

Supporting Information

Amine functionalization of *N,N,N',N'*-tetramethyl-*p*-phenylenediamine applicable to electrosynthesis a wide range of *p*-phenylenediamines in green conditions

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Table of Contents

Figure S1.	CVs of NDPM in solutions with various pHs	p.3
Figure S2.	CVs of NDPM during paired electrolysis at -0.6 V	p.4
Figure S3.	^{13}C NMR and DEPT 135° $^{13}\text{CNMR}$ spectrum of 2a	p.5
Figure S4.	Calculated natural charge of each atom in ADPM _{ox}	p.6
Figure S5.	FT-IR spectrum of NDPM	p.7
Figure S6.	Experimental and simulated ^1H NMR spectrum of NDPM	p.8
Figure S7.	^{13}C NMR spectrum of NDPM	p.9
Figure S8.	Mass spectrum of NDPM	p.10
Figure S9.	FT-IR spectrum of 2a	p.11
Figure S10.	^1H NMR spectrum of 2a	p.12
Figure S11.	^{13}C NMR spectrum of 2a	p.13
Figure S12.	Mass spectrum of 2a	p.14
Figure S13.	FT-IR spectrum of 2b	p.15
Figure S14.	^1H NMR spectrum of 2b	p.16
Figure S15.	^{13}C NMR spectrum of 2b	p.17
Figure S16.	Mass spectrum of 2b	p.18
Figure S17.	FT-IR spectrum of 2c	p.19
Figure S18.	^1H NMR spectrum of 2c	p.20
Figure S19.	^{13}C NMR spectrum of 2c	p.21
Figure S20.	Mass spectrum of 2c	p.22

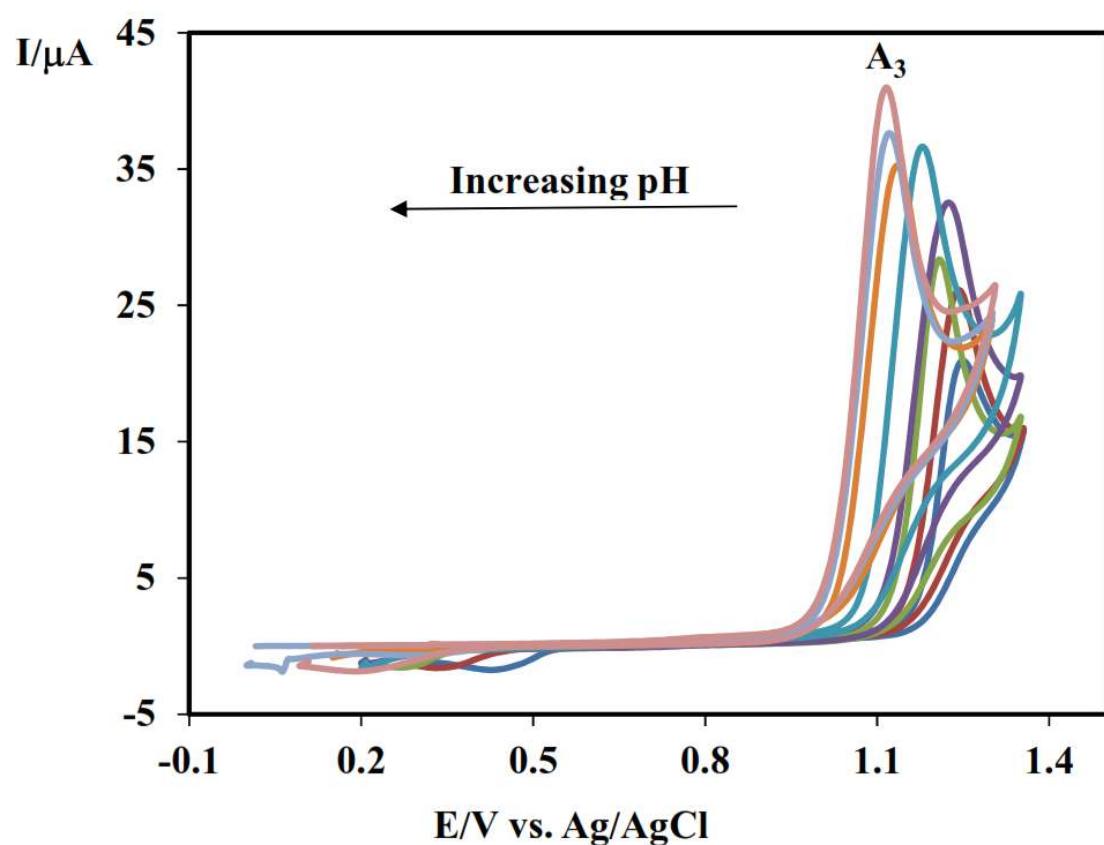


Fig. S1. Cyclic voltammograms of 0.4 mM **1** toward positive going scan in ethanol/ buffered solutions (1 ml ethanol/9 ml buffer) with various pH values; Scan rate: 100 mV s⁻¹.

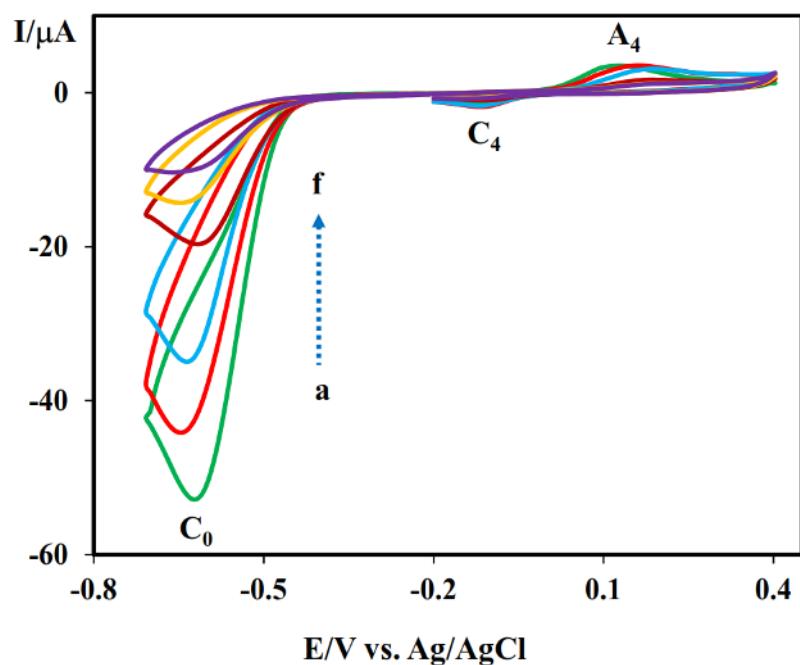


Fig. S2. Cyclic voltammograms of 0.125 mmol of **1** in the presence of 0.125 mmol **4-TSA** in ethanol/acetate buffered solutions (0.2 M, pH = 5.0) (20 mL ethanol/60 mL buffer solution), (a) to (f): progress of electrolysis.

