Electronic Supplementary Information

Potent cyclometalled Pd (II) antitumor complexes bearing α-amino acids: Synthesis, structural characterization, DNA/BSA binding, cytotoxicity and molecular dynamics simulation

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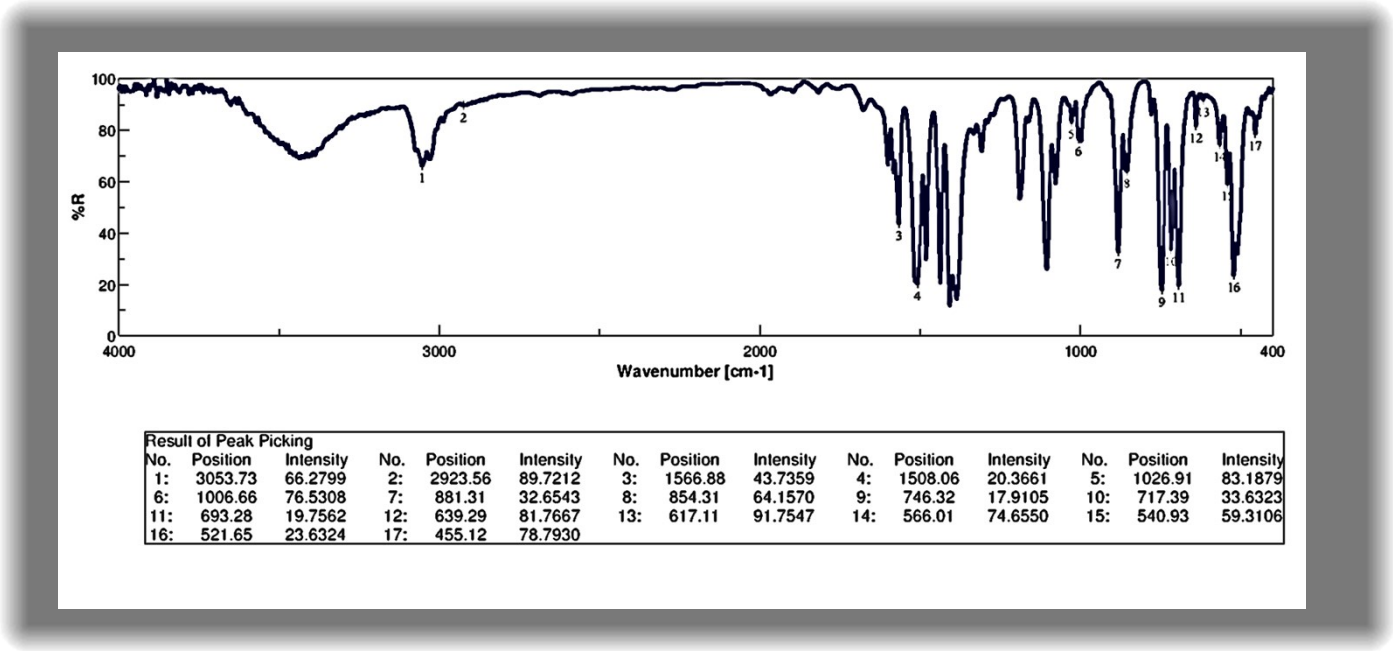


Result of Peak Picking

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1:	3053.73	66.2799	2:	2923.56	89.7212	3:	1566.88	43.7359	4:	1508.06	20.3661	5:	1026.91	83.1879
6:	1006.66	76.5308	7:	881.31	32.6543	8:	854.31	64.1570	9:	746.32	17.9105	10:	717.39	33.6323
11:	693.28	19.7562	12:	639.29	81.7667	13:	617.11	91.7547	14:	566.01	74.6550	15:	540.93	59.3106
16:	521.65	23.6324	17:	455.12	78.7930									

Figure S1. FT-IR spectrum of ylide ligand.

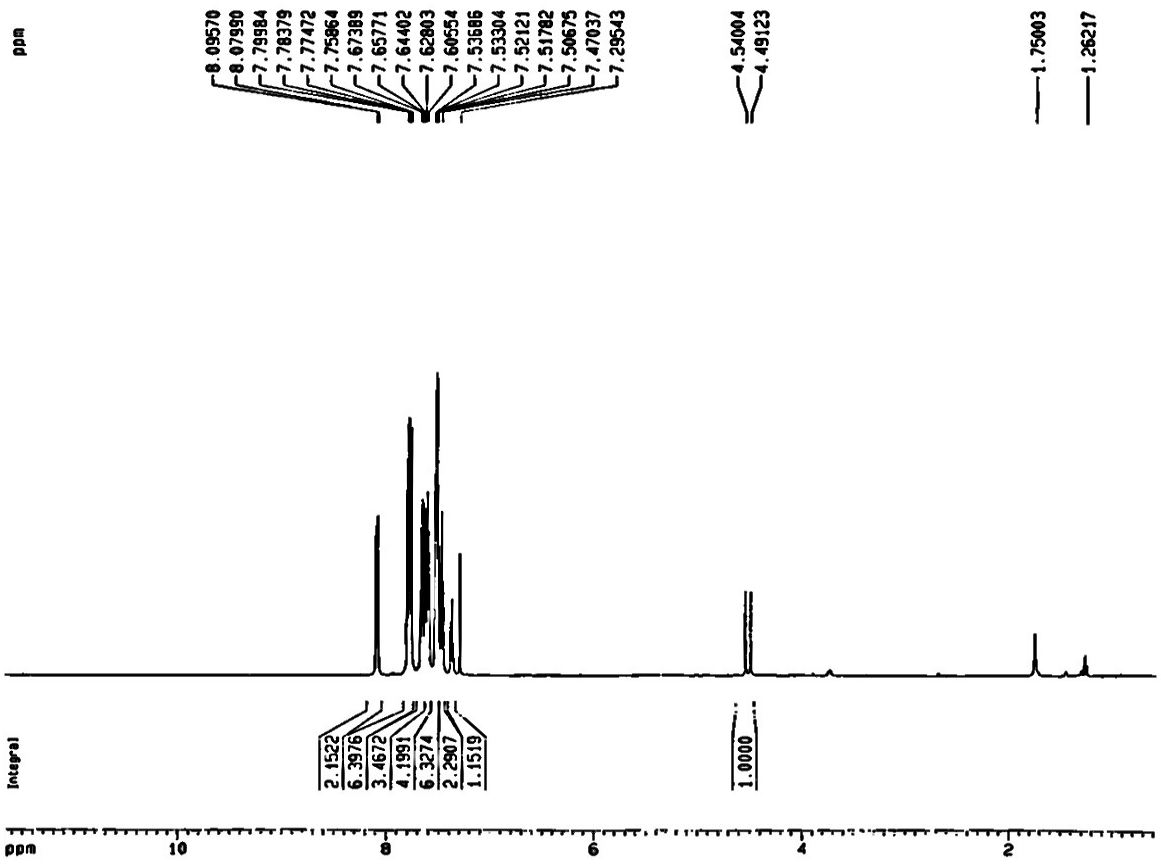


Figure S2. ^{1}H NMR spectrum of ylide ligand in $CDCl_3$ at room temperature.

