Electronic Supplementary Material (ESI) for ChemComm.

Catalyst-controlled Switch of Regioselectivity in the Asymmetric Allylic Alkylation of Oxazolones with MBHCs

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1. General information

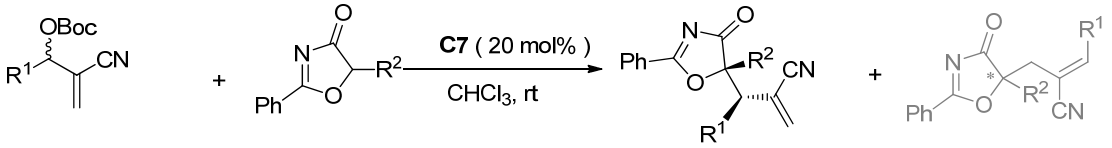
Unless stated otherwise, all reactions were carried out in flame dried glassware. All solvents were purified and dried according to standard methods prior to use. MBHCs **1**[1], oxazol-4(5H) -ones **2**[2] and catalysts **C1-18**[3] were prepared according to literature. ^{1}H and ^{13}C NMR spectra were recorded on a Varian instrument (300 MHz and 75 MHz, respectively) and internally referenced to tetramethylsilane signal or residual protio solvent signals. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet or unresolved, coupling constant(s) in Hz, integration). Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm). IR spectra were recorded on a FT-IR spectrometer and only major peaks were reported in cm^{-1}. Optical rotations were reported as follows: $[\alpha]_D^{rt}$ (c: g/100 mL, in solvent). High resolution mass spectra (HRMS) were obtained by the ESI ionization sources. The ee value determination was carried out using chiral HPLC with Daicel Chiracel column on Waters with a 996 UV-detector.

[1] J. Feng, X. Lu, A. Kong, X. Han, *Tetrahedron* **2007**, *63*, 6035.

[2] B. M., Trost; K., Dogra; M., Franzini, *J. Am. Chem. Soc.* **2004**, *126*, 1944-1945.

[3] (a) T. Okino, Y. Hoashi, Y. Takemoto, *J. Am. Chem. Soc.* **2003**, *125*, 12672. (b) S. Hu, L. Zhang, J. Li, S. Luo, J.-P. Cheng, *Eur. J. Org. Chem.,* 2011, 3347. (c) C. Xu, L. Zhang, S. Luo, *J. Org. Chem.*, 2014, **79**, 11517. (d) X. Bai, Z. Jing, Q. Liu, X. Ye, G. Zhang, X. Zhao, Z. Jiang, *J. Org. Chem.*, 2015, ***80*** , 12686.

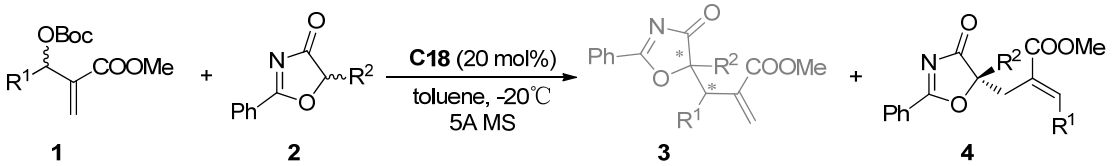
2. General experimental procedure for γ-selective secondary allylation between MBHCs and oxazol-4(5H)-ones



1 **2** **3** **4**

In an ordinary vial, oxazol-4(5H)-ones **2** (0.10 mmol) was added to a stirred mixture of MBHCs **1** (0.10 mmol) and catalyst **C7** (0.02 mmol) in $CHCl_3$ (1.0 mL) at room temperature. The mixture was stirred at this temperature for the requisite amount of time as monitored by TLC. The solvent was removed under vacuum and residue was chromatographed on silica gel (petroleum ether/AcOEt 10:1 - 4:1) and fractions were collected and concentrated in vacuo to provide the pure desired products **3**.

3. General experimental procedure for β-selective secondary allylation between MBHCs and oxazol-4(5H)-ones

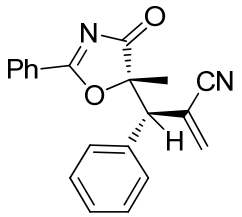


1 **2** **3** **4**

In an ordinary vial, oxazol-4(5H)-ones **2** (0.10 mmol) was added to a stirred mixture of MBHCs **1** (0.30 mmol), catalyst **C18** (0.02 mmol) and 5A MS (100 mg) in Tol (1.0 mL) at -20℃. The mixture was stirred at this temperature for the requisite amount of time as monitored by TLC. The solvent was removed under vacuum and residue was chromatographed on silica gel (petroleum ether/AcOEt 10:1 - 4:1) and fractions were collected and concentrated in vacuo to provide the pure desired products **4**.

4. Characterization of 3 and 4

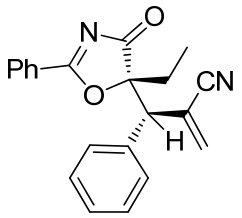
2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3aa'



3aa'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (d, *J* = 1.2, 2H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.65 – 7.58 (m, 4H), 7.52 – 7.43 (m, 3H), 6.01 (s, 1H), 5.88 (s, 1H), 3.99 (s, 1H), 1.42 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.9, 186.4, 135.7, 135.7, 134.2, 130.7, 129.3, 129.1, 128.8, 125.2, 120.5, 117.1, 89.8, 56.2, 21.1. **IR**: 3374, 2923, 2375, 1754, 1602, 1590, 1545, 1451, 1354, 1297, 1148, 1098, 1043, 764, 713 cm^{-1}; **$[\alpha]_D^{rt}$** = -164°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{20}H_{16}N_2O_2$+H, Calc: 317.1285, Found: 317.1293; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 7.5, t_{minor} = 8.6, 95% ee.

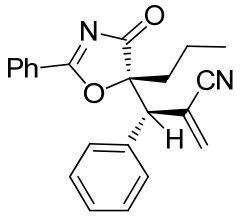
2-((R)-((S)-5-ethyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ba'



3ba'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.5 Hz, 2H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 4H), 7.54 – 7.33 (m, 3H), 6.02 (s, 1H), 5.87 (s, 1H), 4.01 (s, 1H), 1.80 (dd, *J* = 14.5, 7.1 Hz, 2H), 0.75 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.4, 186.9, 135.7, 135.7, 134.3, 130.6, 129.2, 129.2, 129.1, 128.6, 125.0, 120.5, 117.1, 93.5, 55.9, 27.7, 6.9. **IR**: 3363, 2927, 2364, 1753, 1603, 1590, 1546, 1489, 1452, 1358, 1301, 1205, 1151, 1056, 719, 700 cm^{-1}; **$[\alpha]_D^{rt}$** = -140°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{19}N_2O_2$+H, Calc: 331.1441, Found: 331.1450; **HPLC**: DAICEL CHIRALCEL IA, Hexane/EtOH = 80/20, flow rate = 1.0 ml/min, retention time: t_{major} = 8.1, t_{minor} = 6.6, 96% ee.

2-((R)-((S)-4-oxo-2-phenyl-5-propyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ca'

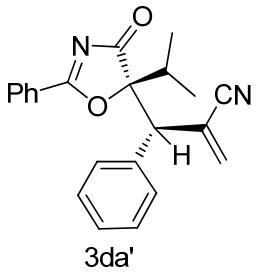


3ca'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 – 8.37 (m, 2H), 7.78 – 7.73 (m, 1H), 7.61 (t, *J* = 7.6 Hz, 4H), 7.55 – 7.37 (m, 3H), 6.01 (s, 1H), 5.87 (s, 1H), 3.99 (s, 1H), 1.74 – 1.67 (m, 2H), 1.20 – 1.12 (m, 2H), 0.75 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.5, 186.9, 135.7, 135.7, 134.3, 130.7, 129.3, 129.2, 129.1, 128.7, 125.0, 120.5, 117.1, 93.2, 56.2, 36.4, 16.0, 13.6. **IR**: 3398, 2925, 2375, 1754, 1603, 1546, 1451, 1354, 1288, 1150, 1107, 1063, 718 cm^{-1}; **$[\alpha]_D^{rt}$** = -112°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{20}N_2O_2$+H, Calc: 345.1598, Found: 345.1607; **HPLC**: DAICEL CHIRALCEL IA, Hexane/EtOH = 95/5, flow rate = 1.0 ml/min, retention time: t_{major} = 15.1, t_{minor}

=11.7, 95% ee.

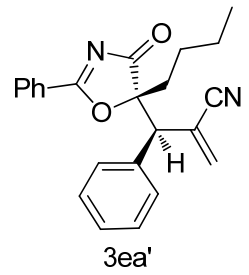
2-((R)-((S)-5-isopropyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3da'



3da'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.5 Hz, 2H), 7.76 (t, *J* = 7.3 Hz, 1H), 7.66 – 7.59 (m, 4H), 7.50 – 7.39 (m, 3H), 6.05 (s, 1H), 5.86 (s, 1H), 4.19 (s, 1H), 2.28 – 2.18 (m, 1H), 1.06 (d, *J* = 6.9 Hz, 3H), 0.80 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 191.3, 186.5, 135.7, 135.5, 134.0, 130.6, 129.4, 129.2, 129.1, 128.7, 124.9, 121.0, 117.2, 95.2, 54.2, 32.0, 16.4, 14.3. **IR**: 3397, 2925, 2375, 1751, 1603, 1549, 1451, 1353, 1298, 1154, 1068, 1029, 740, 719, 701 cm^{-1}; **$[\alpha]_D^{rt}$** = -128°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{20}N_2O_2$+H, Calc: 345.1598, Found: 345.1609; **HPLC**: DAICEL CHIRALCEL IA, Hexane/EtOH = 90/10, flow rate = 1.0 ml/min, retention time: t_{major} = 11.1, t_{minor} = 7.6, 97% ee.

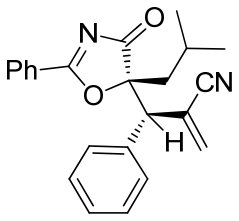
2-((R)-((S)-5-butyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ea'



3ea'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 – 8.38 (m, 2H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.69 – 7.56 (m, 4H), 7.51 – 7.40 (m, 3H), 6.01 (s, 1H), 5.87 (s, 1H), 3.99 (s, 1H), 1.73 – 1.67 (m, 2H), 1.20 – 1.05 (m, 4H), 0.75 – 0.71 (m, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.5, 186.8, 135.7, 135.7, 134.3, 130.7, 129.3, 129.2, 129.1, 128.7, 125.0, 120.5, 117.1, 93.2, 56.1, 34.2, 24.5, 22.3, 13.6. **IR**: 3394, 2924, 2374, 1754, 1604, 1546, 1451, 1356, 1299, 1149, 717 cm^{-1}; **$[\alpha]_D^{rt}$** = -112°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{23}H_{22}N_2O_2$+H, Calc: 359.1754, Found: 359.1766; **HPLC**: DAICEL CHIRALCEL IA, Hexane/EtOH = 95/5, flow rate = 1.0 ml/min, retention time: t_{major} = 16.7, t_{minor} =12.8, 95% ee.

2-((R)-((S)-5-isobutyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3fa'

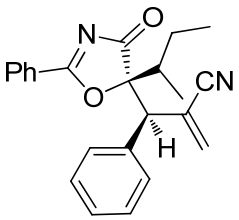


3fa'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 – 8.37 (m, 2H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 4H), 7.53 – 7.37 (m, 3H), 6.01 (s, 1H), 5.87 (s, 1H), 3.93 (s, 1H), 1.73 – 1.70 (m, 2H), 1.58 – 1.45 (m, 1H), 0.79 (d, *J* = 6.6 Hz, 3H), 0.73 (d, *J* = 6.5 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.7, 186.9, 135.8, 134.4, 130.6, 129.3, 129.2, 129.1, 128.7, 125.1, 120.3, 117.1, 93.3, 57.0, 42.8, 24.2, 23.6. **IR**: 3394, 2923, 2375, 1754, 1603, 1547, 1451, 1356, 1292, 1151, 1067, 718 cm^{-1}; **$[\alpha]_D^{rt}$** = -120°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{23}H_{22}N_2O_2$+H, Calc:

359.1754, Found: 359.1764; **HPLC**: DAICEL CHIRALCEL IA, Hexane/EtOH = 95/5, flow rate = 1.0 ml/min, retention time: t_{major} = 15.9, t_{minor} =12.4, 95% ee.

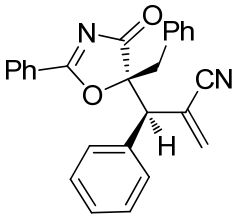
2-((R)-((S)-5-((S)-sec-butyl)-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ga'



3ga'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.5 Hz, 2H), 7.76 (t, *J* = 7.1 Hz, 1H), 7.66 – 7.59 (m, 4H), 7.51 – 7.42 (m, 3H), 6.03 (s, 1H), 5.85 (s, 1H), 4.21 (s, 1H), 1.92 – 1.94 (m, 1H), 1.28 – 1.24 (m, 1H), 1.04 (d, *J* = 6.7 Hz, 3H), 0.97 – 0.82 (m, 1H), 0.76 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 191.5, 186.4, 135.7, 135.5, 134.0, 130.7, 129.4, 129.3, 129.1, 128.6, 124.9, 120.9, 117.2, 95.0, 54.4, 38.6, 22.5, 11.6, 10.4. **IR**: 3389, 2924, 2376, 1752, 1603, 1548, 1450, 1353, 1260, 1119, 715 cm^{-1}; **$[\alpha]_D^{rt}$** = -144°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{23}H_{22}N_2O_2$+H, Calc: 359.1754, Found: 359.1762; **HPLC**: DAICEL CHIRALCEL IA, Hexane/EtOH = 95/5, flow rate = 1.0 ml/min, retention time: t_{major} = 13.2, t_{minor} =10.6, 98% ee.

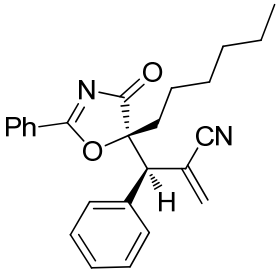
2-((R)-((S)-5-benzyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ha'



3ha'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17 (d, *J* = 7.6 Hz, 2H), 7.30 –7.10 (m, 3H), 7.60 – 7.38 (m, 5H), 7.15 – 7.00 (m, 5H), 6.05 (s, 1H), 5.88 (s, 1H), 4.15 (s, 1H), 3.14 – 2.93 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 191.7, 186.4, 135.9, 135.5, 134.3, 132.1, 130.3, 129.8, 129.5, 129.3, 128.9, 128.8, 128.3, 127.5, 124.9, 120.3, 117.1, 92.9, 55.9, 40.5. **IR**: 3368, 2924, 2367, 1754, 1603, 1548, 1451, 1358, 1296, 1180, 1123, 717, 699 cm^{-1}; **$[\alpha]_D^{rt}$** = -164°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{26}H_{20}N_2O_2$+H, Calc: 393.1598, Found: 393.1606; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/3, flow rate = 1.0 ml/min, retention time: t_{major} = 7.5, t_{minor} =5.8, 90% ee.

2-((R)-((S)-5-hexyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ia'

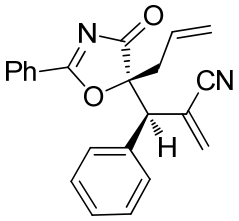


3ia'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.48 – 8.28 (m, 2H), 7.76 (t, *J* = 7.5 Hz, 1H), 7.67 – 7.57 (m, 4H), 7.52 – 7.38 (m, 3H), 6.01 (s, 1H), 5.87 (s, 1H), 3.98 (s, 1H), 1.80 – 1.65 (m, 2H), 1.12 – 1.00 (m, 8H), 0.76 (t, *J* = 6.7 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.5, 186.8, 135.7, 135.7, 134.3, 130.7, 129.3, 129.2, 129.1, 128.7, 125.0, 120.5, 117.2, 93.2, 56.2, 34.5, 31.2, 28.8, 22.4, 22.3, 13.9. **IR**: 3395, 2924, 2373, 1753, 1603, 1546, 1451, 1355, 1296, 1119, 715 cm^{-1}; **$[\alpha]_D^{rt}$** = -113°(c

= 1.00, $CHCl_3$); **HRMS** (ESI): $C_{25}H_{26}N_2O_2$+H, Calc: 387.2067, Found: 387.2077; **HPLC**: DAICEL CHIRALCEL IA, Hexane/EtOH = 95/5, flow rate = 1.0 ml/min, retention time: t_{major} = 12.7, t_{minor} =10.6, 96% ee.

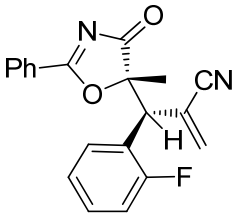
2-((R)-((S)-5-allyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ja'



3ja'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.4 Hz, 2H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.65 – 7.58 (m, 4H), 7.42 – 7.54 (m, 3H), 6.03 (s, 1H), 5.89 (s, 1H), 5.57 – 5.44 (m, 1H), 5.05 (s, 1H), 5.01 (d, *J* = 4.0 Hz, 1H), 4.03 (s, 1H), 2.47 (d, *J* = 7.2 Hz, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 191.8, 186.7, 135.9, 135.7, 134.0, 130.6, 129.4, 129.2, 129.1, 128.8, 128.0, 125.0, 121.9, 120.3, 117.1, 92.1, 55.6, 38.7. **IR**: 3368, 2923, 2372, 1754, 1603, 1548, 1489, 1451, 1357, 1291, 1191, 1115, 720, 701 cm^{-1}; **$[\alpha]_D^{rt}$** = -138°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{19}N_2O_2$+H, Calc: 343.1441, Found: 343.1452; **HPLC**: DAICEL CHIRALCEL IA, Hexane/EtOH = 95/5, flow rate = 1.0 ml/min, retention time: t_{major} = 19.8, t_{minor} =15.0, 95% ee.

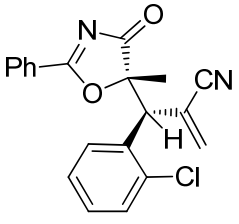
2-((R)-(2-fluorophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryloni trile, 3ab'



3ab'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.49 – 8.24 (m, 2H), 8.04 (m, *J* = 7.5, 1.8 Hz, 1H), 7.76 (t, *J* = 7.5 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 2H), 7.40 (m, *J* = 16.4, 7.4, 1.4 Hz, 2H), 7.21 – 7.08 (m, 1H), 6.09 (s, 1H), 5.94 (s, 1H), 4.55 (s, 1H), 1.47 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.4, 186.3, 160.8 (*J* = 246.0 Hz), 136.8, 135.8, 130.7, 130.4 (*J* = 8.3 Hz), 129.6 (*J* = 2.3 Hz), 129.1, 125.0 (*J* = 3.8 Hz), 121.4 (*J* = 13.5 Hz), 119.0, 116.9, 116.0 (*J* = 22.5 Hz), 115.85, 89.5, 46.6 (*J* = 5.2 Hz), 20.9. **IR**: 3368, 2926, 2373, 1758, 1603, 1547, 1490, 1451, 1354, 1232, 1148, 1104, 762, 709 cm^{-1}; **$[\alpha]_D^{rt}$** = -180°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{20}H_{15}FN_2O_2$+H, Calc: 335.1190, Found: 335.1197; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 6.8, t_{minor} = 7.6, 95% ee.

2-((R)-(2-chlorophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryloni trile, 3ac'

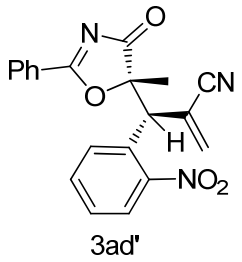


3ac'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.6 Hz, 2H), 8.13 (d, *J* = 7.5 Hz, 1H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 2H), 7.50 (dd, *J* = 7.3, 5.2 Hz, 2H), 7.38 (t, *J* = 7.4 Hz, 1H), 6.11 (s, 1H), 5.95 (s, 1H), 4.78 (s, 1H), 1.47 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.4, 186.2, 137.1,

135.8, 135.1, 131.6, 130.7, 130.3, 129.9, 129.7, 129.1, 127.8, 125.1, 118.5, 116.7, 89.7, 50.9, 20.8. **IR**: 3401, 2927, 2372, 1754, 1603, 1547, 1452, 1353, 1216, 1149, 1089, 1035, 889, 754, 706 cm^{-1}; $[\alpha]_D^{rt}$ = -172°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{20}H_{15}ClN_2O_2$+H, Calc: 351.0895, Found: 351.0905; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/2, flow rate = 1.0 ml/min, retention time: t_{major} = 6.3, t_{minor} = 6.9, 96% ee.

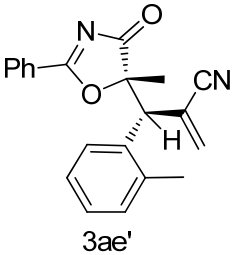
2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(2-nitrophenyl)methyl)acrylonitrile, 3ad'



3ad'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.35 (dd, *J* = 11.9, 7.8 Hz, 3H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.86 (t, *J* = 7.7 Hz, 1H), 7.78 (t, *J* = 7.5 Hz, 1H), 7.62 (t, *J* = 7.7 Hz, 3H), 6.17 (s, 1H), 6.03 (s, 1H), 4.79 (s, 1H), 1.43 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 191.7, 186.2, 150.6, 138.3, 136.0, 133.4, 130.7, 130.6, 129.8, 129.2, 128.1, 125.3, 124.9, 118.2, 116.7, 89.4, 49.1, 21.0. **IR**: 3396, 2924, 2374, 1756, 1603, 1546, 1451, 1353, 1297, 1217, 1150, 1103, 1035, 859, 773, 707 cm^{-1}; $[\alpha]_D^{rt}$ = -268°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{20}H_{15}N_3O_4$+H, Calc: 362.1135, Found: 362.1145; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 14.7, t_{minor} = 10.4, 94% ee.

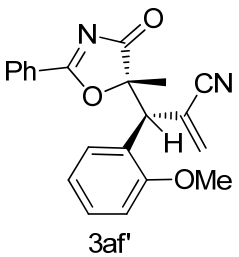
2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(o-tolyl)methyl)acrylonitrile, 3ae'



3ae'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.4 Hz, 2H), 8.01 (d, *J* = 7.7 Hz, 1H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 2H), 7.43 (t, *J* = 7.3 Hz, 1H), 7.36 – 7.26 (m, 2H), 6.00 (s, 1H), 5.90 (s, 1H), 4.32 (s, 1H), 2.37 (s, 3H), 1.45 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.2, 186.4, 137.0, 135.8, 135.6, 132.0, 131.2, 130.7, 129.1, 128.6, 128.4, 127.1, 125.2, 119.9, 116.9, 90.3, 50.9, 20.8, 19.7. **IR**: 3368, 2923, 2370, 1756, 1603, 1548, 1451, 1354, 1295, 1148, 1090, 1036, 887, 732, 710 cm^{-1}; $[\alpha]_D^{rt}$ = -175°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}N_2O_2$+H, Calc: 331.1441, Found: 331.1450; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 7.3, t_{minor} = 8.3, 91% ee.

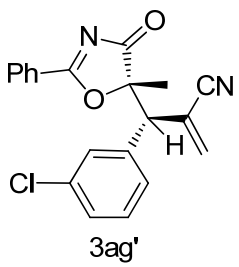
2-((R)-(2-methoxyphenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3af'



3af'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 – 8.21 (m, 2H), 7.98 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.74 (dd, *J* = 10.6, 4.3 Hz, 1H), 7.60 (t, *J* = 7.7 Hz, 2H), 7.39 (td,

J = 8.3, 1.6 Hz, 1H), 7.15 (td, *J* = 7.6, 0.9 Hz, 1H), 6.96 (d, *J* = 8.3 Hz, 1H), 6.02 (s, 1H), 5.87 (s, 1H), 4.80 (s, 1H), 3.86 (s, 3H), 1.44 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.2, 186.3, 157.3, 136.0, 135.6, 130.7, 129.7, 129.2, 129.0, 125.3, 122. 3, 121.1, 119.8, 117.3, 110.9, 90.3, 55.6, 46.4, 20.8. **IR**: 3369, 2924, 2852, 2373, 1756, 1603, 1546, 1491, 1451, 1354, 1248, 1148, 1112, 1025, 888, 762, 711 cm^{-1}; **$[\alpha]_D^{rt}$** = -122°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}N_2O_3$+H, Calc: 347.1390, Found: 347.1401; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 10.2, t_{minor} = 12.1, 96% ee.

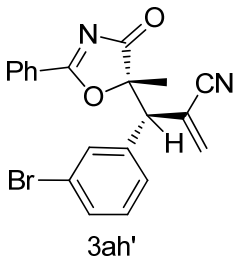


3ag'

2-((R)-(3-chlorophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3ag'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.44 – 8.25 (m, 2H), 7.81 – 7.70 (m, 1H), 7.67 – 7.52 (m, 4H), 7.52 – 7.34 (m, 2H), 6.03 (s, 1H), 5.91 (s, 1H), 3.97 (s, 1H), 1.43 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.4, 186.3, 136.2, 136.0, 135.8, 135.1, 130.7, 130.6, 129.5, 129.1, 129.0, 127.2, 125.0, 119.8, 116.7, 89.4, 55.6, 21.0. **IR**: 3369, 2927, 2367, 1757, 1603, 1546, 1489, 1451, 1353, 1300, 1217, 1148, 1096, 1036, 768, 711, 685 cm^{-1}; **$[\alpha]_D^{rt}$** = -164°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{20}H_{15}ClN_2O_2$+H, Calc: 351.0895, Found: 351.0901; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 6.8, t_{minor} = 7.7, 91% ee.

2-((R)-(3-bromophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3ah'

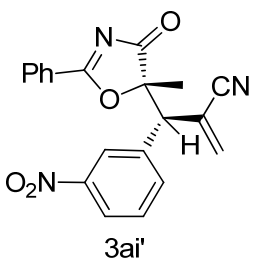


3ah'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.4 Hz, 2H), 7.77 (t, *J* = 7.4 Hz, 1H), 7.63 (m, 5H), 7.39 (t, *J* = 7.8 Hz, 1H), 6.02 (s, 1H), 5.92 (s, 1H), 3.95 (s, 1H), 1.43 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.4, 186.4, 136.3, 136.3, 135.9, 132.5, 132.0, 130.9, 130.7, 129.1, 127.6, 125.0 (s), 123.2 (s), 119.8 (s), 116.7 (s), 89.4 (s), 55.6 (s), 21.1 (s). **IR**: 3373, 2924, 2373, 1754, 1603, 1545, 1451, 1354, 1296, 1216, 1149, 770, 708 cm^{-1}; **$[\alpha]_D^{rt}$** = -144°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{20}H_{15}BrN_2O_2$+H, Calc: 395.0390, Found: 395.0397; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 6.8, t_{minor} = 7.9, 90% ee.

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(3-nitrophenyl)methyl)acrylonitrile, 3ai'

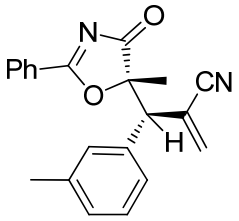
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.51 (t, *J* = 1.8 Hz, 1H), 8.43 – 8.27 (m, 3H), 8.06 (d, *J* = 7.8 Hz,



3ai'

1H), 7.85 – 7.69 (m, 2H), 7.64 (t, *J* = 7.7 Hz, 2H), 6.11 (s, 1H), 5.98 (s, 1H), 4.15 (s, 1H), 1.45 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.0, 186.4, 148.7, 136.8, 136.2, 136.0, 135.1, 130.7, 130.6, 129.2, 124.9, 124.5, 123.9, 119.3, 116.4, 89.0, 55.5, 21.1. **IR**: 3373, 2923, 2373, 1753, 1602, 1545, 1490, 1450, 1351, 1297, 1219, 1149, 1100, 769, 707 cm^{-1}; **$[\alpha]_D^{rt}$** = -211°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{20}H_{15}N_3O_4$+H, Calc: 362.1135, Found: 362.1142; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 22.4, t_{minor} = 37.2, 94% ee.

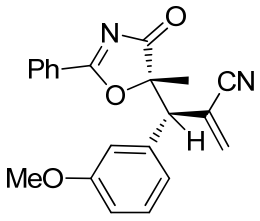
2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(m-tolyl)methyl)acrylonitrile, 3aj'



3aj'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.6 Hz, 2H), 7.75 (t, *J* = 7.3 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 2H), 7.51 (d, *J* = 7.5 Hz, 1H), 7.45 – 7.31 (m, 2H), 7.30 – 7.17 (m, 1H), 6.00 (s, 1H), 5.87 (s, 1H), 3.95 (s, 1H), 2.43 (s, 3H), 1.42 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.9, 186.3, 139.0, 135.7, 135.6, 134.0, 130.6, 130.1, 129.4, 129.2, 129.0, 126.0, 125.2, 120.5, 117.0, 89.8, 56.0, 21.5, 21.0. **IR**: 3372, 2925, 2371, 1758, 1604, 1547, 1489, 1451, 1354, 1301, 1147, 1037, 872, 716 cm^{-1}; **$[\alpha]_D^{rt}$** = -167°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}N_2O_2$+H, Calc: 331.1441, Found: 331.1449; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 7.2, t_{minor} = 8.5, 93% ee.

2-((R)-(3-methoxyphenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryl onitrile, 3ak'

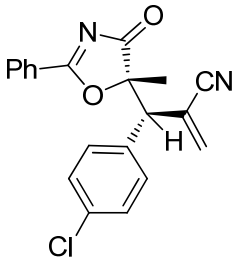


3ak'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.48 – 8.18 (m, 2H), 7.75 (dd, *J* = 10.6, 4.4 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 2H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.19 – 7.15 (m, 1H), 6.96 (dd, *J* = 8.0, 2.2 Hz, 1H), 6.00 (s, 1H), 5.89 (s, 1H), 3.95 (s, 1H), 3.89 (s, 3H), 1.44 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.9, 186.4, 160.0, 135.9, 135.7, 135.5, 130.7, 130.4, 129.1, 125.2, 121.4, 120.3, 117.1, 115.2, 113.8, 89.8, 56.1, 55.3, 21.0. **IR**: 3373, 2926, 2372, 1758, 1603, 1546, 1490, 1451, 1355, 1289, 1263, 1148, 1099, 1038, 955, 872, 788, 716 cm^{-1}; **$[\alpha]_D^{rt}$** = -171°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}N_2O_3$+H, Calc: 347.1390, Found: 347.1398; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/2, flow rate = 1.0 ml/min, retention time: t_{major} = 6.5, t_{minor} = 7.5, 93% ee.

2-((R)-(4-chlorophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryloni

trile, 3al'

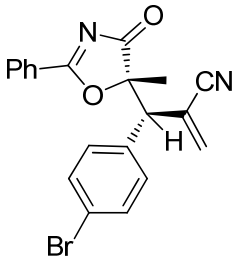


3al'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.4 Hz, 2H), 7.77 (t, *J* = 7.4 Hz, 1H), 7.66 – 7.53 (m, 4H), 7.47 (d, *J* = 8.5 Hz, 2H), 6.02 (s, 1H), 5.90 (s, 1H), 3.98 (s, 1H), 1.41 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.6, 186.4, 136.0, 135.9, 134.9, 132.6, 130.7, 130.6, 129.6, 129.1, 125.0, 120.0, 116.8, 89.5, 55.4, 21.0. **IR**: 3393, 2924, 2373, 1754, 1599, 1545, 1450, 1354, 1293, 1149, 1116, 773, 706, 668 cm^{-1}; **$[\alpha]_D^{rt}$** = -191°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{20}H_{15}ClN_2O_2$+H, Calc: 351.0895, Found: 351.0904; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 6.8, t_{minor} = 7.7, 94% ee.

2-((R)-(4-bromophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylon

itrile, 3am'

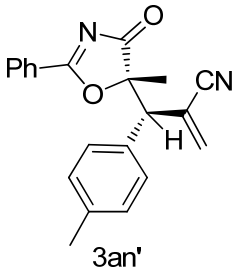


3am'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.5 Hz, 2H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.62 (dd, *J* = 11.9, 6.5 Hz, 4H), 7.53 (d, *J* = 8.4 Hz, 2H), 6.02 (s, 1H), 5.90 (s, 1H), 3.98 (s, 1H), 1.41 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.5, 186.3, 136.0, 135.8, 133.1, 132.5, 130.8, 130.6, 129.1, 125.0, 123.0, 119.8, 116.8, 89.4, 55.4, 21.0. **IR**: 3371, 2928, 2373, 1755, 1603, 1547, 1489, 1452, 1354, 1296, 1216, 1148, 1074, 1012, 889, 778, 726, 703, 511 cm^{-1}; **$[\alpha]_D^{rt}$** = -193°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{20}H_{15}BrN_2O_2$+H, Calc: 395.0390, Found: 395.0399; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 6.9, t_{minor} = 7.9, 90% ee.

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(p-tolyl)methyl)acrylonitrile,

3an'

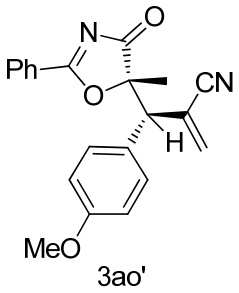


3an'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.38 – 8.36 (m, 2H), 7.74 (d, *J* = 7.5 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.35 – 7.16 (m, 3H), 5.99 (s, 1H), 5.86 (s, 1H), 3.95 (s, 1H), 2.40 (s, 3H), 1.41 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.0, 186.3, 138.6, 135.7, 135.5, 131.1, 130.7, 130.0, 129.1, 125.2, 120.7, 117.1, 90.0, 55.7, 21.2, 21.0. **IR**: 3400, 2924, 2368, 1754, 1617, 1546, 1451, 1354, 1296, 1217, 1148, 1118, 889, 767, 708 cm^{-1}; **$[\alpha]_D^{rt}$** = -203°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}N_2O_2$+H, Calc: 331.1441, Found: 331.1450; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} =

7.3, t_{minor} = 8.5, 95% ee.

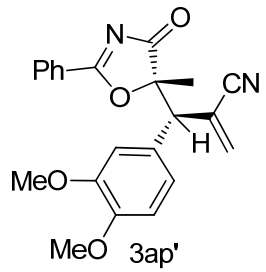
2-((R)-(4-methoxyphenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryl onitrile, 3ao'



3ao'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.3 Hz, 2H), 7.75 (t, *J* = 7.4 Hz, 1H), 7.66 – 7.45 (m, 4H), 7.01 (d, *J* = 8.7 Hz, 2H), 5.98 (s, 1H), 5.86 (s, 1H), 3.94 (s, 1H), 3.86 (s, 3H), 1.41 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.0, 186.3, 159.8, 135.7, 135.3, 130.7, 130.4, 129.1, 126.0, 125.2, 120.8, 117.2, 114.7, 90.1, 55.3, 55.3, 21.0. **IR**: 3397, 2923, 2375, 1753, 1603, 1546, 1512, 1450, 1354, 1253, 1148, 1023, 766, 708 cm^{-1}; **$[\alpha]_D^{rt}$** = -205°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}N_2O_3$+H, Calc: 347.1390, Found: 347.1399; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 8.3, t_{minor} = 9.5, 93% ee.

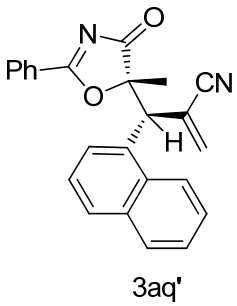
2-((R)-(3,4-dimethoxyphenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)ac rylonitrile, 3ap'



3ap'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.35 (d, *J* = 7.8 Hz, 2H), 7.75 (dd, *J* = 10.8, 4.1 Hz, 1H), 7.60 (t, *J* = 7.7 Hz, 2H), 7.25 – 7.09 (m, 2H), 6.97 (d, *J* = 8.2 Hz, 1H), 6.00 (s, 1H), 5.88 (s, 1H), 4.00 (s, 3H), 3.93 (s, 4H), 1.44 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.8, 186.1, 149.2, 135.6, 135.4, 130.4, 129.0, 126.3, 125.2, 121.7, 120.4, 117.2, 112.0, 111.4, 90.0, 55.9, 55.8, 55.5, 21.0. **IR**: 3369, 2923, 2374, 1756, 1603, 1548, 1516, 1451, 1355, 1265, 1146, 1026, 737 cm^{-1}; **$[\alpha]_D^{rt}$** = -184°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{20}N_2O_4$+H, Calc: 377.1496, Found: 377.1500; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 13.0, t_{minor} = 16.7, 95% ee.

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(naphthalen-1-yl)methyl)acrylon itrile, 3aq'

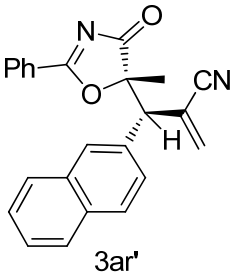


3aq'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.43 (d, *J* = 7.5 Hz, 2H), 8.28 (d, *J* = 7.2 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 8.1 Hz, 2H), 7.77 (t, *J* = 7.3 Hz, 1H), 7.63 – 7.54 (m, 5H), 6.17 (s, 1H), 5.94 (s, 1H), 5.01 (s, 1H), 1.51 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.3, 186.5, 136.0, 135.8, 134.2, 131.6, 130.8, 129.6, 129.5, 129.4, 129.1, 127.2, 126.9, 126.1, 125.7, 125.2, 121.6, 120.3, 116.9, 90.5, 49.6, 20.9. **IR**: 3395, 2923, 2374, 1600, 1545, 1450, 1351, 1297, 1259, 1149, 1121, 854, 779, 709, 663 cm^{-1}; **$[\alpha]_D^{rt}$** = -109°(c = 1.00, $CHCl_3$); **HRMS** (ESI):

$C_{24}H_{18}N_2O_2$+H, Calc: 367.1441, Found: 367.1447; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/2, flow rate = 1.0 ml/min, retention time: t_{major} = 6.4, t_{minor} = 7.5, 94% ee.

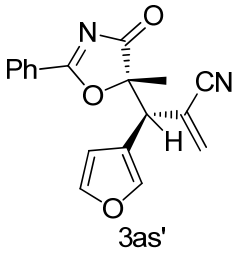
2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(naphthalen-2-yl)methyl)acrylonitrile, 3ar'



3ar'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.42 (d, *J* = 7.4 Hz, 2H), 8.00 (d, *J* = 9.0 Hz, 2H), 7.92 (td, *J* = 7.1, 4.1 Hz, 2H), 7.84 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.77 (t, *J* = 7.4 Hz, 1H), 7.62 (dd, *J* = 14.0, 6.4 Hz, 2H), 7.59 – 7.45 (m, 2H), 6.06 (s, 1H), 5.91 (s, 1H), 4.18 (s, 1H), 1.44 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.9, 186.4, 135.8, 135.8, 133.4, 133.1, 131.6, 130.7, 129.3, 129.1, 129.0, 128.1, 127.7, 126.8, 126.7, 126.1, 125.2, 120.4, 117.1, 89.9, 56.2, 21.2. **IR**: 3384, 2924, 2372, 1753, 1602, 1545, 1451, 1353, 1295, 1213, 1147, 1038, 779, 712 cm^{-1}; **$[\alpha]_D^{rt}$** = -210°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{24}H_{18}N_2O_2$+H, Calc: 367.1441, Found: 367.1447; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/2, flow rate = 1.0 ml/min, retention time: t_{major} = 6.9, t_{minor} = 8.2, 93% ee.

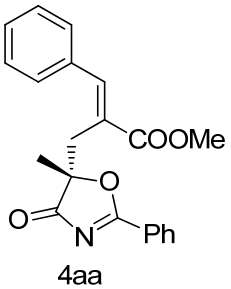
2-((R)-furan-3-yl((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3as'



3as'

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.6 Hz, 2H), 7.75 (t, *J* = 7.4 Hz, 1H), 7.69 – 7.48 (m, 4H), 6.78 (s, 1H), 5.97 (s, 1H), 5.90 (s, 1H), 3.97 (s, 1H), 1.48 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.4, 186.3, 144.0, 141.5, 135.8, 135.6, 130.6, 129.1, 125.2, 120.0, 118.2, 117.1, 110.5, 89.6, 47.0, 21.0. **IR**: 3391, 2923, 2373, 1753, 1600, 1589, 1545, 1451, 1354, 1295, 1248, 1151, 1116, 1028, 873, 770, 712, 609 cm^{-1}; **$[\alpha]_D^{rt}$** = -94°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{18}H_{14}N_2O_3$+H, Calc: 307.1077, Found: 307.1084; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 7.5, t_{minor} = 8.4, 90% ee.

(S,E)-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate 4aa (Table 4., entry 1)

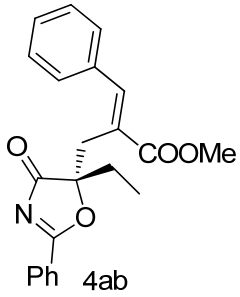


4aa

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 – 7.94 (m, 2H), 7.85 (s, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.44 – 7.28 (m, 5H), 3.73 (s, 3H), 3.41 – 3.20 (m, 2H), 1.51 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 193.2, 184.8, 168.3, 143.4, 135.0, 134.9, 130.0, 129.0, 128.8, 128.8, 128.7, 126.3, 125.6, 86.9, 52.2, 33.3, 21.9. **IR**: 2951, 1758, 1716, 1604, 1551, 1490,

1451, 1359, 1248, 1145, 1121, 764, 706 cm^{-1}; $[\alpha]_D^{rt}$ = -44°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{19}NO_4$+H, Calc: 350.1387, Found: 350.1399; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 17.7, t_{minor} = 25.7, 98% ee.

(S,E)-methyl-2-((5-ethyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate

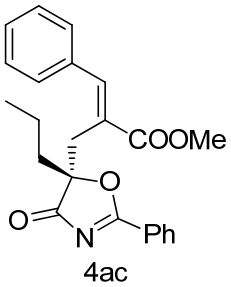


4ab

4ab (Table 4., entry 2)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 – 7.95 (m, 2H), 7.79 (s, 1H), 7.72 – 7.61 (m, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.43 – 7.28 (m, 5H), 3.70 (s, 3H), 3.44 – 3.24 (m, 2H), 2.07 – 1.81 (m, 2H), 0.77 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 192.7, 185.3, 168.3, 143.2, 135.0, 134.9, 130.0, 129.0, 128.8, 126.4, 125.5, 90.4, 52.1, 32.7, 28.9, 7.2. **IR**: 2950, 1756, 1717, 1604, 1551, 1490, 1451, 1362, 1293, 1239, 1204, 1150, 1127, 760, 706 cm^{-1}; $[\alpha]_D^{rt}$ = -31°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{21}NO_4$+H, Calc: 364.1543, Found: 364.1554; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/2, flow rate = 1.0 ml/min, retention time: t_{major} = 7.9, t_{minor} = 9.1, 97% ee.

(S,E)-methyl-2-((4-oxo-2-phenyl-5-propyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate

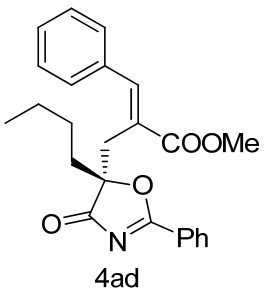


4ac

4ac (Table 4., entry 3)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 – 7.92 (m, 2H), 7.79 (s, 1H), 7.72 – 7.58 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.42 – 7.28 (m, 5H), 3.70 (s, 3H), 3.41 – 3.20 (m, 2H), 1.98 – 1.75 (m, 2H), 1.33 – 0.98 (m, 2H), 0.82 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 192.8, 185.2, 168.4, 143.2, 135.0, 134.9, 130.0, 129.0, 128.8, 128.6, 126.4, 125.5, 90.0, 52.1, 37.8, 32.9, 16.2, 13.7. **IR**: 2958, 1757, 1717, 1604, 1549, 1490, 1451, 1356, 1293, 1203, 1149, 765, 708 cm^{-1}; $[\alpha]_D^{rt}$ = -35°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{23}H_{23}NO_4$+H, Calc: 378.1700, Found: 378.1712; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 13.0, t_{minor} = 18.1, 97% ee.

(S,E)-methyl-2-((5-butyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate



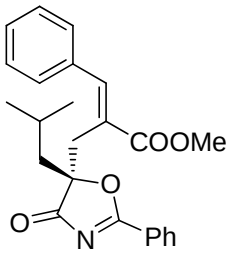
4ad

4ad (Table 4, entry 4)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 – 7.97 (m, 2H), 7.79 (s, 1H), 7.73 – 7.61 (m, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.44 – 7.29 (m, 5H), 3.70 (s, 3H), 3.41 – 3.24 (m, 2H), 2.00 – 1.78 (m, 2H), 1.32 – 0.96 (m, 4H), 0.78 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 192.8, 185.2, 168.3, 143.2, 135.0, 134.9, 130.0, 129.0, 128.8, 128.6, 126.4, 125.5, 90.0, 52.1, 35.5, 32.9, 24.7, 22.4, 13.6. **IR**: 2956, 1757, 1718, 1604,

1551, 1490, 1451, 1359, 1296, 1246, 1180, 1148, 763, 708 cm^{-1}; $[\alpha]_D^{rt}$ = -43°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{24}H_{25}NO_4$+H, Calc: 392.1856, Found: 392.1866; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 11.9, t_{minor} = 15.8, 97% ee.

(S,E)-methyl-2-((5-isobutyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate

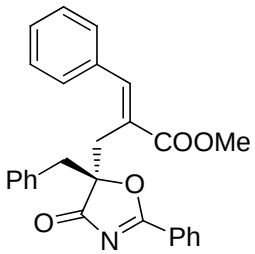


4ae

4ae (Table 4., entry 5)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 – 7.92 (m, 2H), 7.76 (s, 1H), 7.71 – 7.59 (m, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.43 – 7.28 (m, 5H), 3.67 (s, 3H), 3.33 (q, *J* = 14.2 Hz, 2H), 1.91 (dd, *J* = 14.7, 6.2 Hz, 1H), 1.77 (dd, *J* = 14.7, 6.3 Hz, 1H), 1.70 – 1.54 (m, 1H), 0.82 (dd, *J* = 9.0, 6.6 Hz, 6H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 193.0, 185.1, 168.3, 143.2, 135.0, 134.9, 130.0, 128.9, 128.8, 128.7, 128.6, 126.4, 125.6, 90.0, 52.1, 44.2, 33.3, 24.1, 23.8, 23.5. **IR**: 2956, 1757, 1718, 1604, 1551, 1490, 1451, 1357, 1290, 1151, 762, 709 cm^{-1}; $[\alpha]_D^{rt}$ = -20°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{24}H_{25}NO_4$+H, Calc: 392.1856, Found: 392.1867; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/2, flow rate = 1.0 ml/min, retention time: t_{major} = 8.9, t_{minor} = 13.3, 96% ee.

(S,E)-methyl-2-((5-benzyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate

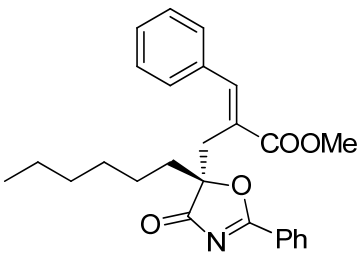


4af

4af (Table 4., entry 6)

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 – 7.81 (m, 2H), 7.79 (s, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.30 (s, 5H), 7.21 – 7.07 (m, 5H), 3.71 (s, 3H), 3.53 – 3.33 (m, 2H), 3.25 – 3.09 (m, 2H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 192.1, 184.9, 168.3, 143.5, 134.9, 134.7, 133.1, 130.2, 129.8, 129.1, 128.8, 128.7, 128.6, 128.3, 127.4, 125.0, 125.4, 89.5, 52.2, 41.7, 32.3. **IR**: 2950, 1757, 1716, 1604, 1551, 1490, 1451, 1362, 1295, 1248, 1180, 1128, 763, 704 cm^{-1}; $[\alpha]_D^{rt}$ = -89°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{27}H_{23}NO_4$+H, Calc: 426.1700, Found: 426.1706; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/2, flow rate = 1.0 ml/min, retention time: t_{major} = 12.8, t_{minor} = 16.7, 97% ee.

(S,E)-methyl-2-((5-hexyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate



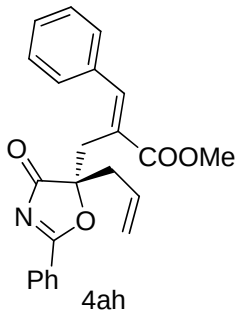
4ag

4ag (Table 4., entry 7)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.3 Hz, 2H), 7.79 (s, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.43 – 7.29 (m, 5H), 3.70 (s, 3H), 3.42 – 3.21 (m, 2H), 1.98 – 1.80 (d, *J* = 9.5 Hz, 2H), 1.32 – 0.97 (m, 8H), 0.81 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 192.8, 185.2, 168.3, 143.2,

135.0, 134.9, 130.0, 129.0, 128.8, 128.6, 126.4 125.5, 90.0, 52.1, 35.7, 32.9, 31.3, 28.9, 22.6, 22.4, 13.9; **IR**: 2928, 1757, 1718, 1604, 1551, 1490, 1451, 1359, 1296, 1243, 1204, 1180, 1147, 764, 708 cm^{-1}; $[\alpha]_D^{rt}$ = -36°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{26}H_{29}NO_4$+H, Calc: 420.2169, Found: 420.2180; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 11.3, t_{minor} = 14.1, 97% ee.

(S,E)-methyl 2-((5-allyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate



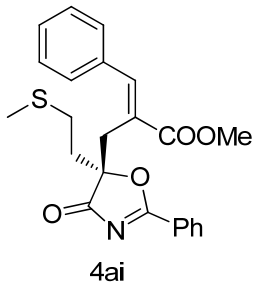
4ah

4ah (Table 4, entry 8)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 – 7.94 (m, 2H), 7.81 (s, 1H), 7.66 (dd, *J* = 10.6, 4.3 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.43 – 7.28 (m, 5H), 5.65 – 5.47 (m, 1H), 5.22 – 4.89 (m, 2H), 3.71 (s, 3H), 3.48 – 3.18 (m, 2H), 2.75 – 2.45 (m, 2H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 192.2, 185.1, 168.3, 143.4, 135.0, 134.8, 130.0, 129.1, 129.0, 128.8, 128.8, 126.1, 125.4, 121.3, 89.0, 52.2, 39.8, 32.3. **IR**: 2951, 1757, 1717, 1604, 1551, 1490, 1451, 1361, 1289, 1183, 763, 713 cm^{-1}; $[\alpha]_D^{rt}$ = -42°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{23}H_{21}NO_4$+H, Calc: 376.1543, Found: 376.1557; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/2, flow rate = 1.0 ml/min, retention time: t_{major} = 12.1, t_{minor} = 16.3, 98% ee.

(S,E)-methyl-2-((5-(2-(methylthio)ethyl)-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-ph

enylacrylate 4ai (Table 4., entry 9)

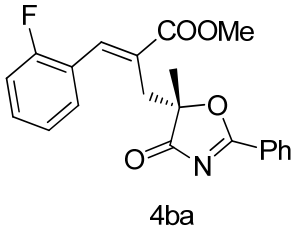


4ai

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 – 7.93 (m, 2H), 7.82 (s, 1H), 7.74 – 7.60 (m, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.43 – 7.28 (m, 5H), 3.70 (s, 3H), 3.48 – 3.22 (m, 2H), 2.38 – 2.11 (m, 4H), 1.99 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 192.0, 185.3, 168.1, 143.5, 135.2, 134.8, 130.0, 128.9, 128.8, 128.7, 125.9, 125.3, 89.0, 52.2, 35.3, 32.8, 27.2, 15.4. **IR**: 2918, 1756, 1716, 1604, 1549, 1490, 1451, 1362, 1295, 1238, 1179, 1131, 765, 705 cm^{-1}; $[\alpha]_D^{rt}$ = -43°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{23}H_{23}NO_4S$+H, Calc: 410.1421, Found: 410.1431; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/2, flow rate = 1.0 ml/min, retention time: t_{major} = 13.7, t_{minor} = 18.3, 98% ee.

(S,E)-methyl-3-(2-fluorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl) acrylate 4ba (Table 4, entry 10)

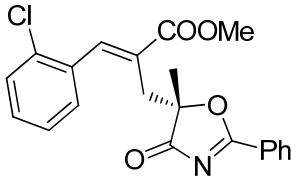
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 5.1, 3.3 Hz, 2H), 7.82 (s, 1H), 7.76 – 7.61 (m, 1H), 7.49 (dd, *J* = 10.8, 4.8 Hz, 2H), 7.41 – 7.27 (m, 2H), 7.14 (td, *J* = 7.6, 0.9 Hz, 1H), 7.06 (dd, *J* = 13.9, 5.3 Hz, 1H), 3.73 (s, 3H), 3.31 – 3.12 (m, 2H), 1.47 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ



4ba

193.1, 184.8, 167.7, 159.8 (J = 247.5 Hz), 136.40 (J = 2.9 Hz), 135.1, 130.6 (J = 8.3 Hz), 130.0, 129.7 (J = 3.0 Hz), 128.9, 128.8, 125.6, 124.2 (J = 3.6 Hz), 122.9 (J = 14.3 Hz), 115.9 (J = 21.0 Hz), 86.7, 52.3, 33.5 (J = 1.8 Hz), 21.6. **IR**: 3405, 2951, 2371, 1758, 1719, 1604, 1551, 1488, 1451, 1359, 1299, 1145, 762, 707 cm^{-1}; $[\alpha]_D^{rt}$ = -3°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}FNO_4$+H, Calc: 368.1293, Found: 368.1301; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 7.0, t_{minor} = 8.3, 96% ee.

(S,E)-methyl-3-(2-chlorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl

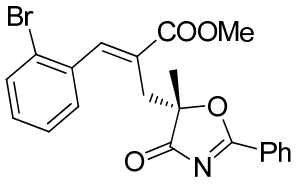


4ca

)acrylate 4ca (Table 4, entry 11)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.16 – 7.97 (m, 2H), 7.88 (s, 1H), 7.76 – 7.60 (m, 1H), 7.51 (t, J = 7.7 Hz, 2H), 7.43 – 7.36 (m, 1H), 7.36 – 7.29 (m, 1H), 7.29 – 7.21 (m, 2H), 3.75 (s, 3H), 3.16 (q, J = 14.2 Hz, 2H), 1.43 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 193.2, 184.8, 167.7, 140.6, 135.1, 133.8, 133.7, 130.1, 129.8, 129.8, 128.8, 128.5, 126.8, 125.7, 86.7, 52.3, 33.0, 21.3. **IR**: 3404, 2951, 2374, 1757, 1720, 1604, 1550, 1490, 1451, 1359, 1293, 1247, 1145, 1121, 762, 707 cm^{-1}; $[\alpha]_D^{rt}$ = -8°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}ClNO_4$+H, Calc: 384.0997, Found: 384.1006; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 7.5, t_{minor} = 8.7, 90% ee.

(S,E)-methyl-3-(2-bromophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl

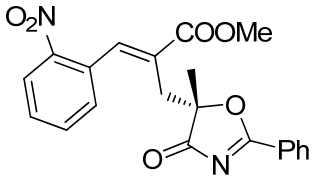


4da

)acrylate 4da (Table 4, entry 12)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 – 8.01 (m, 2H), 7.82 (s, 1H), 7.75 – 7.63 (m, 1H), 7.59 (d, J = 7.9 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.31 (d, J = 4.2 Hz, 2H), 7.25 – 7.10 (m, 1H), 3.75 (s, 3H), 3.15 (q, J = 14.2 Hz, 2H), 1.43 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 193.2, 184.8, 167.7, 142.5, 135.5, 135.1, 132.9, 130.1, 130.0, 129.7, 128.8, 128.1, 127.4, 125.7, 123.8, 86.7, 52.3, 32.9, 21.3. **IR**: 3415, 2951, 2373, 1757, 1720, 1604, 1550, 1490, 1451, 1359, 1292, 1245, 1145, 1124, 762, 707 cm^{-1}; $[\alpha]_D^{rt}$ = -18°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}BrNO_4$+H, Calc: 428.0492, Found: 428.0501; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 7.8, t_{minor} = 8.9, 91% ee.

(S,E)-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(2-nitrophenyl)a

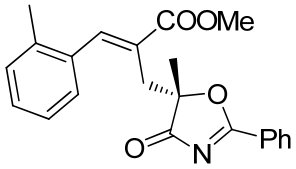


4ea

crylate 4ea (Table 4., entry 13)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 (dd, *J* = 8.3, 1.2 Hz, 1H), 8.12 – 8.04 (m, 3H), 7.77 – 7.60 (m, 2H), 7.61 – 7.48 (m, 3H), 7.34 (d, *J* = 7.6 Hz, 1H), 3.75 (s, 3H), 3.08 (dd, *J* = 42.1, 14.3 Hz, 2H), 1.41 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 193.1, 185.1, 167.5, 147.3, 140.7, 135.2, 134.0, 131.2, 130.6, 130.0, 129.6, 128.8, 127.2, 125.6, 125.2, 86.7, 52.4, 33.2, 21.5. **IR**: 3366, 2951, 2372, 1756, 1719, 1604, 1550, 1490, 1451, 1359, 1288, 1249, 1145, 1122, 759, 707 cm^{-1}; **$[\alpha]_D^{rt}$** = +9.7°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}N_2O_6$+H, Calc: 395.1238, Found: 395.1252; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 11.3, t_{minor} = 11.9, 90% ee.

(S,E)-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(o-tolyl)acrylate

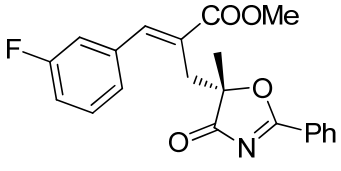


4fa

4fa (Table 4., entry 14)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 5.2, 3.3 Hz, 2H), 7.87 (s, 1H), 7.75 – 7.61 (m, 1H), 7.50 (dd, *J* = 10.7, 4.7 Hz, 2H), 7.26 – 7.13 (m, 4H), 3.71 (s, 3H), 3.31 – 3.04 (m, 2H), 2.25 (s, 3H), 1.42 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 193.1, 184.7, 168.1, 142.9, 136.7, 135.0, 134.2, 130.3, 130.0, 128.8, 128.6, 127.9, 127.1, 125.8, 125.7, 86.8, 52.1, 33.1, 21.7, 20.0. **IR**: 3495, 2950, 2371, 1759, 1718, 1604, 1551, 1490, 1451, 1359, 1295, 1251, 1145, 1123, 764, 707 cm^{-1}; **$[\alpha]_D^{rt}$** = -92°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{21}NO_4$+H, Calc: 364.1543, Found: 364.1559; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 14.2, t_{minor} = 19.6, 97% ee.

(S,E)-methyl-3-(3-fluorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)



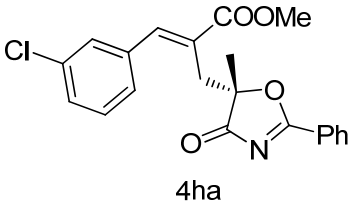
4ga

acrylate 4ga (Table 4., entry 15)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 – 7.98 (m, 2H), 7.77 (s, 1H), 7.72 – 7.62 (m, 1H), 7.55 – 7.41 (m, 2H), 7.41 – 7.28 (m, 1H), 7.21 – 7.08 (m, 2H), 7.07 – 6.94 (m, 1H), 3.73 (s, 3H), 3.38 – 3.22 (m, 2H), 1.52 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.0, 184.8, 167.9, 162.6 (*J* = 245.3 Hz), 141.9 (*J* = 2.2 Hz), 137.0 (*J* = 7.8 Hz), 135.2, 130.3 (*J* = 8.3 Hz), 130.0, 128.8, 127.6, 125.5, 124.6 (*J* = 3.0 Hz), 115.9 (*J* = 4.5 Hz), 115.6 (*J* = 3.0 Hz), 86.8, 52.3, 33.3, 22.0. **IR**: 3408, 2952, 2372, 1758, 1718, 1604, 1589, 1551, 1489, 1451, 1359, 1293, 1235, 1146, 1121, 795, 707 cm^{-1}; **$[\alpha]_D^{rt}$** = -43°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}FNO_4$+H, Calc: 368.1293, Found: 368.1308; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow

rate = 1.0 ml/min, retention time: t_{major} = 7.4, t_{minor} = 9.1, 97% ee.

