Supplementary Information

Synthesis, structural characterization and anticancer activity of 3-(3,5-dinitrobenzoyl)-1*H*-imidazolidine-2-thione

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Table S1 Assignments of vibrational wavelengths by VEDA for the compound

	B3LYP/6-311+ (d,p)
Frequencies	Assignments with TED (%)
STRE NH	3632 (100)
STRE CH	3096 (93)
STRE CH	3219 (100)
STRE CH	3225 (100)
STRE CH	3240 (100)
STRE CH	3007 (93)
STRE CH	3037 (91)
STRE CH	3131 (92)
STRE OC	1771 (89)
STRE ON	1599 (30) +1378 (21) +1368 (20)
STRE ON	1599 (29) +1378 (22) +1368 (17)
STRE ON	1596 (25) +1378 (17)+1368 (22)
STRE ON	1596 (27) + 1378 (20) +1368 (22)
STRE CC	1663 (10)+1447 (13)+1362(13) +1090 (10)
STRE CC	1663 (22) +1447(13)+1362 (14)+1090 (10)
STRE CC	1479 (11) +1362 (18)+1017 (12)
STRE CC	1663 (10) +1631(21) +1596 (11)+1017(10)
STRE CC	1631(12) +1362 (28)
STRE NC	1500 (15) +1273(29)
STRE NC	1316 (25) +1188 (15) +433(14)
STRE NC	1217 (23)+905 (16)
STRE NC	1078 (34)+1055 (21) + 979(10)
STRE NC	929(14) +362 (17)
STRE NC	929 (22)+343(29)
STRE NC	1217 (10)+1078(23)
STRE SC	1217 (14)+1078 (13) +536 (15)
BEND CCC	362 (10)
BEND CNC	1316 (10)+ 979 (28)
BEND HNC	1500 (35)+1273(21)
BEND HCH	1533(71) + 1519 (14)
BEND HCC	1479 (17) + 1256 (27) + 1122 (20)
BEND HCC	1479 (15)+1256 (30) +1122 (17)
BEND HCC	1447 (18) +1256 (25) +1090 (38)
BEND HCN	1227 (43)+1116 (20)
BEND HCN	1316 (22) +1227 (18) +1116 (21)
BEND HCH	1533(11)+1519 (69)
BEND OCC	433(12) +362 (15) +320 (10)

BEND ONC	554 (17)+536 (13) +521 (19)+320 (18)
BEND ONO	929 (10)+855 (28) +744 (27)
BEND ONC	590 (10) + 521(39)+ 362 (10)+ 320 (13)
BEND ONO	929 (17) +855 (21)+764 (17) +744 (17)
BEND CCC	1017 (17) +394 (12)
BEND CCC	1017 (31)
BEND CCC	1479(11) +1017 (16)
BEND NCN	979 (11)+458 (13)+433 (12)
BEND NCC	240 (15) +56 (14)
BEND CNC	225 (12) +186 (16) +157 (10) +56 (11)
BEND CCC	320 (10) +123 (22) +56 (13)+33 (11)
BEND CNC	1217(10)+1055(15) +905(10)
BEND NCC	320(13) +140 (36)
BEND NCC	320(14) +186 (12) +140 (25)
BEND SCN	394 (35) +186 (19)
TORS HNCN	590(24) +554 (32) +536 (18)
TORS HCNC	1500(12) +1370 (11) +1227 (14)+905 (10)
TORS HCCC	975(48)+965 (12)+946 (19)
TORS HCCC	975 (45) +965 (12) +946 (19)
TORS HCCN	965 (40)+957 (40)
TORS HCNC	1500(11) +1370 (22) +905 (12) +170 (11)
TORS HCNC	1396 (32)+1116(11)+905 (20)
TORS HCNC	1396(23)+1246 (23)
TORS ONCC	37(84)
TORS ONCC	42(88)
TORS CCCC	458(14) +198 (17)
TORS CCCC	645(14) +470 (17)
TORS CCCC	946 (11)+ 667 (11) + 645 (17) +198 (10)
TORS NCNC	86 (26)+56 (23)
TORS NCCC	24 (68)
TORS CNCC	123(12) +33 (48) +24(13)
TORS CNCN	170 (47)
OUT OCON	753(29) +717 (40) +470 (10)
OUT OCON	753 (44)+717 (27)
OUT ONCC	776 (49)
OUT SNNC	667 (11) + 645 (24) +621 (28) +170 (13)
OUT NCCC	753 (10) +470 (18) +198 (17)+157 (11)
OUT NCCC	470 (24) +157 (17) +123 (11)
OUT CCCN	225 (39) +86 (12)
OUT CCCC	776 (15) +667 (10) +86 (13)

