Supporting information

I_2-Catalyzed Benzylation of NH-Sulfoximines with Diarylmethanes and Alkylarenes

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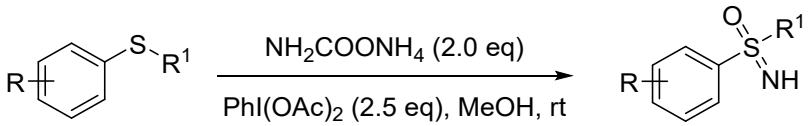
1. General

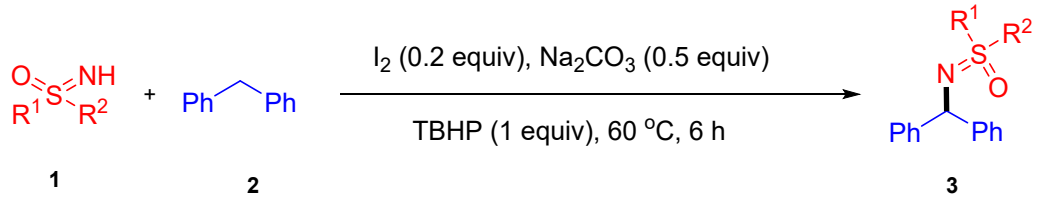
Commercial reagents and solvents were obtained from the commercial providers and used without further purification. The products were purified using a commercial flash chromatography system or a regular glass column. TLC was developed on silica gel 60 F254 glass plates. The chemical shifts are reported in δ (ppm) values (^{1}H and ^{13}C NMR relative to $CDCl_3$, δ 7.26 ppm for ^{1}H NMR and δ 77.16 ppm for ^{13}C NMR). Or alternatively, ^{1}H NMR chemical shifts were referenced to tetramethylsilane signal (0 ppm). Multiplicities are recorded by s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), h (hextet), m (multiplet) and br (broad). Coupling constants (*J*), are reported in Hertz (Hz). Commercial reagents were used without any further purification.

2. General procedures for the synthesis of starting material[1]



Sulfide (5 mmol), NH_2COONH_4 (10 mmol, 2.0 eq) and $PhI(OAc)_2$ (12.5 mmol, 2.5 eq) were added to a 50 mL roundbottom flask. MeOH (10 mL, 0.5M) were added and the reaction mixture stirred at open ambient for 1 h. Then MeOH was removed under reduced pressure, the sulfoximine product were isolated by silica-gel column chromatography.

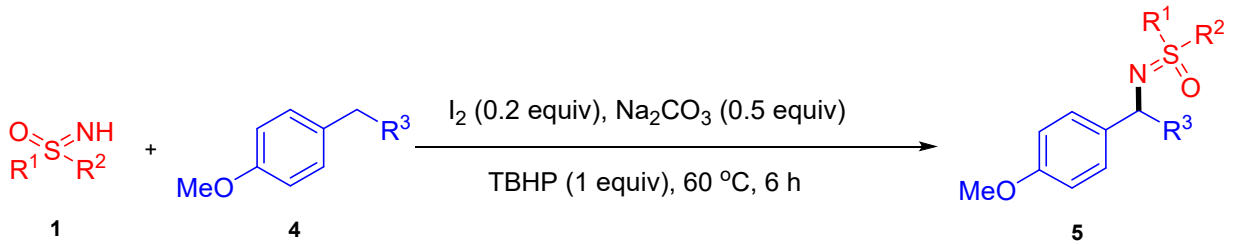
3. General procedure for synthesis of Sulfoximine N-Alkylation.



1 2 3

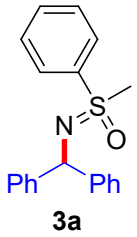
General procedure for synthesis of Sulfoximine N-Alkylation (Method A): Sulfoximine **1** (0.5 mmol), diarylmethane **2** (10 mmol, 20.0 eq) and Na_2CO_3 (26.5 mg, 0.25 mmol) were mixed in a 25 mL Schlenk tube and then I_2 (25.4 mg, 0.1 mmol) and TBHP (45.1 mg, 0.5 mmol) were added.

The reaction mixture was stirred at 60 °C for 6 h. The product was purified by column chromatography on silica gel with pentane/ethyl acetate as eluent to give the corresponding product **3**. The diasteroisomeric ratios were determined by ^{1}H NMR of the product mixtures.



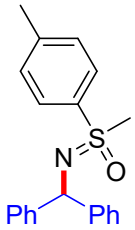
General procedure for synthesis of Sulfoximine N-Alkylation (Method B): Sulfoximine **1** (0.5 mmol), **4** (10 mmol, 20.0 eq) and Na_2CO_3 (26.5 mg, 0.25 mmol) were mixed in a 25 mL Schlenk tube and then I_2 (25.4 mg, 0.1 mmol) and TBHP (45.1 mg, 0.5 mmol) were added. The reaction mixture was stirred at 60 °C for 6 h. The product was purified by column chromatography on silica gel with pentane/ethyl acetate as eluent to give the corresponding product **5**. The diasteroisomeric ratios were determined by ^{1}H NMR of the product mixtures.

4. Characterization data of the products 3 and 5.



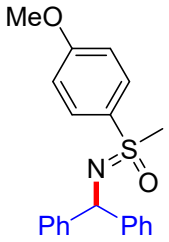
3a

(Benzhydrylimino)(methyl)(phenyl)-λ^6-sulfanone (**3a**)[2], 139.7 mg, 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 7.8 Hz, 2H), 7.49 (t, J = 7.4 Hz, 1H), 7.40 (d, J = 7.9 Hz, 4H), 7.25 – 7.08 (m, 8H), 5.34 (s, 1H), 3.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 145.2, 139.9, 132.7, 129.1, 128.5, 128.12, 128.07, 127.5, 127.4, 126.5, 126.4, 61.4, 45.4.



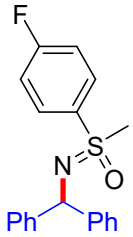
3b

(Benzhydrylimino)(methyl)(p-tolyl)-λ⁶-sulfanone (**3b**), 140.8 mg, 84% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 7.6 Hz, 2H), 7.18 (ddd, *J* = 27.7, 14.0, 7.5 Hz, 10H), 5.32 (s, 1H), 3.05 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 145.3, 143.5, 136.7, 129.7, 128.6, 128.1, 128.0, 127.5, 127.4, 126.4, 126.3, 61.4, 45.5, 21.4. HRMS (ESI): calcd. for $C_{21}H_{22}NOS$ ($[M+H]^+$) 336.1417, found 336.1407.



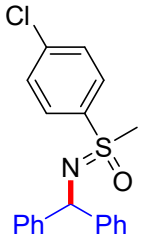
3c

(Benzhydrylimino)(4-methoxyphenyl)(methyl)-λ⁶-sulfanone (**3c**)[3], 154.5 mg, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.8 Hz, 2H), 7.39 (d, *J* = 7.2 Hz, 2H), 7.26 – 7.04 (m, 8H), 6.87 (d, *J* = 8.9 Hz, 2H), 5.32 (s, 1H), 3.79 (s, 3H), 3.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 145.9, 145.5, 131.1, 130.7, 128.1, 127.6, 127.4, 126.42, 126.40, 114.3, 61.4, 55.6, 45.8.



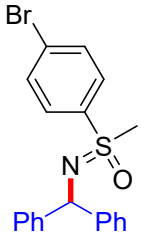
3d

(Benzhydrylimino)(4-fluorophenyl)(methyl)-λ^6-sulfanone (**3d**)[3], 140.7 mg, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 8.7, 5.3 Hz, 2H), 7.39 (d, *J* = 7.0 Hz, 2H), 7.27 – 7.11 (m, 8H), 7.05 (t, *J* = 8.5 Hz, 2H), 5.34 (s, 1H), 3.08 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3 (d, *J* = 253 Hz), 145.4 (d, *J* = 43.3 Hz), 136.0, 131.4 (d, *J* = 9 Hz), 128.2, 127.6, 127.4, 126.6, 116.3 (d, *J* = 23 Hz), 61.3, 45.8. ^{19}F NMR (471 MHz, $CDCl_3$) δ -105.73.



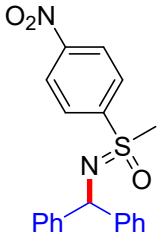
3e

(Benzhydrylimino)(4-chlorophenyl)(methyl)-λ^6-sulfanone (**3e**)[3], 150.9 mg, 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.6 Hz, 2H), 7.38 (d, *J* = 7.1 Hz, 2H), 7.34 (d, *J* = 8.6 Hz, 2H), 7.27 – 7.07 (m, 8H), 5.33 (s, 1H), 3.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 145.0, 139.2, 138.6, 130.0, 129.3, 128.2, 127.5, 127.3, 126.6, 61.3, 45.5.



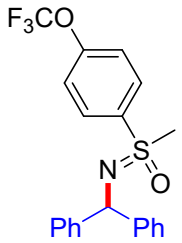
3f

(Benzhydrylimino)(4-bromophenyl)(methyl)-λ^6-sulfanone (**3f**)[3], 179.6 mg, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.7 Hz, 2H), 7.51 (d, *J* = 8.6 Hz, 2H), 7.38 (d, *J* = 7.0 Hz, 2H), 7.27 – 7.09 (m, 8H), 5.32 (s, 1H), 3.07 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 144.9, 139.2, 132.3, 130.2, 128.2, 127.9, 127.6, 127.4, 126.6, 61.4, 45.6.



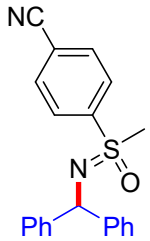
3g

(Benzhydrylimino)(methyl)(4-nitrophenyl)-λ^6-sulfanone (**3g**)[2], 146.4 mg, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.8 Hz, 2H), 7.87 (d, *J* = 8.8 Hz, 2H), 7.40 (d, *J* = 7.1 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.15 (tt, *J* = 15.7, 7.9 Hz, 6H), 5.39 (s, 1H), 3.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.1, 146.8, 145.0, 144.4, 129.8, 128.3, 127.8, 127.3, 126.9, 126.8, 124.1, 61.3, 45.5.



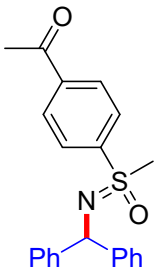
3h

(Benzhydrylimino)(methyl)(4-(trifluoromethoxy)phenyl)-λ^6-sulfanone (**3h**), 156.0 mg, 77% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.8 Hz, 2H), 7.40 (d, *J* = 7.0 Hz, 2H), 7.28 – 7.22 (m, 2H), 7.21 – 7.08 (m, 8H), 5.37 (s, 1H), 3.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 145.4, 144.8, 138.7, 130.7, 128.2(q, *J* = 250.0 Hz), 127.4, 126.7, 121.0, 61.3, 45.6. ^{19}F NMR (471 MHz, $CDCl_3$) δ -57.67. HRMS (ESI): calcd. for $C_{21}H_{19}F_3NO_2S$ ($[M+H]^+$) 406.1083, found 406.1077.



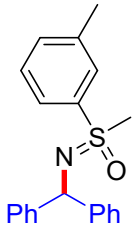
3i

4-(N-benzhydryl-S-methylsulfonimidoyl)benzonitrile (**3i**)[3], 138.4 mg, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.1 Hz, 2H), 7.63 (d, *J* = 8.1 Hz, 2H), 7.39 (d, *J* = 7.6 Hz, 2H), 7.28 (d, *J* = 7.5 Hz, 2H), 7.20 – 7.10 (m, 6H), 5.36 (s, 1H), 3.13 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 144.4, 132.8, 129.1, 128.3, 127.7, 127.3, 126.9, 126.8, 117.5, 116.2, 61.3, 45.4.



3j

(4-Acetylphenyl)(benzhydrylimino)(methyl)-λ^6-sulfanone (**3j**)[3], 132.5 mg, 73% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.5 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 7.1 Hz, 2H), 7.27 – 7.07 (m, 8H), 5.35 (s, 1H), 3.12 (s, 3H), 2.62 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 145.5, 144.9, 144.4, 140.1, 128.9, 128.3, 128.2, 127.6, 127.4, 126.70, 126.67, 61.4, 45.4, 27.0.

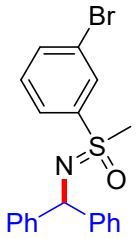


3k

(Benzhydrylimino)(methyl)(m-tolyl)-λ^6-sulfanone (**3k**)[2], 140.8 mg, 84% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 6.3 Hz, 1H), 7.52 (s, 1H), 7.40 (d, *J* = 7.1 Hz, 2H), 7.35 – 7.26 (m, 3H), 7.24 – 7.11 (m, 7H), 5.33 (s, 1H), 3.09 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 145.4, 139.8, 139.3, 133.6, 129.2, 129.0, 128.2, 128.1, 127.7, 127.5, 126.53, 126.52, 125.7, 61.4, 45.6, 21.3.

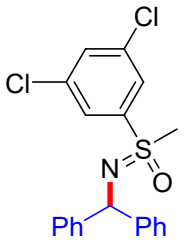
3l

(Benzhydrylimino)(3-chlorophenyl)(methyl)-λ^6-sulfanone (**3l**)[3], 147.4 mg, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.41 (dd, *J* = 15.8, 7.9 Hz, 3H), 7.28 (dd, *J* = 10.1, 7.6 Hz, 2H), 7.22 – 7.04 (m, 7H), 5.35 (s, 1H), 3.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 144.7, 142.0, 135.2, 132.7, 130.3, 128.7, 128.2, 127.6, 127.3, 126.7, 126.6, 126.5, 61.3, 45.5.



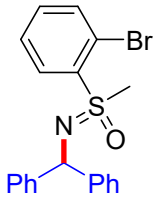
3m

(Benzhydrylimino)(3-bromophenyl)(methyl)-λ^6-sulfanone (**3m**), 167.6 mg, 84% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.63 (dd, *J* = 18.4, 8.0 Hz, 2H), 7.40 (d, *J* = 7.3 Hz, 2H), 7.31 – 7.22 (m, 4H), 7.21 – 7.07 (m, 6H), 5.35 (s, 1H), 3.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 144.7, 142.2, 135.7, 131.6, 130.6, 128.3, 128.2, 127.7, 127.4, 127.0, 126.8, 126.7, 123.1, 61.4, 45.6. HRMS (ESI): calcd. for $C_{20}H_{19}BrNOS$ ($[M+H]^+$) 400.0365, found 400.0358.



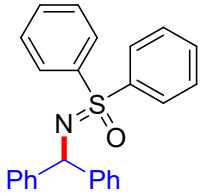
3n

(Benzhydrylimino)(3,5-dichlorophenyl)(methyl)-λ^6-sulfanone (**3n**)[3], 159.5 mg, 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.9 Hz, 2H), 7.40 (d, *J* = 9.4 Hz, 3H), 7.27 (t, *J* = 7.7 Hz, 2H), 7.21 – 7.08 (m, 6H), 5.38 (s, 1H), 3.08 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 144.2, 143.7, 135.9, 132.5, 128.24, 128.20, 127.8, 127.3, 127.0, 126.9, 126.7, 61.3, 45.6.



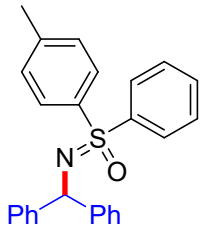
3o

(Benzhydrylimino)(2-bromophenyl)(methyl)-λ^6-sulfanone (**3o**)[3], 175.6 mg, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.8 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.41 – 7.30 (m, 3H), 7.27 – 7.20 (m, 3H), 7.20 – 7.13 (m, 3H), 7.08 (td, *J* = 14.5, 13.3, 8.0 Hz, 3H), 5.33 (s, 1H), 3.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 143.9, 139.5, 135.3, 133.6, 132.4, 128.1, 127.9, 127.8, 127.5, 126.54, 126.48, 120.9, 62.2, 43.5.



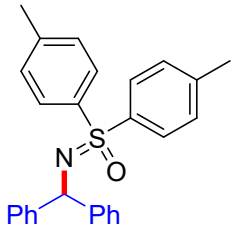
3p

(Benzhydrylimino)diphenyl-λ^6-sulfanone (**3p**)[3], 122.6 mg, 64% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.5 Hz, 4H), 7.45 – 7.33 (m, 10H), 7.24 (t, *J* = 7.6 Hz, 4H), 7.15 (t, *J* = 7.3 Hz, 2H), 5.41 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 141.1, 132.4, 129.0, 128.8, 128.2, 127.5, 126.5, 61.8.



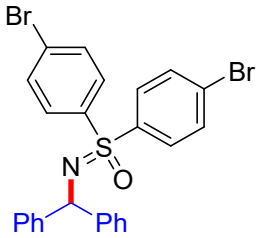
3q

(Benzhydrylimino)(phenyl)(p-tolyl)-λ^6-sulfanone (**3q**), 180.7 mg, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.1 Hz, 2H), 7.80 (d, *J* = 8.4 Hz, 2H), 7.44 – 7.36 (m, 7H), 7.25 (d, *J* = 5.0 Hz, 4H), 7.22 – 7.13 (m, 4H), 5.40 (s, 1H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 146.0, 143.3, 141.4, 138.0, 132.3, 129.8, 129.0, 128.9, 128.7, 128.6, 128.2, 127.57, 127.56, 126.7, 126.5, 61.9, 21.6. HRMS (ESI): calcd. for $C_{26}H_{24}NOS$ ($[M+H]^+$) 398.1573, found 398.1574.



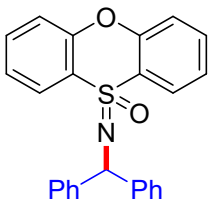
3r

(Benzhydrylimino)di-*p*-tolyl-λ^6-sulfanone (**3r**)[3], 160.4 mg, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.3 Hz, 4H), 7.39 (d, *J* = 7.1 Hz, 4H), 7.24 (d, *J* = 7.7 Hz, 4H), 7.18 (dd, *J* = 7.6, 5.3 Hz, 6H), 5.38 (s, 1H), 2.34 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.2, 143.1, 138.3, 129.8, 128.8, 128.6, 128.2, 127.6, 126.7, 126.5, 61.9, 21.6.



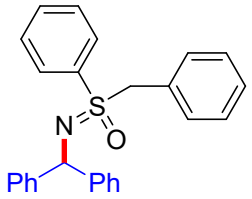
3s

(Benzhydrylimino)bis(4-bromophenyl)-λ^6-sulfanone (**3s**), 215.6 mg, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.6 Hz, 4H), 7.53 (d, *J* = 8.6 Hz, 4H), 7.36 (d, *J* = 7.2 Hz, 4H), 7.25 (d, *J* = 8.0 Hz, 4H), 7.21 – 7.15 (m, 2H), 5.40 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 140.0, 132.5, 130.3, 128.4, 128.0, 127.5, 126.8, 61.8. HRMS (ESI): calcd. for $C_{25}H_{20}Br_2NOS$ ($[M+H]^+$) 539.9627, found 539.9618.



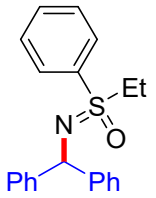
3t

10-(Benzhydrylimino)-10*H*-10λ^4-phenoxathiine 10-oxide (**3t**), 158.8 mg, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 2H), 7.45 (t, *J* = 7.9 Hz, 2H), 7.21 (d, *J* = 10.3 Hz, 5H), 7.10 (dq, *J* = 15.2, 6.9 Hz, 9H), 5.31 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 144.4, 133.4, 128.1, 127.4, 126.6, 124.9, 124.6, 124.5, 118.5, 62.9. HRMS (ESI): calcd. for $C_{25}H_{20}NO_2S$ ([M+H]$^+$) 398.1209, found 398.1201.



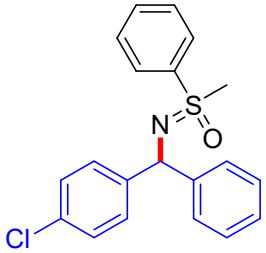
3u

(Benzhydrylimino)(benzyl)(phenyl)-λ^6-sulfanone (**3u**), 162.8 mg, 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (dd, *J* = 14.8, 7.5 Hz, 5H), 7.28 – 7.09 (m, 13H), 6.99 (d, *J* = 6.9 Hz, 2H), 5.42 (s, 1H), 4.38 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.2, 145.6, 137.4, 132.8, 131.3, 129.8, 129.0, 128.7, 128.5, 128.2, 128.1, 127.60, 127.56, 126.52, 126.47, 63.7, 61.5. HRMS (ESI): calcd. for $C_{26}H_{24}NOS$ ([M+H]$^+$) 398.1573, found 398.1564.



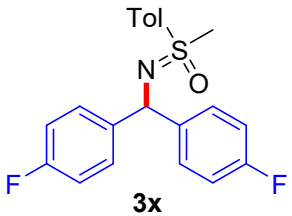
3v

(Benzhydrylimino)(ethyl)(phenyl)-λ^6-sulfanone (**3v**)[3], 137.4 mg, 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.7 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.43 – 7.33 (m, 4H), 7.26 – 7.06 (m, 8H), 5.36 (s, 1H), 3.21 (q, *J* = 20.3, 7.3 Hz, 2H), 1.19 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.2, 145.5, 138.0, 132.6, 129.4, 128.9, 128.07, 128.05, 127.6, 127.4, 126.38, 126.36, 61.1, 51.3, 7.7.



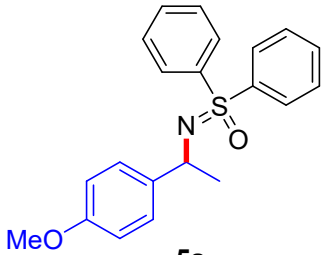
3w

((4-Chlorophenyl)(phenyl)methyl)imino)(methyl)(phenyl)-λ^6-sulfanone (**3w**)[2], 124.2 mg, 70% yield, dr = 1:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 – 7.72 (m, 4H), 7.52 (dt, *J* = 9.4, 7.3 Hz, 2H), 7.44 – 7.35 (m, 6H), 7.32 (d, *J* = 8.3 Hz, 2H), 7.26 – 7.12 (m, 14H), 5.32 (s, 1H), 5.27 (s, 1H), 3.10 (s, 3H), 3.07 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.4, 144.8, 144.5, 143.9, 140.0, 139.7, 132.9, 132.8, 132.2, 132.1, 129.2, 129.0, 128.9, 128.60, 128.4, 128.30, 128.26, 128.24, 128.21, 127.5, 127.4, 126.8, 126.7, 60.9, 60.8, 45.6, 45.5.



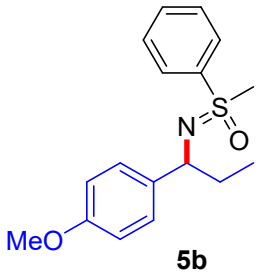
3x

((Bis(4-fluorophenyl)methyl)imino)(methyl)(p-tolyl)-λ^6-sulfanone (**3x**), 146.6 mg, 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.9 Hz, 2H), 7.32 (dd, *J* = 8.4, 5.5 Hz, 2H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.17 (dd, *J* = 8.4, 5.5 Hz, 2H), 6.91 (dt, *J* = 21.9, 8.6 Hz, 4H), 5.27 (s, 1H), 3.09 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6 (q, *J* = 243 Hz, 3.0 Hz), 143.8, 141.4 (d, *J* = 57.3 Hz), 136.7, 129.8, 129.0 (d, *J* = 8.3 Hz), 128.7 (d, *J* = 8.1 Hz), 114.9 (d, *J* = 21.1 Hz), 114.8 (d, *J* = 21.1 Hz), 60.1, 45.6, 21.5. ^{19}F NMR (471 MHz, $CDCl_3$) δ -116.58, -116.78. HRMS (ESI): calcd. for $C_{21}H_{20}F_2NOS$ ($[M+H]^+$) 372.1228, found 372.1223.



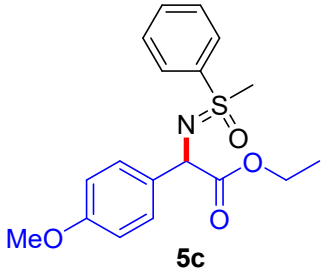
5a

((1-(4-Methoxyphenyl)ethyl)imino)diphenyl-λ^6-sulfanone (**5a**)[4], 87.8 mg, 50% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 8.3, 1.5 Hz, 2H), 7.83 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.52 – 7.42 (m, 4H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 4.36 (q, *J* = 6.6 Hz, 1H), 3.80 (s, 3H), 1.53 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.2, 141.6, 141.0, 139.9, 132.4, 132.3, 129.13, 129.05, 128.6, 127.3, 113.6, 55.4, 53.8, 28.3.



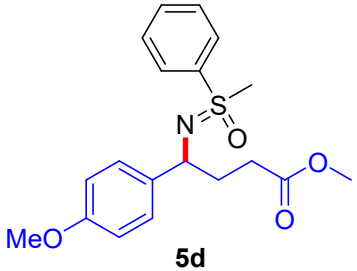
5b

((1-(4-Methoxyphenyl)propyl)imino)(methyl)(phenyl)-λ⁶-sulfanone (**5b**), 90.9 mg, 60% yield, dr = 1:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 6.9 Hz, 2H), 7.65 – 7.54 (m, 5H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.7 Hz, 2H), 7.28 (s, 2H), 7.05 (d, *J* = 8.7 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 6.71 (d, *J* = 8.6 Hz, 2H), 3.98 (t, *J* = 6.9 Hz, 1H), 3.90 (t, *J* = 6.9 Hz, 1H), 3.78 (s, 3H), 3.75 (s, 3H), 3.08 (s, 3H), 2.96 (s, 3H), 1.87 – 1.67 (m, 4H), 0.82 (td, *J* = 7.3, 2.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 158.0, 140.4, 140.2, 138.6, 137.6, 132.8, 132.4, 129.2, 128.9, 128.7, 128.3, 127.9, 127.7, 113.5, 113.3, 59.8, 59.7, 55.2, 55.1, 45.6, 44.9, 33.9, 33.8, 11.2, 11.0. HRMS (ESI): calcd. for $C_{17}H_{22}NO_2S$ ($[M+H]^+$) 304.1366, found 304.1358.



5c

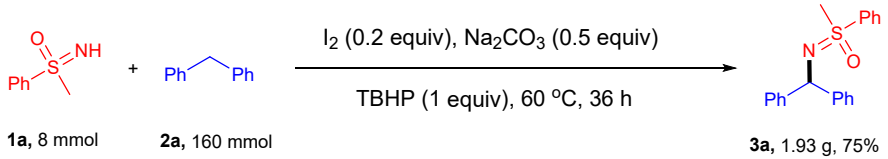
Ethyl 2-(4-methoxyphenyl)-2-((methyl(oxo)(phenyl)-λ⁶-sulfanylidene)amino)acetate (**5c**)[1], 121.5 mg, 70% yield, dr = 1:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.1 Hz, 2H), 7.73 (d, *J* = 7.1 Hz, 2H), 7.63 (d, *J* = 7.2 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 2H), 7.52 (d, *J* = 7.4 Hz, 1H), 7.41 (dt, *J* = 7.5, 3.4 Hz, 4H), 7.27 (d, *J* = 8.7 Hz, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 6.76 (d, *J* = 8.7 Hz, 2H), 4.80 (s, 1H), 4.74 (s, 1H), 4.13 (q, *J* = 11.8, 7.1 Hz, 2H), 4.01 (q, *J* = 7.1 Hz, 2H), 3.76 (s, 3H), 3.75 (s, 3H), 3.18 (s, 3H), 3.15 (s, 3H), 1.18 (t, *J* = 7.1 Hz, 3H), 1.09 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 172.4, 158.9, 158.8, 139.6, 139.2, 133.1, 132.8, 132.2, 131.4, 129.3, 129.1, 128.5, 128.3, 128.2, 113.6, 113.5, 60.9, 60.8, 59.9, 59.7, 55.10, 55.09, 45.33, 45.29, 13.94, 13.92.



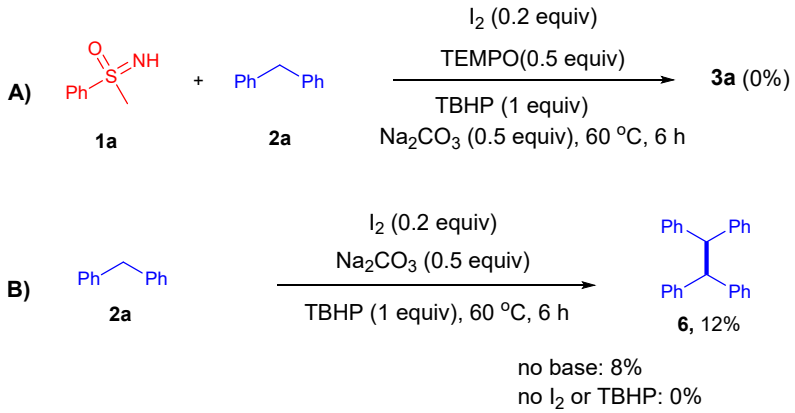
5d

Methyl 4-(4-methoxyphenyl)-4-((methyl(oxo)(phenyl)-λ^6-sulfanylidene)amino)butanoate (**5d**), 101.1 mg, 56% yield, dr = 1:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 6.9 Hz, 2H), 7.63 (d, *J* = 7.6 Hz, 3H), 7.56 (t, *J* = 7.3 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.8 Hz, 2H), 7.29 (s, 2H), 7.08 (d, *J* = 8.7 Hz, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 6.72 (d, *J* = 8.7 Hz, 2H), 4.15 (t, *J* = 6.7 Hz, 1H), 4.06 (t, *J* = 6.7 Hz, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 3.61 (s, 3H), 3.58 (s, 3H), 3.08 (s, 3H), 2.96 (s, 3H), 2.43 – 2.31 (m, 4H), 2.10 – 1.99 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 174.2, 158.5, 158.3, 140.3, 140.1, 137.8, 137.1, 132.8, 132.5, 129.3, 128.9, 128.6, 128.2, 127.8, 127.7, 113.7, 113.5, 57.2, 57.1, 55.3, 55.2, 51.40, 51.38, 45.5, 44.8, 35.9, 35.8, 31.1, 31.0. HRMS (ESI): calcd. for $C_{19}H_{24}NO_4S$ ($[M+H]^+$) 362.1421, found 362.1413.

