Supporting Information

belonging to

Functionalized bis(NHC)-Palladium(II) Complexes via a Post-modification Approach

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Table S1. Selected X-ray crystallographic data for complexes **1a**, **3a·2CH$_3$CN** and **7a**.

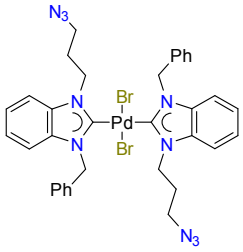
	1a	**3a·2CH$_3$CN**	**7a**
formula	$C_{34}H_{34}Br_4N_4Pd$	$C_{38}H_{40}Br_2N_4O_4Pd \cdot 2CH_3CN$	$C_{58}H_{54}N_4PdS_4$
fw	924.69	965.07	1041.69
color, habit	yellow, block	colourless, rod	orange, block
cryst size [mm]	0.50×0.42×0.26	0.37×0.13×0.07	0.36×0.20×0.10
temp [K]	100(2)	100(2)	100(2)
crystsyst	monoclinic	monoclinic	triclinic
space group	*P*2(1)/n	*P*2(1)/n	*P*-1
a[Å]	10.5266(13)	8.4490(4)	10.6360(9)
b [Å]	8.2026(10)	23.3113(12)	11.3645(9)
c [Å]	19.370(2)	10.4417(4)	11.4680(10)
α [deg]	90.00	90.00	76.226(2)
β [deg]	96.087(3)	94.643(2)	66.087(2)
γ [deg]	90.00	90.00	76.168(2)
V [Å^3]	1663.1(3)	2049.82(16)	1214.77(18)
Z	2	2	1
D_c [g cm^{-3}]	1.847	1.564	1.424
radiation used	Mo Kα	Mo Kα	Mo Kα
μ [mm^{-1}]	5.394	2.451	0.598
θ range [deg]	2.11–27.49	2.14–28.35	1.87–27.49
no. of unique data	11359	20988	16132
max., min. transmn	0.3345, 0.1734	0.7457, 0.6185	0.7456, 0.6211
final R indices	R_1 = 0.0393,	R_1 = 0.0387	R1 = 0.0398,
[$I > 2\sigma(I)$]	wR_2 = 0.1072	wR_2 = 0.0735	wR2 = 0.1038
R indices (all data)	R_1 = 0.0469,	R_1 = 0.0661	R1 = 0.0444,
	wR_2 = 0.1110	wR_2 = 0.0801	wR2 = 0.1079
goodness-of-fit	1.049	1.033	1.076
peak/hole [e Å^{-3}]	1.489/–1.234	0.613/–1.002	0.902/–0.514

Table S2. Selected X-ray crystallographic data for complexes **7b**, **8a** and **9a**.

