

SUPPORTING INFORMATION

DETERMINATION OF THE ABSOLUTE CONFIGURATIONS OF NATURAL PRODUCTS VIA DENSITY FUNCTIONAL THEORY CALCULATIONS OF VIBRATIONAL CIRCULAR DICHROISM, ELECTRONIC CIRCULAR DICHROISM, AND OPTICAL ROTATION: THE IRIDODIDS PLUMERICIN AND ISO-PLUMERICIN

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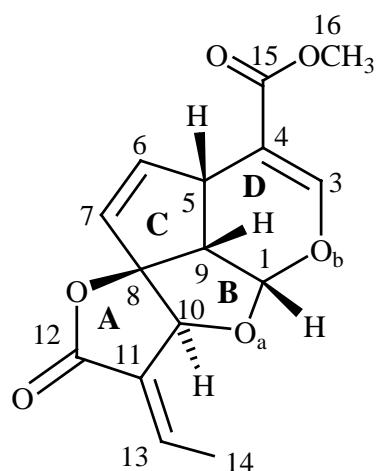
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(1*R*,5*S*,8*S*,9*S*,10*S*)-**1**

B3LYP/6-31G* Plumericin (C₄C₁₅O₁₆) PES scan

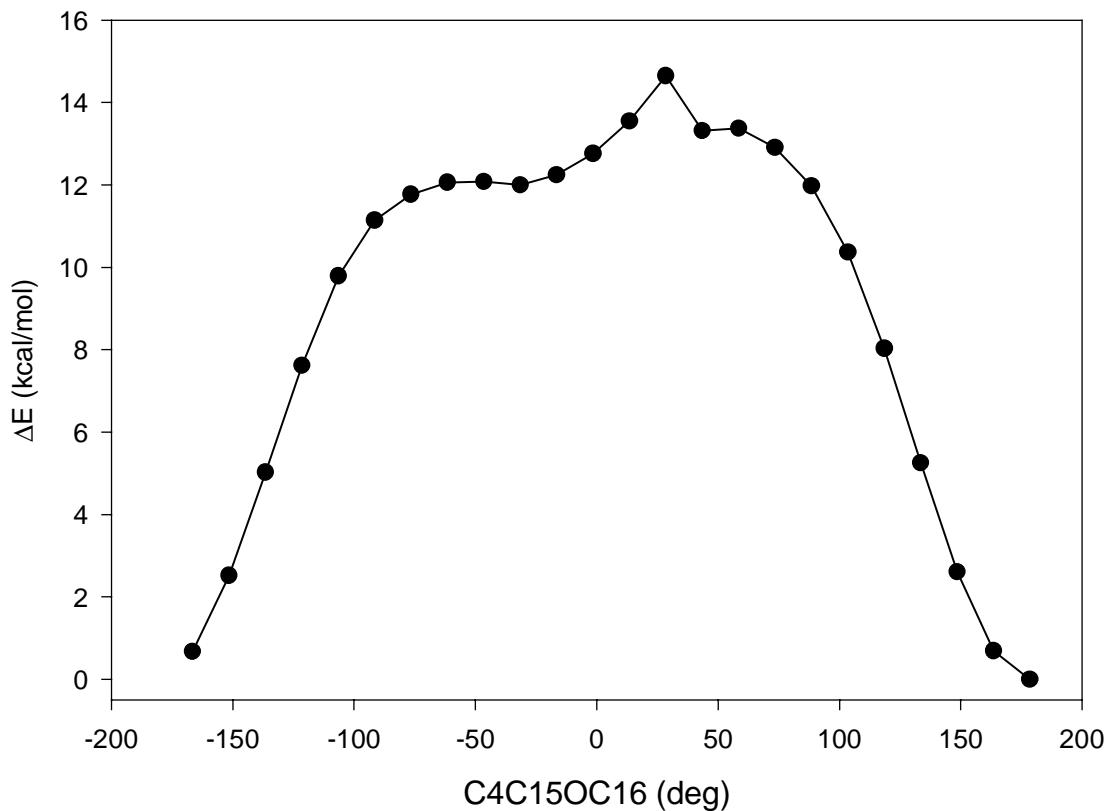
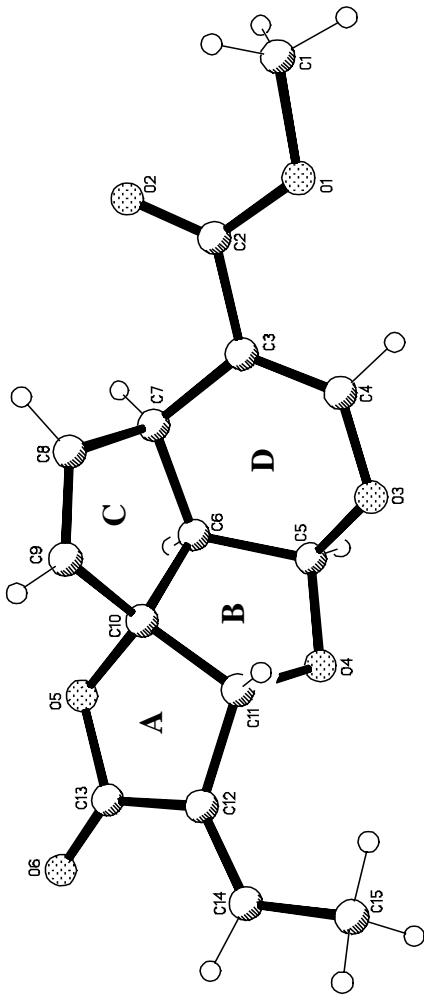


Figure S1. The B3LYP/6-31G* PES scan of **1** with respect to the dihedral angle C₄C₁₅O₁₆. The dihedral angle was varied in 15° steps.

Table S1. Comparison of the “heavy-atom” dihedral angles of the X-ray structure of **1¹⁰** and the MMFF94, B3LYP/6-31G*, B3LYP/TZ2P and B3PW91/TZ2P calculated conformations **a-d** of (IR,5S,8S,9S,10S)-**1**.^a



Plumericin (1) X-ray Structure^b

Ring	Dihedral ^b	MMFF94				B3LYP/6-31G*				B3LYP/TZ2P				B3PW91/TZ2P					
		X-ray		a	b	c	d	a	b	c	d	a	b	c	d	a	b	c	d
		C13 O5	C10 C6	-129.51	-127.64	-127.71	-104.80	-103.91	-124.44	-124.57	-103.53	-102.74	-124.28	-124.38	-104.91	-104.26	-124.58	-124.73	-104.07
A	C13 O5 C10 C9	114.26	117.91	117.86	138.74	139.65	119.14	118.94	138.14	138.87	119.29	119.12	136.98	137.60	118.94	118.70	137.60	138.40	
A	C13 O5 C10 C11	-16.38	-12.91	-13.07	12.84	13.79	-10.75	-10.89	10.46	11.32	-10.42	-10.54	9.39	10.11	-10.78	-10.96	10.16	11.05	
A	C10 O5 C13 O6	-173.69	-174.58	-174.42	174.90	174.47	-176.00	-176.07	176.19	175.85	-176.38	-176.48	176.30	176.04	-176.29	-176.36	176.02	175.68	
A	C10 O5 C13 C12	7.48	5.49	5.58	-5.07	-5.42	4.04	3.86	-3.76	-4.14	3.73	3.54	-3.90	-4.18	3.82	3.67	-4.22	-4.57	
A	O4 C11 C12 C13	95.40	101.68	101.55	126.61	127.38	101.21	100.58	126.02	126.70	101.37	100.78	124.39	125.04	101.02	100.37	125.00	125.78	
A	O4 C11 C12 C14	-83.08	-79.85	-79.94	-52.49	-51.70	-77.20	-78.08	-53.74	-53.07	-78.28	-79.15	-56.22	-55.55	-78.77	-79.72	-55.68	-54.88	
A	C10 C11 C12 C13	-14.67	-11.27	-11.38	11.64	12.52	-10.71	-11.21	10.44	11.16	-10.71	-11.18	8.61	9.27	-11.06	-11.59	9.25	10.07	
A	C10 C11 C12 C14	166.85	167.20	167.13	-167.46	-166.57	170.88	170.14	-169.32	-168.61	169.64	168.89	-172.00	-171.32	169.15	168.33	-171.43	-170.59	
A	C11 C12 C13 O5	5.11	4.22	4.24	-4.76	-5.13	4.73	5.17	-4.81	-5.08	4.89	5.31	-3.47	-3.75	5.10	5.54	-3.74	-4.08	

A	C11 C12 C13 O6	-173.59	-175.71	-175.75	175.28	174.98	-175.23	-174.90	175.25	174.94	-174.99	-174.66	176.31	176.02	-174.78	-174.44	176.01	175.64
A	C14 C12 C13 O5	-176.31	-174.40	-174.41	174.43	174.04	-176.71	-176.05	174.97	174.71	-175.43	-174.75	177.08	176.79	-175.09	-174.39	176.88	176.51
A	C14 C12 C13 O6	4.99	5.67	5.59	-5.53	-5.84	3.33	3.88	-4.97	-5.27	4.69	5.28	-3.13	-3.45	5.03	5.64	-3.38	-3.76
AB	O5 C10 C11 O4	-96.13	-101.24	-101.12	-133.26	-134.46	-103.22	-102.73	-135.18	-136.27	-103.83	-103.37	-133.58	-134.56	-103.41	-102.89	-134.60	-135.77
AB	O5 C10 C11 C12	18.50	14.55	14.71	-14.77	-15.88	12.79	13.19	-12.45	-13.40	12.59	12.96	-10.68	-11.50	13.04	13.47	-11.54	-12.55
AB	C6 C10 C11 O4	22.03	17.09	17.12	-11.82	-12.95	15.40	15.88	-15.23	-16.21	14.86	15.29	-13.77	-14.63	15.38	15.88	-14.60	-15.65
AB	C6 C10 C11 C12	136.66	132.89	132.95	106.68	105.63	131.42	131.81	107.51	106.66	131.28	131.63	109.13	108.42	131.83	132.24	108.47	107.56
AB	C9 C10 C11 O4	140.20	133.64	133.73	103.37	102.33	131.92	132.38	99.43	98.40	131.37	131.78	101.08	100.19	131.57	132.05	99.88	98.78
AB	C9 C10 C11 C12	-105.17	-110.57	-110.45	-138.13	-139.10	-112.06	-111.70	-137.84	-138.73	-112.21	-111.89	-136.02	-136.76	-111.98	-111.59	-137.05	-138.01
B	C11 O4 C5 O3	-83.15	-88.82	-88.76	-157.54	-157.37	-89.80	-89.47	-161.01	-161.29	-90.59	-90.28	-159.17	-159.38	-90.01	-89.73	-160.84	-161.19
B	C11 O4 C5 C6	39.34	37.08	37.15	-27.35	-26.77	34.02	34.34	-34.73	-34.78	33.21	33.52	-32.84	-32.85	33.98	34.27	-34.37	-34.50
B	C5 O4 C11 C10	-38.36	-33.88	-33.96	24.22	24.60	-31.05	-31.57	31.32	31.96	-30.18	-30.66	29.18	29.73	-30.99	-31.51	30.63	31.38
B	C5 O4 C11 C12	-149.52	-144.49	-144.53	-87.52	-87.06	-142.49	-142.89	-82.33	-81.62	-141.96	-142.33	-84.90	-84.32	-142.55	-142.95	-83.24	-82.43
BC	C5 C6 C10 O5	112.46	121.31	121.25	114.66	116.07	117.43	117.13	110.80	111.79	117.48	117.23	110.42	111.34	117.63	117.30	110.57	111.58
BC	C5 C6 C10 C9	-128.49	-121.31	-121.41	-125.72	-124.41	-122.61	-122.81	-126.78	-125.75	-122.45	-122.60	-127.28	-126.37	-122.15	-122.38	-126.82	-125.79
BC	C5 C6 C10 C11	-0.05	4.85	4.86	-4.18	-2.76	3.36	3.07	-4.58	-3.66	3.44	3.19	-4.92	-4.09	3.39	3.07	-4.99	-4.05
BC	C7 C6 C10 O5	-121.97	-114.96	-114.86	-122.71	-121.00	-117.88	-118.02	-126.60	-125.31	-117.79	-117.90	-126.61	-125.41	-117.62	-117.77	-126.65	-125.36
BC	C7 C6 C10 C9	-2.93	2.42	2.47	-3.09	-1.48	2.08	2.04	-4.18	-2.85	2.28	2.27	-4.31	-3.12	2.60	2.55	-4.04	-2.73
BC	C7 C6 C10 C11	125.51	128.59	128.75	118.45	120.17	128.05	127.92	118.03	119.24	128.17	128.06	118.05	119.16	128.15	128.00	117.78	119.01
BD	O3 C5 C6 C7	-24.15	-22.63	-22.73	28.72	27.60	-20.52	-20.62	27.22	26.53	-20.08	-20.20	26.14	25.45	-20.50	-20.57	27.25	26.60
BD	O3 C5 C6 C10	93.54	95.57	95.58	145.29	144.30	97.15	97.16	142.99	142.51	97.66	97.65	142.18	141.70	97.37	97.43	143.21	142.76
BD	O4 C5 C6 C7	-140.94	-143.37	-143.51	-97.71	-99.10	-139.80	-139.90	-92.65	-93.43	-139.48	-139.59	-93.82	-94.58	-140.02	-140.10	-92.78	-93.54
BD	O4 C5 C6 C10	-23.25	-25.16	-25.19	18.86	17.60	-22.13	-22.12	23.12	22.54	-21.73	-21.74	22.21	21.67	-22.15	-22.10	23.17	22.63
C	C3 C7 C8 C9	114.37	122.01	121.70	125.07	125.86	121.26	121.07	124.87	125.75	122.09	121.89	124.84	125.58	121.99	121.77	125.29	126.13
C	C6 C7 C8 C9	-5.65	-0.07	-0.10	0.24	1.27	-0.13	-0.07	0.70	1.77	0.36	0.40	0.48	1.39	0.52	0.54	0.95	1.98
C	C7 C8 C9 C10	4.04	1.70	1.77	-2.35	-2.36	1.55	1.46	-3.62	-3.85	1.17	1.12	-3.49	-3.64	1.21	1.15	-3.79	-3.99
C	C8 C9 C10 O5	120.20	115.92	115.77	124.67	123.66	118.71	118.83	128.06	127.43	118.86	118.94	127.75	127.13	118.76	118.88	128.06	127.42
C	C8 C9 C10 C6	-0.55	-2.56	-2.64	3.40	2.38	-2.27	-2.19	4.90	4.17	-2.17	-2.13	4.90	4.22	-2.39	-2.32	4.91	4.18
C	C8 C9 C10 C11	-118.81	-119.52	-119.62	-112.81	-113.93	-118.94	-118.81	-109.40	-110.09	-118.97	-118.87	-109.88	-110.53	-118.66	-109.37	-110.05	
CD	C5 C6 C7 C3	2.26	-6.31	-6.02	-8.75	-9.95	-5.63	-5.56	-8.73	-10.25	-6.44	-6.35	-8.37	-9.67	-6.37	-6.22	-9.12	-10.61
CD	C5 C6 C7 C8	120.68	114.36	114.48	116.28	114.88	114.48	114.56	116.63	115.31	114.26	114.34	117.21	116.08	113.97	114.11	116.51	115.23
CD	C10 C6 C7 C3	-113.53	-122.19	-122.03	-123.19	-124.57	-121.37	-121.39	-123.08	-124.70	-122.36	-122.35	-123.09	-124.51	-122.29	-122.25	-123.57	-125.17
CD	C10 C6 C7 C8	4.89	-1.52	-1.53	1.85	0.25	-1.26	-1.27	2.29	0.86	-1.66	-1.66	2.49	1.24	-1.95	-1.92	2.07	0.68

D	C2	C3	C4	O3	-176.84	179.92	-179.98	175.75	176.62	-178.96	180.00	176.29	179.54	-179.05	175.84	179.70	175.84	-179.72	179.53	175.79	175.86
D	C7	C3	C4	O3	-3.25	-2.52	-2.28	2.86	1.52	-5.49	-5.67	2.13	1.35	-4.87	-5.15	2.19	1.51	-5.19	-5.48	2.42	1.68
D	C5	O3	C4	C3	-21.77	-28.81	-28.84	18.03	16.81	-24.67	-24.50	17.69	15.92	-25.71	-25.42	16.96	15.35	-25.63	-25.22	16.91	15.19
D	C4	O3	C5	C6	34.21	40.29	40.18	-33.37	-30.93	36.44	36.35	-31.87	-29.40	36.92	36.80	-30.63	-28.35	37.23	36.96	-31.27	-28.87
D	C4	O3	C5	O4	151.10	159.39	159.25	91.70	94.43	155.44	155.28	87.67	90.32	156.01	155.82	89.11	91.52	156.37	156.03	88.49	91.05
D	C2	C3	C7	C6	-174.06	-162.68	-163.12	-179.82	-179.11	-166.54	-166.24	-179.98	-177.65	-164.98	-164.93	-179.40	-177.48	-164.90	-164.97	-178.92	-176.89
D	C2	C3	C7	C8	71.93	81.62	81.41	61.14	61.94	78.21	78.71	61.02	63.51	79.41	79.67	61.47	63.55	79.69	79.83	61.84	64.04
D	C4	C3	C7	C6	12.17	19.65	19.28	-6.73	-4.27	19.70	19.72	-5.62	-3.29	20.12	20.17	-5.56	-3.49	20.35	20.31	-5.35	-3.08
D	C4	C3	C7	C8	-101.83	-96.05	-96.19	-125.76	-123.22	-95.56	-95.33	-124.63	-122.12	-95.48	-95.23	-124.69	-122.46	-95.06	-94.89	-124.59	-122.15
X	C1	O1	C2	O2	0.96	-0.39	0.30	0.24	0.32	-1.33	-0.49	0.85	-0.42	-1.03	-0.43	1.17	-0.39	-1.02	-0.40	1.29	-0.35
X	C1	O1	C2	C3	179.41	-179.84	179.96	179.19	179.21	178.52	179.78	-178.95	178.88	178.82	179.75	-178.55	178.91	178.89	179.71	-178.43	178.94
X	O1	C2	C3	C4	0.54	-3.21	179.00	20.15	-158.24	-7.93	173.99	6.66	-172.43	-6.20	175.20	8.69	-170.47	-6.09	175.52	9.34	-170.33
X	O1	C2	C3	C7	-173.35	179.14	1.31	-166.68	16.88	178.36	-0.27	-178.90	2.27	178.95	0.13	-177.39	3.86	179.20	0.60	-176.99	3.84
X	O2	C2	C3	C4	178.99	177.33	-1.34	-160.88	20.66	171.92	-5.73	-173.14	6.85	173.66	-4.61	-171.04	8.80	173.81	-4.36	-170.38	8.93
X	O2	C2	C3	C7	5.10	-0.32	-179.02	12.29	-164.22	-1.79	-179.99	1.30	-178.46	-1.20	-179.69	2.89	-176.87	-0.90	-179.28	3.29	-176.90
Y	C11	C12	C14	C15	-0.50	1.82	1.83	-1.50	-1.60	-0.12	-0.16	0.35	0.32	0.46	0.45	0.17	0.22	0.51	0.52	0.18	0.21
Y	C13	C12	C14	C15	-178.75	-179.89	-179.84	179.51	179.43	-178.33	-178.65	-179.38	-179.42	-179.15	-179.47	179.49	179.56	-179.26	-179.58	179.42	179.48

^a All angles in degrees.^b Note that the atom numbering used in this Table differs from that in Figure 1 of the paper.

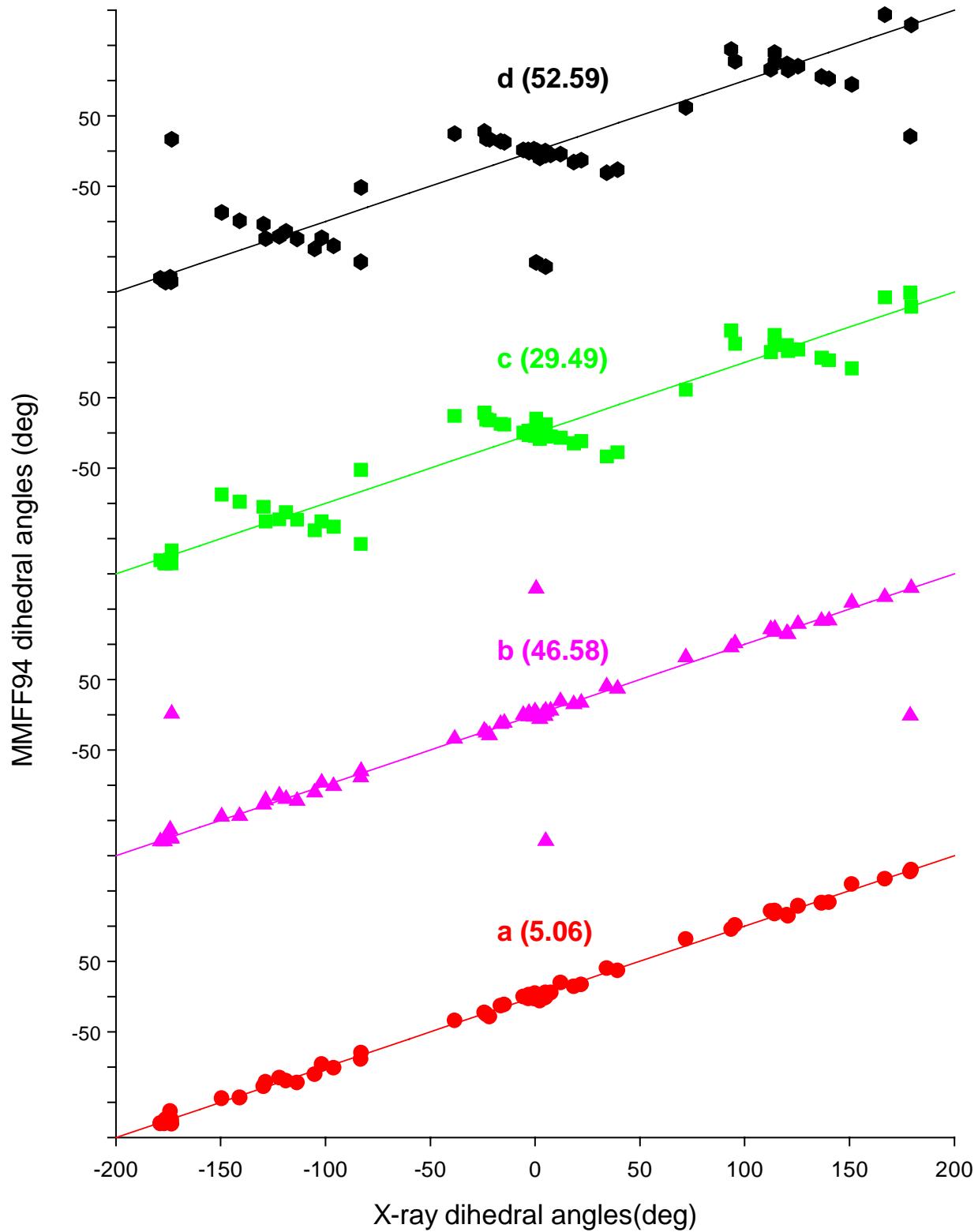


Figure S2a. Comparison of dihedral angles of the X-ray structure of **1** and MMFF94 calculated dihedral angles for the conformations **a-d** of **1**. The numbers in parentheses are the RMS deviations between the calculated and X-ray dihedral angles.

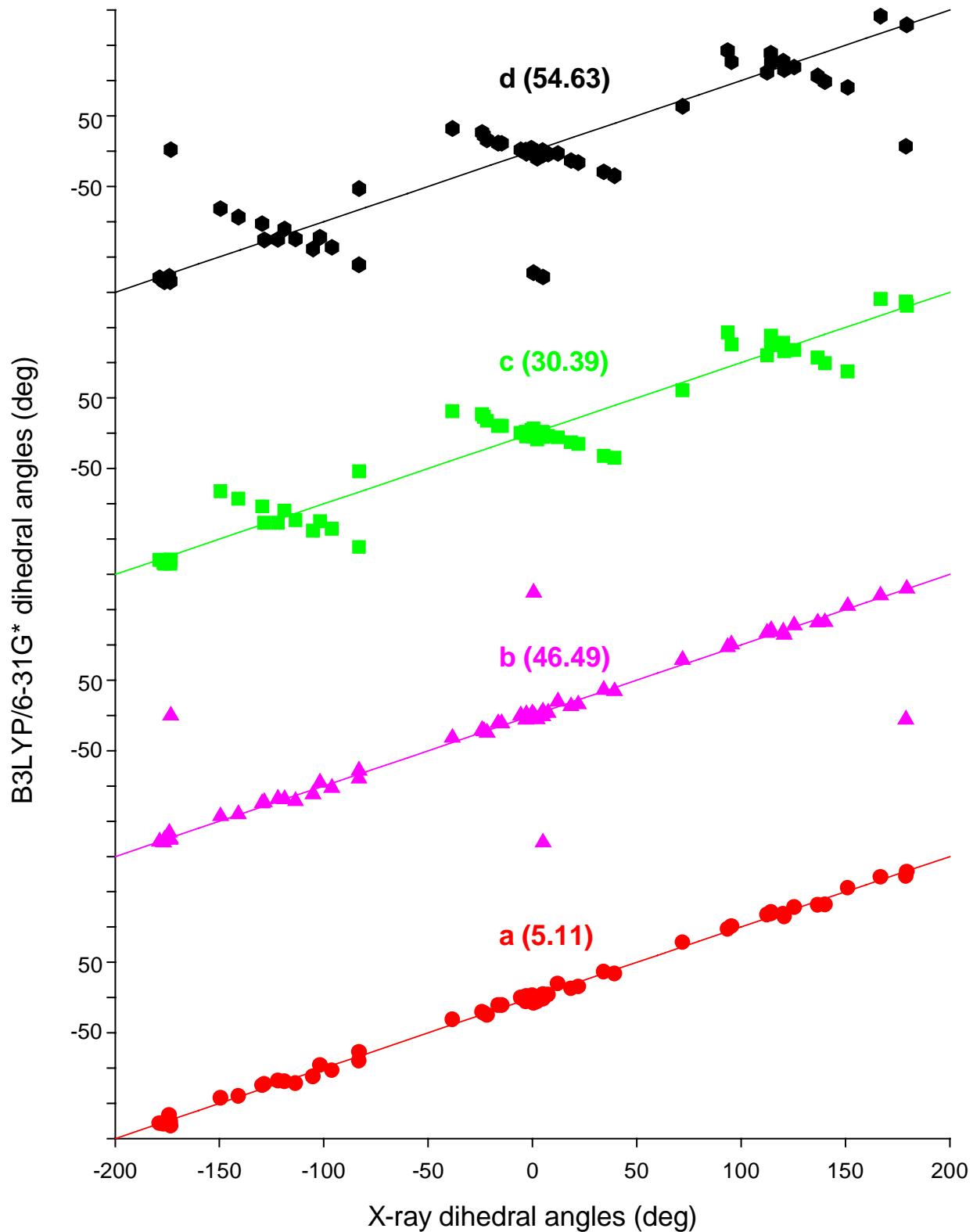


Figure S2b. Comparison of dihedral angles of the X-ray structure of **1** and B3LYP/6-31G* calculated dihedral angles for the conformations **a-d** of **1**. The numbers in parentheses are the RMS deviations between the calculated and X-ray dihedral angles.

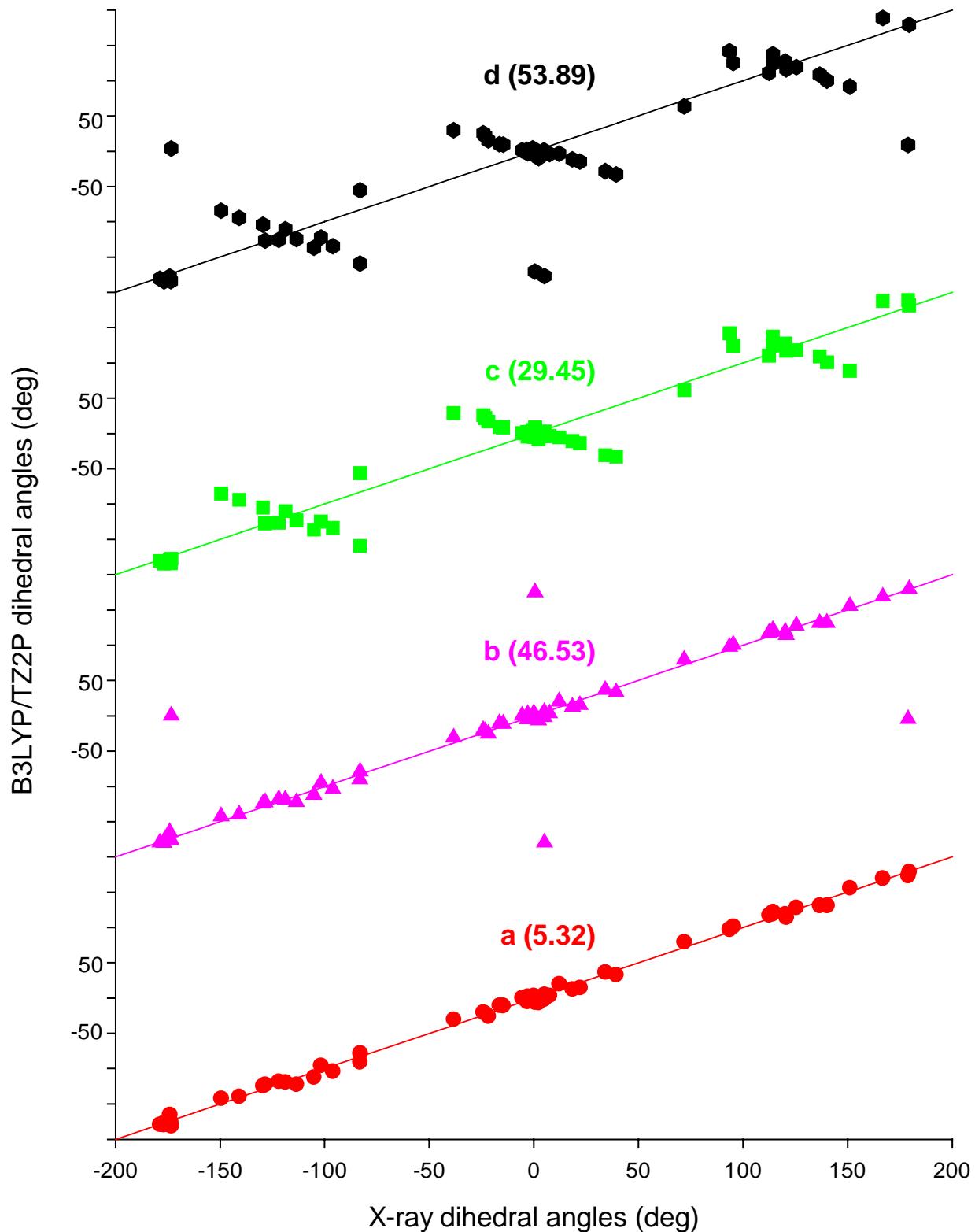
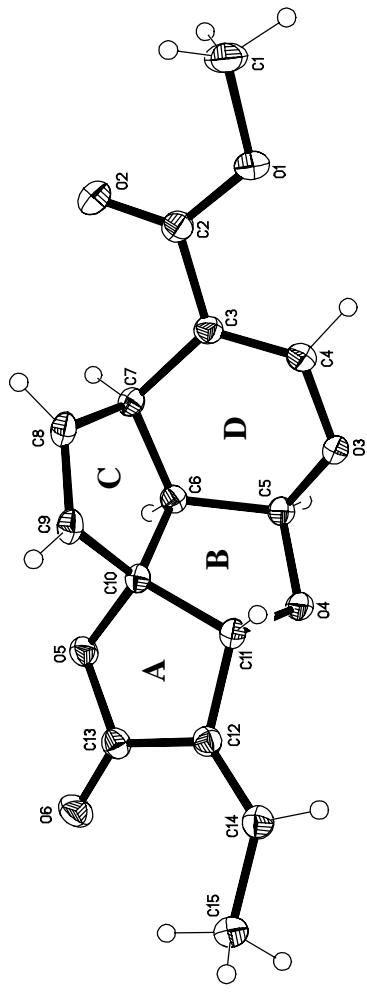


Figure S2c. Comparison of dihedral angles of the X-ray structure of **1** and B3LYP/TZ2P calculated dihedral angles for the conformations **a-d** of **1**. The numbers in parentheses are the RMS deviations between the calculated and X-ray dihedral angles.

Table S2. Comparison of the “heavy-atom” dihedral angles of the X-ray structure of **2¹⁰** and the MMFF94, B3LYP/6-31G*, B3LYP/TZ2P and B3PW91/TZ2P calculated conformations **a-d** of (1R,5S,8S,9S,10S)-**2^a**.