5. Gram scale reaction and Mechanistic studies



Sulfoximine **1a** (8 mmol, 1.24 g), diphenylmethane **2a** (160 mmol, 29.92 g) and Na_2CO_3 (4 mmol, 0.424 g) were mixed in a 100 mL round bottom flask and then I_2 (1.6 mmol, 0.406 g) and TBHP (8 mmol, 0.721 g) were added. The reaction mixture was stirred at 60 °C to reflux 36 h. The product was purified by column chromatography on silica gel with pentane/ethyl acetate as eluent to give the product **3a**, 1.93g, 75%.



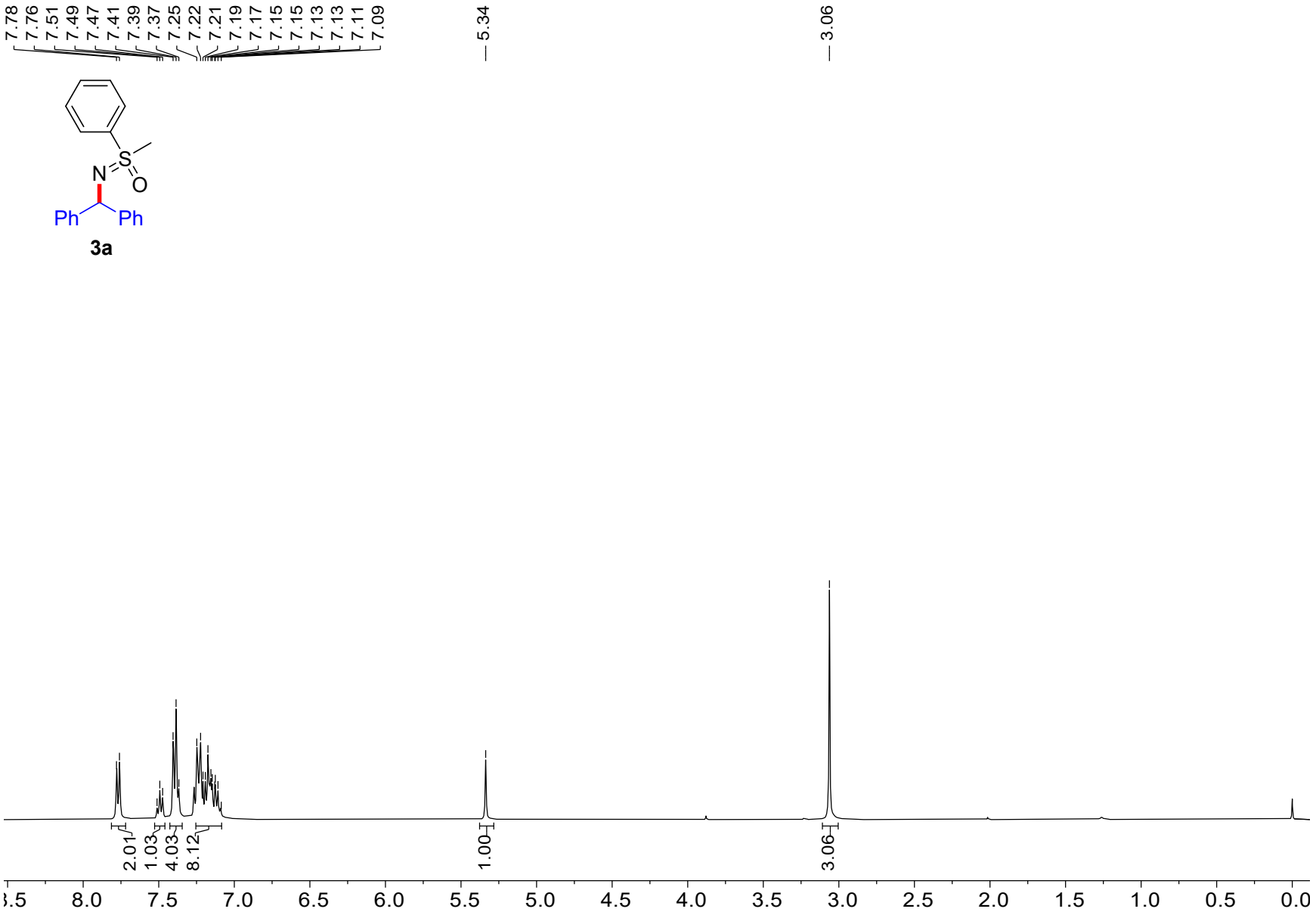
Control experiments A.

Sulfoximines **1a** (77.52 mg, 0.5 mmol), diphenylmethane **2a** (1.683 g, 10 mmol), TEMPO (39.06 mg, 0.25 mmol) and Na_2CO_3 (26.5 mg, 0.25 mmol) were mixed in a 20 mL Schlenk tube and then I_2 (25.4 mg, 0.1 mmol) and TBHP (45.1 mg, 0.5 mmol) were added. The reaction mixture was stirred at 60 °C for 6 h. No product **3a** was formed.

Control experiments B.

Diphenylmethane **2a** (1.683 g, 10 mmol) and Na_2CO_3 (26.5 mg, 0.25 mmol) were mixed in a 20 mL Schlenk tube and then I_2 (25.4 mg, 0.1 mmol) and TBHP (45.1 mg, 0.5 mmol) were added. The reaction mixture was stirred at 60 ^oC for 6 h. Then, the reaction liquid by GC-MS identification analysis to give the formation of dimer-adduct **6** in 12% yield.

6. Copies of NMR spectra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7.22
7.21
7.19
7.17
7.15
7.15
7.13
7.13
7.11
7.09
5.34
3.06
N
S
O
Ph
Ph
2.01
1.03
4.03
8.12
1.00
3.06
8.0
7.5
7.0
6.5
6.0
5.5
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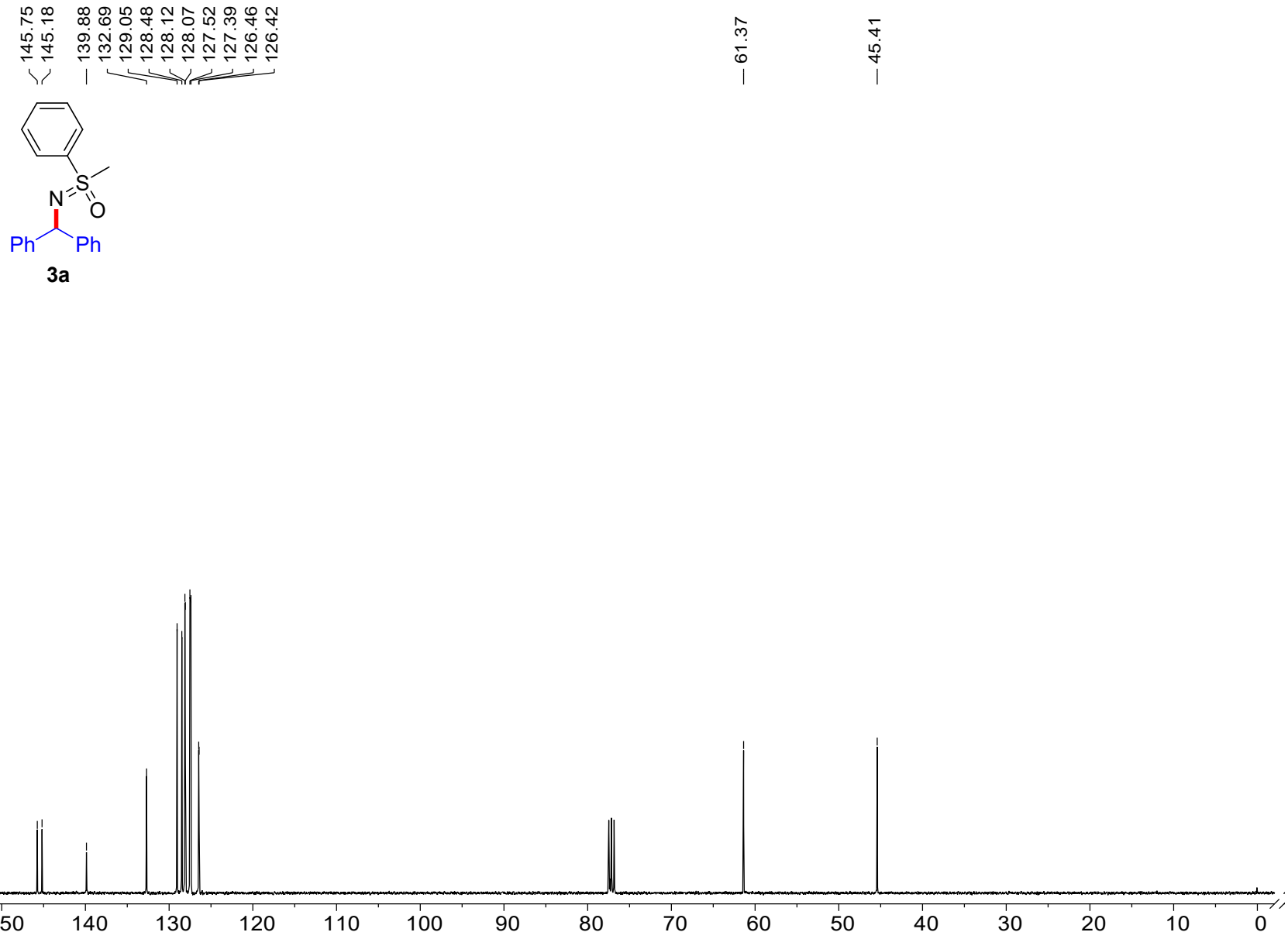
0.0

3a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127.39
126.46
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45.41
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N
O
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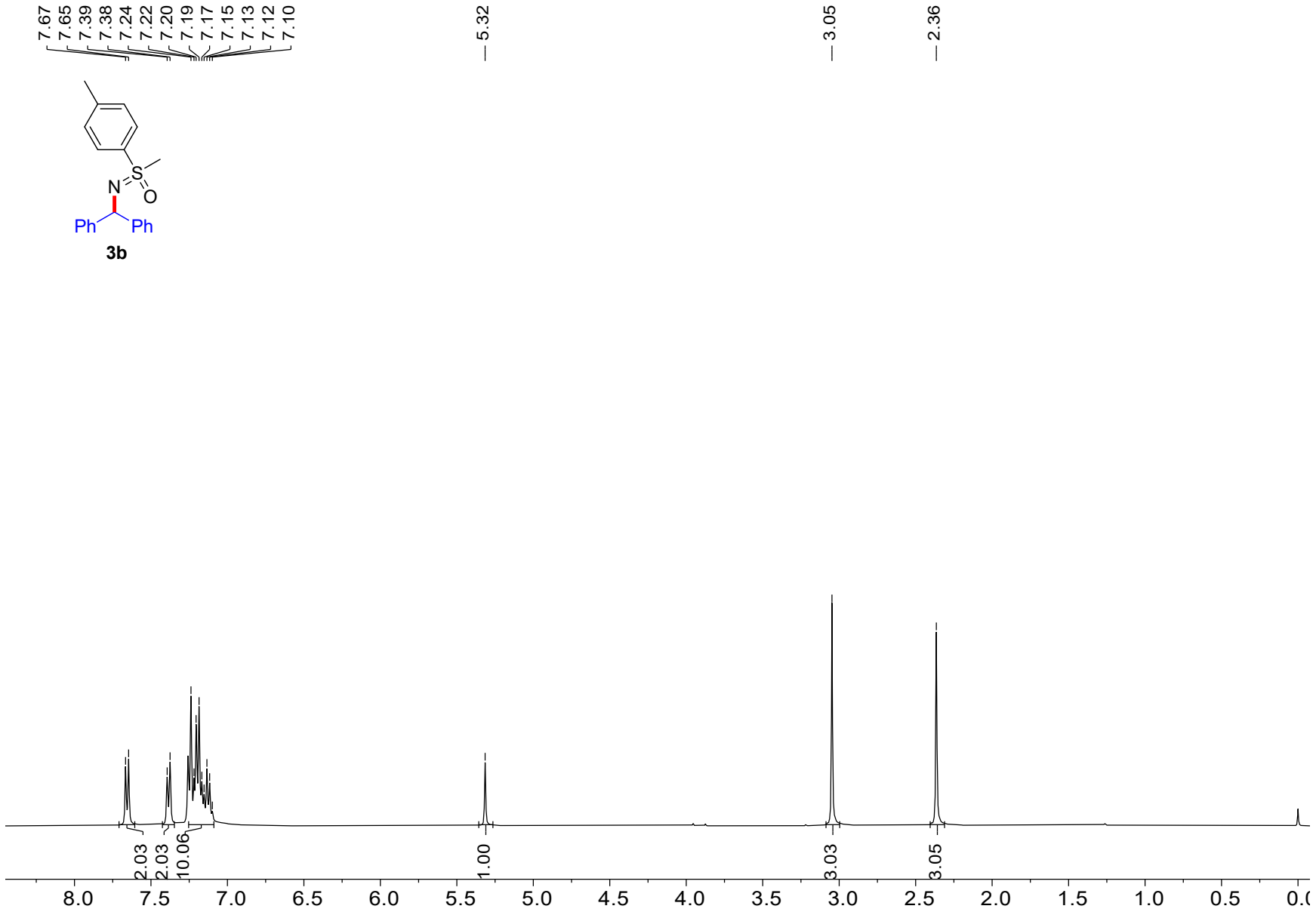
20
10
0

3a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5.32
3.05
2.36
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Ph
Ph
3b
2.03
2.03
10.06
1.00
3.03
3.05
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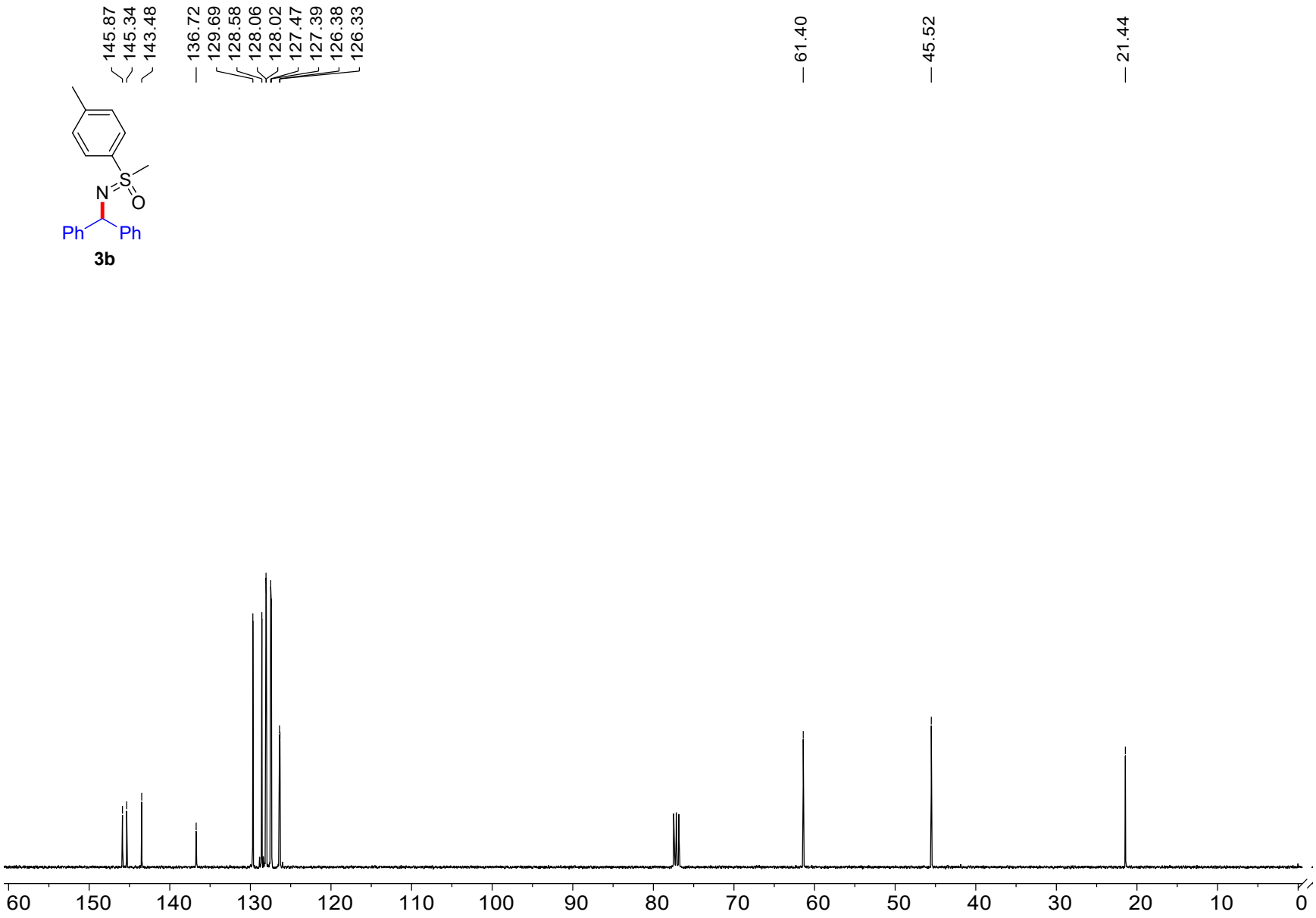
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45.52
21.44
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S
O
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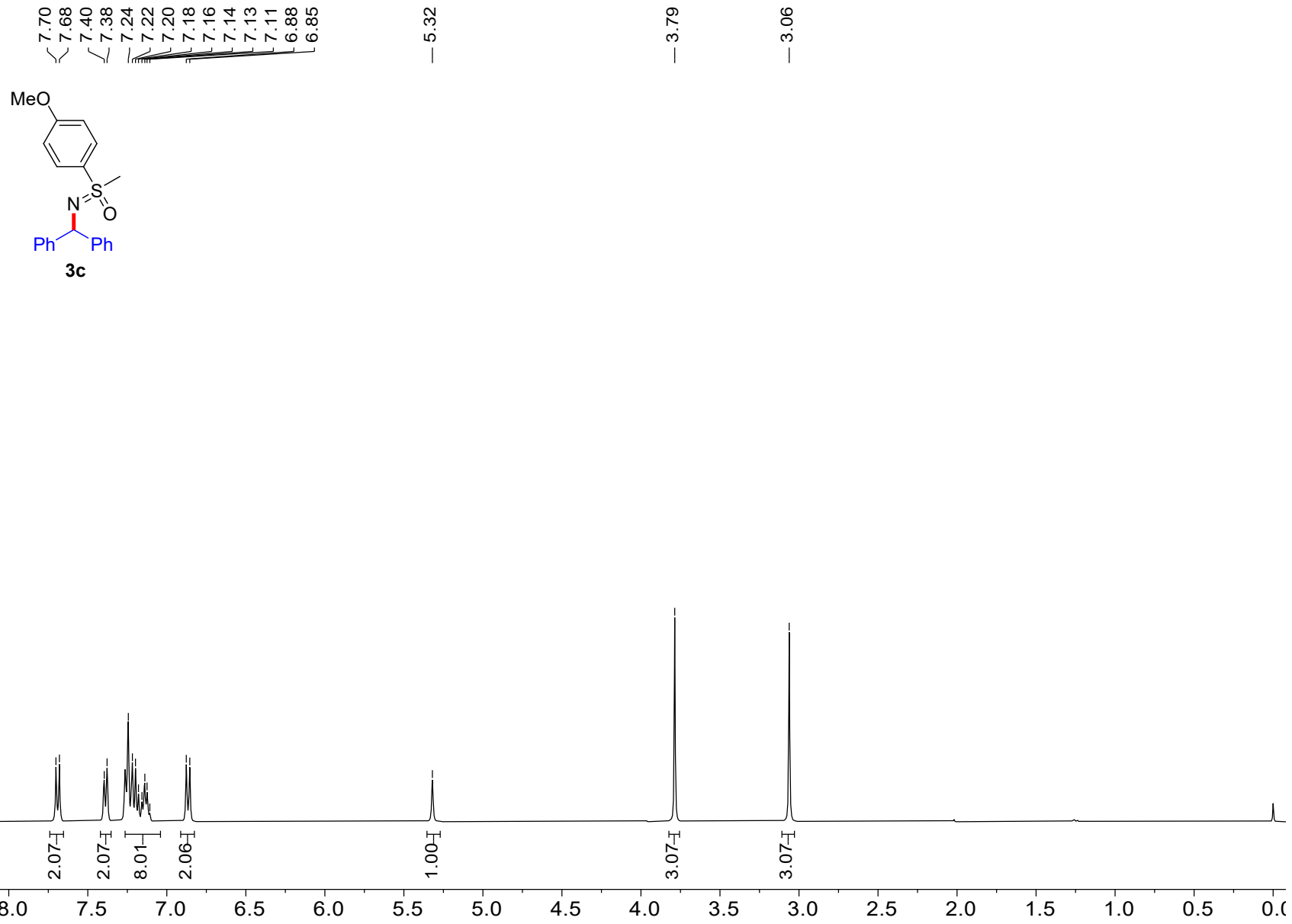
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5.32
3.79
3.06
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S
N
O
Ph
Ph
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2.07
8.01
2.06
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3.07
3.07
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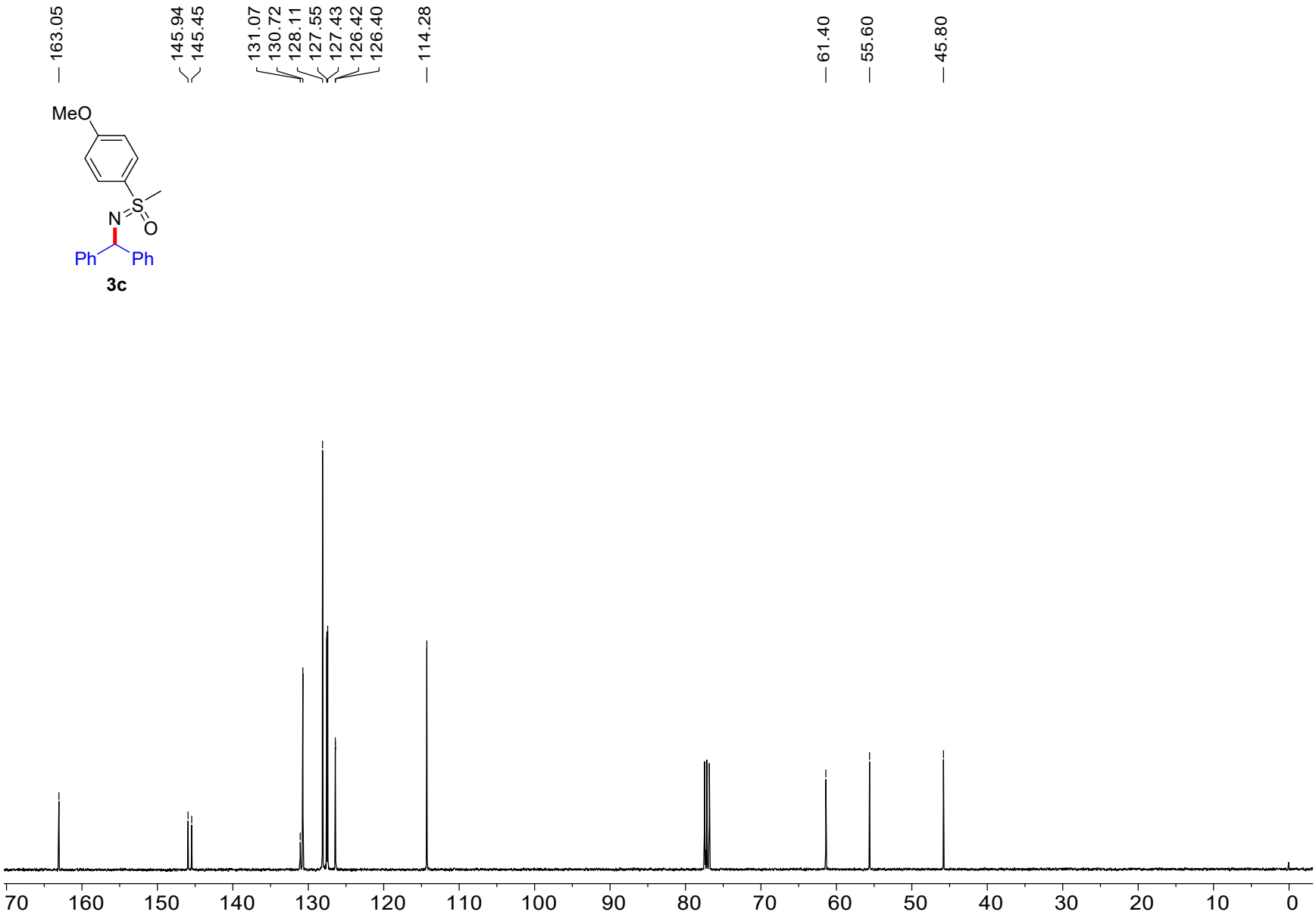
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S
N
O
Ph
Ph
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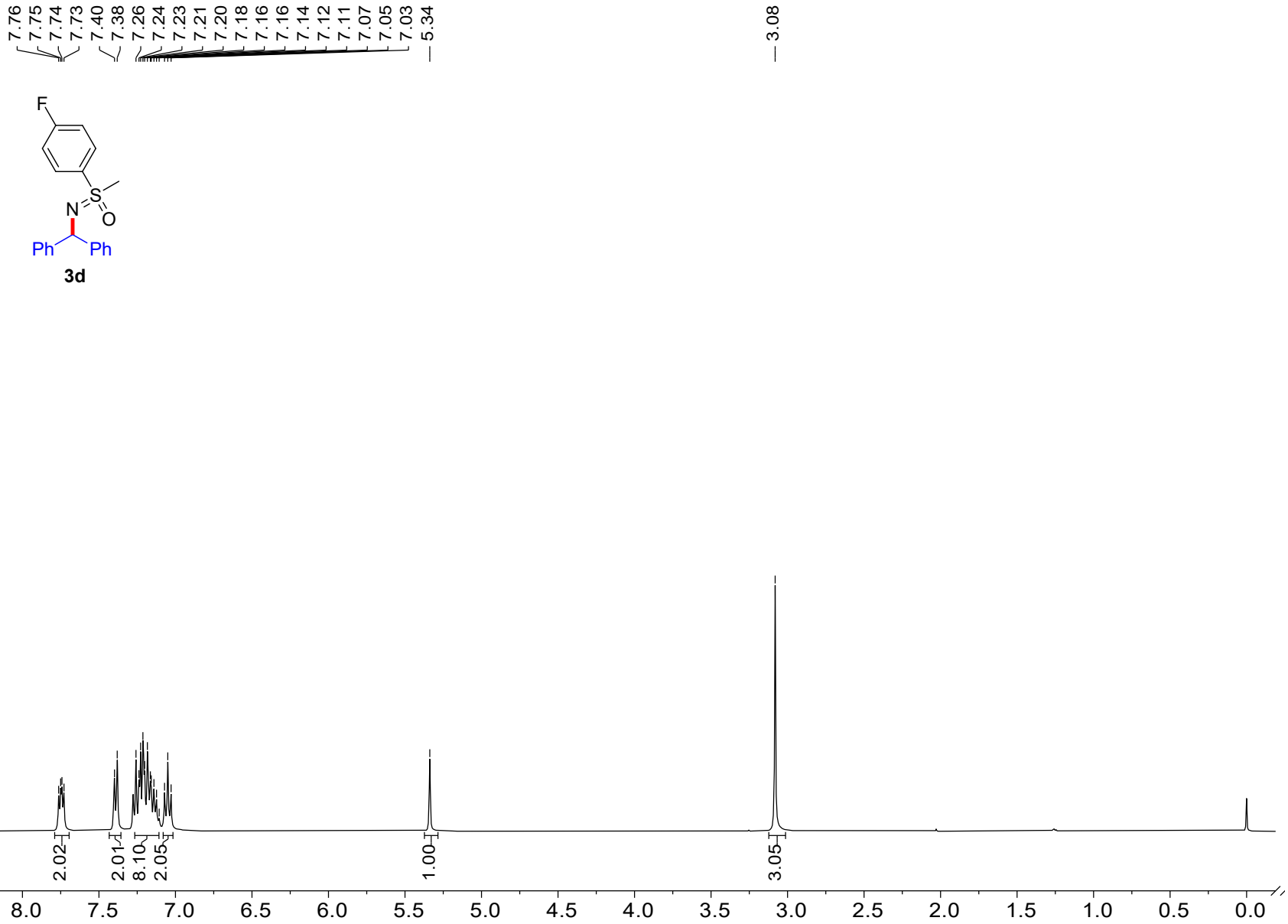
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7.16
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7.03
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O
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Ph
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6.0
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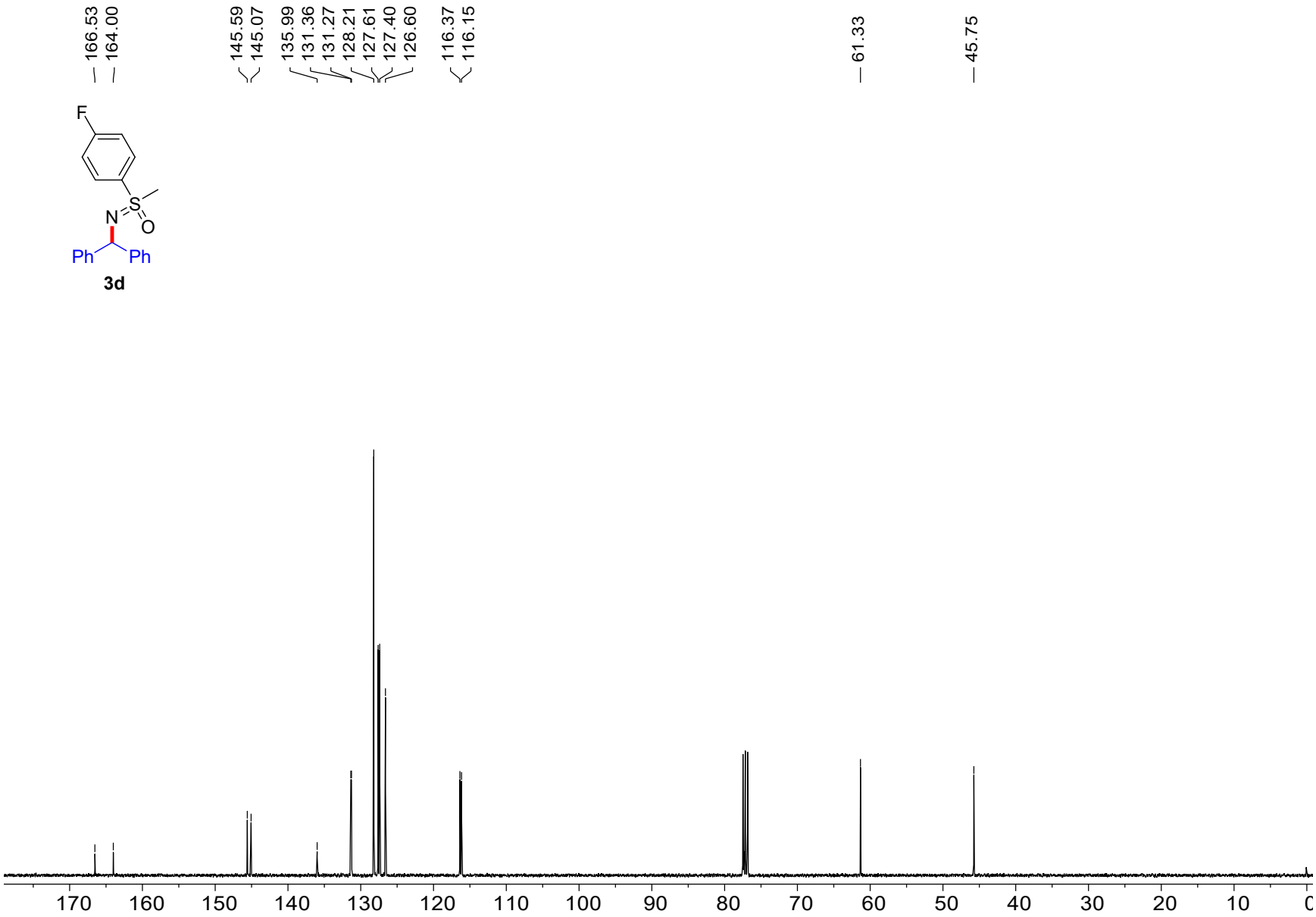
3d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S
N
O
Ph
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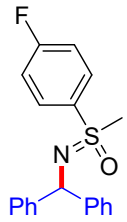
3d


