SUPPORTING INFORMATION

A Multidisciplinary Study of Chemico-physical Properties of Different Classes of 2-Aryl-5(or 6)-nitrobenzimidazoles: NMR, Electrochemical Behaviour, ESR, and DFT Calculations

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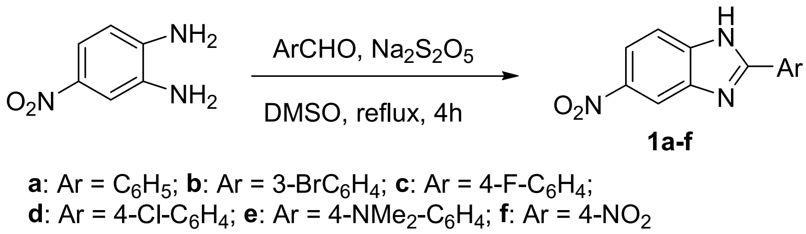
Content **Page**

1. *Synthesis of 5(6)-Nitrobenzimidazole derivative* ***1a–f****. General procedure*



Scheme 1. Synthetic pathway to obtain compounds **1a**-**f.**

The synthetic approach is shown in Scheme 1. *General procedure*: 4-Nitrophenylene diamine (1 mmol) and substituted aromatic aldehydes (1.01 mmol) were refluxed in 15 ml of DMSO in a round bottom flask (100 mL). Sodium metabisulfite ($Na_2S_2O_5$) (1 mmol) was added to the stirring solutions. The reaction mixture was heated until the reaction completion and the progress was checked by TLC. When the reactions were completed the reaction mixtures were cooled to room temperature. Addition of water (30 mL) resulted in the precipitation of crude solid residues. The crude mixtures were chromatographed on silica gel columns to afford the 5(6)-nitrobenzimidazole derivatives **(1a–f)** in high yields. NMR data are reported in main text and Tables S1 and S4 of this section, other data are reported below.

*1.1. 5(6)-Nitro-2-phenyl-1H-benzo[d]imidazole (**1a**)*

Yield: 76 %. Mp: 214–216°C Lit. (Lopez-Alvarado et al., 1995): 213-215 °C. MS: m/z (%): 239 (M^+, 100), 209 (38), 166 (19). Anal. Calcd for $C_{13}H_9N_3O_2$: C, 65.27; H, 3.79, N, 17.56; Found: C, 64.97, H, 3.77, N, 17.55.

*1.2. 2-(3-Bromophenyl)-5(6)-nitro-1H-benzimidazole (**1b**)*

Yield: 80%. Mp: 240–242 °C. MS: m/z (%), 317 (M^+, 100), 289 (29), 192 (21). Anal. Calcd for $C_{13}H_8BrN_3O_2$: C, 49.08; H, 2.53, N, 13.21; Found: C, 49.01, H, 2.51, N, 13.22.

*1.3. 2-(4-Fluorophenyl)-5(6)-nitro-1H-benzo[d]imidazole (**1c**)*

Yield: 81%. Mp: 259–261 °C. Lit. (Shi et al., 2014): 258-260 °C. MS: m/z (%), 257 (M^+, 100), 211 (57), 184 (34). Anal. Calcd for $C_{13}H_8FN_3O_2$: C, 60.70; H, 3.13, N, 16.34; Found: C, 60.60, H, 3.14, N, 16.32.

*1.4. 2-(4-Chlorophenyl)-5(6)-nitro-1H-benzo[d]imidazole (**1d**)*

Yield: 85%) Mp: 308–310 °C. Lit. (Shi et al., 2014): 301–303 °C; MS: m/z (%), 273 (M^+, 100), 227 (70), 200 (33). Anal. Calcd for $C_{13}H_8ClN_3O_2$: C, 57.05; H, 2.95, N, 15.35; Found: C, 57.08, H, 2.92, N, 15.36.

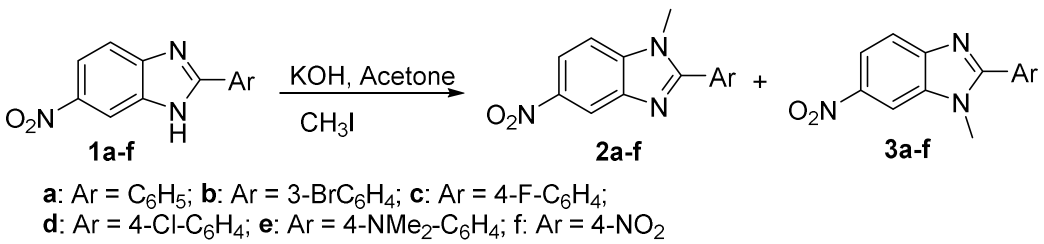
*1.5. N,N-Dimethyl-4-[(5)6-nitro-1H-benzo[d]imidazol-2-yl]aniline **(1e)***

Yield: 82%. Mp: 216–218 °C. Lit. (Leandri et al., 1955): 220 °C; MS: m/z (%), 282 (M^+, 100), 236 (73). Anal. Calcd for $C_{15}H_{14}N_4O_2$: C, 63.82; H, 5.00, N, 19.85; Found: C, 64.01, H, 4.97, N, 19.86.

*1.6. 5(6)-Nitro-2-(4-nitrophenyl)-1H-benzo[d]imidazole **(1f)***

Yield: (80%). Mp: 340–342 °C. Lit. (Feitelson et al., 1952): 340 °C; Anal. Calcd for $C_{13}H_8N_4O_4$: C, 54.93; H, 2.84, N, 19.71; Found: C, 53.98, H, 2.82, N, 19.72.

2. *Synthesis of compounds **2a–f** and **3a–f** by alkylation of 5(6)-nitrobenzimidazole derivatives. General procedure*



Scheme 2. Synthetic pathway to obtain compounds **2a–f** and **3a–f**.

The synthetic approach is shown in Scheme 2. *General procedure:* 5(6)-Nitrobenzimidazole (**1a–f**, 1 g) was dissolved in 15 mL of pure acetone. Potassium hydroxide (3.3 equivalents) was added and the mixture was stirred for 15 minutes at room temperature. Then 2.2 equivalents of iodomethane were added and the mixture was kept under stirring until the reaction was complete. The reaction mixture was filtered and then the solvent was evaporated under reduced pressure. The residue was purified by chromatography on silica gel (eluent: ethyl acetate/hexane 1/9). Yields of known compounds are reported below in parentheses and the related physicochemical data agree with those reported, often partially, in the literature. 1-Methyl-5-nitro-2-phenyl-1H-benzimidazole (**2a**) (Sagitullina et al., 2014) and 1-methyl-6-nitro-2-phenyl-1H-benzimidazole

(**3a**) (Reddy and Rao, 1970) (43% and 47%); 1-methyl-2-(4-chlorophenyl)-5-nitro-1H-benzimidazole (**2d**) (Evans et al., 1996) and 1-methyl-2-(4-chlorophenyl)-6-nitro-1H-benzimidazole (**3d**) (45% and 46%); *N*,*N*-dimethyl-4-(1-methyl-5-nitro-1H-benzoimidazol-2-yl)-aniline (**2e**) (Leandri et al., 1955) and *N*,*N*-dimethyl-4-(1-methyl-6-nitro-1H-benzimidazol-2-yl)-aniline (**3e**) (Leandri et al., 1955) (44% and 47%); 1-methyl-5-nitro-2-(4-nitrophenyl)-1H-benzimidazole (**2f**) (Hui et al., 2019) and 1-methyl-6-nitro-2-(4-nitrophenyl)-1H-benzimidazole (**3f**) (Hui et al., 2019) (45% and 45%). NMR data for unknown compounds are reported in the main text (results and discussion) and in Tables S2, S3, S5, S6, and S7 of this section, other data are reported below.

*2.1. 1-Methyl-2-(3-bromophenyl)-5-nitro-1H-benzimidazole (**2b**)*

Yield: (45%). Mp: 182–184 °C. Lit. (Feitelson et al., 1952): 181–183 °C; MS: m/z (%), 331 (M^+, 100), Anal. Calcd for $C_{14}H_{10}BrN_3O_2$: C, 50.62; H, 3.03, N, 12.65; Found: C, 50.45, H, 3.12, N, 12.93.

*2.2. 1-Methyl-2-(3-bromophenyl)-6-nitro-1H-benzimidazole (**3b**)*

Yield: (45 %). Mp: 228–230 °C. Lit. (Feitelson et al., 1952): 231–232 °C; MS: m/z (%), 331 (M^+, 100), Anal. Calcd for $C_{14}H_{10}BrN_3O_2$: C, 50.62; H, 3.03, N, 12.65; Found: C, 50.51, H, 3.09, N, 12.88.

*2.3. 2-(4-Fluorophenyl)-1-methyl -5-nitro-1H-benzimidazole (**2c**)*

Yield: (45 %). Mp: 208–210 °C. Lit. (Feitelson et al., 1952): 205–207 °C; MS: m/z (%), 271.08 (M^+, 100), Anal. Calcd for $C_{14}H_{10}FN_3O_2$: C, 61.99, H, 3.72, N, 15.49; Found: C, 61.79, H, 3.69, N, 15.46.

*2.4. 2-(4-Fluorophenyl)-1-methyl -6-nitro-1H-benzimidazole (**3c**)*

Yield: (44 %). Mp: 171–173 °C. Lit. (Feitelson et al., 1952): 174–176 °C; MS: m/z (%), 271.08 (M^+, 100), Anal. Calcd for $C_{14}H_{10}FN_3O_2$: C, 61.99, H, 3.72, N, 15.49; Found: C, 61.85, H, 3.73, N, 15.51.

*2.5. 1-Methyl-2-(4-chlorophenyl)-6-nitro-1H-benzimidazole (**3d**)*

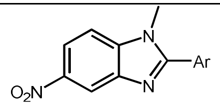
Yield: (46 %). Mp: 226–228 °C. Lit. (Feitelson et al., 1952): 225–227 °C; MS: m/z (%), 287.05 (M^+, 100), Anal. Calcd for $C_{14}H_{10}ClN_3O_2$: C, 58.45, H, 3.50, N, 14.61; Found: C, 58.91, H, 3.75, N, 14.45.

Table S1. ^{1}H NMR data of **1a–f** recorded in DMSO-d$_6$ at +102 °C.[a]

Compound	H-4	H-5	H-7	H-2'/H-6'	H-3'/H-5'	
1a	7.72 d, J=8.8, 1H	8.09 dd, J = 8.8, 2.1, 1H	8.43 d, J = 2.1, 1H	8.20 dd, J_1=8.2 Hz, J_2=2.0 Hz, 2H	7.60-7,52 m, 2H	
1b	7.73 d, J = 8.9, 1H	8.10 dd, J = 8.9, 2.2, 1H	8.43 br.s, 1H	**H-2'** 8.36 dt, J = 1.5, 0.3, 1H; **H-6'** 8.18 dm, J = 7.9, 1H	**H-5'** 7.53 t, J = 7.9, 1H	ddd, J
1c	7.72 d, J = 8.9, 1H	8.09 dd, J = 8.9, 2.3, 1H	8.42 d, J = 2.3, 1H	8.24 dd, J = 9.0, $J_{F\text{-}H}$ = 5.6, 2H	7.38 t, J = 9.0, $J_{F\text{-}H}$ = 9.0, 2H	
1d	7.73 d, J = 8.8, 1H	8.10 dd, J = 8.8, 1.9, 1H	8.44 d, J = 2.3, 1H	8.20 dd, J_1=8.5 Hz, 2H	7.63 d, J = 8.5, 2H	
1e	7.63 d, J = 8.5, 1H	8.07 dd, J = 8.5, 2.2, 1H	8.34 br.s, 1H	8.04 d, J = 8.8, 2H	6.86 d, J = 8.8, 2H	
1f	7.79 d, J = 8.9, 1H	8.13 dd, J = 8.9, 2.2, 1H	8.48 d, J = 2.2, 1H	8.38 d, J = 9.1, 2H	8.42 d, J = 9.1, 2H	

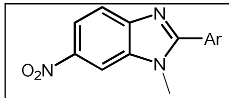
[a] Chemical shifts δ in ppm, J in Hz.

Table S2. ^{1}H NMR data for 1-methyl-5-nitrobenzimidazoles **2a–f** in DMSO-d$_6$ at 25 °C.[a]

 **Compound** (aryl group)	**H-4**	**H-5**	**H-7**	**H-2'/H-6'**	**H-3'/H-5'**	**H-4'**	**NCH$_3$**	**N(CH$_3$)$_2$**
2a (C_6H_5)	7.85 d, J=9.0, 1H	8.20 dd, J_1=9.0, J_2=2.1, 1H	8.55 d, J=2.1, 1H	7.91-7.87 m, 2H	7.64-7.58 m, 2H	7.64-7.58 m, 1H	3.95 s, 3H	
2b (3-Br-C_6H_4)	7.86 d, J=9.0, 1H	8.20 dd, J_1=9.0, J_2=2.3, 1H	8.54 d, J=2.3, 1H	**H-2'** 8.06 t, J=1.8, 1H **H-6'** 7.90 dt, J_1=7,8, J_2=1.2, 1H	7.56 t, J=7.8, 1H	7.81 ddd, J_1=8.0, J_2=1.9, J_3=0.8, 1H	3.95 s, 3H	
2c (4-F-C_6H_4)	7.88 d, J= 8.8, 1H	8.22 dd, J_1=8.8, J_2=2.0 Hz, 1H	8.56 d, J= 2.0, 1H	7.97 dd, $J_{H\text{-}H}$=8.5, $J_{H\text{-}F}$=5.2, 1H	7.46 t, $J_{H\text{-}H,H\text{-}F}$=8.7, 1H		3.95 s, 3H	
2d (4-Cl-C_6H_4)	7.86 d, J=8.9, 1H	8.21 dd, J_1=8.9, J_2=1.9, 1H	8.55 d, J=1.9, 1H	7.92 d, J=8.5, 2H	7.67 d, J=8.5, 2H		3.95 s, 3H	
2e (4-(NMe_2)-C_6H_4)	7.79 d, J=8.8, 1H	8.16 dd, J_1=8.8, J_2=2.0, 1H	8.48 d, J=2.0, 1H	7.76 d, J=9.0, 2H	6.87 d, J=9.0, 2H		3.95 s, 3H	3.02 s, 6H
2f (4-NO_2-C_6H_4)	7.94 d, J= 9.1, 1H	8.26 dd, J_1=9.1, J_2=2.0, 1H	8.62 d, J= 2.0, 1H	8.20 d, J= 8.6, 1H	8.43 d, J= 8.6, 2H		4.01 s, 3H	

[a] Chemical shifts δ in ppm, J in Hz.

Table S3. [1]H NMR data (chemical shifts δ in ppm, *J* in Hz) for 1-methyl-6-nitrobenzimidazoles **3a–f** in DMSO-d_6 at 25 °C.[a]

 **Compound** (aryl group)	**H-4**	**H-5**	**H-7**	**H-2'/H-6'**	**H-3'/H-5'**	**H-4'**	**NCH_3**	**$N(CH_3)_2$**
3a (C_6H_5)	7.85 d, *J*=8.8, 1H	8.15 dd, J_1=8.8, J_2=2.1, 1H	8.66 d, *J*=2.1, 1H	7.93-7.89 m, 2H	7.63-7.60 m, 2H	7.63-7.60 m, 1H	4.00 s, 3H	
3b (3-Br-C_6H_4)	7.84 d, *J*=9.0, 1H	8.13 br.d, *J*=9.0, 1H	8.65 br.s, 1H	**H-2'** 8.07 br.s, 1H **H-6'**7.91 d, J=7.5, 1H	**H-5'** 7.56 t, *J*=8.0, 1H	7.81 br.d. *J*=8.3, 1H	4.00 s, 3H	
3c (4-F-C_6H_4)	7.85 d, *J*= 8.7, 1H	8.15 dd, J_1=8.7, J_2=2.0, 1H	8.67 d, *J*= 2.0, 1H	7.98 dd, J_{H-H}=8.7, J_{H-F}=5.6, 1H	7.46 t, $J_{H-H,H-F}$=8.7, 1H		4.00 s, 3H	
3d (4-Cl-C_6H_4)	7.83 d, *J*=8.9, 1H	8.13 dd, J_1=8.9, J_2=1.9, 1H	8.64 d, *J*=1.9, 1H	7.92 d, *J*=8.6, 2H	7.66 d, *J*=8.6, 2H		3.99 s, 3H	
3e (4-(NMe_2)-C_6H_4)	7.76 d, *J*=8.8, 1H	8.12 dd, J_1=8.8, J_2=2.1, 1H	8.58 d, *J*=2.1, 1H	7.80 d, *J*=8.9, 2H	6.87 d, *J*=8.9, 2H		4.00 s, 3H	3.03 s, 6H
3f (4-NO_2-C_6H_4)	7.92 d, *J*= 8.8, 1H	8.18 dd, J_1=8.8, J_2=1.9, 1H	8.75 d, *J*= 1.9, 1H	8.21 d, *J*= 8.5, 1H	8.42 d, *J*= 8.5, 2H		4.06 s, 3H	

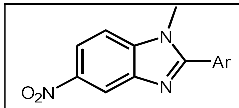
a. Chemical shifts δ in ppm, *J* in Hz.

Table S4. ^{13}C NMR data (chemical shifts δ in ppm) for NH-nitrobenzimidazoles **1a–f** in DMSO-d_6 at 102 °C.

Compound	C-2	C-4	C-5	C-6	C-7	C-3a	C-7a	C-1'	C-2'/C-6'	C-3'/C-5'	C-4'
1a	155.6	114.3 (br)	117.5	142.7	111.6	142.7 (br)	139.2 (br)	129.0	126.8	130.5	128.7
1b	153.8 (−1.8)	114.2 (br)[a]	117.5 (0.0)	142.8 (+0.1)	111.4 (br)[a]	[b]	[b]	131.0 (+2.0)	129.1 ($C_{2'}$) (+2.3) 126.6 ($C_{6'}$) (−0.2)	121.9 ($C_{3'}$) 130.8 ($C_{5'}$)	133.0 (+4.3)
1c	154.6 (−1.0)	114.1 br.s	117.5 (0.0)	143.1 br.s	112.2 br.s	142.6 (br)	139.1 (br)	125.4 (d, J = 3.3 Hz)	129.1 (d, J = 9.0 Hz)	115.7 J_{C-F} = 22.2 Hz	163.9 (d, J = 249.3 Hz)
1d	154.4 (−1.2)	114.2 v. br.	117.6 (+0.4)	142.7 (0.0)	111.4 (v. br.)	142.5 (br.)	139.0 (br.)	127.7 (−1.3)	128.8 (+2.0)	128.3 (−2.2)	135.3 (+6.6)
1e[c]	156.6 (+0.1)	113.4 (v. br.)	116.7 (−0.8)	141.0	110.0 (v. br.)	144.4 (v. br.)	139.1 (v. br.)	115.7 (−13.3)	127.8 (+1.0)	114.4 (−16.1)	151.7 (+23.0)
1f	153.0 (−2.6)	114.6[d] (br)	117.8 (+0.3)	143.1 (+0.4)	112.0[d] (br)	142.7 (br)	139.1 (br)	134.4 (+5.4)	123.5 (−3.3)	127.6 (−2.9)	148.3 (+19.6)

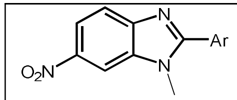
[a.] Tentatively assigned. [b.] Not detected due to high signal broadening. [c.] δ_{NCH3}: 39.1 ppm. [d.] Interchangeable

Table S5. ^{13}C NMR data (chemical shifts δ in ppm) for 1-methyl-5-nitrobenzimidazoles **2a–f** in DMSO-d_6 at 25 °C.

 **Compound** (aryl group)	**C-2**	**C-4**	**C-5**	**C-6**	**C-7**	**C-3a**	**C-7a**	**C1’**	**C-2’/C-6’**	**C-3’/C-5’**	**C-4’**	**NCH$_3$**
2a (C_6H_5)	157.0	111.2	117.9	142.9	115.9	140.9	141.5	129.1	129.4	130.4	128.8	32.3
2b (3-Br-C_6H_4)	155.3 (−1.7)	111.4 (+0.2)	118.4 (+0.5)	143.0 (+0.1)	115.2 (−0.7)	140.8 (+0.1)	141.3 (−0.2)	131.3 (2.2)	**C-2’:**131.8 (+2,4) **C-6’:**128.4 (−0.1)	**C-3’:**121.9 (−8.5) **C-5’:**130.8 (+0.4)	133.2 (+4.4)	32.3 (0.0)
2c (4-F-C_6H_4)	156.1 (−0.9)	111.3 (+0.1)	117.9 (0.0)	142.9 (0.0)	115.9 (0.0)	140.9 (0.0)	141.4 (−0.1)	125.6 (d, J_{C-F}= 3.1 Hz) (−3.5)	131.9 (d, J_{C-F} = 8.7 Hz) (+2.5)	115.9 (d, J_{C-F} =14.5 Hz) (−15.3)	163.3 (d, J_{C-F} = 248.5 Hz) (+34,5)	32.3 (0.0)
2d (4-Cl-C_6H_4)	155.9 (−1.1)	111.4 (+0.2)	118.0 (+0.1)	143.0 (+0.1)	115.1 (−0.8)	140.9 (0.0)	141.4 (−0.1)	127.9 (−1.2)	131.2 (+1.8)	128.9 (−1.5)	135.4 (+6.6)	32.3 (0.0)
2e (4-(NMe_2)-C_6H_4)^a	157.8 (+0.8)	110.6 (−0.6)	117.3 (−0.6)	142.6 (−0.3)	114.2 (−1.7)	141.8 (+0.8)	141.3 (−0.2)	115.5 (−13.6)	130.4 (+1.0)	111.6 (−18.8)	151.4 (+22.6)	32.5 (+0.2)
2f (4-NO_2-C_6H_4)	154.8 (−2.2)	111.7 (+0.5)	118.5 (+0.6)	143.2 (+0.3)	115.6 (−0.3)	141.1 (+0.2)	141.4 (−0.1)	135.1 (+6.0)	128.8 (−0.6)	130.9 (+0.5)	148.3 (+19.5)	35.2 (2.9)

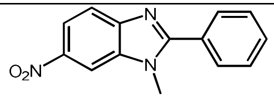
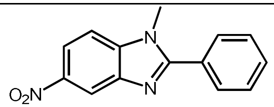
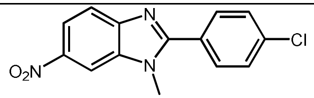
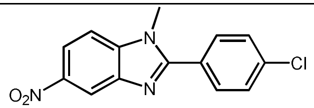
$^a\delta_{NMe2}$ = 39.7 ppm.

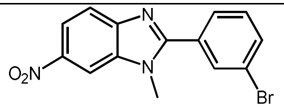
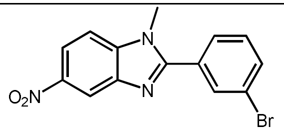
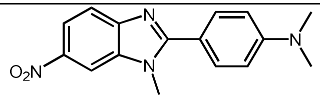
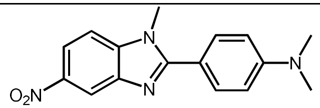
Table S6. ^{13}C NMR data (chemical shifts δ in ppm) for 1-methyl-6-nitrobenzimidazoles **3a–f** in DMSO-d_6 at 25 °C.

 **Compound** (aryl group)	**C-2**	**C-4**	**C-5**	**C-6**	**C-7**	**C-3a**	**C-7a**	**C-1'**	**C-2'/C-6'**	**C-3'/C-5'**	**C-4'**	**NCH_3**
3a (C_6H_5)	158.0	119.2	117.6	146.9	107.9	142.6	136.0	129.0	128.8 (+3.8)	130.5	129.5	32.3
3b (3-Br-C_6H_4)	156.3 (−1.7)	119.3 (+0.1)	117.7 (+0.1)	146.7 (−0.2)	108.0 (+0.1)	142.8 (+0.2)	135.9 (−0.1)	121.9 (−7.1)	**C-2':**131.9 (+3.1) **C-6':**128.4 (−0.4)	**C-3':**131.5 (+1.0) **C-5':**130.9 (+0.4)	133.3	32.3 (0.0)
3c (4-F-C_6H_4)	157.1 (−0.9)	119.2 (0.0)	117.7 (+0.1)	146.8 (−0.1)	107.9 (0.0)	142.6 (0.0)	136.0 (0.0)	125.6 (d, *J* = 2.7 Hz) (−3.4)	132.0 (d, *J* = 8.8 Hz) (+3.2)	115.9 (d, *J* = 21.5 Hz) (−14.6)	163.3 (d, *J* = 249.0 Hz) (+33.8)	32.3 (0.0)
3d (4-Cl-C_6H_4)	156.8 (−1.2)	119.2 (0.0)	117.7 (+0.1)	146.9 (0.0)	107.9 (0.0)	142.7 (+0.1)	136.0 (0.0)	127.1 (−1.9)	131.2 (+2.4)	128.9 (−1.6)	135.5 (+6.0)	32.3 (0.0)
3e (4-(NMe_2)-C_6H_4)[a]	158.9 (+0.9)	118.2 (−1.0)	117.5 (−0.1)	147.5 (+0.6)	107.2 (−0.7)	141.9 (−0.7)	136.2 (+0.2)	115.4 (−13.6)	130.5 (+1.7)	111.5 (−19.0)	151.7 (+22.2)	32.5 (+0.2)
3f (4-NO_2-C_6H_4)	155.8 (−2.2)	119.7 (+0.5)	117.9 (+0.3)	146.6 (−0.3)	108.3 (+0.4)	143.1 (+0.5)	136.2 (+0.2)	135.1 (+6.1)	123.8 (−5.0)	130.9 (+0.4)	148.4 (+18.9)	32.5 (+0.2)

[a] δ_{NMe2} = 39.7 ppm.

Table S7. ^{1}H NMR data (600 MHz, δ in ppm, *J* in Hz) of compounds **2a–f** and **3a–f** recorded in acetone-d$_6$ at 25 °C.

Prodotti	**^{1}H NMR**
 **a**	600 MHz Acetone-d$_6$, 25 °C 8.56 (d, *J*=2.1 Hz, 1H, H_7) 8.20 (dd, J_1=8.8 Hz, J_2=2.1 Hz, 1H, H_5) 7.96 (d, *J*=4.4 Hz, 1H, $H_{2'}$ o $H_{6'}$) 7.95 (d, *J*=2.3 Hz, 1H, $H_{2'}$ o $H_{6'}$) 7.84 (d, *J*=8.8 Hz, 1H, H_4) 7.64 (d, *J*=1.4 Hz, 1H, $H_{3'}$ o $H_{4'}$ o $H_{5'}$) 7.63 (d, *J*=2.1 Hz, 1H, $H_{3'}$ o $H_{4'}$ o $H_{5'}$) 4.13 (s, 3H, NCH_3)
 **a**	600 MHz Acetone-d$_6$, 25 °C 8.57 (d, *J*=2.0 Hz, 1H, H_7) 8.25 (dd, J_1=8.8 Hz, J_2=2.0 Hz, 1H, H_5) 7.94 (d, *J*=4.4 Hz, 1H, $H_{2'}$ o $H_{6'}$) 7.93 (d, *J*=2.0 Hz, 1H, $H_{2'}$ o $H_{6'}$) 7.80 (d, *J*=8.8 Hz, 1H, H_4) 7.63 (d, *J*=1.8 Hz, 1H, $H_{3'}$ o $H_{4'}$ o $H_{5'}$) 7.62 (d, *J*=2.0 Hz, 1H, $H_{3'}$ o $H_{4'}$ o $H_{5'}$) 4.07 (s, 3H, NCH_3)
 **d**	600 MHz Acetone-d$_6$, 25 °C 8.56 (d, *J*=2.1 Hz, 1H, H_7) 8.20 (dd, J_1=8.8 Hz, J_2=2.0 Hz, 1H, H_5) 7.99 (d, *J*=8.5 Hz, 2H, $H_{2'}$) 7.84 (d, *J*=8.8 Hz, 1H, H_4) 7,67 (d, *J*=8.5 Hz, 2H, $H_{3'}$) 4.14 (s, 3H, NCH_3)
 d	600 MHz Acetone-d$_6$, 25 °C 8.57 (d, *J*=2.1 Hz, 1H, H_7) 8.26 (dd, J_1=8.8 Hz, J_2=2.1 Hz, 1H, H_5)

	7.97 (d, *J*=8.5 Hz, 2H, $H_{2'}$) 7.81 (d, *J*=8.8 Hz, 1H, H_4) 7,67 (d, *J*=8.5 Hz, 2H, $H_{3'}$) 4.08 (s, 3H, NCH_3)
 **b**	600 MHz Acetone-d_6, 25 °C 8.58 (d, *J*=2.0 Hz, 1H, H_7) 8.21 (dd, J_1=8.8 Hz, J_2=2.0 Hz, 1H, H_5) 8.13 (t, *J*=1.7 Hz. 1H, $H_{2'}$) 7,97 (d, *J*=7.6 Hz, 1H, $H_{6'}$) 7.85 (d, *J*=8.8 Hz, 1H, H_4) 7.81 (d, *J*=7.9 Hz, 1H, $H_{4'}$) 7.60 (t, *J*=7.9 Hz, 1H $H_{5'}$) 4.15 (s, 3H, NCH_3)
 b	600 MHz Acetone-d_6, 25 °C 8.58 (d, *J*=2.0 Hz, 1H, H_7) 8.27 (dd, J_1=8.8 Hz, J_2=2.0 Hz, 1H, H_5) 8.12 (t, *J*=1.7 Hz. 1H, $H_{2'}$) 7,95 (d, *J*=7.7 Hz, 1H, $H_{6'}$) 7.82 (d, *J*=8.8 Hz, 1H, H_4) 7.81 (d, *J*=7.8 Hz, 1H, $H_{4'}$) 7.60 (t, *J*=7.7 Hz, 1H $H_{5'}$) 4.09 (s, 3H, NCH_3)
 e	600 MHz Acetone-d_6, 25 °C 8.58 (d, *J*=2.1 Hz, 1H, H_7) 8.12 (dd, J_1=8.8 Hz, J_2=2.1 Hz, 1H, H_5) 7.80 (d, *J*=8.9 Hz, 2H, $H_{2'}$) 7.76 (d, *J*=8.8 Hz, 1H, H_4) 6.87 (d, *J*=8.9 Hz, 2H, $H_{3'}$) 4.00 (s, 3H, NCH_3) 3.03 (s, 6H, $N(CH_3)_2$)
 e	600 MHz Acetone-d_6, 25 °C 8.48 (d, *J*=2.0 Hz, 1H, H_7) 8.16 (dd, J_1=8.8 Hz, J_2=2.0 Hz, 1H, H_5) 7.79 (d, *J*=8.8 Hz, 1H, H_4)

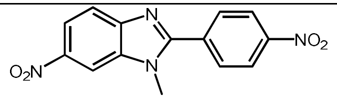
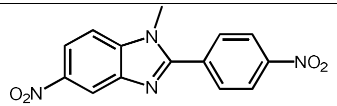
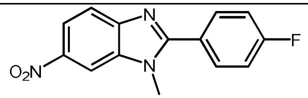
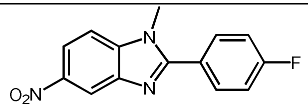
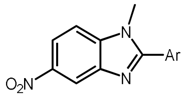
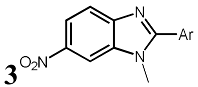
	7.76 (d, *J*=9.0 Hz, 2H, $H_{2'}$) 6.87 (d, *J*=9.0 Hz, 2H, $H_{3'}$) 3.95 (s, 3H, NCH_3) 3.02 (s, 6H, $N(CH_3)_2$)
 f	600 MHz Acetone-d_6, 25 °C 8.75 (d, *J*= 1.9 Hz, 1H, H_7) 8.42 (d, *J*= 8.5 Hz, 2H, $H_{3'}$) 8.21 (d, *J*= 8.5 Hz, 1H, $H_{2'}$) 8.18 (dd, *J1*=8.8 Hz *J2*=1.9 Hz, 1H, H_5) 7.92 (d, *J*= 8.8 Hz, 1H, H_4) 4.06 (s, 3H, NCH_3)
 f	600 MHz Acetone-d_6, 25 °C 8.62 (d, *J*= 2.0 Hz, 1H, H_7) 8.43 (d, *J*= 8.6 Hz, 2H, $H_{3'}$) 8.26 (dd, *J1*=9.1 Hz *J2*=2.0 Hz, 1H, H_5) 8.20 (d, *J*= 8.6 Hz, 1H, $H_{2'}$) 7.94 (d, *J*= 9.1 Hz, 1H, H_4) 4.01 (s, 3H, NCH_3)
 c	600 MHz Acetone-d_6, 25 °C 8.56 (br.s, 1H, H_7) 8.20 (d, *J*=9.0 Hz, 1H, H_5) 8.03 (dd, $J_{H\text{-}H}$=8.0, Hz $J_{H\text{-}F}$=5.3 Hz, 1H, $H_{2'}$) 7.83 (d, *J*=9.0 Hz, 1H, H_4) 7.41 (t, $J_{H\text{-}H,H\text{-}F}$=8.7 Hz, 1H, $H_{3'}$) 4.13 (s, 3H, NCH_3)
 c	600 MHz Acetone-d_6, 25 °C 8.57 (d, *J*= 2.1 Hz, 1H, H_7) 8.25 (dd, J_1=8.8 Hz J_2=2.1 Hz, 1H, H_5) 8.01 (dd, $J_{H\text{-}H}$=8.8, Hz $J_{H\text{-}F}$=5.3 Hz, 1H, $H_{2'}$) 7.80 (d, *J*= 8.8 Hz, 1H, H_4) 7.41 (t, $J_{H\text{-}H,H\text{-}F}$=8.8 Hz, 1H, $H_{3'}$) 4.07 (s, 3H, NCH_3)

Table S8. ^{13}C chemical shift values[a] for mono substituted benzenes.[b]

	C_1	**C_2**	**C_3**	**C_4**
H	128.5	128.5	128.5	128.5
F	163.6 (+35.1)	114.2 (−14.3)	129.4 (+0.9)	124.0 (−4.5)
Cl	134.9 (+6.4)	128.7 (+0.2)	129.5 (+1.0)	126.5 (−2.0)
Br	123.1 (−5.4)	131.9 (+3.4)	126.3 (−2.2)	127.5 (−1.0)
NMe_2	150.9 (+22.4)	112.8 (−15.7)	129.3 (+0.8)	116.7 (−11.8)
NO_2	148.1 (+19.6)	123.2 (−5.3)	129.4 (+0.9)	134.5 (+6.0)

a. Chemical shifts in ppm with respect to TMS. [b]In brackets the difference with respect to benzene.

Table S9. Electrochemical properties of nitrobenzimidazoles **2** and **3**.

Series 2 	**$E_1^{0'}$ (V)**	**$E_2^{0'}$ (V)**
2a	−1.616	
2b	−1.589	
2c	−1.603	
2d	−1.614	
2e	−1.639	
2f	−1.353*	−1,641*
Series  **3**	$E_1^{0'}$ (V)	Ci vuole E?
3a	−1.572	
3b	−1.555	
3c	−1.547	
3d	−1.555	
3e	−1.584	
3f	−1.351*	−1.534*

1 and 2 subscripts indicate the first and second reduction processes. $E^{0'}$ indicates the formal potential.*refers to the reduction of the nitro group on the benzimidazole moiety.

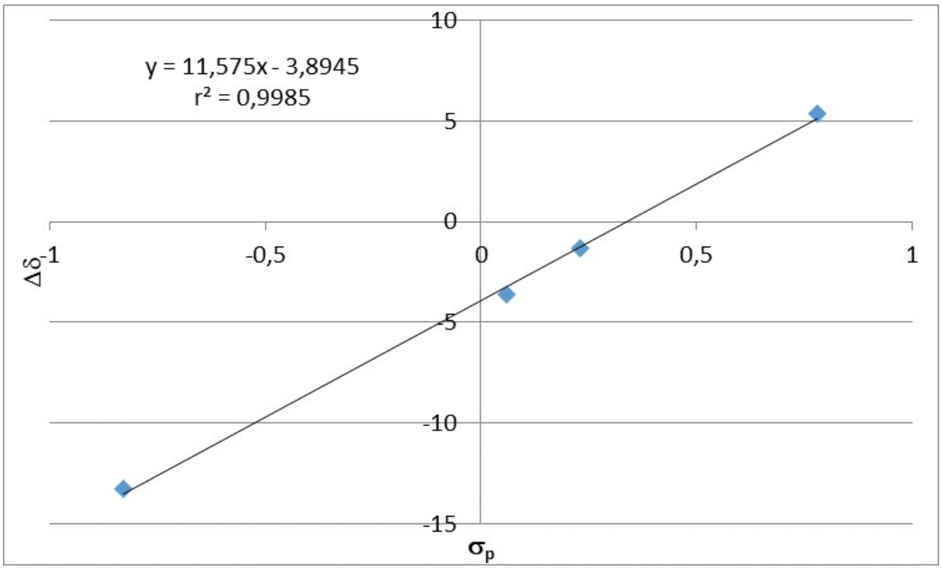


Figure S1. Δδ of $C_{1'}$ *versus* the Hammett constants for series **1.**

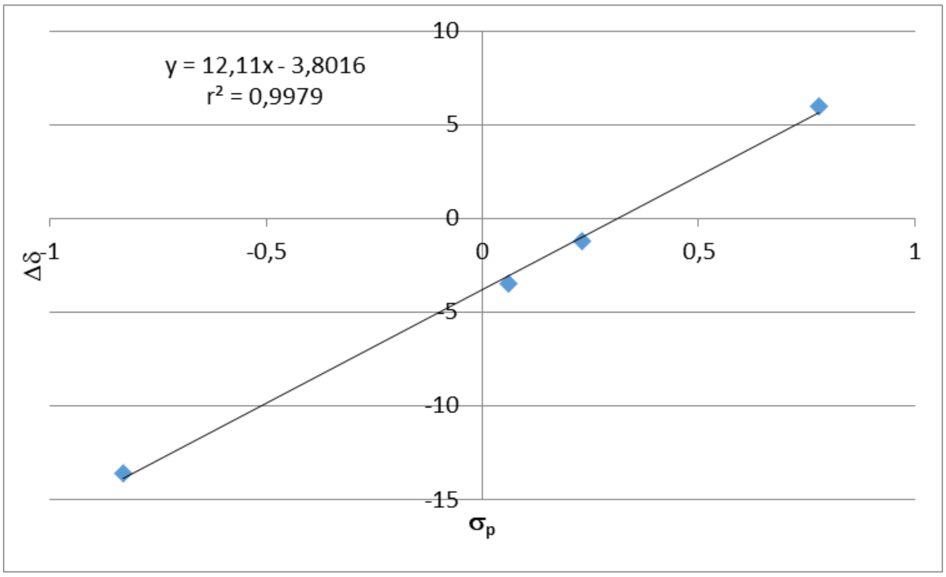


Figure S2. Δδ of $C_{1'}$ *versus* the Hammett constants for series **2.**

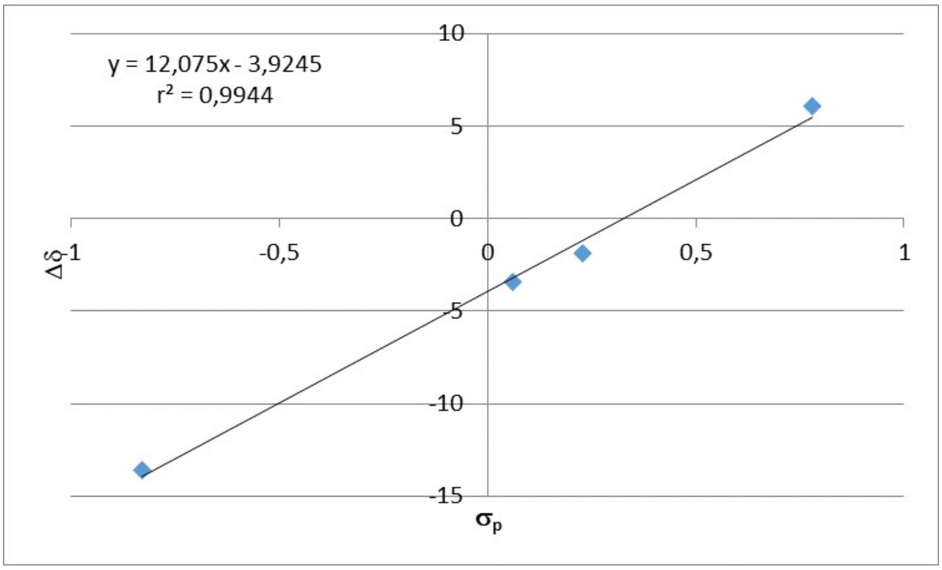


Figure S3. Δδ of $C_{1'}$ *versus* the Hammett constants for series **3.**

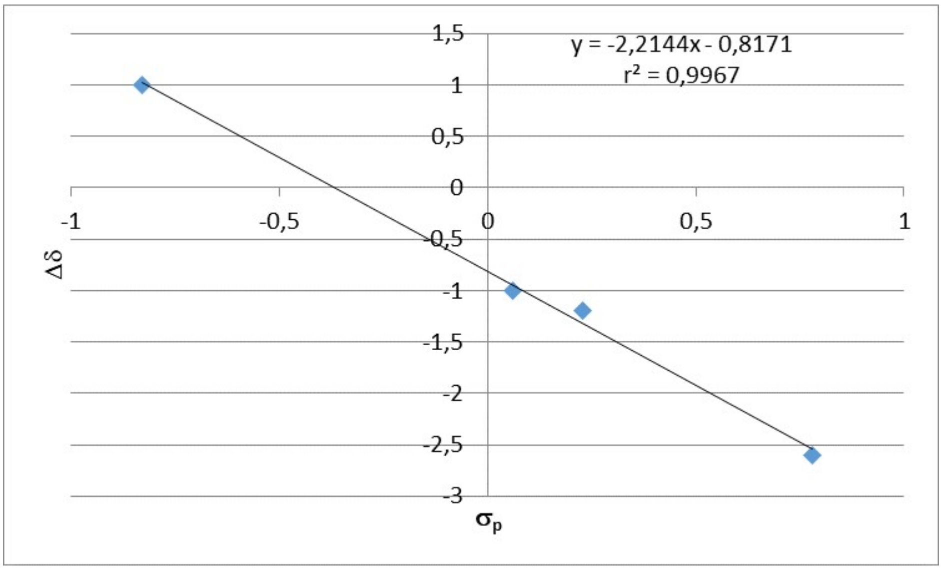


Figure S4. Δδ of C_2 *versus* the Hammett constants for series **1.**

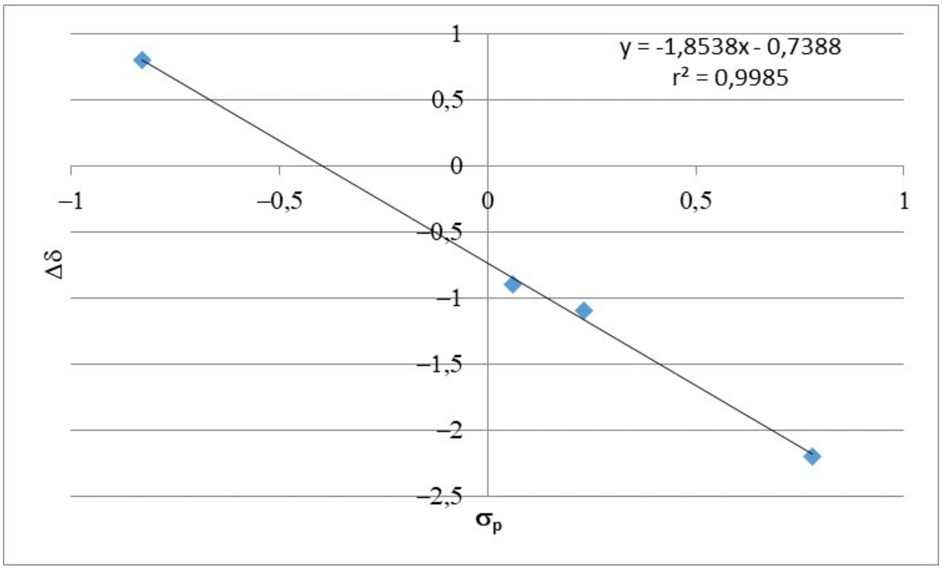


Figure S5. Δδ of C_2 *versus* the Hammett constants for series **2.**

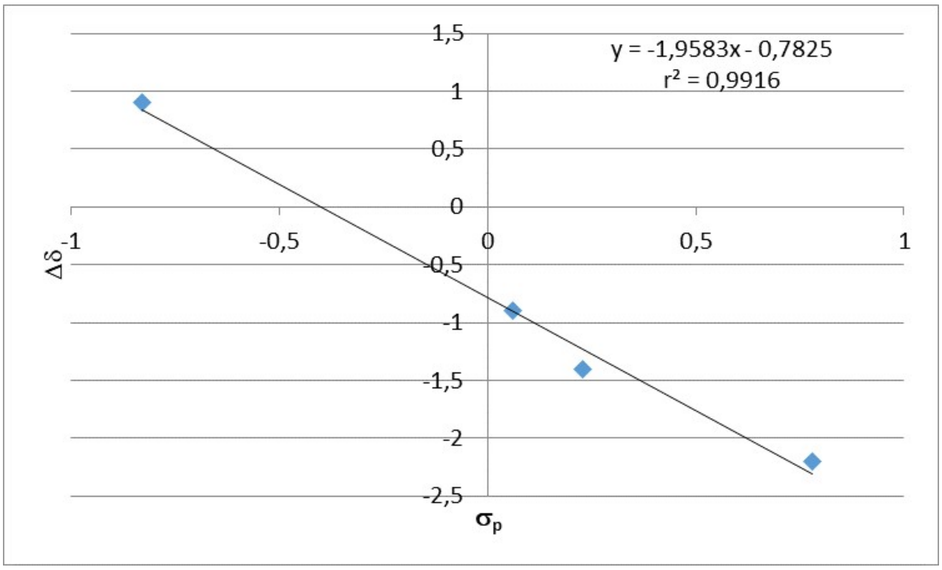


Figure S6. Δδ of C_2 *versus* the Hammett constants for series **3.**

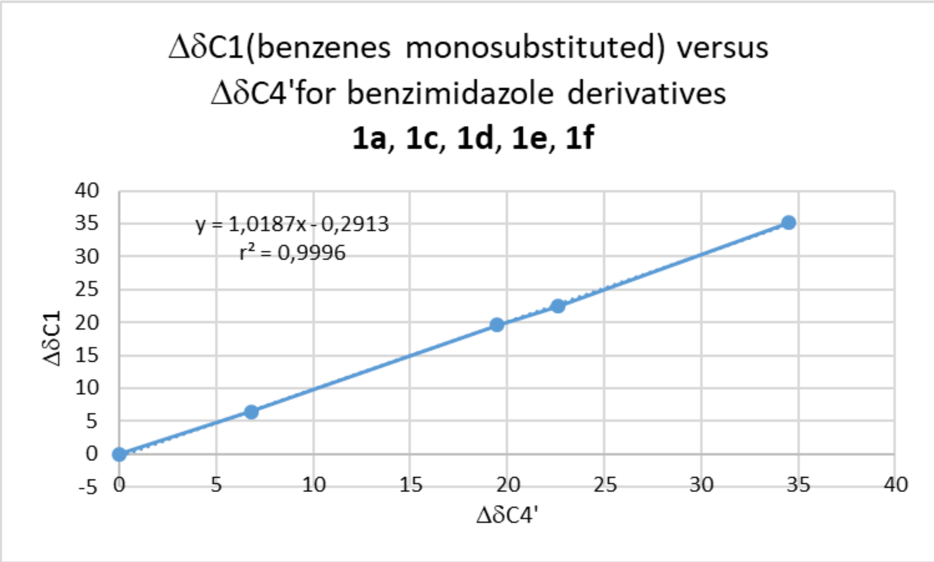


Figure S7. ΔδC1 for monosubstituted benzenes *versus* ΔδC4’ for compounds **1a, 1c, 1d, 1e, and 1f.**

