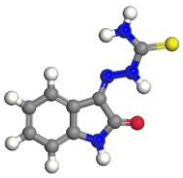
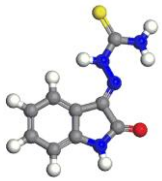
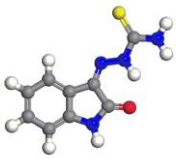
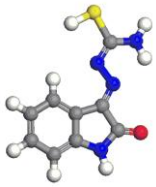
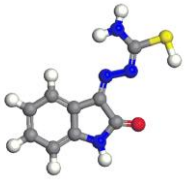
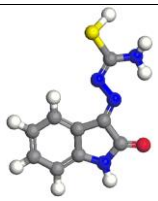
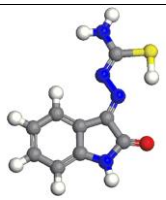
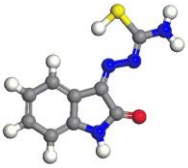
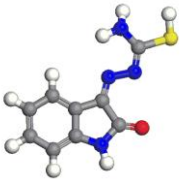
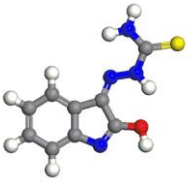
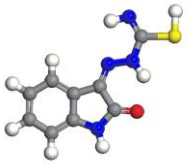
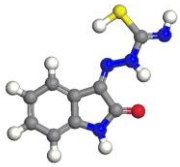
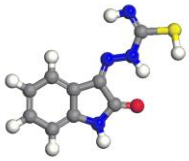
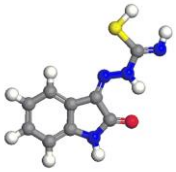
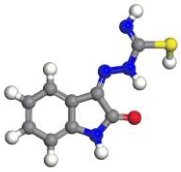
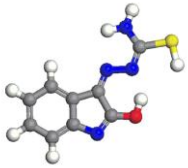
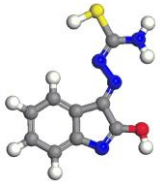
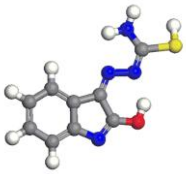
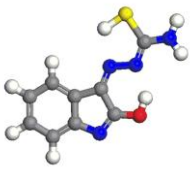
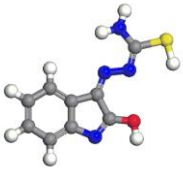
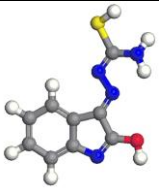
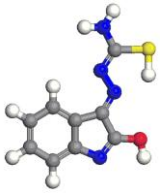
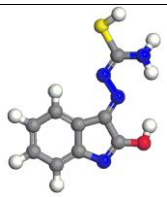
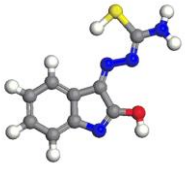
SUPPLEMENTARY INFORMATION

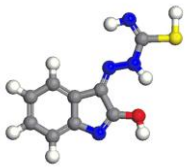
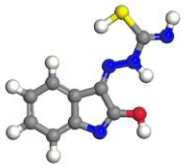
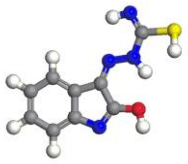
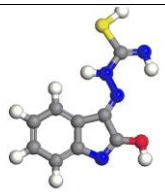
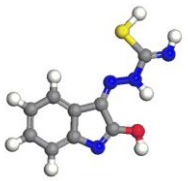
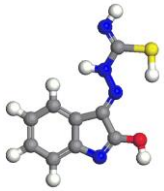
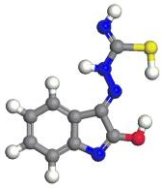
Table A1 B3LYP/6-31G** relative energies (kcal mol^{-1}) of various tautomers and conformers of IBT in the gas phase and aqueous phase

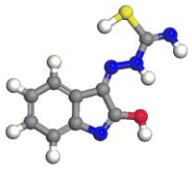
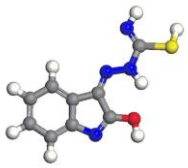
Tautomer	Conformer	Structure	Relative energy	
			Gas phase	Aqueous phase
I	a		0[a]	-16.5
	b		5.7	-11.6
	c		7.7	-13.3
II	a		19.4	4.6
	b		23.2	7.0

	c		20.8	5.4
	d		17.0	1.7
	e		20.3	4.2
	f		25.6	7.4
III	a		17.3	-0.2
	b		19.3	0.6
IV	a		19.7	7.5

	b		18.2	6.5
	c		21.7	8.9
	d		18.3	4.6
	e		23.5	10.0
V	a		31.0	15.9
	b		33.4	17.4
	c		32.2	15.4

	d		29.2	13.2
	e		34.9	17.9
	f		36.5	19.4
	g		35.0	18.0
	h		31.0	14.7
	i		36.4	20.3
	j		34.0	15.4