F
S
N
O
Ph
Ph

3d

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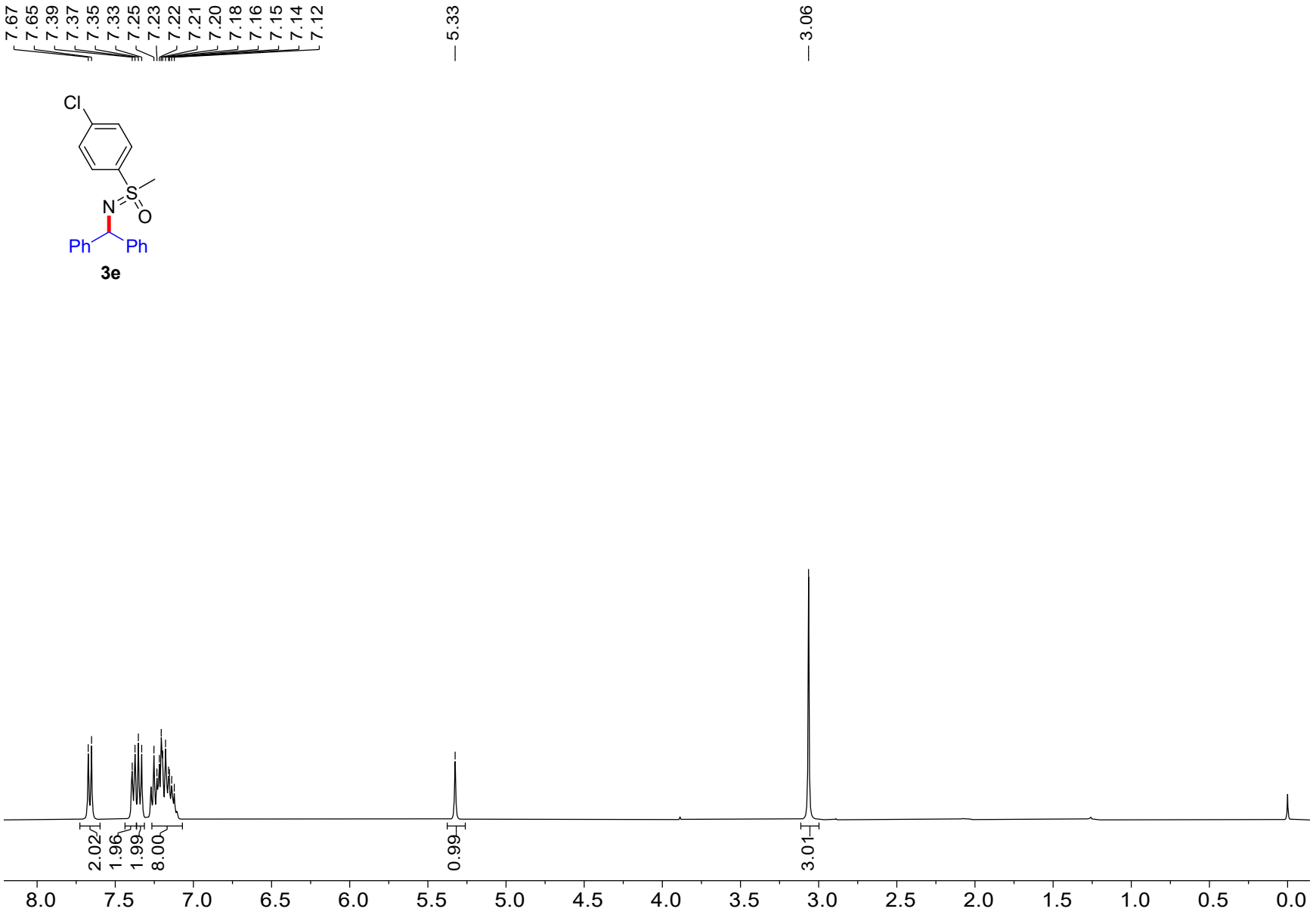
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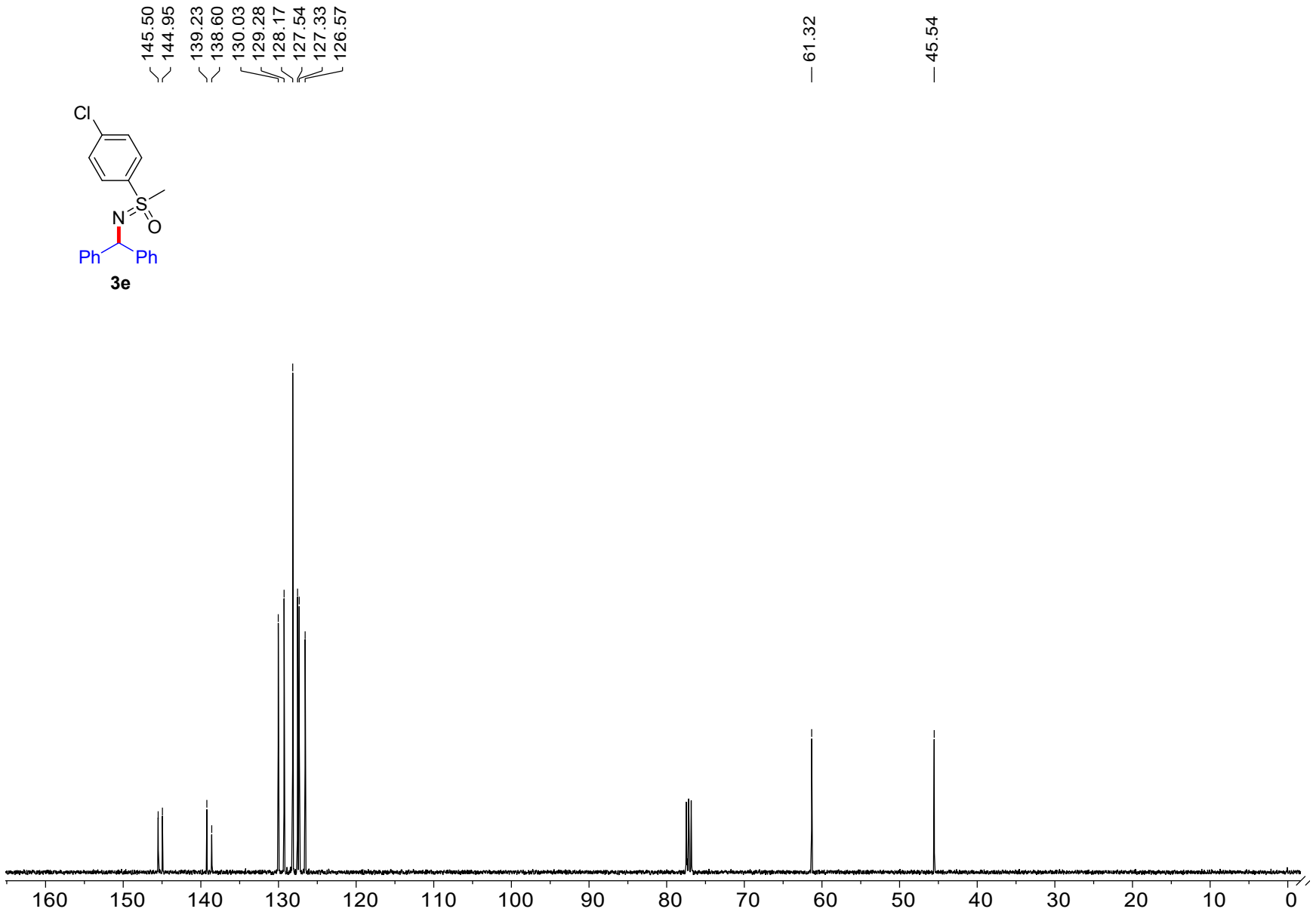
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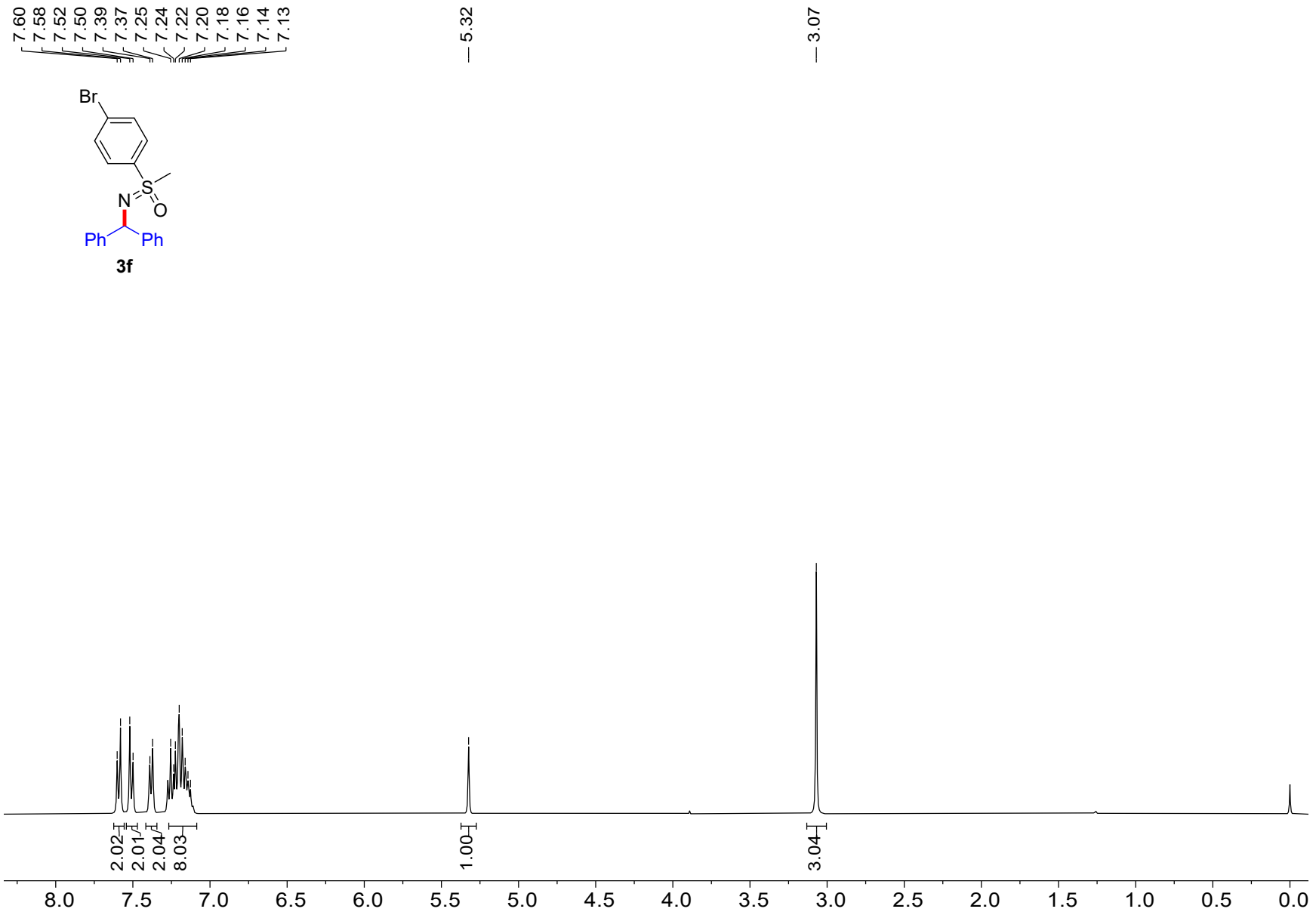
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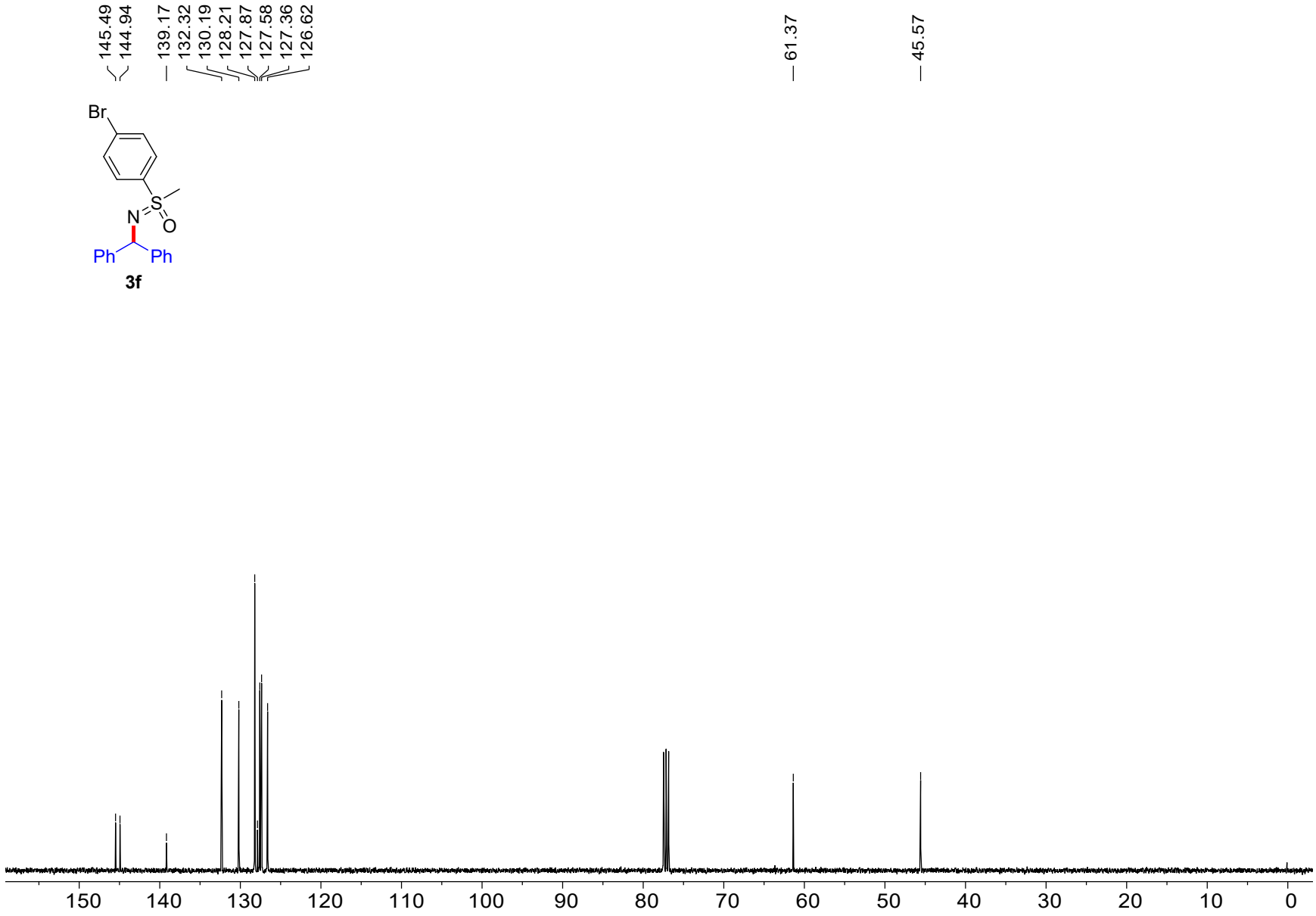
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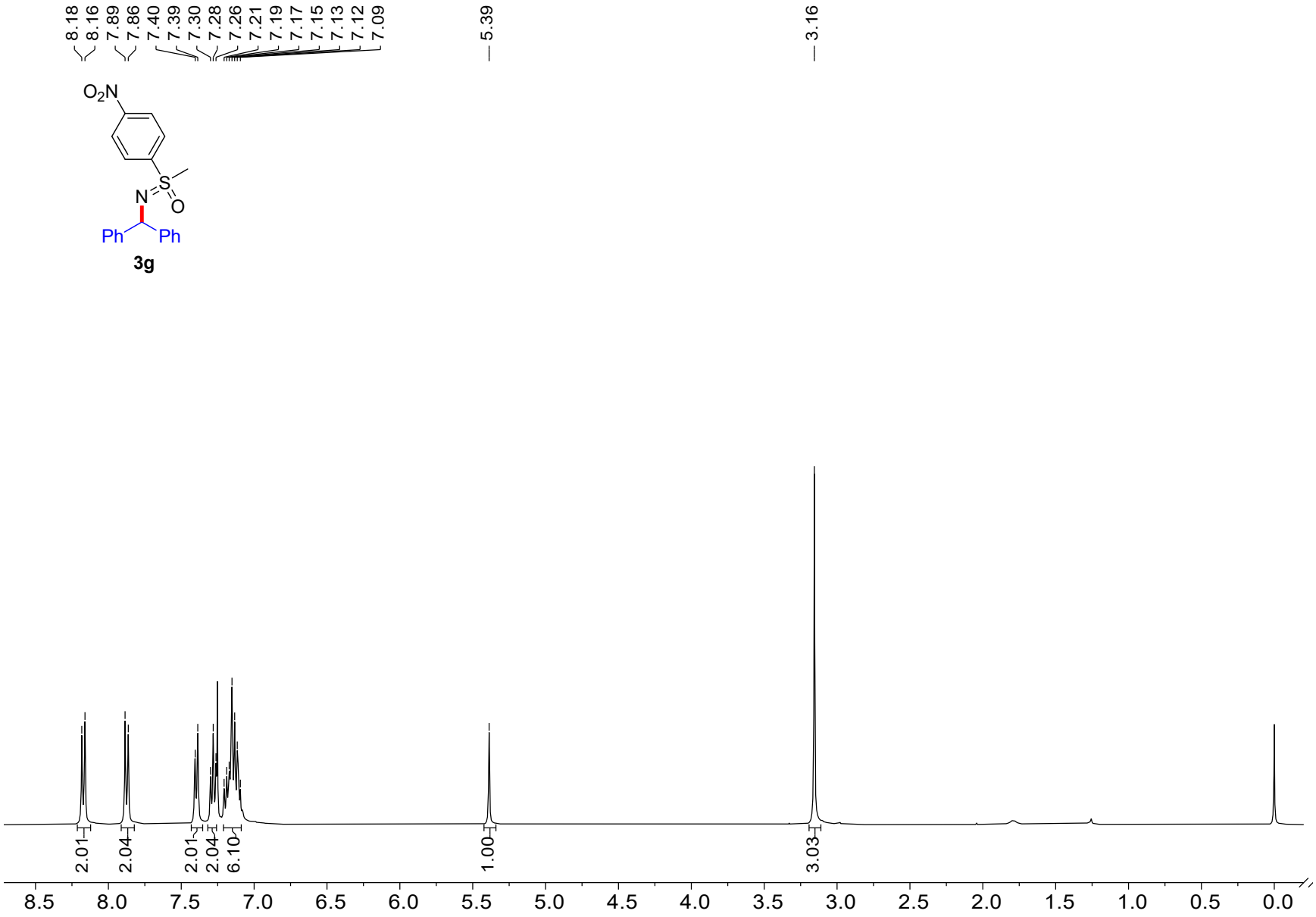
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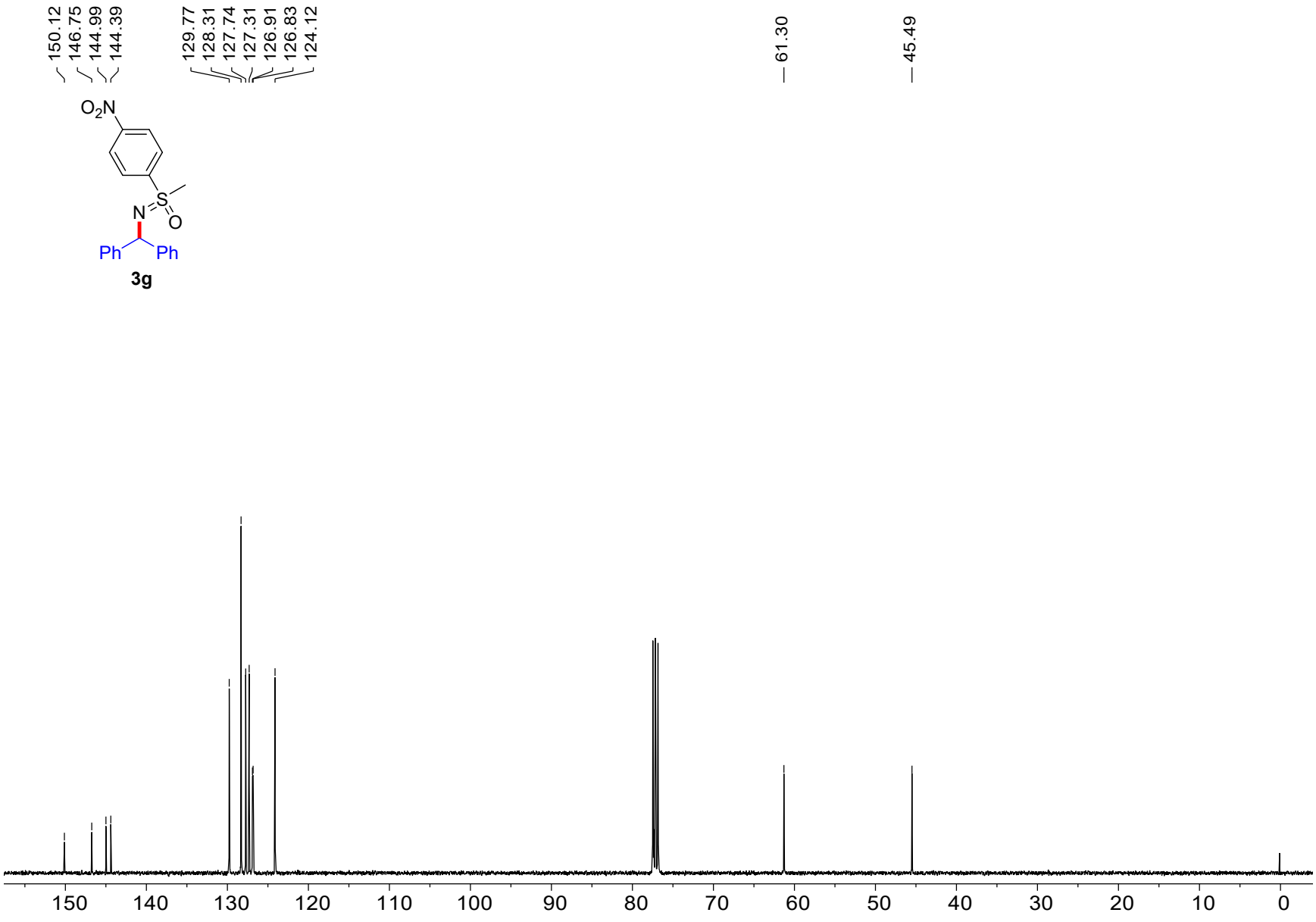
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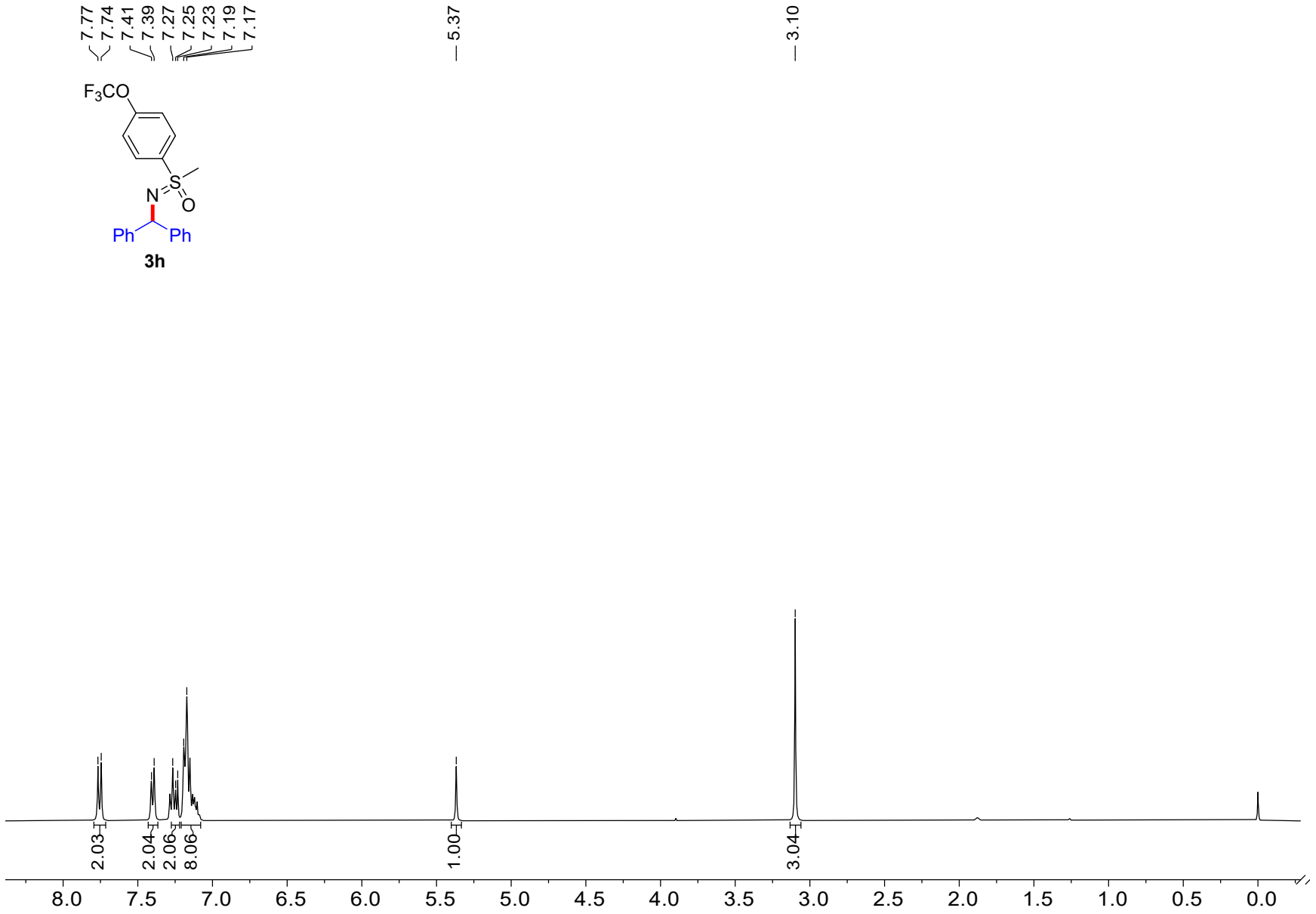
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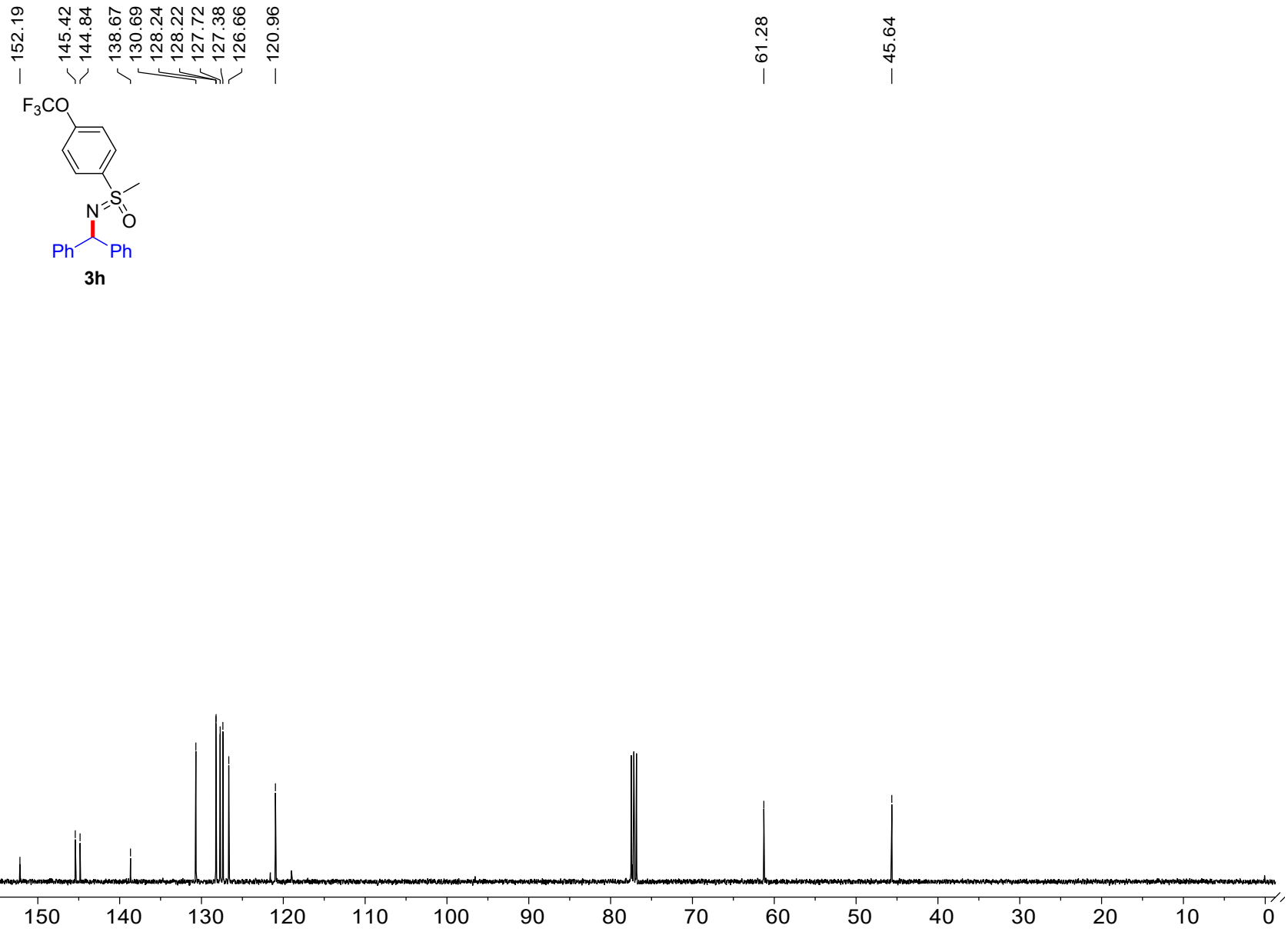
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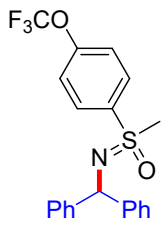
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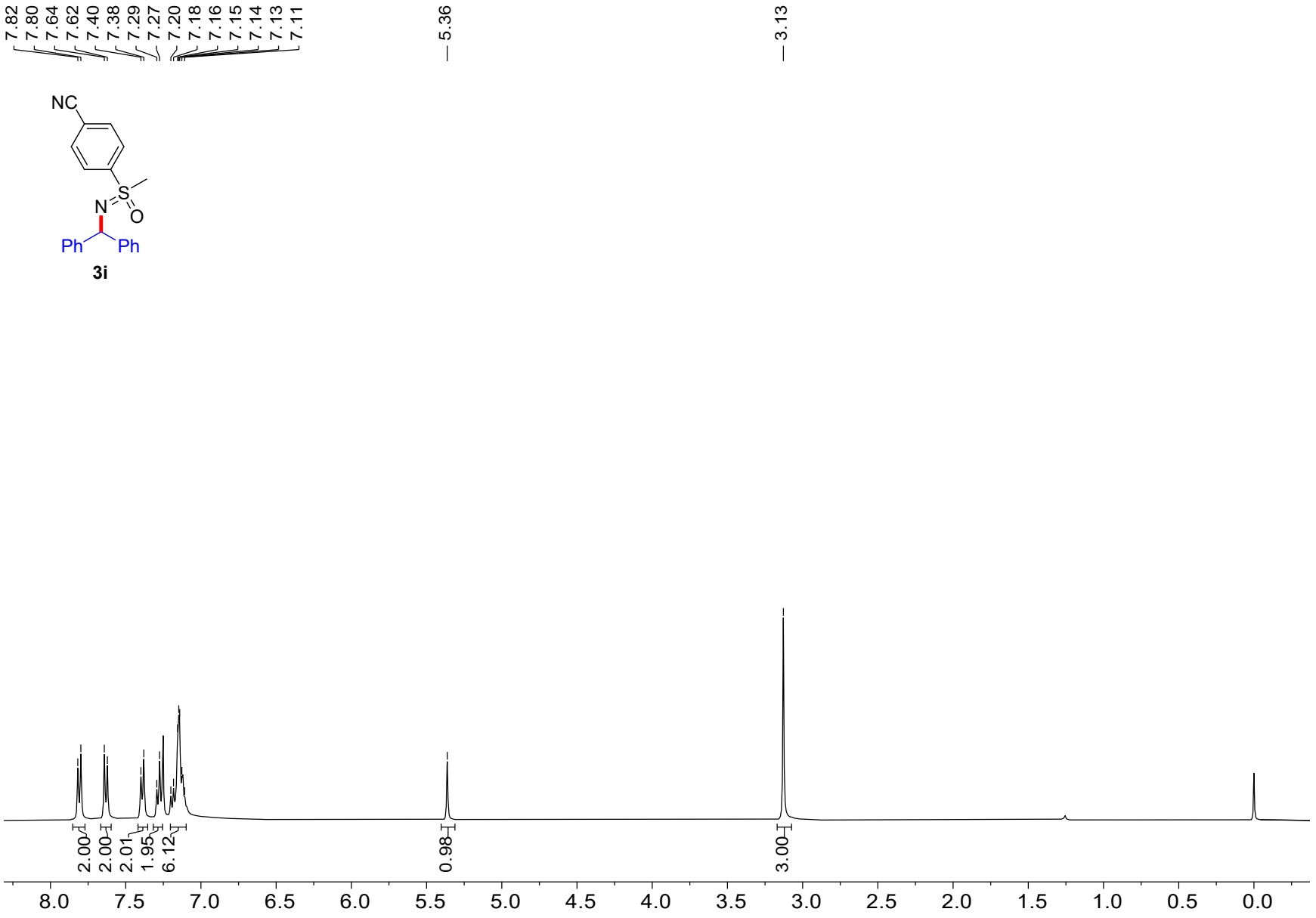
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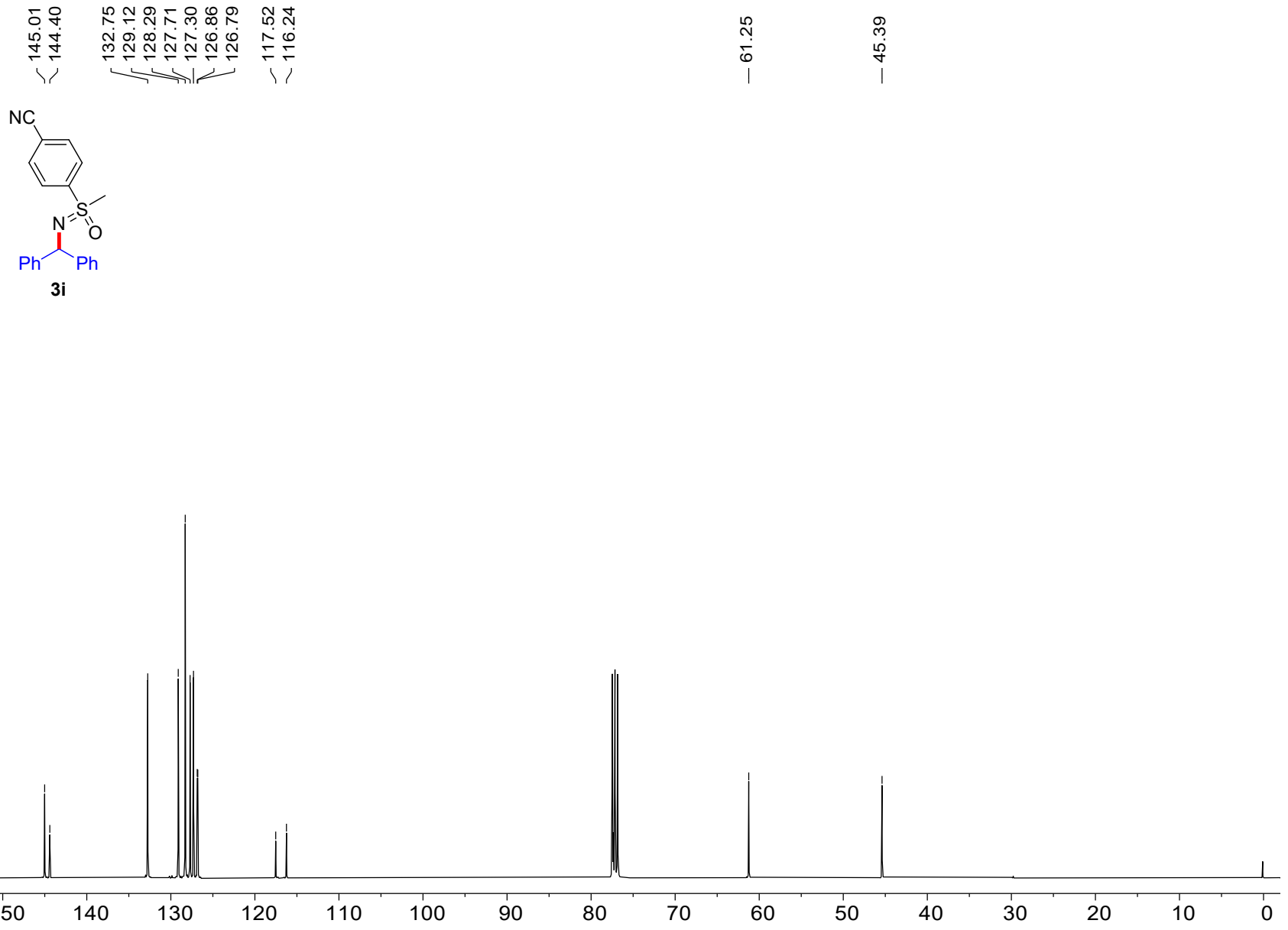
