Optoelectronic and NLO Potential of Styryl-Functionalized Nitroisoxazoles for OLED Technologies

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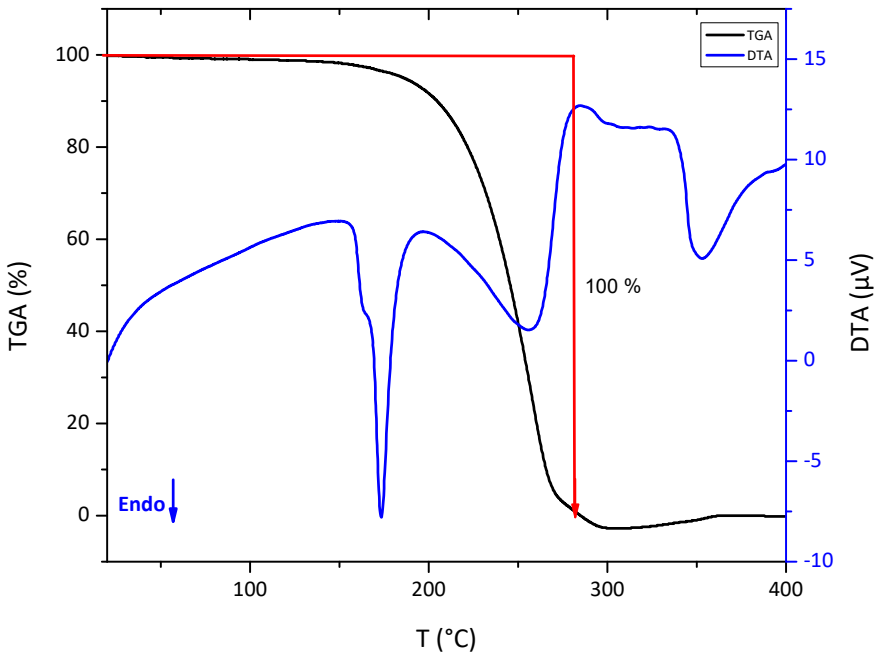

Figure S1. TGA-DTA thermograms of **B1**.

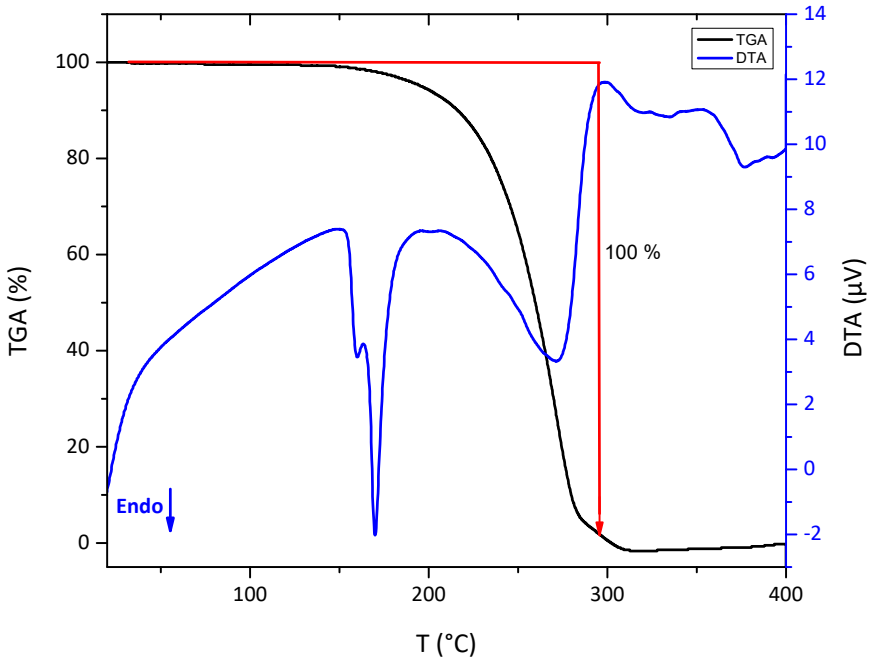

Figure S2. TGA-DTA thermograms of **B2**.

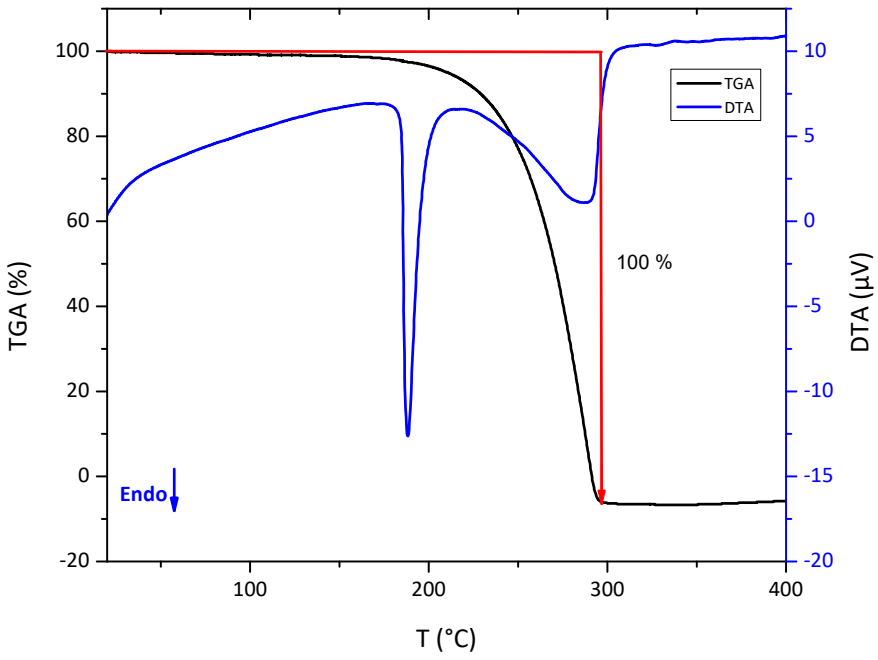

Figure S3. TGA-DTA thermograms of **B3**.

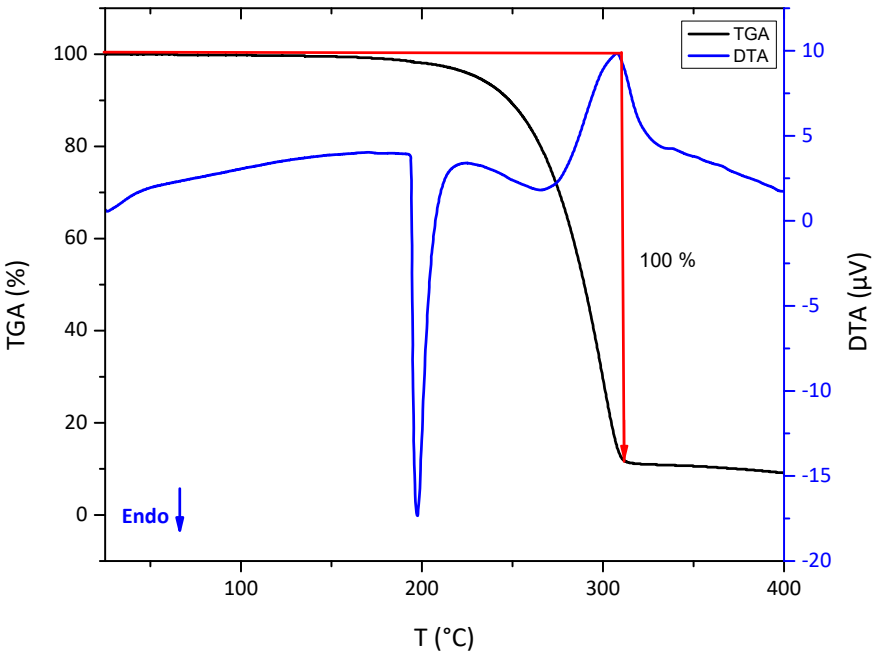

Figure S4. TGA-DTA thermograms of **B4**.

