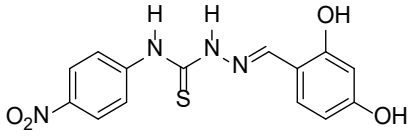
SUPPLEMENTARY MATERIAL

1. NMR (^{1}H and ^{13}C) and FTIR Spectrum of the (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-phenyl-hydrazine-carbothioamide (PBs)



Compound PB12. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-nitro-phenyl)-hydrazine-carbothioamide.

^{1}H NMR (400 MHz, DMSO-d6): δ = 11.94 (s, 1H, NH), 10.28 (s, 1H, OH), 9.91 (s, 1H, CH phenyl), 9.86 (s, 1H, OH), 8.43 (s, 1H, NH), 8.22 (d, 2H, J = 8 Hz, CH phenyl), 8.09 (d, 2H, J = 8 Hz, CH phenyl), 7.89 (m, 1H, CH phenyl), 6.35 (s, 1H, CH=N), 6.32 (d, 1H, J = 4 Hz, CH phenyl). ^{13}C NMR (100 MHz, DMSO-d6): 174.75, 161.55, 159.03, 146.38, 146.14,145.99, 143.62, 142.72, 129.18, 124.91, 124.18, 124.08, 122.61, 111.95, 108.38, 102.83, 56.52. IR (KBr, cm^{-1}): 3561 e 3481 (OH), 3159 e 3010 (NH), 1562 (C=N), 1505(C=S), 1132 (C-N).

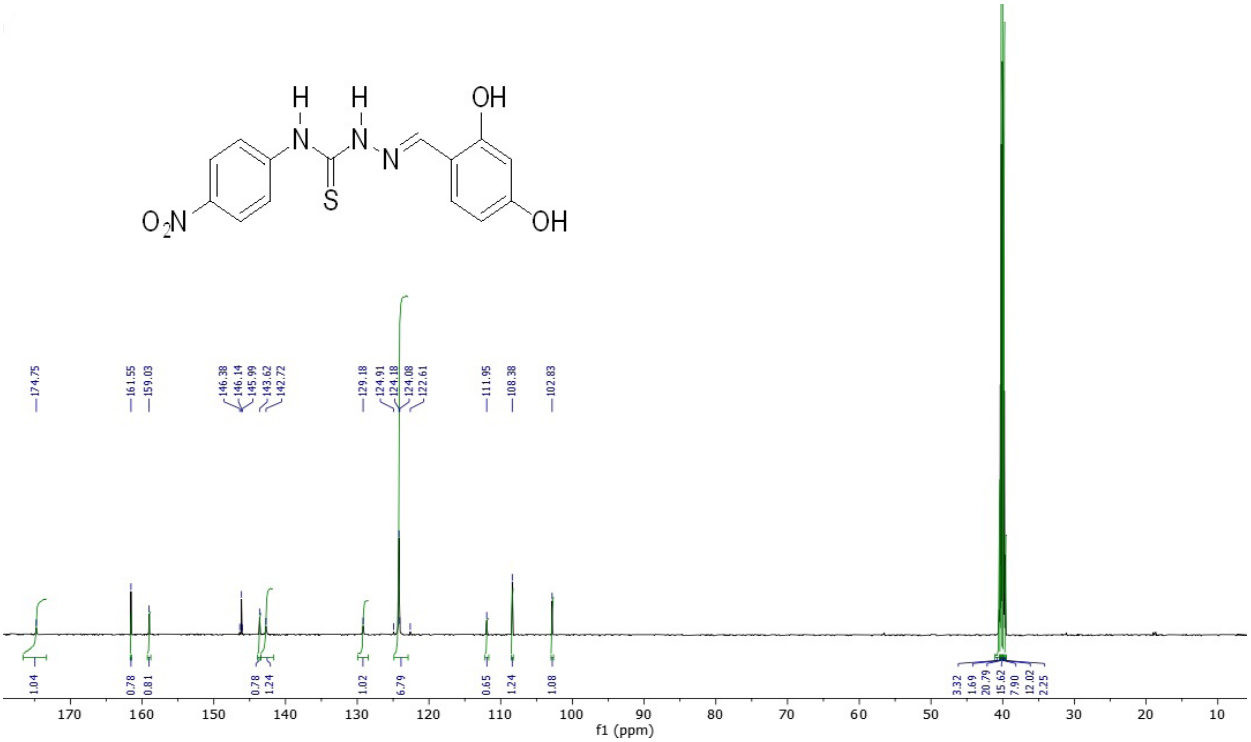


Figure S1. ^{13}C NMR Spectrum of PB12. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-nitro-phenyl)-hydrazine-carbothioamide (100 MHz, DMSO-d_6).

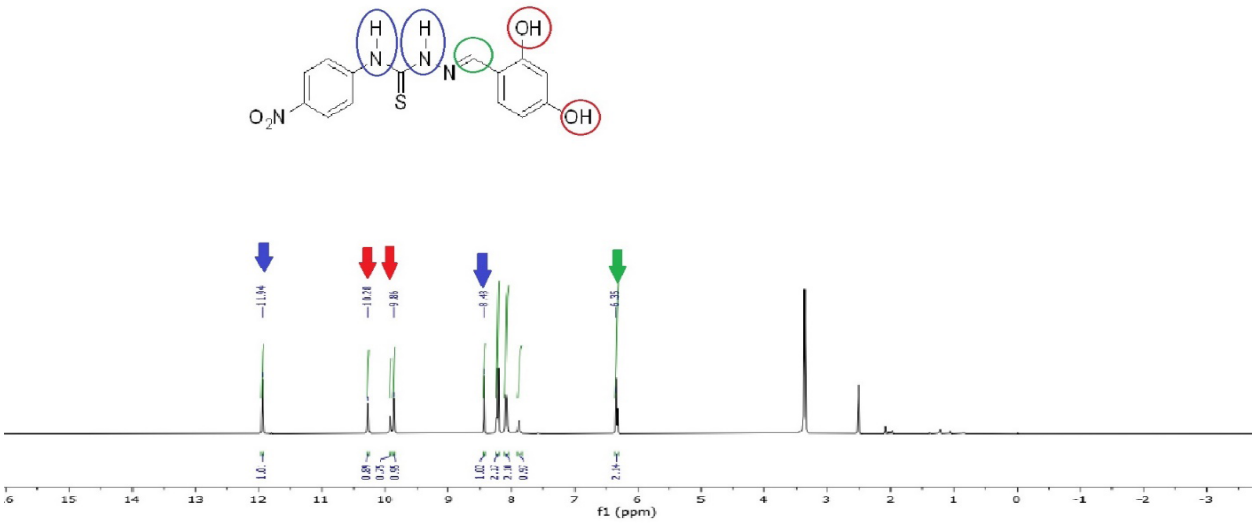


Figure S2. ^{1}H NMR Spectrum of PB12. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-nitrophenyl)-hydrazine-carbothioamide (400 MHz, DMSO-d_6).

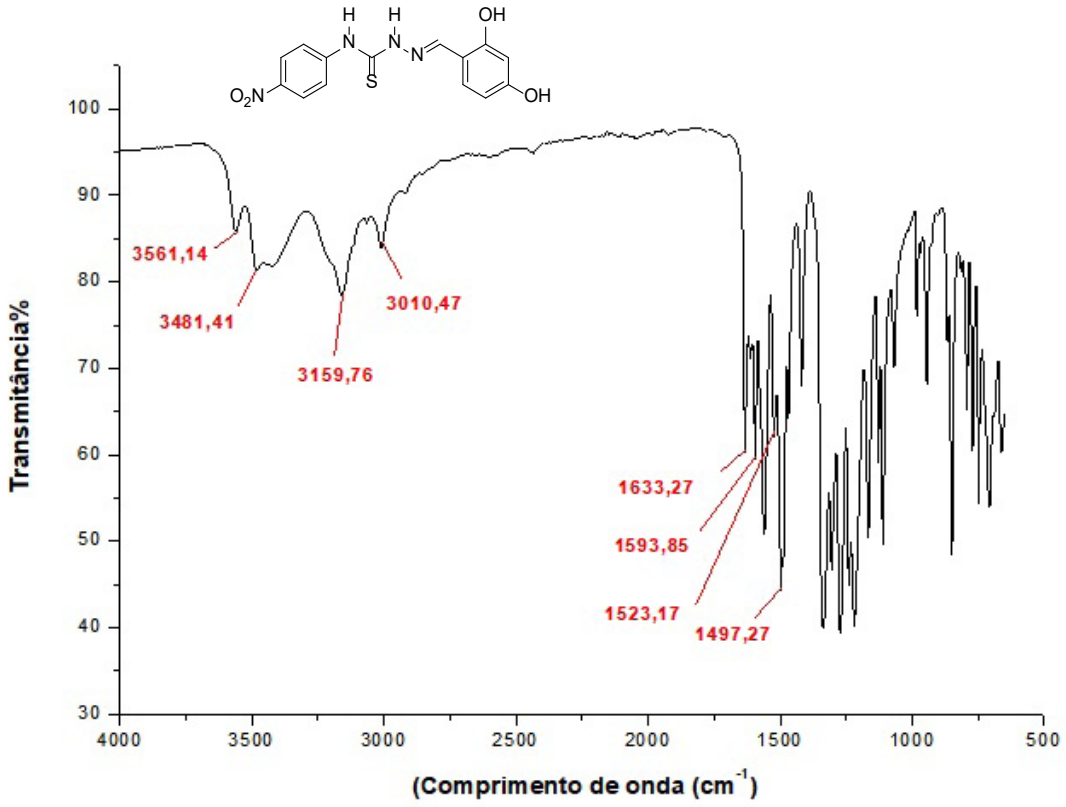
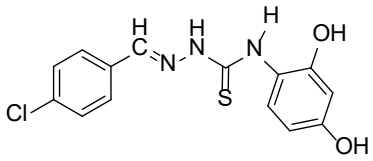


Figure S3. FTIR Spectrum of PB12. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-nitrophenyl)-hydrazine-carbothioamide.