(S,E)-methyl-3-(3-chlorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl

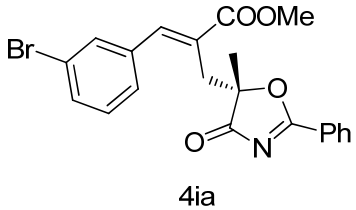


4ha

)acrylate 4ha (Table 4, entry 16)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 – 7.94 (m, 2H), 7.75 (s, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.37 (s, 1H), 7.34 – 7.21 (m, 3H), 3.73 (s, 3H), 3.39 – 3.14 (m, 2H), 1.53 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.9, 184.8, 167.9, 141.7, 136.7, 135.2, 134.6, 130.0, 128.9, 128.8, 128.8, 127.7, 126.9, 125.5, 86.8, 52.3, 33.3, 22.0. **IR**: 2951, 1758, 1719, 1604, 1551, 1490, 1451, 1358, 1290, 1246, 1145, 1121, 792, 706 cm^{-1}; **$[\alpha]_D^{rt}$** = -42°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}ClNO_4$+H, Calc: 384.0997, Found: 384.1013; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 7.7, t_{minor} = 9.6, 94% ee.

(S,E)-methyl-3-(3-bromophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl

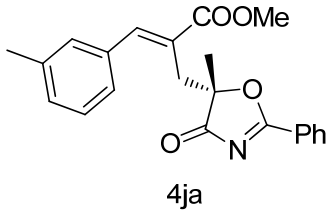


4ia

)acrylate 4ia (Table 4, entry 17)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 – 7.94 (m, 2H), 7.74 (s, 1H), 7.72 – 7.60 (m, 1H), 7.57 – 7.38 (m, 4H), 7.39 – 7.28 (m, 2H), 3.73 (s, 3H), 3.38 – 3.16 (m, 2H), 1.53 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 192.9, 184.8, 167.8, 141.6, 136.9, 135.1, 131.8, 131.7, 130.2, 130.0, 128.8, 127.7, 127.3, 125.5, 122.7, 86.7, 52.3, 33.3, 22.0. **IR**: 2951, 1758, 1718, 1604, 1551, 1490, 1451, 1359, 1289, 1247, 1202, 1145, 1121, 793, 706 cm^{-1}; **$[\alpha]_D^{rt}$** = -37°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}BrNO_4$+H, Calc: 428.0492, Found: 428.0505; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 8.2, t_{minor} = 10.3, 92% ee.

(S,E)-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(m-tolyl)acrylat



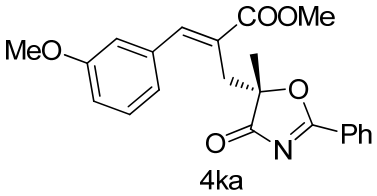
4ja

e 4ja (Table 4., entry 18)

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 – 7.96 (m, 2H), 7.82 (s, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.30 – 7.17 (m, 3H), 7.12 (d, *J* = 6.6 Hz, 1H), 3.73 (s, 3H), 3.42 – 3.15 (m, 2H), 2.30 (s, 3H), 1.52 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.3, 184.8, 168.4, 143.7, 138.3, 135.0, 134.9, 130.1, 129.7, 129.7, 128.8, 128.6, 126.1, 125.7, 87.0, 52.2, 33.3, 21.9, 21.4. **IR**: 2923, 1756, 1718, 1604, 1547, 1490, 1451, 1358, 1237, 1121, 758, 706

cm^{-1}; $[\alpha]_D^{rt}$ = -28°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{21}NO_4$+H, Calc: 364.1543, Found: 364.1560; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 8.3, t_{minor} = 10.6, 95% ee.

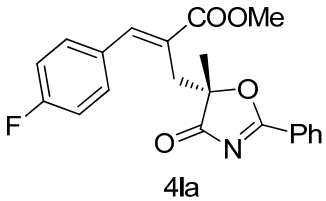
(S,E)-methyl-3-(3-methoxyphenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate 4ka (Table 4., entry 19)



4ka

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 – 7.96 (m, 2H), 7.81 (s, 1H), 7.73 – 7.60 (m, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.35 – 7.23 (m, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.93 (s, 1H), 6.85 (dd, *J* = 8.2, 2.3 Hz, 1H), 3.80 (s, 3H), 3.72 (s, 3H), 3.41 – 3.20 (m, 2H), 1.52 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.2, 184.8, 168.3, 159.6, 143.3, 136.2, 135.0, 130.0, 129.7, 128.8, 126.5, 125.6, 121.3, 114.4, 114.4, 86.9, 55.2, 52.2, 33.4, 21.9. **IR**: 2951, 1757, 1716, 1604, 1551, 1490, 1452, 1359, 1289, 1240, 1145, 1038, 795, 707 cm^{-1}; $[\alpha]_D^{rt}$ = -35°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{21}NO_5$+H, Calc: 380.1492, Found: 380.1510; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 8.9, t_{minor} = 11.6, 97% ee.

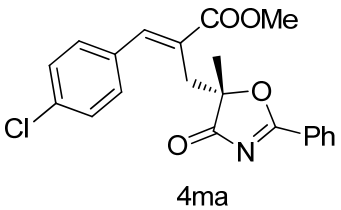
(S,E)-methyl-3-(4-fluorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl) acrylate 4la (Table 4, entry 20)



4la

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 – 7.94 (m, 2H), 7.77 (s, 1H), 7.73 – 7.63(m, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.45 – 7.35 (m, 2H), 7.10 – 7.00 (m, 2H), 3.72 (s, 3H), 3.39 – 3.17 (m, 2H), 1.53 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.1, 184.8, 168.2, 162.7 (*J* = 249 Hz), 161.05, 142.1, 135.2, 131.0 (*J* = 8.3 Hz), 130.9 (*J* = 3.8 Hz), 130.0, 128.8, 126.2 (*J* = 0.75 Hz), 125.5, 115.8 (*J* = 21.8 Hz), 86.9, 52.2, 33.3, 22.0. **IR**: 2952, 1757, 1715, 1603, 1550, 1509, 1490, 1451, 1359, 1227, 1120, 835, 706 cm^{-1}; $[\alpha]_D^{rt}$ = -26°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}FNO_4$+H, Calc: 368.1293, Found: 368.1297; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 7.7, t_{minor} = 9.4, 97% ee.

(S,E)-methyl-3-(4-chlorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate 4ma (Table 4, entry 21)

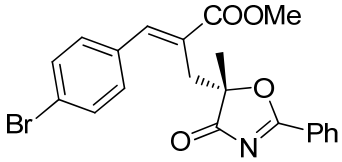


4ma

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 – 7.95 (m, 2H), 7.76 (s, 1H), 7.73 – 7.62 (m, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.38 – 7.29 (m, 4H), 3.72 (s, 3H), 3.38 – 3.23 (m, 2H), 1.53 (s, 3H). **^{13}C NMR** (75

MHz, $CDCl_3$) δ 193.0, 184.8, 168.1, 141.9, 135.2, 134.9, 133.3, 130.3, 130.0, 128.9, 128.8, 126.9, 125.5, 86.9, 52.3, 33.3, 21.9. **IR**: 2951, 1757, 1717, 1604, 1551, 1491, 1451, 1359, 1285, 1246, 1145, 1121, 707 cm^{-1}; $[\alpha]_D^{rt}$ = -28°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}ClNO_4$+H, Calc: 384.0997, Found: 384.0999; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} =8.0, t_{minor} = 9.6, 96% ee.

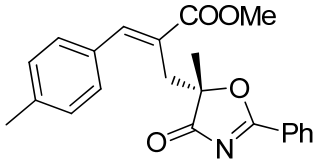
(S,E)-methyl-3-(4-bromophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate 4na (Table 4., entry 22)



4na

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.6 Hz, 2H), 7.73 (s, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.58 – 7.44 (m, 4H), 7.33 – 7.20 (m, 2H), 3.72 (s, 3H), 3.38 – 3.19 (m, 2H), 1.52 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.0, 184.8, 168.0, 142.0, 135.2, 133.7, 131.9, 130.5, 130.0, 128.8, 127.0, 125.5, 123.1, 86.9, 52.3, 33.2, 21.9. **IR**: 2951, 1757, 1717, 1604, 1550, 1489, 1451, 1359, 1284, 1242, 1145, 1120, 707 cm^{-1}; $[\alpha]_D^{rt}$ = -21°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{21}H_{18}BrNO_4$+H, Calc: 428.0492, Found: 428.0494; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} =8.1, t_{minor} = 9.6, 91% ee.

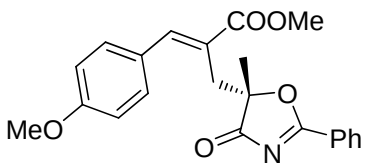
(S,E)-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(p-tolyl)acrylate 4oa (Table 4., entry 23)



4oa

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 – 7.95 (m, 2H), 7.82 (s, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 3.73 (s, 3H), 3.42 – 3.23 (m, 2H), 2.33 (s, 3H), 1.52 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.3, 184.8, 168.4, 143.5, 139.1, 135.0, 132.0, 130.0, 129.4, 129.1, 128.7, 125.6, 125.3, 87.1, 52.1, 33.3, 21.8, 21.3. **IR**: 2951, 1758, 1715, 1604, 1551, 1490, 1451, 1359, 1245, 1145, 1036, 706 cm^{-1}; $[\alpha]_D^{rt}$ = -39°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{21}NO_4$+H, Calc: 364.1543, Found: 364.1551; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} =8.9, t_{minor} = 11.4, 97% ee.

(S,E)-methyl-3-(4-methoxyphenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate 4pa (Table 4., entry 24)

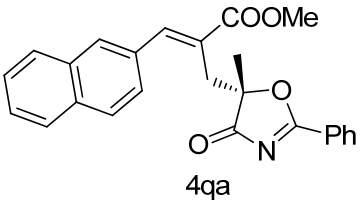


4pa

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 – 7.92 (m, 2H), 7.79 (s, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.53 – 7.35 (m, 4H), 6.88 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H), 3.72 (s, 3H), 3.44 – 3.24 (m, 2H),

1.56 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.4, 184.8, 168.6, 160.1, 143.2, 135.0, 131.1, 130.0, 128.7, 127.3, 125.6, 123.7, 114.1, 87.2, 55.3, 52.1, 33.4, 21.8. **IR**: 2951, 1757, 1711, 1604, 1550, 1512, 1490, 1452, 1360, 1302, 1256, 1178, 1145, 1121, 1035, 835, 707 cm^{-1}; **$[\alpha]_D^{rt}$** = -49°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{22}H_{21}NO_5$+H, Calc: 380.1492, Found: 380.1498; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 10.3, t_{minor} = 13.1, 97% ee.

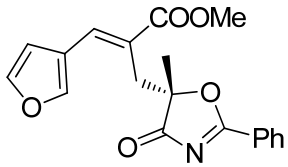
(S,E)-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(naphthalen-2-yl)acrylate 4qa (Table 4., entry 25)



4qa

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.90 (dd, *J* = 6.8, 5.6 Hz, 3H), 7.85 – 7.70 (m, 3H), 7.63 – 7.41 (m, 4H), 7.33 (t, *J* = 7.8 Hz, 2H), 3.77 (s, 3H), 3.54 – 3.31 (m, 2H), 1.53 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 193.2, 184.8, 168.4, 143.5, 135.0, 133.1, 133.0, 132.4, 129.9, 129.3, 128.6, 128.4, 128.3, 127.6, 127.0, 126.6, 126.3, 125.9, 125.5, 87.1, 52.3, 33.4, 21.9. **IR**: 2951, 1756, 1713, 1604, 1549, 1490, 1451, 1359, 1243, 1145, 1119, 737, 707 cm^{-1}; **$[\alpha]_D^{rt}$** = -59°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{25}H_{21}NO_4$+H, Calc: 400.1543, Found: 400.1550; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 9.8, t_{minor} = 12.0, 95% ee.

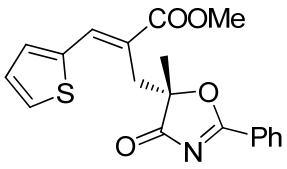
(S,E)-methyl-3-(furan-3-yl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate 4ra (Table 4., entry 26)



4ra

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 – 7.95 (m, 2H), 7.73 (s, 1H), 7.71 – 7.58 (m, 2H), 7.52 – 7.40 (m, 3H), 6.73 (d, *J* = 1.6 Hz, 1H), 3.73 (s, 3H), 3.37 – 3.19 (m, 2H), 1.63 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.3, 185.0, 168.2, 145.9, 144.2, 135.1, 133.6, 130.0, 128.8, 125.6, 123.2, 121.2, 109.9, 87.2, 52.1, 34.2, 21.8. **IR**: 2951, 1756, 1710, 1604, 1549, 1491, 1451, 1359, 1294, 1223, 1167, 1119, 1026, 871, 707 cm^{-1}; **$[\alpha]_D^{rt}$** = +16°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{19}H_{17}NO_5$+H, Calc: 340.1179, Found: 340.1192; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 8.6, t_{minor} = 10.7, 92% ee.

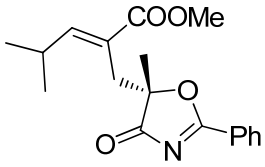
(S,E)-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(thiophen-2-yl)acrylate 4sa (Table 4., entry 27)



4sa

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.98 – 7.88 (m, 0.9 Hz, 2H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.49 – 7.38 (m, 3H), 7.33 (d, *J* = 3.5 Hz, 1H), 7.14 – 7.05 (m, 1H), 3.76 (s, 3H), 3.54 – 3.32 (m, 2H), 1.66 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.1, 184.9, 168.1, 137.5, 136.1, 134.9, 134.1, 130.0, 129.7, 128.7, 127.1, 125.7, 121.5, 87.0, 52.2, 34.4, 21.8. **IR**: 2950, 1757, 1710, 1604, 1550, 1490, 1451, 1359, 1281, 1208, 1145, 1118, 706 cm^{-1}; **$[\alpha]_D^{rt}$** = -51°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{19}H_{17}NO_4S$+H, Calc: 356.0951, Found: 356.0962; **HPLC**: DAICEL CHIRALCEL IC, Hexane/EtOH = 1/1, flow rate = 1.0 ml/min, retention time: t_{major} = 10.2, t_{minor} = 13.7, 96% ee.

(S,E)-methyl-4-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)pent-2-en



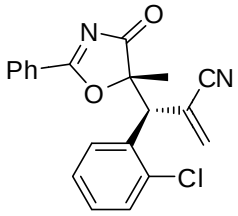
4ta

oate **4ta (Table 4, entry 28)**

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 – 8.08 (m, 2H), 7.77 – 7.63 (m, 1H), 7.53 (t, *J* = 7.7 Hz, 2H), 6.64 (d, *J* = 10.8 Hz, 1H), 3.62 (s, 3H), 3.20 – 2.90 (m, 2H), 2.75 – 2.57 (m, 1H), 1.60 (s, 3H), 1.02 (d, *J* = 6.5 Hz, 3H), 0.97 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.6, 185.1, 168.3, 153.5, 135.1, 130.0, 128.9, 125.8, 122.6, 87.5, 51.8, 33.2, 28.4, 22.2, 22.0, 21.9. **IR**: 2961, 1758, 1718, 1604, 1551, 1491, 1452, 1359, 1281, 1174, 1110, 768, 708 cm^{-1}; **$[\alpha]_D^{rt}$** = +24°(c = 1.00, $CHCl_3$); **HRMS** (ESI): $C_{18}H_{21}NO_4$+H, Calc: 316.1543, Found: 316.1555; **HPLC**: DAICEL CHIRALCEL IC, Hexane/iPrOH = 7/3, flow rate = 1.0 ml/min, retention time: t_{major} = 14.9, t_{minor} = 19.1, 99% ee.

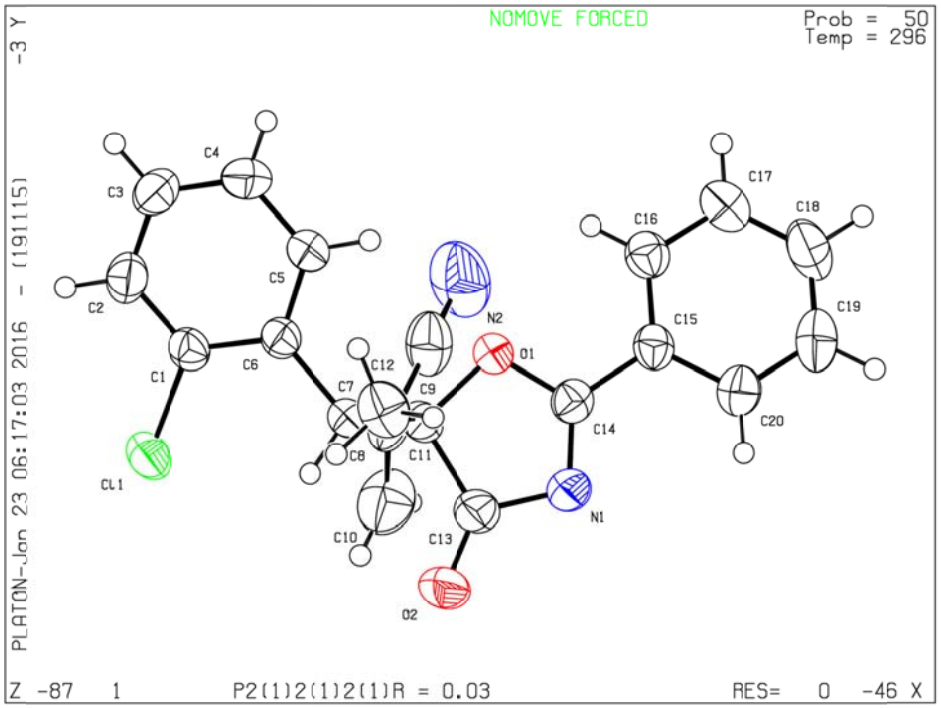
5. Determination of the absolute configuration 3 and 4

X-ray Structure of **3ac':**



3ac'

Datablock: 3ac'



Bond precision:	C-C = 0.0029 A		Wavelength=0.71073
Cell:	a=7.1740(7)	b=14.3271(14)	c=17.4194(17)
	alpha=90	beta=90	gamma=90
Temperature:	296 K		

	Calculated	Reported
Volume	1790.4(3)	1790.4(3)
Space group	P 21 21 21	P2(1)2(1)2(
Hall group	P 2ac 2ab	?
Moiety formula	C20 H15 Cl N2 O2	?
Sum formula	C20 H15 Cl N2 O2	C20 H15 Cl N2 O2
Mr	350.79	350.79

Dx,g cm-3	1.301	1.301
Z	4	4
Mu (mm-1)	0.228	0.228
F000	728.0	728.0
F000'	728.88	
h,k,lmax	8,17,20	8,17,20
Nref	3157[1831]	3155
Tmin,Tmax	0.947,0.955	0.935,0.956
Tmin'	0.934	

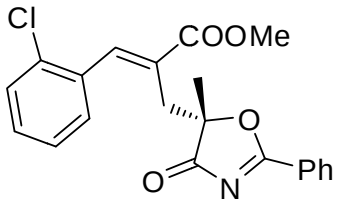
Correction method= # Reported T Limits: Tmin=0.935 Tmax=0.956 AbsCorr = MULTI-SCAN

Data completeness= 1.72/1.00 Theta(max)= 25.000

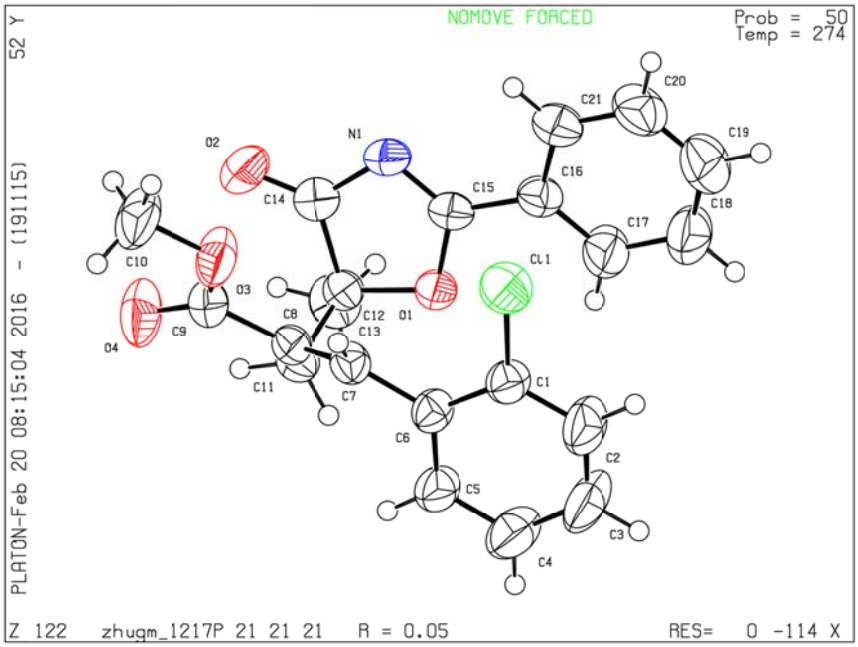
R(reflections)= 0.0280(2865) wR2(reflections)= 0.0661(3155)

S = 1.004 Npar= 227

X-ray Structure of **4ca:**



4ca



Datablock: 4ca

Bond precision: C-C = 0.0046 A Wavelength=0.71073

Cell: a=7.1668(4) b=12.4455(8) c=21.2096(12)
alpha=90 beta=90 gamma=90

Temperature: 274 K

	Calculated	Reported
Volume	1891.78(19)	1891.78(19)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C21 H18 Cl N O4	C21 H18 Cl N O4
Sum formula	C21 H18 Cl N O4	C21 H18 Cl N O4
Mr	383.81	383.81
Dx,g cm-3	1.348	1.348
Z	4	4
Mu (mm-1)	0.228	0.228
F000	800.0	800.0
F000'	800.97	
h,k,lmax	8,15,26	8,15,26
Nref	3722[2150]	3555
Tmin,Tmax	0.949,0.962	0.956,1.000
Tmin'	0.949	

Correction method= # Reported T Limits: Tmin=0.956 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 1.65/0.96 Theta(max)= 26.010

R(reflections)= 0.0538(2476) wR2(reflections)= 0.1143(3555)

S = 1.025 Npar= 246

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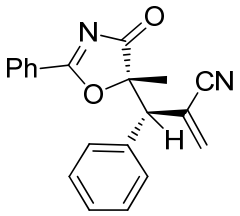
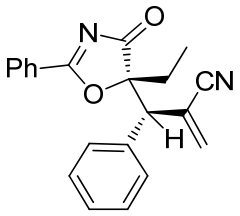
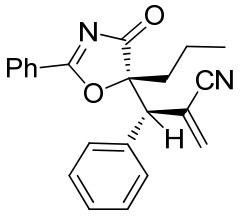
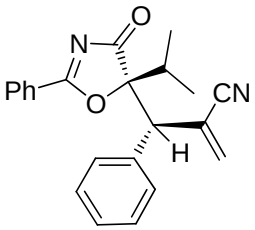
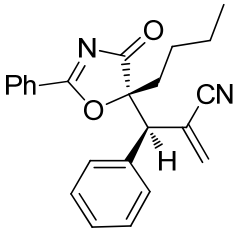
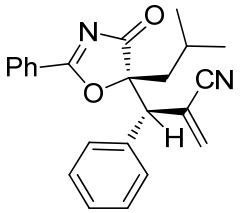
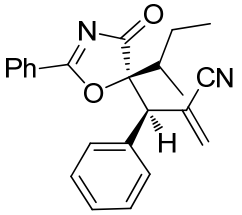
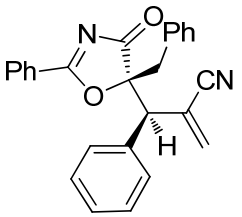
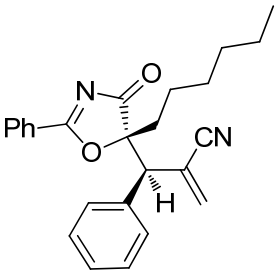
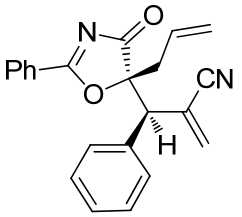
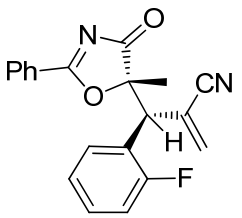
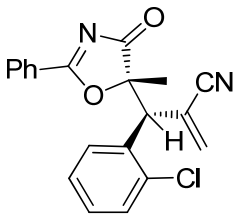
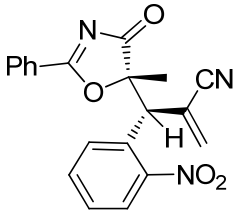
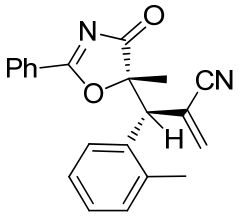
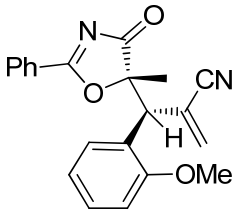
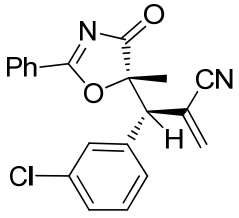
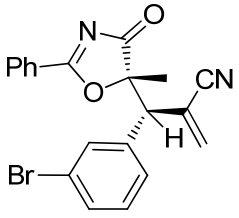
6. HPLC analytic conditions of 3 and 4

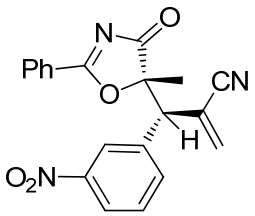
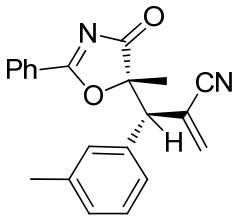
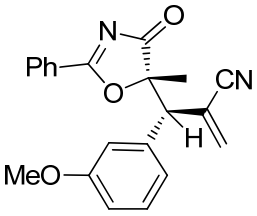
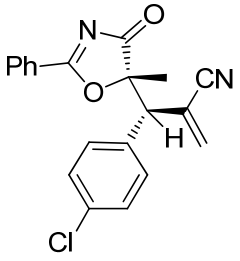
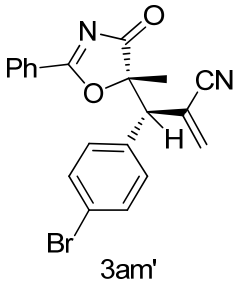
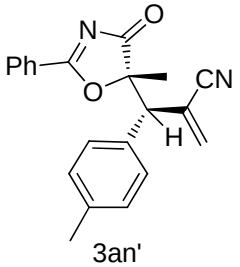
HPLC Analytic Conditions of 3:

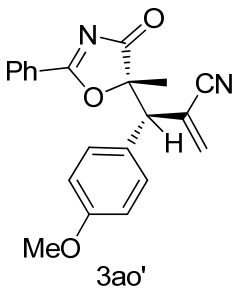
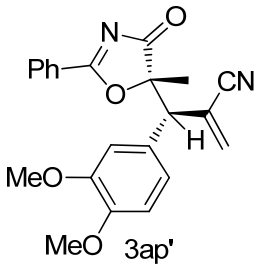
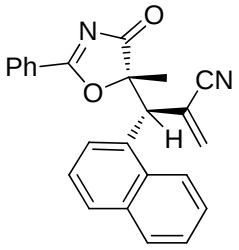
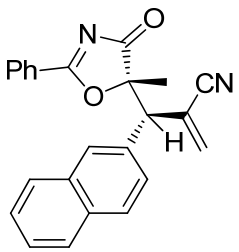
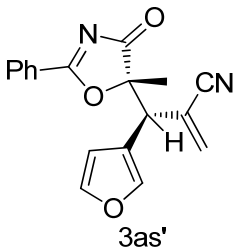
All products are separated by using DAICEL CHIRALCEL column.

entry	product	Chiralcel column	Mobile phase	flow rate ml/min	Retention Time (min)	ee (%)
1	 3aa'	IC	H/I = 1/1	1.0	t_{major} = 7.5, t_{minor} = 8.6	95
2	 3ba'	IA	H/E = 4/1	1.0	t_{major} = 8.1, t_{minor} = 6.6	96
3	 3ca'	IA	H/E = 95/5	1.0	t_{major} = 15.1, t_{minor} = 11.7	95
4	 3da'	IA	H/E = 9/1	1.0	t_{major} = 11.1, t_{minor} = 7.6	97
5	 3ea'	IA	H/E = 95/5	1.0	t_{major} = 16.7, t_{minor} = 12.8	95

6	 3fa'	IA	H/E = 95/5	1.0	t_{major} = 15.9, t_{minor} = 12.4	95
7	 3ga'	IA	H/E = 95/5	1.0	t_{major} = 13.2, t_{minor} = 10.6	98
8	 3ha'	IC	H/I = 1/3	1.0	t_{major} = 7.5, t_{minor} = 5.8	90
9	 3ia'	IA	H/E = 95/5	1.0	t_{major} = 12.7, t_{minor} = 10.6	96
10	 3ja'	IA	H/E = 95/5	1.0	t_{major} = 19.8, t_{minor} = 15.0	95
11	 3ab'	IC	H/I = 1/1	1.0	t_{major} = 6.8, t_{minor} = 7.6	95

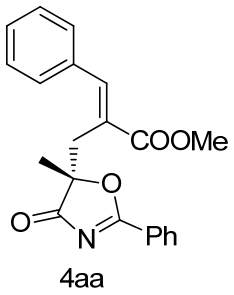
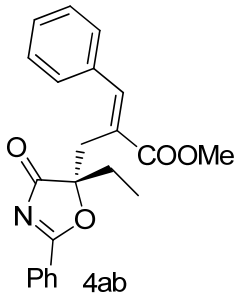
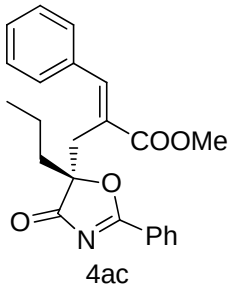
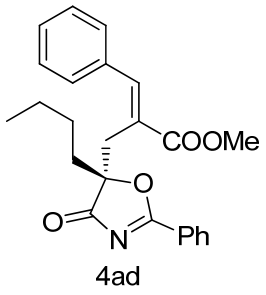
12	 3ac'	IC	H/I = 1/2	1.0	t_{major} = 6.3, t_{minor} = 6.9	96
13	 3ad'	IC	H/I = 1/1	1.0	t_{major} = 14.7, t_{minor} = 10.4	94
14	 3ae'	IC	H/I = 1/1	1.0	t_{major} = 7.3, t_{minor} = 8.3	91
15	 3af'	IC	H/I = 1/1	1.0	t_{major} = 10.2, t_{minor} = 12.1	96
16	 3ag'	IC	H/I = 1/1	1.0	t_{major} = 6.8, t_{minor} = 7.7	91
17	 3ah'	IC	H/I = 1/1	1.0	t_{major} = 6.8, t_{minor} = 7.9	90

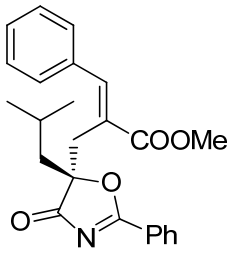
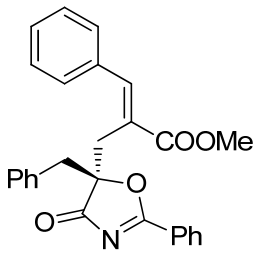
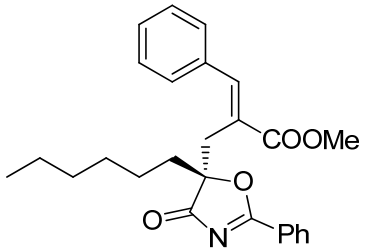
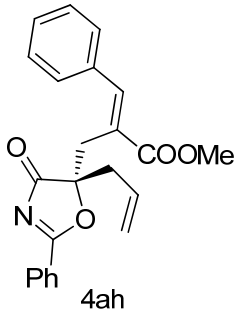
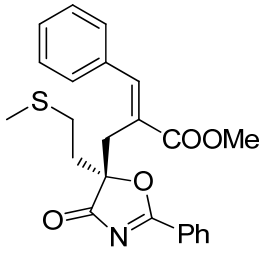
18	 3ai'	IC	H/I = 1/1	1.0	t_{major} = 22.4, t_{minor} = 37.2	94
19	 3aj'	IC	H/I = 1/1	1.0	t_{major} = 7.2, t_{minor} = 8.5	93
20	 3ak'	IC	H/I = 1/1	1.0	t_{major} = 6.5, t_{minor} = 7.5	93
21	 3al'	IC	H/I = 1/1	1.0	t_{major} = 6.8, t_{minor} = 7.7	94
22	 3am'	IC	H/I = 1/1	1.0	t_{major} = 6.9, t_{minor} = 7.9	90
23	 3an'	IC	H/I = 1/1	1.0	t_{major} = 7.3, t_{minor} = 8.5	95

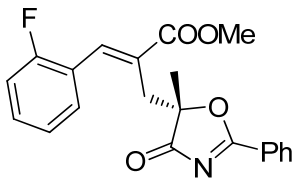
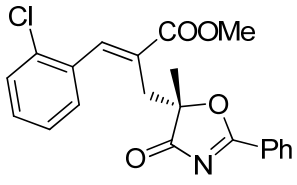
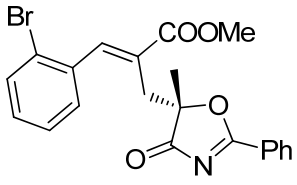
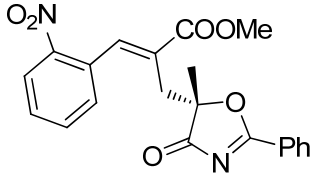
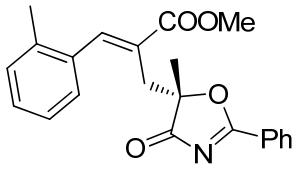
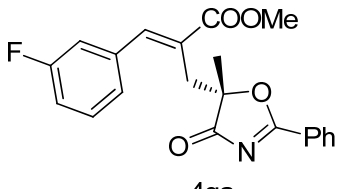
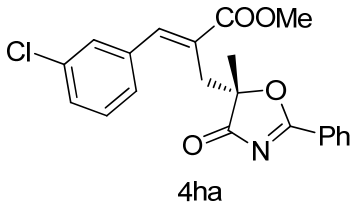
24	 3ao'	IC	H/I = 1/1	1.0	t_{major} = 8.3, t_{minor} = 9.5	93
25	 3ap'	IC	H/I = 1/1	1.0	t_{major} = 13.0, t_{minor} = 16.7	95
26	 3aq'	IC	H/I = 1/1	1.0	t_{major} = 6.4, t_{minor} = 7.5	94
27	 3ar'	IC	H/I = 1/1	1.0	t_{major} = 6.9, t_{minor} = 8.2	93
28	 3as'	IC	H/I = 1/1	1.0	t_{major} = 7.5, t_{minor} = 8.4	90

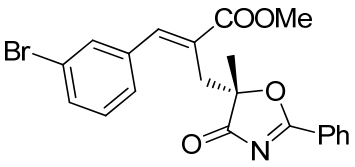
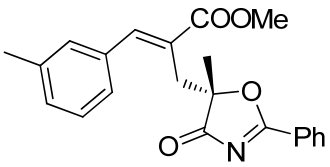
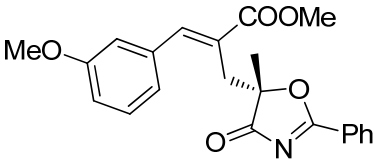
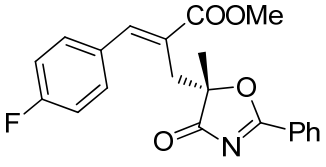
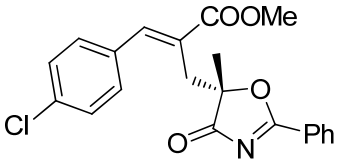
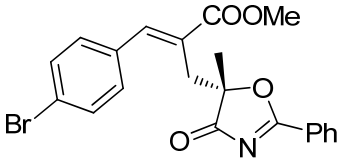
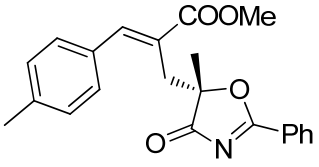
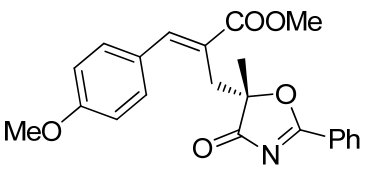
HPLC Analytic Conditions of 4:

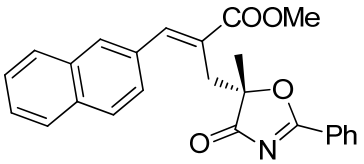
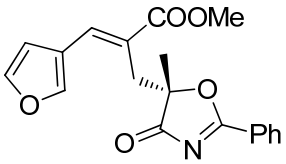
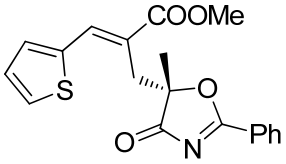
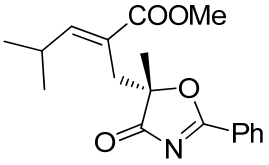
All products are separated by using DAICEL CHIRALCEL column.

entry	product	Chiralcel column	Mobile phase	flow rate ml/min	Retention Time (min)	ee (%)
1	 4aa	IC	H/I = 1/1	1.0	t_{major} = 17.7, t_{minor} = 25.7	98
2	 4ab	IC	H/I = 1/2	1.0	t_{major} = 7.9, t_{minor} = 9.1	97
3	 4ac	IC	H/I = 1/1	1.0	t_{major} = 13.0, t_{minor} = 18.1	97
4	 4ad	IC	H/I = 1/1	1.0	t_{major} = 11.8, t_{minor} = 15.8	97

5	 4ae	IC	H/I = 1/2	1.0	t_{major} = 8.9, t_{minor} = 13.3	96
6	 4af	IC	H/I = 1/2	1.0	t_{major} = 12.8, t_{minor} = 16.7	97
7	 4ag	IC	H/I = 1/1	1.0	t_{major} = 11.3, t_{minor} = 14.1	97
8	 4ah	IC	H/I = 1/2	1.0	t_{major} = 12.1, t_{minor} = 16.3	98
9	 4ai	IC	H/I = 1/2	1.0	t_{major} = 13.7, t_{minor} = 18.3	98

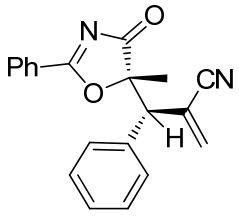
10	 4ba	IC	H/E = 1/1	1.0	t_{major} = 7.0, t_{minor} = 8.3	96
11	 4ca	IC	H/E = 1/1	1.0	t_{major} = 7.5, t_{minor} = 8.7	90
12	 4da	IC	H/E = 1/1	1.0	t_{major} = 7.8, t_{minor} = 8.9	91
13	 4ea	IC	H/E = 1/1	1.0	t_{major} = 11.3, t_{minor} = 11.9	90
14	 4fa	IC	H/I = 1/1	1.0	t_{major} = 14.2, t_{minor} = 19.6	97
15	 4ga	IC	H/E = 1/1	1.0	t_{major} = 7.4, t_{minor} = 9.1	97
16	 4ha	IC	H/E = 1/1	1.0	t_{major} = 7.7, t_{minor} = 9.6	94

17	 4ia	IC	H/E = 1/1	1.0	t_{major} = 8.2, t_{minor} = 10.3	92
18	 4ja	IC	H/E = 1/1	1.0	t_{major} = 8.3, t_{minor} = 10.6	95
19	 4ka	IC	H/E = 1/1	1.0	t_{major} = 8.9, t_{minor} = 11.6	97
20	 4la	IC	H/E = 1/1	1.0	t_{major} = 7.7, t_{minor} = 9.4	97
21	 4ma	IC	H/I = 1/1	1.0	t_{major} = 8.0, t_{minor} = 9.6	96
22	 4na	IC	H/E = 1/1	1.0	t_{major} = 8.1, t_{minor} = 9.6	91
23	 4oa	IC	H/E = 1/1	1.0	t_{major} = 8.9, t_{minor} = 11.4	97
24	 4pa	IC	H/E = 1/1	1.0	t_{major} = 10.3, t_{minor} = 13.1	97

25	 4qa	IC	H/E = 1/1	1.0	t_{major} = 9.8, t_{minor} = 12.0	95
26	 4ra	IC	H/E = 1/1	1.0	t_{major} = 8.6, t_{minor} = 10.7	92
27	 4sa	IC	H/E = 1/1	1.0	t_{major} = 10.2, t_{minor} = 13.7	96
28	 4ta	IC	H/I = 7/3	1.0	t_{major} = 14.9, t_{minor} = 19.1	99

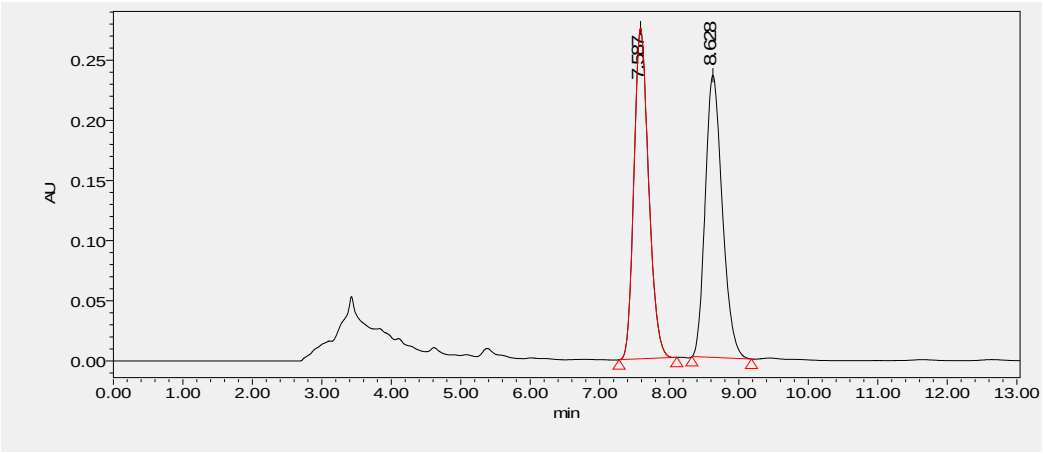
7. Copies of HPLC spectra for 3 and 4

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3aa' (Table 2, entry 1)

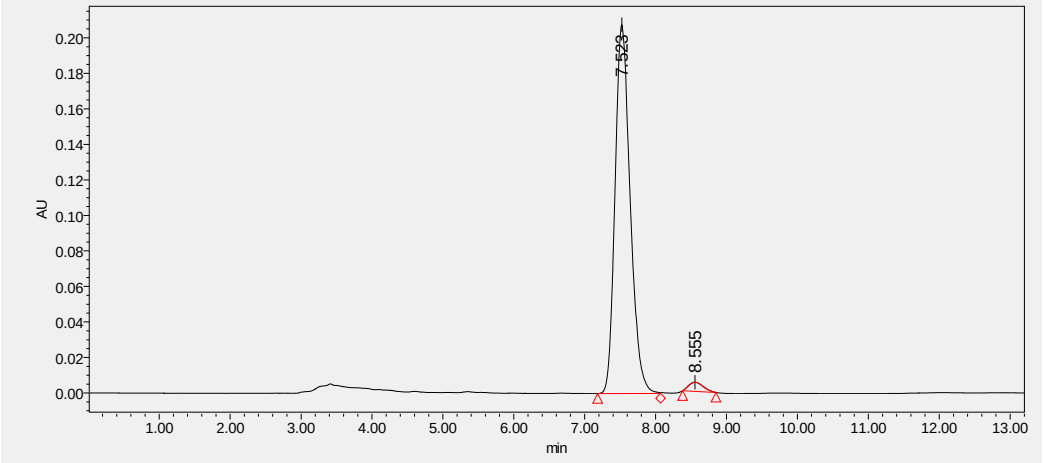


3aa'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min



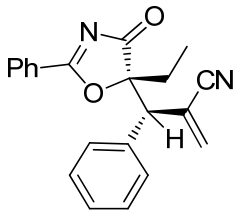
	Retention time	Area	% Area	Height	Integral type
1	7.587	4045023	50.26	274948	bb
2	8.628	4003969	49.74	234566	bb



	Retention time	Area	% Area	Height	Integral type
1	7.523	3077979	97.68	207657	Bv
2	8.555	73264	2.32	5148	bb

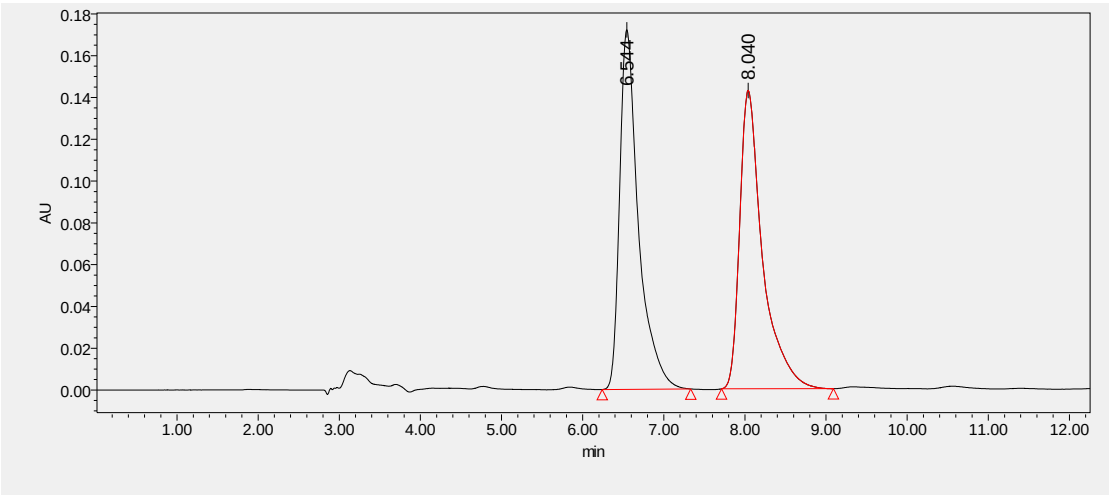
2-((R)-((S)-5-ethyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ba'

(Table 2, entry 2)

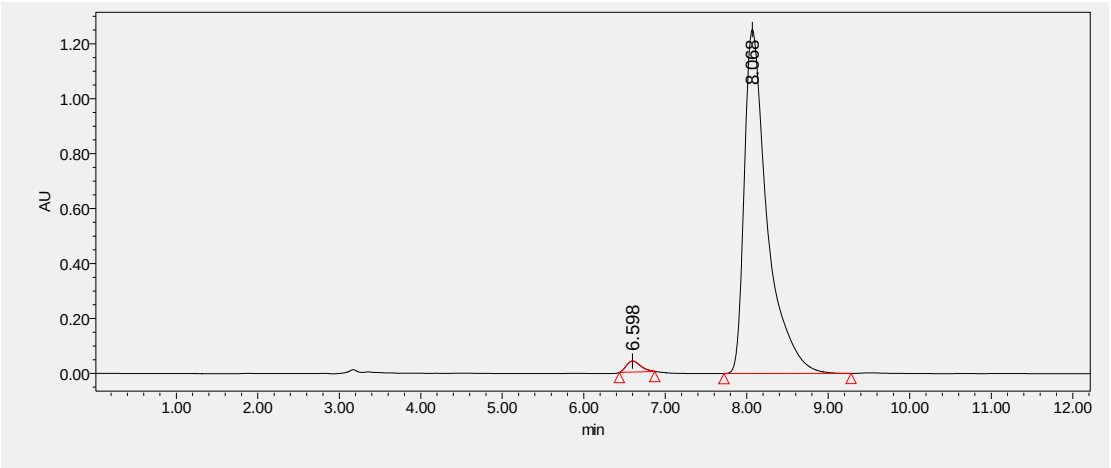


3ba'

Chiralpak IA column, hexane/EtOH (80:20), flow rate 1.0 mL/min



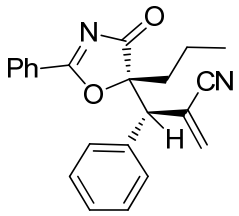
	Retention time	Area	% Area	Height	Integral type
1	6.544	2776991	49.90	172047	bb
2	8.040	2788181	50.10	142797	bb



	Retention time	Area	% Area	Height	Integral type
1	6.598	484052	1.94	40155	bb
2	8.068	24454675	98.06	1252106	bb

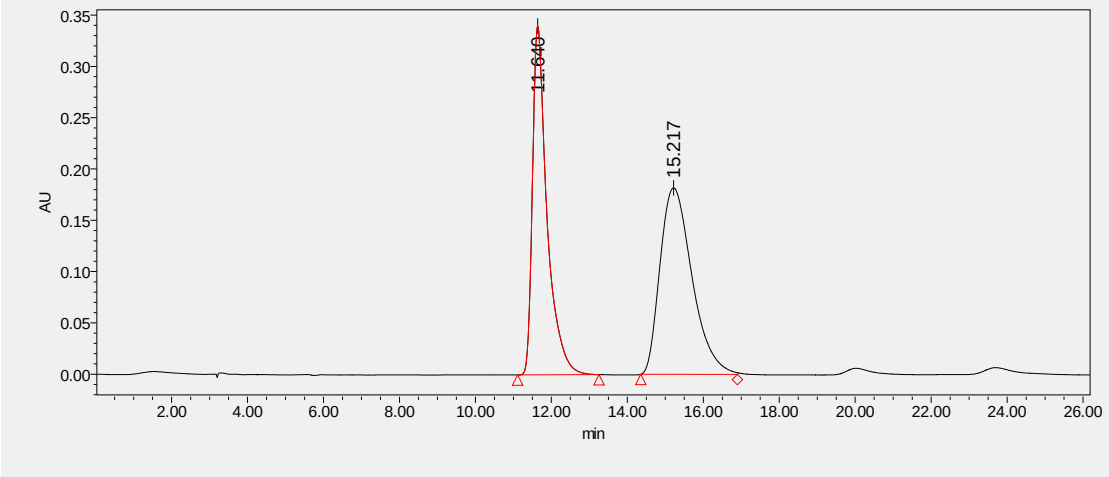
2-((R)-((S)-4-oxo-2-phenyl-5-propyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ca'

(Table 2, entry 3)

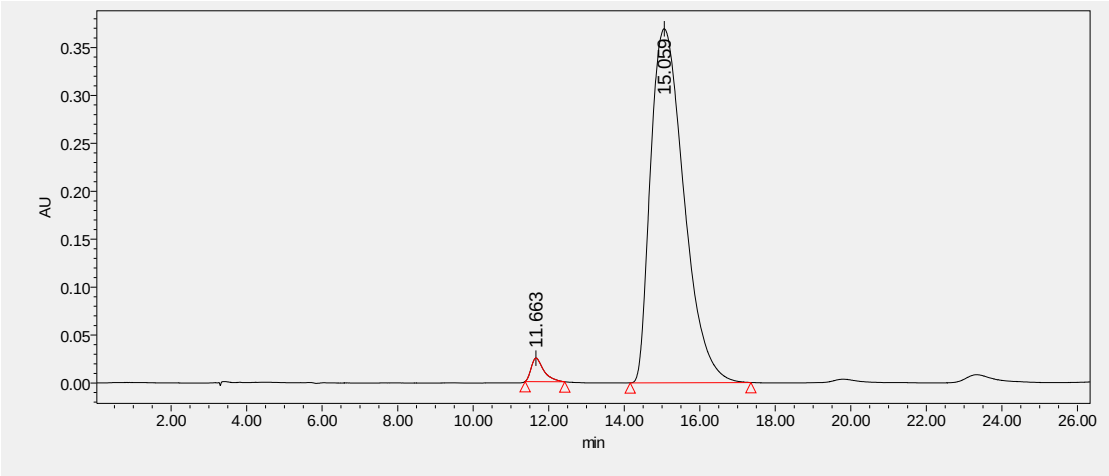


3ca'

Chiralpak IA column, hexane/EtOH (95:5), flow rate 1.0 mL/min

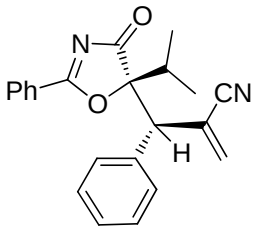


	Retention time	Area	% Area	Height	Integral type
1	11.640	9048691	45.99	339971	bb
2	15.217	10626048	54.01	181679	bv



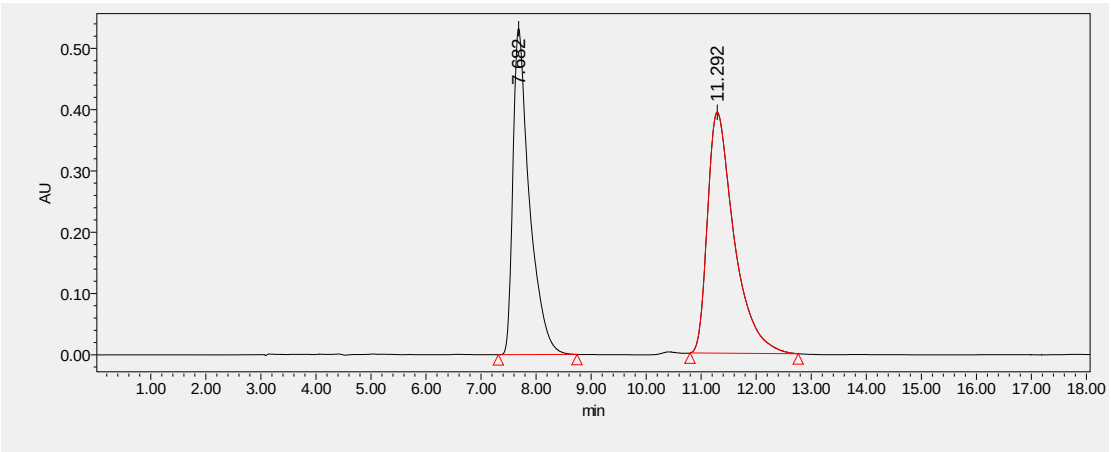
	Retention time	Area	% Area	Height	Integral type
1	11.663	568781	2.45	24562	bb
2	15.059	22639126	97.55	369344	bb

2-((R)-((S)-5-isopropyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3da' (Table 2, entry 4)

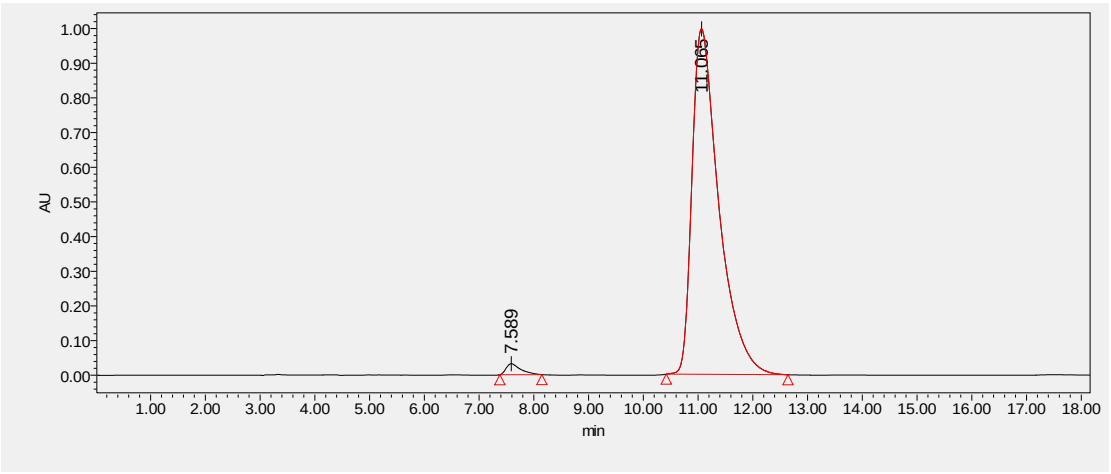


3da'

Chiralpak IA column, hexane/EtOH (90:10), flow rate 1.0 mL/min



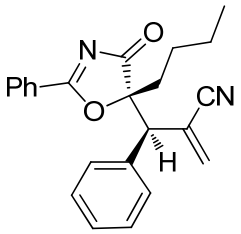
	Retention time	Area	% Area	Height	Integral type
1	7.682	11081483	45.66	532007	bb
2	11.292	13187584	54.34	393102	bb



	Retention time	Area	% Area	Height	Integral type
1	7.589	585679	1.69	31730	bb
2	11.065	34068091	98.31	996447	bb

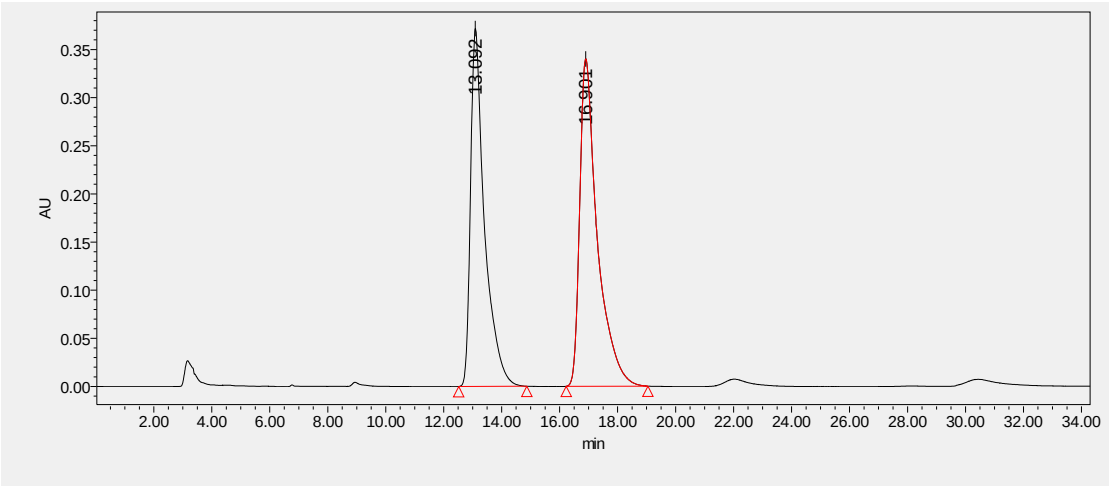
2-((R)-((S)-5-butyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ea'

(Table 2, entry 5)

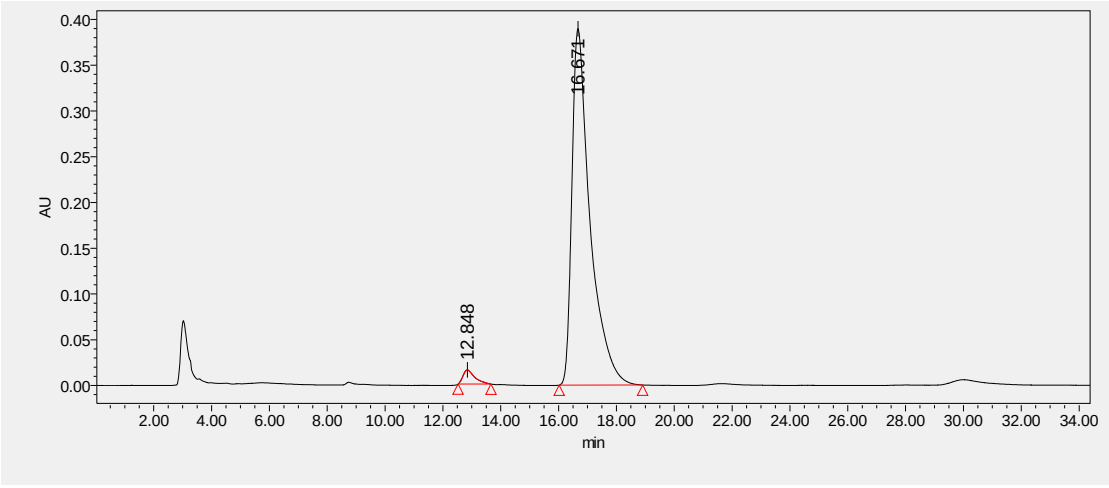


3ea'

