RSC Advances

Electronic Supplementary Information

Chelate *N,O*-palladium(II) complexes: synthesis, characterisation and biological activity

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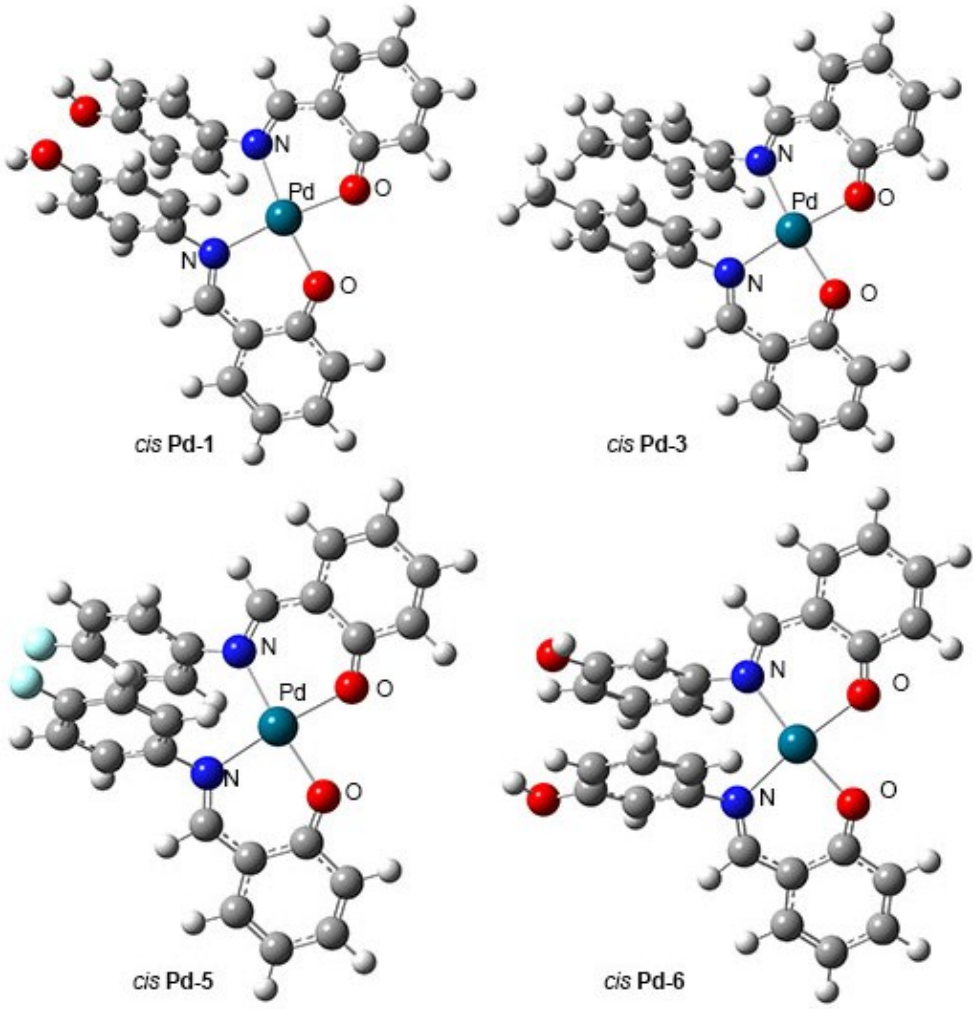


Figure S1**.** The optimised structures of *cis* palladium-Schiff base complexes **Pd-1**, **Pd-3**, **Pd-5**, and **Pd-6**

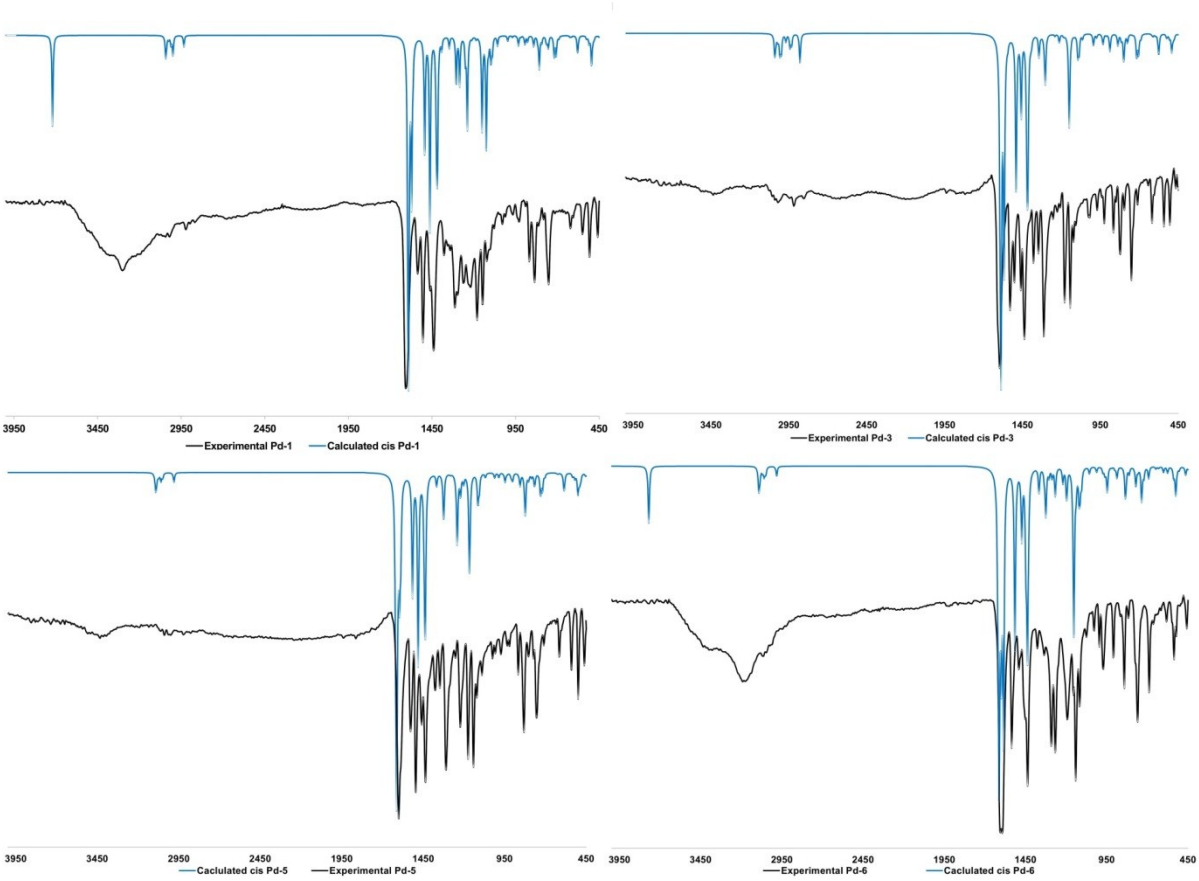


Figure S2. Calculated and experimental IR spectra of *cis* complexes **Pd-1**, **Pd-3**, **Pd-5**, and **Pd-6**

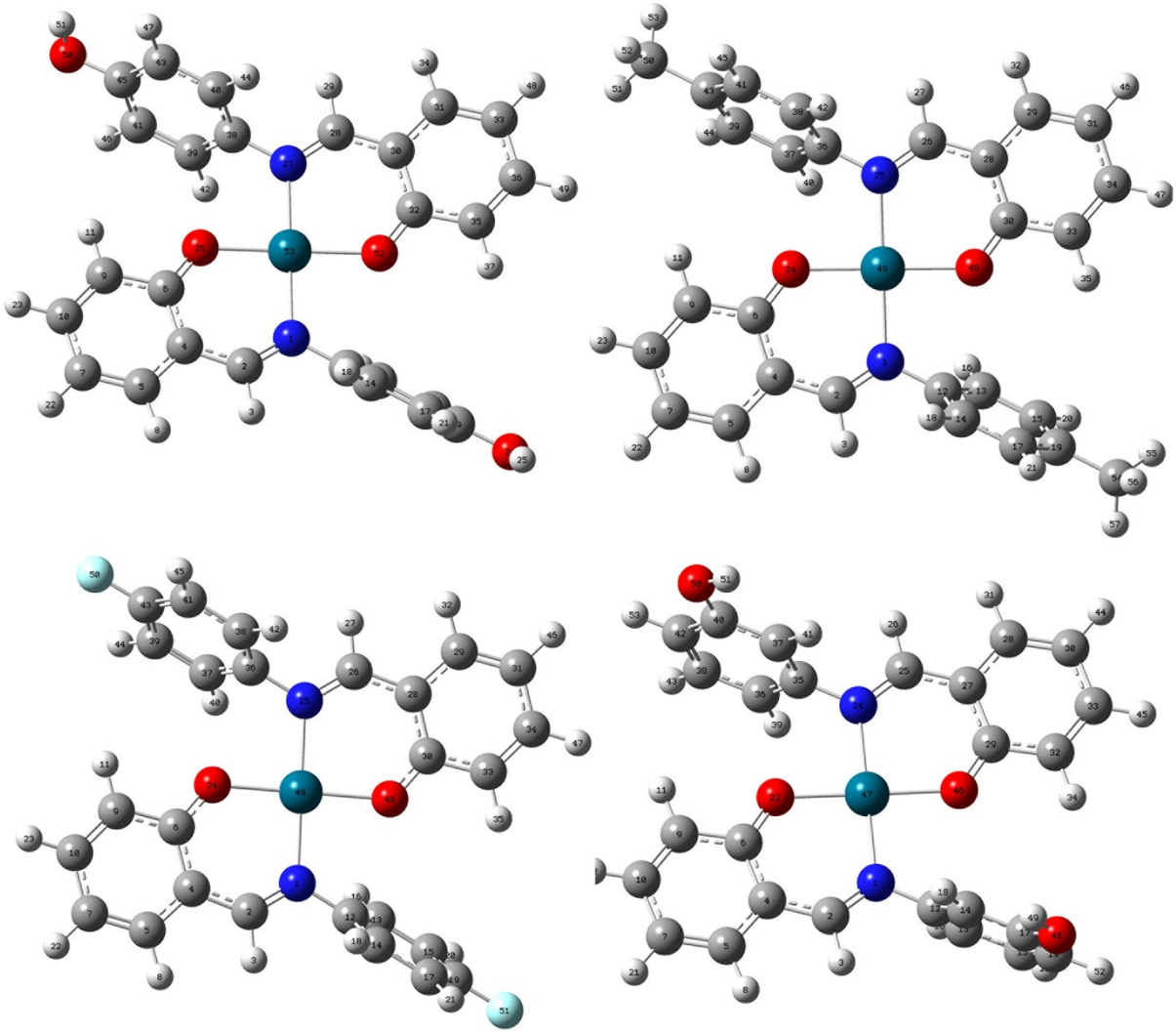


Figure S3. The optimised structures of *trans* palladium-Schiff base complexes **Pd-1**, **Pd-3**, **Pd-5**, and **Pd-6** with atoms labellings used in Tables S1-S4.

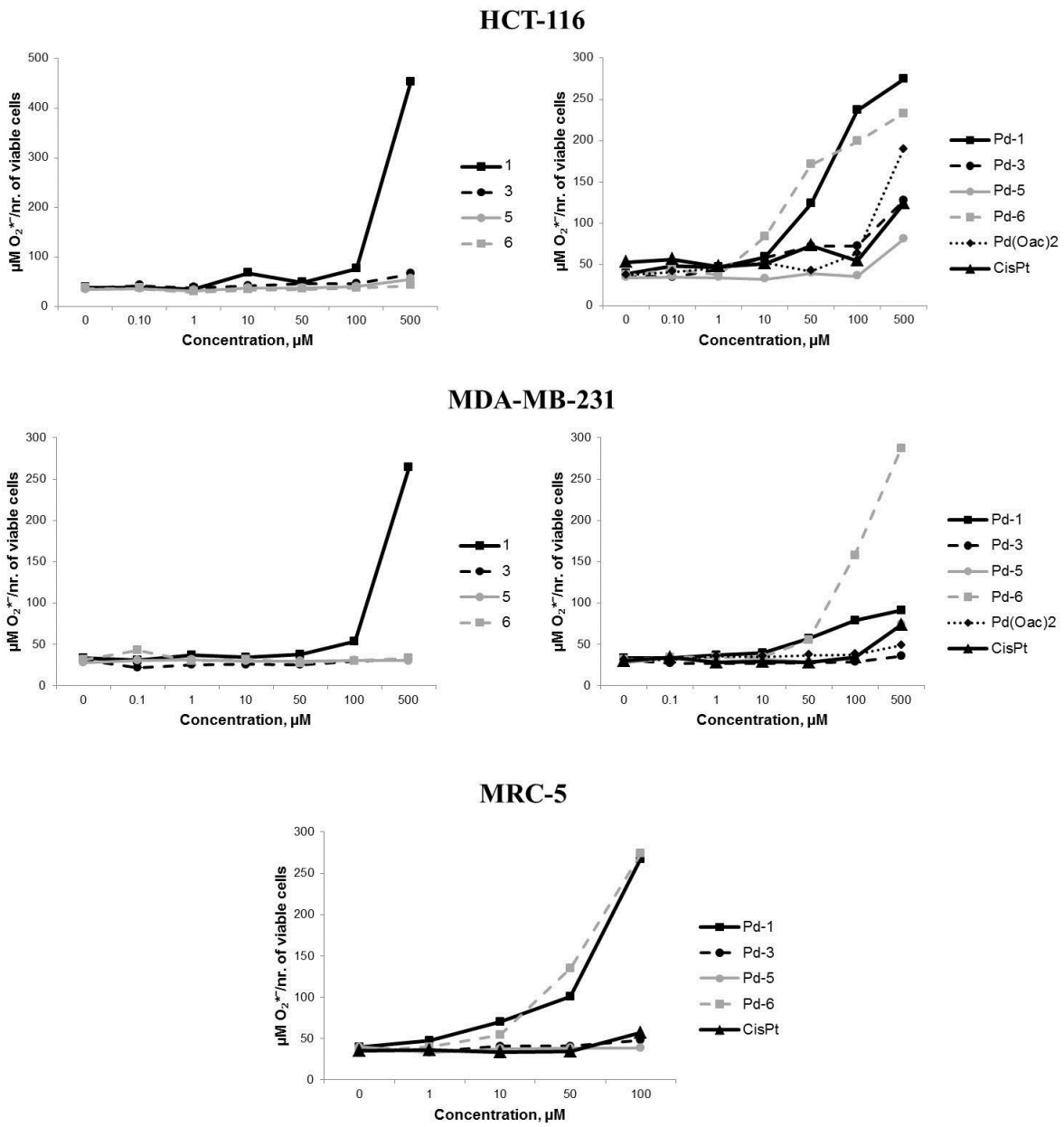


Figure S4. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the $O_2^{\bullet-}$ concentration related to the number of viable cells, after 24 h of exposure

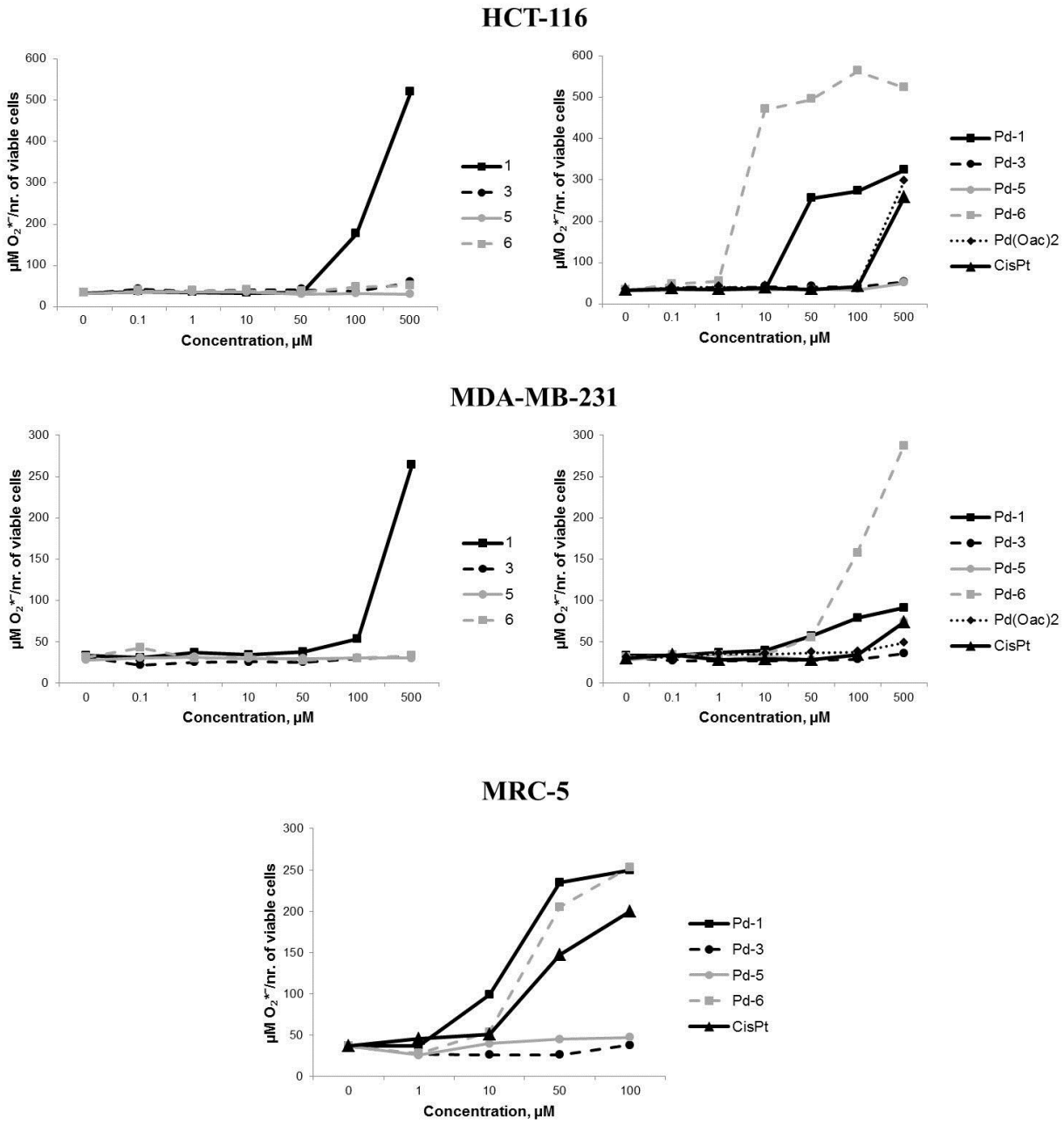


Figure S5. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the $O_2^{\bullet-}$ concentration related to the number of viable cells, after 72 h of exposure

