

Supplementary Information

PhI(OAc)₂ mediated decarboxylative sulfonylation of β -aryl- α,β -unsaturated carboxylic acids:

A synthesis of (*E*)-vinyl sulfones

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Kanchanaburi Campus, Saiyok, Kanchanaburi 71150, Thailand.*

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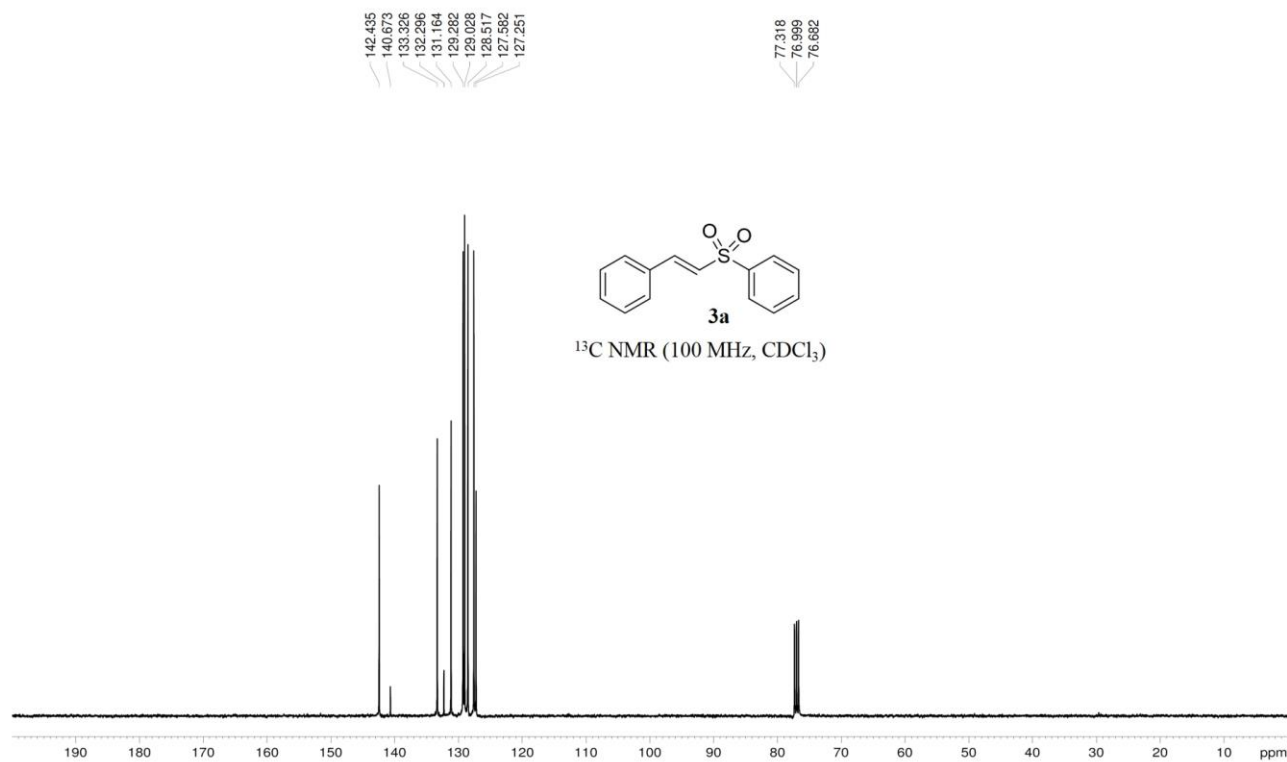
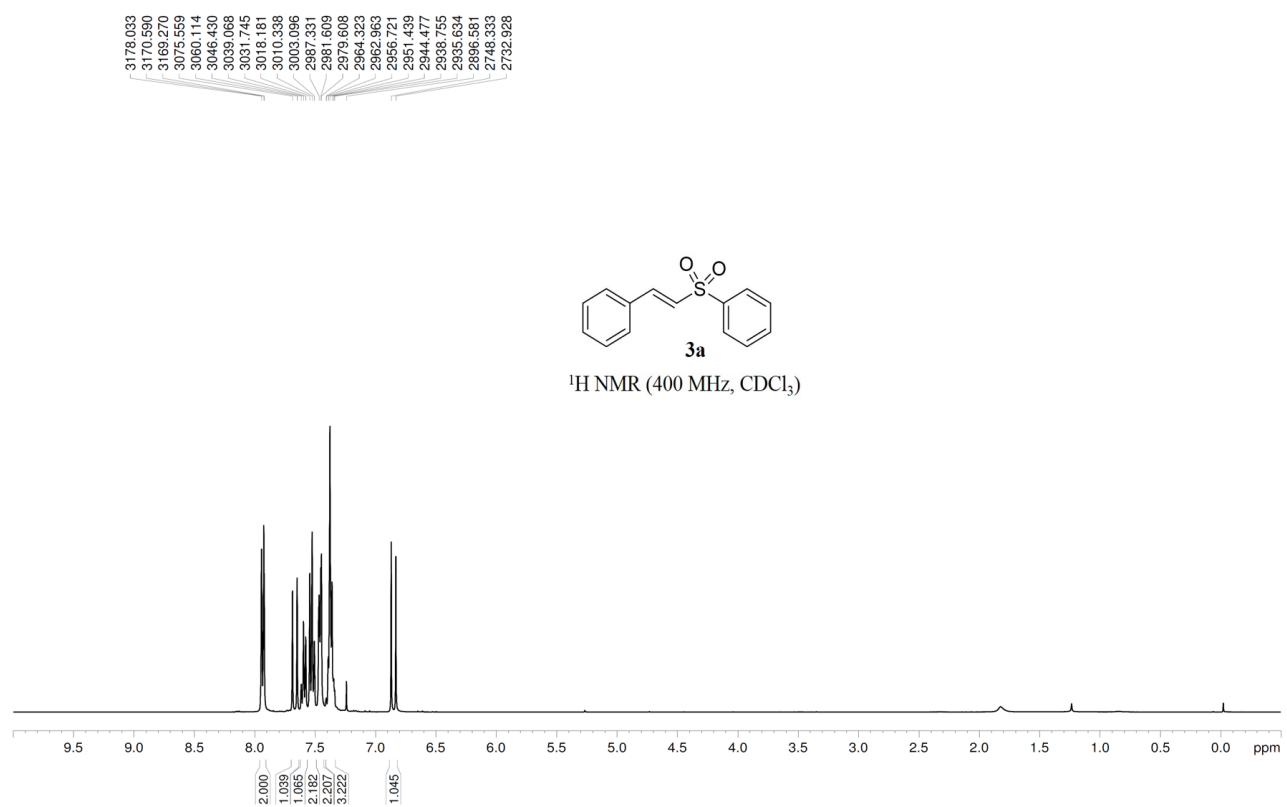
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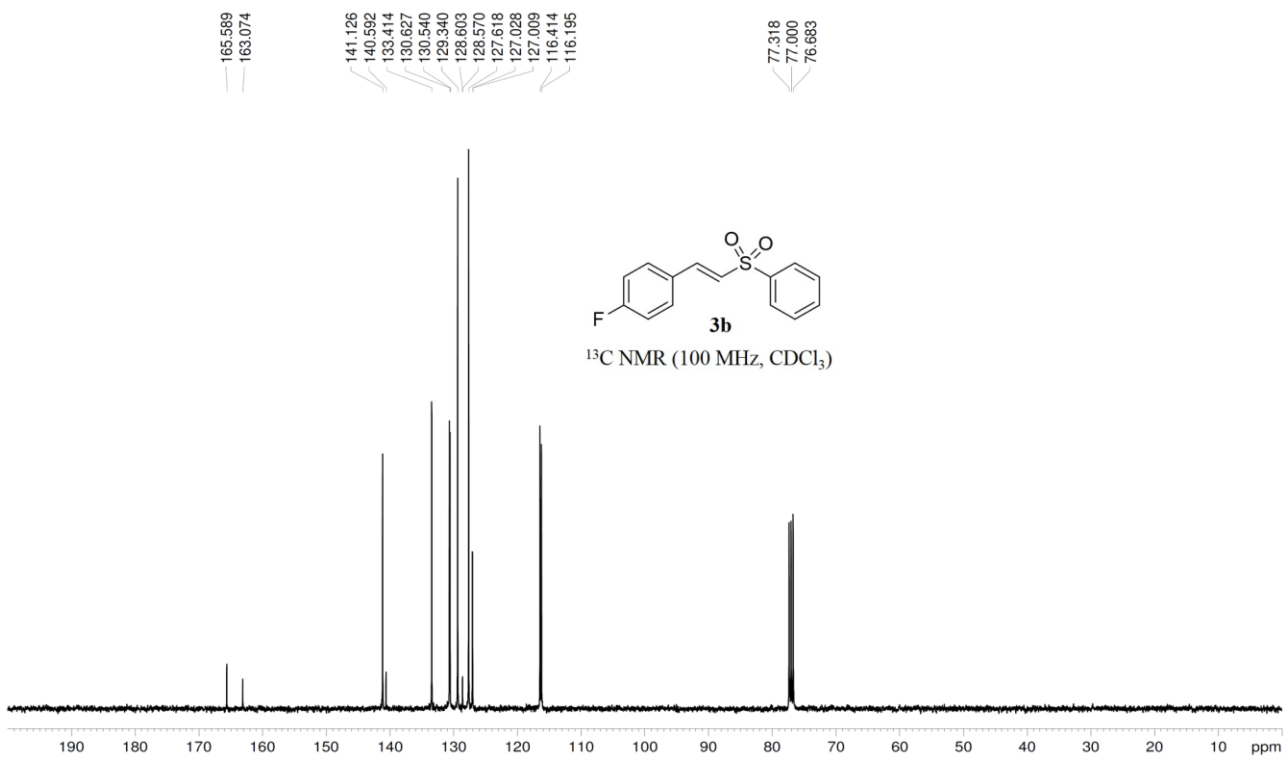
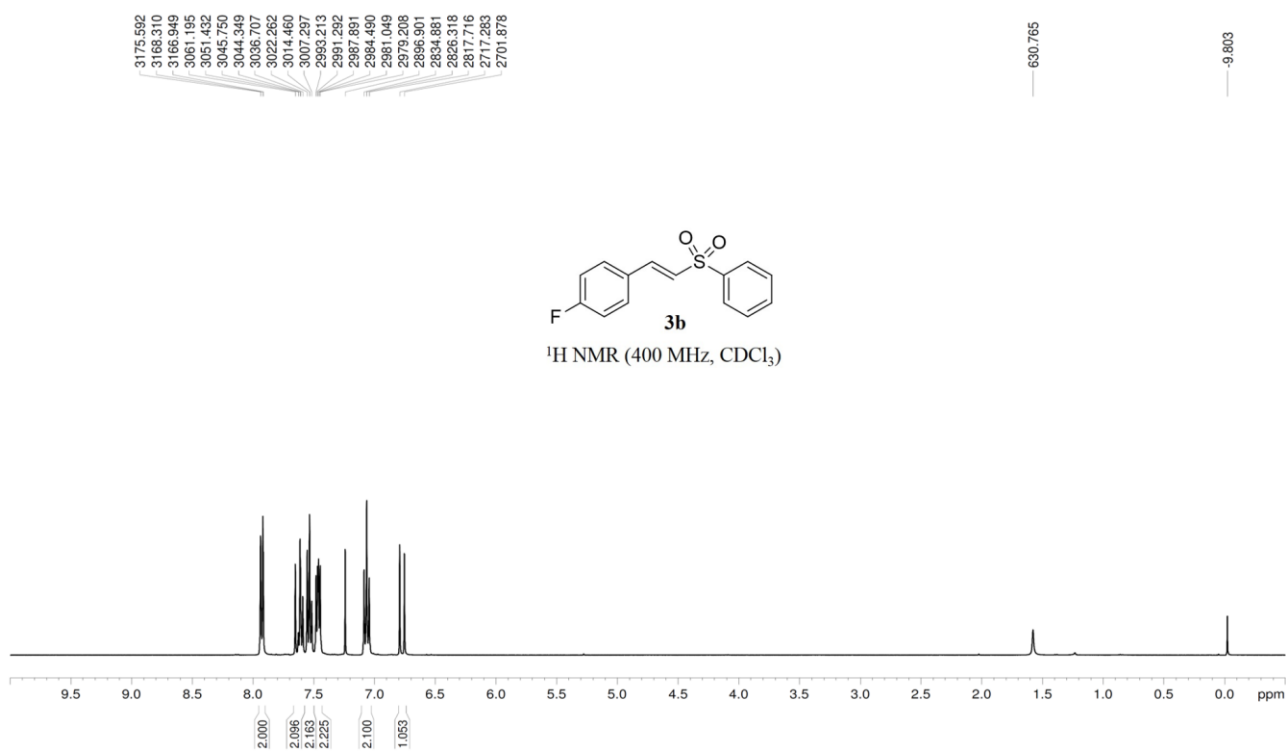
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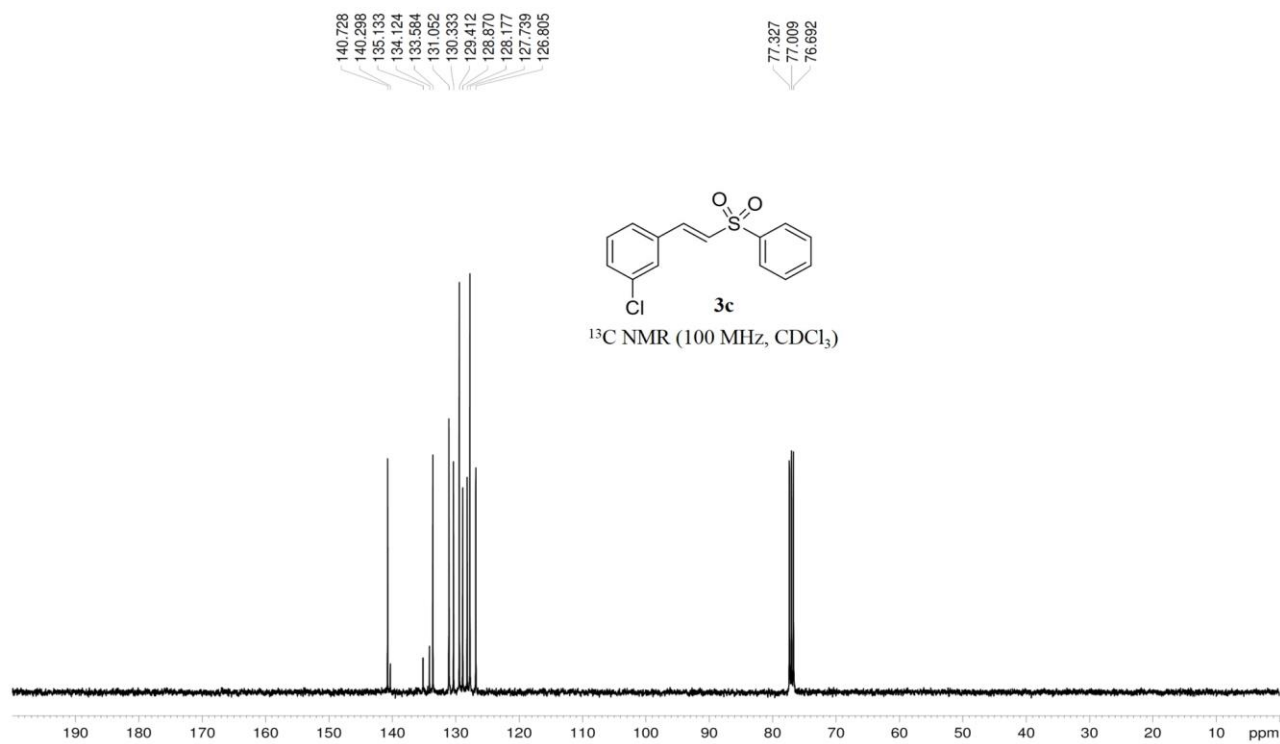
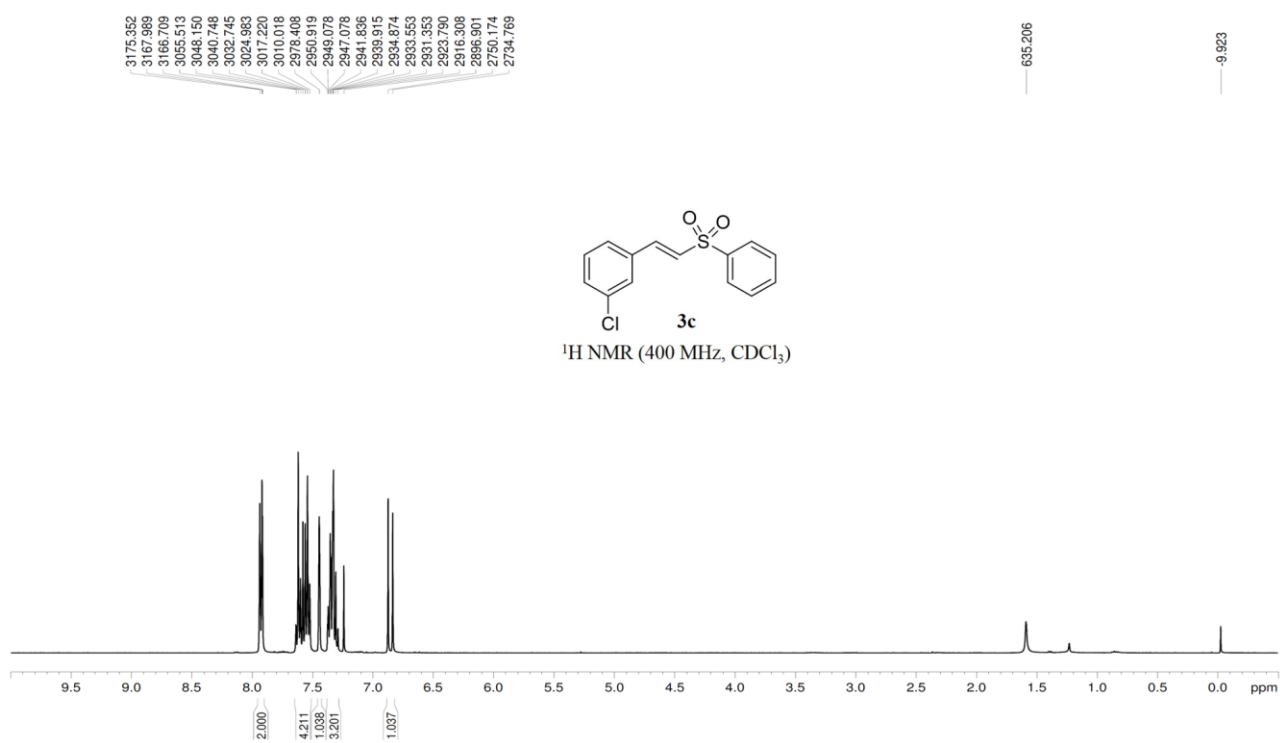
General information

