Supporting Information

Synthesis of Pyrazoline-Derived *N*-Vinyl Nitrones through An Unexpected Selective [3+2] Cycloaddition

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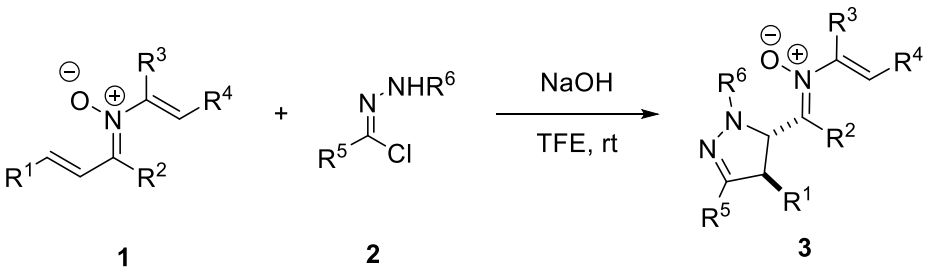
Contents

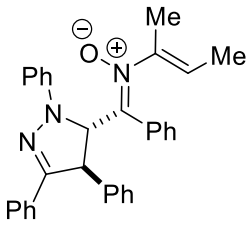
1. General Experimental Information:

^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature using 400 MHz and 600 MHz spectrometers. The data are reported as follows: chemical shift in ppm from internal tetramethylsilane on the δ scale, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), and integration. High resolution mass spectra were acquired on an LTQ FT spectrometer, and were obtained by peak matching. Melting points are reported uncorrected. Analytical thin layer chromatography was performed on 0.25 mm extra hard silica gel plates with UV254 fluorescent indicator. Chromatography was performed using with 300-400 mesh silica gel (SiO_2). Unless otherwise noted, all reagents and solvents were obtained from commercial sources and, where appropriate, purified prior to use. *N*-Vinyl-*α*,*β*-unsaturated nitrones **1a-1v**[1,2], hydrazonoyl chlorides **2a-2s**[3,4] and allenoate[5] were prepared according to the literature methods and their spectral data matched literature values.

2. Synthesis of pyrazoline-derived *N*-vinyl nitrones 3

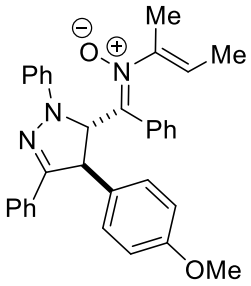


General procedure A: In a Teflon-sealed flask was charged with *N*-vinyl-*α*,*β*-unsaturated nitrones **1** (0.2 mmol), hydrazonoyl chlorides **2** (0.4 mmol, 2.0 equiv.), NaOH (0.0240 g, 0.6 mmol, 3.0 equiv.). Then, TFE (2.0 mL) was added via syringe. The reaction vessel was sealed with a Teflon cap and stirred at room temperature for 5-24 h until the substrate **1** consumed (monitored by TLC). At this time, the solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (the crude residue was dry loaded on silica gel, eluents with a mixed eluents petroleum ether/ethyl acetate = 2/1) to afford compounds **3**.



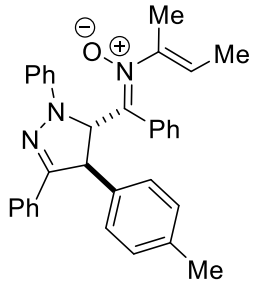
3aa (*Z*/*E* = 20:1)

(*Z*)-N-((*E*)-but-2-en-2-yl)-1-phenyl-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3aa). A yellow solid, R_f = 0.3, 66 mg, 70% yield; M.p: 117-118 °C, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44–7.43 (m, 2H), 7.27–7.26 (m, 2H), 7.22–7.12 (m, 8H), 7.08–7.02 (m, 5H), 6.87–6.85 (m, 2H), 6.75–6.72 (m, 1H), 6.02 (d, *J* = 3.0 Hz, 1H), 5.28–5.23 (m, 1H), 4.58 (d, *J* = 3.0 Hz, 1H), 1.85 (s, 3H), 1.31 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.0, 148.9, 143.6, 141.7, 139.3, 131.7, 131.6, 129.2, 129.1, 129.0, 128.8, 128.3, 128.0, 127.7, 127.5, 126.1, 123.8, 119.3, 112.8, 67.9, 56.9, 14.9, 12.3; HRMS (ESI) m/z calcd for $C_{32}H_{30}N_3O$ $[M + H]^+$: 472.2383; found: 472.2383.



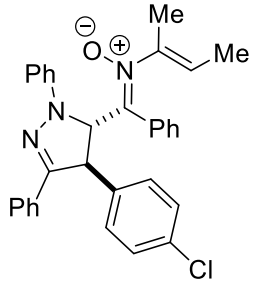
3ba (*Z*/*E* > 20:1)

(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(4-(4-methoxyphenyl)-1,3-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ba). Yellow oil, R_f = 0.3, 40 mg, 40% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.51–7.50 (m, 2H), 7.32–7.28 (m, 2H), 7.25–7.21 (m, 5H), 7.18–7.12 (m, 3H), 7.09–7.07 (m, 2H), 7.04–7.02 (m, 2H), 6.89–6.82 (m, 3H), 5.97 (d, *J* = 2.8 Hz, 1H), 5.33–5.28 (m, 1H), 5.06 (d, *J* = 2.4 Hz, 1H), 3.69 (s, 3H), 1.80 (s, 3H), 1.30 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.5, 150.9, 146.0, 143.4, 141.2, 132.3, 131.6, 131.1, 129.5, 129.4, 129.0, 128.9, 128.5, 127.9, 126.0, 122.3, 119.2, 115.2, 114.4, 112.2, 66.7, 55.0, 54.1, 14.5, 11.8. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O_2$ $[M + H]^+$: 502.2489; found: 502.2480.



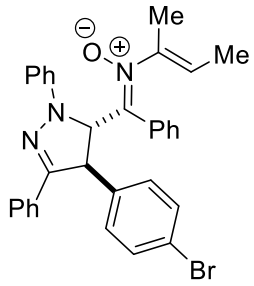
3ca (*Z*/*E* = 10:1)

(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(1,3-diphenyl-4-(p-tolyl)-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ca). A yellow solid, R_f = 0.3, 41 mg, 42% yield; M.p: 173-174 ℃, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44–7.42 (m, 2H), 7.17–7.11 (m, 7H), 7.07–7.00 (m, 7H), 6.86–6.85 (m, 2H), 6.74–6.71 (m, 1H), 6.00 (d, *J* = 3.0 Hz, 1H), 5.26–5.22 (m, 1H), 4.55 (d, *J* = 3.0 Hz, 1H), 2.20 (s, 3H), 1.84 (s, 3H), 1.30 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.1, 148.9, 143.6, 141.7, 137.1, 136.4, 131.8, 131.7, 129.7, 129.2, 129.0, 128.8, 128.3, 128.2, 128.0, 127.5, 126.1, 123.7, 119.2, 112.8, 68.0, 56.5, 21.1, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O$ $[M + H]^+$: 486.2540; found: 486.2541.



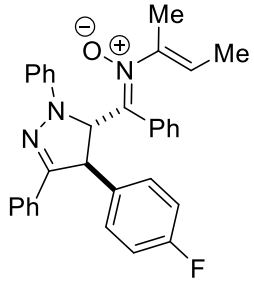
3da (*Z*/*E* = 10:1)

(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(4-(4-chlorophenyl)-1,3-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3da). Yellow oil, R_f = 0.3, 56 mg, 56% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44–7.42 (m, 2H), 7.23–7.21 (m, 2H), 7.18–7.12 (m, 7H), 7.09–7.06 (m, 1H), 7.04–7.00 (m, 4H), 6.84–6.81 (m, 2H), 6.74–6.71 (m, 1H), 5.93 (d, *J* = 3.0 Hz, 1H), 5.28–5.24 (m, 1H), 4.58 (d, *J* = 3.0 Hz, 1H), 1.85 (s, 3H), 1.31 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.6, 149.2, 143.4, 141.6, 137.9, 133.4, 131.4, 131.3, 129.2, 129.1, 128.7, 128.5, 128.4, 128.0, 126.0, 123.9, 119.4, 112.8, 68.1, 56.2, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{32}H_{29}ClN_3O$ $[M + H]^+$: 506.1994; found: 506.1982.



3ea (*Z*/*E* = 10:1)

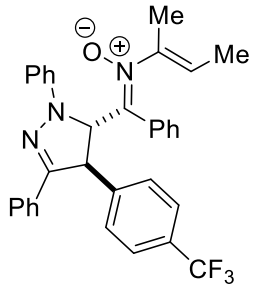
(*Z*)-1-(4-(4-bromophenyl)-1,3-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-*N*-((*E*)-but-2-en-2-yl)-1-phenylmethanimine oxide (3ea). Yellow oil, R_f = 0.3, 67 mg, 61% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44–7.42 (m, 2H), 7.34–7.32 (m, 2H), 7.17–7.12 (m, 7H), 7.06–7.04 (m, 1H), 7.02–6.99 (m, 4H), 6.84–6.82 (m, 2H), 6.74–6.71 (m, 1H), 5.93 (d, *J* = 3.0 Hz, 1H), 5.28–5.24 (m, 1H), 4.56 (d, *J* = 3.0 Hz, 1H), 1.85 (s, 3H), 1.31 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.5, 149.2, 143.4, 141.6, 138.4, 132.1, 131.4, 131.3, 129.5, 129.2, 128.7, 128.5, 128.4, 128.1, 128.0, 126.0, 123.9, 121.5, 119.4, 112.8, 68.1, 56.3, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{32}H_{29}BrN_3O$ $[M + H]^+$: 550.1489; found: 550.1472.



3fa (*Z*/*E* = 10:1)

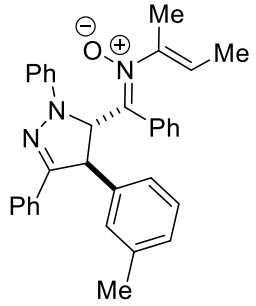
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(4-(4-fluorophenyl)-1,3-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3fa). Yellow oil, R_f = 0.3, 60 mg, 62% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44–7.43 (m, 2H), 7.26–7.24 (m, 2H), 7.18–7.13 (m, 5H), 7.09–7.06 (m, 1H), 7.04–7.01 (m, 4H), 6.91–6.87 (m, 2H), 6.84–6.83 (m, 2H), 6.74–6.71 (m, 1H), 5.94 (d, *J* = 3.0 Hz, 1H), 5.28–5.24 (m, 1H), 4.59 (d, *J* = 3.0 Hz, 1H), 1.85 (s, 3H), 1.31 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.1 (d, *J* = 244.5 Hz), 149.9, 149.3, 143.5, 141.6, 135.1 (d, *J* = 3.0 Hz), 131.5, 131.4, 129.4 (d, *J* = 8.0 Hz), 129.2, 129.1, 128.7, 128.4, 128.3, 128.0, 126.0, 123.9, 119.4, 116.0 (d, *J* = 21.6 Hz), 112.8, 68.2, 56.1, 14.9, 12.3; ^{19}F NMR (470 MHz, $CDCl_3$) δ -114.8. HRMS

(ESI) m/z calcd for $C_{32}H_{29}FN_3O$ $[M + H]^+$: 490.2289; found: 490.2280.



3ga (Z/E = 7:1)

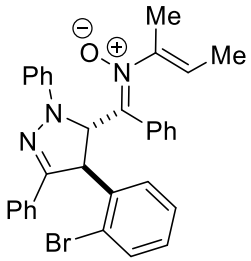
(*Z*)-N-((*E*)-but-2-en-2-yl)-1-(1,3-diphenyl-4-(4-(trifluoromethyl)phenyl)-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ga). Yellow oil, R_f = 0.3, 69 mg, 64% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49–7.41 (m, 6H), 7.18–7.11 (m, 5H), 7.07–7.06 (m, 1H), 7.04–6.98 (m, 4H), 6.84–6.83 (m, 2H), 6.74–6.71 (m, 1H), 5.93 (d, J = 3.0 Hz, 1H), 5.29–5.25 (m, 1H), 4.66 (d, J = 3.0 Hz, 1H), 1.86 (s, 3H), 1.32 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.3, 149.3, 141.6, 131.3, 131.2, 129.9 (q, J = 32.5 Hz), 129.2, 129.1, 128.7, 128.6, 128.5, 128.1, 128.0, 126.8, 126.0 (q, J = 4.0 Hz), 125.9, 125.1 (q, J = 270.1 Hz), 124.0, 119.6, 112.8, 68.2, 56.5, 14.9, 12.3; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.5. HRMS (ESI) m/z calcd for $C_{33}H_{29}F_3N_3O$ $[M + H]^+$: 540.2257; found: 540.2249.



3ha (*Z*/*E* = 17:1)

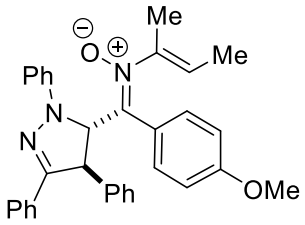
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(1,3-diphenyl-4-(m-tolyl)-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ha). A yellow solid, R_f = 0.3, 68 mg, 70% yield; M.p: 134-135 °C, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43–7.42 (m, 2H), 7.18–7.01 (m, 13H), 6.96–6.94 (m, 1H), 6.85–6.84 (m, 2H), 6.75–6.72 (m, 1H), 6.03 (d, J = 3.0 Hz, 1H), 5.26–5.22 (m, 1H), 4.53 (d, J = 3.0 Hz, 1H), 2.21 (s, 3H), 1.84 (s, 3H), 1.29 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.1, 148.8, 143.6, 141.7, 139.2, 138.7,

131.8, 131.6, 129.2, 129.0, 128.9, 128.8, 128.7, 128.4, 128.3, 128.2, 127.9, 126.1, 124.7, 123.7, 119.2, 112.8, 67.8, 56.8, 21.4, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O$ $[M + H]^+$: 486.2540; found: 486.2532.



3ia (Z/E = 8:1)

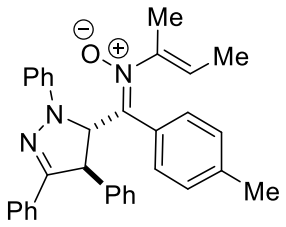
(*Z*)-1-(4-(2-bromophenyl)-1,3-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-N-((*E*)-but-2-en-2-yl)-1-phenylmethanimine oxide (3ia). A yellow solid, R_f = 0.3, 62 mg, 64% yield; M.p: 180-181 °C, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56–7.55 (m, 1H), 7.31–7.26 (m, 6H), 7.10–7.07 (m, 6H), 7.03–6.99 (m, 4H), 6.92–6.90 (m, 1H), 6.83–6.81 (m, 1H), 6.14 (d, J = 2.0 Hz, 1H), 5.23–5.19 (m, 1H), 5.06 (d, J = 3.5 Hz, 1H), 1.83 (s, 3H), 1.28 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.4, 145.6, 143.5, 141.6, 138.9, 133.0, 131.6, 131.1, 129.5, 129.2, 129.1, 128.9, 128.7, 128.5, 128.29, 128.26, 128.22, 125.9, 123.8, 123.4, 119.6, 113.0, 65.8, 55.1, 14.9, 12.2. HRMS (ESI) m/z calcd for $C_{32}H_{29}BrN_3O$ $[M + H]^+$: 550.1489; found: 550.1478.



3ja (*Z*/*E* = 14:1)

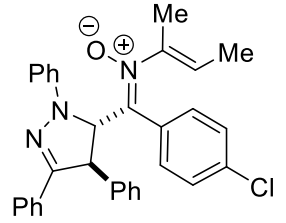
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(4-methoxyphenyl)-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3ja). Yellow oil, R_f = 0.2, 57 mg, 57% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46–7.45 (m, 2H), 7.27–7.25 (m, 2H), 7.22–7.13 (m, 8H), 7.06–7.05 (m, 2H), 6.79–6.78 (m, 2H), 6.75–6.72 (m, 1H), 6.56–6.55 (m, 2H), 5.99 (d, J = 3.0 Hz, 1H), 5.30–5.26 (m, 1H), 4.56 (d, J = 3.5 Hz, 1H), 3.60 (s, 3H), 1.83 (s, 3H), 1.35 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.8, 149.9, 148.7, 143.6, 141.9, 139.4, 131.8, 130.2, 129.2, 129.0, 128.3, 128.2, 127.7, 127.5, 126.1, 123.7, 123.5,

119.2, 113.5, 112.8, 68.0, 56.9, 55.1, 14.9, 12.4. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O_2$ $[M + H]^+$: 502.2489; found: 502.2481.



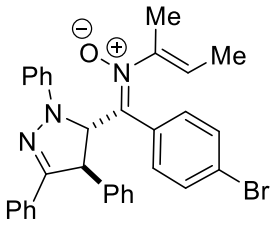
3ka (*Z*/*E* > 20:1)

(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(p-tolyl)-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3ka). Yellow oil, R_f = 0.3, 59 mg, 61% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43–7.42 (m, 2H), 7.28–7.27 (m, 2H), 7.22–7.12 (m, 8H), 7.05–7.03 (m, 2H), 6.89–6.85 (m, 2H), 6.74–6.71 (m, 3H), 6.02 (d, *J* = 3.5 Hz, 1H), 5.28 (q, *J* = 7.0 Hz, 1H), 4.57 (d, *J* = 3.5 Hz, 1H), 2.11 (s, 3H), 1.83 (s, 3H), 1.32 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.9, 149.0, 143.6, 141.8, 139.4, 139.0, 131.8, 129.2, 129.0, 128.7, 128.6, 128.5, 128.3, 127.7, 127.5, 126.1, 123.5, 119.2, 113.5, 112.8, 68.0, 56.9, 21.2, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O$ $[M + H]^+$: 486.2540; found: 486.2534.



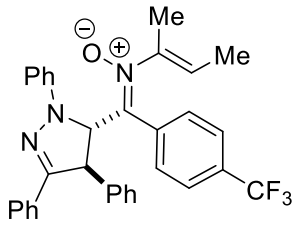
3la (*Z*/*E* = 13:1)

(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(4-chlorophenyl)-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3la). Yellow oil, R_f = 0.3, 68 mg, 67% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46–7.45 (m, 2H), 7.27–7.25 (m, 2H), 7.22–7.19 (m, 2H), 7.17–7.14 (m, 6H), 7.02–7.00 (m, 4H), 6.78–6.72 (m, 3H), 5.96 (d, *J* = 3.0 Hz, 1H), 5.27 (q, *J* = 6.5 Hz, 1H), 4.56 (d, *J* = 3.0 Hz, 1H), 1.84 (s, 3H), 1.34 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.1, 148.0, 143.5, 141.7, 139.1, 135.2, 131.6, 130.2, 130.1, 129.2, 129.1, 128.5, 128.4, 128.3, 127.6, 127.5, 126.1, 124.0, 119.5, 112.7, 68.1, 57.0, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{32}H_{29}ClN_3O$ $[M + H]^+$: 506.1994; found: 506.1983.



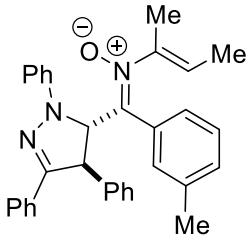
3ma (*Z*/*E* = 15:1)

(*Z*)-1-(4-bromophenyl)-*N*-((*E*)-but-2-en-2-yl)-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3ma). Yellow oil, R_f = 0.3, 67 mg, 61% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47–7.45 (m, 2H), 7.27–7.26 (m, 2H), 7.23–7.20 (m, 2H), 7.18–7.14 (m, 8H), 7.01–6.99 (m, 2H), 6.76–6.70 (m, 3H), 5.96 (d, *J* = 3.0 Hz, 1H), 5.28–5.24 (m, 1H), 4.56 (d, *J* = 3.0 Hz, 1H), 1.85 (s, 3H), 1.35 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.1, 148.1, 143.5, 141.7, 139.1, 132.0, 131.6, 131.3, 130.6, 130.4, 129.3, 129.1, 128.5, 128.4, 127.7, 126.1, 124.1, 123.6, 119.5, 112.8, 68.1, 57.0, 14.9, 12.4. HRMS (ESI) m/z calcd for $C_{32}H_{29}BrN_3O$ $[M + H]^+$: 550.1489; found: 550.1471.



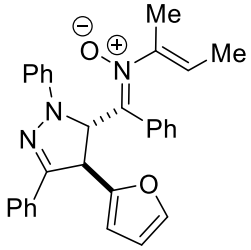
3na (*Z*/*E* = 13:1)

(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(4-(trifluoromethyl)phenyl)-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3na). Yellow oil, R_f = 0.3, 78 mg, 72% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44–7.43 (m, 2H), 7.29–7.27 (m, 4H), 7.23–7.20 (m, 2H), 7.17–7.12 (m, 6H), 6.99–6.95 (m, 4H), 6.75–6.72 (m, 1H), 5.98 (d, *J* = 3.0 Hz, 1H), 5.27 (q, *J* = 7.0 Hz, 1H), 4.57 (d, *J* = 2.5 Hz, 1H), 1.86 (s, 3H), 1.31 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.3, 147.9, 143.4, 141.7, 138.9, 135.4, 131.5, 131.1 (q, *J* = 32.6 Hz), 129.4, 129.3, 129.1, 128.6, 128.4, 127. 7, 127.6, 126.1, 124.9 (q, *J* = 3.5 Hz), 124.6 (q, *J* = 270.6 Hz), 124.4, 119.6, 112.8, 68.2, 57.0, 14.9, 12.3; ^{19}F NMR (470 MHz, $CDCl_3$) δ -63.0. HRMS (ESI) m/z calcd for $C_{33}H_{29}F_3N_3O$ $[M + H]^+$: 540.2257; found: 540.2247.



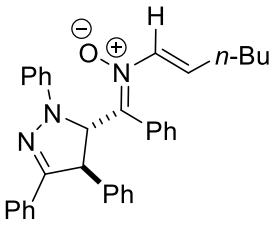
3oa (*Z*/*E* > 20:1)

(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(m-tolyl)-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3oa). Yellow oil, R_f = 0.3, 59 mg, 61% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43–7.42 (m, 2H), 7.28–7.27 (m, 2H), 7.22–7.19 (m, 2H), 7.17–7.12 (m, 6H), 7.05–7.03 (m, 2H), 6.91–6.85 (m, 2H), 6.74–6.71 (m, 1H), 6.62–6.60 (m, 2H), 6.02 (d, J = 3.0 Hz, 1H), 5.28 (q, J = 6.5 Hz, 1H), 4.57 (d, J = 2.5 Hz, 1H), 2.01 (s, 3H), 1.84 (s, 3H), 1.31 (d, J = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.0, 149.1, 143.7, 141.6, 139.3, 137.5, 131.8, 131.5, 129.8, 129.4, 129.1, 129.0, 128.3, 127.8, 127.7, 127.5, 126.0, 125.9, 123.5, 119.2, 112.9, 68.0, 56.8, 21.1, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O$ $[M + H]^+$: 486.2540; found: 486.2534.



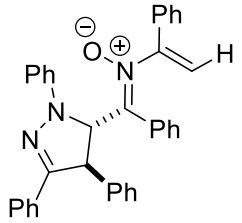
3pa (*Z*/*E* > 20:1)

(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(4-(furan-2-yl)-1,3-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3pa). A yellow oil, R_f = 0.3, 41 mg, 44% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.56–7.55 (m, 3H), 7.33–7.23 (m, 5H), 7.18–7.10 (m, 5H), 7.03–7.01 (m, 2H), 6.88–6.85 (m, 1H), 6.41–6.35 (m, 2H), 6.24 (d, J = 3.5 Hz, 1H), 5.33 (d, J = 3.5 Hz, 1H), 5.31–5.27 (m, 1H), 1.79 (s, 3H), 1.29 (d, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 151.8, 147.2, 145.1, 143.2, 142.9, 141.2, 131.3, 130.9, 129.5, 129.0, 128.6, 128.5, 128.0, 125.8, 122.4, 119.4, 115.2, 112.2, 110.8, 107.8, 63.3, 48.2, 14.5, 11.8. HRMS (ESI) m/z calcd for $C_{30}H_{28}N_3O_2$ $[M + H]^+$: 462.2176; found: 462.2159.



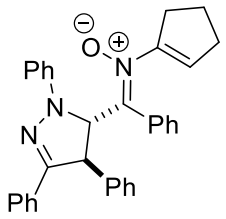
3qa (Z/E > 20:1)

(*Z*)-*N*-((*E*)-hex-1-en-1-yl)-1-phenyl-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3qa). Yellow oil, R_f = 0.4, 28 mg, 28% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.55–7.53 (m, 2H), 7.32–7.22 (m, 15H), 7.05–7.03 (m, 2H), 6.83–6.74 (m, 2H), 6.52–6.50 (m, 1H), 6.12 (brs, 1H), 5.16 (d, J = 3.0 Hz, 1H), 2.01–1.97 (m, 2H), 1.26–1.16 (m, 4H), 0.79–0.76 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 150.8, 146.2, 143.4, 140.4, 131.4, 131.3, 131.0, 130.1, 129.8, 129.5, 129.3, 129.0, 128.4, 128.3, 127.6, 127.4, 126.0, 120.3, 119.1, 112.1, 67.5, 55.3, 30.1, 27.8, 21.5, 13.6. HRMS (ESI) m/z calcd for $C_{34}H_{34}N_3O$ $[M + H]^+$: 500.2696; found: 500.2664.



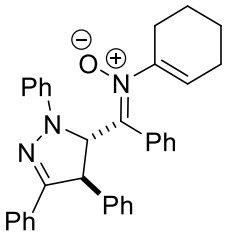
3ra (*Z*/*E* > 20:1)

(*Z*)-1-phenyl-*N*-(1-phenylvinyl)-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3ra). Yellow oil, R_f = 0.3, 69 mg, 67% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44–7.43 (m, 2H), 7.31–7.28 (m, 4H), 7.24–7.19 (m, 6H), 7.17–7.16 (m, 2H), 7.12–7.09 (m, 5H), 7.01–6.98 (m, 1H), 6.88–6.85 (m, 2H), 6.76–6.73 (m, 1H), 6.71–6.69 (m, 2H), 6.16 (d, J = 3.5 Hz, 1H), 5.32 (brs, 1H), 5.06 (brs, 1H), 4.70 (d, J = 3.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 151.2, 149.8, 143.6, 139.1, 133.3, 131.6, 130.8, 129.27, 129.22, 129.20, 129.1, 128.8, 128.6, 128.3, 128.2, 127.8, 127.7, 127.6, 126.1, 125.5, 119.5, 113.0, 111.0, 68.1, 57.1. HRMS (ESI) m/z calcd for $C_{36}H_{30}N_3O$ $[M + H]^+$: 520.2383; found: 520.2370.



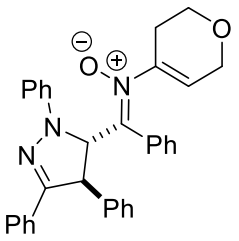
3sa (*Z*/*E* > 20:1)

(*Z*)-*N*-(cyclopent-1-en-1-yl)-1-phenyl-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3sa). Yellow oil, R_f = 0.3, 53 mg, 55% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.55–7.53 (m, 2H), 7.33–7.27 (m, 6H), 7.24–7.14 (m, 7H), 7.10–7.08 (m, 4H), 6.86–6.83 (m, 1H), 6.05 (d, J = 2.4 Hz, 1H), 5.47–5.41 (m, 1H), 5.11 (d, J = 2.4 Hz, 1H), 2.46–2.43 (m, 1H), 2.34–2.30 (m, 1H), 2.09–1.99 (m, 2H), 1.71–1.66 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 150.7, 147.4, 146.3, 143.3, 140.4, 131.1, 131.0, 129.4, 129.3, 129.03, 129.00, 128.5, 128.4, 127.9, 127.5, 127.4, 127.0, 126.0, 119.2, 112.2, 67.0, 55.0, 32.0, 29.9, 21.6. HRMS (ESI) m/z calcd for $C_{33}H_{30}N_3O$ [M + H]$^+$: 484.2383; found: 484.2371.



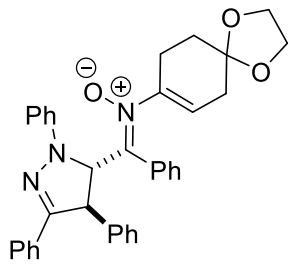
3ta (*Z*/*E* > 20:1)

(*Z*)-*N*-(cyclohex-1-en-1-yl)-1-phenyl-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3ta). Yellow oil, R_f = 0.3, 66 mg, 67% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45–7.44 (m, 2H), 7.28–7.27 (m, 2H), 7.22–7.19 (m, 2H), 7.17–7.12 (m, 6H), 7.07–7.02 (m, 5H), 6.88–6.86 (m, 2H), 6.74–6.71 (m, 1H), 6.01 (d, J = 3.5 Hz, 1H), 5.43–5.39 (m, 1H), 4.60 (d, J = 3.0 Hz, 1H), 2.26–2.21 (m, 2H), 1.73–1.72 (m, 2H), 1.49–1.46 (m, 2H), 1.30–1.27 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.0, 149.2, 144.0, 143.6, 139.3, 131.8, 131.6, 129.2, 129.1, 129.0, 128.8, 128.3, 127.9, 127.7, 127.5, 126.1, 125.9, 119.2, 112.8, 68.0, 56.9, 26.7, 23.8, 21.8, 20.9. HRMS (ESI) m/z calcd for $C_{34}H_{32}N_3O$ [M + H]$^+$: 498.2540; found: 498.2549.



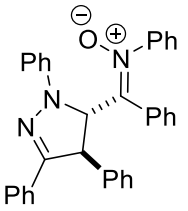
3ua (*Z*/*E* > 20:1)

(*Z*)-*N*-(3,6-dihydro-2H-pyran-4-yl)-1-phenyl-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3ua). Yellow oil, R_f = 0.3, 50 mg, 50% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45–7.43 (m, 2H), 7.28–7.26 (m, 2H), 7.23–7.20 (m, 2H), 7.18–7.10 (m, 7H), 7.08–7.04 (m, 4H), 6.89–6.88 (m, 2H), 6.75–6.72 (m, 1H), 6.02 (d, *J* = 3.0 Hz, 1H), 5.47–5.44 (m, 1H), 4.60 (d, *J* = 3.0 Hz, 1H), 3.85 (d, *J* = 2.0 Hz, 2H), 3.63–3.61 (m, 2H), 2.36–2.30 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.8, 135.4, 142.6, 141.7, 139.1, 132.0, 131.4, 129.3, 129.1, 128.7, 128.6, 128.4, 128.2, 128.1, 127.7, 127.6, 126.2, 123.9, 114.4, 111.3, 67.8, 57.0, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{33}H_{30}N_3O_2$ $[M + H]^+$: 500.2333; found: 500.2328.



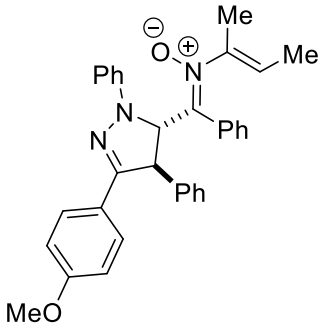
3va (*Z*/*E* > 20:1)

(*Z*)-1-phenyl-*N*-(1,4-dioxaspiro[4.5]dec-7-en-8-yl)-1-((4*R*,5*S*)-1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3va). Yellow oil, R_f = 0.3, 63 mg, 56% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.55–7.54 (m, 2H), 7.33–7.06 (m, 17H), 6.86–6.82 (m, 1H), 6.03 (d, *J* = 2.4 Hz, 1H), 5.37–5.33 (m, 1H), 5.13 (d, *J* = 2.8 Hz, 1H), 3.77–3.76 (m, 4H), 2.53–2.50 (m, 1H), 2.37–2.32 (m, 1H), 1.96–1.87 (m, 2H), 1.54–1.51 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 150.6, 146.7, 143.3, 142.4, 140.4, 131.3, 131.0, 129.4, 129.0, 128.96, 128.91, 128.51, 128.46, 127.8, 127.4, 126.0, 122.3, 119.3, 112.2, 105.6, 66.9, 63.8, 55.0, 33.8, 30.0, 25.5. HRMS (ESI) m/z calcd for $C_{36}H_{34}N_3O_3$ $[M + H]^+$: 556.2595; found: 556.2585.



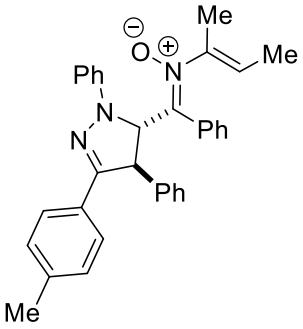
3wa (*Z*/*E* > 20:1)

(*Z*)-*N*,1-diphenyl-1-(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanimine oxide (3wa). Yyellow oil, R_f = 0.3, 57 mg, 58% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49–7.47 (m, 2H), 7.33–7.31 (m, 2H), 7.25–7.21 (m, 2H), 7.17–7.09 (m, 13H), 6.95–6.88 (m, 3H), 6.82–6.80 (m, 2H), 6.76–6.72 (m, 1H), 6.17-6.15 (m, 1H), 4.71-4.70 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 150.1, 146.7, 143.6, 139.4, 131.7, 131.0, 129.8, 129.2, 129.08, 129.05, 128.97, 128.7, 128.3, 127.9, 127.7, 127.6, 126.1, 124.4, 119.4, 112.9, 68.5, 57.1. HRMS (ESI) m/z calcd for $C_{34}H_{28}N_3O$ $[M + H]^+$: 494.2227; found: 494.2214.



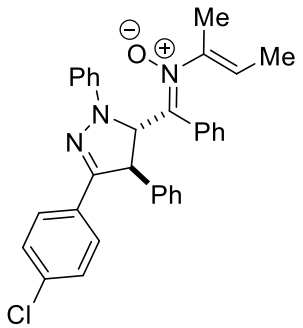
3ab (*Z*/*E* > 20:1)

(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(3-(4-methoxyphenyl)-1,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ab). Yellow oil, R_f = 0.2, 31 mg, 31% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.47–7.45 (m, 2H), 7.31–7.23 (m, 7H), 7.18–7.13 (m, 3H), 7.07–7.03 (m, 4H), 6.83–6.80 (m, 3H), 5.98 (d, J = 2.4 Hz, 1H), 5.33–5.28 (m, 1H), 5.07 (d, J = 2.4 Hz, 1H), 3.69 (s, 3H), 1.80 (s, 3H), 1.30 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.6, 150.7, 146.2, 143.6, 141.2, 140.6, 131.6, 129.7, 129.4, 129.3, 129.0, 128.9, 127.8, 127.6, 127.4, 123.5, 122.3, 118.8, 114.0, 112.0, 66.5, 55.1, 55.1, 14.6, 11.8. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O_2$ $[M + H]^+$: 502.2489; found: 502.2480.



3ac (*Z*/*E* = 15:1)

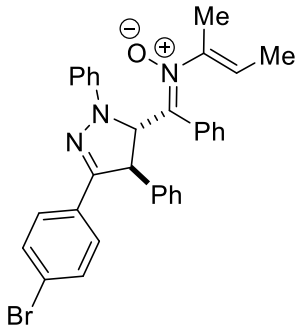
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(1,4-diphenyl-3-(p-tolyl)-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ac). Yellow oil, R_f = 0.2, 43 mg, 44% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34–7.33 (m, 2H), 7.27–7.25 (m, 2H), 7.21–7.18 (m, 2H), 7.17–7.13 (m, 3H), 7.06–7.02 (m, 5H), 6.95–6.74 (m, 2H), 6.86–6.85 (m, 2H), 6.73–6.70 (m, 1H), 6.00 (d, *J* = 3.0 Hz, 1H), 5.27 (q, *J* = 7.0 Hz, 1H), 4.56 (d, *J* = 3.0 Hz, 1H), 2.20 (s, 3H), 1.85 (s, 3H), 1.30 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.2, 149.1, 143.7, 141.7, 139.4, 138.4, 131.7, 129.2, 129.1, 129.0, 128.9, 128.8, 128.0, 127.7, 127.5, 126.1, 123.8, 119.1, 112.7, 67.8, 57.0, 21.3, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O$ $[M + H]^+$: 486.2540; found: 486.2540.



