Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Photophysical and Charge Transport Properties of Pyrazolines

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Spectral data of target compounds

3-(4-methoxystyryl)-4,5-dihydro-5-(4-methoxyphenyl)-1-phenyl-1H-pyrazole (1a)

Fluorescence yellowish green solid; mp: 148-150 ˚C; IR (KBr, cm^{-1}): 3052, 2928, 1599, 1457, 1322, 1280, 1252, 1178, 1101, 1066, 956, 951, 775,676; ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 2.99-2.93 (m, 1H), 3.69-3.62 (m, 1H), 3.76 (s, 3H), 3.81 (s, 3H), 5.20-5.15 (m, 1H), 6.51-6.47 (d, *J* = 16 Hz, 1H), 6.77-6.74 (t, *J* = 6 Hz, 1H), 6.88-6.83 (t, *J* = 10 Hz, 4H), 7.01-6.99 (d, *J* = 8Hz, 2H), 7.10 (s, 1H), 7.16-7.15 (d, *J* = 4 Hz, 2H), 7.18-7.17 (d, *J* = 4 Hz, 1H), 7.25-7.20 (d, *J* = 20 Hz, 2H), 7.38-7.36 (d, *J* = 8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 42.4, 55.2, 55.3, 63.6, 113.3, 114.2, 119.1, 119.6, 126.9, 127.8, 128.9, 129.5, 132.3, 134.5, 144.3, 148.7, 158.9, 159.6; ESI-MS for $C_{25}H_{24}N_2O_2$ Calculated M^+ (m/z) 384.47, found 385.13.

3-(4-(allyloxy) styryl)-5-(4-(allyloxy) phenyl)-4,5-dihydro-1-phenyl-1H-pyrazole (1b)

Fluorescence yellowish green solid; mp: 85-89 ˚C; IR (KBr, cm^{-1}): 3020, 2918, 1597, 1405, 1329, 1243, 1176, 1117, 1056, 924, 863, 744, 694; ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 3.00-2.94 (m, 1H), 3.70-3.62 (m, 1H), 4.50-4.49 (d, *J* = 4 Hz, 2H), 4.55-4.54 (d, *J* = 4 Hz, 2H), 5.20-5.16 (m, 1H), 5.31-5.28 (d, *J* = 12 Hz, 2H), 5.41-5.39 (d, *J* = 8 Hz, 2H), 6.10-5.98 (m, 2H), 6.78-6.74 (t, *J* = 8 Hz, 1H), 6.92-6.84 (m, 5H), 7.00-6.98 (d, *J* = 8 Hz, 2H) 7.06 (s, 1H), 7.16-7.14 (d, *J* = 8 Hz, 2H), 7.20-7.18 (d, *J* = 8 Hz, 2H), 7.37-7.35 (t, *J* = 4 Hz, 2H), 7.46-7.44 (d, *J* = 8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 42.4, 63.6, 68.8, 113.3, 115.1, 115.2, 117.7, 117.8, 119.0, 119.7, 126.9,127.8, 128.9, 129.6, 132.2, 133.0, 133.2, 134.7, 144.3, 148.7, 158.0, 158.6; ESI-MS for $C_{29}H_{28}N_2O_2$ Calculated M^+ (m/z) 436.54, found 437.22.

3-(3,4-dimethoxystyryl)-4,5-dihydro-5-(3,4-dimethoxyphenyl)-1-phenyl-1H-pyrazole (1c)

Fluorescence yellowish green solid; mp: 139-141 ˚C; IR (KBr, cm^{-1}): 3429, 2994, 1654, 1592, 1548, 1477, 1354, 1283, 1154, 1205, 1069, 951, 873, 747, 692; ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 3.03-2.97 (m, 1H), 3.79 (s, 3H), 3.86 (s, 3H), 3.89 (s, 3H), 3.97 (s, 3H), 5.59-5.54 (m, 1H), 6.78-6.74 (d, *J* = 16 Hz, 2H), 6.85-6.81 (t, *J* = 8 Hz, 2H), 6.97-6.93 (t, *J* = 8 Hz, 1H), 7.02-6.99 (d, *J* = 12 Hz, 2H), 7.06-7.04 (d, *J* = 8 Hz, 1H), 7.17-7.15 (d, *J* = 8 Hz, 2H), 7.21-7.19 (d, *J* = 8 Hz, 2H), 7.25 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 41.4, 55.7, 58.7, 60.7, 61.1, 111.5, 111.7, 118.4, 119.1, 122.8, 124.1, 124.6, 126.5, 128.9, 130.8, 135.9,

144.2, 145.6, 146.8, 149.3, 152.8, 153.1; ESI-MS for $C_{27}H_{28}N_2O_4$ Calculated M^+ (m/z) 444.52, found 445.27.

