ELECTRONIC SUPPLEMENTARY INFORMATION

for

Tunable Full-Color Emission of Stilbazoles Containing 2-Halo-3,4-Dicyanopyridine Acceptor

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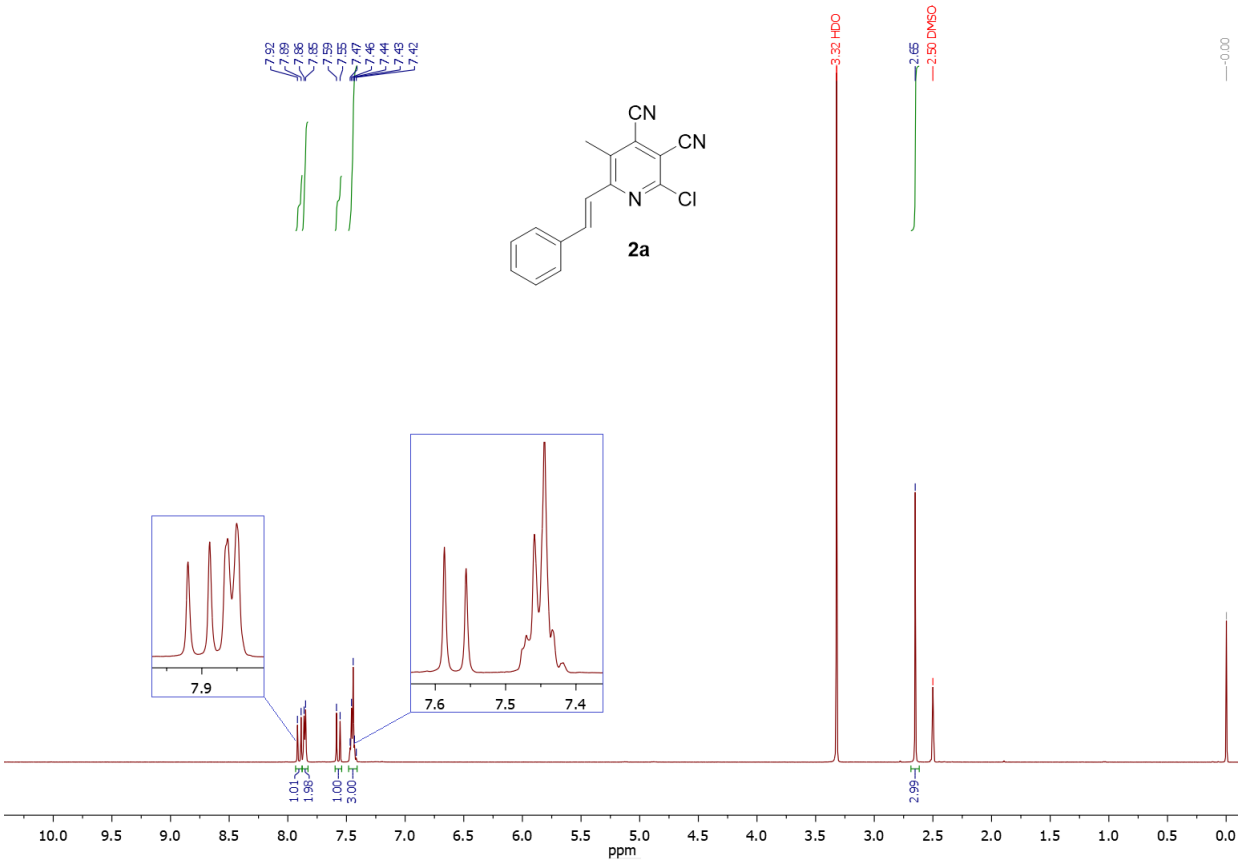

Figure S1 ^{1}H NMR-spectrum of **2a** (500 MHz, DMSO-d_6)

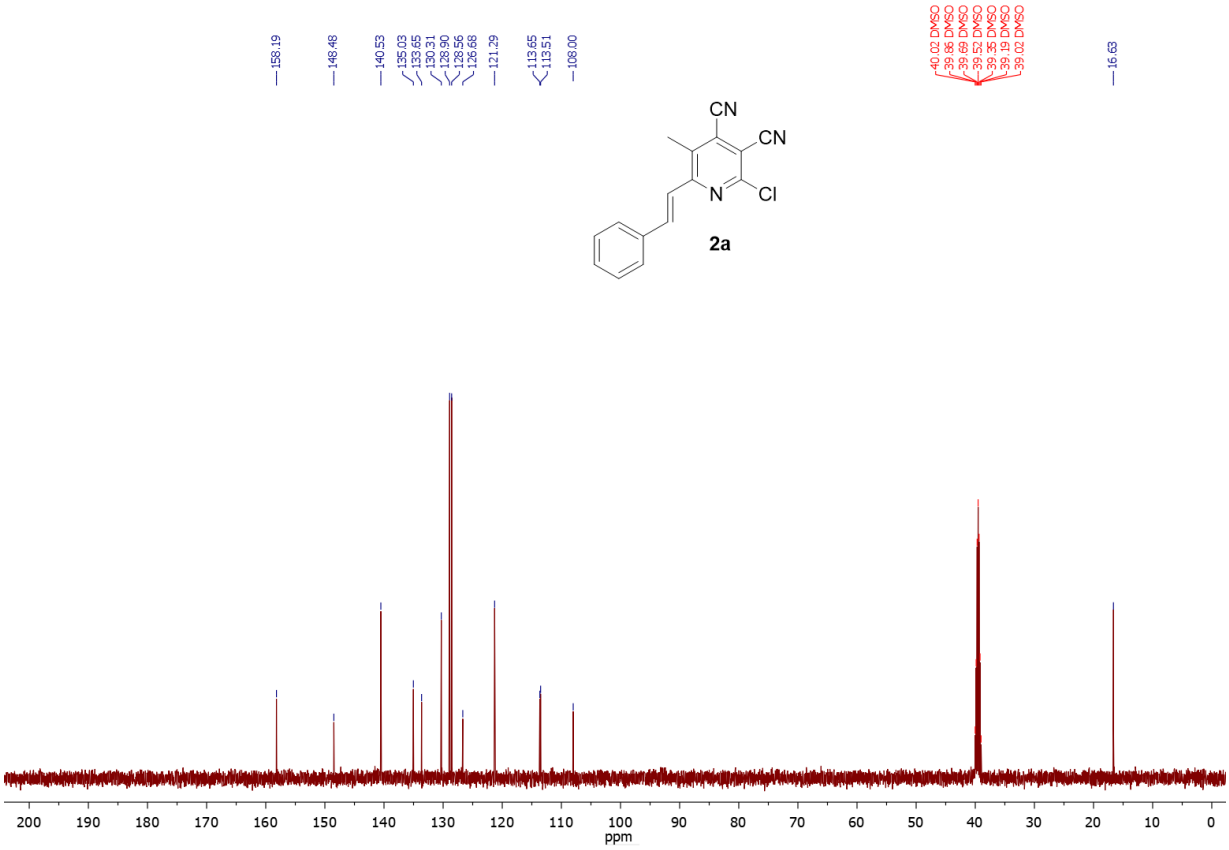

Figure S2 ^{13}C NMR-spectrum of **2a** (126 MHz, DMSO-d_6)

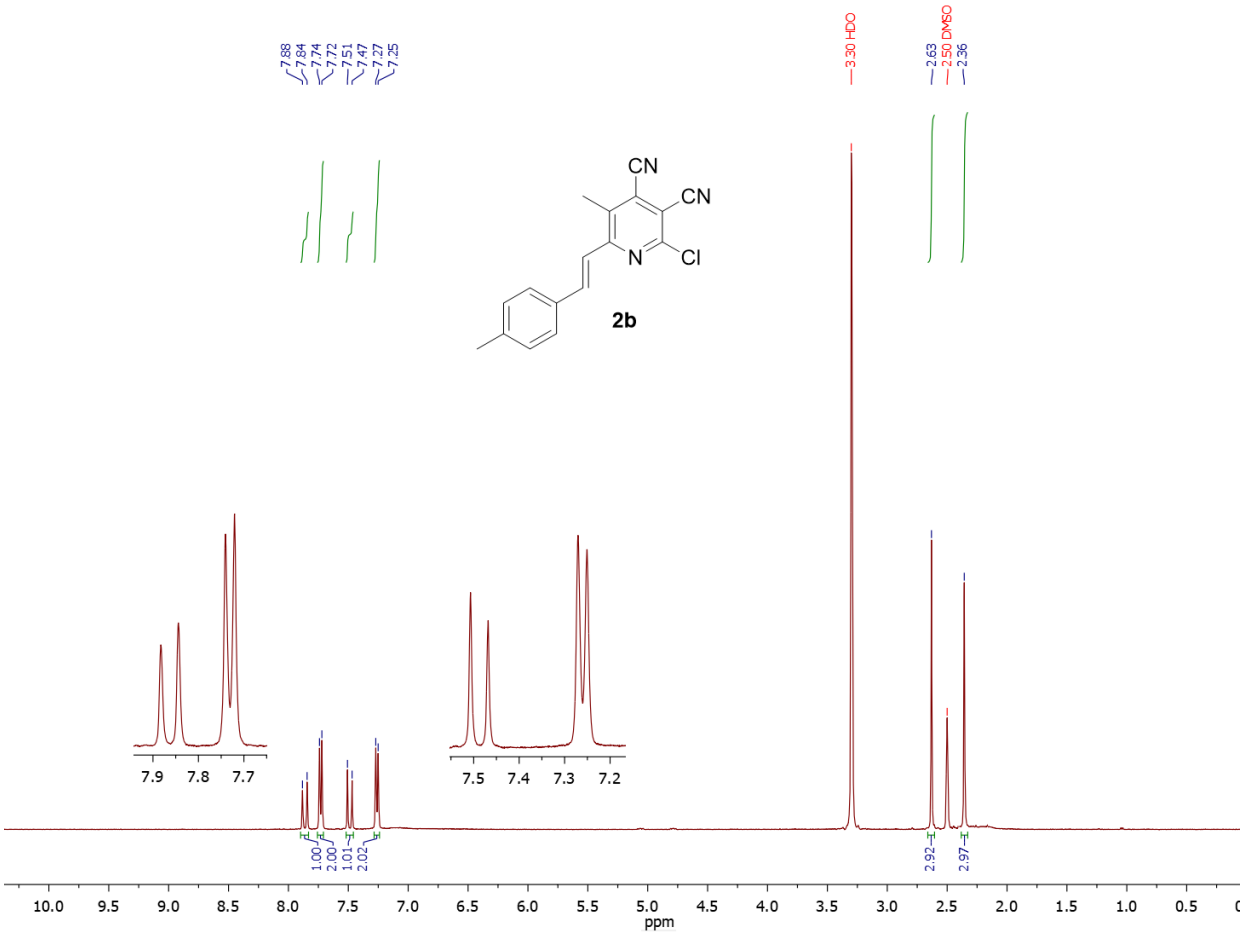

Figure S3 ^{1}H NMR-spectrum of **2b** (500 MHz, DMSO-d_6)

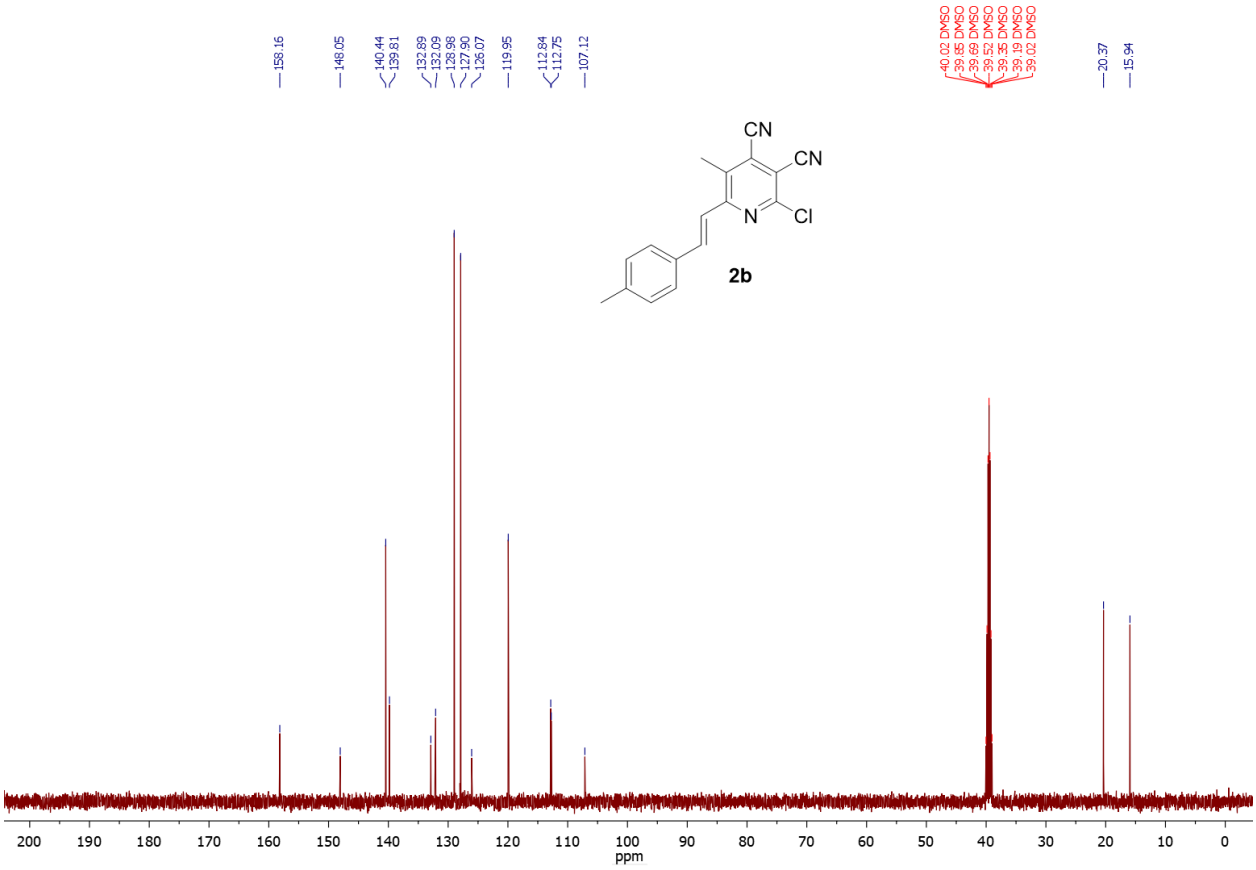

Figure S4 ^{13}C NMR-spectrum of **2b** (126 MHz, DMSO-d_6)

