Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Iodine-mediated Synthesis of (*E*)-Vinyl Sulfones from Sodium Sulfinates and Cinnamic Acids in Aqueous Medium

Jian Gao, Junyi Lai and Gaoqing Yuan*

School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China

E-mail: gqyuan@scut.edu.cn

1. General Information.

Unless otherwise noted, all of solvents and reagents were used as received. ^{1}H and ^{13}C NMR spectra were recorded on a Brüker Advance 400 spectrometer (^{1}H: 400 MHz, ^{13}C: 100 MHz).The chemical shifts were referenced to signals at 7.26 and 77.0 ppm, respectively. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Mass spectra were recorded on a Shimadzu GCMS-QP5050A spectrometer at an ionization voltage of 70 eV equipped with a DB-WAX capillary column. GC-MS was obtained using electron ionization (EI). High-resolution mass spectra (ESI) were obtained with a LCMS-IT-TOF mass spectrometer.

2. Synthesis of 4-methylbenzene-1-sulfonyl iodide.[1]

Sodium 4-methylbenzenesulfinate (5 mmol, 0.89 g) was dissolved in 100 mL water at room temperature. Meanwhile, iodine (2.1 g) was dissolved in 10 mL alcohol at room temperature. Then, the sodium 4-methylbenzenesulfinate solution was added to the iodine solution gradually until a slight excess of iodine was present, and the yellow precipitate was generated continuously. The precipitate was filtered, washed with water, and dried at room temperature. Finally, 4-methylbenzene-1-sulfonyl iodide could be obtained.

MS spectrum of the prepared 4-methylbenzene-1-sulfonyl iodide was given in Figure S-1.

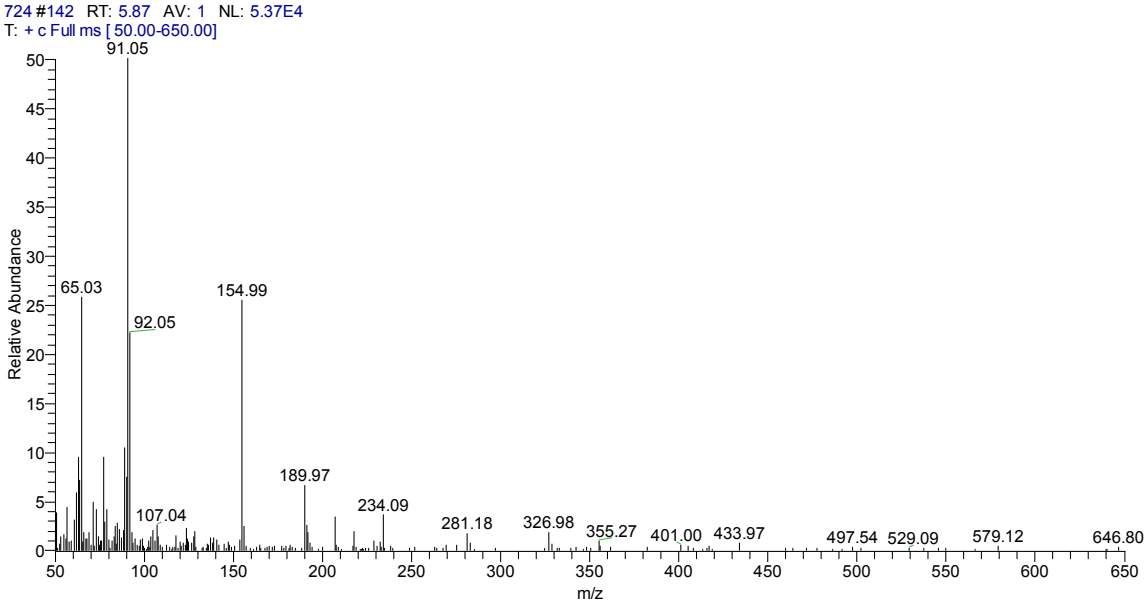
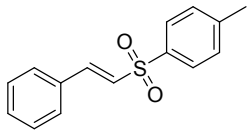


Figure S-1. MS spectrum of the prepared 4-methylbenzene-1-sulfonyl iodide

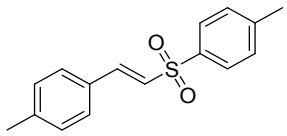
3. General Procedure for the Synthesis of (*E*)-Vinyl Sulfones.

Trans-cinnamic acid **1a** (0.5 mmol), sodium 4-methylbenzenesulfinate **2a** (0.6 mmol), I_2 (1.0 equiv.), K_2CO_3 (1.0 equiv.) and H_2O (2 mL) were added to a 10 mL glass tube at 60 ºC under continuously stirring for 10 h and monitored periodically by TLC. Then the aqueous solution was extracted with diethyl ether (3 × 5 mL) and dried by anhydrous $MgSO_4$. The solvent was removed under reduced pressure by an aspirator, and the crude product was purified by silica gel column chromatography using petroleum ether and ethyl acetate (5:1) as eluent to give the pure product **3a**.

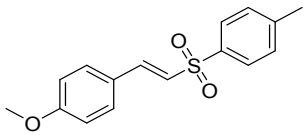
4. Analytical Data for All Products (3a–3t).



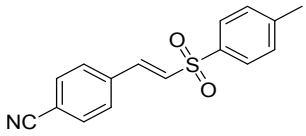
(*E*)-1-methyl-4-(styrylsulfonyl)benzene (3a).[2] Pale Yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.4 Hz, 2H), 7.66 (d, *J* = 15.3 Hz, 1H), 7.46 – 7.33 (m, 7H), 6.85 (d, *J* = 15.3 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 142.0, 137.8, 132.5, 131.1, 130.0, 129.1, 128.5, 127.7, 127.7, 21.6.



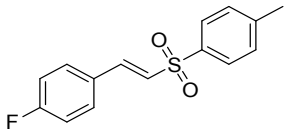
(*E*)-1-methyl-4-((4-methylstyryl)sulfonyl)benzene (3b).[3] Pale Yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.5 Hz, 2H), 7.62 (d, *J* = 15.3 Hz, 1H), 7.39 – 7.30 (m, 4H), 7.18 (d, *J* = 7.5 Hz, 2H), 6.79 (d, *J* = 15.3 Hz, 1H), 2.43 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 142.0, 141.7, 138.0, 129.9, 129.8, 129.7, 128.5, 127.7, 126.5, 21.6, 21.5.



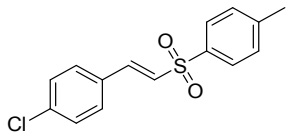
(*E*)-1-methoxy-4-(2-tosylvinyl)benzene (3c).[4] White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.2 Hz, 2H), 7.60 (d, *J* = 15.3 Hz, 1H), 7.41 (d, *J* = 7.4 Hz, 2H), 7.32 (d, *J* = 7.4 Hz, 2H), 6.89 (d, *J* = 7.4 Hz, 2H), 6.71 (d, *J* = 15.3 Hz, 1H), 3.82 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0, 144.1, 141.8, 138.2, 130.3, 129.9, 127.6, 125.1, 124.9, 114.5, 55.4, 21.6.



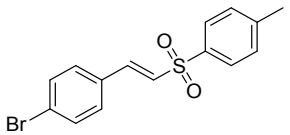
(*E*)-4-(2-tosylvinyl)benzonitrile (3d). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.4 Hz, 2H), 7.79 – 7.45 (m, 5H), 7.37 (d, *J* = 7.5 Hz, 2H), 6.96 (d, *J* = 15.5 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 139.2, 136.9, 136.8, 132.8, 131.4, 130.2, 128.9, 127.9, 118.0, 114.2, 21.7. ESI-HRMS calcd for $C_{16}H_{13}NNaO_2S$ $[M+Na]^+$ 306.0565, found 306.0559.



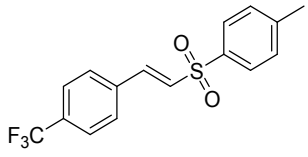
(E)-1-fluoro-4-(2-tosylvinyl)benzene (3e).[2] Colourless oil,^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.6 Hz, 2H), 7.62 (d, *J* = 15.4 Hz, 1H), 7.53 – 7.43 (m, 2H), 7.33 (d, *J* = 7.6 Hz, 2H), 7.06 (t, *J* = 8.0 Hz, 2H), 6.83 (d, *J* = 15.4 Hz, 1H), 2.42 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 163.0, 144.5, 140.6, 137.7, 130.6, 130.6, 130.0, 128.8, 128.7, 127.7, 127.5, 127.5, 116.4, 116.2, 21.6.



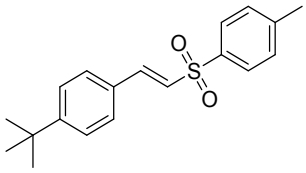
(*E*)-1-chloro-4-(2-tosylvinyl)benzene (3f).[3] White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.2 Hz, 2H), 7.60 (d, *J* = 15.3 Hz, 1H), 7.37 (dd, *J* = 23.0, 6.6 Hz, 6H), 6.85 (d, *J* = 15.4 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 140.4, 137.5, 137.1, 131.0, 130.1, 129.7, 129.4, 128.3, 127.8, 21.6.



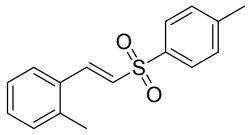
(*E*)-1-bromo-4-(2-tosylvinyl)benzene (3g).[2] White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.6 Hz, 2H), 7.58 (d, *J* = 15.5 Hz, 1H), 7.52 (d, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 13.6 Hz, 4H), 6.85 (d, *J* = 15.4 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 140.5, 137.5, 132.4, 131.4, 130.1, 129.9, 128.4, 127.8, 125.5, 21.6.



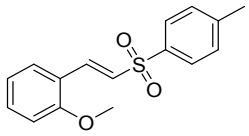
(E)-1-methyl-4-((4-(trifluoromethyl)styryl)sulfonyl)benzene (3h).[5] White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.4 Hz, 2H), 7.79 – 7.61 (m, 3H), 7.58 (d, *J* = 7.6 Hz, 2H), 7.36 (d, *J* = 7.6 Hz, 2H), 6.95 (d, *J* = 15.4 Hz, 1H), 2.44 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 139.9, 137.2, 135.9, 132.7, 132.4, 130.4, 130.1, 128.7, 127.9, 126.1, 126.1, 126.0, 126.0, 122.3, 21.6.



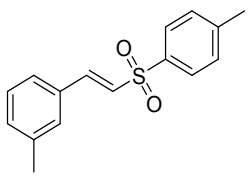
(*E*)-1-(tert-butyl)-4-(2-tosylvinyl)benzene (3i).[5] Pale yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.5 Hz, 2H), 7.64 (d, *J* = 15.3 Hz, 1H), 7.41 (d, *J* = 0.8 Hz, 4H), 7.32 (d, *J* = 7.6 Hz, 2H), 6.81 (d, *J* = 15.3 Hz, 1H), 2.42 (s, 3H), 1.30 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 144.3, 142.0, 138.0, 129.9, 129.7, 128.4, 127.7, 126.6, 126.1, 35.0, 31.1, 21.6.



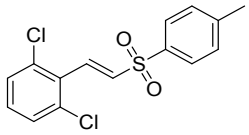
(*E*)-1-methyl-2-(2-tosylvinyl)benzene (3j).[5] Pale yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 15.3 Hz, 1H), 7.83 (d, *J* = 7.7 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 7.4 Hz, 1H), 7.18 (dd, *J* = 15.3, 7.5 Hz, 2H), 6.77 (d, *J* = 15.3 Hz, 1H), 2.43 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 139.6, 138.1, 137.8, 131.4, 131.0, 130.9, 130.0, 128.6, 127.7, 126.9, 126.5, 21.6, 19.8.



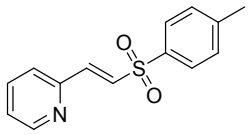
(*E*)-1-methoxy-2-(2-tosylvinyl)benzene (3k).[2] Colourless oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.70 (m, 3H), 7.45 – 7.29 (m, 4H), 7.06 (d, *J* = 15.4 Hz, 1H), 6.93 (dd, *J* = 18.6, 8.2 Hz, 2H), 3.87 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 144.0, 138.3, 138.0, 132.4, 130.7, 129.9, 128.3, 127.7, 121.3, 120.8, 111.3, 55.5, 21.6.



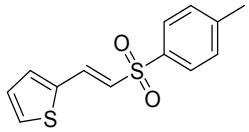
(*E*)-1-methyl-3-(2-tosylvinyl)benzene (3l).[6] Pale yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.7 Hz, 2H), 7.62 (d, *J* = 15.3 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 2H), 7.27 (d, *J* = 5.1 Hz, 4H), 6.83 (d, *J* = 15.4 Hz, 1H), 2.42 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 142.1, 138.8, 137.9, 132.4, 131.9, 130.0, 129.1, 129.0, 127.7, 127.4, 125.8, 21.6, 21.3.



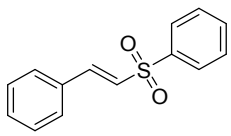
(*E*)-1,3-dichloro-2-(2-tosylvinyl)benzene (3m). Pale yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (t, *J* = 11.5 Hz, 3H), 7.35 (t, *J* = 7.8 Hz, 4H), 7.21 (t, *J* = 7.9 Hz, 1H), 7.13 (d, *J* = 15.8 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 137.1, 135.8, 135.3, 135.3, 130.7, 130.1, 129.8, 129.0, 127.9, 21.7. ESI-HRMS calcd for $C_{16}H_{13}Cl_2NaO_2S$ $[M+Na]^+$ 348.9831, found 348.9827.



(*E*)-2-(2-tosylvinyl)pyridine (3n). Yellow oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 - 8.41 (m, 1H), 7.84 (d, *J* = 6.8 Hz, 2H), 7.73 (t, *J* = 6.7 Hz, 1H), 7.62 (d, *J* = 14.9 Hz, 1H), 7.47 – 7.27 (m, 5H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 150.3, 144.6, 140.0, 137.3, 137.1, 132.2, 130.0, 127.9, 125.4, 124.9, 21.6. ESI-HRMS calcd for $C_{16}H_{13}Cl_2O_2S$ M^+ 260.0743, found 260.0740.

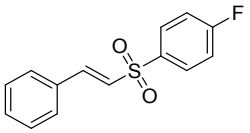


(*E*)-2-(2-tosylvinyl)thiophene (3o).[4] Brown solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.4 Hz, 2H), 7.76 (d, *J* = 15.2 Hz, 1H), 7.42 (d, *J* = 3.9 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 2H), 7.28 (d, *J* = 11.0 Hz, 1H), 7.05 (t, *J* = 3.9 Hz, 1H), 6.64 (d, *J* = 15.1 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 137.9, 137.1, 1346, 132.3, 130.0, 129.9, 128.3, 127.7, 125.9, 21.6.

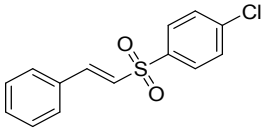


(*E*)-(2-(phenylsulfonyl)vinyl)benzene (3p).[3] Pale yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.3 Hz, 2H), 7.69 (d, *J* = 15.4 Hz, 1H), 7.64 – 7.57 (m, 1H), 7.53 (t, *J* = 7.3 Hz, 2H),

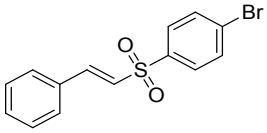
7.47 (d, *J* = 6.4 Hz, 2H), 7.38 (d, *J* = 5.9 Hz, 3H), 6.89 (d, *J* = 15.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.5, 140.8, 133.5, 132.4, 131.3, 129.4, 129.1, 128.6, 127.7, 127.4.



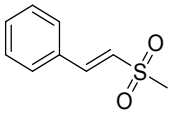
(E)-1-fluoro-4-(styrylsulfonyl)benzene (3q).[2] Colourless oil,^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.87 (m, 2H), 7.68 (d, *J* = 15.3 Hz, 1H), 7.48 (d, *J* = 6.5 Hz, 2H), 7.40 (d, *J* = 6.3 Hz, 3H), 7.22 (t, *J* = 7.8 Hz, 2H), 6.86 (d, *J* = 15.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 164.4, 142.7, 136.9, 136.8, 132.3, 131.4, 130.6, 130.5, 129.1, 128.6, 127.2, 116.8, 116.6.