Chiralpak IA column, hexane/EtOH (95:5), flow rate 1.0 mL/min

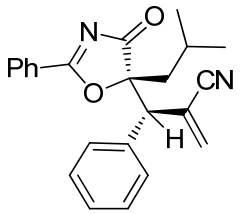


	Retention time	Area	% Area	Height	Integral type
1	13.092	12422244	46.39	371766	bb
2	16.901	14357529	53.61	340069	bb



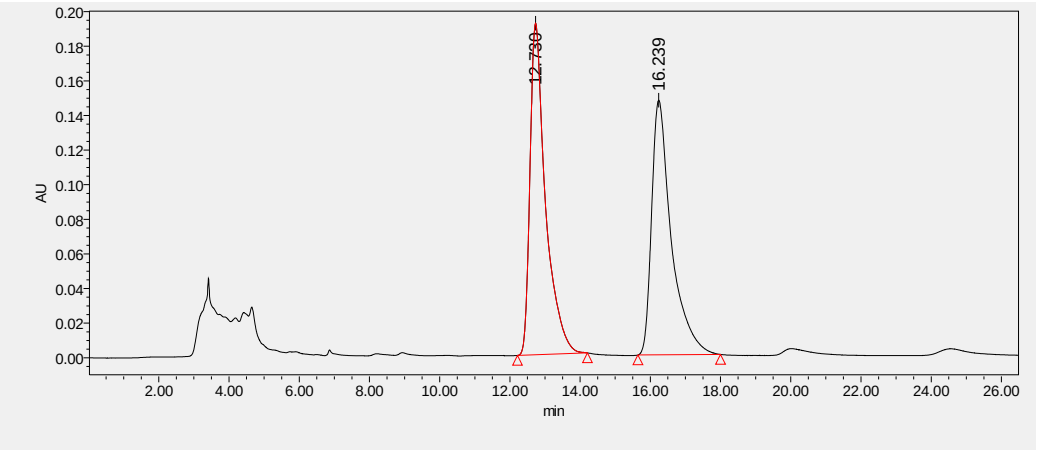
	Retention time	Area	% Area	Height	Integral type
1	12.848	431238	2.48	15435	bb
2	16.671	16936408	97.52	389387	bb

2-((R)-((S)-5-isobutyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3fa' (Table 2, entry 6)

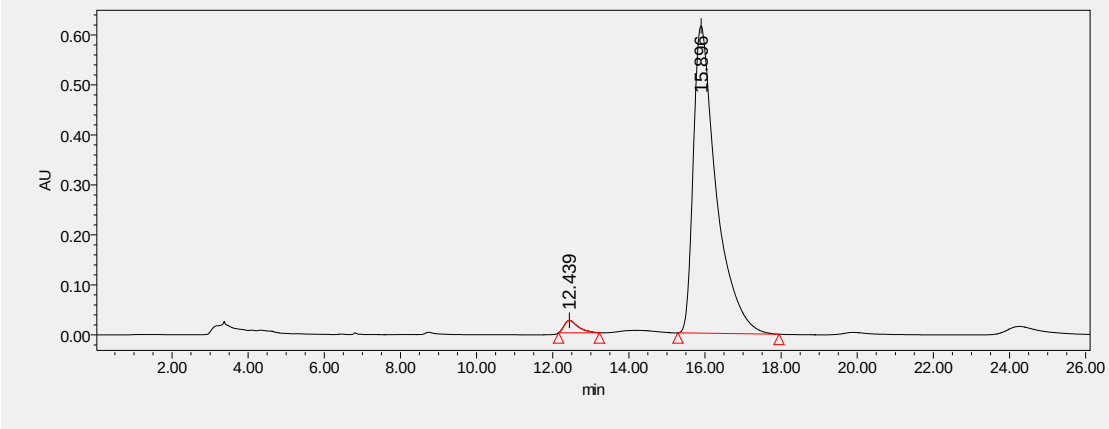


3fa'

Chiralpak IA column, hexane/EtOH (95:5), flow rate 1.0 mL/min

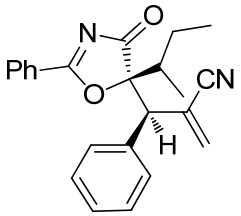


	Retention time	Area	% Area	Height	Integral type
1	12.730	5869271	50.65	191586	bb
2	16.239	5718537	49.35	147121	bb



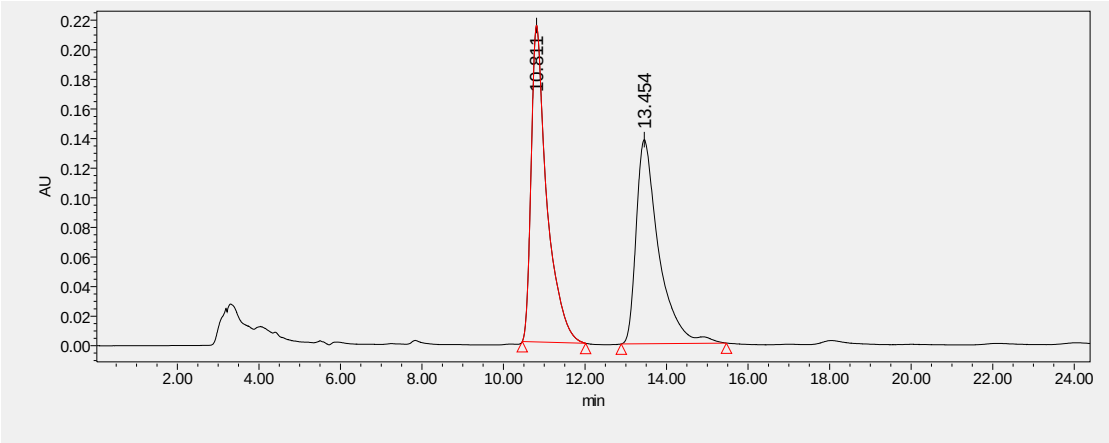
	Retention time	Area	% Area	Height	Integral type
1	12.439	638257	2.43	25021	bb
2	15.896	25645453	97.57	614641	bb

2-((R)-((S)-5-((S)-sec-butyl)-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ga' (Table 2, entry 7)

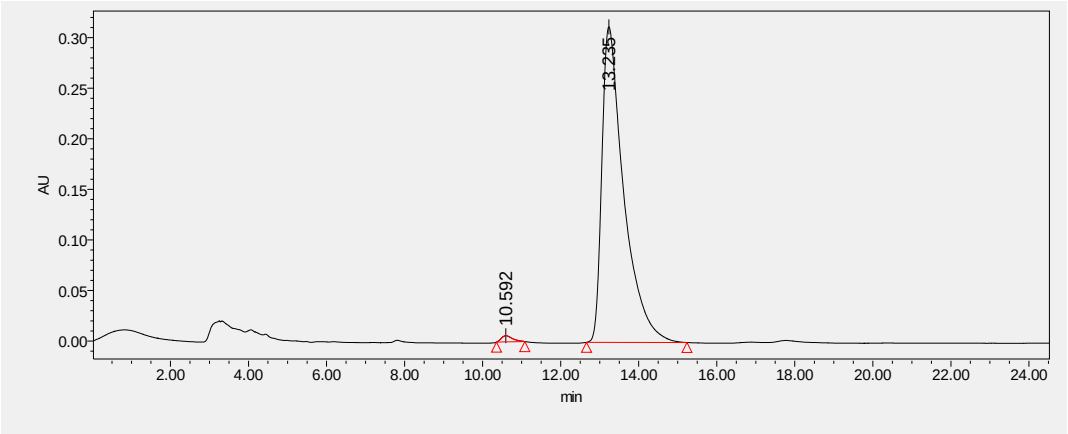


3ga'

Chiralpak IA column, hexane/EtOH (95:5), flow rate 1.0 mL/min

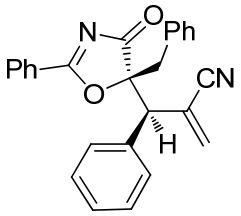


	Retention time	Area	% Area	Height	Integral type
1	10.811	5713717	51.89	213851	bb
2	13.454	5297282	48.11	137830	bb



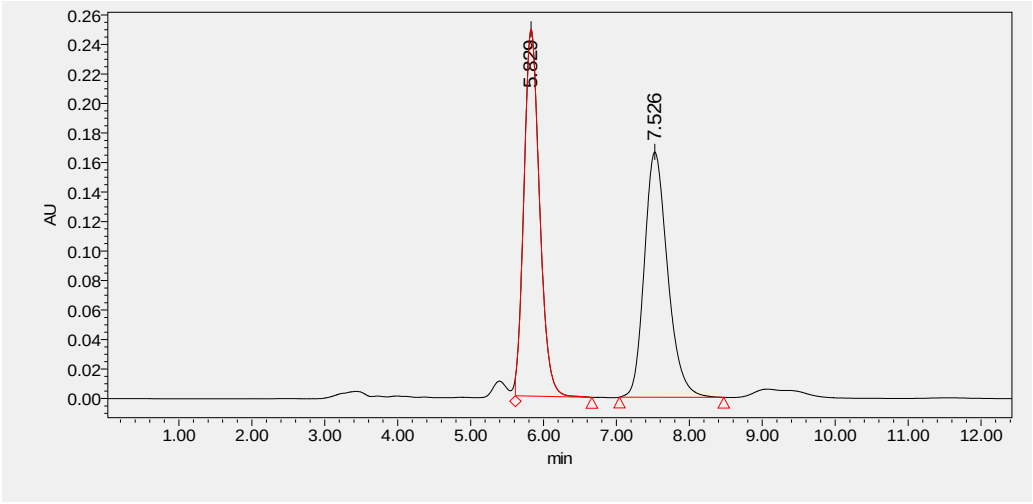
	Retention time	Area	% Area	Height	Integral type
1	10.592	123193	1.00	6164	bb
2	13.235	12157709	99.00	311931	bb

2-((R)-((S)-5-benzyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ha' (Table 2, entry 8)

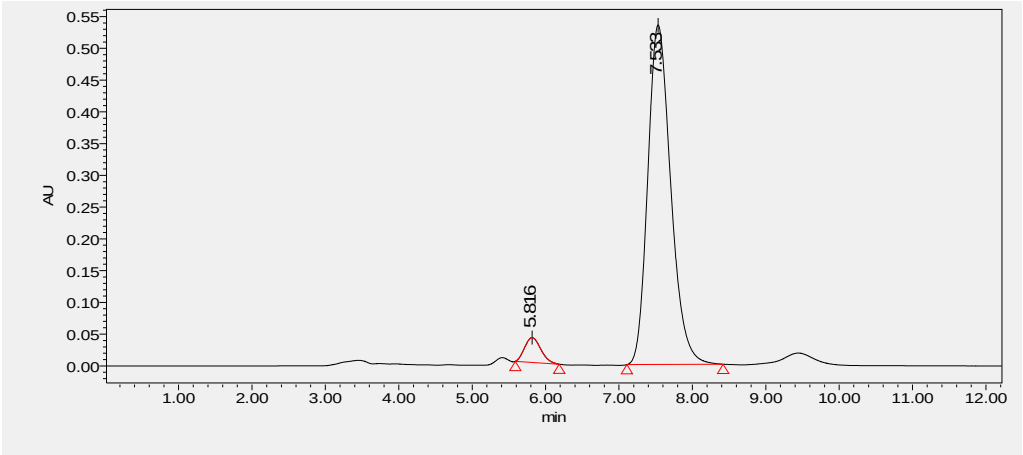


3ha'

Chiralpak IC column, hexane/iPrOH (1:3), flow rate 1.0 mL/min



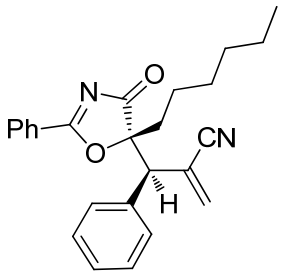
	Retention time	Area	% Area	Height	Integral type
1	5.829	3712401	50.22	248717	vb
2	7.526	3679358	49.78	166280	bb



	Retention time	Area	% Area	Height	Integral type
1	5.816	599129	4.90	39108	bb
2	7.533	11629239	95.10	534510	bb

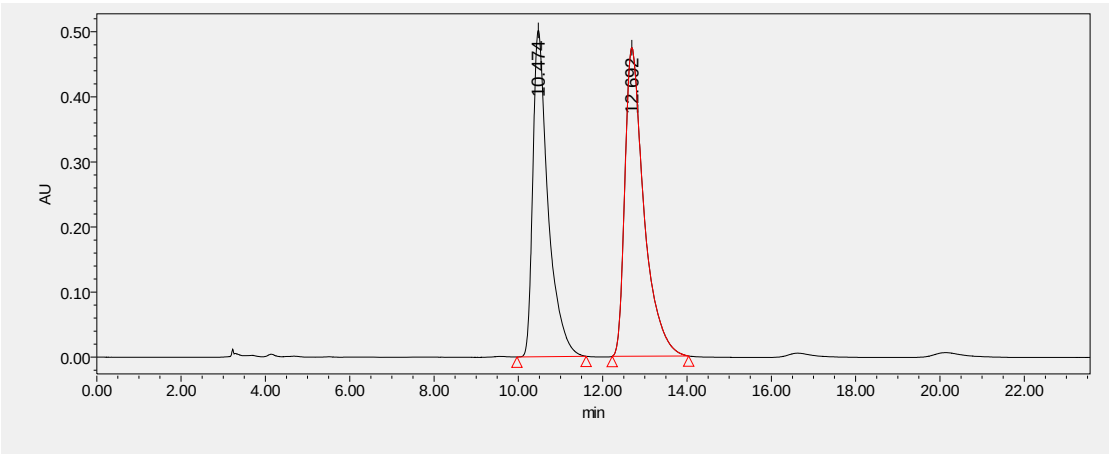
2-((R)-((S)-5-hexyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ia'

(Table 2, entry 9)

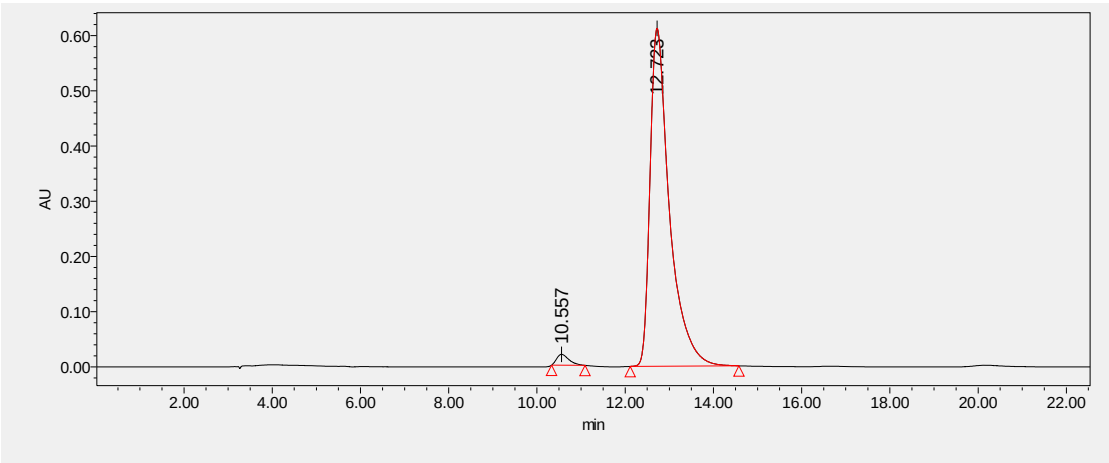


3ia'

Chiralpak IA column, hexane/EtOH (95:5), flow rate 1.0 mL/min



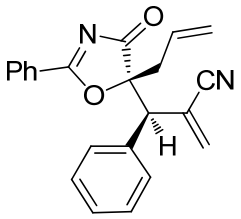
	Retention time	Area	% Area	Height	Integral type
1	10.474	12564485	45.72	501595	bb
2	12.692	14919257	54.28	473956	bb



	Retention time	Area	% Area	Height	Integral type
1	10.557	385052	2.01	19867	bb
2	12.723	18726590	97.99	611913	bb

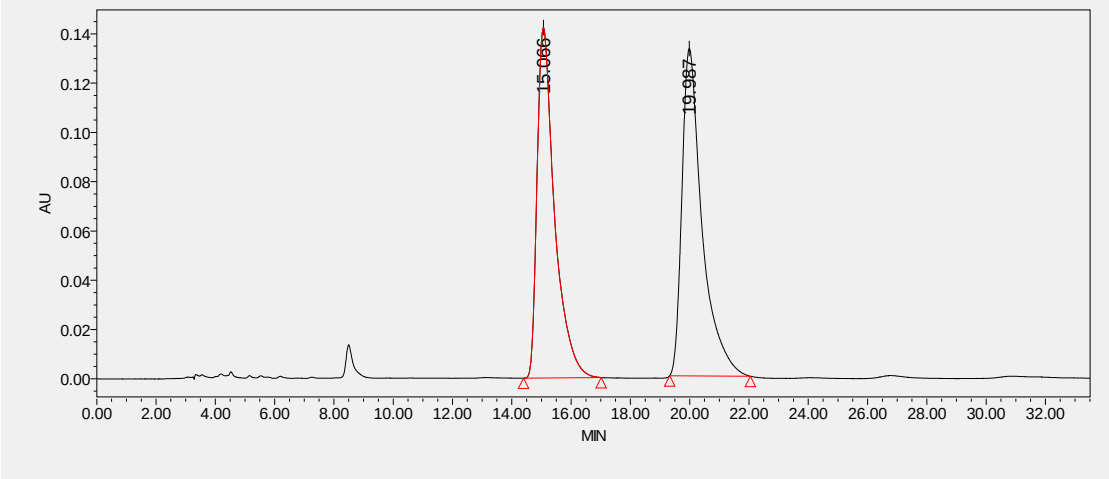
2-((R)-((S)-5-allyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(phenyl)methyl)acrylonitrile, 3ja'

(Table 2, entry 10)

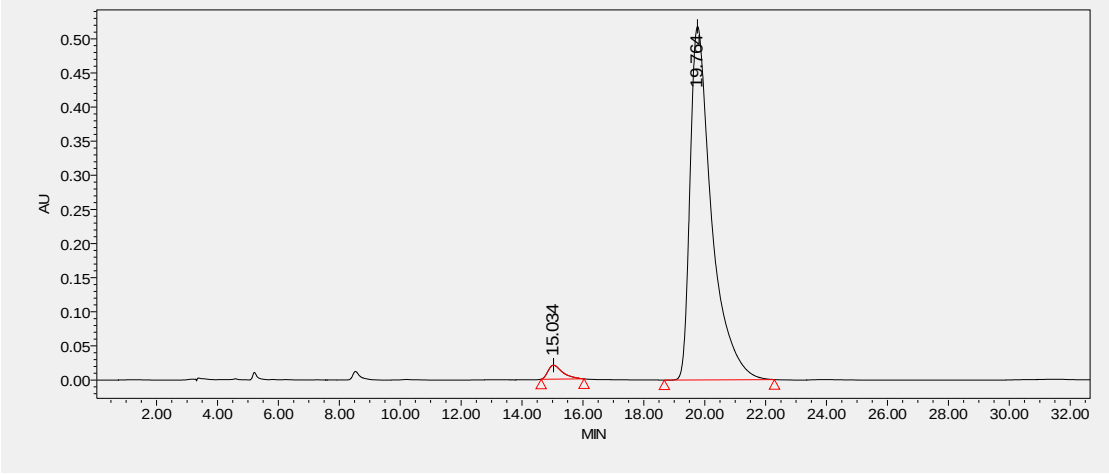


3ja'

Chiralpak IA column, hexane/EtOH (95:5), flow rate 1.0 mL/min

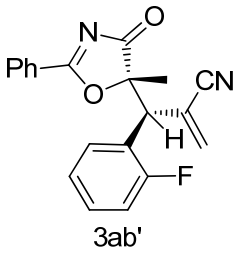


	Retention time	Area	% Area	Height	Integral type
1	15.066	5803184	48.08	142161	bb
2	19.987	6265815	51.92	132860	bb



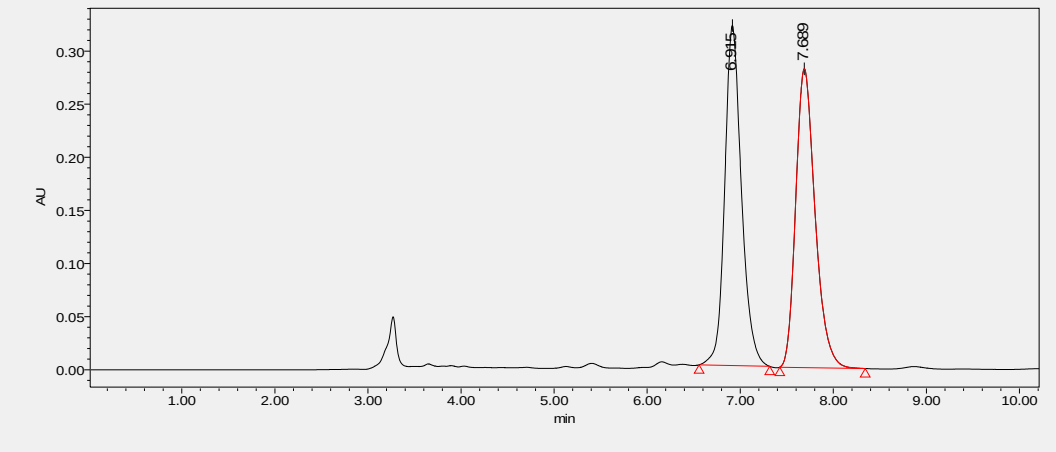
	Retention time	Area	% Area	Height	Integral type
1	15.034	680403	2.61	20426	bb
2	19.764	25409908	97.39	518052	bb

2-((R)-(2-fluorophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryloni trile, 3ab' (Table 2, entry 11)

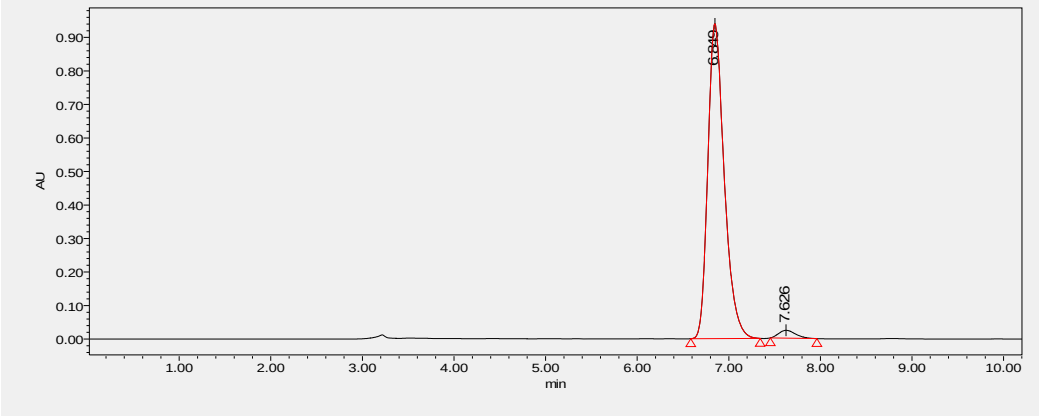


3ab'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

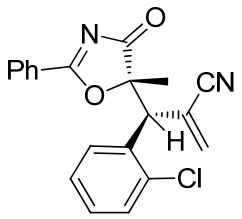


	Retention time	Area	% Area	Height	Integral type
1	6.915	4010217	49.69	320042	bb
2	7.689	4059841	50.31	281262	bb



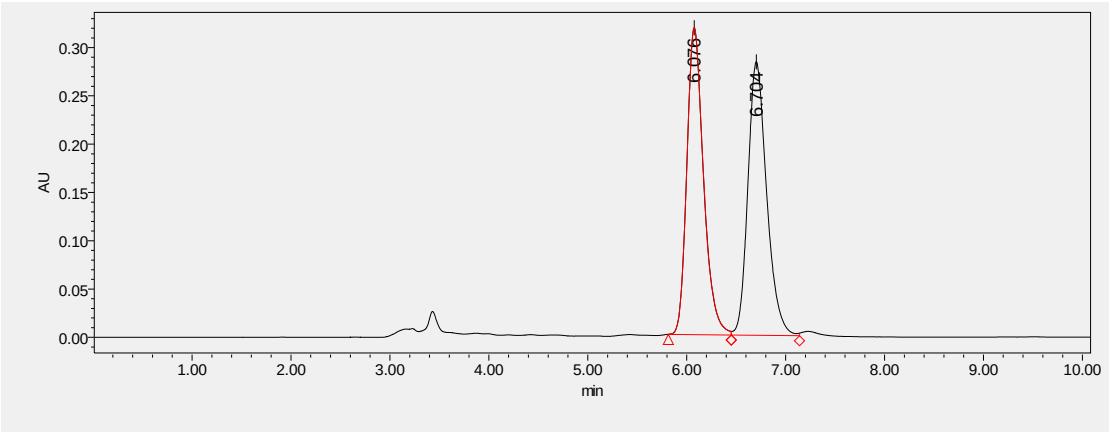
	Retention time	Area	% Area	Height	Integral type
1	6.849	11734463	97.51	939705	bb
2	7.626	299172	2.49	23451	bb

2-((R)-(2-chlorophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryloni trile, 3ac' (Table 2, entry 12)

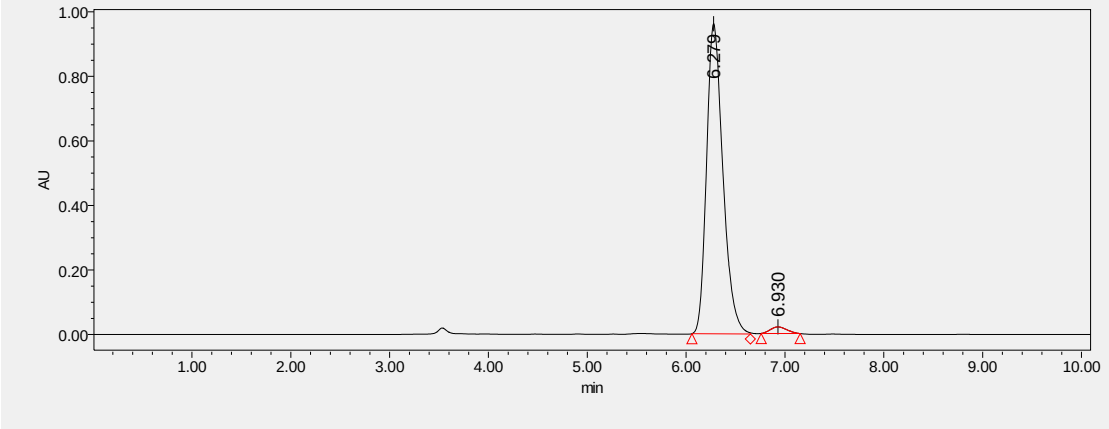


3ac'

Chiralpak IC column, hexane/iPrOH (1:2), flow rate 1.0 mL/min

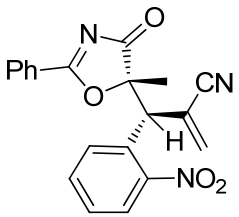


	Retention time	Area	% Area	Height	Integral type
1	6.076	3719364	49.85	317568	bv
2	6.704	3741305	50.15	283128	vv



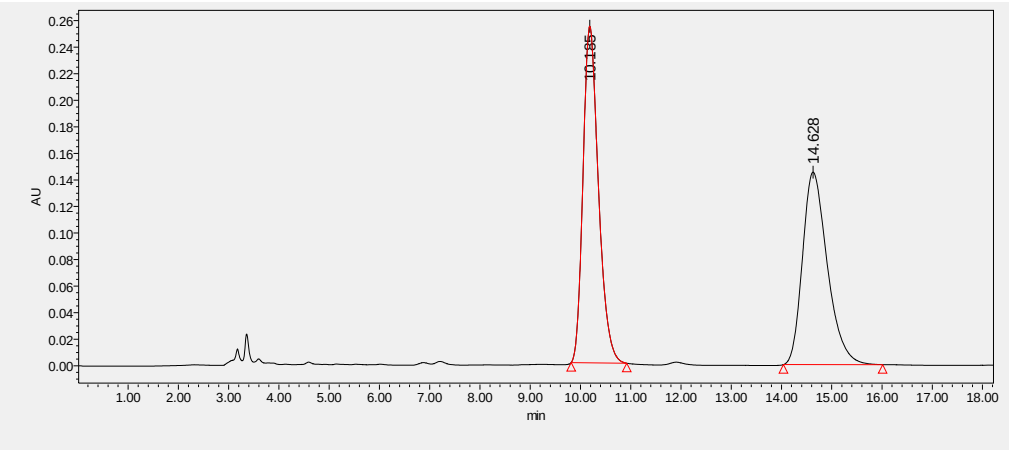
	Retention time	Area	% Area	Height	Integral type
1	6.279	11050102	97.91	960985	bv
2	6.930	235891	2.09	20406	bb

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(2-nitrophenyl)methyl)acrylonitrile, 3ad' (Table 2., entry 13)

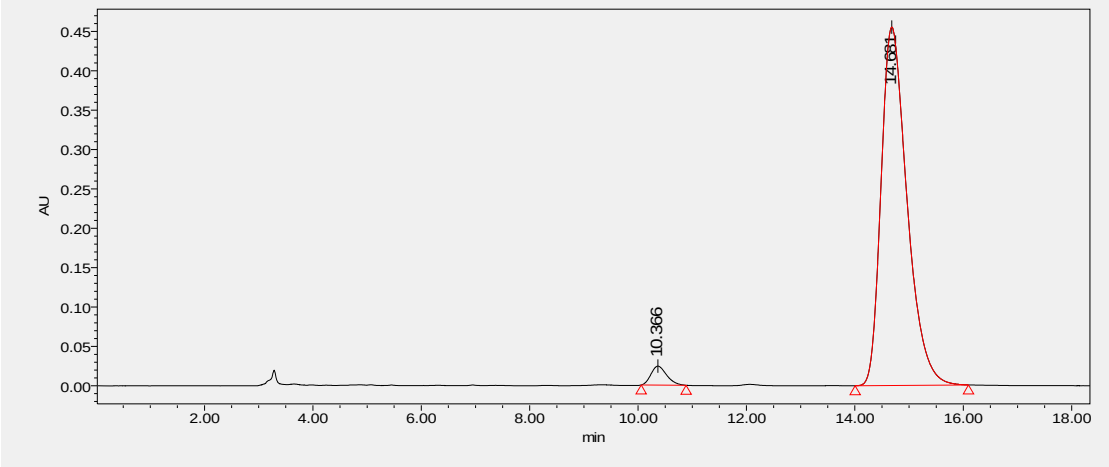


3ad'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min



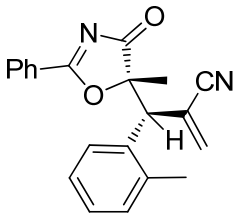
	Retention time	Area	% Area	Height	Integral type
1	10.185	5404436	52.06	253510	bb
2	14.628	4975972	47.94	145012	bb



	Retention time	Area	% Area	Height	Integral type
1	10.366	483097	3.10	24073	bb
2	14.681	15124934	96.90	454997	bb

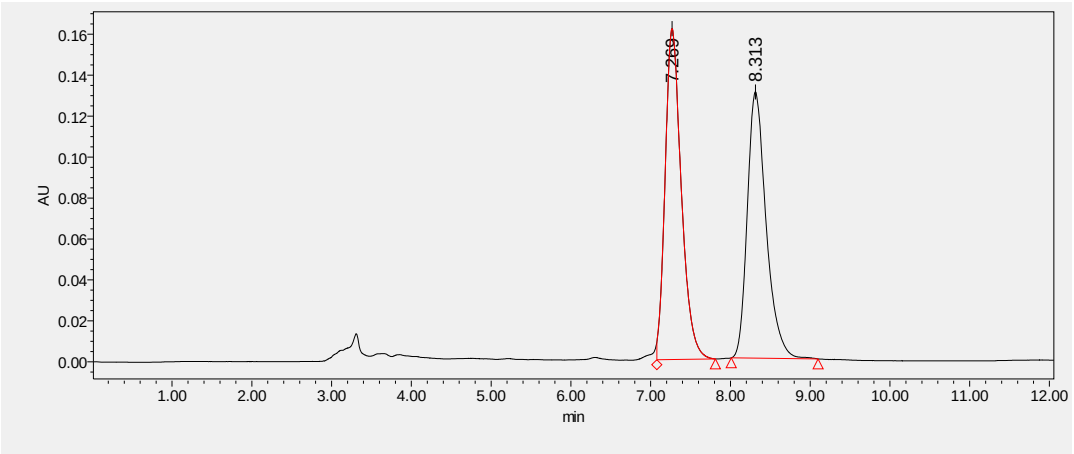
2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(o-tolyl)methyl)acrylonitrile, 3ae'

(Table 2, entry 14)

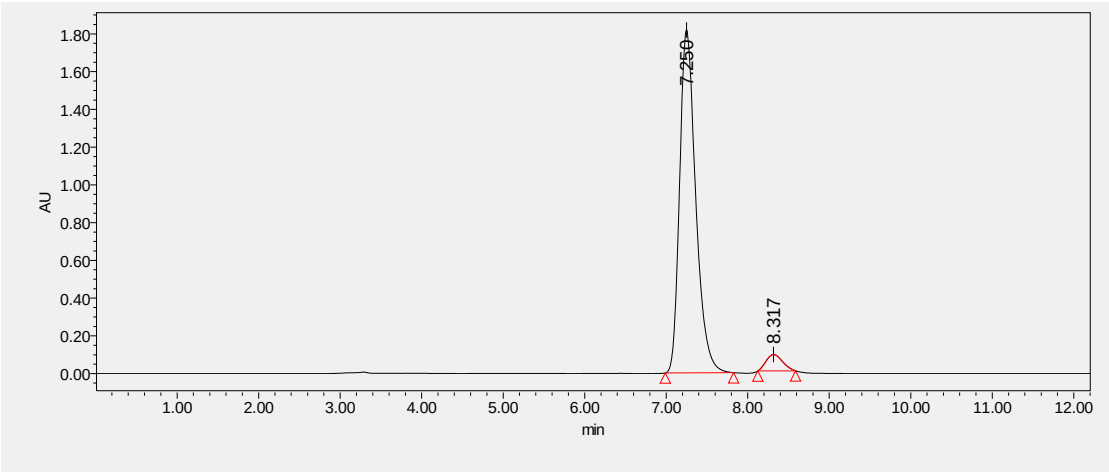


3ae'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

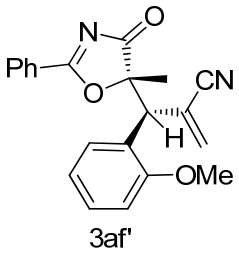


	Retention time	Area	% Area	Height	Integral type
1	7.269	2274523	51.58	161600	vb
2	8.313	2135103	48.42	129985	bb



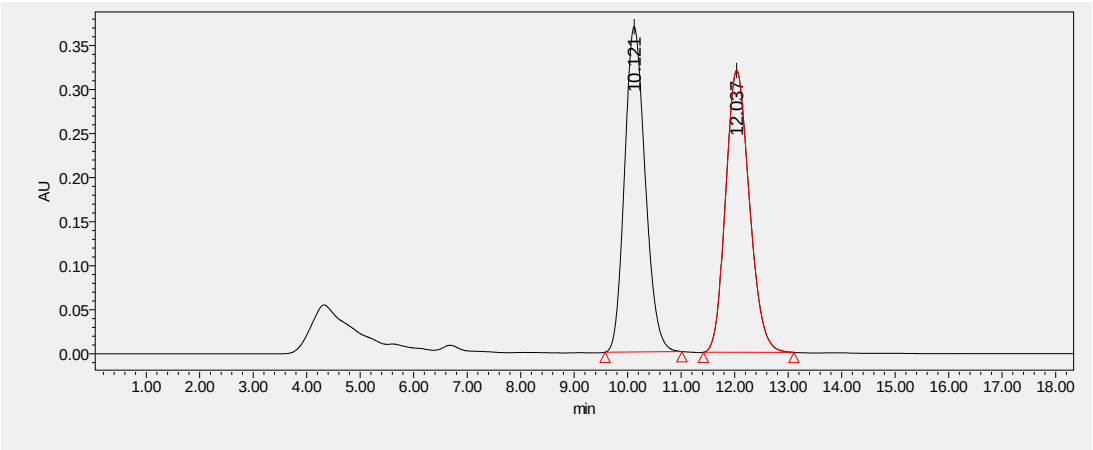
	Retention time	Area	% Area	Height	Integral type
1	7.250	24919960	95.36	1816881	bb
2	8.317	1213272	4.64	86835	bb

2-((R)-(2-methoxyphenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3af' (Table 2, entry 15)

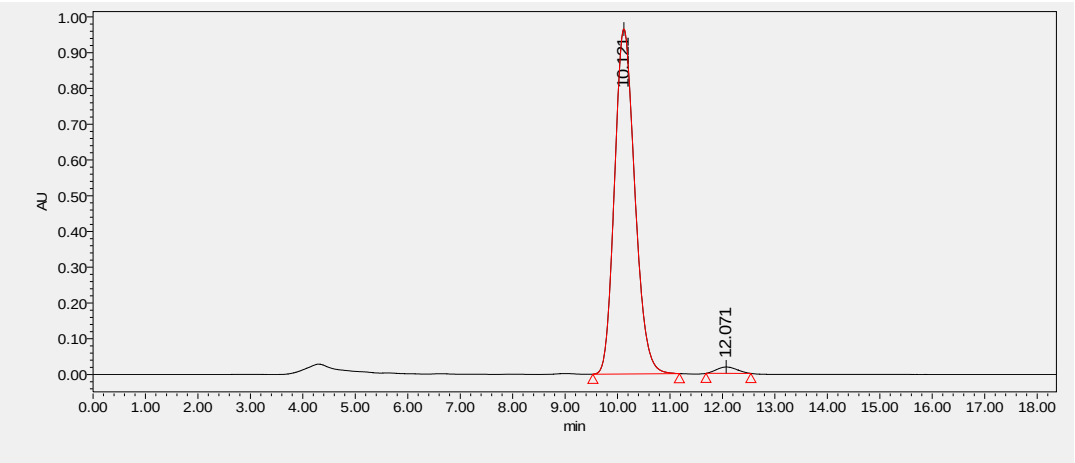


3af'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

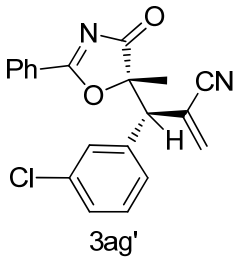


	Retention time	Area	% Area	Height	Integral type
1	10.121	9886967	50.04	369227	bb
2	12.037	9871740	49.96	319961	bb



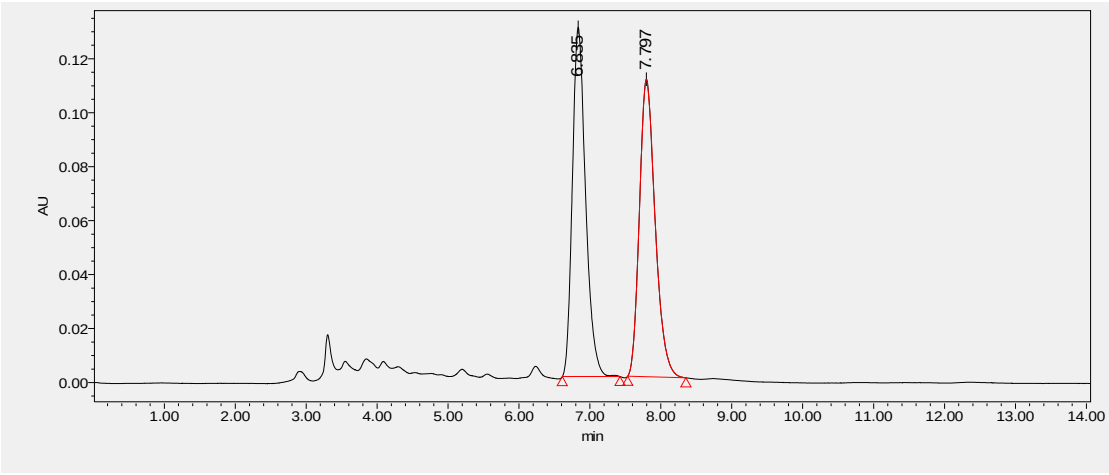
	Retention time	Area	% Area	Height	Integral type
1	10.121	25879644	98.19	964701	bb
2	12.071	476216	1.81	17797	bb

2-((R)-(3-chlorophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryloni trile, 3ag' (Table 2, entry 16)

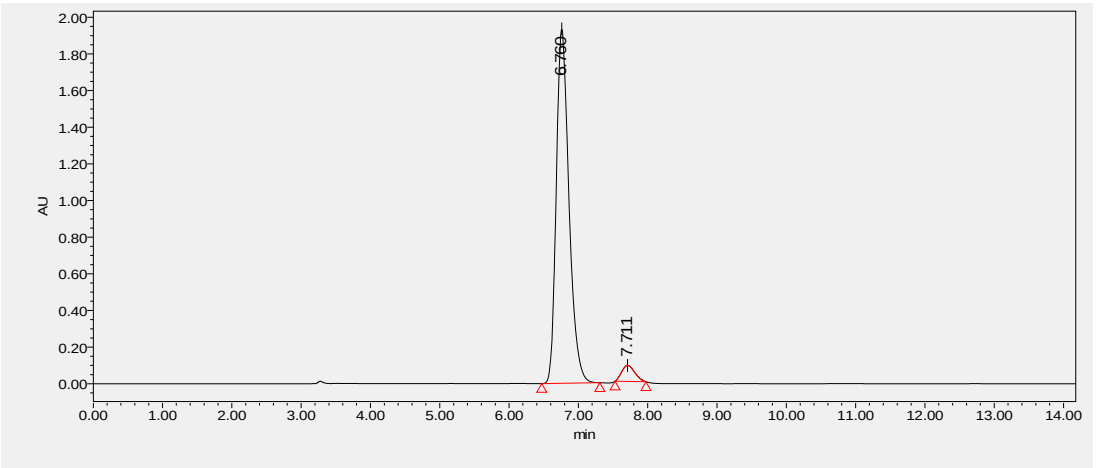


3ag'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

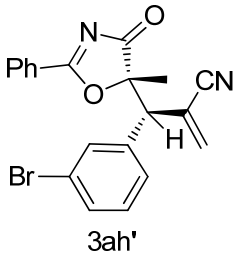


	Retention time	Area	% Area	Height	Integral type
1	6.835	1678849	49.69	129461	bb
2	7.797	1699859	50.31	110259	bb



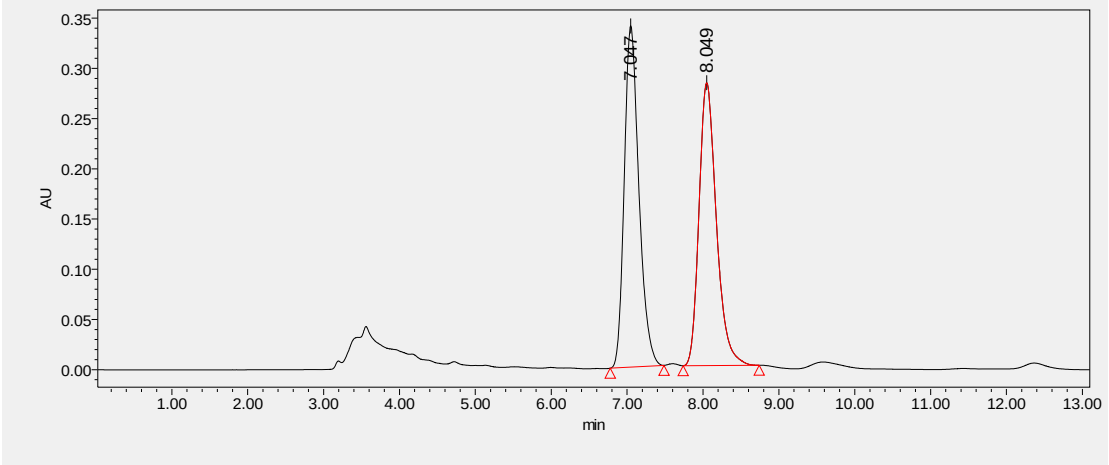
	Retention time	Area	% Area	Height	Integral type
1	6.760	24634883	95.55	1933417	bb
2	7.711	1147454	4.45	87406	bb

2-((R)-(3-bromophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryloni trile, 3ah' (Table 2, entry 17)

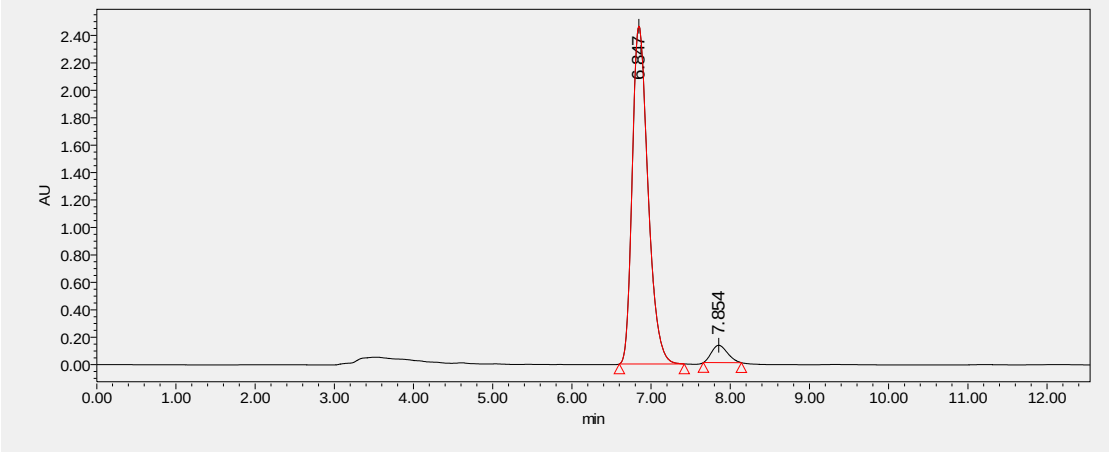


3ah'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

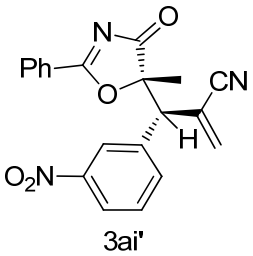


	Retention time	Area	% Area	Height	Integral type
1	7.047	4555451	50.46	339799	bb
2	8.049	4472476	49.54	281657	bb



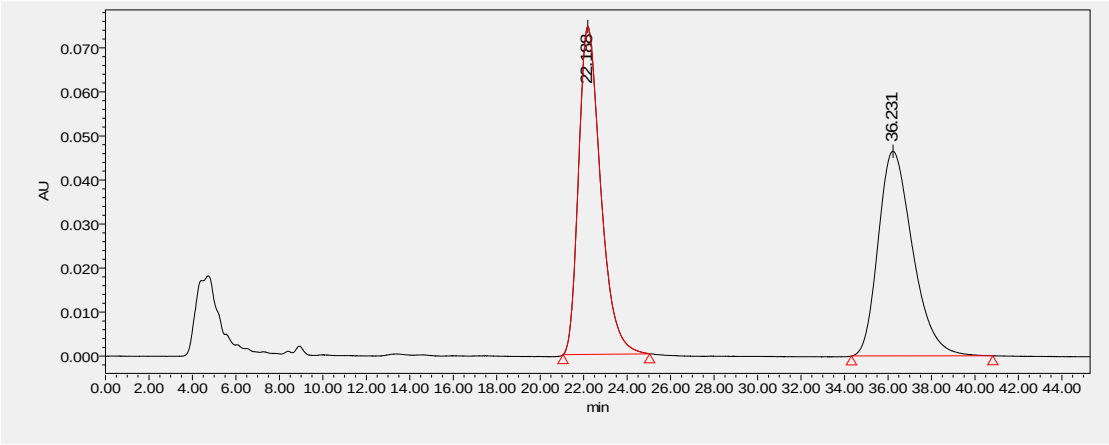
	Retention time	Area	% Area	Height	Integral type
1	6.847	34064342	95.10	2461136	bb
2	7.854	1753530	4.90	126059	bb

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(3-nitrophenyl)methyl)acrylonitrile, 3ai' (Table 2, entry 18)

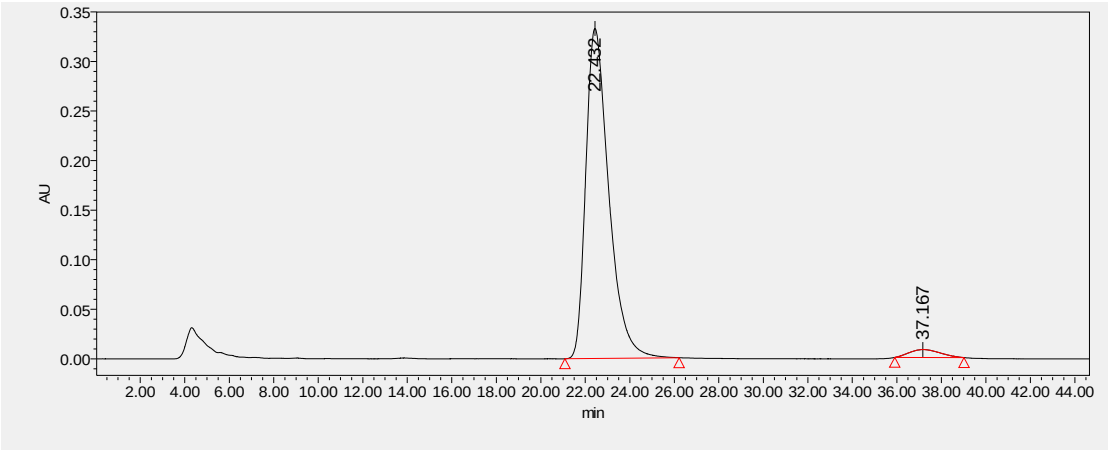


3ai'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

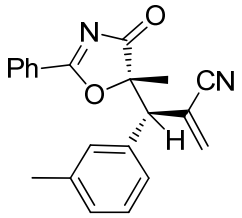


	Retention time	Area	% Area	Height	Integral type
1	22.188	5253040	50.68	74435	bb
2	36.231	5111478	49.32	46482	bb



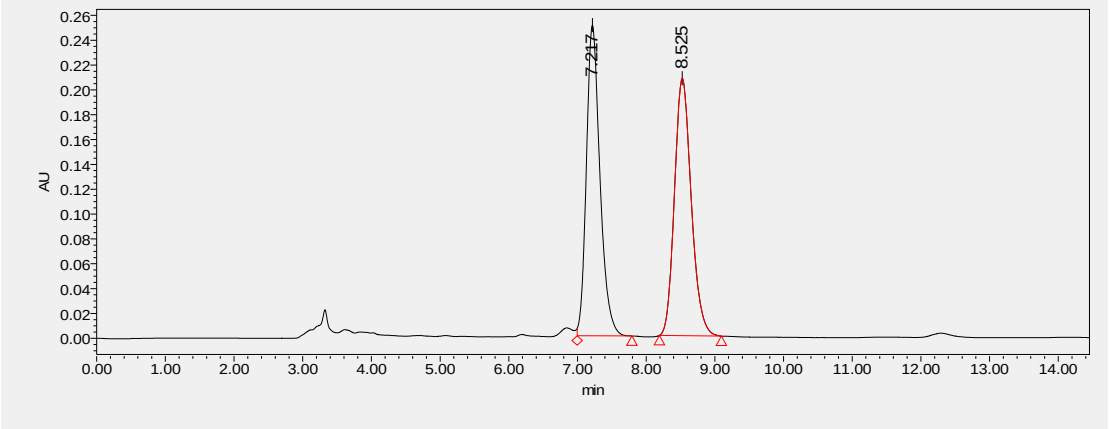
	Retention time	Area	% Area	Height	Integral type
1	22.432	23907420	96.88	332894	bb
2	37.167	770855	3.12	7984	bb

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(m-tolyl)methyl)acrylonitrile, 3aj' (Table 2, entry 19)

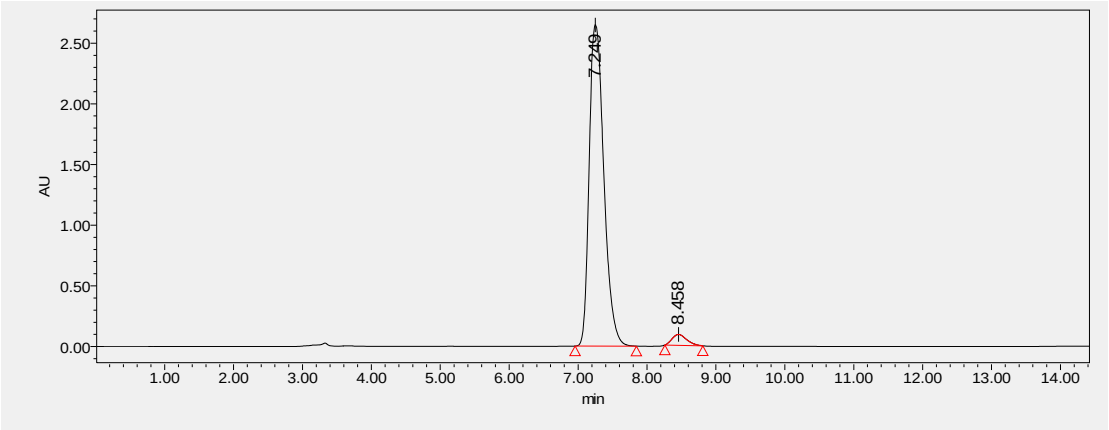


3aj'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

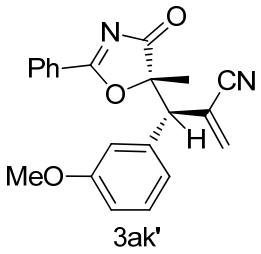


	Retention time	Area	% Area	Height	Integral type
1	7.217	3436743	49.43	250215	vb
2	8.525	3516001	50.57	207277	bb



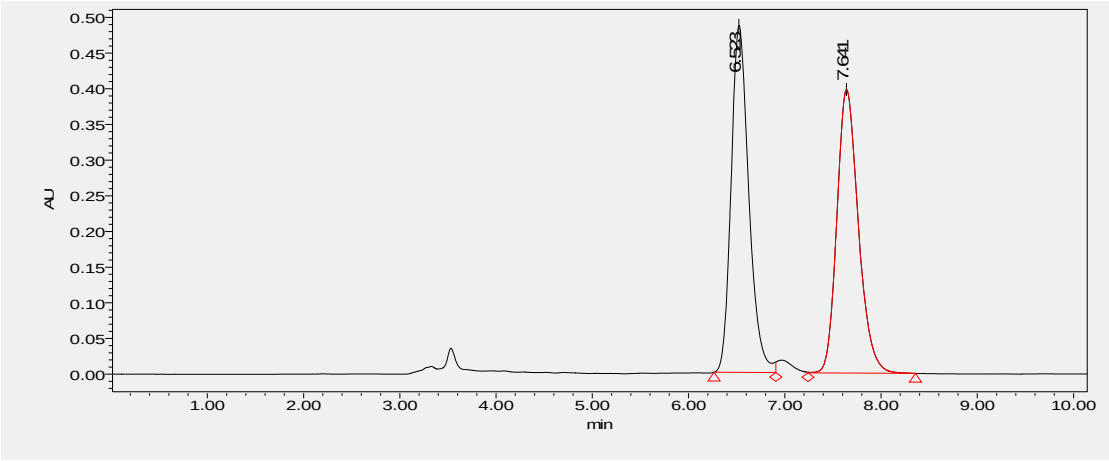
	Retention time	Area	% Area	Height	Integral type
1	7.249	39096962	96.74	2647233	bb
2	8.458	1316279	3.26	89622	bb

2-((R)-(3-methoxyphenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3ak' (Table 2, entry 20)

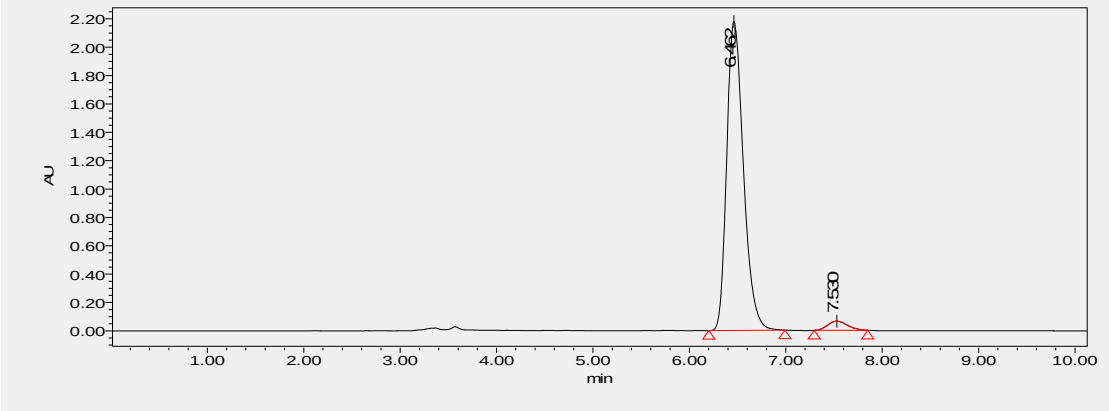


3ak'

Chiralpak IC column, hexane/iPrOH (1:2), flow rate 1.0 mL/min

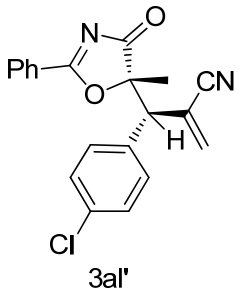


	Retention time	Area	% Area	Height	Integral type
1	6.523	6229785	50.25	486512	bv
2	7.641	6167371	49.75	397407	vb



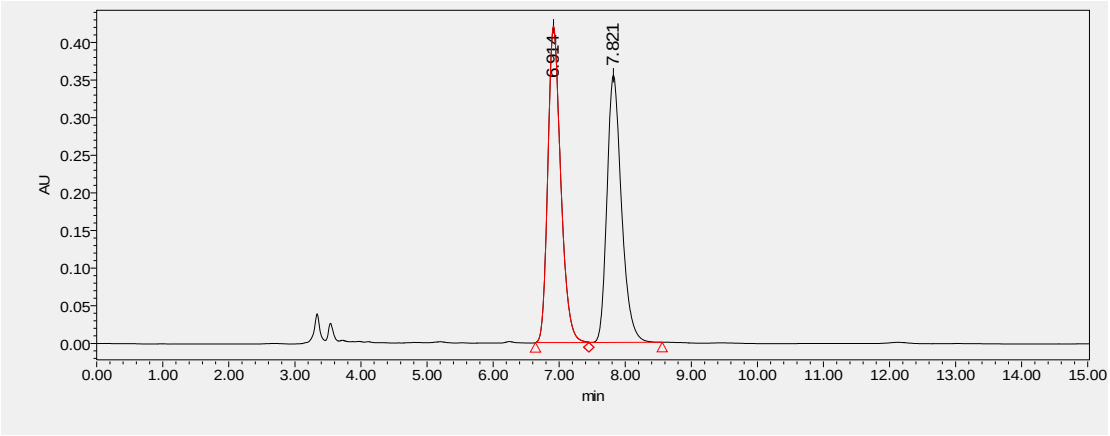
	Retention time	Area	% Area	Height	Integral type
1	6.462	26276270	96.57	2176907	bb
2	7.530	934184	3.43	65162	bb

2-((R)-(4-chlorophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acryloni trile, 3al' (Table 2, entry 21)

