Electronic Supplementary Information

Iodine Promoted Iodosulfonylation of Alkynes with Sulfonyl Hydrazides in an Aqueous Medium: Highly Stereoselective Synthesis of (*E*)-β-Iodo Vinylsulfones

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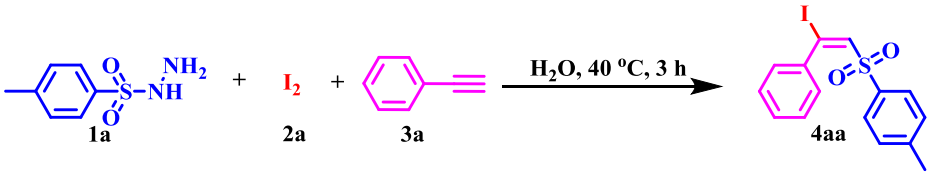
Contents

1. General Information

Unless otherwise noted, all reagents and solvents were obtained from commercial sources and used without further purification. Solvents were dried using standard methods and distilled before use. Reactions were monitored by thin-layer chromatography (TLC) on silica plates (F-254) and visualized under UV light. Melting points were obtained on a Büchi Melting Point B-540 apparatus and were uncorrected. All ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker ARX-600, 600 MHz spectrometers with TMS as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, *J*, are reported in hertz (Hz). Column chromatography was run on silica gel (200-300 mesh) from Qingdao Ocean Chemicals (Qingdao, Shandong, China).

2. General Procedure and Product Characterization

2.1 The Optimal Experimental Conditions



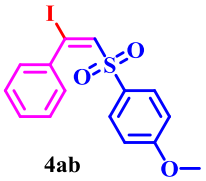
Representative procedure for the synthesis of (*E*)-β-iodo vinylsulfones products:

A mixture of sulfonyl hydrazides (0.27 mmol), alkyne (0.30 mmol), and iodine (0.54 mmol) in water (3.0 mL) was placed in a test tube equipped with a magnetic stirring bar. The reaction mixture was stirred at 40 ℃ for 3h. After the reaction was completed, the mixture was quenched by the addition of satd aq $Na_2S_2O_3$ (8 mL). Further stirring was followed by extraction with ethyl acetate (3 × 10 mL). The organic phase was separated, washed with brine, dried ($MgSO_4$), filtered, and concentrated in vacuo to give the crude product, which was purified by column chromatography on silica gel with a mixture of ethyl acetate/petroleum (1:10, v/v) to afford the desired product **4**.

2.2 Product Characterization

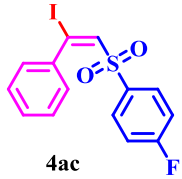
4aa **(*E*)-1-((2-iodo-2-phenylvinyl)sulfonyl)-4-methylbenzene (4aa)[1]**

Yield: 80% (83 mg), white solid, m.p.:78.2 – 79.8 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.46 (d, *J* = 8.3 Hz, 2H), 7.36 (s, 1H), 7.32 – 7.27 (m, 3H), 7.24 – 7.22 (m, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 144.48, 141.19, 139.59, 137.26, 129.70, 129.58, 127.84, 127.81, 127.62, 114.07, 21.55.



4ab **(*E*)-1-((2-iodo-2-phenylvinyl)sulfonyl)-4-methoxybenzene (4ab)** [3]

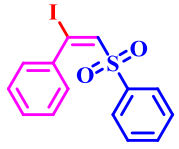
Yield:85% (92 mg), white solid, m.p.:110.3 – 111.2 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.49 (d, *J* = 8.7 Hz, 2H), 7.37 (s, 1H), 7.32 – 7.27 (m, 3H), 7.23 (d, *J* = 6.9 Hz, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 163.55, 141.59, 139.62, 131.68, 130.01, 129.66, 127.87, 127.64, 114.16, 113.52, 55.60.



4ac

(*E*)-1-fluoro-4-((2-iodo-2-phenylvinyl)sulfonyl)benzene (4ac)

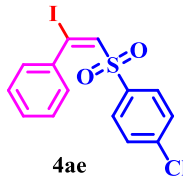
Yield:78% (82 mg), white solid, m.p.: 94.5 – 95.8 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.54 (dd, *J* = 8.7, 5.1 Hz, 2H), 7.40 (s, 1H), 7.33 – 7.27 (m, 3H), 7.20 (d, *J* = 7.3 Hz, 2H), 7.03 (t, *J* = 8.5 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 166.36, 164.66, 141.16, 139.42, 136.14, 130.68, 130.61, 129.86, 127.97, 127.58, 116.25, 116.10, 114.79.



4ad

(*E*)-(1-iodo-2-(phenylsulfonyl)vinyl)benzene (4ad) [3]

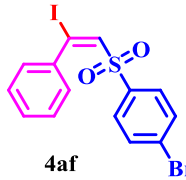
Yield: 75% (75 mg), white solid, m.p.:67.2 – 68.4 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.57 (d, *J* = 7.7 Hz, 2H), 7.54 (d, *J* = 7.4 Hz, 1H), 7.40 – 7.37 (m, 3H), 7.33 – 7.27 (m, 3H), 7.21 (d, *J* = 7.2 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 141.05, 140.18, 139.51, 133.40, 129.77, 128.93, 127.90, 127.75, 127.60, 114.64.



4ae

(*E*)-1-chloro-4-((2-iodo-2-phenylvinyl)sulfonyl)benzene (4ae) [3]

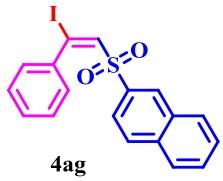
Yield: 81% (88 mg), white solid, m.p.:103.2 – 104.1 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.46 (d, *J* = 8.5 Hz, 2H), 7.39 (s, 1H), 7.34 – 7.32 (m, 3H), 7.29 (t, *J* = 7.4 Hz, 2H), 7.19 (d, *J* = 7.3 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 140.92, 140.16, 139.41, 138.58, 129.90, 129.22, 129.18, 127.97, 127.57, 115.15.



4af

(*E*)-1-bromo-4-((2-iodo-2-phenylvinyl)sulfonyl)benzene (4af) [1]

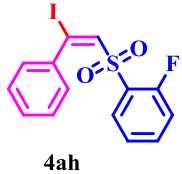
Yield: 73% (88 mg), white solid, m.p.:99.2 – 100.8 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.51 – 7.49 (m, 2H), 7.39 – 7.37 (m, 3H), 7.33 – 7.27 (m, 3H), 7.20 – 7.18 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 140.87, 139.40, 139.12, 132.17, 129.90, 129.27, 128.76, 127.97, 127.56, 115.20.



4ag

(*E*)-2-((2-iodo-2-phenylvinyl)sulfonyl)naphthalene (4ag) [4]

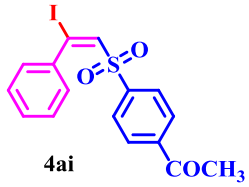
Yield: 70% (79 mg), white solid, m.p.: 78.1 – 79.5 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 8.00 (s, 1H), 7.87 (dd, *J* = 8.3, 2.7 Hz, 2H), 7.79 (d, *J* = 8.2 Hz, 1H), 7.65 (t, *J* = 7.1 Hz, 1H), 7.64 – 7.57 (m, 2H), 7.46 (s, 1H), 7.25 – 7.21 (m, 1H), 7.21 – 7.18 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 141.20, 139.40, 136.79, 135.02, 131.88, 129.92, 129.80, 129.30, 129.28, 129.22, 127.79, 127.57, 127.47, 122.33, 114.72.



4ah

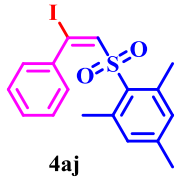
(*E*)-1-fluoro-2-((2-iodo-2-phenylvinyl)sulfonyl)benzene (4ah)

Yield: 61% (64 mg), white solid, m.p.: 115.6 – 116.5 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.52 (t, J = 4.4 Hz, 2H), 7.43 – 7.40 (m, 1H), 7.25 – 7.20 (m, 3H), 7.18 – 7.14 (m, 3H), 7.06 (t, J = 7.6 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 160.07, 158.37, 140.15, 139.35, 135.87, 135.82, 129.83, 129.79, 127.81, 127.45, 124.28, 124.25, 116.93, 116.79, 115.67.



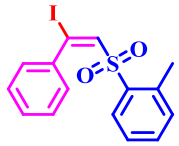
4ai **(*E*)-1-(4-((2-iodo-2-phenylvinyl)sulfonyl)phenyl)ethan-1-one (4ai)**

Yield: 60% (67 mg), white solid, m.p.: 85.3 – 86.5 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.53 (d, J = 8.4 Hz, 2H), 7.49 – 7.46 (m, 3H), 7.36 (s, 1H), 7.32 – 7.27 (m, 3H), 7.22 (d, J = 7.2 Hz, 2H), 2.21 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ_C 163.68, 137.79, 136.35, 134.78, 129.97, 125.06, 124.40, 123.16, 122.85, 114.25, 109.62, 19.97.



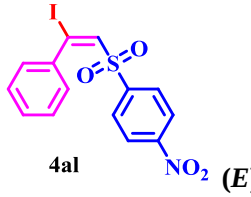
4aj **(*E*)-2-((2-iodo-2-phenylvinyl)sulfonyl)-1,3,5-trimethylbenzene (4aj)**

Yield: 77% (86 mg), white solid, m.p.: 98.3 – 99.1 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.42 (s, 1H), 7.22 (t, J = 7.3 Hz, 1H), 7.17 (t, J = 7.5 Hz, 2H), 7.12 – 7.10 (m, 2H), 6.78 (s, 2H), 2.41 (s, 6H), 2.24 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 143.24, 143.10, 139.51, 139.49, 134.41, 131.79, 129.43, 127.79, 127.13, 112.42, 22.29, 20.87.



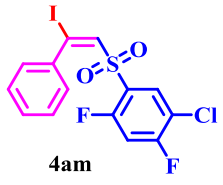
4ak **(*E*)-1-((2-iodo-2-phenylvinyl)sulfonyl)-2-methylbenzene (4ak)** [3]

Yield: 70% (73 mg), white solid, m.p.: 72.1 – 73.3 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.45 – 7.43 (m, 2H), 7.36 (t, J = 7.4 Hz, 1H), 7.23 (t, J = 8.0 Hz, 2H), 7.19 – 7.14 (m, 4H), 7.04 (t, J = 7.6 Hz, 1H), 2.61 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 141.00, 139.25, 138.26, 137.52, 133.28, 132.11, 129.72, 129.32, 127.77, 127.52, 126.04, 114.21, 20.32.



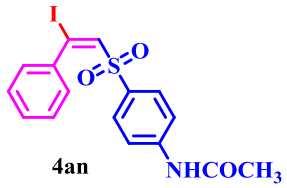
4al **(*E*)-1-((2-iodo-2-phenylvinyl)sulfonyl)-4-nitrobenzene (4al)**

Yield: 30% (33 mg), white solid, m.p.: 104.6 – 105.7 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 8.17 (d, J = 8.7 Hz, 2H), 7.69 (d, J = 8.7 Hz, 2H), 7.44 (s, 1H), 7.35 (t, J = 7.4 Hz, 1H), 7.28 (d, J = 7.8 Hz, 2H), 7.17 (d, J = 7.6 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 150.32, 145.76, 140.24, 139.20, 130.22, 129.14, 128.09, 127.58, 123.90, 116.94.



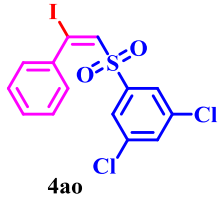
4am **(*E*)-1-chloro-2,4-difluoro-5-((2-iodo-2-phenylvinyl)sulfonyl)benzene (4am)**

Yield: 79% (94 mg), white solid, m.p.: 137.8 – 138.5 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.50 (d, J = 1.1 Hz, 1H), 7.31 (t, J = 7.4 Hz, 2H), 7.24 (t, J = 7.7 Hz, 2H), 7.15 – 7.14 (m, 2H), 6.98 (t, J = 8.6 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 162.30, 162.23, 160.57, 160.50, 158.93, 158.86, 157.21, 157.14, 140.18, 138.96, 131.99, 130.18, 127.86, 127.32, 116.23, 106.65, 106.47, 106.30.



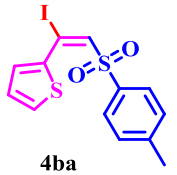
4an **(*E*)-*N*-(4-((2-iodo-2-phenylvinyl)sulfonyl)phenyl)acetamide (4an)**

Yield: 83% (96 mg), white solid, m.p.: 159.2 – 160.1 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.52 (d, J = 8.6 Hz, 2H), 7.48 (d, J = 8.8 Hz, 2H), 7.45 (s, 1H), 7.36 (s, 1H), 7.32 – 7.27 (m, 3H), 7.22 (d, J = 6.9 Hz, 2H), 2.20 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 168.44, 142.55, 141.07, 139.53, 134.69, 129.81, 129.14, 127.91, 127.59, 119.00, 114.40, 24.72.



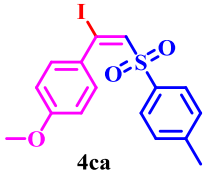
4ao **(*E*)-1,3-dichloro-5-((2-iodo-2-phenylvinyl)sulfonyl)benzene (4ao)**

Yield: 73% (86 mg), white solid, m.p.: 99.3 – 100.5 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.38 (s, 1H), 7.35 (d, J = 7.3 Hz, 1H), 7.31 (t, J = 7.4 Hz, 2H), 7.21 (d, J = 7.3 Hz, 2H), 7.04 (d, J = 4.0 Hz, 2H), 6.99 – 6.96 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 140.13, 139.22, 130.19, 128.04, 127.46, 116.48, 111.53, 111.49, 111.38, 111.34, 109.05.



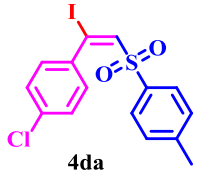
4ba **(*E*)-2-(1-iodo-2-tosylvinyl)thiophene (4ba)** [1]

Yield: 78% (82 mg), white solid, m.p.:96.2 – 97.6 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.59 (d, J = 7.9 Hz, 2H), 7.54 (d, J = 2.8 Hz, 1H), 7.50 (d, J = 4.7 Hz, 1H), 7.31 (s, 1H), 7.24 (d, J = 7.9 Hz, 2H), 7.02 (t, J = 4.2 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 144.61, 141.13, 141.00, 137.03, 131.43, 129.98, 129.62, 127.72, 127.33, 103.38, 21.56.



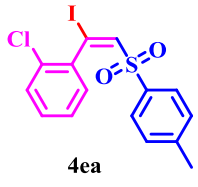
4ca **(*E*)-1-((2-iodo-2-(4-methoxyphenyl)vinyl)sulfonyl)-4-methylbenzene (4ca)**[1]

Yield:83% (93 mg), white solid, m.p.:131.8 – 132.9 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.50 (d, J = 8.1 Hz, 2H), 7.29 (s, 1H), 7.24 (s, 2H), 7.21 (d, J = 8.0 Hz, 2H), 6.80 (d, J = 8.7 Hz, 2H), 3.83 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 160.73, 144.40, 140.21, 137.45, 131.79, 129.88, 129.56, 127.75, 114.78, 113.16, 55.31, 21.54.



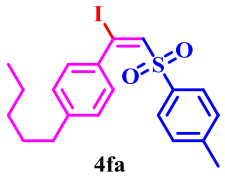
4da **(*E*)-1-chloro-4-(1-iodo-2-tosylvinyl)benzene (4da)**[1]

Yield: 71% (80 mg), white solid, m.p.:146.7 – 147.8 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.50 (d, J = 8.2 Hz, 2H), 7.34 (s, 1H), 7.28 (s, 2H), 7.24 (d, J = 8.1 Hz, 2H), 7.19 (d, J = 8.4 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 144.81, 141.68, 138.00, 137.08, 135.83, 129.72, 129.03, 128.14, 127.81, 111.95, 21.58.



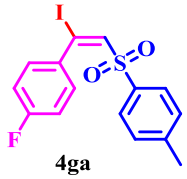
4ea **(*E*)-1-chloro-2-(1-iodo-2-tosylvinyl)benzene (4ea)**

Yield: 66% (74 mg), yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) 7.50 (d, J = 8.2 Hz, 2H), 7.34 (s, 1H), 7.28 (s, 2H), 7.27 – 7.26 (m, 2H) 7.24 (d, J = 8.1 Hz, 2H), 7.19 (d, J = 8.4 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 144.85, 142.23, 137.77, 136.50, 131.04, 130.60, 129.73, 129.66, 128.82, 128.01, 126.47, 108.79, 21.60.



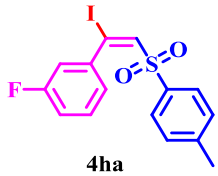
4fa **(*E*)-1-((2-iodo-2-(4-pentylphenyl)vinyl)sulfonyl)-4-methylbenzene (4fa)[1]**

Yield: 80% (98 mg), colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.45 (d, J = 8.2 Hz, 2H), 7.34 (s, 1H), 7.16 (dd, J = 7.8, 6.0 Hz, 4H), 7.07 (d, J = 8.1 Hz, 2H), 2.62 – 2.57 (m, 2H), 2.39 (s, 3H), 1.64 – 1.61 (m, 2H), 1.38 – 1.33 (m, 4H), 0.92 (t, J = 6.9 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 145.15, 144.31, 140.85, 137.33, 136.82, 129.47, 127.82, 127.80, 114.83, 35.73, 31.44, 30.88, 22.45, 21.54, 13.94.



4ga **(*E*)-1-fluoro-4-(1-iodo-2-tosylvinyl)benzene (4ga)[1]**

Yield:75% (81 mg), white solid, m.p.:90.2 – 91.8 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.49 (d, J = 8.2 Hz, 2H), 7.35 (s, 1H), 7.27 (s, 1H), 7.25 – 7.24 (m, 1H), 7.23 (d, J = 8.1 Hz, 2H), 6.98 (t, J = 8.6 Hz, 2H), 2.41 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 163.97, 162.31, 144.72, 141.59, 137.18, 135.62, 129.97, 129.91, 129.68, 127.75, 115.09, 114.95, 112.47, 21.56.



4ha **(*E*)-1-fluoro-3-(1-iodo-2-tosylvinyl)benzene (4ha)**

Yield:70% (76 mg), white solid, m.p.:120.4 – 121.7 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.49 (d, J = 8.2 Hz, 2H), 7.36 (s, 1H), 7.30 – 7.27 (m, 1H), 7.23 (d, J = 8.1 Hz, 2H), 7.05 (d, J = 7.7 Hz, 1H), 7.01 (td, J = 8.4, 2.3 Hz, 1H), 6.86 – 6.81 (m, 1H), 2.41 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ_C 162.47, 160.83, 144.83, 142.01, 141.39, 141.34, 137.02, 129.71, 129.60, 129.54, 127.83, 123.42, 123.39, 116.72, 116.58, 114.69, 114.54, 111.15, 21.54.

