Supporting Information

π-Extended push-pull azo-pyrrole photoswitches: Synthesis, solvatochromism and optical band gaps

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1. General Information

Unless otherwise stated, all the reactions for the synthesis of the compounds **1** and **2** were carried out in open vessel conditions. The synthesis of the palladium complex was conducted under argon atmosphere with standard Schlenk techniques as reported elsewhere.[i] All temperature given for reaction conditions are externally measured. All reactions were monitored by TLC.

2. Materials

Commercial materials were used as received: THF and CH_2Cl_2 purchased from Sigma-Aldrich in anhydrous form. Benzene, THF, Dioxane, $CHCl_3$, Methanol and Ethanol were purchased from Sigma-Aldrich in HPLC and/or spectrophotometric quality. ASTM type 1 ultra-pure water (Millipore-Q system, 18.2 M Ωcm) was used as solvent for the aggregation studies. HCl, $NaNO_2$, *N*-methylpyrrole, 1,2,5-Trimethyl pyrrole, pyridine, aniline, 4-Iodoaniline, 4-nitroaniline, 4-trifluoromethylaniline, ferrocene, t-BuLi (1.7 M), $Cr(CO)_6$, Et_3OBF_4, S_8, $NaBH_4$, $PdCl_2$, PPh_3, phenylboronic acid, 4-nitrophenylboronic acid, 4-trifluoromethylphenyl boronic acid, 4-methansulfonylphenyl boronic acid, 4-(Dimethylamino)phenylboronic acid and K_2CO_3 were purchased from Sigma-Aldrich. Analytical thin layer chromatography was performed on DC-Fertigfolien ALUGRAM® Xtra SIL G/UV254 MACHEREY-NAGEL. Column chromatography was performed on Silica 60, 0.063-0.2 mm MACHEREY-NAGEL.

3. Methods

Microwave irradiation experiments were performed using a Monowave 300 single-mode microwave reactor. The reaction temperature is monitored by an internal fiber-optic (FO) temperature probe (ruby thermometer) protected by a borosilicate immersion well inserted directly into the reaction mixture. Reaction times refer to the hold time at the desired set temperature and not to total irradiation time. A hydraulic sensor integrated in the swiveling cover of the instrument performs pressure sensing. The reusable 10 mL Pyrex vial is sealed with PEEK snap caps and standard PTFE coated silicone septa. Reaction cooling is performed by compressed air automatically after the heating period has elapsed.

The equipment used for irradiation with IR energy was created by employing an empty cylindrical metal vessel in which an Osram lamp (bulb model Thera-Therm, 250 W, 125 V) was inserted.[1] This lamp is special short-wave IR lamp (IR-A) for use in body care and wellness applications, with a maximum radiation at a wavelength of about 1100 nm. The lamp instantly emits a full thermal output as soon as it is switched on. For controlling the temperature, a Digi-Sense variable-time power controller was used. This time controller turned the output load on and off and then repeated the cycle. All the reactions were performed in open atmosphere.

Melting points were obtained on a Stuart Melting Point Apparatus SMP10 and they are uncorrected. All compounds were characterized by IR spectra, recorded on a Perkin-Elmer Spectrum 100 FT-IR spectrophotometer provide with an ATR polarization attachment and all data are expressed in wave numbers (cm^{-1}). NMR spectra were measured on a Bruker Avance 300 Spectrometer, at an operating frequency of 300 MHz for ^{1}H and 75 MHz for ^{13}C, using tetramethylsilane (TMS) as internal reference and $CDCl_3$ as solvent; chemical shifts values are given in parts per million (ppm), relative to TMS. Mass spectrometry analyses were obtained on a JEOL SX102A (EI^+ and FAB^+) and on AccuTOF JMS-T100LC (DART), the values of the signals are expressed in mass/charge units (*m/z*), followed by the relative intensity with reference to a 100% base peak. UV-Vis absorption spectra were recorded at 298 K on a Varian Cary 100 UV-Vis spectrophotometers, using spectrophotometric grade solvents purchased from Sigma-Aldrich Co. and 1 cm quartz cell. The solvatochromic study was performed using 10^{-5} M to 10^{-4} M solutions of azopyrrole dyes in several solvents at room temperature. The aggregation study was carried out using $5x10^{-5}$ M solutions of azopyrrole dyes at different MeOH: H_2O ratios, from 100:0 to 20:80 at room temperature.

^{1}H and ^{13}C NMR Spectra.