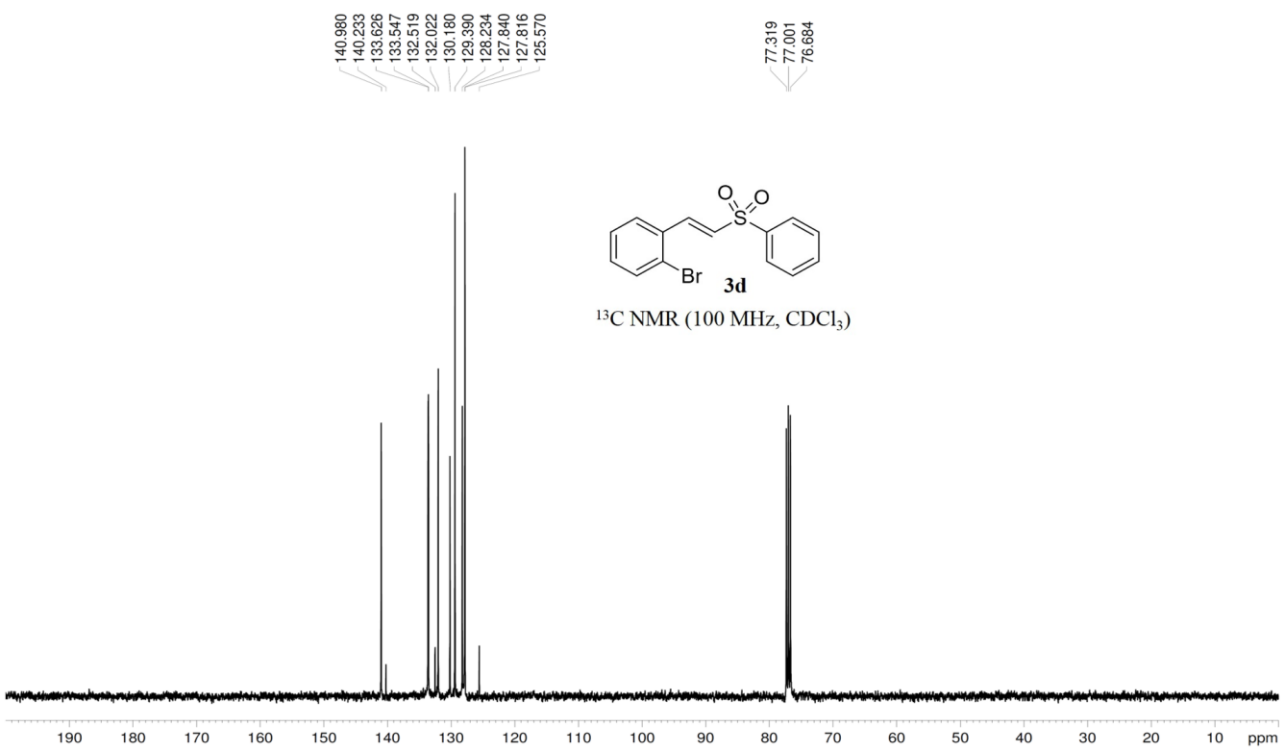
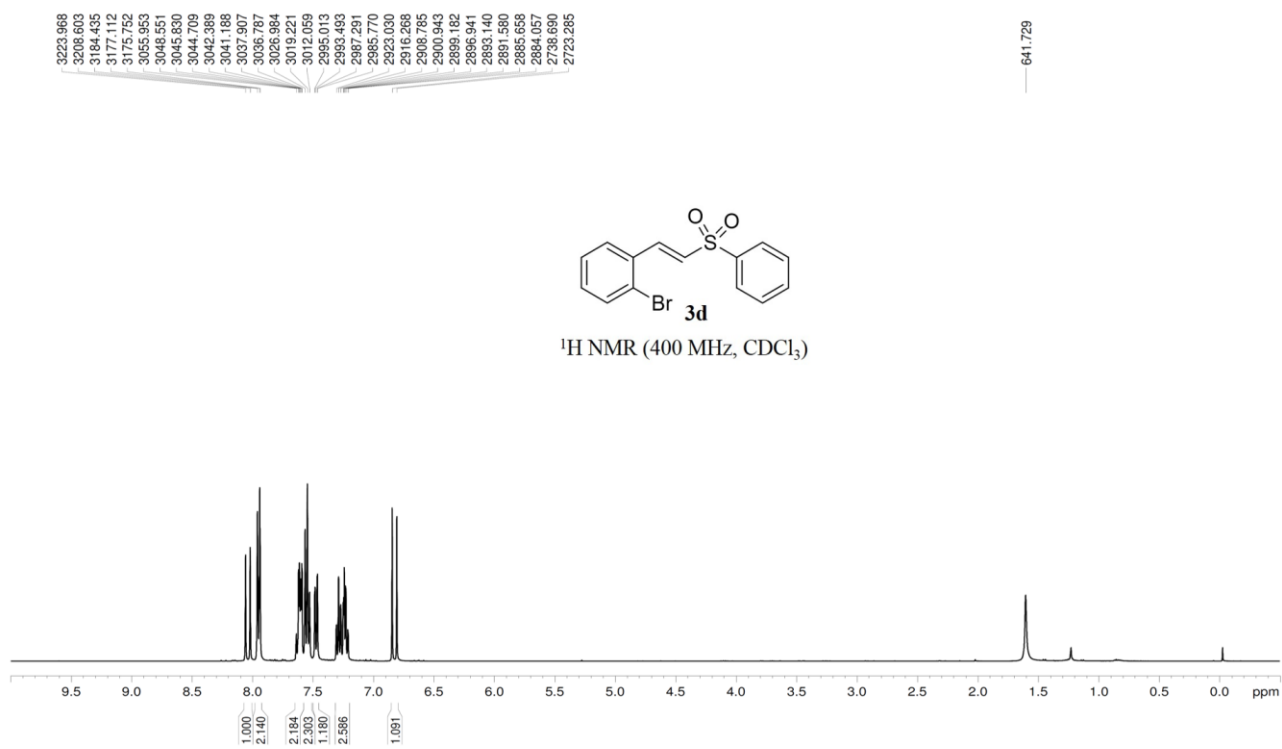
All isolated compounds were characterized on the basis of ^1H NMR and ^{13}C NMR spectroscopic data, IR spectra, and HRMS data. ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker AscendTM spectrometer. ^1H NMR and ^{13}C NMR chemical shifts are reported in ppm using tetramethylsilane (TMS) as an internal standard or residual nondeuterated solvent peak as an internal standard. Infrared spectra were recorded with a Bruker ALPHA FT-IR spectrometer. High-resolution mass spectra (HRMS) were recorded with a Bruker micro TOF spectrometer in the ESI mode. Melting points were recorded with a Sanyo Gallenkamp apparatus. Reactions were monitored by thin-layer chromatography and visualized by UV and a solution of KMnO_4 . Cinnamic acids **1a**, **1g**, **1j**, **1k**, **1n**, **1q** and solvents were obtained from commercial sources and used without further purification. Unless otherwise noted, α,β -unsaturated carboxylic acid were synthesized according to literature procedures via Wittig reaction and Horner-Wadsworth-Emmons reaction. Purification of the reaction products was carried out by column chromatography on silica gel (0.063–0.200 mm). After column chromatography, analytically pure solid was obtained by crystallization from CH_2Cl_2 –hexanes.

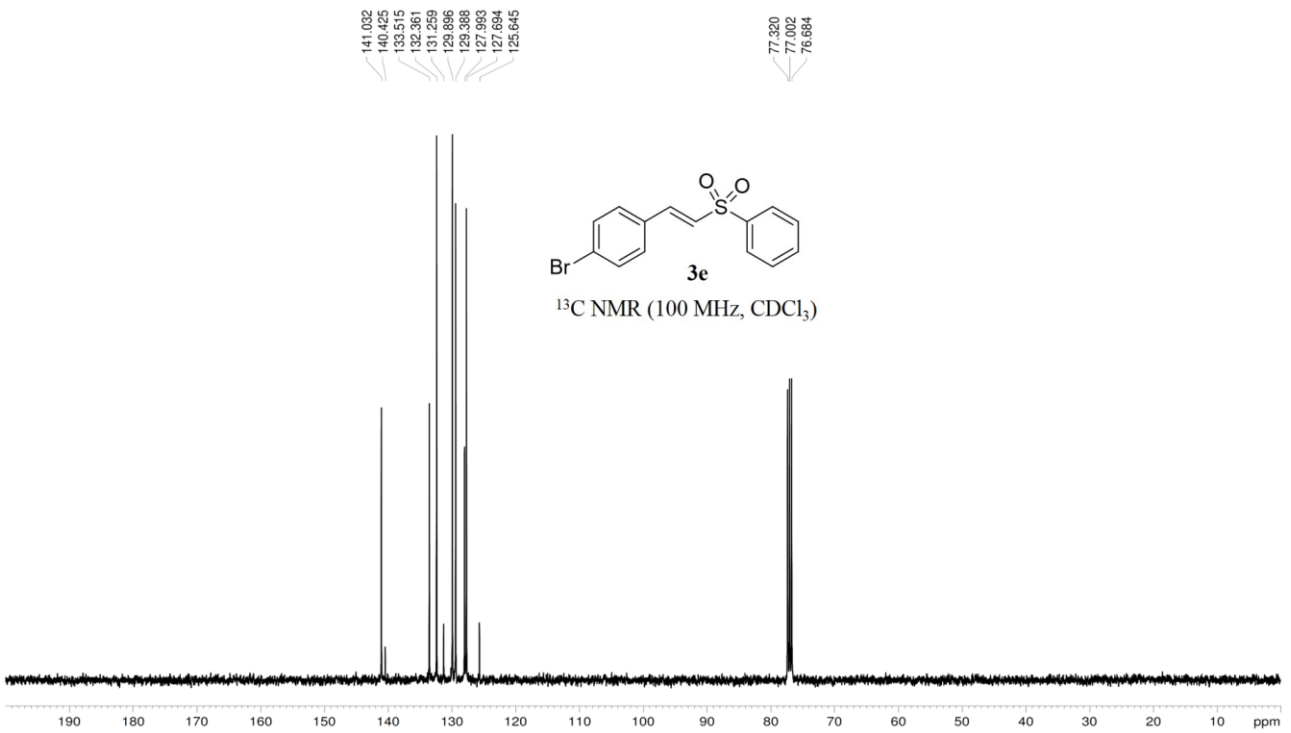
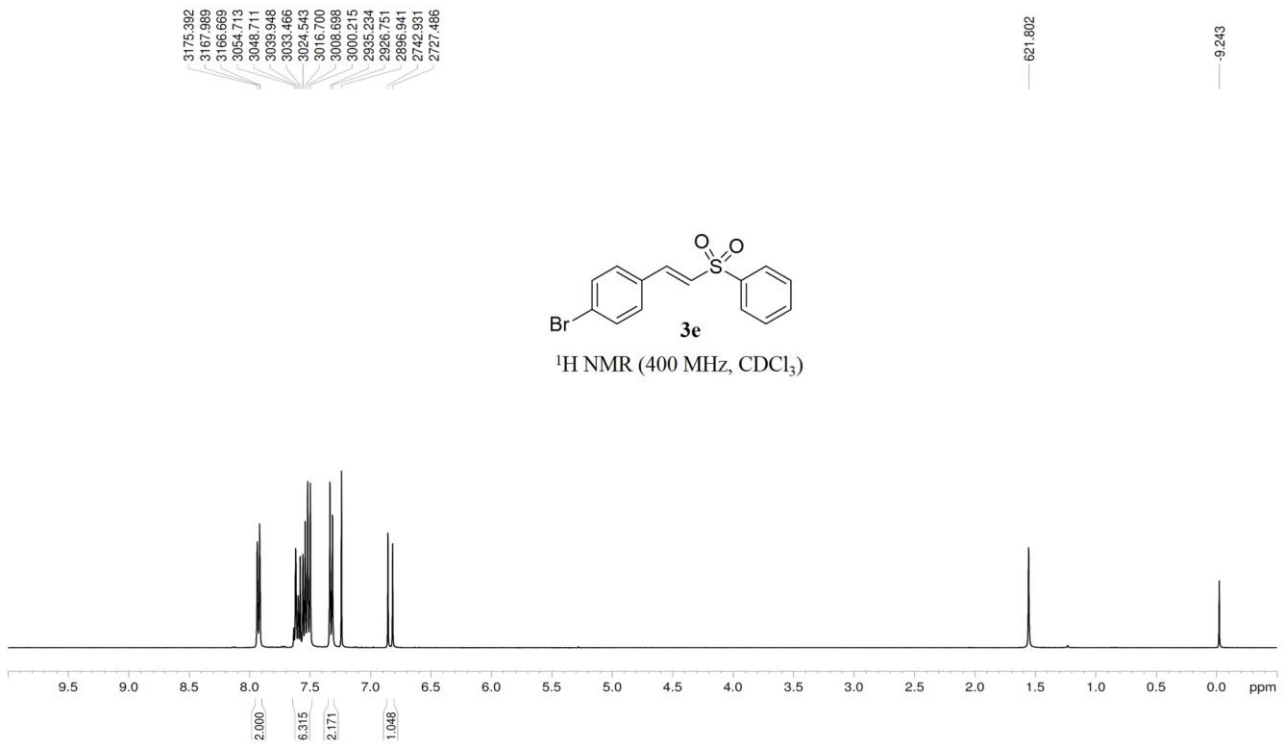
General procedures: Synthesis of vinyl sulfone from β -aryl- α,β -unsaturated carboxylic acid and sodium sulfinite. DIB (161.1 mg, 0.50 mmol) was added to a solution of β -aryl- α,β -unsaturated carboxylic acid (0.25 mmol) and sodium sulfinite (1.0 mmol) in DMF (3 mL) at room temperature and then reaction mixture was stirred at 100 °C under air for 10-30 minutes. After completion of the reaction, the reaction was cooled to room temperature and was diluted with water (10 mL). Further stirring was followed by extraction with EtOAc (2 \times 20 mL). The combined organic extracts were washed with H_2O (20 mL) and brine (20 mL), dried (MgSO_4), filtered, and concentrated (aspirator). The residue was purified by column chromatography using EtOAc–hexanes as eluent to afford the corresponding product.

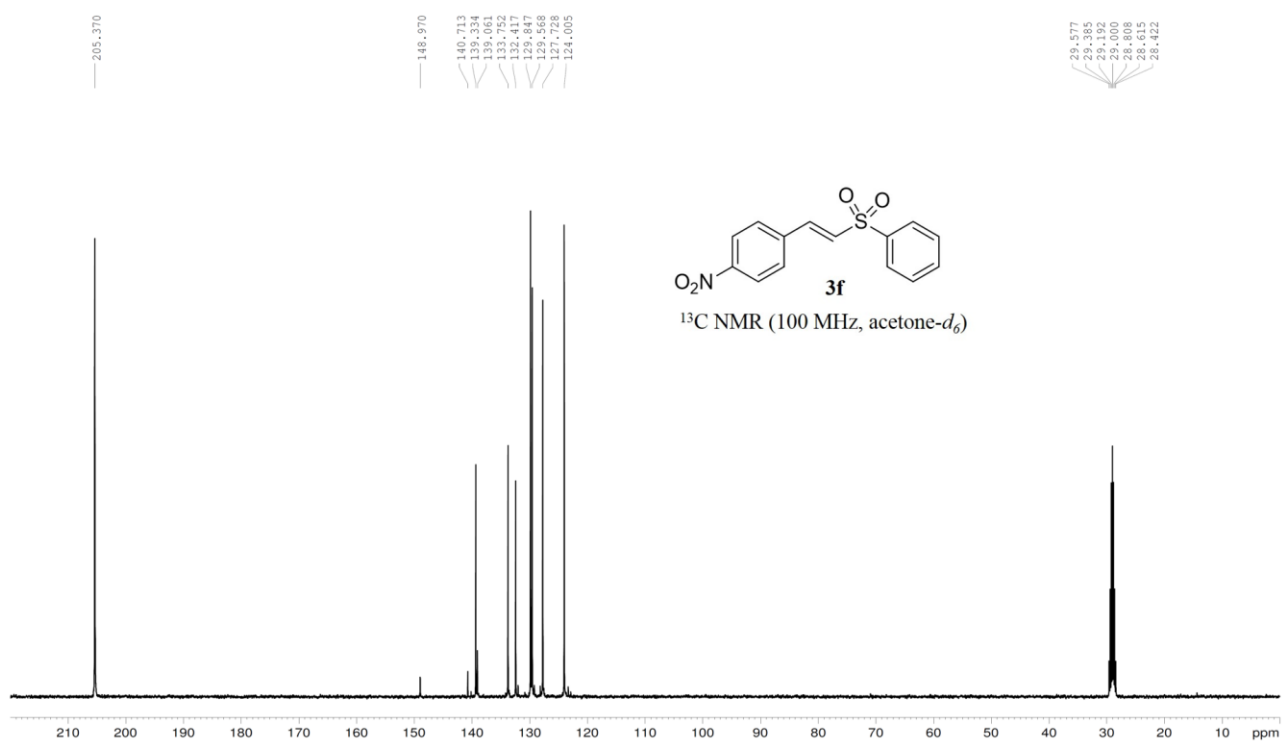
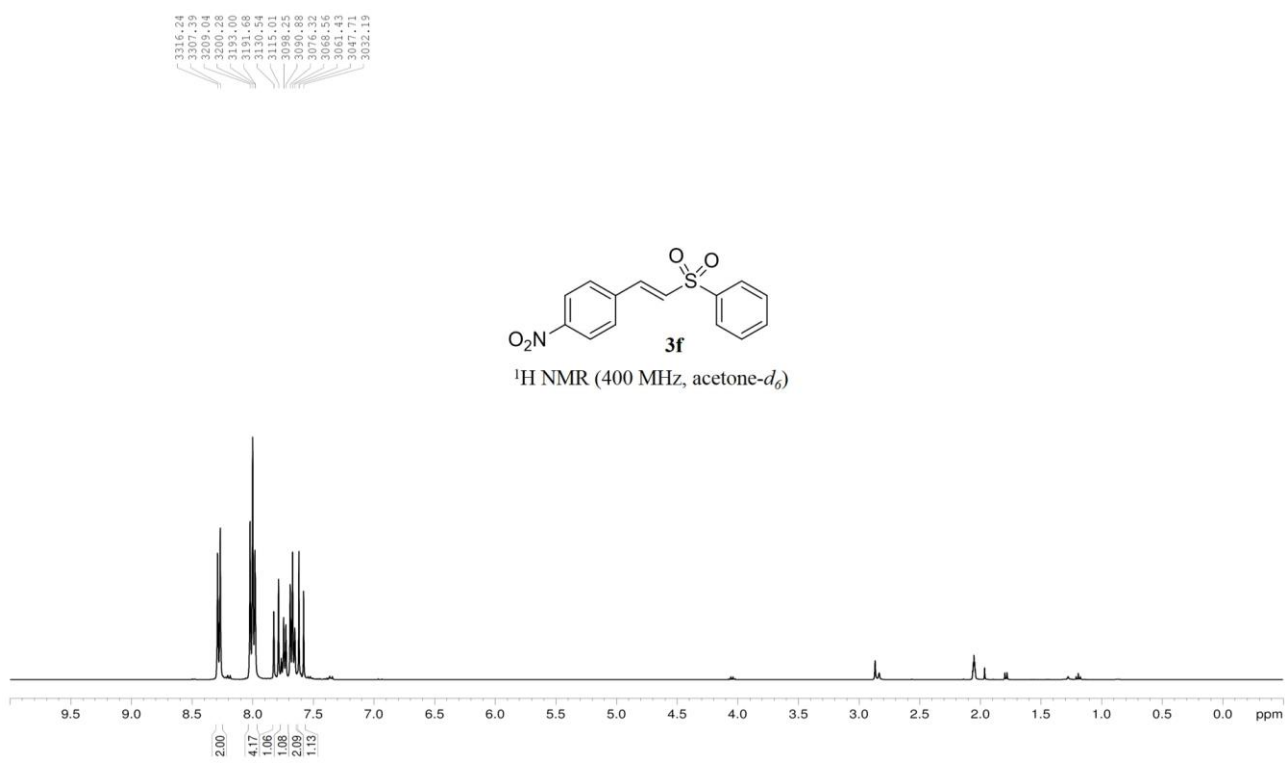
^1H and ^{13}C NMR spectra





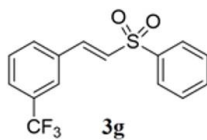




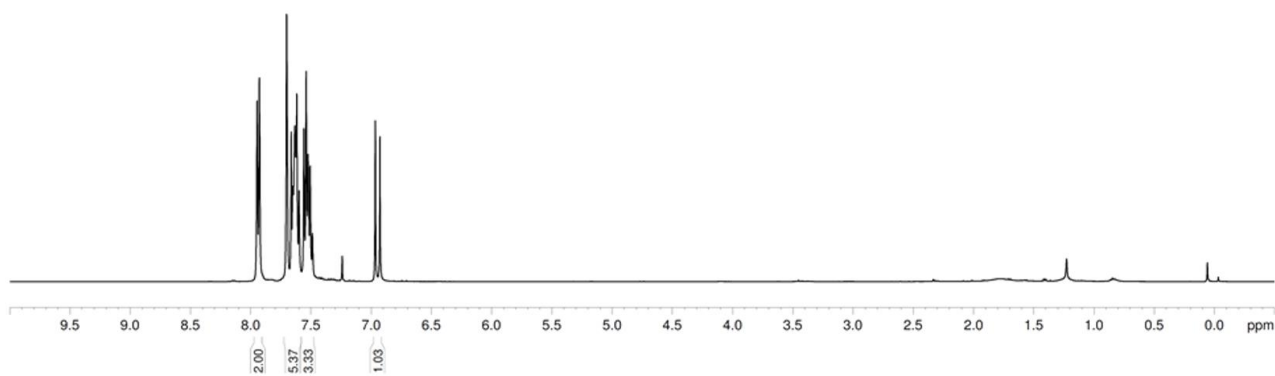


3179.75
3172.35
3171.86
3064.28
3060.95
3053.87
3047.79
3040.19
3037.40
3016.50
3010.90
3009.54
3003.38
2995.61
2987.11
2771.62

490.72



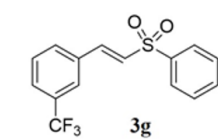
$^1\text{H NMR}$ (400 MHz, CDCl_3)



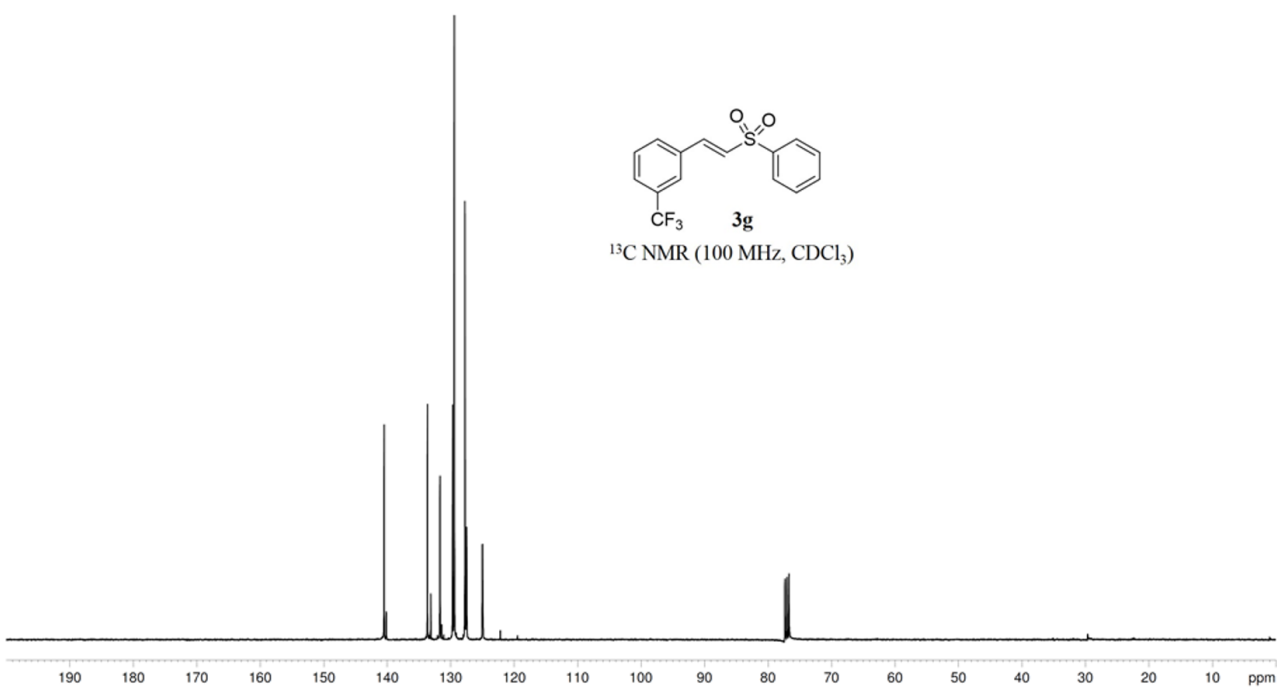
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140.098
133.628
133.112
132.039
131.886
131.386
131.060
129.667
129.400
129.151
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127.937
127.723
127.491
127.456
124.973
124.516
124.904
124.853
122.142