3ad (*Z*/*E* > 20:1)

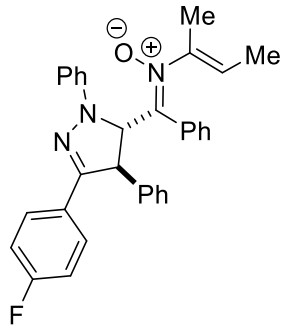
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(3-(4-chlorophenyl)-1,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ad). A yellow solid, R_f = 0.2, 65 mg, 64% yield; M.p: 116-117 °C, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35–7.34 (m, 2H), 7.24–7.16 (m, 7H), 7.10–7.03 (m, 7H), 6.85–6.83 (m, 2H), 6.77–6.74 (m, 1H), 6.04 (d, *J* = 3.0 Hz, 1H), 5.27 (q, *J* = 7.0 Hz, 1H), 4.52 (d, *J* = 3.0 Hz, 1H), 1.85 (s, 3H), 1.30 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.8, 148.4, 143.4, 141.7, 139.0, 134.0, 131.6, 130.2, 129.3, 129.1, 128.8, 128.5, 128.0, 127.7, 127.6, 127.2, 123.8, 119.5, 112.9, 67.9, 56.6, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{32}H_{29}ClN_3O$ $[M + H]^+$: 506.1994; found:

506.1970.



3ae (*Z*/*E* > 20:1)

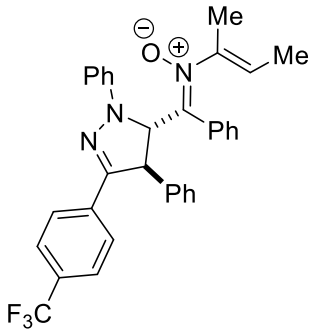
(*Z*)-1-(3-(4-bromophenyl)-1,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-*N*-((*E*)-but-2-en-2-yl)-1-phenylmethanimine oxide (3ae). A yellow solid, R_f = 0.2, 72 mg, 66% yield; M.p: 105-106 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29–7.15 (m, 11H), 7.10–7.03 (m, 5H), 6.85–6.83 (m, 2H), 6.78–6.74 (m, 1H), 6.04 (d, *J* = 3.2 Hz, 1H), 5.27 (q, *J* = 6.8 Hz, 1H), 4.52 (d, *J* = 3.2 Hz, 1H), 1.85 (s, 3H), 1.31 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 148.4, 143.3, 141.7, 138.9, 131.6, 131.5, 130.7, 129.3, 129.1, 128.8, 128.1, 127.7, 127.6, 127.4, 123.8, 122.3, 119.6, 112.9, 67.9, 56.6, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{32}H_{29}BrN_3O$ $[M + H]^+$: 550.1489; found: 550.1470.



3af (*Z*/*E* > 20:1)

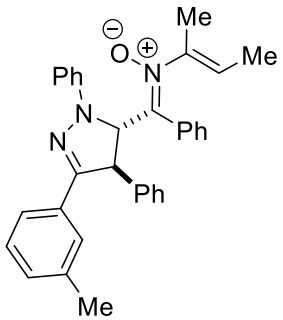
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(3-(4-fluorophenyl)-1,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3af). A yellow oil, R_f = 0.2, 62 mg, 63% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.38 (m, 2H), 7.25–7.15 (m, 7H), 7.09–7.03 (m, 5H), 6.86–6.80 (m, 4H), 6.76–6.73 (m, 1H), 6.03 (d, *J* = 3.5 Hz, 1H), 5.27–5.23 (m, 1H), 4.53 (d, *J* = 3.0 Hz, 1H), 1.85 (s, 3H), 1.30 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.7 (d, *J* = 247.0 Hz), 149.0, 148.6, 143.5, 141.7, 139.0, 131.6, 129.2, 129.1, 128.8, 128.0, 127.9 (d, *J* = 3.5 Hz), 127.8 (d, *J* = 8.0 Hz), 127.7, 127.6, 123.8,

119.3, 115.5 (d, J = 21.6 Hz), 112.8, 67.9, 56.9, 14.9, 12.3; ^{19}F NMR (470 MHz, $CDCl_3$) δ -112.3. HRMS (ESI) m/z calcd for $C_{32}H_{29}FN_3O$ $[M + H]^+$: 490.2289; found: 490.2270.



3ag (Z/E > 20:1)

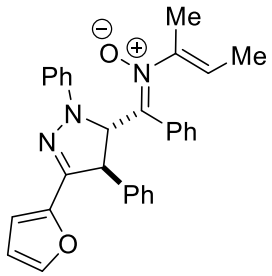
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(1,4-diphenyl-3-(4-(trifluoromethyl)phenyl)-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ag). Yellow oil, R_f = 0.2, 65 mg, 60% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52–7.50 (m, 2H), 7.37–7.36 (m, 2H), 7.25–7.17 (m, 7H), 7.10–7.08 (m, 3H), 7.06–7.03 (m, 2H), 6.85–6.84 (m, 2H), 6.80–6.77 (m, 1H), 6.08 (d, J = 3.0 Hz, 1H), 5.27 (m, J = 7.0 Hz, 1H), 4.57 (d, J = 3.0 Hz, 1H), 1.85 (s, 3H), 1.31 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.3, 148.2, 143.1, 141.7, 138.8, 135.1, 131.5, 129.7 (q, J = 32.1 Hz), 129.3, 129.2, 128.8, 128.1, 127.8, 127.6, 126.0, 125.3 (q, J = 3.5 Hz), 125.1 (q, J = 270.6 Hz), 123.9, 120.0, 113.1, 68.1, 56.5, 14.9, 12.3; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.6. HRMS (ESI) m/z calcd for $C_{33}H_{29}F_3N_3O$ $[M + H]^+$: 540.2257; found: 540.2278.



3ah (*Z*/*E* > 20:1)

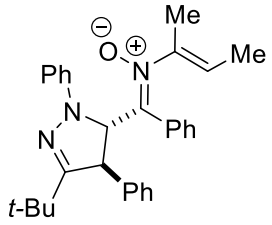
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-((4*R*,5*S*)-1,4-diphenyl-3-(m-tolyl)-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ah). Yellow oil, R_f = 0.2, 55 mg, 57% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.34 (m, 1H), 7.27–7.25 (m, 2H), 7.22–7.14 (m, 6H), 7.09–7.00 (m, 6H), 6.95–6.93 (m, 1H), 6.87–6.85 (m, 2H), 6.74–6.71 (m,1H),

6.00 (d, J = 2.4 Hz, 1H), 5.28–5.23 (m, 1H), 4.58 (d, J = 2.4 Hz, 1H), 2.19 (s, 3H), 1.85 (s, 3H), 1.30 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.2, 149.1, 143.6, 141.7, 139.4, 137.9, 131.64, 131.62, 129.23, 129.18, 129.08, 129.0, 128.8, 128.2, 128.0, 127.7, 127.5, 126.6, 123.8, 123.4, 119.2, 112.8, 67.9, 56.9, 21.4, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{33}H_{31}N_3ONa$ $[M + Na]^+$: 508.2359; found: 508.2354.



3ai (Z/E = 9:1)

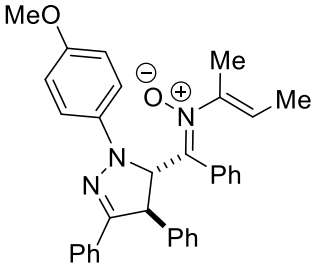
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(3-(furan-2-yl)-1,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide. Yellow oil, R_f = 0.2, 49 mg, 53% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25–7.15 (m, 8H), 7.11–7.08 (m, 5H), 6.91–6.89 (m, 2H), 6.76–6.74 (m, 1H), 6.19–6.15 (m, 1H), 6.13–6.12 (m, 1H), 6.06 (d, J = 4.0 Hz, 1H), 5.27–5.23 (m, 1H), 4.45 (d, J = 4.0 Hz, 1H), 1.83 (s, 3H), 1.29 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.1, 147.1, 143.3, 143.1, 142.4, 141.6, 139.3, 131.4, 129.2, 129.1, 128.9, 128.8, 128.1, 127.6, 127.5, 123.8, 119.5, 113.0, 111.3, 110.2, 67.2, 56.8, 14.8, 12.2. HRMS (ESI) m/z calcd for $C_{30}H_{28}N_3O_2$ $[M + H]^+$: 462.2176; found: 462.2171.



3aj (Z/E = 9:1)

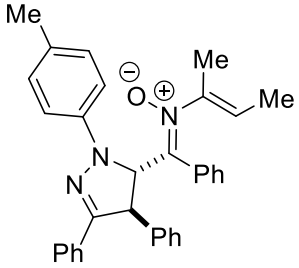
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(3-(tert-butyl)-1,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3aj). Yellow oil, R_f = 0.2, 45 mg, 50% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24–7.22 (m, 10H), 7.11–7.09 (m, 2H), 6.94–6.92 (m, 2H), 6.75–6.72 (m, 1H), 6.08 (d, J = 2.0 Hz, 1H), 5.19 (q, J = 6.8 Hz, 1H), 3.95 (d, J = 2.4 Hz, 1H), 1.81 (s, 3H), 1.26 (d, J = 7.2 Hz, 3H), 0.63 (s, 9H); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 161.3, 147.3, 144.2, 141.6, 140.3, 132.0, 129.4, 129.0, 128.9, 128.2, 127.6, 127.4, 123.8, 118.4, 112.4, 66.1, 56.8, 34.2, 29.1, 15.0, 12.3. HRMS (ESI) m/z calcd for $C_{30}H_{34}N_3O$ $[M + H]^+$: 452.2696; found: 452.2680.



3ak (*Z*/*E* > 20:1)

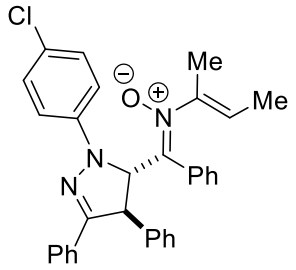
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(1-(4-methoxyphenyl)-3,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ak). Yellow oil, R_f = 0.2, 58 mg, 58% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.50–7.49 (m, 2H), 7.32–7.30 (m, 4H), 7.24–7.21 (m, 3H), 7.18–7.14 (m, 4H), 7.08–7.06 (m, 4H), 6.94–6.92 (m, 2H), 6.00 (d, *J* = 3.0 Hz, 1H), 5.33(q, *J* = 6.5 Hz, 1H), 5.07 (d, *J* = 3.0 Hz, 1H), 3.71 (s, 3H), 1.81 (s, 3H), 1.29 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 152.9, 149.5, 146.2, 141.2, 140.6, 137.7, 131.7, 131.2, 129.1, 129.0, 128.9, 128.4, 128.2, 127.9, 127.4, 127.3, 125.8, 122.3, 114.9, 113.3, 67.2, 55.2, 55.0, 14.5, 11.8. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O_2$ $[M + H]^+$: 502.2489; found: 502.2486.



3al (*Z*/*E* > 20:1)

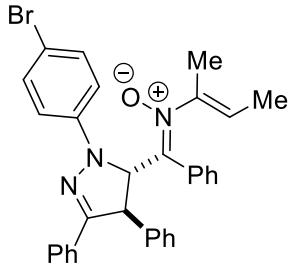
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(3,4-diphenyl-1-(p-tolyl)-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3al). Yellow oil, R_f = 0.2, 52 mg, 54% yield; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.52–7.51 (m, 2H), 7.34–7.29 (m, 4H), 7.22–7.21 (m, 3H), 7.19–7.12 (m, 6H), 7.09–7.04 (m, 4H), 6.03 (d, *J* = 1.5 Hz, 1H), 5.33–5.32 (m, 1H), 5.10 (d, *J* = 2.0 Hz, 1H), 2.24 (s, 3H), 1.82 (s, 3H), 1.28 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 149.9, 146.1, 141.3, 141.2, 140.5, 131.6, 131.1, 129.9,

129.0, 128.9, 128.8, 128.4, 128.3, 127.8, 127.4, 125.9, 122.3, 112.2, 66.8, 54.9, 20.2, 14.5, 11.8. HRMS (ESI) m/z calcd for $C_{33}H_{32}N_3O$ $[M + H]^+$: 486.2540; found: 486.2534.



3am (*Z*/*E* = 10:1)

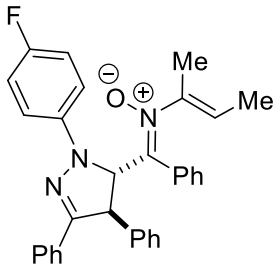
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(1-(4-chlorophenyl)-3,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3am). Yellow oil, R_f = 0.2, 60 mg, 60% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43–7.42 (m, 2H), 7.26–7.20 (m, 4H), 7.17–7.07 (m, 7H), 7.04–7.04 (m, 2H), 7.00–6.98 (m, 2H), 6.85–6.84 (m, 2H), 5.98 (d, *J* = 3.0 Hz, 1H), 5.27 (q, *J* = 7.0 Hz, 1H), 4.59 (d, *J* = 3.0 Hz, 1H), 1.85 (s, 3H), 1.32 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.7, 148.4, 142.2, 141.7, 139.1, 131.5, 131.4, 129.2, 129.1, 129.0, 128.8, 128.6, 128.4, 128.1, 127.7, 127.6, 126.2, 124.0, 123.9, 114.0, 67.9, 57.0, 14.9, 12.3. HRMS (ESI) m/z calcd for $C_{32}H_{29}ClN_3O$ $[M + H]^+$: 506.1994; found: 506.1984.



3an (*Z*/*E* = 11:1)

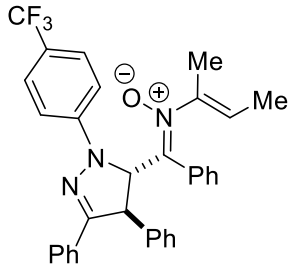
(*Z*)-1-(1-(4-bromophenyl)-3,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-*N*-((*E*)-but-2-en-2-yl)-1-phenylmethanimine oxide (3an). Yellow oil, R_f = 0.2, 67 mg, 61% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43–7.42 (m, 2H), 7.25–7.20 (m, 6H), 7.17–7.04 (m, 7H), 6.95–6.93 (m, 2H), 6.85–6.84 (m, 2H), 5.97 (d, *J* = 3.0 Hz, 1H), 5.27 (q, *J* = 7.0 Hz, 1H), 4.58 (d, *J* = 3.0 Hz, 1H), 1.85 (s, 3H), 1.32 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.8, 148.4, 142.6, 141.7, 139.1, 132.0, 131.4, 129.3, 129.1, 128.7, 128.6, 128.4, 128.2, 128.1, 127.7, 127.6, 126.2, 123.9, 114.4, 111.3, 67.8, 57.0, 14.9,

12.3. HRMS (ESI) m/z calcd for $C_{32}H_{29}BrN_3O$ $[M + H]^+$: 550.1489; found: 550.1444.



3ao (*Z*/*E* = 10:1)

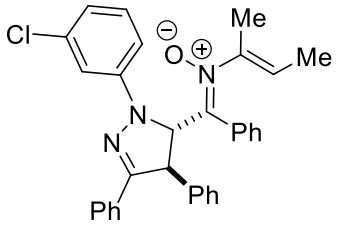
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(1-(4-fluorophenyl)-3,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ao). Yellow oil, R_f = 0.2, 60 mg, 61% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42–7.41 (m, 2H), 7.26–7.19 (m, 4H), 7.16–7.12 (m, 4H), 7.09–7.03 (m, 3H), 7.01–6.98 (m, 2H), 6.87–6.83 (m, 4H), 5.99 (d, J = 3.5 Hz, 1H), 5.25 (q, J = 7.0 Hz, 1H), 4.59 (d, J = 3.5 Hz, 1H), 1.84 (s, 3H), 1.30 (d, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.6 (d, J = 233.1 Hz), 149.0, 147.7, 140.7, 139.2, 138.3, 130.8, 128.3, 128.0, 127.6, 127.6, 127.3, 126.9, 126.8, 125.3, 123.2, 115.2, 115.0, 113.3, 113.2, 68.4, 57.3, 15.8, 13.2; ^{19}F NMR (470 MHz, $CDCl_3$) δ -125.5. HRMS (ESI) m/z calcd for $C_{32}H_{29}FN_3O$ $[M + H]^+$: 490.2289; found: 490.2270.



3ap (*Z*/*E* = 12:1)

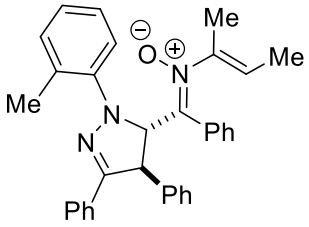
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(3,4-diphenyl-1-(4-(trifluoromethyl)phenyl)-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ap). Yellow oil, R_f = 0.2, 26 mg, 24% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.63–7.57 (m, 4H), 7.32–7.27 (m, 8H), 7.19–7.14 (m, 5H), 7.06–7.05 (m, 2H), 6.00 (d, J = 2.4 Hz, 1H), 5.39–5.38 (m, 1H), 5.23 (d, J = 2.4 Hz, 1H), 1.82 (s, 3H), 1.31 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 153.1, 145.9, 145.5, 141.2, 140.1, 131.2, 130.5, 129.4, 129.2 (q, J = 31.2 Hz), 129.1, 128.9, 128.6, 128.0, 127.6, 127.4, 126.8 (q, J = 3.4 Hz), 126.4, 126.3 (q, J = 269.0 Hz), 122.7, 115.2, 112.0, 66.7, 55.2, 14.6, 11.9; ^{19}F NMR (375 MHz,

DMSO-d_6) δ -59.4. HRMS (ESI) m/z calcd for $C_{33}H_{29}F_3N_3O$ [M + H]$^+$: 540.2257; found: 540.2246.



3aq (*Z*/*E* > 20:1)

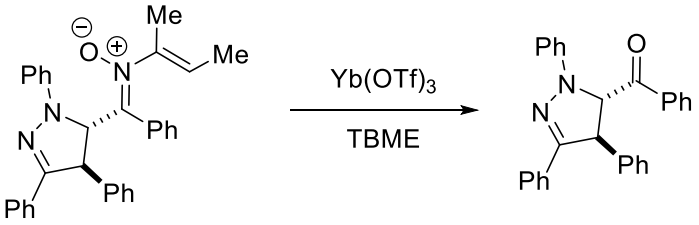
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(1-(3-chlorophenyl)-3,4-diphenyl-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3aq). Yellow oil, R_f = 0.2, 61 mg, 60% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.54–7.53 (m, 2H), 7.34–7.30 (m, 5H), 7.26–7.25 (m, 4H), 7.18–7.13 (m, 4H), 7.06–7.00 (m, 3H), 6.88–6.87 (m, 1H), 6.00 (d, *J* = 3.5 Hz, 1H), 5.38–5.33 (m, 1H), 5.19 (d, *J* = 3.5 Hz, 1H), 1.80 (s, 3H), 1.31 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 152.0, 145.3, 144.4, 141.1, 140.1, 134.2, 131.3, 131.1, 130.6, 129.4, 129.1, 129.0, 128.5, 128.0, 127.6, 127.4, 126.2, 122.5, 118.7, 115.2, 111.8, 110.8, 66.4, 54.8, 14.5, 11.9. HRMS (ESI) m/z calcd for $C_{32}H_{29}ClN_3O$ [M + H]$^+$: 506.1994; found: 506.1979.



3ar (*Z*/*E* = 8:1)

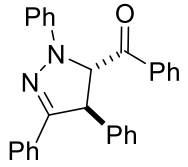
(*Z*)-*N*-((*E*)-but-2-en-2-yl)-1-(3,4-diphenyl-1-(o-tolyl)-4,5-dihydro-1H-pyrazol-5-yl)-1-phenylmethanimine oxide (3ar). Yellow oil, R_f = 0.2, 80 mg, 82% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.52–7.50 (m, 2H), 7.43–7.41 (m, 2H), 7.37–7.33 (m, 2H), 7.29–7.16 (m, 8H), 7.14–7.08 (m, 2H), 6.94–6.89 (m, 3H), 6.02–5.93 (m, 1H), 5.22–5.17 (m, 1H), 5.09 (d, *J* = 5.2 Hz, 1H), 2.21 (s, 3H), 1.70 (s, 3H), 1.25 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 149.7, 146.0, 142.8, 141.3, 140.8, 132.7, 131.8, 131.6, 129.0, 128.8, 128.7, 128.6, 128.4, 128.1, 127.9, 127.7, 127.3, 126.6, 126.2, 125.9, 125.3, 122.2, 70.2, 54.8, 20.6, 14.5, 11.8. (ESI) m/z calcd for $C_{33}H_{32}N_3O$ [M + H]$^+$: 486.2540; found: 486.2527.

3. Synthesis of compound 4



3aa **4**

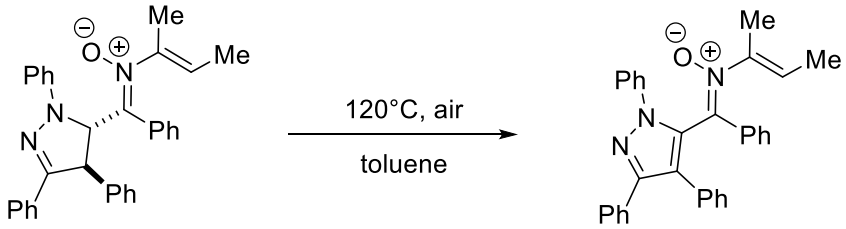
A Teflon-sealed flask was charged with **3aa** (94 mg, 0.2 mmol) and $Yb(OTf)_3$ (0.2 equiv., 0.04 mmol) in air. And then, TBME (2 mL) was added. The reaction vessel was sealed with a Teflon cap and vigorously stirred at at room temperature for 72 h until substrate **3aa** was completely consumed (monitored by TLC). The solvent was removed under reduced pressure and the crude product was purified flash column chromatography (the crude residue was dry loaded with silica gel, 1/50 to 1/30, ethyl acetate/petroleum ether) to provide compound **4**.



4

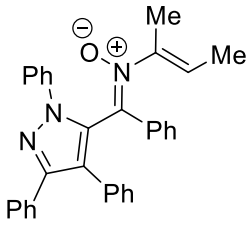
phenyl(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methanone (4). Yellow oil, R_f = 0.3, 40 mg, 50% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, J = 7.5 Hz, 2H), 7.59 (t, J = 7.5 Hz, 1H), 7.54 (d, J = 7.0 Hz, 2H), 7.45 (t, J = 7.5 Hz, 2H), 7.29–7.23 (m, 3H), 7.18–7.11 (m, 7H), 7.00 (d, J = 8.0 Hz, 2H), 6.77 (t, J = 7.0 Hz, 1H), 5.54 (d, J = 4.5 Hz, 1H), 4.54 (d, J = 4.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.8, 148.0, 143.9, 139.3, 134.1, 133.5, 131.5, 129.6, 129.2, 129.1, 128.4, 128.3, 128.1, 127.6, 126.3, 119.5, 112.9, 73.8, 57.0. HRMS (ESI) m/z calcd for $C_{28}H_{23}N_2O$ $[M + H]^+$: 403.1805; found: 403.1802.

4. Synthesis of compound 5



3aa **5**

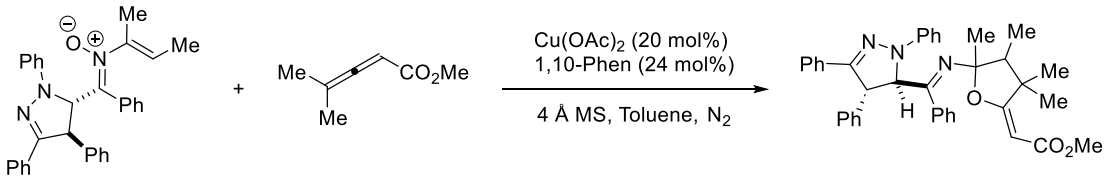
A Teflon-sealed flask was charged with **3aa** (94 mg, 0.2 mmol) in air. And then, toluene (2 mL) was added. The reaction vessel was sealed with a Teflon cap and vigorously stirred at 120 ℃ in an oil bath for 5 h until substrate **3aa** was completely consumed (monitored by TLC). The solvent was removed under reduced pressure and the crude product was purified flash column chromatography (the crude residue was dry loaded with silica gel, 1/50 to 1/30, ethyl acetate/petroleum ether) to provide compound **5**.



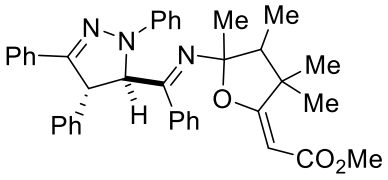
5

(*Z*)-N-((*E*)-but-2-en-2-yl)-1-phenyl-1-(1,3,4-triphenyl-1H-pyrazol-5-yl) methanimine oxide (5). Yellow oil, R_f = 0.3, 49 mg, 52% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, J = 7.5 Hz, 2H), 7.50 (d, J = 8.5 Hz, 2H), 7.42 (d, J = 7.5 Hz, 2H), 7.23–7.22 (m, 5H), 7.20–7.19 (m, 4H), 7.07–7.06 (m, 3H), 7.01–7.00 (m, 2H), 4.48 (q, J = 6.5 Hz, 1H), 1.31 (d, J = 7.0 Hz, 3H), 1.07 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.9, 150.0, 144.9, 139.9, 138.6, 136.5, 132.6, 132.3, 130.4, 129.5, 129.0, 128.4, 128.3, 128.2, 128.1, 127.9, 127.3, 127.0, 123.0, 122.0, 121.9, 108.8, 29.7, 29.3, 14.8, 12.9. HRMS (ESI) m/z calcd for $C_{32}H_{28}N_3O$ $[M + H]^+$: 470.2227; found: 470.2224.

5. Synthesis of compound 6



A Teflon-sealed flask was charged with **3aa** (94 mg, 0.2 mmol), allenoate (0.050 g, 0.40 mmol), $Cu(OAc)_2$ (20 mol%), 1,10-Phen (24 mol%), and 4Å MS (150 mg) under an N_2 atmosphere. And then, toluene (2 mL) was added. The reaction vessel was sealed with a Teflon cap and vigorously stirred at at 120 ℃ in an oil bath for 72 h until substrate **3aa** was completely consumed (monitored by TLC). The solvent was removed under reduced pressure and the crude product was purified flash column chromatography (the crude residue was dry loaded with silica gel, 1/10, ethyl acetate/petroleum ether) to provide compound **6**.

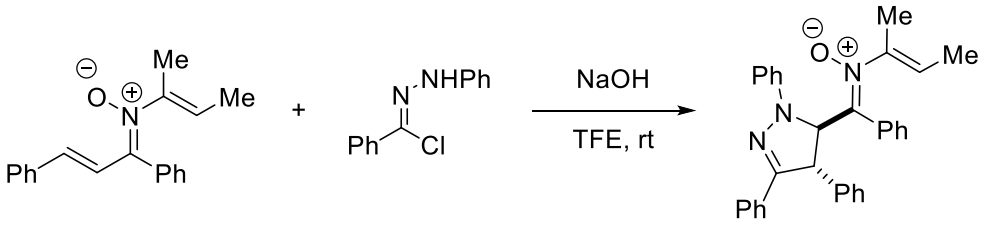


6 (*dr* = 5:1)

Methyl-(*E*)-2-(3,3,4,5-tetramethyl-5-(((*E*)-phenyl(1,3,4-triphenyl-4,5-dihydro-1H-pyrazol-5-yl)methylene)amino)dihydrofuran-2(3H)-ylidene)acetate (6). A yellow solid, R_f = 0.3, 79 mg, 66% yield; Mp: 124-125 ℃, *major isomer*: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, J = 7.0 Hz, 2H), 7.42–7.29 (m, 3H), 7.22–7.16 (m, 6H), 7.14–7.10 (m, 6H), 6.90 (d, J = 6.5 Hz, 2H), 6.77 (t, J = 7.0 Hz, 1H), 4.81 (brs, 1H), 4.55 (d, J = 2.0 Hz, 1H), 4.48 (brs, 1H), 3.35 (s, 3H), 1.58 (q, J = 7.0 Hz, 1H), 1.08 (s, 3H), 0.88 (s, 3H), 0.74 (d, J = 7.0 Hz, 3H), 0.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.0, 166.4, 162.4, 147.9, 145.2, 139.6, 137.6, 132.1, 129.1, 128.7, 128.3, 128.2, 128.1, 128.0, 127.5, 127.0, 126.4, 125.8, 118.9, 113.6, 102.2, 86.8, 77.5, 55.8, 51.6, 50.5, 45.4, 27.3, 25.7, 23.0, 8.8. *minor isomer:* ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (d, J = 7.0 Hz, 2H), 7.22–

7.16 (m, 6H), 7.14–7.10 (m, 6H), 7.02–7.01 (m, 3H), 6.92–6.90 (m, 2H), 6.77 (t, J = 7.0 Hz, 1H), 4.81 (brs, 1H), 4.55 (d, J = 2.0 Hz, 1H), 4.48 (brs, 1H), 3.34 (s, 3H), 1.58 (q, J = 7.0 Hz, 1H), 0.96 (s, 3H), 0.81–0.80 (m, 6H), 0.74 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.0, 166.4, 162.4, 148.4, 144.5, 139.8, 137.6, 131.9, 129.2, 129.0, 128.7, 128.3, 128.2, 128.1, 128.0, 127.6, 127.2, 126.5, 126.0, 113.2, 102.2, 86.8, 78.5, 56.5, 51.6, 50.5, 45.4, 27.3, 25.7, 23.0, 8.8. HRMS (ESI) m/z calcd for $C_{39}H_{39}N_3O_3Na$ $[M + Na]^+$: 620.2884 found: 620.2888.

6. Gram scalable preparation of 3aa



1a (1.0 g, 3.3 mmol) + **2a** → **3aa** (0.933 g, 60%)

In a Teflon-sealed flask was charged with *N*-vinyl-*α,β*-unsaturated nitrone **1a** (1.0 g, 3.3 mmol), hydrazonoyl chloride **2a** (6.6 mmol, 2.0 equiv.), and NaOH (0.396 g, 9.9 mmol, 3.0 equiv.). Then, TFE (16.0 mL) was added via syringe. The reaction vessel was sealed with a Teflon cap and stirred at room temperature for 15 h until substrate **1a** was completely consumed (monitored by TLC). At this time, the solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (the crude residue was dry loaded on silica gel, eluents with a mixed eluents petroleum ether/ethyl acetate = 2/1) to afford **3aa** (0.933 g, 60% yield) as a yellow solid.

7. X-ray structures for compounds 3aa, 3ae, and 6.

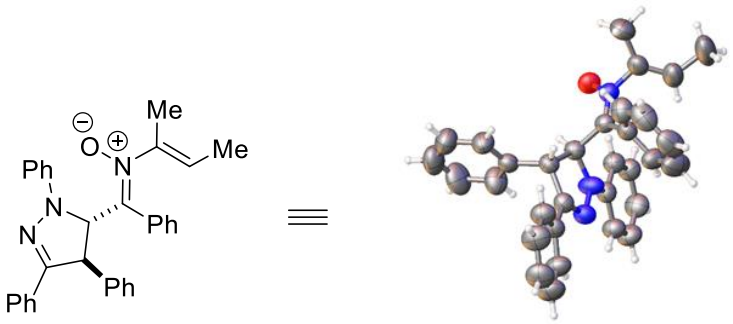


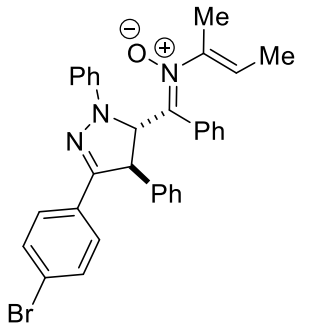
Figure S1: ORTEP diagram of **3aa** at 50% ellipsoid probability.

The preparation of crystal of 3aa: compound **3aa** (50 mg) was dissolved in DCM (3 mL) at room temperature. PE (3 mL) was dropped carefully to the mixture. Then, the flask was capped with thin film. Finally, a needle crystal was obtained for 3 days.

Table S1. Crystal data and structure refinement details for compound **3aa**

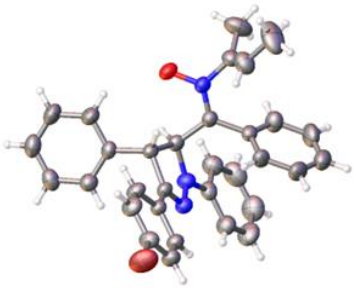
Empirical formula	$C_{32}H_{29}N_3O$
Formula weight (*M*)	471.58
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	18.4332(3)
b/Å	10.5214(2)
c/Å	16.2967(3)
α/°	90

β/°	104.120(2)
γ/°	90
Volume/Å^3	3065.14(10)
Z	4
$\rho_{calc} g/cm^3$	1.377
F (000)	1304.0
2θ range for data collection (°)	9.754 to 146.488
Reflections collected	11579
Independent reflections	3682 [R_{int} = 0.0569, R_{sigma} = 0.0560]
Goodness-of-fit on F^2	1.134
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0582, wR_2 = 0.1746
R indices (all data)	R_1 = 0.0595, ωR_2 = 0.1767



3ae

≡



X-ray of **3ae**

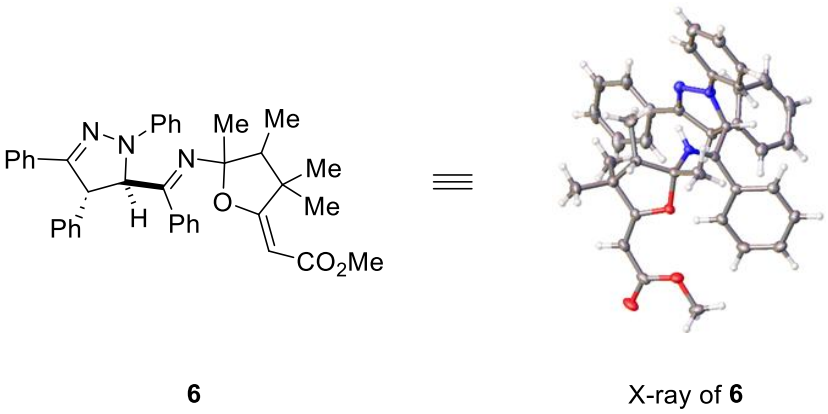
Figure S2: ORTEP diagram of **3ae** at 50% ellipsoid probability.

The preparation of crystal of 3ae: compound **3ae** (50 mg) was dissolved in DCM (3 mL) at room temperature. PE (3 mL) was dropped carefully to the mixture. Then, the flask was capped with thin film. Finally, a needle crystal was obtained for 3 days.

Table S2. Crystal data and structure refinement details for compound **3ae**

Empirical formula	$C_{32}H_{28}BrN_3O$
Formula weight (*M*)	549.14
Crystal system	monoclinic
Space group	Ia
a/Å	18.4332(3)
b/Å	10.5214(2)
c/Å	16.2967(3)
α/°	90
β/°	104.1201(17)
γ/°	90
Volume/Å^3	3065.12(10)
Z	4
$\rho_{calc} g/cm^3$	1.377
F (000)	1304.0
2θ range for data collection (°)	9.754 to 146.488

Reflections collected	11579
Independent reflections	3682 [R_{int} = 0.0569, R_{sigma} = 0.0560]
Goodness-of-fit on F^2	1.134
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0582
	ωR_2 = 0.1746
R indices (all data)	R_1 = 0.0595
	ωR_2 = 0.1767



6 ≡ X-ray of **6**

Figure S3: ORTEP diagram of **6** at 50% ellipsoid probability.

The preparation of crystal of 6: compound **6** (50 mg) was dissolved in DCM (3 mL) at room temperature. PE (3 mL) was dropped carefully to the mixture. Then, the flask was capped with thin film. Finally, a needle crystal was obtained for 3 days.