Isoplumericin (**2**) X-ray Structure^b

Ring	Dihedral ^b	MMFF94				B3LYP/6-31G*				B3LYP/TZ2P				B3PW91/TZ2P				
		X-ray	a	b	c	d	a	b	c	d	a	b	c	d	a	b	c	d
A	C13 O5 C10 C6	-128.96	-127.37	-127.46	-104.39	-103.51	-124.63	-124.67	-103.12	-102.73	-124.29	-124.42	-104.51	-104.04	-124.61	-124.69	-103.56	-103.15
A	C13 O5 C10 C9	114.91	117.97	117.99	138.86	139.77	118.75	118.75	138.42	138.76	119.09	119.00	137.29	137.68	118.70	118.66	138.00	138.33
A	C13 O5 C10 C11	-15.85	-12.94	-13.02	13.33	14.20	-11.26	-11.24	10.74	11.24	-10.72	-10.80	9.66	10.25	-11.13	-11.15	10.53	11.07
A	C10 O5 C13 O6	-174.06	-176.34	-176.21	177.52	177.26	-177.13	-177.10	176.95	176.89	-177.69	-177.58	177.19	177.14	-177.57	-177.50	177.03	176.96
A	C10 O5 C13 C12	7.00	4.18	4.27	-2.83	-3.16	2.57	2.57	-2.97	-3.02	2.18	2.26	-2.83	-2.87	2.33	2.36	-3.00	-3.07
A	O4 C11 C12 C13	95.84	99.74	99.74	130.70	131.48	97.66	97.64	127.82	128.46	98.08	98.01	126.62	127.38	97.74	97.71	127.58	128.23
A	O4 C11 C12 C14	-85.65	-81.60	-81.72	-47.73	-46.93	-82.20	-82.30	-50.06	-49.26	-82.84	-82.99	-51.99	-51.04	-83.22	-83.41	-50.82	-49.98
A	C10 C11 C12 C13	-14.45	-13.35	-13.33	15.77	16.57	-13.85	-13.81	12.08	12.77	-13.64	-13.64	10.67	11.50	-13.98	-13.96	11.69	12.40
A	C10 C11 C12 C14	164.06	165.31	165.21	-162.66	-161.84	166.29	166.25	-165.80	-164.95	165.44	165.36	-167.94	-166.93	165.06	164.93	-166.71	-165.82
A	C11 C12 C13 O5	5.31	6.37	6.30	-8.84	-9.17	7.64	7.62	-6.34	-6.78	7.70	7.66	-5.45	-5.98	7.87	7.84	-6.06	-6.50
A	C11 C12 C13 O6	-173.51	-173.10	-173.19	170.80	170.39	-172.69	-172.75	173.75	173.32	-172.44	-172.52	174.52	174.00	-172.24	-172.32	173.91	173.47

A	C14 C12 C13 O5	-173.21	-172.25	-172.19	169.55	169.21	-172.50	-172.44	171.51	170.91	-171.36	-171.33	173.13	172.42	-171.16	-171.03	172.31	171.70
A	C14 C12 C13 O6	7.97	8.29	8.31	-10.81	-11.24	7.17	7.19	-8.40	-8.99	8.49	8.49	-6.90	-7.59	8.73	8.81	-7.72	-8.33
AB	O5 C10 C11 O4	-96.88	-100.13	-100.08	-136.09	-137.17	-100.71	-100.74	-135.95	-136.79	-101.56	-101.51	-134.75	-135.72	-101.10	-101.13	-136.00	-136.86
AB	O5 C10 C11 C12	18.07	15.91	15.95	-17.71	-18.73	15.06	15.03	-13.62	-14.34	14.61	14.66	-12.11	-12.96	15.08	15.07	-13.25	-14.01
AB	C6 C10 C11 O4	21.05	17.91	17.95	-14.17	-15.21	17.38	17.41	-15.86	-16.57	16.64	16.76	-14.78	-15.57	17.19	17.23	-15.81	-16.50
AB	C6 C10 C11 C12	136.00	133.96	133.98	104.21	103.23	133.15	133.18	106.47	105.88	132.81	132.92	107.87	107.19	133.37	133.43	106.94	106.35
AB	C9 C10 C11 O4	139.34	134.59	134.68	101.06	100.03	134.21	134.23	98.89	98.16	133.41	133.52	100.16	99.32	133.65	133.68	98.76	98.02
AB	C9 C10 C11 C12	-105.70	-109.37	-109.29	-140.56	-141.53	-110.02	-110.00	-138.78	-139.40	-110.42	-110.31	-137.19	-137.93	-110.17	-110.12	-138.49	-139.13
B	C11 O4 C5 O3	-83.11	-88.55	-88.47	-158.25	-157.73	-88.68	-88.53	-161.14	-161.29	-89.68	-89.34	-159.48	-159.82	-89.16	-88.91	-161.23	-161.44
B	C11 O4 C5 C6	39.18	37.32	37.36	-27.49	-26.61	35.06	35.19	-34.82	-34.77	34.08	34.36	-33.08	-33.24	34.80	35.01	-34.66	-34.69
B	C5 O4 C11 C10	-37.66	-34.57	-34.62	25.80	25.93	-32.95	-33.05	31.80	32.20	-31.86	-32.11	29.99	30.59	-32.66	-32.82	31.60	32.05
B	C5 O4 C11 C12	-148.90	-145.60	-145.62	-85.99	-85.77	-144.47	-144.52	-82.00	-81.53	-143.69	-143.88	-84.27	-83.59	-144.27	-144.38	-82.40	-81.87
BC	C5 C6 C10 O5	113.44	120.23	120.25	116.61	118.06	115.30	115.42	110.98	111.79	115.54	115.66	110.92	111.71	115.60	115.78	111.18	111.96
BC	C5 C6 C10 C9	-127.65	-122.06	-122.22	-123.63	-122.24	-124.32	-124.27	-126.56	-125.73	-124.00	-123.96	-126.80	-125.97	-123.77	-123.68	-126.23	-125.40
BC	C5 C6 C10 C11	0.88	4.24	4.23	-2.07	-0.60	1.98	2.01	-4.09	-3.39	2.16	2.20	-4.15	-3.48	2.05	2.13	-4.08	-3.43
BC	C7 C6 C10 O5	-121.06	-115.88	-115.72	-120.80	-118.95	-119.75	-119.48	-126.48	-125.40	-119.48	-119.24	-126.15	-125.16	-119.37	-119.07	-126.09	-125.09
BC	C7 C6 C10 C9	-2.15	1.83	1.80	-1.04	0.75	0.64	0.83	-4.01	-2.91	0.99	1.14	-3.88	-2.84	1.26	1.47	-3.50	-2.45
BC	C7 C6 C10 C11	126.38	128.13	128.25	120.52	122.39	126.93	127.12	118.46	119.43	127.14	127.30	118.78	119.65	127.08	127.28	118.65	119.53
BD	O3 C5 C6 C7	-24.70	-22.60	-22.64	28.03	26.55	-20.36	-20.54	27.13	26.56	-19.89	-20.18	25.94	25.53	-20.23	-20.50	27.04	26.56
BD	O3 C5 C6 C10	93.05	95.67	95.70	144.54	143.30	97.35	97.29	142.81	142.43	97.91	97.72	141.90	141.65	97.69	97.54	142.92	142.61
BD	O4 C5 C6 C7	-141.37	-143.20	-143.27	-98.87	-100.57	-139.55	-139.76	-92.80	-93.49	-139.20	-139.49	-94.09	-94.60	-139.68	-139.96	-93.09	-93.69
BD	O4 C5 C6 C10	-23.63	-24.94	-24.93	17.64	16.18	-21.84	-21.92	22.88	22.38	-21.41	-21.59	21.87	21.52	-21.75	-21.92	22.79	22.37
C	C3 C7 C8 C9	114.55	121.72	121.47	126.01	126.72	120.74	120.48	124.88	125.57	121.60	121.29	124.94	125.60	121.49	121.22	125.44	126.10
C	C6 C7 C8 C9	-5.51	-0.35	-0.41	1.22	2.33	-0.66	-0.65	0.73	1.61	-0.15	-0.19	0.60	1.43	-0.01	0.00	1.12	1.97
C	C7 C8 C9 C10	4.43	1.61	1.65	-2.01	-1.97	1.14	1.26	-3.54	-3.73	0.83	0.98	-3.32	-3.49	0.87	0.99	-3.61	-3.79
C	C8 C9 C10 C5	119.18	116.43	116.31	123.79	122.63	119.81	119.61	128.19	127.68	119.84	119.65	127.64	127.22	119.78	119.56	127.92	127.48
C	C8 C9 C10 C6	-1.28	-2.13	-2.14	1.89	0.71	-1.10	-1.29	4.75	4.14	-1.13	-1.32	4.52	3.95	-1.33	-1.54	4.45	3.87
C	C8 C9 C10 C11	-119.63	-119.14	-119.23	-114.34	-115.53	-118.08	-118.29	-109.62	-110.22	-118.19	-118.39	-110.31	-110.83	-117.99	-118.21	-109.88	-110.41
CD	C5 C6 C7 C3	1.62	-5.68	-5.52	-10.44	-11.49	-4.61	-4.62	-8.96	-10.19	-5.47	-5.42	-8.75	-9.96	-5.35	-5.34	-9.61	-10.83
CD	C5 C6 C7 C8	120.25	115.03	115.15	114.37	112.94	115.66	115.62	116.37	115.28	115.37	115.36	116.75	115.70	115.13	115.07	115.94	114.88
CD	C10 C6 C7 C3	-114.31	-121.69	-121.59	-124.81	-126.18	-120.32	-120.43	-123.16	-124.49	-121.39	-121.41	-124.62	-121.28	-121.35	-123.92	-125.22	
CD	C10 C6 C7 C8	4.33	-0.98	-0.93	0.00	-1.76	-0.05	-0.18	2.17	0.99	-0.55	-0.63	2.15	1.05	-0.80	-0.94	1.63	0.50

D	C2	C3	C4	O3	-176.50	179.81	179.95	176.02	176.90	-179.05	179.93	176.19	176.02	-179.55	179.70	175.77	175.85	-179.71	179.53	175.71	175.83
D	C7	C3	C4	O3	-3.52	-2.44	-2.30	2.51	1.38	-5.16	-5.36	1.95	1.40	-4.54	-4.88	1.94	1.50	-4.86	-5.22	2.12	1.64
D	C5	O3	C4	C3	-22.84	-28.19	-28.23	15.76	14.11	-23.67	-23.68	17.51	15.99	-24.73	-24.66	16.54	15.11	-24.54	-24.46	16.42	14.93
D	C4	O3	C5	C6	35.65	39.61	39.55	-30.68	-27.76	35.18	35.33	-31.57	-29.49	35.67	35.87	-29.99	-28.16	35.82	36.01	-30.54	-28.60
D	C4	O3	C5	O4	152.21	158.57	158.48	94.84	98.01	153.98	154.09	88.05	90.29	154.60	154.72	89.79	91.75	154.81	154.94	89.31	91.40
D	C2	C3	C7	C6	-173.56	-163.21	-163.64	-178.11	-177.29	-167.48	-167.03	-179.68	-177.68	-165.96	-165.77	-178.95	-177.22	-165.99	-165.79	-178.37	-176.63
D	C2	C3	C7	C8	72.33	81.11	80.76	62.89	64.02	77.20	77.89	61.32	63.52	78.37	78.82	61.94	63.83	78.53	79.00	62.43	64.34
D	C4	C3	C7	C6	13.27	18.92	18.72	-4.39	-2.00	18.36	18.53	-5.26	-3.38	18.82	19.04	-4.92	-3.20	18.94	19.21	-4.59	-2.80
D	C4	C3	C7	C8	-100.83	-96.75	-96.88	-123.39	-120.69	-96.96	-96.55	-124.25	-122.19	-96.85	-96.37	-124.03	-122.15	-96.53	-96.00	-123.79	-121.84
X	C1	O1	C2	O2	0.21	-0.33	0.33	0.18	0.37	-1.32	-0.48	0.84	-0.50	-1.06	-0.41	1.20	-0.51	-1.06	-0.39	1.26	-0.50
X	C1	O1	C2	C3	178.57	-179.86	179.95	179.22	179.28	178.57	179.75	-178.90	178.76	178.82	179.75	-178.51	178.76	178.87	179.72	-178.43	178.75
X	O1	C2	C3	C4	-0.25	-2.84	179.61	18.62	-160.33	-7.76	174.46	6.35	-172.32	-5.99	175.47	8.48	-170.62	-5.92	175.81	8.96	-170.45
X	O1	C2	C3	C7	-173.57	179.32	1.88	-167.58	15.23	178.12	-0.19	-179.14	2.30	178.82	0.11	-177.41	3.74	179.04	0.63	-177.16	3.73
X	O2	C2	C3	C4	178.10	177.61	-0.76	-162.31	18.60	172.14	-5.31	-173.39	6.91	173.88	-4.36	-171.23	8.62	174.01	-4.08	-170.73	8.78
X	O2	C2	C3	C7	4.79	-0.23	-178.50	11.48	-165.85	-1.99	-179.95	1.12	-178.47	-1.31	-179.73	2.88	-177.02	-1.03	-179.26	3.14	-177.04
Y	C11	C12	C14	C15	-179.86	-178.42	-178.43	178.07	177.99	178.74	178.80	178.82	178.69	179.19	179.26	178.88	178.75	179.27	179.41	178.83	178.67
Y	C13	C12	C14	C15	-1.64	-0.03	-0.19	-0.03	-0.09	-1.09	-1.13	1.34	1.39	-1.91	-1.93	0.53	0.62	-1.87	-1.93	0.73	0.79

^a All angles in degrees.^b Note that the atom numbering used in this Table differs from that in Figure 3 of the paper.

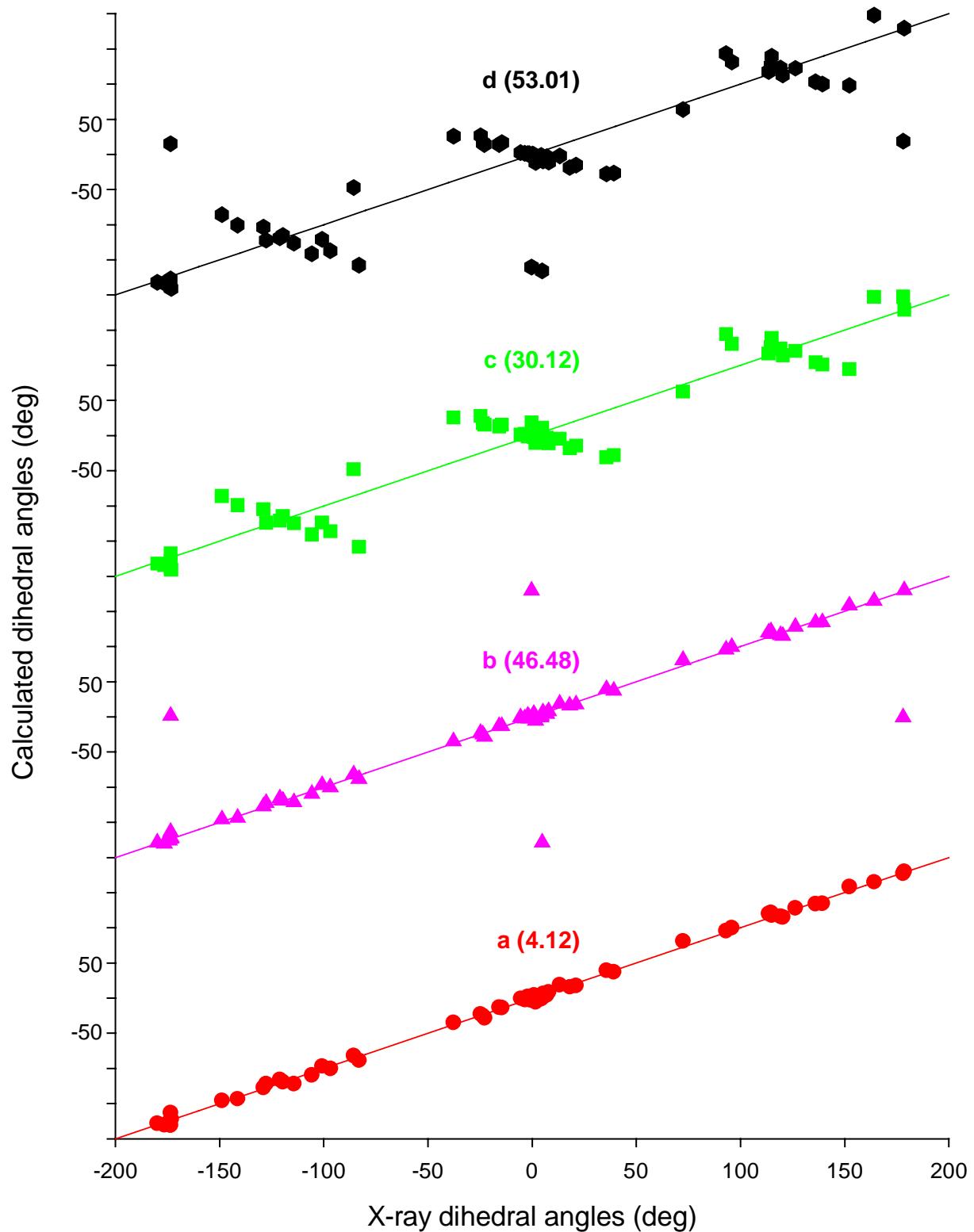


Figure S3a. Comparison of dihedral angles of the X-ray structure of **2** and MMFF94 calculated dihedral angles for the conformations **a-d** of **2**. The numbers in parentheses are the RMS deviations between the calculated and X-ray dihedral angles.

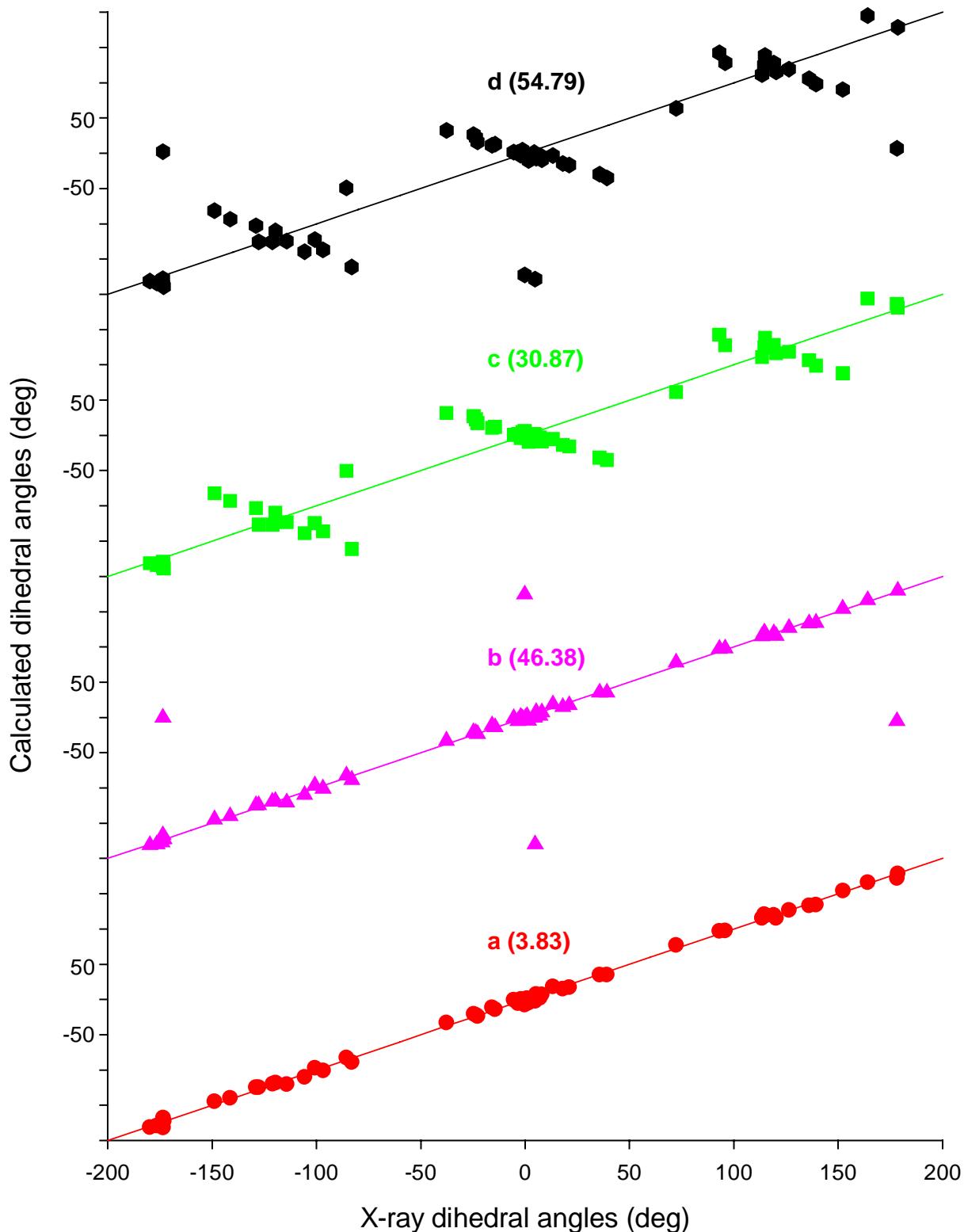


Figure S3b. Comparison of dihedral angles of the X-ray structure of **2** and B3LYP/6-31G* calculated dihedral angles for the conformations **a-d** of **2**. The numbers in parentheses are the RMS deviations between the calculated and X-ray dihedral angles.

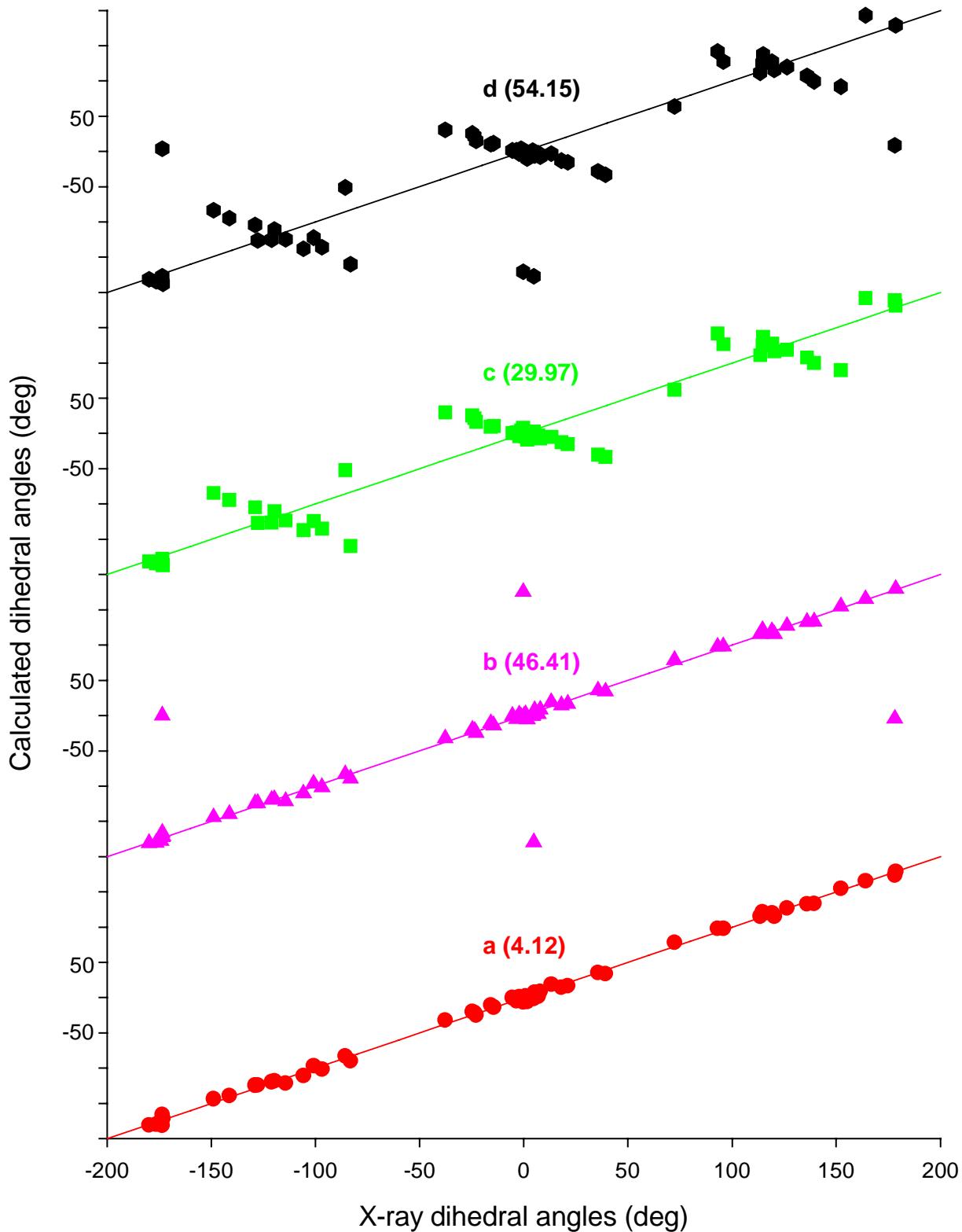


Figure S3c. Comparison of dihedral angles of the X-ray structure of **2** and B3LYP/TZ2P calculated dihedral angles for the conformations **a-d** of **2**. The numbers in parentheses are the RMS deviations between the calculated and X-ray dihedral angles.

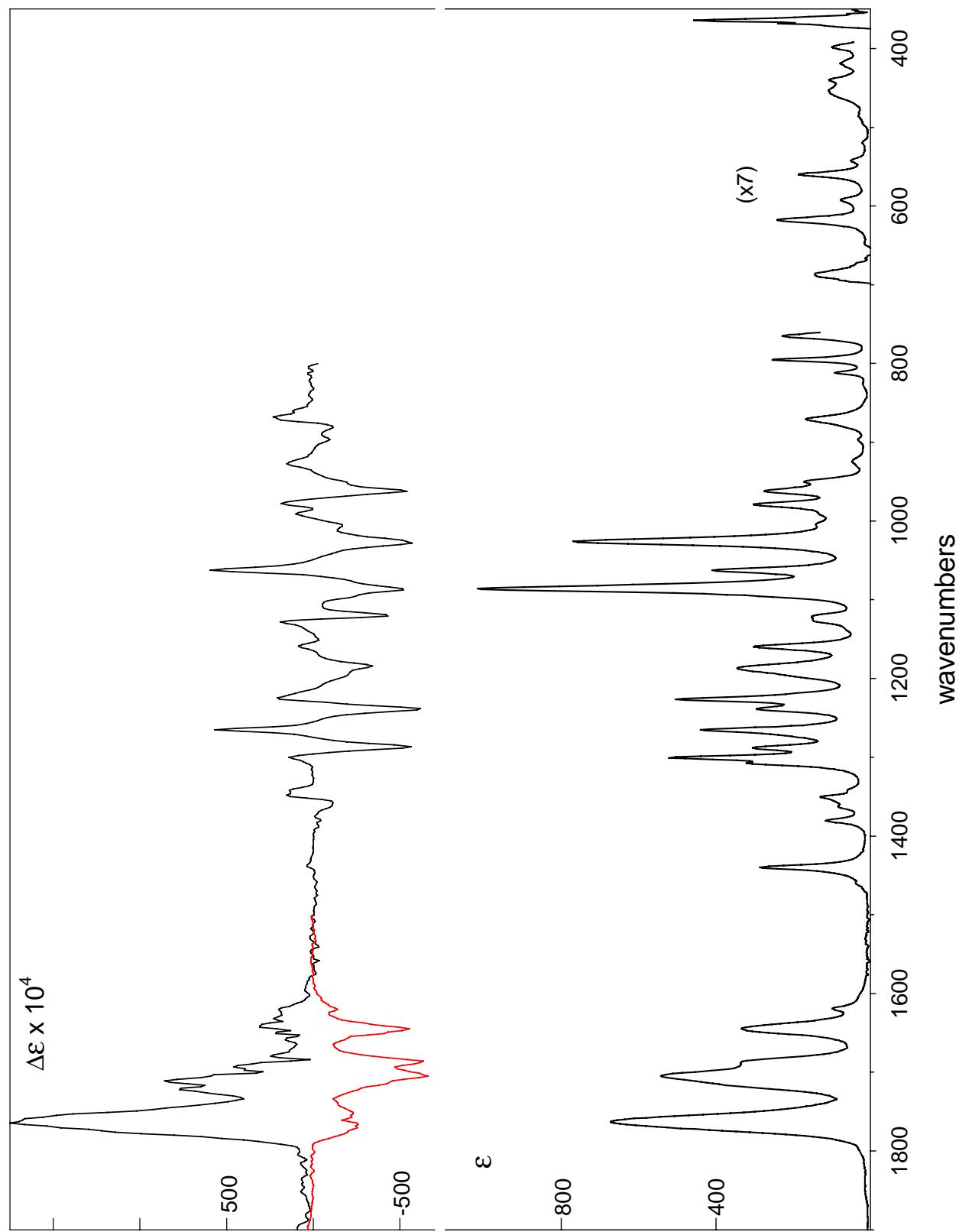


Figure S4. Experimental IR and VCD spectra of (+)-1. The IR spectrum is from Figure 6 of the paper for the range 800 –1500 cm⁻¹. The VCD spectrum above 1500 cm⁻¹ was measured in CDCl₃ solution, 109 μ pathlength. PEM center frequency settings: 1200 cm⁻¹ (black) and 1800 cm⁻¹ (red).

Table S3. Experimental and calculated frequencies (v), dipole strengths (D) and rotational strengths (R) of **1**.^a

v	D	γ	v	R	γ	mode	B3PW91/TZ2P			B3LYP/TZ2P				
							v	D	R	B3PW91/TZ2P				
								D (%) ^c	R (%) ^c	v	D (%) ^c	R (%) ^c		
364.02	132.33	2.75	1d 18	357.02	131.49	24.50	1.37	0.25	357.61	136.44	26.02	1.16	0.22	
			1e 18	358.11	53.24	17.47	2.36	0.78	358.66	54.68	17.98	2.22	0.73	
			1a 18	365.07	120.74	0.13	{	83.18	0.09	365.4	122.61	0.73	86.66	0.52
			1b 18	365.17	152.48	4.20	{	39.08	1.08	365.43	157.19	5.13	38.37	1.25
			1d 19	383.66	3.15	-10.77	0.03	-0.11	384	3.57	-10.62	0.03	-0.09	
			1c 19	386.42	73.35	-18.49	3.26	-0.82	386.65	74.11	-18.15	3.01	-0.74	
			1b 19	398.11	15.13	21.37	{	3.88	5.48	397.47	15.62	22.41	3.81	5.47
			1a 19	400.55	23.23	14.17	{	16.00	9.76	400.02	24.57	15.78	17.37	11.15
			1b 20	418.71	62.15	-18.68	{	15.93	-4.79	417.17	61.63	-19.57	15.04	-4.78
			1a 20	421.94	36.18	-14.28	{	24.92	-9.84	419.75	39.61	-14.46	28.00	-10.22
			1c 20	424.94	5.79	4.67	0.26	0.21	422.69	6.07	4.78	0.25	0.19	
			1d 20	426.69	22.11	3.45	0.23	0.04	426.49	20.07	5.52	0.17	0.05	
			1c 21	440.69	6.78	-1.63	0.30	-0.07	441.06	4.82	-0.8	0.20	-0.03	
			1b 21	445.55	5.55	0.81	{	1.42	0.21	445.01	7.29	1.45	1.78	0.35
			1d 21	446.07	87.23	4.82	{	0.91	0.05	444.16	88.83	3.3	0.76	0.03
			1a 21	447.95	13.88	9.03	{	9.56	6.22	448.02	12.99	8.41	9.18	5.94
			1d 22	464.25	24.97	-10.98	{	0.26	-0.11	463.47	23.89	-11.99	0.20	-0.10
			1a 22	466.45	83.92	6.54	{	57.81	4.51	465.4	89.5	6.39	63.26	4.52
			1b 22	468.68	157.18	33.26	{	40.29	8.52	466.75	159.32	32.68	38.89	7.98
			1c 22	469.19	16.99	-18.10	{	0.75	-0.80	468.49	17.35	-17.81	0.70	-0.72
			1a 23	489.87	2.23	5.71	{	1.54	3.93	488.46	2.7	6.35	1.91	4.49
			1d 23	492.81	6.32	-7.01	{	0.07	-0.07	492.32	4.71	-5.54	0.04	-0.05
			1b 23	493.92	32.27	0.31	{	8.27	0.08	492.67	30.6	-0.61	7.47	-0.15
			1c 23	502.83	43.49	1.61	{	1.93	0.07	501.95	47.22	3.07	1.92	0.12

1d	31	731.39	86.57	-1.73	0.90	-0.02	728.62	87.49	-6.44	0.74	-0.05
1e	31	731.88	81.35	-3.72	3.61	-0.17	729.12	81.1	-7.56	3.29	-0.31
1a	31	739.57	70.73	-0.54	48.73	-0.37	735.75	72.78	-5.02	51.44	-3.55
1b	31	739.97	66.01	-2.98	16.92	-0.76	736.18	68.02	-7.93	16.60	-1.94
1a	32	752.46	91.23	-4.01	62.85	-2.76	748	116.06	-0.66	82.03	-0.47
1b	32	752.64	83.84	-6.76	21.49	-1.73	748.44	109.3	-3.6	26.68	-0.88
1d	32	770.14	100.65	32.18	1.05	0.33	768.24	102.97	32.47	0.88	0.28
1e	32	770.98	87.60	12.33	3.89	0.55	769.4	85.32	12.18	3.46	0.49
1b	33	777.66	135.06	-4.90	{ 34.62	-1.26	773.95	128.85	-11.68	31.45	-2.85
1a	33	779.40	118.85	-10.91		81.88	-7.52	776.29	119.82	-21.09	84.69
1d	33	779.91	40.09	16.57	{ 0.42	0.17	775.45	18.54	24.61	0.16	0.21
1b	34	780.06	116.67	58.61		29.90	15.02	777.76	133.56	60.04	32.60
1e	33	782.84	34.98	35.15	{ 1.55	1.56	777.47	16.34	36.28	0.66	1.47
1a	34	783.75	101.09	56.06		69.64	38.62	781.35	109.01	54.72	77.05
1d	34	787.58	20.00	-24.77	0.21	-0.26	782.89	40.32	-29.23	0.34	-0.25
1e	34	788.91	23.29	-22.72	1.03	-1.01	785.34	40.79	-22.04	1.66	-0.89
1b	35	808.03	171.51	-105.59	{ 43.96	-27.06	804.09	157.99	-110.26	38.57	-26.91
1d	35	808.28	16.75	0.77		0.17	0.01	804.59	20.52	-4.49	0.17
1a	35	809.13	259.43	-83.04	{ 178.72	-57.21	804.82	255.99	-83.09	180.93	-58.73
1e	35	810.64	22.59	0.92		1.00	0.04	806.58	27.4	-4.8	1.11
1b	36	824.42	34.56	2.66	{ 8.86	0.68	819.09	37.88	3.67	9.25	0.90
1d	36	824.88	170.17	-49.27		1.77	-0.51	824.1	158.54	-39.7	1.35
1a	36	824.93	31.78	4.12	{ 21.89	2.84	819.89	39.77	9.78	28.11	6.91
1c	36	826.94	219.74	-28.67		9.76	-1.27	825.39	220.13	-9.47	8.94
1a	37	839.86	21.56	-8.27	{ 14.85	-5.70	836.72	27.21	-11.9	19.23	-8.41
1b	37	843.09	28.89	-20.86		7.40	-5.35	840.27	32.29	-21.54	7.88
1c	37	848.20	28.38	-5.27	1.26	-0.23	843.29	27.2	-2.45	1.10	-0.10
1d	37	849.05	69.95	-38.66	0.73	-0.40	844.56	71.63	-41.03	0.61	-0.35
1c	38	861.76	92.61	-9.71	4.11	-0.43	854.69	88.65	-20.38	3.60	-0.83
1d	38	866.21	21.14	9.20	0.22	0.10	858.58	16.15	5.62	0.14	0.05
		811.72	80.42	2.78							
		827.00	15.66	4.22							

979.22	355.31	4.71	976.60	78.87	4.19	1b 46	999.73	169.65	107.08	{	43.48	27.44	992.06	117.74	114.02	28.74	27.83
			1a 46	999.97	152.55	121.20		105.09	83.49	992.96	108.5	109.97	76.69	77.73			
			1c 46	1009.00	354.80	-97.49	{	15.75	-4.33	996.22	19.53	21.47	0.79	0.87			
990.60	70.09	5.50	991.71	33.18	3.36	1d 46	1009.43	477.26	36.22	{	4.96	0.38	995.63	39.94	36.59	0.34	0.31
			1b 47	1010.93	29.86	15.16		7.65	3.89	1000.46	4.42	3.86	1.08	0.94			
			1a 47	1012.29	33.23	9.43		22.89	6.50	1002.68	6.52	6.38	4.61	4.51			
1003.96	181.74	9.48	1005.28	-40.58	4.53	1b 48	1024.33	63.98	23.04	{	16.40	5.91	1013.3	160.9	10.9	39.28	2.66
			1a 48	1031.84	21.19	-27.14		14.60	-18.70	1020.26	17.32	-14.94	12.24	-10.56			
			1d 47	1035.10	90.17	171.58		0.94	1.78	1020.72	82.59	208.95	0.70	1.78			
			1c 47	1036.21	81.16	185.36		3.60	8.23	1021.58	84.6	204.08	3.43	8.29			
			1e 48	1044.99	48.42	-0.10		2.15	0.00	1030.45	227.42	-72.69	9.23	-2.95			
			1d 48	1046.57	66.05	3.27		0.69	0.03	1030.81	291.94	-86.09	2.48	-0.73			
1025.93	1177.95	5.63	1026.82	-281.22	6.96	1a 49	1048.90	1179.89	-41.08	{	812.83	-28.30	1033.58	1077.14	-53.17	761.32	-37.58
			1b 49	1049.28	1206.52	-57.24		309.23	-14.67	1033.78	1057.77	-72.29	258.20	-17.65			
			1d 49	1054.34	18.30	-28.98		0.19	-0.30	1045.61	618.53	-29	5.26	-0.25			
			1e 49	1056.86	53.77	-50.00		2.39	-2.22	1044.39	906.6	-86.04	36.81	-3.49			
			1c 50	1061.42	978.96	-68.72		43.47	-3.05	1049.08	32.12	-35.39	1.30	-1.44			
			1d 50	1063.60	879.08	-76.51		9.14	-0.80	1047.39	163.32	-71.36	1.39	-0.61			
			1c 51	1068.92	1.82	-4.27		0.08	-0.19	1077.43	4.18	-17.48	0.17	-0.71			
			1a 50	1069.17	1.02	3.74		0.70	2.58	1063.13	24.82	17.26	17.54	12.20			
			1b 50	1069.17	1.19	6.82		0.30	1.75	1061.16	71.89	17.83	17.55	4.35			
			1d 51	1069.46	2.36	-0.63		0.02	-0.01	1077.91	10.31	-24.71	0.09	-0.21			
			1b 51	1072.20	14.88	-79.90		3.81	-20.48	1071.98	493.95	232.06	120.57	56.65			
			1a 51	1073.91	14.92	-55.09		10.28	-37.95	1072.92	301.98	173.1	213.44	122.35			
			1b 52	1085.59	492.74	291.40	{	126.29	74.69	1077.65	18.11	27.41	4.42	6.69			
			1a 52	1086.82	355.30	238.90	{	244.77	164.58	1077.75	19.36	29.9	13.68	21.13			
			1d 52	1103.10	629.92	-75.00		6.55	-0.78	1085.07	881.74	86.76	7.49	0.74			
			1c 52	1103.20	211.95	78.64		9.41	3.49	1085.2	334.92	80.9	13.60	3.28			
			1d 53	1104.63	565.05	38.10		5.88	0.40	1088.52	384.48	-26.22	3.27	-0.22			
			1e 53	1106.04	619.60	-83.17		27.51	-3.69	1090.73	651.42	-33.48	26.45	-1.36			