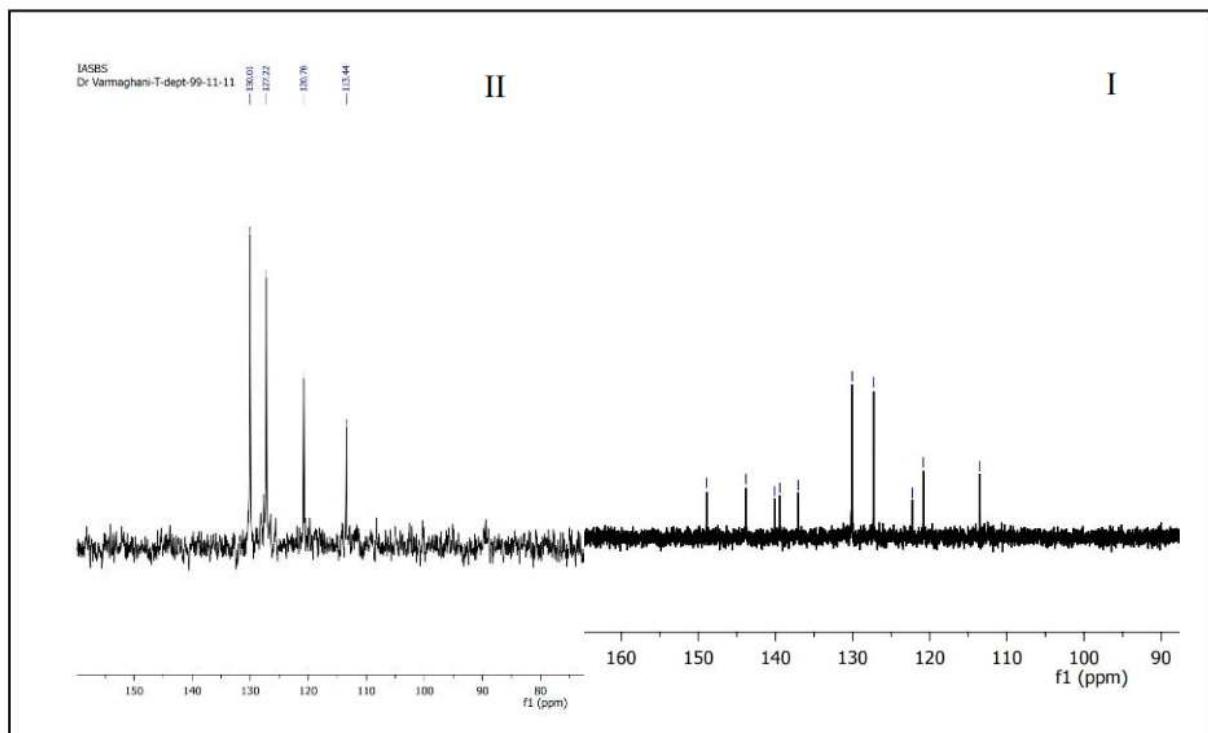


Fig. S3. I: ^{13}C NMR and II: DEPT 135° ^{13}C NMR spectra of **2a**

Atomic Number	Atom type	Charge
1	C	-0.09478
2	C	-0.00915
3	C	0.153914
4	C	-0.12924
5	C	0.067916
6	C	-0.40797
7	H	0.216627
8	H	0.256257
9	H	0.228252
10	N	0.244173
11	N	-0.33294
12	N	0.123167
13	N	-0.31512
14	O	0.261419
15	O	0.231905
16	C	-0.48314
17	C	-0.44068
18	C	-0.38849
19	H	0.192497
20	H	0.272697
21	H	0.231077
22	H	0.172979
23	H	0.27697
24	H	0.225565
25	H	0.327888
26	H	0.343031
27	H	0.287113
28	H	0.261173
29	H	0.226884