Table S3. Crystal data and structure refinement details for compound **6**

Empirical formula	$C_{39}H_{39}N_3O_3$

Formula weight (*M*)	598.74
Crystal system	orthorhombic
Space group	Pbca
a/Å	13.4977(2)
b/Å	20.1520(3)
c/Å	23.7070(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	6448.44(17)
Z	8
$\rho_{calc} g/cm^3$	1.233
F (000)	2552.0
2θ range for data collection (°)	7.458 to 153.762
Reflections collected	24910
Independent reflections	6319 [R_{int} = 0.0874, R_{sigma} = 0.0525]
Goodness-of-fit on F^2	1.049
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0654
	ωR_2 = 0.1831
R indices (all data)	R_1 = 0.0696

	ωR_2 = 0.1884

8. References

[1] Chen, C.-H.; Wu, Q.-Y.; Wei, C.; Liang, C.; Su, G.-F.; Mo, D.-L. *Green Chem.* **2018**, *20*, 2722-2729.

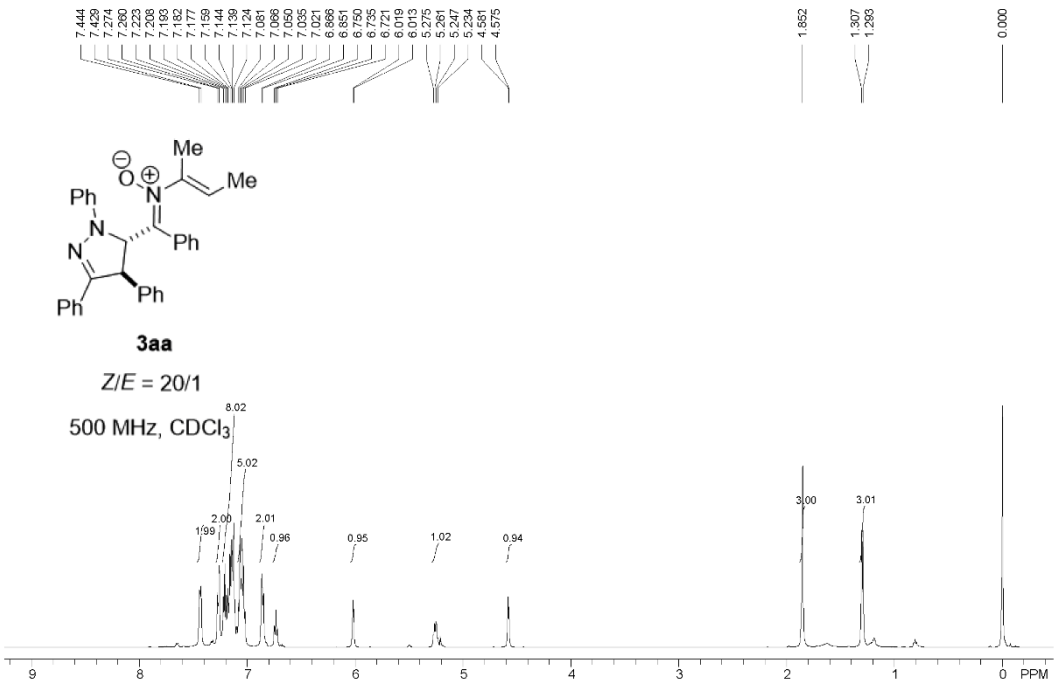
[2] Kontokosta, D.; Meller, D. S.; Mo, D.-L.; Pace, W. H.; Simpson, R. A.; Anderson, L. L. *Beilstein J. Org. Chem*. **2015**, *11*, 2097-2104.

[3] Zhao, X.; Zhou, Y.; Li, B.-L.; Du, G.; Yu, Z. *Org. Chem. Front*. **2022**, *9*, 1336-1342.

[4] Du, S.; Wang, W.-F.; Song, Y.; Chen, Z.; Wu, X.-F. *Org. Lett.* **2021**, *23*, 974-978.

[5] Rout, L.; Harned, A. M. *Chem. Eur. J.* **2009**, *15*, 12926-12928.

9. NMR spectra for compounds 3, 4, 5 and 6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Ph
Ph
Ph
3aa
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2.00
1.99
2.01
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3.01
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6
5
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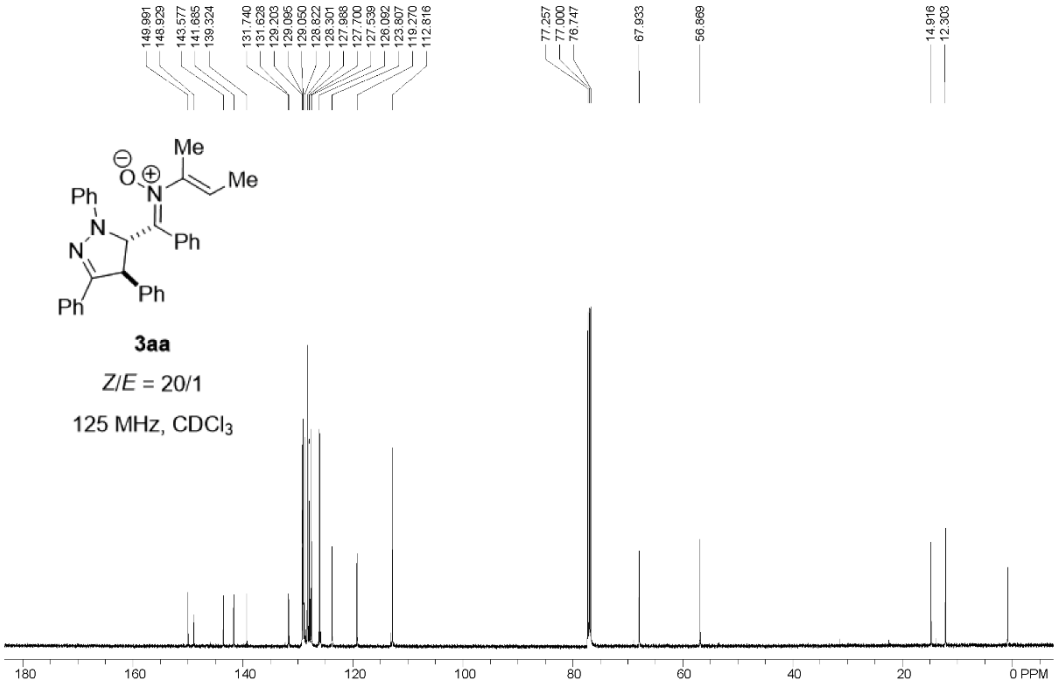
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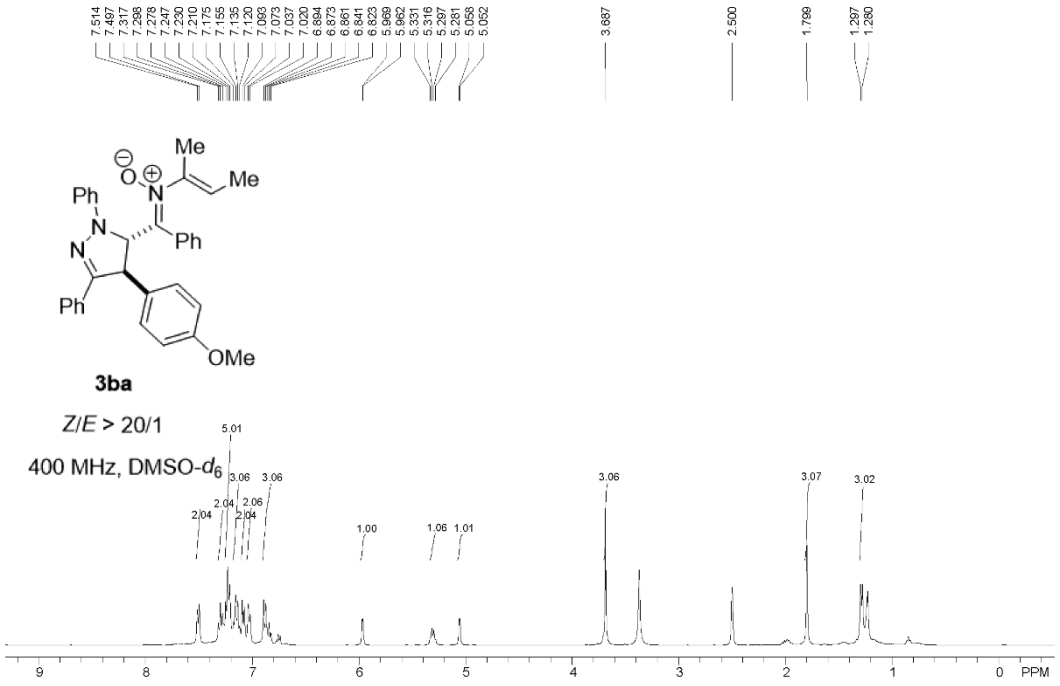
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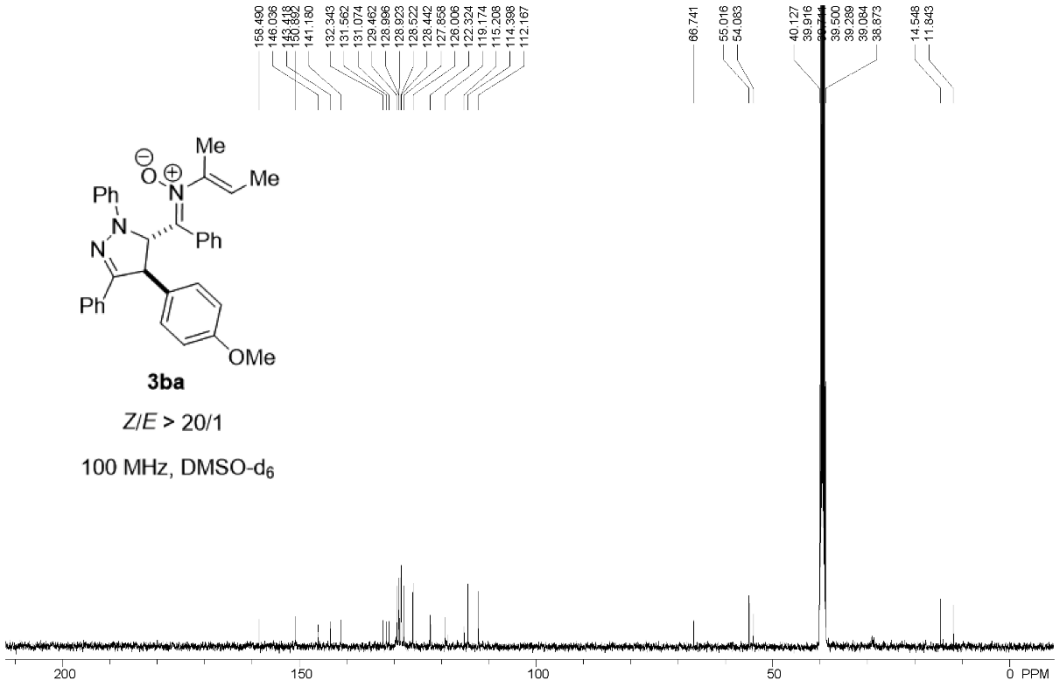
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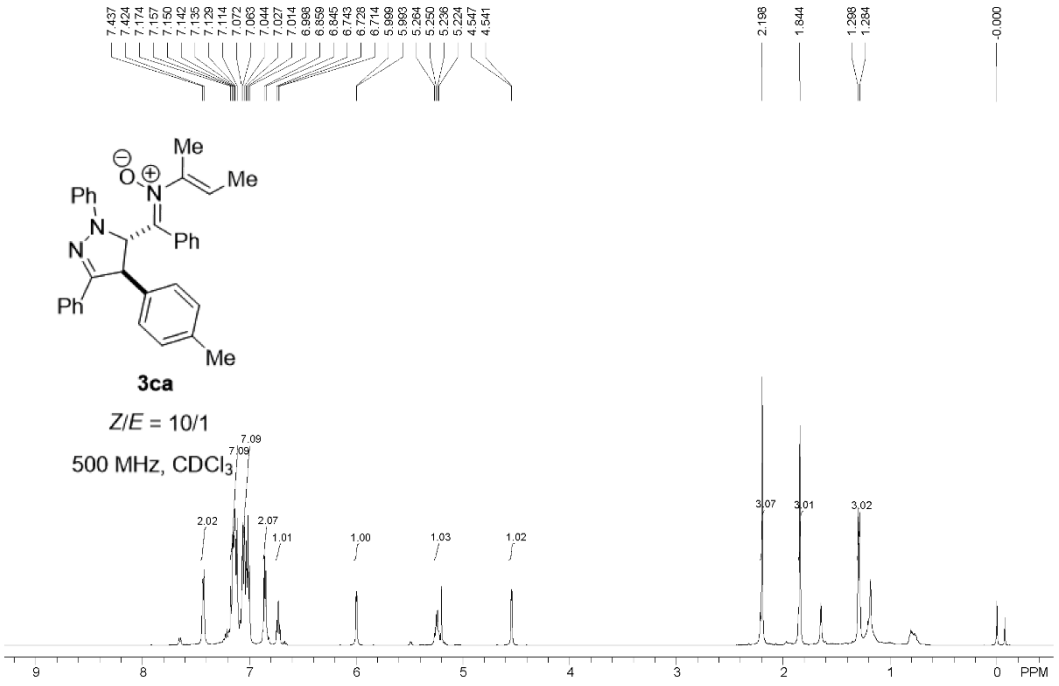
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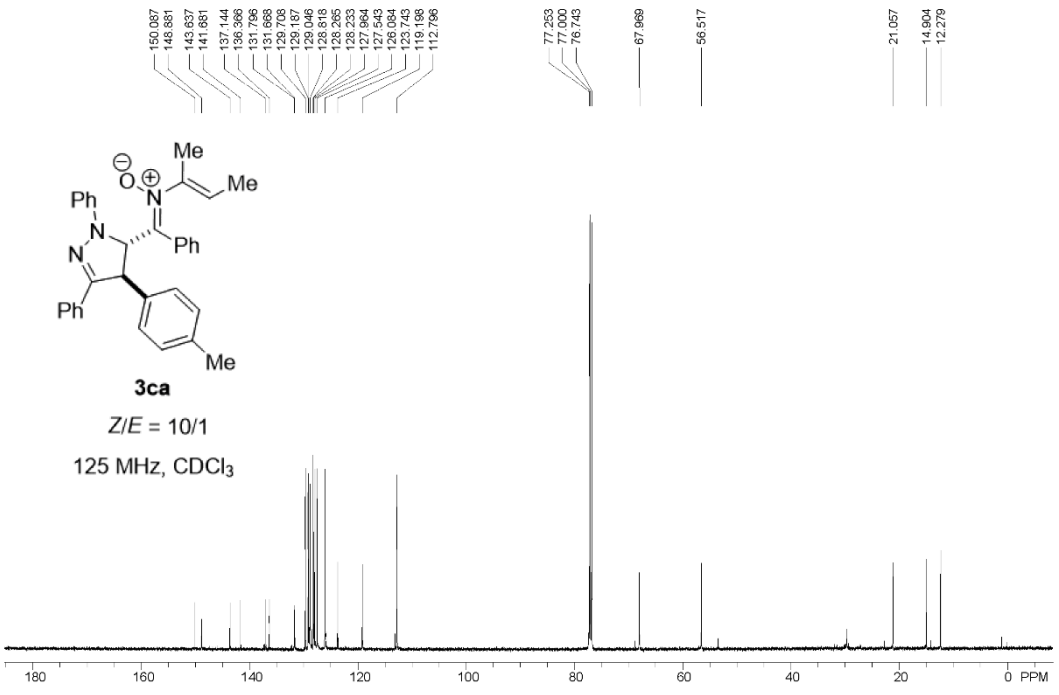
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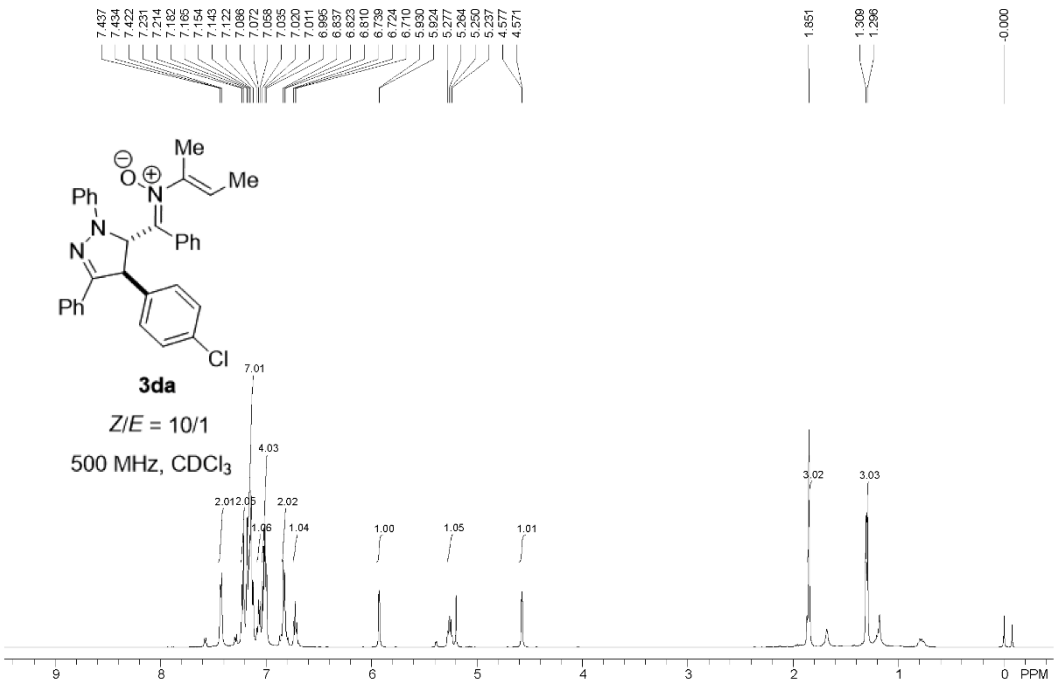
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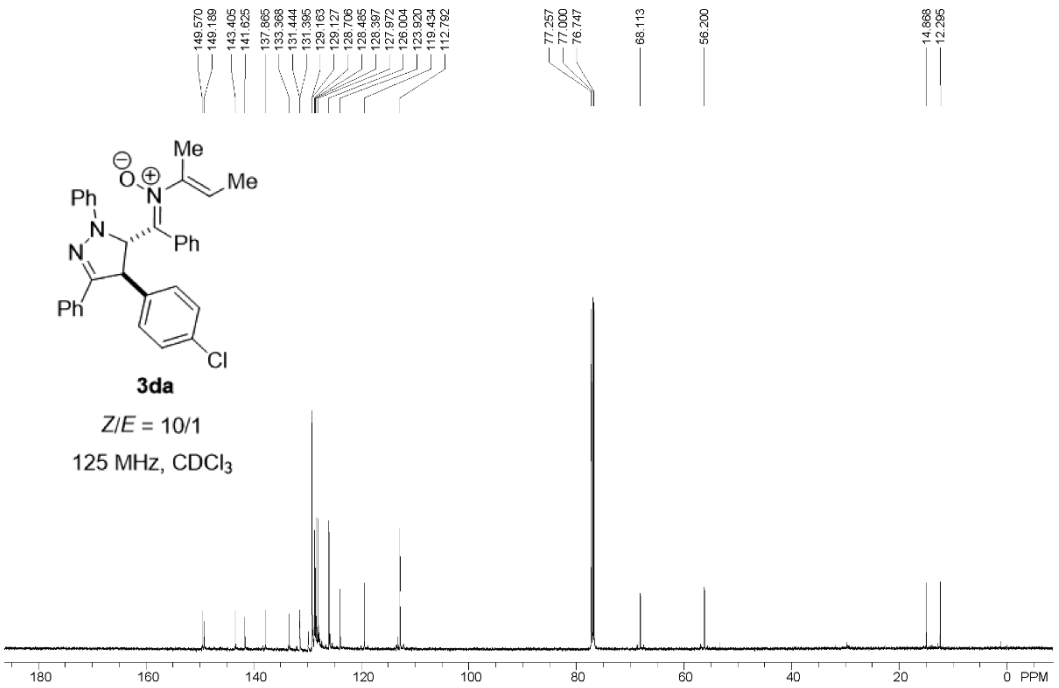
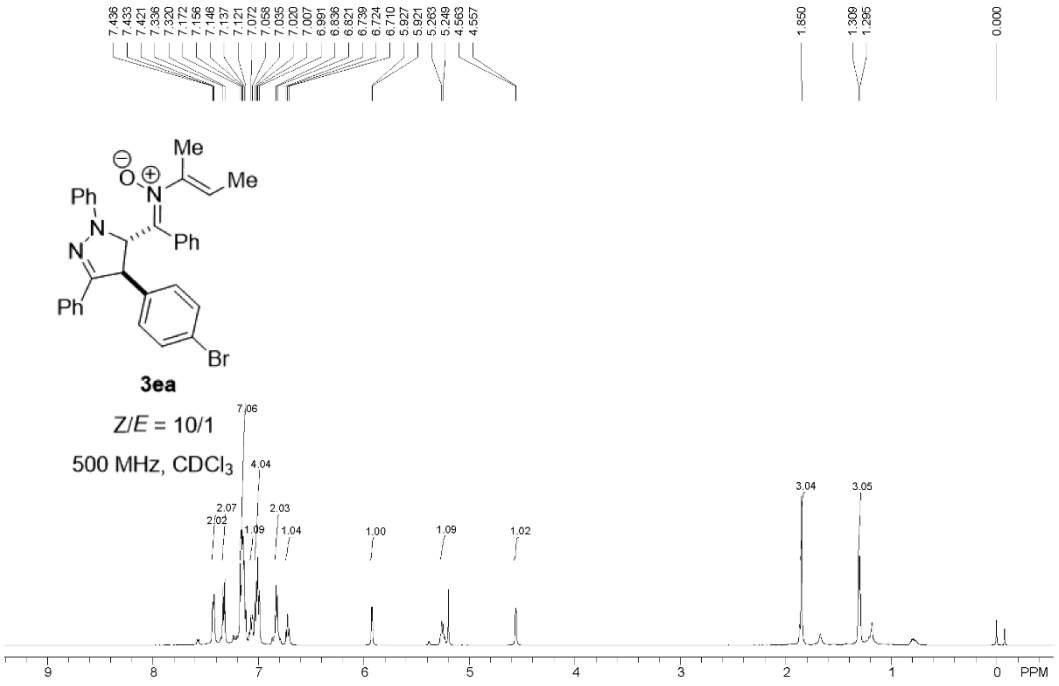
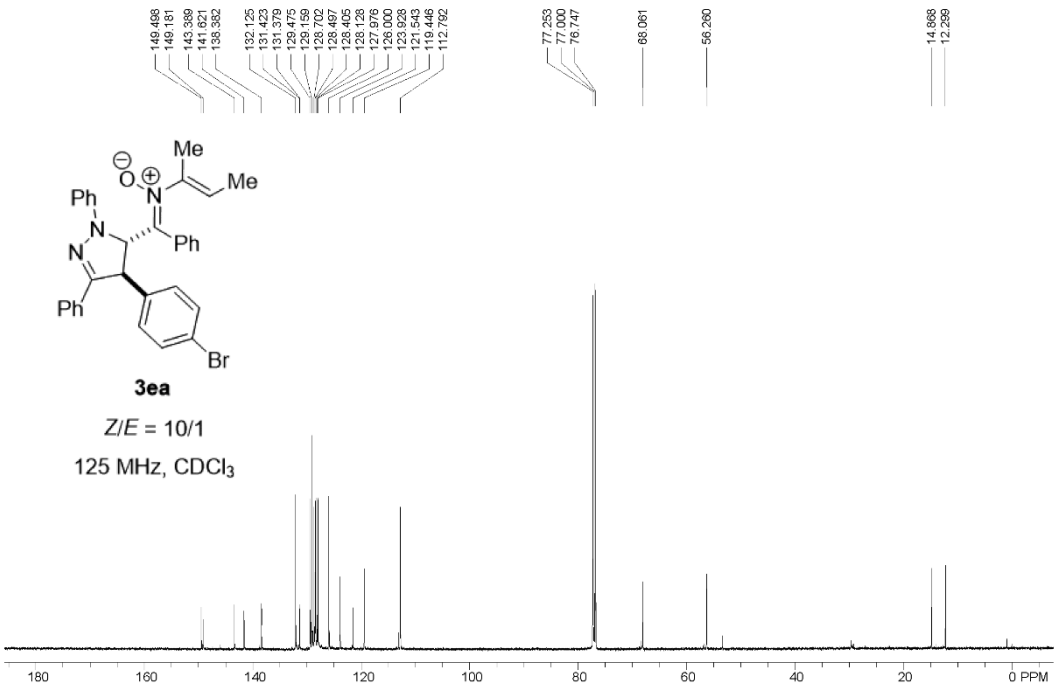
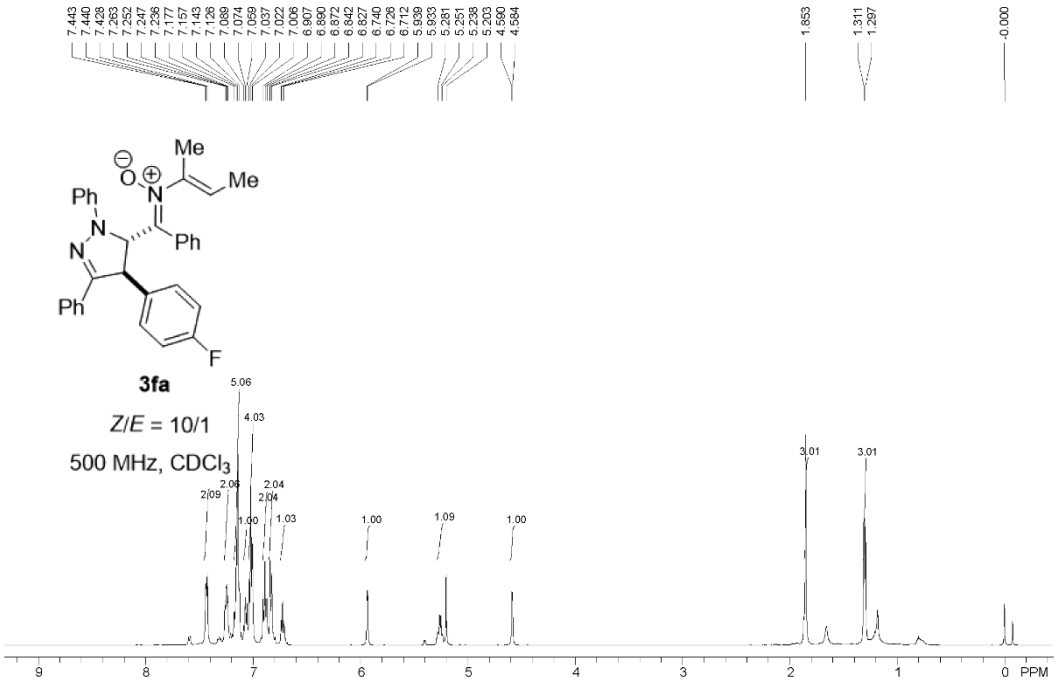
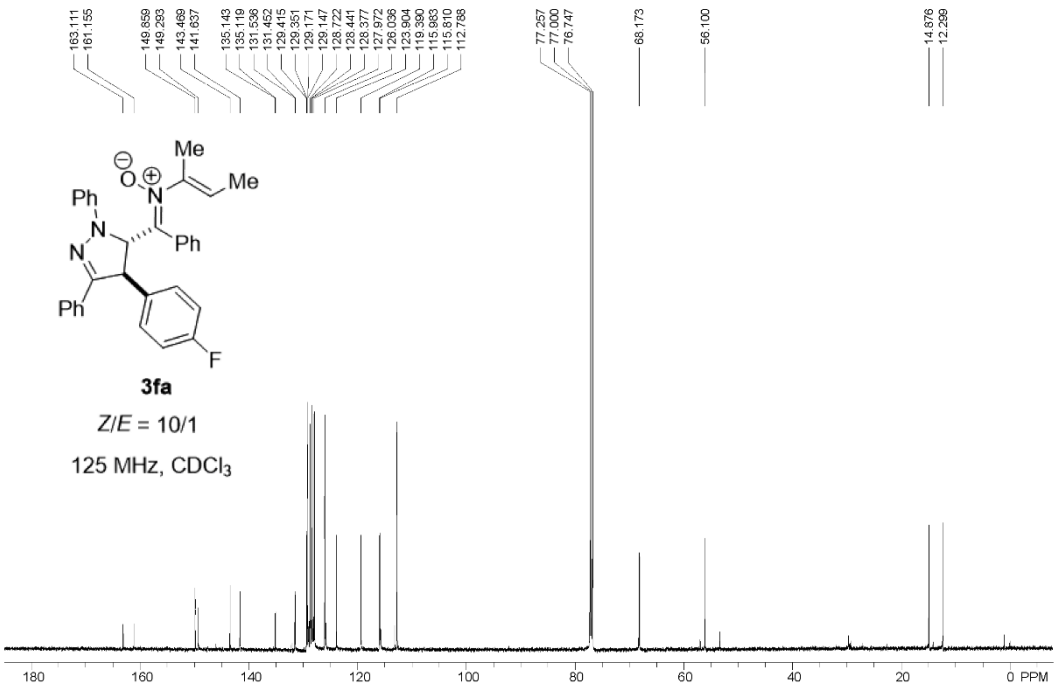
1
0 PPM


149.570
149.189
143.405
141.625
137.865
133.388
131.444
131.395
129.163
129.127
128.706
128.465
128.397
127.972
126.004
123.920
119.434
112.782
77.257
77.000
76.747
68.113
56.200
14.868
12.295
Me
Me
Ph
Ph
Ph
Cl
3da
Z/E = 10/1
125 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0 PPM


7.436
7.433
7.421
7.336
7.320
7.172
7.156
7.146
7.137
7.121
7.072
7.058
7.035
7.020
7.007
6.991
6.836
6.821
6.739
6.724
6.710
5.927
5.921
5.283
5.249
4.563
4.557
1.850
1.309
1.295
0.000
Me
Me
Ph
N
O
N
Ph
N
Ph
Ph
Br
3ea
Z/E = 10/1
500 MHz, CDCl3
7.06
4.04
2.07
2.02
2.03
1.09
1.04
1.00
1.09
1.02
3.04
3.05
9
8
7
6
5
4
3
2
1
0
PPM


149.498
149.181
143.389
141.621
138.382
132.125
131.423
131.379
129.475
129.159
128.702
128.497
128.405
128.128
127.976
126.000
123.928
121.543
119.446
112.792
77.253
77.000
76.747
68.061
56.260
14.868
12.299
Me
Me
Ph
N
O
N
Ph
N
Ph
Ph
Br
3ea
Z/E = 10/1
125 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0 PPM

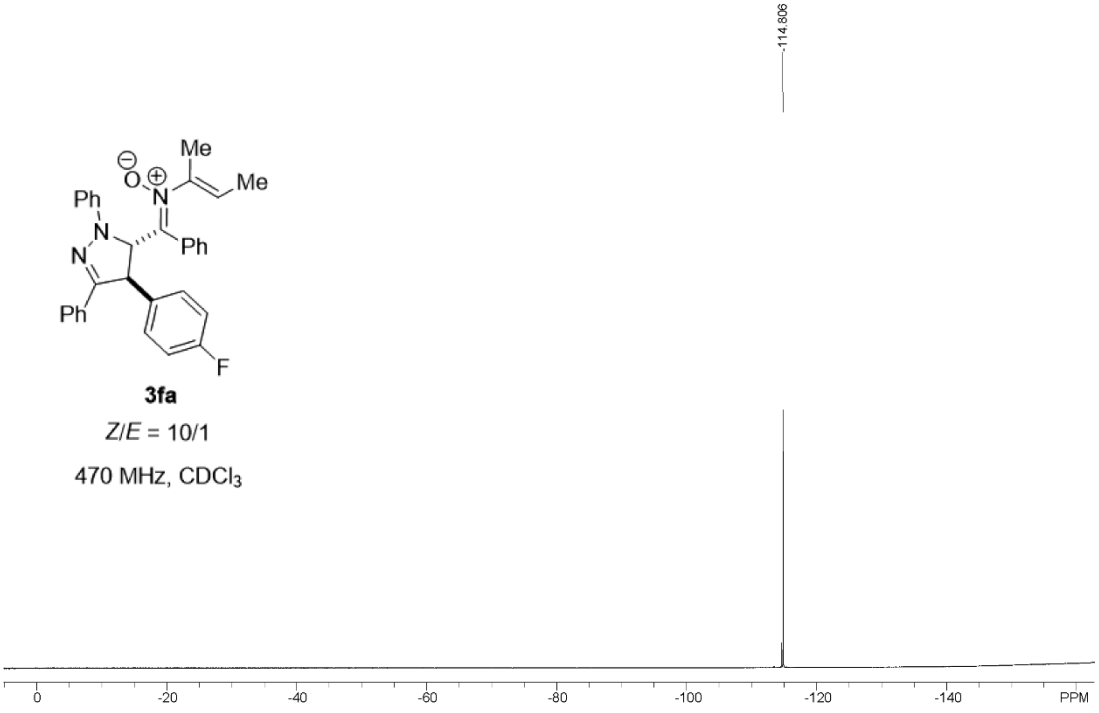

7.443
7.440
7.428
7.263
7.252
7.247
7.236
7.177
7.157
7.143
7.126
7.089
7.074
7.059
7.037
7.022
7.006
6.907
6.890
6.872
6.842
6.827
6.740
6.726
6.712
5.939
5.933
5.281
5.251
5.238
5.203
4.590
4.584
1.853
1.311
1.297
0.000
Me
Me
Ph
Ph
Ph
F
3fa
Z/E = 10/1
500 MHz, CDCl3
5.06
4.03
2.09
2.06
2.04
2.04
1.00
1.03
1.00
1.09
1.00
3.01
3.01
9
8
7
6
5
4
3
2
1
0 PPM

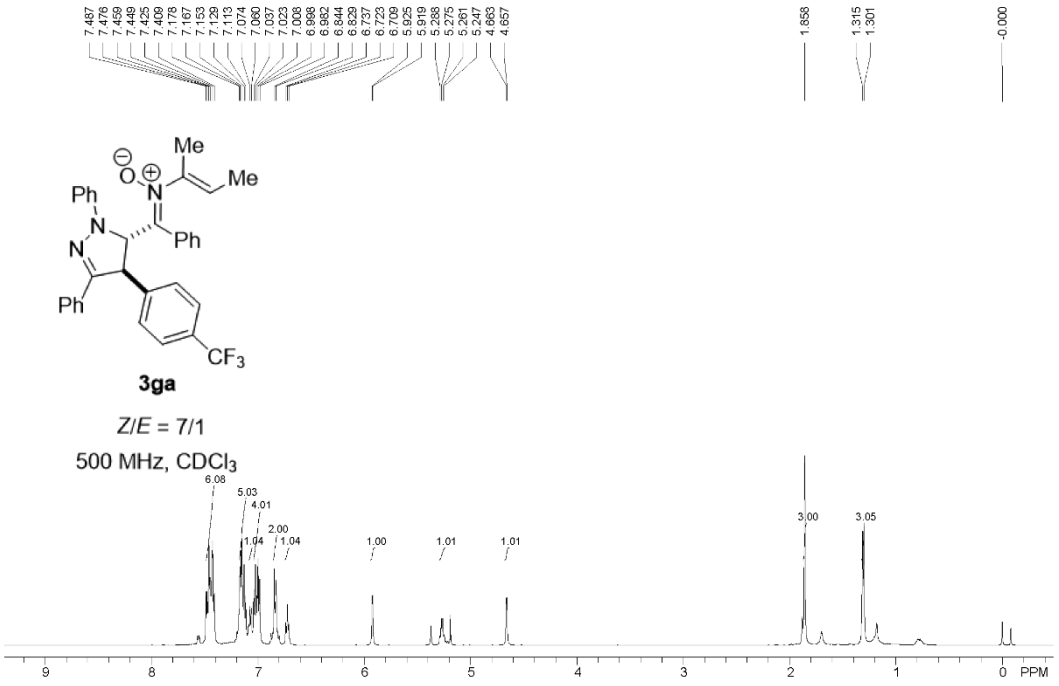

163.111
161.155
149.859
149.293
143.469
141.637
135.143
135.119
131.536
131.452
129.415
129.351
129.171
129.147
128.722
128.441
128.377
127.972
126.036
123.904
119.380
115.983
115.810
112.788
77.257
77.000
76.747
68.173
56.100
14.876
12.299
Me
Me
Ph
Ph
Ph
F
3fa
Z/E = 10/1
125 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0 PPM

