Supplementary Material

3a-(4-Chlorophenyl)-1-thioxo-2,3,3a,4-tetrahydroimidazo[1,5-*a*]quinazolin-5(1H)-one

Contents

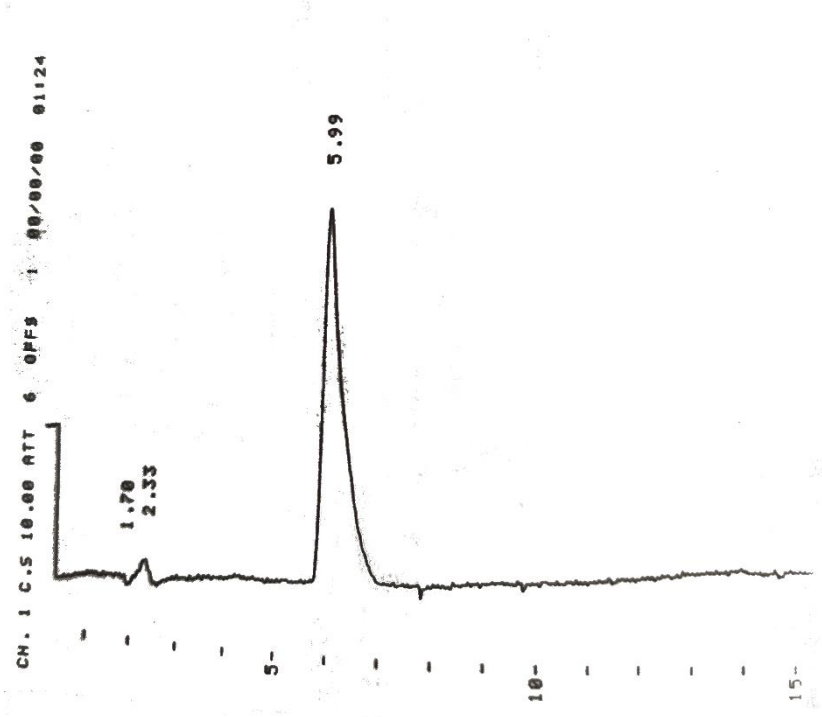

Figure S1. Analytical HPLC chromatogram of tile compound (RP18, CH_3CN/ H_2O 1:1, t_R 5.99 min).