Fig. S4: Calculated natural charge of each atom in ADPM_{ox}

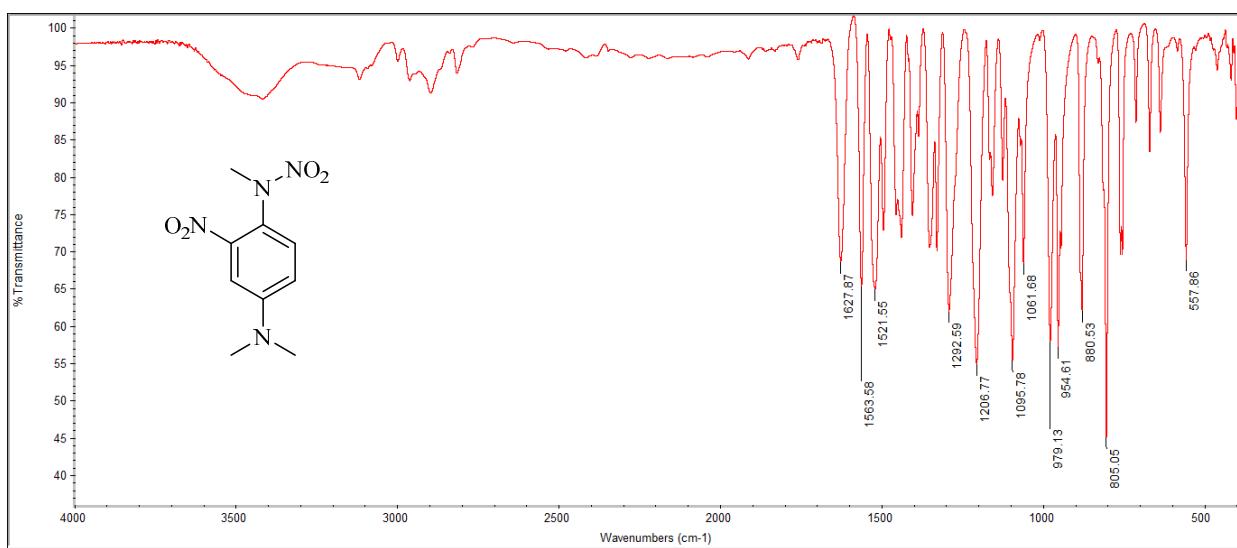


Figure S5. FT-IR spectrum of NDPM

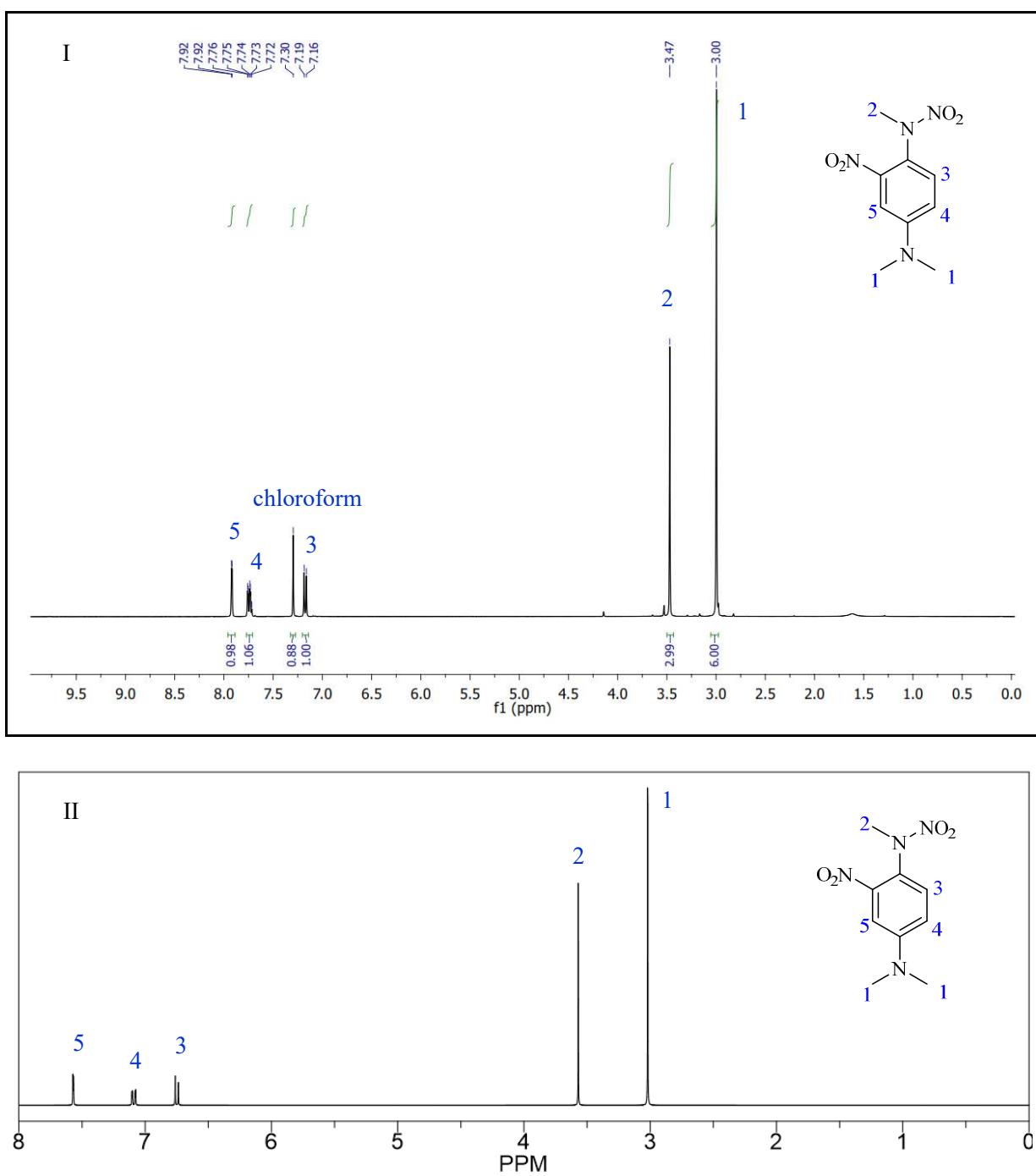


Figure S6. I: Experimental and II: simulated ^1H NMR spectra of NDPM

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Sample code:MA-2 in CDCl₃ (Abbasi)

-145.19

-138.26

-132.80

~124.50

~119.09

~117.26

77.36
76.72

-42.52

-31.53

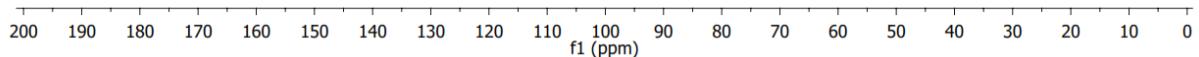
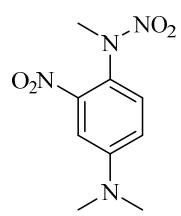


