

Table 1S. Experimental and calculated ^{13}C chemical shifts (ppm) for forms A and B of Irbesartan.

Atom	A form Exp. ^a	B form Exp. ^a	A form Calc.	B form Calc.
C10	43.4	44.1	46.28	45.85
C11	137.5	135.9	141.99	139.73
C12	130	127.7	128.47	128.13
C13	130.9	129	130.59	130.57
C14	138.4	140	142.90	146.22
C15	130.9	131.4	131.62	131.50
C16	128.1	129	130.79	131.11
C17	141.4	141.3	147.80	145.75
C18	123.7	125.3	126.71	129.65
C19	130.9	133.8	129.34	133.18
C2	165.9	167.2	163.12	163.18
C20	130.9	125.3	127.90	128.08
C21	131.8	127.7	132.01	130.56
C22	135.5	132.5	134.21	132.78
C23	156.3	164.9	155.22	166.79
C28	28.4	27	35.35	32.13
C29	29.6	27	36.54	29.36
C30	21.5	21.7	29.22	27.04
C31	11.6	15.4	17.07	14.95
C4	76	74.2	83.58	82.10
C5	182.6	185	187.19	186.11
C6	41.2	37	43.47	42.93
C7	26.3	27	30.85	28.15
C8	24.8	27	28.39	27.32
C9	35.5	29.8	40.28	41.71

^a Taken from Ref. 3.

Table 2S. Experimental and calculated ^{15}N chemical shifts (ppm) for forms A and B of Irbesartan. OA: original assignment, taken from Ref. 3. PA: assignment proposed in this work.

Compound	OA ^a	PA	Exp. ^a	Calc.
A Form	N25	N24	-143.6	-168.66
	N24	N27	-54.6	-51.90
	N27	N25	13.4	16.50
	N26	N26	-13.3	-27.69
	N1	N1	-211.3	-210.15
	N3	N3	-135.1	-113.83
B Form	N27	N27	-50.7	-51.74
	N24	N24	-79.3	-88.05
	N25	N25	-88.7	-124.04
	N26	N26	-3.2	-8.95
	N1	N1	-213.9	-207.06
	N3	N3	-138.8	-122.78

^a Taken from Ref. 3.

Table 3S. Experimental and calculated ¹H chemical shifts (ppm) for forms A and B of Irbesartan.

Atom	DCM ^a	DMSO ^b	A form Calc.	B form Calc.
H(NH)	-	16.22	10.99	11.86
H10a	4.66	4.66	5.52	5.53
H10b	-	-	3.82	3.82
H12	7.09	7.08	7.21	7.21
H13	7.18	7.08	6.77	7.05
H15	7.18	7.08	7.78	7.78
H16	7.09	7.08	7.70	7.92
H19	7.88	7.65	7.46	8.59
H20	7.55	7.56	7.61	7.68
H21	7.64	7.66	7.74	7.65
H22	7.48	7.52	7.70	7.50
H28a	2.15	2.27	2.17	1.98
H28b	-	-	2.26	2.39
H29a	1.47	1.46	1.46	1.47
H29b	-	-	1.46	2.02
H30a	1.27	1.25	1.34	1.66
H30b	-	-	1.41	1.23
H31a	0.83	0.79	0.83	0.95
H31b	-	-	1.20	0.77
H31c	-	-	0.88	0.39
H6a	1.62	1.64	1.57	1.45
H6b	1.81	1.83	2.05	2.15
H7a	1.71	1.83	2.18	2.20
H7b	-	-	1.79	1.87
H8a	1.71	1.83	1.79	1.89
H8b	-	-	1.92	2.08
H9a	1.81	1.83	2.09	2.10
H9b	1.62	1.64	1.52	1.47

^a Taken from Ref. 3, DCM: dichloromethane.

^b Taken from Ref. 3, DMSO: dimethylsulfoxide.