3fa

Z/*E* = 10/1

470 MHz, $CDCl_3$

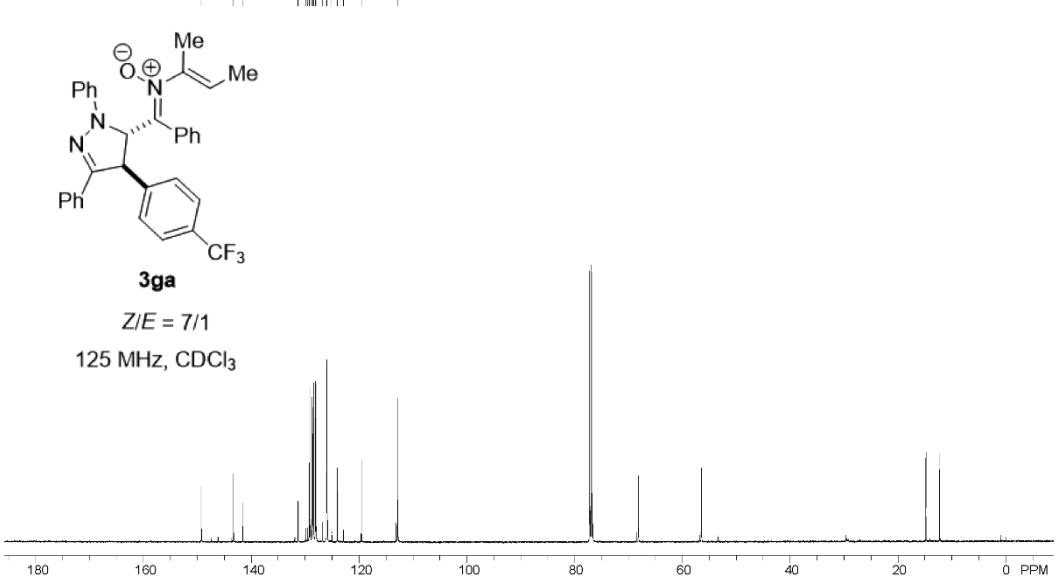




3ga

Z/*E* = 7/1

500 MHz, $CDCl_3$



3ga

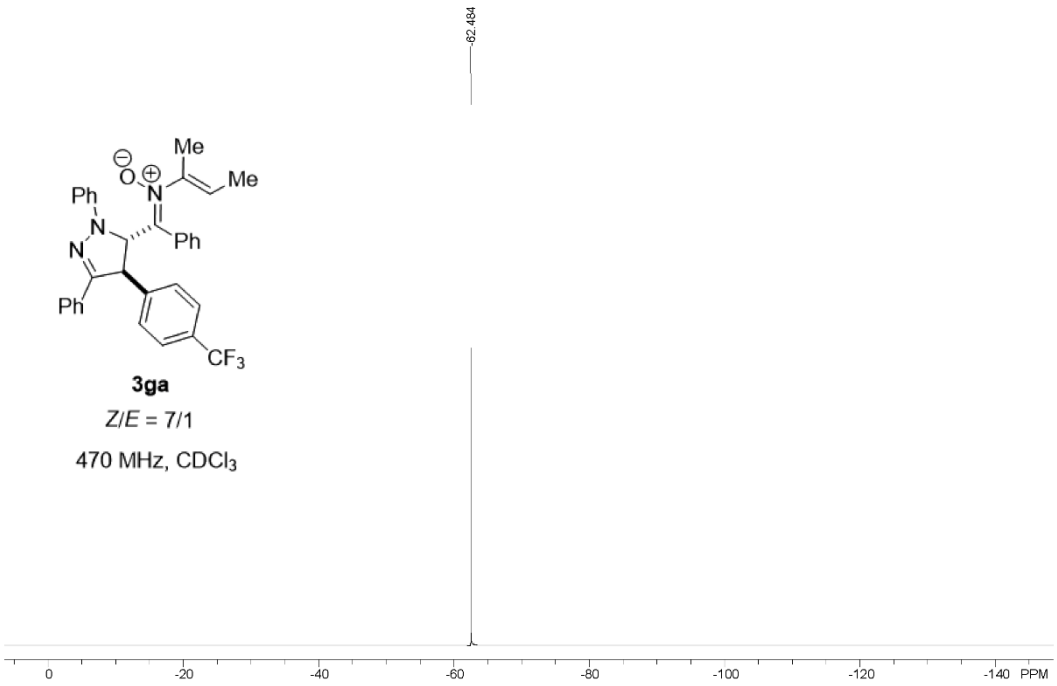
Z/*E* = 7/1

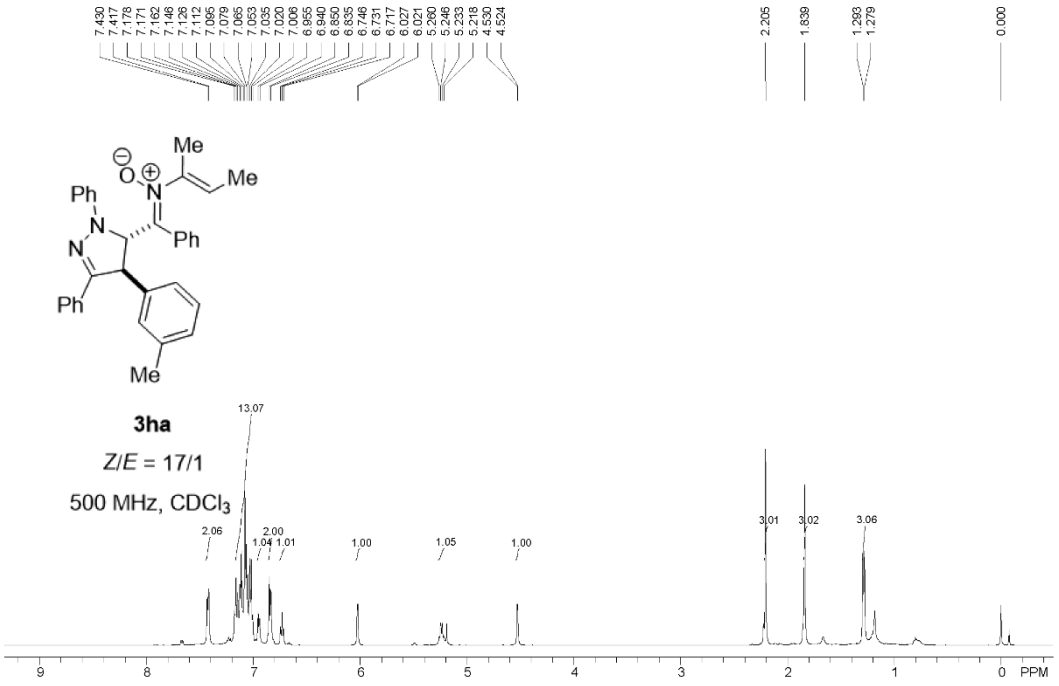
125 MHz, $CDCl_3$

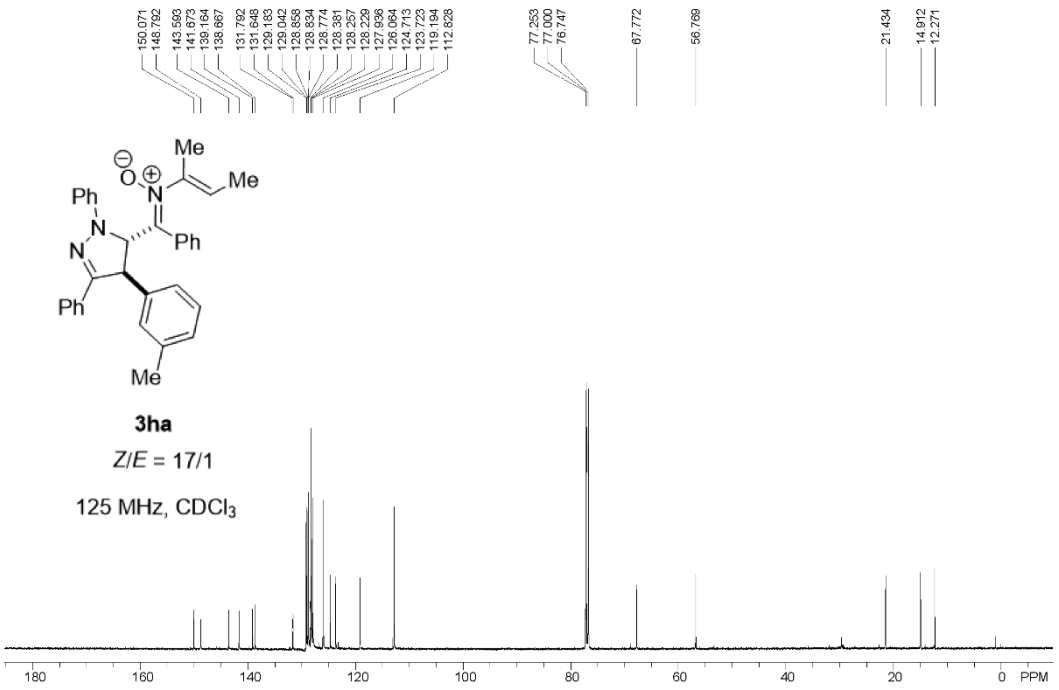
3ga

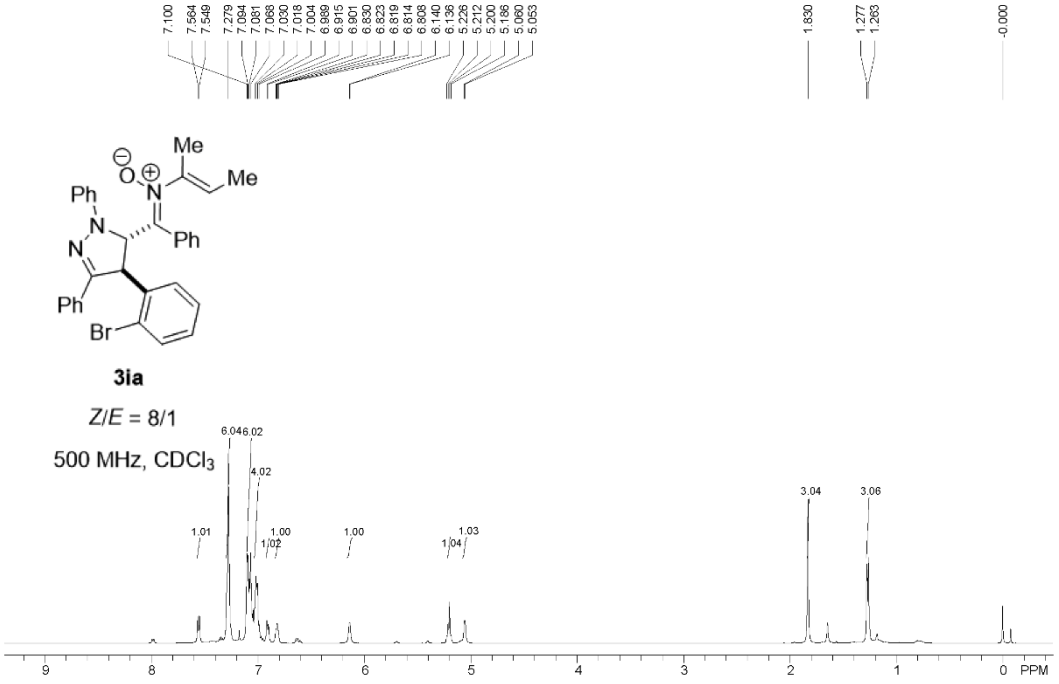
Z/*E* = 7/1

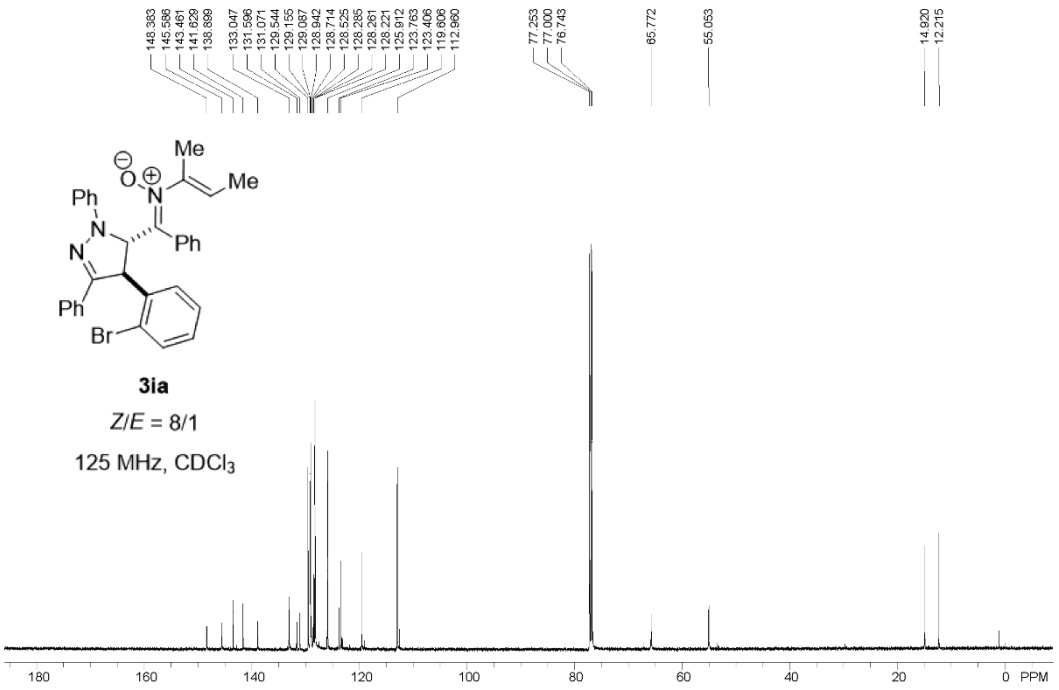
470 MHz, $CDCl_3$

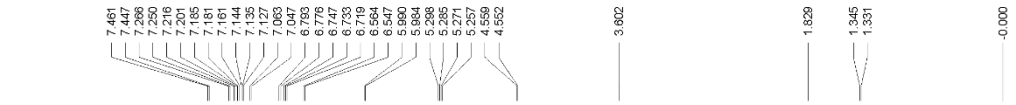


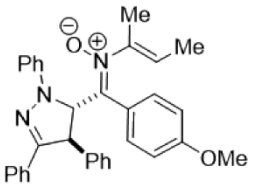

7.430
7.417
7.178
7.171
7.162
7.146
7.126
7.112
7.095
7.079
7.065
7.053
7.035
7.020
7.006
6.955
6.940
6.850
6.835
6.746
6.731
6.717
6.027
6.021
5.260
5.246
5.233
5.218
4.530
4.524
2.205
1.839
1.293
1.279
0.000
Me
Me
Ph
N
O
N
Ph
N
Ph
Ph
Me
3ha
Z/E = 17/1
500 MHz, CDCl3
13.07
2.06
2.00
1.04
1.01
1.00
1.05
1.00
3.01
3.02
3.06
9
8
7
6
5
4
3
2
1
0
PPM


150.071
148.792
143.593
141.673
139.164
138.667
131.792
131.648
129.183
129.042
128.858
128.834
128.774
128.381
128.257
128.229
127.936
126.084
124.713
123.723
119.194
112.828
77.253
77.000
76.747
67.772
56.769
21.434
14.912
12.271
Me
Me
Ph
N
O
N
Ph
N
Ph
Ph
Me
3ha
Z/E = 17/1
125 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0
PPM


7.100
7.564
7.549
7.279
7.094
7.081
7.066
7.030
7.018
7.004
6.889
6.915
6.901
6.830
6.823
6.819
6.814
6.808
6.140
6.136
5.226
5.212
5.200
5.186
5.060
5.053
1.830
1.277
1.263
0.000
Me
Me
Ph
Ph
Ph
Br
3ia
Z/E = 8/1
500 MHz, CDCl3
6.04
6.02
4.02
1.01
1.00
1.02
1.00
1.03
1.04
3.04
3.06
9
8
7
6
5
4
3
2
1
0
PPM


148.383
145.588
143.461
141.629
138.889
133.047
131.596
131.071
129.544
129.155
129.087
128.942
128.714
128.525
128.285
128.261
128.221
125.912
123.763
123.406
119.606
112.960
77.253
77.000
76.743
65.772
55.053
14.920
12.215
Me
Me
Ph
Ph
Ph
Br
3ia
Z/E = 8/1
125 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0
PPM

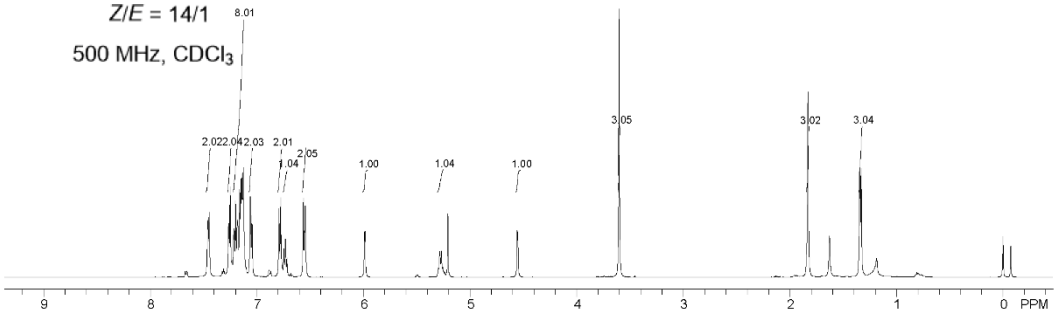


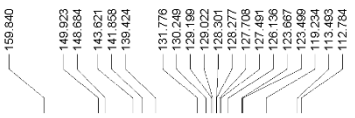


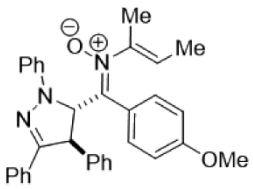
3ja

Z/*E* = 14/1

500 MHz, $CDCl_3$



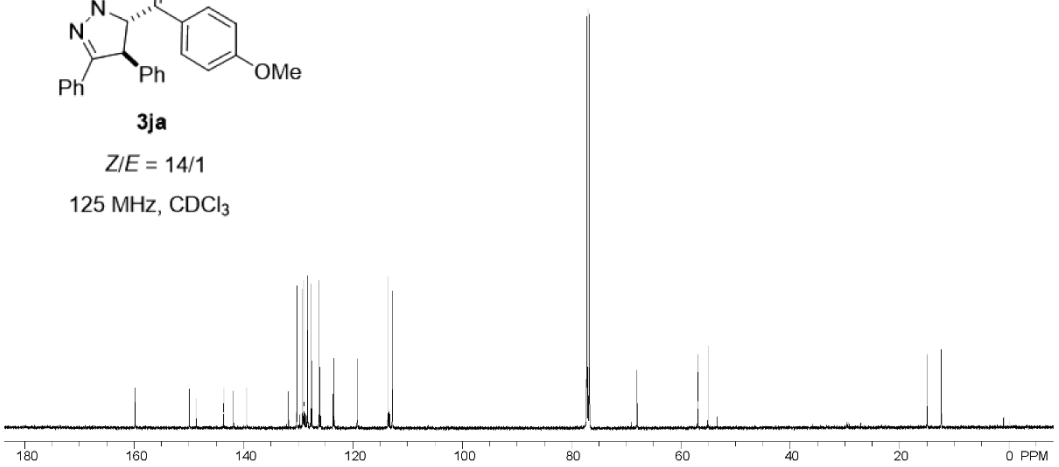


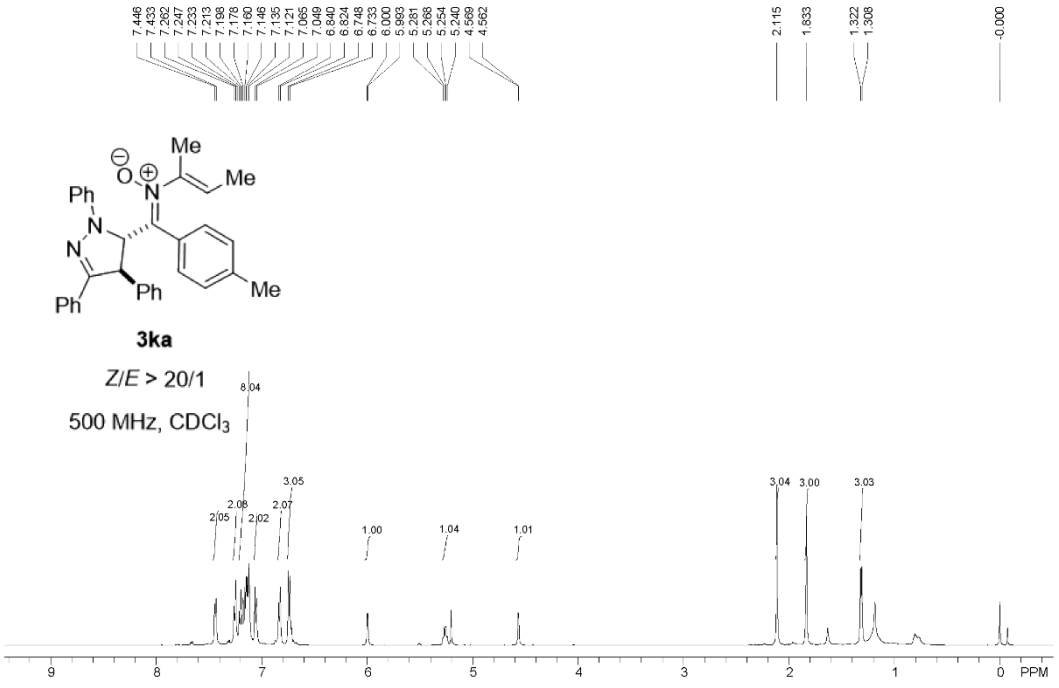


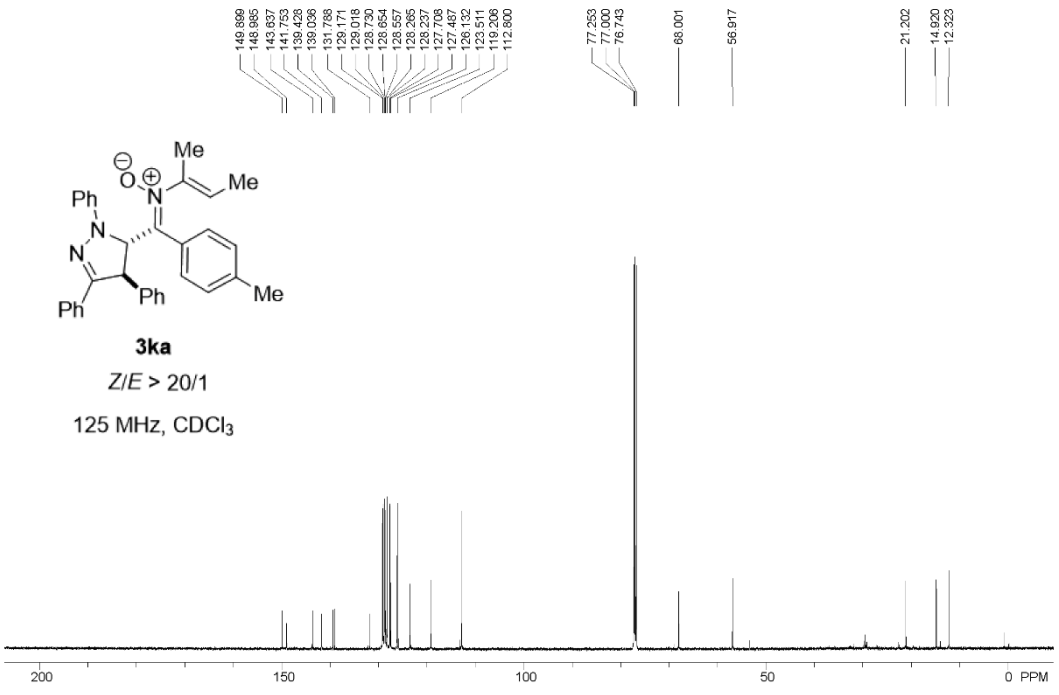
3ja

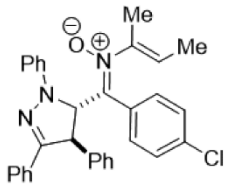
Z/*E* = 14/1

125 MHz, $CDCl_3$




7.446
7.433
7.262
7.247
7.233
7.213
7.198
7.178
7.160
7.146
7.135
7.121
7.065
7.049
6.840
6.824
6.748
6.733
6.000
5.993
5.281
5.266
5.254
5.240
4.569
4.562
2.115
1.833
1.322
1.308
0.000
Me
Me
Ph
Ph
Ph
Me
3ka
Z/E > 20/1
500 MHz, CDCl3
8.04
3.05
2.08
2.07
2.05
2.02
1.00
1.04
1.01
3.04
3.00
3.03
9
8
7
6
5
4
3
2
1
0 PPM

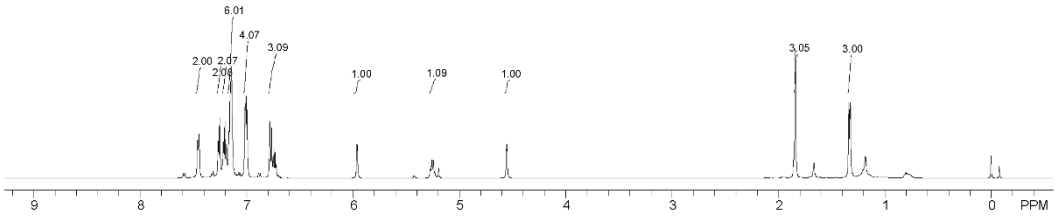

149.899
148.985
143.637
141.753
139.428
139.036
131.788
129.171
129.018
128.730
128.654
128.557
128.265
128.237
127.708
127.487
126.132
123.511
119.206
112.800
77.253
77.000
76.743
68.001
56.917
21.202
14.920
12.323
Me
Me
Ph
Ph
Ph
Me
3ka
Z/E > 20/1
125 MHz, CDCl3
200
150
100
50
0 PPM