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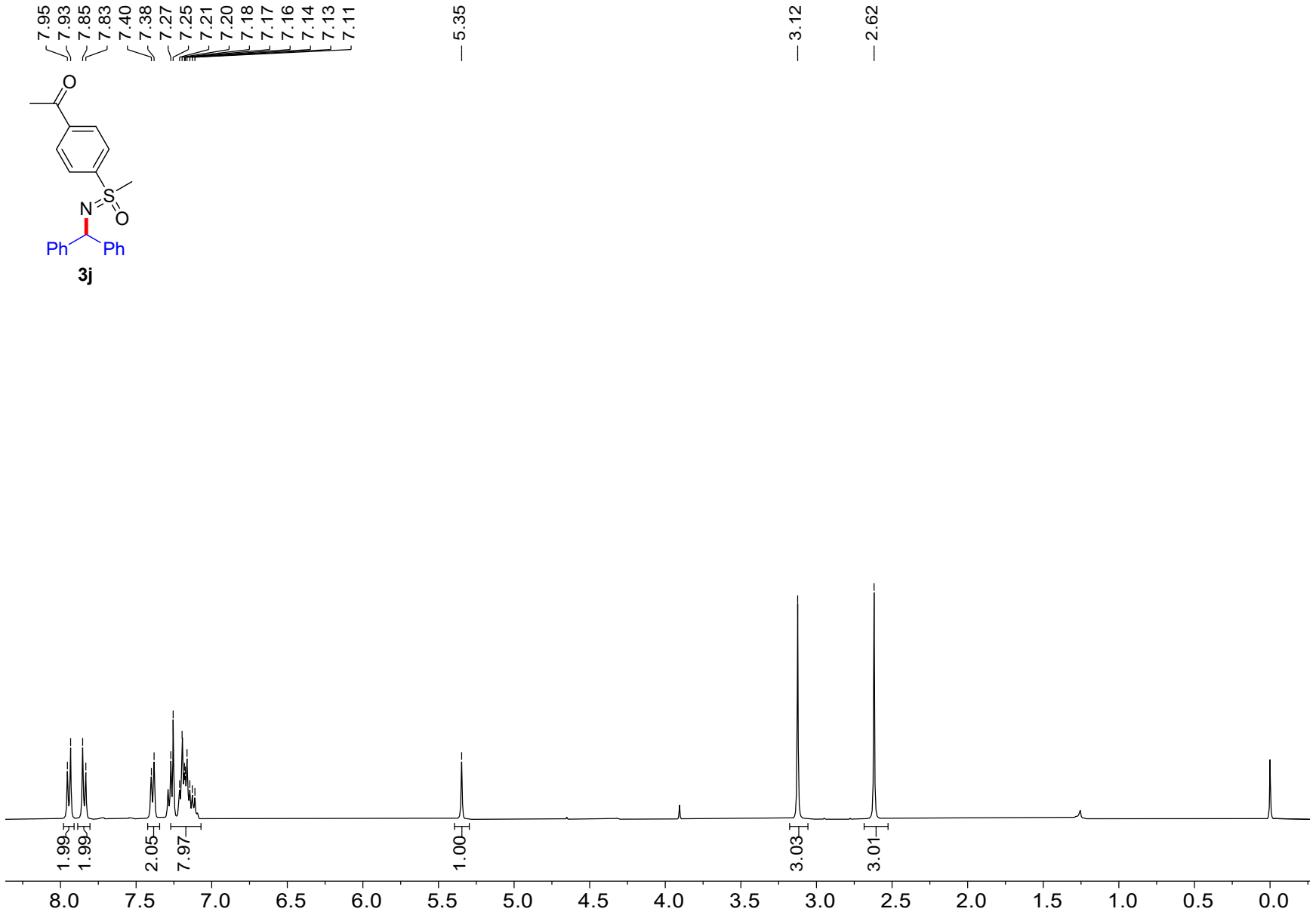
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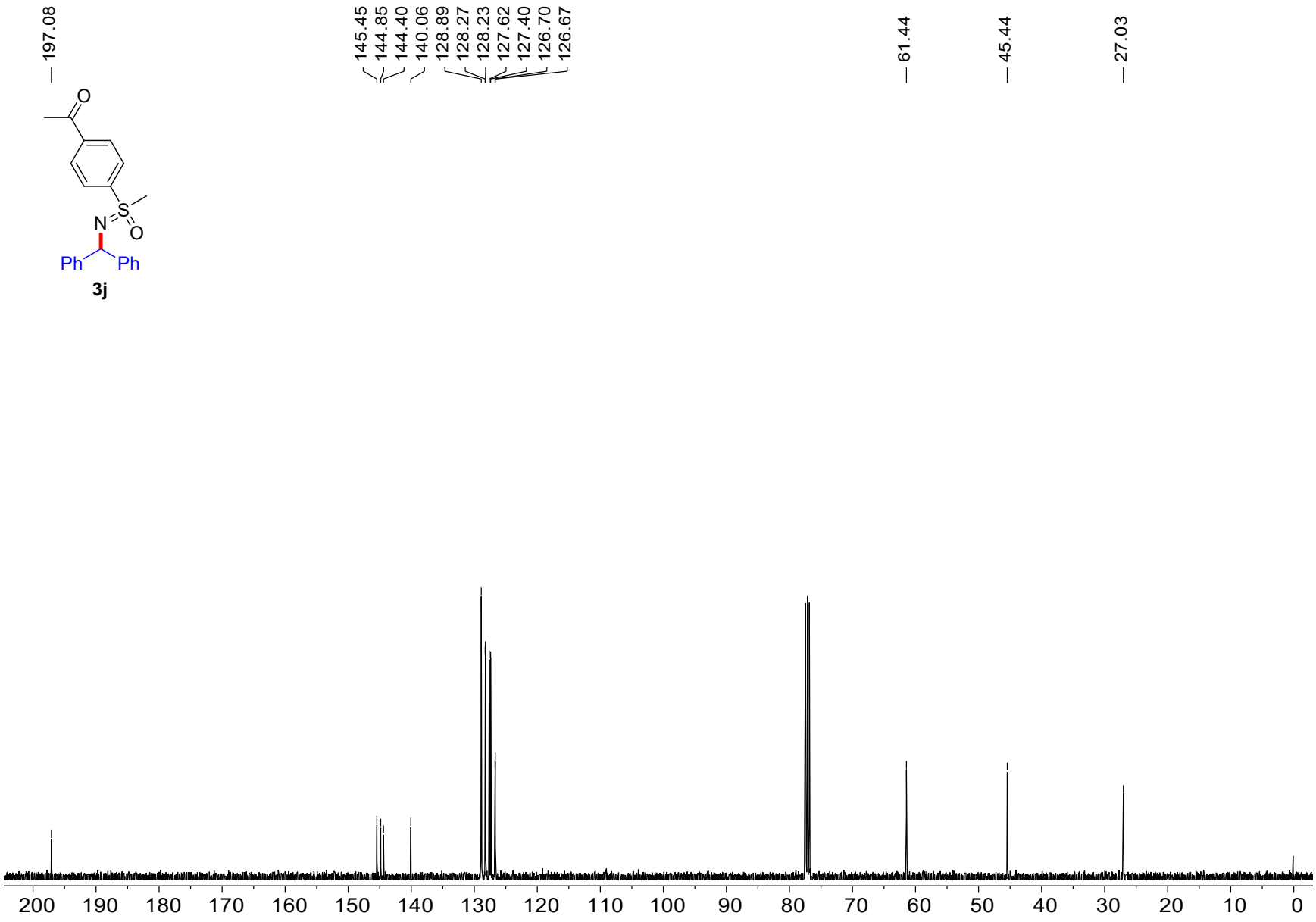
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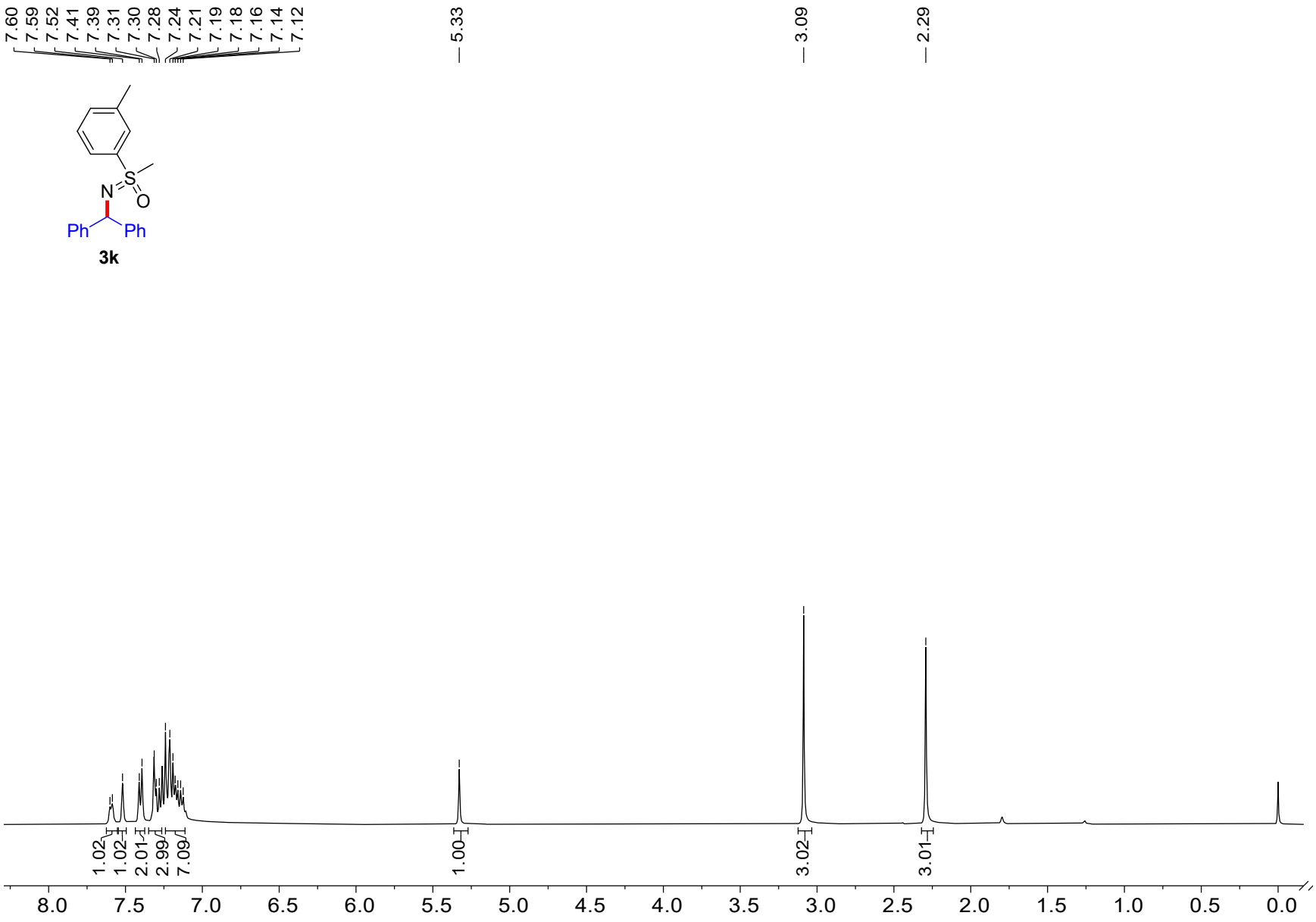
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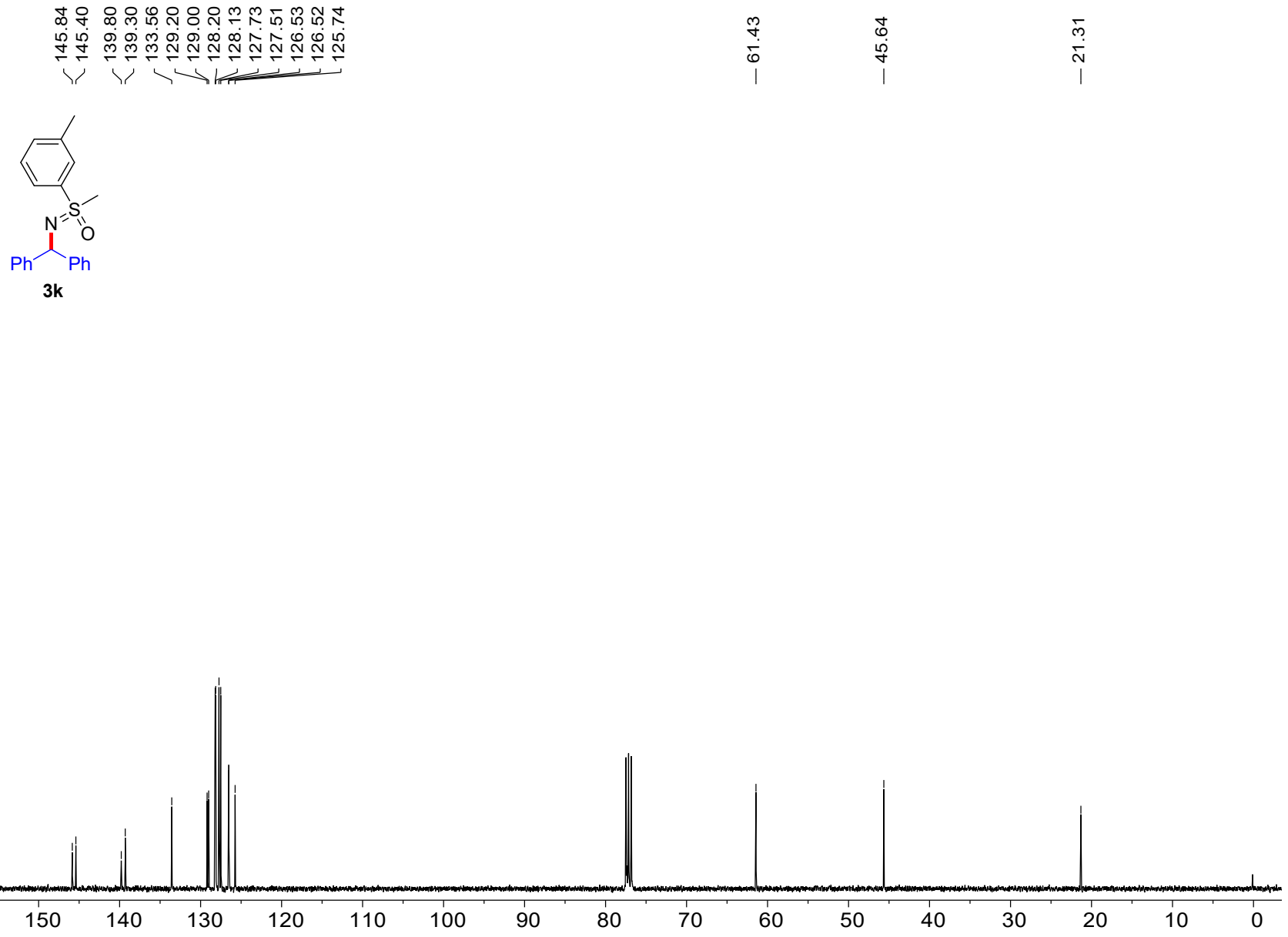
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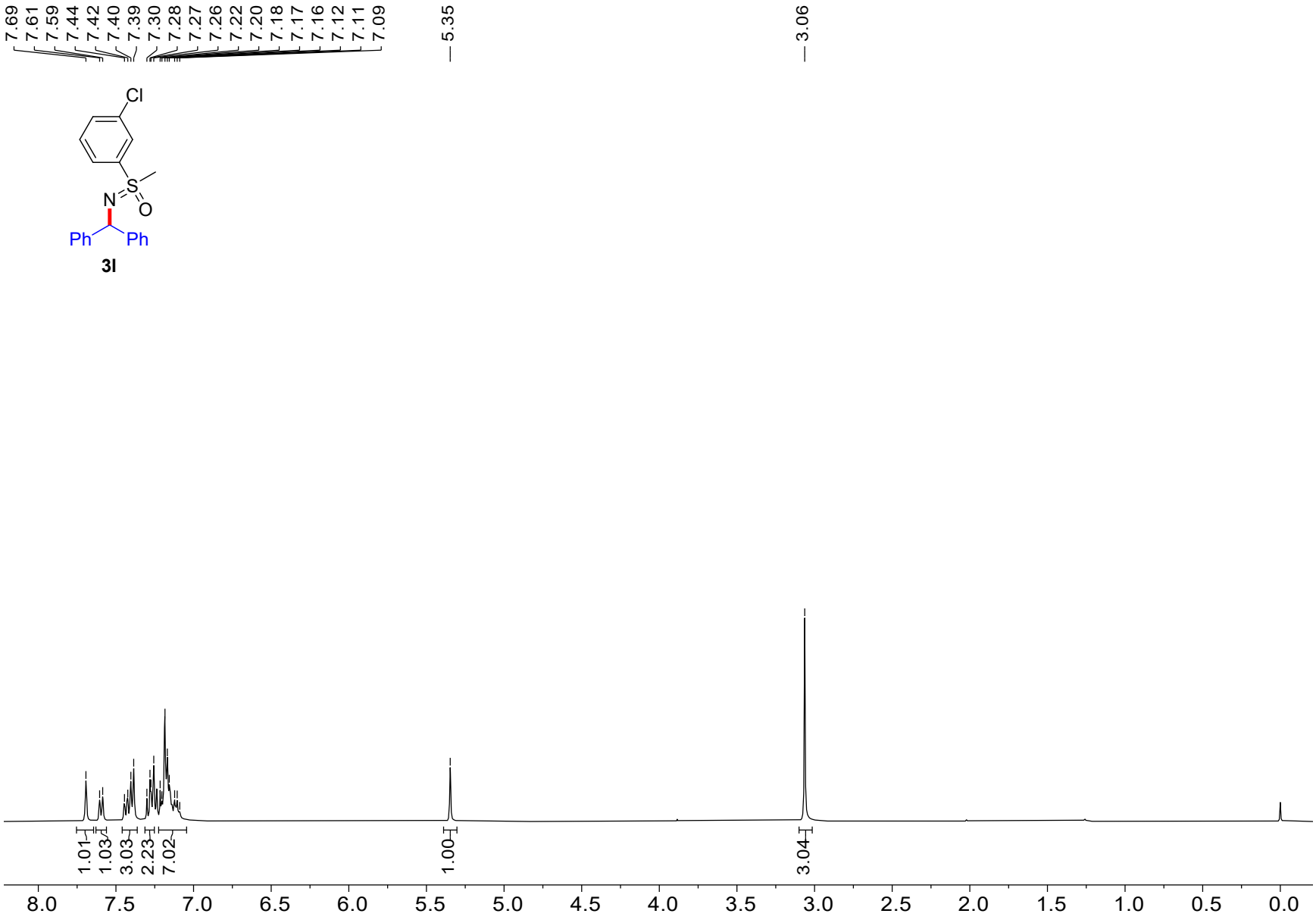
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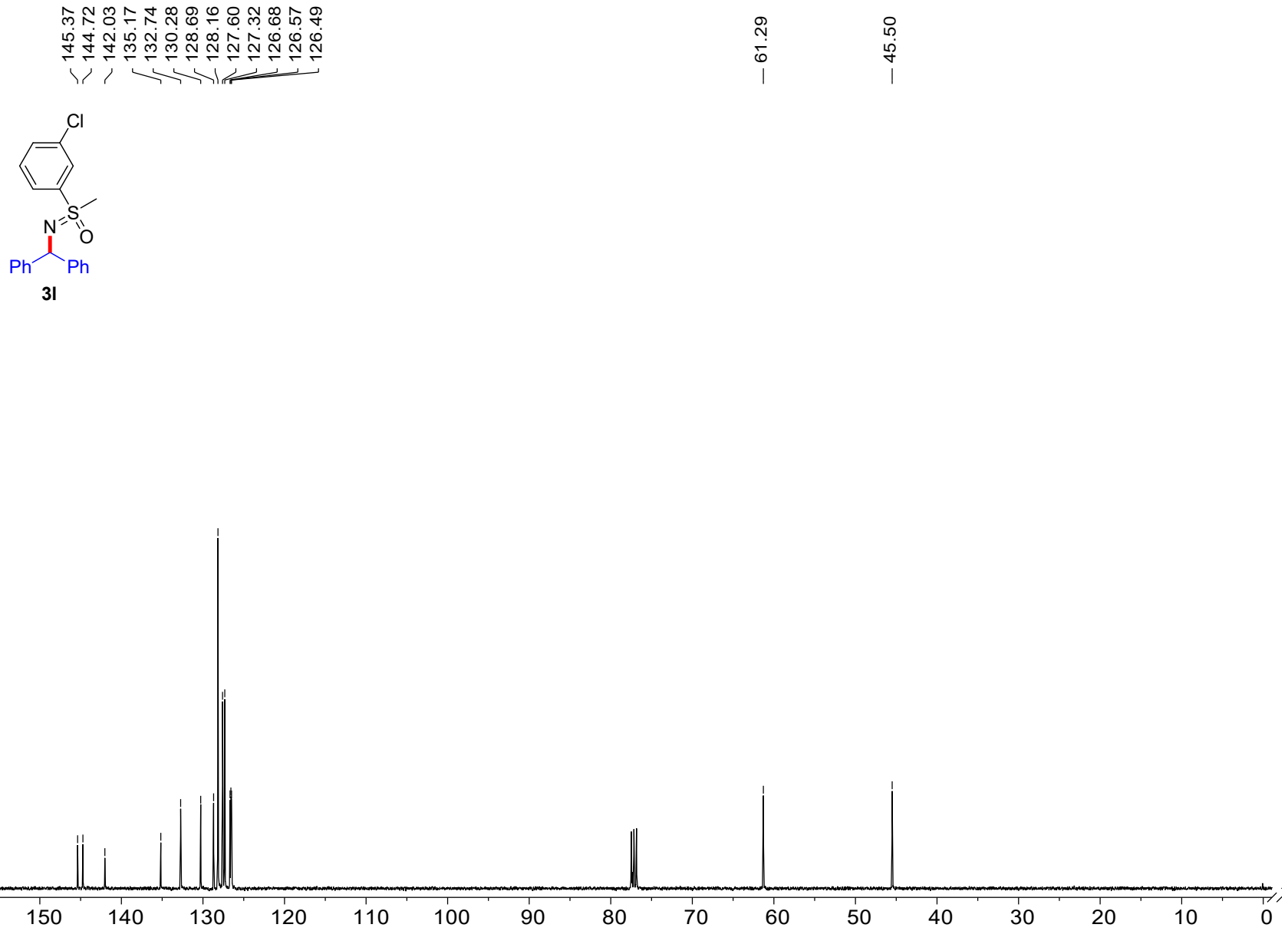
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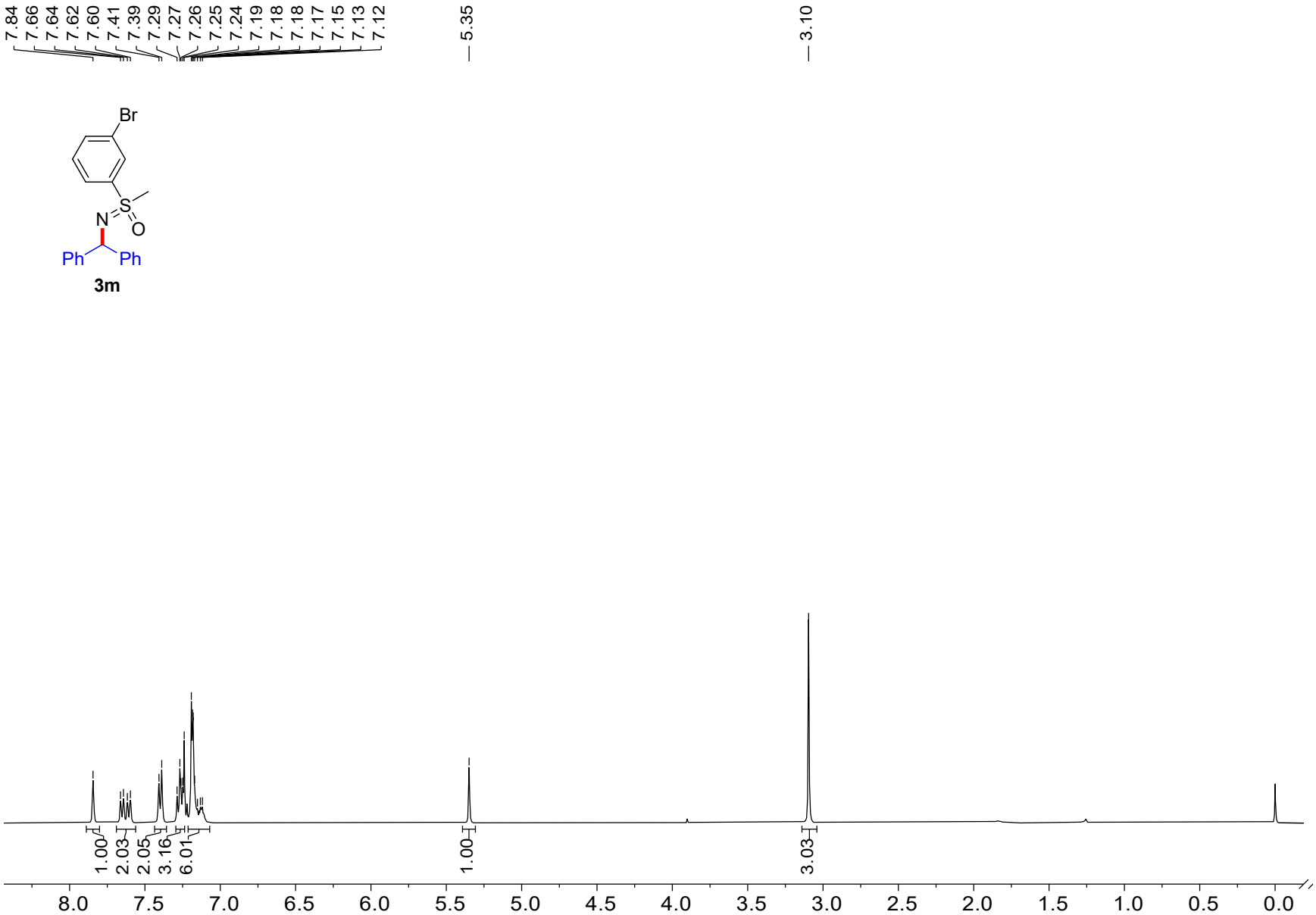
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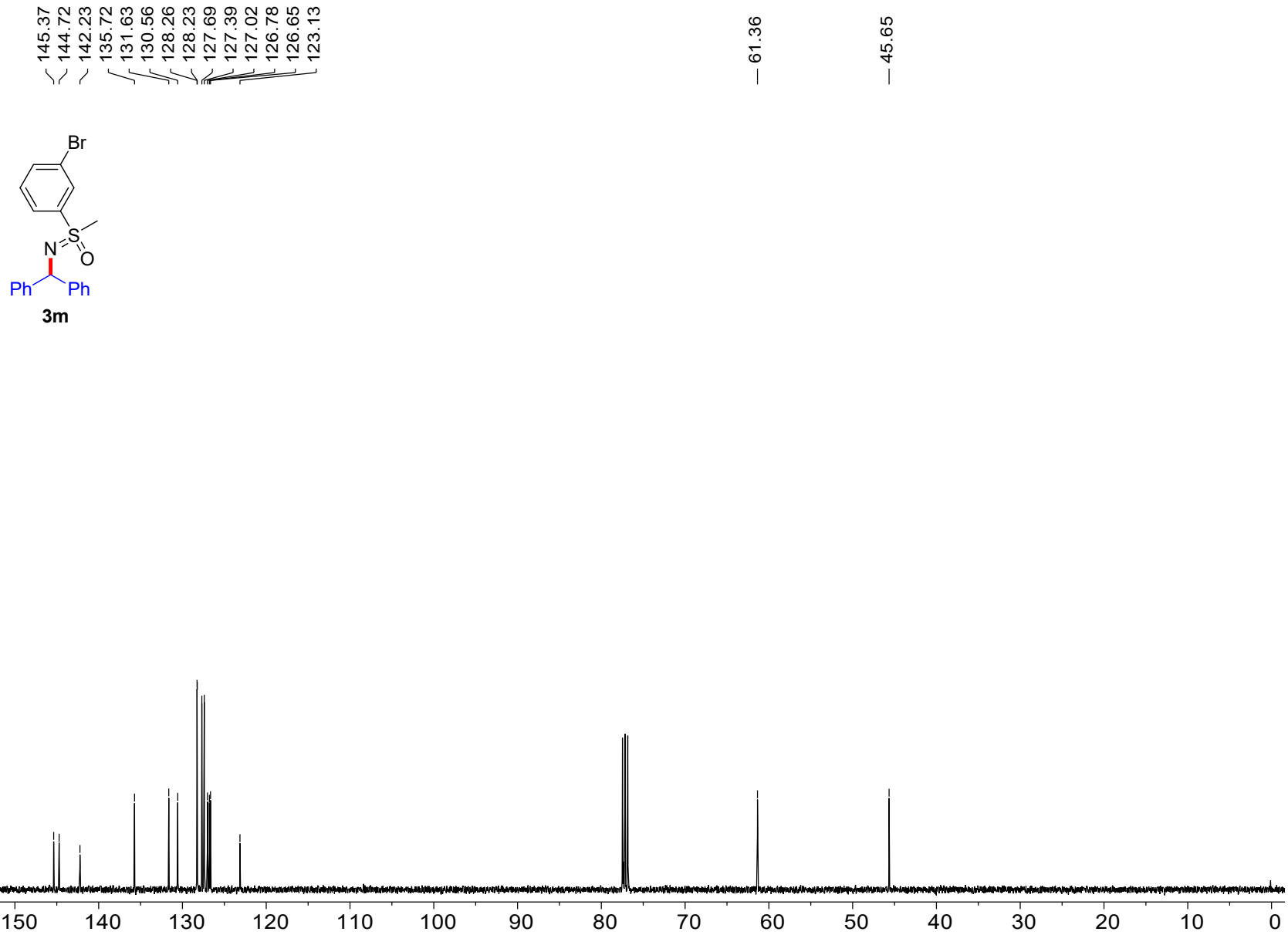
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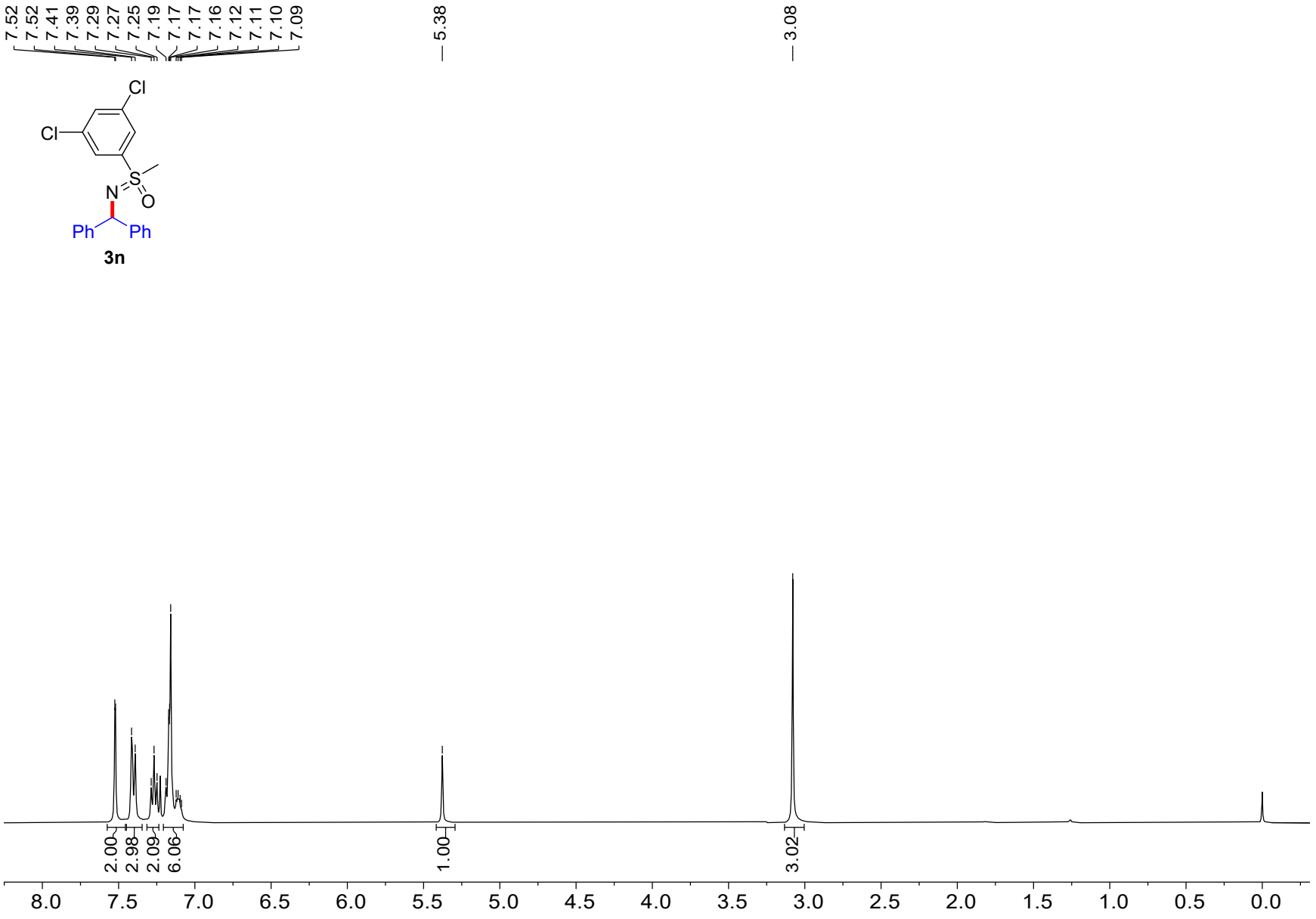
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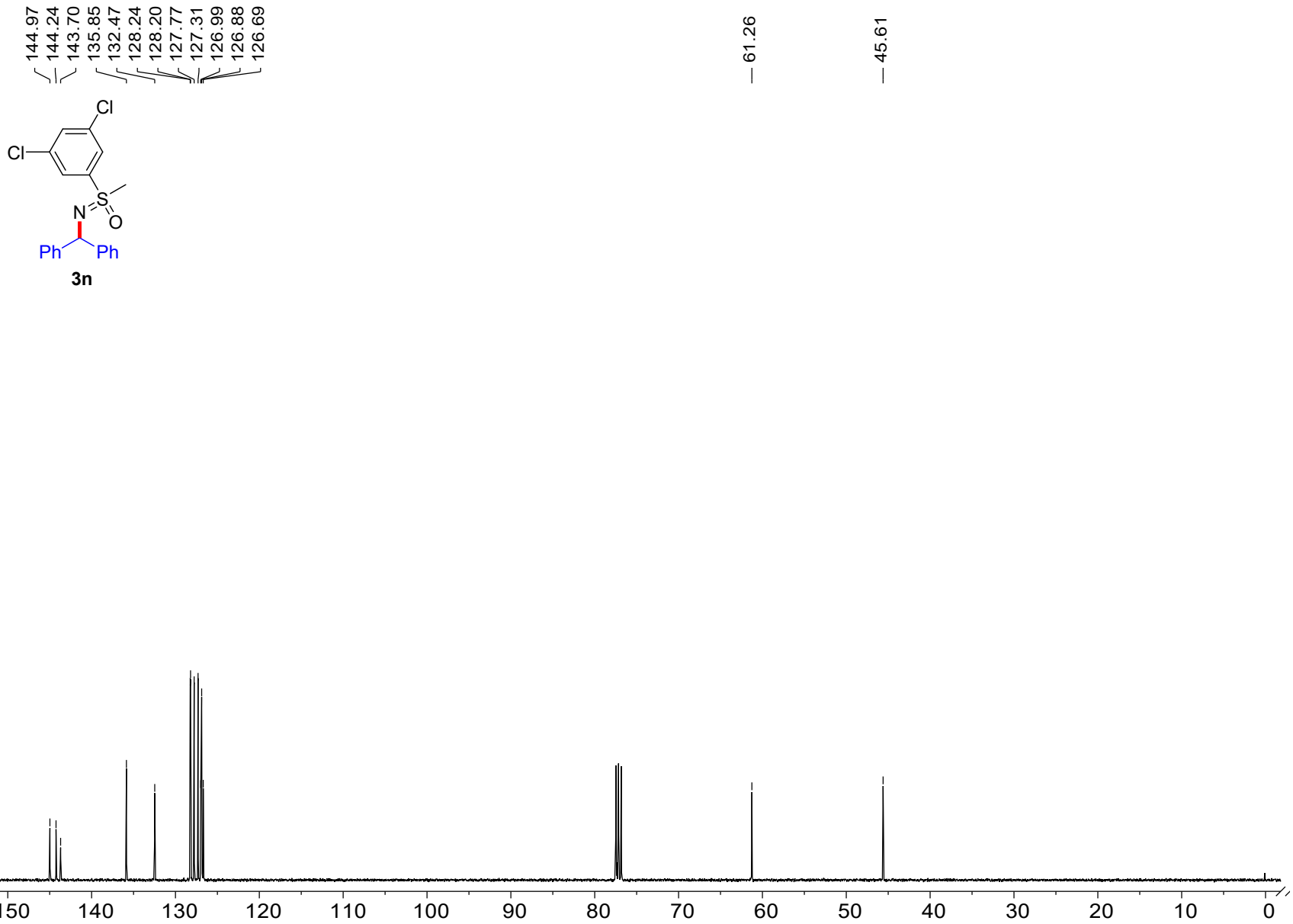
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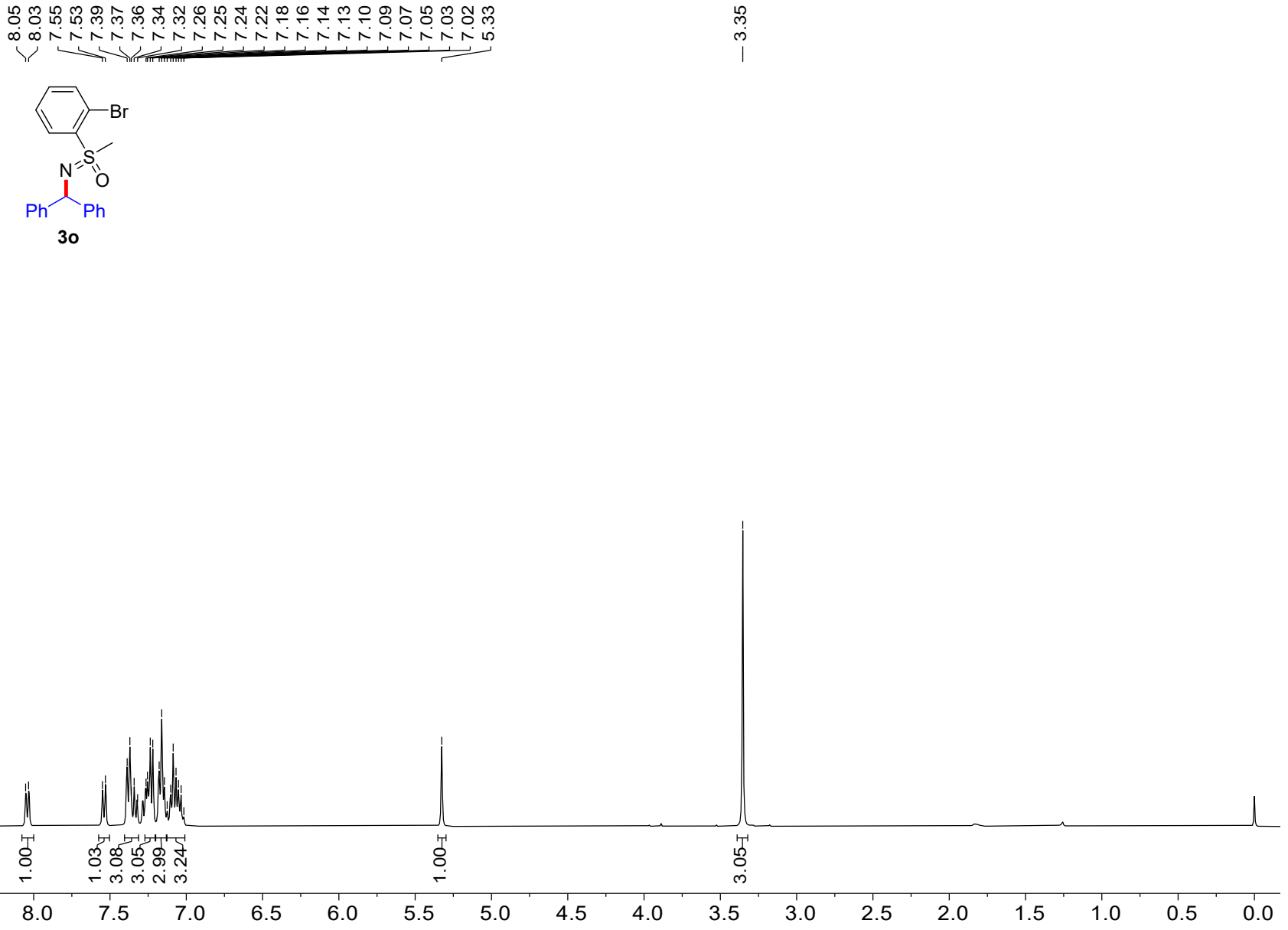
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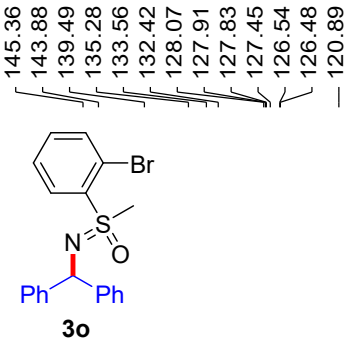