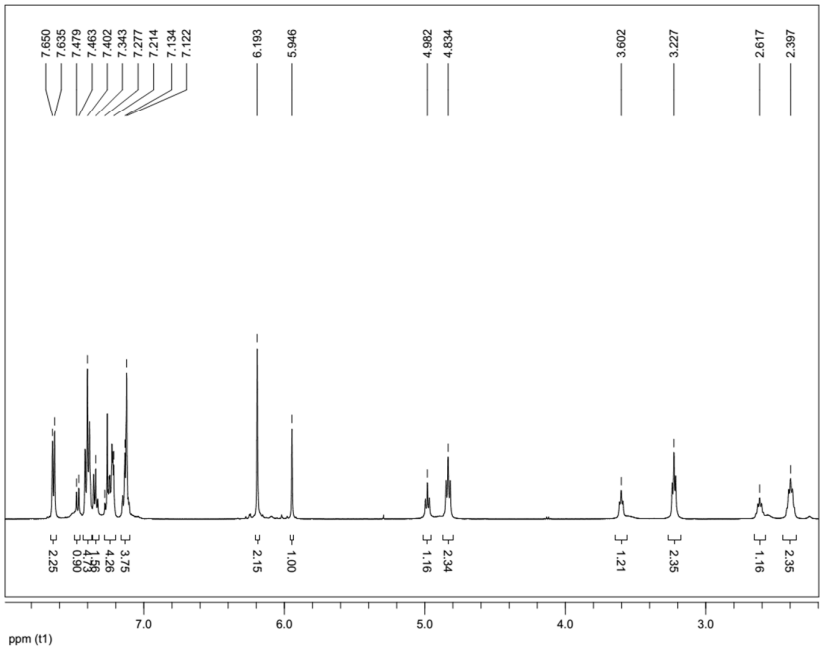
	7b	**8a**	**9a**
formula	$C_{50}H_{50}N_4PdS_4$	$C_{38}H_{34}N_8PdS_4$	$C_{36}H_{22}Br_2N_6PdS_2$
fw	941.58	837.37	868.93
color, habit	yellow, plate	yellow, block	Pale-yellow, block
cryst size [mm]	0.36×0.14×0.12	0.54×0.34×0.14	0.14×0.12×0.04
temp [K]	100(2)	223(2)	100(2)
crystsyst	triclinic	monoclinic	monoclinic
space group	*P*-1	*P*2(1)/n	*C*2/c
a[Å]	9.0012(18)	10.9426(8)	25.707(3)
b [Å]	11.220 (2)	9.6095(7)	9.3604(12)
c [Å]	12.316(2)	18.7276(14)	16.538(2)
α [deg]	73.186(6)	90.00	90.00
β [deg]	75.788(6)	103.262(2)	116.555(4)
γ [deg]	69.685(6)	90.00	90.00
V [Å^3]	1101.9(4)	1916.7(2)	3559.7 (8)
Z	1	2	4
D_c [g cm^{-3}]	1.419	1.451	1.621
radiation used	Mo Kα	Mo Kα	Mo Kα
μ [mm^{-1}]	0.651	0.741	2.918
θ range [deg]	2.33–27.50	1.98–27.50	2.35–27.50
no. of unique data	39984	13088	25486
max., min. transmn	0.7457, 0.7005	0.9033, 0.6903	0.7457, 0.6576
final R indices	R_1 = 0.0231,	R_1 = 0.0564,	R1 = 0.0501,
[I> 2σ(I)]	wR_2 = 0.0564	wR_2 = 0.1302	wR2 = 0.1304
R indices (all data)	R_1 = 0.0252,	R_1 = 0.0694,	R1 = 0.0693,
	wR_2 = 0.0572	wR_2 = 0.1367	wR2 = 0.1404
goodness-of-fit	1.044	1.130	1.047
peak/hole [e Å^{-3}]	1.355/–0.287	1.127/–0.674	1.902/–1.902

