Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPORTING INFORMATION

Real-time probing of mercury through an efficient "turn-on" strategy with potentialities as in field mapping kit and live cell imaging

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7	**7**	**Table S1.** Crystal data and structure refinement for TS.
8	**8**	**Table S2.** Crystal data and structure refinement for complex.

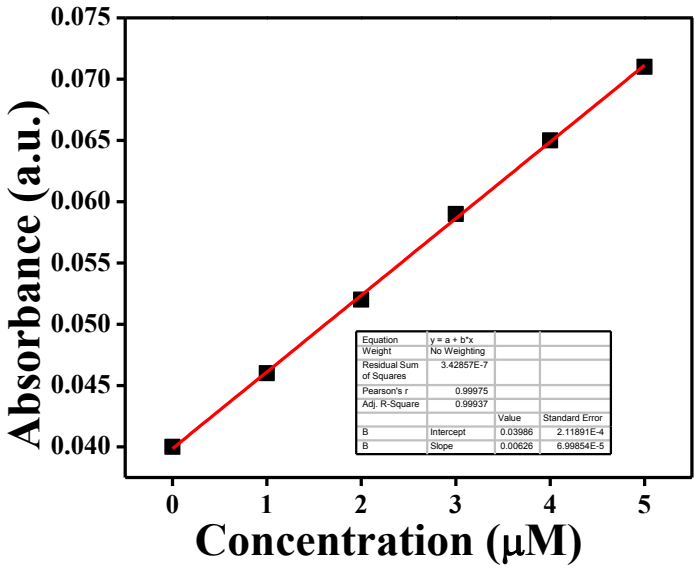

