
13	1	0	2.451085	4.279121	-0.246343
14	1	0	1.569039	4.221598	1.273548
15	6	0	0.797041	2.894782	-0.246498
16	1	0	0.774764	2.837282	-1.338644
17	6	0	-2.253059	0.965029	0.590337
18	6	0	1.944781	0.720448	-0.594129
19	6	0	-3.034288	-0.269869	-0.014819
20	6	0	-2.738644	-0.453993	-1.524930
21	6	0	-3.706100	-0.227674	-2.511103
22	1	0	-4.707962	0.062691	-2.228278
23	6	0	-3.406247	-0.378929	-3.865096
24	1	0	-4.180554	-0.199265	-4.603013
25	6	0	-2.129722	-0.755136	-4.268269
26	1	0	-1.896331	-0.866742	-5.321278
27	6	0	-1.154417	-0.988843	-3.301494
28	1	0	-0.149309	-1.275631	-3.584970
29	6	0	-1.459444	-0.850278	-1.951156
30	1	0	-0.682163	-1.057911	-1.226928

31	6	0	-2.638042	-1.544541	0.789092
32	6	0	-2.555281	-2.795327	0.163389
33	1	0	-2.710910	-2.878242	-0.903531
34	6	0	-2.278784	-3.952286	0.890832
35	1	0	-2.218833	-4.903228	0.373043
36	6	0	-2.082784	-3.889085	2.266078
37	1	0	-1.866265	-4.787618	2.833152
38	6	0	-2.181010	-2.655558	2.905055
39	1	0	-2.051031	-2.588901	3.980025
40	6	0	-2.462342	-1.499714	2.180448
41	1	0	-2.562440	-0.554372	2.694494
42	6	0	-4.541049	0.026980	0.207716
43	6	0	-5.450601	-0.990965	0.503652
44	1	0	-5.099300	-2.004936	0.641548
45	6	0	-6.813467	-0.722897	0.632782
46	1	0	-7.495574	-1.532897	0.866860
47	6	0	-7.295399	0.571289	0.470509
48	1	0	-8.353781	0.781254	0.577111
49	6	0	-6.399752	1.596849	0.173816
50	1	0	-6.756926	2.613027	0.047320
51	6	0	-5.041789	1.325276	0.044160
52	1	0	-4.366148	2.138742	-0.190638
53	6	0	2.977295	-0.312154	0.016652
54	6	0	2.694070	-1.717811	-0.579507
55	6	0	2.436342	-2.841181	0.210776
56	1	0	2.397747	-2.755059	1.287434
57	6	0	2.233933	-4.097777	-0.364400
58	1	0	2.033414	-4.948439	0.277352
59	6	0	2.291594	-4.257821	-1.742612
60	1	0	2.133968	-5.232745	-2.190379
61	6	0	2.567527	-3.149439	-2.542822
62	1	0	2.631910	-3.259019	-3.620011
63	6	0	2.772423	-1.899531	-1.970402
64	1	0	2.993907	-1.054021	-2.604726
65	6	0	4.399705	0.118638	-0.434134
66	6	0	5.443816	-0.816618	-0.393122
67	1	0	5.237213	-1.832872	-0.081023
68	6	0	6.740741	-0.464908	-0.752176
69	1	0	7.527593	-1.209884	-0.709405
70	6	0	7.026493	0.832306	-1.174245
71	1	0	8.034972	1.105658	-1.463382
72	6	0	6.000381	1.768765	-1.227112
73	1	0	6.202917	2.780573	-1.560685
74	6	0	4.702288	1.416113	-0.856706
75	1	0	3.925798	2.167444	-0.908681

76	6	0	2.857087	-0.304671	1.558737
77	6	0	3.934948	-0.025946	2.404890
78	1	0	4.909021	0.188287	1.986983
79	6	0	3.777713	-0.016515	3.792591
80	1	0	4.632849	0.201421	4.422822
81	6	0	2.538502	-0.280917	4.363283
82	1	0	2.416744	-0.271978	5.440560
83	6	0	1.450570	-0.553393	3.533995
84	1	0	0.473874	-0.757094	3.956965
85	6	0	1.609200	-0.563836	2.153112
86	1	0	0.747660	-0.776745	1.531008
87	7	0	-1.301363	1.569278	-0.168731
88	7	0	1.632326	1.781649	0.196889
89	8	0	-2.523081	1.371217	1.712460
90	8	0	1.507360	0.614170	-1.728972
91	1	0	-1.124822	1.243706	-1.108426
92	1	0	1.959172	1.784002	1.151414

4b (conf. 1)

1	6	0	-0.602833	-0.487798	-2.087707
2	1	0	-1.497838	0.128821	-2.032232
3	6	0	-0.675469	-1.311329	-3.391564
4	1	0	-1.598898	-1.898213	-3.369785
5	1	0	0.159036	-2.014872	-3.421199
6	6	0	-0.631928	-0.431747	-4.645401
7	1	0	-0.667173	-1.065458	-5.537263
8	1	0	-1.515990	0.216756	-4.683262
9	6	0	0.631928	0.431747	-4.645401
10	1	0	0.667173	1.065458	-5.537263
11	1	0	1.515990	-0.216756	-4.683262
12	6	0	0.675469	1.311329	-3.391564
13	1	0	1.598898	1.898213	-3.369785
14	1	0	-0.159036	2.014872	-3.421199
15	6	0	0.602833	0.487798	-2.087707
16	1	0	1.497838	-0.128821	-2.032232
17	6	0	0.262926	-2.370975	-0.740043
18	6	0	-0.262926	2.370975	-0.740043
19	6	0	-0.006620	-3.600569	0.241550
20	6	0	1.072878	-4.688409	-0.048961
21	6	0	2.428666	-4.376974	0.137807
22	1	0	2.711806	-3.376218	0.431264
23	6	0	3.418364	-5.332285	-0.049441
24	1	0	4.457894	-5.058661	0.094366
25	6	0	3.082244	-6.635333	-0.417484

26	1	0	3.855384	-7.381830	-0.561928
27	6	0	1.744476	-6.964290	-0.587568
28	1	0	1.460200	-7.974127	-0.862756
29	6	0	0.749878	-6.000141	-0.403564
30	1	0	-0.282075	-6.292734	-0.536796
31	6	0	0.209253	-3.210068	1.722945
32	6	0	0.166956	-4.210767	2.708010
33	1	0	-0.054338	-5.231401	2.421002
34	6	0	0.439009	-3.925504	4.040404
35	1	0	0.396748	-4.720473	4.776691
36	6	0	0.789485	-2.631658	4.425263
37	1	0	1.018888	-2.410361	5.461440
38	6	0	0.857479	-1.633928	3.460879
39	1	0	1.143977	-0.626030	3.737159
40	6	0	0.563851	-1.920589	2.125531
41	1	0	0.631108	-1.124153	1.395777
42	6	0	-1.418536	-4.150859	-0.070850
43	6	0	-1.744476	-4.412166	-1.410737
44	1	0	-1.005249	-4.235063	-2.183284
45	6	0	-2.992982	-4.909046	-1.769263
46	1	0	-3.213019	-5.101622	-2.813521
47	6	0	-3.954418	-5.161876	-0.791692
48	1	0	-4.928556	-5.549664	-1.067202
49	6	0	-3.647644	-4.907151	0.540205
50	1	0	-4.384894	-5.092524	1.313632
51	6	0	-2.394640	-4.405395	0.895495
52	1	0	-2.193476	-4.201317	1.938409
53	6	0	0.006620	3.600569	0.241550
54	6	0	-0.209253	3.210068	1.722945
55	6	0	-0.166956	4.210767	2.708010
56	1	0	0.054338	5.231401	2.421002
57	6	0	-0.439009	3.925504	4.040404
58	1	0	-0.396748	4.720473	4.776691
59	6	0	-0.789485	2.631658	4.425263
60	1	0	-1.018888	2.410361	5.461440
61	6	0	-0.857479	1.633928	3.460879
62	1	0	-1.143977	0.626030	3.737159
63	6	0	-0.563851	1.920589	2.125531
64	1	0	-0.631108	1.124153	1.395777
65	6	0	1.418536	4.150859	-0.070850
66	6	0	1.744476	4.412166	-1.410737
67	1	0	1.005249	4.235063	-2.183284
68	6	0	2.992982	4.909046	-1.769263
69	1	0	3.213019	5.101622	-2.813521
70	6	0	3.954418	5.161876	-0.791692

71	1	0	4.928556	5.549664	-1.067202
72	6	0	3.647644	4.907151	0.540205
73	1	0	4.384894	5.092524	1.313632
74	6	0	2.394640	4.405395	0.895495
75	1	0	2.193476	4.201317	1.938409
76	6	0	-1.072878	4.688409	-0.048961
77	6	0	-2.428666	4.376974	0.137807
78	1	0	-2.711806	3.376218	0.431264
79	6	0	-3.418364	5.332285	-0.049441
80	1	0	-4.457894	5.058661	0.094366
81	6	0	-3.082244	6.635333	-0.417484
82	1	0	-3.855384	7.381830	-0.561928
83	6	0	-1.744476	6.964290	-0.587568
84	1	0	-1.460200	7.974127	-0.862756
85	6	0	-0.749878	6.000141	-0.403564
86	1	0	0.282075	6.292734	-0.536796
87	7	0	-0.672216	-1.377804	-0.889856
88	7	0	0.672216	1.377804	-0.889856
89	8	0	1.296102	-2.349022	-1.396093
90	8	0	-1.296102	2.349022	-1.396093
91	6	0	1.904865	1.237543	-0.112450
92	1	0	1.808550	1.691077	0.868460
93	1	0	2.104030	0.173221	0.024286
94	1	0	2.762011	1.687242	-0.623697
95	6	0	-1.904865	-1.237543	-0.112450
96	1	0	-1.808550	-1.691077	0.868460
97	1	0	-2.104030	-0.173221	0.024286
98	1	0	-2.762011	-1.687242	-0.623697

4b (conf. 5)

1	6	0	0.490773	-2.085620	0.725462
2	1	0	-0.130376	-1.981980	1.612927
3	6	0	1.302150	-3.393108	0.865203
4	1	0	1.875980	-3.338899	1.796549
5	1	0	2.017191	-3.464781	0.043290
6	6	0	0.417242	-4.643442	0.868020
7	1	0	1.046310	-5.535343	0.951666
8	1	0	-0.242052	-4.637681	1.744778
9	6	0	-0.430639	-4.695590	-0.404705
10	1	0	-1.068474	-5.585206	-0.407968
11	1	0	0.227606	-4.775274	-1.278757
12	6	0	-1.302300	-3.440599	-0.511528
13	1	0	-1.880408	-3.456485	-1.440613
14	1	0	-2.013921	-3.431002	0.316928
15	6	0	-0.477235	-2.135273	-0.486401

16	1	0	0.146393	-2.113296	-1.377961
17	6	0	2.384940	-0.788053	-0.194459
18	6	0	-2.350303	-0.747850	0.331655
19	6	0	3.561538	0.267756	-0.039266
20	6	0	2.917281	1.634959	-0.385690
21	6	0	2.319894	1.770628	-1.649855
22	1	0	2.323535	0.923742	-2.325853
23	6	0	1.752380	2.972872	-2.055644
24	1	0	1.306198	3.048385	-3.040939
25	6	0	1.764985	4.078532	-1.206226
26	1	0	1.333517	5.020334	-1.525413
27	6	0	2.328668	3.953292	0.058304
28	1	0	2.338841	4.798904	0.737487
29	6	0	2.891325	2.742125	0.467029
30	1	0	3.318763	2.678862	1.458602
31	6	0	4.308399	0.199993	1.315717
32	6	0	5.276394	1.166952	1.630357
33	1	0	5.454524	1.990057	0.950522
34	6	0	6.046610	1.073286	2.784363
35	1	0	6.782837	1.840357	2.997855
36	6	0	5.890890	-0.007487	3.649935
37	1	0	6.494128	-0.084700	4.547260
38	6	0	4.966055	-0.995836	3.333766
39	1	0	4.845816	-1.857551	3.981113
40	6	0	4.188836	-0.893046	2.180322
41	1	0	3.489971	-1.686629	1.954010
42	6	0	4.677015	-0.075632	-1.074185
43	6	0	5.296446	0.912387	-1.843362
44	1	0	4.945838	1.935001	-1.801915
45	6	0	6.371645	0.607879	-2.680484
46	1	0	6.829369	1.397223	-3.266766
47	6	0	6.850731	-0.692998	-2.762952
48	1	0	7.682892	-0.932909	-3.415325
49	6	0	6.249344	-1.686672	-1.990842
50	1	0	6.612355	-2.707460	-2.039444
51	6	0	5.183580	-1.380019	-1.154846
52	1	0	4.740069	-2.168471	-0.562798
53	6	0	-3.588256	0.216256	0.041835
54	6	0	-3.195883	1.710238	0.143150
55	6	0	-4.213080	2.679236	0.166743
56	1	0	-5.247683	2.365780	0.100672
57	6	0	-3.921335	4.030773	0.302317
58	1	0	-4.729800	4.753469	0.315752
59	6	0	-2.599505	4.453671	0.440253
60	1	0	-2.370186	5.506895	0.557688

61	6	0	-1.582492	3.507689	0.437433
62	1	0	-0.549130	3.811508	0.549253
63	6	0	-1.878495	2.150997	0.286903
64	1	0	-1.061627	1.441309	0.287451
65	6	0	-4.185878	-0.172828	-1.331965
66	6	0	-4.426153	-1.530110	-1.595117
67	1	0	-4.195194	-2.269367	-0.836947
68	6	0	-4.970737	-1.947661	-2.805109
69	1	0	-5.146051	-3.003905	-2.977478
70	6	0	-5.293272	-1.013738	-3.788621
71	1	0	-5.717845	-1.335555	-4.732805
72	6	0	-5.062547	0.335103	-3.542306
73	1	0	-5.305094	1.075308	-4.296914
74	6	0	-4.514022	0.750076	-2.328052
75	1	0	-4.334001	1.804926	-2.170473
76	6	0	-4.637456	-0.019425	1.170567
77	6	0	-4.287929	0.265238	2.499780
78	1	0	-3.285436	0.598432	2.728794
79	6	0	-5.207085	0.127443	3.530746
80	1	0	-4.904584	0.348220	4.548598
81	6	0	-6.511608	-0.289172	3.263054
82	1	0	-7.230359	-0.394549	4.068171
83	6	0	-6.877723	-0.558778	1.951691
84	1	0	-7.889395	-0.873708	1.719967
85	6	0	-5.949246	-0.423940	0.915782
86	1	0	-6.270468	-0.633681	-0.094715
87	7	0	1.396814	-0.899061	0.749358
88	7	0	-1.375119	-0.948283	-0.612665
89	8	0	2.361265	-1.487285	-1.200898
90	8	0	-2.305913	-1.348509	1.397860
91	6	0	-1.271849	-0.265303	-1.903531
92	1	0	-1.674783	-0.880123	-2.715198
93	1	0	-1.796302	0.682952	-1.894356
94	1	0	-0.217936	-0.065226	-2.104506
95	6	0	1.203780	-0.024753	1.905277
96	1	0	1.500621	-0.519036	2.836138
97	1	0	1.772652	0.892150	1.808037
98	1	0	0.145788	0.234067	1.977981

4b (conf. 7)

1	6	0	-0.212032	0.741662	2.281994
2	1	0	-1.299944	0.809047	2.297871
3	6	0	0.313370	1.419013	3.570900
4	1	0	-0.008391	2.461348	3.553104
5	1	0	1.410921	1.408411	3.555050

6	6	0	-0.182967	0.742115	4.851212
7	1	0	0.237274	1.248053	5.726031
8	1	0	-1.272195	0.853478	4.918851
9	6	0	0.182967	-0.742115	4.851212
10	1	0	-0.237274	-1.248053	5.726031
11	1	0	1.272195	-0.853478	4.918851
12	6	0	-0.313370	-1.419013	3.570900
13	1	0	0.008391	-2.461348	3.553104
14	1	0	-1.410921	-1.408411	3.555050
15	6	0	0.212032	-0.741662	2.281994
16	1	0	1.299944	-0.809047	2.297871
17	6	0	-0.507863	2.686155	0.881772
18	6	0	0.507863	-2.686155	0.881772
19	6	0	-0.087742	3.722483	-0.240502
20	6	0	-0.294200	2.976256	-1.582941
21	6	0	0.679661	2.838187	-2.574577
22	1	0	1.673847	3.235926	-2.422226
23	6	0	0.392953	2.192651	-3.778485
24	1	0	1.167080	2.108402	-4.533127
25	6	0	-0.869816	1.661577	-4.010555
26	1	0	-1.093112	1.165541	-4.947910
27	6	0	-1.844339	1.766818	-3.019399
28	1	0	-2.832323	1.349683	-3.179449
29	6	0	-1.558381	2.413291	-1.822729
30	1	0	-2.329533	2.505467	-1.066326
31	6	0	-1.039744	4.955273	-0.163511
32	6	0	-1.650835	5.491198	-1.299515
33	1	0	-1.541517	5.003981	-2.258949
34	6	0	-2.413078	6.659223	-1.226241
35	1	0	-2.876078	7.049129	-2.126194
36	6	0	-2.578112	7.315036	-0.013614
37	1	0	-3.172984	8.219604	0.046569
38	6	0	-1.963822	6.796745	1.126431
39	1	0	-2.078707	7.297622	2.081455
40	6	0	-1.200889	5.639093	1.049995
41	1	0	-0.729671	5.262125	1.946869
42	6	0	1.318035	4.333921	-0.020341
43	6	0	1.844339	5.227765	-0.966490
44	1	0	1.284072	5.445556	-1.866726
45	6	0	3.057454	5.873729	-0.755861
46	1	0	3.436573	6.555682	-1.508956
47	6	0	3.771648	5.665206	0.422645
48	1	0	4.714417	6.173110	0.590876
49	6	0	3.247446	4.812993	1.387167
50	1	0	3.776565	4.654331	2.320379