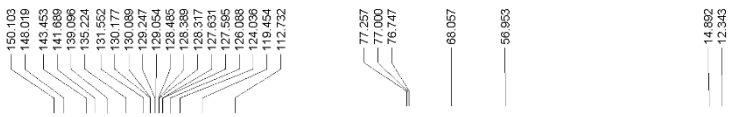


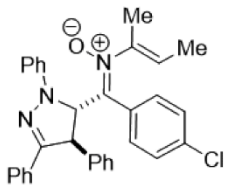
3la

Z/*E* = 13/1

500 MHz, $CDCl_3$



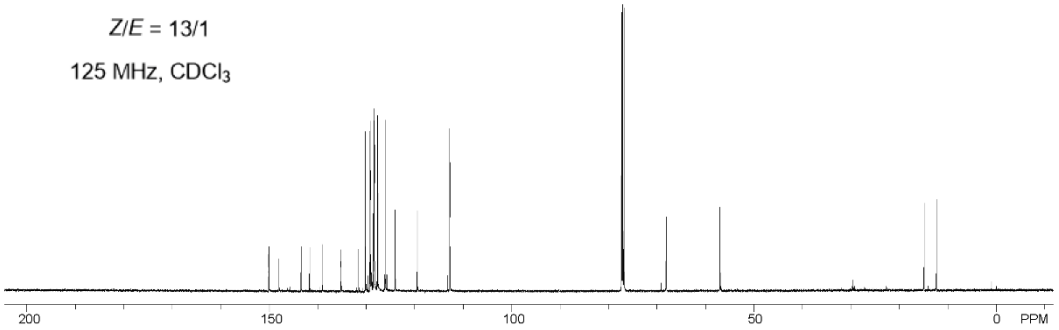


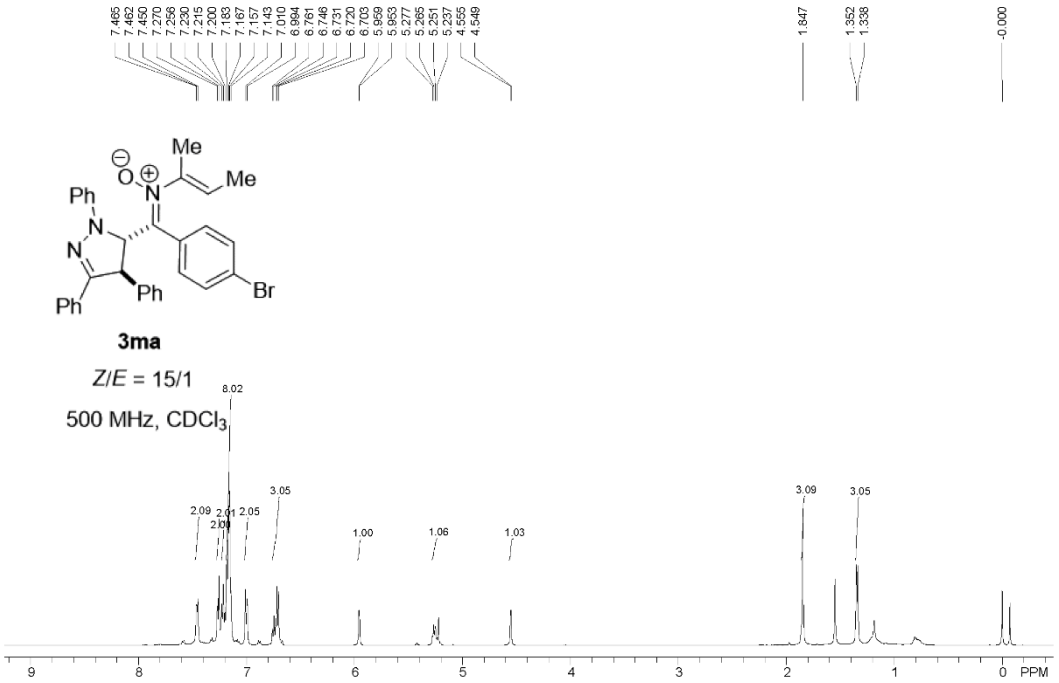


3la

Z/*E* = 13/1

125 MHz, $CDCl_3$

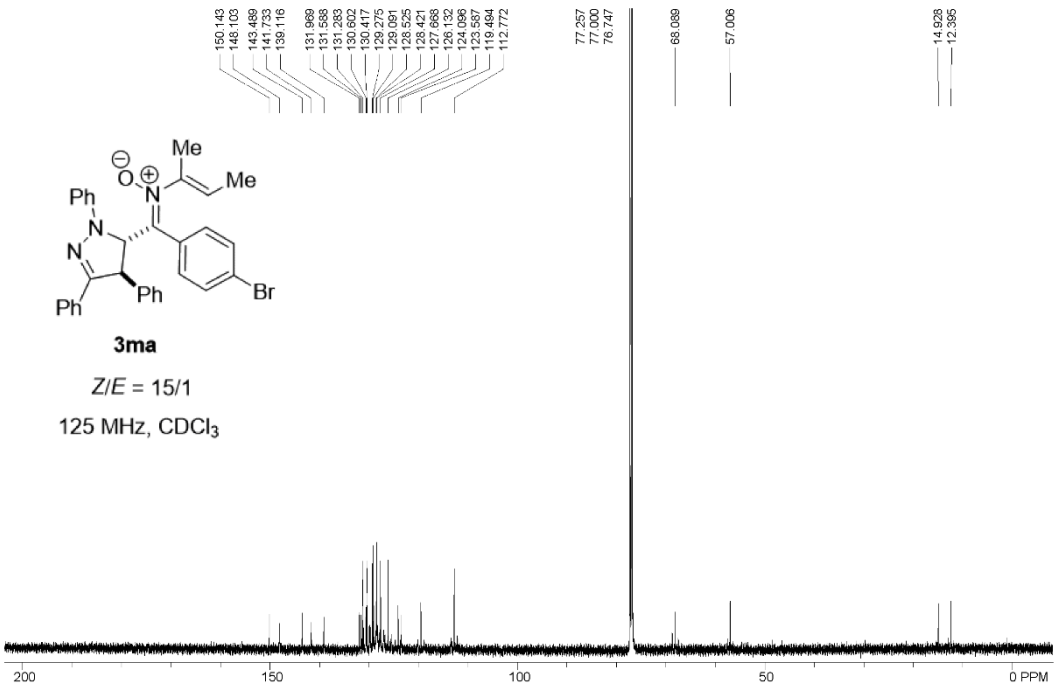




3ma

Z/*E* = 15/1

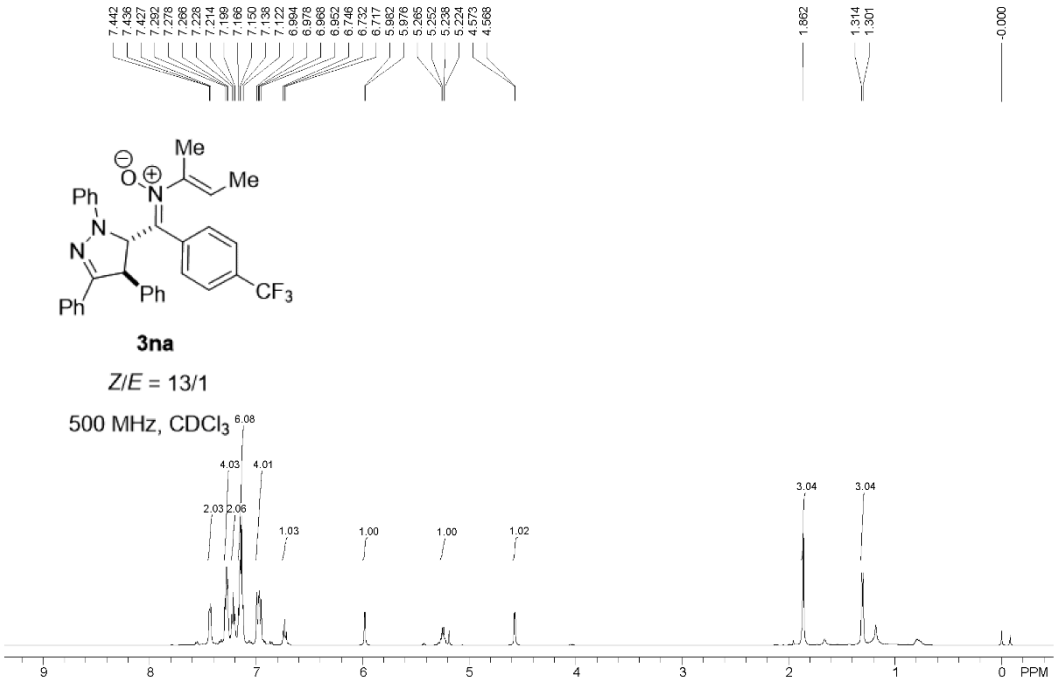
500 MHz, $CDCl_3$



3ma

Z/*E* = 15/1

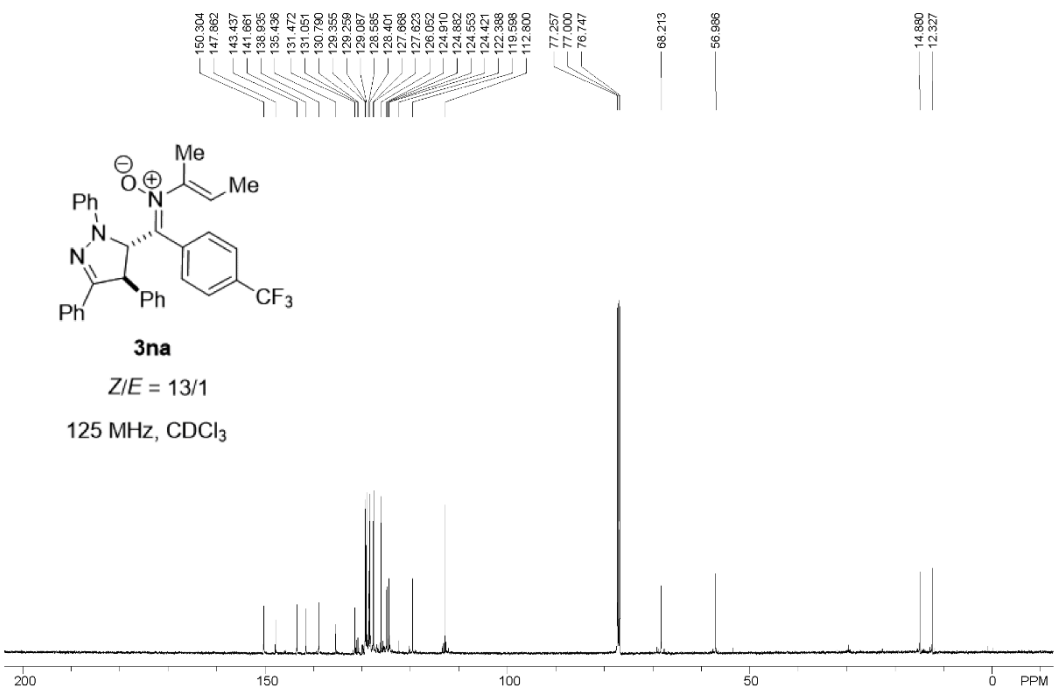
125 MHz, $CDCl_3$



3na

Z/*E* = 13/1

500 MHz, $CDCl_3$



3na

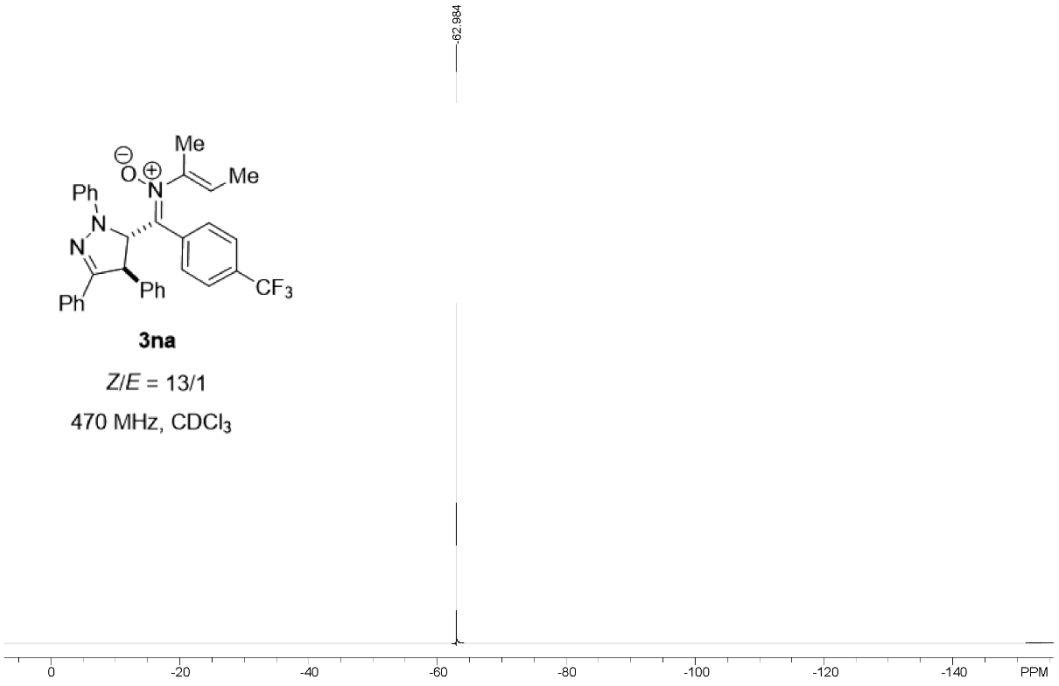
Z/*E* = 13/1

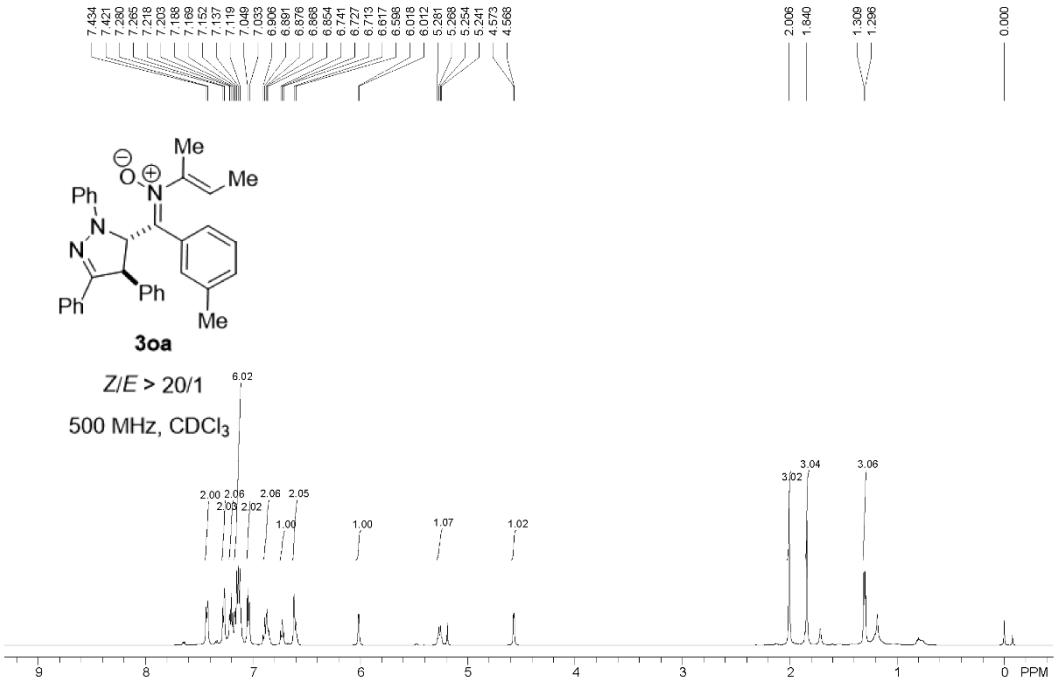
125 MHz, $CDCl_3$

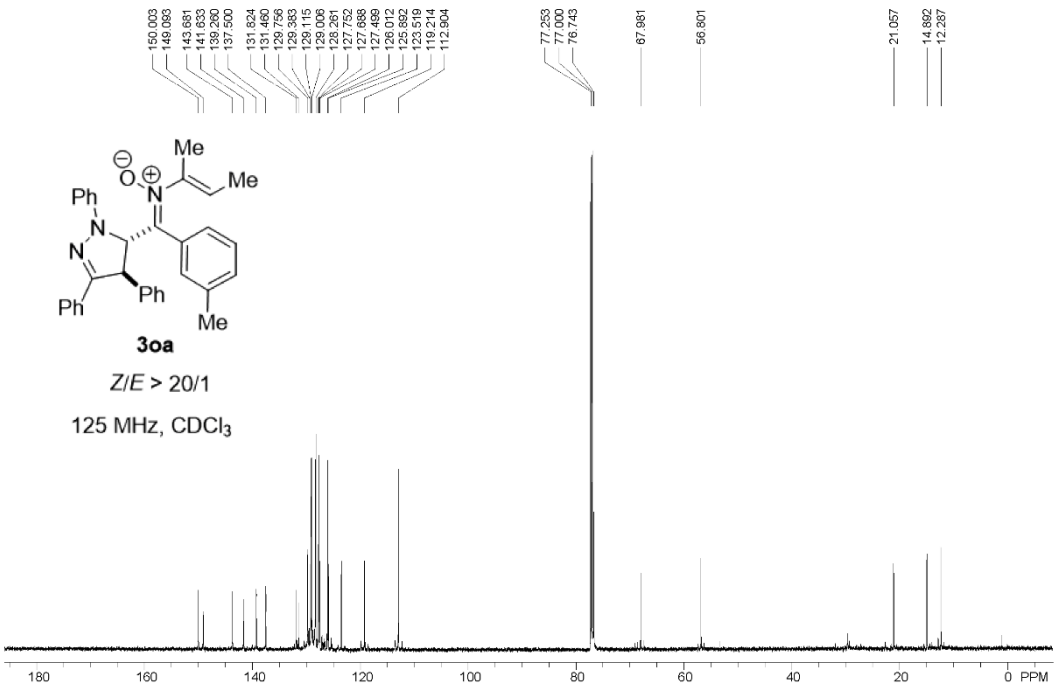
3na

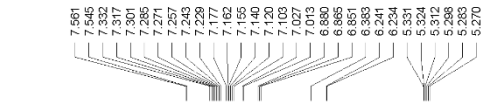
Z/*E* = 13/1

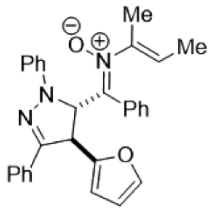
470 MHz, $CDCl_3$




7.434
7.421
7.280
7.265
7.218
7.203
7.188
7.169
7.152
7.137
7.119
7.049
7.033
6.906
6.891
6.876
6.868
6.854
6.741
6.727
6.713
6.617
6.596
6.016
6.012
5.281
5.268
5.254
5.241
4.573
4.568
2.006
1.840
1.309
1.296
0.000
Me
Me
Ph
Ph
Ph
Me
3oa
Z/E > 20/1
500 MHz, CDCl3
6.02
2.00
2.06
2.03
2.02
2.06
2.05
1.00
1.00
1.07
1.02
3.02
3.04
3.06
9
8
7
6
5
4
3
2
1
0 PPM


150.003
149.093
143.681
141.633
139.260
137.500
131.824
131.460
129.736
129.383
129.115
129.006
128.261
127.752
127.688
127.489
126.012
125.892
123.519
119.214
112.804
77.253
77.000
76.743
67.981
56.801
21.057
14.892
12.287
Me
Me
Ph
Ph
Ph
Me
3oa
Z/E > 20/1
125 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0 PPM

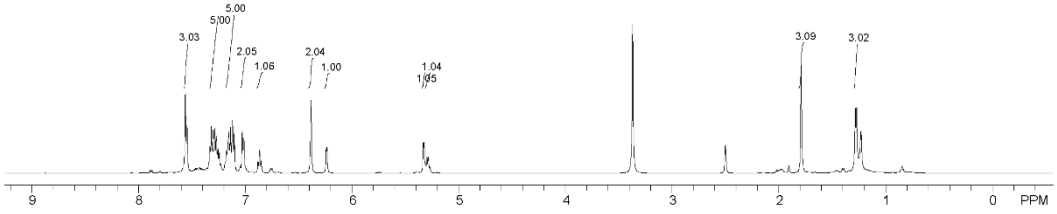


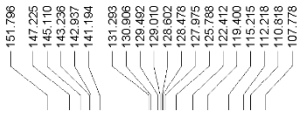


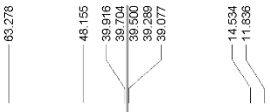
3pa

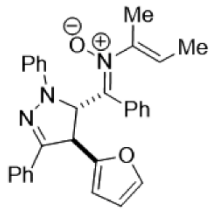
Z/*E* > 20/1

500 MHz, DMSO-d_6





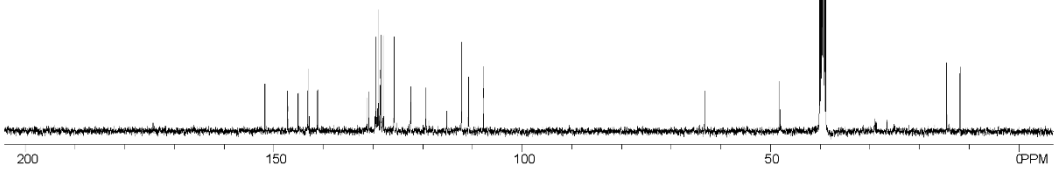


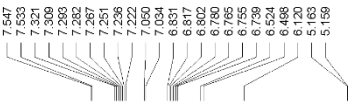


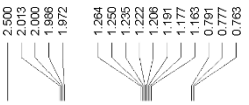
3pa

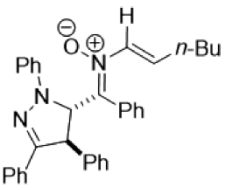
Z/*E* > 20/1

100 MHz, DMSO-d_6





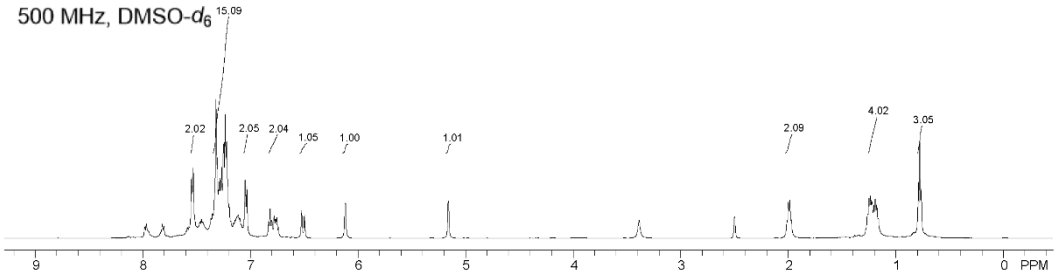


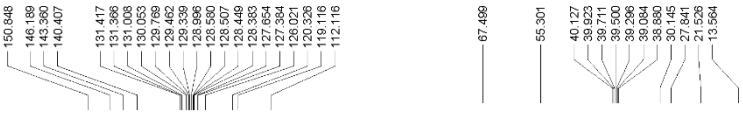


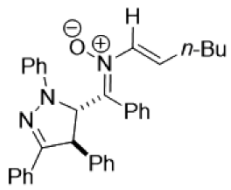
3qa

Z/*E* > 20/1

500 MHz, DMSO-d_6



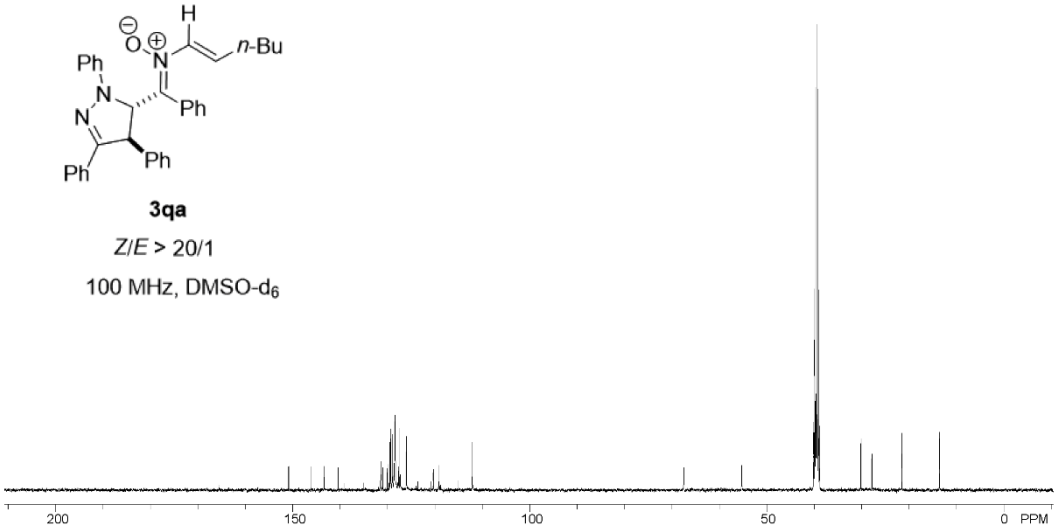


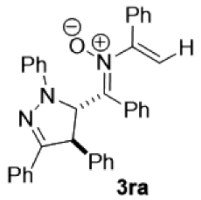


3qa

Z/*E* > 20/1

100 MHz, DMSO-d_6

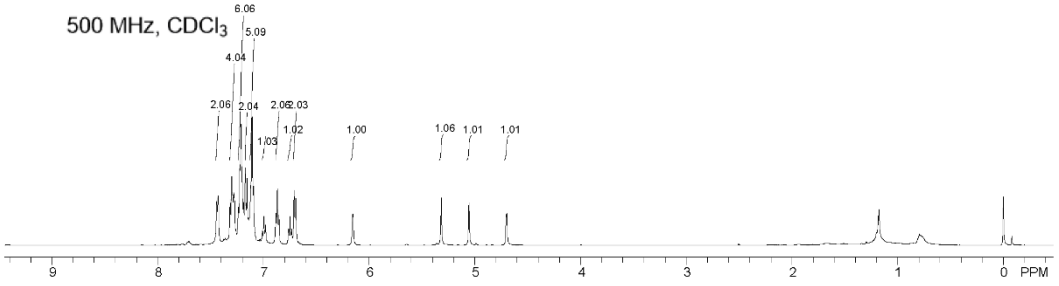


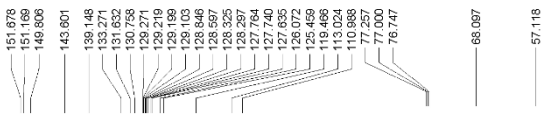


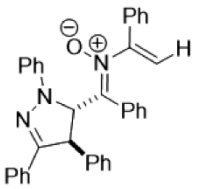
3ra

Z/*E* > 20/1

500 MHz, $CDCl_3$



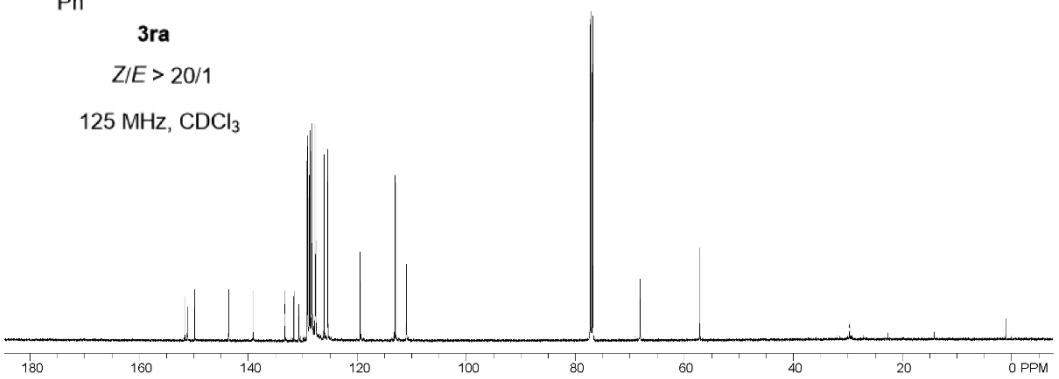


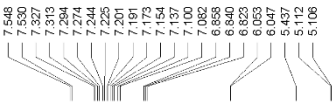


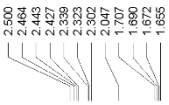
3ra

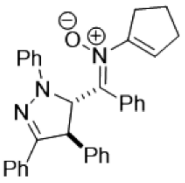
Z/*E* > 20/1

125 MHz, $CDCl_3$





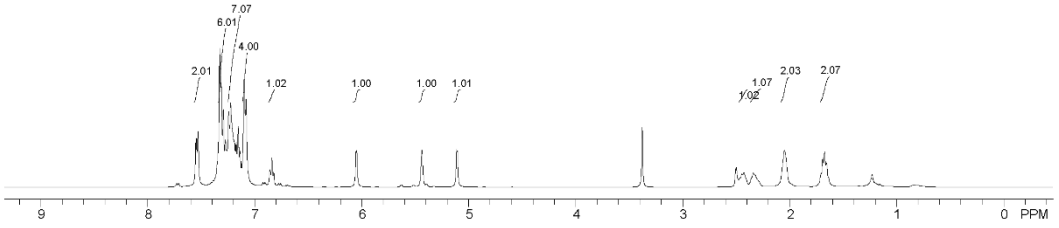


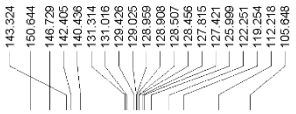


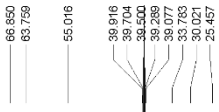
3sa

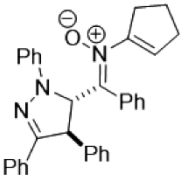
Z/*E* > 20/1

400 MHz, DMSO-d_6





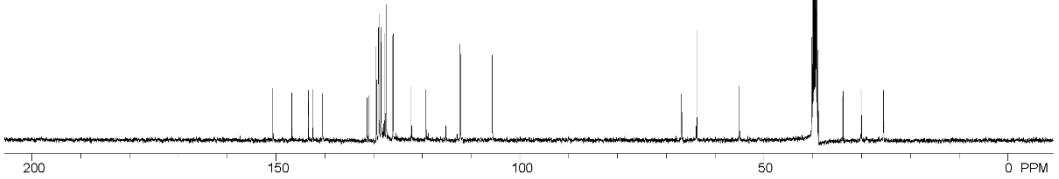


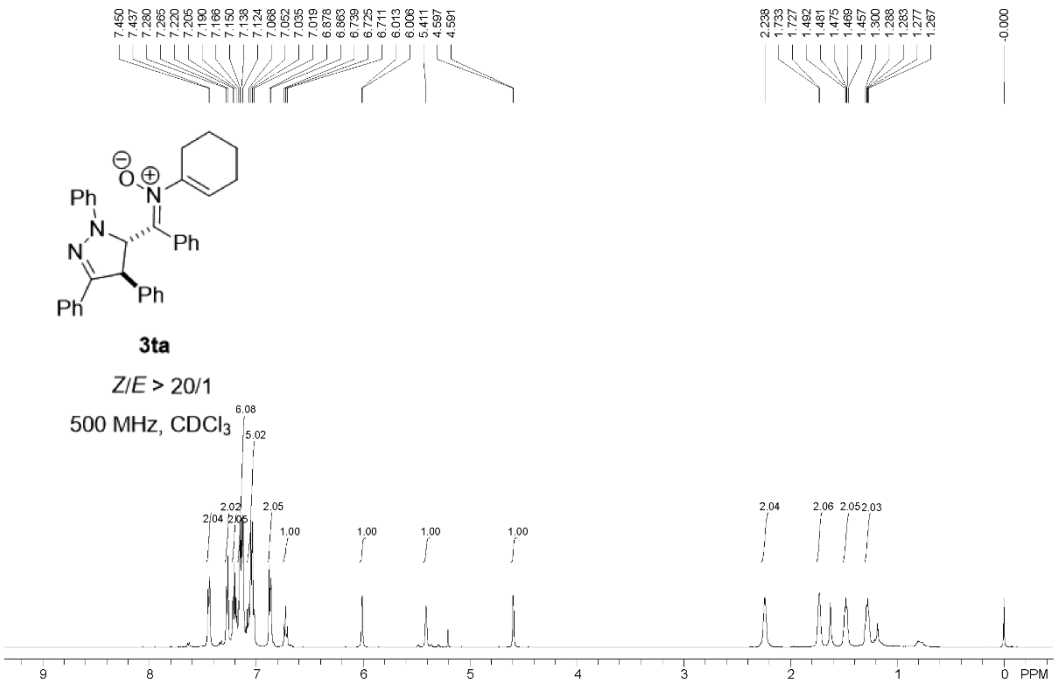


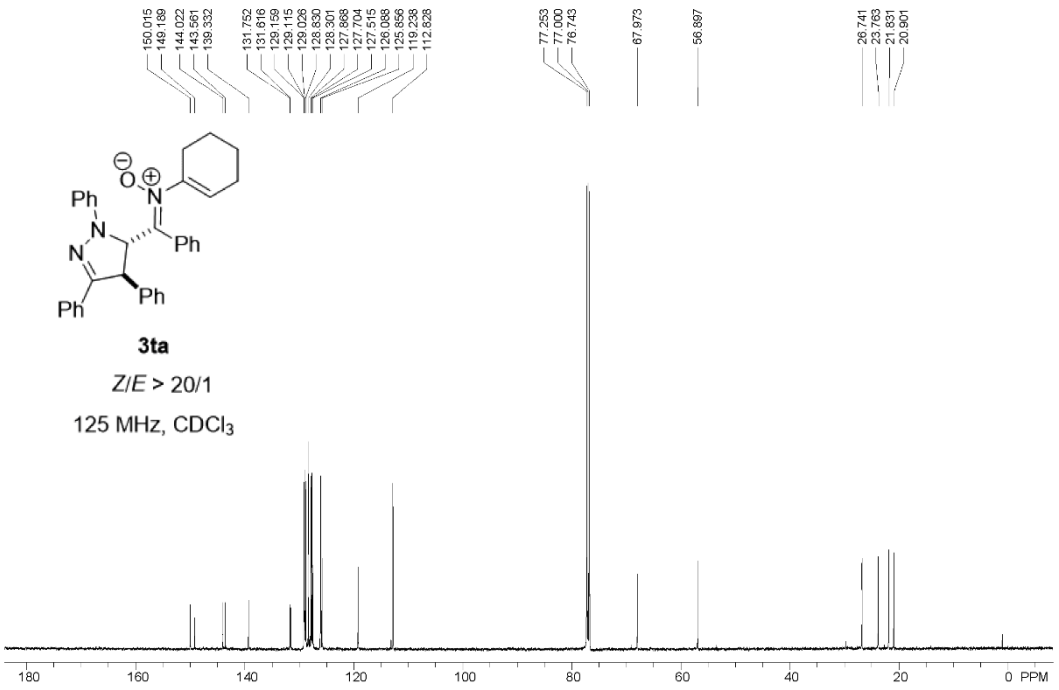
3sa

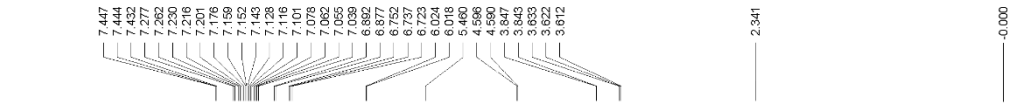
Z/*E* > 20/1

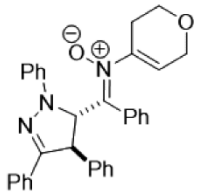
100 MHz, DMSO-d_6




7.450
7.437
7.280
7.265
7.220
7.205
7.190
7.166
7.150
7.138
7.124
7.068
7.052
7.035
7.019
6.876
6.863
6.739
6.725
6.711
6.013
6.006
5.411
4.597
4.591
2.238
1.733
1.727
1.492
1.481
1.475
1.469
1.457
1.300
1.288
1.283
1.277
1.267
0.000
Ph
N
N
Ph
Ph
Ph
O
N
3ta
Z/E > 20/1
500 MHz, CDCl3
6.08
5.02
2.04
2.02
2.05
2.05
1.00
1.00
1.00
1.00
2.04
2.06
2.05
2.03
9
8
7
6
5
4
3
2
1
0 PPM


150.015
149.189
144.022
143.561
138.332
131.752
131.616
129.159
129.115
129.026
128.830
128.301
127.868
127.704
127.515
126.088
125.856
119.238
112.828
77.253
77.000
76.743
67.973
56.897
26.741
23.763
21.831
20.901
Ph
N
N
Ph
Ph
Ph
O
N
3ta
Z/E > 20/1
125 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0 PPM

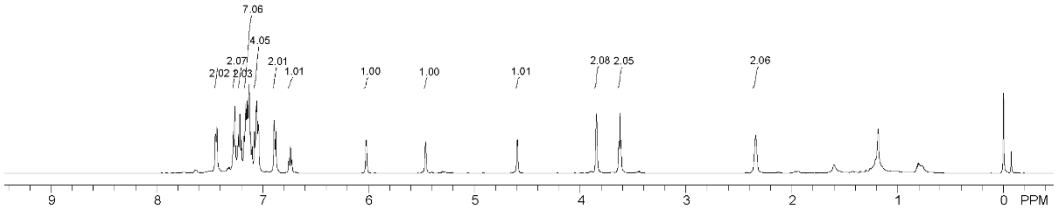


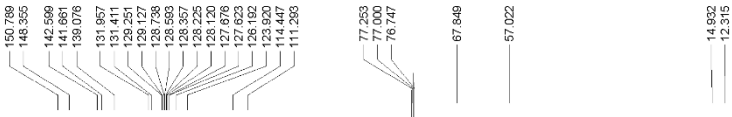


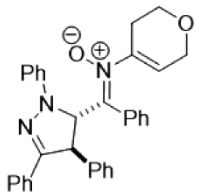
3ua

Z/*E* > 20/1

500 MHz, $CDCl_3$



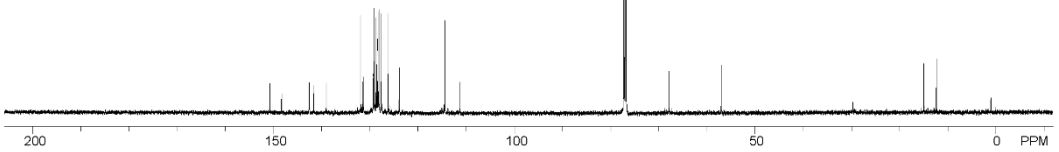


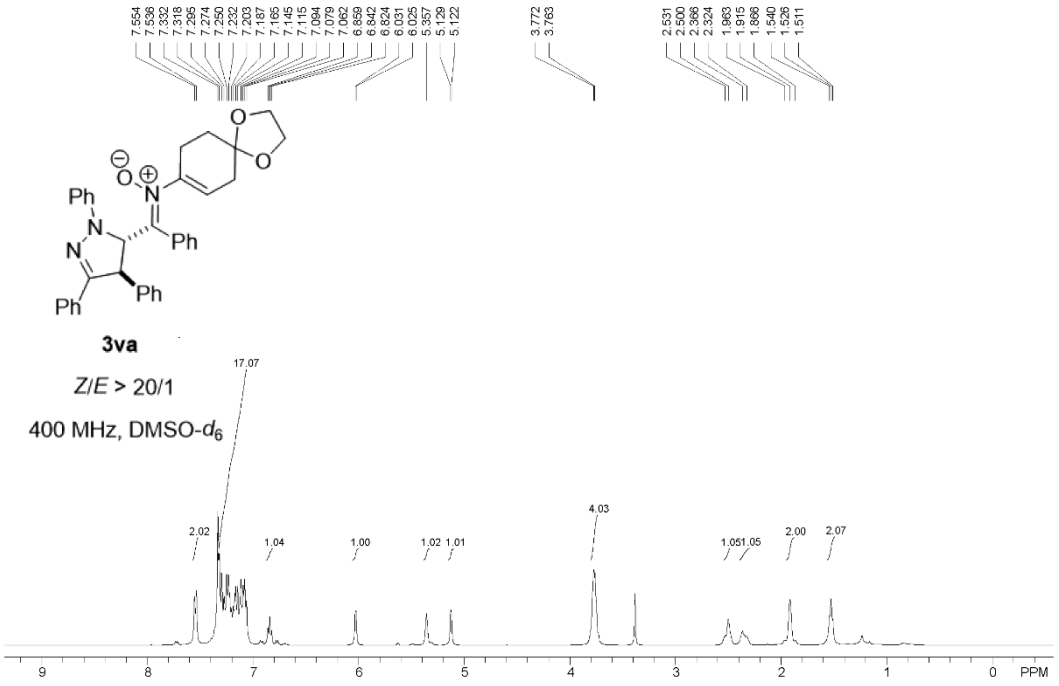


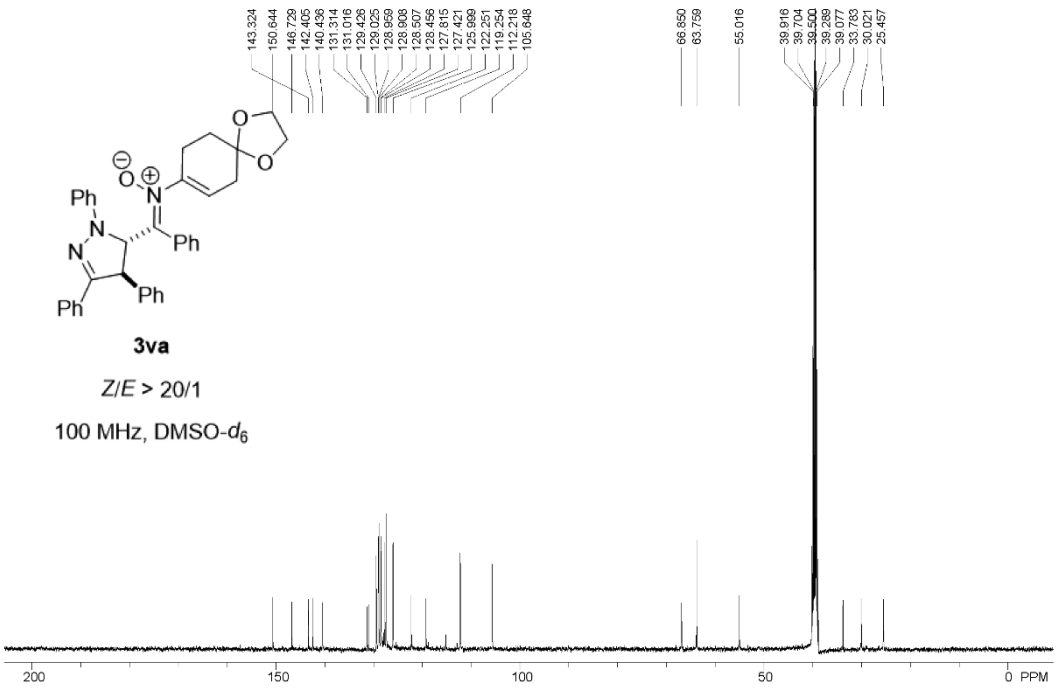
3ua

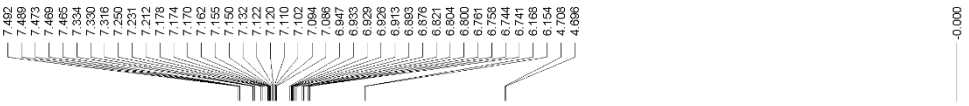
Z/*E* > 20/1

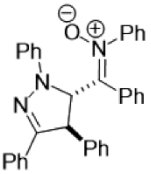
125 MHz, $CDCl_3$




7.554
7.536
7.332
7.318
7.295
7.274
7.250
7.232
7.203
7.187
7.165
7.145
7.115
7.094
7.079
7.062
6.859
6.842
6.824
6.031
6.025
5.357
5.129
5.122
3.772
3.763
2.531
2.500
2.366
2.324
1.963
1.915
1.886
1.540
1.526
1.511
O
O
O
N
Ph
N
Ph
Ph
N
Ph
Ph
3va
Z/E > 20/1
400 MHz, DMSO-d6
17.07
2.02
1.04
1.00
1.02
1.01
4.03
1.05
1.05
2.00
2.07
9
8
7
6
5
4
3
2
1
0
PPM


143.324
150.644
146.729
142.465
140.436
131.314
131.016
129.426
129.025
128.959
128.908
128.507
128.456
127.815
127.421
125.969
122.251
119.254
112.218
105.648
66.850
63.759
55.016
39.916
39.704
39.500
39.289
39.077
33.783
30.021
25.457
O
O
O
N
Ph
N
Ph
Ph
N
Ph
Ph
3va
Z/E > 20/1
100 MHz, DMSO-d6
200
150
100
50
0
PPM