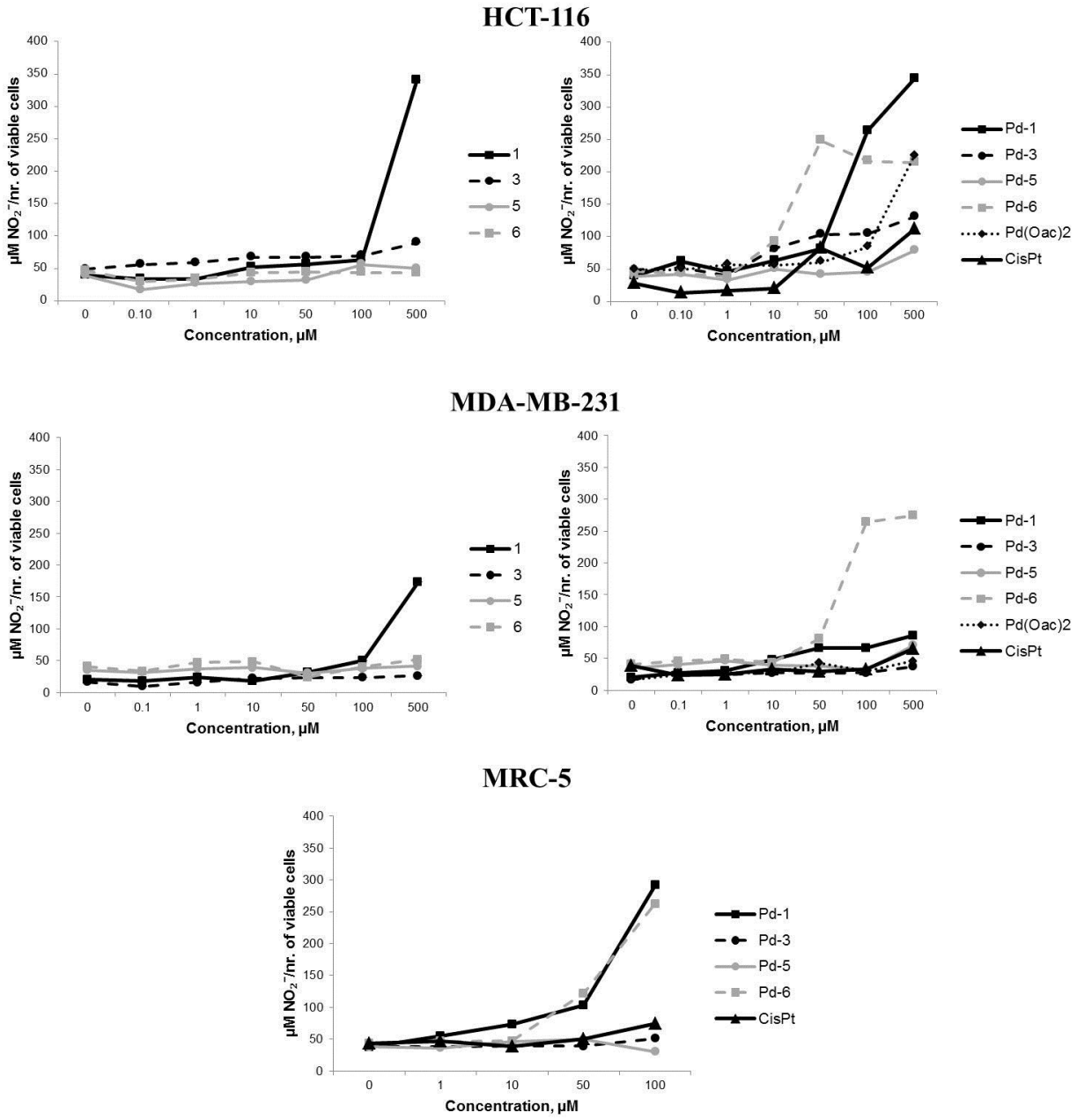


Figure S6. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the NO_2^- concentration related to the number of viable cells, after 24 h of exposure

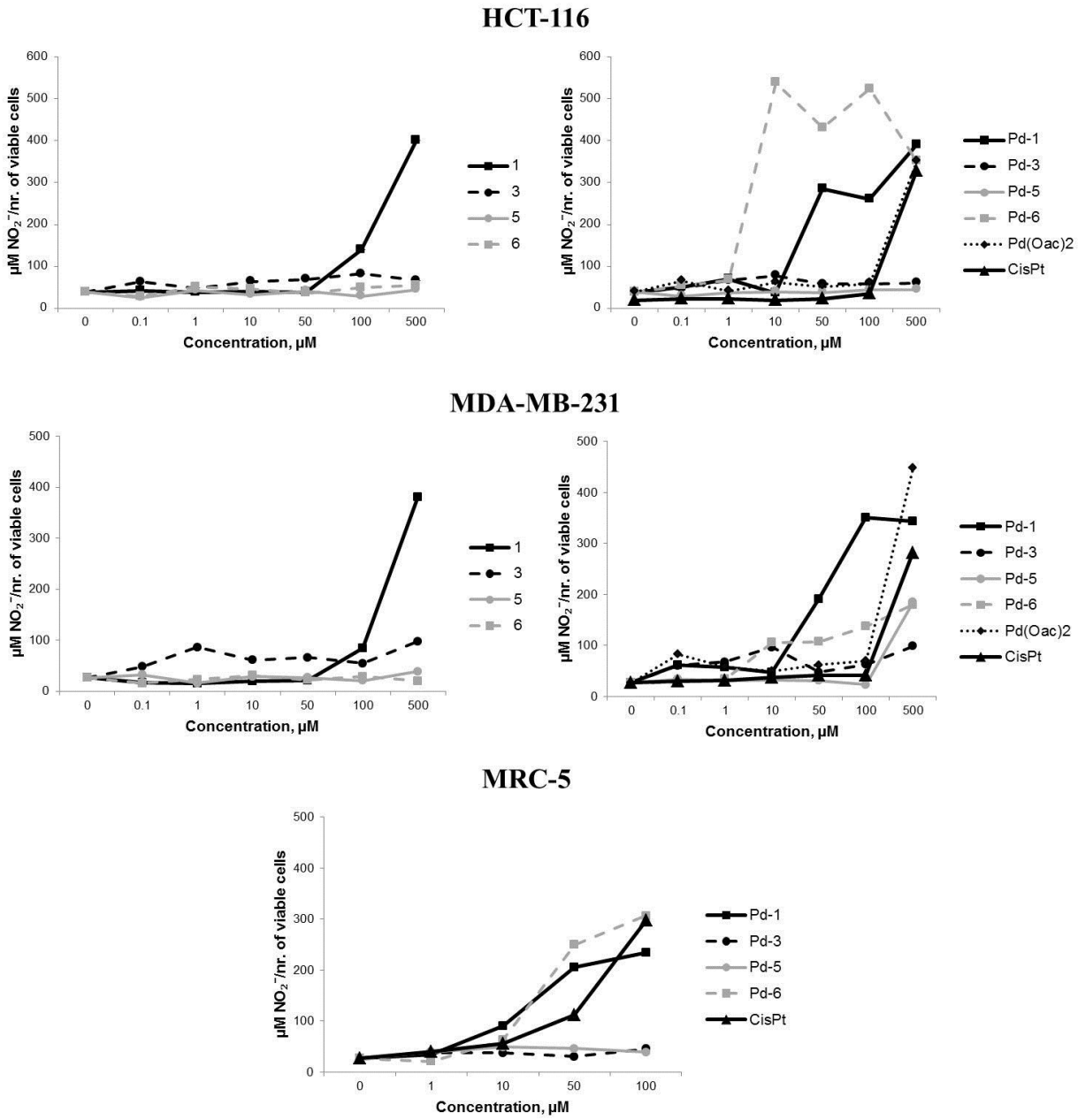


Figure S7. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the NO_2^- concentration related to the number of viable cells, after 72 h of exposure

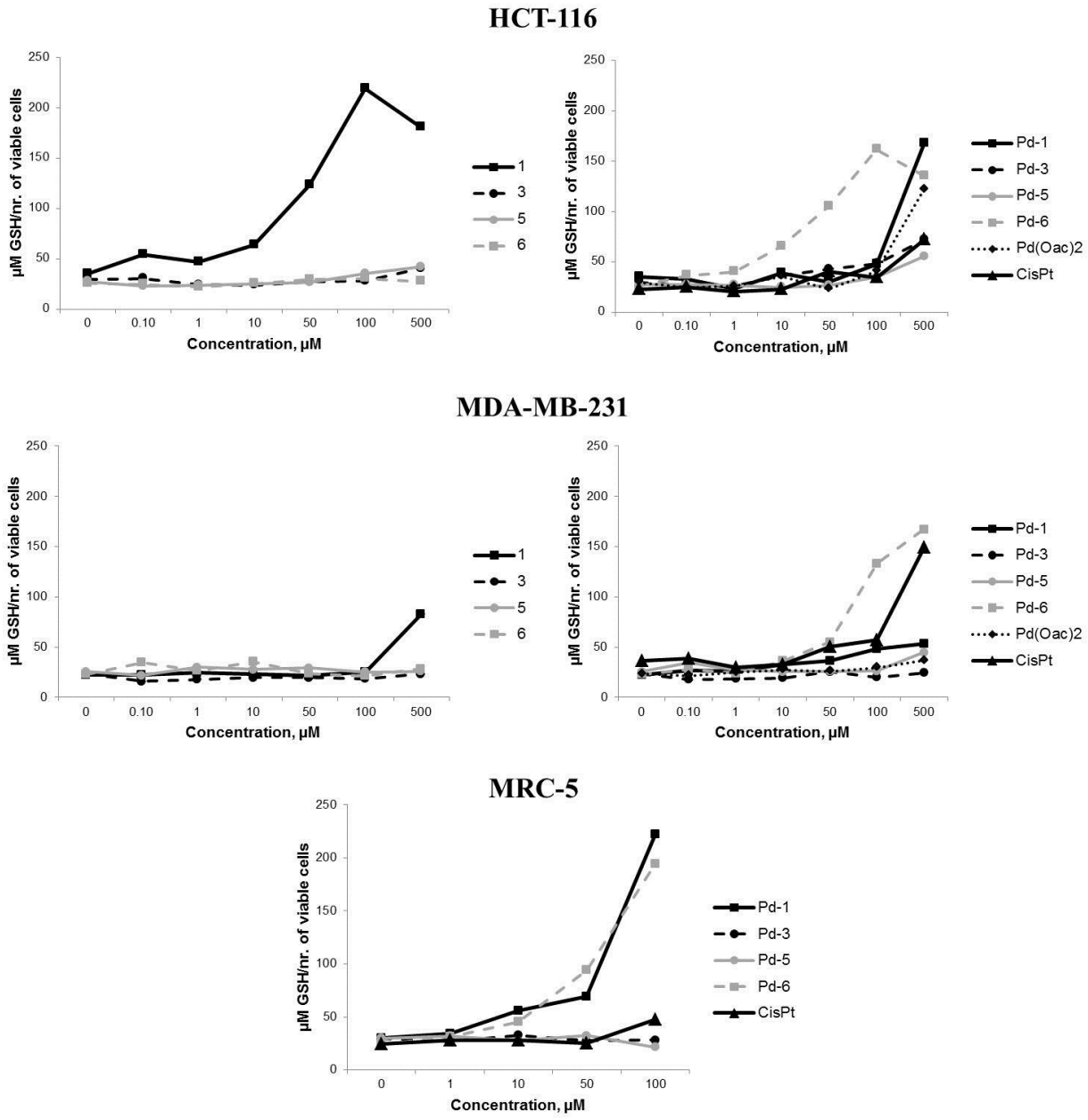


Figure S8. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the reduced glutathione (GSH) concentration related to the number of viable cells, after 24 h of exposure

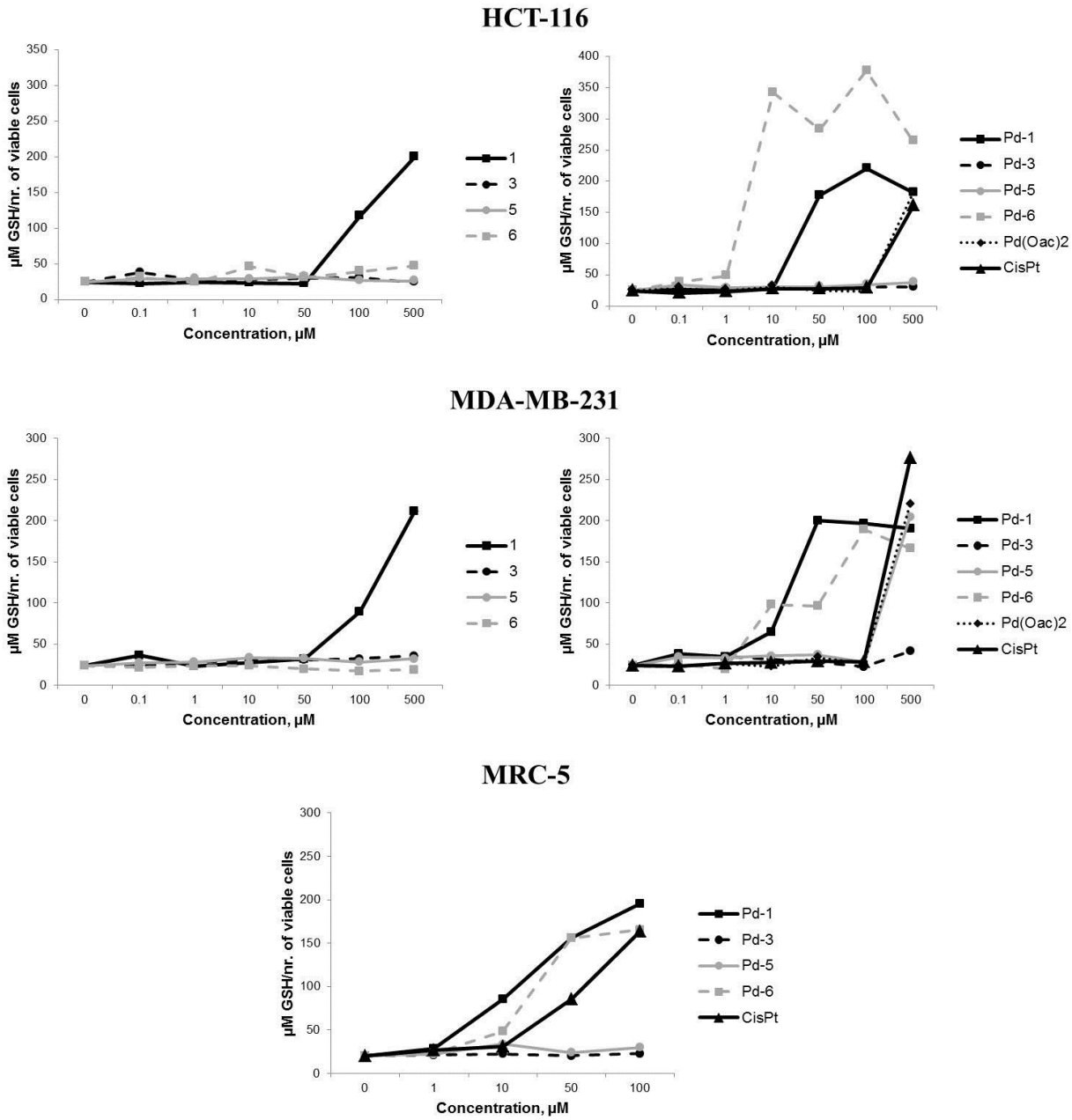


Figure S9. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the reduced glutathione (GSH) concentration related to the number of viable cells, after 72 h of exposure

Table S1. ^{13}C NMR chemical shifts for the investigated Schiff bases and corresponding *cis* palladium complexes. R and AAE stand for correlation coefficient and Average Absolute Error.