3-(3,4,5-trimethoxystyryl)-4,5-dihydro-5-(3,4,5-trimethoxyphenyl)-1-phenyl-1H-pyrazole (1d)

Fluorescence yellowish green solid; mp: 180-182 ˚C; IR (KBr, cm^{-1}): 3427, 2926, 1595, 1501, 1459, 1421, 1331, 1238, 1127, 1056, 963, 875,746; ^1H NMR ($CDCl_3$, 400 MHz): δ (ppm) 3.05-2.98 (m, 1H), 3.69-3.65 (m, 1H), 3.82-3.81 (d, *J* = 4 Hz, 9H), 3.88-3.86 (d, *J* = 8 Hz, 9H), 5.17-5.12 (m, 1H), 6.50-6.46 (t, *J* = 8 Hz, 3H), 6.68 (s, 2H), 6.83-6.79 (t, *J* = 8 Hz, 1H), 7.03-7.01 (d, *J* = 8 Hz, 2H), 7.22-7.18 (d, *J* = 16 Hz, 1H) 7.26 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ (ppm) 42.3, 56.0, 56.1, 60.8, 60.9, 64.7, 102.3, 103.6, 113.4, 119.5, 121.1, 128.9, 132.2, 132.7, 137.1, 138.2, 138.3, 144.4,148.5, 153.4, 153.8; ESI-MS for $C_{29}H_{32}N_2O_6$ Calculated M^+ (m/z) 504.57, found 505.13.

Table S1. Photophysical properties of pyrazolines in different solvents

compound	Solvents	Absorbance (nm)	Fluorescence (nm)	Stokes Shift (cm^{-1})
1a	Heptane	285, 382	451	4005
	Dichloromethane	286, 385	471	4743
	Acetonitrile	276, 381	472	5060
	Methanol	285, 380	485	5697
1b	Heptane	285, 383	449	3838
	Dichloromethane	286, 385	470	4697
	Acetonitrile	285, 381	474	5150
	Methanol	285, 379	484	5724
1c	Heptane	301, 381	449	4073
	Dichloromethane	305, 384	477	4900
	Acetonitrile	304, 383	480	5276
	Methanol	301, 382	488	5770
1d	Heptane	301, 381	451	3818
	Dichloromethane	305, 384	473	4278
	Acetonitrile	304,383	480	3786
	Methanol	301, 383	490	5770

Table S2. Photophysical properties of pyrazolines in different solvents

Compound	Wavelength (nm)	Osc. Strength	Major contributions
1a	415	0.916	HOMO→LUMO (78%)
	308	0.150	H-2→LUMO (33%), H-1→LUMO (53%)
	299	0.194	H-2→LUMO (23%), H-1→LUMO (20%), HOMO→L+3 (37%)
	254	0.105	HOMO→L+5 (48%), HOMO→L+6 (13%)
	227	0.105	H-6->LUMO (13%), H-1->L+2 (53%)
1b	416	0.937	HOMO→LUMO (79%)
	305	0.145	H-1→LUMO (31%), HOMO→L+2 (32%), HOMO->L+3 (20%)
	302	0.099	HOMO→L+2 (57%), HOMO→L+3 (17%)
	254	0.116	H-5→LUMO (11%), HOMO→L+7 (47%), HOMO→L+8 (14%)
	248	0.078	H-5→LUMO (41%), HOMO→L+7 (17%), HOMO→L+8 (18%)
1c	415	0.945	HOMO→LUMO (79%)
	313	0.135	H-2→LUMO (16%), H-1→LUMO (63%)
	297	0.141	H-3→LUMO (15%), H-1→LUMO (11%), HOMO→L+3 (59%)
	254	0.115	HOMO→L+5 (57%), HOMO→L+6 (13%)
	224	0.094	H-2→L+2 (60%)
1d	334	0.102	H-3→LUMO (55%)
	306	0.075	H-6→LUMO (44%)
	291	0.143	H-8→LUMO (12%), HOMO→L+1 (62%)
	262	0.105	H-2→L+1 (21%), HOMO→L+2 (44%), HOMO→L+6 (11%)
	257	0.142	H-2→L+1 (14%), H-1→L+2 (13%), HOMO→L+2 (38%), HOMO→L+6 (12%)