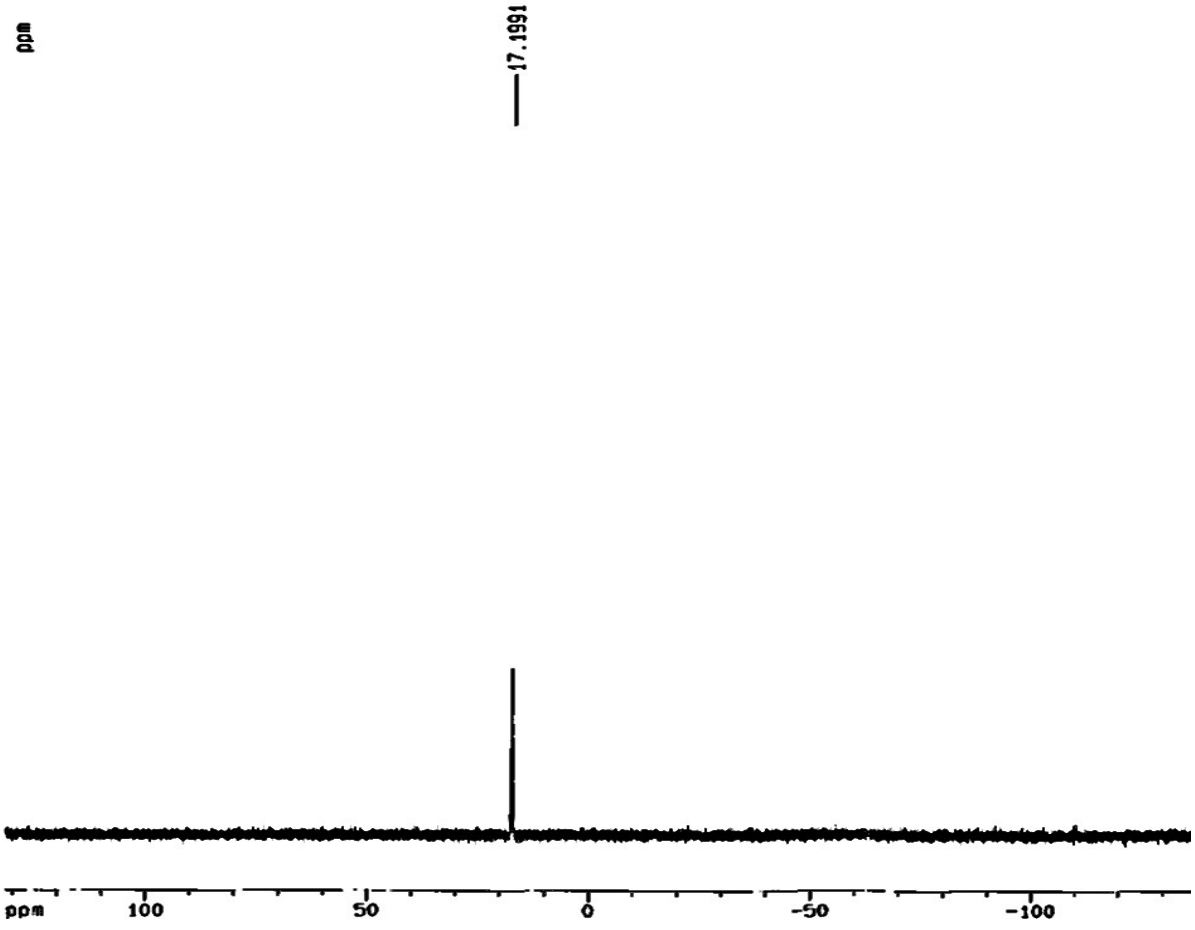
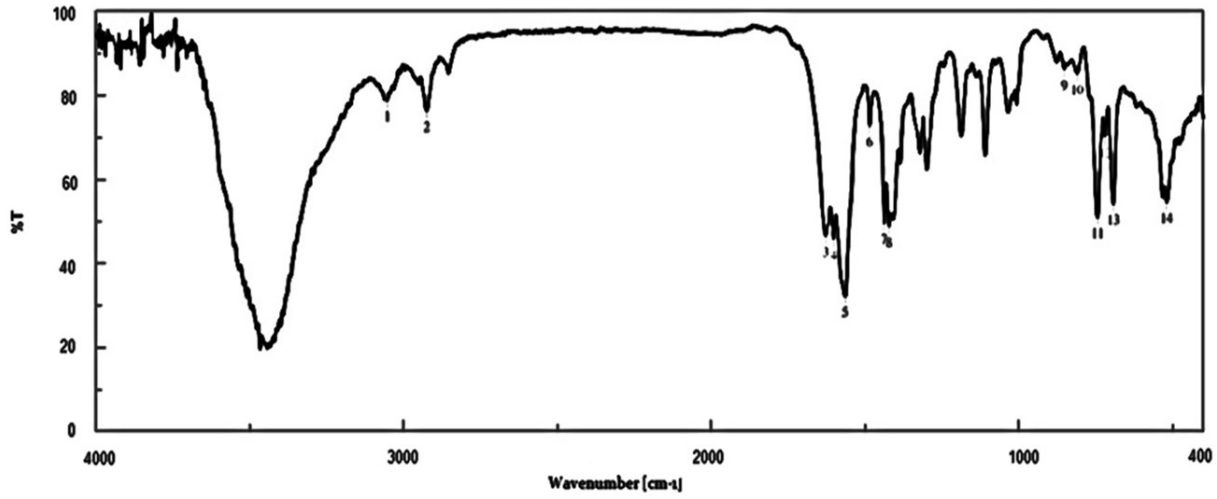
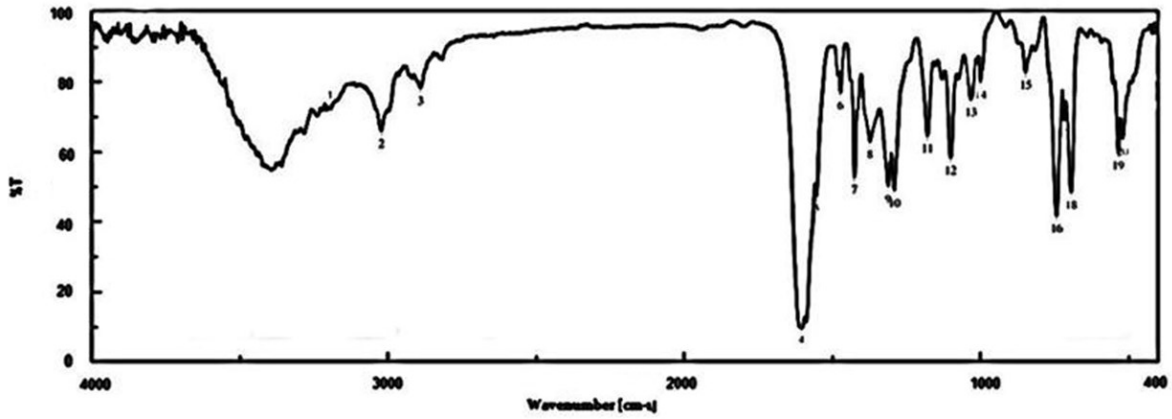


Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of ylide ligand in $CDCl_3$ at room temperature.



Result of Peak Picking												
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1:	3052.76	78.5240	2:	2924.52	75.3023	3:	1626.66	43.3499	4:	1601.59	42.0132
5:	1563.99	33.2071	6:	1483.96	70.5048	7:	1436.71	47.8768	8:	1421.28	47.5345
9:	851.42	84.2311	10:	809.96	82.6911	11:	743.42	46.6169	12:	719.32	68.1446
13:	692.32	50.2191	14:	518.76	51.3982						

Figure S4. FT-IR spectrum of dinuclear ylide palladacycle



Result of Peak Picking												
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1:	3232.11	73.1965	2:	3057.58	65.5504	3:	2923.56	77.6717	4:	1618.96	10.3999
5:	1566.88	44.6860	6:	1484.92	74.7020	7:	1436.71	52.7064	8:	1383.68	61.2251
9:	1321.96	49.7196	10:	1300.75	47.8549	11:	1186.97	62.5425	12:	1107.90	60.7642
13:	1038.48	72.2283	14:	1005.70	79.9275	15:	851.42	82.0512	16:	745.35	42.4436
17:	719.32	67.7553	18:	696.21	47.4153	19:	534.19	61.9037	20:	518.76	63.7632