Compound	C=N		Ar C-O$^-$		Ar C-N		Ar C				CH_3	
	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.		Calc.		Exp.	Calc.
Pd-1	164.26	168.03	163.22	165.39	155.88	155.37	140.92	120.43	145.05	126.25	/	/
							135.22	119.74	138.72	121.33		
							134.84	114.70	137.88	121.18		
							125.70	114.36	127.98	112.79		
R 0.99 AAE 3												
Pd-3	165.26	168.41	162.68	165.79	147.12	149.68	136.07	124.40	138.38	127.55	21.10	20.83
							135.00	120.70	136.81	125.90		
							134.38	120.33	130.81	121.30		
R 0.99 AAE 2							128.63	115.03	129.59	112.53		
Pd-5	165.20	168.45	163.66	165.94	163.07	161.93	158.78	126.23	148.93	120.22	/	/
							145.40	126.07	138.28	114.61		
							135.49	120.31	126.82	114.73		
R 0.97 AAE 6							134.51	114.89	121.10	112.79		
Pd-6	164.28	168.57	163.31	165.53	157.19	156.30	150.23	120.04	155.02	120.87	/	/
							135.35	115.45	139.00	116.64		
							135.11	114.82	138.32	113.03		
							128.78	113.37	131.67	111.72		
R 0.99 AAE 2							120.30	112.04	121.50	109.48		

Table S2. Interatomic distances, angles, and dihedral angles in **Pd–1**

Bond (Å)		Angle (°)		Dihedral angle (°)	
N1-C2	1.294	N1-C2-H3	116.141	N1-C2-C4-C5	178.784
C2-H3	1.096	N1-C2-C4	128.924	N1-C2-C4-C6	0.258
C2-C4	1.424	C2-C4-C5	116.808	C2-C4-C5-C7	-178.638
C4-C5	1.414	C2-C4-C6	123.806	C2-C4-C5-H8	1.179
C4-C6	1.427	C2-C5-C7	122.094	C2-C4-C6-C9	178.374
C5-C7	1.369	C4-C5-H8	117.981	C4-C6-C9-C10	0.213
C5-H8	1.088	C4-C6-C9	117.237	C4-C6-C9-H11	179.846
C6-C9	1.419	C6-C9-C10	121.551	C2-N1-C12-C12	178.993
C9-C10	1.370	C6-C9-H11	116.641	C2-N1-C12-C13	117.554
C9-H11	1.086	C2-N1-C12	118.093	C2-N1-C12-C14	-64.394
N1-C12	1.422	N1-C12-C13	119.933	N1-C12-C13-C15	179.575
C12-C13	1.392	N1-C12-C14	120.481	N1-C12-C13-H16	0.096
C12-C14	1.387	C12-C13-C15	120.431	N1-C12-C14-C17	-179.071
C13-C15	1.380	C12-C13-H16	118.962	N1-C12-C14-H18	-0.339
C13-H16	1.085	C12-C14-C17	120.287	C12-C14-C17-C19	0.256
C14-C17	1.388	C12-C14-H18	119.472	C12-C13-C15-H20	179.474
C14-H18	1.086	C14-C17-C19	119.864	C12-C14-C17-H21	179.725
C17-C19	1.388	C13-C15-H20	121.308	C4-C5-C7-H22	179.981
C15-H20	1.085	C14-C17-H21	120.084	C6-C9-C10-H23	179.862
C17-H21	1.088	C5-C7-H22	120.866	C14-C17-C19-O24	179.804
C7-H22	1.084	C9-C10-H23	119.193	C17-C19-O24-H25	-0.429
C10-H23	1.087	C17-C19-O24	122.713	C2-C4-C6-O26	-1.524
C19-O24	1.358	C19-O24-O25	109.820		
024-H25	0.961	C4-C6-O26	125.530		
C6-O26	1.286	N1-Pd-N27	179.390		
Pd-N (both)	2.061	O26-Pd-O52	177.482		
PD-O (both)	2.026	N1-Pd-O52	88.581		
		N27-Pd-O52	91.406		
		N1-Pd-O26	91.406		
		N27-Pd-O26	88.581		

Table S3. Interatomic distances, angles, and dihedral angles in **Pd–3**

Bond (Å)		Angle (°)		Dihedral angle (°)	
N1-C2	1.294	N1-C2-H3	116.171	N1-C2-C4-C5	179.15729
C2-H3	1.096	N1-C2-C4	128.853	N1-C2-C4-C6	0.5652605
C2-C4	1.424	C2-C4-C5	116.859	C2-C4-C5-C7	-178.79058
C4-C5	1.414	C2-C4-C6	123.767	C2-C4-C5-H8	1.1141541
C4-C6	1.427	C2-C5-C7	122.092	C2-C4-C6-C9	178.5333
C5-C7	1.369	C4-C5-H8	117.981	C4-C6-C9-C10	0.1743852
C5-H8	1.088	C4-C6-C9	117.258	C4-C6-C9-H11	179.68515
C6-C9	1.420	C6-C9-C10	121.538	C4-C2-N1-C12	179.27036
C9-C10	1.370	C6-C9-H11	116.529	C2-N1-C12-C13	117.31902
C9-H11	1.086	C2-N1-C12	118.085	C2-N1-C12-C14	-64.665833
N1-C12	1.423	N1-C12-C13	119.860	N1-C12-C13-C15	179.46597
C12-C13	1.390	N1-C12-C14	120.366	N1-C12-C13-H16	0.3931708
C12-C14	1.387	C12-C13-C15	119.832	N1-C12-C14-C17	-178.96398
C13-C15	1.383	C12-C13-H16	119.061	N1-C12-C14-H18	-0.540895
C13-H16	1.086	C12-C14-C17	119.908	C12-C14-C17-C19	0.0085509
C14-C17	1.388	C12-C14-H18	119.392	C12-C13-C15-H20	179.69999
C14-H18	1.087	C14-C17-C19	121.114	C12-C14-C17-H21	179.49016
C17-C19	1.391	C13-C15-H20	119.452	C4-C5-C7-H22	-179.93577
C15-H20	1.088	C14-C17-H21	119.477	C6-C9-C10-H23	179.77455
C17-H21	1.088	C5-C7-H22	120.855	C2-C4-C6-O24	-1.3216427
C7-H22	1.084	C9-C10-H23	119.223	C14-C17-C19-C54	-178.74571
C10-H23	1.087	C4-C6-O24	125.574		
C6-O24	1.286	C14-C17-C19	121.158		
C54-H	1.094	N1-Pd-N25	179.177		
Pd-O (both)	2.024	O24-Pd-O48	177.599		
Pd-N (both)	2.060	N1-Pd-O48	88.592		
		N25-Pd-O48	91.389		
		N1-Pd-O24	91.388		
		N25-Pd-O24	88.595		

Table S4. Interatomic distances, angles, and dihedral angles in **Pd–5**

Bond (Å)		Angle (°)		Dihedral angle (°)	
N1-C2	1.295	N1-C2-H3	116.184	N1-C2-C4-C5	178.942
C2-H3	1.096	N1-C2-C4	128.858	N1-C2-C4-C6	0.288
C2-C4	1.423	C2-C4-C5	116.795	C2-C4-C5-C7	-178.799
C4-C5	1.415	C2-C4-C6	123.818	C2-C4-C5-H8	1.060
C4-C6	1.427	C2-C5-C7	122.059	C2-C4-C6-C9	178.608
C5-C7	1.369	C4-C5-H8	118.000	C4-C6-C9-C10	0.117
C5-H8	1.088	C4-C6-C9	117.252	C4-C6-C9-H11	179.662
C6-C9	1.419	C6-C9-C10	121.536	C4-C2-N1-C12	179.166
C9-C10	1.370	C6-C9-H11	116.673	C2-N1-C12-C13	117.131
C9-H11	1.086	C2-N1-C12	118.102	C2-N1-C12-C14	-64.699
N1-C12	1.422	N1-C12-C13	119.681	N1-C12-C13-C15	179.579
C12-C13	1.391	N1-C12-C14	120.245	N1-C12-C13-H16	0.207
C12-C14	1.389	C12-C13-C15	120.167	N1-C12-C14-C17	-179.179
C13-C15	1.383	C12-C13-H16	119.093	N1-C12-C14-H18	-0.399
C13-H16	1.085	C12-C14-C17	120.257	C12-C14-C17-C19	0.269
C14-C17	1.388	C12-C14-H18	119.418	C12-C13-C15-H20	179.493
C14-H18	1.086	C14-C17-C19	118.541	C12-C14-C17-H21	179.795
C17-C19	1.380	C13-C15-H20	121.704	C4-C5-C7-H22	-179.982
C15-H20	1.085	C14-C17-H21	121.759	C6-C9-C10-H23	179.825
C17-H21	1.084	C5-C7-H22	120.868	C2-C4-C6-O24	-1.235
C7-H22	1.084	C9-C10-H23	119.183	C14-C17-C19-C54	-2.485
C10-H23	1.087	C4-C6-O24	125.540		
C6-O24	1.287	N1-Pd-N25	179.299		
C19-F	1.340	O24-Pd-O48	177.739		
Pd-O (both)	2.025	N1-Pd-O48	88.591		
Pd-N (both)	2.060	N25-Pd-O48	91.396		
		N1-Pd-O24	91.396		
		N25-Pd-O24	88.590		

Table S5. Interatomic distances, angles, and dihedral angles in **Pd–6**

Bond (Å)		Angle (°)		Dihedral angle (°)	
N1-C2	1.293	N1-C2-H3	116.241	N1-C2-C4-C5	178.802
C2-H3	1.096	N1-C2-C4	128.583	N1-C2-C4-C6	-0.524
C2-C4	1.424	C2-C4-C5	116.920	C2-C4-C5-C7	-179.269
C4-C5	1.414	C2-C4-C6	123.713	C2-C4-C5-H8	0.549
C4-C6	1.427	C2-C5-C7	122.036	C2-C4-C6-C9	179.171
C5-C7	1.369	C4-C5-H8	117.999	C4-C6-C9-C10	0.093
C5-H8	1.088	C4-C6-C9	117.288	C4-C6-C9-H11	-179.920
C6-C9	1.420	C6-C9-C10	121.481	C4-C2-N1-C12	179.535
C9-C10	1.370	C6-C9-H11	116.468	C2-N1-C12-C13	103.736
C9-H11	1.086	C2-N1-C12	118.423	C2-N1-C12-C14	-78.703
N1-C12	1.424	N1-C12-C13	119.912	N1-C12-C13-C15	178.134
C12-C13	1.386	N1-C12-C14	119.118	N1-C12-C13-H16	-0.305
C12-C14	1.388	C12-C13-C15	118.891	N1-C12-C14-C17	-177.770
C13-C15	1.387	C12-C13-H16	119.418	N1-C12-C14-H18	0.419
C13-H16	1.085	C12-C14-C17	119.495	C12-C14-C17-C19	-0.648
C14-C17	1.389	C12-C14-H18	119.520	C12-C13-C15-H20	179.818
C14-H18	1.088	C14-C17-C19	121.044	C12-C14-C17-H21	179.908
C15-C19	1.386	C13-C15-H20	119.584	C6-C9-C10-H22	-179.995
C15-H20	1.086	C5-C7-H21	120.871	C2-C4-C6-O23	-0.886
C7-H21	1.084	C9-C10-H22	119.194	C4-C6-O23-Pd	0.219
C10-H20	1.087	C4-C6-O24	125.650	C12-C14-C17-O48	179.874
C6-O23	1.286	C6-O23-Pd	127.156	C14-C17-O48-H49	-2.919
C17-O48	1.357	C14-C17-O48	122.307		
O48-H49	0.961	N1-Pd-N24	179.826		
C19-H52	1.085	O23-Pd-O46	178.593		
Pd-N (both)	2.055	N1-Pd-O46	88.710		
Pd-O (both)	2.025	N24-Pd-O46	91.287		
		N1-Pd-O23	91.287		
		N24-Pd-O23	88.711		

Table S6. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the $O_2^{\bullet-}$ concentration after 24 h of exposure. *p < 0.05 as compared to the control cells

Superoxide anion radical, $O_2^{\bullet-}$ (µM)										
HCT-116										
	Schiff bases				**Complexes**					
µM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	37.07±0.28	37.07±0.28	37.07±0.28	37.07±0.28	37.07±0.28	37.07±0.28	37.07±0.28	37.07±0.28	37.07±0.28	40.03±0.33
0.1	41.15±0.91*	39.18±0.55	40.82±0.60*	38.17±0.62	35.04±0.29	38.17±1.28	37.94±0.30	33.99±0.01*	39.37±0.50*	46.16±2.58*
1	39.46±1.69	36.75±1.27	38.15±0.91	31.61±0.15*	39.32±0.48*	44.15±0.53*	38.60±0.12*	32.23±0.19*	42.51±0.31*	50.57±0.53*
10	49.45±0.65*	37.29±1.18	40.62±0.55*	31.65±0.17*	37.88±1.23	41.79±0.50*	38.98±0.67*	32.16±0.44*	41.30±0.12*	45.87±1.15*
50	43.78±0.79*	40.25±1.40	39.51±0.97*	32.43±0.55*	36.57±0.25	41.30±0.38*	43.62±0.56*	33.36±0.16*	39.10±0.92	38.05±0.43
100	40.09±0.35	36.58±1.52	36.03±0.77	31.79±0.11*	39.19±0.72	41.05±0.95*	35.89±0.35	36.71±0.50	41.67±0.92*	31.88±0.22*
500	64.04±1.06*	41.37±0.78*	41.25±0.28*	33.01±0.55*	42.36±0.62*	54.85±0.47*	51.47±0.19*	46.96±0.52*	40.96±0.90*	31.64±0.42*
MDA-MB-231										
	Schiff bases				**Complexes**					
µM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	31.02±0.19	31.02±0.19	31.02±0.19	31.02±0.19	31.02±0.19	31.02±0.19	31.02±0.19	31.02±0.19	31.02±0.19	30.56±0.36
0.1	30.74±0.14	31.65±0.17	35.02±0.27*	34.03±0.71*	29.46±1.34	31.15±0.21	32.51±0.74	34.81±0.21*	30.95±0.36	32.41±0.18*
1	30.97±0.08	32.67±0.23*	33.51±0.40*	28.39±0.32*	32.02±0.49	31.97±0.20	29.79±0.17	32.82±0.31*	30.53±0.38	31.61±0.19*
10	31.44±0.19	32.24±0.20*	32.94±0.03*	30.61±0.72	32.00±1.61	32.15±0.76	34.46±1.08*	27.45±0.27*	31.61±0.42	31.81±0.23*
50	34.70±0.11*	31.73±0.24	30.96±0.08	27.06±0.59*	35.70±0.41*	31.73±0.20	31.21±0.35	30.00±0.85	32.77±0.87	30.45±0.10
100	40.02±0.16*	31.71±0.30	32.54±0.14*	29.95±0.22	36.64±0.07*	34.65±0.05*	38.93±0.67*	30.24±0.57	30.95±0.22	29.81±0.03*
500	61.67±1.17*	32.24±0.17*	31.06±0.11	28.82±0.07*	37.43±1.37*	36.01±0.13*	47.63±0.56*	48.46±0.47*	31.16±0.73	30.24±0.23
MRC-5										
µM					**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	-	-	-	-	37.53±0.15	37.53±0.15	37.53±0.15	37.53±0.15	-	37.53±0.15
1	-	-	-	-	37.05±1.10	35.51±2.20	35.39±3.43	39.20±2.98	-	40.97±0.72*
10	-	-	-	-	37.91±0.43	39.54±0.04	39.02±0.64	44.03±0.41*	-	38.98±0.27
50	-	-	-	-	38.93±0.22	40.95±0.31	39.73±0.56	42.21±0.63*	-	40.23±0.15*
100	-	-	-	-	38.38±0.78	41.28±0.15	40.70±0.99	46.58±0.30*	-	41.63±0.14*

Table S7. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the $O_2^{\bullet-}$ concentration after 72 h of exposure. *p < 0.05 as compared to the control cells