1085.80	1531.24	5.75	1086.49	-215.47	6.28	1b 53	1112.81	1523.40	-63.33	{ 390.45	-16.23	1095.77	1689.61	-29	412.43	-7.08				
						1a 53	1115.81	1339.92	-126.47	923.07	-87.13	1099.47	1747.59	-127.8	1235.20	-90.33				
						1b 54	1118.23	144.54	39.19	{ 37.05	10.04	1105.57	16.69	-36.4	4.07	-8.89				
						1c 54	1118.39	338.90	1.49	{ 15.05	0.07	1109.19	306.18	22.91	12.43	0.93				
						1a 54	1119.64	286.60	30.02	{ 197.44	20.68	1107.81	70.78	20.66	50.03	14.60				
						1d 54	1123.98	131.21	57.83	{ 1.36	0.60	1115.4	183.3	28.78	1.56	0.24				
						1b 55	1138.10	68.91	-109.85	{ 17.66	-28.15	1135.59	50.57	2.22	12.34	0.54				
						1a 55	1140.56	125.38	-125.86	{ 86.37	-86.70	1135.11	11.81	-30.56	8.35	-21.60				
						1d 55	1141.08	207.18	-235.24	{ 2.15	-2.45	1131.59	202.23	-232.15	1.72	-1.97				
						1c 55	1146.81	185.17	-225.65	{ 8.22	-10.02	1138.62	119.08	-246.59	4.83	-10.01				
						1b 56	1148.72	48.89	41.16	{ 12.53	10.55	1138.07	106.91	-61.88	26.10	-15.10				
						1a 56	1151.01	84.87	124.42	{ 58.47	85.71	1143.32	155.24	39.92	109.72	28.22				
						1d 56	1156.71	368.84	201.85	{ 3.84	2.10	1144.19	396.35	211.86	3.37	1.80				
						1c 56	1158.68	434.70	202.74	{ 19.30	9.00	1147.53	466.66	205.76	18.95	8.35				
						1b 57	1170.68	2.96	2.24	{ 0.76	0.57	1173.13	6.11	4.22	1.49	1.03				
						1d 57	1171.00	2.49	0.39	{ 0.03	0.00	1171.91	150.41	30.72	1.28	0.26				
						1a 57	1171.09	1.88	-0.04	{ 1.30	-0.03	1173.35	2.32	0.07	1.64	0.05				
						1c 57	1171.09	2.18	-0.67	{ 0.10	-0.03	1170.54	166.24	22.38	6.75	0.91				
						1e 58	1178.83	40.40	7.79	{ 1.79	0.35	1173.27	2.38	0.96	0.10	0.04				
						1d 58	1178.91	27.23	15.88	{ 0.28	0.17	1173.59	3.28	-0.72	0.03	-0.01				
						1b 58	1182.99	513.63	82.67	{ 131.64	21.19	1176.93	524.14	85.75	127.94	20.93				
						1c 59	1185.87	233.35	34.72	{ 10.36	1.54	1181.55	149.07	18.28	6.05	0.74				
						1d 59	1186.32	273.81	5.30	{ 2.85	0.06	1181.2	162.66	-6.79	1.38	-0.06				
							1184.77	-127.77	6.50	1a 59	1204.52	24.56	-20.84	{ -14.36	1196.63	61.4	-27.54	43.40	-19.47	
										1b 59	1204.89	73.96	-36.21	{ 18.96	-9.28	1196.57	63.67	-27.34	15.54	-6.67
										1b 60	1207.34	343.90	11.78	{ 88.14	{ 3.02	1204.53	616.71	4.19	150.54	1.02
										1c 60	1210.27	178.53	7.32	{ 54.71	{ 4.75	1205.62	652.8	64.23	5.55	0.55
										1a 60	1210.93	203.84	3.01	{ 9.05	{ 0.13	1211.11	494.65	-25.91	20.08	-1.05

1220.34	68.55	3.81	1220.49	25.71	3.51	1b 61	1225.95	575.12	43.20	{	147.40	11.07	1220.08	229.02	16.79	55.90	4.10
1226.44	392.61	3.84	1225.88	45.98	2.92	1a 61	1226.71	235.62	-99.57	{	2.45	-1.04	1222.89	130.18	-105.27	1.11	-0.89
						1d 62	1237.05	1072.99	192.13		427.24	28.31	1214.82	289.49	-52.75	204.61	-37.28
						1c 62	1238.83	1042.16	188.52		46.27	8.37	1229.93	910.51	93.11	7.74	0.79
						1b 62	1244.14	598.96	-36.60	{	153.51	-9.38	1234.81	584.8	-76.82	142.75	-18.75
						1a 62	1244.37	561.76	-51.72	{	387.00	-35.63	1235.12	628.36	-61.21	444.12	-43.26
						1d 63	1260.15	62.29	-110.74	{	0.65	-1.15	1258.41	90.98	-28.79	0.77	-0.24
						1c 63	1262.50	50.02	-85.99		2.22	-3.82	1260.47	32	-4.82	1.30	-0.20
						1d 64	1283.34	167.51	54.49		1.74	0.57	1282.56	8.33	-32.18	0.07	-0.27
						1e 64	1284.20	215.11	39.27		9.55	1.74	1283.4	200.67	7.96	8.15	0.32
						1b 64	1290.63	212.35	88.03	{	54.43	22.56	1287.63	407.89	87.16	99.57	21.28
						1a 64	1292.40	147.44	81.62	{	101.57	56.23	1287.74	493.41	-22.09	348.74	-15.61
						1d 65	1300.01	52.87	10.64	{	13.55	2.73	1294.5	92.11	31.97	22.48	7.80
						1c 65	1300.52	124.45	6.31	{	5.53	0.28	1297.48	502.05	31.7	20.38	1.29
						1d 65	1304.23	103.74	-35.81	{	1.08	-0.37	1294.18	608.23	76.6	5.17	0.65
						1b 66	1305.52	41.47	-93.69	{	10.63	-24.01	1306.41	31.2	-76.3	7.62	-18.62
						1d 66	1307.65	444.52	-9.43	{	4.62	-0.10	1305.41	43.33	-41.41	0.37	-0.35
						1a 66	1308.83	63.46	17.46	{	43.72	12.03	1309.93	79.3	3.4	56.05	2.40
						1e 66	1309.58	15.29	33.97	{	0.68	1.51	1309.67	324.73	49.57	13.18	2.01
						1d 67	1313.75	165.43	-37.18	{	1.72	-0.39	1315.17	43.9	-57.06	0.37	-0.49
						1b 67	1315.99	157.61	-14.35	{	40.40	-3.68	1315.63	142.08	-39.08	34.68	-9.54
						1a 67	1316.43	54.87	-39.60	{	37.80	-27.28	1319.7	154.57	-87.66	109.25	-61.96
						1c 67	1318.36	891.22	-93.73	{	39.57	-4.16	1315.12	301.3	-154.16	12.23	-6.26
						1b 68	1321.38	365.24	43.38	{	93.61	11.12	1326.07	84.54	28.98	20.64	7.07

1300.37	319.11	3.30	1299.33	35.44	3.51	1a 68	1327.14	461.80	-31.53	{	318.13	-21.72	1328.13	260.39	-15.51	184.04	-10.96
						1b 69	1329.88	10.23	7.97	{	2.62	2.04	1337.14	0.31	4.46	0.08	1.09
						1a 69	1334.01	247.48	10.39	{	170.49	7.16	1340.65	47.16	11.94	33.33	8.44
						1d 68	1334.51	73.01	45.27	{	0.76	0.47	1341.49	70.21	29.33	0.60	0.25
1308.13	202.87	4.17	1304.48	13.35	4.92	1c 68	1336.68	217.16	54.21	{	9.64	2.41	1343.21	105.42	35.23	4.28	1.43
						1d 69	1341.12	17.81	23.55	{	0.19	0.24	1346.32	11.61	26.8	0.10	0.23
						1c 69	1343.13	34.62	0.98	{	1.54	0.04	1347.97	29.85	14.93	1.21	0.61
						1e 70	1363.48	14.09	-35.09	{	0.63	-1.56	1368.51	14.24	-33.93	0.58	-1.38
						1d 70	1363.54	22.81	-33.41	{	0.24	-0.35	1368.42	21.12	-32.56	0.18	-0.28
1341.01	47.30	5.87	1342.32	23.75	3.31	1a 70	1368.86	25.06	32.34	{	17.26	22.28	1369.58	21.68	28.61	15.32	20.22
						1b 70	1369.50	0.32	3.08	{	0.08	0.79	1369.59	1.33	6.8	0.32	1.66
						1c 71	1376.61	33.65	6.70	{	1.49	0.30	1377.42	32.5	10.31	1.32	0.42
						1e 71	1377.27	63.60	19.71	{	43.81	13.58	1378.19	48.42	19.99	34.22	14.13
1350.01	46.99	2.93	1348.90	23.90	2.72	1a 71	1377.71	53.35	11.98	{	0.55	0.12	1379.42	54.07	6.11	0.46	0.05
						1b 71	1378.33	60.33	23.29	{	15.46	5.97	1378.97	39.47	19.21	9.63	4.69
						1d 72	1383.35	22.43	-2.59	{	0.23	-0.03	1385.25	12.16	0.49	0.10	0.00
						1c 72	1383.47	6.64	2.50	{	0.29	0.11	1386.15	2.15	4.57	0.09	0.19
						1b 72	1384.11	20.26	1.41	{	5.19	0.36	1385.46	12.7	-7.02	3.10	-1.71
						1a 72	1384.82	6.77	-17.07	{	4.66	-11.76	1388.29	22.58	-23.9	15.96	-16.89
1353.51	33.19	4.98				1b 73	1388.66	26.20	-21.29	{	6.72	-5.46	1390.85	17.09	-9.28	4.17	-2.27
1355.98	30.22	5.46	1356.49	-19.99	3.41	1a 73	1390.12	17.08	-19.41	{	0.18	-0.20	1388.68	0.79	1.17	0.01	0.01
1363.04	52.77	4.82	1362.70	-19.70	4.21	1d 73	1391.12	42.49	-17.23	{	29.27	-11.87	1393.13	15.93	-5.45	11.26	-3.85
						1b 74	1393.99	44.84	-23.28	{	11.49	-5.97	1394.02	55.86	-21.14	13.64	-5.16
						1e 73	1401.76	96.76	-14.67	{	4.30	-0.65	1399.74	44.56	-3.38	1.81	-0.14
						1e 74	1404.16	37.34	-4.07	{	1.66	-0.18	1414.77	26.42	0.58	1.07	0.02
						1d 74	1404.72	34.76	-2.97	{	0.36	-0.03	1415.32	26.96	0.68	0.23	0.01
						1b 75	1406.33	34.02	-7.26	{	8.72	-1.86	1415.59	24.14	-2.13	5.89	-0.52
						1a 74	1406.75	36.37	3.05	{	25.06	2.10	1403.84	36.82	-3.63	26.02	-2.57
						1a 75	1407.35	76.48	-11.57	{	52.69	-7.97	1416.26	24.4	-1.55	17.25	-1.10

1d	75	1428.91	17.13	8.22	0.18	0.09	1431.26	21.62	6.86	0.18	0.06
1e	75	1429.86	12.91	14.55	0.57	0.65	1431.14	13.62	12.77	0.55	0.52
1b	76	1466.70	65.74	1.16	16.85	0.30	1472.81	43.88	0.28	10.71	0.07
1d	76	1467.74	63.78	-2.15	0.66	-0.02	1474.01	42.98	-1.72	0.37	-0.01
1e	76	1469.23	29.23	12.14	1.30	0.54	1476.04	69.38	-4.04	2.82	-0.16
1439.72	219.88	4.06	1437.26	5.76	2.73	1a 76	1470.50	17.36	4.14	11.96	2.85
1c	77	1470.81	115.30	-1.75	5.12	-0.08	1479.07	33	15.31	1.34	0.62
1b	77	1470.90	19.98	6.22	5.12	1.59	1480.66	18.63	5.99	4.55	1.46
1a	77	1470.91	119.09	4.59	82.04	3.16	1480.14	19.97	6.77	14.11	4.79
1d	77	1471.36	34.64	14.83	0.36	0.15	1481.22	31.79	13.96	0.27	0.12
1b	78	1477.45	68.37	-2.75	17.52	-0.70	1486.84	23.81	-0.09	5.81	-0.02
1a	78	1478.65	66.38	-3.54	45.73	-2.44	1488.09	64.61	-2.4	45.67	-1.70
1b	79	1478.68	24.87	0.44	6.37	0.11	1486.92	66.6	-1.49	16.26	-0.36
1d	78	1479.31	24.83	-1.64	0.26	-0.02	1487.54	23.06	-1.61	0.20	-0.01
1c	78	1480.02	58.28	-1.06	2.59	-0.05	1488.77	23.84	1.17	0.97	0.05
1d	79	1480.13	60.60	-1.07	0.63	-0.01	1489.57	59.35	-0.1	0.50	0.00
1a	79	1480.35	25.69	1.57	17.70	1.08	1488.28	24.31	0.49	17.18	0.35
1c	79	1481.05	25.87	0.51	1.15	0.02	1489.58	57.62	-0.65	2.34	-0.03
1b	80	1495.71	28.66	2.64	7.35	0.68	1502.95	28.66	2.73	7.00	0.67
1d	80	1496.02	28.69	2.93	0.30	0.03	1503.31	28.58	3.03	0.24	0.03
1c	80	1496.67	26.29	-0.73	1.17	-0.03	1503.87	26.58	-0.84	1.08	-0.03
1a	80	1496.72	26.06	-1.31	17.95	-0.90	1503.84	26.85	-1.33	18.98	-0.94
1b	81	1681.61	717.71	15.00	183.95	3.84	1666.05	792.27	7.5	193.39	1.83
1a	81	1685.46	140.52	9.26	96.80	6.38	1673.71	268.22	7.9	189.58	5.58
1d	81	1689.26	560.01	-65.96	5.82	-0.69	1673.54	706.26	-85.12	6.00	-0.72
1b	82	1689.29	99.35	3.63	25.46	0.93	1678.73	29.37	4.41	7.17	1.08
1c	81	1691.99	112.42	-12.51	4.99	-0.56	1680.38	188.51	-25.92	7.65	-1.05
1a	82	1693.61	326.41	15.83	224.86	10.91	1680.62	179.97	13.96	127.20	9.87
1d	82	1698.43	211.71	-19.48	2.20	-0.20	1687.26	73.39	-2.06	0.62	-0.02
1c	82	1704.31	306.86	-37.61	13.62	-1.67	1690.89	217.64	-22.81	8.84	-0.93

1d	83	1736.55	252.33	-16.40	2.62	-0.17	1723.53	254.4	-18.12	2.16	-0.15
1e	83	1736.61	250.27	-16.48	11.11	-0.73	1723.58	250.18	-20.71	10.16	-0.84
1b	83	1745.18	241.89	-28.71	{ 62.00	-7.36	1731.63	245.39	-29.4	59.90	-7.18
1a	83	1745.36	242.16	-25.72	{ 166.82	-17.72	1731.92	242.31	-29.75	171.26	-21.03
1a	84	1760.07	672.65	67.63	{ 463.39	46.59	1738.66	686.93	71.88	485.52	50.80
1c	84	1761.24	649.83	78.49	{ 28.85	3.48	1740.21	662.12	82.43	26.88	3.35
1b	84	1775.06	597.30	31.53	{ 153.09	8.08	1755.11	594.58	34.63	145.14	8.45
1d	84	1778.67	563.76	47.23	{ 5.86	0.49	1758.95	560.73	48.77	4.77	0.41
1c	85	1841.91	935.52	23.13	{ 41.54	1.03	1822.87	939.26	22	38.13	0.89
1d	85	1842.53	910.28	8.07	{ 9.47	0.08	1823.34	914.07	7.54	7.77	0.06
1a	85	1843.31	955.67	24.68	{ 658.36	17.00	1824.29	956.31	24.01	675.92	16.97
1b	85	1843.31	928.34	13.36	{ 237.93	3.42	1824.28	929.58	12.83	226.91	3.13

^a Frequencies, ν , in cm^{-1} ; dipole strengths, D, in $10^{-40} \text{ esu}^2\text{cm}^2$; rotational strengths, R, in $10^{-44} \text{ esu}^2\text{cm}^2$; Lorentzian bandwidths, γ , in cm^{-1} . Experimental rotational strengths are for (+)-1; calculated rotational strengths are for (1R,5S,8S,9S,10S)-1.

^b From Lorentzian fitting.

^c D (%); population-weighted dipole strengths; R (%); population-weighted rotational strengths.

Table S4. Experimental and calculated frequencies (v), dipole strengths (D) and rotational strengths (R) of **2^a**.

v	D	γ	Expt ^b	B3PW91/TZ2P						B3LYP/TZ2P						
				v	R	γ	mode	v	D	R	D (%) ^c	R (%) ^c	v	D	R	D (%) ^c
2d 18	356.80	16.77	7.62	0.21	0.10			356.22	20.16	9.26	0.20	0.09				
2c 18	357.48	30.13	-15.41	1.91	-0.98			356.87	32.25	-13.94	1.63	-0.70				
2a 18	357.85	48.54	8.65	35.46	6.32			357.53	50.72	9.68	38.22	7.29				
2b 18	360.03	68.14	19.36	13.18	3.74			359.72	71.63	20.86	13.34	3.88				
2c 19	390.14	31.75	1.27	2.02	0.08			390.08	34.67	0.55	1.75	0.03				
2d 19	393.03	17.04	0.92	0.21	0.01			393.45	17.81	0.42	0.17	0.00				
2a 19	399.92	34.20	-1.24	24.99	-0.91			399.09	41.20	-2.13	31.05	-1.61				
2b 19	403.41	7.53	-3.57	1.46	-0.69			403.20	9.80	-6.47	1.82	-1.20				
2c 20	420.99	6.83	3.76	{ 0.43	0.24			420.40	11.02	8.89	0.56	0.45				
2d 20	422.47	50.47	-10.20	{ 0.63	-0.13			422.41	43.77	-10.25	0.42	-0.10				
2b 20	424.94	86.44	0.26	{ 16.72	0.05			423.91	97.13	6.74	18.09	1.25				
2d 21	428.99	51.37	24.30	{ 0.64	0.30			427.55	63.90	28.31	0.62	0.27				
2c 21	431.00	30.70	5.82	{ 1.95	0.37			430.39	27.32	3.55	1.38	0.18				
2a 20	431.52	67.60	8.63	{ 49.39	6.31			431.17	74.74	13.59	56.32	10.24				
2b 21	435.81	72.84	15.89	14.09	3.07			434.00	63.81	12.21	11.88	2.27				
2a 21	440.14	17.61	12.00	12.87	8.77			438.33	12.52	7.20	9.44	5.43				
2b 22	451.07	38.09	16.57	{ 7.37	3.20			450.47	46.42	18.50	8.64	3.44				
2a 22	452.47	35.29	14.23	{ 25.78	10.40			451.84	40.85	16.27	30.78	12.26				
2c 22	459.19	25.83	10.27	1.64	0.65			459.33	23.49	10.59	1.19	0.53				
2d 22	462.25	43.89	3.97	0.55	0.05			461.62	41.23	2.76	0.40	0.03				
2a 23	473.39	56.46	-6.43	41.25	-4.70			473.02	55.70	-8.00	41.98	-6.03				
2d 23	481.36	38.96	-14.34	{ 0.49	-0.18			480.37	35.54	-15.20	0.34	-0.15				
2b 23	482.42	118.95	20.80	{ 23.00	4.02			481.54	113.68	17.01	21.17	3.17				
2c 23	489.87	66.26	-22.56	4.21	-1.43			488.49	69.94	-22.44	3.53	-1.13				

2d 24	516.75	41.91	-1.89	0.52	-0.02	513.82	44.97	-1.51	0.44	-0.01
2c 24	526.78	74.01	16.28	4.70	1.03	526.35	51.85	-1.75	2.62	-0.09
2d 25	528.62	57.32	32.75	0.72	0.41	529.59	59.67	33.09	0.58	0.32
2a 24	530.29	9.15	2.72	6.68	1.99	529.09	10.08	3.31	7.60	2.49
2c 25	530.95	17.87	20.09	1.13	1.28	530.19	48.00	37.19	2.42	1.88
2b 24	531.95	20.28	-16.15	3.92	-3.12	530.52	21.76	-15.51	4.05	-2.89
2b 25	558.03	16.40	9.67	{	3.17	1.87	555.50	17.82	9.38	3.32
2a 25	560.71	58.87	-8.91	{	43.01	-6.51	557.67	68.64	-9.68	51.73
2b 26	564.21	13.59	-10.47	{	2.63	-2.02	561.80	15.08	-11.86	2.81
2c 26	581.96	4.67	-1.86	{	0.30	-0.12	579.98	5.49	-2.36	0.28
2a 26	582.48	5.93	7.94	{	4.33	5.80	581.47	3.78	5.56	2.85
2d 26	594.49	13.57	-1.08	0.17	-0.01	592.58	16.18	-1.11	0.16	-0.01
2a 27	603.43	2.88	-5.13	{	2.10	-3.75	601.59	4.54	-6.31	3.42
2b 27	610.74	4.50	-5.72	{	0.87	-1.11	609.52	8.09	-7.07	1.51
2d 27	612.57	22.05	-16.23	0.28	-0.20	608.74	25.90	-20.72	0.25	-0.20
2c 27	613.07	26.81	-18.83	1.70	-1.20	609.28	32.53	-23.86	1.64	-1.20
2a 28	646.25	59.71	-1.89	43.62	-1.38	644.94	71.70	-2.03	54.03	-1.53
2b 28	647.07	47.35	-1.29	9.16	-0.25	645.89	55.41	-1.55	10.32	-0.29
2d 28	671.10	52.75	4.16	0.66	0.05	670.88	51.54	0.26	0.50	0.00
2c 28	673.76	48.56	-6.91	3.08	-0.44	671.32	33.84	-9.97	1.71	-0.50
2d 29	680.05	1.87	-4.16	0.02	-0.05	675.78	4.58	0.78	0.04	0.01
2c 29	680.44	3.31	-0.17	0.21	-0.01	678.34	19.27	4.30	0.97	0.22
2a 29	694.59	18.21	30.09	13.30	21.98	692.64	22.59	26.82	17.02	20.21
2b 29	695.15	16.97	31.28	3.28	6.05	693.24	18.92	28.47	3.52	5.30
2c 30	705.26	45.95	51.50	2.92	3.27	704.09	46.52	51.80	2.35	2.62
2d 30	707.44	56.92	56.36	0.71	0.70	706.13	60.03	58.04	0.58	0.56
2a 30	726.34	61.87	20.32	45.20	14.85	718.51	78.27	24.76	58.98	18.66
2b 30	726.82	53.86	18.03	10.42	3.49	719.10	67.63	21.31	12.59	3.97

2c	31	741.36	3.61	-4.43	0.23	-0.28	738.49	3.94	-2.99	0.20	-0.15	
2d	31	741.63	3.57	-6.19	0.04	-0.08	738.64	3.03	-4.74	0.03	-0.05	
2a	31	745.05	127.36	17.61	93.05	12.87	743.25	147.74	21.67	111.34	16.33	
2b	31	745.80	118.94	19.75	23.00	3.82	744.20	141.49	24.58	26.35	4.58	
2a	32	766.36	16.05	-22.57	11.73	-16.49	761.56	27.92	-22.07	21.04	-16.63	
2b	32	767.30	20.34	-24.48	3.93	-4.73	762.61	32.31	-22.48	6.02	-4.19	
2d	32	771.45	101.80	12.94	1.27	0.16	769.43	98.00	9.99	0.95	0.10	
2c	32	772.54	83.28	-6.60	5.29	-0.42	771.05	75.72	-5.98	3.82	-0.30	
2b	33	778.74	85.04	-8.73	16.45	-1.69	774.87	91.81	-15.74	17.10	-2.93	
2d	33	779.63	44.41	14.79	0.56	0.18	775.16	16.82	30.67	0.16	0.30	
2a	33	780.71	82.21	-21.69	60.06	-15.85	777.43	86.61	-27.13	65.27	-20.45	
2b	34	781.27	147.93	31.33	28.61	6.06	779.40	142.95	30.16	26.62	5.62	
2c	33	782.79	39.77	37.52	2.53	2.38	777.24	14.48	36.47	0.73	1.84	
2a	34	784.41	124.46	43.52	90.93	31.80	782.51	122.07	36.99	91.99	27.88	
2d	34	786.47	23.23	-30.48	0.29	-0.38	780.60	57.71	-38.15	0.56	-0.37	
2c	34	788.11	22.45	-30.19	1.43	-1.92	783.27	52.78	-27.09	2.67	-1.37	
2b	35	808.29	162.68	-104.64	{	31.46	-20.24	804.06	148.91	-106.53	27.73	-19.84
2a	35	809.29	250.12	-84.69	{	182.74	-61.87	804.55	242.84	-83.34	183.00	-62.81
2d	35	812.69	24.17	-1.64	0.30	-0.02	809.80	22.14	-6.02	0.21	-0.06	
2c	35	813.77	31.36	-8.62	1.99	-0.55	810.99	30.19	-12.38	1.52	-0.63	
2d	36	823.43	176.76	-65.59	{	2.21	-0.82	822.20	171.66	-65.80	1.67	-0.64
2c	36	825.91	227.72	-41.61	{	14.46	-2.64	824.44	238.12	-35.07	12.03	-1.77
2a	36	826.12	22.68	-7.02	{	16.57	-5.13	820.99	38.80	-6.60	29.24	-4.97
2b	36	826.17	20.16	-11.19	{	3.90	-2.16	820.93	28.65	-14.69	5.33	-2.74
2c	37	835.39	38.86	-5.52	{	2.47	-0.35	830.86	39.82	-2.83	2.01	-0.14
2d	37	835.97	53.25	-23.59	{	0.67	-0.29	831.42	54.14	-23.25	0.53	-0.23
2a	37	840.26	13.43	-7.47	{	9.81	-5.46	837.47	20.70	-11.47	15.60	-8.64
2b	37	843.28	23.02	-20.76	{	4.45	-4.01	840.61	28.44	-21.81	5.30	-4.06
2c	38	858.98	55.78	30.86	{	3.54	1.96	850.97	43.94	23.50	2.22	1.19
2d	38	864.11	14.88	10.19	{	0.19	0.13	855.77	7.16	3.93	0.07	0.04
		810.79	87.03	3.88								
		826.04	18.32	4.94								

2a	44	978.31	103.87	18.73	$\begin{cases} 75.89 \\ 13.68 \end{cases}$	966.41	595.07	120.49	448.44	90.80
2b	44	978.56	25.62	32.12	$\begin{cases} 4.95 \\ 6.21 \end{cases}$	969.25	50.83	11.04	9.46	2.06
2d	44	982.90	92.67	1.94	$\begin{cases} 1.16 \\ 0.02 \end{cases}$	970.67	167.29	81.43	1.62	0.79
2a	45	983.86	42.59	-11.11	$\begin{cases} 31.12 \\ -8.12 \end{cases}$	970.45	103.27	0.75	77.82	0.57
2d	45	989.42	127.01	-63.38	$\begin{cases} 1.59 \\ -0.79 \end{cases}$	981.50	320.00	91.05	3.10	0.88
2b	45	989.95	15.68	-14.39	$\begin{cases} 3.03 \\ -2.78 \end{cases}$	974.33	98.84	-52.25	18.40	-9.73
2c	44	990.17	128.60	37.38	$\begin{cases} 8.17 \\ 2.37 \end{cases}$	972.81	148.64	112.55	7.51	5.68
2c	45	992.23	33.78	1.36	$\begin{cases} 2.15 \\ 0.09 \end{cases}$	986.92	165.73	-18.00	8.37	-0.91
2a	46	993.66	144.18	10.46	$\begin{cases} 105.34 \\ 7.64 \end{cases}$	986.81	78.93	23.79	59.48	17.93
2b	46	993.97	173.51	-40.90	$\begin{cases} 33.56 \\ -7.91 \end{cases}$	986.36	62.83	41.02	11.70	7.64
2b	47	1009.39	55.34	-7.71	$\begin{cases} 10.70 \\ -1.49 \end{cases}$	1000.76	14.38	1.33	2.68	0.25
2c	46	1009.94	338.65	-77.97	$\begin{cases} 21.50 \\ -4.95 \end{cases}$	995.69	107.93	-25.29	5.45	-1.28
2a	47	1011.15	78.23	-13.25	$\begin{cases} 57.15 \\ -9.68 \end{cases}$	1003.08	25.46	0.02	19.19	0.02
985.55	71.29	3.67	984.96	-15.68	3.11	2d	46	1009.55	368.08	66.64
2c	46	1009.94	338.65	-77.97	21.50	-4.95	995.37	167.99	16.41	1.63
2a	47	1026.11	47.98	37.60	{	9.28	7.27	1015.33	106.55	20.84
2b	48	1026.11	28.15	-13.68	{	20.57	-9.99	1020.72	13.90	-5.22
2c	47	1043.67	63.13	-15.89	{	4.01	-1.01	1030.58	223.95	-17.59
1004.92	52.67	4.58	1008.10	-51.03	7.81	2a	48	1053.27	987.57	-65.88
2d	47	1046.28	35.38	14.26	0.44	0.18	1031.64	235.71	3.04	2.29
2a	49	1053.27	1010.27	-101.40	{	721.52	-48.13	1038.38	961.94	-79.29
2b	49	1053.34	338.15	-97.62	{	195.39	-19.61	1038.32	965.84	-112.43
2d	49	1058.25	1023.74	-115.03	{	68.49	-10.35	1035.52	1346.56	-251.94
2c	49	1059.21	323.09	-43.39	{	20.52	-1.22	1037.34	1292.15	-243.26
2a	50	1070.71	0.59	-4.85	{	0.43	-3.54	1067.54	184.87	226.52
2c	50	1070.77	18.58	48.49	{	1.18	3.08	1057.13	79.18	286.12
2b	50	1071.35	0.59	-4.12	{	0.11	-0.80	1065.99	338.08	265.22
2d	50	1071.39	11.64	30.81	{	0.15	0.39	1058.61	114.55	269.94
2c	51	1076.83	70.73	203.97	{	4.49	12.95	1080.31	9.05	0.39
2d	51	1078.47	101.86	202.18	{	1.27	2.53	1080.41	16.55	10.40
1028.36	1053.71	4.58	1028.31	-471.57	5.62	2c	48	1053.93	1078.60	-162.96

1058.05	240.96	5.62	1057.21	356.33	9.05	2b 51	1082.97	300.47	226.31	{	58.11	43.77	1079.53	1.37	-0.92	0.26	-0.17
						2a 51	1084.38	210.32	195.33	{	153.66	142.71	1078.96	1.41	-2.65	1.06	-2.00
						2d 52	1101.35	459.36	-8.09		5.74	-0.10	1086.93	577.79	-12.38	5.60	-0.12
						2c 52	1102.87	245.03	34.80		15.56	2.21	1088.55	332.60	33.99	16.80	1.72
						2a 52	1110.34	270.97	2.67	{	197.97	1.95	1098.75	1923.60	-110.93	1449.62	-83.60
						2b 52	1110.79	477.32	13.72	{	92.31	2.65	1095.97	1960.36	7.33	365.02	1.36
						2b 53	1112.90	1165.56	-74.73		225.42	-14.45	1101.43	11.57	8.32	2.15	1.55
1085.31	1620.21	5.22	1085.71	-363.53	9.79	2a 53	1113.85	943.49	-90.15	{	689.31	-65.86	1100.73	17.34	2.21	13.07	1.67
						2c 53	1115.67	566.30	-54.79	{	35.96	-3.48	1100.87	768.03	-87.88	38.79	-4.44
						2b 54	1117.41	291.17	0.30		56.31	0.06	1103.95	60.03	-99.11	11.18	-18.45
						2d 53	1117.73	531.19	-39.34	{	6.64	-0.49	1101.85	623.54	-54.28	6.05	-0.53
						2a 54	1118.93	613.08	-48.26	{	447.92	-35.26	1104.99	69.81	-41.24	52.61	-31.08
						2c 54	1123.38	147.71	-50.74		9.38	-3.22	1114.36	53.09	-8.00	2.68	-0.40
						2d 54	1125.85	79.94	-30.40		1.00	-0.38	1118.56	8.23	-41.46	0.08	-0.40
1117.99	42.41	2.58	1118.35	-29.64	2.55	2a 55	1140.22	13.44	-85.31	{	9.82	-62.33	1129.92	164.30	66.96	123.82	50.46
						2b 55	1140.91	27.78	-97.02	{	5.37	-18.76	1129.59	239.12	93.66	44.52	17.44
						2d 55	1142.16	125.14	-233.93	{	1.56	-2.92	1132.95	202.48	-207.95	1.96	-2.02
										{	43.22	21.15	1140.39	80.25	-78.85	14.94	-14.68
1123.60	250.96	4.23	1123.97	24.44	2.07	2b 56	1143.90	223.49	109.38	{	4.62	-10.10	1134.85	184.90	-80.34	9.34	-4.06
						2c 55	1145.33	72.68	-159.13	{	4.62	-10.10	1134.85	184.90	-80.34	9.34	-4.06
						2a 56	1147.10	302.37	141.93	{	220.91	103.69	1143.78	170.77	4.71	128.69	3.55
						2d 56	1150.29	665.10	260.94	{	8.31	3.26	1136.41	661.75	273.77	6.42	2.66
						2c 56	1154.43	768.58	164.57	{	48.80	10.45	1143.96	656.27	85.83	33.14	4.33
						2b 57	1171.18	2.06	0.26		0.13	0.02	1171.73	168.11	14.87	8.49	0.75
						2d 57	1171.19	3.35	2.08		0.04	0.03	1173.20	92.59	15.40	0.90	0.15
						2a 57	1171.40	1.82	0.32		1.33	0.23	1173.61	2.31	0.92	1.74	0.69
						2c 57	1171.55	3.05	1.88		0.59	0.36	1173.74	5.56	2.88	1.04	0.54
						2d 58	1181.15	63.99	9.61		4.06	0.61	1173.30	2.52	1.71	0.13	0.09
						2a 58	1182.23	73.71	14.87		0.92	0.19	1173.66	99.32	5.19	0.96	0.05
						2b 58	1188.22	1018.78	170.37	{	197.03	32.95	1178.68	854.18	133.54	159.05	24.87
						2a 58	1188.57	973.31	159.73	{	711.10	116.70	1178.63	845.38	157.21	637.08	118.47

2c	59	1195.92	635.61	-70.27	40.36	-4.46	1189.46	431.68	-61.02	21.80	-3.08
2d	59	1196.02	671.20	-93.09	8.39	-1.16	1189.28	381.41	-94.37	3.70	-0.92
2b	59	1206.76	441.24	-6.70	85.34	-1.30	1199.31	387.52	-0.79	72.16	-0.15
2d	60	1207.55	298.07	-5.60	3.73	-0.07	1205.29	544.55	17.28	5.28	0.17
1185.67	365.41	5.51	1183.32	-72.07	4.85	2a	59	1208.11	252.11	-17.82	184.19
2c	60	1209.66	152.87	-5.01	9.71	-0.32	1210.05	362.07	-103.65	18.28	-5.23
2b	60	1209.77	48.79	-78.71	9.44	-15.22	1206.25	302.07	-123.23	56.25	-22.95
2a	60	1210.83	136.82	4.95	99.96	3.62	1212.32	204.07	-0.99	153.79	-0.75
2c	61	1219.64	29.68	-238.03	1.88	-15.11	1212.69	42.70	-68.34	2.16	-3.45
2d	61	1221.18	62.38	-138.00	0.78	-1.73	1216.68	230.17	-32.86	2.23	-0.32
2b	61	1227.96	322.83	-173.03	62.44	-33.46	1221.44	138.34	-82.07	25.76	-15.28
1189.82	233.66	7.29	1193.84	-296.38	7.99	2d	62	1229.33	874.43	284.50	10.93
2c	62	1229.77	882.59	327.63	56.04	20.80	1220.07	622.85	229.93	31.45	11.61
2a	61	1230.64	285.06	-230.60	208.26	-168.48	1216.72	194.05	-216.43	146.24	-163.10
1215.72	122.89	3.21	1215.80	101.23	4.06	2b	62	1239.40	230.11	105.89	{ 44.50
2a	62	1239.45	237.82	119.80	{ 173.75	87.53	1235.11	188.36	60.36	141.95	45.49
2d	63	1259.28	118.15	-34.10	1.48	-0.43	1258.92	120.27	-5.67	1.17	-0.05
2c	63	1260.34	102.90	-55.95	6.53	-3.55	1259.01	38.12	-11.38	1.93	-0.57
2b	63	1264.22	48.82	-81.42	{ 9.44	-15.75	1262.72	41.30	-61.67	7.69	-11.48
1240.42	132.23	7.34	1239.47	-114.31	5.74	2b	63	1265.10	52.72	-81.89	{ 38.52
2a	63	1272.86	30.05	32.54	1.91	2.07	1276.36	109.57	34.47	5.53	1.74
2c	64	1273.53	16.54	19.91	0.21	0.25	1276.45	3.83	-10.08	0.04	-0.10
2d	64	1297.82	262.52	-16.11	{ 191.80	-11.77	1297.25	114.24	59.09	86.09	44.53
1262.62	122.84	5.18	1262.42	16.76	2.35	2b	64	1289.13	70.29	23.82	{ 13.59
2a	64	1291.98	27.47	21.76	{ 20.07	15.90	1288.85	512.92	-6.98	386.54	-5.26
2a	65	1297.82	262.52	-16.11	{ 191.80	-11.77	1297.25	114.24	59.09	86.09	44.53
2c	65	1300.26	126.47	26.47	8.03	1.68	1294.89	398.46	-14.73	20.12	-0.74
2b	65	1301.97	100.72	20.93	{ 19.48	4.05	1294.85	17.45	4.82	3.25	0.90
2b	66	1303.85	197.81	44.31	38.26	8.57	1303.39	131.04	1.77	24.40	0.33
2d	65	1304.41	276.17	-1.05	3.45	-0.01	1292.82	465.13	7.51	4.51	0.07