Figure S5. FT-IR spectrum of **Pd-F**

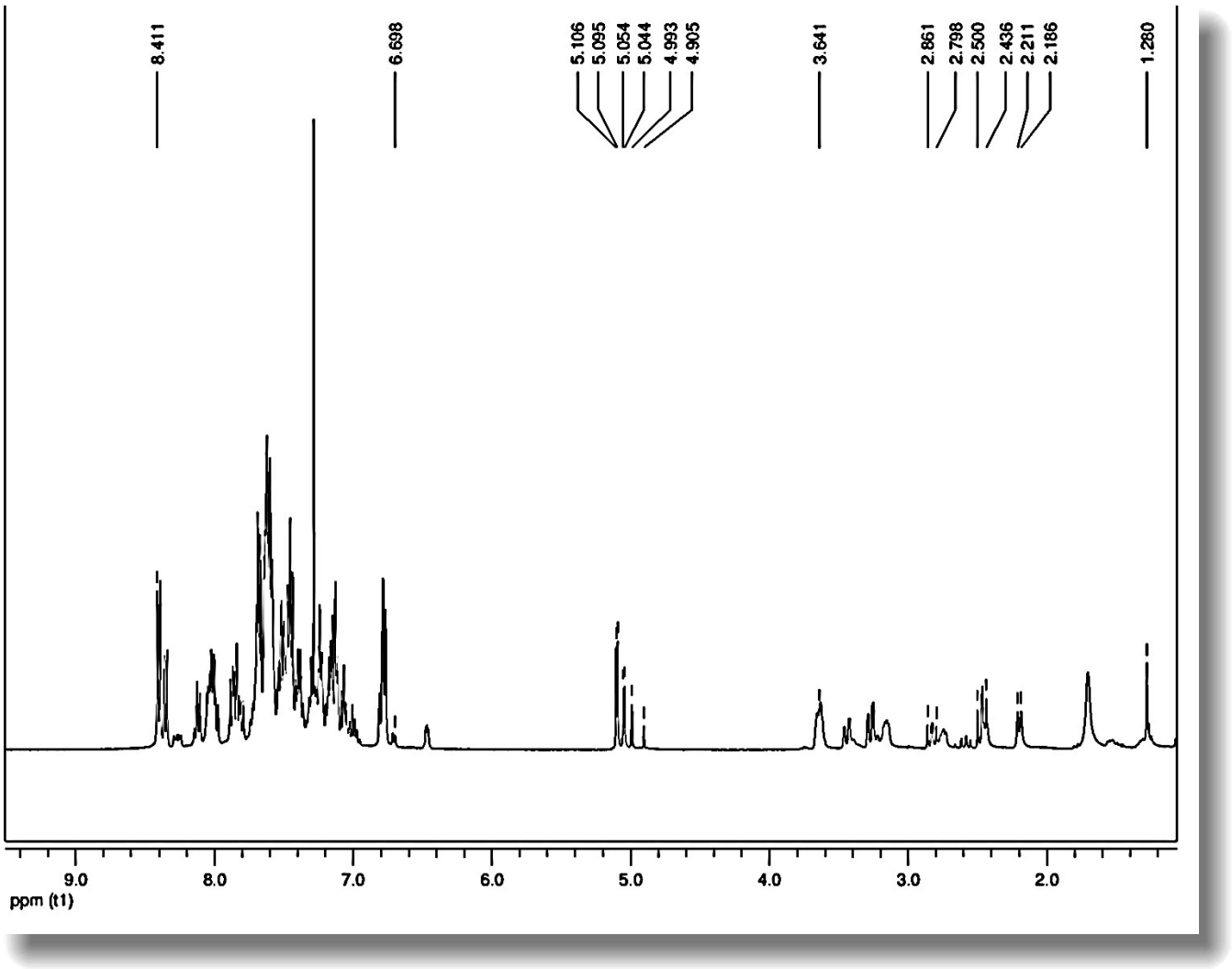
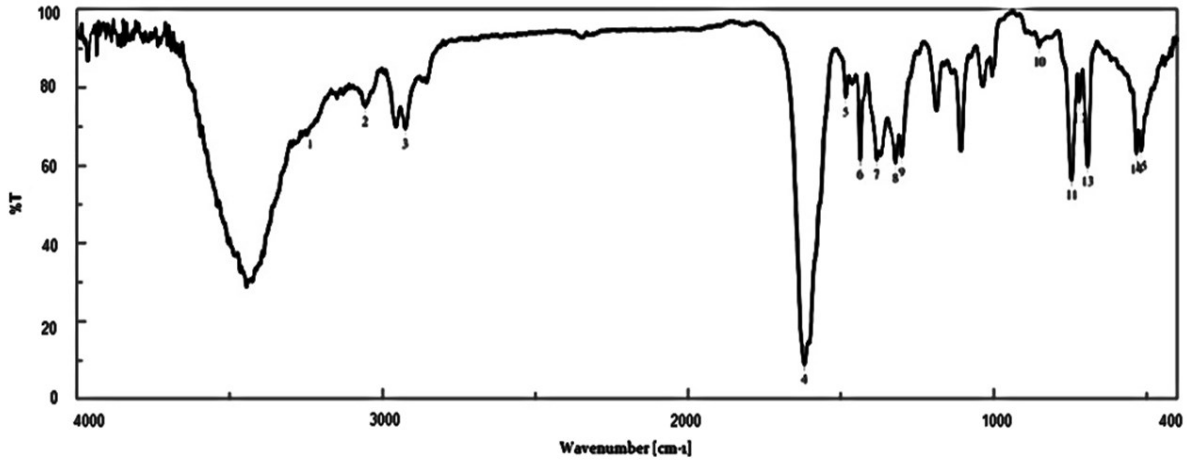


Figure S6. ^{1}H NMR spectrum of **Pd-F** in $CDCl_3$ at room temperature.



Result of Peak Picking												
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1:	3236.93	68.8397	2:	3056.62	75.6448	3:	2925.48	70.8178	4:	1619.91	8.5749
5:	1483.96	78.8414	6:	1436.71	60.8866	7:	1383.68	61.8124	8:	1321.96	60.3890
9:	1300.75	63.2098	10:	851.42	90.3352	11:	745.35	58.2539	12:	719.32	76.0670
13:	693.28	60.9841	14:	533.22	65.5526	15:	517.79	65.9078			

Figure S7. FT-IR spectrum of **Pd-V**

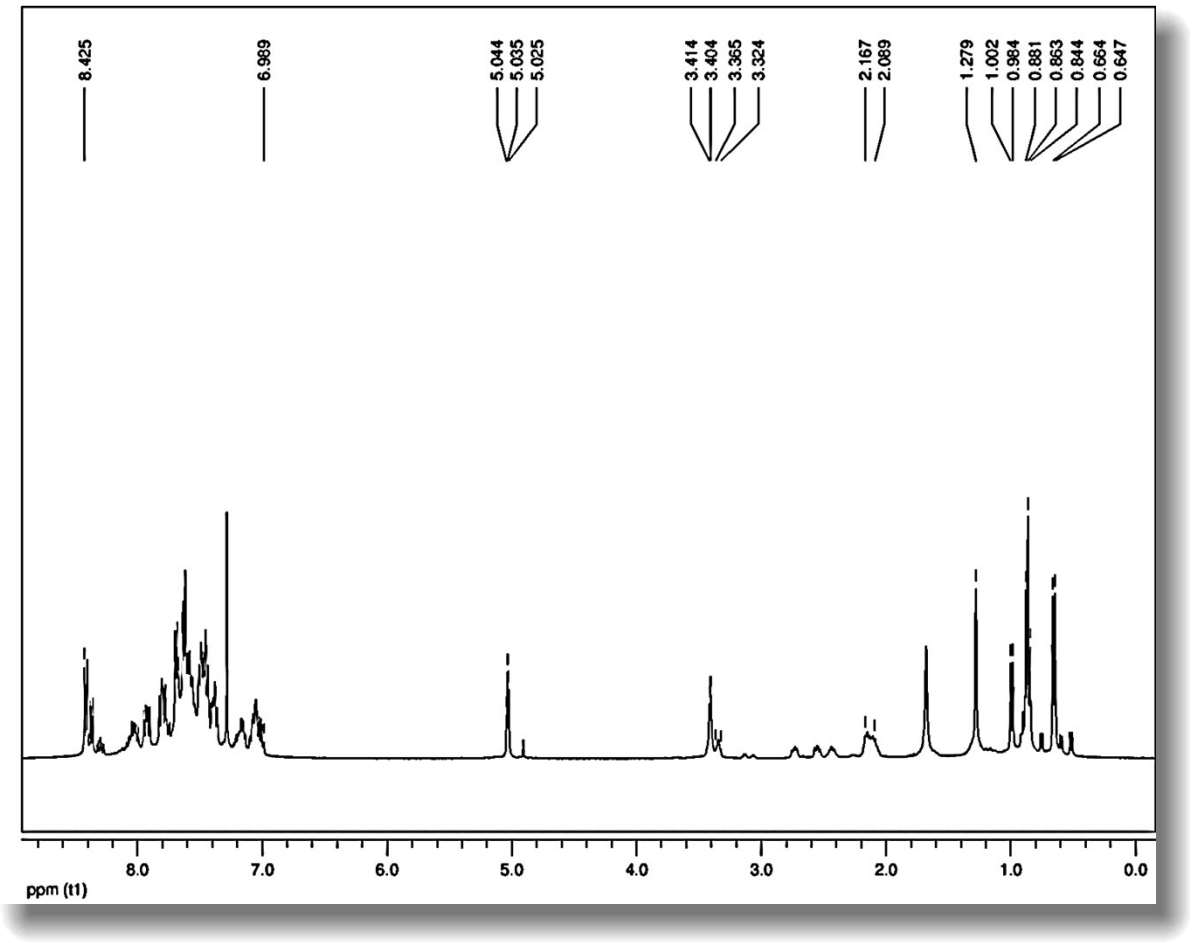
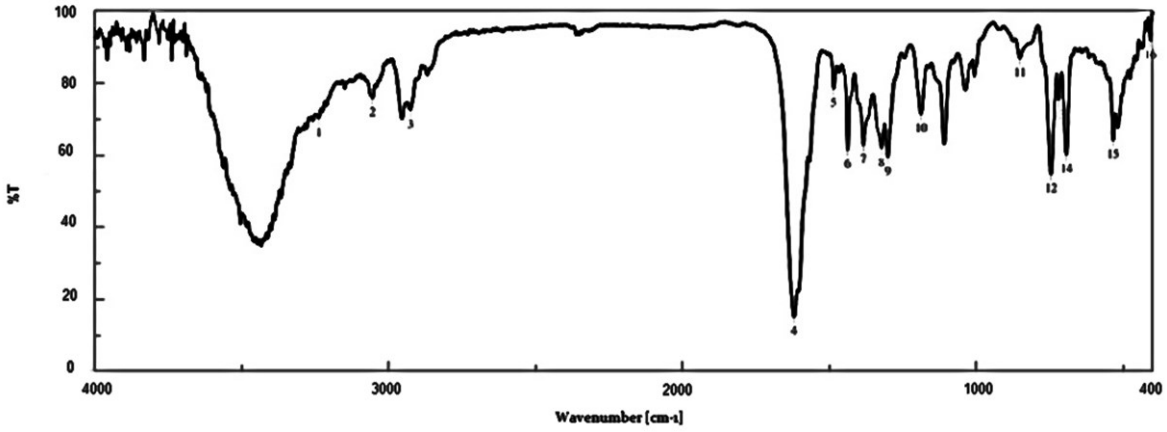


Figure S8. ^{1}H NMR spectrum of **Pd-V** in $CDCl_3$ at room temperature.