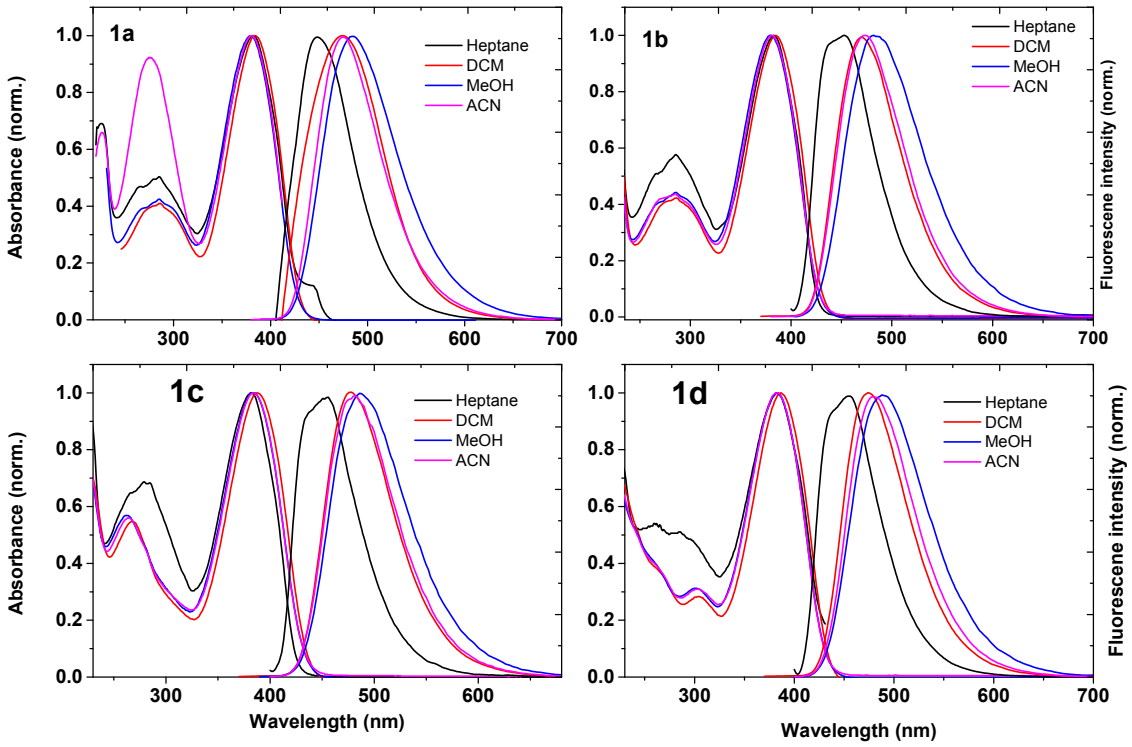

Figure S1. UV-visible absorption and fluorescence emission of pyrazolines derivatives **1a-d** in different solvents.

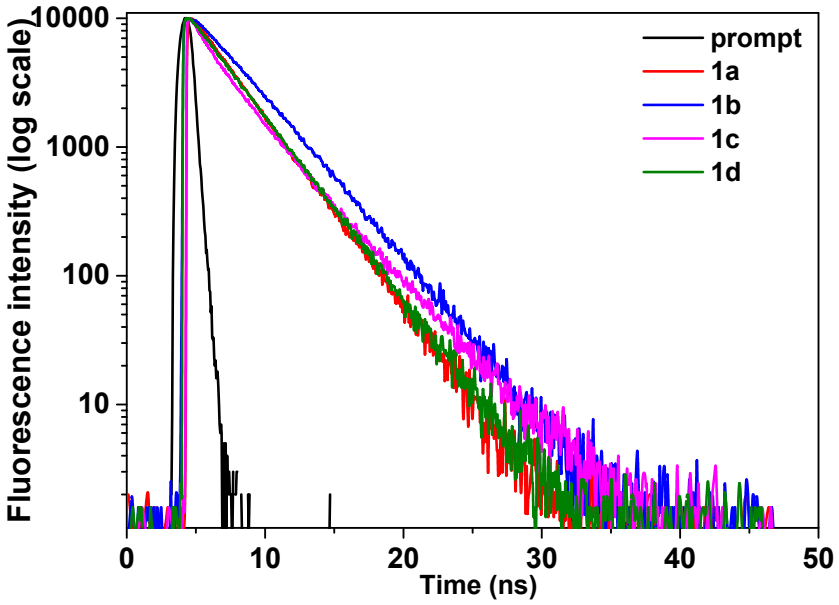

Figure S2. Fluorescence lifetime decay profiles of pyrazolines **1a-1d** dissolved in acetonitrile. The samples are excited at 375 nm and the decay profiles were monitored at respective emission aximum