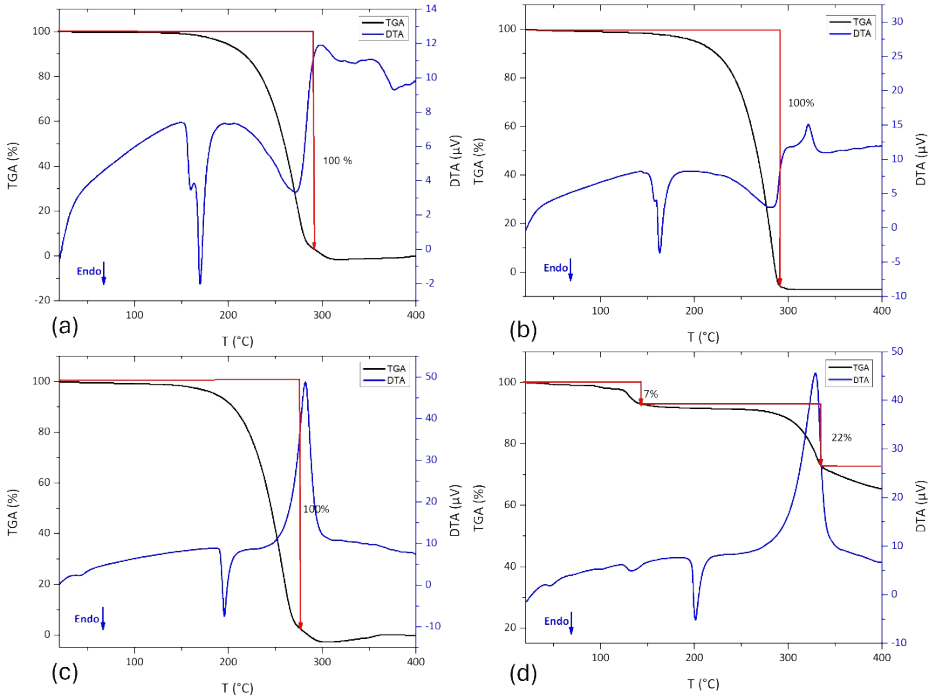

Figure S5. TGA (black line) - DTA (blue line) thermograms of (a) **B5**, (b) **B6**, (c) **B7**, (d) **B8** compounds.

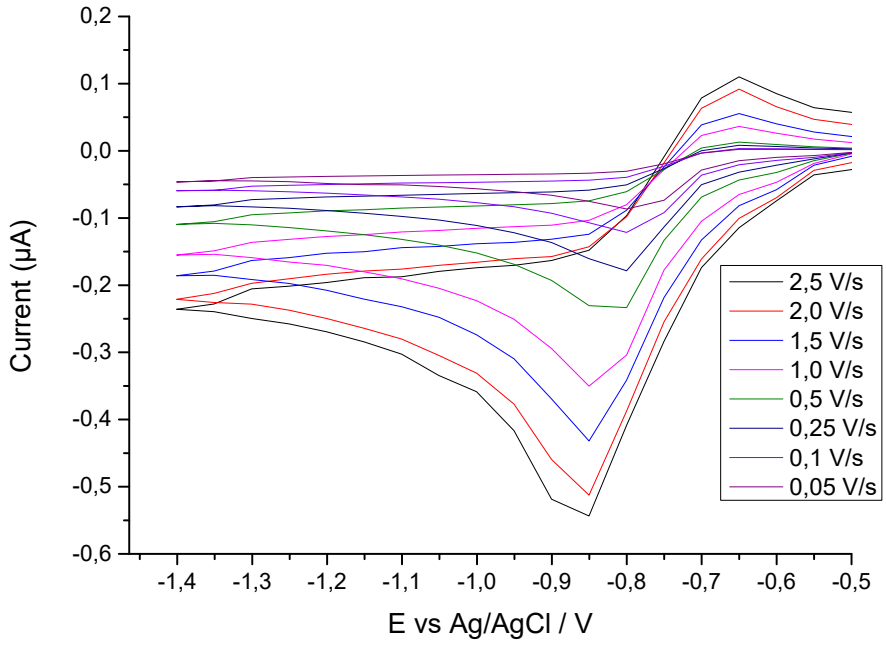

Figure S6. Voltammogram of **B2**.

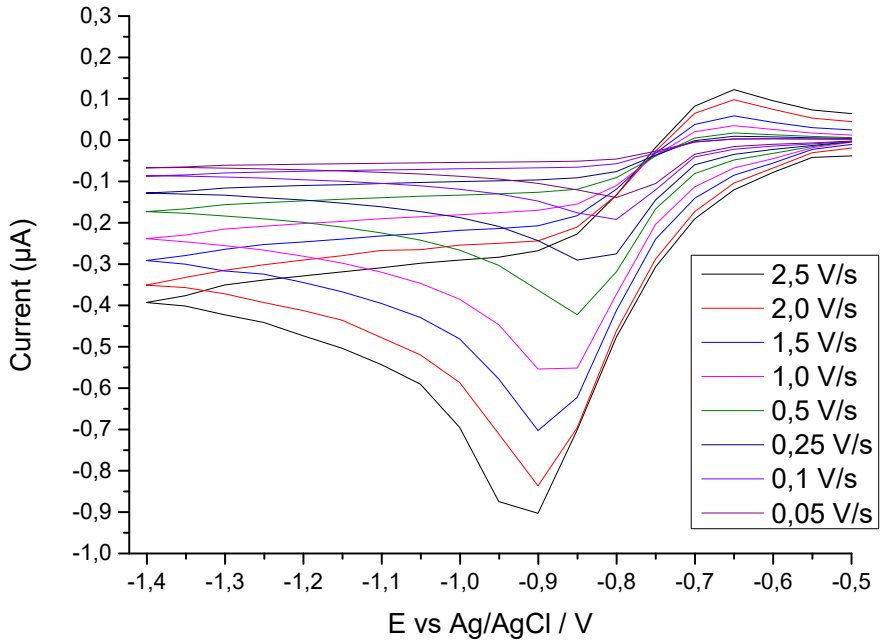

Figure S7. Voltammograms of **B3**.

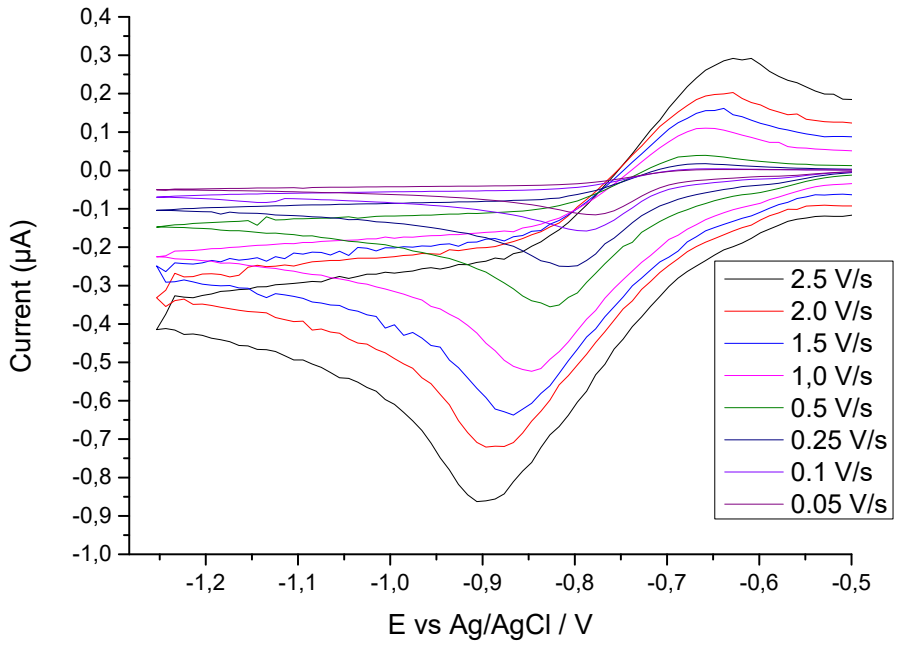

Figure S8. Voltammogram of **B4**.

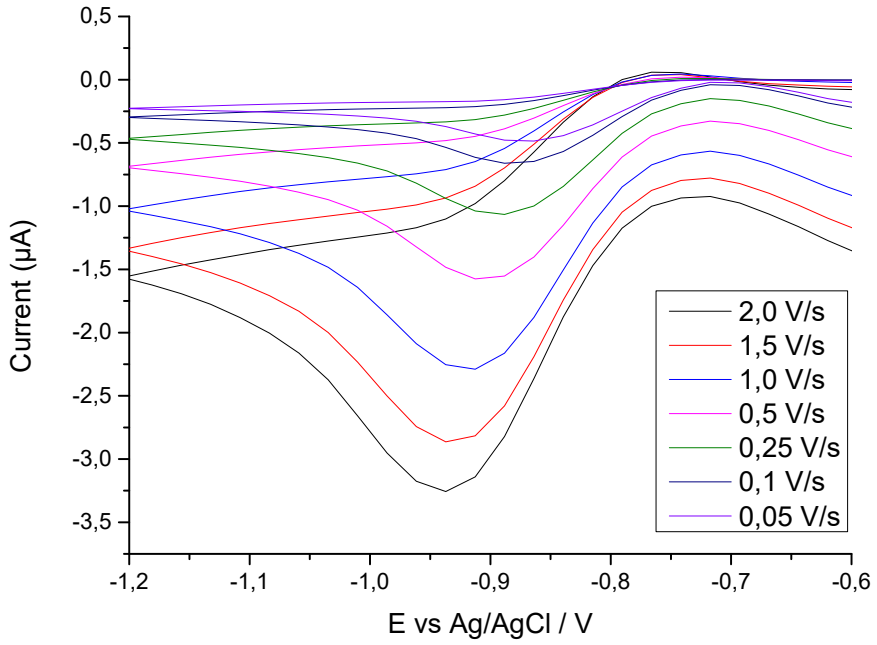

Figure S9. Voltammogram of **B6**.