Result of Peak Picking												
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1:	3236.93	69.2208	2:	3054.69	74.0300	3:	2925.48	72.3635	4:	1619.91	14.6495
5:	1483.96	75.3263	6:	1436.71	59.9066	7:	1383.68	61.5247	8:	1321.96	61.0451
9:	1300.75	60.8150	10:	1187.94	69.8372	11:	851.42	88.5585	12:	745.35	53.4646
13:	719.32	72.6676	14:	693.28	59.2243	15:	534.19	63.1967	16:	407.87	92.9936

Figure S9. FT-IR spectrum of **Pd-L**

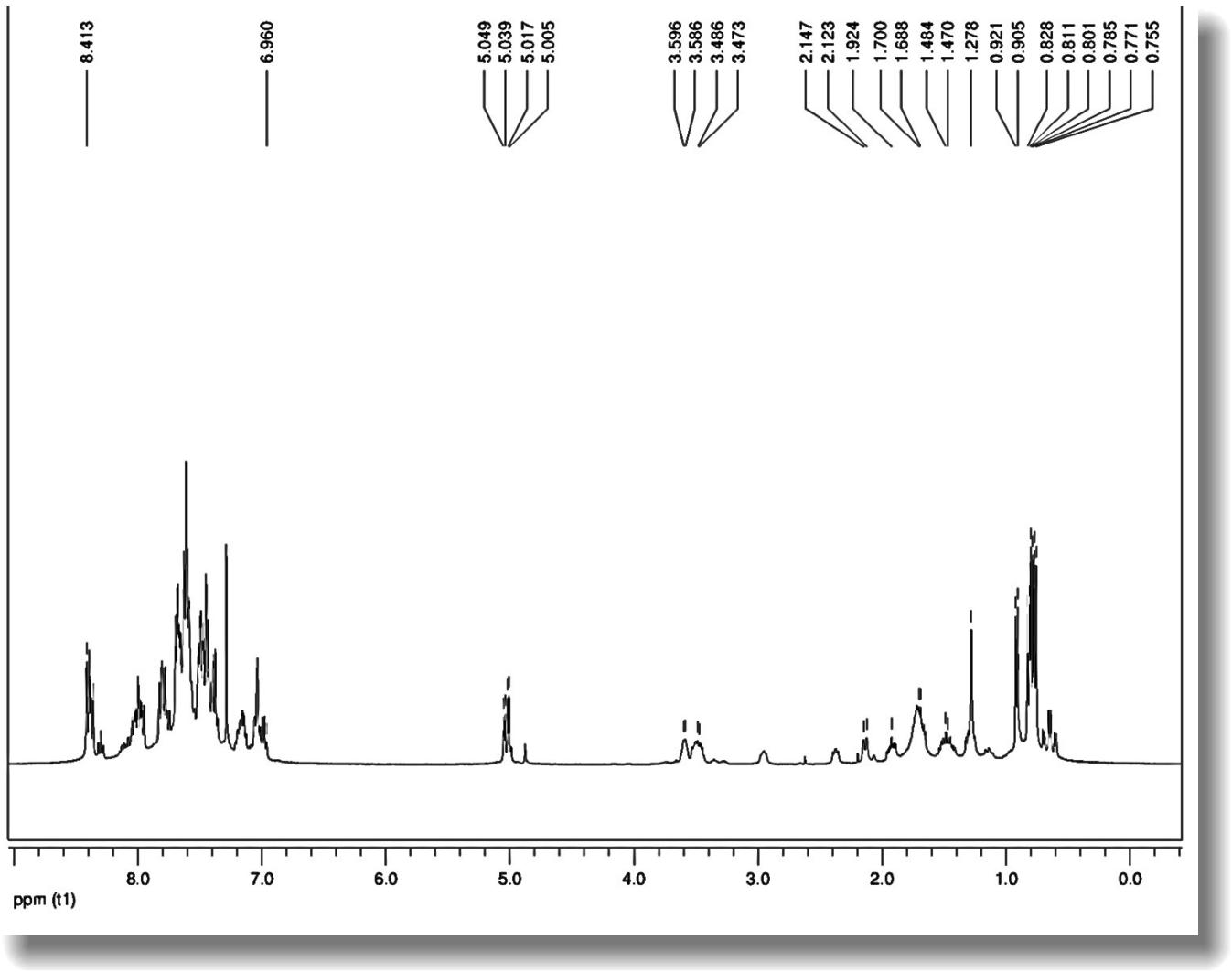


Figure S10. ^{1}H NMR spectrum of **Pd-L** in $CDCl_3$ at room temperature.

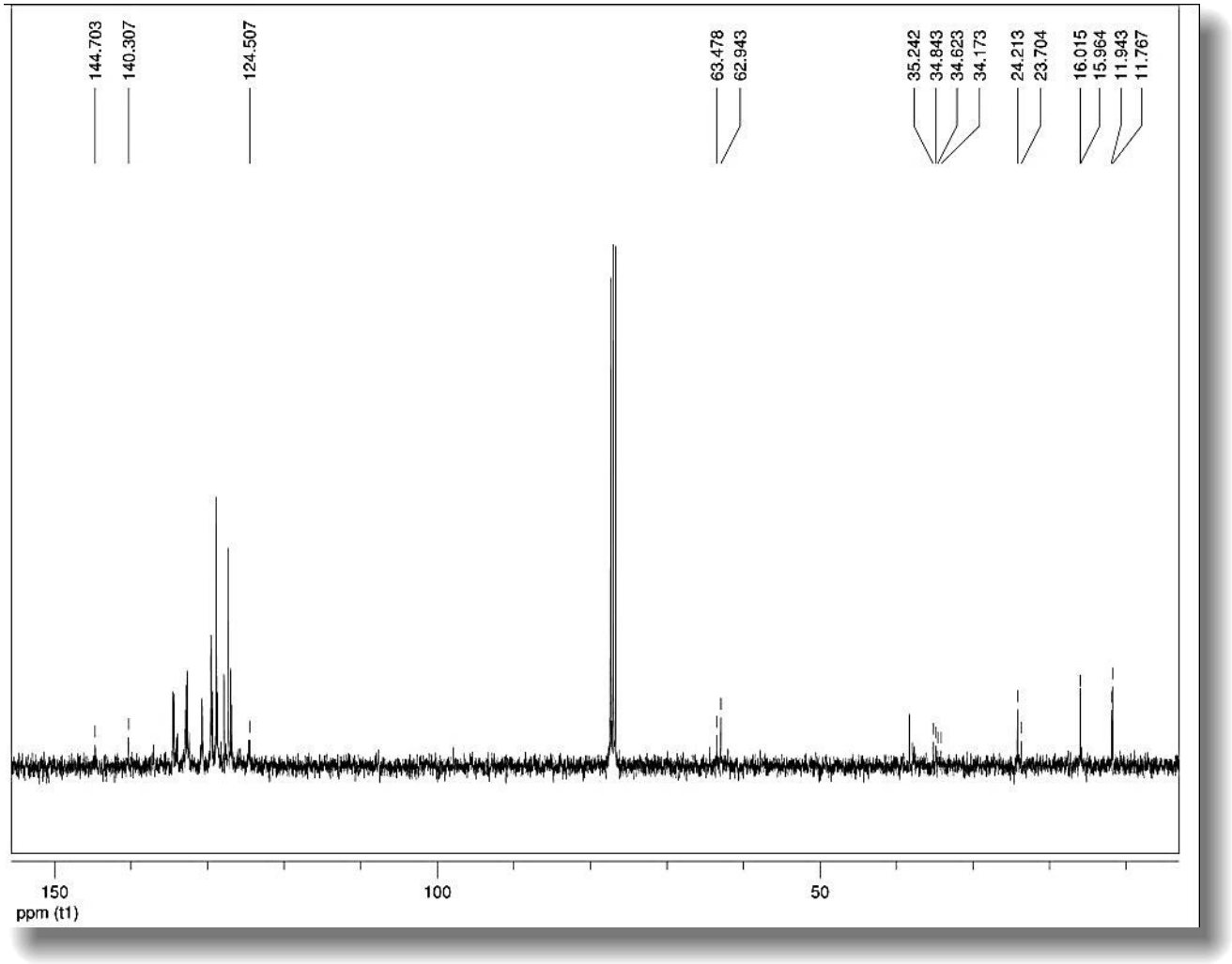


Figure S11. ^{13}C-{^{1}H} NMR spectrum of **Pd-L** in $CDCl_3$ at room temperature.