Figure S1: Calibration curve for probe **TS**

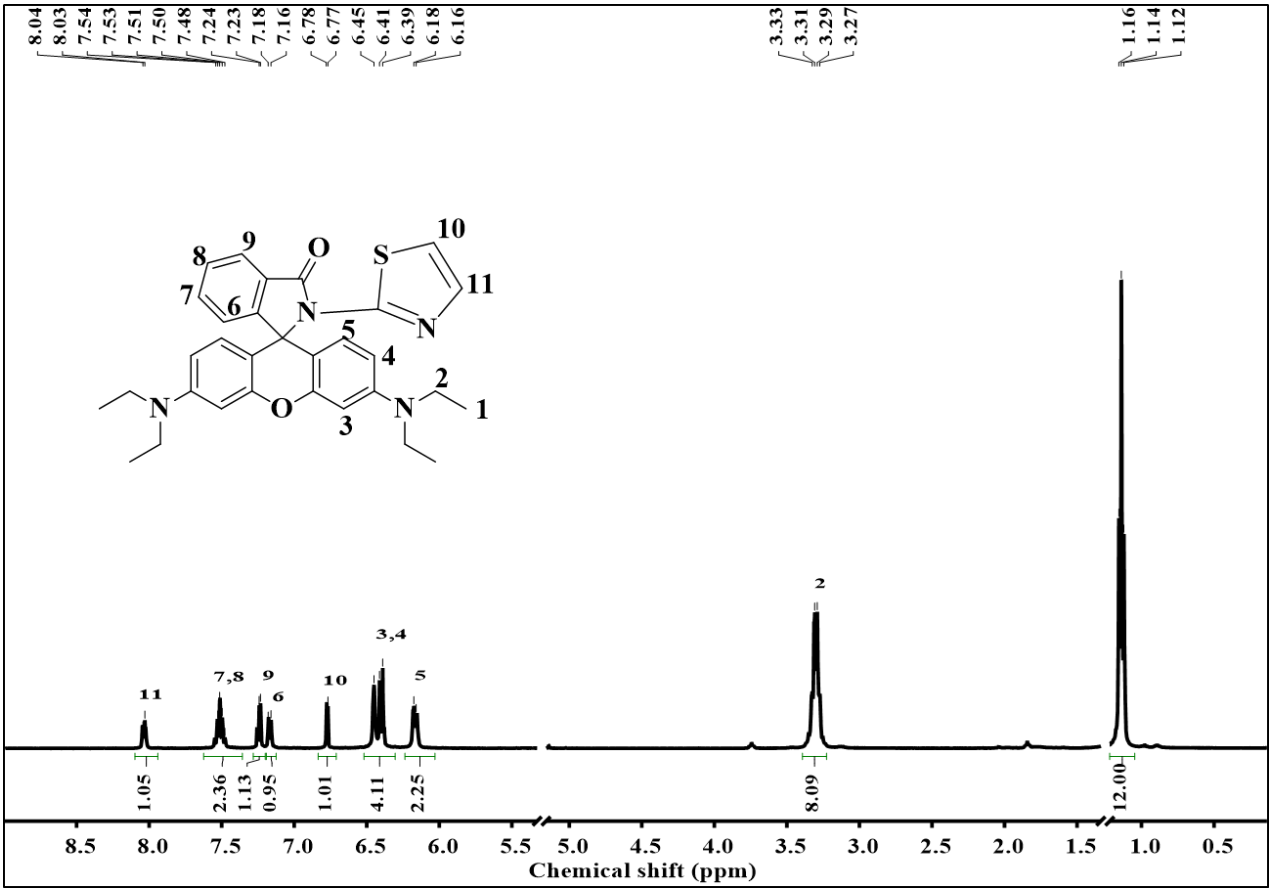

Figure S2: ^{1}H NMR spectra of TS in $CDCl_3$

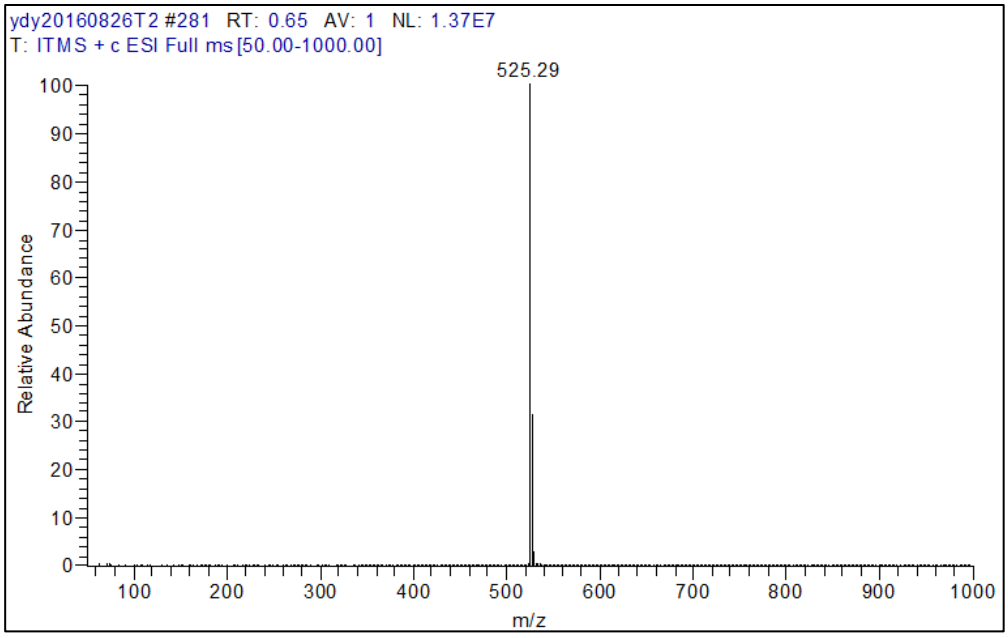

Figure S3: Mass spectra of TS.

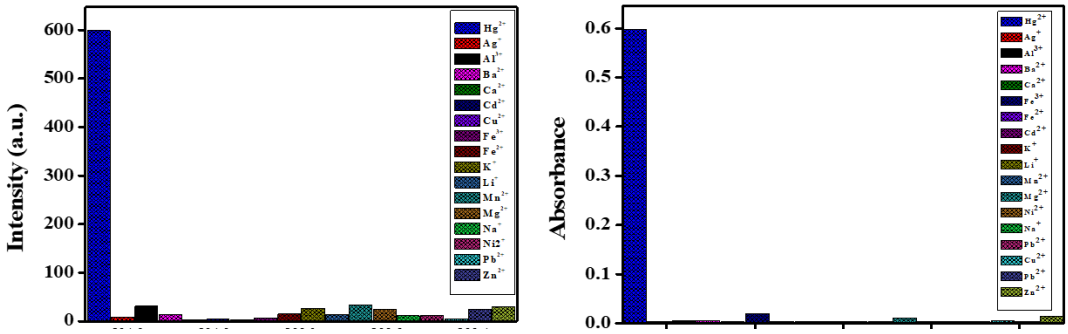

Figure S4: (B) Fluorescence (B) UV-Visible response of TS (5 μM) towards Hg^{2+} among miscellaneous metal cations in MeCN/H_2O (7:3 v/v, HEPES buffer 10 mM pH 7.0).