Compound PB13. (*E*)-*N*-(4-chloro-phenyl)-2-(2,4-dihydroxy-benzylidene)-hydrazine-carbothioamide

^{1}H NMR (400 MHz, DMSO-d6): δ = 6.33 (s, 1H, C=N), 6.30 (d, 1H, J = 4Hz, CH phenyl), 7.40 (d, 2H J = 8 Hz, phenyl), 7.87 (m, 1H, CH phenyl), 8.38 (s, 1H, NH), 9.81 (s, 1H, OH), 9.85 (s, 1H, CH phenyl), 9.96 (s, 1H, OH), 11.65 (s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d6): 175.53, 161.26, 158.76, 141.94, 138.74, 129.35, 129.16, 128.31, 127.41, 112.15, 108.28, 102.80, 40.58. IR (KBr, cm^{-1}): 3647 - 3389 (OH), 3143 - 2986 (NH), 1562 (C=N), 1505(C=S), 1132 (C-N). IR (KBr, cm^{-1}): 3647 e 3389 (OH), 3143 e 2986 (NH), 1565 (C=N), 1508(C=S), 1135 (C-N).

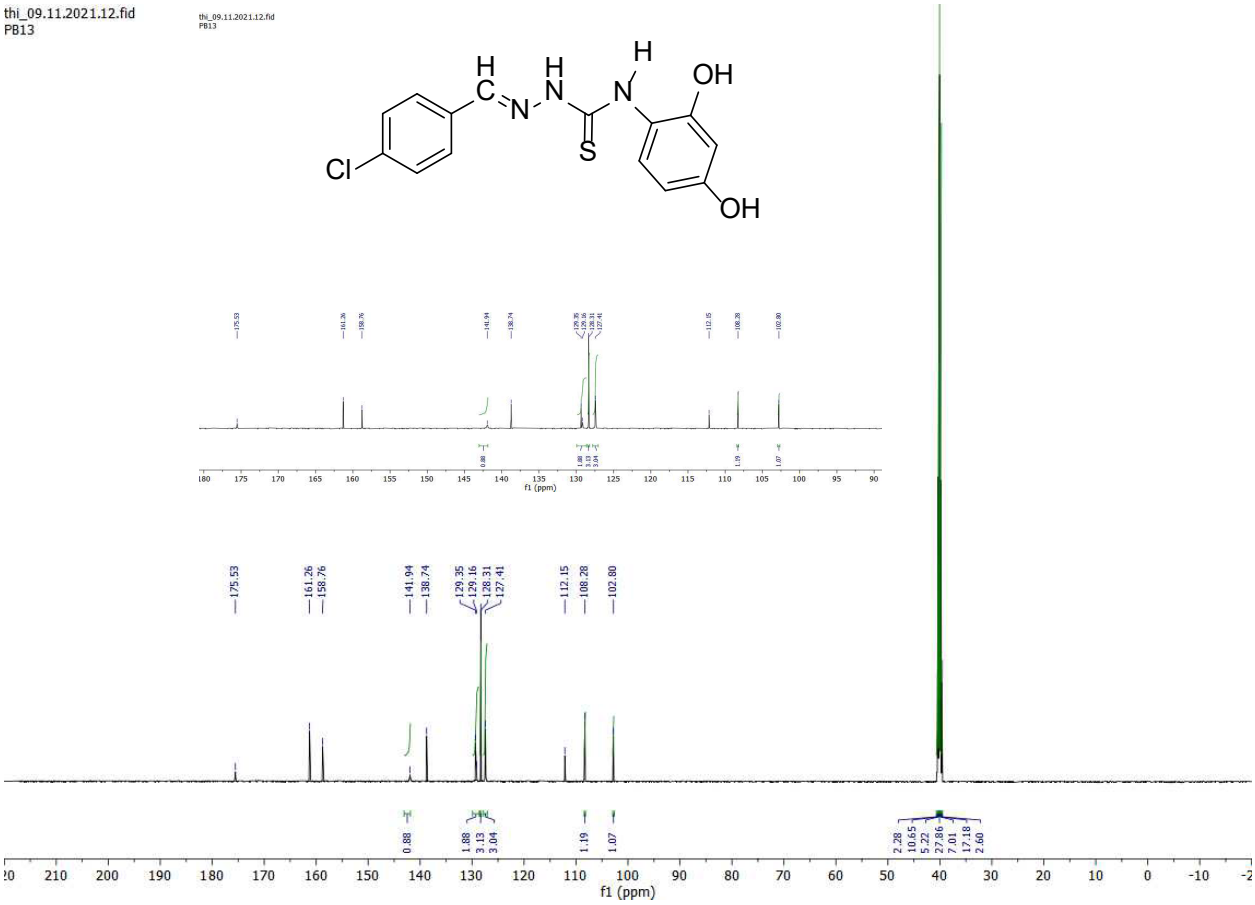


Figure S4. **^{13}C NMR Spectrum of PB13. ((*E*)-*N*-(4-chloro-phenyl)-2-(2,4-dihydroxy-benzylidene)-hydrazine-carbothioamide (100 MHz, DMSO-d$_6$).**

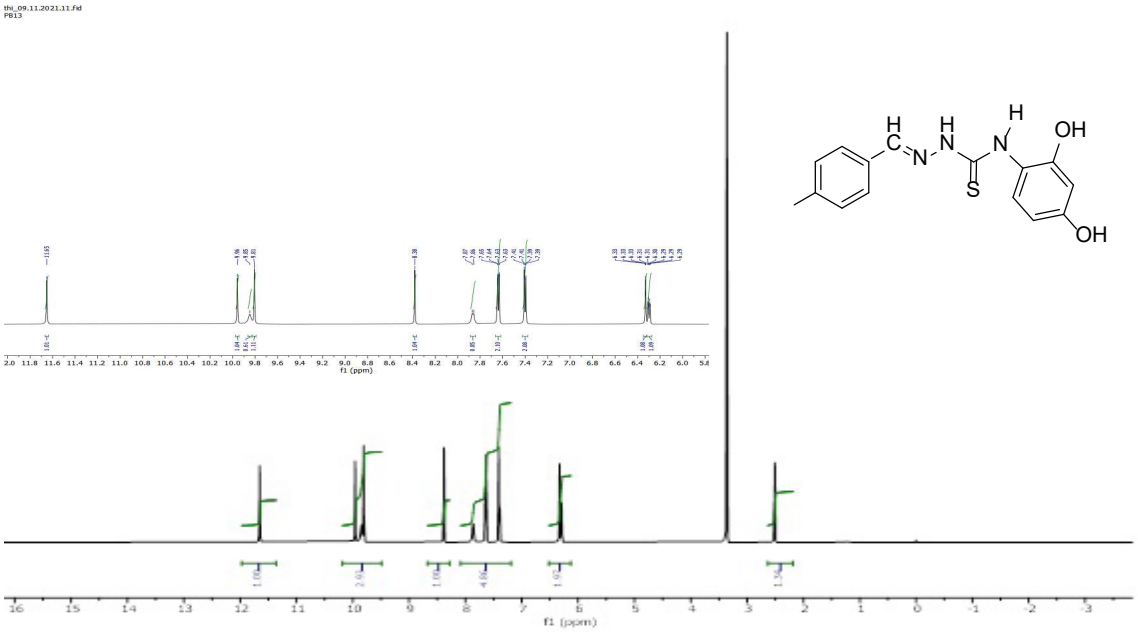


Figure S5. ^{1}H NMR Spectrum of PB13. ((*E*)-*N*-(4-chloro-phenyl)-2-(2,4-dihydroxy-benzylidene)-hydrazine-carbothioamide (400 MHz, DMSO-d_6).

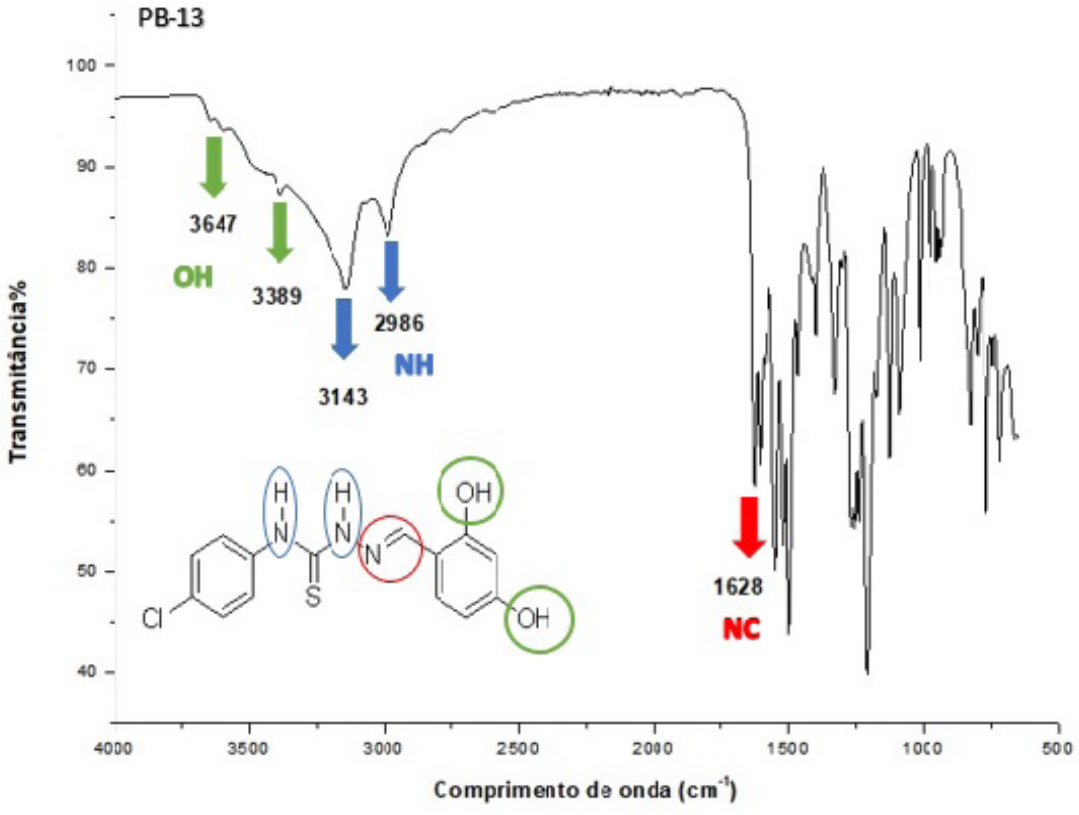
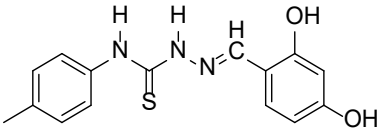


Figure S6. FTIR Spectrum of PB13. ((*E*)-*N*-(4-chloro-phenyl)-2-(2,4-dihydroxy-benzylidene)-hydrazine-carbothioamide.