Superoxide anion radical, $O_2^{\bullet-}$ (μM)										
HCT-116										
	Schiff bases				**Complexes**					
μM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	31.78±0.09	31.78±0.09	31.78±0.09	31.78±0.09	31.78±0.09	31.78±0.09	31.78±0.09	31.78±0.09	31.78±0.09	31.78±0.09
0.1	37.65±0.23*	34.08±0.66*	34.97±0.48	37.84±1.38*	31.63±0.41	31.82±0.14	33.21±1.02	31.95±0.54	31.82±0.14	29.89±0.77
1	36.29±0.88*	32.73±0.57	35.20±0.45*	35.28±1.85*	31.02±0.15	33.58±1.17	33.18±0.23	34.38±0.15*	33.58±1.17	29.37±0.18
10	34.71±0.55*	33.78±0.91	34.33±0.52*	32.21±0.41	31.25±0.15	31.60±0.25	32.65±0.18	44.43±0.69*	31.60±0.25	31.29±0.96
50	35.70±0.46*	34.98±0.59*	29.47±0.50	31.24±1.06	33.18±0.14	31.11±0.17	33.15±0.81	45.16±0.83*	31.11±0.17	32.27±1.01
100	38.65±0.61*	33.84±0.67	32.06±1.40	32.25±0.93	34.26±0.49*	31.58±0.51	32.99±1.51	50.55±1.25*	31.58±0.51	32.04±0.69
500	67.01±1.23*	41.35±0.63*	29.57±2.62	32.98±0.53	41.40±0.26*	33.54±0.21	40.69±1.77*	50.44±0.52*	33.54±0.21	29.19±0.37
MDA-MB-231										
	Schiff bases				**Complexes**					
μM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	25.92±0.22	25.92±0.22	25.92±0.22	25.92±0.22	25.92±0.22	25.92±0.22	25.92±0.22	25.92±0.22	25.92±0.22	28.71±0.31
0.1	27.64±0.15	26.00±0.18	29.89±0.76*	30.45±0.28*	20.05±0.22*	23.60±0.18	26.73±0.04	25.59±0.08	25.17±0.29	29.08±0.08
1	25.33±0.72	26.04±0.06	29.81±0.40*	29.64±0.52*	19.71±1.51*	22.08±0.28*	27.56±0.27	25.49±0.30	24.60±0.34	29.20±0.28
10	25.56±0.05	25.08±0.13	28.19±0.66*	27.04±0.24	21.64±0.07*	23.72±0.15	26.07±0.07	25.07±0.03	25.40±0.12	29.01±0.07
50	26.93±0.07	24.53±0.15	25.36±0.24	28.64±0.32*	22.63±0.22*	24.36±0.38	27.53±0.11	25.76±0.14	25.47±0.09	28.87±0.44
100	36.19±0.13*	24.49±0.04	26.93±0.28	25.77±0.16	22.32±0.10*	25.12±0.19	28.91±0.27*	26.29±0.11	24.61±0.35	28.14±0.19
500	63.24±0.39*	24.20±0.54	26.91±0.31	24.48±0.06	27.93±0.60	28.76±0.08*	34.00±1.43*	32.11±0.54*	30.23±0.10*	27.16±0.11
MRC-5										
μM					**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	-	-	-	-	37.11±0.26	37.11±0.26	37.11±0.26	37.11±0.26	-	37.11±0.26
1	-	-	-	-	38.85±0.19	34.72±0.09*	32.51±0.60*	30.85±0.78*	-	37.99±1.26
10	-	-	-	-	36.93±0.41	36.00±0.66	36.21±0.99	33.92±0.67*	-	35.78±0.68
50	-	-	-	-	36.23±0.30	35.88±0.17	43.00±0.99*	30.93±0.40*	-	37.84±1.63
100	-	-	-	-	37.66±0.13	36.52±0.44	44.48±2.01*	35.30±0.29	-	32.82±1.17*

Table S8. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the NO_2^- concentration after 24 h of exposure. *p < 0.05 as compared to the control cells

Nitrites, NO_2^- (µM)										
HCT-116										
	Schiff bases				**Complexes**					
µM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	43.21±0.34	43.21±0.34	43.21±0.34	43.21±0.34	43.21±0.34	43.21±0.34	43.21±0.34	43.21±0.34	43.21±0.34	28.37±0.27
0.1	41.65±0.63	46.39±0.81	19.77±1.02*	28.18±2.23*	51.92±1.17*	51.76±0.83*	47.24±2.34*	31.20±1.26*	42.40±1.45	10.96±0.43*
1	41.96±1.42	50.83±0.22*	31.92±2.20*	33.92±4.00*	45.46±2.08	35.96±0.64*	39.14±5.08	31.18±0.81*	47.40±0.24*	18.11±1.37*
10	43.62±3.41	54.13±0.99*	32.46±3.44*	37.64±2.21*	47.17±1.15*	52.40±1.89*	62.07±1.55*	33.25±2.13*	39.31±0.25*	18.00±0.98*
50	57.30±1.42*	52.43±2.19*	34.13±1.64*	38.04±0.73*	27.90±0.46*	53.31±1.96*	47.86±1.59*	45.42±2.56	50.96±0.17*	43.36±1.86*
100	38.91±2.45	49.54±2.05*	51.54±0.42*	34.60±0.38*	50.86±0.60*	53.93±0.83*	46.64±3.25	37.38±3.04*	49.46±1.74*	29.72±0.52
500	55.95±3.18*	51.01±0.24*	38.10±4.15*	31.40±2.18*	61.74±0.51*	50.89±0.79*	51.95±1.01*	40.51±1.27	43.92±1.69	31.26±1.47
MDA-MB-231										
	Schiff bases				**Complexes**					
µM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	28.21±0.22	28.21±0.22	28.21±0.22	28.21±0.22	28.21±0.22	28.21±0.22	28.21±0.22	28.21±0.22	28.21±0.22	39.00±0.30
0.1	27.08±0.49	24.43±0.41	26.21±0.94	18.51±1.81*	35.79±2.31*	57.98±2.98*	28.74±1.09	32.48±1.30*	42.51±1.15*	22.59±1.78*
1	29.86±0.31	35.59±1.78*	29.10±1.17	31.83±1.38*	38.89±0.57*	49.56±1.85*	35.20±3.68*	33.22±1.53*	41.90±1.05*	28.10±1.32*
10	24.31±0.57	47.55±3.22*	31.08±1.30	32.49±1.75*	57.43±0.49*	56.90±0.78*	30.72±1.98	24.22±0.98*	42.09±0.32*	36.17±1.18*
50	43.59±2.10*	50.72±3.48*	22.87±0.89*	16.65±1.90*	61.86±5.69*	52.17±3.67*	30.87±3.22*	31.20±2.47*	65.91±2.88*	31.55±0.88*
100	56.11±1.07*	42.50±3.91*	29.57±0.26	28.06±0.95	45.37±0.09*	56.72±3.08*	27.63±1.09	35.56±2.96*	43.10±0.33*	28.88±1.77*
500	60.24±1.02*	45.67±1.40*	30.89±1.31	31.72±0.97*	52.31±1.73*	64.79±1.16*	32.99±0.51*	32.63±1.17*	50.95±1.46*	26.87±0.47*
MRC-5										
µM					**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	-	-	-	-	40.27±0.27	40.27±0.24	40.27±0.27	40.27±0.27	-	40.27±0.27
1	-	-	-	-	48.57±2.13*	46.28±1.65*	44.50±1.98*	40.03±1.43	-	45.68±1.42*
10	-	-	-	-	44.82±0.72*	44.15±1.22*	54.72±2.20*	33.75±1.49*	-	39.36±1.06
50	-	-	-	-	45.23±2.62*	45.19±0.48*	58.43±1.23*	33.44±1.42*	-	50.88±0.06*
100	-	-	-	-	47.90±0.62*	49.92±3.45*	36.22±1.16*	39.14±1.83	-	47.17±2.30*

Table S9. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the NO_2^- concentration after 72 h of exposure. *p < 0.05 as compared to the control cells

Nitrites, NO_2^- (µM)										
HCT-116										
	Schiff bases				**Complexes**					
µM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	37.88±0.32	37.88±0.32	37.88±0.32	37.88±0.32	37.88±0.32	37.88±0.32	37.88±0.32	37.88±0.32	37.88±0.32	18.69±0.19
0.1	43.54±2.03*	51.42±1.42*	25.75±3.43*	28.00±1.29*	47.52±1.51*	37.42±1.92	28.57±0.22*	36.29±2.20	53.72±1.16*	18.63±1.21
1	41.50±4.74*	42.10±0.90*	42.74±2.29*	47.98±1.31*	63.50±1.46*	56.38±0.28*	35.67±1.41	42.88±0.61*	33.84±3.37*	18.21±0.13
10	43.85±0.39*	54.29±2.74*	31.62±0.55*	37.08±0.51	32.90±0.94*	59.95±0.35*	39.16±1.53	50.91±2.08*	50.80±1.29*	15.18±0.72*
50	39.43±1.07	59.00±1.31*	40.98±2.62	31.46±2.87*	37.14±2.13	43.91±2.06*	35.48±0.84	39.36±1.92	47.53±1.71*	20.82±0.42
100	30.71±1.51*	74.06±1.12*	29.58±3.60*	33.38±1.22*	32.76±0.89*	46.19±2.13*	43.09±1.73*	47.02±2.07*	44.81±0.59*	26.69±2.85*
500	51.64±3.00*	47.43±3.88*	44.19±3.02*	34.90±1.00*	49.76±1.75*	38.75±1.60	36.33±0.83	33.82±1.37*	39.79±2.24	37.12±1.11*
MDA-MB-231										
	Schiff bases				**Complexes**					
µM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	26.51±0.24	26.51±0.24	26.51±0.24	26.51±0.24	26.51±0.24	26.51±0.24	26.51±0.24	26.51±0.24	26.51±0.24	26.51±0.24
0.1	17.44±0.44*	48.32±2.61*	31.05±0.95*	16.61±0.98*	50.43±0.96*	55.52±1.36*	30.46±2.59	28.21±1.51	63.90±5.25*	29.62±0.26
1	16.19±0.54*	75.03±2.29*	14.60±1.00*	20.64±3.50*	49.57±3.55*	56.22±2.37*	25.04±0.75	33.91±1.56*	53.71±1.04*	28.97±0.53
10	20.18±0.49*	53.53±1.29*	25.90±0.72	30.95±1.40*	25.46±0.94	78.20±4.11*	28.23±1.41	22.41±0.71*	50.33±0.56*	37.18±0.78*
50	16.94±0.19*	56.11±1.93*	23.71±0.70*	24.85±0.46	30.12±0.17*	42.94±2.13*	27.17±0.97	20.93±1.27*	59.13±2.55*	38.89±0.89*
100	24.28±0.87	46.30±2.57*	19.75±1.40*	31.17±0.62*	61.31±0.95*	62.02±0.05*	22.64±1.84*	19.10±0.26*	68.01±0.86*	39.79±0.77*
500	49.56±0.79*	62.75±2.58*	29.76±1.43*	22.93±0.56*	51.22±0.60*	72.93±4.24*	23.00±1.18	24.13±1.60	50.80±1.84*	31.87±1.00*
MRC-5										
µM					**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	-	-	-	-	26.40±0.28	26.40±0.28	26.40±0.28	26.40±0.28	-	26.40±0.28
1	-	-	-	-	35.99±2.19*	49.51±1.18*	49.40±2.49*	22.59±0.75	-	33.68±3.14*
10	-	-	-	-	33.84±1.62*	51.09±2.10*	44.14±1.48*	39.57±0.38*	-	39.16±2.01*
50	-	-	-	-	31.65±2.73*	40.79±1.19*	43.69±1.70*	37.57±1.70*	-	28.73±0.93
100	-	-	-	-	35.34±0.49*	43.26±1.37*	36.80±1.72*	42.69±1.30*	-	48.75±1.18*

Table S10. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the reduced glutathione (GSH) concentration after 24 h of exposure. *p < 0.05 as compared to the control cells

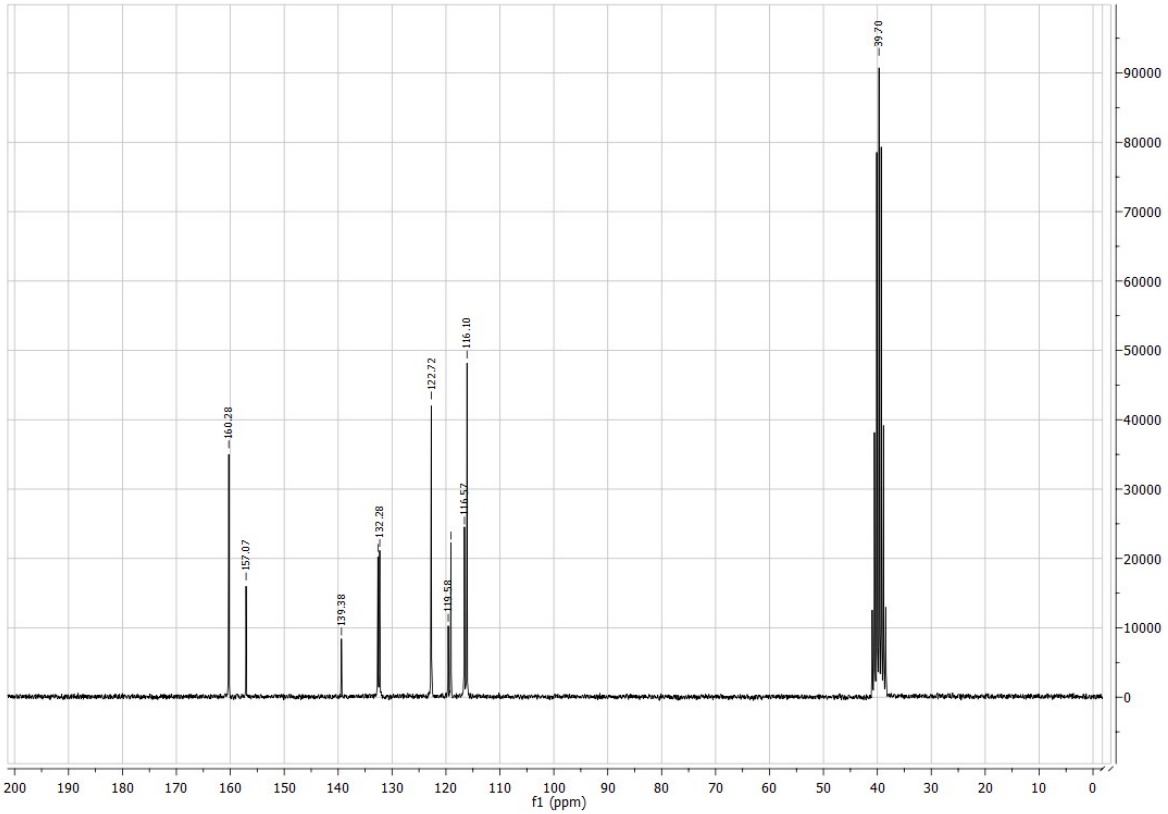
GSH (µM)										
HCT-116										
	Schiff bases				**Complexes**					
µM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	29.56±0.25	29.56±0.25	29.56±0.25	29.56±0.25	29.56±0.25	29.56±0.25	29.56±0.25	29.56±0.25	29.56±0.25	22.85±0.25
0.1	35.35±1.36*	28.05±0.58	26.30±1.66	28.93±0.69	31.45±1.40	29.19±0.26	29.56±0.59	31.78±0.59	23.77±0.22*	20.6±0.20*
1	35.16±0.87*	23.24±0.11*	27.87±0.82	27.02±1.40	23.03±0.83*	25.77±1.16*	30.33±0.70	39.45±0.86*	23.95±0.05*	22.23±0.54
10	36.46±0.96*	21.29±0.49*	27.50±2.19	27.23±0.14	25.43±1.70*	26.02±0.42*	29.41±0.93	28.70±3.22	27.92±1.11	20.28±0.98*
50	32.76±0.40	23.81±0.73*	27.84±0.80	30.98±2.93	23.98±0.68*	24.49±0.41*	29.22±0.34	23.40±0.88*	21.49±0.24*	21.21±0.08
100	32.55±1.52	22.24±0.39*	31.38±0.60	29.65±0.25	22.71±0.31*	27.52±0.33	34.61±0.58*	33.91±1.94	26.89±0.85*	20.21±0.08*
500	25.09±1.27*	25.59±0.52*	31.37±1.03	24.47±0.85*	21.29±0.29*	31.07±1.24	35.30±0.59*	31.09±1.80	26.50±0.36*	20.22±1.77
MDA-MB-231										
	Schiff bases				**Complexes**					
µM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	23.68±0.24	23.68±0.24	23.68±0.24	23.68±0.24	23.68±0.24	23.68±0.24	23.68±0.24	23.68±0.24	23.68±0.24	36.24±0.24
0.1	24.23±1.18	23.43±0.54	20.90±0.15*	28.88±1.30*	26.03±1.42	20.61±0.02	28.66±1.21*	29.64±0.32*	21.64±1.63	36.27±1.18
1	22.90±1.15	23.50±0.21	26.81±0.98*	26.67±1.30	24.50±0.81	22.70±0.21	23.58±1.78	24.34±0.87	21.82±0.43	33.79±0.51
10	23.32±0.30	24.49±1.11	25.54±0.40	35.80±2.19*	29.20±0.36*	23.62±0.29	23.09±0.34	30.23±1.11*	25.00±0.05	35.66±0.43
50	21.84±0.14	24.78±0.48	25.31±0.27	24.25±0.74	25.24±0.75	29.22±1.05*	24.02±0.45	31.54±0.22*	23.39±0.27	53.53±1.31*
100	21.43±0.28	19.99±0.08*	22.59±0.90	22.33±0.21	24.74±0.67	24.44±0.66	25.94±0.63	26.80±1.00*	24.63±0.62	48.74±1.96*
500	21.64±0.12	23.67±0.16	22.07±0.16	25.77±0.69	24.33±0.62	25.09±1.23	24.08±0.59	29.66±1.24*	23.98±1.32	60.8±4.12*
MRC-5										
µM					**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	-	-	-	-	27.27±0.11	27.27±0.11	27.27±0.11	27.27±0.11	-	27.27±0.11
1	-	-	-	-	26.12±0.45	27.85±0.71	33.58±0.86*	31.95±0.46*	-	32.17±1.20
10	-	-	-	-	29.41±0.57*	31.03±1.12*	27.39±1.69	37.86±1.20*	-	32.98±1.22*
50	-	-	-	-	25.99±0.27	26.91±1.15	32.41±1.76*	30.39±0.92*	-	29.69±2.25
100	-	-	-	-	31.16±0.98*	23.32±0.54*	22.11±0.09*	34.11±0.23*	-	35.59±1.16*