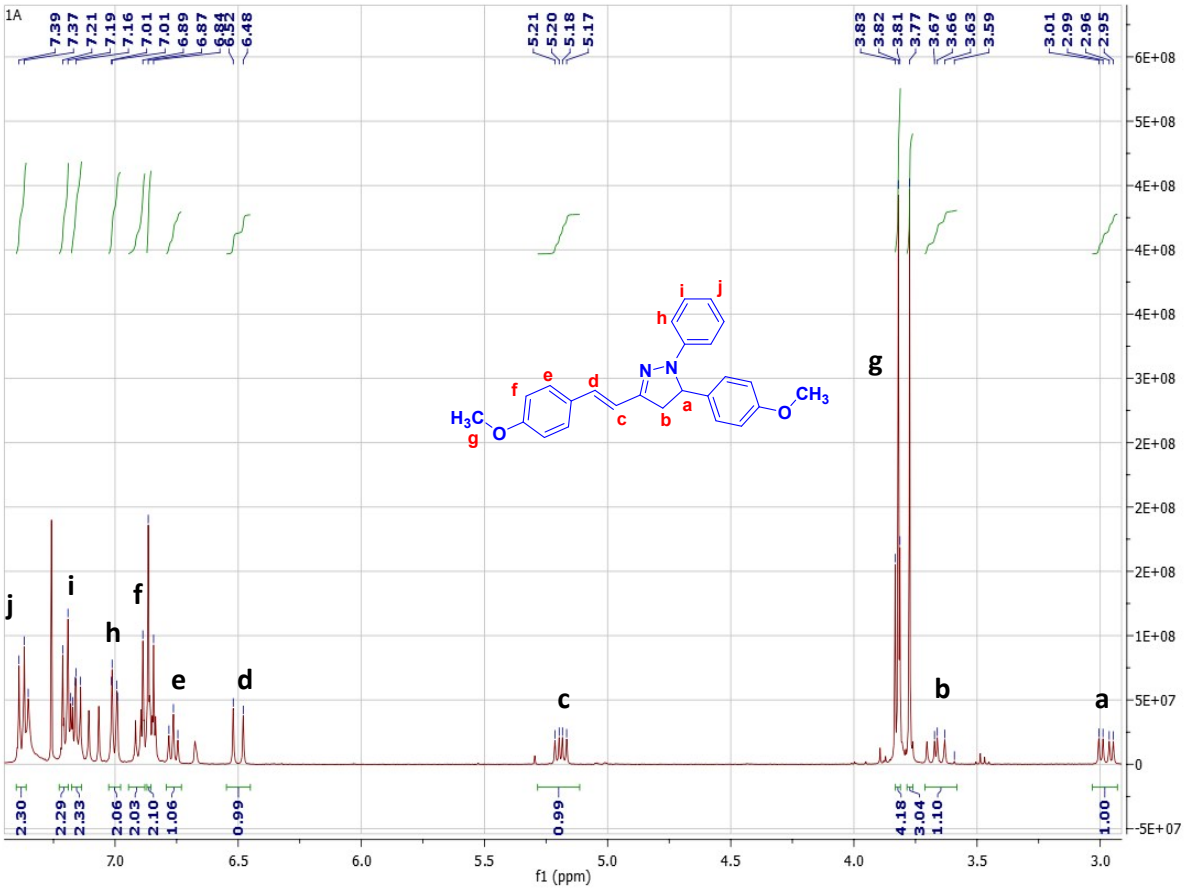

Fig. S3 ^{1}H-NMR spectrum of **1a** in $CDCl_3$.