(*E*)-1-chloro-4-(styrylsulfonyl)benzene (3r).[7] White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.4 Hz, 2H), 7.69 (d, *J* = 15.4 Hz, 1H), 7.56 – 7.45 (m, 4H), 7.40 (d, *J* = 6.7 Hz, 3H), 6.85 (d, *J* = 15.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 140.1, 139.3, 132.2, 131.4, 129.7, 129.2, 128.7, 126.9.



(*E*)-1-bromo-4-(styrylsulfonyl)benzene (3s).[2] White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.8 Hz, 2H), 7.75 – 7.61 (m, 3H), 7.48 (d, *J* = 6.4 Hz, 2H), 7.39 (d, *J* = 6.6 Hz, 3H), 6.86 (d, *J* = 15.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 139.8, 132.7, 132.2, 131.5, 129.2, 129.2, 128.7, 128.7, 126.9.



(*E*)-(2-(methylsulfonyl)vinyl)benzene (3t).[7] Yellow oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 15.5 Hz, 1H), 7.52 (d, *J* = 6.4 Hz, 2H), 7.43 (d, *J* = 6.0 Hz, 3H), 6.95 (d, *J* = 15.5 Hz, 1H), 3.03 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 132.1, 131.4, 129.2, 128.6, 126.3, 43.3.

Reference:

1 M. Hong, Y. Li, B. Li and Y. Li, *Macromol. Rapid Commun.*, 2012, **33**, 998.

2 R. Q. Guo, Q. W. Gui and D. D. Wang, *Catal. Lett.*, 2014, **144**, 1377.

3 V. Nair, A. Augustine, T. G. George and L. G. Nair, *Tetrahedron Lett.*, 2001, **42**, 6763.

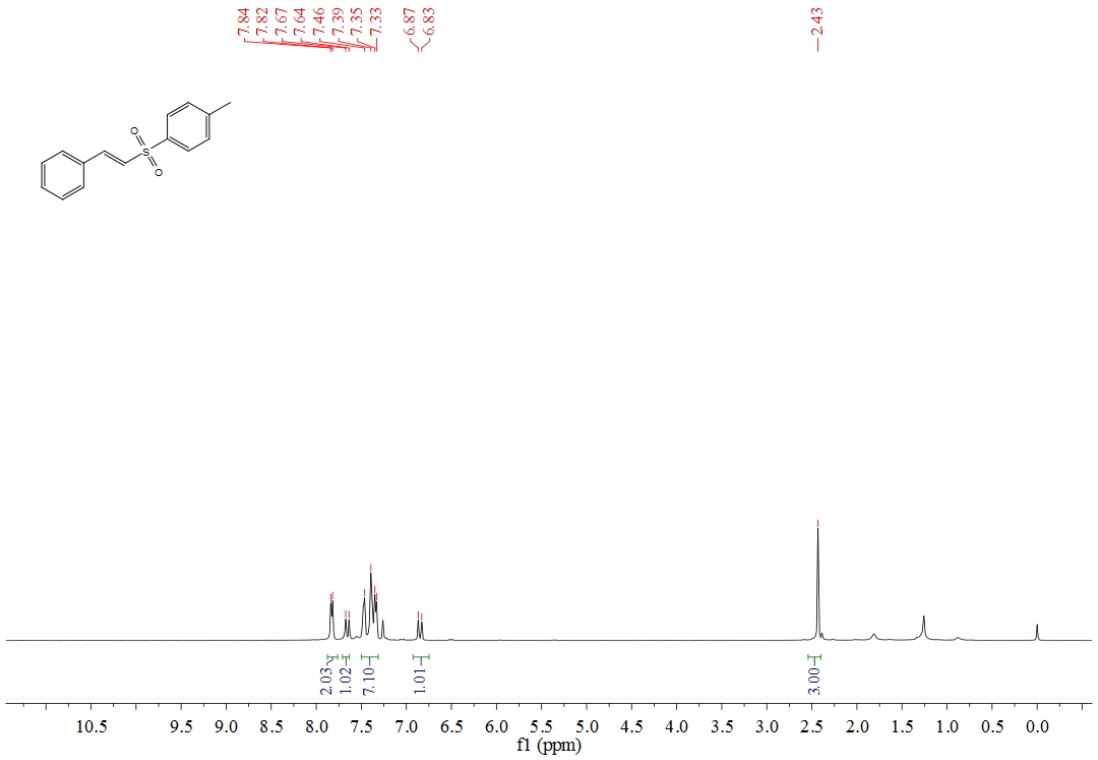
4 B. V. Rokade and K. R. Prabhu, *J. Org. Chem.*, 2014, **79**, 8110.

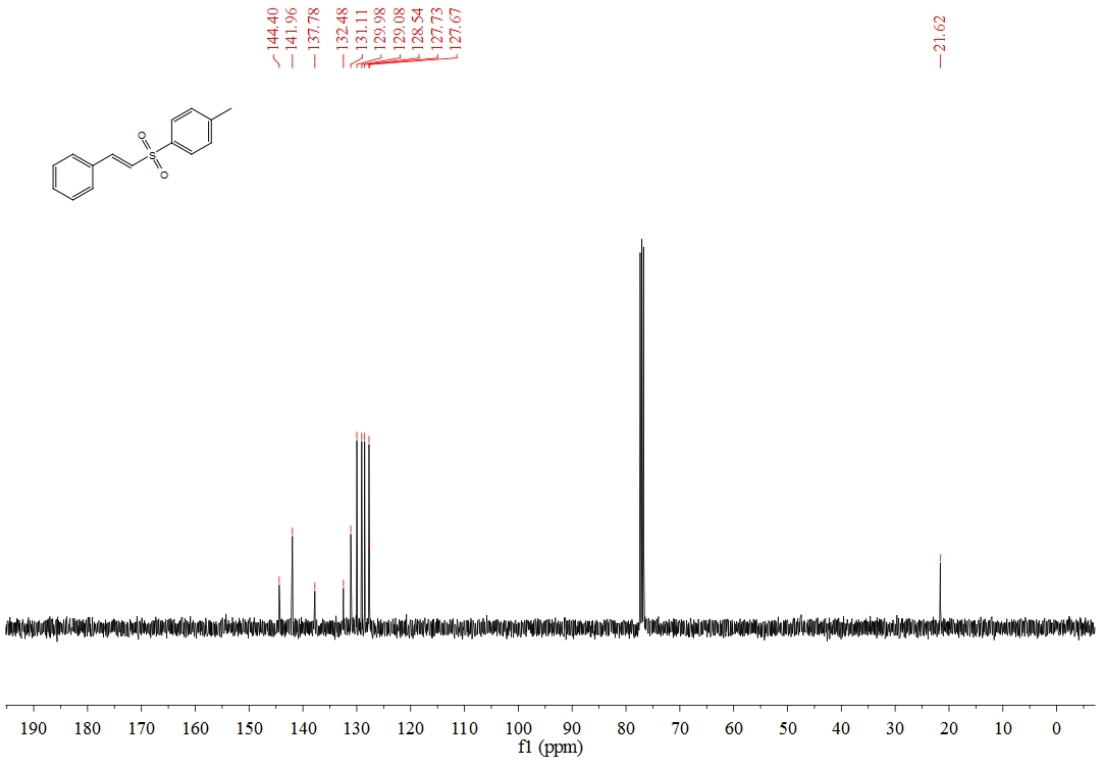
5 S. Tang, Y. Wu, W. Q. Liao, R. P. Bai, C. Liu and A. W. Lei, *Chem. Commun.*, 2014, **50**, 4496.

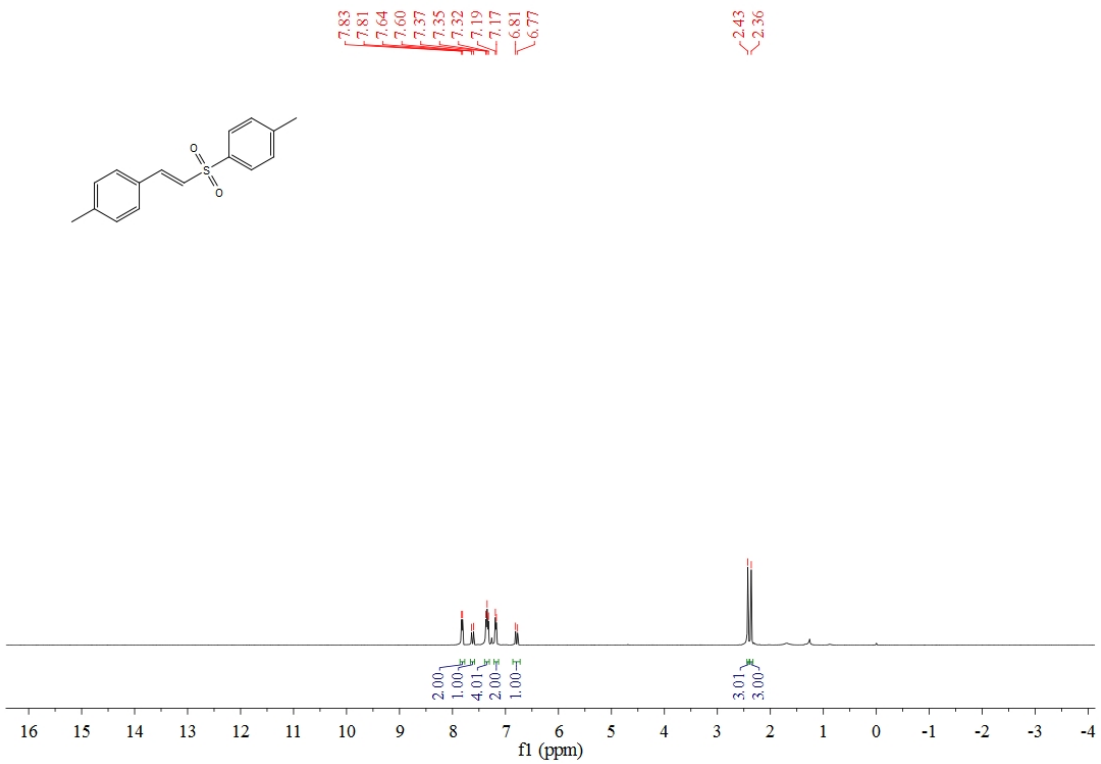
6 G. S. Deng and J. Y. Zou, *Arkivoc*, 2010, **2**, 186.

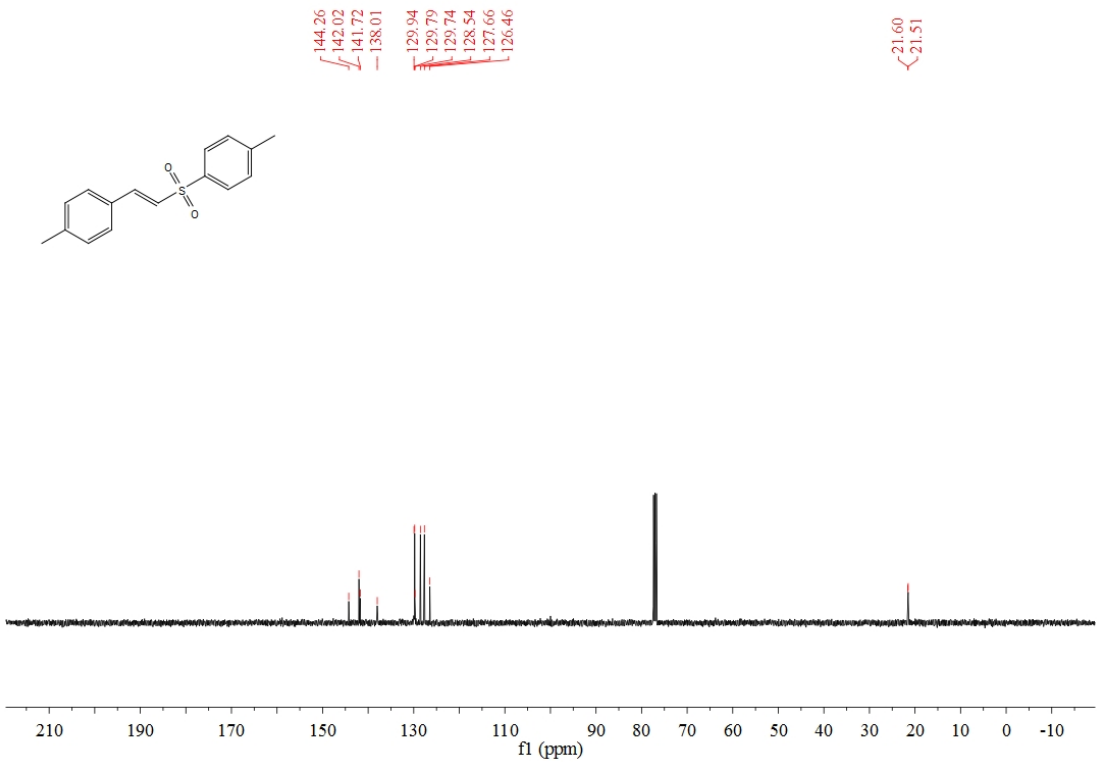
7 Y. L. Xu, X. T. Tang, W. G. Hu, W. Q. Wu and H. F. Jiang, *Green Chem.*, 2014, **16**, 3720.

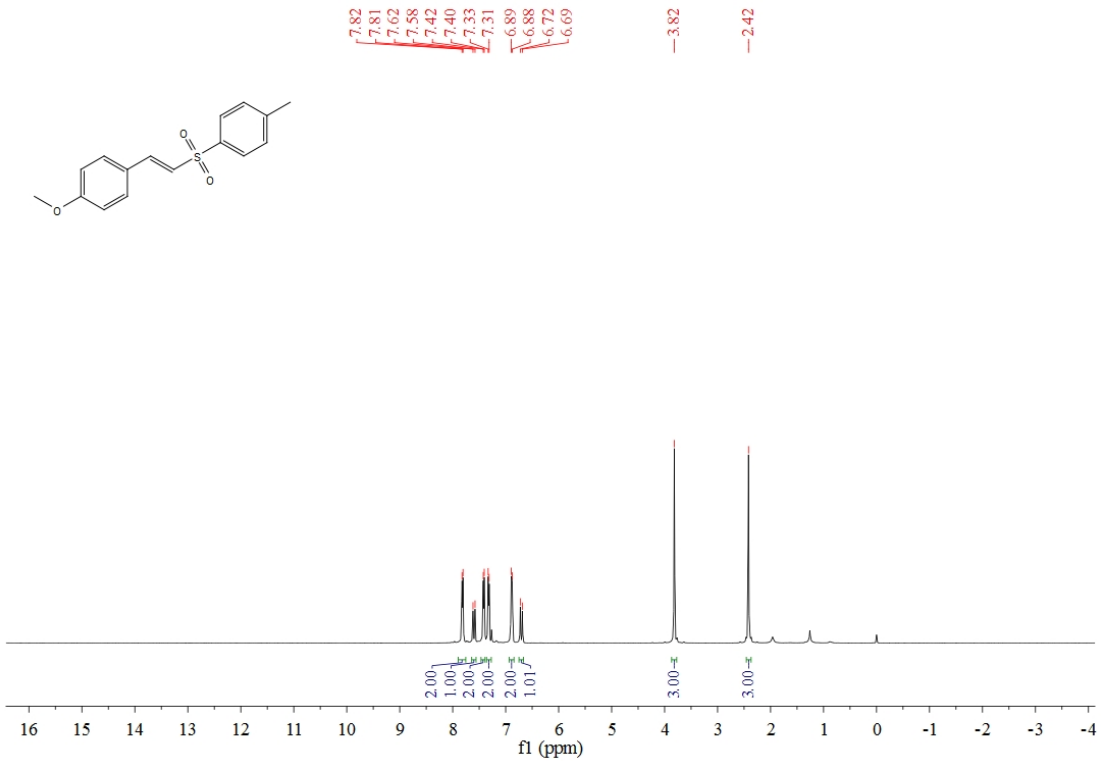
5. NMR Spectra for All Compounds.