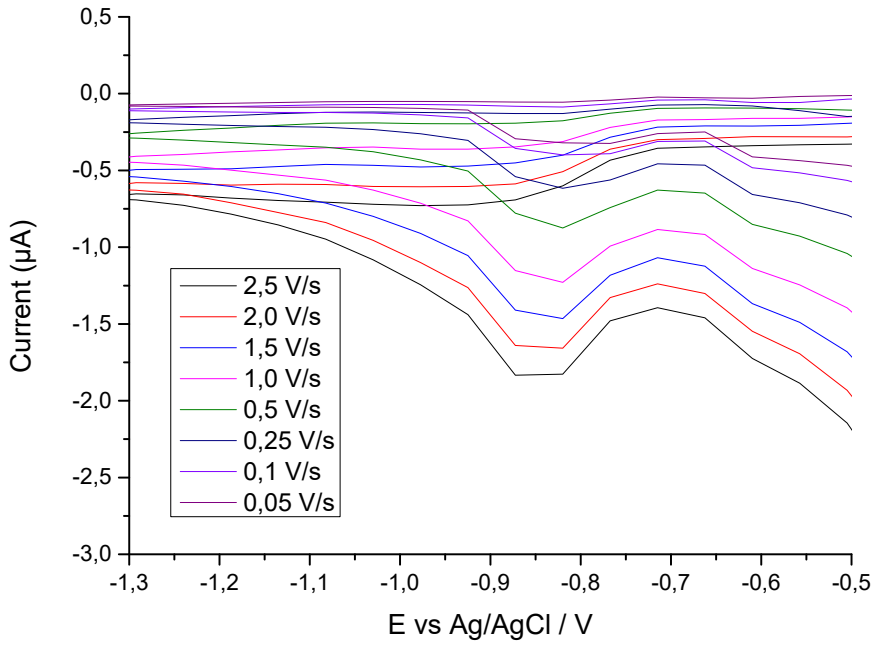

Figure S10. Voltammogram of **B8**.

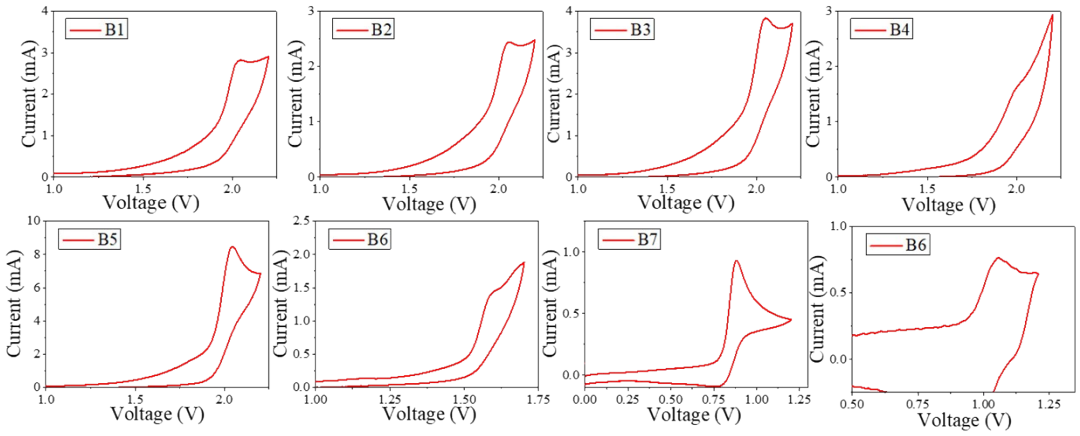

Figure S11. voltammograms of oxidation for **B1-8** compounds.

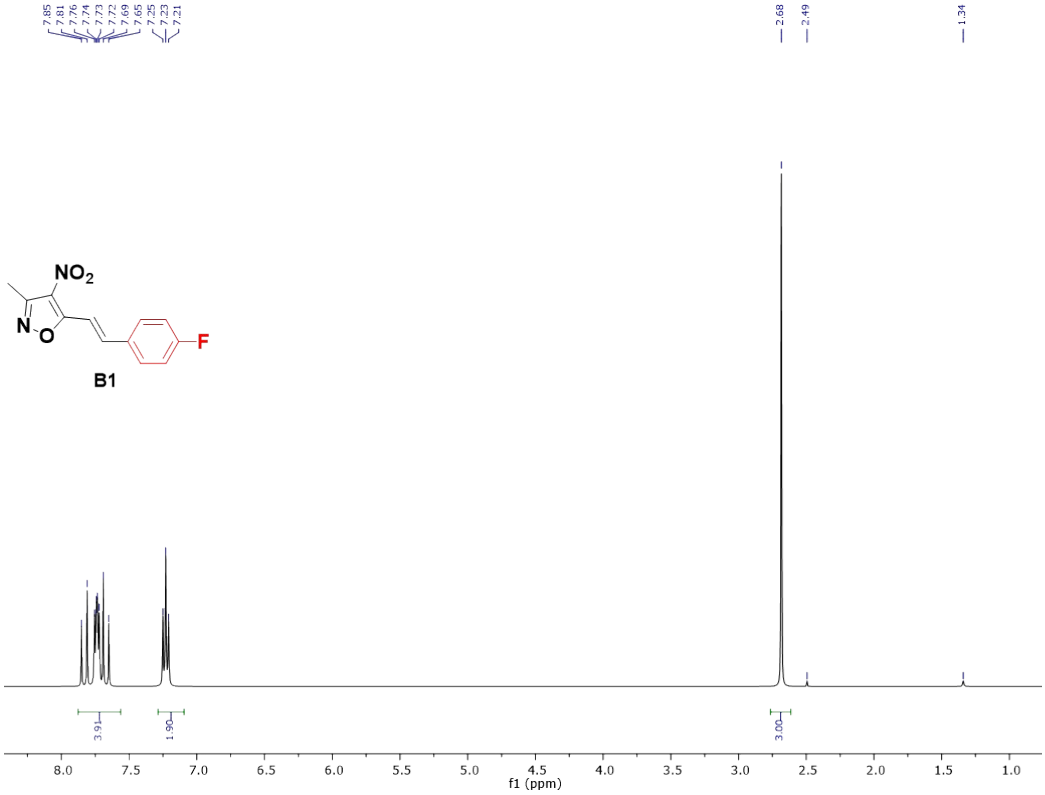

Figure S12. ^{1}H NMR spectrum of **B1**.

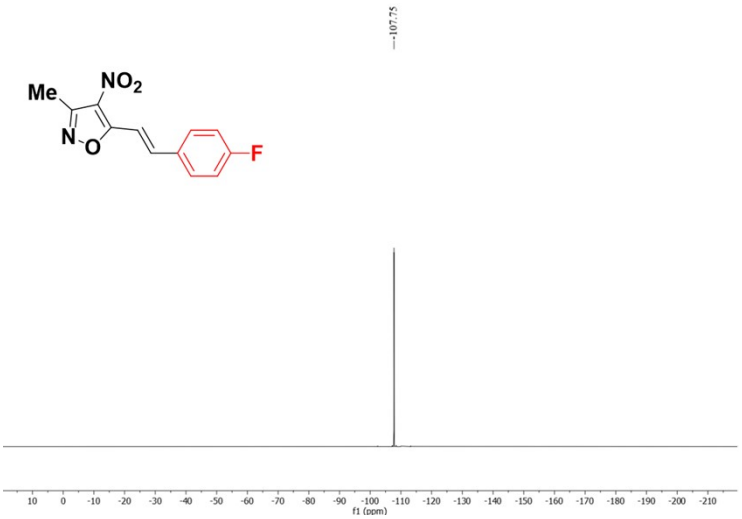

Figure S13. ^{19}F NMR spectrum of **B1**.