51	6	0	2.034978	4.158897	1.167850
52	1	0	1.649172	3.512980	1.944927
53	6	0	0.087742	-3.722483	-0.240502
54	6	0	1.039744	-4.955273	-0.163511
55	6	0	1.650835	-5.491198	-1.299515
56	1	0	1.541517	-5.003981	-2.258949
57	6	0	2.413078	-6.659223	-1.226241
58	1	0	2.876078	-7.049129	-2.126194
59	6	0	2.578112	-7.315036	-0.013614
60	1	0	3.172984	-8.219604	0.046569
61	6	0	1.963822	-6.796745	1.126431
62	1	0	2.078707	-7.297622	2.081455
63	6	0	1.200889	-5.639093	1.049995
64	1	0	0.729671	-5.262125	1.946869
65	6	0	-1.318035	-4.333921	-0.020341
66	6	0	-1.844339	-5.227765	-0.966490
67	1	0	-1.284072	-5.445556	-1.866726
68	6	0	-3.057454	-5.873729	-0.755861
69	1	0	-3.436573	-6.555682	-1.508956
70	6	0	-3.771648	-5.665206	0.422645
71	1	0	-4.714417	-6.173110	0.590876
72	6	0	-3.247446	-4.812993	1.387167
73	1	0	-3.776565	-4.654331	2.320379
74	6	0	-2.034978	-4.158897	1.167850
75	1	0	-1.649172	-3.512980	1.944927
76	6	0	0.294200	-2.976256	-1.582941
77	6	0	-0.679661	-2.838187	-2.574577
78	1	0	-1.673847	-3.235926	-2.422226
79	6	0	-0.392953	-2.192651	-3.778485
80	1	0	-1.167080	-2.108402	-4.533127
81	6	0	0.869816	-1.661577	-4.010555
82	1	0	1.093112	-1.165541	-4.947910
83	6	0	1.844339	-1.766818	-3.019399
84	1	0	2.832323	-1.349683	-3.179449
85	6	0	1.558381	-2.413291	-1.822729
86	1	0	2.329533	-2.505467	-1.066326
87	7	0	0.223411	1.538899	1.102205
88	7	0	-0.223411	-1.538899	1.102205
89	8	0	-1.528067	2.890180	1.526087
90	8	0	1.528067	-2.890180	1.526087
91	6	0	-1.467133	-1.157223	0.438310
92	1	0	-1.669814	-1.812507	-0.398475
93	1	0	-2.318475	-1.212407	1.124637
94	1	0	-1.387076	-0.138608	0.056484
95	6	0	1.467133	1.157223	0.438310

96	1	0	1.387076	0.138608	0.056484
97	1	0	1.669814	1.812507	-0.398475
98	1	0	2.318475	1.212407	1.124637

4b (conf. 8)

1	6	0	0.578596	-0.514736	2.358786
2	1	0	1.499839	0.060076	2.419973
3	6	0	0.461317	-1.390173	3.625899
4	1	0	1.265375	-2.131638	3.618193
5	1	0	-0.483376	-1.941314	3.592892
6	6	0	0.534732	-0.548586	4.906084
7	1	0	0.423070	-1.193642	5.783418
8	1	0	1.527435	-0.087080	4.980563
9	6	0	-0.534732	0.548586	4.906084
10	1	0	-0.423070	1.193642	5.783418
11	1	0	-1.527435	0.087080	4.980563
12	6	0	-0.461317	1.390173	3.625899
13	1	0	-1.265375	2.131638	3.618193
14	1	0	0.483376	1.941314	3.592892
15	6	0	-0.578596	0.514736	2.358786
16	1	0	-1.499839	-0.060076	2.419973
17	6	0	-0.276512	-2.137628	0.702188
18	6	0	0.276512	2.137628	0.702188
19	6	0	-0.016169	-3.353737	-0.294286
20	6	0	0.845025	-4.347279	0.529310
21	6	0	2.078671	-4.851252	0.109024
22	1	0	2.489629	-4.556232	-0.847147
23	6	0	2.806733	-5.734027	0.908151
24	1	0	3.760591	-6.108765	0.553405
25	6	0	2.319093	-6.128492	2.148720
26	1	0	2.884731	-6.814804	2.768705
27	6	0	1.094247	-5.627012	2.586929
28	1	0	0.698766	-5.920780	3.552981
29	6	0	0.369960	-4.748656	1.788187
30	1	0	-0.584029	-4.372406	2.138646
31	6	0	-1.393946	-3.979982	-0.654459
32	6	0	-1.653991	-5.345600	-0.528693
33	1	0	-0.910054	-6.004474	-0.101495
34	6	0	-2.870109	-5.889687	-0.949809
35	1	0	-3.043120	-6.954604	-0.838737
36	6	0	-3.848131	-5.076505	-1.506441
37	1	0	-4.793588	-5.496492	-1.831190
38	6	0	-3.596563	-3.711236	-1.647458
39	1	0	-4.348140	-3.062107	-2.083406
40	6	0	-2.385436	-3.174318	-1.232788

41	1	0	-2.208678	-2.114340	-1.357310
42	6	0	0.595486	-2.967505	-1.662714
43	6	0	0.815070	-3.971976	-2.619712
44	1	0	0.585051	-5.001774	-2.375730
45	6	0	1.297868	-3.669799	-3.887579
46	1	0	1.459194	-4.469513	-4.602024
47	6	0	1.557846	-2.347385	-4.245488
48	1	0	1.928840	-2.109231	-5.235874
49	6	0	1.321406	-1.337902	-3.320415
50	1	0	1.499035	-0.301505	-3.583494
51	6	0	0.845025	-1.647384	-2.045014
52	1	0	0.674956	-0.842360	-1.343338
53	6	0	0.016169	3.353737	-0.294286
54	6	0	1.393946	3.979982	-0.654459
55	6	0	1.653991	5.345600	-0.528693
56	1	0	0.910054	6.004474	-0.101495
57	6	0	2.870109	5.889687	-0.949809
58	1	0	3.043120	6.954604	-0.838737
59	6	0	3.848131	5.076505	-1.506441
60	1	0	4.793588	5.496492	-1.831190
61	6	0	3.596563	3.711236	-1.647458
62	1	0	4.348140	3.062107	-2.083406
63	6	0	2.385436	3.174318	-1.232788
64	1	0	2.208678	2.114340	-1.357310
65	6	0	-0.595486	2.967505	-1.662714
66	6	0	-0.815070	3.971976	-2.619712
67	1	0	-0.585051	5.001774	-2.375730
68	6	0	-1.297868	3.669799	-3.887579
69	1	0	-1.459194	4.469513	-4.602024
70	6	0	-1.557846	2.347385	-4.245488
71	1	0	-1.928840	2.109231	-5.235874
72	6	0	-1.321406	1.337902	-3.320415
73	1	0	-1.499035	0.301505	-3.583494
74	6	0	-0.845025	1.647384	-2.045014
75	1	0	-0.674956	0.842360	-1.343338
76	6	0	-0.845025	4.347279	0.529310
77	6	0	-2.078671	4.851252	0.109024
78	1	0	-2.489629	4.556232	-0.847147
79	6	0	-2.806733	5.734027	0.908151
80	1	0	-3.760591	6.108765	0.553405
81	6	0	-2.319093	6.128492	2.148720
82	1	0	-2.884731	6.814804	2.768705
83	6	0	-1.094247	5.627012	2.586929
84	1	0	-0.698766	5.920780	3.552981
85	6	0	-0.369960	4.748656	1.788187

86	1	0	0.584029	4.372406	2.138646
87	7	0	0.761206	-1.364853	1.149972
88	7	0	-0.761206	1.364853	1.149972
89	8	0	-1.411525	-1.960762	1.128211
90	8	0	1.411525	1.960762	1.128211
91	6	0	-2.179172	1.561460	0.837007
92	1	0	-2.691778	2.072962	1.658927
93	1	0	-2.316519	2.144519	-0.063541
94	1	0	-2.638414	0.582066	0.687522
95	6	0	2.179172	-1.561460	0.837007
96	1	0	2.691778	-2.072962	1.658927
97	1	0	2.316519	-2.144519	-0.063541
98	1	0	2.638414	-0.582066	0.687522

5 (conf. 1)

1	6	0	0.720139	0.289210	2.314775
2	1	0	0.780453	1.055823	3.088787
3	6	0	1.757638	-0.780292	2.596681
4	6	0	-1.757638	0.780292	2.596681
5	6	0	-0.720139	-0.289210	2.314775
6	1	0	-0.780453	-1.055823	3.088787
7	6	0	1.519353	2.219088	0.995553
8	6	0	-1.519353	-2.219088	0.995553
9	6	0	1.844164	2.680654	-0.461441
10	6	0	0.437400	2.792385	-1.074798
11	6	0	-0.108853	1.781931	-1.866044
12	1	0	0.513801	0.950073	-2.170794
13	6	0	-1.443424	1.821364	-2.262442
14	1	0	-1.856891	1.014208	-2.858599
15	6	0	-2.246335	2.895386	-1.895051
16	1	0	-3.283292	2.928470	-2.208291
17	6	0	-1.708657	3.914971	-1.115921
18	1	0	-2.324022	4.756897	-0.820060
19	6	0	-0.386395	3.854109	-0.690839
20	1	0	0.011685	4.629511	-0.045599
21	6	0	2.609406	4.010515	-0.477141
22	6	0	2.377083	4.956806	-1.475388
23	1	0	1.581175	4.801897	-2.194147
24	6	0	3.153112	6.108301	-1.562493
25	1	0	2.951854	6.830669	-2.344749
26	6	0	4.178031	6.329911	-0.653128
27	1	0	4.780996	7.227988	-0.715841
28	6	0	4.427157	5.384605	0.336203
29	1	0	5.228372	5.541794	1.048430

30	6	0	3.656183	4.233230	0.419812
31	1	0	3.864253	3.508154	1.194888
32	6	0	2.761914	1.676694	-1.181431
33	6	0	2.920482	1.762225	-2.569041
34	1	0	2.344109	2.492918	-3.126445
35	6	0	3.815263	0.939014	-3.237937
36	1	0	3.923832	1.026989	-4.312609
37	6	0	4.577153	0.010492	-2.531132
38	1	0	5.276525	-0.632184	-3.053044
39	6	0	4.443735	-0.070414	-1.152350
40	1	0	5.034148	-0.779300	-0.583370
41	6	0	3.550783	0.762549	-0.481909
42	1	0	3.483914	0.686141	0.597594
43	6	0	-1.844164	-2.680654	-0.461441
44	6	0	-2.609406	-4.010515	-0.477141
45	6	0	-2.377083	-4.956806	-1.475388
46	1	0	-1.581175	-4.801897	-2.194147
47	6	0	-3.153112	-6.108301	-1.562493
48	1	0	-2.951854	-6.830669	-2.344749
49	6	0	-4.178031	-6.329911	-0.653128
50	1	0	-4.780996	-7.227988	-0.715841
51	6	0	-4.427157	-5.384605	0.336203
52	1	0	-5.228372	-5.541794	1.048430
53	6	0	-3.656183	-4.233230	0.419812
54	1	0	-3.864253	-3.508154	1.194888
55	6	0	-2.761914	-1.676694	-1.181431
56	6	0	-2.920482	-1.762225	-2.569041
57	1	0	-2.344109	-2.492918	-3.126445
58	6	0	-3.815263	-0.939014	-3.237937
59	1	0	-3.923832	-1.026989	-4.312609
60	6	0	-4.577153	-0.010492	-2.531132
61	1	0	-5.276525	0.632184	-3.053044
62	6	0	-4.443735	0.070414	-1.152350
63	1	0	-5.034148	0.779300	-0.583370
64	6	0	-3.550783	-0.762549	-0.481909
65	1	0	-3.483914	-0.686141	0.597594
66	6	0	-0.437400	-2.792385	-1.074798
67	6	0	0.108853	-1.781931	-1.866044
68	1	0	-0.513801	-0.950073	-2.170794
69	6	0	1.443424	-1.821364	-2.262442
70	1	0	1.856891	-1.014208	-2.858599
71	6	0	2.246335	-2.895386	-1.895051
72	1	0	3.283292	-2.928470	-2.208291
73	6	0	1.708657	-3.914971	-1.115921
74	1	0	2.324022	-4.756897	-0.820060

75	6	0	0.386395	-3.854109	-0.690839
76	1	0	-0.011685	-4.629511	-0.045599
77	7	0	0.972393	0.969714	1.056260
78	7	0	-0.972393	-0.969714	1.056260
79	8	0	1.655612	2.928085	1.964973
80	8	0	-1.655612	-2.928085	1.964973
81	1	0	1.035484	0.392921	0.226831
82	1	0	-1.035484	-0.392921	0.226831
83	6	0	2.326372	-0.863894	3.865815
84	6	0	3.269835	-1.842893	4.158755
85	6	0	3.656183	-2.749227	3.178653
86	6	0	3.091911	-2.673551	1.909115
87	6	0	2.146837	-1.696878	1.617607
88	6	0	-2.146837	1.696878	1.617607
89	6	0	-3.091911	2.673551	1.909115
90	6	0	-3.656183	2.749227	3.178653
91	6	0	-3.269835	1.842893	4.158755
92	6	0	-2.326372	0.863894	3.865815
93	1	0	2.033455	-0.148730	4.627660
94	1	0	3.706898	-1.892024	5.148989
95	1	0	4.393328	-3.511263	3.401905
96	1	0	3.384229	-3.376779	1.138177
97	1	0	1.720574	-1.655251	0.619797
98	1	0	-1.720574	1.655251	0.619797
99	1	0	-3.384229	3.376779	1.138177
100	1	0	-4.393328	3.511263	3.401905
101	1	0	-3.706898	1.892024	5.148989
102	1	0	-2.033455	0.148730	4.627660

5 (conf. 5)

1	6	0	0.606771	-0.286066	2.450531
2	1	0	1.282255	0.131255	3.197274
3	6	0	0.275679	-1.704707	2.899310
4	6	0	-0.207321	2.149560	2.214484
5	6	0	-0.588483	0.669224	2.259909
6	1	0	-1.306270	0.518640	3.070307
7	6	0	2.674067	-0.025264	1.085280
8	6	0	-2.595059	-0.035560	0.967740
9	6	0	3.166244	-0.023152	-0.395434
10	6	0	2.991960	-1.402487	-1.052643
11	6	0	3.214886	-1.533635	-2.427696
12	1	0	3.462131	-0.653827	-3.011903
13	6	0	3.143901	-2.771677	-3.049421
14	1	0	3.316515	-2.845132	-4.116834
15	6	0	2.877288	-3.918142	-2.303855

16	1	0	2.829822	-4.886528	-2.787477
17	6	0	2.691869	-3.807648	-0.933383
18	1	0	2.498389	-4.689483	-0.333645
19	6	0	2.746293	-2.560400	-0.313900
20	1	0	2.595139	-2.510252	0.757148
21	6	0	2.313957	1.095690	-1.027513
22	6	0	1.361379	0.891424	-2.024011
23	1	0	1.196968	-0.092038	-2.444181
24	6	0	0.601134	1.959343	-2.502576
25	1	0	-0.113104	1.778446	-3.298522
26	6	0	0.749612	3.229945	-1.963503
27	1	0	0.154049	4.056117	-2.334172
28	6	0	1.669471	3.433301	-0.937934
29	1	0	1.777082	4.411245	-0.484446
30	6	0	2.448655	2.379842	-0.485624
31	1	0	3.168068	2.542882	0.311093
32	6	0	4.666823	0.290750	-0.470461
33	6	0	5.178807	1.175376	-1.418054
34	1	0	4.506734	1.723053	-2.067777
35	6	0	6.552311	1.371744	-1.538839
36	1	0	6.929589	2.065560	-2.280936
37	6	0	7.431589	0.686612	-0.713422
38	1	0	8.500103	0.842529	-0.802595
39	6	0	6.928912	-0.206574	0.228862
40	1	0	7.605637	-0.751319	0.876445
41	6	0	5.561559	-0.408017	0.343864
42	1	0	5.183640	-1.108515	1.077679
43	6	0	-3.189315	-0.106068	-0.468280
44	6	0	-4.382083	-1.068872	-0.527408
45	6	0	-5.402314	-0.854854	-1.454506
46	1	0	-5.397301	0.044188	-2.060950
47	6	0	-6.431364	-1.776730	-1.607242
48	1	0	-7.215887	-1.589638	-2.330921
49	6	0	-6.452169	-2.933450	-0.837568
50	1	0	-7.254061	-3.652719	-0.952976
51	6	0	-5.432632	-3.161275	0.079147
52	1	0	-5.436119	-4.061015	0.683099
53	6	0	-4.404233	-2.239439	0.231143
54	1	0	-3.622029	-2.432857	0.954521
55	6	0	-3.600116	1.367099	-0.649353
56	6	0	-2.750039	2.302341	-1.238204
57	1	0	-1.816724	1.983293	-1.682770
58	6	0	-3.066706	3.657584	-1.233428
59	1	0	-2.385796	4.365548	-1.691481
60	6	0	-4.233521	4.100958	-0.625625

61	1	0	-4.481054	5.155999	-0.619116
62	6	0	-5.076669	3.178515	-0.012108
63	1	0	-5.980443	3.513243	0.482925
64	6	0	-4.761627	1.826135	-0.019248
65	1	0	-5.405309	1.117436	0.488089
66	6	0	-2.192366	-0.647908	-1.506357
67	6	0	-1.295464	-1.666417	-1.159731
68	1	0	-1.244778	-2.019509	-0.134057
69	6	0	-0.477093	-2.258186	-2.115364
70	1	0	0.216604	-3.037738	-1.822213
71	6	0	-0.549101	-1.852714	-3.444204
72	1	0	0.093615	-2.311456	-4.186626
73	6	0	-1.455887	-0.863921	-3.806805
74	1	0	-1.538171	-0.553475	-4.842105
75	6	0	-2.273390	-0.272763	-2.847716
76	1	0	-2.989899	0.481938	-3.151585
77	7	0	1.360239	-0.336379	1.205117
78	7	0	-1.287447	0.326068	1.025118
79	8	0	3.365746	0.300130	2.028929
80	8	0	-3.281793	-0.210099	1.953413
81	1	0	0.879043	-0.697141	0.390337
82	1	0	-0.845828	0.633522	0.165598
83	6	0	1.365767	-2.537375	3.177540
84	6	0	1.176968	-3.857730	3.556014
85	6	0	-0.114306	-4.370192	3.666836
86	6	0	-1.200485	-3.545121	3.416035
87	6	0	-1.011894	-2.214680	3.038087
88	6	0	-1.194992	3.056312	1.815154
89	6	0	-0.934018	4.418262	1.760550
90	6	0	0.322249	4.902531	2.114284
91	6	0	1.308676	4.010539	2.511573
92	6	0	1.051093	2.641729	2.557673
93	1	0	2.370183	-2.128270	3.103494
94	1	0	2.033230	-4.484902	3.775267
95	1	0	-0.268141	-5.401537	3.960814
96	1	0	-2.208967	-3.928764	3.519220
97	1	0	-1.881027	-1.589755	2.873333
98	1	0	-2.183209	2.694049	1.548076
99	1	0	-1.718333	5.097679	1.447265
100	1	0	0.528123	5.966102	2.080532
101	1	0	2.293534	4.372369	2.784095
102	1	0	1.859186	1.979955	2.844720