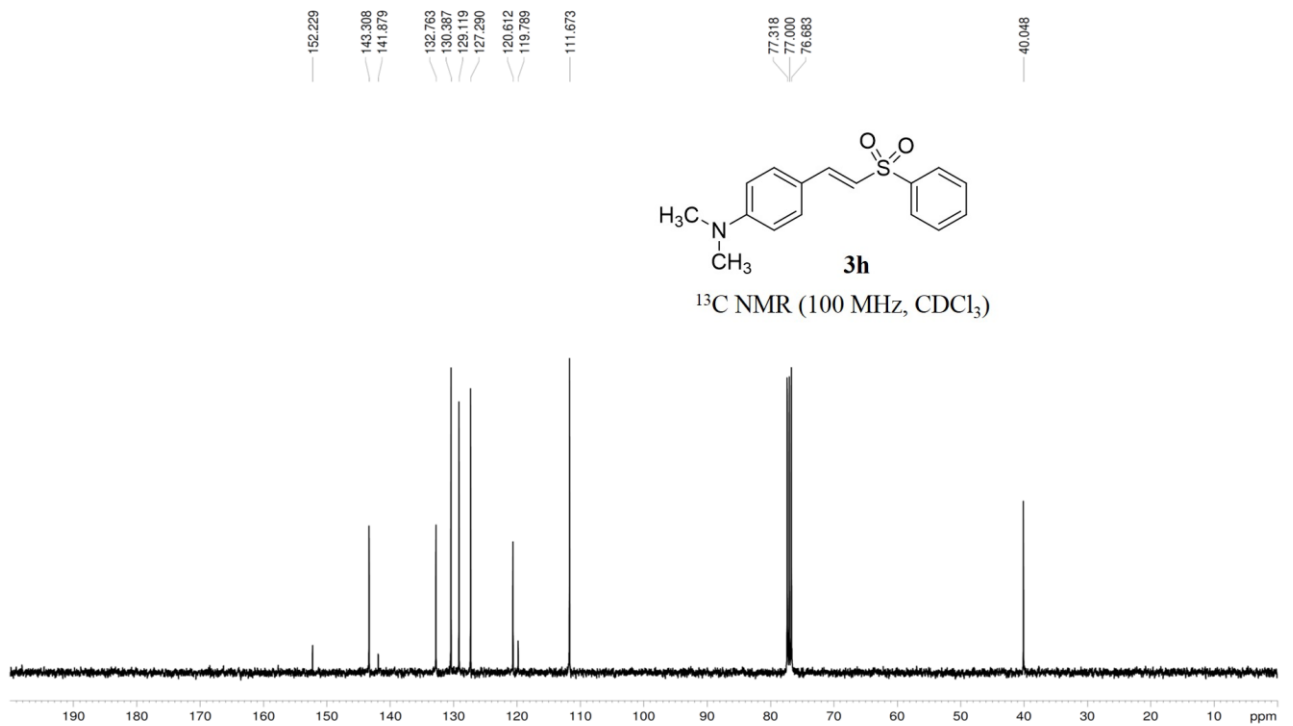
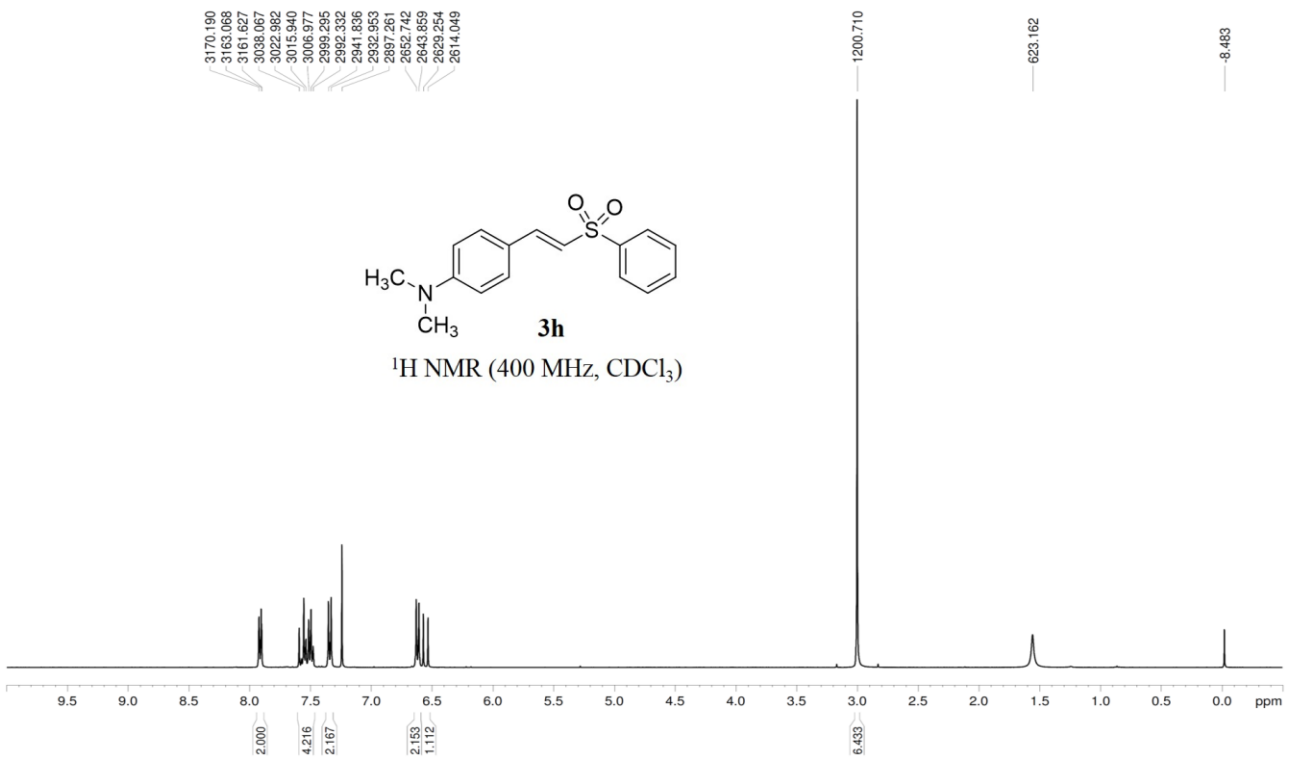
77.307
76.990
76.671

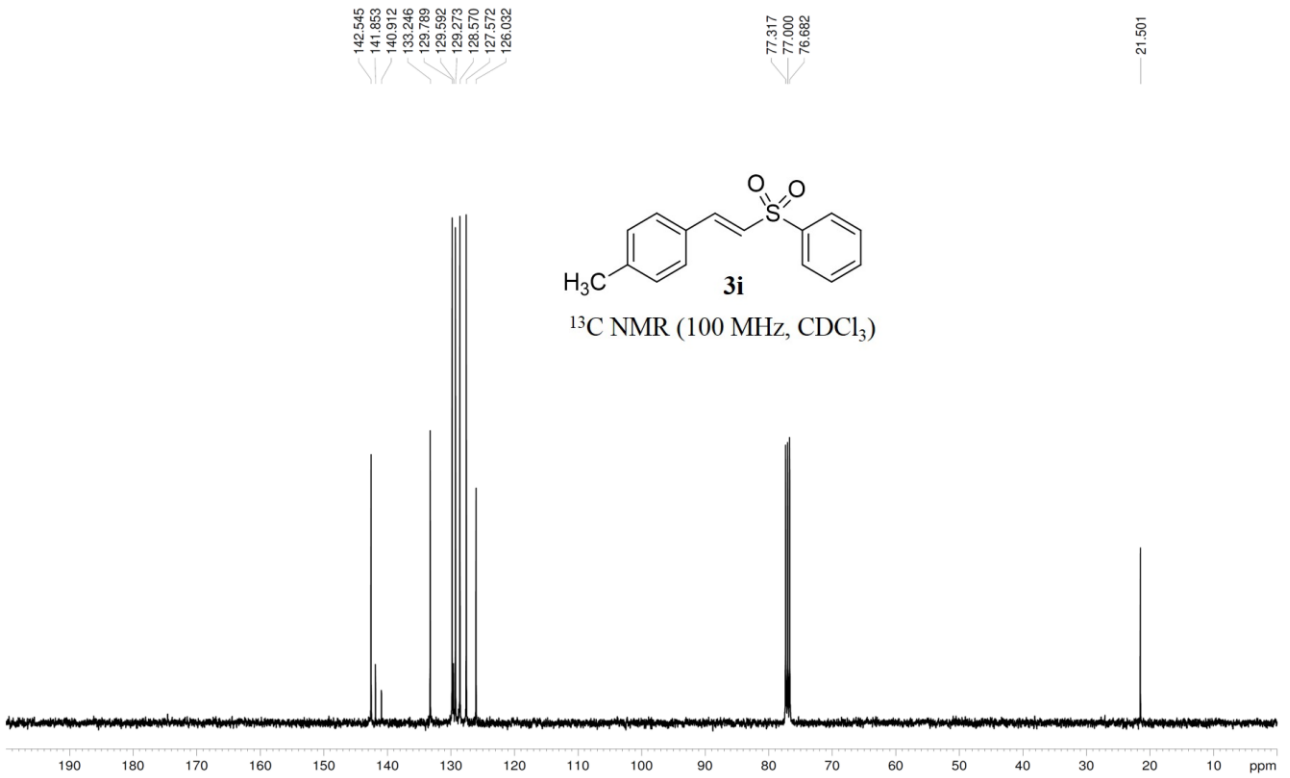
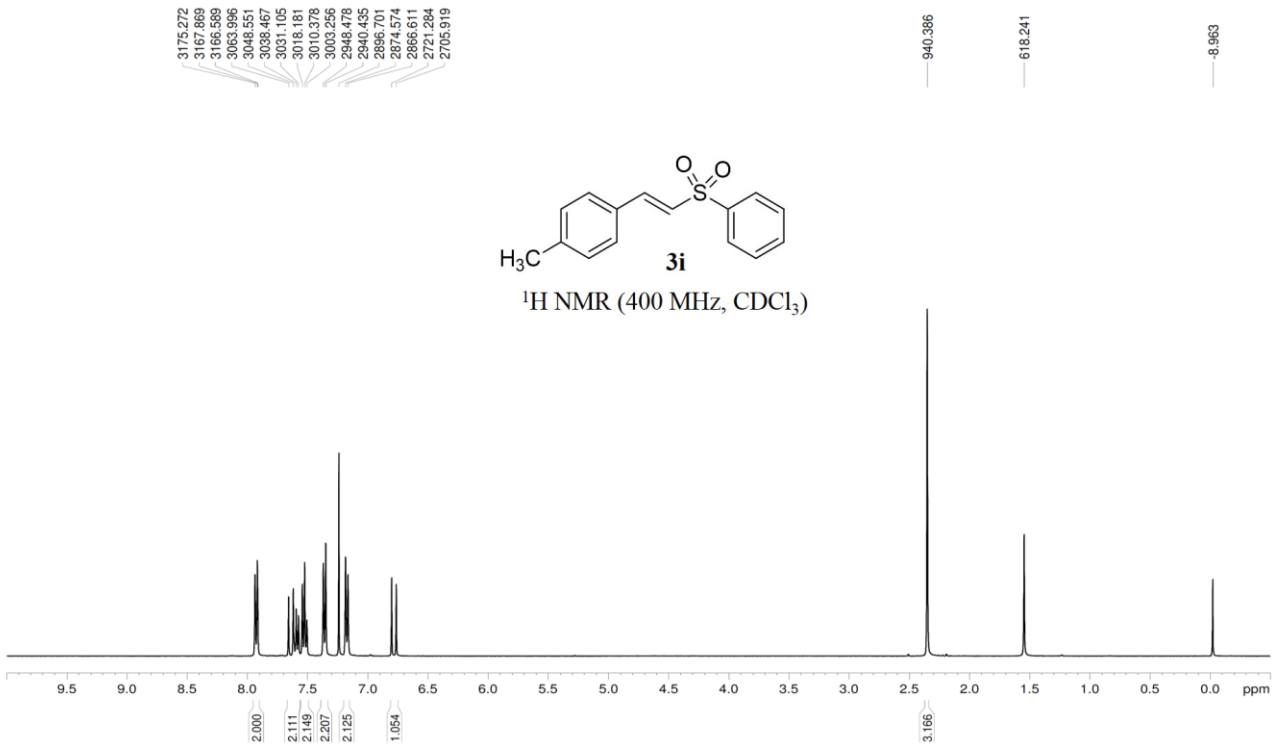
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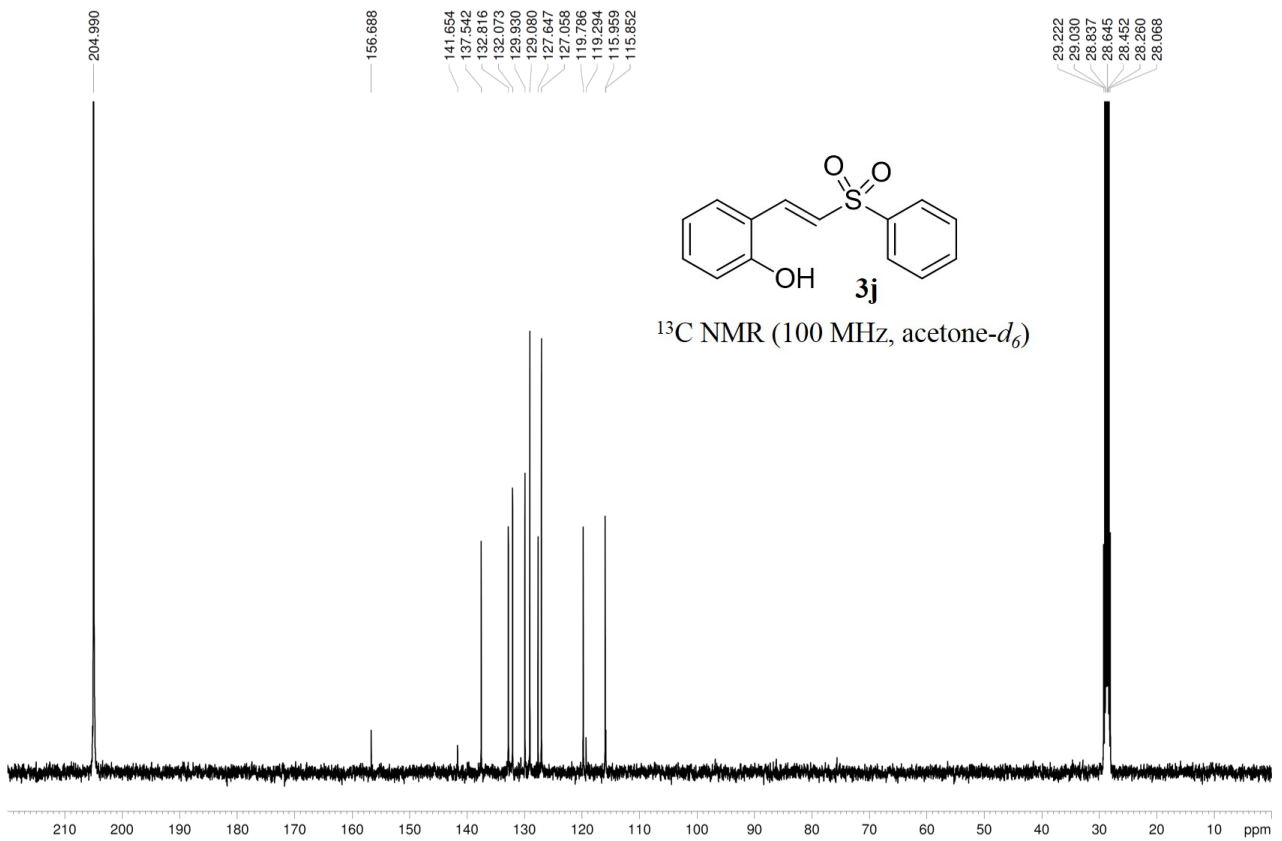
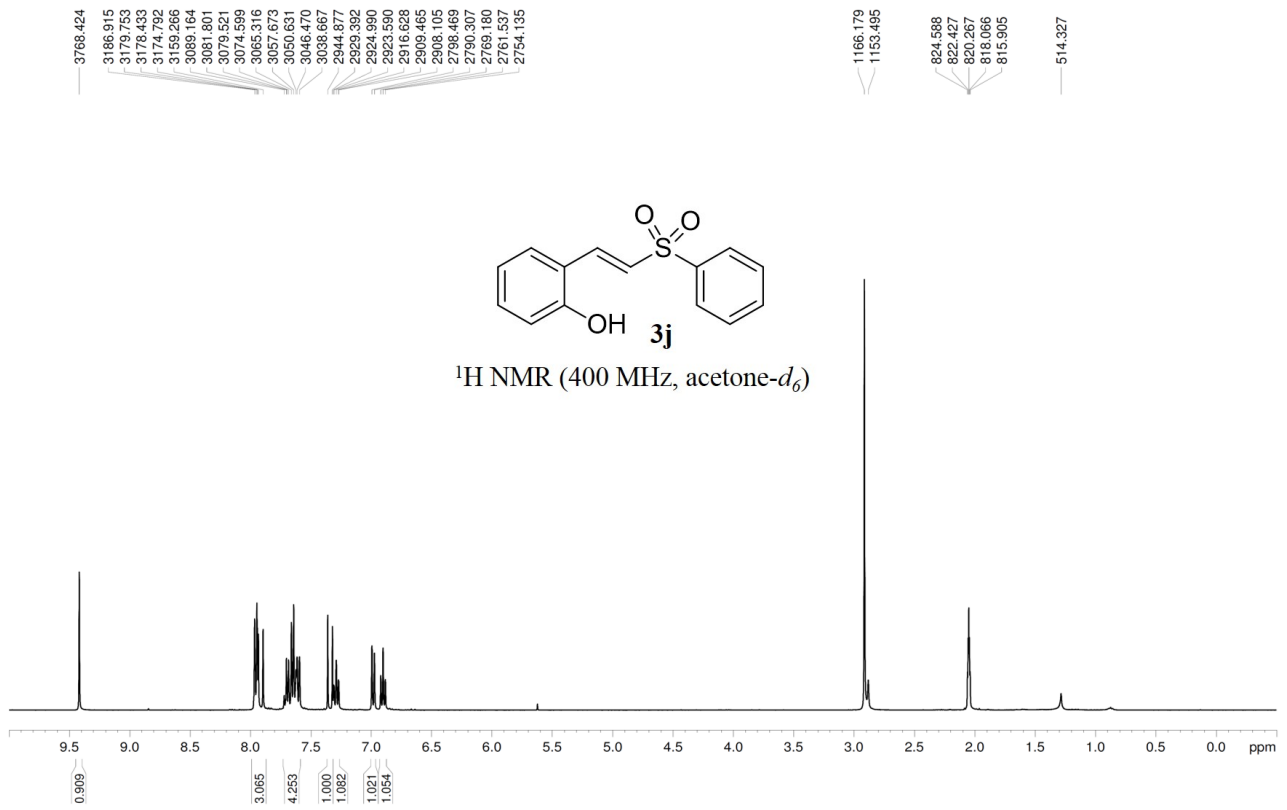


$^{13}\text{C NMR}$ (100 MHz, CDCl_3)

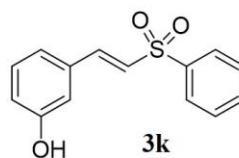




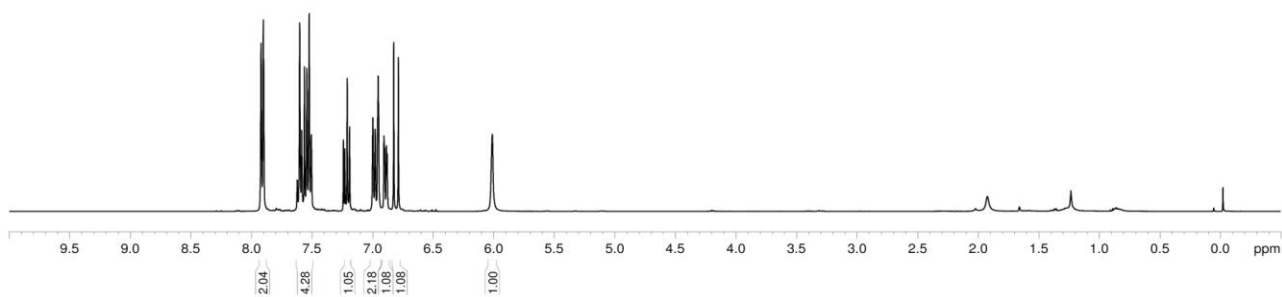




3168.75
3161.51
3160.19
3041.35
3034.67
3018.55
3018.02
3010.22
3002.98
2897.02
2892.26
2876.49
2876.49
2799.67
2791.87
2783.90
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2777.98
2760.86
2760.86
2754.66
2752.77
2730.77
2715.36
2405.18