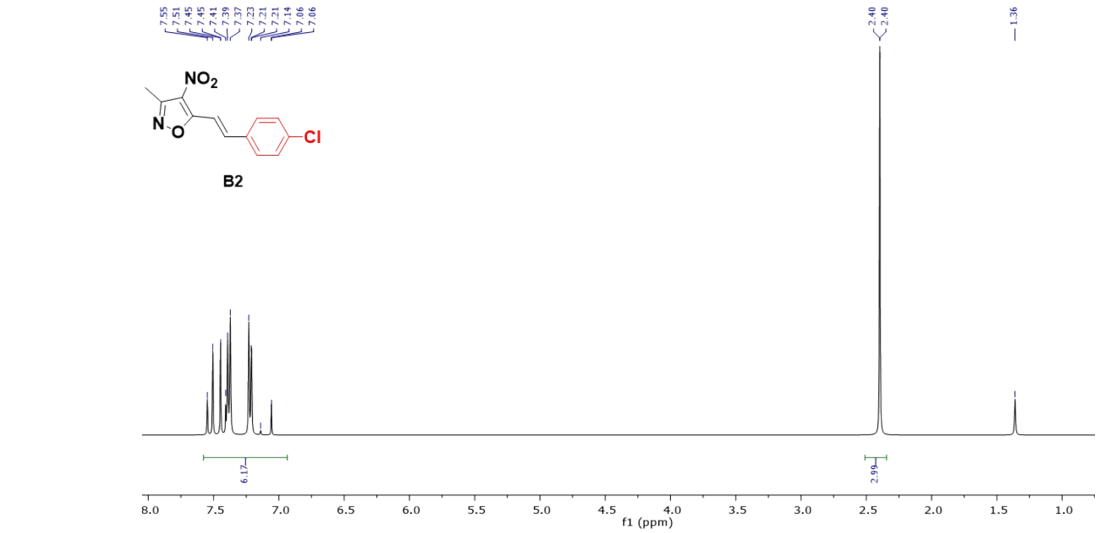

Figure S14. ^{1}H NMR spectrum of **B2**.

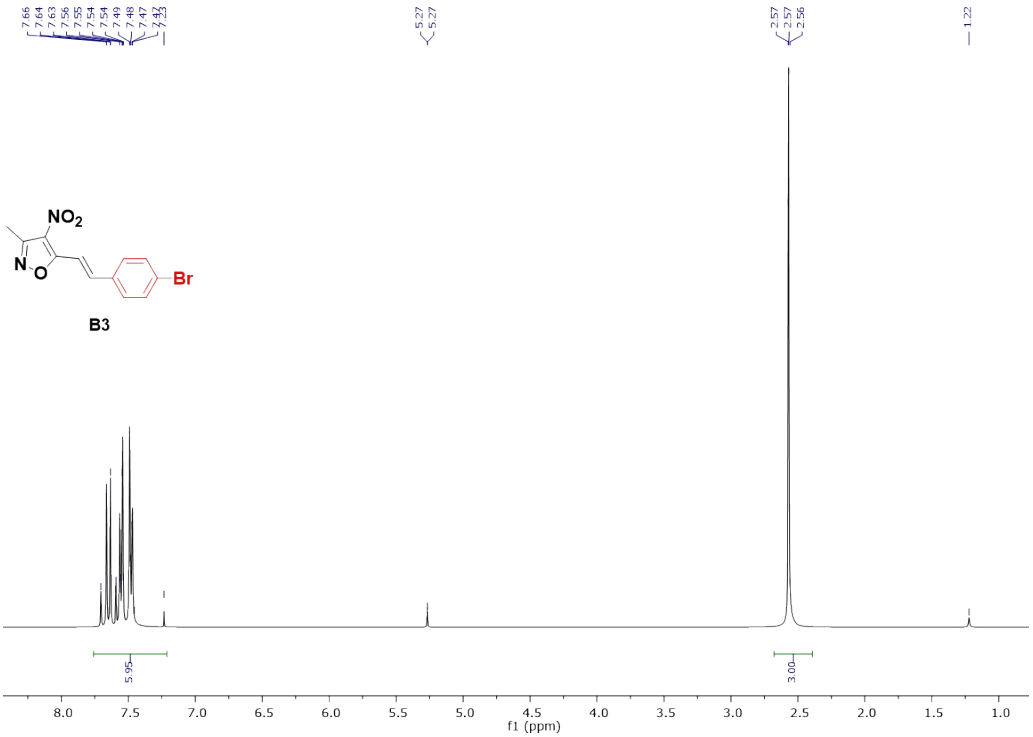

Figure S15. ^{1}H NMR spectrum of **B3**.

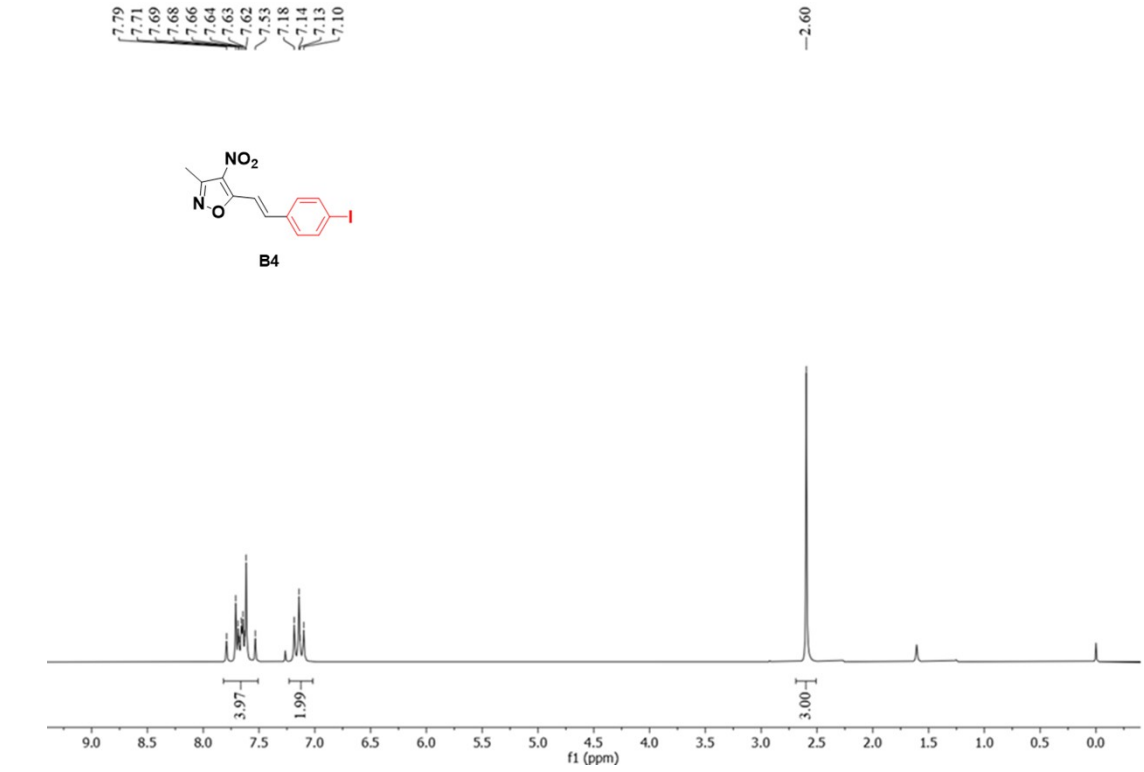

Figure S16. ^{1}H NMR spectrum of **B4**.