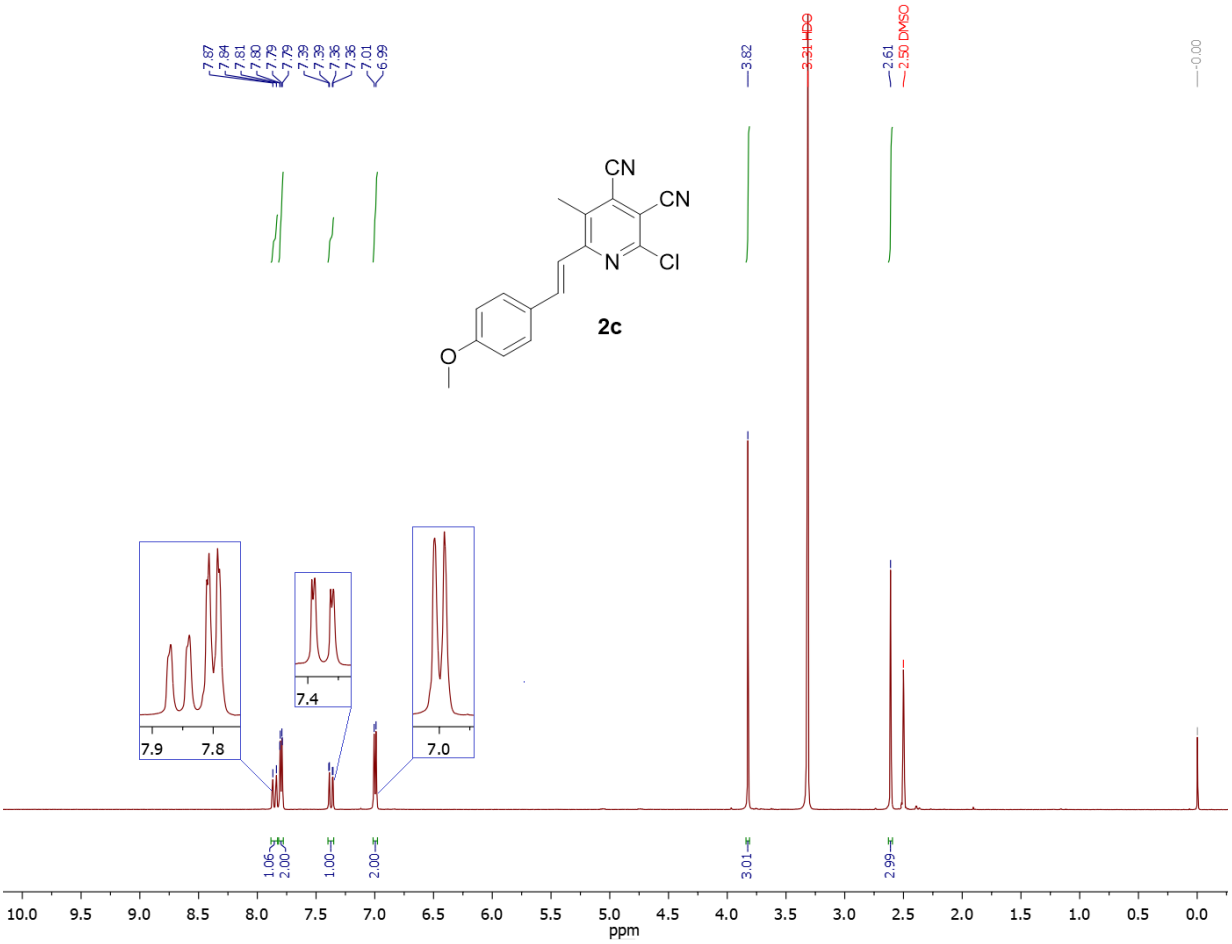

Figure S5 ^{1}H NMR-spectrum of **2c** (500 MHz, DMSO-d_6)

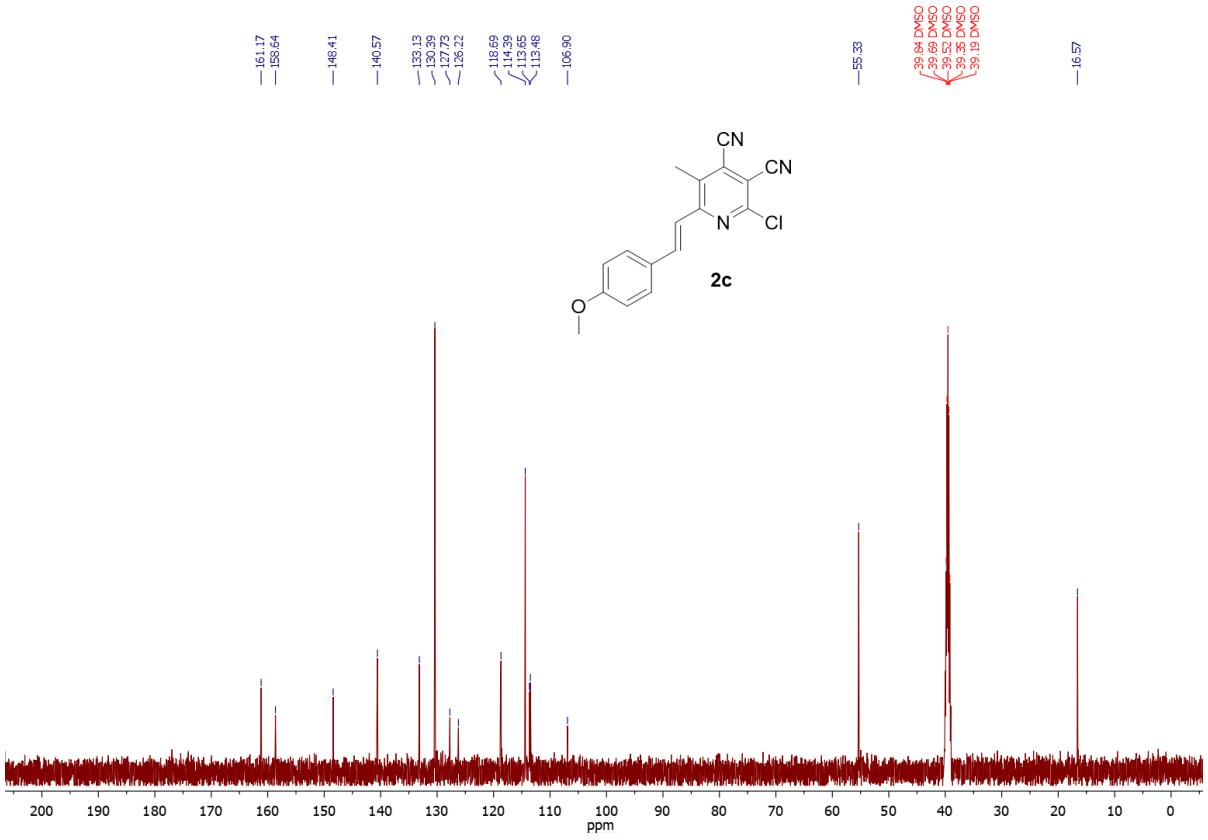

Figure S6 ^{13}C NMR-spectrum of **2c** (126 MHz, DMSO-d_6)

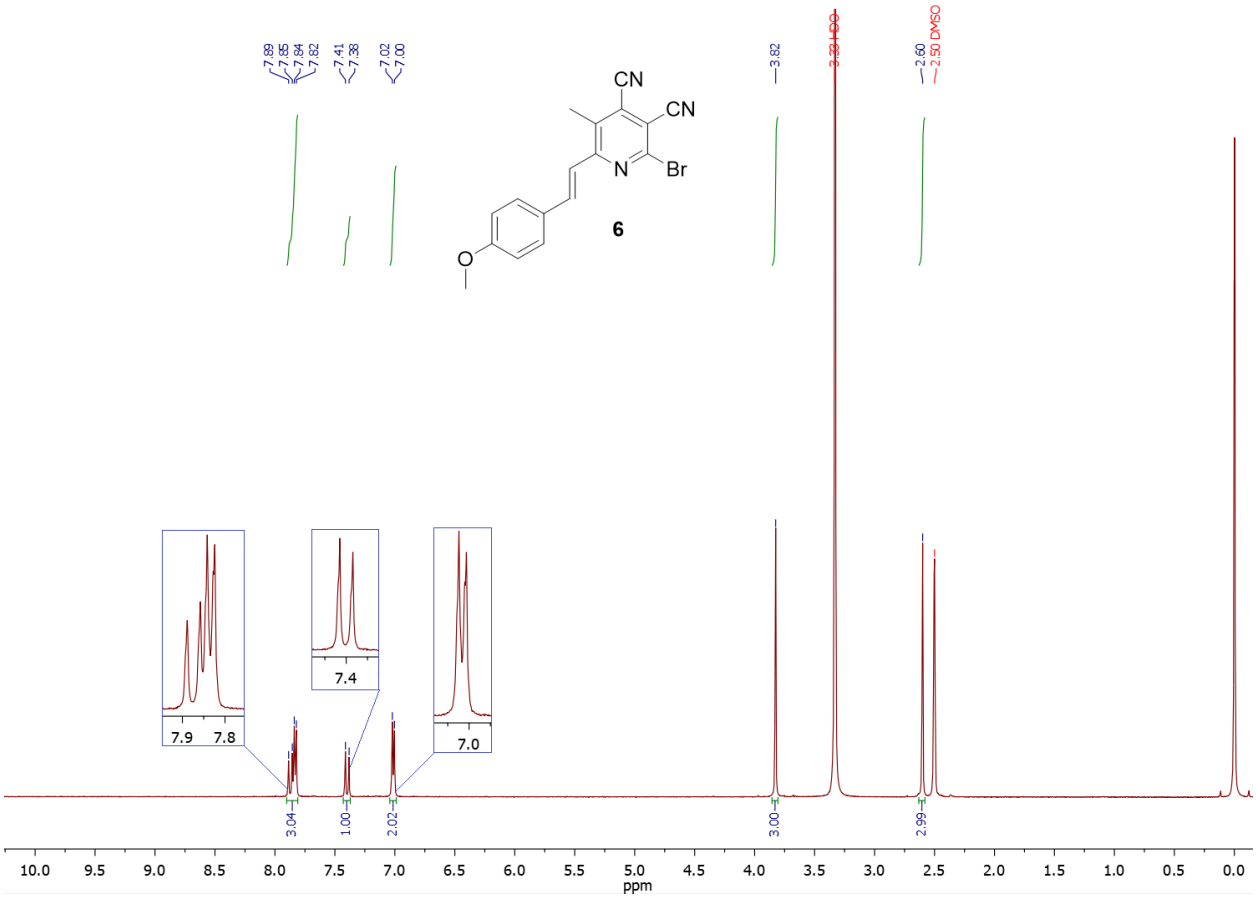

Figure S7 ^{1}H NMR-spectrum of **6** (500 MHz, DMSO-d_6)