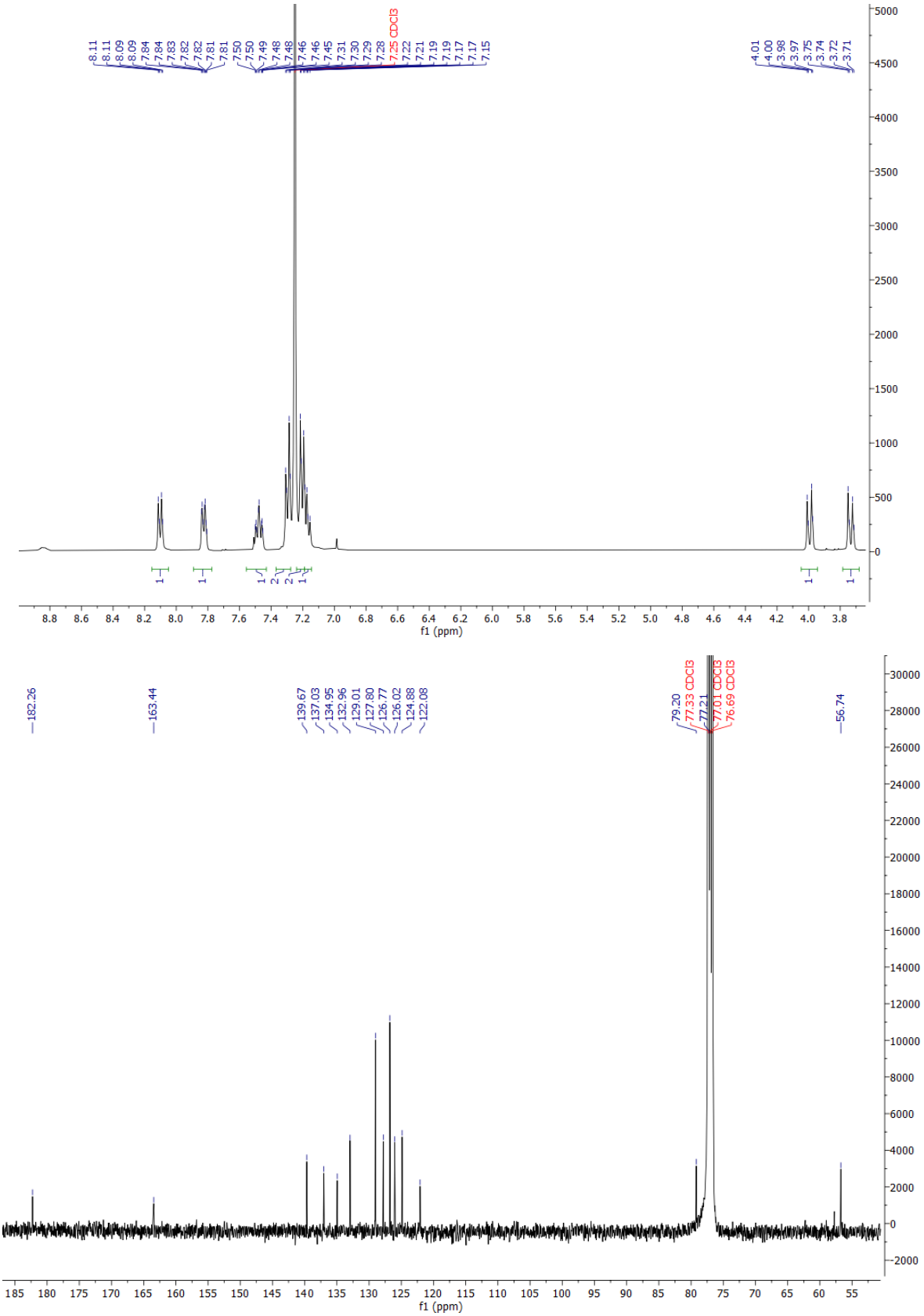

Figure S2. ^{1}HNMR (400MHz) and ^{13}CNMR (100 MHz) spectra of title compound in $CDCl_3$ /CD_3OD.

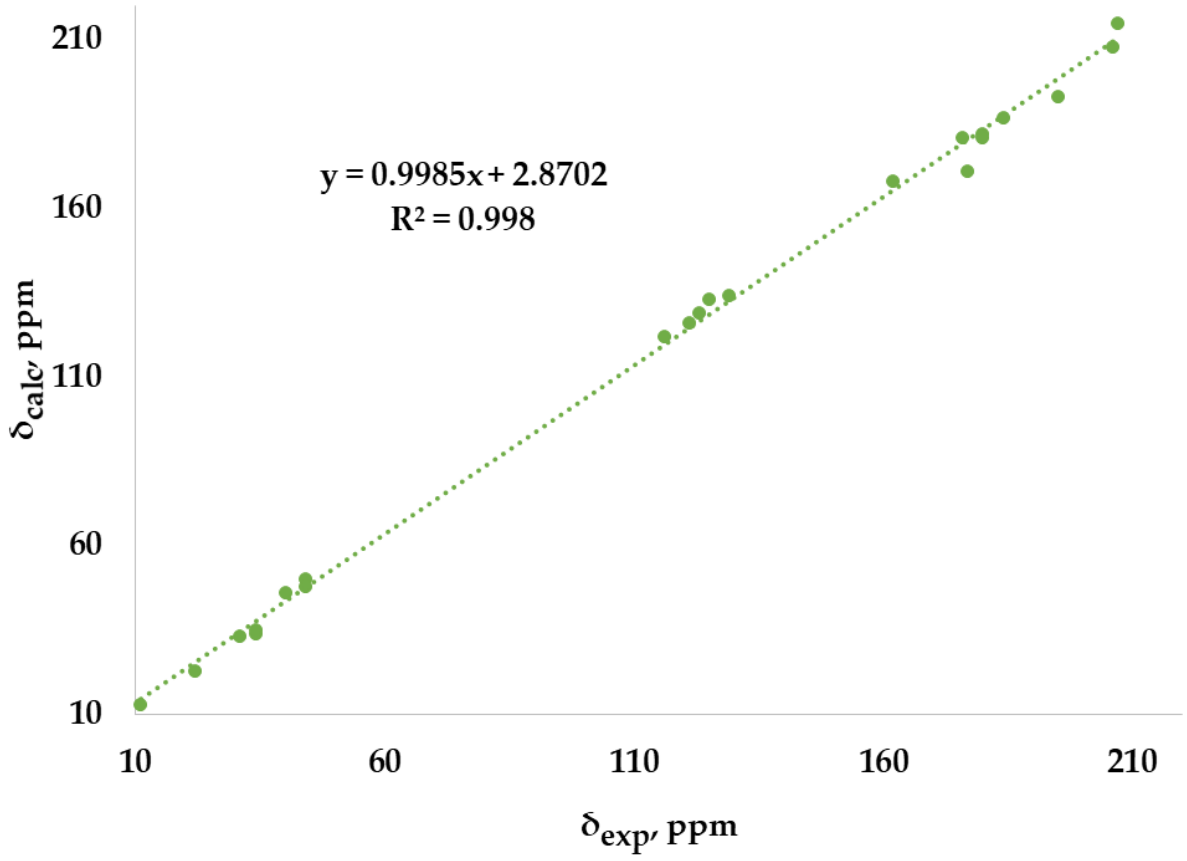

Figure S3. Correlation plot of calculated vs. experimental ^{13}CNMR chemical shifts for the model compounds (acetone, acetamide, thioacetamide, imidazolin-2-one, thiourea, phenylthiourea, cyanothioacetamide, ethyl dithioacetate, and N,N'-diethylthiobarbituric acid) in the validation of the adopted BP86 /Jgauss-TZP2 level of theory.