3 The structural confirmation of the representative compound 4aa

Figure.1S. The structures of the representative compound **4aa** and **4aa'**

The chemical structures of the target compounds were confirmed by ^{1}H NMR, and ^{13}C NMR. ^{1}H NMR spectroscopy showed that all the protons of **4aa** resonated with the expected chemical shifts (**Figure 2SA**, ^{1}H NMR (600 MHz, $CDCl_3$) δ_H 7.46 (d, J = 8.3 Hz, 2H), 7.36 (s, 1H), 7.32 – 7.27 (m, 3H), 7.24 – 7.22 (m, 2H), 7.19 (d, J = 8.0 Hz, 2H), 2.39 (s, 3H)). In addition, the configuration of alkene double bond was consistent with Wang's work[4] (**4aa**, *E*-configuration, **Figure 2SB**, ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.48 (d, J = 8.3 Hz, 2H), 7.38 (s, 1H), 7.34 – 7.28 (m, 3H), 7.26 – 7.24 (m, 2H), 7.21 (d, J = 8.0 Hz, 2H), 2.42 (s, 3H)), instead of Liu's work[2] (**4aa',** *Z*-configuration, **Figure 2SC**, ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.95 (d, J = 8.0 Hz, 2H), 7.45 (d, J = 7.6 Hz, 2H), 7.35 (t, J = 9.2 Hz, 5H), 7.25 (s, 1H), 2.46 (s, 3H)). The result of ^{13}C NMR experiment further confirmed its chemical structure. Thus, all the related compounds were assigned the same *E*-configuration by analogy unambiguously.

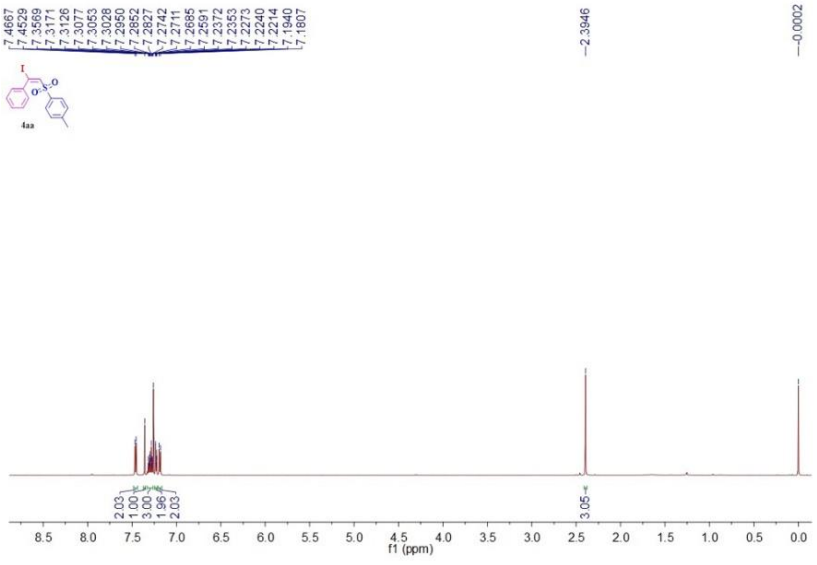
Reference

[1] X. Q. Li, X. S. Xu, X. H. Shi, *Tetrahedron Lett.* **2013**, *54*, 3071–3074.

[2] J. P. Wan, D. Q. Hu, F. C. Bai, L. Wei, Y. Y. Liu, *RSC Adv.*, **2016**, *6*, 73132–73135.

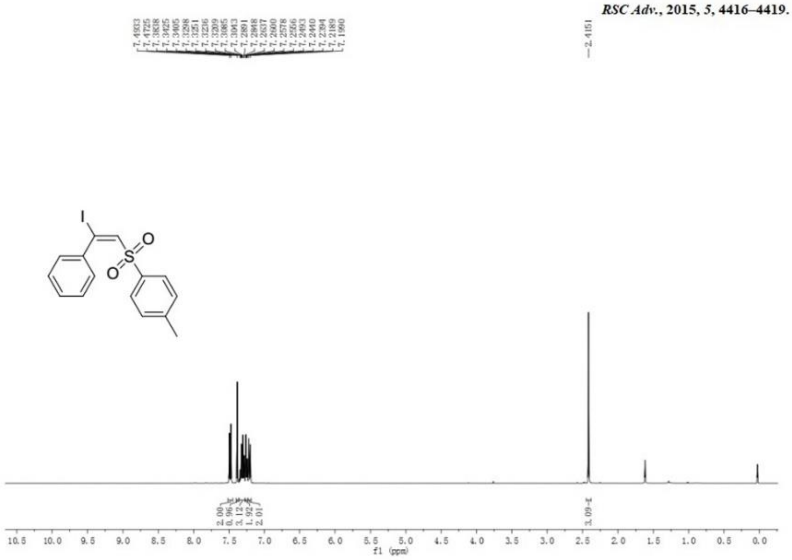
[3] Y. D Sun, A. Abdukader, D. Lu, H. Y. Zhang, C. J. Liu, *Green Chem.*, **2017**, *19*, 1255–1258.

[4] W. Wei, J. W. Wen, D. S. Yang, H. J. Jing, J. M. You, H. Wang, *RSC Adv.*, **2015**, *5*, 4416–4419.



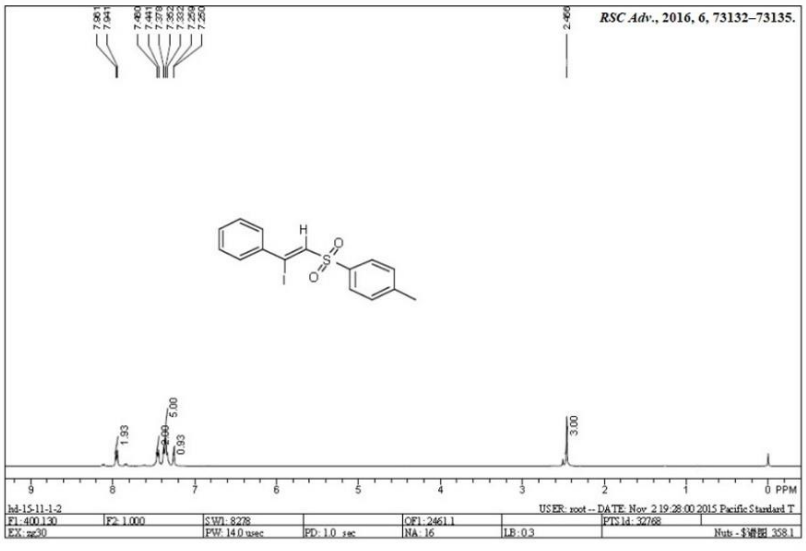
A

RSC Adv., 2015, *5*, 4416–4419.

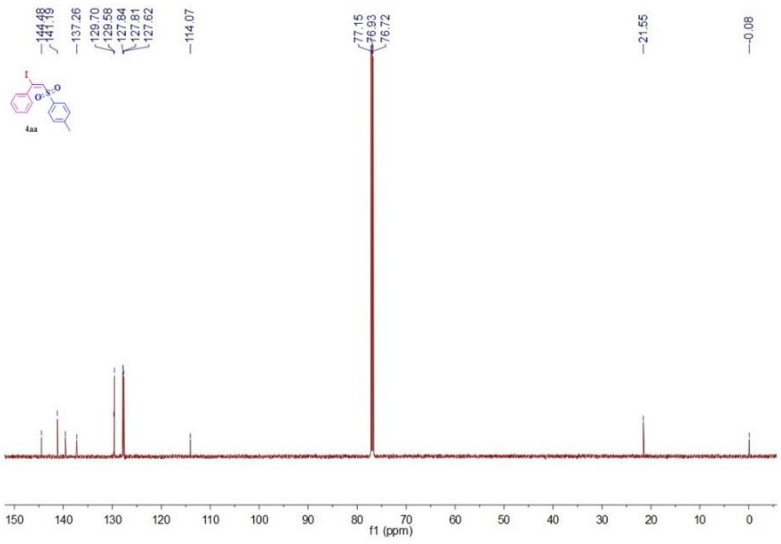


B

RSC Adv., 2016, *6*, 73132–73135.



C



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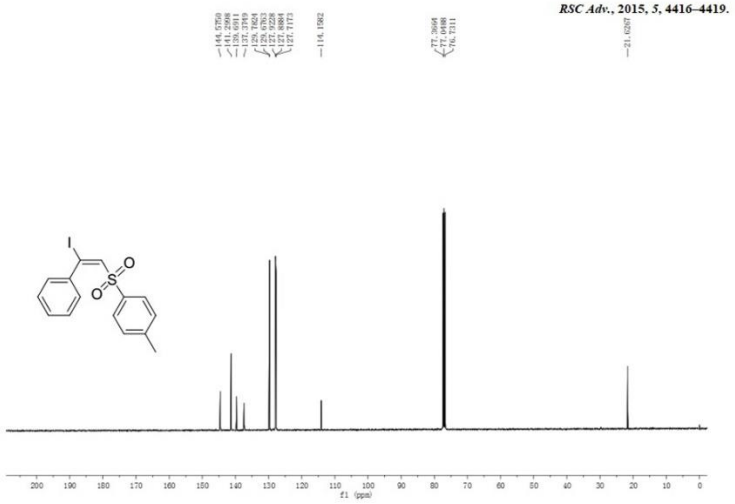
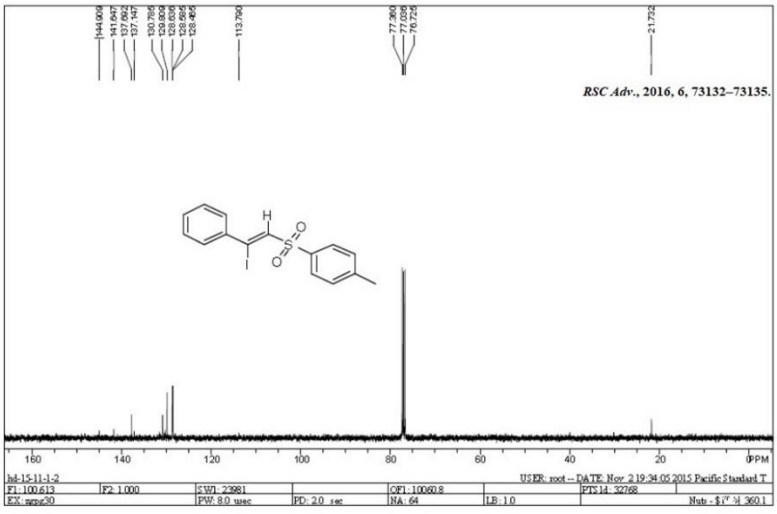


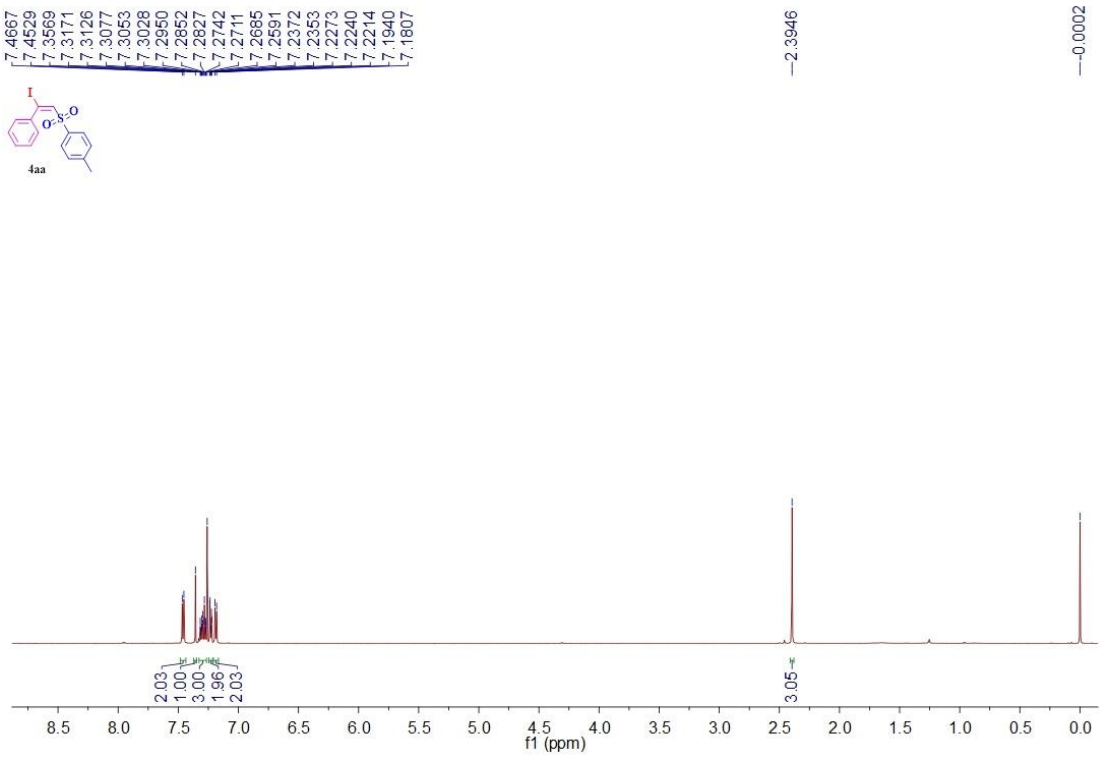
B'

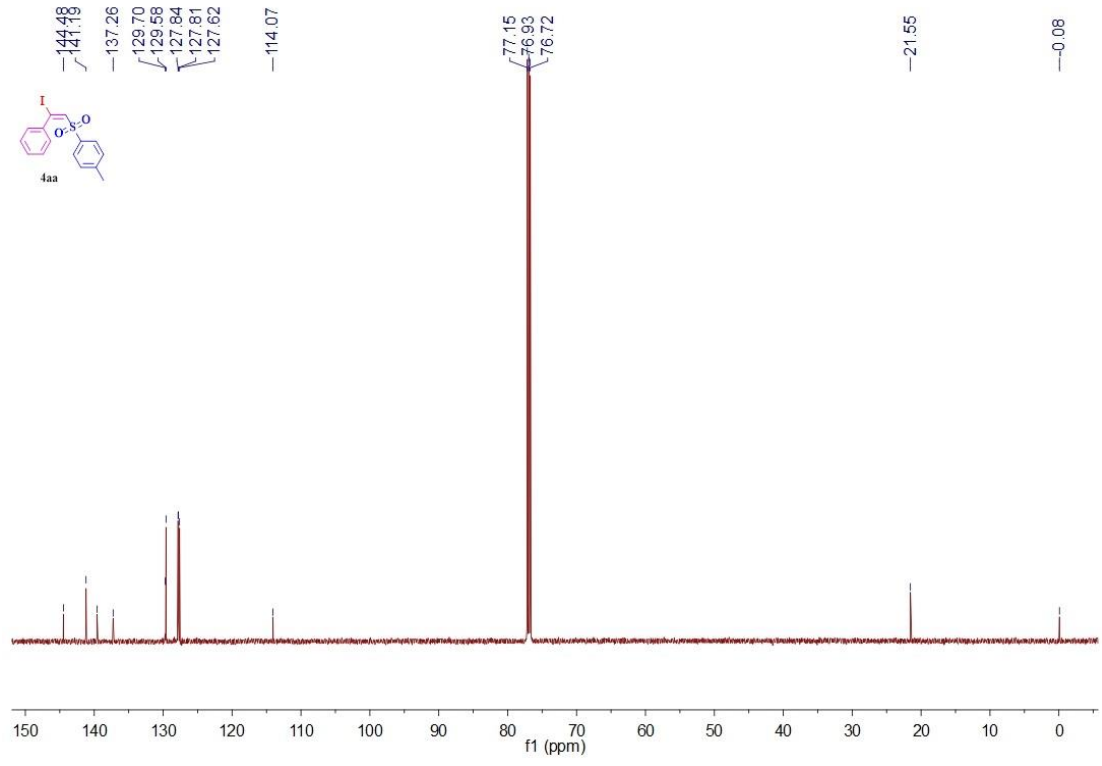


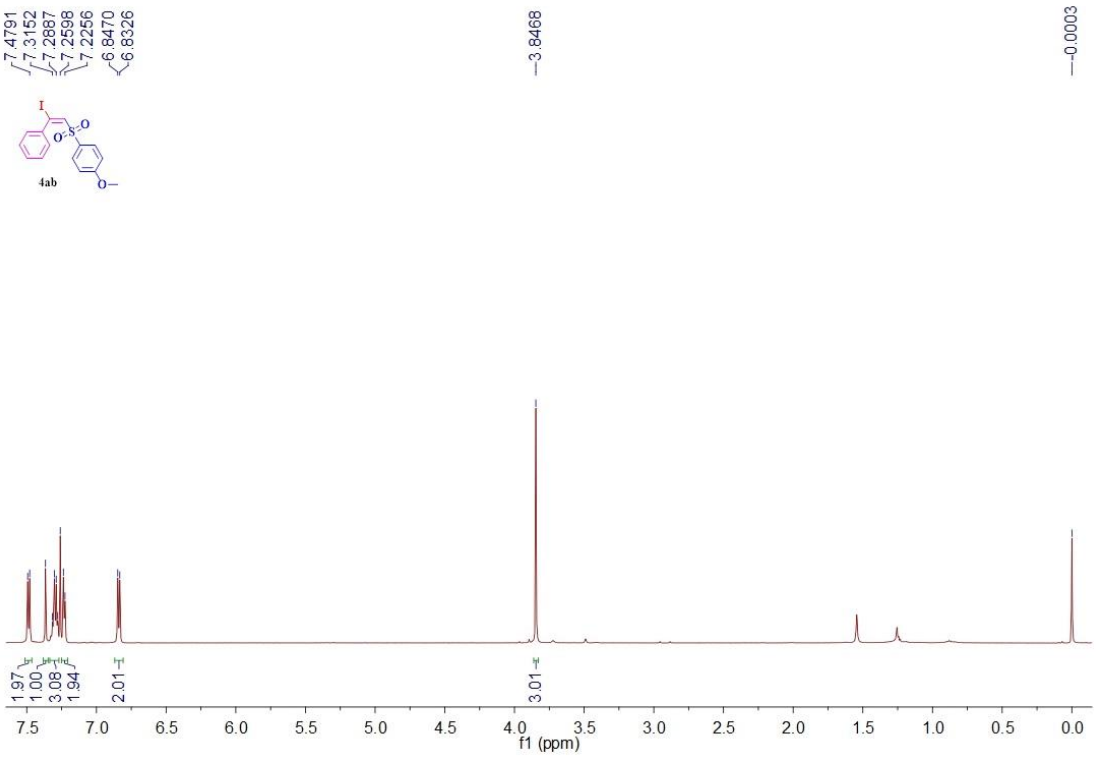
C'

Figure. 2S. The [1]HNMR and [13]CNMR of the representative compound **4aa** and **4aa'**, A and A': our work; B and B': Wang's work; C and C': Liu's work.

