Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supplementary Information

Hydroamination of alkenyl *N*-arylhydrazones mediated by *t*-BuOK for synthesis of nitrogen-heterocycles

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Table of Contents

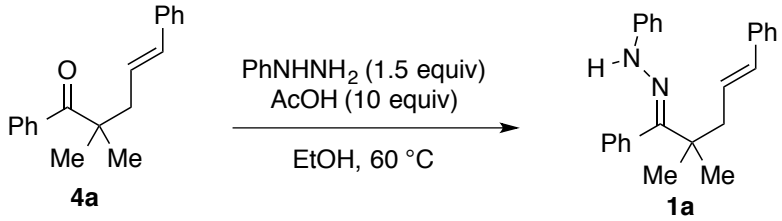
1. General

^{1}H NMR spectra were recorded on a Bruker Avance 400 MHz spectrometer in $CDCl_3$ [using TMS (for ^{1}H, δ = 0.00) as internal standard]. ^{13}C NMR spectra on a Bruker Avance 400 MHz spectrometer in $CDCl_3$ [using $CDCl_3$ (for ^{13}C, δ = 77.00) as internal standard]. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, br = broad. IR spectra were recorded on a Shimadzu IR IRAffinity-1 FT-IR Spectrometer. High-resolution mass spectra were obtained with a Waters Q-Tof Premier mass spectrometer. Melting points are uncorrected and were recorded on a MPA 100 OptiMelt Automated Melting Point System. Flash chromatography was performed using Merck silica gel 60 with distilled solvents. *o*-Xylene was distilled over CaH_2. *t*-BuOK (≥98%, reagent grade, CAS Number 865-47-4) was purchased from Sigma-Aldrich, Et_3COH (≥99%, reagent grade, CAS Number 597-49-9) was purchased from TCI and used as received. Ketones **4a-o**[1] and **4p**[2] were prepared by following the literature methods.

2.4. Synthesis of Alkenyl Hydrazones 1

Synthesis of hydrazones 1a-d, f-k, o-p: These hydrazones were prepared by condensation of the corresponding ketones **4** with phenylhydrazine or *p*-methoxyphenylhydrazine (for **1j**) in the presence of AcOH. All these hydrazones were isolated as a single isomer.

Typical Procedure: [3] preparation of (*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1a**)

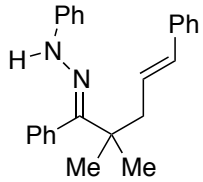


To a 2-neck round bottom flask containing ketone **4a** (1.283 g, 4.85 mmol) in EtOH (10 mL) was added phenylhydrazine (0.72 mL, 7.28 mmol) and AcOH (0.28 mL, 4.85 mmol). The solution was stirred at 60 °C under a N_2 atmosphere until **4a** was completely consumed. After the mixture was cooled down to room temperature, the solvent was removed under reduced pressure and the resulting crude product was purified immediately by flash column

[1] X. Peng, B. M. K. Tong, H. Hirao and S. Chiba, *Angew. Chem. Int. Ed.,* 2014, **53**, 1959.
[2] a) A. J. A. Van Der Weerdt and H. Crefontain, *Tetrahedron*, 1981, **37**, 2121; b) T. Nishikata, Y. Noda, R. Fujimoto and T. Sakashita, *J. Am. Chem. Soc.,* 2013, **135**, 16372.
[3] X. Zhu, Y.-F. Wang, W. Ren, F.-L. Zhang and S. Chiba, *Org. Lett*. 2013, **15**, 3214.

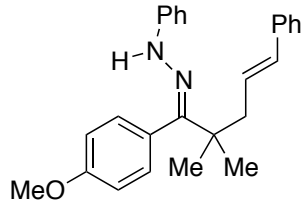
chromatography (hexane:ethyl acetate = 100:1) to yield (*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1a**) (1.596 g, 4.50 mmol, 93% yield), which was used immediately or stored under -20 °C under a N_2 atmosphere as hydrazones are not very stable with moisture and air.[4]

(*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1a**):



Yellow solid; mp. 109-110 °C; IR (NaCl) 3422, 1647, 1603 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 1.22 (6H, s), 2.50 (2H, d, *J* = 6.2 Hz), 6.38 (1H, td, *J* = 6.2, 15.9 Hz), 6.43 (1H, d, *J* = 15.9 Hz), 6.75-9.79 (2H, m), 6.93 (2H, d, *J* = 7.6 Hz), 7.13-7.20 (5H, m), 7.25-7.30 (3H, m), 7.34-7.39 (2H, m), 7.41-7.52 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.6, 41.5, 44.2, 112.6, 119.3, 126.1, 126.9, 127.7, 128.5, 128.6, 128.7, 129.1, 129.2, 132.3, 133.5, 137.8, 145.4, 153.3; EIHRMS: Found: *m/z* 355.2179. Calcd for $C_{25}H_{27}N_2$: $(M+H)^+$ 355.2174.

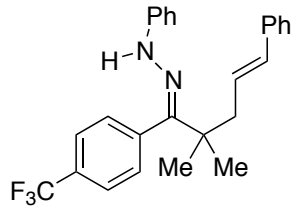
(*Z*)-1-((*E*)-1-(4-methoxyphenyl)-2,2-dimethyl-5-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1b**):



95% yield from ketone **4b** and phenylhydrazine; Yellow solid; mp. 98-99 °C; IR (NaCl) 3418, 1645, 1607 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 1.20 (6H, s), 2.48 (2H, d, *J* = 6.3 Hz), 3.87 (3H, s), 6.35 (1H, td, *J* = 6.3, 15.9 Hz), 6.42 (1H, d, *J* = 15.9 Hz), 6.75-9.78 (1H, m), 6.83 (1H, s), 6.92-6.95 (2H, m), 6.99-7.08 (4H, m), 7.16-7.20 (3H, m), 7.25-7.30 (3H, m), 7.34-7.36 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.6, 41.7, 44.2, 55.3, 112.6, 114.6, 119.2, 125.4, 126.1, 126.9, 127.8, 128.5, 129.1, 130.0, 132.2, 137.9, 145.5, 153.2, 159.6; EIHRMS: Found: *m/z* 385.2291. Calcd for $C_{26}H_{29}N_2O$: $(M+H)^+$ 385.2280.

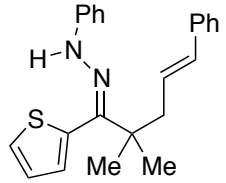
[4] For the reaction of hydrazones with molecular oxygen, see: M. Harej and D. Dolenc, *J. Org. Chem*. 2007, **72**, 7214.

(*Z*)-1-((*E*)-2,2-Dimethyl-5-phenyl-1-(4-(trifluoromethyl)phenyl)pent-4-en-1-ylidene)-2-phenylhydrazine (**1c**):



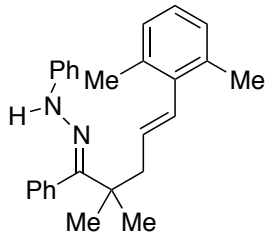
97% yield from ketone **4c** and phenylhydrazine; Yellow solid; mp. 80-81 °C; IR (NaCl) 3422, 1638, 1603 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.22 (6H, s), 2.50 (2H, d, J = 6.8 Hz), 6.37 (1H, td, J = 6.8, 15.9 Hz), 6.44 (1H, d, J = 15.9 Hz), 6.65 (1H, s), 7.80 (1H, t, J = 7.2 Hz), 6.95 (2H, t, J = 7.9 Hz), 7.20 (3H, t, J = 7.7 Hz), 7.26-7.36 (6H, m), 7.77 (2H, d, J = 8.0 Hz),; ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.6, 41.6, 44.2, 112.7, 119.8, 123.9 (q, $^{1}J_{C\text{-}F}$ = 270.8 Hz), 126.1, 126.2 (q, $^{3}J_{C\text{-}F}$ = 3.6 Hz), 127.0, 127.2, 128.5, 129.2, 129.3, 130.9 (q, $^{2}J_{C\text{-}F}$ = 32.8 Hz), 132.7, 137.5, 137.7, 145.1, 151.5; ESIHRMS: Found: m/z 423.2037. Calcd for $C_{26}H_{26}N_2F_3$: $(M+H)^+$ 423.2048.

(*Z*)-1-((*E*)-2,2-dimethyl-5-phenyl-1-(thiophen-2-yl)pent-4-en-1-ylidene)-2-phenylhydrazine (**1d**):



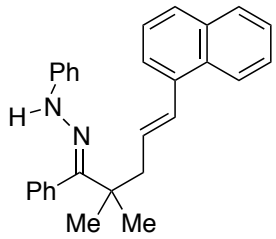
96% yield from ketone **4d** and phenylhydrazine; Yellow solid; mp. 77-78 °C; IR (NaCl) 3420, 1647, 1601 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.26 (6H, s), 2.50 (2H, d, J = 7.1 Hz), 6.29 (1H, td, J = 7.1, 15.8 Hz), 6.41 (1H, d, J = 15.8 Hz), 8.00 (1H, t, J = 7.3 Hz), 6.94-6.97 (3H, m), 7.16-7.22 (4H, m), 7.24-7.29 (3H, m), 7.34 (2H, d, J = 7.5 Hz), 7.51 (1H, d, J = 5.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.4, 41.7, 44.2, 112.7, 119.7, 126.1, 126.9, 127.4, 127.5, 128.2, 128.5, 129.1, 131.4, 132.4, 137.8, 144.9, 145.3; EIHRMS: Found: *m/z* 361.1748. Calcd for $C_{23}H_{25}N_2S$: $(M+H)^+$ 361.1738.

(*Z*)-1-((*E*)-5-(2,6-Dimethylphenyl)-2,2-dimethyl-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1f**):



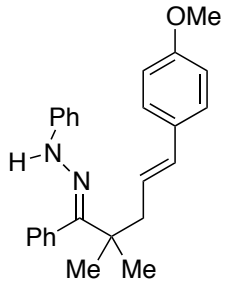
98% yield from ketone **4f** and phenylhydrazine; yellow solid; mp. 109-110 °C; IR (NaCl) 3420, 1645, 1597 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.25 (6H, s), 2.29 (6H, s), 2.52 (2H, d, *J* = 7.2 Hz), 5.83 (1H, td, *J* = 7.2, 16.1 Hz), 6.38 (1H, d, *J* = 16.1 Hz), 6.74-6.77 (2H, m), 6.89 (2H, d, *J* = 8.4 Hz), 7.00 (3H, s), 7.14-7.18 (4H, m), 7.41-7.47 (1H, m), 7.49 (2H, t, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.1, 26.5, 41.5, 44.6, 112.5, 119.2, 126.2, 127.6, 128.6, 128.7, 129.0, 129.2, 130.0, 132.5, 133.5, 136.0, 137.7, 145.4, 153.0; ESIHRMS: Found: m/z 383.2490. Calcd for $C_{27}H_{31}N_2$: $(M+H)^+$ 383.2487.

(*Z*)-1-((*E*)-2,2-Dimethyl-5-(naphthalene-1-yl)-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1g**):



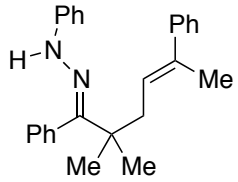
98% yield from ketone **4g** and phenylhydrazine; Yellow viscous oil; IR (NaCl) 3420, 1601, 1504 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.28 (6H, s), 2.63 (2H, dd, *J* = 1.0, 7.3 Hz), 6.37 (1H, td, *J* = 7.3, 15.0 Hz), 6.75-6.79 (2H, m), 6.95 (2H, d, *J* = 7.7 Hz), 7.14-7.20 (5H, m), 7.37-7.51 (6H, m), 7.55 (1H, d, *J* = 7.1 Hz), 7.72 (1H, d, *J* = 8.2 Hz), 7.80-7.83 (1H, m), 8.09-8.12 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.7, 41.6, 44.6, 112.6, 119.3, 123.8, 124.0, 125.6, 125.7, 125.8, 127.3, 128.4, 128.6, 128.7, 129.1, 129.2, 129.7, 131.0, 131.1, 133.5, 133.6, 135.7, 145.4, 153.1; ESIHRMS: Found: m/z 405.2330. Calcd for $C_{29}H_{29}N_2$: $(M+H)^+$ 405.2331.

(*Z*)-1-((*E*)-5-(4-Methoxyphenyl)-2,2-dimethyl-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1h**):



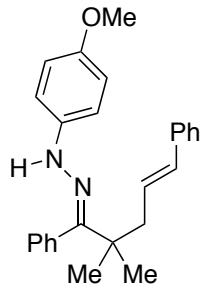
98% yield from ketone **4h** and phenylhydrazine; white solid; mp. 87-88 °C; IR (NaCl) 2964, 1601, 1504 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21 (6H, s), 2.47 (2H, d, *J* = 7.1 Hz), 3.78 (3H, s), 6.21 (1H, td, *J* = 7.1, 15.8 Hz), 6.36 (1H, d, *J* = 15.8 Hz), 6.74-6.78 (2H, m), 6.82 (2H, d, *J* = 8.6 Hz), 6.92 (2H, d, *J* = 8.2 Hz), 7.13-7.20 (4H, m), 7.28 (2H, d, *J* = 8.6 Hz), 7.41-7.44 (1H, m), 7.48 (2H, t, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.5, 41.5, 44.2, 55.3, 112.6, 113.9, 119.3, 125.4, 127.1, 128.6, 128.7, 129.0, 129.1, 130.7, 131.7, 133.6, 145.4, 153.4, 158.7; ESIHRMS: Found: m/z 385.2275. Calcd for $C_{26}H_{29}N_2O$: $(M+H)^+$ 385.2280.

(*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylhex-4-en-1-ylidene)-2-phenylhydrazine (**1i**):



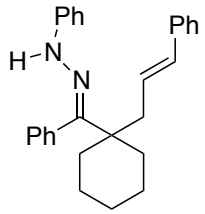
97% yield from ketone **4i** and phenylhydrazine; Yellow solid; mp. 90-91 °C; IR (NaCl) 3017, 1601, 1502 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.25 (6H, s), 2.02 (3H, s), 2.44 (2H, d, *J* = 7.1 Hz), 5.95 (1H, t, *J* = 7.1 Hz), 6.76 (2H, t, *J* = 8.6 Hz), 6.93 (2H, d, *J* = 7.7 Hz), 7.12-7.23 (5H, m), 7.29 (2H, t, *J* = 5.5 Hz), 7.37-7.50 (5H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.2, 26.5, 39.5, 41.9, 112.6, 119.3, 125.4, 125.7, 126.5, 128.2, 128.5, 128.7, 129.0, 129.1, 133.6, 136.1, 144.2, 145.4, 153.3; ESIHRMS: Found: m/z 369.2337. Calcd for $C_{26}H_{29}N_2$: $(M+H)^+$ 369.2331.

(*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylpent-4-en-1-ylidene)-2-(-4-methoxyphenyl)hydrazine (**1j**):



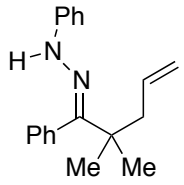
86% yield from ketone **4j** and *p*-methoxyphenylhydrazine; Yellow oil; IR (NaCl) 3017, 1601, 1502 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21 (6H, s), 2.49 (2H, d, *J* = 6.1 Hz), 3.74 (3H, s), 6.36 (1H, dt, *J* = 6.1, 15.9 Hz), 6.42 (1H, d, *J* = 15.9 Hz), 6.61 (1H, m), 6.75-6.79 (2H, m), 6.86-6.90 (2H, m), 7.13-7.22 (3H, m), 7.26-7.30 (2H, m), 7.32-7.35 (2H, m), 7.36-7.46 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.6, 41.5, 44.2, 55.8, 113.7, 114.7, 126.0, 126.9, 127.8, 128.4, 128.5, 128.7, 129.1, 132.3, 133.7, 137.9, 139.8, 152.8, 153.3; ESIHRMS: Found: m/z 385.2271. Calcd for $C_{26}H_{29}N_2O$: $(M+H)^+$ 385.2280.

(*Z*)-1-((1-cinnamylcyclohexyl)(phenyl)methylene)-2-phenylhydrazine (**1k**)**:**



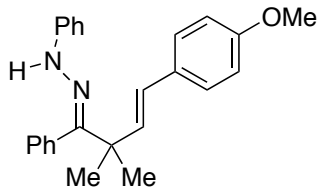
93% yield from ketone **4k** and phenylhydrazine; Yellow viscous oil; IR (NaCl) 3337, 2930, 1601, 1504 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.37-1.69 (8H, m), 1.90-1.95 (2H, m), 2.46 (2H, d, *J* = 6.8 Hz), 6.33 (1H, dt, *J* = 6.8, 15.8 Hz), 6.43 (1H, d, *J* = 15.8 Hz), 6.76 (1H, t, *J* = 7.3 Hz), 6.85 (1H, s), 6.92 (2H, d, *J* = 7.7 Hz), 7.15-7.19 (5H, m), 7.23-7.27 (2H, m), 7.33 (2H, d, *J* = 7.3 Hz), 7.40-7.46 (1H, m), 7.50 (2H, t, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.5, 26.2, 34.2, 41.7, 44.8, 112.6, 119.2, 126.1, 126.9, 127.2, 128.4, 128.5, 128.6, 129.0, 129.1, 132.0, 133.4, 137.8, 145.5, 151.1; ESIHRMS: Found: m/z 395.2480. Calcd for $C_{28}H_{31}N_2$: $(M+H)^+$ 395.2487.

(*Z*)-1-(2,2-Dimethyl-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1o**):[5]



91% yield from ketone **4o** and phenylhydrazine; Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.17 (6H, s), 2.33 (2H, d, *J* = 7.2 Hz), 5.06 (1H, d, *J* = 16.8 Hz), 5.07 (1H, d, *J* = 11.2 Hz), 5.94 (1H, tdd, *J* = 7.2, 11.2, 16.8 Hz), 6.73 (1H, s br), 6.76 (1H, t, *J* = 7.6 Hz), 6.91 (2H, d, *J* = 8.4 Hz), 7.13 (2H, d, *J* = 7.6 Hz), 7.18 (2H, t, *J* = 7.6 Hz), 7.42 (1H, dd, *J* = 7.2, 7.6 Hz), 7.48 (1H, d, *J* = 7.6 Hz), 7.50 (1H, d, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.3, 41.0, 44.9, 112.5, 117.0, 119.3, 128.5, 128.6, 129.06, 129.10, 133.5, 135.7, 145.4, 153.2.

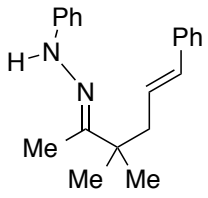
(*Z*)-1-((E)-4-(4-methoxyphenyl)-2,2-dimethyl-1-phenylbut-3-en-1-ylidene)-2-phenylhydrazine (**1p**):



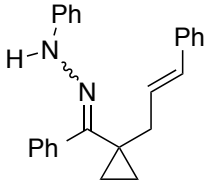
93% yield from ketone **4p** and phenylhydrazine; Yellow solid; mp. 107-108 °C; IR (NaCl) 3337, 1601, 1504, 1248, 1215 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.40 (6H, s), 3.79 (3H, s), 6.20 (1H, d, *J* = 6.2 Hz), 6.25 (1H, d, *J* = 6.2 Hz), 6.77 (1H, t, *J* = 7.3 Hz), 6.83-6.85 (3H, m), 6.94 (2H, d, *J* = 7.8 Hz), 7.10-7.12 (2H, m), 7.18 (2H, t, *J* = 8.1 Hz), 7.28 (2H, d, *J* = 8.7 Hz), 7.36-7.45 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.1, 43.6, 55.3, 112.6, 114.0, 119.4, 126.7, 127.3, 128.5, 128.8, 128.9, 129.1, 130.5, 133.4, 135.4, 145.4, 152.4, 158.9; ESIHRMS: Found: m/z 371.2127. Calcd for $C_{25}H_{27}N_2O$: $(M+H)^+$ 371.2123.

[5] X. Y. Duan, X. L. Yang, R. Fang, X. X. Peng, W. Yu and B. Han, *J. Org. Chem.* 2013, **78**, 10692.

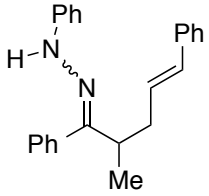
As hydrazones **1e** and **1l-n** (shown below) were not stable enough to be characterized, we used these hydrazones soon after preparation. The yields of hydroamination products **2** were calculated from the corresponding ketones **4** in 2-step manner (for detailed procedures, see section 3).



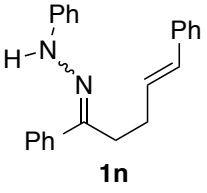
1e



1l



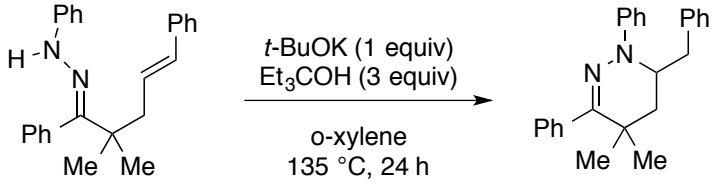
1m



1n

3. KO*t*-Bu-Mediated Hydroamination of Alkenyl Hydrazones 1

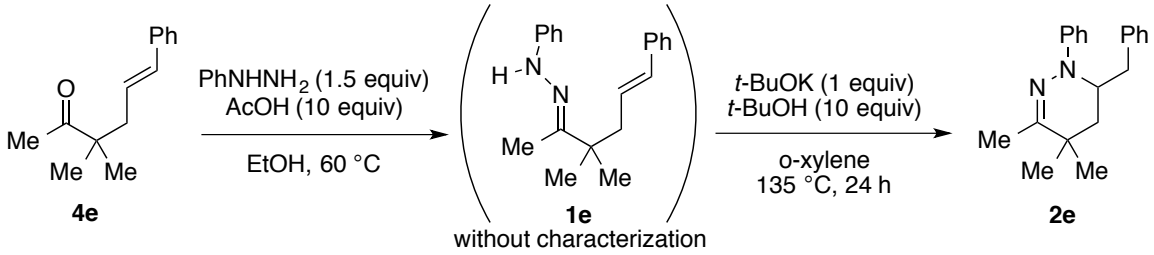
3.1 Typical Procedure A: the reaction of hydrazone **1a** (Table 1, entry 2)



1a **2a**

To a 25 mL Schlenk tube containing (*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1a**) (177.2 mg, 0.50 mmol) and *t*-BuOK (56.0 mg, 0.50 mmol) in *o*-xylene (5.0 mL) was added Et_3COH (210 μL, 1.50 mmol) and the solution was stirred at 135 °C for 24 h. Upon completion of the reaction, the solution was cooled to room temperature. After dilution with water and ethyl acetate, the mixture was extracted with ethyl acetate. The combined extracts were washed with brine, dried over $MgSO_4$, and concentrated in vacuo. The resulting crude material was purified by flash column chromatography (hexane:Et_2O = 50:1) to yield 6-benzyl-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**1a**) (149.6 mg, 0.42 mmol) in 84 % yield.

3.2 Typical Procedure B: Two-Step Procedure from Ketones 4 (for synthesis of 2e, 2l-n)

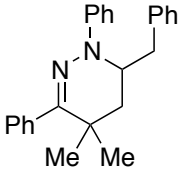


4e **1e** without characterization **2e**

To a 25 mL 2-neck round bottom flask containing ketone **4e** (101.2 mg, 0.50 mmol) in EtOH (4 mL) was added $PhNHNH_2$ (74 μL, 0.75 mmol) and AcOH (29 μL, 0.50 mmol). The solution was stirred at 60 °C under a N_2 atmosphere. After the mixture was cooled down to room temperature, the solvent was removed under reduced pressure and the resulting crude product was treated through a short silica gel pad (hexane:ethyl acetate = 20:1) afforded the corresponding hydrazone **2e**, which was used immediately for the next hydroamination.

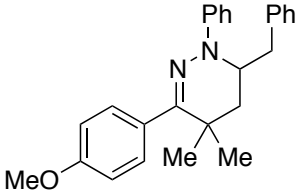
To a 25 mL Schlenk tube containing hydrazone **2e** obtained above and *t*-BuOK (56.1 mg, 0.50 mmol) in *o*-xylene (5.0 mL) was added *t*-BuOH (465 μL, 5.00 mmol) and the solution was stirred at 135 °C for 24 h. Upon completion of the reaction, the solution was cooled to room temperature. After dilution with water and ethyl acetate, the mixture was extracted with ethyl acetate. The combined extracts were washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The resulting crude material was purified by flash column chromatography (hexane:Et_2O = 50:1) to yield 6-benzyl-3,4,4-trimethyl-1-phenyl-1,4,5,6-tetrahydropyridazine (**2e**) (112.6 mg, 0.385 mmol) in 77% yield (from ketone **4e**).

6-Benzyl-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2a**):



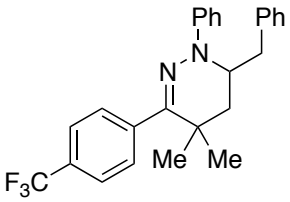
84% yield; Yellow oil; IR (NaCl) 2972, 1597, 1493 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.22 (3H, s), 1.33 (3H, s), 1.85 (2H, d, *J* = 6.3 Hz), 2.74 (1H, dd, *J* = 10.3, 13.8 Hz), 3.29 (1H, dd, *J* = 3.6, 13.8 Hz), 4.26 (1H, dtd, *J* = 3.6, 6.3, 10.3 Hz), 6.93 (1H, t, *J* = 7.1 Hz), 7.22-7.28 (3H, m), 7.29-7.38 (9H, m), 7.50 (2H, d, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.9, 29.2, 31.4, 37.3, 39.8, 52.8, 117.2, 120.8, 126.4, 127.3, 127.8, 128.4, 128.5, 128.8, 129.2, 138.4, 138.9, 146.5, 151.0; ESIHRMS: Found: m/z 355.2171. Calcd for $C_{25}H_{27}N_2$: $(M+H)^+$ 355.2174.

6-Benzyl-3-(4-methoxyphenyl)-4,4-dimethyl-1-phenyl-1,4,5,6-tetrahydropyridazine (**2b**):



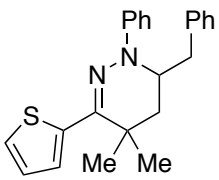
79% yield from hydrazone **1b** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 41 h) by procedure A; Yellow oil; IR (NaCl) 2959, 1597, 1495 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.21 (3H, s), 1.26 (3H, s), 1.84 (2H, d, *J* = 6.2 Hz), 2.73 (1H, dd, *J* = 10.3, 13.8 Hz), 3.27 (1H, dd, *J* = 3.6, 13.8 Hz), 4.24 (1H, dtd, *J* = 3.6, 6.2, 10.3 Hz), 6.86-6.93 (3H, m), 7.22-7.25 (3H, m), 7.28-7.37 (6H, m), 7.44 (2H, d, *J* = 8.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.9, 29.2, 31.4, 37.3, 39.9, 52.7, 55.2, 113.2, 117.0, 120.6, 126.4, 128.5, 128.8, 129.2, 129.6, 131.7, 138.5, 146.6, 150.9, 158.9; ESIHRMS: Found: m/z 385.2273. Calcd for $C_{26}H_{29}N_2O$: $(M+H)^+$ 385.2280.

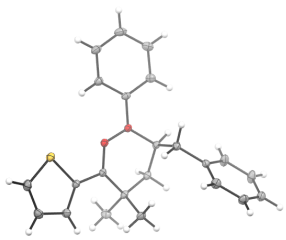
6-Benzyl-4,4-dimethyl-1-phenyl-3-(4-(trifluoromethyl)phenyl)-1,4,5,6-tetrahydropyridazine (**2c**):



63% yield from hydrazone **1c** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 48 h) by procedure A; Yellow oil; IR (NaCl) 2964, 1597, 1495, 1325 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.24 (3H, s), 1.35 (3H, s), 1.85 (2H, d, *J* = 6.4 Hz), 2.73 (1H, dd, *J* = 10.2, 13.8 Hz), 3.30 (1H, dd, *J* = 3.6, 13.8 Hz), 4.28 (1H, dtd, *J* = 3.6, 6.4, 10.2 Hz), 6.95-6.99 (1H, m), 7.22-7.27 (3H, m), 7.31-7.38 (6H, m), 7.59 (2H, d, *J* = 8.4 Hz), 7.64 (2H, d, *J* = 8.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.9, 29.0, 31.2, 37.5, 39.9, 52.7, 117.6, 121.4, 124.3 (q, $^1J_{C\text{-}F}$ = 270.2 Hz), 124.8 (q, $^3J_{C\text{-}F}$ = 3.6 Hz), 125.9 (q, $^2J_{C\text{-}F}$ = 39.7 Hz), 126.5, 128.5, 128.6, 128.9, 129.2, 129.3, 138.2, 142.4, 146.2, 148.7; ESIHRMS: Found: m/z 423.2042. Calcd for $C_{26}H_{26}N_2F_3$: $(M+H)^+$ 423.2048.

6-Benzyl-4,4-dimethyl-1-phenyl-3-(thiophen-2-yl)-1,4,5,6-tetrahydropyridazine (**2d**):

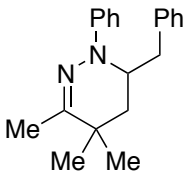


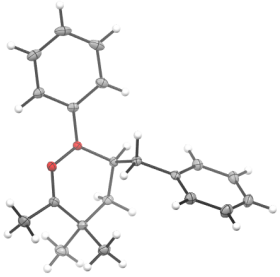


X-ray

92% yield from hydrazone **1d** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 17 h) by procedure A; Pale yellow crystal (CCDC 1001827); mp. 139-140 °C; IR (NaCl) 3019, 1597, 1495 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.34 (3H, s), 1.58 (3H, s), 1.90 (1H, dd, *J* = 5.3, 14.1 Hz), 1.94 (1H, dd, *J* = 4.7, 14.1 Hz), 2.78 (1H, dd, *J* = 10.8, 14.0 Hz), 3.18 (1H, dd, *J* = 4.1, 14.0 Hz), 4.28-4.34 (1H, m), 6.91-6.95 (1H, m), 6.98 (1H, dd, *J* = 3.7, 5.2 Hz), 7.17-7.20 (2H, m), 7.22-7.25 (3H, m), 7.30-7.39 (6H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.5, 29.9, 30.7, 35.8, 39.0, 52.3, 115.8, 120.6, 124.3, 124.8, 126.4, 126.9, 128.6, 129.0, 129.1, 138.3, 143.9, 144.7, 146.0; ESIHRMS: Found: m/z 361.1741. Calcd for $C_{23}H_{25}N_2S$: $(M+H)^+$ 361.1738.

6-Benzyl-3,4,4-trimethyl-1-phenyl-1,4,5,6-tetrahydropyridazine (**2e**):

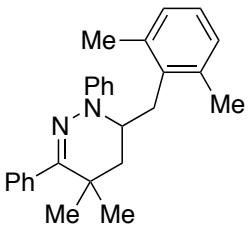




X-ray

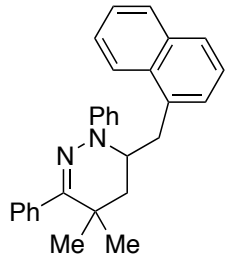
77% yield in two steps from ketone **4e** (0.5 mmol) with *t*-BuOK (1 equiv) and *t*-BuOH (10 equiv) (hydroamination for 24 h) by procedure B; Pale yellow crystal (CCDC 1001792); mp. 95-96 °C; IR (NaCl) 2961, 1643, 1595, 1495 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.08 (3H, s), 1.26 (3H, s), 1.77 (1H, d, *J* = 5.7 Hz), 1.99 (3H, s), 2.62 (1H, dd, *J* = 10.6, 13.8 Hz), 3.08 (1H, dd, *J* = 3.8, 13.8 Hz), 4.06 (1H, dtd, *J* = 3.8, 5.7, 10.6 Hz), 6.90-6.94 (1H, m), 7.17-7.23 (3H, m), 7.28-7.33 (6H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.9, 28.3, 28.4, 31.2, 36.6, 38.3, 53.0, 116.9, 120.6, 126.2, 128.5, 128.9, 129.2, 138.7, 147.2, 151.2; ESIHRMS: Found: m/z 293.2022. Calcd for $C_{20}H_{25}N_2$: $(M+H)^+$ 293.2018.

6-(2,6-Dimethylbenzyl-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2f**):



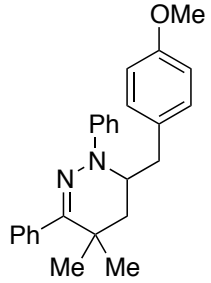
69% yield from hydrazone **1f** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 47 h) by procedure A; Yellow oil; IR (NaCl) 2961, 1597, 1495 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.21 (3H, s), 1.32 (3H, s), 1.81 (1H, dd, *J* = 4.4, 13.3 Hz), 1.99 (1H, dd, *J* = 7.4, 13.3 Hz), 2.24 (6H, s), 2.74 (1H, dd, *J* = 6.4, 13.8 Hz), 3.31 (1H, dd, *J* = 7.4, 13.8 Hz), 4.16-4.22 (1H, m), 6.87 (1H, t, *J* = 7.2 Hz), 6.91-6.99 (3H, m), 7.04-7.06 (2H, m), 7.11-7.15 (2H, m), 7.27-7.36 (3H, m), 7.51 (2H, d, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.6, 29.1, 29.6, 32.0, 33.3, 42.3, 52.3, 118.9, 121.7, 126.1, 127.3, 127.8, 128.3, 128.4, 128.6, 136.0, 136.7, 139.0, 147.2, 151.9; ESIHRMS: Found: m/z 383.2486. Calcd for $C_{27}H_{31}N_2$: $(M+H)^+$ 383.2487.

4,4-Dimethyl-6-(naphthalene-1-ylmethyl)-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2g**):



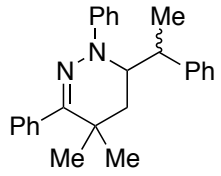
79% yield from hydrazone **1g** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 22 h) by procedure A; Yellow oil; IR (NaCl) 3052, 2959, 1593 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.18 (3H, s), 1.23 (3H, s), 1.79 (1H, dd, *J* = 5.0, 13.5 Hz), 1.96 (1H, dd, *J* = 8.0, 13.5 Hz), 3.11 (1H, dd, *J* = 9.3, 14.2 Hz), 3.70 (1H, dd, *J* = 4.5, 14.2 Hz), 4.34-4.41 (1H, m), 6.97 (1H, t, *J* = 7.0 Hz), 7.26-7.39 (9H, m), 7.45-7.51 (4H, m), 7.72 (1H, d, *J* = 7.9 Hz), 7.83-7.86 (1H, m), 7.88-7.90 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.9(1), 28.9(4), 31.7, 35.3, 41.5, 52.8, 119.5, 122.0, 123.6, 125.4, 125.5, 126.0, 127.1, 127.2, 127.3, 127.8, 128.5, 128.8, 128.9, 132.2, 133.9, 134.6, 138.9, 147.2, 152.0; ESIHRMS: Found: m/z 405.2330. Calcd for $C_{29}H_{29}N_2$: $(M+H)^+$ 405.2331.

6-(4-methoxybenzyl)-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2h**):



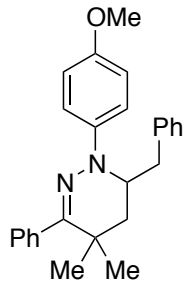
77% yield from hydrazone **1h** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 47 h) by procedure A; Yellow oil; IR (NaCl) 2959, 1597, 1512 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.22 (3H, s), 1.33 (3H, s), 1.84 (2H, d, *J* = 6.3 Hz), 2.69 (1H, dd, *J* = 10.2, 13.9 Hz), 3.20 (1H, dd, *J* = 3.6, 13.9 Hz), 3.80 (3H, s), 4.20 (1H, dtd, *J* = 3.6, 6.3, 10.2 Hz), 6.86 (2H, d, *J* = 8.5 Hz), 6.92 (1H, t, *J* = 7.0 Hz), 7.14 (2H, d, *J* = 8.5 Hz), 7.26-7.37 (7H, m), 7.50 (2H, d, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.9, 29.2, 31.4, 36.4, 39.8, 52.9, 55.2, 114.0, 117.2, 120.8, 127.2, 127.7, 128.4, 128.8, 130.1, 130.3, 139.0, 146.6, 150.9, 158.2; ESIHRMS: Found: m/z 385.2282. Calcd for $C_{26}H_{29}N_2O$: $(M+H)^+$ 385.2280.

4,4-Dimethyl-1,3-diphenyl-6-(1-phenylethyl)-1,4,5,6-tetrahydropyridazine (**2i**):



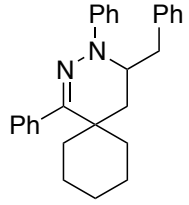
74% yield from hydrazone **1i** (0.3 mmol) with *t*-BuOK (1 equiv) and *t*-BuOH (10 equiv) (for 48 h) by procedure A as 1:1 diastereomeric mixture; each isomer (**a** and **b**) was separated by column chromatography for charaterization (the relative stereochemistry of each isomer was not assigned); Yellow oil; isomer (**a**): IR (NaCl) 2965, 1597, 1487 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.15 (3H, s), 1.25 (3H, s), 1.30 (3H, d, *J* = 7.3 Hz), 1.65 (1H, dd, *J* = 7.9, 13.4 Hz), 1.88 (1H, dd, *J* = 6.3, 13.4 Hz), 3.68 (1H, dq, *J* = 6.5, 7.3 Hz), 4.38 (1H, ddd, *J* = 6.3, 6.5, 7.9 Hz), 6.87-6.90 (1H, m), 7.13 (2H, d, *J* = 7.1 Hz), 7.19-7.36 (13H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.5, 28.2, 29.1, 31.6, 38.0, 38.3, 55.9, 116.0, 119.7, 126.3, 127.3, 127.7, 128.1, 128.3, 128.4, 128.9, 138.7, 142.5, 147.1, 153.7; ESIHRMS: Found: m/z 369.2333. Calcd for $C_{26}H_{29}N_2$: $(M+H)^+$ 369.2331. isomer (**b**): IR (NaCl) 3059, 1597, 1487 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.11 (3H, s), 1.16 (3H, d, *J* = 7.1 Hz), 1.24 (3H, s), 1.38 (1H, dd, *J* = 6.1, 13.3 Hz), 1.86 (1H, dd, *J* = 11.5, 13.3 Hz), 3.69 (1H, dq, *J* = 4.6, 7.1 Hz), 4.38 (1H, ddd, *J* = 4.6, 6.1, 11.5 Hz), 6.93 (1H, t, *J* = 7.2 Hz), 7.20-7.34 (10H, m), 7.39 (2H, d, *J* = 8.1 Hz), 7.44 (2H, d, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.1, 26.4, 28.4, 32.0, 35.9, 37.4, 56.7, 118.9, 121.2, 126.3, 127.3, 127.6, 127.7, 128.2, 128.3, 128.7, 138.7, 142.9, 146.4, 152.8; ESIHRMS: Found: m/z 369.2329. Calcd for $C_{26}H_{29}N_2$: $(M+H)^+$ 369.2331.

6-Benzyl-1-(4-methoxyphenyl)-4,4-dimethyl-3-phenyl-1,4,5,6-tetrahydropyridazine (**2j**):



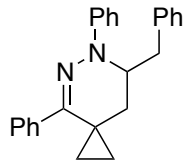
79% yield from hydrazone **1j** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 24 h) by procedure A; yellow oil; IR (NaCl) 2957, 1504, 1464 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.21 (3H, s), 1.24 (3H, s), 1.75 (1H, dd, *J* = 4.8, 13.5 Hz), 1.81 (1H, dd, *J* = 8.6, 13.5 Hz), 2.61 (1H, dd, *J* = 10.2, 13.6 Hz), 3.18 (1H, dd, *J* = 3.6, 13.6 Hz), 3.78 (3H, s), 3.95 (1H, dddd, *J* = 3.6, 4.8, 8.6, 10.2 Hz), 6.87-6.90 (2H, d, *J* = 8.5 Hz), 7.16 (2H, d, *J* = 7.0 Hz), 7.20-7.32 (8H, m), 7.44-7.47 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.7, 29.4, 31.9, 38.6, 40.8, 54.2, 55.6, 114.2, 122.0, 126.3, 127.1, 127.7, 128.4, 128.5, 129.2, 138.4, 139.0, 141.0, 150.9, 155.6; ESIHRMS: Found: m/z 385.2278. Calcd for $C_{26}H_{29}N_2O$: $(M+H)^+$ 385.2280.