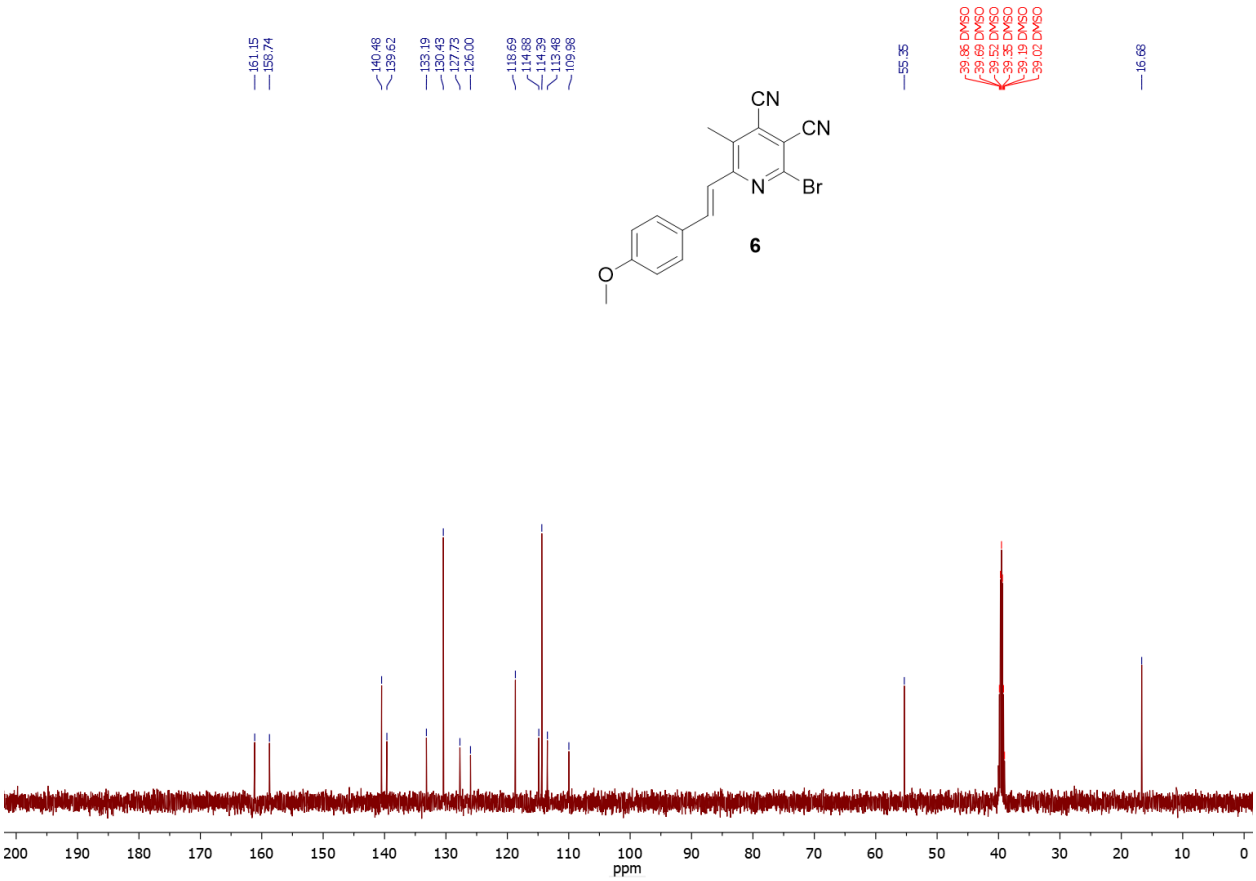

Figure S8 ^{13}C NMR-spectrum of **6** (126 MHz, DMSO-d_6)

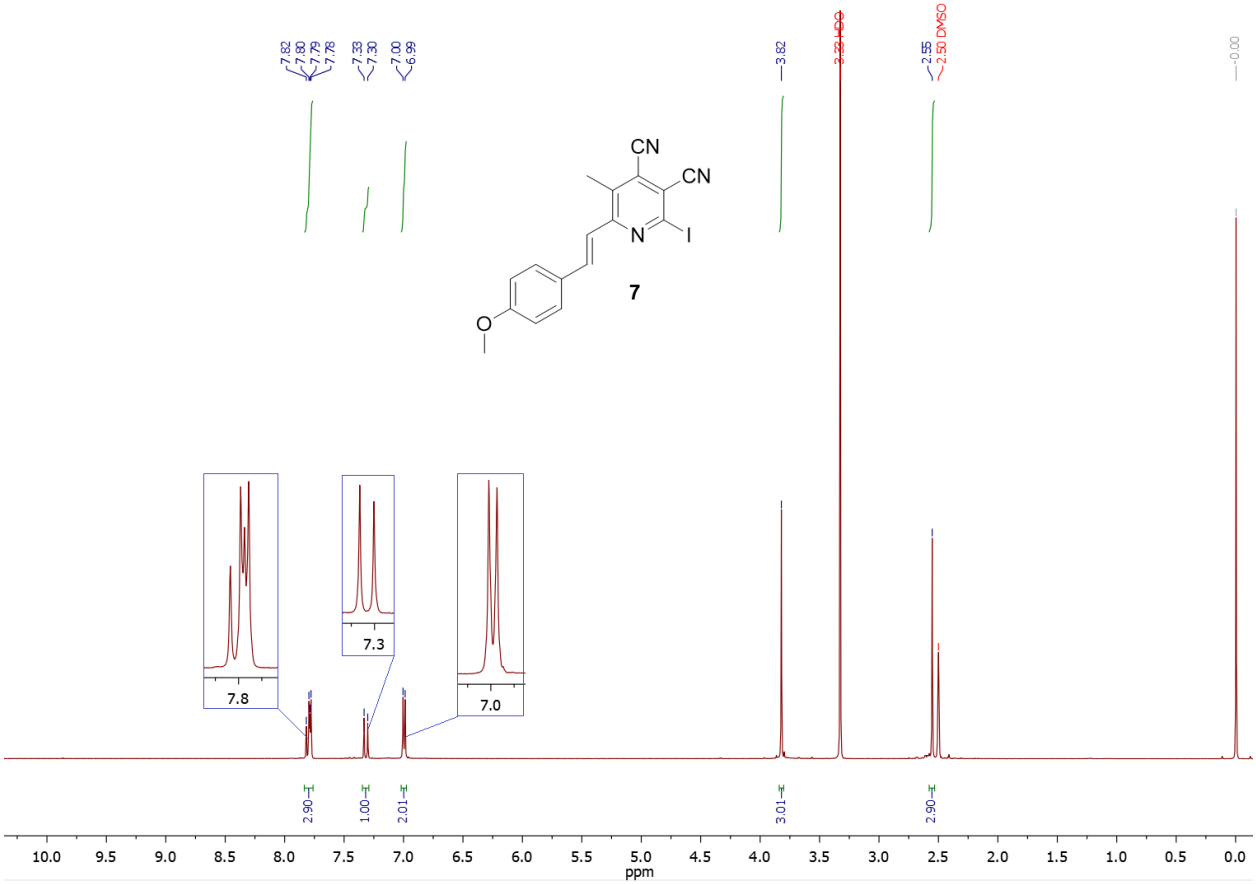

Figure S9 ^{1}H NMR-spectrum of **7** (500 MHz, DMSO-d_6)

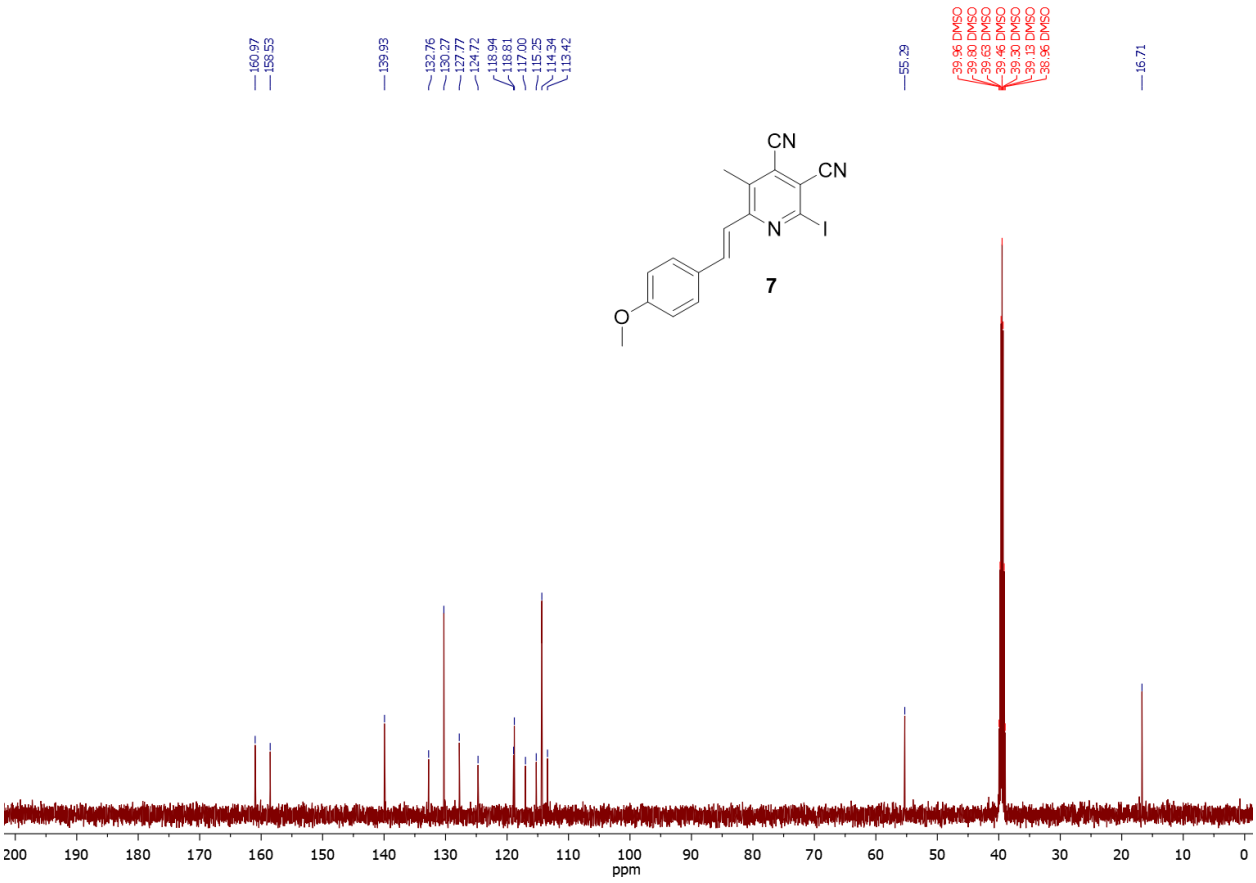

Figure S10 ^{13}C NMR-spectrum of **7** (126 MHz, DMSO-d_6)

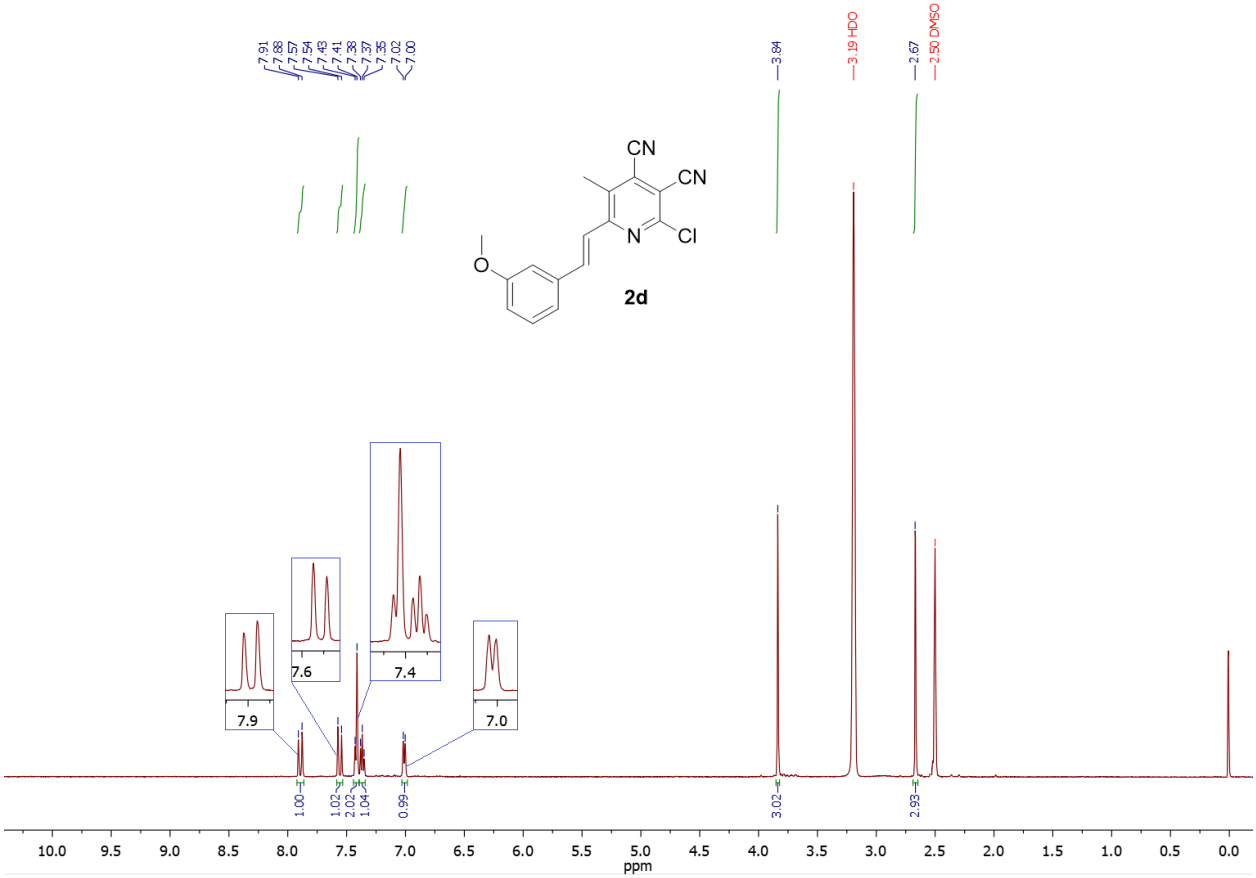

Figure S11 ^{1}H NMR-spectrum of **2d** (500 MHz, DMSO-d_6)