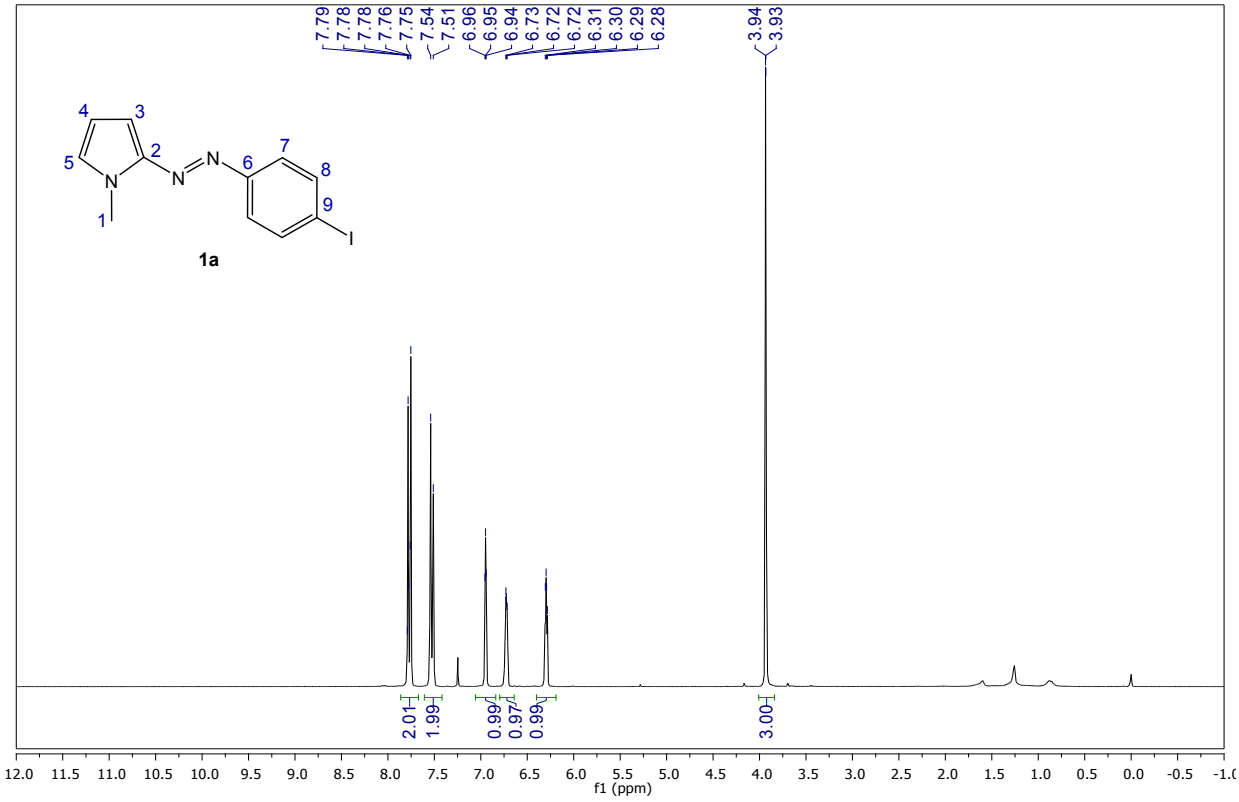


Figure S1. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **1a**

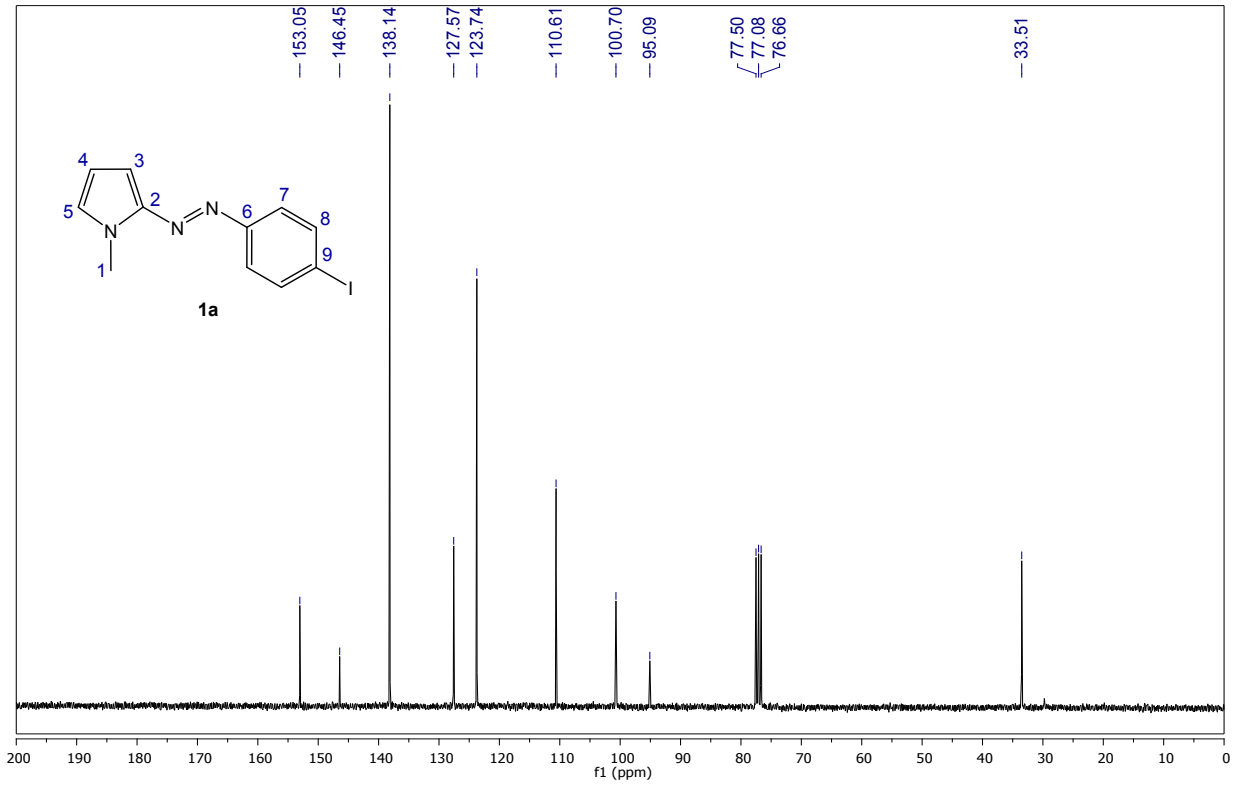


Figure S2. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **1a**

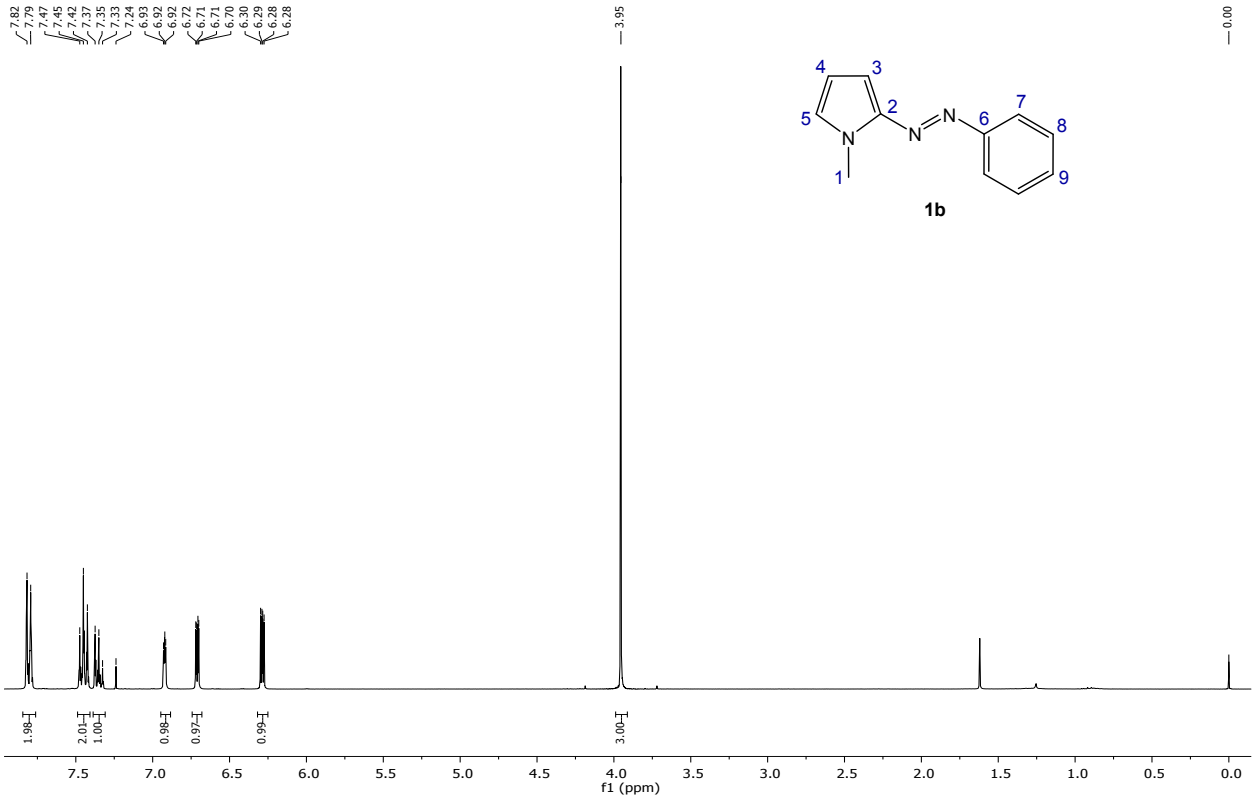


Figure S3. ^{1}H NMR spectrum of compound **1b**

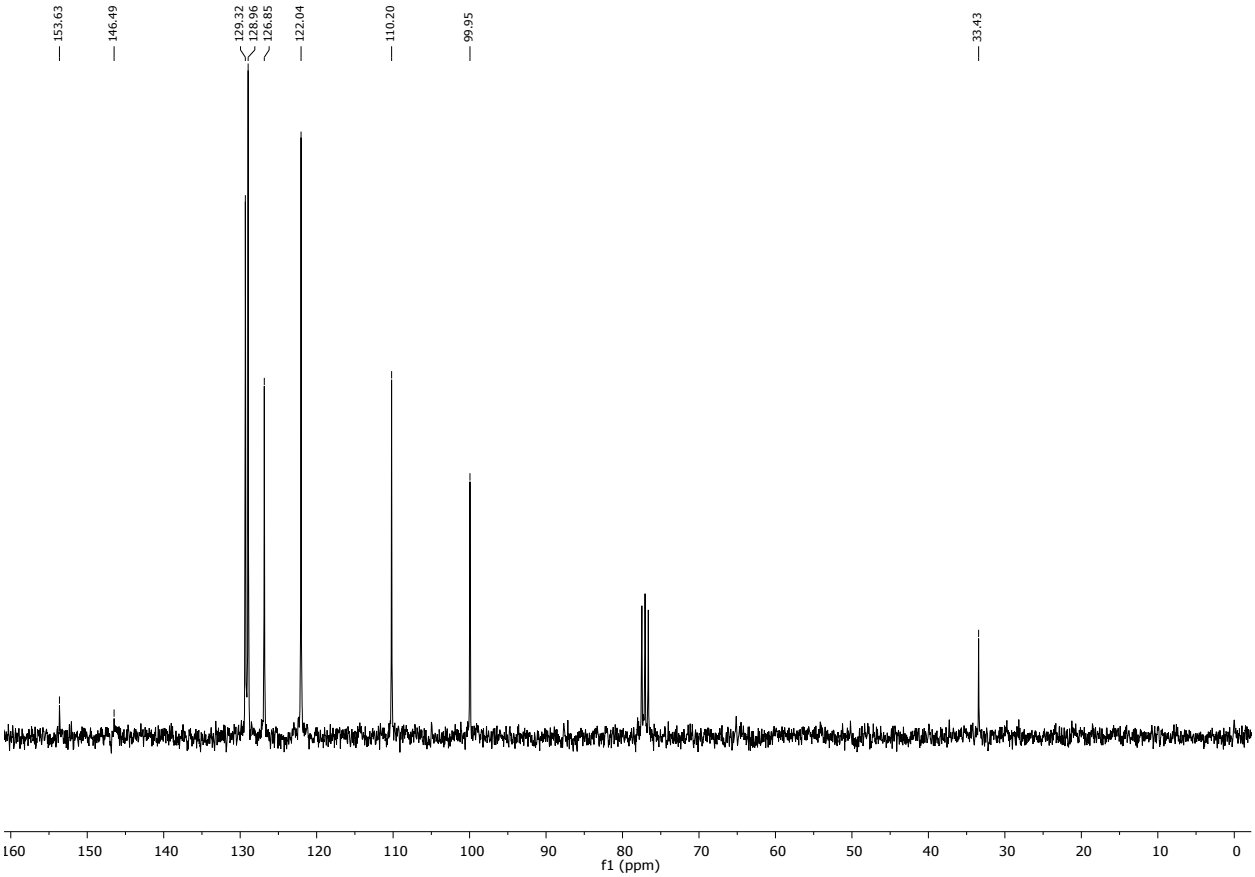


Figure S4. ^{13}C NMR spectrum of compound **1b**

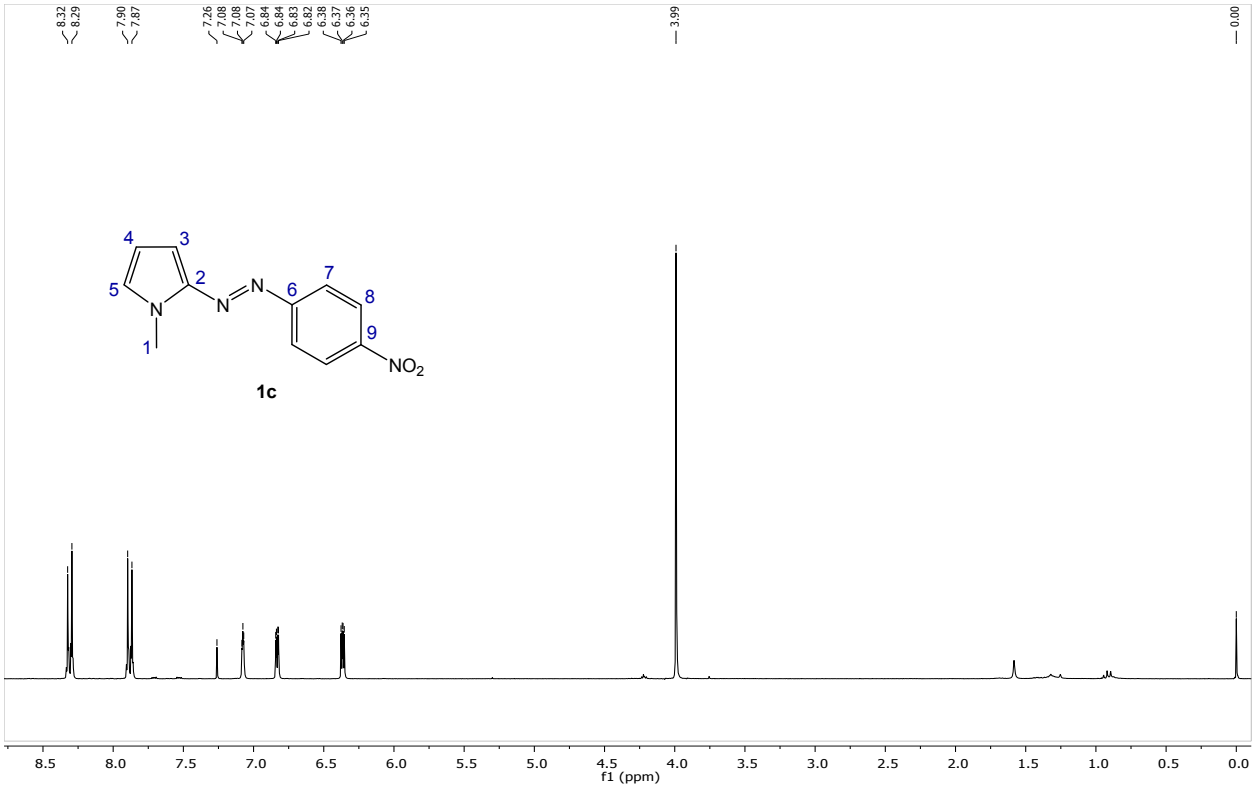


Figure S5. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **1c**

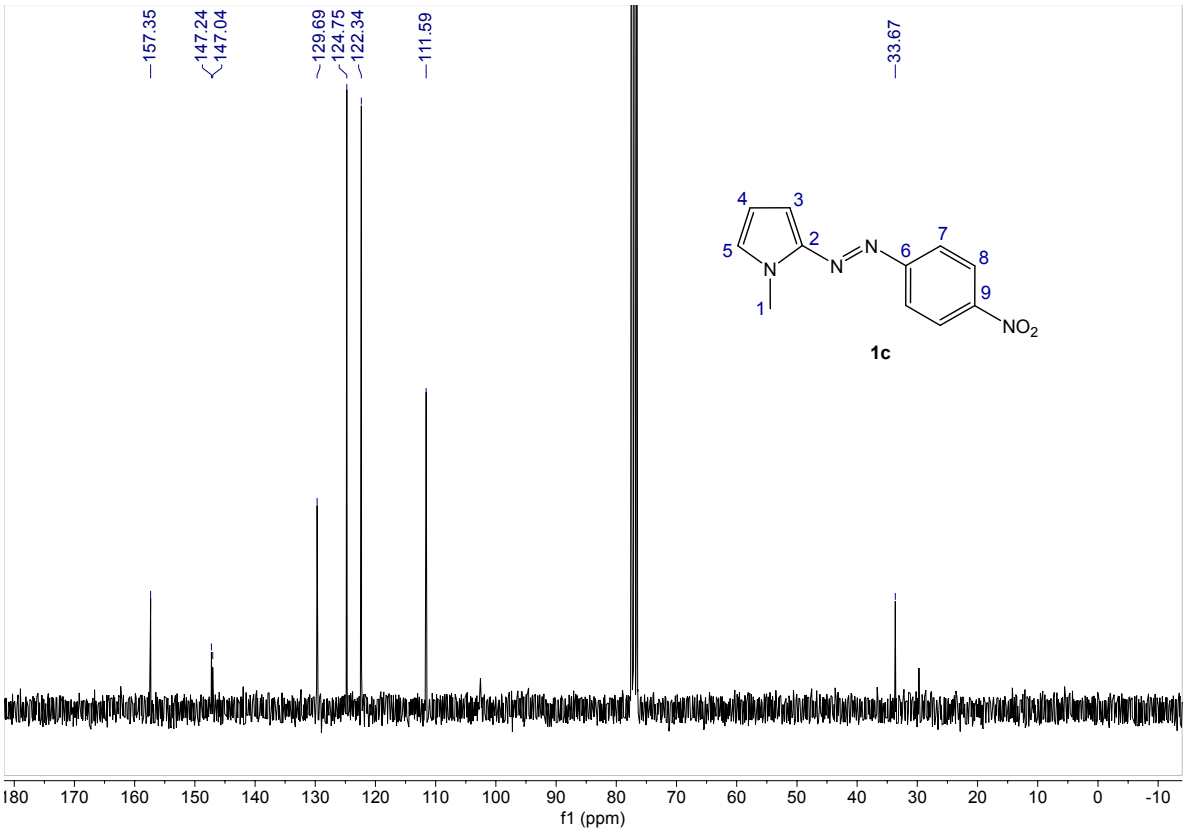


Figure S6. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **1c**

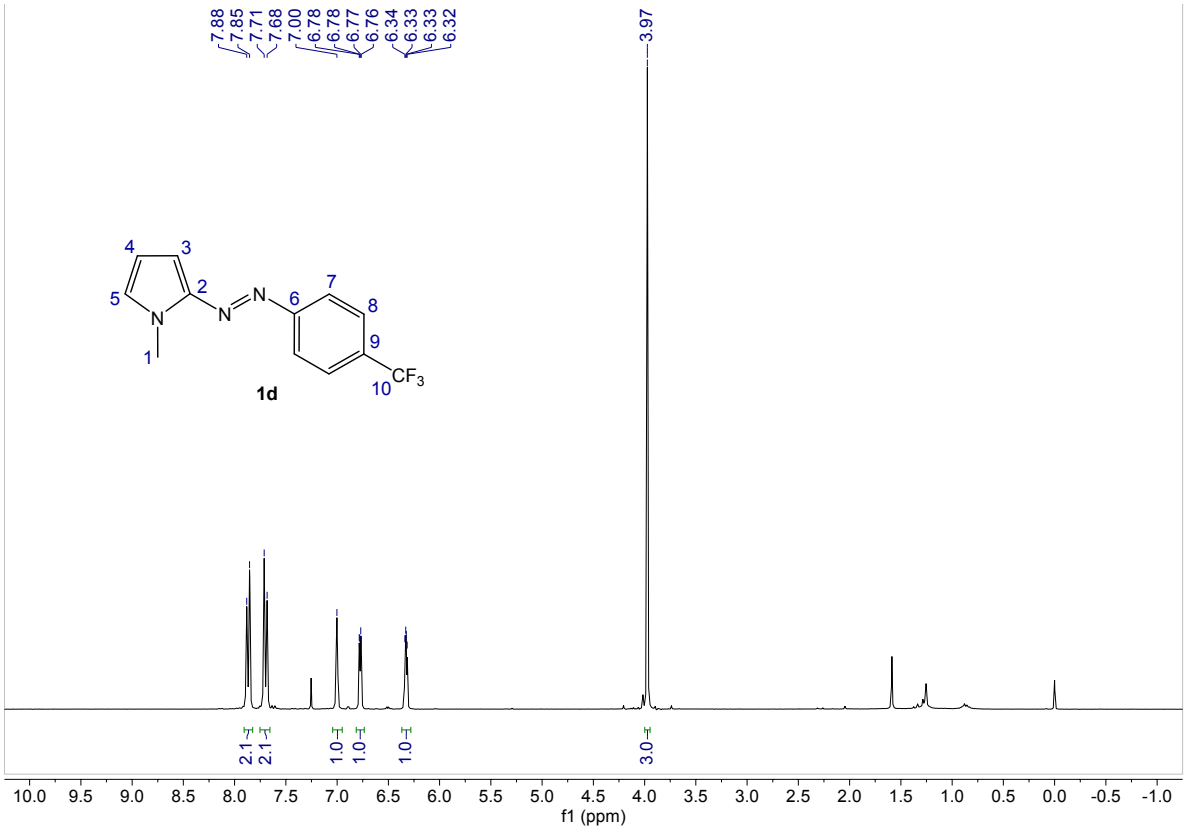


Figure S7. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **1d**

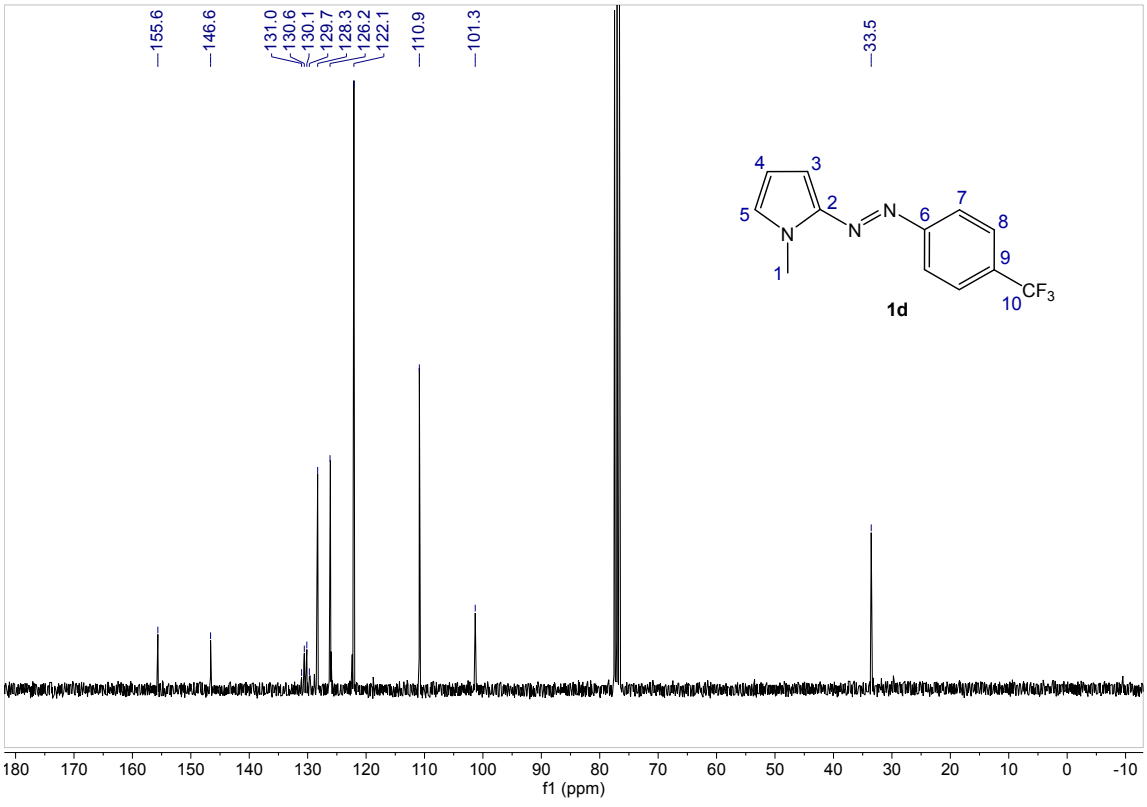


Figure S8. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **1d**

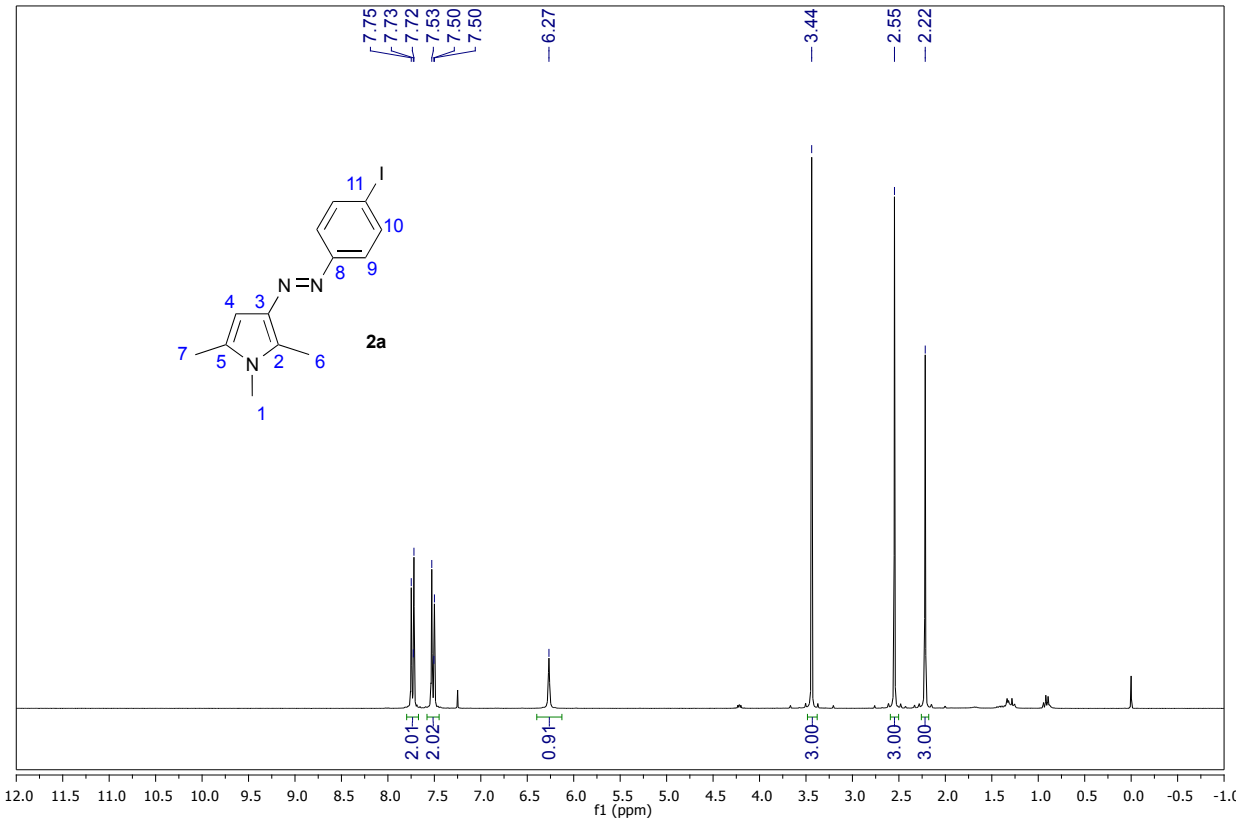


Figure S9. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **2a**

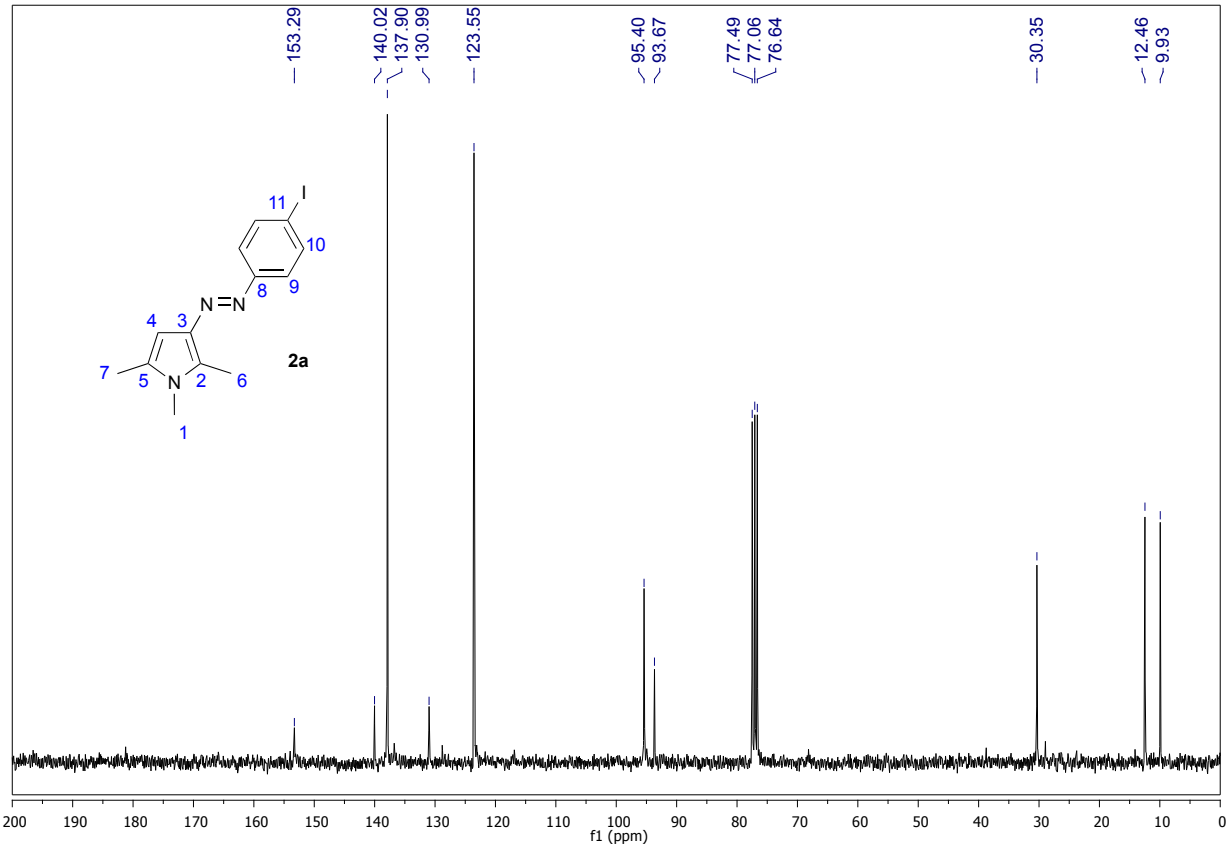


Figure S10. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **2a**

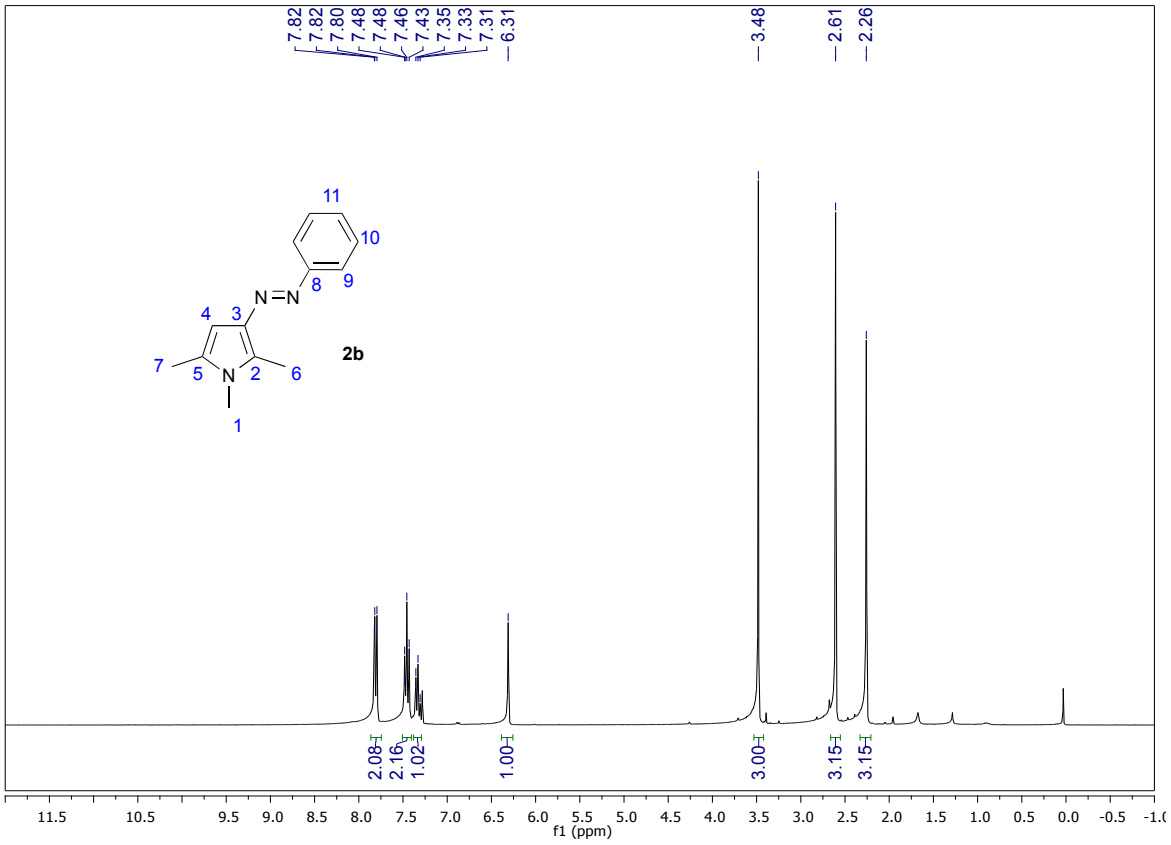


Figure S11. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **2b**

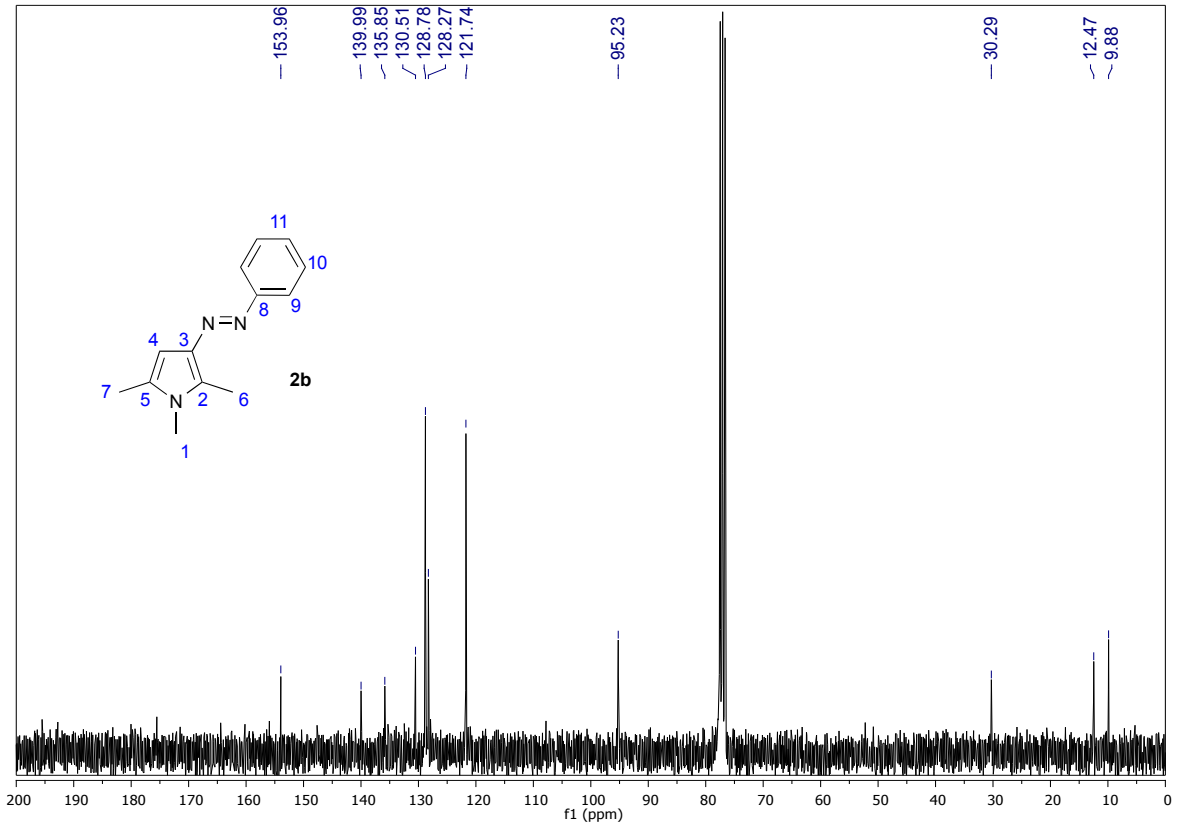


Figure S12. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **2b**

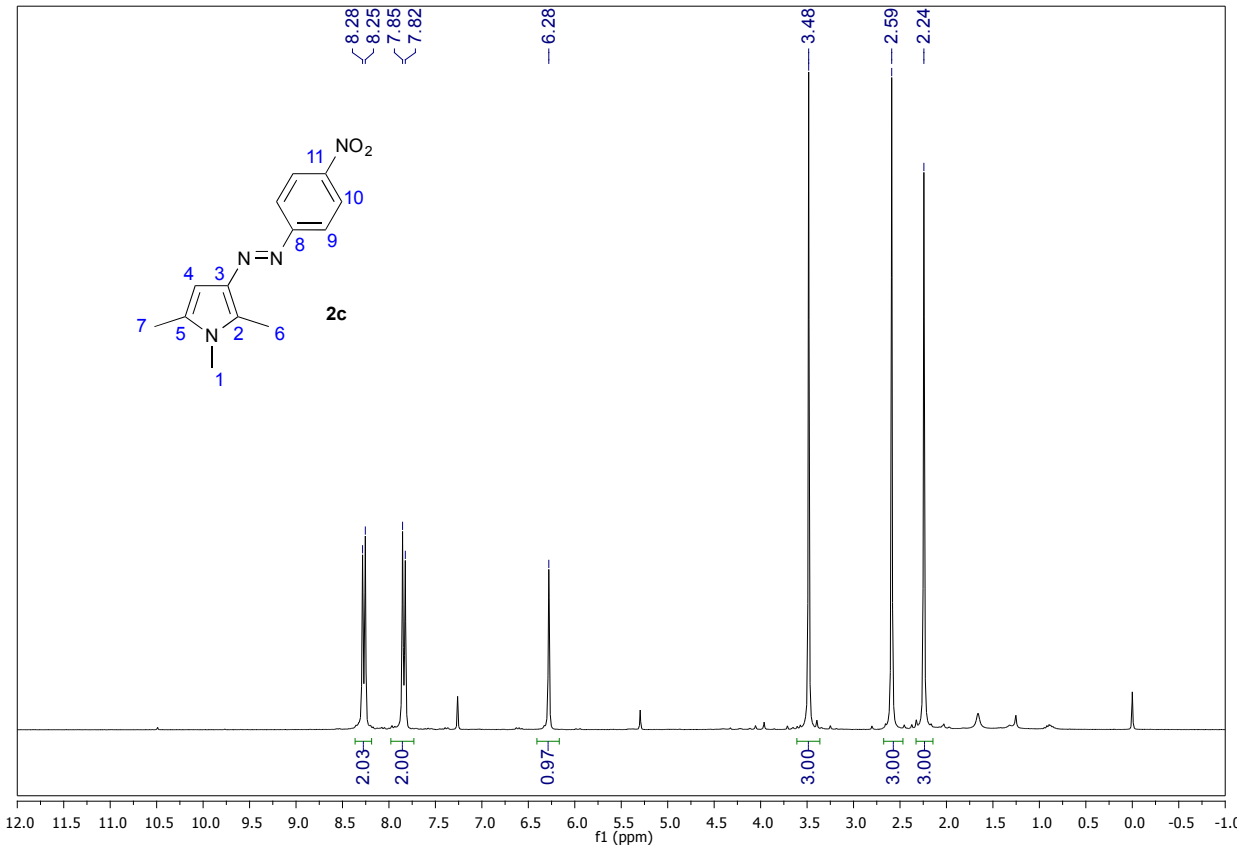


Figure S13. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **2c**

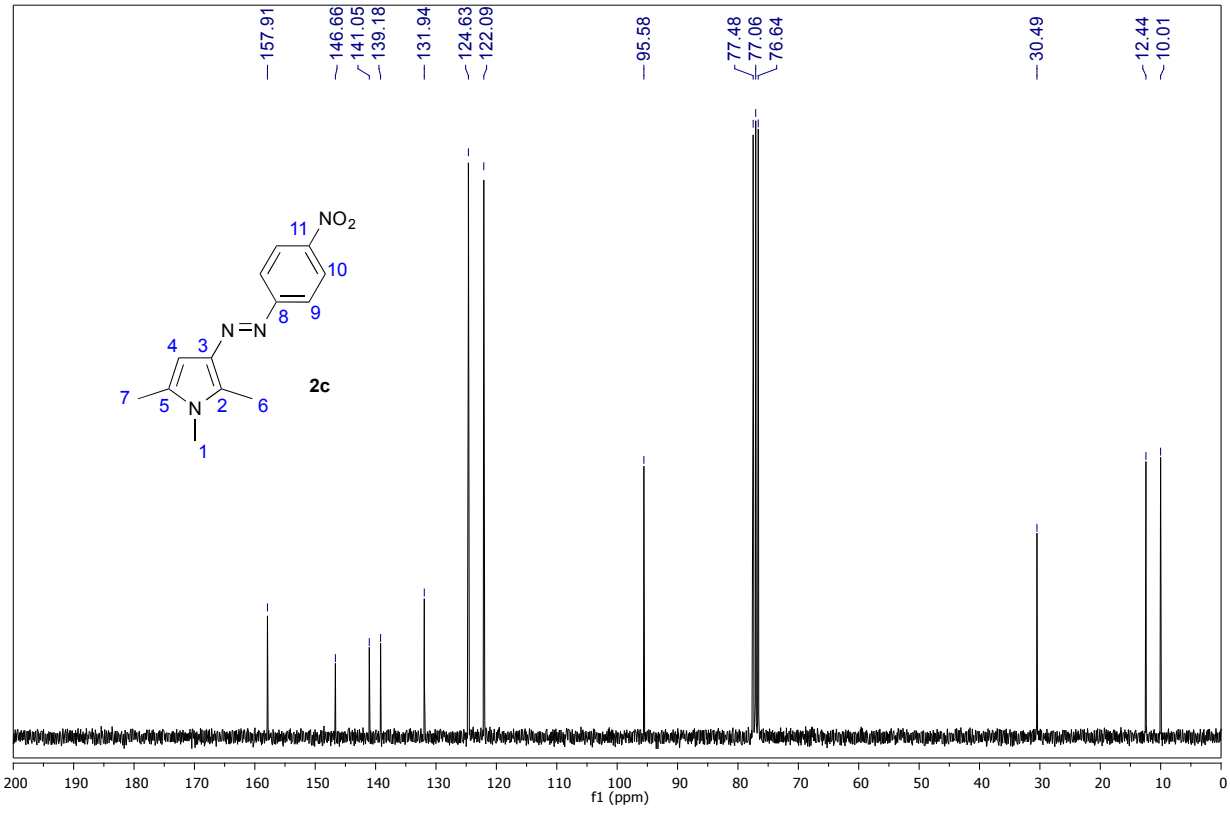


Figure S14. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **2c**

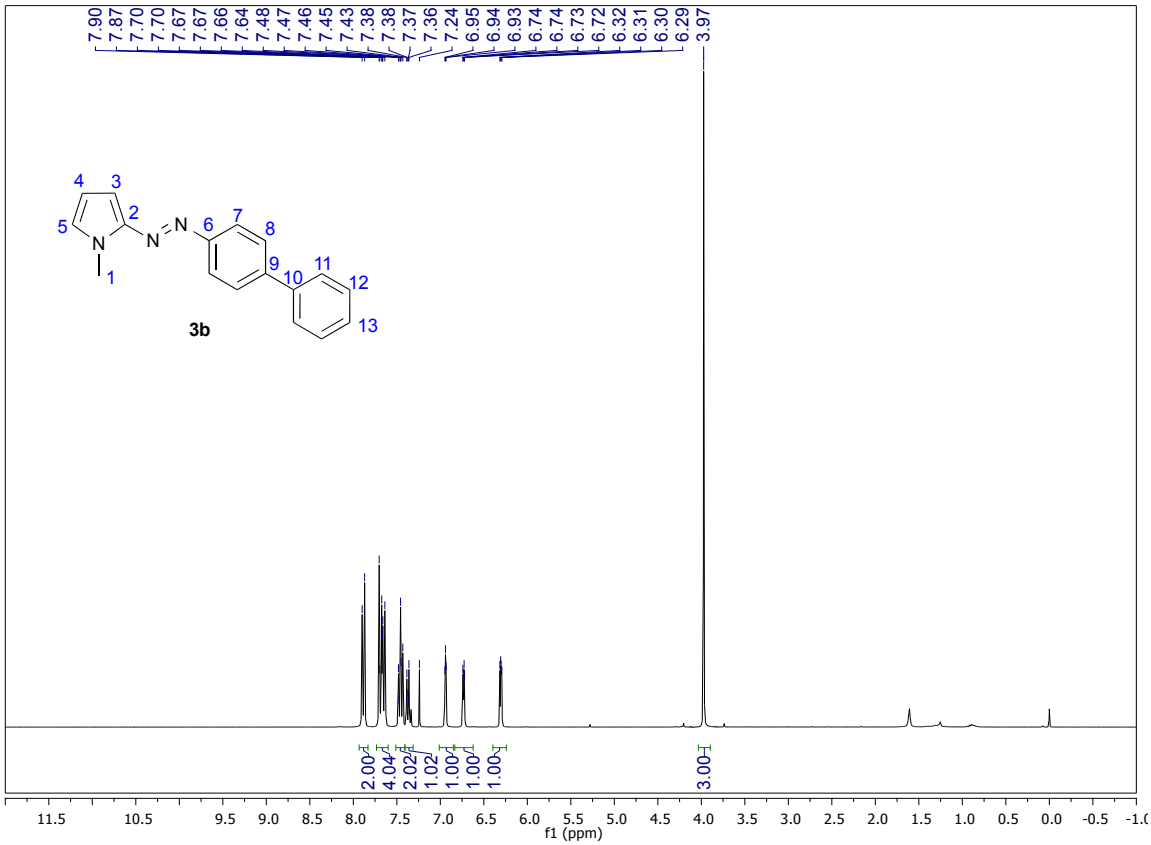


Figure S15. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **3b**

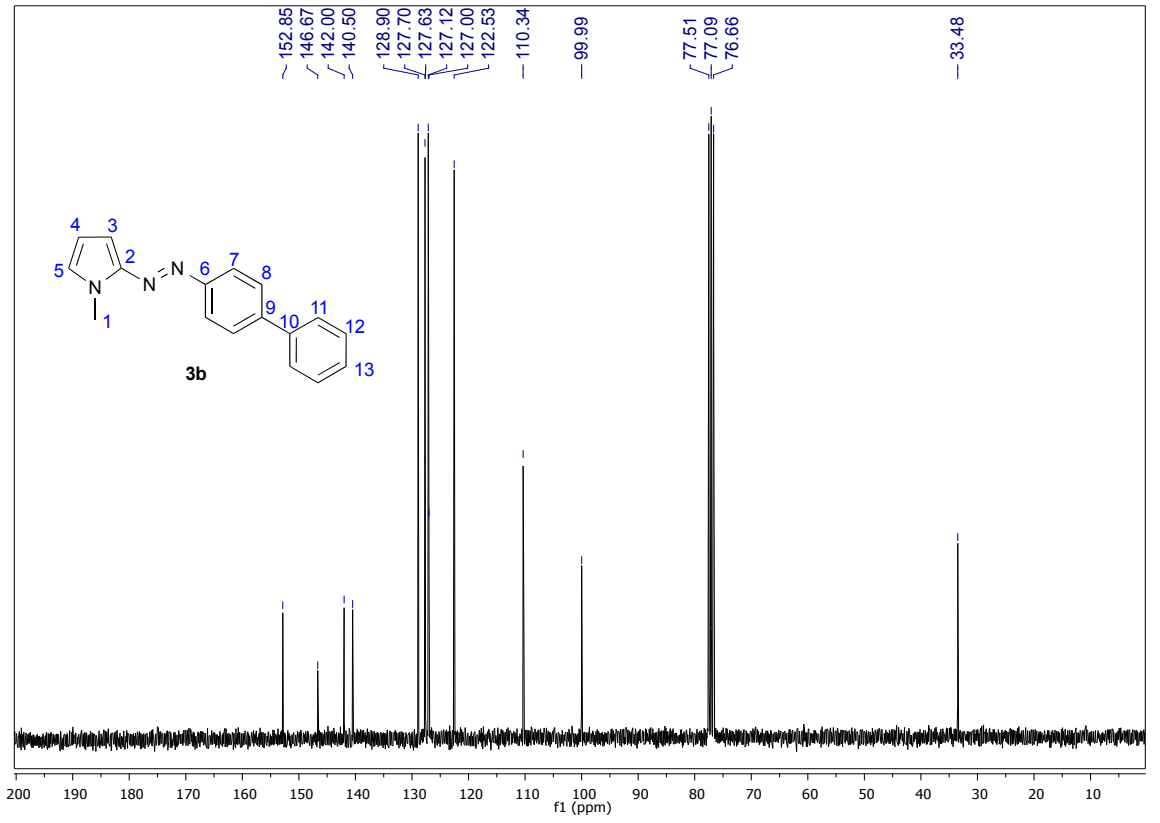


Figure S16. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **3b**

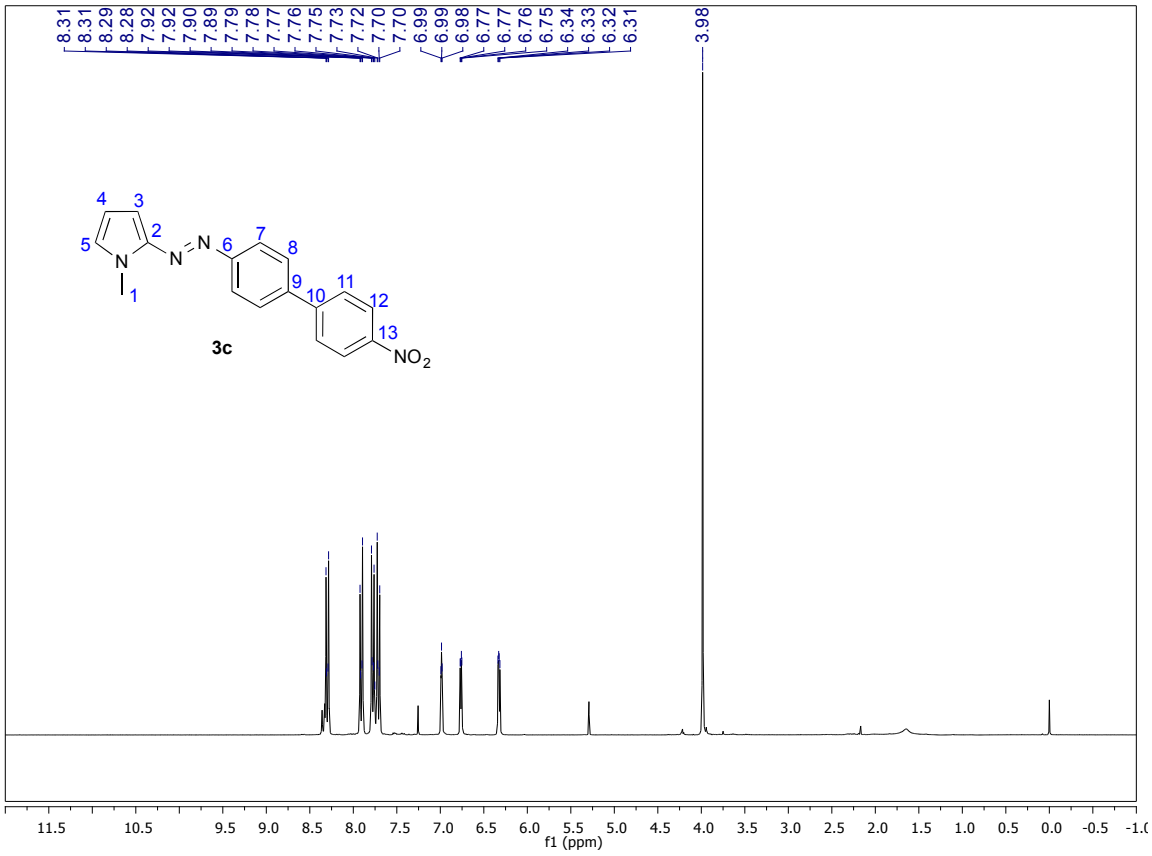


Figure S17. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **3c**

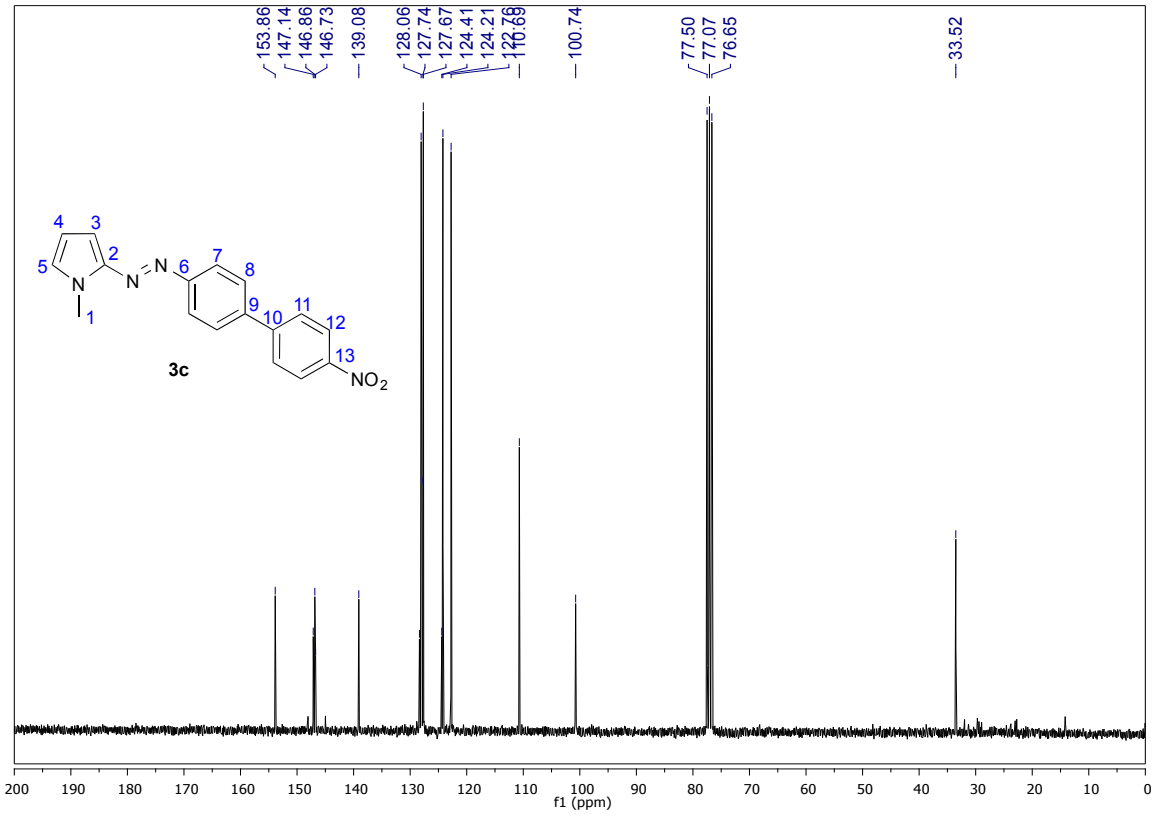


Figure S18. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **3c**

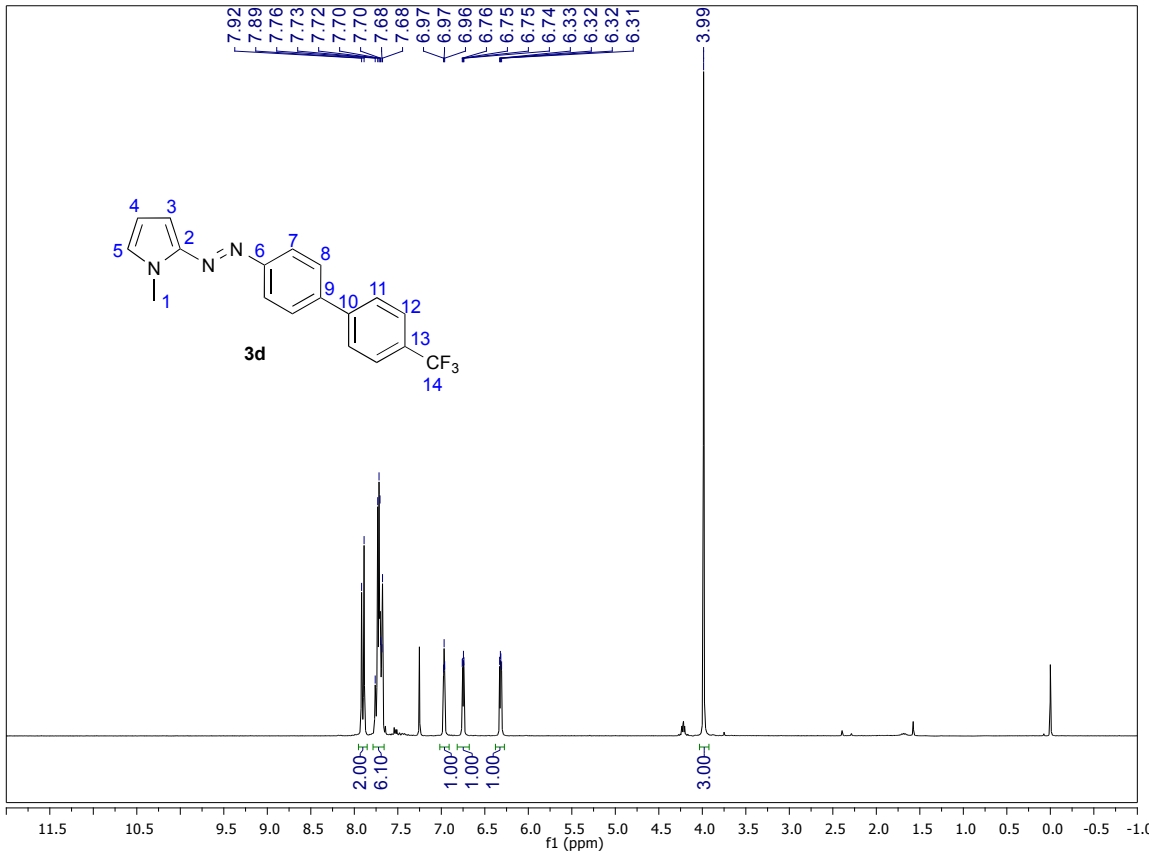


Figure S19. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **3d**

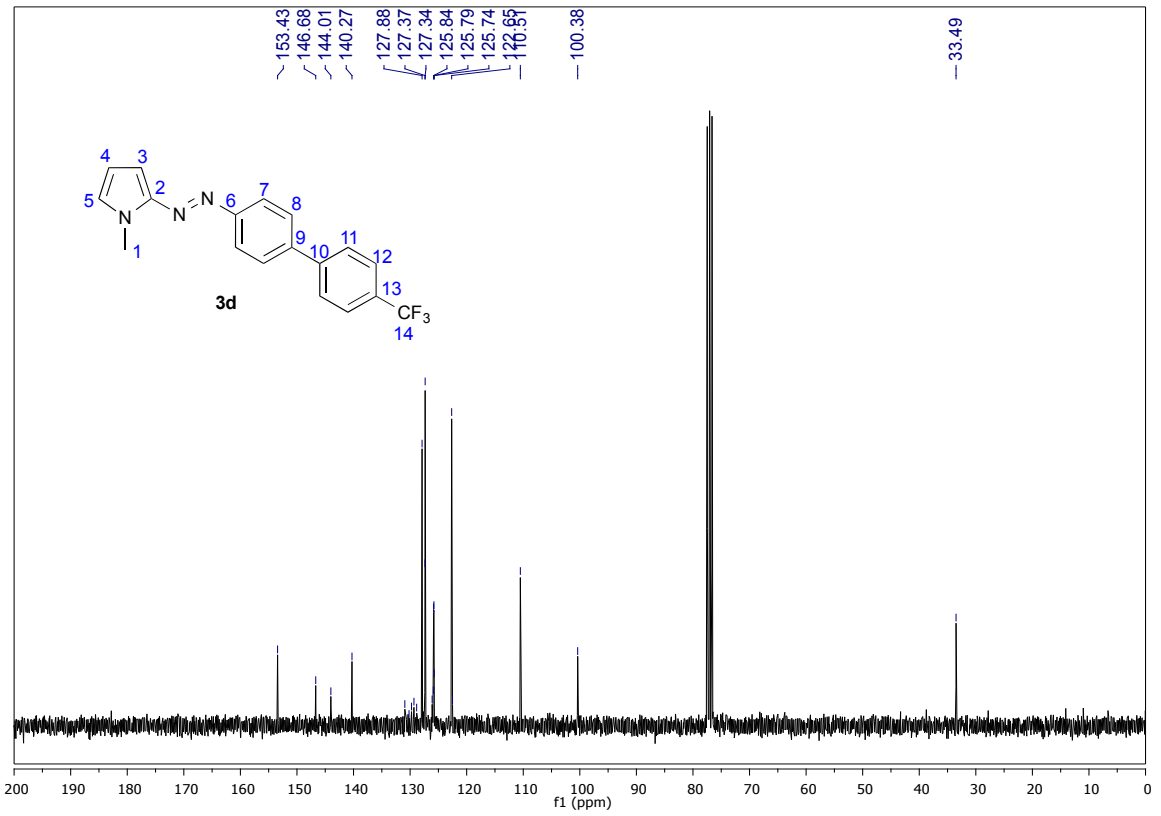


Figure S20. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **3d**

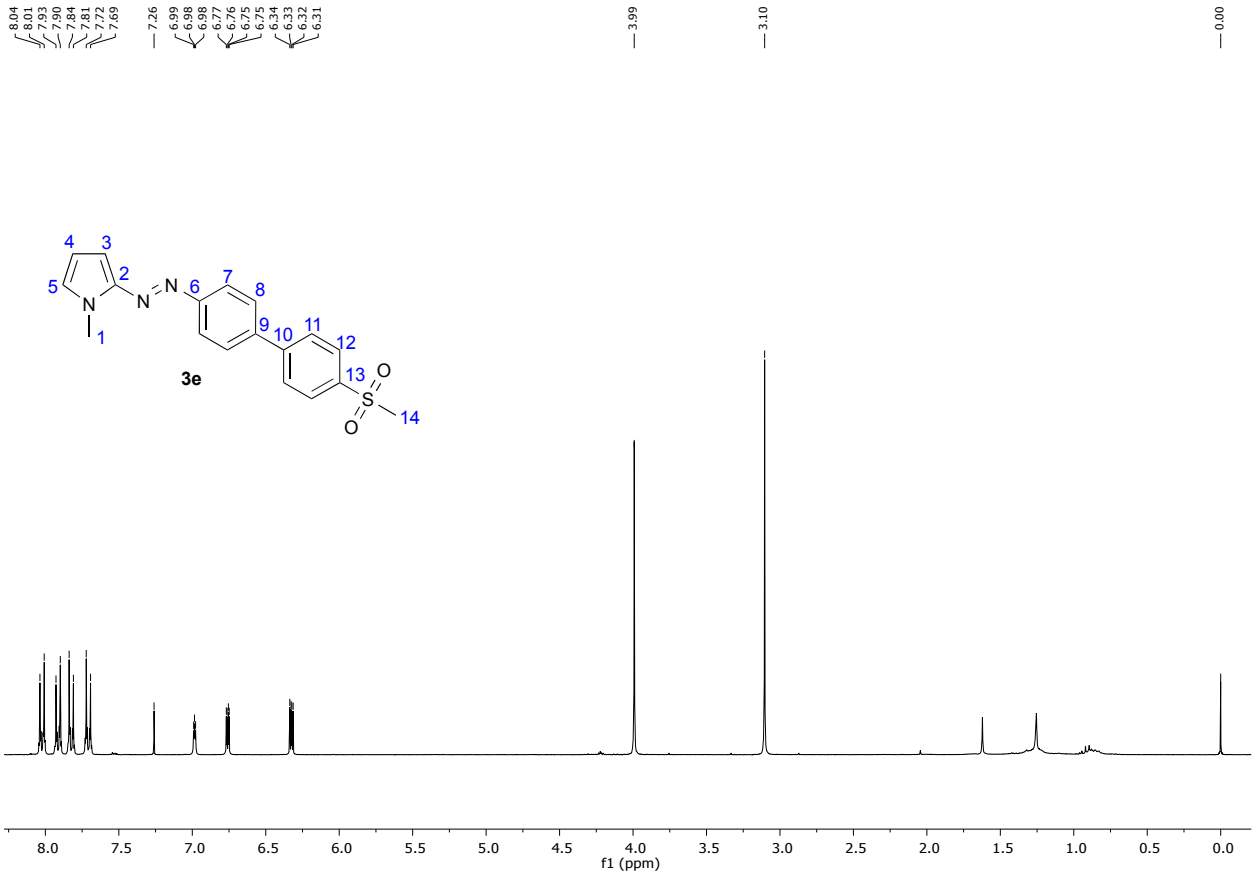


Figure S23. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **3e**

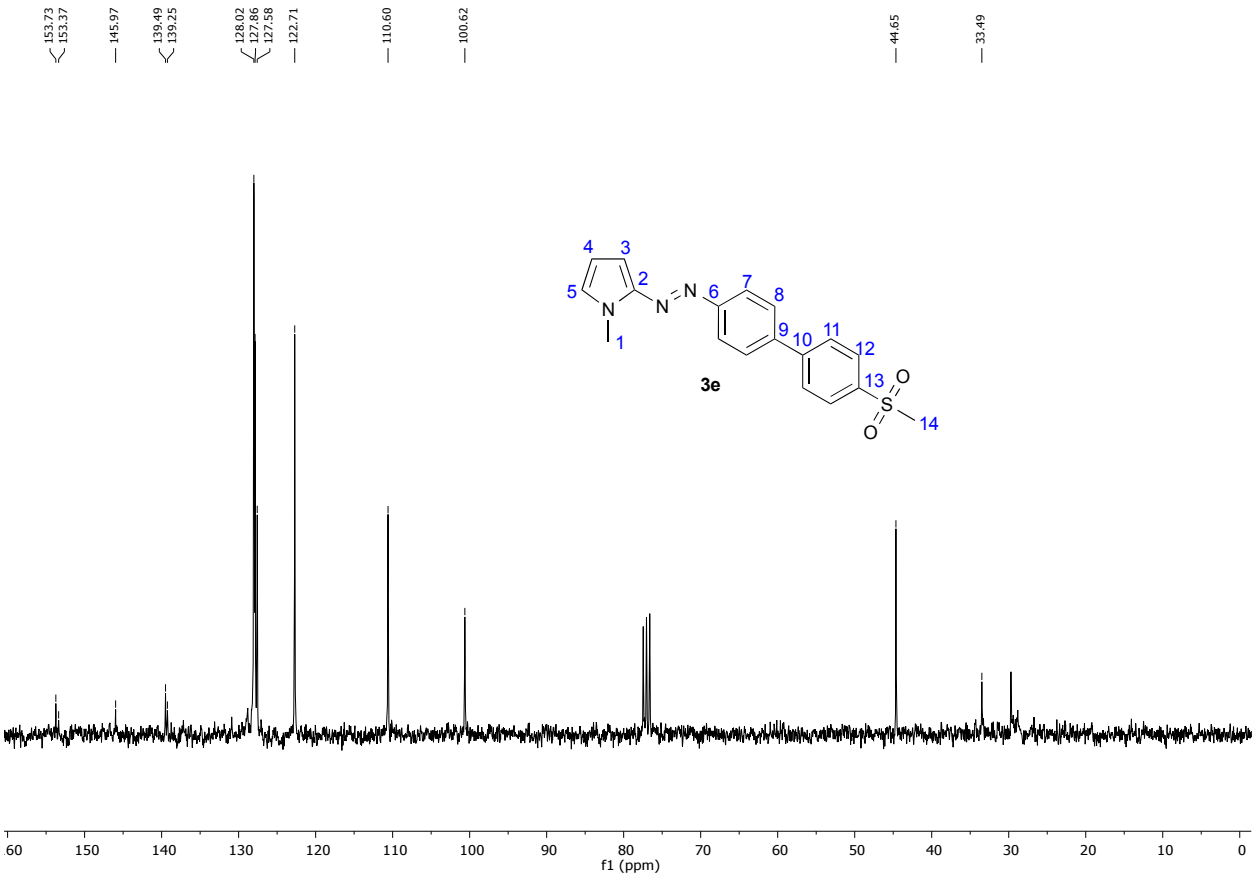


Figure S24. ^{13}C NMR spectrum (300 MHz, $CDCl_3$) of compound **3e**

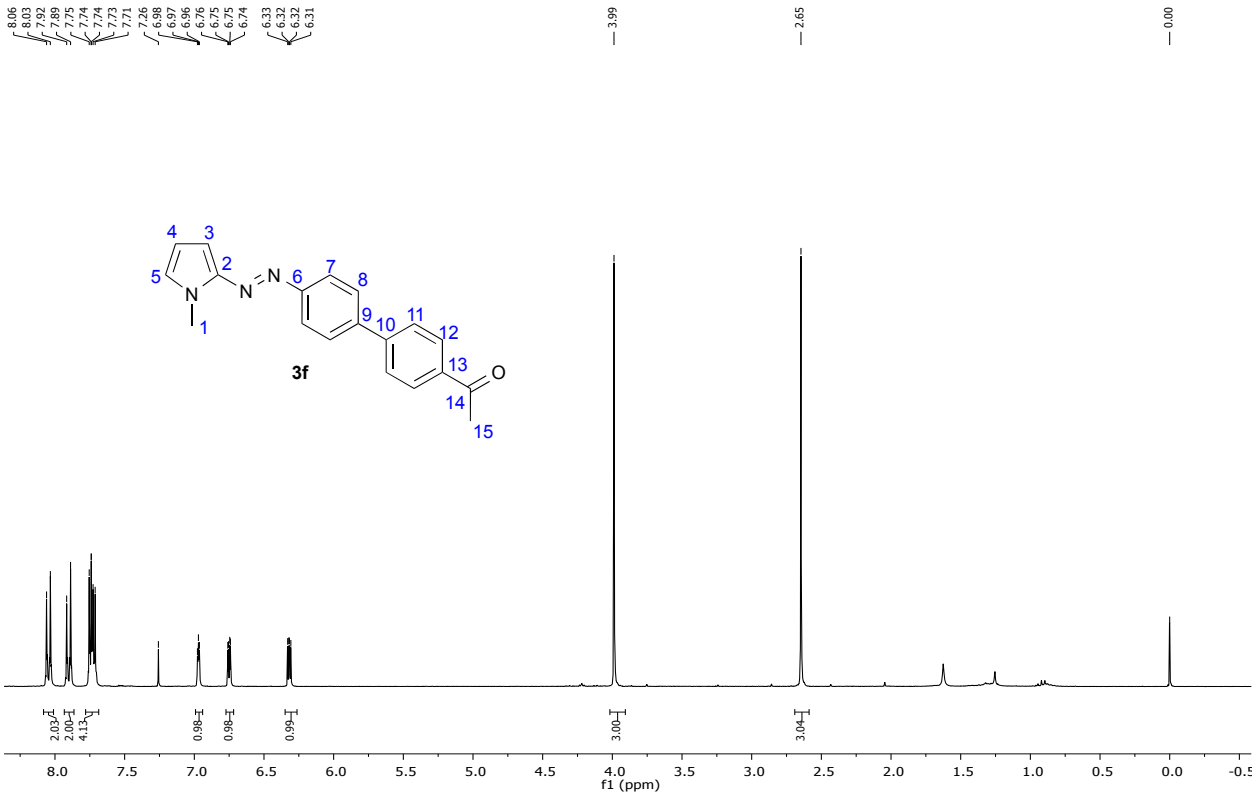


Figure S21. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **3f**

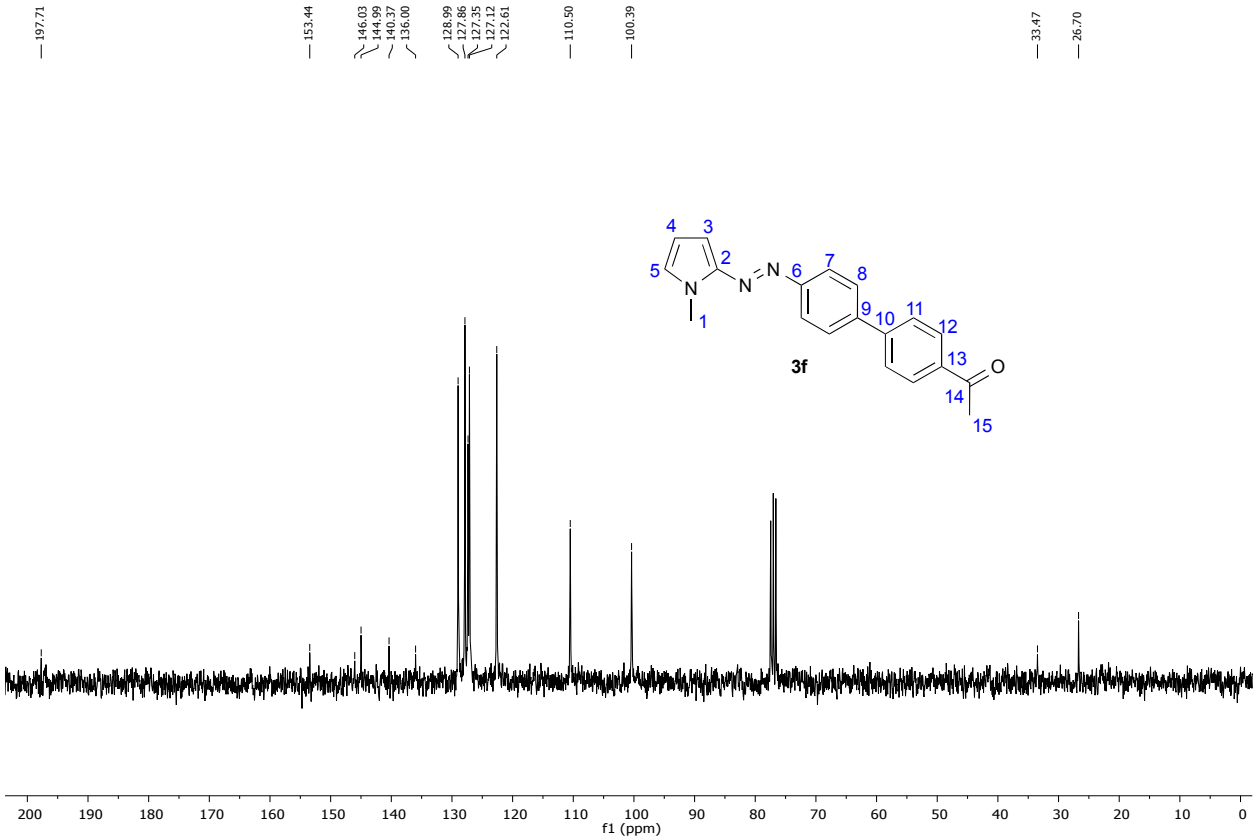


Figure S22. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **3f**

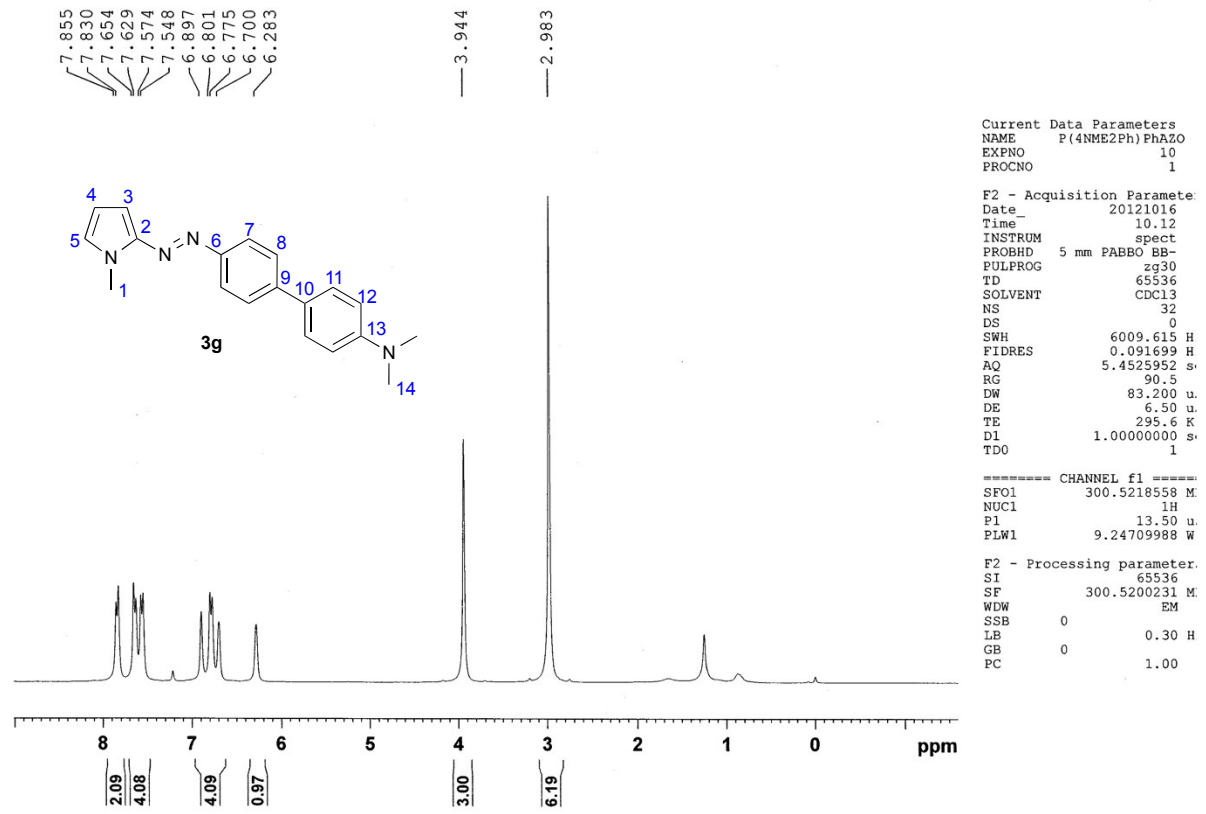


Figure S25. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **3g**

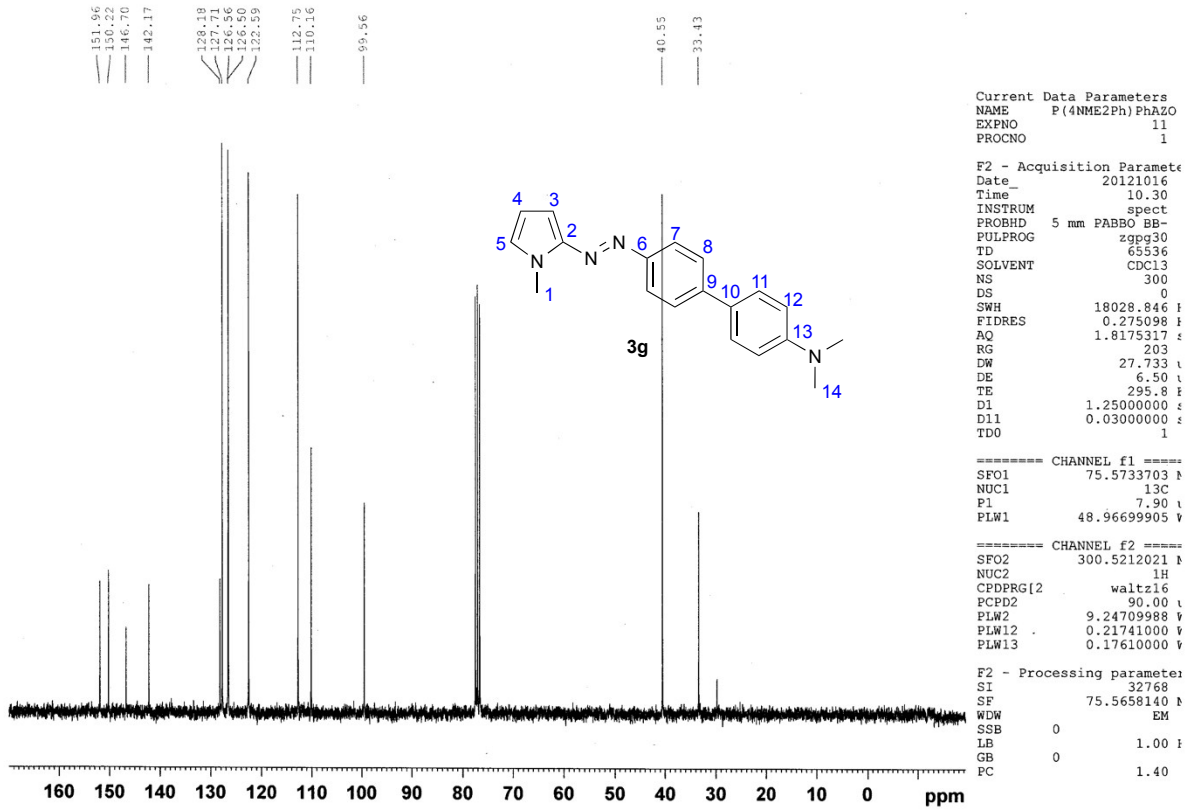