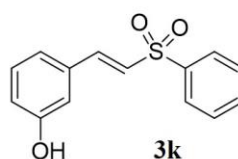


$^1\text{H NMR}$ (400 MHz, CDCl_3)

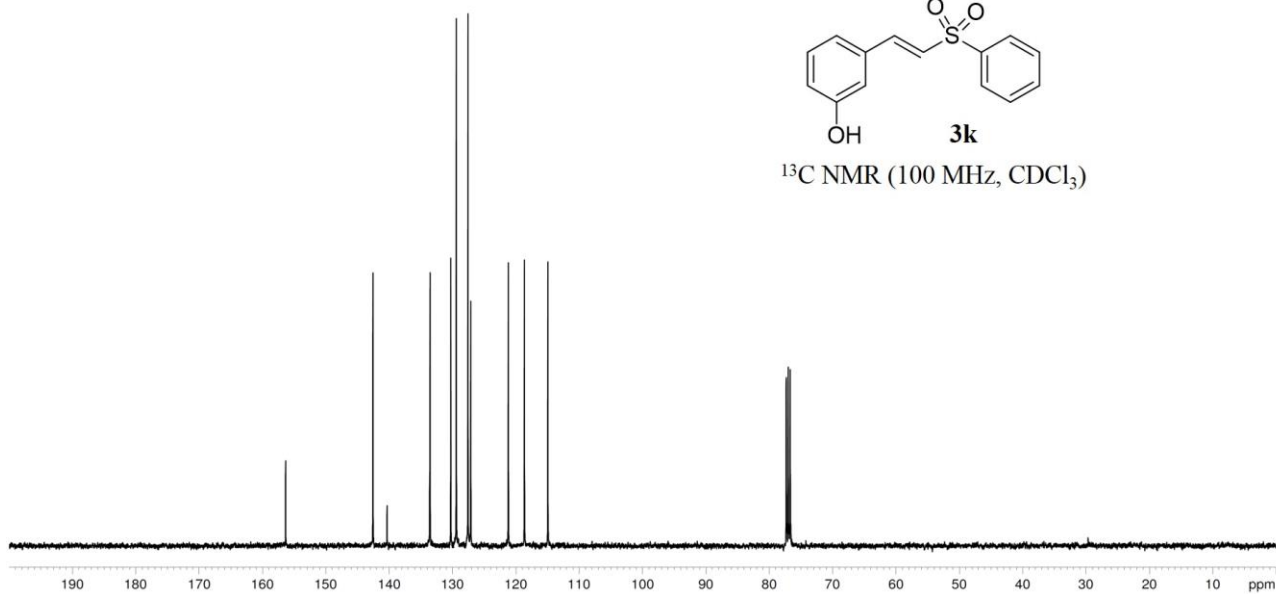


156.340
142.559
140.330
133.593
132.546
130.775
129.561
127.121
127.121
121.188
118.646
114.546

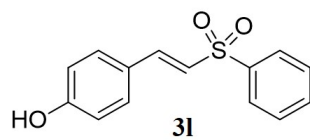
77.318
77.000
76.683



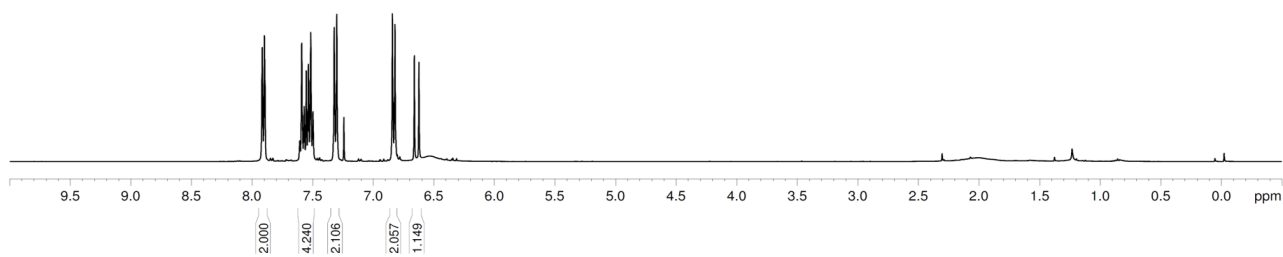
$^{13}\text{C NMR}$ (100 MHz, CDCl_3)



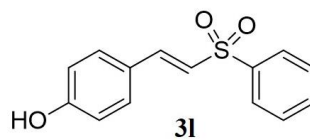
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3159.787
3043.349
3036.667
3028.664
3021.742
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2921.029
2897.381
2737.329
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2665.026
2649.701



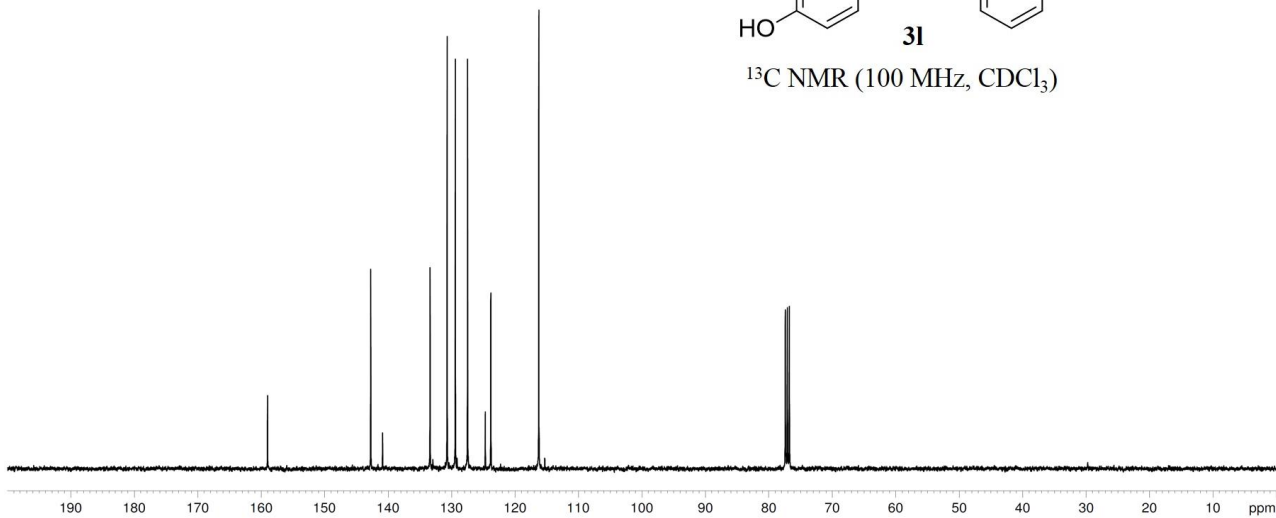
$^1\text{H NMR}$ (400 MHz, CDCl_3)

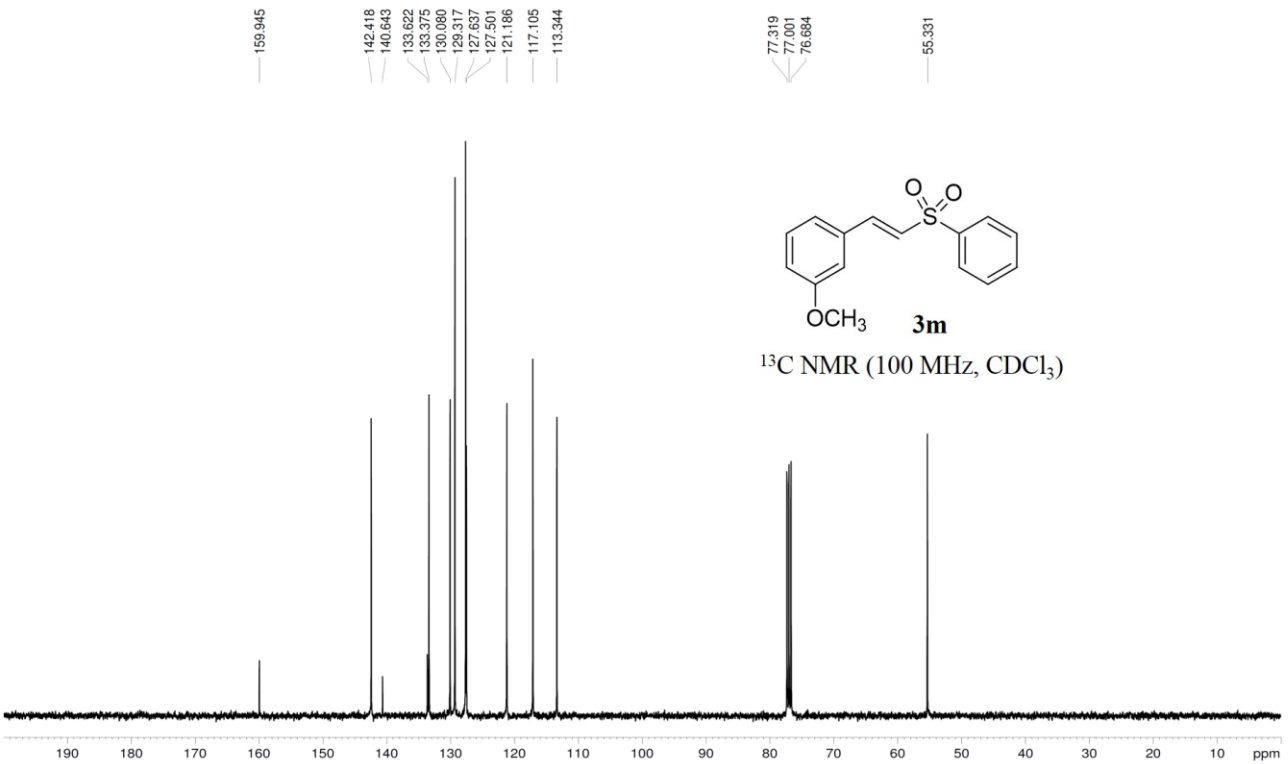
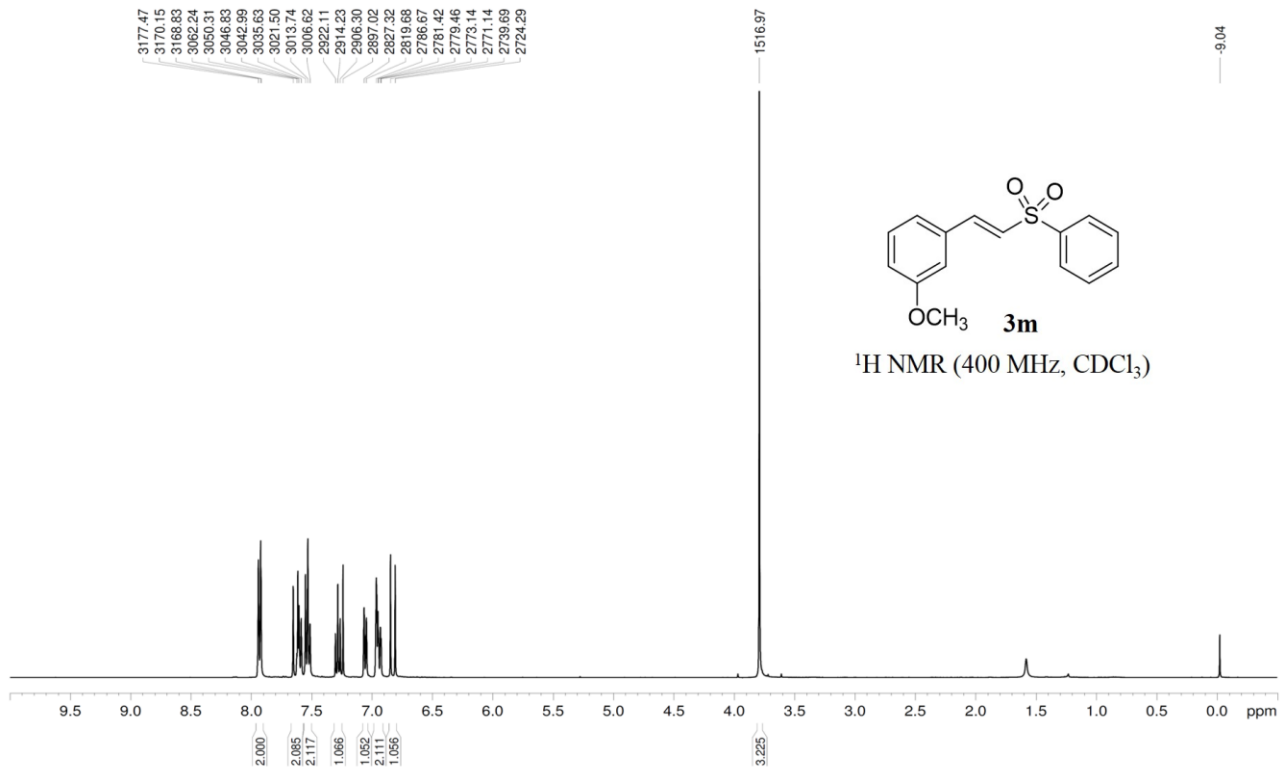


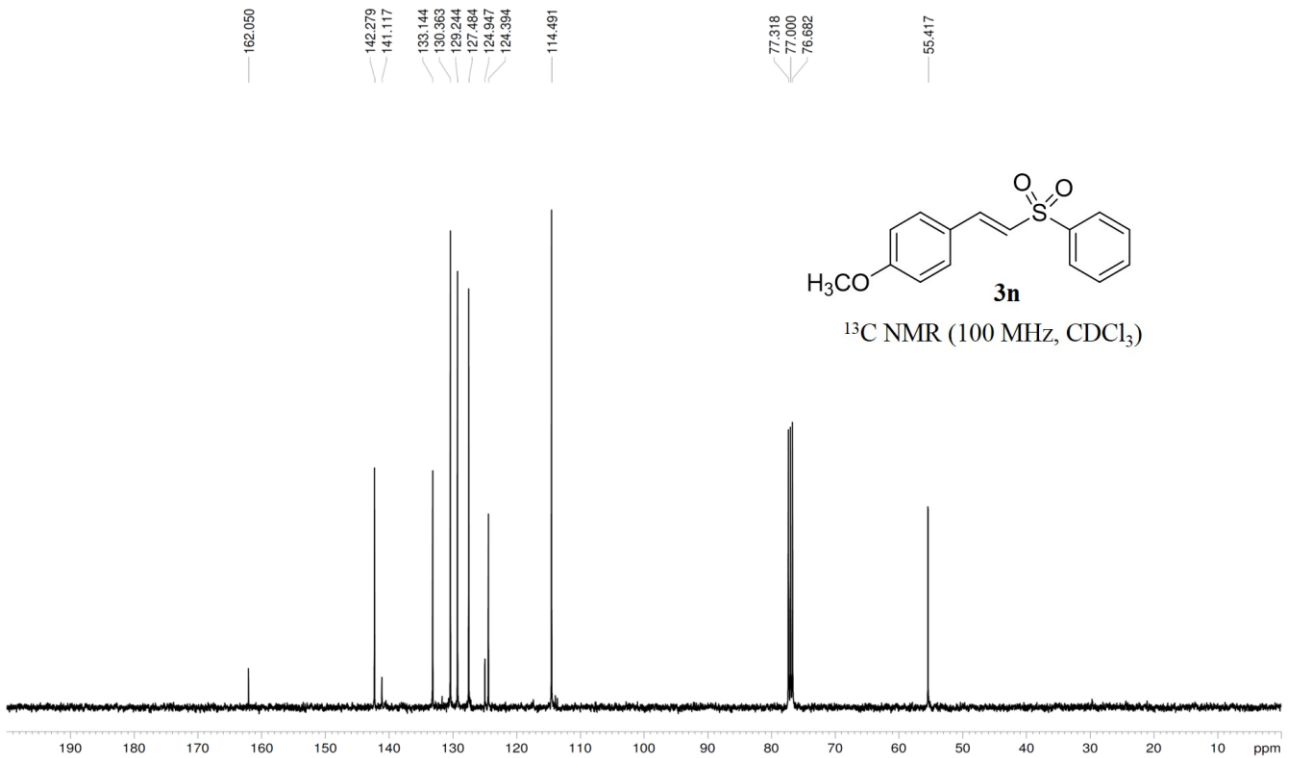
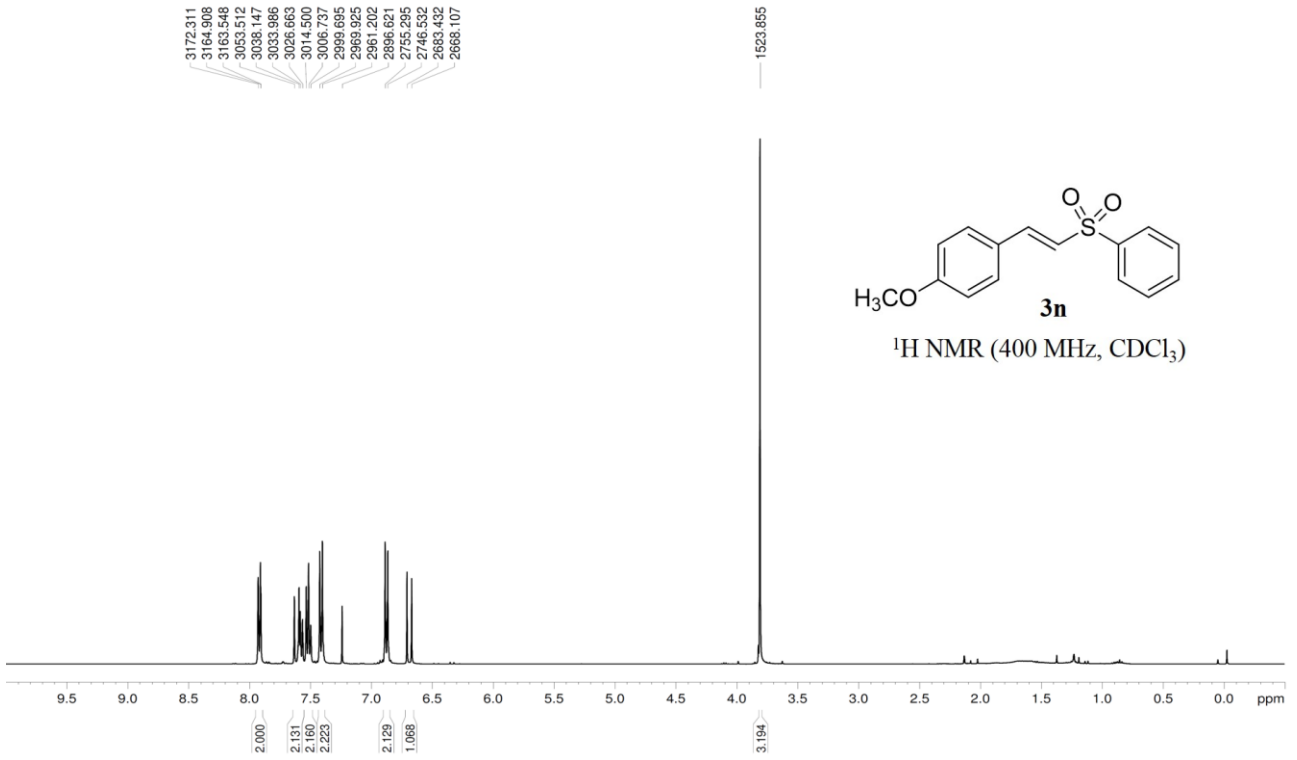
158.977
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133.362
130.672
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116.216
77.367
77.050
76.732