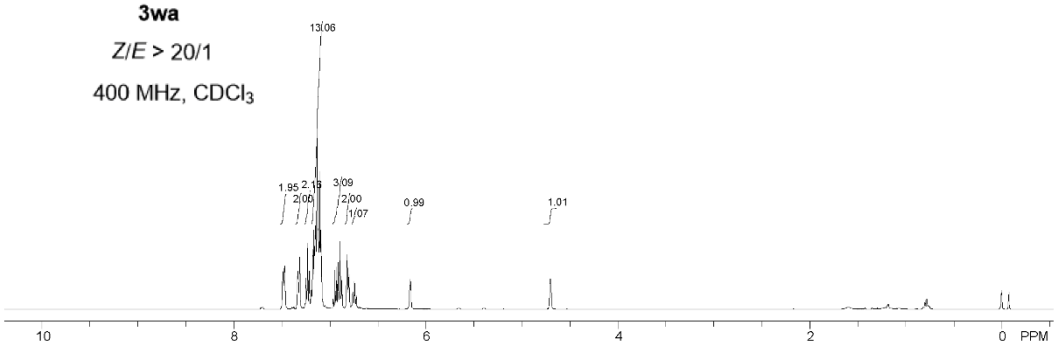


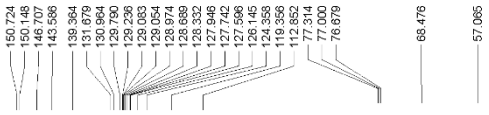


3wa

Z/*E* > 20/1

400 MHz, $CDCl_3$

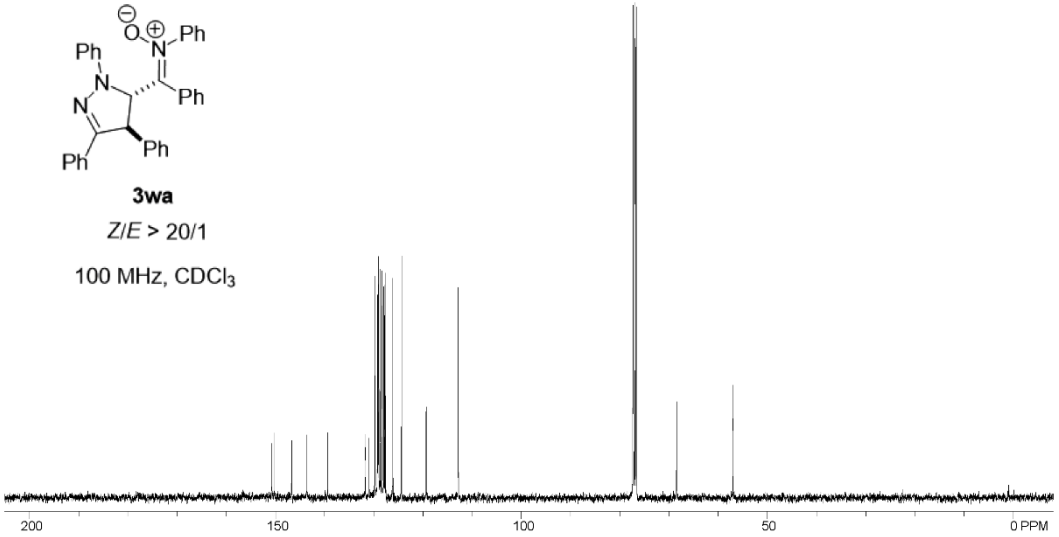


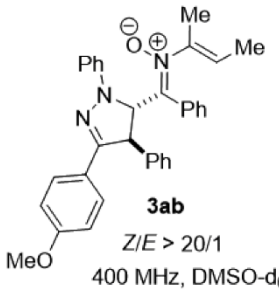


3wa

Z/*E* > 20/1

100 MHz, $CDCl_3$

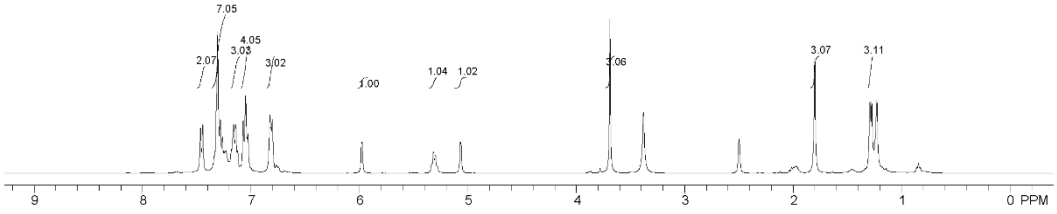


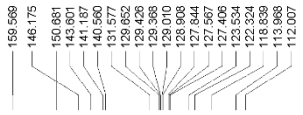


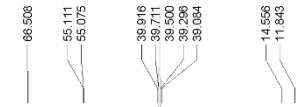
3ab

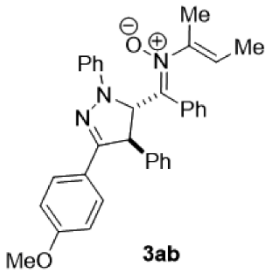
Z/*E* > 20/1

400 MHz, DMSO-d_6





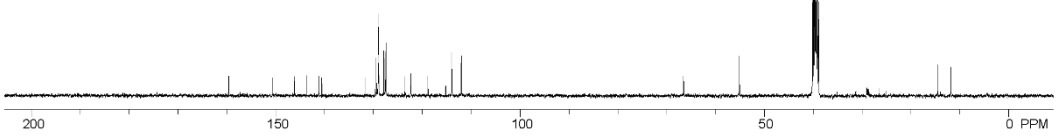


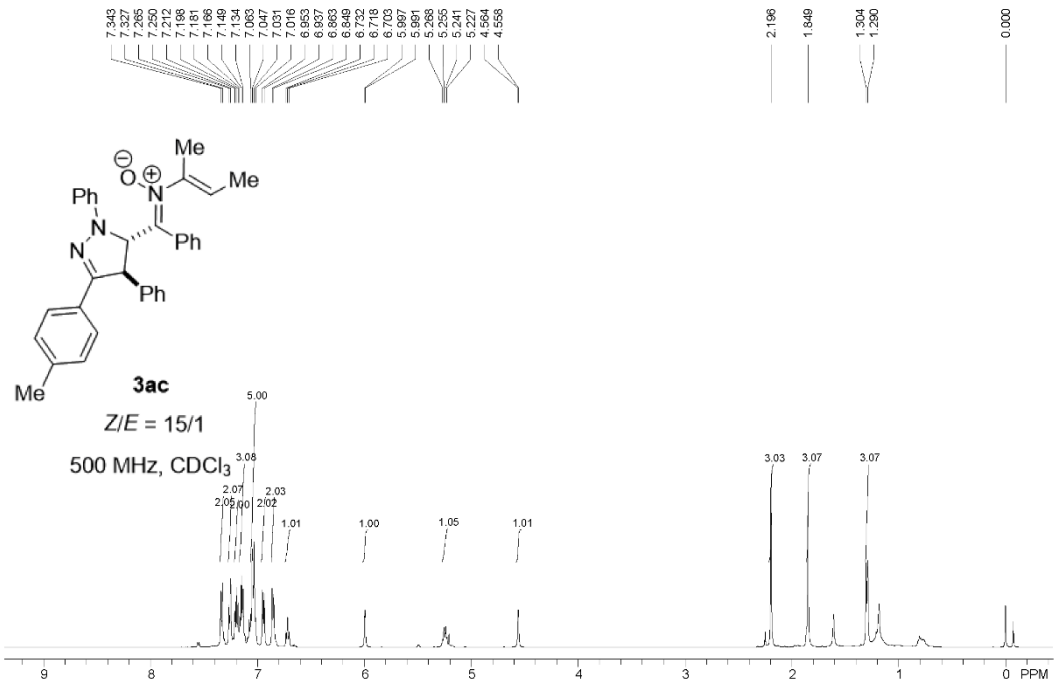


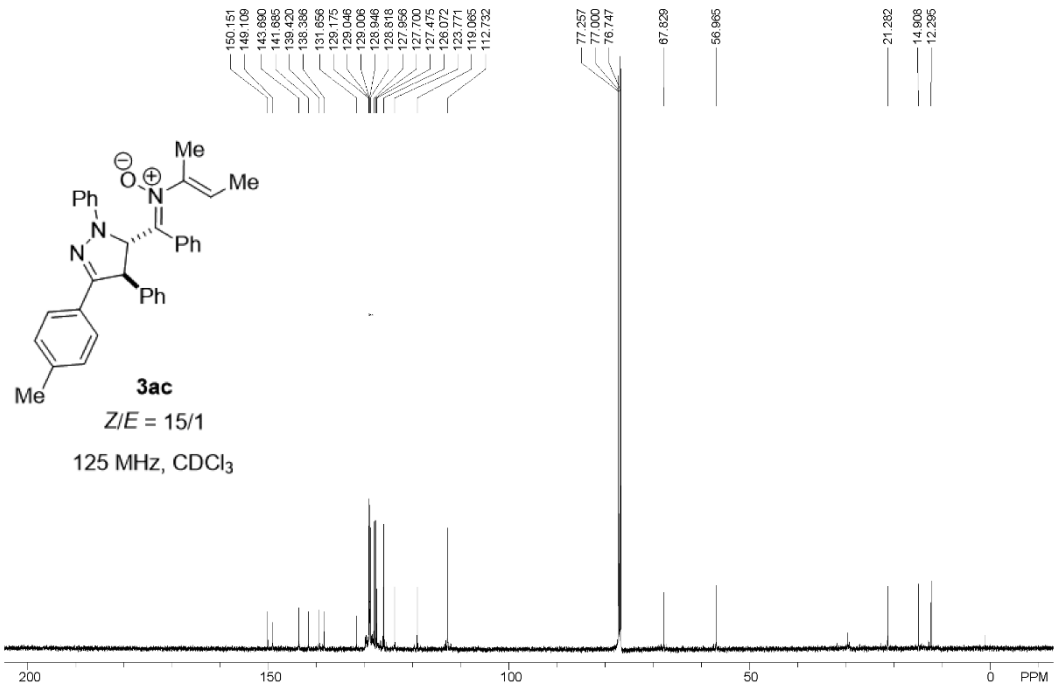
3ab

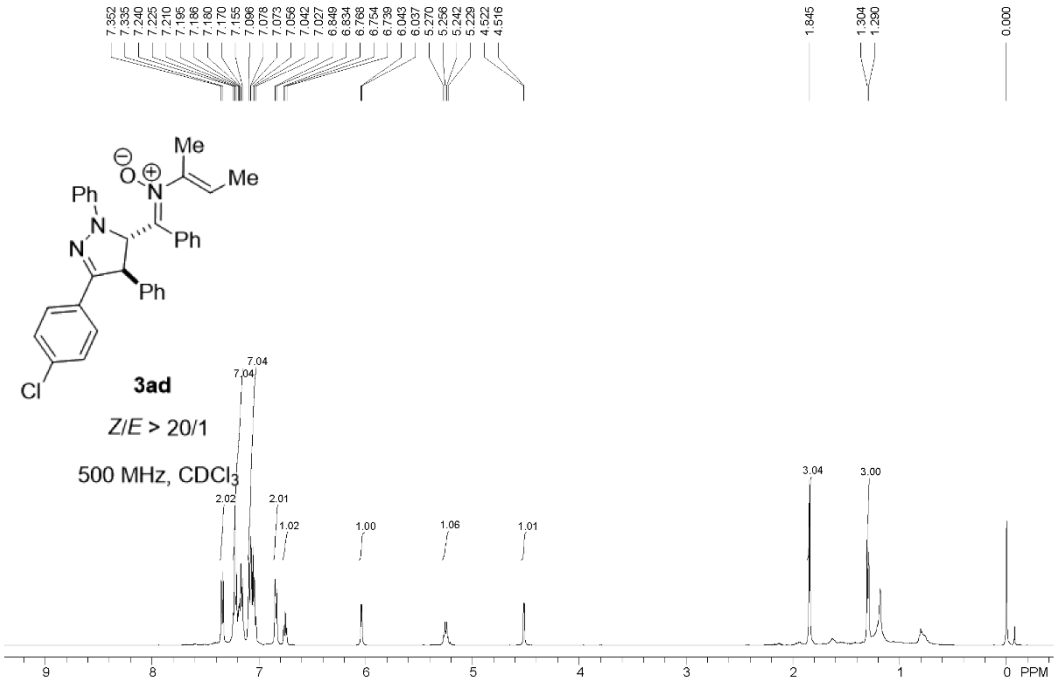
Z/*E* > 20/1

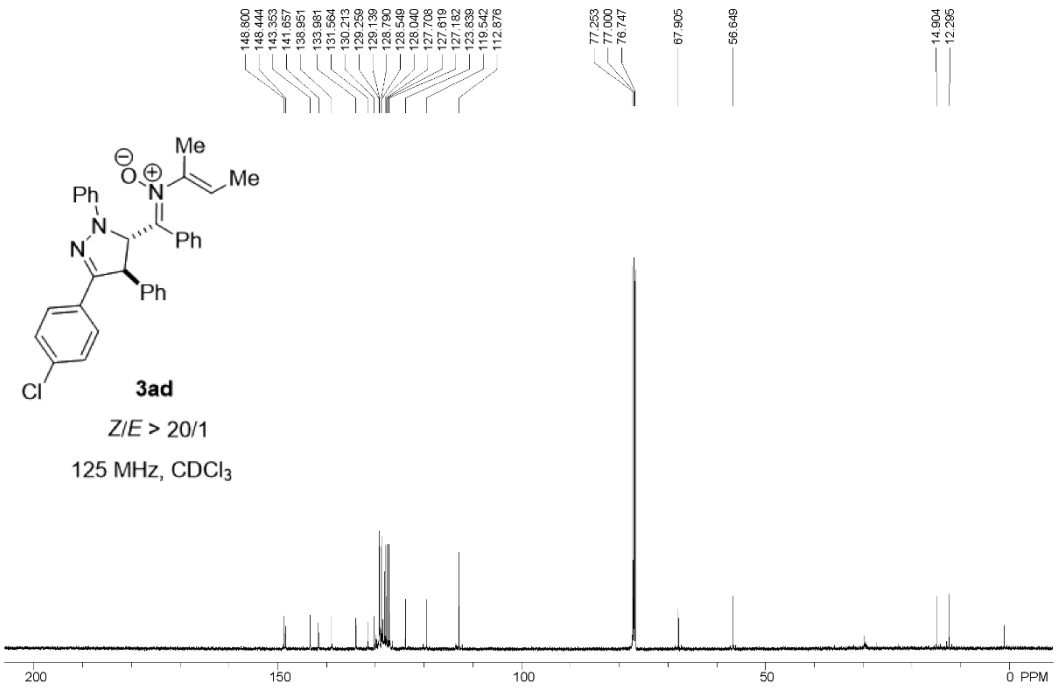
100 MHz, DMSO-d_6

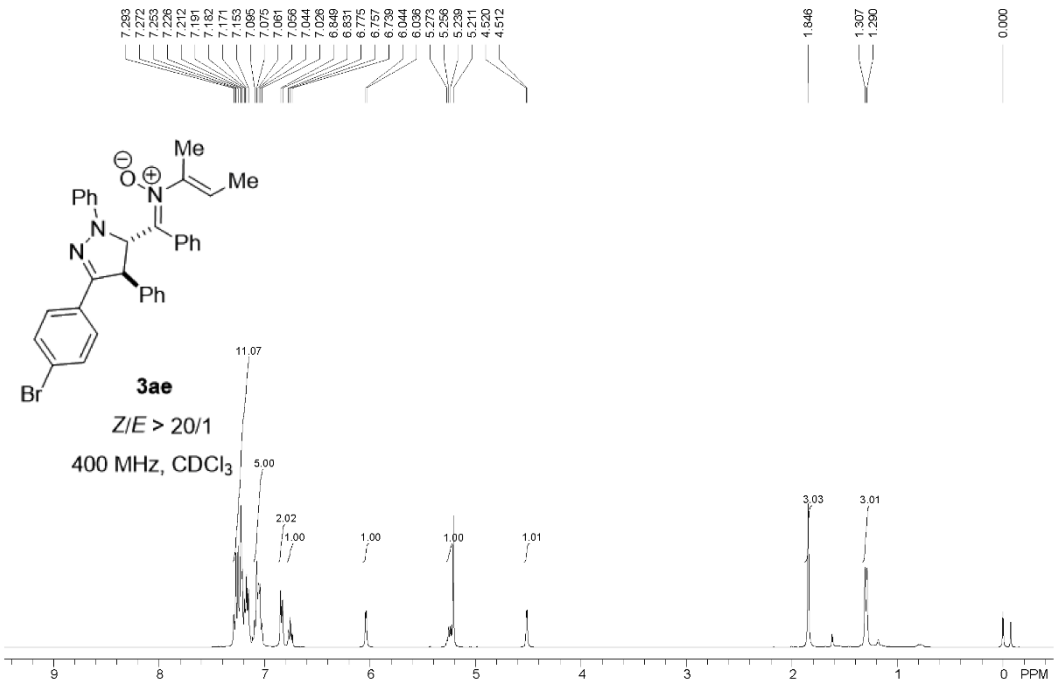


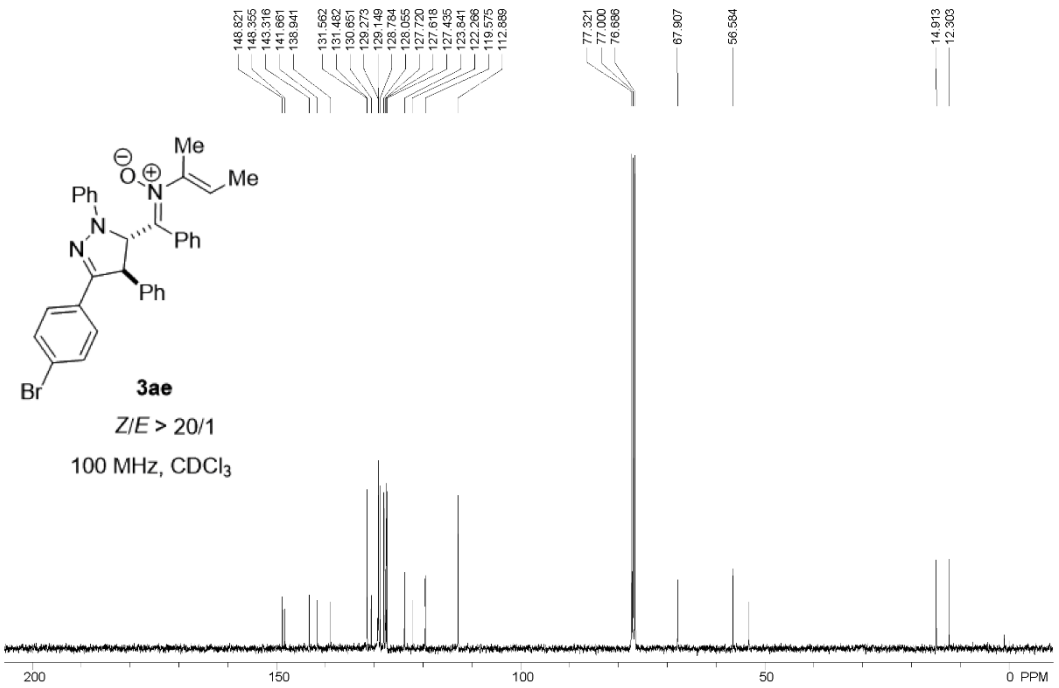

7.343
7.327
7.285
7.250
7.212
7.198
7.181
7.166
7.149
7.134
7.063
7.047
7.031
7.016
6.853
6.837
6.803
6.849
6.732
6.718
6.703
5.997
5.991
5.268
5.255
5.241
5.227
4.564
4.558
2.196
1.849
1.304
1.290
0.000
Me
Me
Ph
Ph
Ph
Me
3ac
Z/E = 15/1
500 MHz, CDCl3
5.00
3.08
2.07
2.05
2.00
2.03
2.02
1.01
1.00
1.05
1.01
3.03
3.07
3.07
9
8
7
6
5
4
3
2
1
0
PPM

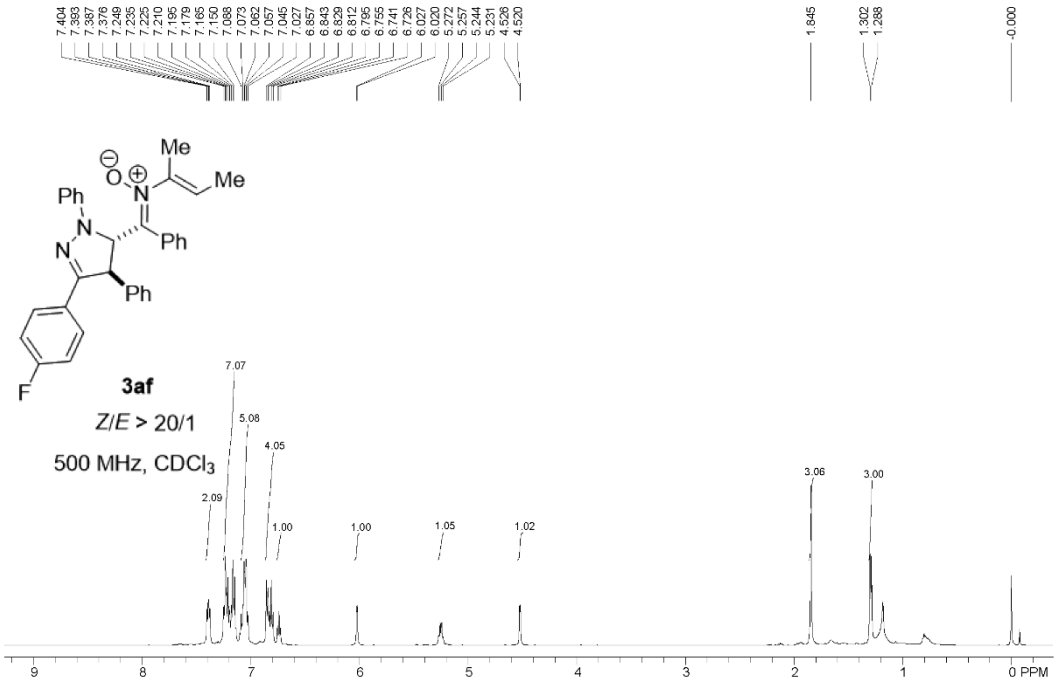

150.151
149.109
143.690
141.685
139.420
138.388
131.658
129.175
129.048
129.006
128.946
128.818
127.956
127.700
127.475
126.072
123.771
119.065
112.732
77.257
77.000
76.747
67.829
56.965
21.282
14.908
12.295
Me
Me
Ph
Ph
Ph
Me
3ac
Z/E = 15/1
125 MHz, CDCl3
200
150
100
50
0
PPM

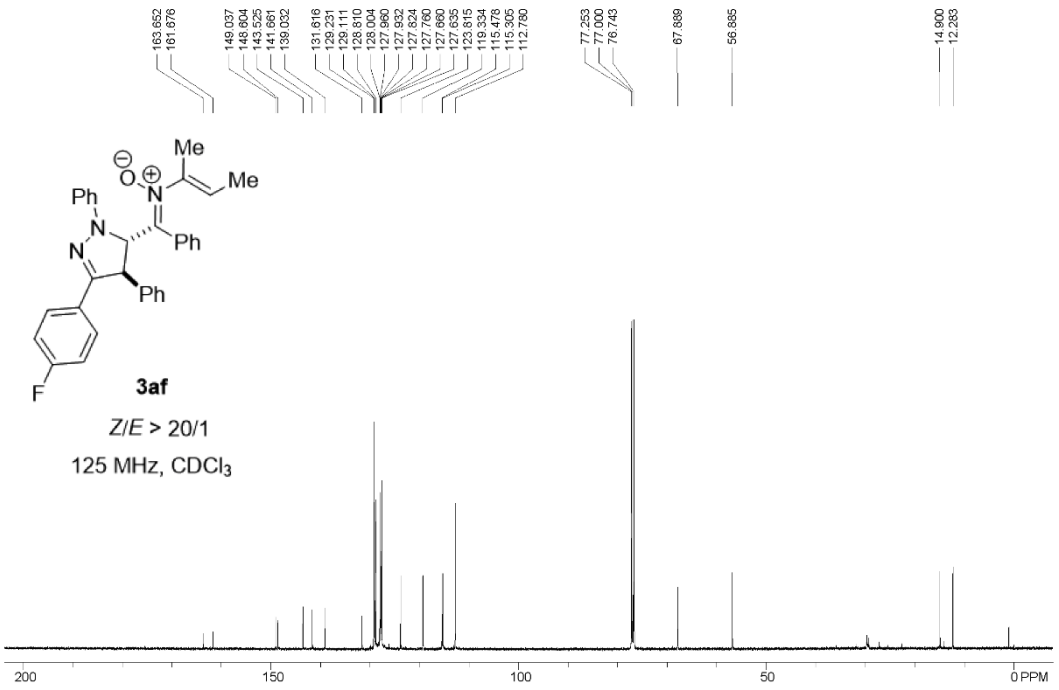

7.352
7.335
7.240
7.225
7.210
7.195
7.188
7.180
7.170
7.155
7.098
7.078
7.073
7.056
7.042
7.027
6.849
6.834
6.788
6.754
6.739
6.043
6.037
5.270
5.256
5.242
5.228
4.522
4.516
1.845
1.304
1.290
0.000
Me
Me
Ph
Ph
Ph
Ph
Cl
3ad
Z/E > 20/1
500 MHz, CDCl3
7.04
7.04
2.02
2.01
1.02
1.00
1.06
1.01
3.04
3.00
9
8
7
6
5
4
3
2
1
0 PPM


148.800
148.444
143.353
141.657
138.951
133.981
131.564
130.213
129.259
129.139
128.790
128.549
128.040
127.708
127.619
127.182
123.839
119.542
112.876
77.253
77.000
76.747
67.905
56.649
14.904
12.295
Me
Me
Ph
Ph
Ph
Ph
Cl
3ad
Z/E > 20/1
125 MHz, CDCl3
200
150
100
50
0 PPM


7.293
7.272
7.253
7.226
7.212
7.191
7.182
7.171
7.153
7.095
7.075
7.061
7.056
7.044
7.028
6.849
6.831
6.775
6.757
6.739
6.044
6.038
5.273
5.256
5.239
5.211
4.520
4.512
1.846
1.307
1.290
0.000
Me
Me
Ph
Ph
Ph
Ph
Br
3ae
Z/E > 20/1
400 MHz, CDCl3
11.07
5.00
2.02
1.00
1.00
1.00
1.01
3.03
3.01
9
8
7
6
5
4
3
2
1
0 PPM


148.821
148.355
143.316
141.661
138.941
131.562
131.462
130.651
129.273
129.149
128.784
128.055
127.720
127.618
127.435
123.841
122.268
119.575
112.869
77.321
77.000
76.686
67.907
56.584
14.913
12.303
Me
Me
Ph
Ph
Ph
Ph
Br
3ae
Z/E > 20/1
100 MHz, CDCl3
200
150
100
50
0 PPM

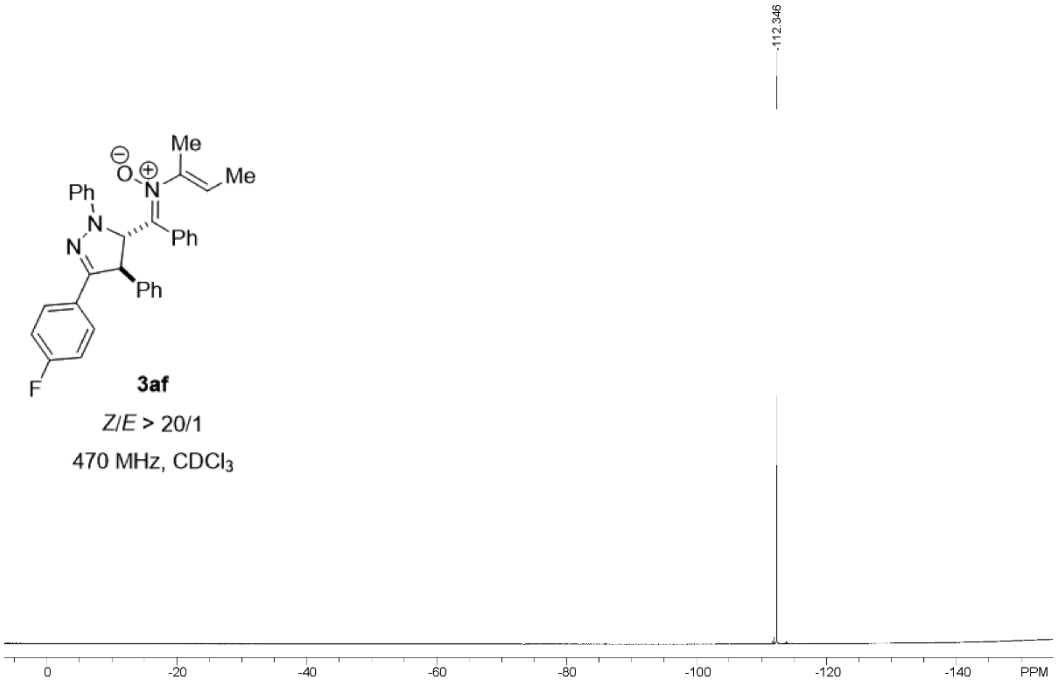

7.404
7.393
7.387
7.376
7.249
7.235
7.225
7.210
7.195
7.179
7.165
7.150
7.088
7.073
7.062
7.057
7.045
7.027
6.857
6.843
6.829
6.812
6.795
6.755
6.741
6.726
6.027
6.020
5.272
5.257
5.244
5.231
4.528
4.520
1.845
1.302
1.288
0.000
Me
Me
Ph
Ph
Ph
Ph
F
3af
Z/E > 20/1
500 MHz, CDCl3
7.07
5.08
4.05
2.09
1.00
1.00
1.05
1.02
3.06
3.00
9
8
7
6
5
4
3
2
1
0 PPM

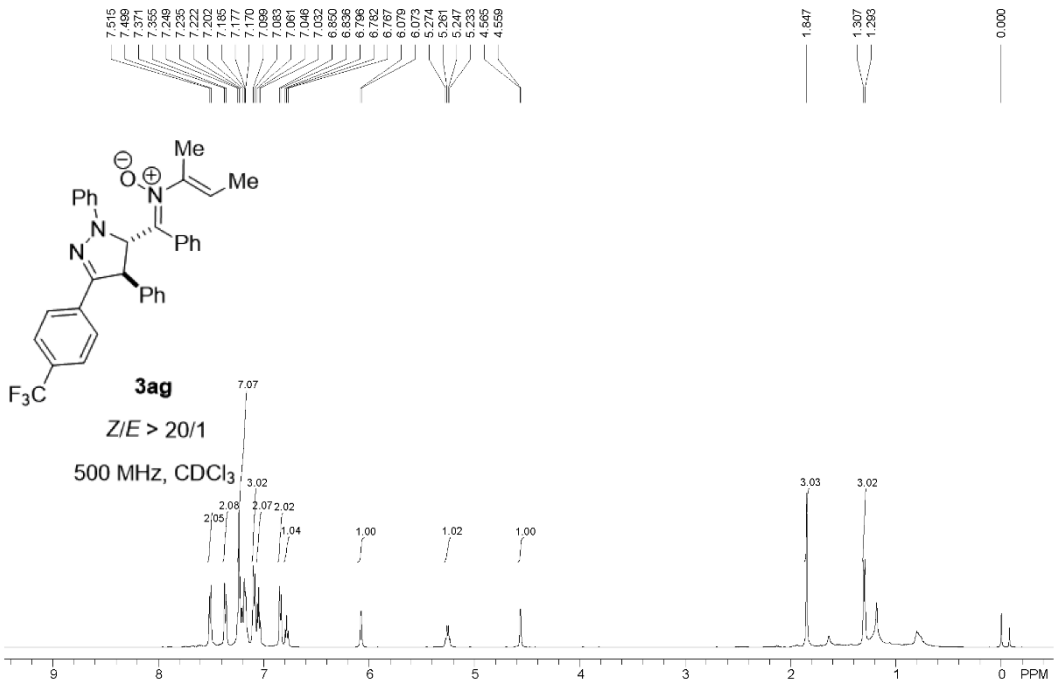

163.652
161.676
149.037
148.604
143.525
141.661
139.032
131.616
129.231
129.111
128.810
128.004
127.960
127.932
127.824
127.760
127.660
127.635
123.815
119.334
115.478
115.305
112.780
77.253
77.000
76.743
67.889
56.885
14.900
12.283
Me
Me
Ph
Ph
Ph
Ph
F
3af
Z/E > 20/1
125 MHz, CDCl3
200
150
100
50
0 PPM

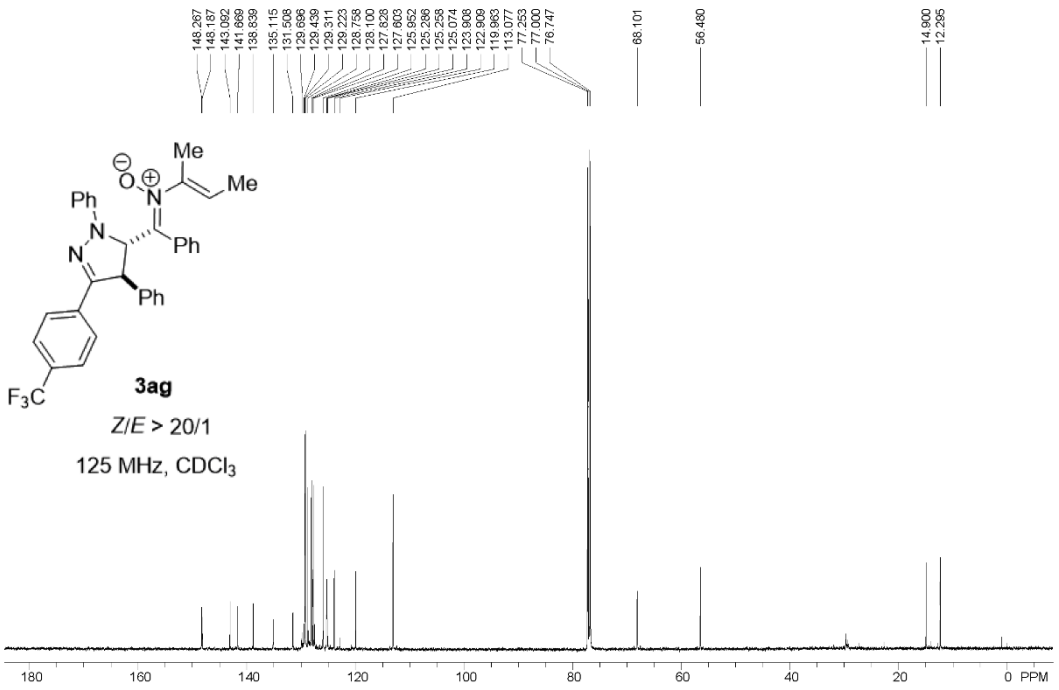
3af

Z/*E* > 20/1

470 MHz, $CDCl_3$



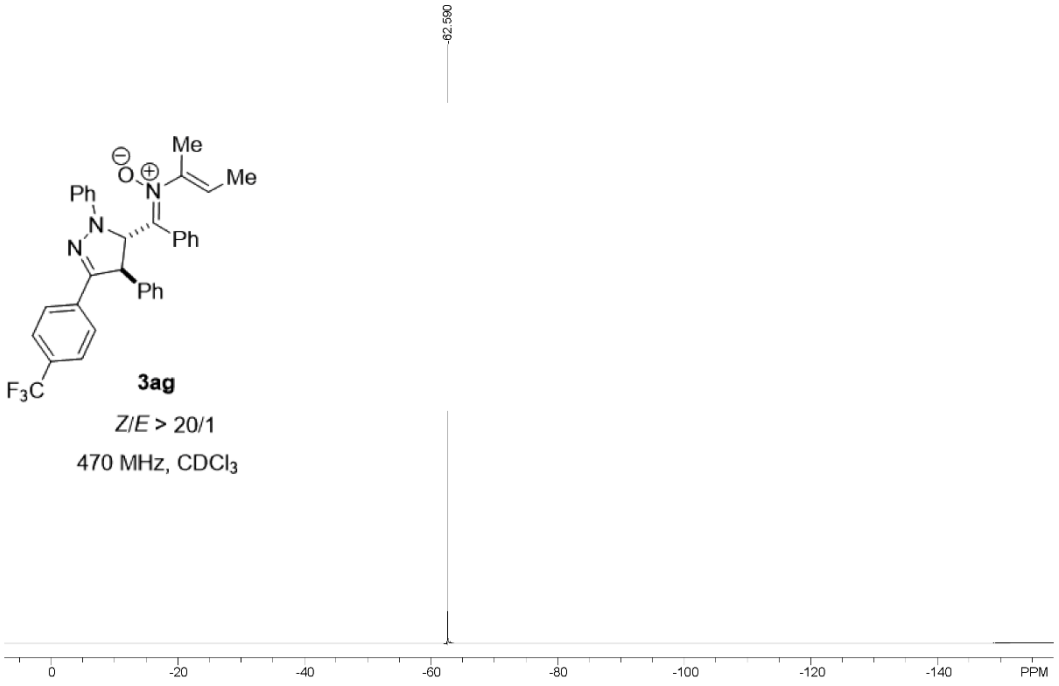

7.515
7.499
7.371
7.355
7.249
7.235
7.222
7.202
7.185
7.177
7.170
7.088
7.083
7.061
7.046
7.032
6.850
6.838
6.798
6.782
6.767
6.079
6.073
5.274
5.261
5.247
5.233
4.565
4.559
1.847
1.307
1.293
0.000
Me
Me
Ph
Ph
Ph
Ph
F3C
3ag
Z/E > 20/1
500 MHz, CDCl3
7.07
3.02
2.08
2.07
2.02
2.05
1.04
1.00
1.02
1.00
3.03
3.02
9
8
7
6
5
4
3
2
1
0 PPM