VI	a		38.0	23.4
	b		35.8	22.4
	c		40.4	25.0
	d		41.0	24.2
	e		36.1	20.5
	f		37.8	22.9
	g		40.5	21.3

	h		39.9	23.2
	i		41.7	24.4

[a]Energy= -1040.223613 Ha

Table A2 Bond lengths and Wiberg bond orders of various bonds of IBT (Isatin-3-thiosemicarbazone)

Bond	**Bond length (in Å)**	**Bond order**
C8-C9	1.396	1.43
C7-C8	1.397	1.44
C6-C7	1.399	1.42
C5-C6	1.385	1.41
C4-C5	1.410	1.28
C4-C9	1.391	1.38
C9-H9a	1.083	0.92
C8-H8a	1.083	0.92
C7-H7a	1.084	0.92
C6-H6a	1.084	0.92

C3-C4	1.456	1.10
C2-C3	1.503	1.00
C2-N1	1.378	1.14
N1-C5	1.404	1.05
N1-H1a	1.009	0.80
C2-O10	1.222	1.14
C3-N11	1.295	1.62
N11-N12	1.335	1.20
N12-H12a	1.022	0.74
O10-H12a	2.025	0.02
N12-C13	1.384	1.10
C13-S14	1.667	1.55
C13-N15	1.345	1.25
N15-H15a	1.005	0.81
N15-H15b	1.009	0.80
N11-H15b	2.251	0.01

Table A3 Natural, ESP and Mulliken charges on various atoms of IBT

Atom	**Natural charge**	**ESP charge**	**Mulliken charge**
C9	-0.149	-0.08	-0.16
C6	-0.227	-0.37	-0.18

C7	-0.181	-0.06	-0.14
C8	-0.228	-0.22	-0.14
H9a	0.214	0.13	0.15
H6a	0.214	0.19	0.16
H7a	0.210	0.13	0.15
H8a	0.211	0.14	0.16
C2	0.615	0.66	0.25
N1	-0.588	-0.70	-0.22
C5	0.166	0.45	0.06
C4	-0.097	-0.13	-0.04
C3	0.088	0.07	-0.19
O10	-0.598	-0.52	-0.36
H1a	0.412	0.40	0.31
N11	-0.214	-0.31	0.04
N12	-0.395	0.32	-0.10
C13	0.242	-0.05	0.04
N15	-0.770	-0.42	-0.43
S14	-0.184	-0.30	-0.27
H12a	0.436	0.09	0.30
H15b	0.411	0.27	0.29
H15a	0.411	0.29	0.30

Table A4 Vibrational frequencies (cm^{-1}) and intensities ($km\ mol^{-1}$) of IBT

Frequency	**Intensity**
69.50	0.18
82.51	0.05
99.52	1.37
140.91	0.06
167.14	0.04
198.41	4.02
249.11	22.05
268.24	25.69
296.15	139.76
338.96	5.76
356.68	17.80
424.36	16.65
427.99	2.48
453.86	13.43
460.54	6.37
487.47	7.24
505.67	113.11
573.50	3.14
574.64	16.56

577.09	0.15
609.25	3.01
634.58	1.45
670.44	11.66
723.29	53.05
143.42	7.42
751.13	19.17
770.24	40.05
790.94	45.06
841.16	70.14
863.73	0.11
868.39	21.51
937.29	1.75
950.68	1.99
973.86	0.01
1008.26	5.86
1032.66	36.70
1088.61	29.84
1143.67	261.55
1155.37	155.60
1180.28	62.94

1207.44	71.36
1239.69	5.73
1262.01	451.98
1290.66	4.04
1325.63	38.88
1379.38	74.50
1391.99	65.44
1449.73	130.95
1465.37	34.91
1479.80	369.45
1560.25	264.37
1579.68	56.91
1587.35	78.07
1612.43	92.56
1714.36	295.60
3083.78	0.24
3090.85	2.80
3100.23	5.61
3105.13	3.53
3346.02	81.00
3468.04	51.53

3529.27	77.95
3611.71	115.10