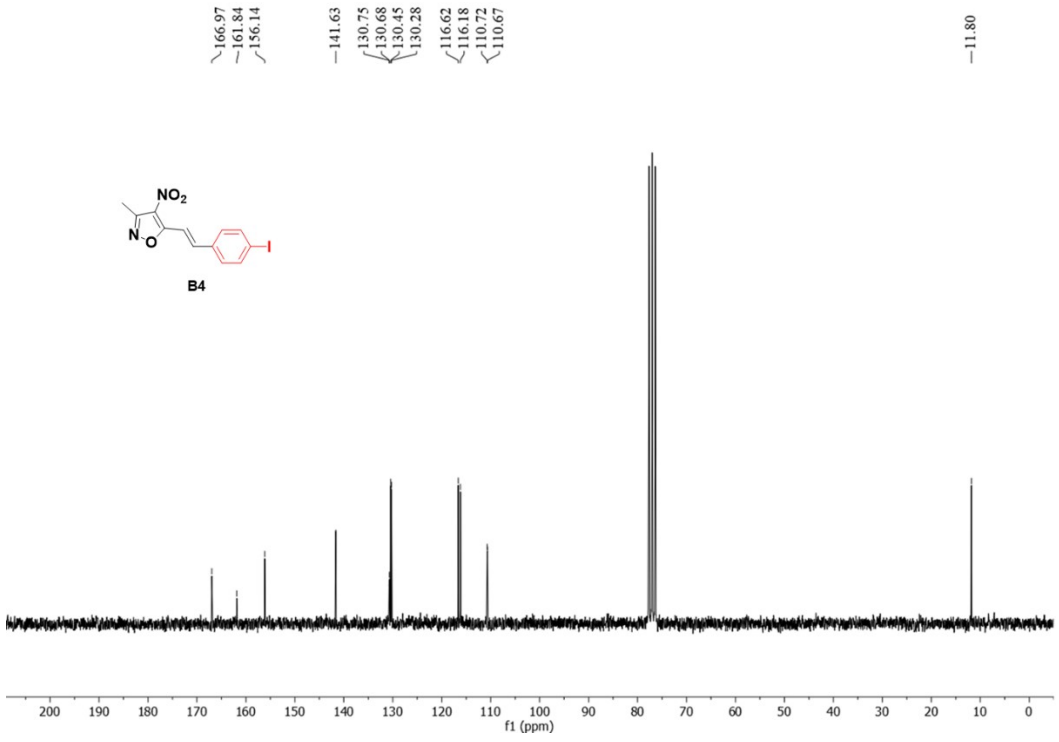

Figure S17. ^{13}C NMR spectrum of **B4**.

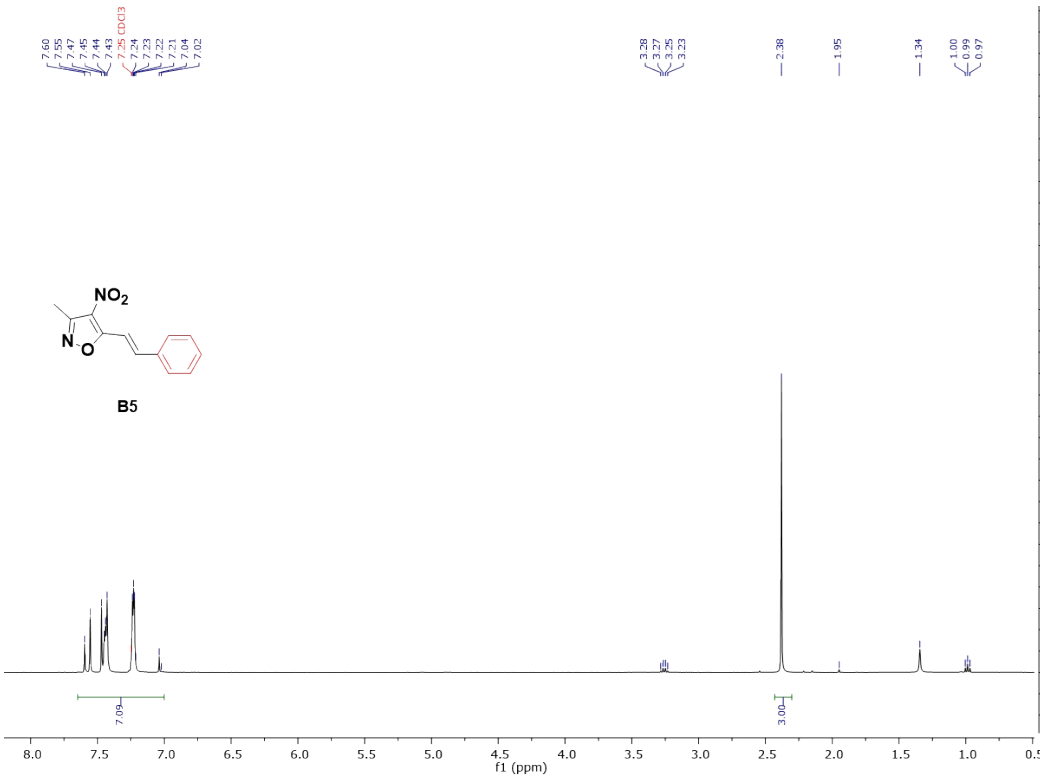

Figure S18. ^{1}H NMR spectrum of **B5**.

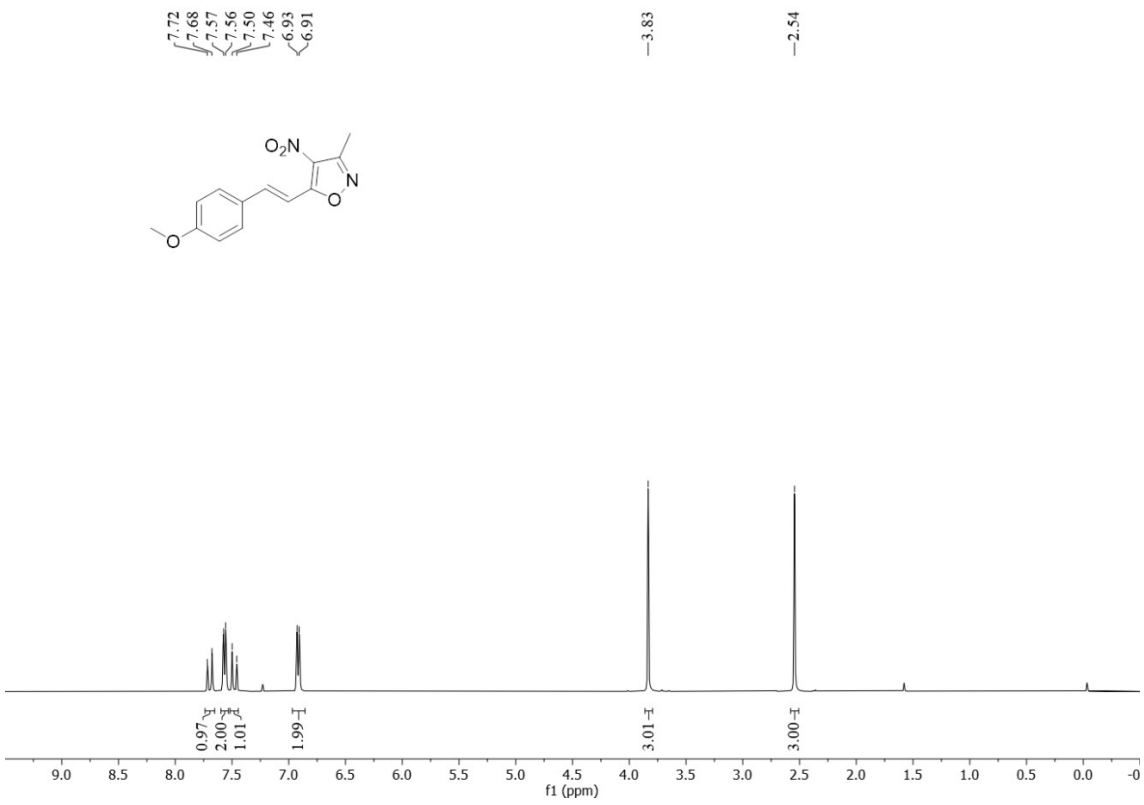

Figure S19. ^{1}H NMR spectrum of **B6**.