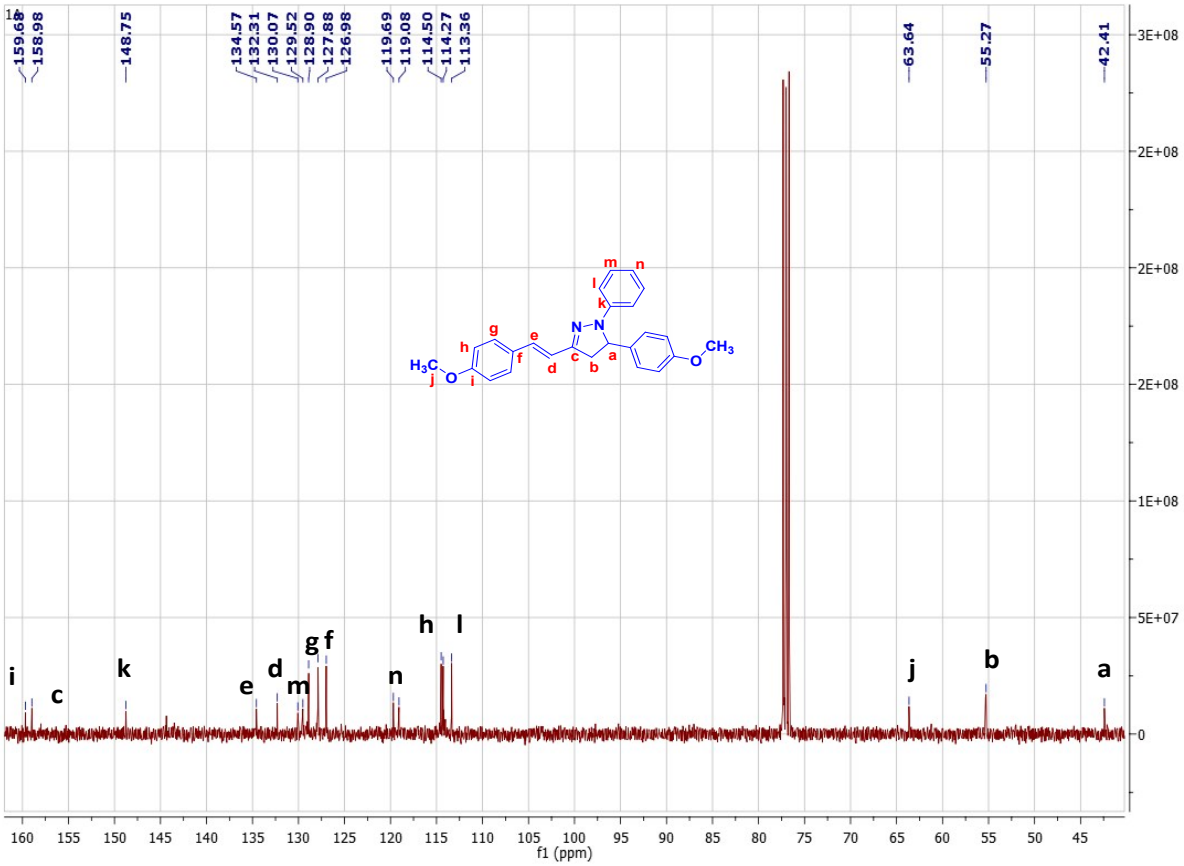

Fig.S4 ^{13}C-NMR spectrum of **1a** in $CDCl_3$

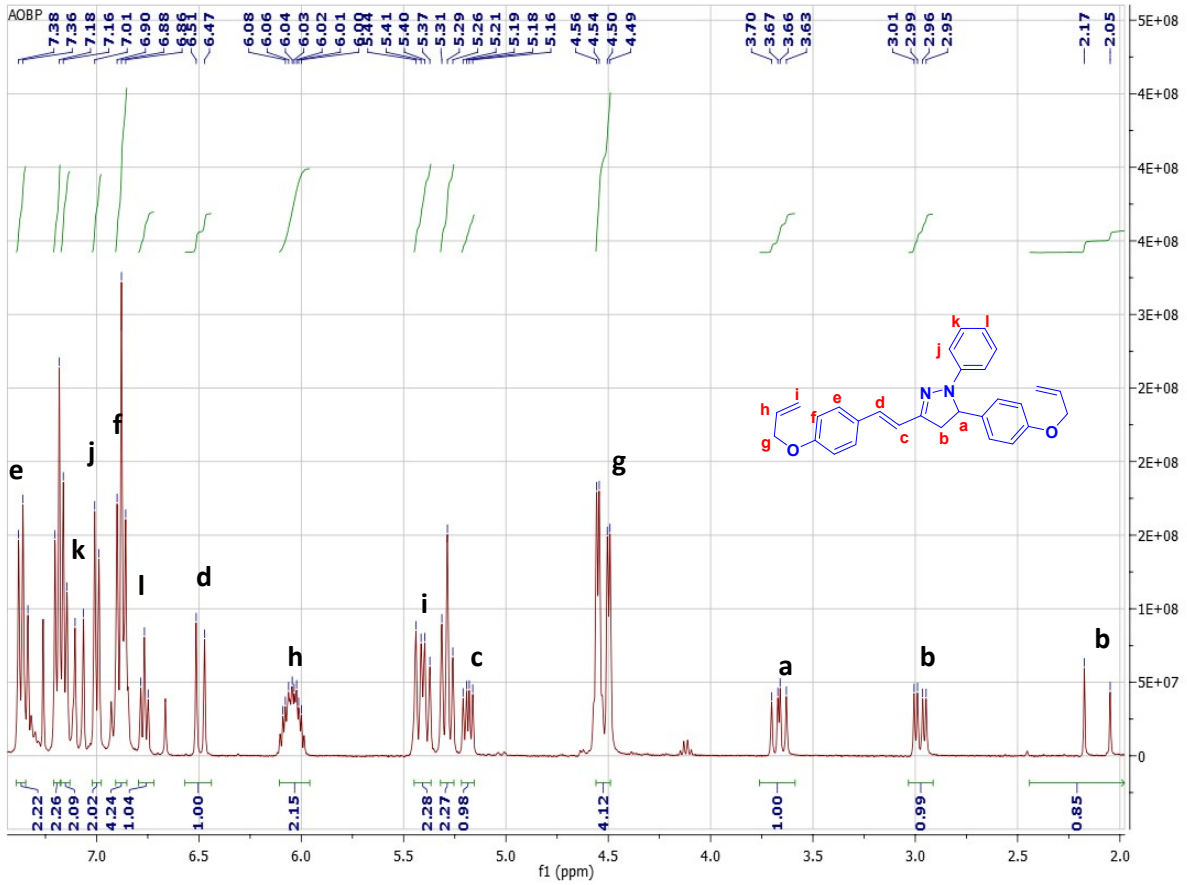

Fig. S5 ^{1}H-NMR spectrum of **1b** in $CDCl_3$