Table S2. The regression analysis between experimental and theoretical ^{1}H NMR chemical shifts for the compound

Atom No	Experimental	Theoretical	Regression graph and R_2 value
27	10.07	10.37	
12	8.90	9.37	
11	8.74	9.19	
19	8.74	9.19	
4	4.20	3.96	
6	3.65	3.86	
5	3.65	3.80	
3	4.20	3.63	

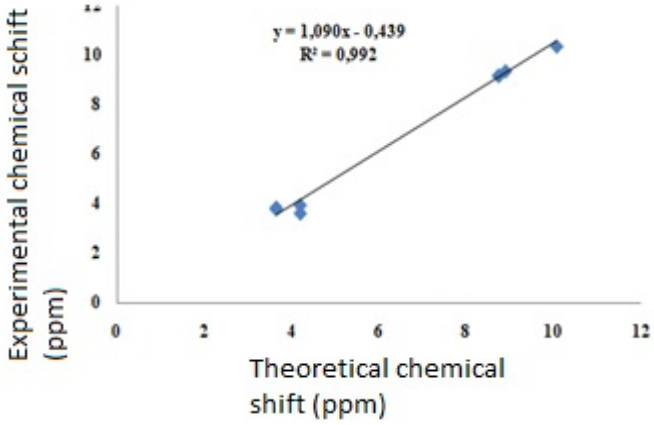
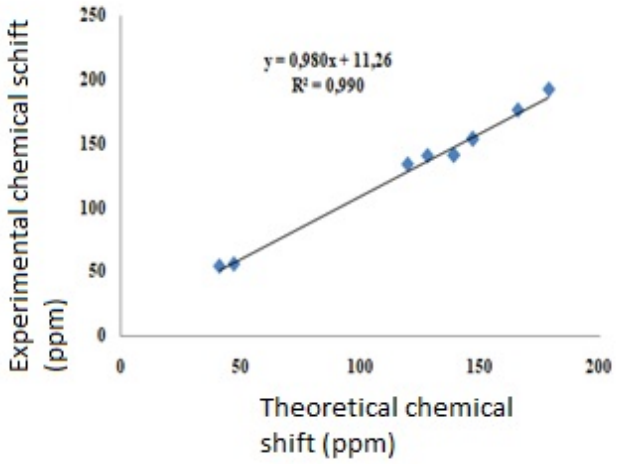


Table S3 The regression analysis between experimental and theoretical ^{13}C NMR chemical shifts for the compound

Atom No	Experimental	Theoretical	Regression graph and R_2 value
7	178.70	191.87	
13	165.78	175.80	
16	146.93	153.75	
17	146.93	153.18	
9	138.96	140.82	
10	138.96	140.70	
8	128.07	140.26	
18	119.81	133.65	
2	47.26	56.03	
1	41.25	54.28	