5 (conf. 60)

1	6	0	0.581852	0.879712	-2.256314

2	1	0	0.944753	0.858411	-3.287526
3	6	0	-0.035095	2.250713	-2.024763
4	6	0	0.186825	-1.619590	-2.215952
5	6	0	-0.487379	-0.255412	-2.176518
6	1	0	-1.106649	-0.171965	-3.073024
7	6	0	1.803484	0.339899	-0.136215
8	6	0	-2.706250	-0.371361	-1.165423
9	6	0	3.222843	0.257669	0.497894
10	6	0	4.267637	-0.404735	-0.412043
11	6	0	3.905292	-1.464463	-1.249125
12	1	0	2.868493	-1.775732	-1.324927
13	6	0	4.865013	-2.148667	-1.986956
14	1	0	4.552629	-2.964073	-2.629090
15	6	0	6.205780	-1.798469	-1.888822
16	1	0	6.954832	-2.331808	-2.461636
17	6	0	6.580758	-0.767060	-1.034857
18	1	0	7.625272	-0.497219	-0.933870
19	6	0	5.621542	-0.081200	-0.299757
20	1	0	5.931300	0.709384	0.374003
21	6	0	3.460270	1.753976	0.778167
22	6	0	2.830732	2.340044	1.880177
23	1	0	2.284937	1.711859	2.573974
24	6	0	2.866420	3.715829	2.070463
25	1	0	2.369917	4.149216	2.930431
26	6	0	3.523215	4.533571	1.156711
27	1	0	3.549626	5.606697	1.303486
28	6	0	4.137969	3.963193	0.048835
29	1	0	4.641235	4.589836	-0.677636
30	6	0	4.101384	2.585707	-0.141749
31	1	0	4.567833	2.162758	-1.023409
32	6	0	3.210168	-0.602241	1.768408
33	6	0	4.108020	-0.339313	2.803035
34	1	0	4.739368	0.541214	2.757988
35	6	0	4.203755	-1.192601	3.896751
36	1	0	4.905180	-0.968038	4.691528
37	6	0	3.408574	-2.329844	3.968150
38	1	0	3.483932	-2.997511	4.818020
39	6	0	2.518948	-2.604148	2.935822
40	1	0	1.897251	-3.492108	2.971776
41	6	0	2.418037	-1.747824	1.846237
42	1	0	1.713800	-1.977656	1.056298
43	6	0	-3.450708	-0.410437	0.208940
44	6	0	-3.356245	0.909451	0.992638
45	6	0	-3.844135	0.924997	2.304917
46	1	0	-4.215132	0.004430	2.742752

47	6	0	-3.870761	2.094692	3.046402
48	1	0	-4.250746	2.078982	4.061092
49	6	0	-3.422260	3.287349	2.483186
50	1	0	-3.447273	4.206050	3.057236
51	6	0	-2.951440	3.288130	1.179891
52	1	0	-2.605134	4.206733	0.722623
53	6	0	-2.914247	2.107640	0.436309
54	1	0	-2.535874	2.143693	-0.578786
55	6	0	-4.951555	-0.656610	0.001308
56	6	0	-5.673438	-1.534067	0.808654
57	1	0	-5.162673	-2.129536	1.555758
58	6	0	-7.053787	-1.658172	0.672442
59	1	0	-7.593543	-2.348419	1.310138
60	6	0	-7.733587	-0.902697	-0.271543
61	1	0	-8.807100	-1.000993	-0.381985
62	6	0	-7.023566	-0.011954	-1.071345
63	1	0	-7.543504	0.588882	-1.808078
64	6	0	-5.649487	0.113884	-0.932107
65	1	0	-5.108783	0.812724	-1.557027
66	6	0	-2.743614	-1.577567	0.923702
67	6	0	-2.942135	-2.876496	0.441198
68	1	0	-3.646673	-3.036582	-0.368054
69	6	0	-2.238945	-3.948943	0.972303
70	1	0	-2.408656	-4.946011	0.583084
71	6	0	-1.309694	-3.741999	1.989794
72	1	0	-0.765429	-4.579996	2.411054
73	6	0	-1.084956	-2.453162	2.456972
74	1	0	-0.351385	-2.270658	3.233428
75	6	0	-1.794008	-1.377631	1.925542
76	1	0	-1.579462	-0.378640	2.285075
77	7	0	1.776348	0.625023	-1.457319
78	7	0	-1.386104	-0.077003	-1.063283
79	8	0	0.805227	0.281323	0.560222
80	8	0	-3.237065	-0.664789	-2.216096
81	1	0	2.656626	0.599957	-1.948118
82	1	0	-0.964199	0.131612	-0.165116
83	6	0	-1.100995	2.646230	-2.837645
84	6	0	-1.693076	3.891366	-2.674705
85	6	0	-1.225210	4.762294	-1.694031
86	6	0	-0.165945	4.374469	-0.884215
87	6	0	0.429078	3.126026	-1.047545
88	6	0	0.185916	-2.471484	-1.114747
89	6	0	0.852115	-3.693925	-1.167971
90	6	0	1.530138	-4.076102	-2.319247
91	6	0	1.526251	-3.233224	-3.428339

92	6	0	0.856328	-2.017137	-3.375273
93	1	0	-1.481679	1.973555	-3.599737
94	1	0	-2.520264	4.181024	-3.311742
95	1	0	-1.685512	5.735150	-1.565292
96	1	0	0.207994	5.040592	-0.115084
97	1	0	1.259717	2.852056	-0.408597
98	1	0	-0.335045	-2.183566	-0.209088
99	1	0	0.837026	-4.343021	-0.299065
100	1	0	2.049550	-5.026245	-2.358376
101	1	0	2.036970	-3.528190	-4.337774
102	1	0	0.844515	-1.375074	-4.251358

5 (conf. 61)

1	6	0	-0.816727	2.297670	0.388044
2	1	0	-0.632497	2.270965	1.467125
3	6	0	-1.398428	3.639283	0.002752
4	6	0	1.517208	3.196301	-0.038099
5	6	0	0.539300	2.068968	-0.336123
6	1	0	0.358554	2.029319	-1.413719
7	6	0	-1.772229	0.035734	0.707001
8	6	0	1.870863	0.052882	-0.758638
9	6	0	-2.801637	-0.983972	0.123766
10	6	0	-2.385285	-1.461534	-1.284925
11	6	0	-1.422197	-0.840271	-2.077984
12	1	0	-0.833098	-0.015538	-1.701726
13	6	0	-1.162730	-1.287666	-3.373965
14	1	0	-0.395349	-0.787079	-3.953928
15	6	0	-1.856787	-2.366126	-3.898575
16	1	0	-1.657731	-2.709885	-4.906815
17	6	0	-2.799162	-3.017730	-3.104195
18	1	0	-3.337077	-3.876025	-3.489683
19	6	0	-3.051243	-2.575487	-1.814397
20	1	0	-3.781705	-3.094919	-1.203921
21	6	0	-2.848262	-2.212976	1.044182
22	6	0	-4.014223	-2.661805	1.657750
23	1	0	-4.946395	-2.128991	1.520227
24	6	0	-4.004939	-3.812041	2.447092
25	1	0	-4.924884	-4.145579	2.912854
26	6	0	-2.830592	-4.524495	2.630600
27	1	0	-2.822162	-5.415666	3.247269
28	6	0	-1.663457	-4.092543	2.004191
29	1	0	-0.739718	-4.644904	2.124250
30	6	0	-1.673532	-2.954888	1.212432
31	1	0	-0.764209	-2.644486	0.706127
32	6	0	-4.146406	-0.236106	0.078298

33	6	0	-4.601550	0.368345	1.258014
34	1	0	-4.011195	0.267633	2.164310
35	6	0	-5.788462	1.082355	1.282982
36	1	0	-6.121524	1.539660	2.207063
37	6	0	-6.546368	1.217943	0.120952
38	1	0	-7.472424	1.779907	0.136335
39	6	0	-6.099414	0.636924	-1.054909
40	1	0	-6.674575	0.741936	-1.967237
41	6	0	-4.904577	-0.084279	-1.079355
42	1	0	-4.570446	-0.522375	-2.011273
43	6	0	2.728275	-1.085289	-0.093739
44	6	0	1.975696	-2.419293	-0.267107
45	6	0	2.104886	-3.450543	0.669379
46	1	0	2.707103	-3.301752	1.557336
47	6	0	1.478594	-4.675613	0.469935
48	1	0	1.602308	-5.462246	1.206006
49	6	0	0.694098	-4.889713	-0.658267
50	1	0	0.184391	-5.835504	-0.798660
51	6	0	0.575746	-3.879244	-1.603928
52	1	0	-0.027968	-4.024798	-2.492245
53	6	0	1.230846	-2.665326	-1.420078
54	1	0	1.168389	-1.903560	-2.184507
55	6	0	4.065263	-1.140975	-0.854490
56	6	0	4.724173	-2.347934	-1.074613
57	1	0	4.260297	-3.280566	-0.779176
58	6	0	5.976179	-2.376741	-1.684591
59	1	0	6.466398	-3.329262	-1.848511
60	6	0	6.588652	-1.198722	-2.085732
61	1	0	7.560199	-1.221925	-2.564886
62	6	0	5.937816	0.013424	-1.874032
63	1	0	6.399355	0.942215	-2.187989
64	6	0	4.690642	0.040565	-1.267177
65	1	0	4.198600	0.994846	-1.116038
66	6	0	2.968375	-0.766274	1.398111
67	6	0	4.170850	-0.232335	1.862290
68	1	0	5.005001	-0.102804	1.186364
69	6	0	4.322138	0.139094	3.197315
70	1	0	5.269194	0.548755	3.529059
71	6	0	3.275975	-0.012586	4.095940
72	1	0	3.394293	0.283182	5.131537
73	6	0	2.075908	-0.561718	3.652466
74	1	0	1.245109	-0.696205	4.334866
75	6	0	1.931566	-0.946489	2.326521
76	1	0	0.982652	-1.367419	2.010530
77	7	0	-1.757900	1.234084	0.070552

78	7	0	1.083481	0.787027	0.063984
79	8	0	-1.053247	-0.207210	1.656065
80	8	0	1.912968	0.257845	-1.956818
81	1	0	-2.485848	1.424356	-0.602679
82	1	0	1.027868	0.551245	1.042928
83	6	0	-1.899549	3.843028	-1.283984
84	6	0	-2.376270	5.090871	-1.666565
85	6	0	-2.346258	6.152042	-0.767882
86	6	0	-1.842388	5.957347	0.512912
87	6	0	-1.373296	4.705751	0.895875
88	6	0	1.589971	4.304102	-0.881090
89	6	0	2.448400	5.357451	-0.591872
90	6	0	3.246577	5.314072	0.546484
91	6	0	3.183797	4.210374	1.389676
92	6	0	2.325006	3.155431	1.098837
93	1	0	-1.900538	3.029165	-2.004297
94	1	0	-2.764521	5.235825	-2.667602
95	1	0	-2.711744	7.127033	-1.066786
96	1	0	-1.811225	6.781510	1.215308
97	1	0	-0.964766	4.558623	1.889765
98	1	0	0.966820	4.340939	-1.768731
99	1	0	2.497224	6.210187	-1.258529
100	1	0	3.919475	6.133093	0.770946
101	1	0	3.809690	4.163090	2.273230
102	1	0	2.306854	2.289691	1.754862

5 (conf. 69)

1	6	0	-0.568494	0.526979	2.178581
2	1	0	-1.509147	-0.019496	2.233988
3	6	0	-0.451667	1.403770	3.413824
4	6	0	0.451667	-1.403770	3.413824
5	6	0	0.568494	-0.526979	2.178581
6	1	0	1.509147	0.019496	2.233988
7	6	0	0.379452	1.811861	0.234434
8	6	0	-0.379452	-1.811861	0.234434
9	6	0	-0.007211	2.729491	-0.980488
10	6	0	-1.401356	2.388438	-1.527768
11	6	0	-1.727448	1.054527	-1.804035
12	1	0	-1.011890	0.265042	-1.603899
13	6	0	-2.965598	0.703990	-2.320563
14	1	0	-3.184310	-0.340555	-2.503218
15	6	0	-3.908626	1.692015	-2.589948
16	1	0	-4.878304	1.424534	-2.992663
17	6	0	-3.598583	3.019557	-2.331091
18	1	0	-4.325622	3.797745	-2.531825

19	6	0	-2.357943	3.366317	-1.799953
20	1	0	-2.144714	4.407589	-1.594820
21	6	0	0.005886	4.180560	-0.445867
22	6	0	0.350133	5.239839	-1.290011
23	1	0	0.662784	5.036917	-2.307294
24	6	0	0.289801	6.555265	-0.844988
25	1	0	0.559502	7.359208	-1.519650
26	6	0	-0.109434	6.839687	0.455950
27	1	0	-0.147638	7.864584	0.805246
28	6	0	-0.459277	5.795451	1.301793
29	1	0	-0.773849	5.995511	2.319465
30	6	0	-0.410956	4.479701	0.851945
31	1	0	-0.706273	3.689783	1.530535
32	6	0	1.071105	2.582413	-2.074090
33	6	0	0.777471	2.156160	-3.368684
34	1	0	-0.228331	1.855887	-3.632167
35	6	0	1.762726	2.133462	-4.356456
36	1	0	1.504245	1.801862	-5.355083
37	6	0	3.054340	2.547813	-4.070639
38	1	0	3.815333	2.543638	-4.842156
39	6	0	3.361731	2.970474	-2.778927
40	1	0	4.366443	3.297347	-2.537386
41	6	0	2.385569	2.982609	-1.793261
42	1	0	2.632492	3.323179	-0.797403
43	6	0	0.007211	-2.729491	-0.980488
44	6	0	-0.005886	-4.180560	-0.445867
45	6	0	-0.350133	-5.239839	-1.290011
46	1	0	-0.662784	-5.036917	-2.307294
47	6	0	-0.289801	-6.555265	-0.844988
48	1	0	-0.559502	-7.359208	-1.519650
49	6	0	0.109434	-6.839687	0.455950
50	1	0	0.147638	-7.864584	0.805246
51	6	0	0.459277	-5.795451	1.301793
52	1	0	0.773849	-5.995511	2.319465
53	6	0	0.410956	-4.479701	0.851945
54	1	0	0.706273	-3.689783	1.530535
55	6	0	-1.071105	-2.582413	-2.074090
56	6	0	-0.777471	-2.156160	-3.368684
57	1	0	0.228331	-1.855887	-3.632167
58	6	0	-1.762726	-2.133462	-4.356456
59	1	0	-1.504245	-1.801862	-5.355083
60	6	0	-3.054340	-2.547813	-4.070639
61	1	0	-3.815333	-2.543638	-4.842156
62	6	0	-3.361731	-2.970474	-2.778927
63	1	0	-4.366443	-3.297347	-2.537386

64	6	0	-2.385569	-2.982609	-1.793261
65	1	0	-2.632492	-3.323179	-0.797403
66	6	0	1.401356	-2.388438	-1.527768
67	6	0	1.727448	-1.054527	-1.804035
68	1	0	1.011890	-0.265042	-1.603899
69	6	0	2.965598	-0.703990	-2.320563
70	1	0	3.184310	0.340555	-2.503218
71	6	0	3.908626	-1.692015	-2.589948
72	1	0	4.878304	-1.424534	-2.992663
73	6	0	3.598583	-3.019557	-2.331091
74	1	0	4.325622	-3.797745	-2.531825
75	6	0	2.357943	-3.366317	-1.799953
76	1	0	2.144714	-4.407589	-1.594820
77	7	0	-0.653607	1.292246	0.935623
78	7	0	0.653607	-1.292246	0.935623
79	8	0	1.544510	1.655259	0.554772
80	8	0	-1.544510	-1.655259	0.554772
81	1	0	-1.582094	1.405219	0.557941
82	1	0	1.582094	-1.405219	0.557941
83	6	0	0.555339	2.364444	3.536248
84	6	0	0.653607	3.129638	4.693103
85	6	0	-0.238629	2.934137	5.743372
86	6	0	-1.233995	1.970856	5.631376
87	6	0	-1.339489	1.213488	4.470317
88	6	0	-0.555339	-2.364444	3.536248
89	6	0	-0.653607	-3.129638	4.693103
90	6	0	0.238629	-2.934137	5.743372
91	6	0	1.233995	-1.970856	5.631376
92	6	0	1.339489	-1.213488	4.470317
93	1	0	1.259198	2.510165	2.723905
94	1	0	1.433512	3.877693	4.776190
95	1	0	-0.156513	3.528647	6.645602
96	1	0	-1.929846	1.808242	6.445714
97	1	0	-2.110410	0.454152	4.386403
98	1	0	-1.259198	-2.510165	2.723905
99	1	0	-1.433512	-3.877693	4.776190
100	1	0	0.156513	-3.528647	6.645602
101	1	0	1.929846	-1.808242	6.445714
102	1	0	2.110410	-0.454152	4.386403

6 (conf. 1)