Figure S26. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **3g**

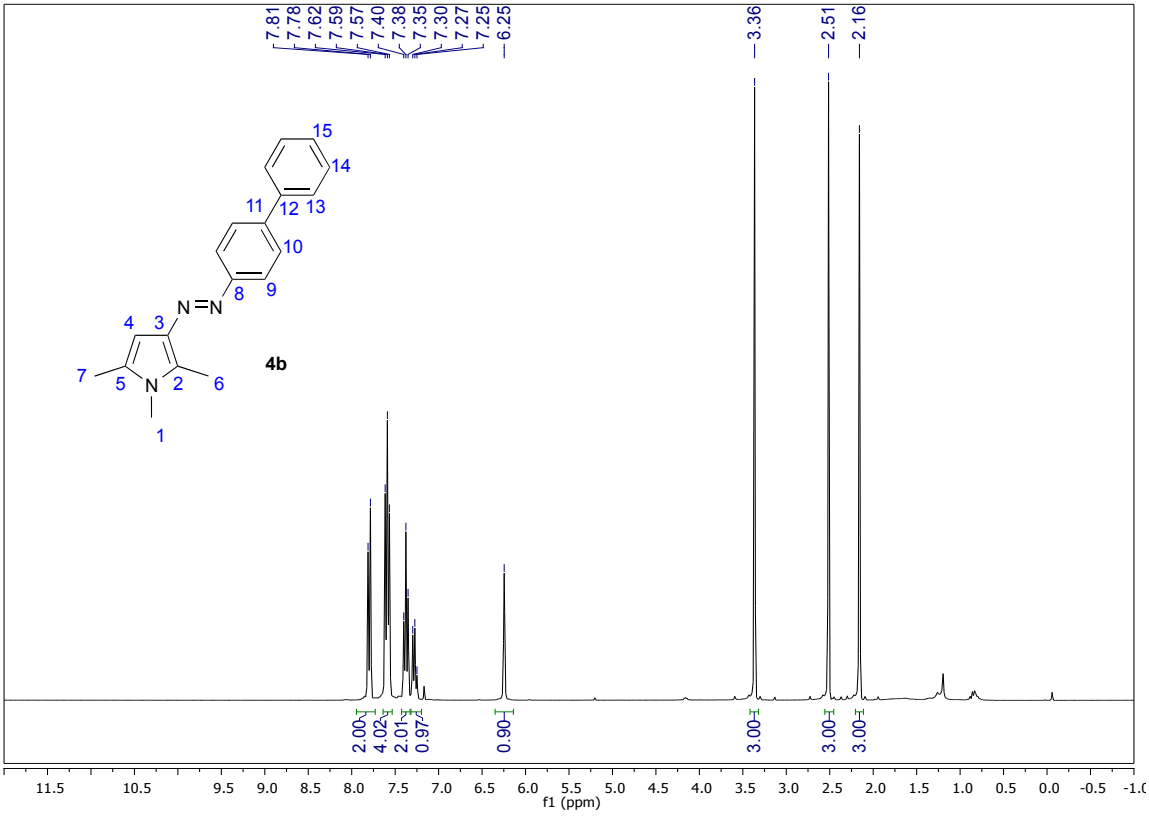


Figure S27. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4b**

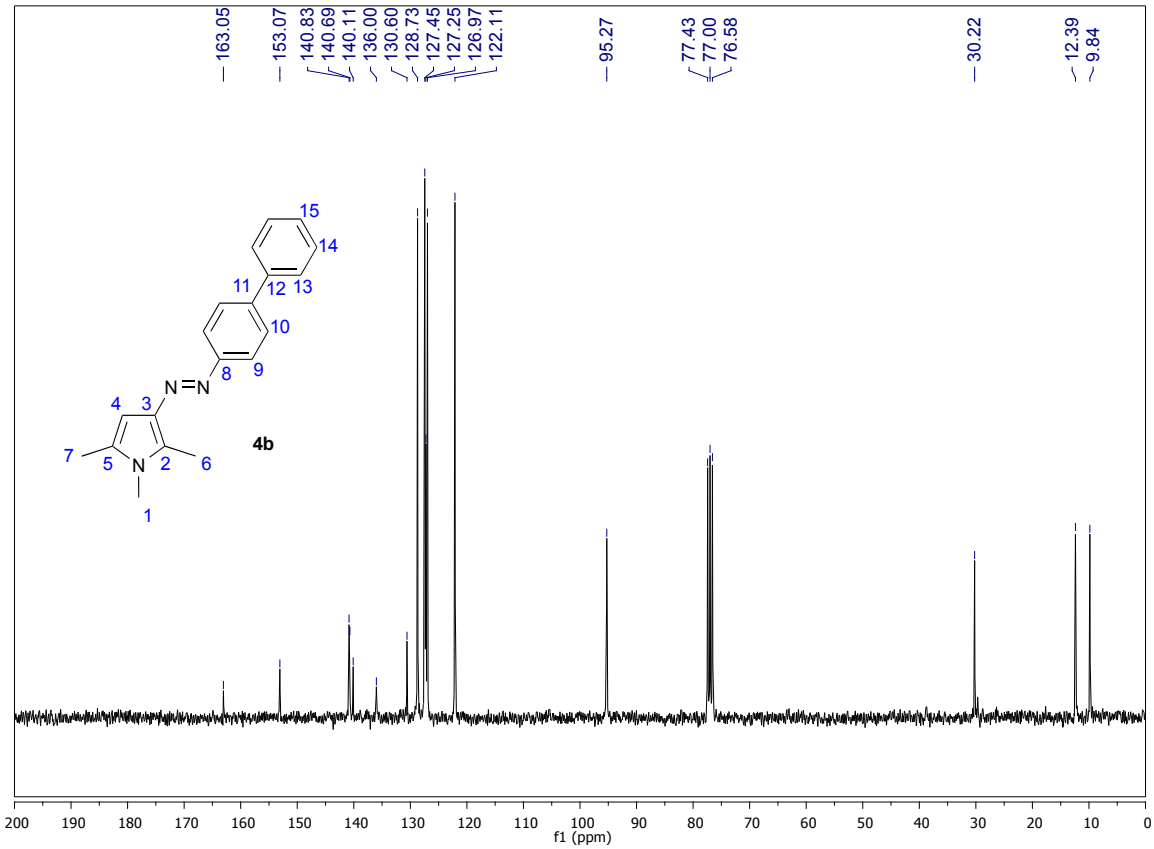


Figure S28. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **4b**.

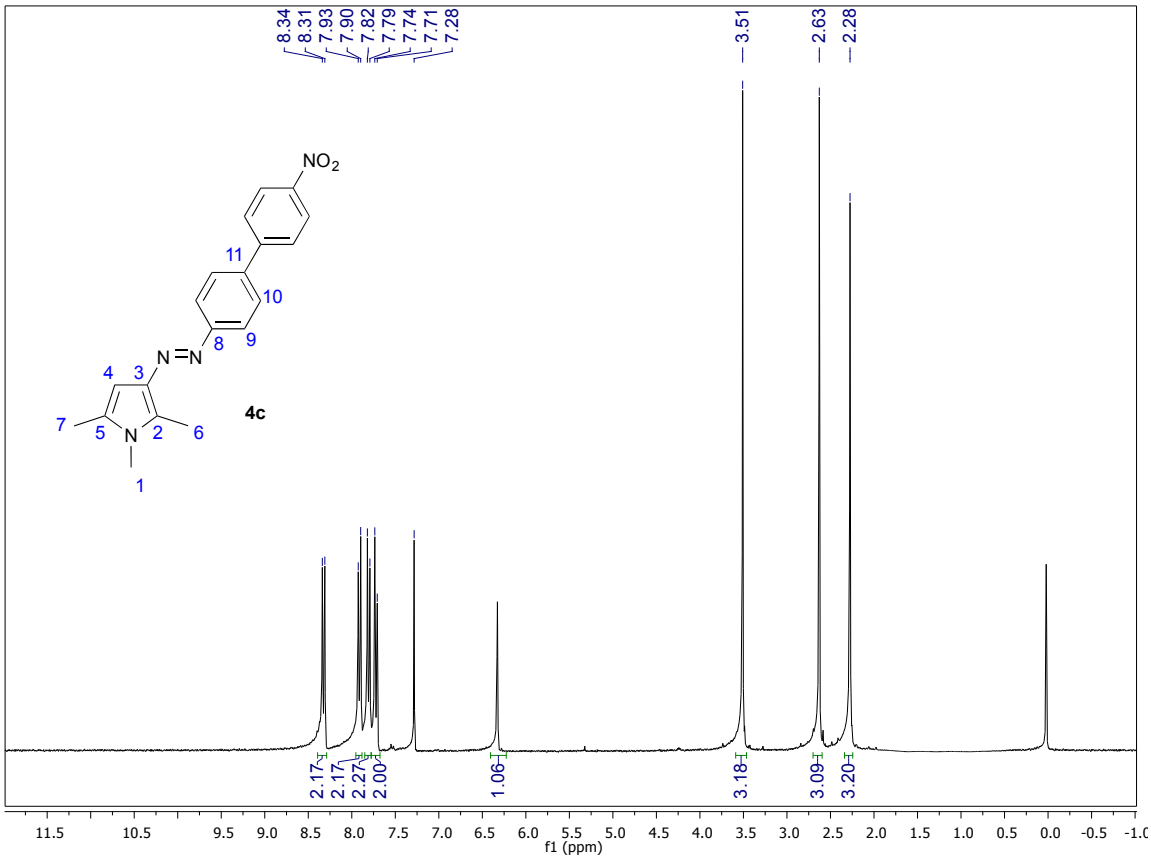


Figure S29. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4c**

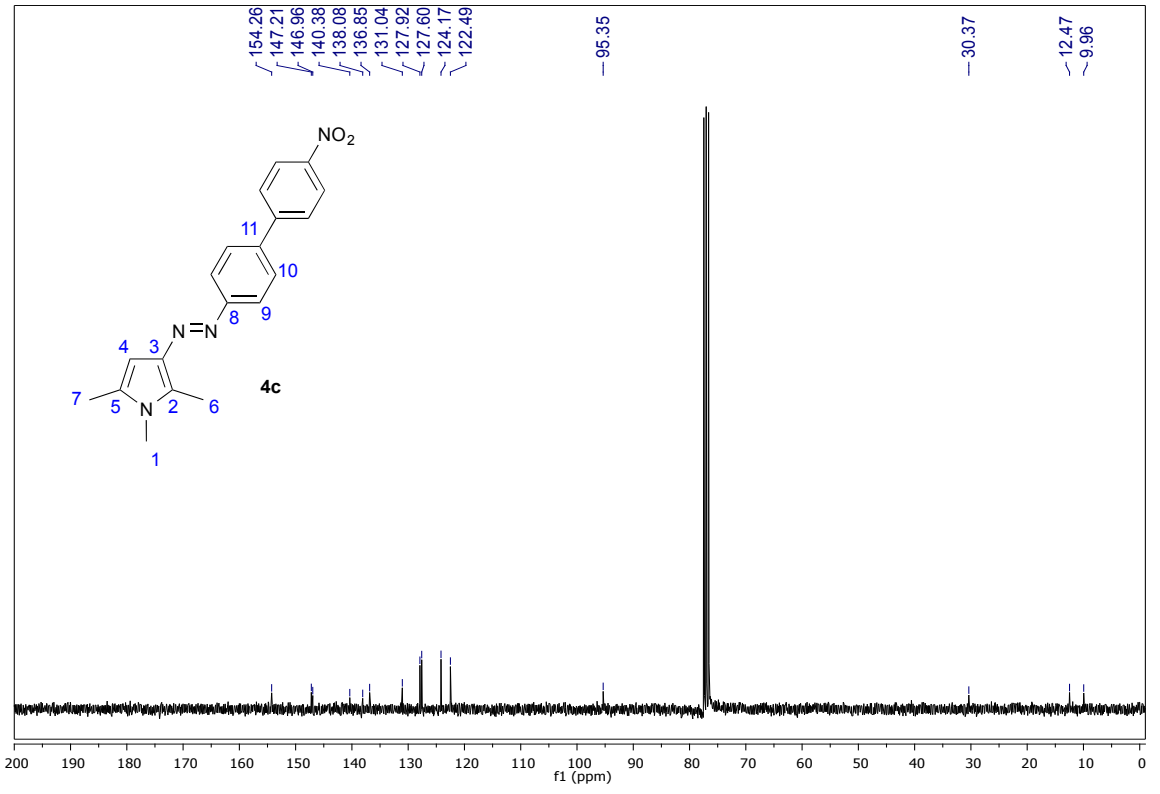


Figure S30. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **4c**.

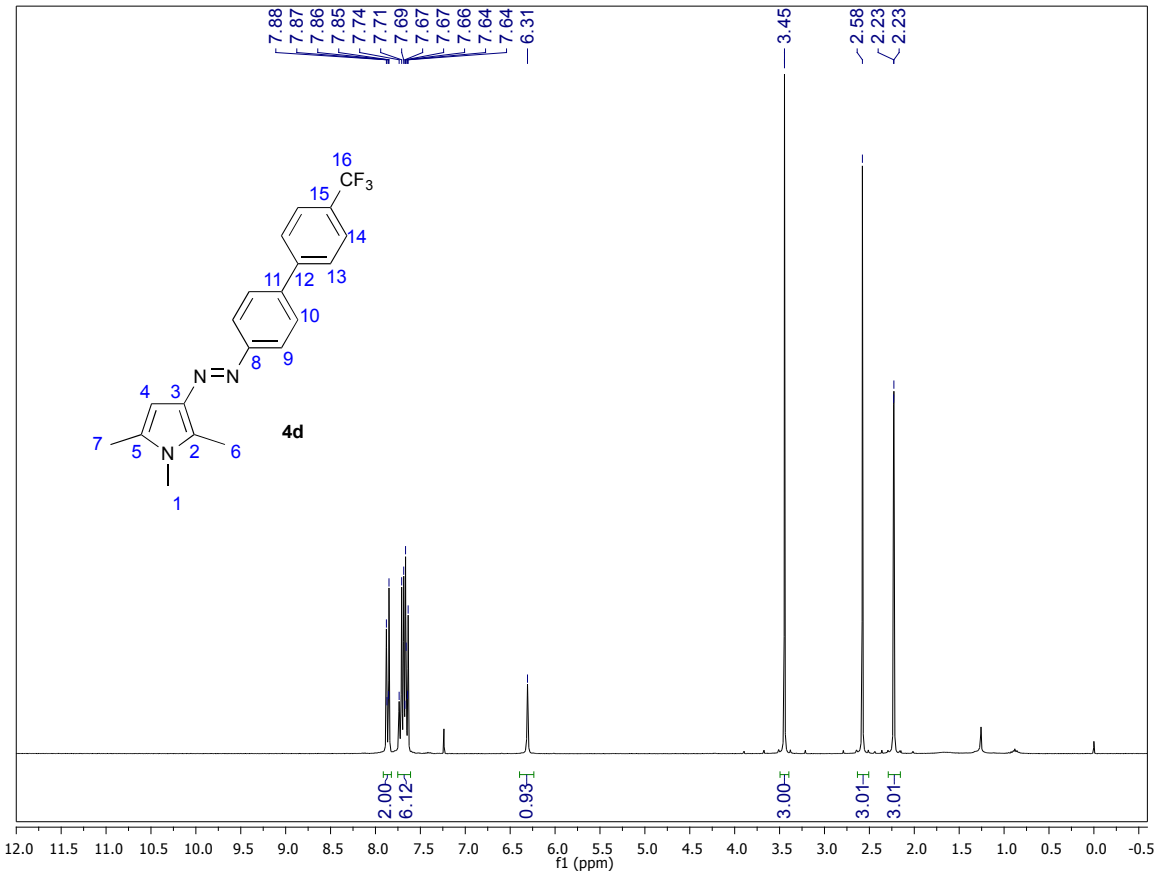


Figure S31. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4d.**

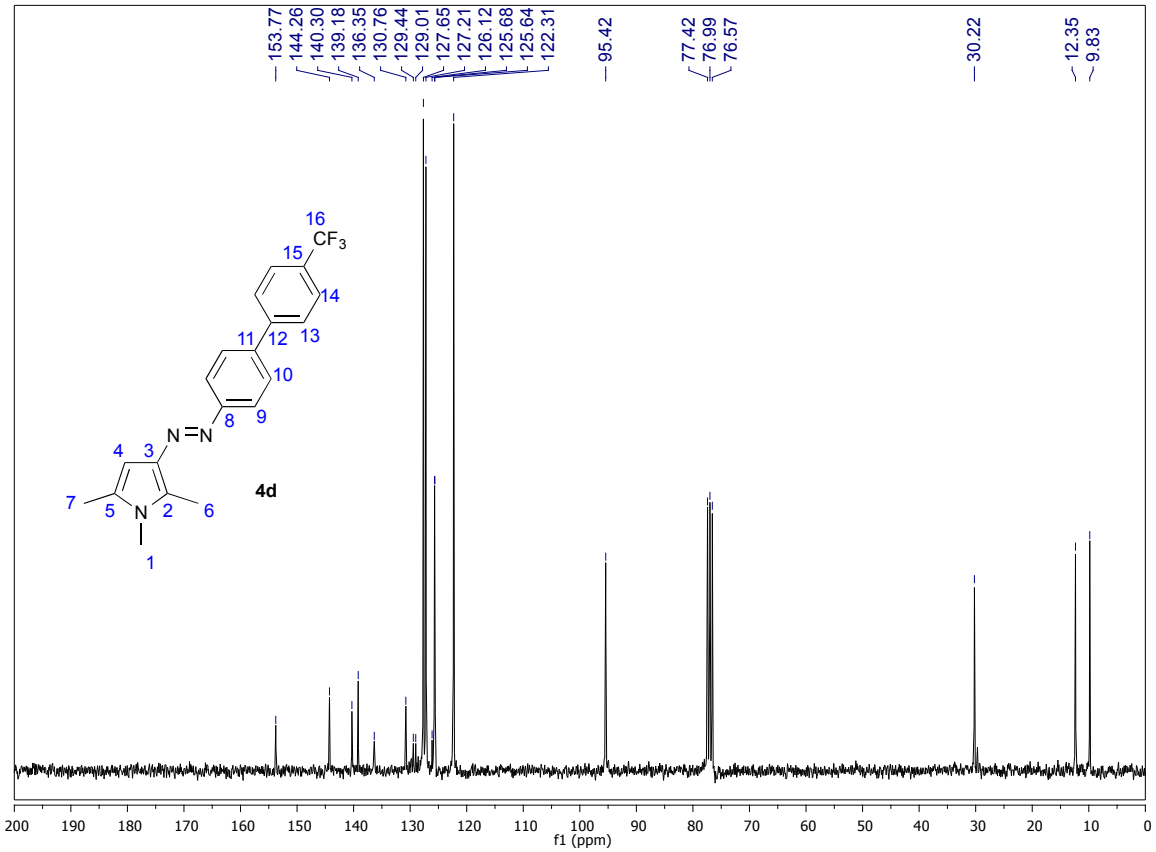


Figure S32. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **4d.**

8. Structure determination by X-ray crystallography

Suitable X-ray quality crystals of **1c**, **2a**, **2b** and **4d** were grown by slow evaporation of chloroform at room temperature. Crystals of each compound were mounted on a glass fiber at room temperature, and then placed on a Bruker Smart Apex CCD (for **1c**), Bruker D8 Venture κ geometry diffractometer 208039-1 (for **2a**, **2b**, **4b**), both equipped with Mo-K α radiation; decay was negligible in both cases. Details of crystallographic data collected for these compounds are provided in SI. Systematic absences and intensity statistics were used in space group determination. The structure was solved using direct methods.[ii] Anisotropic structure refinements were achieved using full matrix, least-squares technique on all non-hydrogen atoms. All hydrogen atoms were placed in idealized positions, based on hybridization, with isotropic thermal parameters fixed at 1.2 times the value of the attached atom. Structure solutions and refinements were performed using SHELXTL V6.10.[iii] The experimental and refinement details of the X-ray crystallographic structure of compounds **1c**, **2a**, **2b** and **4d** can be obtained free of charge from the Cambridge Crystallographic Data Centre (http://www.ccdc.cam.ac.uk).

Table S1. X-ray Data Collection and Structure Refinement Details for **1c**, **2a**, **2b** and **4d**

	1c	**2a**	**2b**	**4d**
Formula	$C_{11}H_{10}N_4O_2$	$C_{13}H_{14}IN_3$	$C_{13}H_{15}N_3$	$C_{20}H_{18}F_3N_3$
MW g^{-1} mol^{-1}	230.23	339.17	213.28	357.37
Crystal size (mm^3)	0.35x0.21x0.06	0.35x0.16x0.14	0.37 × 0.14 × 0.11	0.40x0.26x0.07
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P*-1	$P2_1/n$	$P2_1/n$	$P2_1/c$
a/Å	7.345(5)	11.538(10)	8.564 (4)	14.409(2)
b/Å	7.435(6)	9.5869(9)	22.313 (11)	7.2189(10)
c/Å	11.625(9)	12.6216(11)	25.094 (12)	17.976(3)
α/(°)	74.87(3)	90	90	90
β/(°)	89.96(3)	106.002(2)	93.048 (7)	107.935(7)
γ/(°)	65:91(3)	90	90	90
Volume/ $Å^3$	555.4	1340.4	47788(4)	1778.9(5)
Z	2	4	16	4
d_c/Mg m^{-3}	1.377	1.681	1.186	1.334
Θ/°	3.06 to 27.41	2.71 to 27.41	2.44 to 27.31	2.38 to 27.48