4. NMR Spectra of New Compounds



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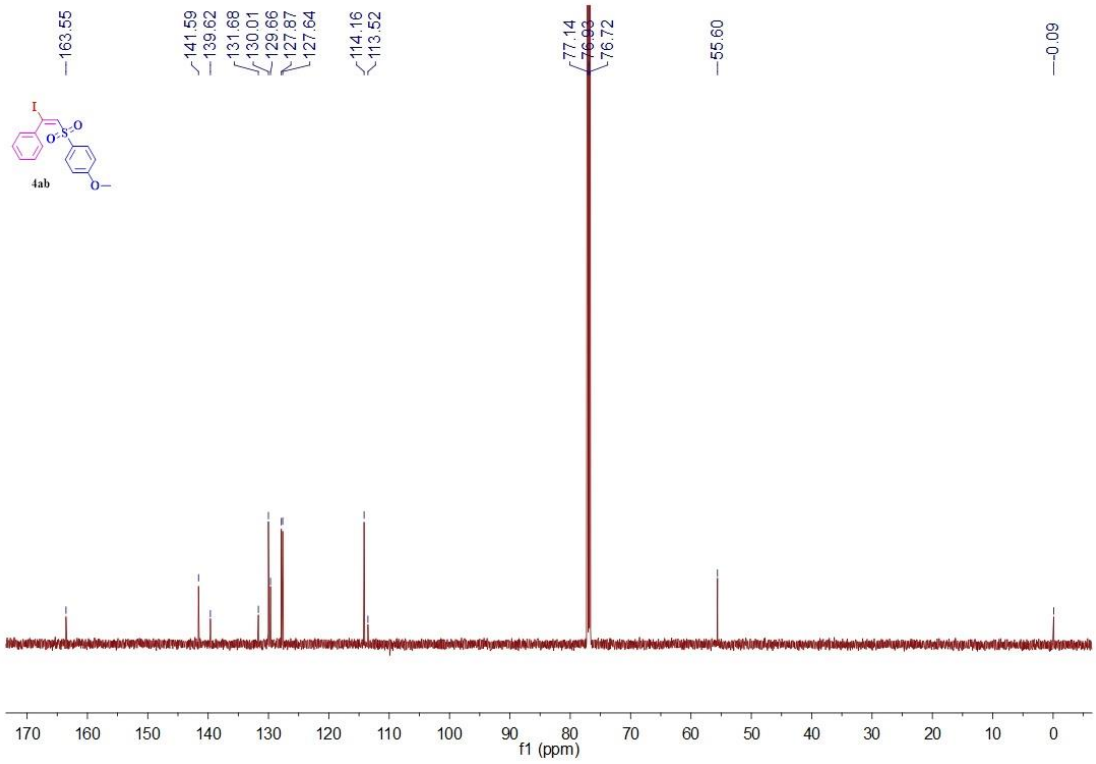
1.00
3.08
1.94
2.01
3.01
f1 (ppm)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139.62
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127.64
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77.14
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76.72
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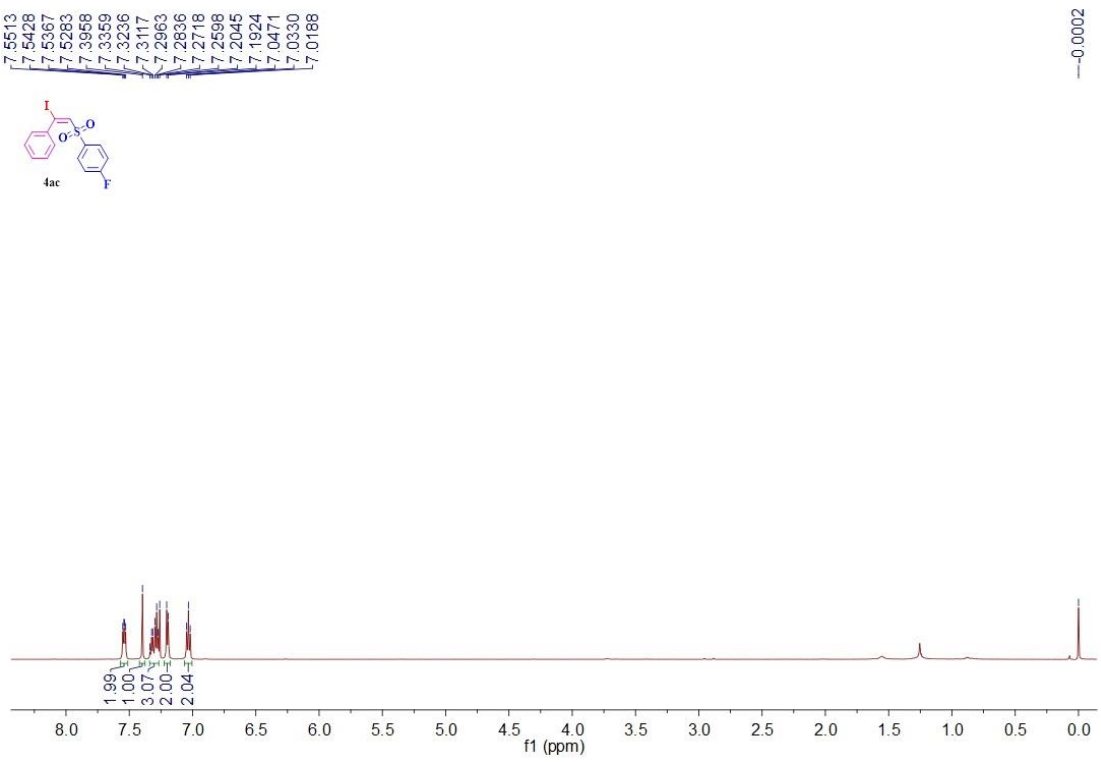
0.09
4ab
f1 (ppm)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7.2598
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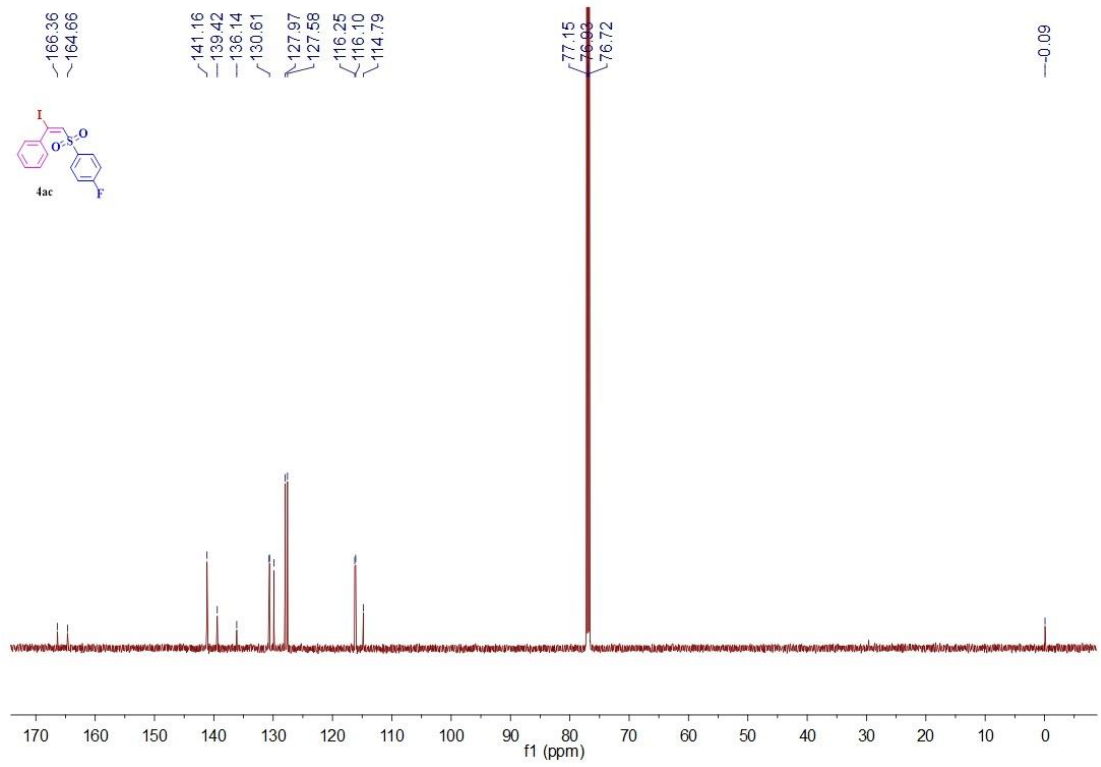
1.00
3.07
2.00
2.04
f1 (ppm)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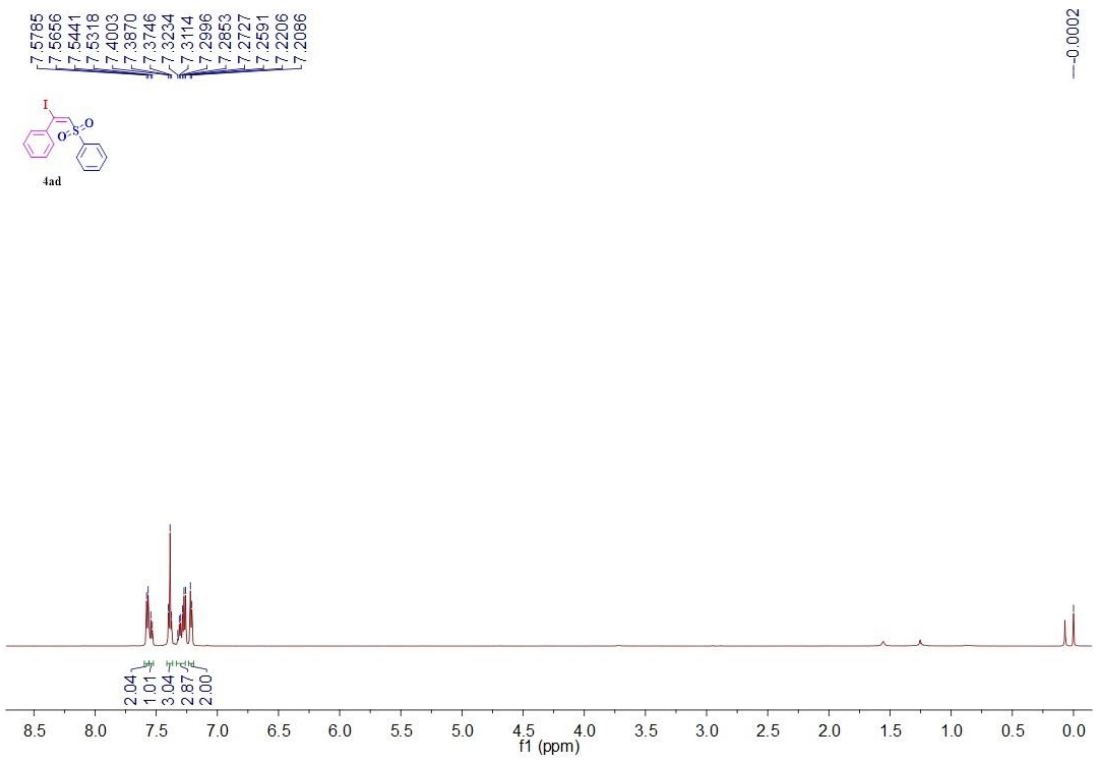
f1 (ppm)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7.2996
7.2853
7.2727