1280.00	138.17	3.47	1280.18	73.17	2.87	2a 66	1306.98	257.37	135.21	{	2.50	-0.48	1303.88	131.94	-6.74	1.28	-0.07
						2c 66	1309.09	11.73	37.08	{	188.03	98.78	1306.11	286.70	91.65	216.06	69.07
						2d 67	1313.43	216.62	-15.50	2.71	0.74	2.35	1308.80	420.30	115.53	21.23	5.83
						2b 67	1317.85	310.77	-19.48	{	60.10	-0.19	1314.46	32.45	-43.19	0.31	-0.42
1289.87	256.26	3.19	1289.29	-17.14	2.67	2c 67	1318.22	877.68	-86.60	{	55.73	-5.50	1314.28	343.87	-175.84	17.37	-8.88
						2a 67	1319.48	246.25	-66.53	{	179.91	-48.61	1320.75	247.54	-107.32	186.55	-80.88
1292.31	56.52	1.95				2b 68	1324.44	77.41	-9.91	{	14.97	-1.92	1330.31	15.58	2.99	2.90	0.56
1305.84	299.92	4.14	1304.82	-57.12	5.69	2a 68	1331.53	449.98	-27.47	{	328.76	-20.07	1332.82	135.14	-15.03	101.84	-111.33
						2d 68	1333.81	77.50	40.84	{	0.97	0.51	1341.48	68.88	27.95	0.67	0.27
						2c 68	1336.28	279.72	43.44	{	17.76	2.76	1342.86	127.39	29.63	6.43	1.50
						2b 69	1339.29	1.53	-0.55	{	0.30	-0.11	1342.22	0.75	2.05	0.14	0.38
						2a 69	1339.39	3.97	-1.68	{	2.90	-1.23	1342.81	13.08	7.67	9.86	5.78
						2c 69	1346.28	18.31	4.83	{	1.16	0.31	1349.15	19.97	13.76	1.01	0.69
						2d 69	1346.52	28.08	14.40	{	0.35	0.18	1348.81	21.24	16.74	0.21	0.16
1339.08	40.96	3.68	1338.85	21.47	3.61	2a 70	1366.39	42.99	20.08	{	31.41	14.67	1367.67	27.08	20.39	20.41	15.37
						2b 70	1366.66	13.56	3.86	{	2.62	0.75	1367.43	3.68	6.02	0.69	1.12
						2d 70	1372.44	36.35	23.63	{	0.45	0.30	1375.07	7.37	4.20	0.07	0.04
						2c 70	1372.46	23.33	15.89	{	1.48	1.01	1375.45	4.92	-4.14	0.25	-0.21
						2c 71	1377.34	47.53	-4.06	{	3.02	-0.26	1377.97	37.45	7.60	1.89	0.38
						2d 71	1378.51	39.25	6.17	{	0.49	0.08	1379.82	57.96	-0.71	0.56	-0.01
										{	52.31	14.16	1378.89	48.47	19.55	36.53	14.73
1350.23	51.51	3.47	1349.79	40.43	3.82	2a 71	1378.56	71.60	19.38	{	11.50	5.18	1379.24	35.09	18.20	6.53	3.39
						2b 71	1379.24	59.44	26.79	{	24.61	-0.54	1387.52	143.52	-18.31	1.39	-0.18
						2d 72	1380.04	159.72	-43.12	{	2.00	-2.39	1387.50	23.78	-13.25	4.43	-2.47
						2c 72	1380.17	122.77	-32.80	{	7.80	-2.08	1388.35	129.39	-18.93	6.53	-0.96
						2a 72	1384.69	90.39	-2.49	{	66.04	-1.82	1390.99	33.50	-22.03	25.25	-16.60
						2b 72	1384.72	127.24	-12.38	{	10.00	-5.04	1393.95	167.13	-30.74	31.12	-5.72
										{	0.19	-0.23	1388.96	0.57	0.54	0.01	0.01
1358.36	203.35	3.88	1358.24	-66.52	3.90	2b 73	1388.50	51.72	-26.04	{	38.07	-23.70	1394.58	103.42	-3.73	77.94	-2.81
										{	5.78	-4.00	1394.78	7.32	4.13	1.36	0.77

1642.03	258.53	7.24	2b 81	1682.18	703.49	14.20 {	136.05	2.75	1666.45	803.87	5.39	149.68	1.00
			2a 81	1685.60	146.66	8.91 {	107.15	6.51	1673.73	273.67	7.37	206.24	5.55
			2b 82	1689.48	131.13	-0.38 {	25.36	-0.07	1678.80	35.34	1.78	6.58	0.33
			2d 81	1689.74	580.43	-68.77 {	7.26	-0.86	1673.97	716.11	-87.88	6.95	-0.85
			2c 81	1692.91	117.90	-11.69 {	7.49	-0.74	1681.14	198.68	-25.64	10.03	-1.29
			2a 82	1693.90	330.60	13.70 {	241.54	10.01	1680.86	183.74	12.14	138.47	9.15
			2d 82	1699.00	196.62	-23.01 {	2.46	-0.29	1687.92	70.56	-5.24	0.68	-0.05
			2c 82	1704.73	302.96	-43.22 {	19.24	-2.74	1691.35	208.01	-27.50	10.50	-1.39
			2d 83	1728.12	213.98	-5.57 {	2.67	-0.07	1715.38	204.99	-8.08	1.99	-0.08
			2c 83	1728.34	212.76	-5.43 {	13.51	-0.34	1715.56	202.89	-8.41	10.25	-0.42
			2b 83	1734.17	206.16	-20.11 {	39.87	-3.89	1721.08	196.74	-19.34	36.63	-3.60
			2a 83	1734.44	206.01	-16.45 {	150.51	-12.02	1721.32	196.54	-15.85	148.11	-11.94
			2a 84	1759.60	667.53	66.24 {	487.70	48.39	1738.45	677.56	66.52	510.61	50.13
			2c 84	1761.17	646.51	71.52 {	41.05	4.54	1739.99	657.44	73.41	33.20	3.71
			2b 84	1775.41	598.25	31.86 {	115.70	6.16	1755.29	594.24	34.27	110.65	6.38
			2d 84	1778.72	568.41	48.28 {	7.11	0.60	1758.83	563.72	49.35	5.47	0.48
			2c 85	1830.80	869.19	-10.95 {	55.19	-0.70	1811.43	879.76	-9.07	44.43	-0.46
			2d 85	1831.71	840.49	-27.29 {	10.51	-0.34	1812.37	851.47	-24.98	8.26	-0.24
			2a 85	1832.29	896.41	40.09 {	654.92	29.29	1813.45	906.37	38.57	683.04	29.07
			2b 85	1832.52	866.69	28.12 {	167.62	5.44	1813.44	876.65	26.66	163.23	4.96

^a Frequencies, ν , in cm^{-1} ; dipole strengths, D, in $10^{-40} \text{ esu}^2 \text{ cm}^2$; rotational strengths, R, in $10^{-44} \text{ esu}^2 \text{ cm}^2$; Lorentzian bandwidths, γ , in cm^{-1} . Experimental rotational strengths are for (+)-2; calculated rotational strengths are for (1R,5S,8S,9S,10S)-2.

^b From Lorentzian fitting.

^c D (%): population-weighted dipole strengths; R (%): population-weighted rotational strengths.

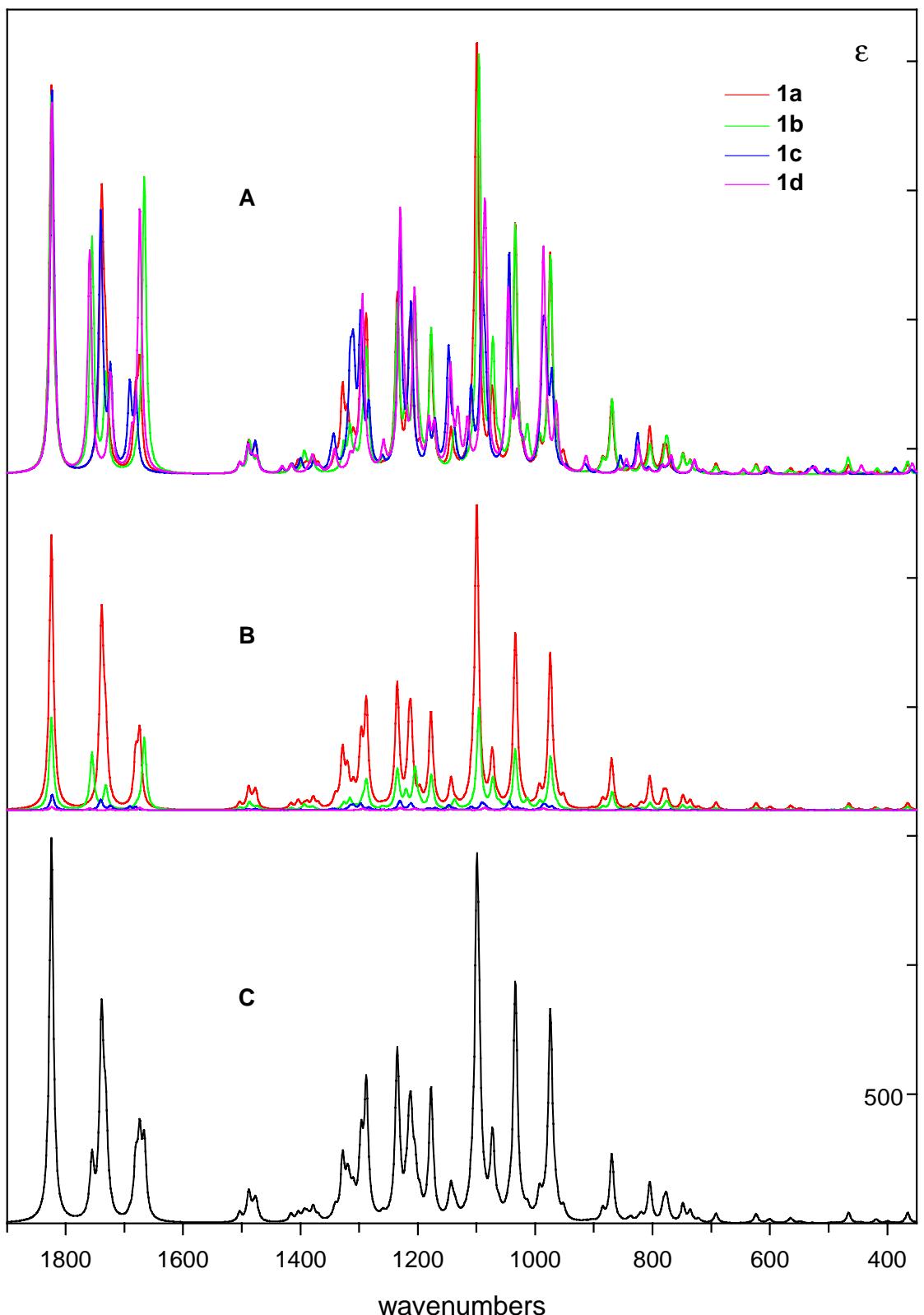


Figure S5. B3LYP/TZ2P IR spectra of **1**. A: Spectra of conformations **1a** – **1d**. B: Spectra of conformations **1a** – **1d**, weighted by the B3LYP/TZ2P populations (Table 1). C: Conformationally averaged IR spectrum of **1** (the sum of the spectra in B). Bandshapes are Lorentzian; $\gamma = 4.0$ cm⁻¹.

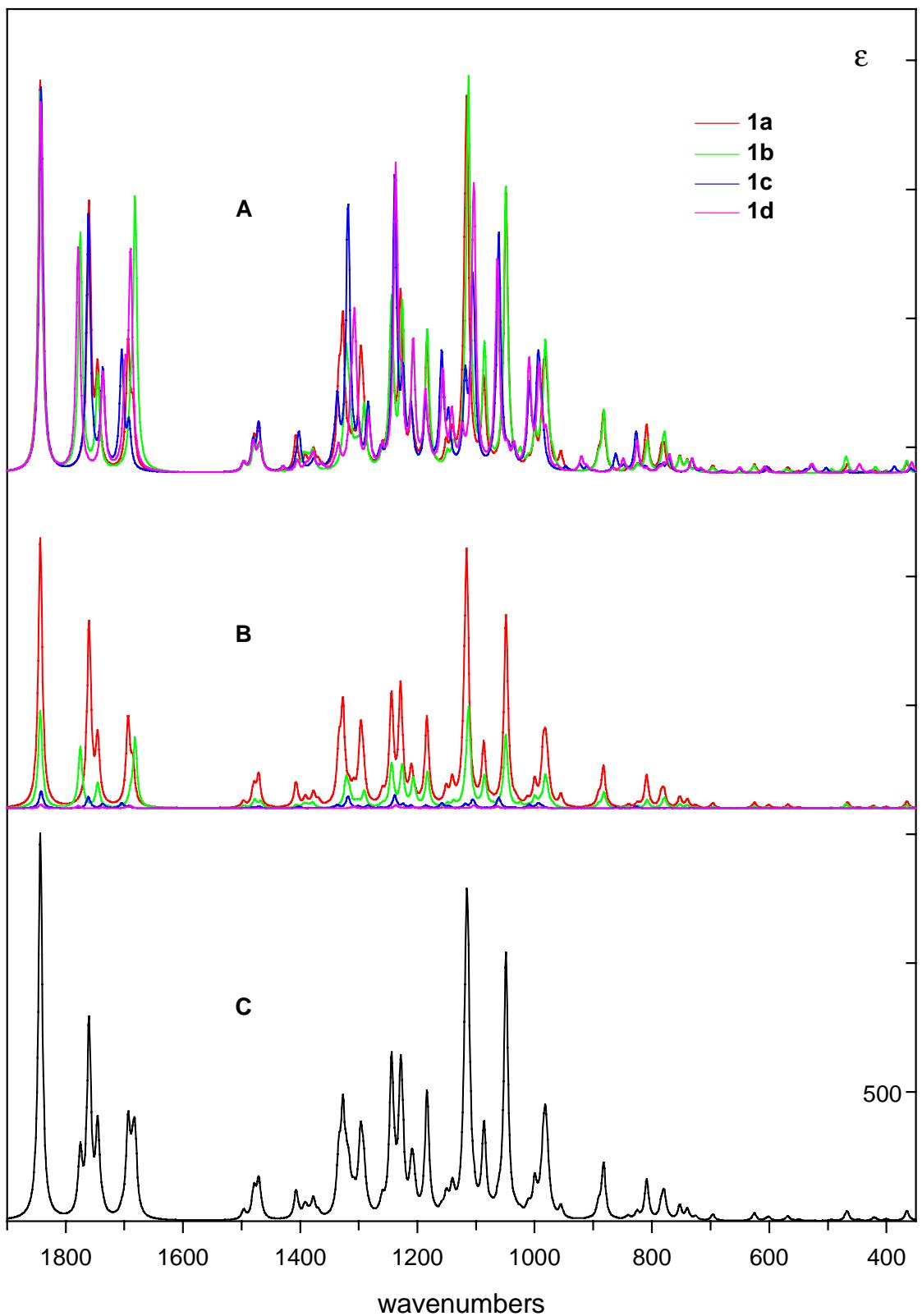


Figure S6. B3PW91/TZ2P IR spectra of **1**. A: Spectra of conformations **1a** – **1d**. B: Spectra of conformations **1a** – **1d**, weighted by the B3PW91/TZ2P populations (Table 1). C: Conformationally averaged IR spectrum of **1** (the sum of the spectra in B). Bandshapes are Lorentzian; $\gamma = 4.0$ cm⁻¹.

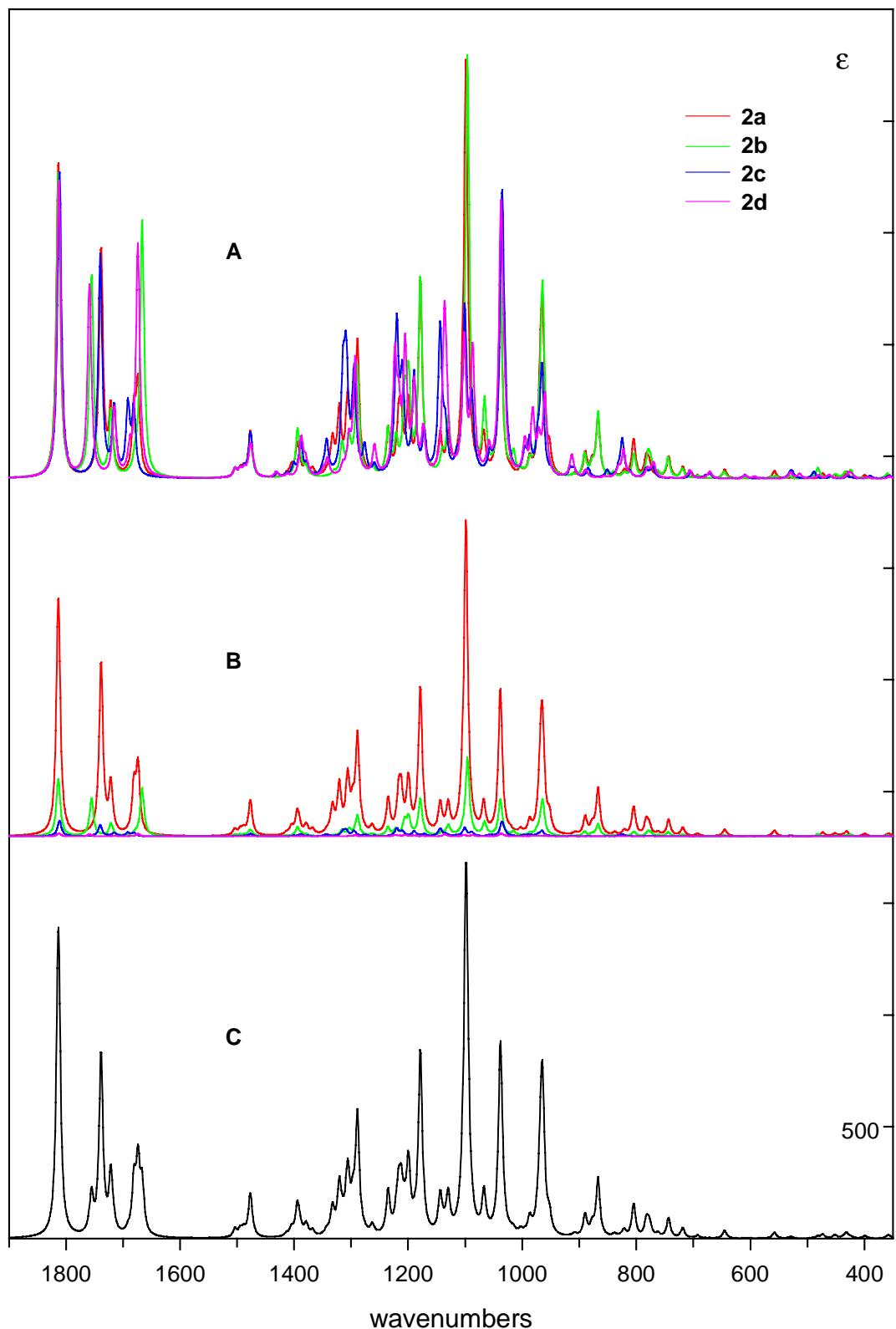


Figure S7. B3LYP/TZ2P IR spectra of **2**. A: Spectra of conformations **2a** – **2d**. B: Spectra of conformations **2a** – **2d**, weighted by the B3LYP/TZ2P populations (Table 2). C: Conformationally averaged IR spectrum of **2** (the sum of the spectra in B). Bandshapes are Lorentzian; $\gamma = 4.0 \text{ cm}^{-1}$.

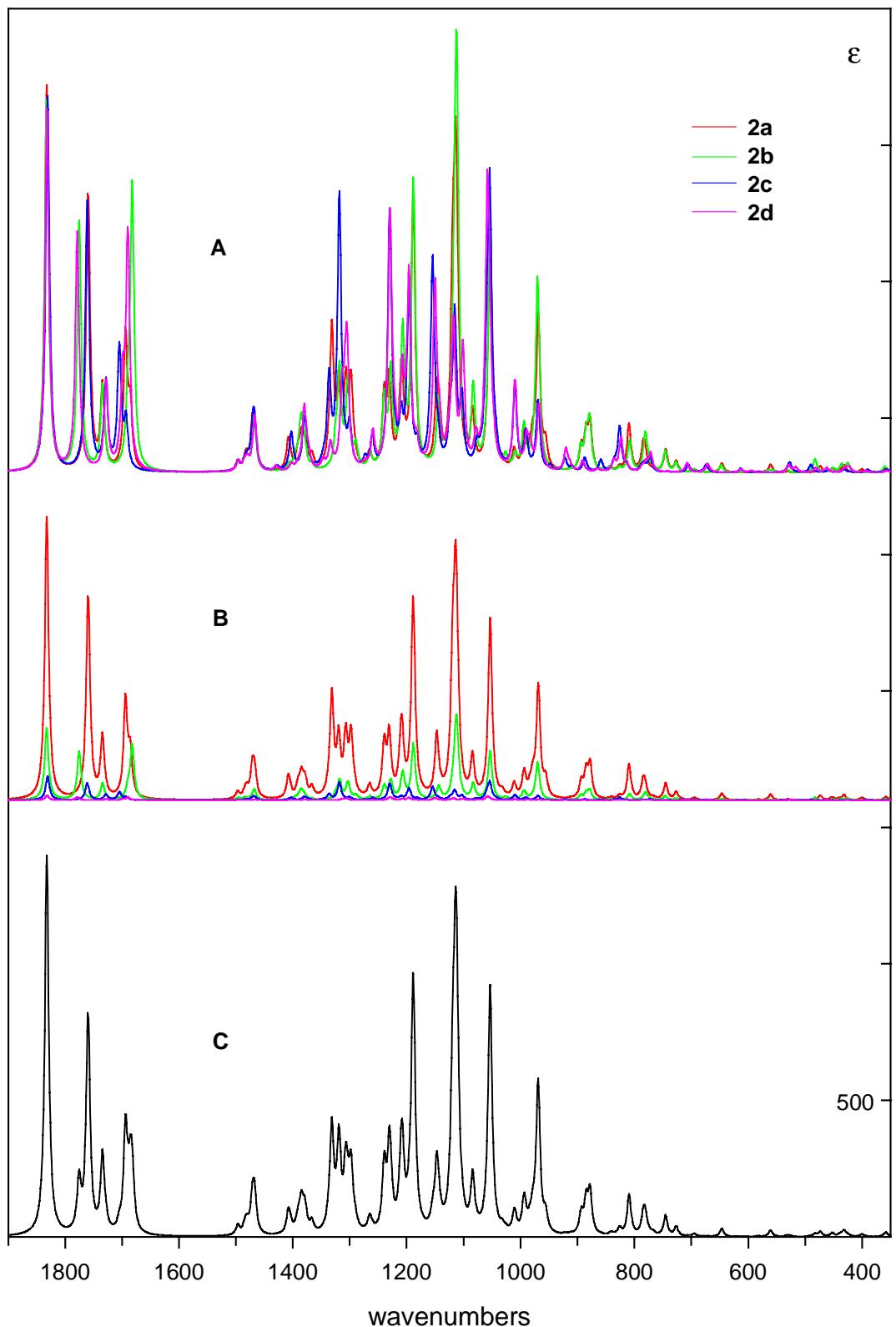


Figure S8. B3PW91/TZ2P IR spectra of **2**. A: Spectra of conformations **2a** – **2d**. B: Spectra of conformations **2a** – **2d**, weighted by the B3PW91/TZ2P populations (Table 2). C: Conformationally averaged IR spectrum of **2** (the sum of the spectra in B). Bandshapes are Lorentzian; $\gamma = 4.0$ cm⁻¹.

IR peak fit results of Plumericin from 350 to 700 cm⁻¹
 $r^2=0.98373$

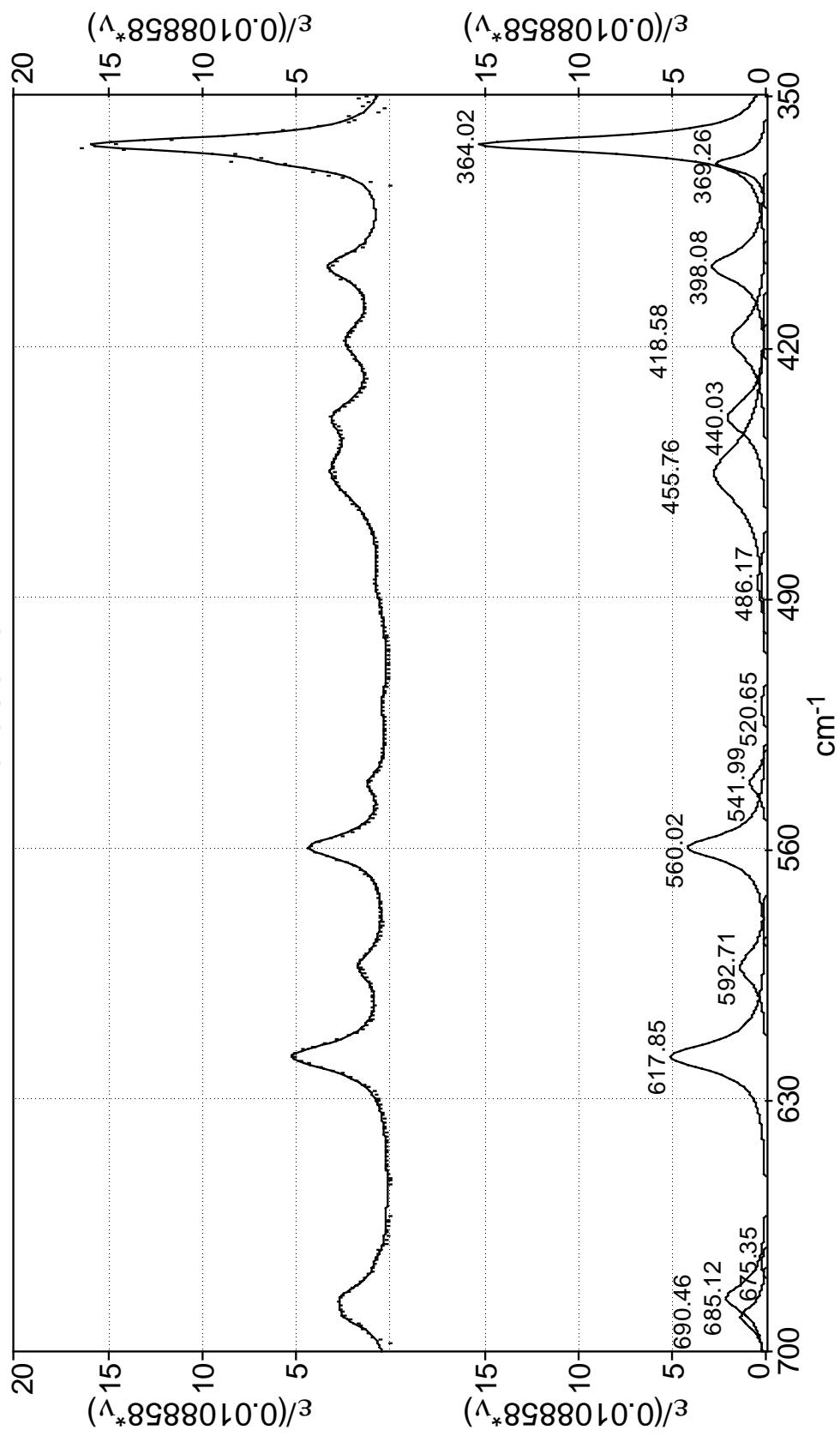


Figure S9a. The Lorentzian fitting of the experimental IR spectrum of **1** over the range 350 – 700 cm⁻¹.

IR peak fit results of Plumericin from 750 to 950 cm⁻¹

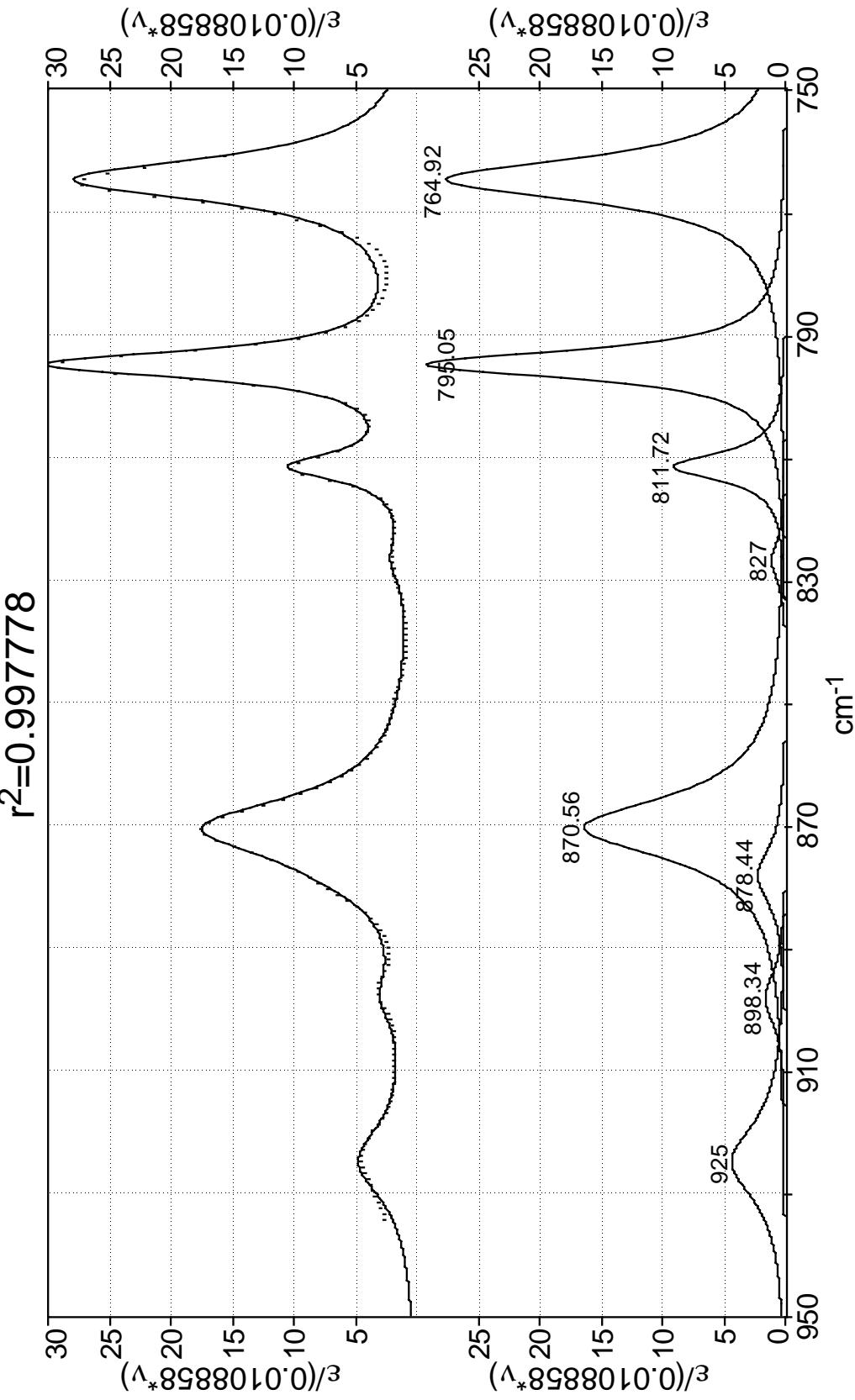


Figure S9b. The Lorentzian fitting of the experimental IR spectrum of **1** over the range 750 – 950 cm⁻¹.

IR peak fit results of Plumericin from 900 to 1150 cm⁻¹
 $r^2=0.998821$

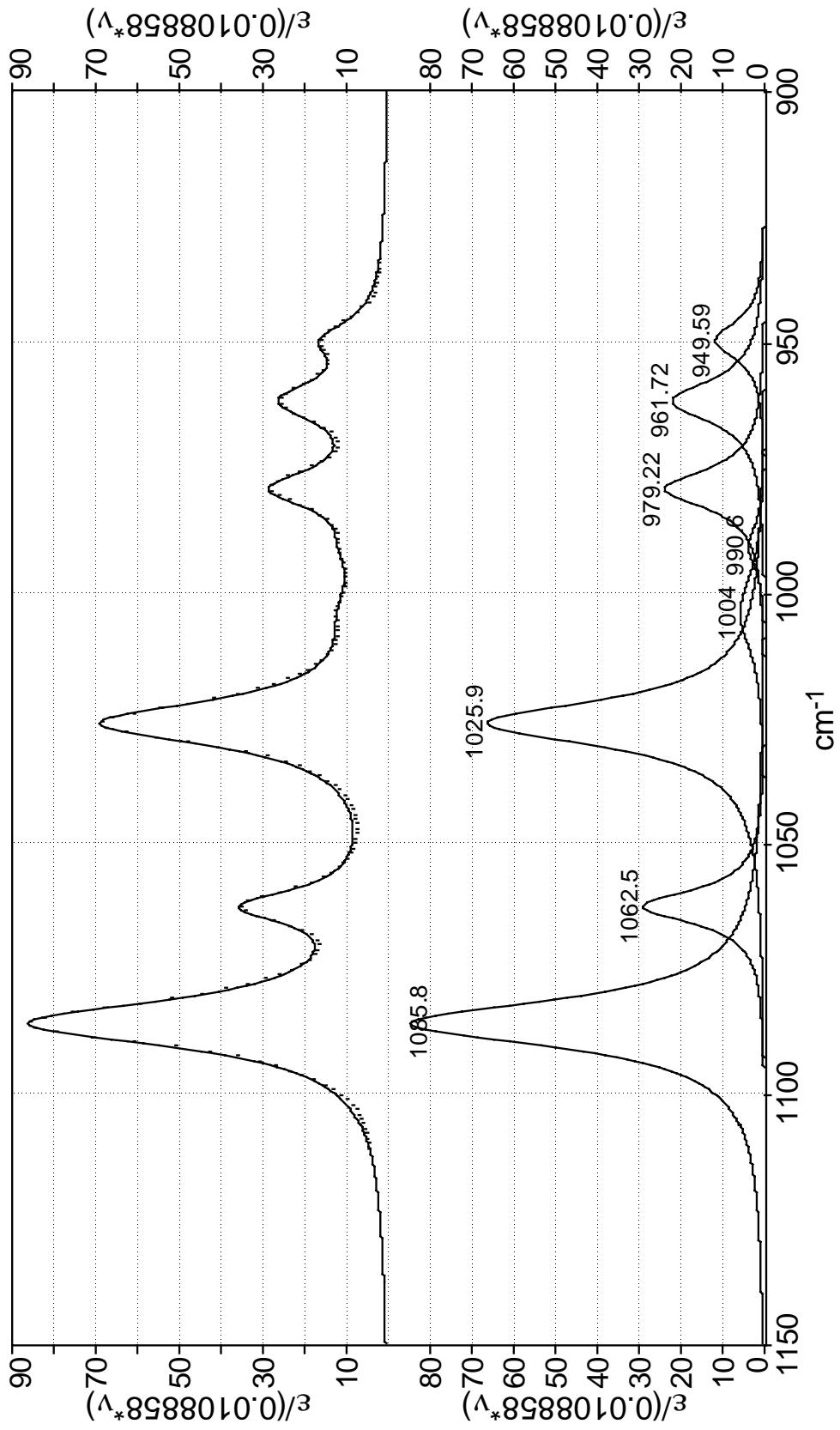


Figure S9c. The Lorentzian fitting of the experimental IR spectrum of **1** over the range 900 – 1150 cm⁻¹.