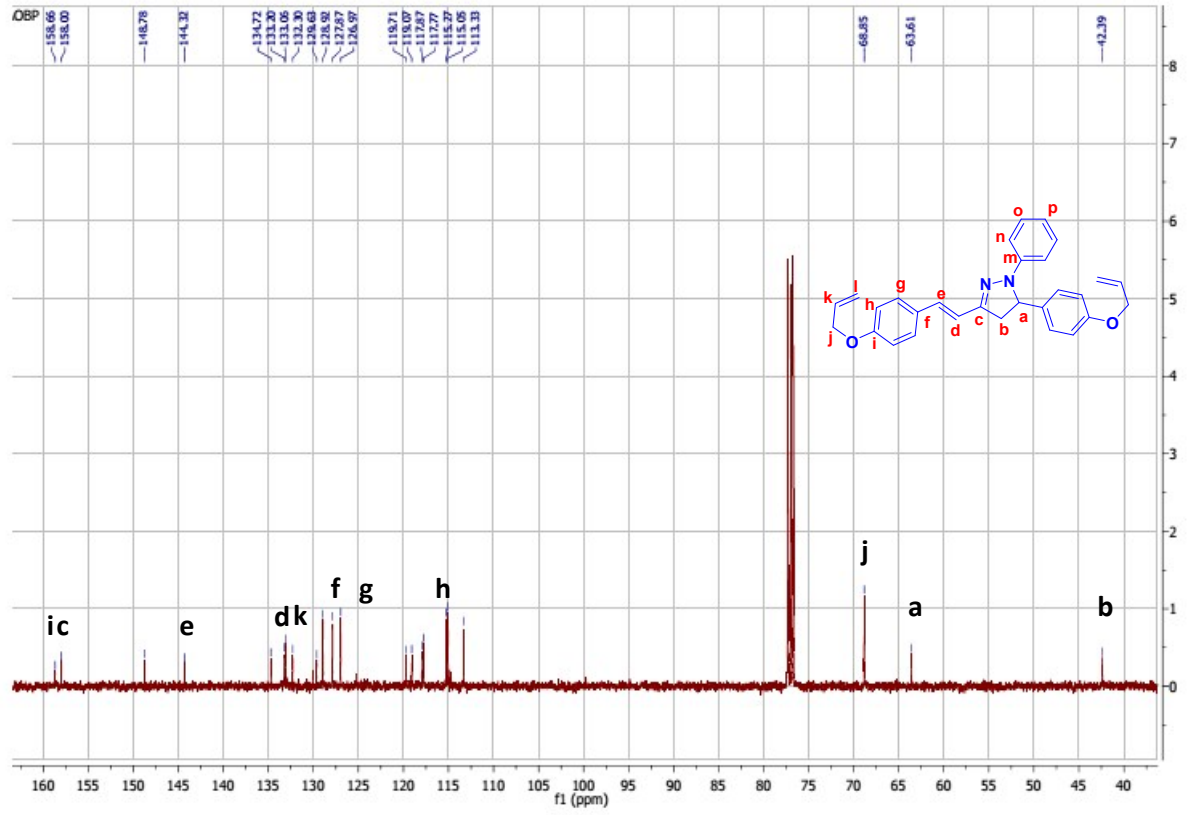

Fig. S6 ^{13}C-NMR spectrum of **1b** in $CDCl_3$

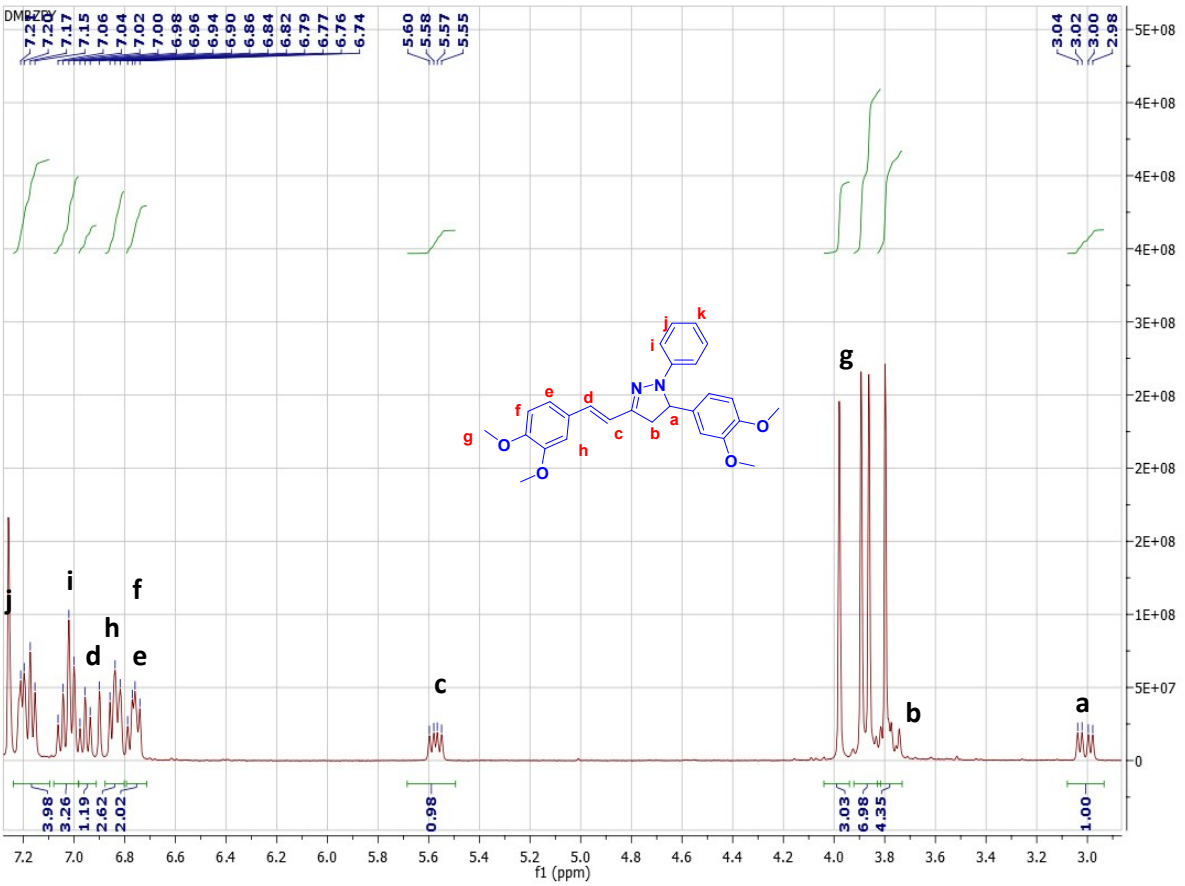