Table S11. Effects of Schiff bases and their complexes on HCT-116, MDA-MB-231 and MRC-5 cell lines, expressed as the reduced glutathione (GSH) concentration after 72 h of exposure. *p < 0.05 as compared to the control cells

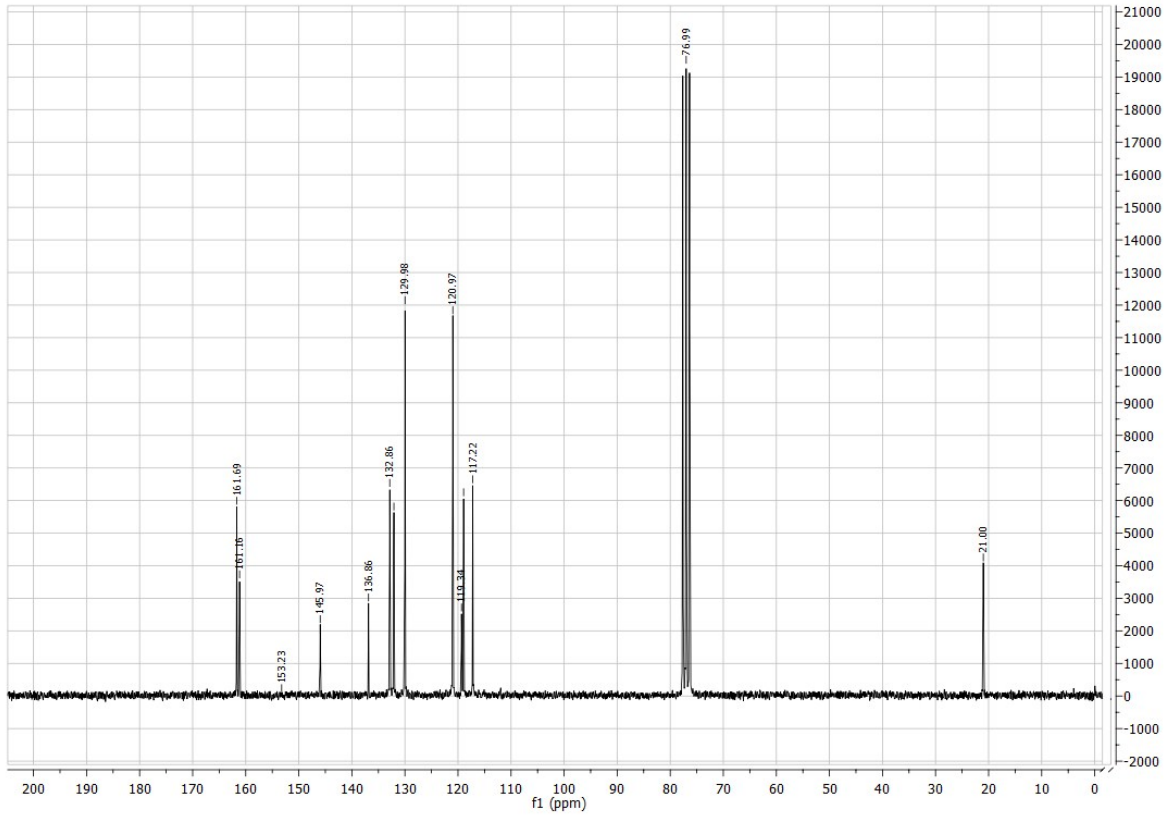
GSH (μM)										
HCT-116										
Schiff bases					**Complexes**					
μM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	24.47±0.23	24.47±0.23	24.47±0.23	24.47±0.23	24.47±0.23	24.47±0.23	24.47±0.23	24.47±0.23	24.47±0.23	24.47±0.23
0.1	23.50±0.12	31.25±0.06*	29.26±0.88*	31.57±1.35*	24.97±0.25	18.46±1.09*	34.51±0.68*	26.16±1.29	23.58±0.68	17.56±0.62*
1	25.57±0.18	24.22±1.29	29.39±0.76*	22.50±0.51	23.24±1.15	21.48±0.67	28.66±0.62*	30.73±0.82*	20.86±0.63	19.70±1.32*
10	25.70±0.48	23.38±0.13	28.23±0.18*	37.86±0.65*	24.51±0.28	23.13±0.44	30.12±0.48*	32.32±0.37*	25.50±0.28*	22.58±0.44
50	22.61±0.13	25.33±0.40	31.57±0.67*	26.76±0.79	23.13±1.62	21.59±1.69	29.16±0.61*	25.83±0.19	23.25±0.63	25.97±0.77
100	25.62±0.53	27.48±1.52	27.12±0.51*	26.99±1.54	27.76±0.47*	23.68±0.37	33.28±0.25*	33.85±0.46*	18.19±0.11*	22.24±0.40
500	25.73±0.80	17.05±0.16*	26.11±1.90	30.48±0.96*	23.25±0.71	19.49±0.65*	31.02±0.18*	25.46±0.84	20.60±1.54*	18.33±1.05*
MDA-MB-231										
Schiff bases					**Complexes**					
μM	**1**	**3**	**5**	**6**	**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	24.18±0.13	24.18±0.13	24.18±0.13	24.18±0.13	24.18±0.13	24.18±0.13	24.18±0.13	24.18±0.13	24.18±0.13	24.18±0.13
0.1	39.71±0.78*	24.28±0.29	25.95±0.49	23.04±1.77	31.80±0.60*	33.30±0.43*	31.27±1.74*	25.67±0.30	23.39±1.17	23.40±0.81
1	23.86±0.83	24.43±0.41	26.86±0.63	20.84±0.49	30.17±1.78*	29.28±0.74*	26.94±1.79	20.34±1.16*	24.20±0.66	25.13±0.88
10	27.33±0.75	27.07±0.89	30.59±0.23*	23.91±0.61	34.81±0.84*	25.45±0.53	31.25±0.72*	20.76±0.80*	22.93±0.14	28.38±1.91
50	26.69±0.64	26.16±0.51	29.00±1.05*	21.78±0.72	31.61±0.11*	25.26±1.09	32.55±1.16*	18.88±0.94*	32.01±0.96*	27.69±0.21
100	25.43±0.47	27.44±0.66	26.72±0.08	18.98±0.34*	34.49±0.37*	22.25±0.02	27.13±0.91	26.26±1.34	26.98±0.64	27.69±0.35
500	27.58±0.90	23.01±0.63	24.80±1.13	21.36±0.45	28.47±0.47*	30.91±0.94*	25.56±0.63	22.29±0.34	24.92±1.83	31.34±4.12*
MRC-5										
μM					**Pd-1**	**Pd-3**	**Pd-5**	**Pd-6**	**$Pd(OAc)_2$**	**CisPt**
0	-	-	-	-	20.38±0.18	20.38±0.18	20.38±0.18	20.38±0.18	-	20.38±0.18
1	-	-	-	-	30.49±0.43*	27.57±1.84*	27.36±1.05*	25.53±0.30*	-	22.38±0.23
10	-	-	-	-	31.91±1.13*	30.40±1.07*	30.81±0.76*	30.52±0.28*	-	21.75±0.59
50	-	-	-	-	24.10±0.53	27.92±2.08*	22.94±0.46	23.50±1.33	-	22.08±0.20
100	-	-	-	-	29.51±1.11*	21.68±0.42	28.16±0.52*	23.09±1.44	-	26.81±0.50*

NMR spectra of the compounds investigated

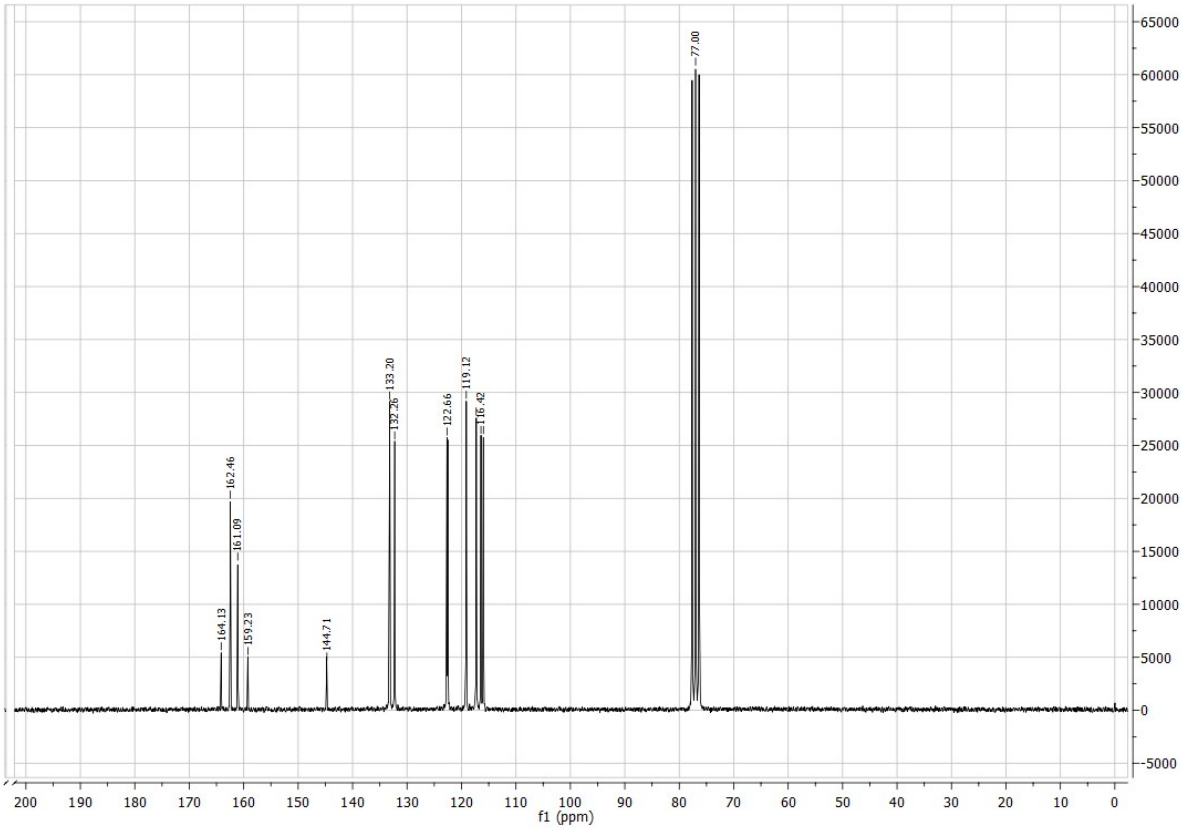
1 ^{13}C NMR (DMSO)



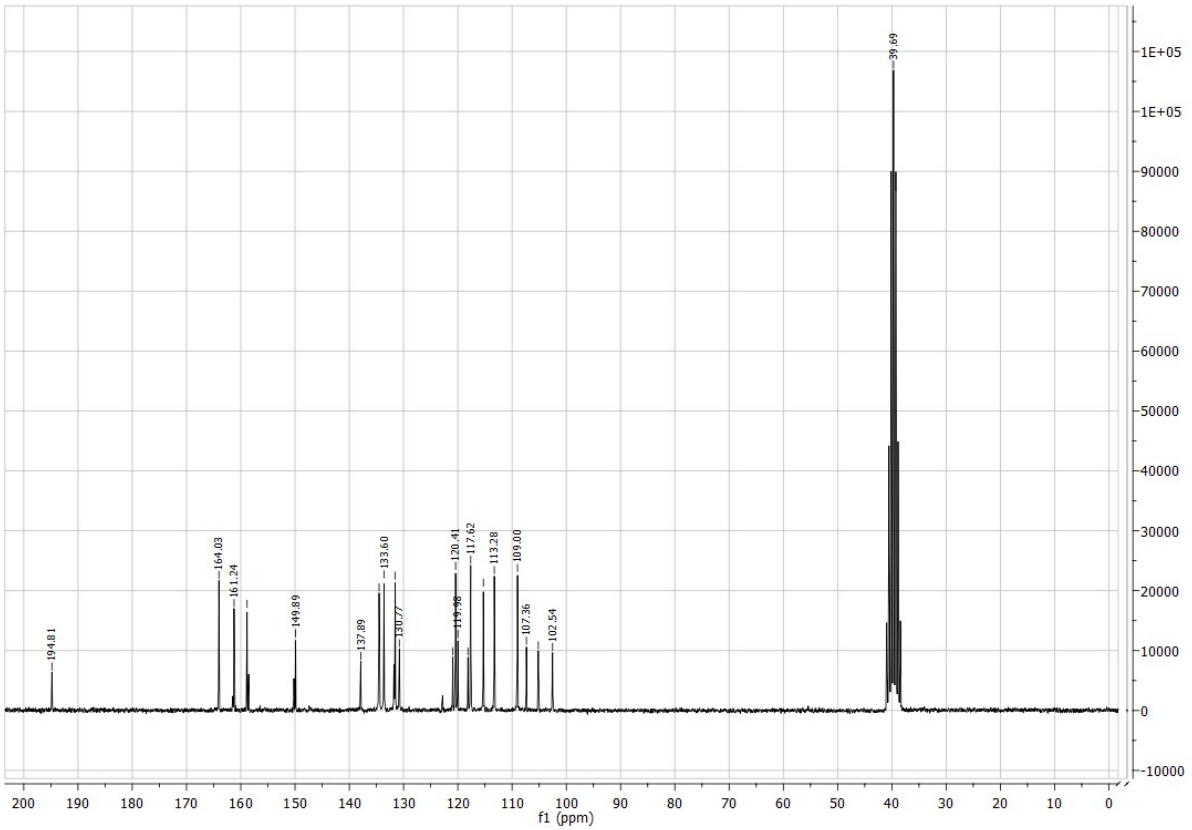
3 ^{13}C NMR ($CDCl_3$)



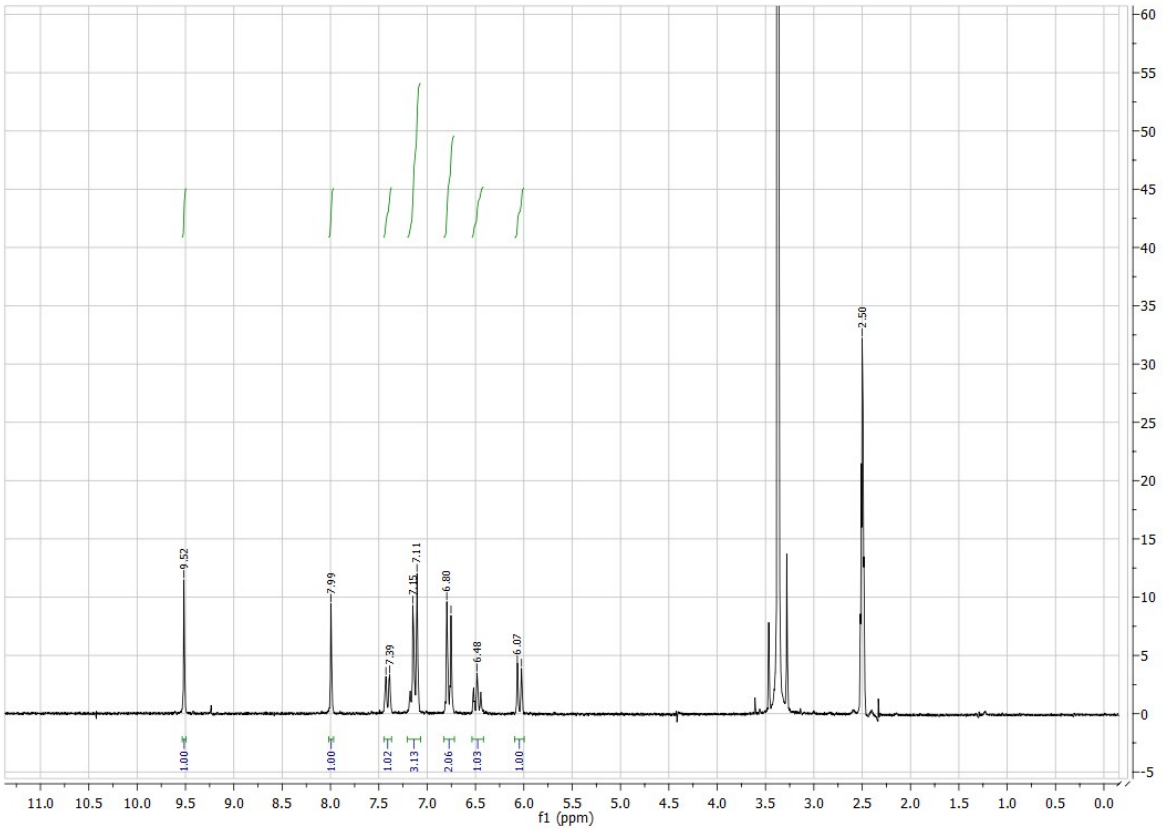
5 ^{13}C NMR ($CDCl_3$)