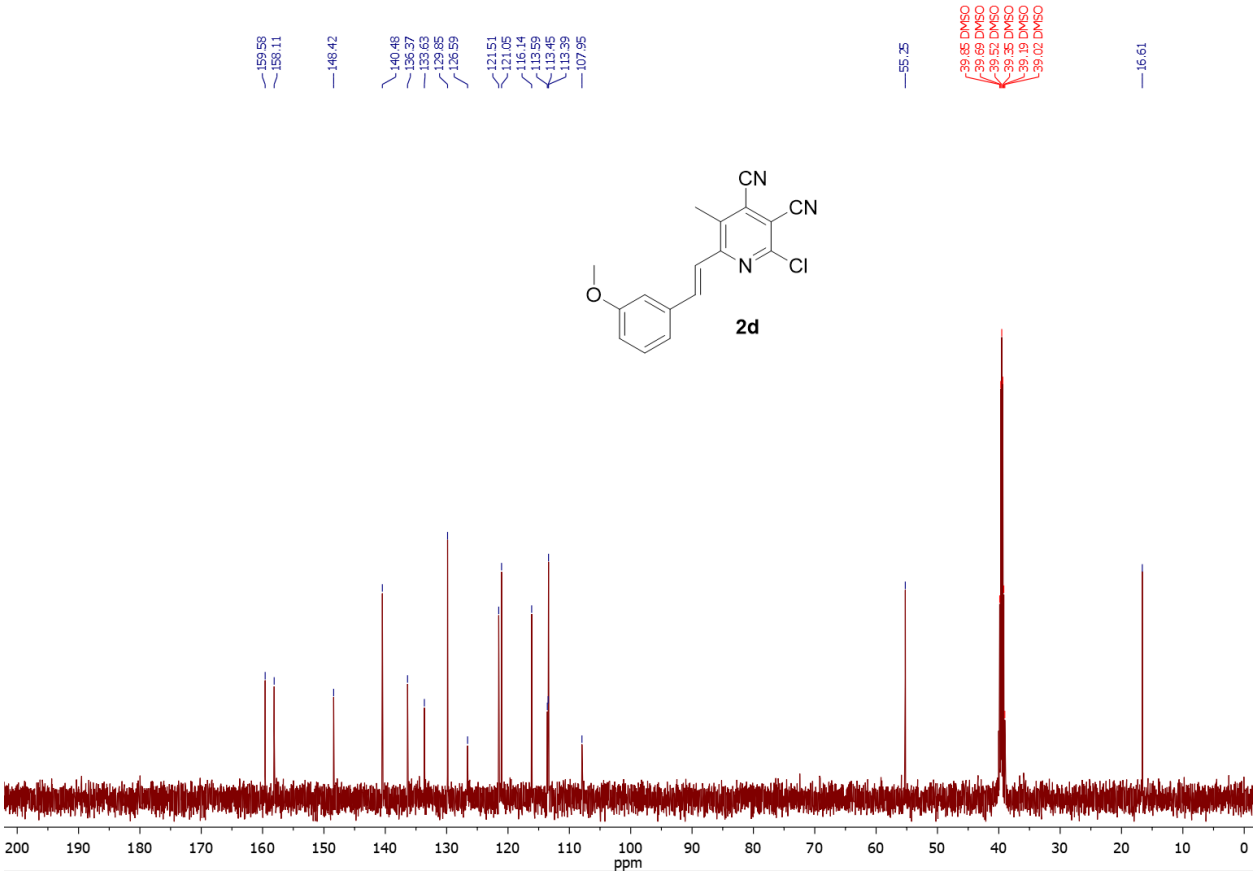

Figure S12 ^{13}C NMR-spectrum of **2d** (126 MHz, DMSO-d_6)

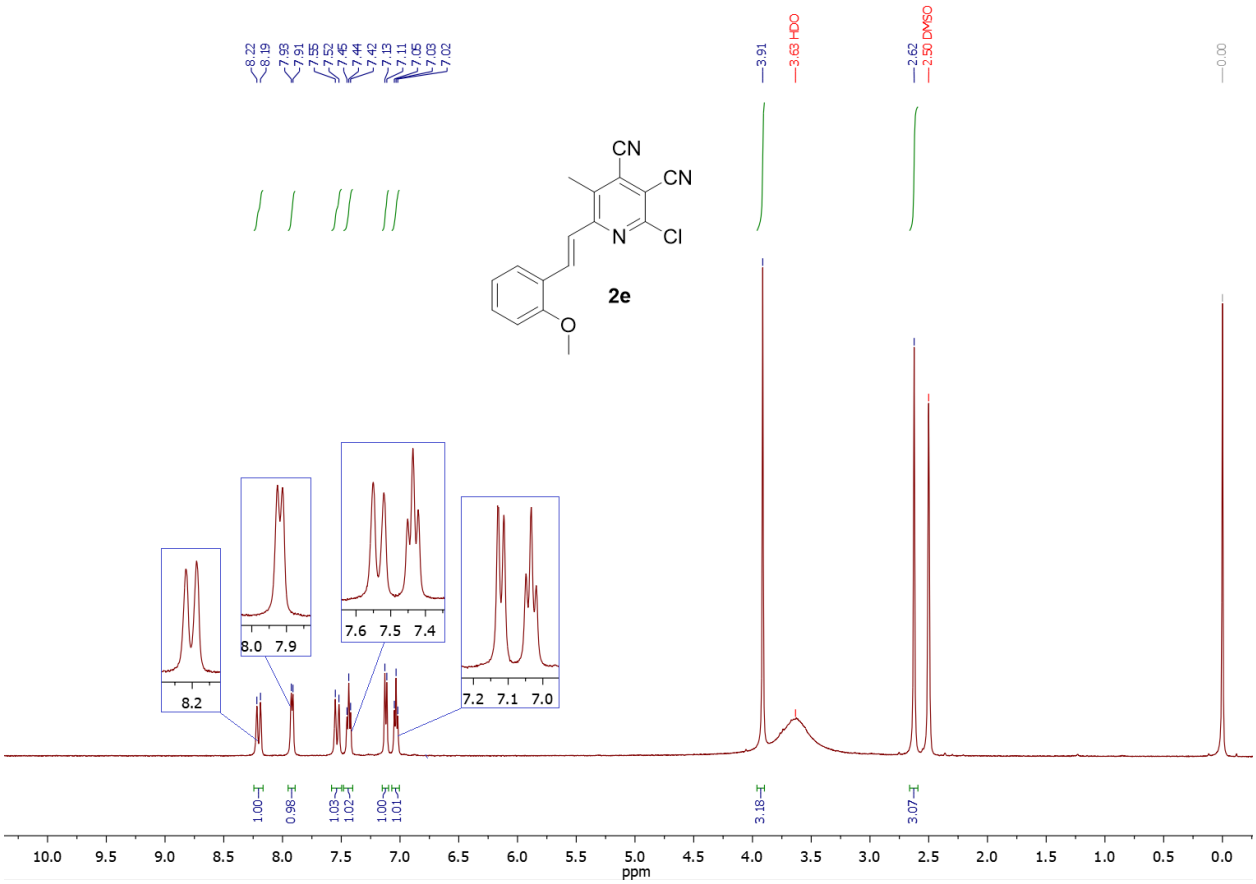

Figure S13 ^{1}H NMR-spectrum of **2e** (500 MHz, DMSO-d_6)

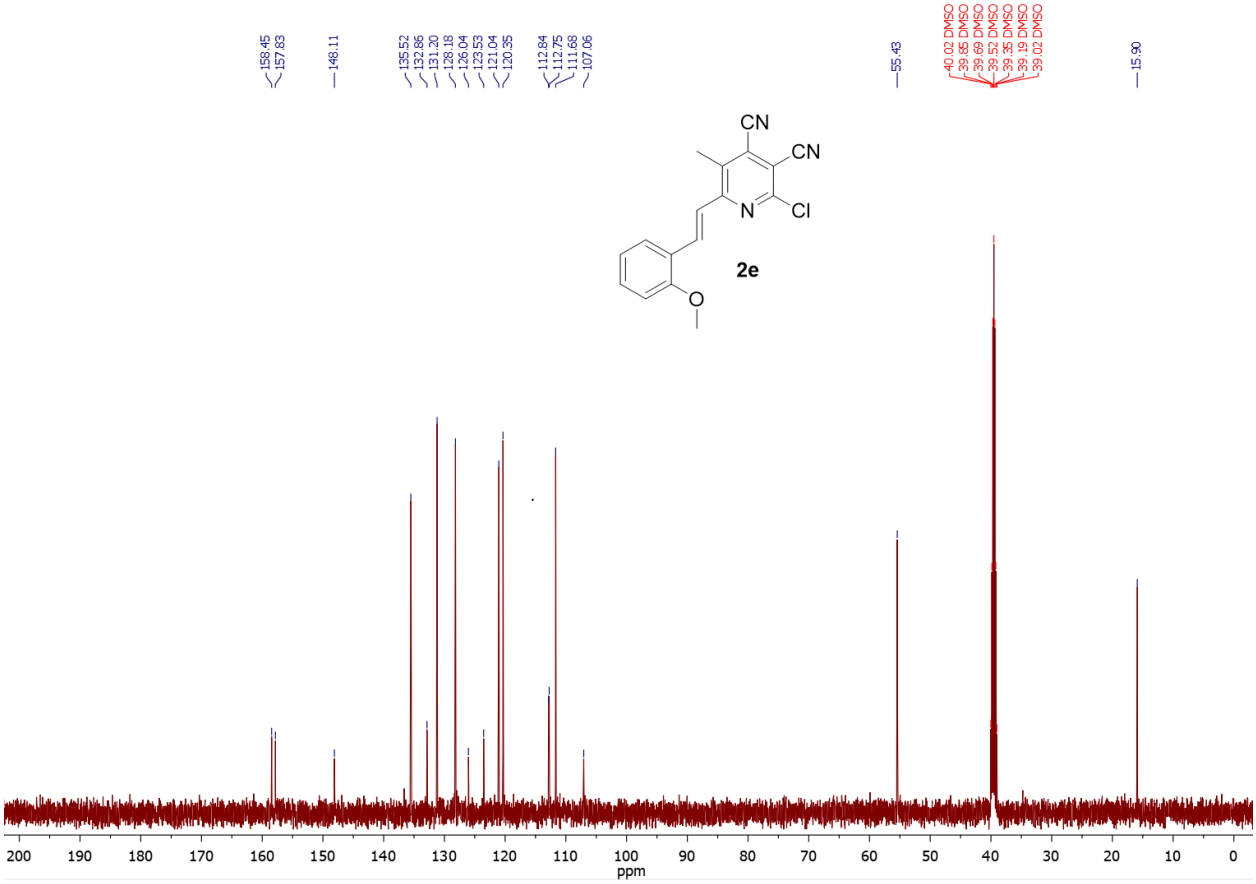

Figure S14 ^{13}C NMR-spectrum of **2e** (126 MHz, DMSO-d_6)