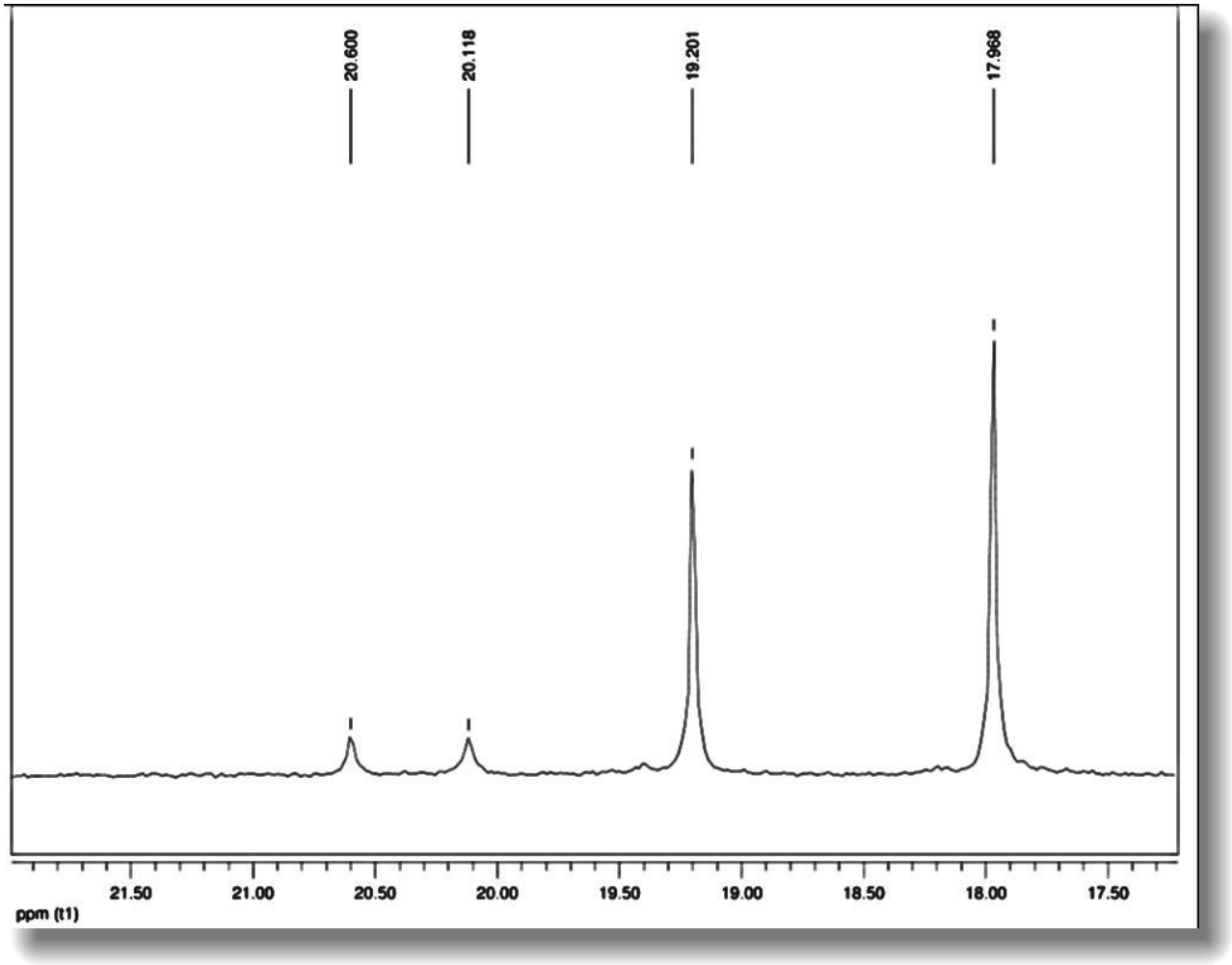
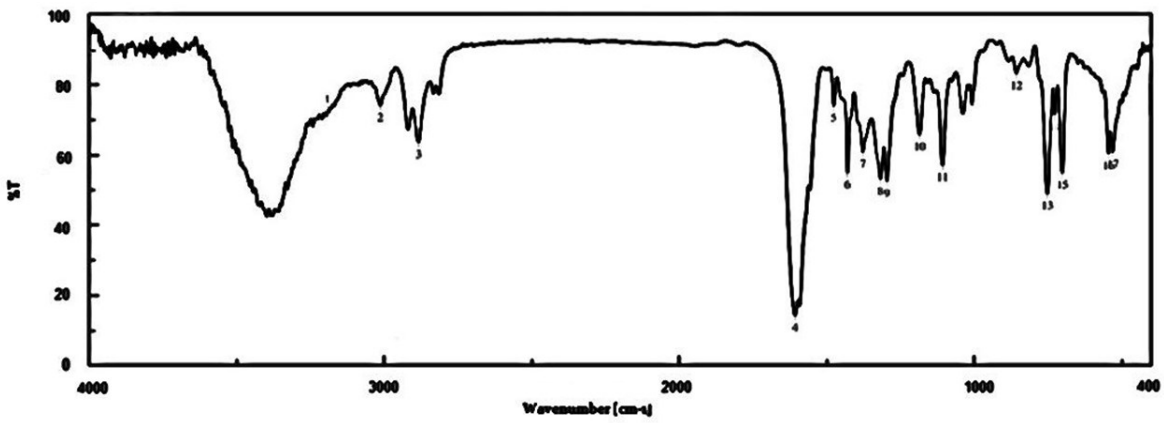


Figure S12. ^{31}P-$\{^{1}H\}$ NMR spectrum (expansion) of **Pd-L** in $CDCl_3$ at room temperature.



Result of Peak Picking

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1:	3238.86	71.4566	2:	3055.66	75.8120	3:	2923.56	64.7972	4:	1618.95	13.5965
5:	1483.96	74.7596	6:	1436.71	54.0159	7:	1383.68	62.9768	8:	1322.93	51.7243
9:	1300.75	51.3200	10:	1187.94	67.2505	11:	1107.90	59.3889	12:	852.38	85.9677
13:	745.35	48.9435	14:	719.32	72.9277	15:	693.28	53.9626	16:	533.22	60.6382
17:	517.79	60.8948									