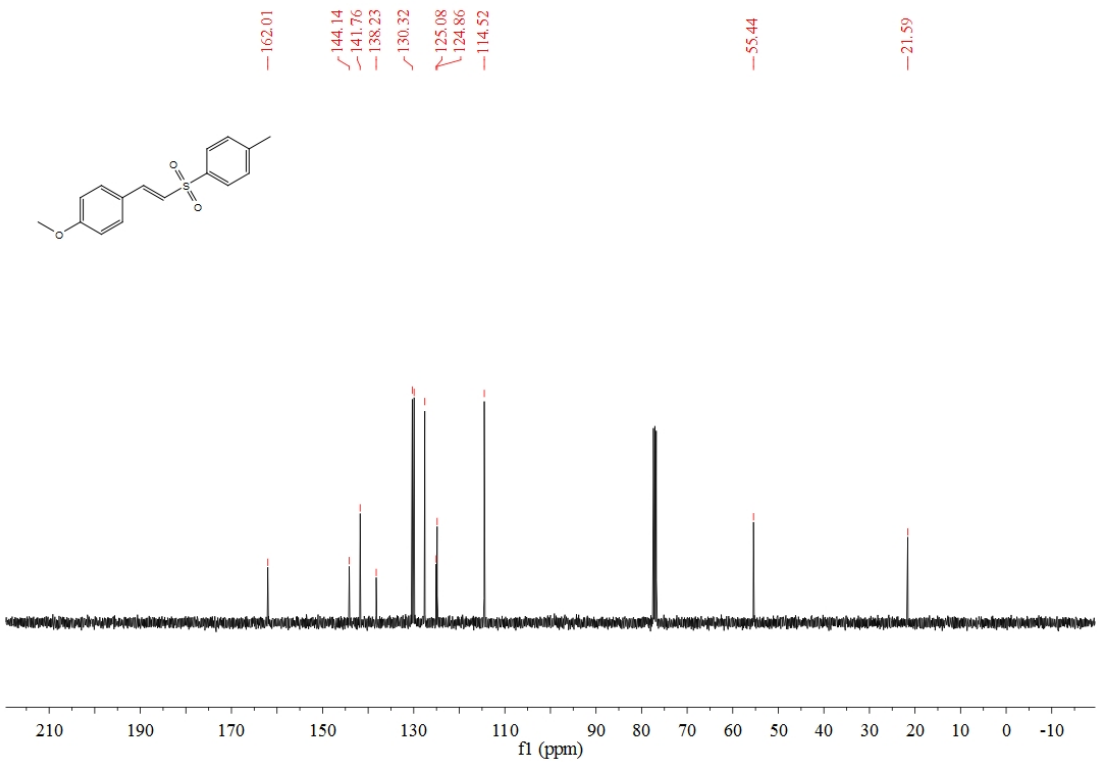

7.84
7.82
7.67
7.64
7.46
7.39
7.35
7.33
6.87
6.83
2.43
2.03
1.02
7.10
1.01
3.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

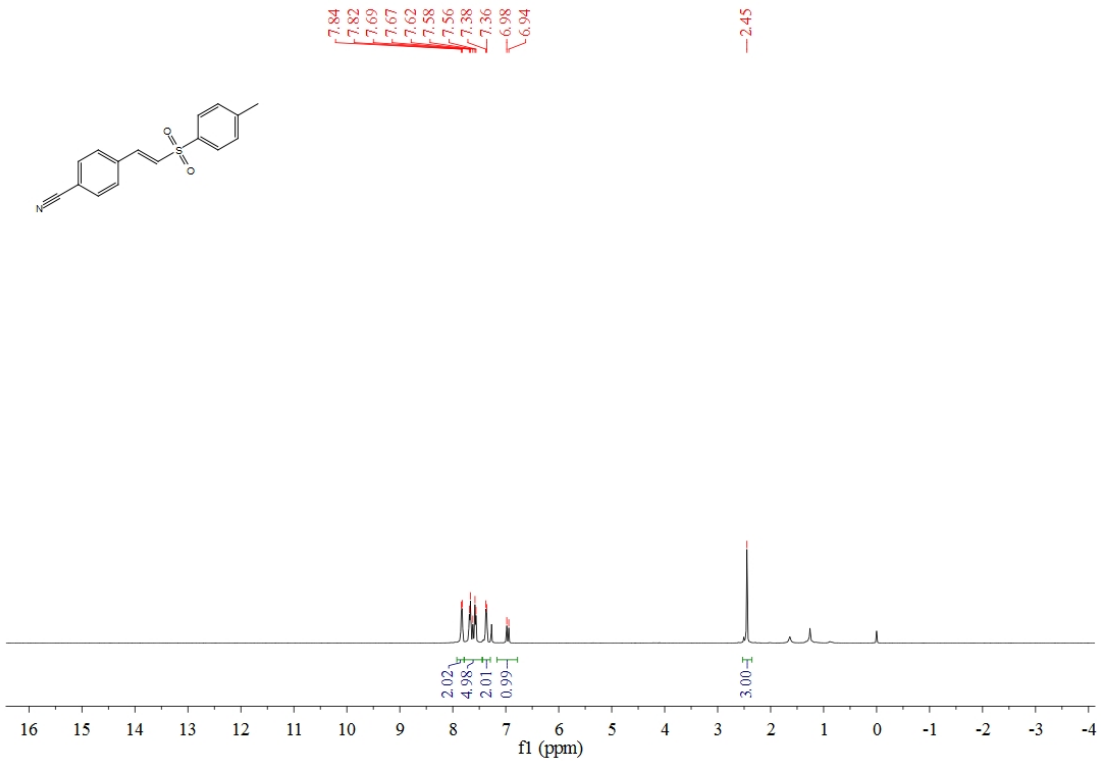

144.40
141.96
137.78
132.48
131.11
129.98
129.08
128.54
127.73
127.67
21.62
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

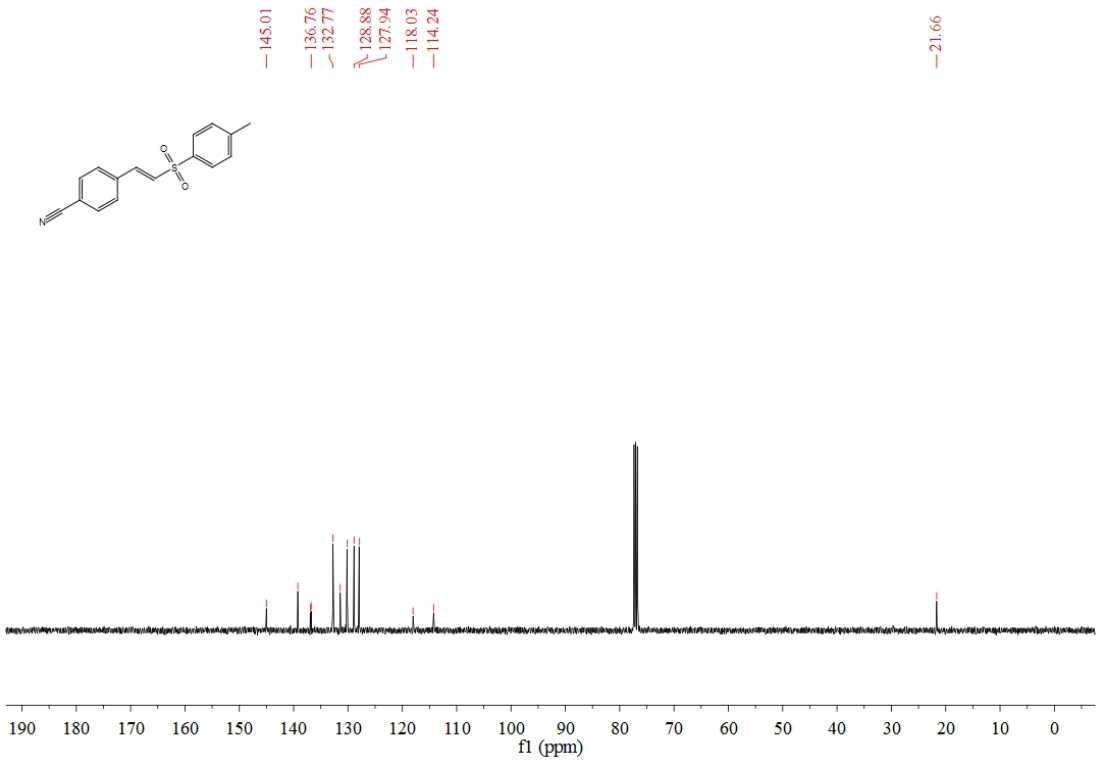

7.83
7.81
7.64
7.60
7.37
7.35
7.32
7.19
7.17
6.81
6.77
2.43
2.36
2.00
1.00
4.01
2.00
1.00
3.01
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

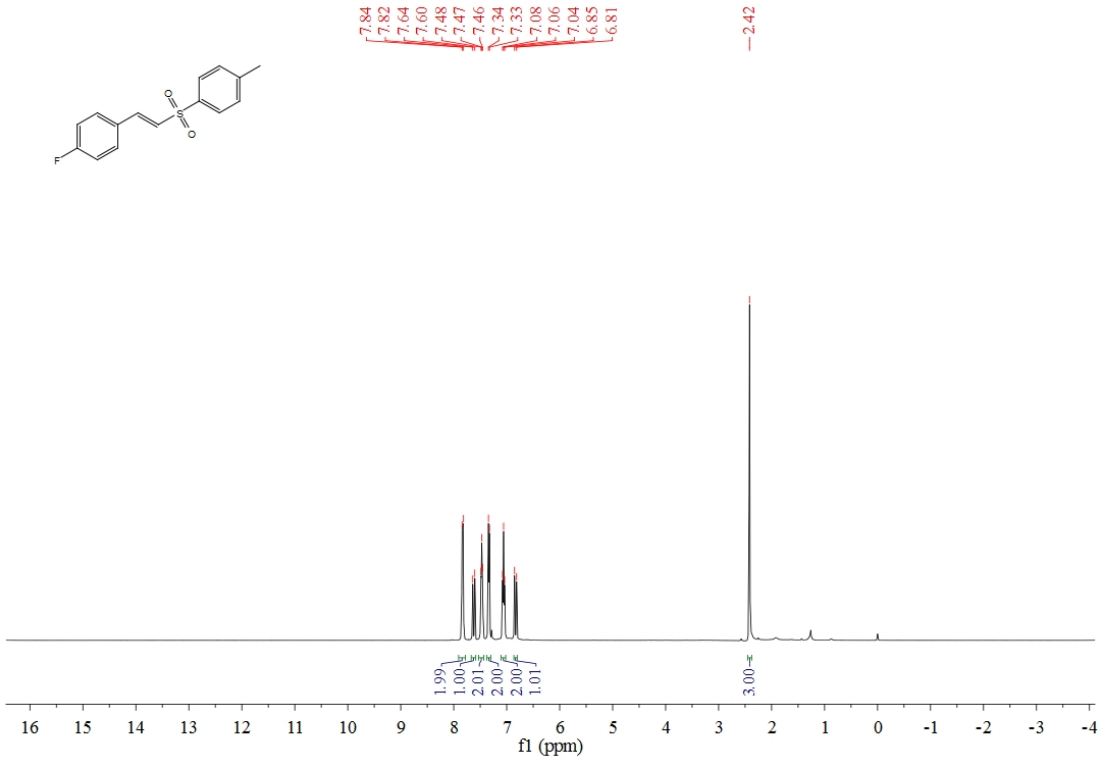

144.26
142.02
141.72
138.01
129.94
129.79
129.74
128.54
127.66
126.46
21.60
21.51
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

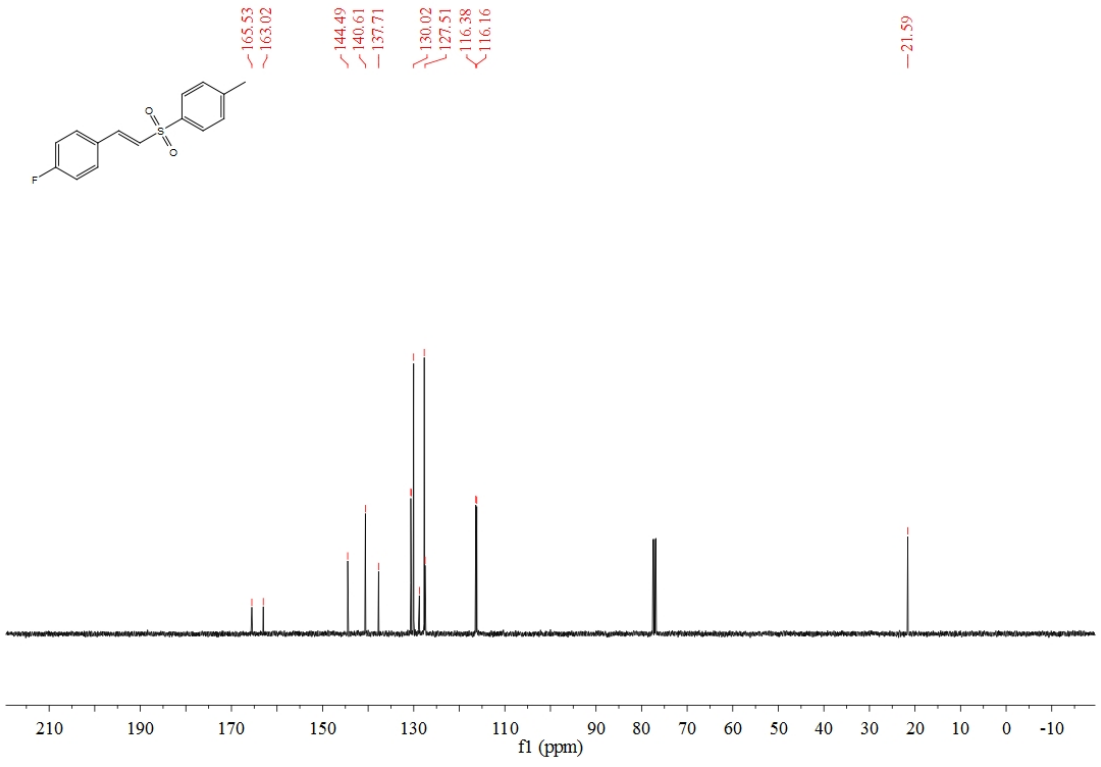

7.82
7.81
7.62
7.58
7.42
7.40
7.33
7.31
6.89
6.88
6.72
6.69
3.82
2.42
2.00
1.00
2.00
2.00
2.00
1.01
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

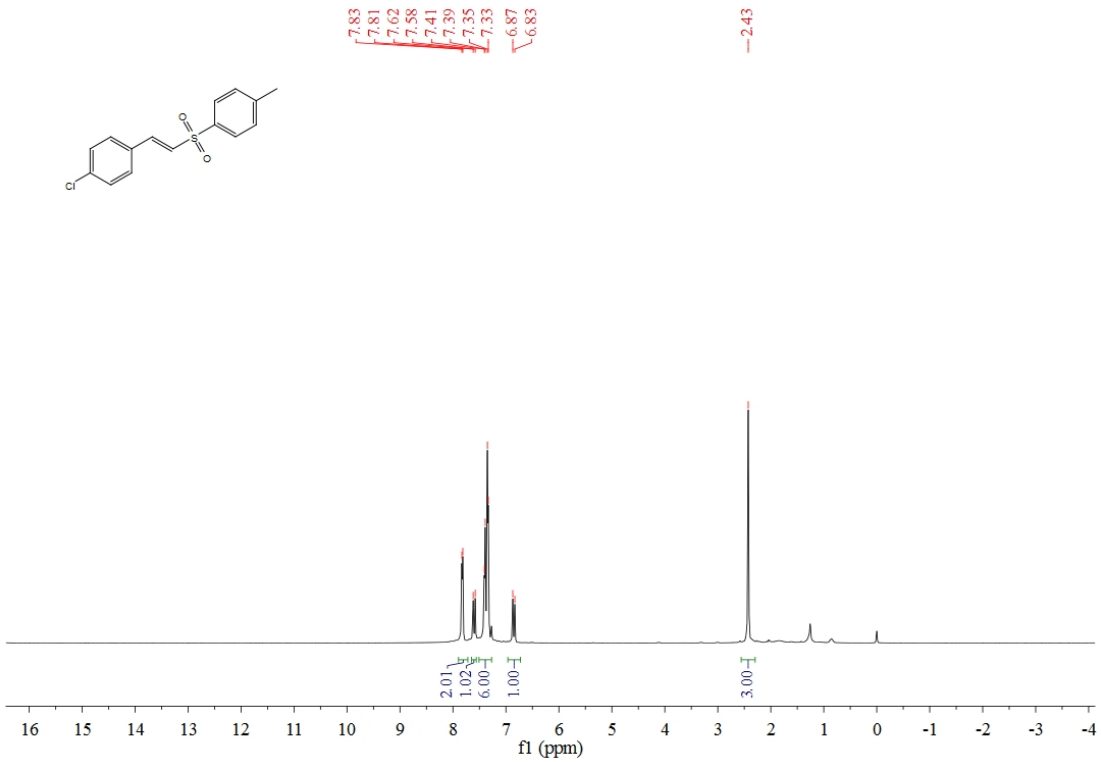

162.01
144.14
141.76
138.23
130.32
125.08
124.86
114.52
55.44
21.59
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