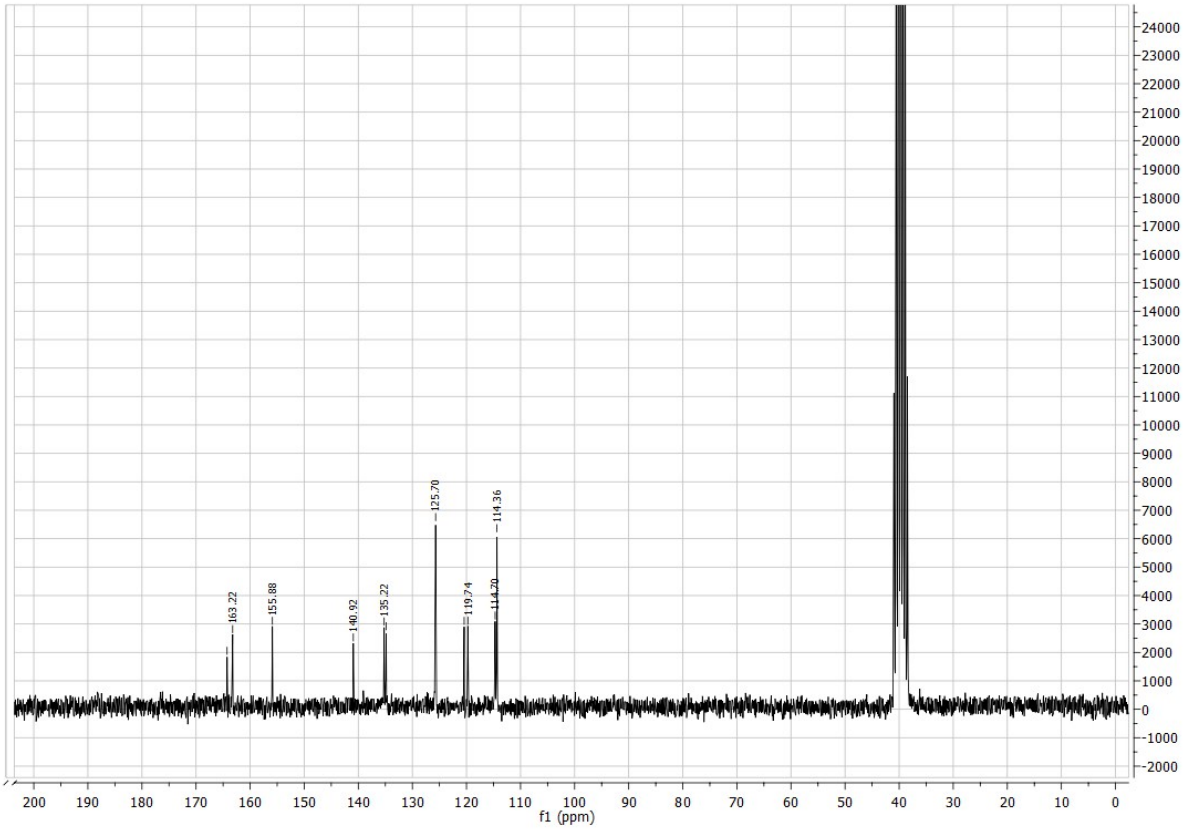
6 ^{13}C NMR (DMSO)



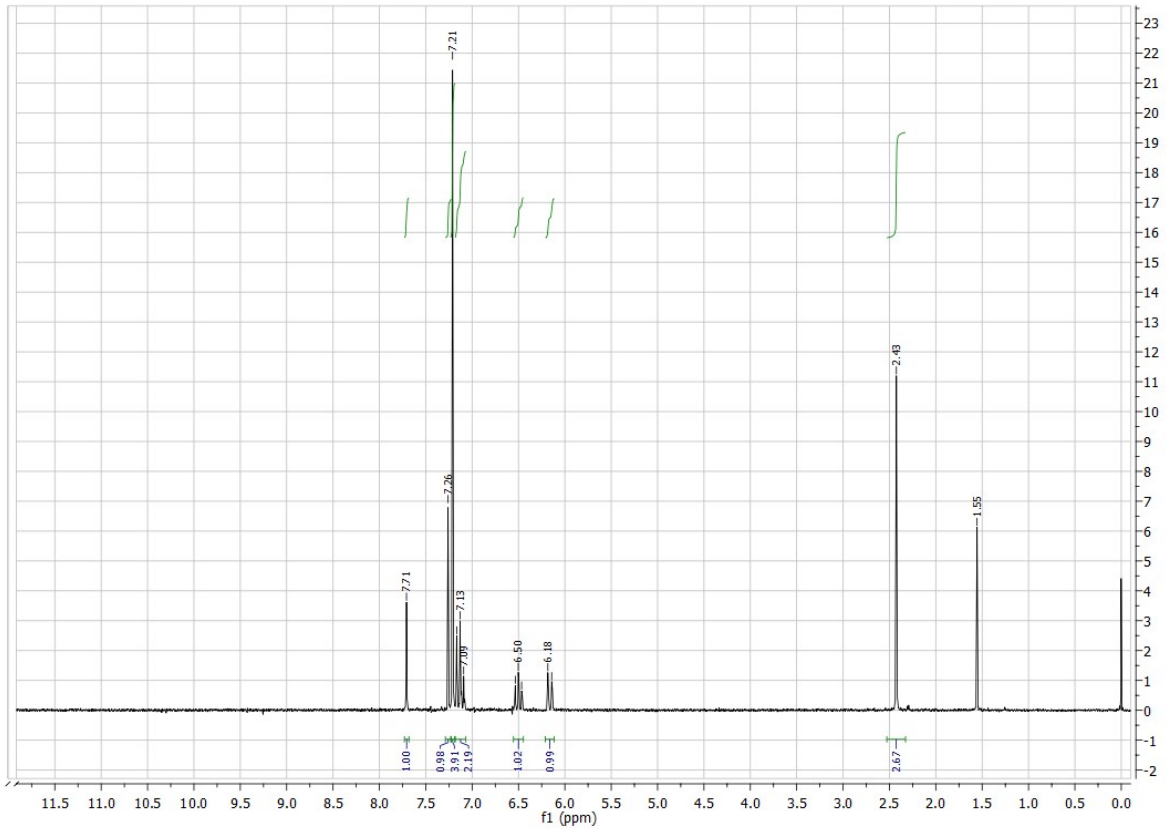
Pd-1 ^{1}H NMR (DMSO)



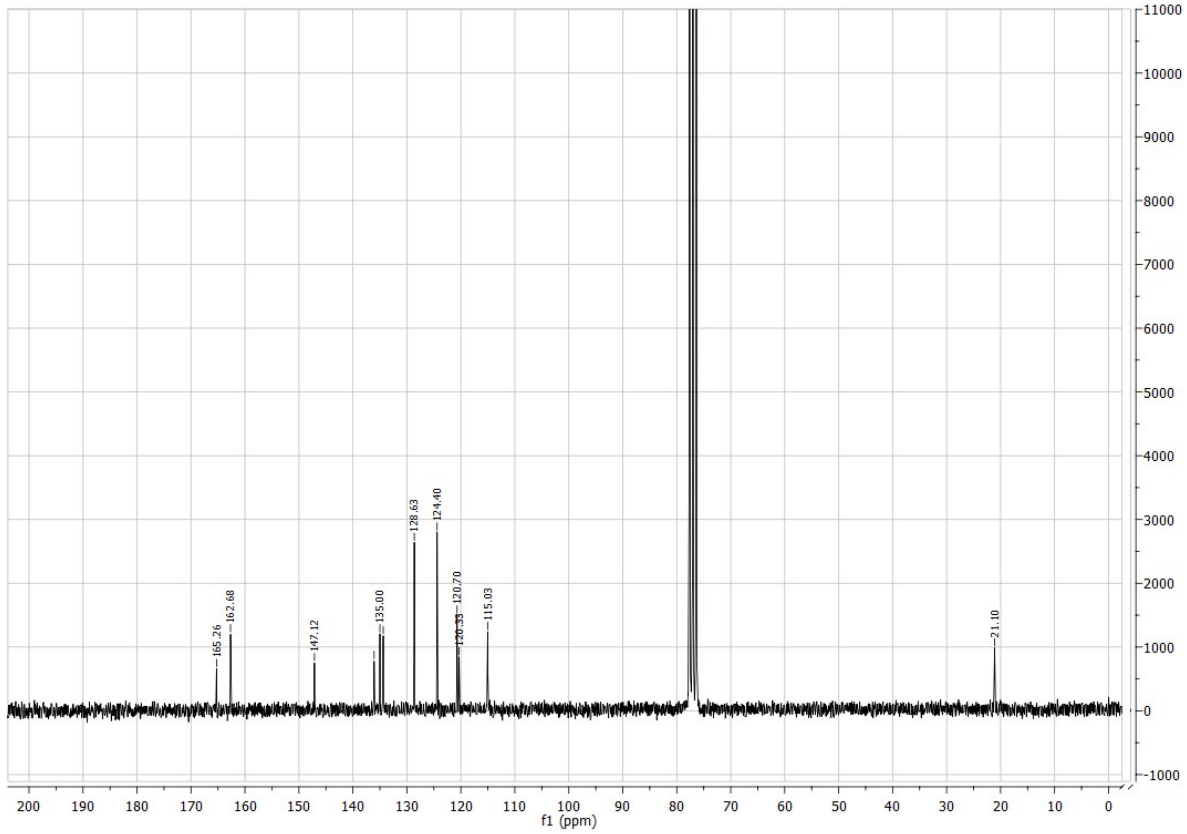
Pd-1 ^{13}C NMR (DMSO)



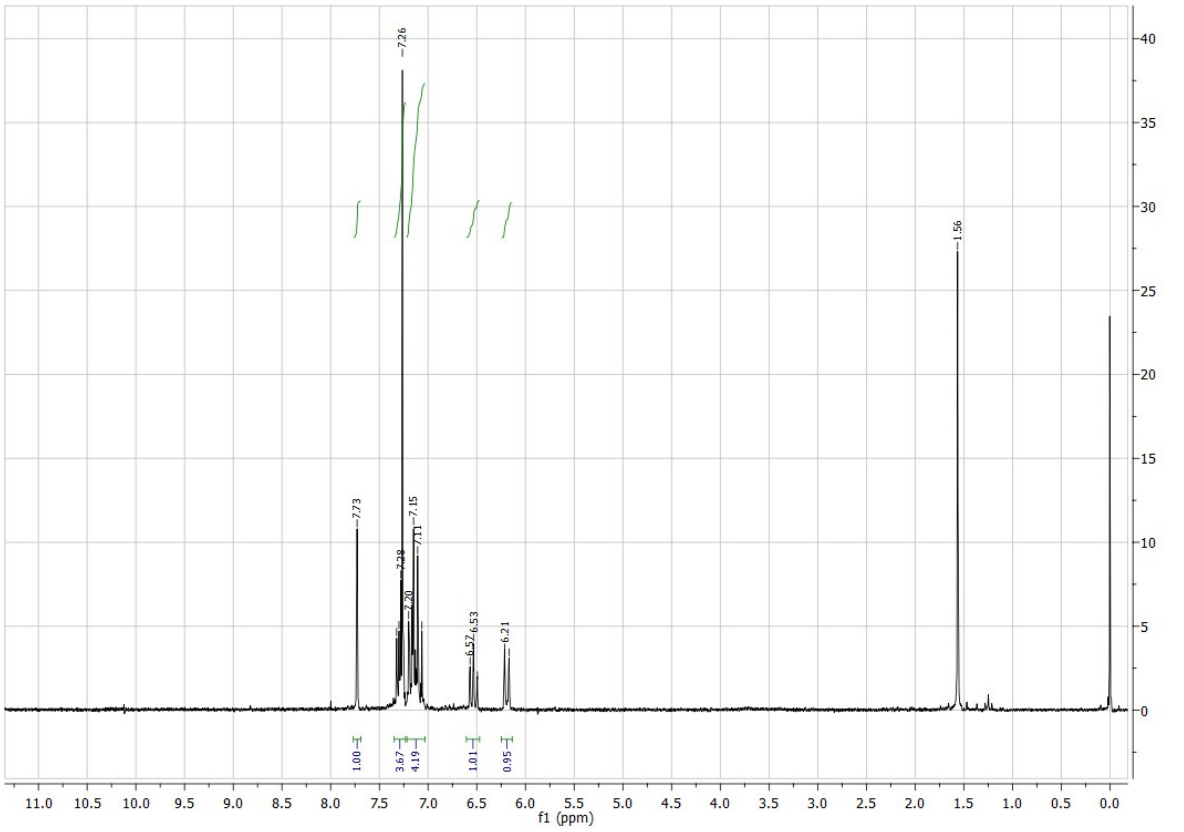
Pd-3 ^{1}H NMR ($CDCl_3$)



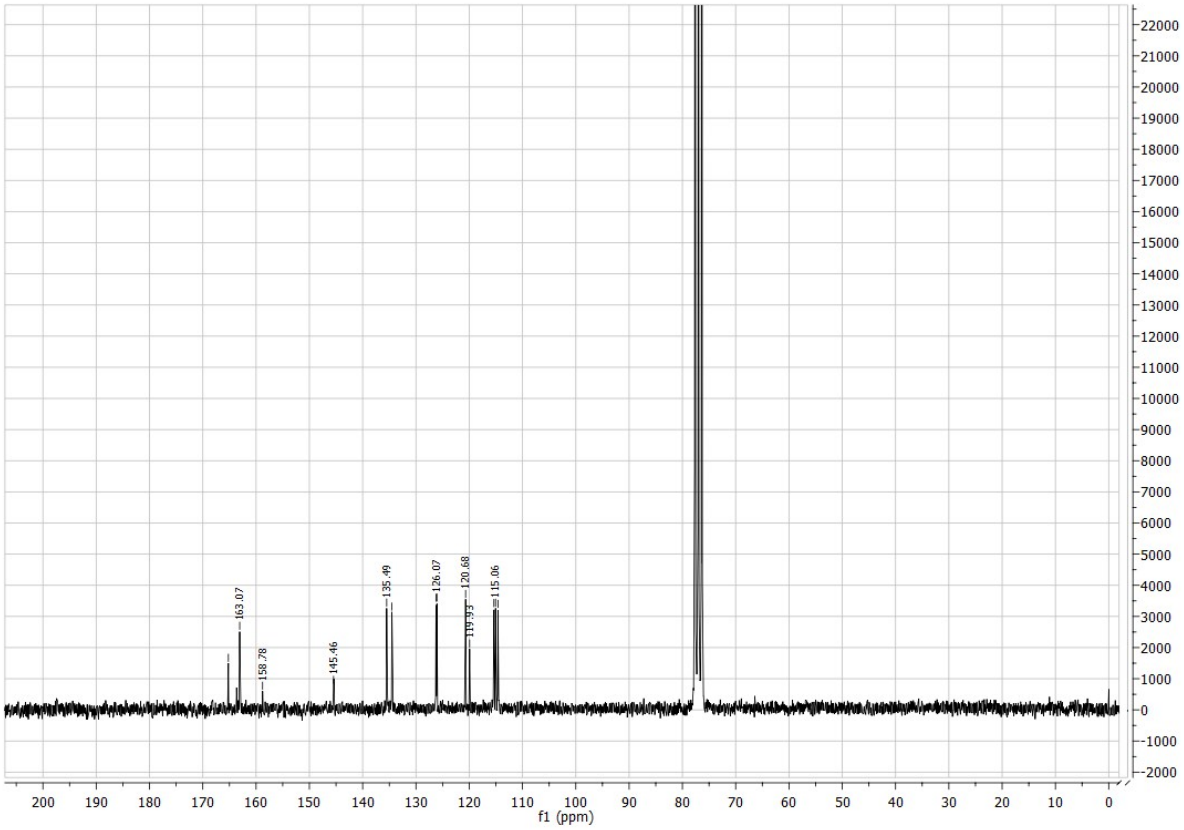
Pd-3 ^{13}C NMR ($CDCl_3$)