Figure S13. FT-IR spectrum of **Pd-I**

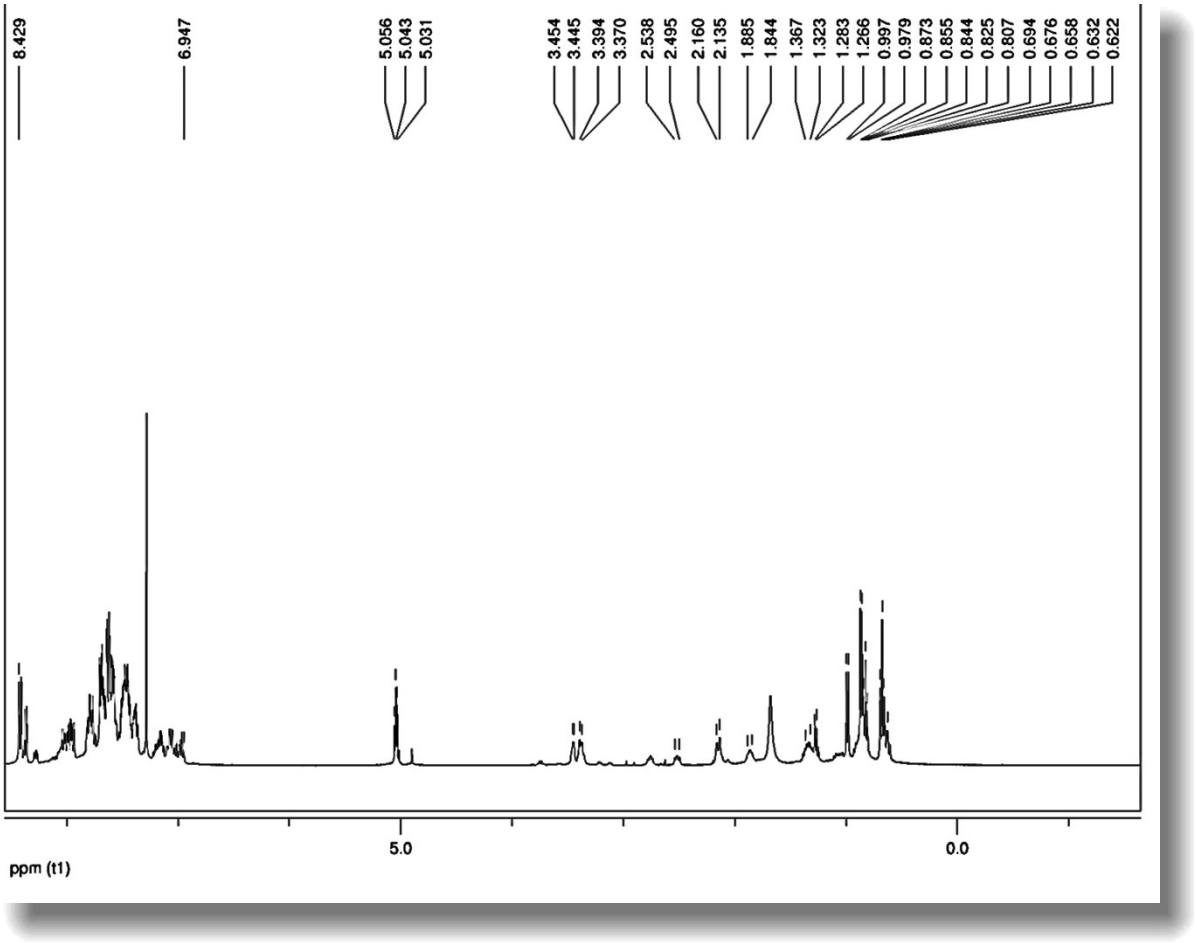


Figure S14. ^{1}H NMR spectrum of **Pd-I** in $CDCl_3$ at room temperature.

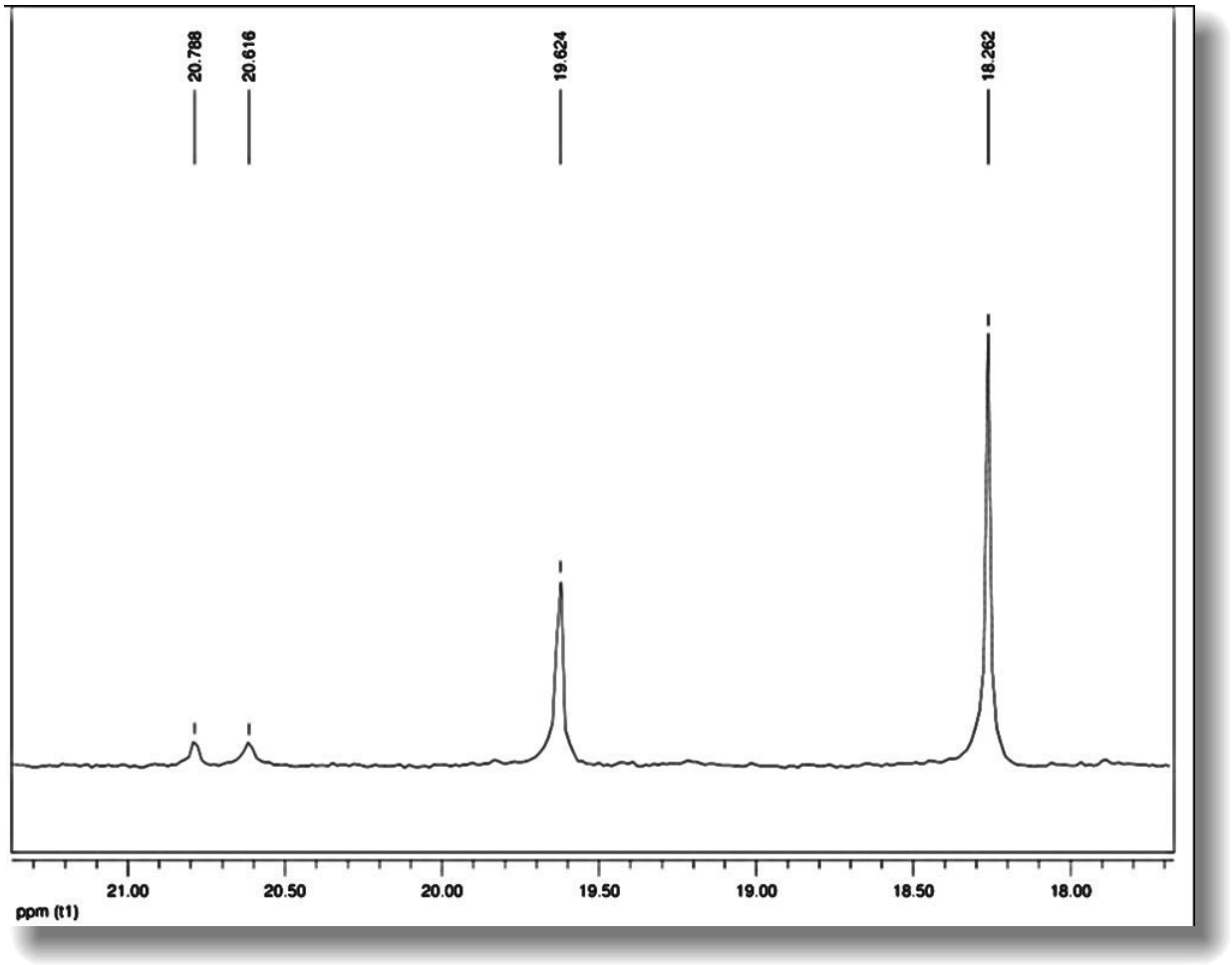
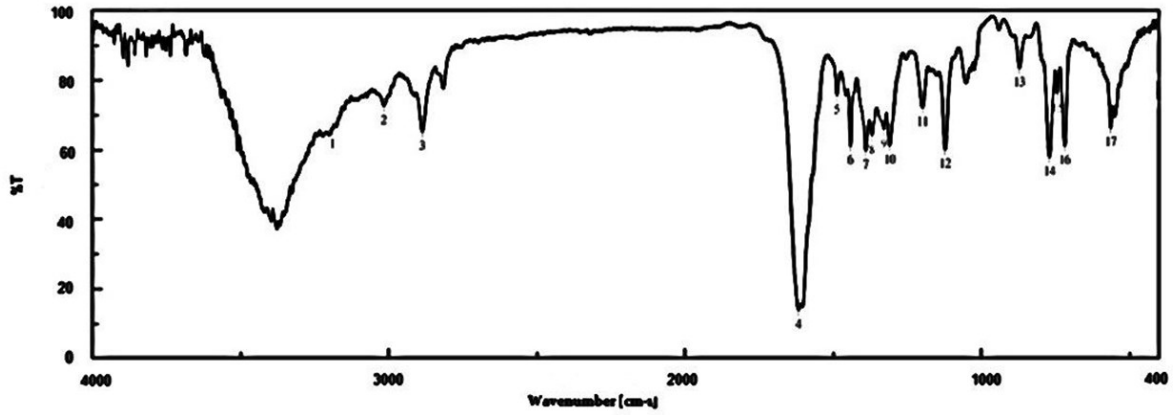


Figure S15. ^{31}P-{^{1}H} NMR spectrum (expansion) of **Pd-I** in $CDCl_3$ at room temperature.