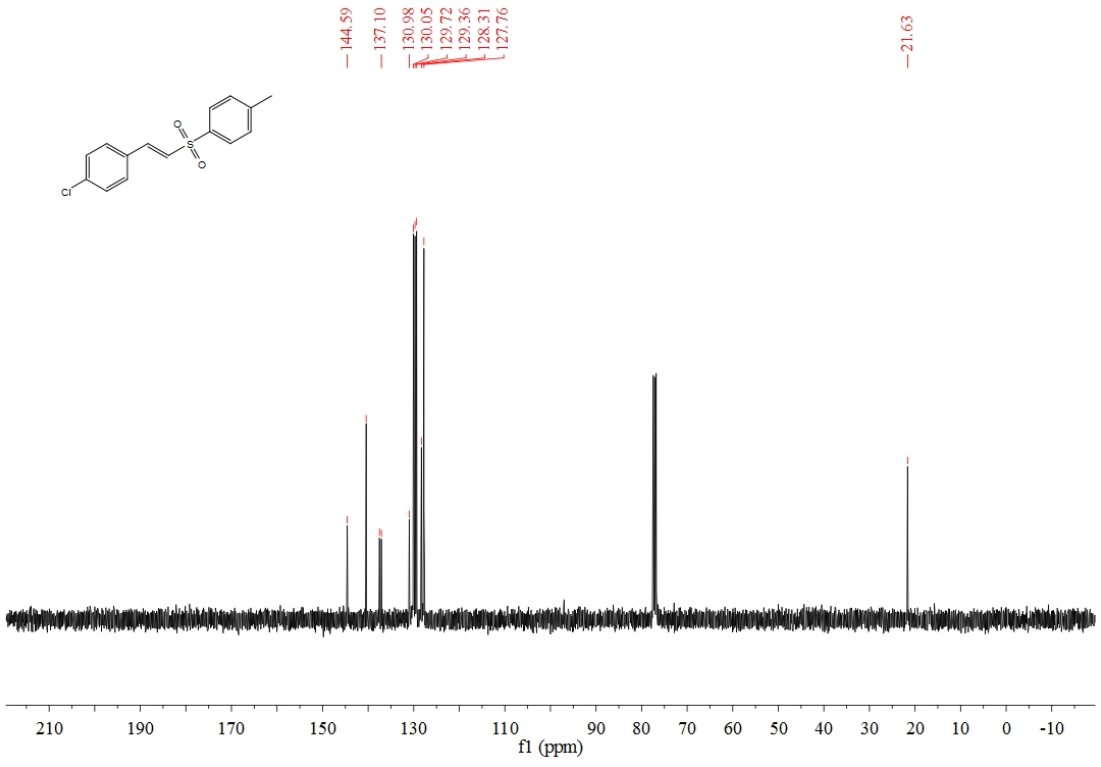

7.84
7.82
7.69
7.67
7.62
7.58
7.56
7.38
7.36
6.98
6.94
2.45
2.02
4.98
2.01
0.99
3.00
f1 (ppm)

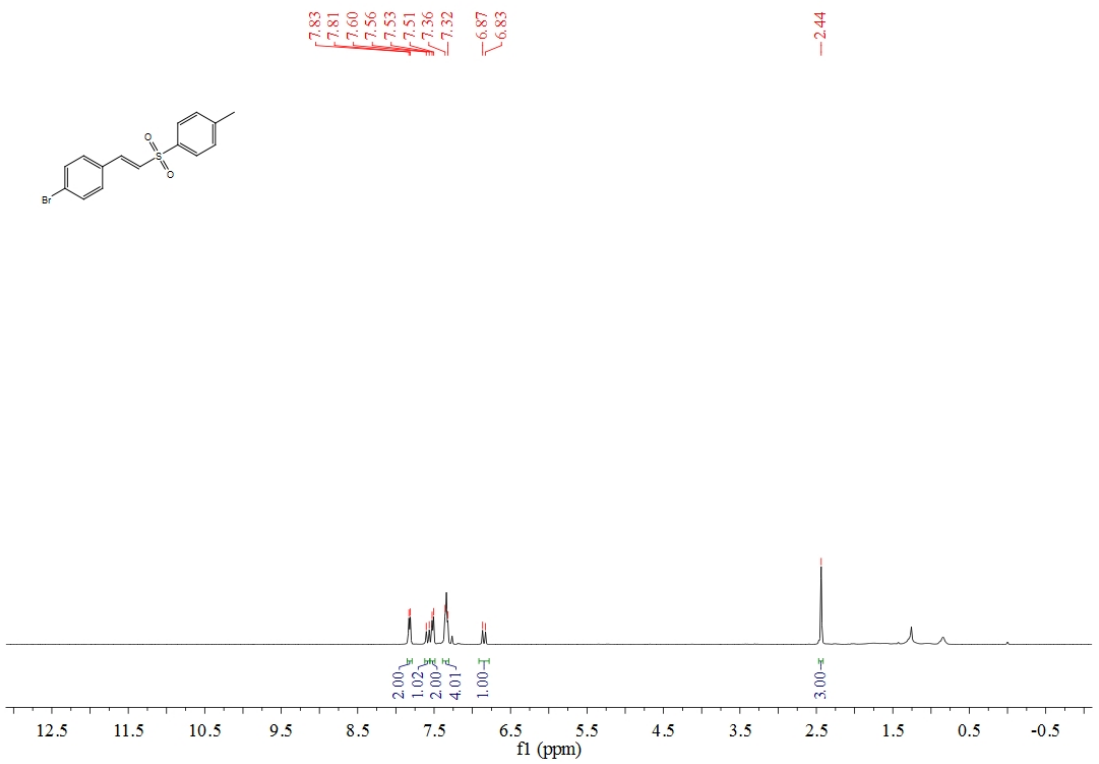

145.01
136.76
132.77
128.88
127.94
118.03
114.24
21.66
f1 (ppm)

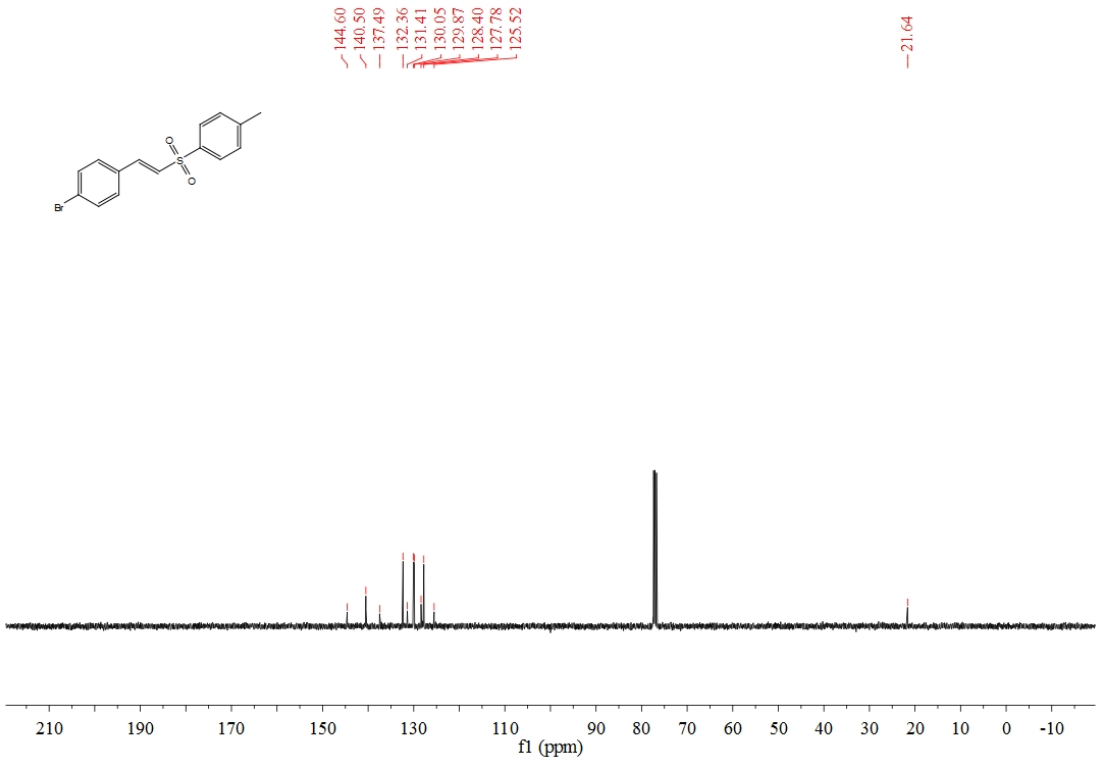

7.84
7.82
7.64
7.60
7.48
7.47
7.46
7.34
7.33
7.08
7.06
7.04
6.85
6.81
2.42
1.99
1.00
2.01
2.00
2.00
1.01
3.00
f1 (ppm)

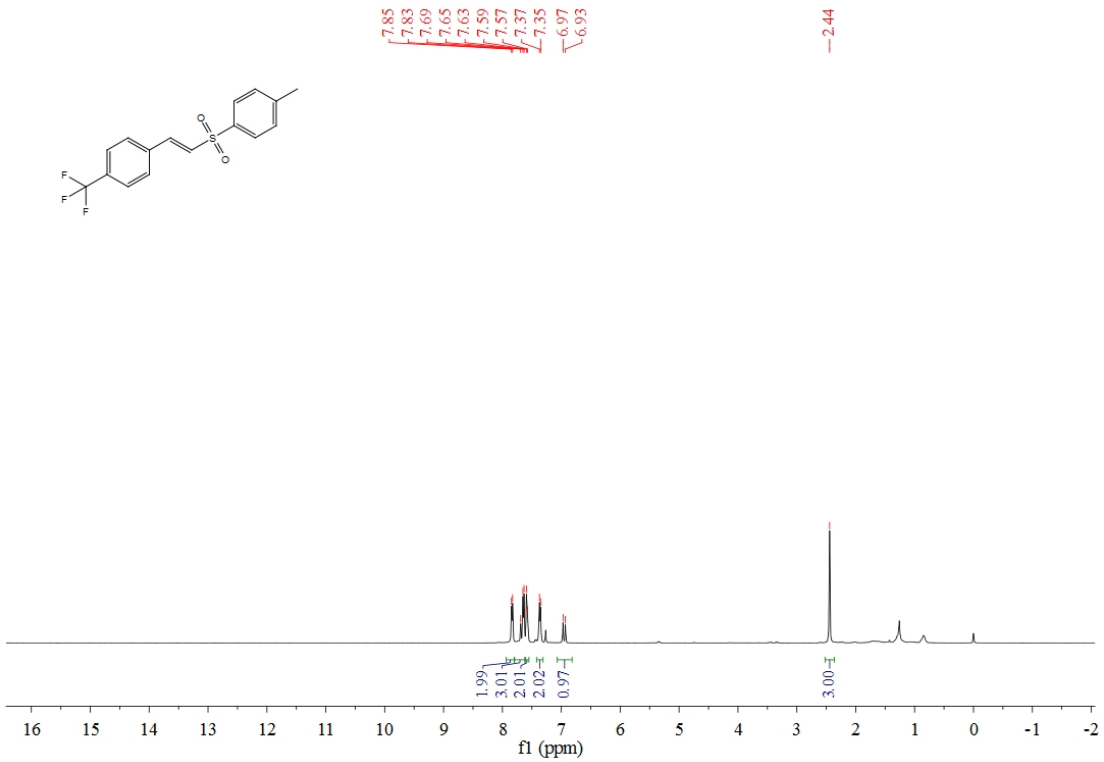

165.53
163.02
144.49
140.61
137.71
130.02
127.51
116.38
116.16
21.59
f1 (ppm)

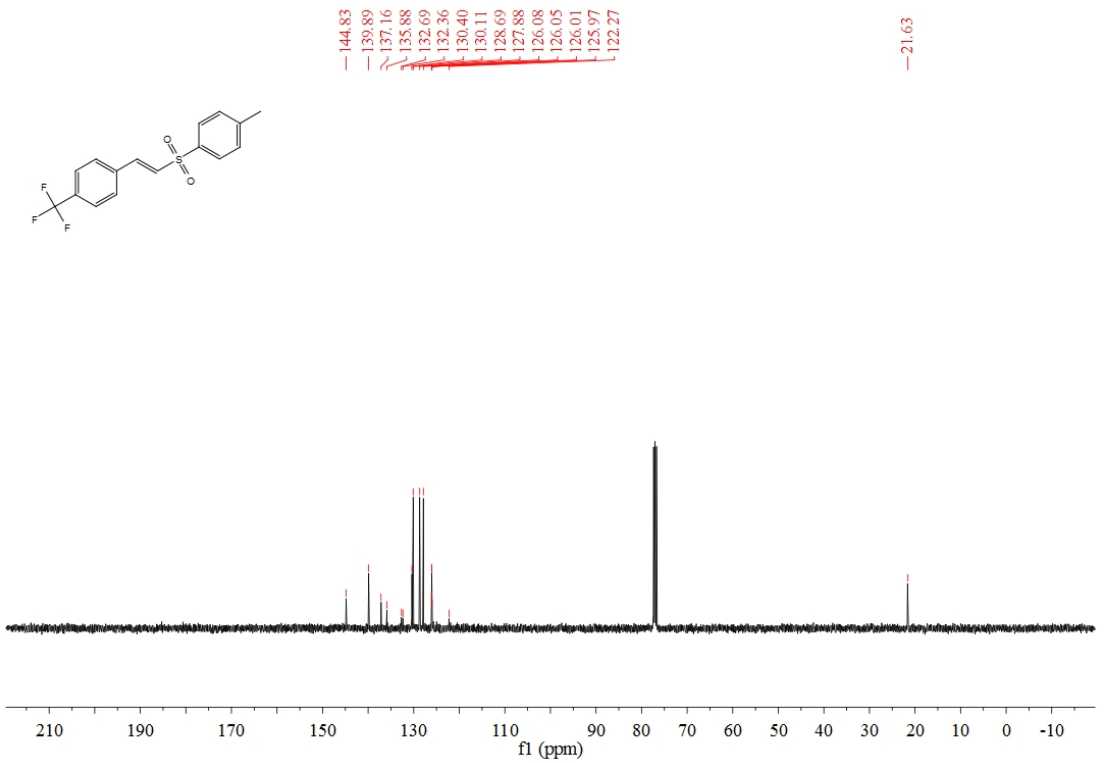

7.83
7.81
7.62
7.58
7.41
7.39
7.35
7.33
6.87
6.83
2.43
Cl
O
S
O
2.01
1.02
6.00
1.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