Fig. S7 ^{1}H-NMR spectrum of **1c** in $CDCl_3$

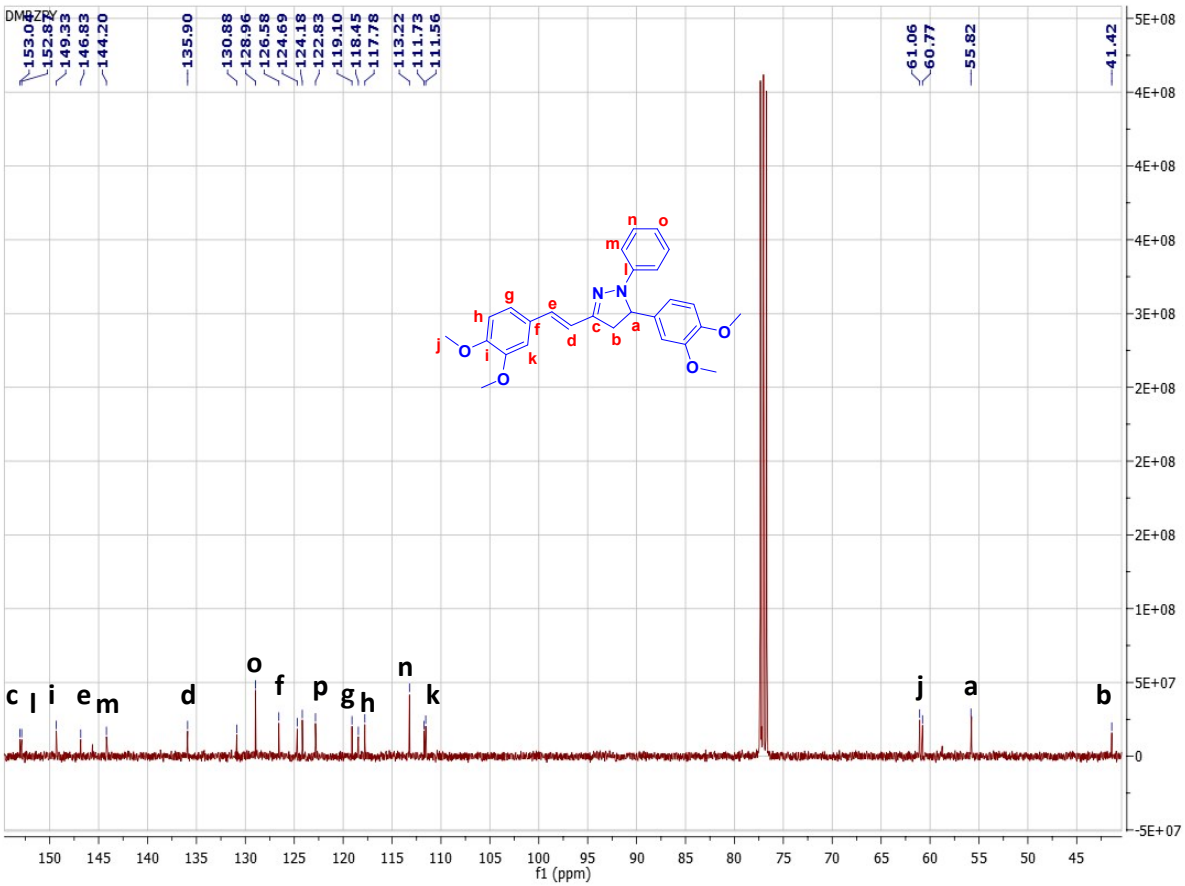

Fig. S8 ^{13}C-NMR spectrum of **1c** in $CDCl_3$

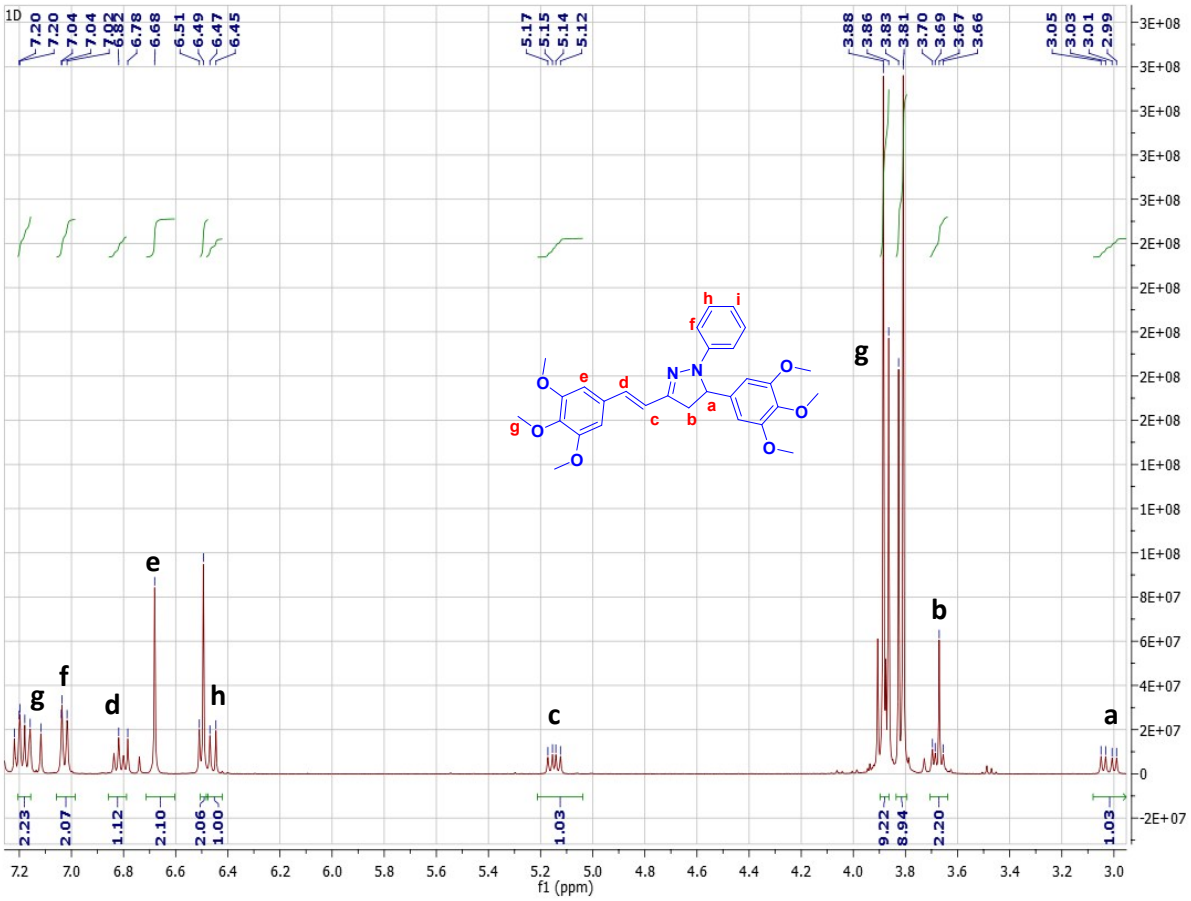