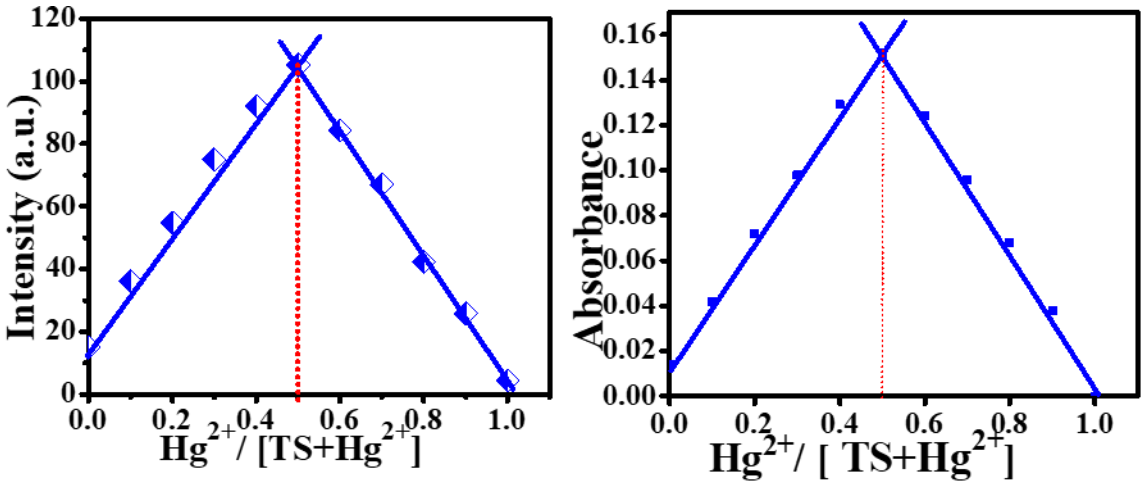

Figure S5: Job's plot to show 1:1 binding stoichiometry between metal ion and TS. The total concentration of TS and Hg^{2+} remain 10 μM during the experiment.

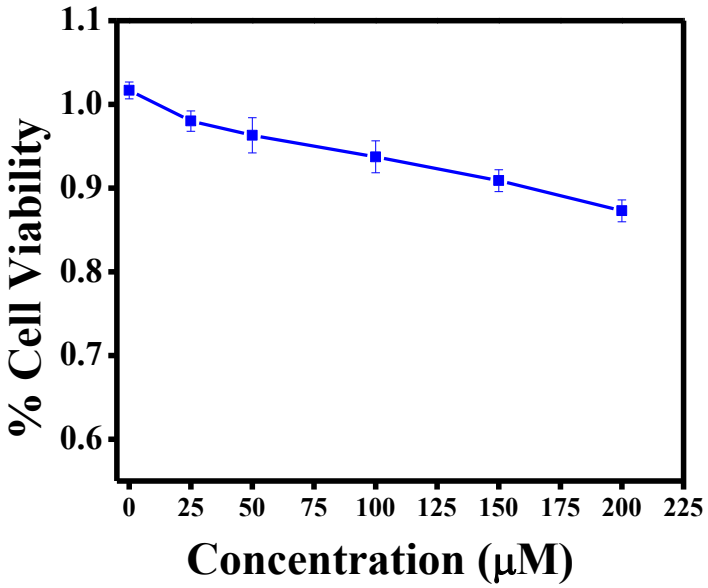

Figure S6: Check of viability of **TS** on HeLa Cells. Here % of Viability was calculated with respect to the growth considering 100% without **TS**.

Table S1. Crystal data and structure refinement for TS.

Identification code	**TS**
Empirical formula	C31 H31 N4 O2 S
Formula weight	523.66
Temperature/K	173.01
Crystal system	Orthorhombic
Space group	Pbca
a/Å	13.1565(3)
b/Å	17.4978(4)
c/Å	23.4603(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	5400.8 (2)/A3
Z	8
ρ_{calc}g/cm^3	1.288 mg/m^3
μ/mm^{-1}	1.345 mm-1
F(000)	2216
Crystal size/mm^3	0.05 x 0.04 x 0.03 mm
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	4.608 to 66.743 deg.
Index ranges	-15<=h<=15, -20<=k<=20, -27<=l<=27
Reflections collected	48375
Independent reflections	4760 [R(int) = 0.0371]
Data/restraints/parameters	4760 / 229 / 347
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R1 = 0.0608, wR2 = 0.1927
Final R indexes [all data]	R1 = 0.0669, wR2 = 0.2015
Largest diff. peak/hole / e Å^{-3}	1.211 and -0.487

Table S2. Selected bond lengths of TS.