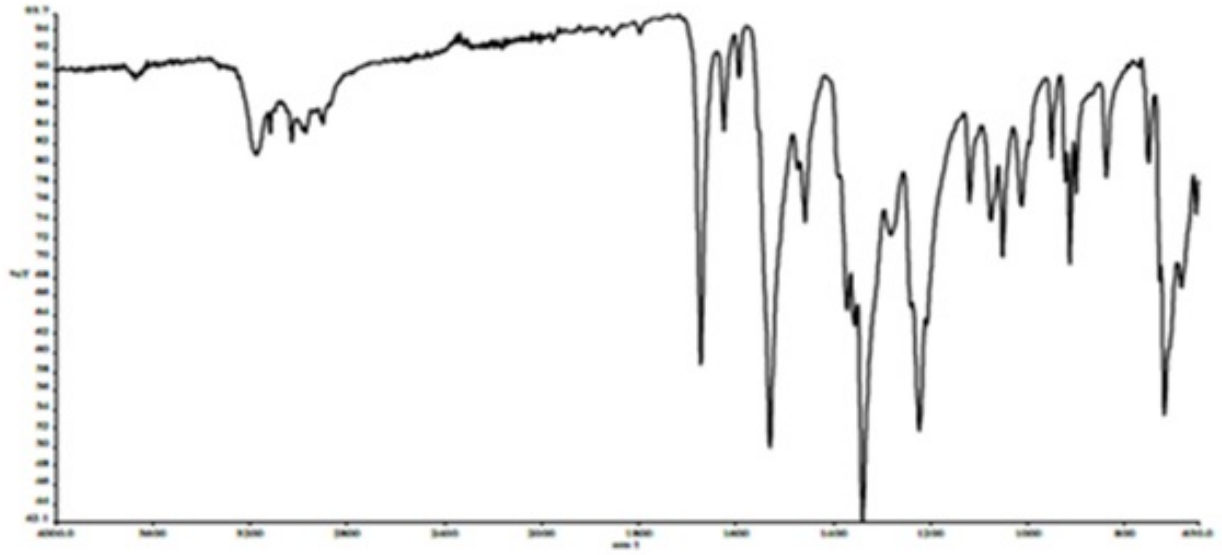


Figure S1 — Experimental IR spectrum of the compound

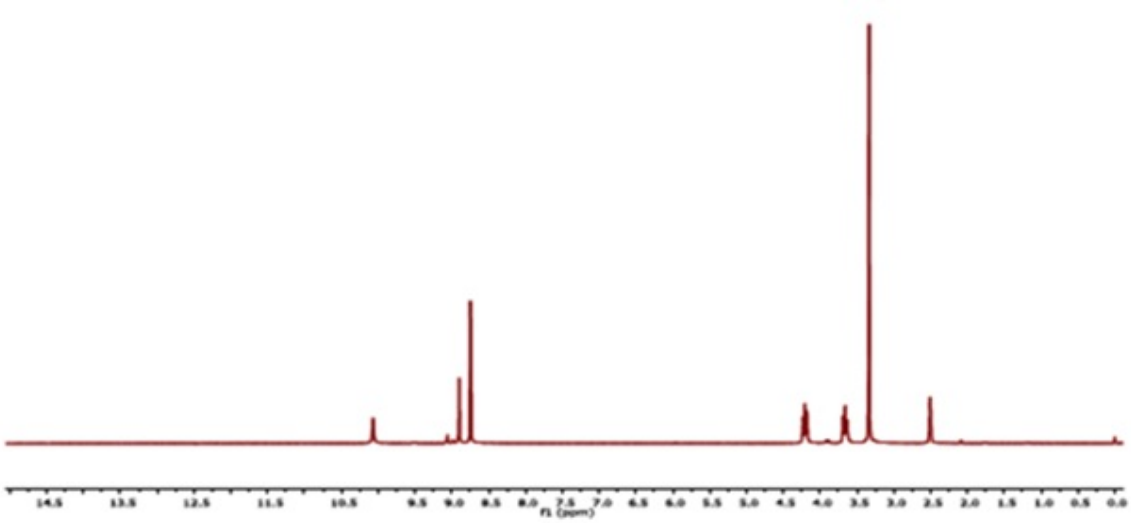


Figure S2 — ^{1}H NMR spectrum of the compound (DMSO-d_6, 300 MHz)

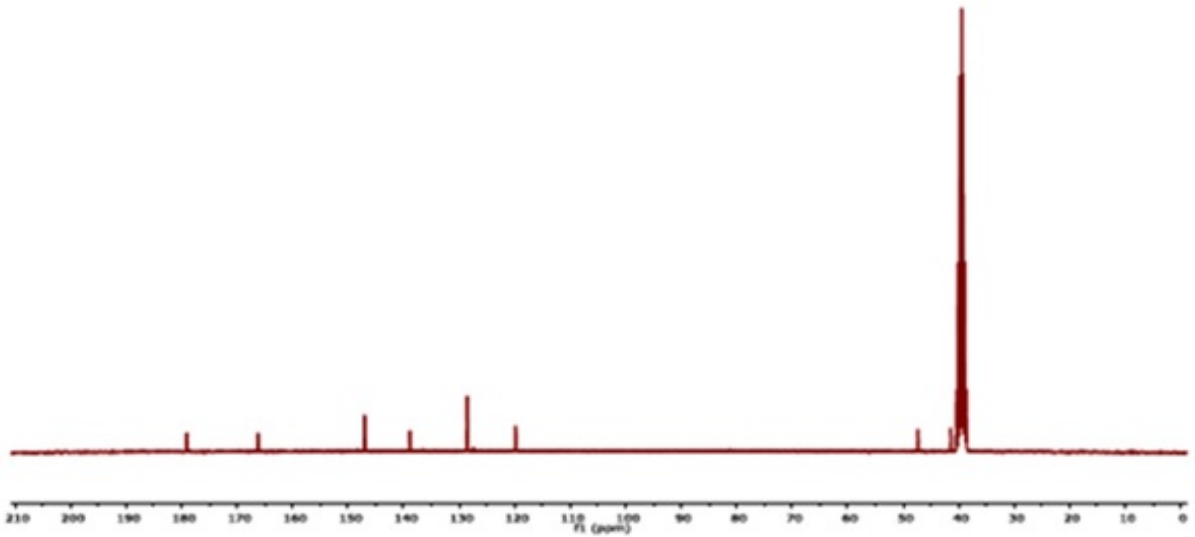


Figure S3 — ^{13}C NMR spectrum of the compound (DMSO-d_6, 300 MHz)