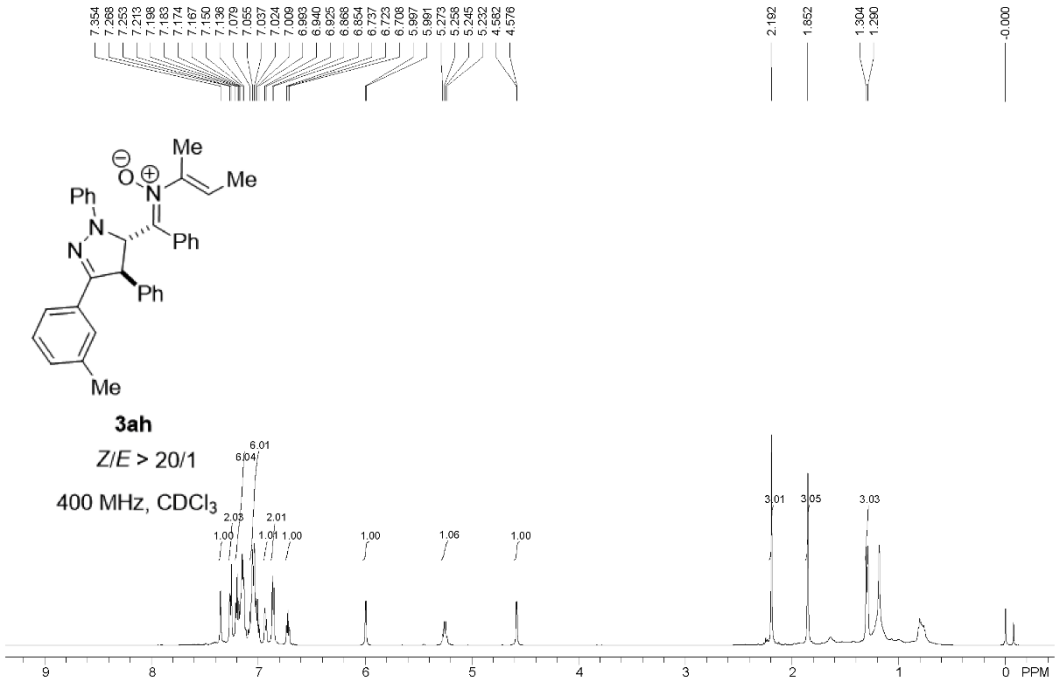

148.267
148.187
143.092
141.669
138.839
135.115
131.508
129.696
129.439
129.311
129.223
128.758
128.100
127.828
127.603
125.952
125.286
125.258
125.074
123.908
122.909
119.963
113.077
77.253
77.000
76.747
68.101
56.480
14.900
12.295
Me
Me
Ph
Ph
Ph
Ph
F3C
3ag
Z/E > 20/1
125 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0 PPM

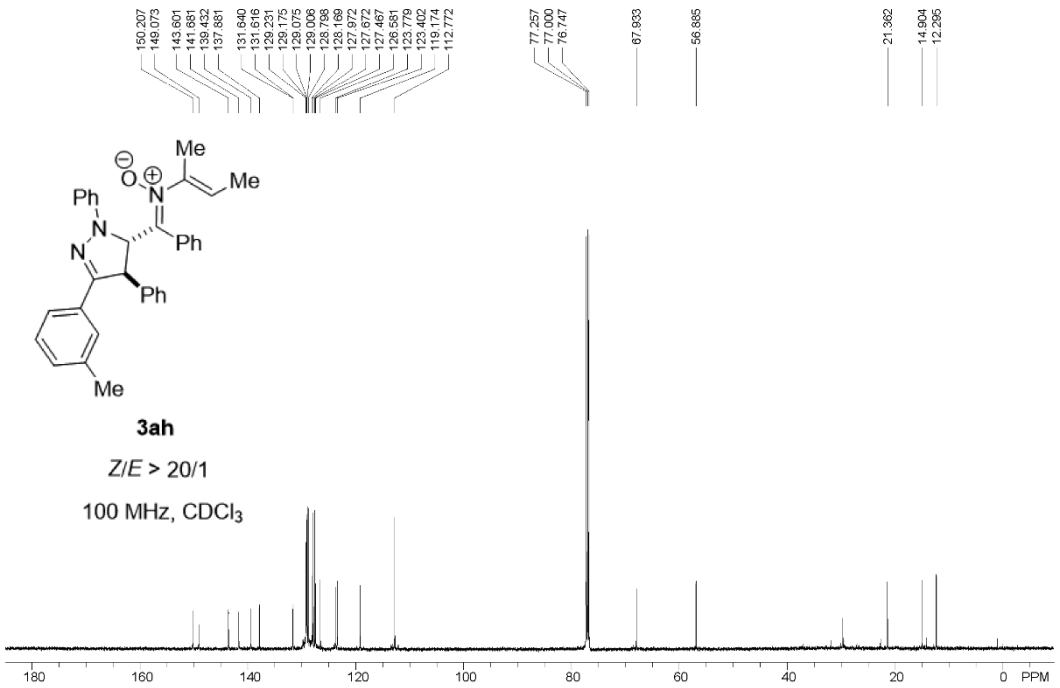
3ag

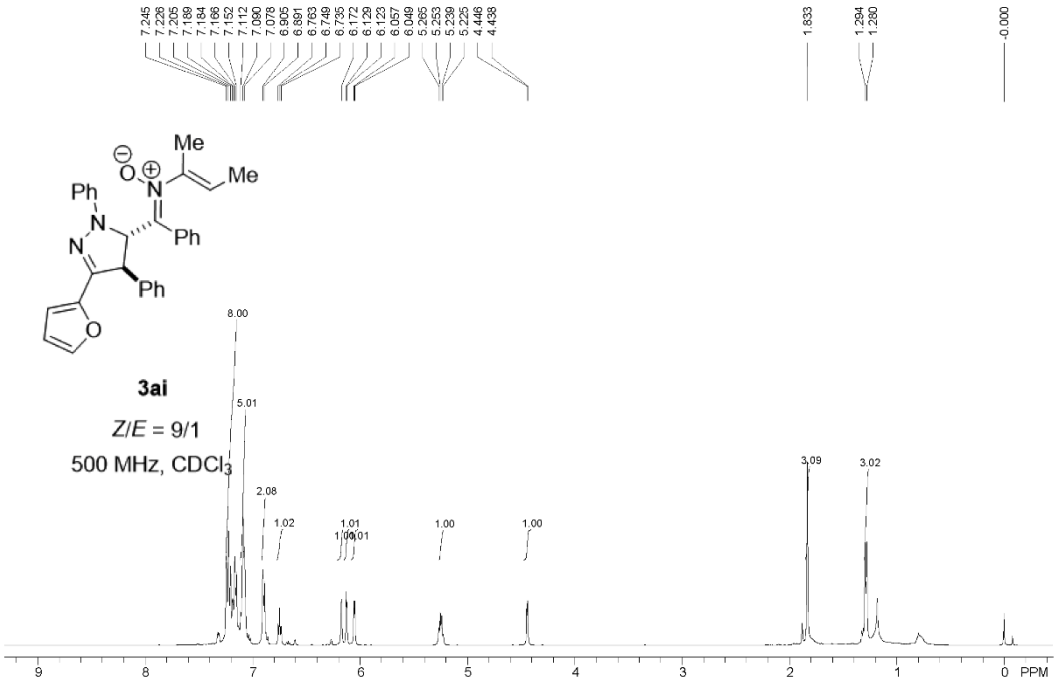
Z/*E* > 20/1

470 MHz, $CDCl_3$




7.354
7.268
7.253
7.213
7.198
7.183
7.174
7.167
7.150
7.136
7.079
7.055
7.037
7.024
7.009
6.993
6.940
6.925
6.885
6.854
6.737
6.723
6.708
5.997
5.991
5.273
5.258
5.245
5.232
4.582
4.576
2.192
1.852
1.304
1.290
0.000
Me
Me
Ph
Ph
Ph
Me
3ah
Z/E > 20/1
400 MHz, CDCl3
6.01
6.04
2.03
2.01
1.00
1.01
1.00
1.00
1.06
1.00
3.01
3.05
3.03
9
8
7
6
5
4
3
2
1
0
PPM

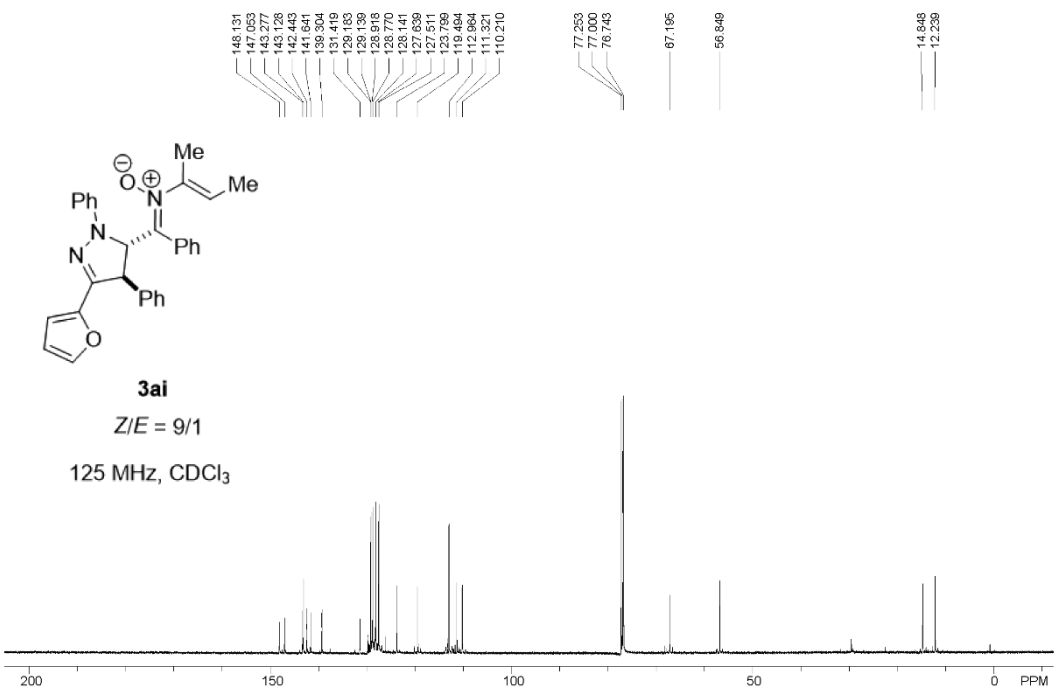

150.207
149.073
143.601
141.681
139.432
137.881
131.640
131.616
129.231
129.175
129.075
129.006
128.798
128.169
127.972
127.672
127.467
126.581
123.779
123.402
119.174
112.772
77.257
77.000
76.747
67.933
56.885
21.362
14.904
12.285
Me
Me
Ph
Ph
Ph
Me
3ah
Z/E > 20/1
100 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0
PPM



3ai

Z/*E* = 9/1

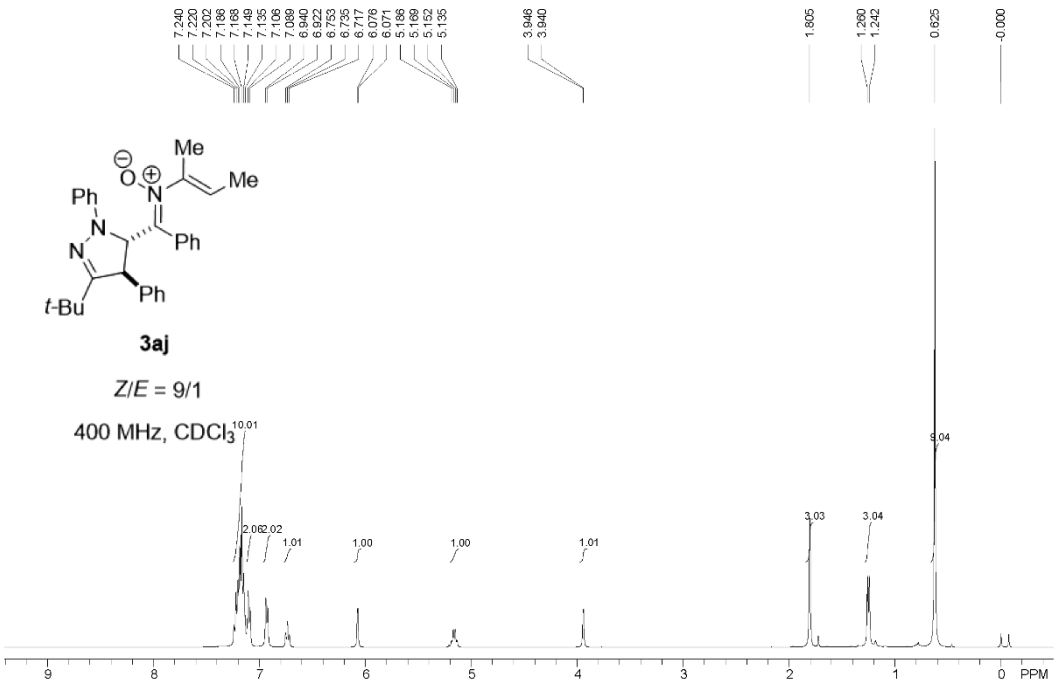
500 MHz, $CDCl_3$

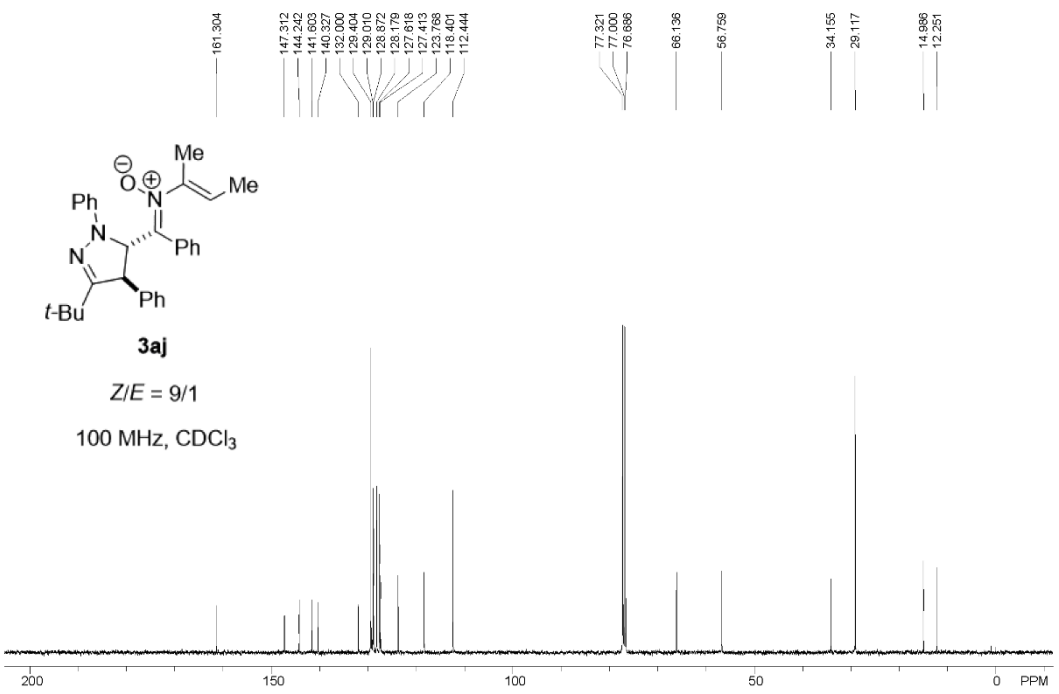


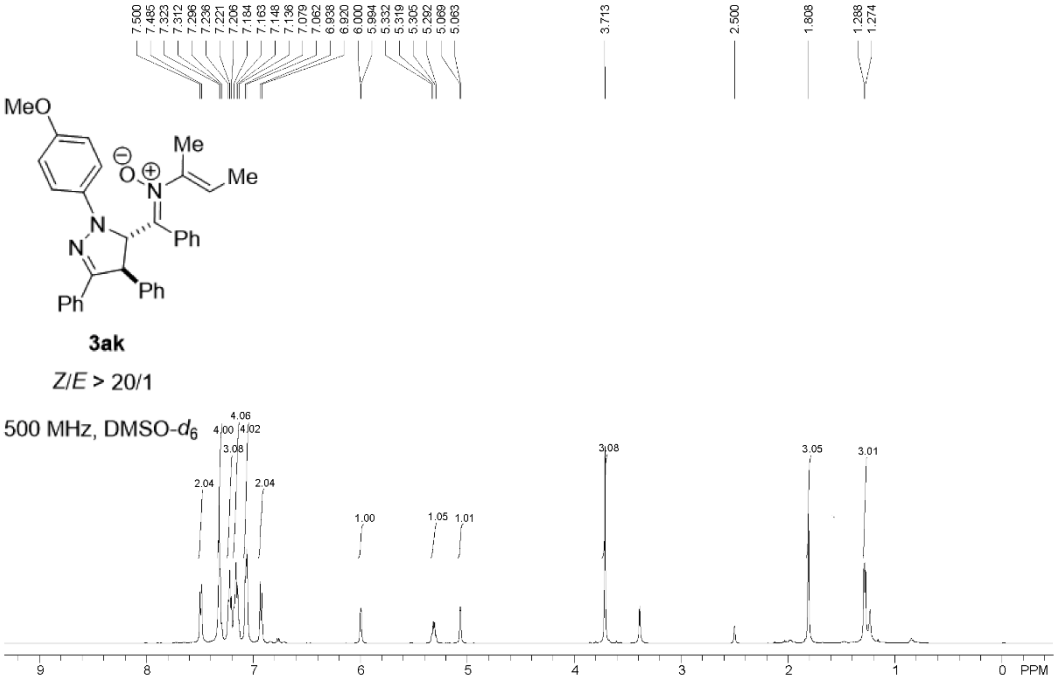
3ai

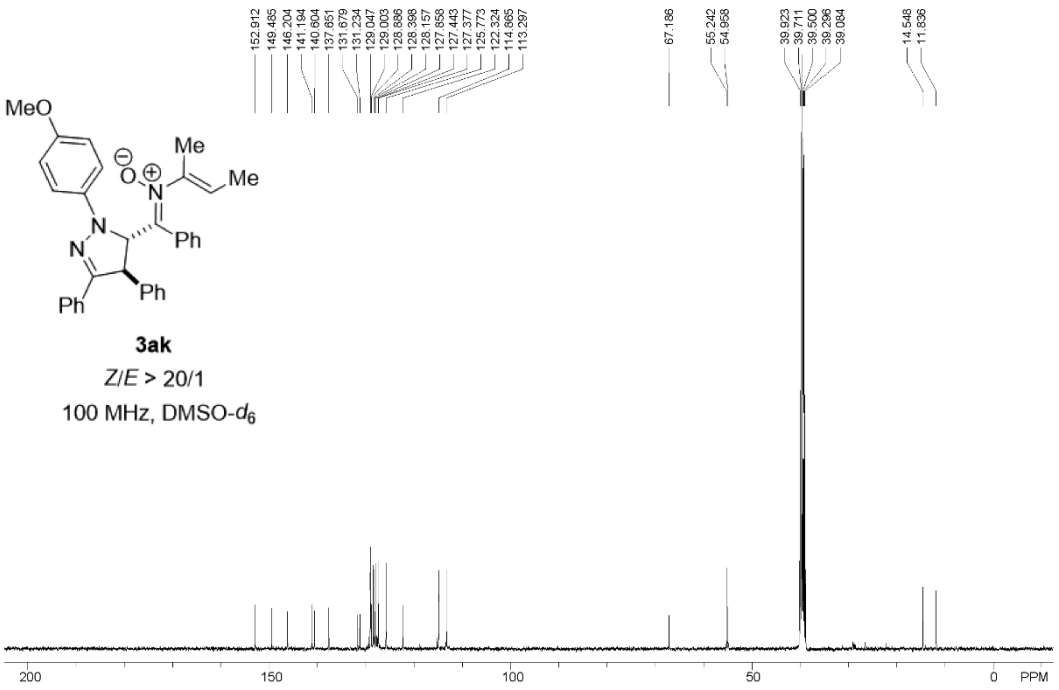
Z/*E* = 9/1

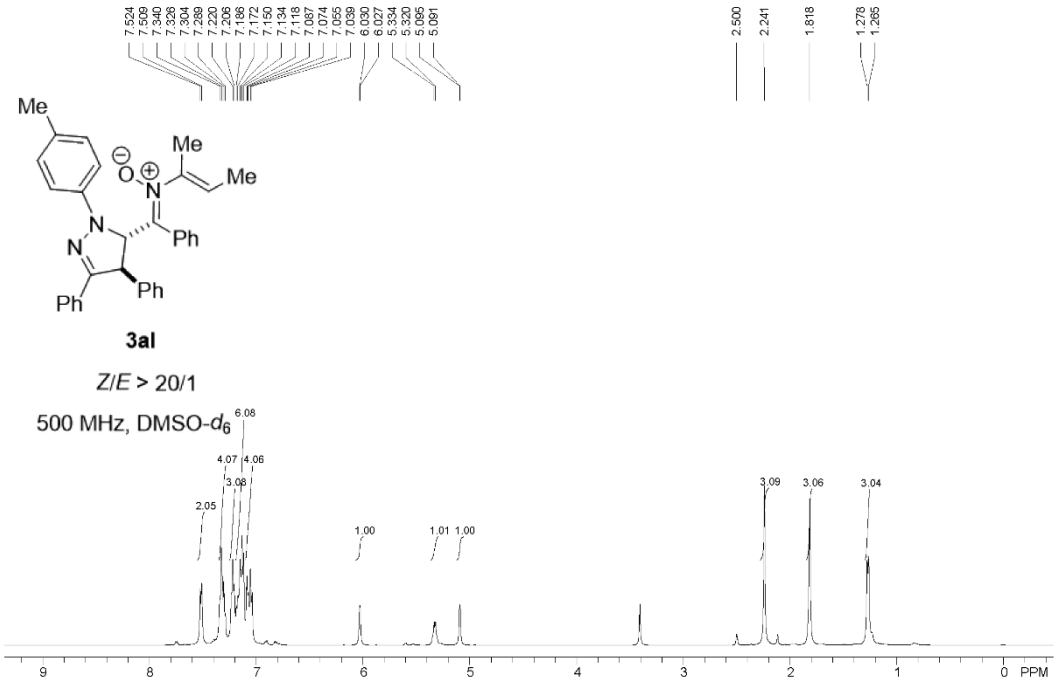
125 MHz, $CDCl_3$


7.240
7.220
7.202
7.188
7.168
7.149
7.135
7.106
7.088
6.940
6.922
6.753
6.735
6.717
6.076
6.071
5.186
5.169
5.152
5.135
3.946
3.940
1.805
1.260
1.242
0.625
0.000
Me
Me
Ph
Ph
Ph
t-Bu
3aj
Z/E = 9/1
400 MHz, CDCl3
10.01
2.06
2.02
1.01
1.00
1.00
1.01
3.03
3.04
9.04
9
8
7
6
5
4
3
2
1
0
PPM


161.304
147.312
144.242
141.603
140.327
132.000
129.404
129.010
128.872
128.179
127.618
127.413
123.768
118.401
112.444
77.321
77.000
76.688
66.136
56.759
34.155
29.117
14.986
12.251
Me
Me
Ph
Ph
Ph
t-Bu
3aj
Z/E = 9/1
100 MHz, CDCl3
200
150
100
50
0
PPM


7.500
7.485
7.323
7.312
7.298
7.236
7.221
7.206
7.184
7.163
7.148
7.136
7.079
7.062
6.938
6.920
6.000
5.994
5.332
5.319
5.305
5.292
5.069
5.063
3.713
2.500
1.808
1.288
1.274
MeO
Me
Me
Ph
Ph
Ph
3ak
Z/E > 20/1
500 MHz, DMSO-d6
4.06
4.00
4.02
3.08
2.04
2.04
1.00
1.05
1.01
3.08
3.05
3.01
9
8
7
6
5
4
3
2
1
0
PPM

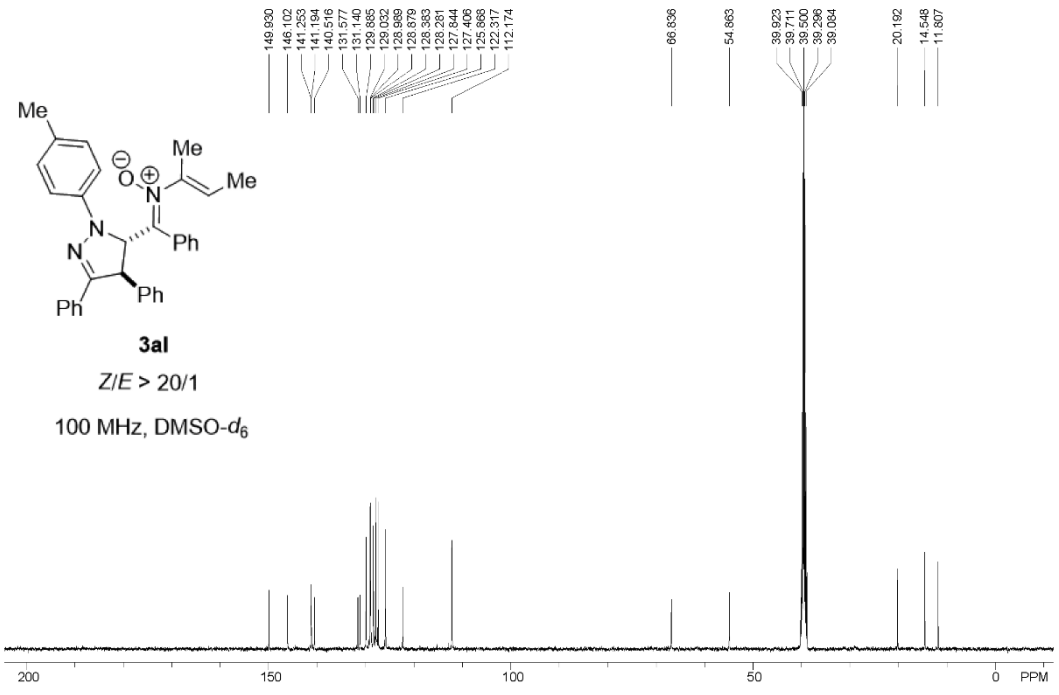

152.912
149.485
146.204
141.194
140.604
137.851
131.679
131.234
129.047
129.003
128.886
128.398
128.157
127.858
127.443
127.377
125.773
122.324
114.865
113.297
67.186
55.242
54.958
39.923
39.711
39.500
39.296
39.084
14.548
11.836
MeO
Me
Me
Ph
Ph
Ph
3ak
Z/E > 20/1
100 MHz, DMSO-d6
200
150
100
50
0
PPM



3al

Z/*E* > 20/1

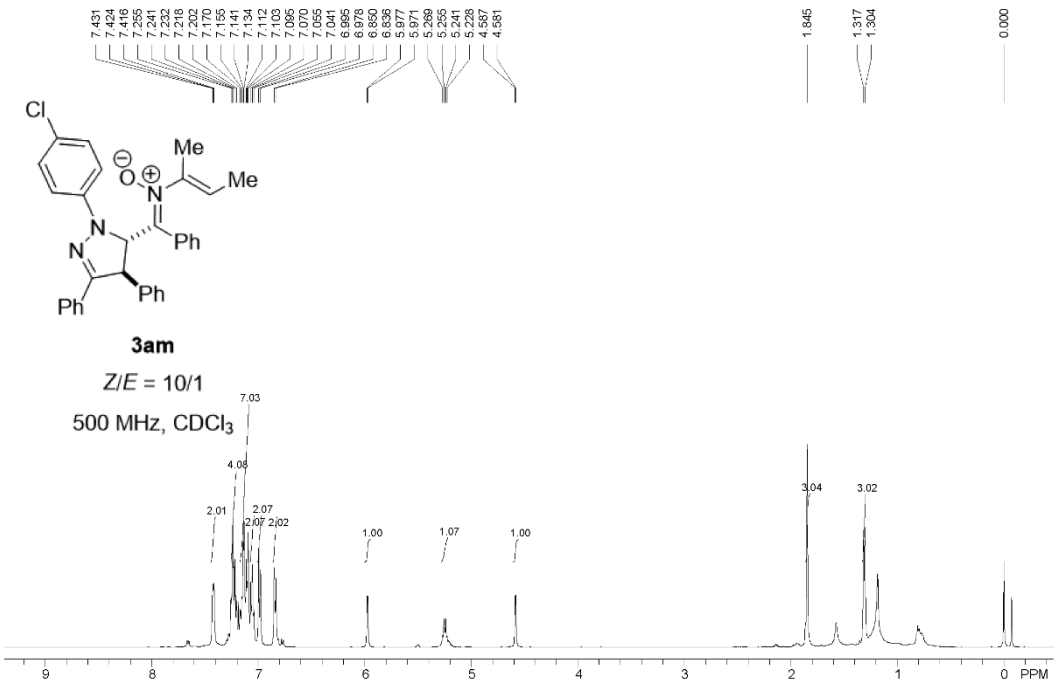
500 MHz, DMSO-d_6

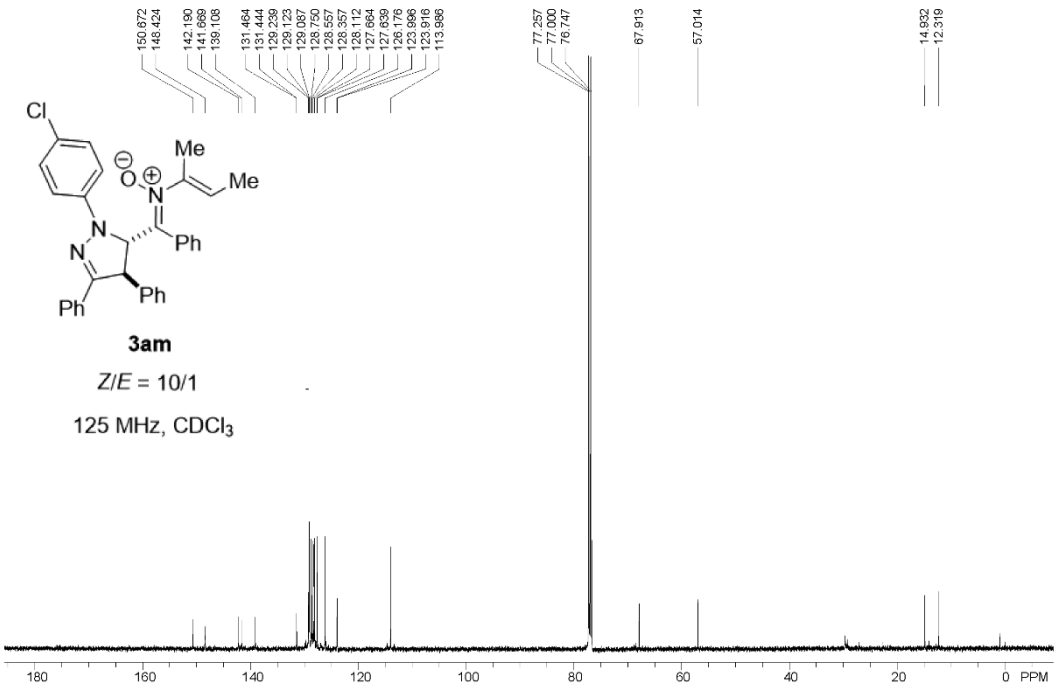


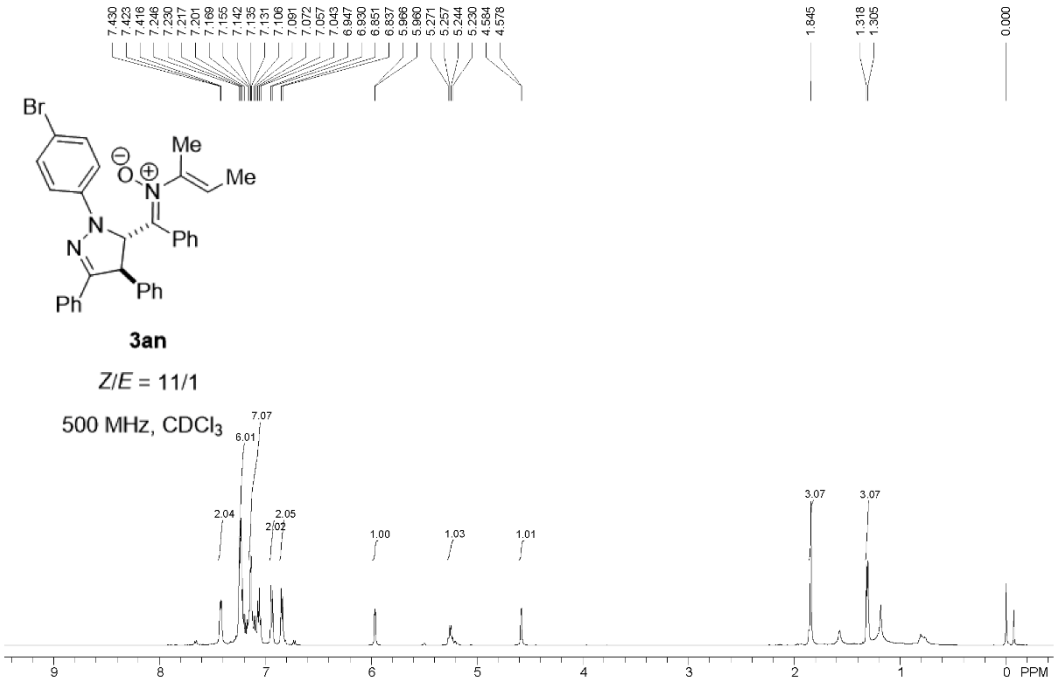
3al

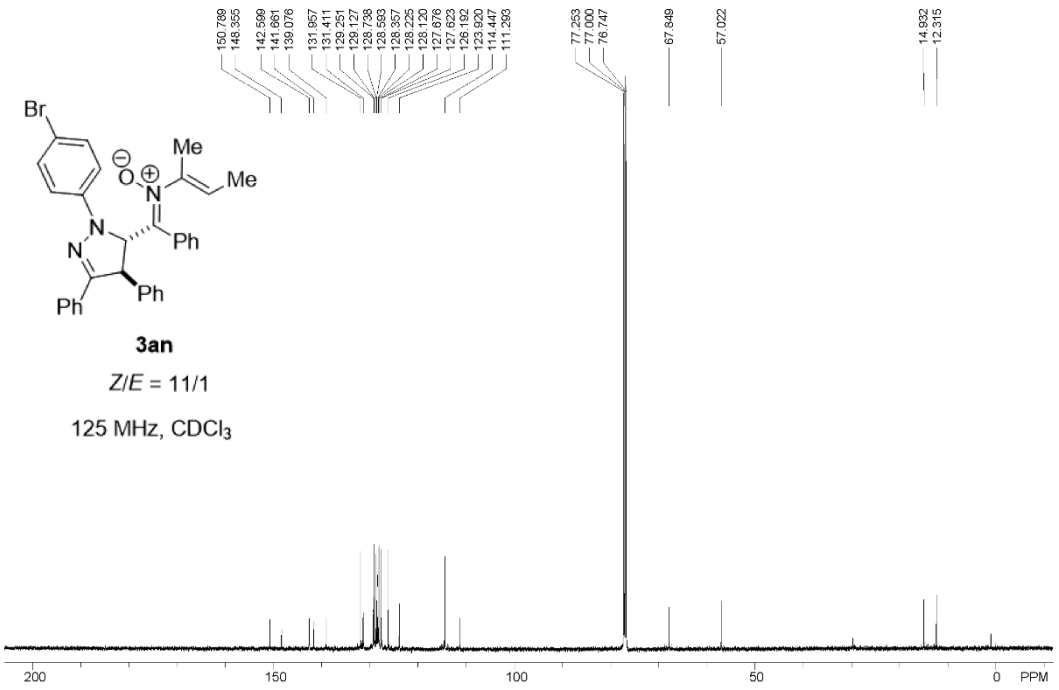
Z/*E* > 20/1

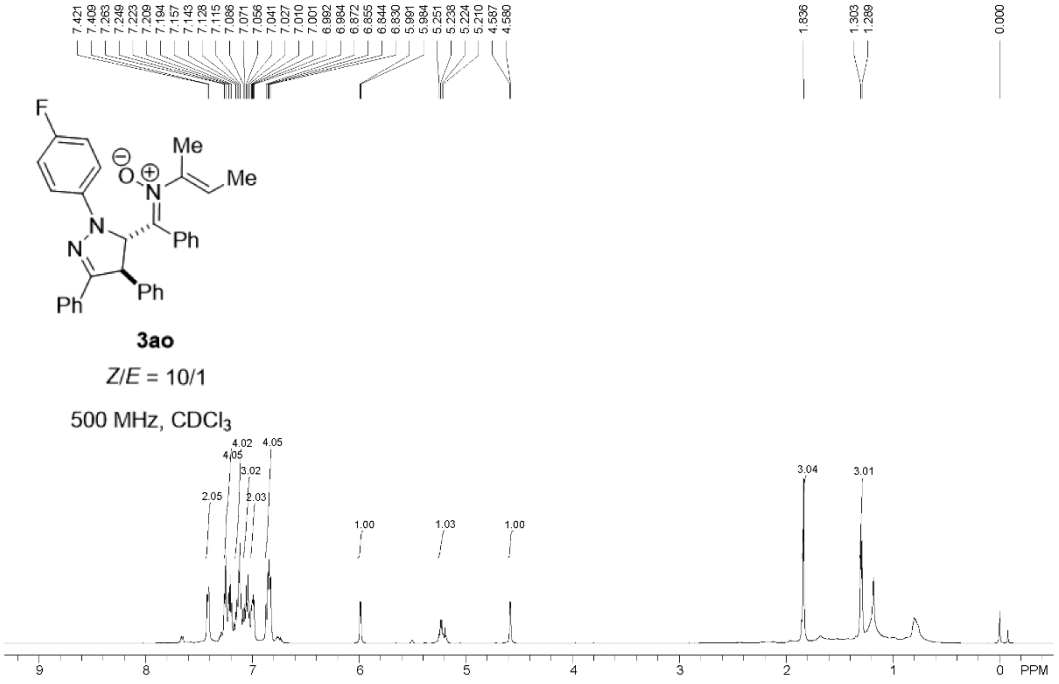
100 MHz, DMSO-d_6


7.431
7.424
7.416
7.255
7.241
7.232
7.216
7.202
7.170
7.165
7.141
7.134
7.112
7.103
7.096
7.070
7.055
7.041
6.995
6.978
6.850
6.836
5.977
5.971
5.269
5.255
5.241
5.228
4.587
4.581
1.845
1.317
1.304
0.000
Cl
Me
Me
Ph
Ph
Ph
3am
Z/E = 10/1
500 MHz, CDCl3
7.03
4.08
2.01
2.07
2.07
2.02
1.00
1.07
1.00
3.04
3.02
9
8
7
6
5
4
3
2
1
0
PPM