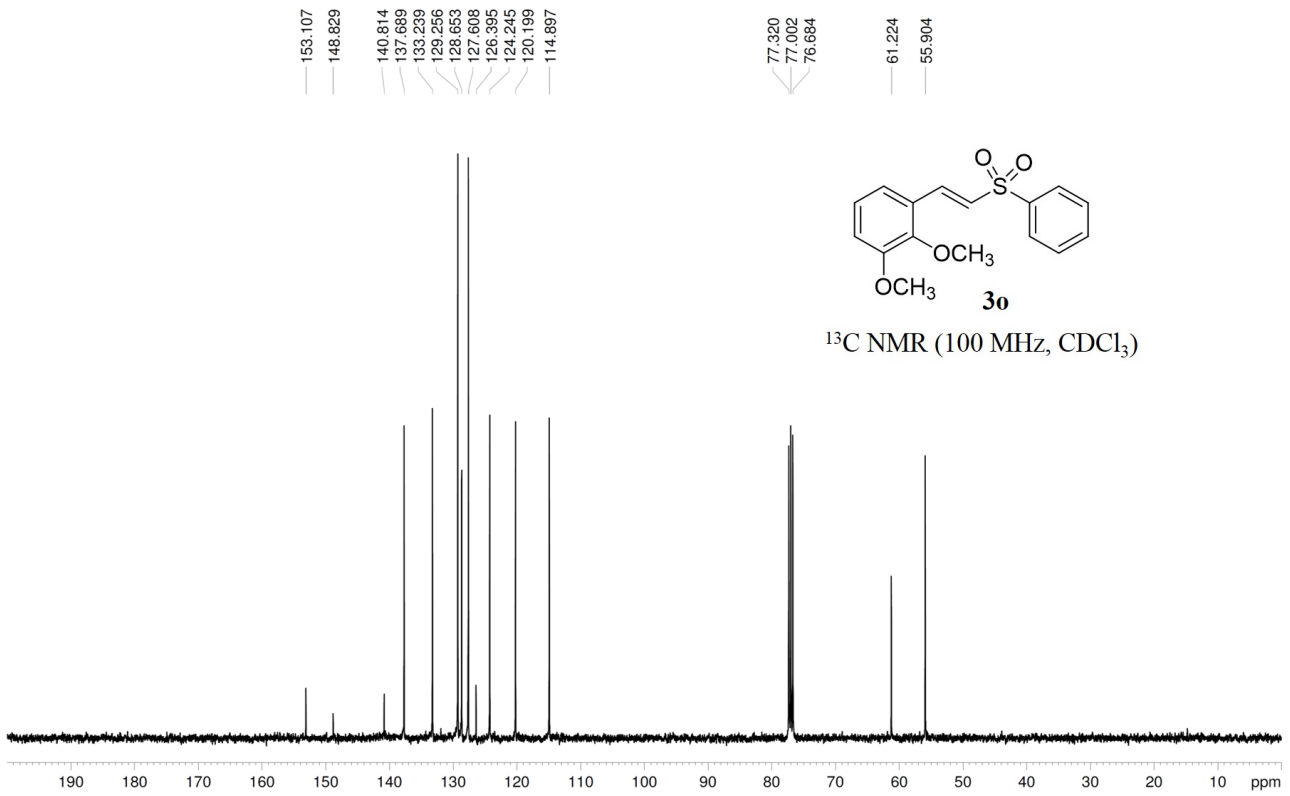
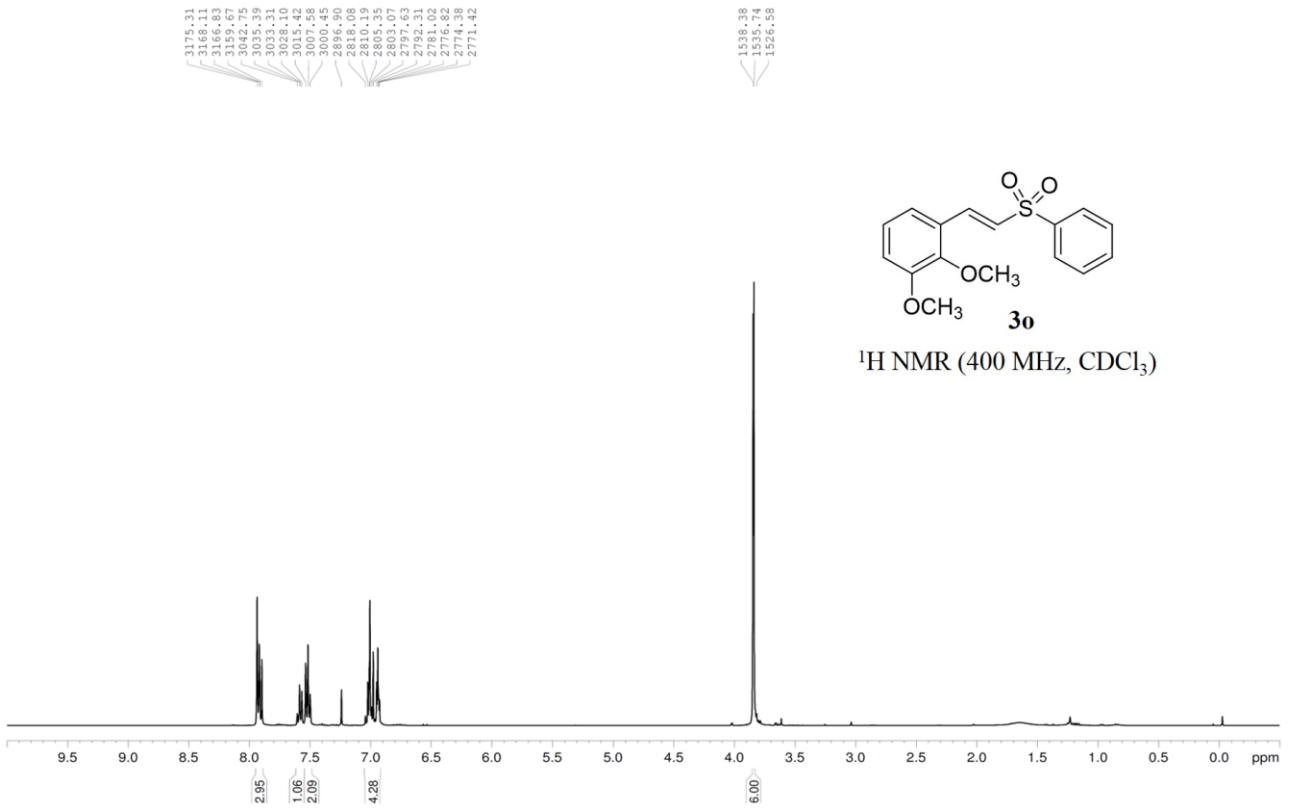


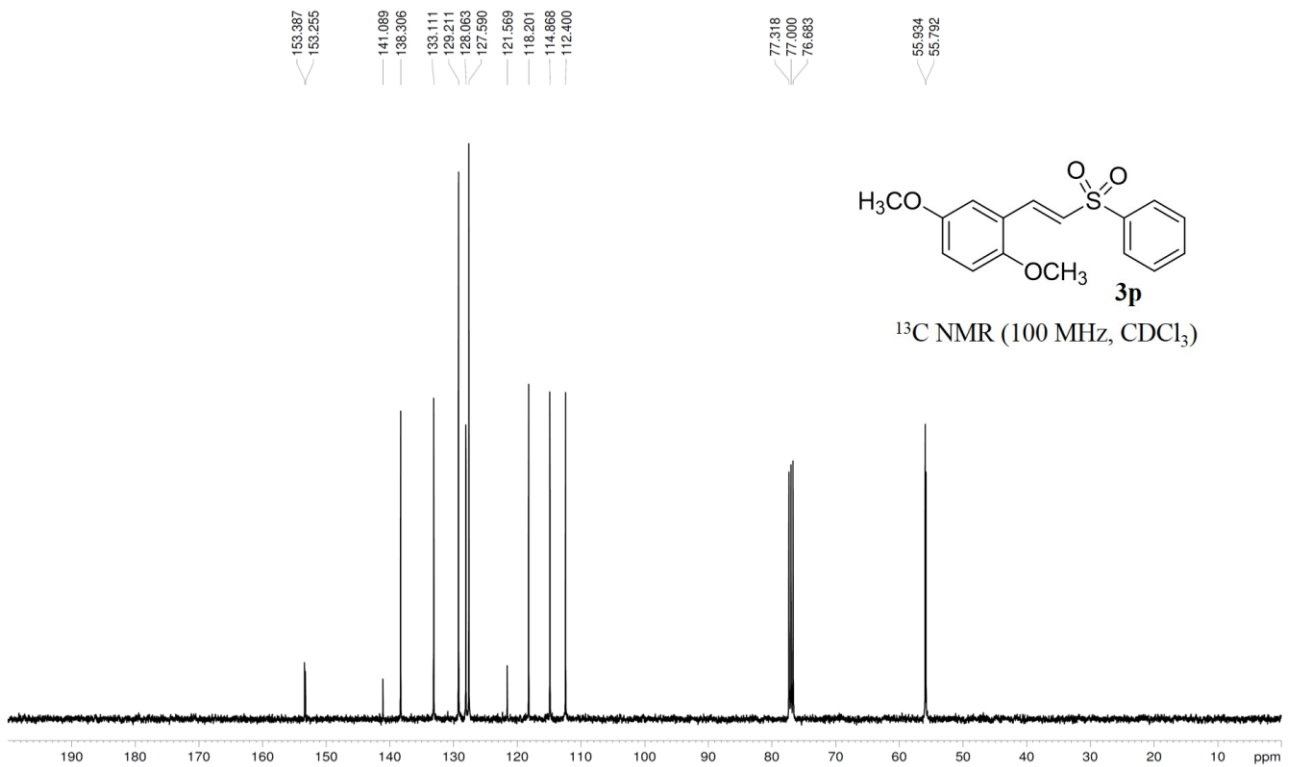
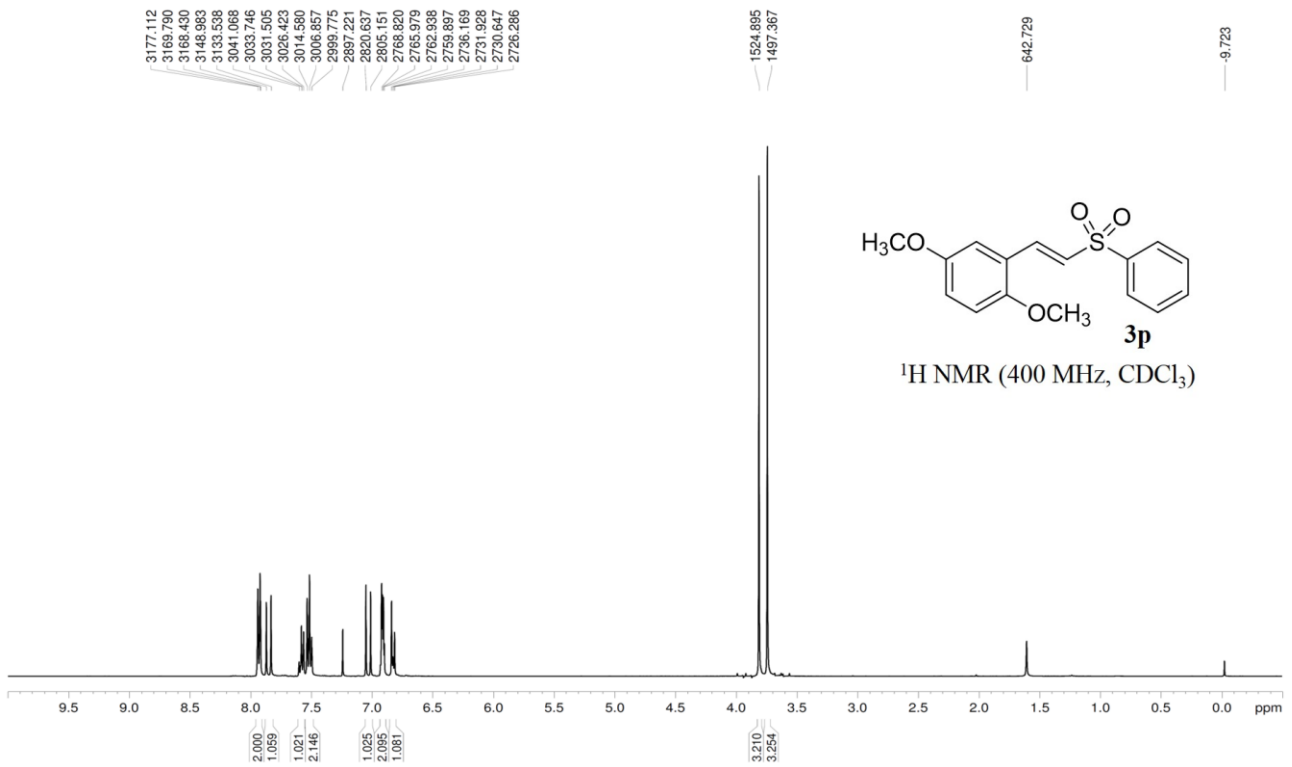
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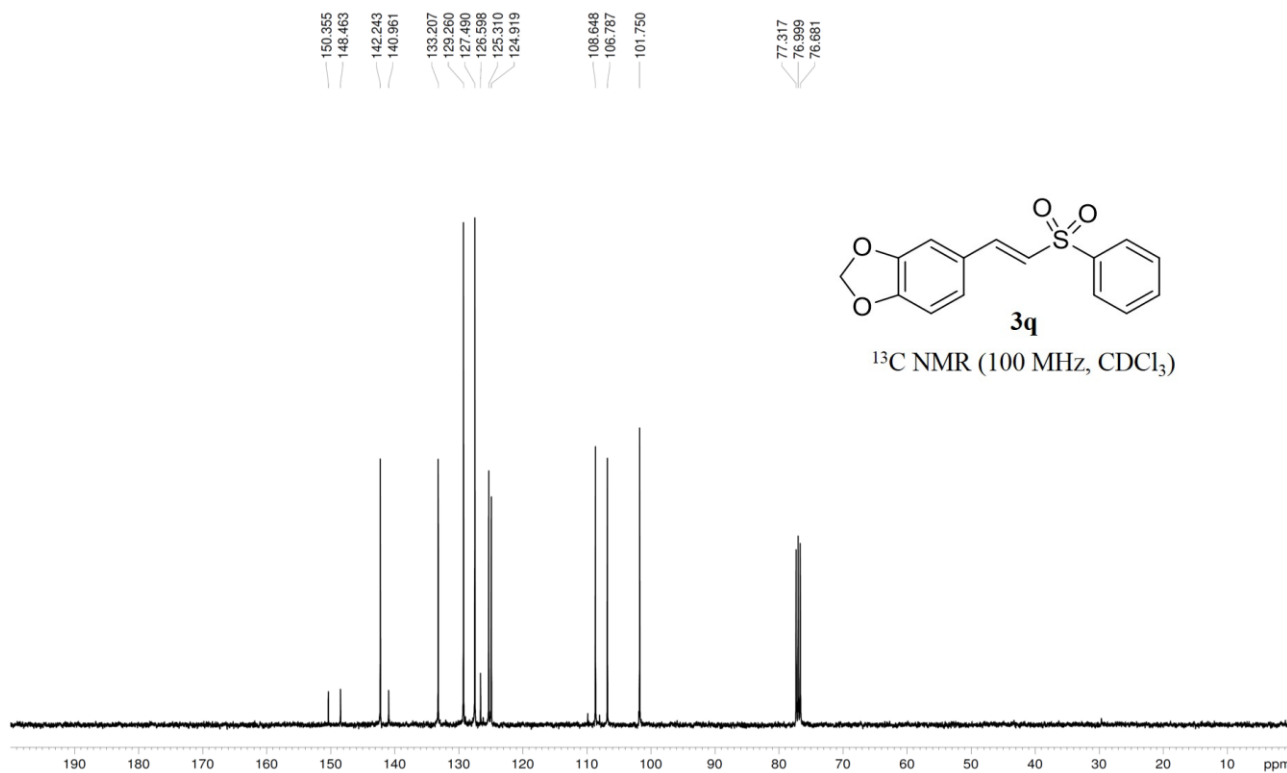
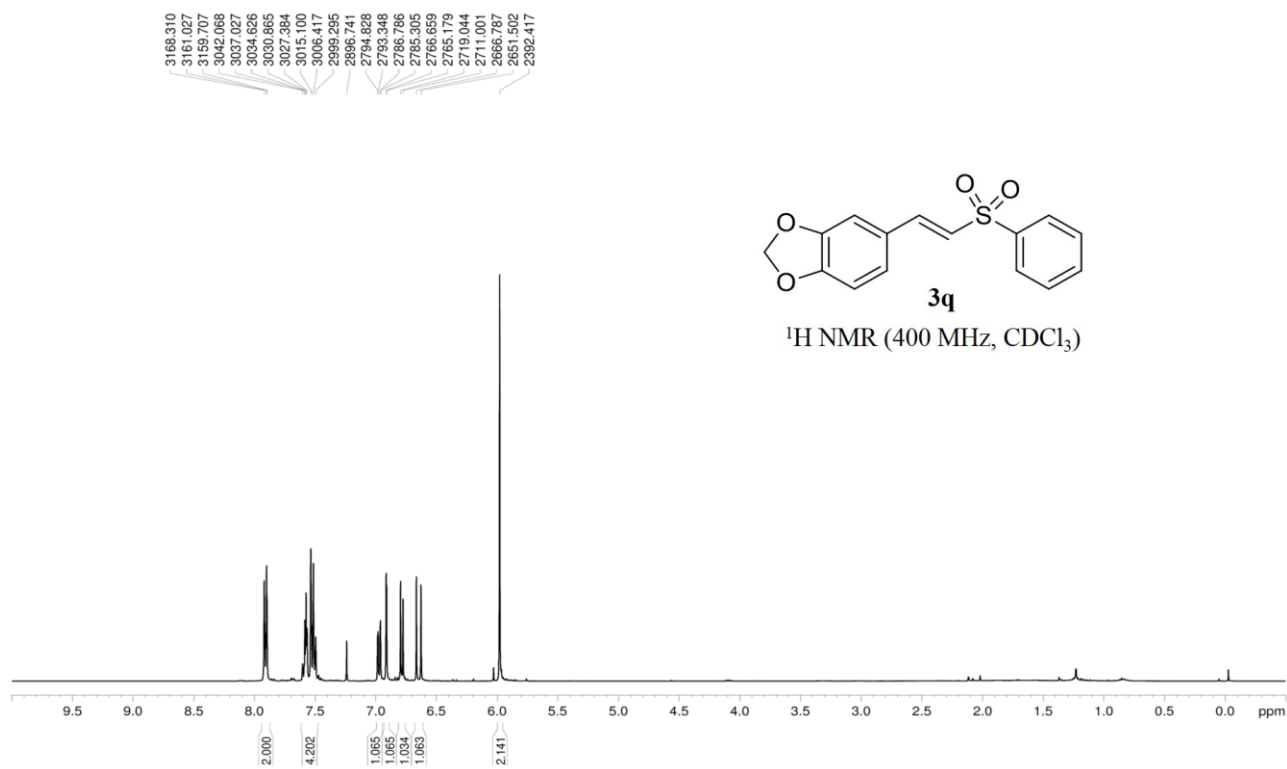


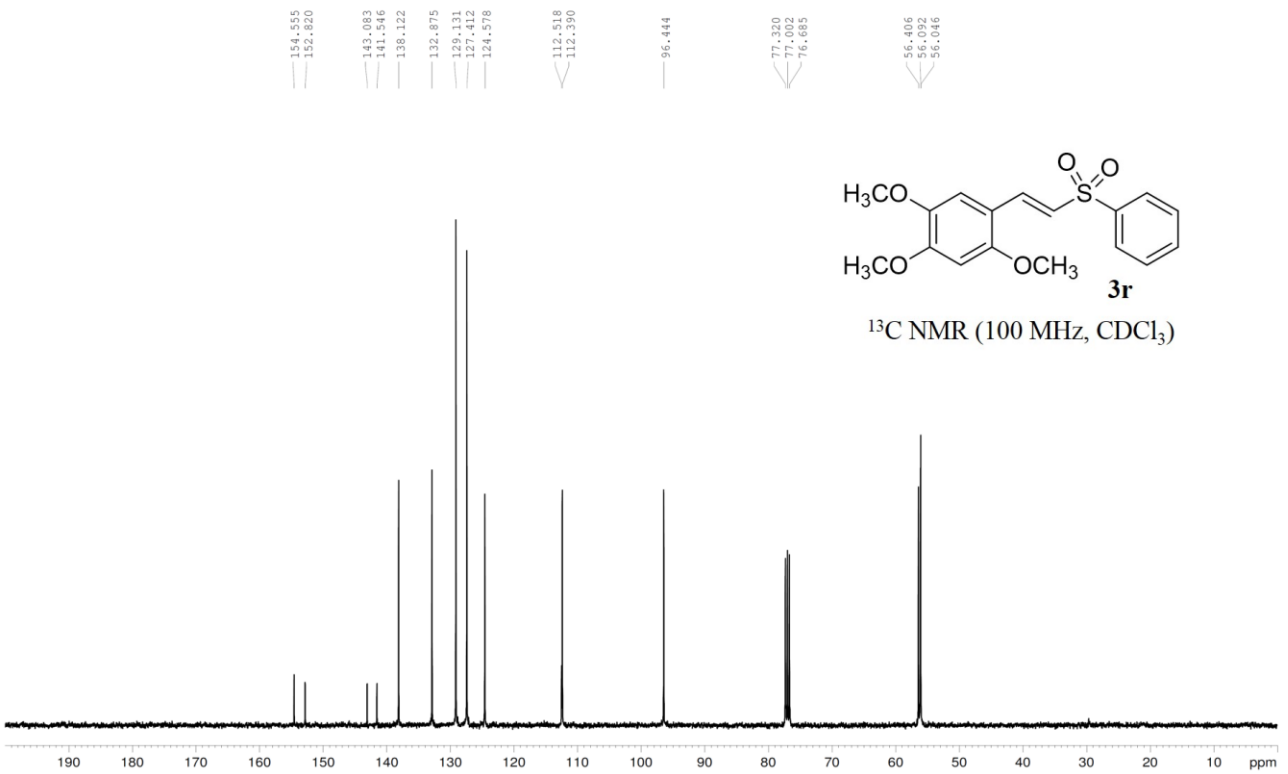
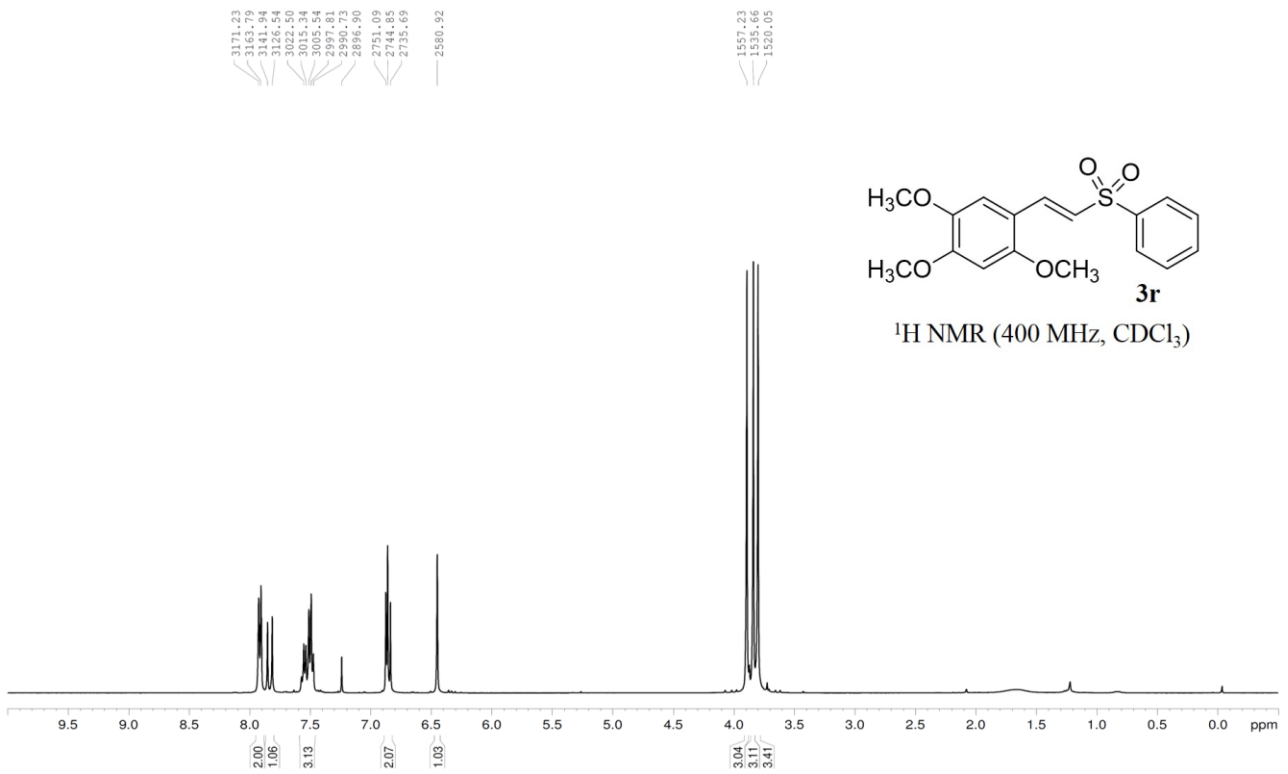