Result of Peak Picking

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1:	3236.93	63.8176	2:	3058.55	72.7119	3:	2924.52	63.4432	4:	1617.02	15.6650
5:	1483.96	78.5100	6:	1436.71	61.1186	7:	1383.68	60.3101	8:	1362.46	62.7457
9:	1321.96	63.8063	10:	1300.75	61.1425	11:	1186.97	72.4522	12:	1108.87	60.4609
13:	850.45	85.0784	14:	746.32	59.2041	15:	719.32	78.6663	16:	693.28	61.0861
17:	533.22	64.1202									

Figure S16. FT-IR spectrum of **Pd-A**

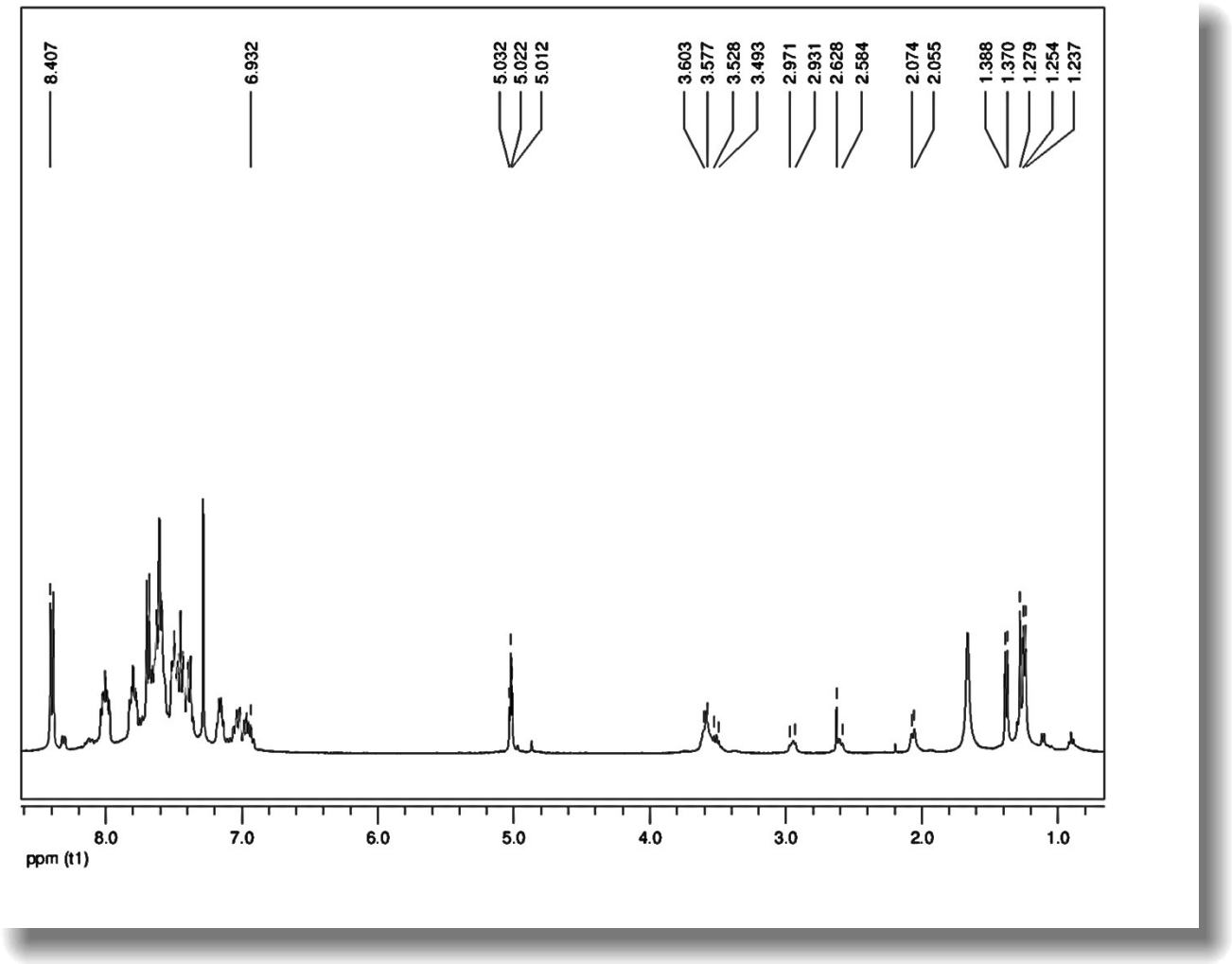


Figure S17. ^{1}H NMR spectrum of **Pd-A** in $CDCl_3$ at room temperature.

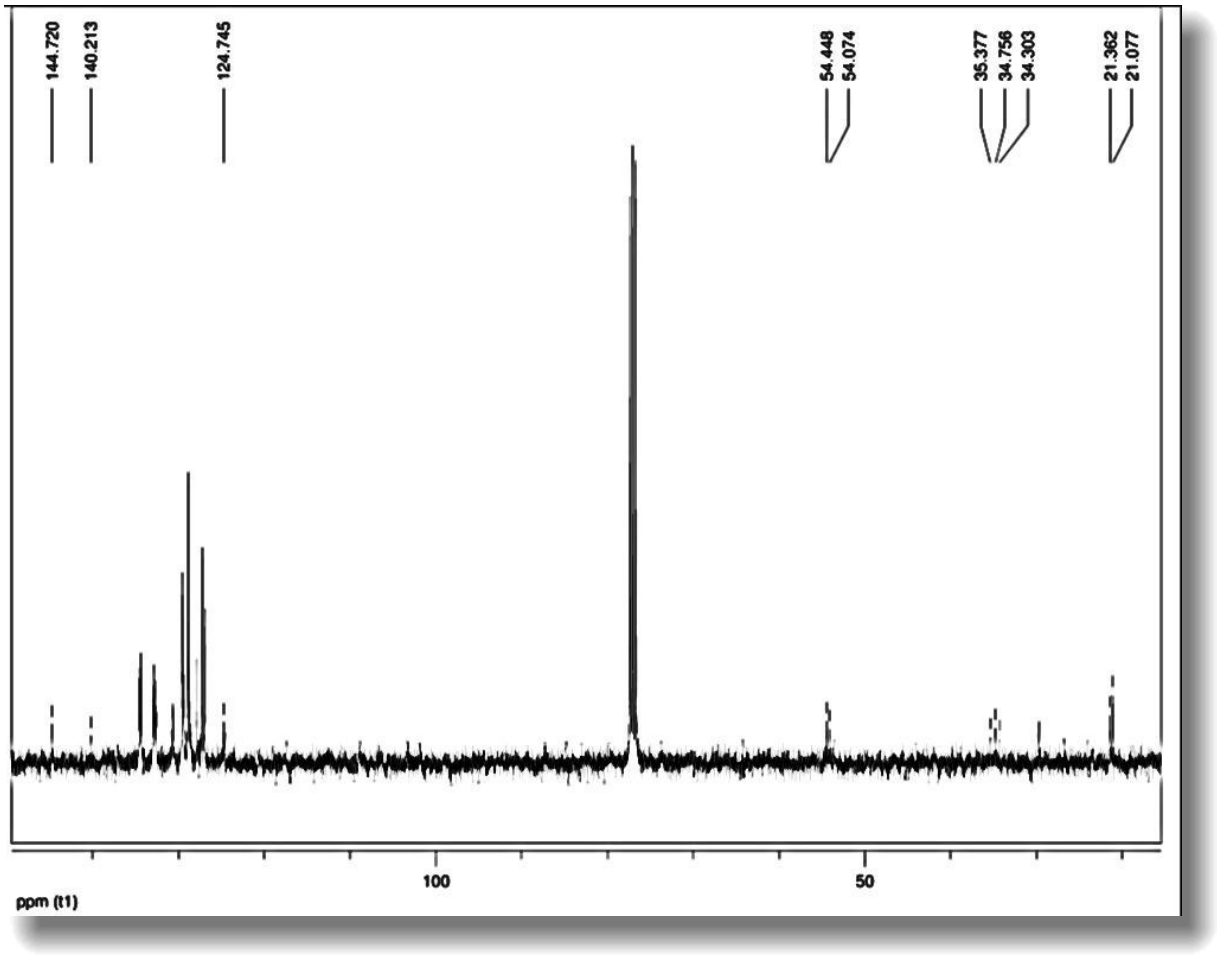


Figure S18. ^{13}C-{^{1}H} NMR spectrum of **Pd-A** in $CDCl_3$ at room temperature.