Index Ranges	-9≤*h*≤*9* -9≤*k*≤9 -14≤*l*≤*14*	-14≤*h*≤*14* -12≤*k*≤12 -16≤*l*≤*16*	-10≤*h*≤*10* -28≤*k*≤28 -32≤*l*≤*32*	-18≤*h*≤*18* -9≤*k*≤9 -23≤*l*≤*23*
Reflections collected	11624	16497	112168	26053
Independent reflections	2445 [*R*(int)=0.0812]	3070 [*R*(int)=0.0239]	10535 [*R*(int)= 0.135]	3932 [*R*(int)= 0.034]
Data/parameters	2445/229	3070/157	10535/589	3932/295
Final *R* indices	*R*1=0.0951	*R*1=0.0307	*R1=0.069*	*R1=0.047*
[*I*>2σ(*I*)]	*wR*2=0.2496	*wR*2=0.0768	*wR2=0.173*	*wR2=0.154*
R indices (all data)	*R*1=0.1516	*R*1=0.0452	*R1=0.2051*	*R1=0.0651*
	*wR*2=0.2184	*wR*2=0.0700	*wR2=0.1283*	*wR2=0.1398*
GoF(F^2)	1.152	1.049	0.999	1.080
Absorptions corrections	Multi-scan	Multi-scan	Multi-scan	Multi-scan
CCDC	1950956	1950957	1950959	1950958

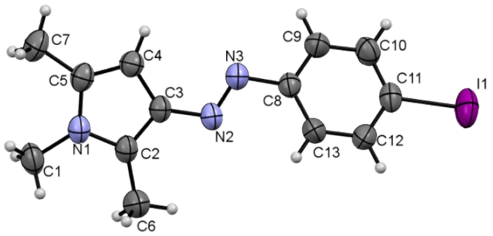


Figure S33. ORTEP view of **2a** with thermal ellipsoids at 30% probability level. Selected bond lengths (Å) and angles (°):I(1)-C(11) 2.099(2); N(1)-C(1) 1.457(3); N(2)-N(3) 1.262(3); N(2)-C(3) 1.386(3); N(3)-C(8) 1.427(3); N(3)-N(2)-C(3) 114.3(2); N(2)-N(3)-C(8) 113.1(2), C(10)-C(11)-I(1) 120.1(2), C(11)-C(12)-I(1) 119.2(2).

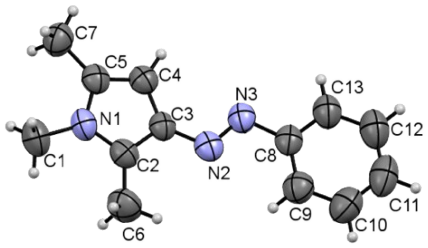
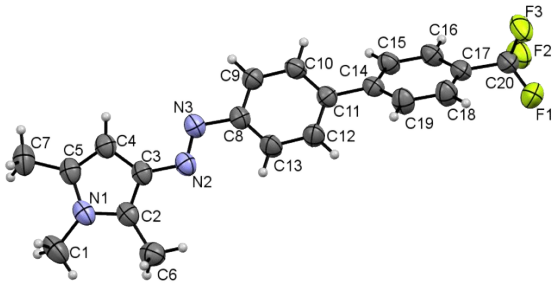


Figure S34. ORTEP view of **2b** with thermal ellipsoids at 30% probability level. Selected bond lengths (Å) and angles (°): N(1)-C(1) 1.461(4); N(2)-N(3) 1.270(3); N(2)-C(3) 1.378(3); N(3)-C(8) 1.424(3); C(5)-N(1)-C(2) 109.4(2), C(5)-N(1)-C(1) 124.7(2); C(2)-N(1)-C(1) 125.8(2), N(3)-N(2)-C(3) 115.3(2); N(2)-N(3)-C(8) 112.7(2). Torsion angle C(8)-N(3)-(N2)-C(3) 178.5(2).



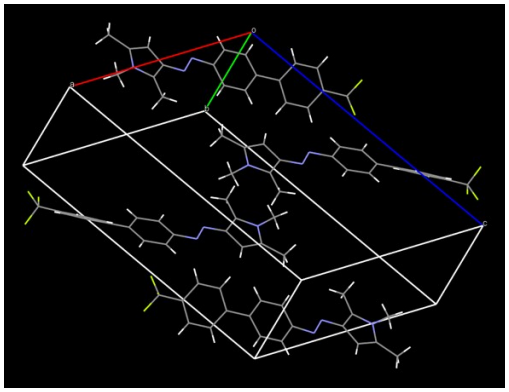
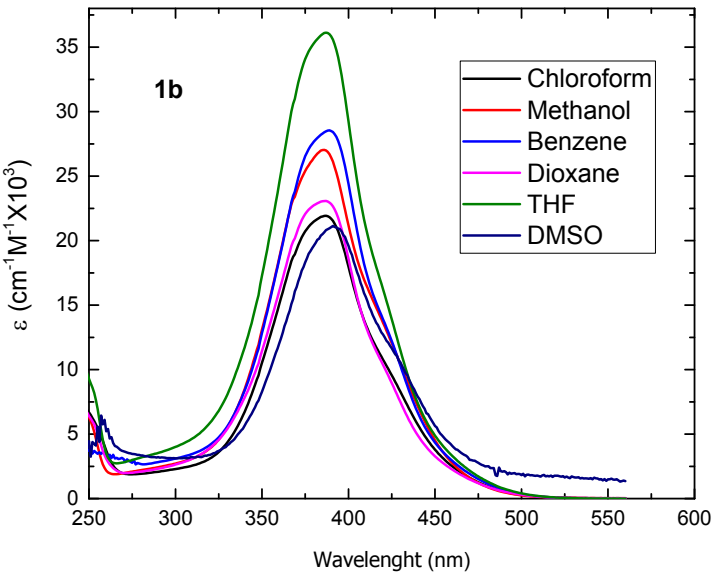


Figure S35. ORTEP view of **4d** with thermal ellipsoids at 30% probability level. Selected bond lengths (Å) and angles (°): N(2)-N(3) 1.263(3); N(2)-C(3) 1.385(1); N(3)-C(8) 1.428(1); C(11)-C(14) 1.485(1); C(2)-N(1)-C(1) 125.1(3), N(3)-N(2)-C(3) 114.7(3); N(2)-N(3)-C(8) 113.1(1); C(12)-C(11)-C(14) 120.4(5); C(11)-C(14)-C(19) 121.3(7). Torsion angle C(10)-C(11)-C(14)-C(15) 33.4(2).

9. UV-Visible studies

9.1 UV-Visible studies of compound **1b**



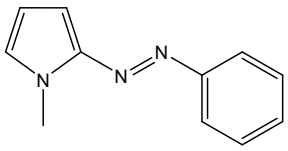


Figure S36 . UV-visible spectra of compound **1b** in different solvents.

Table S2. UV-visible spectroscopic data for **1b** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
1b	λ_{max}= 386 ε= 21915	λ_{max}= 385 ε= 27022	λ_{max}= 389 ε= 28545	λ_{max}= 386 ε= 23067	λ_{max}= 387 ε= 36121	λ_{max}= 391 ε= 21135	$\lambda_{max\ MeOH}$= 385 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$= 424

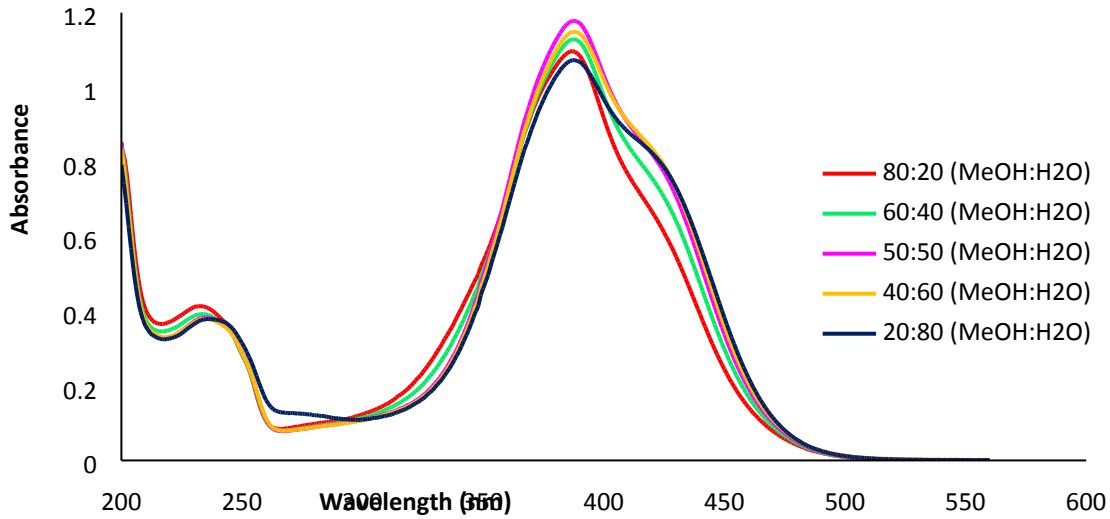
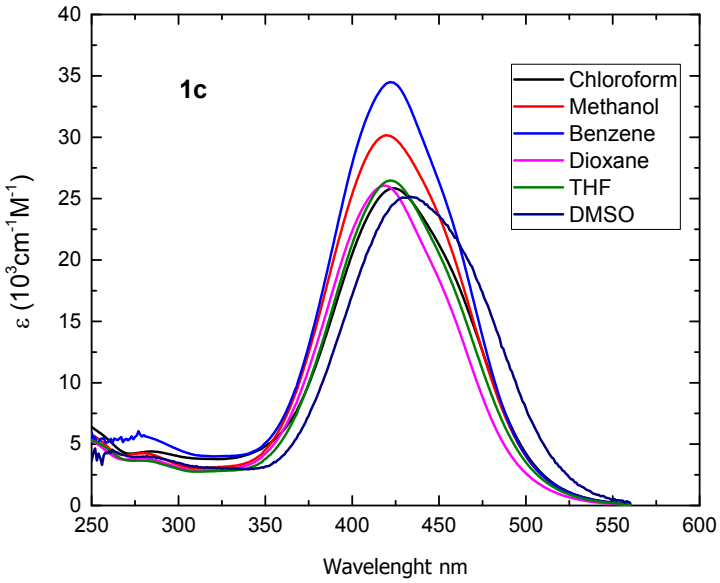


Figure S37 . UV-visible spectra of compound **1b** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

9.2 UV-Visible studies of compound **1c**



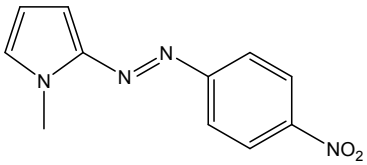


Figure S38 . UV-visible spectra of compound **1c** in different solvents.