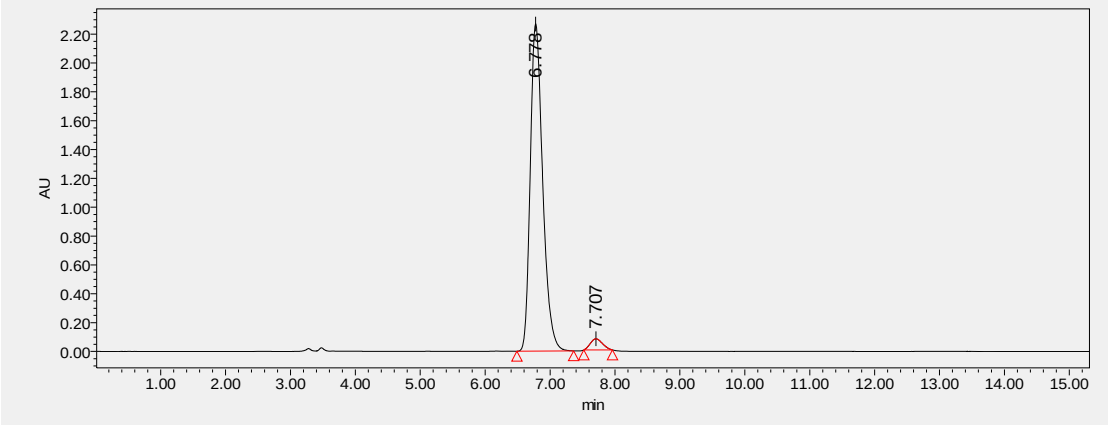


3al'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

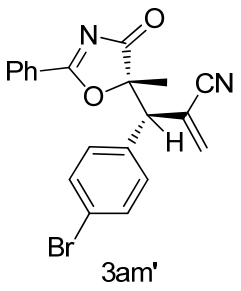


	Retention time	Area	% Area	Height	Integral type
1	6.914	5708833	51.26	420382	bv
2	7.821	5427851	48.74	355160	vb



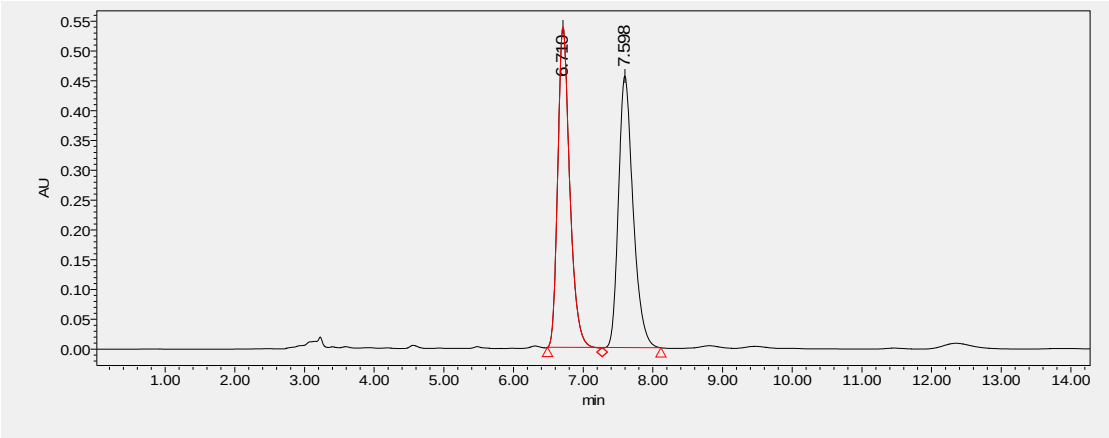
	Retention time	Area	% Area	Height	Integral type
1	6.778	30204702	96.78	2268251	bb
2	7.707	1006249	3.22	77298	bb

2-((R)-(4-bromophenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3am' (Table 2, entry 22)

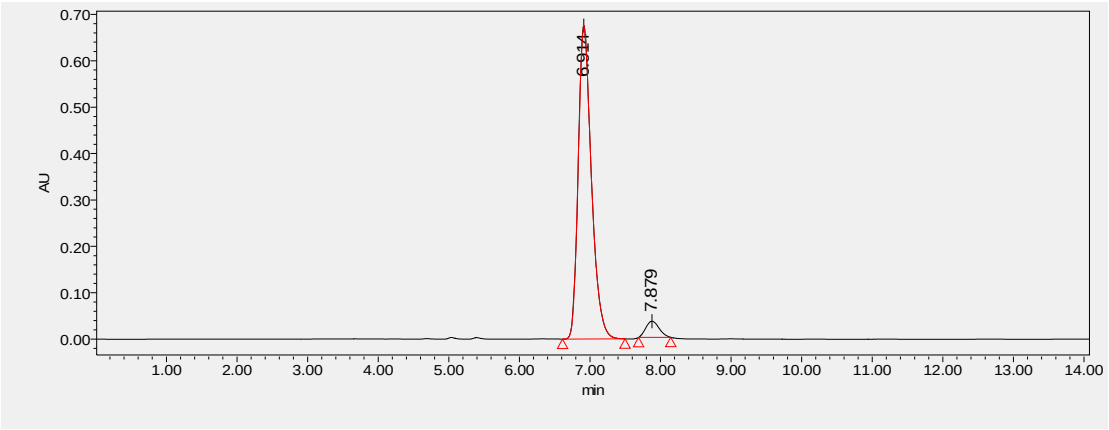


3am'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

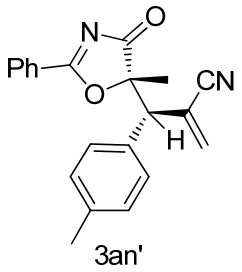


	Retention time	Area	% Area	Height	Integral type
1	6.710	6431317	49.23	537507	bv
2	7.598	6633025	50.77	455630	vb



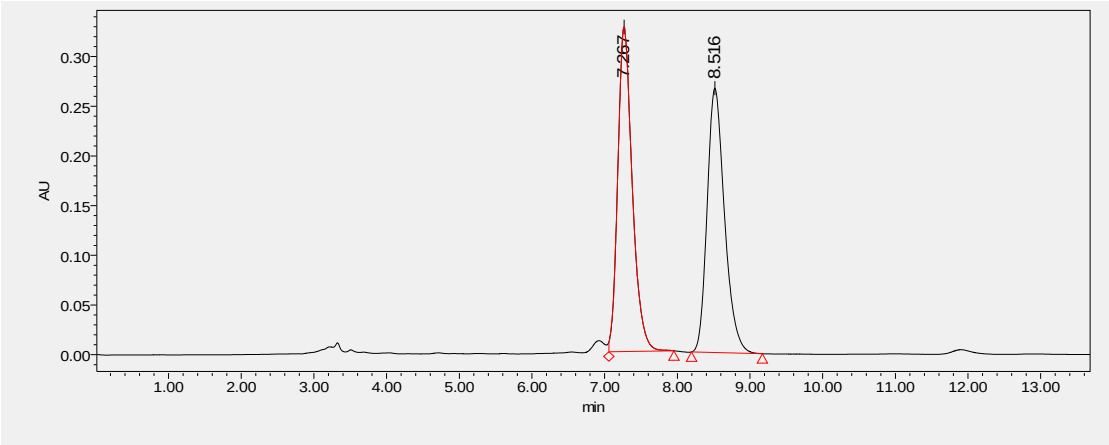
	Retention time	Area	% Area	Height	Integral type
1	6.914	8769952	95.05	675552	bb
2	7.879	456662	4.95	34851	bb

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(p-tolyl)methyl)acrylonitrile, 3an' (Table 2, entry 23)

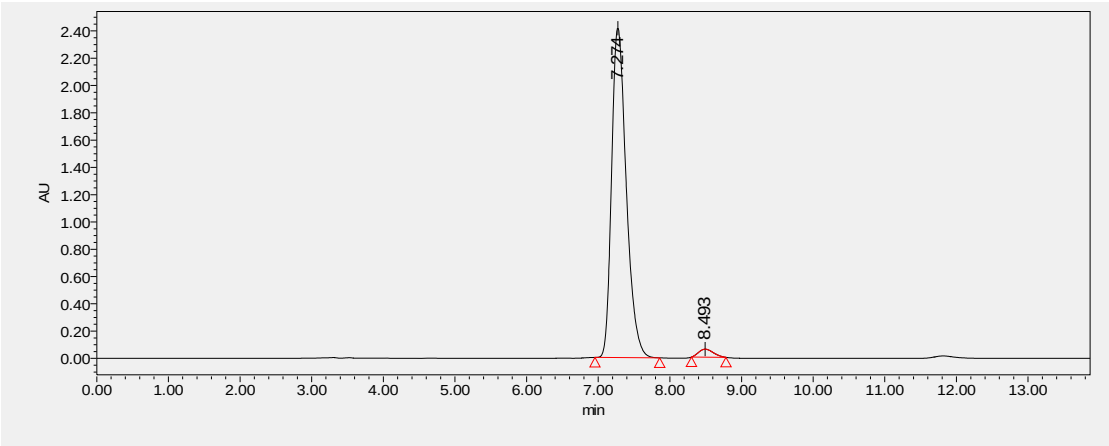


3an'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

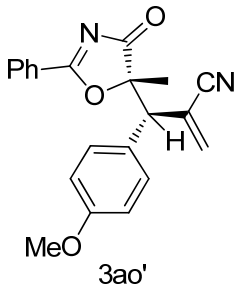


	Retention time	Area	% Area	Height	Integral type
1	7.267	4516644	50.58	326641	vb
2	8.516	4413103	49.42	265865	bb



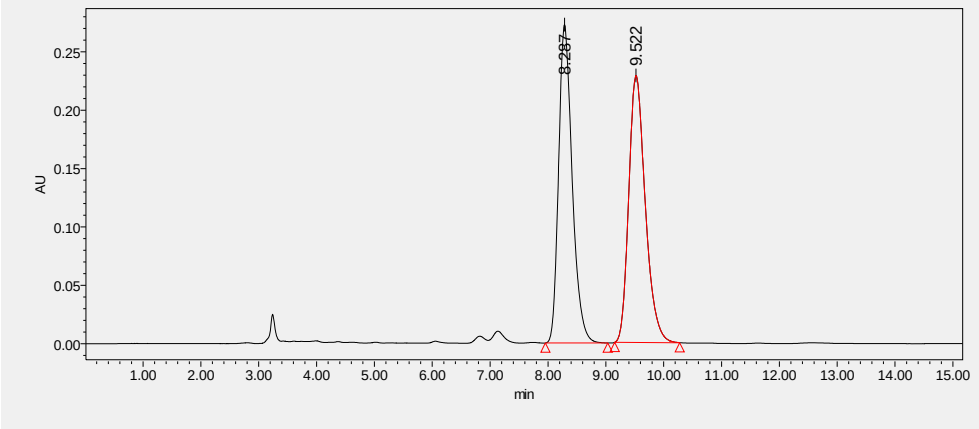
	Retention time	Area	% Area	Height	Integral type
1	7.274	34356356	97.61	2415648	bb
2	8.493	843014	2.39	58987	bb

2-((R)-(4-methoxyphenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3ao' (Table 2, entry 24)

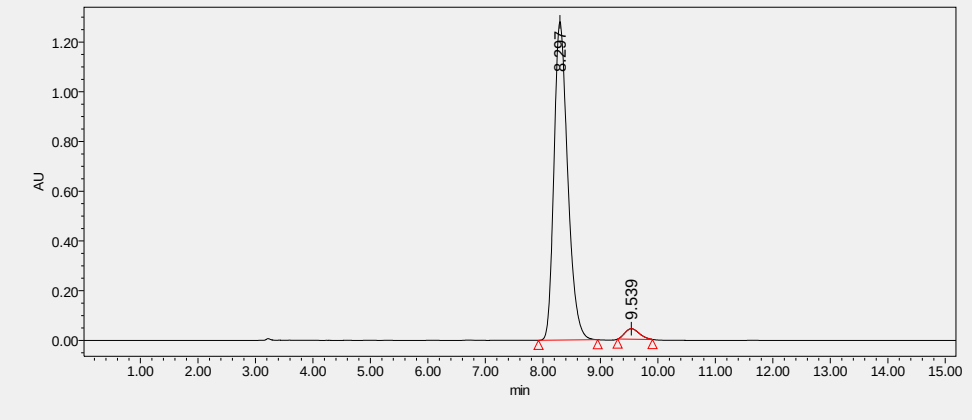


3ao'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

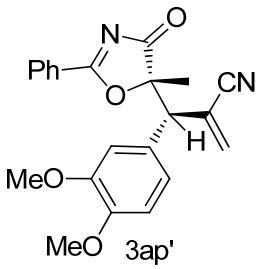


	Retention time	Area	% Area	Height	Integral type
1	8.287	4452438	49.50	272710	bb
2	9.522	4541678	50.50	228702	bb

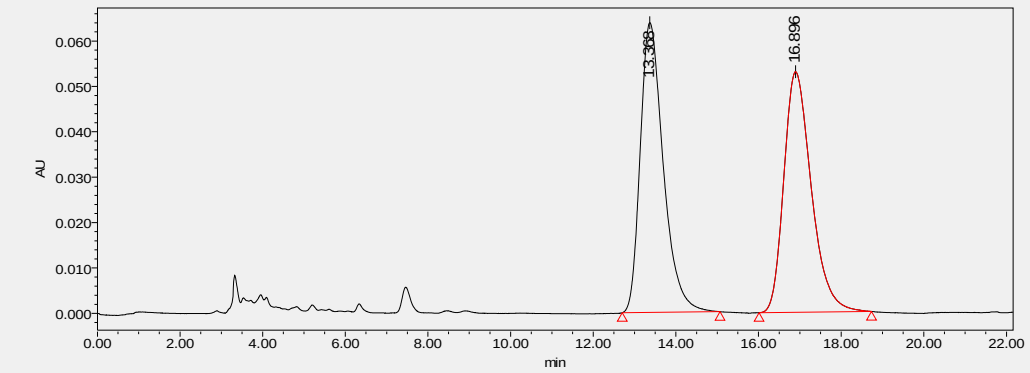


	Retention time	Area	% Area	Height	Integral type
1	8.297	21208890	96.66	1279758	bb
2	9.539	732292	3.34	42327	bb

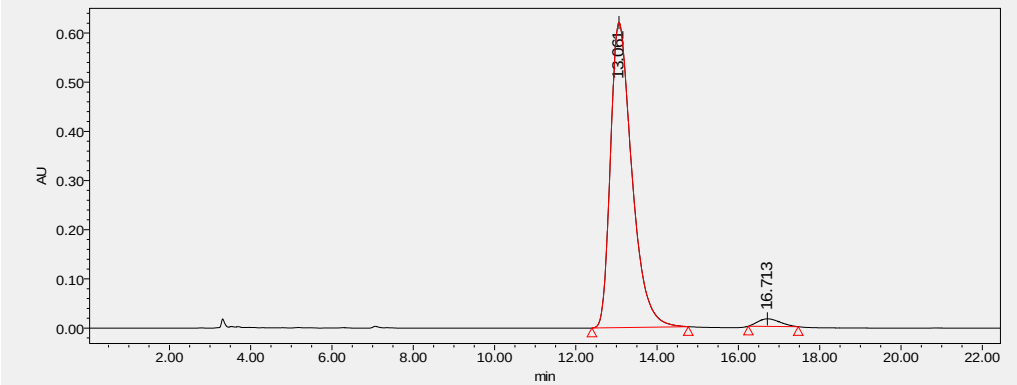
2-((R)-(3,4-dimethoxyphenyl)((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3ap' (Table 2, entry 25)



Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

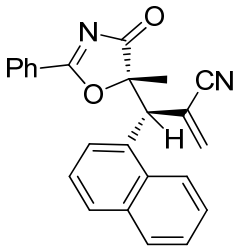


	Retention time	Area	% Area	Height	Integral type
1	13.368	2468753	50.27	63815	bb
2	16.896	2442607	49.73	53005	bb



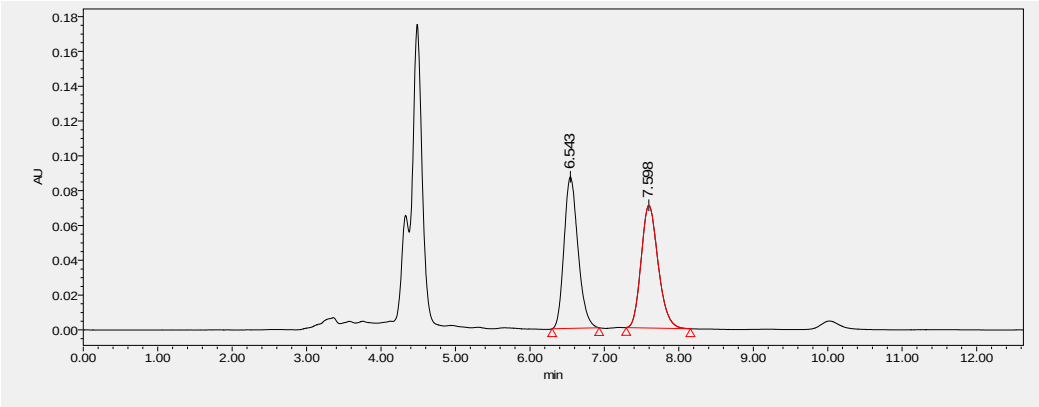
	Retention time	Area	% Area	Height	Integral type
1	13.061	22733965	97.51	620357	bb
2	16.713	581396	2.49	15325	bb

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(naphthalen-1-yl)methyl)acrylonitrile, 3aq' (Table 2, entry 26)

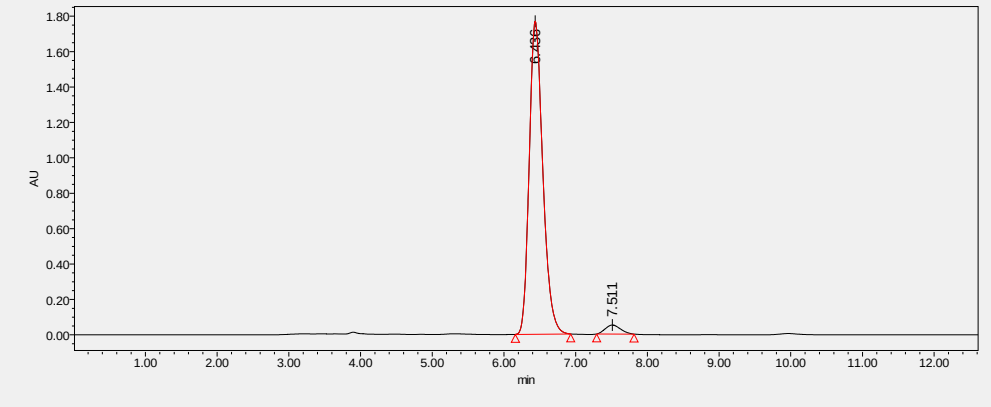


3aq'

Chiralpak IC column, hexane/iPrOH (1:2), flow rate 1.0 mL/min

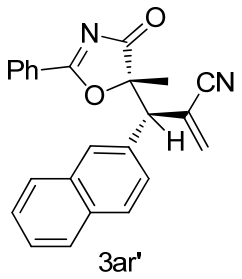


	Retention time	Area	% Area	Height	Integral type
1	6.543	1135317	50.38	87082	bb
2	7.598	1118046	49.62	70514	bb



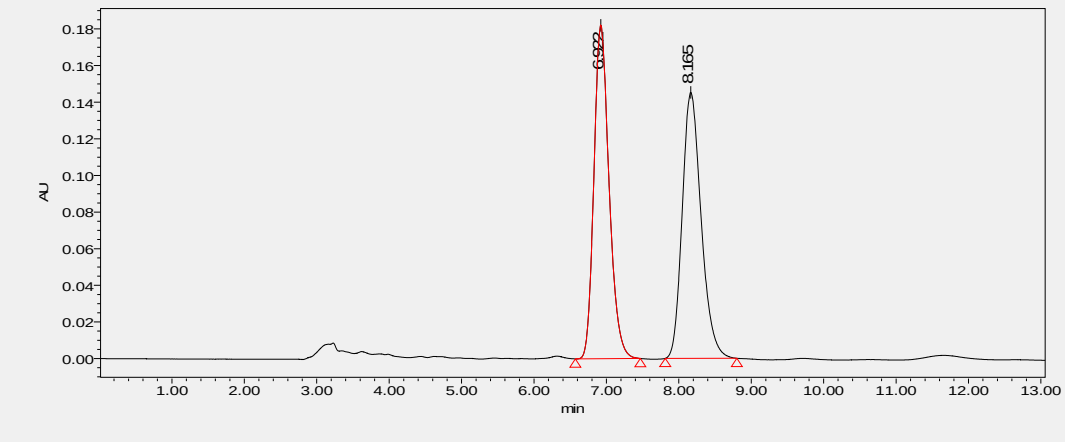
	Retention time	Area	% Area	Height	Integral type
1	6.436	23295308	96.91	1768663	bb
2	7.511	741604	3.09	50249	bb

2-((R)-((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)(naphthalen-2-yl)methyl)acrylonitrile, 3ar' (Table 2, entry 27)

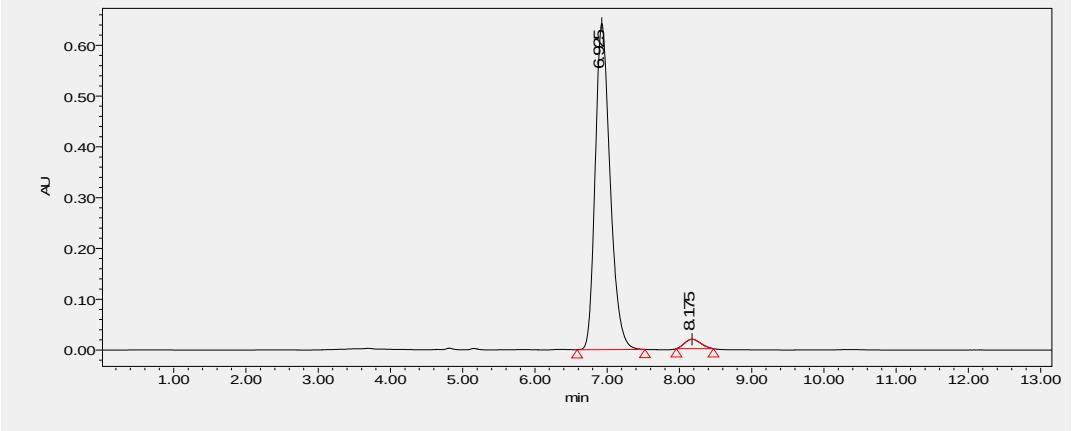


3ar'

Chiralpak IC column, hexane/iPrOH (1:2), flow rate 1.0 mL/min

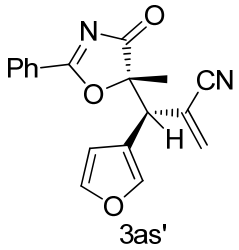


	Retention time	Area	% Area	Height	Integral type
1	6.922	2652343	50.16	182061	bb
2	8.165	2635295	49.84	145166	bb



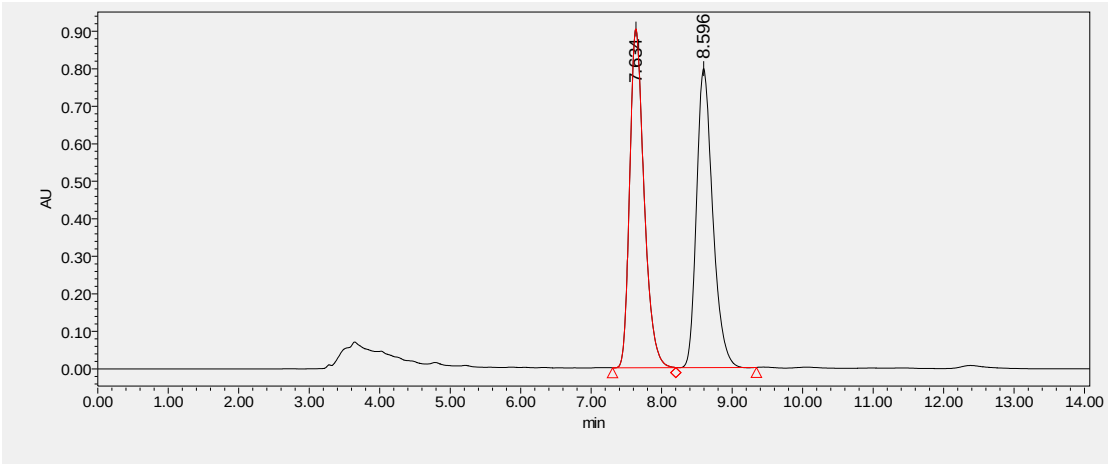
	Retention time	Area	% Area	Height	Integral type
1	6.925	9243887	97.01	641944	bb
2	8.175	285109	2.99	18496	bb

2-((R)-furan-3-yl((S)-5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylonitrile, 3as' (Table 2, entry 28)

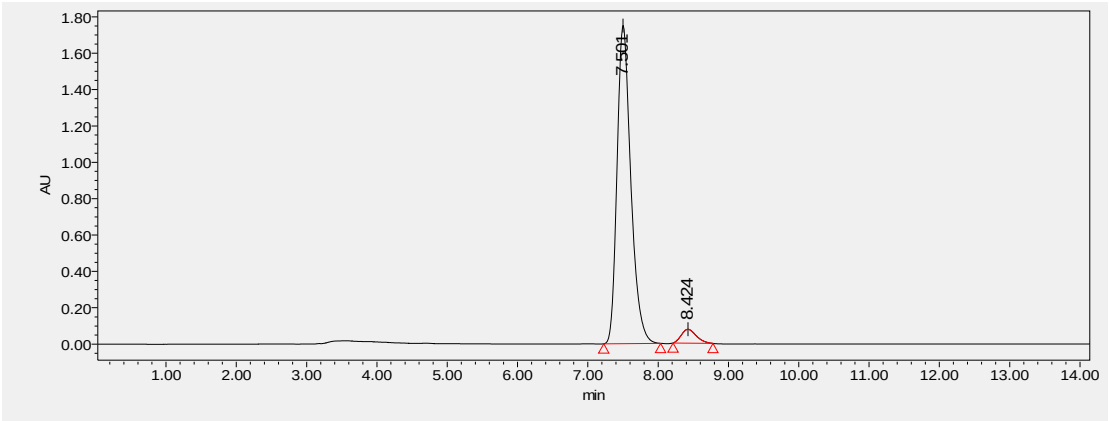


3as'

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

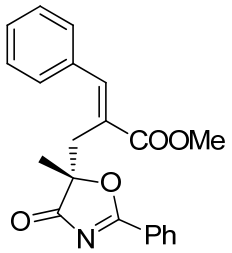


	Retention time	Area	% Area	Height	Integral type
1	7.634	12815189	50.20	902636	bv
2	8.596	12713856	49.80	796504	vb



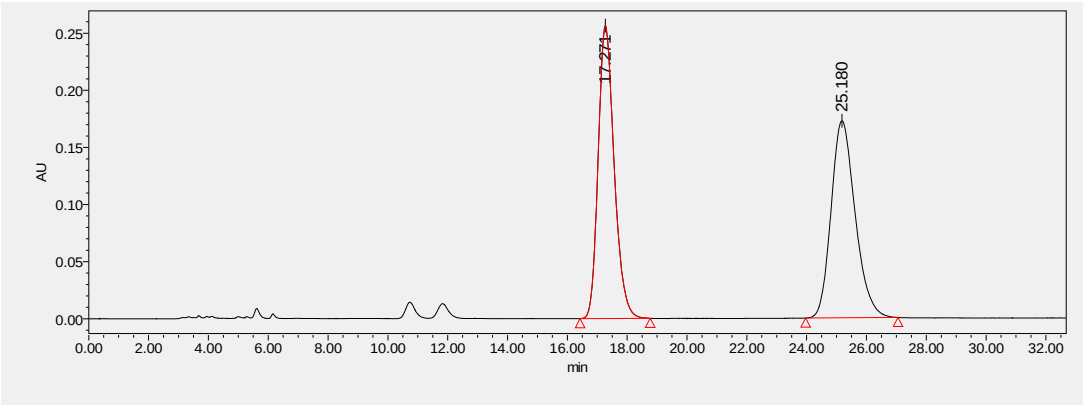
	Retention time	Area	% Area	Height	Integral type
1	7.501	23820047	95.51	1748989	bb
2	8.424	1120709	4.49	76031	bb

(S,E)-methyl 2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate, 4aa (Table 4, entry 1)

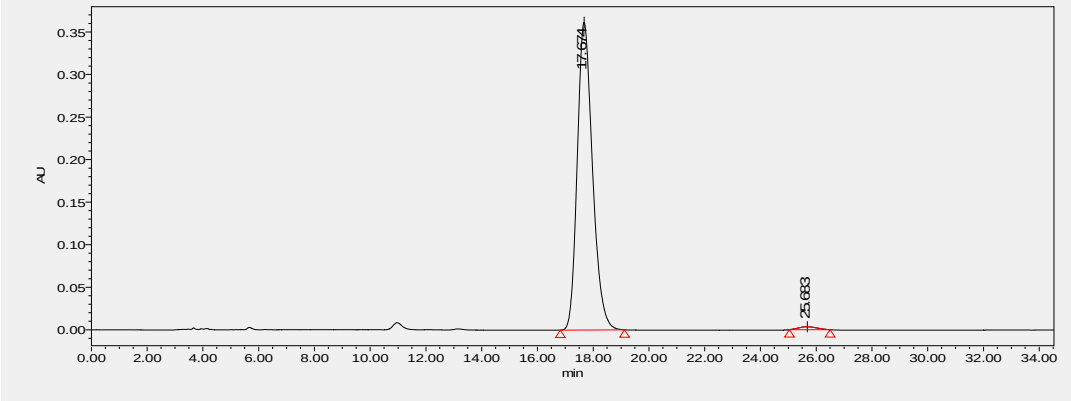


4aa

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

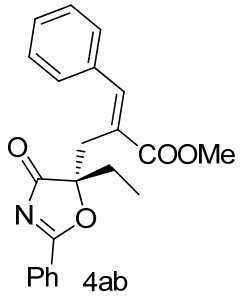


	Retention time	Area	% Area	Height	Integral type
1	17.271	9508934	49.70	256451	bb
2	25.180	9625471	50.30	172499	bb



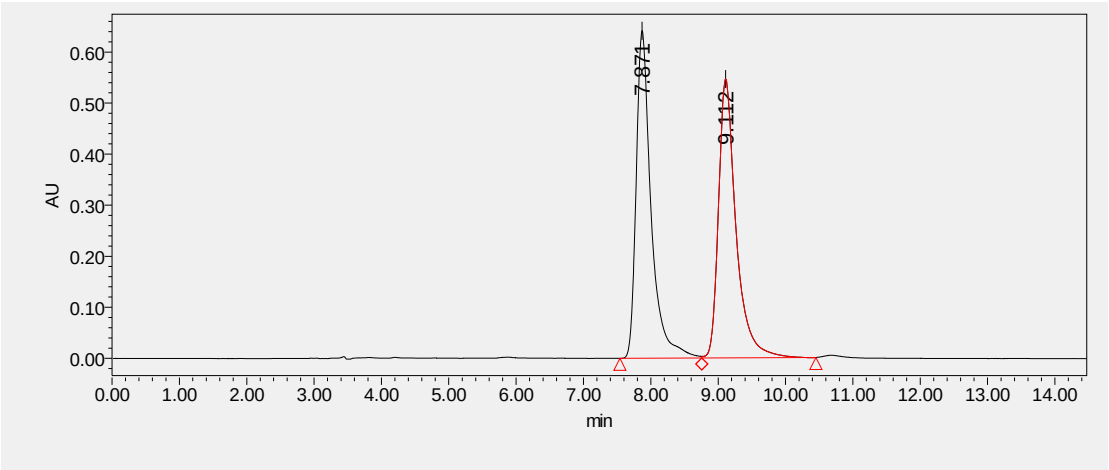
	Retention time	Area	% Area	Height	Integral type
1	17.674	13750489	98.85	361749	BB
2	25.683	160646	1.15	3497	bb

(S,E)-methyl 2-((5-ethyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate, 4ab (Table 4, entry 2)

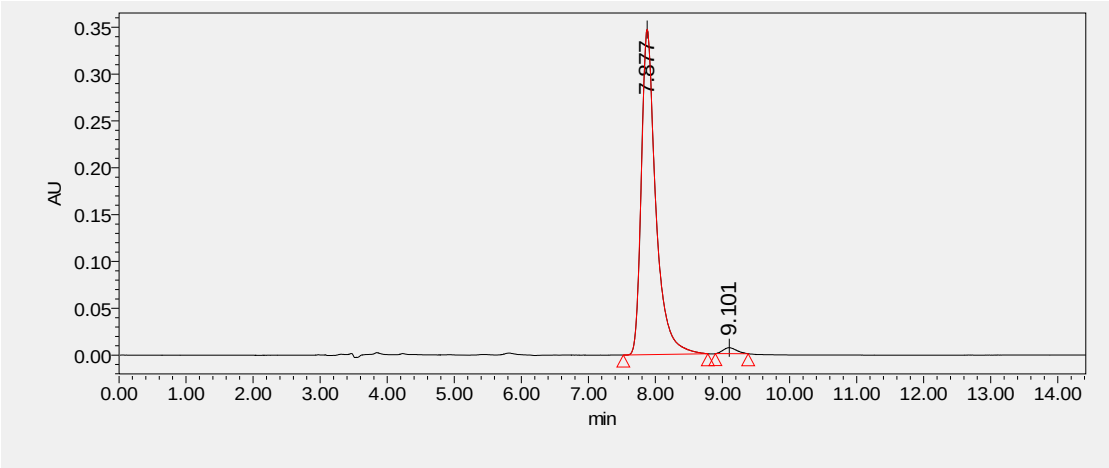


4ab

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

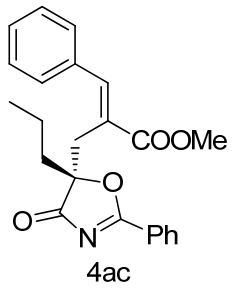


	Retention time	Area	% Area	Height	Integral type
1	7.871	9884606	50.02	641439	bv
2	9.112	9876896	49.98	546126	vb



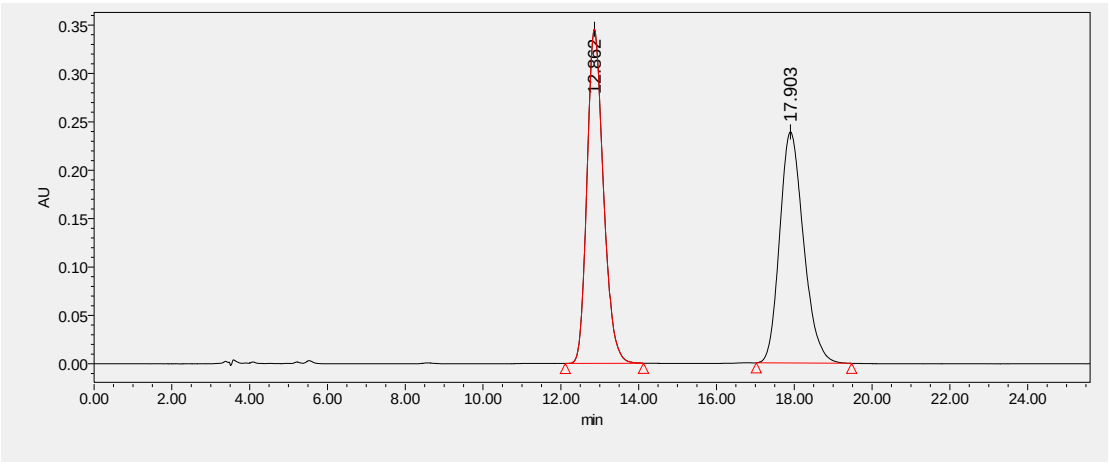
	Retention time	Area	% Area	Height	Integral type
1	7.877	5214426	98.31	347089	bb
2	9.101	89520	1.69	6343	bb

(S,E)-methyl 2-((4-oxo-2-phenyl-5-propyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate, 4ac (Table 4, entry 3)

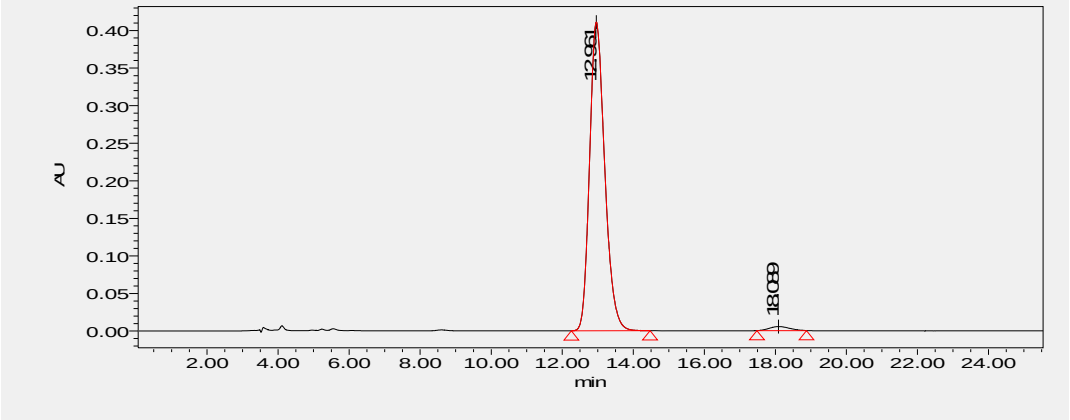


4ac

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

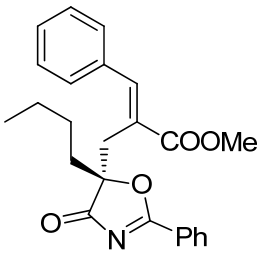


	Retention time	Area	% Area	Height	Integral type
1	12.862	10135812	49.93	345241	bb
2	17.903	10164181	50.07	238753	bb



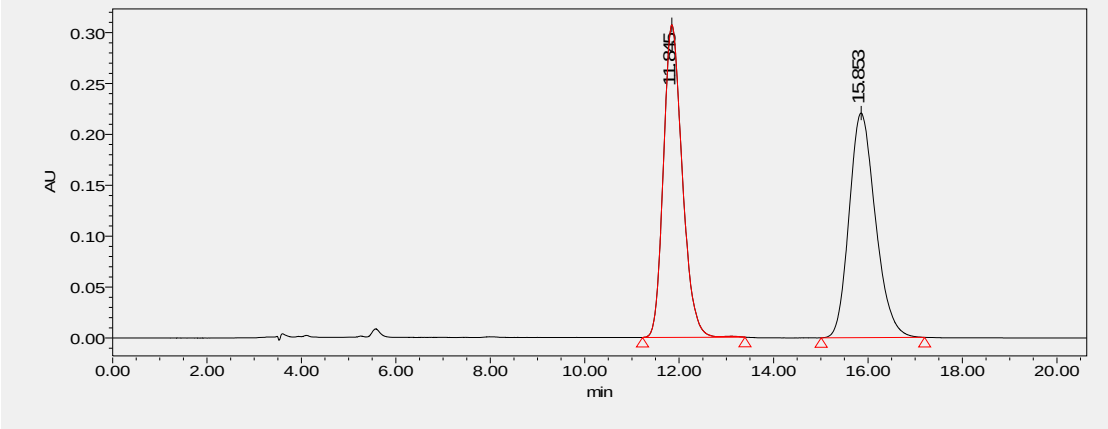
	Retention time	Area	% Area	Height	Integral type
1	12.961	12203058	98.30	410763	bb
2	18.089	211666	1.70	5390	BB

(S,E)-methyl 2-((5-butyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate, 4ad (Table 4, entry 4)

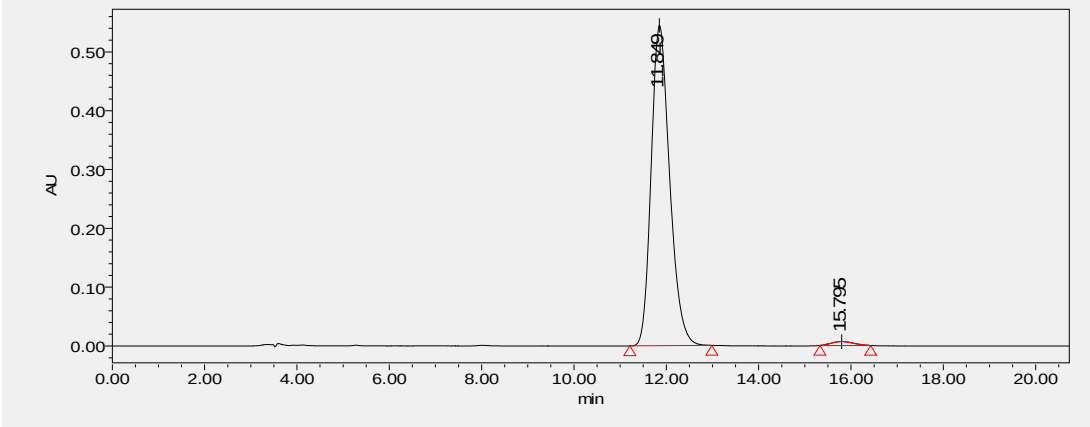


4ad

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

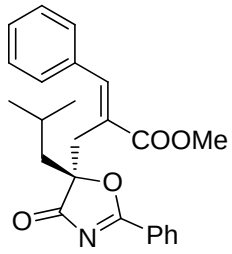


	Retention time	Area	% Area	Height	Integral type
1	11.845	8514853	49.94	307035	bb
2	15.853	8535075	50.06	220623	BB



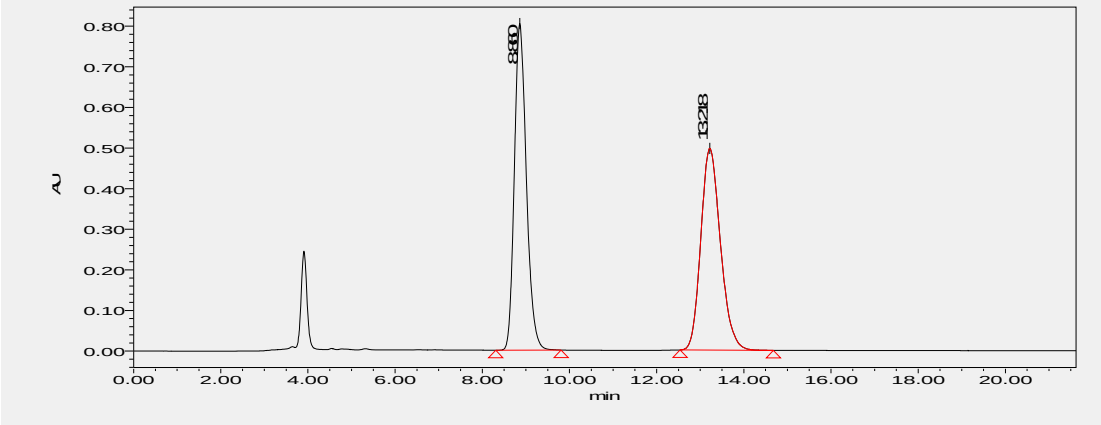
	Retention time	Area	% Area	Height	Integral type
1	11.849	15165332	98.56	544529	BB
2	15.795	221313	1.44	6655	bb

(S,E)-methyl 2-((5-isobutyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate, 4ae (Table 4, entry 5)

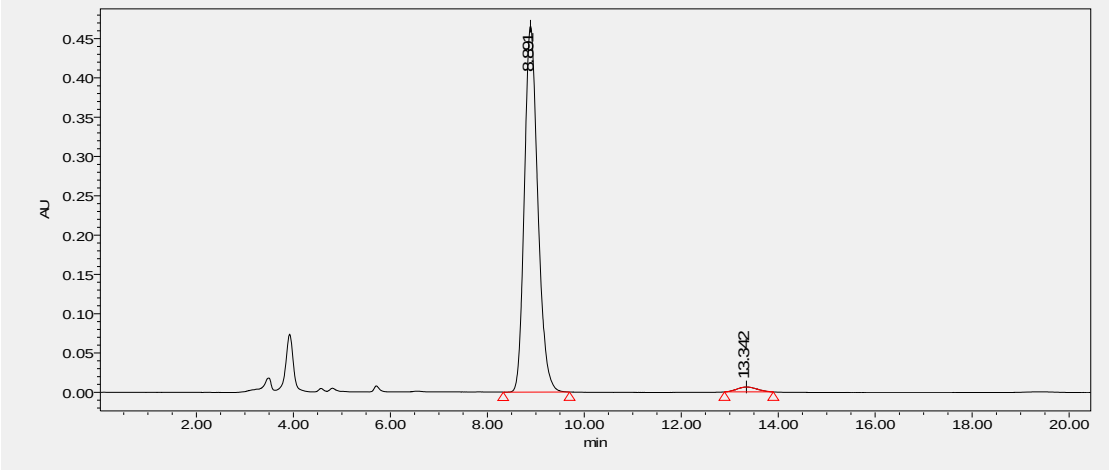


4ae

Chiralpak IC column, hexane/iPrOH (1:2), flow rate 1.0 mL/min

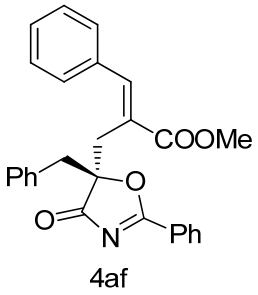


	Retention time	Area	% Area	Height	Integral type
1	8.860	15422583	49.82	804246	bb
2	13.218	15534469	50.18	496631	bb



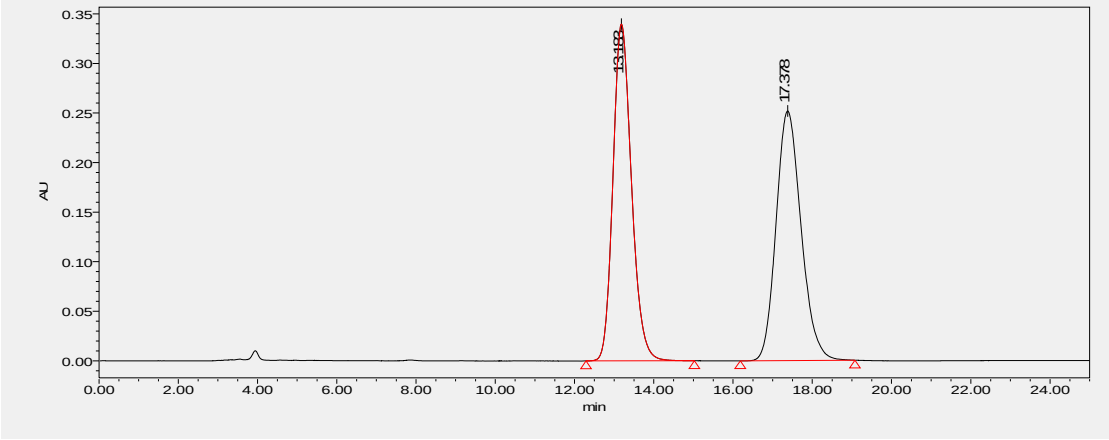
	Retention time	Area	% Area	Height	Integral type
1	8.891	8943277	98.02	465598	bb
2	13.342	180850	1.98	6246	bb

(S,E)-methyl 2-((5-benzyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate, 4af (Table 4., entry 6)

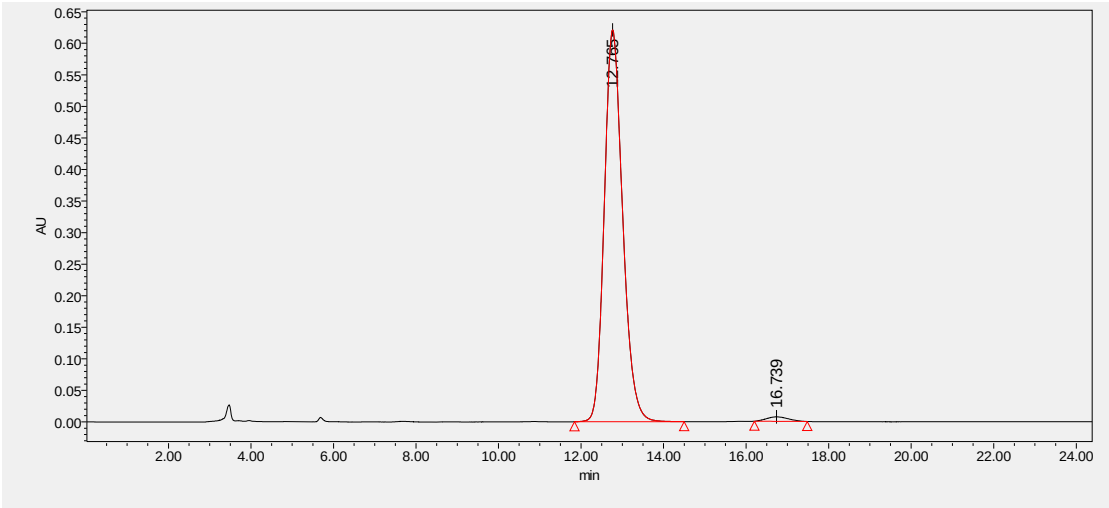


4af

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

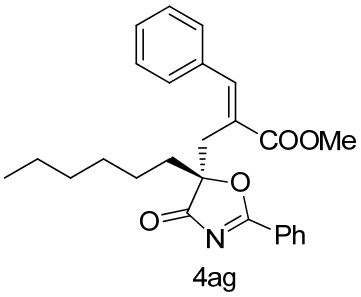


	Retention time	Area	% Area	Height	Integral type
1	13.183	11025366	50.00	339740	bb
2	17.378	11024287	50.00	251793	bb



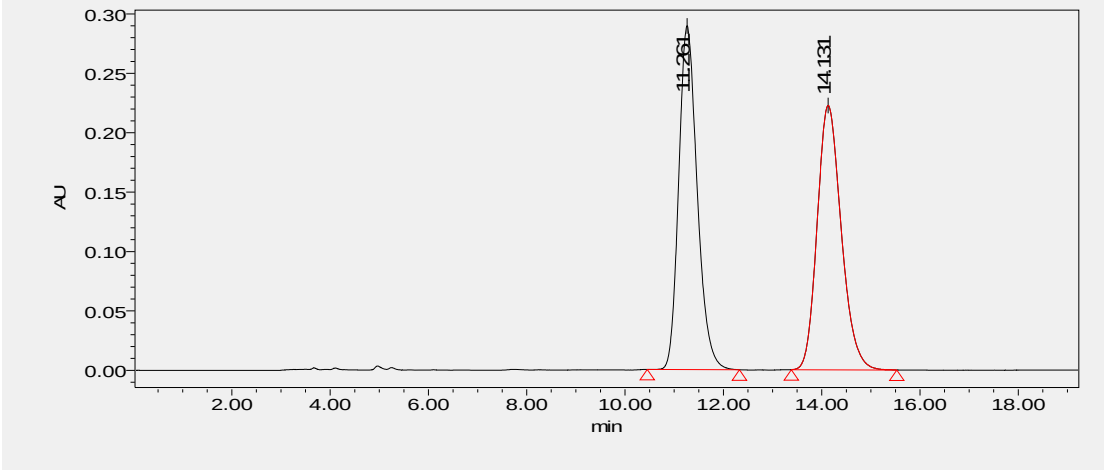
	Retention time	Area	% Area	Height	Integral type
1	12.765	19742251	98.66	621009	bb
2	16.739	267584	1.34	7078	bb

(S,E)-methyl 2-((5-hexyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate, 4ag (Table 4, entry 7)

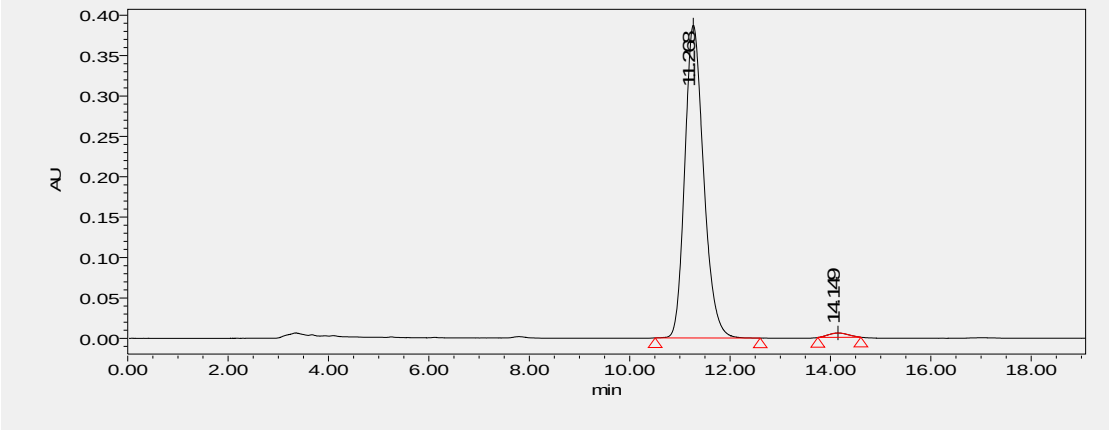


4ag

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

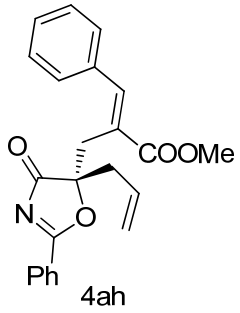


	Retention time	Area	% Area	Height	Integral type
1	11.261	7561376	49.98	289259	bb
2	14.131	7566573	50.02	222522	bb



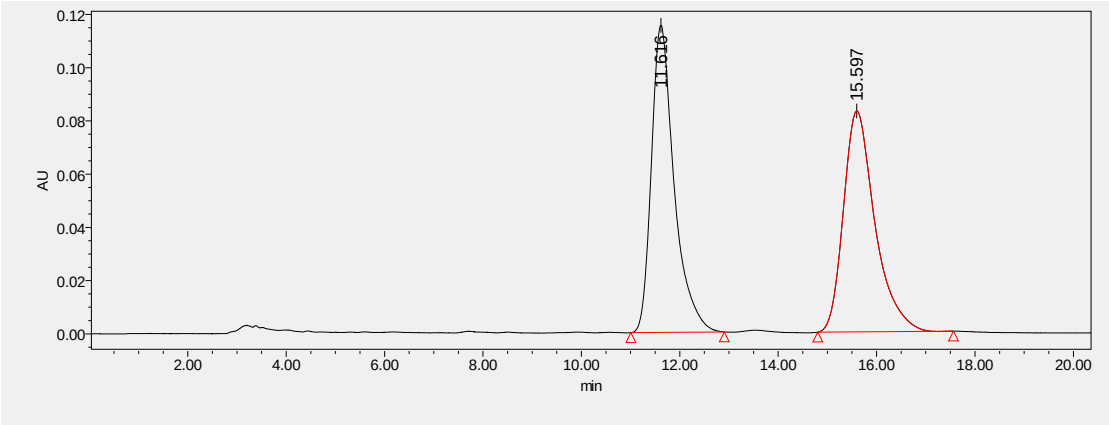
	Retention time	Area	% Area	Height	Integral type
1	11.268	10127459	98.54	387427	bb
2	14.149	149773	1.46	5430	bb

(S,E)-methyl 2-((5-allyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate, 4ah (Table 4, entry 8)

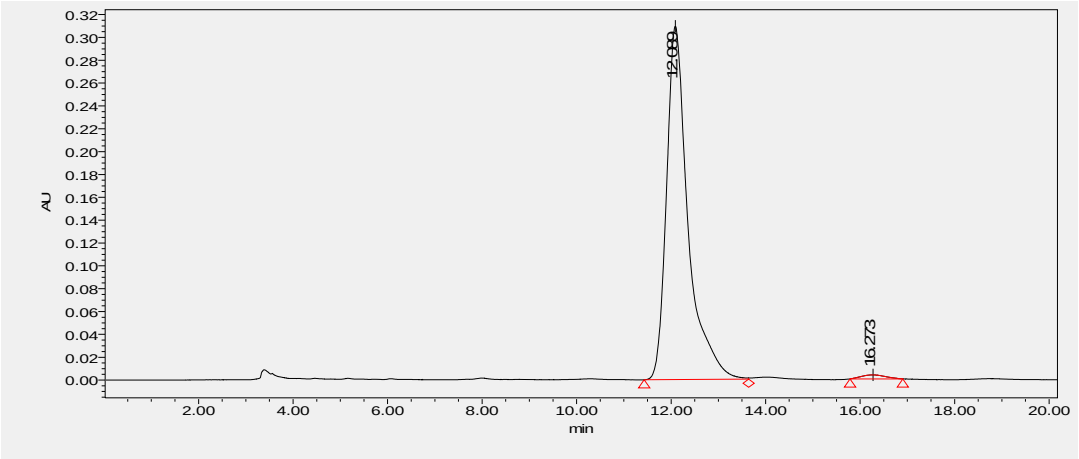


4ah

Chiralpak IC column, hexane/iPrOH (1:2), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	11.616	3705163	50.15	115367	bb
2	15.597	3683498	49.85	82997	bb

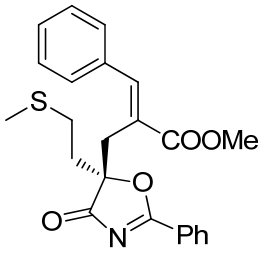


	Retention time	Area	% Area	Height	Integral type
1	12.089	9795353	98.77	309437	BV
2	16.273	122165	1.23	3490	bb

(S,E)-methyl

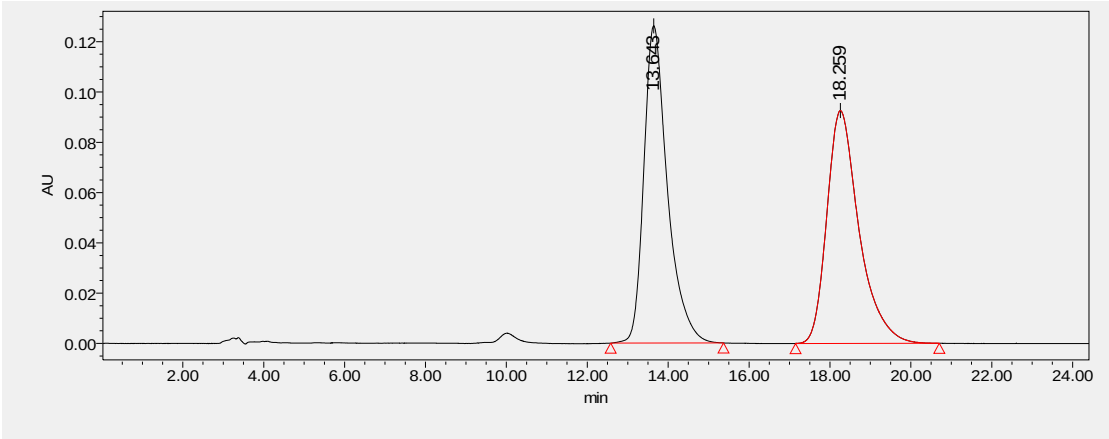
2-((5-(2-(methylthio)ethyl)-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-phenylacrylate,

4ai (Table 4, entry 9)

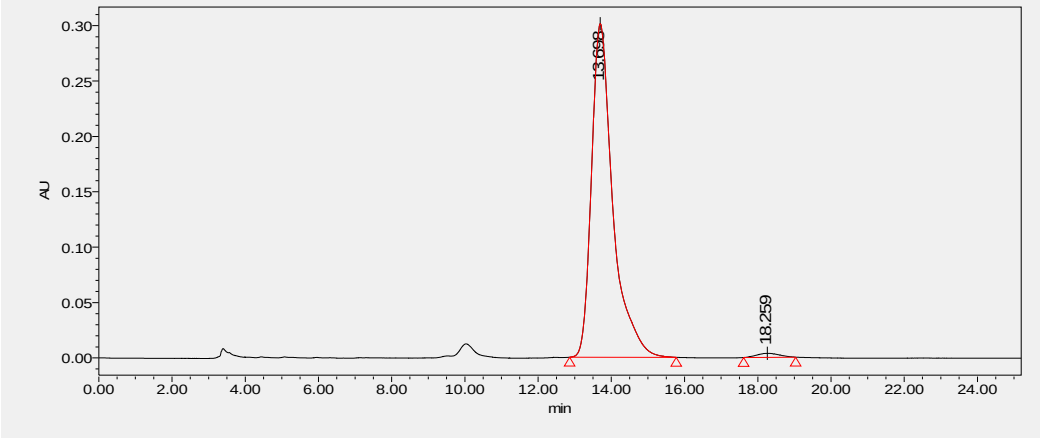


4ai

Chiralpak IC column, hexane/iPrOH (1:2), flow rate 1.0 mL/min

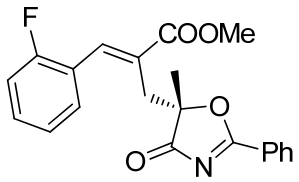


	Retention time	Area	% Area	Height	Integral type
1	13.643	5112712	50.01	126185	bb
2	18.259	5110235	49.99	92623	bb