Table S3. Selected X-ray crystallographic data for complexes **13.**

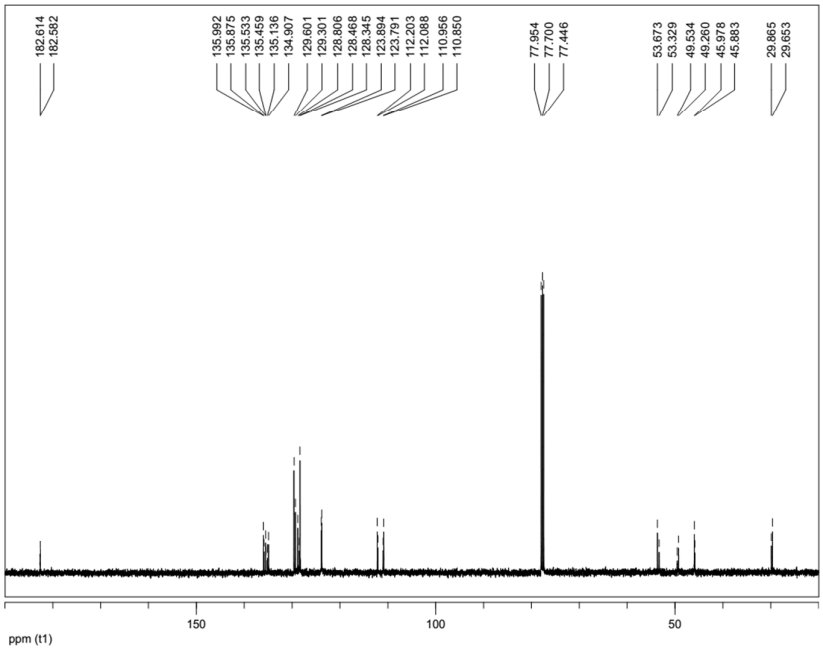
	13
formula	$C_{36}H_{34}I_2N_6PdS_2$
fw	975.01
color, habit	yellow, block
cryst size [mm]	0.40×0.40×0.40
temp [K]	100(2)
crystsyst	monoclinic
space group	*P*2(1)/n
a[Å]	7.8570(10)
b [Å]	20.915(3)
c [Å]	11.3480(15)
α [deg]	90.00
β [deg]	109.728(3)
γ [deg]	90.00
V [Å^3]	1755.3(4)
Z	2
D_c [g cm^{-3}]	1.845
radiation used	Mo Kα
μ [mm^{-1}]	2.442
θ range [deg]	1.95–27.50
no. of unique data	12380
max., min. transmn	0.7673, 0.6022
final R indices	R_1 = 0.0294,
[$I > 2\sigma(I)$]	wR_2 = 0.0725
R indices (all data)	R_1 = 0.0306,
	wR_2 = 0.0731
goodness-of-fit	1.141
peak/hole [e Å^{-3}]	1.284/–0.457

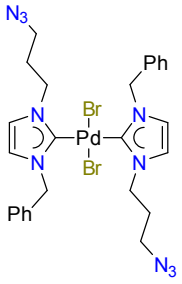


Compound **5a**, ^{1}H NMR spectrum (500 MHz, $CDCl_3$):

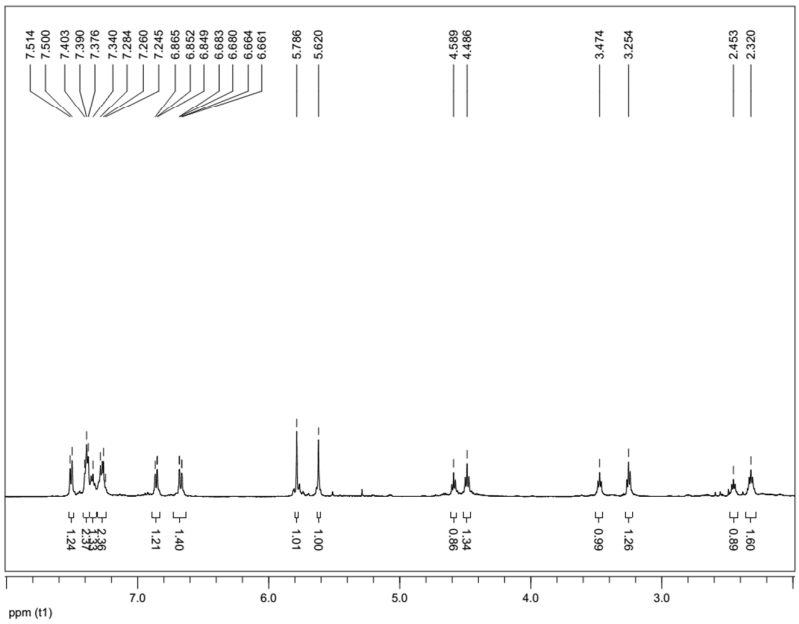


Compound **5a**, ^{13}C NMR spectrum (125.77 MHz, $CDCl_3$):