1 C1	-0.5876	1.6409	0.5006	C
2 H2	-0.2084	1.1667	1.4043	H
3 C3	0.5538	1.6748	-0.5781	C
4 H4	0.1914	1.2267	-1.5020	H

5	C5	-2.0501	-0.3300	0.7210 C
6	C6	2.0121	-0.3155	-0.7652 C
7	C7	-3.2559	-1.1650	0.1453 C
8	C8	-2.6670	-2.5727	-0.1414 C
9	C9	-3.3462	-3.7476	0.1874 C
10	H10	-4.3011	-3.7003	0.6926 H
11	C11	-2.8025	-4.9972	-0.1140 C
12	H12	-3.3498	-5.8938	0.1562 H
13	C13	-1.5662	-5.0950	-0.7423 C
14	H14	-1.1390	-6.0660	-0.9667 H
15	C15	-0.8743	-3.9304	-1.0711 C
16	H16	0.0978	-3.9828	-1.5469 H
17	C17	-1.4211	-2.6859	-0.7759 C
18	H18	-0.8566	-1.8018	-1.0505 H
19	C19	-3.8313	-0.5188	-1.1424 C
20	C20	-3.6794	-1.0844	-2.4118 C
21	H21	-3.1492	-2.0195	-2.5248 H
22	C22	-4.2107	-0.4654	-3.5447 C
23	H23	-4.0777	-0.9311	-4.5149 H
24	C24	-4.9061	0.7329	-3.4352 C
25	H25	-5.3182	1.2120	-4.3160 H
26	C26	-5.0719	1.3093	-2.1765 C
27	H27	-5.6172	2.2403	-2.0704 H
28	C28	-4.5468	0.6884	-1.0484 C
29	H29	-4.7067	1.1371	-0.0749 H
30	C30	-4.3869	-1.2546	1.2118 C
31	C31	-5.6992	-1.5256	0.7941 C
32	H32	-5.9161	-1.6317	-0.2613 H
33	C33	-6.7385	-1.6645	1.7096 C
34	H34	-7.7402	-1.8758	1.3513 H
35	C35	-6.4944	-1.5310	3.0739 C
36	H36	-7.3027	-1.6323	3.7897 H
37	C37	-5.1974	-1.2723	3.5041 C
38	H38	-4.9855	-1.1745	4.5633 H
39	C39	-4.1535	-1.1446	2.5879 C
40	H40	-3.1494	-0.9750	2.9471 H
41	C41	3.2472	-1.0776	-0.1390 C
42	C42	4.5517	-0.5377	-0.7852 C
43	C43	5.7285	-1.2942	-0.6776 C
44	H44	5.7022	-2.2510	-0.1707 H
45	C45	6.9282	-0.8446	-1.2185 C
46	H46	7.8207	-1.4521	-1.1170 H
47	C47	6.9822	0.3720	-1.8969 C
48	H48	7.9146	0.7198	-2.3272 H
49	C49	5.8226	1.1276	-2.0226 C

50	H50	5.8427	2.0710	-2.5574 H
51	C51	4.6223	0.6790	-1.4695 C
52	H52	3.7377	1.2904	-1.5842 H
53	C53	3.1354	-2.5835	-0.4966 C
54	C54	3.1212	-3.5917	0.4700 C
55	H55	3.1485	-3.3392	1.5208 H
56	C56	3.0784	-4.9394	0.1060 C
57	H57	3.0673	-5.6986	0.8801 H
58	C58	3.0531	-5.3046	-1.2339 C
59	H59	3.0220	-6.3507	-1.5183 H
60	C60	3.0777	-4.3082	-2.2102 C
61	H61	3.0666	-4.5757	-3.2612 H
62	C62	3.1233	-2.9675	-1.8471 C
63	H63	3.1476	-2.2102	-2.6172 H
64	C64	3.2333	-0.8525	1.3921 C
65	C65	2.0579	-1.1374	2.1099 C
66	H66	1.1742	-1.4990	1.5957 H
67	C67	1.9925	-0.9486	3.4855 C
68	H68	1.0677	-1.1708	4.0050 H
69	C69	3.1024	-0.4707	4.1827 C
70	H70	3.0530	-0.3234	5.2558 H
71	C71	4.2678	-0.1754	3.4857 C
72	H72	5.1360	0.2063	4.0115 H
73	C73	4.3316	-0.3605	2.1027 C
74	H74	5.2474	-0.1143	1.5826 H
75	N75	-1.7194	0.8280	0.0846 N
76	N76	1.7069	0.8807	-0.1810 N
77	O77	-1.4235	-0.7346	1.6904 O
78	O78	1.3979	-0.7380	-1.7297 O
79	H79	-2.2360	1.1002	-0.7388 H
80	H80	2.1763	1.1280	0.6784 H
81	C81	0.2447	3.7756	1.3940 C
82	C82	1.3025	3.7997	0.4722 C
83	C83	2.5267	4.3543	0.8262 C
84	C84	2.6922	4.8962	2.1039 C
85	C85	1.6417	4.8737	3.0174 C
86	C86	0.4131	4.3082	2.6658 C
87	H87	3.3464	4.3706	0.1155 H
88	H88	3.6432	5.3350	2.3836 H
89	H89	1.7766	5.2954	4.0070 H
90	H90	-0.4036	4.2872	3.3799 H
91	C91	-1.3740	3.8069	-0.4465 C
92	C92	-2.5991	4.3795	-0.7665 C
93	C93	-2.7697	4.9878	-2.0132 C
94	C94	-1.7230	5.0133	-2.9312 C

95 C95 -0.4918 4.4346 -2.6125 C
96 C96 -0.3180 3.8382 -1.3699 C
97 H97 -3.4143 4.3610 -0.0507 H
98 H98 -3.7209 5.4426 -2.2652 H
99 H99 -1.8621 5.4859 -3.8969 H
100 H100 0.3236 4.4561 -3.3280 H
101 C101 0.9430 3.1654 -0.8603 C
102 C102 -1.0068 3.1099 0.8511 C
103 H103 1.7587 3.2125 -1.5829 H
104 H104 -1.8237 3.1039 1.5738 H

6 (conf. 31)
1 C1 -0.5655 1.5297 0.4500 C
2 H2 -0.1731 1.0901 1.3655 H
3 C3 0.5810 1.5730 -0.6264 C
4 H4 0.2351 1.0649 -1.5246 H
5 C5 -1.9985 -0.4775 0.6831 C
6 C6 2.0972 -0.3691 -0.6859 C
7 C7 -3.3356 -1.1514 0.1813 C
8 C8 -3.7006 -2.3462 1.0975 C
9 C9 -4.9696 -2.5032 1.6611 C
10 H10 -5.7287 -1.7468 1.5136 H
11 C11 -5.2888 -3.6336 2.4162 C
12 H12 -6.2825 -3.7269 2.8406 H
13 C13 -4.3446 -4.6320 2.6180 C
14 H14 -4.5898 -5.5102 3.2050 H
15 C15 -3.0804 -4.4967 2.0444 C
16 H16 -2.3362 -5.2741 2.1785 H
17 C17 -2.7651 -3.3738 1.2894 C
18 H18 -1.7850 -3.2979 0.8405 H
19 C19 -3.1485 -1.7448 -1.2387 C
20 C20 -4.2350 -2.3921 -1.8486 C
21 H21 -5.1854 -2.4453 -1.3308 H
22 C22 -4.1092 -2.9864 -3.0983 C
23 H23 -4.9663 -3.4773 -3.5462 H
24 C24 -2.8837 -2.9675 -3.7647 C
25 H25 -2.7816 -3.4382 -4.7362 H
26 C26 -1.7931 -2.3557 -3.1599 C
27 H27 -0.8248 -2.3485 -3.6468 H
28 C28 -1.9219 -1.7487 -1.9085 C
29 H29 -1.0364 -1.3055 -1.4727 H
30 C30 -4.3984 -0.0267 0.2409 C
31 C31 -5.0591 0.4769 -0.8820 C
32 H32 -4.8683 0.0520 -1.8582 H
33 C33 -5.9702 1.5307 -0.7680 C

34	H34	-6.4712	1.8976	-1.6570 H
35	C35	-6.2333	2.1052	0.4692 C
36	H36	-6.9452	2.9182	0.5577 H
37	C37	-5.5677	1.6242	1.5984 C
38	H38	-5.7569	2.0647	2.5712 H
39	C39	-4.6612	0.5778	1.4825 C
40	H40	-4.1482	0.2167	2.3671 H
41	C41	3.4053	-1.0582	-0.1366 C
42	C42	4.1220	-0.1488	0.8938 C
43	C43	4.1706	-0.4445	2.2594 C
44	H44	3.7030	-1.3454	2.6317 H
45	C45	4.8240	0.4019	3.1572 C
46	H46	4.8460	0.1434	4.2101 H
47	C47	5.4448	1.5621	2.7103 C
48	H48	5.9548	2.2165	3.4081 H
49	C49	5.4065	1.8731	1.3515 C
50	H50	5.8912	2.7708	0.9839 H
51	C51	4.7554	1.0292	0.4586 C
52	H52	4.7523	1.2755	-0.5968 H
53	C53	4.3725	-1.3726	-1.3192 C
54	C54	5.7579	-1.4079	-1.0991 C
55	H55	6.1562	-1.1688	-0.1220 H
56	C56	6.6468	-1.7513	-2.1153 C
57	H57	7.7113	-1.7678	-1.9080 H
58	C58	6.1738	-2.0703	-3.3844 C
59	H59	6.8634	-2.3328	-4.1790 H
60	C60	4.8016	-2.0558	-3.6140 C
61	H61	4.4117	-2.3131	-4.5930 H
62	C62	3.9110	-1.7225	-2.5953 C
63	H63	2.8490	-1.7420	-2.7868 H
64	C64	2.9408	-2.3826	0.5278 C
65	C65	3.7337	-3.5333	0.4947 C
66	H66	4.6647	-3.5344	-0.0562 H
67	C67	3.3403	-4.6952	1.1576 C
68	H68	3.9739	-5.5744	1.1115 H
69	C69	2.1436	-4.7314	1.8659 C
70	H70	1.8365	-5.6362	2.3788 H
71	C71	1.3408	-3.5933	1.9014 C
72	H72	0.4009	-3.5955	2.4414 H
73	C73	1.7346	-2.4336	1.2391 C
74	H74	1.0750	-1.5756	1.2880 H
75	N75	-1.6871	0.6928	0.0556 N
76	N76	1.7809	0.8640	-0.2042 N
77	O77	-1.3060	-0.9437	1.5715 O
78	O78	1.3790	-0.9438	-1.4923 O

79 H79 -2.3229 1.0530 -0.6418 H
80 H80 2.3627 1.2810 0.5076 H
81 C81 0.1797 3.7427 1.2504 C
82 C82 1.2283 3.7825 0.3188 C
83 C83 2.4173 4.4302 0.6314 C
84 C84 2.5591 5.0435 1.8792 C
85 C85 1.5198 5.0003 2.8046 C
86 C86 0.3252 4.3455 2.4935 C
87 H87 3.2271 4.4637 -0.0896 H
88 H88 3.4825 5.5548 2.1264 H
89 H89 1.6362 5.4777 3.7710 H
90 H90 -0.4845 4.3130 3.2151 H
91 C91 -1.4477 3.6079 -0.5801 C
92 C92 -2.7089 4.0796 -0.9251 C
93 C93 -2.9178 4.6084 -2.2023 C
94 C94 -1.8750 4.6548 -3.1236 C
95 C95 -0.6095 4.1705 -2.7812 C
96 C96 -0.3983 3.6507 -1.5107 C
97 H97 -3.5239 4.0363 -0.2108 H
98 H98 -3.8977 4.9834 -2.4751 H
99 H99 -2.0443 5.0667 -4.1121 H
100 H100 0.2014 4.2019 -3.5015 H
101 C101 0.8970 3.0659 -0.9787 C
102 C102 -1.0393 2.9935 0.7480 C
103 H103 1.7073 3.1160 -1.7074 H
104 H104 -1.8529 2.9830 1.4741 H

6 (conf. 32)
1 C1 0.5775 1.5939 -0.6596 C
2 H2 0.2289 1.0826 -1.5551 H
3 C3 -0.5688 1.5565 0.4169 C
4 H4 -0.1742 1.1361 1.3402 H
5 C5 2.0467 -0.3828 -0.6500 C
6 C6 -1.9728 -0.4642 0.6791 C
7 C7 3.3656 -1.0647 -0.1178 C
8 C8 2.9140 -2.3538 0.6209 C
9 C9 3.6993 -3.5103 0.6163 C
10 H10 4.6122 -3.5435 0.0369 H
11 C11 3.3209 -4.6378 1.3442 C
12 H12 3.9484 -5.5221 1.3196 H
13 C13 2.1460 -4.6338 2.0892 C
14 H14 1.8501 -5.5119 2.6526 H
15 C15 1.3501 -3.4902 2.0966 C
16 H16 0.4242 -3.4638 2.6594 H
17 C17 1.7310 -2.3640 1.3715 C

18	H18	1.0778	-1.5004	1.4011	H
19	C19	4.1297	-0.1204	0.8454	C
20	C20	4.2147	-0.3527	2.2214	C
21	H21	3.7448	-1.2274	2.6489	H
22	C22	4.9066	0.5239	3.0593	C
23	H23	4.9560	0.3142	4.1220	H
24	C24	5.5307	1.6519	2.5407	C
25	H25	6.0710	2.3296	3.1918	H
26	C26	5.4567	1.9000	1.1705	C
27	H27	5.9434	2.7717	0.7473	H
28	C28	4.7672	1.0259	0.3372	C
29	H29	4.7366	1.2236	-0.7279	H
30	C30	4.2824	-1.4422	-1.3217	C
31	C31	5.6749	-1.4869	-1.1547	C
32	H32	6.1147	-1.2102	-0.2056	H
33	C33	6.5181	-1.8874	-2.1888	C
34	H34	7.5898	-1.9100	-2.0230	H
35	C35	5.9909	-2.2550	-3.4229	C
36	H36	6.6450	-2.5620	-4.2314	H
37	C37	4.6110	-2.2307	-3.5991	C
38	H38	4.1792	-2.5251	-4.5496	H
39	C39	3.7660	-1.8405	-2.5620	C
40	H40	2.6969	-1.8536	-2.7105	H
41	C41	-3.2975	-1.1622	0.1917	C
42	C42	-3.2707	-1.4780	-1.3240	C
43	C43	-4.4497	-1.8930	-1.9620	C
44	H44	-5.3765	-1.9338	-1.4026	H
45	C45	-4.4493	-2.2765	-3.2981	C
46	H46	-5.3767	-2.5899	-3.7650	H
47	C47	-3.2621	-2.2738	-4.0293	C
48	H48	-3.2593	-2.5772	-5.0703	H
49	C49	-2.0809	-1.8972	-3.4014	C
50	H50	-1.1421	-1.9115	-3.9435	H
51	C51	-2.0814	-1.5060	-2.0614	C
52	H52	-1.1320	-1.2467	-1.6095	H
53	C53	-4.3842	-0.1399	0.6131	C
54	C54	-5.0999	0.6455	-0.2949	C
55	H55	-4.9605	0.5094	-1.3591	H
56	C56	-6.0026	1.6144	0.1485	C
57	H57	-6.5511	2.2024	-0.5792	H
58	C58	-6.1997	1.8249	1.5086	C
59	H59	-6.9040	2.5743	1.8521	H
60	C60	-5.4778	1.0617	2.4262	C
61	H61	-5.6128	1.2185	3.4908	H
62	C62	-4.5809	0.0961	1.9836	C

63 H63 -4.0179 -0.4825 2.7062 H
64 C64 -3.4764 -2.5331 0.8856 C
65 C65 -4.7142 -2.9521 1.3816 C
66 H66 -5.5622 -2.2799 1.3629 H
67 C67 -4.8830 -4.2334 1.9079 C
68 H68 -5.8548 -4.5301 2.2873 H
69 C69 -3.8159 -5.1230 1.9432 C
70 H70 -3.9442 -6.1190 2.3525 H
71 C71 -2.5800 -4.7219 1.4375 C
72 H72 -1.7387 -5.4061 1.4468 H
73 C73 -2.4138 -3.4464 0.9102 C
74 H74 -1.4479 -3.1635 0.5157 H
75 N75 1.7782 0.8857 -0.2376 N
76 N76 -1.6748 0.6979 0.0320 N
77 O77 1.2831 -0.9900 -1.3887 O
78 O78 -1.3085 -0.8817 1.6128 O
79 H79 2.3889 1.3283 0.4334 H
80 H80 -2.2671 0.9989 -0.7283 H
81 C81 -0.4014 3.6593 -1.5653 C
82 C82 -1.4572 3.6195 -0.6419 C
83 C83 -2.7171 4.0856 -0.9992 C
84 C84 -2.9189 4.6044 -2.2816 C
85 C85 -1.8700 4.6461 -3.1964 C
86 C86 -0.6055 4.1685 -2.8414 C
87 H87 -3.5353 4.0481 -0.2879 H
88 H88 -3.8974 4.9764 -2.5639 H
89 H89 -2.0337 5.0500 -4.1891 H
90 H90 0.2104 4.1976 -3.5562 H
91 C91 1.2125 3.8122 0.2748 C
92 C92 2.3987 4.4632 0.5912 C
93 C93 2.5308 5.0861 1.8353 C
94 C94 1.4842 5.0500 2.7526 C
95 C95 0.2922 4.3920 2.4376 C
96 C96 0.1565 3.7789 1.1985 C
97 H97 3.2142 4.4915 -0.1237 H
98 H98 3.4522 5.5994 2.0857 H
99 H99 1.5928 5.5351 3.7160 H
100 H100 -0.5228 4.3644 3.1533 H
101 C101 -1.0560 3.0196 0.6947 C
102 C102 0.8928 3.0842 -1.0195 C
103 H103 -1.8750 3.0097 1.4147 H
104 H104 1.7078 3.1323 -1.7432 H

6 (conf. 37)
1 C1 0.5337 0.5780 -1.5142 C

2	H2	1.4455	0.2147	-1.0438 H
3	C3	-0.5337	-0.5780	-1.5142 C
4	H4	-1.4455	-0.2147	-1.0438 H
5	C5	0.7040	2.0803	0.4457 C
6	C6	-0.7040	-2.0803	0.4457 C
7	C7	0.1454	3.4055	1.0983 C
8	C8	1.0903	3.8739	2.2354 C
9	C9	1.5641	5.1859	2.3261 C
10	H10	1.3207	5.9079	1.5585 H
11	C11	2.3494	5.5969	3.4050 C
12	H12	2.7014	6.6220	3.4466 H
13	C13	2.6731	4.7035	4.4181 C
14	H14	3.2847	5.0201	5.2557 H
15	C15	2.1904	3.3971	4.3502 C
16	H16	2.4222	2.6897	5.1388 H
17	C17	1.4036	2.9903	3.2795 C
18	H18	1.0297	1.9774	3.2539 H
19	C19	-1.2282	3.1254	1.7629 C
20	C20	-1.8614	4.1613	2.4679 C
21	H21	-1.3896	5.1350	2.5270 H
22	C22	-3.0777	3.9563	3.1083 C
23	H23	-3.5453	4.7759	3.6430 H
24	C24	-3.6857	2.7008	3.0779 C
25	H25	-4.6305	2.5379	3.5843 H
26	C26	-3.0580	1.6598	2.4055 C
27	H27	-3.4966	0.6689	2.3818 H
28	C28	-1.8413	1.8702	1.7526 C
29	H29	-1.3898	1.0223	1.2563 H
30	C30	0.0611	4.4425	-0.0475 C
31	C31	-1.1348	5.0145	-0.4873 C
32	H32	-2.0664	4.7625	0.0013 H
33	C33	-1.1511	5.9149	-1.5562 C
34	H34	-2.0943	6.3462	-1.8728 H
35	C35	0.0268	6.2565	-2.2085 C
36	H36	0.0142	6.9604	-3.0331 H
37	C37	1.2282	5.6799	-1.7916 C
38	H38	2.1563	5.9316	-2.2930 H
39	C39	1.2413	4.7827	-0.7312 C
40	H40	2.1814	4.3414	-0.4189 H
41	C41	-0.1454	-3.4055	1.0983 C
42	C42	-1.0903	-3.8739	2.2354 C
43	C43	-1.5641	-5.1859	2.3261 C
44	H44	-1.3207	-5.9079	1.5585 H
45	C45	-2.3494	-5.5969	3.4050 C
46	H46	-2.7014	-6.6220	3.4466 H