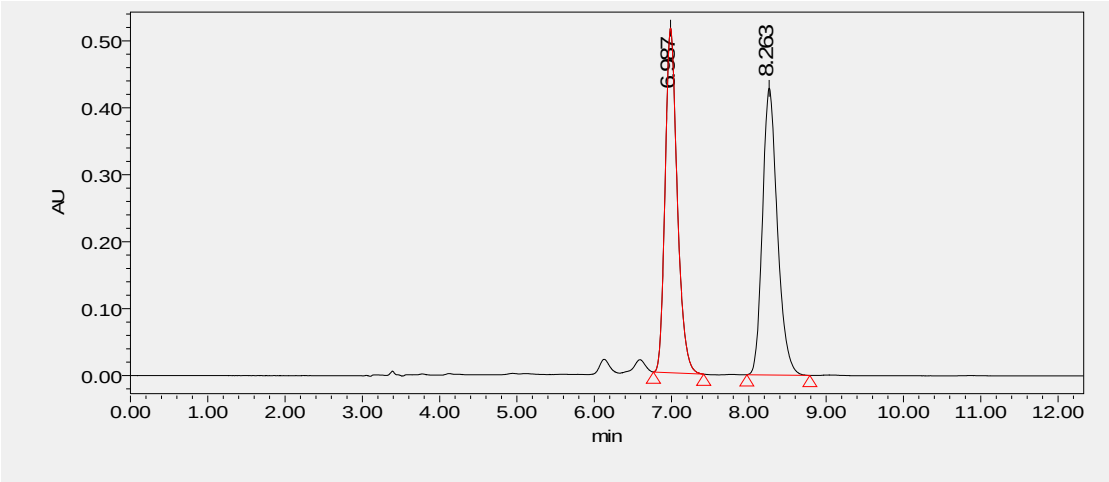
	Retention time	Area	% Area	Height	Integral type
1	13.698	12194746	98.75	301026	bb
2	18.259	154681	1.25	3633	BB

(S,E)-methyl-3-(2-fluorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl) acrylate, 4ba (Table 4, entry 10)

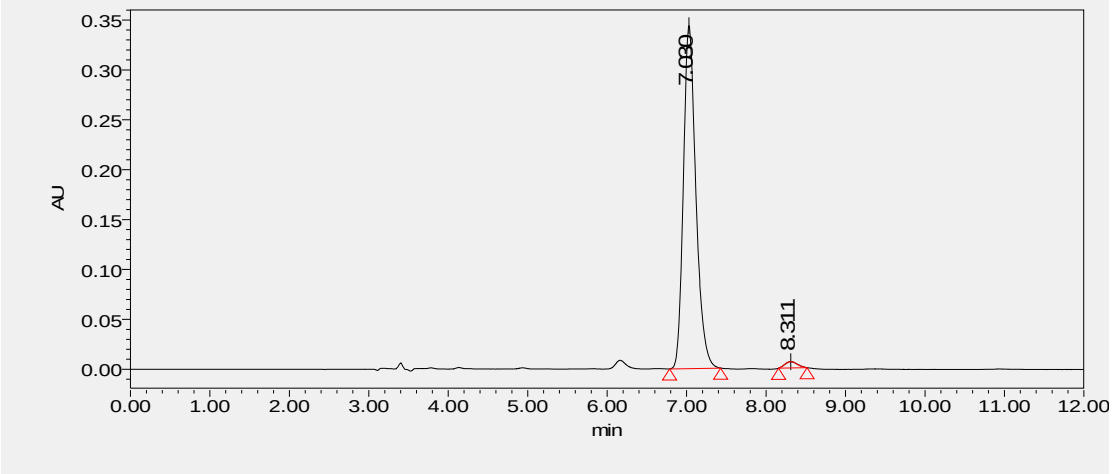


4ba

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	6.987	5616521	49.39	514823	bb
2	8.263	5754701	50.61	428109	bb

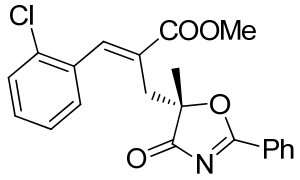


	Retention time	Area	% Area	Height	Integral type
1	7.030	3759237	98.19	343605	bb
2	8.311	69280	1.81	6352	bb

(S,E)-methyl

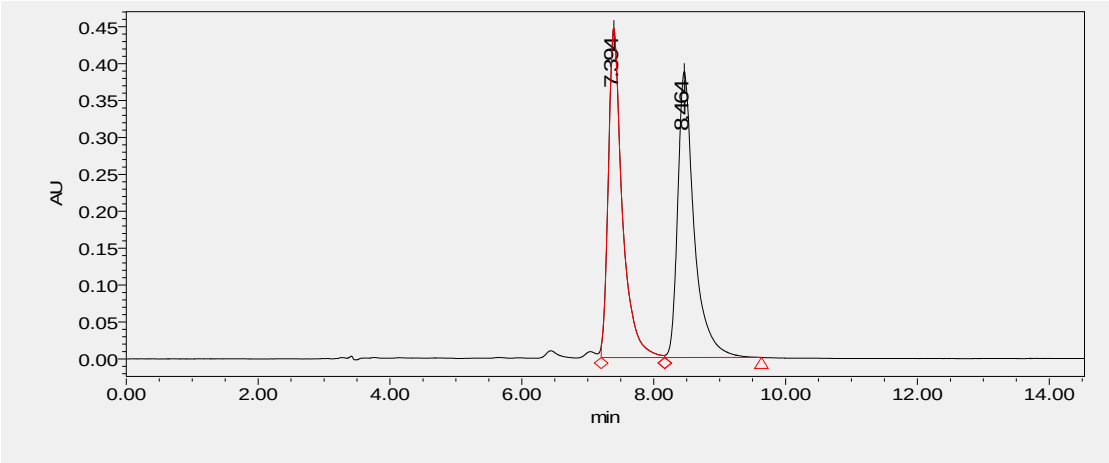
3-(2-chlorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate, 4ca

(Table 4, entry 11)

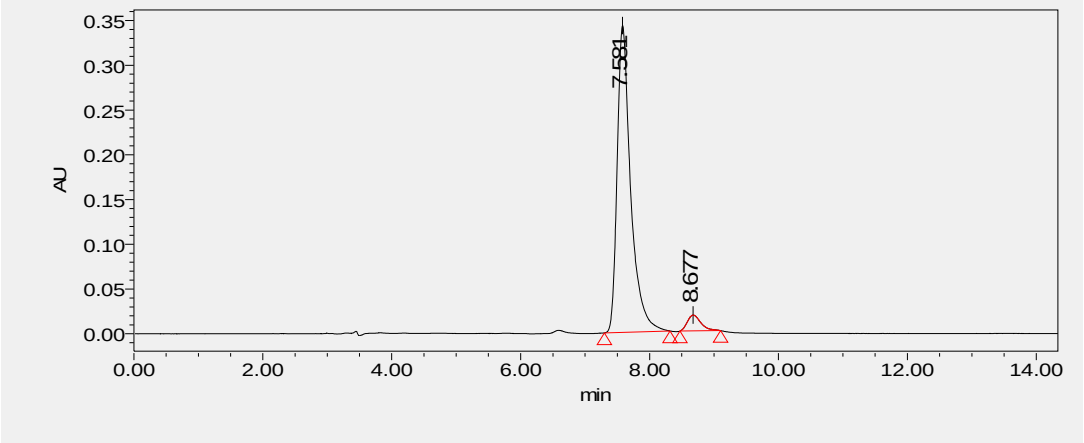


4ca

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	7.394	6597440	49.61	446000	vv
2	8.464	6702032	50.39	387557	vb

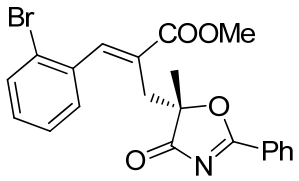


	Retention time	Area	% Area	Height	Integral type
1	7.581	4984521	95.03	342754	bb
2	8.677	260453	4.97	17744	bb

(S,E)-methyl

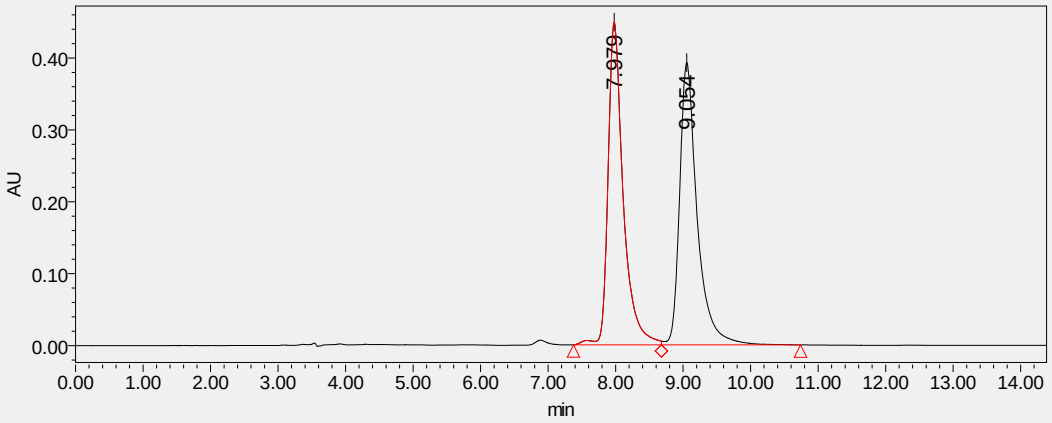
3-(2-bromophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate, 4da

(Table 4, entry 12)

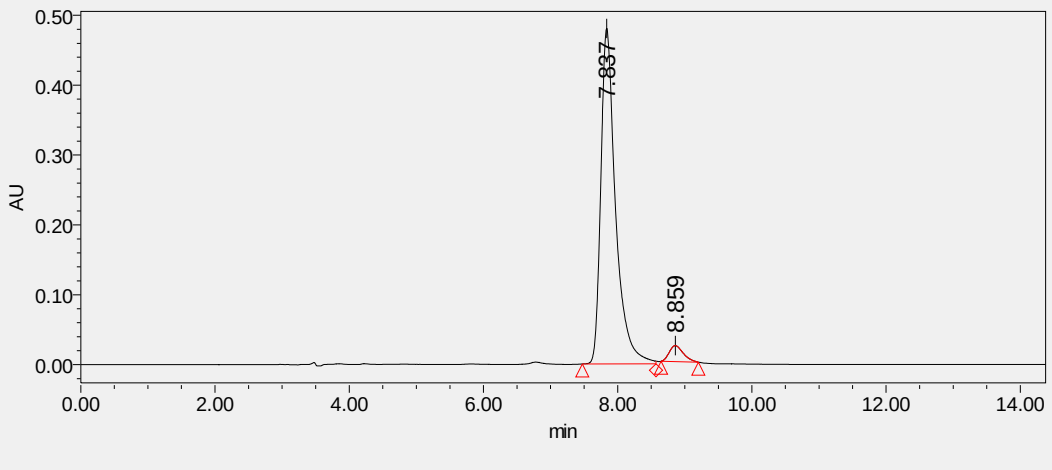


4da

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	7.979	7005261	49.72	448634	bv
2	9.054	7082978	50.28	392592	vb

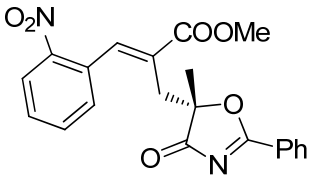


	Retention time	Area	% Area	Height	Integral type
1	7.837	7325357	95.65	480246	bv
2	8.859	333429	4.35	22921	bb

(S,E)-methyl

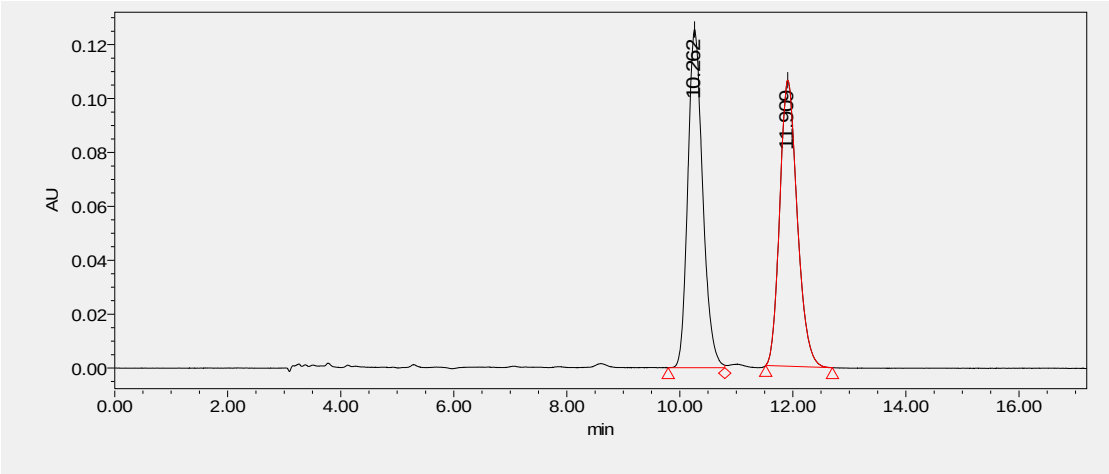
2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(2-nitrophenyl)acrylate, 4ea

(Table 4, entry 13)

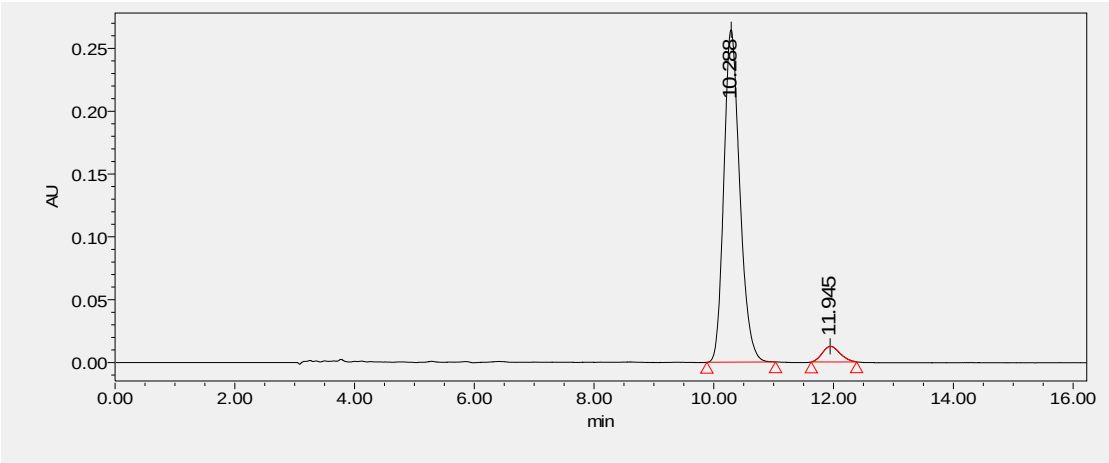


4ea

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min

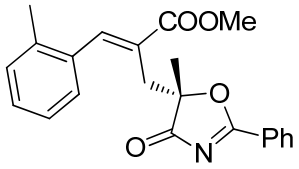


	Retention time	Area	% Area	Height	Integral type
1	10.262	2299486	50.18	125506	bv
2	11.909	2282924	49.82	106075	bb



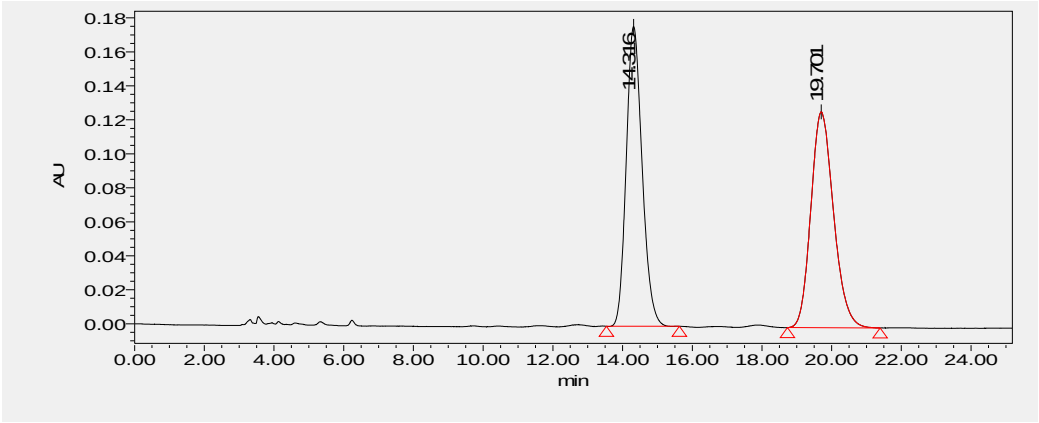
	Retention time	Area	% Area	Height	Integral type
1	10.288	4886726	95.07	264490	bb
2	11.945	253185	4.93	12376	bb

(S,E)-methyl 2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(o-tolyl)acrylate, 4fa (Table 4, entry 14)

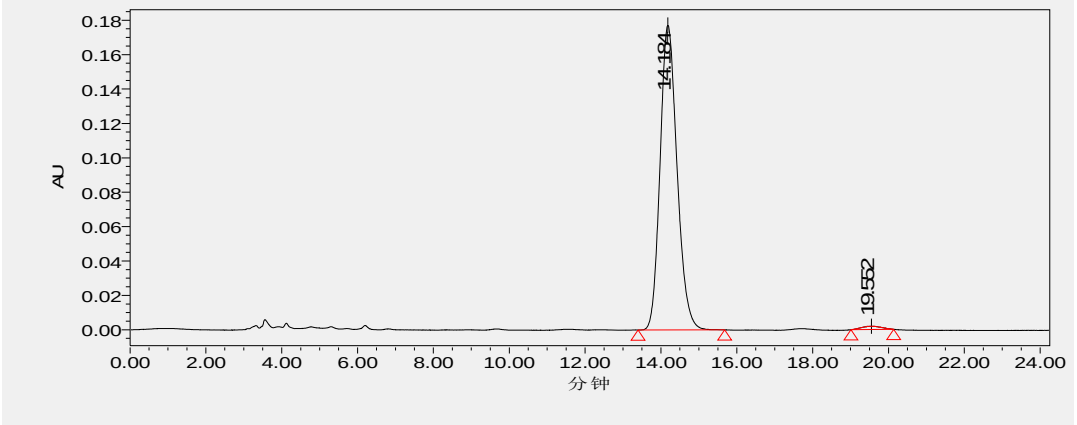


4fa

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	14.316	5596382	49.34	176436	bb
2	19.701	5745689	50.66	127009	bb

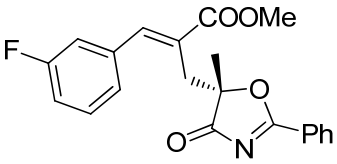


	Retention time	Area	% Area	Height	Integral type
1	14.184	5515147	98.73	177269	bb
2	19.552	71117	1.27	1919	bb

(S,E)-methyl

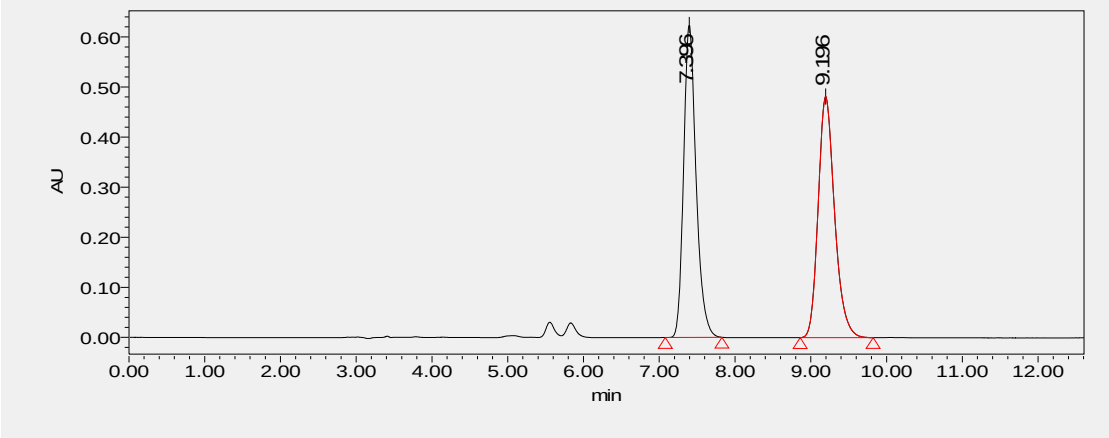
3-(3-fluorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate, 4ga

(Table 4, entry 15)

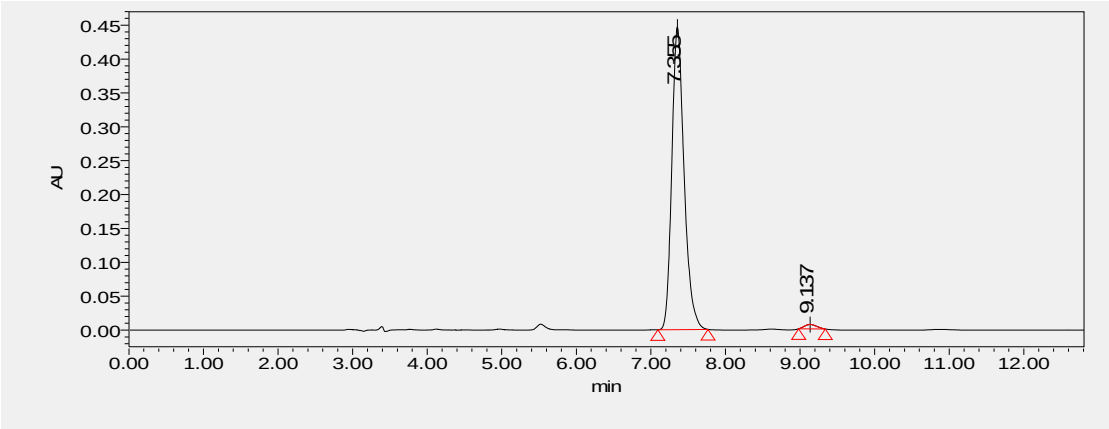


4ga

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	7.396	7124057	49.59	623652	bb
2	9.196	7241927	50.41	481393	bb

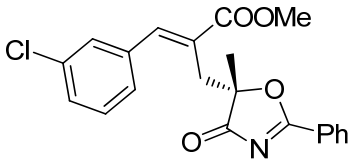


	Retention time	Area	% Area	Height	Integral type
1	7.355	5120186	98.56	446650	bb
2	9.137	75001	1.44	6489	bb

(S,E)-methyl

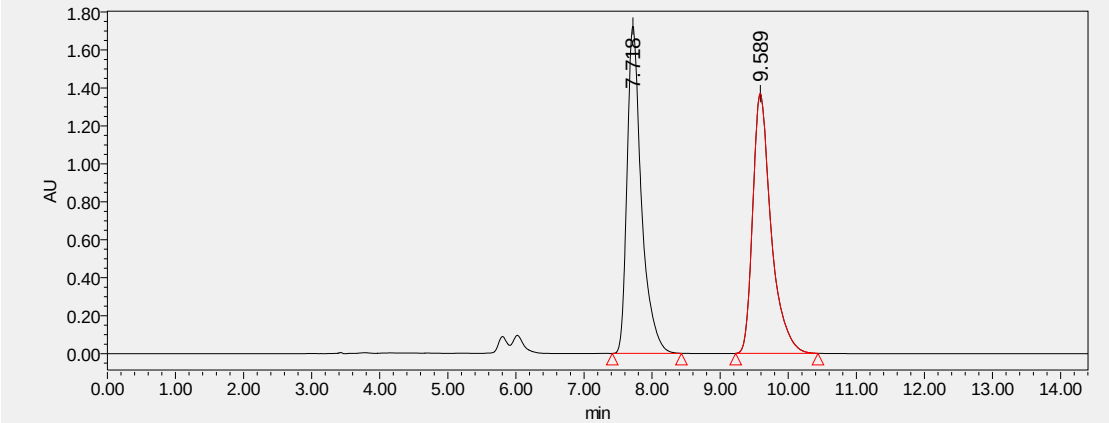
3-(3-chlorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate, 4ha

(Table 4, entry 16)

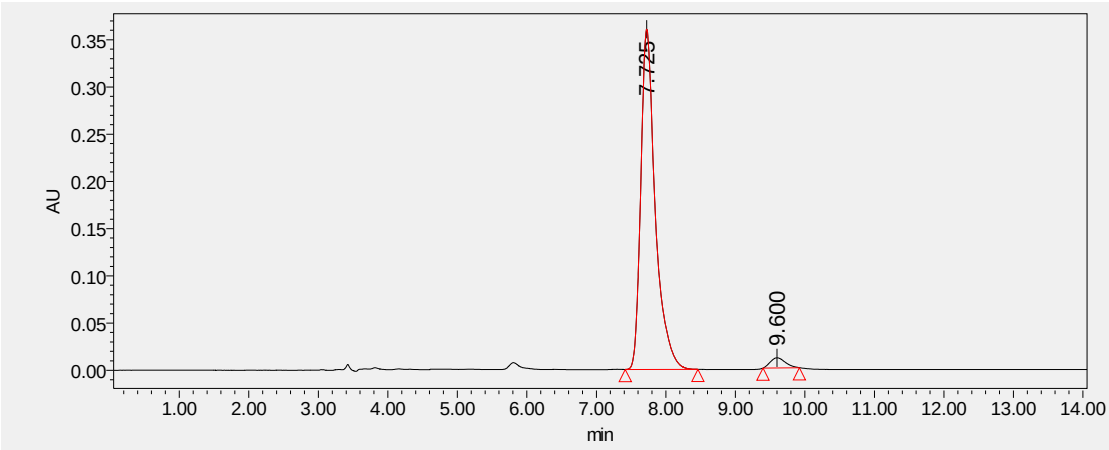


4ha

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	7.718	25284312	49.60	1724815	bb
2	9.589	25696058	50.40	1369375	bb

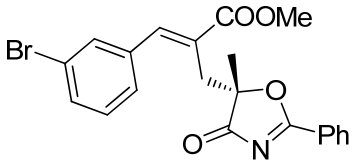


	Retention time	Area	% Area	Height	Integral type
1	7.725	5210543	97.01	360236	bb
2	9.600	160661	2.99	10770	bb

(S,E)-methyl

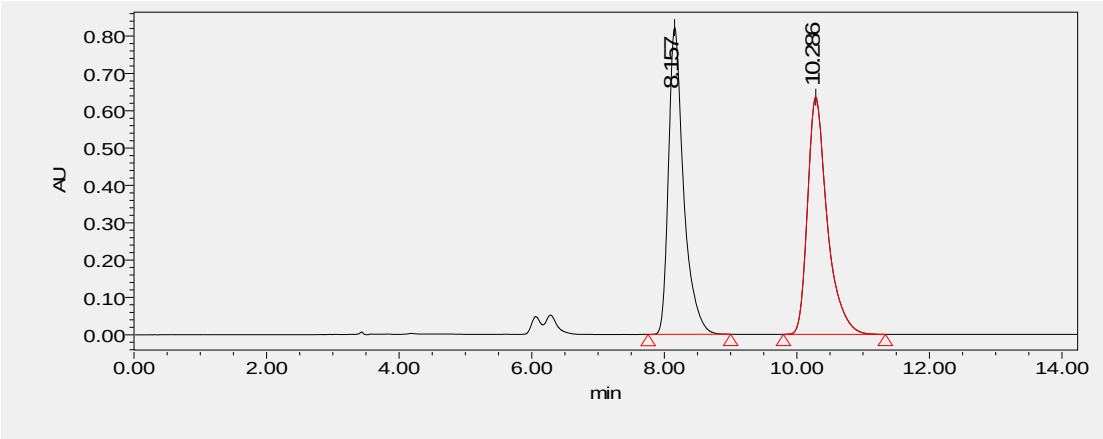
3-(3-bromophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate, 4ia

(Table 4, entry 17)

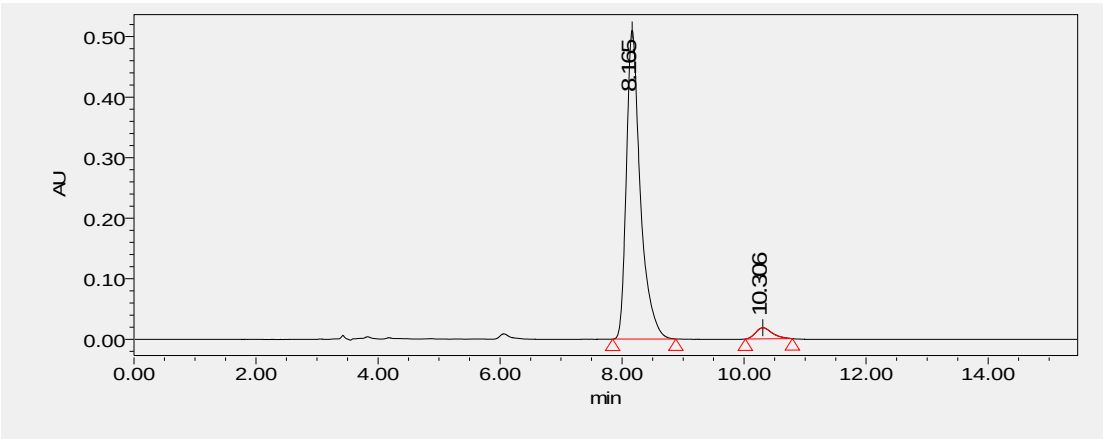


4ia

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



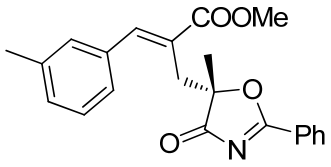
	Retention time	Area	% Area	Height	Integral type
1	8.157	12990832	49.77	821762	bb
2	10.286	13113358	50.23	635362	bb



	Retention time	Area	% Area	Height	Integral type
1	8.165	8081154	95.87	510269	bb
2	10.306	348271	4.13	18395	bb

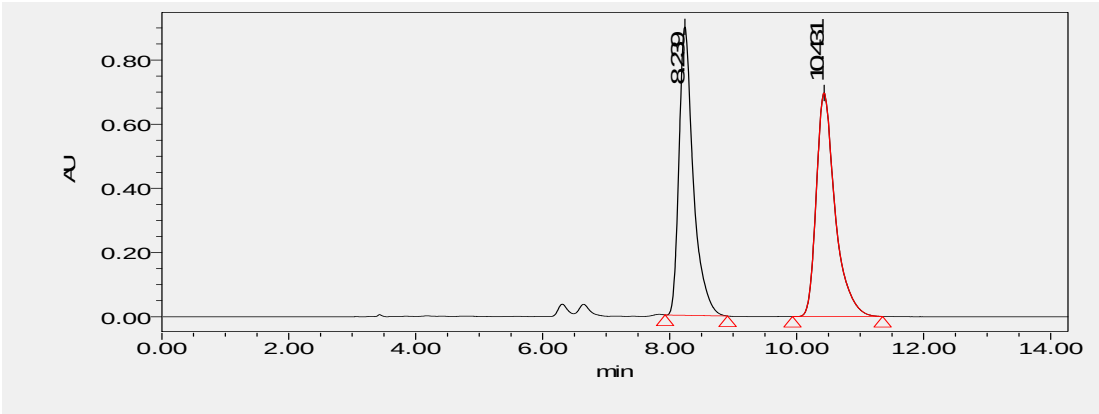
(S,E)-methyl

2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(m-tolyl)acrylate, 4ja (Table 4, entry 18)

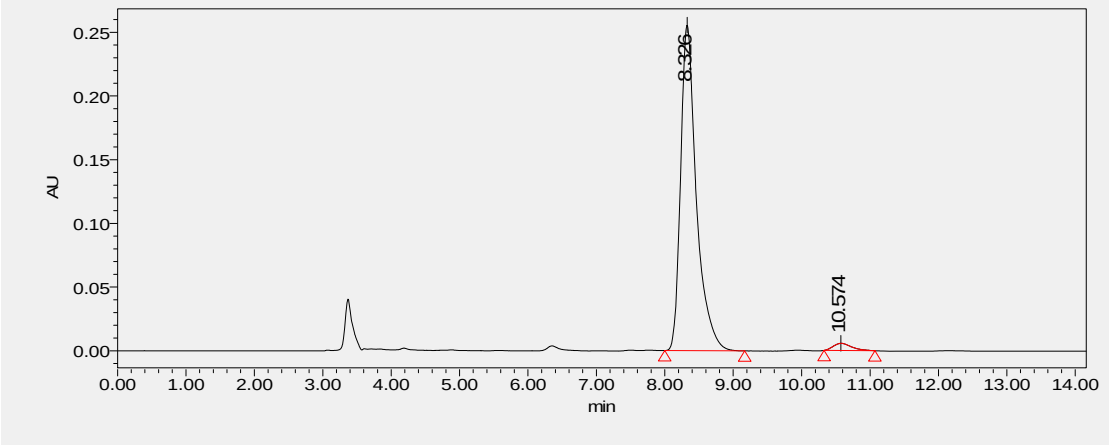


4ja

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	8.239	14303294	49.58	899077	bb
2	10.431	14543928	50.42	696719	bb

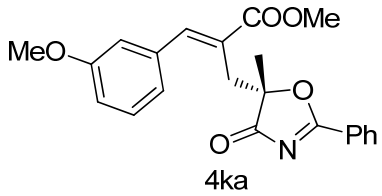


	Retention time	Area	% Area	Height	Integral type
1	8.326	4088275	97.50	255529	bb
2	10.574	104916	2.50	5634	bb

(S,E)-methyl

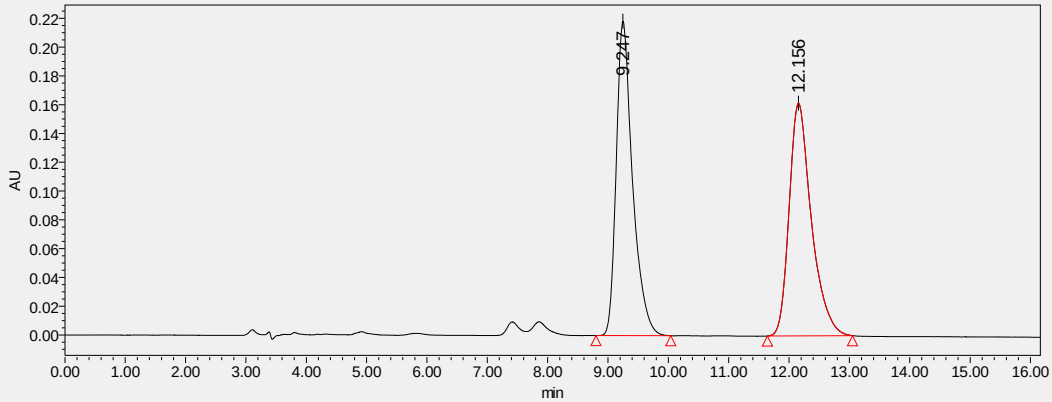
3-(3-methoxyphenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate,

4ka (Table 4, entry 19)

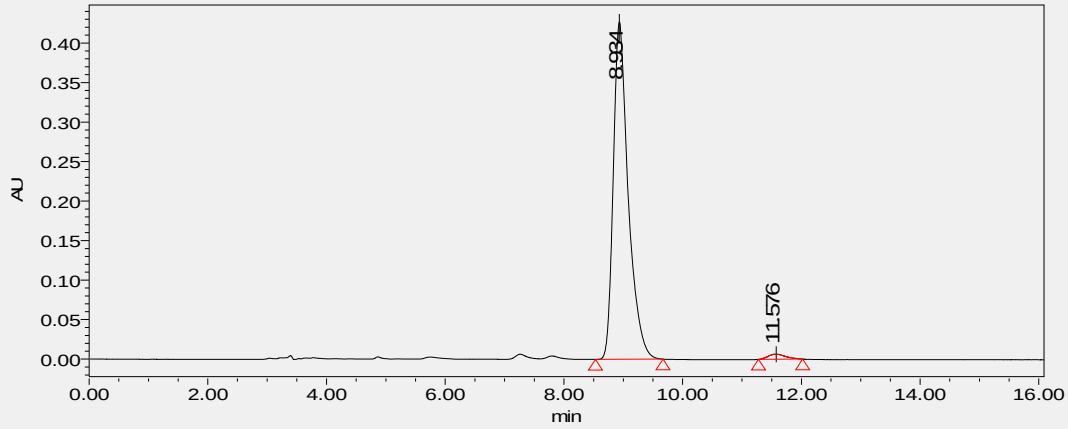


4ka

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min

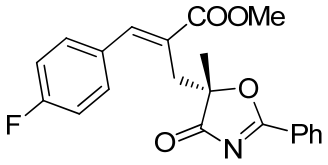


	Retention time	Area	% Area	Height	Integral type
1	9.247	4104140	49.84	218518	bb
2	12.156	4130501	50.16	161617	bb



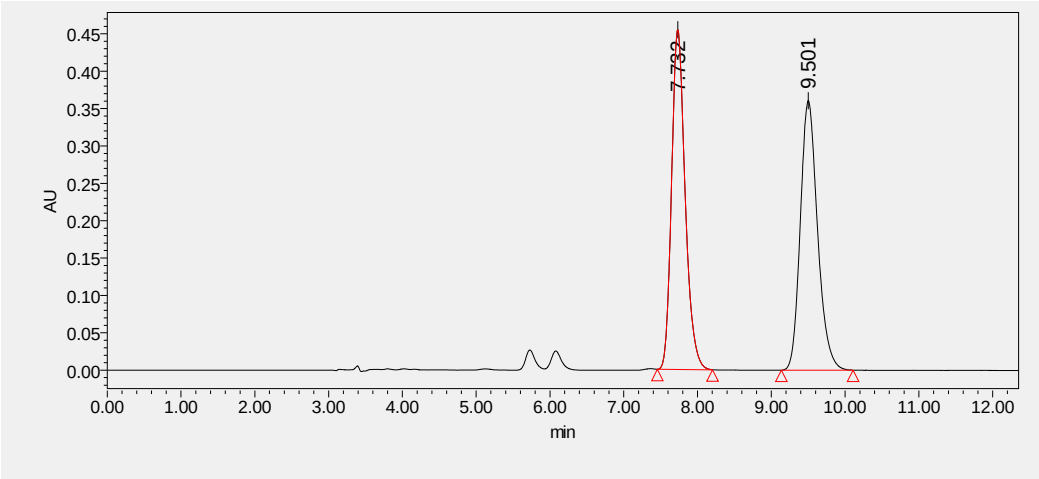
	Retention time	Area	% Area	Height	Integral type
1	8.934	7445831	98.27	426965	bb
2	11.576	131252	1.73	6449	bb

(S,E)-methyl
3-(4-fluorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate, 4la
(Table 4, entry 20)

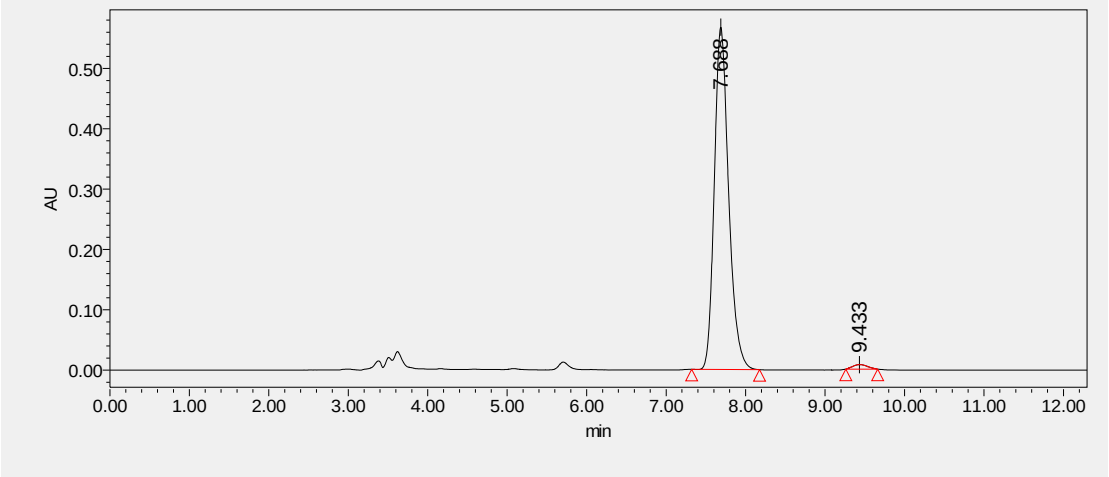


4la

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	7.732	5805636	49.81	454595	bb
2	9.501	5849595	50.19	360460	bb

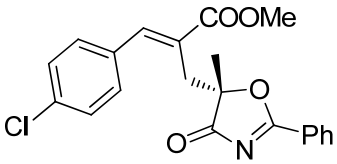


	Retention time	Area	% Area	Height	Integral type
1	7.688	7108044	98.67	567305	bb
2	9.433	95664	1.33	7482	bb

(S,E)-methyl

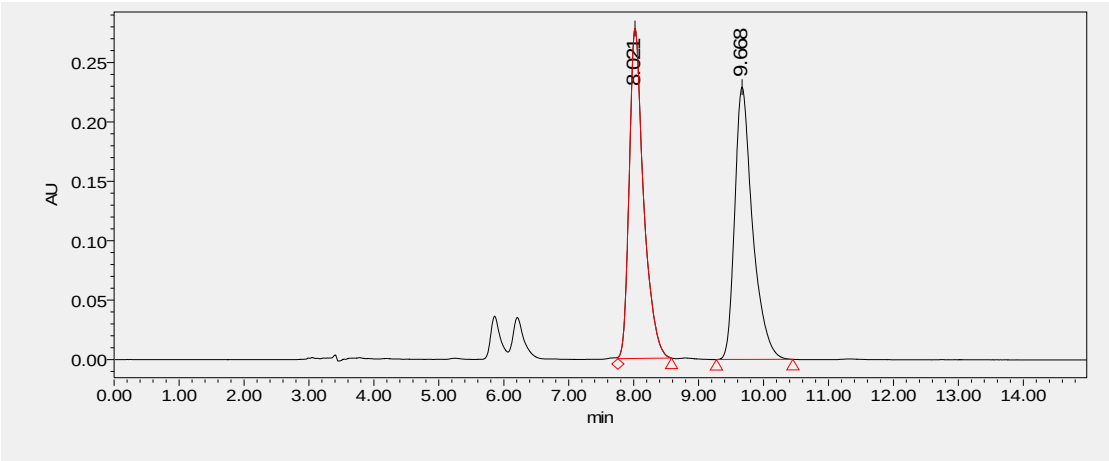
3-(4-chlorophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate,

4ma (Table 4, entry 21)

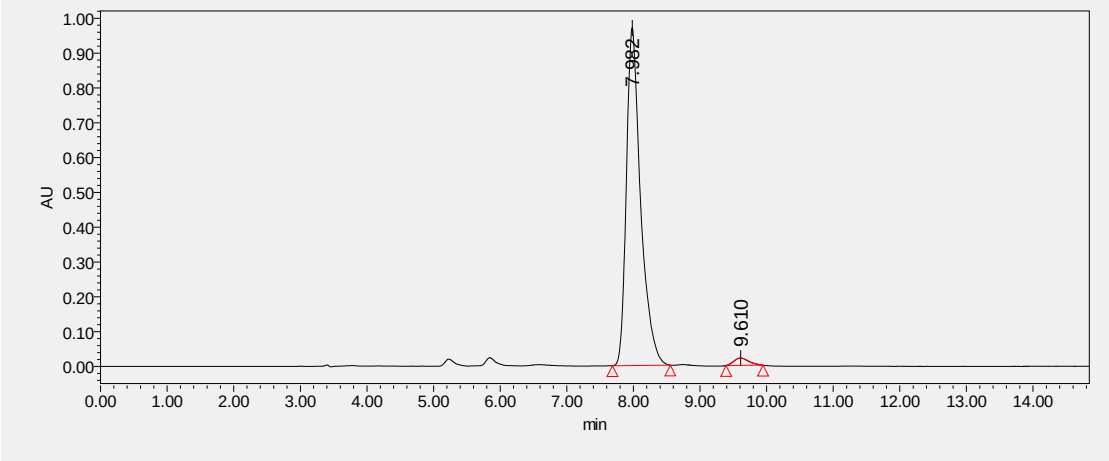


4ma

Chiralpak IC column, hexane/iPrOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	8.021	4266814	49.38	277596	vb
2	9.668	4373343	50.62	229274	bb

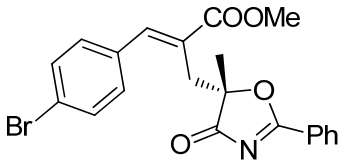


	Retention time	Area	% Area	Height	Integral type
1	7.982	14383808	97.76	969537	bb
2	9.610	330249	2.24	21051	bb

(S,E)-methyl

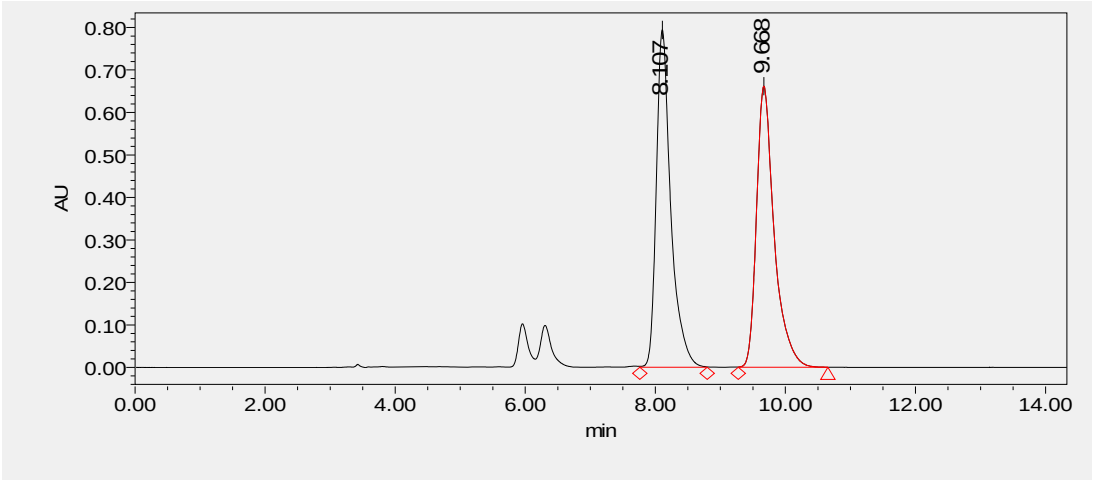
3-(4-bromophenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate, 4na

(Table 4, entry 22)

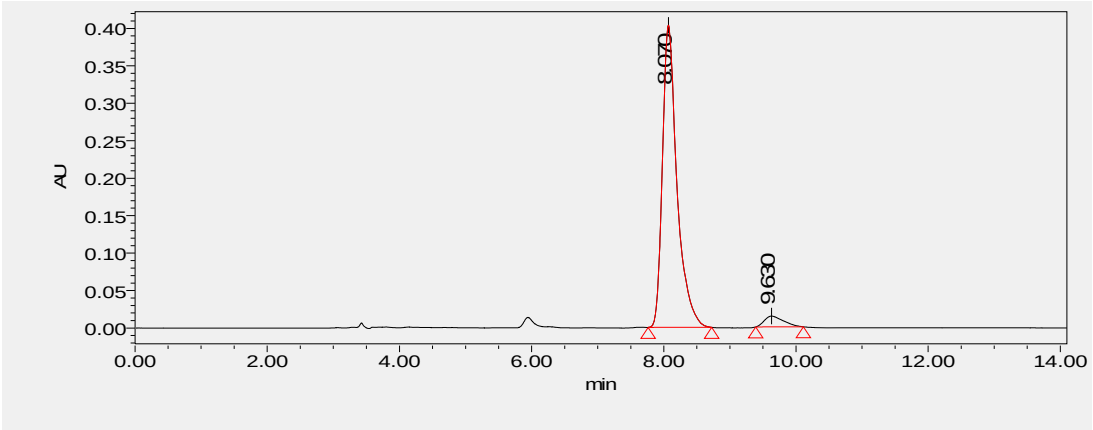


4na

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min

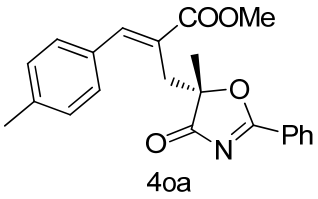


	Retention time	Area	% Area	Height	Integral type
1	8.107	13700475	49.60	793858	Vv
2	9.668	13924102	50.40	661583	vB



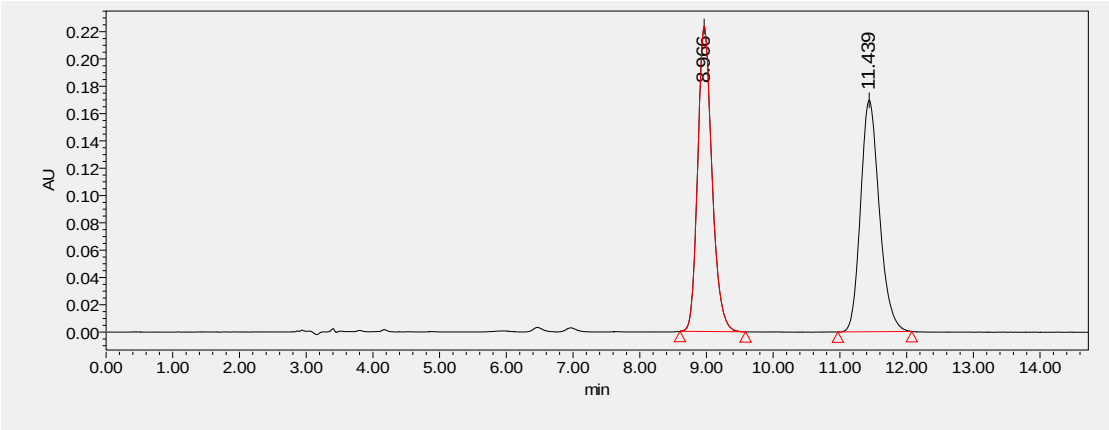
	Retention time	Area	% Area	Height	Integral type
1	8.070	6174877	95.52	403329	bb
2	9.630	289807	4.48	14399	bb

(S,E)-methyl 2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(p-tolyl)acrylate, 4oa (Table 4, entry 23)

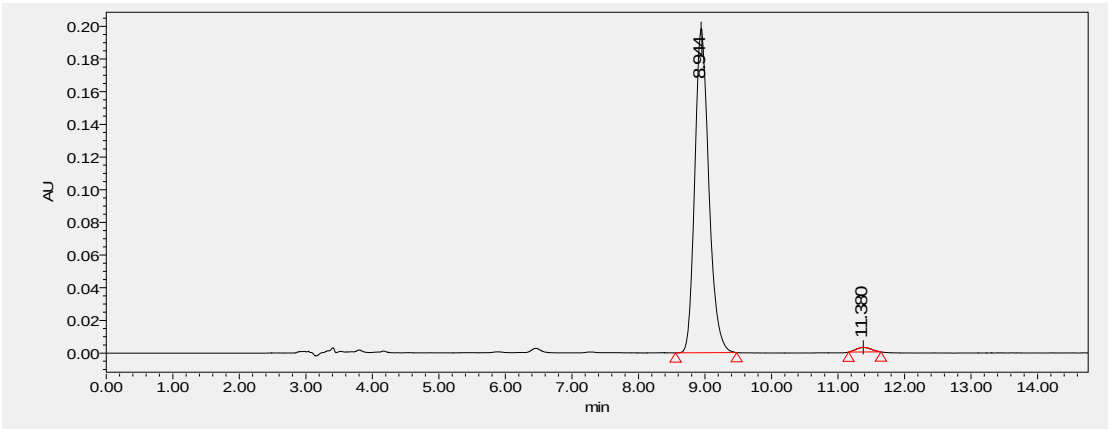


4oa

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	8.966	3325137	50.03	223374	bb
2	11.439	3321048	49.97	169650	bb

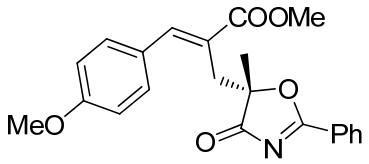


	Retention time	Area	% Area	Height	Integral type
1	8.944	2913915	98.51	198361	bb
2	11.380	44060	1.49	2834	bb

(S,E)-methyl

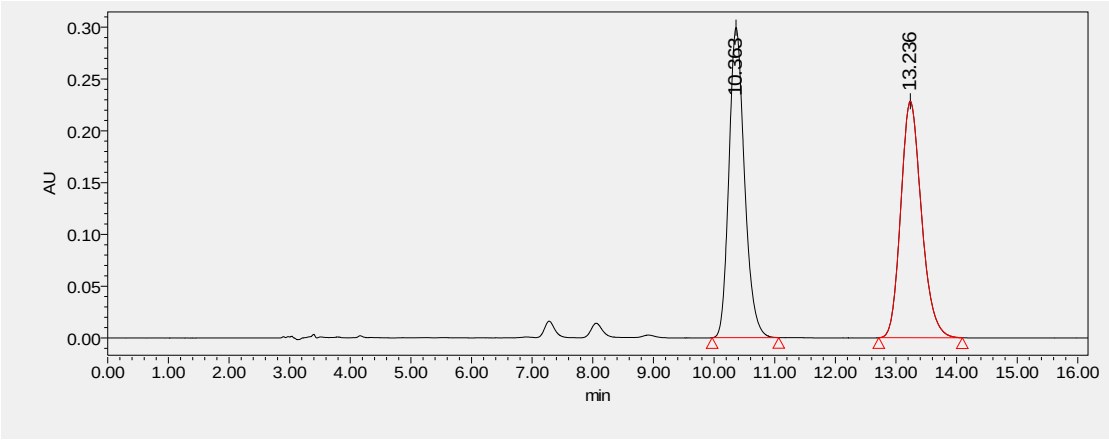
3-(4-methoxyphenyl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate,

4pa (Table 4, entry 24)

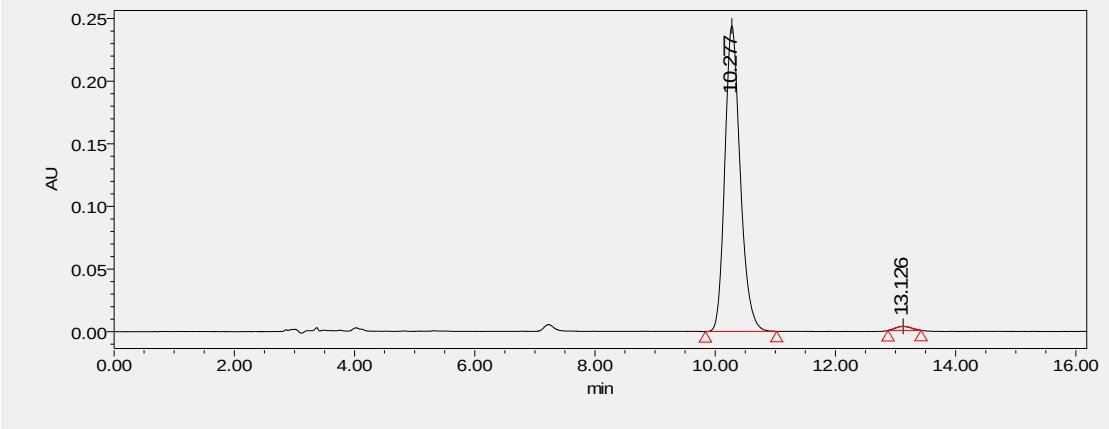


4pa

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min

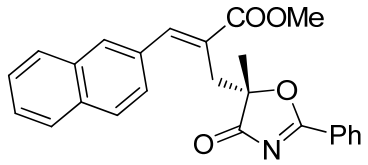


	Retention time	Area	% Area	Height	Integral type
1	10.363	5325563	49.57	299273	bb
2	13.236	5417262	50.43	228308	bb



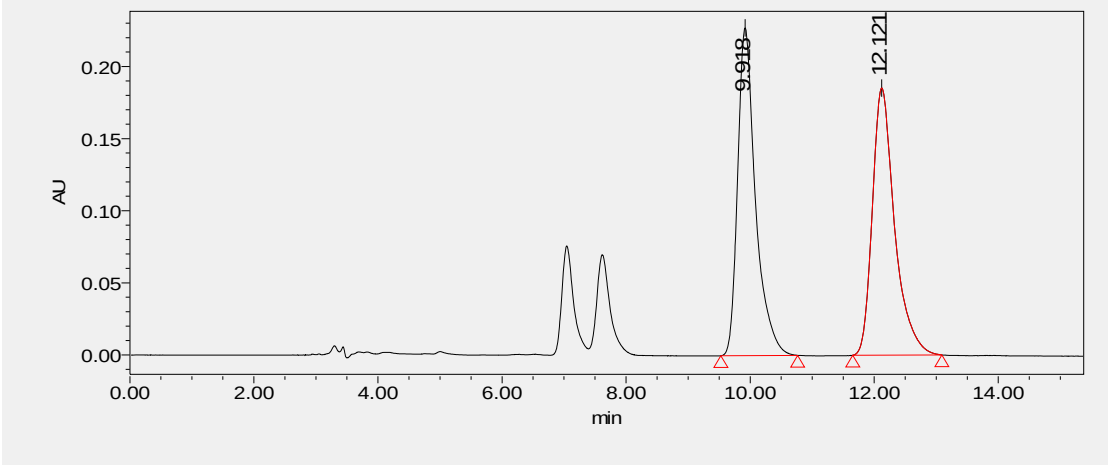
	Retention time	Area	% Area	Height	Integral type
1	10.277	4340825	98.67	243893	BB
2	13.126	58521	1.33	3234	bb

(S,E)-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(naphthalen-2-yl)acrylate, 4qa (Table 4, entry 25)

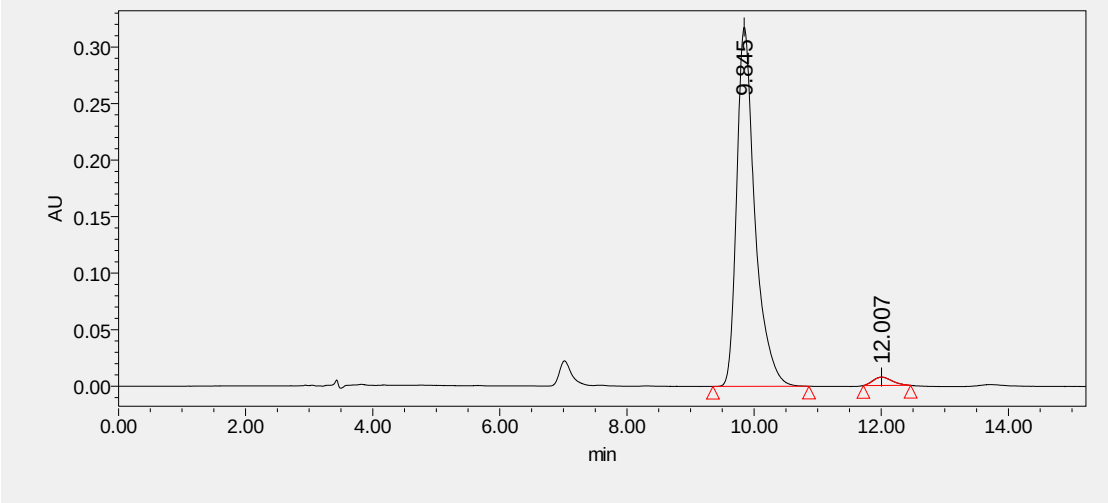


4qa

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	9.918	4536108	49.61	227203	bb
2	12.121	4607740	50.39	185183	bb

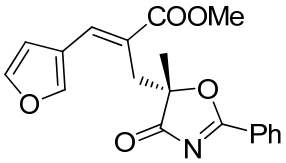


	Retention time	Area	% Area	Height	Integral type
1	9.845	6321454	97.62	317726	bb
2	12.007	153833	2.38	7422	bb