Fig. S9 ^{1}H-NMR spectrum of **1d** in $CDCl_3$

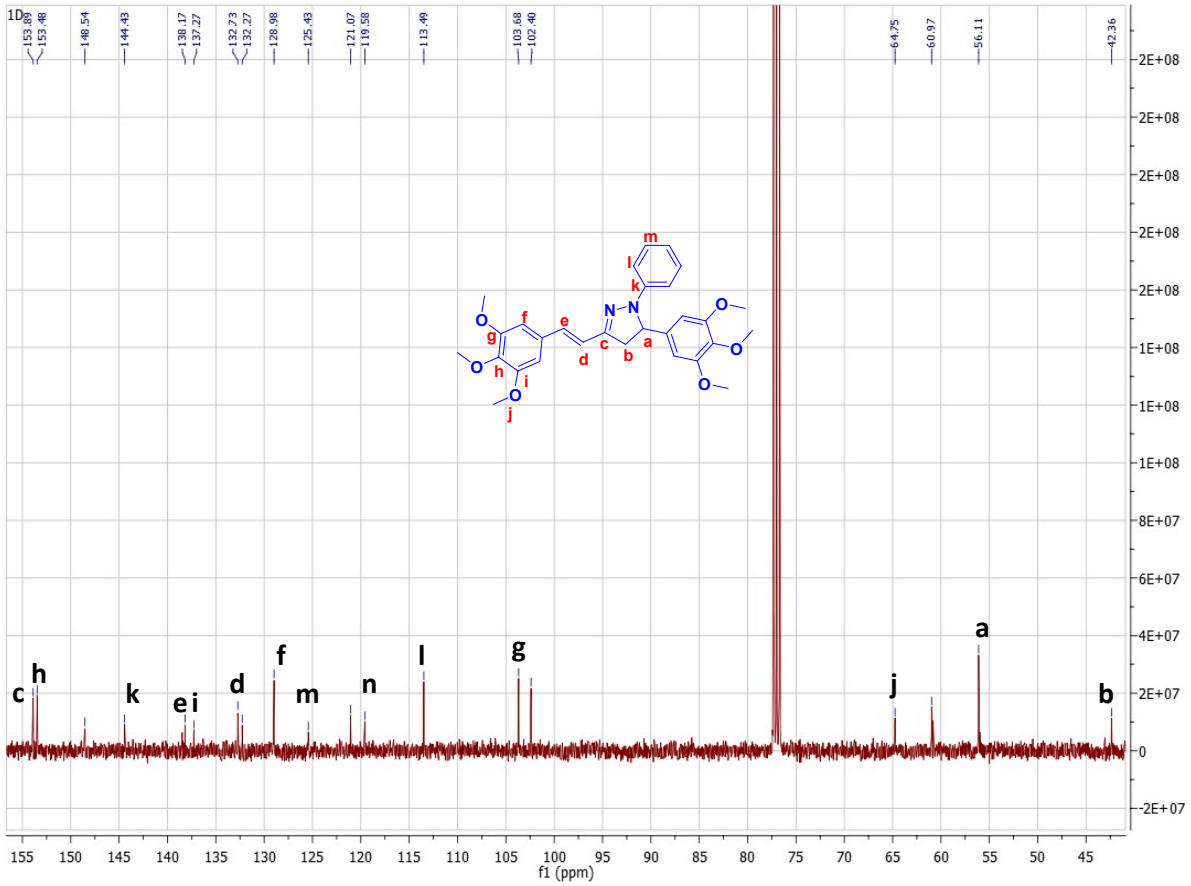

Fig. S10 ^{13}C-NMR spectrum of **1d** in $CDCl_3$.