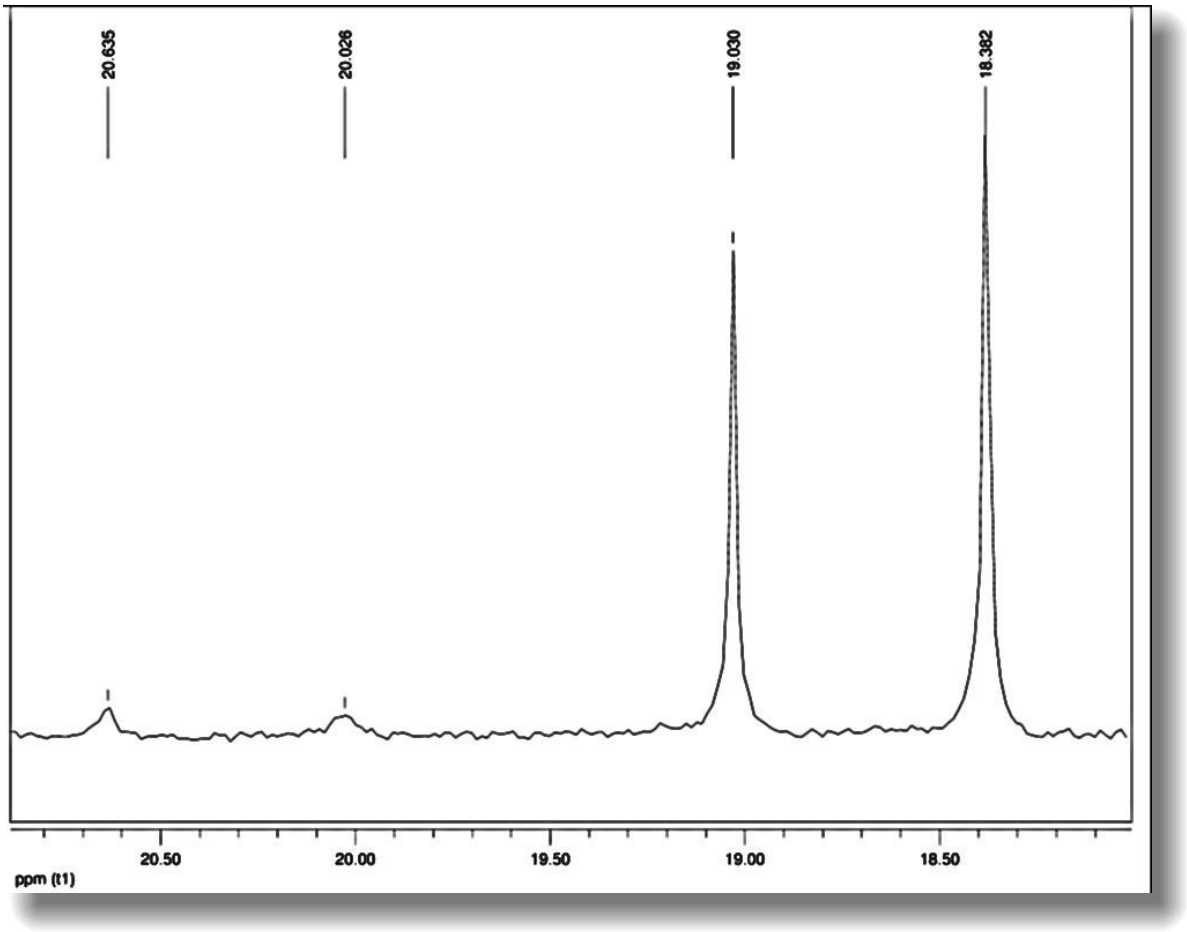


Figure S19. ^{31}P-{^{1}H} NMR spectrum of **Pd-A** in $CDCl_3$ at room temperature.

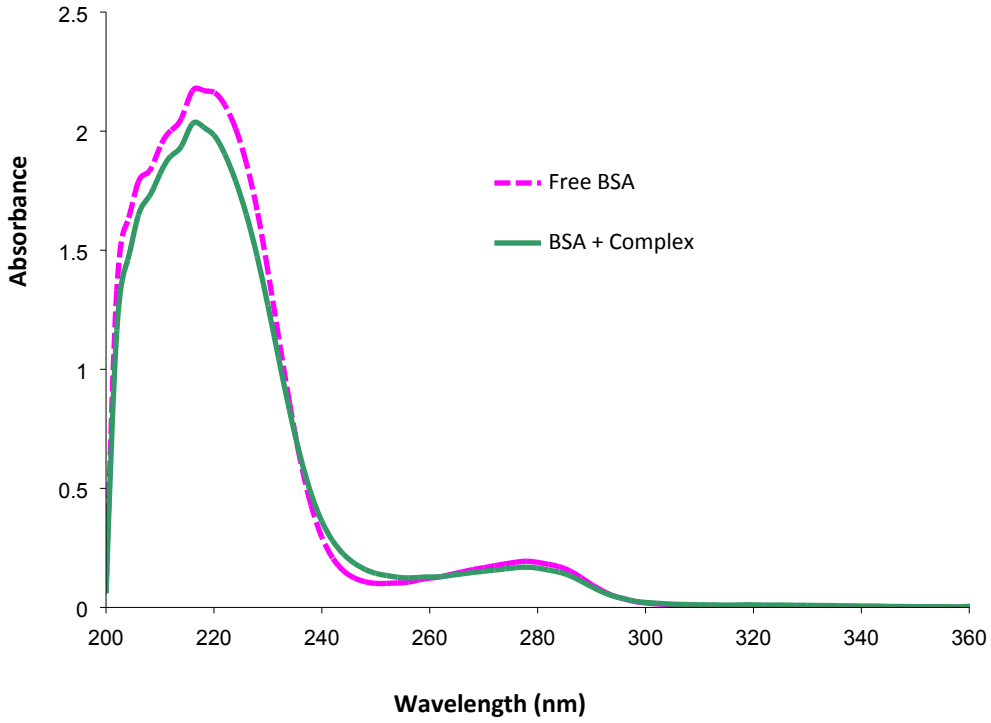


Figure S20. UV absorption spectra of *C*(BSA)=2×10^{-6} M in the absence and presence of **Pd-F**. *C*(complex)= 0-6×10^{-6} M in 5 mM Tris-HCl with 50 Mm NaCl.

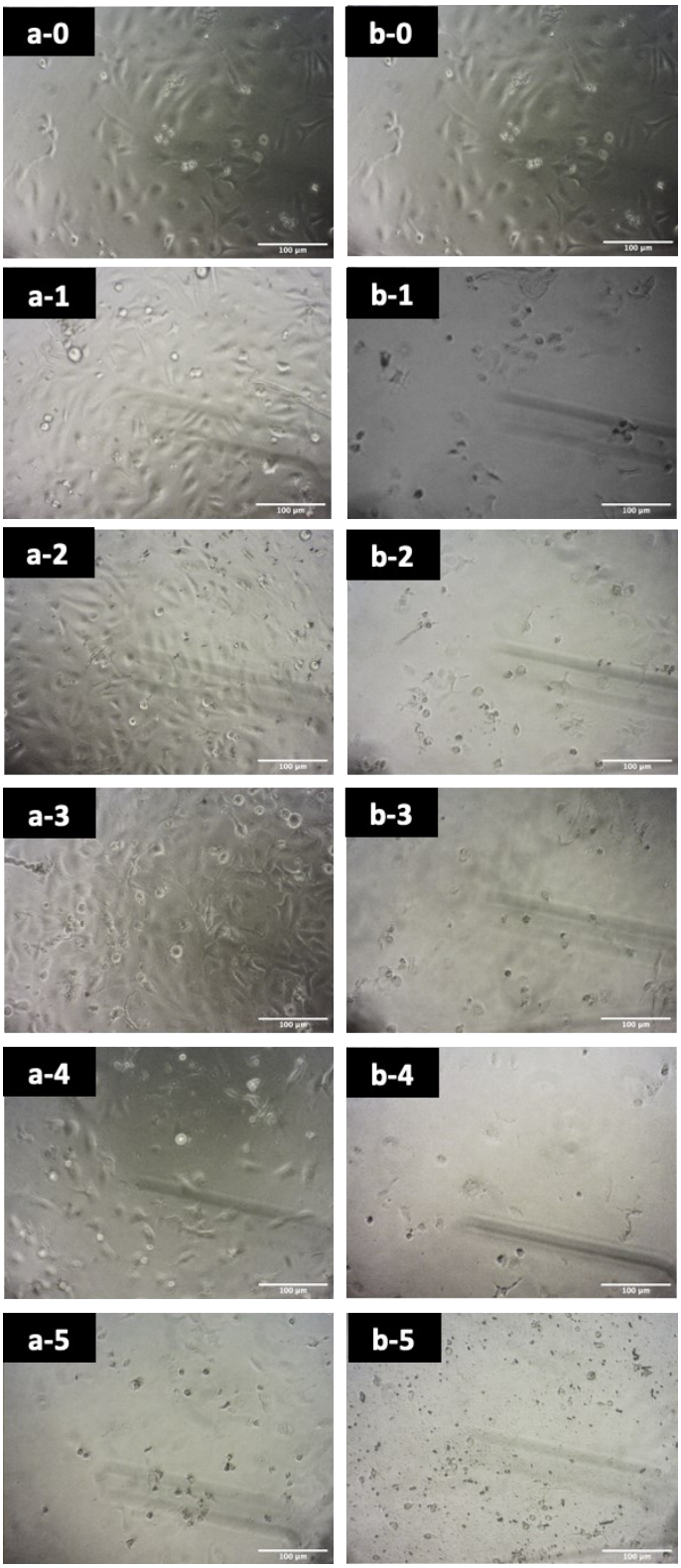


Figure S21. Morphological evaluation of **Pd-F** treated normal HUVEC cell, (0: Control, 1: 5 µg/ml, 2: 10 µg/ml, 3: 15 µg/ml, 4: 25 µg/ml and 5: 50 µg/ml).