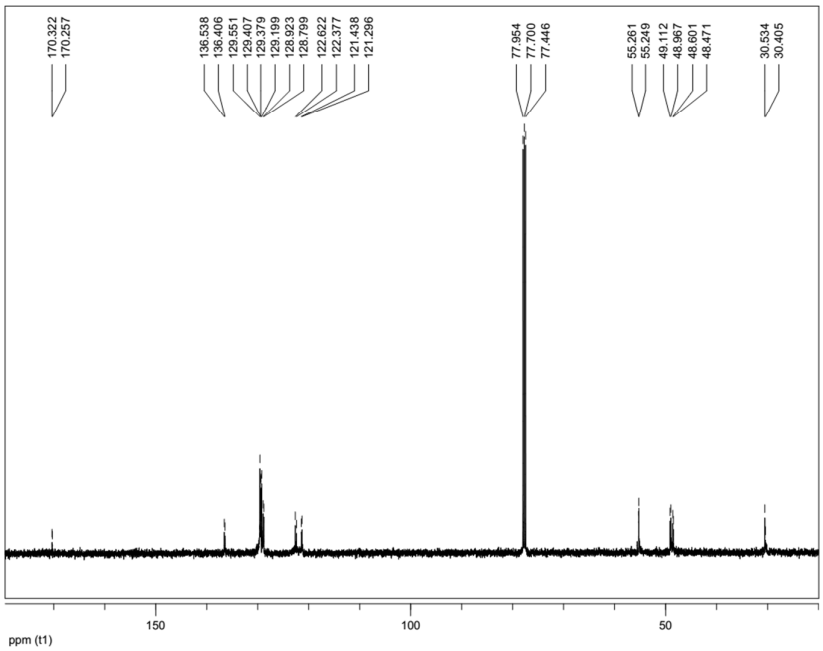


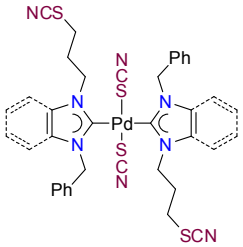


Compound **5b**, ^{1}H NMR spectrum (500 MHz, $CDCl_3$):

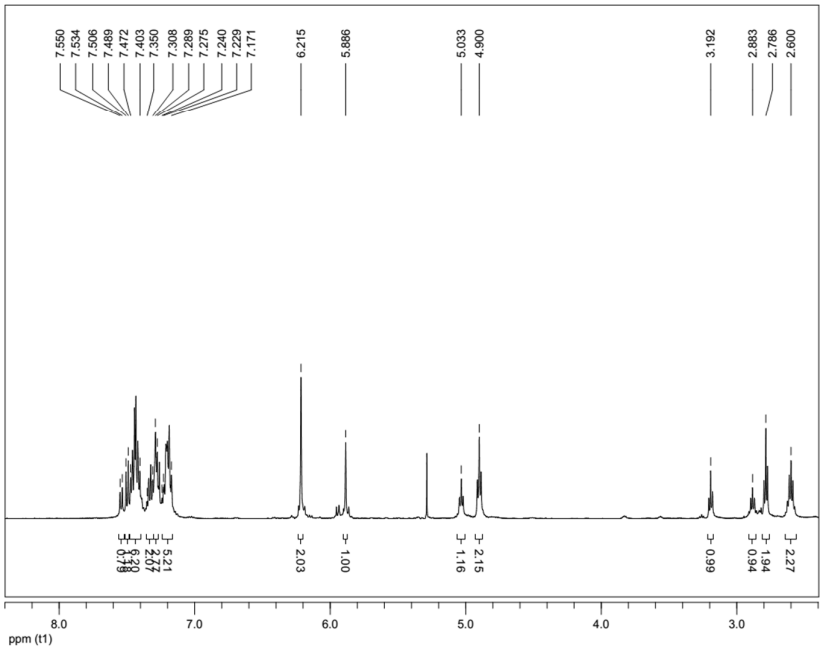


Compound **5b**, ^{13}C NMR spectrum (125.77 MHz, $CDCl_3$):