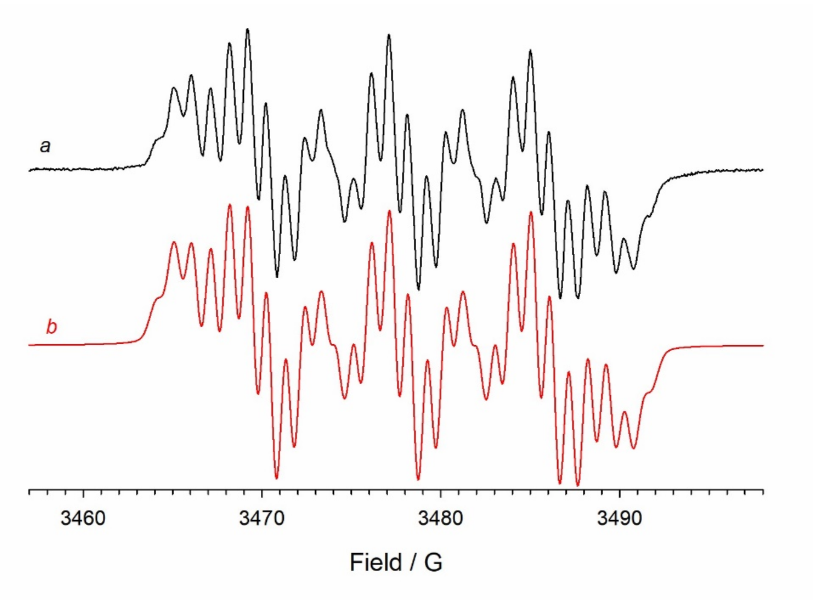


Figure S8. ESR spectrum of the radical species electrogenerated from **2f** (*a*) in 0.1 M Bu_4NClO_4 -ACN. The corresponding theoretical simulation is reported in red (*b*).

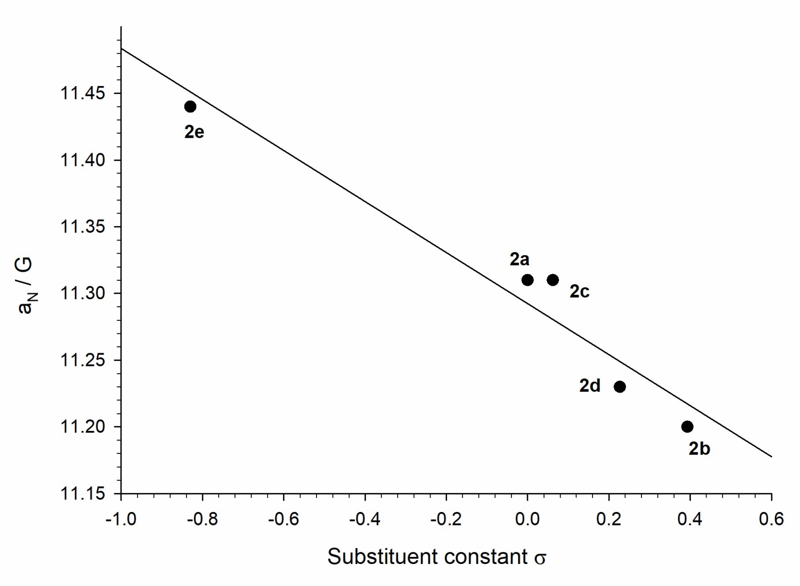


Figure S9. Plot of a_N *vs*. σ substituent constants for compounds **2**. ($r^2 = 0.943$, $\rho = -0.19$).

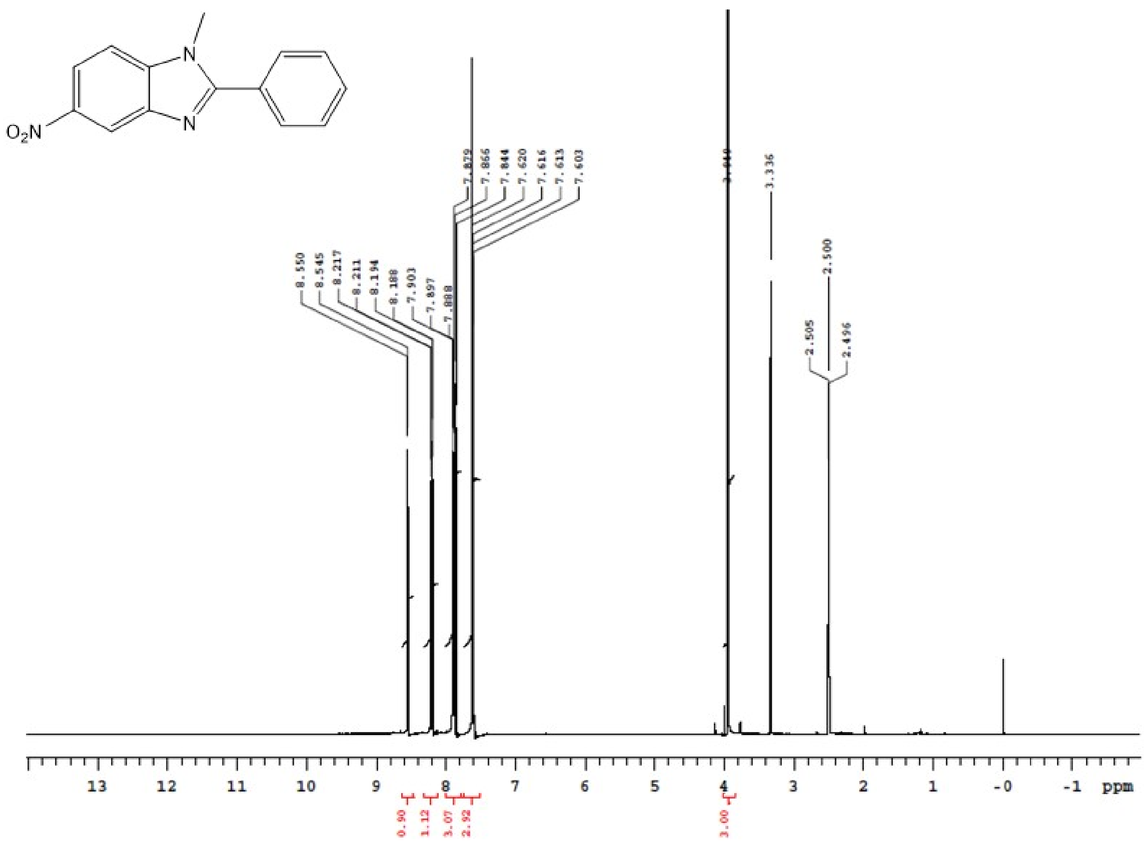


Figure S10. ^{1}H NMR spectrum of compound **2a** in DMSO-d$_6$ at 25 °C.

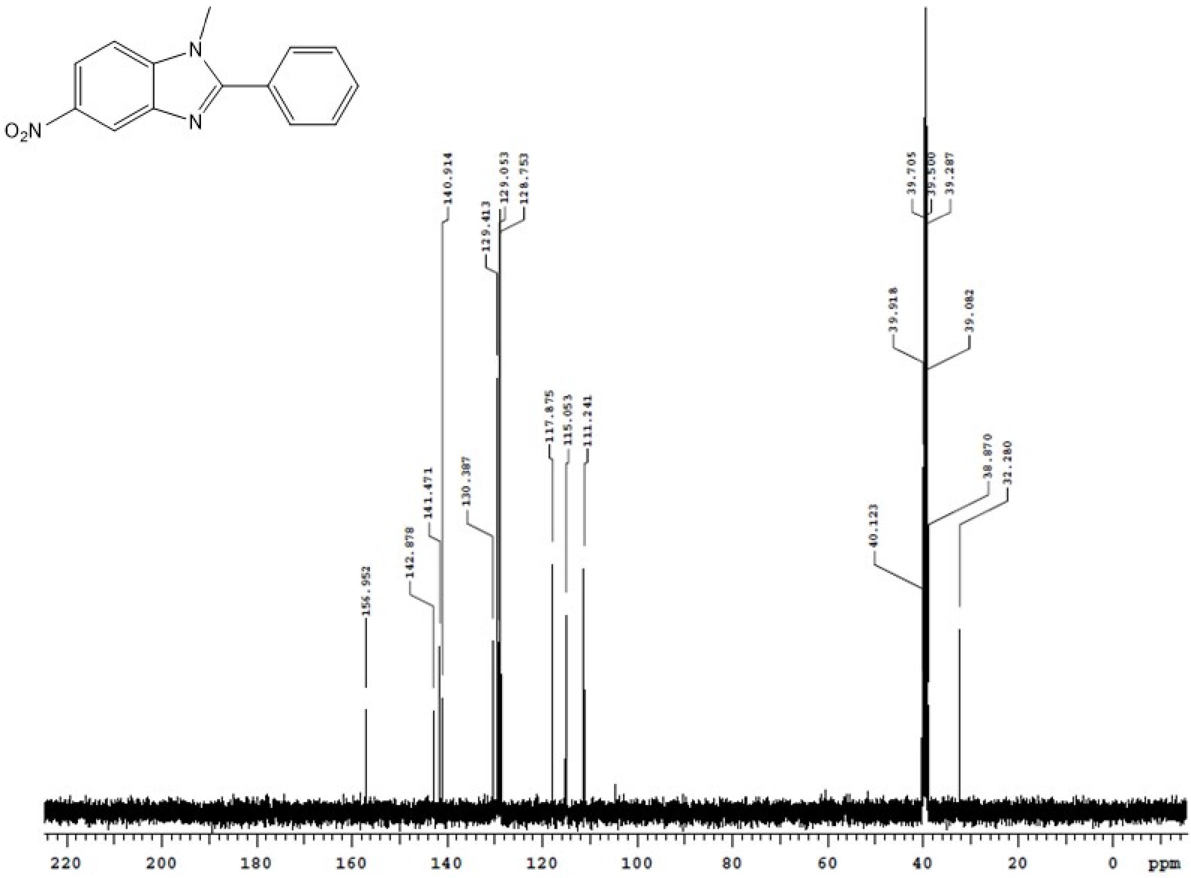


Figure S11. ^{13}C NMR spectrum of compound **2a** in DMSO-d_6 at 25 °C.

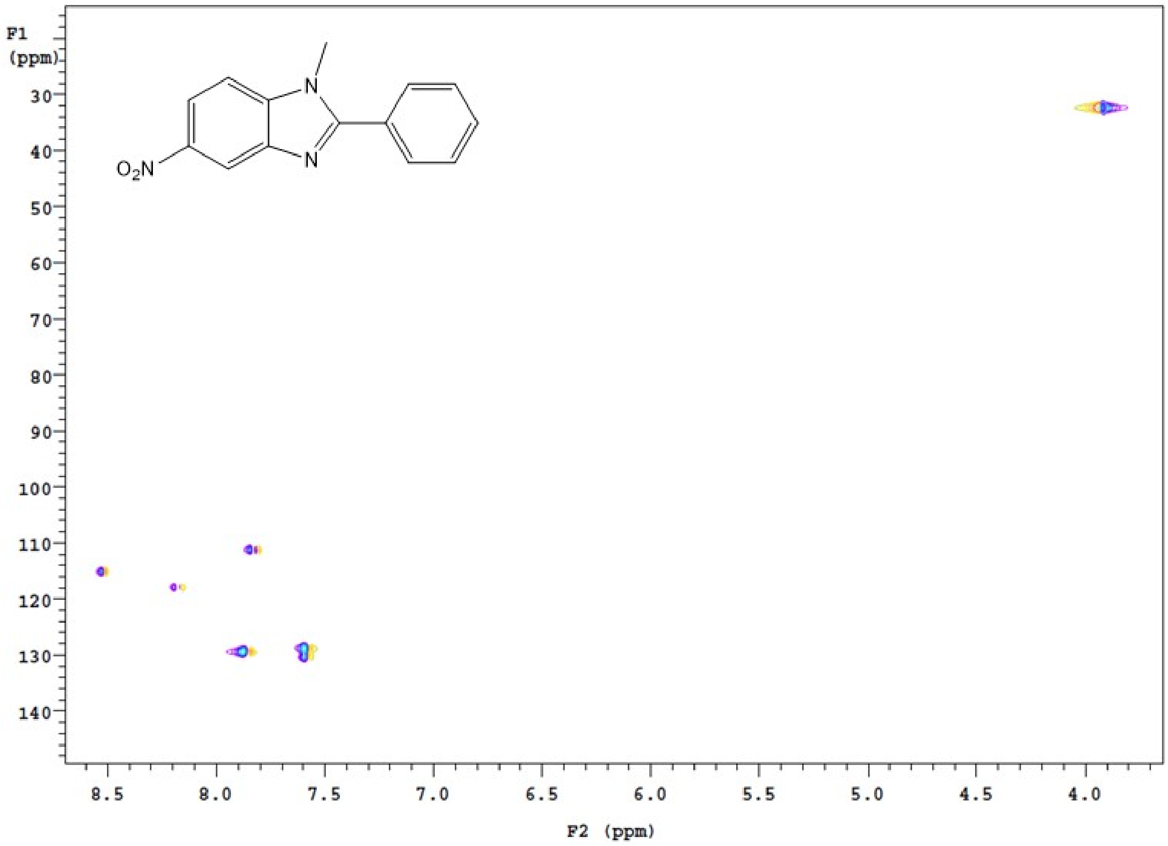


Figure S12. HSQC spectrum of compound **2a** in DMSO-d$_6$ at 25 °C.

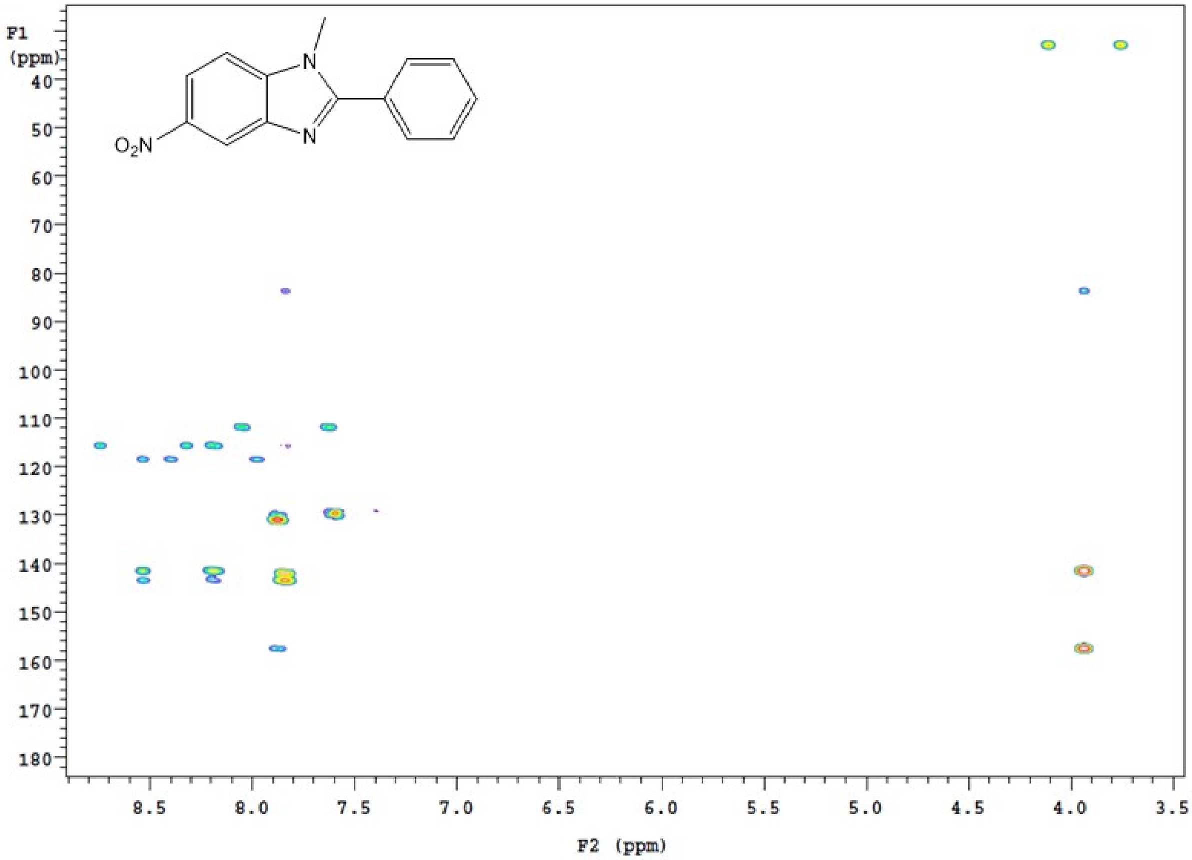


Figure S13. HMBC spectrum of compound **2a** in DMSO-d_6 at 25 °C.

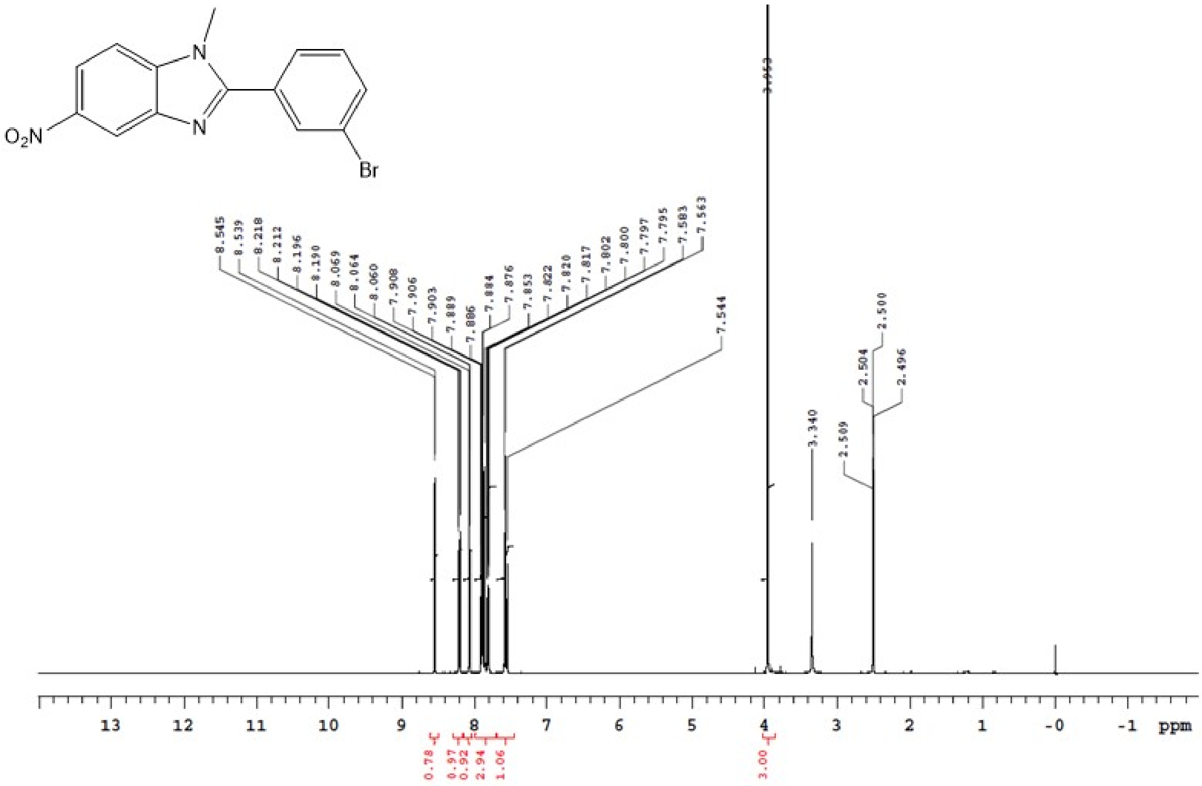


Figure S14. ^{1}H NMR spectrum of compound **2b** in DMSO-d_6 at 25 °C.

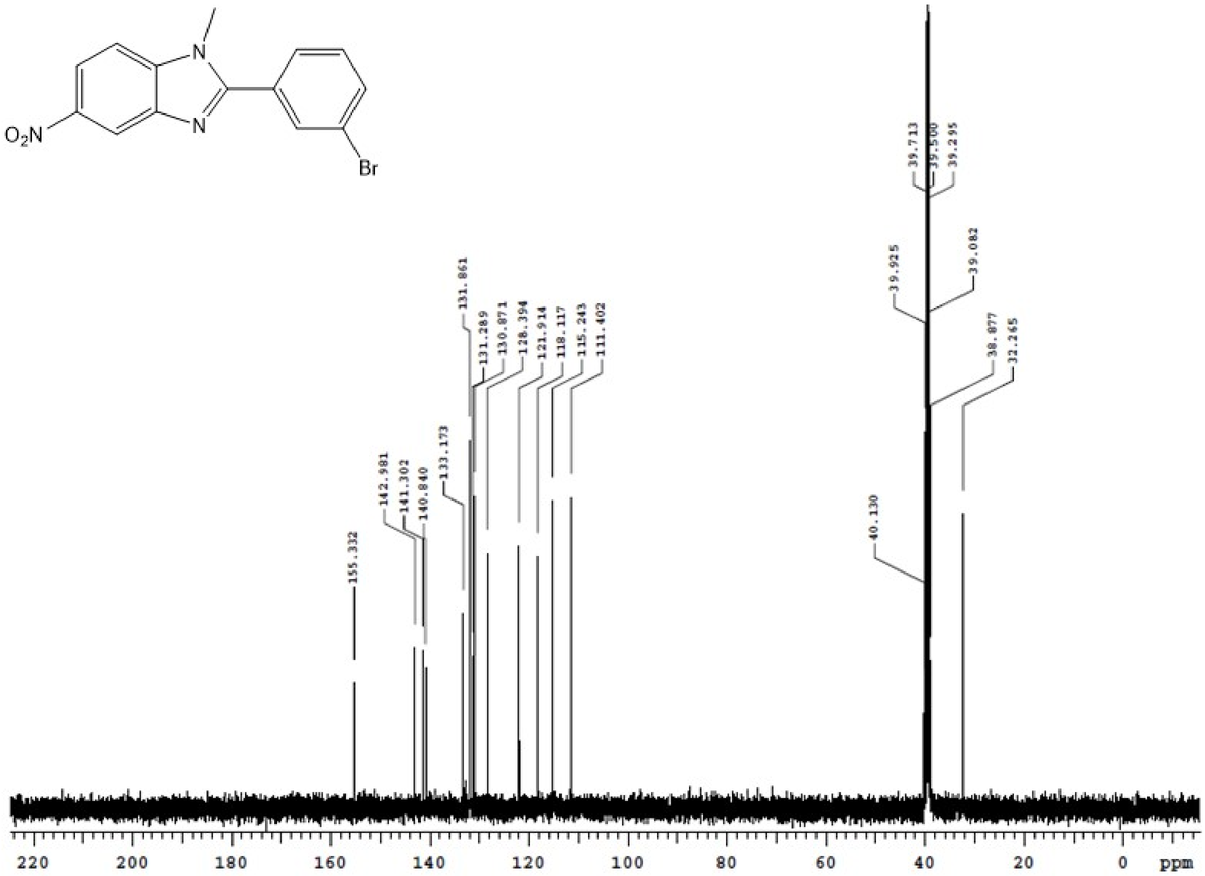


Figure S15. ^{13}C NMR spectrum of compound **2b** in DMSO-d_6 at 25 °C.

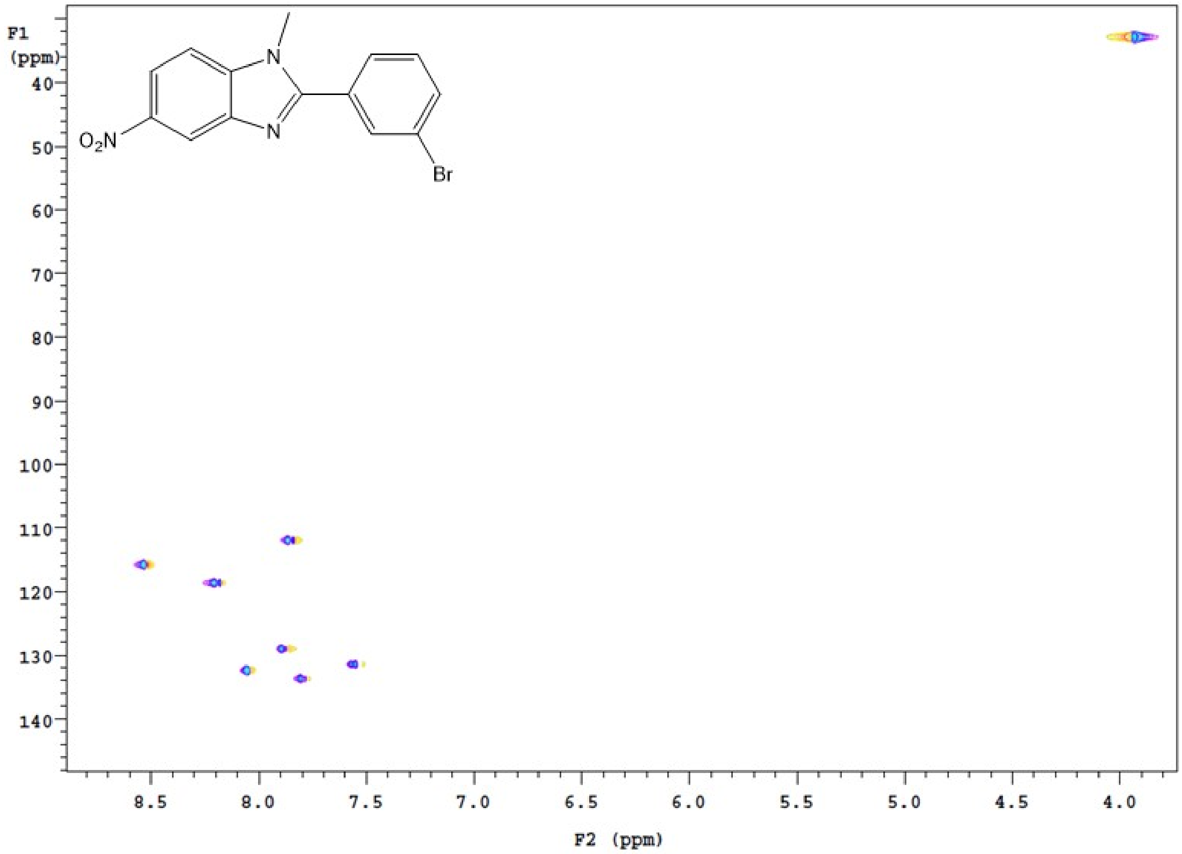


Figure S16. HSQC spectrum of compound **2b** in DMSO-d_6 at 25 °C.

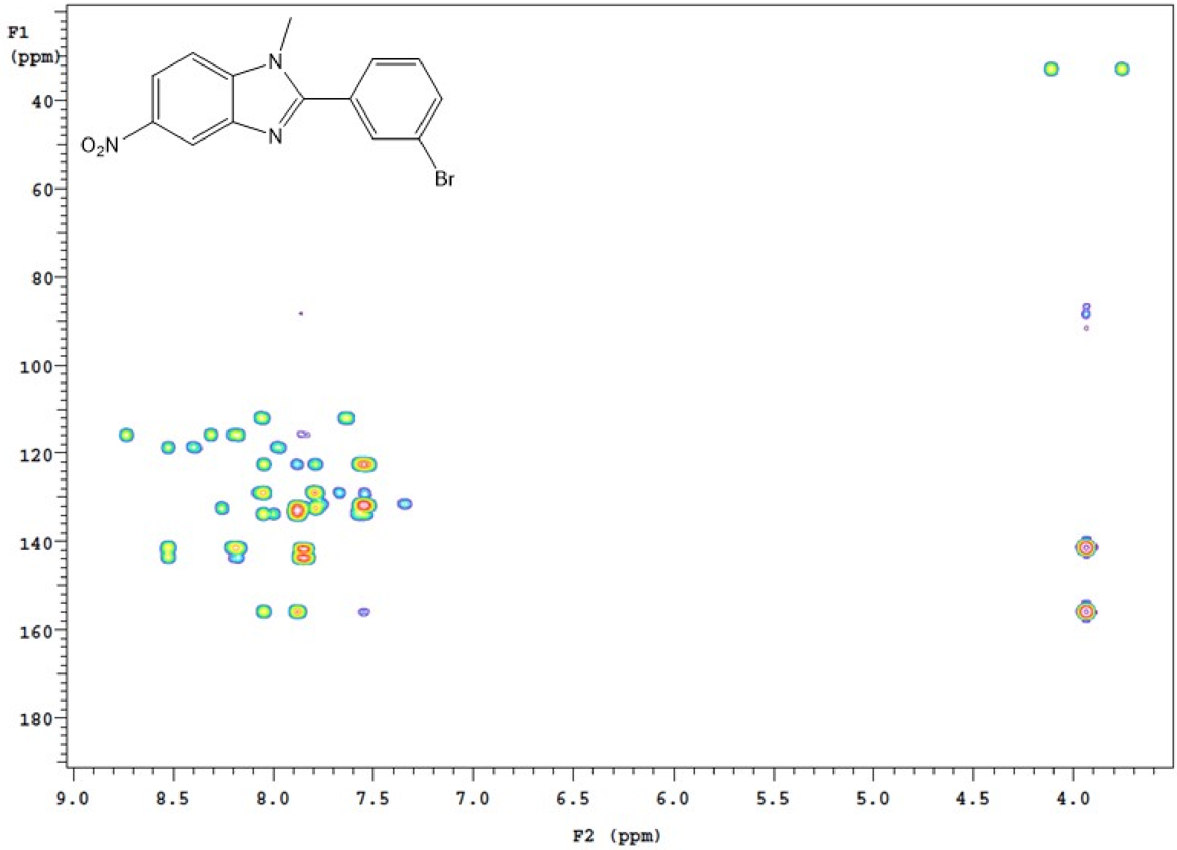


Figure S17. HMBC spectrum of compound **2b** in DMSO-d_6 at 25 °C.

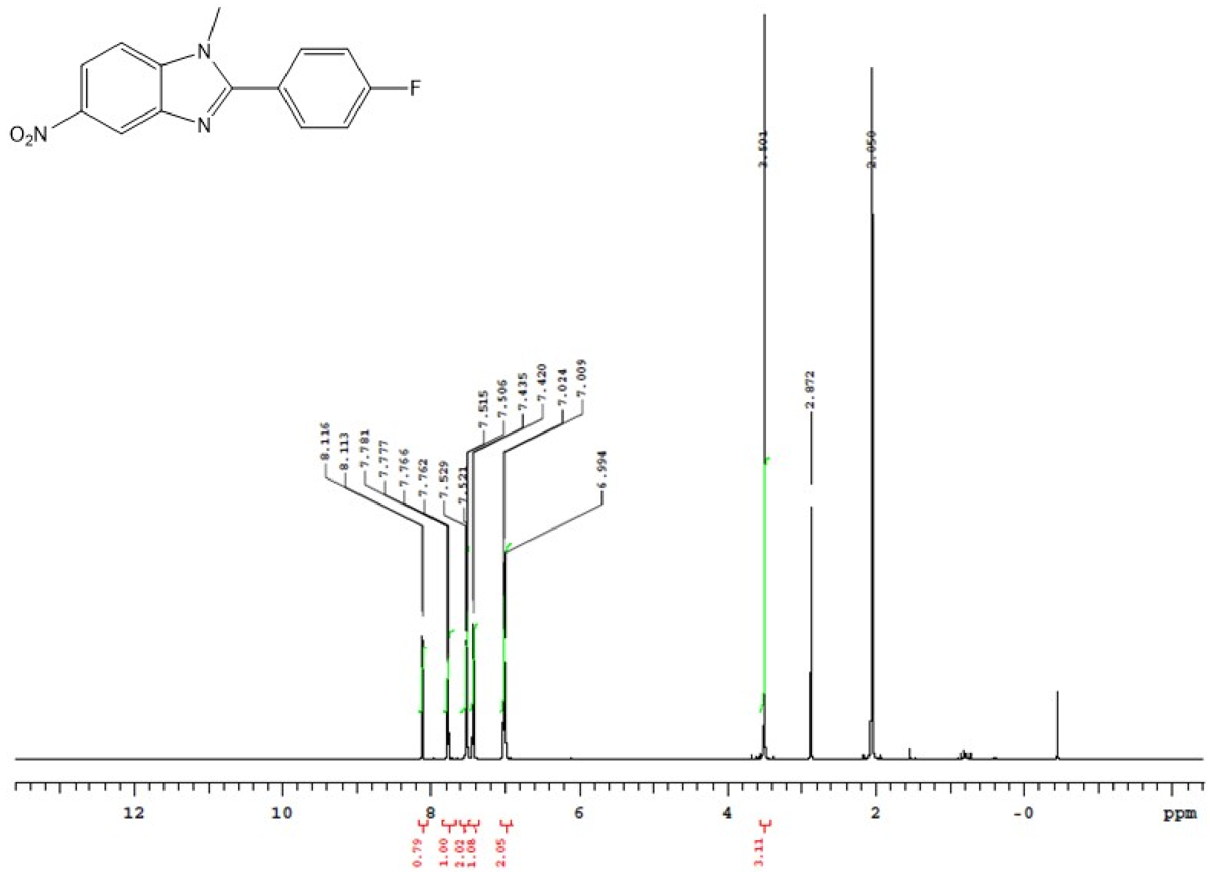
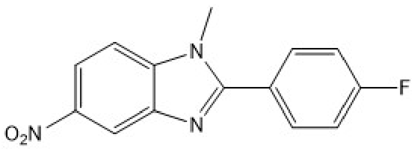


Figure S18. ^{1}H NMR spectrum of compound **2c** in DMSO-d_6 at 25 °C.



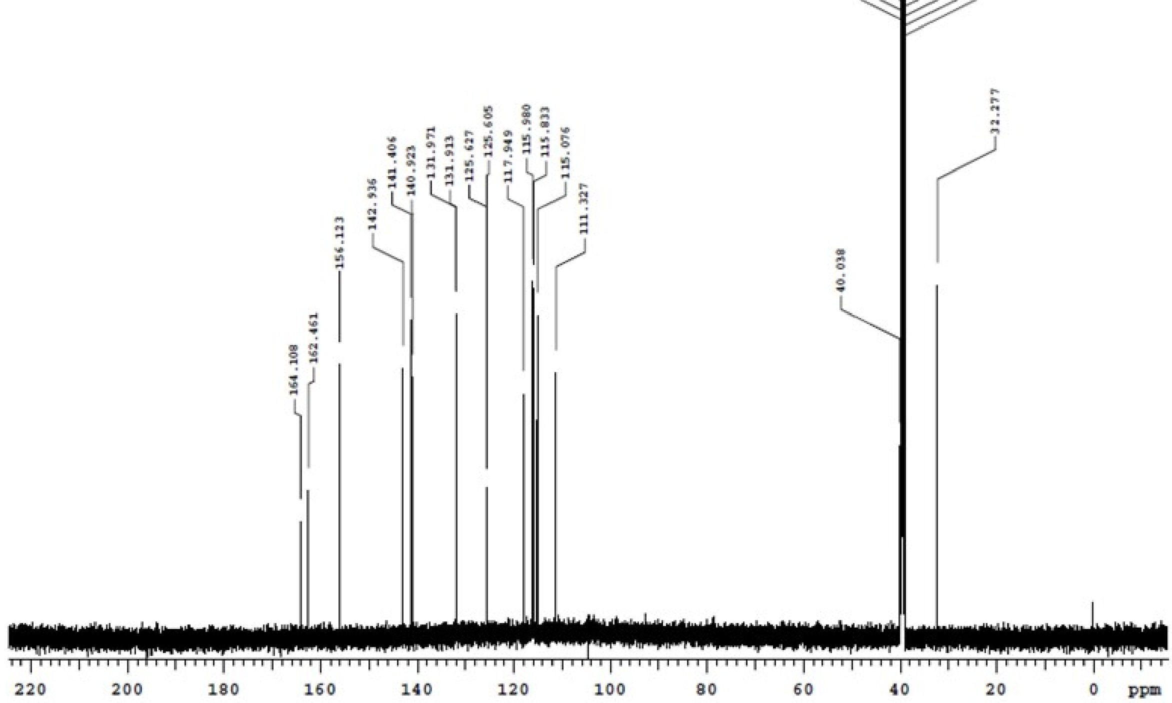


Figure S19. ^{13}C NMR spectrum of compound **2c** in DMSO-d_6 at 25 °C.