150.872
148.424
142.190
141.669
139.108
131.464
131.444
129.239
129.123
129.087
128.750
128.557
128.357
128.112
127.664
127.639
126.176
123.996
123.916
113.986
77.257
77.000
76.747
67.913
57.014
14.932
12.319
Cl
Me
Me
Ph
Ph
Ph
3am
Z/E = 10/1
125 MHz, CDCl3
180
160
140
120
100
80
60
40
20
0
PPM


7.490
7.423
7.416
7.246
7.230
7.217
7.201
7.169
7.155
7.142
7.135
7.131
7.106
7.091
7.072
7.057
7.043
6.947
6.930
6.851
6.837
5.988
5.960
5.271
5.257
5.244
5.230
4.584
4.576
1.845
1.318
1.305
0.000
Br
Me
Me
Ph
Ph
Ph
3an
Z/E = 11/1
500 MHz, CDCl3
7.07
6.01
2.04
2.05
2.02
1.00
1.03
1.01
3.07
3.07
9
8
7
6
5
4
3
2
1
0 PPM

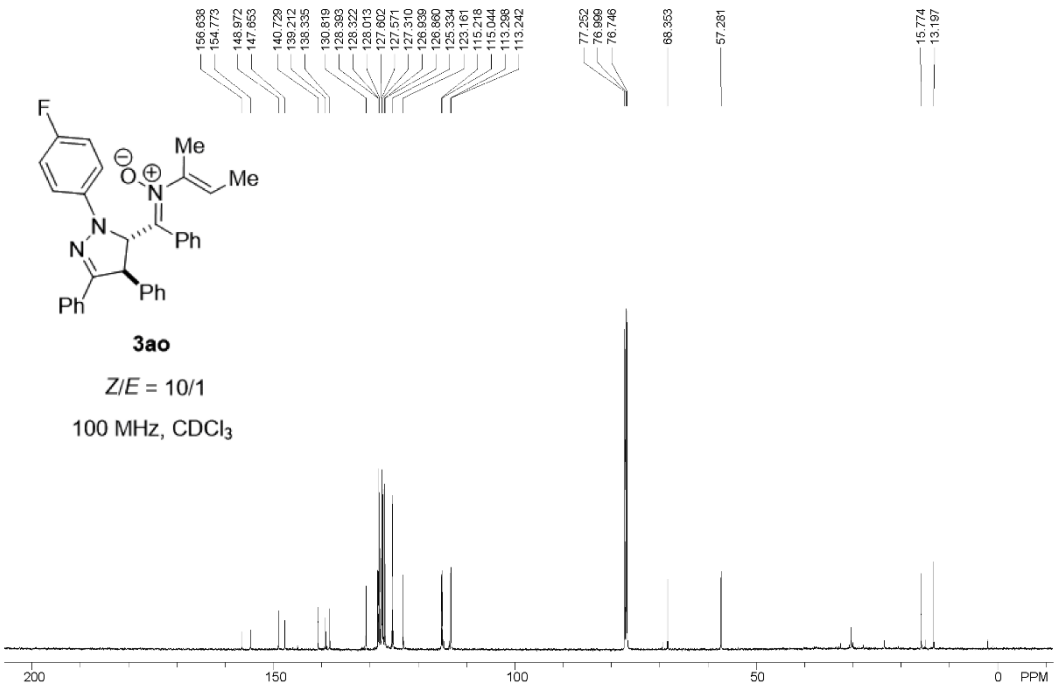

150.789
148.355
142.599
141.661
139.076
131.957
131.411
129.251
129.127
128.738
128.583
128.357
128.225
128.120
127.676
127.623
126.192
123.920
114.447
111.293
77.253
77.000
76.747
67.849
57.022
14.932
12.315
Br
Me
Me
Ph
Ph
Ph
3an
Z/E = 11/1
125 MHz, CDCl3
200
150
100
50
0 PPM



3ao

Z/*E* = 10/1

500 MHz, $CDCl_3$



3ao

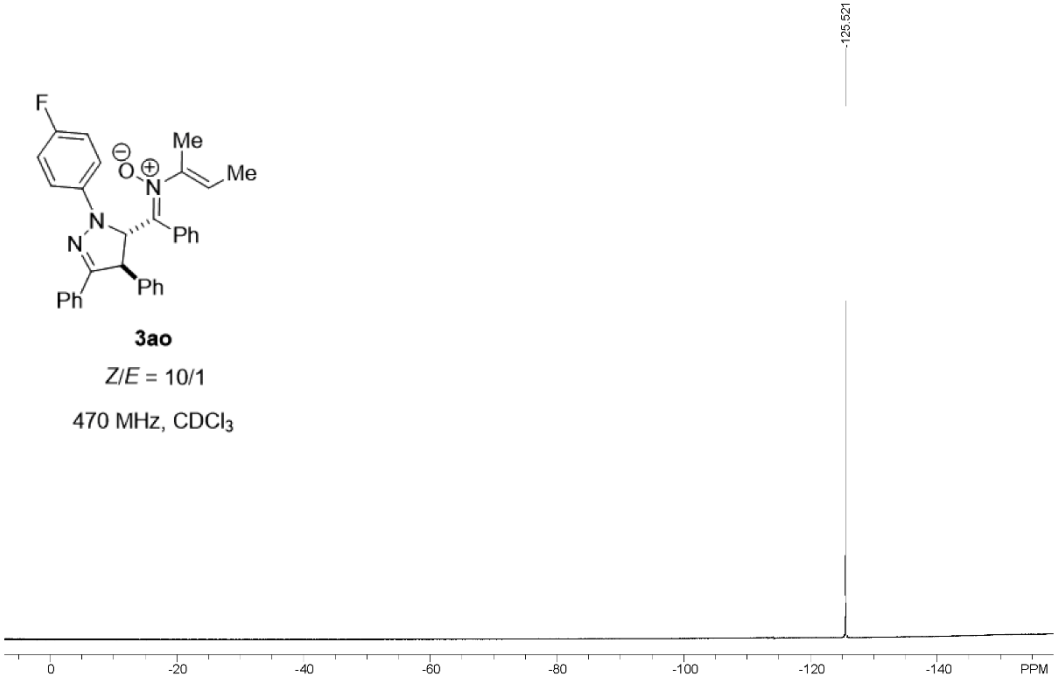
Z/*E* = 10/1

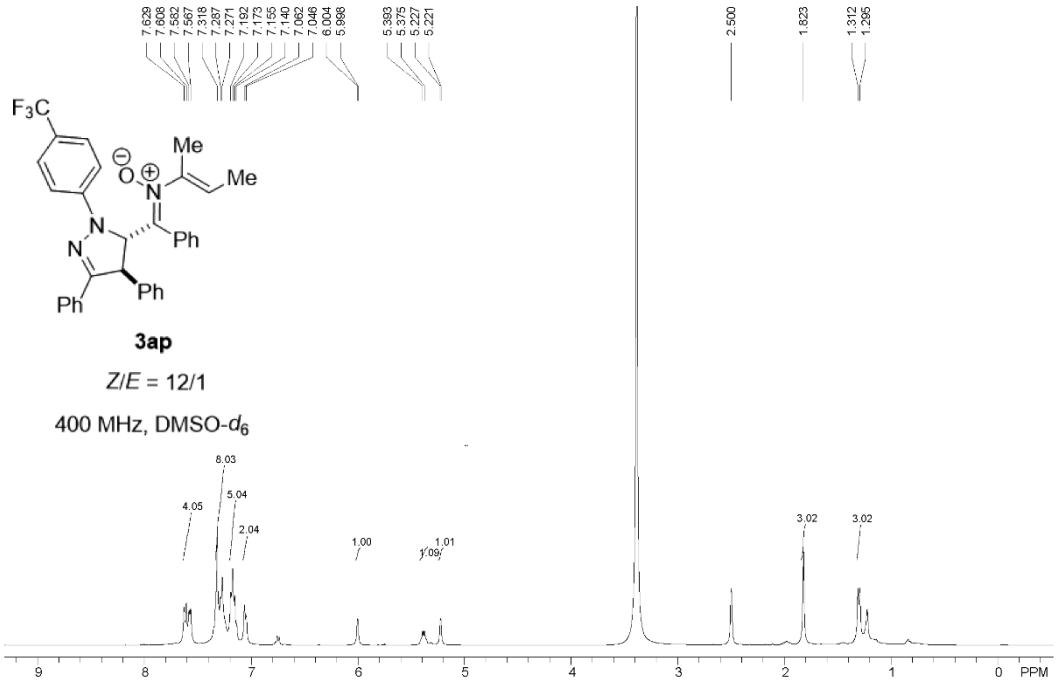
100 MHz, $CDCl_3$

3ao

Z/*E* = 10/1

470 MHz, $CDCl_3$

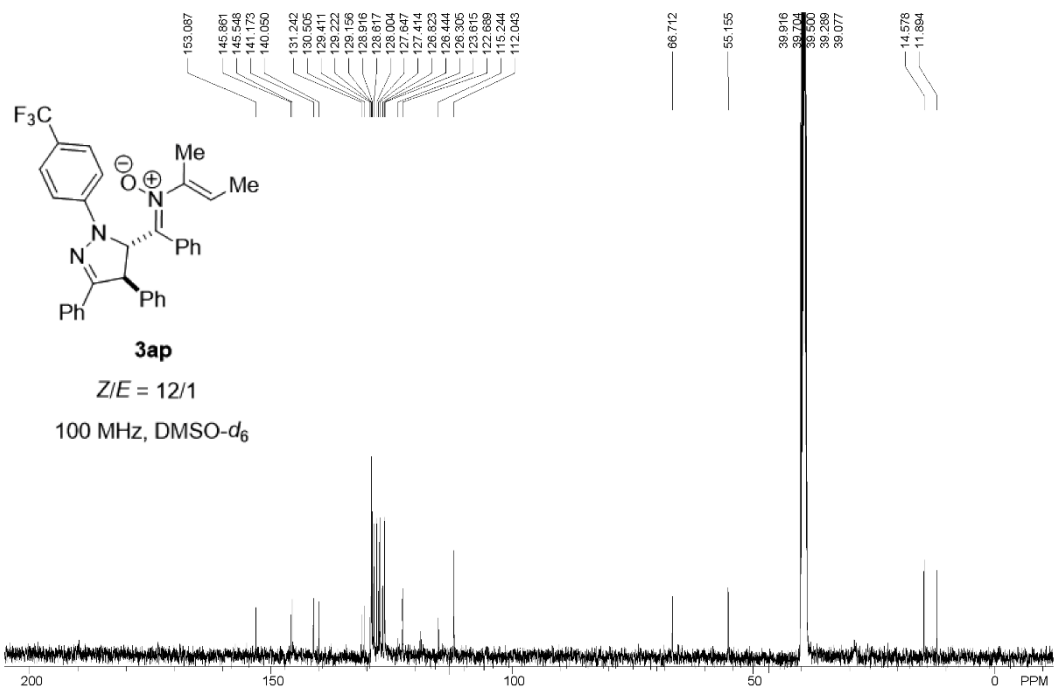




3ap

Z/*E* = 12/1

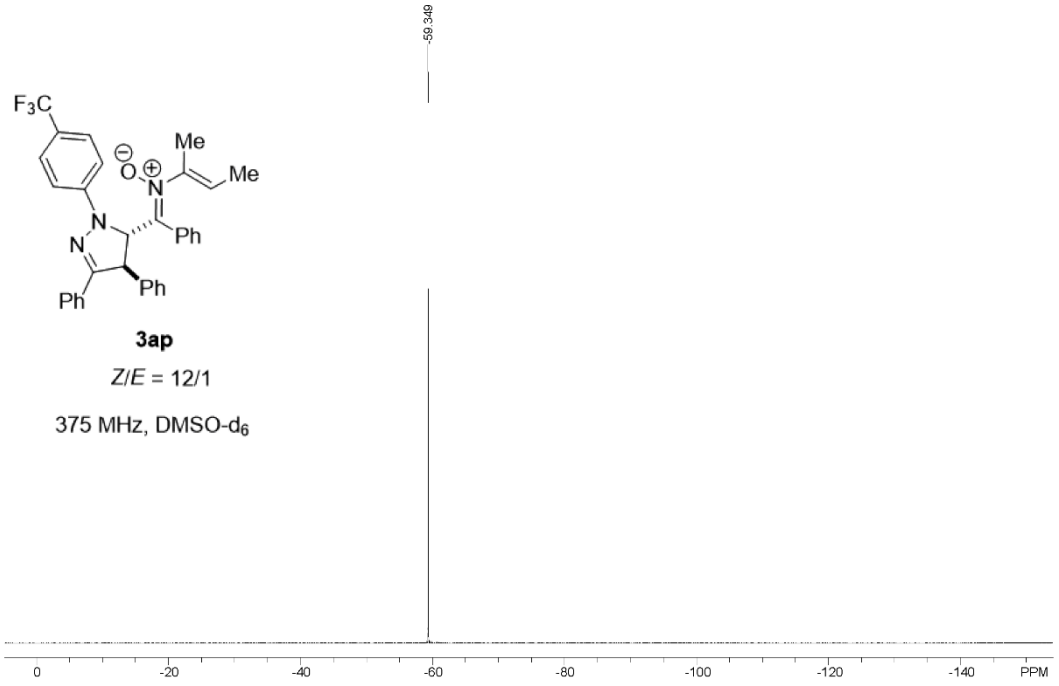
400 MHz, DMSO-d_6



3ap

Z/*E* = 12/1

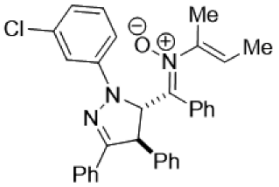
100 MHz, DMSO-d_6



3ap

Z/*E* = 12/1

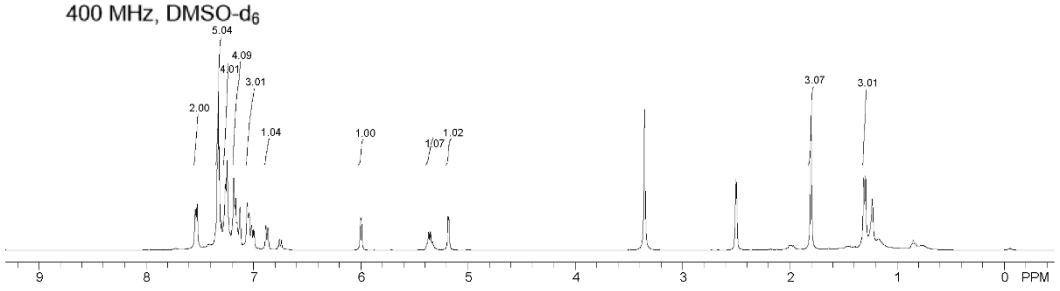
375 MHz, DMSO-d_6

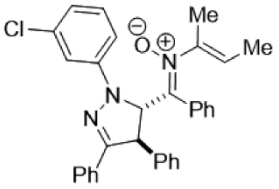


3aq

Z/*E* > 20/1

400 MHz, DMSO-d_6

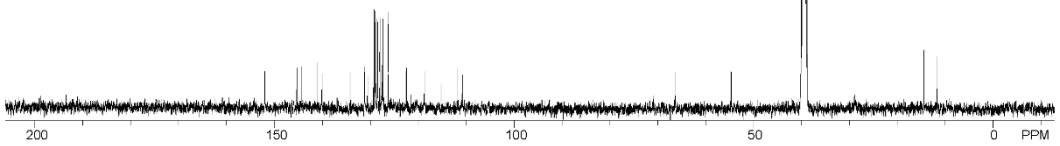


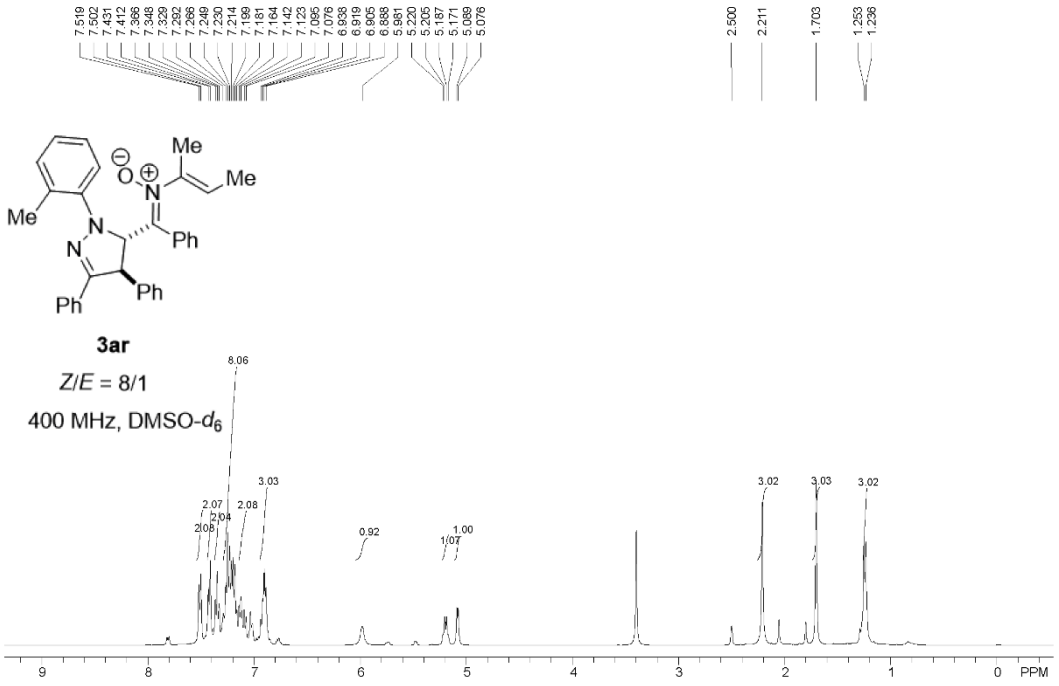


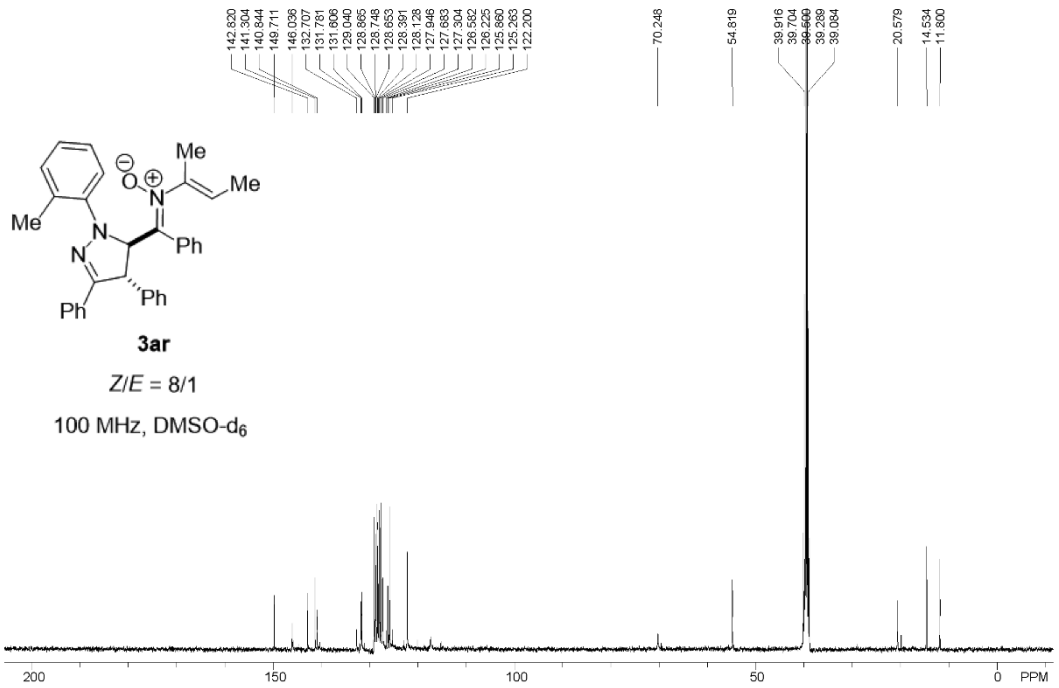
3aq

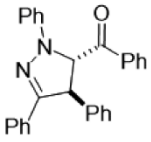
Z/*E* > 20/1

100 MHz, DMSO-d_6



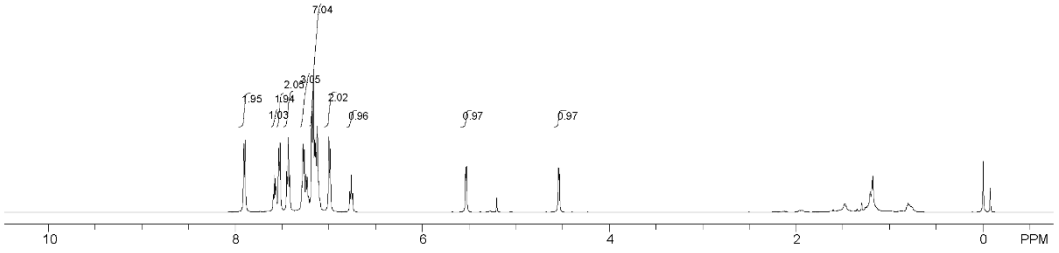

7.519
7.502
7.431
7.412
7.368
7.348
7.329
7.282
7.266
7.249
7.230
7.214
7.199
7.181
7.164
7.142
7.123
7.095
7.076
6.838
6.819
6.805
6.888
5.981
5.220
5.205
5.187
5.171
5.089
5.076
2.500
2.211
1.703
1.253
1.236
Me
Me
N
O
N
Me
Ph
N
Ph
Ph
3ar
Z/E = 8/1
400 MHz, DMSO-d6
8.06
3.03
2.07
2.04
2.08
2.08
0.92
1.00
1.07
3.02
3.03
3.02
9
8
7
6
5
4
3
2
1
0
PPM

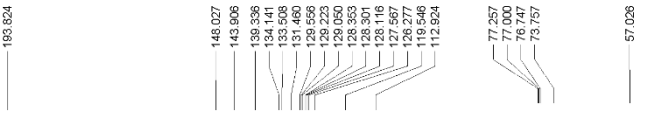

142.820
141.304
140.844
140.711
146.038
132.707
131.761
131.608
129.040
128.865
128.748
128.653
128.391
128.128
127.946
127.683
127.304
126.582
126.225
125.860
125.263
122.200
70.248
54.819
39.916
39.704
39.289
39.084
20.579
14.534
11.800
Me
Me
N
O
N
Me
Ph
N
Ph
Ph
3ar
Z/E = 8/1
100 MHz, DMSO-d6
200
150
100
50
0
PPM

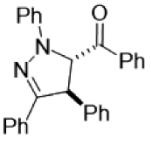


4

500 MHz, $CDCl_3$

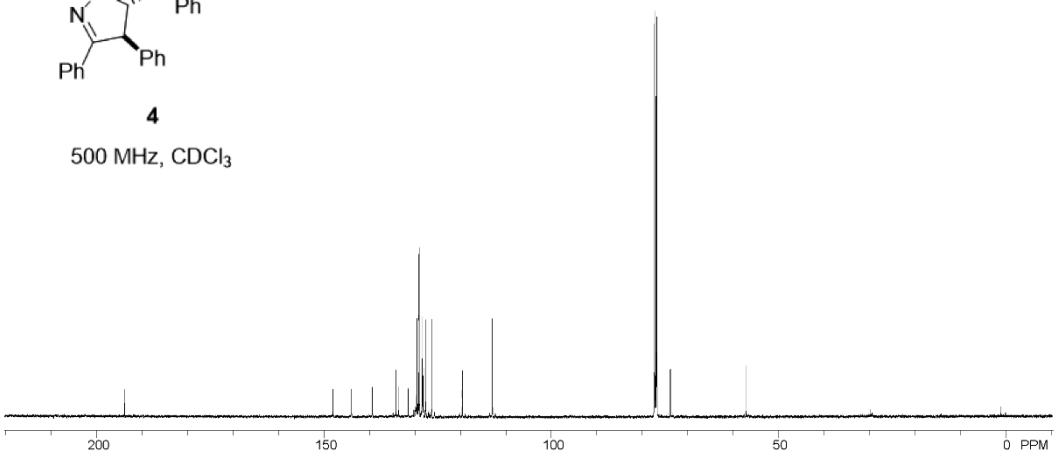


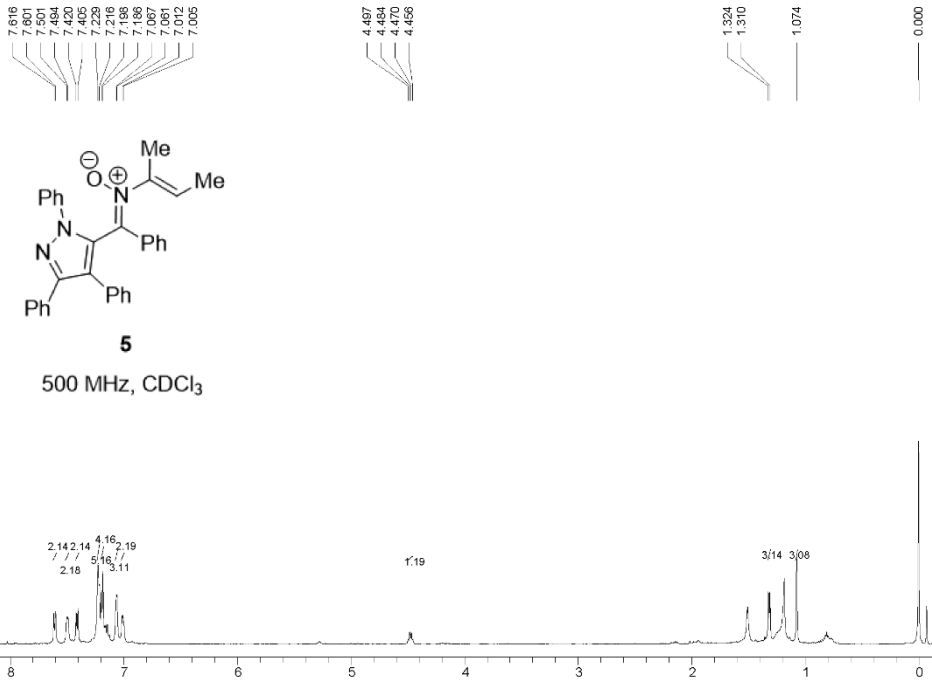


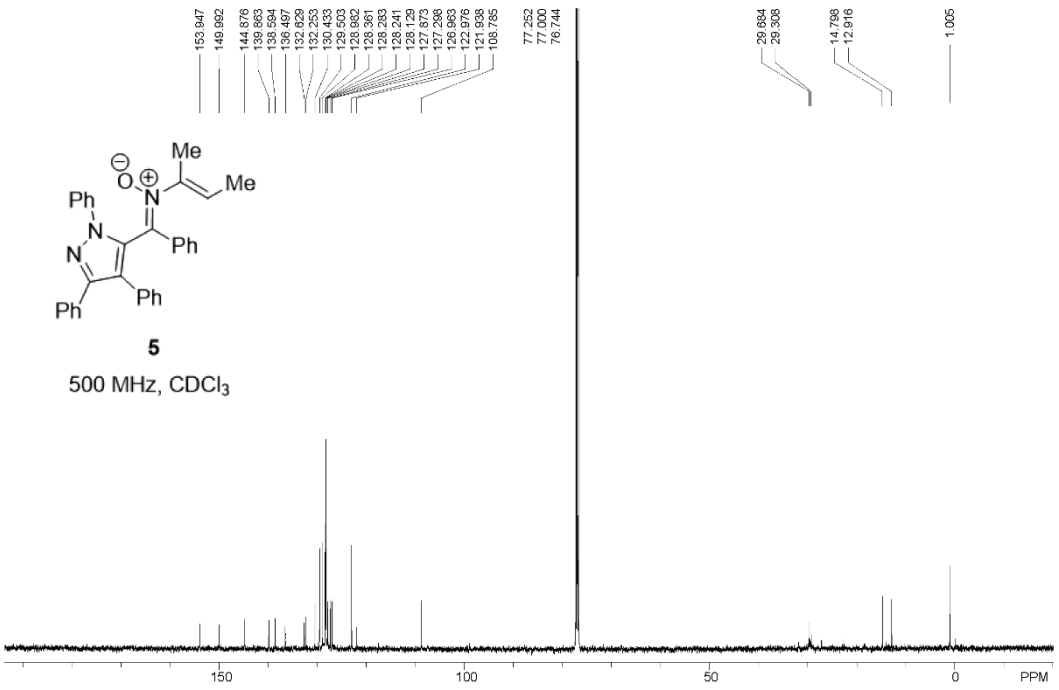


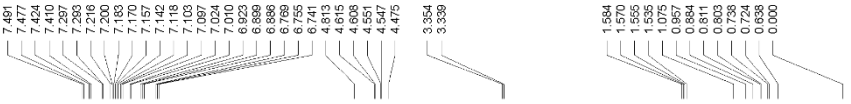
4

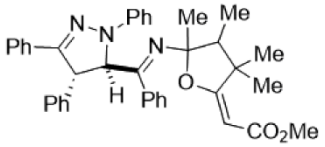
500 MHz, $CDCl_3$




7.616
7.601
7.501
7.484
7.420
7.405
7.229
7.216
7.198
7.188
7.067
7.061
7.012
7.005
4.497
4.484
4.470
4.456
1.324
1.310
1.074
0.000
Me
Me
Ph
Ph
Ph
Ph
Ph
5
500 MHz, CDCl3
2.14
2.14
2.18
4.16
5.16
2.19
3.11
1.19
3.14
3.08
8
7
6
5
4
3
2
1
0
PPM


153.947
149.992
144.876
139.863
138.594
136.497
132.629
132.253
130.433
129.503
128.982
128.361
128.283
128.241
128.129
127.873
127.298
126.963
122.976
121.938
108.785
77.252
77.000
76.744
29.884
29.308
14.798
12.916
1.005
Me
Me
Ph
Ph
Ph
Ph
Ph
5
500 MHz, CDCl3
150
100
50
0
PPM

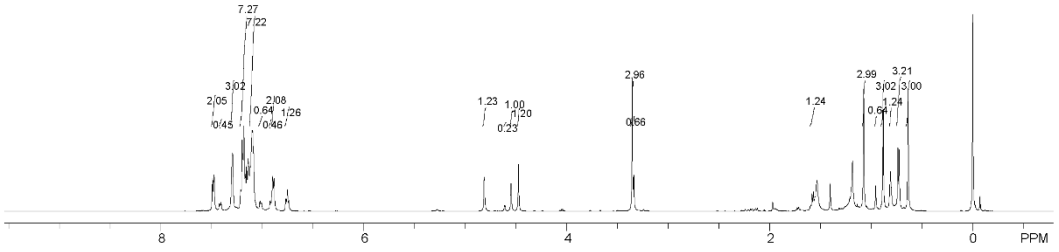


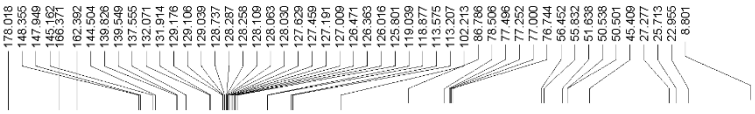


6

dr = 5:1

500 MHz, $CDCl_3$





6

dr = 5:1

125 MHz, $CDCl_3$