Atom	Atom	Bond length/Å	Atom	Atom	Bond length/Å
S(1)	C(31)	1.714(3)	C(11)	C(12)	1.515(3)
S(1)	C(29)	1.747(3)	C(11)	C(22)	1.537(3)
O(1)	C(13)	1.377(3)	C(12)	C(13)	1.384(3)
O(1)	C(7)	1.377(3)	C(12)	C(17)	1.390(3)
N(1)	C(5)	1.389(4)	C(13)	C(14)	1.382(3)
N(1)	C(3)	1.444(5)	C(14)	C(15)	1.401(3)
N(1)	C(2)	1.479(5)	C(14)	H(14)	0.9500
C(1)	C(2)	1.518(7)	C(15)	C(16)	1.410(4)
C(1)	H(1A)	0.9800	C(16)	C(17)	1.381(4)
C(1)	H(1B)	0.9800	C(16)	H(16)	0.9500
C(1)	H(1C)	0.9800	C(17)	H(17)	0.9500
O(2)	C(28)	1.213(3)	C(18)	C(19)	1.513(5)
N(2)	C(15)	1.373(3)	C(18)	H(18A)	0.9800
N(2)	C(19)	1.453(4)	C(18)	H(18A)	0.9801
N(2)	C(20)	1.457(4)	C(18)	H(18A)	0.9802
C(2)	H(2A)	0.9900	C(18)	H(18A)	0.9803
C(2)	H(2B)	0.9900	C(18)	H(18A)	0.9804
N(3)	C(29)	1.298(3)	C(18)	H(18A)	0.9805
N(3)	C(30)	1.375(3)	C(18)	H(18A)	0.9806
C(3)	C(4)	1.389(7)	C(18)	H(18A)	0.9807
C(3)	H(3)	0.9500	C(18)	H(18A)	0.9808
N(4)	C(28)	1.377(3)	C(18)	H(18A)	0.9809
N(4)	C(29)	1.384(3)	C(18)	H(18A)	0.9810
N(4)	C(11)	1.507(3)	C(18)	H(18A)	0.9811
C(4)	H(4A)	0.9800	C(18)	H(18A)	0.9812
C(4)	H(4B)	0.9800	C(18)	H(18A)	0.9813
C(4)	H(4C)	0.9800	C(18)	H(18A)	0.9814
C(5)	C(6)	1.405(4)	C(18)	H(18A)	0.9815
C(5)	C(10)	1.405(4)	C(18)	H(18A)	0.9816
C(6)	C(7)	1.389(4)	C(18)	H(18A)	0.9817
C(6)	H(6)	0.9500	C(18)	H(18A)	0.9818
C(7)	C(8)	1.386(3)	C(18)	H(18A)	0.9819
C(8)	C(9)	1.399(3)	C(18)	H(18A)	0.9820
C(8)	C(11)	1.498(3)	C(18)	H(18A)	0.9821
C(9)	C(10)	1.373(4)	C(18)	H(18A)	0.9822
C(9)	H(9)	0.9500	C(18)	H(18A)	0.9823
C(10)	H(10)	0.9500	C(18)	H(18A)	0.9824

Table S3. Selected bond Angels of TS.