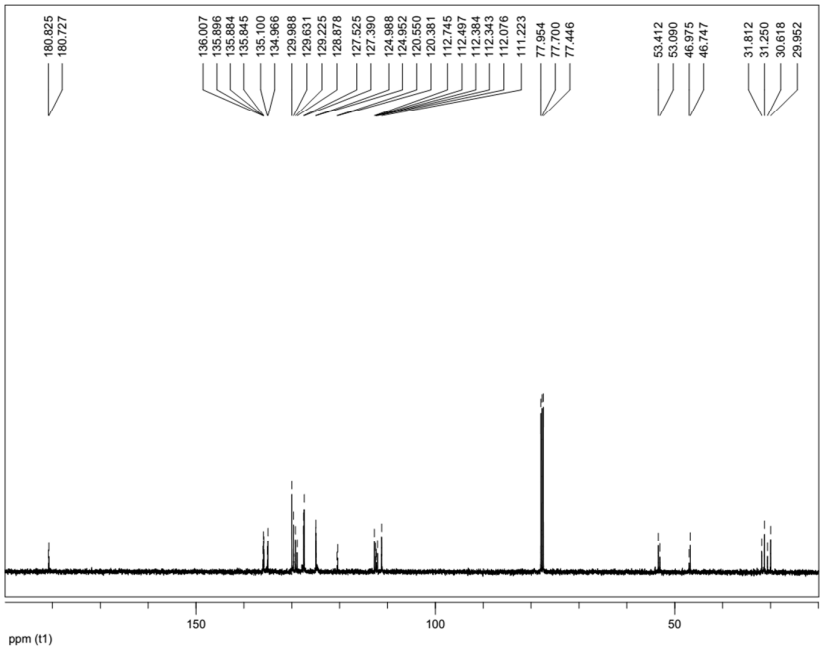


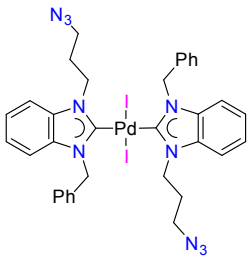


Compound **8a**, ^{1}H NMR spectrum (500 MHz, $CDCl_3$):

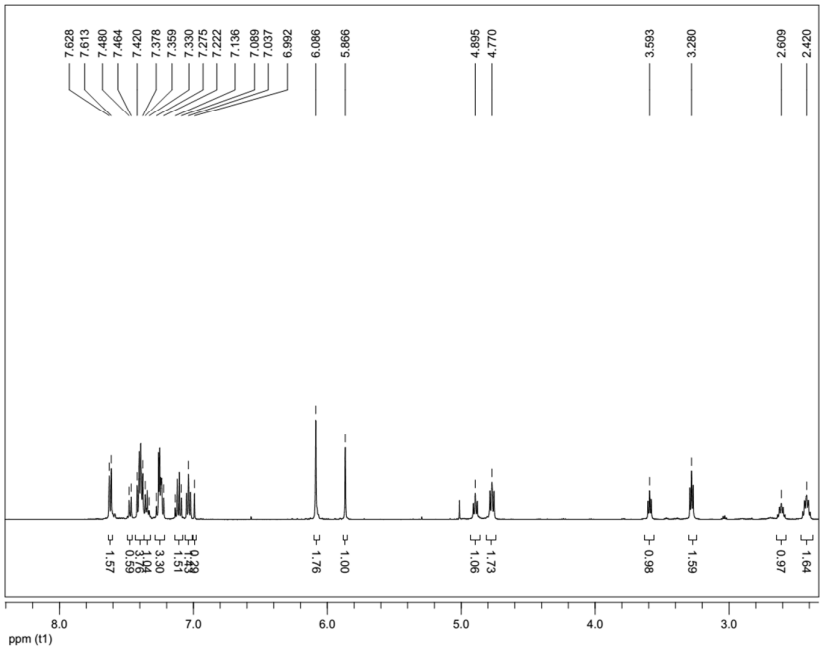


Compound **8a**, ^{13}C NMR spectrum (125.77 MHz, $CDCl_3$):