Compound PB17. (*E*) 2-(2,4-dihydroxy-benzylidene)-*N*-(*p*-tolyl)-hydrazine-carbothioamide

^{1}H RMN (400 MHz, DMSO-d6): δ = 11.51 (s, 1H, NH), 9.83 (s, 1H, OH), 9.77 (s, 1H, CH phenyl), 9.78 (s, 1H, OH), 8.37 (s, 1H, NH), 7.85 (m, 1H, CH phenyl), 7.44 (d, 2H, J = 8 Hz, CH phenyl), 7.15 (d, 2H, J = 8 Hz, CH phenyl), 6.33 (s, 1H, HC=N), 6.29 (d, 1H, J = 4 Hz, CH phenyl), 2.31 (s, 3H, CH3). ^{13}C RMN (100 MHz, DMSO-d6): 206.86, 175.70, 161.14, 158.67, 141.62, 137.17, 134.55, 129.17, 128.93, 125.77, 112.24, 08.27, 102.82, 40.59. IR (KBr, cm^{-1}): 3647 e 3389 (OH), 3038 e 2983 (NH), 1630 (C=N), 508 (C=S), 1135 (C-N).

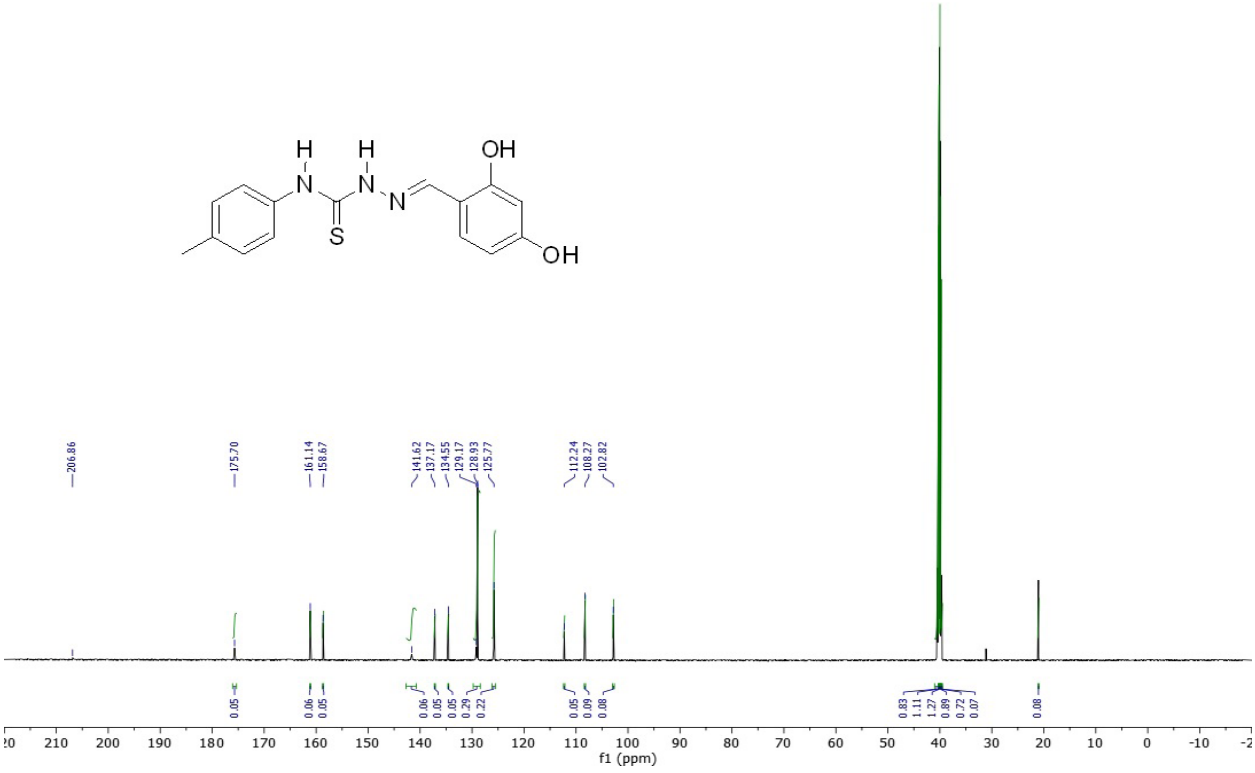


Figure S7. ^{13}**C NMR Spectrum of PB17. (*E*) 2-(2,4-dihydroxy-benzylidene)-*N*-(*p*-tolyl)-hydrazine-carbothioamide (100 MHz, DMSO-d$_6$).**

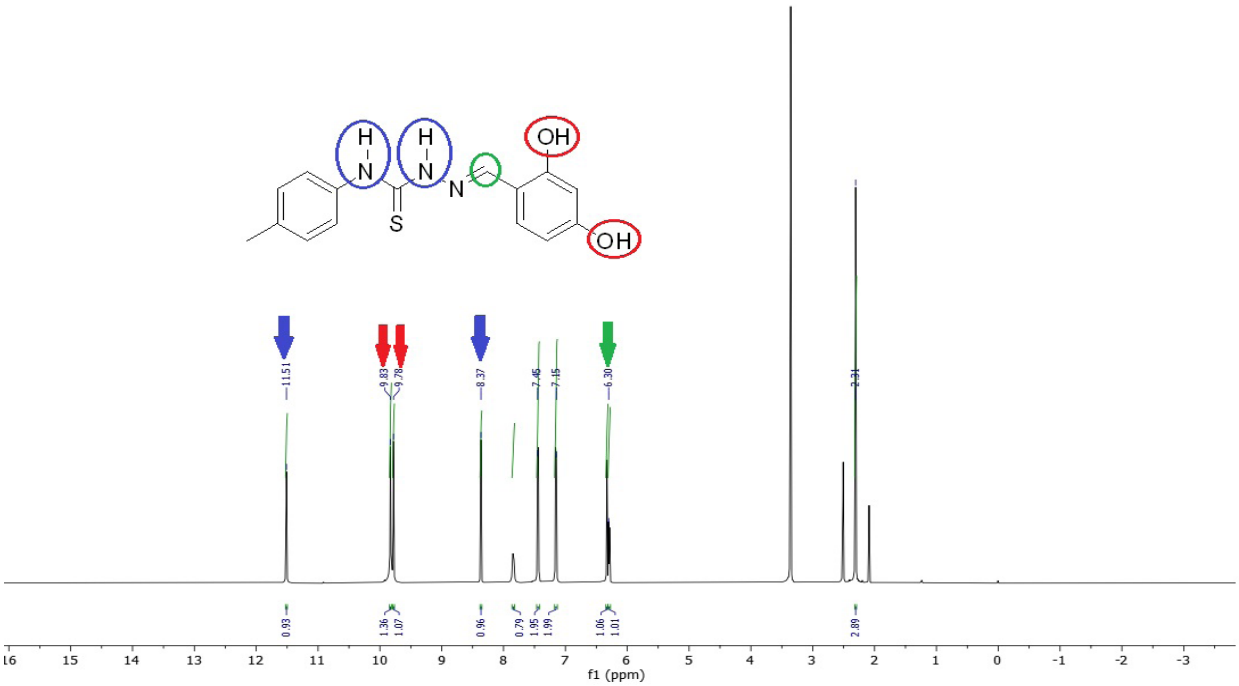


Figure S8. ^{1}H NMR Spectrum of PB17. (*E*) 2-(2,4-dihydroxy-benzylidene)-*N*-(*p*-tolyl)-hydrazine-carbothioamide (400 MHz, DMSO-d_6)

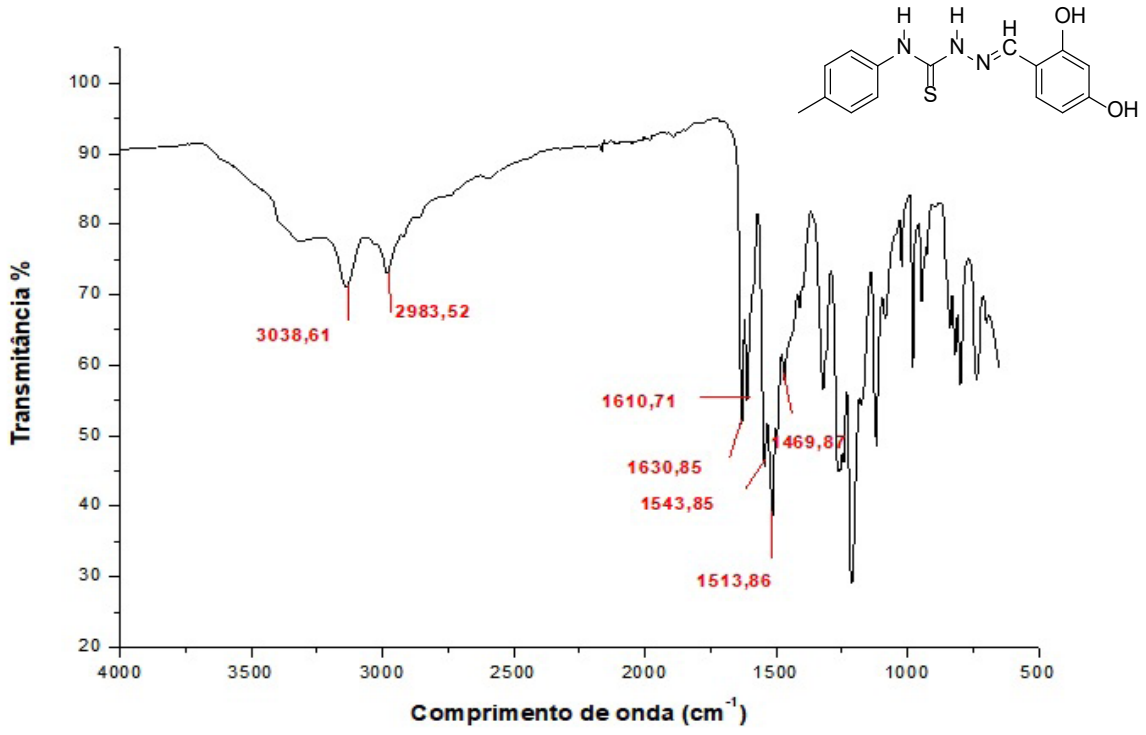
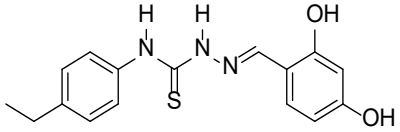


Figure S9. FTIR Spectrum of PB17. (*E*) 2-(2,4-dihydroxy-benzylidene)-*N*-(*p*-tolyl)-hydrazine-carbothioamide.