IR peak fit results of Plumericin from 1100 to 1350 cm⁻¹
 $r^2=0.998893$

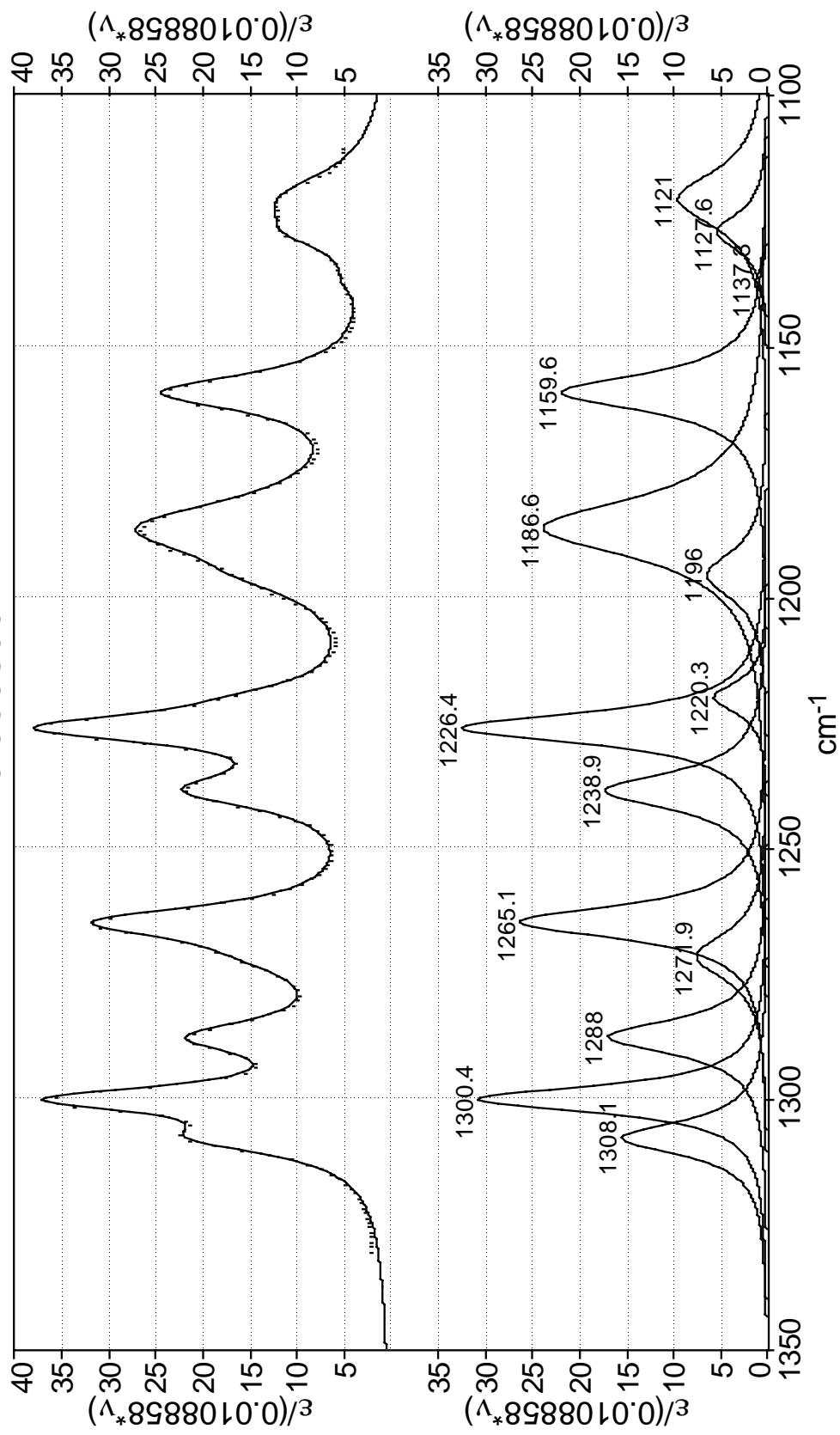


Figure S9d. The Lorentzian fitting of the experimental IR spectrum of **1** over the range 1100 – 1350 cm⁻¹.

IR peak fit results of Plumericin from 1300 to 1500 cm⁻¹
 $r^2=0.992949$

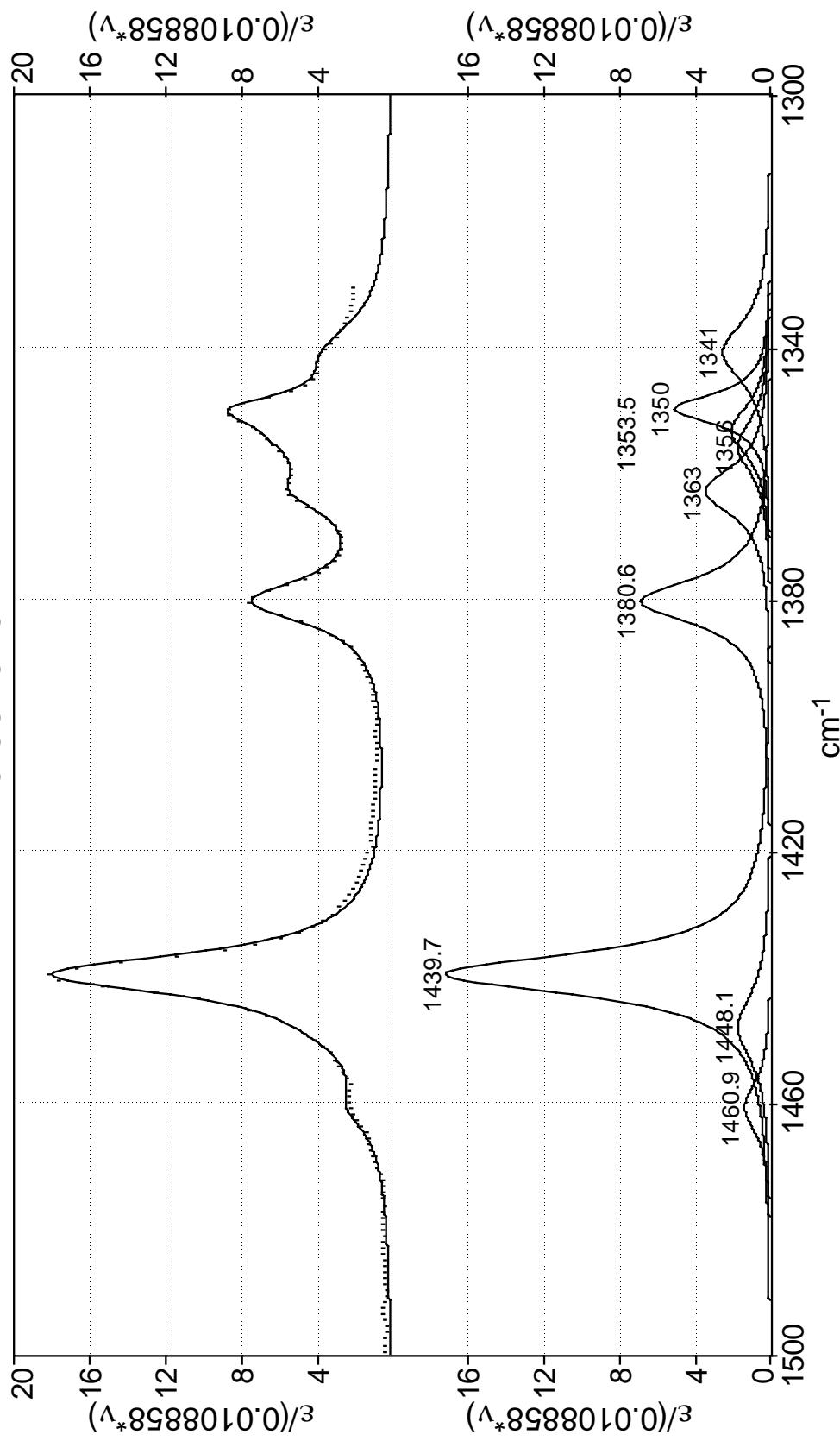


Figure S9e. The Lorentzian fitting of the experimental IR spectrum of **1** over the range 1300 – 1500 cm⁻¹.

IR peak fit results of Plumericin from 1550 to 1850 cm⁻¹
 $r^2=0.996324$

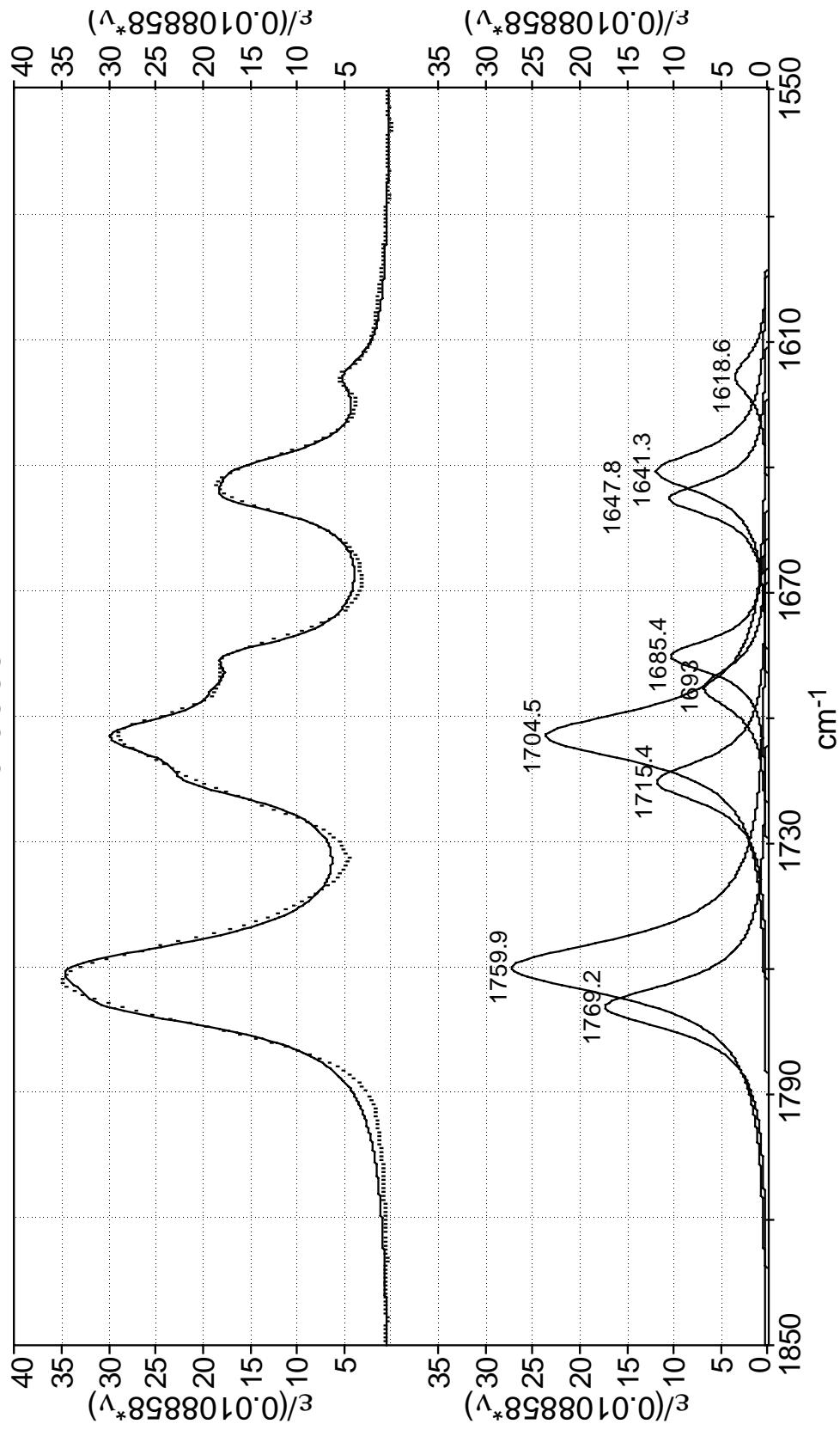


Figure S9f. The Lorentzian fitting of the experimental IR spectrum of **1** over the range 1550 – 1850 cm⁻¹.

IR peak fit results of Isoplumericin from 350 to 650 cm⁻¹
 $r^2=0.997146$

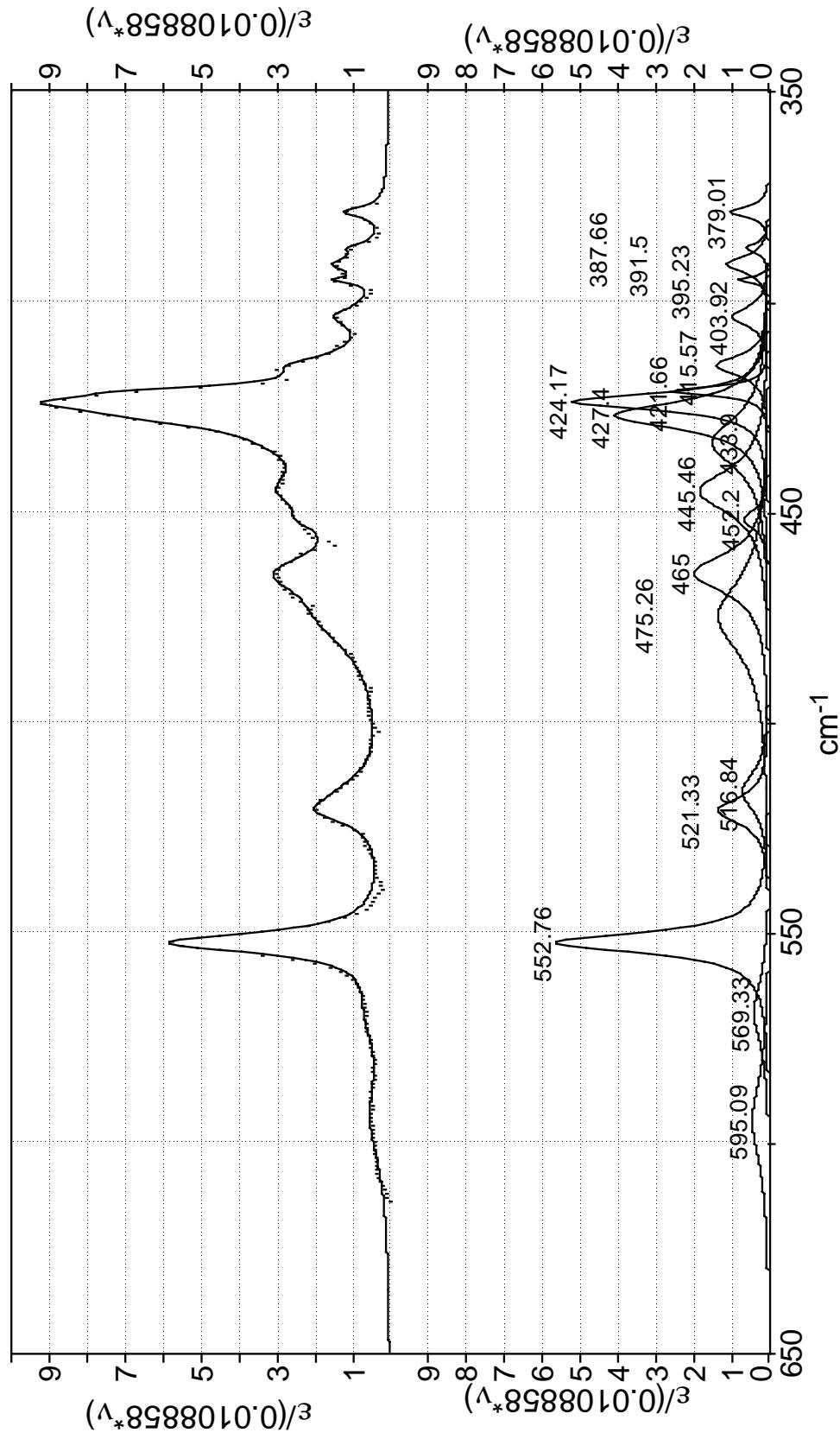


Figure S10a. The Lorentzian fitting of the experimental IR spectrum of **2** over the range 350 – 650 cm⁻¹.

IR peak fit results of Isoplumericin from 780 to 900 cm⁻¹
 $r^2=0.998158$

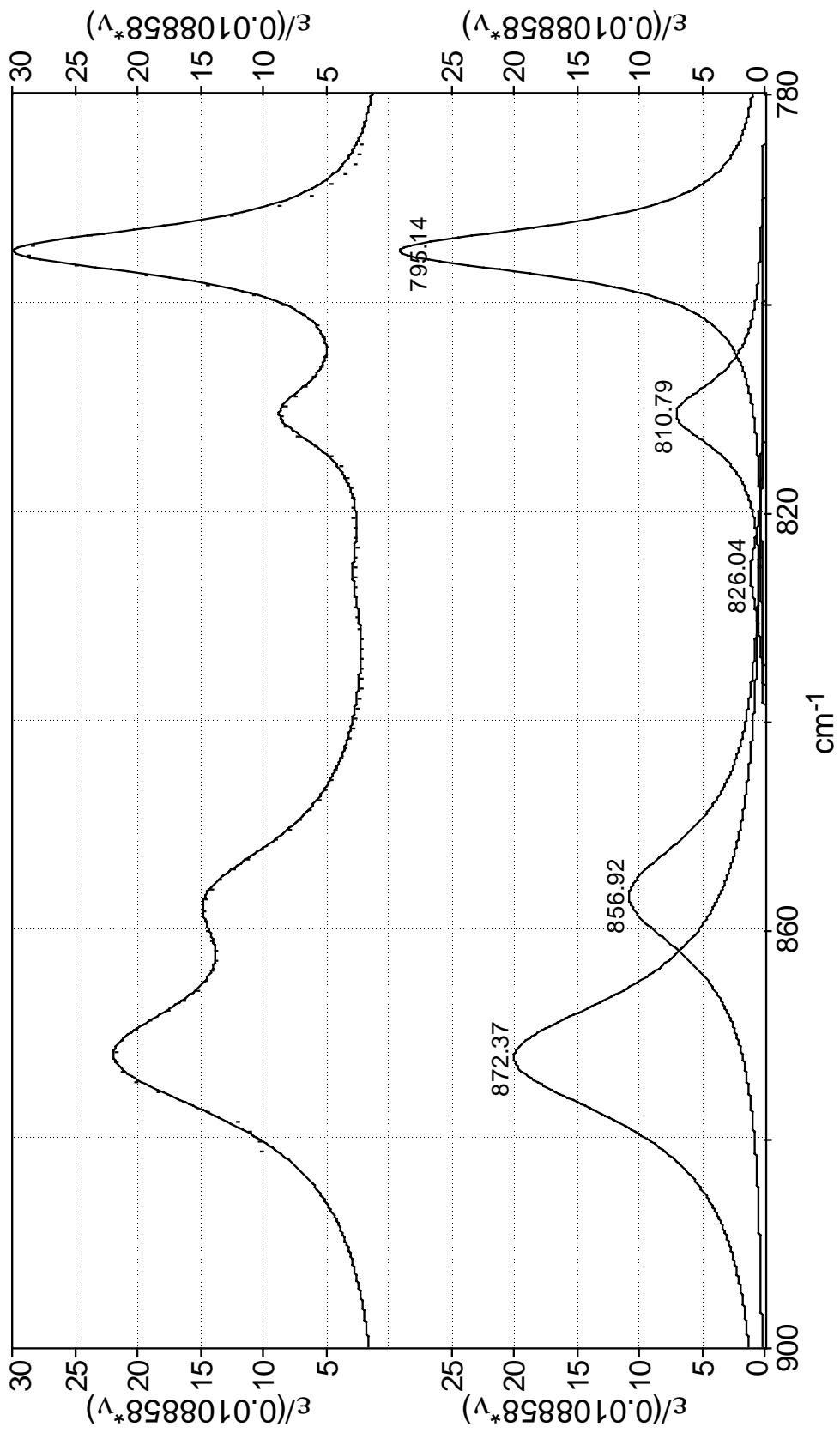


Figure S10b. The Lorentzian fitting of the experimental IR spectrum of **2** over the range 780 – 900 cm⁻¹.

IR peak fit results of Isoplumericin from 900 to 1150 cm⁻¹
 $r^2=0.998545$

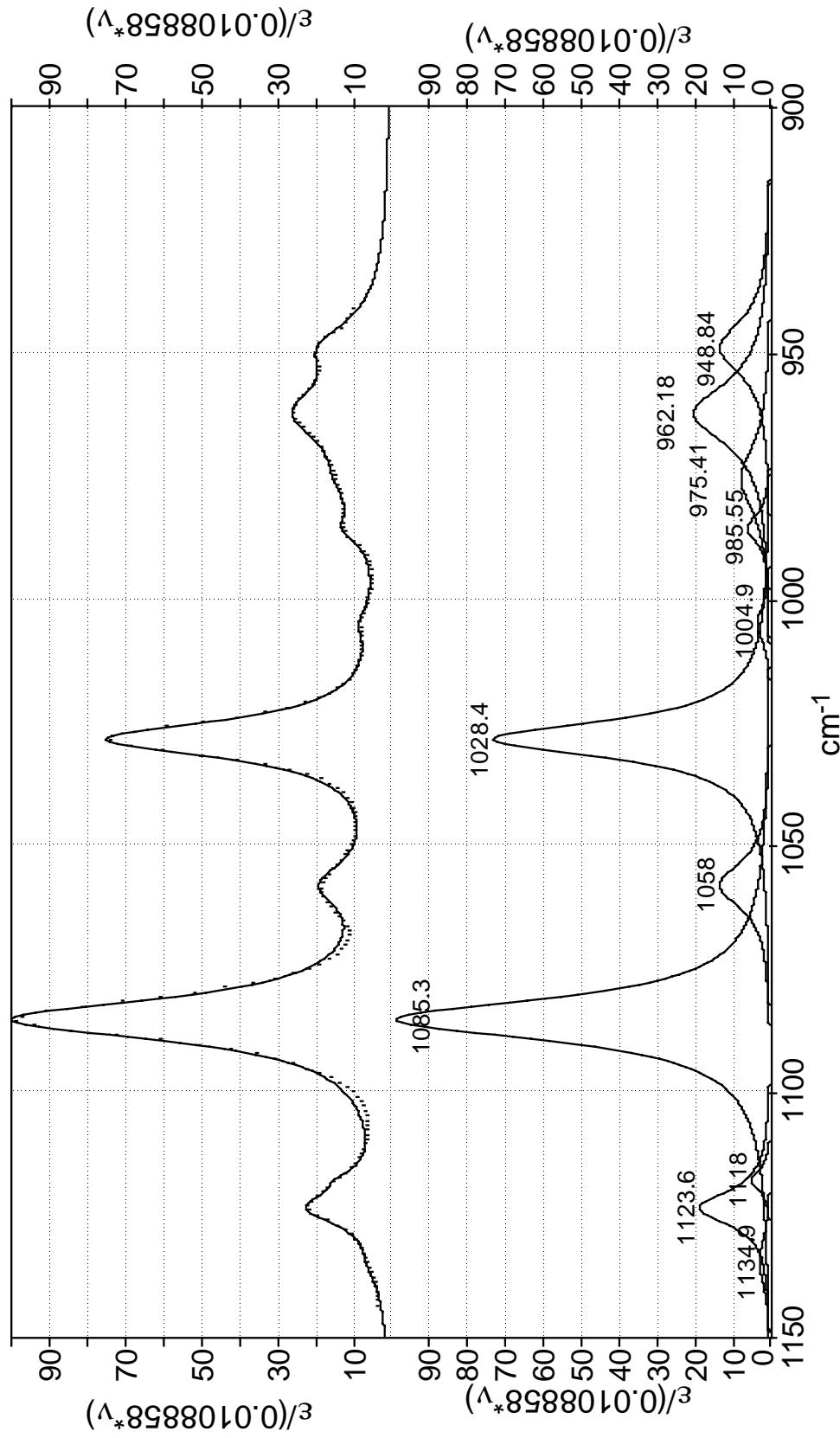


Figure S10c. The Lorentzian fitting of the experimental IR spectrum of **2** over the range 900 – 1150 cm⁻¹.

IR peak fit results of Isoplumericin from 1125 to 1250 cm⁻¹
 $r^2=0.999314$

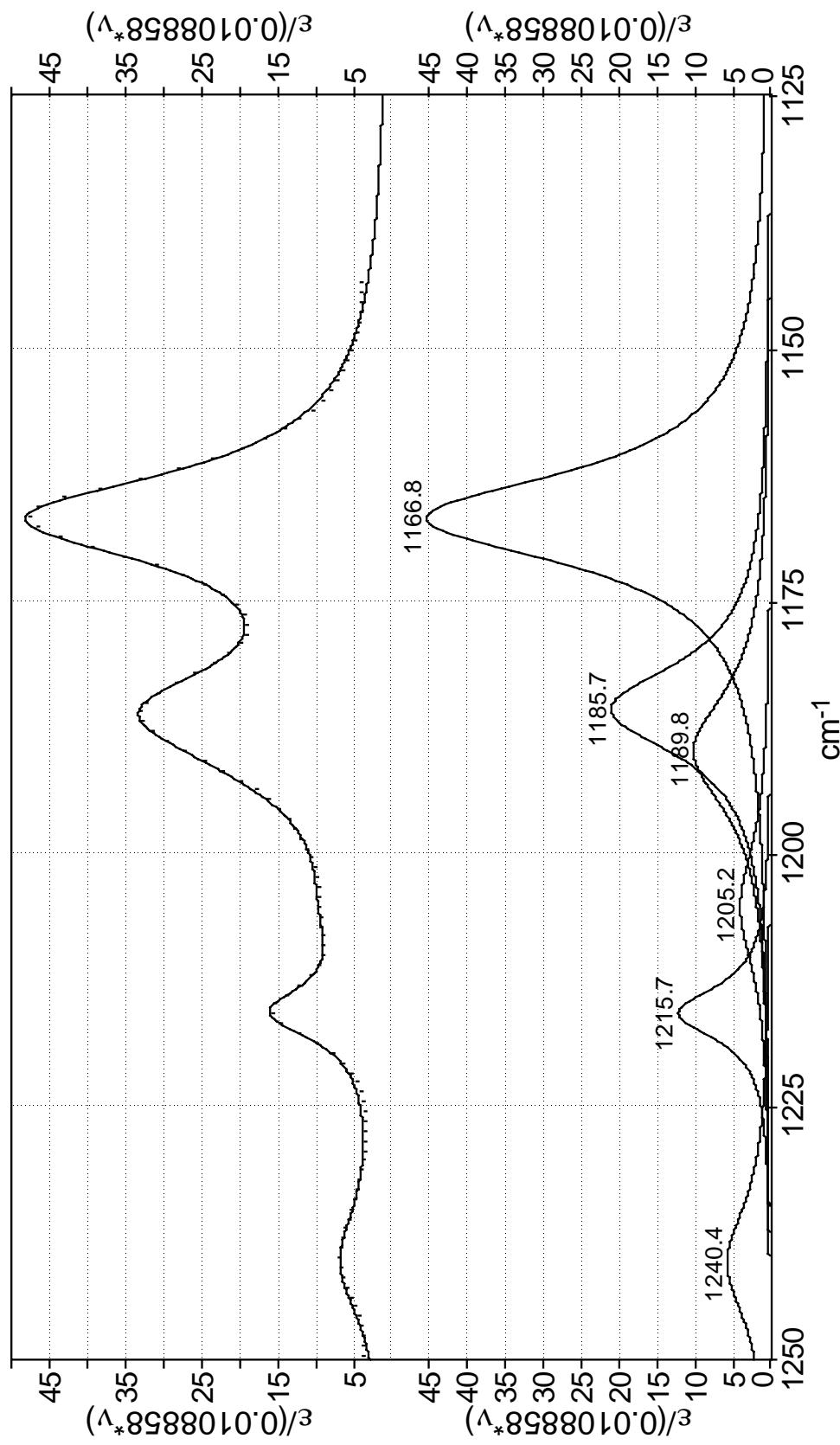


Figure S10d. The Lorentzian fitting of the experimental IR spectrum of **2** over the range 1125 – 1250 cm⁻¹.

IR peak fit results of Isoplumericin from 1200 to 1500 cm⁻¹
 $r^2=0.9985$

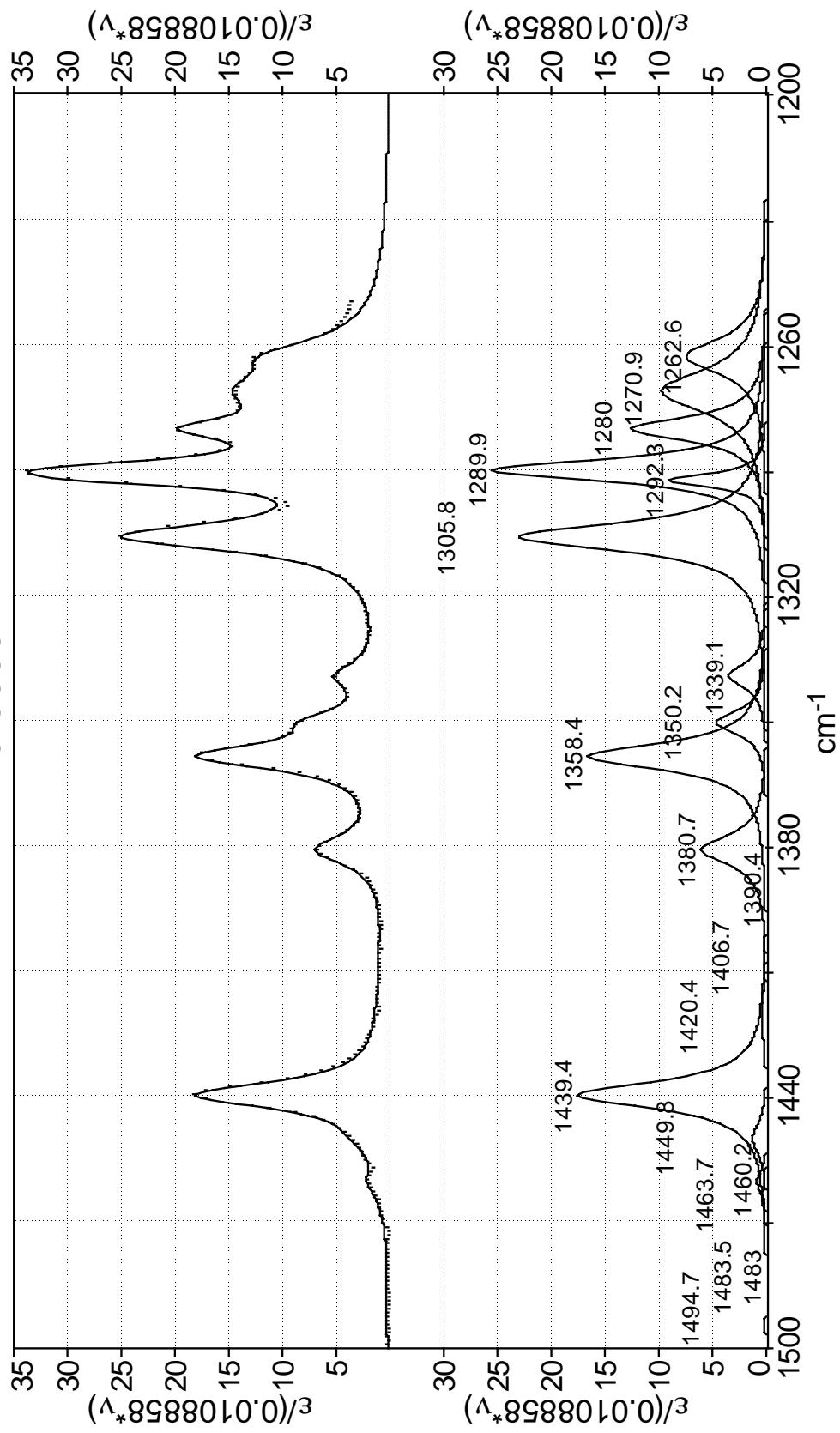


Figure S10e. The Lorentzian fitting of the experimental IR spectrum of **2** over the range 1200 – 1500 cm⁻¹.

IR peak fit results of Isoplumericin from 1600 to 1800 cm⁻¹
 $r^2=0.996884$

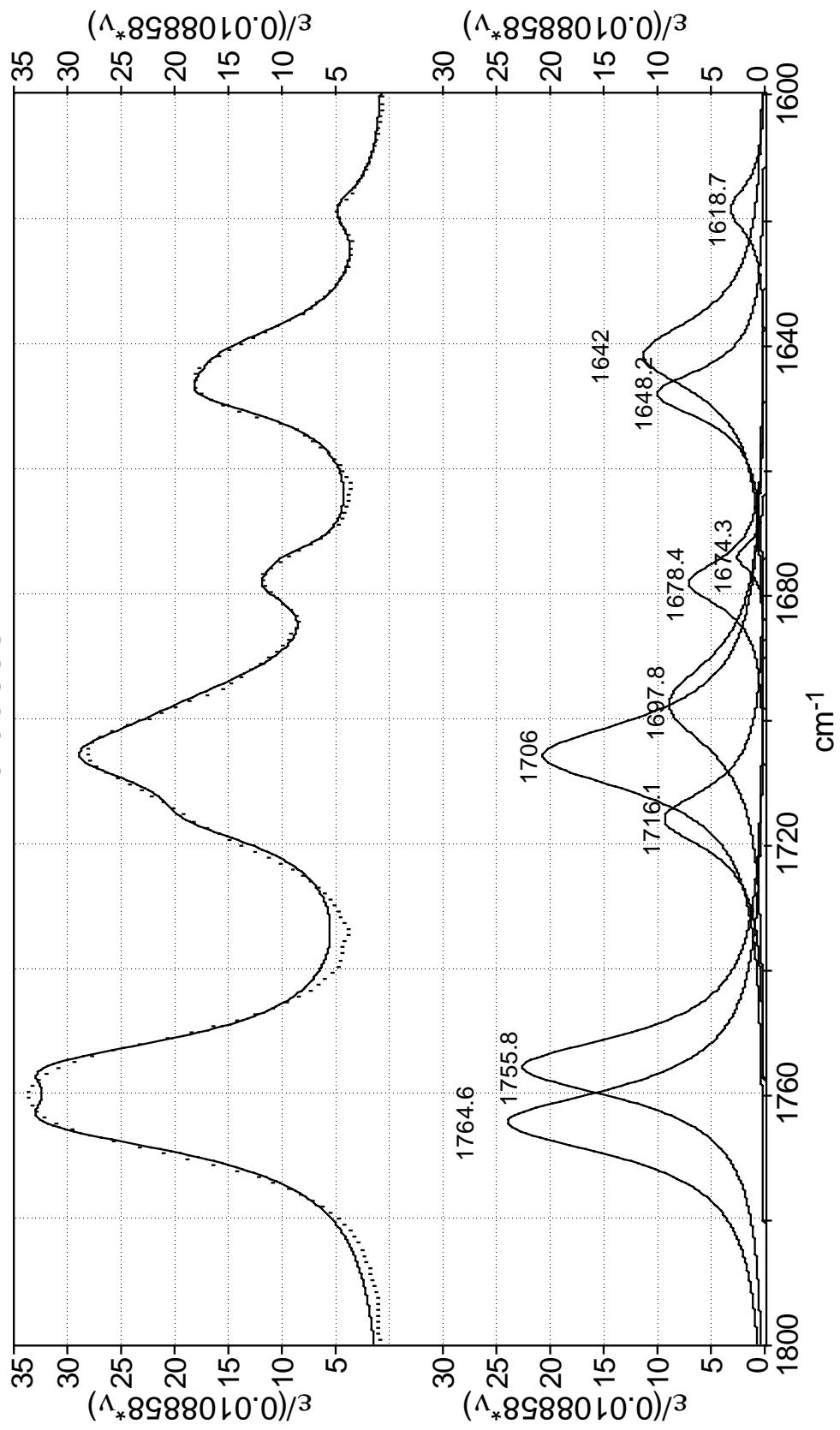


Figure S10f. The Lorentzian fitting of the experimental IR spectrum of **2** over the range 1600 – 1800 cm⁻¹.

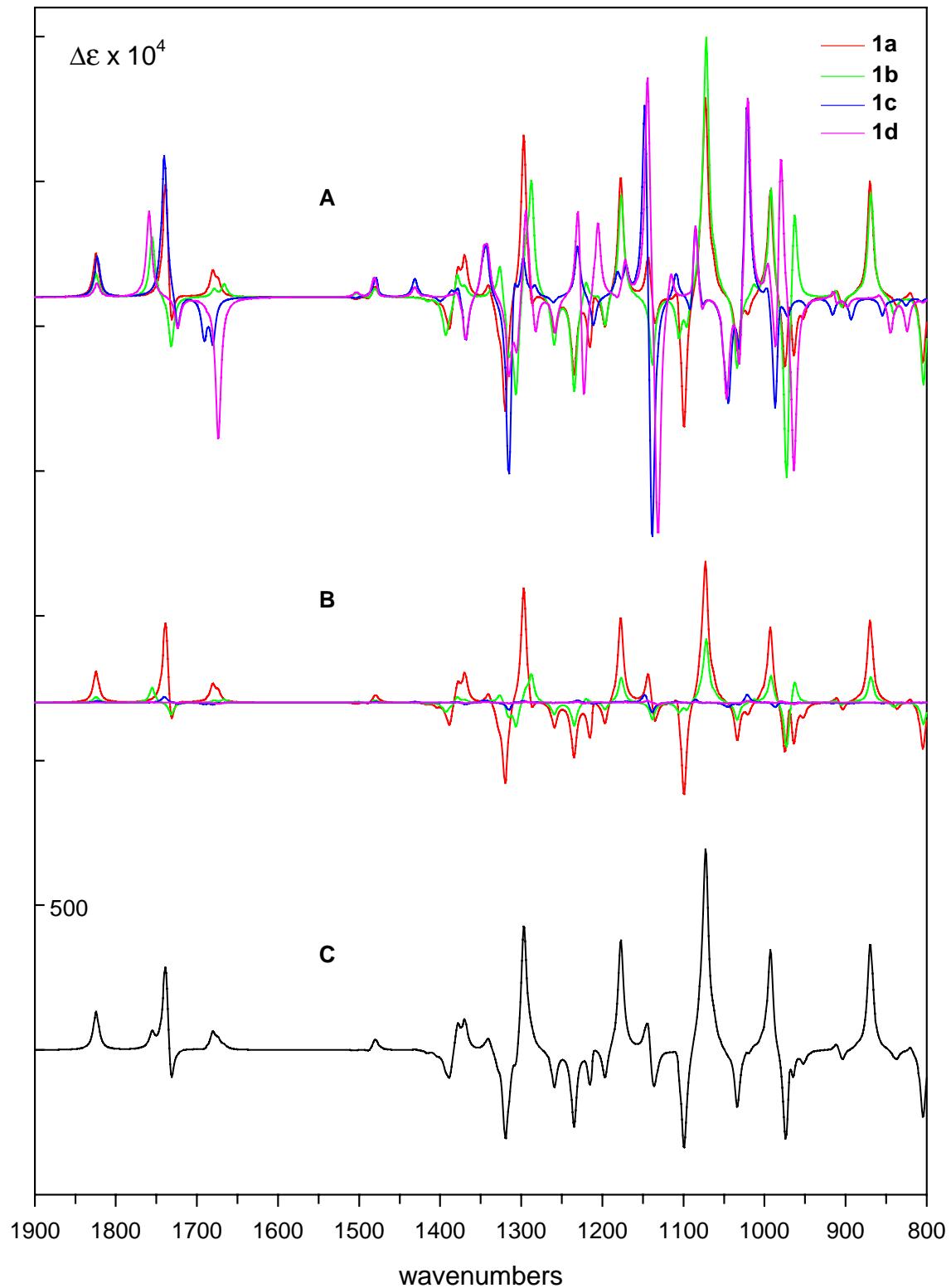


Figure S11. B3LYP/TZ2P VCD spectra of (1R,5S,8S,9S,10S)-**1**. A: Spectra of conformations **1a** – **1d**. B: Spectra of conformations **1a** – **1d**, weighted by the B3LYP/TZ2P populations (Table 1). C: Conformationally averaged VCD spectrum of **1** (the sum of the spectra in B). Bandshapes are Lorentzian; $\gamma = 4.0$ cm⁻¹.