Figure S7. ¹³C NMR spectrum of NDPM

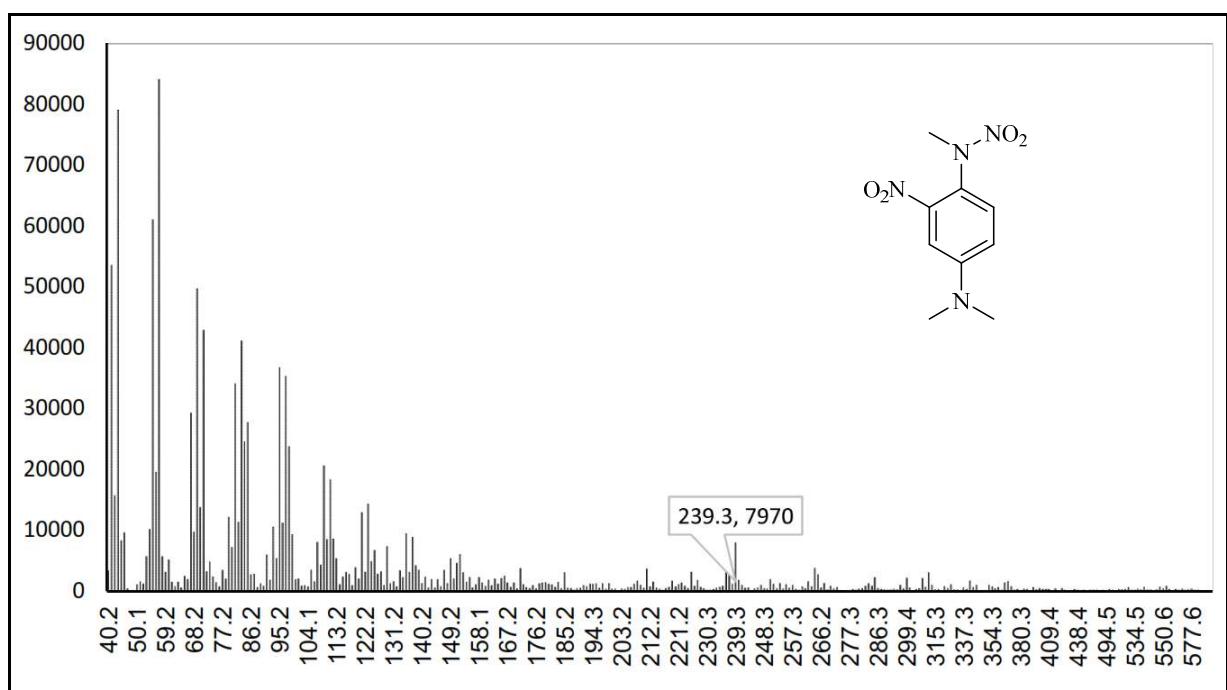


Figure S8. Mass spectrum of NDPM

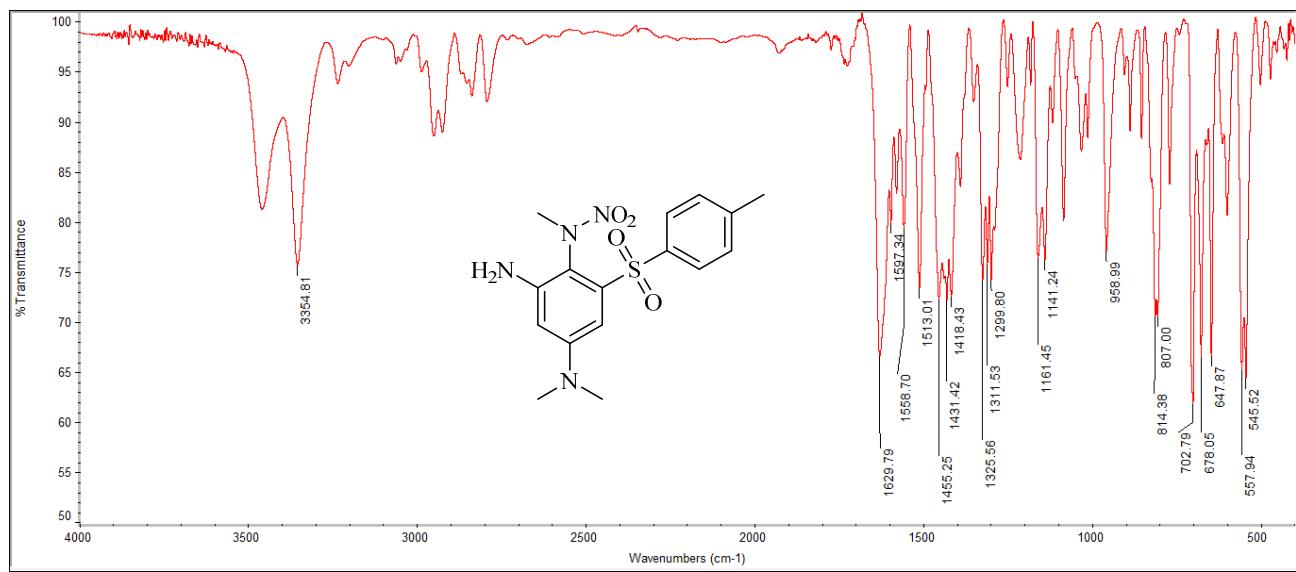


Figure S9. FT-IR spectrum of **2a**

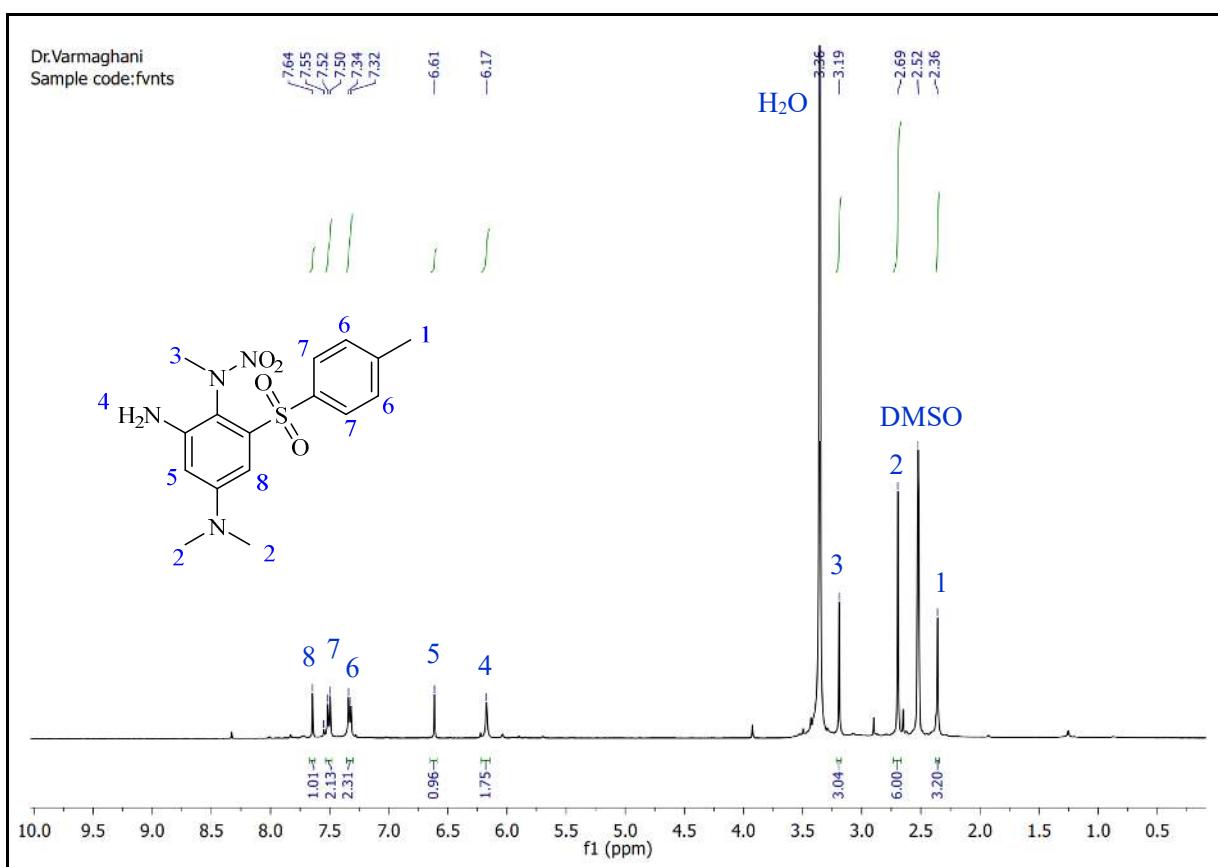


Figure S10. ^1H NMR spectrum of **2a**

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Sample code:MA (Abbasi) C-NMR

-146.90

-141.83

-140.12

-135.43

-137.05

-130.05

-127.25

-122.25

-120.83

-113.50

-42.94

-40.63

-40.43

-40.22

-39.80

-39.59

-39.38

-37.08

-21.45

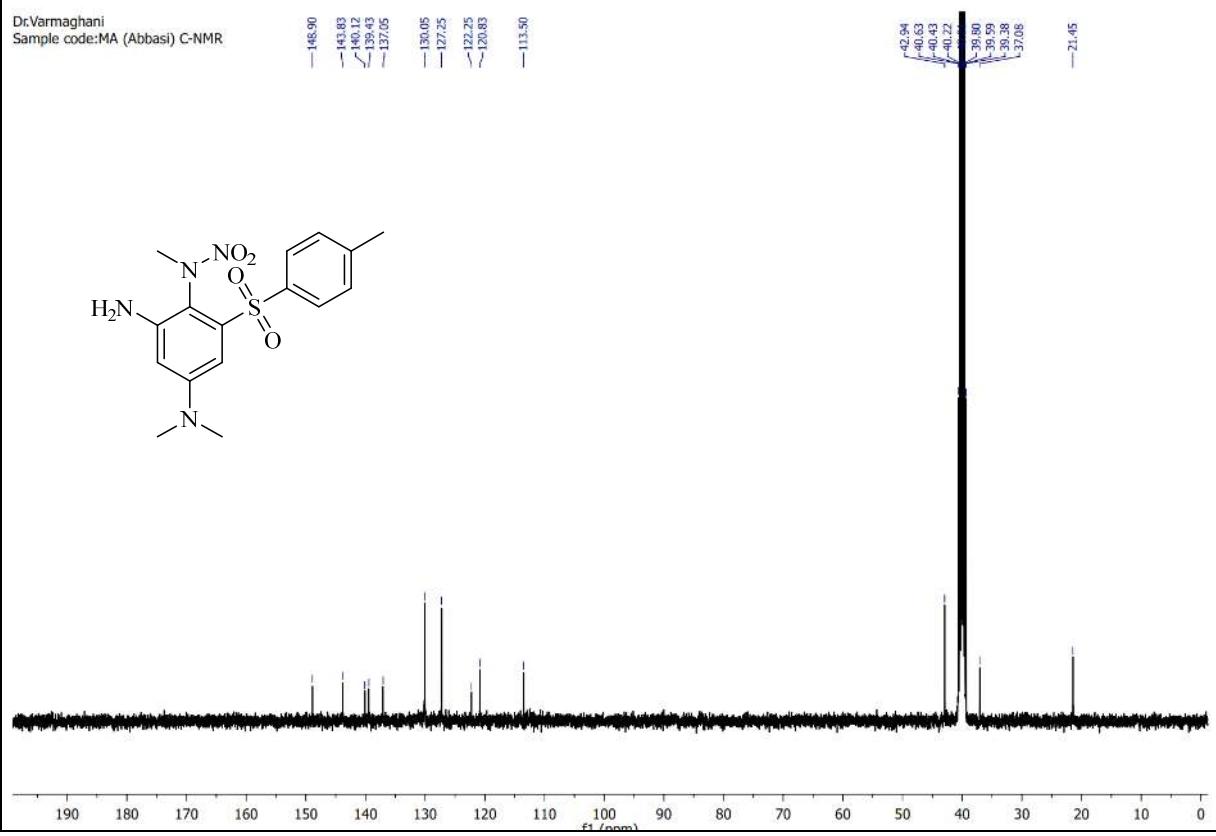
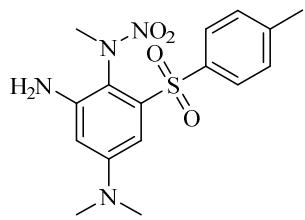