Compound PB18. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-ethyl-phenyl)-hydrazine-carbothioamide

^{1}H RMN (400 MHz, DMSO-d_6): δ = 11.54 (s, 1H, NH), 9.85 (s, 1H, OH), 9.82 (s, 1H, CH phenyl), 9.80 (s, 1H, OH), 8.36 (s, 1H, NH), 7.86 (m, 1H, CH phenyl), 7.46 (d, 2H, J = 8 Hz, CH phenyl), 7.18 (d, 2H, J = 8 Hz, CH phenyl), 6.33 (s, 1H, HC=N), 6.29 (d, 1H, J = 4 Hz, CH phenyl), 2.60 (q, 2H, CH_2), 1.19 (t, 3H, CH_3). ^{13}C RMN (400 MHz, DMSO-d_6): 206.88, 175.64, 161.14, 158.67, 141.55, 140.95, 137.35, 129.13, 127.72, 125.84, 112.24, 108.26, 102.80, 40.58.

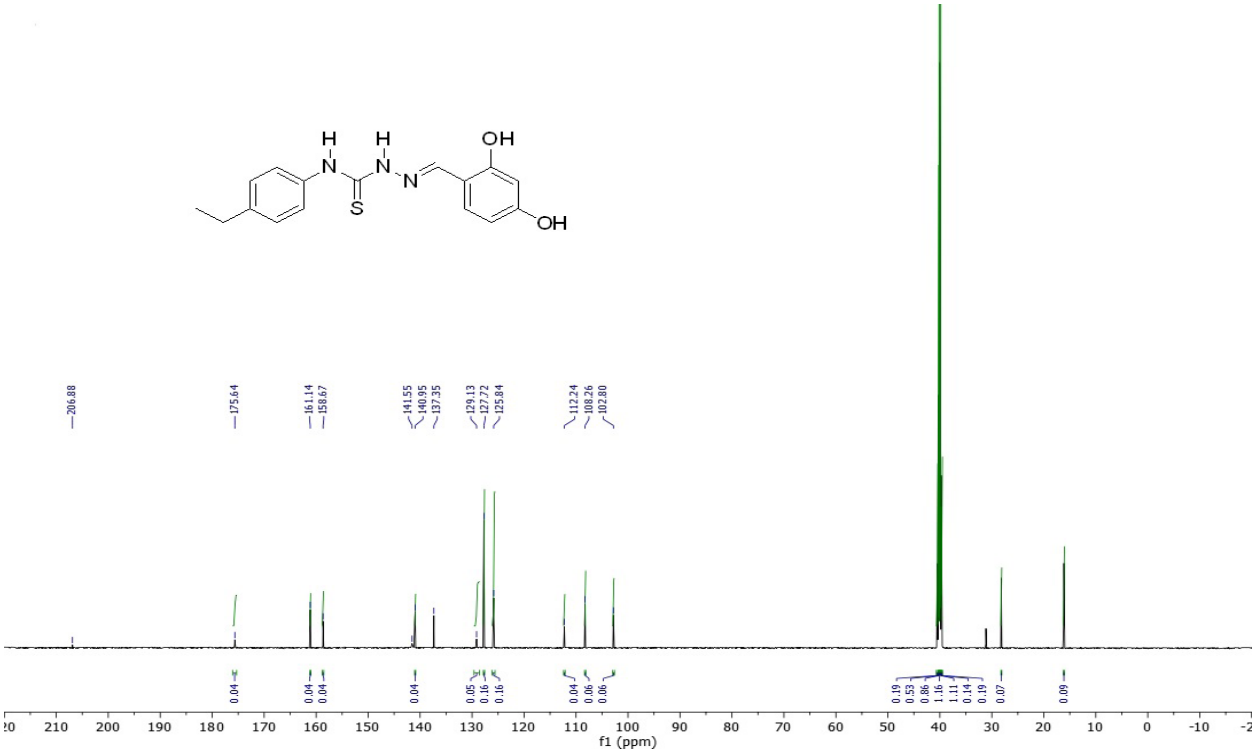


Figure S10. ^{13}**C NMR Spectrum of PB18. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-ethyl-phenyl)-hydrazine-carbothioamide (100 MHz, DMSO-d_6).**

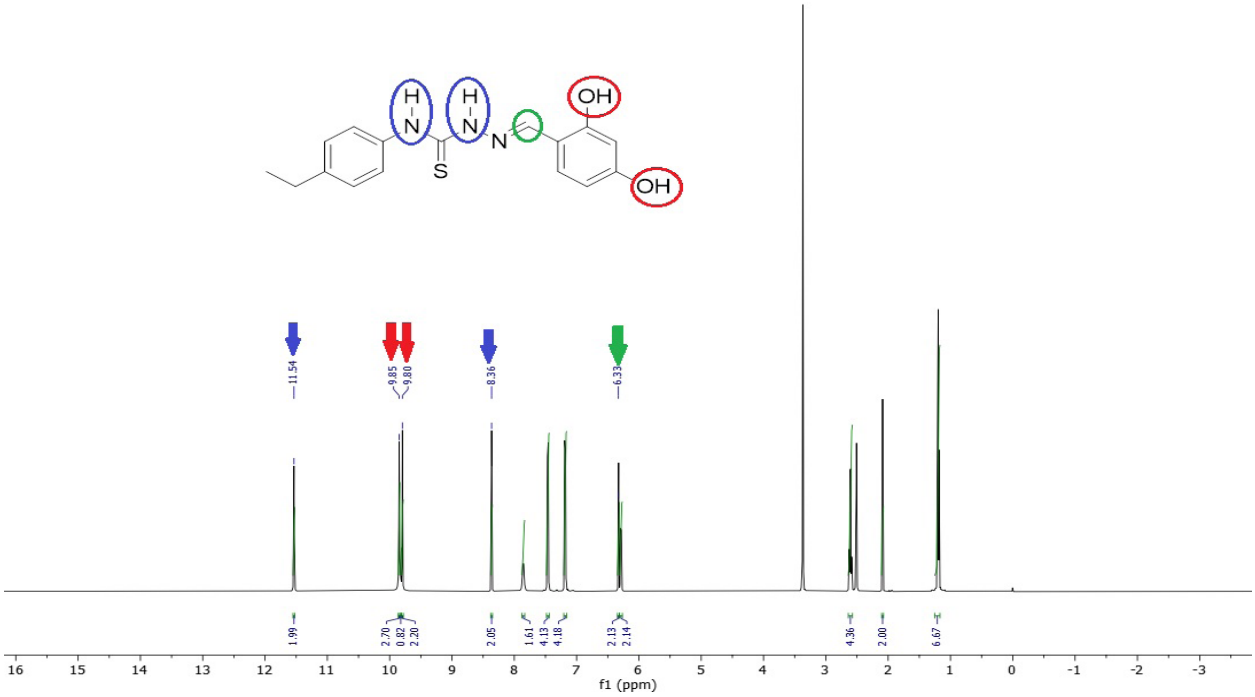
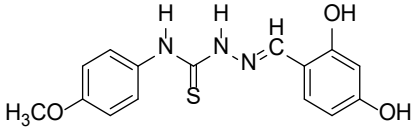


Figure S11. ^{1}H NMR Spectrum of PB18. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-ethyl-phenyl)-hydrazine-carbothioamide (400 MHz, DMSO-d_6).



Compound PB19: (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-methoxy-phenyl)-hydrazine-carbothioamide

^{1}H RMN (400 MHz, DMSO-d6): δ = 11.47 (s, 1H, NH), 9.80 (s, 1H, OH), 9.77 (s, 1H, CH phenyl), 9.76 (s, 1H, OH), 8.35 (s, 1H, NH), 7.85 (m, 1H, CH phenyl), 7.41 (d, 2H, J= 8 Hz, CH phenyl) 6.92 (d, 2H, J = 8 Hz, CH phenyl) 6.33 (s, 1H, HC=N), 6.29 (d, 1H, J = 4 Hz, CH phenyl) 3.77 (s, 3H, OCH3). RMN C13 (400 MHz, DMSO-d6): 176.04, 165.64, 161.09, 158.62, 157.23, 141.51, 132.66, 129.17, 127.63, 113.70, 112.28, 109.12, 108.24, 102.81, 102.69, 55.72, 40.59.

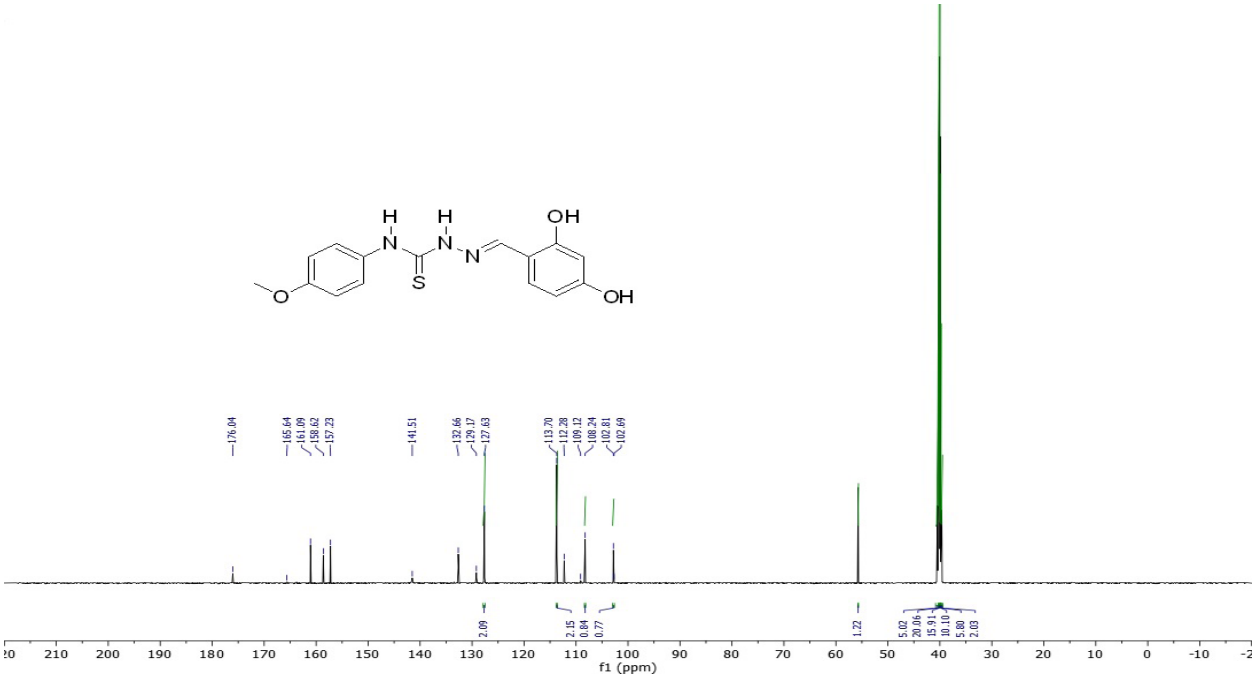


Figure S12. ^{13}C NMR Spectrum of PB19. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-methoxy-phenyl)-hydrazine-carbothioamide (100 MHz, DMSO-d_6).