Atom	Atom	Atom	Angle/ °	Atom	Atom	Atom	Angle/ °
C(31)-	S(1)-	C(29)	87.78(13)	C(15)-	C(14)-	H(14)	119.6
C(13)-	O(1)-	C(7)	118.22(17)	N(2)-	C(15)-	C(14)	121.3(2)
C(5)-	N(1)-	C(3)	122.0(3)	N(2)-	C(15)-	C(16)	121.6(2)
C(5)-	N(1)-	C(2)	119.3(3)	C(14)-	C(15)-	C(16)	117.1(2)
C(3)-	N(1)-	C(2)	114.5(3)	C(17)-	C(16)-	C(15)	120.4(2)
C(2)-	C(1)-	H(1A)	109.5	C(17)-	C(16)-	H(16)	119.8
C(2)-	C(1)-	H(1B)	109.5	C(15)-	C(16)-	H(16)	119.8
H(1A)-	C(1)-	H(1B)	109.5	C(16)-	C(17)-	C(12)	122.6(2)
C(2)-	C(1)-	H(1C)	109.5	C(16)-	C(17)-	H(17)	118.7
H(1A)-	C(1)-	H(1C)	109.5	C(12)-	C(17)-	H(17)	118.7
H(1B)-	C(1)-	H(1C)	109.5	C(19)-	C(18)-	H(18A)	109.5
C(15)-	N(2)-	C(19)	121.4(2)	C(19)-	C(18)-	H(18B)	109.5
C(15)-	N(2)-	C(20)	121.4(2)	H(18A)-	C(18)-	H(18B)	109.5
C(19)-	N(2)-	C(20)	115.8(2)	C(19)-	C(18)-	H(18C)	109.5
N(1)-	C(2)-	C(1)	114.4(3)	H(18A)-	C(18)-	H(18C)	109.5
N(1)-	C(2)-	H(2A)	108.7	H(18B)-	C(18)-	H(18C)	109.5
C(1)-	C(2)-	H(2A)	108.7	N(2)-	C(19)-	C(18)	112.8(3)
N(1)-	C(2)-	H(2B)	108.7	N(2)-	C(19)-	H(19A)	109.0
C(1)-	C(2)-	H(2B)	108.7	C(18)-	C(19)-	H(19A)	109.0
H(2A)-	C(2)-	H(2B)	107.6	N(2)-	C(19)-	H(19B)	109.0
C(29)-	N(3)-	C(30)	109.5(2)	C(18)-	C(19)-	H(19B)	109.0
C(4)-	C(3)-	N(1)	116.8(4)	H(19A)-	C(19)-	H(19B)	107.8
C(4)-	C(3)-	H(3)	121.6	N(2)-	C(20)-	C(21)	113.4(2)
N(1)-	C(3)-	H(3)	121.6	N(2)-	C(20)-	H(20A)	108.9
C(28)-	N(4)-	C(29)	124.4(2)	C(21)-	C(20)-	H(20A)	108.9
C(28)-	N(4)-	C(11)	114.67(19)	N(2)-	C(20)-	H(20B)	108.9
C(29)-	N(4)-	C(11)	120.78(19)	C(21)-	C(20)-	H(20B)	108.9
C(3)-	C(4)-	H(4A)	109.5	H(20A)-	C(20)-	H(20B)	107.7
C(3)-	C(4)-	H(4B)	109.5	C(20)-	C(21)-	H(21A)	109.5
H(4A)-	C(4)-	H(4B)	109.5	C(20)-	C(21)-	H(21B)	109.5
C(3)-	C(4)	-H(4C)	109.5	H(21A)-	C(21)-	H(21B)	109.5
H(4A)-	C(4)-	H(4C)	109.5	C(20)-	C(21)-	H(21C)	109.5
H(4B)-	C(4)-	H(4C)	109.5	H(21A)-	C(21)-	H(21C)	109.5
N(1)-	C(5)-	C(6)	121.7(3)	H(21B)-	C(21)-	H(21C)	109.5
N(1)-	C(5)-	C(10)	120.6(3)	C(23)-	C(22)-	C(27)	121.8(2)
C(6)-	C(5)-	C(10)	117.6(2)	C(23)-	C(22)-	C(11)	127.0(2)
C(7)-	C(6)-	C(5)	119.9(2)	C(27)-	C(22)-	C(11)	111.2(2)
C(7)-	C(6)-	H(6)	120.0	C(22)-	C(23)-	C(24)	118.4(3)
C(5)-	C(6)-	H(6)	120.0	C(22)-	C(23)-	H(23)	120.8

O(1)-	C(7)-	C(8)	122.8(2)	C(24)-	C(23)-	H(23)	120.8
O(1)-	C(7)-	C(6)	114.4(2)	C(23)-	C(24)-	C(25)	120.1(3)
C(8)-	C(7)-	C(6)	122.7(2)	C(23)-	C(24)-	H(24)	120.0
C(7)-	C(8)-	C(9)	116.5(2)	C(25)-	C(24)-	H(24)	120.0
C(7)-	C(8)-	C(11)	122.3(2)	C(26)-	C(25)-	C(24)	120.8(3)
C(9)-	C(8)-	C(11)	121.1(2)	C(26)-	C(25)-	H(25)	119.6
C(10)-	C(9)-	C(8)	122.2(2)	C(24)-	C(25)-	H(25)	119.6
C(10)-	C(9)-	H(9)	118.9	C(25)-	C(26)-	C(27)	120.0(3)
C(8)-	C(9)-	H(9)	118.9	C(25)-	C(26)-	H(26)	120.0
C(9)-	C(10)-	C(5)	120.9(2)	C(27)-	C(26)-	H(26)	120.0
C(9)-	C(10)-	H(10)	119.6	C(22)-	C(27)-	C(26)	119.0(3)
C(5)-	C(10)-	H(10)	119.6	C(22)-	C(27)-	C(28)	109.7(2)
C(8)-	C(11)-	N(4)	111.68(19)	C(26)-	C(27)-	C(28)	131.3(3)
C(8)-	C(11)-	C(12)	110.61(19)	O(2)-	C(28)-	N(4)	126.0(2)
N(4)-	C(11)-	C(12)	111.45(19)	O(2)-	C(28)-	C(27)	128.5(2)
C(8)-	C(11)-	C(22)	111.63(19)	N(4)-	C(28)-	C(27)	105.5(2)
N(4)-	C(11)-	C(22)	98.88(18)	N(3)-	C(29)-	N(4)	122.8(2)
C(12)-	C(11)-	C(22)	112.12(19)	N(3)-	C(29)-	S(1)	115.34(19)
C(13)-	C(12)-	C(17)	116.6(2)	N(4)-	C(29)-	S(1)	121.85(18)
C(13)-	C(12)-	C(11)	121.7(2)	C(31)-	C(30)-	N(3)	116.4(3)
C(17)-	C(12)-	C(11)	121.6(2)	C(31)-	C(30)-	H(30)	121.8
O(1)-	C(13)-	C(14)	114.5(2)	N(3)-	C(30)-	H(30)	121.8
O(1)-	C(13)-	C(12)	123.1(2)	C(30)-	C(31)-	S(1)	111.0(2)
C(14)-	C(13)-	C(12)	122.4(2)	C(30)-	C(31)-	H(31)	124.5
C(13)-	C(14)-	C(15)	120.9(2)	S(1)-	C(31)-	H(31)	124.5
C(13)-	C(14)-	H(14)	119.6				