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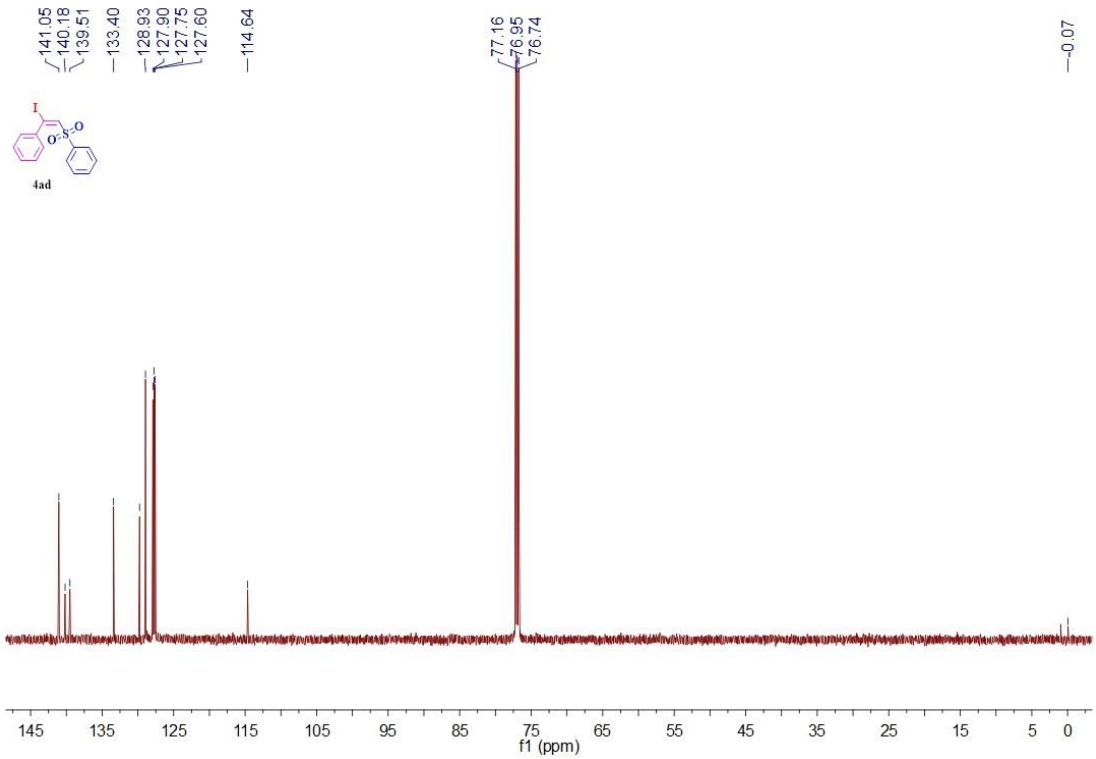
2.00
f1 (ppm)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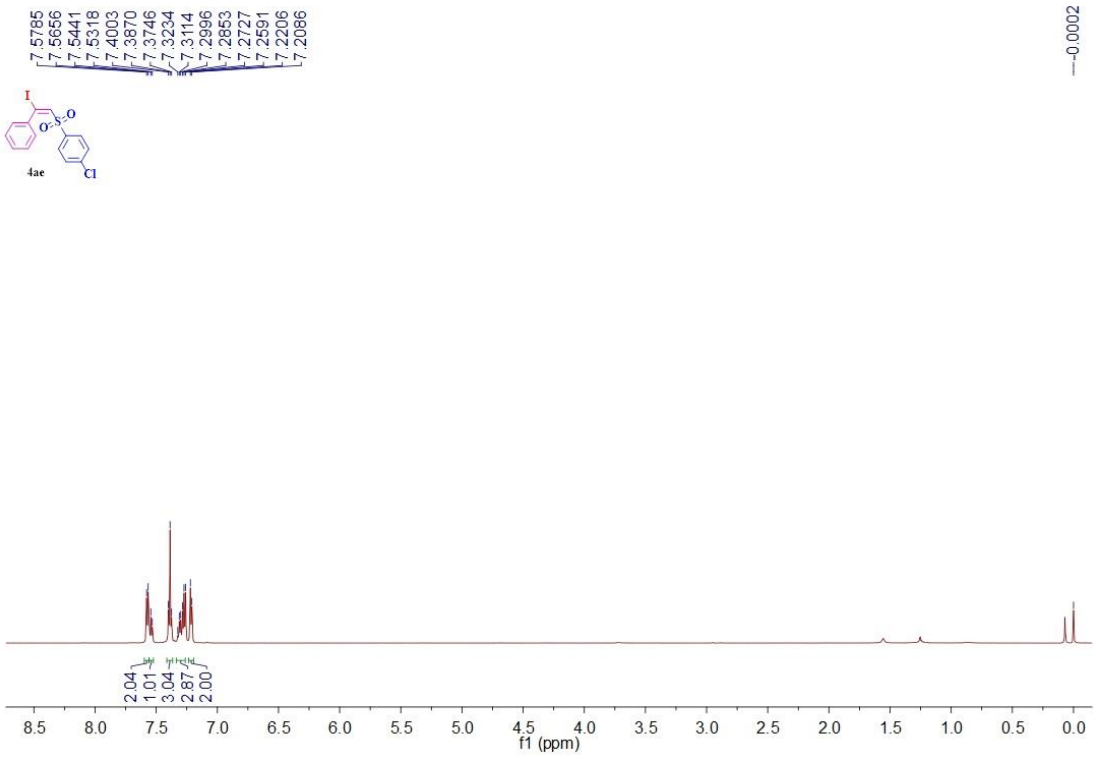
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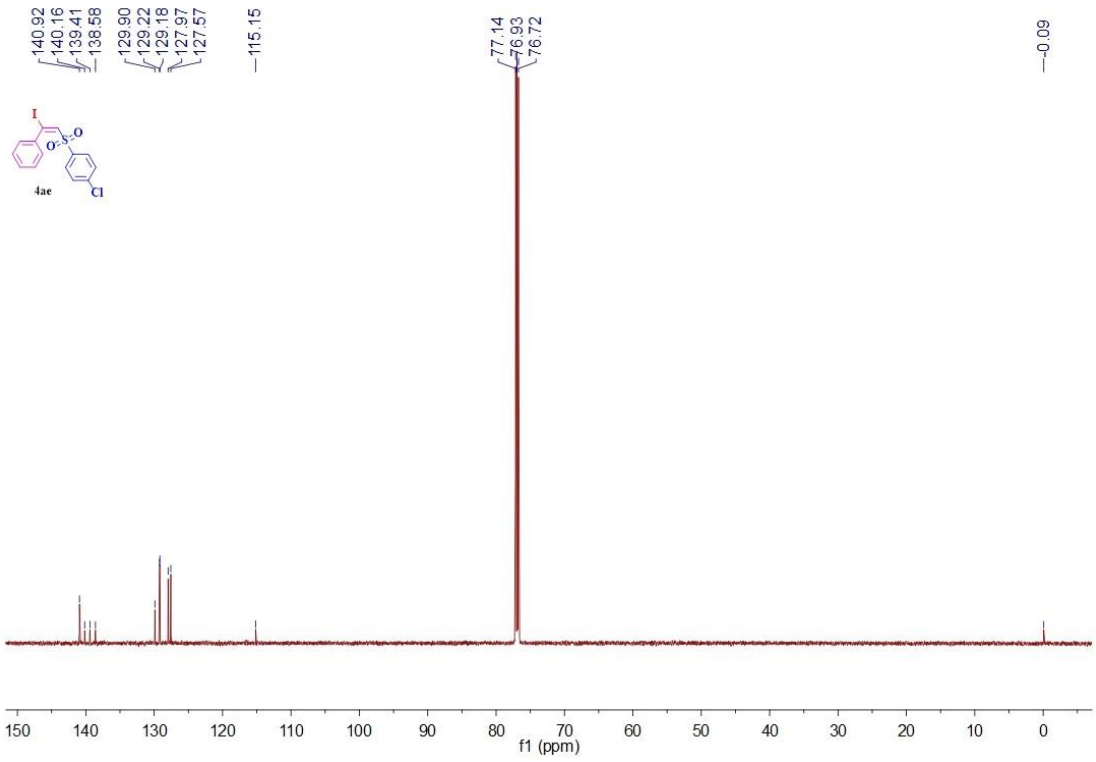
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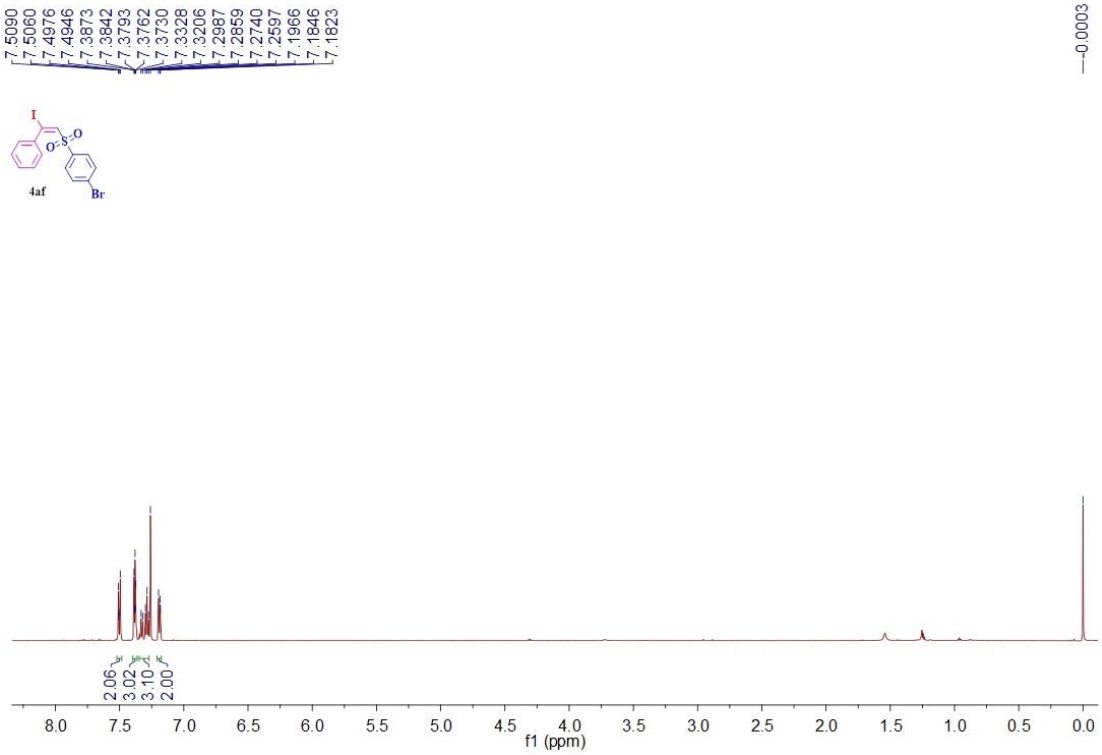
f1 (ppm)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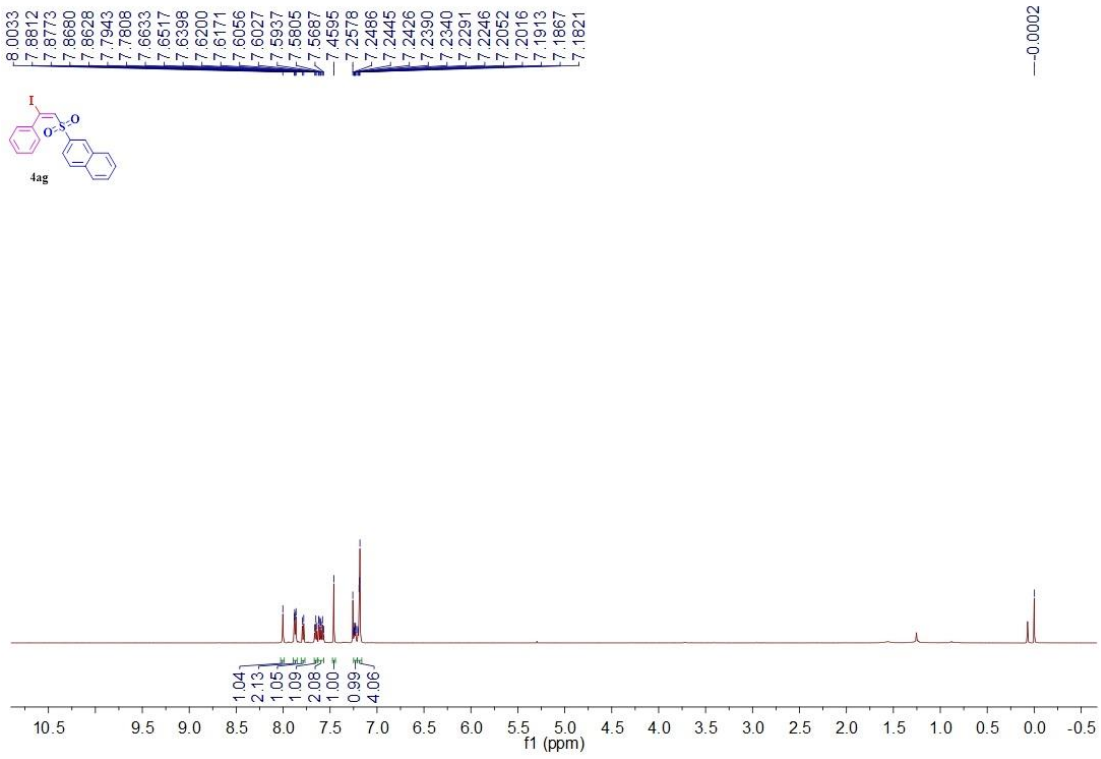
Br
f1 (ppm)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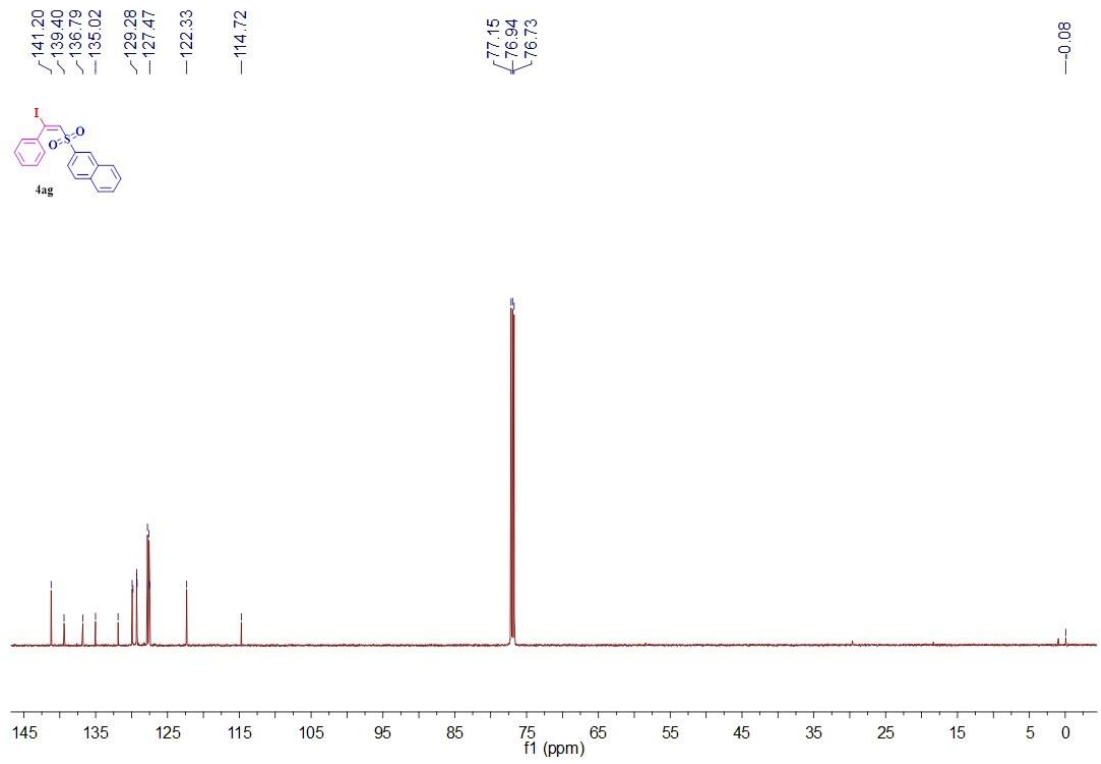
f1 (ppm)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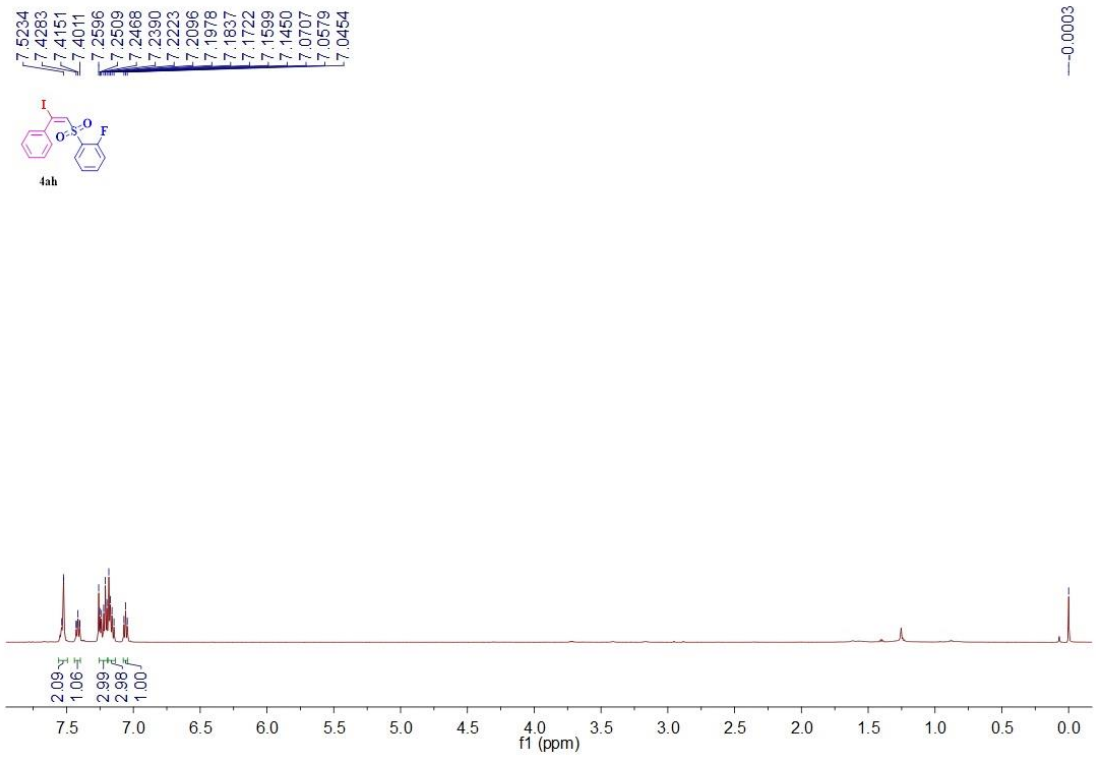
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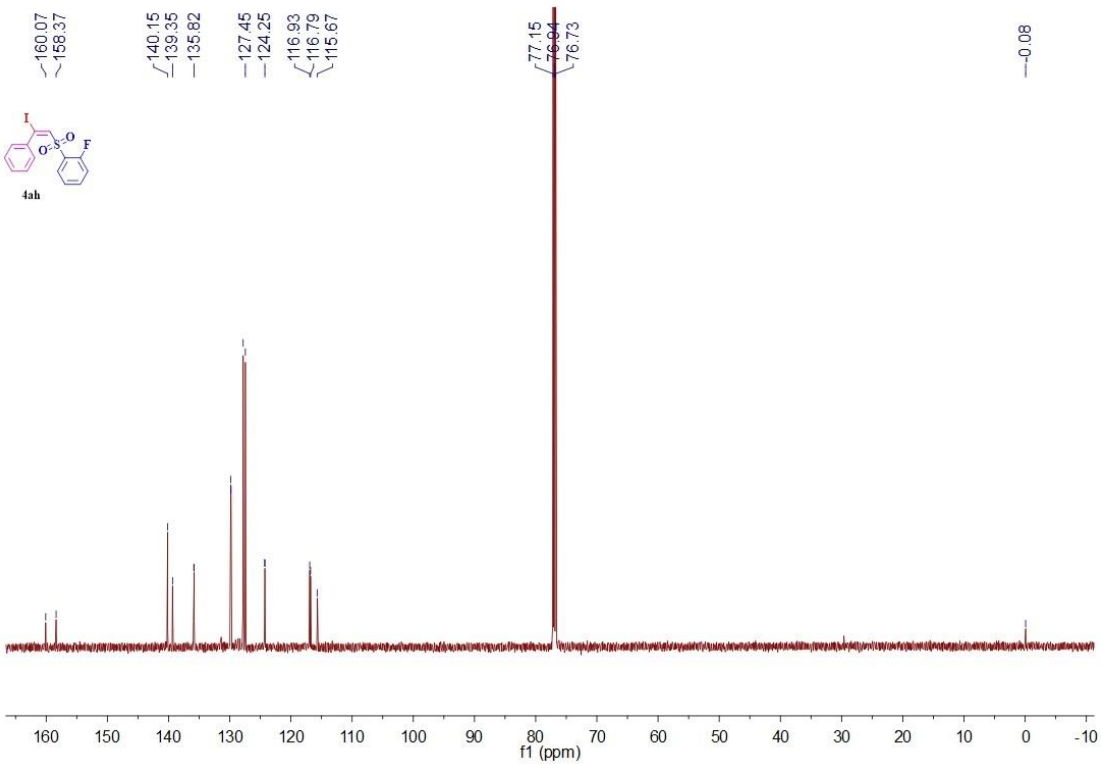
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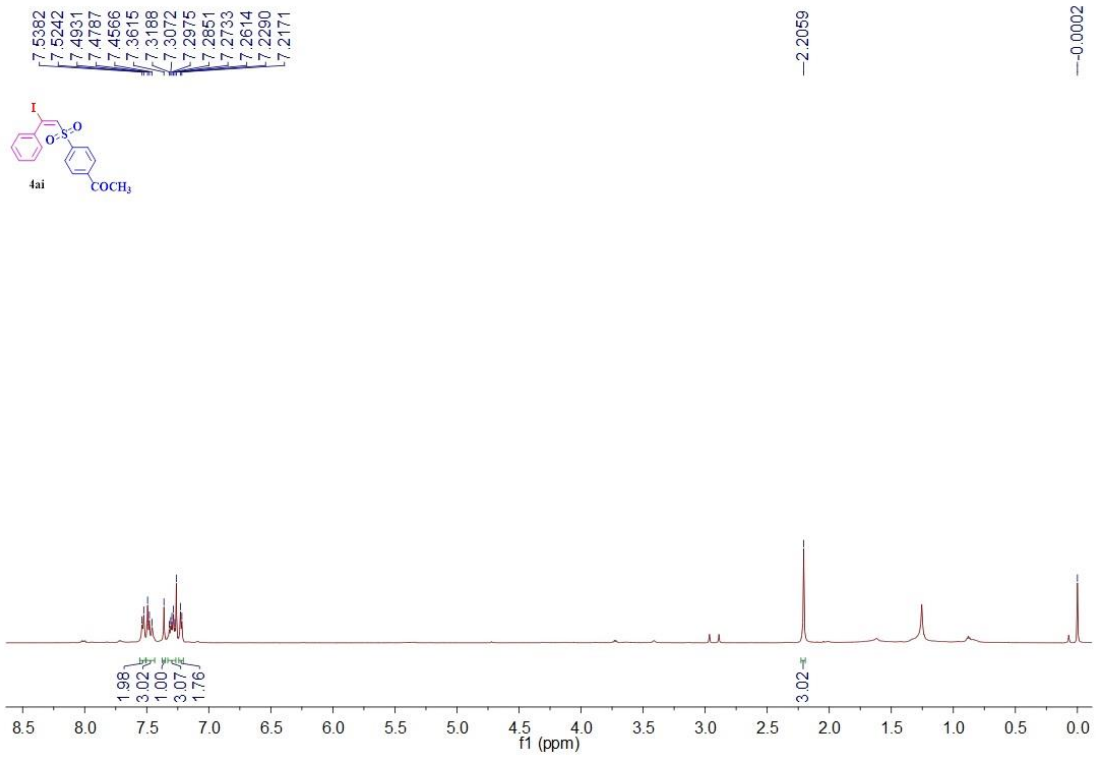