4-Benzyl-1,3-diphenyl-2,3-diazaspiro[5.5]undec-1-ene (**2k**):



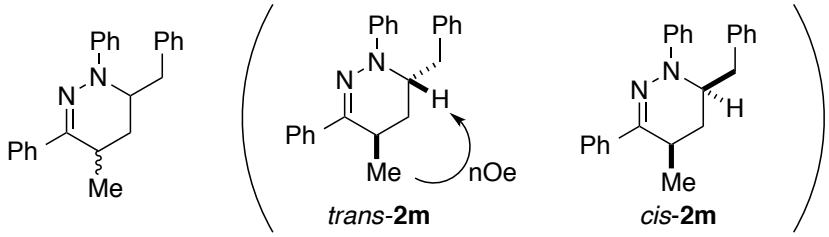
54% yield from hydrazone **1k** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 48 h) by procedure A; Yellow oil; IR (NaCl) 2934, 1597, 1495 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.98-1.09 (1H, m), 1.17-1.19 (2H, m), 1.22-1.80 (7H, m), 1.96 (1H, dd, *J* = 6.4, 14.0 Hz), 2.10 (1H, dd, *J* = 5.6, 14.0 Hz), 2.77 (1H, dd, *J* = 10.4, 14.0 Hz), 3.20 (1H, dd, *J* = 3.6, 14.0 Hz), 4.23-4.29 (1H, m), 6.88-6.92 (1H, m), 7.22-7.26 (4H, m), 7.28-7.36 (8H, m), 7.38-7.41 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.6, 20.9, 25.4, 31.7, 34.5, 35.3, 35.4, 36.3, 52.7, 116.7, 120.6, 126.3, 127.2, 127.6, 128.5, 128.8, 129.1, 129.4, 138.6, 138.9, 146.6, 154.0; ESIHRMS: Found: m/z 395.2483. Calcd for $C_{28}H_{31}N_2$: $(M+H)^+$ 395.2487.

7-Benzyl-4,6-diphenyl-5,6-diazaspiro[2.5]oc-4-ene (**2l**):



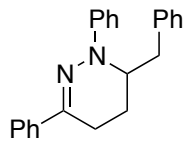
93% yield in two steps from ketone **4l** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (hydroamination for 21 h) by procedure B; Yellow oil; IR (NaCl) 1597, 1495 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.64 (1H, ddd, *J* = 4.9, 5.9, 11.0 Hz), 0.76 (1H, ddd, *J* = 4.3, 5.9, 9.6 Hz), 1.00 (1H, ddd, *J* = 4.9, 5.8, 9.9 Hz), 1.12 (1H, m), 1.38 (1H, dd, *J* = 2.0, 13.6 Hz), 2.43 (1H, dd, *J* = 4.4, 13.6 Hz), 3.09 (1H, dd, *J* = 9.7, 13.9 Hz), 3.13 (1H, dd, *J* = 5.5, 13.9 Hz), 4.56 (1H, dddd, *J* = 2.0, 4.4, 5.5, 9.7 Hz), 6.82-6.86 (1H, m), 7.21-7.37 (14H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 9.9, 14.9, 16.6, 31.5, 34.7, 54.4, 113.8, 119.3, 126.4, 127.6, 127.9, 128.7, 128.9, 129.0, 137.2, 138.8, 146.3, 148.5; ESIHRMS: Found: m/z 353.2021. Calcd for $C_{25}H_{25}N_2$: $(M+H)^+$ 353.2018.

6-Benzyl-4-methyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2m**):



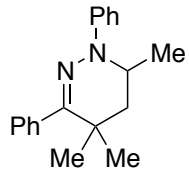
76% yield in two steps from ketone **4m** (0.5 mmol) with *t*-BuOK (1 equiv) and *t*-BuOH (10 equiv) (hydroamination for 24 h) by procedure B; (isolated as an inseparable isomers, *trans/cis* = 4:1); Yellow oil; IR (NaCl) 3026, 2959, 1599, 1489 cm^{-1}; ^1H NMR for major *trans*-isomer (400 MHz, $CDCl_3$): δ 1.13 (3H, d, *J* = 6.9 Hz), 1.74 (1H, ddd, *J* = 4.4, 11.4, 14.9 Hz), 2.13 (1H, ddd, *J* = 2.8, 7.4, 14.9 Hz), 2.75 (1H, dd, *J* = 10.8, 13.6 Hz), 3.02 (1H, dd, *J* = 4.2, 13.6 Hz), 3.06-3.21 (1H, m), 4.33-4.39 (1H, m), 6.87-6.92 (1H, m), 7.24-7.44 (12H, m), 7.67-7.69 (2H, m); ^{13}C NMR for major *trans*-isomer (100 MHz, $CDCl_3$): δ 19.5, 23.4, 30.6, 34.4, 52.7, 113.9, 119.7, 126.5, 126.6, 127.4, 128.1, 128.7, 129.1, 129.2, 138.3, 138.4, 146.3, 146.7; EIHRMS: Found: *m/z* 341.2008. Calcd for $C_{24}H_{25}N_2$: $(M+H)^+$ 341.2018.

6-Benzyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2n**):



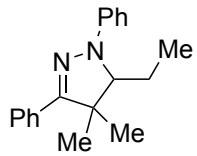
81% yield in two steps from ketone **4n** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (hydroamination for 18 h) by procedure B; Yellow solid, mp. 96-97 °C; IR (NaCl) 1589, 1489 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.84-1.94 (1H, m), 2.00-2.07 (1H, m), 2.67-2.75 (3H, m), 3.05 (1H, dd, *J* = 4.1, 13.8 Hz), 4.38-4.43 (1H, m), 6.91 (1H, t, *J* = 7.2 Hz), 7.24-7.30 (3H, m), 7.32-7.46 (9H, m), 7.86-7.88 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.0, 19.4, 34.5, 51.9, 113.7, 119.7, 124.5, 126.6, 127.7, 128.3, 128.8, 129.1(6), 129.1(9), 138.2, 138.8, 139.3, 146.3; ESIHRMS: Found: m/z 327.1857. Calcd for $C_{23}H_{23}N_2$: $(M+H)^+$ 327.1861.

4,4,6-trimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2o**):



39% yield from hydrazone **1o** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 48 h) by procedure A; Yellow solid, mp. 73-74 °C; IR (NaCl) 2968, 1597, 1493 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.29 (3H, s), 1.32 (3H, d, *J* = 7.2 Hz), 1.33 (3H, s), 1.86 (1H, dd, *J* = 7.1, 13.5 Hz), 1.99 (1H, dd, *J* = 5.0, 13.5 Hz), 4.06-4.14 (1H, m), 6.88-6.93 (1H, m), 7.22-7.34 (7H, m), 7.50-7.52 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.7, 28.9, 29.4, 31.6, 44.2, 47.1, 117.5, 120.8, 127.1, 127.7, 128.4, 128.7, 139.1, 146.8, 150.0; ESIHRMS: Found: m/z 279.1866. Calcd for $C_{19}H_{23}N_2$: $(M+H)^+$ 279.1861.

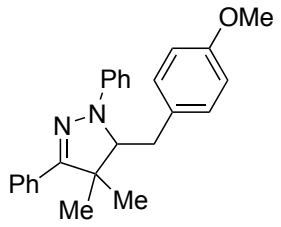
5-Ethyl-4,4-dimethyl-1,3-diphenyl-4,5-dihydro-1*H*-pyrazole (**3o**):



8% yield; Yellow solid, mp. 73-74 °C; IR (NaCl) 2970, 1595, 1495 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.83 (3H, t, *J* = 7.5 Hz), 1.42 (3H, s), 1.43 (3H, s), 1.59-1.70 (1H, m), 1.85-1.96 (1H, m), 3.86 (1H, dd, *J* = 2.6, 6.8 Hz), 6.80-6.84 (1H, m), 7.15-7.17 (2H, m), 7.24-7.38 (5H,

m), 7.70-7.72 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 10.1, 18.9, 20.3, 28.2, 49.3, 72.6, 114.3, 119.0, 126.8, 128.1, 128.3, 129.0, 132.7, 144.9, 155.3; ESIHRMS: Found: m/z 279.1855. Calcd for $C_{19}H_{23}N_2$: $(M+H)^+$ 279.1861.

5-(4-methoxybenzyl)-4,4-dimethyl-1,3-diphenyl-4,5-dihydro-1*H*-pyrazole (**3p**):



90% yield from hydrazone **1p** (0.5 mmol) with *t*-BuOK (1 equiv) and Et_3COH (3 equiv) (for 18 h) by procedure A; Yellow oil; IR (NaCl) 2970, 1595, 1514, 1495 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.31 (3H, s), 1.36 (3H, s), 2.85 (1H, dd, *J* = 8.9, 14.9 Hz), 3.05 (1H, dd, *J* = 3.8, 14.9 Hz), 3.78 (3H, s), 4.16 (1H, dd, *J* = 3.8, 8.9 Hz), 6.80-6.86 (3H, m), 7.14 (4H, t, *J* = 8.6 Hz), 7.25 (2H, t, *J* = 7.9 Hz), 7.33-7.37 (3H, m), 7.69 (2H, d, *J* = 7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.0, 27.6, 32.2, 50.6, 55.2, 72.8, 113.9, 114.9, 119.6, 126.9, 128.2, 128.3, 128.9, 130.0, 130.5, 132.7, 144.9, 156.0, 158.0; ESIHRMS: Found: m/z 371.2126. Calcd for $C_{25}H_{27}N_2O$: $(M+H)^+$ 371.2123.

4. DFT Calculation

4.1. Mehtod

Density functional theory (DFT) calculations were performed using Gaussian 09 at the B3LYP/6-311+G(d,p) level, with the solvent effect of *o*-xylene (for the reaction of hydrazone) or chlorobenzene (for the reaction of oxime) taken into account by the self-consistent reaction field (SCRF) IEFPCM method. All optimized geometries were subjected to frequency calculations to characterize the local minima or saddle points and to evaluate zero-point energy (ZPE) values.

4.2. Full reference for Gaussian 09

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

4.3. Reaction Energy Profiles

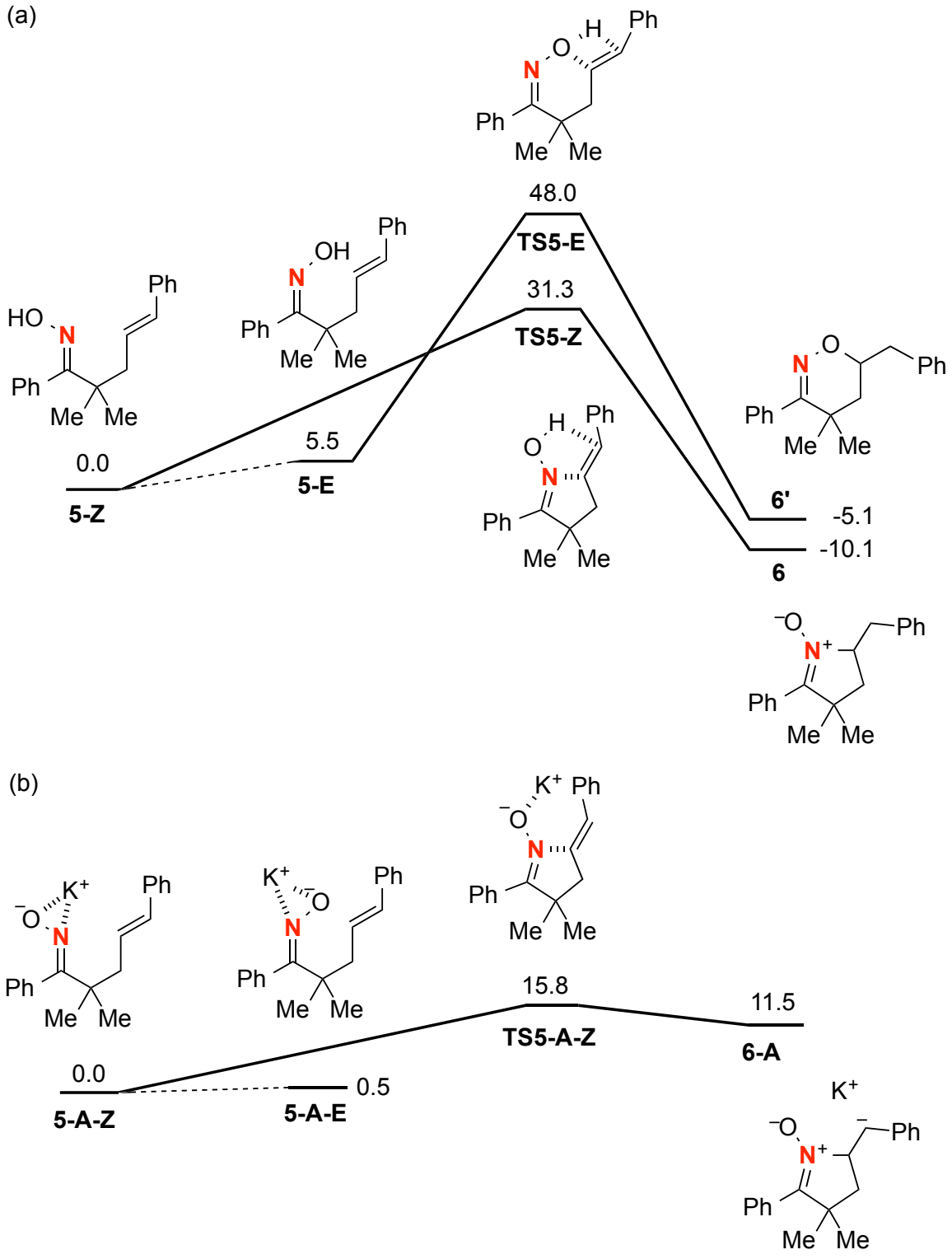


Figure S1. Energy diagrams (in kcal mol^{-1}) for the reaction of (a) the neutral and (b) deprotonated oxime substrate, which were determined at the B3LYP(SCRF,chlorobenzene)/6-311+G(d,p) level with ZPE corrections.

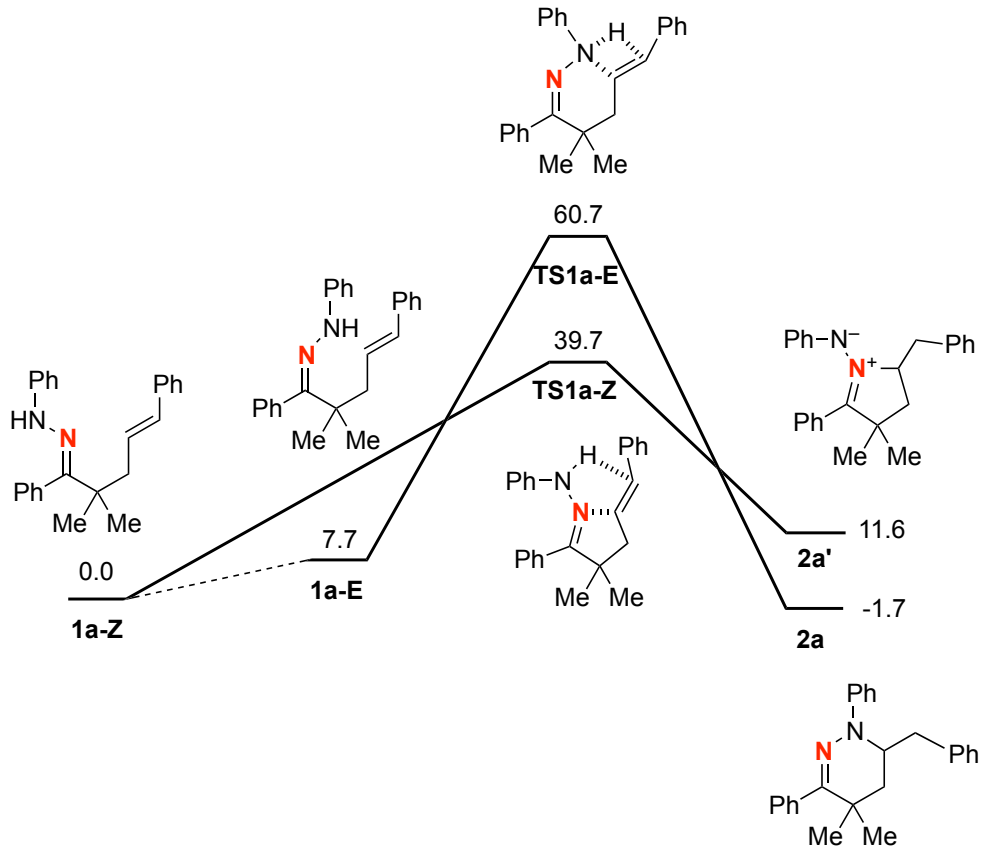


Figure S2. Energy diagram (in kcal mol^{-1}) for the reaction of the neutral hydrazone substrate, which was determined at the B3LYP(SCRF,*o*-xylene)/6-311+G(d,p) level with ZPE corrections.

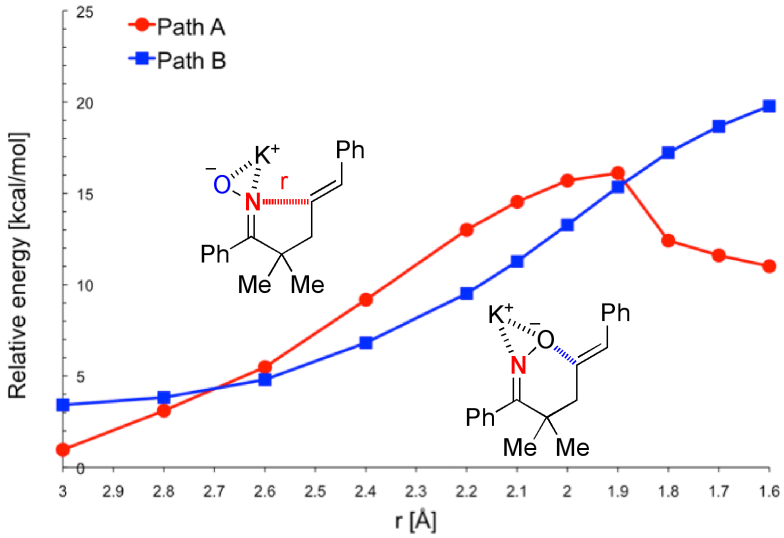


Figure S3. Variation of energy (in kcal mol^{-1}) for the reaction of deprotonate oxime with decreasing N–C or O–C bond distance, as obtained from relaxed energy calculations.

4.4. Reaction of oxime

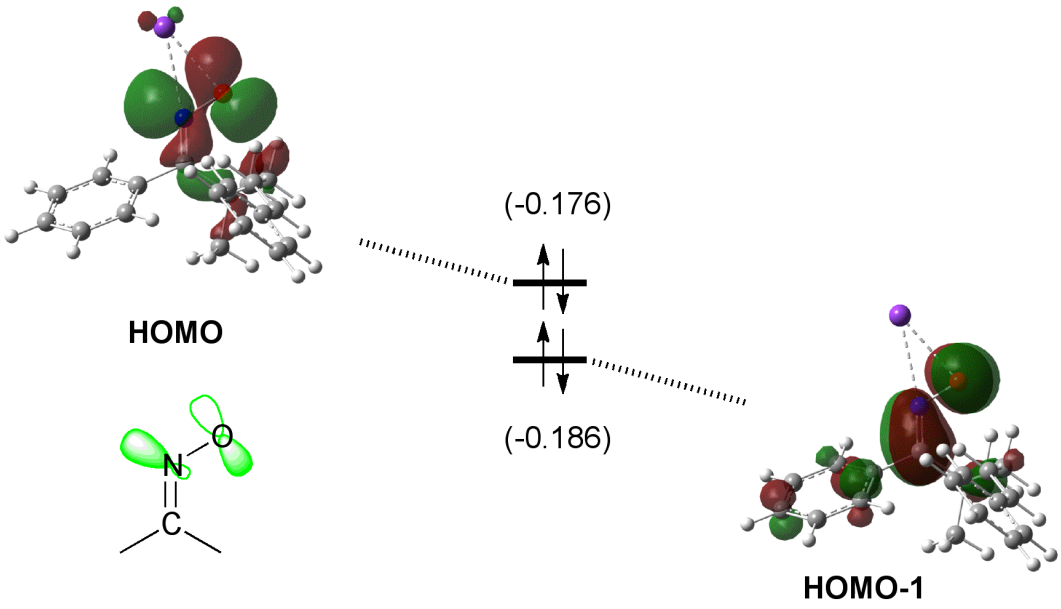


Figure S4. HOMO and HOMO-1 of **5-A-E**. The values in parentheses are orbital energy levels in hartrees.

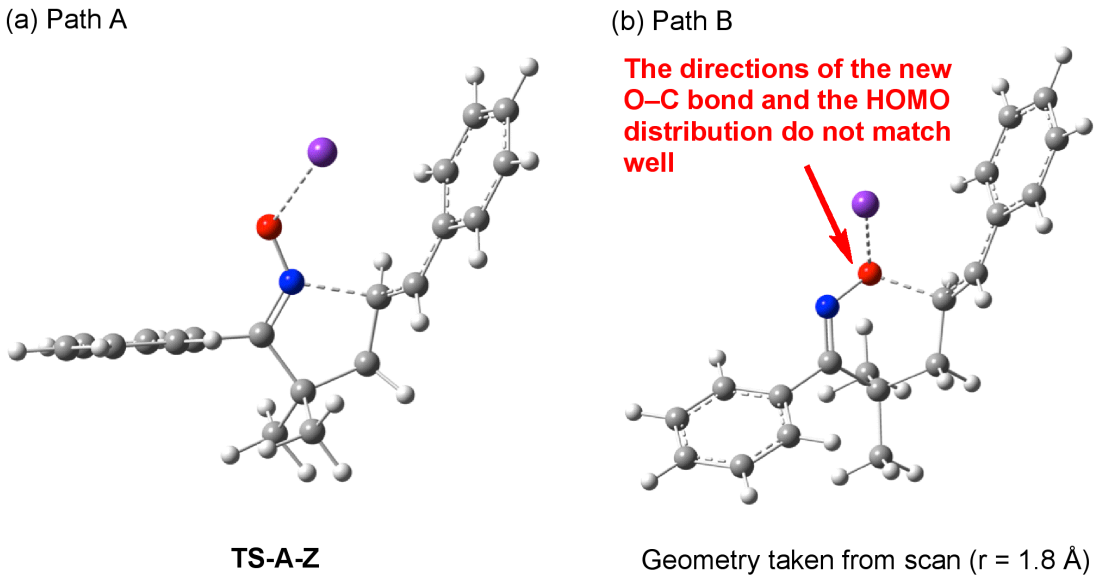


Figure S5. (a) Top view of the geometry of **TS5-A-Z** (path A). (b) Geometry of **5-A-E** at r = 1.8 Å (path B).

4.5. Raw DFT Energy Data

Table S1. Raw energy energy data obtained from DFT calculations at the B3LYP(SCRF)/6-311+G(d,p) level.

(a) Oxime

	E [au]	ZPE [au]	ΔE [kcal mol^{-1}]	Δ(E+ZPE) [kcal mol^{-1}]
5-Z	-866.814657	0.351632	0.0	0.0
TS5-Z	-866.763714	0.350529	32.0	31.3
6	-866.834236	0.355184	-12.3	-10.1
5-E	-866.806077	0.351760	5.4	5.5
TS5-E	-866.732462	0.345957	51.6	48.0
6'	-866.825198	0.354090	-6.6	-5.1

	E [au]	ZPE [au]	ΔE [kcal mol^{-1}]	Δ(E+ZPE) [kcal mol^{-1}]
5-A-Z	-1466.216073	0.339107	0.0	0.0
TS5-A-Z	-1466.190391	0.338618	16.1	15.8
6-A	-1466.198531	0.339863	11.0	11.5
5-A-E	-1466.215389	0.339193	0.4	0.5

(b) Hydrazone

	E [au]	ZPE [au]	ΔE [kcal mol^{-1}]	Δ(E+ZPE) [kcal mol^{-1}]
1a-Z	-1078.063815	0.444012	0.0	0.0
TS1a-Z	-1077.997235	0.440718	41.8	39.7
2a'	-1078.047977	0.446681	10.0	11.6
1a-E	-1078.051864	0.444358	7.5	7.7
TS1a-E	-1077.963745	0.440654	62.8	60.7
2a	-1078.069349	0.446945	-3.5	-1.7

	E [au]	ZPE [au]	ΔE [kcal mol^{-1}]	Δ(E+ZPE) [kcal mol^{-1}]
1a-Z	-1078.063815	0.444012		
t-BuOK	-833.131450	0.122269		
t-BuOH	-233.754969	0.134790		
1a + t-BuOK	-1911.195266	0.566281	0.0	1.3
1a-A-Z	-1677.442333	0.431431		
1a-A-Z + t-BuOH	-1911.197302	0.566221	0.8	0.0
1a'	-1078.049756	0.444334		
1a' + t-BuOH	-1911.181207	0.566603	9.6	10.3
1a-A-E	-1677.437319	0.431106		
1a-A-E + t-BuOH	-1911.192288	0.565896	2.9	2.9
TS1a-A-E	-1677.410678	0.431968		
TS1a-A-E + t-BuOH	-1911.165647	0.566758	23.2	20.2
2a-A	-1677.413605	0.433122		
2a-A + t-BuOH	-1911.168574	0.567912	21.7	19.1

4.6. XYZ Coordinates of Optimized Geometries

* XYZ coordinates of other oxime species are described in the Supporting Information of *Angew. Chem. Int. Ed*. 2014, **53**, 1959–1962 (DOI: 10.1002/anie.201308617).

N-OH

=== 5-E ===

C	-3.354042	-0.477102	0.420260
C	-3.561855	-1.005150	1.698821
C	-2.519483	-1.622168	2.389052
C	-1.254571	-1.716889	1.809695
C	-1.037024	-1.184713	0.539401
C	-2.080089	-0.568020	-0.151024
H	-4.541900	-0.928787	2.156186
H	-2.695189	-2.023772	3.380823
H	-0.443182	-2.194974	2.346735
H	-0.053312	-1.241395	0.086819
H	-1.896509	-0.142925	-1.130838
C	-4.484035	0.194919	-0.316163
N	-4.634223	1.404023	0.076379
O	-5.653077	2.133353	-0.566733
H	-5.575785	3.000650	-0.152715
C	-5.255484	-0.594446	-1.399008
C	-5.148654	-2.110375	-1.109459
H	-5.601781	-2.362130	-0.147274
H	-5.686117	-2.660333	-1.886296
H	-4.115808	-2.461380	-1.099222
C	-6.764087	-0.257567	-1.443826
H	-7.261834	-0.980515	-2.096823
H	-7.210426	-0.343010	-0.449661
H	-6.970003	0.742783	-1.812382
C	-4.593084	-0.352533	-2.799126
H	-3.586670	-0.781870	-2.795071
H	-5.180734	-0.952594	-3.507624
C	-4.532221	1.061566	-3.294578
C	-3.404180	1.667199	-3.688089
H	-5.475948	1.595143	-3.344189
H	-2.474011	1.103241	-3.635815
C	-3.259898	3.036085	-4.209550
C	-4.321486	3.957052	-4.270660
C	-2.000865	3.457099	-4.669354
C	-4.128998	5.237714	-4.777260
H	-5.305578	3.673714	-3.916142
C	-1.806389	4.740334	-5.176889
H	-1.165764	2.765060	-4.628006
C	-2.870707	5.638096	-5.234361
H	-4.963084	5.930054	-4.813504
H	-0.823643	5.037681	-5.525930
H	-2.724390	6.637887	-5.627042

=== TS5-E ===

C	-3.252124	-0.831687	0.778590
C	-4.118625	-1.490103	1.662486
C	-3.616623	-2.236589	2.726475
C	-2.239709	-2.342665	2.923210
C	-1.368727	-1.689674	2.052124
C	-1.871253	-0.938736	0.990707
H	-5.191542	-1.403686	1.535617
H	-4.302590	-2.730049	3.405961
H	-1.850450	-2.925775	3.750126
H	-0.296710	-1.763164	2.197866
H	-1.192187	-0.428139	0.318268
C	-3.770176	0.010943	-0.342700
N	-3.368345	1.235002	-0.299565
O	-3.872096	2.052935	-1.278796
H	-3.161156	2.385999	-2.334997
C	-4.663372	-0.571186	-1.461693
C	-4.578500	-2.109836	-1.505589
H	-4.970700	-2.569238	-0.598692
H	-5.168248	-2.478764	-2.349597
H	-3.548729	-2.452729	-1.636269
C	-6.134464	-0.149971	-1.247044
H	-6.752461	-0.492647	-2.083227
H	-6.531860	-0.602882	-0.335938
H	-6.239168	0.931648	-1.154830
C	-4.129951	-0.081986	-2.850366
H	-3.079000	-0.366931	-2.951016
H	-4.679986	-0.632222	-3.626758
C	-4.297307	1.365054	-3.165129
C	-3.269202	2.184351	-3.683200
H	-5.311788	1.747895	-3.148149
H	-2.353408	1.669055	-3.967603
C	-3.521323	3.466075	-4.392309
C	-4.627999	4.284120	-4.111871
C	-2.611761	3.901857	-5.368223
C	-4.825277	5.480408	-4.796783
H	-5.335589	3.996788	-3.341768
C	-2.805735	5.102013	-6.049619
H	-1.745728	3.289267	-5.597453
C	-3.916488	5.897305	-5.770620
H	-5.687743	6.094481	-4.561586
H	-2.088358	5.413411	-6.801084
H	-4.069653	6.831057	-6.299404

=== 6' ===

C	-3.662706	-0.545710	0.709718
C	-4.899492	-0.622361	1.360425
C	-4.980506	-1.081092	2.674953
C	-3.827011	-1.469860	3.354596
C	-2.589970	-1.389104	2.715990
C	-2.508611	-0.928298	1.403011
H	-5.799906	-0.302102	0.849885
H	-5.944544	-1.125802	3.169126
H	-3.890529	-1.825559	4.376747
H	-1.686641	-1.679797	3.240539
H	-1.544052	-0.859006	0.913380
C	-3.557257	-0.036399	-0.700106
N	-3.124501	1.170085	-0.765587
O	-2.967628	1.786483	-2.013143
H	-2.111152	1.840618	-4.460402
C	-3.877092	-0.965165	-1.878441
C	-3.134978	-2.306847	-1.699159
H	-3.488173	-2.848787	-0.819919
H	-3.310145	-2.934564	-2.577636
H	-2.056701	-2.157235	-1.601040
C	-5.394535	-1.247304	-1.957947
H	-5.592503	-1.908550	-2.806870
H	-5.755417	-1.747060	-1.057336
H	-5.976400	-0.332998	-2.094887
C	-3.387563	-0.286574	-3.173593
H	-2.308131	-0.430954	-3.288887
H	-3.874586	-0.745665	-4.038991
C	-3.669498	1.204002	-3.134060
C	-3.196298	1.954165	-4.382314
H	-4.740811	1.385622	-2.979518
H	-3.635486	1.446027	-5.246925
C	-3.572194	3.420186	-4.413986

C	-2.657194	4.410587	-4.041507
C	-4.855046	3.815729	-4.813032
C	-3.013577	5.758858	-4.062262
H	-1.658598	4.123943	-3.729664
C	-5.216728	5.161978	-4.833859
H	-5.577319	3.063772	-5.116592
C	-4.295499	6.139579	-4.457445
H	-2.289492	6.511258	-3.769415
H	-6.214495	5.447390	-5.148912
H	-4.573146	7.187509	-4.475379

N-O^{-}(K^{+})

=== 5-A-E ===

C	-2.175332	-0.948386	0.507604
C	-2.570603	-1.089004	1.848171
C	-1.643085	-1.040097	2.888594
C	-0.289028	-0.851365	2.613015
C	0.123124	-0.709085	1.287343
C	-0.807361	-0.757876	0.250429
H	-3.620661	-1.243997	2.068249
H	-1.977809	-1.156319	3.914223
H	0.435640	-0.815910	3.418979
H	1.172014	-0.551648	1.059088
H	-0.467274	-0.624622	-0.769802
C	-3.205358	-0.951528	-0.579112
N	-4.110723	-0.027382	-0.430195
O	-5.116148	0.094916	-1.307527
C	-3.216541	-2.017271	-1.698256
C	-2.030711	-2.996951	-1.612426
H	-1.972246	-3.472031	-0.629986
H	-2.167612	-3.786296	-2.358851
H	-1.071006	-2.519172	-1.813271
C	-4.512957	-2.852031	-1.547654
H	-4.581800	-3.589456	-2.355378
H	-4.508223	-3.396204	-0.598116
H	-5.388924	-2.204938	-1.580368
C	-3.226319	-1.354994	-3.113966
H	-3.251311	-2.154028	-3.864255
H	-4.159029	-0.787770	-3.183308
C	-2.082692	-0.431142	-3.397294
C	-1.205361	-0.576709	-4.400969
H	-1.996903	0.423332	-2.728731
H	-1.311397	-1.445498	-5.049334
C	-0.083469	0.311209	-4.748084
C	0.188137	1.519178	-4.079084
C	0.769398	-0.055079	-5.803371
C	1.266629	2.315972	-4.447973
H	-0.450443	1.842385	-3.265055
C	1.849894	0.742788	-6.175049
H	0.579369	-0.980997	-6.336794
C	2.105700	1.933839	-5.498132
H	1.453794	3.242597	-3.916047
H	2.490797	0.433068	-6.993339
H	2.944361	2.558637	-5.783703
K	-5.630894	2.045167	0.236334

N-NH-Ph

=== 1a-Z ===

C	-3.628407	-1.115804	-0.089650
C	-4.887481	-0.572635	-0.380942
C	-6.053772	-1.208926	0.043958
C	-5.979837	-2.394327	0.773071
C	-4.733156	-2.937258	1.081948
C	-3.567674	-2.301523	0.657243
H	-4.959135	0.354125	-0.938595
H	-7.018688	-0.775838	-0.194666
H	-6.886477	-2.889549	1.101661
H	-4.666164	-3.855799	1.654149
H	-2.601833	-2.727850	0.904440
C	-2.362994	-0.421878	-0.513673
N	-1.760562	0.416420	0.255162
N	-2.271897	0.700796	1.473444
H	-3.118299	0.237793	1.786009
C	-1.756760	-0.709719	-1.895262
C	-0.359846	-0.083869	-2.034274
H	0.328014	-0.495218	-1.292346
H	0.036526	-0.302224	-3.030404
H	-0.383098	0.998137	-1.906510
C	-1.637760	-2.236428	-2.103445
H	-1.195035	-2.442785	-3.081989
H	-0.993237	-2.686589	-1.343198
H	-2.610002	-2.732737	-2.063769
C	-2.696074	-0.153297	-3.017170
H	-2.296745	-0.479429	-3.983267
H	-3.675173	-0.637041	-2.910126
C	-2.873173	1.336895	-3.024782
C	-2.670009	2.118806	-4.093029
H	-3.196876	1.785120	-2.088266
H	-2.353272	1.644250	-5.020678
C	-2.839661	3.578593	-4.178239
C	-3.086782	4.394682	-3.059882
C	-2.745991	4.199879	-5.434414
C	-3.244946	5.768926	-3.198768
H	-3.145709	3.955425	-2.070918
C	-2.904662	5.576950	-5.575267
H	-2.549062	3.590700	-6.310843
C	-3.156879	6.369115	-4.457212
H	-3.431458	6.377590	-2.320734
H	-2.829369	6.029733	-6.557795
H	-3.278301	7.441358	-4.561037
C	-1.640546	1.592047	2.336077
C	-2.209800	1.821767	3.599922
C	-0.462306	2.267230	1.983071
C	-1.611744	2.709031	4.487806
H	-3.120594	1.302370	3.881372
C	0.123243	3.152020	2.884687
H	-0.022115	2.091489	1.011363
C	-0.439994	3.383114	4.140054
H	-2.066279	2.873136	5.458779
H	1.033871	3.667187	2.598087
H	0.024131	4.073869	4.833873

=== TS1a-Z ===

C	-3.071299	-0.892689	0.415636
C	-3.745339	-1.983880	0.987613
C	-3.402171	-2.444161	2.255102
C	-2.365228	-1.839299	2.963839
C	-1.681004	-0.762205	2.401667
C	-2.037962	-0.281524	1.146711
H	-4.551073	-2.468339	0.452939
H	-3.943826	-3.277661	2.687094
H	-2.094917	-2.202525	3.948699
H	-0.872929	-0.287233	2.945733
H	-1.509631	0.563706	0.725631
C	-3.394897	-0.420875	-0.942401
N	-3.335386	0.815615	-1.326152
N	-2.921176	1.970092	-0.776015
H	-2.787721	2.556391	-1.795672
C	-3.715291	-1.323070	-2.155764
C	-2.880852	-2.613878	-2.156558

H	-3.179043	-3.303736	-1.365246
H	-3.014765	-3.125700	-3.113727
H	-1.816142	-2.398773	-2.035978
C	-5.222361	-1.661770	-2.233792
H	-5.417846	-2.237098	-3.142910
H	-5.553089	-2.264922	-1.386297
H	-5.841012	-0.761934	-2.264957
C	-3.306788	-0.404500	-3.345834
H	-2.230580	-0.488592	-3.527581
H	-3.829662	-0.685999	-4.261702
C	-3.640848	1.015170	-2.920618
C	-2.934220	2.216277	-3.357739
H	-4.723284	1.167892	-2.917600
H	-1.930668	2.031685	-3.743380
C	-3.630348	3.322160	-4.018369
C	-4.979476	3.668207	-3.770069
C	-2.934712	4.149598	-4.931063
C	-5.586275	4.751626	-4.399582
H	-5.564517	3.093428	-3.059136
C	-3.539920	5.236936	-5.551508
H	-1.896747	3.920192	-5.154079
C	-4.877168	5.551186	-5.297523
H	-6.624383	4.979244	-4.177256
H	-2.964305	5.840987	-6.246254
H	-5.351796	6.395971	-5.783343
C	-3.559566	2.546138	0.339673
C	-3.020746	3.754595	0.812127
C	-4.684690	2.007289	0.977930
C	-3.603605	4.409176	1.890021
H	-2.149987	4.171174	0.318569
C	-5.257869	2.672069	2.061110
H	-5.119425	1.077909	0.633413
C	-4.725594	3.872520	2.525945
H	-3.177169	5.343815	2.237247
H	-6.129230	2.242259	2.543163
H	-5.174894	4.382401	3.369910

=== 2a' ===

C	-3.018383	-0.560125	0.323939
C	-3.500965	-1.805863	0.763020
C	-2.919649	-2.459332	1.845771
C	-1.835718	-1.889710	2.510980
C	-1.344203	-0.654218	2.087468
C	-1.932779	0.008547	1.017479
H	-4.346766	-2.264025	0.267669
H	-3.317591	-3.414209	2.170591
H	-1.382544	-2.398624	3.354015
H	-0.502545	-0.200674	2.598597
H	-1.545697	0.970826	0.707623
C	-3.566697	0.097076	-0.864069
N	-3.658476	1.420569	-1.004190
N	-3.541418	2.447084	-0.165497
H	-3.157092	3.788049	-2.167275
C	-3.999418	-0.611734	-2.149378
C	-3.155211	-1.847517	-2.498271
H	-3.333813	-2.678996	-1.814819
H	-3.408913	-2.186386	-3.507061
H	-2.087518	-1.615334	-2.476038
C	-5.499841	-0.993520	-2.102935
H	-5.799804	-1.431320	-3.060099
H	-5.710145	-1.728094	-1.322646
H	-6.130750	-0.120314	-1.917537
C	-3.771261	0.510359	-3.192482
H	-2.748885	0.446046	-3.576082
H	-4.452134	0.429857	-4.040692
C	-3.951528	1.817535	-2.430494
C	-3.059516	2.979183	-2.892194
H	-4.994133	2.148855	-2.430840
H	-2.015971	2.650439	-2.876005
C	-3.431256	3.462336	-4.277940
C	-4.575497	4.247488	-4.473164
C	-2.650846	3.139700	-5.393354
C	-4.932627	4.689565	-5.745205
H	-5.186003	4.524346	-3.619166
C	-3.003170	3.581980	-6.668862
H	-1.753115	2.544144	-5.262530
C	-4.147303	4.356503	-6.849504
H	-5.819181	5.300828	-5.873680
H	-2.380920	3.324606	-7.519020
H	-4.421487	4.704073	-7.839180
C	-3.965280	2.337640	1.152810
C	-3.452423	3.306954	2.043170
C	-4.949515	1.454409	1.649490
C	-3.898811	3.390645	3.355675
H	-2.704785	3.997681	1.669396
C	-5.402249	1.559136	2.961031
H	-5.379566	0.698307	1.005720
C	-4.880670	2.517748	3.830748
H	-3.479738	4.145605	4.012924
H	-6.169889	0.875357	3.308995
H	-5.229749	2.581867	4.854772