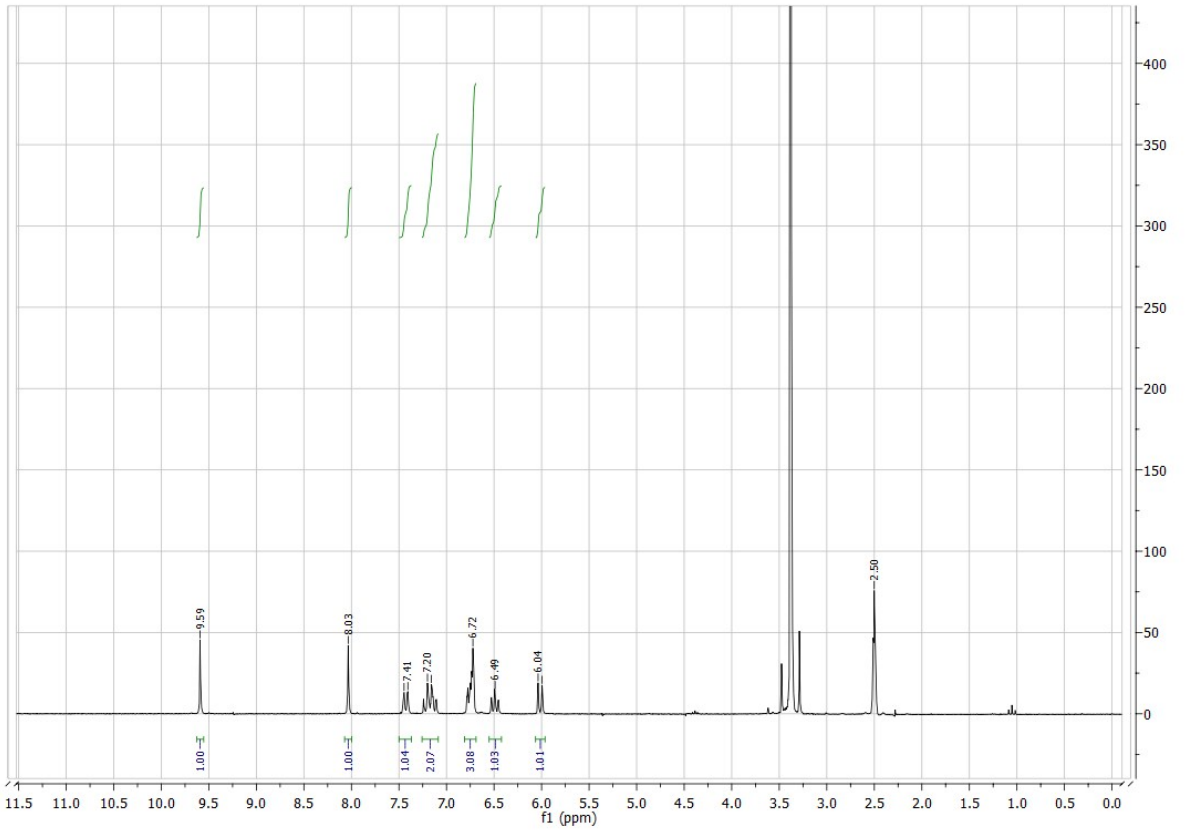
Pd-5 ^{1}H NMR ($CDCl_3$)



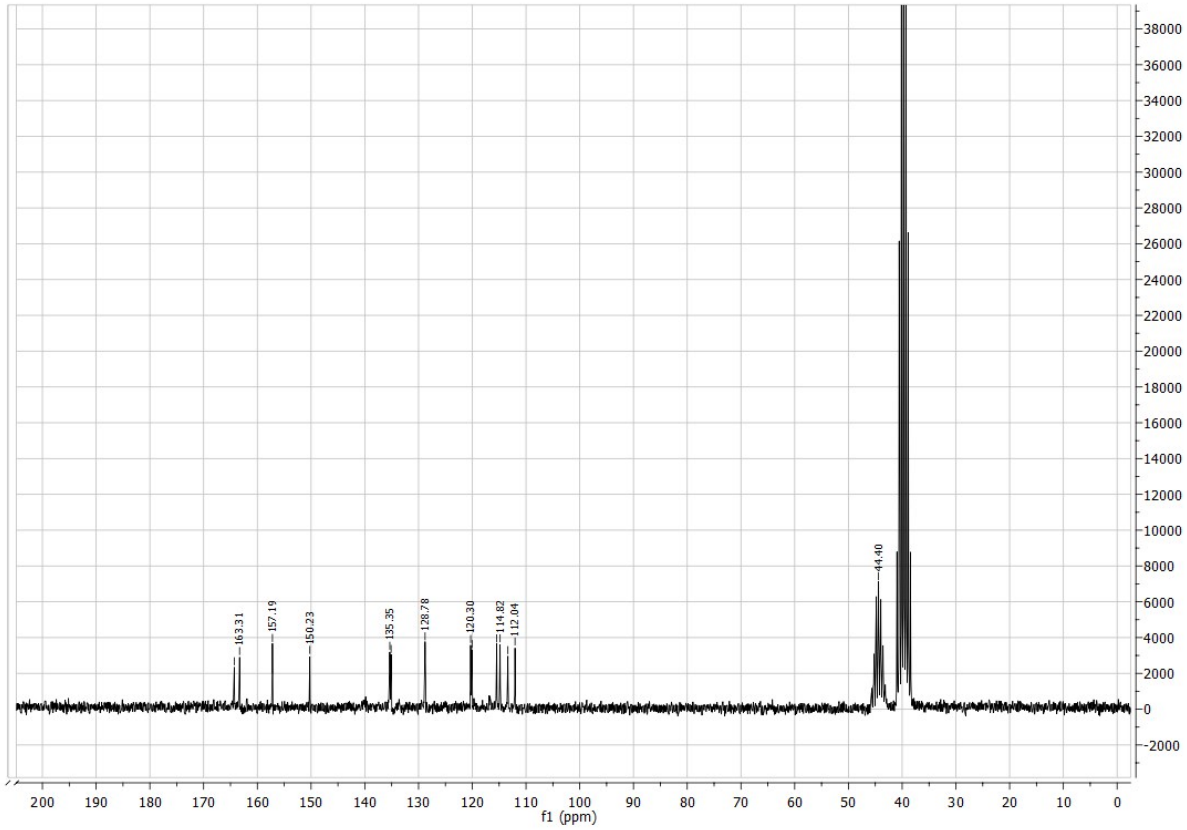
Pd-5 ^{13}C NMR ($CDCl_3$)



Pd-6 ^{1}H NMR (DMSO)



Pd-6 ^{13}C NMR (DMSO)



Cartesian coordinates of the optimised structures

1

0 1

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C	-0.70906500	-0.56953400	-0.15990400
H	-0.35028700	-1.58427400	-0.39474900
C	-2.14375500	-0.40368500	-0.10668100
C	-2.97443400	-1.50474700	-0.35325800
C	-2.73481800	0.84599600	0.18723000
C	-4.34795600	-1.39397800	-0.31304800
H	-2.50739100	-2.46117200	-0.57901800
C	-4.12542400	0.95077800	0.22813500
C	-4.91635500	-0.15373700	-0.01963600
H	-4.55702700	1.91998100	0.45620600
C	1.49544400	0.17457500	0.02703900
C	2.32259100	1.18375100	-0.47194100
C	2.08652800	-0.98221500	0.53284900
C	3.69332700	1.02608900	-0.51265600
H	1.86181900	2.09371100	-0.84457600
C	3.46363400	-1.13992300	0.50820200
H	1.46846100	-1.75302600	0.98424600
C	4.27100300	-0.14146600	-0.02335300
H	4.33939100	1.80081700	-0.91234300
H	3.91566600	-2.03952900	0.92137500
H	-4.97699100	-2.25593700	-0.50608600
H	-5.99698200	-0.05142700	0.01555500
O	5.62328700	-0.23905400	-0.07349800
H	5.90530700	-1.07974000	0.29666900
O	-2.01165100	1.93826100	0.42754000
H	-1.05816500	1.69547900	0.35243600

3

0 1

N	0.08930400	0.40421000	0.04184500
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C	-2.16167700	-0.40341800	-0.10839400
C	-2.98735300	-1.50640300	-0.36315400
C	-2.75782100	0.84284600	0.18994800
C	-4.36124300	-1.40067500	-0.32698800
H	-2.51596900	-2.45986700	-0.59226000
C	-4.14903700	0.94251300	0.22628200
C	-4.93487600	-0.16373300	-0.02931700
H	-4.58495700	1.90902100	0.45754700
C	1.47390500	0.18314100	0.03335700
C	2.29832500	1.17567300	-0.49750500
C	2.06270500	-0.95933100	0.57443900
C	3.67001600	1.00425000	-0.52848600
H	1.83873200	2.07635700	-0.89391000
C	3.44035600	-1.11389500	0.54924000
H	1.44083100	-1.71153600	1.05205900
C	4.26806300	-0.14455200	-0.01012100
H	4.29752100	1.78345100	-0.95542700
H	3.88567800	-2.00350200	0.98914600
H	-4.98674500	-2.26376700	-0.52624700
H	-6.01598200	-0.06544600	0.00276100
O	-2.03956300	1.93625600	0.43828800
H	-1.08473200	1.69806000	0.36411900
C	5.75351000	-0.32451200	-0.05993700
H	6.07499200	-0.68855500	-1.04304000
H	6.27728900	0.61930900	0.12082600
H	6.09511700	-1.04939200	0.68427200

5

0 1

N	0.12156300	0.40642700	0.04528400

C	-0.69650400	-0.55919400	-0.15855600
H	-0.33286200	-1.57026300	-0.40157500
C	-2.13072700	-0.39874200	-0.10814700
C	-2.95587500	-1.50107600	-0.36978400
C	-2.72734300	0.84597900	0.19589800
C	-4.32938900	-1.39556200	-0.33460600
H	-2.48416300	-2.45323700	-0.60338000
C	-4.11856100	0.94517600	0.23126300
C	-4.90345800	-0.15992400	-0.03125300
H	-4.55510200	1.91025400	0.46703200
C	1.50478800	0.18019600	0.03460800
C	2.32867700	1.16651600	-0.50983500
C	2.08740400	-0.96430300	0.58203900
C	3.70118500	0.99717600	-0.55337000
H	1.86940500	2.06373400	-0.91292100
C	3.46238100	-1.13739500	0.55441700
H	1.46161500	-1.70974600	1.06381700
C	4.24535400	-0.15689000	-0.02168100
H	4.35487500	1.74725100	-0.98507400
H	3.93453300	-2.01352700	0.98597500
H	-4.95465300	-2.25749100	-0.53920900
H	-5.98458900	-0.06208800	-0.00011600
O	-2.01015700	1.93855200	0.45078700
H	-1.05556700	1.70321000	0.37684700
F	5.57435800	-0.32036100	-0.04896000

6

0 1

N	-0.19885100	-0.56587400	0.01886000
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H	0.14506800	1.36162900	-0.67364600
C	2.00125400	0.36438100	-0.17162200
C	2.76311600	1.48078900	-0.54205800
C	2.66447900	-0.78898200	0.30560400
C	4.13773800	1.47755900	-0.44685300
H	2.24085700	2.36106200	-0.91091200
C	4.05652100	-0.78578000	0.39877500
C	4.77811000	0.33163800	0.02818500
H	4.54429000	-1.68226100	0.76764300
C	-1.59260700	-0.44284700	-0.06139300
C	-2.32669500	-1.53867500	-0.51008300
C	-2.25676700	0.72141200	0.33002200
C	-3.70694100	-1.44620200	-0.60171000
H	-1.79898300	-2.44272800	-0.79505000
C	-3.64135000	0.79238600	0.24544800
H	-1.69307200	1.55769300	0.73956000
C	-4.37353000	-0.29062100	-0.22777700
H	-4.27777600	-2.29555100	-0.96421800
H	4.71363300	2.34941300	-0.73678600
H	5.86105000	0.31405300	0.10790300
O	2.00976300	-1.88884300	0.67150300
H	1.04517600	-1.73169400	0.53822900
H	-5.45413900	-0.21112800	-0.27757700
O	-4.33471500	1.89535100	0.62418600
H	-3.73066000	2.56835200	0.94881000

Pd-1

0 1

N	-1.09810100	-1.74370300	0.06270300
C	-0.56008900	-2.91359400	-0.06425000
H	-1.25277400	-3.76227400	-0.10100700
C	0.81924000	-3.26103000	-0.13782900
C	1.12517500	-4.63697400	-0.25061800
C	1.88161600	-2.31102900	-0.07347600
C	2.41478400	-5.09356400	-0.30153300
H	0.29758900	-5.34206100	-0.29416400
C	3.20768000	-2.81483700	-0.12507900

C	3.46094600	-4.15668100	-0.23655600
H	4.00898900	-2.08292900	-0.07795800
C	-2.51772900	-1.65872000	0.09036900
C	-3.16244700	-1.17200600	1.22397100
C	-3.26568100	-2.01977400	-1.01986100
C	-4.53868300	-1.07694600	1.25870600
H	-2.56534600	-0.86101300	2.07546900
C	-4.64985800	-1.91702600	-0.99509900
H	-2.75873500	-2.36424600	-1.91690300
C	-5.28785700	-1.44566500	0.14444100
H	-5.05637200	-0.70758100	2.13792700
H	-5.23326900	-2.19702200	-1.86973800
H	2.62662900	-6.15341600	-0.38782600
H	4.49136600	-4.50028700	-0.27503500
O	-6.63694300	-1.31807800	0.23045700
H	-7.04342500	-1.59131200	-0.59626100
O	1.73966300	-1.03657200	0.02922500
N	1.09810400	1.74369500	0.06287600
C	0.56008500	2.91359400	-0.06396900
H	1.25276600	3.76228000	-0.10065100
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H	-0.29760300	5.34208200	-0.29361200
C	-3.20768700	2.81482700	-0.12480300
C	-3.46095700	4.15668400	-0.23612700
H	-4.00899300	2.08291200	-0.07776800
C	2.51773100	1.65871600	0.09053100
C	3.16245500	1.17192300	1.22409600
C	3.26568300	2.01986800	-1.01966700
C	4.53869100	1.07686500	1.25882200
H	2.56535800	0.86086700	2.07557400
C	4.64986100	1.91712500	-0.99491500
H	2.75873800	2.36441100	-1.91668400
C	5.28786200	1.44567300	0.14458600
H	5.05638100	0.70743500	2.13801600
H	5.23326900	2.19719500	-1.86953100
H	-2.62665100	6.15343800	-0.38717100
H	-4.49137600	4.50029400	-0.27456900
O	6.63695000	1.31808600	0.23059000
H	7.04342900	1.59140800	-0.59610000
O	-1.73966000	1.03655400	0.02931300
Pd	0.00000300	-0.00000700	0.07376700

Pd-3

0 1

N	-1.11039300	-1.73516700	0.05864600
C	-0.58272000	-2.90812300	-0.08082500
H	-1.28208900	-3.75112400	-0.12144600
C	0.79385200	-3.26441100	-0.16494200
C	1.09056000	-4.64037400	-0.29882600
C	1.86266300	-2.32222500	-0.09238100
C	2.37708500	-5.10400500	-0.36448500
H	0.25836800	-5.33961300	-0.34823700
C	3.18536600	-2.83307800	-0.15974600
C	3.42954900	-4.17460100	-0.29264700
H	3.98997200	-2.10487800	-0.10871400
C	-2.52938400	-1.63976700	0.10114700
C	-3.15678800	-1.16036200	1.24503100
C	-3.28901200	-1.98390000	-1.00768100
C	-4.53502800	-1.05748800	1.28169200
H	-2.54912400	-0.85787000	2.09234700
C	-4.67136100	-1.86674100	-0.96299600
H	-2.78989800	-2.31892100	-1.91295800
C	-5.31722300	-1.40731400	0.18012400
H	-5.01988800	-0.68612700	2.18183800

H	-5.25937900	-2.13052300	-1.83899600
H	2.58167200	-6.16372700	-0.46823200
H	4.45739300	-4.52433000	-0.34418200
O	1.73050000	-1.04889500	0.03156900
N	1.11038500	1.73509600	0.05878500
C	0.58269900	2.90805800	-0.08062400
H	1.28206300	3.75106900	-0.12112900
C	-0.79386800	3.26435300	-0.16478100
C	-1.09058700	4.64036100	-0.29818900
C	-1.86267300	2.32212000	-0.09275800
C	-2.37711300	5.10399000	-0.36383300
H	-0.25840400	5.33963800	-0.34721800
C	-3.18537900	2.83296700	-0.16011300
C	-3.42957200	4.17453700	-0.29250700
H	-3.98997400	2.10472600	-0.10948800
C	2.52938200	1.63974100	0.10128100
C	3.15682300	1.16042700	1.24517600
C	3.28898200	1.98387600	-1.00757300
C	4.53507700	1.05765900	1.28183300
H	2.54919100	0.85792600	2.09250900
C	4.67133500	1.86682200	-0.96289300
H	2.78983300	2.31883400	-1.91285500
C	5.31724000	1.40750100	0.18025400
H	5.01996600	0.68637400	2.18199300
H	5.25932800	2.13060800	-1.83890800
H	-2.58170700	6.16374900	-0.46718500
H	-4.45741500	4.52426900	-0.34403700
O	-1.73050000	1.04874000	0.03062400
Pd	0.00000900	-0.00004400	0.07350800
C	6.81032700	1.30719200	0.23915700
H	7.13117300	0.43678200	0.81976100
H	7.24680100	1.22774900	-0.76057500
H	7.24718600	2.19219200	0.71711400
C	-6.81029700	-1.30681900	0.23904700
H	-7.13101400	-0.43573000	0.81870900
H	-7.24685100	-1.22844900	-0.76073200
H	-7.24718800	-2.19123600	0.71805000