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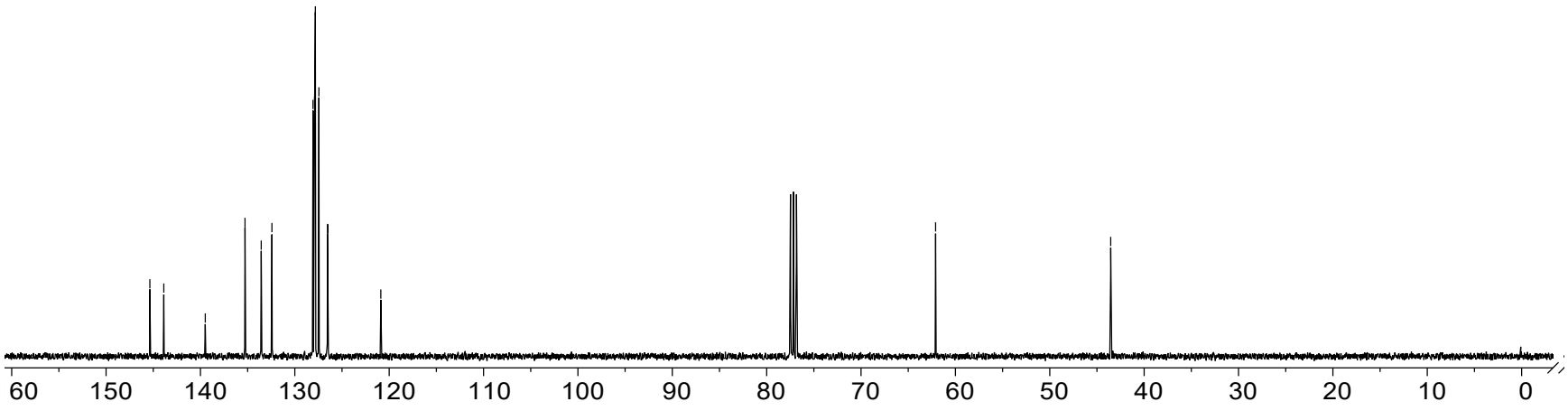
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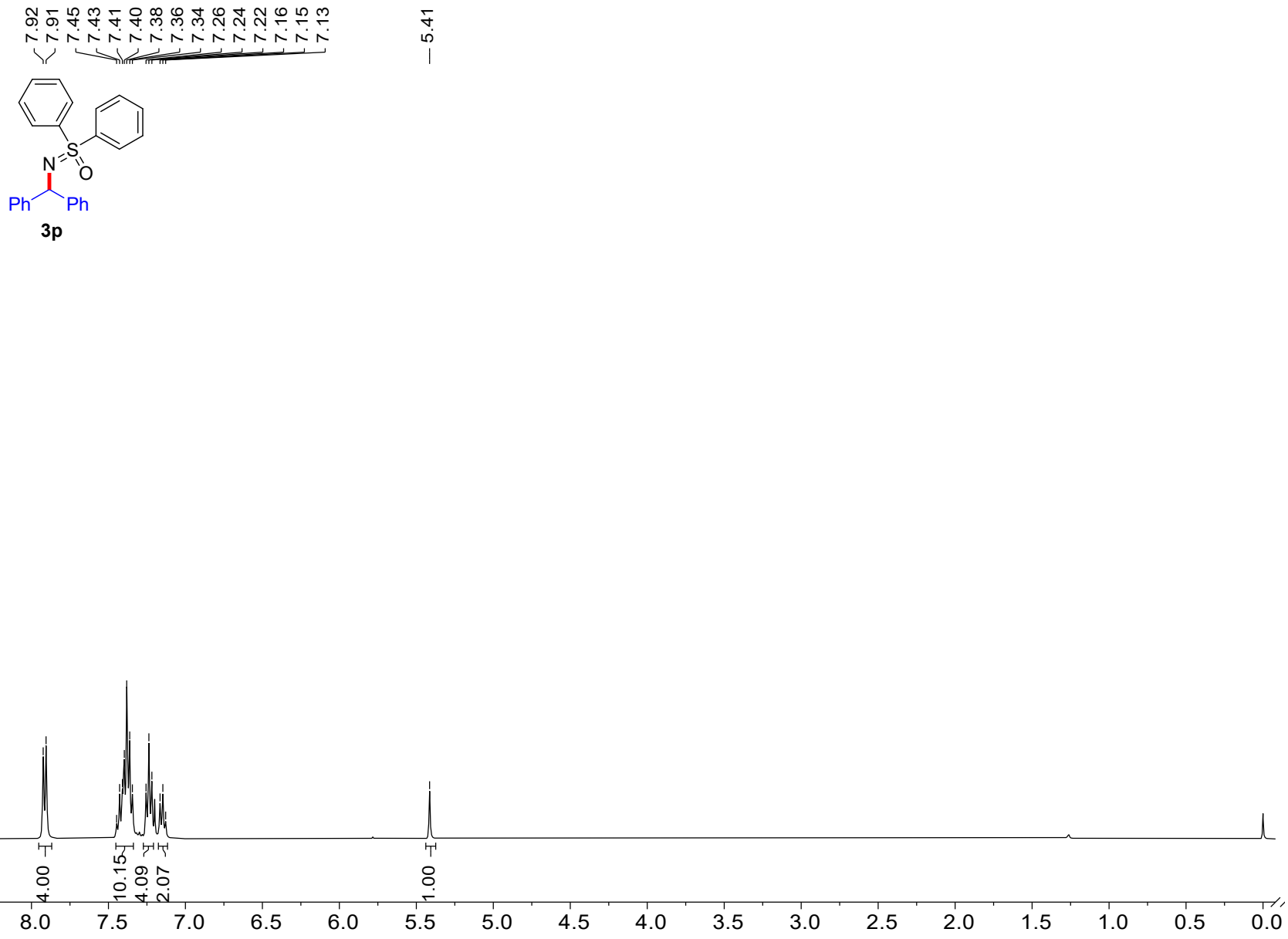
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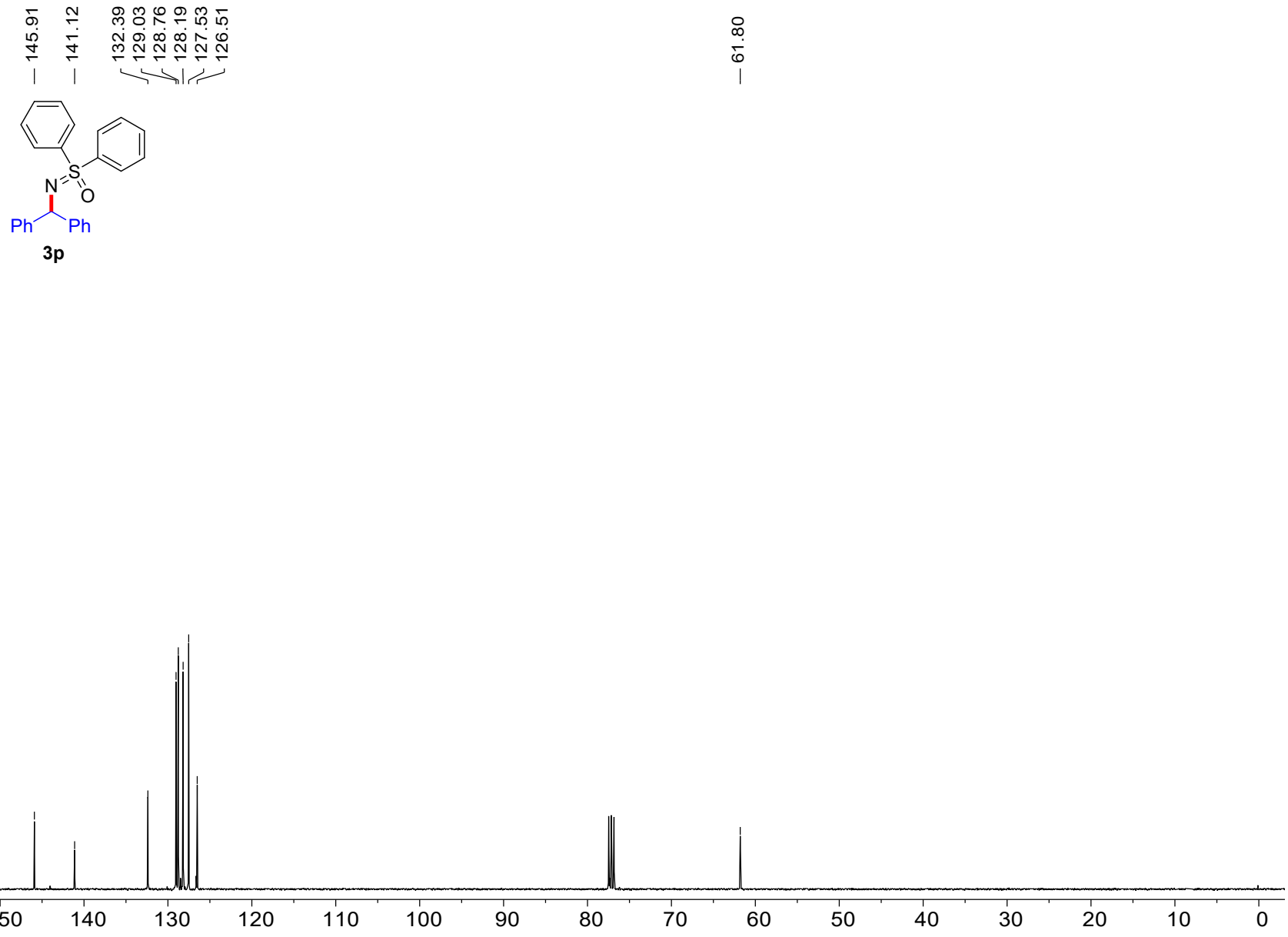
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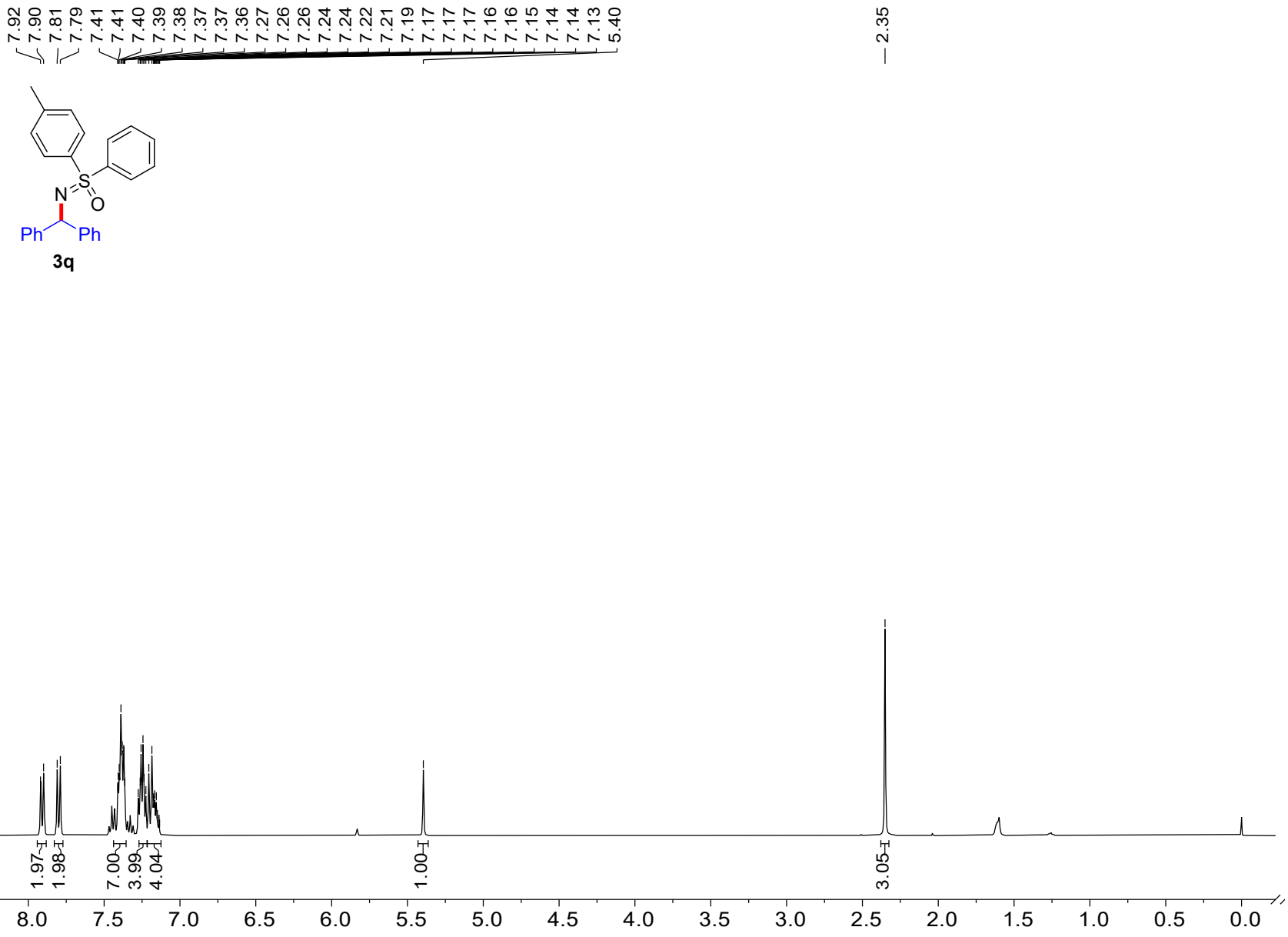
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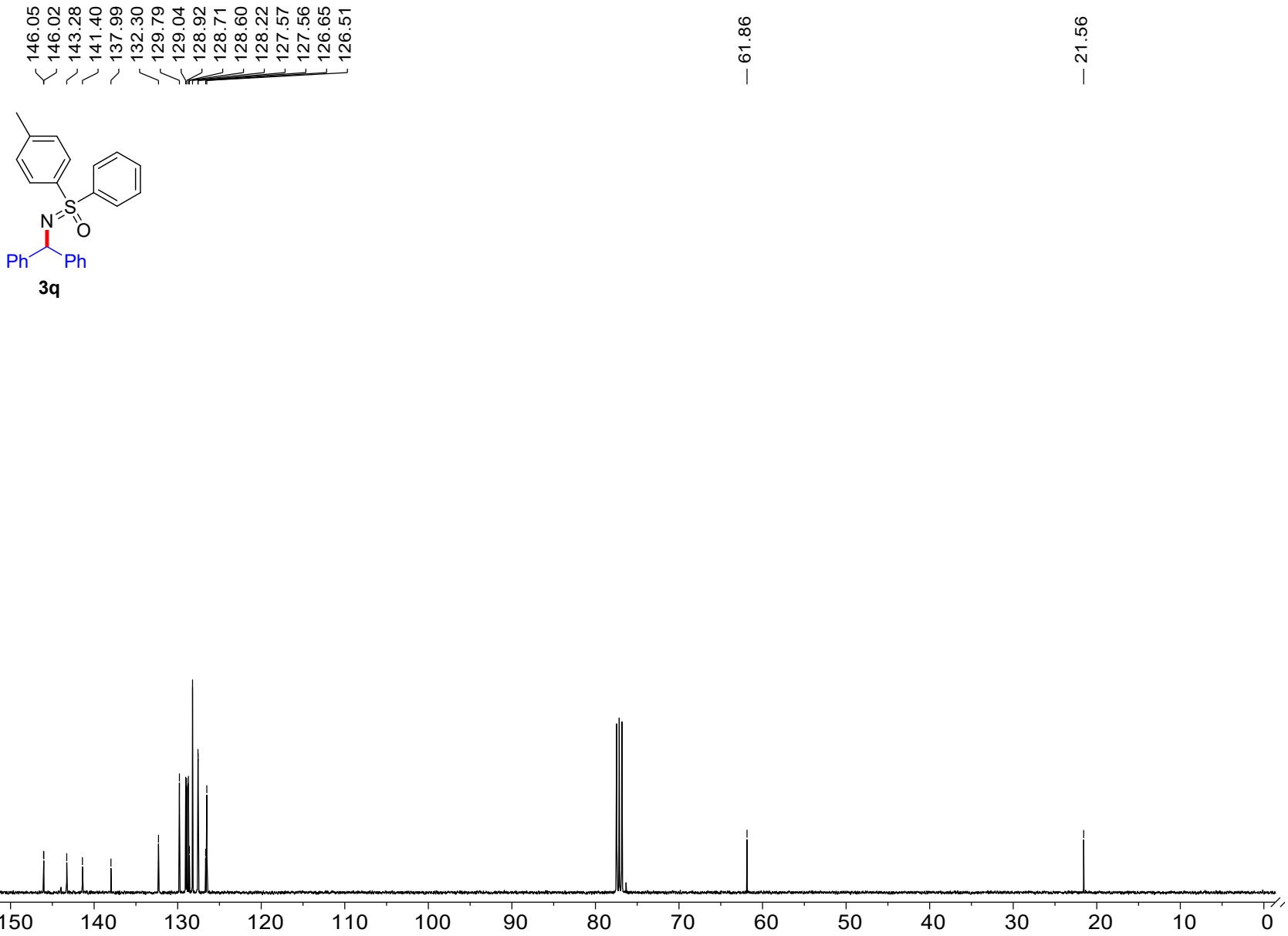
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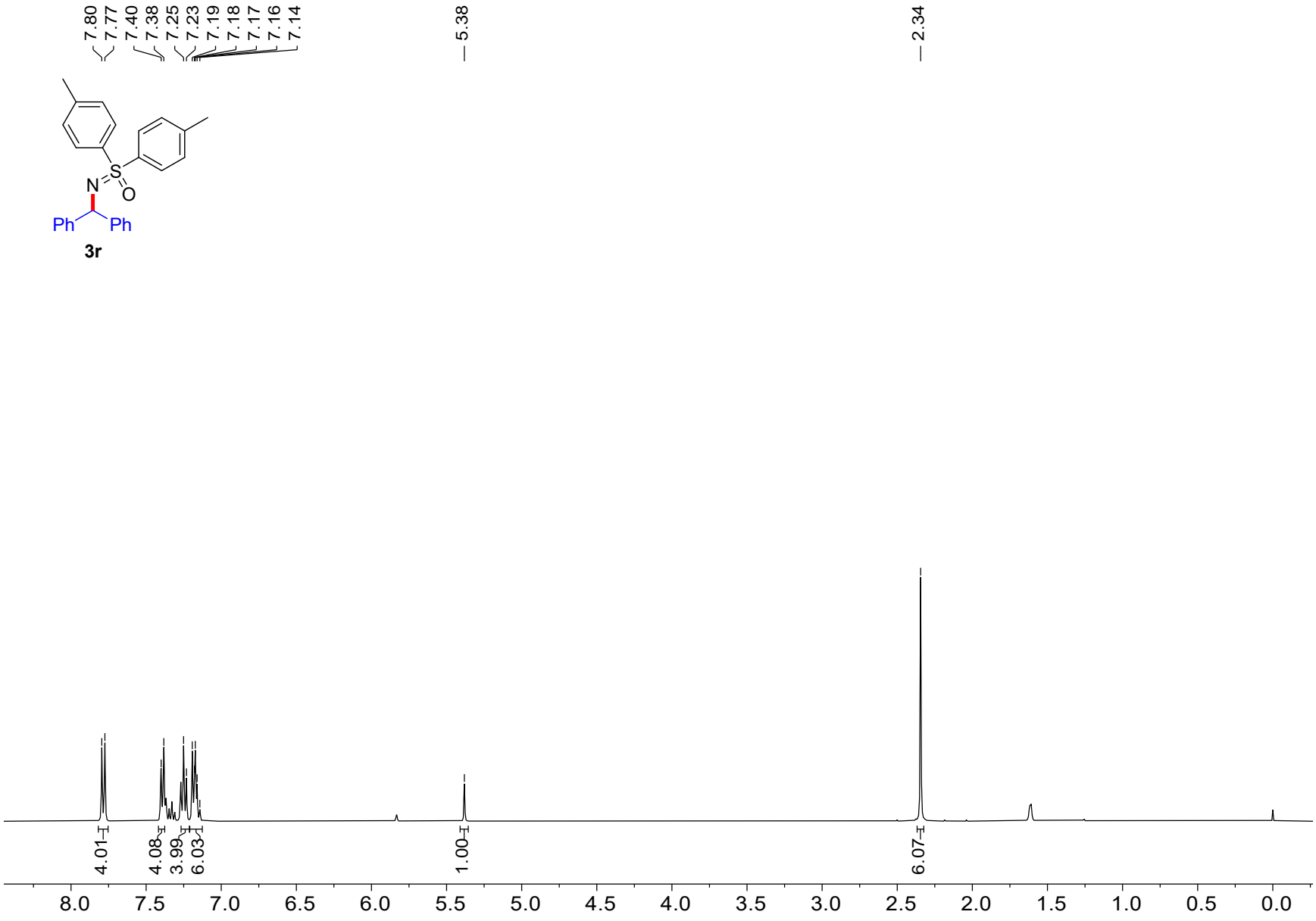
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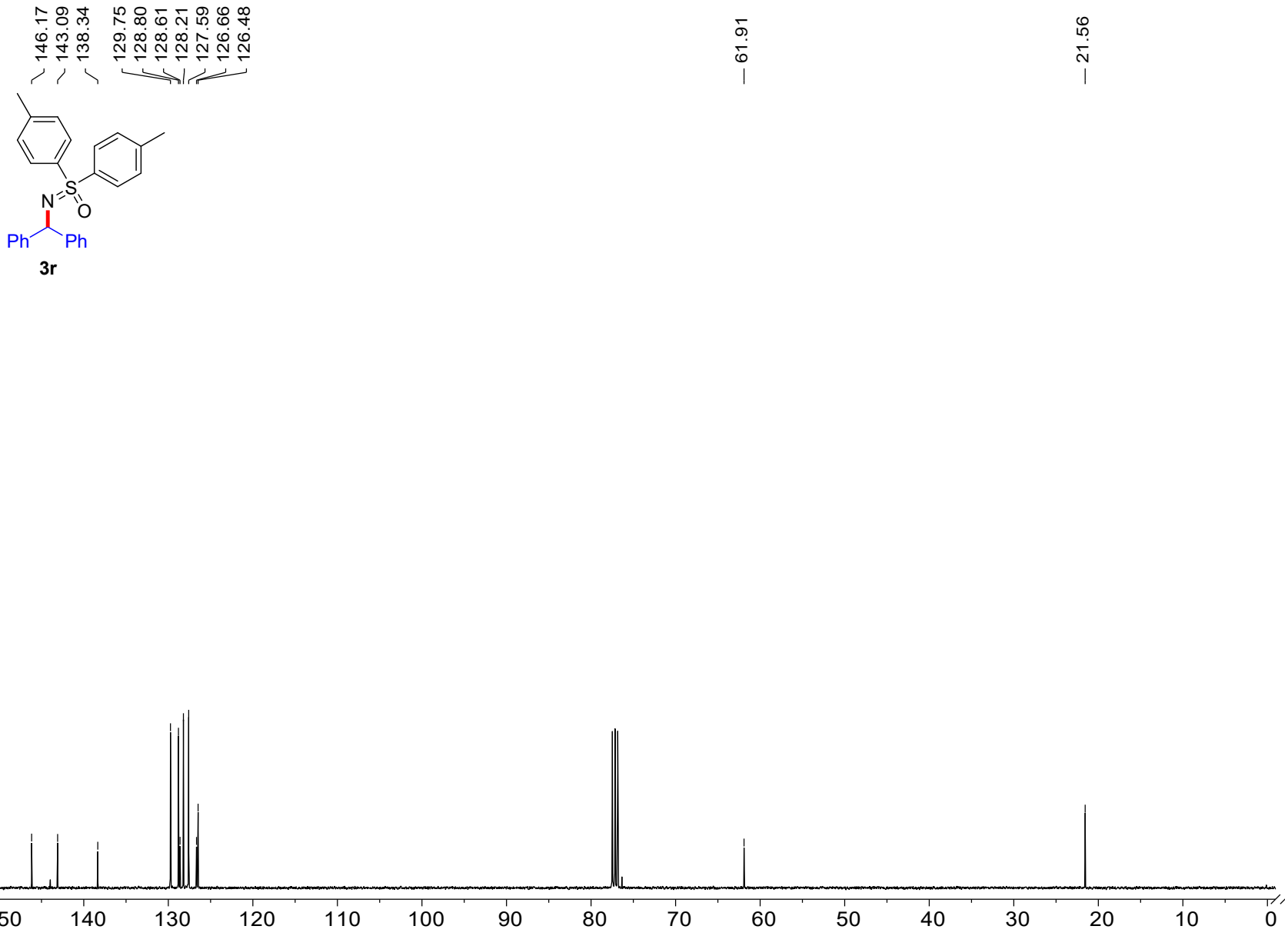
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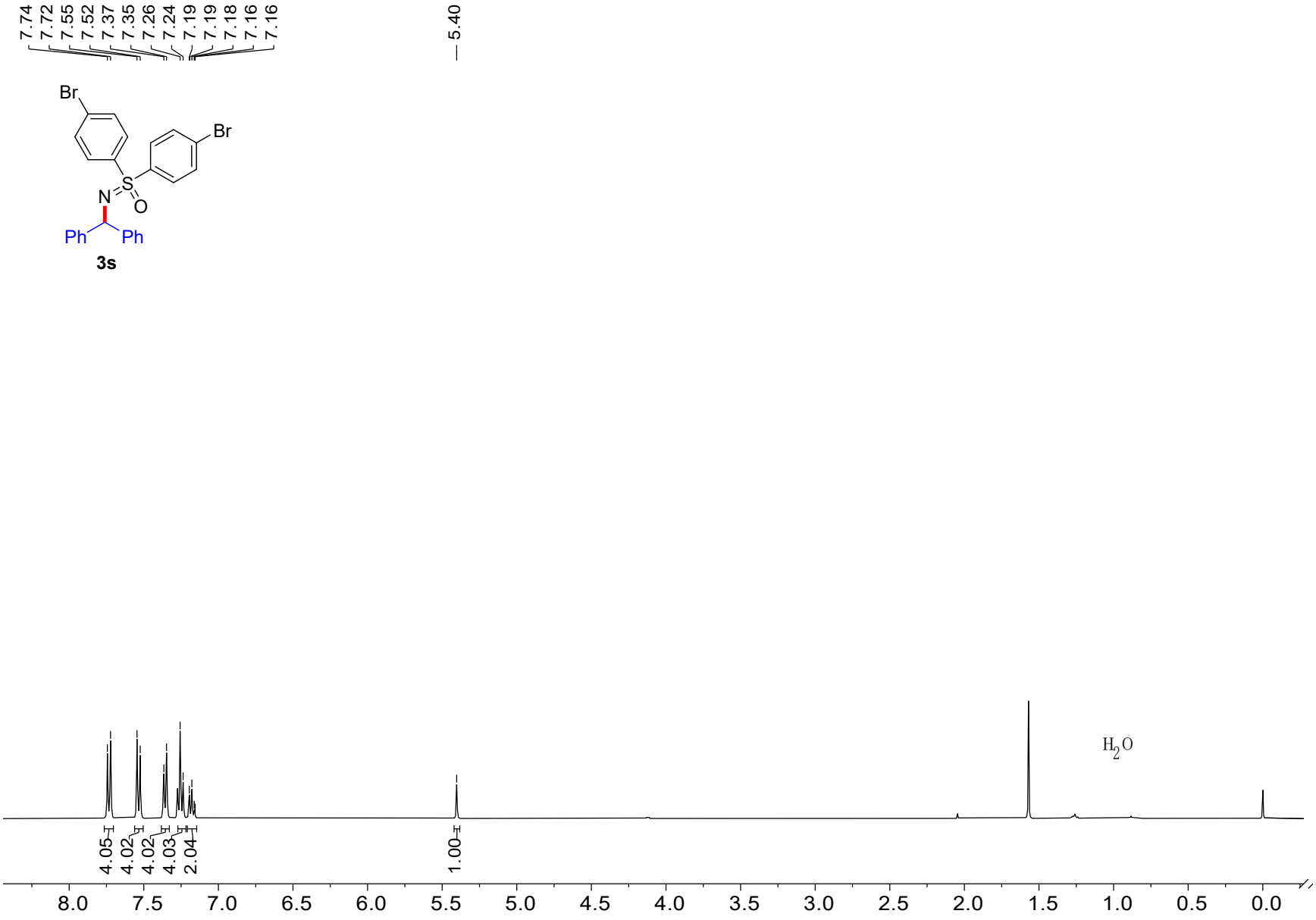
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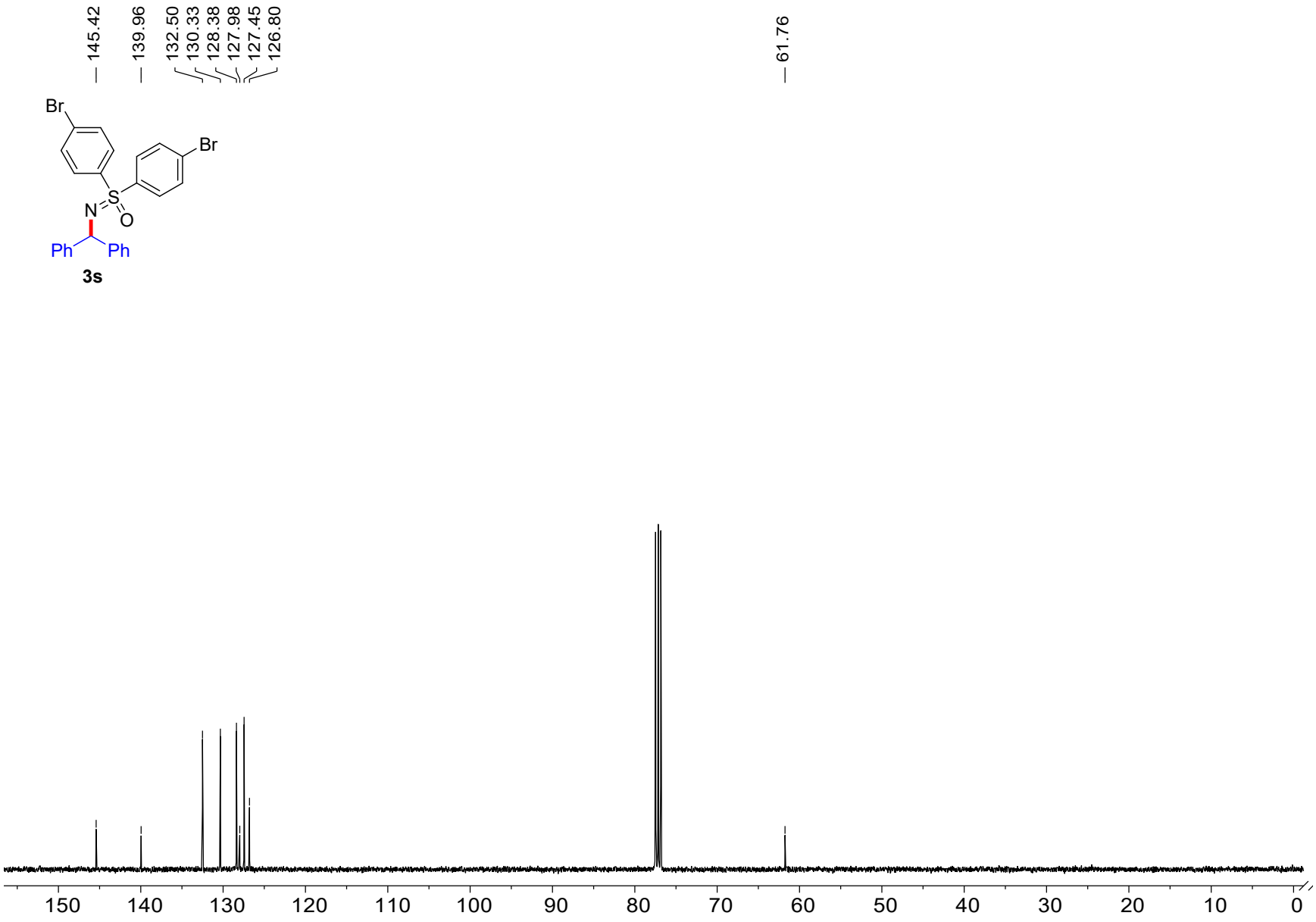
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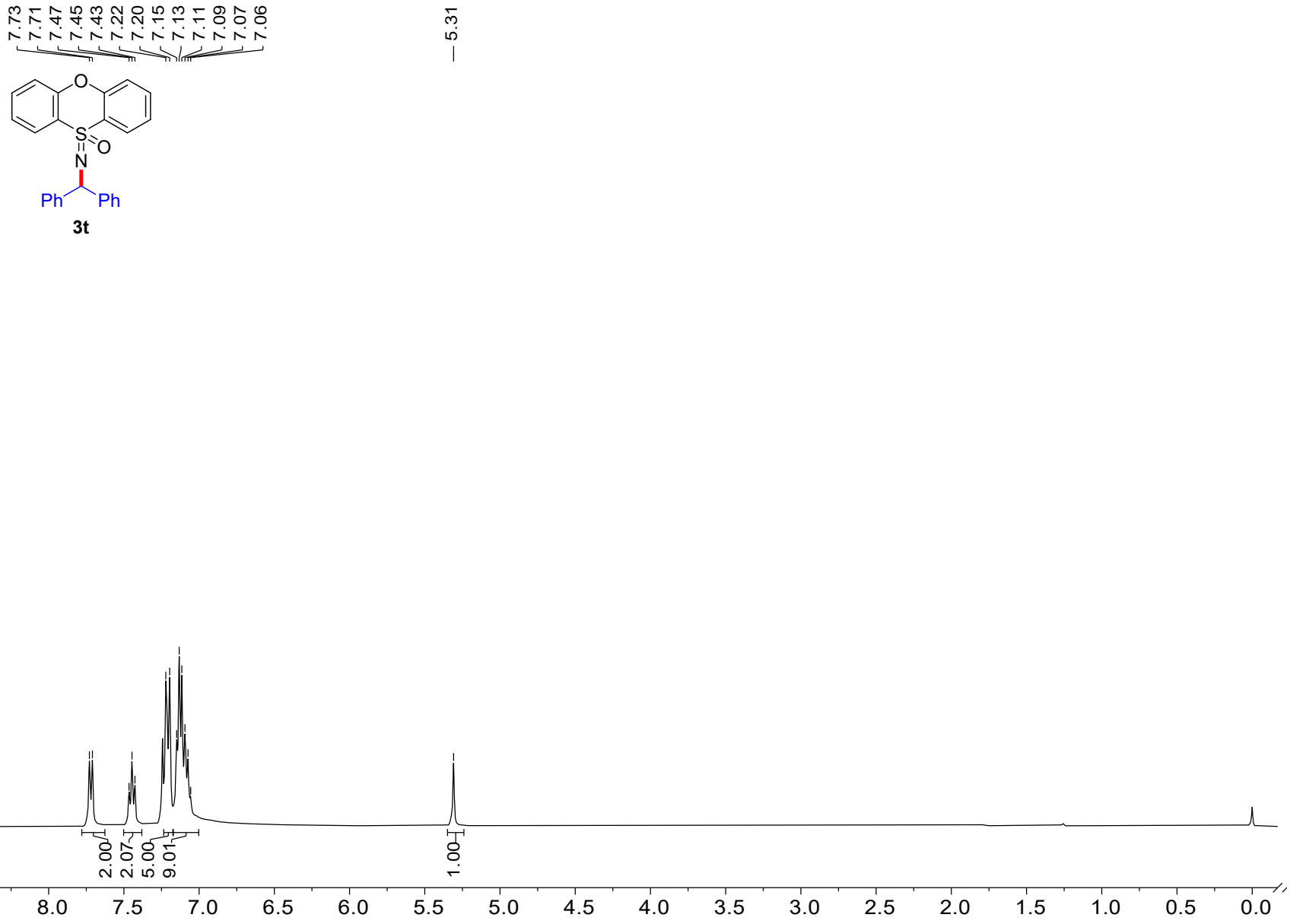
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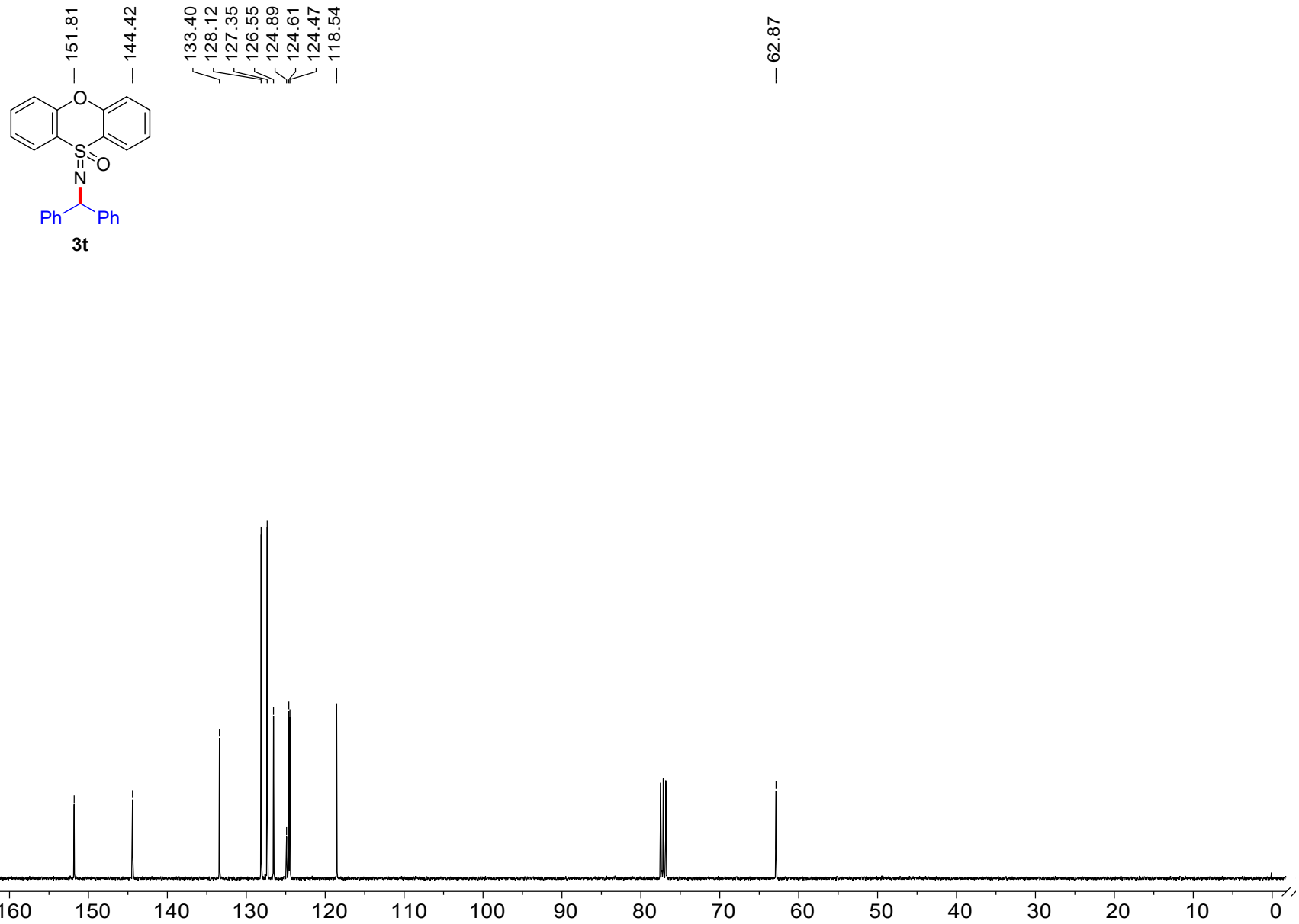