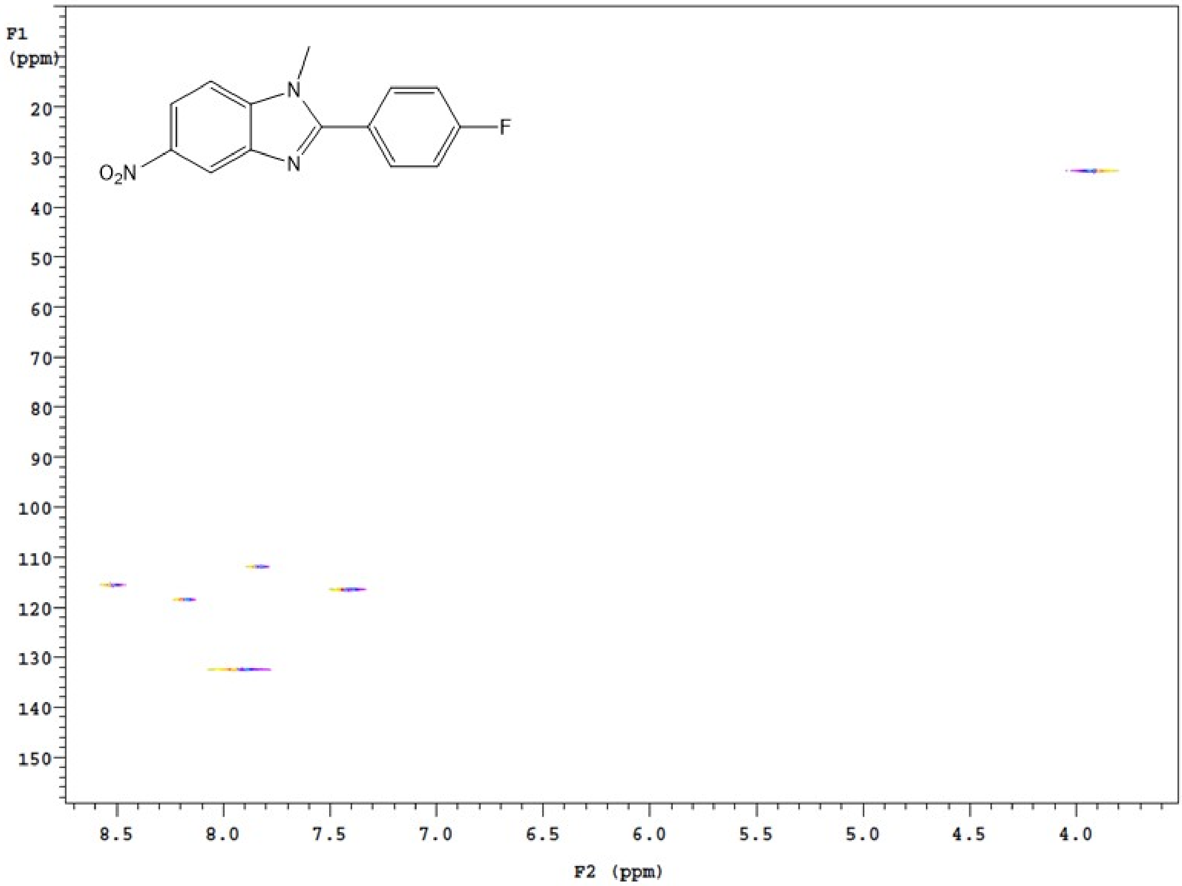


Figure S20. HSQC spectrum of compound **2c** in DMSO-d_6 at 25 °C.

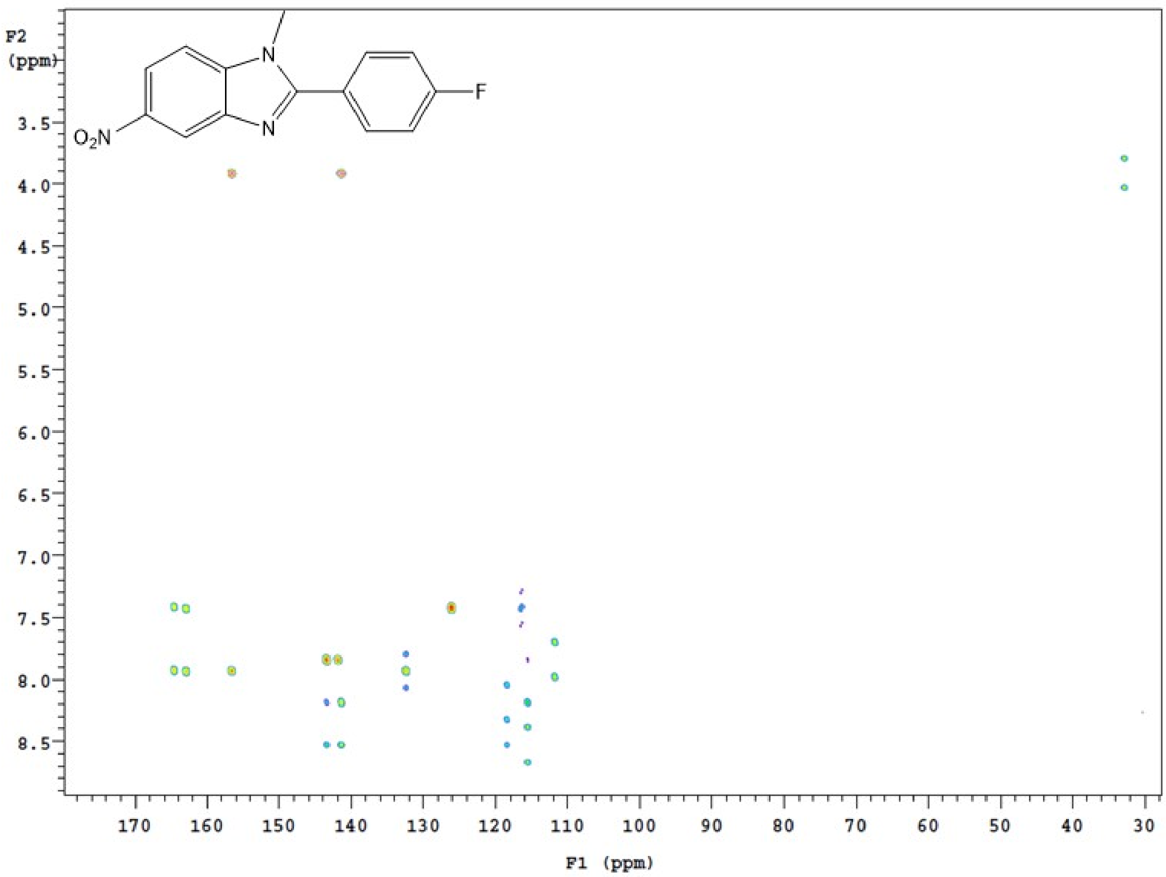


Figure S21. HMBC spectrum of compound **2c** in DMSO-d_6 at 25 °C.

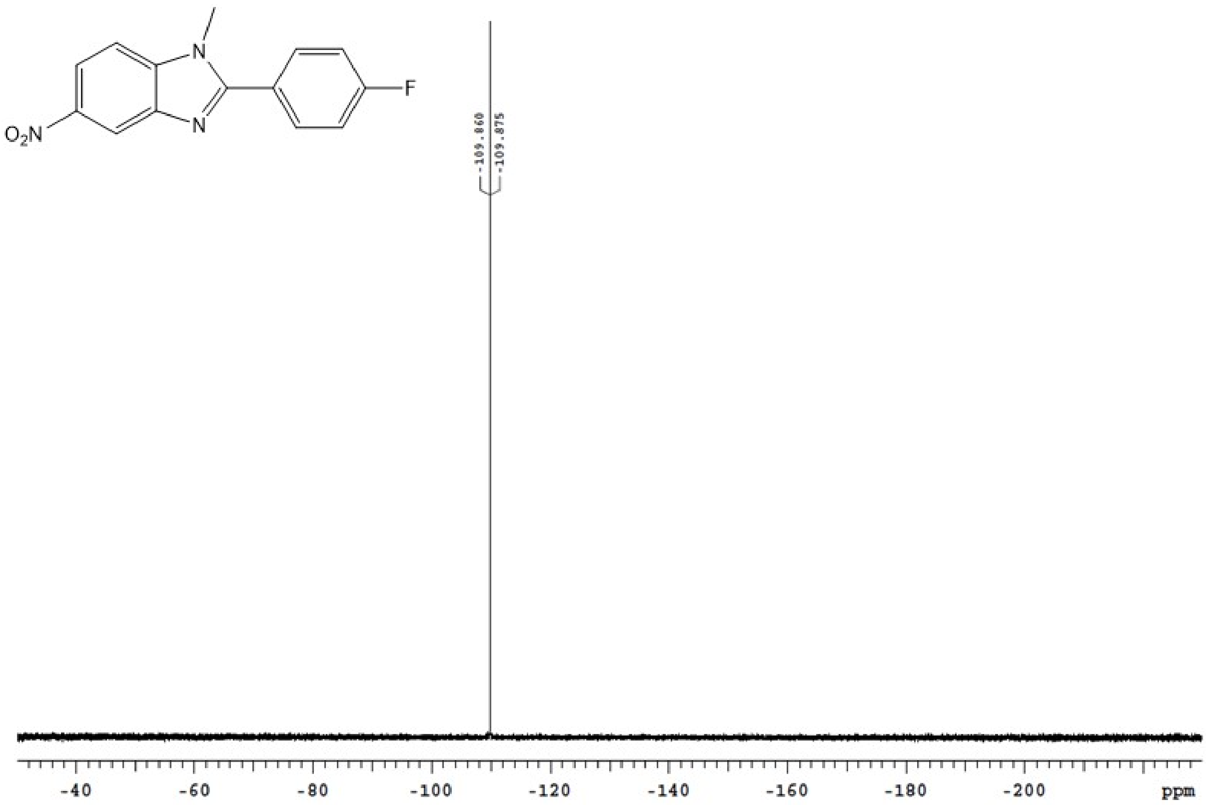


Figure S22. ^{19}F NMR spectrum of compound **2c** in DMSO-d_6 at 25 °C.

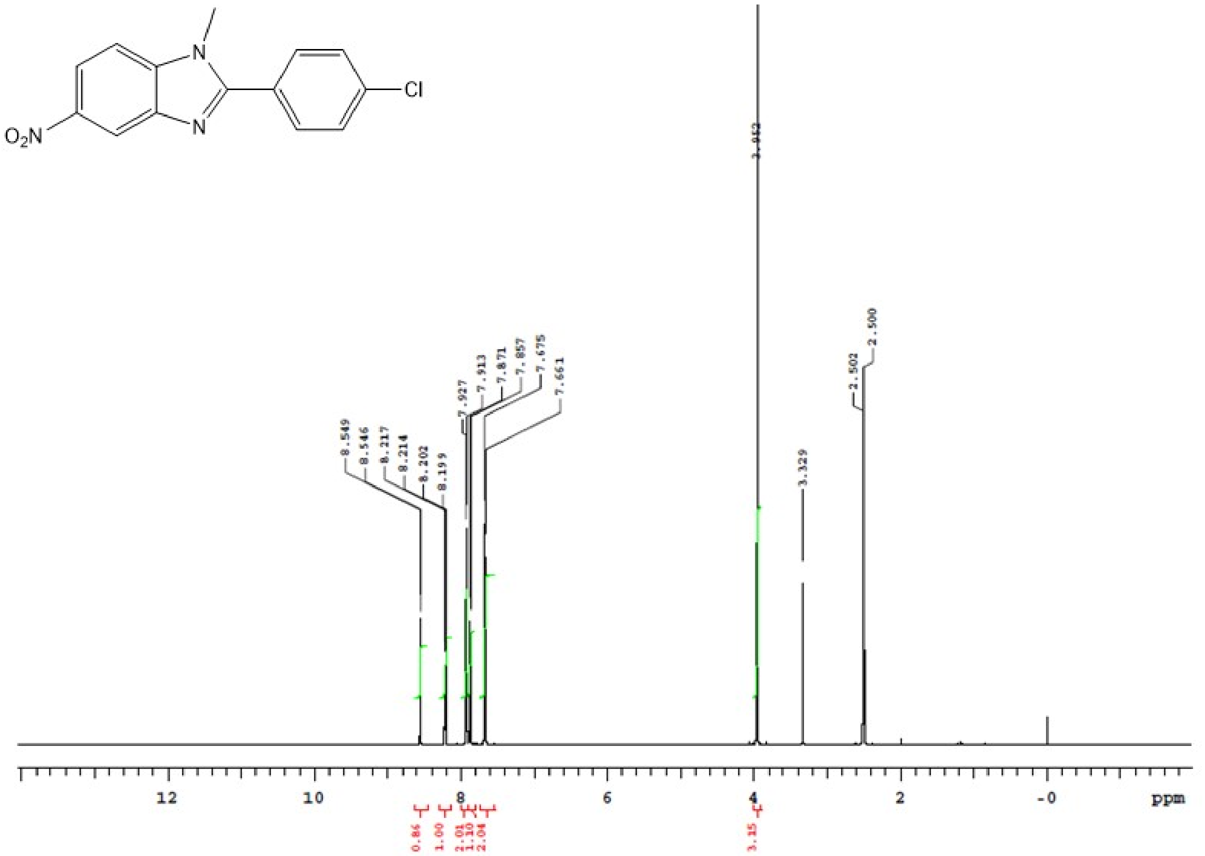


Figure S23. ^{1}H NMR spectrum of compound **2d** in DMSO-d_6 at 25 °C.

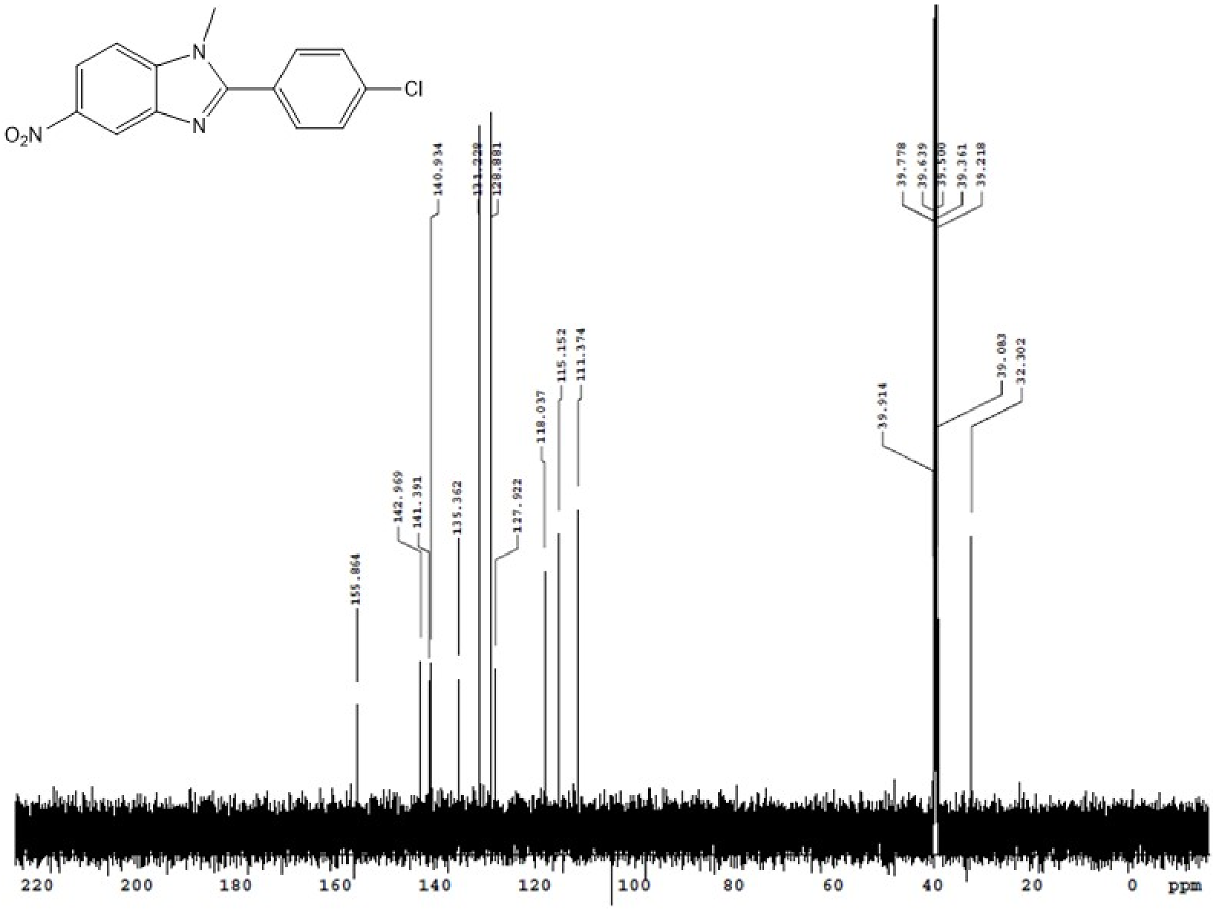


Figure S24. ^{13}C NMR spectrum of compound **2d** in DMSO-d_6 at 25 °C.

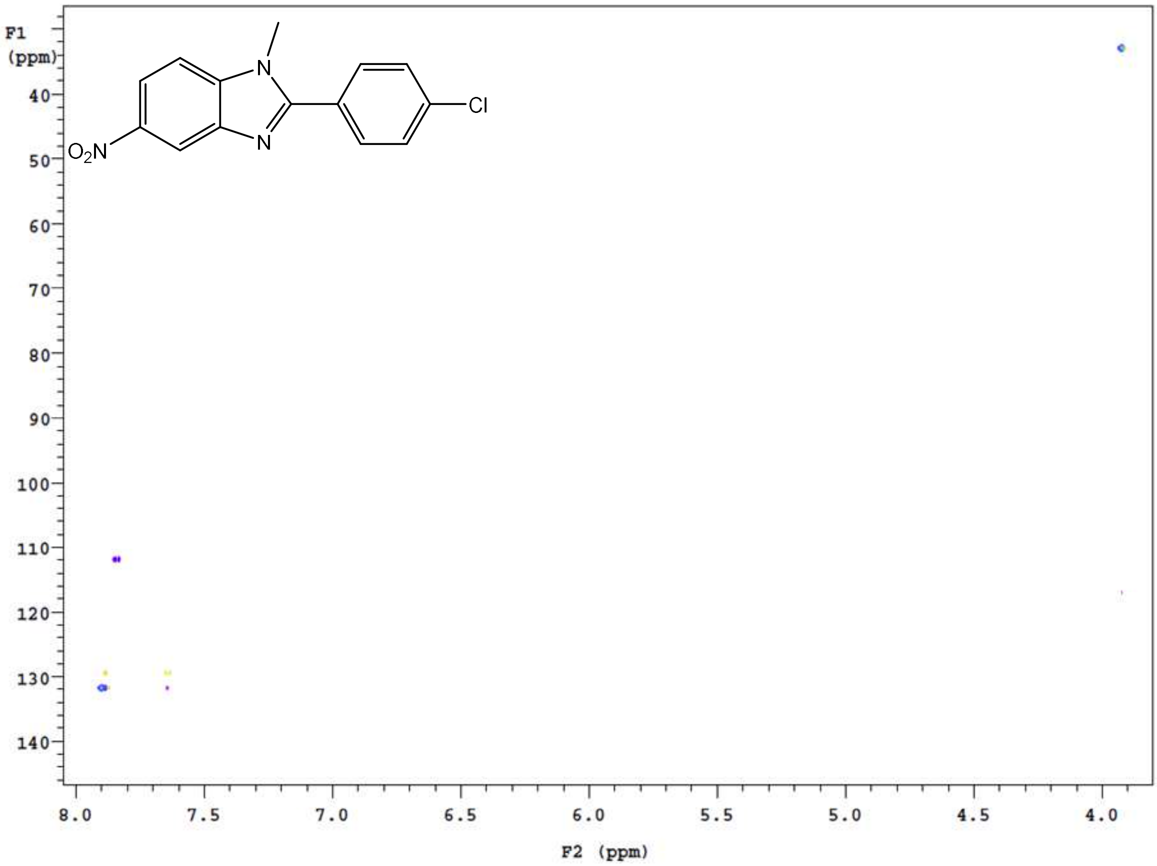


Figure S25. HSQC spectrum of compound **2d** in DMSO-d_6 at 25 °C.

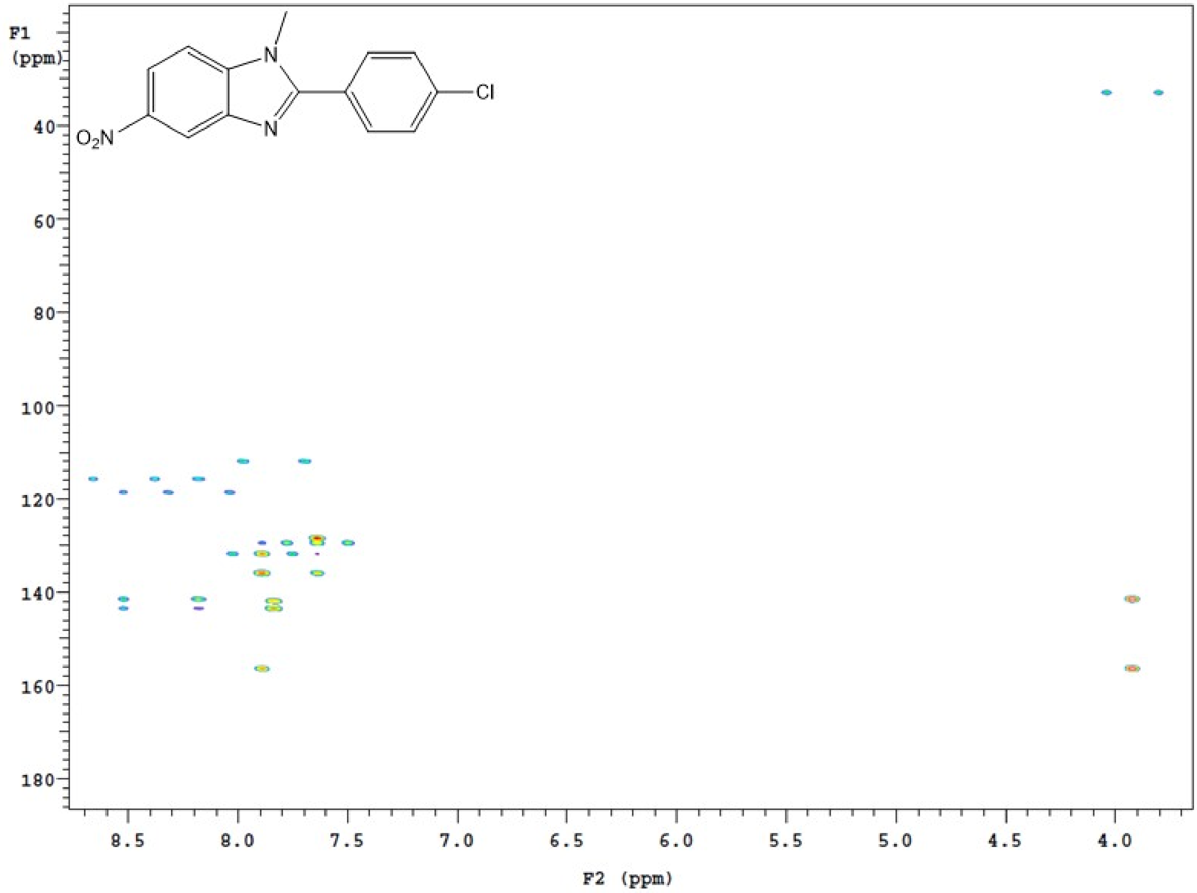


Figure S26. HMBC spectrum of compound **2d** in DMSO-d$_6$ at 25 °C.

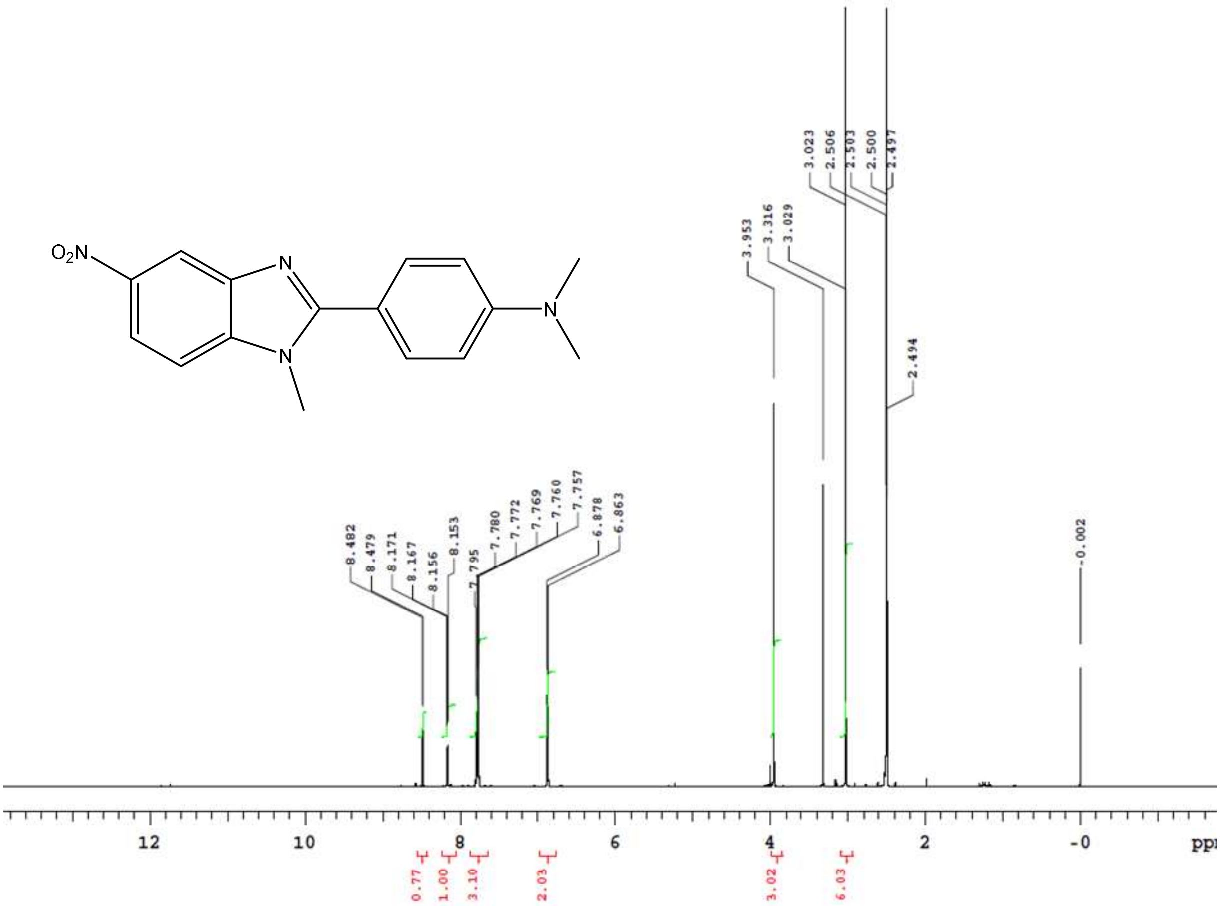


Figure S27. ^{1}H NMR spectrum of compound **2e** in DMSO-d_6 at 25 °C.

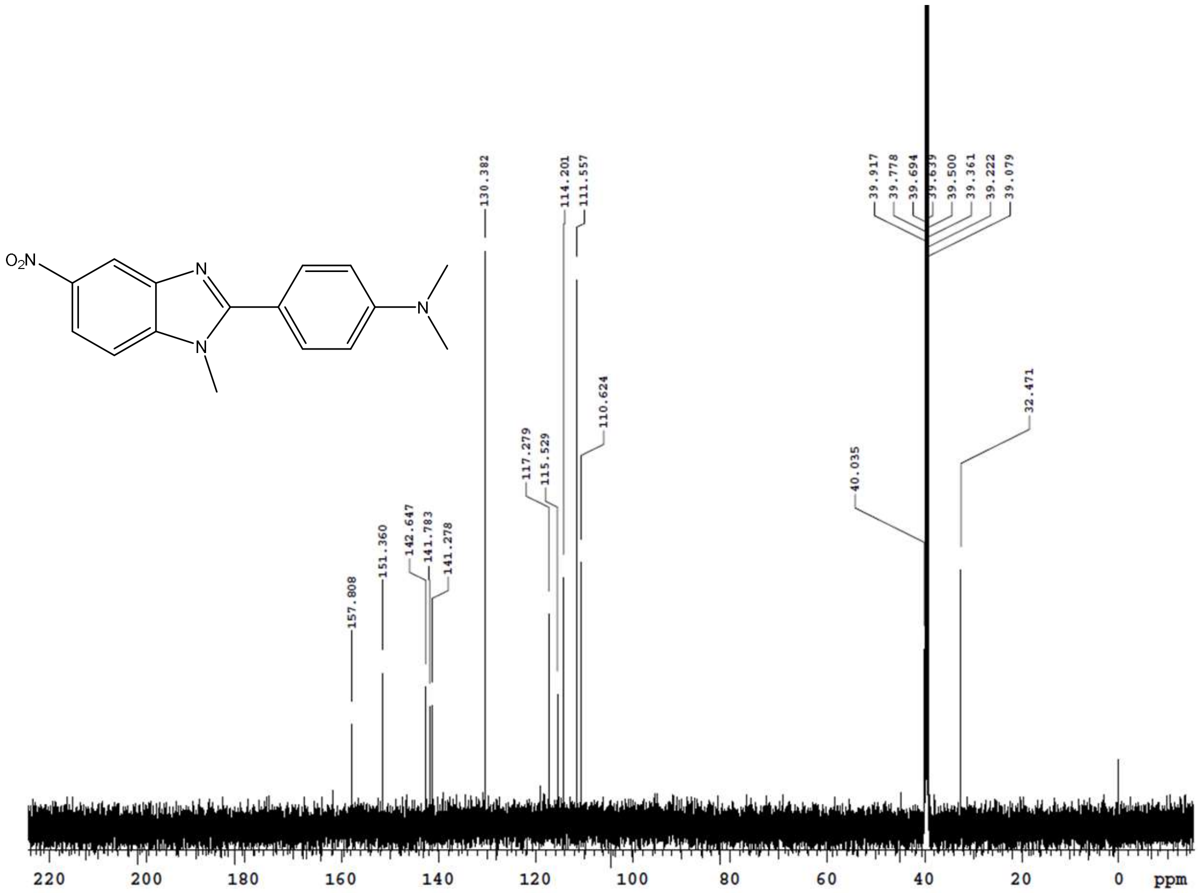


Figure S28. ^{13}C NMR spectrum of compound **2e** in DMSO-d_6 at 25 °C.

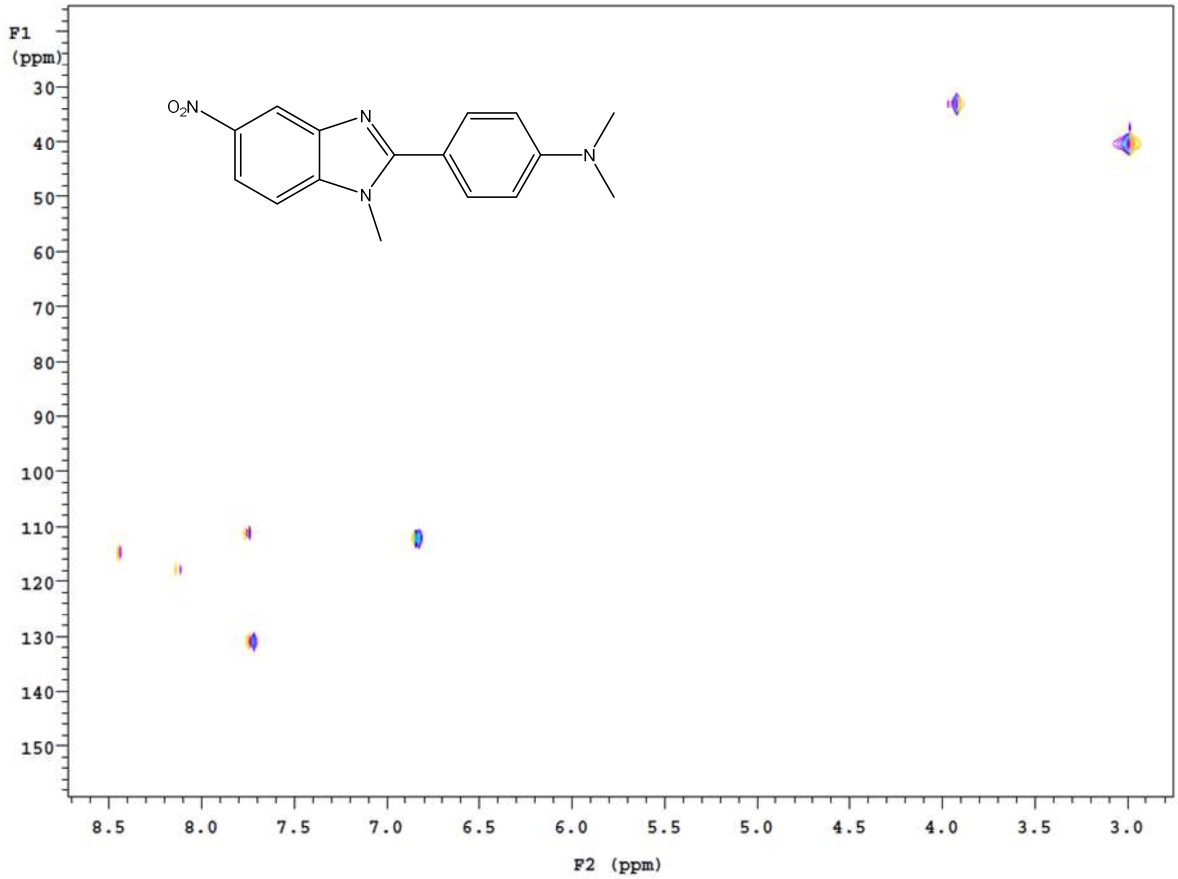


Figure S29. HSQC spectrum of compound **2e** in DMSO-d_6 at 25 °C.

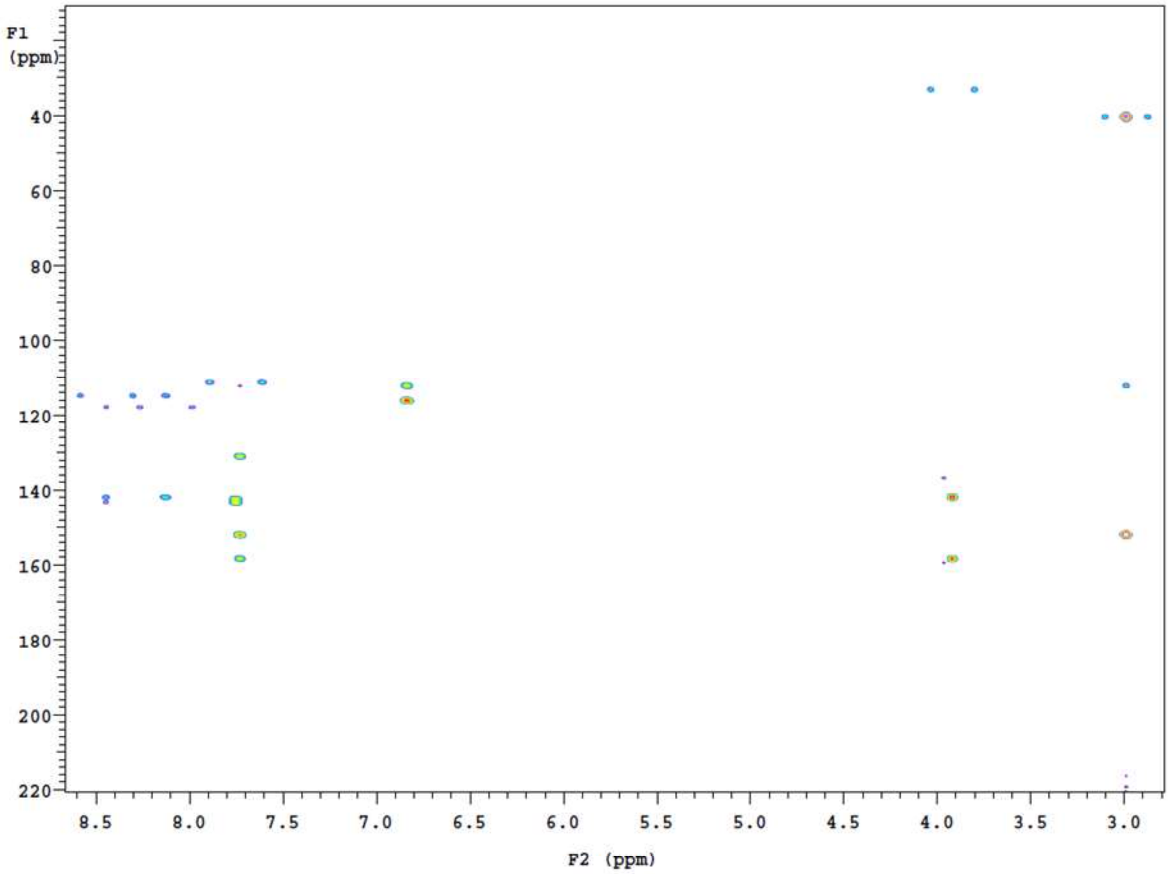


Figure S30. HMBC spectrum of compound **2e** in DMSO-d_6 at 25 °C.

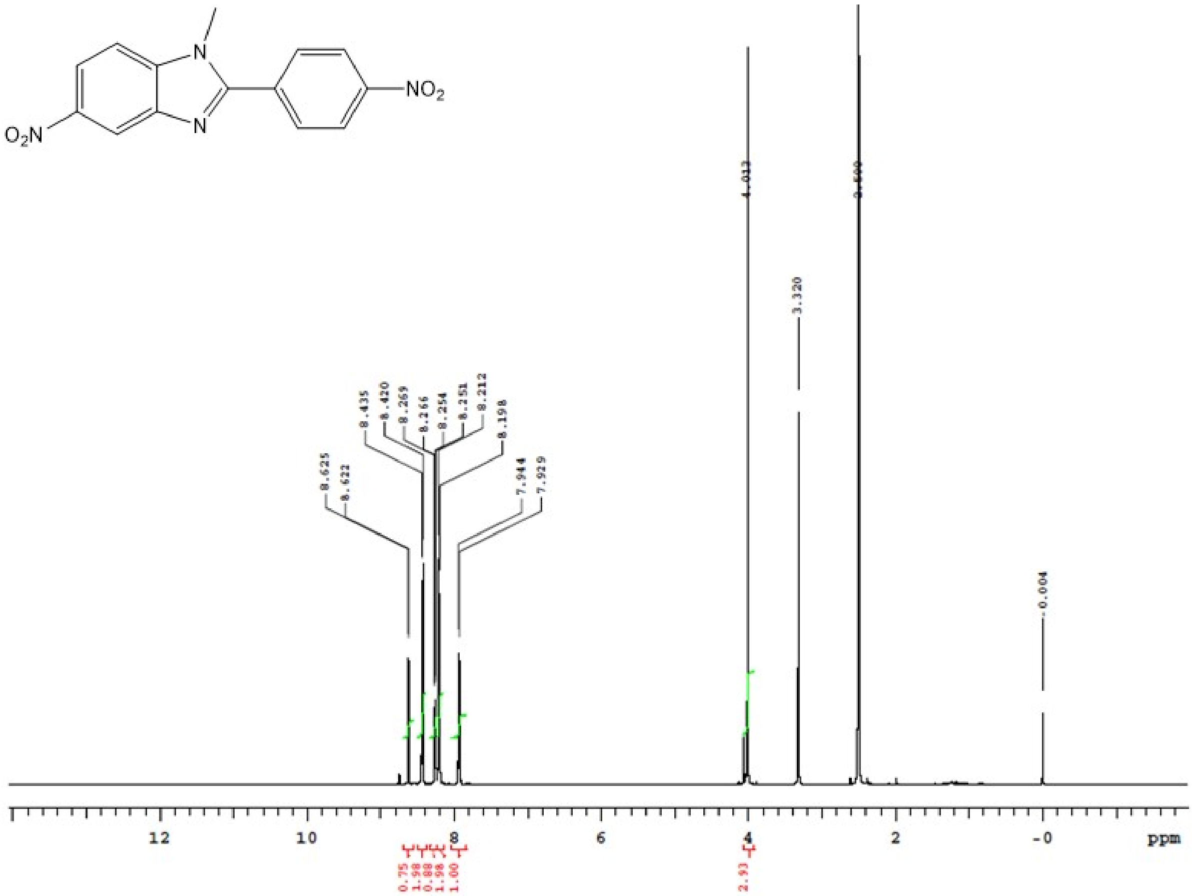


Figure S31. ^{1}H NMR spectrum of compound **2f** in DMSO-d_6 at 25 °C.

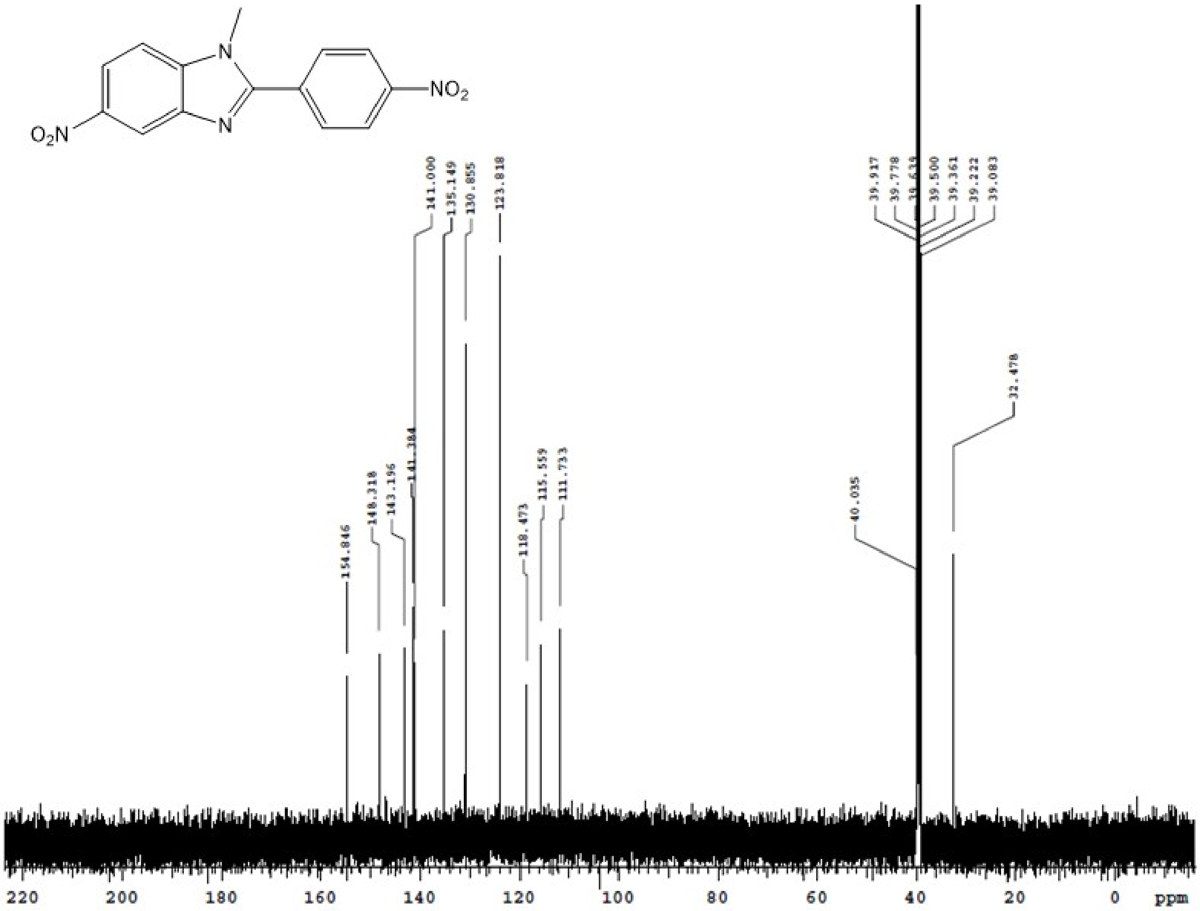


Figure S32. ^{13}C NMR spectrum of compound **2f** in DMSO-d_6 at 25 °C.