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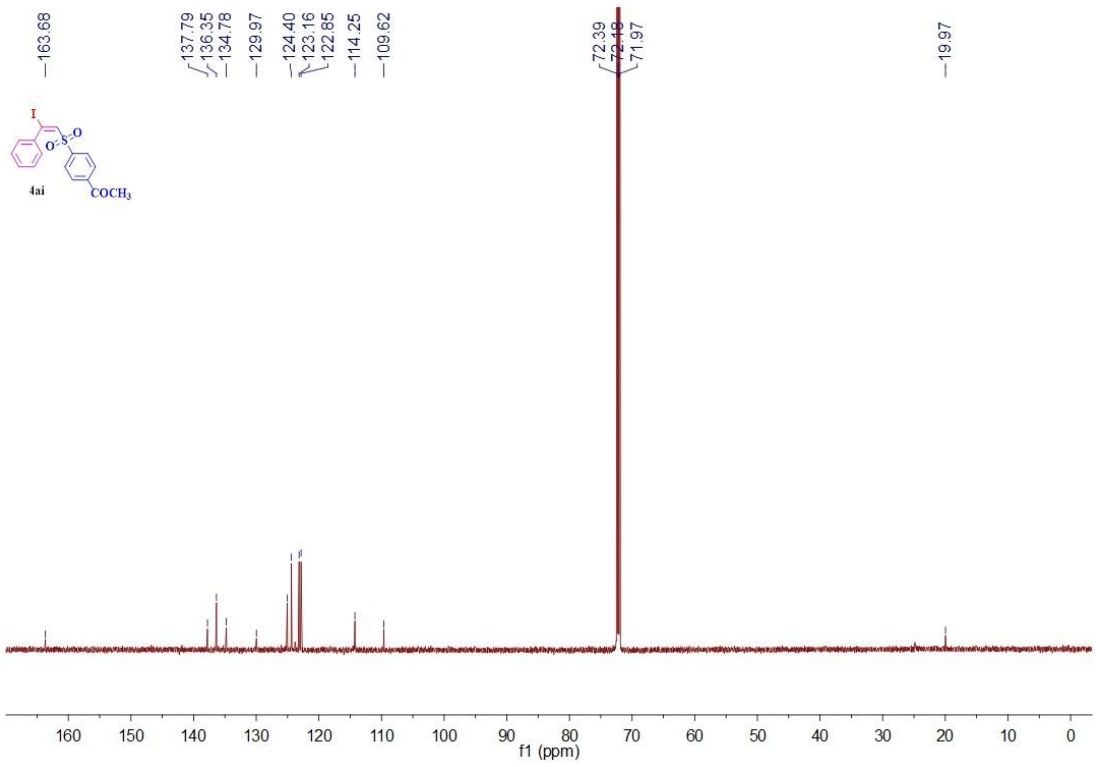
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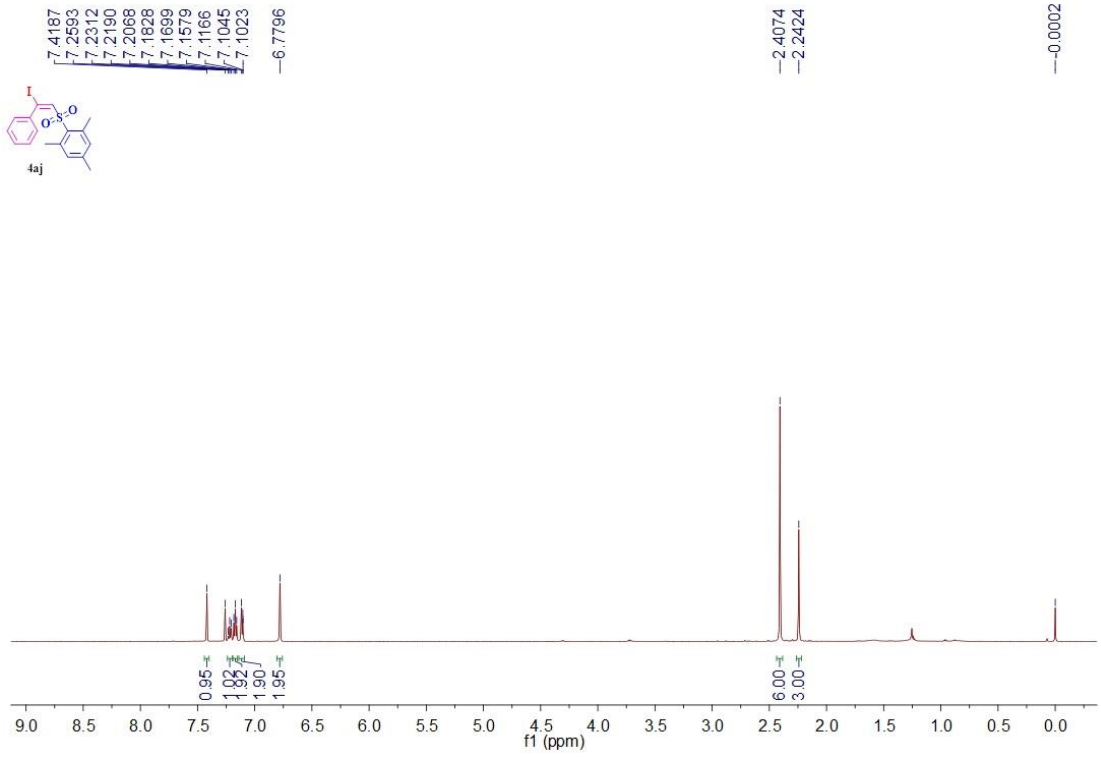
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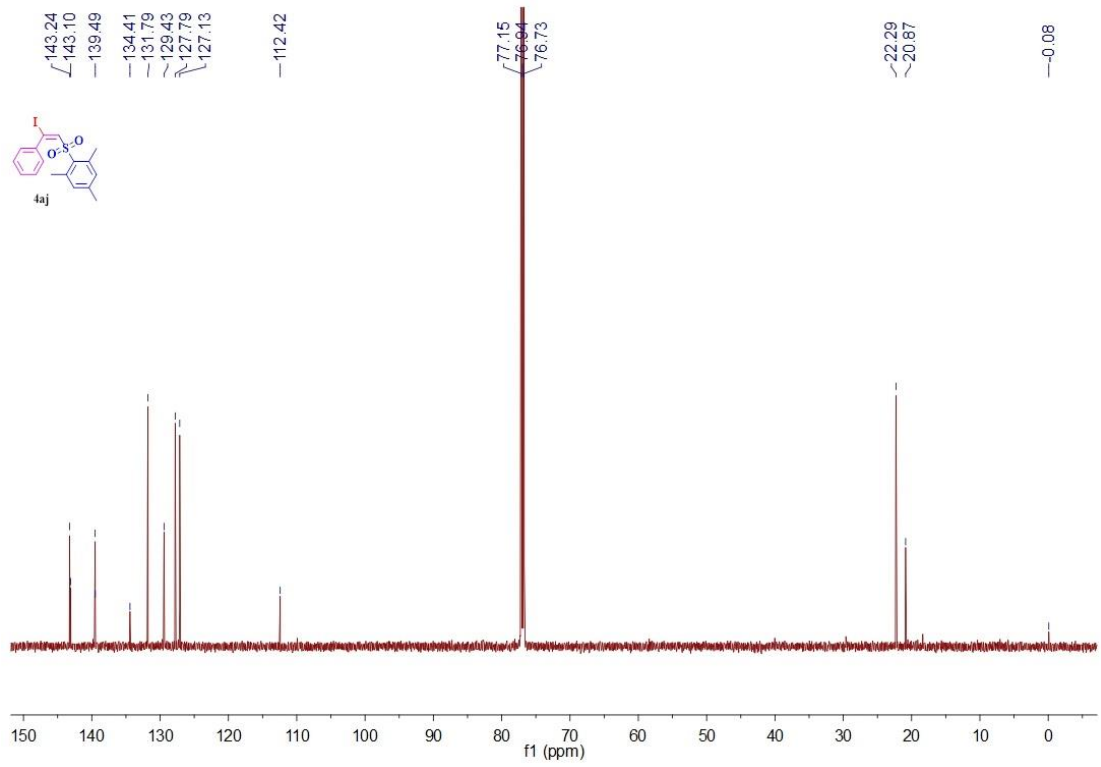
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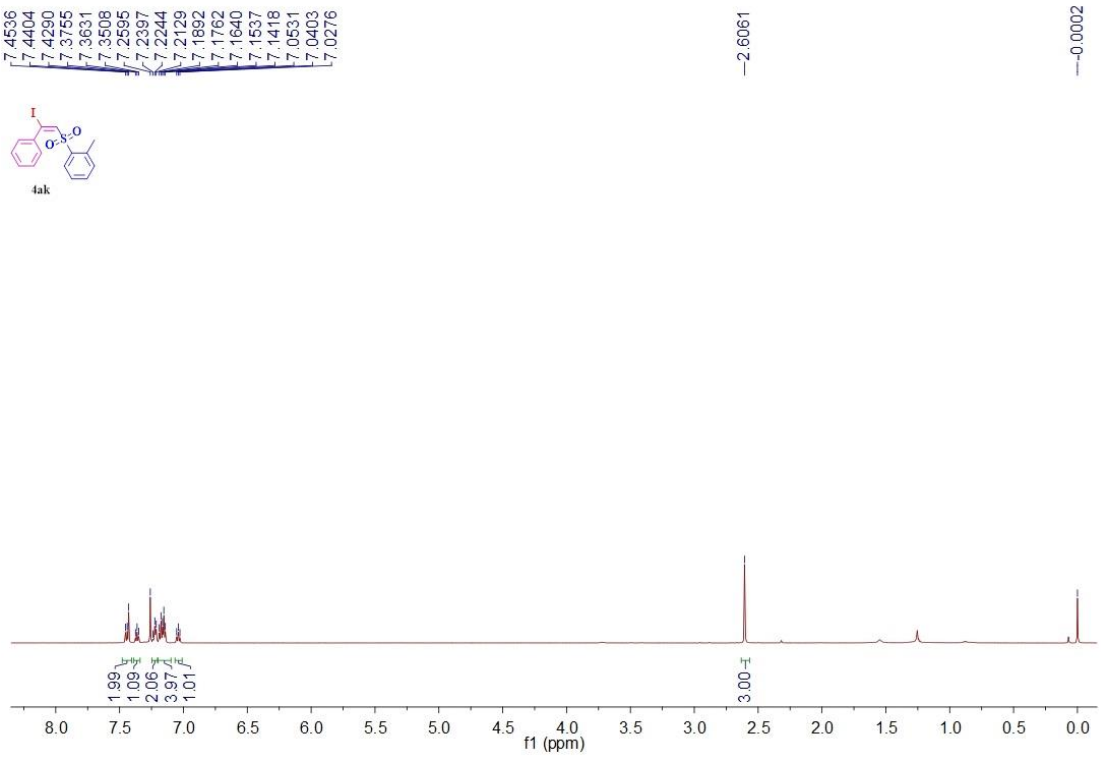
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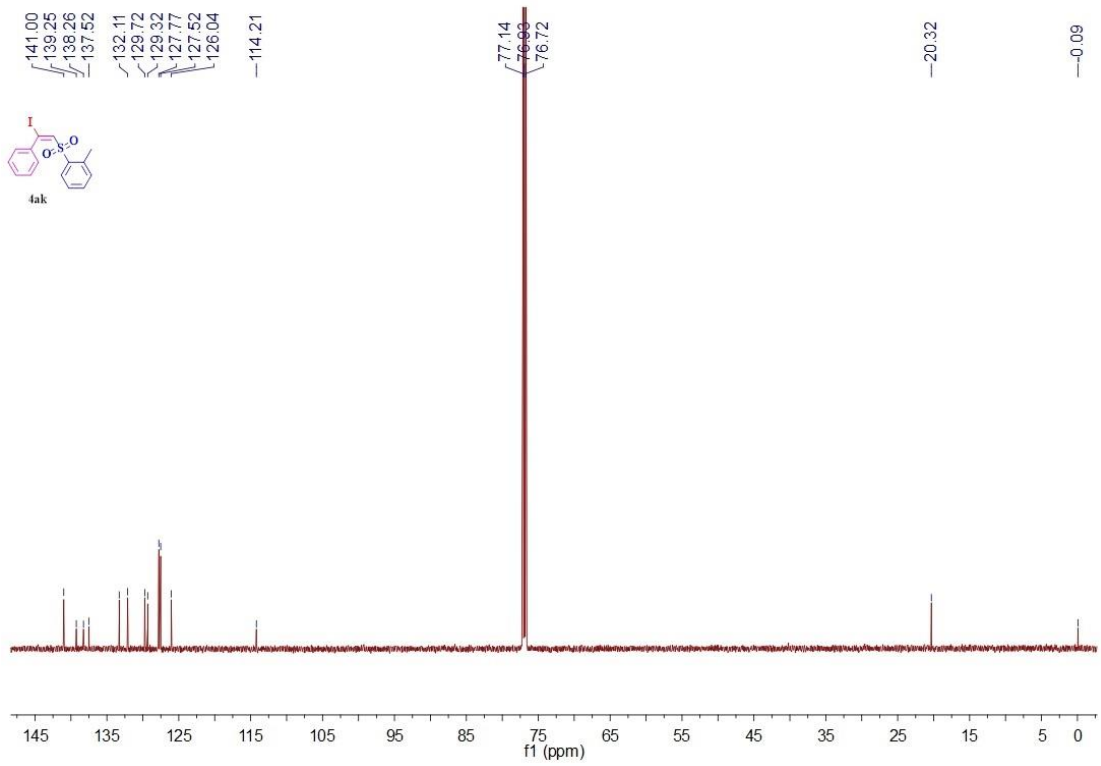
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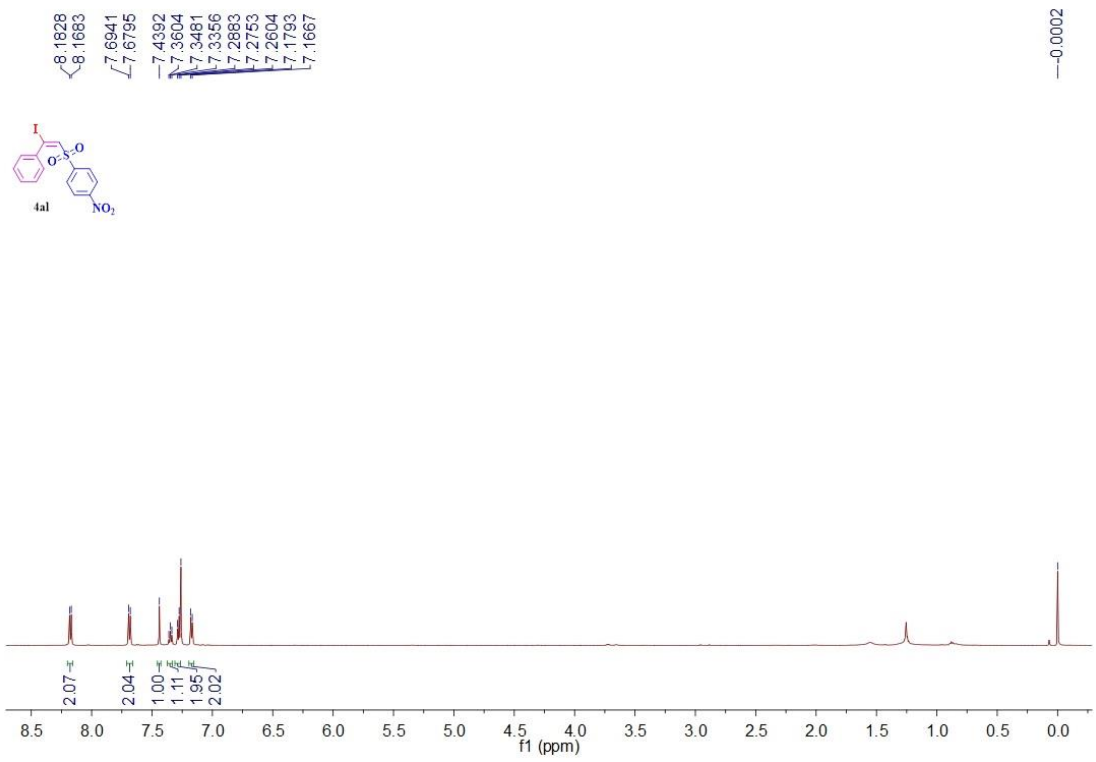
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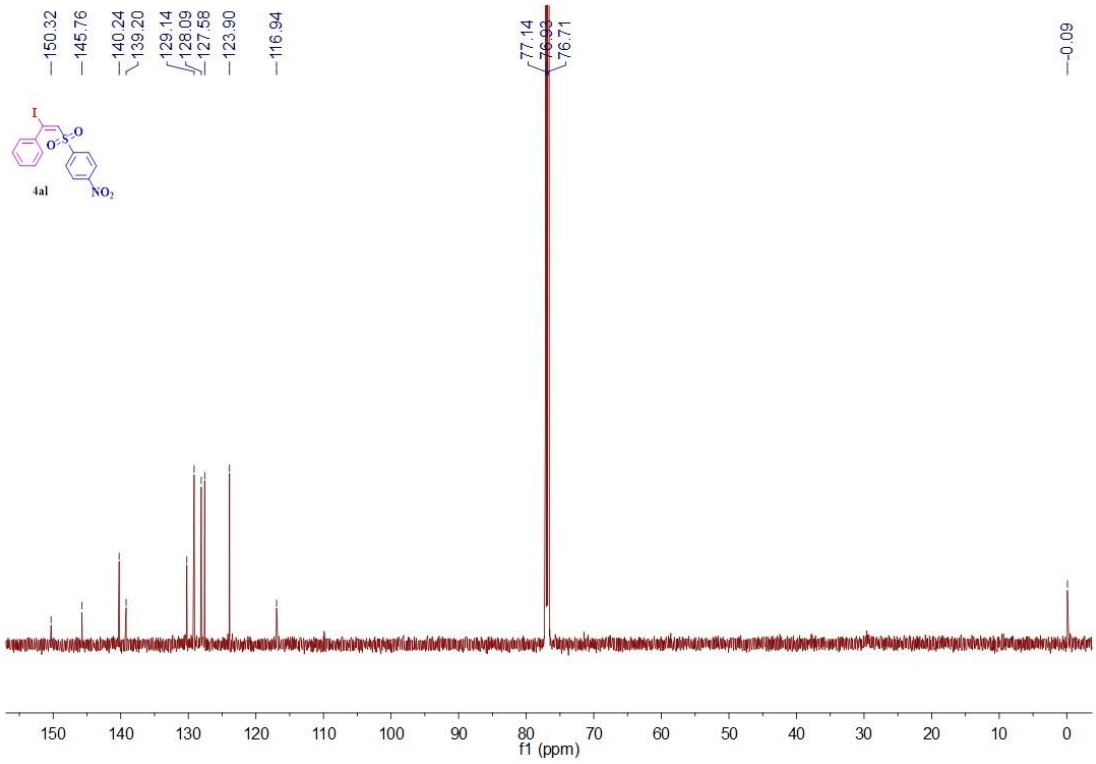
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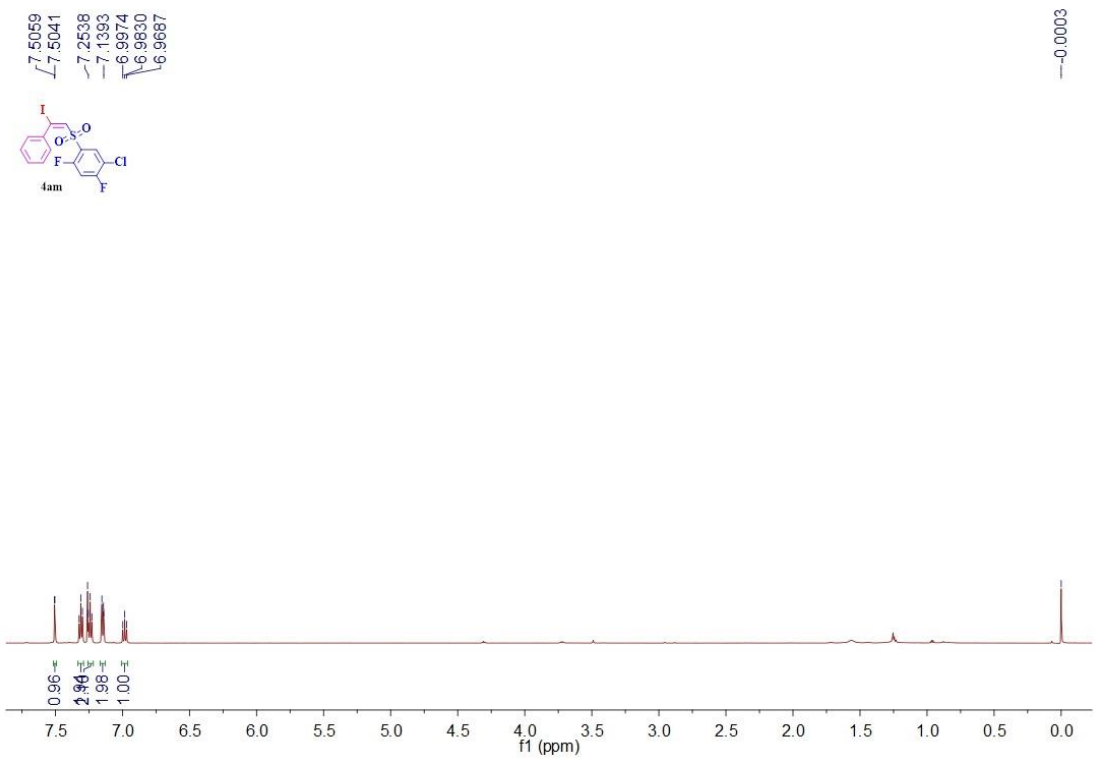
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7.2538