=== 1a-E ===

C	-3.568265	-1.318495	0.001530
C	-4.883100	-1.465642	-0.461022
C	-5.806755	-2.236270	0.242985
C	-5.432040	-2.880505	1.421302
C	-4.128105	-2.738984	1.894180
C	-3.207887	-1.963051	1.192115
H	-5.200189	-0.959437	-1.365432
H	-6.822188	-2.326778	-0.126946
H	-6.150001	-3.482282	1.967032
H	-3.825717	-3.232378	2.811452
H	-2.197505	-1.848318	1.566797
C	-2.563330	-0.456642	-0.712115
N	-2.127602	0.491330	0.046546
N	-1.236846	1.424424	-0.341600
H	-1.038289	1.569684	-1.322425
C	-2.146525	-0.805755	-2.167826
C	-0.632196	-0.574347	-2.417422
H	-0.029646	-0.882227	-1.560211
H	-0.321272	-1.173151	-3.277203
H	-0.378929	0.458734	-2.660833
C	-2.394865	-2.310124	-2.434248
H	-2.071660	-2.553004	-3.449974
H	-1.820871	-2.930982	-1.741316
H	-3.444284	-2.587533	-2.339665
C	-2.983772	-0.002894	-3.222624
H	-2.607107	-0.277505	-4.214287
H	-4.018058	-0.362187	-3.174563
C	-2.986579	1.491330	-3.083579
C	-2.470599	2.332552	-3.991576
H	-3.468938	1.886549	-2.192487
H	-2.005432	1.899993	-4.876347
C	-2.459527	3.803655	-3.954101
C	-3.036244	4.556315	-2.915670
C	-1.843154	4.499958	-5.006768
C	-2.992432	5.945532	-2.932814
H	-3.522588	4.055788	-2.086680
C	-1.799737	5.892295	-5.025543
H	-1.394136	3.938508	-5.819934
C	-2.374286	6.622152	-3.987177
H	-3.441811	6.504964	-2.119897
H	-1.318159	6.405139	-5.850730

H	-2.343396	7.705713	-3.996830
C	-0.867835	2.446986	0.537454
C	-0.075155	3.496861	0.047278
C	-1.240448	2.441416	1.889141
C	0.337301	4.518524	0.895594
H	0.213138	3.510431	-0.998964
C	-0.820995	3.473506	2.724629
H	-1.852929	1.634312	2.266266
C	-0.030619	4.516909	2.241905
H	0.948008	5.322077	0.498804
H	-1.117893	3.458462	3.767894
H	0.291761	5.314256	2.901023

=== TS1a-E===

C	-3.172075	-1.558214	0.077956
C	-4.359822	-2.106477	0.582444
C	-4.332963	-3.257447	1.366806
C	-3.123080	-3.889772	1.648079
C	-1.936088	-3.355522	1.147949
C	-1.959651	-2.197459	0.376510
H	-5.310677	-1.627018	0.390136
H	-5.260447	-3.657967	1.760247
H	-3.105534	-4.789318	2.252746
H	-0.989425	-3.839754	1.359646
H	-1.036905	-1.778224	-0.004575
C	-3.149603	-0.300979	-0.731601
N	-2.249535	0.531382	-0.338119
N	-2.057526	1.761240	-1.042479
H	-1.101753	1.928584	-1.751704
C	-4.084488	-0.098637	-1.938416
C	-4.391816	-1.441149	-2.633591
H	-5.002701	-2.100143	-2.016584
H	-4.937777	-1.245172	-3.560878
H	-3.473512	-1.975527	-2.889927
C	-5.412621	0.572710	-1.515560
H	-6.038646	0.718256	-2.400522
H	-5.975989	-0.039784	-0.810280
H	-5.254146	1.549372	-1.056132
C	-3.332551	0.780903	-2.957838
H	-2.499516	0.197656	-3.363800
H	-3.993302	1.012741	-3.798337
C	-2.784417	2.091781	-2.417324
C	-1.593721	2.603669	-3.181948
H	-3.575162	2.811142	-2.205683
H	-1.308948	1.948900	-4.004305
C	-1.388778	4.016710	-3.479046
C	-2.055276	5.079371	-2.824624
C	-0.448474	4.391386	-4.471831
C	-1.796767	6.411593	-3.139056
H	-2.784174	4.866796	-2.050665
C	-0.188471	5.720310	-4.778702
H	0.082391	3.608641	-5.006169
C	-0.860482	6.752303	-4.115314
H	-2.334925	7.192988	-2.610993
H	0.541030	5.956194	-5.547537
H	-0.660988	7.790206	-4.356058
C	-2.034480	2.850192	-0.059026
C	-0.815106	3.445896	0.244824
C	-3.206279	3.266187	0.568510
C	-0.771125	4.483543	1.175064
H	0.088453	3.106202	-0.245771
C	-3.155448	4.301387	1.498165
H	-4.150196	2.784817	0.346720
C	-1.938766	4.913805	1.800464
H	0.177166	4.954223	1.405841
H	-4.065957	4.626549	1.987949
H	-1.902918	5.720910	2.522933

=== 2a ===

C	-3.584900	-1.350169	0.015049
C	-4.882508	-1.876677	-0.082381
C	-5.240767	-3.042103	0.594106
C	-4.310109	-3.716254	1.381154
C	-3.014469	-3.209267	1.486228
C	-2.658458	-2.045653	0.812301
H	-5.635956	-1.371714	-0.670181
H	-6.254151	-3.418710	0.507142
H	-4.588930	-4.624411	1.903696
H	-2.276100	-3.725293	2.090397
H	-1.651787	-1.656517	0.895005
C	-3.154240	-0.090273	-0.668016
N	-2.305108	0.601439	0.015901
N	-1.686335	1.727873	-0.459665
H	-0.953167	4.115017	-1.479951
C	-3.615305	0.276047	-2.089583
C	-3.617933	-0.958003	-3.015931
H	-4.370102	-1.692051	-2.724576
H	-3.832704	-0.645055	-4.042530
H	-2.643937	-1.454814	-3.011056
C	-5.022386	0.923676	-2.096482
H	-5.259685	1.264059	-3.109711
H	-5.804071	0.225279	-1.796761
H	-5.078004	1.785604	-1.428674
C	-2.594333	1.286384	-2.650701
H	-1.667555	0.763274	-2.912561
H	-2.989471	1.726254	-3.569169
C	-2.246654	2.392888	-1.659071
C	-1.264456	3.419721	-2.261752
H	-3.161284	2.932111	-1.368636
H	-0.366916	2.892881	-2.599306
C	-1.860330	4.212043	-3.406600
C	-2.792733	5.228205	-3.158623
C	-1.495898	3.958190	-4.733397
C	-3.349752	5.962035	-4.204027
H	-3.078426	5.454295	-2.135953
C	-2.048809	4.691628	-5.783534
H	-0.767353	3.182709	-4.947481
C	-2.980224	5.694858	-5.522513
H	-4.066535	6.746984	-3.988934
H	-1.748775	4.480479	-6.804128
H	-3.409500	6.267541	-6.336876
C	-1.206076	2.552200	0.618246
C	0.123990	2.977599	0.628603
C	-2.052660	2.916798	1.669458
C	0.596274	3.778700	1.667428
H	0.787001	2.665313	-0.169191
C	-1.575890	3.708962	2.711659
H	-3.076726	2.562514	1.673032
C	-0.251606	4.147328	2.711137
H	1.631488	4.101172	1.667775
H	-2.238707	3.981983	3.525346
H	0.119063	4.762910	3.522884

=== 1a' ===

C	-3.728809	-0.704690	-0.164848
C	-5.023236	-0.358319	-0.569440
C	-6.079859	-1.260331	-0.453012
C	-5.861848	-2.525387	0.089063
C	-4.582074	-2.875010	0.518099
C	-3.525924	-1.973929	0.394183
H	-5.212047	0.629702	-0.975019
H	-7.072799	-0.970214	-0.778286
H	-6.682114	-3.227757	0.185557
H	-4.404185	-3.851791	0.954502

H	-2.541876	-2.254020	0.746352
C	-2.602044	0.310896	-0.305364
N	-1.834211	0.312274	0.957878
N	-1.917069	1.387187	1.574341
H	-3.048825	1.303124	-0.425673
C	-1.618317	0.082839	-1.513647
C	-0.550202	1.193302	-1.495394
H	0.107108	1.097201	-0.628323
H	0.069851	1.129677	-2.394416
H	-0.999393	2.189304	-1.471656
C	-0.915959	-1.285087	-1.438952
H	-0.172026	-1.358456	-2.237785
H	-0.398579	-1.414257	-0.486047
H	-1.619548	-2.110989	-1.564543
C	-2.404433	0.134960	-2.860708
H	-1.707213	-0.160260	-3.651910
H	-3.182208	-0.637728	-2.829751
C	-3.028525	1.449153	-3.234978
C	-2.710138	2.145784	-4.334083
H	-3.795848	1.835306	-2.569195
H	-1.934637	1.743564	-4.984408
C	-3.283567	3.423388	-4.787182
C	-4.349976	4.070095	-4.137380
C	-2.744484	4.038266	-5.929201
C	-4.847695	5.279426	-4.609123
H	-4.799847	3.624424	-3.257753
C	-3.241793	5.250364	-6.403250
H	-1.922464	3.556674	-6.449065
C	-4.296685	5.878229	-5.744666
H	-5.671560	5.757892	-4.090892
H	-2.805018	5.702687	-7.286775
H	-4.688337	6.820690	-6.110104
C	-1.209119	1.447139	2.817066
C	-1.192778	2.699124	3.436255
C	-0.571435	0.355080	3.420893
C	-0.531156	2.869014	4.650782
H	-1.699873	3.525464	2.951879
C	0.081522	0.529644	4.634604
H	-0.600383	-0.611391	2.935025
C	0.106147	1.784978	5.251225
H	-0.516439	3.842388	5.127285
H	0.573064	-0.313410	5.107273
H	0.618170	1.912225	6.198326

N-N^{-}(K^{+})-Ph

=== 1a-A-Z ===

C	-1.903974	-0.556566	0.553342
C	-1.785797	-1.291249	1.751128
C	-0.545229	-1.550209	2.322431
C	0.626163	-1.071409	1.727452
C	0.534685	-0.338538	0.547925
C	-0.712957	-0.086682	-0.030185
H	-2.684942	-1.657296	2.227791
H	-0.488927	-2.132174	3.236309
H	1.592531	-1.274366	2.175395
H	1.433032	0.034290	0.066841
H	-0.750418	0.480611	-0.951531
C	-3.255225	-0.320889	-0.044755
N	-4.278416	0.108807	0.647003
N	-4.122383	0.487563	1.930308
C	-3.518241	-0.626641	-1.538363
C	-2.800000	-1.920840	-1.977285
H	-3.164412	-2.775851	-1.400727
H	-2.994395	-2.121189	-3.035911
H	-1.718482	-1.862694	-1.840112
C	-5.027638	-0.828245	-1.783899
H	-5.191533	-1.103220	-2.831006
H	-5.418560	-1.627441	-1.150964
H	-5.607314	0.067631	-1.562954
C	-3.025005	0.540057	-2.468969
H	-1.944648	0.476203	-2.625624
H	-3.480110	0.380795	-3.456494
C	-3.382389	1.912181	-1.981247
C	-2.522566	2.939031	-1.895500
H	-4.416771	2.052240	-1.678956
H	-1.493909	2.774988	-2.214411
C	-2.799849	4.299532	-1.401124
C	-4.061740	4.712222	-0.931298
C	-1.752491	5.237646	-1.371593
C	-4.259760	6.003962	-0.454225
H	-4.899038	4.023981	-0.945325
C	-1.951990	6.532411	-0.896528
H	-0.772722	4.946053	-1.736757
C	-3.207335	6.922310	-0.433648
H	-5.242065	6.297556	-0.101212
H	-1.127469	7.236697	-0.892558
H	-3.367671	7.929023	-0.065536
K	-2.440898	2.468780	1.485828
C	-5.308489	0.843789	2.547681
C	-5.224882	1.342532	3.873138
C	-6.606522	0.750444	1.980569
C	-6.356414	1.739099	4.575989
H	-4.247199	1.388263	4.344615
C	-7.729457	1.153106	2.695140
H	-6.706928	0.351643	0.980138
C	-7.626136	1.655179	3.996394
H	-6.248864	2.110256	5.590967
H	-8.707962	1.066736	2.230825
H	-8.509284	1.959476	4.546372

=== 1a-A-E ===

C	-1.902333	-0.836655	0.600007
C	-2.236429	-1.545693	1.767534
C	-1.253617	-2.052149	2.615191
C	0.096916	-1.861571	2.319498
C	0.448142	-1.158890	1.167239
C	-0.537412	-0.656138	0.318341
H	-3.283602	-1.703698	1.997586
H	-1.542593	-2.606218	3.502242
H	0.864044	-2.259617	2.974355
H	1.493811	-0.998217	0.926791
H	-0.239612	-0.101431	-0.563343
C	-2.987340	-0.261062	-0.256904
N	-3.814757	0.495433	0.409046
N	-4.788200	1.202846	-0.223456
C	-3.135670	-0.640254	-1.750613
C	-2.089556	-1.674020	-2.214129
H	-2.079481	-2.553312	-1.565407
H	-2.346792	-2.007546	-3.224404
H	-1.077177	-1.270687	-2.251258
C	-4.528812	-1.294508	-1.940067
H	-4.676488	-1.552693	-2.994173
H	-4.599549	-2.216539	-1.355560
H	-5.323691	-0.618167	-1.628393
C	-3.061405	0.612272	-2.684179
H	-3.168221	0.266890	-3.718960
H	-3.925245	1.237418	-2.442645
C	-1.817244	1.435623	-2.554770
C	-0.920563	1.642051	-3.529552
H	-1.658305	1.895639	-1.580873
H	-1.089224	1.154754	-4.488619
C	0.307622	2.450391	-3.459269
C	0.615821	3.300722	-2.382088

C	1.230456	2.378413	-4.516265
C	1.799361	4.030144	-2.358656
H	-0.081926	3.401083	-1.558581
C	2.416550	3.108959	-4.495307
H	1.012404	1.734838	-5.362489
C	2.709424	3.938037	-3.414363
H	2.012366	4.680509	-1.516970
H	3.110961	3.030635	-5.324640
H	3.629993	4.510159	-3.394911
K	-3.371584	2.641312	1.972673
C	-5.794130	1.614329	0.613781
C	-6.678481	2.628967	0.144692
C	-6.055977	1.098973	1.918227
C	-7.718359	3.104639	0.926576
H	-6.517593	3.019565	-0.855000
C	-7.105660	1.595890	2.692739
H	-5.459980	0.271237	2.283152
C	-7.945030	2.603488	2.218552
H	-8.368616	3.878023	0.528677
H	-7.283396	1.166897	3.675183
H	-8.765543	2.974265	2.821603

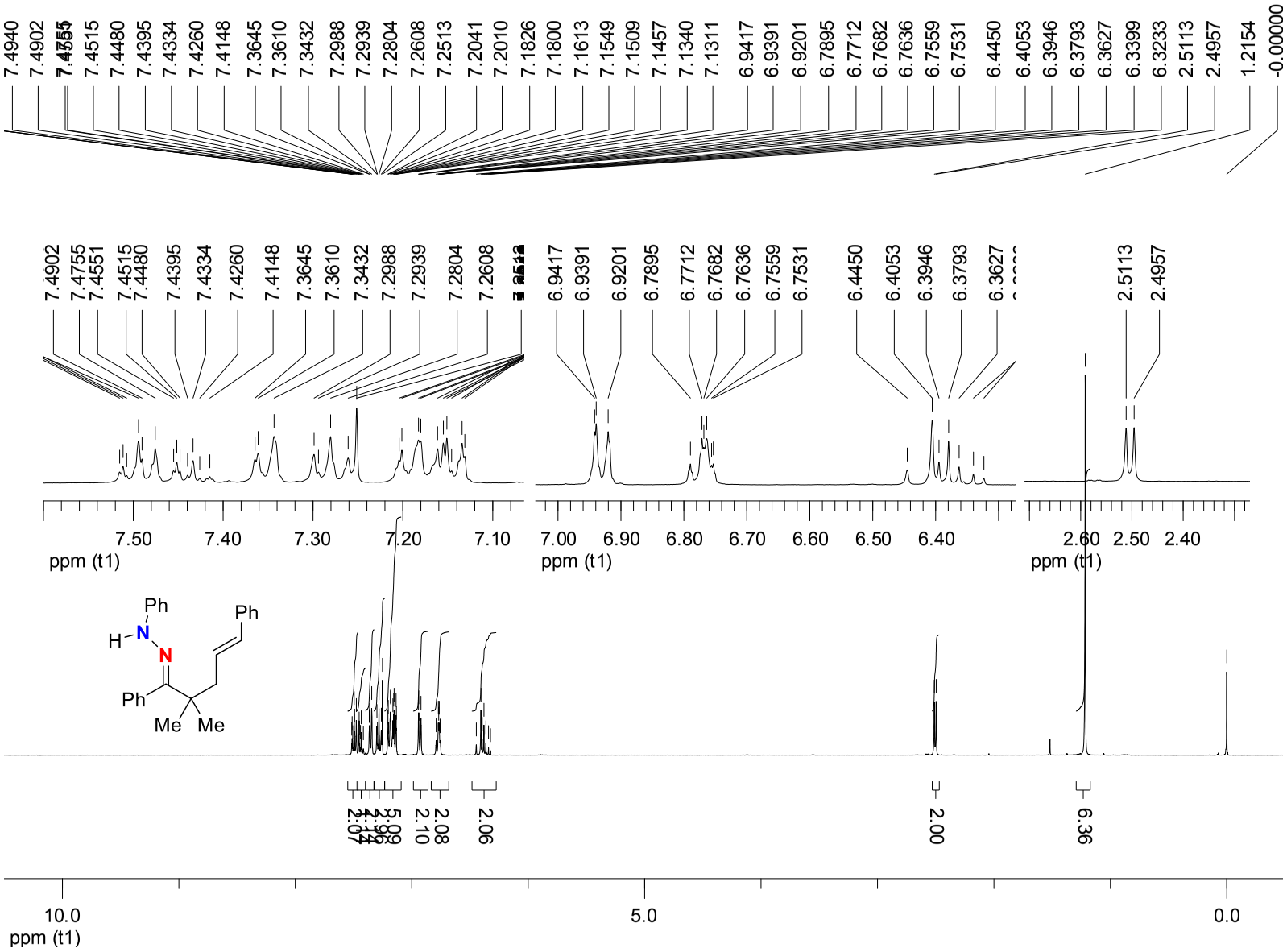
=== TS1a-A-E ===

C	-1.729688	-1.716324	0.280657
C	-2.243847	-2.171096	1.505933
C	-1.467940	-2.939977	2.370850
C	-0.155552	-3.268646	2.032350
C	0.371320	-2.820647	0.821654
C	-0.407616	-2.056246	-0.046187
H	-3.262506	-1.916168	1.773218
H	-1.890665	-3.285520	3.308025
H	0.449346	-3.867926	2.703497
H	1.392932	-3.063690	0.550486
H	0.025412	-1.707690	-0.975205
C	-2.581112	-0.846668	-0.591550
N	-3.044160	0.205432	0.009777
N	-3.798459	1.059656	-0.737909
C	-3.062657	-1.307649	-1.980052
C	-2.032770	-2.169905	-2.736466
H	-1.747739	-3.061354	-2.174650
H	-2.476029	-2.499723	-3.680606
H	-1.127868	-1.608683	-2.980592
C	-4.310935	-2.190724	-1.707383
H	-4.733162	-2.536732	-2.656289
H	-4.053073	-3.070256	-1.110717
H	-5.079475	-1.623251	-1.177731
C	-3.492316	-0.097666	-2.888384
H	-3.078941	-0.239188	-3.891702
H	-4.579901	-0.102001	-2.981898
C	-3.064307	1.258348	-2.359821
C	-1.660570	1.533898	-2.370046
H	-3.700388	2.066391	-2.711050
H	-0.989321	0.699035	-2.545547
C	-1.044241	2.818066	-2.263898
C	-1.743255	4.030291	-1.975804
C	0.374104	2.952181	-2.394840
C	-1.085188	5.253245	-1.876581
H	-2.818490	4.008732	-1.840740
C	1.017941	4.176329	-2.285281
H	0.958246	2.063379	-2.618603
C	0.300712	5.352148	-2.025801
H	-1.669124	6.146009	-1.672029
H	2.096079	4.219224	-2.410453
H	0.805319	6.307419	-1.943463
K	-1.116492	2.117250	0.584668
C	-4.359445	2.122823	-0.030482
C	-5.137734	3.081832	-0.719170
C	-4.249785	2.264526	1.373916
C	-5.718995	4.149391	-0.047611
H	-5.304535	2.972003	-1.783005
C	-4.845943	3.338520	2.033086
H	-3.742228	1.496610	1.942940
C	-5.572393	4.300848	1.334098
H	-6.306886	4.866883	-0.610543
H	-4.751888	3.410645	3.112282
H	-6.035506	5.131944	1.852501

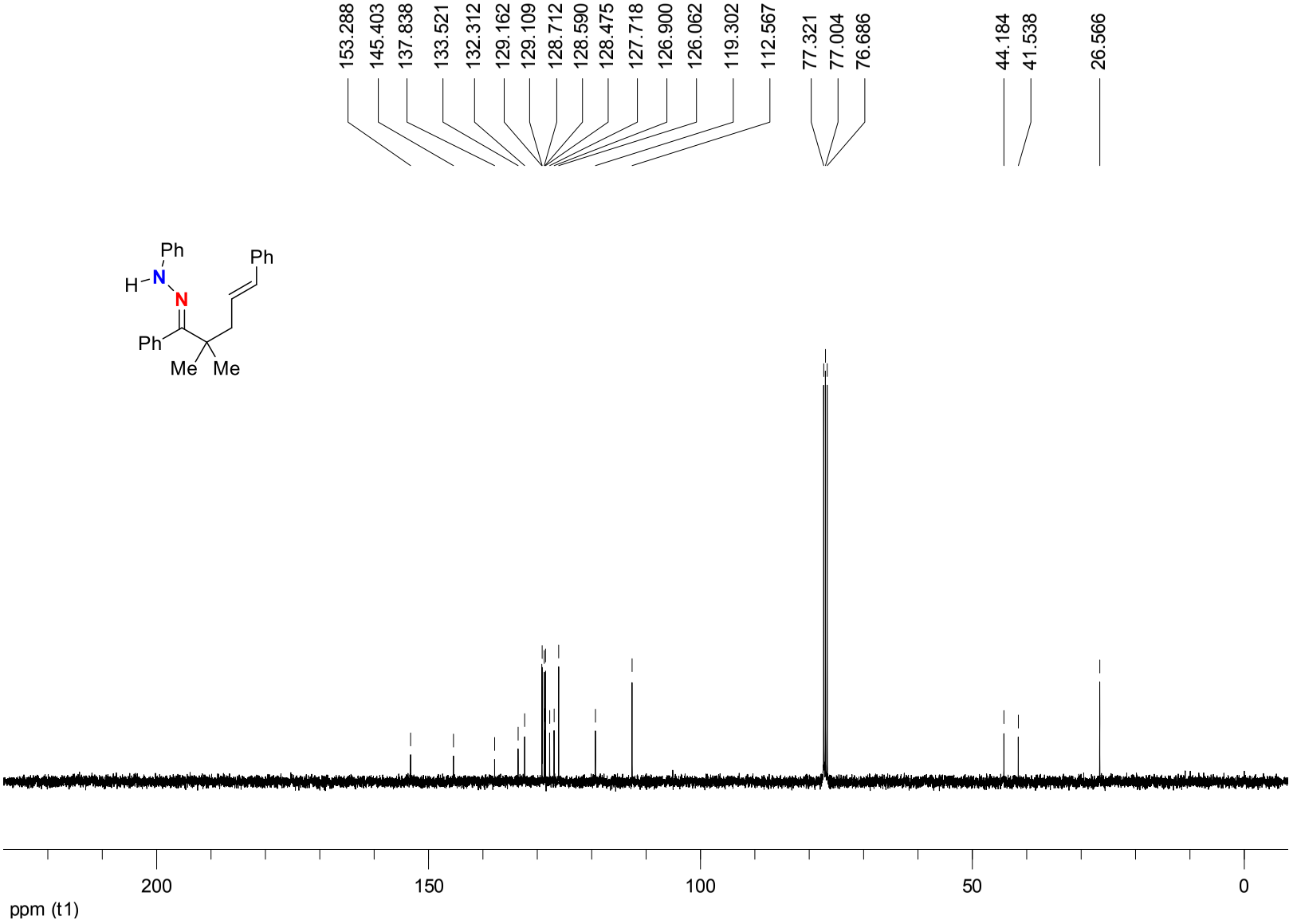
=== 2a-A ===

C	-1.791270	-1.761962	0.375141
C	-2.438812	-2.223727	1.530694
C	-1.789800	-3.072225	2.424885
C	-0.474679	-3.469792	2.185104
C	0.183842	-3.011109	1.045368
C	-0.469019	-2.168038	0.146136
H	-3.458758	-1.911754	1.722166
H	-2.311978	-3.423480	3.308077
H	0.032174	-4.129844	2.879963
H	1.209505	-3.306979	0.854269
H	0.062272	-1.810787	-0.727160
C	-2.510093	-0.817444	-0.542597
N	-2.891331	0.273868	0.037044
N	-3.520723	1.229871	-0.715207
C	-2.948909	-1.266564	-1.946868
C	-1.819286	-1.941089	-2.754503
H	-1.467304	-2.854603	-2.271886
H	-2.207972	-2.216674	-3.739136
H	-0.966233	-1.279269	-2.909514
C	-4.061756	-2.329311	-1.733357
H	-4.446390	-2.653060	-2.705260
H	-3.679512	-3.209084	-1.209918
H	-4.895645	-1.919421	-1.157776
C	-3.553509	-0.065555	-2.740627
H	-3.284384	-0.146283	-3.796910
H	-4.644003	-0.113775	-2.678178
C	-3.111087	1.295726	-2.196801
C	-1.664822	1.588760	-2.419736
H	-3.751820	2.069502	-2.622302
H	-1.060516	0.785321	-2.821992
C	-1.069830	2.867263	-2.398903
C	-1.717989	4.073363	-1.957989
C	0.315349	3.039421	-2.760245
C	-1.056475	5.299365	-1.918900
H	-2.761641	4.045870	-1.667127
C	0.954978	4.264364	-2.706818
H	0.864842	2.169360	-3.111005
C	0.286051	5.426966	-2.282545
H	-1.609749	6.176573	-1.593211
H	1.997440	4.325347	-3.008475
H	0.791212	6.384684	-2.247719
K	-0.855348	2.208629	0.422793
C	-4.225457	2.207244	-0.006066
C	-5.005784	3.177366	-0.671071
C	-4.216605	2.233577	1.407849
C	-5.701255	4.145559	0.045254
H	-5.086803	3.172458	-1.748851
C	-4.917729	3.212573	2.106523
H	-3.685502	1.461987	1.947140
C	-5.660811	4.184958	1.438981
H	-6.290158	4.874642	-0.500987
H	-4.889922	3.201772	3.191377
H	-6.208705	4.940774	1.988725

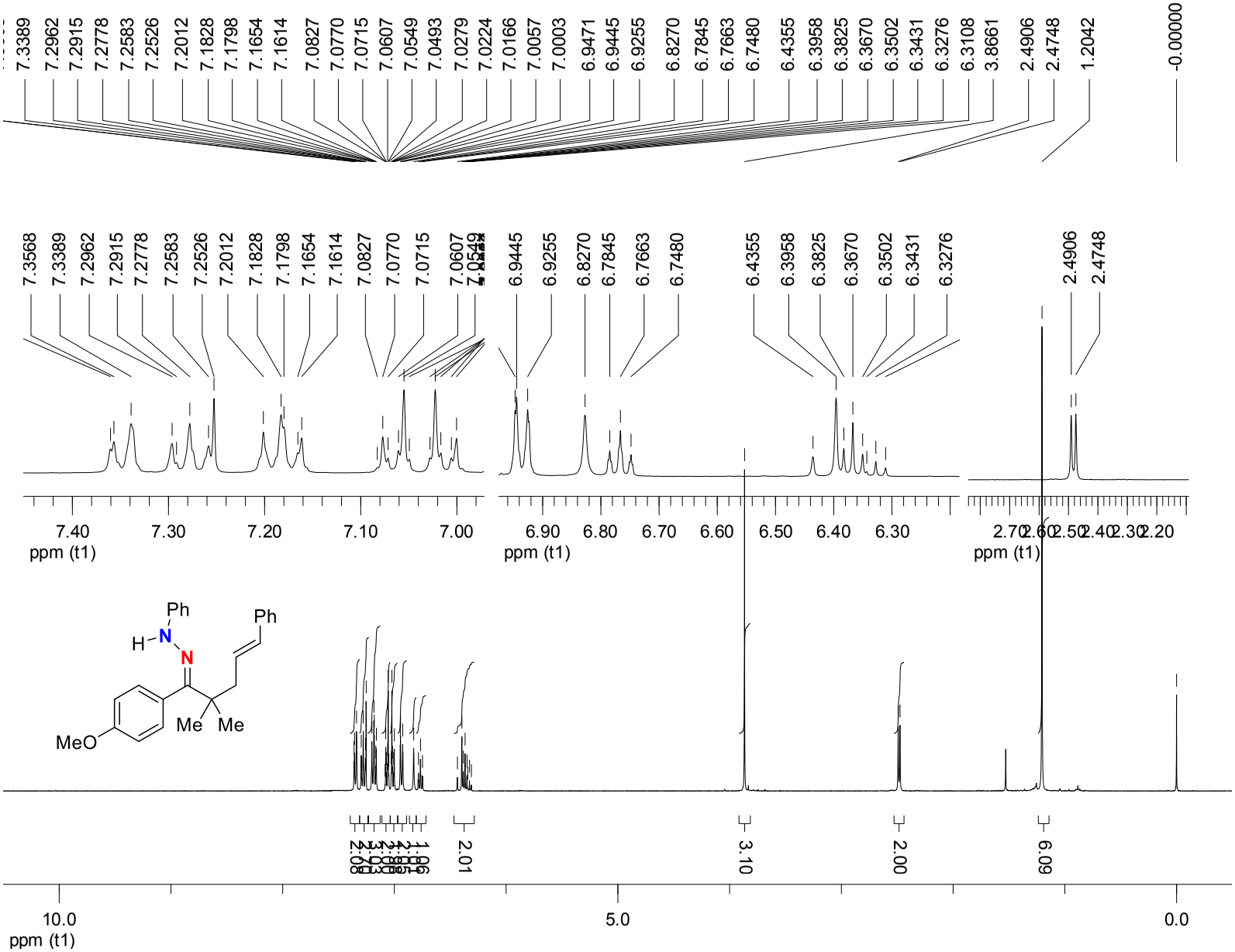
(*Z*)-1-((*E*)- 2,2-dimethyl-1,5-diphenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1a**) (400 MHz, $CDCl_3$)



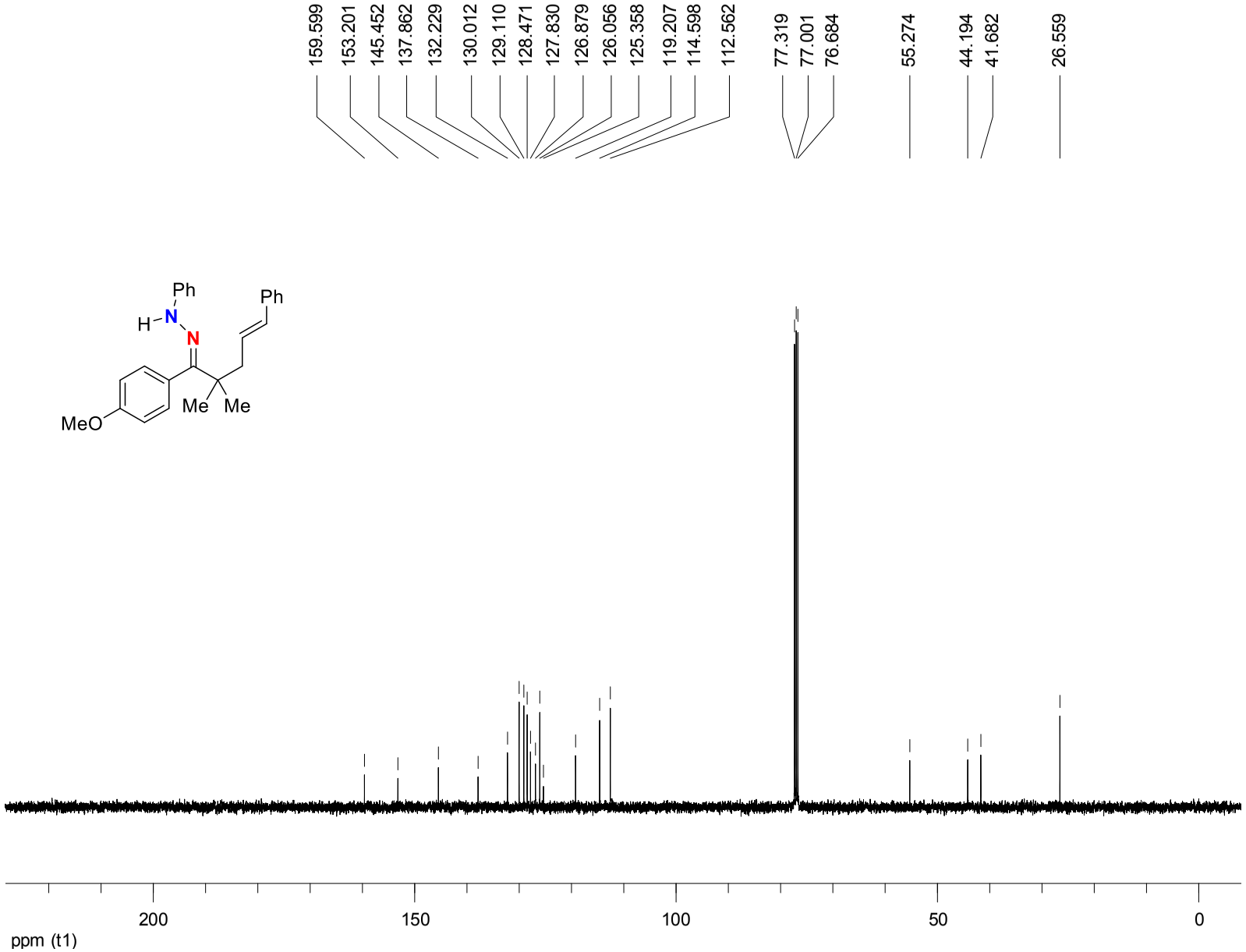
(*Z*)-1-((*E*)- 2,2-dimethyl-1,5-diphenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1a**) (100 MHz, $CDCl_3$)



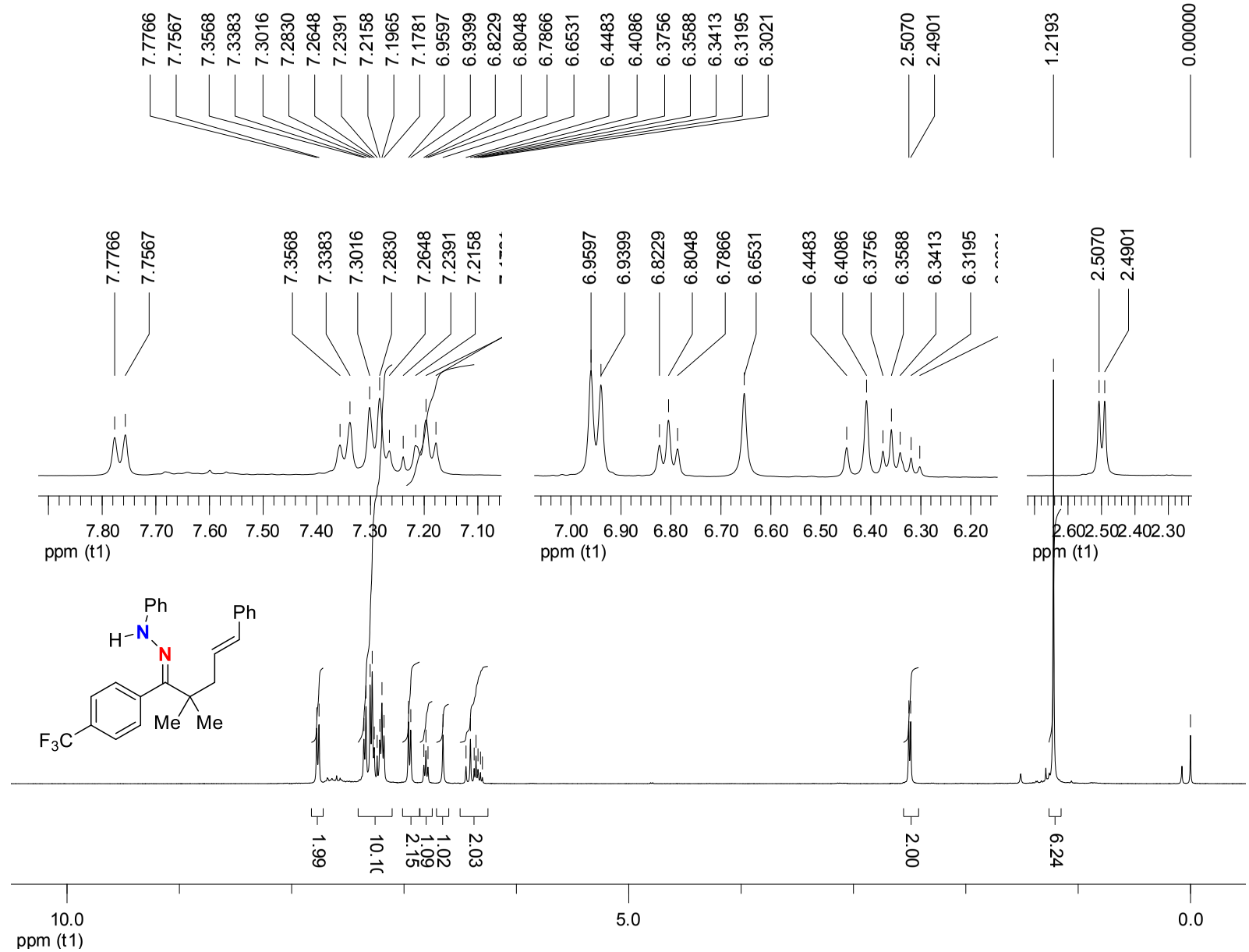
(*Z*)-1-((*E*)-1-(4-methoxyphenyl)-2,2-dimethyl-5-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1b**) (400 MHz, $CDCl_3$)