47	C47	-2.6731	-4.7035	4.4181 C
48	H48	-3.2847	-5.0201	5.2557 H
49	C49	-2.1904	-3.3971	4.3502 C
50	H50	-2.4222	-2.6897	5.1388 H
51	C51	-1.4036	-2.9903	3.2795 C
52	H52	-1.0297	-1.9774	3.2539 H
53	C53	1.2282	-3.1254	1.7629 C
54	C54	1.8614	-4.1613	2.4679 C
55	H55	1.3896	-5.1350	2.5270 H
56	C56	3.0777	-3.9563	3.1083 C
57	H57	3.5453	-4.7759	3.6430 H
58	C58	3.6857	-2.7008	3.0779 C
59	H59	4.6305	-2.5379	3.5843 H
60	C60	3.0580	-1.6598	2.4055 C
61	H61	3.4966	-0.6689	2.3818 H
62	C62	1.8413	-1.8702	1.7526 C
63	H63	1.3898	-1.0223	1.2563 H
64	C64	-0.0611	-4.4425	-0.0475 C
65	C65	1.1348	-5.0145	-0.4873 C
66	H66	2.0664	-4.7625	0.0013 H
67	C67	1.1511	-5.9149	-1.5562 C
68	H68	2.0943	-6.3462	-1.8728 H
69	C69	-0.0268	-6.2565	-2.2085 C
70	H70	-0.0142	-6.9604	-3.0331 H
71	C71	-1.2282	-5.6799	-1.7916 C
72	H72	-2.1563	-5.9316	-2.2930 H
73	C73	-1.2413	-4.7827	-0.7312 C
74	H74	-2.1814	-4.3414	-0.4189 H
75	N75	0.1190	1.7358	-0.7369 N
76	N76	-0.1190	-1.7358	-0.7369 N
77	O77	1.5845	1.4056	0.9526 O
78	O78	-1.5845	-1.4056	0.9526 O
79	H79	-0.5758	2.3519	-1.1343 H
80	H80	0.5758	-2.3519	-1.1343 H
81	C81	1.3841	-0.2771	-3.6617 C
82	C82	0.4657	-1.3379	-3.6566 C
83	C83	0.8134	-2.5681	-4.2022 C
84	C84	2.0812	-2.7347	-4.7668 C
85	C85	2.9907	-1.6805	-4.7758 C
86	C86	2.6457	-0.4466	-4.2176 C
87	H87	0.1078	-3.3918	-4.1888 H
88	H88	2.3563	-3.6905	-5.1982 H
89	H89	3.9722	-1.8167	-5.2157 H
90	H90	3.3571	0.3727	-4.2201 H
91	C91	-0.4657	1.3379	-3.6566 C

92 C92 -0.8134 2.5681 -4.2022 C
93 C93 -2.0812 2.7347 -4.7668 C
94 C94 -2.9907 1.6805 -4.7758 C
95 C95 -2.6457 0.4466 -4.2176 C
96 C96 -1.3841 0.2771 -3.6617 C
97 H97 -0.1078 3.3918 -4.1888 H
98 H98 -2.3563 3.6905 -5.1982 H
99 H99 -3.9722 1.8167 -5.2157 H
100 H100 -3.3571 -0.3727 -4.2201 H
101 C101 -0.8533 -0.9777 -2.9954 C
102 C102 0.8533 0.9777 -2.9954 C
103 H103 -1.5720 -1.7977 -3.0155 H
104 H104 1.5720 1.7977 -3.0155 H

6 (conf. 62)
1 C1 0.5179 1.5489 -0.5336 C
2 H2 0.1153 1.0200 -1.3954 H
3 C3 -0.5845 1.6046 0.5892 C
4 H4 -0.1839 1.1374 1.4885 H
5 C5 2.0360 -0.3884 -0.6945 C
6 C6 -1.9628 -0.4364 0.5838 C
7 C7 3.3374 -1.1127 -0.1724 C
8 C8 3.9283 -0.3903 1.0667 C
9 C9 3.8532 -0.9209 2.3586 C
10 H10 3.3822 -1.8804 2.5192 H
11 C11 4.3838 -0.2352 3.4523 C
12 H12 4.3113 -0.6761 4.4403 H
13 C13 5.0019 0.9981 3.2817 C
14 H14 5.4144 1.5290 4.1322 H
15 C15 5.0888 1.5419 2.0014 C
16 H16 5.5710 2.5005 1.8476 H
17 C17 4.5635 0.8549 0.9119 C
18 H18 4.6611 1.2833 -0.0786 H
19 C19 4.3944 -1.1394 -1.3173 C
20 C20 5.7594 -1.2198 -1.0025 C
21 H21 6.0747 -1.2175 0.0329 H
22 C22 6.7304 -1.3068 -1.9971 C
23 H23 7.7763 -1.3684 -1.7165 H
24 C24 6.3622 -1.3141 -3.3394 C
25 H25 7.1160 -1.3759 -4.1164 H
26 C26 5.0119 -1.2485 -3.6673 C
27 H27 4.7036 -1.2638 -4.7071 H
28 C28 4.0388 -1.1717 -2.6719 C
29 H29 2.9952 -1.1508 -2.9495 H
30 C30 2.9044 -2.5598 0.1836 C

31	C31	3.7225	-3.6620	-0.0758 C
32	H32	4.6665	-3.5295	-0.5868 H
33	C33	3.3346	-4.9471	0.3047 C
34	H34	3.9870	-5.7860	0.0877 H
35	C35	2.1186	-5.1547	0.9471 C
36	H36	1.8141	-6.1547	1.2357 H
37	C37	1.2916	-4.0635	1.2070 C
38	H38	0.3333	-4.2002	1.6949 H
39	C39	1.6811	-2.7815	0.8313 C
40	H40	1.0079	-1.9597	1.0432 H
41	C41	-3.3115	-1.1414	0.1811 C
42	C42	-3.0269	-2.1647	-0.9515 C
43	C43	-4.1168	-2.7462	-1.6200 C
44	H44	-5.1265	-2.4664	-1.3431 H
45	C45	-3.9273	-3.6709	-2.6408 C
46	H46	-4.7889	-4.1061	-3.1354 H
47	C47	-2.6372	-4.0277	-3.0320 C
48	H48	-2.4857	-4.7426	-3.8332 H
49	C49	-1.5499	-3.4496	-2.3884 C
50	H50	-0.5375	-3.7017	-2.6817 H
51	C51	-1.7400	-2.5307	-1.3542 C
52	H52	-0.8661	-2.1092	-0.8808 H
53	C53	-4.3685	-0.1338	-0.3482 C
54	C54	-5.5151	0.2264	0.3673 C
55	H55	-5.7099	-0.2152	1.3344 H
56	C56	-6.4350	1.1376	-0.1541 C
57	H57	-7.3184	1.3881	0.4230 H
58	C58	-6.2306	1.7138	-1.4025 C
59	H59	-6.9472	2.4200	-1.8066 H
60	C60	-5.0992	1.3587	-2.1353 C
61	H61	-4.9266	1.7866	-3.1162 H
62	C62	-4.1900	0.4412	-1.6195 C
63	H63	-3.3381	0.1491	-2.2225 H
64	C64	-3.7822	-1.8406	1.4841 C
65	C65	-3.8208	-1.1053	2.6788 C
66	H66	-3.5050	-0.0678	2.6807 H
67	C67	-4.2480	-1.6794	3.8700 C
68	H68	-4.2631	-1.0851	4.7771 H
69	C69	-4.6438	-3.0160	3.9002 C
70	H70	-4.9736	-3.4694	4.8282 H
71	C71	-4.5967	-3.7616	2.7288 C
72	H72	-4.8862	-4.8067	2.7368 H
73	C73	-4.1673	-3.1806	1.5340 C
74	H74	-4.1218	-3.7905	0.6430 H
75	N75	1.6995	0.8030	-0.1274 N

76 N76 -1.7952 0.8695 0.2462 N
77 O77 1.3599 -0.8951 -1.5777 O
78 O78 -1.1110 -1.0577 1.2008 O
79 H79 2.2565 1.1574 0.6360 H
80 H80 -2.5096 1.3409 -0.2896 H
81 C81 -0.3970 3.6707 -1.4193 C
82 C82 -1.3827 3.7248 -0.4214 C
83 C83 -2.6188 4.3007 -0.6877 C
84 C84 -2.8700 4.8319 -1.9564 C
85 C85 -1.8930 4.7765 -2.9466 C
86 C86 -0.6517 4.1907 -2.6815 C
87 H87 -3.3818 4.3421 0.0826 H
88 H88 -3.8300 5.2889 -2.1675 H
89 H89 -2.0936 5.1913 -3.9280 H
90 H90 0.1090 4.1483 -3.4541 H
91 C91 1.3451 3.7402 0.2962 C
92 C92 2.5821 4.3355 0.5112 C
93 C93 2.8373 4.9705 1.7298 C
94 C94 1.8637 4.9998 2.7246 C
95 C95 0.6201 4.3996 2.5111 C
96 C96 0.3618 3.7770 1.2965 C
97 H97 3.3407 4.3143 -0.2642 H
98 H98 3.7977 5.4441 1.8996 H
99 H99 2.0687 5.4935 3.6677 H
100 H100 -0.1403 4.4267 3.2847 H
101 C101 -0.9334 3.0992 0.8891 C
102 C102 0.8890 3.0121 -0.9562 C
103 H103 -1.6964 3.1598 1.6667 H
104 H104 1.6527 2.9942 -1.7346 H

6 (conf. 68)
1 C1 0.5413 0.5690 -1.7089 C
2 H2 1.4585 0.1899 -1.2611 H
3 C3 -0.5413 -0.5690 -1.7089 C
4 H4 -1.4585 -0.1899 -1.2611 H
5 C5 0.7371 1.9604 0.3208 C
6 C6 -0.7371 -1.9604 0.3208 C
7 C7 0.1237 3.1666 1.1385 C
8 C8 0.8553 4.4680 0.7106 C
9 C9 1.5296 4.5975 -0.5071 C
10 H10 1.5790 3.7620 -1.1925 H
11 C11 2.1536 5.7938 -0.8626 C
12 H12 2.6787 5.8601 -1.8094 H
13 C13 2.1086 6.8919 -0.0114 C

14	H14	2.5941	7.8213	-0.2869 H
15	C15	1.4368	6.7798	1.2045 C
16	H16	1.3947	7.6241	1.8837 H
17	C17	0.8251	5.5826	1.5615 C
18	H18	0.3216	5.5096	2.5173 H
19	C19	0.4020	2.9337	2.6484 C
20	C20	-0.6135	2.8966	3.6074 C
21	H21	-1.6480	2.9991	3.3113 H
22	C22	-0.3201	2.7324	4.9627 C
23	H23	-1.1312	2.7047	5.6819 H
24	C24	0.9964	2.6062	5.3864 C
25	H25	1.2254	2.4757	6.4384 H
26	C26	2.0209	2.6567	4.4419 C
27	H27	3.0553	2.5682	4.7559 H
28	C28	1.7291	2.8251	3.0940 C
29	H29	2.5365	2.8673	2.3778 H
30	C30	-1.3935	3.2531	0.8497 C
31	C31	-2.0211	4.4237	0.4139 C
32	H32	-1.4409	5.3226	0.2559 H
33	C33	-3.3968	4.4555	0.1748 C
34	H34	-3.8567	5.3783	-0.1615 H
35	C35	-4.1703	3.3160	0.3601 C
36	H36	-5.2376	3.3406	0.1709 H
37	C37	-3.5571	2.1369	0.7843 C
38	H38	-4.1386	1.2330	0.9246 H
39	C39	-2.1884	2.1060	1.0263 C
40	H40	-1.7413	1.1716	1.3468 H
41	C41	-0.1237	-3.1666	1.1385 C
42	C42	-0.4020	-2.9337	2.6484 C
43	C43	0.6135	-2.8966	3.6074 C
44	H44	1.6480	-2.9991	3.3113 H
45	C45	0.3201	-2.7324	4.9627 C
46	H46	1.1312	-2.7047	5.6819 H
47	C47	-0.9964	-2.6062	5.3864 C
48	H48	-1.2254	-2.4757	6.4384 H
49	C49	-2.0209	-2.6567	4.4419 C
50	H50	-3.0553	-2.5682	4.7559 H
51	C51	-1.7291	-2.8251	3.0940 C
52	H52	-2.5365	-2.8673	2.3778 H
53	C53	1.3935	-3.2531	0.8497 C
54	C54	2.0211	-4.4237	0.4139 C
55	H55	1.4409	-5.3226	0.2559 H
56	C56	3.3968	-4.4555	0.1748 C
57	H57	3.8567	-5.3783	-0.1615 H
58	C58	4.1703	-3.3160	0.3601 C

59	H59	5.2376	-3.3406	0.1709 H
60	C60	3.5571	-2.1369	0.7843 C
61	H61	4.1386	-1.2330	0.9246 H
62	C62	2.1884	-2.1060	1.0263 C
63	H63	1.7413	-1.1716	1.3468 H
64	C64	-0.8553	-4.4680	0.7106 C
65	C65	-1.5296	-4.5975	-0.5071 C
66	H66	-1.5790	-3.7620	-1.1925 H
67	C67	-2.1536	-5.7938	-0.8626 C
68	H68	-2.6787	-5.8601	-1.8094 H
69	C69	-2.1086	-6.8919	-0.0114 C
70	H70	-2.5941	-7.8213	-0.2869 H
71	C71	-1.4368	-6.7798	1.2045 C
72	H72	-1.3947	-7.6241	1.8837 H
73	C73	-0.8251	-5.5826	1.5615 C
74	H74	-0.3216	-5.5096	2.5173 H
75	N75	0.1489	1.7026	-0.8857 N
76	N76	-0.1489	-1.7026	-0.8857 N
77	O77	1.7067	1.3320	0.7103 O
78	O78	-1.7067	-1.3320	0.7103 O
79	H79	-0.7129	2.1788	-1.1102 H
80	H80	0.7129	-2.1788	-1.1102 H
81	C81	1.3837	-0.2707	-3.8585 C
82	C82	0.4714	-1.3368	-3.8495 C
83	C83	0.8226	-2.5627	-4.4022 C
84	C84	2.0883	-2.7224	-4.9730 C
85	C85	2.9928	-1.6638	-4.9821 C
86	C86	2.6441	-0.4332	-4.4195 C
87	H87	0.1184	-3.3882	-4.3943 H
88	H88	2.3658	-3.6749	-5.4101 H
89	H89	3.9730	-1.7942	-5.4264 H
90	H90	3.3518	0.3894	-4.4229 H
91	C91	-0.4714	1.3368	-3.8495 C
92	C92	-0.8226	2.5627	-4.4022 C
93	C93	-2.0883	2.7224	-4.9730 C
94	C94	-2.9928	1.6638	-4.9821 C
95	C95	-2.6441	0.4332	-4.4195 C
96	C96	-1.3837	0.2707	-3.8585 C
97	H97	-0.1184	3.3882	-4.3943 H
98	H98	-2.3658	3.6749	-5.4101 H
99	H99	-3.9730	1.7942	-5.4264 H
100	H100	-3.3518	-0.3894	-4.4229 H
101	C101	-0.8480	-0.9819	-3.1880 C
102	C102	0.8480	0.9819	-3.1880 C
103	H103	-1.5654	-1.8032	-3.2099 H

104 H104 1.5654 1.8032 -3.2099 H

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1 C1 -0.5780 1.5213 0.5108 C
2 H2 -0.2122 1.0642 1.4284 H
3 C3 0.5798 1.5253 -0.5542 C
4 H4 0.2214 1.0487 -1.4648 H
5 C5 -2.0751 -0.4392 0.7171 C
6 C6 2.0935 -0.4255 -0.7173 C
7 C7 -3.3955 -1.1065 0.1657 C
8 C8 -3.8520 -2.2392 1.1211 C
9 C9 -5.1608 -2.3358 1.6021 C
10 H10 -5.8897 -1.5754 1.3561 H
11 C11 -5.5598 -3.4112 2.3984 C
12 H12 -6.5826 -3.4575 2.7562 H
13 C13 -4.6571 -4.4149 2.7257 C
14 H14 -4.9642 -5.2497 3.3459 H
15 C15 -3.3537 -4.3413 2.2356 C
16 H16 -2.6393 -5.1229 2.4699 H
17 C17 -2.9590 -3.2739 1.4384 C
18 H18 -1.9481 -3.2442 1.0589 H
19 C19 -3.1192 -1.7799 -1.2043 C
20 C20 -4.1567 -2.4917 -1.8274 C
21 H21 -5.1280 -2.5488 -1.3505 H
22 C22 -3.9565 -3.1414 -3.0394 C
23 H23 -4.7774 -3.6813 -3.4987 H
24 C24 -2.7040 -3.1135 -3.6537 C
25 H25 -2.5448 -3.6268 -4.5955 H
26 C26 -1.6613 -2.4345 -3.0361 C
27 H27 -0.6730 -2.4114 -3.4805 H
28 C28 -1.8667 -1.7727 -1.8233 C
29 H29 -1.0176 -1.2711 -1.3800 H
30 C30 -4.4385 0.0340 0.0788 C
31 C31 -5.0165 0.4648 -1.1175 C
32 H32 -4.7653 -0.0274 -2.0473 H
33 C33 -5.9219 1.5293 -1.1362 C
34 H34 -6.3580 1.8389 -2.0795 H
35 C35 -6.2626 2.1862 0.0395 C
36 H36 -6.9705 3.0074 0.0250 H
37 C37 -5.6799 1.7784 1.2410 C
38 H38 -5.9306 2.2837 2.1673 H
39 C39 -4.7777 0.7222 1.2566 C
40 H40 -4.3313 0.4172 2.1967 H
41 C41 3.4120 -1.0884 -0.1513 C
42 C42 4.4206 0.0531 0.1185 C