Table S3. UV-visible spectroscopic data for **1c** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
1c	λ_{max}= 242 ε= 25845	λ_{max}= 420 ε= 30157	λ_{max}= 422 ε= 34488	λ_{max}= 419 ε= 26052	λ_{max}= 422 ε= 26476	λ_{max}= 433 ε= 25171	$\lambda_{max\ MeOH}$= 420 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$= 425

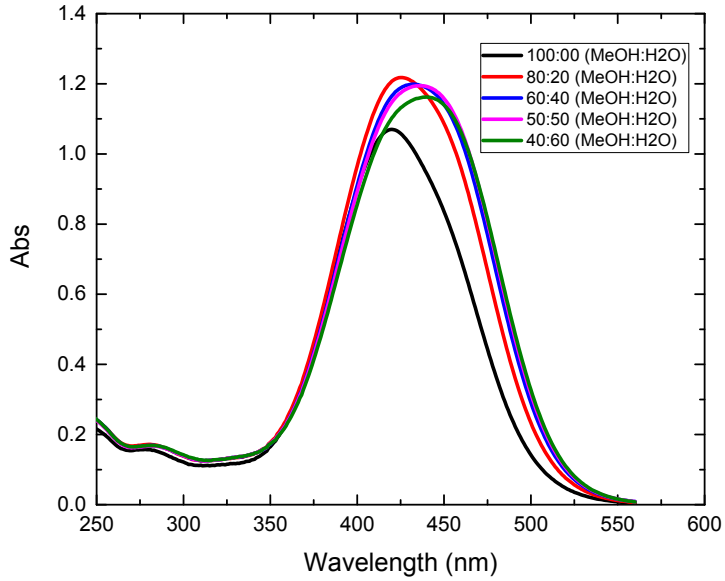


Figure S39 . UV-visible spectra of compound **1c** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

9.3 UV-Visible studies of compound **1d**

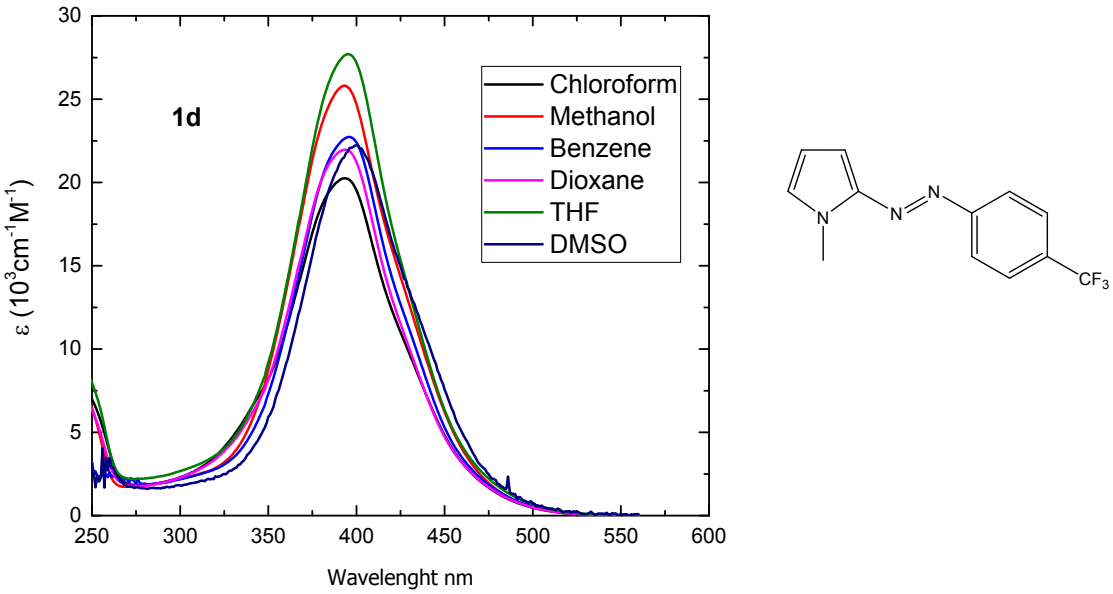


Figure S40 . UV-visible spectra of compound **1d** in different solvents.

Table S4. UV-visible spectroscopic data for **1d** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
1d	λ_{max}= 394 ε= 20248	λ_{max}= 393 ε= 25812	λ_{max}= 396 ε= 22731	λ_{max}= 394 ε= 21965	λ_{max}= 395 ε= 27714	λ_{max}= 400 ε= 22232	$\lambda_{max\ MeOH}$= 393 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$= 422

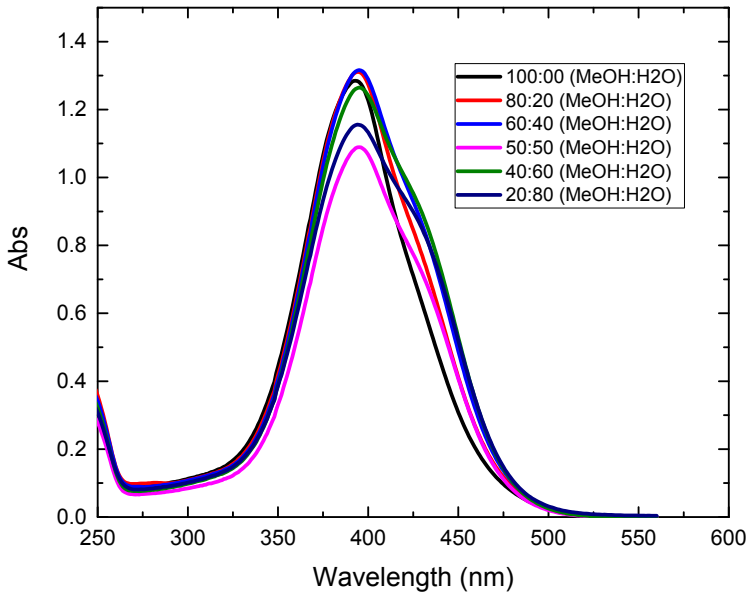
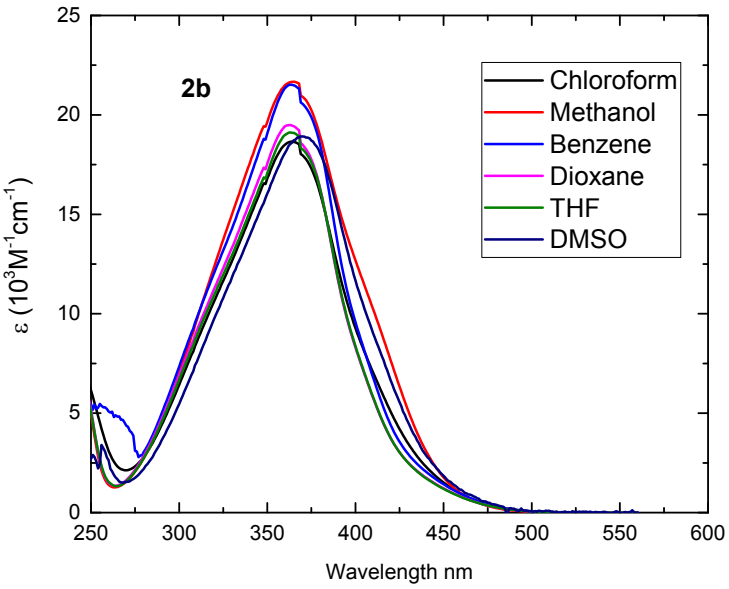


Figure S41 . UV-visible spectra of compound **1d** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

9.4 UV-Visible studies of compound **2b**



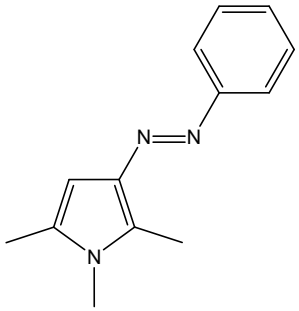


Figure S42 . UV-visible spectra of compound **2b** in different solvents.

Table S5. UV-visible spectroscopic data for **2b** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
2b	λ_{max}= 364 ε= 18660	λ_{max}= 364 ε= 21662	λ_{max}= 363 ε= 21521	λ_{max}= 362 ε= 19484	λ_{max}= 363 ε= 19124	λ_{max}= 370 ε= 19014	$\lambda_{max\ MeOH}$= 364 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$ = 409

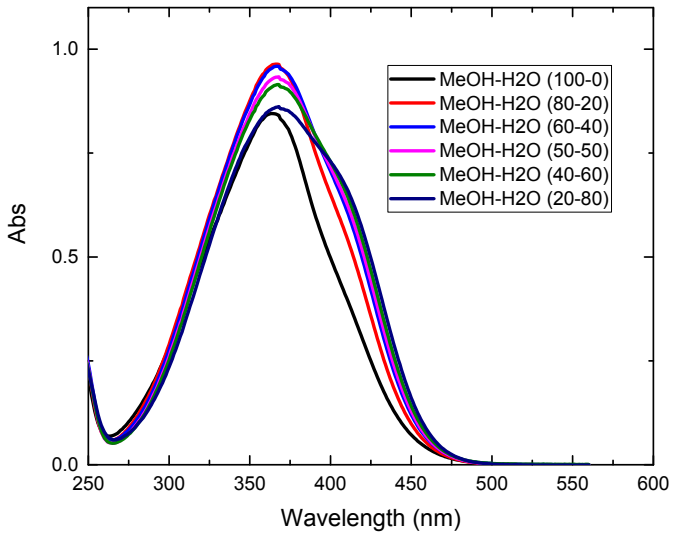
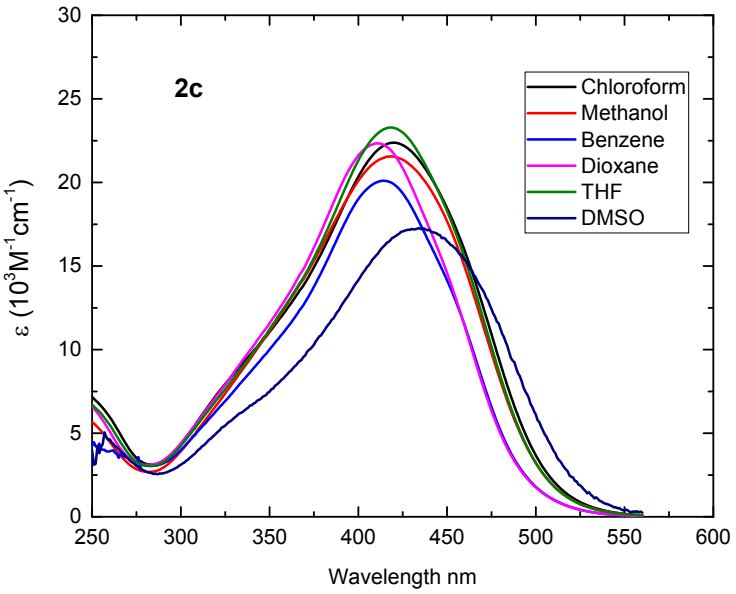


Figure S43 . UV-visible spectra of compound **2b** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

9.5 UV-Visible studies of compound **2c**



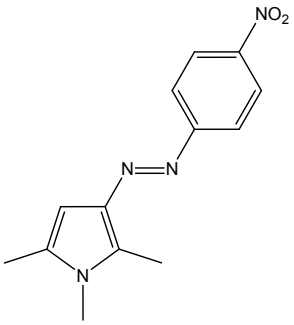


Figure S44 . UV-visible spectra of compound **2c** in different solvents.

Table S6. UV-visible spectroscopic data for **2c** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
2c	λ_{max}= 420 ε= 22380	λ_{max}= 419 ε= 21551	λ_{max}= 414 ε= 20099	λ_{max}= 411 ε= 22337	λ_{max}= 418 ε= 23285	λ_{max}= 434 ε= 17509	$\lambda_{max\ MeOH}$= 419 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$ = 428

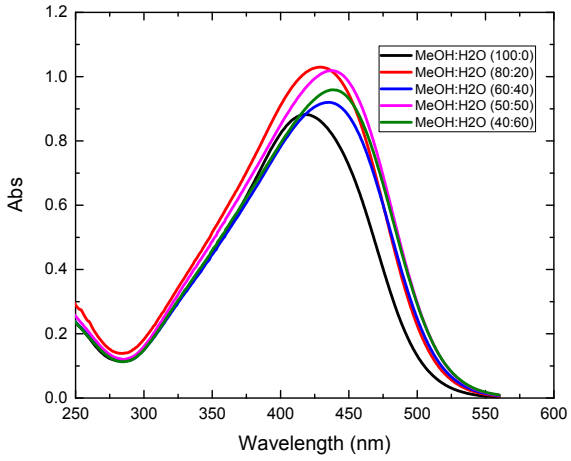


Figure S45 . UV-visible spectra of compound **2c** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

9.6 UV-Visible studies of compound **3b**

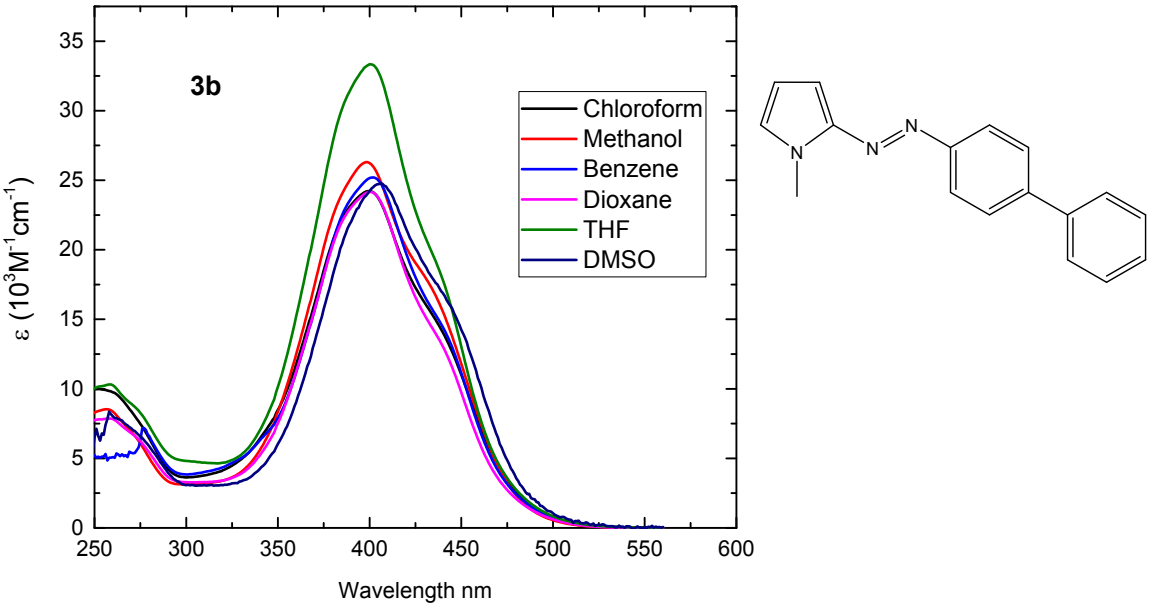


Figure S46 . UV-visible spectra of compound **3b** in different solvents.

Table S7. UV-visible spectroscopic data for **3b** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
3b	λ_{max}= 400 ε= 24216	λ_{max}= 398 ε= 26304	λ_{max}= 401 ε= 25193	λ_{max}= 400 ε= 24165	λ_{max}= 400 ε= 33341	λ_{max}= 406 ε= 24766	$\lambda_{max\ MeOH}$= 398 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$ = 435

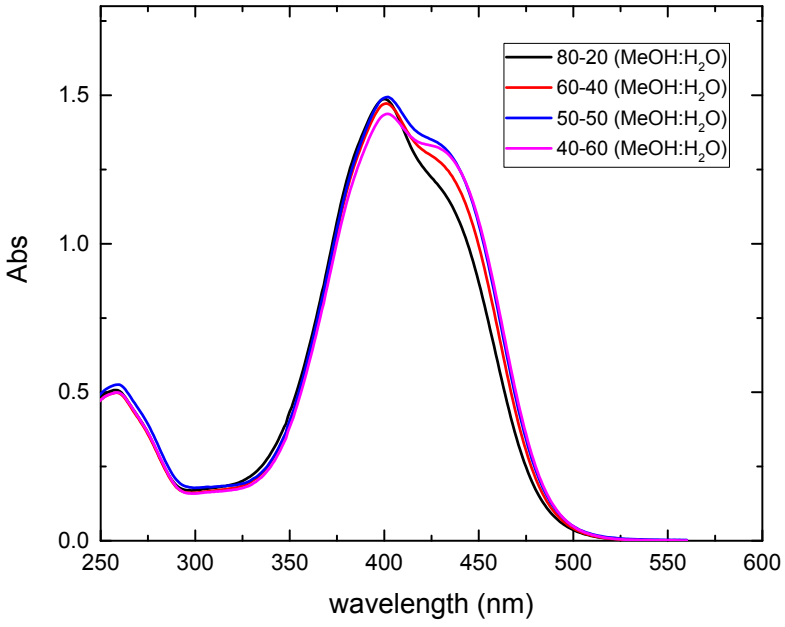


Figure S47 . UV-visible spectra of compound **3b** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

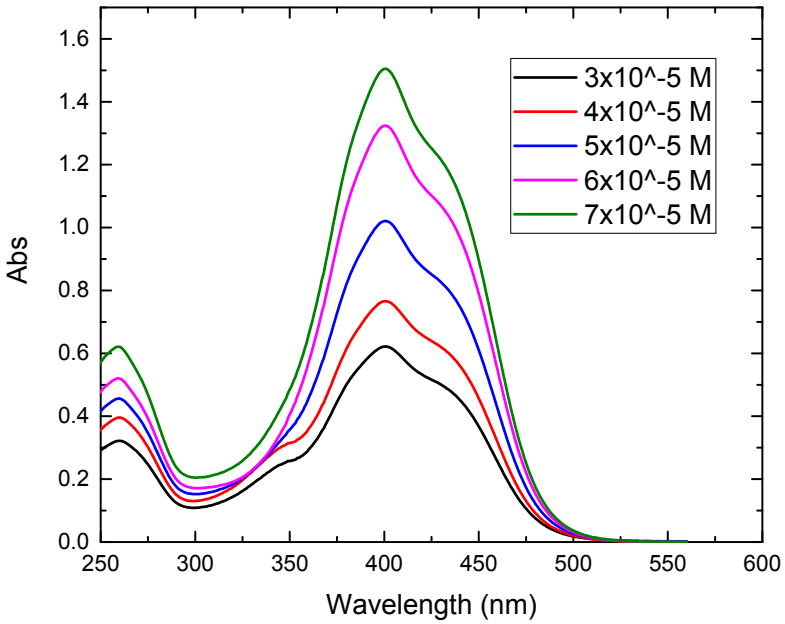


Figure S48 . UV-visible spectra of compound **3b** at different concentrations using MeOH/H_2O (80:20).

9.7 UV-Visible studies of compound **3c**

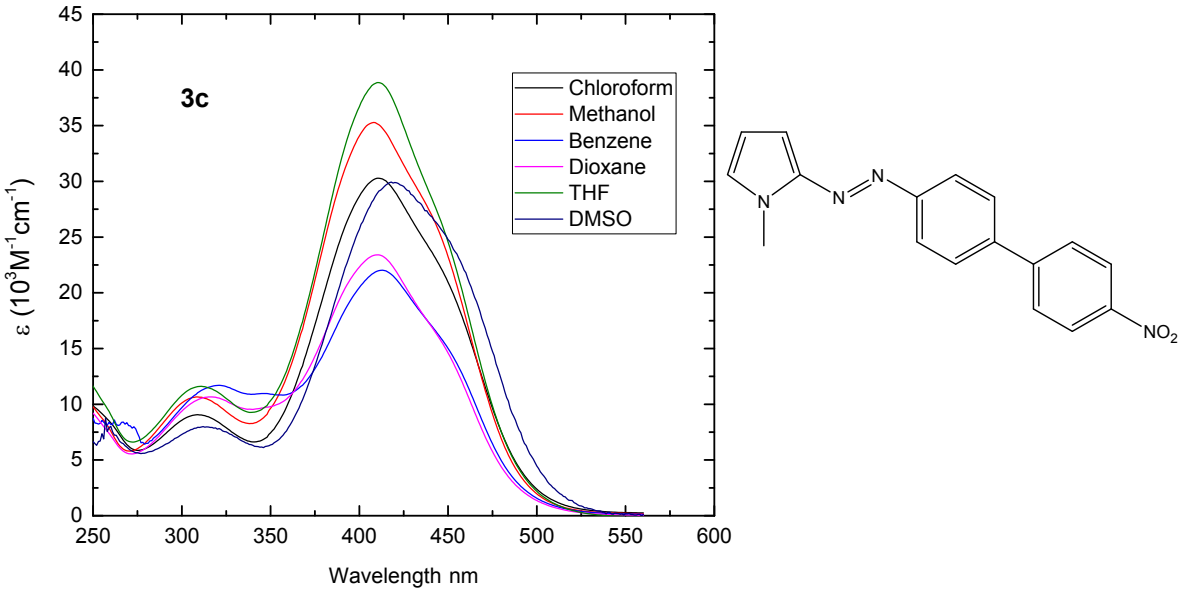


Figure S49 . UV-visible spectra of compound **3c** in different solvents.

Table S8. UV-visible spectroscopic data for **3c** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
3c	λ_{max}= 411 ε= 29848	λ_{max}= 409 ε= 34780	λ_{max}= 413 ε= 21888	λ_{max}= 410 ε= 23410	λ_{max}= 411 ε= 38857	λ_{max}= 420 ε= 29892	$\lambda_{max\ MeOH}$= 409 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$= 437

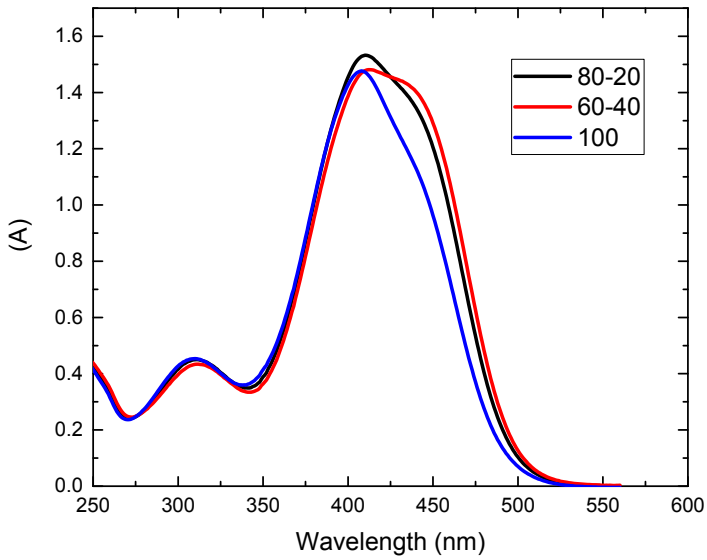


Figure S50 . UV-visible spectra of compound **3c** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

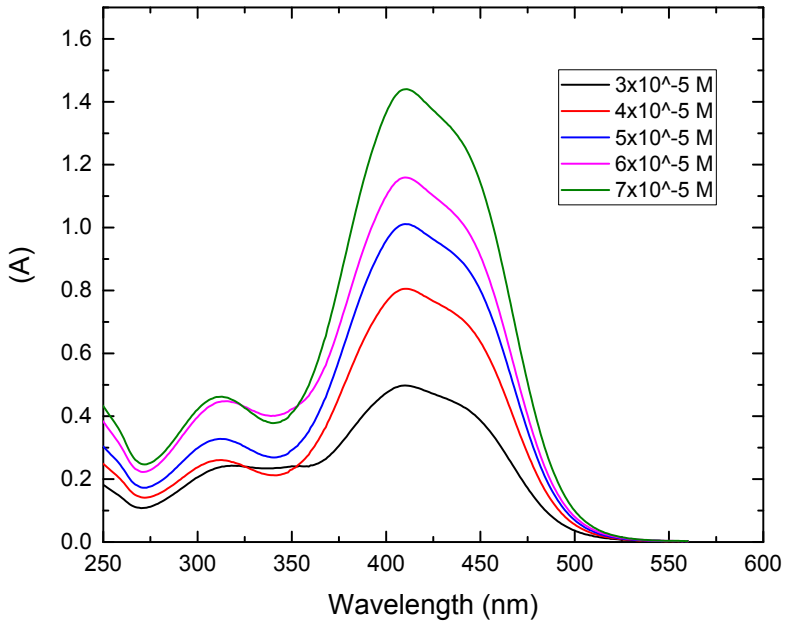


Figure S51 . UV-visible spectra of compound **3c** at different concentrations using MeOH/H_2O (80:20).

9.8 UV-Visible studies of compound **3d**

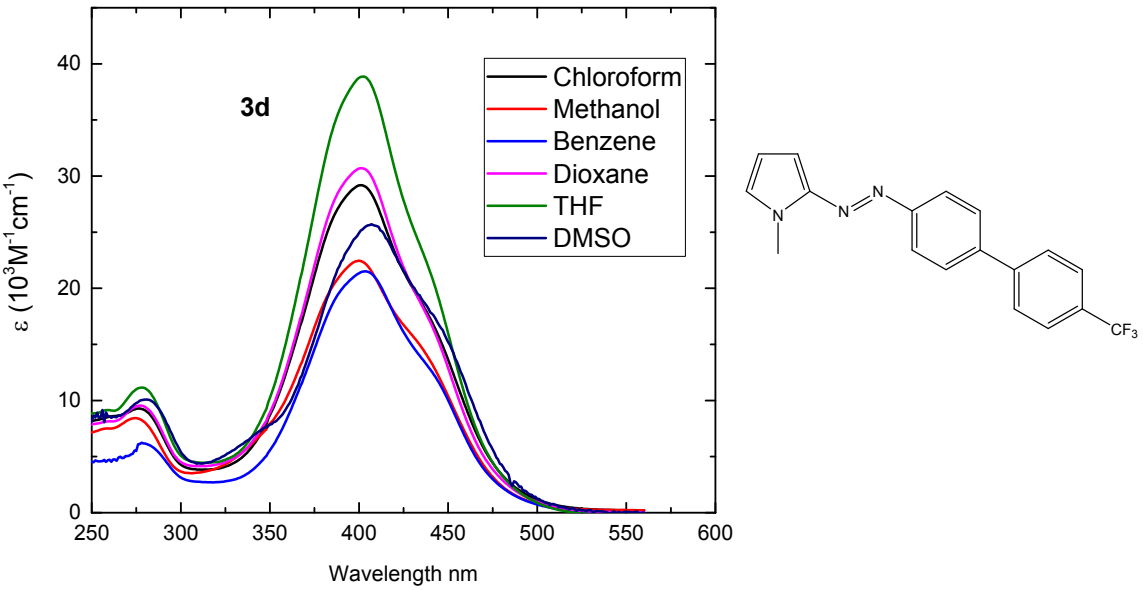


Figure S52 . UV-visible spectra of compound **3d** in different solvents.

Table S9. UV-visible spectroscopic data for **3d** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
3d	λ_{max}= 401 ε= 28761	λ_{max}= 400 ε= 21982	λ_{max}= 404 ε= 21511	λ_{max}= 402 ε= 30689	λ_{max}= 402 ε= 38857	λ_{max}= 406 ε= 25632	$\lambda_{max\ MeOH}$= 400 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$= 434

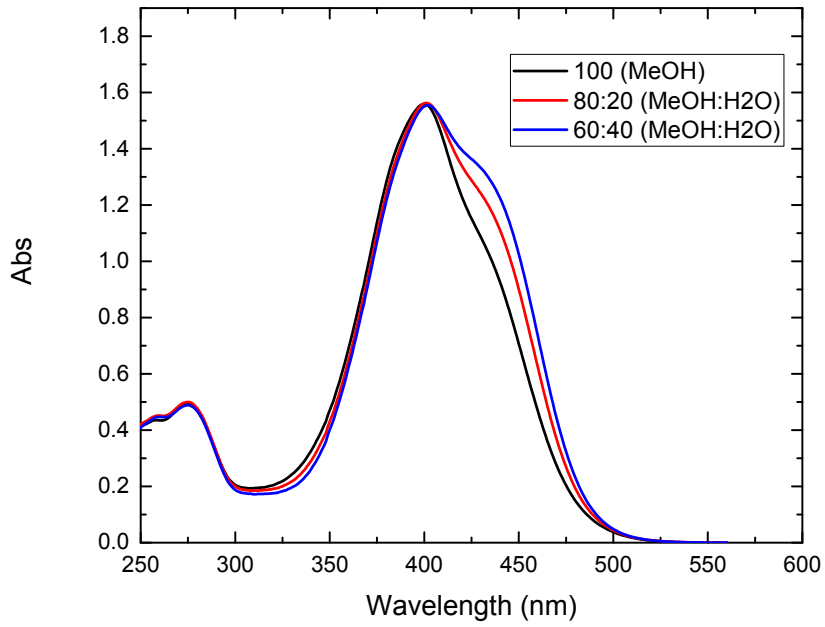


Figure S53 . UV-visible spectra of compound **3d** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

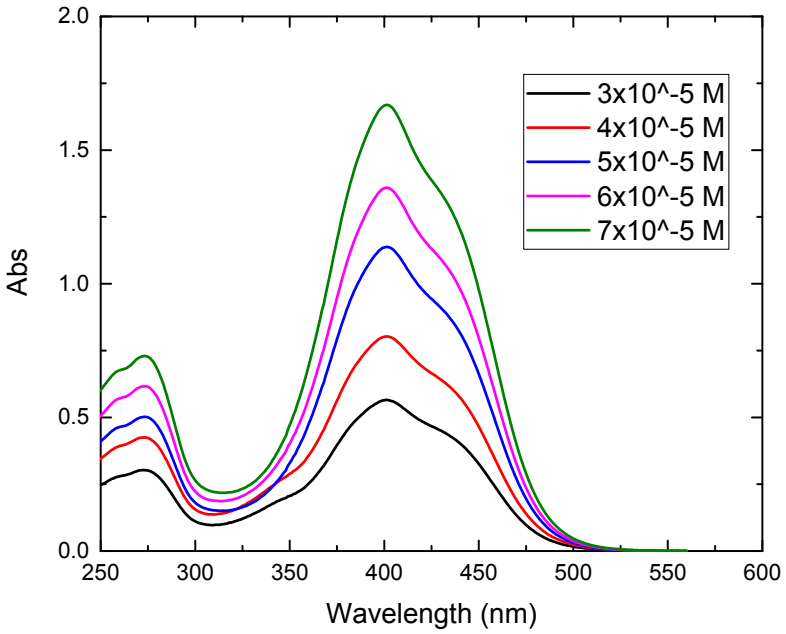


Figure S54 . UV-visible spectra of compound **3d** at different concentrations using MeOH/H_2O (80:20).