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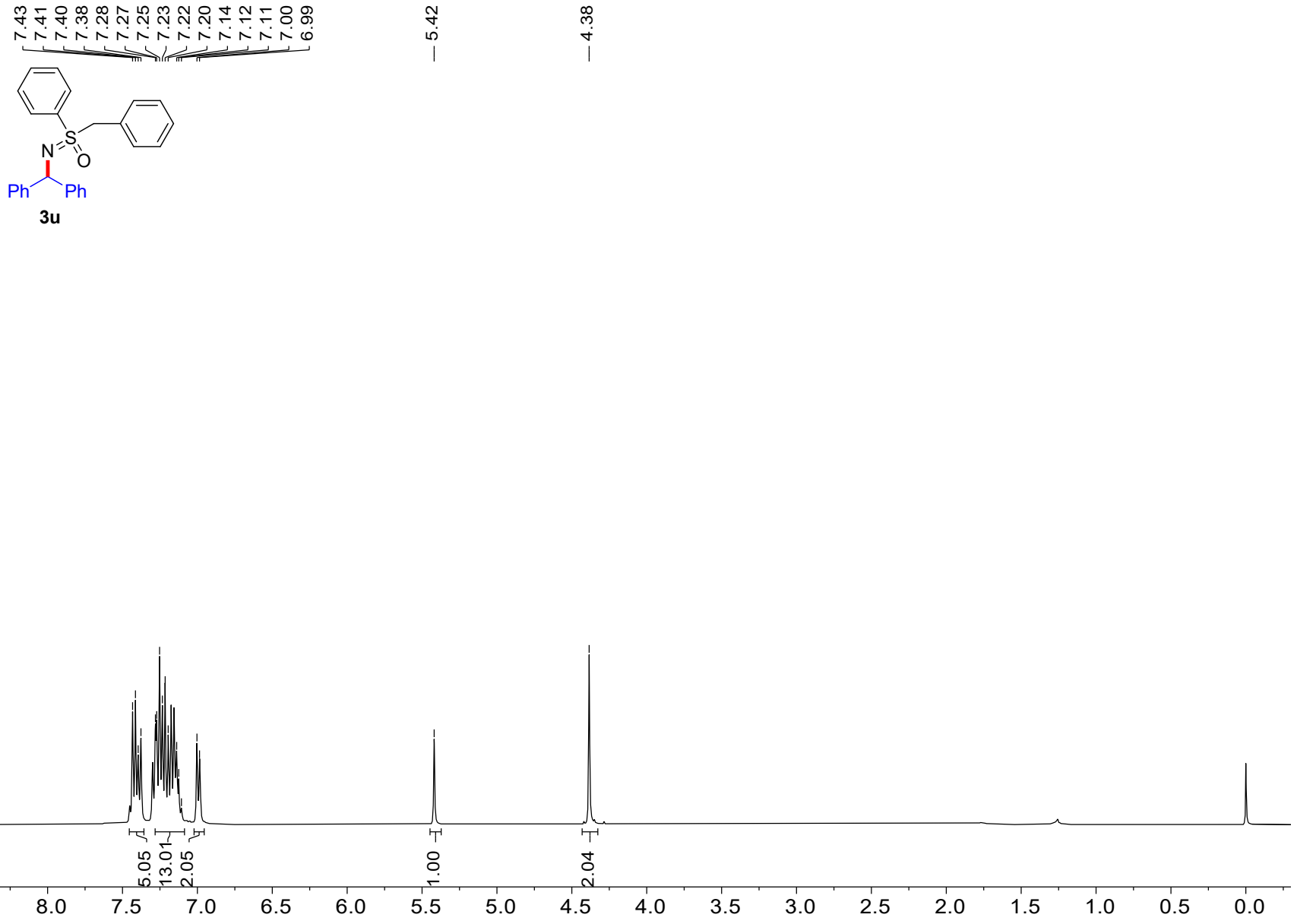
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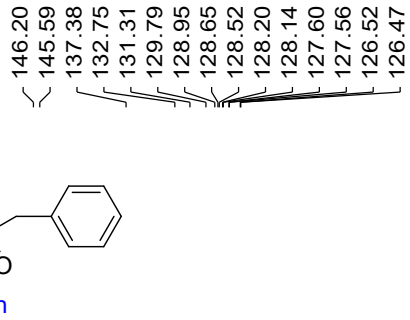
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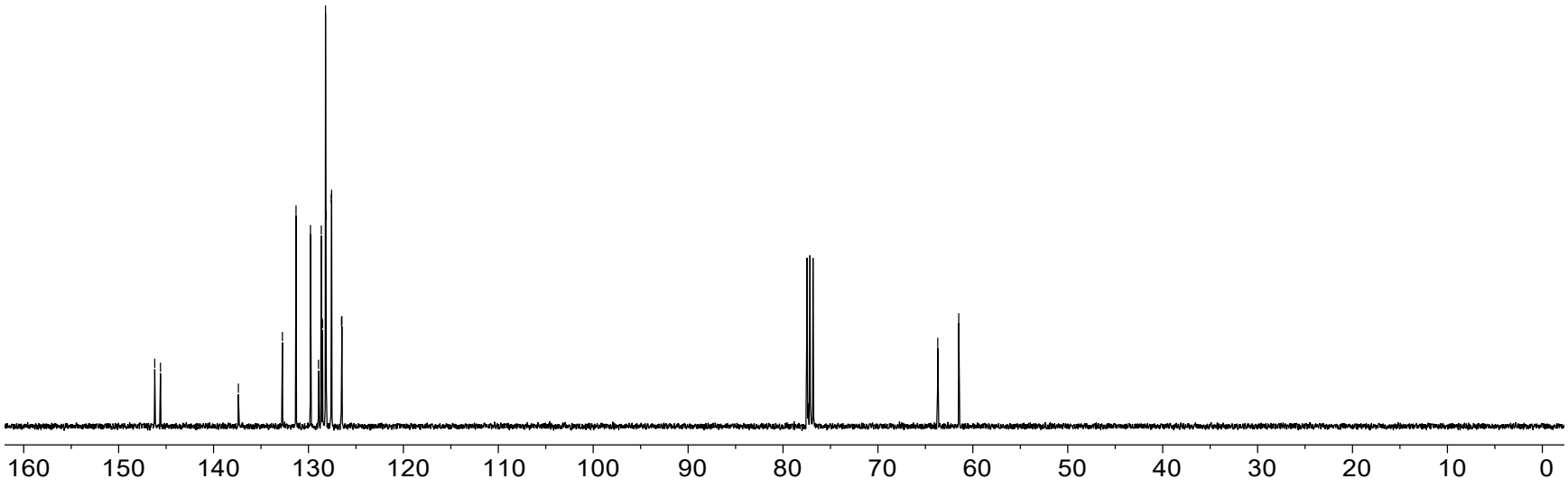
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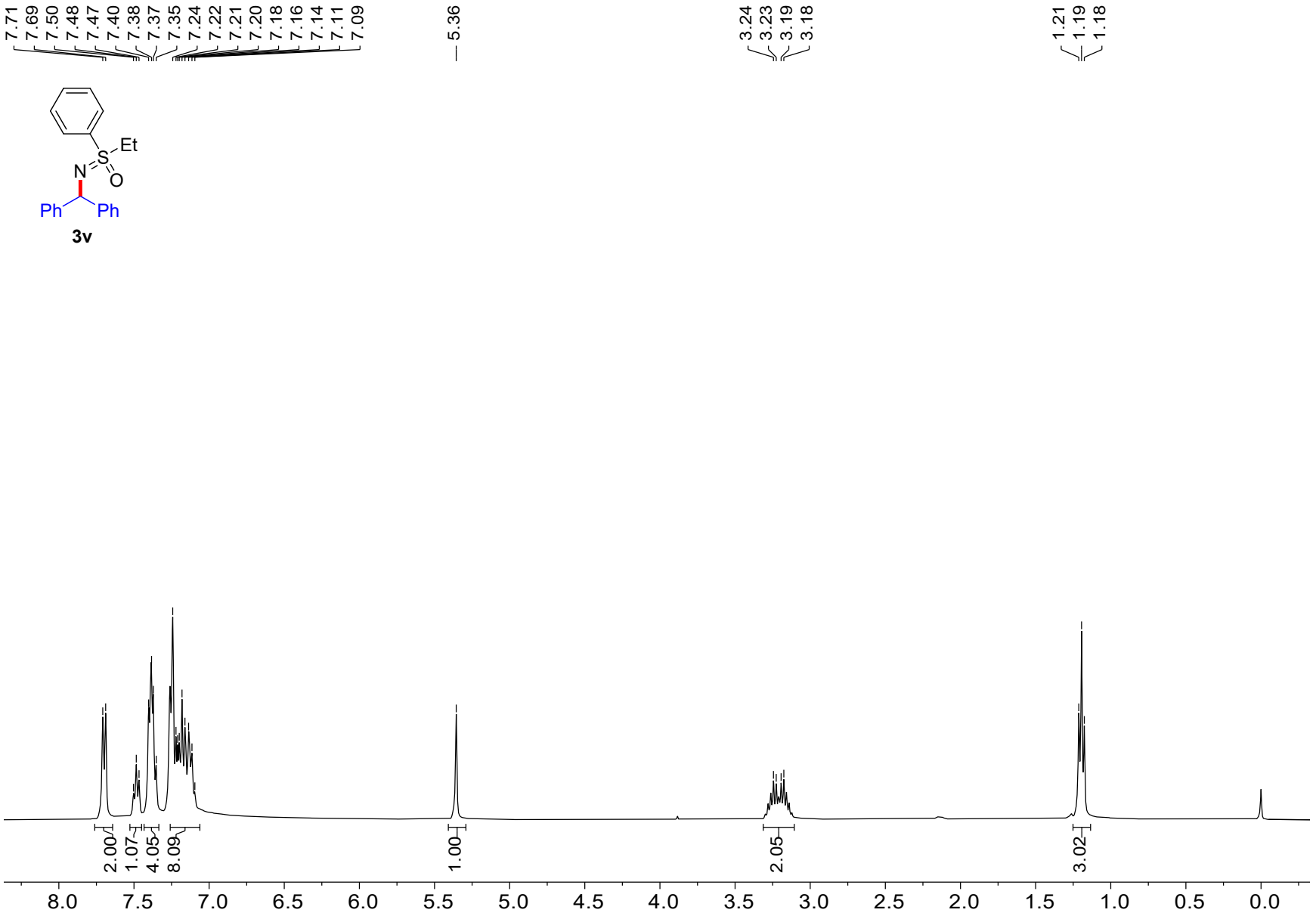
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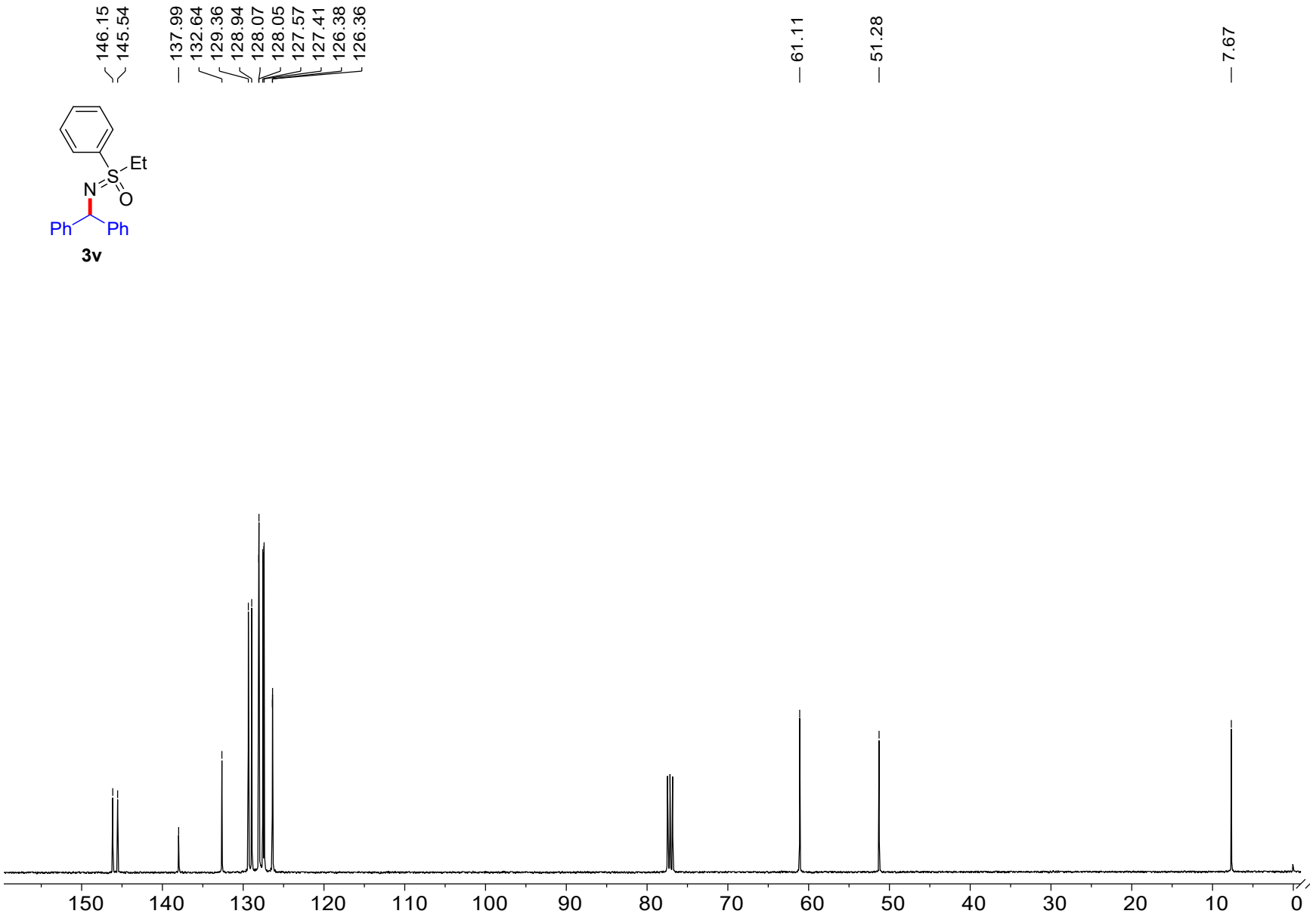
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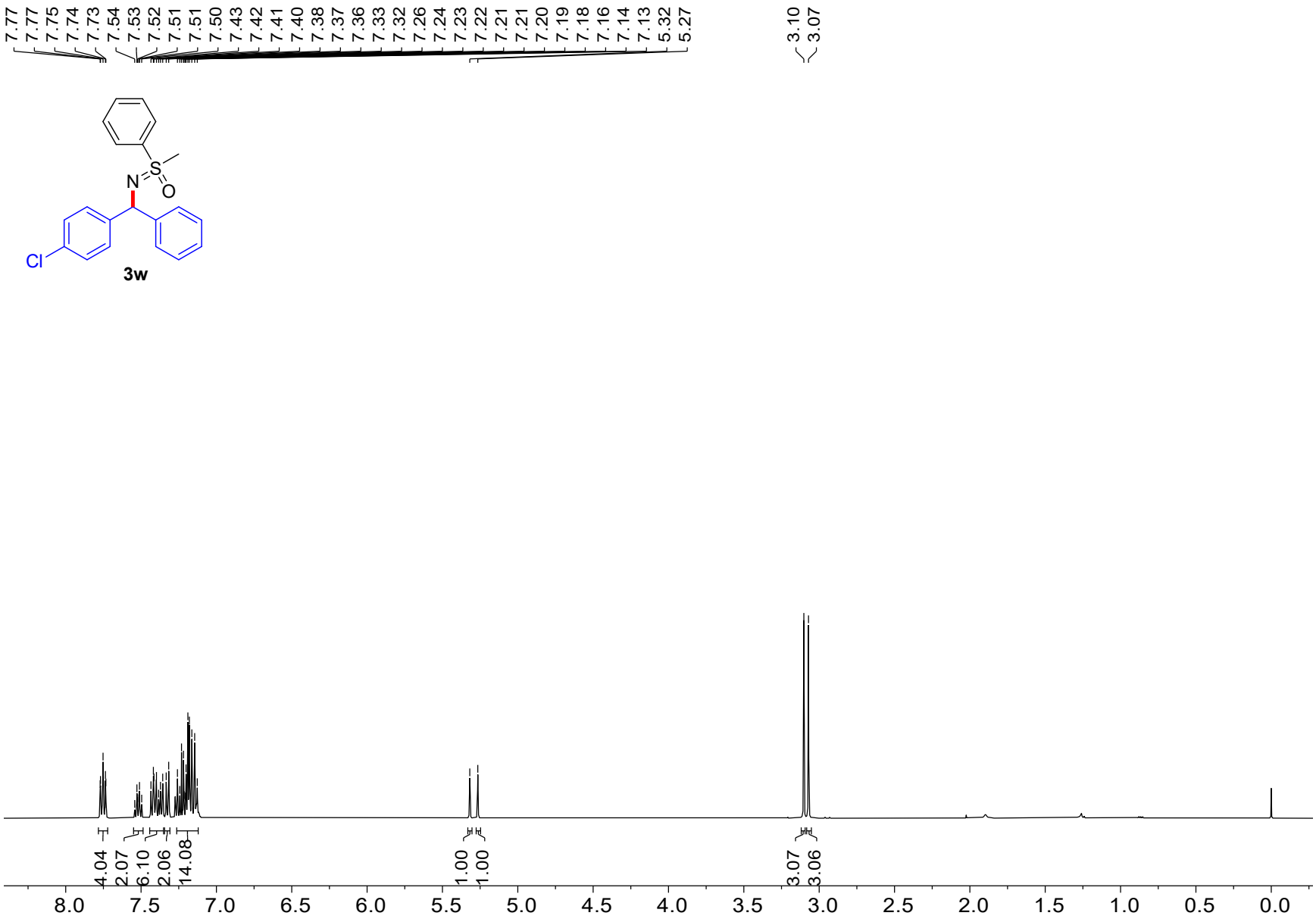
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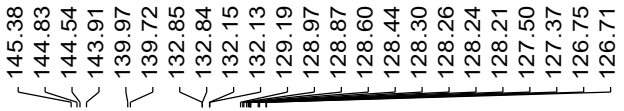
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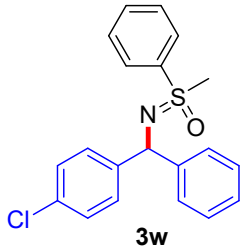
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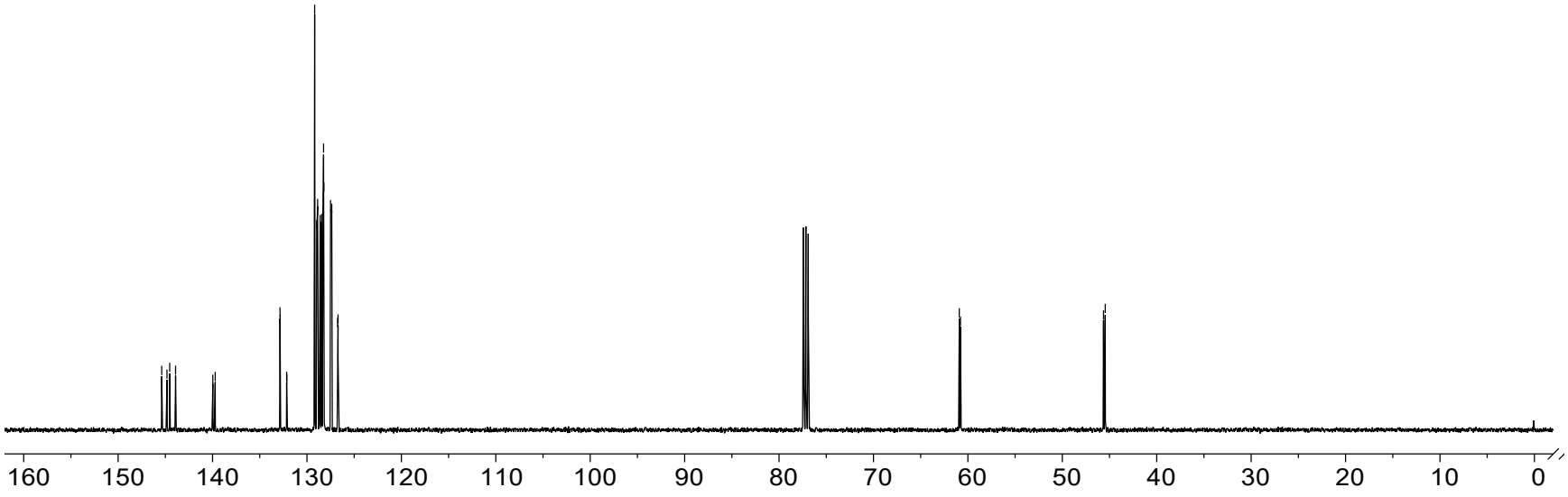
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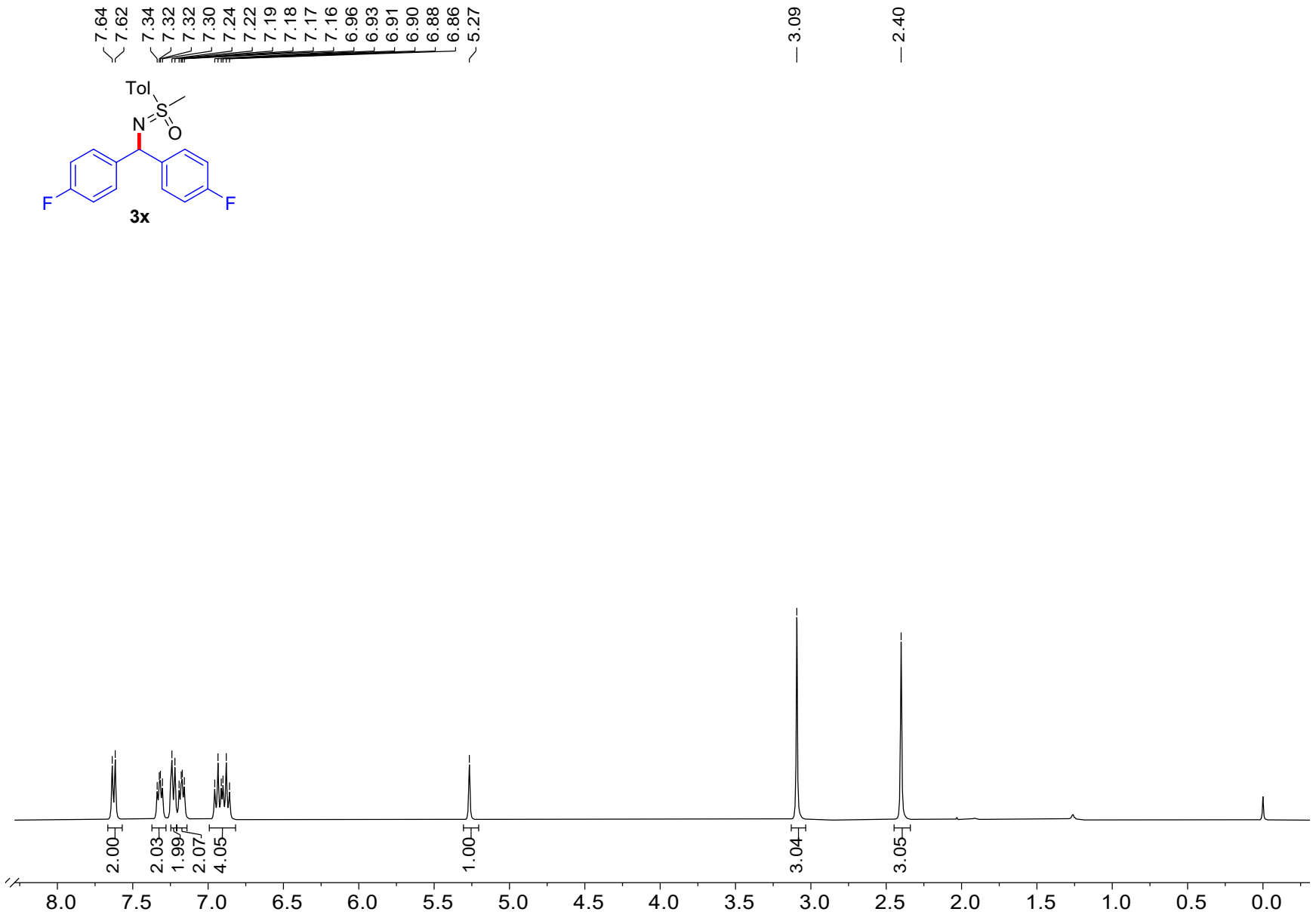
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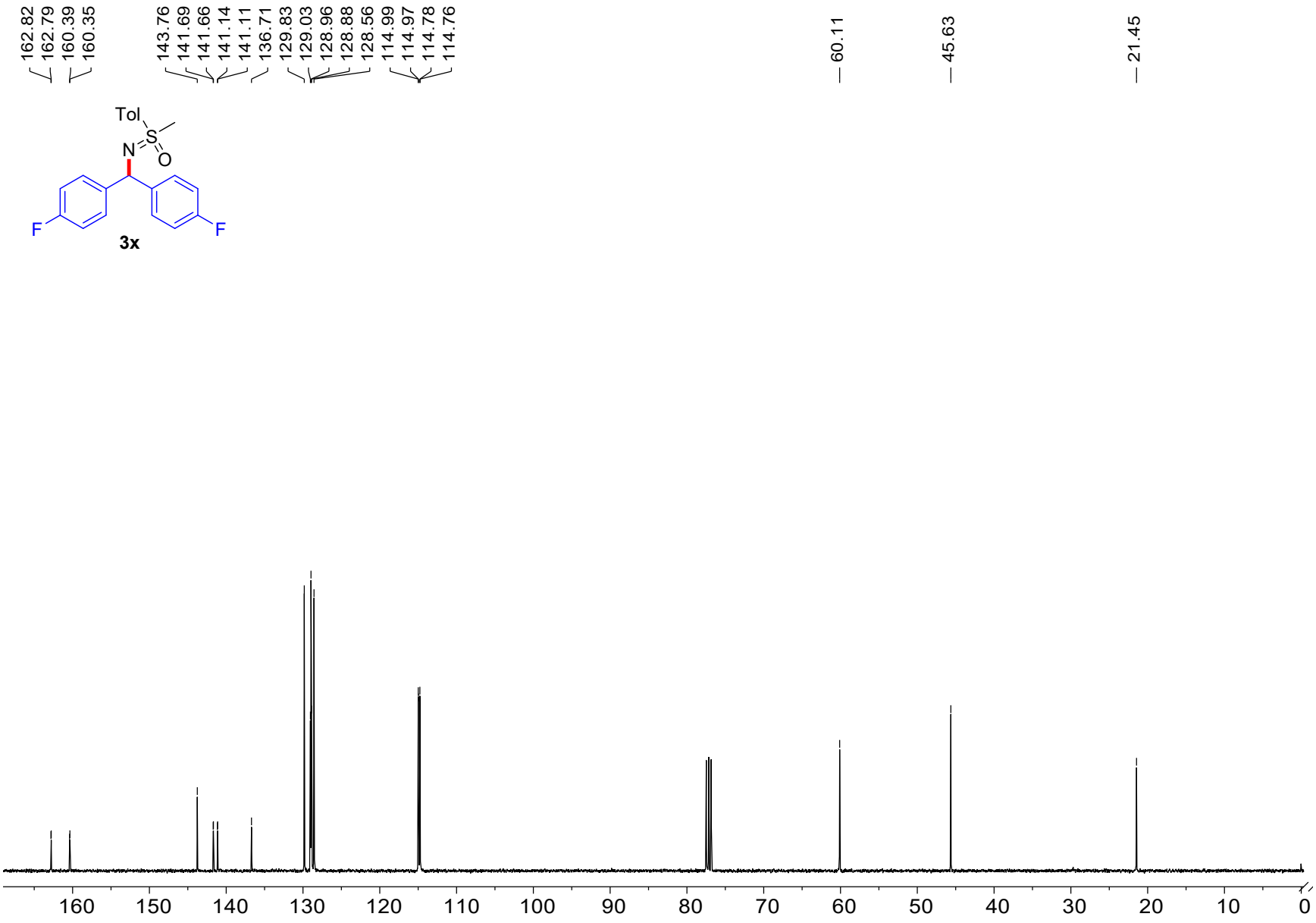
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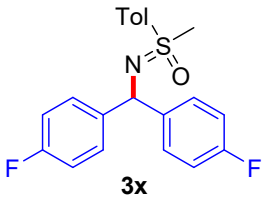