Table S4. Crystal data and structure refinement for Complex.

Identification code	**TS-Hg^{2+}**
Empirical formula	C31 H32 Cl3 Hg N4 O2 S
Formula weight	831.61
Temperature/K	173.01
Crystal system	Monoclinic
Space group	P2(1)/n
a/Å	13.9541(3)
b/Å	10.2955(3)
c/Å	24.0087(6)
α/°	90
β/°	97.9520(10)
γ/°	90
Volume/$Å^3$	3416.03 (15)/A3
Z	4
$\rho_{calc}g/cm^3$	1.617 mg/m3
μ/mm^{-1}	11.0775 mm-1
F(000)	9180
Crystal size/mm^3	0.05 x 0.04 x 0.03 mm
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	3.469 to 66.621 deg.
Index ranges	-16<=h<=16, -11<=k<=12, -28<=l<=22
Reflections collected	19708
Independent reflections	5942 [R(int) = 0.0481]
Data/restraints/parameters	5942 / 365 / 383
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R1 = 0.0383, wR2 = 0.0956
Final R indexes [all data]	R1 = 0.0669, wR2 = 0.2015
Largest diff. peak/hole / e $Å^{-3}$	1.482 and -0.872

TableS5. Selected bond lengths of TS-Hg^{2+}.

Atom	Atom	Bond length/ Å	Atom	Atom	Bond Length/ Å
Hg(1)	Cl(1)	2.3811(16)	C(9)	H(9)	0.9500
Hg(1)	N(4)	2.423(5)	C(10)	H(10)	0.9500
Hg(1)	Cl(2)	2.4400(13)	C(11)	C(12)	1.407(6)
Hg(1)	Cl(3)	2.4565(17)	C(11)	C(22)	1.495(6)
S(1)	C(29)	1.716(6)	C(12)	C(17)	1.416(7)
S(1)	C(31)	1.730(8)	C(12)	C(13)	1.428(6)
O(1)	C(7)	1.369(5)	C(13)	C(14)	1.368(6)
O(1)	C(13)	1.368(6)	C(14)	C(15)	1.418(7)
N(1)	C(5)	1.343(7)	C(14)	H(14)	0.9500
N(1)	C(4)	1.471(7)	C(15)	C(16)	1.430(7)
N(1)	C(2)	1.480(7)	C(16)	C(17)	1.360(6)
C(1)	C(2)	1.519(8)	C(16)	H(16)	0.9500
C(1)	H(1A)	0.9800	C(17)	H(17)	0.9500
C(1)	H(1B)	0.9800	C(18)	C(19)	1.524(7)
C(1)	H(1C)	0.9800	C(18)	H(18A)	0.9900
O(2)	C(28)	1.216(6)	C(18)	H(18B)	0.9900
N(2)	C(15)	1.348(6)	C(19)	H(19A)	0.9800
N(2)	C(20)	1.461(6)	C(19)	H(19B)	0.9800
N(2)	C(18)	1.470(6)	C(19)	H(19C)	0.9800
C(2)	H(2A)	0.9900	C(20)	C(21)	1.499(8)
C(2)	H(2B)	0.9900	C(20)	H(20A)	0.9900
N(3)	C(28)	1.366(6)	C(20)	H(20B)	0.9900
N(3)	C(29)	1.395(6)	C(21)	H(21A)	0.9800
C(3)	C(4)	1.507(9)	C(21)	H(21B)	0.9800
C(3)	H(3A)	0.9800	C(21)	H(21C)	0.9800
C(3)	H(3B)	0.9800	C(22)	C(23)	1.390(7)
C(3)	H(3C)	0.9800	C(22)	C(27)	1.411(7)
N(4)	C(29)	1.311(7)	C(23)	C(24)	1.392(7)
N(4)	C(30)	1.378(8)	C(23)	H(23)	0.9500
C(4)	H(4A)	0.9900	C(24)	C(25)	1.374(8)
C(4)	H(4B)	0.9900	C(24)	H(24)	0.9500
C(5)	C(6)	1.411(7)	C(25)	C(26)	1.380(7)
C(5)	C(10)	1.439(7)	C(25)	H(25)	0.9500
C(6)	C(7)	1.372(7)	C(26)	C(27)	1.387(7)
C(6)	H(6)	0.9500	C(26)	H(26)	0.9500
C(7)	C(8)	1.408(6)	C(27)	C(28)	1.495(6)
C(8)	C(11)	1.404(7)	C(30)	C(31)	1.320(11)
C(8)	C(9)	1.428(6)	C(30)	H(30)	0.9500
C(9)	C(10)	1.350(7)	C(31)	H(31)	0.9500