(S,E)-methyl

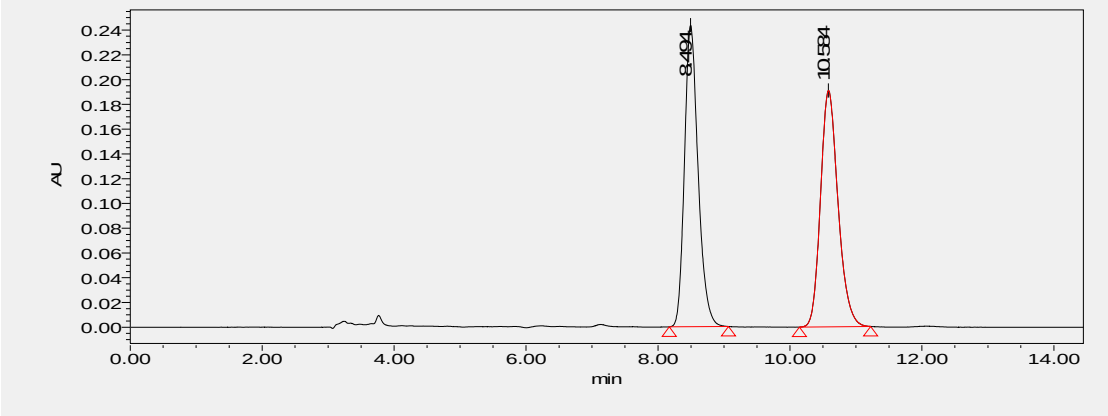
3-(furan-3-yl)-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)acrylate, 4ra

(Table 4, entry 26)

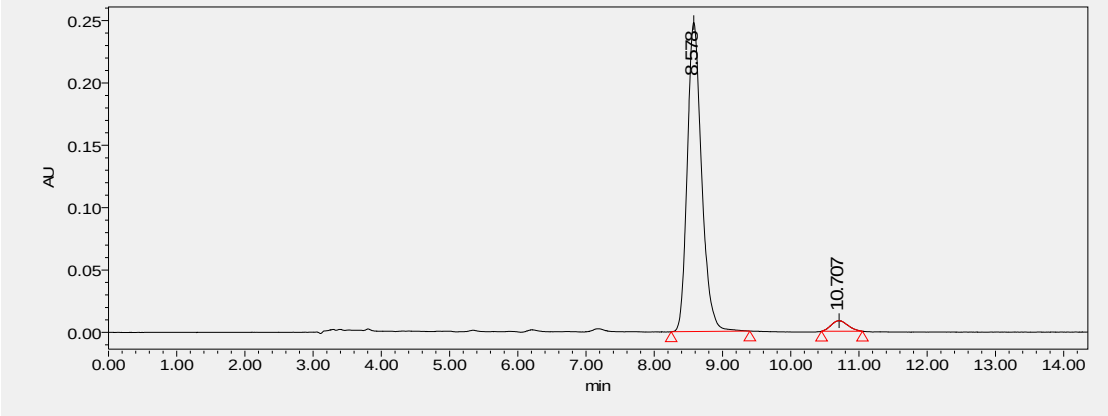


4ra

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	8.494	3497065	49.84	243560	bb
2	10.584	3519279	50.16	190870	bb

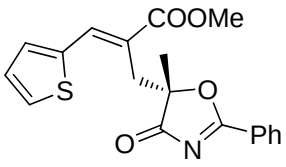


	Retention time	Area	% Area	Height	Integral type
1	8.578	3611804	96.18	247819	bb
2	10.707	143618	3.82	8469	bb

(S,E)-methyl

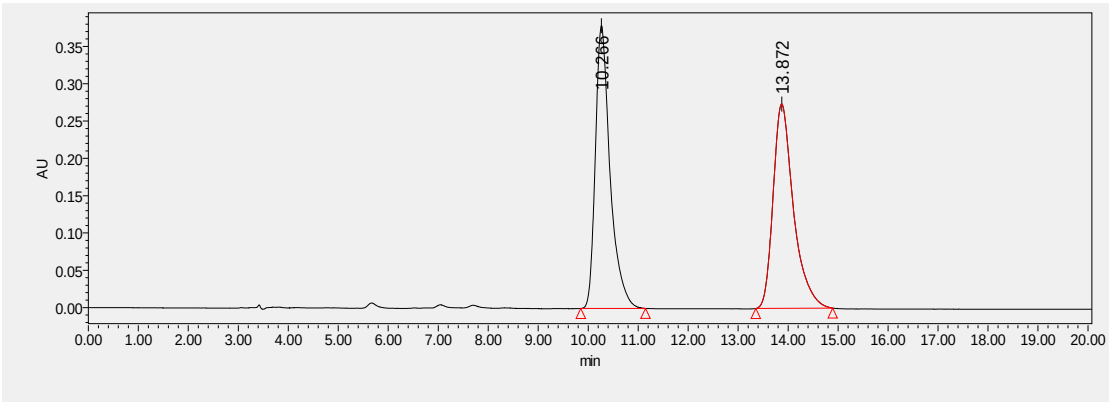
2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)-3-(thiophen-2-yl)acrylate, 4sa

(Table 4, entry 27)

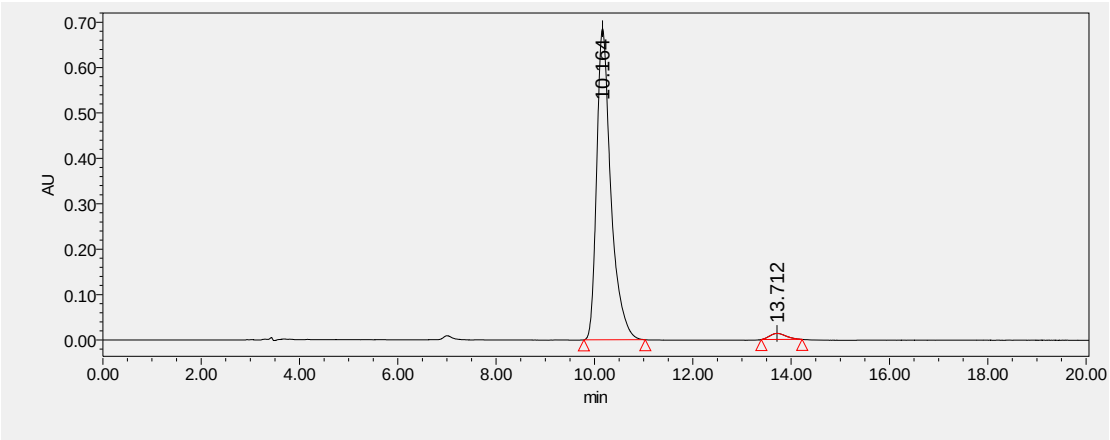


4sa

Chiralpak IC column, hexane/EtOH (1:1), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	10.266	7743868	50.00	379044	bb
2	13.872	7744736	50.00	273859	bb

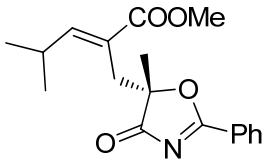


	Retention time	Area	% Area	Height	Integral type
1	10.164	13702094	97.78	685265	bb
2	13.712	311357	2.22	13358	bb

(S,E)-methyl

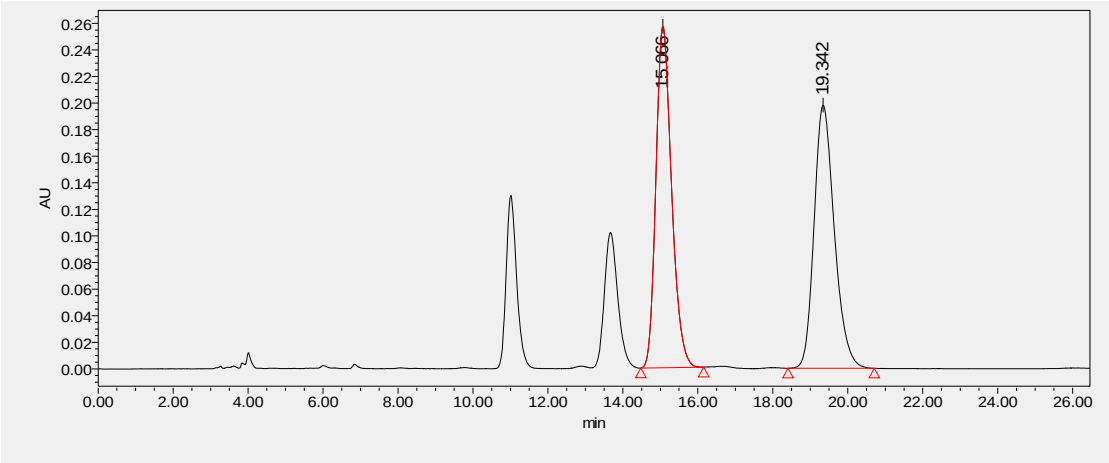
4-methyl-2-((5-methyl-4-oxo-2-phenyl-4,5-dihydrooxazol-5-yl)methyl)pent-2-enoate, 4ta

(Table 4, entry 28)

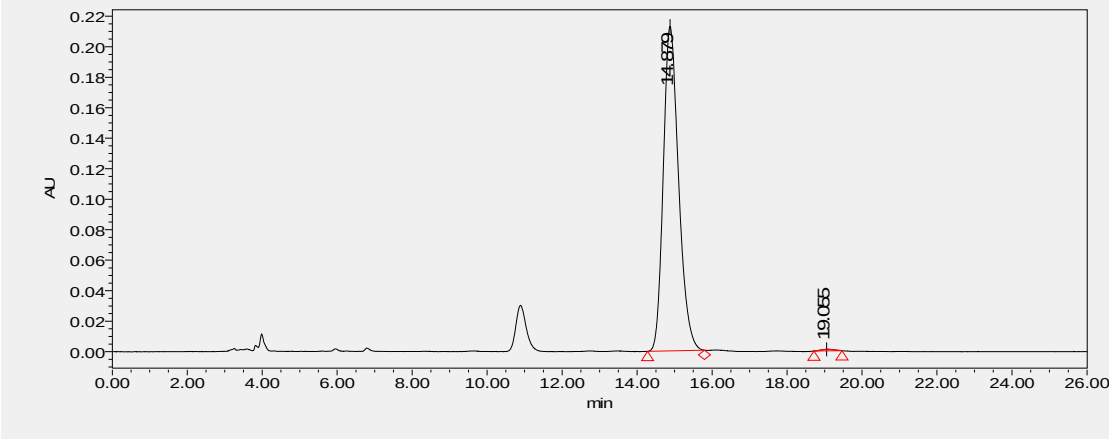


4ta

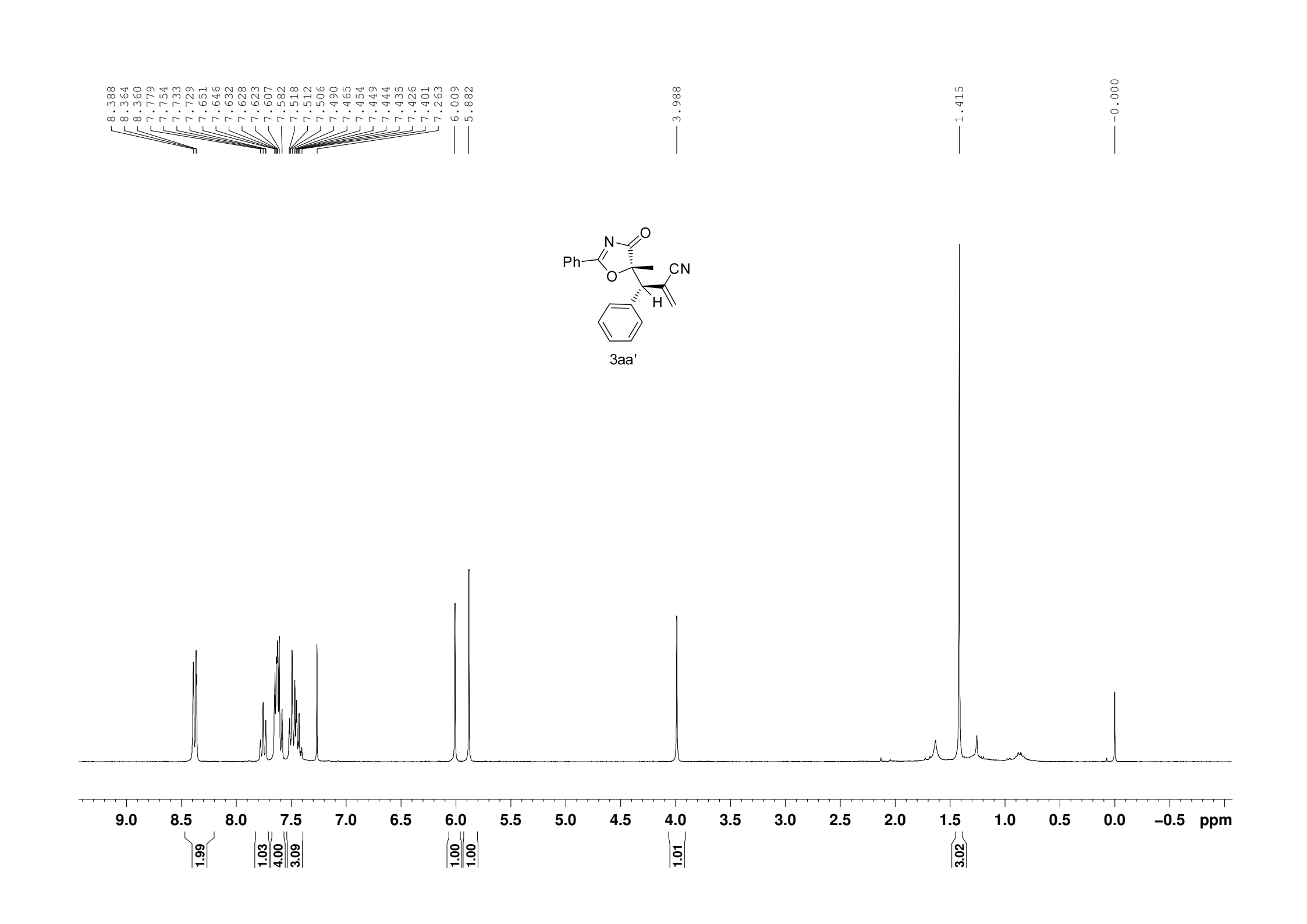
Chiralpak IC column, hexane/iPrOH (7:3), flow rate 1.0 mL/min



	Retention time	Area	% Area	Height	Integral type
1	15.066	7441450	50.07	256926	bb
2	19.342	7420788	49.93	198008	bb



	Retention time	Area	% Area	Height	Integral type
1	14.879	6051575	99.59	213035	bv
2	19.055	24864	0.41	1016	bb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7.582
7.518
7.512
7.506
7.490
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7.454
7.449
7.444
7.435
7.426
7.401
7.263
6.009
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1.415
-0.000
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O
Ph
O
CN
H
3aa'
9.0
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8.0
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7.0
6.5
6.0
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4.0
3.5
3.0
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1.5
1.0
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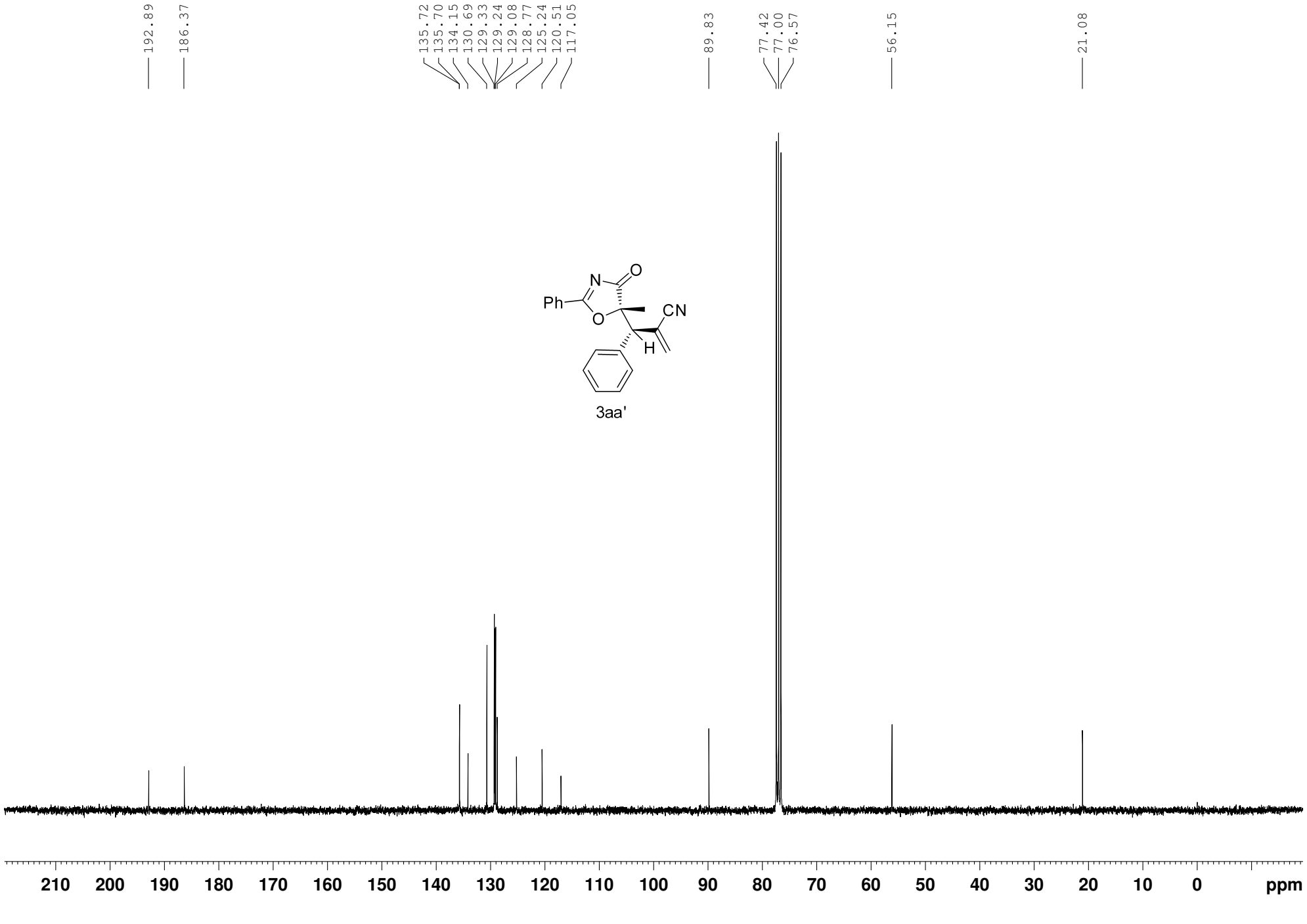
3.02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120.51
117.05
89.83
77.42
77.00
76.57
56.15
21.08
N
O
Ph
O
CN
H
3aa'
210
200
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140
130
120
110
100
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60
50
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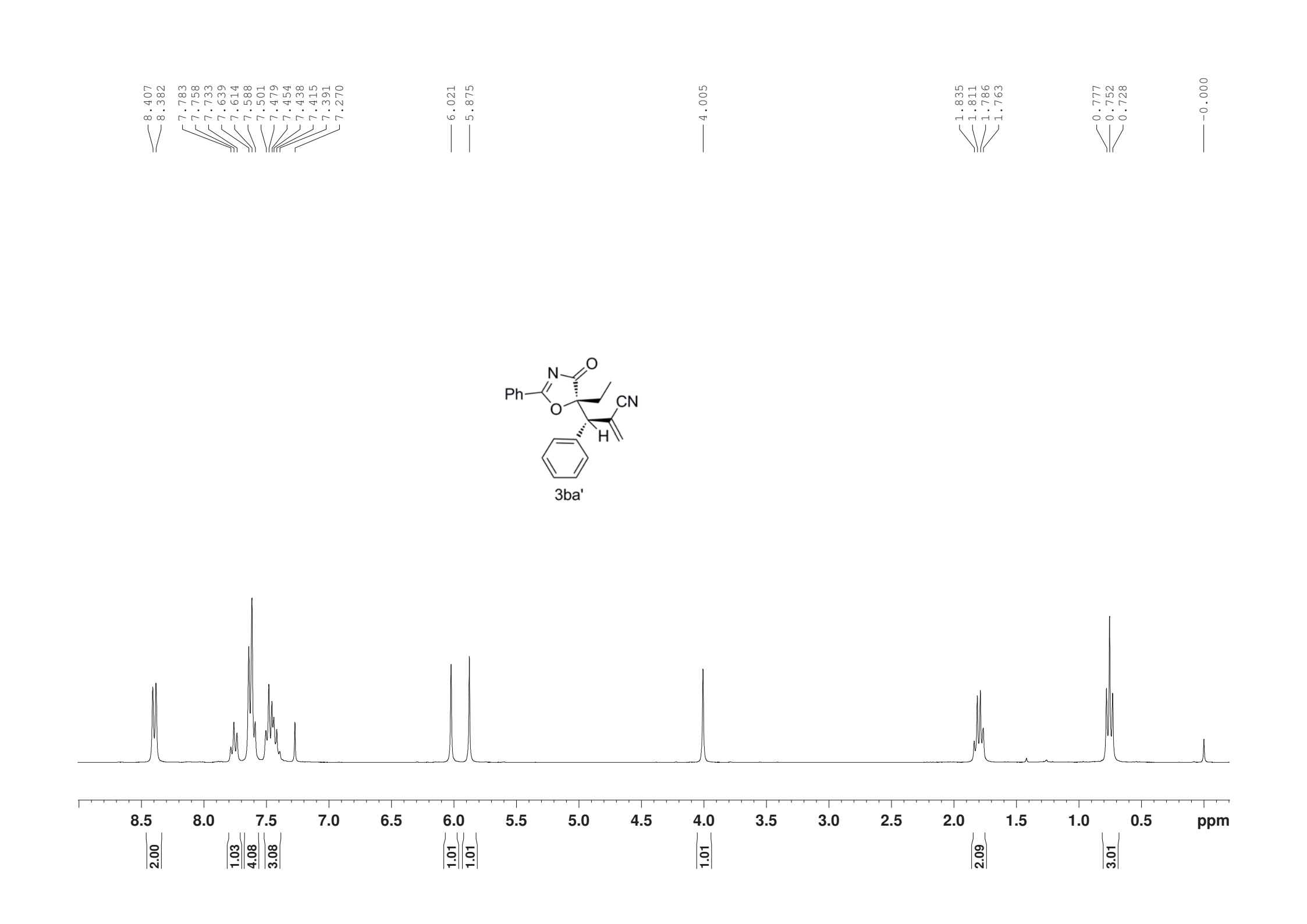
20
10
0
ppm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7.588
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7.438
7.415
7.391
7.270
6.021
5.875
4.005
1.835
1.811
1.786
1.763
0.777
0.752
0.728
0.000
Ph
N
O
O
CN
H
3ba'
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7.0
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6.0
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5.0
4.5
4.0
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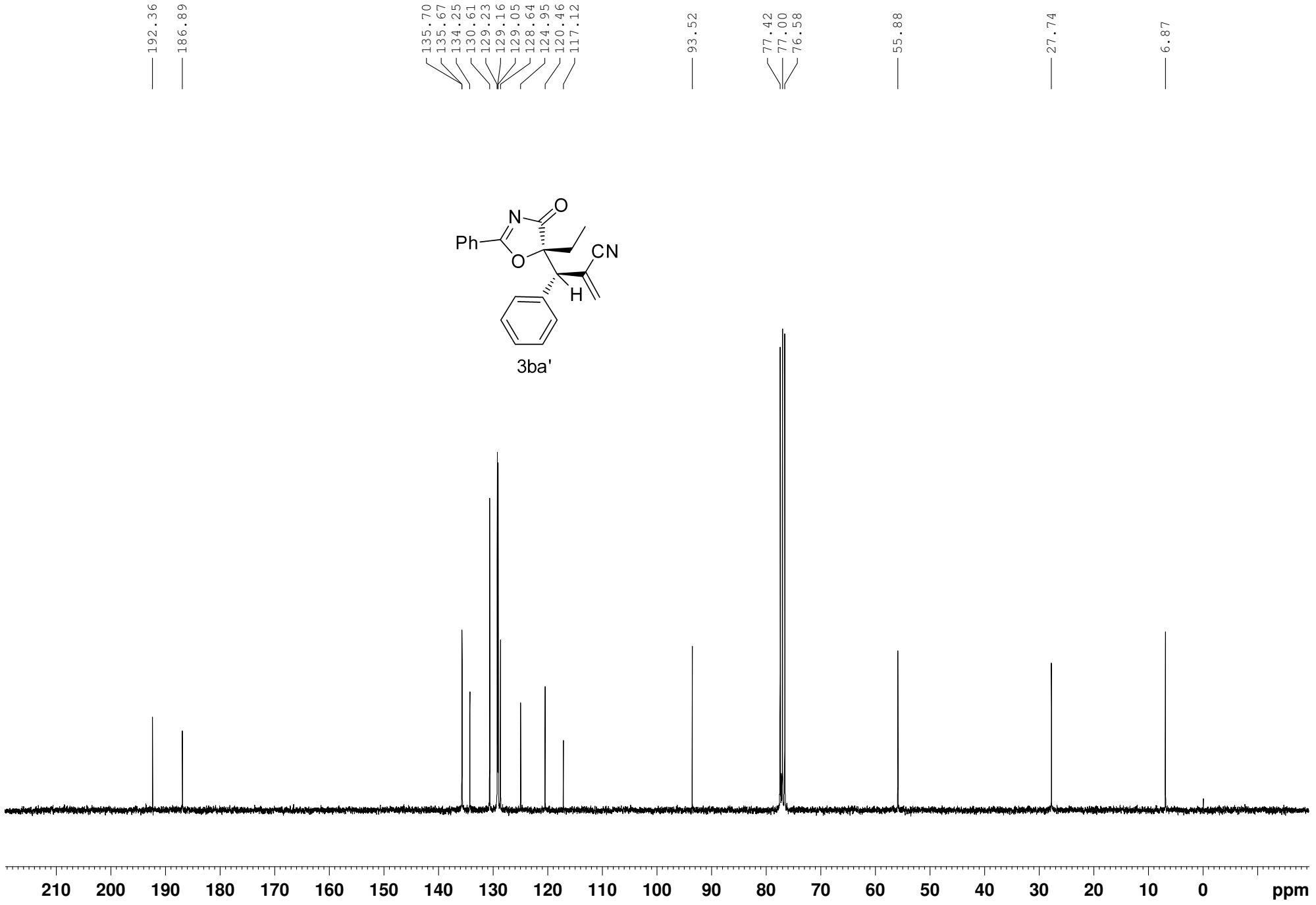
2.09
3.01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117.12
93.52
77.42
77.00
76.58
55.88
27.74
6.87
N
O
Ph
O
CN
H
3ba'
210
200
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140
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100
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60
50
40
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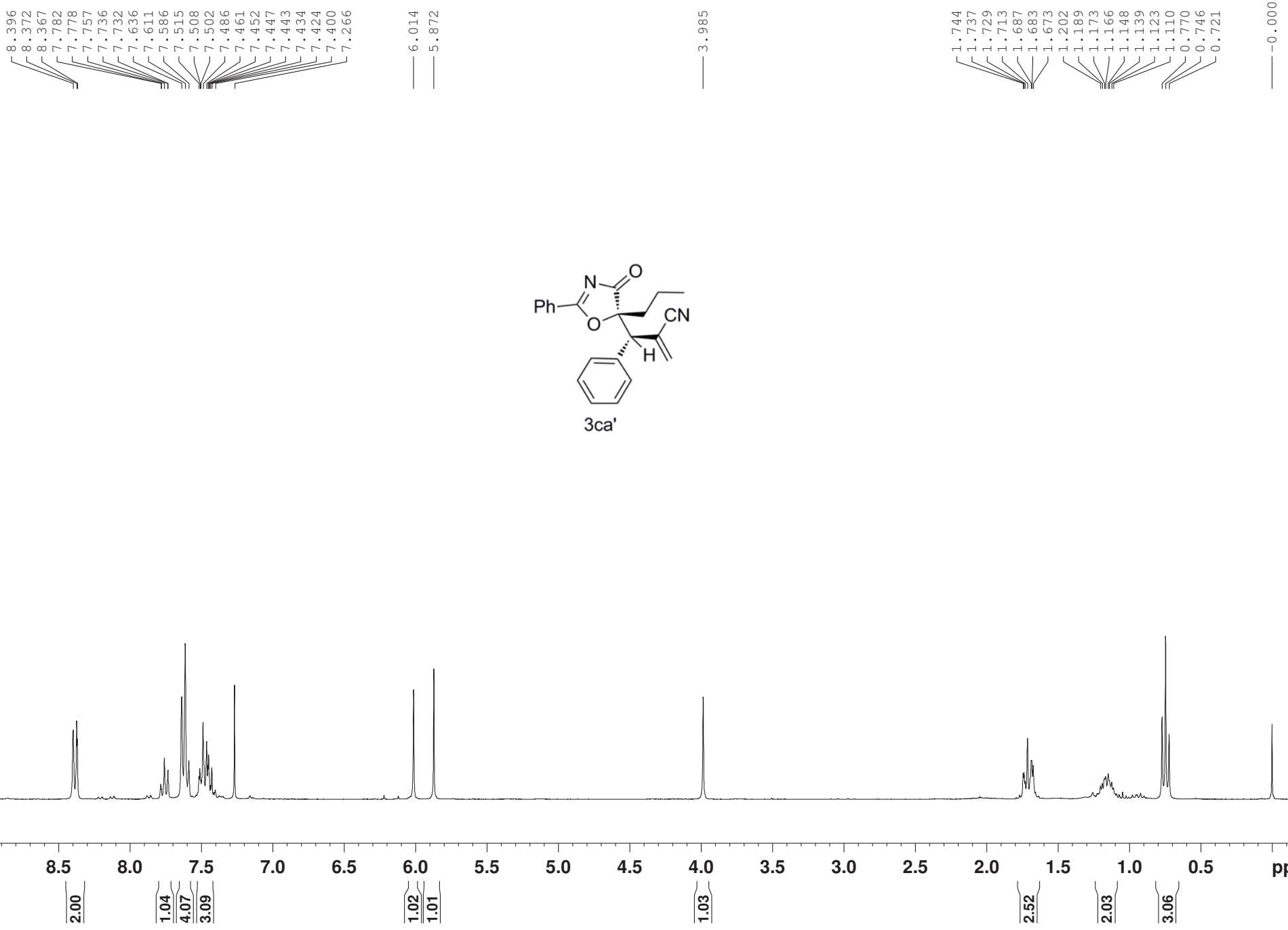
20
10
0
ppm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7.461
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7.447
7.443
7.434
7.424
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1.737
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1.202
1.189
1.173
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1.139
1.123
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O
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O
CN
H
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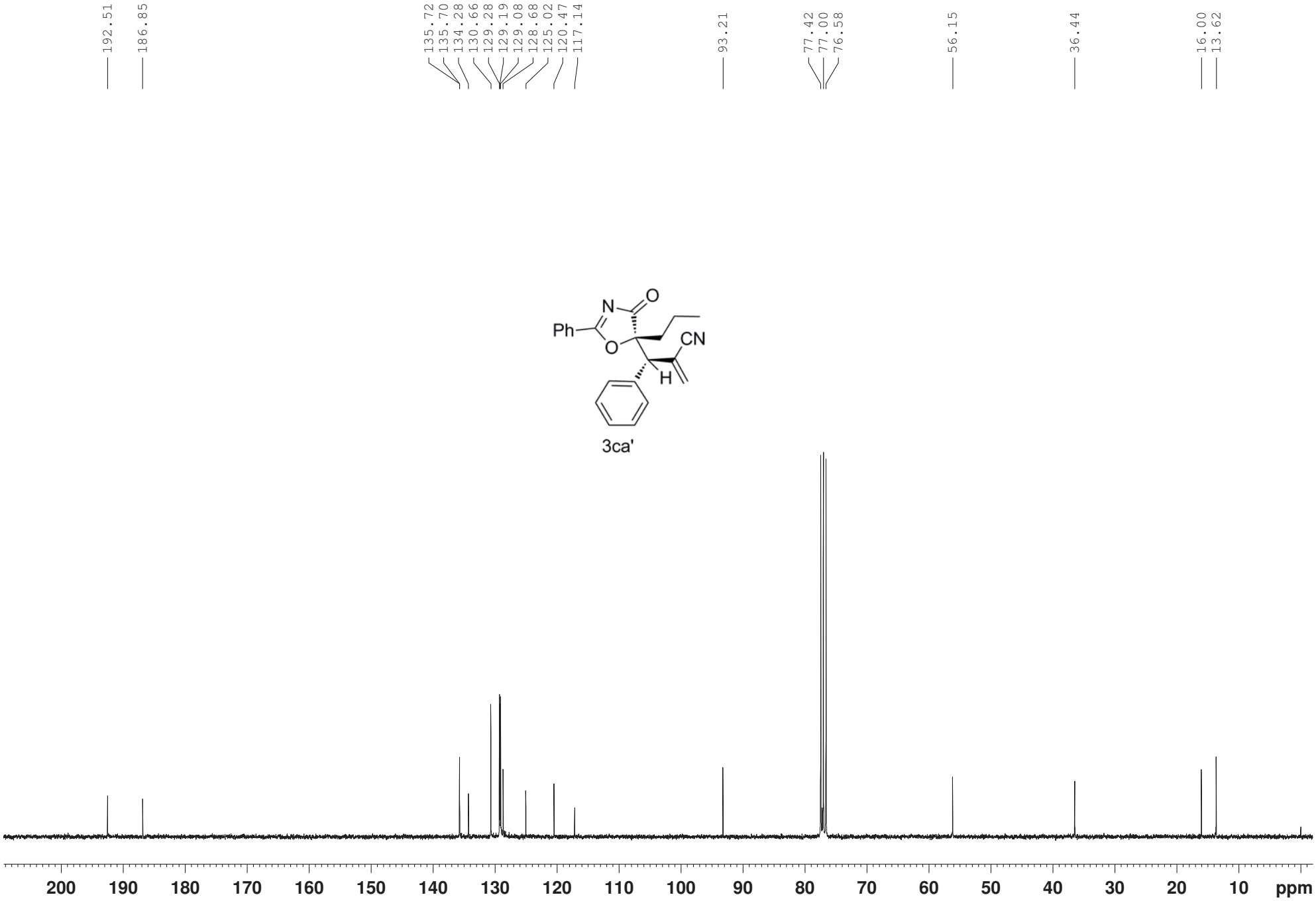
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93.21
77.42
77.00
76.58
56.15
36.44
16.00
13.62
N
O
Ph
O
CN
H
3ca'
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


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7.755
7.731
7.663
7.638
7.612
7.586
7.503
7.480
7.455
7.438
7.415
7.391
7.265
6.046
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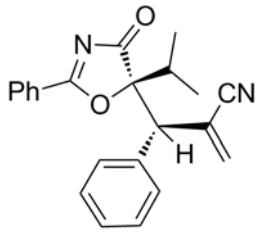
O
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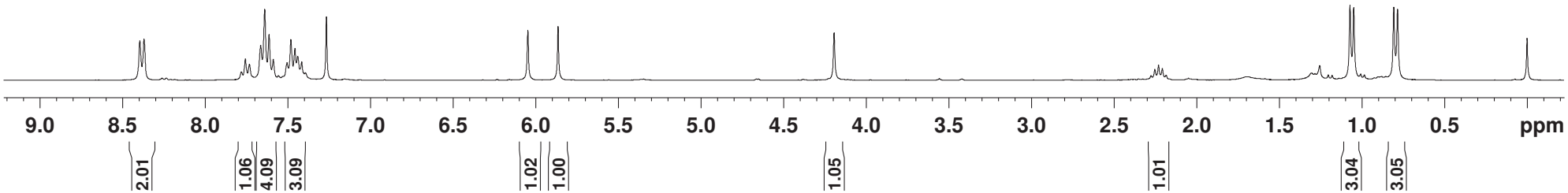
Ph
O
CN
H

3da'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4.0
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3.0
2.5
2.0
1.5
1.0
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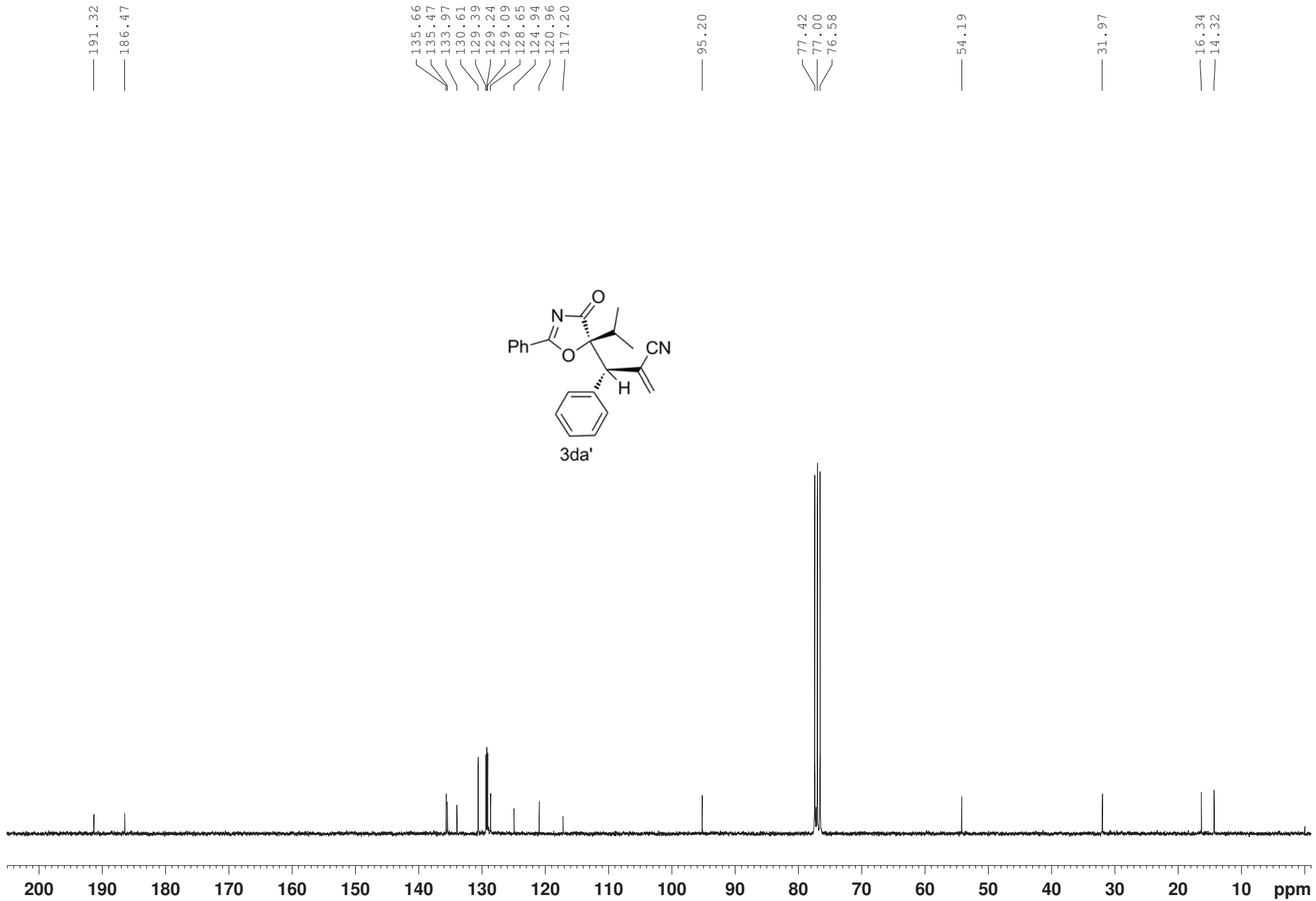
3.09
1.02
1.00
1.05
1.01
3.04
3.05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128.65
124.94
120.96
117.20
95.20
77.42
77.00
76.58
54.19
31.97
16.34
14.32
O
N
Ph
O
CN
H
3da'
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150
140
130
120
110
100
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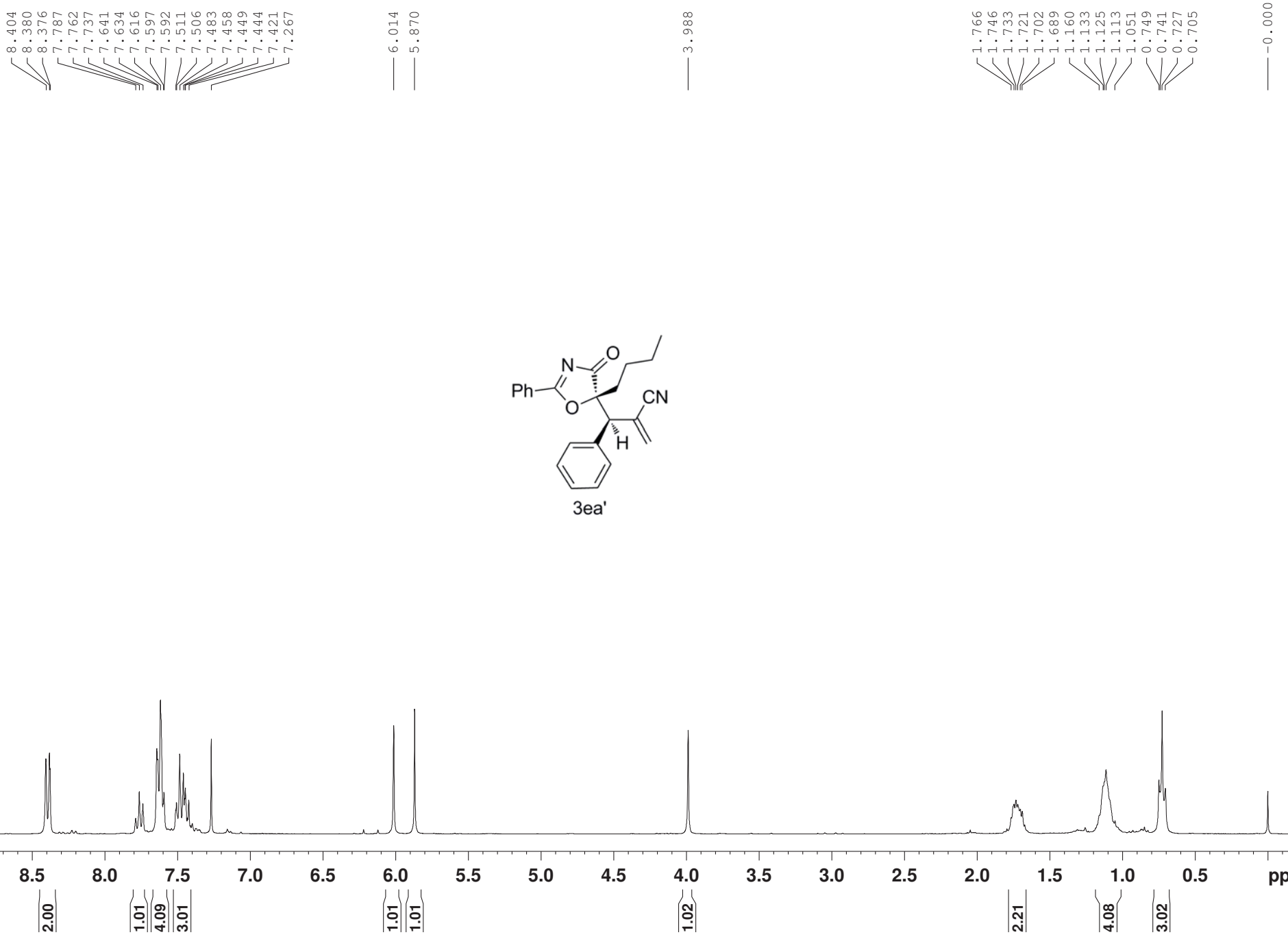
70
60
50
40
30
20
10
ppm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7.511
7.506
7.483
7.458
7.449
7.444
7.421
7.267
6.014
5.870
3.988
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1.733
1.721
1.702
1.689
1.160
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1.125
1.113
1.051
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0.741
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0.705
0.000
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N
O
CN
H
3ea'
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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1.01
1.02
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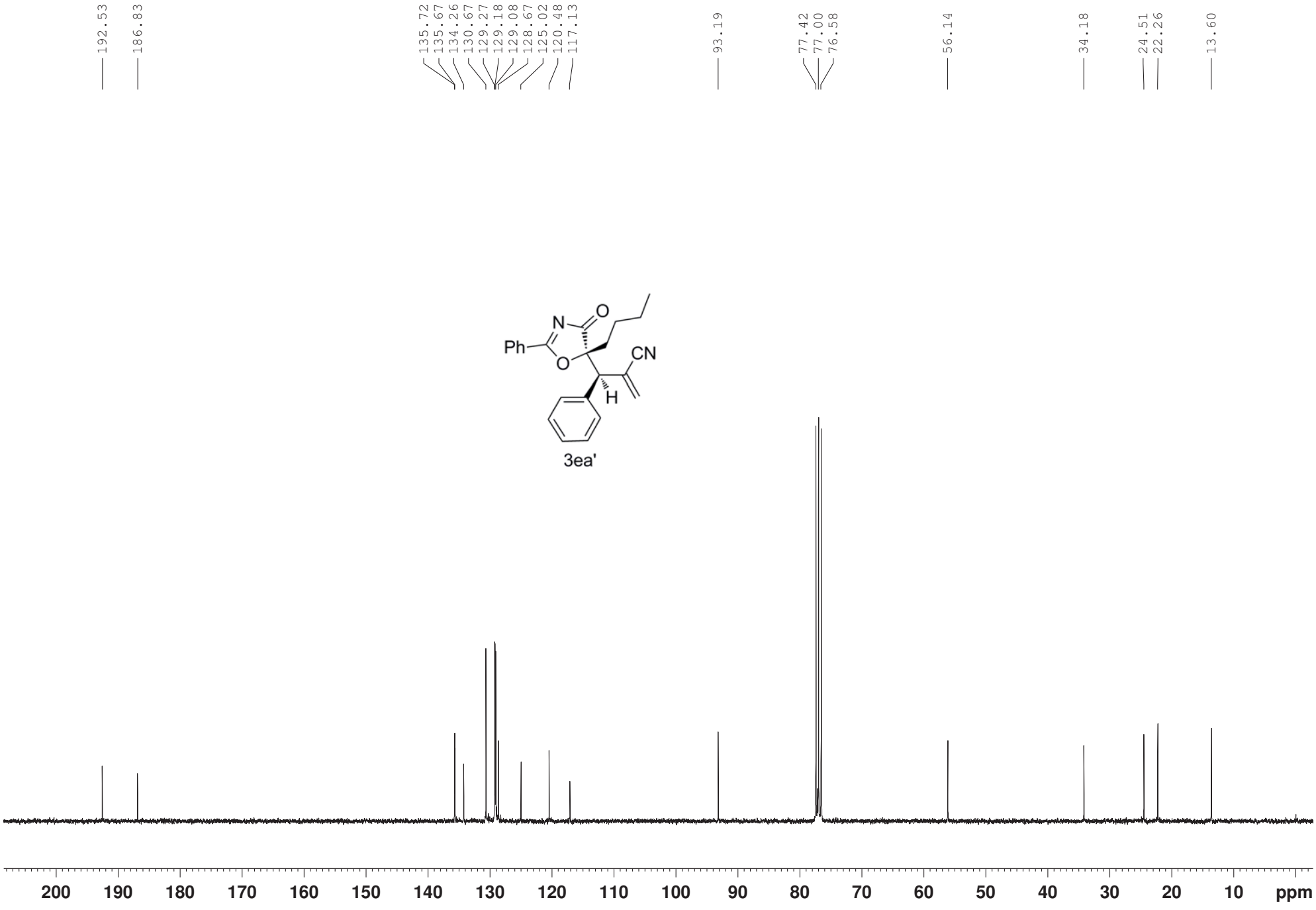
4.08
3.02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129.18
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125.02
120.48
117.13
93.19
77.42
77.00
76.58
56.14
34.18
24.51
22.26
13.60
Ph
N
O
O
CN
H
3ea'
200
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180
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150
140
130
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110
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70
60
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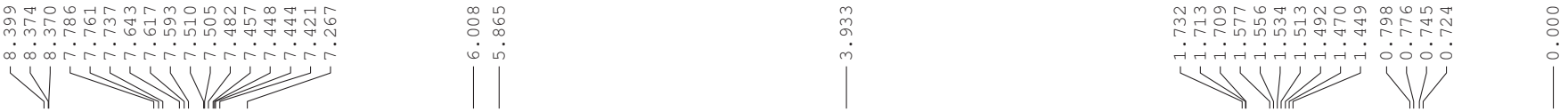
10
ppm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7.510
7.505
7.482
7.457
7.448
7.444
7.421
7.267
6.008
5.865
3.933
1.732
1.713
1.709
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1.470
1.449
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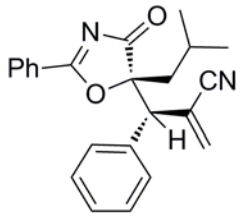
0.724
0.000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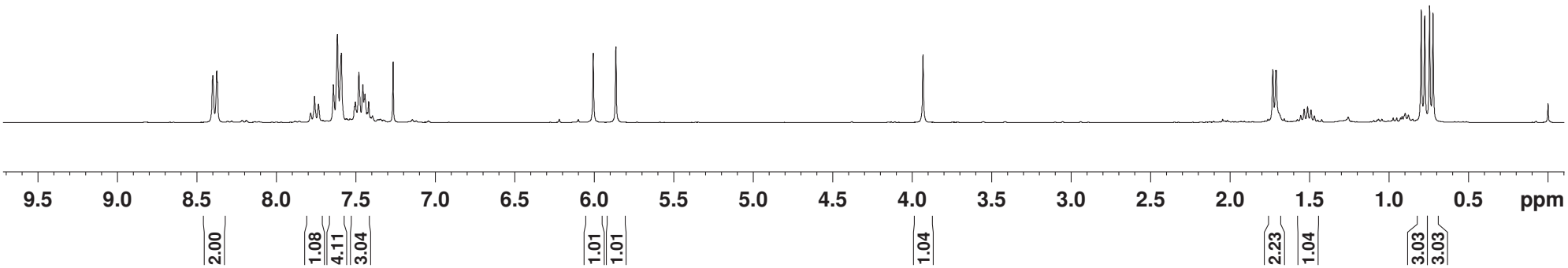
Ph
O
CN
H

3fa'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2.5
2.0
1.5
1.0
0.5
ppm
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1.01
1.01
1.04
2.23
1.04
3.03
3.03

192.73
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129.13
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76.58
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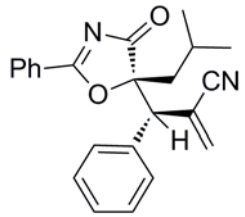
42.83
24.19
23.55



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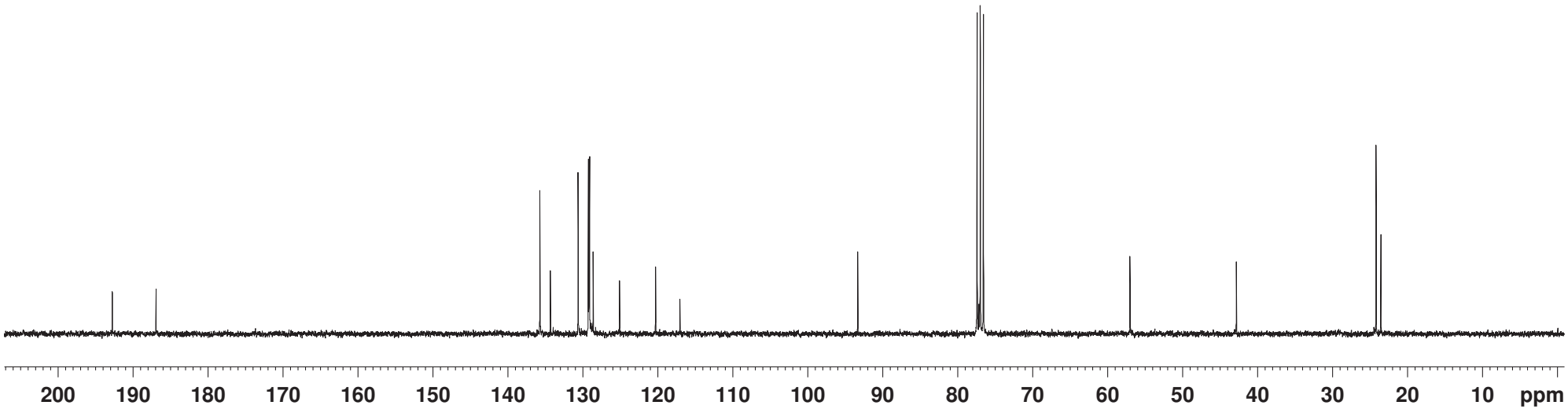

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7.590
7.507
7.485
7.461
7.445
7.421
7.265
6.033
5.852
4.213
1.938
1.917
1.637
1.295
1.271
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1.025
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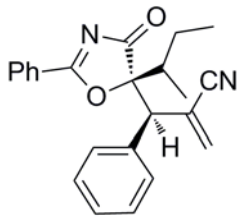
0.736
0.000



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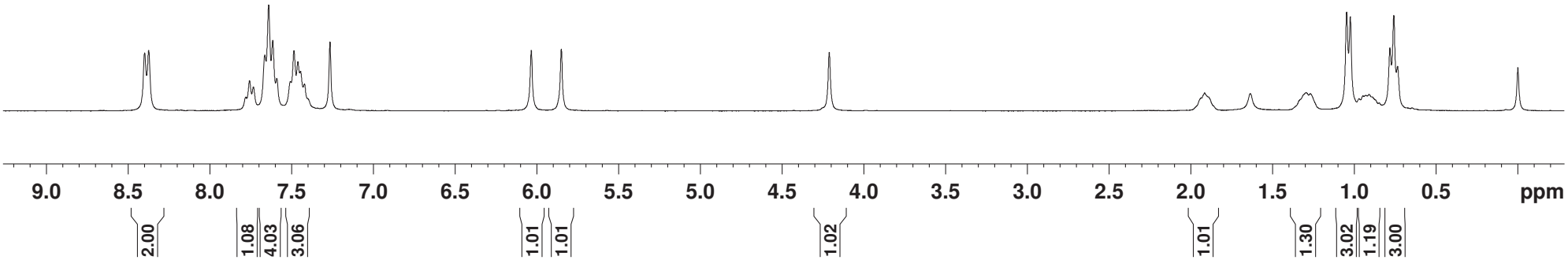