9.8 UV-Visible studies of compound **3e**

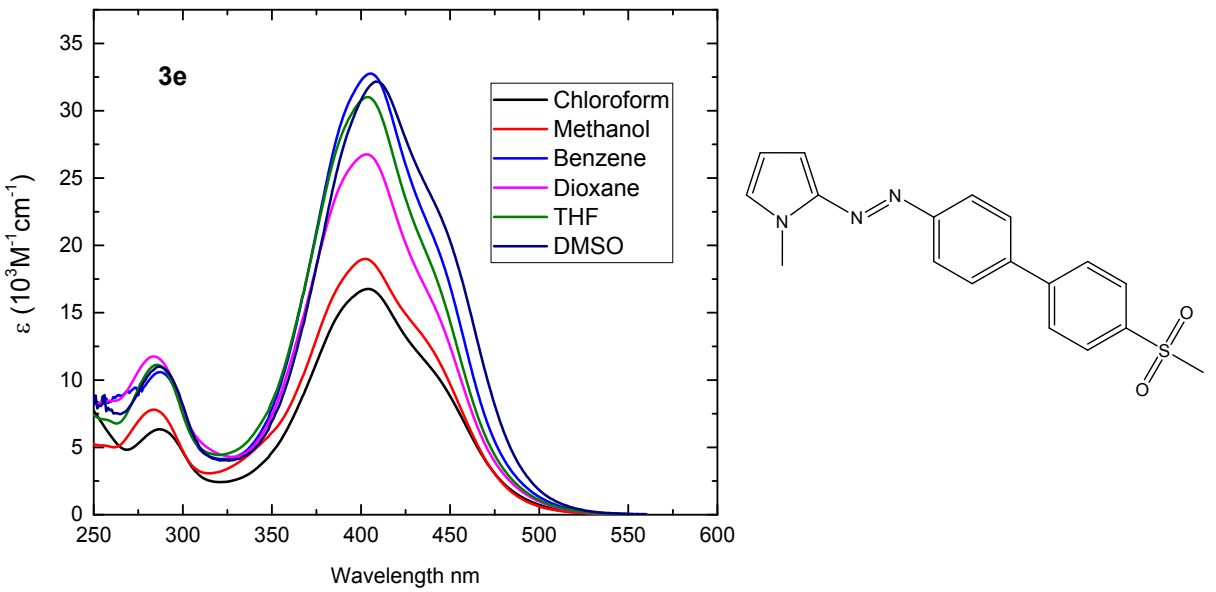


Figure S55 . UV-visible spectra of compound **3e** in different solvents.

Table S10. UV-visible spectroscopic data for **3e** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
3e	λ_{max}= 404 ε= 16768	λ_{max}= 402 ε= 18991	λ_{max}= 405 ε= 32757	λ_{max}= 403 ε= 26758	λ_{max}= 403 ε= 31005	λ_{max}= 409 ε= 32153	$\lambda_{max\ MeOH}$= 402 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$= 438

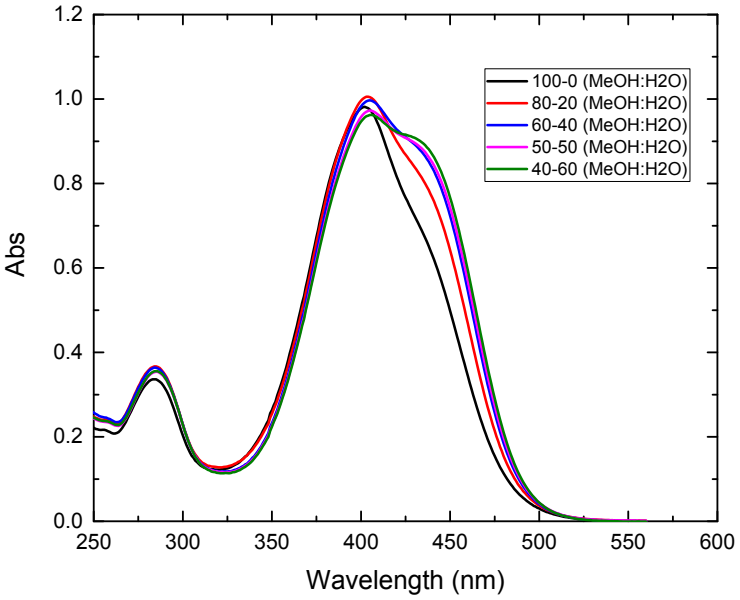


Figure S56 . UV-visible spectra of compound **3e** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

9.9 UV-Visible studies of compound **3f**

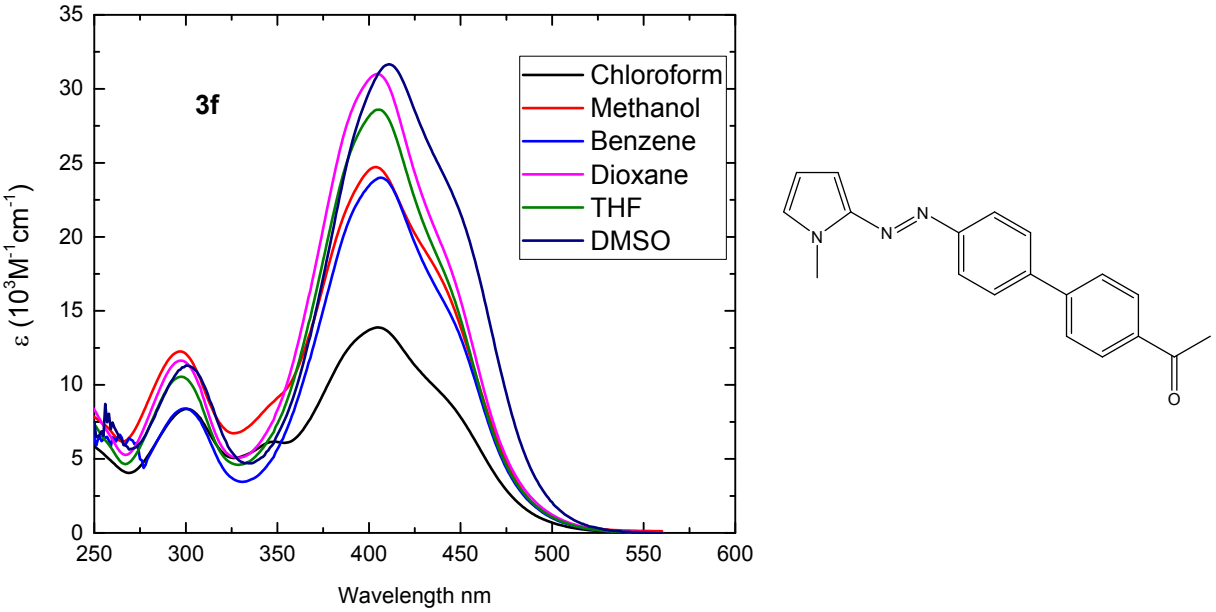
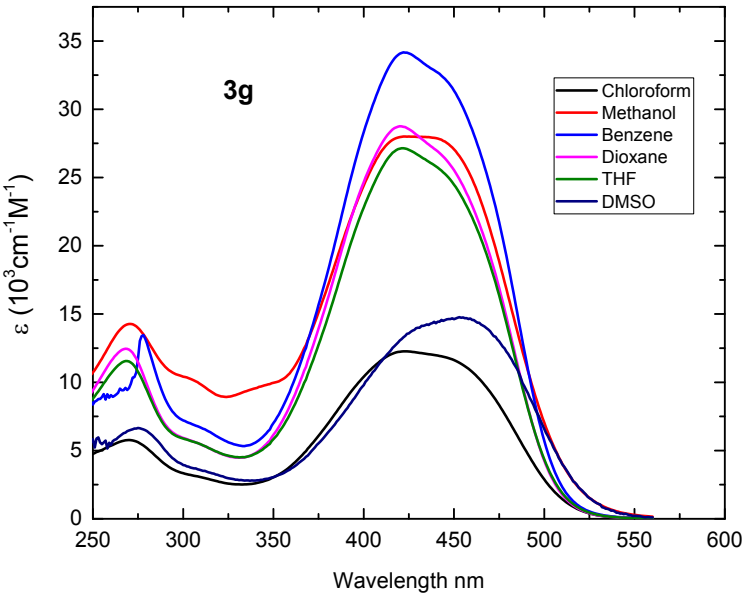


Figure S57 . UV-visible spectra of compound **3f** in different solvents.

Table S11. UV-visible spectroscopic data for **3f** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
3f	λ_{max}= 405 ε= 13881	λ_{max}= 403 ε= 24714	λ_{max}= 406 ε= 23999	λ_{max}= 405 ε= 31005	λ_{max}= 405 ε= 28597	λ_{max}= 412 ε= 31595	Highly photosensitive

9.10 UV-Visible studies of compound **3g**



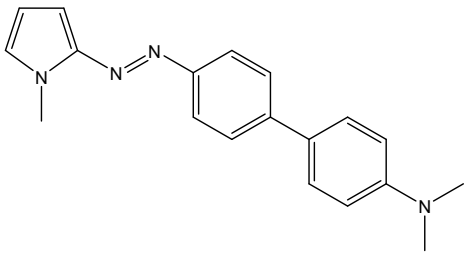


Figure S58 . UV-visible spectra of compound **3g** in different solvents.

Table S12. UV-visible spectroscopic data for **3g** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
3g	λ_{max}= 423 ε= 12267	λ_{max}= 425 ε= 28005	λ_{max}= 423 ε= 34150	λ_{max}= 421 ε= 28748	λ_{max}= 421 ε= 27145	λ_{max}= 452 ε= 14893	$\lambda_{max\ MeOH}$= 425 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$= 446

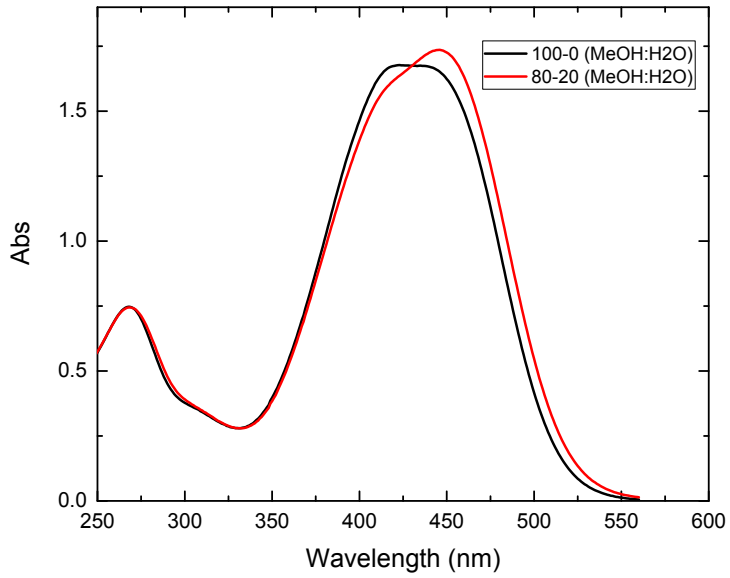
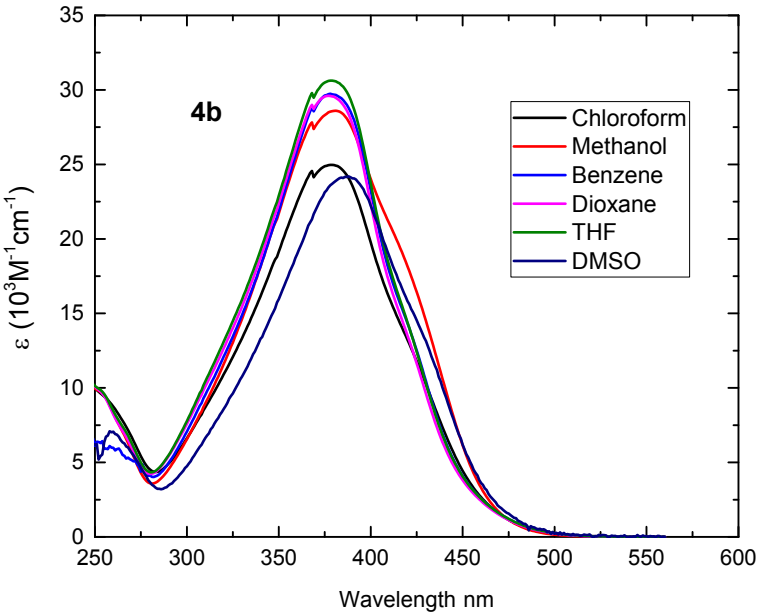


Figure S59 . UV-visible spectra of compound **3g** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

9.11 UV-Visible studies of compound **4b**



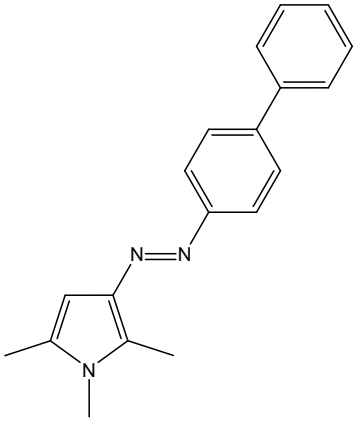


Figure S60 . UV-visible spectra of compound **4b** in different solvents.

Table S13. UV-visible spectroscopic data for **4b** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
4b	λ_{max}= 378 ε= 24971	λ_{max}= 380 ε= 28595	λ_{max}= 378 ε= 29739	λ_{max}= 377 ε= 29604	λ_{max}= 378 ε= 30619	λ_{max}= 387 ε= 24153	$\lambda_{max\ MeOH}$= 380 $\lambda_{max\ (MeOH/H2O,\ 80:20)}$ = 415

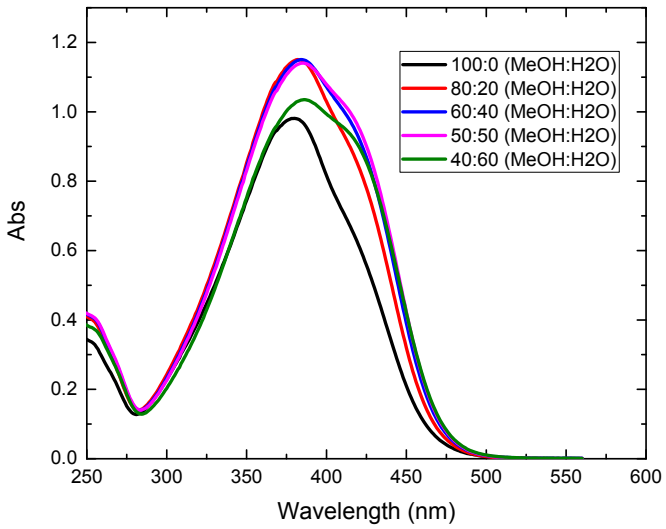
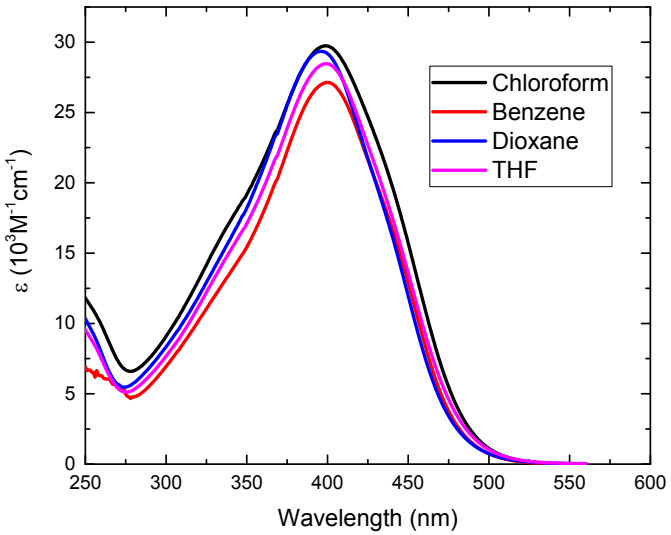


Figure S61 . UV-visible spectra of compound **4b** (5 x 10^{-5} M) in different ratios MeOH/H_2O.

9.11 UV-Visible studies of compound **4c**



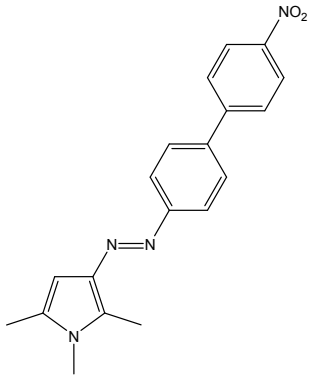


Figure S62 . UV-visible spectra of compound **4c** in different solvents.

Table S14. UV-visible spectroscopic data for **4c** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	Aggregation
4c	λ_{max}= 398 ε= 29736	λ_{max}= 395 ε= 27560	λ_{max}= 399 ε= 27135	λ_{max}= 396 ε= 29350	λ_{max}= 400 ε= 28463	Not soluble

9.12 UV-Visible studies of compound **4d**

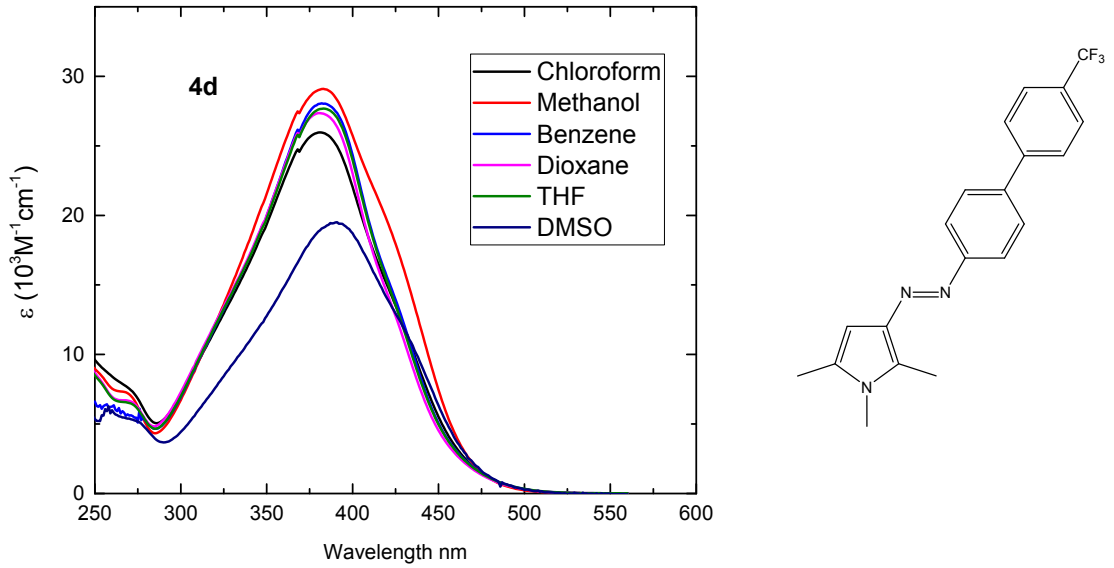


Figure S63. UV-visible spectra of compound **4d** in different solvents.

Table S14. UV-visible spectroscopic data for **4d** acquired in different solvents.

Compound	Chloroform	Methanol	Benzene	Dioxane	THF	DMSO	Aggregation
4d	λ_{max}= 381 ε= 25964	λ_{max}= 382 ε= 29088	λ_{max}= 381 ε= 28032	λ_{max}= 380 ε= 27353	λ_{max}= 383 ε= 27683	λ_{max}= 390 ε= 19461	$\lambda_{max\ MeOH}$= 382 $\lambda_{max\ (MeOH/H20\ 80:20)}$≈ 417

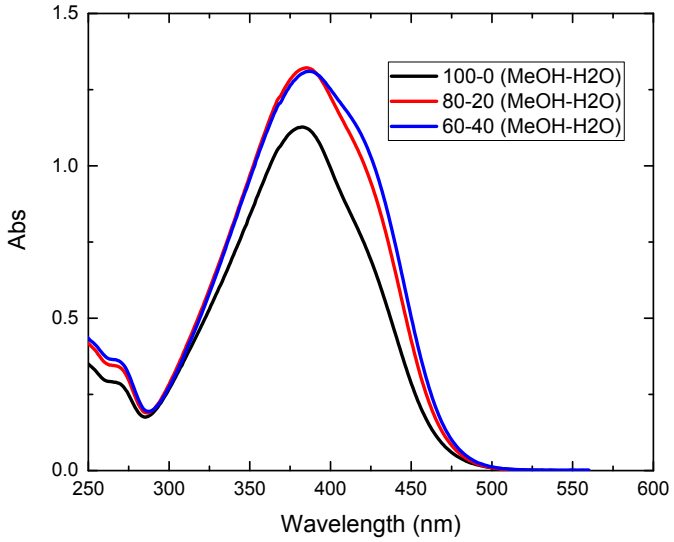
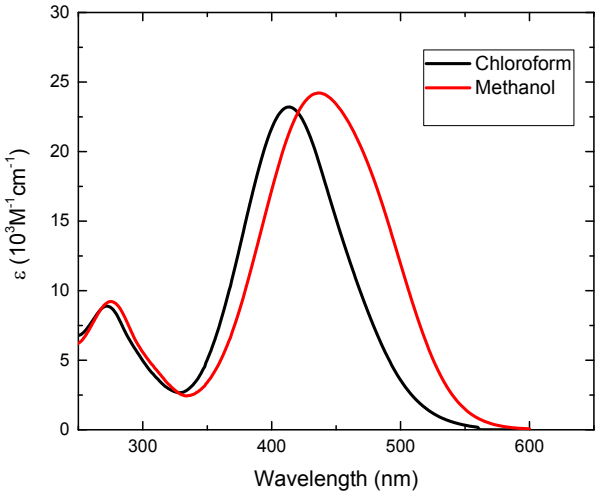


Figure S64 . UV-visible spectra of compound **4d** (5 x 10^{-5} M) in different ratios MeOH/H_2O.



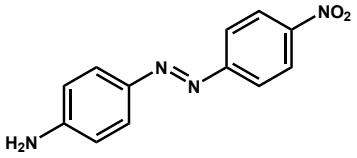


Figure S65 . UV-visible spectra of Disperse Orange 3 in $CHCl_3$ and MeOH.

Chloroform	**Methanol**
λ_{max}= 413	λ_{max}= 435
ε= 23203	ε= 24190

10. Photoisomerization of compounds 3b, 4b and 4c

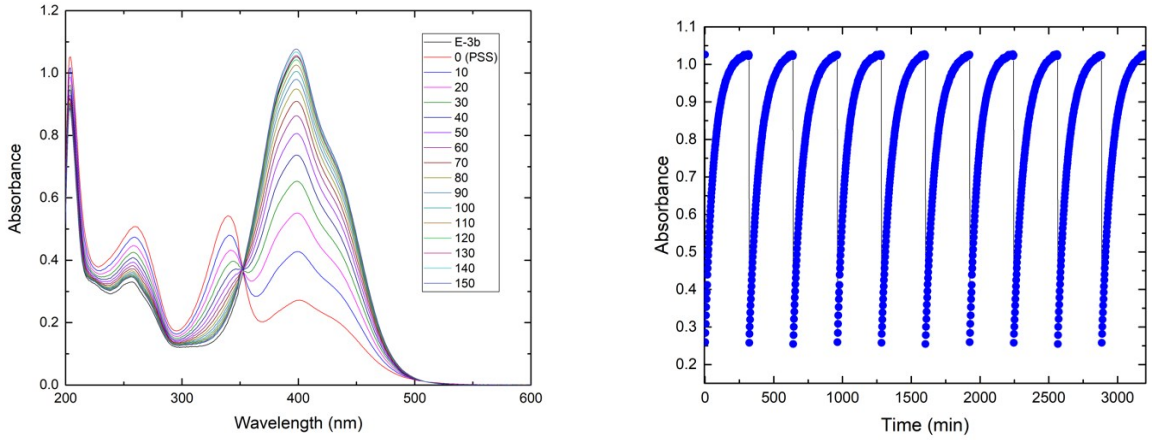


Figure S66. (Left) UV-vis spectra for **3b** (2x 10^{-5}M, MeOH) after 485 irradiation (PSS) and cis →trans return. (Right) **3b** was irradiated ten times for 1 minute (5.0 mW).

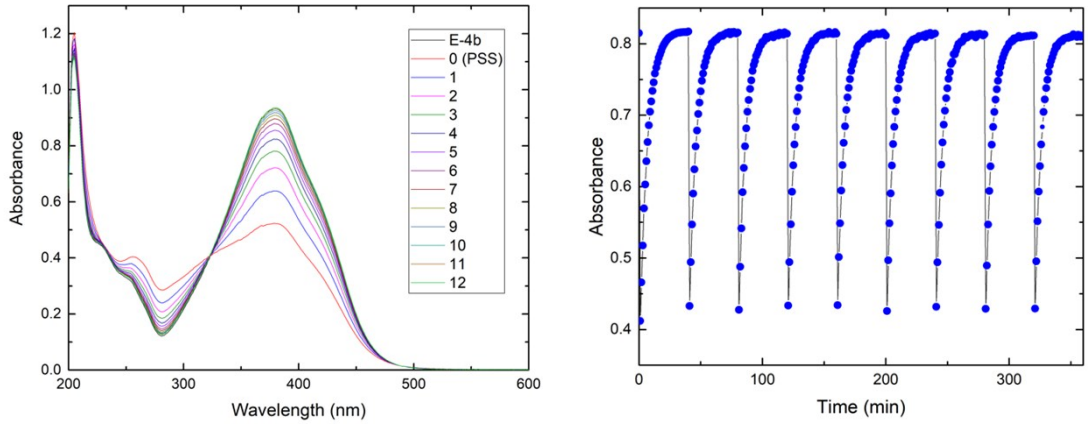


Figure S67. (Left) UV-vis spectra for **4b** (2x 10^{-5}M, MeOH) after 485 irradiation (PSS) and cis →trans return. (Right) **4b** was irradiated ten times for 1 minute (5.0 mW).

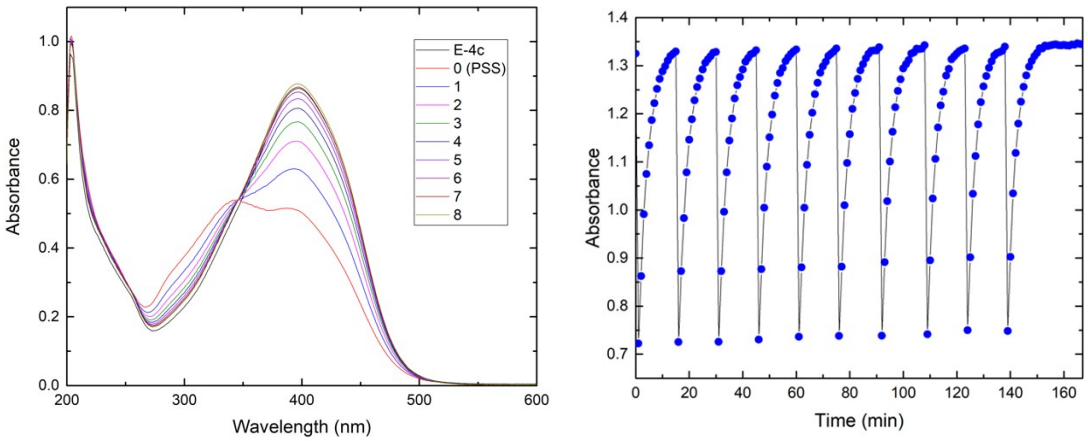


Figure S68. (Left) UV-vis spectra for **4c** (2x 10^{-5}M, MeOH) after 485 irradiation (PSS) and cis →trans return. (Right) **4c** was irradiated ten times for 1 minute (5.0 mW).