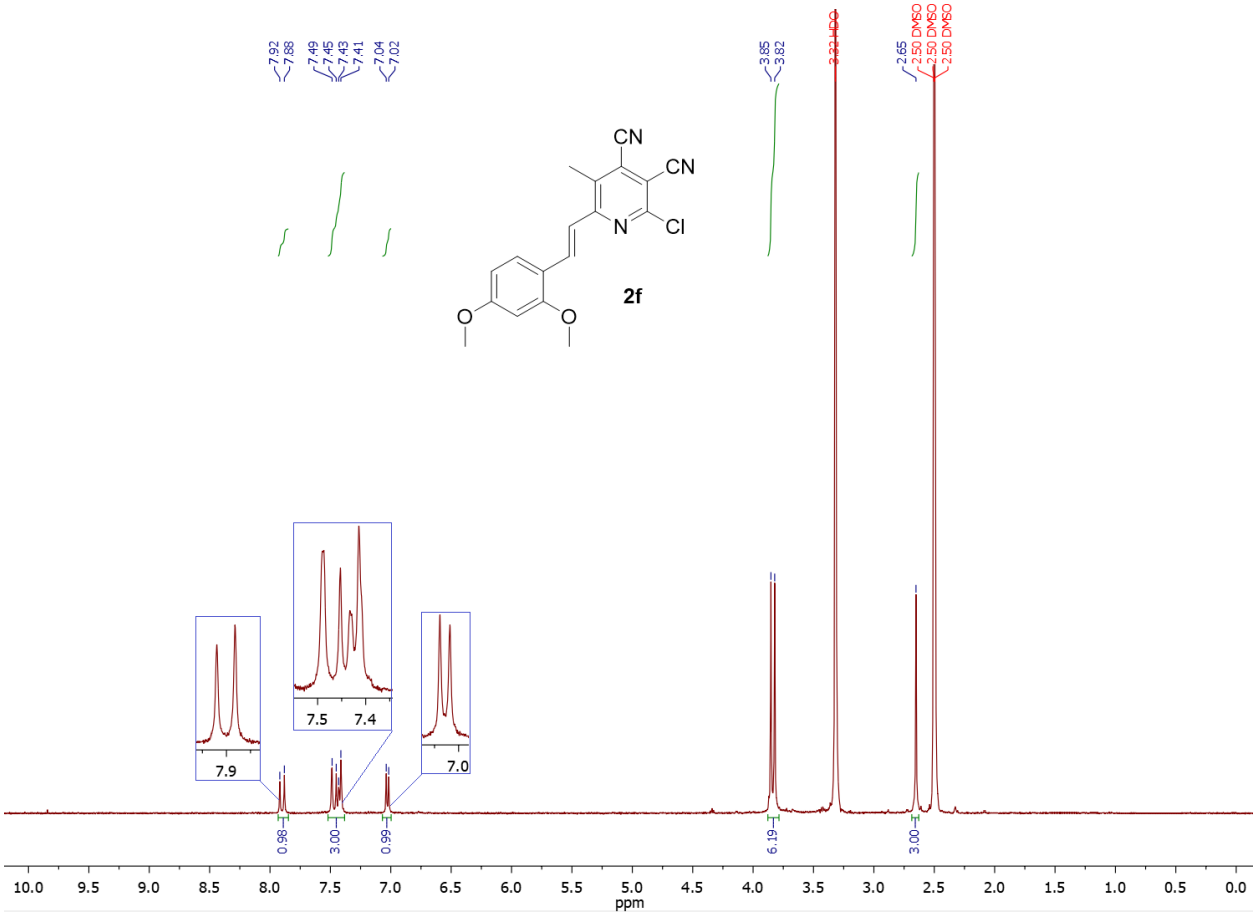

Figure S15 ^{1}H NMR-spectrum of **2f** (500 MHz, DMSO-d_6)

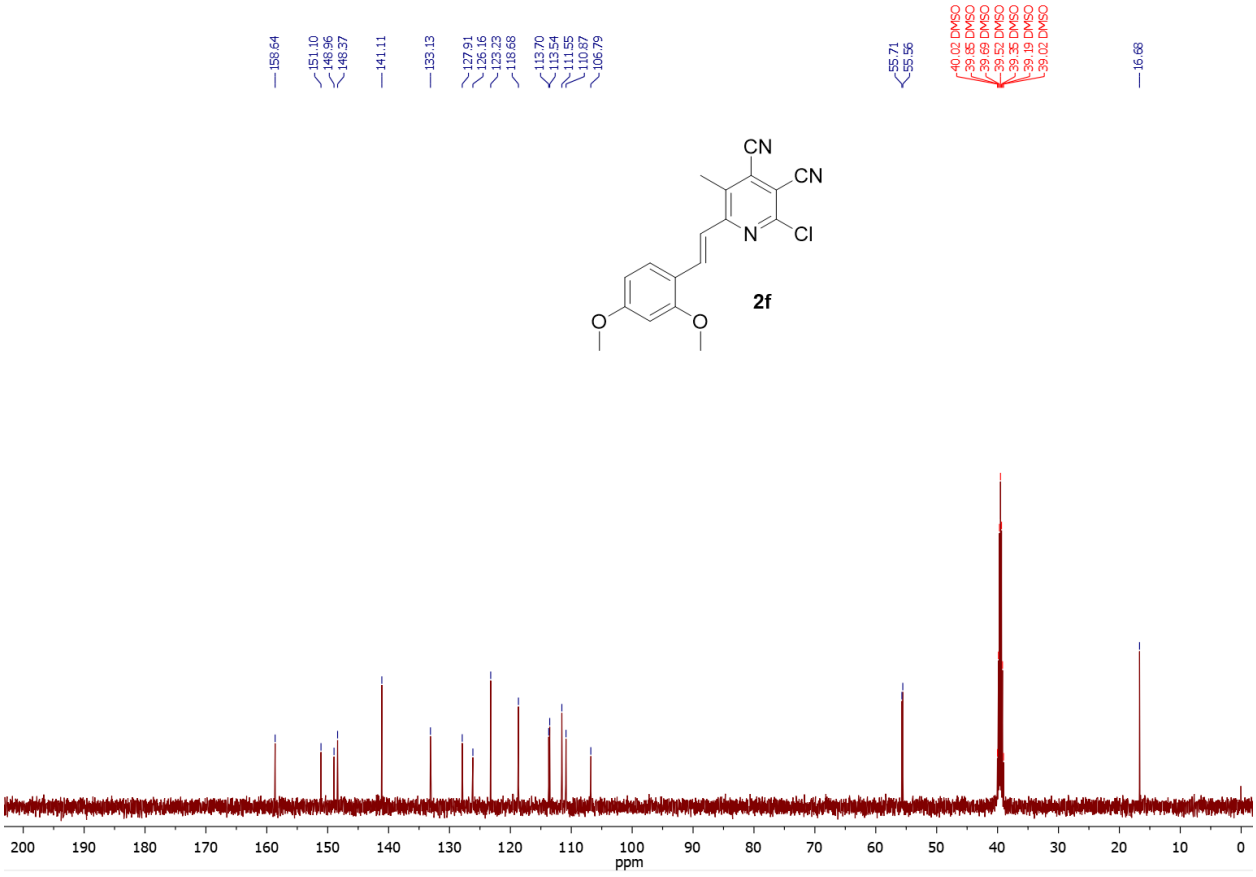

Figure S16 ^{13}C NMR-spectrum of **2f** (126 MHz, DMSO-d_6)

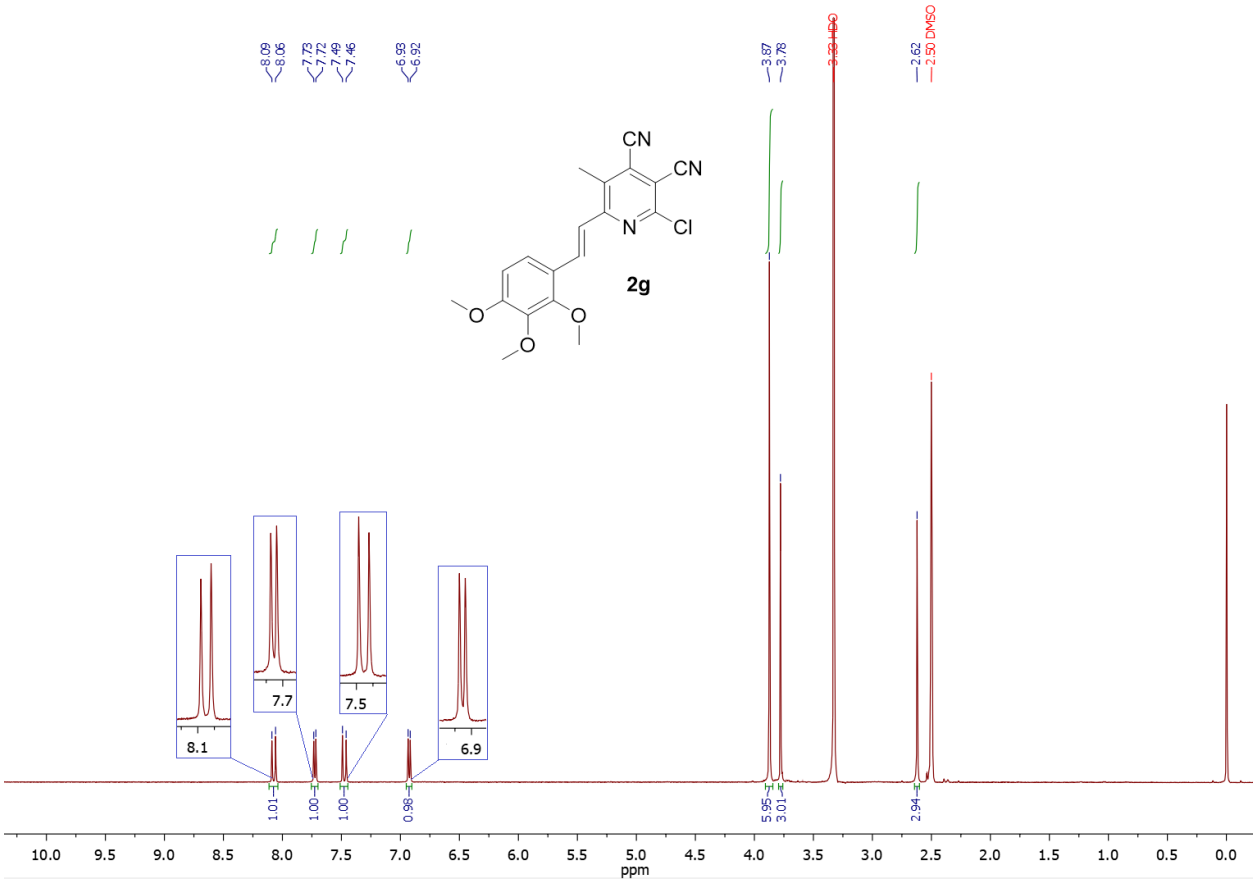

Figure S17 ^{1}H NMR-spectrum of **2g** (500 MHz, DMSO-d_6)

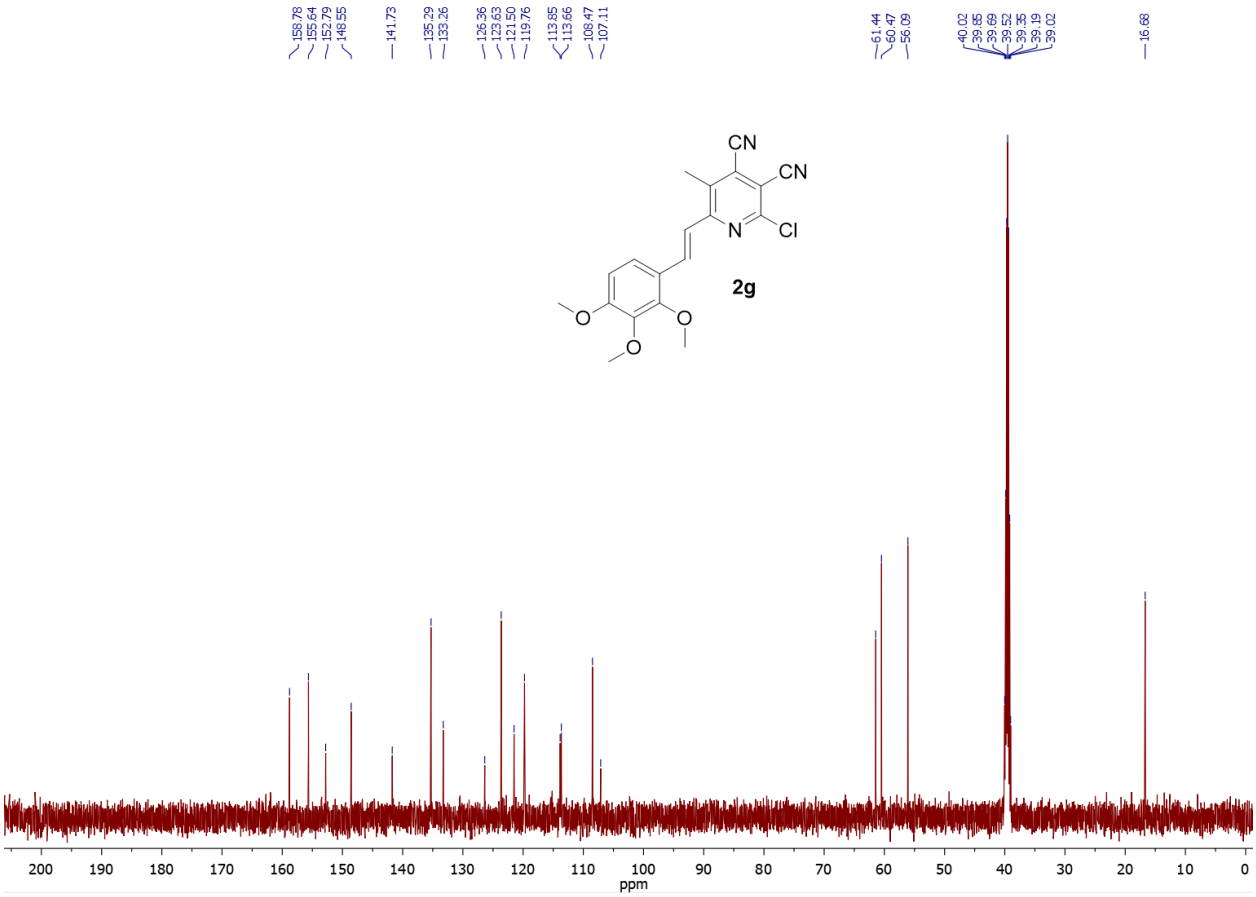

Figure S18 ^{13}C NMR-spectrum of **2g** (126 MHz, DMSO-d_6)