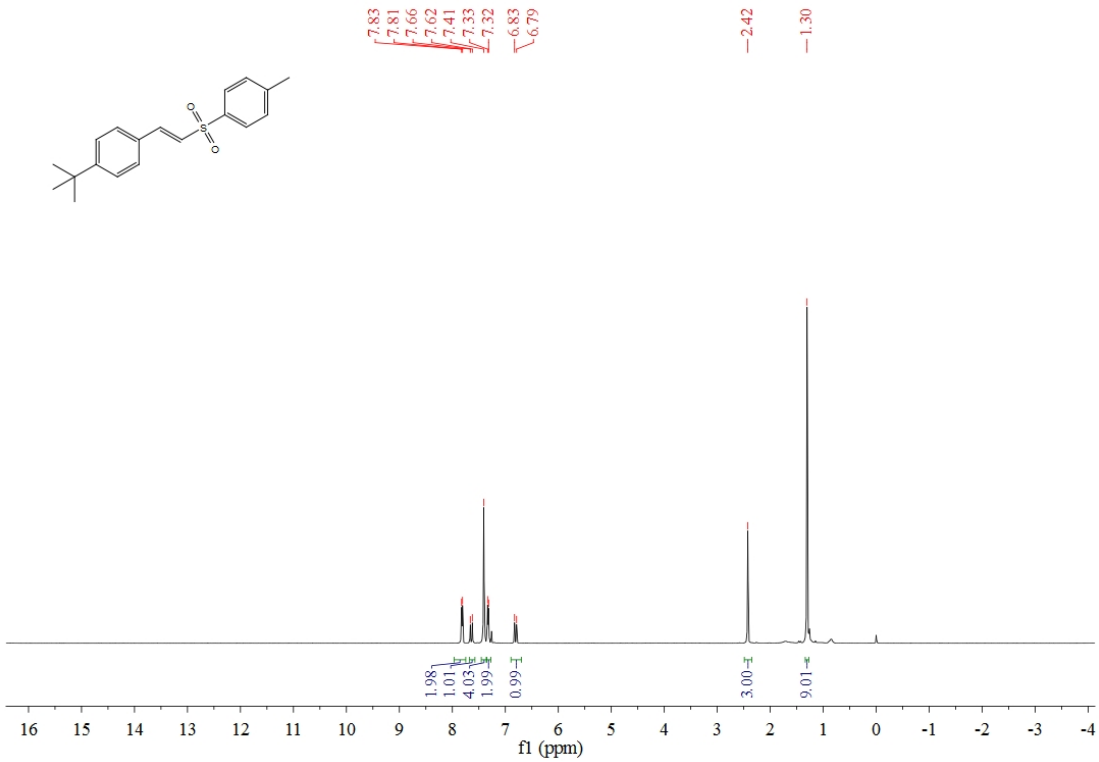

144.59
137.10
130.98
130.05
129.72
129.36
128.31
127.76
21.63
Cl
O
S
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

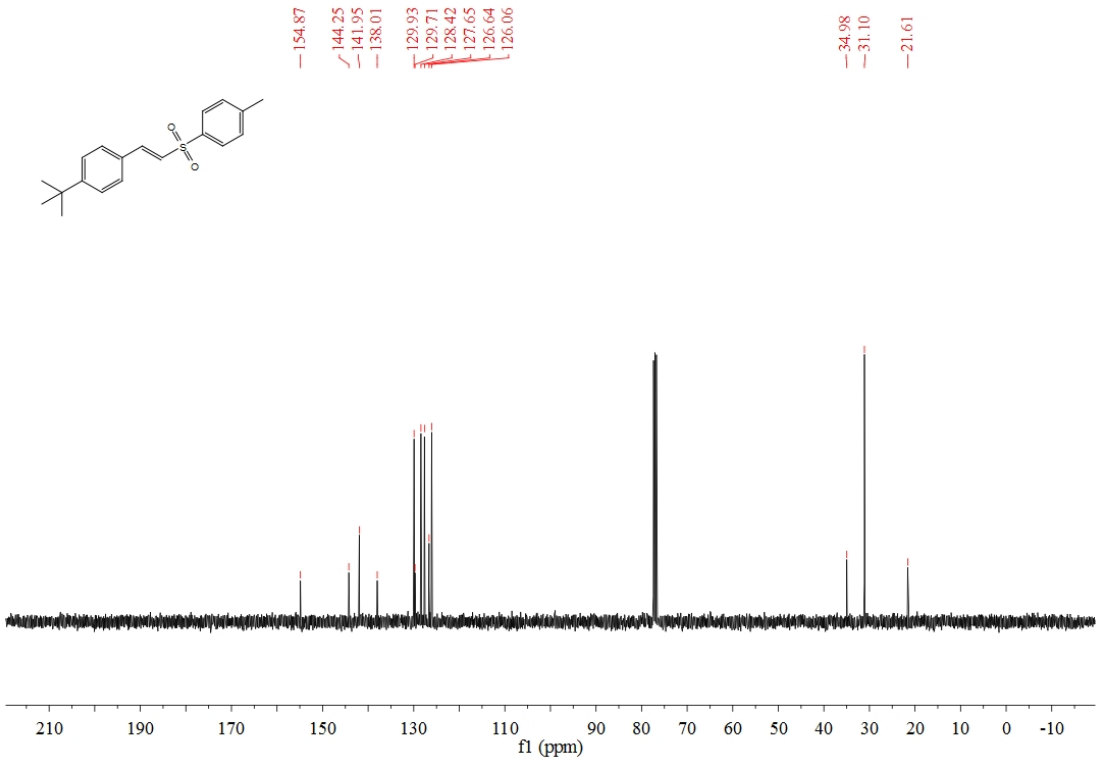

7.83
7.81
7.60
7.56
7.53
7.51
7.36
7.32
6.87
6.83
2.44
Br
2.00
1.02
2.00
4.01
1.00
3.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

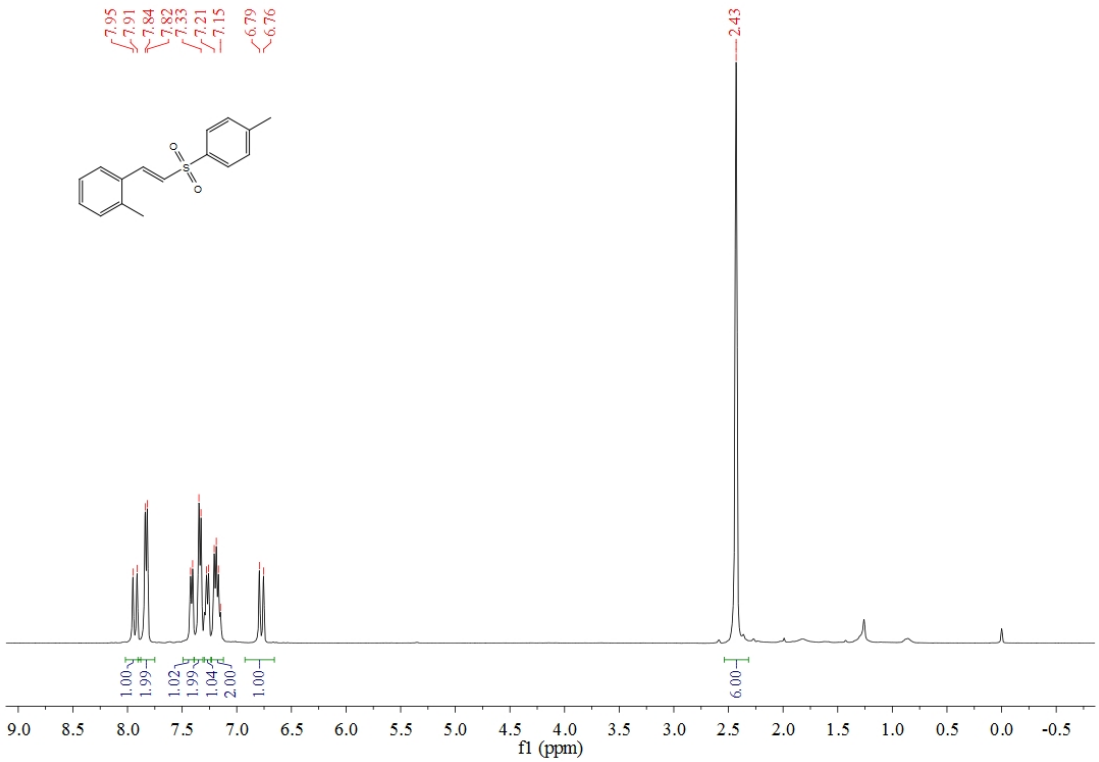

144.60
140.50
137.49
132.36
131.41
130.05
129.87
128.40
127.78
125.52
21.64
Br
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

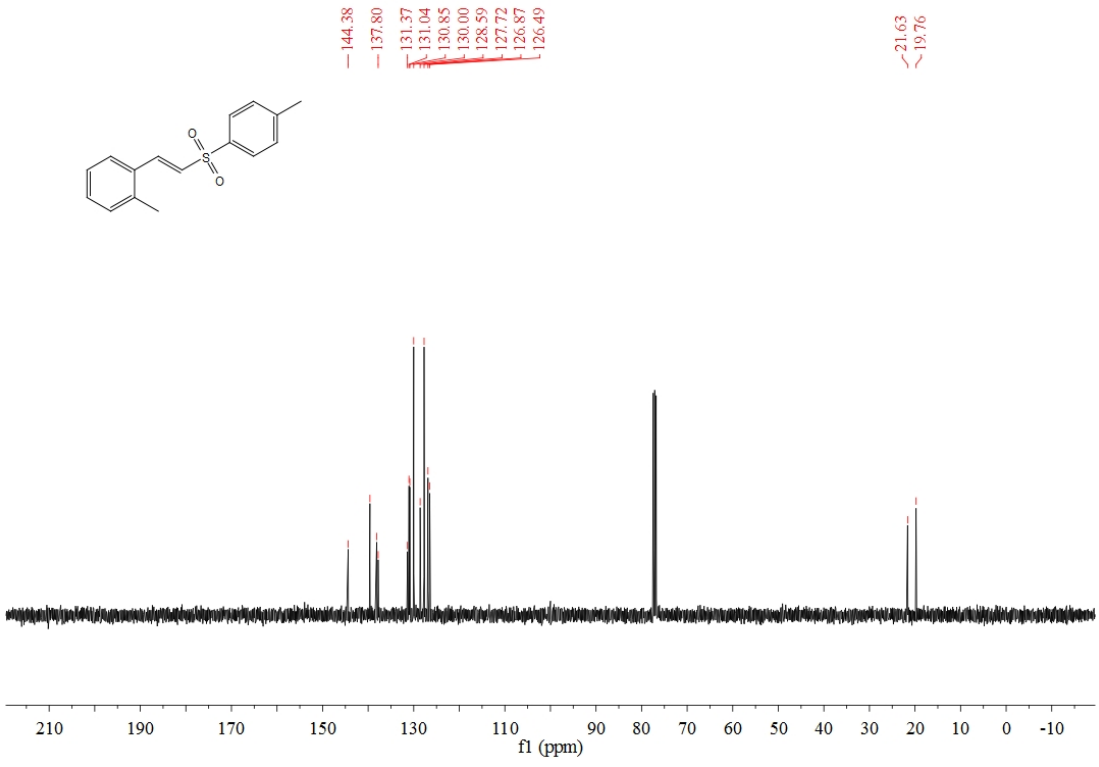

7.85
7.83
7.69
7.65
7.63
7.59
7.57
7.37
7.35
6.97
6.93
2.44
1.99
3.01
2.01
2.02
0.97
3.00
f1 (ppm)

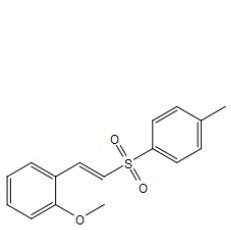

144.83
139.89
137.16
135.88
132.69
132.36
130.40
130.11
128.69
127.88
126.08
126.05
126.01
125.97
122.27
21.63
f1 (ppm)


7.83
7.81
7.66
7.62
7.41
7.33
7.32
6.83
6.79
2.42
1.30
1.98
1.01
4.03
1.99
0.99
3.00
9.01
f1 (ppm)

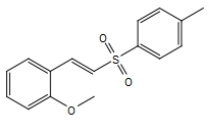

154.87
144.25
141.95
138.01
129.93
129.71
128.42
127.65
126.64
126.06
34.98
31.10
21.61
f1 (ppm)


7.95
7.91
7.84
7.82
7.33
7.21
7.15
6.79
6.76
2.43
1.00
1.99
1.02
1.99
1.04
2.00
1.00
6.00
9.0 8.5 8.0 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 -0.5
f1 (ppm)

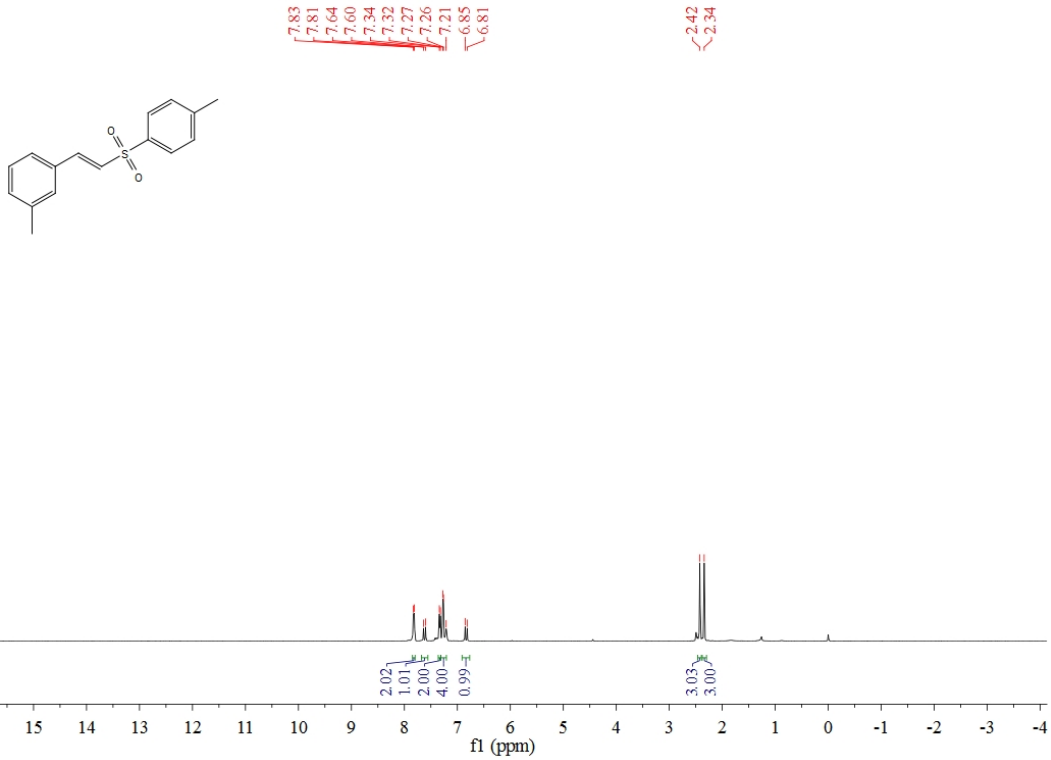

144.38
137.80
131.37
131.04
130.85
130.00
128.59
127.72
126.87
126.49
21.63
19.76
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