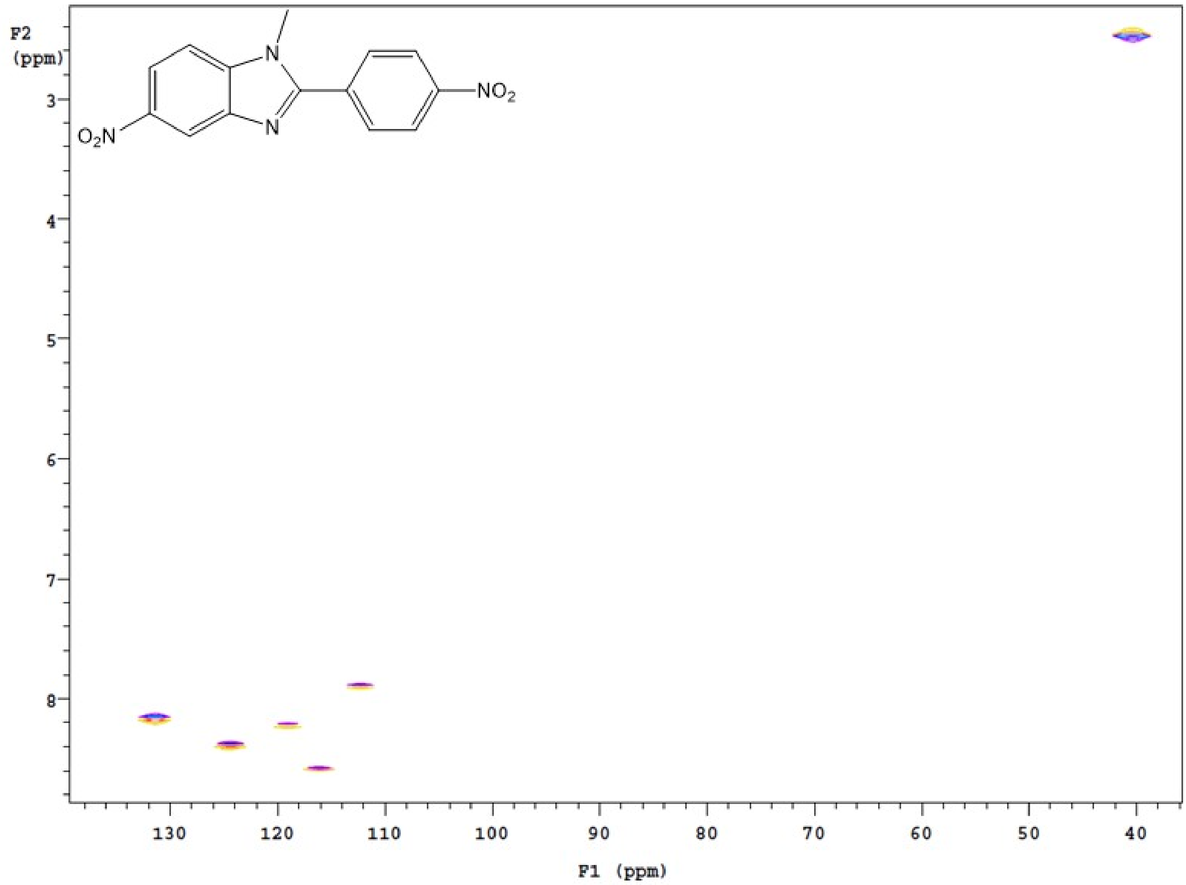


Figure S33. HSQC spectrum of compound **2f** in DMSO-d_6 at 25 °C.

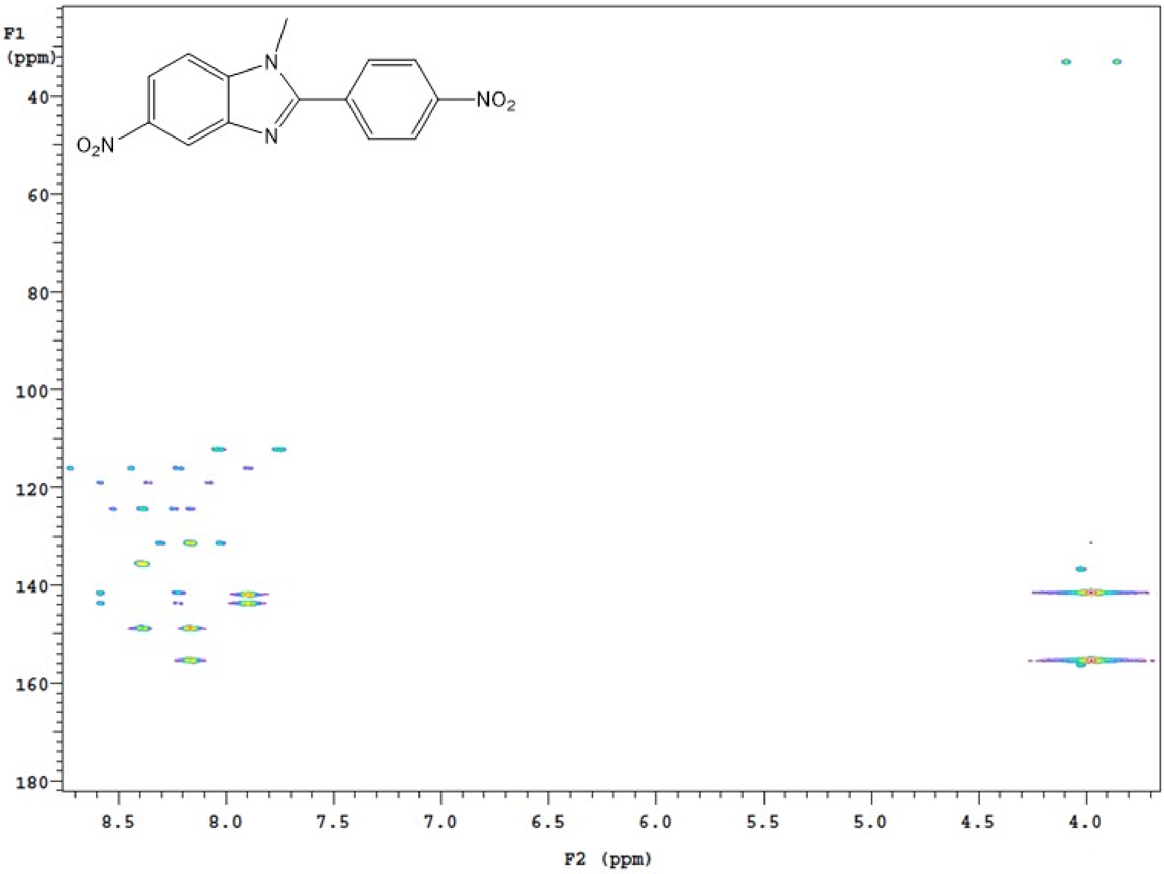


Figure S34. HMBC spectrum of compound **2f** in DMSO-d_6 at 25 °C.

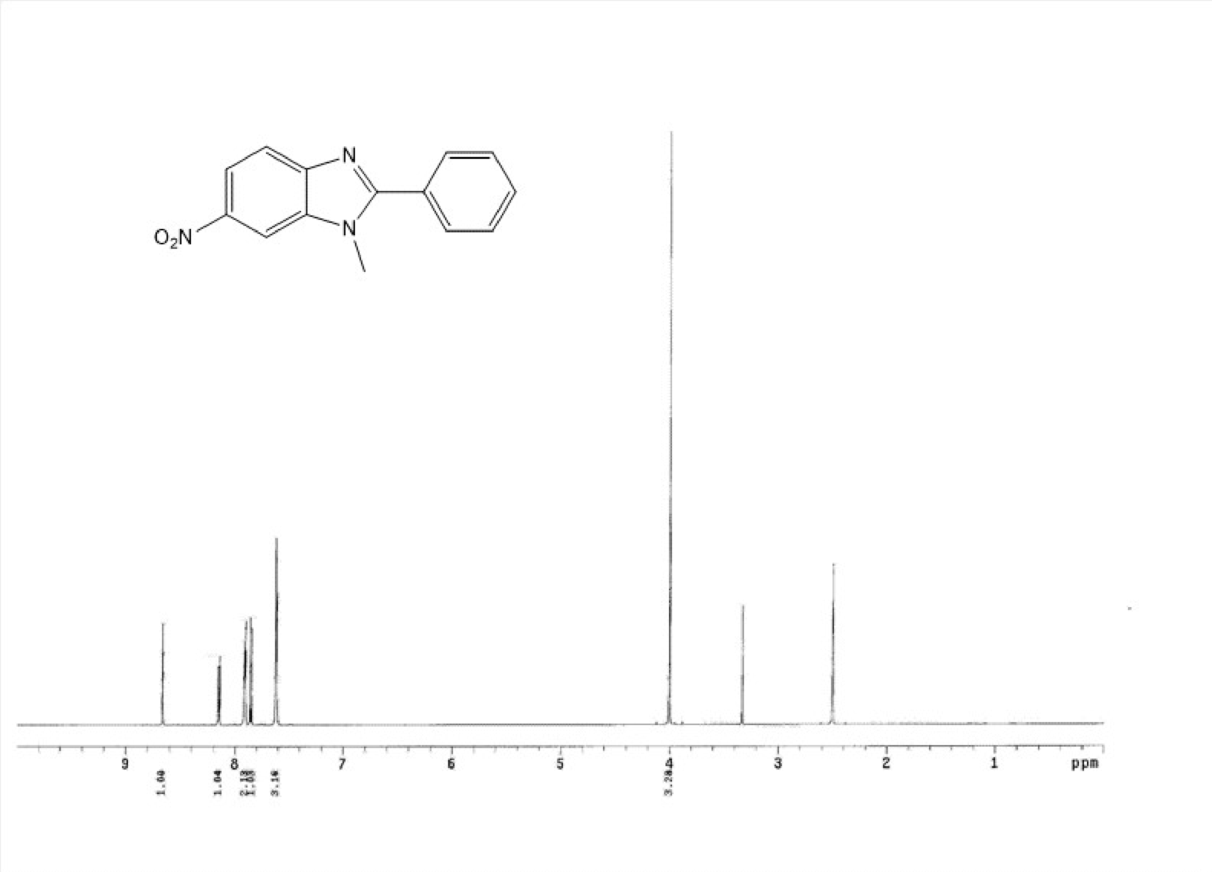


Figure S35. ^{1}H NMR spectrum of compound **3a** in DMSO-d$_6$ at 25 °C.

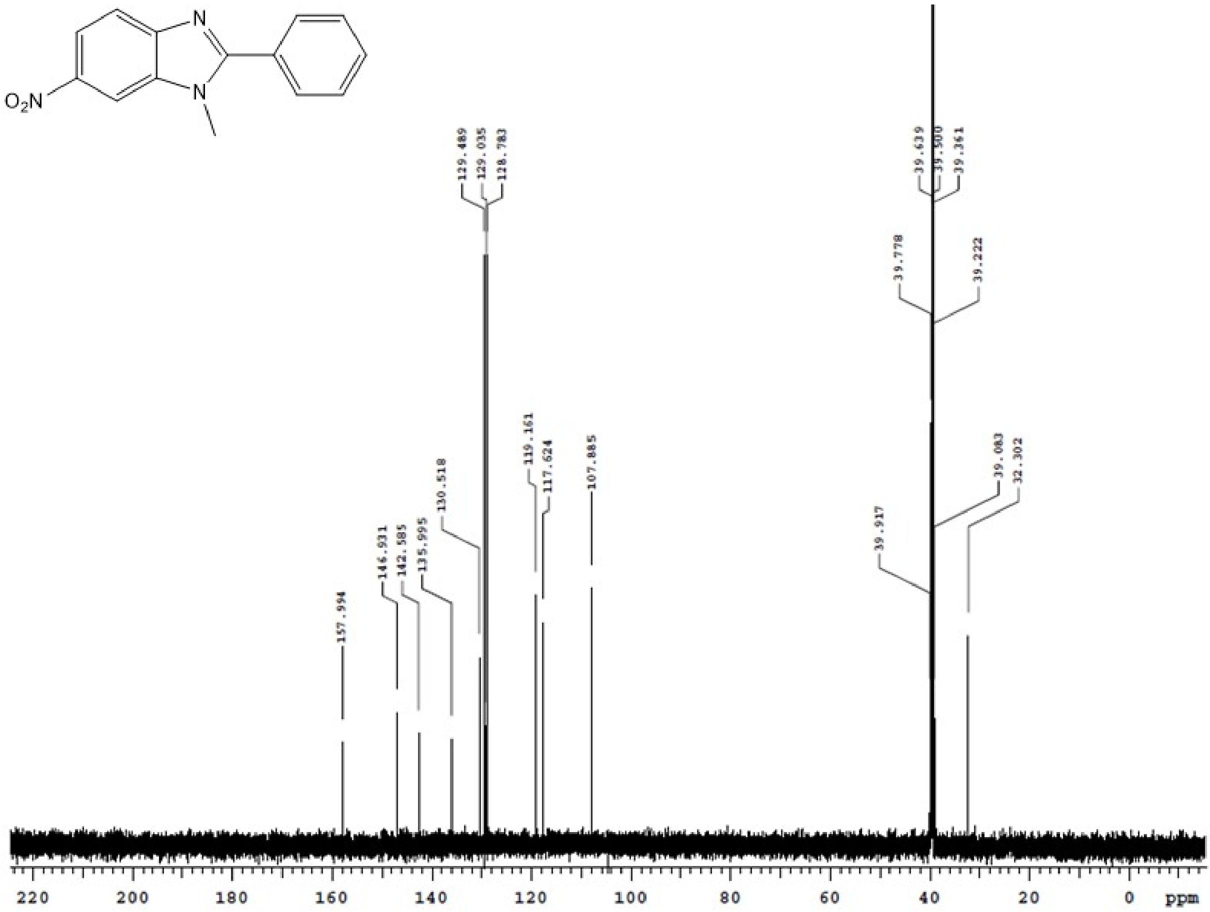


Figure S36. ^{13}C NMR spectrum of compound **3a** in DMSO-d_6 at 25 °C.

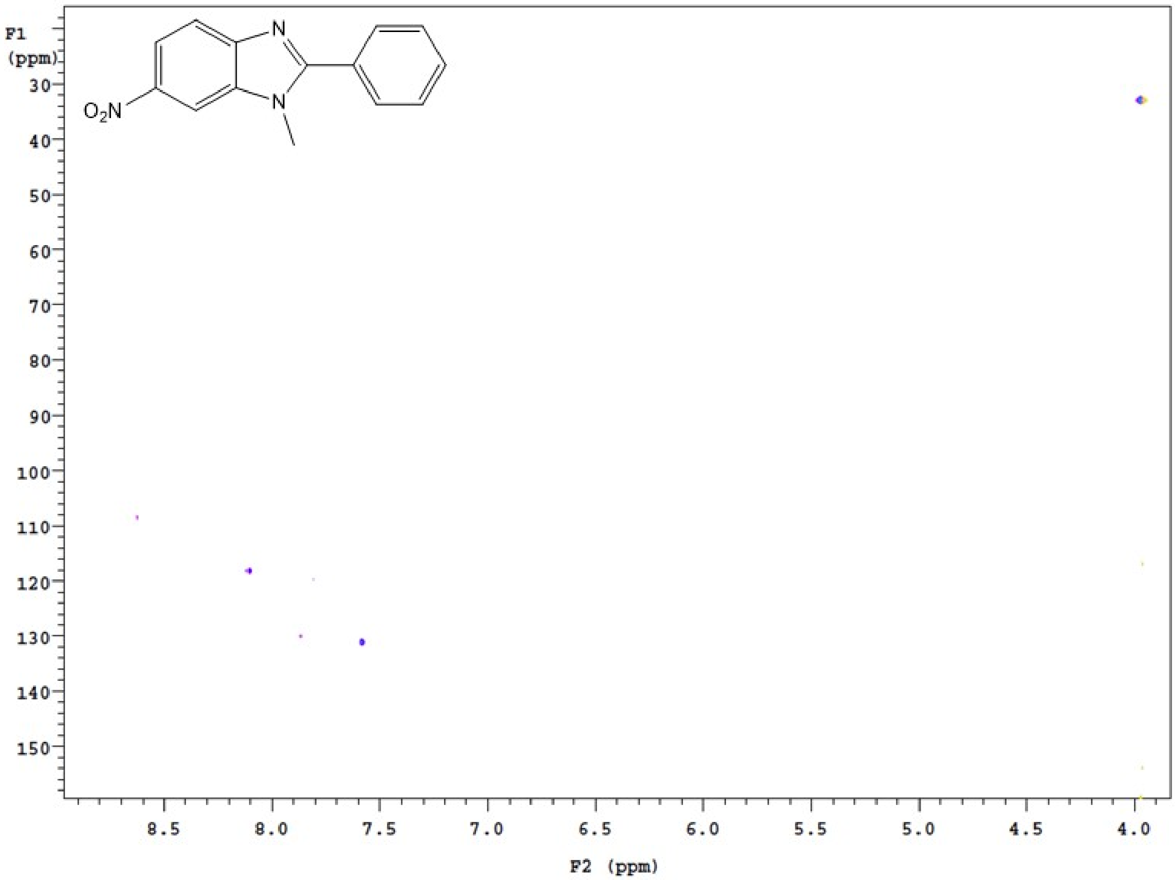


Figure S37. HSQC spectrum of compound **3a** in DMSO-d$_6$ at 25 °C.

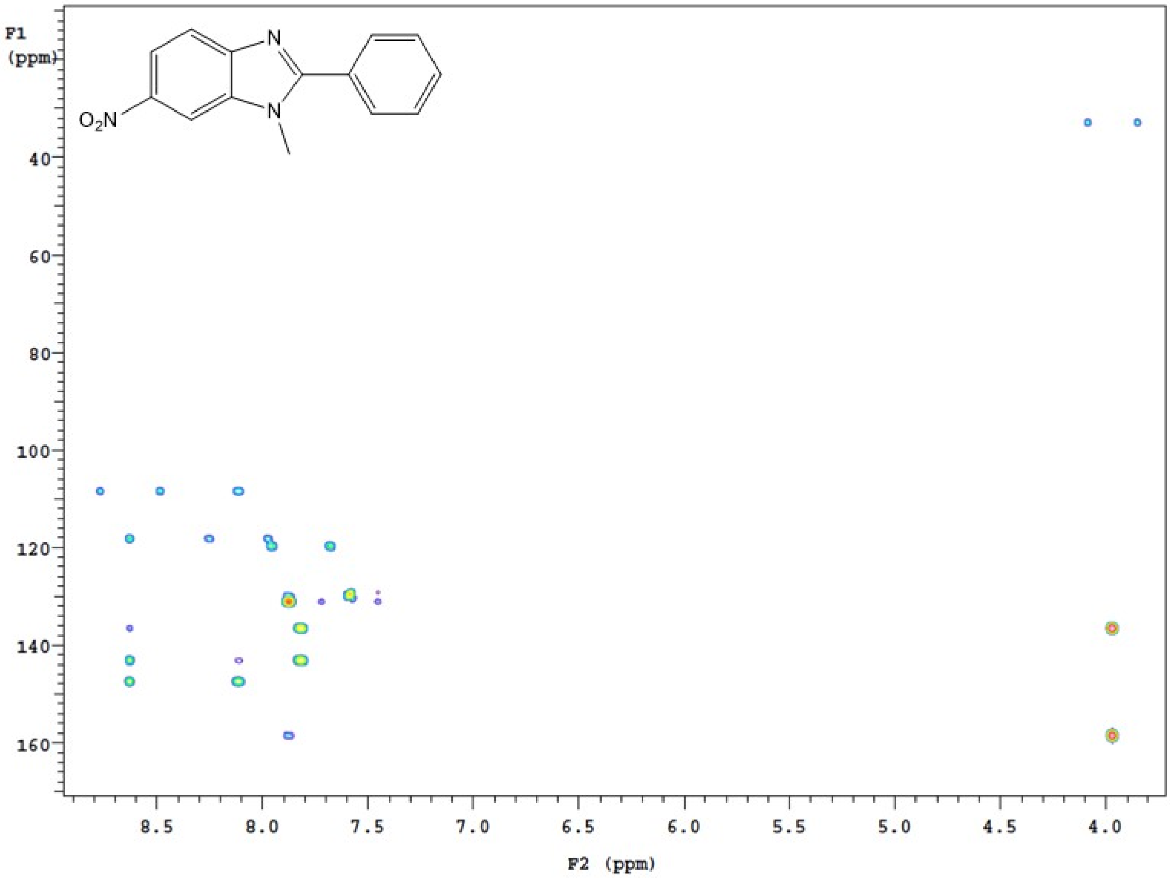


Figure S38. HMBC spectrum of compound **3a** in DMSO-d_6 at 25 °C.

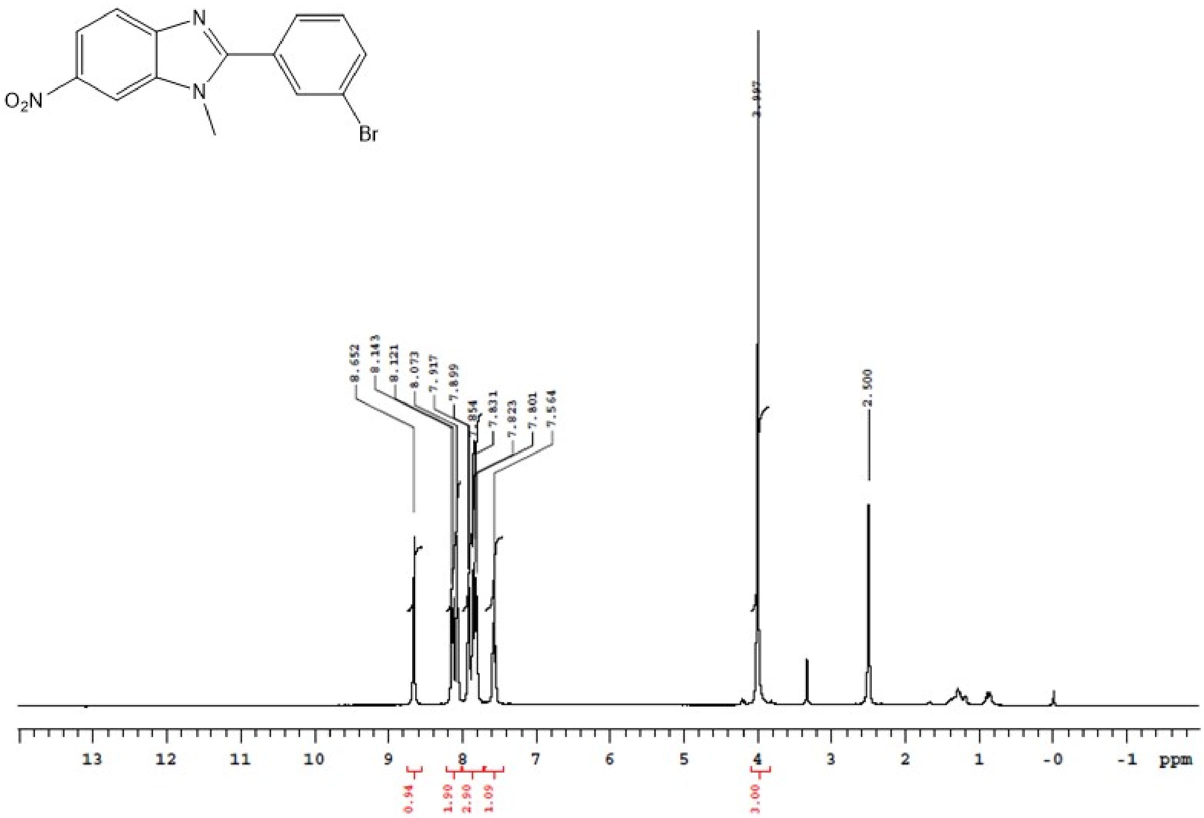


Figure S39. ^{1}H NMR spectrum of compound **3b** in DMSO-d_6 at 25 °C.

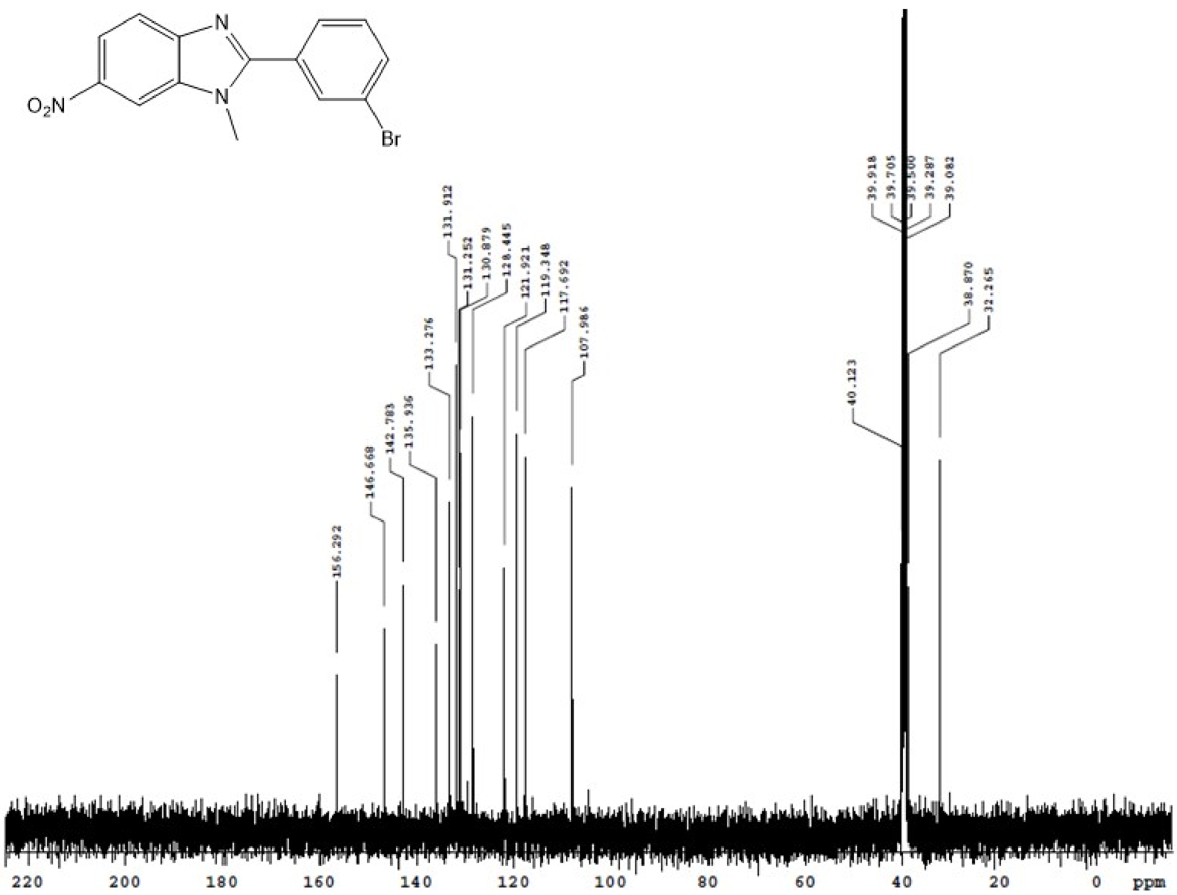


Figure S40. ^{13}C NMR spectrum of compound **3b** in DMSO-d_6 at 25 °C.

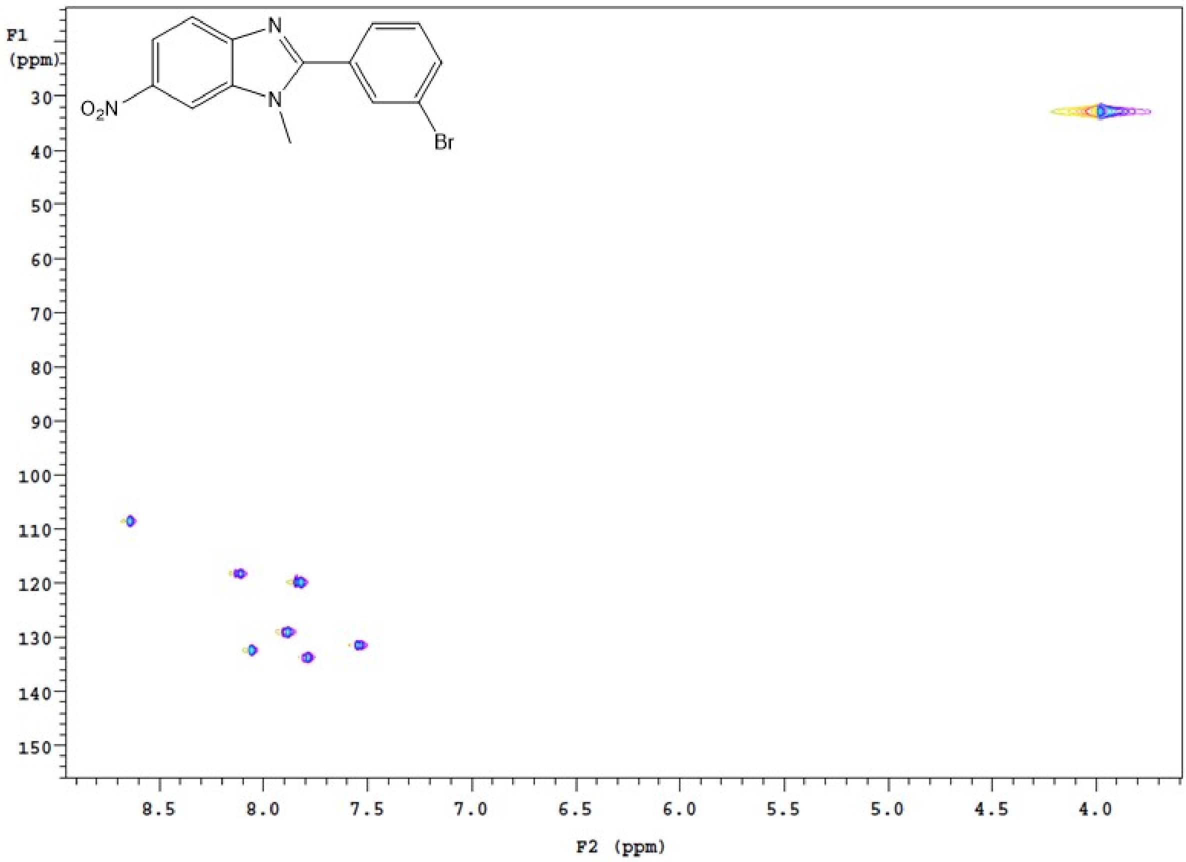


Figure S41. HSQC spectrum of compound **3b** in DMSO-d_6 at 25 °C.

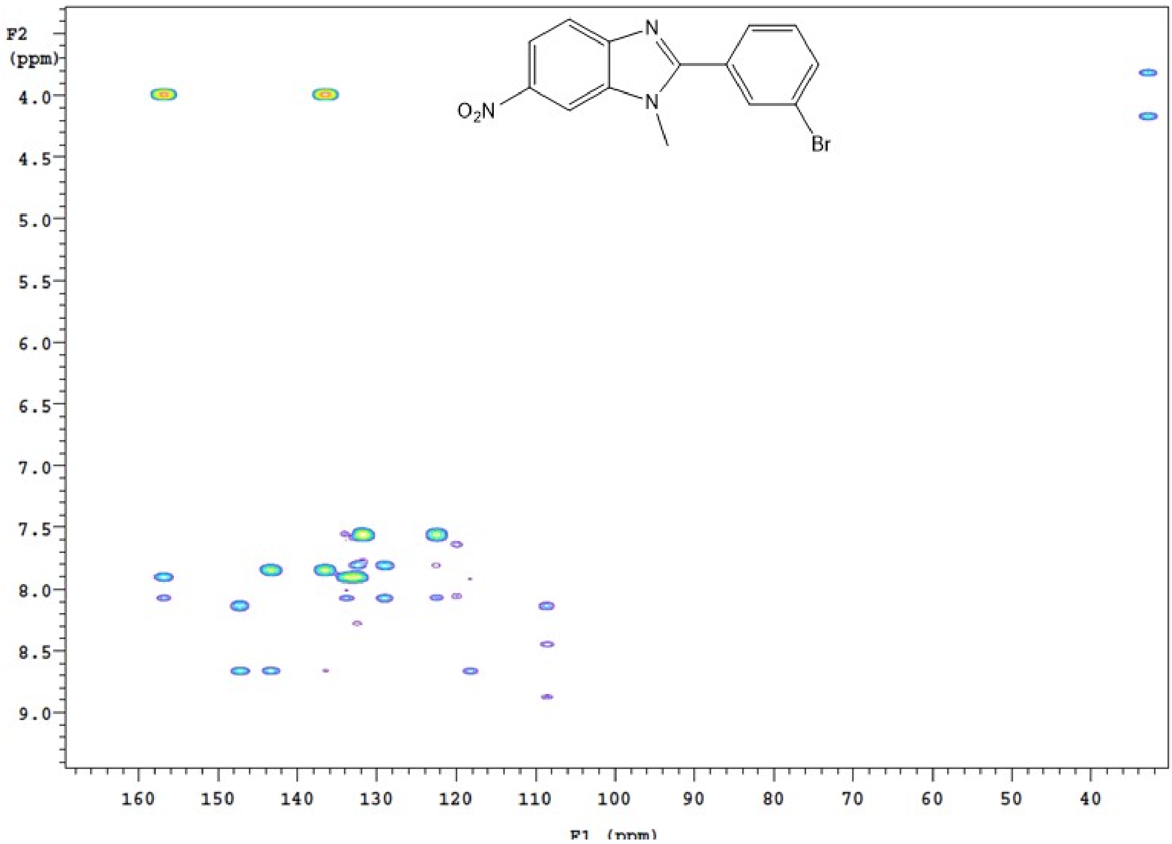


Figure S42. HMBC spectrum of compound **3b** in DMSO-d_6 at 25 °C.

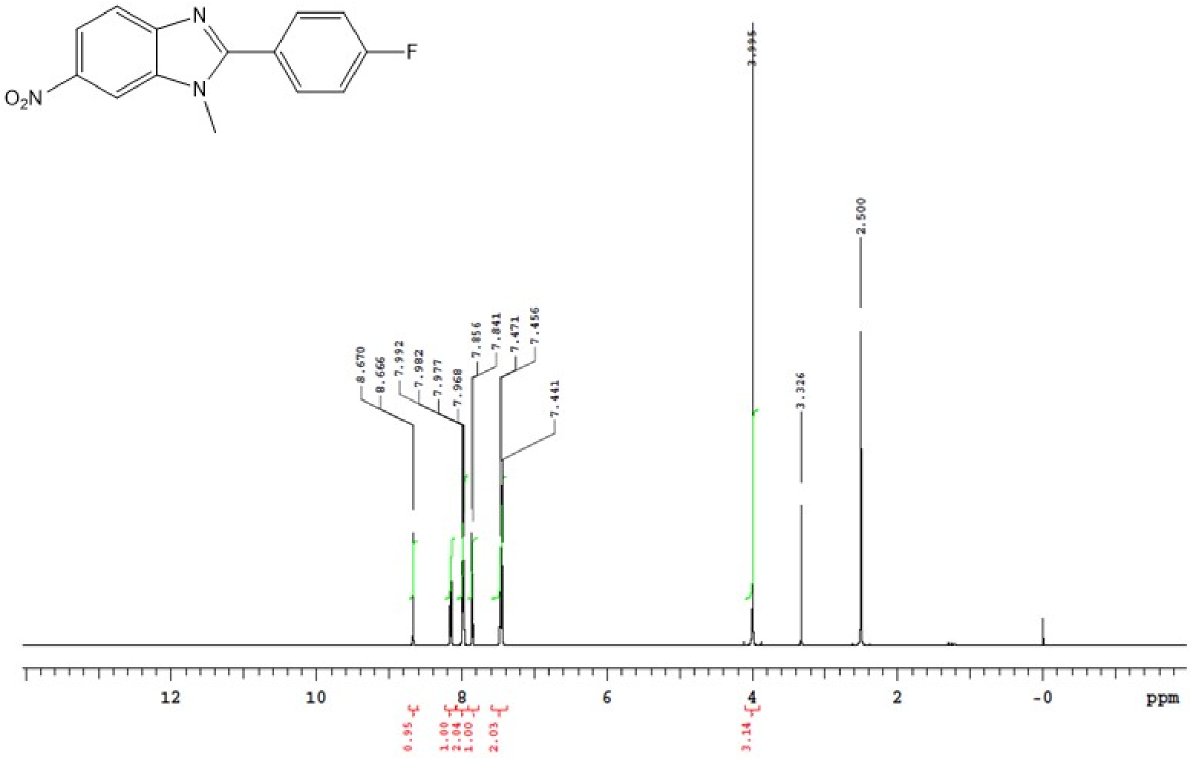


Figure S43. ^{1}H NMR spectrum of compound **3c** in DMSO-d_6 at 25 °C.

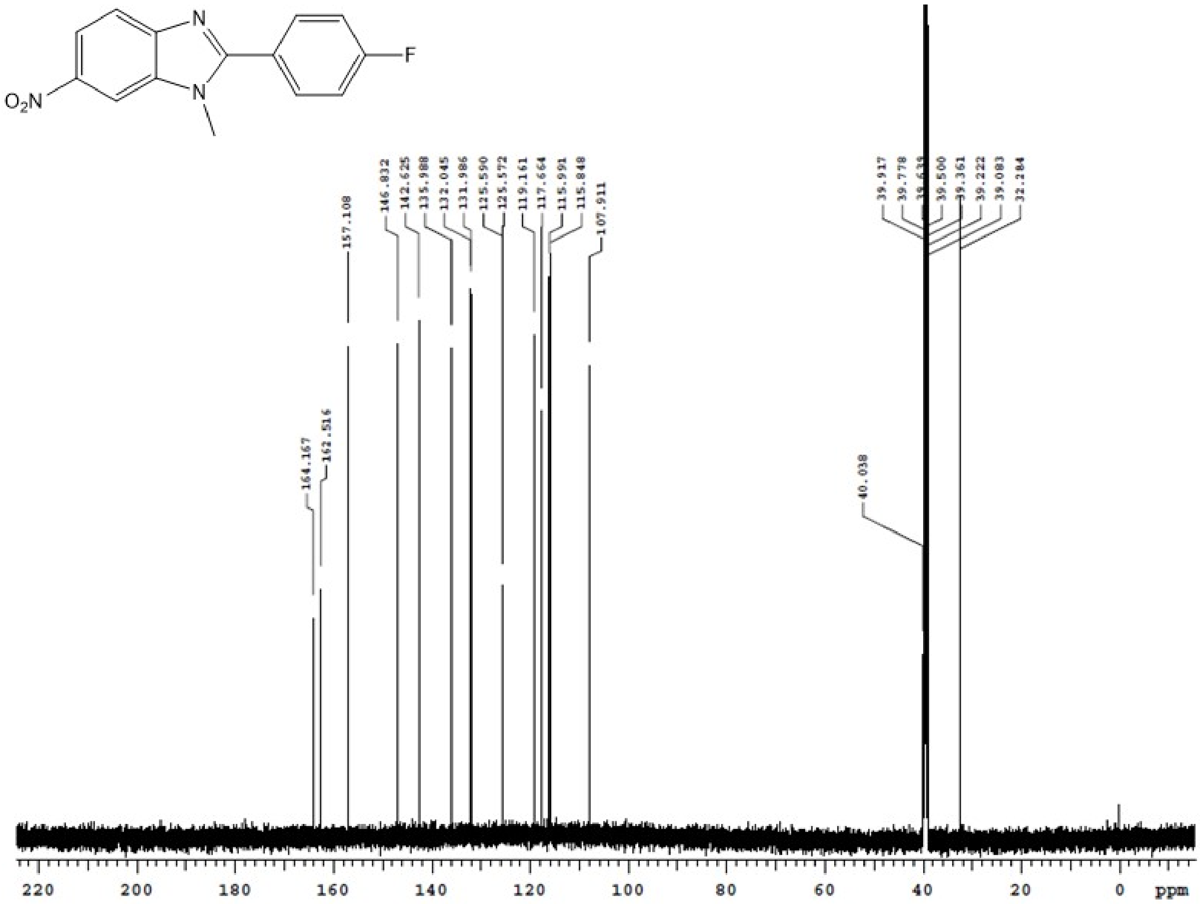


Figure S44. ^{13}C NMR spectrum of compound **3c** in DMSO-d_6 at 25 °C.