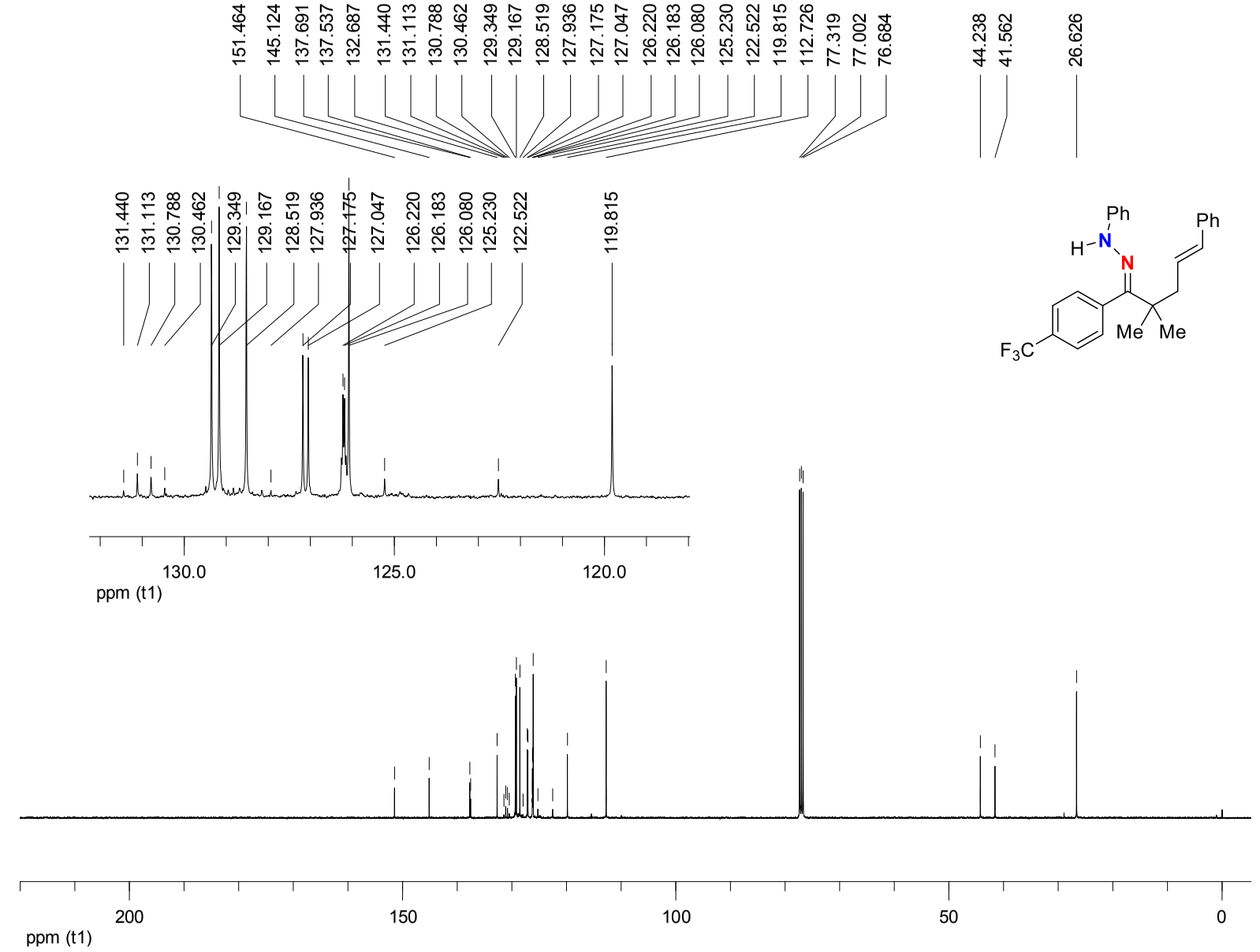
(*Z*)-1-((*E*)-1-(4-methoxyphenyl)-2,2-dimethyl-5-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1b**) (100 MHz, $CDCl_3$)



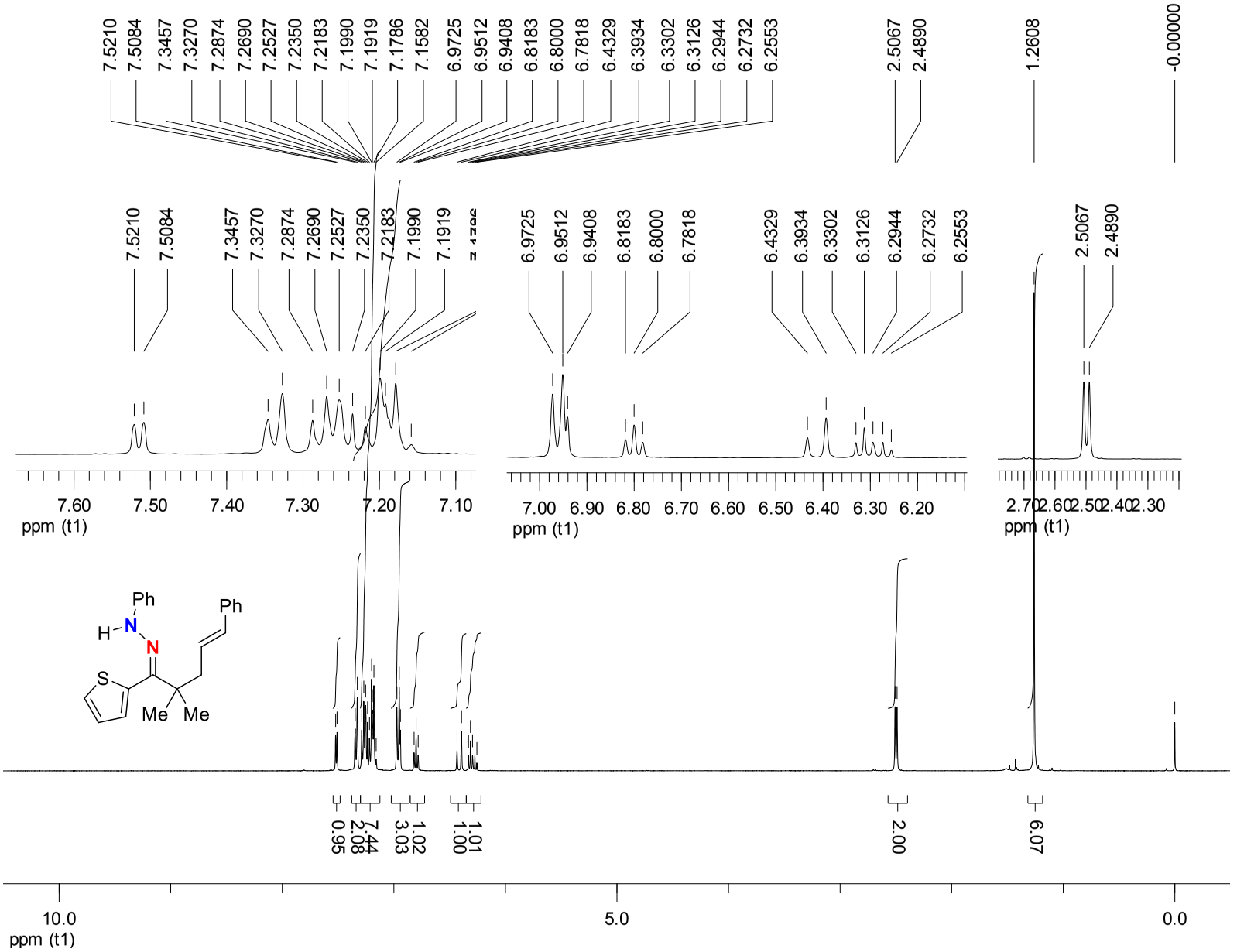
(*Z*)-1-((*E*)-2,2-Dimethyl-5-phenyl-1-(4-(trifluoromethyl)phenyl)pent-4-en-1-ylidene)-2-phenylhydrazine (**1c**) (400 MHz, $CDCl_3$)



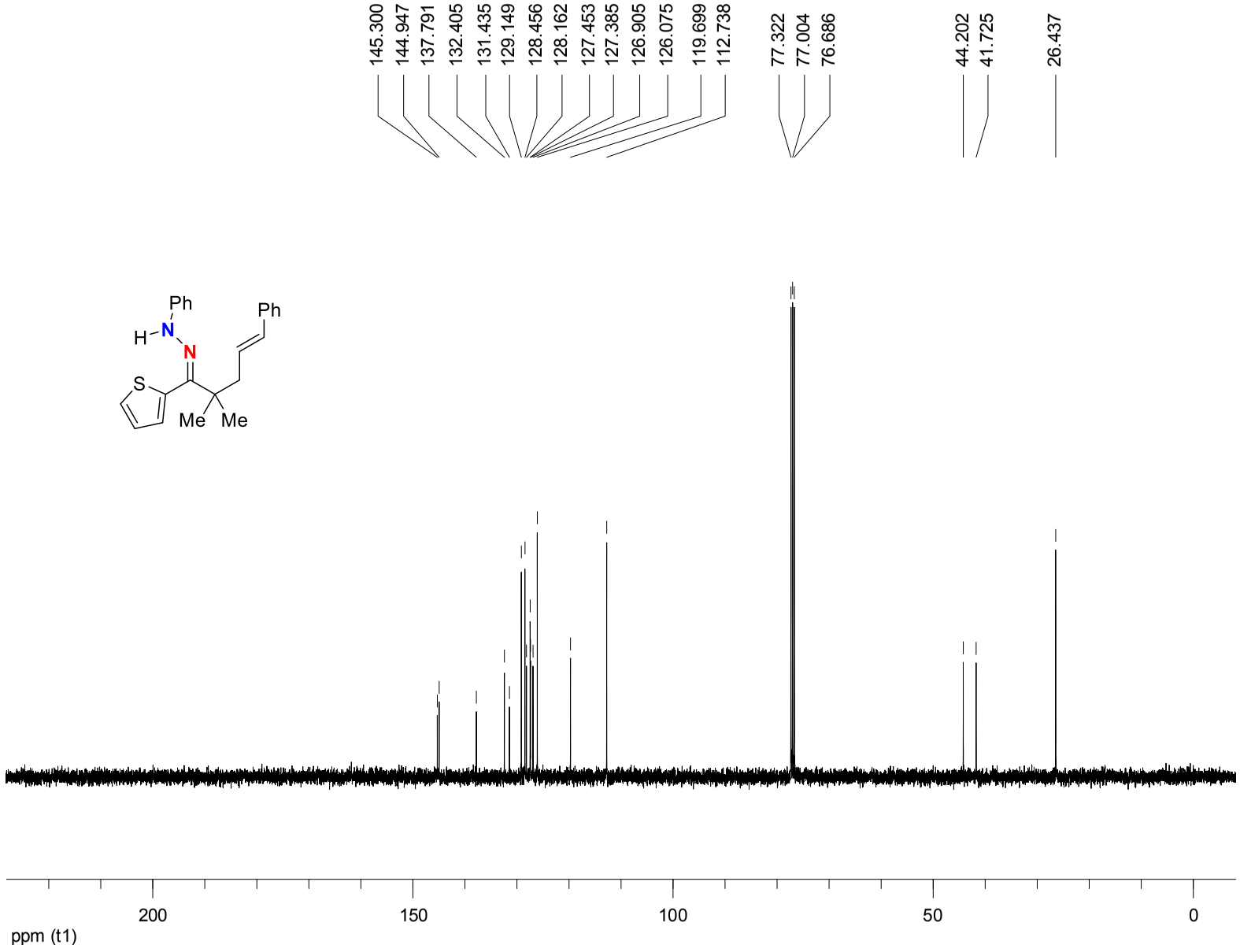
(*Z*)-1-((*E*)-2,2-Dimethyl-5-phenyl-1-(4-(trifluoromethyl)phenyl)pent-4-en-1-ylidene)-2-phenylhydrazine (**1c**) (100 MHz, $CDCl_3$)



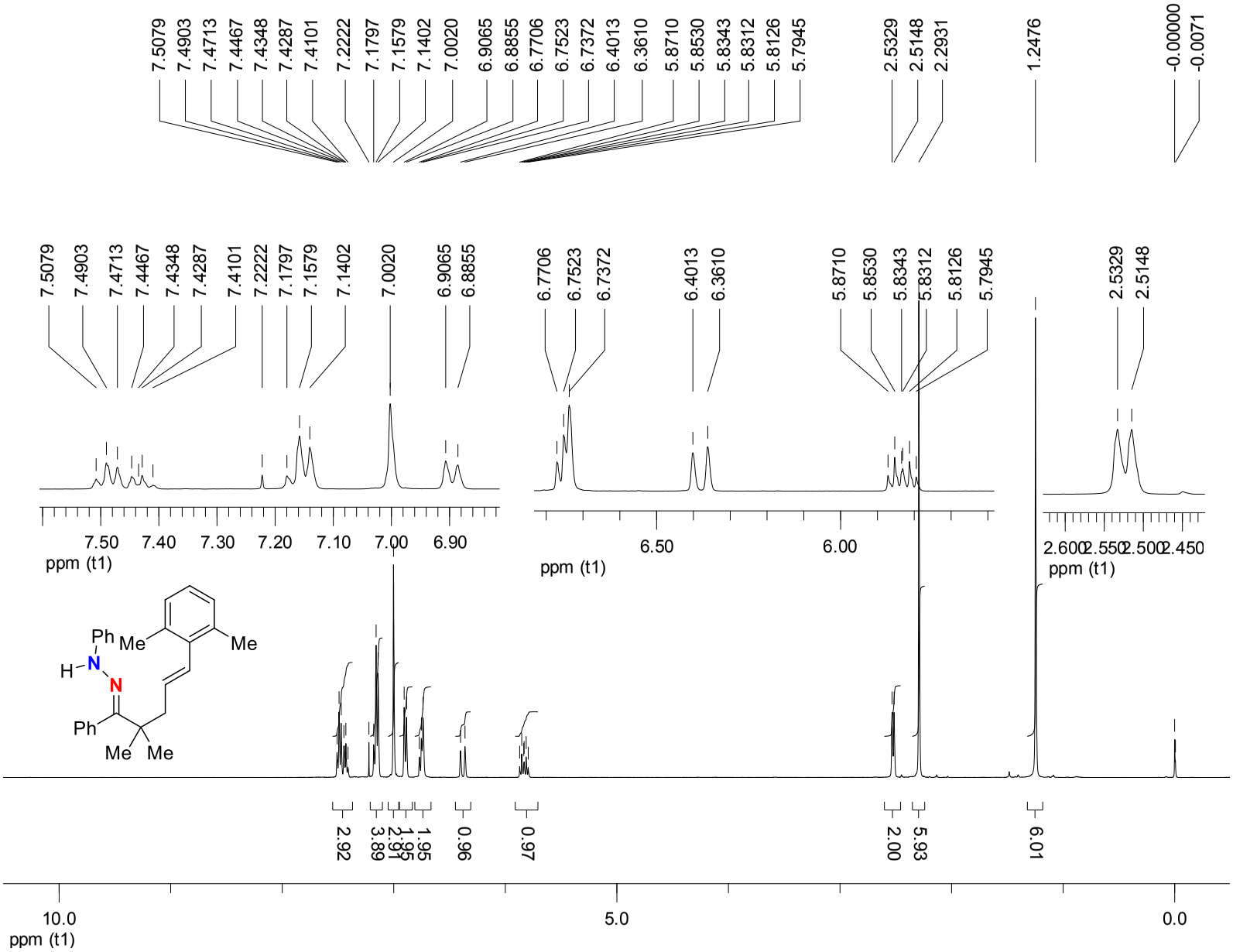
(*Z*)-1-((*E*)-2,2-dimethyl-5-phenyl-1-(thiophen-2-yl)pent-4-en-1-ylidene)-2-phenylhydrazine (**1d**) (400 MHz, $CDCl_3$)



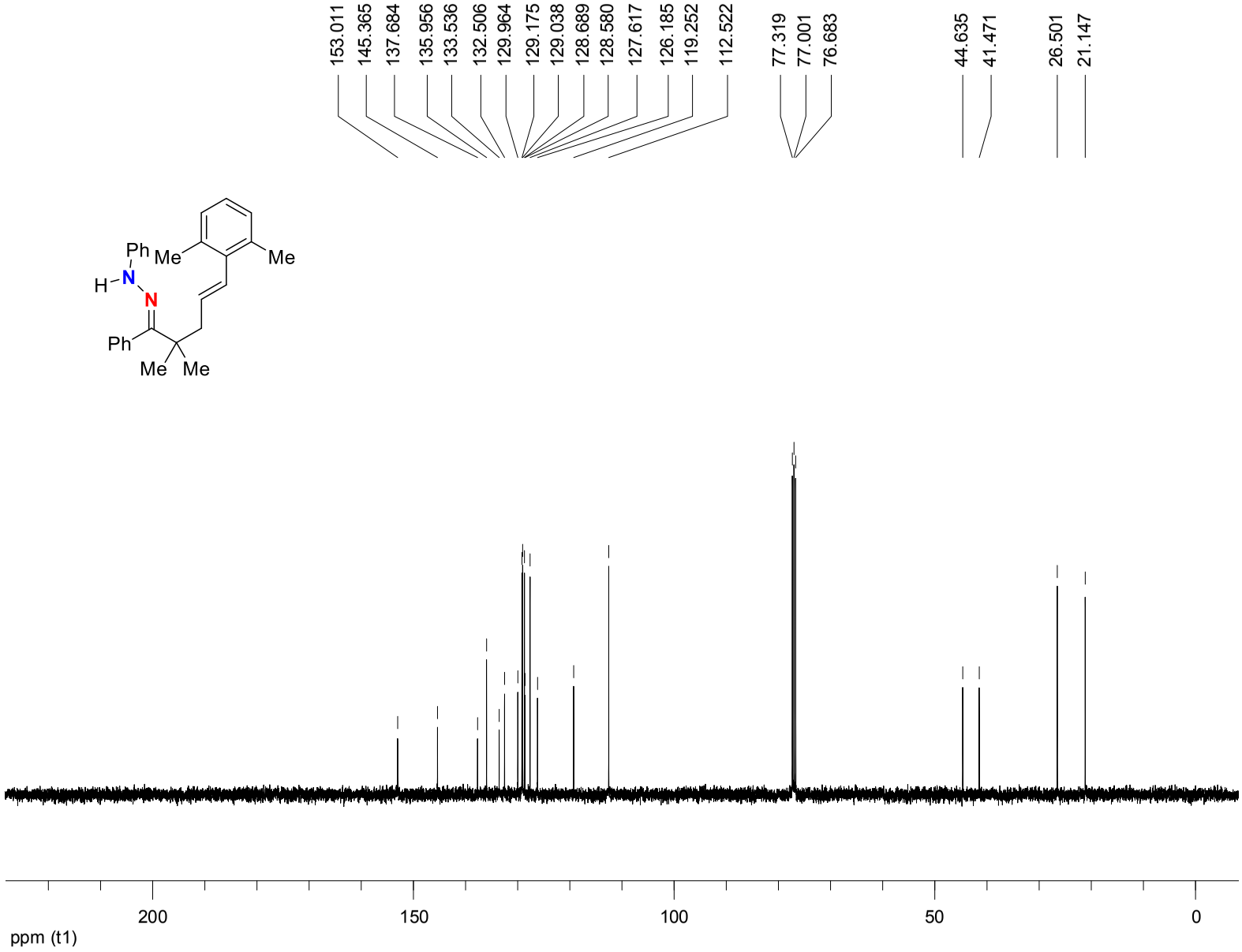
(*Z*)-1-((*E*)-2,2-dimethyl-5-phenyl-1-(thiophen-2-yl)pent-4-en-1-ylidene)-2-phenylhydrazine (**1d**) (100 MHz, $CDCl_3$)



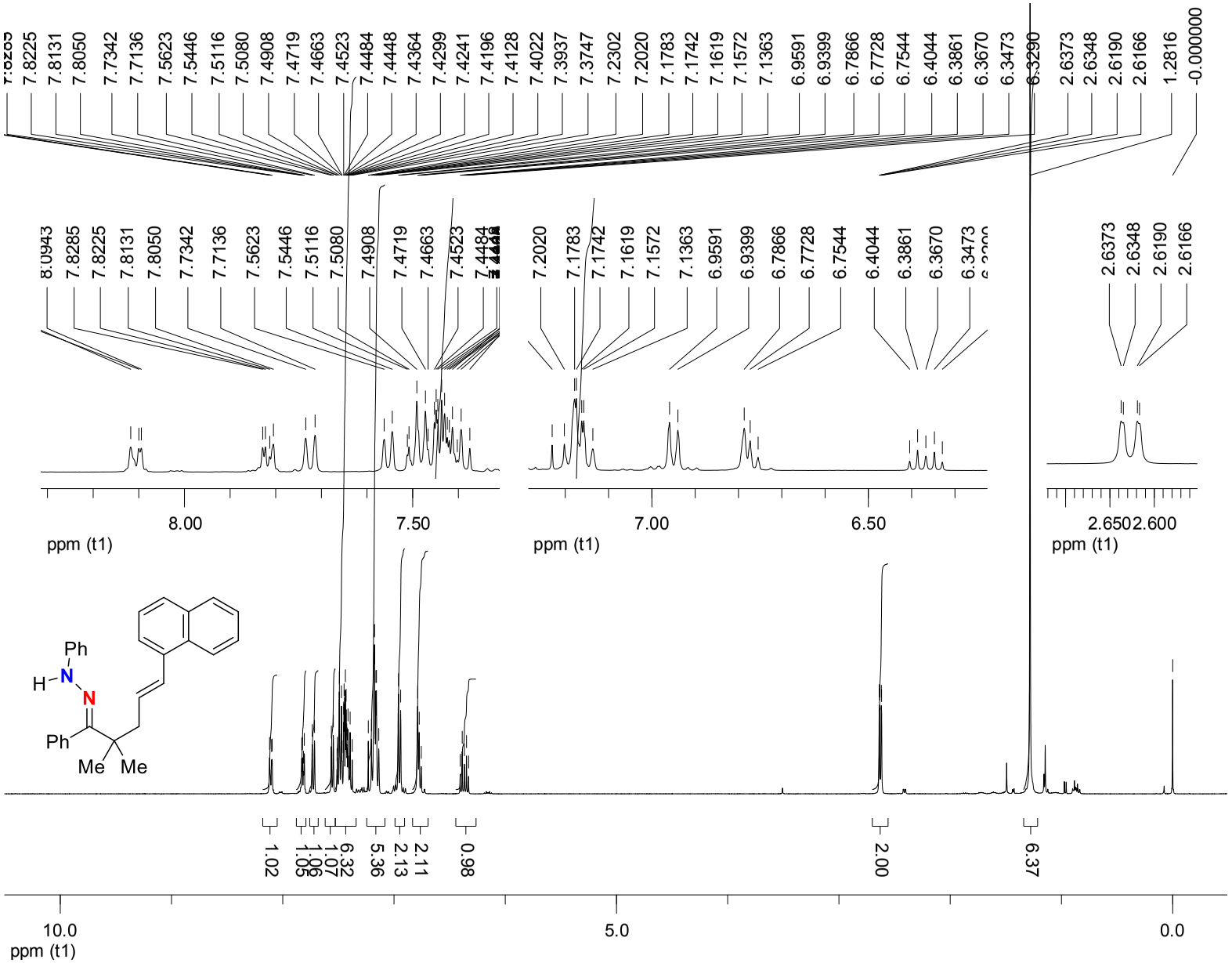
(*Z*)-1-((*E*)-5-(2,6-Dimethylphenyl)-2,2-dimethyl-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1f**) (400 MHz, $CDCl_3$)



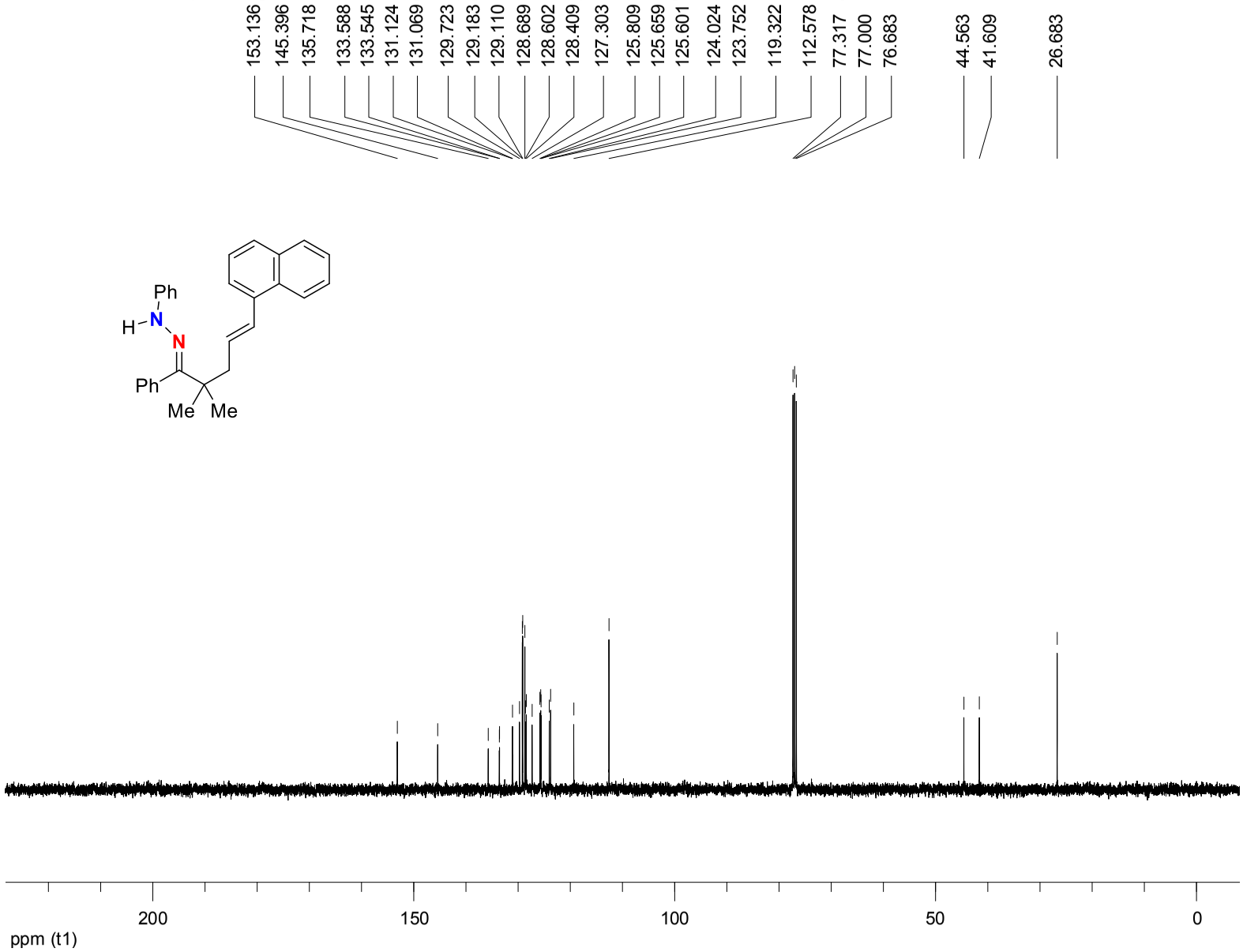
(*Z*)-1-((*E*)-5-(2,6-Dimethylphenyl)-2,2-dimethyl-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1f**) (100 MHz, $CDCl_3$)



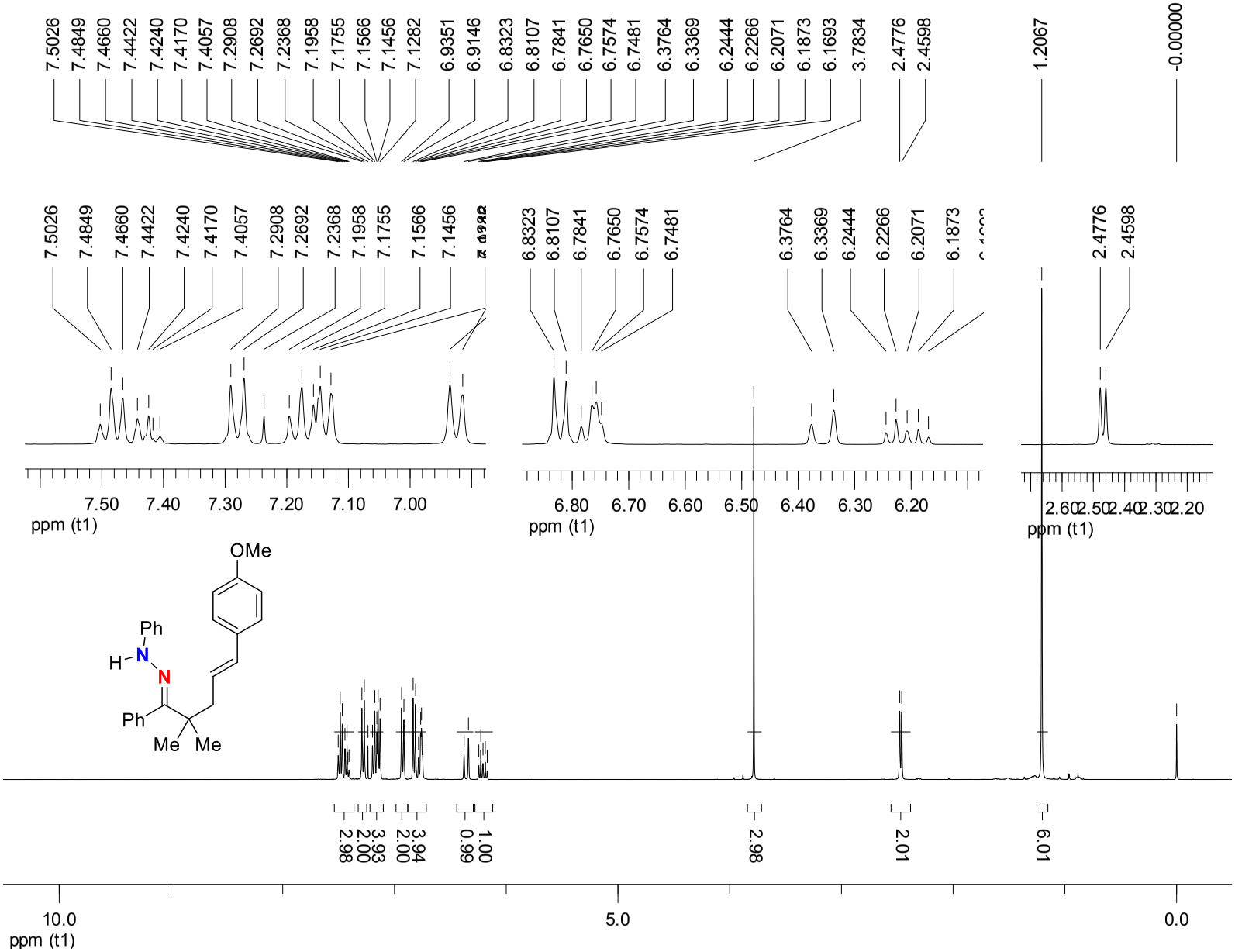
(*Z*)-1-((*E*)-2,2-Dimethyl-5-(naphthalene-1-yl)-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1g**) (400 MHz, $CDCl_3$)



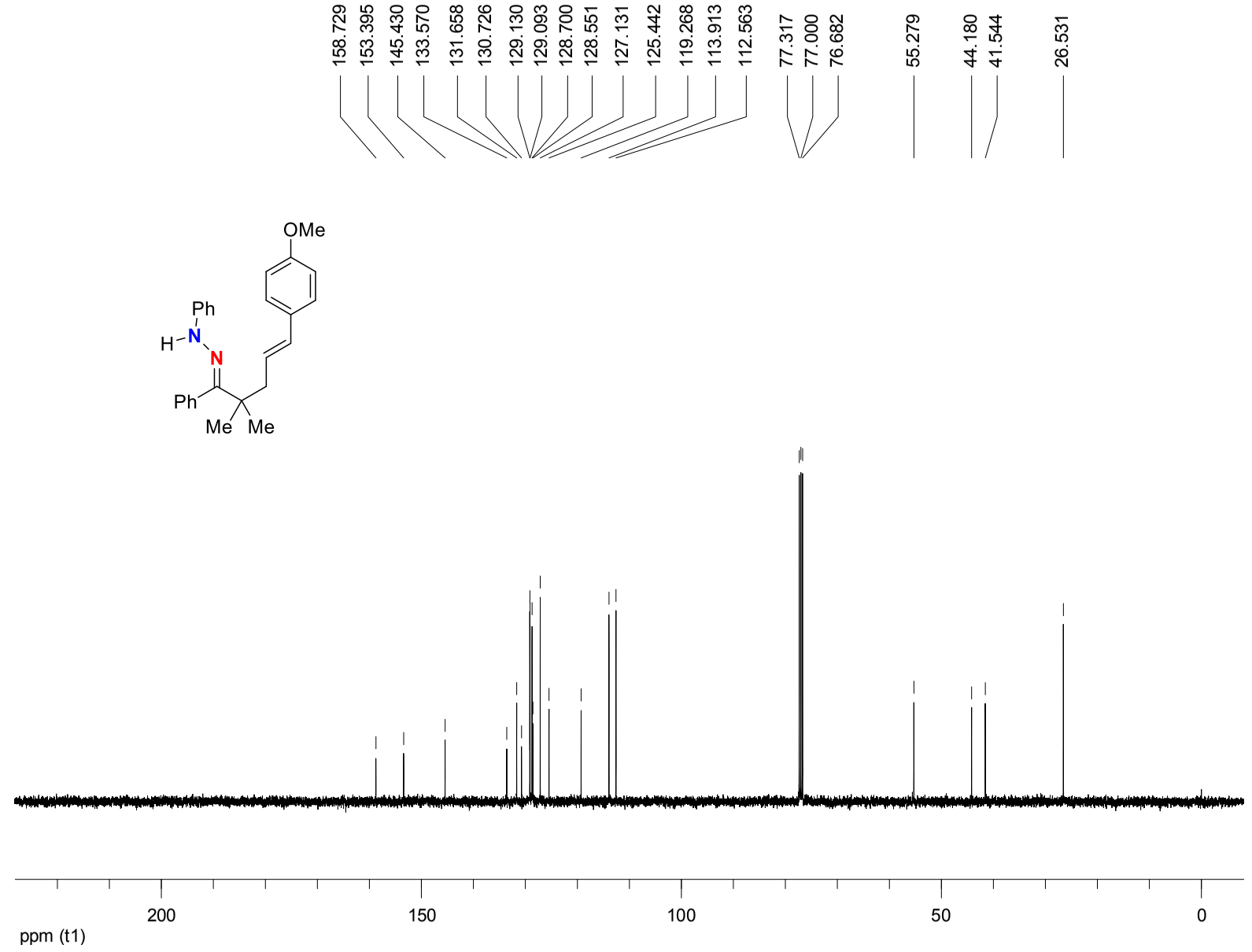
(*Z*)-1-((*E*)-2,2-Dimethyl-5-(naphthalene-1-yl)-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine (**1g**) (100 MHz, $CDCl_3$)



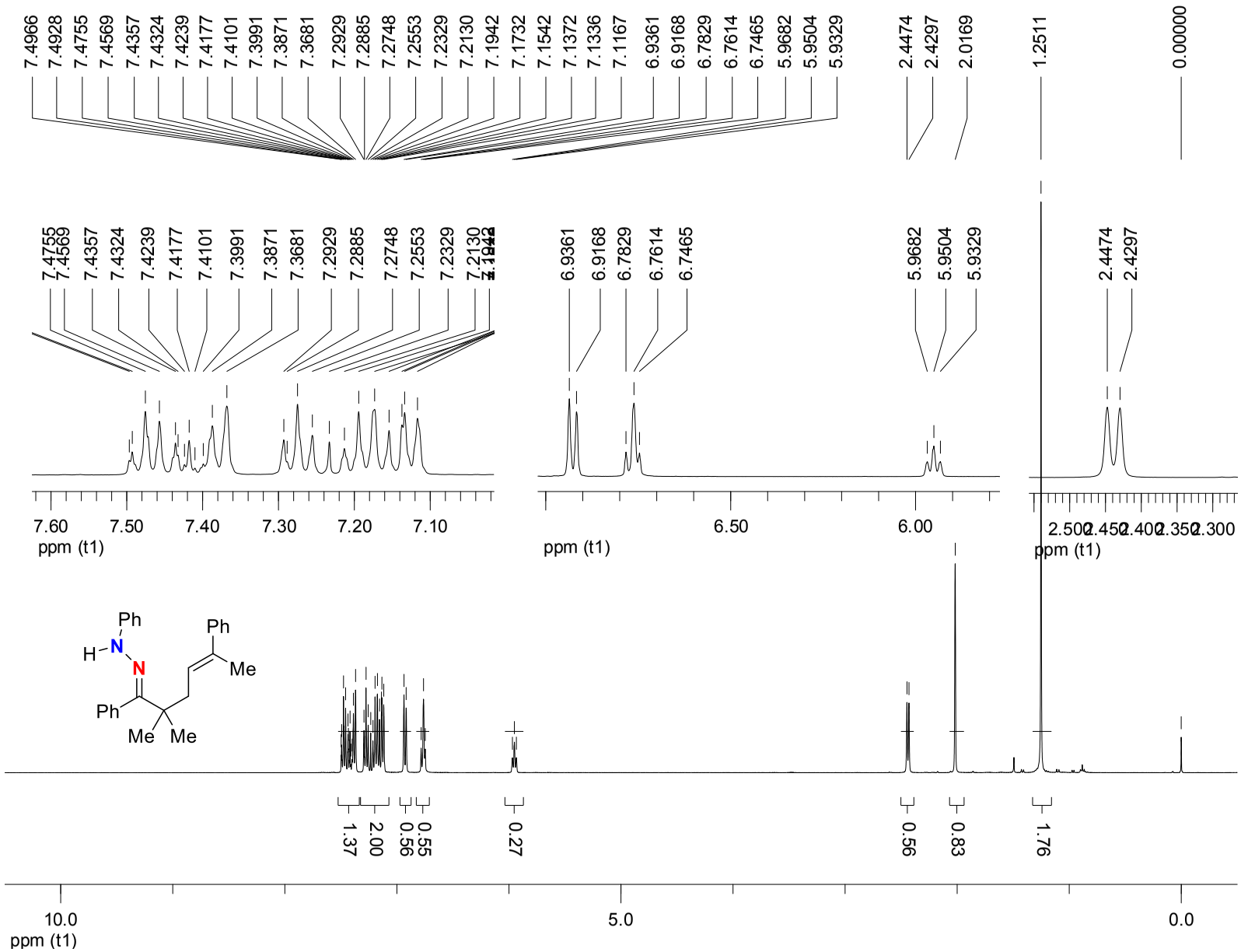
(*Z*)-1-((*E*)-5-(4-Methoxyphenyl)-2,2-dimethyl-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine **(1h)** (400 MHz, $CDCl_3$)