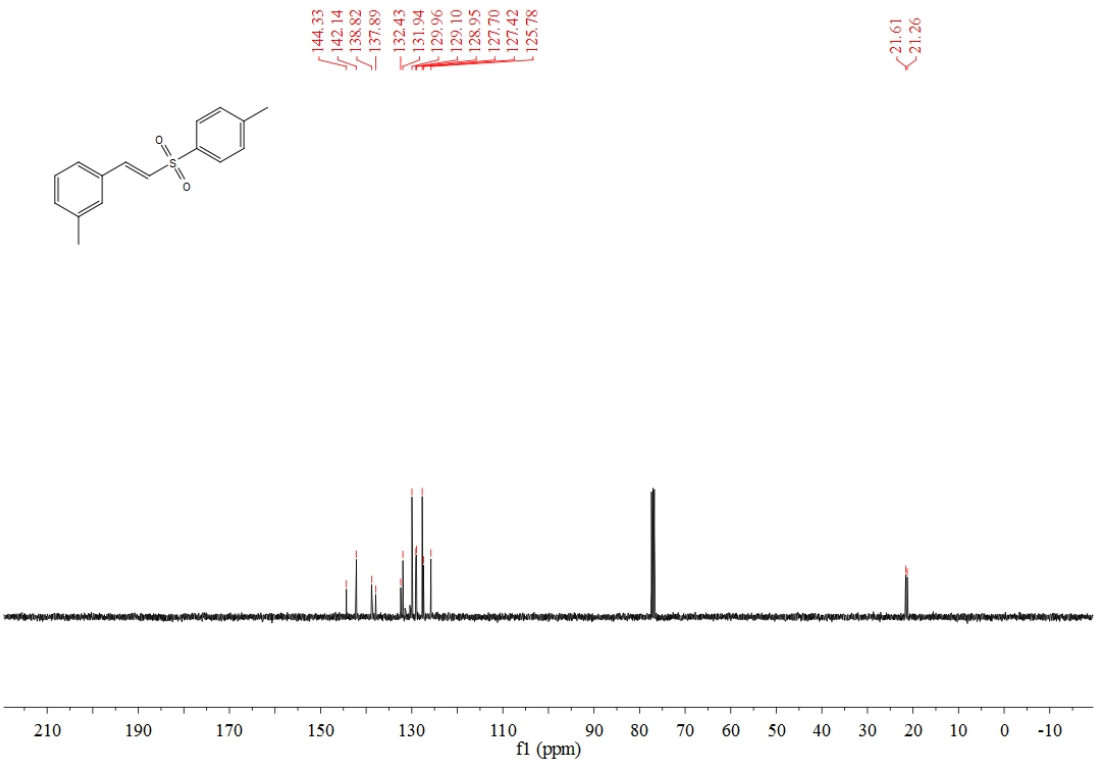


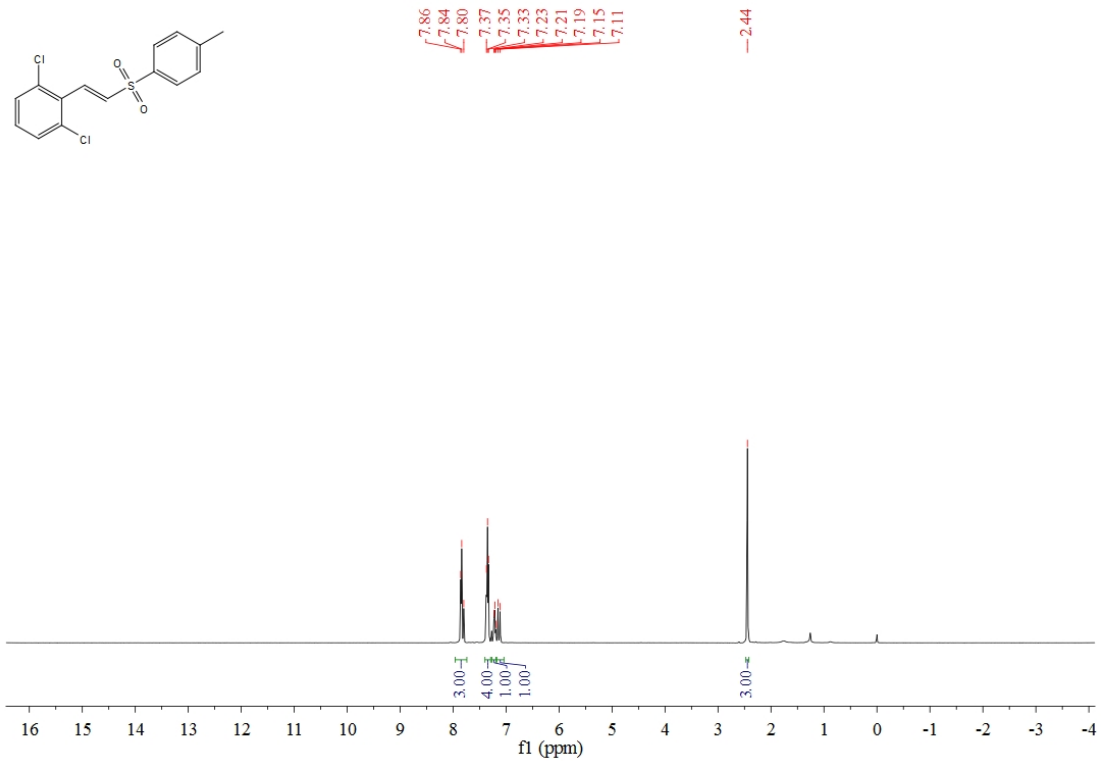
7.88
7.84
7.82
7.33
7.04
6.96
6.95
6.92
6.90
3.87
2.42
2.99
4.00
1.00
1.99
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

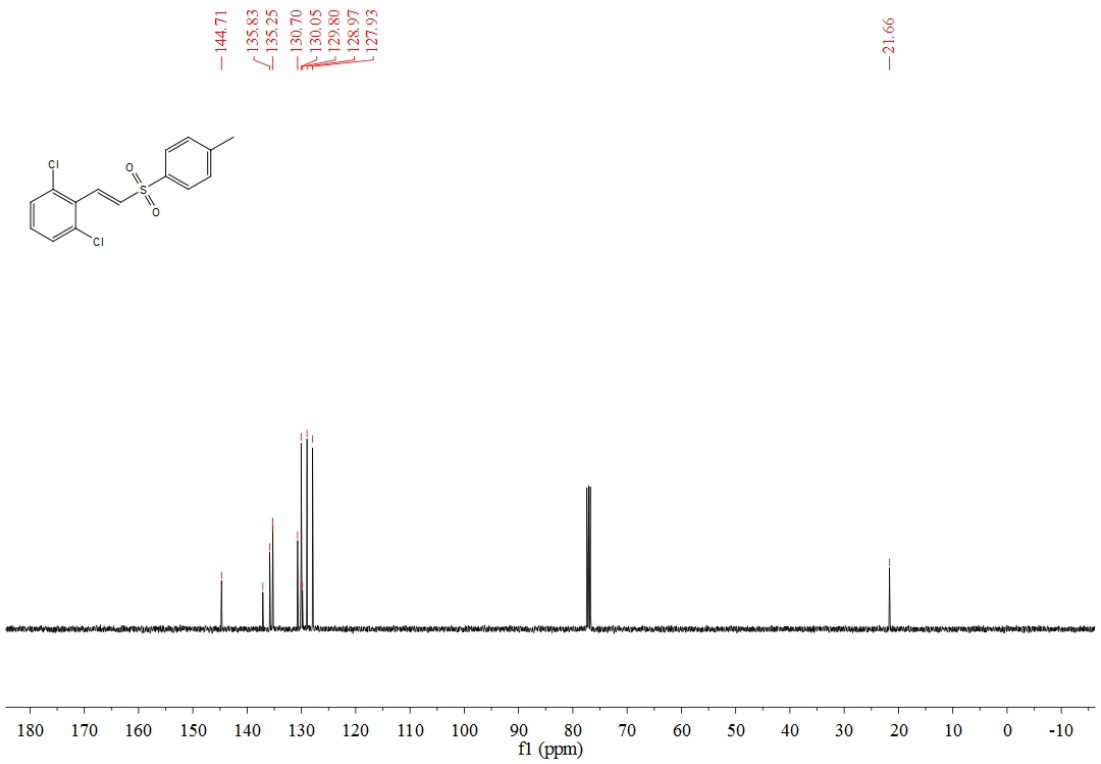


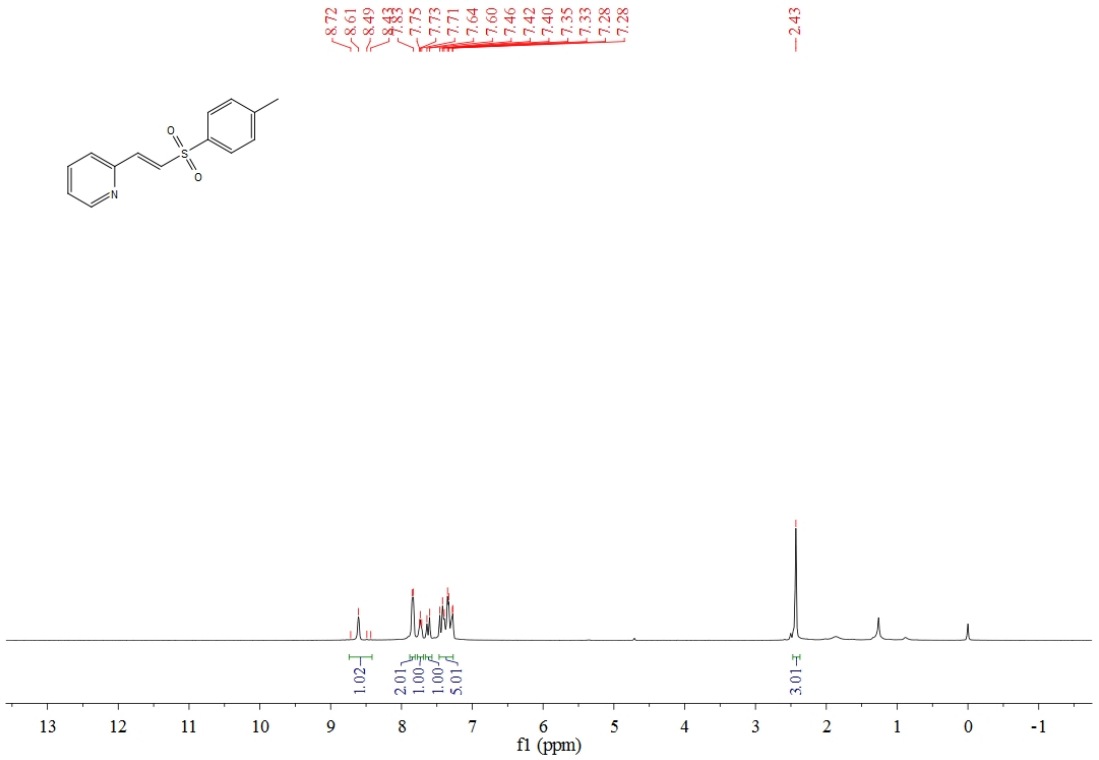
158.82
144.04
138.02
129.87
127.65
121.32
120.78
111.26
55.50
21.59
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

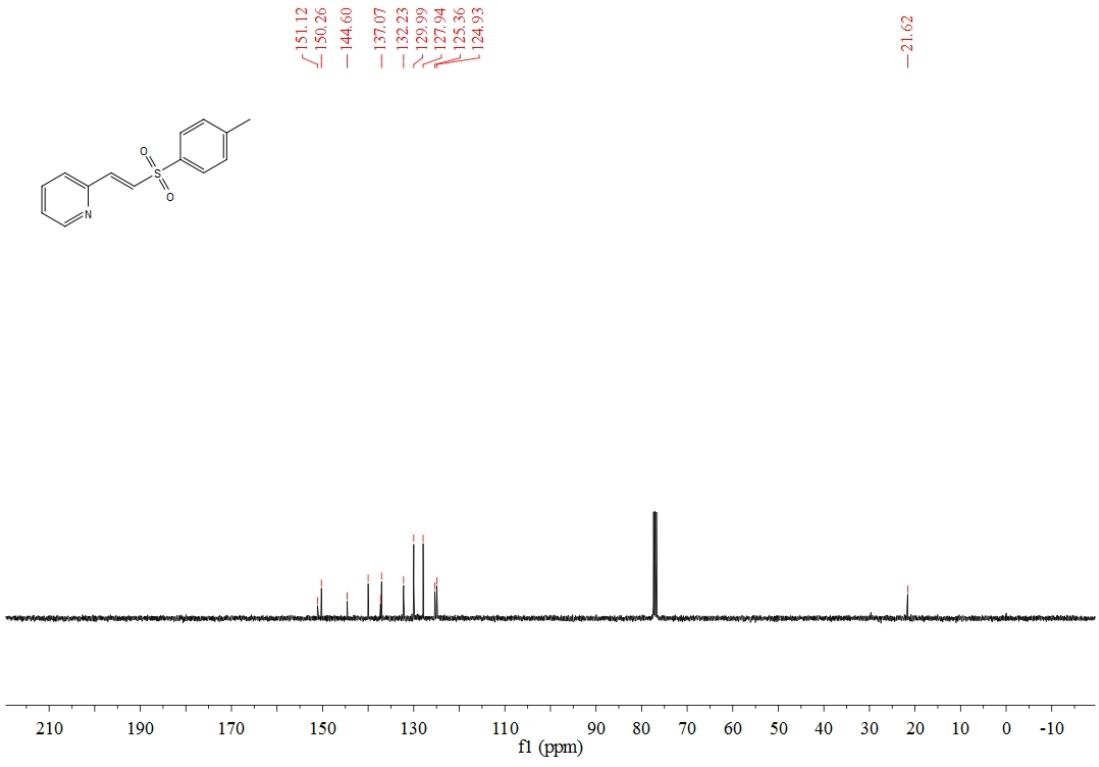

7.83
7.81
7.64
7.60
7.34
7.32
7.27
7.26
7.21
6.85
6.81
2.42
2.34
O
S
O
2.02
1.01
2.00
4.00
0.99
3.03
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

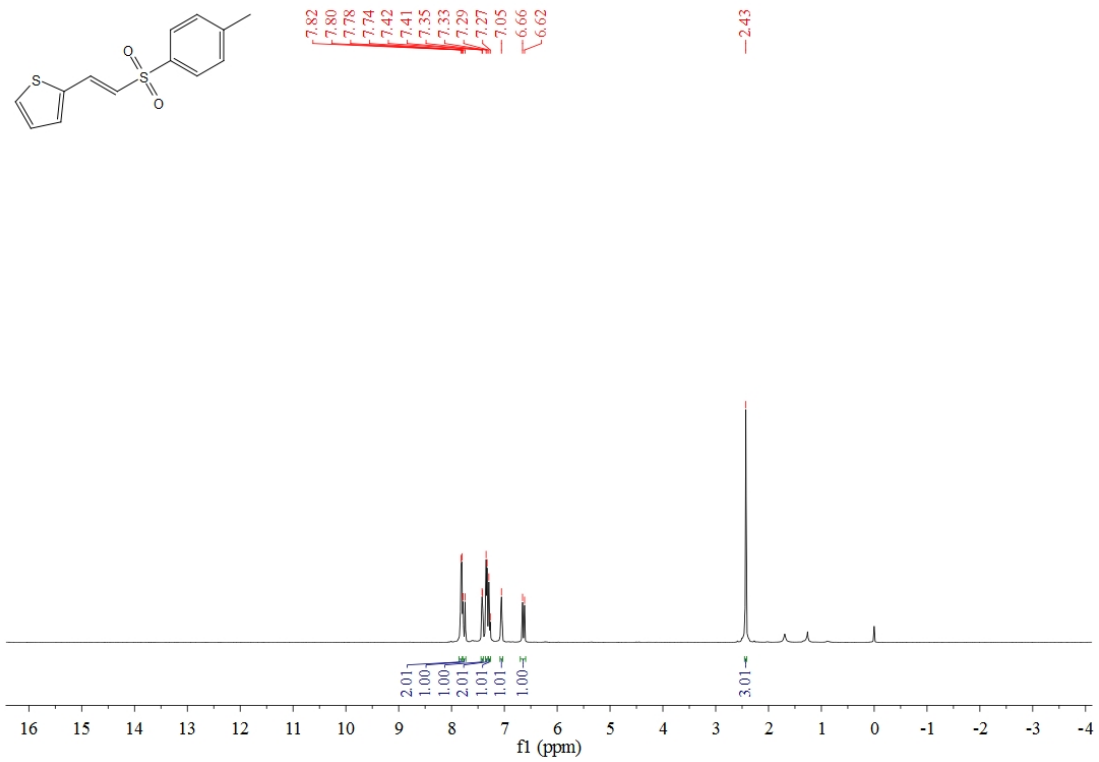

144.33
142.14
138.82
137.89
132.43
131.94
129.96
129.10
128.95
127.70
127.42
125.78
21.61
21.26
O
S
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