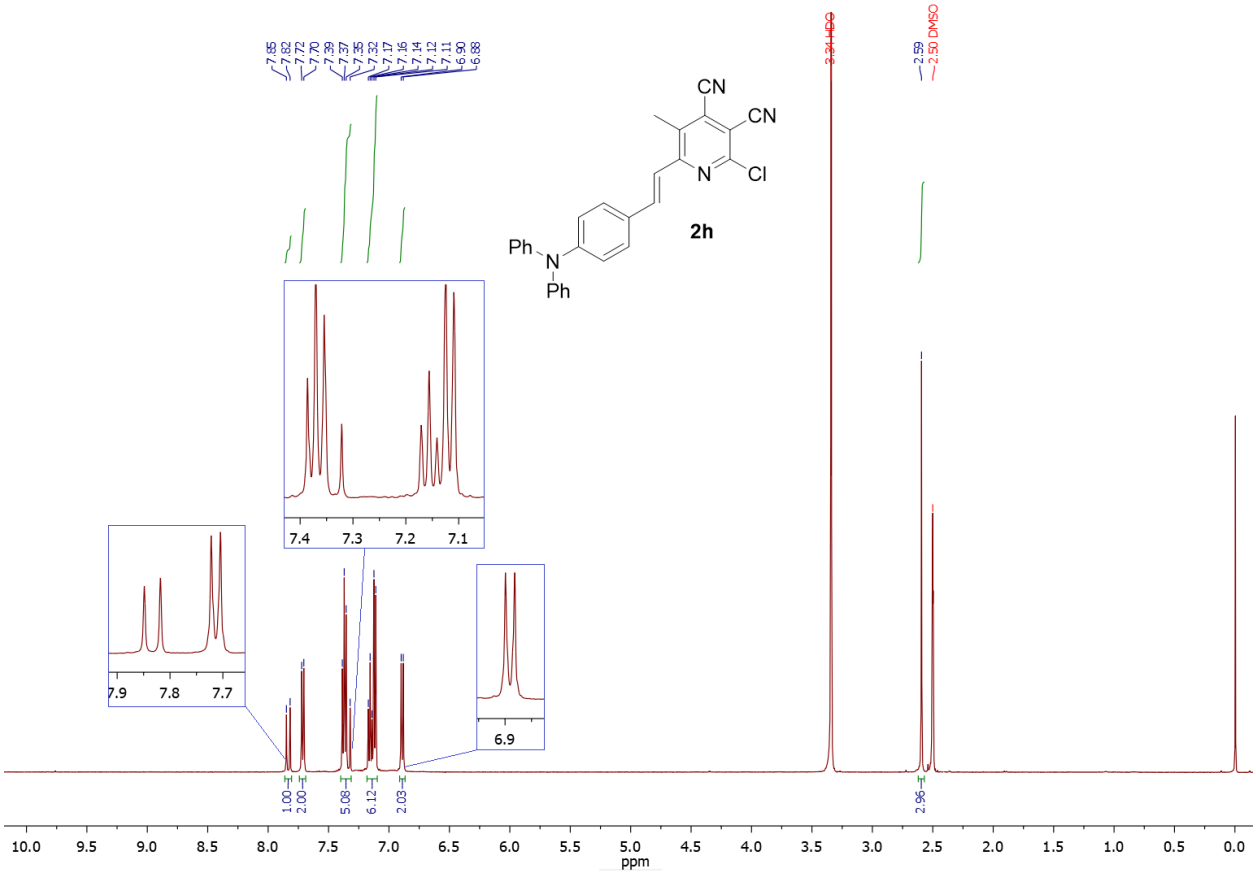

Figure S19 ^{1}H NMR-spectrum of **2h** (500 MHz, DMSO-d_6)

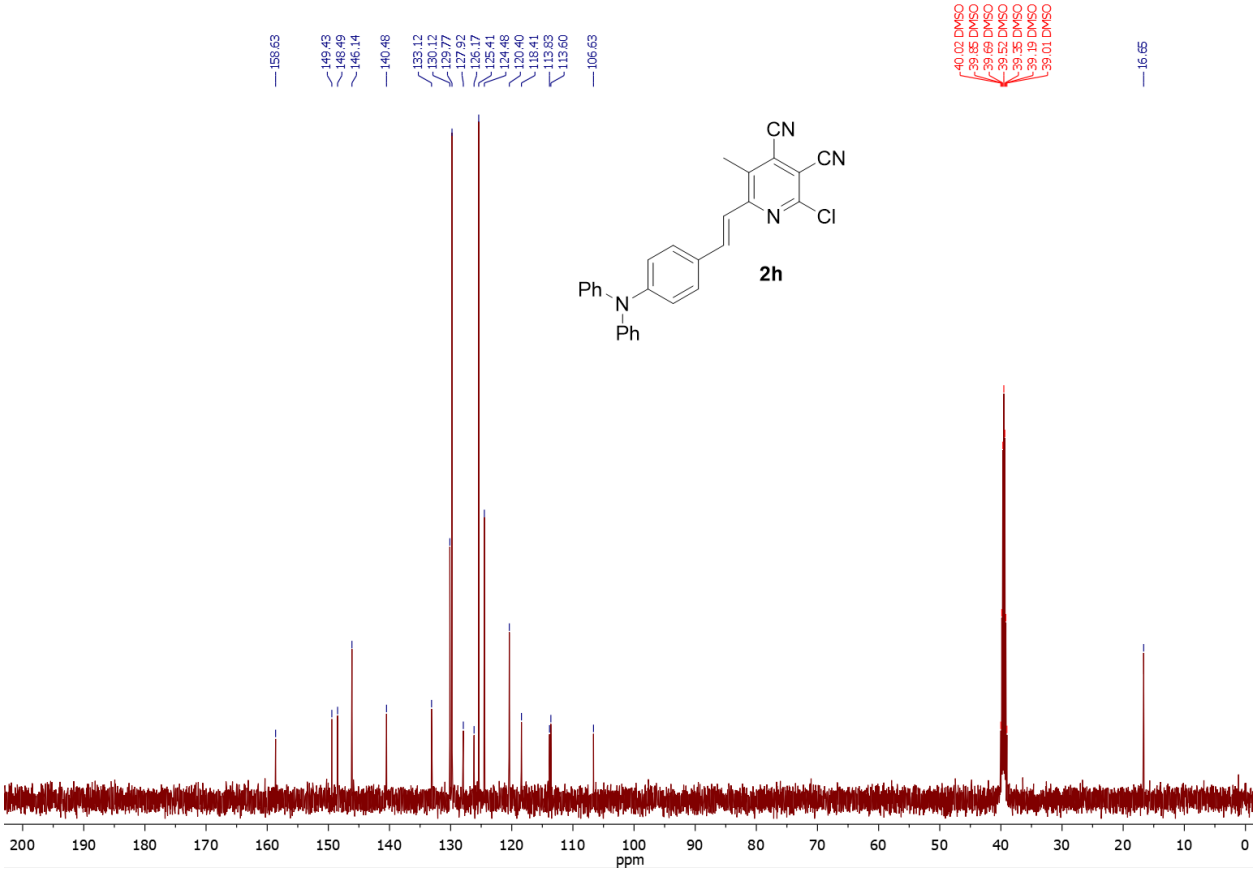

Figure S20 ^{13}C NMR-spectrum of **2h** (126 MHz, DMSO-d_6)

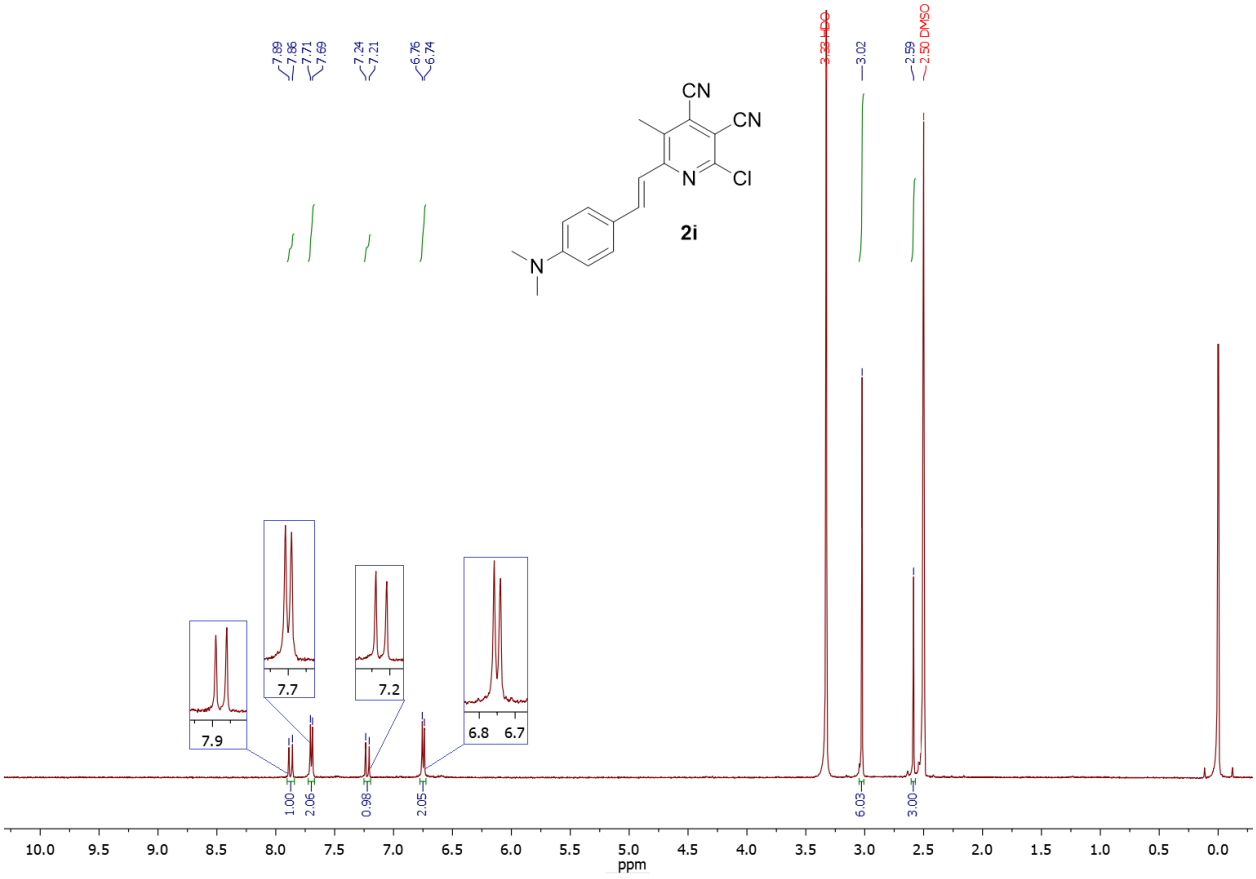

Figure S21 ^{1}H NMR-spectrum of **2i** (500 MHz, DMSO-d_6)

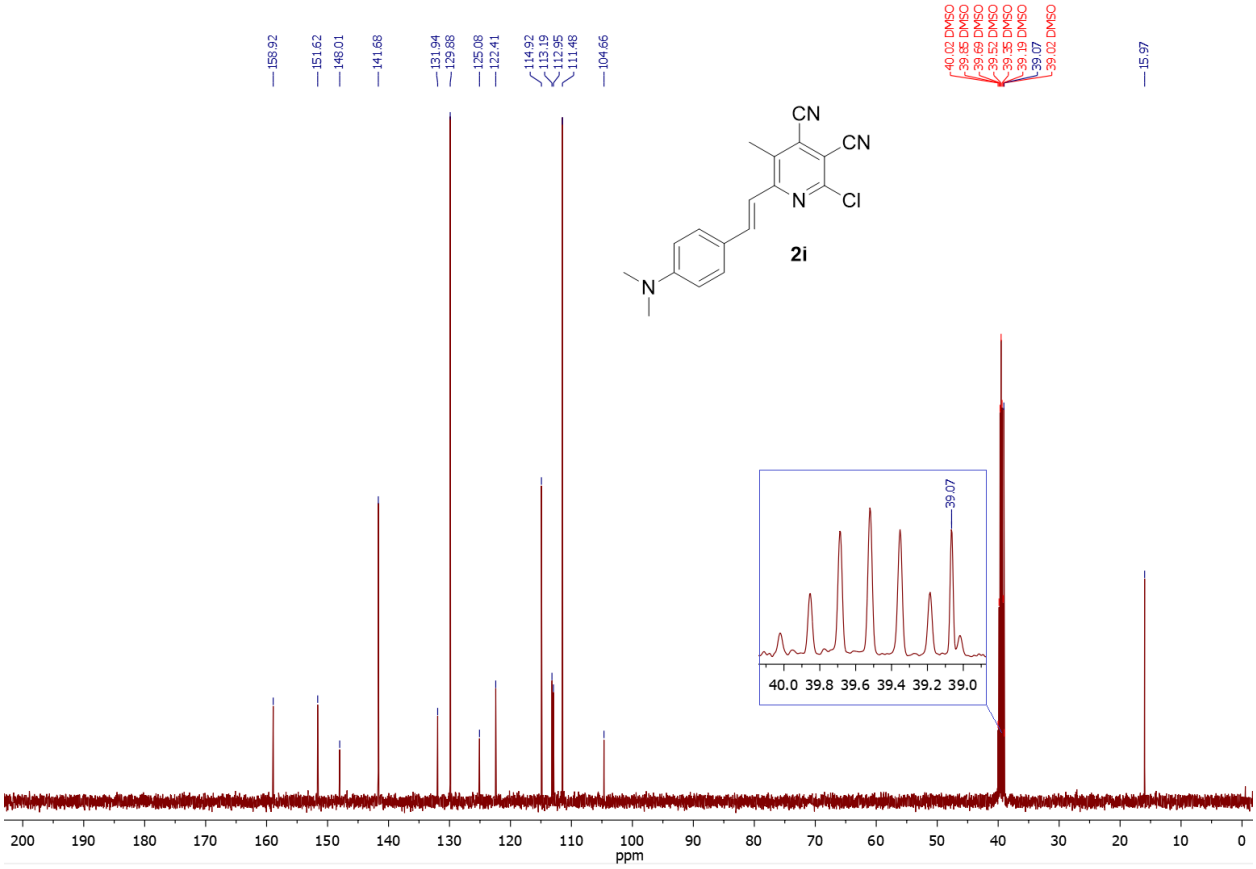

Figure S22 ^{13}C NMR-spectrum of **2i** (126 MHz, DMSO-d_6)