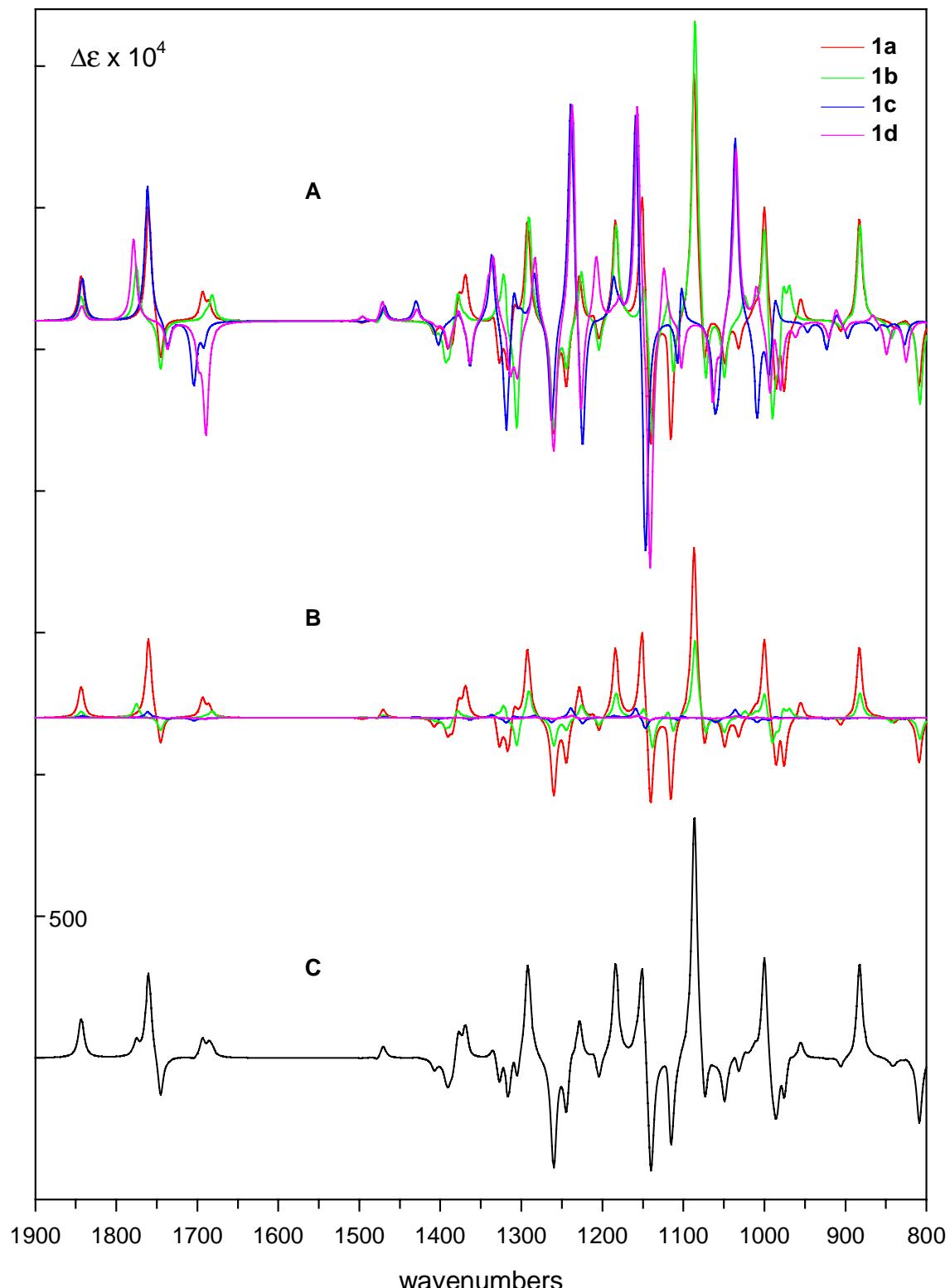


Figure S12. B3PW91/TZ2P VCD spectra of (1R,5S,8S,9S,10S)-1. A: Spectra of conformations **1a** – **1d**. B: Spectra of conformations **1a** – **1d**, weighted by the B3PW91/TZ2P populations (Table 1). C: Conformationally averaged VCD spectrum of **1** (the sum of the spectra in B). Bandshapes are Lorentzian; $\gamma = 4.0$ cm⁻¹.

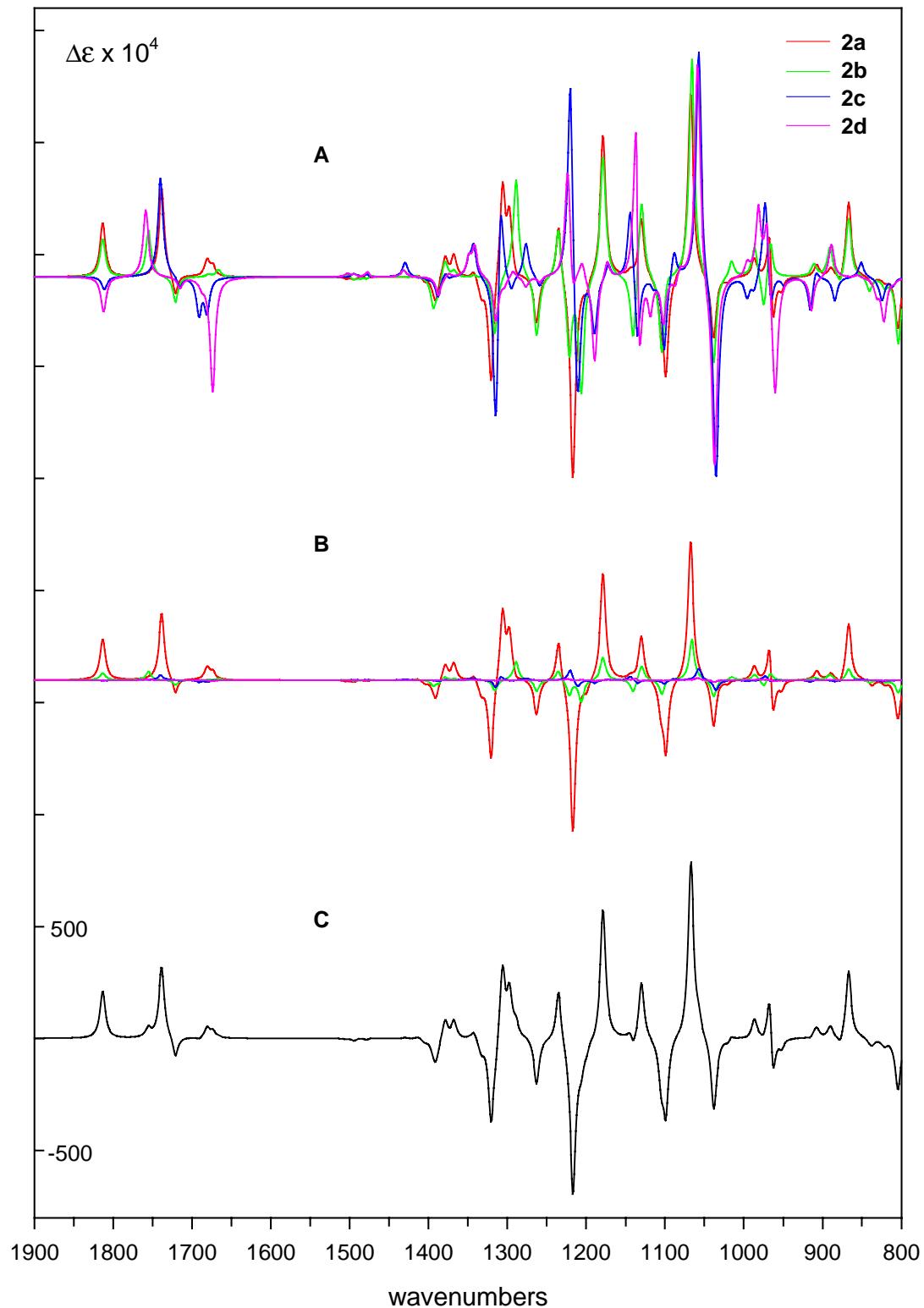


Figure S13. B3LYP/TZ2P VCD spectra of (1R,5S,8S,9S,10S)-**2**. A: Spectra of conformations **2a** – **2d**. B: Spectra of conformations **2a** – **2d**, weighted by the B3LYP/TZ2P populations (Table 2). C: Conformationally averaged VCD spectrum of **2** (the sum of the spectra in B). Bandshapes are Lorentzian; $\gamma = 4.0$ cm⁻¹.

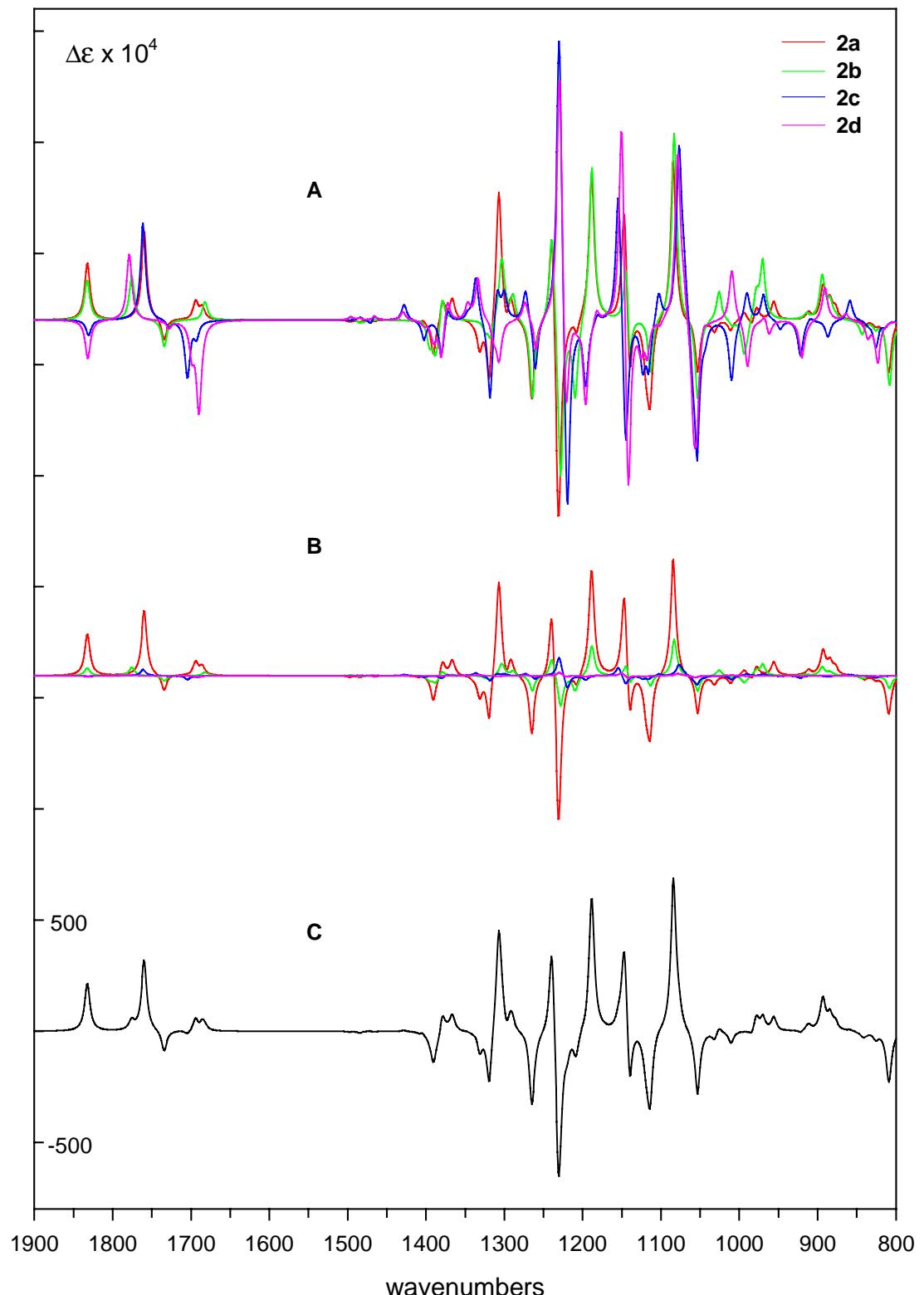


Figure S14. B3PW91/TZ2P VCD spectra of (1R,5S,8S,9S,10S)-2. A: Spectra of conformations **2a** – **2d**. B: Spectra of conformations **2a** – **2d**, weighted by the B3PW91/TZ2P populations (Table 2). C: Conformationally averaged VCD spectrum of **2** (the sum of the spectra in B). Bandshapes are Lorentzian; $\gamma = 4.0$ cm⁻¹.

VCD peak fit results of (+)-Plumericin from 825 to 1075 cm⁻¹
 $r^2=0.993794$

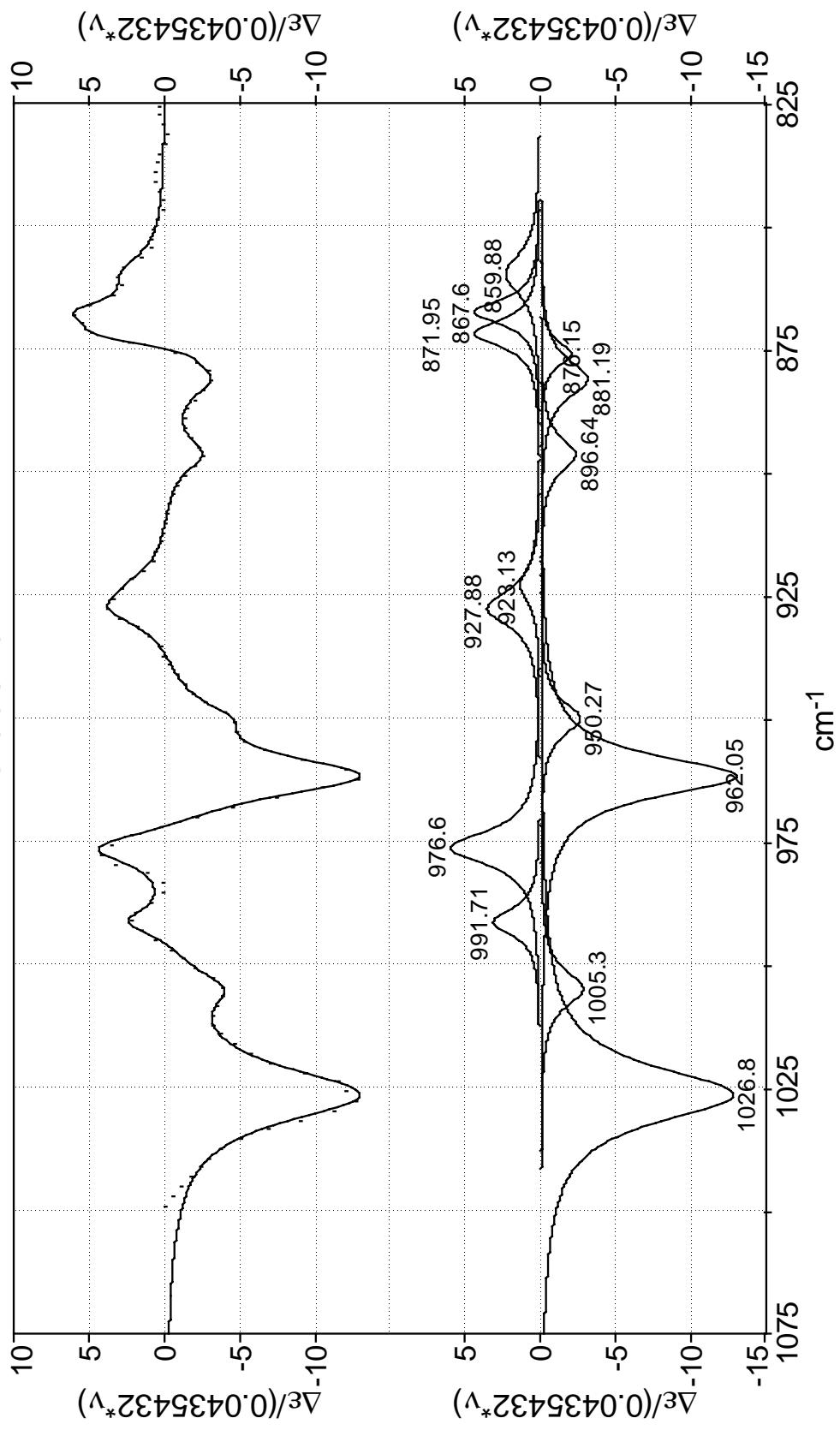


Figure S15a. The Lorentzian fitting of the experimental VCD spectrum of (+)-1 over the range 825 – 1075 cm⁻¹.

VCD peak fit results of (+)-Plumericin from 1025 to 1225 cm⁻¹
 $r^2=0.995323$

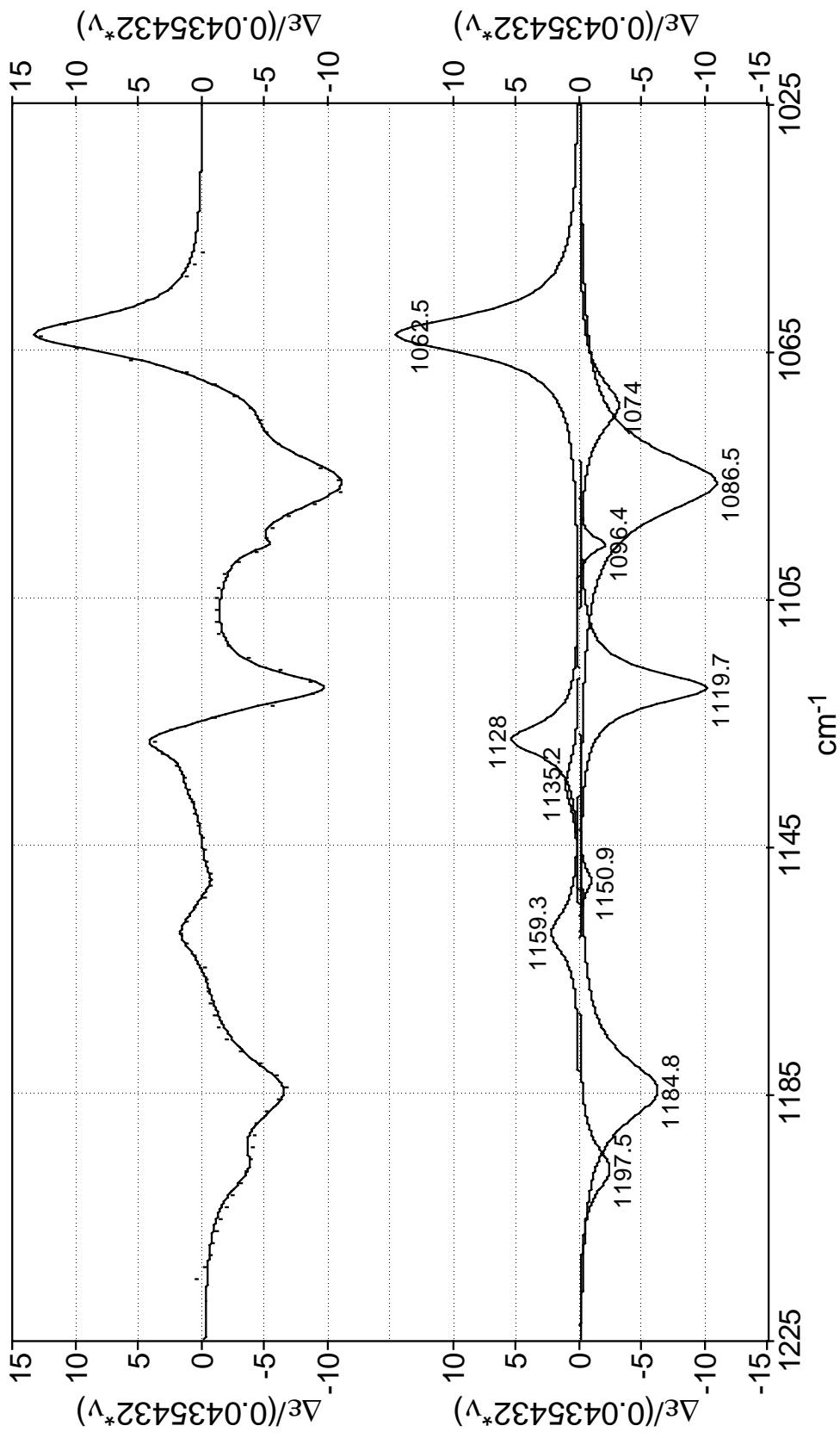


Figure S15b. The Lorentzian fitting of the experimental VCD spectrum of (+)-1 over the range 1025 – 1225 cm⁻¹.

VCD peak fit results of (+)-Plumericin from 1200 to 1450 cm⁻¹
 $r^2=0.998708$

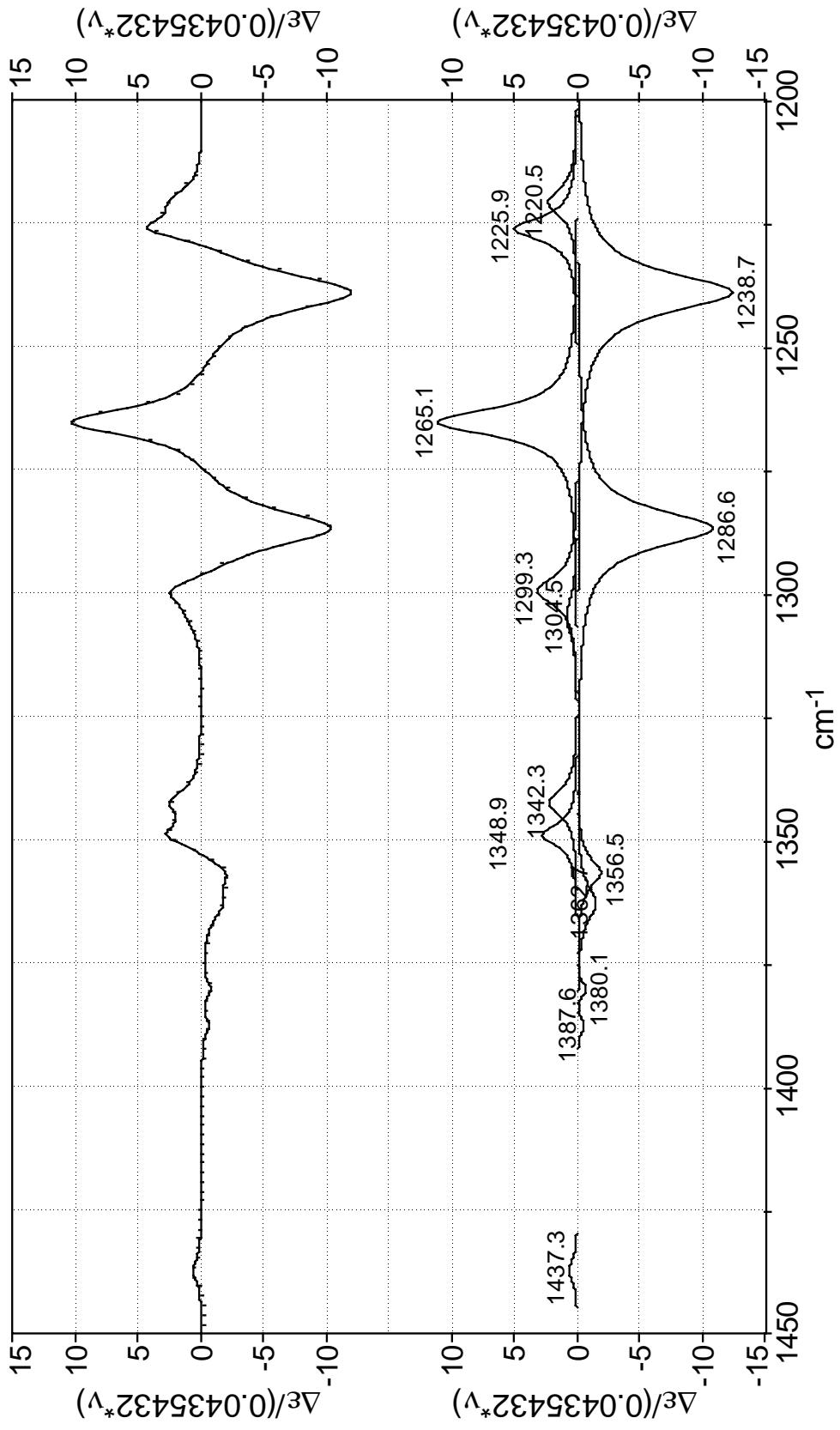


Figure S15c. The Lorentzian fitting of the experimental VCD spectrum of (+)-1 over the range 1200–1450 cm⁻¹.

VCD peak fit results of (+)-Isoplumericin from 790 to 890 cm⁻¹
 $r^2=0.992716$

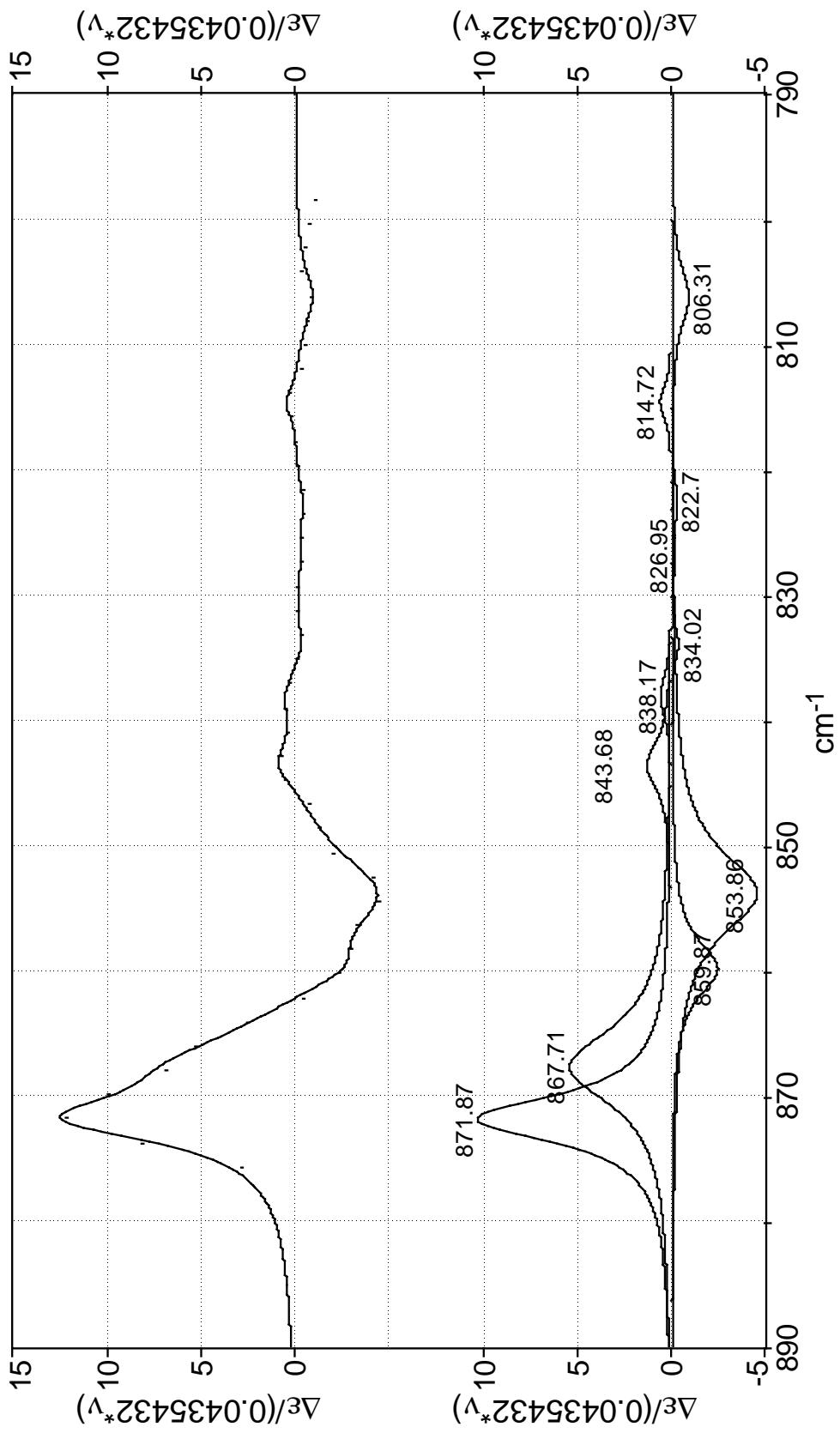


Figure S16a. The Lorentzian fitting of the experimental VCD spectrum of (+)-2 over the range 790 – 890 cm⁻¹.

VCD peak fit results of (+)-Isoplumericin from 950 to 1150 cm⁻¹
 $r^2=0.997569$

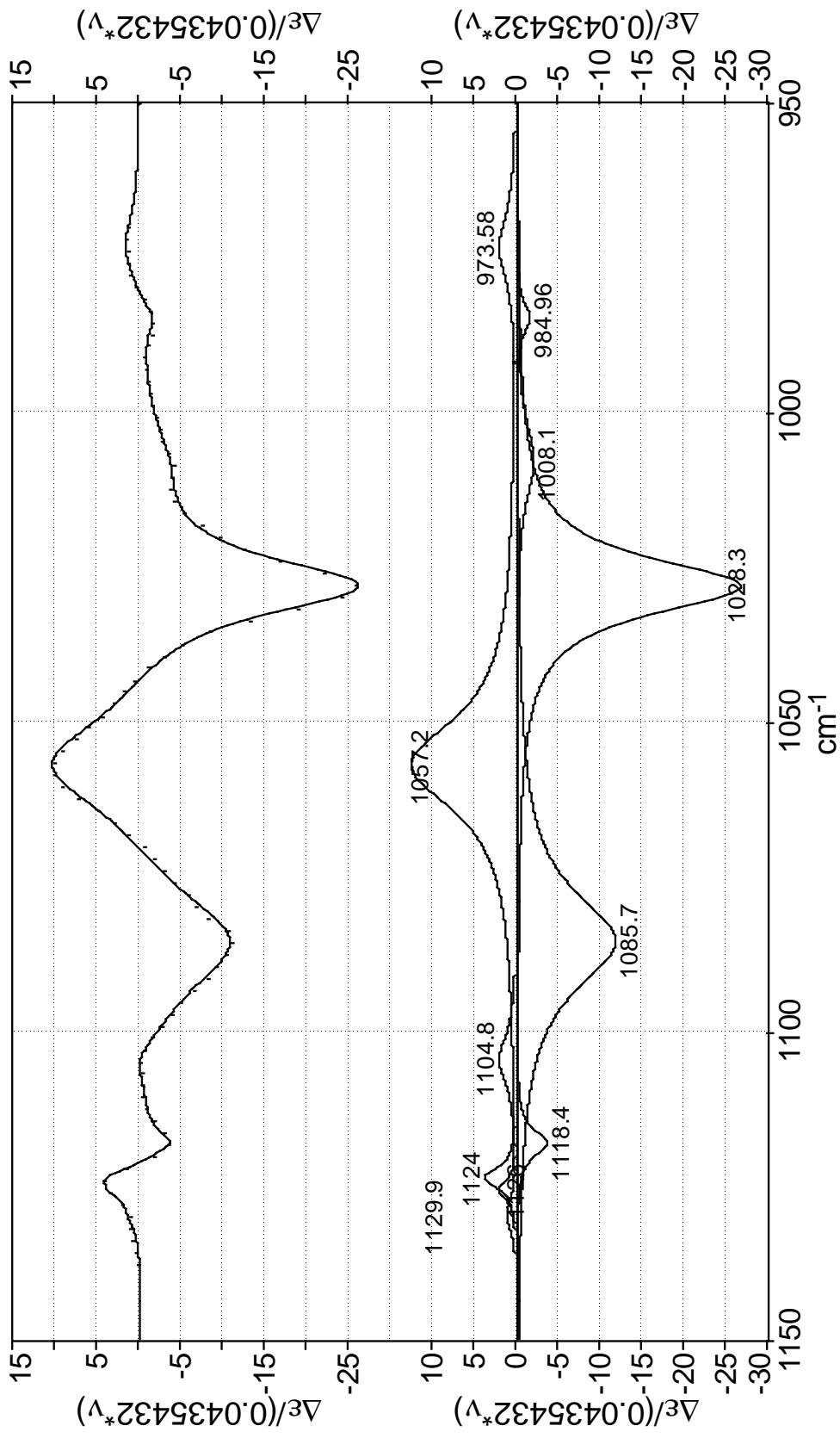


Figure S16b. The Lorentzian fitting of the experimental VCD spectrum of (+)-2 over the range 950 – 1150 cm⁻¹.

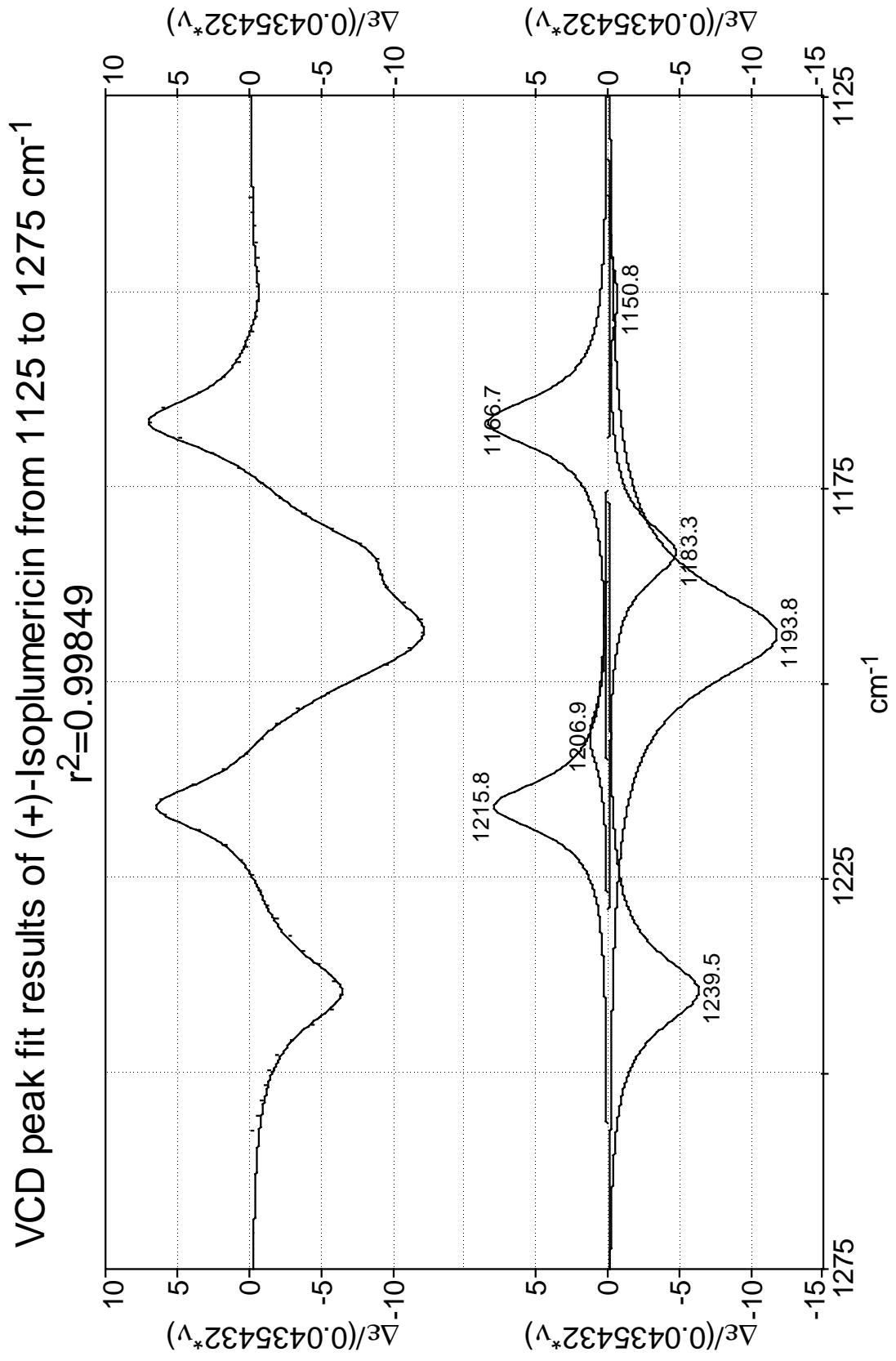


Figure S16c. The Lorentzian fitting of the experimental VCD spectrum of (+)-2 over the range 1125 – 1275 cm⁻¹.