Table S1. ^{13}CNMR chemical shifts (ppm) of title compound: experimental and BP86 /Jgauss-TZP2 calculated values for the thioamide (NHC=S) and iminethiol (N=CSH) tautomers.

		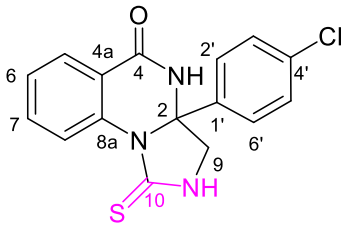	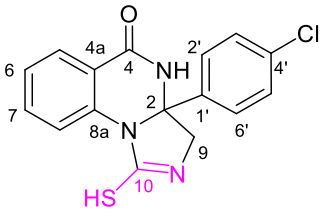
Assignment	Experimental	Calculated	Calculated
C(2)	79.20	85.74	89.23
C(4)	163.44	164.30	163.10
C(4a)	124.88	124.41	129.05
C(5)	127.80	131.54	132.34
C(6)	126.02	127.97	130.46
C(7)	132.96	136.41	137.16
C(8)	122.08	124.49	129.47
C(8a)	134.95	141.20	142.17
C(9)	56.74	61.74	78.29
C(10)	182.26	181.84	162.72
C(1′)	139.67	147.30	147.31
C(2′)	126.77	129.90	132.39
C(3′)	129.01	131.62	131.30
C(4′)	137.03	147.34	146.54
C(5′)	129.01	133.51	132.06
C(6′)	126.77	130.36	132.21

Table S2. xyz Coordinates of geometry-optimized structures of title compounds and its tautomer.

34			
Compound (as thioamide form)			
O	-1.22612	2.67275	2.34424
C	-1.16228	1.69145	1.63573
C	-1.53748	1.68083	0.20370
C	-1.83108	2.89291	-0.40813
H	-1.73901	3.78962	0.18940
C	-2.24047	2.92893	-1.72630
H	-2.46977	3.87280	-2.20145
C	-2.35467	1.73989	-2.43580
H	-2.66657	1.75733	-3.47188
C	-2.06652	0.52092	-1.84643
H	-2.15413	-0.39711	-2.40314
C	-1.65898	0.48593	-0.51750
N	-1.31795	-0.69376	0.15559
C	-1.75919	-1.97703	-0.01651
N	-1.09041	-2.73972	0.89105
H	-1.43790	-3.66826	1.05468
C	-0.46747	-1.95306	1.92614
H	0.50291	-2.35290	2.21424
H	-1.10786	-1.85856	2.80839
S	-2.86216	-2.57500	-1.09005
C	-0.33723	-0.58052	1.23761
C	1.05697	-0.35751	0.65608
C	1.88981	0.65274	1.11415
H	1.54875	1.33903	1.87706
C	3.16505	0.81234	0.59087
H	3.80981	1.60446	0.94305
C	3.60332	-0.04944	-0.39724
Cl	5.19699	0.14277	-1.05823
C	2.78525	-1.06308	-0.87344
H	3.14002	-1.72179	-1.65290
C	1.51626	-1.21034	-0.34536
H	0.87473	-1.99676	-0.72216
N	-0.76489	0.47101	2.12188
H	-0.44118	0.47065	3.07643

34			
Iminethiol tautomer			
O	-1.27079	1.79753	2.86903
C	-1.11845	1.08964	1.89603
C	-1.39255	1.54649	0.50870
C	-1.63198	2.89258	0.26782
H	-1.57780	3.57315	1.10685
C	-1.94696	3.32605	-1.00741
H	-2.13369	4.37470	-1.19419
C	-2.01481	2.40999	-2.05032
H	-2.24332	2.74760	-3.05266
C	-1.76783	1.06492	-1.82558
H	-1.77594	0.35208	-2.63892
C	-1.46867	0.62848	-0.54016
N	-1.18682	-0.72533	-0.26777
C	-2.12519	-1.77211	-0.20640
N	-1.80259	-2.77042	0.50365
C	-0.49532	-2.47835	1.05828
H	0.26937	-3.06381	0.54289
H	-0.45184	-2.73565	2.11737
S	-3.61466	-1.76860	-1.13145
H	-3.67320	-0.43679	-1.29272
C	-0.25765	-0.96876	0.83267
C	1.16633	-0.62910	0.42696
C	2.00273	0.12223	1.23963
H	1.63719	0.51993	2.17613
C	3.31203	0.38572	0.86237
H	3.96055	0.97300	1.49624
C	3.78116	-0.10603	-0.34110
Cl	5.41735	0.22095	-0.82386
C	2.96153	-0.85453	-1.17295
H	3.34181	-1.22495	-2.11404
C	1.66100	-1.11158	-0.78234
H	1.01119	-1.68312	-1.43274
N	-0.71515	-0.21243	1.98320
H	-0.51883	-0.55146	2.91161

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