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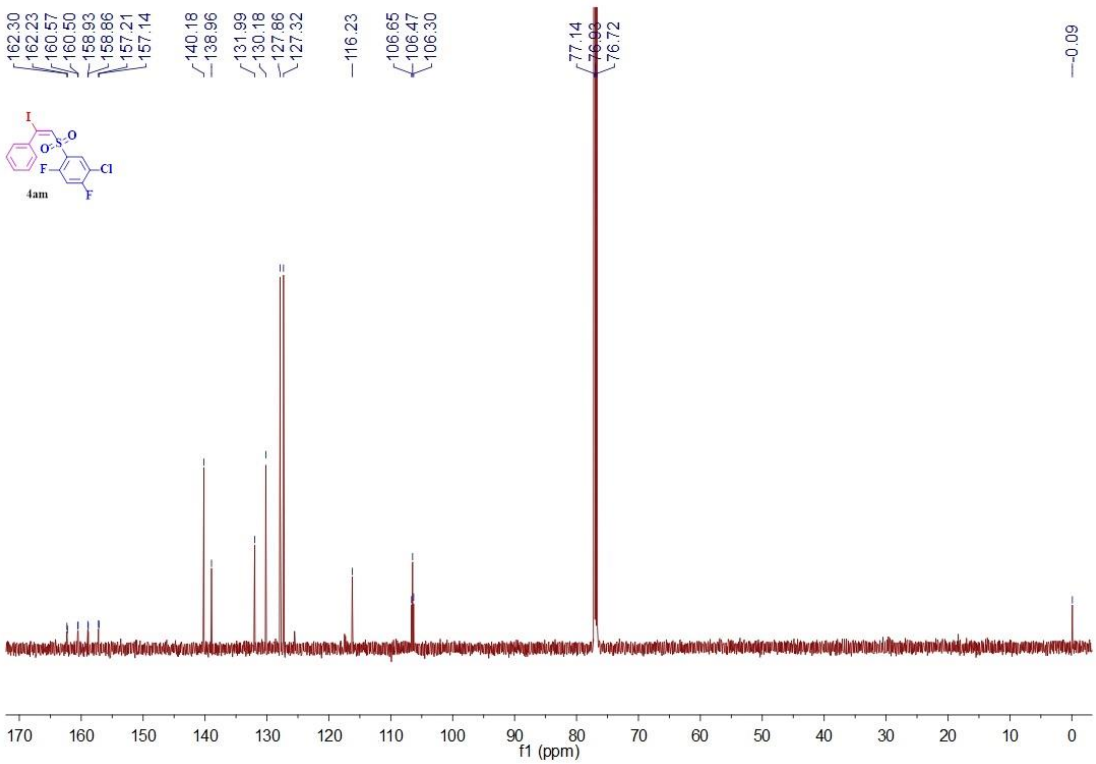
6.9974
6.9830
6.9687
0.0003
4am
0.96
2.94
1.98
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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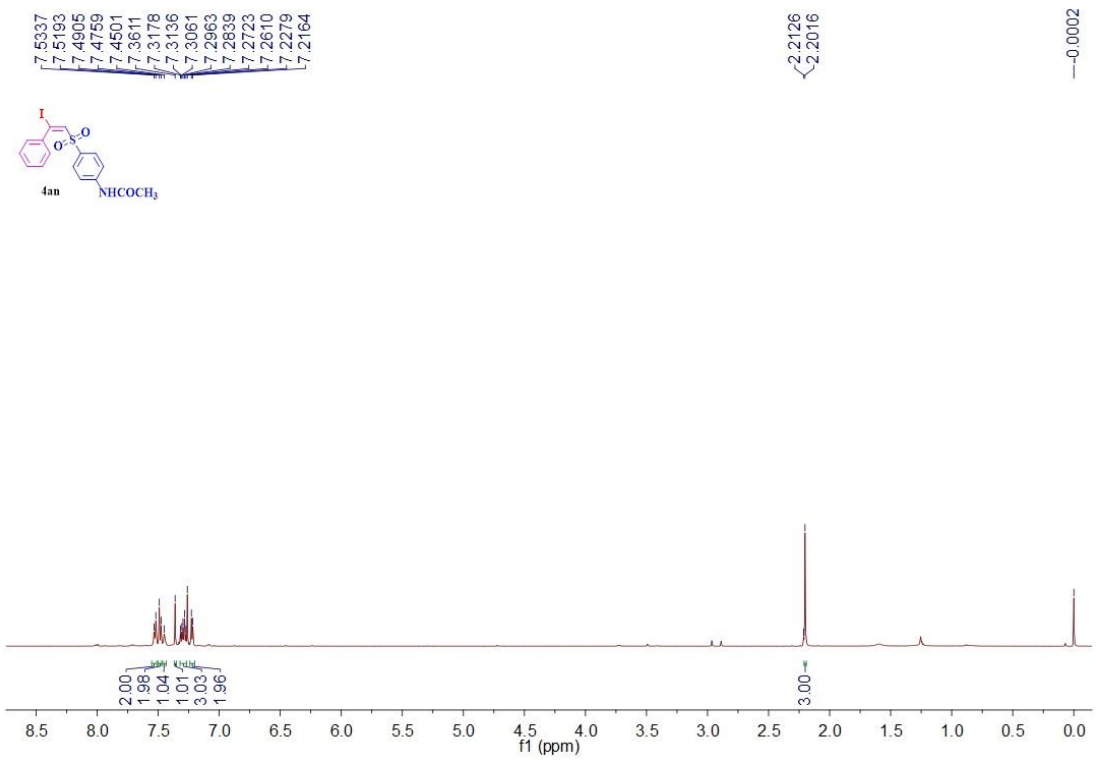
162.23
160.57
160.50
158.93
158.86
157.21
157.14
140.18
138.96
131.99
130.18
127.86
127.32
116.23
106.65
106.47
106.30
77.14
76.99
76.72
0.09
4am
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4501
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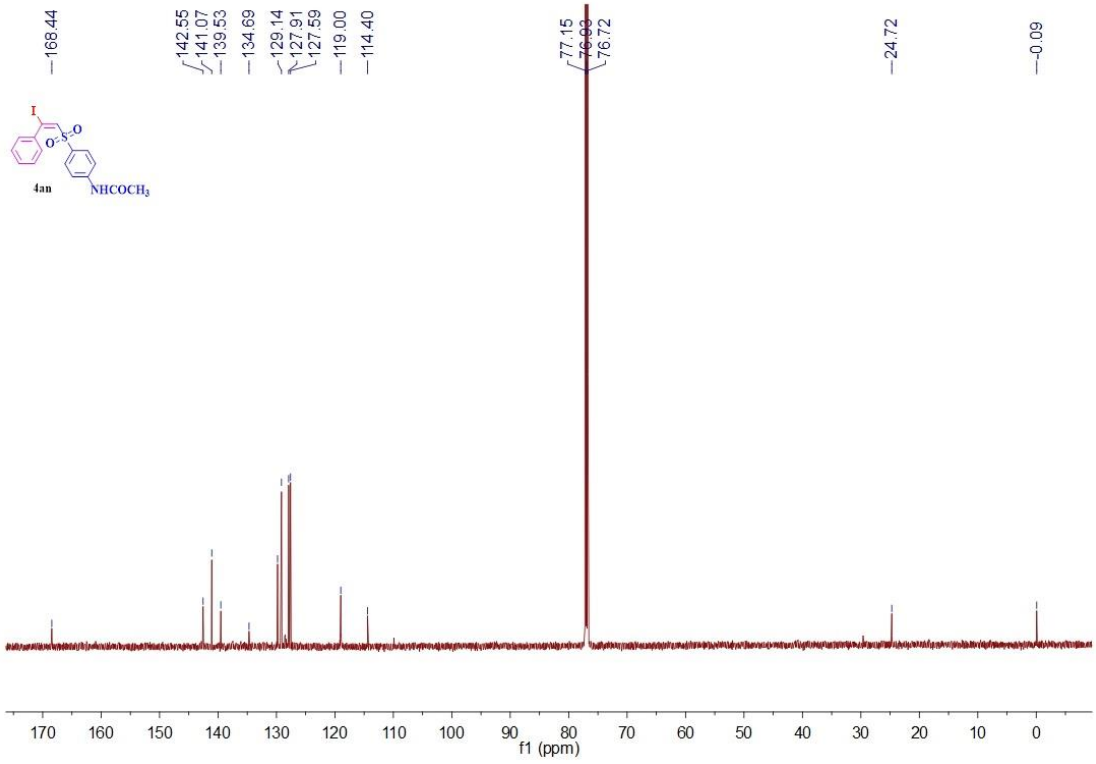
7.3178
7.3136
7.3061
7.2963
7.2839
7.2723
7.2610
7.2279
7.2164
2.2126
2.2016
0.0002
4an
NHCOCH3
2.00
1.98
1.04
1.01
3.03
1.96
3.00
f1 (ppm)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141.07
139.53
134.69
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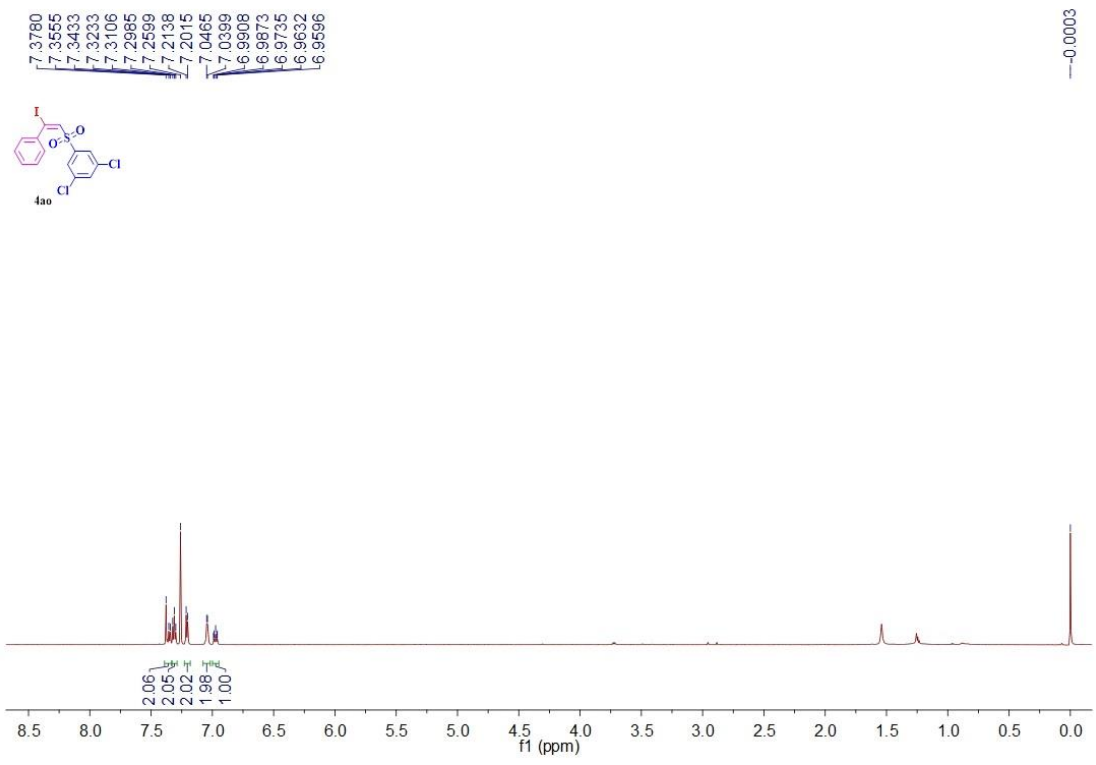
127.91
127.59