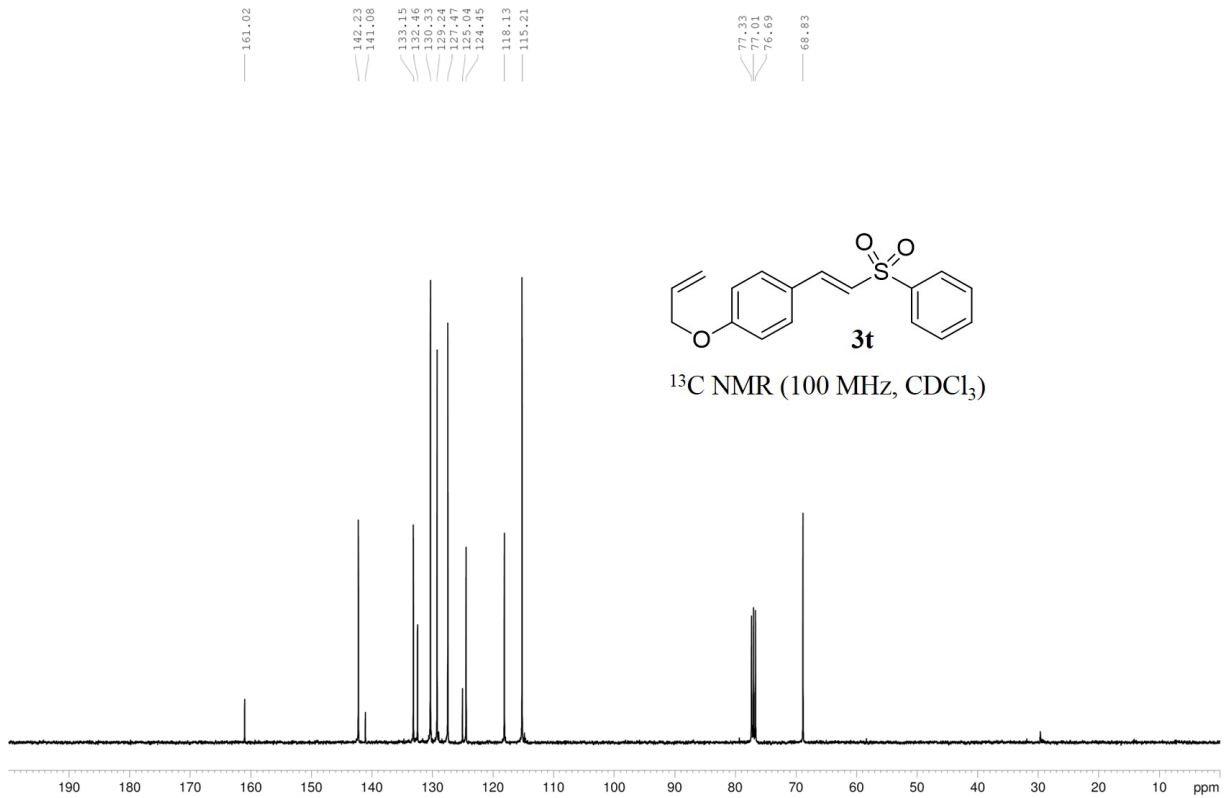
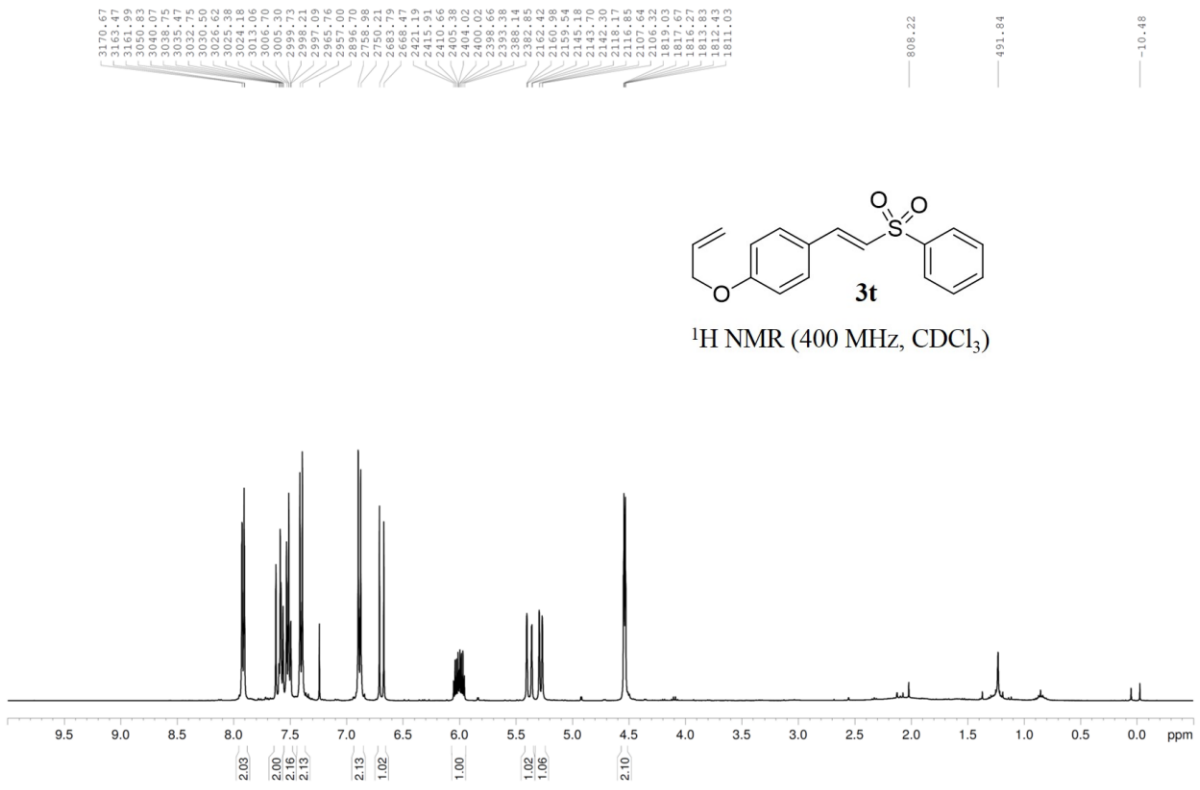




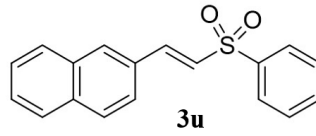




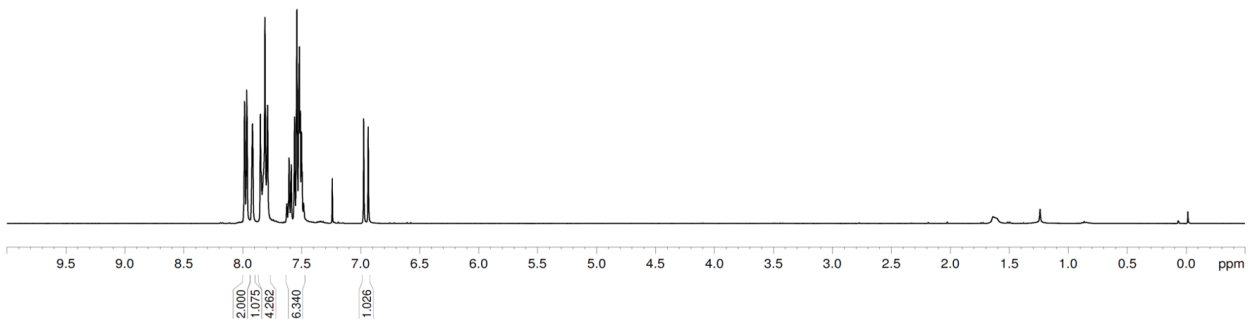




3194.398
3187.196
3185.955
3167.709
3140.701
3138.460
3131.217
3125.296
3116.493
3050.671
3043.469
3041.148
3036.027
3024.983
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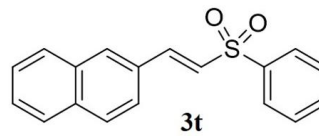


$^1\text{H NMR}$ (400 MHz, CDCl_3)

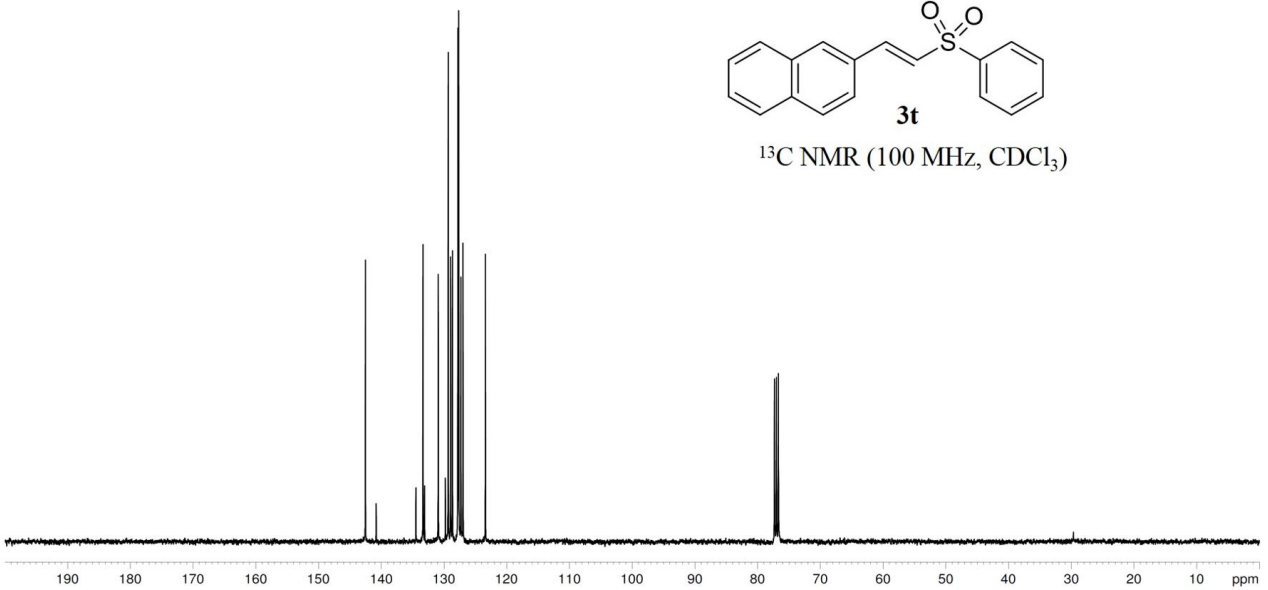


142.526
140.803
134.478
133.343
133.078
130.908
129.783
129.525
128.858
128.655
127.785
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127.239
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123.399

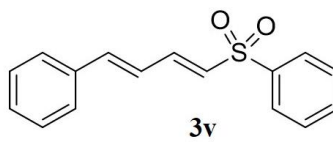
77.321
77.004
76.686



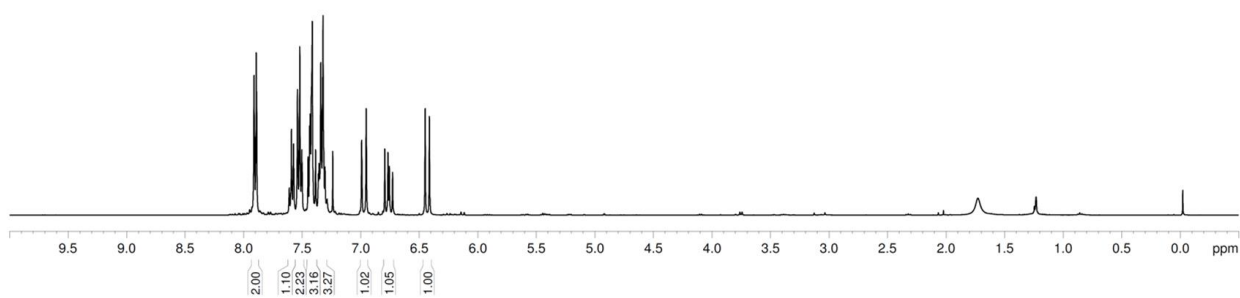
$^{13}\text{C NMR}$ (100 MHz, CDCl_3)



3155.51
3155.11
3155.67
3045.27
3037.51
3035.71
3030.54
3017.10
3009.34
3003.74
3003.74
2981.05
2975.61
2973.93
2969.46
2955.36
2946.00
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2941.32
2941.32
2929.71
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2666.19



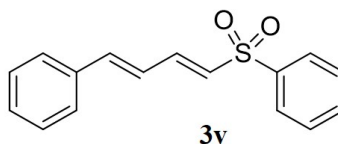
$^1\text{H NMR}$ (400 MHz, CDCl_3)



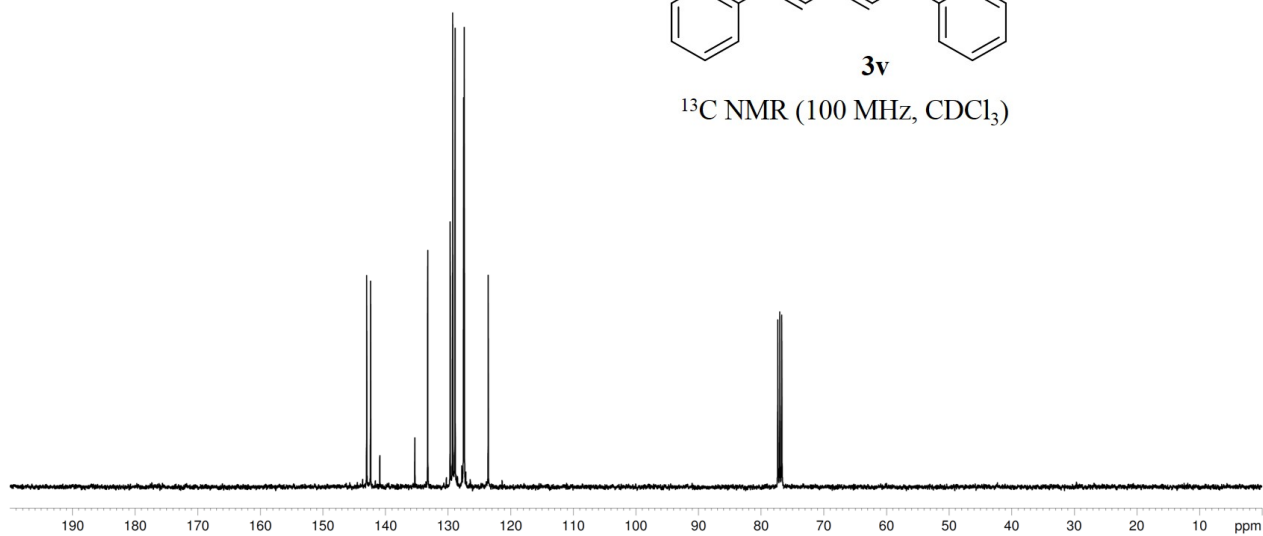
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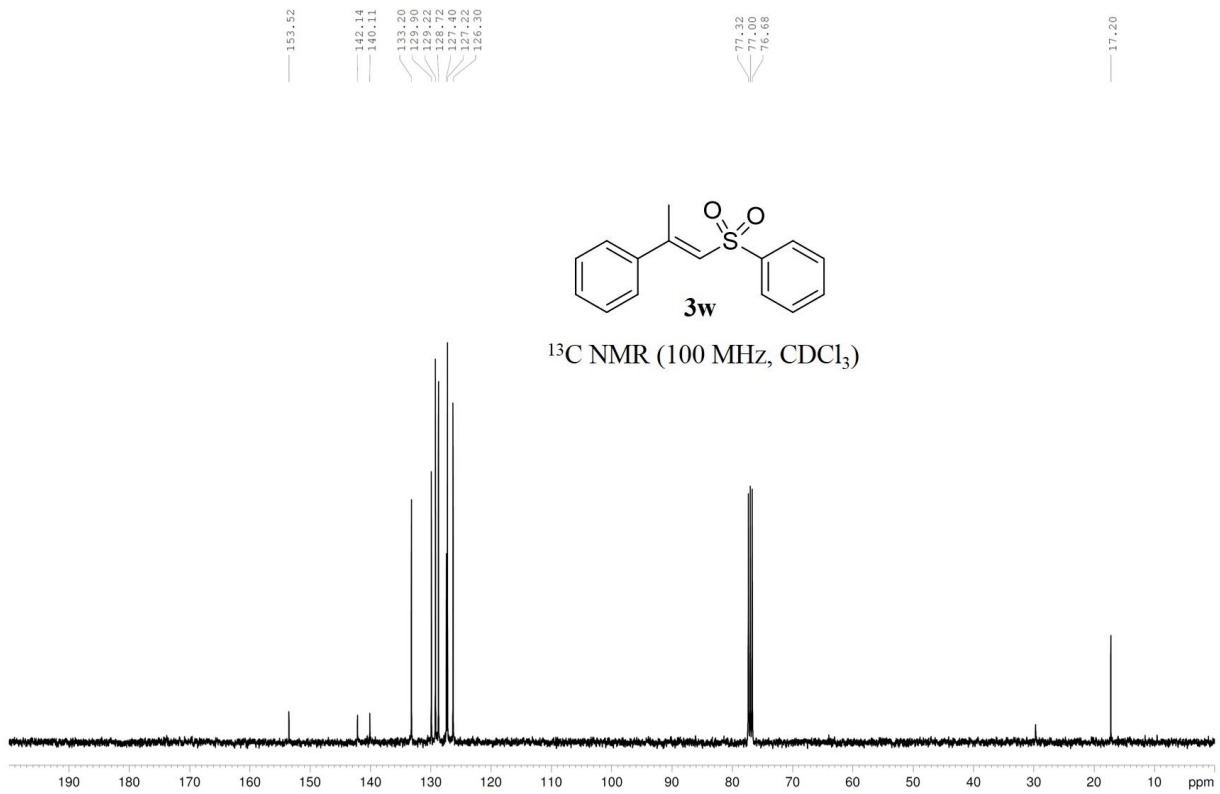
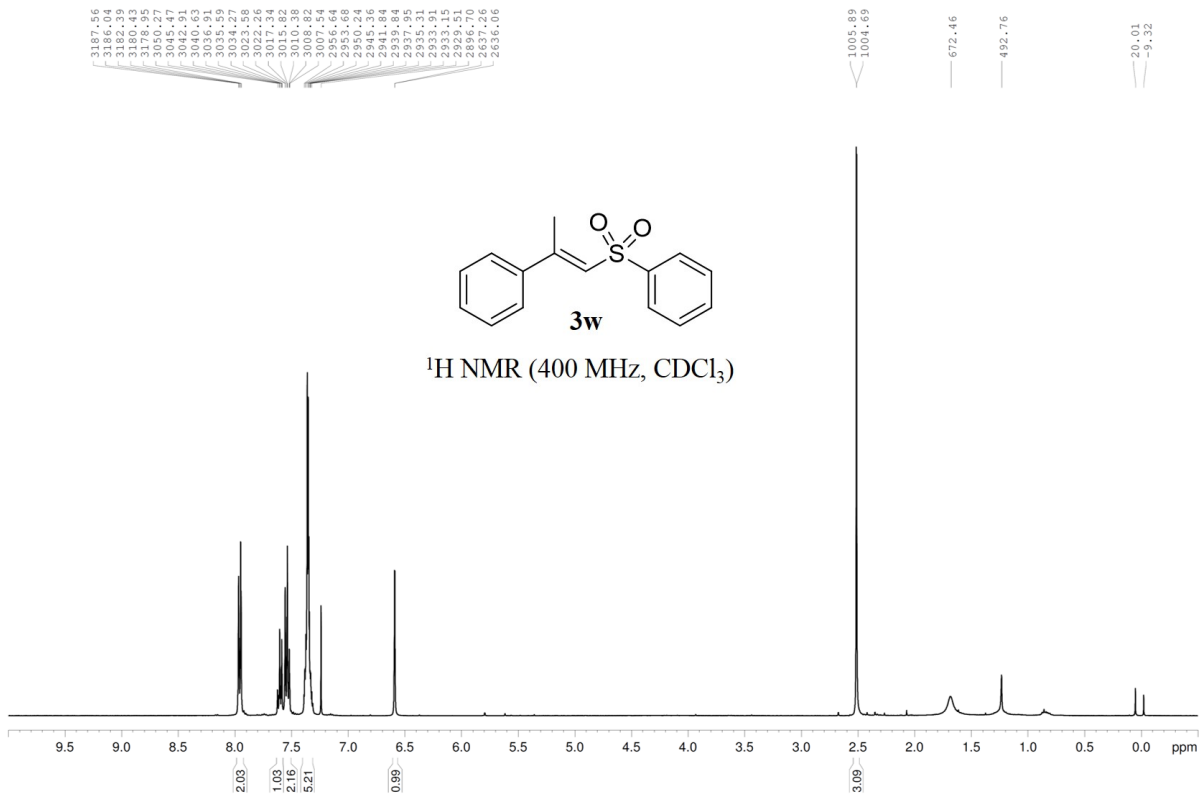
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142.39
146.90
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135.30
129.65
129.65
128.87
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127.51
123.58
123.58