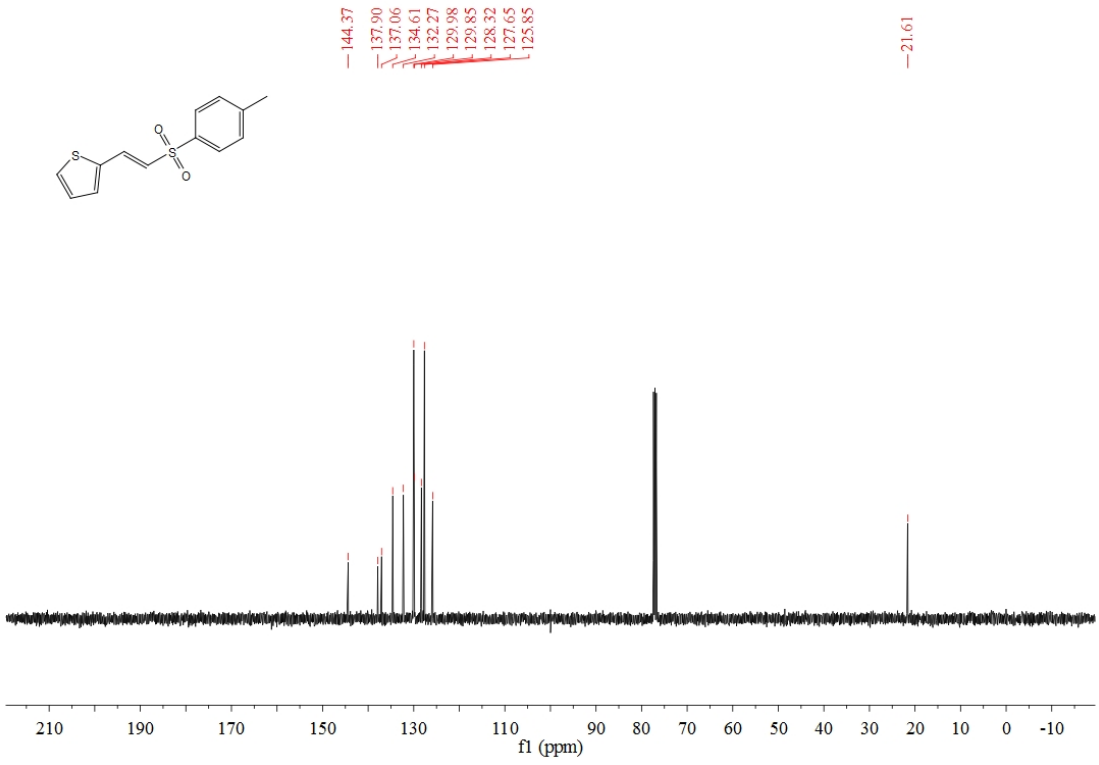

7.86
7.84
7.80
7.37
7.35
7.33
7.23
7.21
7.19
7.15
7.11
2.44
Cl
Cl
O
S
O
3.00
4.00
1.00
1.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

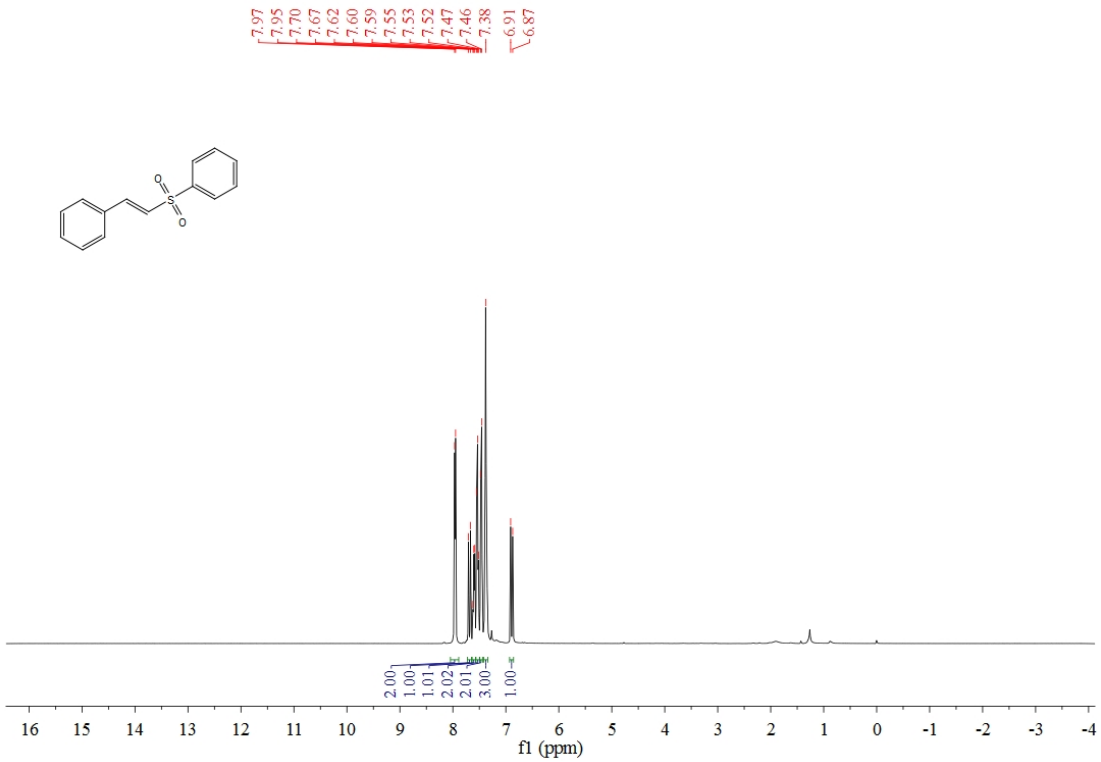

144.71
135.83
135.25
130.70
130.05
129.80
128.97
127.93
21.66
Cl
Cl
O
S
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

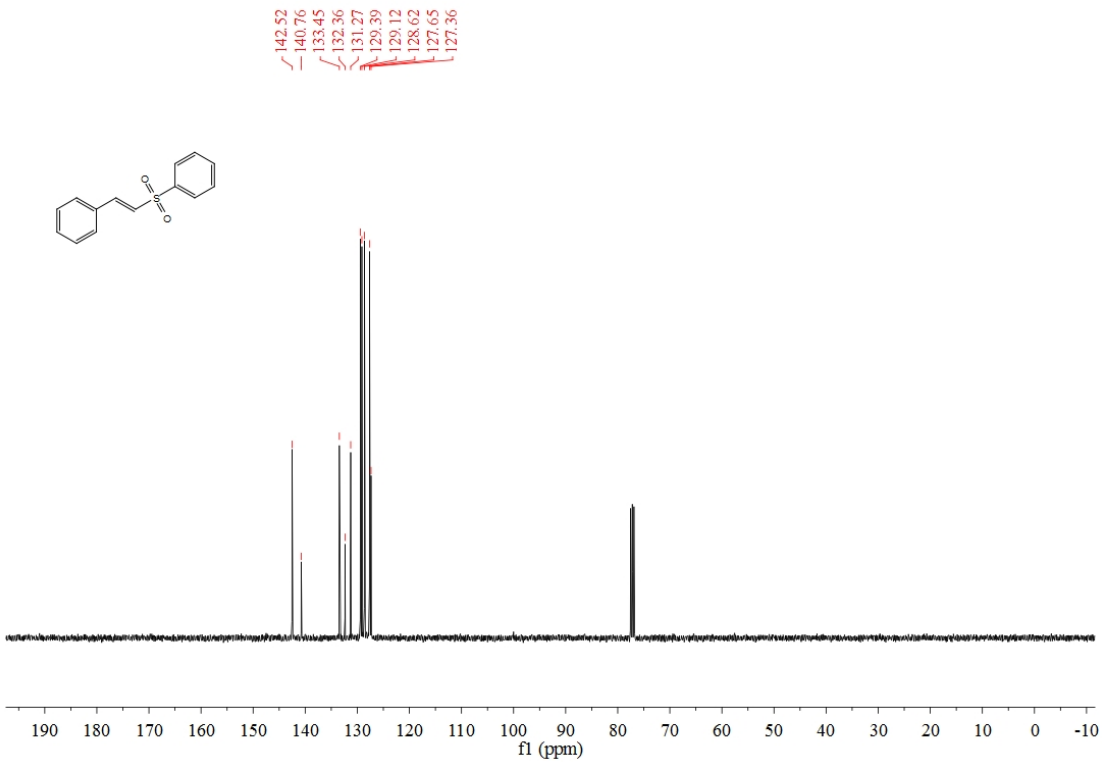

8.72
8.61
8.49
7.75
7.73
7.71
7.64
7.60
7.46
7.42
7.40
7.35
7.33
7.28
7.28
2.43
1.02
2.01
1.00
1.00
5.01
3.01
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

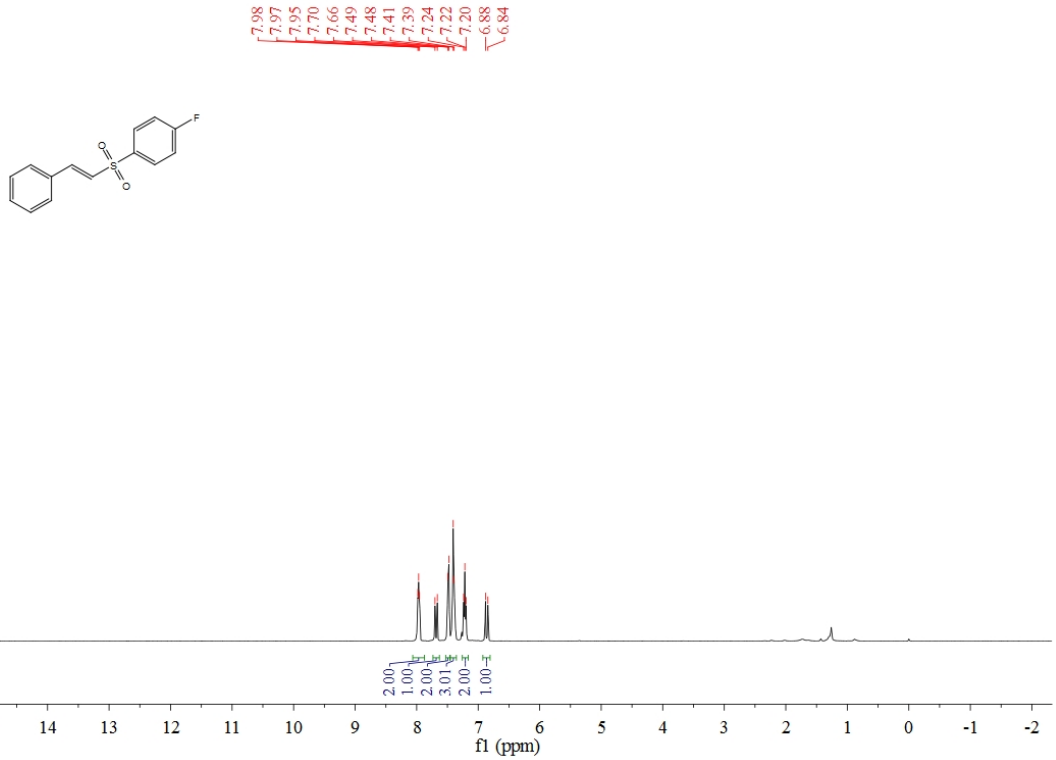

151.12
150.26
144.60
137.07
132.23
129.99
127.94
125.36
124.93
21.62
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

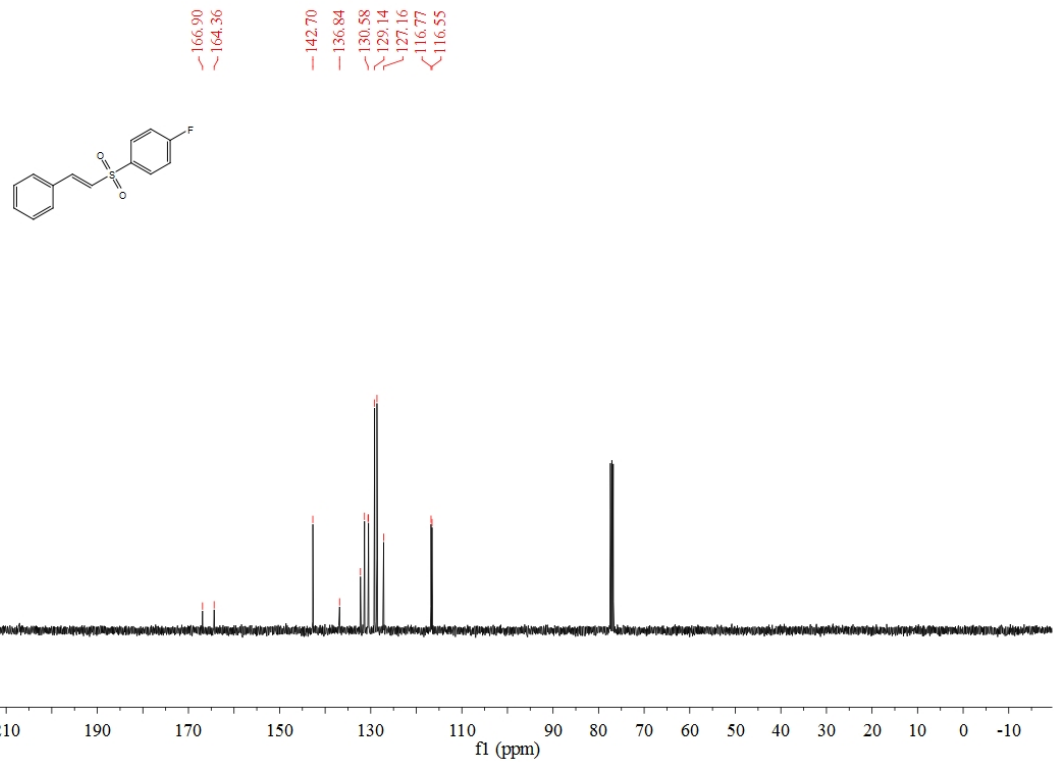

7.82
7.80
7.78
7.74
7.42
7.41
7.35
7.33
7.29
7.27
7.05
6.66
6.62
2.43
2.01
1.00
1.00
2.01
1.01
1.01
1.00
3.01
f1 (ppm)

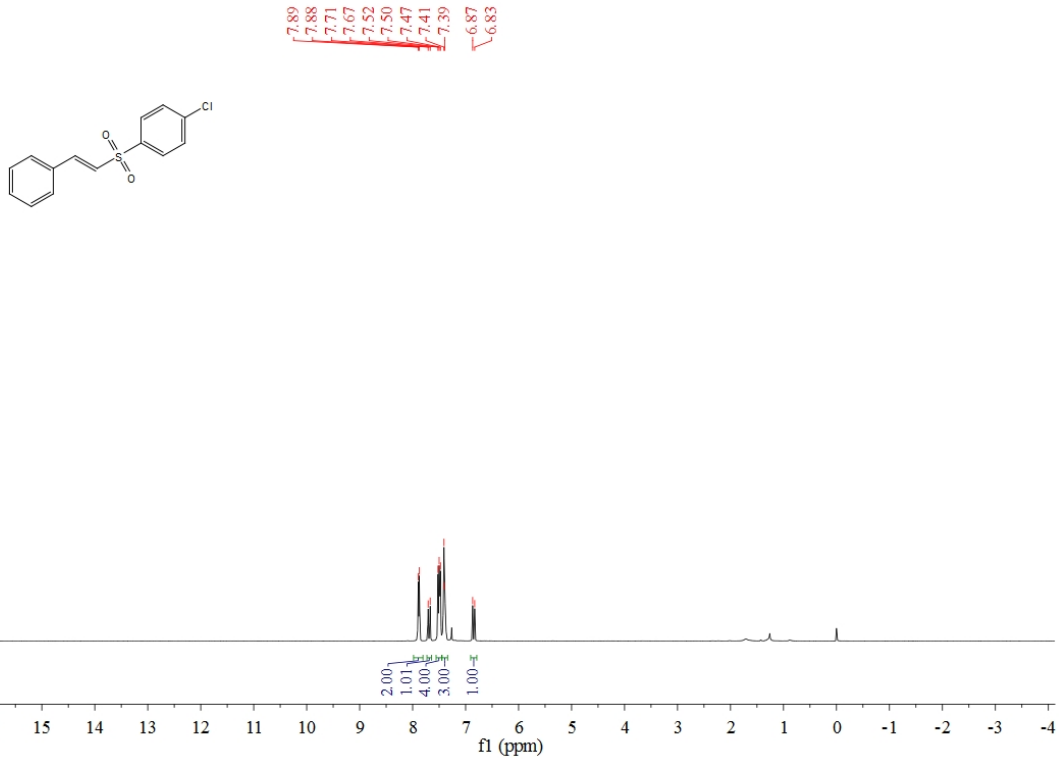

144.37
137.90
137.06
134.61
132.27
129.98
129.85
128.32
127.65
125.85
21.61
f1 (ppm)