Figure S11. ^{13}C NMR spectrum of **2a**

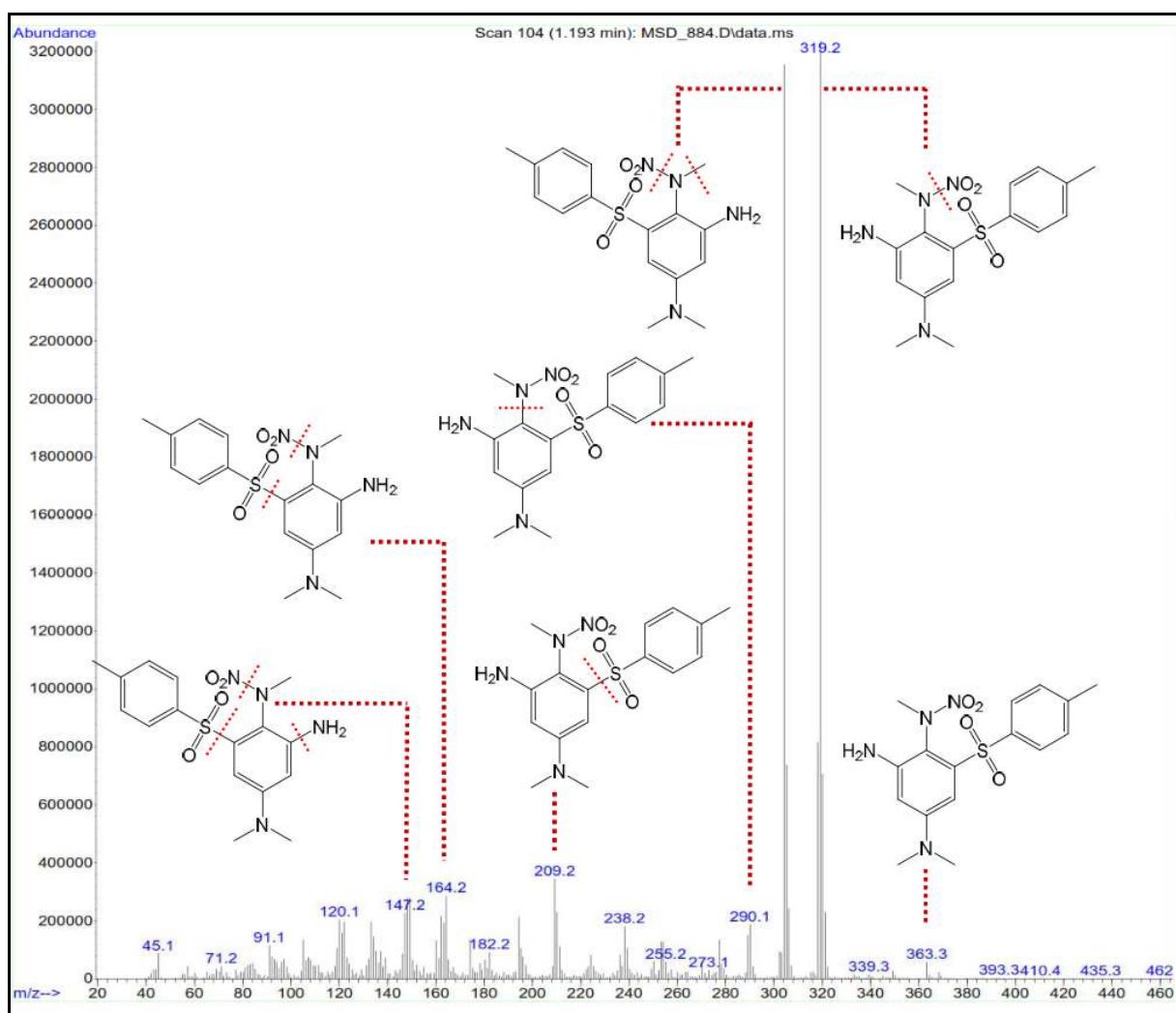


Figure S12. Mass spectrum of **2a**

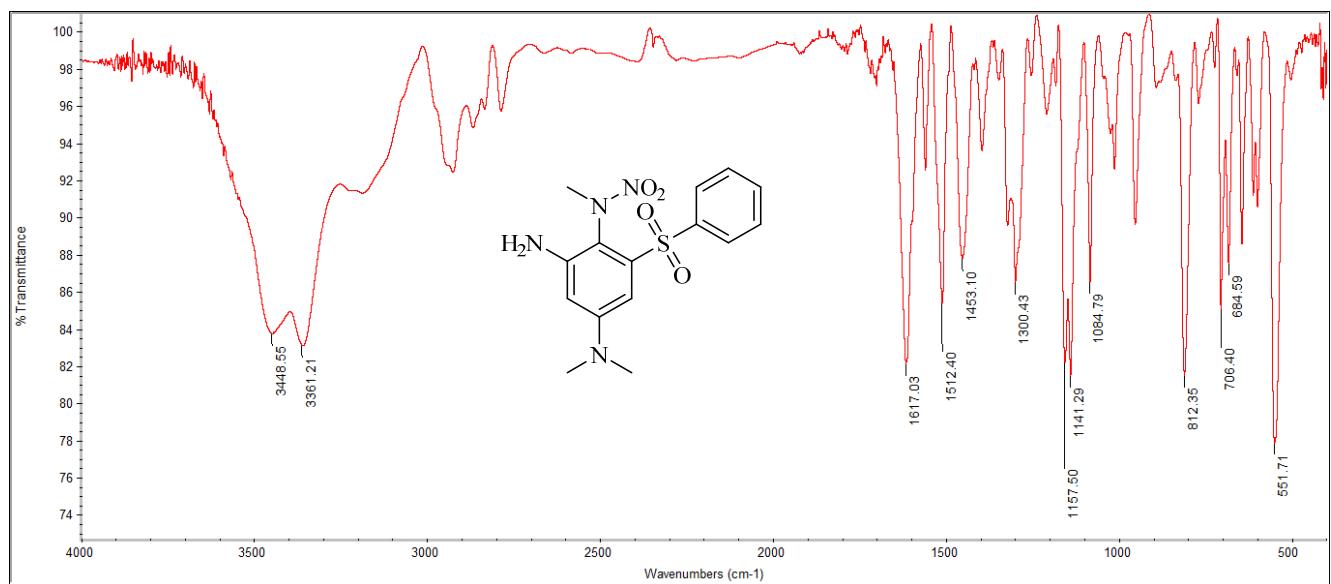


Figure S13. FT-IR spectrum of **2b**

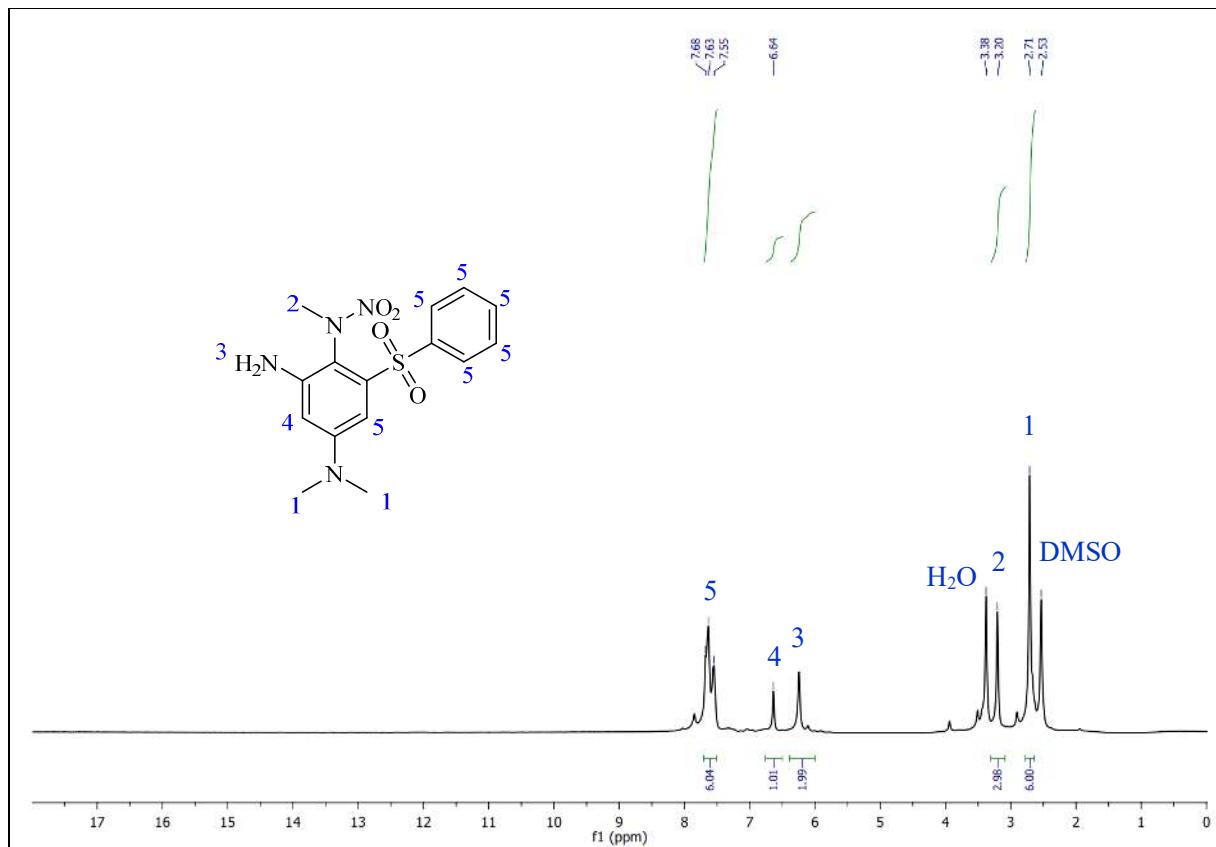


Figure S14. ^1H NMR spectrum of **2b**