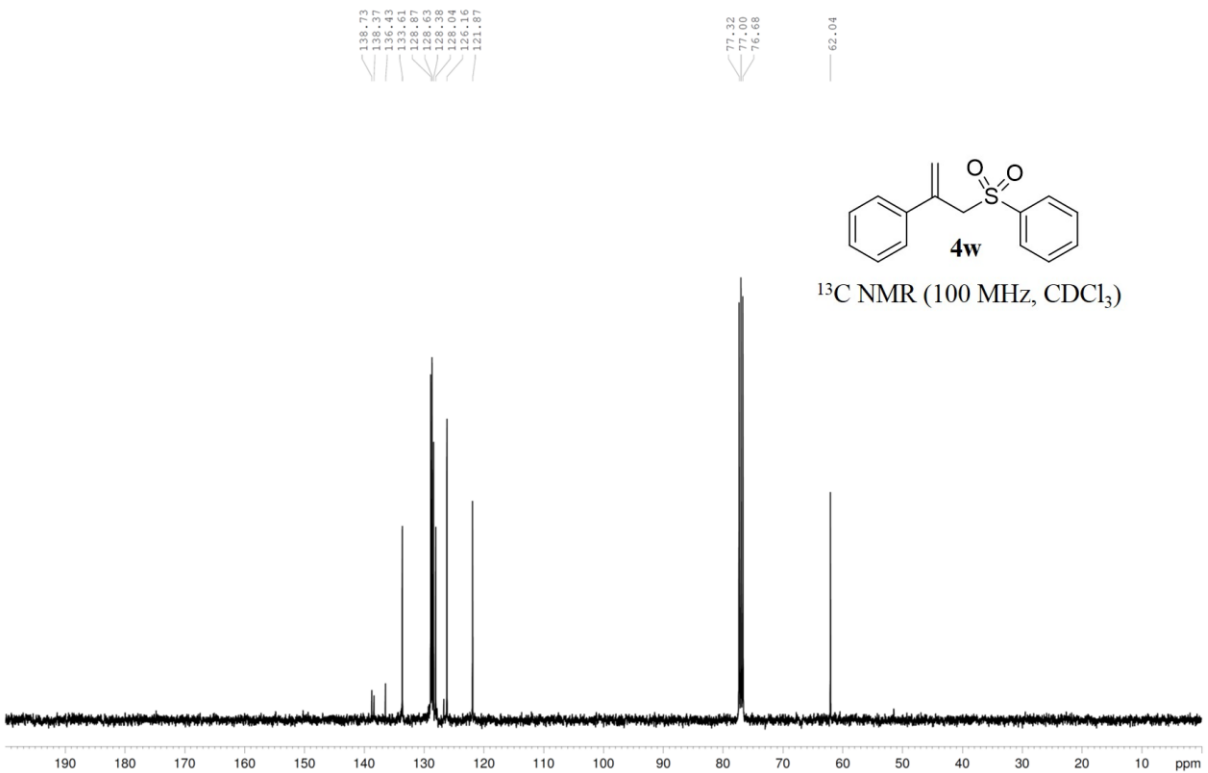
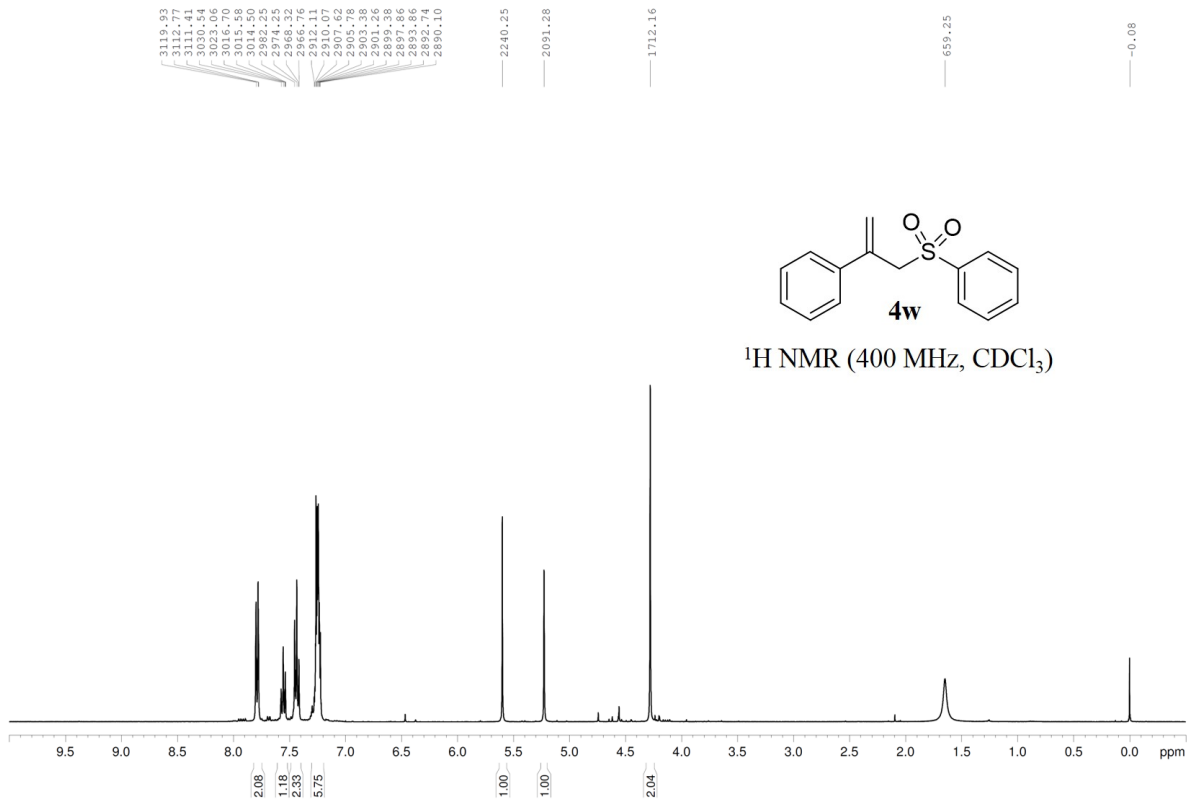
77.32
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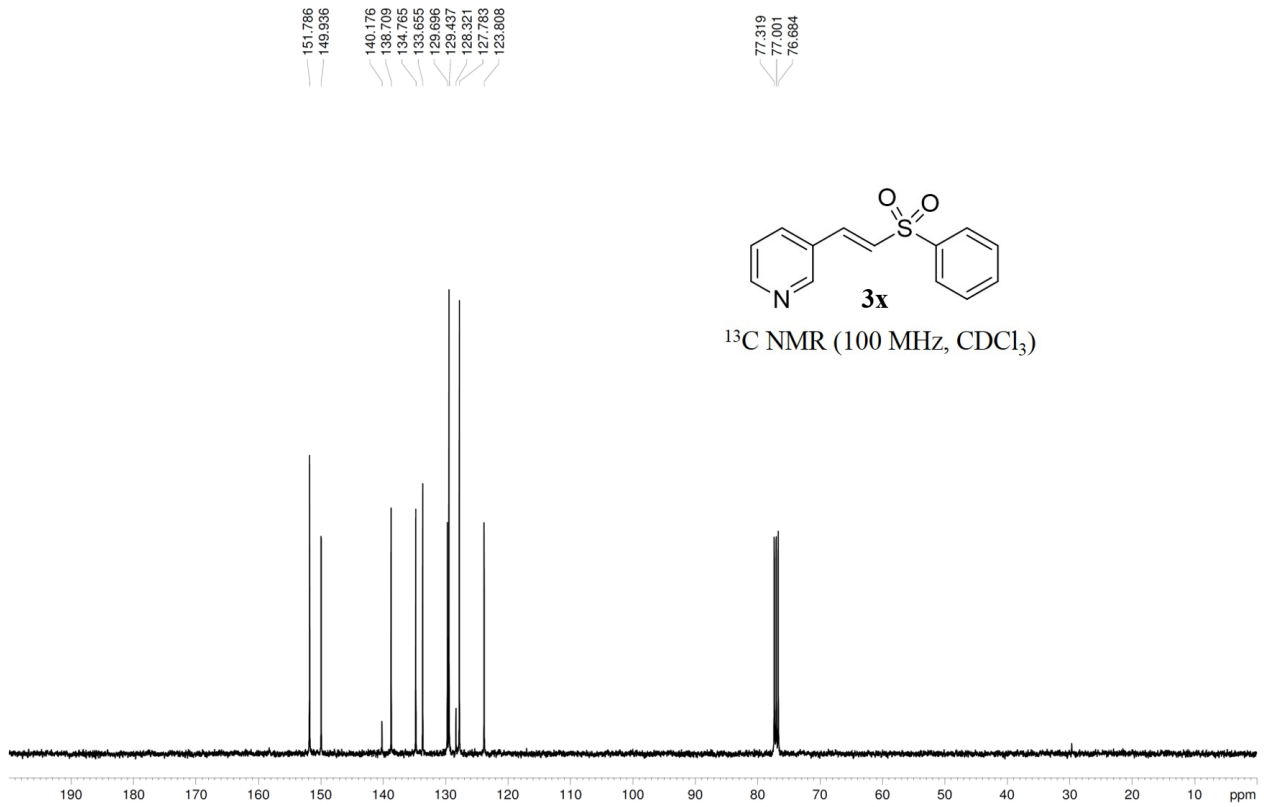
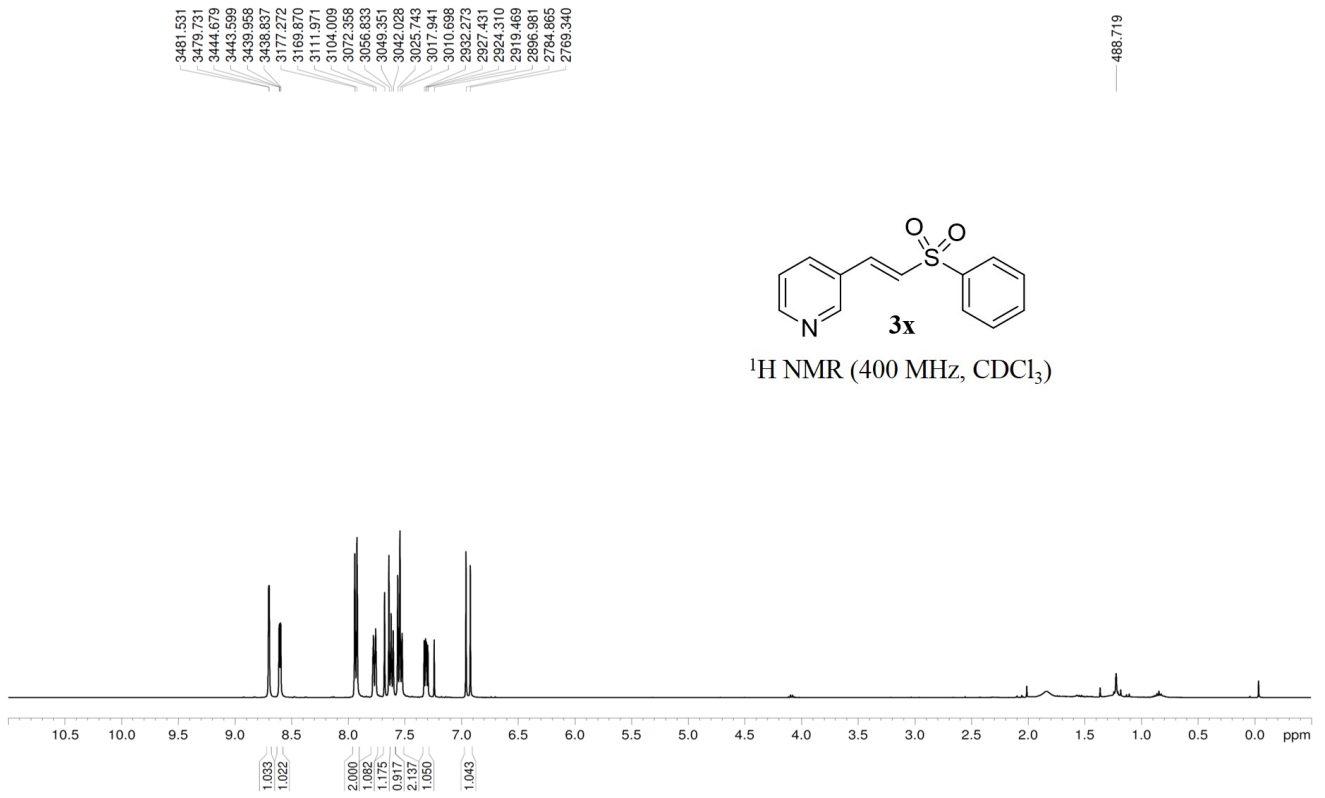


$^{13}\text{C NMR}$ (100 MHz, CDCl_3)





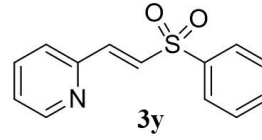




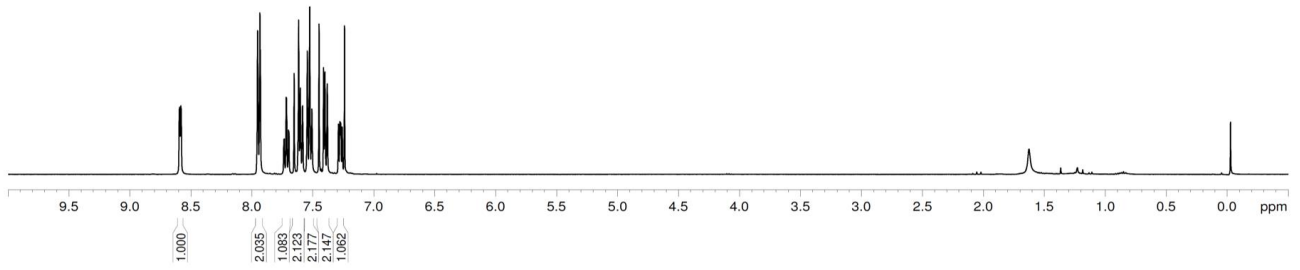
3438.317
3433.876
3181.954
3174.512
3096.206
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3047.390
3041.868
3034.546
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3004.056
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650.491

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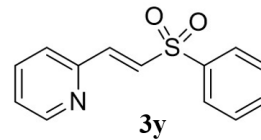


$^1\text{H NMR}$ (400 MHz, CDCl_3)

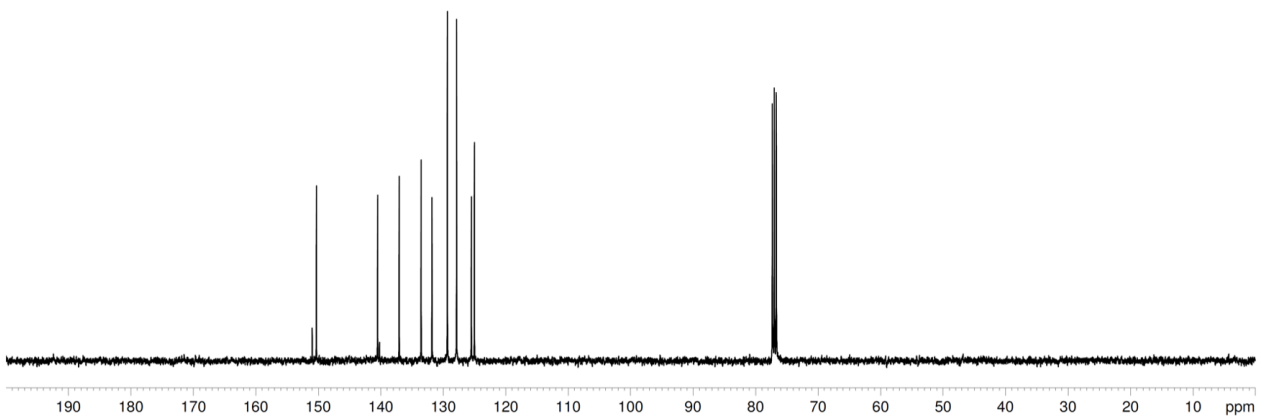


150.972
150.295
140.503
140.190
137.047
133.536
131.805
129.340
127.864
125.481
125.005

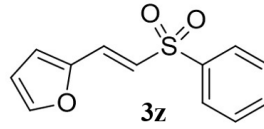
77.320
77.002
76.685



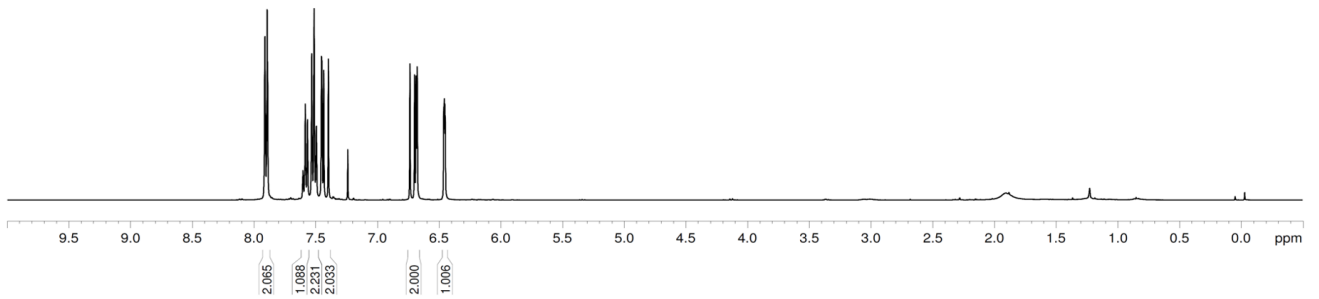
$^{13}\text{C NMR}$ (100 MHz, CDCl_3)



3165.709
3156.226
3156.866
3042.349
3034.986
3032.865
3027.664
3013.659
3005.857
2998.734
2981.969
2980.929
2974.847
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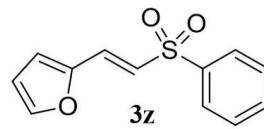


$^1\text{H NMR}$ (400 MHz, CDCl_3)

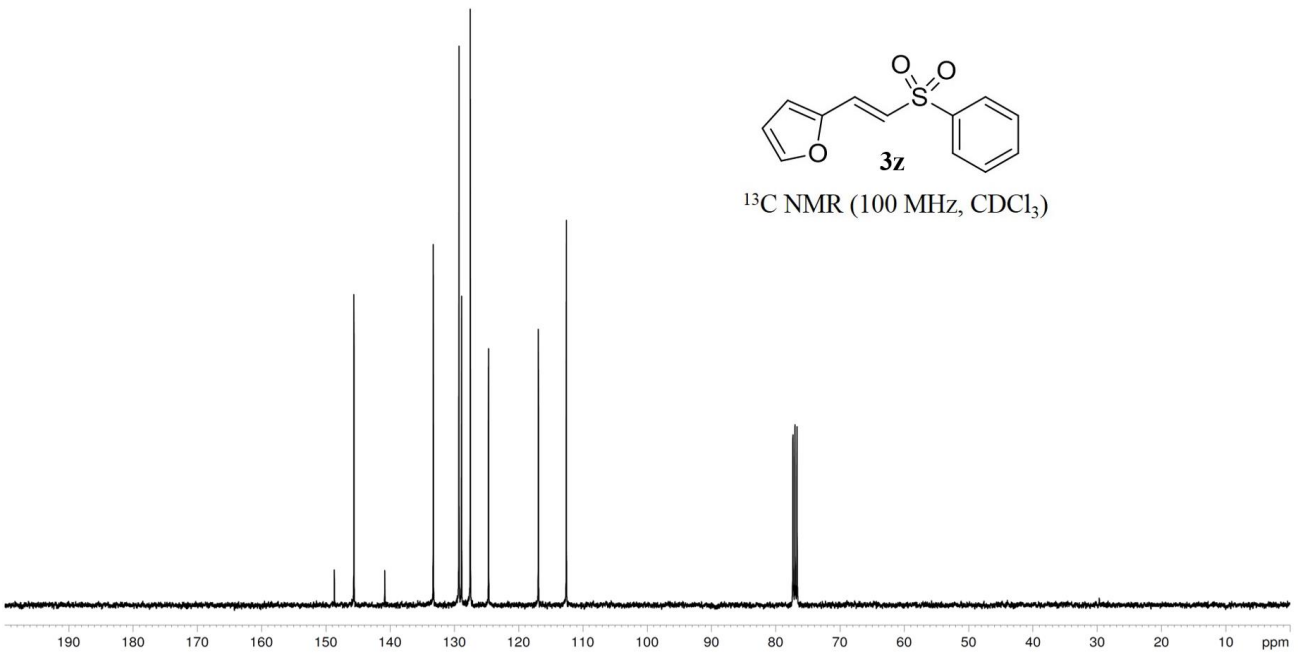


148.669
145.631
140.826
133.270
129.274
128.867
127.510
124.682
116.925
112.560

77.319
77.002
76.684

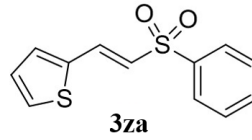


$^{13}\text{C NMR}$ (100 MHz, CDCl_3)