Table S6. Bond angles of TS-Hg.

Atom	Atom	Atom	Angle	Atom	Atom	Atom	Angle
Cl(1)-	Hg(1)-	N(4)	96.18(12)	O(1)-	C(13)-	C(12)	120.5(4)
Cl(1)-	Hg(1)-	Cl(2)	124.24(6)	C(13)-	C(14)-	C(15)	119.8(4)
N(4)-	Hg(1)-	Cl(2)	98.58(13)	C(13)-	C(14)-	H(14)	120.1
Cl(1)-	Hg(1)-	Cl(3)	128.86(6)	C(15)-	C(14)-	H(14)	120.1
N(4)-	Hg(1)-	Cl(3)	95.98(13)	N(2)-	C(15)-	C(14)	121.1(4)
Cl(2)-	Hg(1)-	Cl(3)	102.56(5)	N(2)-	C(15)-	C(16)	121.7(4)
C(29)-	S(1)-	C(31)	87.8(3)	C(14)-	C(15)-	C(16)	117.2(4)
C(7)-	O(1)-	C(13)	120.6(4)	C(17)-	C(16)-	C(15)	121.6(4)
C(5)-	N(1)-	C(4)	121.7(4)	C(17)-	C(16)-	H(16)	119.2
C(5)-	N(1)-	C(2)	122.0(5)	C(15)-	C(16)-	H(16)	119.2
C(4)-	N(1)-	C(2)	116.3(4)	C(16)-	C(17)-	C(12)	122.5(4)
C(2)-	C(1)-	H(1A)	109.5	C(16)-	C(17)-	H(17)	118.7
C(2)-	C(1)-	H(1B)	109.5	C(12)-	C(17)-	H(17)	118.7
H(1A)-	C(1)-	H(1B)	109.5	N(2)-	C(18)-	C(19)	113.8(4)
C(2)-	C(1)-	H(1C)	109.5	N(2)-	C(18)-	H(18A)	108.8
H(1A)-	C(1)-	H(1C)	109.5	C(19)-	C(18)-	H(18A)	108.8
H(1B)-	C(1)-	H(1C)	109.5	N(2)-	C(18)-	H(18B)	108.8
C(15)-	N(2)-	C(20)	122.7(4)	C(19)-	C(18)-	H(18B)	108.8
C(15)-	N(2)-	C(18)	120.5(4)	H(18A)-	C(18)-	H(18B)	107.7
C(20)-	N(2)-	C(18)	116.4(4)	C(18)-	C(19)-	H(19A)	109.5
N(1)-	C(2)-	C(1)	113.2(5)	C(18)-	C(19)-	H(19B)	109.5
N(1)-	C(2)-	H(2A)	108.9	H(19A)-	C(19)-	H(19B)	109.5
C(1)-	C(2)-	H(2A)	108.9	C(18)-	C(19)-	H(19C)	109.5
N(1)-	C(2)-	H(2B)	108.9	H(19A)-	C(19)-	H(19C)	109.5
C(1)-	C(2)-	H(2B)	108.9	H(19B)-	C(19)-	H(19C)	109.5
H(2A)-	C(2)-	H(2B)	107.8	N(2)-	C(20)-	C(21)	112.8(4)
C(28)-	N(3)-	C(29)	123.2(4)	N(2)-	C(20)-	H(20A)	109.0
C(4)-	C(3)-	H(3A)	109.5	C(21)-	C(20)-	H(20A)	109.0
C(4)-	C(3)-	H(3B)	109.5	N(2)-	C(20)-	H(20B)	109.0
H(3A)-	C(3)-	H(3B)	109.5	C(21)-	C(20)-	H(20B)	109.0
C(4)-	C(3)-	H(3C)	109.5	H(20A)-	C(20)-	H(20B)	107.8
H(3A)-	C(3)-	H(3C)	109.5	C(20)-	C(21)-	H(21A)	109.5
H(3B)-	C(3)-	H(3C)	109.5	C(20)-	C(21)-	H(21B)	109.5
C(29)-	N(4)-	C(30)	109.9(5)	H(21A)-	C(21)-	H(21B)	109.5
C(29)-	N(4)-	Hg(1)	123.0(3)	C(20)-	C(21)-	H(21C)	109.5
C(30)-	N(4)-	Hg(1)	122.0(4)	H(21A)-	C(21)-	H(21C)	109.5
N(1)-	C(4)-	C(3)	113.5(6)	H(21B)-	C(21)-	H(21C)	109.5
N(1)-	C(4)-	H(4A)	108.9	C(23)-	C(22)-	C(27)	118.2(4)