43	C43	4.9391	0.3394	1.3836 C
44	H44	4.6531	-0.2658	2.2332 H
45	C45	5.8283	1.4009	1.5739 C
46	H46	6.2159	1.5975	2.5673 H
47	C47	6.2134	2.1982	0.5037 C
48	H48	6.9083	3.0173	0.6507 H
49	C49	5.6917	1.9353	-0.7643 C
50	H50	5.9791	2.5505	-1.6100 H
51	C51	4.8044	0.8826	-0.9499 C
52	H52	4.4067	0.6917	-1.9406 H
53	C53	3.9625	-2.1121	-1.1801 C
54	C54	5.2867	-2.0949	-1.6277 C
55	H55	5.9655	-1.3222	-1.2942 H
56	C56	5.7674	-3.0728	-2.5010 C
57	H57	6.8005	-3.0316	-2.8288 H
58	C58	4.9328	-4.0919	-2.9414 C
59	H59	5.3032	-4.8515	-3.6209 H
60	C60	3.6154	-4.1335	-2.4863 C
61	H61	2.9538	-4.9305	-2.8078 H
62	C62	3.1393	-3.1641	-1.6120 C
63	H63	2.1199	-3.2237	-1.2612 H
64	C64	3.0670	-1.8848	1.1355 C
65	C65	4.0490	-2.7133	1.7010 C
66	H66	5.0219	-2.7879	1.2299 H
67	C67	3.7909	-3.4528	2.8493 C
68	H68	4.5694	-4.0831	3.2654 H
69	C69	2.5350	-3.3969	3.4544 C
70	H70	2.3302	-3.9802	4.3453 H
71	C71	1.5475	-2.5961	2.8943 C
72	H72	0.5572	-2.5449	3.3318 H
73	C73	1.8120	-1.8449	1.7470 C
74	H74	1.0045	-1.2485	1.3463 H
75	N75	-1.7249	0.7260	0.1009 N
76	N76	1.7432	0.7575	-0.1356 N
77	O77	-1.4112	-0.9184	1.6209 O
78	O78	1.4161	-0.9389	-1.5920 O
79	H79	-2.3363	1.1040	-0.6088 H
80	H80	2.3557	1.1611	0.5589 H
81	C81	0.2480	3.6852	1.3480 C
82	C82	1.3137	3.6840	0.4353 C
83	C83	2.5349	4.2485	0.7841 C
84	C84	2.6882	4.8266	2.0475 C
85	C85	1.6294	4.8307	2.9516 C
86	C86	0.4042	4.2545	2.6054 C
87	H87	3.3623	4.2394	0.0829 H

88 H88 3.6373 5.2720 2.3235 H
89 H89 1.7551 5.2812 3.9297 H
90 H90 -0.4190 4.2539 3.3122 H
91 C91 -1.3568 3.6475 -0.5100 C
92 C92 -2.5911 4.1765 -0.8688 C
93 C93 -2.7568 4.7296 -2.1419 C
94 C94 -1.6978 4.7435 -3.0457 C
95 C95 -0.4597 4.2019 -2.6896 C
96 C96 -0.2911 3.6577 -1.4228 C
97 H97 -3.4186 4.1592 -0.1678 H
98 H98 -3.7158 5.1481 -2.4256 H
99 H99 -1.8334 5.1742 -4.0314 H
100 H100 0.3635 4.2079 -3.3966 H
101 C101 0.9676 3.0085 -0.8803 C
102 C102 -0.9963 3.0007 0.8160 C
103 H103 1.7909 3.0322 -1.5952 H
104 H104 -1.8203 3.0169 1.5302 H

6 (conf. 73)
1 C1 0.5802 -1.6707 0.3860 C
2 H2 0.1731 -1.2731 1.3141 H
3 C3 -0.5578 -1.6972 -0.6974 C
4 H4 -0.1952 -1.2125 -1.6021 H
5 C5 1.8620 0.4202 0.6458 C
6 C6 -1.9406 0.3438 -0.7120 C
7 C7 3.1429 1.2062 0.1889 C
8 C8 4.2478 0.4339 0.9562 C
9 C9 5.0277 -0.5647 0.3617 C
10 H10 4.9352 -0.7688 -0.6970 H
11 C11 5.9364 -1.3103 1.1121 C
12 H12 6.5373 -2.0684 0.6215 H
13 C13 6.0739 -1.0851 2.4782 C
14 H14 6.7829 -1.6622 3.0611 H
15 C15 5.2839 -0.1133 3.0888 C
16 H16 5.3675 0.0656 4.1551 H
17 C17 4.3797 0.6322 2.3385 C
18 H18 3.7588 1.3707 2.8293 H
19 C19 3.0586 2.6941 0.6029 C
20 C20 4.2136 3.4046 0.9470 C
21 H21 5.1643 2.8907 1.0159 H
22 C22 4.1662 4.7722 1.2100 C
23 H23 5.0770 5.2967 1.4778 H
24 C24 2.9594 5.4598 1.1281 C
25 H25 2.9191 6.5235 1.3353 H
26 C26 1.8050 4.7668 0.7712 C

27	H27	0.8559	5.2853	0.6954 H
28	C28	1.8543	3.4014	0.5066 C
29	H29	0.9434	2.8917	0.2269 H
30	C30	3.3177	1.2374	-1.3486 C
31	C31	4.5790	1.4562	-1.9201 C
32	H32	5.4528	1.5269	-1.2849 H
33	C33	4.7317	1.6031	-3.2954 C
34	H34	5.7208	1.7688	-3.7082 H
35	C35	3.6221	1.5494	-4.1359 C
36	H36	3.7401	1.6641	-5.2075 H
37	C37	2.3600	1.3648	-3.5811 C
38	H38	1.4803	1.3438	-4.2145 H
39	C39	2.2063	1.2162	-2.2032 C
40	H40	1.2018	1.1048	-1.8116 H
41	C41	-3.1930	1.0775	-0.0847 C
42	C42	-2.9500	2.6099	-0.1414 C
43	C43	-3.0077	3.4252	0.9920 C
44	H44	-3.1954	2.9936	1.9650 H
45	C45	-2.8346	4.8078	0.8965 C
46	H46	-2.8856	5.4127	1.7952 H
47	C47	-2.6037	5.4034	-0.3373 C
48	H48	-2.4695	6.4768	-0.4135 H
49	C49	-2.5590	4.6036	-1.4789 C
50	H50	-2.3880	5.0525	-2.4512 H
51	C51	-2.7366	3.2286	-1.3839 C
52	H52	-2.7038	2.6268	-2.2800 H
53	C53	-3.3830	0.5905	1.3717 C
54	C54	-4.5926	0.0792	1.8498 C
55	H55	-5.4464	0.0041	1.1901 H
56	C56	-4.7211	-0.3414	3.1754 C
57	H57	-5.6721	-0.7331	3.5194 H
58	C58	-3.6411	-0.2633	4.0462 C
59	H59	-3.7406	-0.5927	5.0744 H
60	C60	-2.4246	0.2371	3.5815 C
61	H61	-1.5683	0.2999	4.2434 H
62	C62	-2.2962	0.6583	2.2625 C
63	H63	-1.3347	1.0332	1.9273 H
64	C64	-4.4385	0.7508	-0.9542 C
65	C65	-4.5276	-0.3947	-1.7513 C
66	H66	-3.6971	-1.0857	-1.8020 H
67	C67	-5.6762	-0.6697	-2.4938 C
68	H68	-5.7110	-1.5606	-3.1113 H
69	C69	-6.7670	0.1910	-2.4484 C
70	H70	-7.6592	-0.0213	-3.0266 H
71	C71	-6.6959	1.3339	-1.6544 C

72 H72 -7.5355 2.0187 -1.6084 H
73 C73 -5.5456 1.6110 -0.9223 C
74 H74 -5.5050 2.5109 -0.3217 H
75 N75 1.6691 -0.7802 0.0283 N
76 N76 -1.7290 -0.9368 -0.2858 N
77 O77 1.1560 0.8055 1.5635 O
78 O78 -1.2372 0.8620 -1.5633 O
79 H79 2.2422 -1.0166 -0.7684 H
80 H80 -2.2468 -1.2651 0.5169 H
81 C81 -0.1431 -3.8797 1.1733 C
82 C82 -1.2161 -3.8965 0.2688 C
83 C83 -2.4115 -4.5170 0.6117 C
84 C84 -2.5339 -5.1305 1.8614 C
85 C85 -1.4687 -5.1150 2.7578 C
86 C86 -0.2688 -4.4845 2.4175 C
87 H87 -3.2415 -4.5296 -0.0872 H
88 H88 -3.4624 -5.6202 2.1326 H
89 H89 -1.5695 -5.5934 3.7254 H
90 H90 0.5591 -4.4698 3.1186 H
91 C91 1.4465 -3.7407 -0.6909 C
92 C92 2.6958 -4.2221 -1.0648 C
93 C93 2.8732 -4.7516 -2.3463 C
94 C94 1.8093 -4.7905 -3.2436 C
95 C95 0.5548 -4.2997 -2.8716 C
96 C96 0.3752 -3.7789 -1.5965 C
97 H97 3.5238 -4.1924 -0.3643 H
98 H98 3.8436 -5.1347 -2.6413 H
99 H99 1.9535 -5.2029 -4.2358 H
100 H100 -0.2727 -4.3276 -3.5731 H
101 C101 -0.9049 -3.1846 -1.0359 C
102 C102 1.0711 -3.1339 0.6492 C
103 H103 -1.7300 -3.2300 -1.7481 H
104 H104 1.8992 -3.1297 1.3587 H

6 (conf. 81)
1 C1 0.6192 1.6184 -0.6419 C
2 H2 0.2638 1.1985 -1.5846 H
3 C3 -0.4832 1.4207 0.4505 C
4 H4 -0.0521 0.9267 1.3229 H
5 C5 2.0256 -0.3908 -0.5394 C
6 C6 -2.4377 -0.0162 0.7940 C
7 C7 3.4179 -1.0376 -0.1862 C
8 C8 4.0068 -1.7675 -1.4309 C
9 C9 5.3943 -1.9642 -1.5116 C
10 H10 6.0403 -1.5720 -0.7367 H

11	C11	5.9685	-2.6603	-2.5717 C
12	H12	7.0443	-2.7946	-2.6008 H
13	C13	5.1684	-3.1767	-3.5872 C
14	H14	5.6126	-3.7136	-4.4180 H
15	C15	3.7910	-2.9977	-3.5165 C
16	H16	3.1501	-3.3992	-4.2939 H
17	C17	3.2132	-2.3116	-2.4486 C
18	H18	2.1399	-2.2081	-2.4011 H
19	C19	3.1113	-2.0576	0.9434 C
20	C20	3.6690	-3.3377	0.9655 C
21	H21	4.3138	-3.6612	0.1600 H
22	C22	3.3993	-4.2188	2.0135 C
23	H23	3.8446	-5.2076	2.0042 H
24	C24	2.5620	-3.8399	3.0572 C
25	H25	2.3472	-4.5278	3.8672 H
26	C26	1.9933	-2.5675	3.0455 C
27	H27	1.3264	-2.2582	3.8420 H
28	C28	2.2679	-1.6904	2.0018 C
29	H29	1.8159	-0.7053	2.0164 H
30	C30	4.4303	0.0395	0.2817 C
31	C31	4.9279	0.1070	1.5857 C
32	H32	4.6085	-0.6166	2.3229 H
33	C33	5.8463	1.0919	1.9561 C
34	H34	6.2160	1.1166	2.9751 H
35	C35	6.2881	2.0294	1.0307 C
36	H36	7.0035	2.7911	1.3189 H
37	C37	5.8057	1.9737	-0.2773 C
38	H38	6.1489	2.6896	-1.0161 H
39	C39	4.8941	0.9907	-0.6449 C
40	H40	4.5475	0.9458	-1.6708 H
41	C41	-3.4607	-1.0427	0.1686 C
42	C42	-4.9141	-0.7125	0.6218 C
43	C43	-5.9922	-1.0155	-0.2229 C
44	H44	-5.8095	-1.4321	-1.2043 H
45	C45	-7.3100	-0.7984	0.1739 C
46	H46	-8.1180	-1.0452	-0.5062 H
47	C47	-7.5872	-0.2691	1.4303 C
48	H48	-8.6116	-0.0940	1.7402 H
49	C49	-6.5291	0.0230	2.2859 C
50	H50	-6.7246	0.4250	3.2743 H
51	C51	-5.2110	-0.2047	1.8948 C
52	H52	-4.4041	0.0040	2.5804 H
53	C53	-3.0205	-2.4232	0.7272 C
54	C54	-3.9381	-3.3443	1.2374 C
55	H55	-4.9893	-3.0936	1.2816 H

56	C56	-3.5178	-4.5914	1.7010 C
57	H57	-4.2510	-5.2875	2.0939 H
58	C58	-2.1718	-4.9386	1.6667 C
59	H59	-1.8454	-5.9063	2.0316 H
60	C60	-1.2458	-4.0276	1.1613 C
61	H61	-0.1912	-4.2761	1.1292 H
62	C62	-1.6656	-2.7855	0.6956 C
63	H63	-0.9231	-2.1064	0.2913 H
64	C64	-3.4006	-1.0188	-1.3798 C
65	C65	-3.0572	-2.1362	-2.1457 C
66	H66	-2.8048	-3.0667	-1.6568 H
67	C67	-3.0371	-2.0749	-3.5406 C
68	H68	-2.7672	-2.9594	-4.1069 H
69	C69	-3.3594	-0.8949	-4.1999 C
70	H70	-3.3410	-0.8478	-5.2830 H
71	C71	-3.7113	0.2285	-3.4514 C
72	H72	-3.9691	1.1575	-3.9476 H
73	C73	-3.7377	0.1633	-2.0631 C
74	H74	-4.0274	1.0426	-1.5003 H
75	N75	1.8744	0.9426	-0.3322 N
76	N76	-1.5639	0.5857	-0.0539 N
77	O77	1.0956	-1.0722	-0.9507 O
78	O78	-2.3892	0.1953	1.9979 O
79	H79	2.6193	1.4747	0.0928 H
80	H80	-1.5422	0.2961	-1.0188 H
81	C81	-0.4614	3.7425	-1.2695 C
82	C82	-1.4695	3.5709	-0.3104 C
83	C83	-2.7504	4.0521	-0.5516 C
84	C84	-3.0217	4.7123	-1.7532 C
85	C85	-2.0193	4.8807	-2.7059 C
86	C86	-0.7323	4.3915	-2.4676 C
87	H87	-3.5314	3.9192	0.1895 H
88	H88	-4.0173	5.0974	-1.9429 H
89	H89	-2.2364	5.3964	-3.6346 H
90	H90	0.0491	4.5225	-3.2094 H
91	C91	1.2320	3.7314	0.5078 C
92	C92	2.4173	4.3724	0.8475 C
93	C93	2.5925	4.8437	2.1520 C
94	C94	1.5904	4.6667	3.1021 C
95	C95	0.4002	4.0174	2.7617 C
96	C96	0.2202	3.5553	1.4643 C
97	H97	3.1987	4.5108	0.1073 H
98	H98	3.5127	5.3487	2.4230 H
99	H99	1.7326	5.0347	4.1120 H
100	H100	-0.3793	3.8776	3.5030 H

101 C101 -0.9964 2.8290 0.9236 C
102 C102 0.8700 3.1478 -0.8477 C
103 H103 -1.7754 2.6962 1.6720 H
104 H104 1.6495 3.3049 -1.5953 H

6 (conf. 87)
1 C1 0.5947 1.5754 -0.7110 C
2 H2 0.1922 1.0704 -1.5893 H
3 C3 -0.4969 1.5287 0.4222 C
4 H4 -0.0700 1.0652 1.3095 H
5 C5 1.9520 -0.4619 -0.5175 C
6 C6 -1.9633 -0.4431 0.7039 C
7 C7 3.3142 -1.1379 -0.1085 C
8 C8 3.6483 -2.0961 -1.2824 C
9 C9 3.5636 -1.6217 -2.6005 C
10 H10 3.2423 -0.6027 -2.7852 H
11 C11 3.8743 -2.4334 -3.6847 C
12 H12 3.7958 -2.0371 -4.6912 H
13 C13 4.2741 -3.7533 -3.4797 C
14 H14 4.5123 -4.3917 -4.3230 H
15 C15 4.3495 -4.2420 -2.1815 C
16 H16 4.6439 -5.2704 -2.0030 H
17 C17 4.0376 -3.4227 -1.0950 C
18 H18 4.0865 -3.8377 -0.0982 H
19 C19 3.1034 -1.9138 1.2197 C
20 C20 4.2296 -2.3819 1.9159 C
21 H21 5.2215 -2.1819 1.5277 H
22 C22 4.0989 -3.0928 3.1039 C
23 H23 4.9871 -3.4460 3.6164 H
24 C24 2.8346 -3.3406 3.6372 C
25 H25 2.7302 -3.8869 4.5681 H
26 C26 1.7121 -2.8716 2.9652 C
27 H27 0.7187 -3.0393 3.3653 H
28 C28 1.8424 -2.1713 1.7645 C
29 H29 0.9428 -1.8284 1.2751 H
30 C30 4.4377 -0.0894 0.1163 C
31 C31 5.4927 0.1079 -0.7805 C
32 H32 5.5681 -0.5027 -1.6691 H
33 C33 6.4718 1.0736 -0.5427 C
34 H34 7.2807 1.1953 -1.2548 H
35 C35 6.4209 1.8676 0.5973 C
36 H36 7.1839 2.6154 0.7816 H
37 C37 5.3837 1.6777 1.5089 C
38 H38 5.3315 2.2768 2.4108 H
39 C39 4.4141 0.7074 1.2752 C