Pd-5

0 1

N	1.09241400	1.74600300	0.05818700
C	0.55199000	2.91551700	-0.06834600
H	1.24250600	3.76588900	-0.10581400
C	-0.82723800	3.25856100	-0.14175400
C	-1.13700800	4.63399500	-0.25744000
C	-1.88703000	2.30557800	-0.07726500
C	-2.42762400	5.08584600	-0.31173500
H	-0.31165900	5.34154900	-0.30109500
C	-3.21413700	2.80479400	-0.13389900
C	-3.47107100	4.14563600	-0.24824400
H	-4.01355500	2.07068600	-0.08976800
C	2.51166900	1.66383800	0.08980600
C	3.14847100	1.18437800	1.22933800
C	3.25818800	2.02415500	-1.02438400
C	4.52791500	1.09202800	1.26778600
H	2.54805800	0.87601800	2.07902100
C	4.64239800	1.92793600	-0.99963400
H	2.74815400	2.36278300	-1.92154200
C	5.25045000	1.46386100	0.14846400
H	5.05062500	0.72942700	2.14619200
H	5.24886700	2.19954000	-1.85664100
H	-2.64298600	6.14466900	-0.40076500
H	-4.50234000	4.48580900	-0.29119600
O	-1.74175600	1.03129800	0.03080500
N	-1.09241600	-1.74600400	0.05813600
C	-0.55199100	-2.91551500	-0.06841700
H	-1.24250600	-3.76588700	-0.10590900

C	0.82723700	-3.25855800	-0.14182700
C	1.13700300	-4.63398800	-0.25756600
C	1.88703100	-2.30558000	-0.07729100
C	2.42761800	-5.08584200	-0.31187500
H	0.31165300	-5.34153800	-0.30125400
C	3.21413600	-2.80480000	-0.13394100
C	3.47106800	-4.14563800	-0.24834000
H	4.01355700	-2.07069700	-0.08977500
C	-2.51167000	-1.66383800	0.08975100
C	-3.14847500	-1.18439600	1.22929000
C	-3.25818500	-2.02413100	-1.02444900
C	-4.52791900	-1.09204300	1.26773400
H	-2.54806300	-0.87605100	2.07898000
C	-4.64239500	-1.92791000	-0.99970200
H	-2.74814700	-2.36274500	-1.92161000
C	-5.25045000	-1.46385500	0.14840200
H	-5.05063100	-0.72945700	2.14614400
H	-5.24886100	-2.19949700	-1.85671700
H	2.64297600	-6.14466200	-0.40094600
H	4.50233500	-4.48581100	-0.29130200
O	1.74176200	-1.03130500	0.03083600
Pd	0.00000200	-0.00000500	0.07076000
F	-6.58658600	-1.36704100	0.18079500
F	6.58658600	1.36705000	0.18086000

Pd-6

0 1

N	-1.03292700	-1.77648300	0.18333300
C	-0.46213000	-2.93525800	0.12931200
H	-1.13025800	-3.80422600	0.10860300
C	0.92887500	-3.23998700	0.10692600
C	1.28408500	-4.60850700	0.07162500
C	1.95721400	-2.25036800	0.13220000
C	2.58945400	-5.01973600	0.06255500
H	0.48247800	-5.34401200	0.05443000
C	3.30100200	-2.70778800	0.12322800
C	3.60168200	-4.04376100	0.08973700
H	4.07284300	-1.94346400	0.14406700
C	-2.45581800	-1.72124300	0.18492600
C	-3.13639000	-1.46437500	1.36511700
C	-3.13916800	-1.87637800	-1.01337400
C	-4.52058800	-1.37647500	1.33514400
H	-2.57561900	-1.31213500	2.28134900
C	-4.52502600	-1.77745800	-1.02834400
H	-2.57983300	-2.04416100	-1.93188600
C	-5.22070300	-1.52773300	0.14894400
H	-5.06513200	-1.17865700	2.25337600
H	2.84036000	-6.07415500	0.03681700
H	4.64368700	-4.35264400	0.08403700
O	1.77246600	-0.97803700	0.16140600
N	1.03294400	1.77637300	0.18337900
C	0.46212400	2.93513200	0.12919400
H	1.13023700	3.80410800	0.10834200
C	-0.92888500	3.23984400	0.10684700
C	-1.28411000	4.60835600	0.07131700
C	-1.95721700	2.25022800	0.13245300
C	-2.58948400	5.01957300	0.06232400
H	-0.48251200	5.34386400	0.05387800
C	-3.30101000	2.70763500	0.12358300
C	-3.60170300	4.04359800	0.08984800
H	-4.07283400	1.94330200	0.14469500
C	2.45582900	1.72115300	0.18487800
C	3.13645900	1.46348400	1.36486500
C	3.13914100	1.87712900	-1.01333800
C	4.52065400	1.37564400	1.33478100
H	2.57572400	1.31058500	2.28100900
C	4.52500200	1.77825800	-1.02842800

H	2.57977300	2.04550900	-1.93172200
C	5.22072700	1.52773700	0.14865900
H	5.06523500	1.17720100	2.25285600
H	-2.84039900	6.07398400	0.03639400
H	-4.64371000	4.35247500	0.08422500
O	-1.77245900	0.97790200	0.16185200
Pd	0.00000800	-0.00006300	0.18648000
O	-5.24970500	-1.91676400	-2.16688900
H	-4.66124200	-2.03972000	-2.91658600
O	5.24963200	1.91836700	-2.16690700
H	4.66113300	2.04181500	-2.91649500
H	-6.30241600	-1.45383100	0.11117700
H	6.30243900	1.45387900	0.11080300

cis Pd-1

N	-1.09810100	-1.74370300	0.06270300
C	-0.56008900	-2.91359400	-0.06425000
H	-1.25277400	-3.76227400	-0.10100700
C	0.81924000	-3.26103000	-0.13782900
C	1.12517500	-4.63697400	-0.25061800
C	1.88161600	-2.31102900	-0.07347600
C	2.41478400	-5.09356400	-0.30153300
H	0.29758900	-5.34206100	-0.29416400
C	3.20768000	-2.81483700	-0.12507900
C	3.46094600	-4.15668100	-0.23655600
H	4.00898900	-2.08292900	-0.07795800
C	-2.51772900	-1.65872000	0.09036900
C	-3.16244700	-1.17200600	1.22397100
C	-3.26568100	-2.01977400	-1.01986100
C	-4.53868300	-1.07694600	1.25870600
H	-2.56534600	-0.86101300	2.07546900
C	-4.64985800	-1.91702600	-0.99509900
H	-2.75873500	-2.36424600	-1.91690300
C	-5.28785700	-1.44566500	0.14444100
H	-5.05637200	-0.70758100	2.13792700
H	-5.23326900	-2.19702200	-1.86973800
H	2.62662900	-6.15341600	-0.38782600
H	4.49136600	-4.50028700	-0.27503500
O	-6.63694300	-1.31807800	0.23045700
H	-7.04342500	-1.59131200	-0.59626100
O	1.73966300	-1.03657200	0.02922500
N	1.09810400	1.74369500	0.06287600
C	0.56008500	2.91359400	-0.06396900
H	1.25276600	3.76228000	-0.10065100
C	-0.81924600	3.26103200	-0.13750800
C	-1.12518700	4.63698700	-0.25014200
C	-1.88162200	2.31101700	-0.07325500
C	-2.41479800	5.09357800	-0.30100100
H	-0.29760300	5.34208200	-0.29361200
C	-3.20768700	2.81482700	-0.12480300
C	-3.46095700	4.15668400	-0.23612700
H	-4.00899300	2.08291200	-0.07776800
C	2.51773100	1.65871600	0.09053100
C	3.16245500	1.17192300	1.22409600
C	3.26568300	2.01986800	-1.01966700
C	4.53869100	1.07686500	1.25882200
H	2.56535800	0.86086700	2.07557400
C	4.64986100	1.91712500	-0.99491500
H	2.75873800	2.36441100	-1.91668400
C	5.28786200	1.44567300	0.14458600
H	5.05638100	0.70743500	2.13801600
H	5.23326900	2.19719500	-1.86953100
H	-2.62665100	6.15343800	-0.38717100
H	-4.49137600	4.50029400	-0.27456900
O	6.63695000	1.31808600	0.23059000
H	7.04342900	1.59140800	-0.59610000
O	-1.73966000	1.03655400	0.02931300
Pd	0.00000300	-0.00000700	0.07376700

cis Pd-3

N	-1.11039300	-1.73516700	0.05864600
C	-0.58272000	-2.90812300	-0.08082500
H	-1.28208900	-3.75112400	-0.12144600
C	0.79385200	-3.26441100	-0.16494200
C	1.09056000	-4.64037400	-0.29882600
C	1.86266300	-2.32222500	-0.09238100
C	2.37708500	-5.10400500	-0.36448500
H	0.25836800	-5.33961300	-0.34823700
C	3.18536600	-2.83307800	-0.15974600

C	3.42954900	-4.17460100	-0.29264700
H	3.98997200	-2.10487800	-0.10871400
C	-2.52938400	-1.63976700	0.10114700
C	-3.15678800	-1.16036200	1.24503100
C	-3.28901200	-1.98390000	-1.00768100
C	-4.53502800	-1.05748800	1.28169200
H	-2.54912400	-0.85787000	2.09234700
C	-4.67136100	-1.86674100	-0.96299600
H	-2.78989800	-2.31892100	-1.91295800
C	-5.31722300	-1.40731400	0.18012400
H	-5.01988800	-0.68612700	2.18183800
H	-5.25937900	-2.13052300	-1.83899600
H	2.58167200	-6.16372700	-0.46823200
H	4.45739300	-4.52433000	-0.34418200
O	1.73050000	-1.04889500	0.03156900
N	1.11038500	1.73509600	0.05878500
C	0.58269900	2.90805800	-0.08062400
H	1.28206300	3.75106900	-0.12112900
C	-0.79386800	3.26435300	-0.16478100
C	-1.09058700	4.64036100	-0.29818900
C	-1.86267300	2.32212000	-0.09275800
C	-2.37711300	5.10399000	-0.36383300
H	-0.25840400	5.33963800	-0.34721800
C	-3.18537900	2.83296700	-0.16011300
C	-3.42957200	4.17453700	-0.29250700
H	-3.98997400	2.10472600	-0.10948800
C	2.52938200	1.63974100	0.10128100
C	3.15682300	1.16042700	1.24517600
C	3.28898200	1.98387600	-1.00757300
C	4.53507700	1.05765900	1.28183300
H	2.54919100	0.85792600	2.09250900
C	4.67133500	1.86682200	-0.96289300
H	2.78983300	2.31883400	-1.91285500
C	5.31724000	1.40750100	0.18025400
H	5.01996600	0.68637400	2.18199300
H	5.25932800	2.13060800	-1.83890800
H	-2.58170700	6.16374900	-0.46718500
H	-4.45741500	4.52426900	-0.34403700
O	-1.73050000	1.04874000	0.03062400
Pd	0.00000900	-0.00004400	0.07350800
C	6.81032700	1.30719200	0.23915700
H	7.13117300	0.43678200	0.81976100
H	7.24680100	1.22774900	-0.76057500
H	7.24718600	2.19219200	0.71711400
C	-6.81029700	-1.30681900	0.23904700
H	-7.13101400	-0.43573000	0.81870900
H	-7.24685100	-1.22844900	-0.76073200
H	-7.24718800	-2.19123600	0.71805000

cis Pd-5

N	1.09241400	1.74600300	0.05818700
C	0.55199000	2.91551700	-0.06834600
H	1.24250600	3.76588900	-0.10581400
C	-0.82723800	3.25856100	-0.14175400
C	-1.13700800	4.63399500	-0.25744000
C	-1.88703000	2.30557800	-0.07726500
C	-2.42762400	5.08584600	-0.31173500
H	-0.31165900	5.34154900	-0.30109500
C	-3.21413700	2.80479400	-0.13389900
C	-3.47107100	4.14563600	-0.24824400
H	-4.01355500	2.07068600	-0.08976800
C	2.51166900	1.66383800	0.08980600
C	3.14847100	1.18437800	1.22933800
C	3.25818800	2.02415500	-1.02438400
C	4.52791500	1.09202800	1.26778600

H	2.54805800	0.87601800	2.07902100
C	4.64239800	1.92793600	-0.99963400
H	2.74815400	2.36278300	-1.92154200
C	5.25045000	1.46386100	0.14846400
H	5.05062500	0.72942700	2.14619200
H	5.24886700	2.19954000	-1.85664100
H	-2.64298600	6.14466900	-0.40076500
H	-4.50234000	4.48580900	-0.29119600
O	-1.74175600	1.03129800	0.03080500
N	-1.09241600	-1.74600400	0.05813600
C	-0.55199100	-2.91551500	-0.06841700
H	-1.24250600	-3.76588700	-0.10590900
C	0.82723700	-3.25855800	-0.14182700
C	1.13700300	-4.63398800	-0.25756600
C	1.88703100	-2.30558000	-0.07729100
C	2.42761800	-5.08584200	-0.31187500
H	0.31165300	-5.34153800	-0.30125400
C	3.21413600	-2.80480000	-0.13394100
C	3.47106800	-4.14563800	-0.24834000
H	4.01355700	-2.07069700	-0.08977500
C	-2.51167000	-1.66383800	0.08975100
C	-3.14847500	-1.18439600	1.22929000
C	-3.25818500	-2.02413100	-1.02444900
C	-4.52791900	-1.09204300	1.26773400
H	-2.54806300	-0.87605100	2.07898000
C	-4.64239500	-1.92791000	-0.99970200
H	-2.74814700	-2.36274500	-1.92161000
C	-5.25045000	-1.46385500	0.14840200
H	-5.05063100	-0.72945700	2.14614400
H	-5.24886100	-2.19949700	-1.85671700
H	2.64297600	-6.14466200	-0.40094600
H	4.50233500	-4.48581100	-0.29130200
O	1.74176200	-1.03130500	0.03083600
Pd	0.00000200	-0.00000500	0.07076000
F	-6.58658600	-1.36704100	0.18079500
F	6.58658600	1.36705000	0.18086000

cis Pd-6

N	-1.03292700	-1.77648300	0.18333300
C	-0.46213000	-2.93525800	0.12931200
H	-1.13025800	-3.80422600	0.10860300
C	0.92887500	-3.23998700	0.10692600
C	1.28408500	-4.60850700	0.07162500
C	1.95721400	-2.25036800	0.13220000
C	2.58945400	-5.01973600	0.06255500
H	0.48247800	-5.34401200	0.05443000
C	3.30100200	-2.70778800	0.12322800
C	3.60168200	-4.04376100	0.08973700
H	4.07284300	-1.94346400	0.14406700
C	-2.45581800	-1.72124300	0.18492600
C	-3.13639000	-1.46437500	1.36511700
C	-3.13916800	-1.87637800	-1.01337400
C	-4.52058800	-1.37647500	1.33514400
H	-2.57561900	-1.31213500	2.28134900
C	-4.52502600	-1.77745800	-1.02834400
H	-2.57983300	-2.04416100	-1.93188600
C	-5.22070300	-1.52773300	0.14894400
H	-5.06513200	-1.17865700	2.25337600
H	2.84036000	-6.07415500	0.03681700
H	4.64368700	-4.35264400	0.08403700
O	1.77246600	-0.97803700	0.16140600
N	1.03294400	1.77637300	0.18337900
C	0.46212400	2.93513200	0.12919400
H	1.13023700	3.80410800	0.10834200
C	-0.92888500	3.23984400	0.10684700

C	-1.28411000	4.60835600	0.07131700
C	-1.95721700	2.25022800	0.13245300
C	-2.58948400	5.01957300	0.06232400
H	-0.48251200	5.34386400	0.05387800
C	-3.30101000	2.70763500	0.12358300
C	-3.60170300	4.04359800	0.08984800
H	-4.07283400	1.94330200	0.14469500
C	2.45582900	1.72115300	0.18487800
C	3.13645900	1.46348400	1.36486500
C	3.13914100	1.87712900	-1.01333800
C	4.52065400	1.37564400	1.33478100
H	2.57572400	1.31058500	2.28100900
C	4.52500200	1.77825800	-1.02842800
H	2.57977300	2.04550900	-1.93172200
C	5.22072700	1.52773700	0.14865900
H	5.06523500	1.17720100	2.25285600
H	-2.84039900	6.07398400	0.03639400
H	-4.64371000	4.35247500	0.08422500
O	-1.77245900	0.97790200	0.16185200
Pd	0.00000800	-0.00006300	0.18648000
O	-5.24970500	-1.91676400	-2.16688900
H	-4.66124200	-2.03972000	-2.91658600
O	5.24963200	1.91836700	-2.16690700
H	4.66113300	2.04181500	-2.91649500
H	-6.30241600	-1.45383100	0.11117700
H	6.30243900	1.45387900	0.11080300