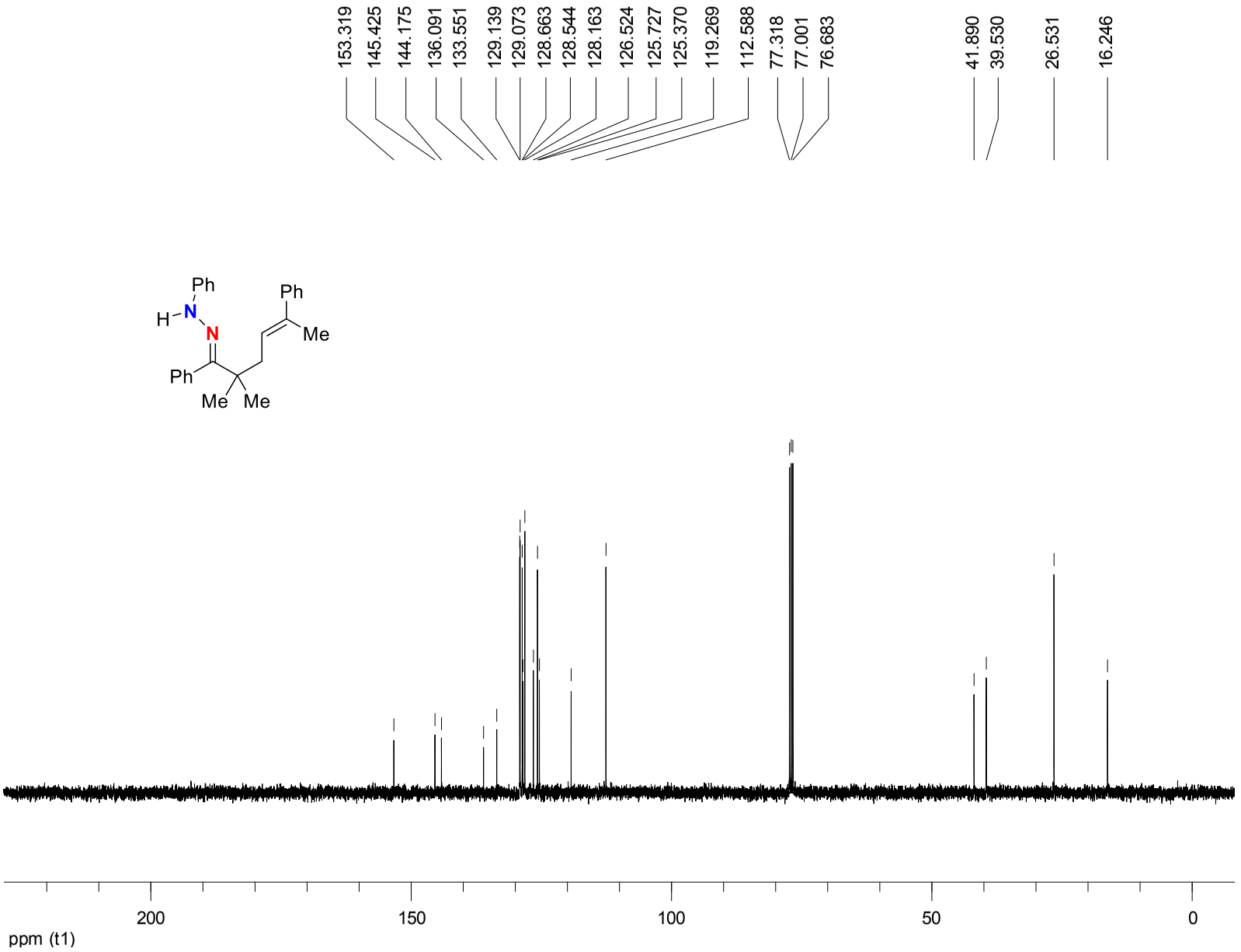
(*Z*)-1-((*E*)-5-(4-Methoxyphenyl)-2,2-dimethyl-1-phenylpent-4-en-1-ylidene)-2-phenylhydrazine **(1h)** (100 MHz, $CDCl_3$)



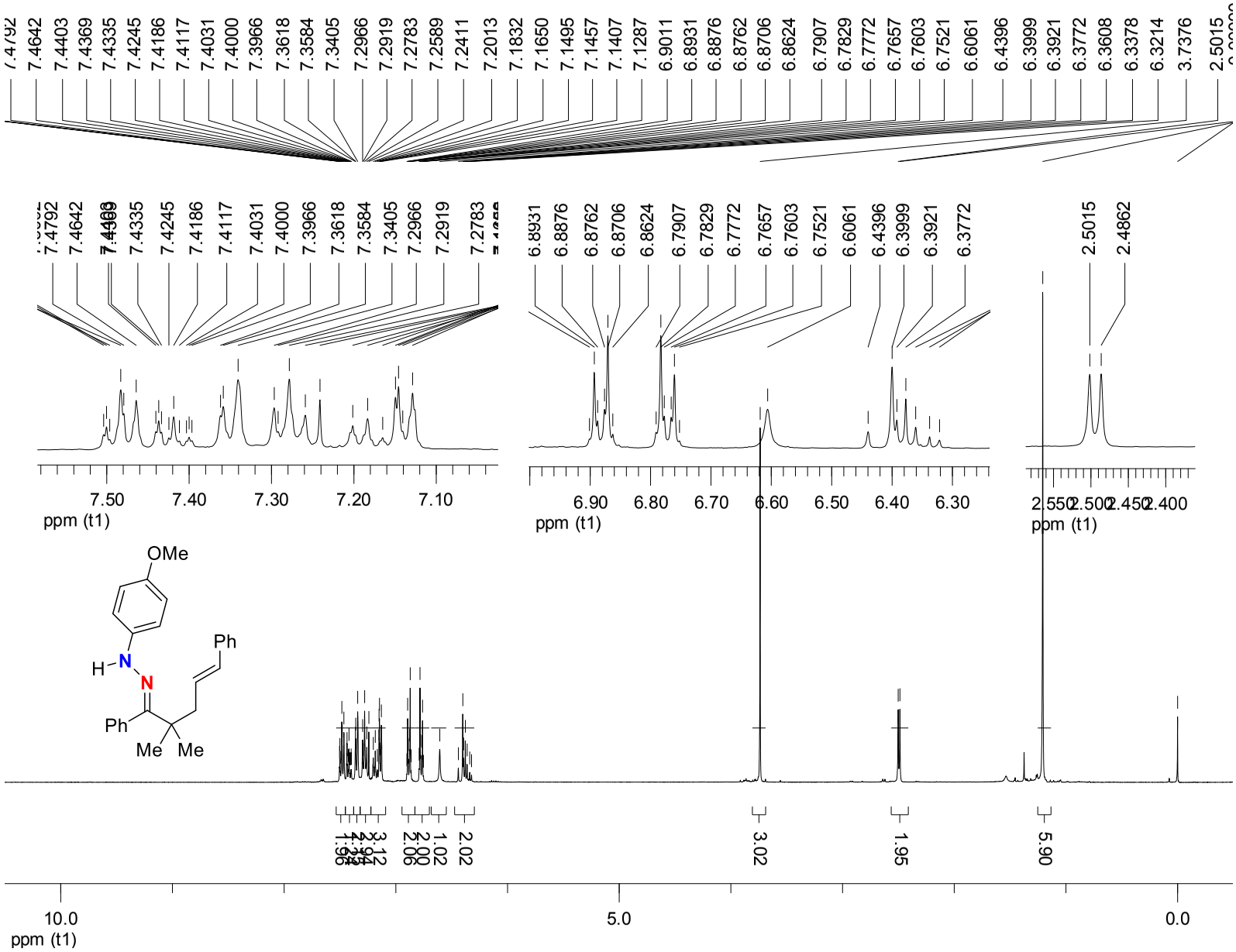
(*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylhex-4-en-1-ylidene)-2-phenylhydrazine (**1i**) (400 MHz, $CDCl_3$)



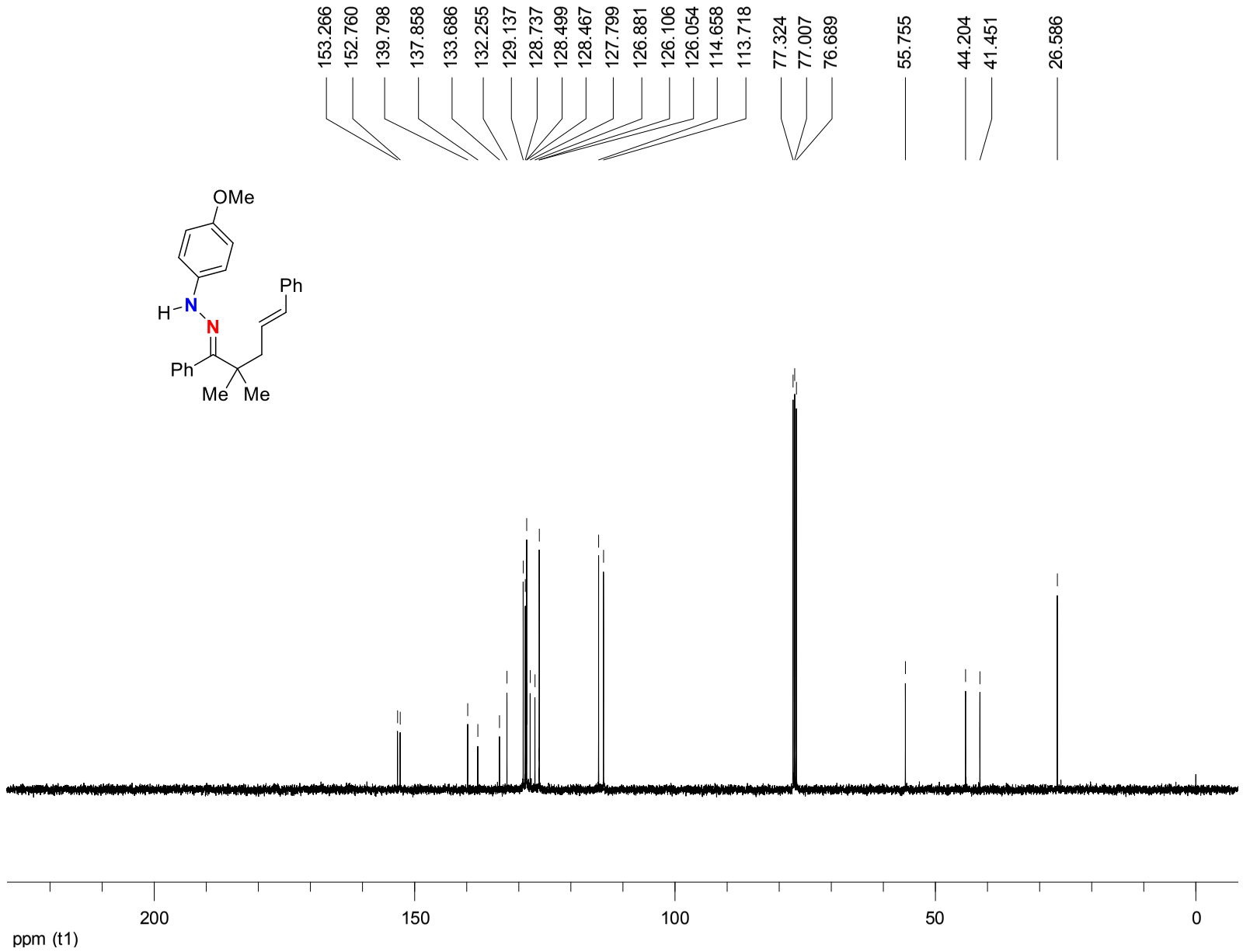
(*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylhex-4-en-1-ylidene)-2-phenylhydrazine (**1i**) (100 MHz, $CDCl_3$)



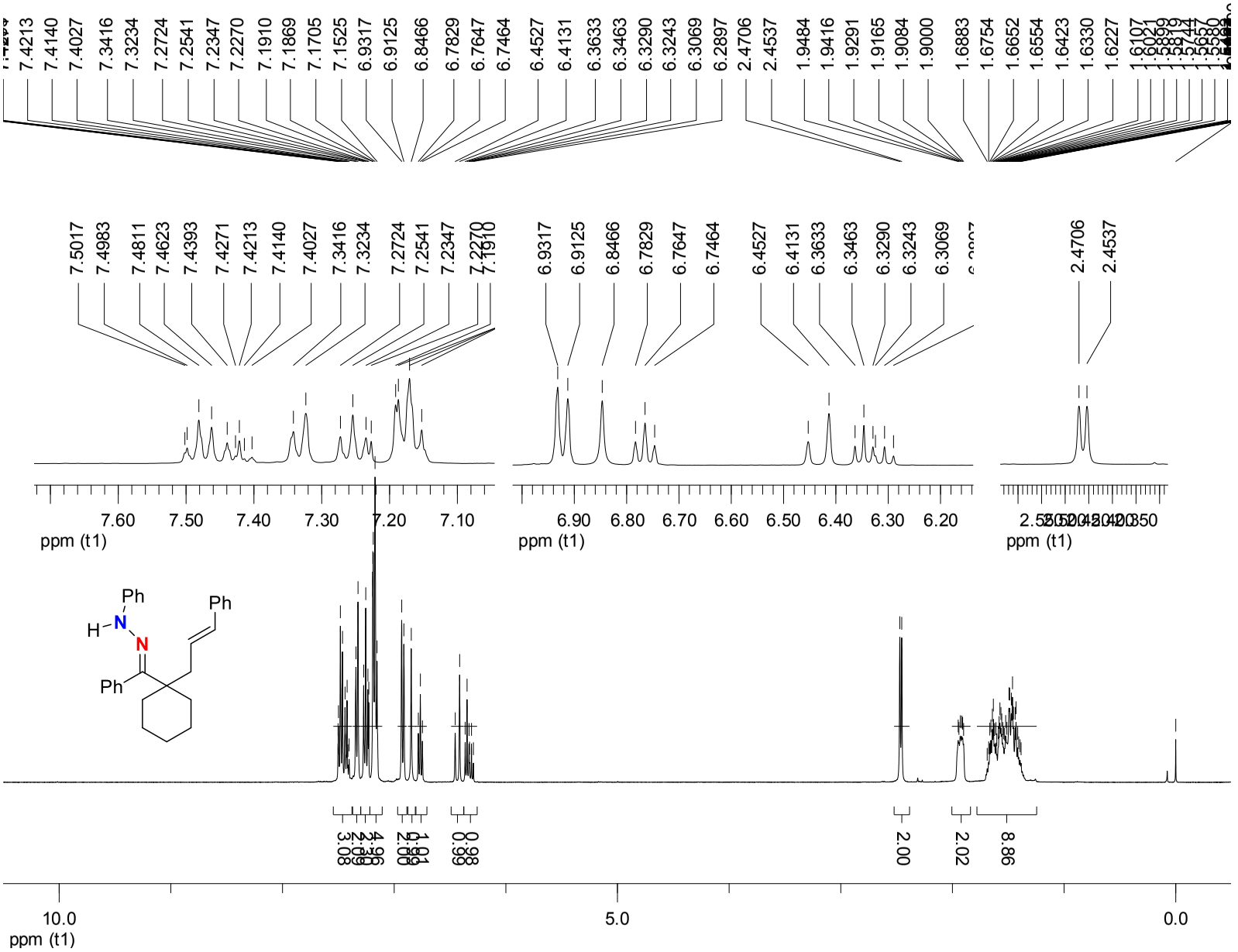
(*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylpent-4-en-1-ylidene)-2-(-4-methoxyphenyl)hydrazine **(1j)** (400 MHz, $CDCl_3$)



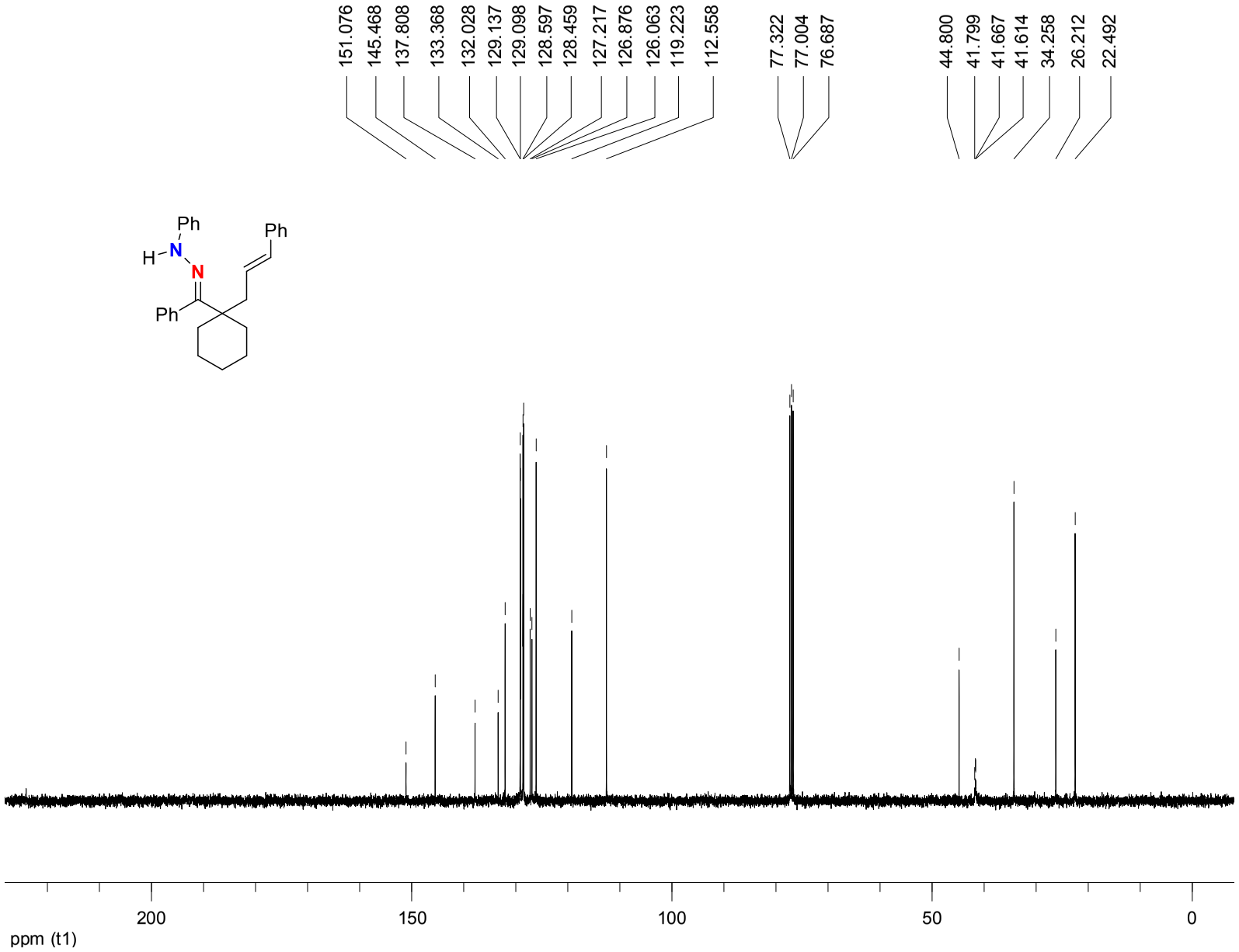
(*Z*)-1-((*E*)-2,2-dimethyl-1,5-diphenylpent-4-en-1-ylidene)-2-(-4-methoxyphenyl)hydrazine **(1j)** (100 MHz, $CDCl_3$)



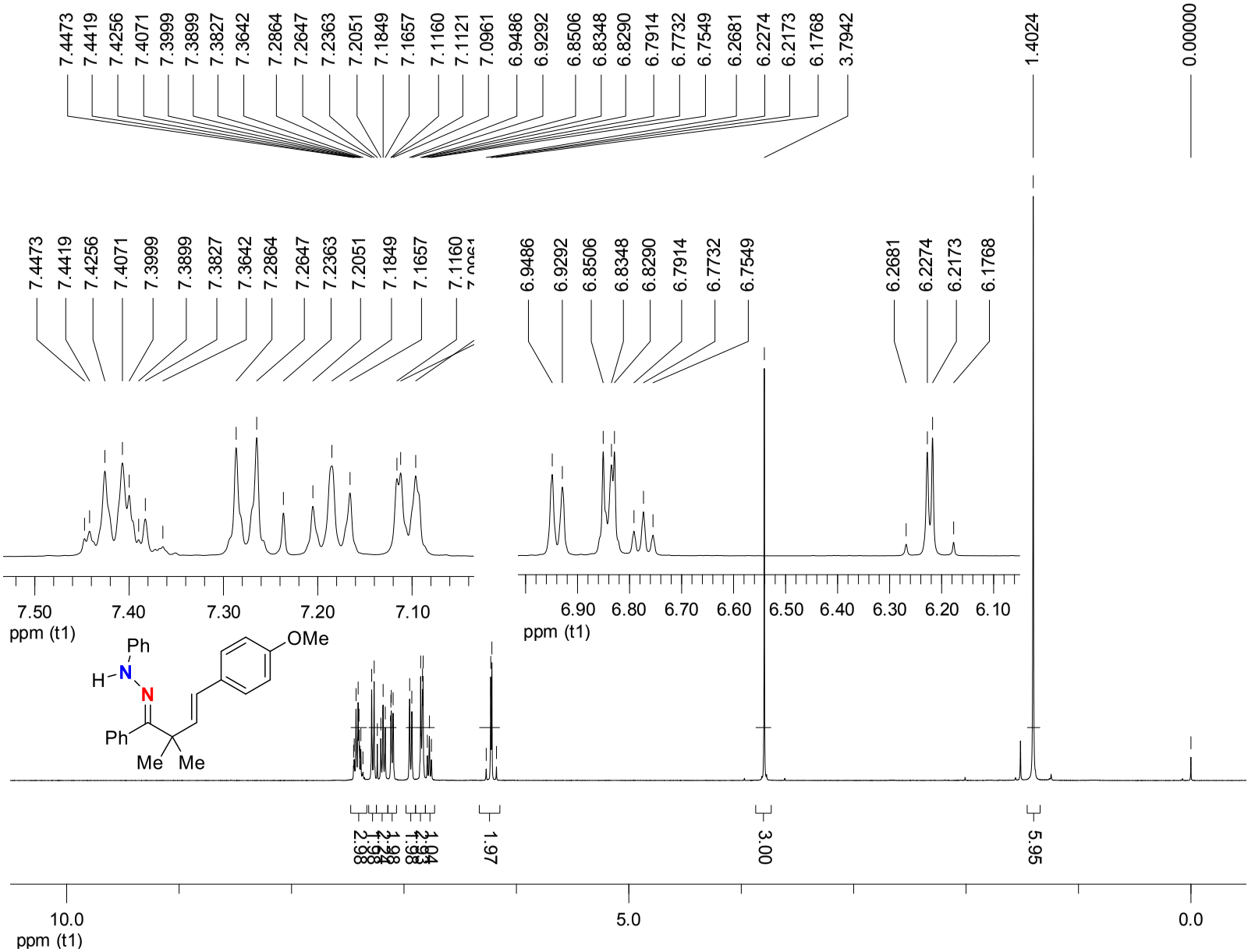
(Z)-1-((1-cinnamylcyclohexyl)(phenyl)methylene)-2-phenylhydrazine **(1k)** (400 MHz, $CDCl_3$)



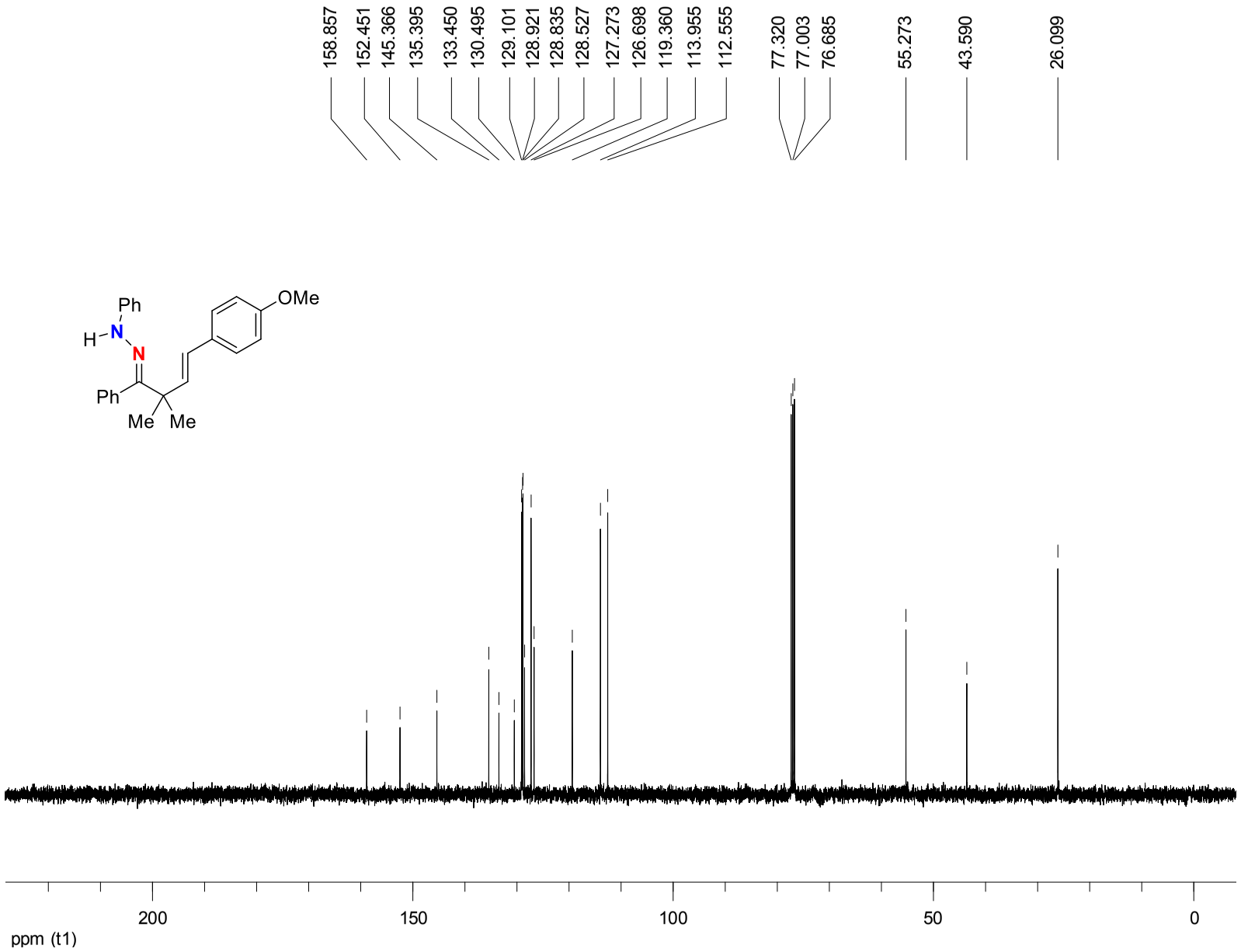
(Z)-1-((1-cinnamylcyclohexyl)(phenyl)methylene)-2-phenylhydrazine **(1k)** (100 MHz, $CDCl_3$)



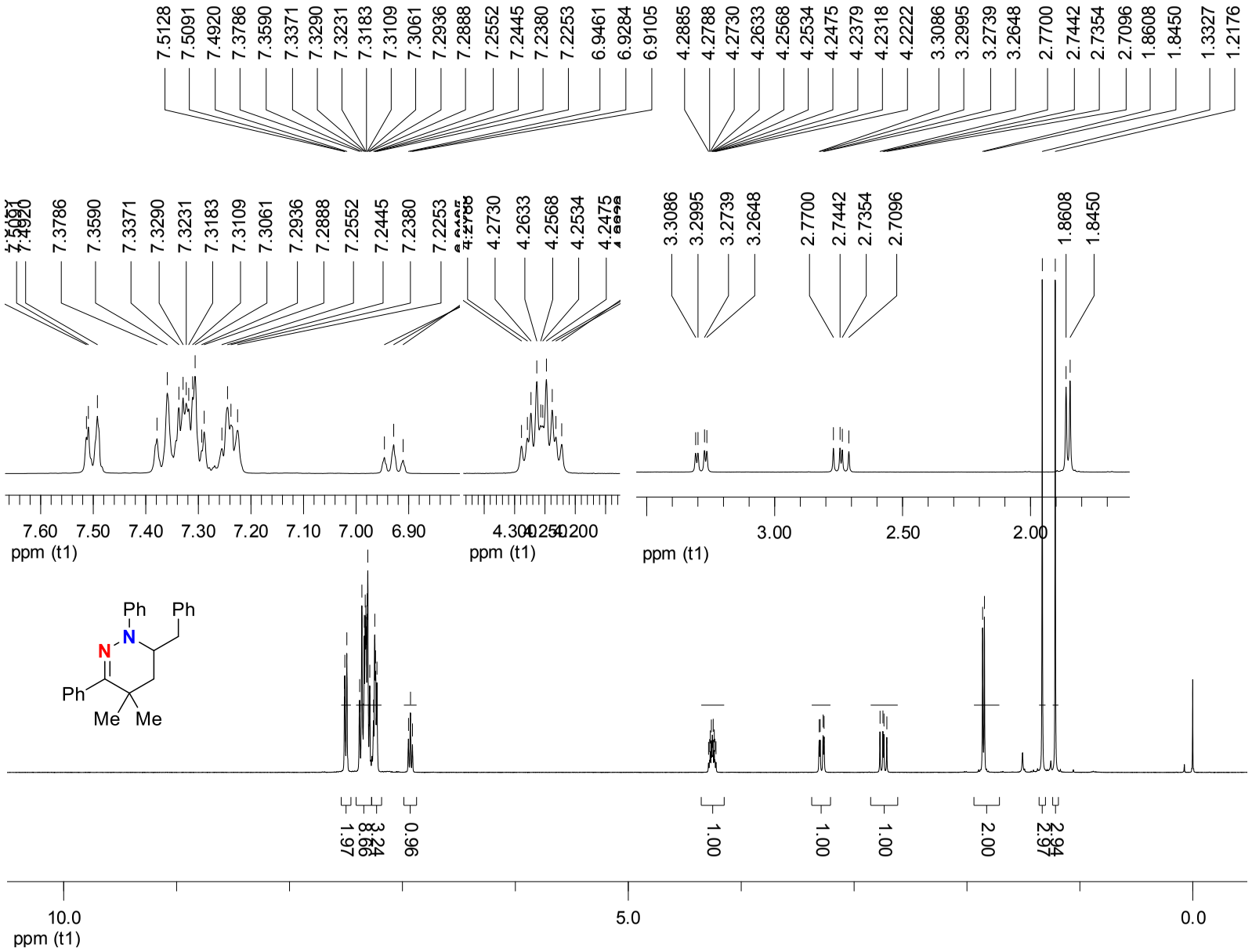
(Z)-1-((E)-4-(4-methoxyphenyl)-2,2-dimethyl-1-phenylbut-3-en-1-ylidene)-2-phenylhydrazine **(1p)** (400 MHz, $CDCl_3$)



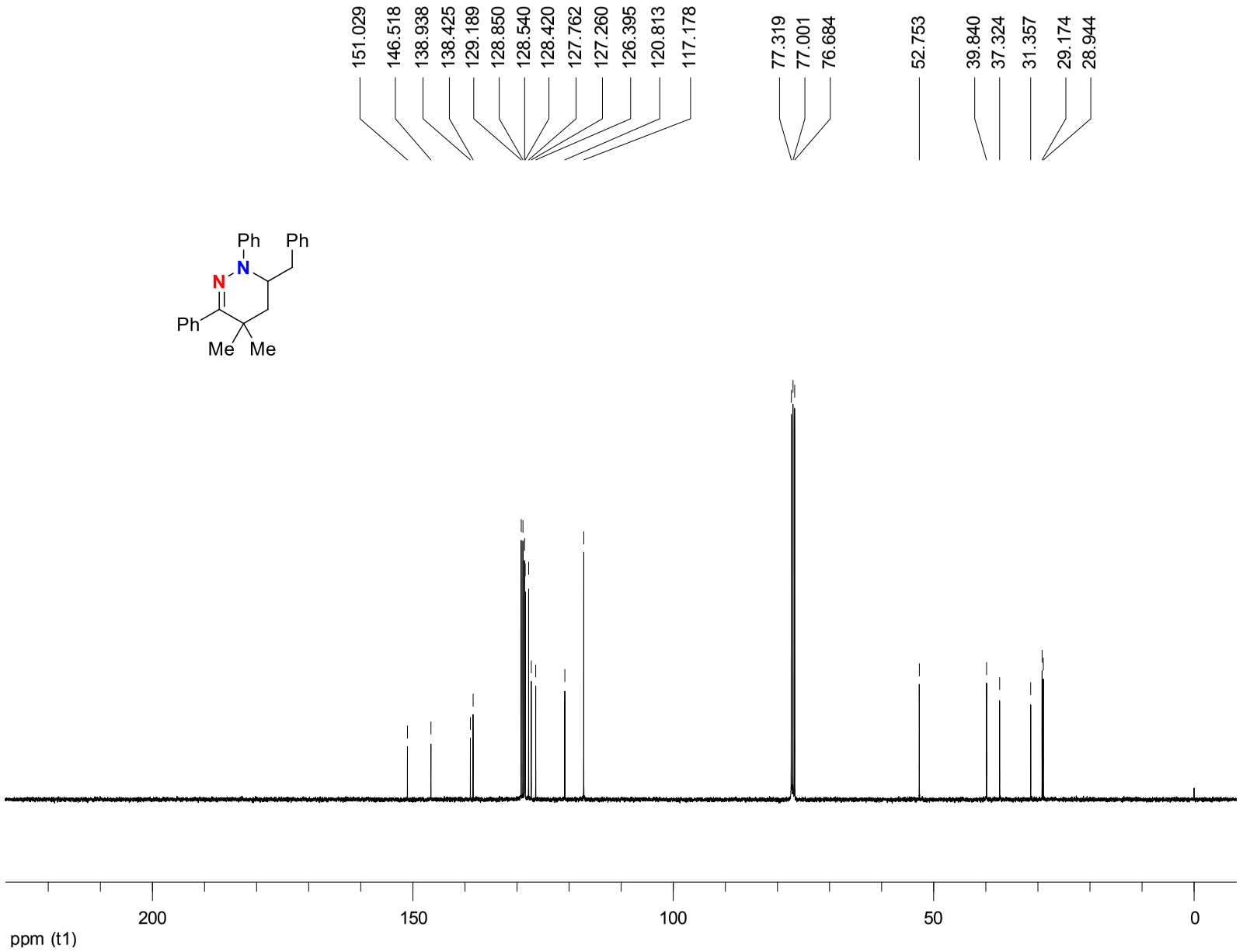
(Z)-1-((E)-4-(4-methoxyphenyl)-2,2-dimethyl-1-phenylbut-3-en-1-ylidene)-2-phenylhydrazine **(1p)** (100 MHz, $CDCl_3$)



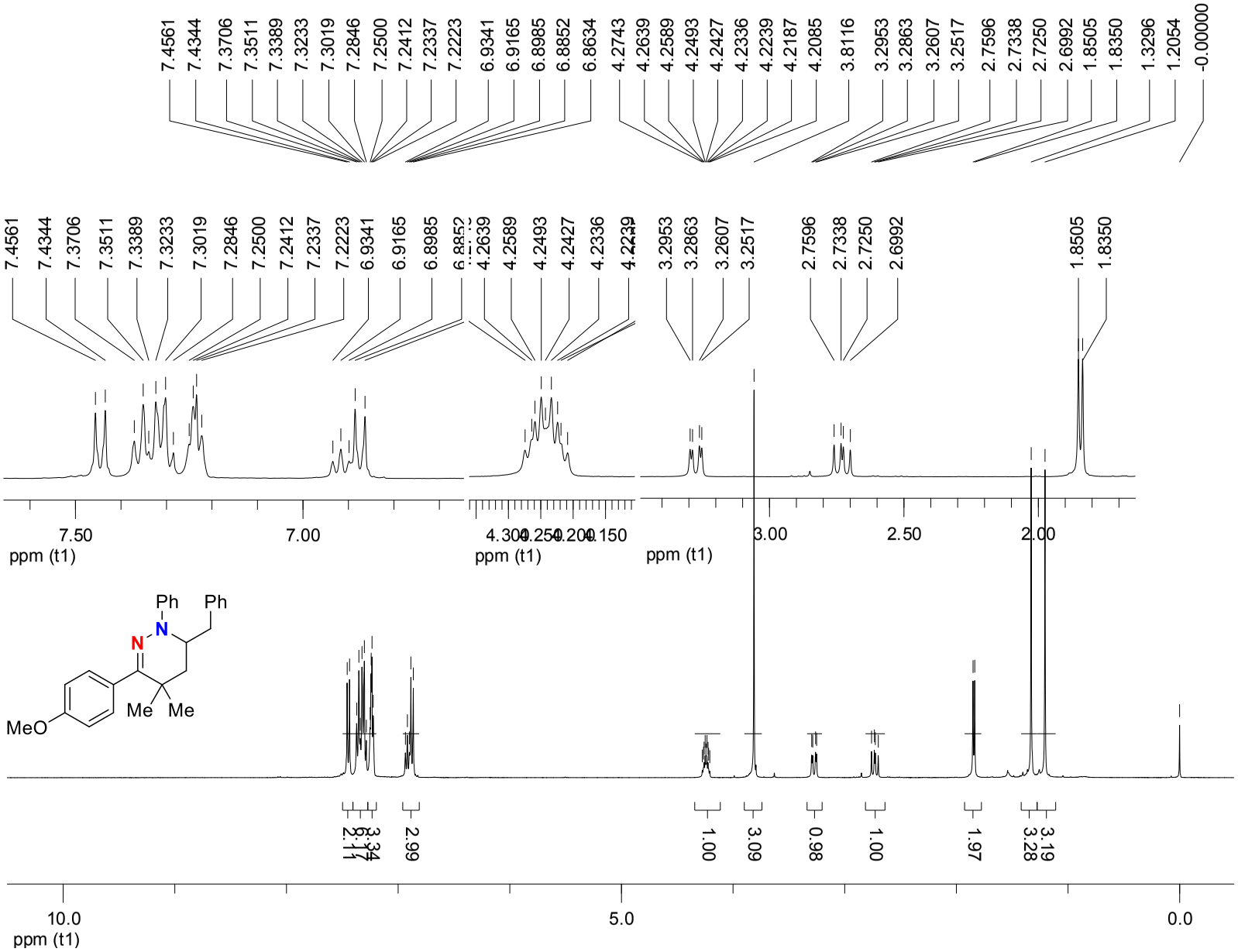
6-Benzyl-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine **(2a)** (400 MHz, $CDCl_3$)



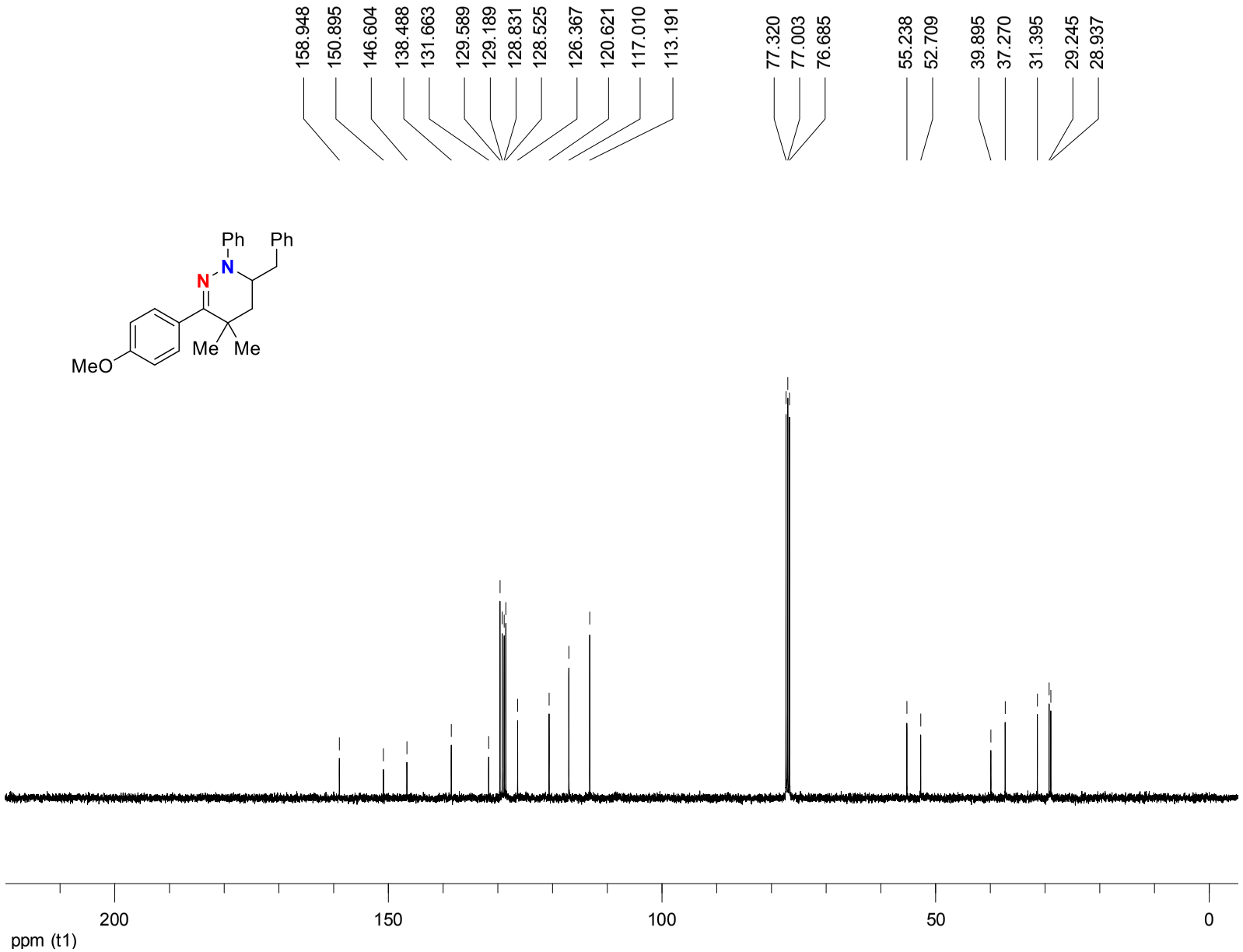
6-Benzyl-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine **(2a)** (100 MHz, $CDCl_3$)