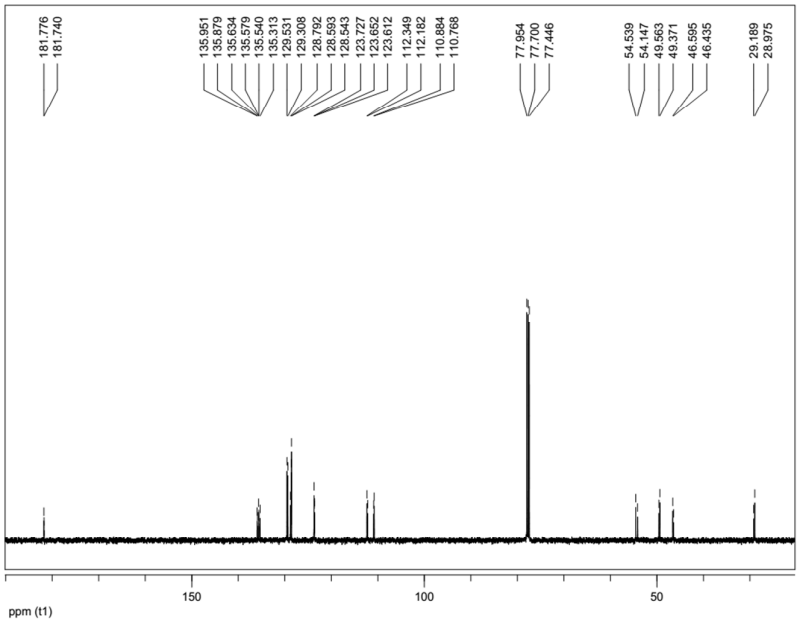


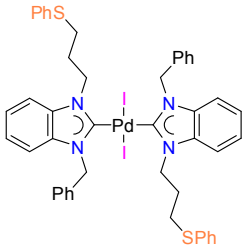


Compound **10**, ^{1}H NMR spectrum (500 MHz, $CDCl_3$):

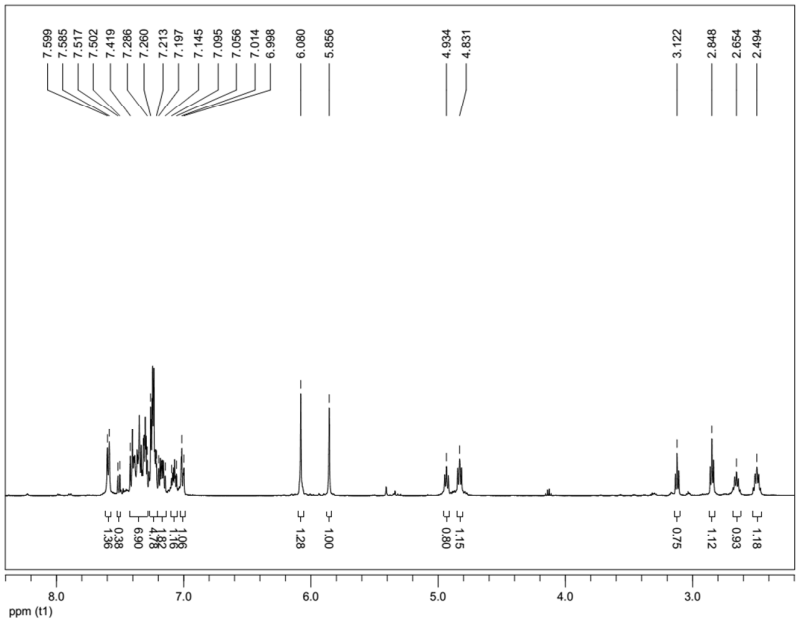


Compound **10**, ^{13}C NMR spectrum (125.77 MHz, $CDCl_3$):