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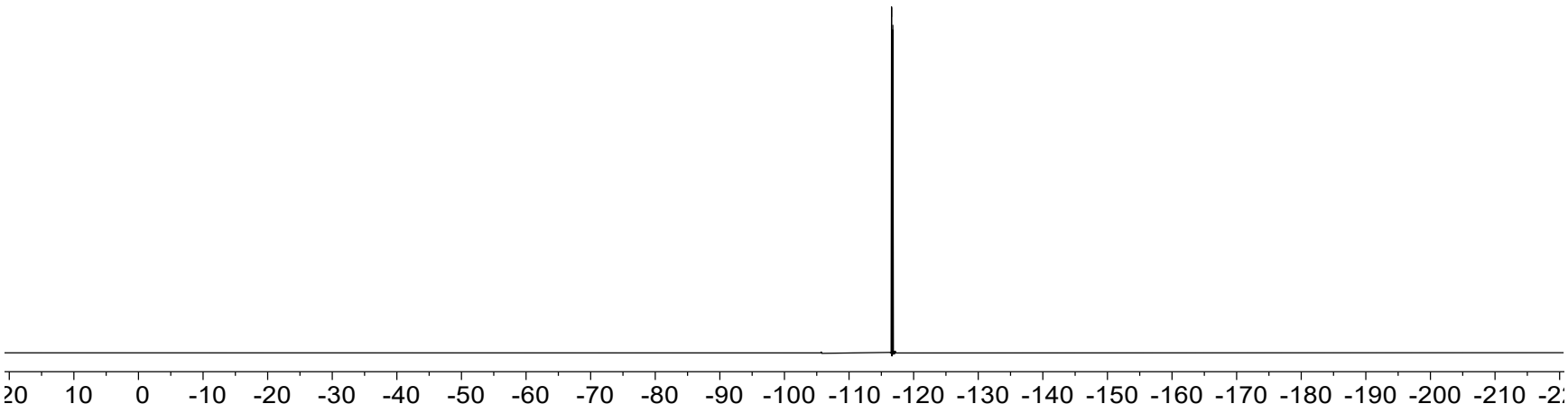