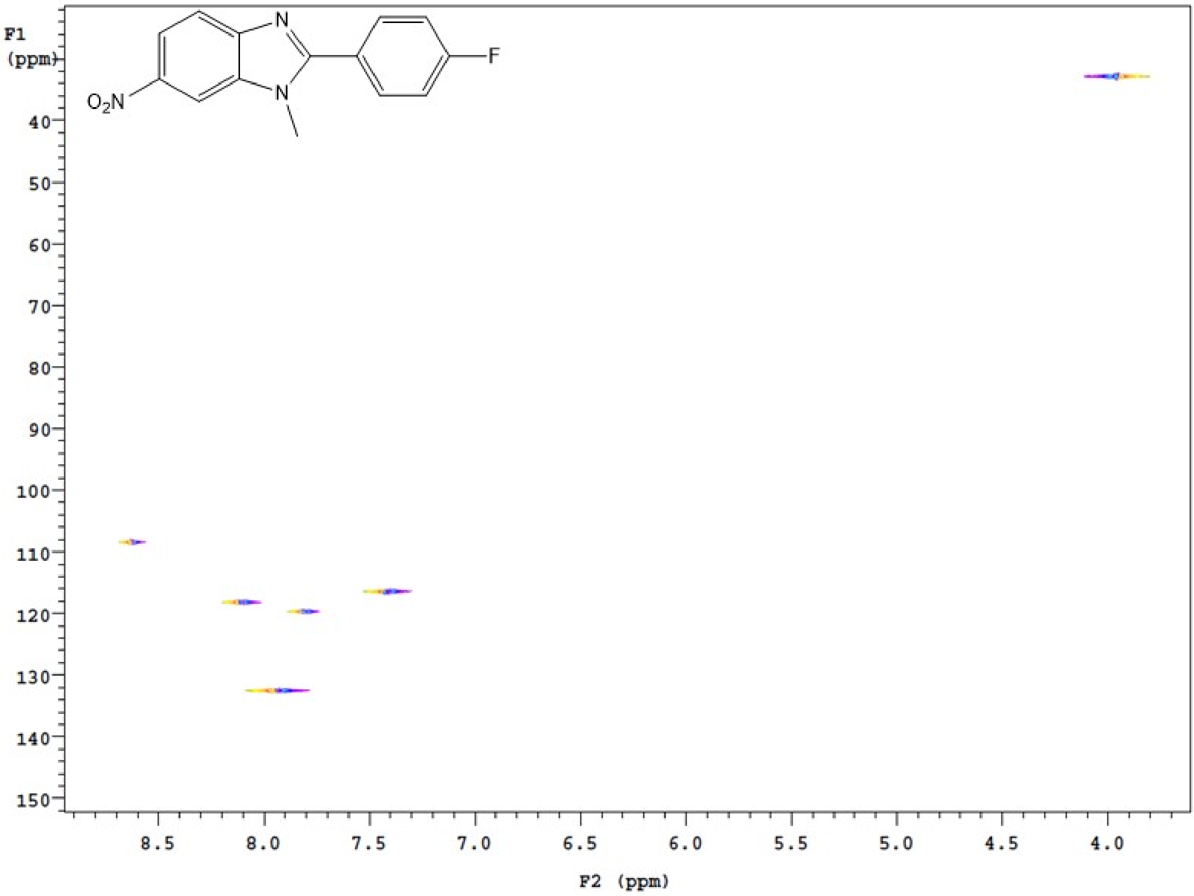


Figure S45. HSQC spectrum of compound **3c** in DMSO-d_6 at 25 °C.

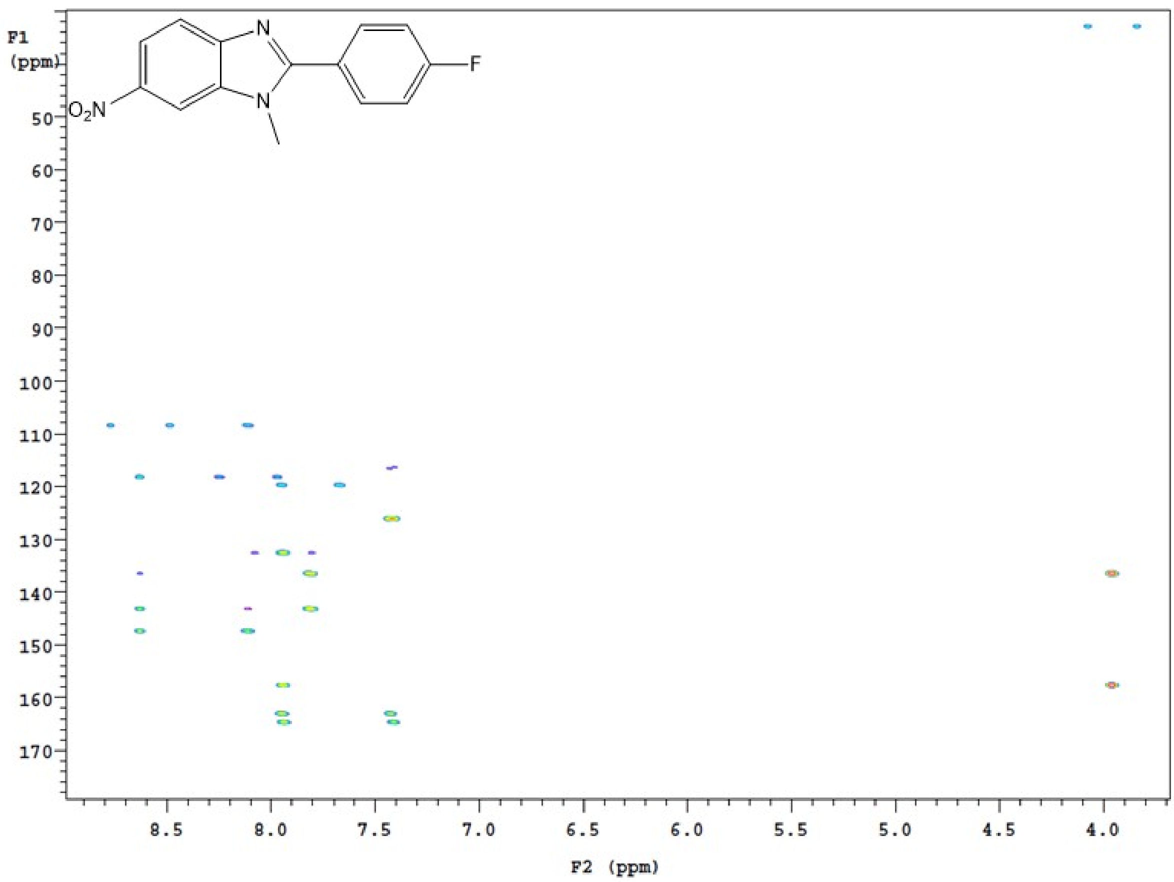


Figure S46. HMBC spectrum of compound **3c** in DMSO-d$_6$ at 25 °C.

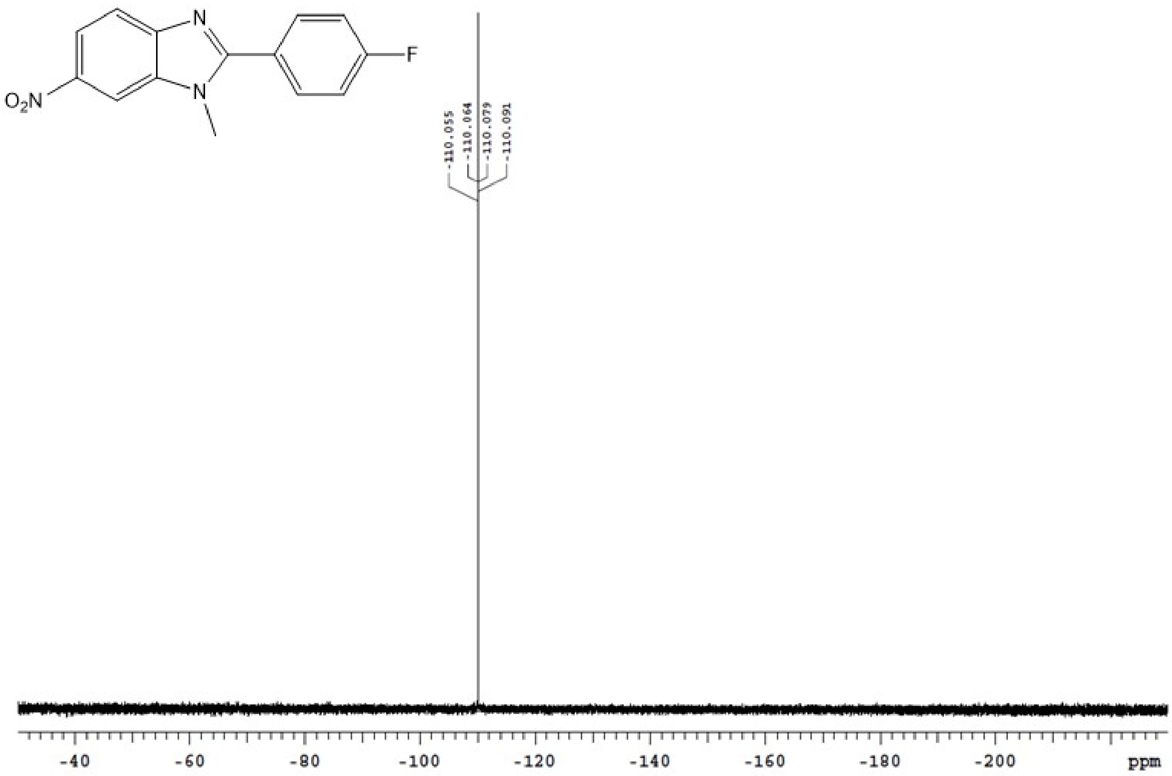


Figure S47. ^{19}F NMR spectrum of compound **3c** in DMSO-d_6 at 25 °C.

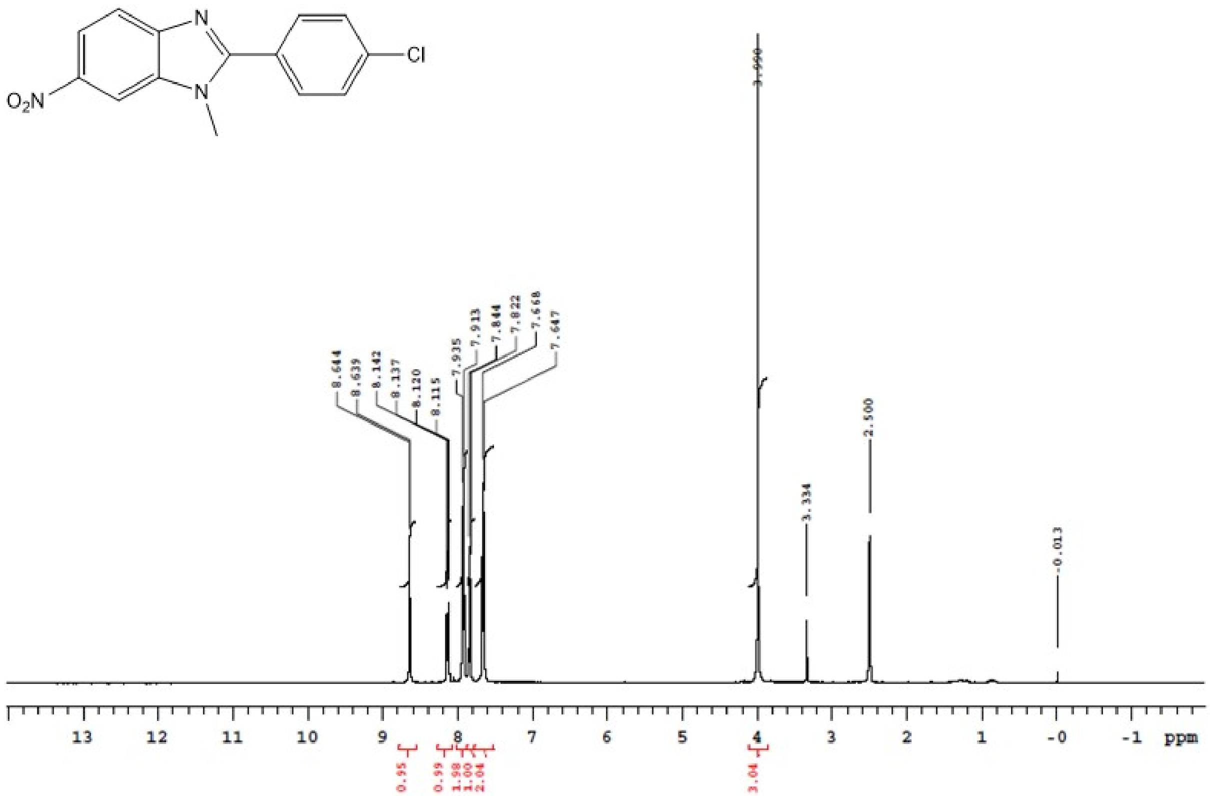


Figure S48. ^{1}H NMR spectrum of compound **3d** in DMSO-d$_6$ at 25 °C.

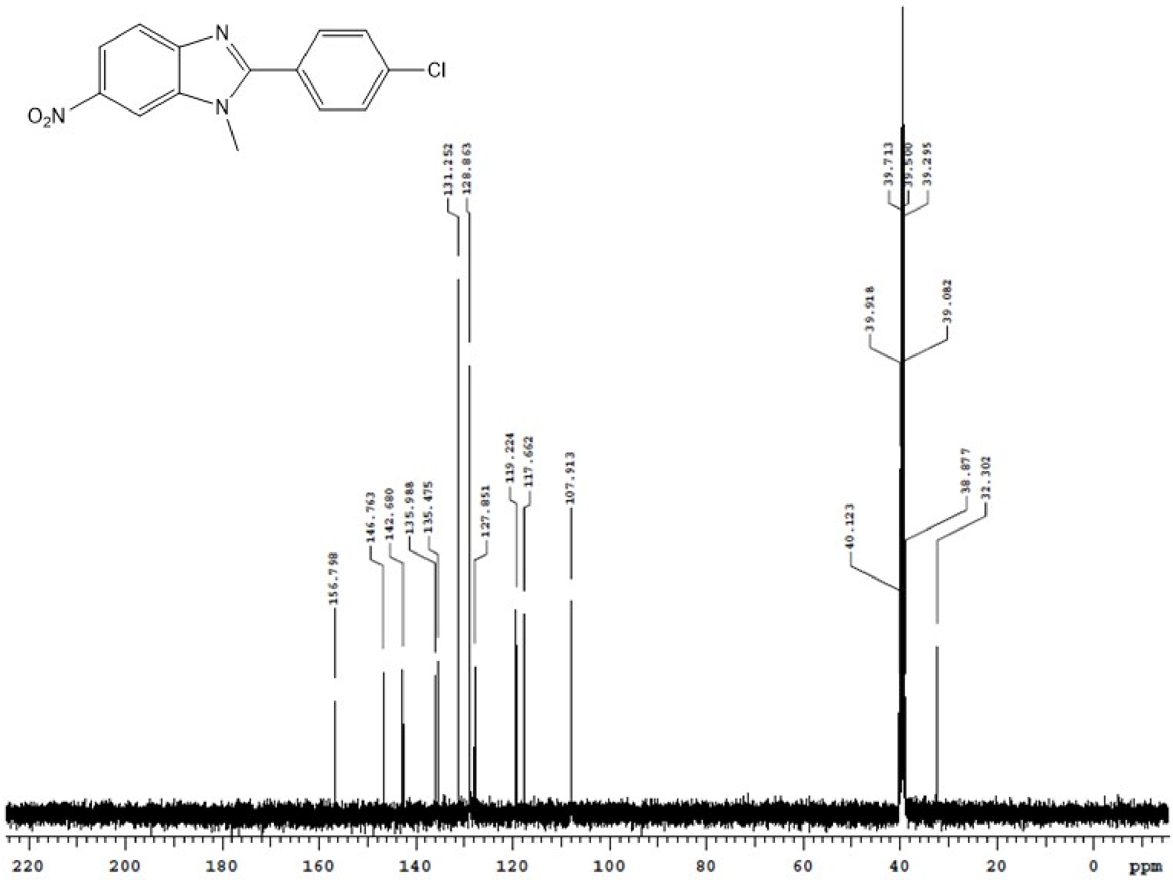


Figure S49. ^{13}C NMR spectrum of compound **3d** in DMSO-d_6 at 25 °C.

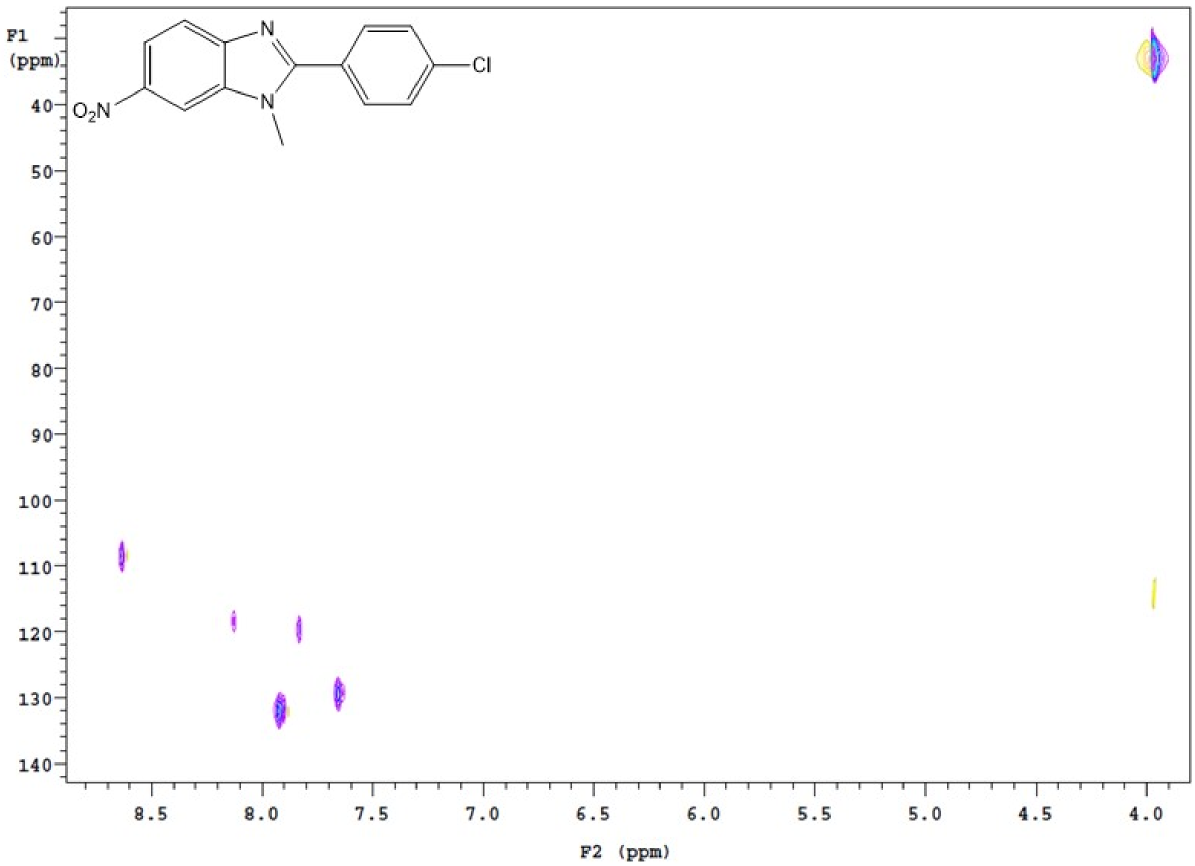


Figure S50. HSQC spectrum of compound **3d** in DMSO-d_6 at 25 °C.

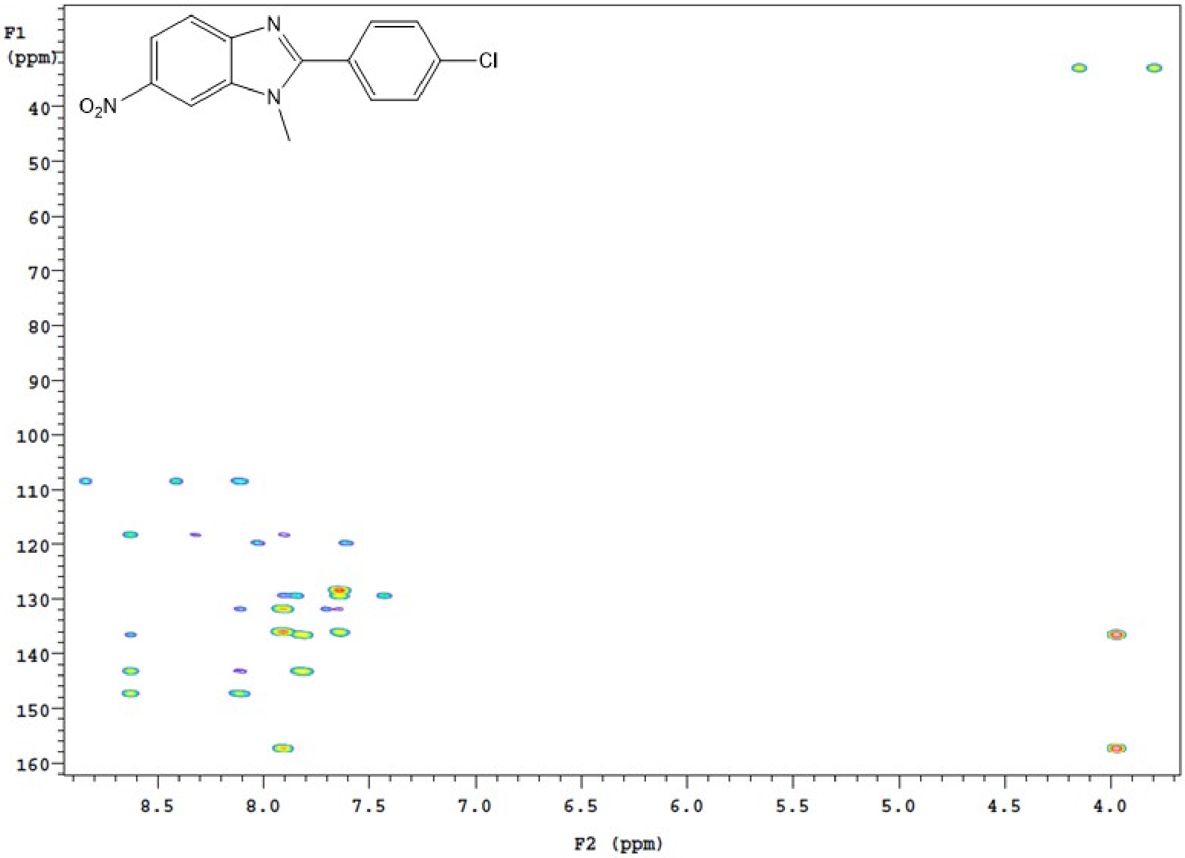


Figure S51. HMBC spectrum of compound **3d** in DMSO-d_6 at 25 °C.

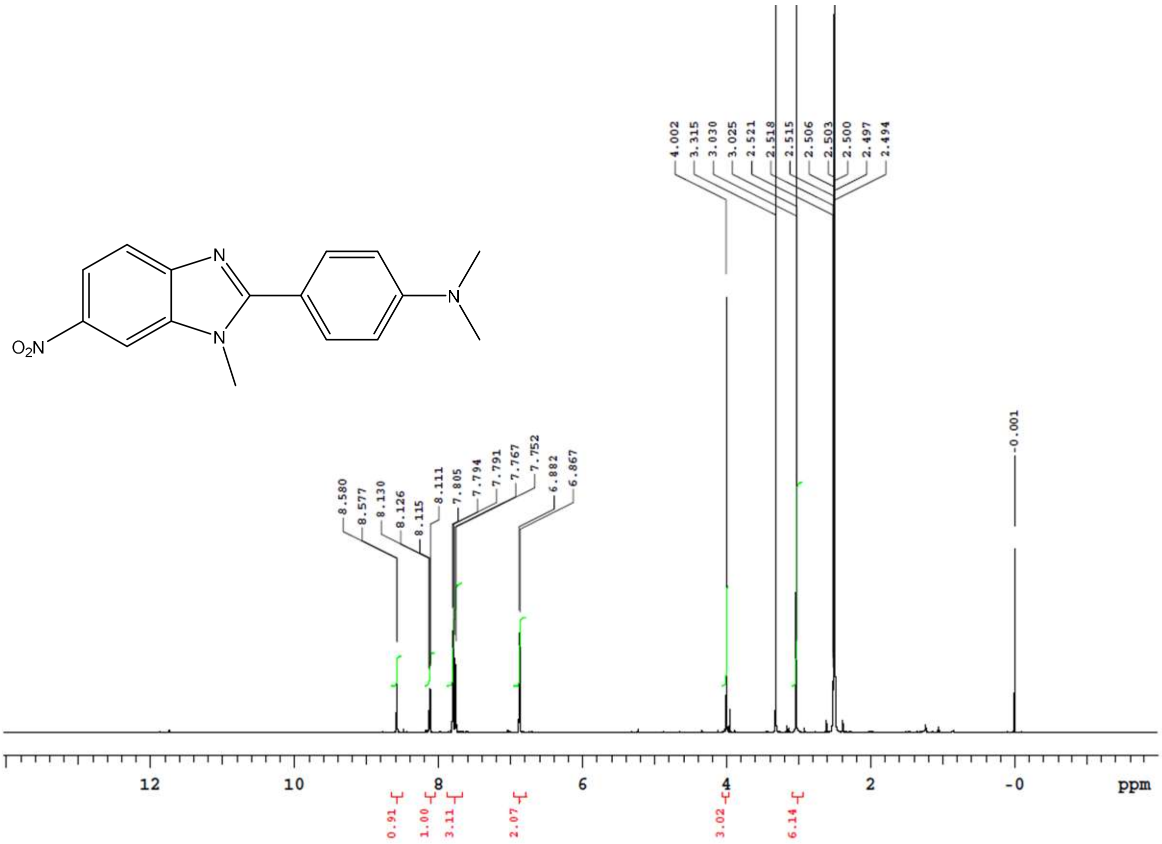


Figure S52. [1]H NMR spectrum of compound **3e** in DMSO-d$_6$ at 25 °C.

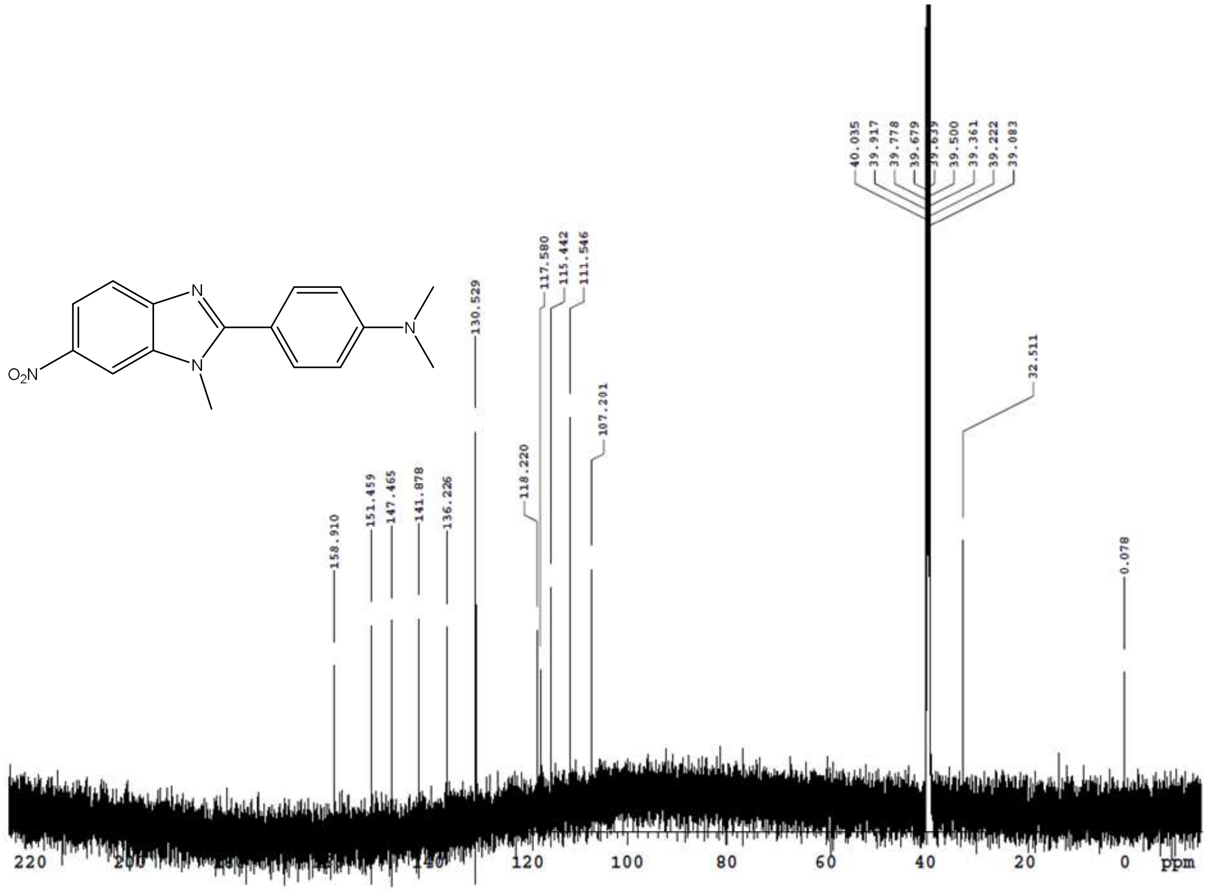


Figure S53. ^{13}C NMR spectrum of compound **3e** in DMSO-d_6 at 25 °C.

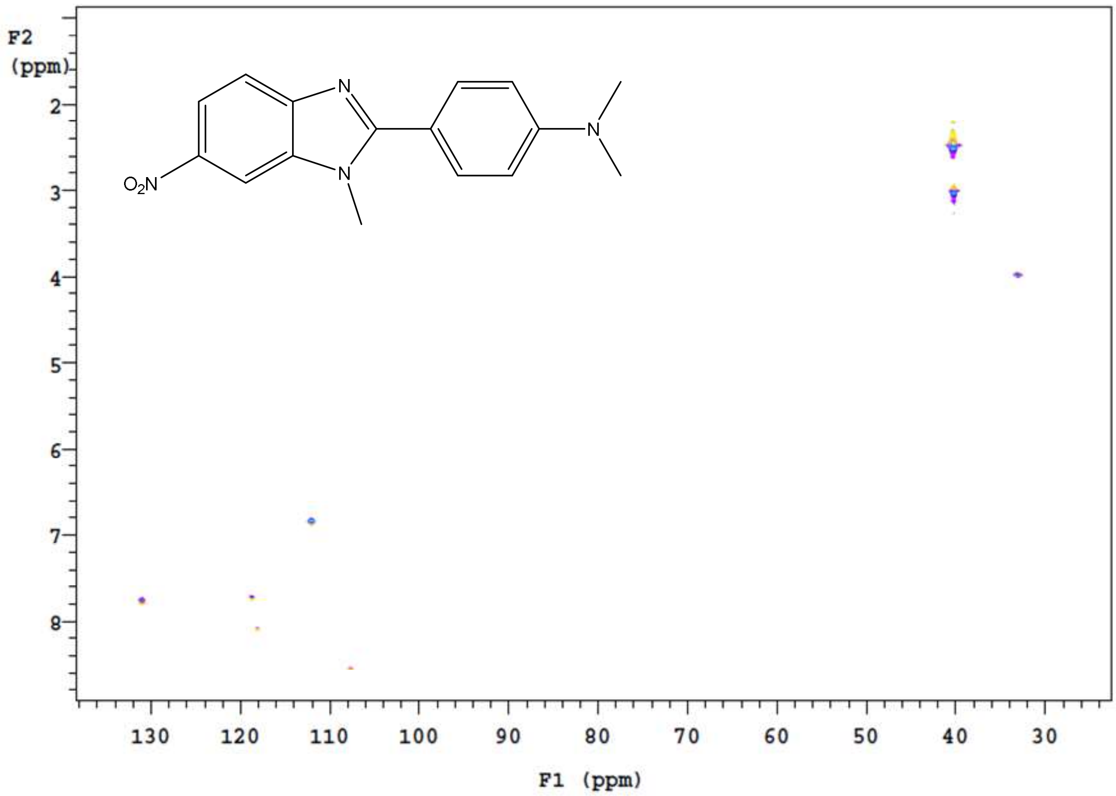


Figure S54. HSQC spectrum of compound **3e** in DMSO-d_6 at 25 °C.

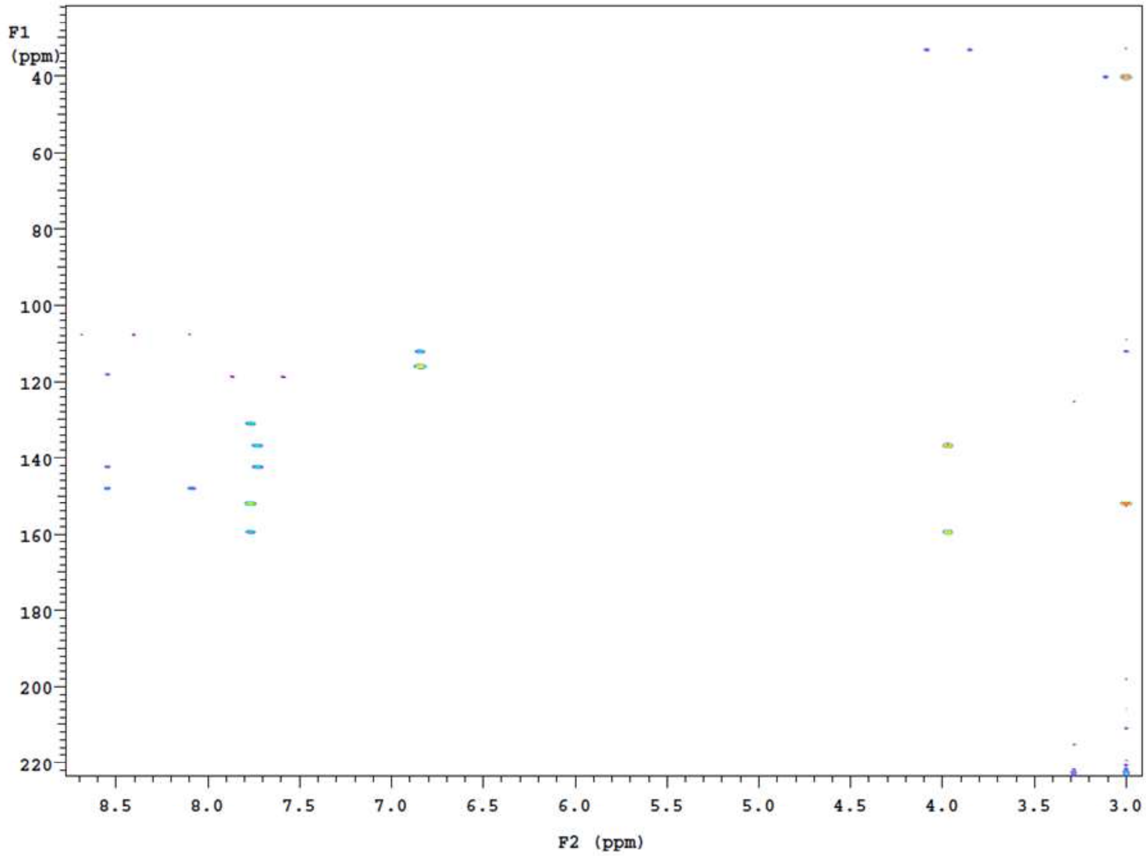


Figure S55. HMBC spectrum of compound **3e** in DMSO-d_6 at 25 °C.

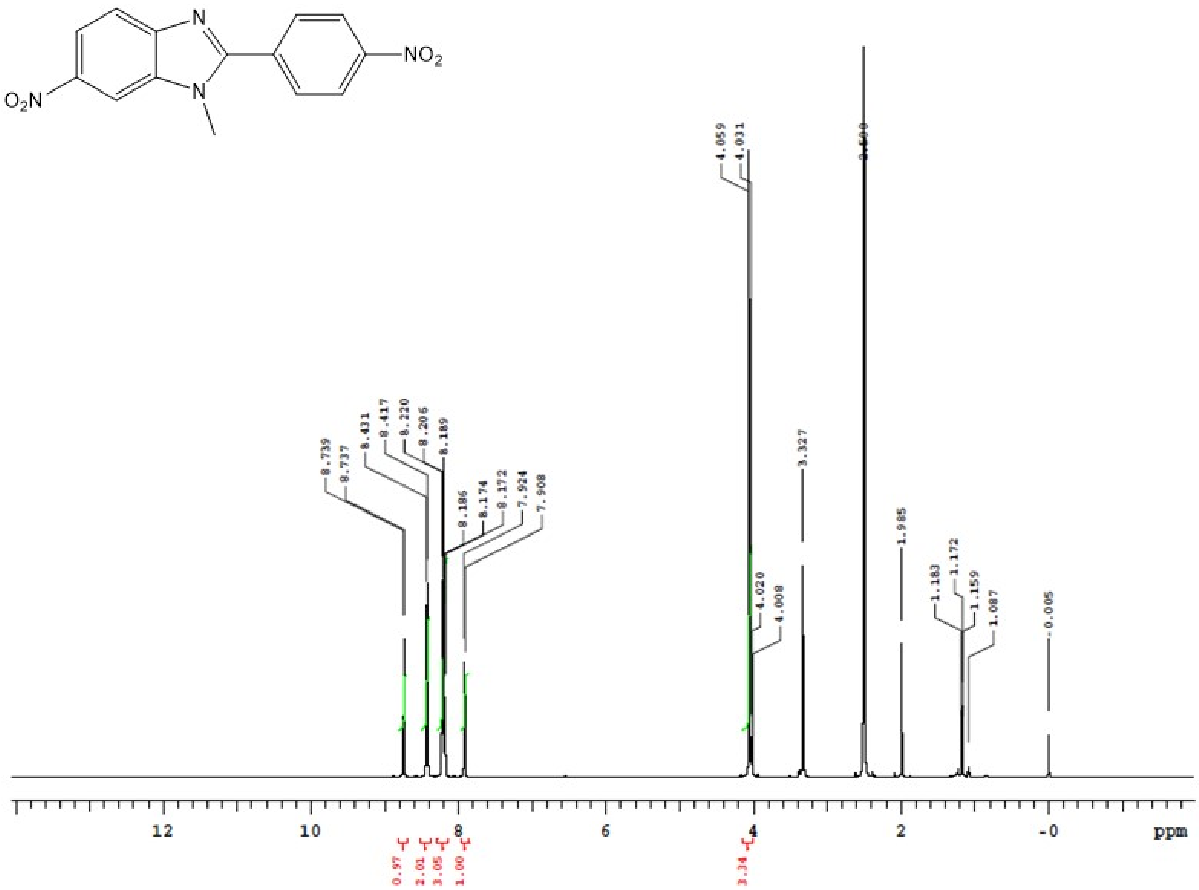


Figure S56. ^{1}H NMR spectrum of compound **3f** in DMSO-d_6 at 25 °C.

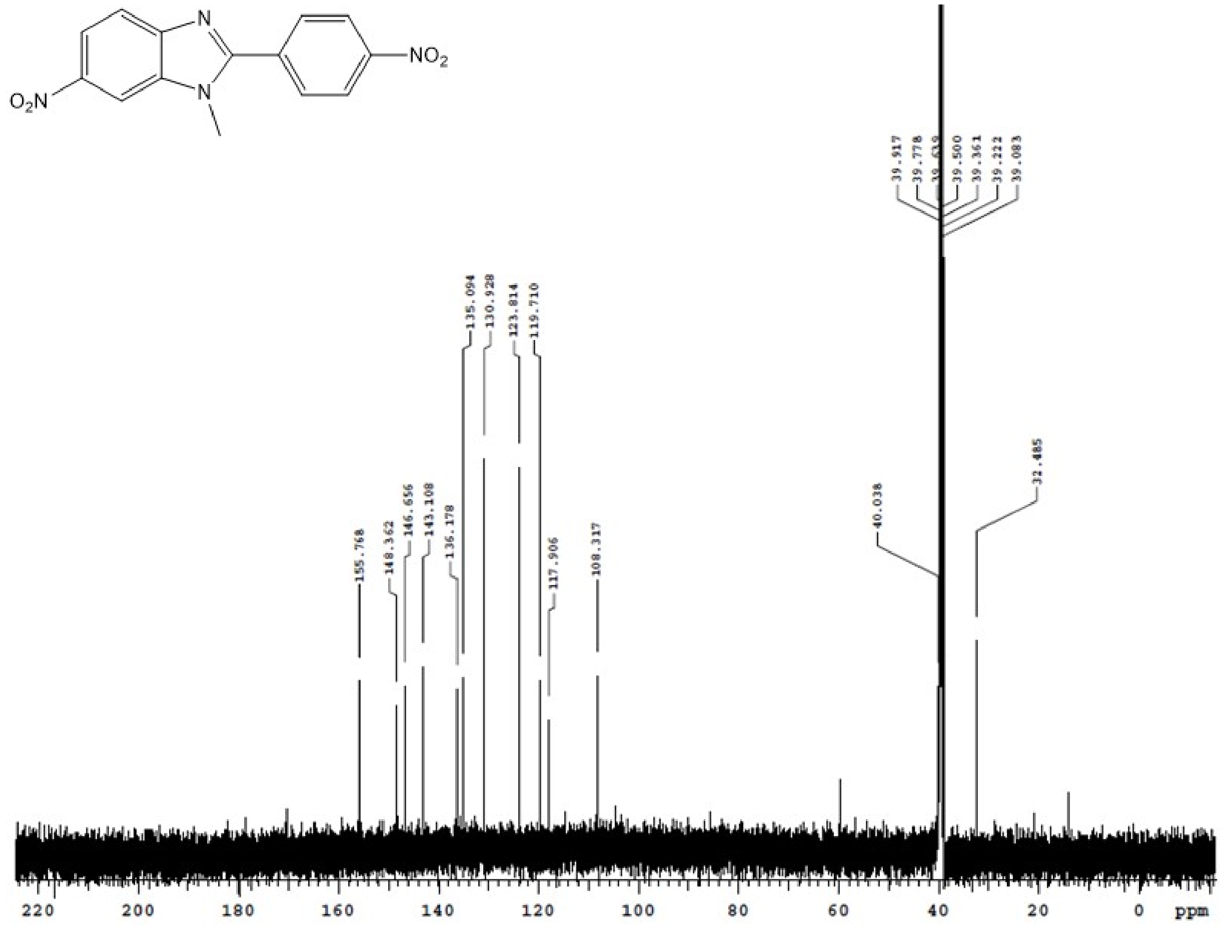


Figure S57. ^{13}C NMR spectrum of compound **3f** in DMSO-d_6 at 25 °C.