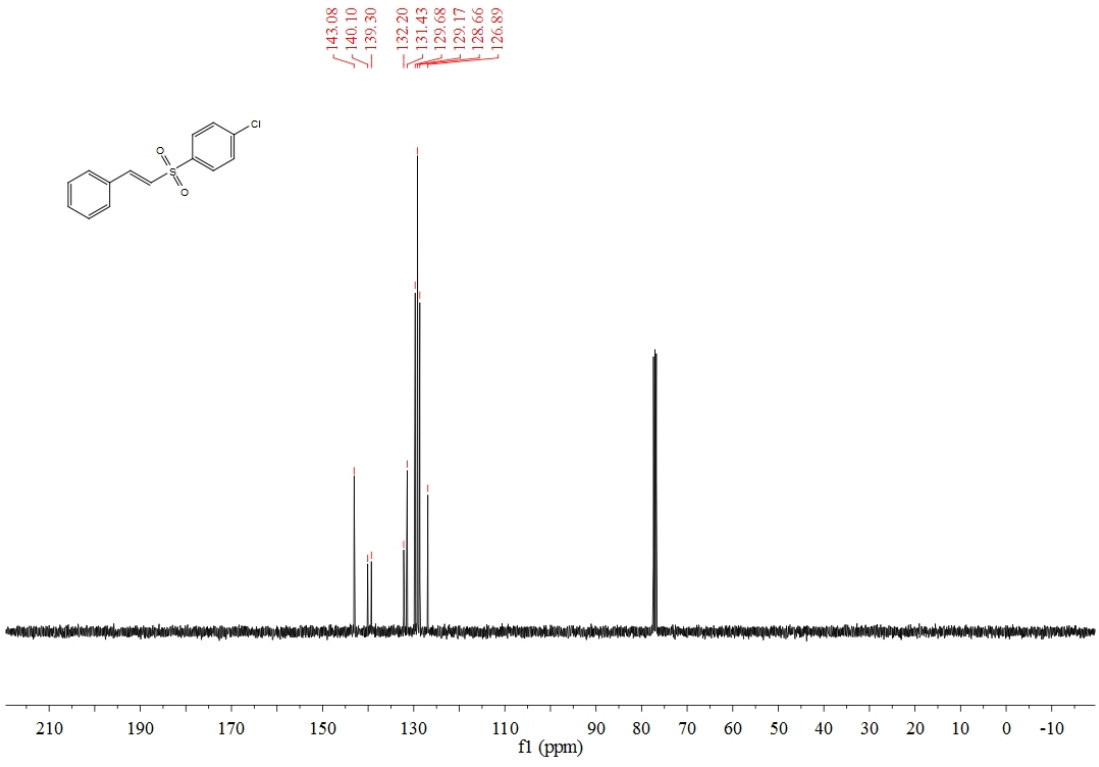

7.97
7.95
7.70
7.67
7.62
7.60
7.59
7.55
7.53
7.52
7.47
7.46
7.38
6.91
6.87
2.00
1.00
1.01
2.02
2.01
3.00
1.00
f1 (ppm)

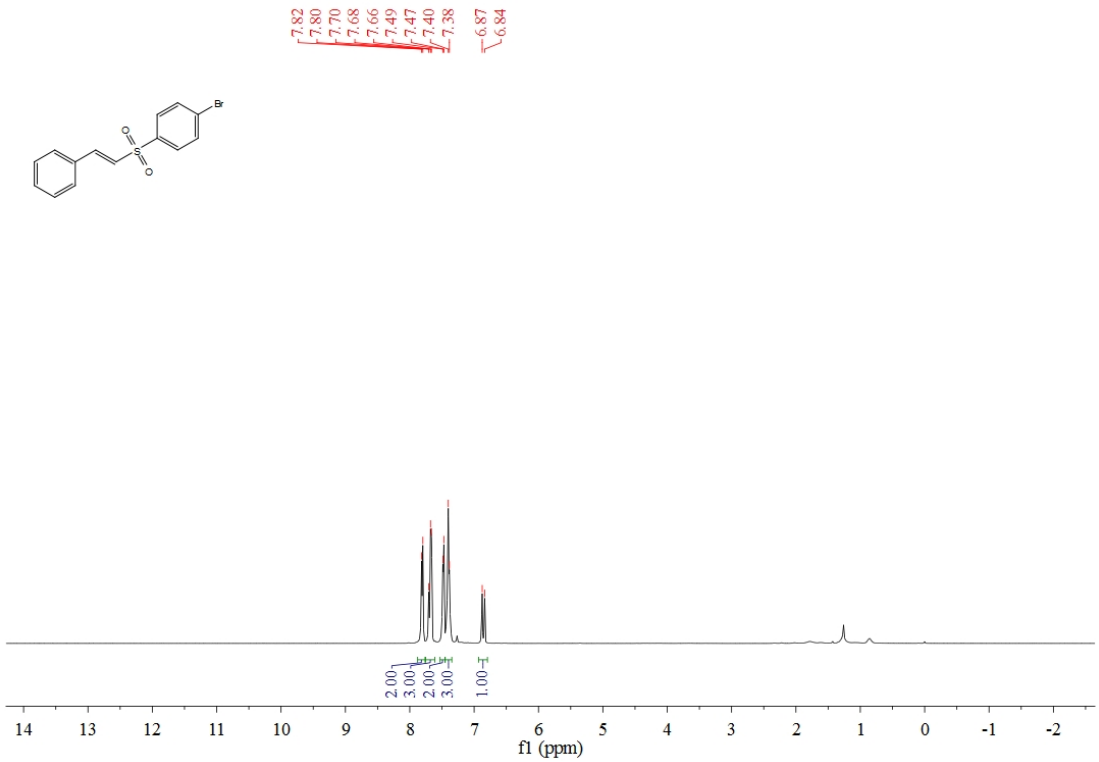

142.52
140.76
133.45
132.36
131.27
129.39
129.12
128.62
127.65
127.36
f1 (ppm)

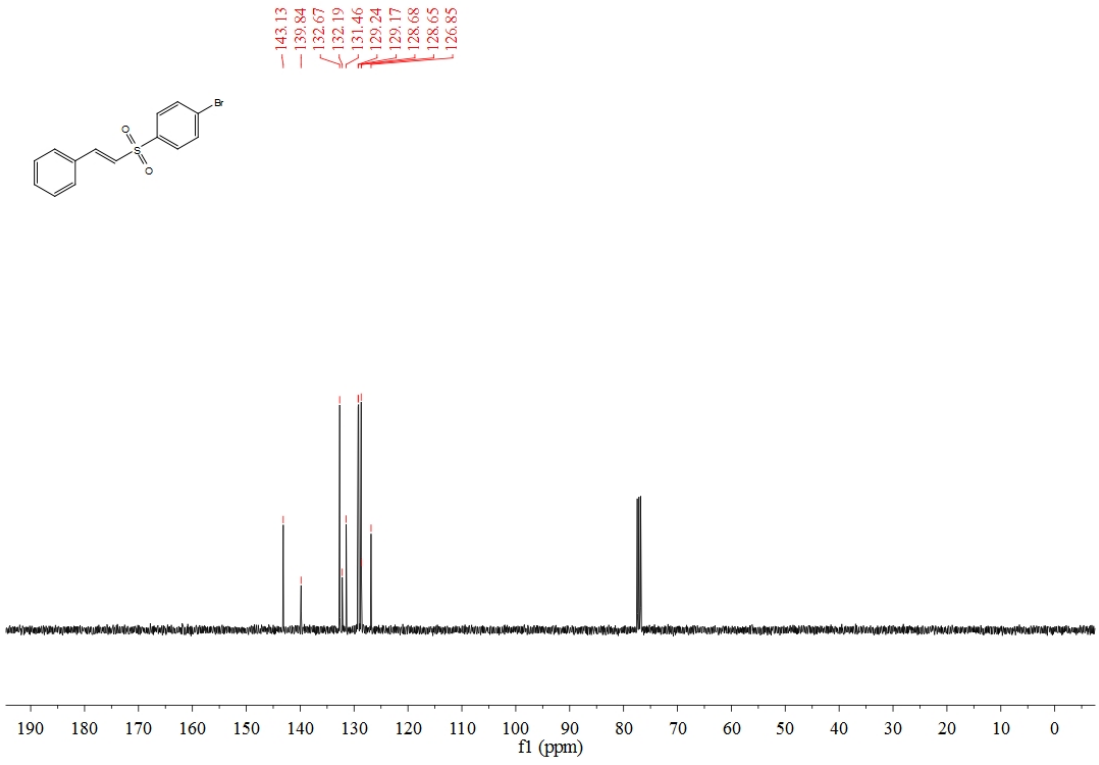

7.98
7.97
7.95
7.70
7.66
7.49
7.48
7.41
7.39
7.24
7.22
7.20
6.88
6.84
F
O
S
O
2.00
1.00
2.00
3.01
2.00
1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

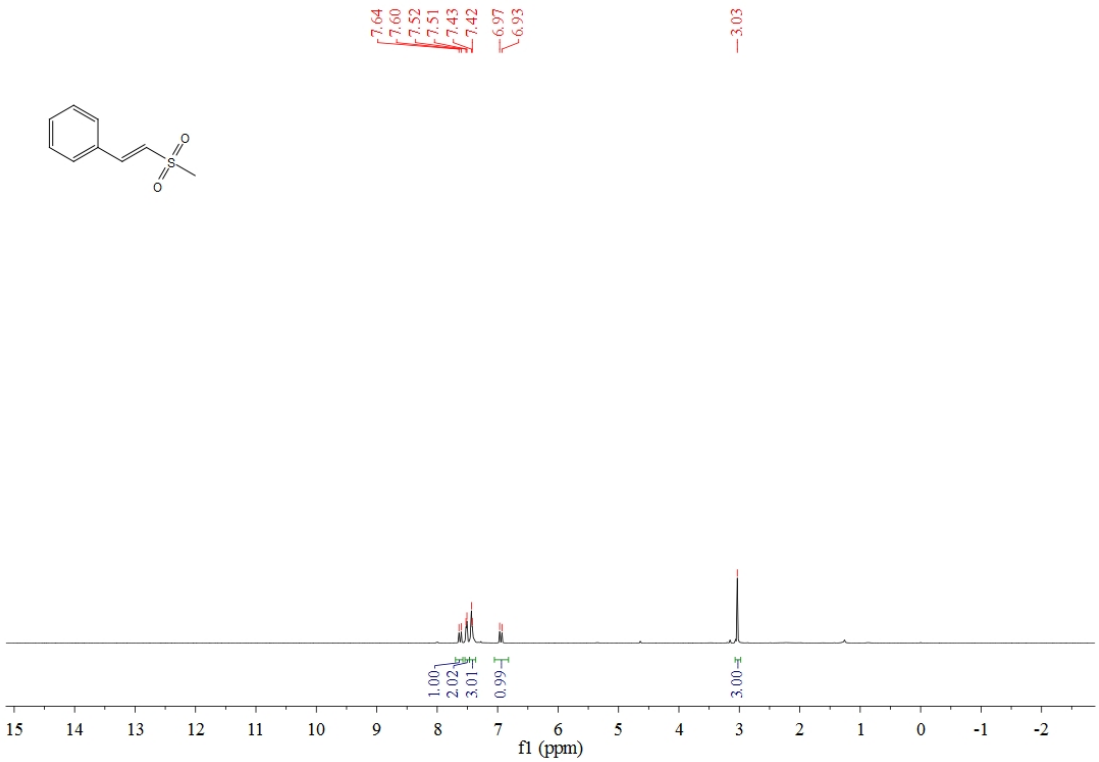

166.90
164.36
142.70
136.84
130.58
129.14
127.16
116.77
116.55
F
O
S
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

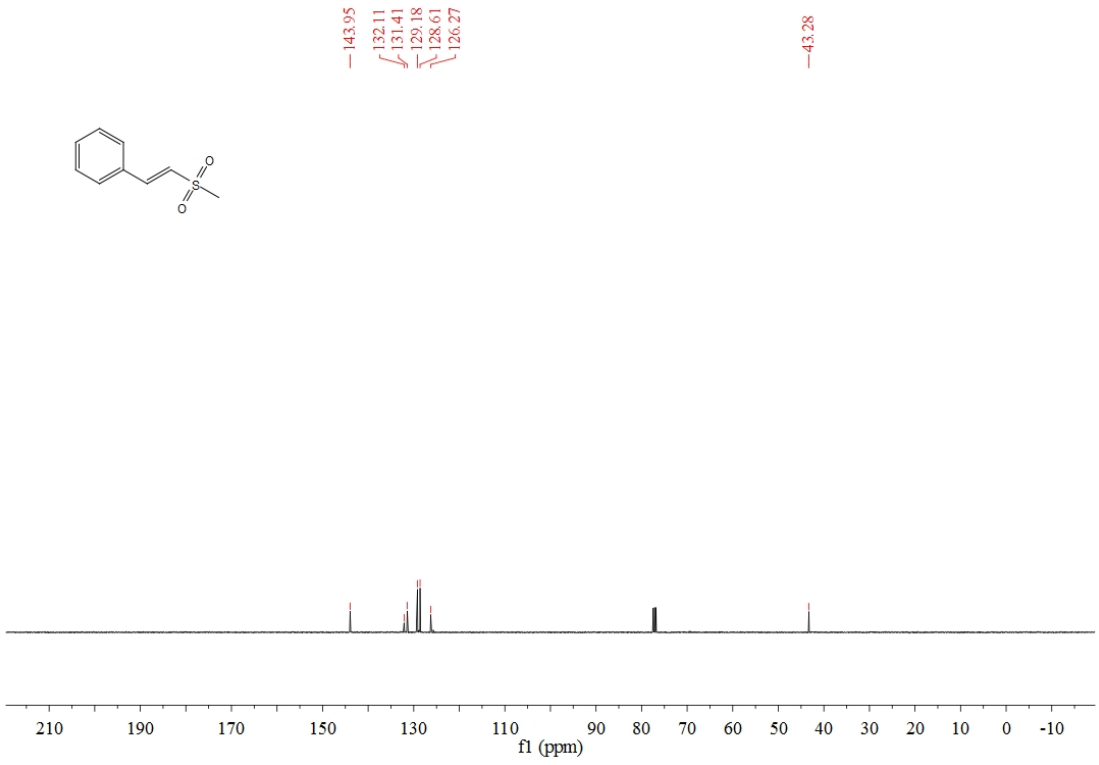

7.89
7.88
7.71
7.67
7.52
7.50
7.47
7.41
7.39
6.87
6.83
Cl
O
S
O
2.00
1.01
4.00
3.00
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


143.08
140.10
139.30
132.20
131.43
129.68
129.17
128.66
126.89
Cl
O
S
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.82
7.80
7.70
7.68
7.66
7.49
7.47
7.40
7.38
6.87
6.84
Br
O
S
O
2.00
3.00
2.00
3.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


143.13
139.84
132.67
132.19
131.46
129.24
129.17
128.68
128.65
126.85
Br
O
S
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.64
7.60
7.52
7.51
7.43
7.42
6.97
6.93
3.03
1.00
2.02
3.01
0.99
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


143.95
132.11
131.41
129.18
128.61
126.27
43.28
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)