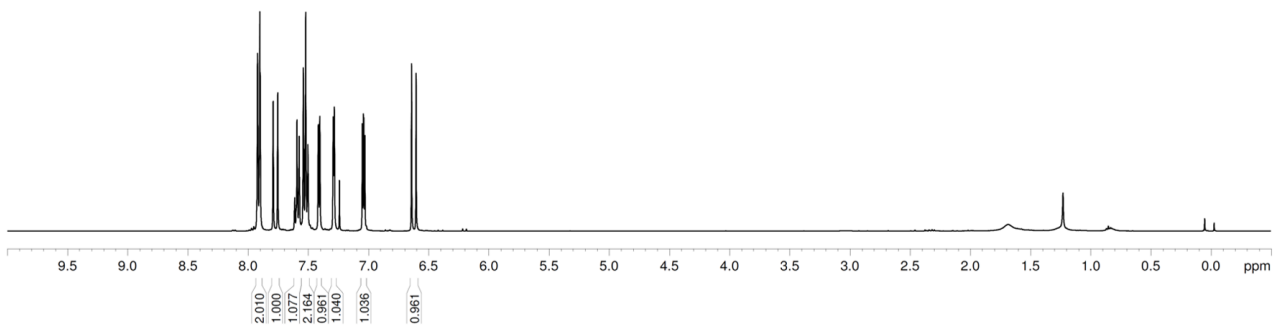


3169.030
3161.787
3160.347
3117.213
3102.088
3045.630
3044.429
3040.708
3038.267
3036.107
3032.105
3030.905
3029.664
3017.060
3010.498
3009.258
3003.656
3002.136
2967.164
2962.082
2917.508
2913.947
2896.781
2881.077
2817.355
2816.035
2812.314
2657.183
2642.059

491.440

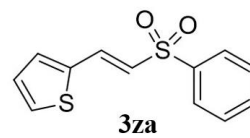


$^1\text{H NMR}$ (400 MHz, CDCl_3)

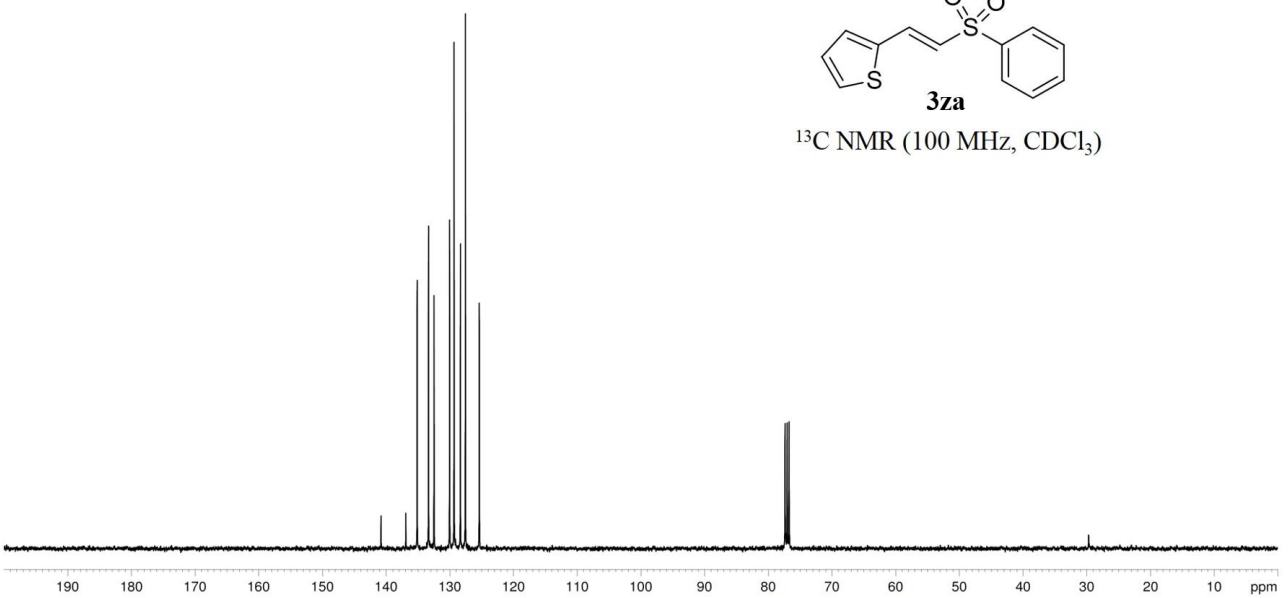


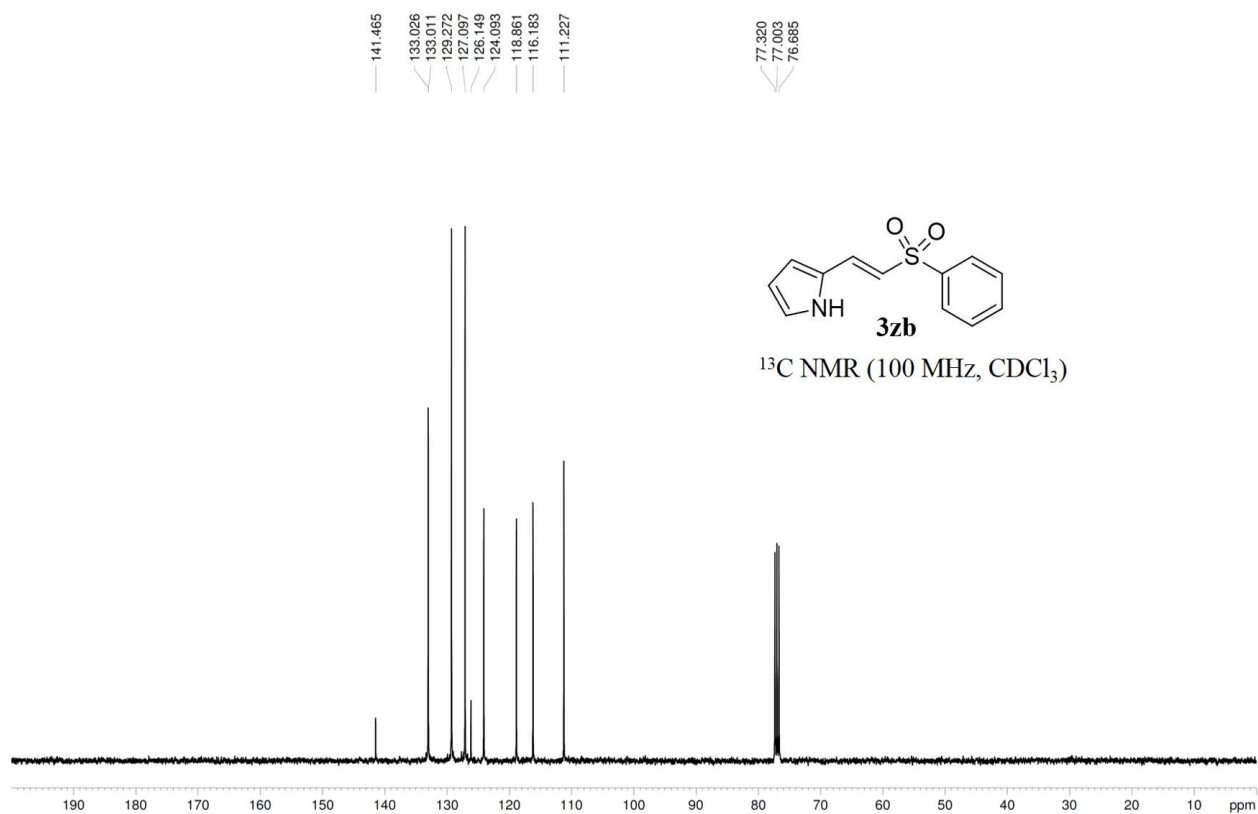
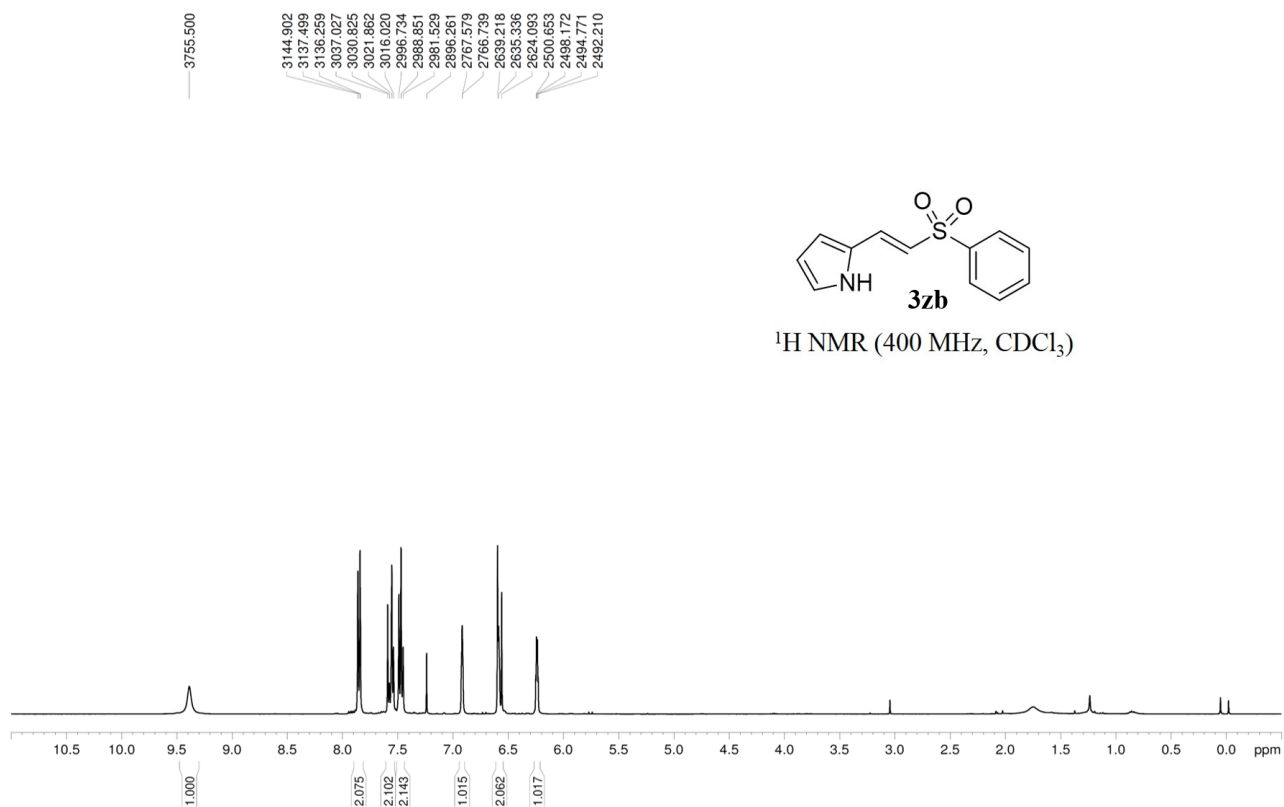
140.760
136.880
135.092
133.312
132.442
129.997
128.295
127.524
125.329

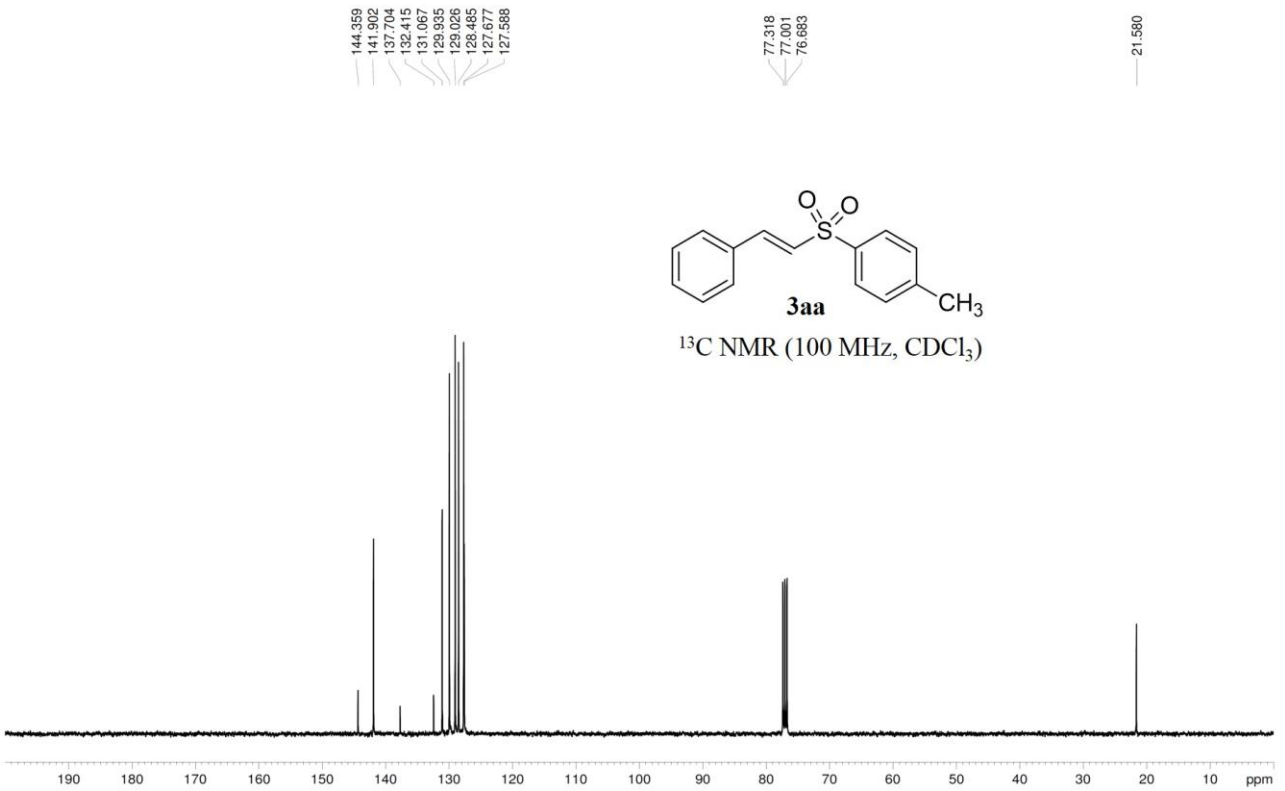
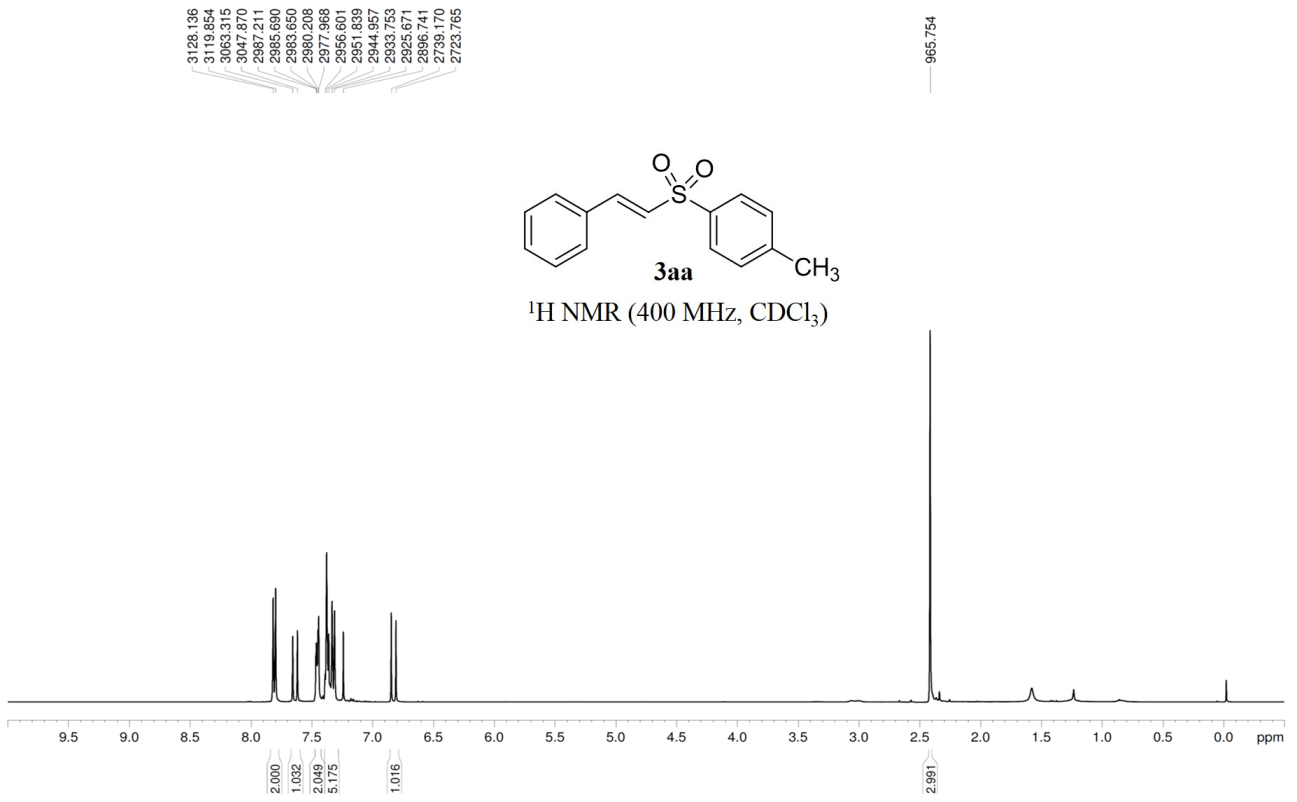
77.320
77.002
76.685



$^{13}\text{C NMR}$ (100 MHz, CDCl_3)



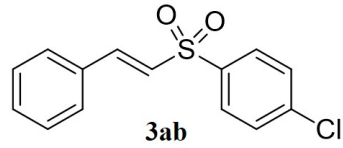




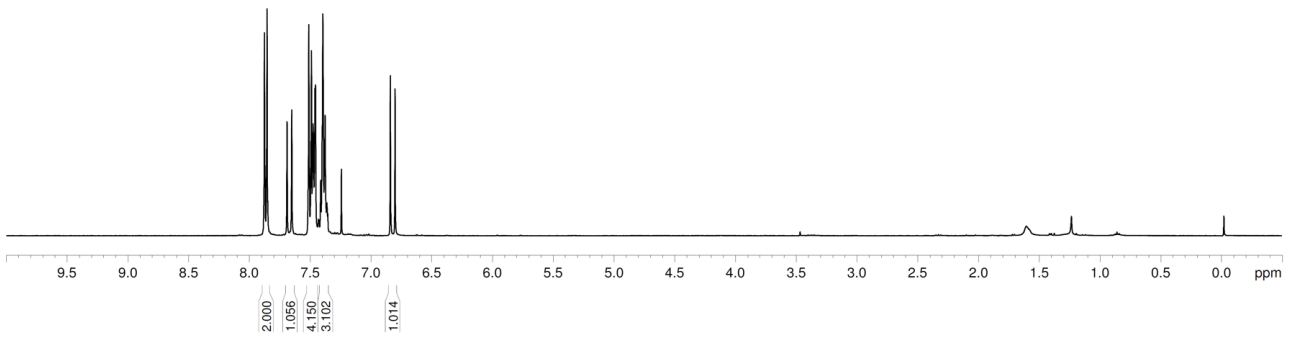
3150.744
3148.943
3142.141
3139.780
3076.320
3060.915
3004.736
2996.134
2991.812
2990.532
2984.530
2982.649
2972.766
2971.005
2965.484
2958.561
2950.919
2944.757
2942.116
2887.301
2736.009
2720.604

493.200

-9.003

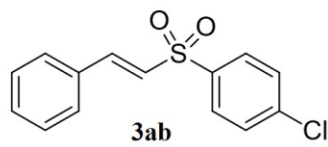


$^1\text{H NMR}$ (400 MHz, CDCl_3)



143.035
140.078
139.218
132.144
131.397
129.643
129.124
128.614
126.809

77.321
77.003
76.685



$^{13}\text{C NMR}$ (100 MHz, CDCl_3)