40	H40	3.6380	0.5509	2.0154 H
41	C41	-3.2987	-1.1201	0.2203 C
42	C42	-3.3845	-1.2564	-1.3188 C
43	C43	-4.6232	-1.4678	-1.9413 C
44	H44	-5.5302	-1.4645	-1.3495 H
45	C45	-4.7116	-1.7040	-3.3093 C
46	H46	-5.6842	-1.8607	-3.7629 H
47	C47	-3.5583	-1.7533	-4.0899 C
48	H48	-3.6256	-1.9407	-5.1557 H
49	C49	-2.3202	-1.5804	-3.4808 C
50	H50	-1.4091	-1.6429	-4.0653 H
51	C51	-2.2305	-1.3390	-2.1097 C
52	H52	-1.2459	-1.2382	-1.6688 H
53	C53	-4.3577	-0.1798	0.8519 C
54	C54	-5.0587	0.7857	0.1219 C
55	H55	-4.9337	0.8532	-0.9506 H
56	C56	-5.9273	1.6757	0.7550 C
57	H57	-6.4671	2.4054	0.1614 H
58	C58	-6.1024	1.6289	2.1341 C
59	H59	-6.7809	2.3173	2.6253 H
60	C60	-5.3894	0.6897	2.8776 C
61	H61	-5.5027	0.6482	3.9553 H
62	C62	-4.5260	-0.1986	2.2451 C
63	H63	-3.9639	-0.9108	2.8361 H
64	C64	-3.3990	-2.5704	0.7488 C
65	C65	-4.6209	-3.1059	1.1670 C
66	H66	-5.5015	-2.4774	1.2092 H
67	C67	-4.7310	-4.4455	1.5382 C
68	H68	-5.6913	-4.8330	1.8607 H
69	C69	-3.6185	-5.2786	1.4940 C
70	H70	-3.7003	-6.3199	1.7852 H
71	C71	-2.3984	-4.7604	1.0637 C
72	H72	-1.5223	-5.3977	1.0150 H
73	C73	-2.2905	-3.4248	0.6905 C
74	H74	-1.3345	-3.0514	0.3505 H
75	N75	1.8272	0.8812	-0.3584 N
76	N76	-1.6423	0.7142	0.0597 N
77	O77	1.0433	-1.1422	-0.9717 O
78	O78	-1.3256	-0.8660	1.6528 O
79	H79	2.5835	1.4095	0.0514 H
80	H80	-2.2005	1.0014	-0.7306 H
81	C81	-0.4252	3.6668	-1.5183 C
82	C82	-1.4138	3.6289	-0.5235 C
83	C83	-2.6862	4.1246	-0.7834 C
84	C84	-2.9673	4.6704	-2.0393 C

85 C85 -1.9846 4.7098 -3.0252 C
86 C86 -0.7080 4.2030 -2.7683 C
87 H87 -3.4529 4.0879 -0.0168 H
88 H88 -3.9557 5.0653 -2.2458 H
89 H89 -2.2097 5.1348 -3.9968 H
90 H90 0.0567 4.2314 -3.5377 H
91 C91 1.3138 3.7682 0.2078 C
92 C92 2.5262 4.4022 0.4508 C
93 C93 2.7503 5.0020 1.6937 C
94 C94 1.7699 4.9581 2.6812 C
95 C95 0.5521 4.3159 2.4390 C
96 C96 0.3239 3.7266 1.2022 C
97 H97 3.2911 4.4365 -0.3180 H
98 H98 3.6911 5.5051 1.8866 H
99 H99 1.9493 5.4263 3.6424 H
100 H100 -0.2113 4.2826 3.2092 H
101 C101 -0.9319 2.9944 0.7691 C
102 C102 0.8957 3.0658 -1.0732 C
103 H103 -1.6993 2.9817 1.5435 H
104 H104 1.6594 3.1198 -1.8510 H

6 (conf. 90)
1 C1 0.2874 0.7225 -1.3894 C
2 H2 1.2906 0.7354 -0.9599 H
3 C3 -0.2874 -0.7225 -1.3894 C
4 H4 -1.2906 -0.7354 -0.9599 H
5 C5 0.0002 2.7256 -0.0007 C
6 C6 -0.0002 -2.7256 -0.0007 C
7 C7 -0.9380 3.5748 0.9440 C
8 C8 -0.3225 3.4440 2.3633 C
9 C9 -0.3778 4.4970 3.2805 C
10 H10 -0.8089 5.4450 2.9872 H
11 C11 0.1222 4.3493 4.5738 C
12 H12 0.0690 5.1844 5.2637 H
13 C13 0.6923 3.1459 4.9761 C
14 H14 1.0867 3.0334 5.9797 H
15 C15 0.7569 2.0886 4.0712 C
16 H16 1.2026 1.1445 4.3641 H
17 C17 0.2536 2.2378 2.7822 C
18 H18 0.3168 1.4007 2.0973 H
19 C19 -2.3866 3.0276 0.9216 C
20 C20 -3.0038 2.4710 2.0455 C

21	H21	-2.4690	2.4198	2.9839 H
22	C22	-4.3100	1.9818	1.9825 C
23	H23	-4.7616	1.5563	2.8717 H
24	C24	-5.0278	2.0364	0.7936 C
25	H25	-6.0403	1.6524	0.7450 H
26	C26	-4.4304	2.5935	-0.3366 C
27	H27	-4.9747	2.6467	-1.2726 H
28	C28	-3.1317	3.0866	-0.2700 C
29	H29	-2.6921	3.5313	-1.1551 H
30	C30	-0.9270	5.0704	0.5049 C
31	C31	-2.0827	5.8551	0.6249 C
32	H32	-3.0054	5.4122	0.9744 H
33	C33	-2.0741	7.2127	0.3082 C
34	H34	-2.9869	7.7889	0.4126 H
35	C35	-0.9062	7.8228	-0.1367 C
36	H36	-0.8978	8.8775	-0.3885 H
37	C37	0.2536	7.0604	-0.2443 C
38	H38	1.1775	7.5206	-0.5778 H
39	C39	0.2494	5.7063	0.0815 C
40	H40	1.1618	5.1340	0.0101 H
41	C41	0.9380	-3.5748	0.9440 C
42	C42	2.3866	-3.0276	0.9216 C
43	C43	3.0038	-2.4710	2.0455 C
44	H44	2.4690	-2.4198	2.9839 H
45	C45	4.3100	-1.9818	1.9825 C
46	H46	4.7616	-1.5563	2.8717 H
47	C47	5.0278	-2.0364	0.7936 C
48	H48	6.0403	-1.6524	0.7450 H
49	C49	4.4304	-2.5935	-0.3366 C
50	H50	4.9747	-2.6467	-1.2726 H
51	C51	3.1317	-3.0866	-0.2700 C
52	H52	2.6921	-3.5313	-1.1551 H
53	C53	0.9270	-5.0704	0.5049 C
54	C54	2.0827	-5.8551	0.6249 C
55	H55	3.0054	-5.4122	0.9744 H
56	C56	2.0741	-7.2127	0.3082 C
57	H57	2.9869	-7.7889	0.4126 H
58	C58	0.9062	-7.8228	-0.1367 C
59	H59	0.8978	-8.8775	-0.3885 H
60	C60	-0.2536	-7.0604	-0.2443 C
61	H61	-1.1775	-7.5206	-0.5778 H
62	C62	-0.2494	-5.7063	0.0815 C
63	H63	-1.1618	-5.1340	0.0101 H
64	C64	0.3225	-3.4440	2.3633 C
65	C65	0.3778	-4.4970	3.2805 C

66 H66 0.8089 -5.4450 2.9872 H
67 C67 -0.1222 -4.3493 4.5738 C
68 H68 -0.0690 -5.1844 5.2637 H
69 C69 -0.6923 -3.1459 4.9761 C
70 H70 -1.0867 -3.0334 5.9797 H
71 C71 -0.7569 -2.0886 4.0712 C
72 H72 -1.2026 -1.1445 4.3641 H
73 C73 -0.2536 -2.2378 2.7822 C
74 H74 -0.3168 -1.4007 2.0973 H
75 N75 -0.5251 1.6008 -0.5593 N
76 N76 0.5251 -1.6008 -0.5593 N
77 O77 1.1754 3.0160 -0.1644 O
78 O78 -1.1754 -3.0160 -0.1644 O
79 H79 -1.5110 1.4134 -0.4653 H
80 H80 1.5110 -1.4134 -0.4653 H
81 C81 1.3883 0.2576 -3.5381 C
82 C82 0.9283 -1.0679 -3.5340 C
83 C83 1.7020 -2.0792 -4.0907 C
84 C84 2.9401 -1.7640 -4.6577 C
85 C85 3.3990 -0.4487 -4.6560 C
86 C86 2.6246 0.5681 -4.0913 C
87 H87 1.3433 -3.1033 -4.0917 H
88 H88 3.5439 -2.5469 -5.1030 H
89 H89 4.3603 -0.2109 -5.0976 H
90 H90 2.9832 1.5921 -4.0877 H
91 C91 -0.9283 1.0679 -3.5340 C
92 C92 -1.7020 2.0792 -4.0907 C
93 C93 -2.9401 1.7640 -4.6577 C
94 C94 -3.3990 0.4487 -4.6560 C
95 C95 -2.6246 -0.5681 -4.0913 C
96 C96 -1.3883 -0.2576 -3.5381 C
97 H97 -1.3433 3.1033 -4.0917 H
98 H98 -3.5439 2.5469 -5.1030 H
99 H99 -4.3603 0.2109 -5.0976 H
100 H100 -2.9832 -1.5921 -4.0877 H
101 C101 -0.4265 -1.2243 -2.8723 C
102 C102 0.4265 1.2243 -2.8723 C
103 H103 -0.7930 -2.2503 -2.8761 H
104 H104 0.7930 2.2503 -2.8761 H

7 (conf. 1)

1	6	0	-0.905216	3.546544	-1.164230
2	6	0	-0.944545	3.607754	-2.559766
3	6	0	-0.150643	2.762640	-3.325593
4	6	0	0.703630	1.845387	-2.726709

5	6	0	0.761529	1.768606	-1.328657
6	6	0	-0.055869	2.614356	-0.539266
7	6	0	-0.006468	2.512881	0.956715
8	6	0	0.912626	3.285321	1.693109
9	6	0	0.957574	3.148002	3.082980
10	6	0	0.109391	2.260425	3.735267
11	6	0	-0.810528	1.500192	3.025410
12	6	0	-0.878979	1.628283	1.633134
13	6	0	1.850829	4.243706	0.996301
14	6	0	-1.763451	4.483374	-0.345281
15	7	0	-1.833640	0.928466	0.858462
16	6	0	-2.561223	-0.183768	1.201520
17	8	0	-2.442281	-0.760031	2.267365
18	6	0	-3.494267	-0.748201	0.067399
19	6	0	-4.762569	-1.427266	0.647526
20	6	0	-5.252214	-1.188428	1.935088
21	6	0	-6.457844	-1.750255	2.356542
22	6	0	-7.199798	-2.559980	1.504390
23	6	0	-6.726564	-2.800185	0.215883
24	6	0	-5.527970	-2.235733	-0.204966
25	6	0	-4.052388	0.354717	-0.865944
26	6	0	-4.180002	0.184027	-2.248715
27	6	0	-4.808814	1.146463	-3.037768
28	6	0	-5.330371	2.299883	-2.462078
29	6	0	-5.226773	2.477675	-1.083840
30	6	0	-4.602092	1.514788	-0.298532
31	6	0	-2.551571	-1.768808	-0.622435
32	6	0	-2.527663	-3.105082	-0.204423
33	6	0	-1.626591	-4.012979	-0.755266
34	6	0	-0.717529	-3.602290	-1.726169
35	6	0	-0.703327	-2.268563	-2.126925
36	6	0	-1.605399	-1.362085	-1.573787
37	7	0	1.642085	0.895329	-0.655823
38	6	0	5.324692	2.294266	1.477378
39	6	0	2.431327	-0.102647	-1.179034
40	6	0	3.479766	-0.696648	-0.160904
41	8	0	2.396832	-0.440311	-2.346667
42	6	0	2.832571	-1.270465	1.123287
43	6	0	3.665483	-1.702007	2.168306
44	6	0	3.139987	-2.291670	3.311028
45	6	0	1.763238	-2.478248	3.436918
46	6	0	0.926130	-2.082457	2.401747
47	6	0	1.458184	-1.491485	1.253053
48	6	0	4.227980	-1.885585	-0.810487
49	6	0	5.615449	-2.024855	-0.721157

50	6	0	6.259885	-3.154406	-1.227617
51	6	0	5.526836	-4.167953	-1.832685
52	6	0	4.140303	-4.046778	-1.915680
53	6	0	3.499636	-2.924318	-1.405262
54	6	0	4.415125	0.514635	0.094879
55	6	0	5.138692	1.038860	-0.988845
56	6	0	5.947569	2.159160	-0.838437
57	6	0	6.050792	2.790605	0.400920
58	6	0	4.508967	1.171178	1.324954
59	1	0	-1.603820	4.320735	-3.041943
60	1	0	-0.190170	2.817372	-4.407852
61	1	0	1.323066	1.191326	-3.318692
62	1	0	1.664882	3.740785	3.652438
63	1	0	0.160163	2.156960	4.813352
64	1	0	-1.461819	0.803327	3.527709
65	1	0	2.560515	3.717827	0.351583
66	1	0	1.309152	4.950233	0.362027
67	1	0	2.427173	4.814510	1.726181
68	1	0	-2.441986	3.941493	0.318560
69	1	0	-1.154473	5.133948	0.289309
70	1	0	-2.367882	5.115753	-0.997169
71	1	0	-1.963481	1.283265	-0.079093
72	1	0	-4.687718	-0.585254	2.629663
73	1	0	-6.810449	-1.552254	3.362842
74	1	0	-8.134461	-2.997696	1.836504
75	1	0	-7.292623	-3.424671	-0.466466
76	1	0	-5.182889	-2.428102	-1.213665
77	1	0	-3.795878	-0.709658	-2.721589
78	1	0	-4.891619	0.985940	-4.106909
79	1	0	-5.820416	3.047008	-3.075929
80	1	0	-5.643090	3.362372	-0.615138
81	1	0	-4.561958	1.659385	0.774979
82	1	0	-3.217458	-3.439024	0.558621
83	1	0	-1.634357	-5.043048	-0.416877
84	1	0	-0.019514	-4.310493	-2.158021
85	1	0	0.020690	-1.920703	-2.854407
86	1	0	-1.559990	-0.330452	-1.899157
87	1	0	1.713820	1.049775	0.341105
88	1	0	5.385774	2.778642	2.445725
89	1	0	4.739136	-1.589146	2.079339
90	1	0	3.808702	-2.613351	4.102008
91	1	0	1.351529	-2.935388	4.329618
92	1	0	-0.146279	-2.216355	2.477585
93	1	0	0.776884	-1.218837	0.458033
94	1	0	6.209726	-1.250619	-0.253941

95	1	0	7.338243	-3.234868	-1.144660
96	1	0	6.025643	-5.044614	-2.230589
97	1	0	3.553561	-4.832900	-2.378328
98	1	0	2.422196	-2.857649	-1.467265
99	1	0	5.061906	0.562158	-1.959026
100	1	0	6.497472	2.540308	-1.691752
101	1	0	6.685141	3.661562	0.521141
102	1	0	3.946304	0.813081	2.176432

7 (conf. 2)

1	6	0	-0.771766	-3.490708	1.566168
2	6	0	-0.720794	-3.502309	2.961751
3	6	0	0.178057	-2.690704	3.643452
4	6	0	1.041654	-1.849378	2.955924
5	6	0	1.008216	-1.821745	1.556756
6	6	0	0.100035	-2.645847	0.851910
7	6	0	0.105884	-2.658251	-0.648479
8	6	0	0.955173	-3.553394	-1.329061
9	6	0	0.964379	-3.563551	-2.725788
10	6	0	0.141879	-2.703117	-3.441505
11	6	0	-0.707691	-1.819376	-2.788882
12	6	0	-0.735143	-1.791391	-1.386943
13	6	0	1.847296	-4.506926	-0.567313
14	6	0	-1.761842	-4.374859	0.842910
15	7	0	-1.611563	-0.946377	-0.665988
16	6	0	-2.408055	0.063002	-1.156407
17	8	0	-2.387975	0.411805	-2.321401
18	6	0	-3.431277	0.684691	-0.123154
19	6	0	-3.753409	2.142271	-0.558181
20	6	0	-4.316746	2.377866	-1.823032
21	6	0	-4.651983	3.663433	-2.231141
22	6	0	-4.450724	4.750718	-1.381648
23	6	0	-3.917396	4.530359	-0.117940
24	6	0	-3.573887	3.239281	0.289179
25	6	0	-4.743148	-0.144670	-0.216215
26	6	0	-5.944743	0.418692	0.237457
27	6	0	-7.135796	-0.299326	0.205156
28	6	0	-7.160777	-1.599814	-0.295069
29	6	0	-5.980214	-2.168758	-0.758401
30	6	0	-4.784618	-1.450449	-0.715246
31	6	0	-2.841138	0.646028	1.304876
32	6	0	-1.572098	1.205254	1.537240
33	6	0	-1.017944	1.232154	2.812135
34	6	0	-1.724200	0.702719	3.891693
35	6	0	-2.975324	0.137474	3.677618

36	6	0	-3.526955	0.104506	2.395900
37	7	0	1.897830	-1.023045	0.801426
38	6	0	1.355321	4.008600	-0.190963
39	6	0	2.621941	0.067140	1.217567
40	6	0	3.446432	0.790615	0.089410
41	8	0	2.574133	0.511547	2.349779
42	6	0	4.725728	1.463330	0.651331
43	6	0	5.379123	2.415360	-0.143806
44	6	0	6.584504	2.984086	0.251955
45	6	0	7.176171	2.605723	1.455387
46	6	0	6.545553	1.653921	2.248676
47	6	0	5.333974	1.086942	1.852607
48	6	0	3.977542	-0.179640	-0.994600
49	6	0	4.024374	0.158274	-2.351805
50	6	0	4.628426	-0.685165	-3.282919
51	6	0	5.206768	-1.883741	-2.878666
52	6	0	5.185112	-2.226780	-1.528454
53	6	0	4.583515	-1.382517	-0.600999
54	6	0	2.413305	1.831542	-0.415399
55	6	0	1.432668	1.493883	-1.358258
56	6	0	0.443971	2.403159	-1.729582
57	6	0	0.405094	3.669500	-1.150715
58	6	0	2.342588	3.098025	0.178265
59	1	0	-1.391100	-4.153035	3.512369
60	1	0	0.209171	-2.709408	4.727077
61	1	0	1.727781	-1.205972	3.482260
62	1	0	1.623027	-4.248378	-3.247957
63	1	0	0.156824	-2.715925	-4.525620
64	1	0	-1.342457	-1.149130	-3.344073
65	1	0	2.543711	-3.978223	0.088674
66	1	0	1.266269	-5.180518	0.069175
67	1	0	2.433423	-5.114628	-1.258292
68	1	0	-2.540738	-3.784387	0.350641
69	1	0	-1.281756	-4.975468	0.066357
70	1	0	-2.254186	-5.051779	1.543069
71	1	0	-1.617740	-1.080401	0.337129
72	1	0	-4.490721	1.548786	-2.492483
73	1	0	-5.078765	3.814553	-3.216669
74	1	0	-4.717341	5.752717	-1.699397
75	1	0	-3.767559	5.359607	0.564799
76	1	0	-3.169886	3.101120	1.281905
77	1	0	-5.948868	1.433536	0.615233
78	1	0	-8.047949	0.163902	0.564881
79	1	0	-8.089980	-2.157252	-0.329128
80	1	0	-5.981243	-3.175419	-1.161565