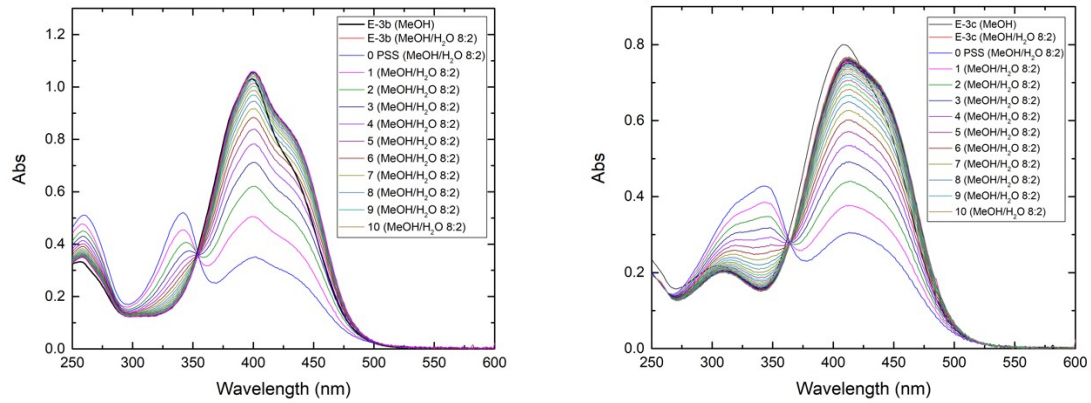


Figure S69. (Left) UV-vis spectra for **3b** (2x 10^{-5}M, MeOH:H_2O /80:20 after 485 irradiation (PSS) and cis →trans return. (Right) UV-vis spectra for **3c** (2x 10^{-5}M, MeOH:H_2O /80:20 after 485 irradiation (PSS) and cis →trans return.

11. Graphical determination of Optical band-gap for compounds 1b-d, 2b-c, 3b-d and 4b-d

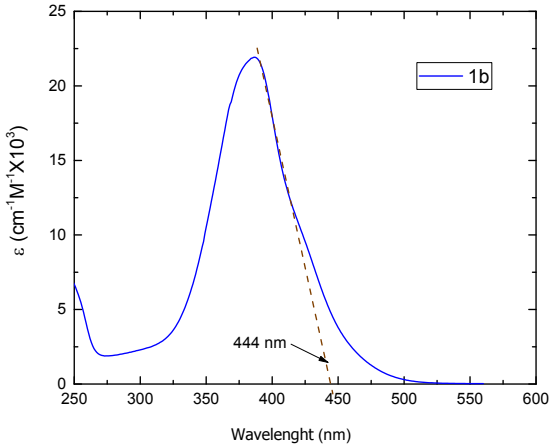


Figure S70. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **1b**

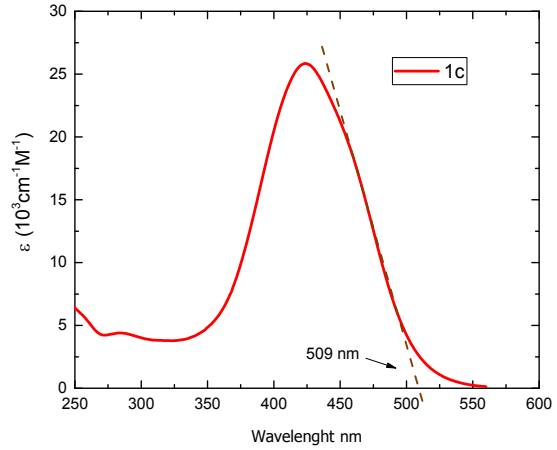


Figure S71. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **1c**

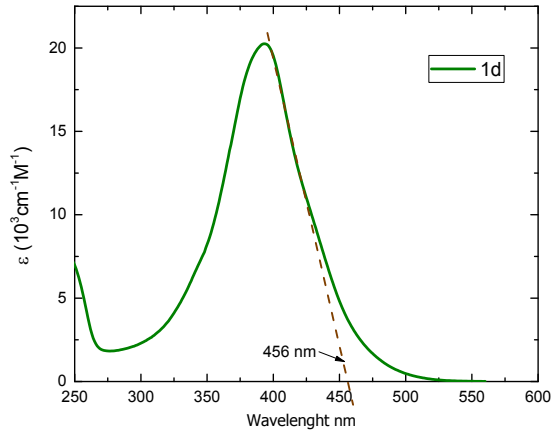


Figure S72. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **1d**

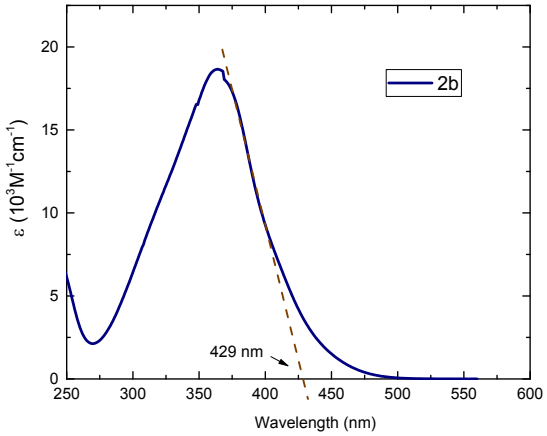


Figure S73. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **2b**

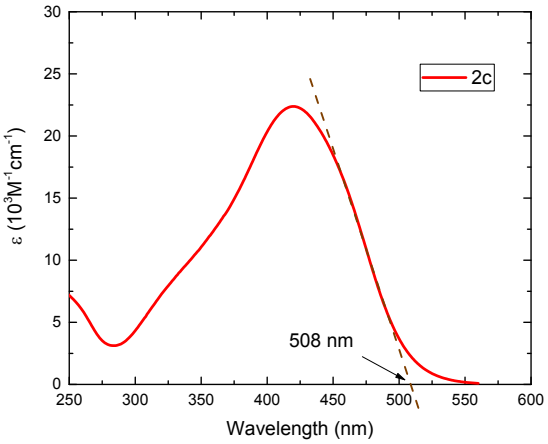


Figure S74. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **2c**

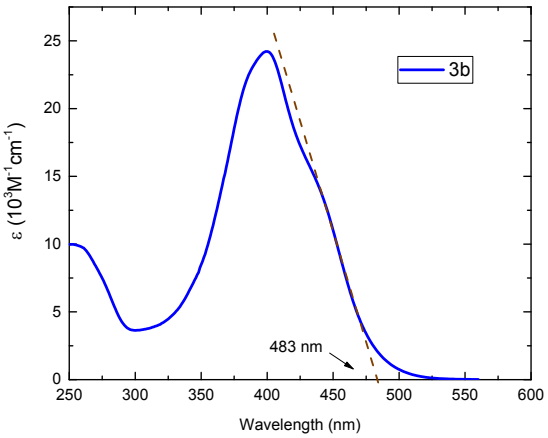


Figure S75. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **3b**

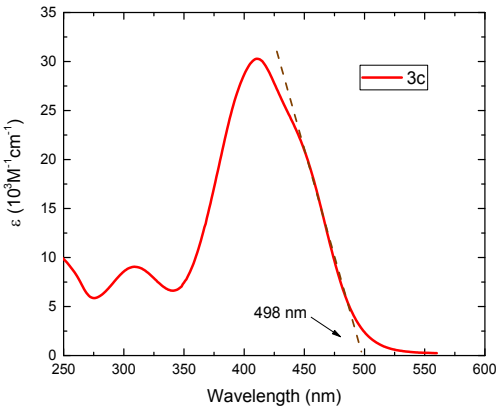


Figure S76. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **3c**

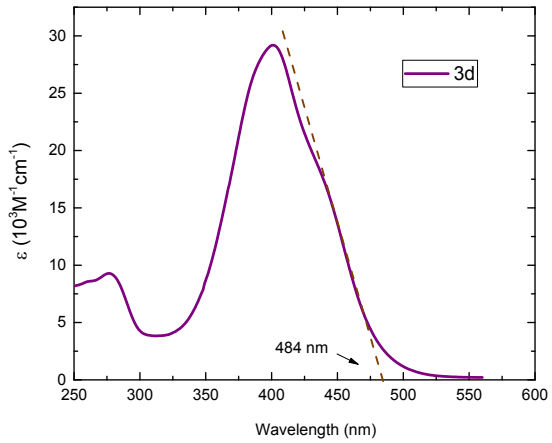


Figure S77. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **3d**

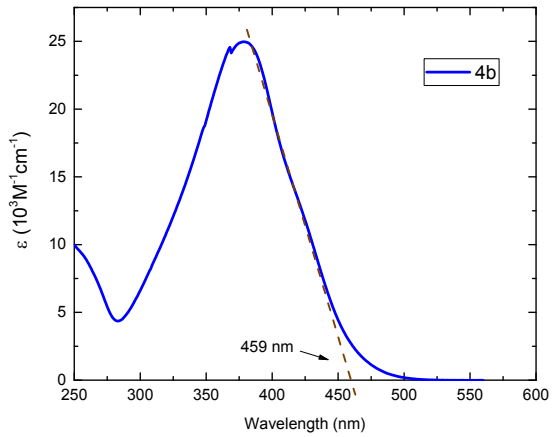


Figure S78. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **4b**

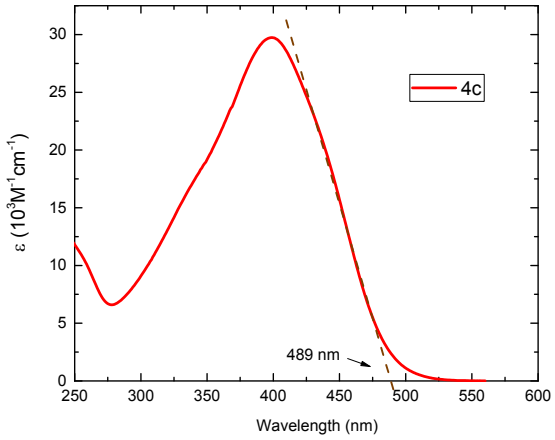


Figure S79. Absorption spectrum in $CHCl_3$ and optical onset band gap for compound **4c**

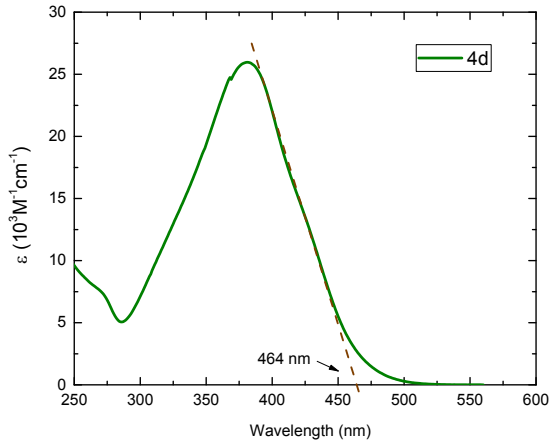


Figure S80. Absorption spectrum in $CHCl_3$ and optical onset band gap for **compound 4d**

12. Theoretical calculations.

The data results were obtained from DMol3 numerical-based density-functional module implemented in the Materials Studio 6.0 software package from Accelrys Inc., employing DFT, PBE (Perdew-Burke-Ernzerhof correlation),[iv] Gradient General Approximation (GGA). All the calculations were running in conjunction with the double numerical basis set DNP, which has a polarization d-function added on all non-hydrogen atoms. The calculations involve: the geometric optimization of *trans* isomer in vacuum and chloroform mediums, the energies of orbital frontiers (HOMO and LUMO), the energy of band gap from the difference between the HOMO and LUMO energies, and finally the dipole moment. PBE is a DFT hybrid approach and is acceptable to be used in geometry of molecules and calculations of electronic properties with a small positive bias,[v] moreover, using the double numerical basis set (DNP)[vi] the accuracy usually is increased.

Table S6. Frontier molecular orbitals of *E* and *Z*-azopyrrole dyes calculated at the PBE-D/DNP level of theory, using $CHCl_3$ as implicit solvent (COSMO model). Frontier orbital gaps, optical energies gaps and molecular dipole moments.

Entry	Compound	E(*E*)-E(*Z*), (eV)	E_{gap} (eV)	λ_{onset} (nm)[a]	Optical E_{gap} (eV)[a]	Dipole Moment (D)
1	*E*-**1b**	-0.37	2.12	444	2.79	3.49
2	*Z*-**1b**		2.37			4.76
3	*E*-**1c**	-0.37	1.75	509	2.44	11.28
4	*Z*-**1c**		1.93			9.53
5	*E*-**1d**	-0.36	2.09	456	2.72	7.35
6	*Z*-**1d**		2.48			6.59
7	*E*-**2b**	-0.38	2.27	429	2.89	6.31
8	*Z*-**2b**		2.57			8.18
9	*E*-**2c**	-0.37	1.70	508	2.44	15.41
10	*Z*-**2c**		1.78			12.24
11	*E*-**2d**	-0.37	2.62	-	-[b]	9.39
12	*Z*-**2d**		2.61			9.39
13	*E*-**3b**	-0.39	1.99	483	2.56	3.39
14	*Z*-**3b**		2.29			4.82
15	*E*-**3c**	-0.38	1.60	498	2.49	10.70
16	*Z*-**3c**		1.71			9.76
17	*E*-**3d**	-0.38	1.98	484	2.56	6.98
18	*Z*-**3d**		2.22			6.76
19	*E*-**4b**	-0.38	2.15	459	2.70	6.26
20	*Z*-**4b**		2.40			8.26
21	*E*-**4c**	-0.39	1.52	489	2.53	15.12
22	*Z*-**4c**		1.53			11.49
23	*E*-**4d**	-0.41	2.09	464	2.67	11.04
24	*Z*-**4d**		2.56			8.44

12.1 Optimized Molecular Geometries for arylazopyroles 1b-d, 2b-d, 3b-d and 4b-d.

***Z*-1b**			***E*-1b**		
C	5.17995	-4.17097	C	0.12776	-0.56954
C	6.44437	-3.60571	C	0.02059	-0.05630
C	6.27788	-2.22788	C	1.31414	0.26322
C	4.89962	-1.97489	C	2.18513	-0.06464
N	4.25575	-3.19496	N	1.43232	-0.57001
H	4.88157	-5.20228	H	-0.63446	-0.93109
H	7.38030	-4.14113	H	-0.90150	0.07310
H	7.06008	-1.49142	H	1.62281	0.69097
C	2.82209	-3.39569	C	1.95839	-1.07429
H	2.34116	-2.43903	H	2.97927	-0.71223
H	2.48878	-3.76463	H	1.96700	-2.16881
H	2.54811	-4.11895	H	1.34826	-0.71341
N	4.05426	-0.88905	N	3.53976	0.02659
N	4.40308	0.29881	N	4.16791	0.48495
C	5.76312	0.64493	C	5.56048	0.57858
C	6.29860	0.53503	C	6.25172	0.18663
C	6.51582	1.22386	C	6.27124	1.10608
C	7.59487	0.97284	C	7.62962	0.32678
H	5.69420	0.10477	H	5.69032	-0.22359
C	7.81572	1.64934	C	7.65245	1.24500
H	6.07649	1.32823	H	5.71078	1.39977
C	8.36145	1.52310	C	8.33568	0.85581
H	8.00867	0.88340	H	8.16386	0.02198
H	8.40245	2.08819	H	8.19625	1.65644
H	9.37362	1.86309	H	9.41522	0.96203

***Z*-1c**			***E*-1c**		
C	5.07752	-4.20637	C	0.17330	-0.58086
C	6.36533	-3.68687	C	0.03473	-0.09027
C	6.25669	-2.30416	C	1.31193	0.24342
C	4.88974	-2.00180	C	2.20691	-0.05269
N	4.19505	-3.19810	N	1.47970	-0.55519
H	4.73860	-5.22806	H	-0.57334	-0.94333
H	7.27666	-4.25672	H	-0.89853	0.00937
H	7.06895	-1.59645	H	1.59753	0.65564
C	2.75671	-3.34473	C	2.04108	-1.00043
H	2.29547	-2.39342	H	2.64860	-0.21036
H	2.45282	-3.61816	H	2.66855	-1.88304
H	2.43130	-4.12090	H	1.22281	-1.24995
N	4.09849	-0.88309	N	3.55468	0.05247
N	4.51130	0.28654	N	4.17536	0.51366
C	5.87299	0.59236	C	5.56356	0.61073
C	6.41921	0.44394	C	6.24697	0.23353

C 6.61996 1.19998 2.91856	C 6.28091 1.12640 2.78777
C 7.71225 0.86913 0.36456	C 7.62013 0.37189 0.45722
H 5.82005 -0.00473 -0.16542	H 5.67866 -0.16475 -0.30050
C 7.91847 1.61675 2.66996	C 7.65745 1.26891 2.72154
H 6.17216 1.33533 3.89754	H 5.72797 1.40895 3.67746
C 8.44917 1.44308 1.39617	C 8.30882 0.88850 1.55382
H 8.16465 0.76512 -0.61462	H 8.17694 0.09032 -0.42876
H 8.52719 2.07812 3.43863	H 8.23559 1.66506 3.54759
N 9.81377 1.88275 1.13199	N 9.75797 1.03375 1.47293
O 10.25209 1.72249 0.00269	O 10.30493 0.69136 0.43493
O 10.43740 2.38197 2.05659	O 10.33777 1.48890 2.44750

***Z*-1d**	***E*-1d**
C -2.42554 -3.13004 -0.19313	C -0.11956 -0.30371 0.12433
C -3.48738 -3.76673 -0.85156	C -0.02555 -0.14642 1.50812
C -3.26219 -5.14459 -0.76769	C 1.33243 -0.01032 1.81462
C -2.07654 -5.33008 -0.07054	C 2.03631 -0.08639 0.61857
N -1.58152 -4.12641 0.28221	N 1.15959 -0.25765 -0.39744
H -4.32945 -3.28144 -1.31766	H -0.87127 -0.12907 2.17905
H -3.89071 -5.92919 -1.16414	H 1.77048 0.13666 2.79163
H -1.55605 -6.24045 0.19222	H 3.09861 -0.02810 0.42737
C -0.33242 -3.90393 0.98014	C 1.50156 -0.44087 -1.79048
H -0.21413 -4.65927 1.75973	H 2.47869 0.00810 -1.97640
H 0.51570 -3.96070 0.29083	H 1.53807 -1.50283 -2.05192
H -0.35880 -2.91016 1.42461	H 0.75357 0.04658 -2.41557
N -2.05745 -1.85152 0.15717	N -1.15690 -0.47102 -0.74579
N -2.63211 -0.79849 -0.20870	N -2.30204 -0.51864 -0.21059
C -3.71842 -0.81262 -1.12210	C -3.35635 -0.69074 -1.12583
C -5.01676 -0.59830 -0.65292	C -4.63885 -0.70834 -0.56861
C -3.47595 -0.88175 -2.49771	C -3.20364 -0.84193 -2.51217
C -6.07039 -0.50194 -1.55207	C -5.75553 -0.87286 -1.37587
H -5.18764 -0.51094 0.41528	H -4.73144 -0.58647 0.50576
C -4.53106 -0.77439 -3.39184	C -4.31794 -1.00687 -3.31580
H -2.45961 -1.01682 -2.85379	H -2.20497 -0.82508 -2.93356
C -5.83145 -0.59276 -2.92221	C -5.59643 -1.02263 -2.75131
H -7.08098 -0.34044 -1.19105	H -6.75059 -0.87840 -0.94386
H -4.34691 -0.82328 -4.46013	H -4.20616 -1.11698 -4.38985
C -6.97585 -0.54304 -3.88807	C -6.79032 -1.26075 -3.62624
F -7.98490 0.21635 -3.43050	F -7.90924 -0.73486 -3.10228
F -7.48592 -1.76788 -4.11865	F -7.02159 -2.57459 -3.80389
F -6.60257 -0.04820 -5.07973	F -6.62593 -0.72781 -4.84898

***Z*-2b**			***E*-2b**		
C	-1.72687	-3.74736	C	-0.01488	-0.29309	0.13049
C	-2.01480	-2.53929	3.27348	C	0.00965	-0.21067	1.52009
C	-3.19880	-2.74798	4.06003	C	1.37567	-0.18946	1.93445
C	-3.58046	-4.04748	3.87394	C	2.13904	-0.25794	0.80286
N	-2.67731	-4.64612	3.00470	N	1.28261	-0.31766	-0.29189
H	-3.71345	-2.03902	4.68801	H	1.72880	-0.12820	2.95268
C	-2.76449	-6.01826	2.56640	C	1.72241	-0.42809	-1.66098
H	-2.75425	-6.70084	3.42161	H	2.44325	0.35918	-1.90032
H	-3.68181	-6.19063	1.99408	H	2.19179	-1.39943	-1.85269
H	-1.91135	-6.25082	1.92963	H	0.86637	-0.32182	-2.32728
C	-4.73133	-4.79913	4.44288	C	3.61712	-0.27168	0.63477
H	-5.40819	-5.17787	3.66691	H	3.97216	-1.17865	0.12983
H	-4.41267	-5.65880	5.04560	H	3.98072	0.58699	0.05639
H	-5.30926	-4.13789	5.09127	H	4.09276	-0.23229	1.61652
C	-0.60592	-4.05117	1.70766	C	-1.19171	-0.34605	-0.77259
H	0.04520	-4.84565	2.09165	H	-1.22323	0.50140	-1.46836
H	-0.95795	-4.35675	0.71516	H	-1.22208	-1.26722	-1.36697
H	-0.01212	-3.14231	1.59830	H	-2.09091	-0.31011	-0.15518
N	-1.14785	-1.48267	3.01956	N	-1.15754	-0.16323	2.25114
N	-1.24064	-0.33014	3.49983	N	-0.99364	-0.08654	3.49939
C	-2.28474	0.03844	4.39514	C	-2.19477	-0.04025	4.24017
C	-2.08266	-0.05065	5.77452	C	-2.04311	0.05139	5.62649
C	-3.45061	0.62742	3.89988	C	-3.48236	-0.08000	3.68774
C	-3.06203	0.40867	6.64872	C	-3.15841	0.10353	6.45479
H	-1.16057	-0.48625	6.14753	H	-1.03445	0.08016	6.02745
C	-4.42427	1.08368	4.78204	C	-4.59134	-0.02790	4.51869
H	-3.58440	0.71528	2.82587	H	-3.58349	-0.15155	2.61032
C	-4.23849	0.97169	6.15841	C	-4.43607	0.06401	5.90345
H	-2.90332	0.32814	7.72065	H	-3.03078	0.17491	7.53116
H	-5.33337	1.53223	4.39080	H	-5.58863	-0.05904	4.08804
H	-4.99925	1.33254	6.84407	H	-5.30996	0.10428	6.54737

***Z*-2c**			***E*-2c**		
C	-0.75874	3.69225	C	-0.02590	-0.29944	0.14631
C	-1.39975	2.50162	3.95099	C	0.00535	-0.22119	1.54009
C	-2.53988	2.85512	4.75055	C	1.37431	-0.19599	1.94877
C	-2.55234	4.21803	4.84857	C	2.13026	-0.25841	0.81399
N	-1.46427	4.71512	4.14034	N	1.26608	-0.32115	-0.27884
H	-3.26731	2.20111	5.20289	H	1.73277	-0.13836	2.96521
C	-1.15268	6.12019	4.02057	C	1.70468	-0.39761	-1.65178
H	-1.97256	6.66090	3.53803	H	2.30398	0.47805	-1.92015
H	-0.97222	6.56412	5.00434	H	2.30556	-1.29670	-1.82086
H	-0.25467	6.24233	3.41596	H	0.83638	-0.43517	-2.30898
C	-3.50152	5.12004	5.55420	C	3.60658	-0.26596	0.63387

H	-3.00821	5.72019	6.32846	H	3.96095	-1.17793	0.13799
H	-4.00135	5.81625	4.86975	H	3.95801	0.58674	0.04010
H	-4.27472	4.52321	6.04130	H	4.09076	-0.21097	1.61050
C	0.46522	3.86376	2.77060	C	-1.20738	-0.35173	-0.75000
H	0.27567	4.45106	1.86444	H	-1.24058	0.49641	-1.44414
H	1.27153	4.35583	3.32709	H	-1.23771	-1.27247	-1.34466
H	0.80834	2.87198	2.47235	H	-2.10461	-0.31834	-0.13007
N	-0.83298	1.32645	3.48785	N	-1.15373	-0.18210	2.27057
N	-1.27043	0.17488	3.71004	N	-0.98946	-0.11165	3.52295
C	-2.42474	-0.09555	4.47840	C	-2.19174	-0.07263	4.25345
C	-2.29935	-0.38334	5.84425	C	-2.04659	0.00543	5.64432
C	-3.66325	-0.25215	3.84151	C	-3.47813	-0.10611	3.69040
C	-3.40635	-0.78225	6.57519	C	-3.15828.	0.04993	6.46990
H	-1.32869	-0.28582	6.31933	H	-1.04140	0.02979	6.05211
C	-4.77321	-0.65075	4.56813	C	-4.59364	-0.06220	4.50576
H	-3.74073	-0.05382	2.77753	H	-3.57336	-0.16656	2.61249
C	-4.63294	-0.90575	5.92916	C	-4.42005	0.01536	5.88689
H	-3.34251	-0.99985	7.63487	H	-3.07303	0.11042	7.54816
H	-5.74608	-0.76858	4.10554	H	-5.59917	-0.08633	4.10233
N	-5.79950	-1.31769	6.69663	N	-5.59732	0.06160	6.74543
O	-5.64697	-1.53521	7.88996	O	-5.41809	0.12951	7.95270
O	-6.86380	-1.41770	6.10343	O	-6.69450	0.02973	6.20717

***Z*-2d**				***E*-2d**			
C	-0.95751	3.71472	3.32296	C	-0.02301	-0.29990	0.14272
C	-1.53872	2.52041	3.76049	C	0.00767	-0.22743	1.53466
C	-2.64279	2.87169	4.61045	C	1.37576	-0.19750	1.94353
C	-2.69282	4.23666	4.65902	C	2.13325	-0.25160	0.80829
N	-1.66275	4.73794	3.87237	N	1.27091	-0.31389	-0.28383
H	-3.32291	2.21428	5.12702	H	1.73345	-0.14231	2.96044
C	-1.40255	6.14532	3.68306	C	1.70875	-0.38232	-1.65685
H	-2.26352	6.64315	3.22632	H	2.30325	0.49743	-1.92328
H	-1.18344	6.63317	4.63787	H	2.31416	-1.27752	-1.83138
H	-0.54255	6.27046	3.02593	H	0.83992	-0.42164	-2.31342
C	-3.62891	5.13658	5.38462	C	3.60998	-0.25109	0.62963
H	-3.11284	5.77908	6.10868	H	3.97014	-1.15963	0.13134
H	-4.18742	5.79265	4.70566	H	3.95821	0.60512	0.03878
H	-4.35513	4.53569	5.93507	H	4.09293	-0.19656	1.60697
C	0.21202	3.89126	2.42576	C	-1.20411	-0.35397	-0.75442
H	-0.04614	4.43943	1.51197	H	-1.24237	0.49683	-1.44527
H	1.03381	4.42573	2.91686	H	-1.23154	-1.27243	-1.35298
H	0.56671	2.89881	2.14353	H	-2.10084	-0.32712	-0.13324
N	-0.95877	1.34582	3.30424	N	-1.15410	-0.19652	2.26845
N	-1.33792	0.18691	3.58946	N	-0.98822	-0.13180	3.51862
C	-2.44008	-0.07359	4.44463	C	-2.19037	-0.09874	4.25568

C	-2.22817	-0.28090	5.81108	C	-2.04368	-0.03785	5.64442
C	-3.70942	-0.28800	3.89907	C	-3.47709	-0.12507	3.69897
C	-3.28582	-0.65327	6.62868	C	-3.15800	-0.00126	6.47091
H	-1.23203	-0.14490	6.22001	H	-1.03777	-0.02334	6.05169
C	-4.76416	-0.65987	4.72073	C	-4.58809	-0.08870	4.52363
H	-3.85685	-0.15764	2.83169	H	-3.57717	-0.17727	2.62076
C	-4.55793	-0.83786	6.08825	C	-4.43312	-0.02665	5.91108
H	-3.12407	-0.81144	7.69017	H	-3.04240	0.03907	7.54892
H	-5.75110	-0.82308	4.29975	H	-5.58624	-0.11691	4.09795
C	-5.71000	-1.17730	6.98231	C	-5.64359	0.07159	6.78876
F	-6.65041	-1.89091	6.34075	F	-6.68842	-0.60085	6.27563
F	-6.31935	-0.07119	7.45378	F	-6.04430	1.34749	6.94482
F	-5.32148	-1.88883	8.05378	F	-5.41396	-0.41665	8.01902

***Z*-3b**				***E*-3b**			
C	3.45882	5.02085	-0.05825	C	0.23034	-0.68238	0.32750
C	4.83362	4.91128	-0.20806	C	0.07029	-0.07202	1.56414
C	5.20225	3.63287	0.22681	C	1.33819	0.33738	1.99555
C	4.03218	2.97764	0.63306	C	2.24768	-0.03504	1.00669
N	2.97780	3.85986	0.43363	N	1.54229	-0.65599	-0.00797
H	2.79644	5.84941	-0.26664	H	-0.49940	-1.13006	-0.33238
H	5.48957	5.67885	-0.59353	H	-0.86952	0.06011	2.08149
H	6.19678	3.21678	0.23400	H	1.60566	0.85141	2.90645
C	1.59356	3.59813	0.76613	C	2.11884	-1.22926	-1.20344
H	1.44550	2.51942	0.79426	H	3.14340	-0.87110	-1.29337
H	1.33996	4.01554	1.74566	H	2.12769	-2.32235	-1.14874
H	0.94818	4.04493	0.00690	H	1.54525	-0.91828	-2.08005
N	3.65591	1.72176	1.05845	N	3.60075	0.09903	0.86377
N	4.43591	0.78869	1.36407	N	4.18354	0.66494	1.83302
C	5.84481	0.97126	1.40441	C	5.57280	0.79986	1.67841
C	6.64634	0.36385	0.43662	C	6.31549	0.35119	0.57627
C	6.44583	1.62052	2.48666	C	6.23900	1.43491	2.73148
C	8.02969	0.44934	0.52685	C	7.68518	0.54051	0.54071
H	6.17540	-0.17454	-0.38014	H	5.79941	-0.15279	-0.23344
C	7.82866	1.68602	2.57503	C	7.61225	1.62194	2.68901
H	5.82133	2.07906	3.24745	H	5.64773	1.78328	3.57274
C	8.64965	1.11113	1.59467	C	8.36416	1.17894	1.59302
H	8.64272	-0.03765	-0.22645	H	8.25481	0.16328	-0.30425
H	8.28368	2.21647	3.40695	H	8.10883	2.14314	3.50232
C	10.12285	1.18929	1.69215	C	9.82752	1.37451	1.54239
C	10.91110	1.36933	0.54793	C	10.47096	1.68126	0.33573
C	10.76860	1.08592	2.93126	C	10.60986	1.25782	2.69927
C	12.29637	1.44247	0.63911	C	11.84796	1.86454	0.28742
H	10.42851	1.47878	-0.41940	H	9.87928	1.80411	-0.56710
C	12.15366	1.16192	3.02333	C	11.98685	1.44131	2.65123