VCD peak fit results of (+)-Isoplumericin from 1250 to 1500 cm⁻¹
 $r^2=0.993084$

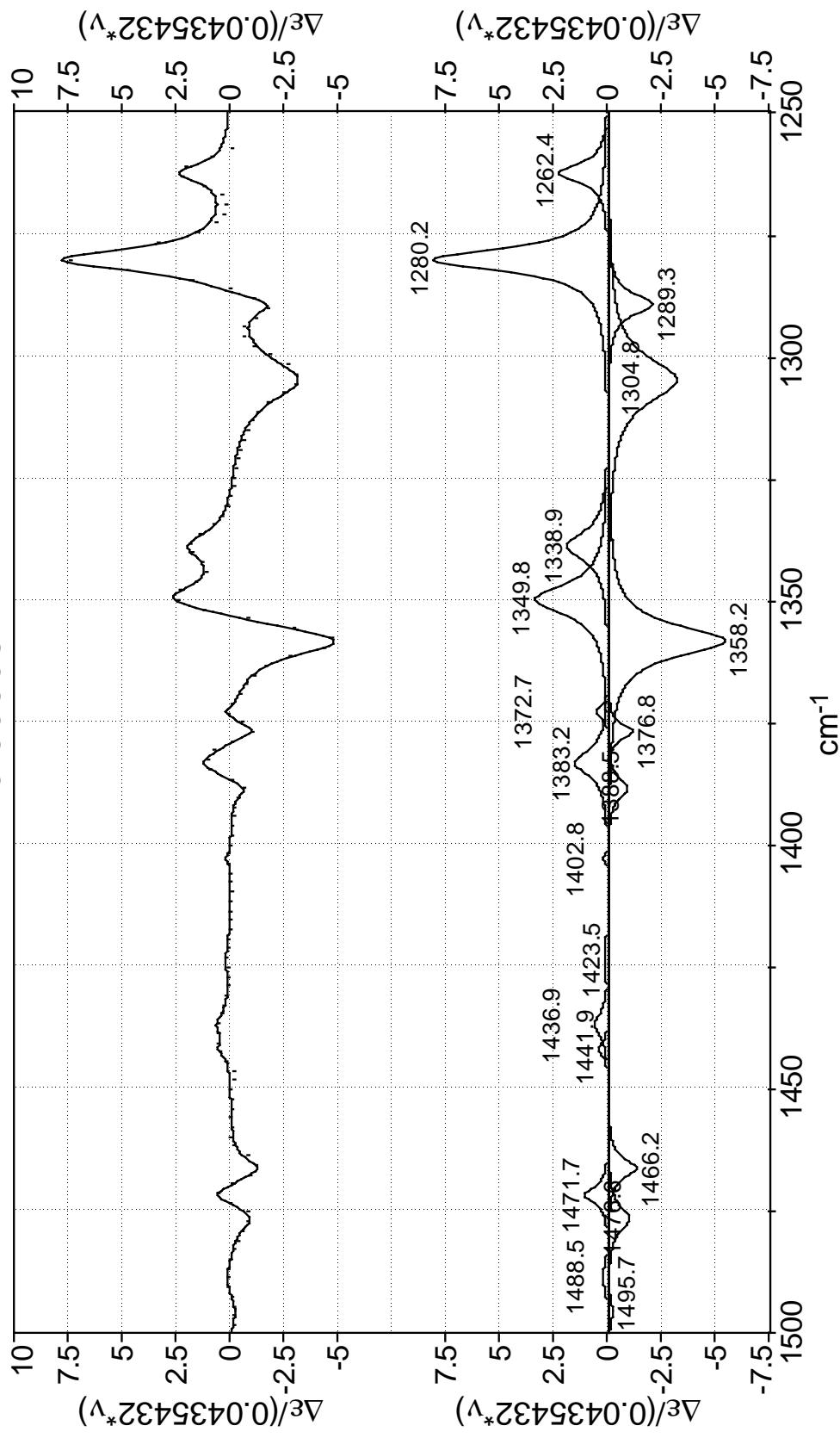


Figure S16d. The Lorentzian fitting of the experimental VCD spectrum of (+)-2 over the range 1250 – 1500 cm⁻¹.

Table S5. B3LYP/aug-cc-pVDZ//B3LYP/6-31G* calculated excitation energies, oscillator strengths and rotational strengths of the lowest 20 electronic excitations of **1a-1d**.^a

#	eV	Excitation Energy				λ Max. (nm)		
		v (cm ⁻¹)	λ (nm)	f	R _{velocity}	R _{length}	$\sigma = 0.2\text{ eV}$	$\sigma = 0.4\text{ eV}$
1a	1	4.53	36512	274	0.0008	-3.36	-3.47	
	2	4.64	37427	267	0.0034	6.11	6.21	268
	3	5.05	40720	246	0.0222	-51.99	-51.95	249
	4	5.16	41590	240	0.0194	24.06	24.82	
	5	5.17	41738	240	0.1300	17.31	18.45	
	6	5.42	43714	229	0.0261	37.36	37.95	229
	7	5.59	45084	222	0.1125	25.11	25.44	
	8	5.72	46125	217	0.0359	-5.69	-6.06	
	9	5.78	46598	215	0.0263	-38.65	-39.48	
	10	5.79	46716	214	0.0040	10.24	10.51	
	11	5.80	46751	214	0.0035	13.51	13.89	
	12	5.88	47416	211	0.1467	-12.00	-11.90	211
	13	5.94	47932	209	0.0372	11.05	11.24	
	14	5.99	48344	207	0.2487	-20.16	-20.50	206
	15	6.18	49865	201	0.0055	4.53	4.63	
	16	6.21	50058	200	0.0037	0.62	0.62	
	17	6.25	50388	198	0.0007	-9.81	-10.12	
	18	6.41	51664	194	0.0092	13.98	14.26	
	19	6.44	51929	193	0.0033	-10.68	-10.82	
	20	6.45	52026	192	0.0055	10.86	11.34	192

1	4.53	36575	273	0.0005	-3.77	-3.85	271
2	4.57	36891	271	0.0031	6.28	6.32	
3	4.97	40067	250	0.0249	-14.30	-14.78	253
4	5.17	41665	240	0.1273	13.08	14.92	
5	5.21	41992	238	0.0038	9.10	9.29	238
6	5.48	44226	226	0.0731	3.80	3.75	226
7	5.53	44641	224	0.0811	48.23	48.90	
8	5.61	45224	221	0.0004	-0.07	-0.07	
9	5.74	46279	216	0.0417	-42.04	-43.12	
1b	10	5.74	46333	216	0.0223	30.17	30.72
	11	5.84	47063	212	0.0497	-26.18	-26.01
	12	5.91	47642	210	0.1507	1.42	1.36
	13	5.98	48237	207	0.1123	15.53	15.61
	14	6.04	48681	205	0.1272	-21.36	-21.66
	15	6.11	49302	203	0.0045	3.99	4.00
	16	6.18	49836	201	0.0054	2.41	2.48
	17	6.30	50800	197	0.0006	-4.61	-4.93
	18	6.40	51618	194	0.0051	-8.13	-8.27
	19	6.40	51642	194	0.0060	4.47	4.55
	20	6.41	51690	193	0.0048	-7.67	-7.61

1	4.43	35731	280	0.0004	1.62	1.60	280	
2	4.70	37935	264	0.0159	0.66	0.70		
3	4.86	39160	255	0.0113	-8.18	-8.08	258	
4	5.08	40990	244	0.0007	9.05	9.23	247	
5	5.34	43053	232	0.0209	9.53	9.57		
6	5.36	43240	231	0.1987	-59.82	-61.49	230	225
7	5.61	45210	221	0.0021	-1.08	-1.05		
8	5.65	45552	220	0.0020	-2.22	-2.26		
9	5.69	45926	218	0.0237	-12.58	-12.71	217	
1c	10	5.72	46128	217	0.0398	12.00	12.22	
	11	5.77	46507	215	0.2542	-57.56	-58.87	
	12	5.90	47612	210	0.0751	-6.66	-7.01	
	13	5.91	47671	210	0.0079	17.90	18.58	
	14	5.98	48218	207	0.0404	24.81	25.12	205
	15	6.27	50543	198	0.0016	5.88	6.20	198
	16	6.32	50974	196	0.0012	4.55	4.63	
	17	6.35	51219	195	0.0264	-8.23	-8.55	
	18	6.35	51227	195	0.0045	5.95	6.13	
	19	6.36	51300	195	0.0126	-3.67	-3.75	
	20	6.38	51467	194	0.0026	-0.52	-0.42	

1	4.44	35782	279	0.0006	2.03	2.03	281	
2	4.62	37254	268	0.0140	-0.69	-0.68		
3	4.91	39615	252	0.0133	-8.58	-8.45	254	
4	5.05	40705	246	0.0012	4.43	4.57		
5	5.34	43053	232	0.1811	-45.03	-46.37	232	227
6	5.50	44352	225	0.0052	0.47	0.44		
7	5.55	44791	223	0.0104	0.66	0.77		
8	5.60	45159	221	0.0645	-1.39	-1.81		
9	5.63	45397	220	0.0029	-3.83	-3.74		
1d	10	5.73	46221	216	0.0117	-7.70	-7.72	217
	11	5.77	46503	215	0.2854	-35.78	-36.19	
	12	5.83	47041	213	0.0015	2.21	2.22	
	13	5.93	47856	209	0.0847	14.52	14.87	
	14	6.06	48866	205	0.0259	15.45	15.62	205
	15	6.20	50003	200	0.0010	0.04	0.05	
	16	6.27	50600	198	0.0033	-1.18	-0.96	
	17	6.29	50736	197	0.0191	-3.93	-4.27	
	18	6.35	51188	195	0.0014	0.43	0.40	
	19	6.38	51432	194	0.0084	-7.36	-7.26	194
	20	6.40	51608	194	0.0063	-4.66	-4.50	

^a f: Oscillator Strengths. R values in 10^{-40} esu²cm².

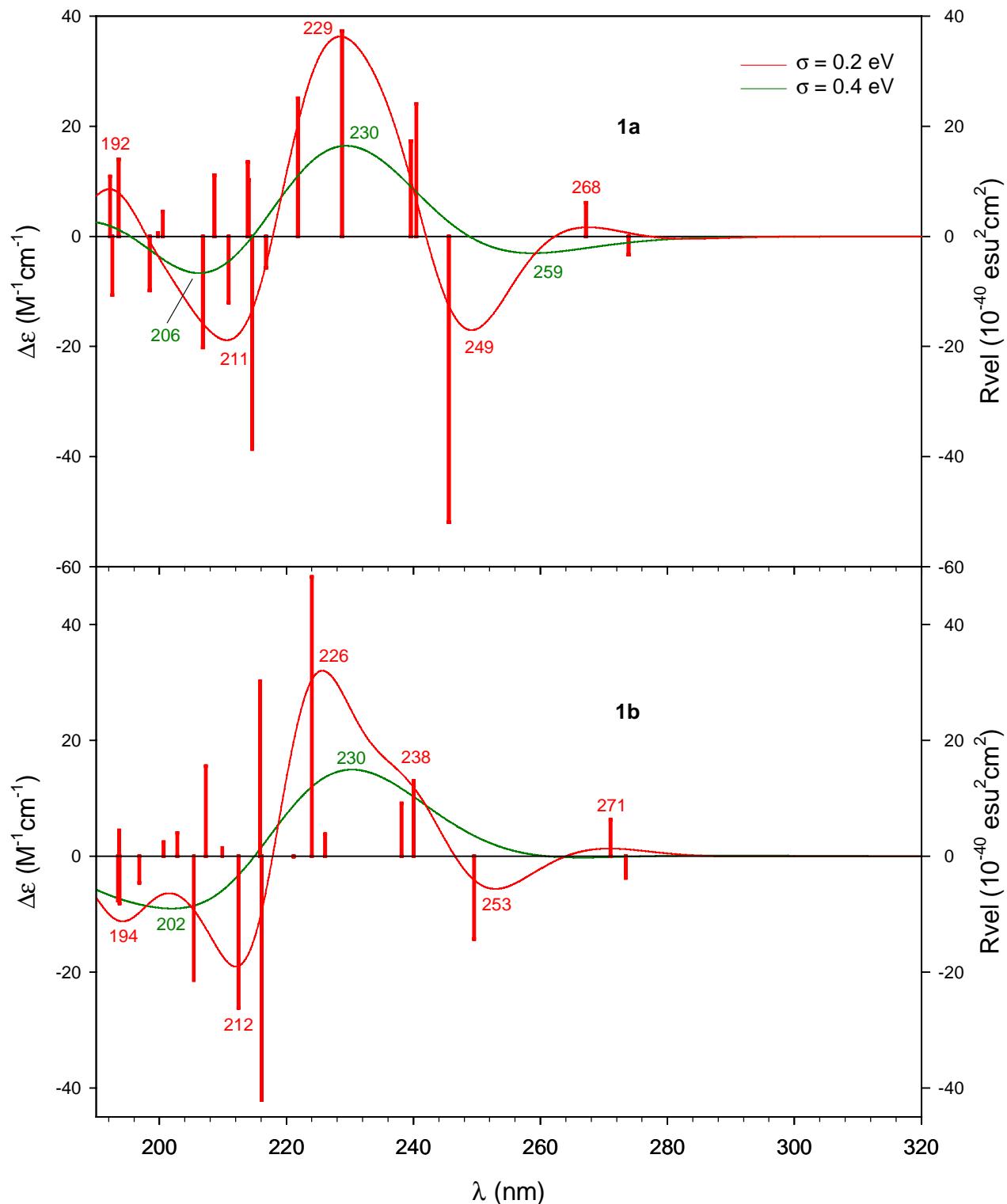


Figure S17a. B3LYP/aug-cc-pVDZ//B3LYP/6-31G* velocity rotational strengths and simulated ECD spectra of conformations **1a** and **1b**.

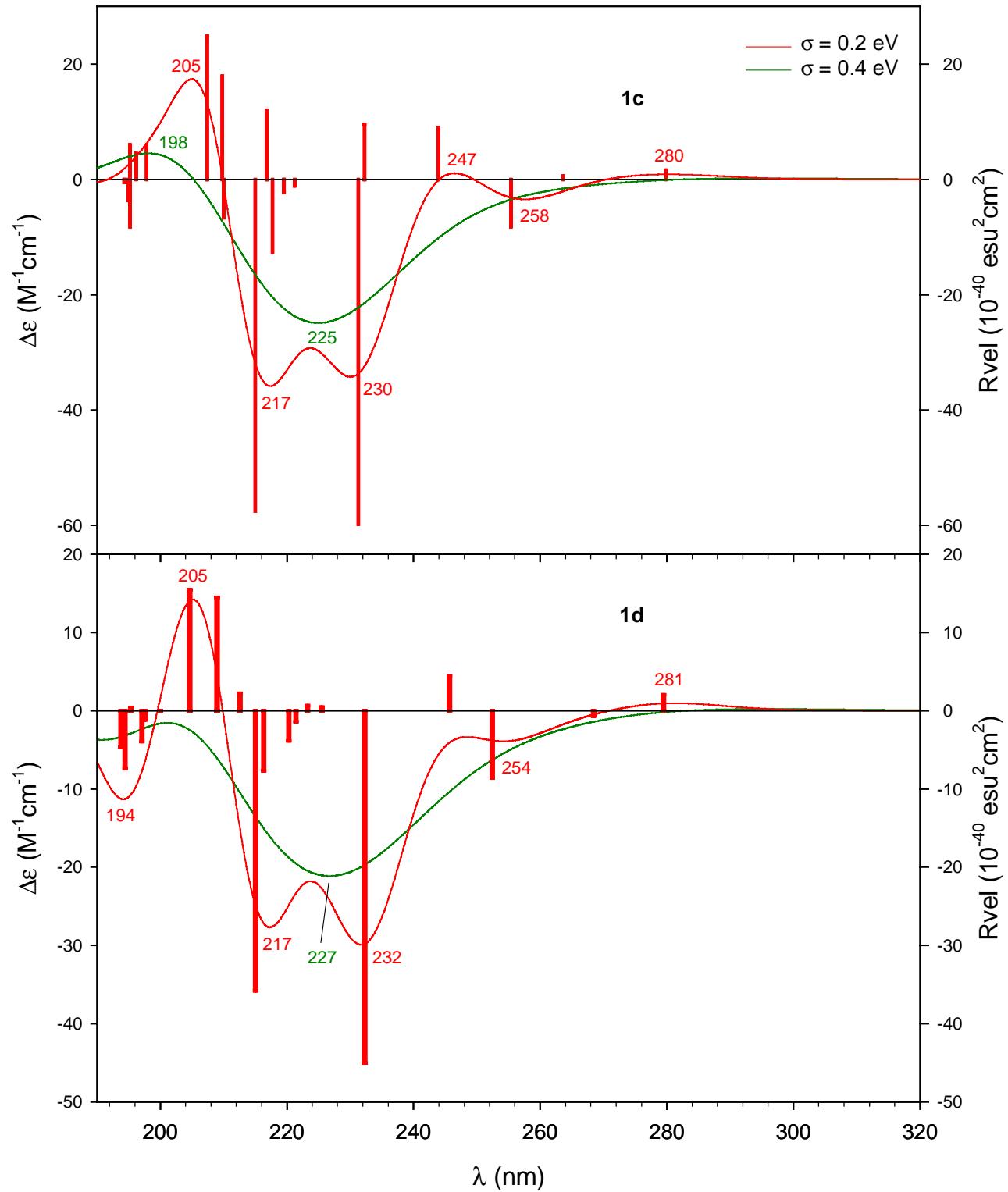


Figure S17b. B3LYP/aug-cc-pVDZ//B3LYP/6-31G* velocity rotational strengths and simulated ECD spectra of conformations **1c** and **1d**.

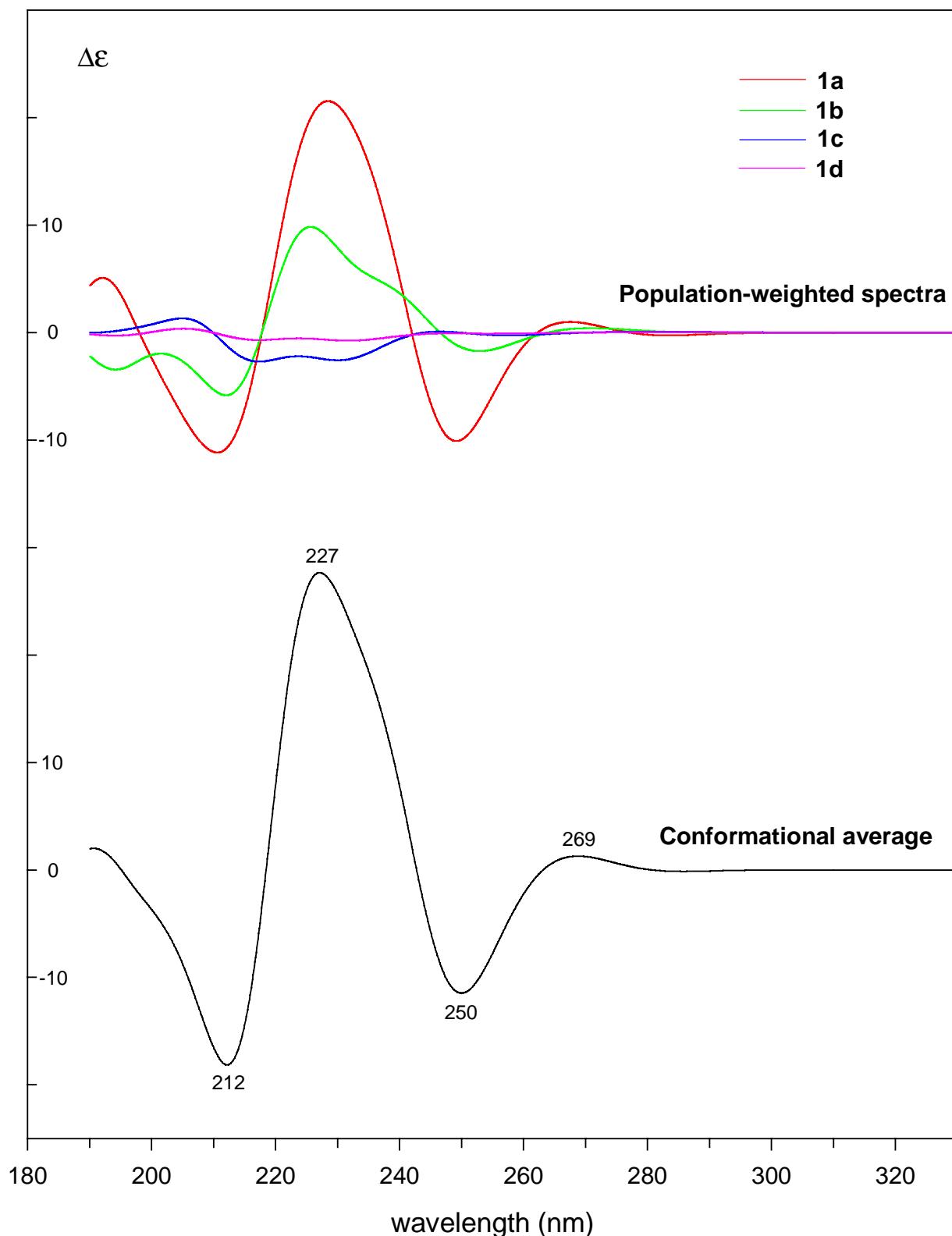


Figure S18a. B3LYP/aug-cc-pVDZ//B3LYP/6-31G* calculated ECD spectra of (1R,5S,8S,9S,10S)-1. Gaussian bandwidth, $\sigma = 0.2$ eV.

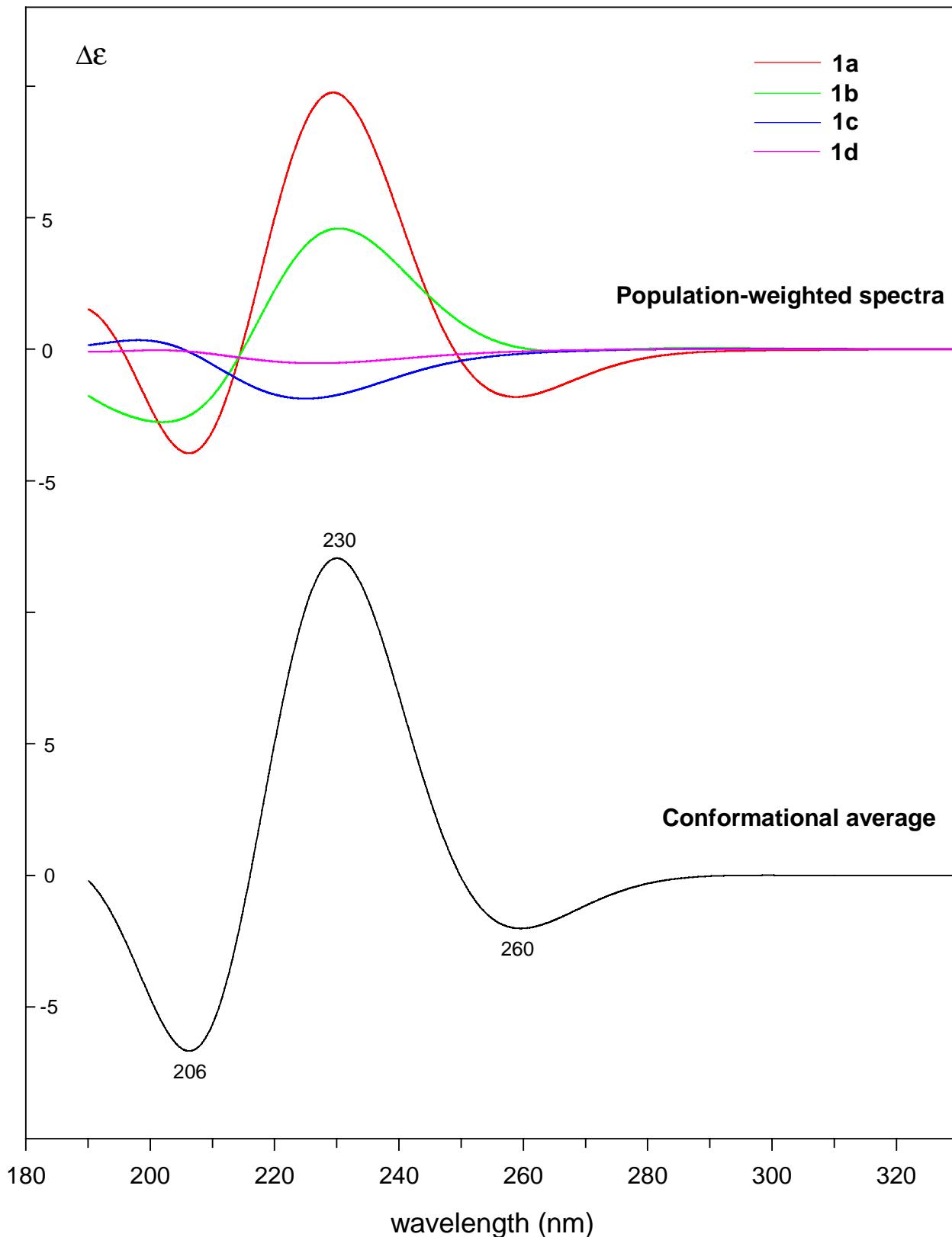


Figure S18b. B3LYP/aug-cc-pVDZ//B3LYP/6-31G* calculated ECD spectra of (1R,5S,8S,9S,10S)-1. Gaussian bandwidth, $\sigma = 0.4$ eV.

Table S6. B3LYP/aug-cc-pVDZ//B3LYP/6-31G* calculated excitation energies, oscillator strengths and rotational strengths of the lowest 20 electronic excitations of **2a-2d**.^a

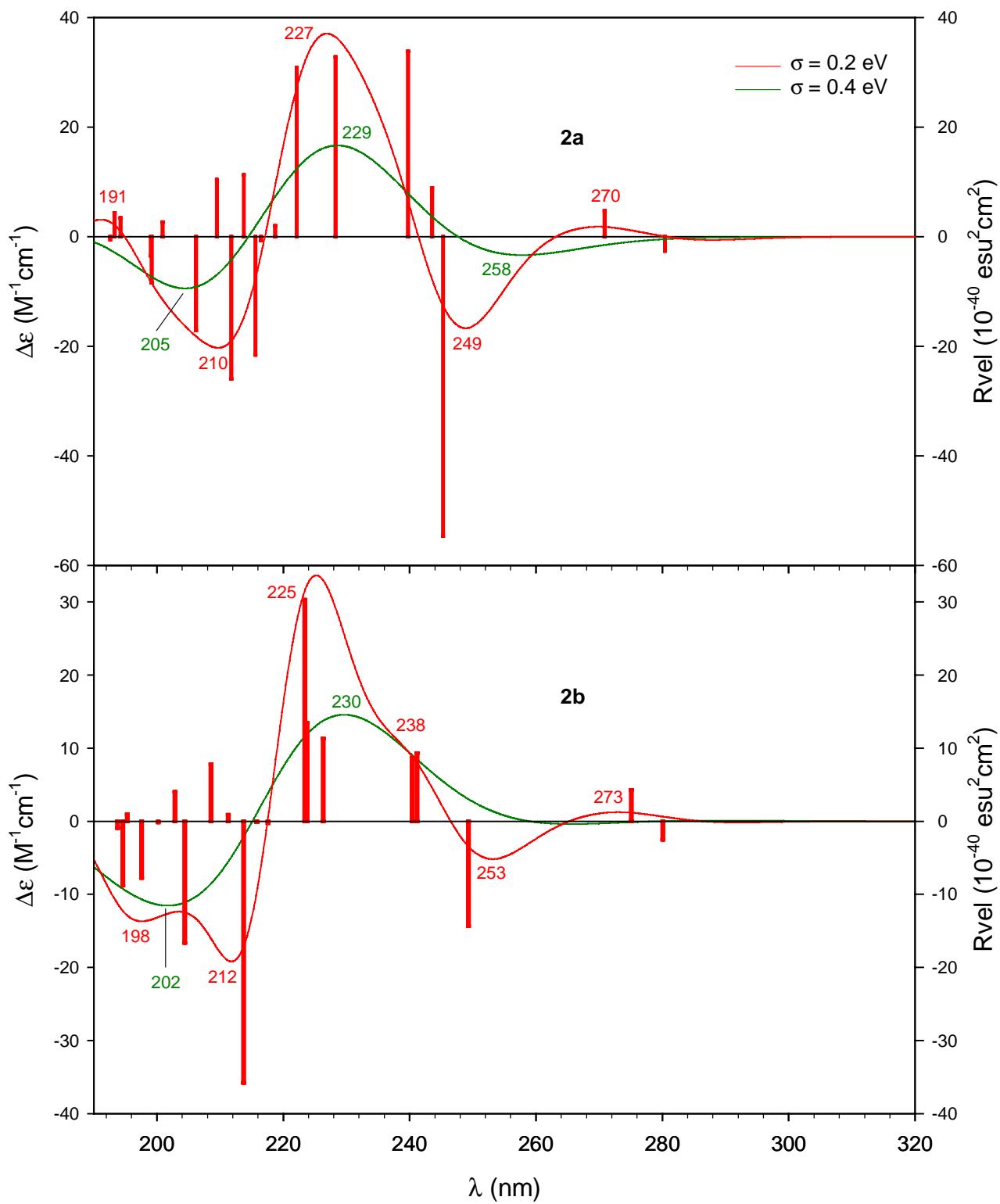
#	Excitation Energy					λ Max. (nm)		
	eV	v (cm ⁻¹)	λ (nm)	f	R _{velocity}	R _{length}	$\sigma = 0.2\text{ eV}$	$\sigma = 0.4\text{ eV}$
2a	1	4.42	35663	280	0.0012	-2.57	-2.73	
	2	4.58	36918	271	0.0023	4.73	4.88	270
	3	5.05	40768	245	0.0243	-54.67	-54.65	249
	4	5.09	41059	244	0.0043	8.90	9.30	
	5	5.17	41712	240	0.1404	33.84	35.29	
	6	5.43	43802	228	0.0229	32.82	33.33	227
	7	5.58	45019	222	0.1259	30.92	31.38	
	8	5.67	45723	219	0.0059	2.00	2.20	
	9	5.73	46198	216	0.0012	-0.66	-0.58	
	10	5.75	46384	216	0.0137	-21.54	-21.80	
	11	5.80	46784	214	0.0062	11.31	11.41	
	12	5.85	47223	212	0.3310	-25.96	-26.52	
	13	5.92	47737	209	0.0821	10.44	10.59	210
	14	6.01	48504	206	0.0484	-17.13	-17.34	205
	15	6.17	49776	201	0.0073	2.70	2.70	
	16	6.22	50203	199	0.0011	-8.38	-8.40	
	17	6.23	50244	199	0.0009	-3.47	-3.67	
	18	6.38	51475	194	0.0042	3.43	3.56	
	19	6.41	51736	193	0.0083	4.33	4.53	
	20	6.44	51918	193	0.0010	-0.52	-0.25	191

1	4.43	35702	280	0.0011	-2.51	-2.68	
2	4.51	36353	275	0.0020	4.27	4.40	273
3	4.97	40114	249	0.0264	-14.36	-14.84	253
4	5.14	41461	241	0.0026	9.31	9.60	
5	5.16	41597	240	0.1201	8.72	10.47	238
6	5.48	44185	226	0.0944	11.32	11.39	225
7	5.54	44689	224	0.0248	13.49	13.68	
8	5.55	44765	223	0.0500	30.34	30.79	
9	5.70	45956	218	0.0074	-0.27	0.01	
2b	10	5.74	46335	216	0.0056	-0.11	-0.14
	11	5.80	46790	214	0.0905	-35.82	-36.11
	12	5.87	47324	211	0.2806	0.90	0.66
	13	5.95	47950	209	0.0691	7.80	7.92
	14	6.07	48924	204	0.0348	-16.65	-16.85
	15	6.11	49300	203	0.0068	4.02	4.02
	16	6.19	49943	200	0.0026	-0.18	-0.14
	17	6.27	50610	198	0.0016	-7.76	-8.03
	18	6.35	51195	195	0.0030	0.98	0.97
	19	6.37	51387	195	0.0075	-8.81	-8.71
	20	6.40	51610	194	0.0010	-0.94	-1.00

1	4.31	34744	288	0.0010	0.94	0.92		
2	4.62	37227	269	0.0138	-2.15	-2.12	263	
3	4.78	38558	259	0.0174	-5.04	-4.81		
4	5.09	41014	244	0.0005	7.59	7.76	248	
5	5.33	43026	232	0.0538	7.33	7.27		
6	5.36	43223	231	0.1695	-56.13	-57.46	230	229
7	5.53	44627	224	0.0101	-4.45	-4.47		
8	5.60	45159	221	0.0331	-6.08	-6.15		
9	5.63	45397	220	0.0234	-2.23	-2.23		
2c	10	5.71	46034	217	0.1854	33.98	34.64	
	11	5.72	46130	217	0.1039	-47.73	-48.63	
	12	5.86	47297	211	0.0308	8.21	8.36	
	13	5.92	47726	210	0.0011	3.28	3.33	
	14	6.00	48356	207	0.0191	14.70	14.86	207
	15	6.27	50543	198	0.0026	0.76	0.80	205
	16	6.30	50834	197	0.0029	3.67	3.53	
	17	6.31	50922	196	0.0123	4.13	3.71	
	18	6.33	51028	196	0.0137	-16.29	-16.40	
	19	6.37	51348	195	0.0059	-2.75	-2.76	195
	20	6.37	51417	194	0.0067	-5.22	-5.20	

1	4.31	34790	287	0.0012	1.24	1.24		
2	4.53	36540	274	0.0118	-2.70	-2.68		
3	4.84	39003	256	0.0207	-5.14	-4.89	260	
4	5.05	40718	246	0.0012	4.50	4.63		
5	5.33	43003	233	0.1866	-45.46	-46.88	232	231
6	5.47	44094	227	0.0115	-2.03	-2.02		
7	5.49	44318	226	0.0022	1.70	1.73		
8	5.55	44755	223	0.0140	-2.66	-2.66		
9	5.60	45130	222	0.0722	-2.82	-3.27		
2d	10	5.71	46019	217	0.2541	-13.30	-13.37	
	11	5.72	46125	217	0.0425	3.39	3.19	
	12	5.84	47083	212	0.0014	2.79	2.81	
	13	5.89	47501	211	0.0348	7.71	7.86	
	14	6.08	49015	204	0.0140	9.82	9.93	208
	15	6.20	49993	200	0.0008	0.15	0.13	
	16	6.26	50505	198	0.0162	-5.33	-5.87	
	17	6.27	50543	198	0.0002	-0.44	-0.48	
	18	6.29	50736	197	0.0031	-1.12	-1.00	
	19	6.38	51419	194	0.0146	-24.71	-24.83	195
	20	6.40	51645	194	0.0047	2.21	2.31	193

^a f: Oscillator Strengths. R values in 10^{-40} esu 2 cm 2 .