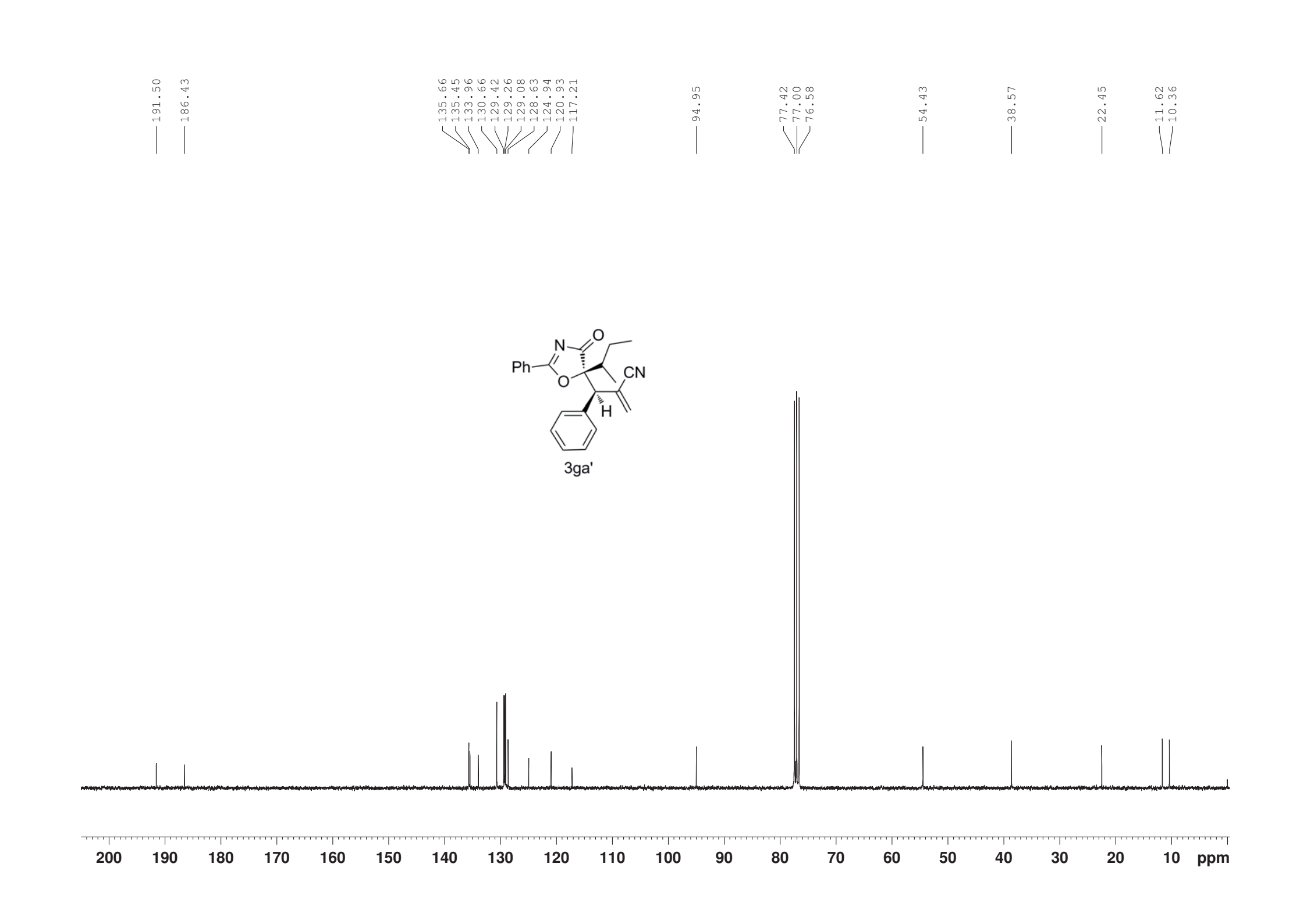
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120.93
117.21
94.95
77.42
77.00
76.58
54.43
38.57
22.45
11.62
10.36
N
O
Ph
O
CN
H
3ga'
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180
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150
140
130
120
110
100
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70
60
50
40
30
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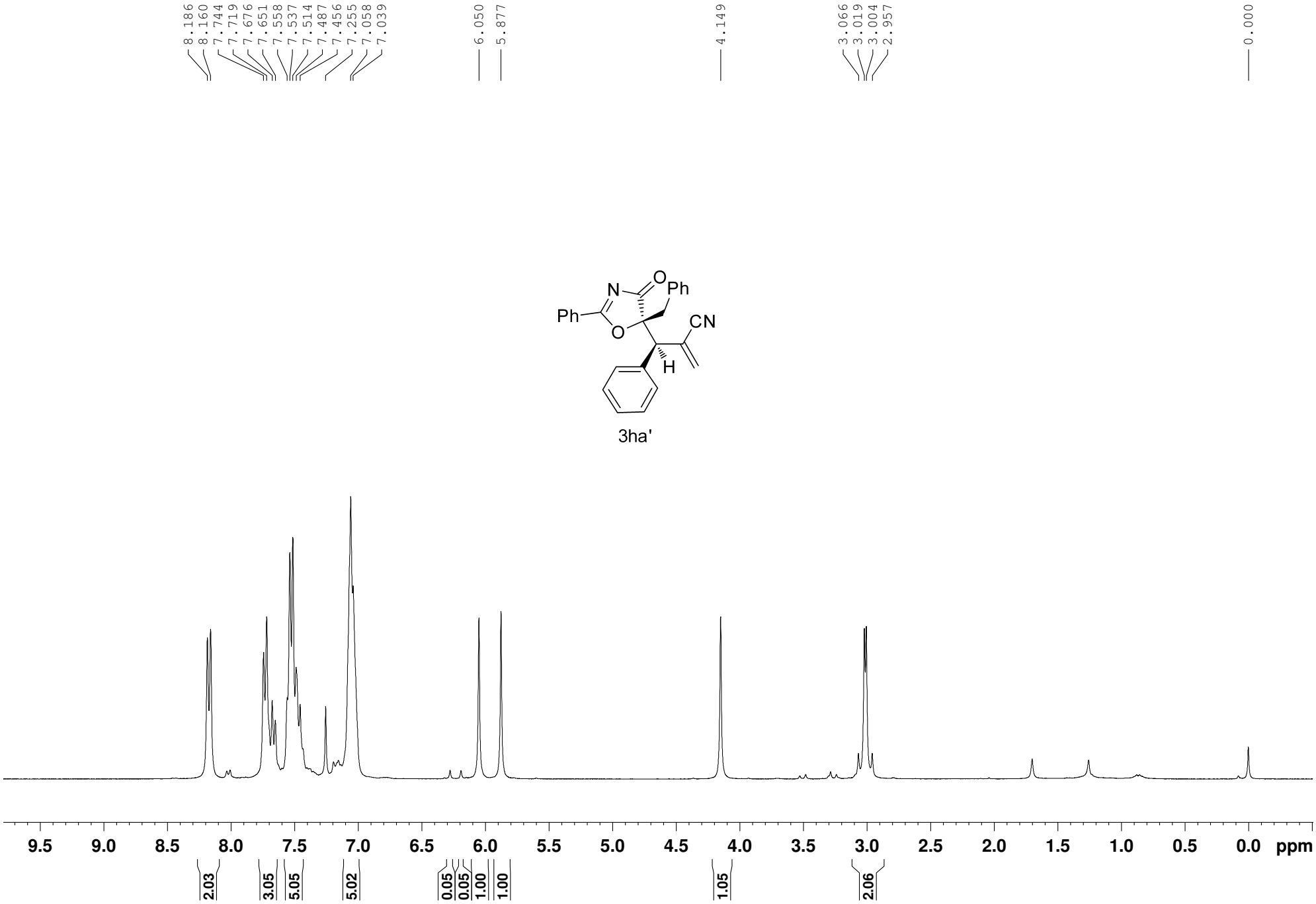
10
ppm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7.487
7.456
7.255
7.058
7.039
6.050
5.877
4.149
3.066
3.019
3.004
2.957
0.000
N
O
Ph
Ph
O
CN
H
3ha'
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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0.05
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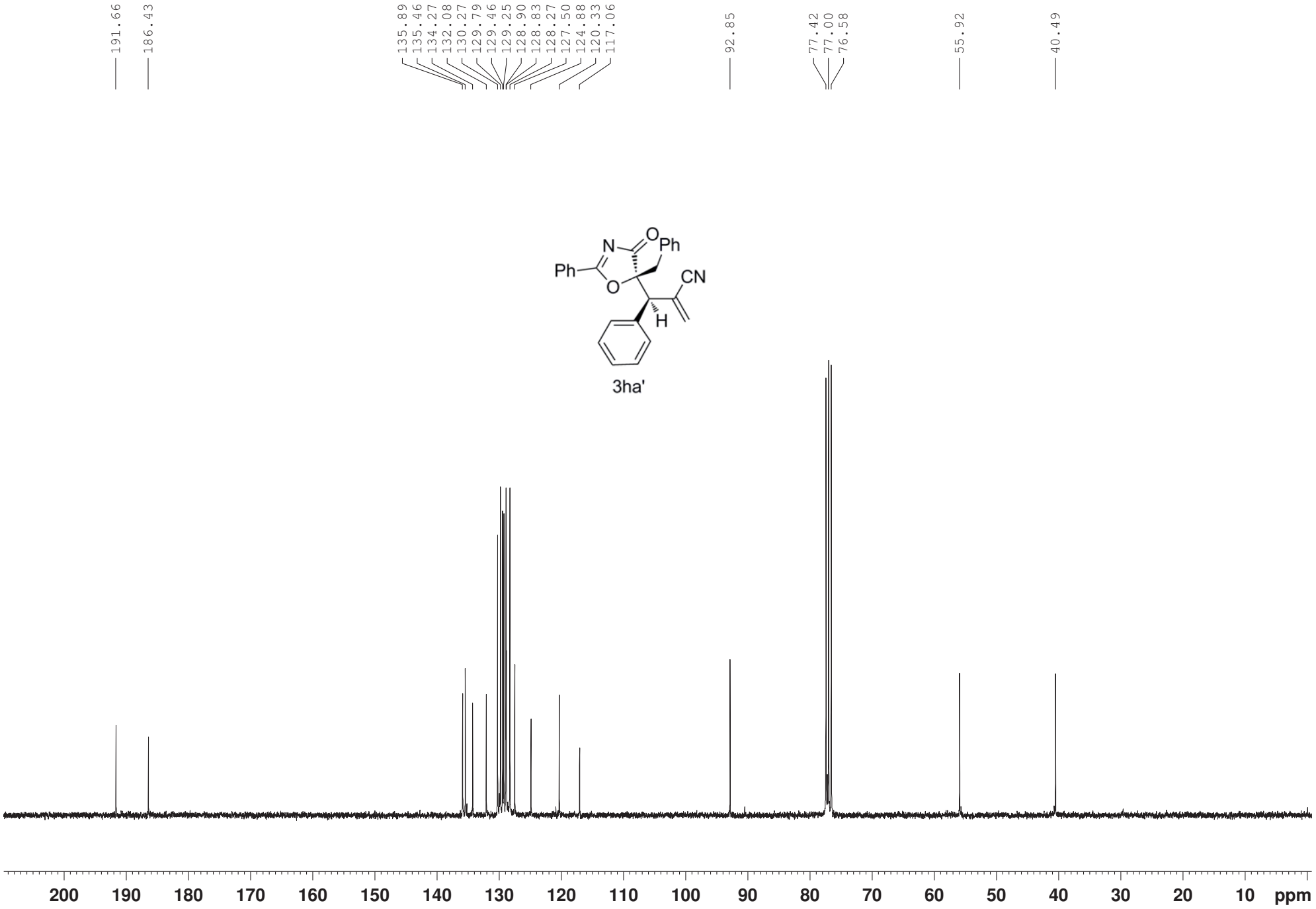
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128.83
128.27
127.50
124.88
120.33
117.06
92.85
77.42
77.00
76.58
55.92
40.49
N
O
Ph
Ph
O
CN
H
3ha'
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


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8.371
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7.762
7.737
7.642
7.636
7.630
7.615
7.608
7.591
7.512
7.506
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7.450
7.445
7.431
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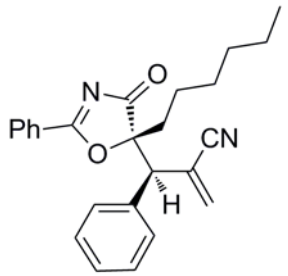
0.738
-0.000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Ph
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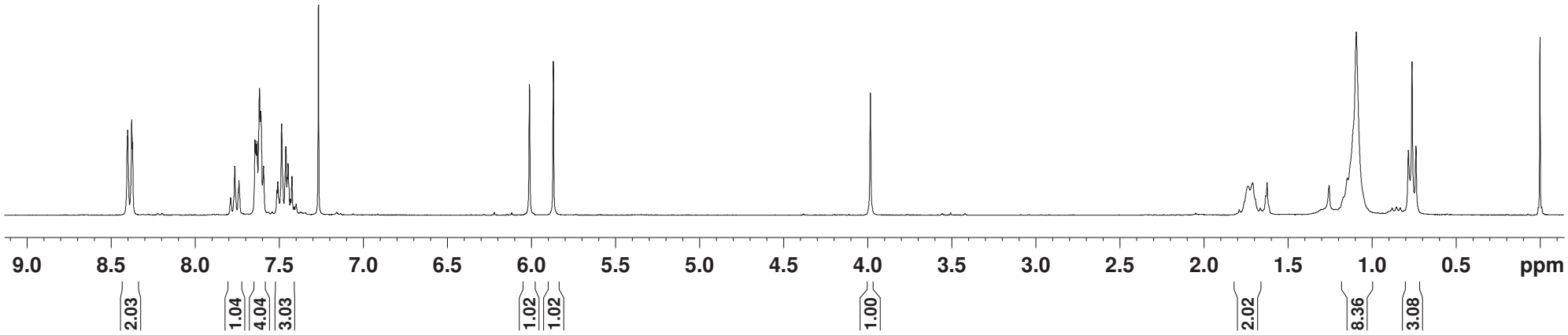
CN
H

3ia'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2.0
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1.02
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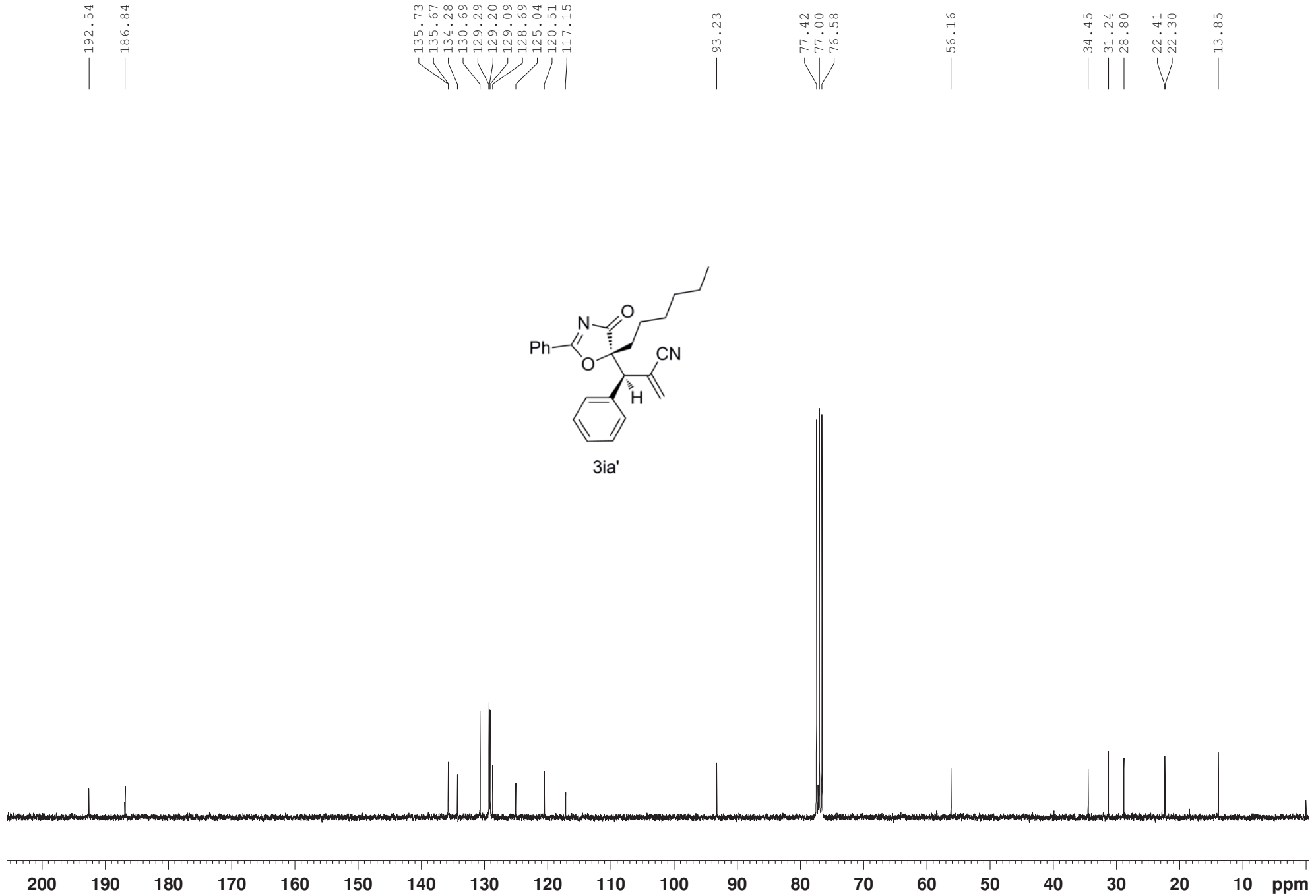
8.36
3.08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128.69
125.04
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117.15
93.23
77.42
77.00
76.58
56.16
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31.24
28.80
22.41
22.30
13.85
N
O
Ph
O
CN
H
3ia'
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180
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160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


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7.732
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7.630
7.607
7.582
7.519
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7.472
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7.434
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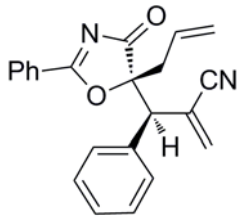
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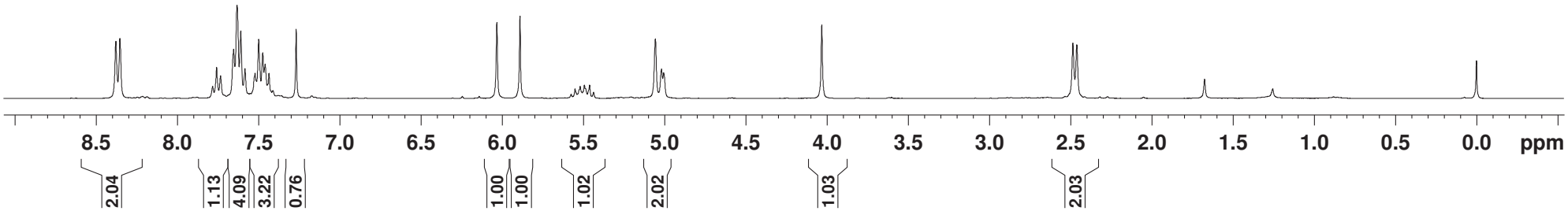
3ja'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2.0
1.5
1.0
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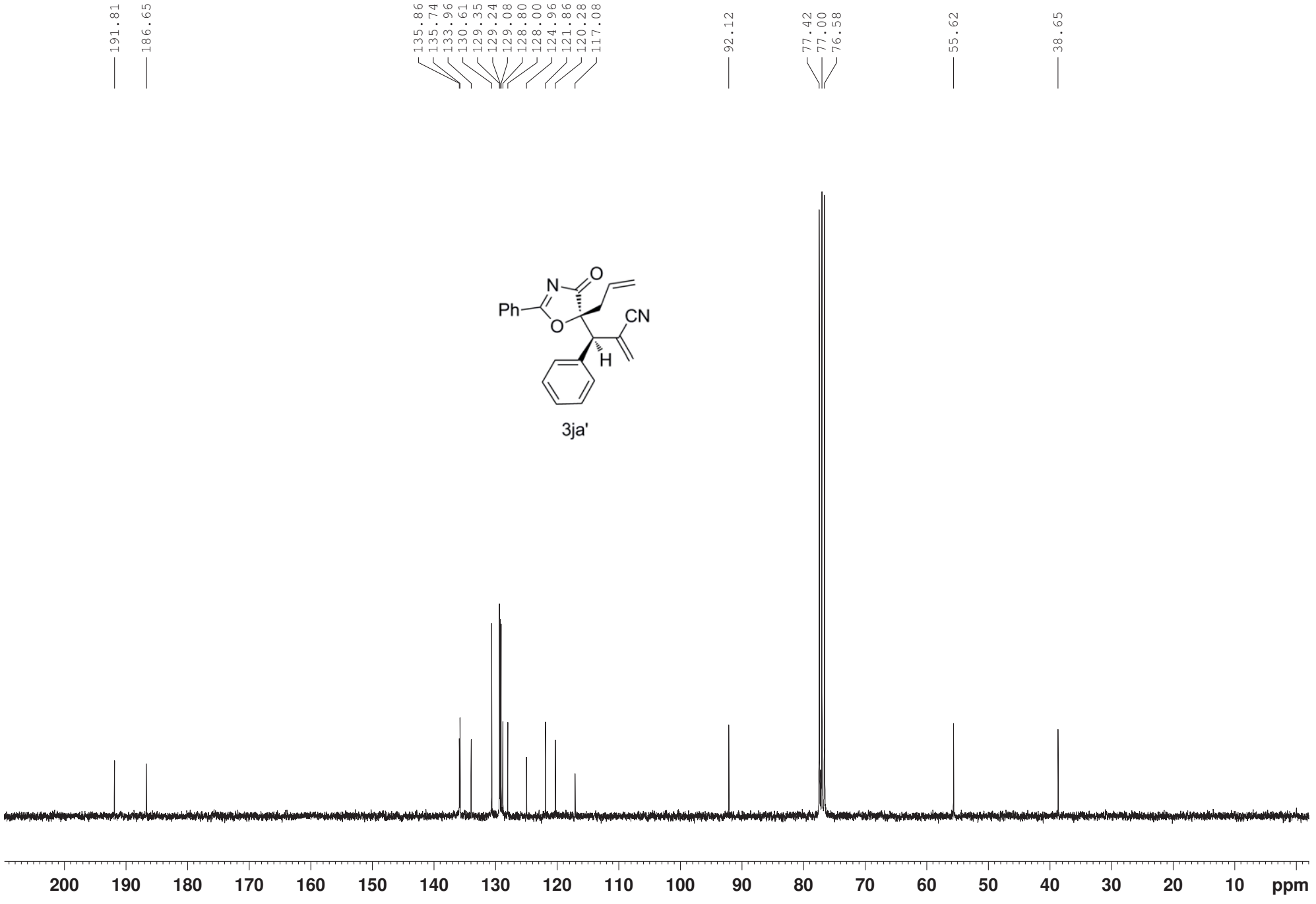
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77.00
76.58
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Ph
O
CN
H
3ja'
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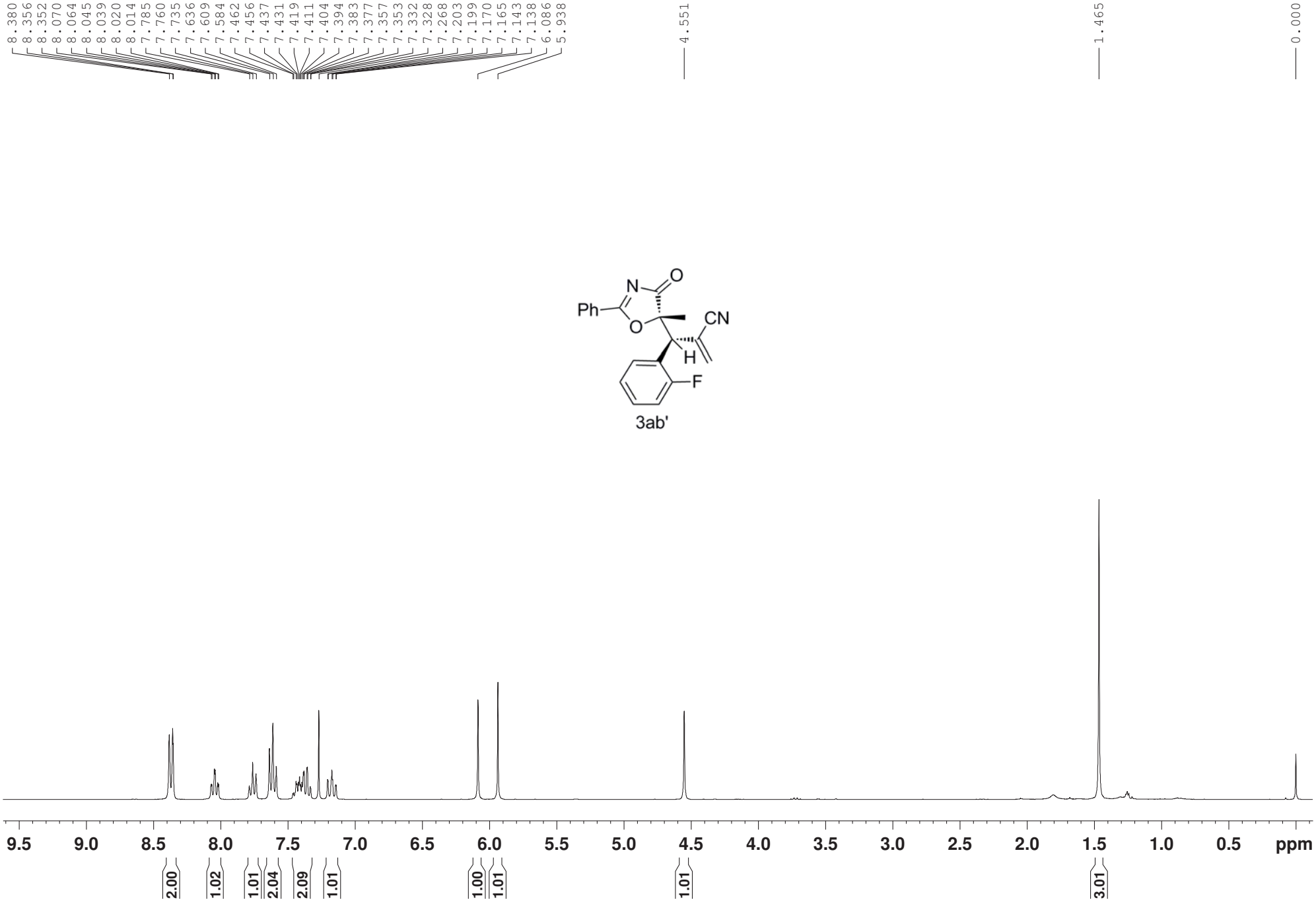
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F
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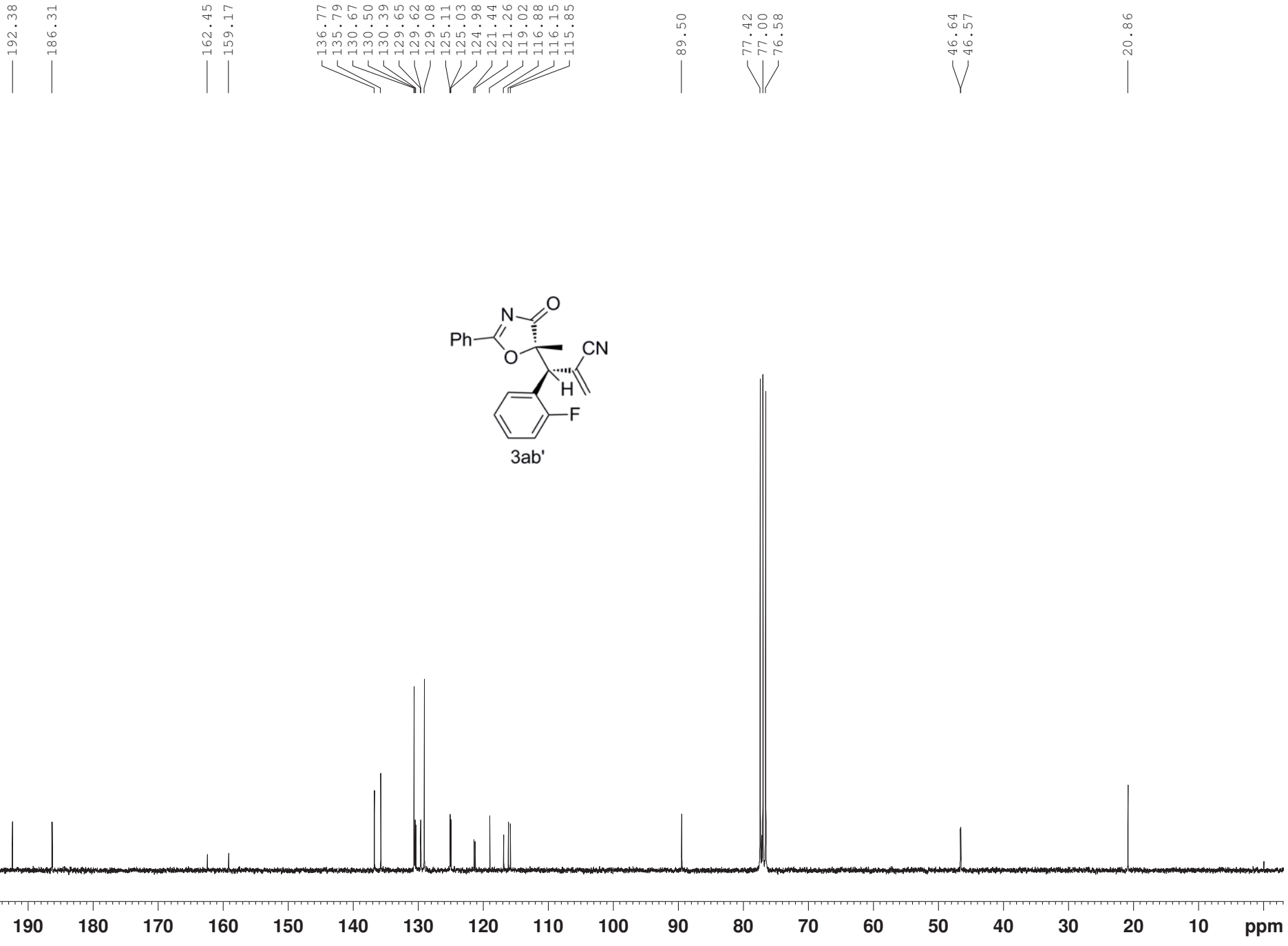
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O
Ph
O
CN
H
F
3ab'
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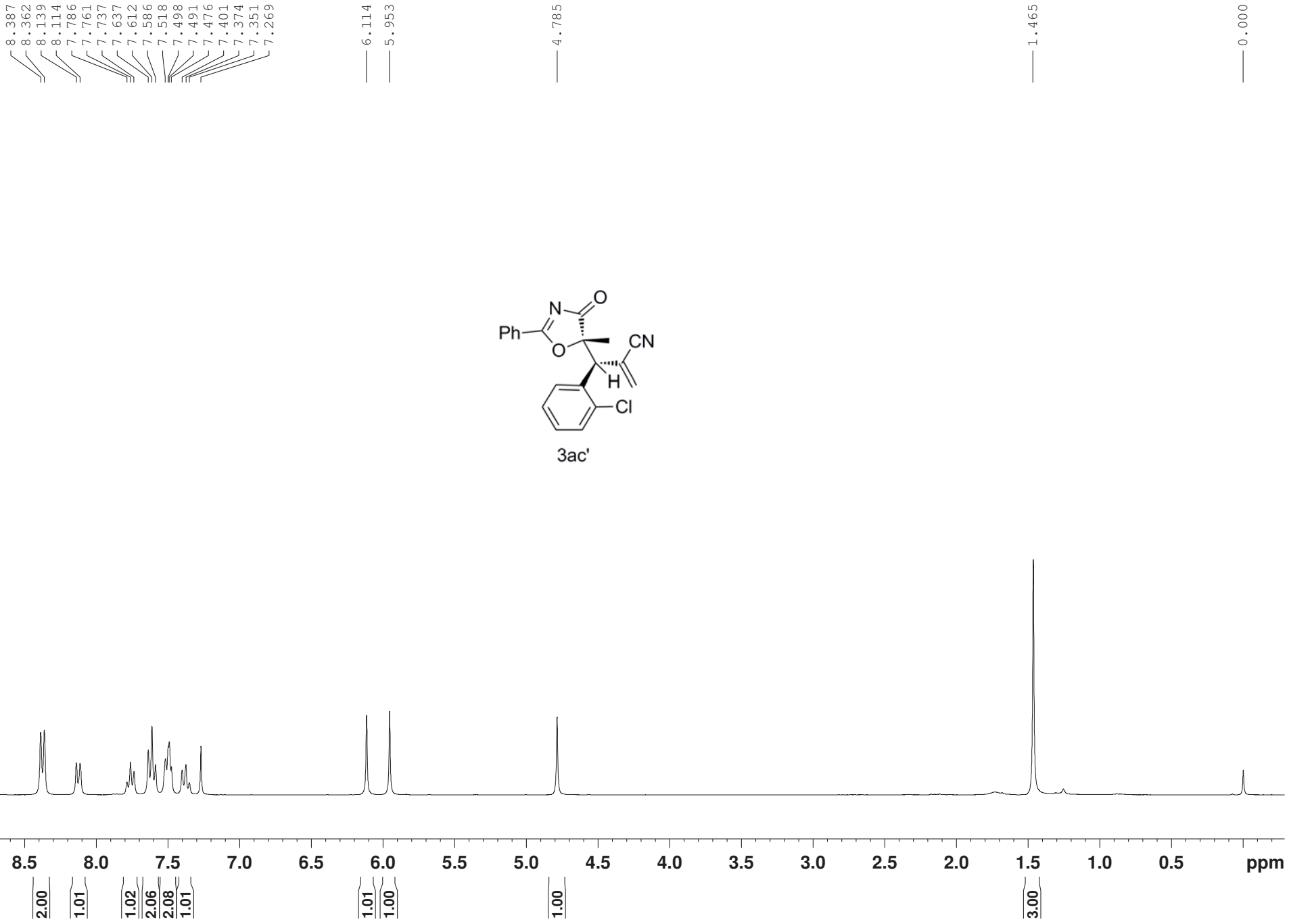
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7.476
7.401
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7.351
7.269
6.114
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4.785
1.465
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O
O
CN
H
Cl
3ac'
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6.5
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1.0
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1.02
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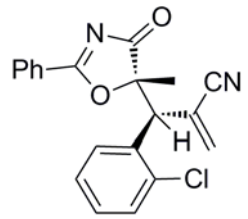

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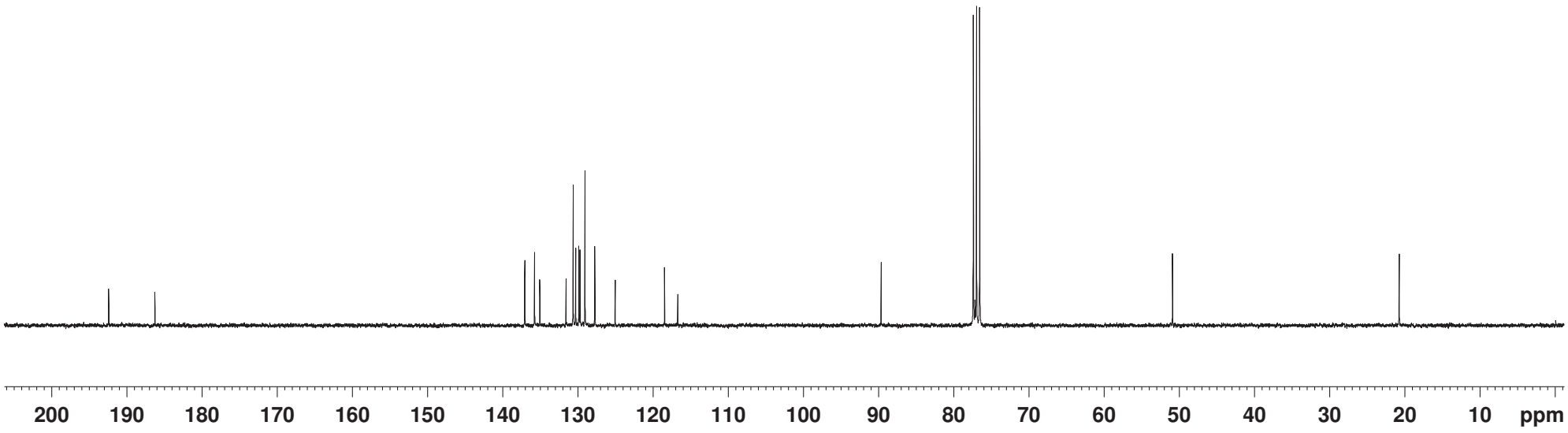

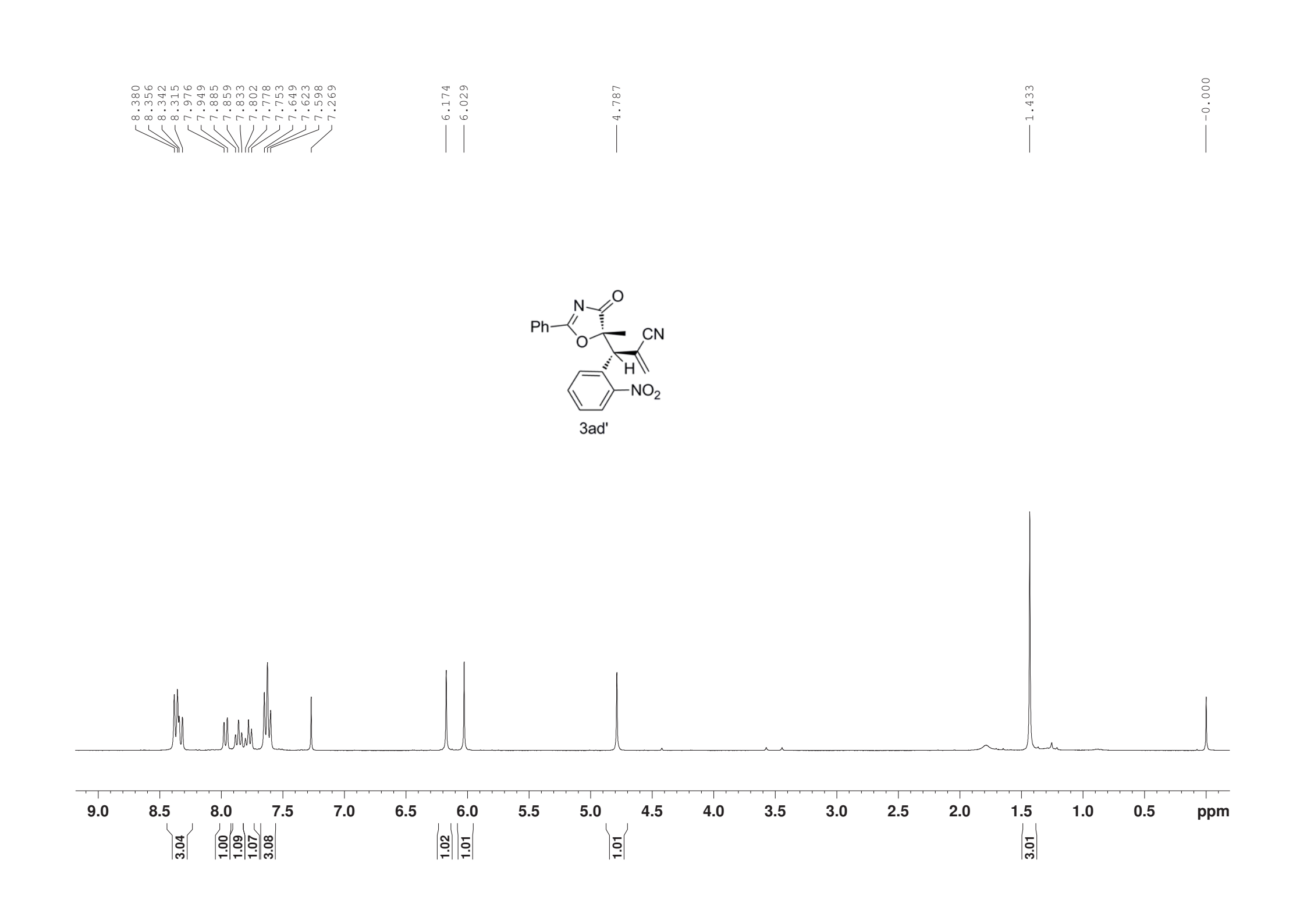
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7.623
7.598
7.269
6.174
6.029
4.787
1.433
-0.000
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O
Ph
O
CN
H
NO2
3ad'
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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1.07
3.08
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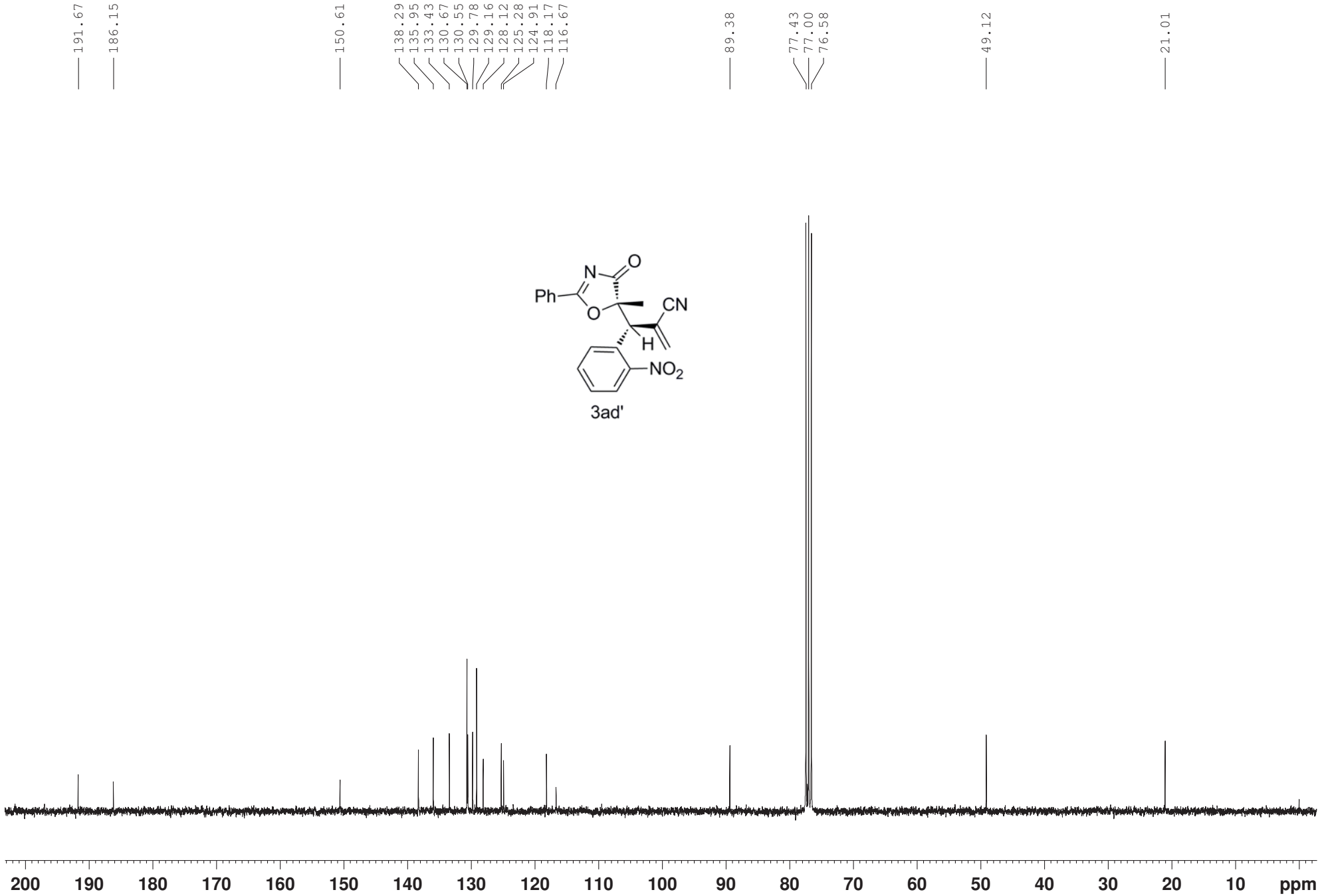
1.01
3.01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77.43
77.00
76.58
49.12
21.01
N
O
Ph
O
CN
H
NO2
3ad'
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150
140
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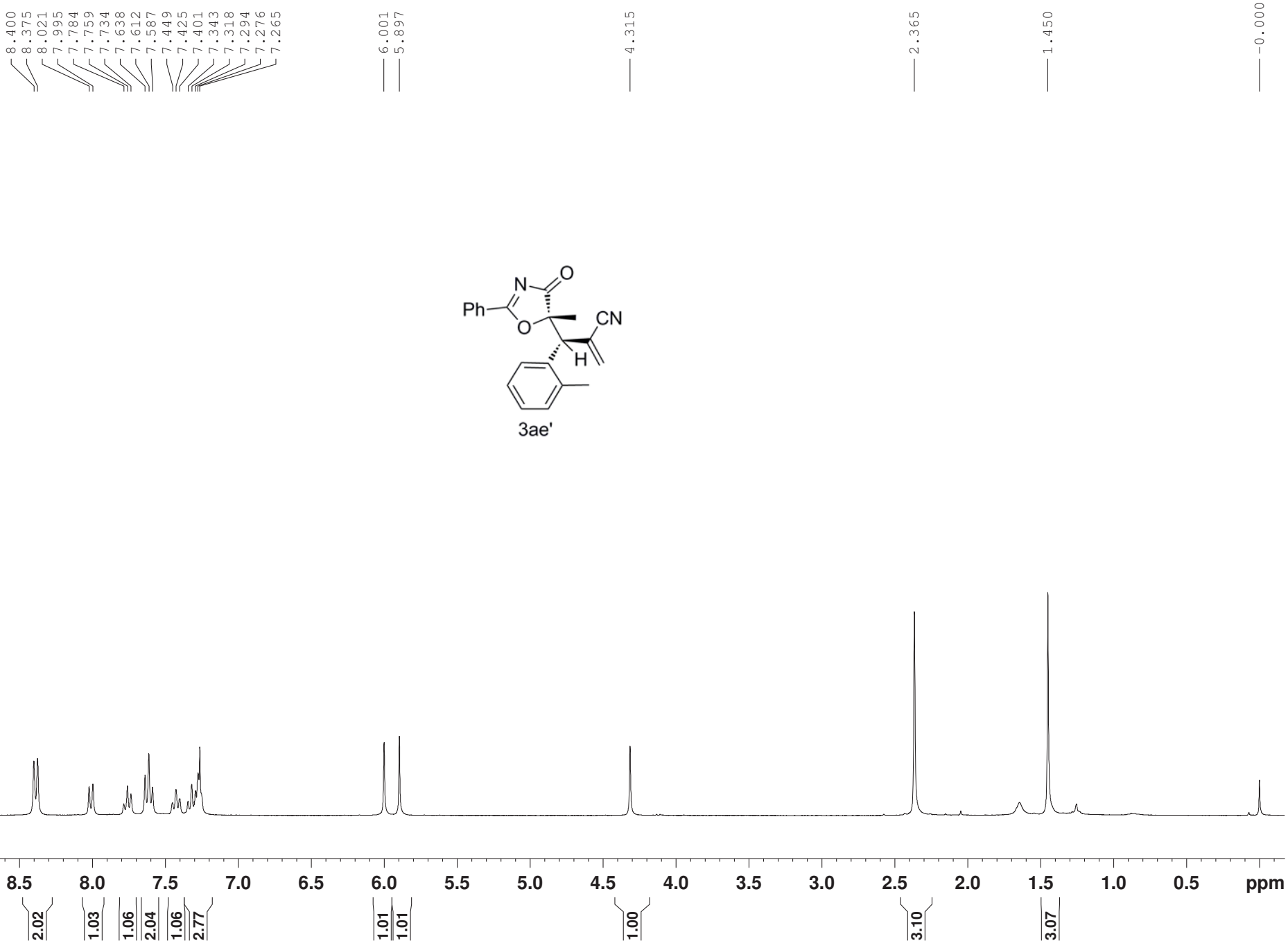
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1.450
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Ph
O
CN
H
3ae'
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.0
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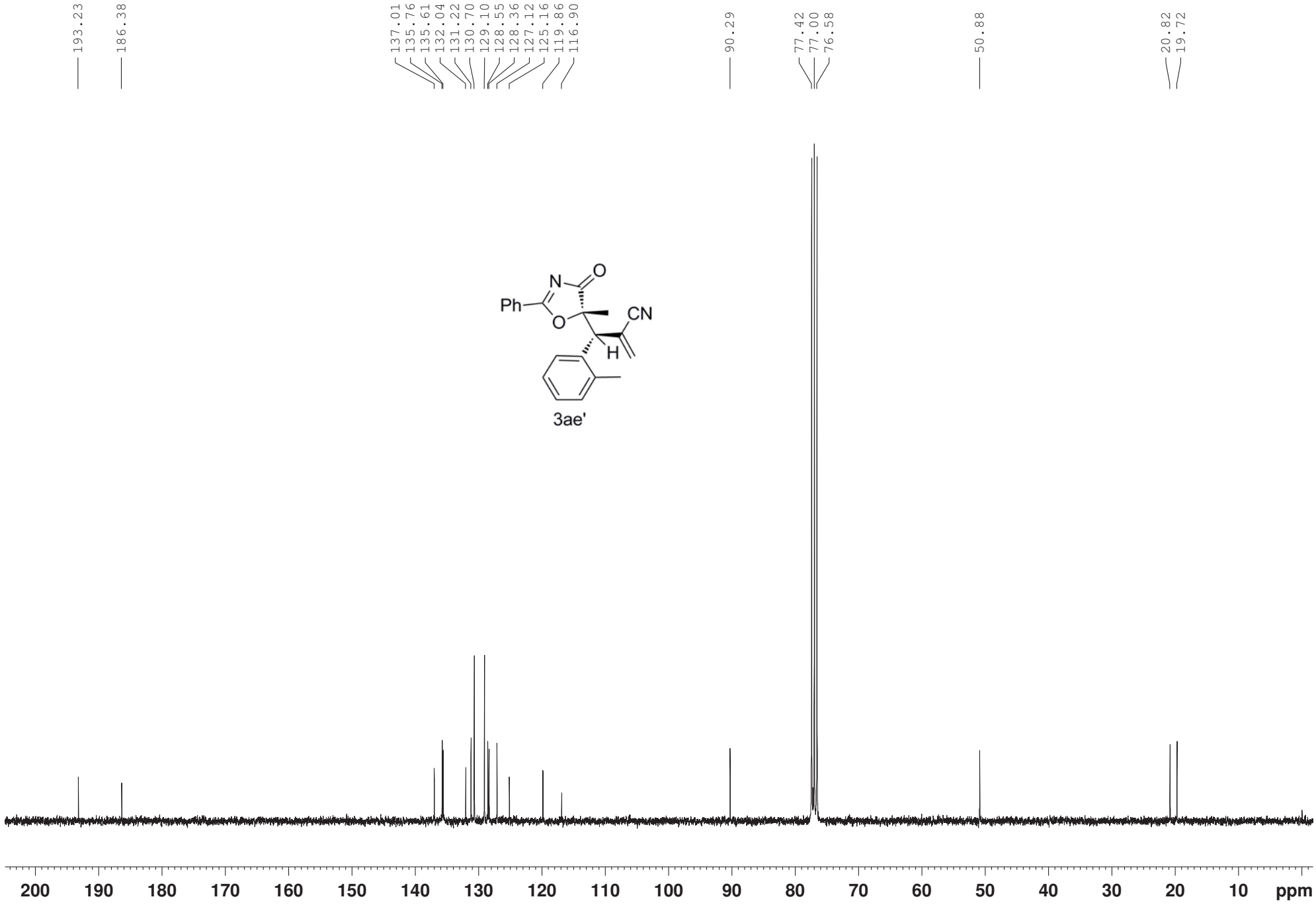
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19.72
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Ph
O
CN
H
3ae'
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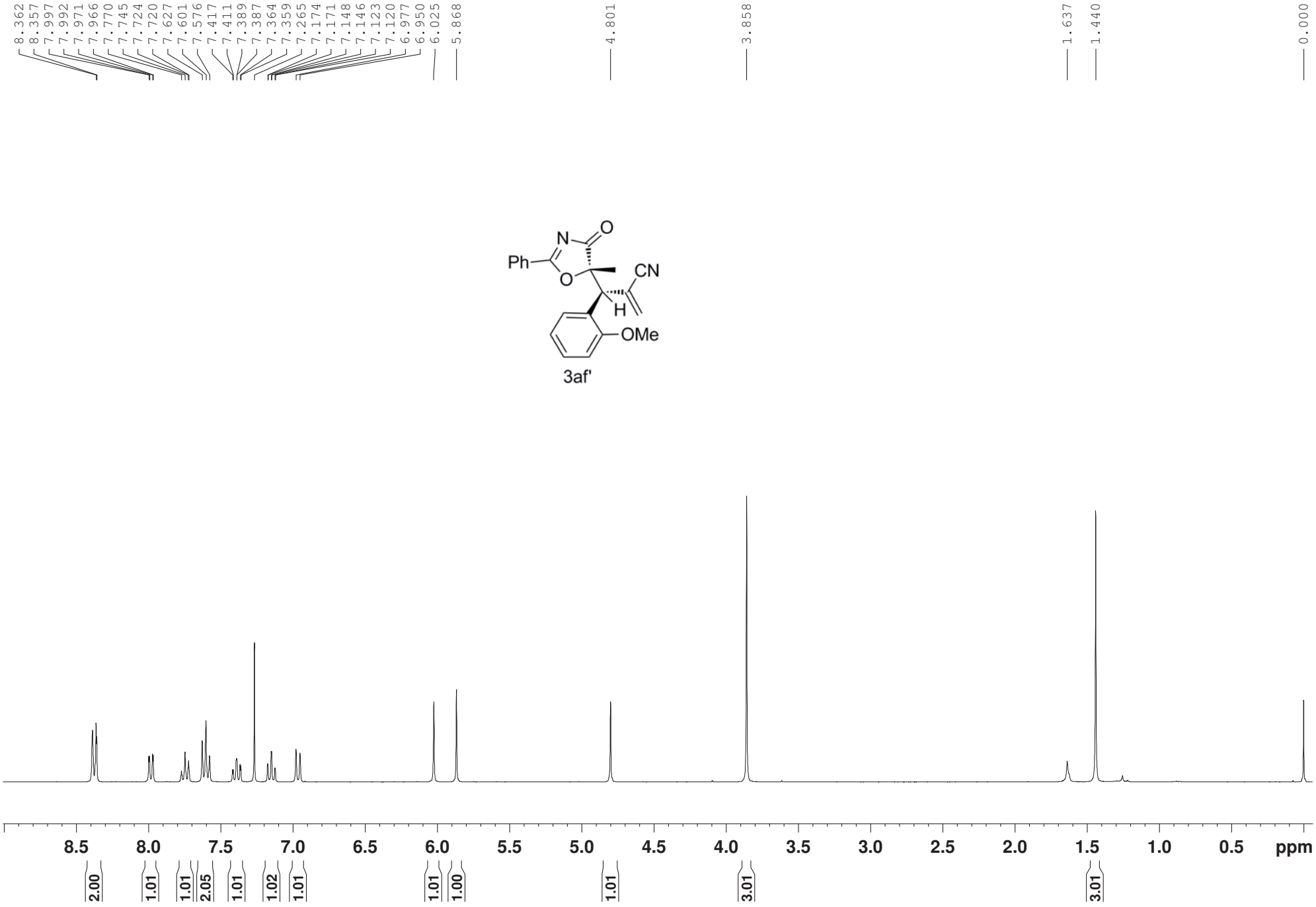
ppm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CN
H
OMe
3af'
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7.5
7.0
6.5
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5.0
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4.0
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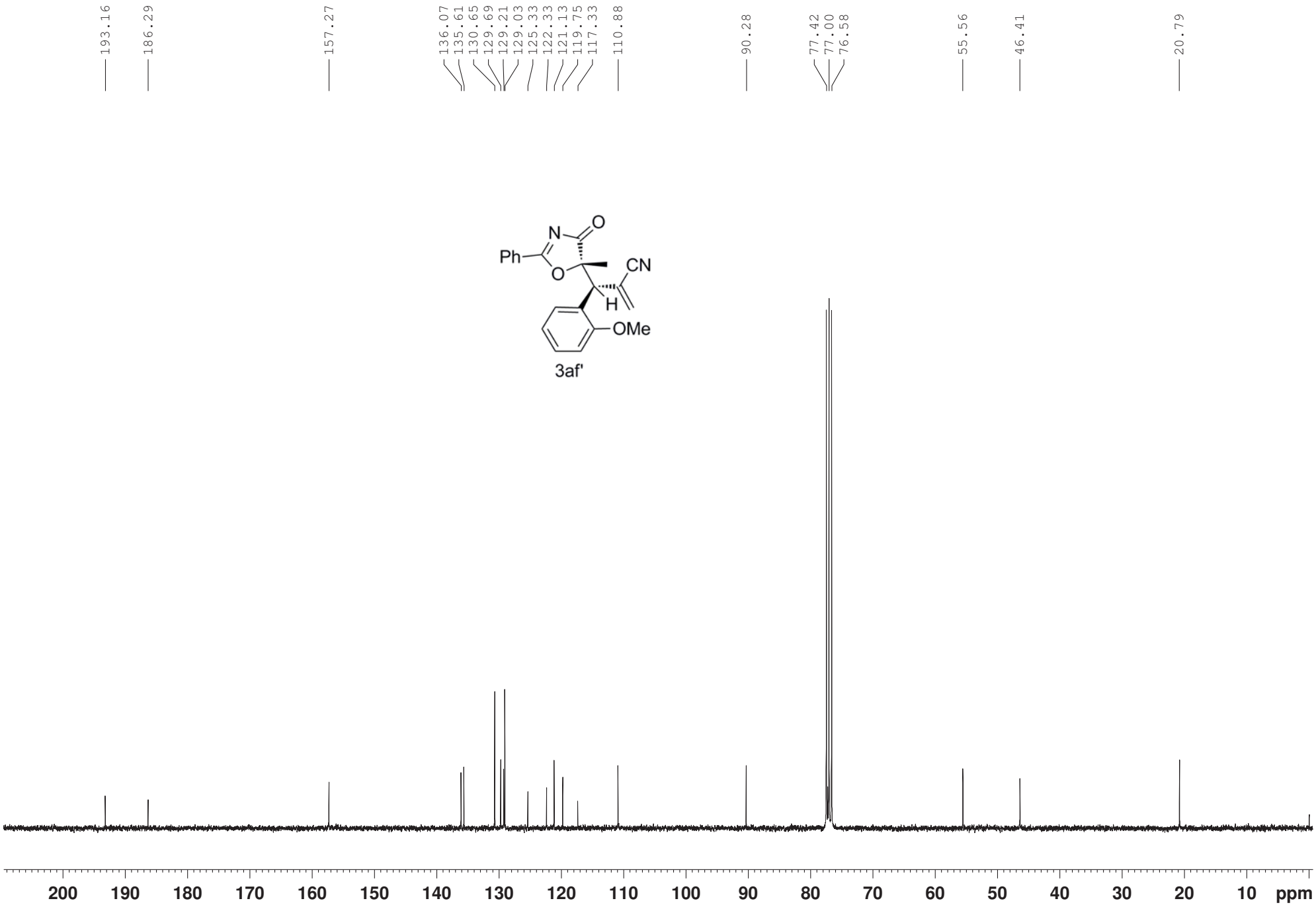
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90.28
77.42
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55.56
46.41
20.79
N
O
Ph
O
CN
H
OMe
3af'
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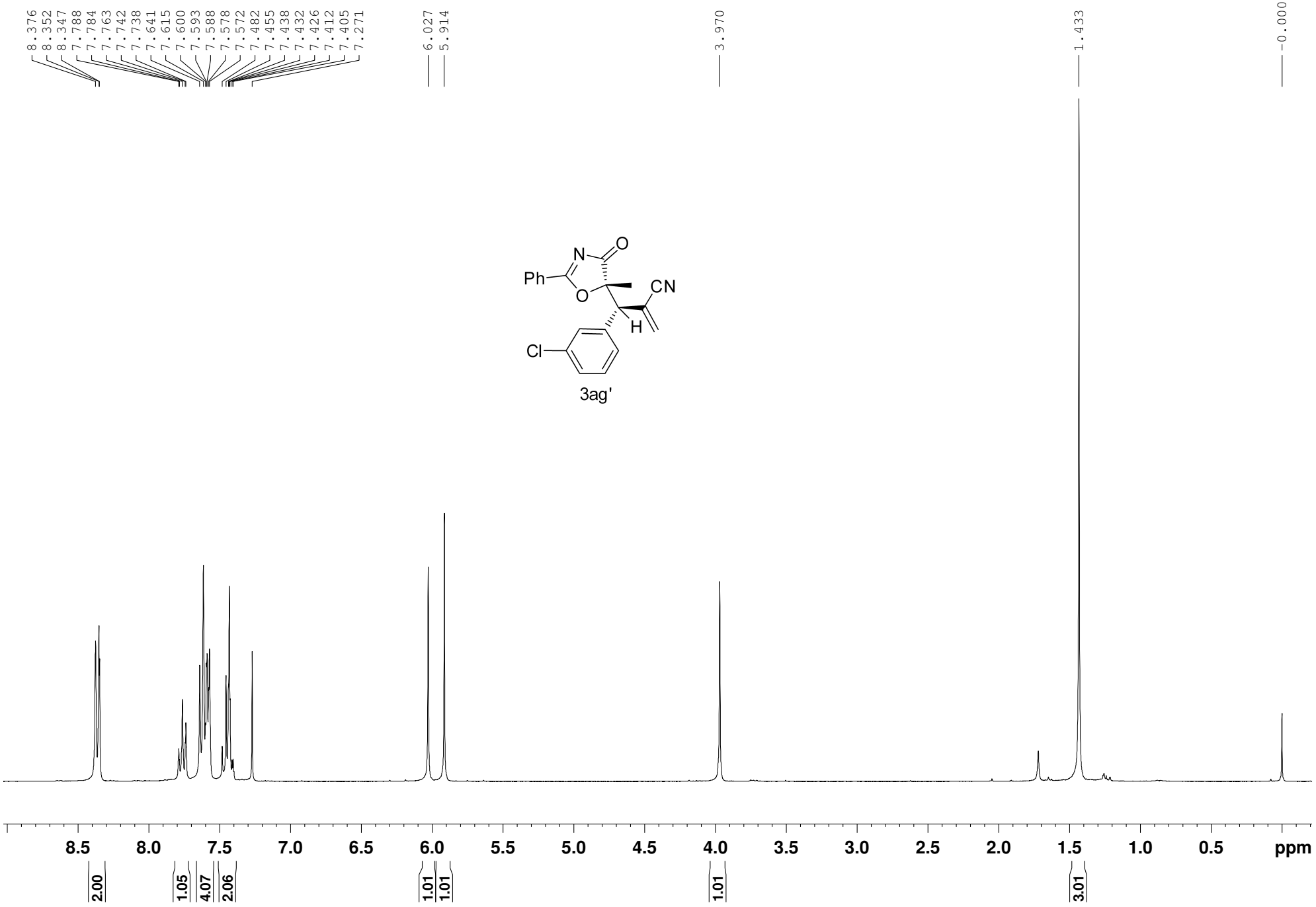
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7.578
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6.027
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O
CN
H
Cl
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7.5
7.0
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6.0
5.5
5.0
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4.0
3.5
3.0
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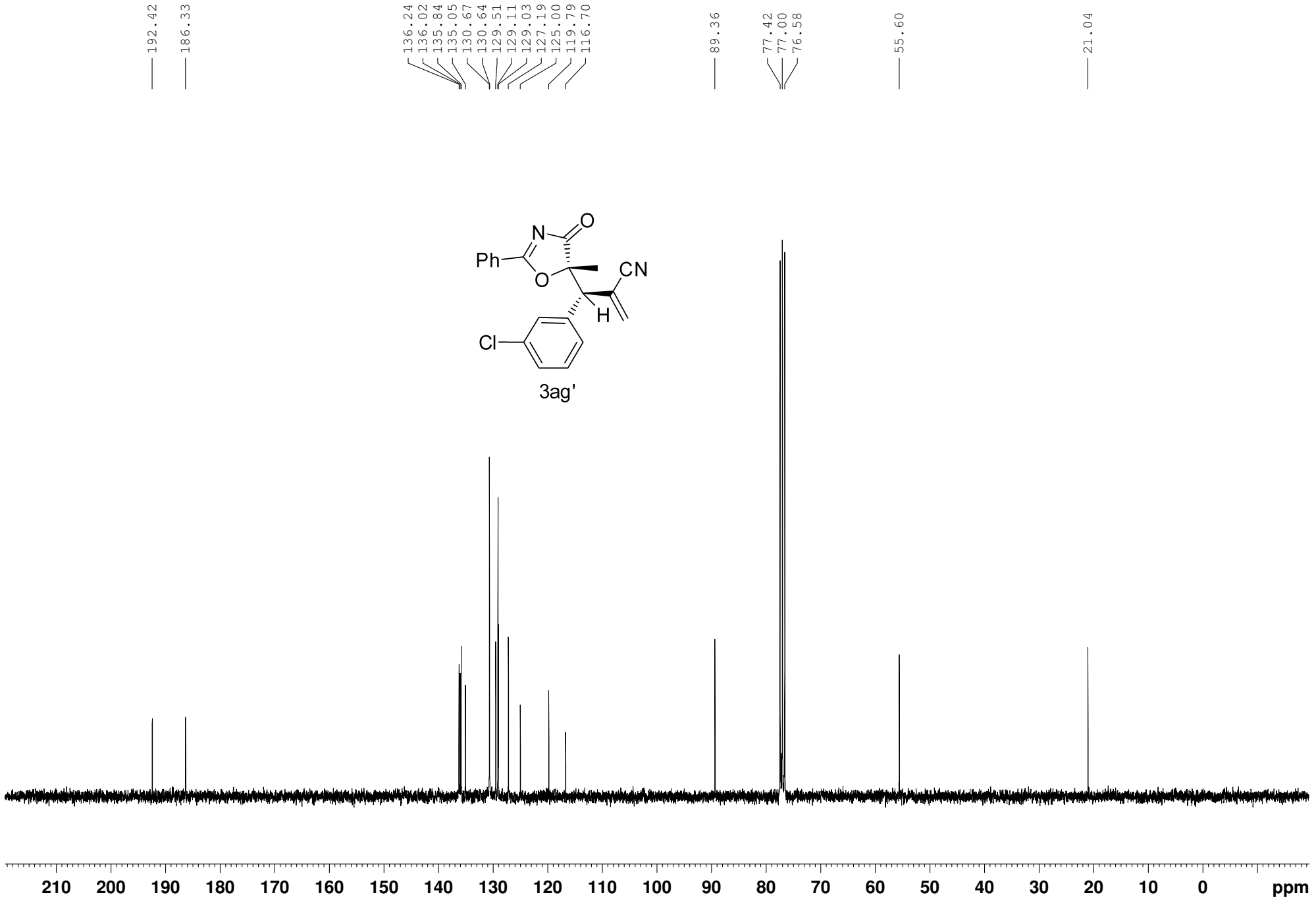
3.01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O
Ph
O
CN
H
Cl
3ag'
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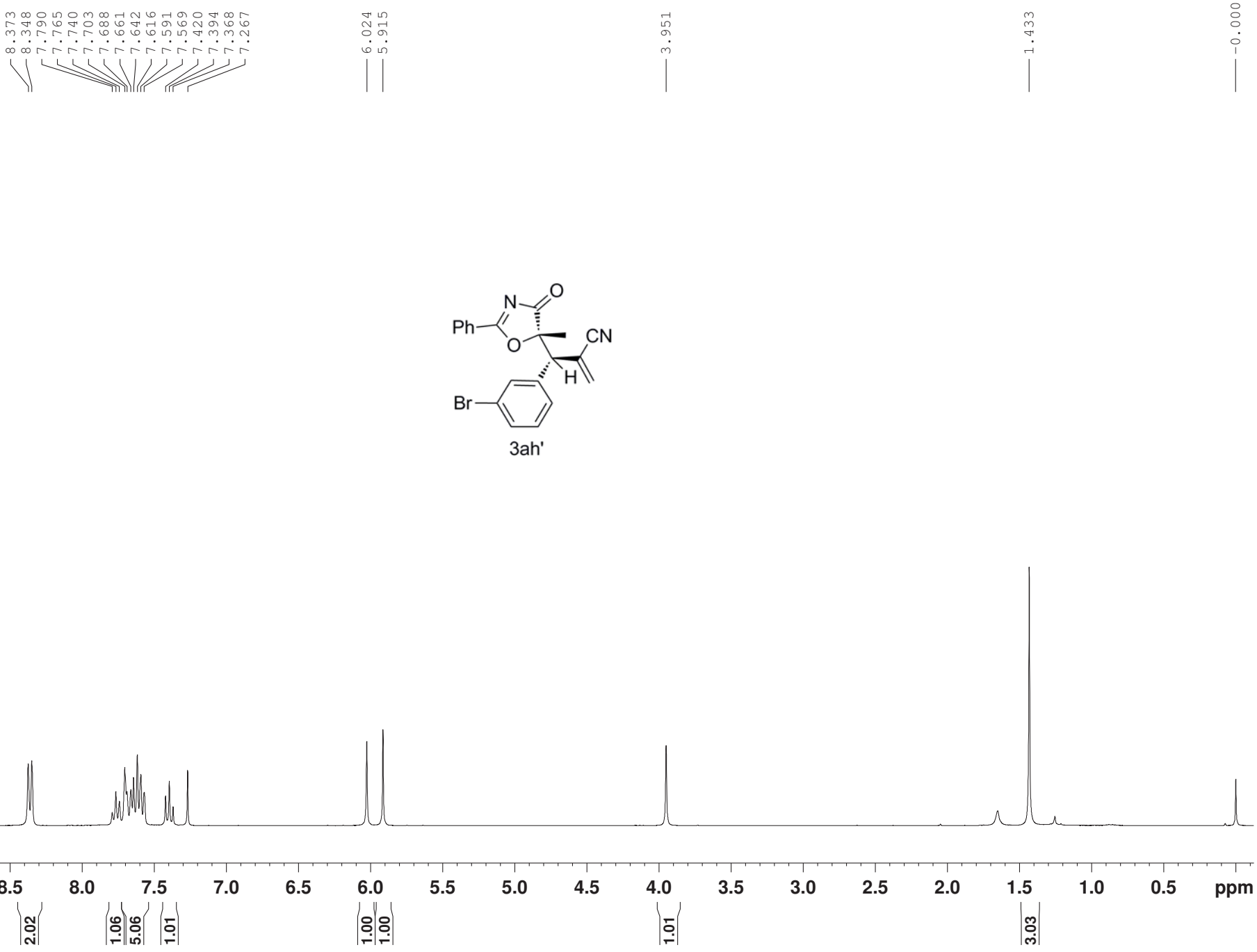
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CN
H
Br
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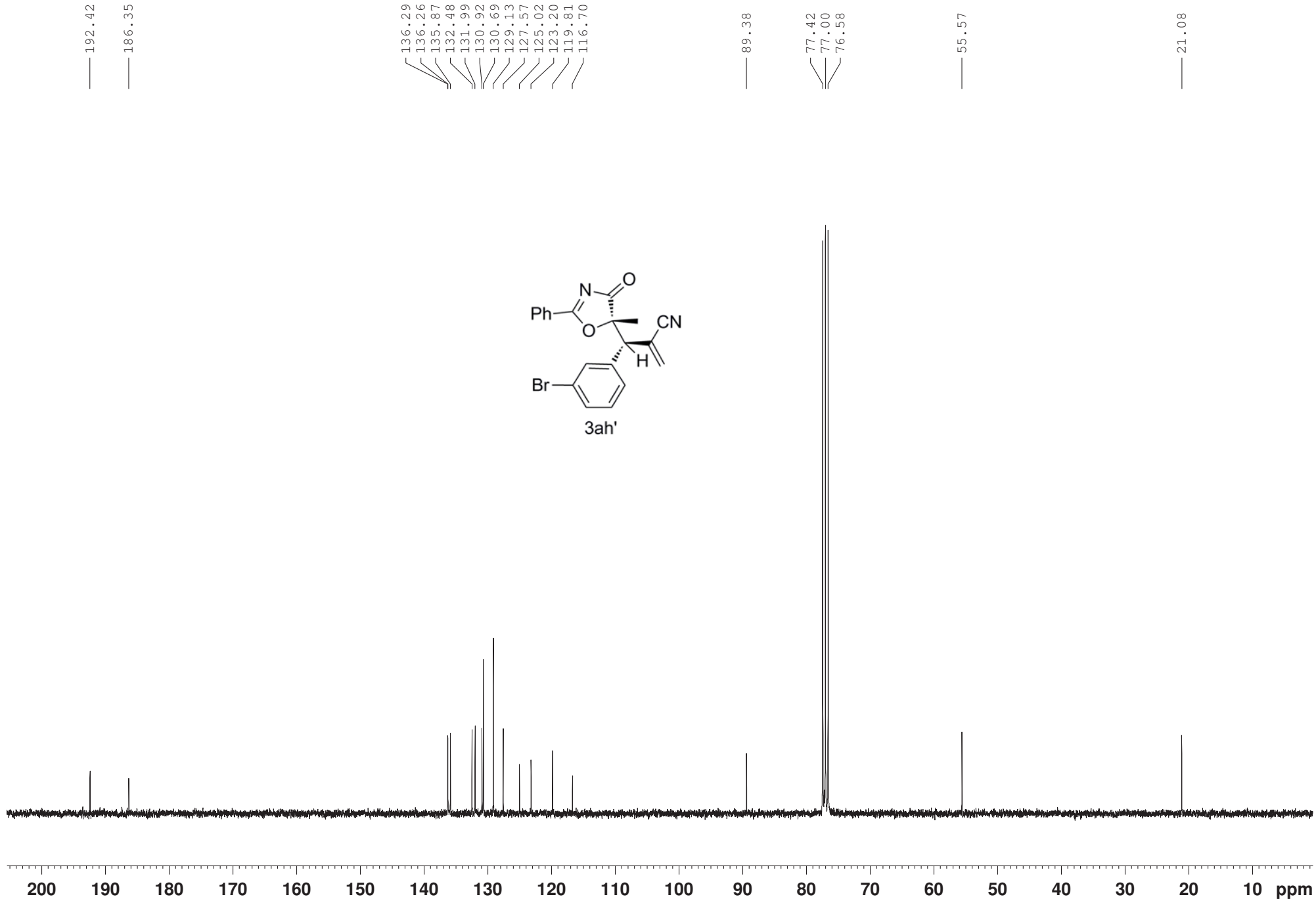
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21.08
N
O
Ph
O
CN
H
Br
3ah'
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10
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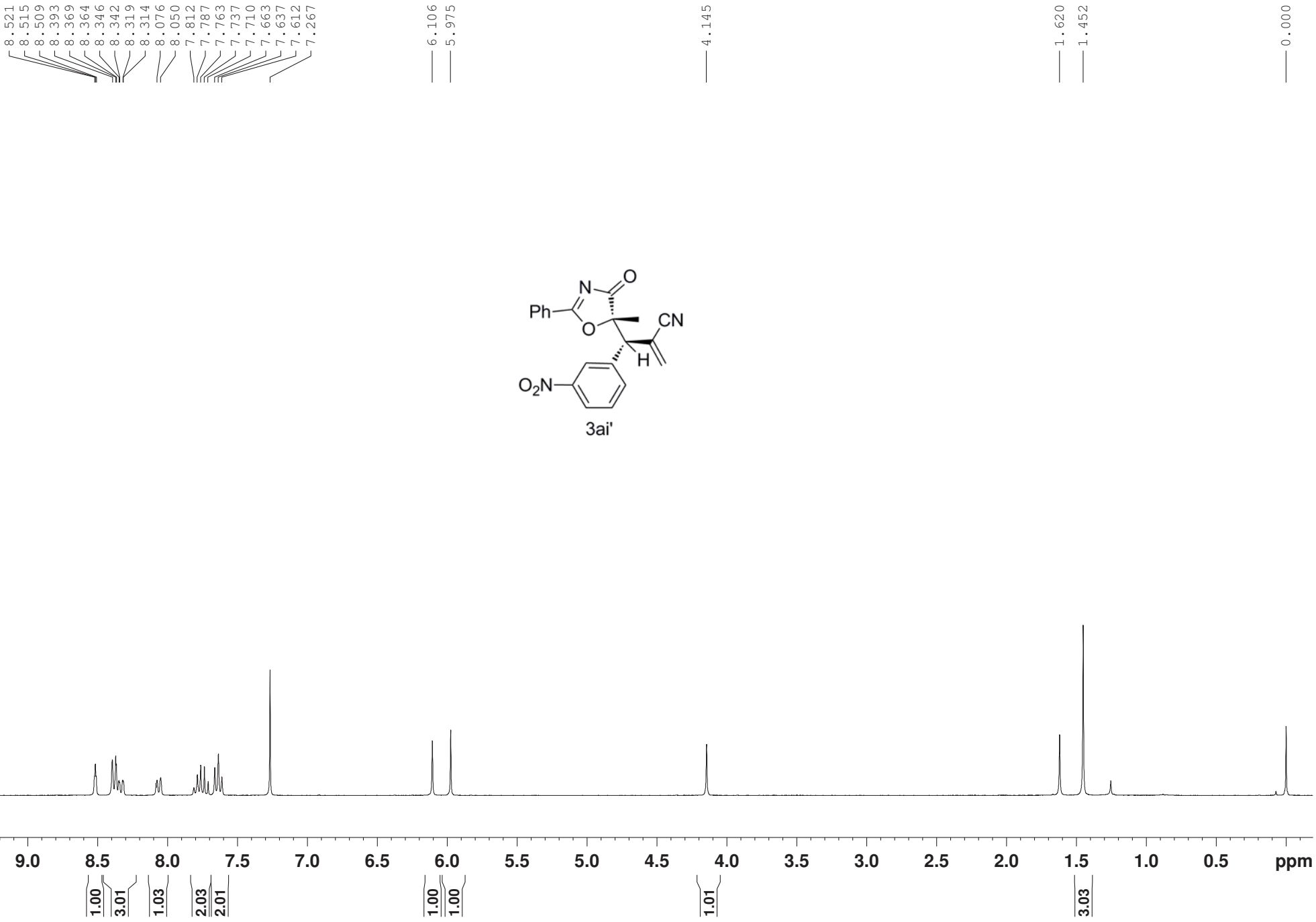
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4.145
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1.452
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CN
H
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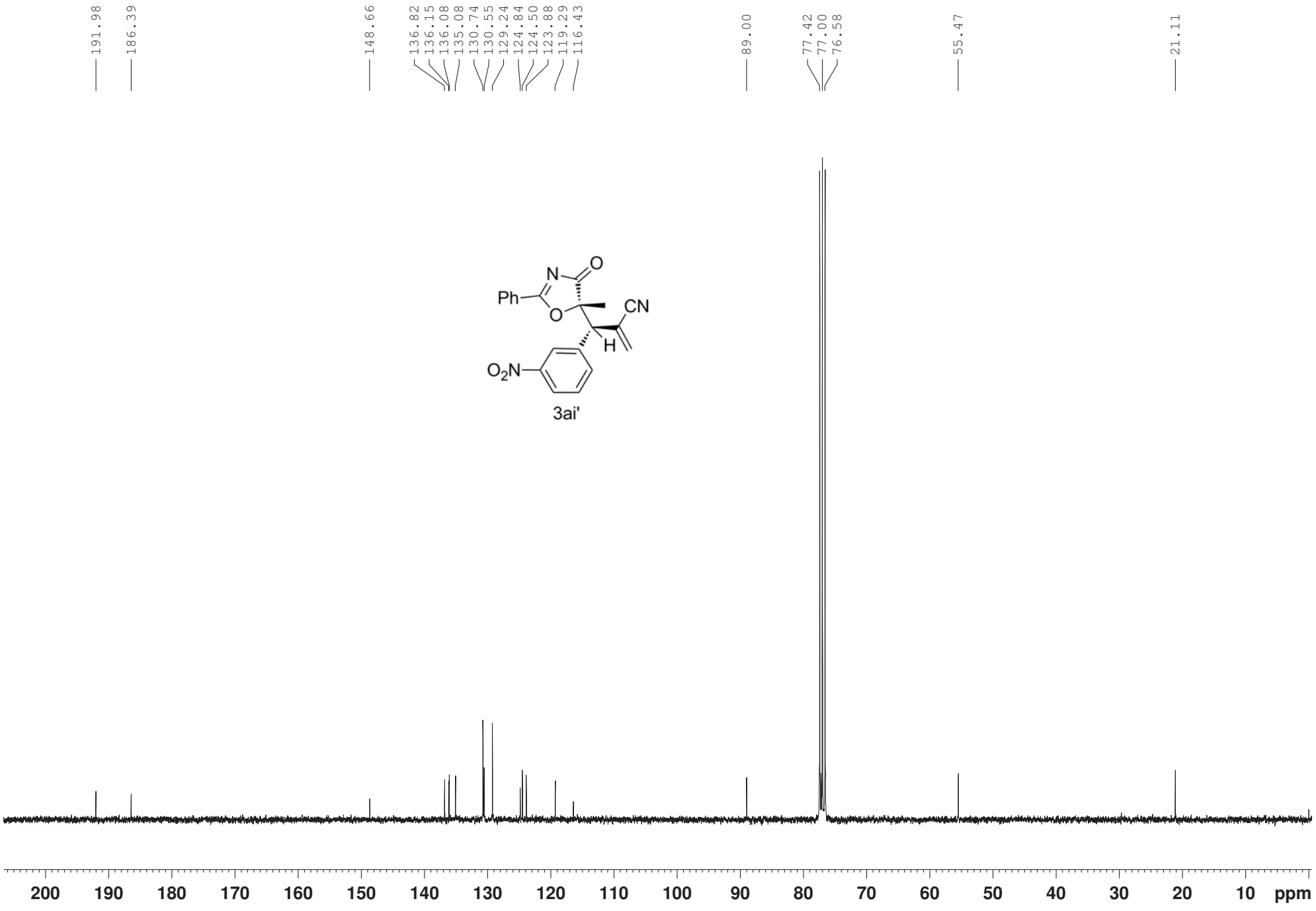
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Ph
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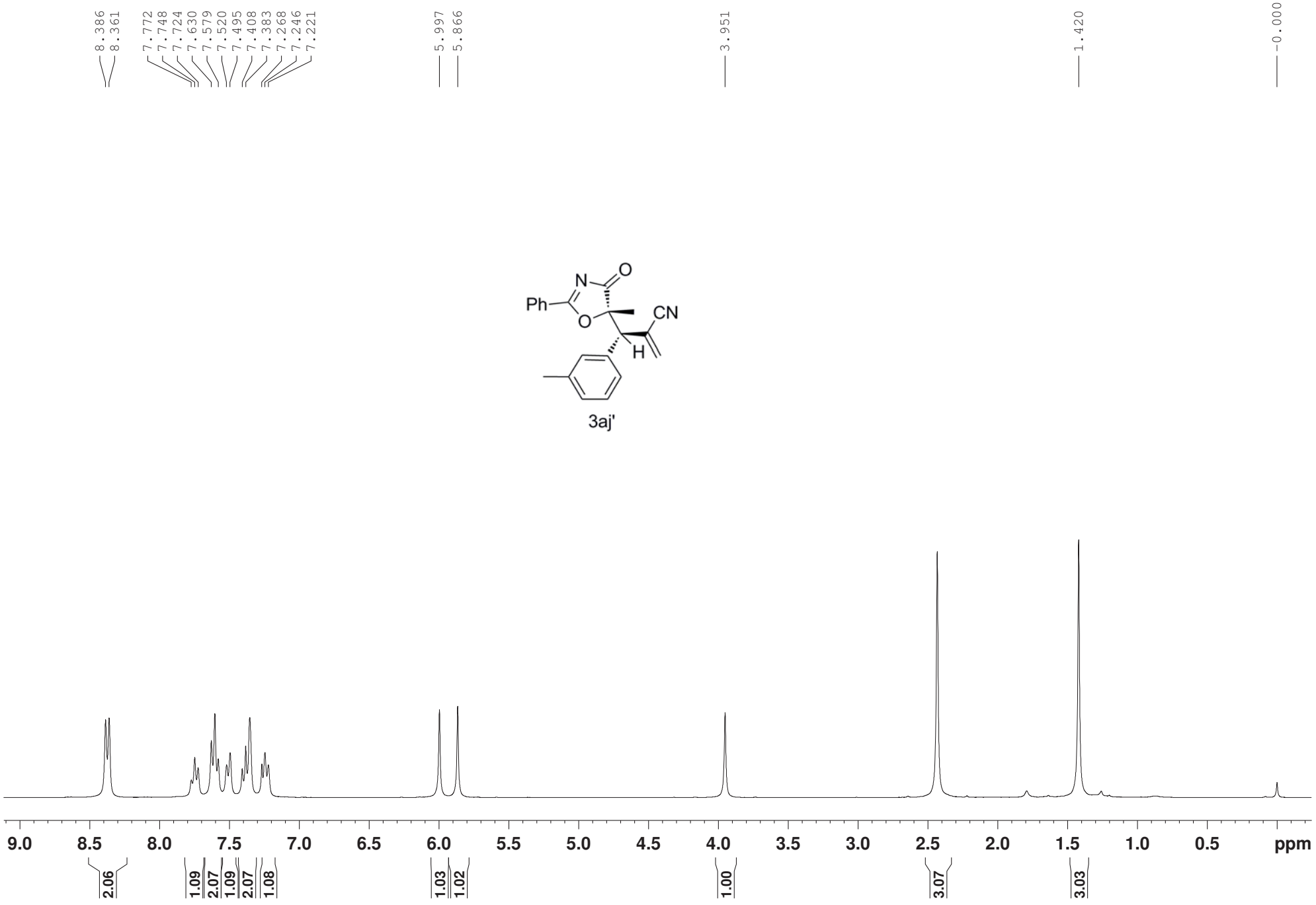
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O
CN
H
3aj'
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3.07
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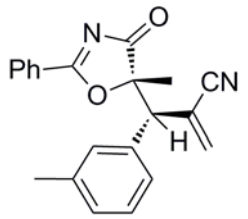