119.00
114.40
77.15
76.72
24.72
0.09
4an
NHCOCH3
f1 (ppm)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7.3433
7.3233
7.3106
7.2985
7.2599
7.2138
7.2015
7.0465
7.0399
6.9908
6.9873
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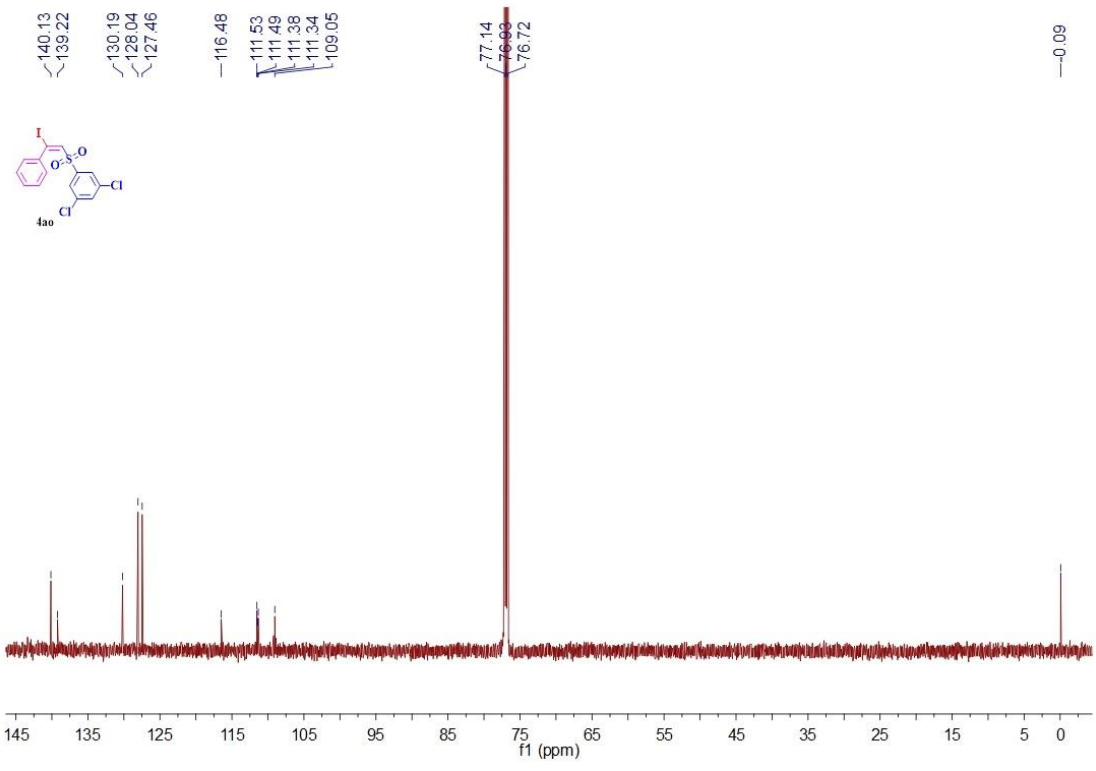
6.9596
0.0003
4ao
2.06
2.05
2.02
1.98
1.00
f1 (ppm)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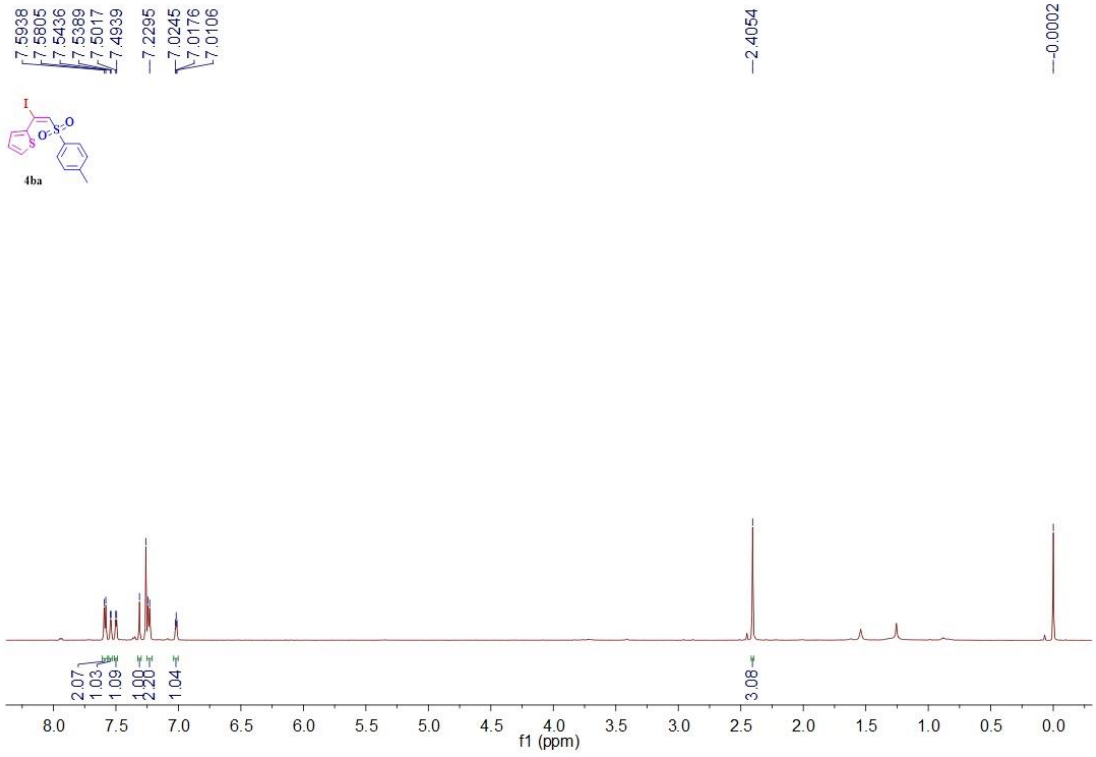
139.22
130.19
128.04
127.46
116.48
111.53
111.49
111.38
111.34
109.05
77.14
76.93
76.72
0.09
4ao
f1 (ppm)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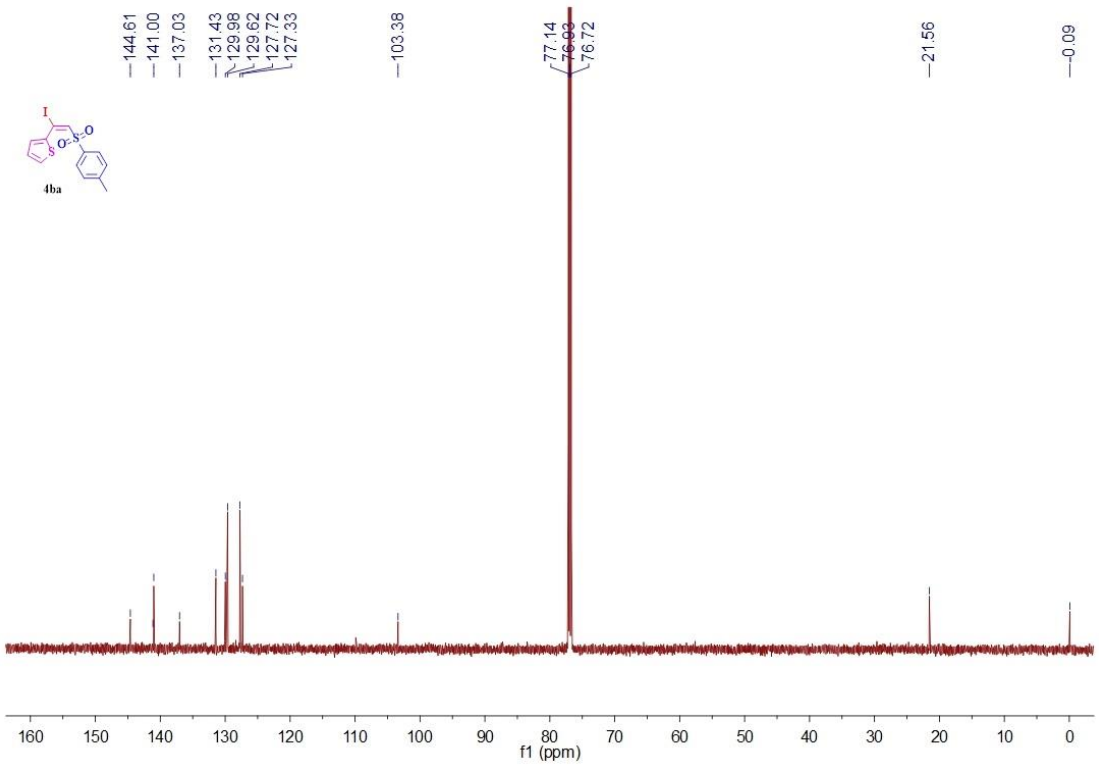
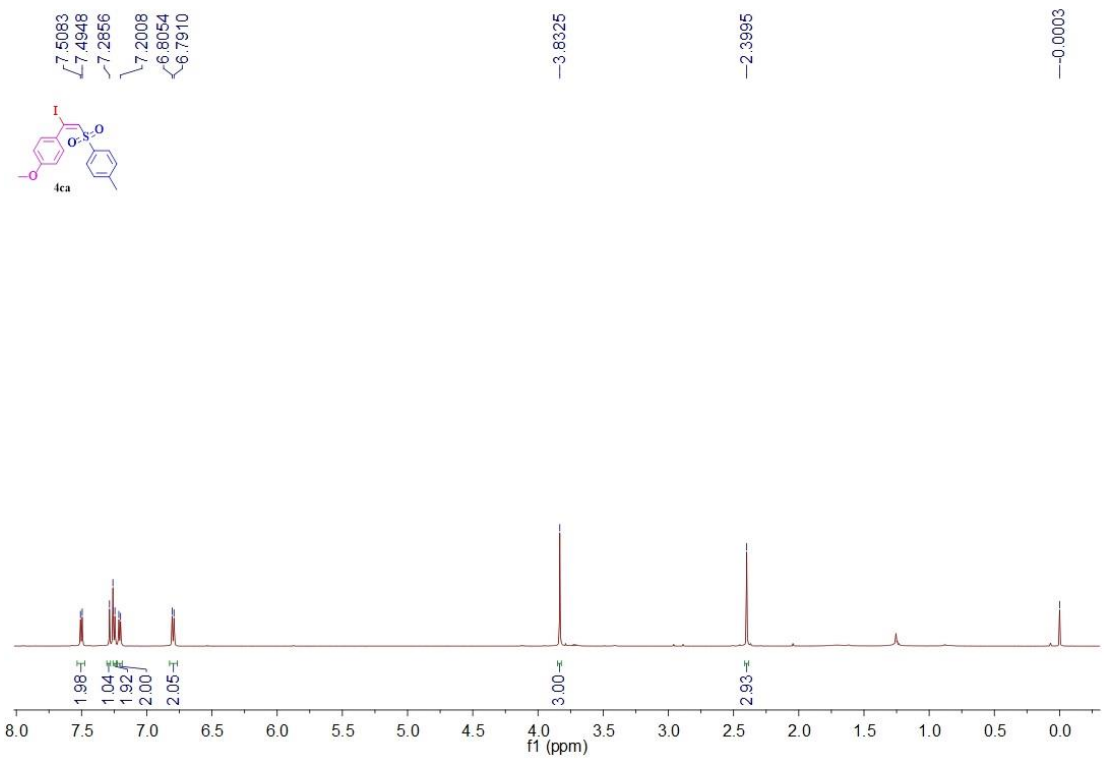
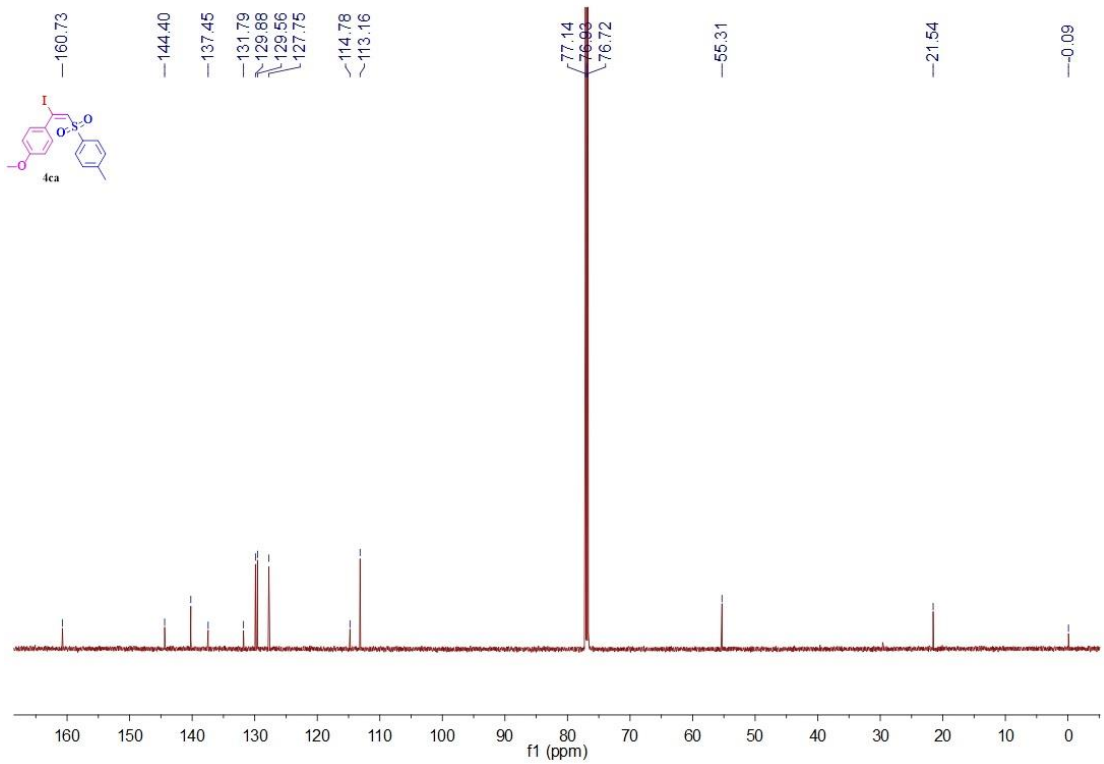
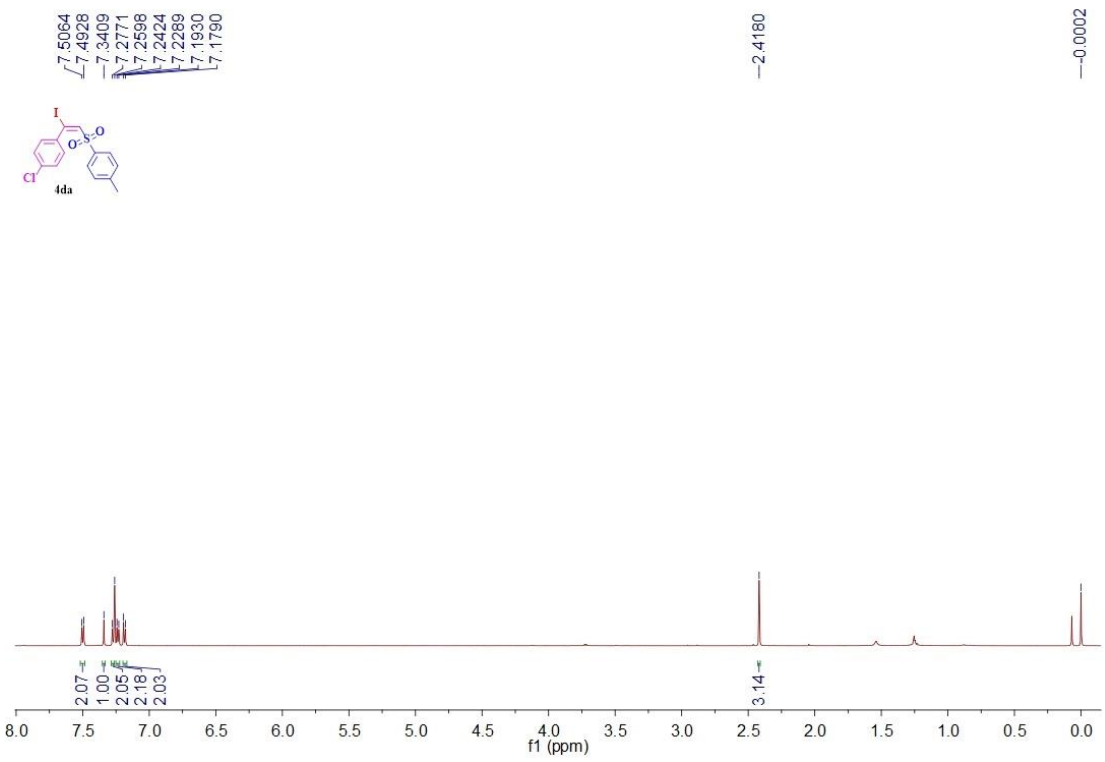
7.5436
7.5389
7.5017
7.4939
7.2295
7.0245
7.0176
7.0106
2.4054
0.0002
4ba
2.07
1.03
1.09
1.98
2.20
1.04
3.08
f1 (ppm)