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Sample code:MASB (Abbasi)

-149.06
-142.90
-139.34
-137.23
-133.48
-129.62
-127.16
-121.81
-120.94
-120.79
-113.48

-42.94
-37.03

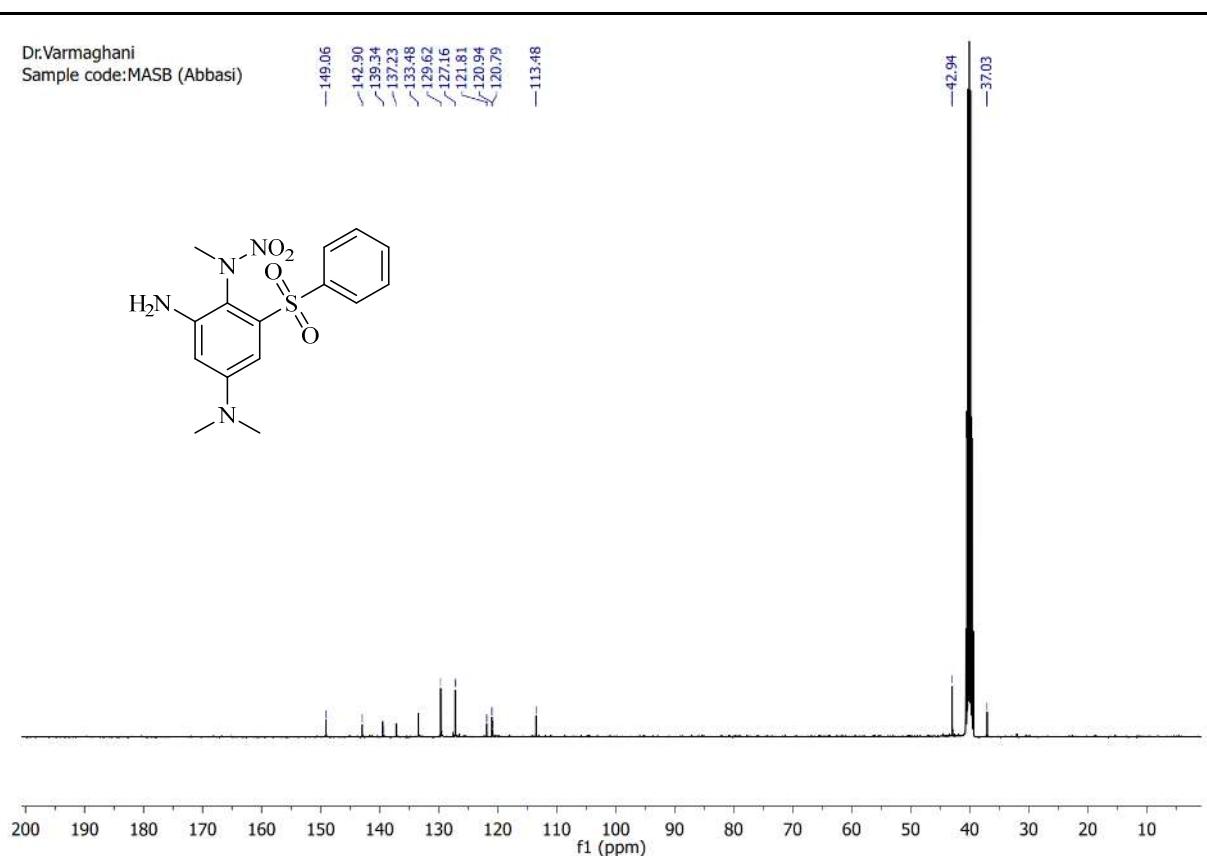
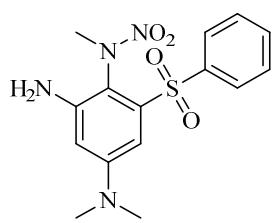