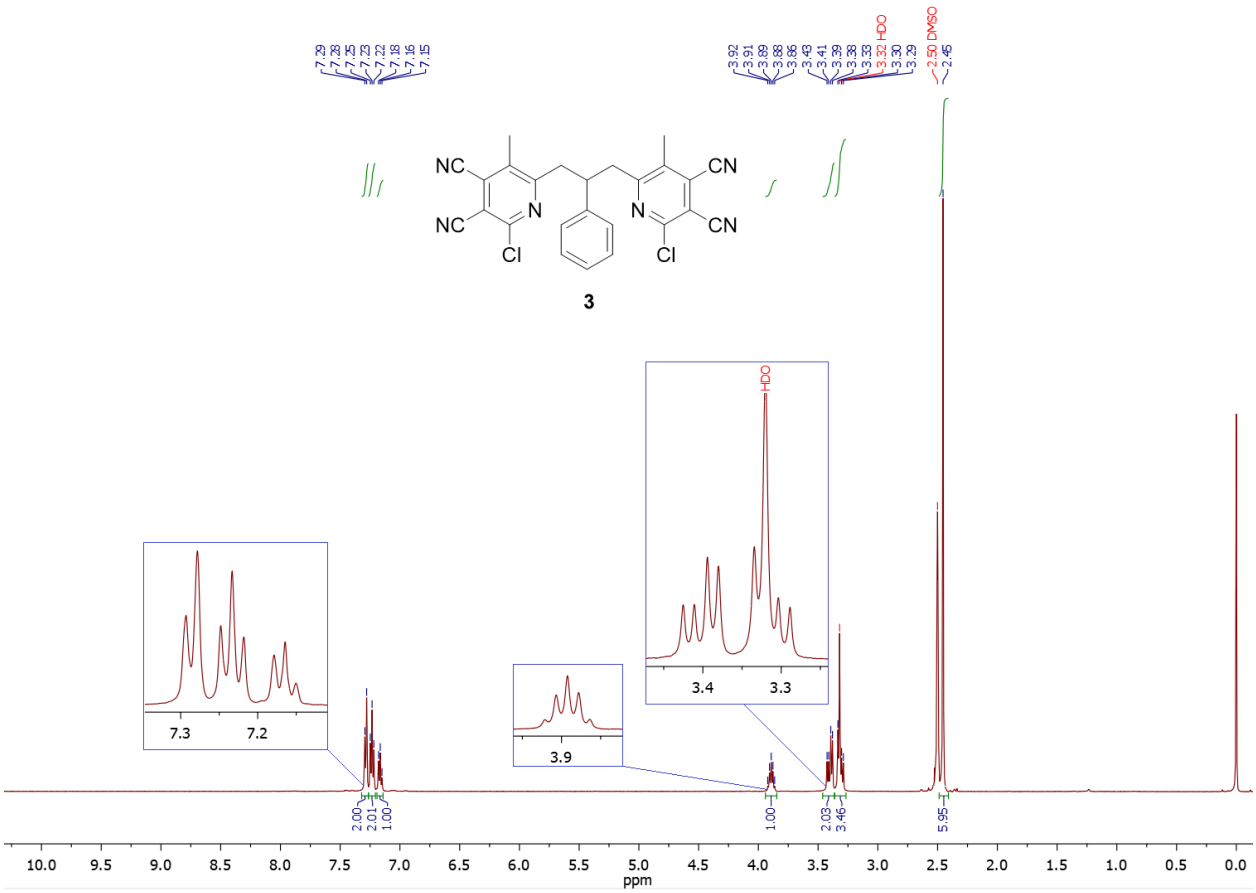

Figure S23 ^{1}H NMR-spectrum of **3** (500 MHz, DMSO-d_6)

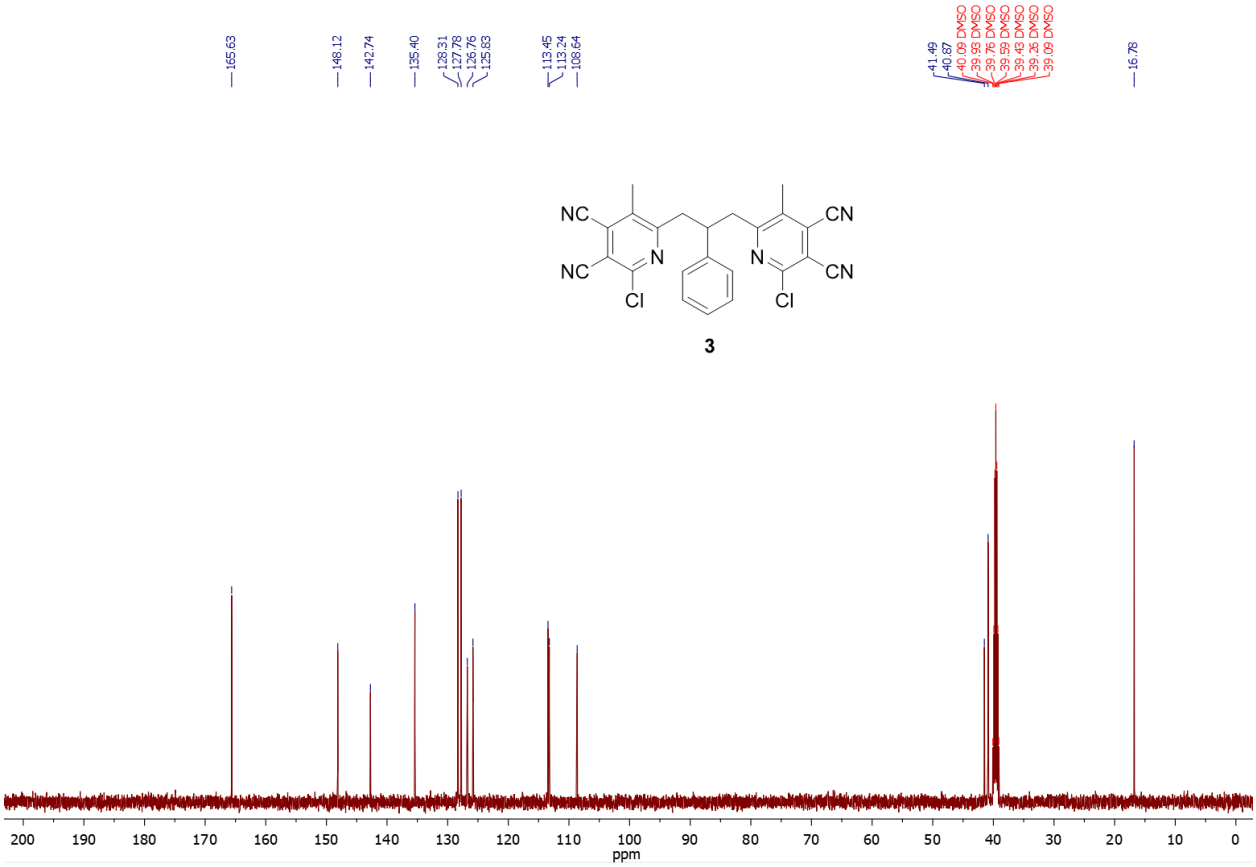

Figure S24 ^{13}C NMR-spectrum of **3** (126 MHz, DMSO-d_6)

2. Photo-physical characteristics of compounds 2, 6 and 7

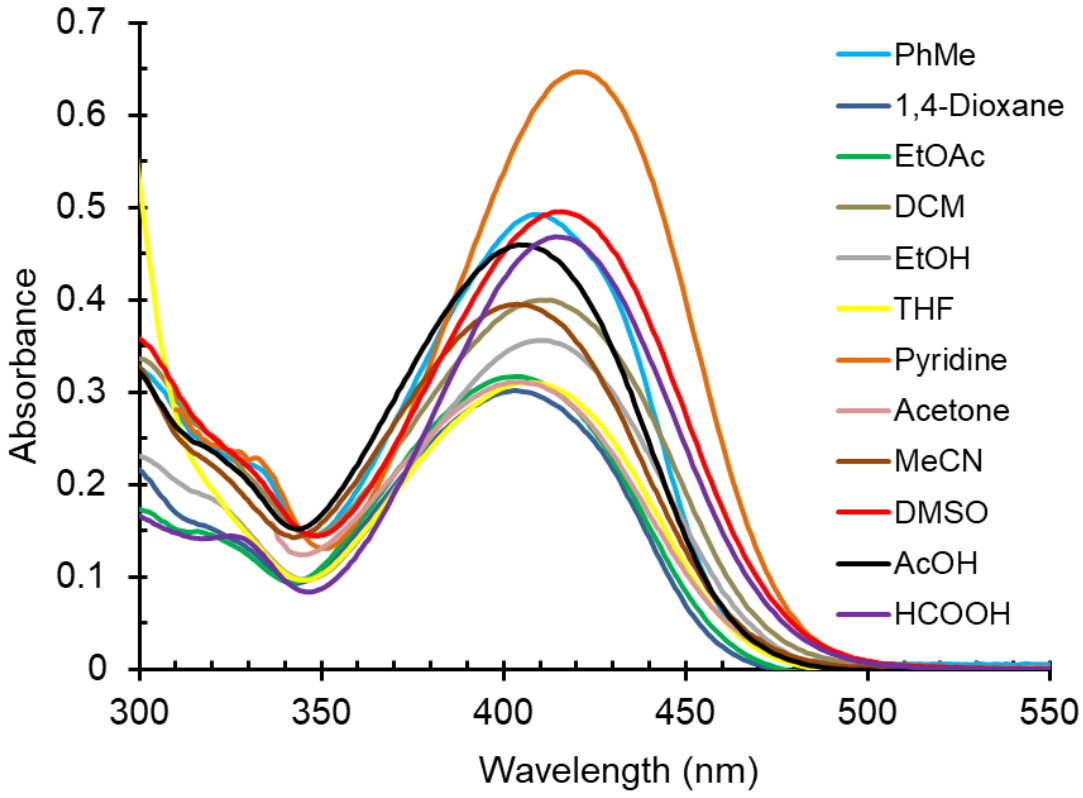

Figure S25 Absorption spectra of **2c** in various solvents (3×10^{-5} M)

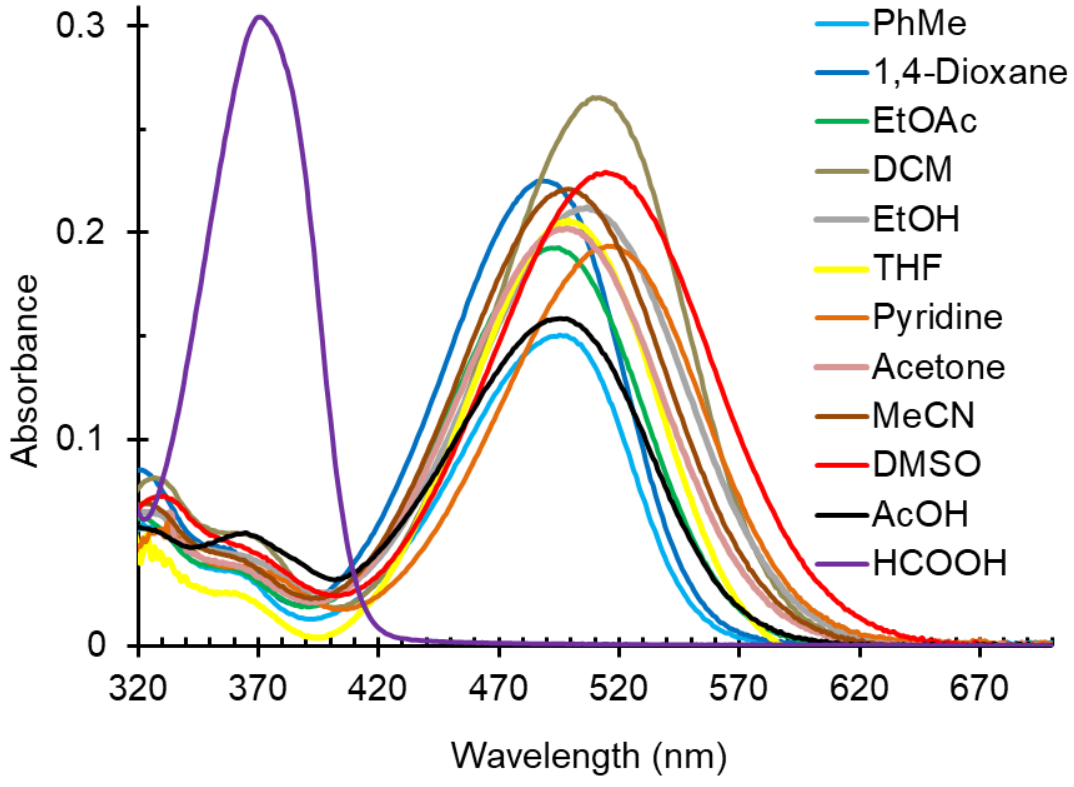

Figure S26 Absorption spectra of **2i** in various solvents (10^{-5} M)

