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Palladium(II) Complexes with Thiosemicarbazones. Syntheses, Characterization, Cytotoxicity against Breast Cancer Cells and Anti-*Mycobacterium tuberculosis* Activity

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Table S1. Hydrogen bonds (distances in pm and angles in °) for complexes **1-3**, calculated for distances d(H···A) < r(A) + 200.0 pm and angles ∠ (D–H···A) > 110° (D = H–donor, A = H–acceptor)

D–H···A	d(H···A)	∠ (D–H···A)	d(D···A)	Symmetry operation
Complex **1**				
N(4)–H(41a)···O(4)	205.3	177.69	291.2	
N(4)–H(41b)···O(2)	223.1	151.91	301.7	
O(4)–H(4a)···O(1)	231.7	150.42	309.1	–x+3, –y+1, –z+1
O(4)–H(4a)···O(3)	242.8	155.95	322.9	–x+3, –y+1, –z+1
O(4)–H(4b)···N(3)	256.1	135.37	328.2	–x+2, –y+1, –z+1
Complex **2**				
N(4)–H(41)···O(1)	259.2	145.41	333.6	
N(4)–H(41)···O(2)	206.5	149.85	284.2	
Complex **3**				
O(4b)–H(411b)···O(1b)	214.9	135.67	282.0	x-1, y, z
N(4)–H(41)···O(4b)	206.1	162.88	289.4	x-1, y, z

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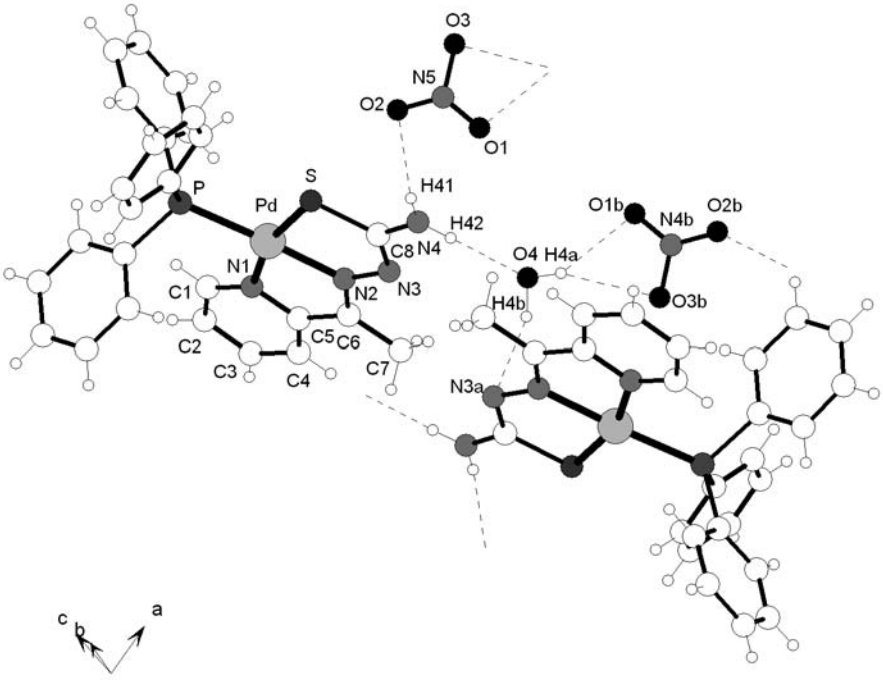

Figure S1. View of the crystal structure of [Pd(aptsc)(PPh_3)](NO_3)·H_2O (**1**) toward the direction [001], showing the hydrogen bonds as dashed lines.