C(3)-	C(4)-	H(4A)	108.9	C(23)-	C(22)-	C(11)	117.1(4)
N(1)-	C(4)-	H(4B)	108.9	C(27)-	C(22)-	C(11)	124.5(4)
C(3)-	C(4)-	H(4B)	108.9	C(22)-	C(23)-	C(24)	121.0(5)
H(4A)-	C(4)-	H(4B)	107.7	C(22)-	C(23)-	H(23)	119.5
N(1)-	C(5)-	C(6)	121.8(5)	C(24)-	C(23)-	H(23)	119.5
N(1)-	C(5)-	C(10)	121.6(5)	C(25)-	C(24)-	C(23)	120.0(5)
C(6)-	C(5)-	C(10)	116.6(4)	C(25)-	C(24)-	H(24)	120.0
C(7)-	C(6)-	C(5)	120.2(5)	C(23)-	C(24)-	H(24)	120.0
C(7)-	C(6)-	H(6)	119.9	C(24)-	C(25)-	C(26)	120.1(5)
C(5)-	C(6)-	H(6)	119.9	C(24)-	C(25)-	H(25)	120.0
O(1)-	C(7)-	C(6)	115.2(4)	C(26)-	C(25)-	H(25)	120.0
O(1)-	C(7)-	C(8)	120.8(4)	C(25)-	C(26)-	C(27)	120.6(5)
C(6)-	C(7)-	C(8)	123.9(4)	C(25)-	C(26)-	H(26)	119.7
C(11)-	C(8)-	C(7)	119.7(4)	C(27)-	C(26)-	H(26)	119.7
C(11)-	C(8)-	C(9)	125.1(4)	C(26)-	C(27)-	C(22)	120.0(4)
C(7)-	C(8)-	C(9)	115.3(4)	C(26)-	C(27)-	C(28)	121.4(4)
C(10)-	C(9)-	C(8)	122.0(5)	C(22)-	C(27)-	C(28)	118.5(4)
C(10)-	C(9)-	H(9)	119.0	O(2)-	C(28)-	N(3)	122.3(4)
C(8)-	C(9)-	H(9)	119.0	O(2)-	C(28)-	C(27)	123.2(4)
C(9)-	C(10)-	C(5)	122.0(4)	N(3)-	C(28)-	C(27)	114.5(4)
C(9)-	C(10)-	H(10)	119.0	N(4)-	C(29)-	N(3)	120.2(5)
C(5)-	C(10)-	H(10)	119.0	N(4)-	C(29)-	S(1)	115.4(4)
C(8)-	C(11)-	C(12)	119.3(4)	N(3)-	C(29)-	S(1)	124.4(4)
C(8)-	C(11)-	C(22)	120.7(4)	C(31)-	C(30)-	N(4)	115.4(7)
C(12)-	C(11)-	C(22)	119.5(4)	C(31)-	C(30)-	H(30)	122.3
C(11)-	C(12)-	C(17)	125.8(4)	N(4)-	C(30)-	H(30)	122.3
C(11)-	C(12)-	C(13)	119.0(4)	C(30)-	C(31)-	S(1)	111.4(6)
C(17)-	C(12)-	C(13)	115.0(4)	C(30)-	C(31)-	H(31)	124.3
C(14)-	C(13)-	O(1)	115.6(4)	S(1)-	C(31)-	H(31)	124.3