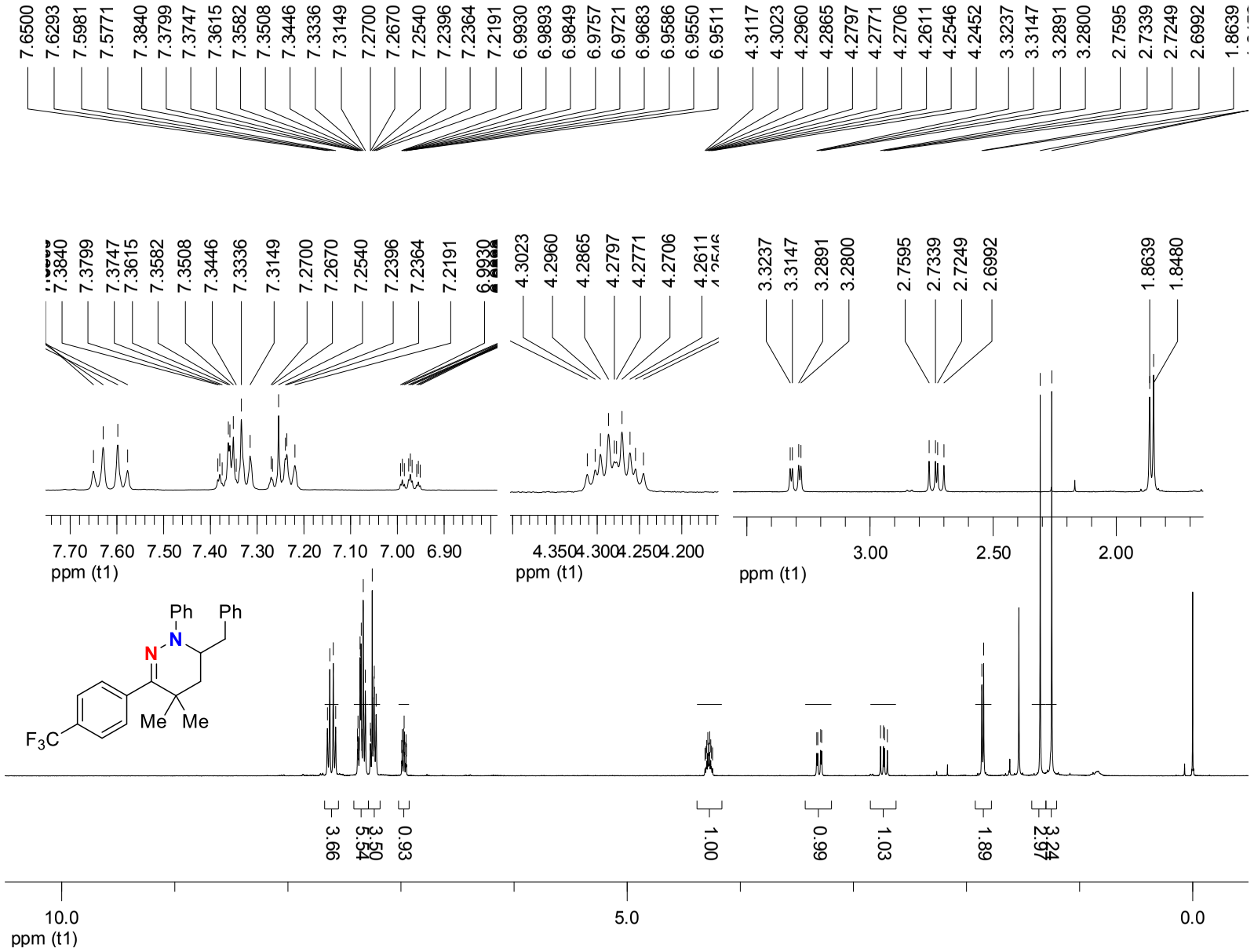
6-Benzyl-3-(4-methoxyphenyl)-4,4-dimethyl-1-phenyl-1,4,5,6-tetrahydropyridazine **(2b)** (400 MHz, $CDCl_3$)



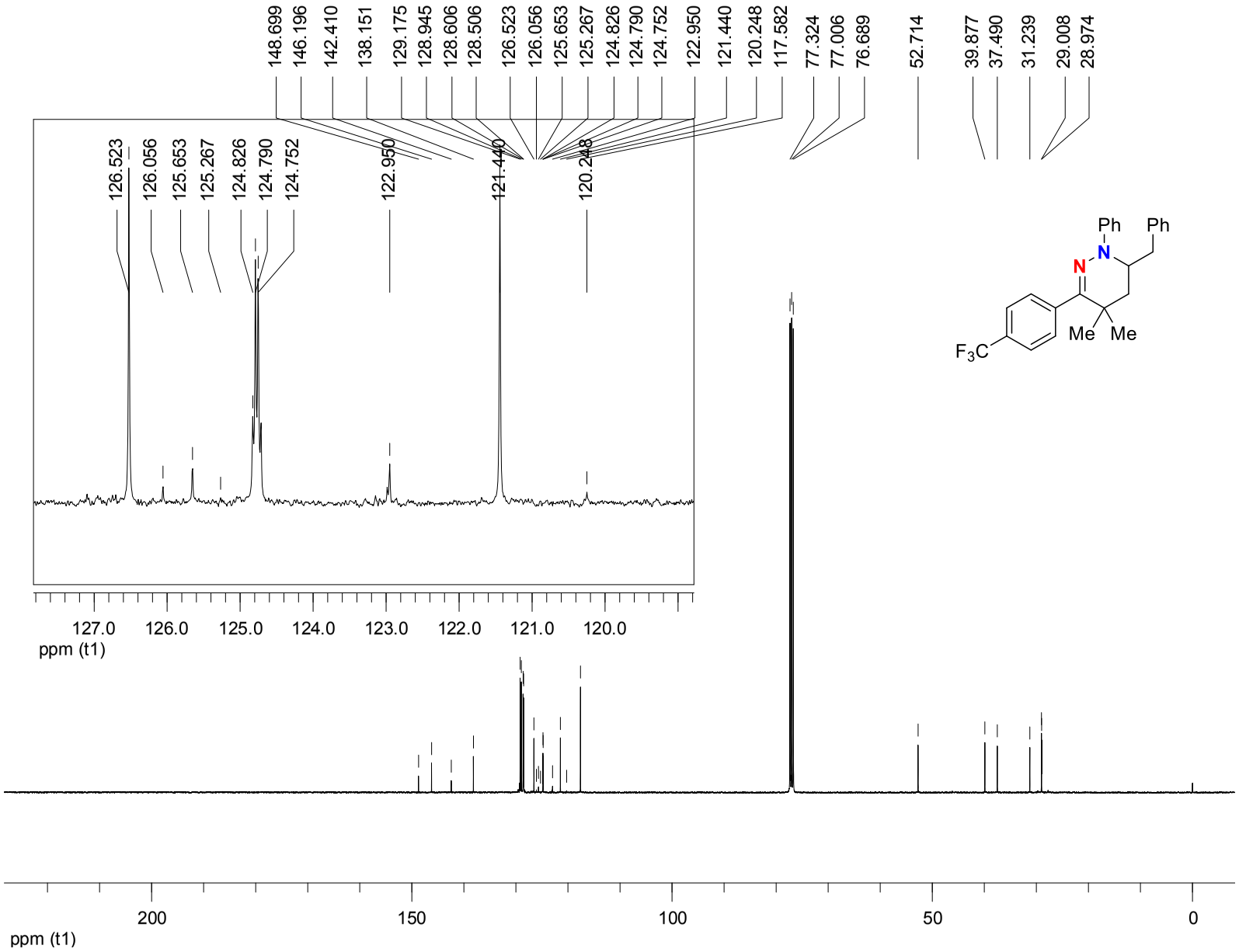
6-Benzyl-3-(4-methoxyphenyl)-4,4-dimethyl-1-phenyl-1,4,5,6-tetrahydropyridazine **(2b)** (100 MHz, $CDCl_3$)



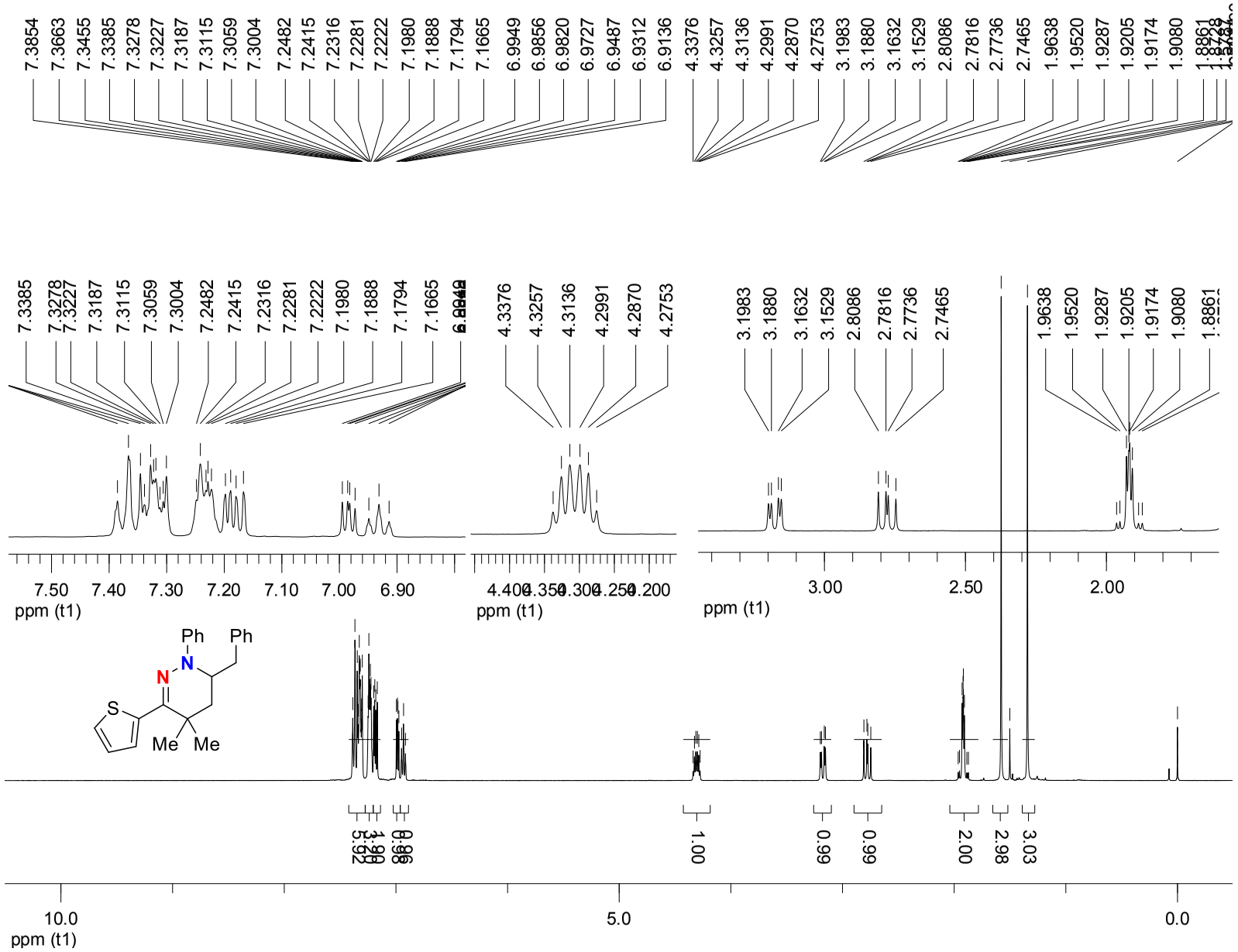
6-Benzyl-4,4-dimethyl-1-phenyl-3-(4-(trifluoromethyl)phenyl)-1,4,5,6-tetrahydropyridazine **(2c)** (400 MHz, $CDCl_3$)



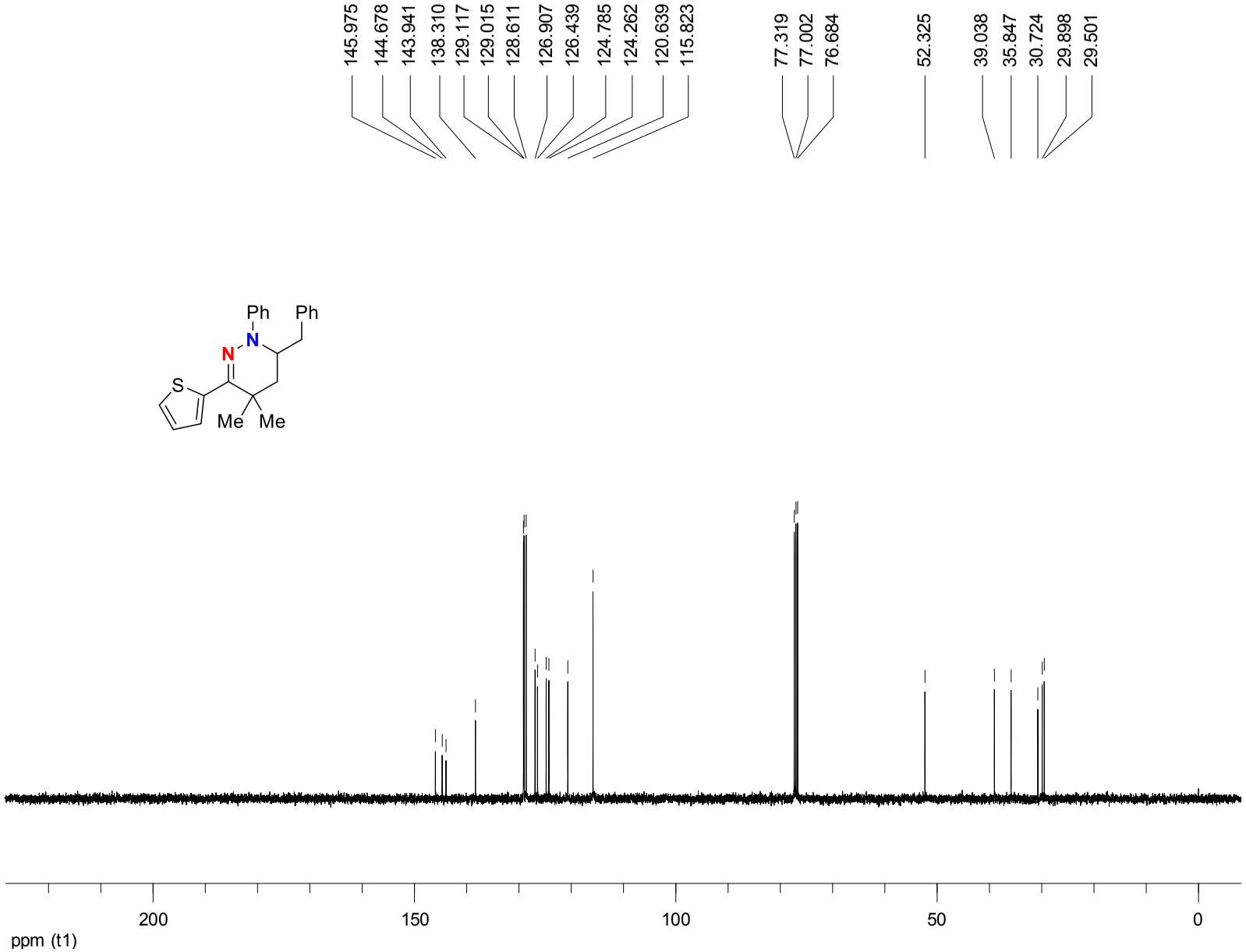
6-Benzyl-4,4-dimethyl-1-phenyl-3-(4-(trifluoromethyl)phenyl)-1,4,5,6-tetrahydropyridazine **(2c)** (100 MHz, $CDCl_3$)



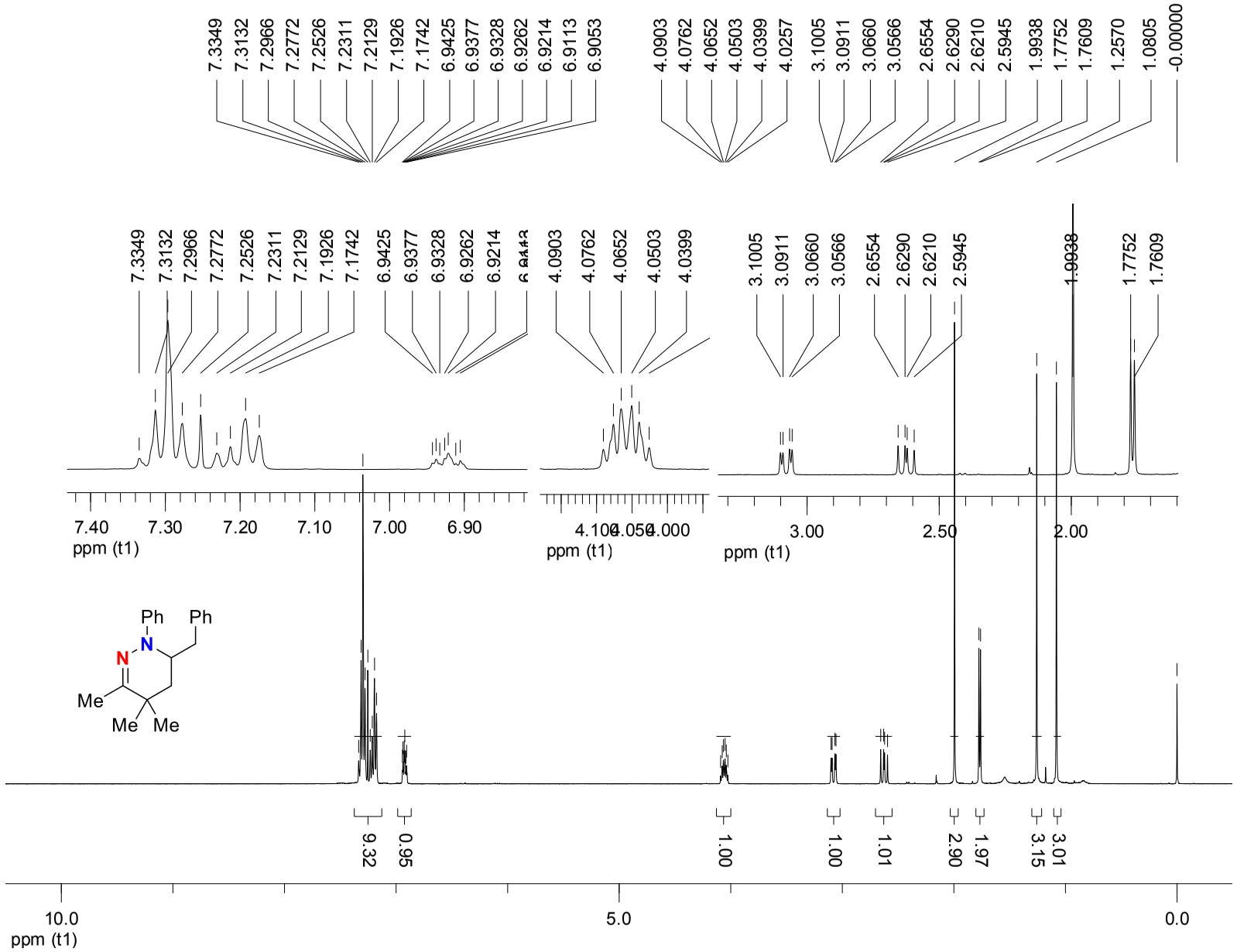
6-Benzyl-4,4-dimethyl-1-phenyl-3-(thiophen-2-yl)-1,4,5,6-tetrahydropyridazine **(2d)** (400 MHz, $CDCl_3$)



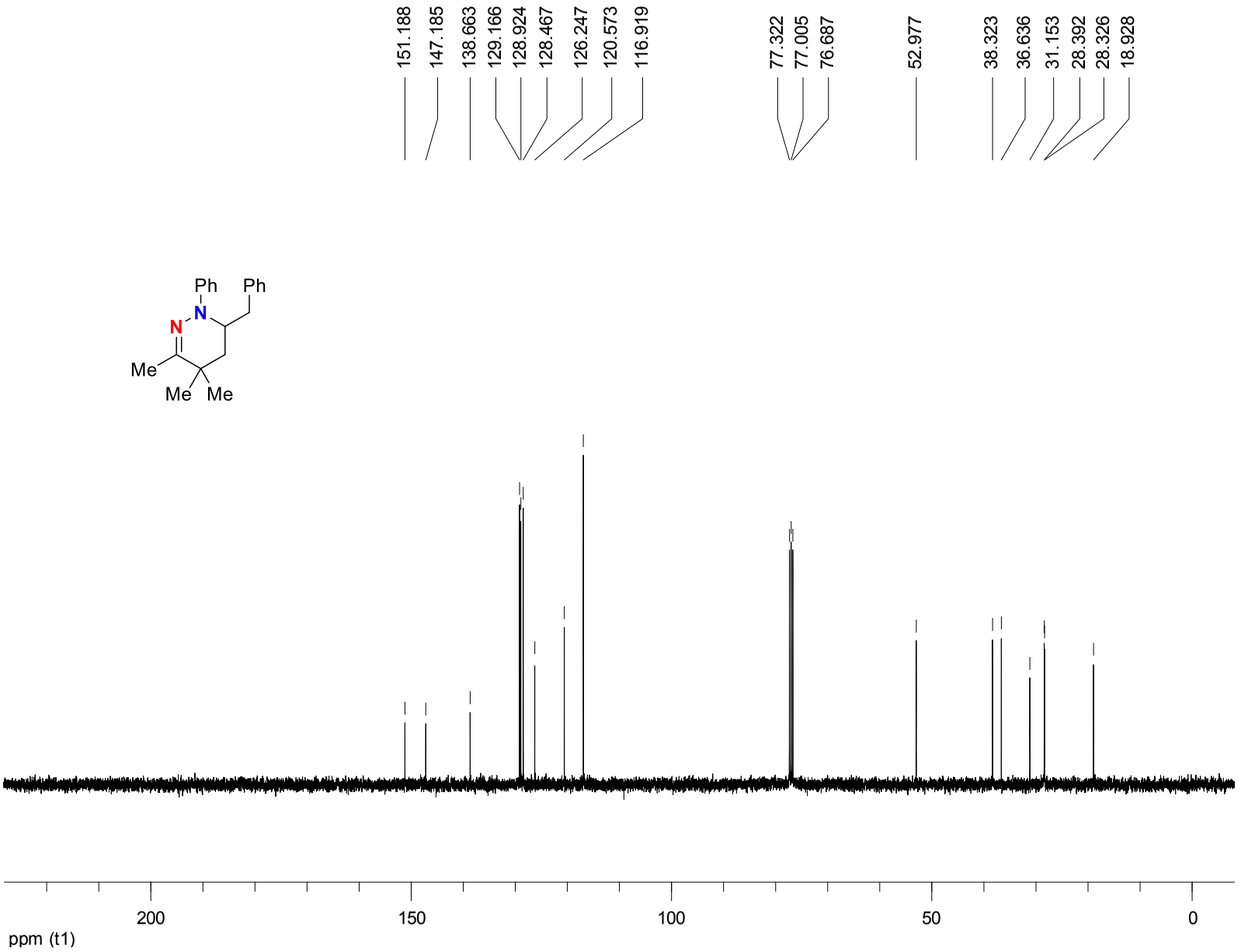
6-Benzyl-4,4-dimethyl-1-phenyl-3-(thiophen-2-yl)-1,4,5,6-tetrahydropyridazine **(2d)** (100 MHz, $CDCl_3$)



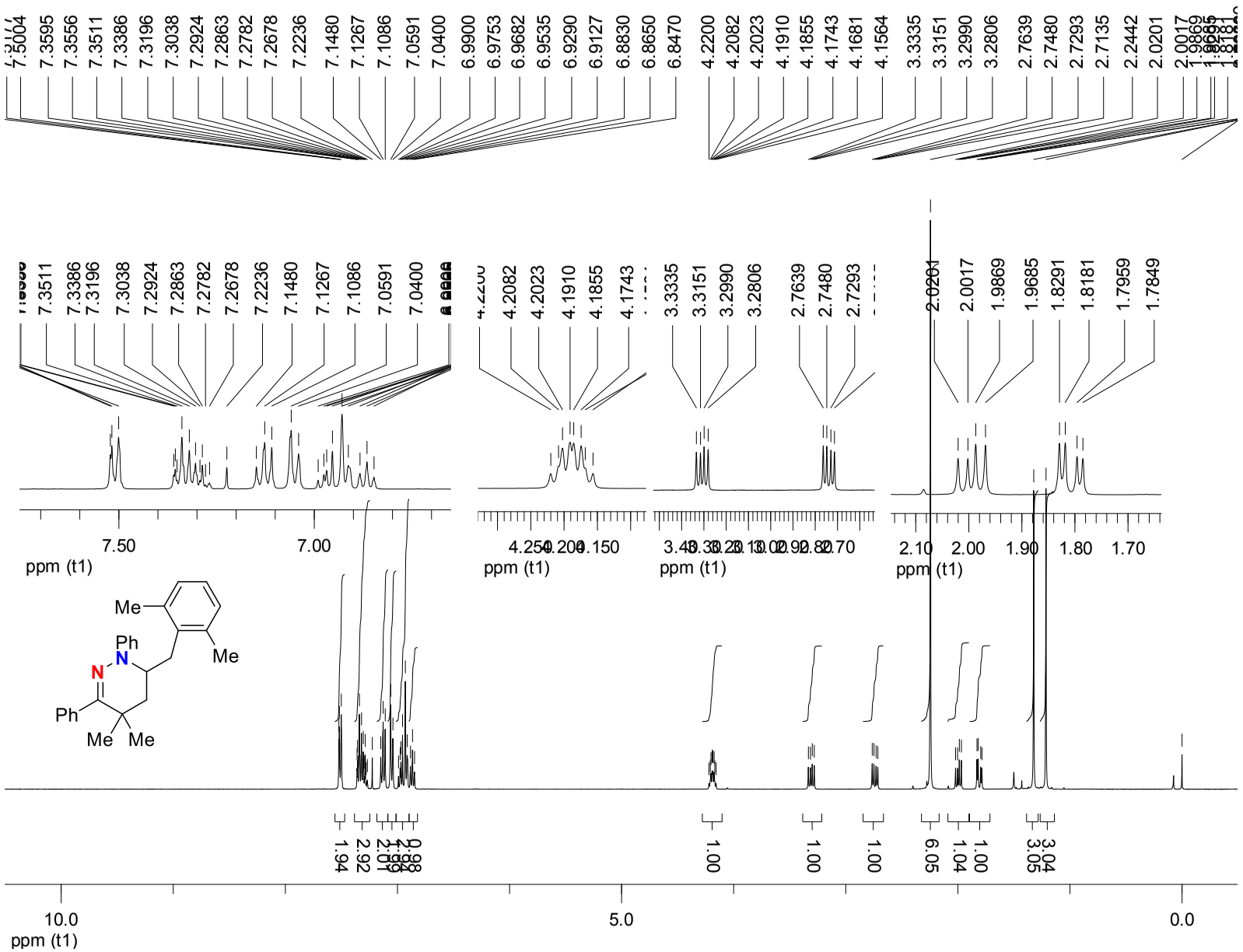
6-Benzyl-3,4,4-trimethyl-1-phenyl-1,4,5,6-tetrahydropyridazine (**2e**) (400 MHz, $CDCl_3$)



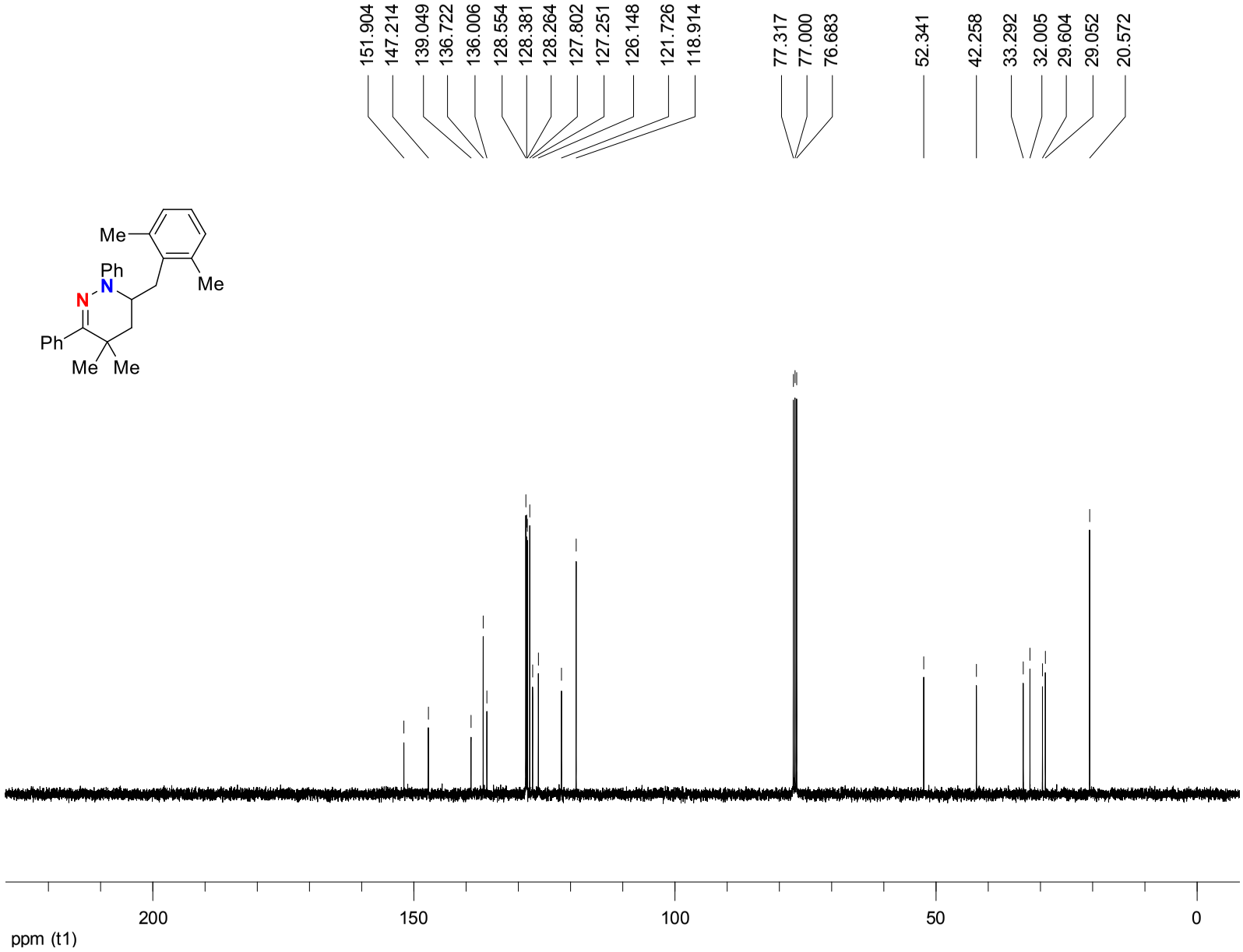
6-Benzyl-3,4,4-trimethyl-1-phenyl-1,4,5,6-tetrahydropyridazine (**2e**) (100 MHz, $CDCl_3$)



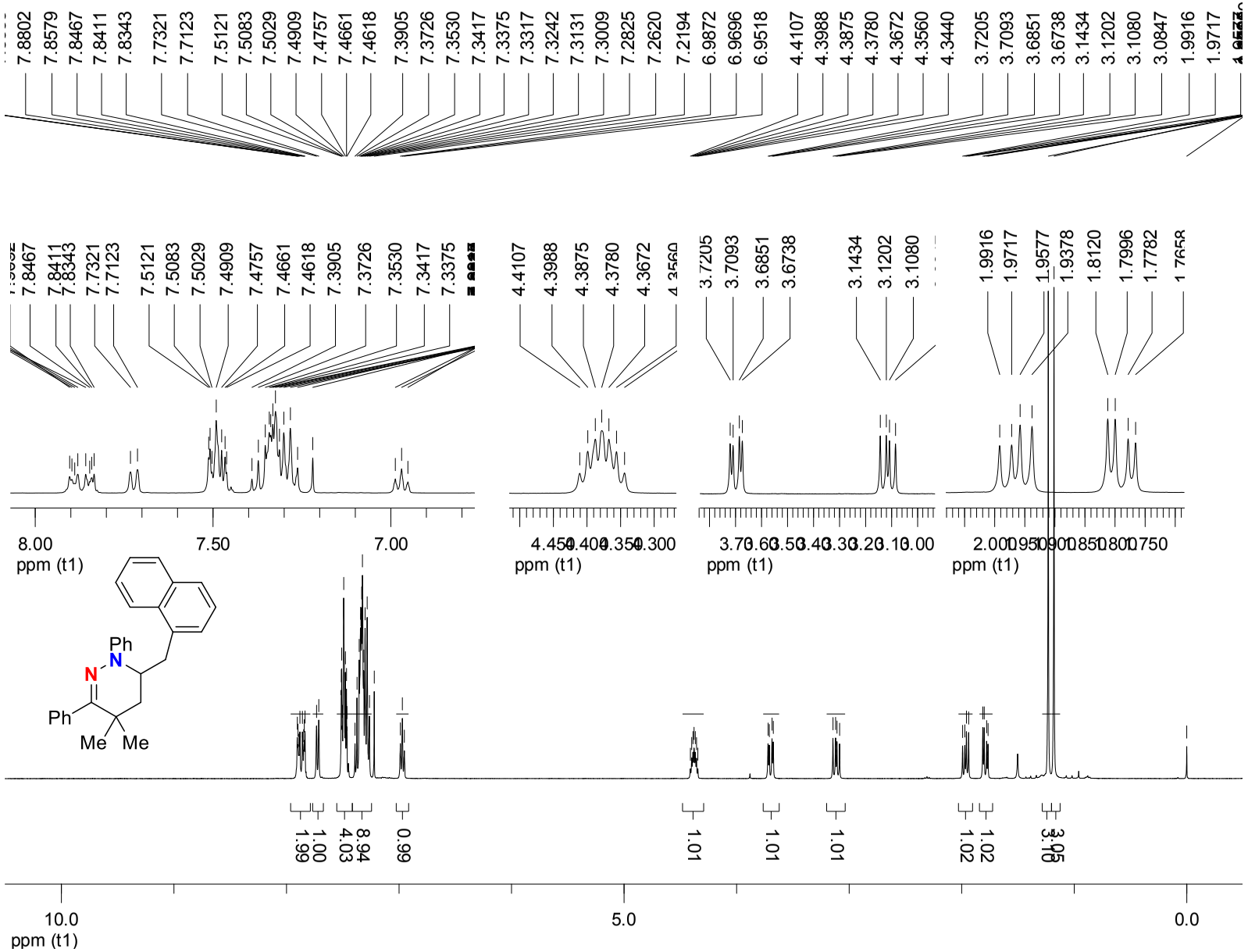
6-(2,6-Dimethylbenzyl-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2f**) (400 MHz, $CDCl_3$)



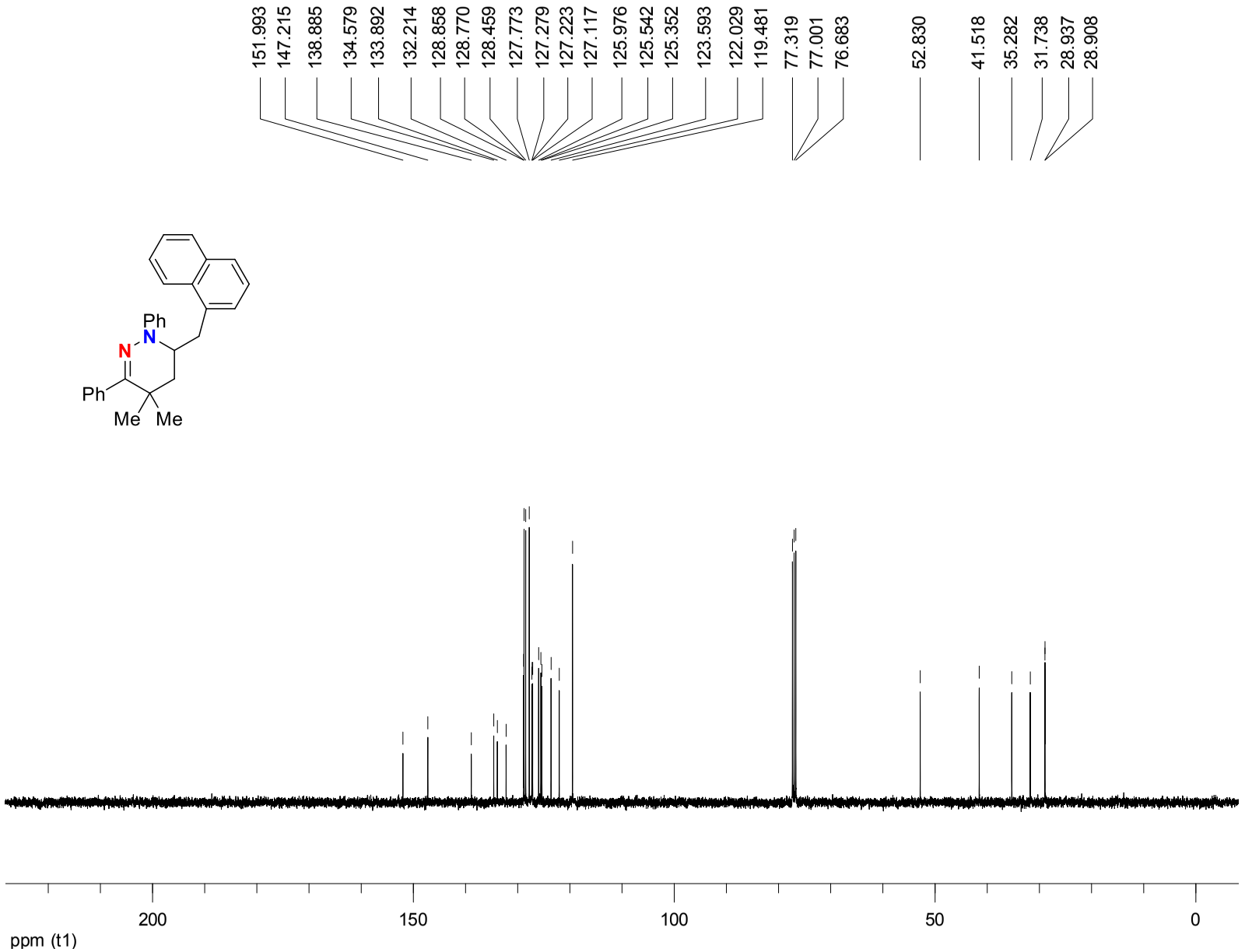
6-(2,6-Dimethylbenzyl-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2f**) (100 MHz, $CDCl_3$)