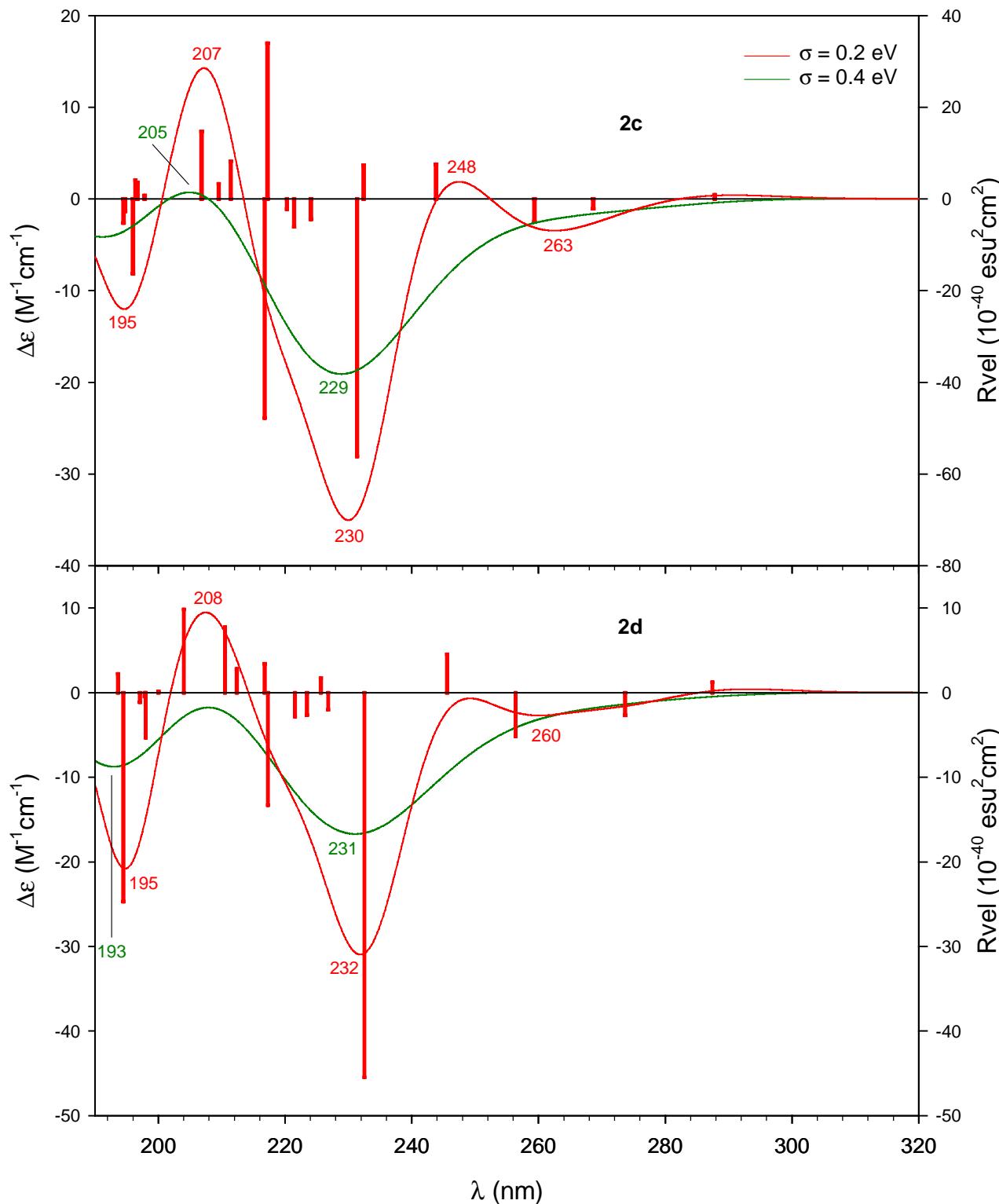


Figure S19b. B3LYP/aug-cc-pVDZ//B3LYP/6-31G* velocity rotational strengths and simulated ECD spectra of conformations **2c** and **2d**.

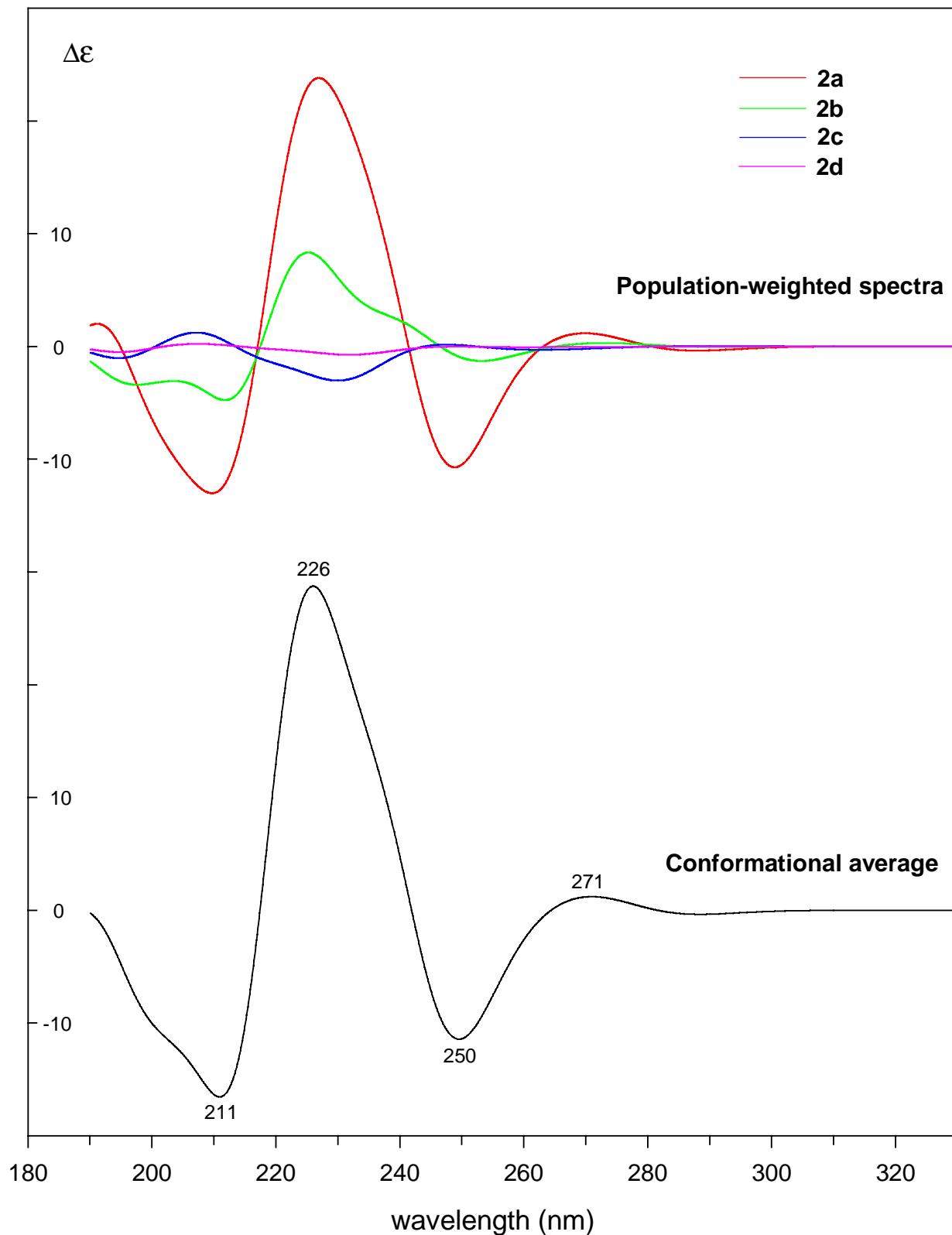


Figure S20a. B3LYP/aug-cc-pVDZ//B3LYP/6-31G* calculated ECD spectra of (1R,5S,8S,9S,10S)-**2**. Gaussian bandwidth, $\sigma = 0.2$ eV.

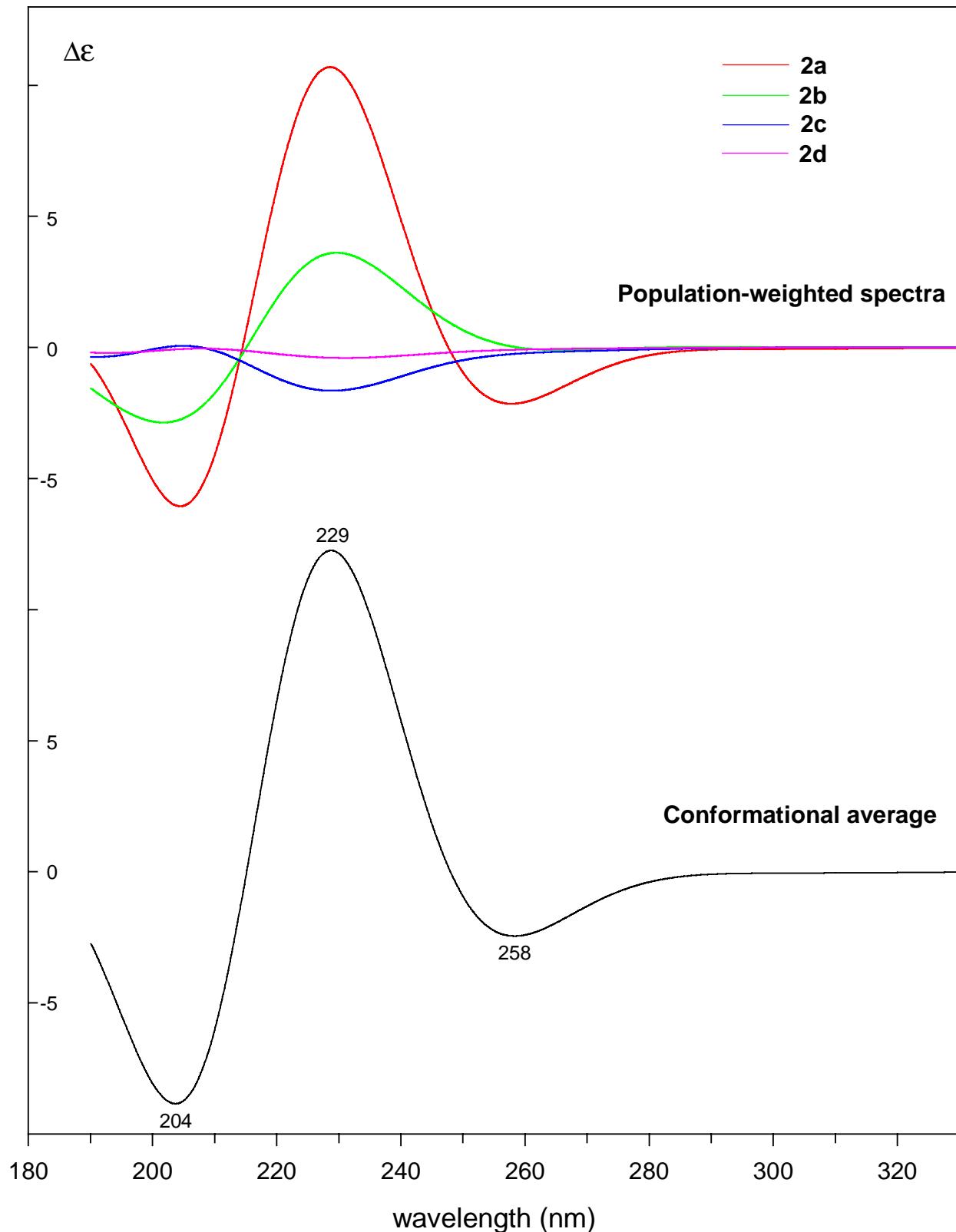


Figure S20b. B3LYP/aug-cc-pVDZ//B3LYP/6-31G* calculated ECD spectra of (1R,5S,8S,9S,10S)-**2**. Gaussian bandwidth, $\sigma = 0.4$ eV.

#B3LYP/6-31G* Opt

Plumericin conformation **1a**

C	1.787121	1.685454	-0.073664
H	2.361687	2.567898	0.187900
C	2.330787	0.456204	-0.154719
C	3.759910	0.224159	0.102042
C	1.463383	-0.764215	-0.371381
C	0.064805	-0.421601	-0.956524
O	0.485571	1.968503	-0.275644
C	-0.295830	1.066577	-1.105663
O	4.260233	-0.885450	0.178337
O	4.475962	1.367789	0.250681
C	5.870243	1.182520	0.535829
H	-0.196777	1.443367	-2.127280
O	-1.627798	1.202350	-0.733652
C	-1.923707	0.260378	0.325412
C	-0.991388	-0.951145	0.049056
H	-0.089437	-0.905507	-1.923847
H	2.004114	-1.467974	-1.014360
C	1.124518	-1.439776	0.948130
C	-0.186174	-1.520937	1.180444
O	-1.842713	-1.971371	-0.537585
H	-1.730386	0.730800	1.294618
C	-3.172967	-1.653711	-0.440350
C	-3.300377	-0.297483	0.159664
O	-4.042721	-2.405375	-0.804856
C	-4.488999	0.252214	0.436225
C	-4.728090	1.614060	1.003623
H	1.911301	-1.787475	1.609866
H	-0.655386	-1.960775	2.055388
H	-5.365825	-0.355703	0.211858
H	-3.800003	2.159915	1.191729
H	-5.300335	1.548650	1.938491
H	-5.336560	2.208632	0.309340
H	6.360427	0.637041	-0.274951
H	6.285052	2.187075	0.626600
H	6.004436	0.626296	1.467665

#B3LYP/6-31G* Opt

Plumericin conformation **1b**

C	1.844239	1.774770	-0.120201
H	2.457590	2.638460	0.118049
C	2.360174	0.532374	-0.187280
C	3.807865	0.396253	0.054503
C	1.460564	-0.671405	-0.371418
C	0.062111	-0.299538	-0.944842
O	0.550546	2.090764	-0.311380
C	-0.262673	1.194978	-1.115959
O	4.595195	1.311686	0.212229
O	4.183503	-0.911466	0.089775
C	5.582992	-1.137616	0.316312
H	-0.166895	1.551014	-2.145175
O	-1.586476	1.369081	-0.730622
C	-1.888189	0.457455	0.352531
C	-0.995237	-0.784346	0.081613
H	-0.116483	-0.795308	-1.901863
H	1.963339	-1.401120	-1.015630
C	1.116891	-1.316828	0.962771
C	-0.192482	-1.359415	1.211543
O	-1.883153	-1.787196	-0.479481
H	-1.662877	0.940456	1.308550
C	-3.202819	-1.430084	-0.366484
C	-3.282138	-0.065442	0.221912
O	-4.098605	-2.160673	-0.709902
C	-4.449940	0.515923	0.521819
C	-4.642539	1.886012	1.086621
H	1.898393	-1.672769	1.626611
H	-0.662274	-1.770351	2.100088
H	-5.346408	-0.071346	0.321354
H	-3.697178	2.406522	1.260634
H	-5.203564	1.839962	2.029370
H	-5.243543	2.494973	0.398314
H	5.889686	-0.719927	1.278987
H	5.709144	-2.220867	0.309648
H	6.180067	-0.675819	-0.474529

#B3LYP/6-31G* Opt

Plumericin conformation **1c**

C	1.842392	0.168960	-1.450836
H	2.893151	0.104411	-1.706844
C	0.931695	-0.720400	-1.882822
C	1.330271	-1.839918	-2.754626
C	-0.547879	-0.548798	-1.610136
C	-0.864582	0.661141	-0.679839
O	1.586000	1.270915	-0.709527
C	0.352911	1.348222	-0.025366
O	0.538703	-2.606905	-3.276248
O	2.672104	-1.938476	-2.929734
C	3.100583	-3.002715	-3.792124
H	0.185463	2.423178	0.105037
O	0.536581	0.724775	1.239094
C	-0.742772	0.387118	1.764213
C	-1.651469	0.078863	0.532887
H	-1.475881	1.400201	-1.201085
H	-1.036278	-0.407598	-2.584995
C	-1.213326	-1.721587	-0.913744
C	-1.841141	-1.370947	0.207560
O	-2.908951	0.750319	0.770729
H	-0.589696	-0.484897	2.407592
C	-2.838538	1.608719	1.840493
C	-1.493797	1.492385	2.464227
O	-3.765176	2.312552	2.157380
C	-1.112086	2.289195	3.470986
C	0.213282	2.271636	4.163211
H	-1.171028	-2.717673	-1.338736
H	-2.406961	-2.027772	0.861235
H	-1.844564	3.022098	3.811066
H	0.905190	1.552427	3.720216
H	0.082611	2.038464	5.228805
H	0.676984	3.266075	4.121742
H	2.688395	-2.876205	-4.796924
H	4.189050	-2.938884	-3.814121
H	2.780760	-3.970880	-3.397768

#B3LYP/6-31G* Opt

Plumericin conformation **1d**

C	-1.221667	1.868685	-1.199982
H	-1.649649	2.847137	-1.387661
C	-0.048980	1.494634	-1.741087
C	0.603761	2.491767	-2.614878
C	0.504384	0.096219	-1.566250
C	-0.381021	-0.799180	-0.643729
O	-2.031201	1.105324	-0.435885
C	-1.509667	-0.079556	0.127458
O	0.236243	3.639484	-2.785982
O	1.690874	1.968684	-3.243817
C	2.370682	2.867346	-4.134239
H	-2.384951	-0.727497	0.249516
O	-0.976431	0.263744	1.399718
C	-0.077489	-0.763552	1.799969
C	0.557339	-1.319920	0.487409
H	-0.792125	-1.640591	-1.204582
H	0.564854	-0.356822	-2.566072
C	1.878505	0.014008	-0.925948
C	1.911465	-0.782462	0.141024
O	0.560291	-2.759083	0.608971
H	0.656633	-0.289451	2.458882
C	-0.195402	-3.184067	1.675069
C	-0.691383	-1.995474	2.418419
O	-0.378576	-4.354226	1.901277
C	-1.542143	-2.111629	3.446480
C	-2.115126	-0.993076	4.256806
H	2.724622	0.547844	-1.343264
H	2.784235	-1.016145	0.743120
H	-1.844961	-3.125747	3.709595
H	-1.801746	-0.011665	3.894997
H	-1.824064	-1.099770	5.310687
H	-3.212306	-1.032873	4.236571
H	2.733721	3.744644	-3.592373
H	3.204070	2.296547	-4.545324
H	1.700209	3.197718	-4.931897

#B3PW91/TZ2P Opt

Plumericin conformation **1a**

C	1.976827	1.432918	-0.181587
H	2.669801	2.240619	0.013586
C	2.353760	0.147101	-0.197466
C	3.748334	-0.246958	0.024254
C	1.336192	-0.952404	-0.323171
C	-0.005302	-0.469807	-0.913271
O	0.724017	1.866868	-0.370173
C	-0.173466	1.031181	-1.140323
O	4.107781	-1.399093	0.124714
O	4.599332	0.796416	0.108636
C	5.964676	0.447856	0.349529
H	-0.036957	1.333968	-2.178910
O	-1.467368	1.354051	-0.774406
C	-1.867339	0.518491	0.328443
C	-1.102988	-0.805551	0.116254
H	-0.227859	-0.976935	-1.850279
H	1.767508	-1.758112	-0.920906
C	0.936923	-1.491833	1.031242
C	-0.364565	-1.398895	1.271795
O	-2.075544	-1.737336	-0.405342
H	-1.605520	1.005945	1.268595
C	-3.348270	-1.254957	-0.319591
C	-3.297709	0.130086	0.207867
O	-4.299828	-1.906793	-0.640369
C	-4.397419	0.825536	0.490425
C	-4.455781	2.216871	1.005479
H	1.677111	-1.892591	1.710750
H	-0.867814	-1.723668	2.173017
H	-5.342529	0.319301	0.311244
H	-3.470112	2.644625	1.177651
H	-5.031027	2.255983	1.934082
H	-4.982787	2.855069	0.290803
H	6.350657	-0.174332	-0.456643
H	6.504147	1.390031	0.392325
H	6.065033	-0.090634	1.290949

#B3PW91/TZ2P Opt

Plumericin conformation **1b**

C	1.841934	1.761838	-0.122451
H	2.463469	2.619546	0.102818
C	2.349070	0.522157	-0.171523
C	3.795111	0.387106	0.055899
C	1.447277	-0.671191	-0.336323
C	0.066282	-0.303432	-0.922991
O	0.556544	2.078636	-0.312569
C	-0.248516	1.179740	-1.110993
O	4.575648	1.297867	0.208872
O	4.172180	-0.911368	0.079041
C	5.569284	-1.132519	0.289608
H	-0.137988	1.522229	-2.140199
O	-1.570603	1.360820	-0.746590
C	-1.886740	0.463393	0.333941
C	-0.998953	-0.774644	0.087020
H	-0.100157	-0.803006	-1.875546
H	1.946459	-1.414717	-0.960290
C	1.092110	-1.287574	0.998239
C	-0.213446	-1.329235	1.230248
O	-1.875448	-1.777475	-0.470968
H	-1.671300	0.948780	1.286895
C	-3.189359	-1.421968	-0.376510
C	-3.272659	-0.058675	0.200254
O	-4.072720	-2.150623	-0.725444
C	-4.434148	0.512536	0.512873
C	-4.627861	1.868972	1.084258
H	1.860076	-1.631388	1.678239
H	-0.687576	-1.725223	2.118656
H	-5.325209	-0.077948	0.315437
H	-3.688781	2.382374	1.281549
H	-5.207177	1.813602	2.009445
H	-5.211764	2.482727	0.392739
H	5.882385	-0.722750	1.248812
H	5.701997	-2.210800	0.274538
H	6.154429	-0.665297	-0.501109

#B3PW91/TZ2P Opt

Plumericin conformation **1c**

C	1.905514	1.397804	-0.691722
H	2.625617	2.203212	-0.684800
C	2.229007	0.145130	-0.352968
C	3.608673	-0.190919	0.022800
C	1.250970	-0.990333	-0.480202
C	-0.163921	-0.531629	-0.904955
O	0.704347	1.814411	-1.128852
C	-0.407598	0.981398	-0.915360
O	4.001423	-1.326231	0.175088
O	4.405716	0.885477	0.178237
C	5.765187	0.592637	0.509909
H	-1.1111305	1.265342	-1.701669
O	-0.939790	1.313908	0.353526
C	-1.750059	0.240347	0.795570
C	-1.131686	-1.046947	0.188395
H	-0.433629	-0.957406	-1.868478
H	1.661202	-1.675378	-1.230027
C	1.009346	-1.775288	0.784549
C	-0.273246	-1.843219	1.111397
O	-2.222913	-1.817447	-0.341664
H	-1.709262	0.247829	1.885440
C	-3.390682	-1.109824	-0.355962
C	-3.160878	0.205736	0.284027
O	-4.396367	-1.557804	-0.826725
C	-4.118355	1.129699	0.353388
C	-4.009071	2.472827	0.978020
H	1.825953	-2.236425	1.321302
H	-0.688523	-2.371558	1.959388
H	-5.072176	0.863749	-0.095686
H	-3.027821	2.658598	1.408258
H	-4.771369	2.586576	1.753736
H	-4.211437	3.250695	0.236556
H	6.231803	-0.007295	-0.270224
H	6.259696	1.556407	0.594151
H	5.822709	0.052617	1.453849

#B3PW91/TZ2P Opt

Plumericin conformation **1d**

C	1.760388	1.775320	-0.546967
H	2.406155	2.641256	-0.493853
C	2.224177	0.546748	-0.292339
C	3.657780	0.460551	0.035822
C	1.367918	-0.677707	-0.464066
C	-0.086400	-0.345762	-0.881018
O	0.518397	2.094040	-0.941770
C	-0.495408	1.130628	-0.807291
O	4.394069	1.397055	0.240063
O	4.081850	-0.822738	0.070458
C	5.472361	-0.992990	0.359746
H	-1.212192	1.381083	-1.593389
O	-1.087133	1.324809	0.463868
C	-1.784709	0.145380	0.815399
C	-1.005206	-1.026916	0.163878
H	-0.299167	-0.737800	-1.872711
H	1.836819	-1.292891	-1.239426
C	1.196279	-1.531766	0.767706
C	-0.074026	-1.757655	1.069682
O	-1.985096	-1.896389	-0.425355
H	-1.780626	0.093981	1.904907
C	-3.225730	-1.324718	-0.450019
C	-3.165629	-0.020690	0.249555
O	-4.159353	-1.863101	-0.971329
C	-4.222245	0.788191	0.317560
C	-4.286550	2.107716	0.996368
H	2.047465	-1.921251	1.307565
H	-0.436796	-2.362295	1.890349
H	-5.123915	0.437438	-0.178576
H	-3.348812	2.383533	1.472764
H	-5.084535	2.103699	1.743981
H	-4.548407	2.888607	0.276989
H	5.716037	-0.570851	1.333544
H	5.644539	-2.065803	0.354944
H	6.083546	-0.506086	-0.398664

#B3LYP/6-31G* Opt

Isoplumericin conformation **2a**

C	1.874229	-1.636489	0.615918
H	2.588923	-2.183177	1.222154
C	0.973824	-2.246700	-0.178173
C	0.904649	-3.711680	-0.282980
C	-0.097978	-1.455305	-0.894528
C	0.226677	0.061738	-0.987885
O	1.987807	-0.304489	0.778825
C	1.490771	0.568966	-0.271805
O	0.020795	-4.304503	-0.878819
O	1.921708	-4.349013	0.351251
C	1.871479	-5.782238	0.298628
H	2.338446	0.740538	-0.940423
O	1.162062	1.785342	0.314256
C	-0.213534	1.731289	0.765818
C	-0.920511	0.817186	-0.267230
H	0.271648	0.392370	-2.028171
H	-0.250516	-1.893434	-1.887555
C	-1.409824	-1.476323	-0.125329
C	-1.840367	-0.262597	0.221749
O	-1.613695	1.728038	-1.161699
H	-0.245227	1.336122	1.786072
C	-1.635796	3.013822	-0.686755
C	-0.869926	3.064288	0.591121
O	-2.215642	3.892130	-1.279353
C	-0.778205	4.106171	1.431607
H	-1.983264	5.531468	0.353131
H	-1.897899	-2.416639	0.109741
H	-2.747427	-0.038688	0.775045
C	-1.400728	5.457131	1.270966
H	-0.616875	6.226716	1.263185
H	-0.179840	3.960554	2.332506
H	-2.042646	5.680369	2.133868
H	1.905172	-6.131544	-0.736737
H	2.749769	-6.124892	0.846933
H	0.956901	-6.155347	0.767820

#B3LYP/6-31G* Opt

Isoplumericin conformation **2b**

C	-1.973229	-1.725994	-0.506965
H	-2.835760	-2.199568	-0.965886
C	-0.777572	-2.342526	-0.438274
C	-0.697866	-3.705163	-0.994490
C	0.445468	-1.612871	0.074990
C	0.088464	-0.341516	0.899068
O	-2.240106	-0.488107	-0.053841
C	-1.393478	0.062485	0.991113
O	-1.631415	-4.356723	-1.426692
O	0.580187	-4.173436	-0.977347
C	0.749787	-5.500615	-1.497534
H	-1.869088	-0.214508	1.935585
O	-1.440397	1.447418	0.885158
C	-0.406418	1.882700	-0.031034
C	0.744568	0.866673	0.180989
H	0.483960	-0.407887	1.915229
H	1.052484	-2.304609	0.669597
C	1.280251	-1.050546	-1.066241
C	1.425482	0.274245	-1.017376
O	1.698397	1.551514	1.035672
H	-0.801275	1.881920	-1.051866
C	1.420862	2.888257	1.164524
C	0.167690	3.190026	0.416332
O	2.142591	3.620506	1.798307
C	-0.355196	4.403817	0.184257
H	1.103429	5.612392	1.212434
H	1.677930	-1.701661	-1.838225
H	1.973808	0.884471	-1.728726
C	0.183033	5.723287	0.639882
H	-0.566787	6.234590	1.258753
H	-1.278485	4.439606	-0.396344
H	0.363615	6.374779	-0.225816
H	0.438050	-5.546836	-2.544474
H	1.814411	-5.717873	-1.403849
H	0.158574	-6.217751	-0.921907

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Isoplumericin conformation **2c**

C	2.171737	0.125338	-1.333785
H	3.226368	0.100220	-1.580597
C	1.296206	-0.788282	-1.787510
C	1.739853	-1.880454	-2.671927
C	-0.190564	-0.673421	-1.525514
C	-0.558687	0.515118	-0.586506
O	1.871169	1.207449	-0.580541
C	0.627993	1.236875	0.089246
O	0.979063	-2.668344	-3.208123
O	3.085065	-1.927690	-2.842303
C	3.554963	-2.963453	-3.717565
H	0.422119	2.304256	0.225990
O	0.817544	0.609631	1.351140
C	-0.456846	0.229965	1.853283
C	-1.335518	-0.107476	0.613274
H	-1.189081	1.238284	-1.107507
H	-0.676279	-0.541139	-2.502973
C	-0.817284	-1.876571	-0.845505
C	-1.466561	-1.560415	0.273719
O	-2.620550	0.509940	0.849465
H	-0.286061	-0.633779	2.503236
C	-2.597558	1.366729	1.922459
C	-1.245969	1.320609	2.543125
O	-3.573281	2.010058	2.227721
C	-0.782456	2.127772	3.509784
H	-2.532661	3.347620	3.823574
H	-0.733804	-2.866568	-1.278582
H	-2.011697	-2.244416	0.916993
C	-1.517154	3.232812	4.201636
H	-0.970920	4.178617	4.085572
H	0.252376	1.971126	3.819443
H	-1.556933	3.032524	5.281198
H	3.138752	-2.840297	-4.721106
H	4.640173	-2.857407	-3.737450
H	3.272638	-3.948280	-3.335960

#B3LYP/6-31G* Opt

Isoplumericin conformation **2d**

C	-2.422761	1.026735	-0.336269
H	-3.284297	1.685061	-0.349520
C	-1.760635	0.706619	-1.461941
C	-2.291516	1.292999	-2.710034
C	-0.621852	-0.291377	-1.465565
C	-0.267411	-0.817946	-0.039637
O	-2.171023	0.554752	0.902793
C	-0.935079	-0.083383	1.145294
O	-3.183434	2.117657	-2.787925
O	-1.666500	0.783497	-3.805976
C	-2.143512	1.281408	-5.065684
H	-1.144491	-0.771072	1.972171
O	-0.021719	0.921280	1.567149
C	1.296144	0.418868	1.399688
C	1.250836	-0.527980	0.165508
H	-0.457992	-1.890397	0.033133
H	-0.930335	-1.134216	-2.100406
C	0.702624	0.235639	-1.988070
C	1.708122	0.063357	-1.131957
O	2.018495	-1.697561	0.525167
H	1.940464	1.290158	1.246040
C	2.320440	-1.728581	1.865510
C	1.806930	-0.484780	2.500255
O	2.910110	-2.664706	2.349795
C	1.754147	-0.220935	3.814912
H	2.625501	-2.040031	4.578349
H	0.779870	0.680312	-2.973633
H	2.746218	0.336449	-1.295039
C	2.220696	-1.094054	4.937120
H	1.393072	-1.286821	5.632935
H	1.307582	0.732868	4.101416
H	2.993198	-0.570965	5.517418
H	-2.009609	2.364658	-5.127162
H	-1.545663	0.776044	-5.824982
H	-3.203998	1.049072	-5.193524

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Isoplumericin conformation **2a**

C	1.861596	-1.635529	0.623055
H	2.576439	-2.189051	1.217417
C	0.960409	-2.239211	-0.164125
C	0.906419	-3.698933	-0.287295
C	-0.107699	-1.447796	-0.865795
C	0.223209	0.056016	-0.966312
O	1.972382	-0.312586	0.793686
C	1.480641	0.555191	-0.256289
O	0.043659	-4.284581	-0.903485
O	1.909481	-4.334894	0.352670
C	1.871519	-5.761634	0.273171
H	2.326897	0.714636	-0.924876
O	1.161811	1.772159	0.318238
C	-0.209540	1.733694	0.759401
C	-0.914877	0.820446	-0.260936
H	0.276160	0.376465	-2.005089
H	-0.272327	-1.886283	-1.852339
C	-1.405675	-1.458939	-0.091049
C	-1.830864	-0.246802	0.241605
O	-1.601147	1.719234	-1.159978
H	-0.252609	1.348889	1.779090
C	-1.617703	3.003271	-0.700841
C	-0.858669	3.060135	0.573481
O	-2.183301	3.873164	-1.301370
C	-0.782504	4.094345	1.413759
H	-1.982618	5.515416	0.340682
H	-1.896575	-2.390122	0.158001
H	-2.732467	-0.020592	0.795456
C	-1.402786	5.434867	1.254862
H	-0.621244	6.200236	1.252385
H	-0.194614	3.944935	2.316656
H	-2.040154	5.653453	2.116128
H	1.928719	-6.090866	-0.763307
H	2.737812	-6.108985	0.829464
H	0.955160	-6.148554	0.717042

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Isoplumericin conformation **2b**

C	1.991054	1.760967	0.067033
H	2.655037	2.557246	0.379744
C	2.436728	0.509992	-0.115038
C	3.874060	0.282779	0.093243
C	1.481049	-0.614216	-0.409210
C	0.113751	-0.117571	-0.929860
O	0.724843	2.162286	-0.083741
C	-0.132793	1.390128	-0.956897
O	4.696216	1.132987	0.344921
O	4.189725	-1.026611	-0.028877
C	5.574071	-1.334775	0.153323
H	-0.021321	1.834131	-1.946354
O	-1.439752	1.589626	-0.550021
C	-1.770917	0.606685	0.449801
C	-0.962410	-0.639482	0.042918
H	-0.089554	-0.506608	-1.925779
H	1.942121	-1.298144	-1.124254
C	1.107284	-1.371615	0.845465
C	-0.196113	-1.374152	1.093427
O	-1.910921	-1.507884	-0.614327
H	-1.503222	0.986426	1.436672
C	-3.199096	-1.089815	-0.451401
C	-3.190872	0.179264	0.318344
O	-4.119049	-1.718309	-0.893896
C	-4.250690	0.813939	0.823927
H	-5.808467	-0.496461	0.141442
H	1.862938	-1.834565	1.465992
H	-0.680132	-1.849946	1.936175
C	-5.678861	0.423831	0.702353
H	-6.235519	1.226028	0.209226
H	-4.050865	1.724453	1.384504
H	-6.119726	0.314541	1.697135
H	5.902404	-1.050970	1.152251
H	5.656925	-2.409509	0.016620
H	6.183408	-0.809132	-0.580414

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Isoplumericin conformation **2c**

C	-1.989375	-1.520156	-0.433680
H	-2.725848	-2.303447	-0.326906
C	-2.301191	-0.224649	-0.318966
C	-3.687545	0.188483	-0.064860
C	-1.295788	0.862060	-0.581601
C	0.123250	0.321801	-0.876414
O	-0.780942	-2.019560	-0.744360
C	0.338974	-1.177373	-0.633644
O	-4.059535	1.339951	-0.112118
O	-4.515955	-0.836147	0.221195
C	-5.880778	-0.470838	0.439318
H	1.059895	-1.593299	-1.341567
O	0.830146	-1.307100	0.688173
C	1.650775	-0.189522	0.963817
C	1.064147	0.992373	0.155831
H	0.431900	0.581890	-1.886250
H	-1.664758	1.430424	-1.442207
C	-1.083466	1.827361	0.557128
C	0.187910	1.927628	0.917175
O	2.183404	1.666499	-0.443188
H	1.603020	-0.026155	2.040947
C	3.343051	0.955899	-0.320743
C	3.070215	-0.267927	0.468490
O	4.364478	1.348280	-0.811127
C	3.911661	-1.282190	0.680351
H	5.621992	-0.570144	-0.407517
H	-1.909481	2.375268	0.987441
H	0.582921	2.572816	1.690706
C	5.309608	-1.417756	0.194346
H	5.413613	-2.339739	-0.384473
H	3.525833	-2.114272	1.265734
H	5.985624	-1.518499	1.048537
H	-6.298481	0.006198	-0.446255
H	-6.402031	-1.400314	0.651082
H	-5.965647	0.212707	1.282845

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Isoplumericin conformation **2d**

C	1.863943	1.845569	-0.301875
H	2.537885	2.680801	-0.168200
C	2.299551	0.582993	-0.227619
C	3.742301	0.417872	0.019988
C	1.399002	-0.587218	-0.513792
C	-0.059193	-0.168021	-0.823659
O	0.617035	2.244080	-0.595218
C	-0.419828	1.297522	-0.543915
O	4.516913	1.300797	0.305025
O	4.125375	-0.870493	-0.126597
C	5.521305	-1.112920	0.069763
H	-1.157453	1.664683	-1.261693
O	-0.959798	1.340430	0.764508
C	-1.681383	0.145385	0.979856
C	-0.956987	-0.952441	0.166051
H	-0.322048	-0.422520	-1.847769
H	1.817993	-1.112857	-1.378431
C	1.250249	-1.582182	0.610477
C	-0.013307	-1.810179	0.937497
O	-1.984639	-1.723212	-0.477155
H	-1.658438	-0.043660	2.053692
C	-3.211827	-1.129218	-0.382919
C	-3.082932	0.101576	0.431288
O	-4.174101	-1.610334	-0.911862
C	-4.020525	1.032524	0.620355
H	-5.614277	0.188136	-0.547573
H	2.110027	-2.055846	1.062283
H	-0.361751	-2.500539	1.694216
C	-5.404846	1.048786	0.079938
H	-5.570607	1.968675	-0.487620
H	-3.734262	1.887660	1.229218
H	-6.120350	1.070265	0.907219
H	5.822159	-0.829059	1.077168
H	5.658881	-2.179859	-0.082927
H	6.112814	-0.546317	-0.647802