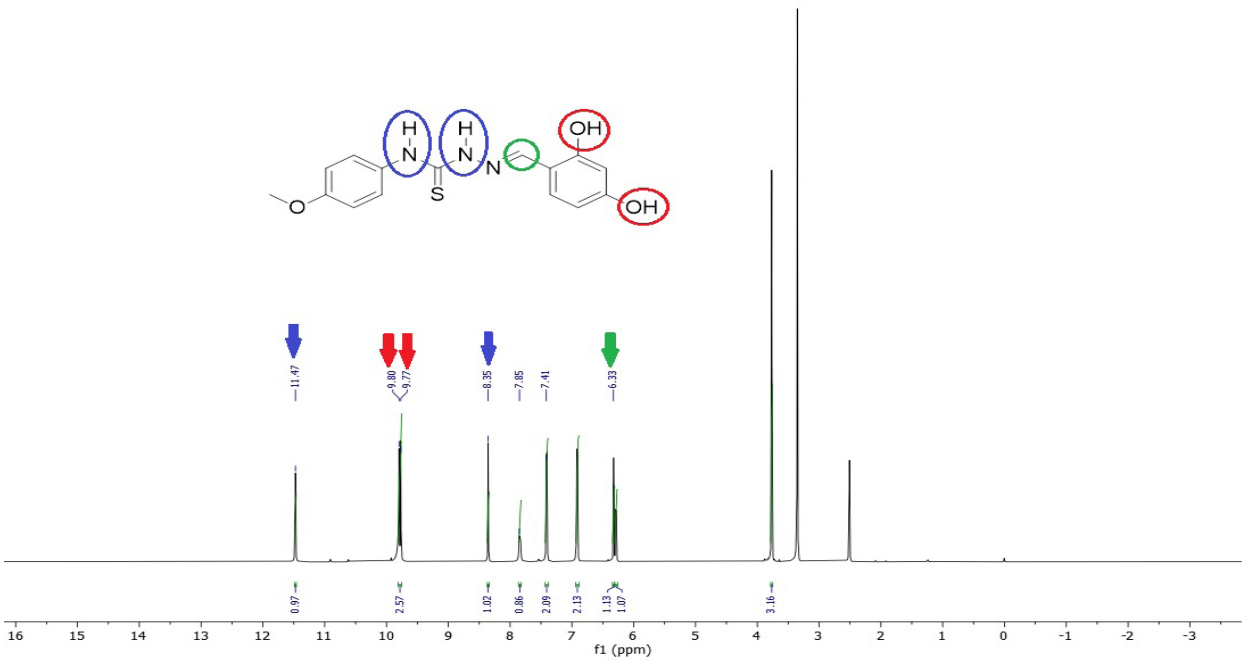


Figure S13. ^{1}H NMR Spectrum of PB19. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-methoxy-phenyl)-hydrazine-carbothioamide (400 MHz, DMSO-d_6).

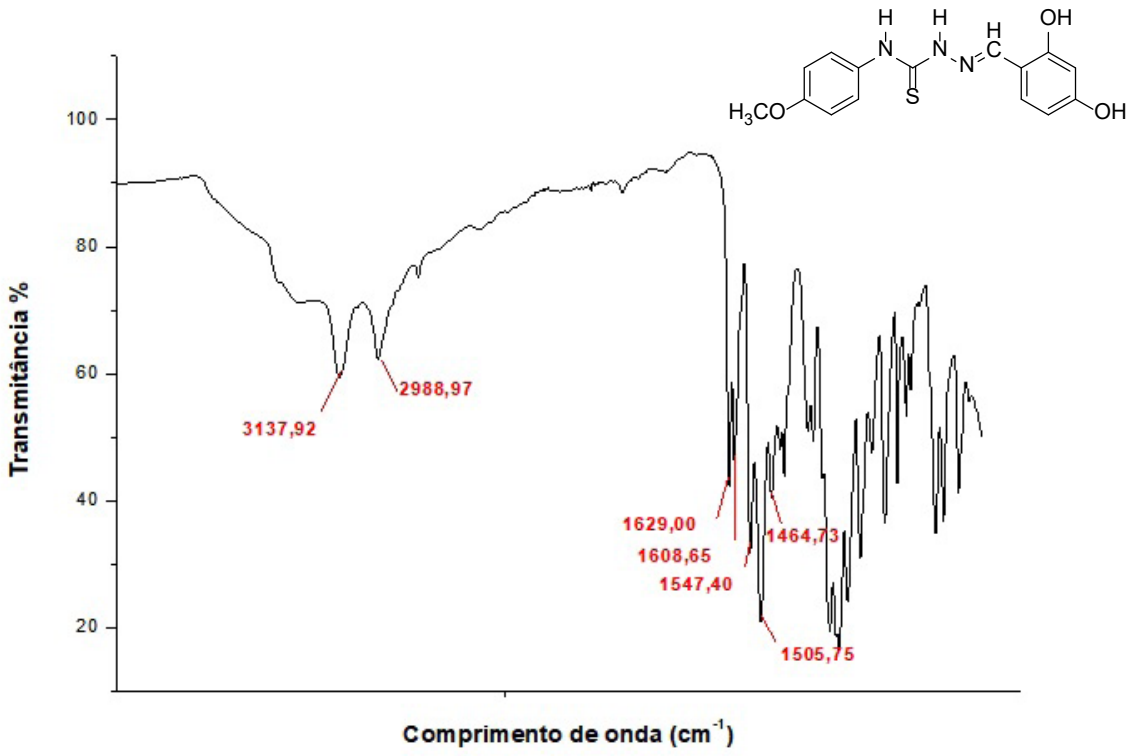
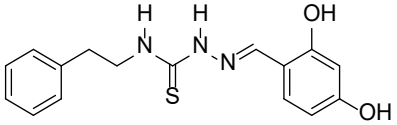


Figure S14. FTIR Spectrum of PB19. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-(4-methoxy-phenyl)-hydrazine-carbothioamide.



Compound PB20. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-phenethyl-hydrazine-carbothioamide

^{1}H NMR (400 MHz, DMSO-d_6): δ = 11.25 (s, 1H, NH), 9.78 (s, 1H, OH), 9.77 (s, 1H, CH phenyl), 9.76 (s, 1H, OH), 8.35 (s, 1H, NH), 7.64 (m, 1H, CH phenyl), 7.33 – 7.22 (m, 5H, CH phenyl), 6.29 (d, 1H, J = 4 Hz, CH phenyl), 6.30 (s, 1H, CH=N), 3.77 (m, 2H, CH_2), 2.91 (t, 2H, J = 8 Hz, CH_2). ^{13}C NMR (400 MHz, DMSO-d_6): 176.88, 160.94, 158.45, 140.87, 139.82, 129.08, 128.90, 128.57, 126.62, 112.35, 108.21, 102.84, 45.40, 40.59.

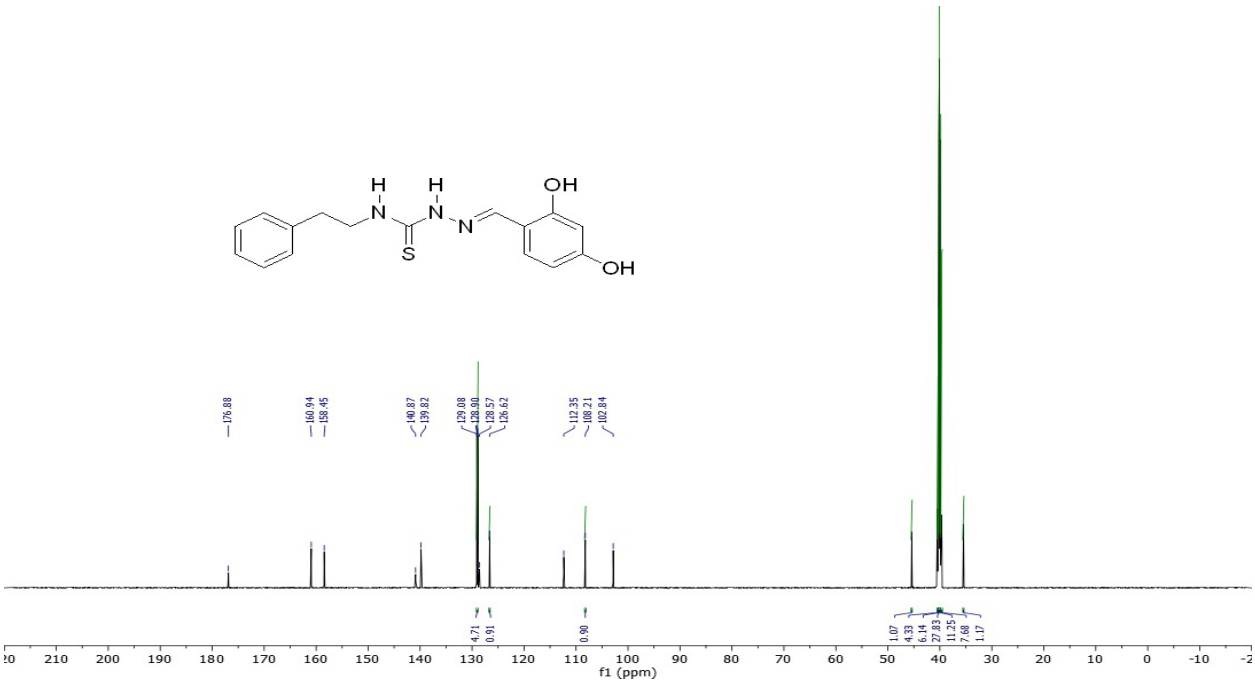


Figure S15. ^{13}C NMR Spectrum of PB20. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-phenethyl-hydrazine-carbothioamide (100 MHz, DMSO-d_6).