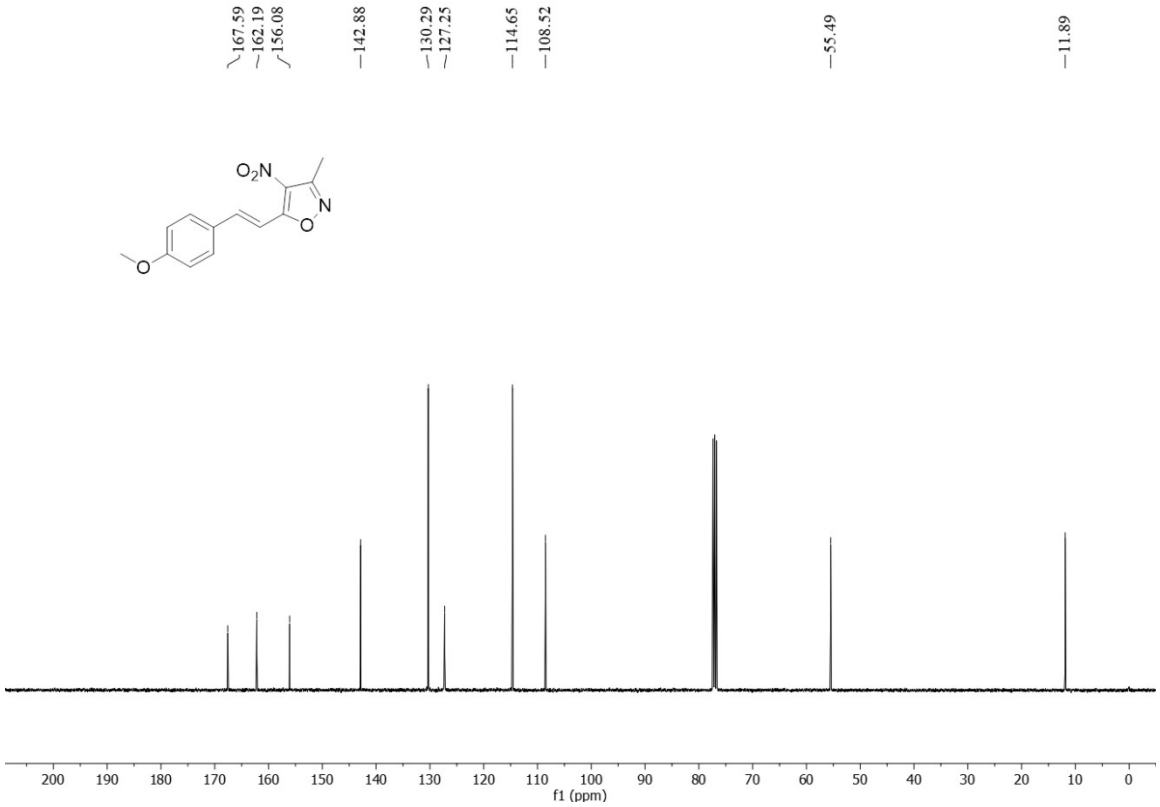

Figure S20. ^{13}C NMR spectrum of **B6**.

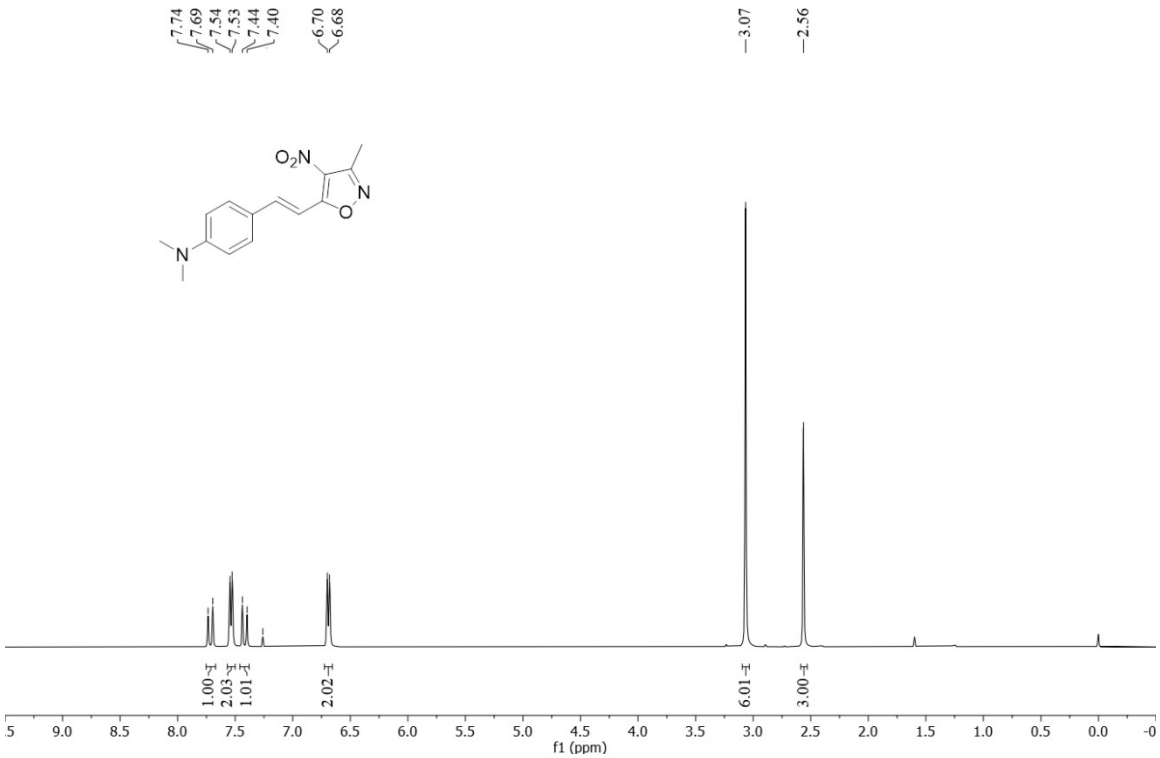

Figure S21. ^{1}H NMR spectrum of **B7**.

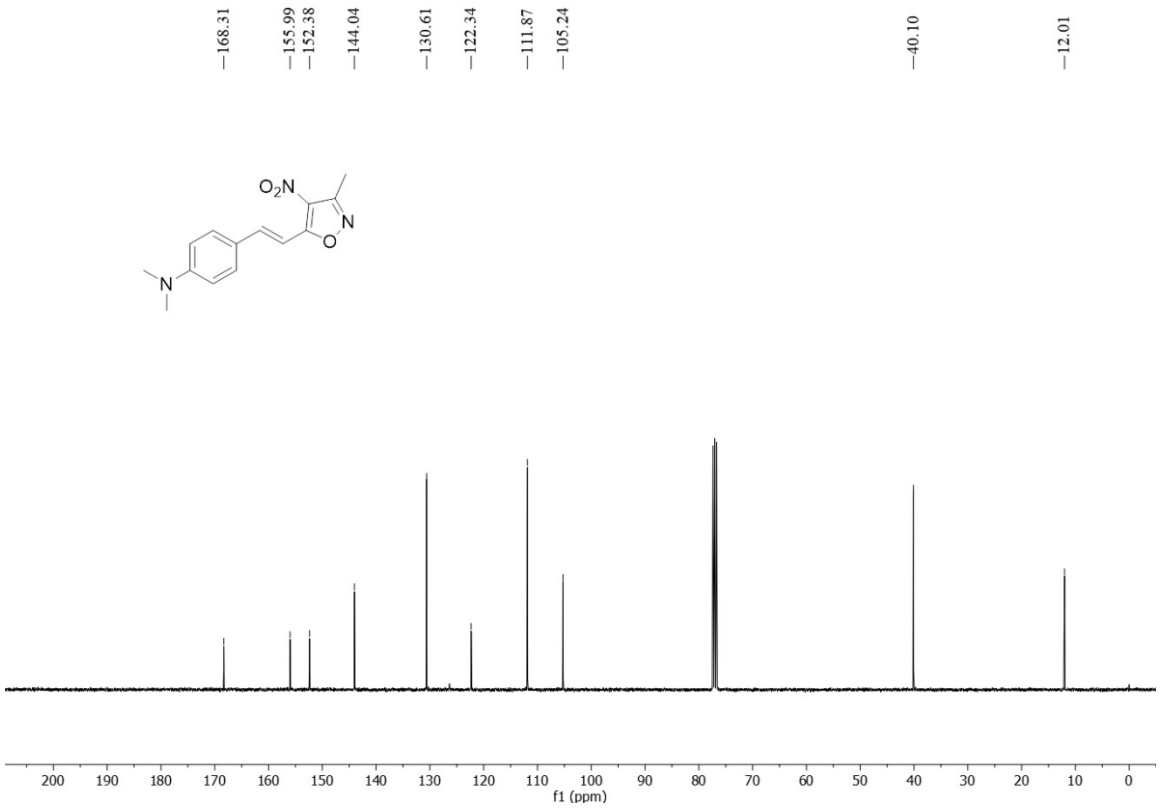

Figure S22. ^{13}C NMR spectrum of **B7**.