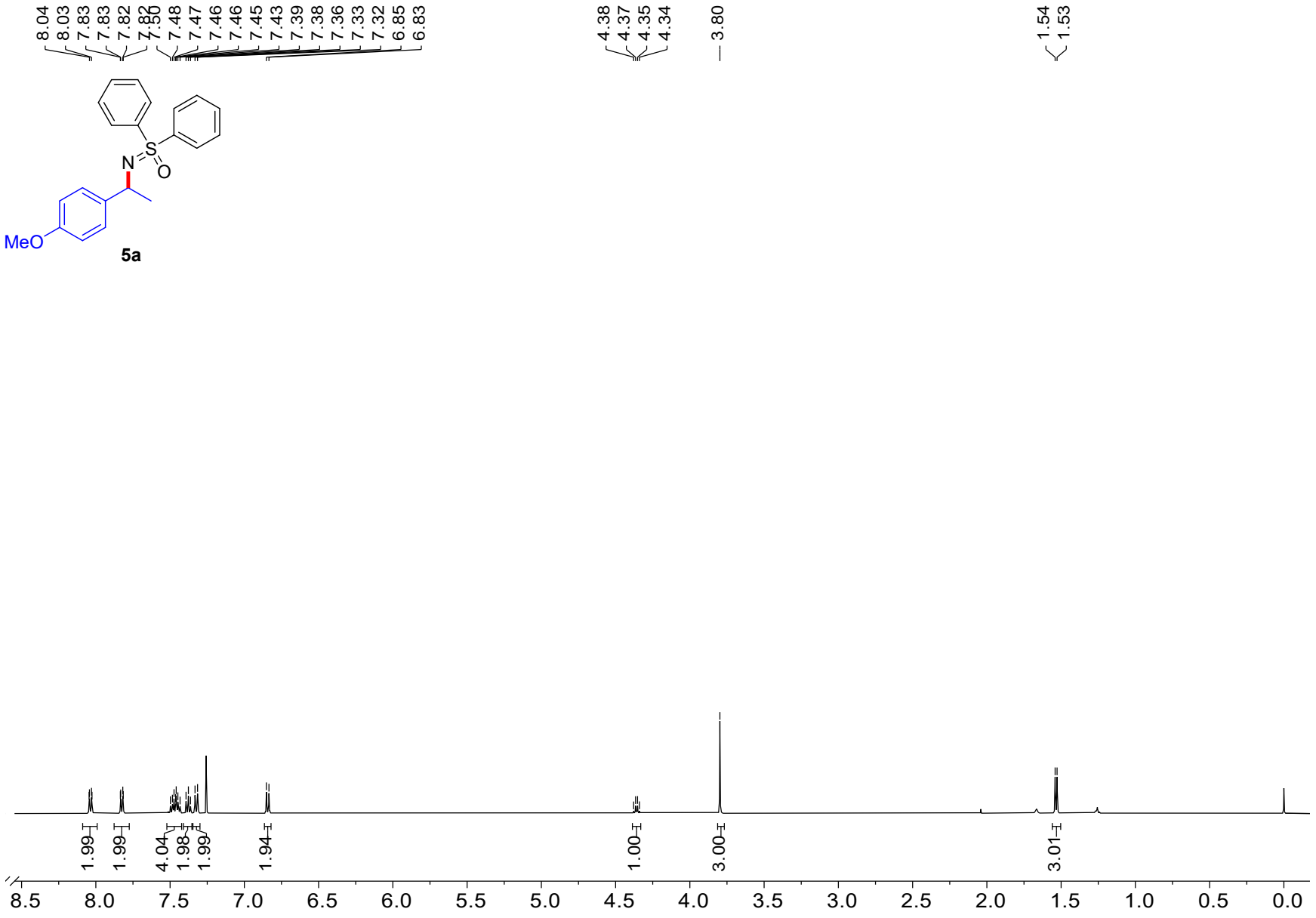
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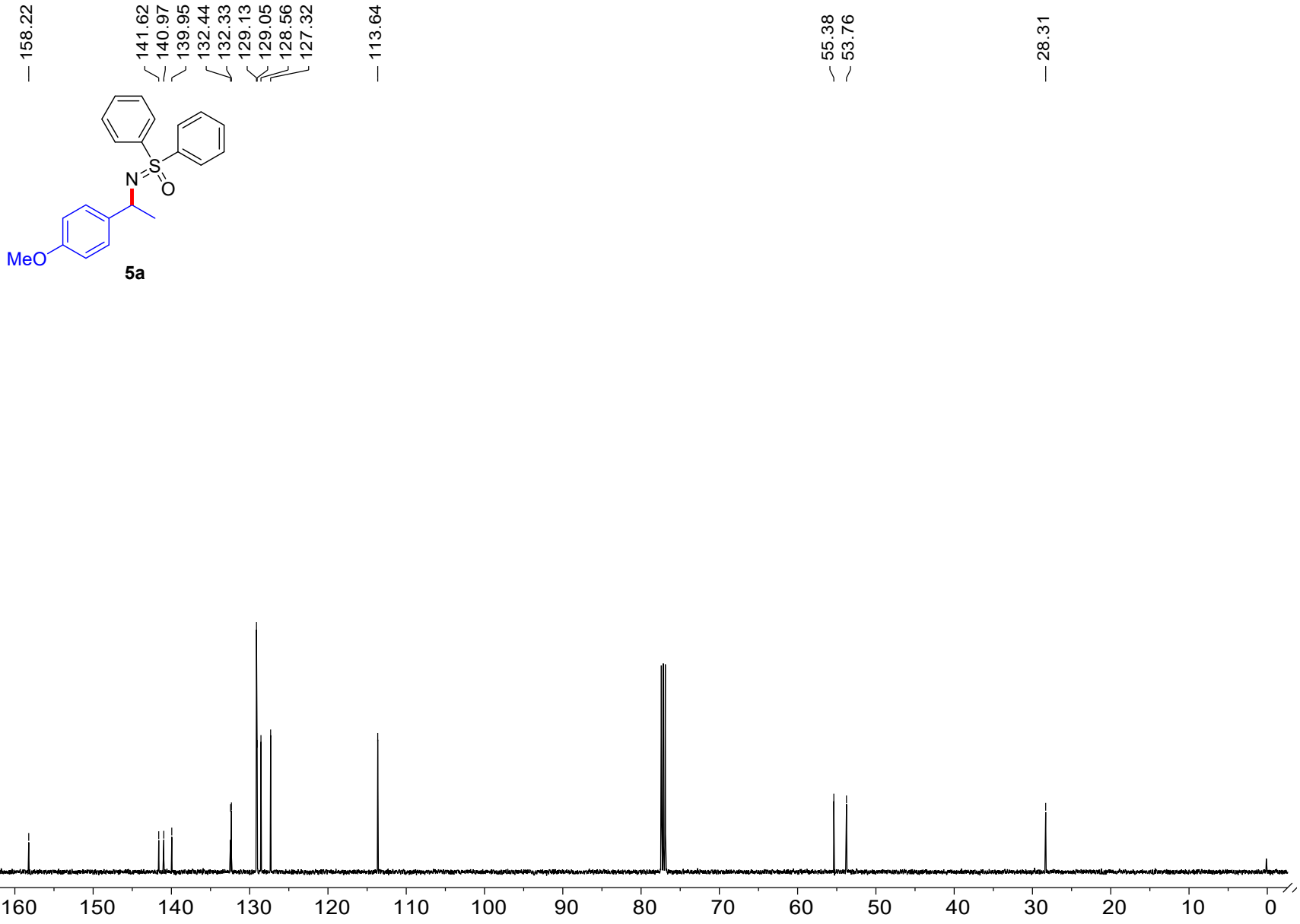
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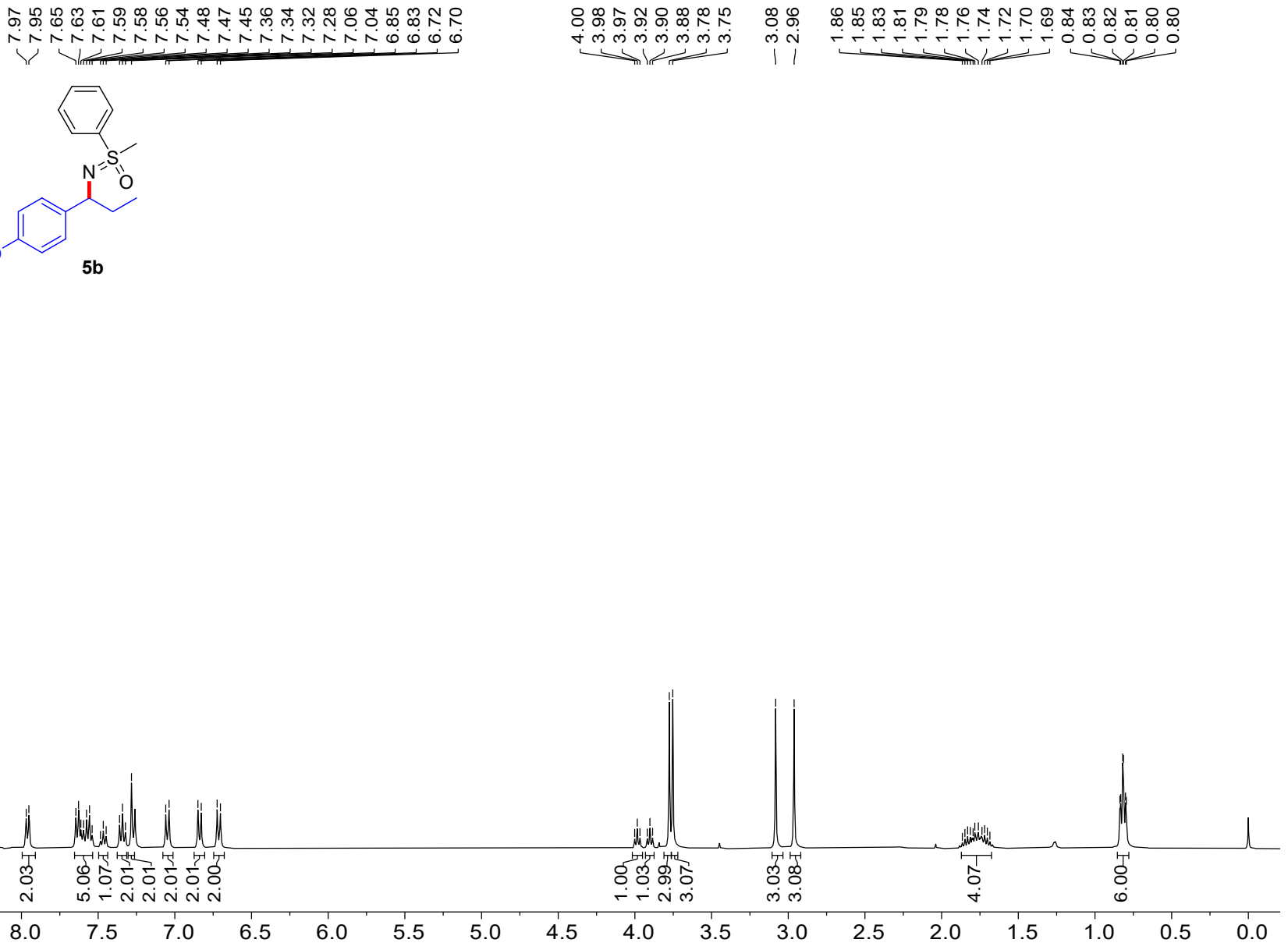
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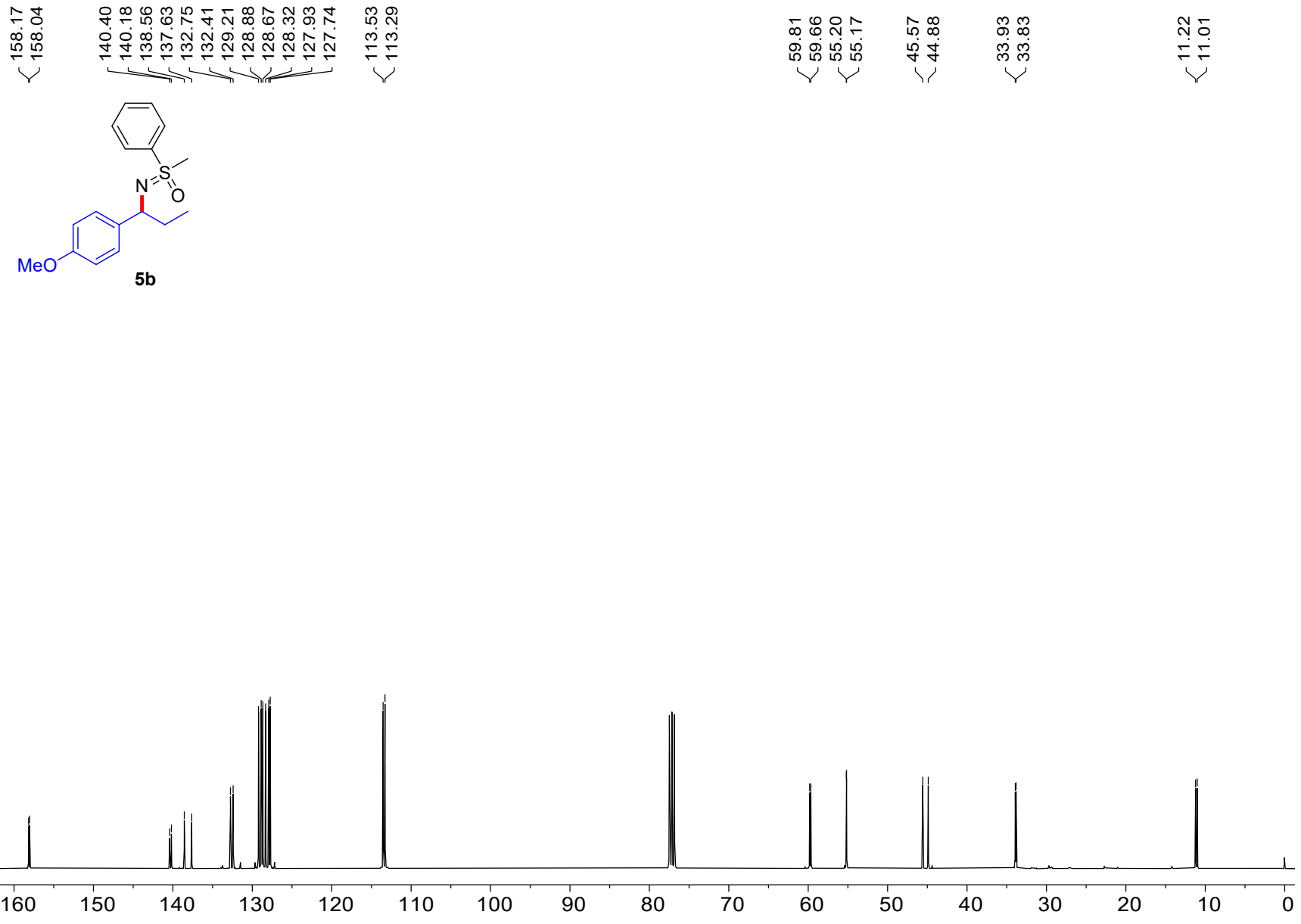
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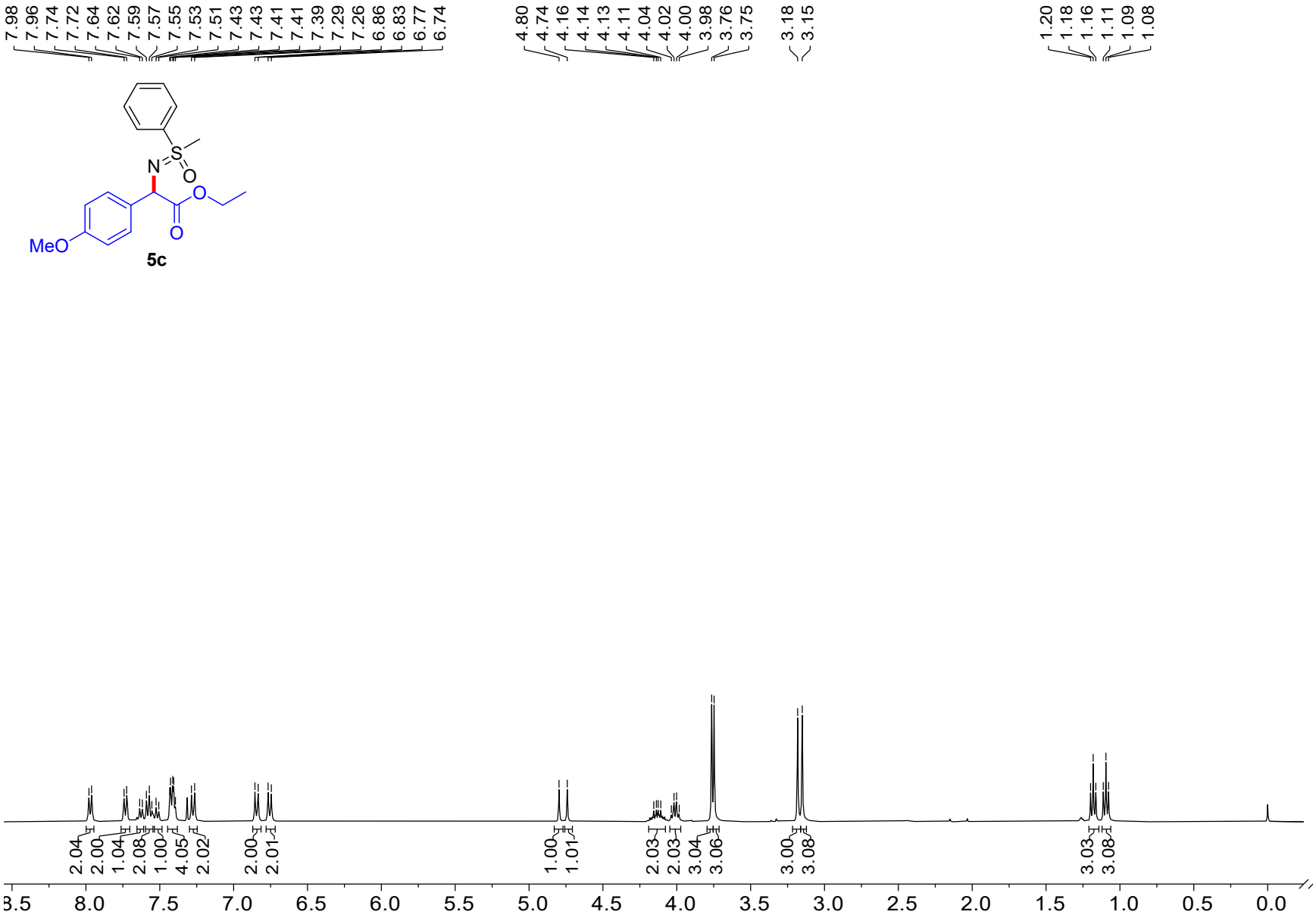
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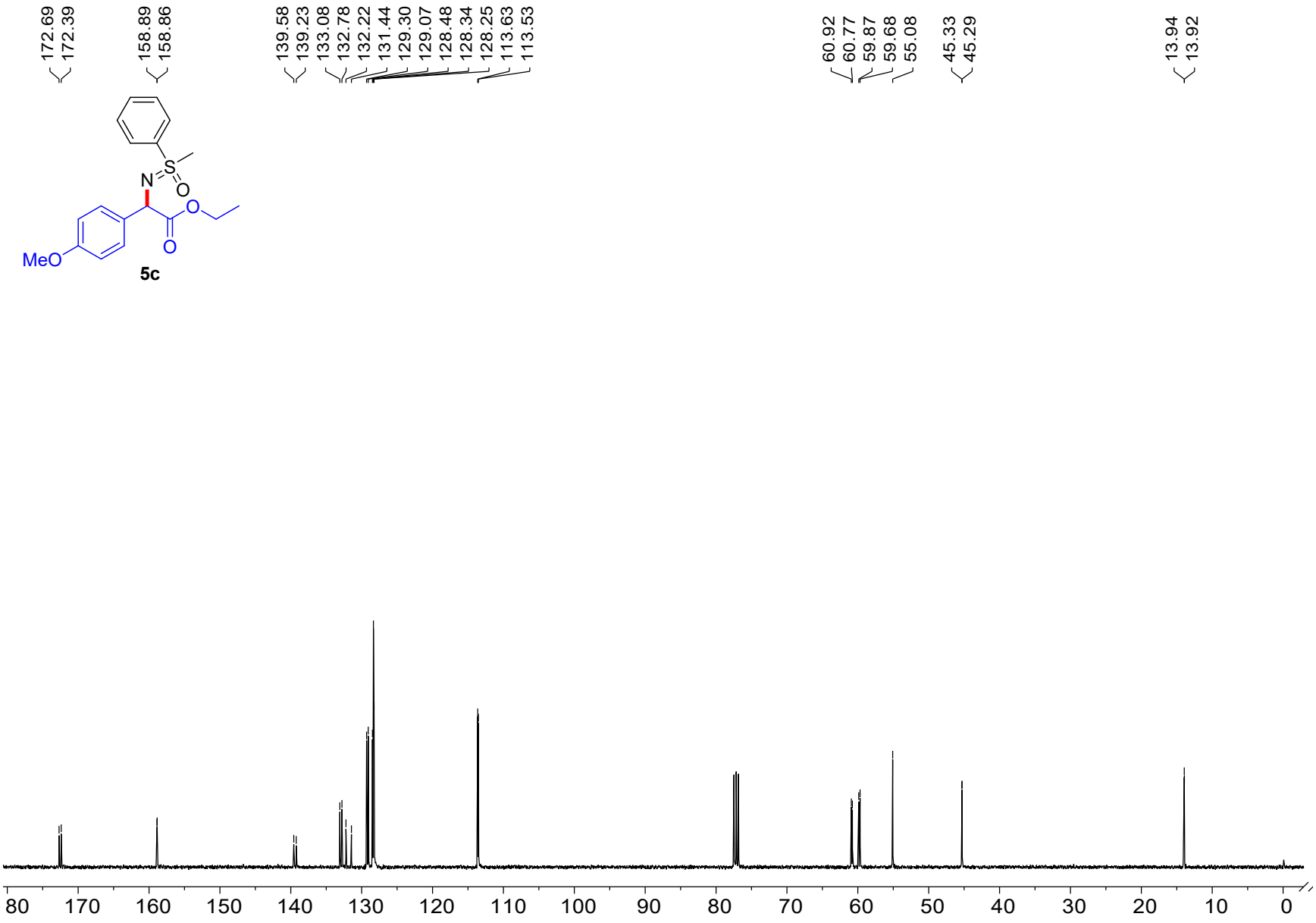
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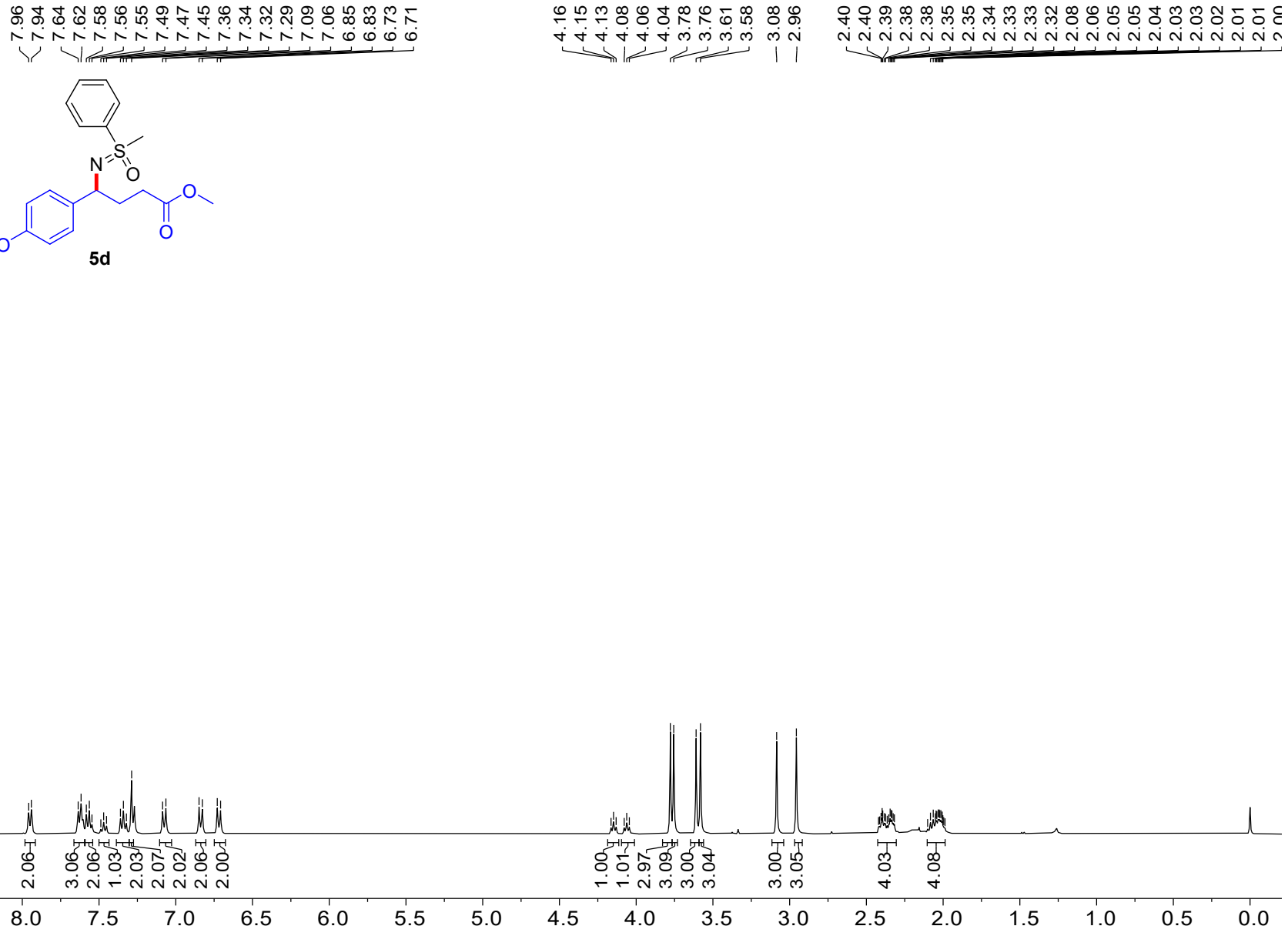
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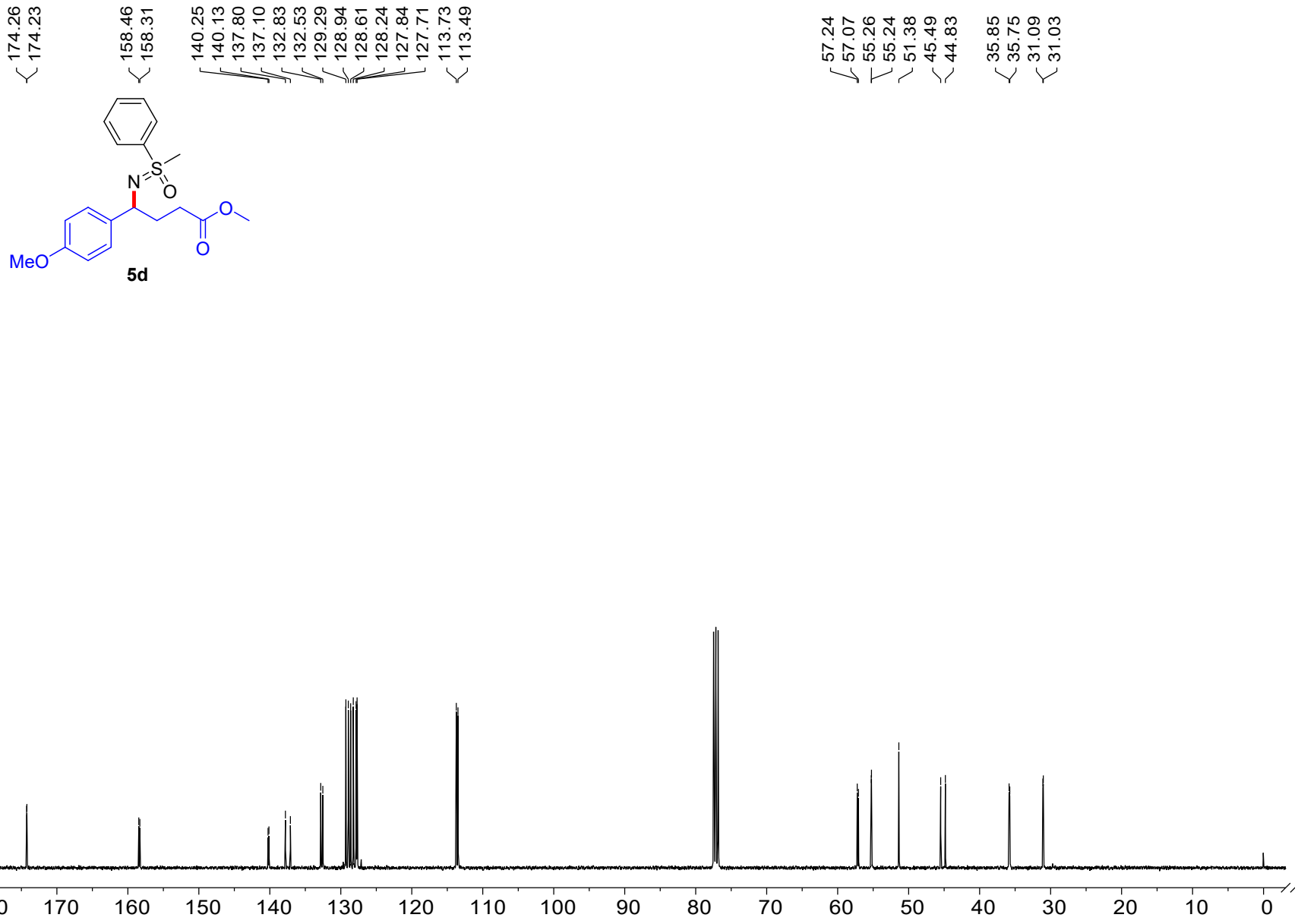
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5d
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160
150
140
130
120
110
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90
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70
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50
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7. References

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