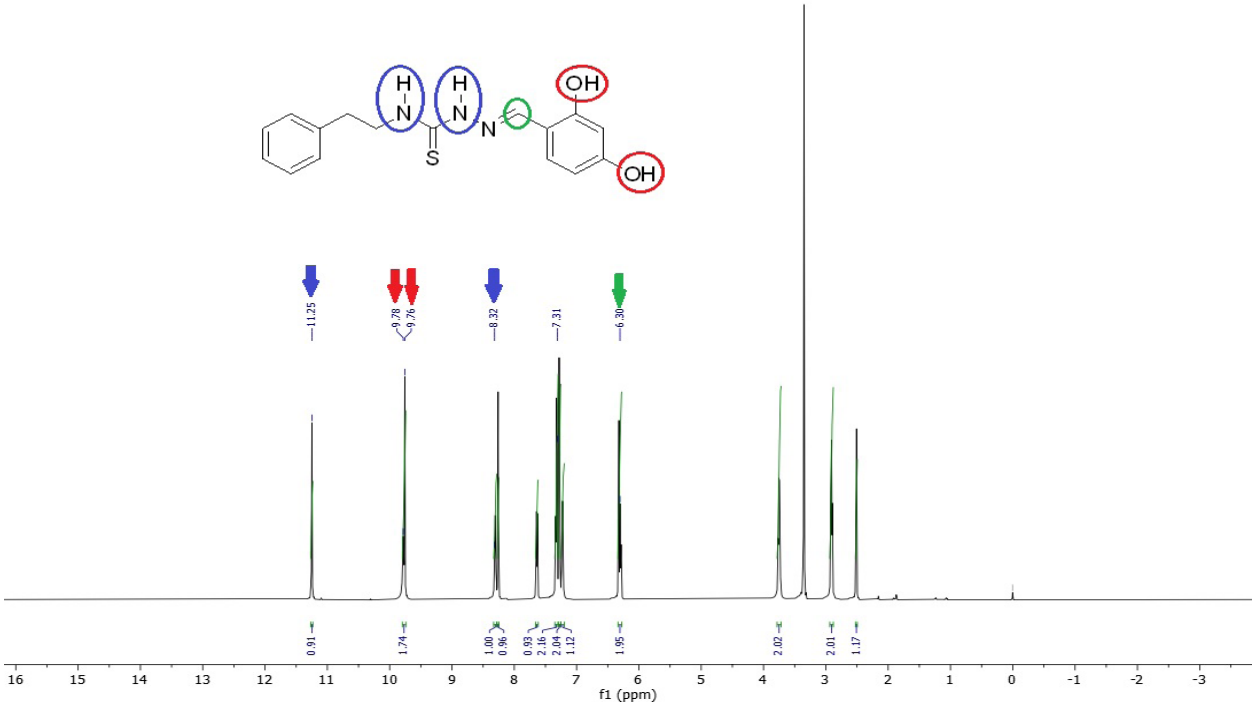


Figure S16. ^{1}H NMR Spectrum of PB20. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-phenethyl-hydrazine-carbothioamide (400 MHz, DMSO-d_6).

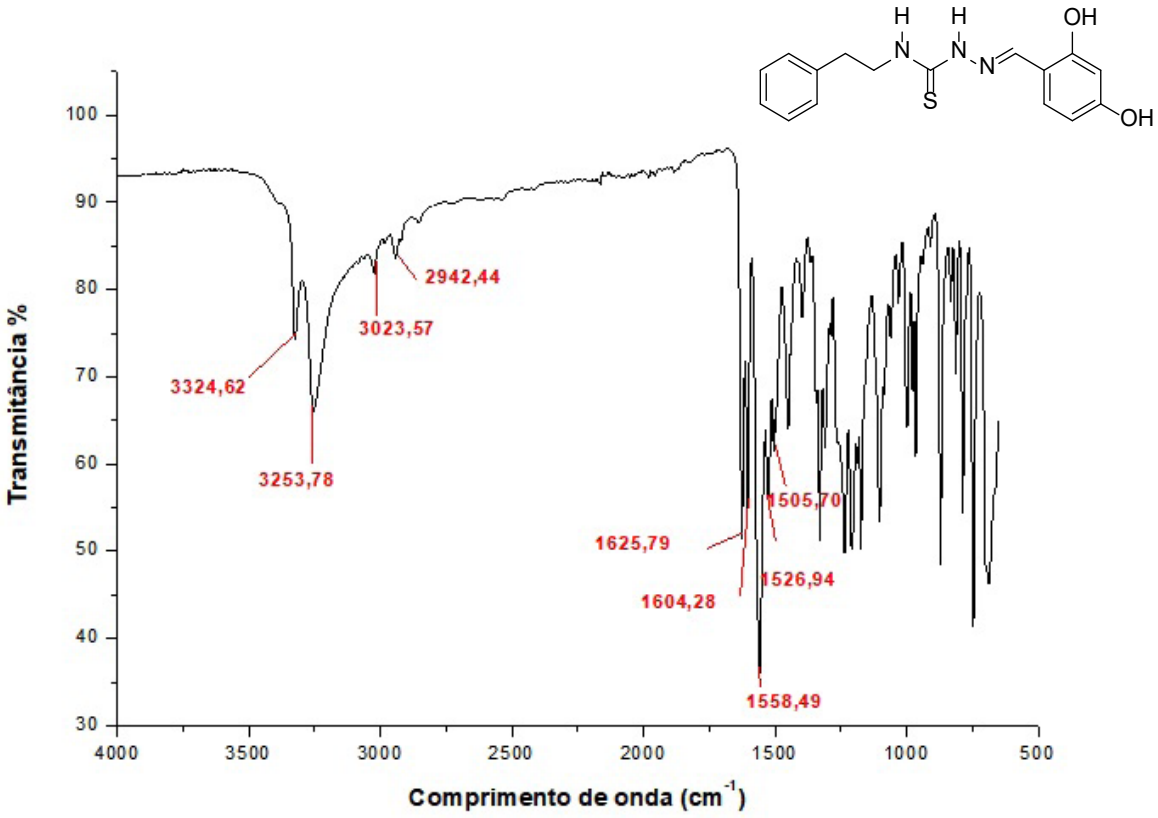


Figure S17. FTIR Spectrum of PB20. (*E*)-2-(2,4-dihydroxy-benzylidene)-*N*-phenethyl-hydrazine-carbothioamide.

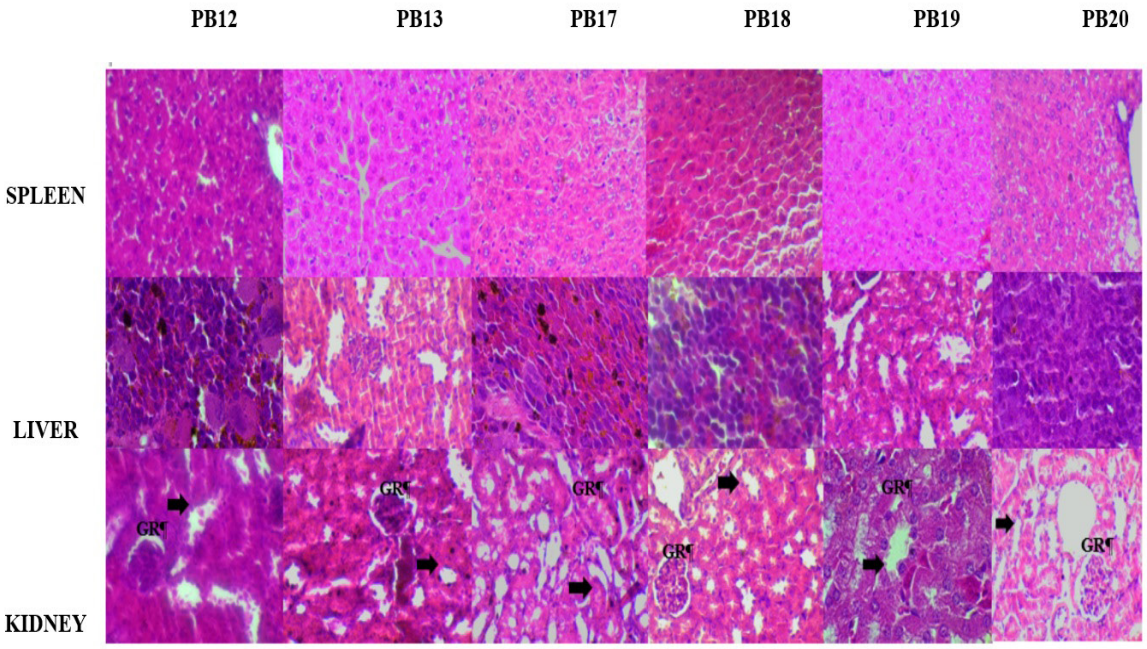


Figure S18. Photomicrograph of histological analysis of spleens, livers and kidneys from mice treated with thiosemicarbazonic compounds. Caption: Representative photomicrographs of the spleen, liver and kidney of female mice from the groups treated with a single dose of 2000mg/kg po. Spleen: Lymph nodes (Nd) are well defined in treated groups. We can visualize the pulps of the organ without hyperactivation and with well-defined contours. Hematoxylin and eosin staining was used. Livers: the centrilobular vein (cv) is seen in all images with the presence of well-organized hepatocyte cords. Kidneys: Renal glomeruli (Gr) and convoluted tubes (arrowheads) preserved in order. Bowman's intracapsular space is well delimited and of normal diameter. Magnification: 400x and 100x objectives.

Table SI. Cytotoxic activity promoted by thiosemicarbazone compounds against J774 Macrophage strains, Vero cells, V79 fibroblasts, HepG2 and against erythrocytes respectively.