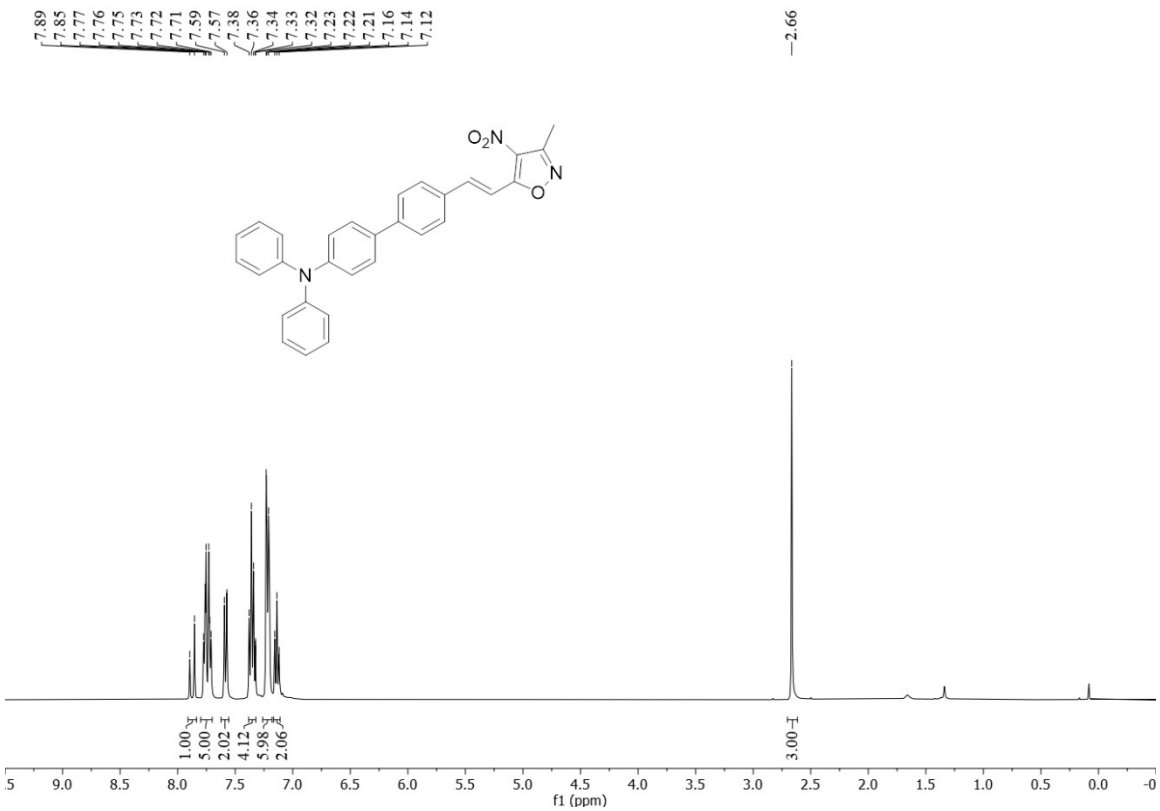

Figure S23. ^{1}H NMR spectrum of **B8**.

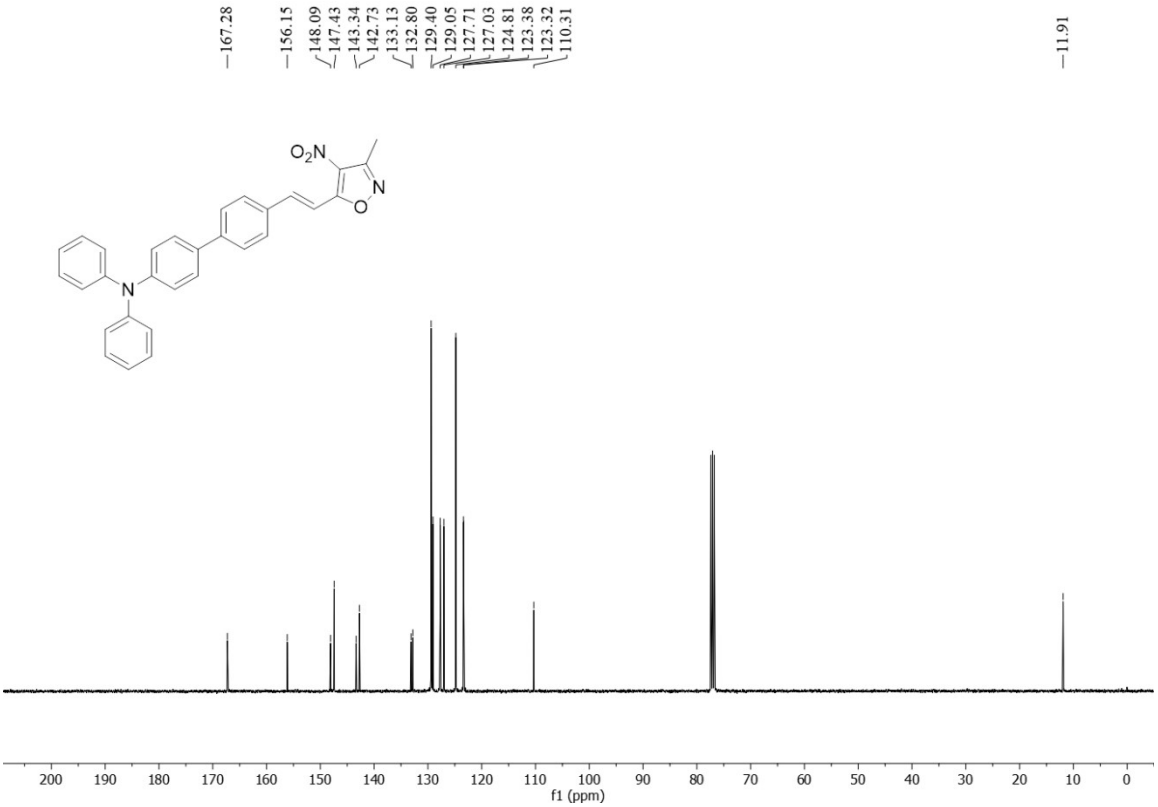

Figure S24. ^{13}C NMR spectrum of **B8**.

Compound	PLQY (%)
B1	3.04
B2	4.93
B3	8.5
B4	15.7
B5	2.9
B6	210
B7	110

Table s1. PL Quantum Yield in solid state.

Global reactivity descriptors

Hardness (η)

$$\eta = \frac{1}{2}(E_{LUMO} - E_{HOMO}) \quad (3)$$

Global softness (S)

$$S = \frac{1}{2\eta} \quad (4)$$

Chemical potential (μ)

$$\mu = -\frac{1}{2}(E_{HOMO} + E_{LUMO}) \quad (5)$$

Electronegativity (χ)

$$\chi = -\mu \quad (6)$$

Electrophilicity index (ω)

$$\omega = \frac{\mu^2}{2\eta} \quad (7)$$

NLO parameters

Average dipole moment

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2} \quad (8)$$

Linear polarizability

$$\alpha_0 = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad (9)$$

Total polarizability

$$\Delta\alpha = \frac{1}{\sqrt{2}}\sqrt{(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6(\alpha_{xy}{}^2 + \alpha_{yz}{}^2 + \alpha_{xz}{}^2)} \quad (10)$$

First-order hyperpolarizability

$$\beta_{tot} = \left[(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxy} + \beta_{zyy})^2\right]^{1/2} \quad (11)$$

Second-order hyperpolarizability

$$\gamma_{ave} = \frac{1}{5}[\gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz} + 2[\gamma_{xxyy} + \gamma_{yyzz} + \gamma_{xxzz}]] \quad (12)$$

Compound	**Excitation**	**E_{calc}**[a]	**f_{os}**[b]	**Major contribution (%)**	**Excited**	**λ_{abs}**[c]	**%D**[d]

	vertical (*nm*)	(*eV*)			state	(*nm*)	
B1	374.17	3.3135	0.8549	H → L (100%)	S_1	364	2.8
	271.32	4.5697	0.2705	H → L+1 (92%)	S_5	267	1.6
B2	375.50	3.3019	0.9554	H → L (99%)	S_1	365	2.9
	272.37	4.5520	0.2745	H → L+1 (89%)	S_5	272	0.1
B3	379.27	3.2690	0.9860	H → L (99%)	S_1	366	3.6
	274.51	4.5166	0.2262	H → L+1 (67%)	S_5	274	0.2
B4	384.27	3.2264	1.0085	H → L (99%)	S_1	373	3.0
	275.78	4.4957	0.3035	H → L+1 (95%)	S_7	274	0.6
B5	369.70	3.3537	0.8459	H → L (99%)	S_1	364	1.6
	269.05	4.6083	0.2711	H → L+1 (92%)	S_5	267	0.8
B6	402.78	3.0782	0.9615	H → L (100%)	S_1	396	1.7
	286.17	4.3326	0.3233	H → L+1 (93%)	S_4	285	0.4
B7	460.23	2.6939	1.0395	H → L (100%)	S_1	482	4.5
	319.02	3.8865	0.3500	H → L+1 (92%)	S_2	319	0.0
B8	548.25	2.2614	0.6381	H → L (99%)	S_1	446	22.9
	383.69	3.2313	0.9856	H-1 → L (93%)	S_2	333	15.2

Table S2. Main electronic transitions of **B1-8** calculated in chloroform. [a]Calculated transition energy. [b]Oscillator strength. [c]Experimental absorption maxima. [d]Percent deviation. H: HOMO, L: LUMO