Figure S15. ¹³C NMR spectrum of **2b**

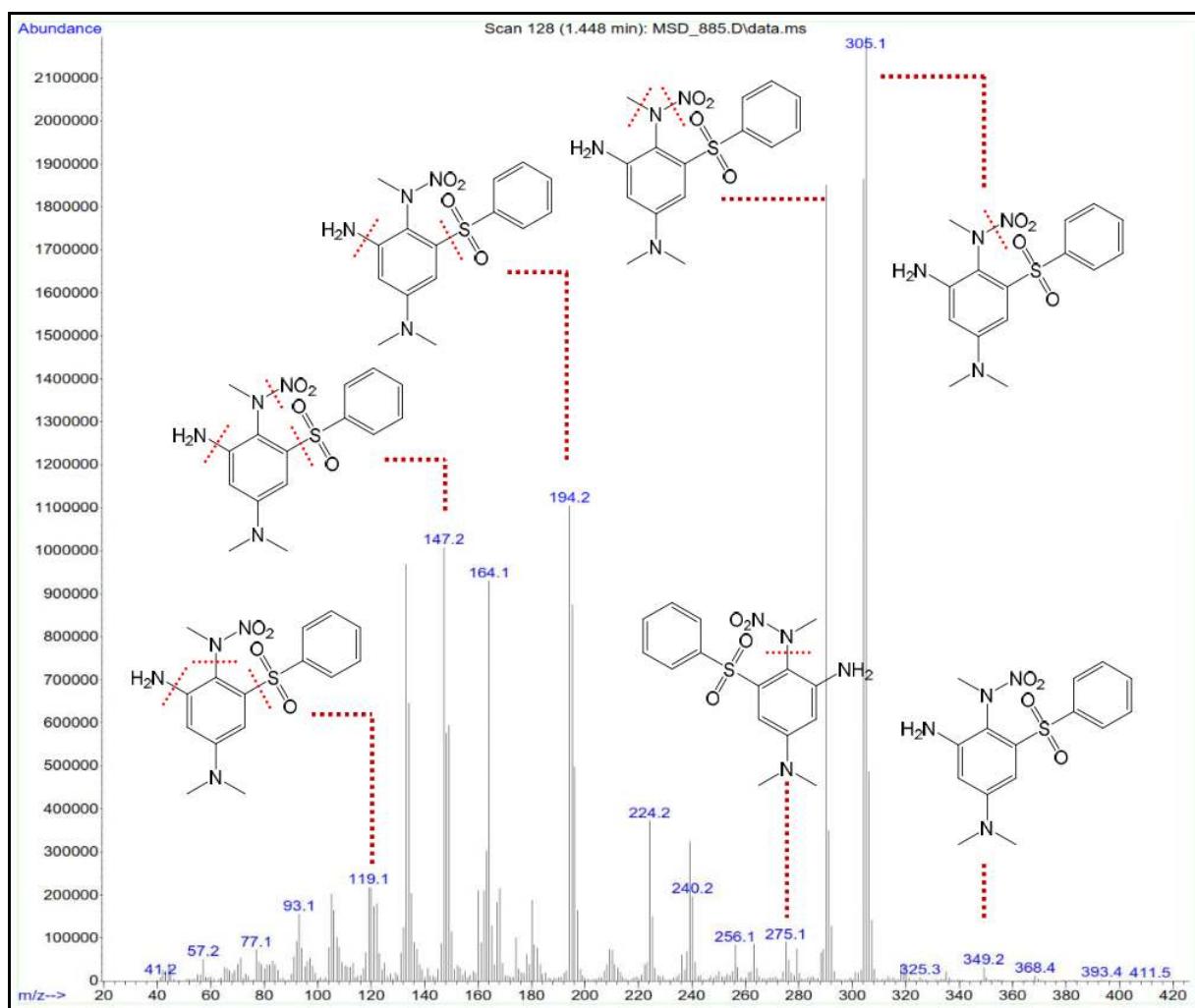


Figure S16. Mass spectrum of **2b**

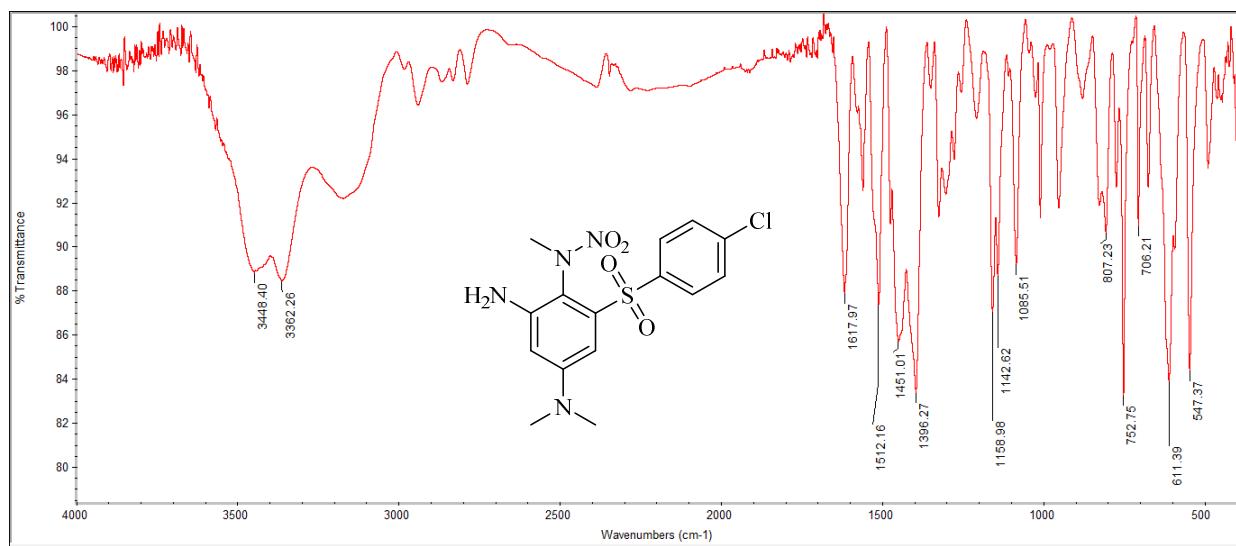


Figure S17. FT-IR spectrum of **2c**

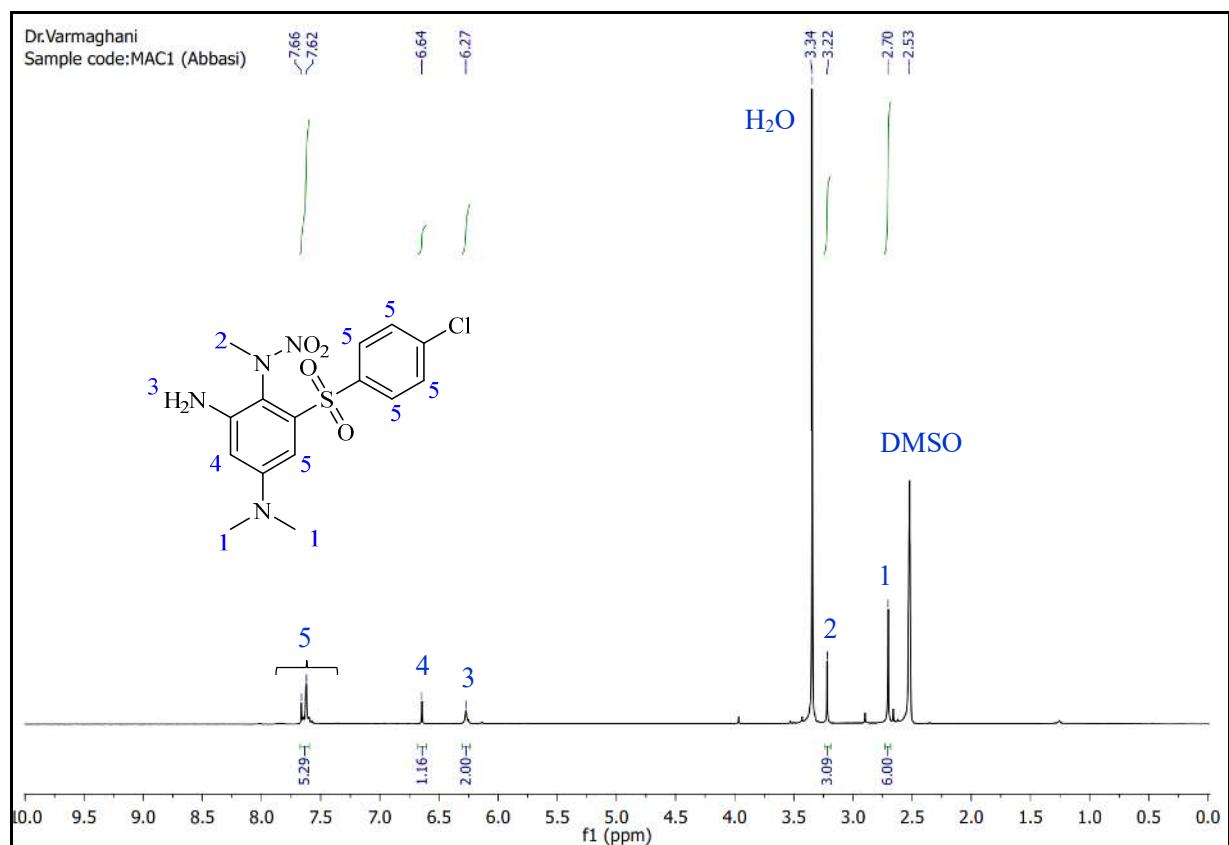