Compounds (PB)	Macrophages J774(IC_{50} µM)	Vero cells (IC_{50} µM)	Fibroblasts V79 (IC_{50} µM)	Erythrocytes (%)
PB12	74.11 ± 5.1	85.34 ± 2.5	81.45 ± 1.3	< 10
PB13	49.27 ± 0.9	60.12 ± 1.0	62.65 ± 0.1	< 10
PB17	65.01 ± 1.9	67.56 ± 0.8	71.21 ± 0.3	< 10
PB18	31.85 ± 1.3	45.21 ± 2.0	49.45 ± 0.9	< 10
PB19	55.01 ± 1.9	65.02 ± 1.0	67.23 ± 0.2	< 10
PB20	67.02 ± 0.6	73.09 ± 0.5	75.04 ± 1.1	< 10
Dox	1.22 ± 0.01	1.43 ± 0.02	1.54 ± 0.00	< 10
*m*AMSA	3.1 ± 0.03	1.16 ± 0.02	1.32 ± 0.01	< 10

Mean ± Standard deviation; Dox: Doxorubicin; mAMSA: Amsacrine.

Table SII. Evaluation of water and feed consumption, average weight of the animals and relative weight (g/10 g of animal body weight) of the organs of mice without treatment and those treated with compounds PB12, PB13, PB17, PB18, PB19 and PB20 all administered orally.

Parameters	Control	Gavage
Water consumption (mL)	26.79 ± 1.88	26.92 ± 1.38
Food consumption (g)	17.35 ± 0.41	17.85 ± 0.51
Average weight (g)	35.09 ± 0.85	34.81 ± 0.49
Organ Control	**Control**	**Gavage**
Kidney (g)	0.54 ± 0.08	0.55 ± 0.09
Spleen (g)	0.28 ± 0.03	0.28 ± 0.07
Liver (g)	2.37 ± 0.58	2.36 ± 0.61

Mean ± Standard deviation.

Table SIII. Hematological and biochemical parameters of mice not treated and treated with compounds PB12, PB13, PB17, PB18, PB19 and PB20 all orally.

Hematological Parameters	Control	PB12	PB13	PB17	PB18	PB19	PB20
RBC	10.5 ± 0.70	8.91 ± 0.73	9.93 ± 0.01	9.36 ± 0.57	9.86 ± 0.70	10.37 ± 0.1	9.93 ± 0.57
HCT	55.0 ±0.41	44.36 ± 0.23	50.56 ± 0.21	47.26 ± 0.51	51.75 ± 0.12	52.95 ± 0.01	51.56 ± 1.52
HB	15.5 ± 0.70	13.4 ± 0.08	15.2 ± 0.01	14.1 ± 0.70	15.8 ± 0.70	16.0 ± 0.02	15.2 ± 0.27
MCV	54.0 ±1.41	49.08 ± 0.45	50.93 ± 0.03	50.5 ± 1.15	42.55 ± 1.41	51.10 ± 0.02	59.93 ± 0.07
MCH	15.5 ± 0.21	15.1 ± 0.23	15.2 ± 0.09	15.0 ± 0.57	16.0 ± 0.70	15.45 ± 0.70	16.2 ± 0.51
MCHC	28.5 ± 0.11	30.33 ± 0.6	30.06 ± 0.01	29.83 ± 0.57	30.5 ± 0.01	30.25 ± 0.57	29.06 ± 0.57
WBC	4.5 ± 0.01	3.84 ± 0.01	4.19 ± 0.02	3.88 ± 0.01	3.95 ± 0.12	5.58 ± 0.12	4.19 ± 0.52
PLT	0.73 ± 0.0	0.55± 0.08	0.83± 0.0	0.79 ± 0.01	0.42 ± 0.0	0.74 ± 0.0	0.57± 0.002
NEUT	12.0 ± 1.7	14.66 ± 0.03	8.66 ± 0.05	7.33 ± 0.15	8.5 ± 0.01	8.50 ± 0.01	8.0 ± 0.01
LIMPH	85 ± 9.89	85.33 ± 5.03	90.66 ± 3.21	91.66 ± 1.54	91 ± 0.70	91.50 ± 0.40	91.33 ± 0.09
MONO	1.5 ± 0.01	0.2 ± 0.2	0.16 ± 0.11	0.33 ± 0.15	1.0 ± 0.0	0.21 ± 0.06	0.0 ± 0.0
EO	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.01	0.5 ± 0.0	0.5 ± 0.0	0.20 ± 0.02	0.0 ± 0.0
BASO	0.2 ± 0.0	0.2 ± 0.0	0.3 ± 0.05	0.2 ± 0.0	0.4 ± 0.01	0.21 ± 0.01	0.0 ± 0.0
Biochemical Parameters	**Control**	**PB12**	**PB13**	**PB17**	**PB18**	**PB19**	**PB20**
ALB	3.97 ± 0.09	3.9. ± 0.04	3.8 ± 0.01	3.8 ± 0.01	4.5 ± 0.70	4.0 ± 0.1	39.0 ± 0.57
ALT	45.0 ± 0.0	41.66 ± 1.1	51.33 ± 0.3	51.33 ± 0.8	42.5 ± 2.12	52.0 ± 3.46	44.0 ± 0.0
AMYL	2311 ± 10.1	1996.33 ± 10.5	2491.33 ± 5.90	2379.33 ± 4.32	1990.5 ± 2.34	2407 ± 1.12	2355.66 ± 1.65
AST	92.0 ± 0.0	98.33 ± 4.04	71.0 ± 13.0	71.0 ± 13.0	94.5 ± 2.12	79.66 ± 0.78	94.5 ± 0.3
ALP	9.0 ± 0.01	9.33 ± 5.50	1.33 ± 0.02	1.33 ± 0.09	8.0 ± 0.12	1.66 ± 0.0	1.66 ± 0.01
GGT	8.0 ± 0.02	5.0 ± 0.02	6.66 ± 0.01	6.66 ± 0.01	6.0 ± 0.0	6.66 ± 0.02	6.33 ± 0.03
GLUC	108 ± 1.0	108 ± 1.3	106.33 ± 6.61	103.33 ± 4.72	102.5 ± 7.7	110.66 ± 1.19	128.33 ± 0.43
CRE	0.2 ± 0.0	0.23± 0.0	0.10 ± 0.0	0.08 ± 0.0	0.15 ± 0.0	0.11 ± 0.0	0.116 ± 0.0
CHO	103.5 ± 9.80	120.33 ± 2.02	88.33 ± 2.30	117.33 ± 2.00	158 ± 0.89	121.33 ± 6.50	113.66 ± 0.05
BIL	0.13 ± 0.0	0.18 ± 0.0	0.18 ± 0.0	0.08 ± 0.0	0.19 ± 0.0	0.14 ± 0.0	0.14 ± 0.0
LIP	11.5 ± 0.26	47.66 ± 0.08	34.33 ± 0.44	39 ± 0.2	25.1 ± 0.1	27.66 ± 0.85	28.66 ± 0.52
Na	157.5 ± 0.7	147 ± 2.64	148.66 ± 1.52	149 ± 2	146 ± 2.82	148.33 ± 2.88	147.66 ± 0.57
Cl	106 ±1.41	100.66 ± 0.57	103 ± 1.0	105.33 ± 1.15	100.05 ± 0.70	101.33 ± 2.51	102.66 ± 2.51
K	4.5 ± 0.65	42.33 ± 0.08	42.33 ± 0.45	45 ± 0.21	42.5 ± 0.53	48.0 ± 0.84	47.33 ± 0.50
TP	5.0 ± 0.0	5.7 ± 0.06	5.03 ± 0.02	5.03 ± 0.01	5.7 ± 0.01	5.16 ± 0.07	4.9 ± 0.01
UR	5.0 ± 0.76	4.1 ± 0.01	3.81 ± 0.07	5.1 ± 0.1	4.7 ± 0.02	4.23± 0.35	50.0 ± 0.84
TG	109.0 ± 0.2	159.26 ± 2.74	51.33 ± 1.65	168.23 ± 1.04	115.8 ± 0.70	145.63 ± 0.58	132.83 ± 0.52

Mean ± Standard deviation; RBC: Red Blood Cells (106/mm3); HCT: Hematocrit (%); HB: Hemoglobin (g/dL); MCV: Mean Corpuscular Volume (%); MCH: Mean Corpuscular Hemoglobin (%); MCHC: Mean Corpuscular Hemoglobin Concentration (%); PLT: Platelets (10^3/mm^3); WBC: White Blood Cells (10^3/mm^3). ALB: albumin (g/dL); ALT: alanine aminotransferase (U/L); AST: aspartate aminotransferase (U/L); ALP: alkaline phosphatase (U/L); BIL: bilirubin (mg/dL); GGT: gamma-glutamyl transferase; TP:total protein (g/dL); RH: blood urea (mg/dL); CRE: creatinine (mg/dL); TC: total cholesterol (mg/dL) TG: triglycerides (mg/dL).

Table SIV. ***In vitro*** **antioxidant activity promoted by the compounds 2,4-dihydroxy-benzylidene-thiosemicarbazones**

Compounds PB	Radicals DPPH EC_{50} (µM)	ABTS Radicals EC_{50} (µM)	OH Radicals EC_{50} (µM)	Radicals NO EC_{50} (µM)	Iron ion reduction (TPTZ) EC_{50} (µM)	Iron ion reduction (potassium ferrocyanide) EC_{50} (µM)
PB12	1150 ± 1.0	955 ± 0.3	1485 ± 0.1	1498 ± 0.1	>1500	>1500
PB13	>1500	>1500	>1500	>1500	>1500	>1500
PB17	729.06 ± 0.9	84.25 ± 0.1	1245 ± 1.0	1100 ± 0.9	>1500	>1500
PB18	>1500	>1500	>1500	>1500	>1500	>1500
PB19	598.90 ± 0.2	475.17 ± 0.5	1300.4 ± 0.4	1479 ± 1.0	>1500	>1500
PB20	>1500	>1500	>1500	>1500	>1500	>1500
AA	43.99 ± 0.2	76.06 ± 0.3	83.56 ± 0.7	1000.2 ±0.3	1235.4 ± 1.1	1123.0± 0.1
BHT	85.77 ± 1.2	27.78 ± 0.4	75.49 ± 0.5	978.6	1100.9 ± 0.1	1016 ± 0.8

Mean ± standard deviation; ascorbic acid (AA) and butylated hydroxytoluene (BHT).

Table SV. Values obtained in the measurement of liver enzymes CAT, SOD, GPx and GR promoted by PB compounds respectively.