144.61
141.00
137.03
131.43
129.98
129.62
127.72
127.33
103.38
77.14
76.72
21.56
0.09
4ba
f1 (ppm)


7.5083
7.4948
7.2856
7.2008
6.8054
6.7910
3.8325
2.3995
0.0003
4ca
1.98
1.04
1.92
2.00
2.05
3.00
2.93
f1 (ppm)


160.73
144.40
137.45
131.79
129.88
129.56
127.75
114.78
113.16
77.14
76.93
76.72
55.31
21.54
0.09
4ca
f1 (ppm)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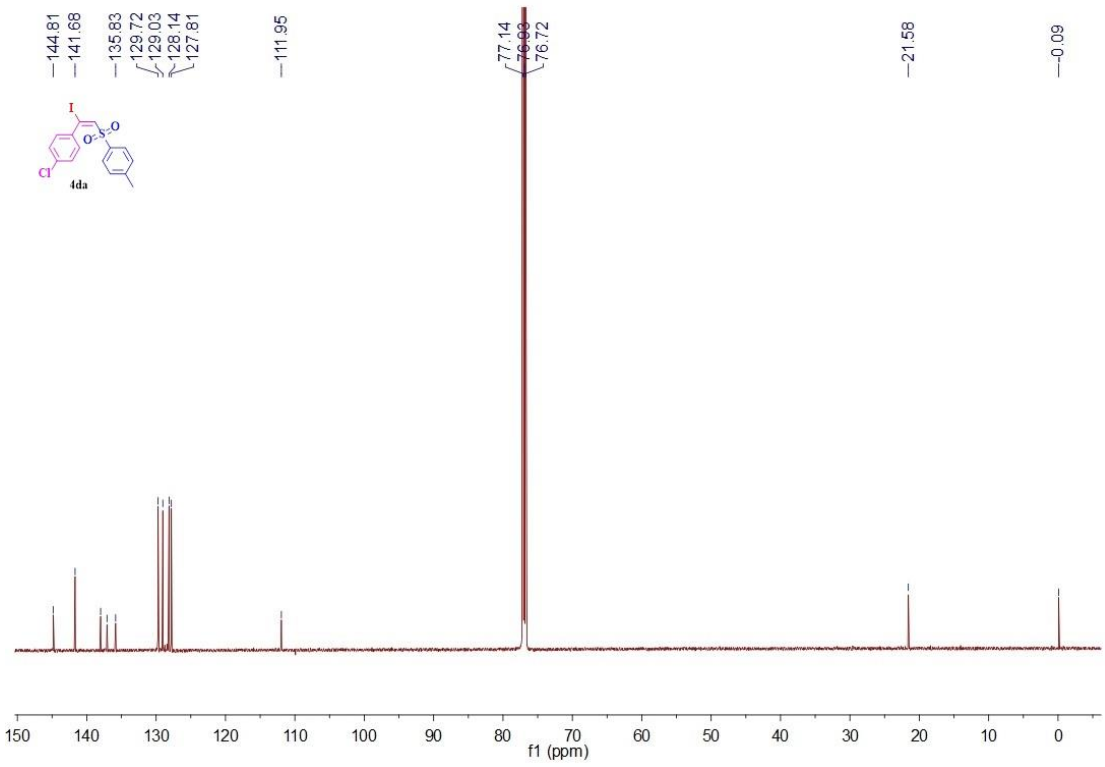
7.4928
7.3409
7.2771
7.2598
7.2424
7.2289
7.1930
7.1790
2.4180
0.0002
4da
2.07
1.00
2.05
2.18
2.03
3.14
f1 (ppm)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141.68
135.83
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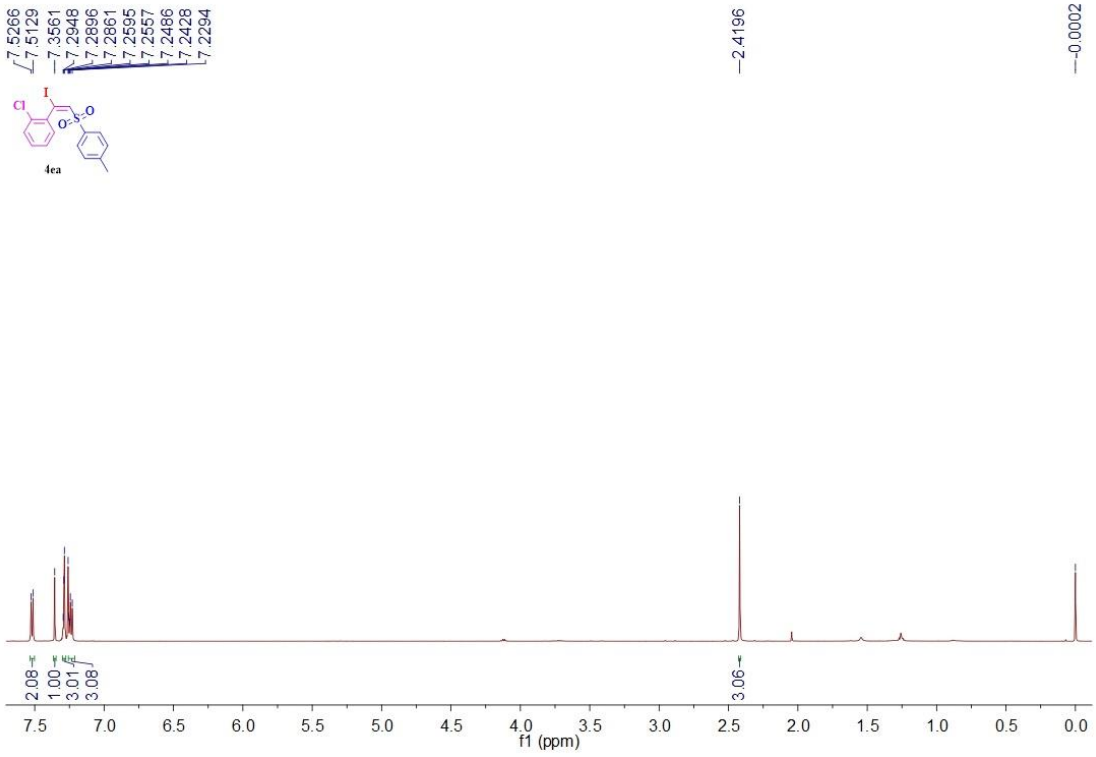
129.03
128.14
127.81
111.95
77.14
76.72
21.58
0.09
4da
f1 (ppm)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7.5129
7.3561
7.2948
7.2896
7.2861
7.2595
7.2557
7.2486
7.2428
7.2294
2.4196
0.0002
4ea
2.08
1.00
3.01
3.08
3.06
7.5
7.0
6.5
6.0
5.5
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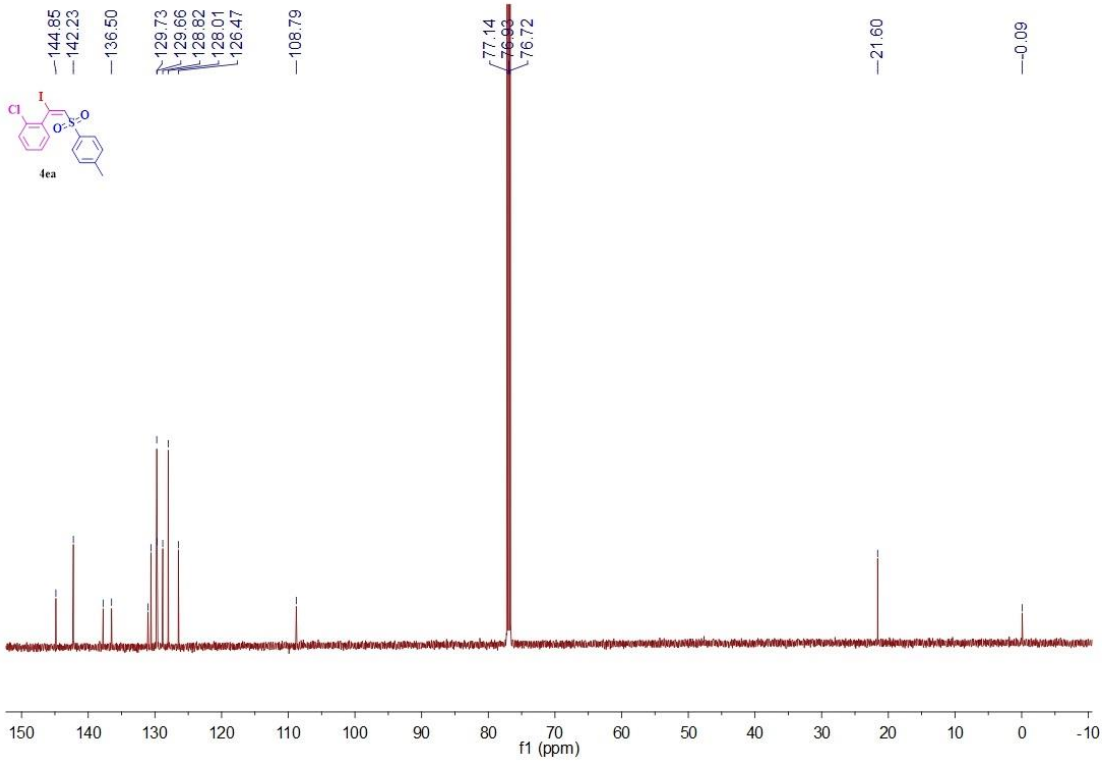
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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142.23
136.50
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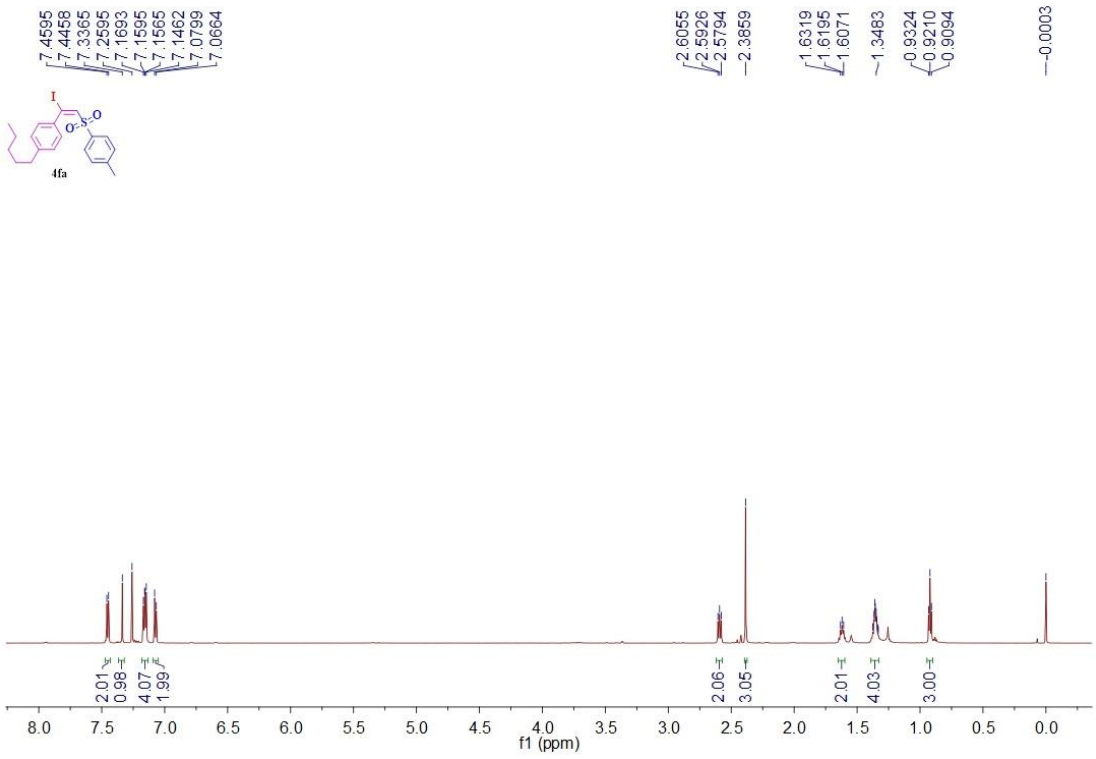
129.66
128.82
128.01
126.47
108.79
77.14
76.93
76.72
21.60
0.09
4ea
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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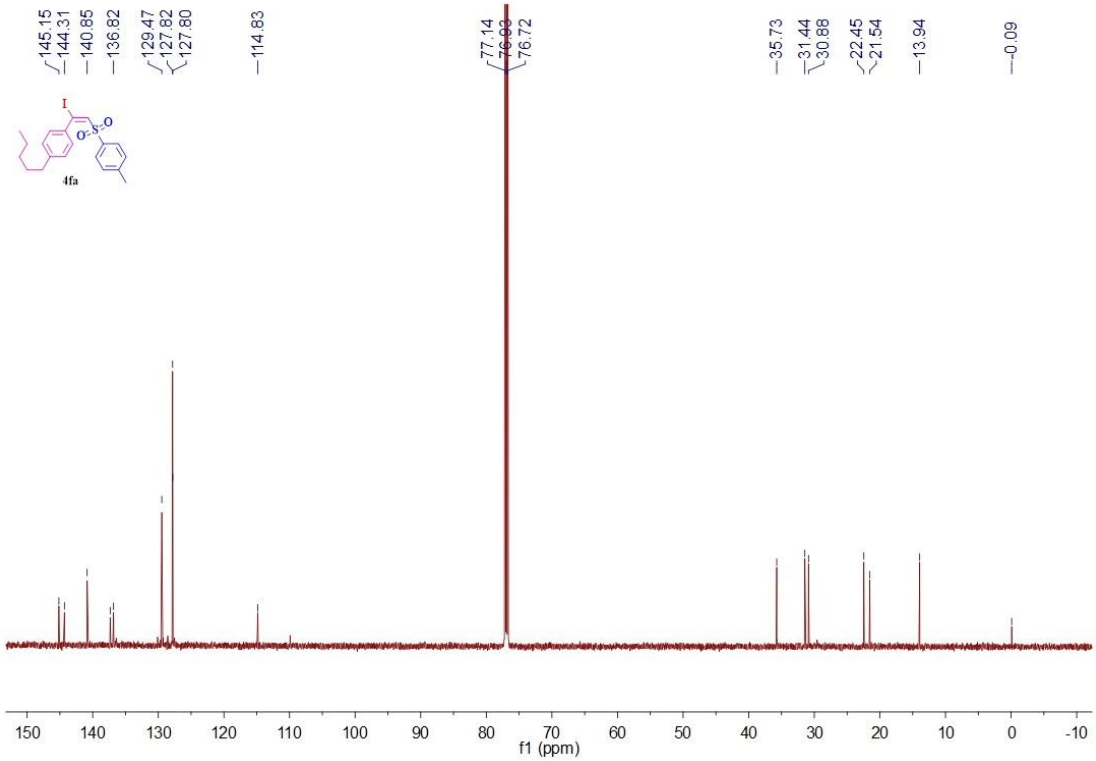
7.1565
7.1462
7.0799
7.0664
2.6055
2.5926
2.5794
2.3859
1.6319
1.6195
1.6071
1.3483
0.9324
0.9210
0.9094
0.0003
4fa
2.01
0.98
4.07
1.99
2.06
3.05
2.01
4.03
3.00
f1 (ppm)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140.85
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127.82
127.80
114.83
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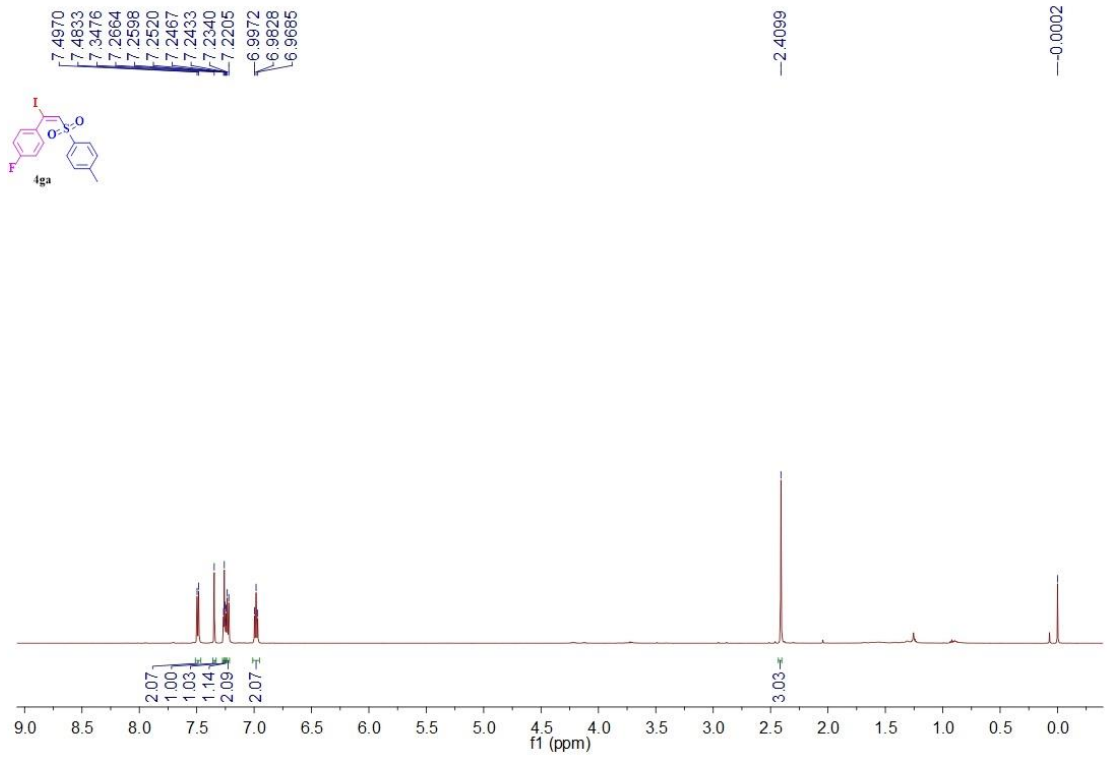
76.72
35.73
31.44
30.88
22.45
21.54
13.94
0.09
4fa
f1 (ppm)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7.2433
7.2340
7.2205
6.9972
6.9828
6.9685
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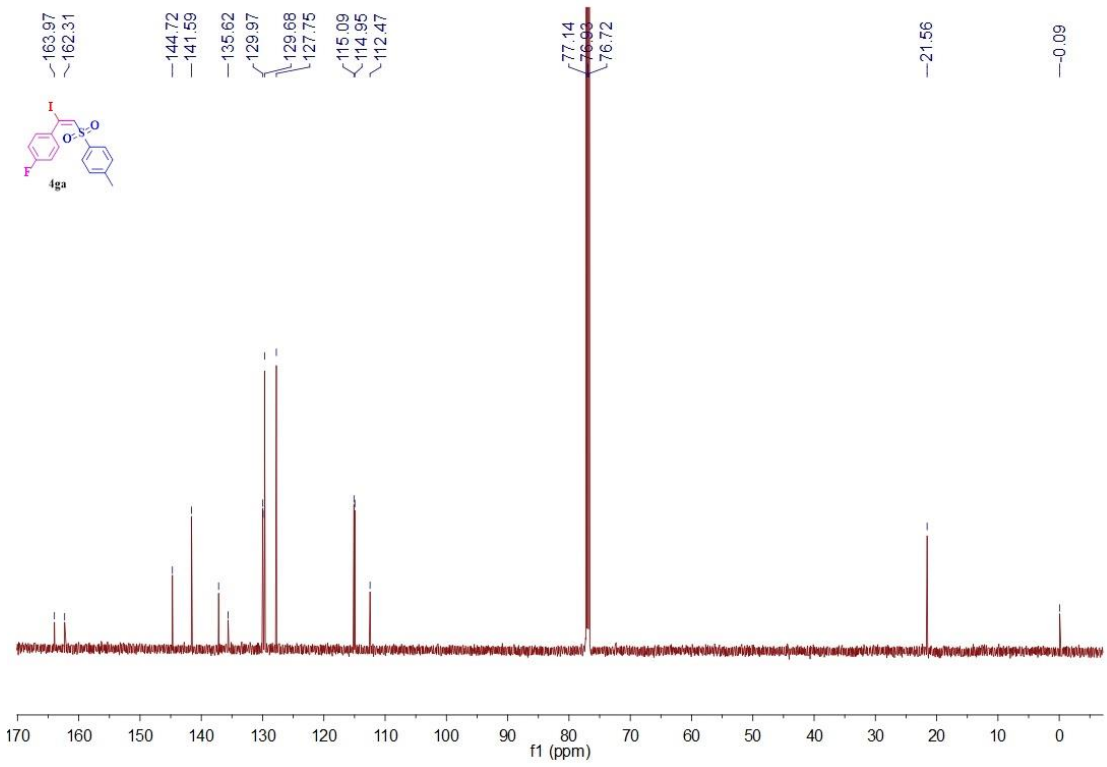
4ga
2.07
1.00
1.03
1.14
2.09
2.07
3.03
f1 (ppm)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141.59
135.62
129.97
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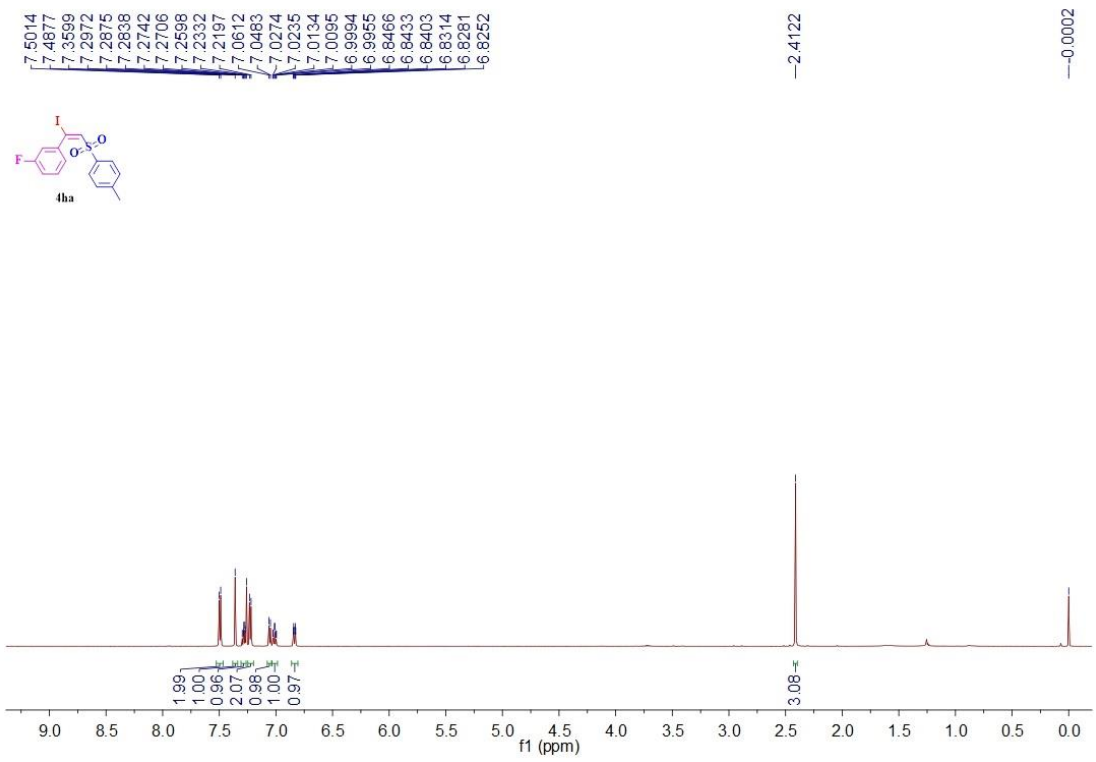
127.75
115.09
114.95
112.47
77.14
76.93
76.72
21.56
0.09
4ga
f1 (ppm)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7.0612
7.0483
7.0274
7.0235
7.0134
7.0095
6.9994
6.9955
6.8466
6.8433
6.8403
6.8314
6.8281
6.8252
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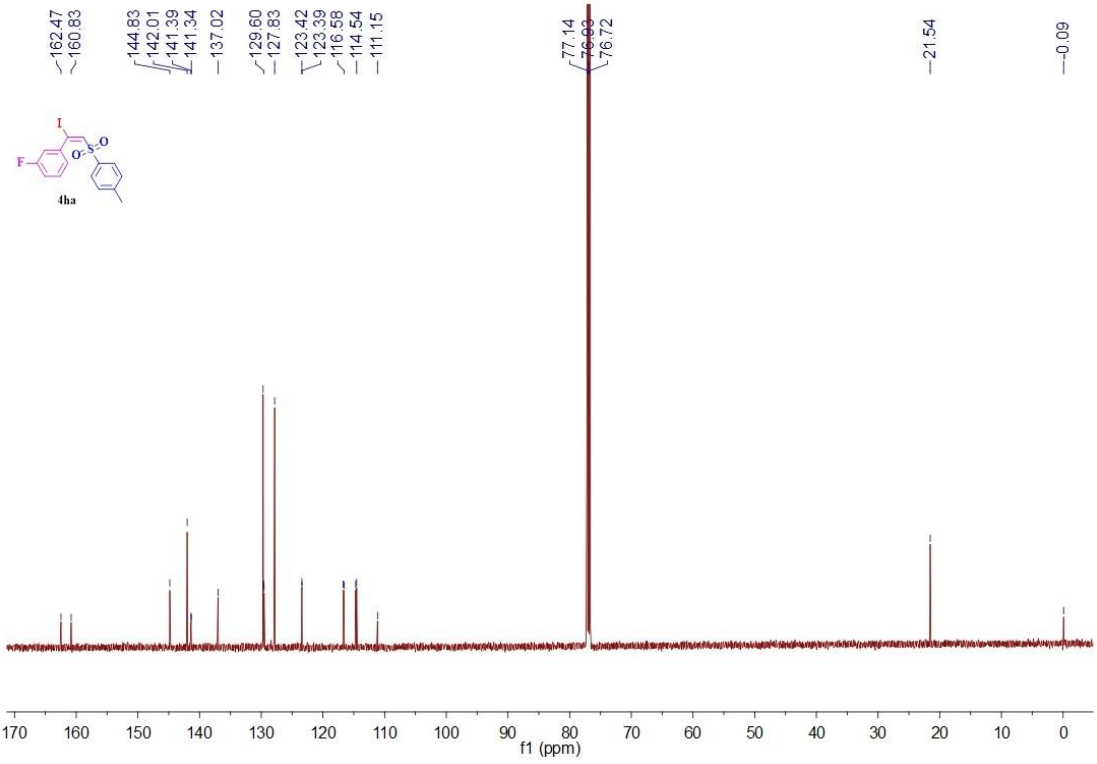
1.00
0.96
2.07
0.98
1.00
0.97
3.08
f1 (ppm)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141.39
141.34
137.02
129.60
127.83
123.42
123.39
116.58
114.54
111.15
77.14
76.90
76.72
21.54
0.09
4ha
f1 (ppm)