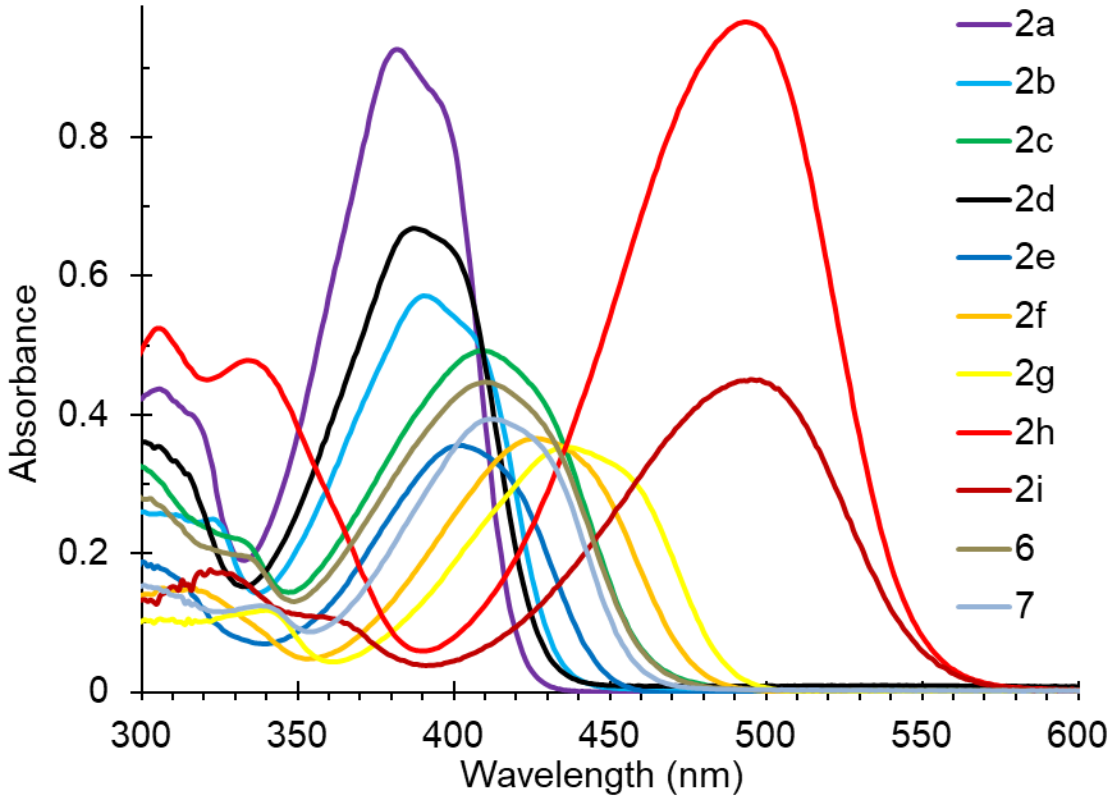

Figure S27 Absorption spectra of **2, 6** and **7** in toluene at 3×10^{-5} M

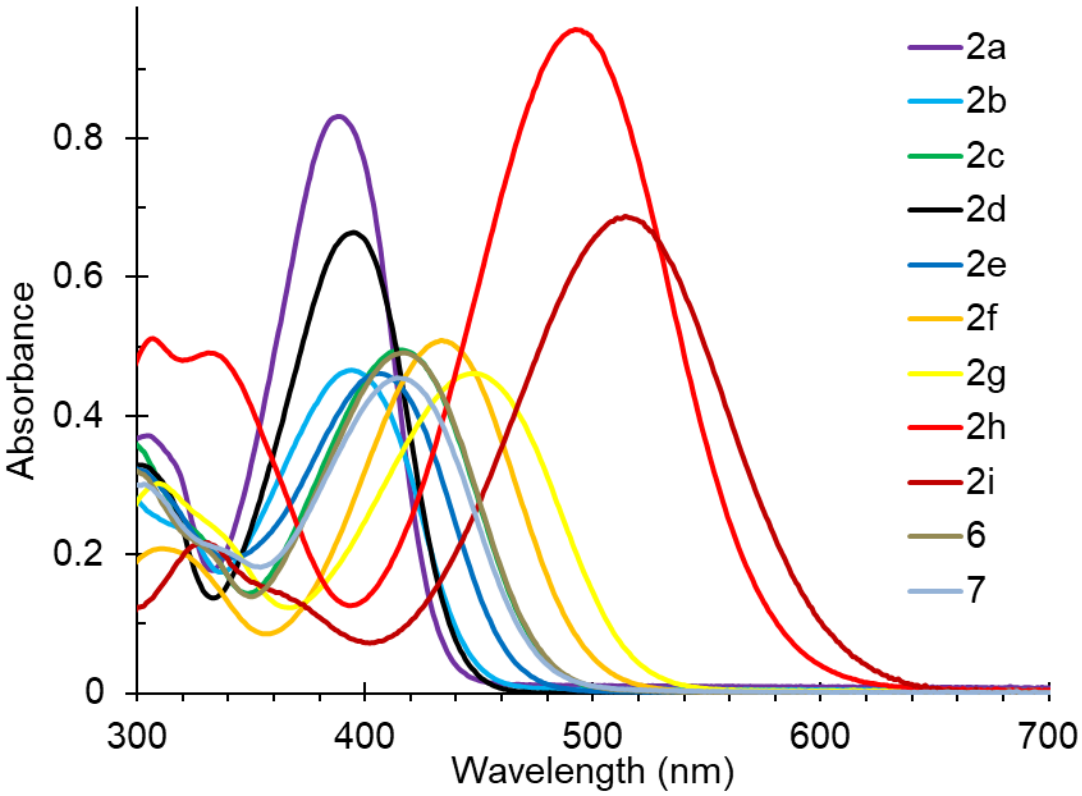

Figure S28. Absorption spectra of **2,6** and **7** in DMSO at 3×10^{-5} M

Table S1. Solvatochromic characteristics of **2c**

Solvent	λ_{abs}, nm[a]	ε, M^{-1} cm^{-1}	λ_{em}, nm[b]	Stokes shift		Φ_{em},%[c]
				nm	cm^{-1}	
PhMe	409	16400	482	73	3703	3.9
1,4-Dioxane	403	10100	493	90	4530	3.0
DCM	410	13300	523	113	5270	3.2
THF	408	10300	517	109	5167	4.5
EtOAc	404	10600	515	111	5335	3.8
AcOH	404	15300	529	125	5849	4.3
HCOOH	414	15600	565	151	6455	4.4
EtOH	411	11900	546	135	6016	6.1
Pyridine	420	21600	545	125	5461	13.6
Acetone	405	10400	541	136	6207	6.2
MeCN	403	13200	549	146	6599	7.7
DMSO	416	16500	562	146	6245	14.1

[a] Absorption maxima of solutions with concentration of 3×10^{-5} M

[b] Emission maxima of solutions with concentration of 3×10^{-5} M (absorption maxima were used for excitation)

[c] The relative emission quantum yield (Φ_{em}) was measured using 7-hydroxy-4-methylcoumarin in phosphate buffer with pH 10 (Φ_{em} 0.7) using 330 nm as excitation wavelength.

Table S2. Photo-physical characteristics of **2a-i**, **6** and **7** in DMSO

Compound	λ_{abs}, nm[a]	ε, M^{-1} cm^{-1}	λ_{em}, nm[b]	Stokes shift		Φ_{em},%
				nm	cm^{-1}	
2a	388	27700	488	100	5281	1.2[c]
2b	394	15500	510	116	5773	4.4[c]
2c	416	16500	562	146	6245	14.1[c]
6	417	16400	563	146	6219	17.7[c]
7	414	15200	563	149	6393	13.8[c]
2d	395	22200	563	168	7554	9.8[c]
2e	406	15400	558	152	6709	0.7[c]
2f	434	16900	611	177	6675	2.3[d]
2g	447	15400	587	140	5336	6.0[d]
2h	492	31900	655, 697	163, 205	5058, 5978	0.2[d]
2i	515	22900	710	196	5371	0.2 [d]

[a] Absorption maxima of solutions with concentration of 3×10^{-5} M

[b] Emission maxima of solutions with concentration of 3×10^{-5} M (absorption maxima were used for excitation)

[c] The relative emission quantum yield (Φ_{em}) was measured using 7-hydroxy-4-methylcoumarin in phosphate buffer with pH 10 (Φ_{em} 0.7) using 330 nm as excitation wavelength

[d] The relative emission quantum yield (Φ_{em}) was measured using Rhodamine 6G in ethanol (Φ_{em} 0.95) using 450 nm as excitation wavelength.

3. Calculation of charge-transfer properties of compounds 2c and 2i

The change in the dipole moment Δμ (in Debyes) upon transition between the ground and excited states for compounds **2c** and **2i** was estimated using the Lippert–Mataga equation:

$$\Delta\nu = \nu_{abs} - \nu_{em} = f(\varepsilon_r, n)\,\frac{2(\Delta\mu)^2}{hca^3} + const$$

where $\Delta\nu$ is the Stokes shift value found as the difference between absorption (ν_{abs}) and emission (ν_{em}) maxima wavenumbers (in cm^{-1}) in corresponding solvent; h is Planck's constant (6.6262×10^{-27} erg×s); c is the speed of light in vacuum (2.9979×10^{10} cm/s); a is the cavity radius (in Å) in which the solute resides estimated from the van der Waals volume ($V_{VDW} = \frac{4}{3}\pi a^3$) of the fluorophore molecule; $f(\varepsilon_r, n)$ is the orientation polarizability (Lippert-Mataga polarity function) of the solvent defined as:

$$f(\varepsilon_r, n) = \frac{\varepsilon_r - 1}{2\varepsilon_r + 1} - \frac{n^2 - 1}{n^2 + 1}$$

where ε_r is the static dielectric constant and n is the optical refractivity index of the solvent (Table S4).

The van der Waals volumes (V_{VDW}) of molecule **2c** and **2i** were calculated by the following reported formula[1]:

$$V_{VDW} = \sum(all\ atom\ contributions) - 5.92N_B - 14.7R_A - 3.8R_{NA}$$

where N_B = $(Number\ of\ atoms - 1 + R_A + R_{NA})$; R_A is the number of aromatic rings; R_{NA} is the number of non-aromatic rings; and V_{vdW} for C = 20.58 $Å^3$; for H = 7.24 $Å^3$; for O = 14.71 $Å^3$; for N = 15.60 $Å^3$; for Cl = 22.45 $Å^3$

Table S3. Calculated Van Der Waals Volume (V_{VDW}) and cavity radius (a).

Dye	Molecular Formula	∑(all atom contributions)	N_B	Vvdw (Å³)	a (Å)
2c	$C_{17}H_{12}ClN_3O$	520.7	35	284.1	4.1
2i	$C_{18}H_{15}ClN_4$	563.8	39	303.6	4.2

[1]Y. H. Zhao, M. H. Abraham, and A.M. Zissimos, Fast Calculation of van der Waals Volume as a Sum of Atomic and Bond Contributions and Its Application to Drug Compounds *J. Org. Chem.* 2003, 68, 7368-7373 https://doi.org/10.1021/jo034808o

Table S4. Solvent parameters and Stokes shift values of fluorophores

Solvent	ε_r	n	f	$\Delta\nu$ (**2c**)	$\Delta\nu$ (**2i**)
PhMe	2.38	1.4969	0.013	3703	3049
1,4-Dioxane	2.25	1.4224	0.025	4530	3965
DCM	8.93	1.4241	0.217	5270	4051
THF	7.53	1.4073	0.209	5167	4536
EtOAc	6.02	1.3724	0.200	5335	4553
AcOH	6.15	1.3716	0.202	5849	4258
EtOH	24.5	1.3614	0.289	6016	4503
Pyridine	12.4	1.5102	0.212	5461	4447
Acetone	20.7	1.3587	0.284	6207	5526
MeCN	37.5	1.3441	0.305	6599	5631
DMSO	46.7	1.4783	0.263	6245	5371