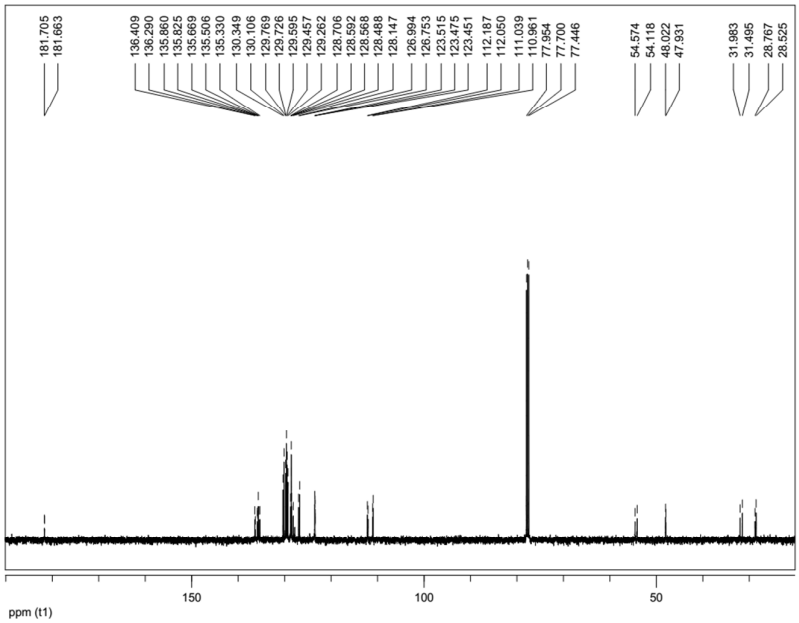


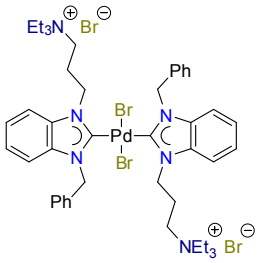


Compound **11**, ^{1}H NMR spectrum (500 MHz, $CDCl_3$):

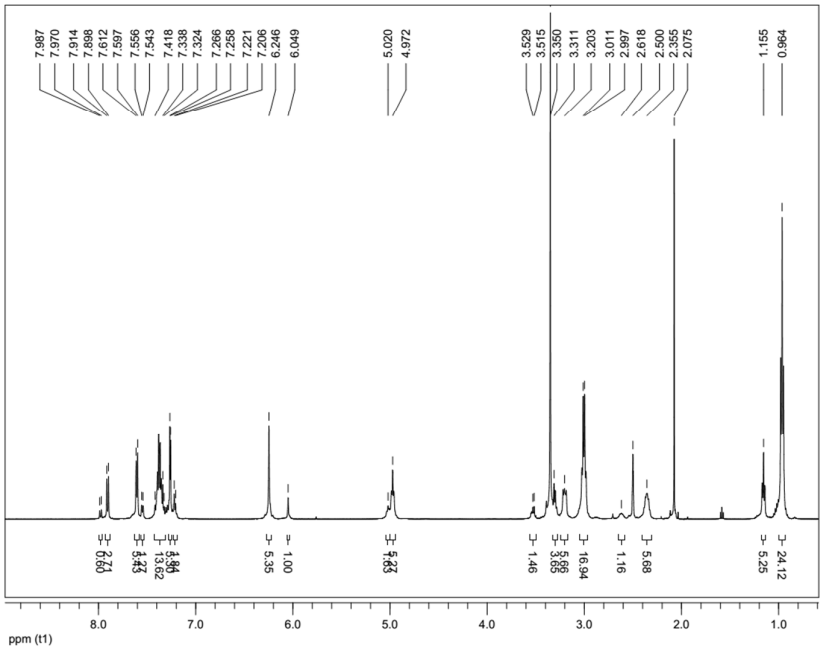


Compound **11**, ^{13}C NMR spectrum (125.77 MHz, $CDCl_3$):





Compound **14**, ^{1}H NMR spectrum (500 MHz, d_6-DMSO):



Compound **14**, ^{13}C NMR spectrum (125.77 MHz, d_6-DMSO):