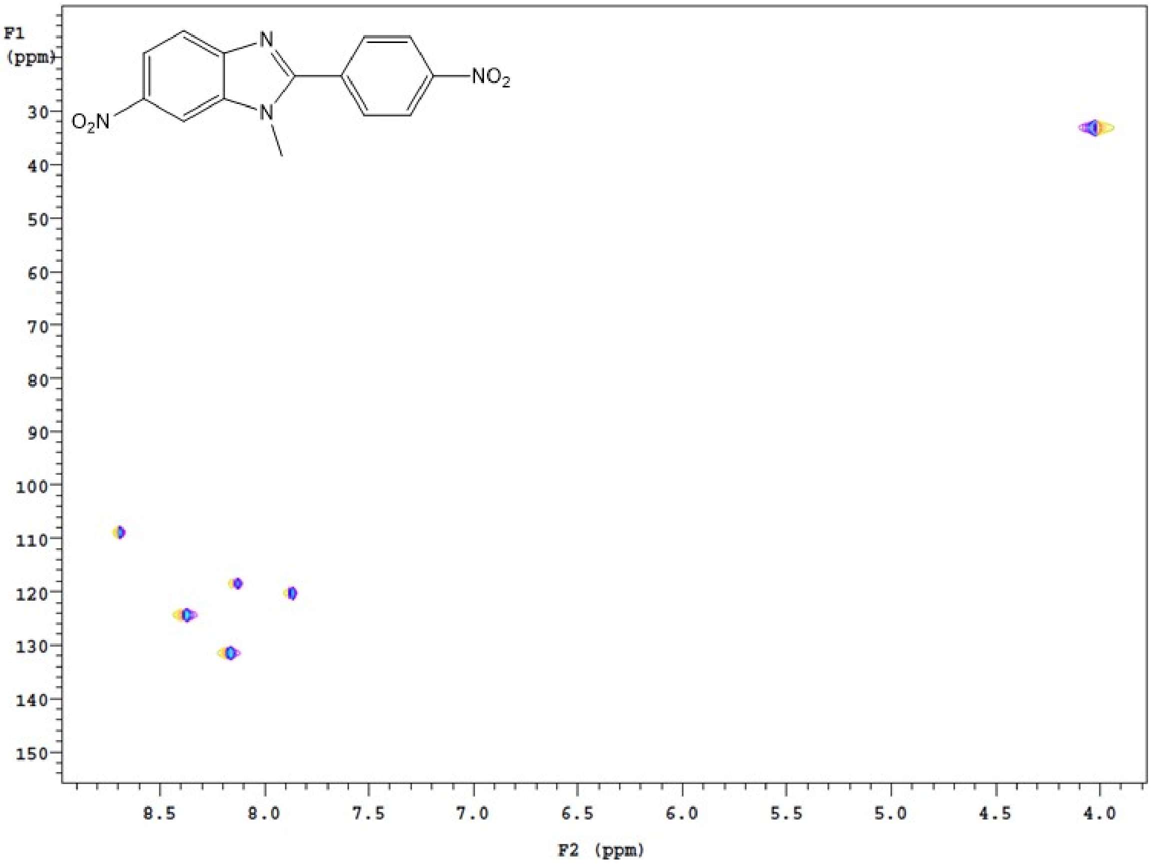


Figure S58. HSQC spectrum of compound **3f** in DMSO-d_6 at 25 °C.

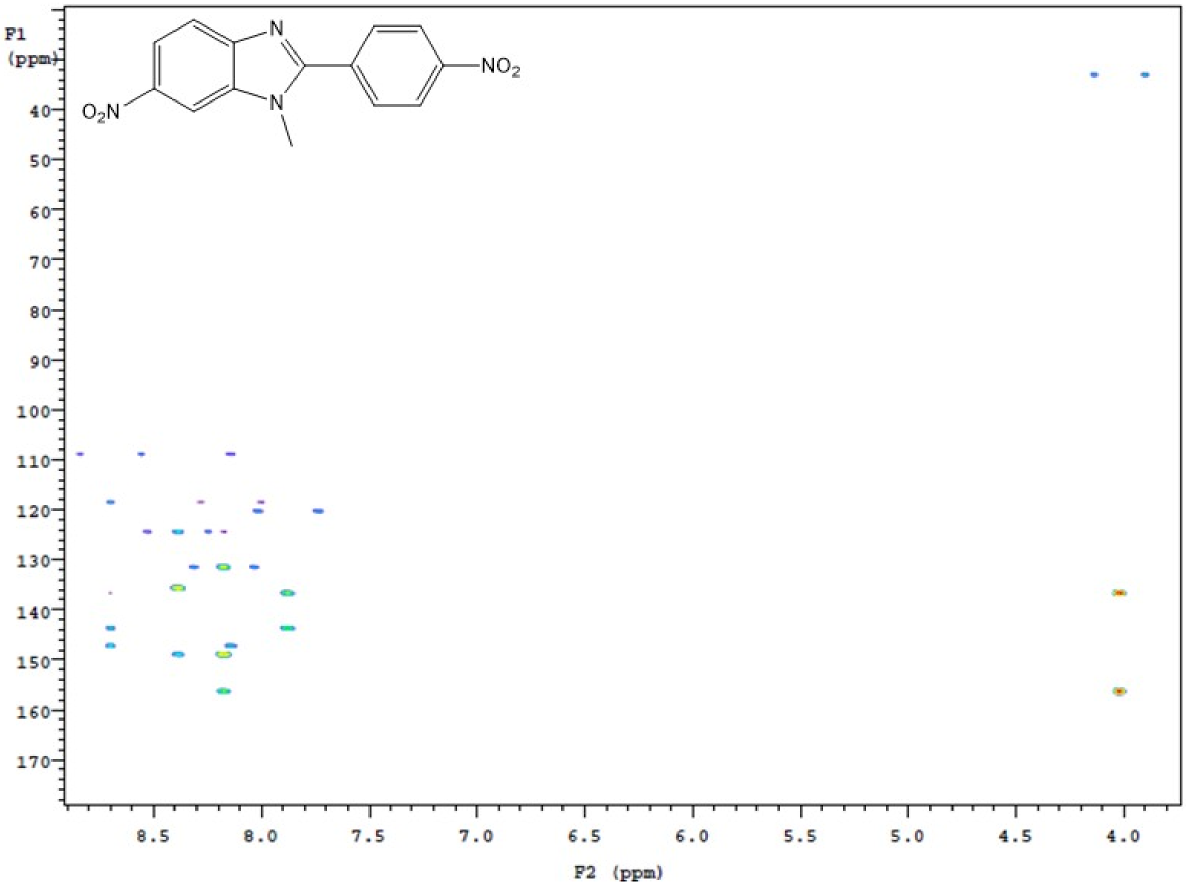


Figure S59. HMBC spectrum of compound **3f** in DMSO-d$_6$ at 25 °C.

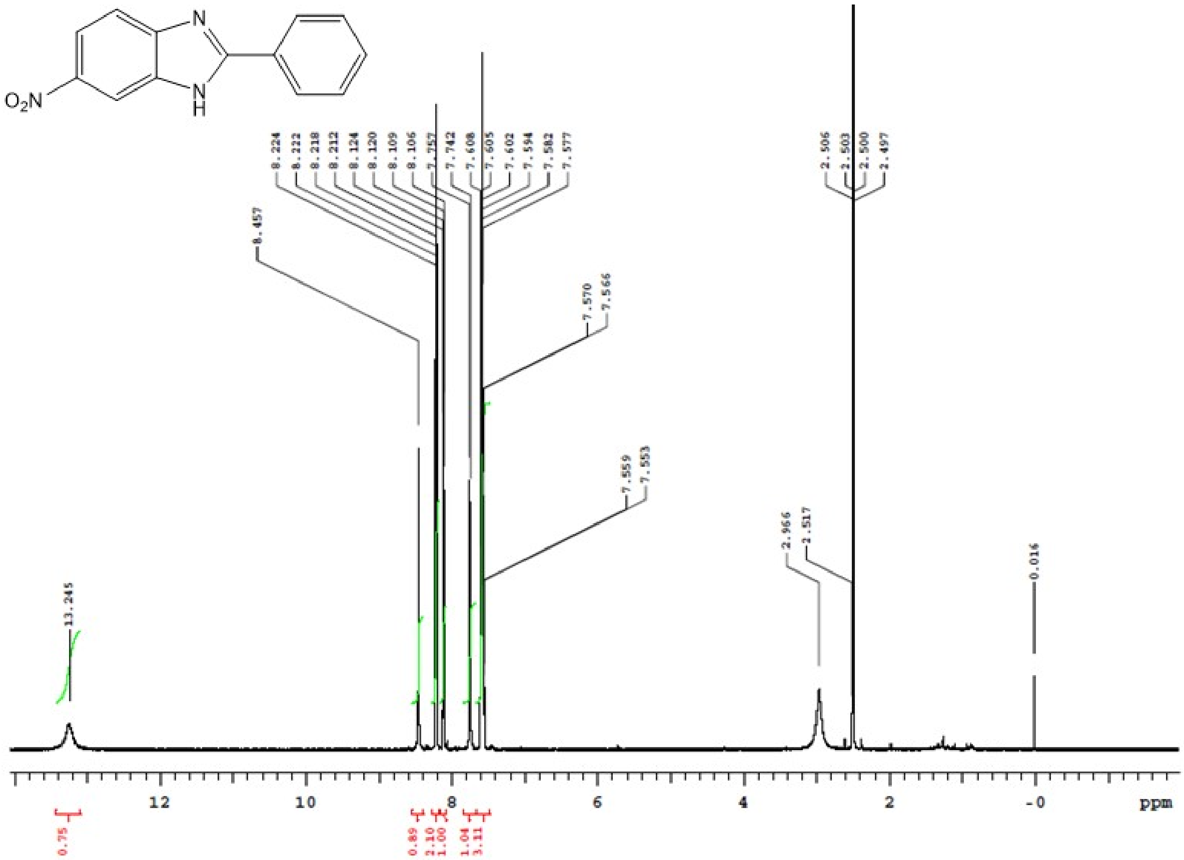


Figure S60. ^{1}H NMR spectrum of compound **1a** in DMSO-d_6 at 102 °C.

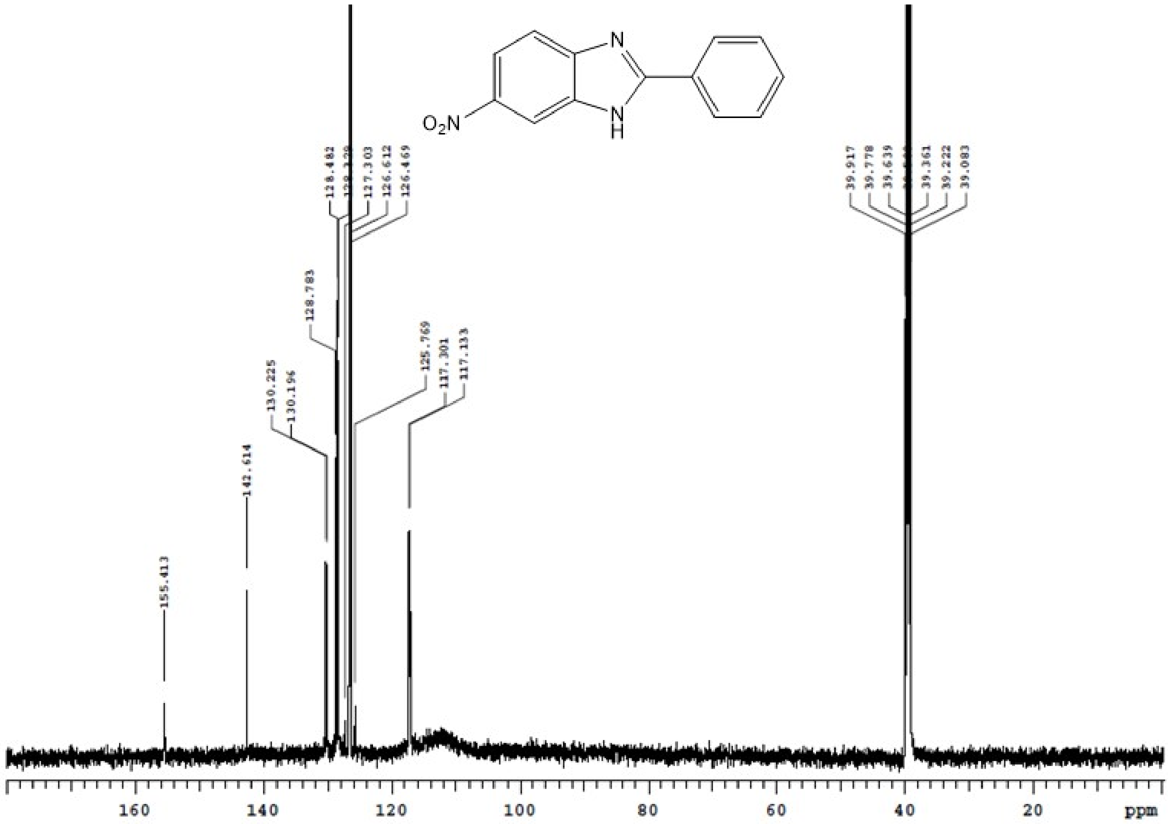


Figure S61. ^{13}C NMR spectrum of compound **1a** in DMSO-d_6 at 102 °C.

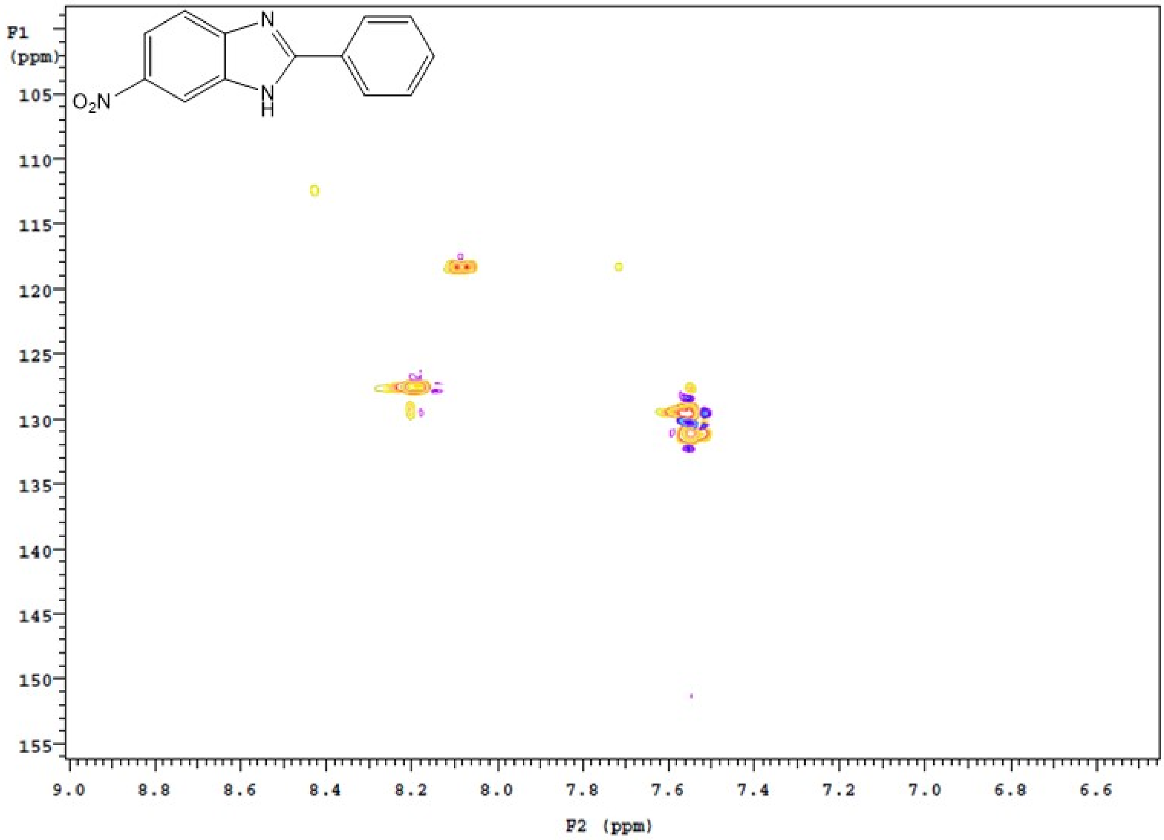


Figure S62. HSQC spectrum of compound **1a** in DMSO-d_6 at 102 °C.

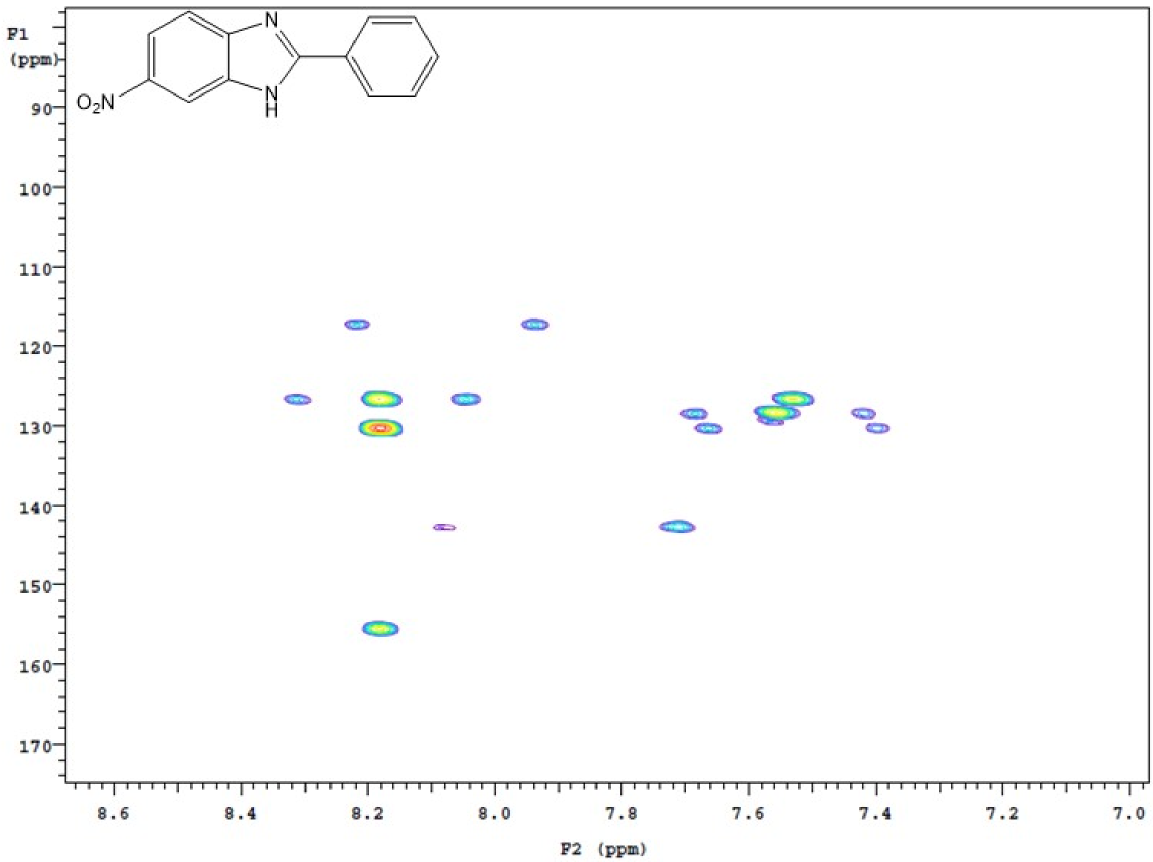


Figure S63. HMBC spectrum of compound **1a** in DMSO-d_6 at 102 °C.

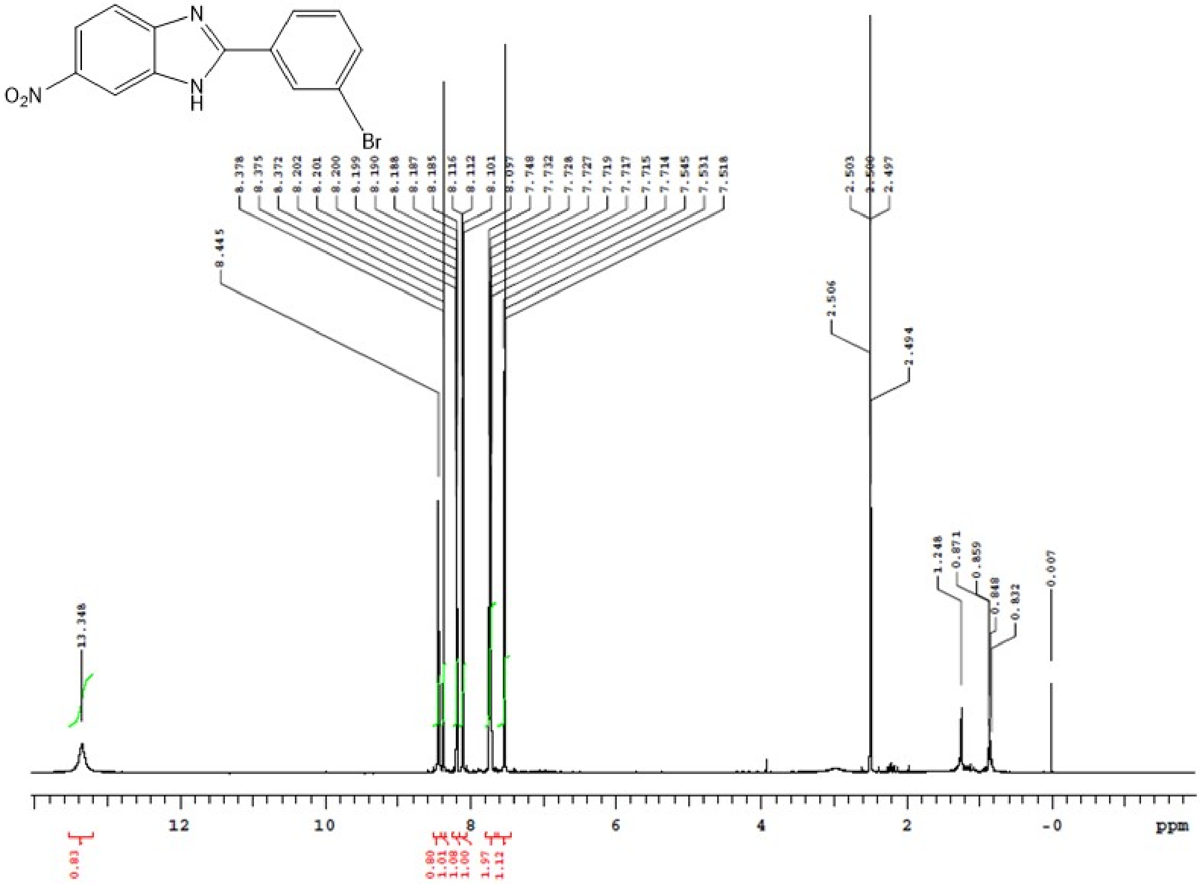


Figure S64. ^{1}H NMR spectrum of compound **1b** in DMSO-d_6 at 102 °C.

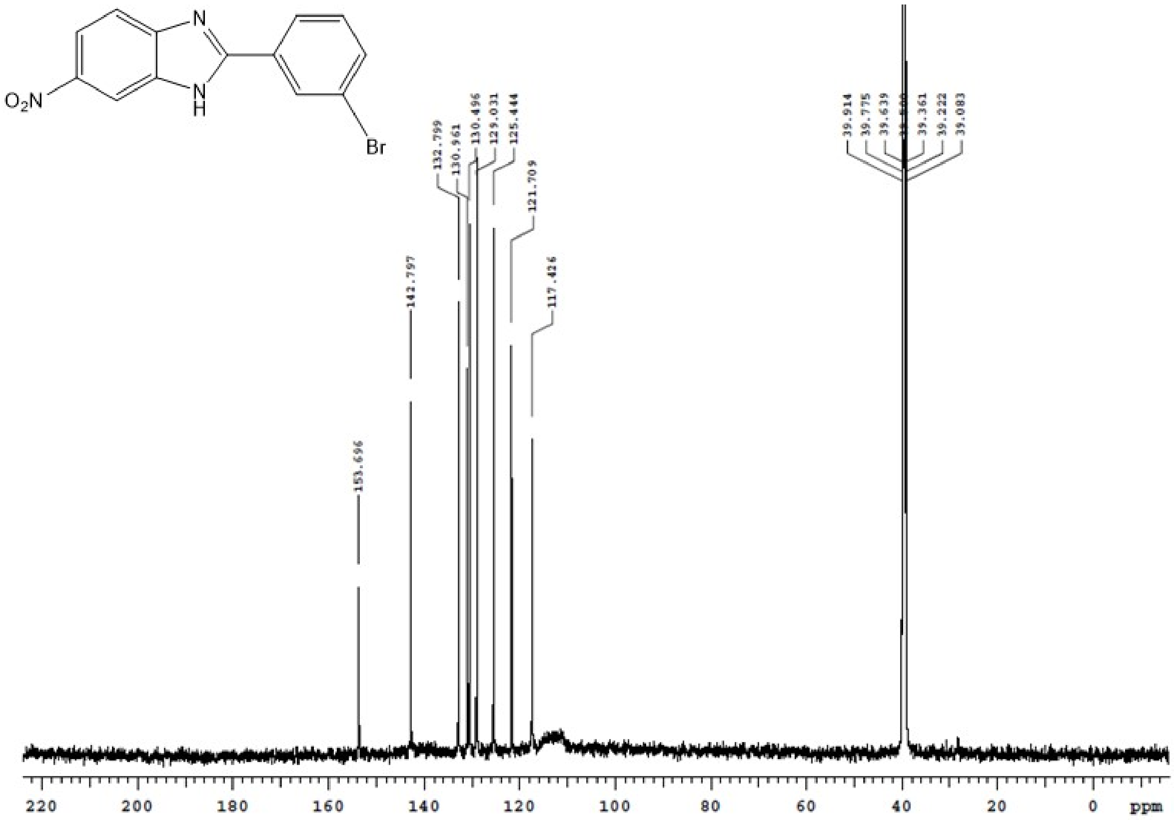


Figure S65. ^{13}C NMR spectrum of compound **1b** in DMSO-d_6 at 102 °C.

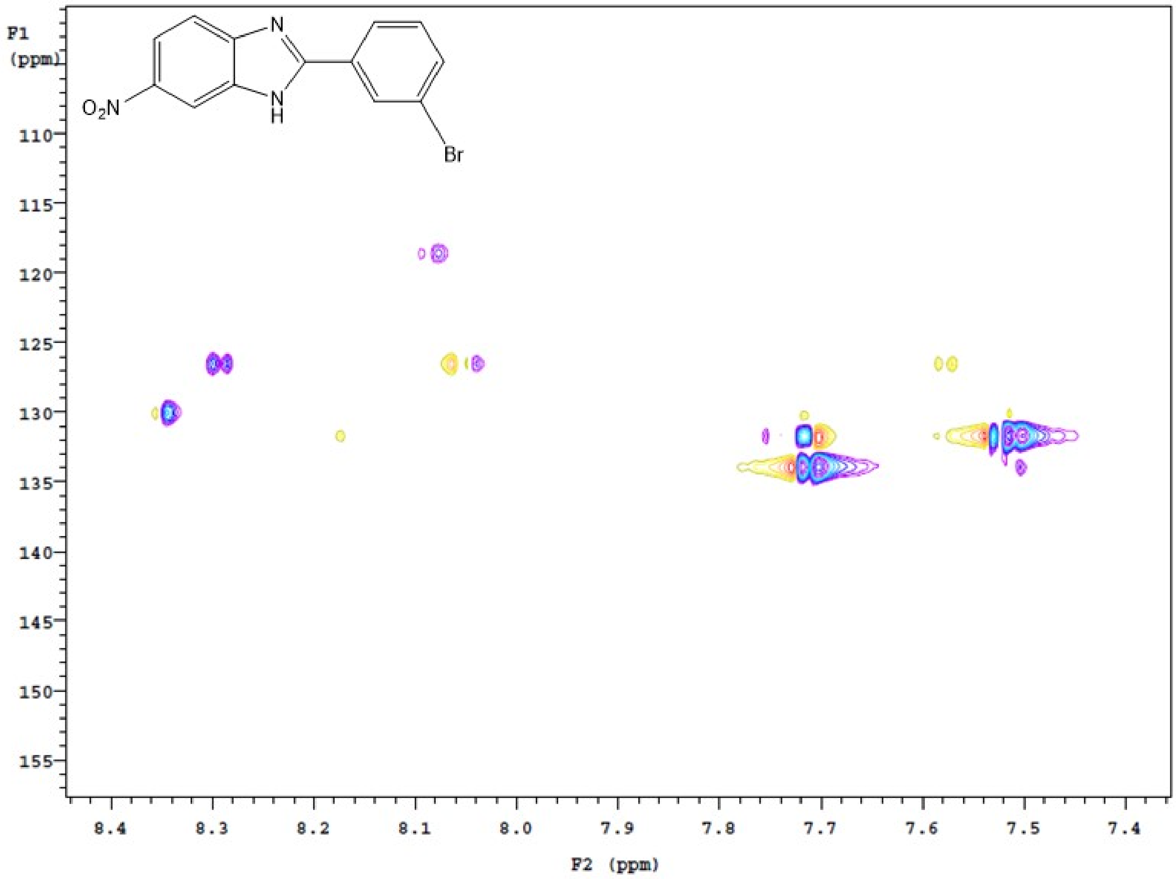


Figure S66. HSQC spectrum of compound **1b** in DMSO-d_6 at 102 °C.

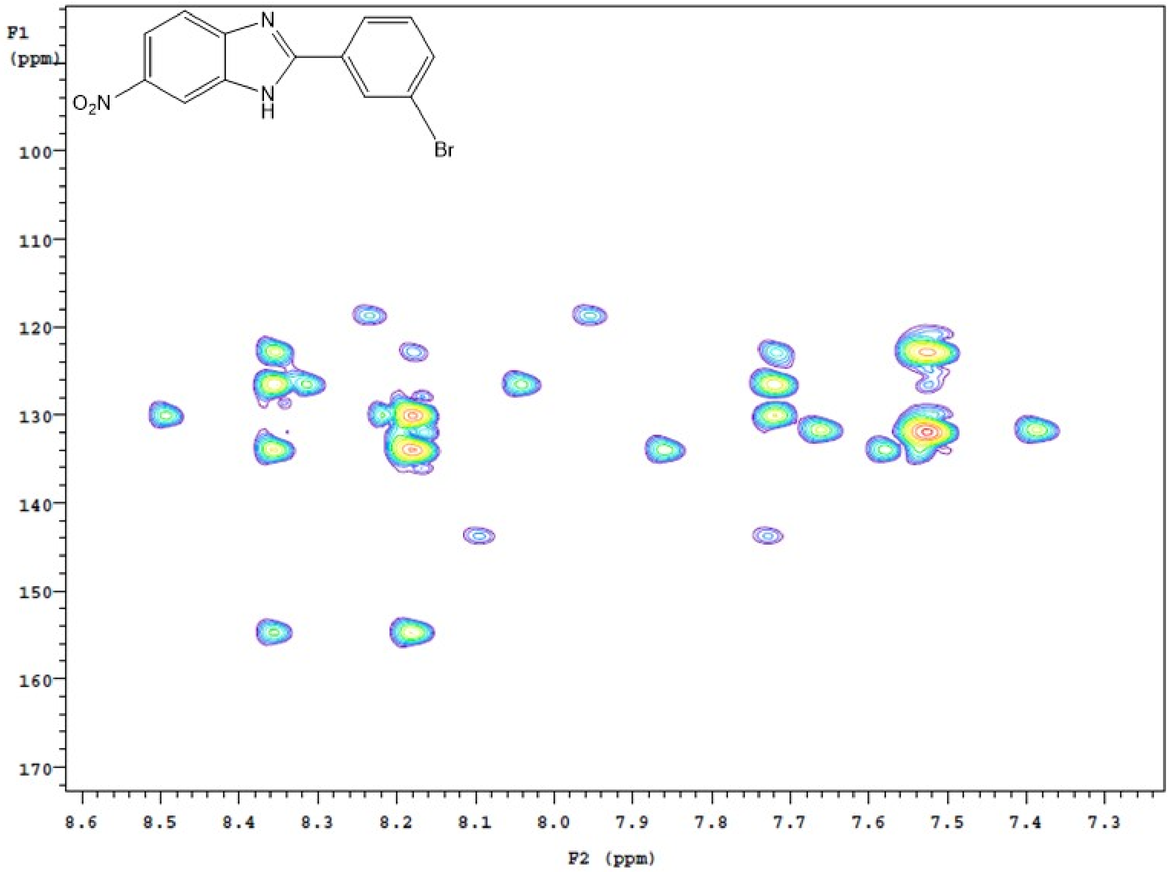


Figure S67. HMBC spectrum of compound **1b** in DMSO-d_6 at 102 °C.

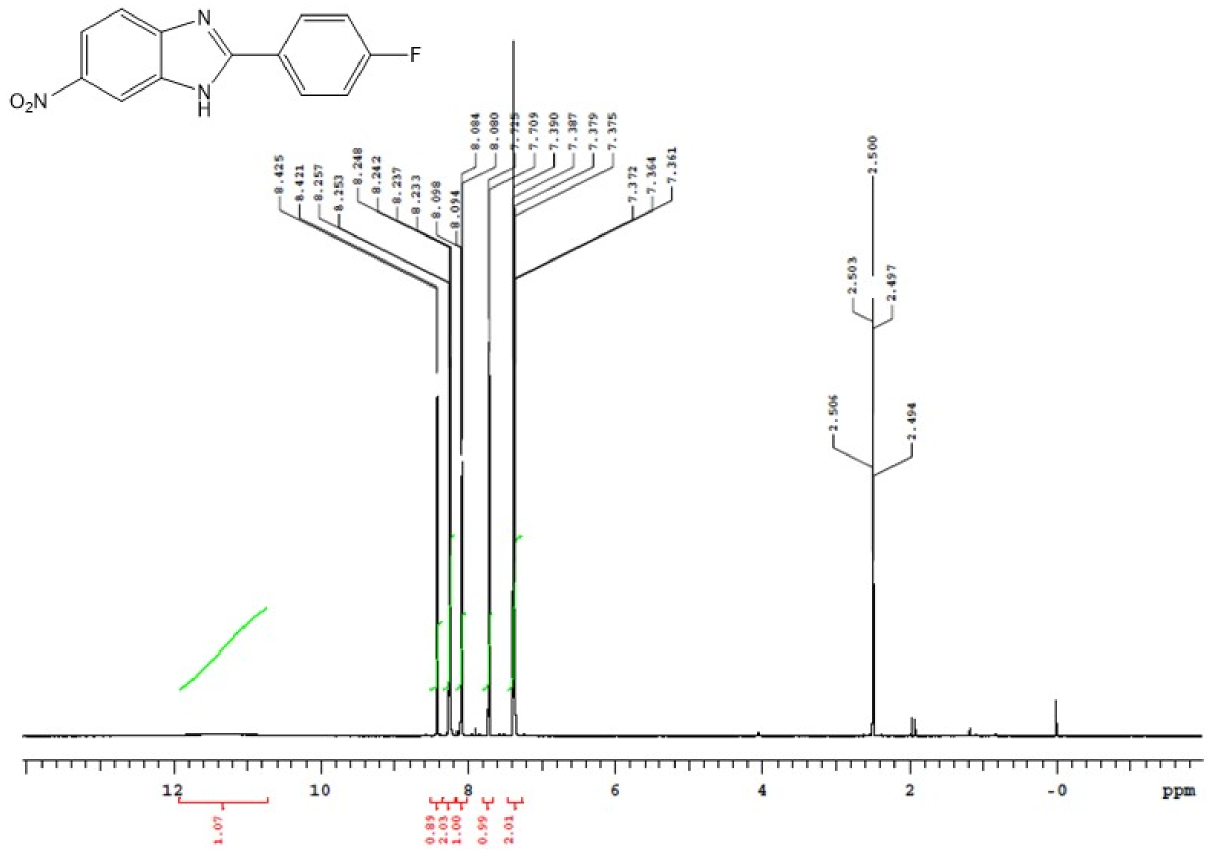


Figure S68. ¹H NMR spectrum of compound **1c** in DMSO-d_6 at 102 °C.

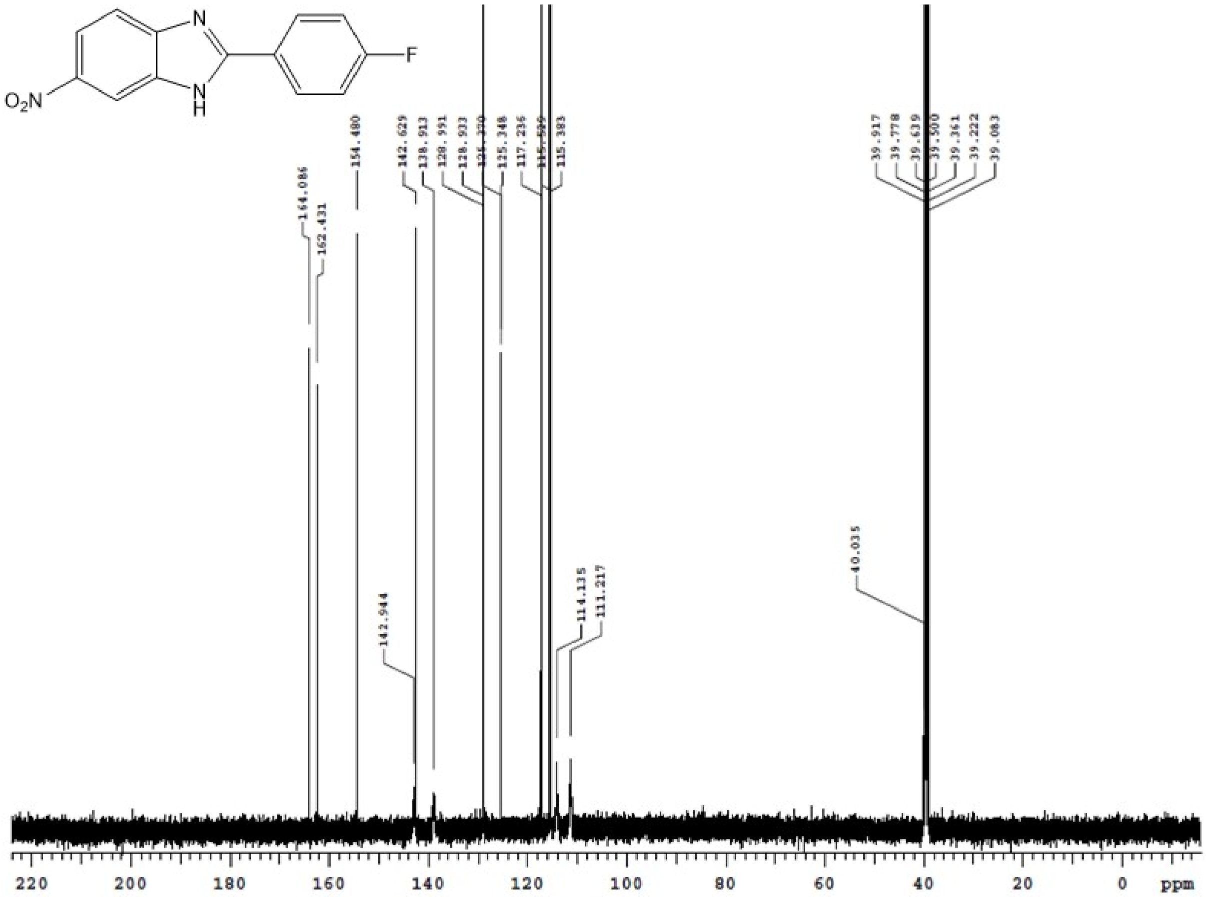


Figure S69. ^{13}C NMR spectrum of compound **1c** in DMSO-d_6 at 102 °C.

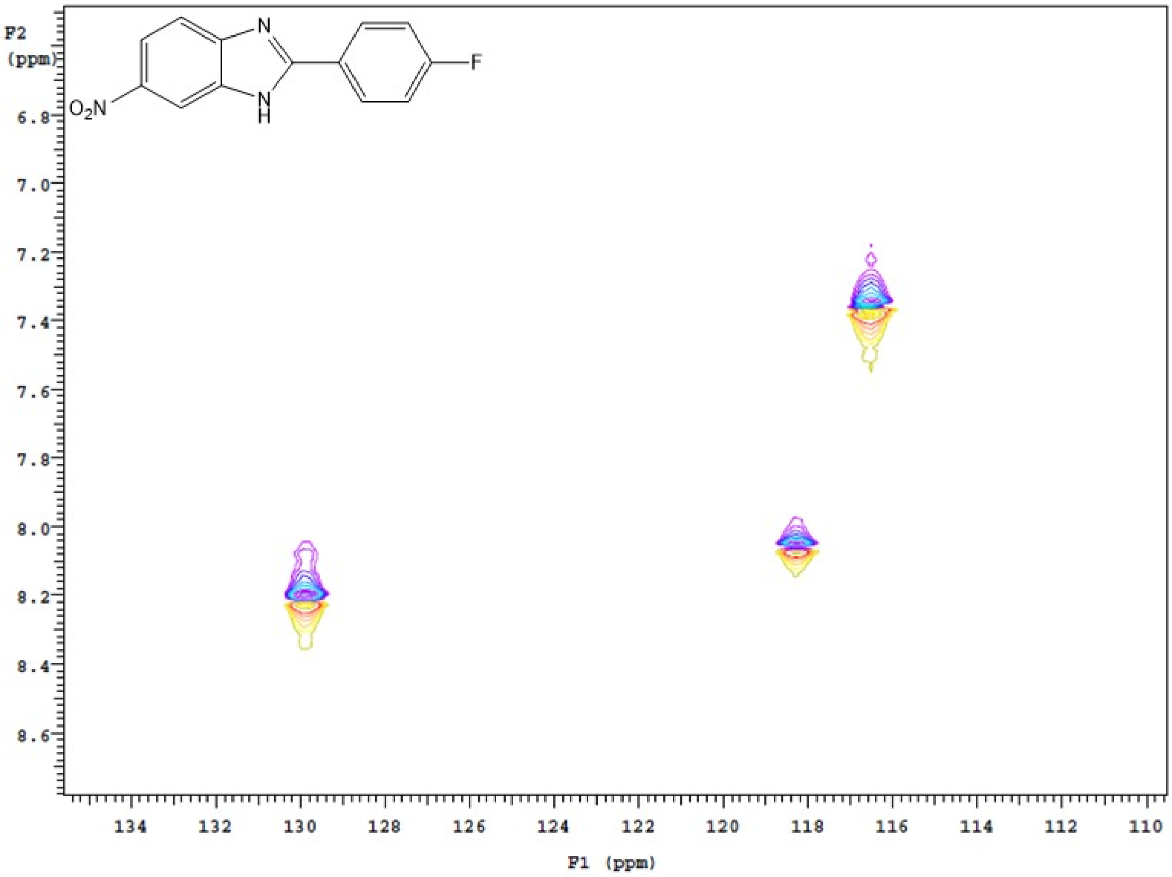


Figure S70. HSQC spectrum of compound **1c** in DMSO-d$_6$ at 102 °C.