Figure S18. ^1H NMR spectrum of **2c**

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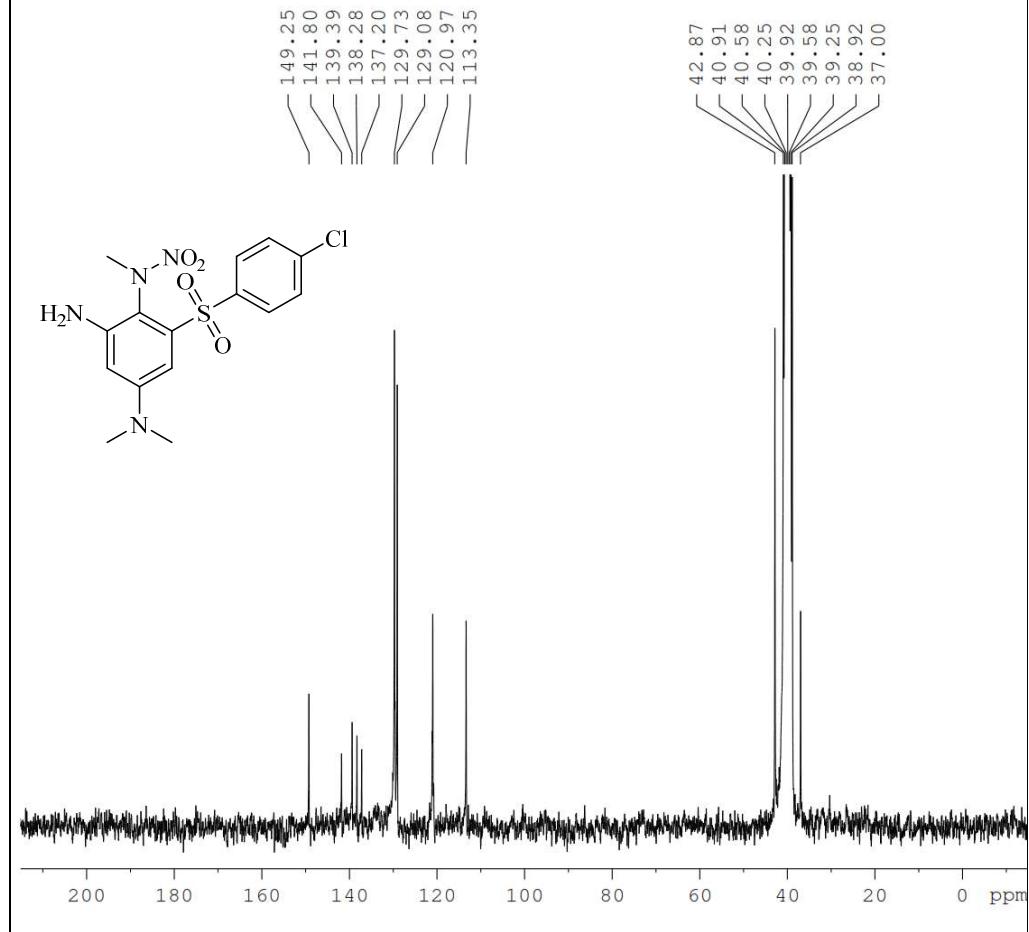


Figure S19. ^{13}C NMR spectrum of **2c**

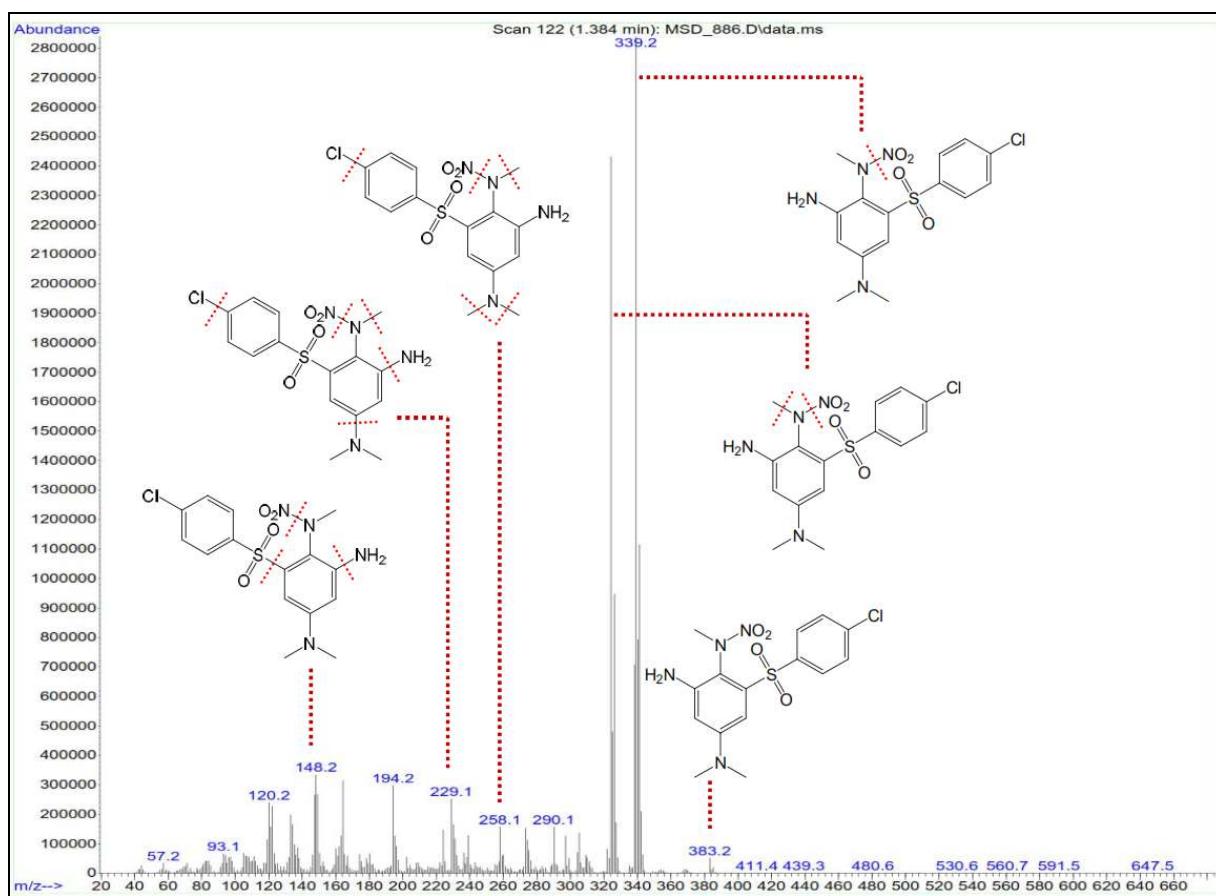


Figure S20. Mass spectrum of **2c**