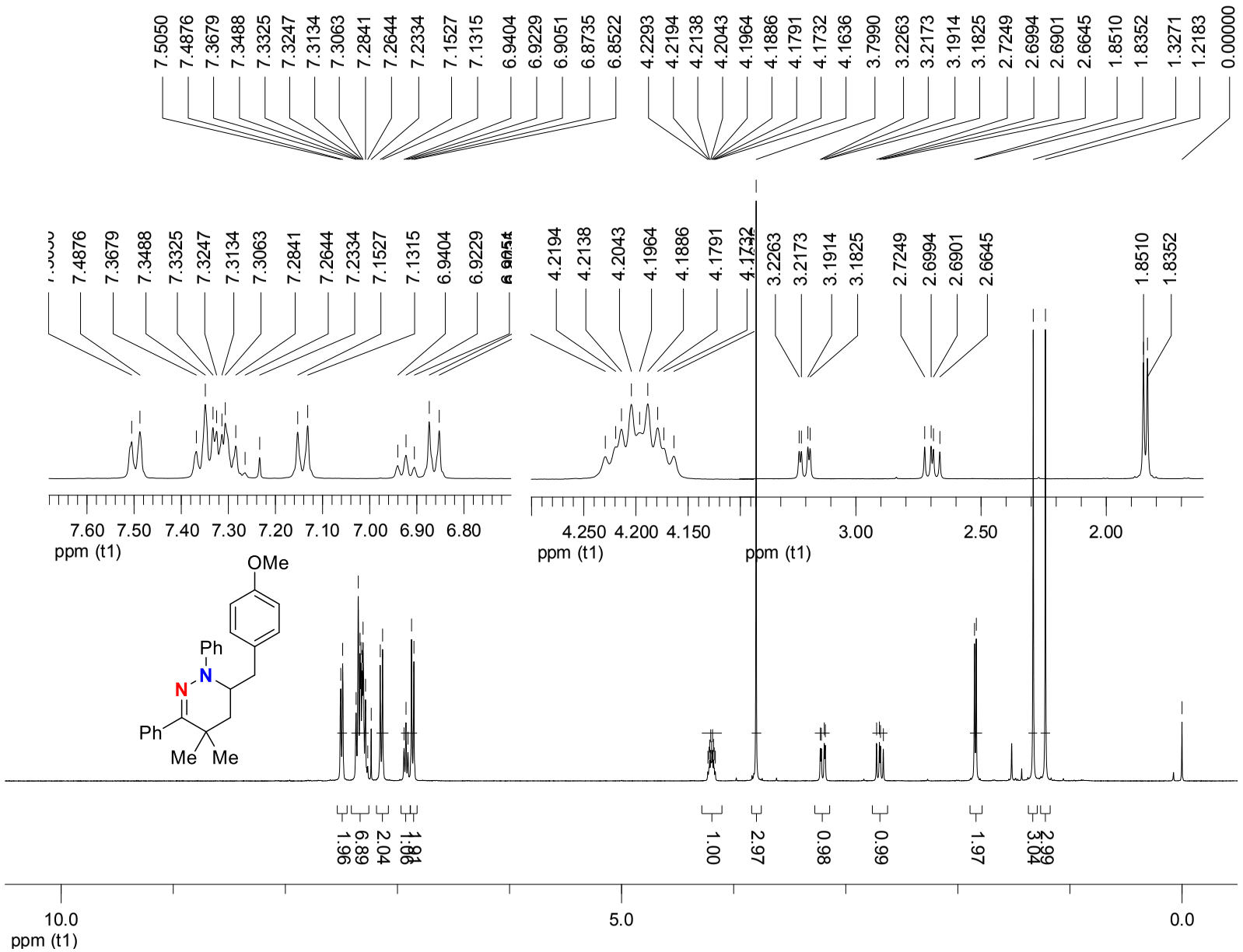
4,4-Dimethyl-6-(naphthalene-1-ylmethyl)-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2g**) (400 MHz, $CDCl_3$)



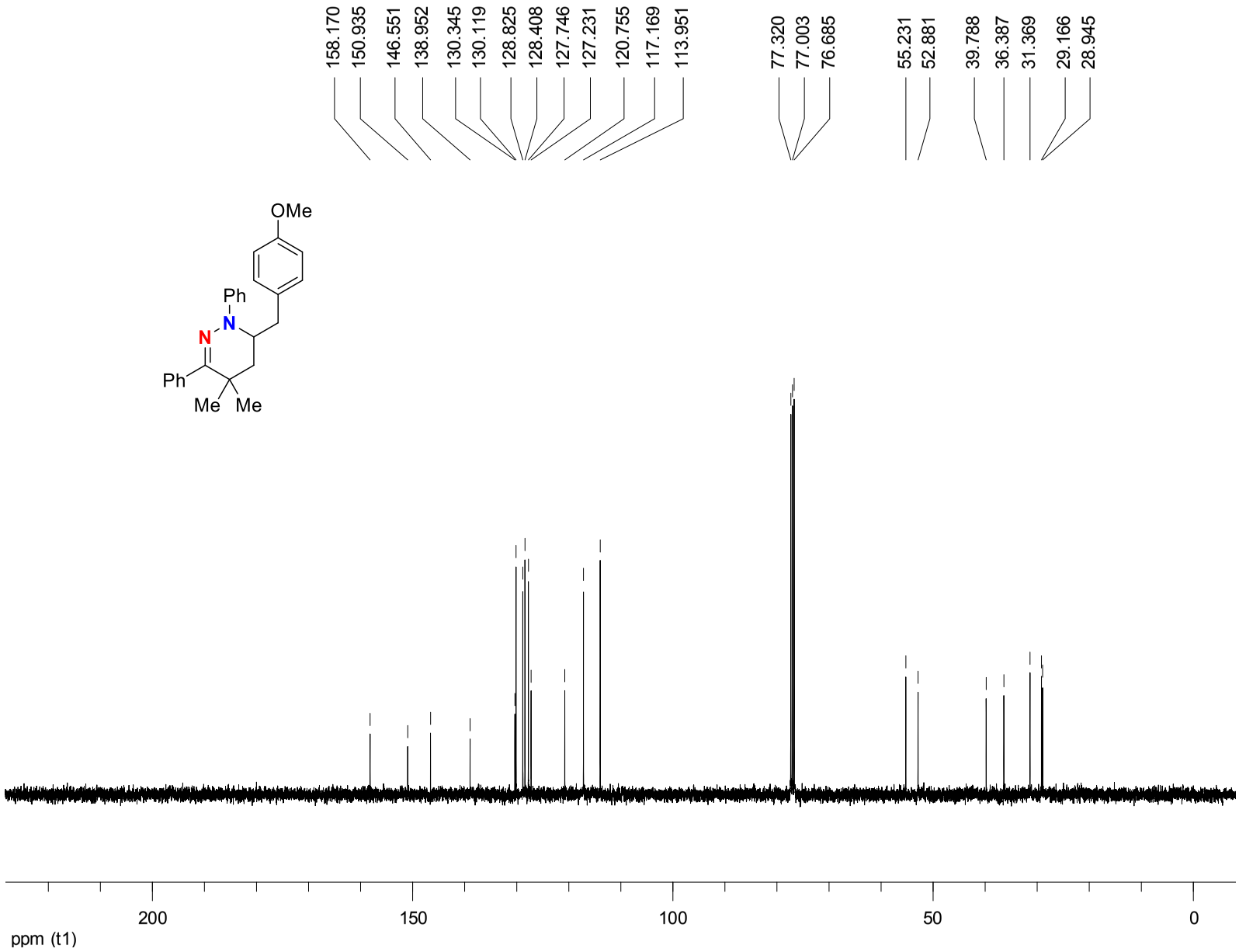
4,4-Dimethyl-6-(naphthalene-1-ylmethyl)-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2g**) (100 MHz, $CDCl_3$)



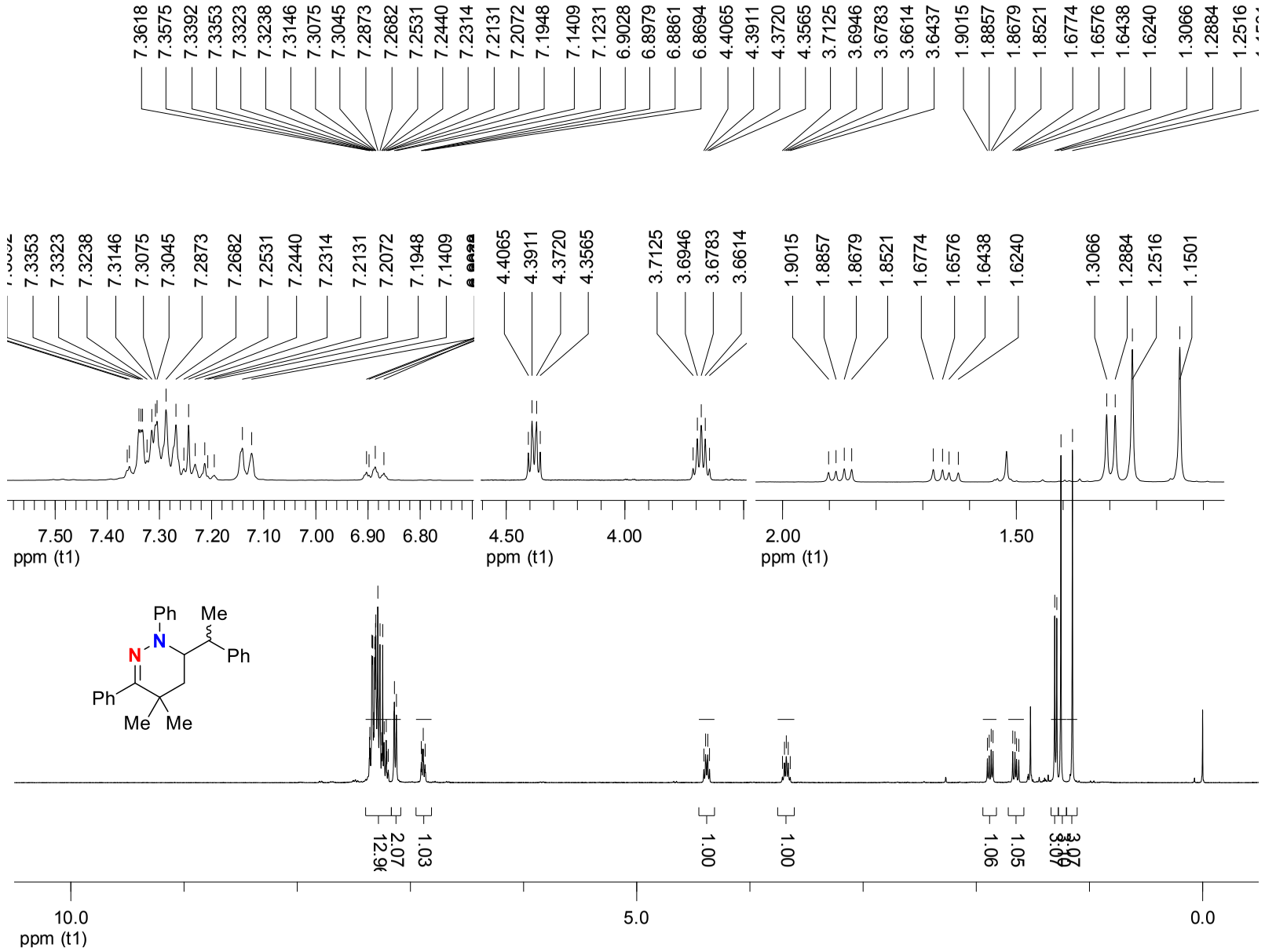
6-(4-methoxybenzyl)-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine **(2h)** (400 MHz, $CDCl_3$)



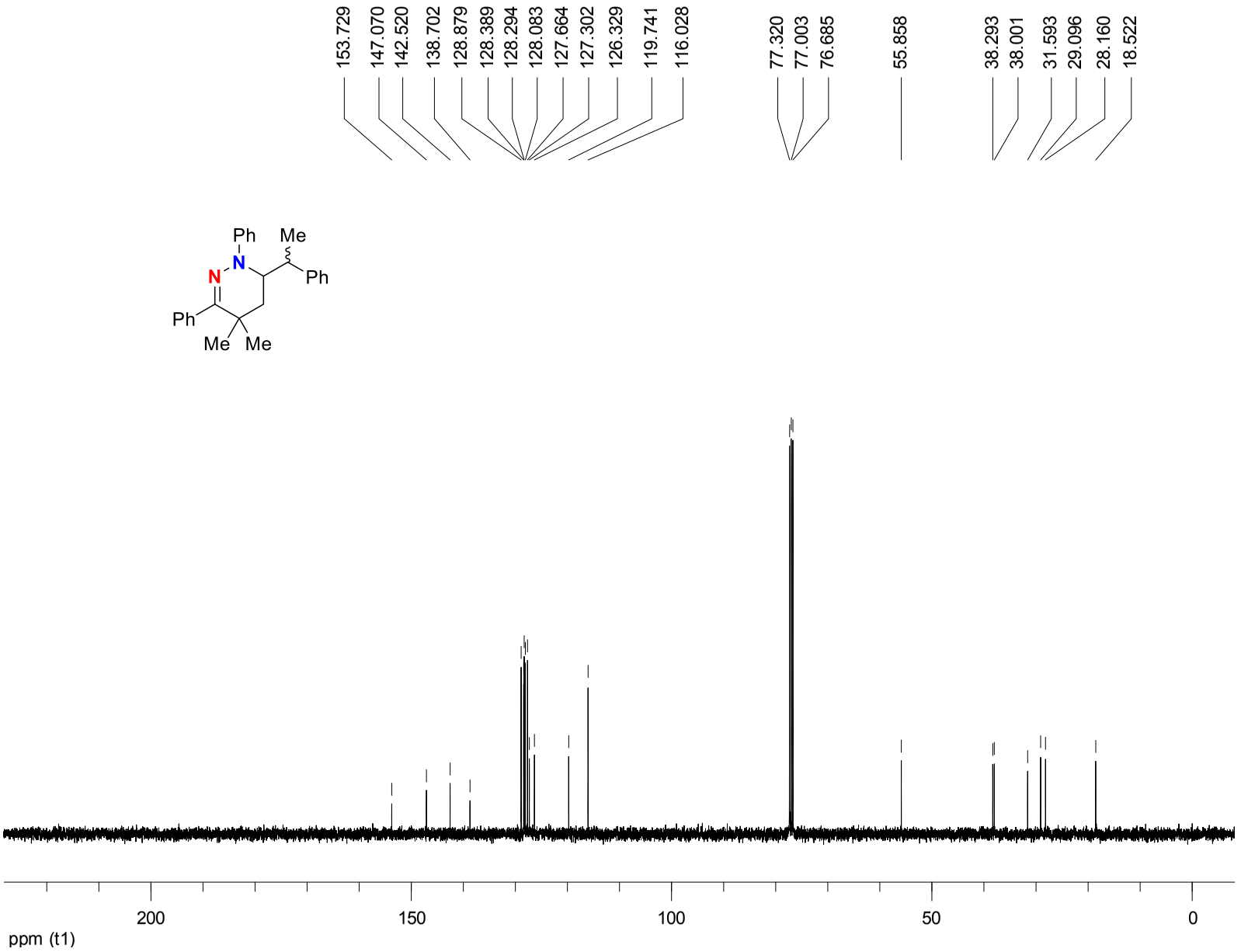
6-(4-methoxybenzyl)-4,4-dimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine **(2h)** (100 MHz, $CDCl_3$)



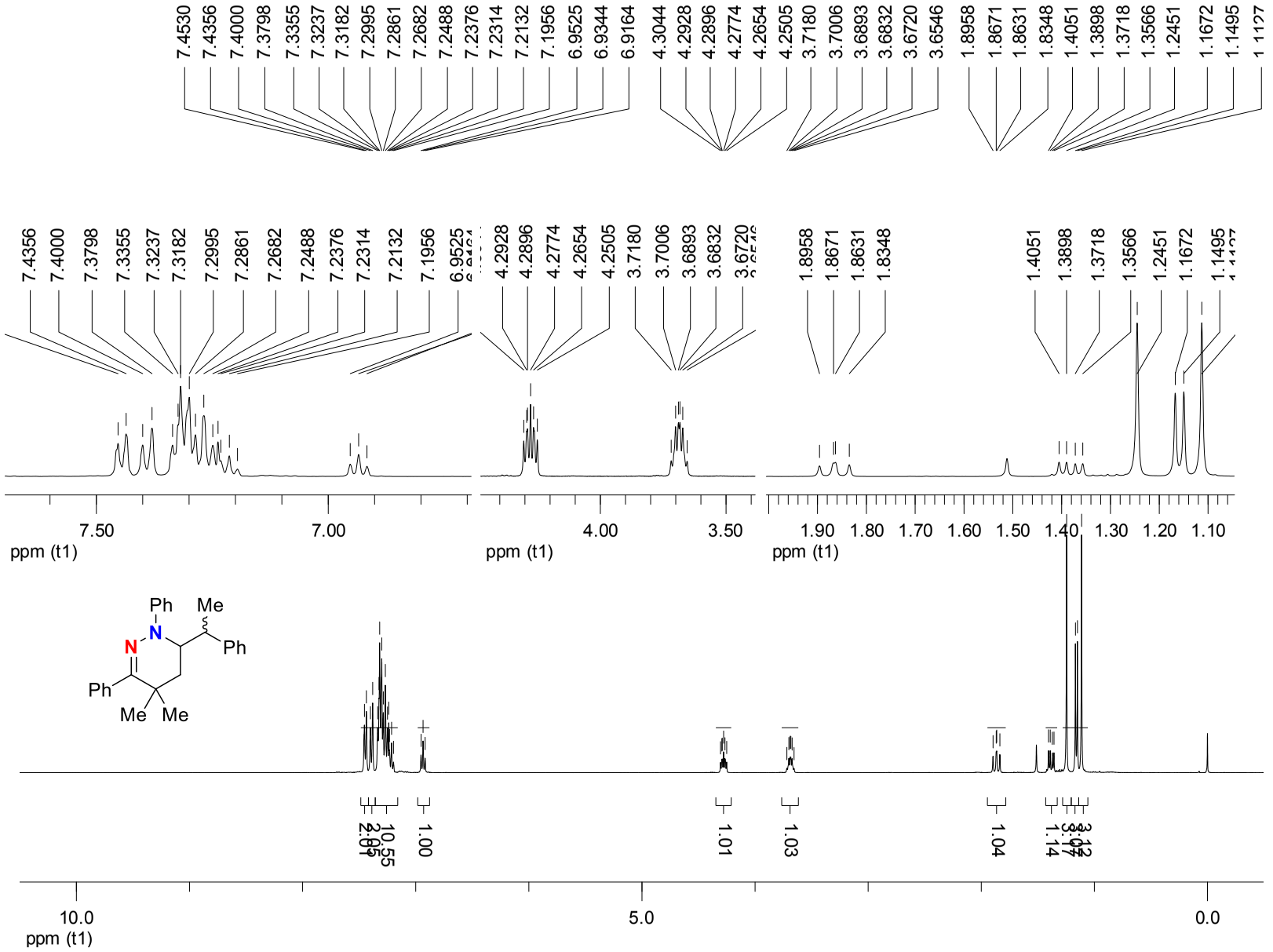
4,4-Dimethyl-1,3-diphenyl-6-(1-phenylethyl)-1,4,5,6-tetrahydropyridazine **(2i)**-isomer (**a**) (400 MHz, $CDCl_3$)



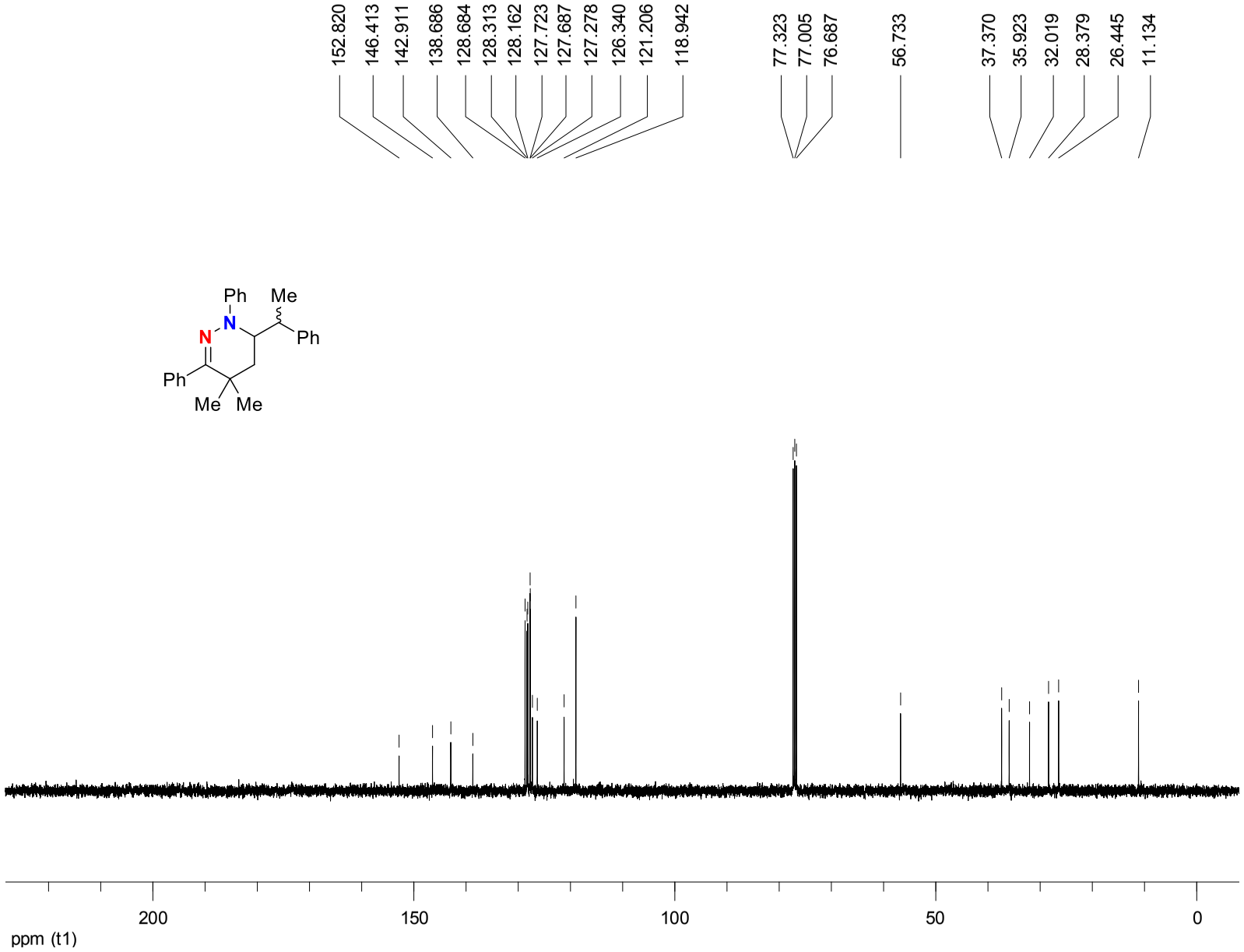
4,4-Dimethyl-1,3-diphenyl-6-(1-phenylethyl)-1,4,5,6-tetrahydropyridazine **(2i)**-isomer (**a**) (100 MHz, $CDCl_3$)



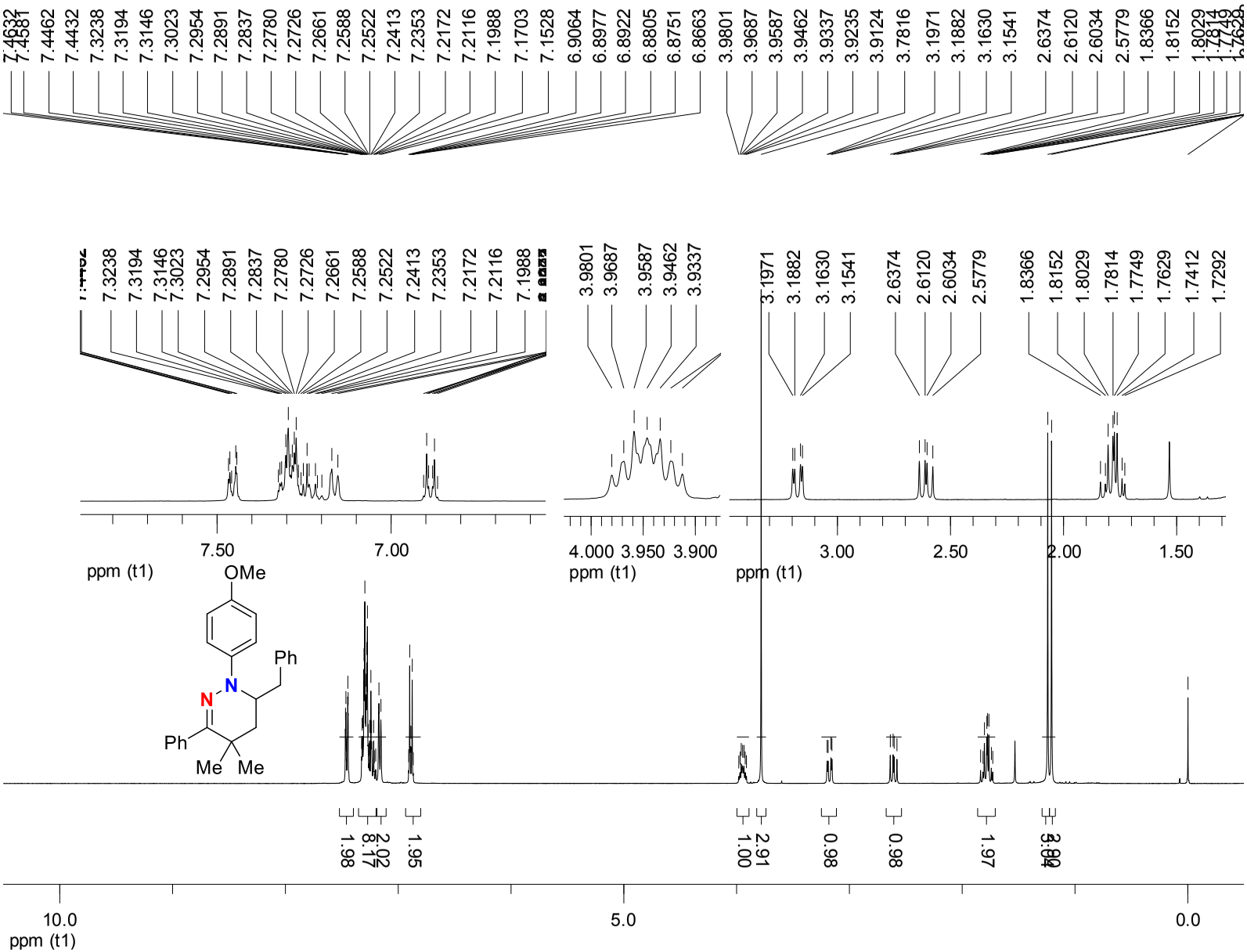
4,4-Dimethyl-1,3-diphenyl-6-(1-phenylethyl)-1,4,5,6-tetrahydropyridazine (**2i**)-isomer (**b**) (400 MHz, $CDCl_3$)



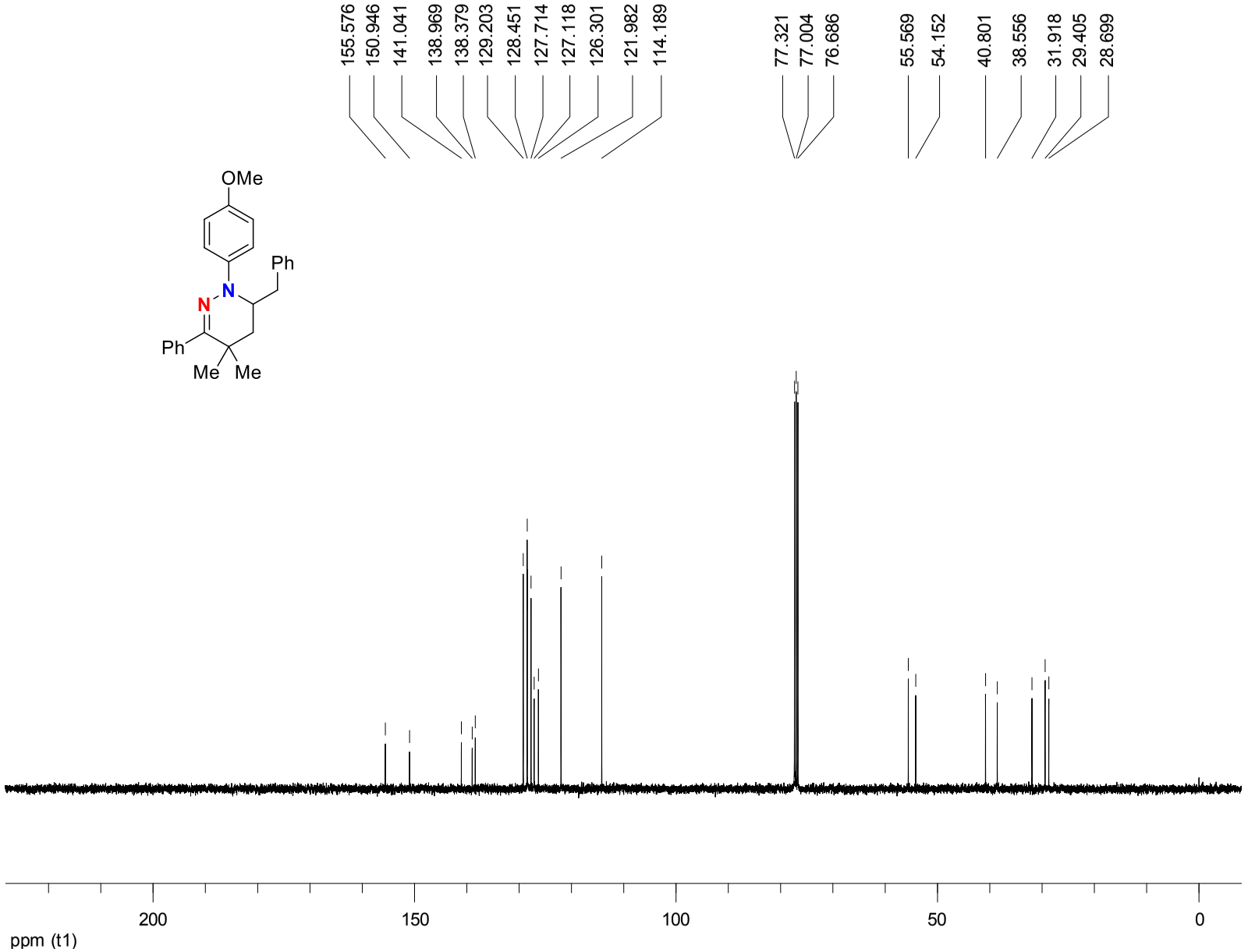
4,4-Dimethyl-1,3-diphenyl-6-(1-phenylethyl)-1,4,5,6-tetrahydropyridazine (**2i**)-isomer (**b**) (100 MHz, $CDCl_3$)



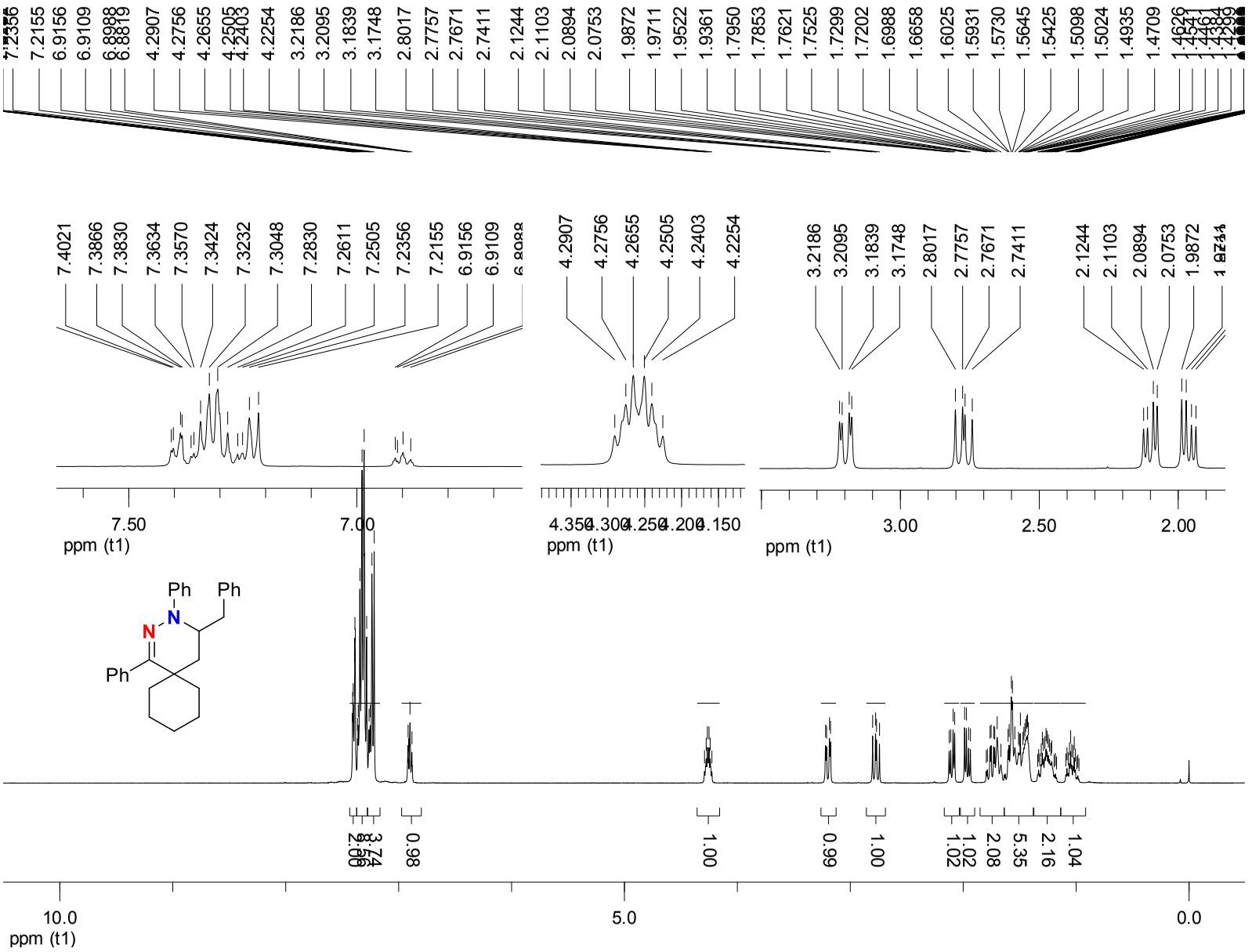
6-Benzyl-1-(4-methoxyphenyl)-4,4-dimethyl-3-phenyl-1,4,5,6-tetrahydropyridazine **(2j)** (400 MHz, $CDCl_3$)



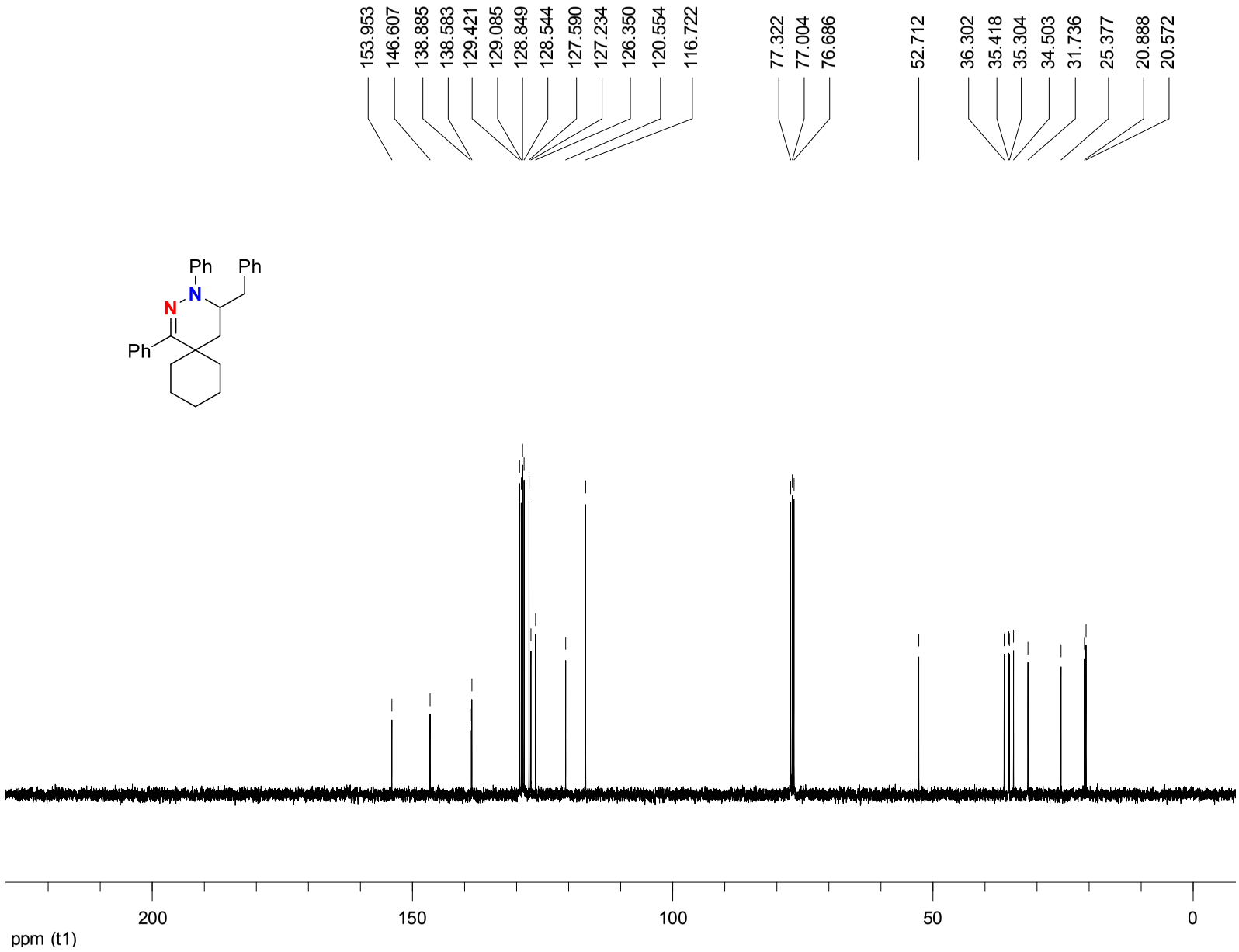
6-Benzyl-1-(4-methoxyphenyl)-4,4-dimethyl-3-phenyl-1,4,5,6-tetrahydropyridazine **(2j)** (100 MHz, $CDCl_3$)



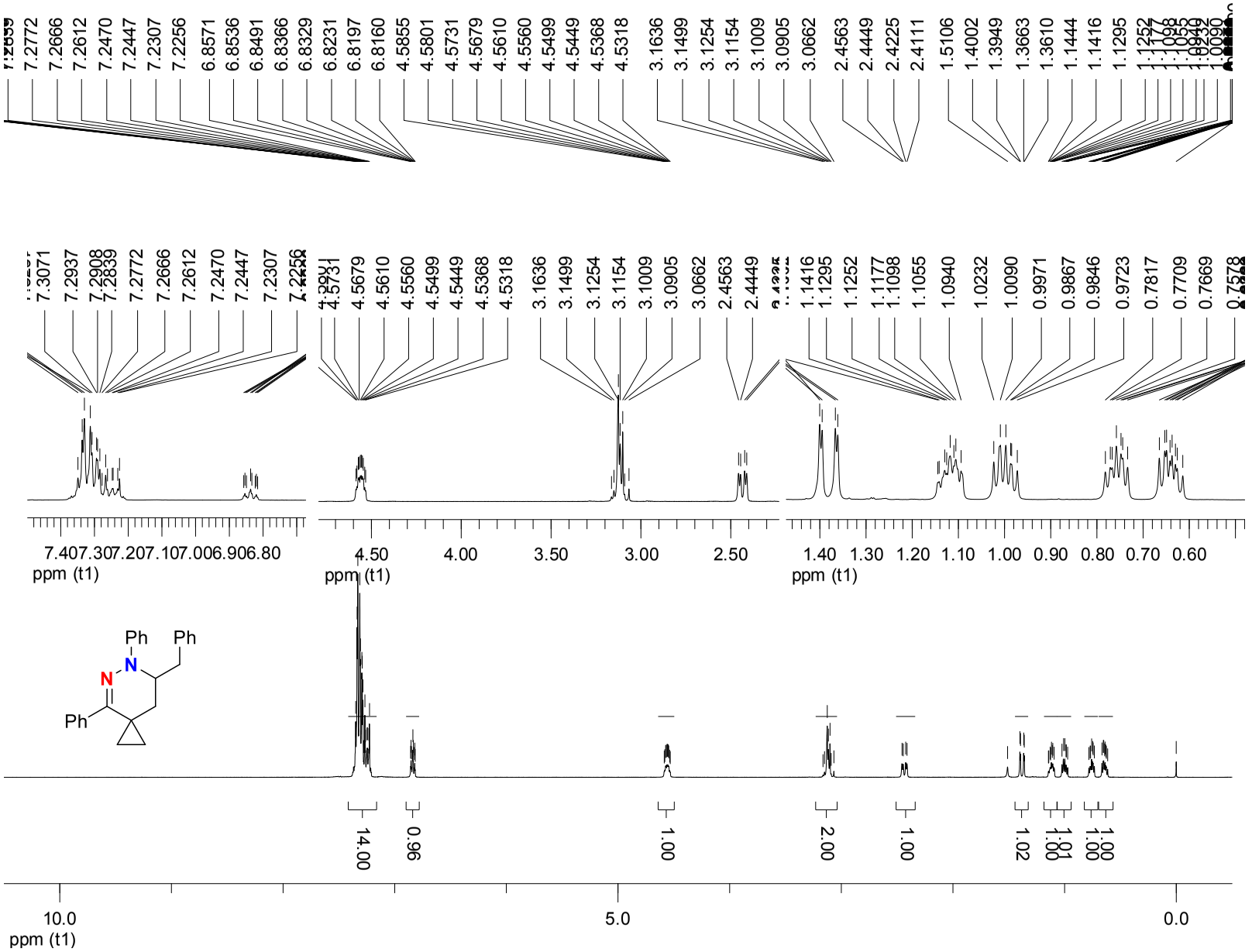
4-Benzyl-1,3-diphenyl-2,3-diazaspiro[5.5]undec-1-ene (**2k**) (400 MHz, $CDCl_3$)