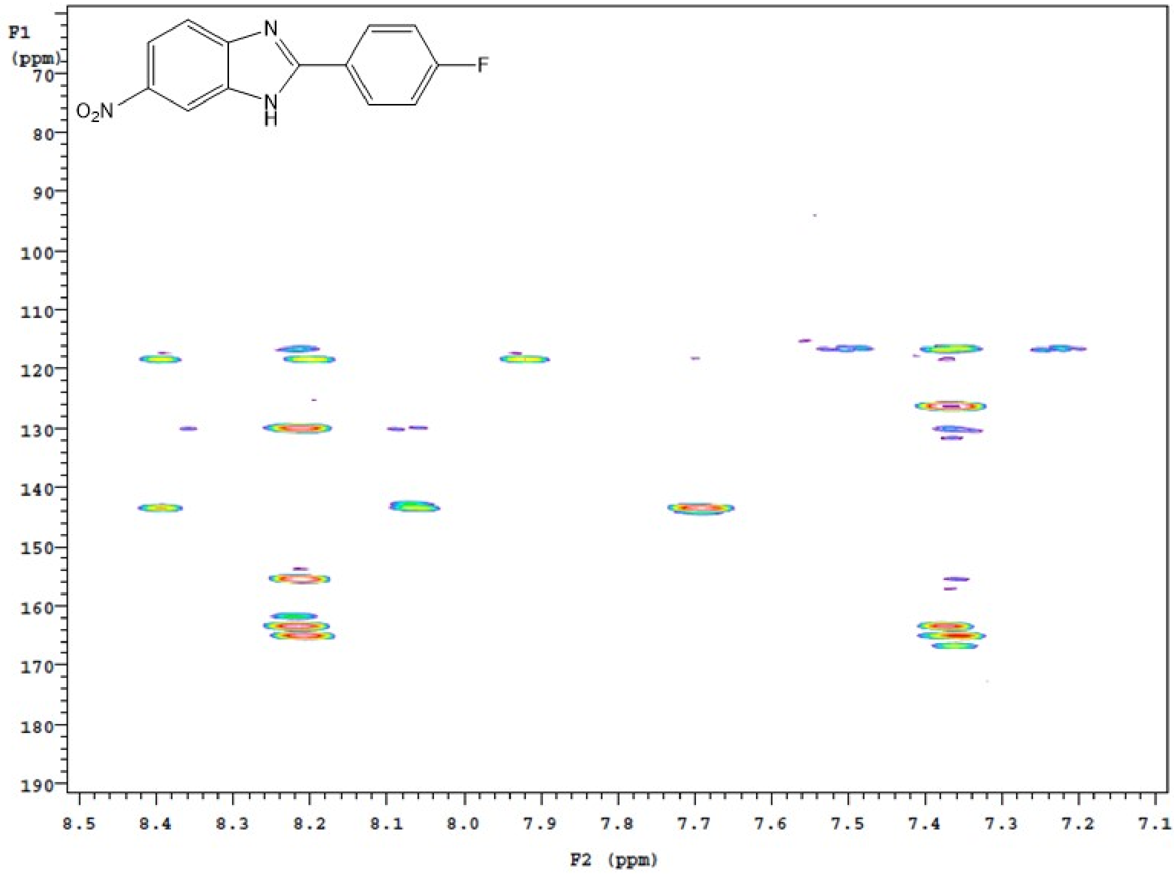


Figure S71. HMBC spectrum of compound **1c** in DMSO-d_6 at 102 °C.

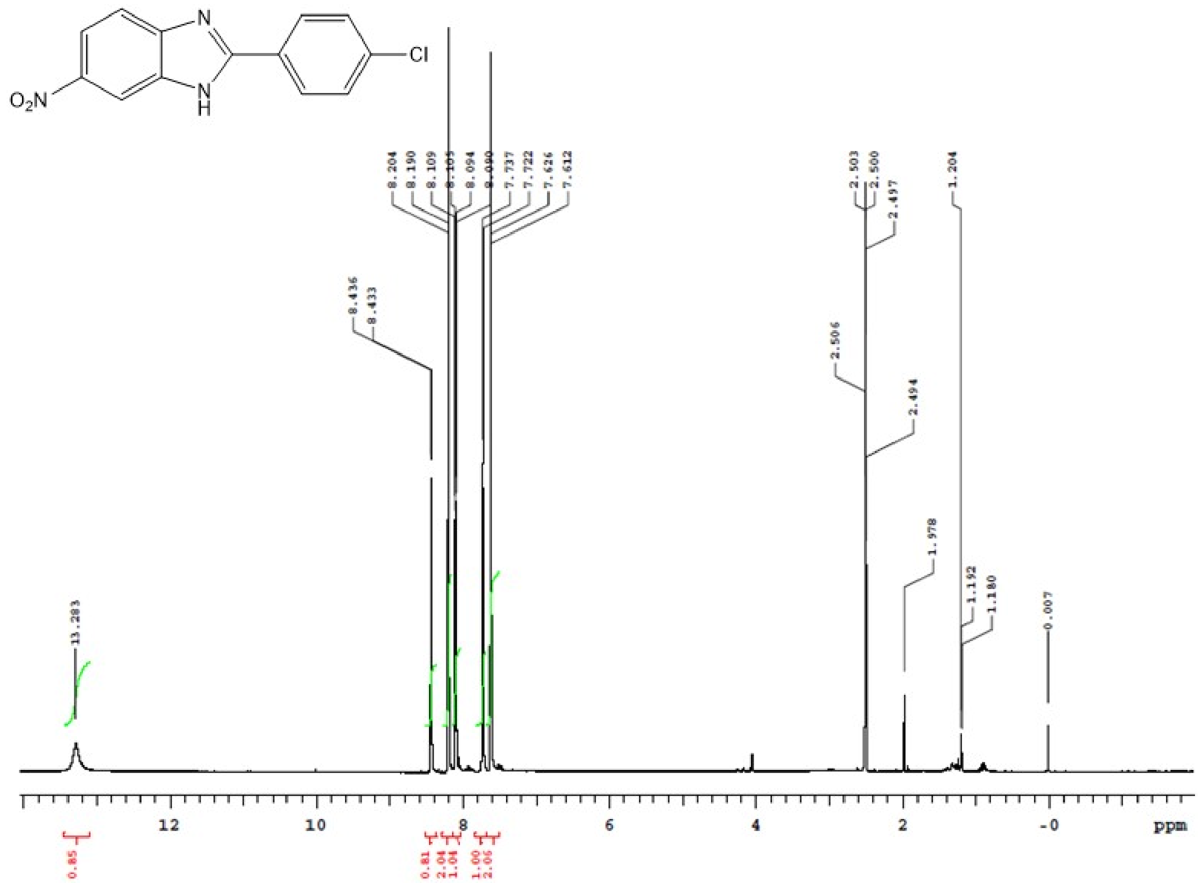


Figure S72. ^{1}H NMR spectrum of compound **1d** in DMSO-d_6 at 102 °C.

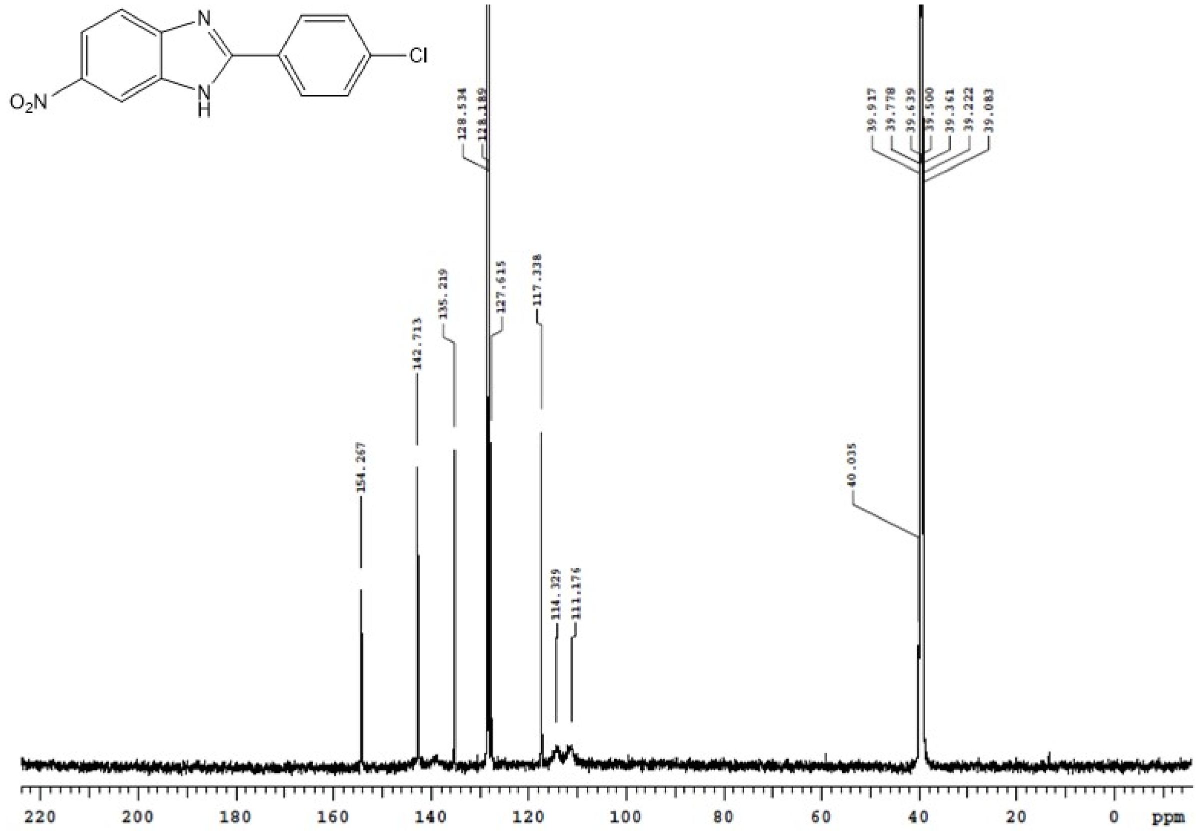


Figure S73. ^{13}C NMR spectrum of compound **1d** in DMSO-d_6 at 102 °C.

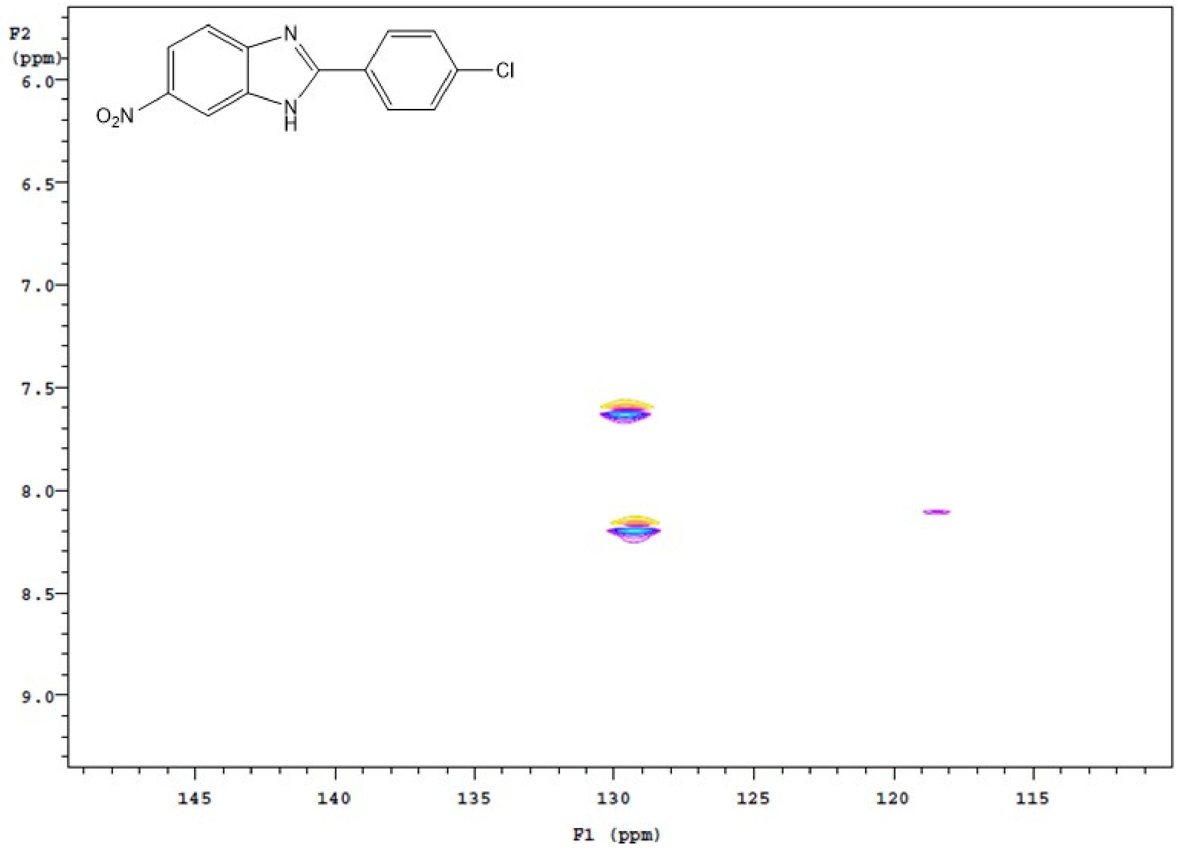


Figure S74. HSQC spectrum of compound **1d** in DMSO-d_6 at 102 °C.

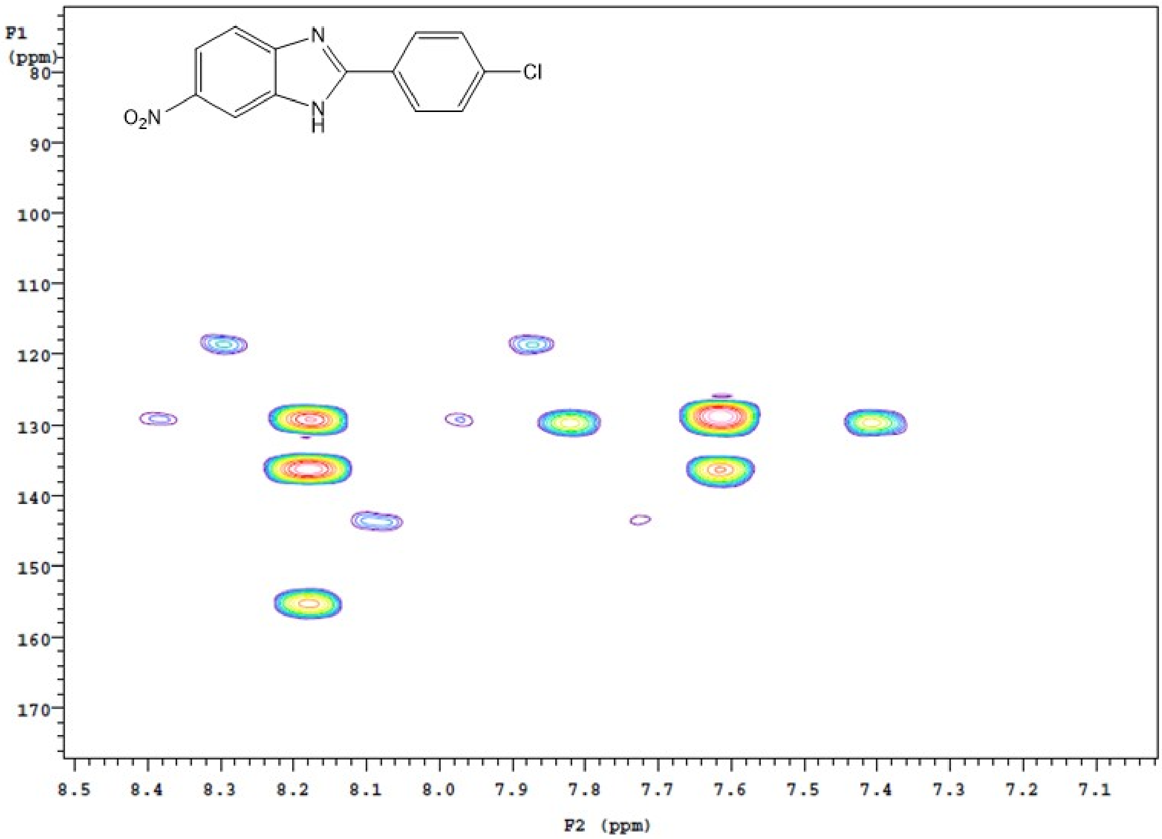


Figure S75. HMBC spectrum of compound **1d** in DMSO-d_6 at 102 °C.

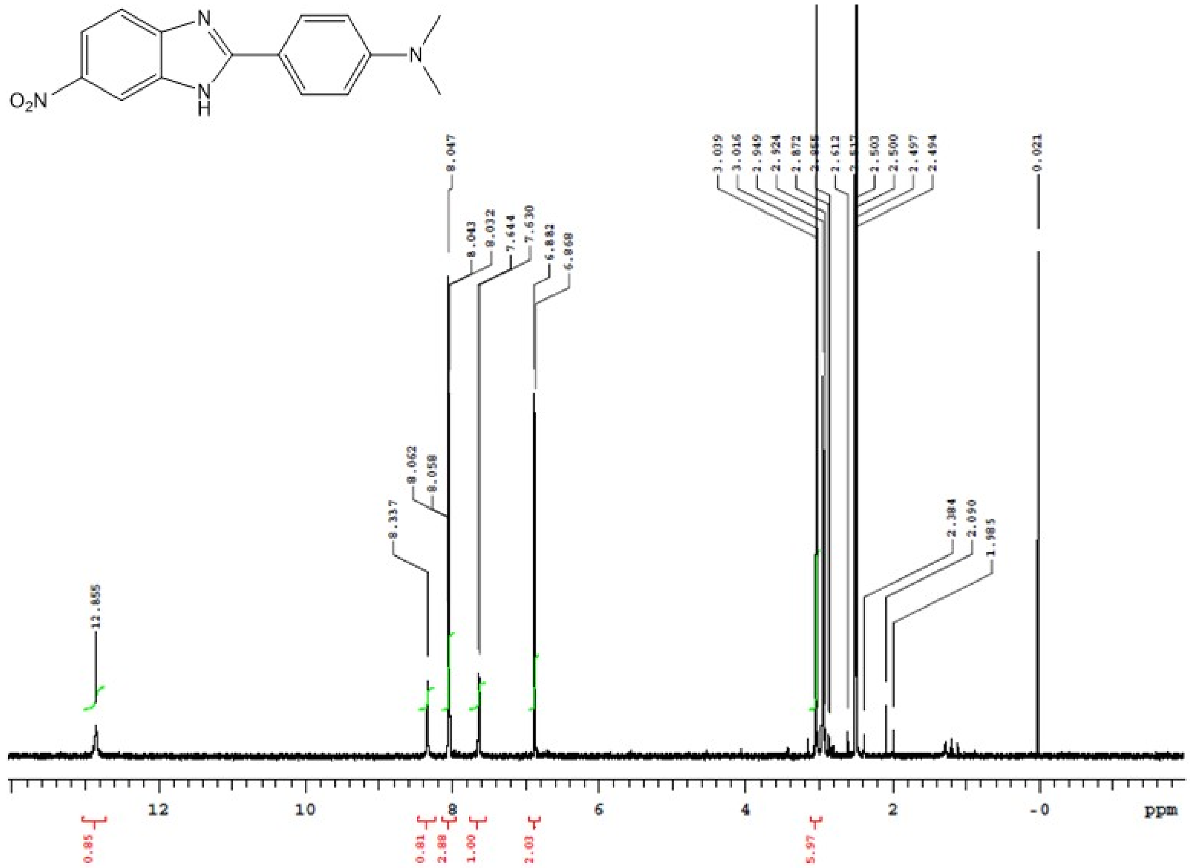


Figure S76. ^{1}H NMR spectrum of compound **1e** in DMSO-d_6 at 102 °C.

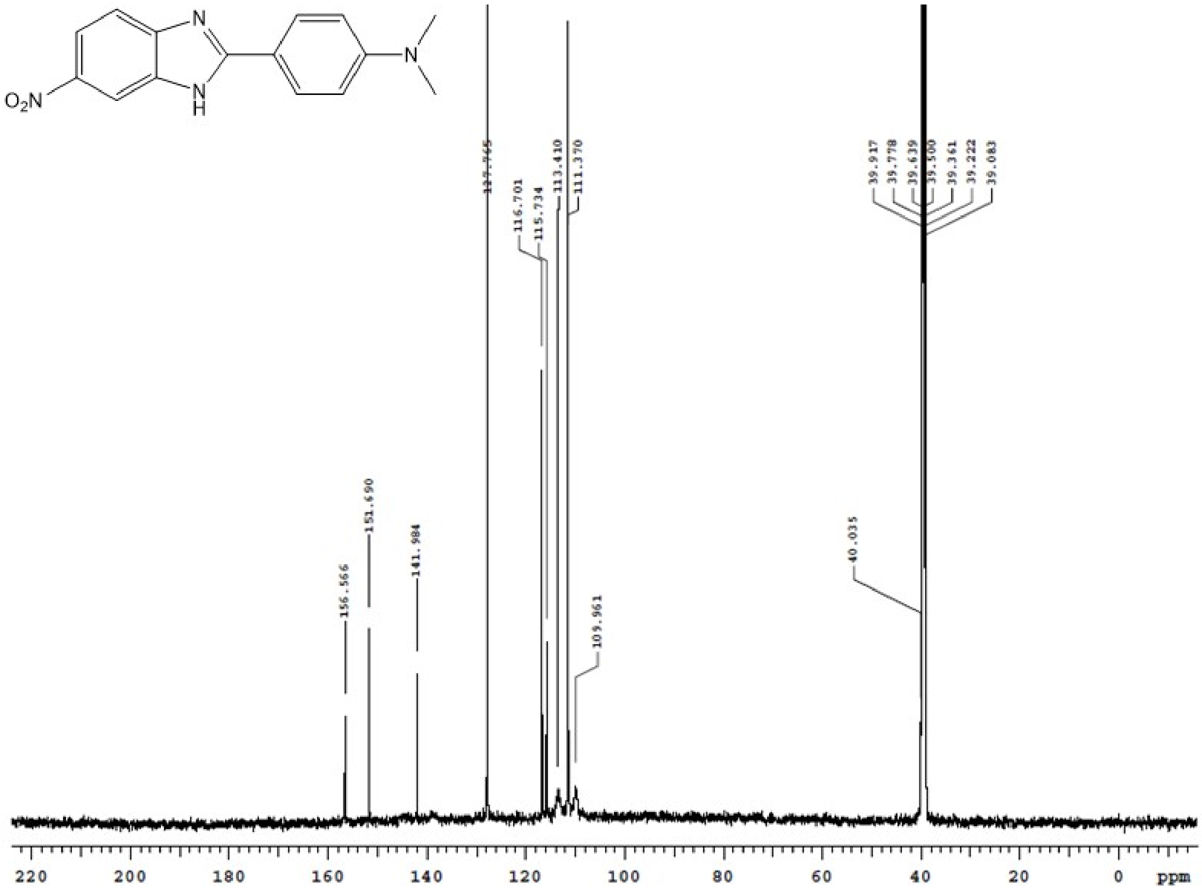


Figure S77. ^{13}C NMR spectrum of compound **1e** in DMSO-d_6 at 102 °C.

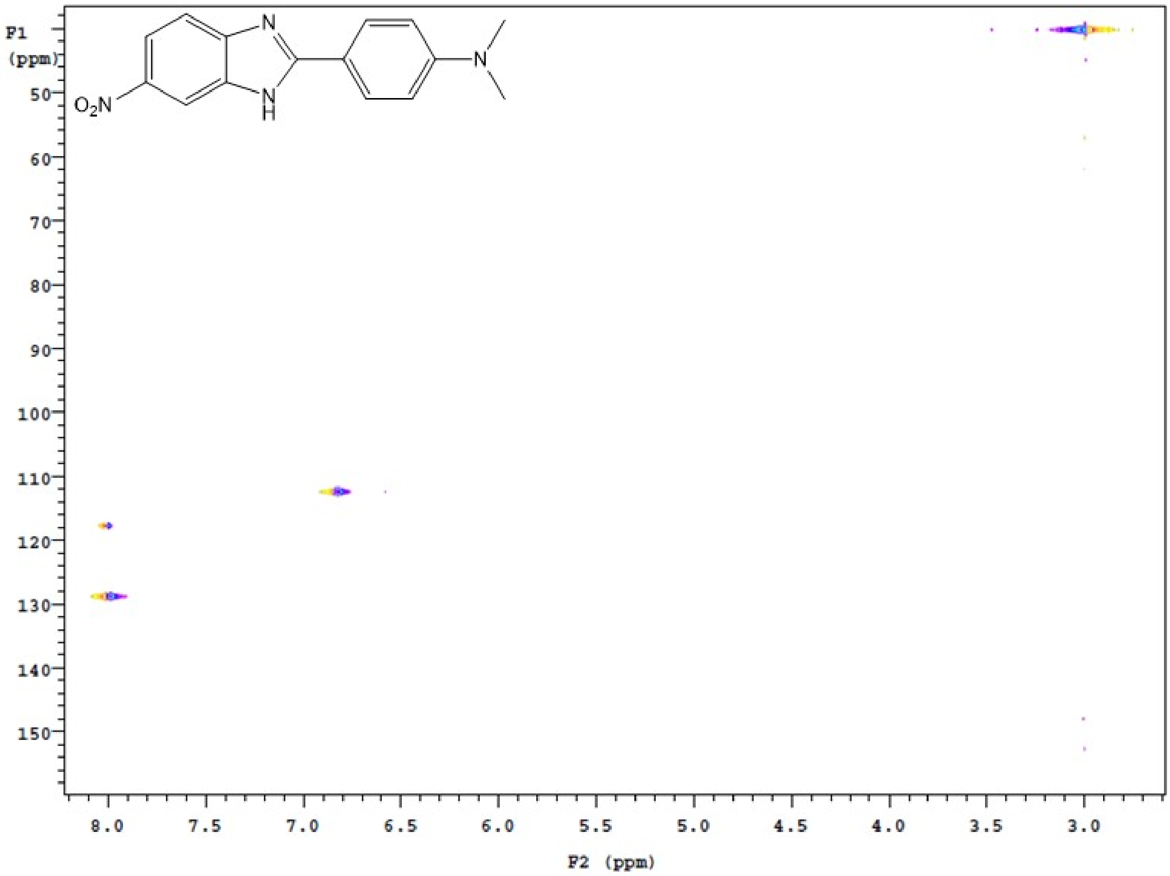


Figure S78. HSQC spectrum of compound **1e** in DMSO-d_6 at 102 °C.

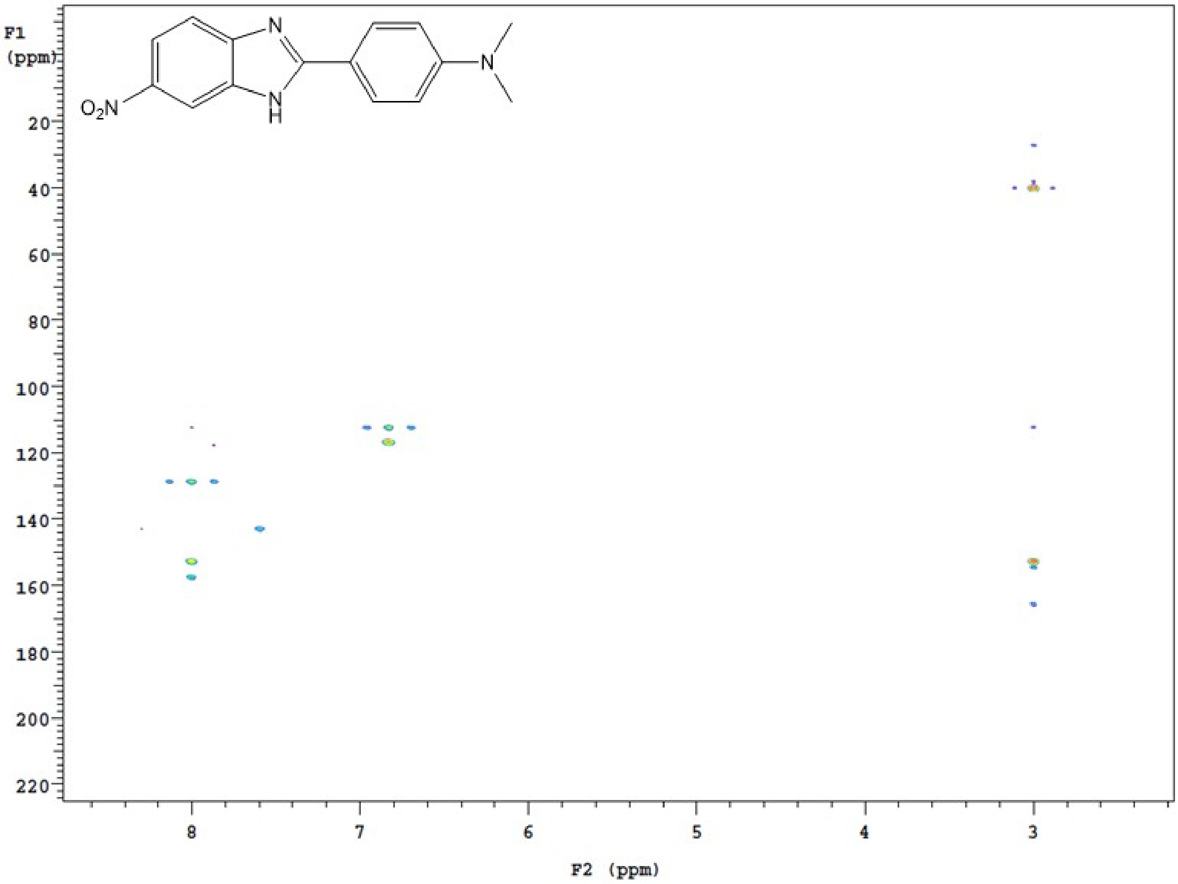


Figure S79. HMBC spectrum of compound **1e** in DMSO-d_6 at 102°C.

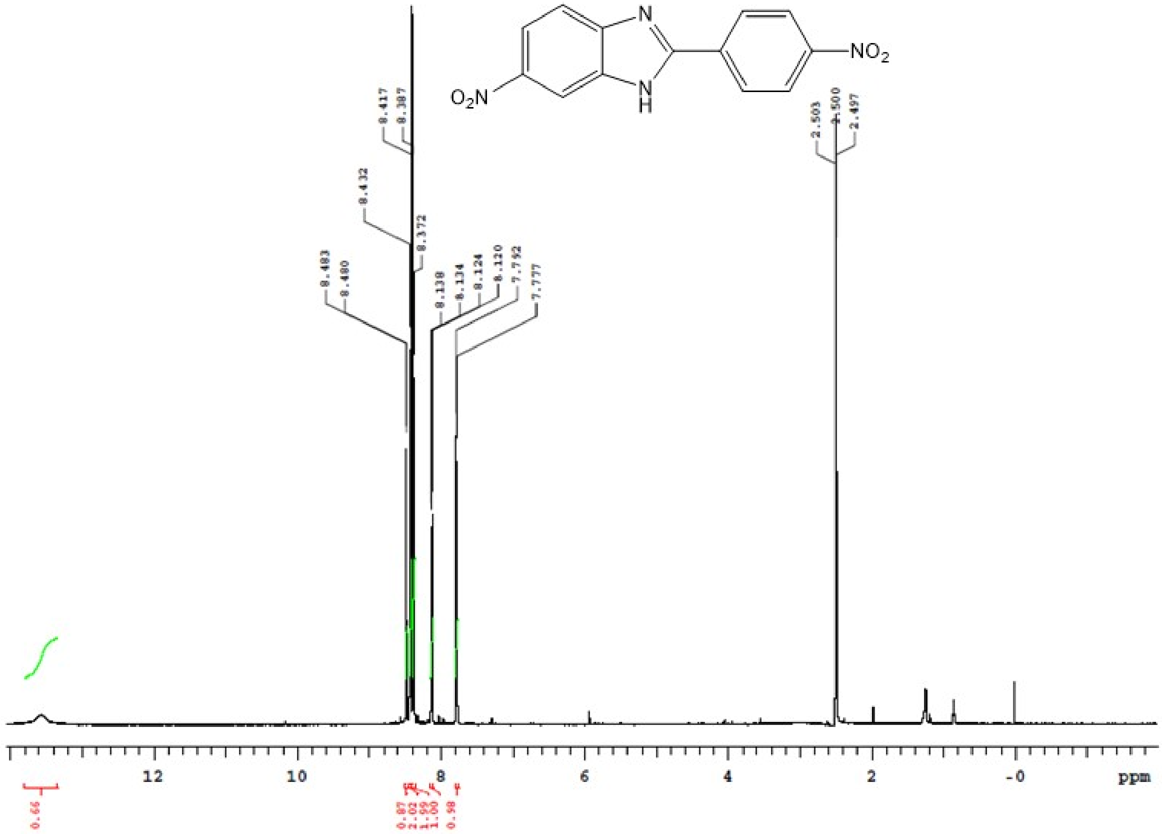


Figure S80. ^{1}H NMR spectrum of compound **1f** in DMSO-d_6 at 102 °C.

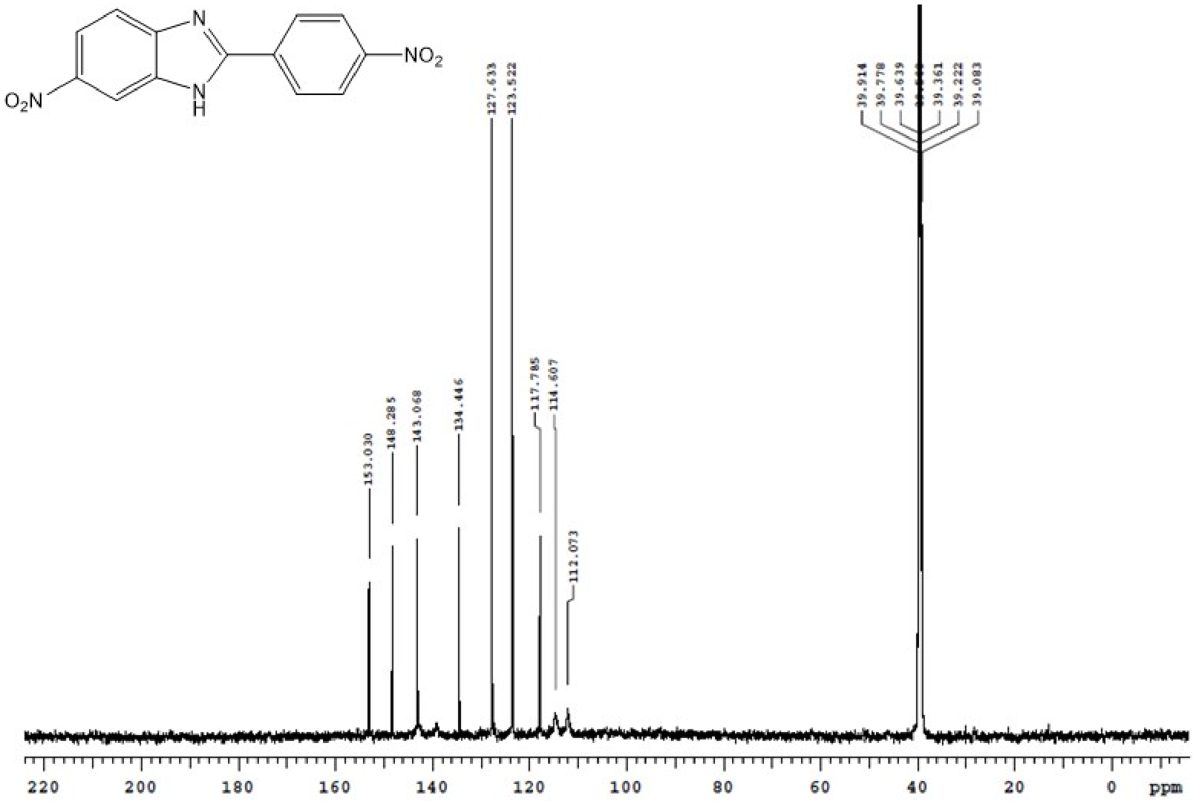


Figure S81. ^{13}C NMR spectrum of compound **1f** in DMSO-d_6 at 102 °C.

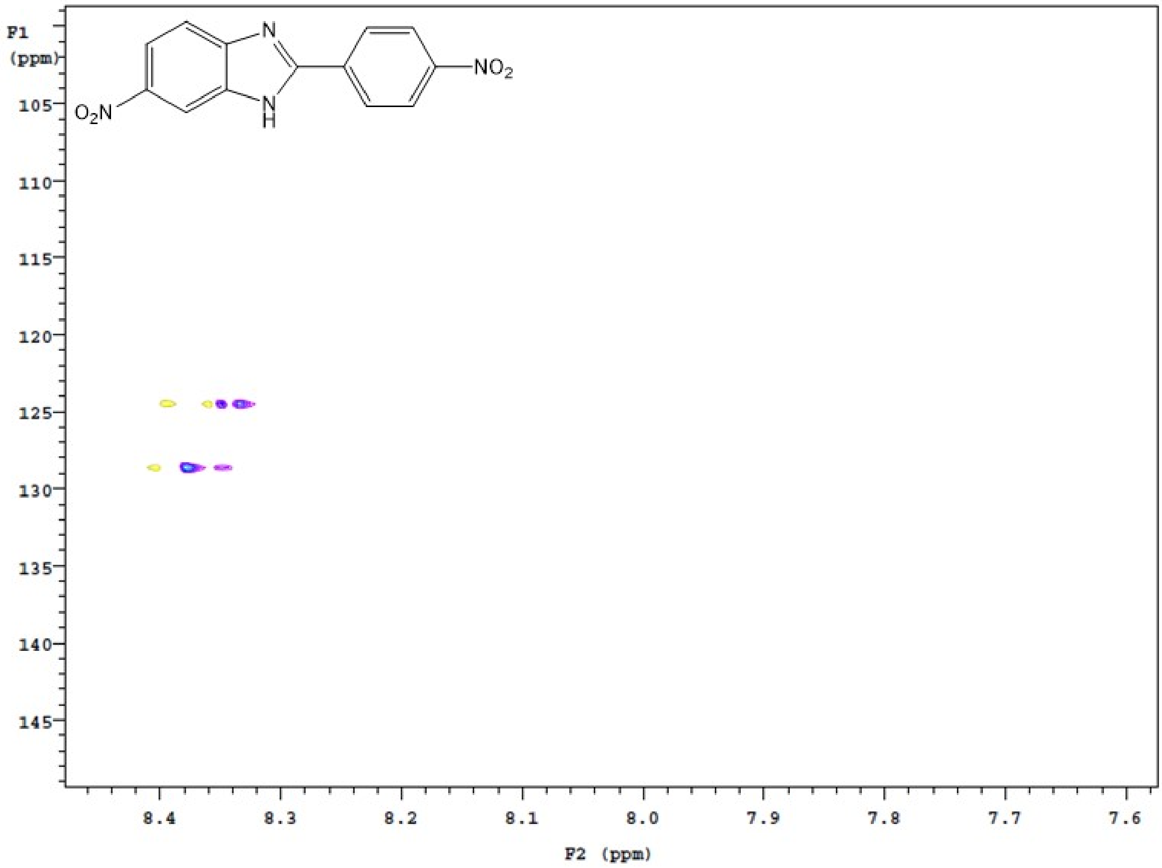


Figure S82. HSQC spectrum of compound **1f** in DMSO-d_6 at 102 °C.

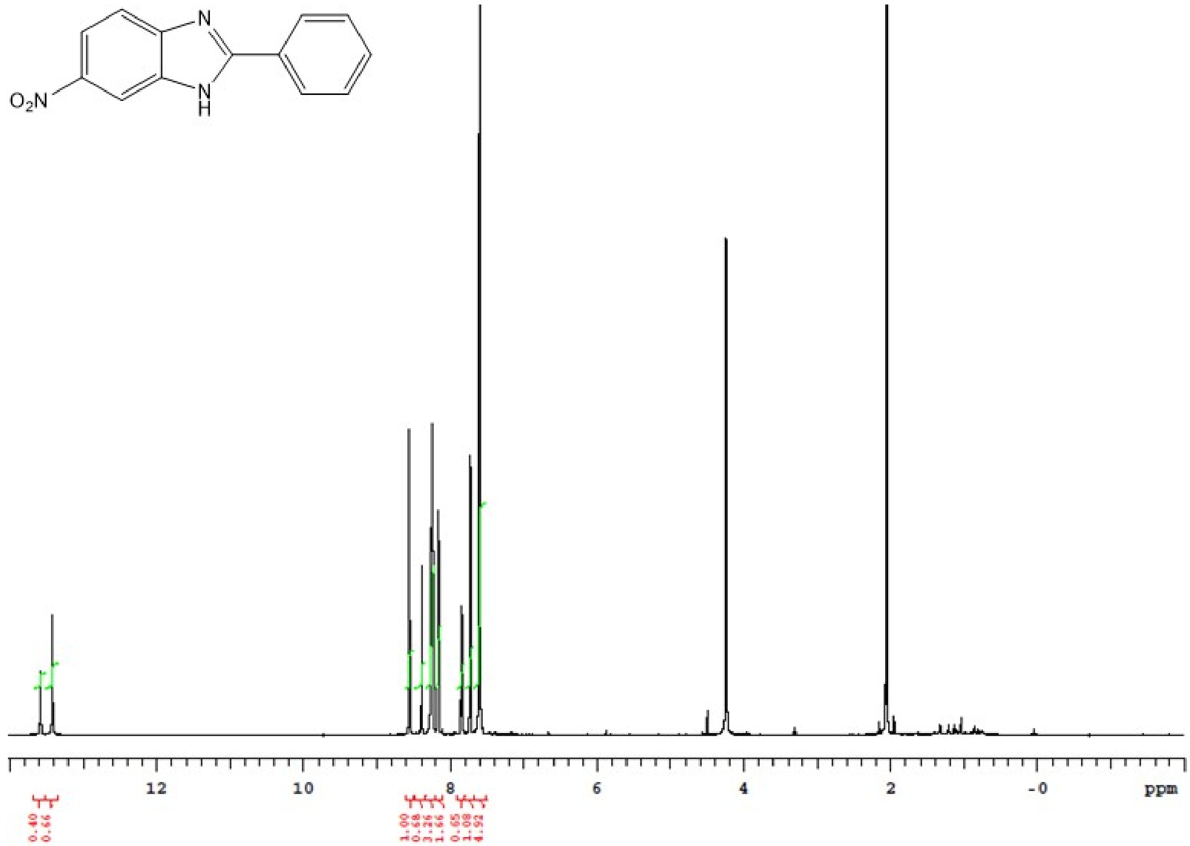


Figure S83. ^{1}H NMR spectrum of compound **1a** in acetone-d_6 at −76 °C.