Compounds PB	SOD (U SO/mg protein)	CAT ($\Delta E \cdot min^{-1} \cdot mg^{-1}$ protein)	GPx ($\Delta E \cdot min^{-1} \cdot mg^{-1}$ protein)	GR ($\Delta E \cdot min^{-1} \cdot mg^{-1}$ protein)
PB12	28.90 ± 0.1#	0.43 ± 0.0[9]#	0.81 ± 0.0[7]#	2.25 ± 0.[1]#
PB13	24.53 ± 0.7	0.34± 0.01	0.681 ± 0.03	2.15 ± 0.2
PB17	39.57 ± 0.02#	0.61 ± 0.02#	0.97 ± 0.0[4]#	2.55 ± 0.06
PB18	24.56 ± 0.4	0.345 ± 0.03	0.68 ± 0.04	2.15 ± 0.0[3]#
PB19	30.29 ± 0.7#	0.52 ± 0.02#	0.89 ± 0.0[1]#	2.32 ± 0.1[2]#
PB20	24.51± 0.6	0.349 ± 0.01	0.683± 0.02	2.148 ± 0.2
Control	24.49 ± 0.1	0.35 ± 0.02	0.68 ± 0.01	2.15 ± 0.1

Mean ± standard deviation; enzymes evaluated superoxide dismutase (SOD), catalase (CAT), glutathione peroxidase (GPx) and glutathione reductase (GR)). #Show statistically significant p < 0.05 compared to control.

Table SVI. Results of *in vitro* antitumor activity promoted by PB compounds against different tumor cells.

Antitumor activity	PB12	PB13	PB17	PB18	PB19	PB20	Dox	mAMSA
DU145 (IC_{50} µM)	2.13 ± 0.4	1.97 ± 0.1	1.83 ± 0.2	2.33 ± 0.1	1.34 ± 0.3	2.04 ± 0.1	1.23 ± 0.01	0.8 ± 0.3
SI[a]	34.74	25.01	35.52	13.66	41.05	32.85	0.99	3.88
SI[b]	40.06	30.51	36.91	19.40	48.52	35.82	1.16	1.45
SI[c]	38.23	31.80	38.91	21.22	50.17	36.78	1.25	1.65
HCT-8 (IC_{50} µM)	5.12 ± 0.1	5.32 ± 0.2	5.19 ± 0.3	5.98 ± 0.11	5.88± 0.1	5.23 ± 0.8	1.34 ± 0.2	1.44 ± 0.2
SI[a]	14.47	9.26	12.52	5.32	9.35	12.81	0.91	2.15
SI[b]	16.66	11.30	13.01	7.56	11.05	13.97	1.06	0.85
SI[c]	15.90	11.77	13.72	8.26	11.43	14.34	1.14	0.92
HEp-2 (IC_{50} µM)	4.33 ± 0.4	4.69 ± 0.3	4.74 ± 0.1	4.73 ± 0.5	4.99 ± 0.1	4.23 ± 0.8	1.85 ± 0.01	1.95 ± 0.01
SI[a]	17.11	10.50	13.71	6.73	11.02	15.84	0.65	1.59
SI[b]	19.70	12.81	14.25	9.55	13.03	17.27	0.77	0.59
SI[c]	18.81	13.35	15.02	10.45	13.47	17.73	0.83	0.68
HepG2 (IC_{50} µM)	88.11 ± 1.2	50.36 ± 0.1	70.85 ± 1.1	50.43 ± 0.9	66.36 ± 1.0	74.35 ± 0.7	1.12 ± 0.1	3.72 ± 0.09
SI[a]	0.84	0.97	0.91	0.63	0.82	0.90	1.08	1.92
SI[b]	0.96	1.19	0.95	0.89	0.97	0.98	1.27	0.59
SI[c]	0.92	1.24	1.00	0.98	1.01	1.0	1.37	0.68
HL-60 (IC_{50} µM)	6.98 ± 0.0	6.73 ± 0.2	6.93 ± 0.9	5.99 ± 0.1	6.02 ± 0.2	6.83± 0.1	1.43 ± 0.01	0.9 ± 0.01
SI[a]	10.61	7.32	9.38	5.31	9.13	9.81	0.85	3.44
SI[b]	12.22	8.93	9.74	7.54	10.80	10.70	1.0	1.29
SI[c]	11.66	9.30	10.27	8.25	11.16	10.98	1.07	1.47
HT-29 (IC_{50} µM)	10.3 ± 0.2	10.9 ± 0.1	10.93 ± 0.5	9.91 ± 0.4	9.34 ± 0.2	9.12 ± 0.8	1.74 ± 0.01	1.15 ± 0.17
SI[a]	7.19	4.52	5.94	3.21	5.88	7.34	0.70	2.7
SI[b]	8.28	5.51	6.18	4.56	6.96	8.01	0.82	1.01
SI[c]	7.90	5.74	6.51	4.98	7.19	8.22	0.88	1.15
Jurkat (IC_{50} µM)	3.24 ± 0.5	3.99 ± 0.2	3.50 ± 0.0	3.64 ± 0.1	3.75 ± 0.1	4.01 ± 0.1	1.66 ± 0.01	1.44 ± 0.11
SI[a]	22.87	12.34	18.57	8.75	14.66	16.71	0.73	2.15
SI[b]	26.33	15.06	19.30	12.42	17.47	18.22	0.86	0.81
SI[c]	25.13	15.70	20.34	13.58	17.92	18.71	0.92	0.92
MCF-7 (IC_{50} µM)	1.32 ± 0.0	1.29 ± 0.3	1.12 ± 0.1	1.43 ± 0.1	1.23 ± 0.1	1.92 ± 0.1	1.02 ± 0.3	1.02 ± 0.09
SI[a]	56.14	38.19	58.04	22.27	44.72	34.90	1.19	3.04
SI[b]	64.65	46.60	60.32	31.61	52.86	38.06	1.40	1.14
SI[c]	61.70	48.56	63.58	34.58	54.65	39.08	1.50	1.29
NCI-H292 (IC_{50} µM)	5.44 ± 0.1	4.95 ± 0.5	4.83 ± 0.3	5.50 ± 0.2	5.11± 0.3	5.79 ± 0.2	1.98 ± 0.01	2.0 ± 0.01
SI[a]	13.62	9.95	13.45	5.79	10.76	11.57	0.61	1.55
SI[b]	15.68	12.14	13.98	8.22	12.72	12.62	0.72	0.58
SI[c]	14.97	12.65	14.74	8.99	13.15	12.96	0.77	0.66
SF-295 (IC_{50} µM)	10.4 ± 0.5	10.3 ± 0.4	10.9 ± 0.5	10.2 ± 0.1	10.8 ± 0.9	10.6 ± 0.1	1.46 ± 0.0	3.0 ± 0.01
SI[a]	7.12	4.78	5.96	3.12	5.09	6.32	0.83	1.03
SI[b]	8.20	5.83	6.19	4.43	6.02	6.89	0.97	0.39
SI[c]	7.83	6.08	6.53	4.84	6.22	7.07	1.05	0.44
T-47D (IC_{50} µM)	2.43 ± 0.0	2.99 ± 0.4	3.01 ± 0.4	3.12 ± 0.4	3.45 ± 0.6	3.92 ± 0.1	1.11 ± 0.01	1.25 ± 0.38
SI[a]	30.49	16.47	21.59	10.20	15.94	17.09	1.09	2.4
SI[b]	35.11	20.10	22.44	14.49	18.84	18.64	1.28	0.9
SI[c]	33.51	20.95	23.65	15.84	19.48	19.14	1.38	1.02

Mean ± standard deviation; Selectivity index: SI[a]= (CC_{50} macrophages/IC_{50} tumor cell), SI[b]= (CC_{50} vero cells/IC_{50} tumor cell); SI[c]= (CC_{50} fibroblast V79/IC_{50} tumor cell); Dox: Doxorubicin; mAMSA: Amsacrine.

Table SVII. Results of *in vivo* antitumor activity promoted by PB compounds.

Groups	Mean tumor mass (g)	Inhibition (%)	Linear equation	IC_{50} (mg/kg)
G2:PB12 (0 mg/kg)	1.649 ± 0.6	0.0	y = 3.63x + 1.605 R^2 = 0.99	13.33
G2:PB12 (10 mg/kg)	0.97 ± 0.01	41.17		
G2:PB12 (20 mg/kg)	0.45 ± 0.03	72.71		
G2:PB12 (40 mg/kg)	0.34 ± 0.09	79.38		
G3:PB13 (0 mg/kg)	1.653 ± ± 0.00	0.0	y = 3.57x + 2.9 R^2 = 0.98	13.19
G3:PB13 (10 mg/kg)	0.90 ± 0.02	44.48		
G3:PB13 (20 mg/kg)	0.47± 0.01	71.56		
G3:PB13 (40mg/kg)	0.35 ± 0.00	78.82		
G4:PB17 (0 mg/kg)	1.658 ± 0.1	0.0	y = 3.55x + 2.99 R^2 = 0.97	13.24
G4:PB17 (10 mg/kg)	0.92 ± 0.00	44.51		
G4:PB17 (20 mg/kg)	0.48 ± 0.02	71.04		
G4:PB17 (40mg/kg)	0.30 ± 0.01	81.90		
G5:PB18 (0 mg/kg)	1.647 ± 0.3	0.0	y = 1.04x + 31.08 R^2 = 0.99	18.19
G5:PB18 (10 mg/kg)	0.97 ± 0.03	41.10		
G5:PB18 (20 mg/kg)	0.78 ± 0.00	52.64		
G5:PB18 (40mg/kg)	0.45 ± 0.02	72.67		
G6:PB19 (0 mg/kg)	1.620 ± 0.4	0.0	y = 0.52x + 35.79 R^2 = 0.88	27.30
G6:PB19 (10 mg/kg)	0.99 ± 0.03	38.88		
G6:PB19 (20 mg/kg)	0.83± 0.00	49.37		
G6:PB19 (40mg/kg)	0.72 ± 0.02	55.55		
G7:PB20 (0 mg/kg)	1.625 ± 0.11	0.0	y = 0.52x + 36.6 R^2 = 0.99	25.76
G7:PB20 (10 mg/kg)	0.95 ± 0.03	41.53		
G7:PB20 (20 mg/kg)	0.85 ± 0.01	47.67		
G7:PB20 (40mg/kg)	0.69 ± 0.00	57.53		

Mean ± standard deviation; the lines were obtained through the best linear fit.