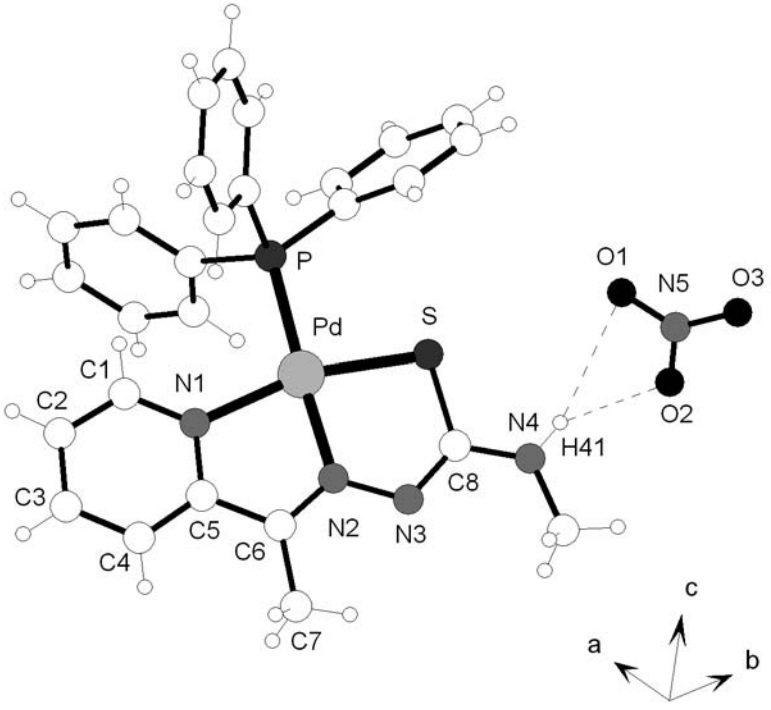

Figure S2. View of the crystal structure of [Pd(apmtsc)(PPh_3)](NO_3) (**2**) parallel to the plane *ab*, showing the hydrogen bonds as dashed lines.

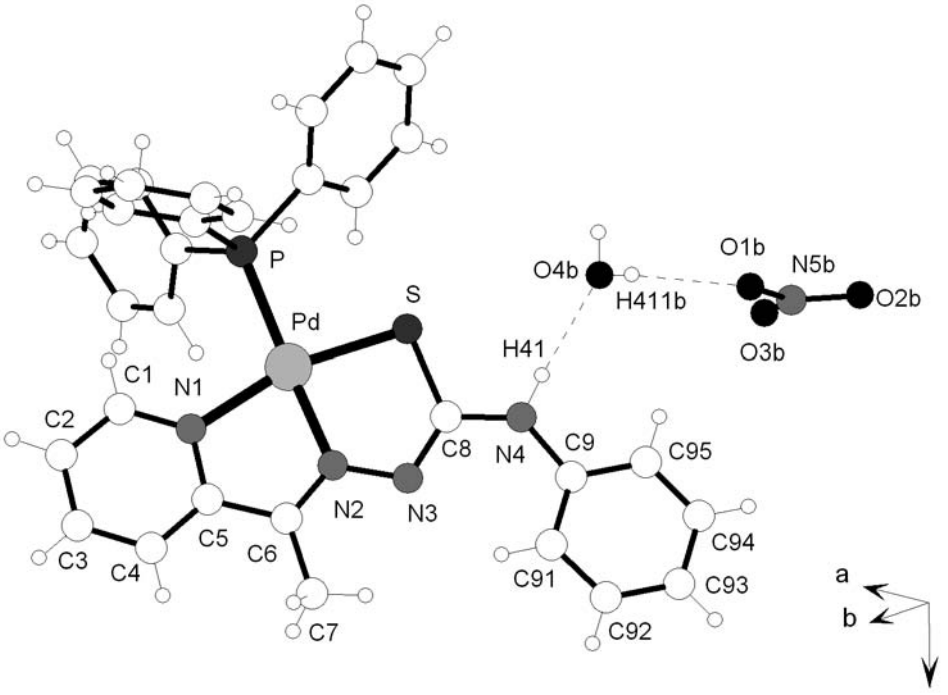

Figure S3. View of the crystal structure of [Pd(apptsc)(PPh_3)](NO_3)·H_2O (**3**) toward the direction [010], showing the hydrogen bonds as dashed lines.