81	1	0	-3.887041	-1.924606	-1.089414
82	1	0	-1.011686	1.631692	0.712865
83	1	0	-0.028531	1.649627	2.955844
84	1	0	-1.293555	0.722076	4.886330
85	1	0	-3.530950	-0.287226	4.506419
86	1	0	-4.500471	-0.344437	2.254899
87	1	0	1.960800	-1.261917	-0.178791
88	1	0	1.327789	4.984184	0.281878
89	1	0	4.940296	2.717866	-1.086907
90	1	0	7.062816	3.720881	-0.383957
91	1	0	8.116099	3.046818	1.767654
92	1	0	6.991234	1.347454	3.188699
93	1	0	4.857621	0.368412	2.502104
94	1	0	3.594651	1.090675	-2.692436
95	1	0	4.647075	-0.396849	-4.328048
96	1	0	5.677122	-2.538428	-3.603454
97	1	0	5.646293	-3.148732	-1.192245
98	1	0	4.604545	-1.655587	0.447659
99	1	0	1.426578	0.512747	-1.816215
100	1	0	-0.307926	2.106492	-2.451004
101	1	0	-0.368866	4.373874	-1.432502
102	1	0	3.060980	3.373020	0.938631

7 (conf. 3)

1	6	0	0.764864	1.516463	3.591250
2	6	0	1.928637	2.286129	3.528260
3	6	0	2.941453	1.968562	2.630072
4	6	0	2.827995	0.868305	1.791255
5	6	0	1.676014	0.075764	1.845588
6	6	0	0.627894	0.408809	2.731885
7	6	0	-0.627894	-0.408809	2.731885
8	6	0	-0.764864	-1.516463	3.591250
9	6	0	-1.928637	-2.286129	3.528260
10	6	0	-2.941453	-1.968562	2.630072
11	6	0	-2.827995	-0.868305	1.791255
12	6	0	-1.676014	-0.075764	1.845588
13	6	0	0.334675	-1.884939	4.561246
14	6	0	-0.334675	1.884939	4.561246
15	7	0	-1.555193	1.106577	1.072179
16	6	0	-2.144579	1.367799	-0.140115
17	8	0	-2.789178	0.528021	-0.744486
18	6	0	-1.894469	2.798024	-0.752567
19	6	0	-0.970929	2.529191	-1.972211
20	6	0	-1.312287	2.910958	-3.271768
21	6	0	-0.455697	2.648309	-4.341617

22	6	0	0.752579	1.992062	-4.135167
23	6	0	1.100448	1.591680	-2.846632
24	6	0	0.245565	1.857584	-1.782468
25	6	0	-3.234250	3.456991	-1.202612
26	6	0	-3.227851	4.836722	-1.466697
27	6	0	-4.370806	5.499788	-1.899381
28	6	0	-5.564153	4.801658	-2.071739
29	6	0	-5.586676	3.435860	-1.816898
30	6	0	-4.435551	2.766851	-1.396432
31	6	0	-1.250687	3.766508	0.274518
32	6	0	-1.984164	4.114353	1.422801
33	6	0	-1.489289	5.024808	2.348412
34	6	0	-0.245565	5.624217	2.146478
35	6	0	0.487721	5.298300	1.012483
36	6	0	-0.008967	4.378690	0.085943
37	7	0	1.555193	-1.106577	1.072179
38	6	0	0.455697	-2.648309	-4.341617
39	6	0	2.144579	-1.367799	-0.140115
40	6	0	1.894469	-2.798024	-0.752567
41	8	0	2.789178	-0.528021	-0.744486
42	6	0	3.234250	-3.456991	-1.202612
43	6	0	4.435551	-2.766851	-1.396432
44	6	0	5.586676	-3.435860	-1.816898
45	6	0	5.564153	-4.801658	-2.071739
46	6	0	4.370806	-5.499788	-1.899381
47	6	0	3.227851	-4.836722	-1.466697
48	6	0	1.250687	-3.766508	0.274518
49	6	0	1.984164	-4.114353	1.422801
50	6	0	1.489289	-5.024808	2.348412
51	6	0	0.245565	-5.624217	2.146478
52	6	0	-0.487721	-5.298300	1.012483
53	6	0	0.008967	-4.378690	0.085943
54	6	0	0.970929	-2.529191	-1.972211
55	6	0	-0.245565	-1.857584	-1.782468
56	6	0	-1.100448	-1.591680	-2.846632
57	6	0	-0.752579	-1.992062	-4.135167
58	6	0	1.312287	-2.910958	-3.271768
59	1	0	2.034532	3.143320	4.183585
60	1	0	3.836080	2.579426	2.585275
61	1	0	3.612534	0.621416	1.093321
62	1	0	-2.034532	-3.143320	4.183585
63	1	0	-3.836080	-2.579426	2.585275
64	1	0	-3.612534	-0.621416	1.093321
65	1	0	1.244529	-2.199752	4.041964
66	1	0	0.611792	-1.042273	5.199881

67	1	0	0.019694	-2.709231	5.203197
68	1	0	-0.019694	2.709231	5.203197
69	1	0	-1.244529	2.199752	4.041964
70	1	0	-0.611792	1.042273	5.199881
71	1	0	-0.930534	1.811492	1.437865
72	1	0	-2.251285	3.411501	-3.461983
73	1	0	-0.745693	2.955530	-5.340639
74	1	0	1.412341	1.781616	-4.969375
75	1	0	2.020724	1.052968	-2.657040
76	1	0	0.542401	1.529346	-0.793496
77	1	0	-2.315365	5.404042	-1.332591
78	1	0	-4.327227	6.565356	-2.096501
79	1	0	-6.459877	5.316166	-2.401445
80	1	0	-6.504139	2.872770	-1.949808
81	1	0	-4.473901	1.700645	-1.238683
82	1	0	-2.966252	3.682062	1.578521
83	1	0	-2.081209	5.277137	3.221301
84	1	0	0.139271	6.341503	2.862634
85	1	0	1.452404	5.760581	0.835678
86	1	0	0.576454	4.152412	-0.794341
87	1	0	0.930534	-1.811492	1.437865
88	1	0	0.745693	-2.955530	-5.340639
89	1	0	4.473901	-1.700645	-1.238683
90	1	0	6.504139	-2.872770	-1.949808
91	1	0	6.459877	-5.316166	-2.401445
92	1	0	4.327227	-6.565356	-2.096501
93	1	0	2.315365	-5.404042	-1.332591
94	1	0	2.966252	-3.682062	1.578521
95	1	0	2.081209	-5.277137	3.221301
96	1	0	-0.139271	-6.341503	2.862634
97	1	0	-1.452404	-5.760581	0.835678
98	1	0	-0.576454	-4.152412	-0.794341
99	1	0	-0.542401	-1.529346	-0.793496
100	1	0	-2.020724	-1.052968	-2.657040
101	1	0	-1.412341	-1.781616	-4.969375
102	1	0	2.251285	-3.411501	-3.461983

7 (conf. 4)

1	6	0	1.456848	0.884751	3.431388
2	6	0	2.853517	0.916122	3.363745
3	6	0	3.537824	0.098171	2.471985
4	6	0	2.853517	-0.780598	1.642649
5	6	0	1.457652	-0.835226	1.699752
6	6	0	0.749154	0.013152	2.579581
7	6	0	-0.749154	-0.013152	2.579581

8	6	0	-1.456848	-0.884751	3.431388
9	6	0	-2.853517	-0.916122	3.363745
10	6	0	-3.537824	-0.098171	2.471985
11	6	0	-2.853517	0.780598	1.642649
12	6	0	-1.457652	0.835226	1.699752
13	6	0	-0.730773	-1.797516	4.394754
14	6	0	0.730773	1.797516	4.394754
15	7	0	-0.712975	1.767817	0.932363
16	6	0	-1.106863	2.433405	-0.208620
17	8	0	-2.157362	2.186328	-0.777284
18	6	0	-0.093497	3.537993	-0.735257
19	6	0	0.995827	2.868894	-1.618104
20	6	0	1.381136	1.535704	-1.462690
21	6	0	2.402250	0.978087	-2.234041
22	6	0	3.064069	1.754061	-3.180211
23	6	0	2.692561	3.088298	-3.346168
24	6	0	1.670444	3.635299	-2.577191
25	6	0	-0.882416	4.545123	-1.614502
26	6	0	-0.859890	5.924828	-1.385148
27	6	0	-1.532173	6.809126	-2.230897
28	6	0	-2.237077	6.333156	-3.327535
29	6	0	-2.251634	4.962886	-3.582478
30	6	0	-1.578213	4.081737	-2.744559
31	6	0	0.536897	4.245413	0.488856
32	6	0	1.916418	4.350575	0.680915
33	6	0	2.437609	5.015955	1.794002
34	6	0	1.590297	5.584880	2.735755
35	6	0	0.208915	5.479230	2.563645
36	6	0	-0.307404	4.815858	1.457863
37	7	0	0.712975	-1.767817	0.932363
38	6	0	-2.437609	-5.015955	1.794002
39	6	0	1.106863	-2.433405	-0.208620
40	6	0	0.093497	-3.537993	-0.735257
41	8	0	2.157362	-2.186328	-0.777284
42	6	0	-0.995827	-2.868894	-1.618104
43	6	0	-1.670444	-3.635299	-2.577191
44	6	0	-2.692561	-3.088298	-3.346168
45	6	0	-3.064069	-1.754061	-3.180211
46	6	0	-2.402250	-0.978087	-2.234041
47	6	0	-1.381136	-1.535704	-1.462690
48	6	0	0.882416	-4.545123	-1.614502
49	6	0	0.859890	-5.924828	-1.385148
50	6	0	1.532173	-6.809126	-2.230897
51	6	0	2.237077	-6.333156	-3.327535
52	6	0	2.251634	-4.962886	-3.582478

53	6	0	1.578213	-4.081737	-2.744559
54	6	0	-0.536897	-4.245413	0.488856
55	6	0	0.307404	-4.815858	1.457863
56	6	0	-0.208915	-5.479230	2.563645
57	6	0	-1.590297	-5.584880	2.735755
58	6	0	-1.916418	-4.350575	0.680915
59	1	0	3.401645	1.588693	4.014540
60	1	0	4.620451	0.135242	2.424392
61	1	0	3.383285	-1.415522	0.951199
62	1	0	-3.401645	-1.588693	4.014540
63	1	0	-4.620451	-0.135242	2.424392
64	1	0	-3.383285	1.415522	0.951199
65	1	0	-0.315888	-2.671871	3.884065
66	1	0	0.100749	-1.291019	4.888085
67	1	0	-1.414688	-2.164311	5.162550
68	1	0	0.315888	2.671871	3.884065
69	1	0	-0.100749	1.291019	4.888085
70	1	0	1.414688	2.164311	5.162550
71	1	0	0.201763	1.994200	1.298050
72	1	0	0.891823	0.903713	-0.736229
73	1	0	2.668029	-0.061275	-2.077724
74	1	0	3.857265	1.325885	-3.783388
75	1	0	3.195748	3.707645	-4.080759
76	1	0	1.392641	4.670585	-2.727825
77	1	0	-0.308921	6.330745	-0.547353
78	1	0	-1.493953	7.873092	-2.025443
79	1	0	-2.760892	7.018712	-3.983840
80	1	0	-2.785509	4.575559	-4.443228
81	1	0	-1.588200	3.026594	-2.971540
82	1	0	2.596016	3.914531	-0.038611
83	1	0	3.512711	5.084530	1.916224
84	1	0	1.995990	6.103655	3.596930
85	1	0	-0.466275	5.915518	3.291359
86	1	0	-1.382780	4.747731	1.335345
87	1	0	-0.201763	-1.994200	1.298050
88	1	0	-3.512711	-5.084530	1.916224
89	1	0	-1.392641	-4.670585	-2.727825
90	1	0	-3.195748	-3.707645	-4.080759
91	1	0	-3.857265	-1.325885	-3.783388
92	1	0	-2.668029	0.061275	-2.077724
93	1	0	-0.891823	-0.903713	-0.736229
94	1	0	0.308921	-6.330745	-0.547353
95	1	0	1.493953	-7.873092	-2.025443
96	1	0	2.760892	-7.018712	-3.983840
97	1	0	2.785509	-4.575559	-4.443228

98	1	0	1.588200	-3.026594	-2.971540
99	1	0	1.382780	-4.747731	1.335345
100	1	0	0.466275	-5.915518	3.291359
101	1	0	-1.995990	-6.103655	3.596930
102	1	0	-2.596016	-3.914531	-0.038611

7 (conf. 6)

1	6	0	-0.855805	-3.370497	1.304183
2	6	0	-0.792911	-3.524056	2.691382
3	6	0	0.161359	-2.838525	3.434766
4	6	0	1.061067	-1.976295	2.822745
5	6	0	1.011529	-1.802333	1.432675
6	6	0	0.055269	-2.508120	0.663213
7	6	0	0.058157	-2.413487	-0.835268
8	6	0	0.943804	-3.229595	-1.569660
9	6	0	0.920417	-3.181760	-2.965361
10	6	0	0.038471	-2.338403	-3.629119
11	6	0	-0.840805	-1.528782	-2.922891
12	6	0	-0.841353	-1.564040	-1.522167
13	6	0	1.907534	-4.159733	-0.869469
14	6	0	-1.881705	-4.143954	0.508727
15	7	0	-1.716734	-0.757758	-0.752131
16	6	0	-2.858039	-0.128333	-1.179795
17	8	0	-3.244347	-0.167022	-2.334173
18	6	0	-3.721582	0.634040	-0.096838
19	6	0	-4.888053	-0.317827	0.306338
20	6	0	-5.433915	-1.233311	-0.603052
21	6	0	-6.513948	-2.039712	-0.248632
22	6	0	-7.087822	-1.941139	1.015005
23	6	0	-6.572158	-1.019068	1.921131
24	6	0	-5.486691	-0.219345	1.570543
25	6	0	-2.876430	1.037206	1.140018
26	6	0	-2.435110	2.350977	1.340899
27	6	0	-1.649145	2.691019	2.441879
28	6	0	-1.285156	1.726652	3.375339
29	6	0	-1.721426	0.416140	3.198631
30	6	0	-2.507474	0.078957	2.100060
31	6	0	-4.303303	1.898337	-0.785784
32	6	0	-5.568260	2.388248	-0.451871
33	6	0	-6.057274	3.568223	-1.012348
34	6	0	-5.291244	4.284891	-1.924356
35	6	0	-4.028765	3.807817	-2.270486
36	6	0	-3.543280	2.631338	-1.708510
37	7	0	1.900841	-0.947458	0.746536
38	6	0	2.638726	3.105043	-2.588349

39	6	0	2.871292	-0.118464	1.261410
40	6	0	3.703525	0.646884	0.161773
41	8	0	3.111840	-0.021364	2.447995
42	6	0	4.726525	1.600140	0.829364
43	6	0	6.040530	1.707160	0.364455
44	6	0	6.921584	2.645700	0.902385
45	6	0	6.503920	3.498125	1.917389
46	6	0	5.192387	3.410033	2.381363
47	6	0	4.313592	2.479119	1.840001
48	6	0	4.399034	-0.495620	-0.619928
49	6	0	4.096791	-0.825124	-1.943495
50	6	0	4.726944	-1.899048	-2.576310
51	6	0	5.660112	-2.670465	-1.894336
52	6	0	5.950482	-2.369829	-0.563156
53	6	0	5.325015	-1.299915	0.065247
54	6	0	2.812565	1.564030	-0.711348
55	6	0	1.501411	1.900019	-0.360126
56	6	0	0.766212	2.815937	-1.114681
57	6	0	1.326209	3.416288	-2.235532
58	6	0	3.371961	2.199756	-1.830977
59	1	0	-1.487555	-4.195947	3.183630
60	1	0	0.211101	-2.976155	4.509523
61	1	0	1.798499	-1.438805	3.395853
62	1	0	1.595929	-3.816125	-3.528459
63	1	0	0.028169	-2.308420	-4.713031
64	1	0	-1.536264	-0.887149	-3.437144
65	1	0	2.706505	-3.606523	-0.367257
66	1	0	1.407327	-4.762689	-0.107904
67	1	0	2.376352	-4.833984	-1.587846
68	1	0	-2.587800	-3.477998	0.004575
69	1	0	-1.412261	-4.753216	-0.268389
70	1	0	-2.453764	-4.805122	1.161562
71	1	0	-1.491540	-0.687682	0.231089
72	1	0	-5.025904	-1.306965	-1.601455
73	1	0	-6.909153	-2.743511	-0.972833
74	1	0	-7.928791	-2.568627	1.288033
75	1	0	-7.012606	-0.916723	2.906874
76	1	0	-5.107525	0.490934	2.293636
77	1	0	-2.716494	3.126394	0.642561
78	1	0	-1.327903	3.719163	2.566812
79	1	0	-0.674122	1.990507	4.230817
80	1	0	-1.451024	-0.351812	3.912372
81	1	0	-2.853630	-0.943439	2.006093
82	1	0	-6.191468	1.846658	0.246599
83	1	0	-7.045306	3.919013	-0.735338

84	1	0	-5.672972	5.198472	-2.366109
85	1	0	-3.419666	4.347746	-2.987117
86	1	0	-2.564580	2.278859	-2.007071
87	1	0	1.803253	-0.956390	-0.260197
88	1	0	3.098316	3.577613	-3.449346
89	1	0	6.391435	1.055819	-0.425214
90	1	0	7.935368	2.704577	0.521702
91	1	0	7.187616	4.225770	2.340196
92	1	0	4.848991	4.071596	3.169071
93	1	0	3.300345	2.433676	2.213194
94	1	0	3.367155	-0.248554	-2.496109
95	1	0	4.478408	-2.127001	-3.606688
96	1	0	6.152052	-3.500962	-2.387990
97	1	0	6.665829	-2.970282	-0.012250
98	1	0	5.555993	-1.079326	1.100908
99	1	0	1.034731	1.465704	0.514667
100	1	0	-0.245512	3.057918	-0.811218
101	1	0	0.754459	4.126659	-2.821739
102	1	0	4.400708	1.998130	-2.102933