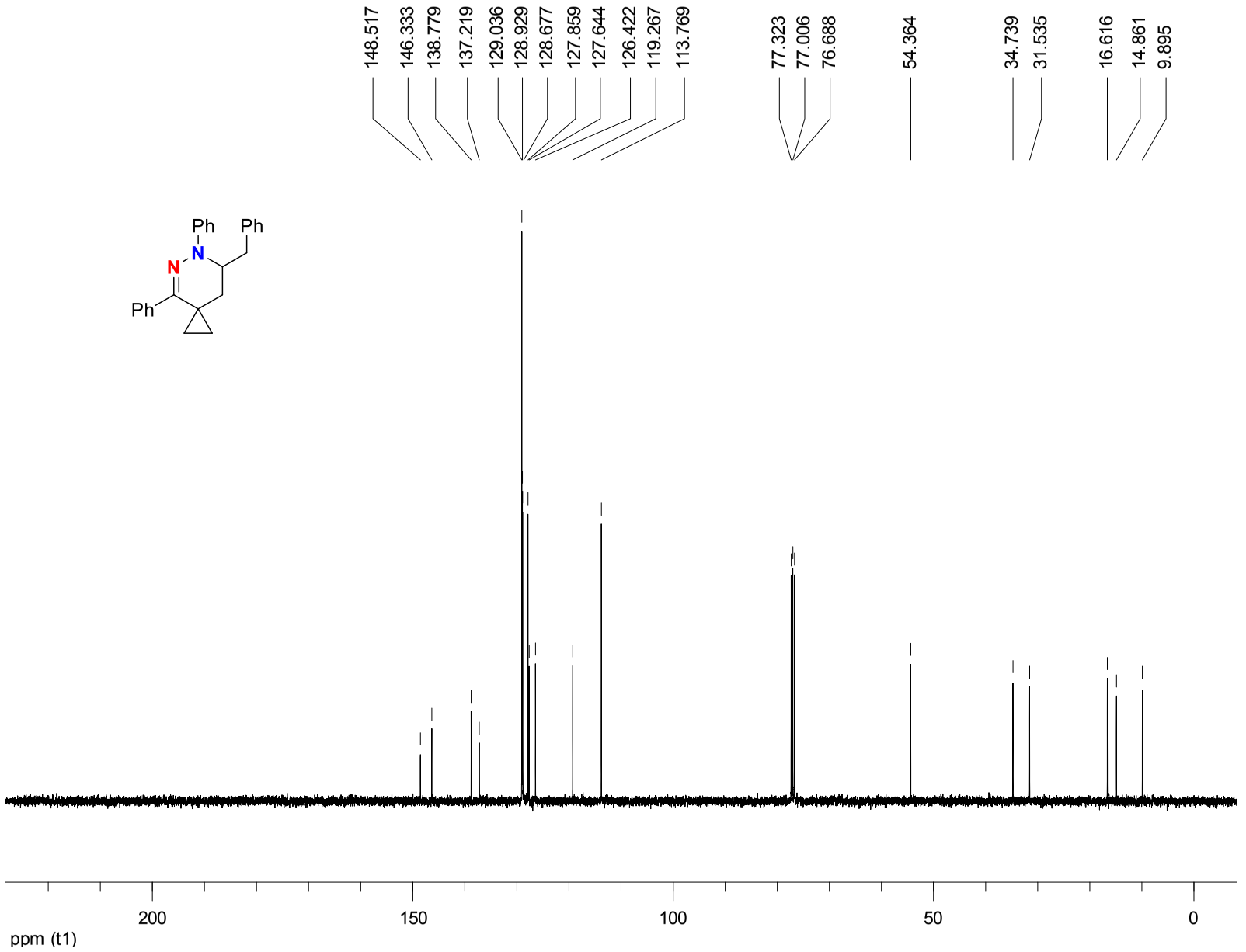
4-Benzyl-1,3-diphenyl-2,3-diazaspiro[5.5]undec-1-ene (**2k**) (100 MHz, $CDCl_3$)



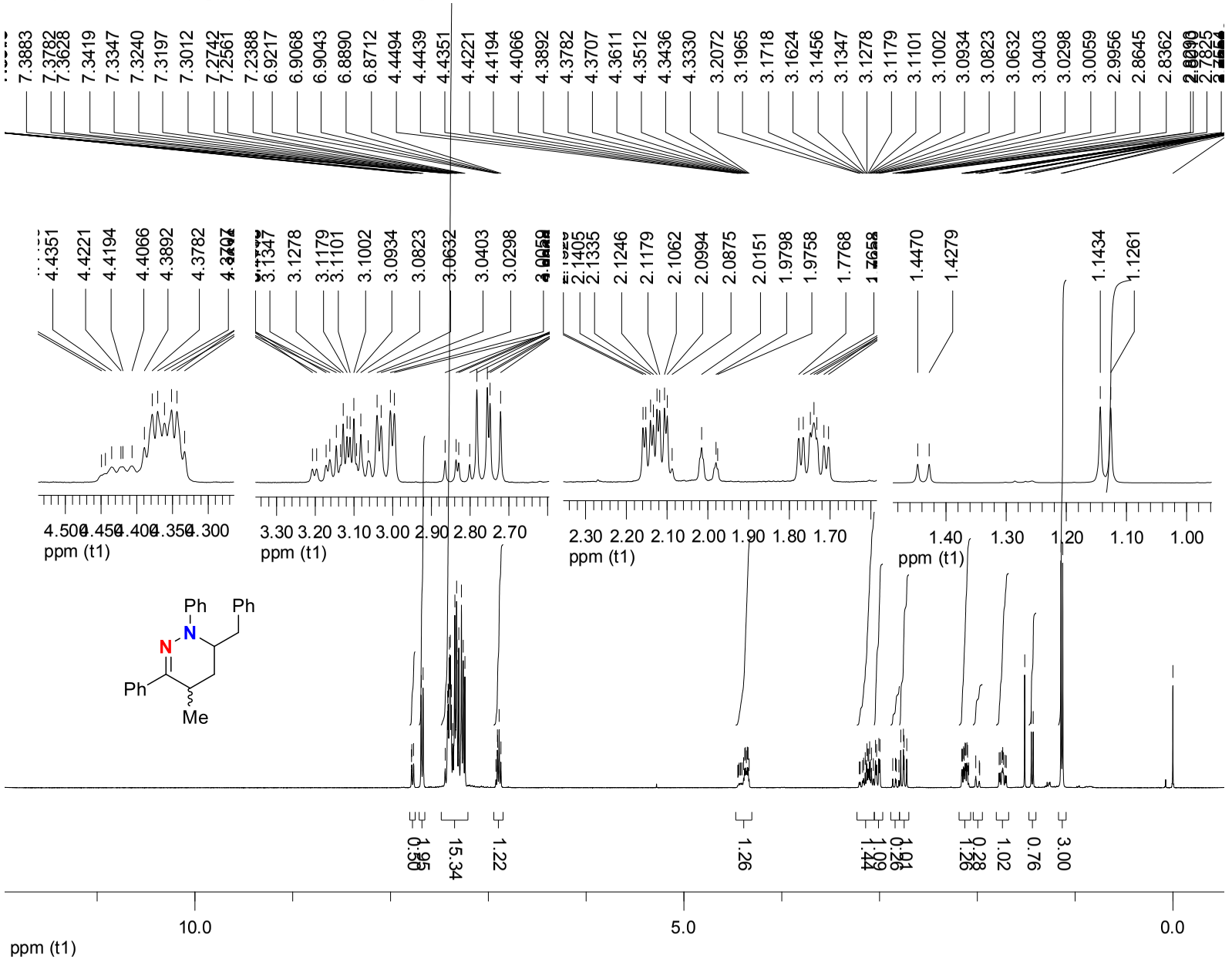
7-Benzyl-4,6-diphenyl-5,6-diazaspiro[2.5]oc-4-ene (**2l**) (400 MHz, $CDCl_3$)



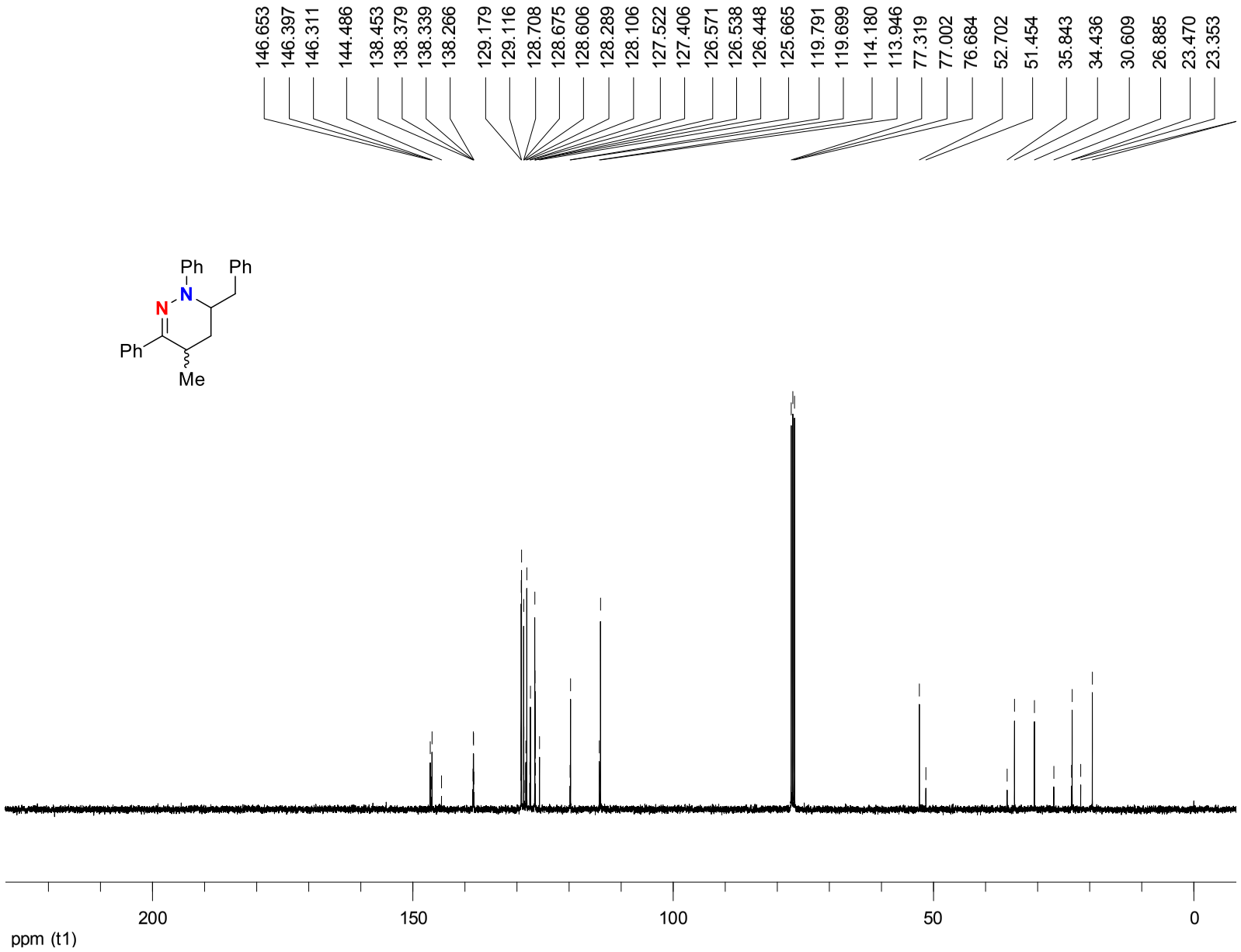
7-Benzyl-4,6-diphenyl-5,6-diazaspiro[2.5]oc-4-ene (**2l**) (100 MHz, $CDCl_3$)



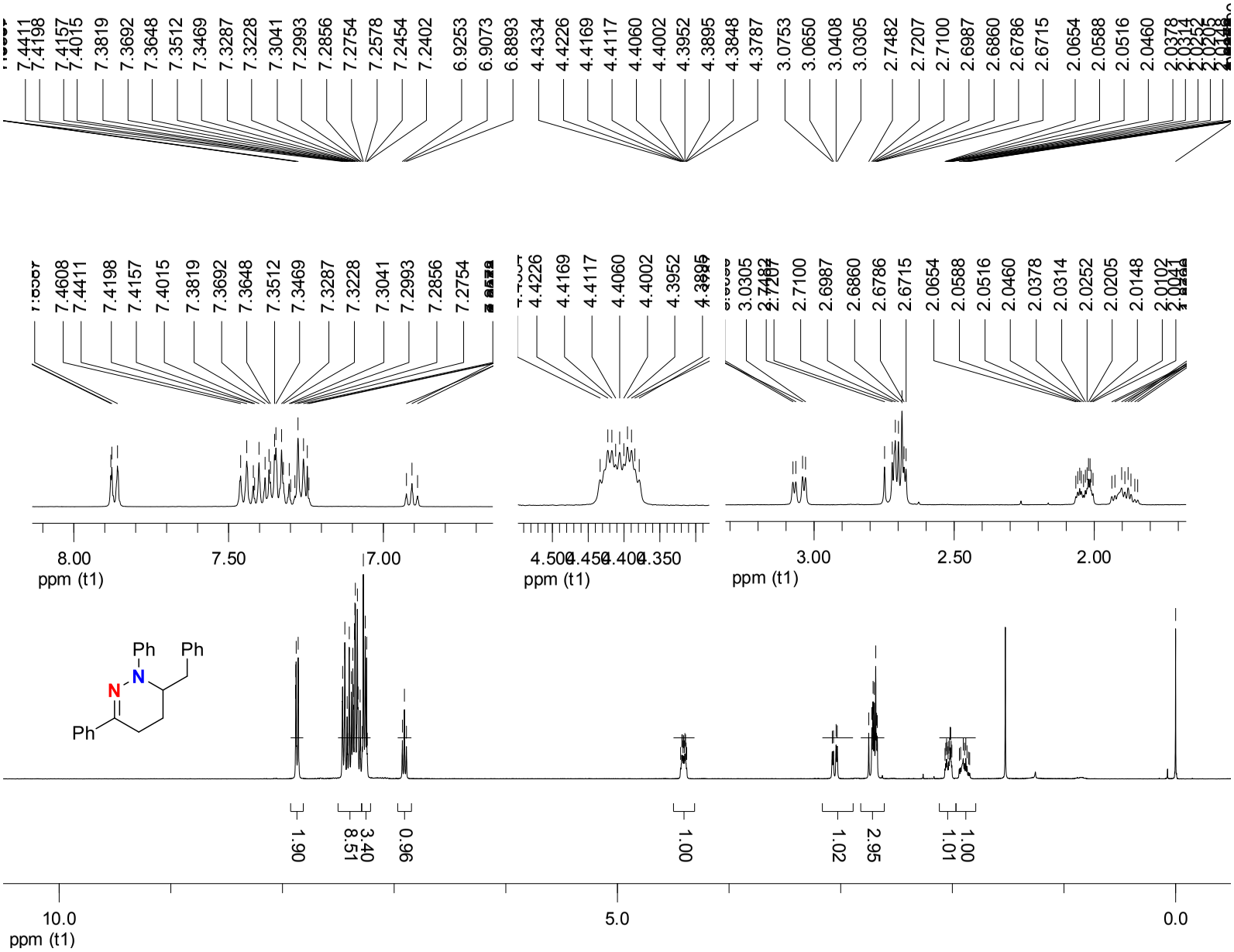
6-Benzyl-4-methyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine **(2m)** (400 MHz, $CDCl_3$)



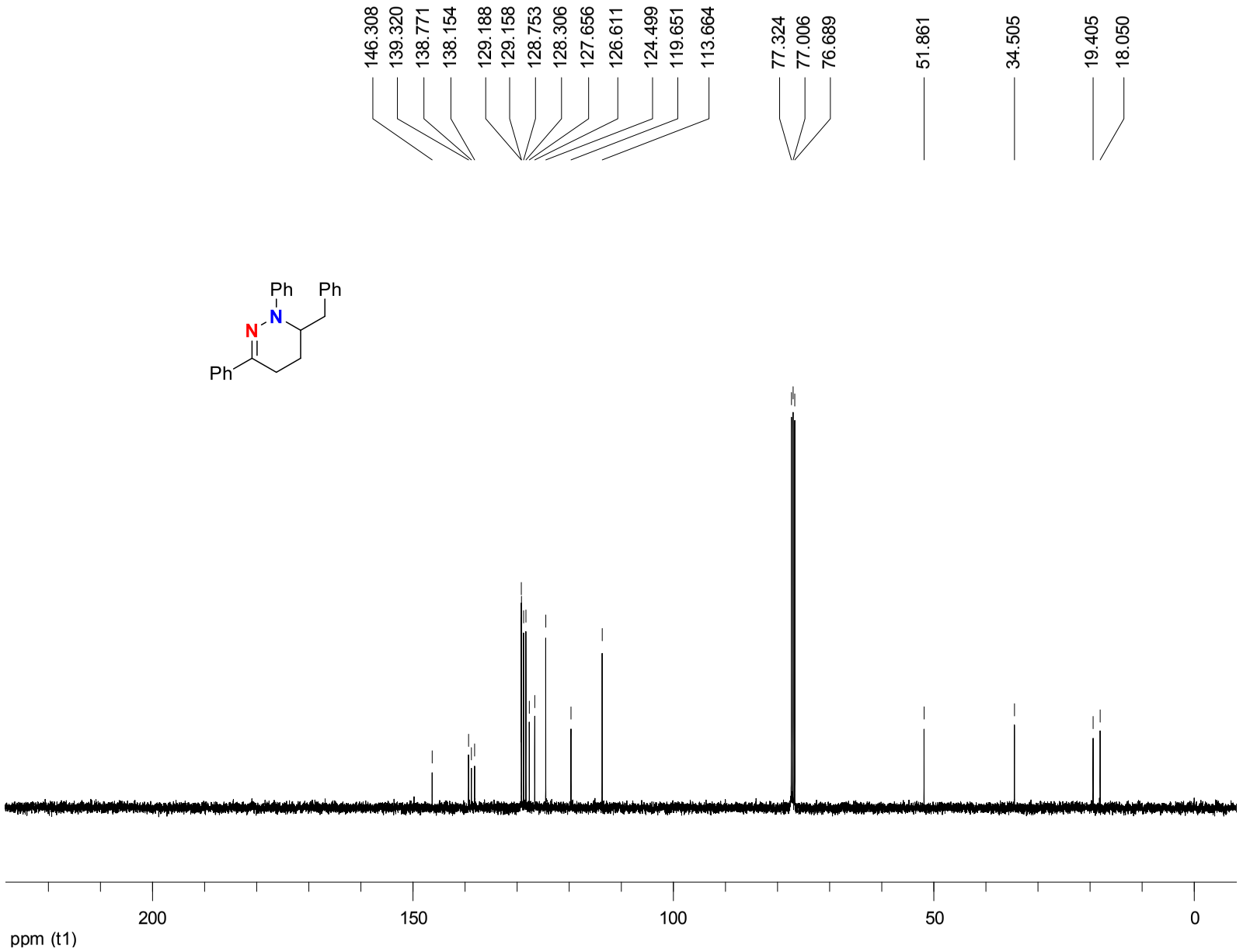
6-Benzyl-4-methyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine **(2m)** (100 MHz, $CDCl_3$)



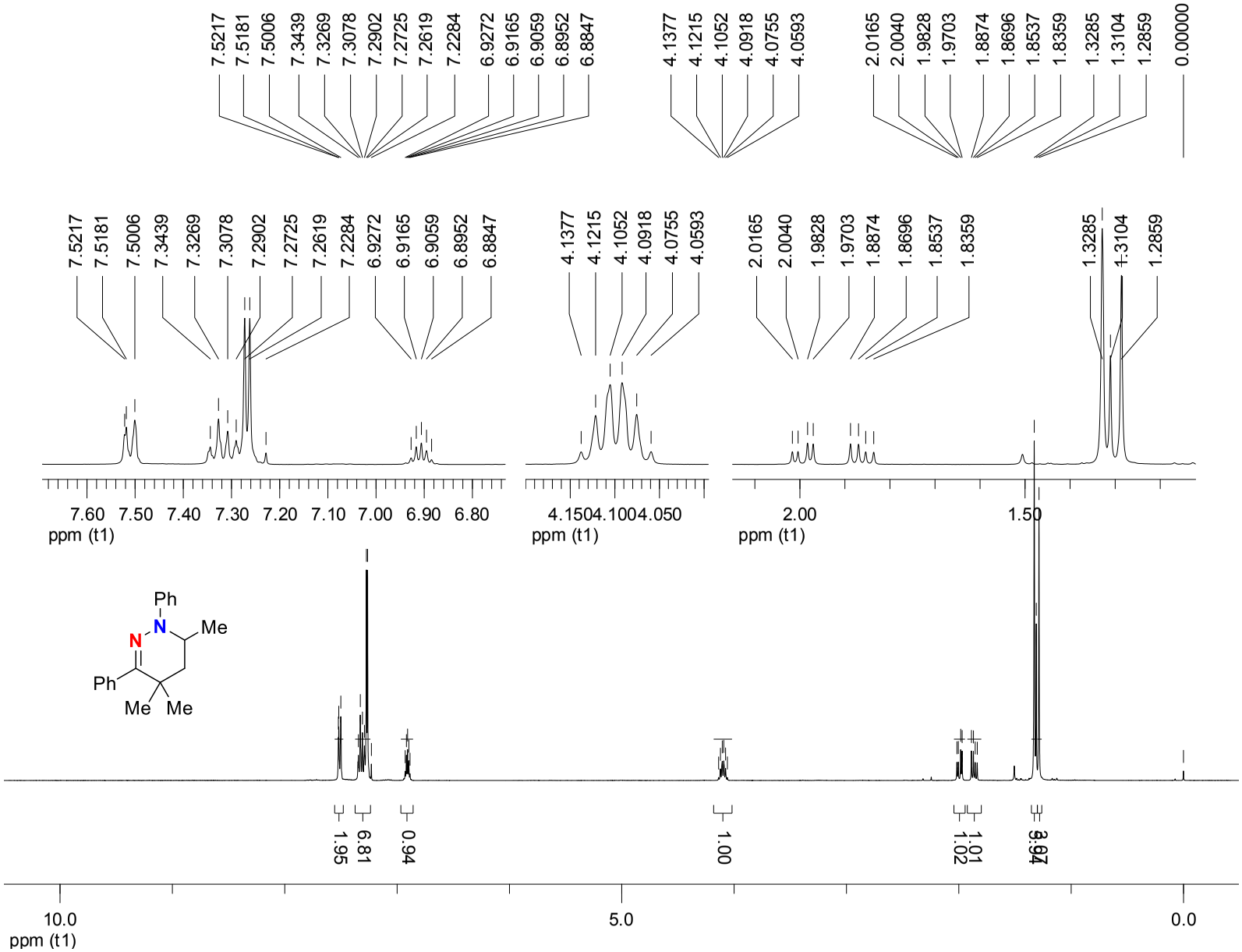
6-Benzyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2n**) (400 MHz, $CDCl_3$)



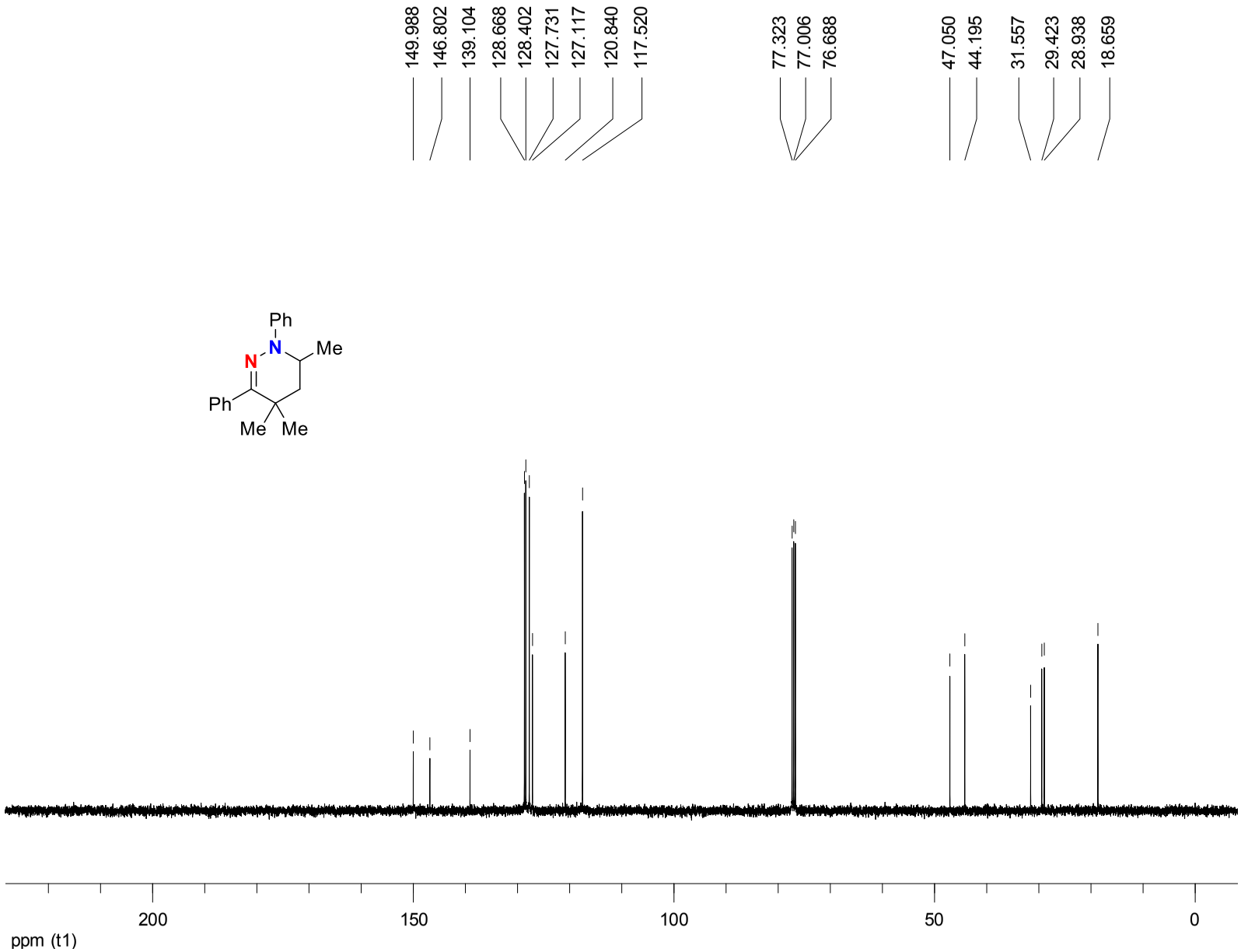
6-Benzyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine (**2n**) (100 MHz, $CDCl_3$)



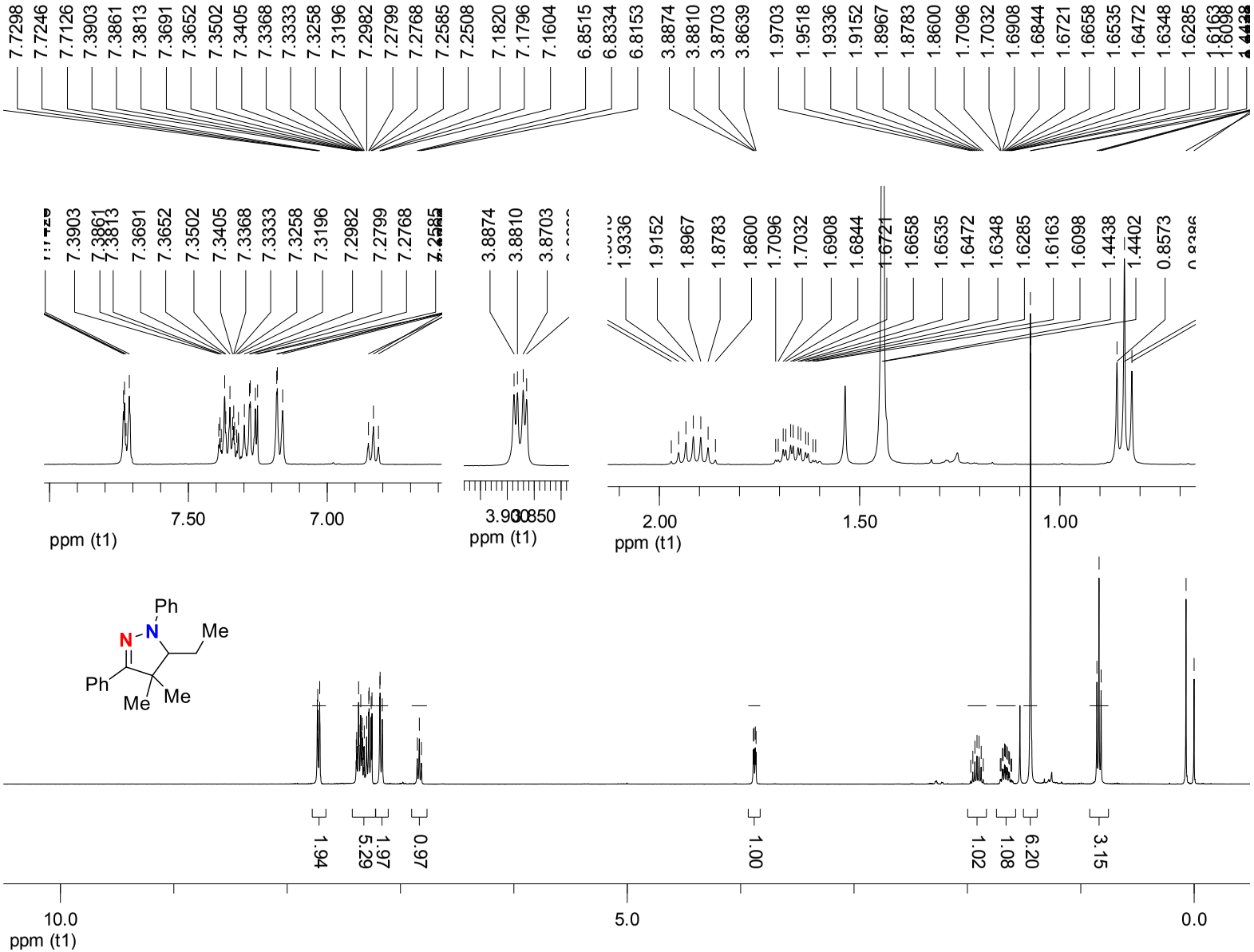
4,4,6-trimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine **(2o)** (400 MHz, $CDCl_3$)



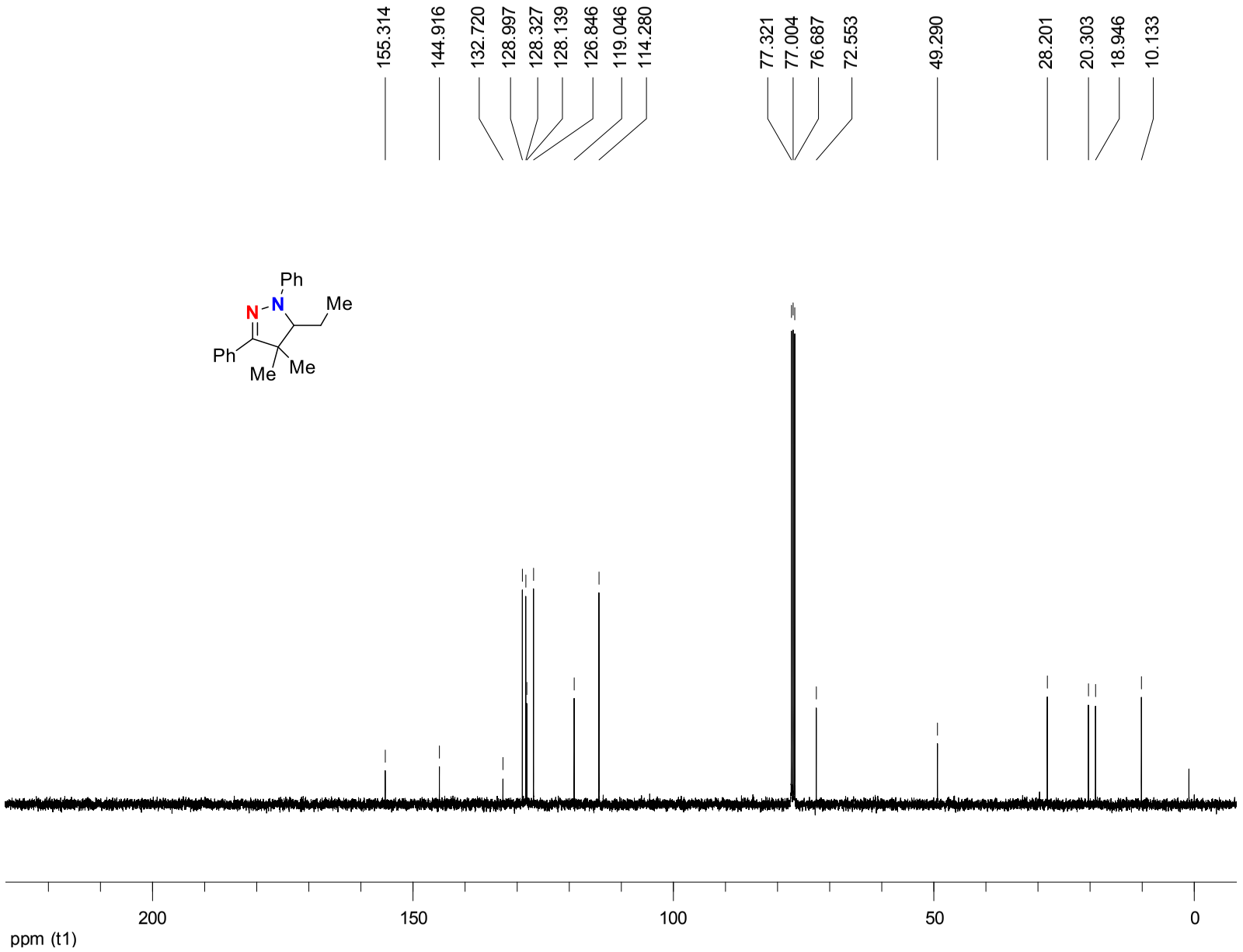
4,4,6-trimethyl-1,3-diphenyl-1,4,5,6-tetrahydropyridazine **(2o)** (100 MHz, $CDCl_3$)



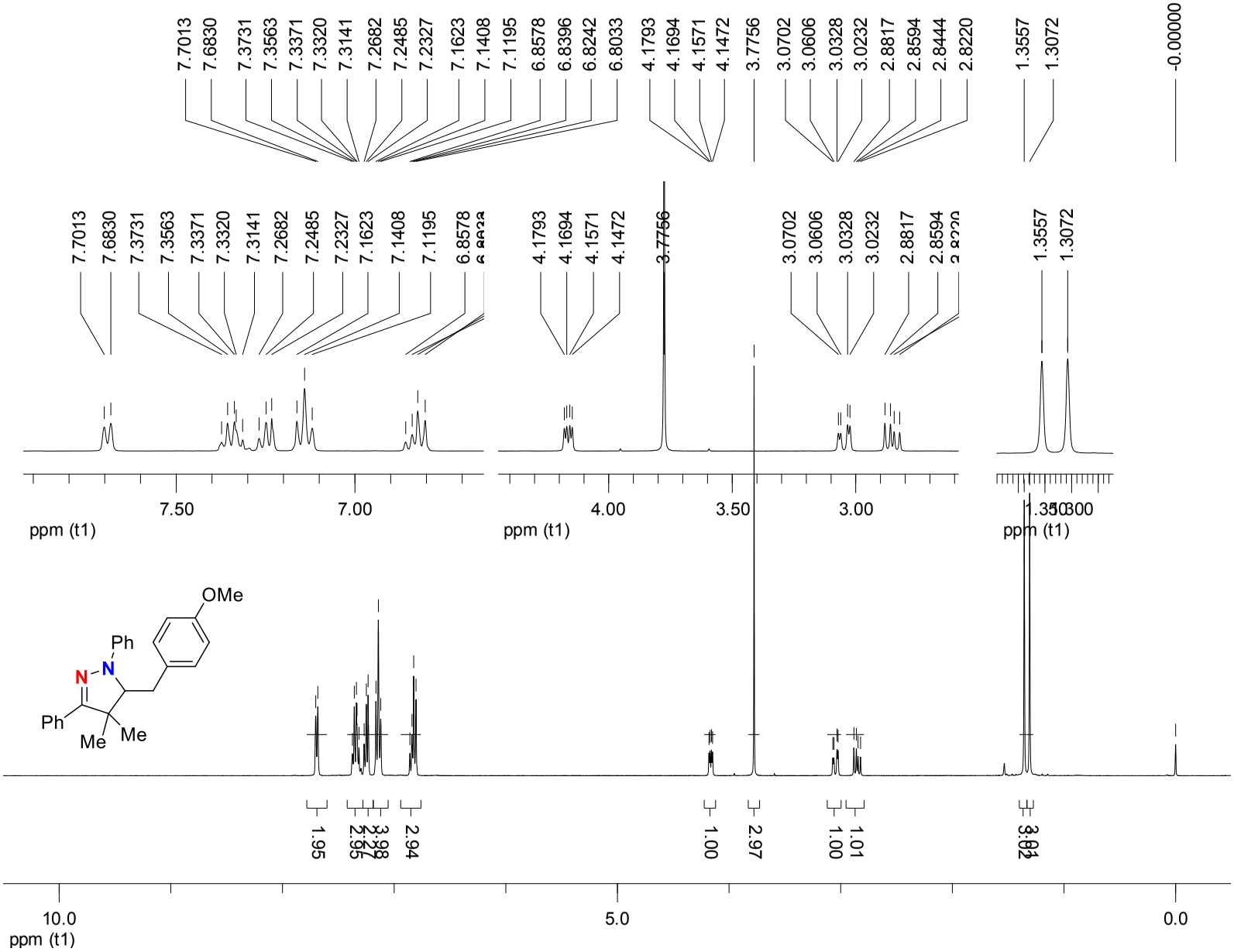
5-Ethyl-4,4-dimethyl-1,3-diphenyl-4,5-dihydro-1*H*-pyrazole **(3o)** (400 MHz, $CDCl_3$)



5-Ethyl-4,4-dimethyl-1,3-diphenyl-4,5-dihydro-1*H*-pyrazole **(3o)** (100 MHz, $CDCl_3$)



5-(4-methoxybenzyl)-4,4-dimethyl-1,3-diphenyl-4,5-dihydro-1*H*-pyrazole (**3p**) (400 MHz, $CDCl_3$)



5-(4-methoxybenzyl)-4,4-dimethyl-1,3-diphenyl-4,5-dihydro-1*H*-pyrazole (**3p**) (100 MHz, $CDCl_3$)