Parameters	B1	B4	B7
CCDC number	2423120	2423121	2423122
Empirical formula	$C_{12}H_9FN_2O_3$	$C_{12}H_9IN_2O_3$	$C_{14}H_{15}N_3O_3$
M_r	248.21	356.11	273.29
Temperature/K	296.15	296.15	296.15
Crystal system	Monoclinic.	Triclinic	orthorhombic
Space group	P21/n	P-1	Pna21
a/Å	7.3988(8)	8.1177(16)	22.0846(11)
b/Å	11.3929(12)	8.4258(18)	4.0685(3)
c/Å	13.6438(15)	10.345(2)	29.5491(18)
α/°	90	89.257(10)	90
ß/°	101.437(4)	73.519(9)	90
γ/°	90	68.680(9)	90
V/(Å^3)	1127.3(2)	628.9(2)	2655.0(3)
Z,Z′	4,1	2,1	8,2
D/(g/cm^3)	1.463	1.881	1.367
μ/mm^{-1}	0.118	2.548	0.098
F(000)	512.0	344.0	1152.0
Crystal size/(mm)	0.091 × 0.072 × 0.029	0.113 × 0.112 × 0.056	0.15 × 0.07 × 0.036
Radiation	MoKα	MoKα	MoKα

2Θ range for data collection/°	4.696 to 52.8	4.126 to 54.96	4.606 to 55.22
Reflections collected	15629	13461	31056
Independent reflections	2307 [Rint = 0.1104, Rsigma = 0.0655]	2775 [Rint = 0.1447, Rsigma = 0.1267]	6095 [Rint = 0.1045, Rsigma = 0.0821]
Data/ restraints/ parameters	2307/0/164	2775/0/164	6095/1/367
Goodness-of-fit on F2	1.044	1.020	0.989
Final R indexes [I>=2σ (I)]	R1= 0.0794, wR2= 0.2271	R1= 0.0450, wR2= 0.0974	R1= 0.0712, wR2= 0.1803
Final R indexes [all data]	R1= 0.1563, wR2= 0.2817	R1= 0.1363, wR2= 0.1147	R1= 0.1508, wR2= 0.2350
$\Delta\rho_{max}$, Δ_{min} (e Å^{-3})	0.60/-0.21	1.27/-0.74	0.51/-0.23
Flack parameter			-1.8(10)

Table S3. Crystal data and refinement parameters for compounds **B1**, **B4**, and **B7.**

Torsion angle	B1	B4
Isoxazole ring-NO2		
C(1)-C(2)-C(2)-N(4)	0.8(5)	0.9(7)
C(1)-C(2)-C(3)-(C6)	-178.4(5)	-179.2(5)
C(1)-C(2)-N(7)-O(17)	173.1(5)	-176.4(5)
C(1)-C(2)-N(7)-O(18)	-8.1(7)	2.5(9)
C(2)-C(3)-N(4)-O(5)	-0.4(5)	-0.8(6)
C(3)-C(2)-N(7)-O(17)	-7.4(7)	5.6(9)
C(3)-C(2)-N(7)-O(18)	171.5(4)	-175.4(5)
C(3)-N(4)-O(5)-C(1)	-0.2(5)	0.4(6)
O(5)-C(1)-C(2)-C(3)	-0.8(5)	-0.6(6)
O(5)-C(1)-C(2-N(7)	178.8(4)	-178.9(5)
C(1)-C(8)-C(9)-C(10)	179.3(5)	178.8(5)
C(2)-C(1)-O(5)-N(4)	0.6(5)	0.2(6)
C(6)-C(3)-N(4)-O(5)	178.9(4)	179.4(4)
N(7)-C(2)-C(3)-N(4)	-178.9(4)	179.1(5)
N(7)-C(2)-C(3)-C(6)	2.0(8)	-1.0(10)
C-C=C-C		
O(5)-C(1)-C(8)-C(9)	7.0(8)	2.8(9)
C(2)-C(1)-C(8)-C(9)	-173.8(5)	179.8(6)

C(8)-C(1)-O(5)-N(4)	-179.9(4)	178.0(4)
C(8)-C(1)-C(2)-C(3)	179.9(5)	-177.9(6)
C(8)-C(1)-C(2)-N(7)	-0.5(9)	3.9(11)
C(8)-C(9)-C(1O)-C(11)	171.0(5)	178.4(6)
C(8)-C(9)-C(10)-C(15)	-6.6(8)	-2.3(9)
Aromatic ring- -C=-C		
C(9)-C(10)-C(11)-C(12)	-176.8(5)	178.2(5)
C(9)-C(10)-C(15)-C(14)	176.2(4)	-178.2(5)
C(10)-C(11)-C(12)-C(13)	0.0(7)	0.8(9)
C(11)-C(10)-C(15)-C(14)	-1.5(7)	1.1(8)
C(11)-C(12)-C(13)-C(14)	-0.4(8)	-0.4(9)
C(11)-C(12)-C(13)-F(16)	179.6(4)	-179.7(4)
C(12)-C(13)-C(14)-C(15)	-0.1(8)	0.3(9)
C(13)-C(14)-C(15)-C(10)	1.1(7)	-0.8(9)
C(15)-C(10)-C(11)-C(12)	0.9(7)	-1.2(8)
F(16)-C(13)-C(14)-C(15)	179.8(4)	179.7(4)

Table S4. Torsion angles (º) for **B1** and **B4**

Torsion angle	Molecule A	Molecule B
Isoxazole ring-NO_2		
C(1)-C(2)-C(3)-N(4)	-3.8(10)	3.3(10)
C(2)-C(1)-O(5)-N(4)	-1.0(10)	1.2(10)
C(3)-C(2)-N(18)-O(19)	3.3(13)	6.1(13)
C(3)-C(2)-N(18)-O(20)	-176.3(9)	-175.1(9)
C(6)-C(3)-N(4)-O(5)	-177.5(9)	-179.3(9)
C(2)-C(3)-N(4)-O(5)	3.1(10)	-2.4(10)
C(1)-C(2)-N(18)-O(19)	-172.2(8)	-176.7(10)
C(1)-C(2)-N(18)-O(20)	8.2(14)	2.0(13)
C(1)-C(2)-C(3)-(C6)	177.0(10)	179.8(10)
C(3)-N(4)-O(5)-C(1)	-1.4(11)	0.8(10)
O(5)-C(1)-C(2)-C(3)	2.8(9)	-2.6(10)

O(5)-C(1)-C(2-N(18)	179.0(7)	179.7(7)
C-C=C-C		
C(1)-C(7)-C(8)-C(9)	179.6(8)	178.5(8)
C(2)-C(1)-C(7)-C(8)	179.0(10)	174.8(10)
O(5)-C(1)-C(7)-C(8)	-3.8(12)	1.4(13)
C(7)-C(1)-C(2)-C(3)	-179.8(9)	-176.5(9)
C(7)-C(1)-C(2)-N(18)	-3.5(15)	5.9(15)
C(7)-C(1)-O(5)-N(4)	-178.9(7)	176.4(7)
C(7)-C(8)-C(9)-C(10)	178.3(9)	179.8(9)
C(7)-C(8)-C(9)-C(14)	-2.4(14)	-2.8(14)
C(8)-C(9)-C(10)-C(11)	176.9(8)	179.0(9)
C(8)-C(9)-C(14)-C(13)	-178.3(8)	-176.4(8)
Aromatic ring		
C(9)-C(10)-C(11)-C(12)	1.9(14)	-2.9(17)
C(10)-C(9)-C(14)-C(13)	1.1(11)	1.2(10)
C(10)-C(11)-C(12)-C(13)	0.2(13)	1.8(13)
C(10)-C(11)-C(12)-N(15)	-179.9(8)	-176.7(8)
C(11)-C(12)-C(13)-C(14)	-1.7(11)	0.6(11)
C(11)-C(12)-N(15)-C(16)	179.7(8)	-178.9(8)
C(11)-C(12)-N(15)-C(17)	-2.5(12)	-3.1(12)
C(12)-C(13)-C(14)-C(9)	1.0(11)	-2.1(11)
C(13)-C(12)-N(15)-C(16)	-0.4(10)	2.6(11)
C(13)-C(12)-N(15)-C(17)	177.4(8)	178.5(8)
C(14)-C(9)-C(10)-C(11)	-2.5(12)	1.4(14)
N(15)-C(12)-C(13)-C(14)	178.4(7)	179.1(7)
N(18)-C(2)-C(3)-N(4)	-179.9(8)	-179.1(8)
N(18)-C(2)-C(3)-C(6)	0.8(15)	-2.6(15)

Table S5. Selected torsion angles (°) in **B7**.