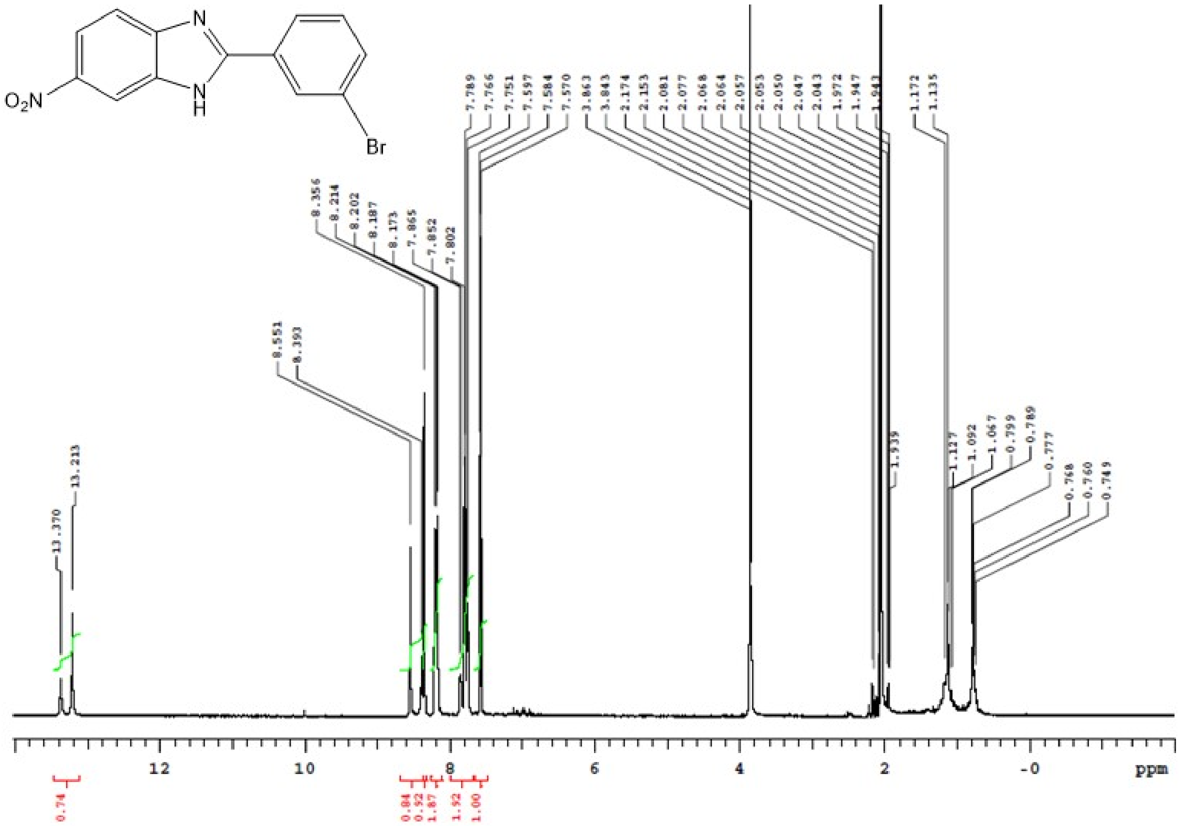


Figure S84. ^{1}H NMR spectrum of compound **1b** in acetone-d_6 at −76 °C.

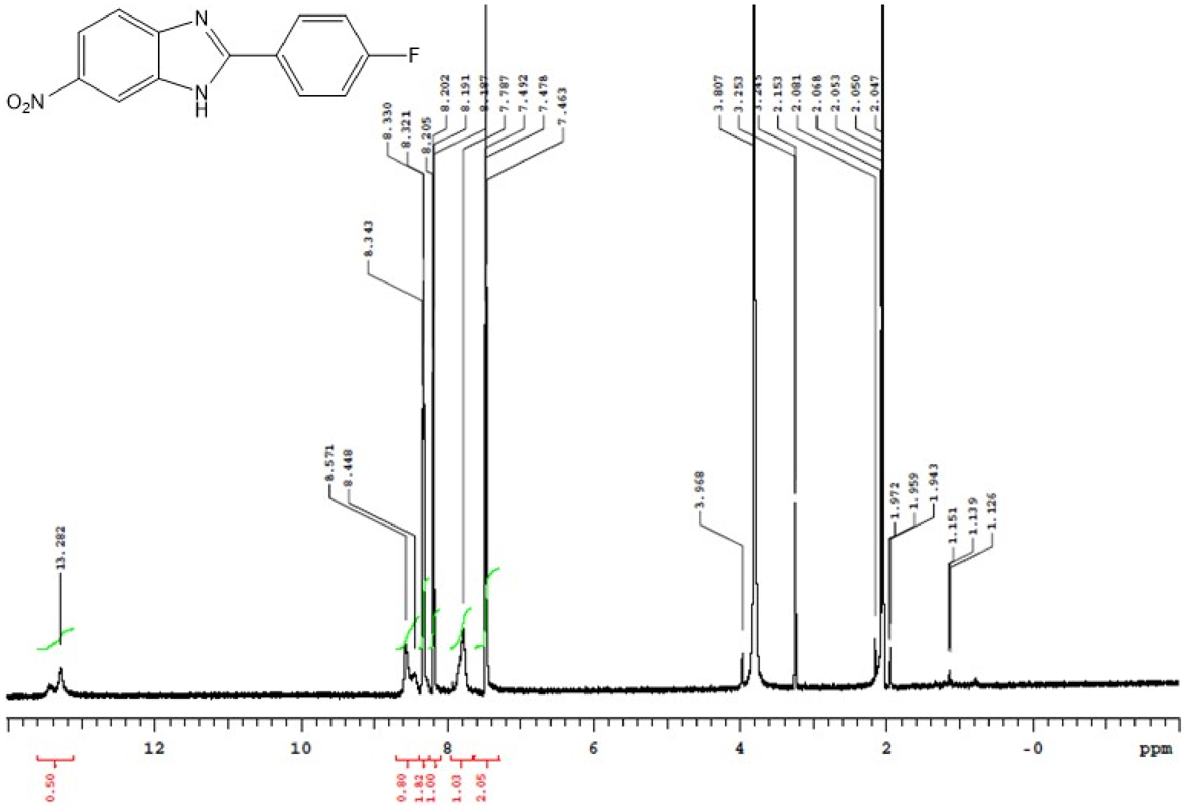


Figure S85. [1]H NMR spectrum of compound **1c** in acetone-d_6 at −76 °C.

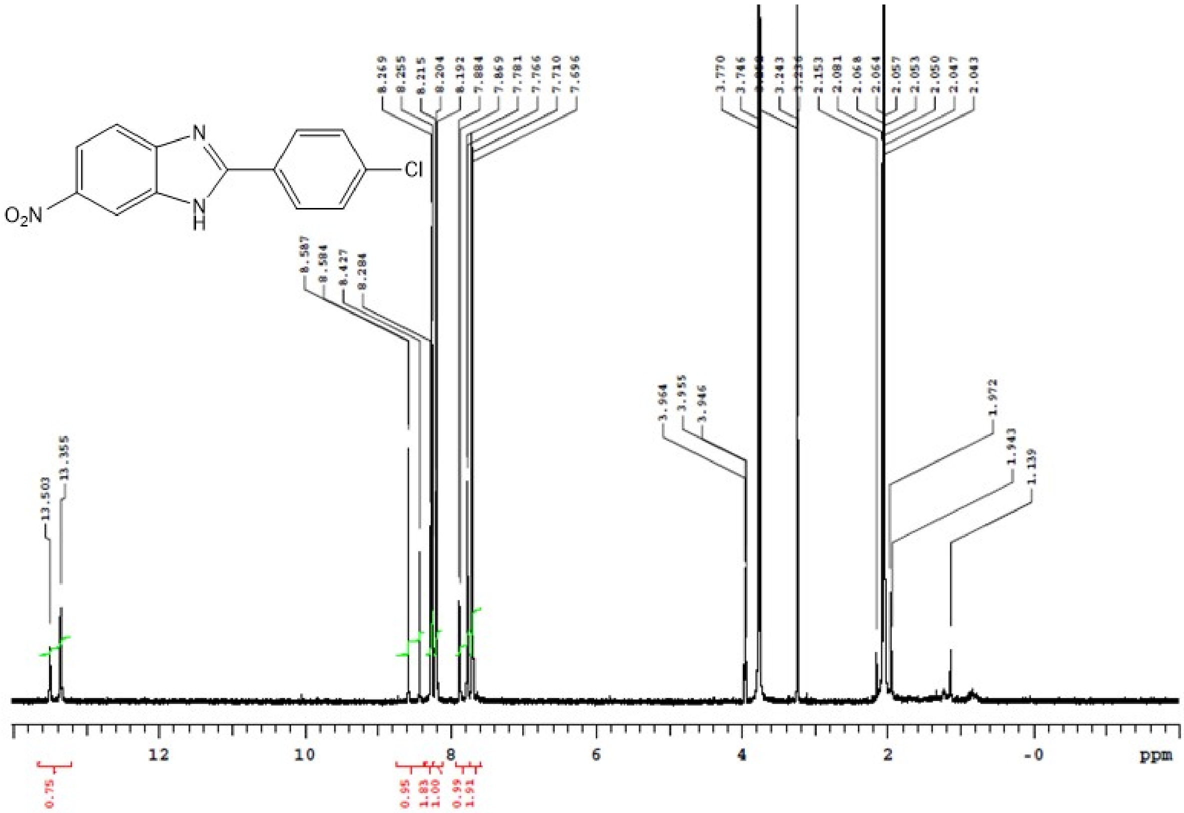


Figure S86. ^{1}H NMR spectrum of compound **1d** in acetone-d_6 at −76 °C.

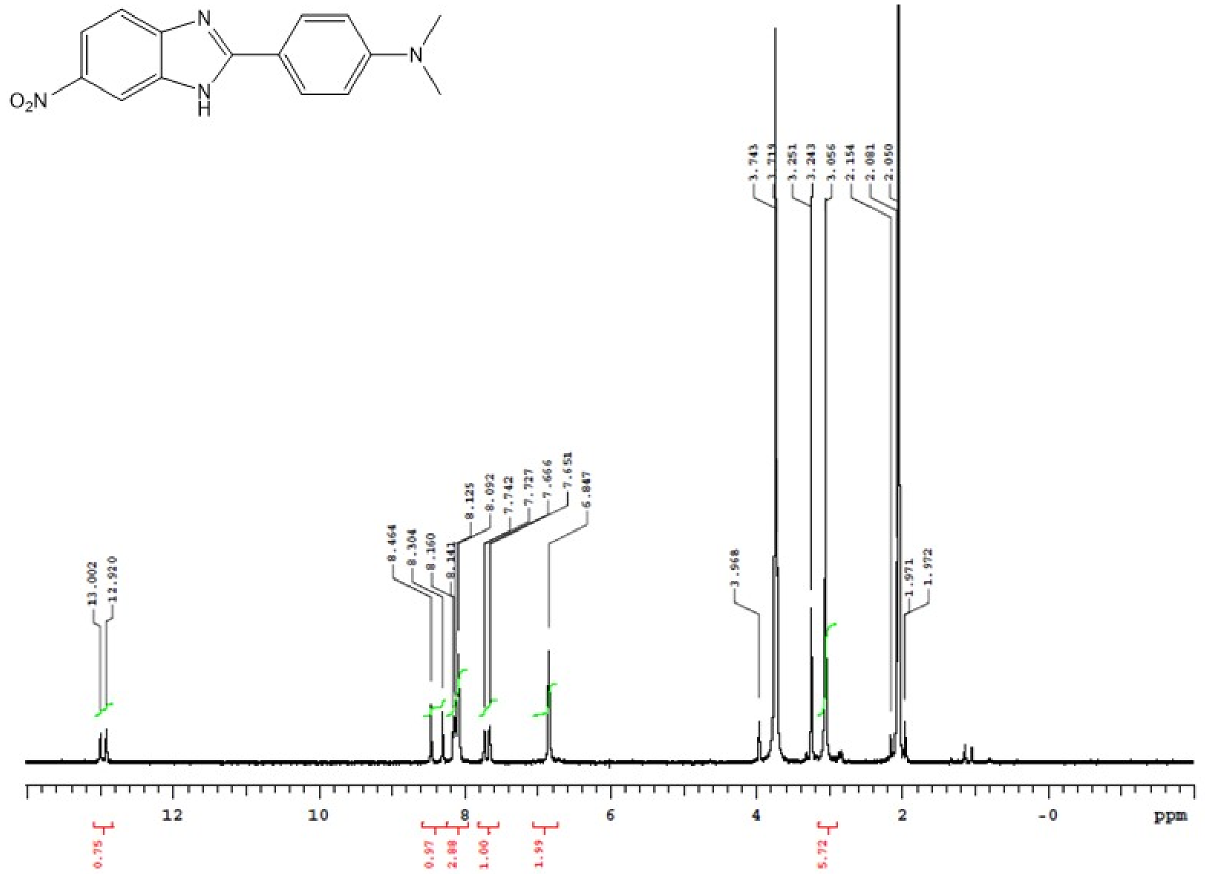


Figure S87. ^{1}H NMR spectrum of compound **1e** in acetone-d_6 at −76 °C.

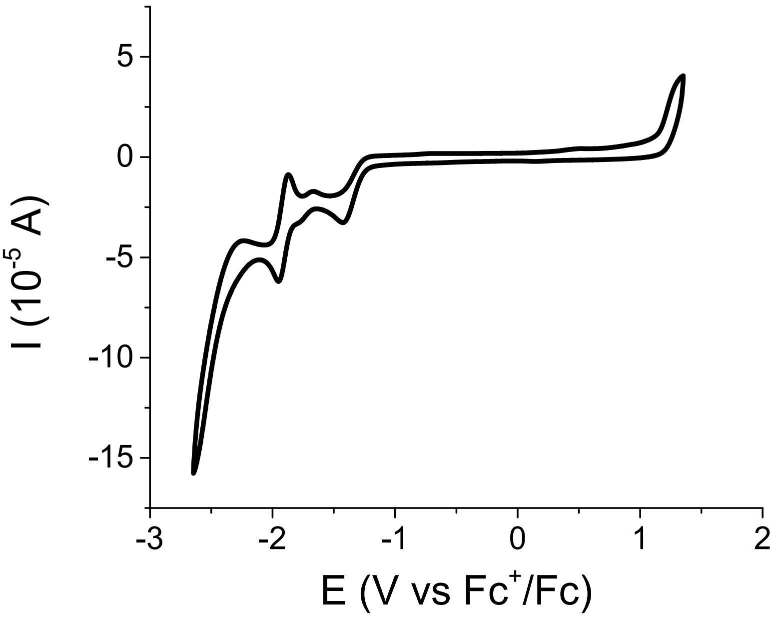


Figure S88. Cyclic voltammogram of **1a** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

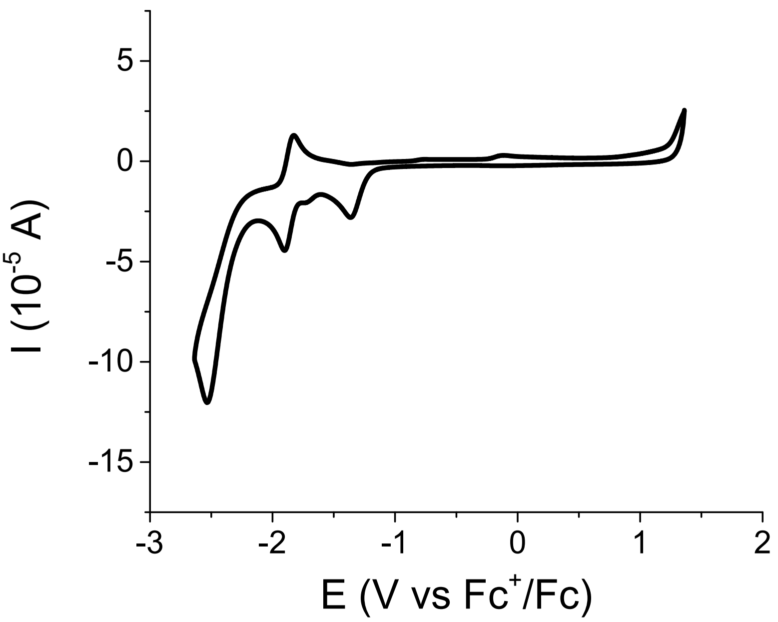


Figure S89. Cyclic voltammogram of **1b** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

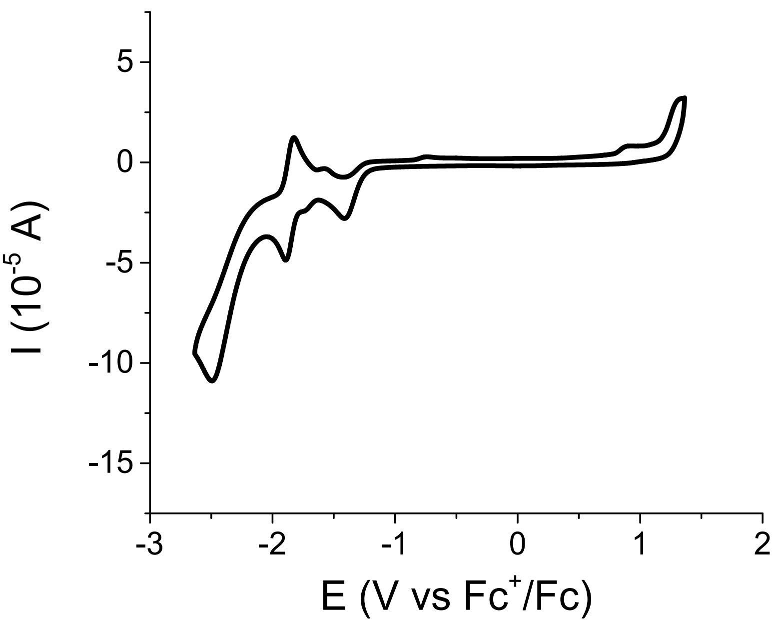


Figure S90. Cyclic voltammogram of **1c** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

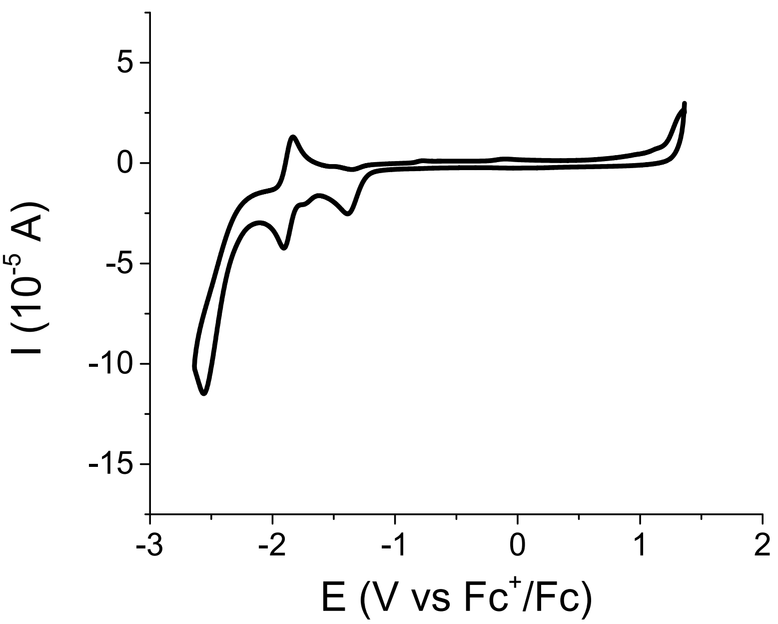


Figure S91. Cyclic voltammogram of **1d** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$. This figure corresponds to Fig. 8 of main text.

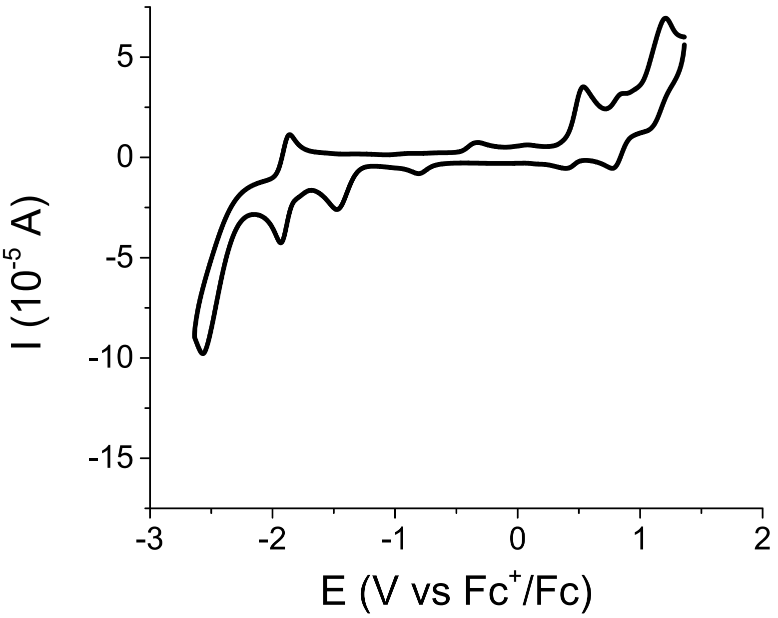


Figure S92. Cyclic voltammogram of **1e** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

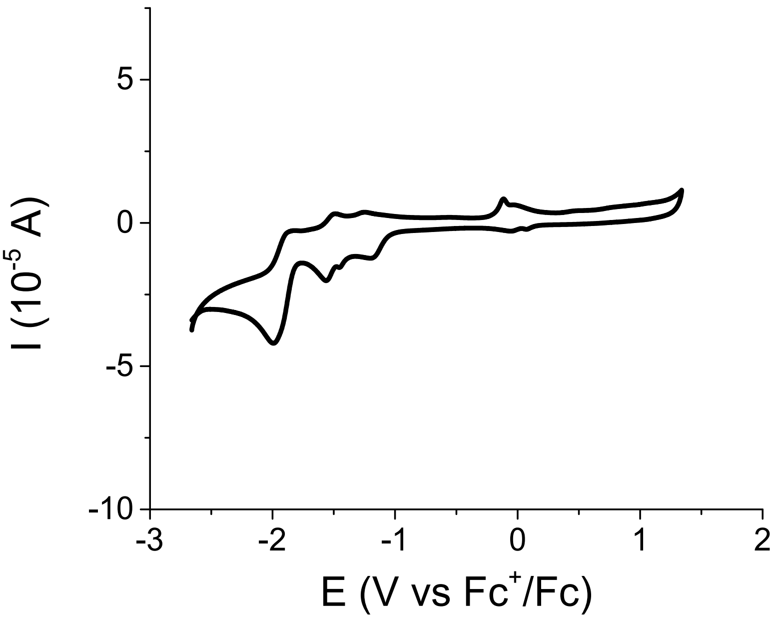


Figure S93. Cyclic voltammogram of **1f** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

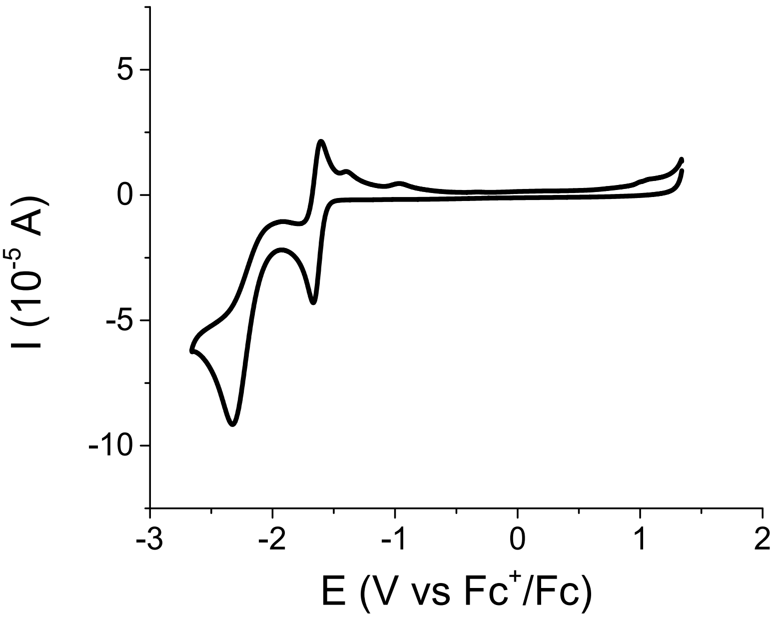


Figure S94. Cyclic voltammogram of **2a** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$. This Figure is included in Fig. 7 of main text.

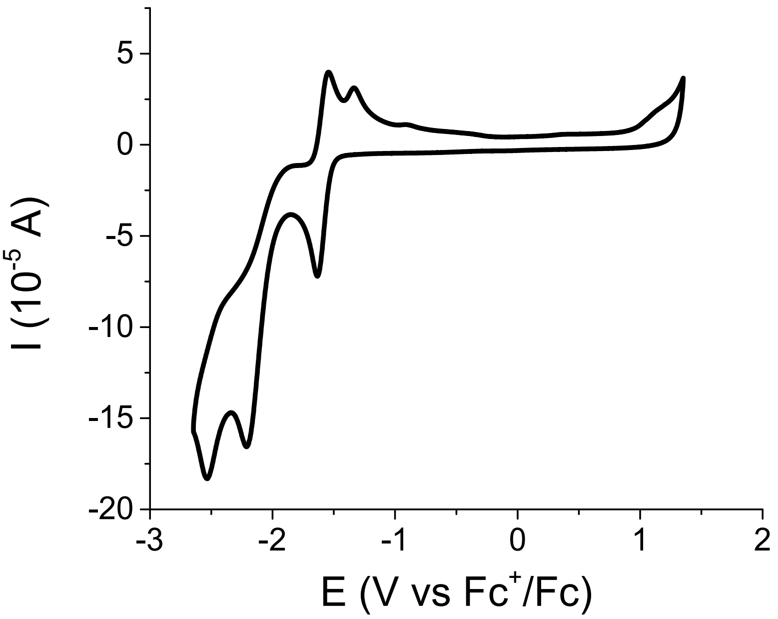


Figure S95. Cyclic voltammogram of **2b** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

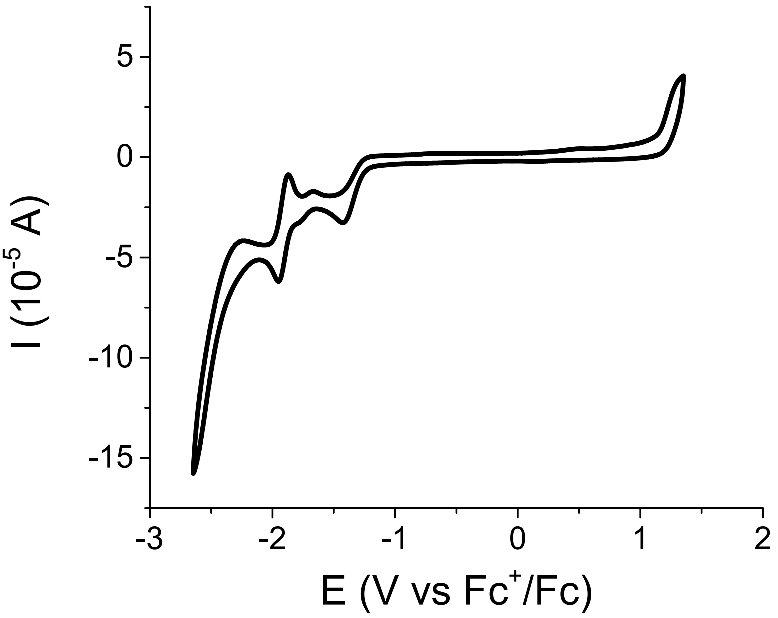


Figure S96. Cyclic voltammogram of **2c** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

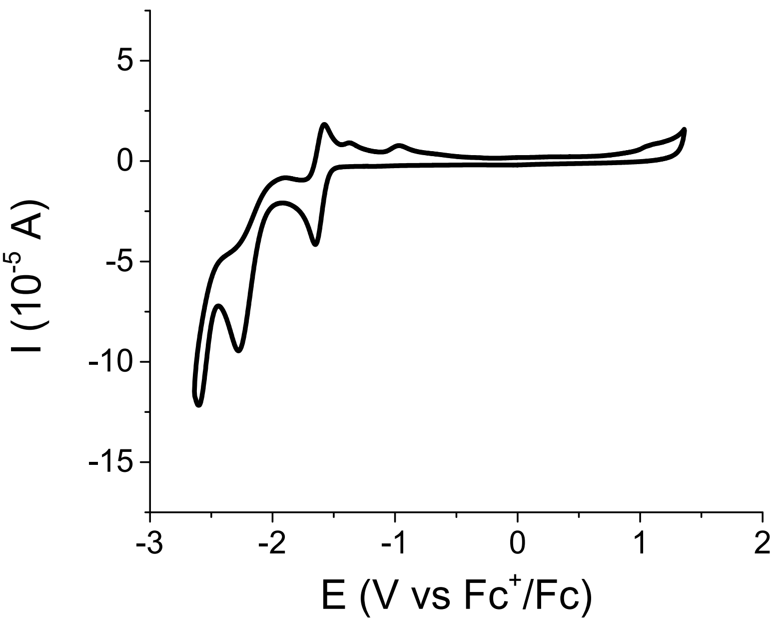


Figure S97. Cyclic voltammogram of **2d** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

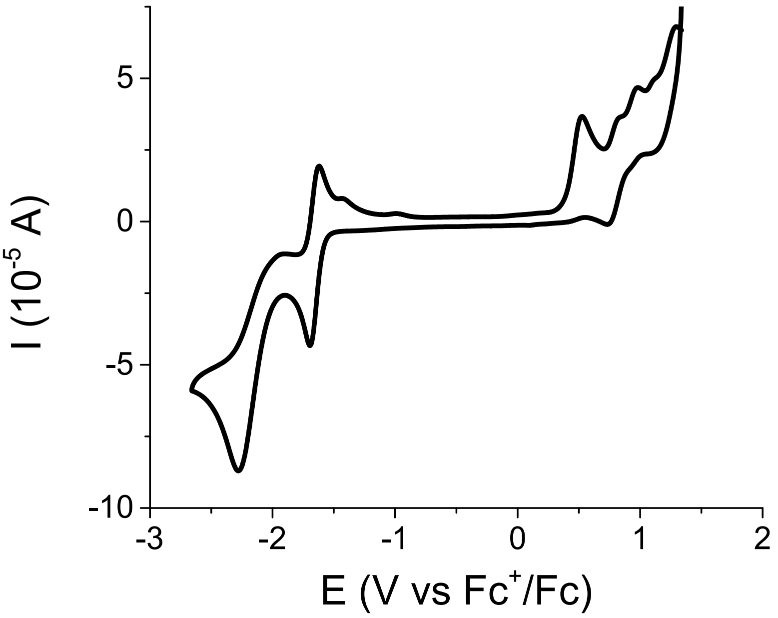


Figure S98. Cyclic voltammogram of **2e** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

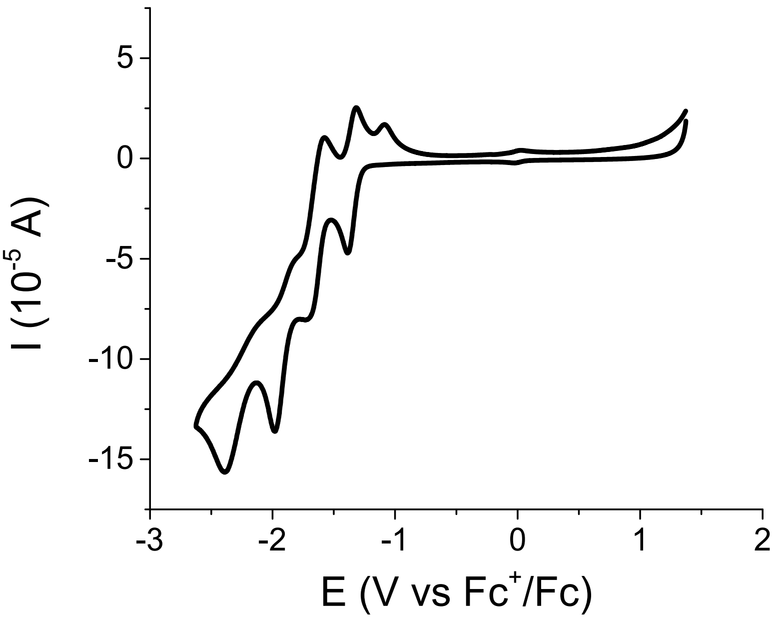


Figure S99. Cyclic voltammogram of **2f** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

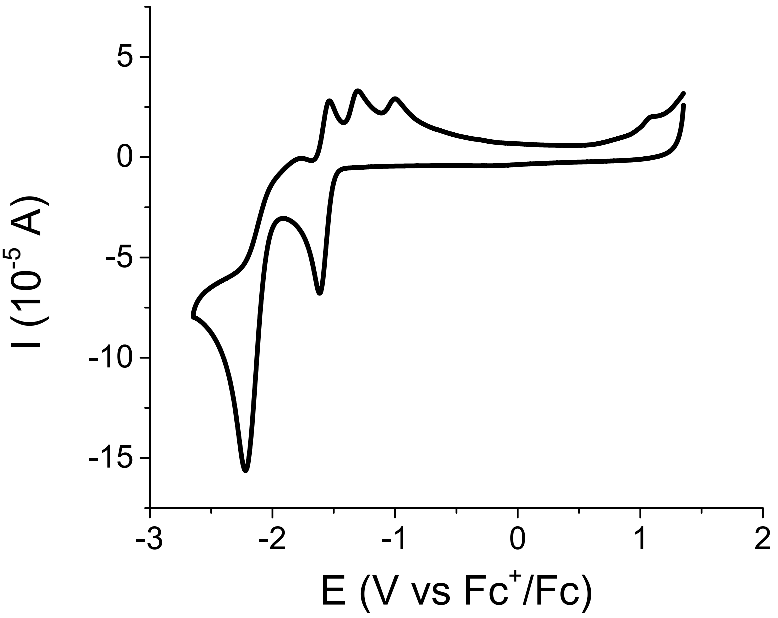


Figure S100. Cyclic voltammogram of **3a** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

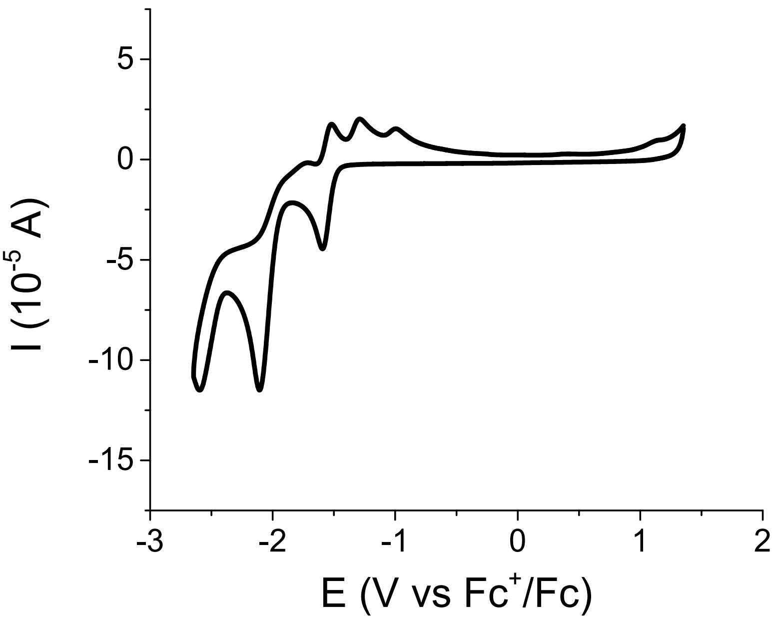


Figure S101. Cyclic voltammogram of **3b** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

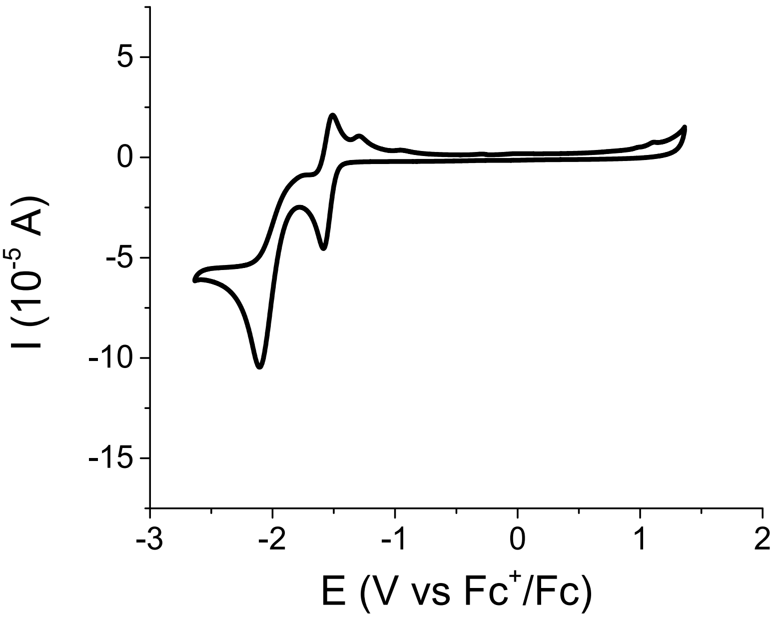


Figure S102. Cyclic voltammogram of **3c** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

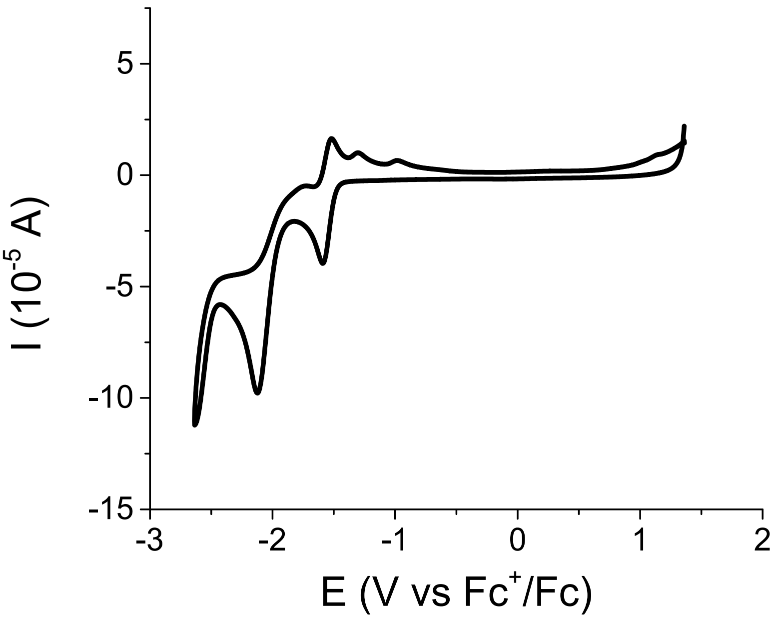


Figure S103. Cyclic voltammogram of **3d** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

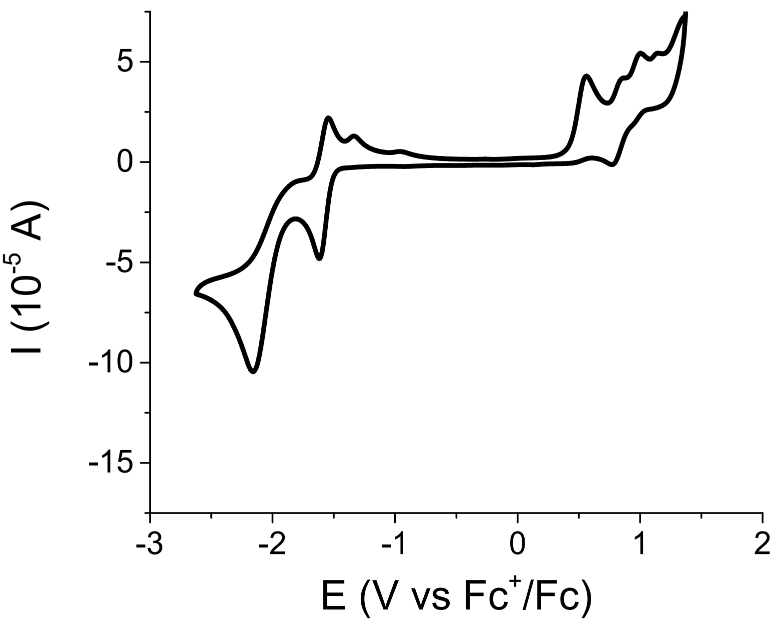


Figure S104. Cyclic voltammogram of **3e** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

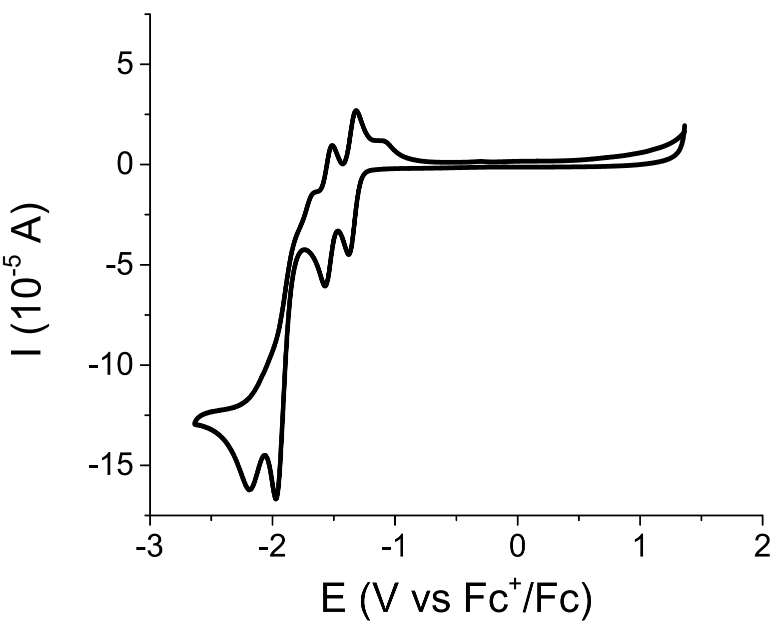


Figure S105. Cyclic voltammogram of **3f** (2 mM) recorded at a scan rate of 0.05 V s^{-1} in acetonitrile containing 0.1 M $TBAPF_6$.

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