H	10.17768	0.91688	3.82722
C	12.92427	1.34000	1.87757
H	12.88734	1.58988	-0.26048
H	12.63364	1.07112	3.99367
H	14.00639	1.39795	1.94911

H	10.13421	0.99250	3.63926
C	12.61242	1.74532	1.44503
H	12.32485	2.11066	-0.65710
H	12.57511	1.33699	3.55852
H	13.68834	1.88834	1.40742

***Z*-3c**			
C	4.74264	-4.23726	2.40849
C	6.05802	-3.82402	2.56720
C	6.07230	-2.42826	2.47495
C	4.75064	-2.01098	2.26449
N	3.95913	-3.15244	2.23987
H	4.31889	-5.23178	2.40254
H	6.90678	-4.47167	2.73457
H	6.93317	-1.78620	2.56804
C	2.53149	-3.17580	1.99939
H	2.12170	-2.20232	2.26484
H	2.31522	-3.37494	0.94522
H	2.07459	-3.95410	2.61393
N	4.05436	-0.82696	2.17687
N	4.56376	0.31718	2.11153
C	5.96500	0.51633	2.01265
C	6.62239	0.33464	0.79150
C	6.66341	1.05182	3.09694
C	7.96540	0.65736	0.67245
H	6.07395	-0.06806	-0.05444
C	8.01254	1.35357	2.97308
H	6.13818	1.22989	4.03005
C	8.69020	1.16293	1.76142
H	8.47045	0.48509	-0.27388
H	8.54043	1.78110	3.82087
C	10.12211	1.49596	1.63320
C	10.63143	2.04282	0.44499
C	11.00920	1.27235	2.69795
C	11.97589	2.35506	0.31743
H	9.95680	2.25158	-0.37942
C	12.35545	1.58266	2.58790
H	10.64073	0.82361	3.61518
C	12.82194	2.12039	1.39451
H	12.37998	2.78585	-0.59096
H	13.05219	1.40739	3.39895
N	14.23923	2.44714	1.26927
O	14.62011	2.91708	0.20810
O	14.95731	2.22998	2.23333

***E*-3c**			
C	0.25267	-0.62811	0.25082
C	0.09116	-0.18427	1.55773
C	1.35732	0.16724	2.03784
C	2.26776	-0.07213	1.00723
N	1.56274	-0.55430	-0.07973
H	-0.47684	-0.98758	-0.46120
H	-0.84927	-0.12005	2.08642
H	1.62334	0.56131	3.00716
C	2.14549	-0.98502	-1.33097
H	2.99780	-0.34922	-1.56918
H	2.48828	-2.02266	-1.27110
H	1.39625	-0.89985	-2.12003
N	3.61746	0.07966	0.87701
N	4.20844	0.50878	1.91075
C	5.59581	0.66207	1.75864
C	6.32266	0.35940	0.59739
C	6.27633	1.15394	2.87746
C	7.69165	0.55199	0.56759
H	5.79347	-0.03508	-0.26289
C	7.64918	1.34155	2.84298
H	5.69682	1.39077	3.76422
C	8.38393	1.04540	1.68712
H	8.24781	0.28650	-0.32730
H	8.15607	1.75170	3.71158
C	9.84477	1.24389	1.64516
C	10.47793	1.68408	0.47192
C	10.63664	0.99710	2.77794
C	11.85025	1.87206	0.42460
H	9.88023	1.90891	-0.40578
C	12.00976	1.18217	2.74750
H	10.16992	0.62761	3.68558
C	12.59952	1.61805	1.56706
H	12.35031	2.22040	-0.47127
H	12.63356	0.98634	3.61149
N	14.04555	1.81442	1.52628
O	14.53548	2.19631	0.47447
O	14.67674	1.58460	2.54650

***Z*-3d**			***E*-3d**		
C	3.51102	-5.19003	C	0.22384	-0.11364
C	4.88926	-5.14855	C	0.16721	0.20134
C	5.28337	-3.81061	C	1.46961	0.11024
C	4.12538	-3.05210	C	2.29563	-0.26036
N	3.05272	-3.93513	N	1.50724	-0.38578
H	2.83200	-6.03120	H	-0.56120	-0.15962
H	5.53007	-6.00040	H	-0.72634	0.47411
H	6.28687	-3.42603	H	1.81565	0.29387
C	1.67196	-3.57221	C	1.96758	-0.81837
H	1.55156	-2.51355	H	3.02530	-0.57639
H	1.39847	-3.74491	H	1.84080	-1.89847
H	1.02282	-4.16817	H	1.40207	-0.29866
N	3.77627	-1.72424	N	3.63641	-0.48959
N	4.57560	-0.76088	N	4.29638	-0.37987
C	5.98029	-0.95156	C	5.67446	-0.61081
C	6.78806	-0.61557	C	6.43053	-0.49193
C	6.57432	-1.31926	C	6.32268	-0.94502
C	8.16998	-0.69341	C	7.80114	-0.69997
H	6.32262	-0.29160	H	5.91374	-0.22393
C	7.95608	-1.37732	C	7.69052	-1.14921
H	5.94487	-1.56636	H	5.73214	-1.04921
C	8.78150	-1.07530	C	8.45852	-1.03192
H	8.78721	-0.41676	H	8.37620	-0.57517
H	8.40488	-1.69033	H	8.17851	-1.43530
C	10.25285	-1.14398	C	9.91796	-1.25397
C	10.90235	-0.74663	C	10.68852	-0.83643
C	11.03814	-1.60422	C	10.57169	-1.88461
C	12.28432	-0.81024	C	12.06012	-1.04388
H	10.31748	-0.35413	H	10.20866	-0.31570
C	12.42050	-1.66629	C	11.94335	-2.09380
H	10.55566	-1.93826	H	9.99223	-2.23732
C	13.04795	-1.27007	C	12.69180	-1.67418
H	12.77507	-0.48431	H	12.64670	-0.70064
H	13.01585	-2.02410	H	12.43627	-2.58528
C	14.53606	-1.39167	C	14.16410	-1.95143
F	14.89610	-2.60432	F	14.42439	-3.13167
F	15.15921	-1.22160	F	14.71050	-2.00095
F	15.03528	-0.48672	F	14.82209	-1.01248

***Z*-4b**				***E*-4b**			
C	0.34649	-1.30232	0.57648	C	-0.02787	-0.41667	0.15835
C	0.13227	-0.32116	1.54819	C	-0.01188	-0.22298	1.53740
C	1.03190	0.76180	1.26333	C	1.34505	-0.03232	1.93833
C	1.75039	0.40633	0.15597	C	2.11152	-0.11359	0.80988
N	1.32947	-0.85380	-0.24959	N	1.26597	-0.34973	-0.26980
H	1.14024	1.69345	1.79468	H	1.68988	0.14157	2.94635
C	1.87236	-1.56090	-1.38447	C	1.71357	-0.48138	-1.63454
H	1.71184	-0.99834	-2.30968	H	2.17001	0.44764	-1.99232
H	2.94679	-1.72988	-1.26159	H	2.44771	-1.28766	-1.72862
H	1.37995	-2.52828	-1.47906	H	0.86320	-0.71572	-2.27469
C	2.81515	1.14560	-0.57405	C	3.58311	0.00907	0.63065
H	3.76891	0.60349	-0.58327	H	4.03221	-0.90352	0.21902
H	2.54395	1.34598	-1.61807	H	3.85535	0.83589	-0.03719
H	2.98693	2.10700	-0.08645	H	4.05065	0.19878	1.59863
C	-0.34256	-2.60855	0.42477	C	-1.19434	-0.65503	-0.72813
H	-0.82377	-2.71136	-0.55498	H	-1.30709	0.12568	-1.49013
C	0.34017	-3.45710	0.55373	H	-1.13627	-1.62063	-1.24516
H	-1.11207	-2.66757	1.19623	H	-2.09233	-0.65652	-0.10797
N	-0.87334	-0.57186	2.47437	N	-1.17665	-0.23691	2.27237
N	-1.16950	0.16204	3.44490	N	-1.01821	-0.05105	3.51092
C	-0.42820	1.32839	3.77634	C	-2.21359	-0.06560	4.25636
C	0.77910	1.22718	4.47389	C	-2.07315	0.13248	5.63272
C	-0.98349	2.58959	3.55119	C	-3.49635	-0.25984	3.72526
C	1.43452	2.37340	4.90032	C	-3.18361	0.13838	6.46394
H	1.20229	0.24534	4.66371	H	-1.07342	0.29077	6.02574
C	-0.31324	3.73098	3.97074	C	-4.60025	-0.25258	4.55954
H	-1.94204	2.66319	3.04650	H	-3.59850	-0.42383	2.65808
C	0.90914	3.64895	4.65114	C	-4.47029	-0.05348	5.94460
H	2.38793	2.28071	5.41347	H	-3.05828	0.32280	7.52709
H	-0.76265	4.70515	3.79830	H	-5.58721	-0.43195	4.14146
C	1.61579	4.86682	5.10207	C	-5.65731	-0.04583	6.82444
C	2.29891	4.89245	6.32530	C	-5.60616	-0.60366	8.10907
C	1.62165	6.02803	4.31771	C	-6.86600	0.52049	6.39710
C	2.96591	6.03668	6.74788	C	-6.72293	-0.59498	8.93675
H	2.28151	4.01274	6.96258	H	-4.68721	-1.07302	8.44893
C	2.28510	7.17387	4.74148	C	-7.98333	0.52834	7.22400
H	1.11991	6.02105	3.35396	H	-6.91892	0.98305	5.41549
C	2.96163	7.18344	5.95835	C	-7.91715	-0.02916	8.49812
H	3.48207	6.03582	7.70385	H	-6.66269	-1.04105	9.92552
H	2.28170	8.06051	4.11360	H	-8.90737	0.98064	6.87491
H	3.48089	8.07812	6.28919	H	-8.78989	-0.02287	9.14454

***Z*-4c**			***E*-4c**		
C	-0.91259	3.68252	C	-0.04121	-0.36832	0.17318
C	-1.63501	2.60835	3.41594	C	-0.01553	-0.17886	1.55421
C	-2.82466	3.14860	4.01301	C	1.34824	-0.03332	1.95242
C	-2.78249	4.50336	3.83608	C	2.10800	-0.13579	0.82191
N	-1.61176	4.81671	3.15619	N	1.25126	-0.33793	-0.25745
H	-3.62250	2.61693	4.50574	H	1.70155	0.12749	2.95962
C	-1.22130	6.15884	2.79481	C	1.69318	-0.50873	-1.62027
H	-1.94862	6.60766	2.11095	H	2.31229	0.33629	-1.93599
H	-1.14002	6.79251	3.68315	H	2.27528	-1.42924	-1.73545
H	-0.25113	6.13372	2.29956	H	0.82686	-0.56420	-2.27914
C	-3.74901	5.55582	4.24935	C	3.58231	-0.06269	0.63923
H	-3.30239	6.28653	4.93487	H	3.99538	-0.98140	0.20473
H	-4.14975	6.11346	3.39389	H	3.88229	0.76910	-0.01027
H	-4.59143	5.09174	4.76558	H	4.05967	0.08785	1.60923
C	0.38043	3.64867	2.15951	C	-1.21660	-0.56905	-0.71057
H	0.30129	4.08521	1.15705	H	-1.30792	0.21841	-1.46847
H	1.17409	4.18222	2.69617	H	-1.18657	-1.53318	-1.23210
H	0.67763	2.60362	2.05903	H	-2.11324	-0.54672	-0.08905
N	-1.10377	1.34237	3.21490	N	-1.17675	-0.15788	2.28922
N	-1.58404	0.27314	3.65546	N	-1.01372	0.02509	3.52873
C	-2.71248	0.22655	4.51294	C	-2.21120	0.04009	4.26947
C	-2.57018	0.46576	5.88402	C	-2.07167	0.25137	5.64447
C	-3.93838	-0.23033	4.02180	C	-3.49523	-0.14030	3.73545
C	-3.64757	0.28340	6.73737	C	-3.18369	0.28163	6.47182
H	-1.61297	0.80559	6.26732	H	-1.07115	0.39877	6.03908
C	-5.01551	-0.39405	4.88068	C	-4.60194	-0.10511	4.56444
H	-4.03332	-0.45590	2.96419	H	-3.59594	-0.31568	2.67015
C	-4.89399	-0.14080	6.25423	C	-4.47122	0.10487	5.94799
H	-3.53000	0.50422	7.79474	H	-3.05719	0.47593	7.53300
H	-5.95819	-0.76179	4.48489	H	-5.58897	-0.27540	4.14297
C	-6.03894	-0.32665	7.16544	C	-5.65741	0.13712	6.82361
C	-5.85070	-0.81211	8.46948	C	-5.60463	-0.38425	8.12635
C	-7.34552	-0.02136	6.75169	C	-6.86830	0.68987	6.37645
C	-6.92072	-0.98458	9.33314	C	-6.71381	-0.35612	8.95657
H	-4.85288	-1.08451	8.79878	H	-4.68698	-0.84322	8.48048
C	-8.42677	-0.19201	7.60150	C	-7.98741	0.72309	7.19320
H	-7.50987	0.38072	5.75684	H	-6.92208	1.12464	5.38335
C	-8.19878	-0.67140	8.88601	C	-7.89442	0.19857	8.47686
H	-6.78958	-1.36671	10.33851	H	-6.68844	-0.76337	9.96031
H	-9.43846	0.04806	7.29668	H	-8.92475	1.15499	6.86328
N	-9.33097	-0.85032	9.78875	N	-9.06747	0.23087	9.34415
O	-9.09934	-1.27412	10.91097	O	-8.95418	-0.23526	10.46781
O	-10.44187	-0.56463	9.36784	O	-10.09168	0.72197	8.89405

***Z*-4d**			***E*-4d**		
C	-0.79978	-3.82056 3.00302	C	-0.04405	-0.41087 0.17063
C	-1.41953	-2.72738 3.61507	C	-0.01544	-0.20377 1.54823
C	-2.29605	-3.24791 4.62708	C	1.34269	0.01489 1.93122
C	-2.18551	-4.60996 4.59207	C	2.09669	-0.06244 0.79444
N	-1.27700	-4.94691 3.59644	N	1.24168	-0.31883 -0.27394
H	-2.92641	-2.69893 5.30767	H	1.69637	0.20674 2.93287
C	-0.91508	-6.30261 3.25760	C	1.67811	-0.50204 -1.63660
H	-0.47791	-6.81665 4.11919	H	2.32921	0.32044 -1.94568
H	-1.78972	-6.86794 2.92088	H	2.22498	-1.44372 -1.75826
H	-0.18064	-6.29190 2.45282	H	0.81136	-0.51847 -2.29736
C	-2.86095	-5.64828 5.41571	C	3.56399	0.08316 0.59785
H	-3.46785	-6.33268 4.81003	H	4.01820	-0.81475 0.16100
H	-2.14860	-6.25950 5.98361	H	3.81693	0.92780 -0.05527
H	-3.52677	-5.16456 6.13282	H	4.04193	0.25927 1.56329
C	0.20115	-3.81226 1.90664	C	-1.21522	-0.68306 -0.69954
H	1.13632	-4.30536 2.19698	H	-1.35281	0.08793 -1.46749
H	-0.17055	-4.30494 1.00020	H	-1.14150	-1.65167 -1.20835
H	0.42019	-2.77080 1.66574	H	-2.10636	-0.69658 -0.06983
N	-1.03556	-1.46735 3.17517	N	-1.17063	-0.23126 2.29503
N	-1.51827	-0.38045 3.56743	N	-1.00473	-0.02736 3.53023
C	-2.61164	-0.30505 4.46983	C	-2.19406	-0.06113 4.28457
C	-2.39735	0.11549 5.78450	C	-2.04995	0.16680 5.65610
C	-3.92136	-0.48304 4.01297	C	-3.47404	-0.30265 3.76601
C	-3.47372	0.30265 6.64059	C	-3.15424	0.15557 6.49506
H	-1.38152	0.29372 6.12360	H	-1.05282	0.36131 6.03899
C	-4.99123	-0.27951 4.87195	C	-4.57245	-0.31084 4.60722
H	-4.08833	-0.79449 2.98635	H	-3.57815	-0.49030 2.70304
C	-4.79121	0.10774 6.20436	C	-4.43767	-0.08266 5.98710
H	-3.29133	0.64102 7.65690	H	-3.02651	0.36366 7.55355
H	-6.00180	-0.45302 4.51213	H	-5.55593	-0.52743 4.19869
C	-5.93474	0.31366 7.11644	C	-5.61718	-0.09305 6.87532
C	-5.85033	-0.04122 8.46992	C	-5.53843	-0.61741 8.17298
C	-7.13531	0.87022 6.65414	C	-6.84894	0.41825 6.44337
C	-6.92332	0.14876 9.32898	C	-6.64534	-0.62733 9.00979
H	-4.93757	-0.49287 8.84701	H	-4.60405	-1.05007 8.51756
C	-8.21345	1.05807 7.50752	C	-7.95967	0.40866 7.27498
H	-7.21254	1.18647 5.61822	H	-6.92861	0.85021 5.45032
C	-8.11054	0.69745 8.84899	C	-7.86069	-0.11402 8.56246
H	-6.84258	-0.13094 10.37444	H	-6.57343	-1.05135 10.00609
H	-9.13165	1.50333 7.13855	H	-8.90644	0.80873 6.92684
C	-9.29140	0.84305 9.76026	C	-9.04323	-0.07209 9.48242
F	-10.04987	-0.26889 9.77183	F	-9.01816	-1.07613 10.37474
F	-8.91744	1.07025 11.03061	F	-9.08535	1.07380 10.18688
F	-10.09126	1.85512 9.38572	F	-10.20304	-0.15695 8.80947

12.2 TD-DFT Studies. The calculation of the excited states of the push-pull azo-pyrrole compounds was performed with the Cam-B3LYP functional[vii] and the 6-311++G(d,p) basis within the time-dependent DFT formalism as implemented in Gaussian 09.[viii] The Cam-B3LYP functional has demonstrated to properly reproduce excited state properties such as absorption energies.[ix] 50 states were obtained with chloroform as implicit solvent modeled with PCM method. Atomic population and energies were calculated within the atoms-in-molecules approach at basal and excited states, to determine the electron charge transfer and atomic energy changes after the electronic excitation.[x] The calculations involve the geometry optimization of *trans* and *cis* isomers.

Table S7. Energetic and electronic features of the excited state associated with the λ_{max} of each molecule.

Compound	Isomer	Excited State f_{os}	Excited State Energy	Donor-Acceptor Electron Transfer and group energies changes	Orbital transitions	
1b	*Z*	6 (0.5757)	4.07 eV; 304.43 nm	0.189 e A: 1.726 eV D: 2.345 eV	45 -> 50 48 -> 50 **49H -> 50L**	0.12706 -0.40180 **0.54788**
	E	4 (0.9682)	3.17 eV; 391.03 nm	0.1803 e A: 1.112 eV D: 2.067 eV	49H -> 50L	0.69945
1c	*Z*	8 (0.5468)	3.80 eV 326.55 nm	0.250 e A: 0.283 eV D: 3.512 eV	56 -> 61 59 -> 61 59 -> 62 **60H -> 61L** 60 -> 62	0.14075 0.14529 -0.36886 **0.47757** 0.26243
	E	5 (1.1816)	2.91 eV 426.08 nm	0.203 e A: 1.124 eV D: 1.782 eV	60H -> 61L 0.67122 60 -> 62 0.18726	
1d	*Z*	6 (0.5845)	4.02 eV 308.09 nm	0.191 e A: 2.805 eV D: 1.224 eV	61 -> 66 64 -> 66 64 -> 67 **65H -> 66L**	0.10430 -0.34627 0.12549 **0.58169**
	E	4 (1.0175)	3.13 eV 396.78 nm	0.175 e A: 1.893 eV D: 1.230 eV	**65H -> 66L**	0.69863
2b	*Z*	6 (0.5700)	4.30 eV 288.44 nm	0.324 e A: 0.528 eV D: 3.770 eV	**57H -> 58L**	**0.68757**
	E	5 (1.0060)	3.46 eV 358.78 nm	0.229 e A: 0.884 eV D: 2.572 eV	56 -> 58 **57H -> 58L**	0.10875 **0.69061**
2c	*Z*	7 (0.6576)	3.83 eV 323.42 nm	0.318 e A: -2.093 eV D: 5.927 eV	65 -> 69L **67 -> 69L** 67 -> 76 68H -> 70	0.16137 **0.60087** 0.10198 -0.28553
	E	6 (1.1836)	3.07 eV 403.48 nm	0.288 e A: 0.163 eV D: 2.911 eV	67 -> 69 **68H -> 69L** 68 -> 70	0.14004 **0.64823** -0.21264
2d	*Z*	6 (0.5968)	4.23 eV 292.85 nm	0.316 e A: 1.581 eV D: 2.656 eV	72 -> 75 **73H -> 74L**	-0.14634 **0.67966**
	E	5 (1.0394)	3.38 eV 366.82 nm	0.246 e A: 1.379 eV D: 2.000 eV	72 -> 74 **73H -> 74L**	0.11019 **0.68911**

Table S7. (Continuation) Energetic and electronic features of the excited state associated with the λ_{max} of each molecule.

Compound	Isomer	Excited State f_{os}	Excited State Energy	Donor-Acceptor Electron Transfer and group energies changes	Orbital transitions	
3b	*Z*	7 (0.6140)	3.99 eV 310.96 nm	0.159 e A: 2.044 eV D: 1.948 eV	63 -> 70	-0.12654
					67 -> 70	-0.28426
					68 -> 70	0.44482
					68 -> 71	-0.12258
					69H -> 70L	**-0.39741**
					69 -> 71	-0.10907
	E	4 (1.3026)	3.04 eV 408.21 nm	0.172 e A: -0.185 eV D: 3.225 eV	**69 H-> 70L**	**0.6931**
3c	*Z*	8 (0.8975)	3.79 eV 327.40 nm	0.263 e A: -0.473 eV D: 4.258 eV	77 -> 81	-0.21983
					77 -> 82	-0.15693
					79 -> 81	0.20574
					79 -> 82	-0.28798
					80H -> 81L	**0.47010**
					80 -> 82	0.16568
					80 -> 83	-0.11906
	E	6 (1.4954)	2.96 eV 418.31 nm	0.186 e A: 1.247 eV D: 1.716 eV	**80H -> 81L**	**0.55342**
					80 -> 82	0.41624
3d	*Z*	7 (0.6518)	3.97 eV 311.96 nm	0.171 e A: 3.006 eV D: 0.965 eV	82 -> 86	-0.22465
					84 -> 86	-0.41795
					84 -> 87	0.19502
					85H -> 86L	**0.44403**
	E	4 (1.3187)	3.03 eV 409.14 nm	0.164 e A: 1.816 eV D: 1.213	**85 H-> 86L**	**0.69038**
4b	*Z*	8 (0.7861)	4.20 eV 295.50 nm	0.287 e A: 1.328 eV D: 2.869 eV	74 -> 78	-0.15387
					76 -> 78	-0.33901
					76 -> 79	0.26299
					77H -> 78L	**0.50925**
	E	5 (1.3809)	3.31 eV 374.86 nm	0.196 e A: 0.724 eV D: 2.584 eV	**77H -> 78L**	**0.68696**
4c	*Z*	8 (0.9536)	3.75 eV 330.38 nm	0.369 e A: -2.423 eV D: 6.178 eV	82 -> 89	0.11509
					85 -> 89	0.26655
					87 -> 89	0.41754
					87 -> 90	-0.12432
					87 -> 92	-0.12235
					88H -> 89L	**-0.39078**
					88 -> 90	-0.11600
	E	6 (1.6044)	3.17 eV 391.53 nm	0.251 e A: 0.629 eV D: 2.536 eV	87 -> 89	0.13335
					88H -> 89L	**0.50721**
					88 -> 90	0.44546
4d	*Z*	7 (0.8544)	4.16 eV 298.15 nm	0.281 e A: 1.828 eV D: 2.333 eV	90 -> 94	0.14165
					92 -> 95	-0.36180
					93H -> 94L	**0.51424**
					93 -> 95	0.19689
	E	5 (1.4086)	3.29 eV 377.33 nm	0.209 e A: 1.833 eV D: 1.452 eV	**93H -> 94L**	**0.67880**
					93 -> 95	0.12146

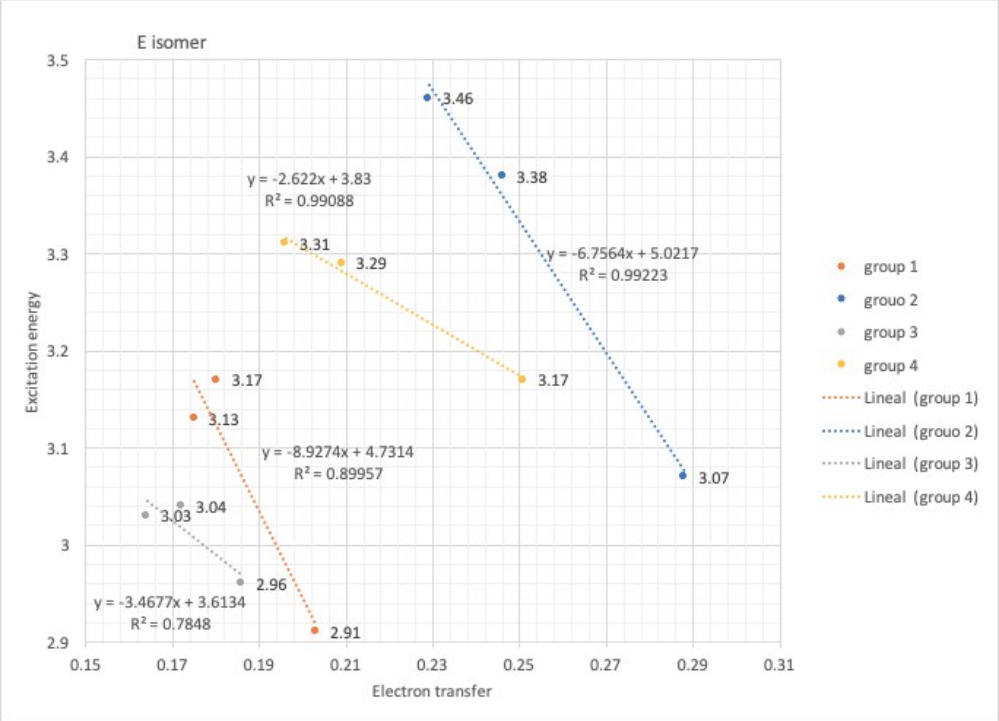


Figure S81. Relationship between Electron transfer and excitation energy for *E*-isomers

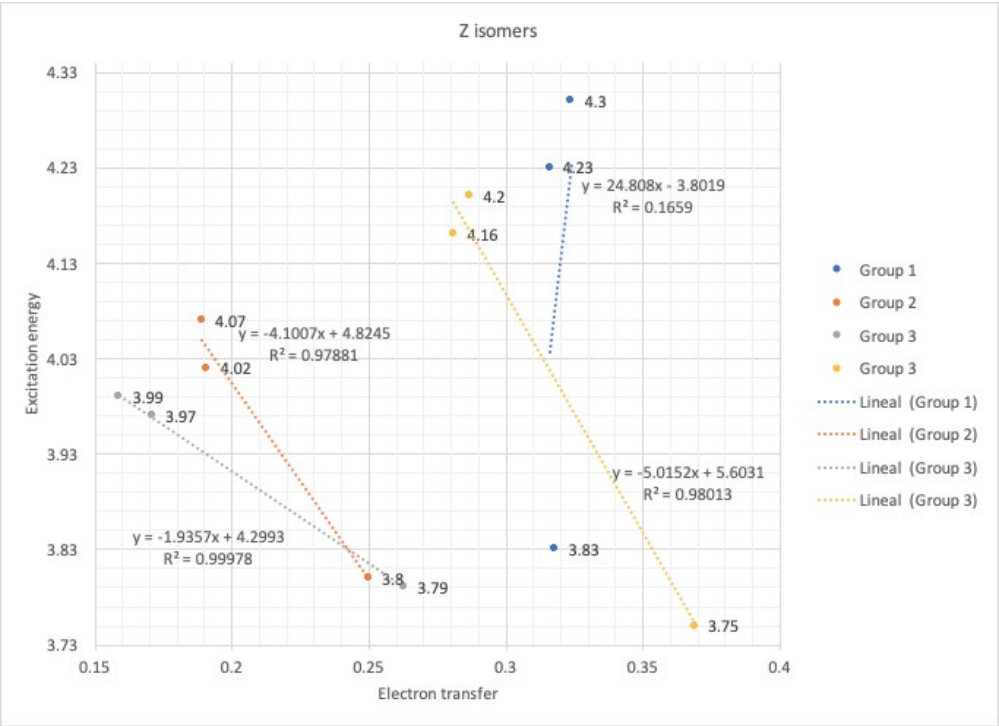


Figure S82. Relationship between Electron transfer and excitation energy for *Z*- isomers.

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