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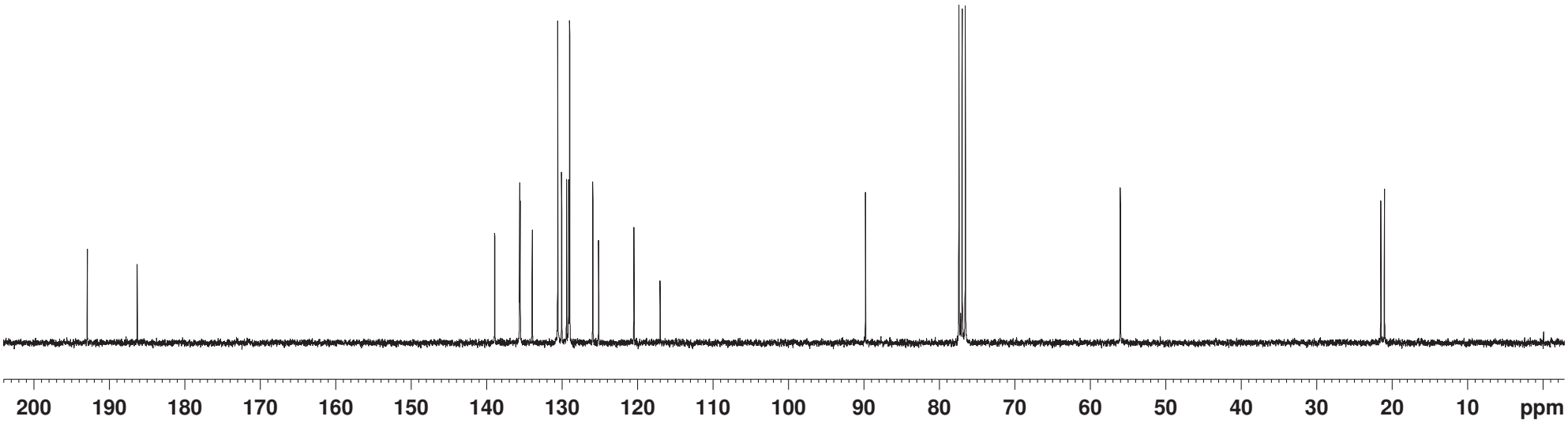

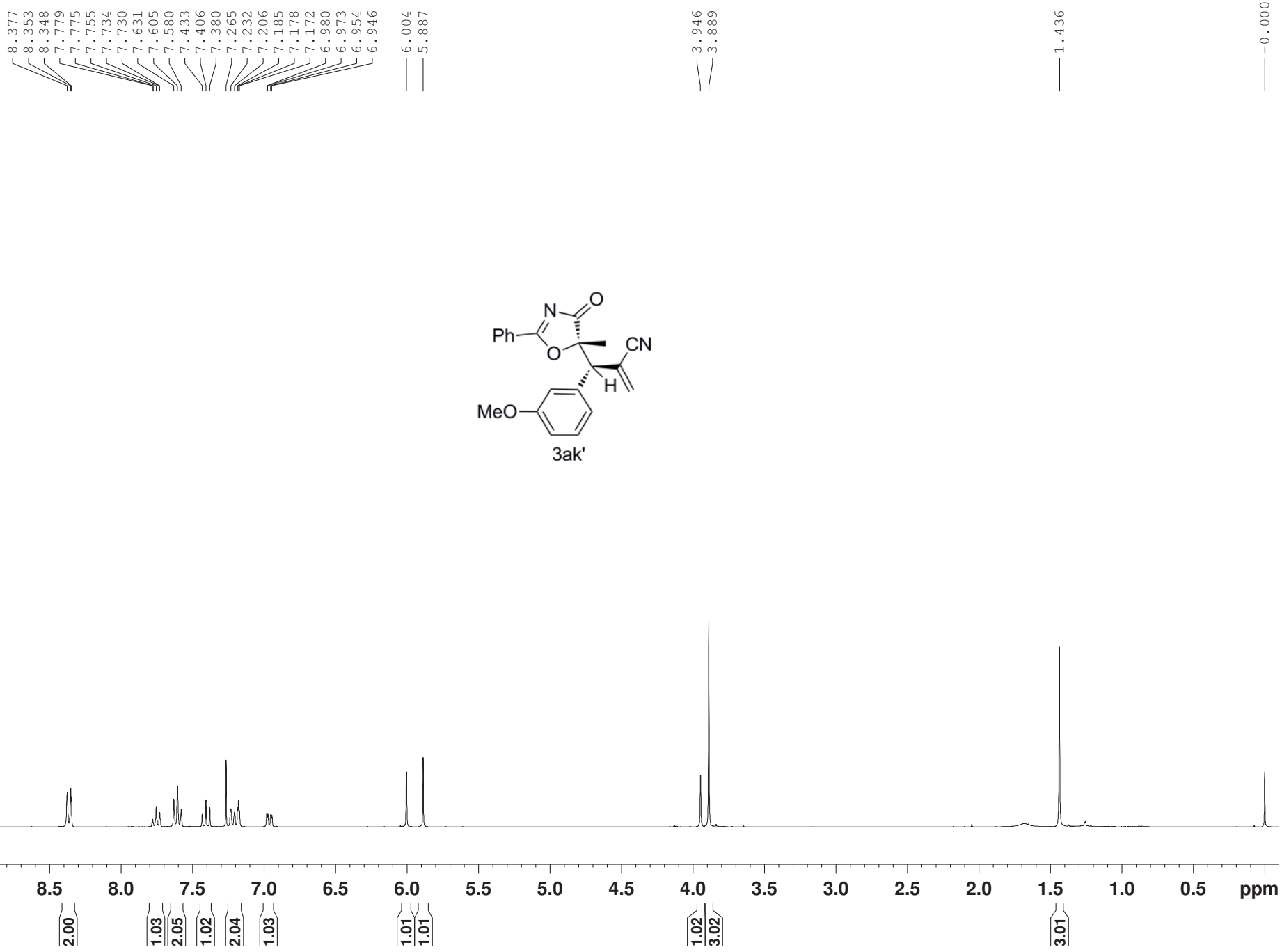
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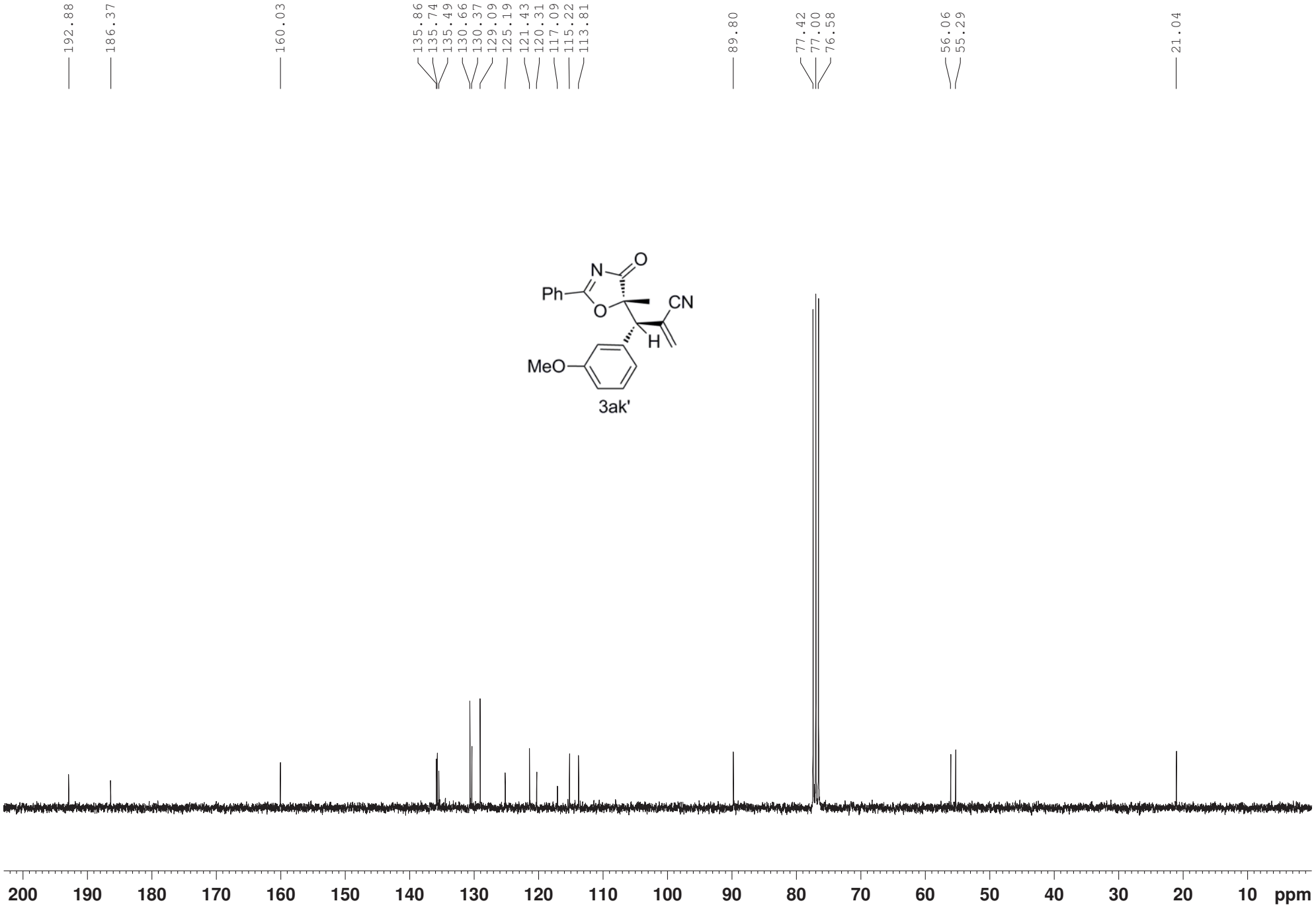
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O
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O
CN
H
MeO
3ak'
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130
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40
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20
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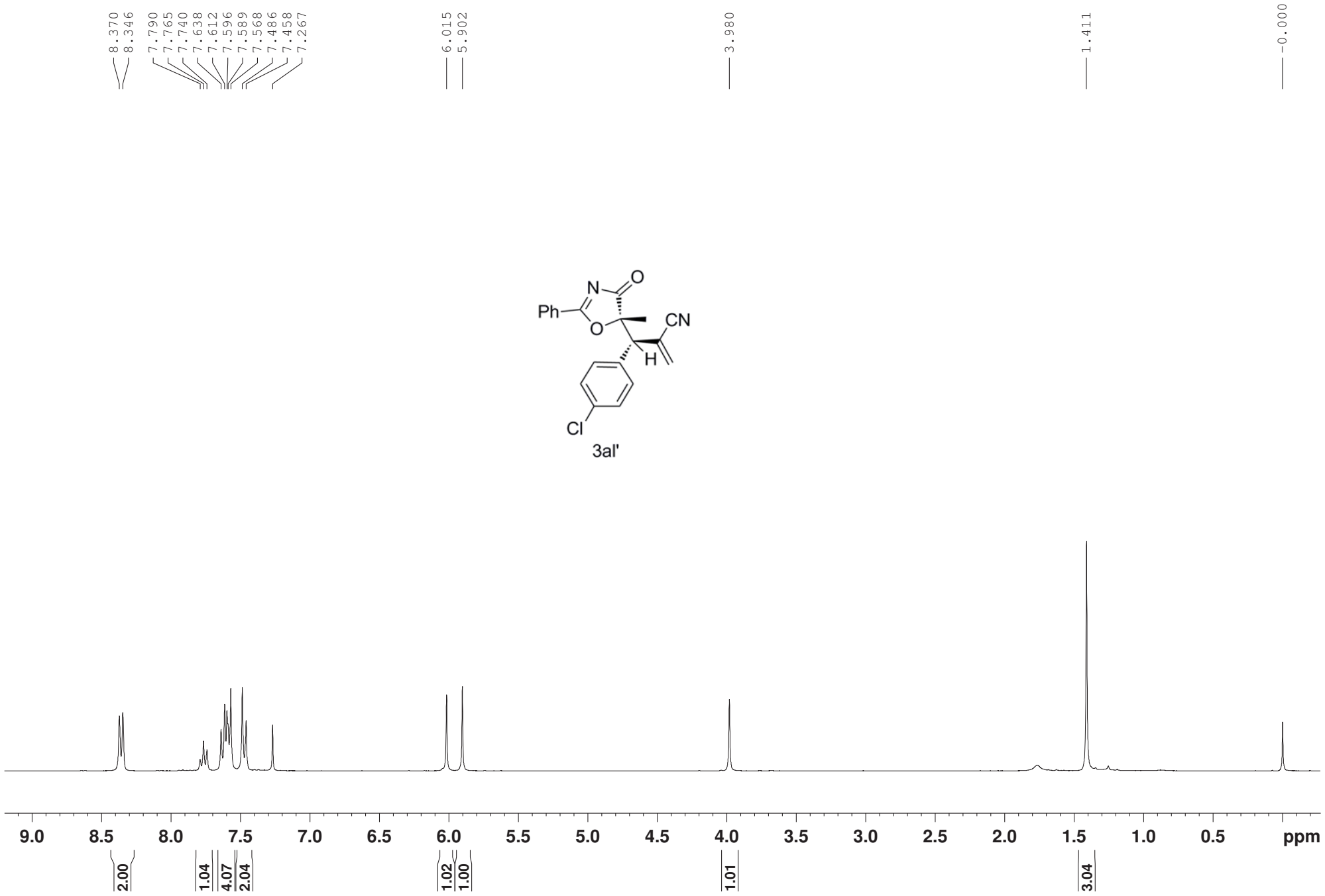
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7.458
7.267
6.015
5.902
3.980
1.411
0.000
N
O
Ph
O
CN
H
Cl
3al'
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
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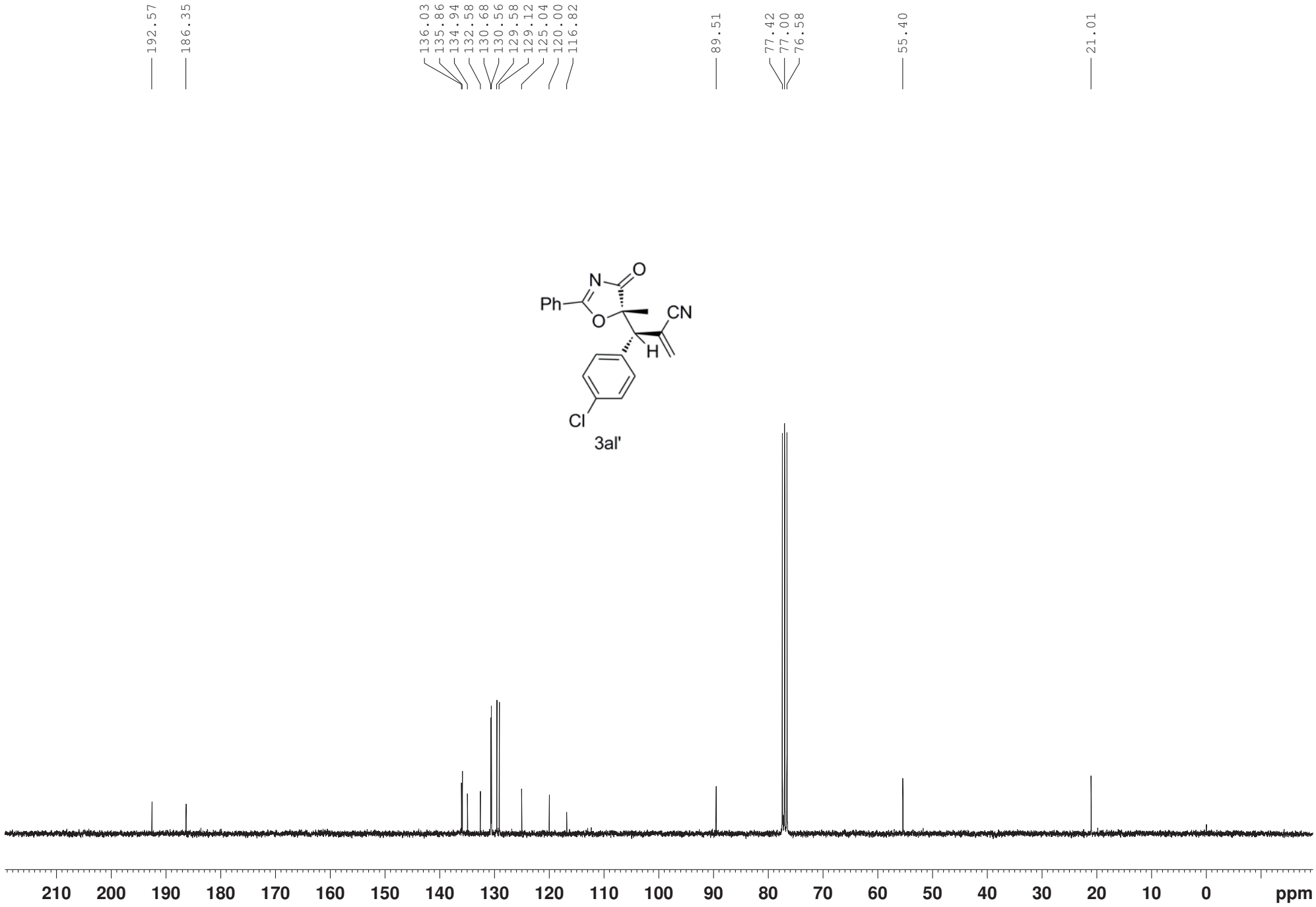
3.04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89.51
77.42
77.00
76.58
55.40
21.01
N
O
Ph
O
CN
H
Cl
3al'
210
200
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100
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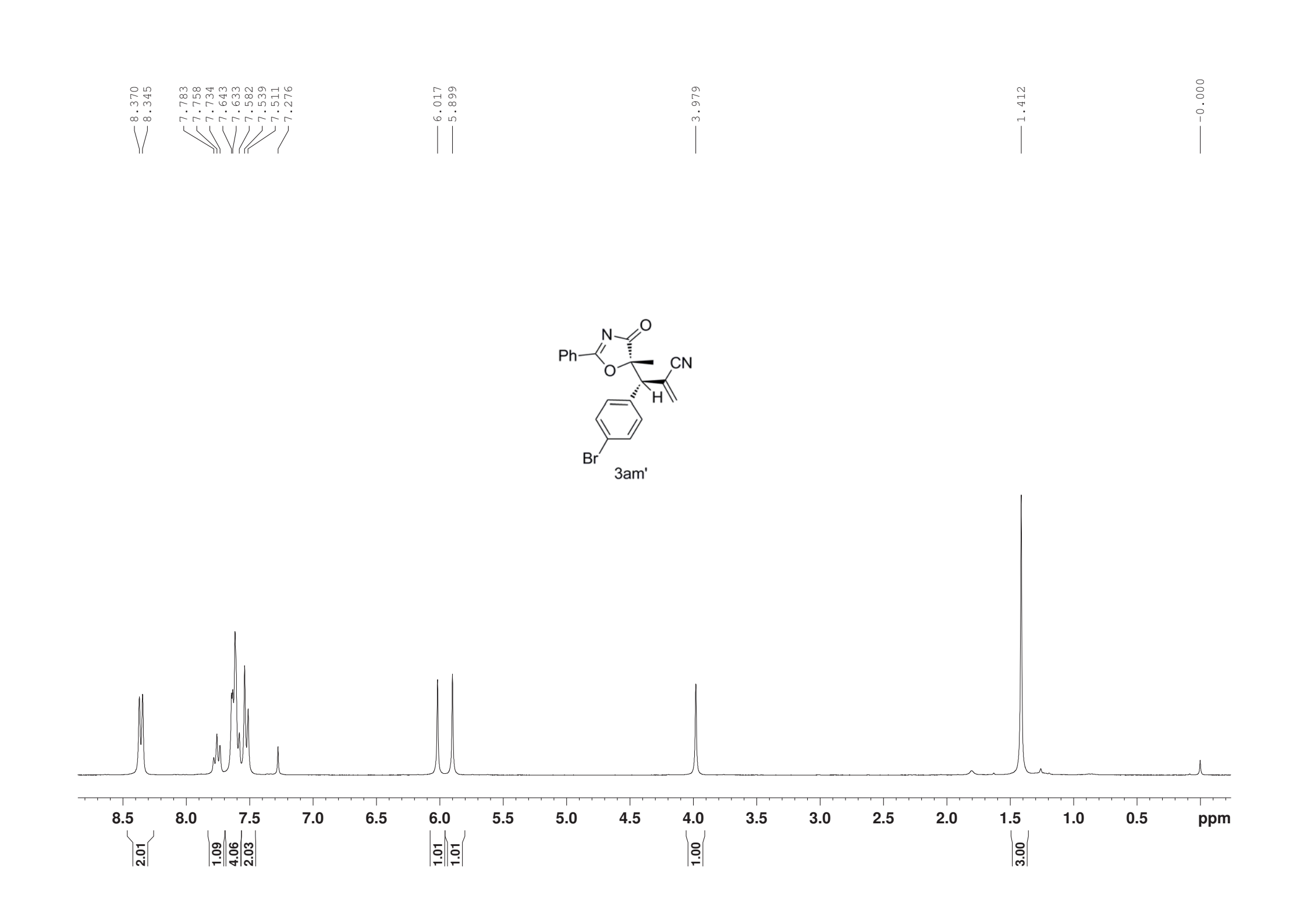
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O
Ph
O
CN
H
Br
3am'
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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2.0
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1.0
0.5
ppm
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4.06
2.03
1.01
1.01
1.00
3.00

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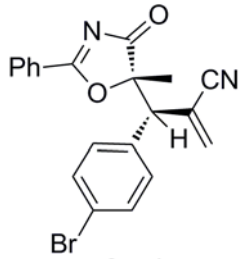

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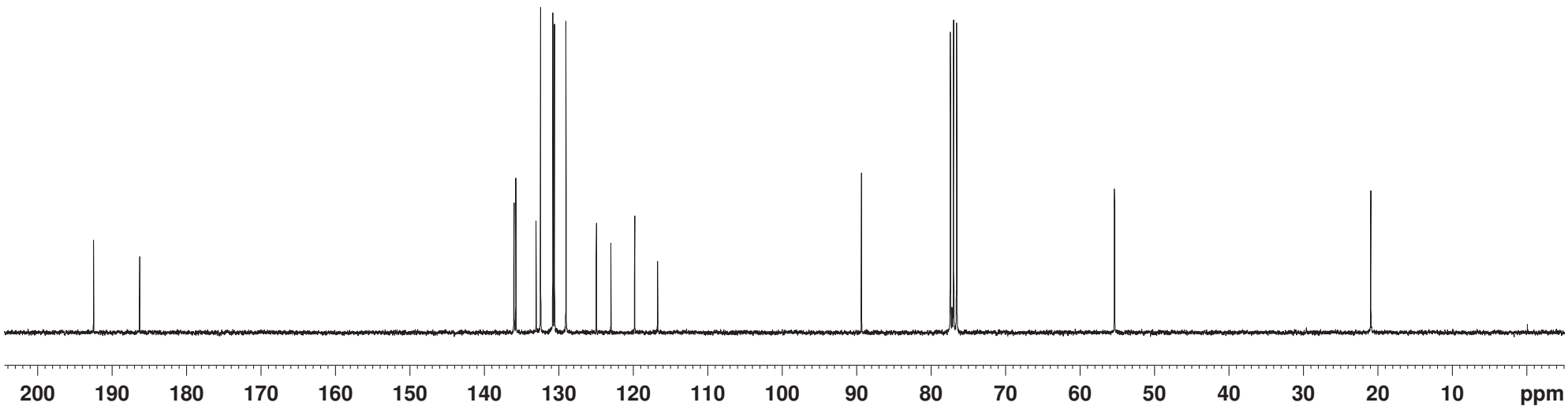

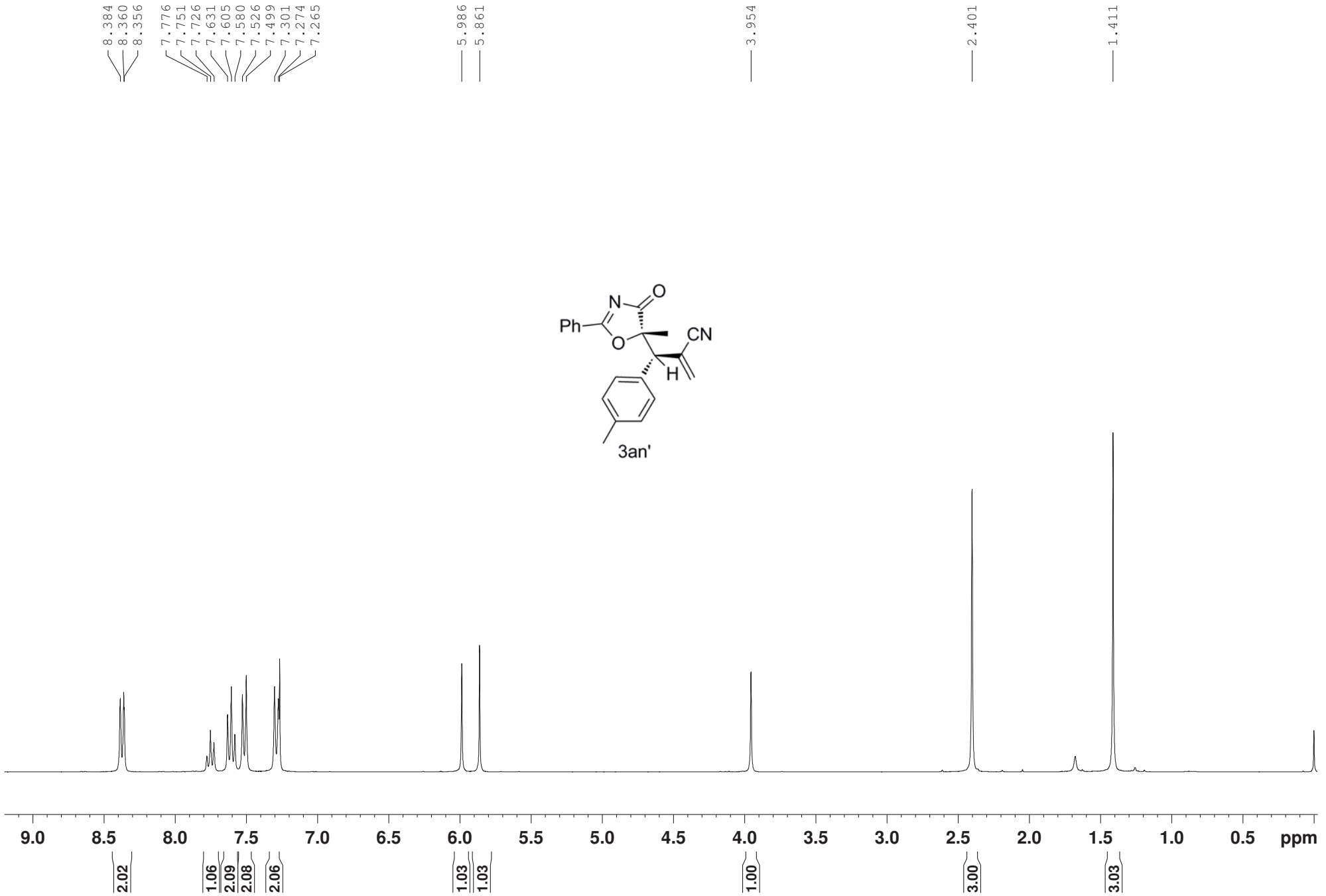
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7.274
7.265
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5.861
3.954
2.401
1.411
Ph
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O
O
CN
H
3an'
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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2.0
1.5
1.0
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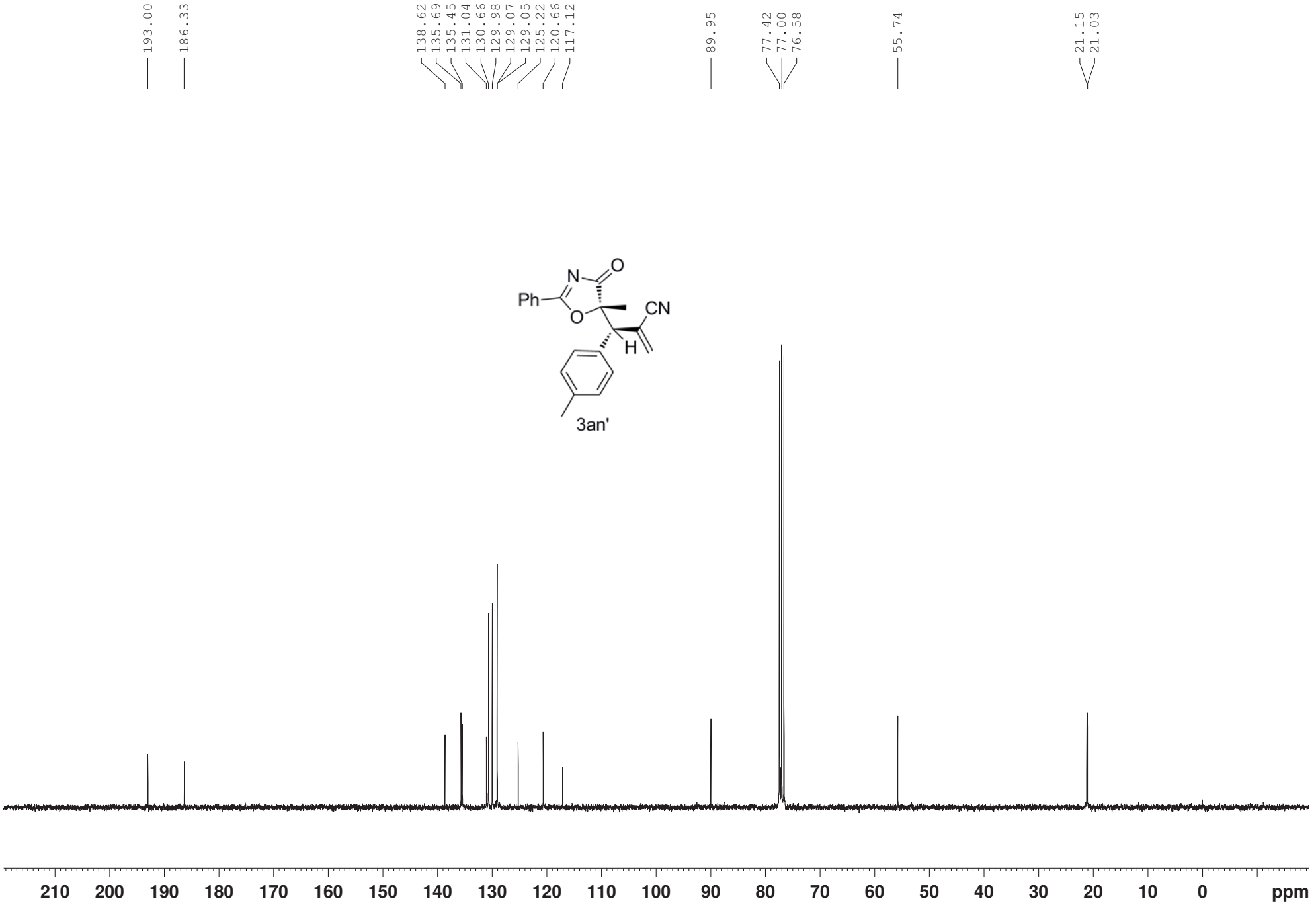
3.00
3.03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77.42
77.00
76.58
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21.15
21.03
N
O
Ph
O
CN
H
3an'
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200
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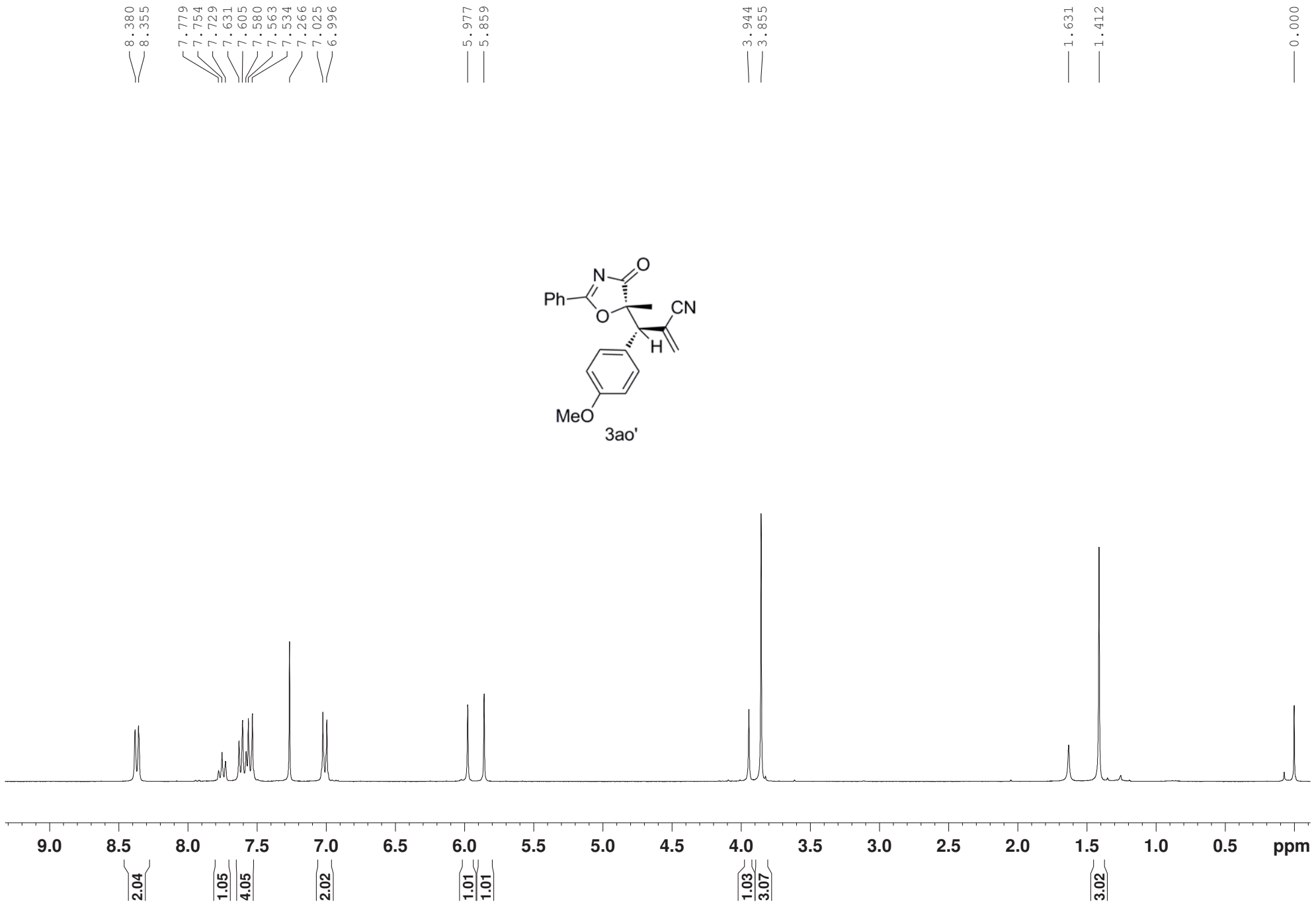
ppm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7.025
6.996
5.977
5.859
3.944
3.855
1.631
1.412
0.000
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N
O
O
CN
H
MeO
3ao'
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8.5
8.0
7.5
7.0
6.5
6.0
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5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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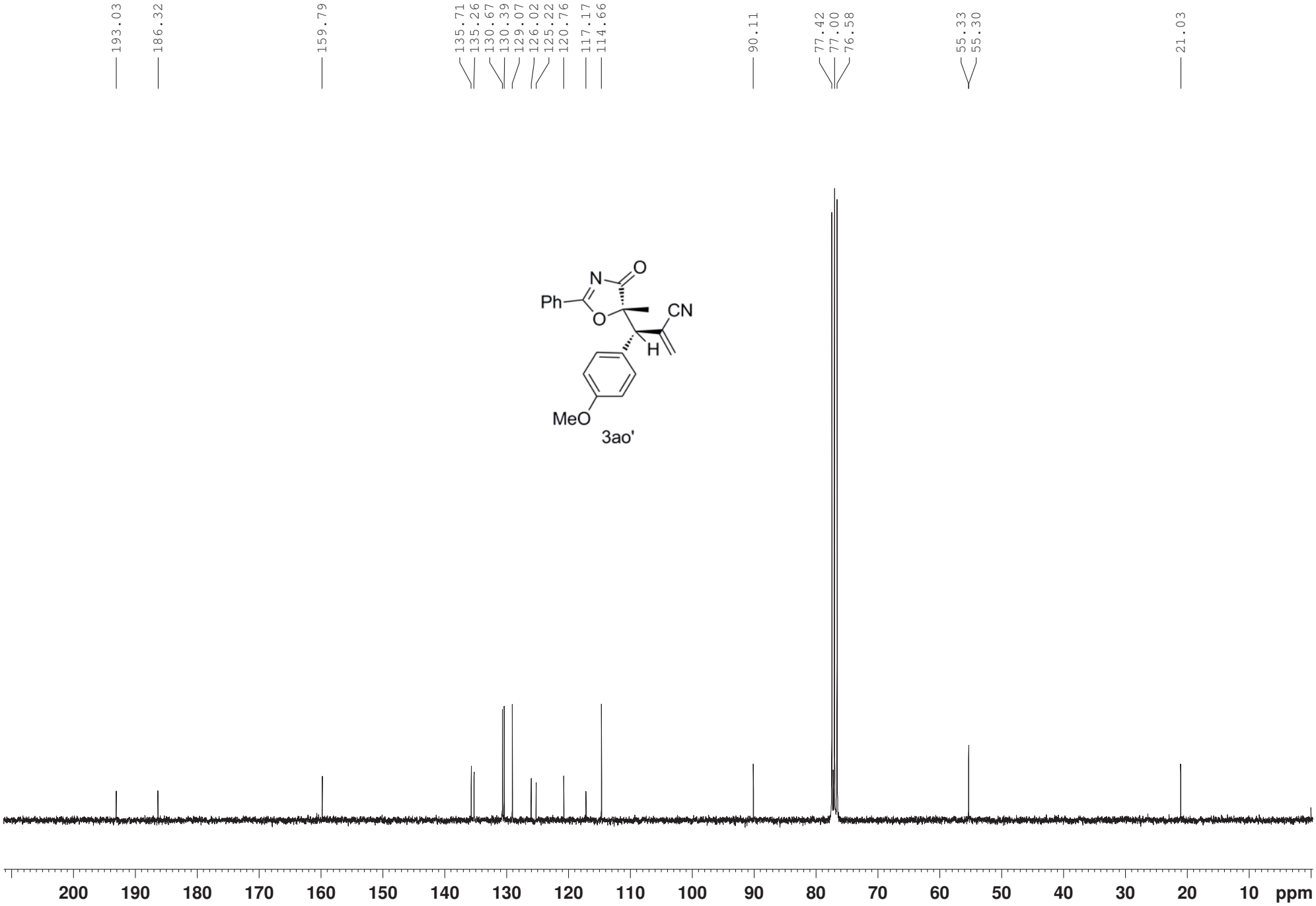
1.05
4.05
2.02
1.01
1.01
1.03
3.07
3.02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114.66
90.11
77.42
77.00
76.58
55.33
55.30
21.03
N
O
Ph
O
CN
H
MeO
3ao'
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140
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70
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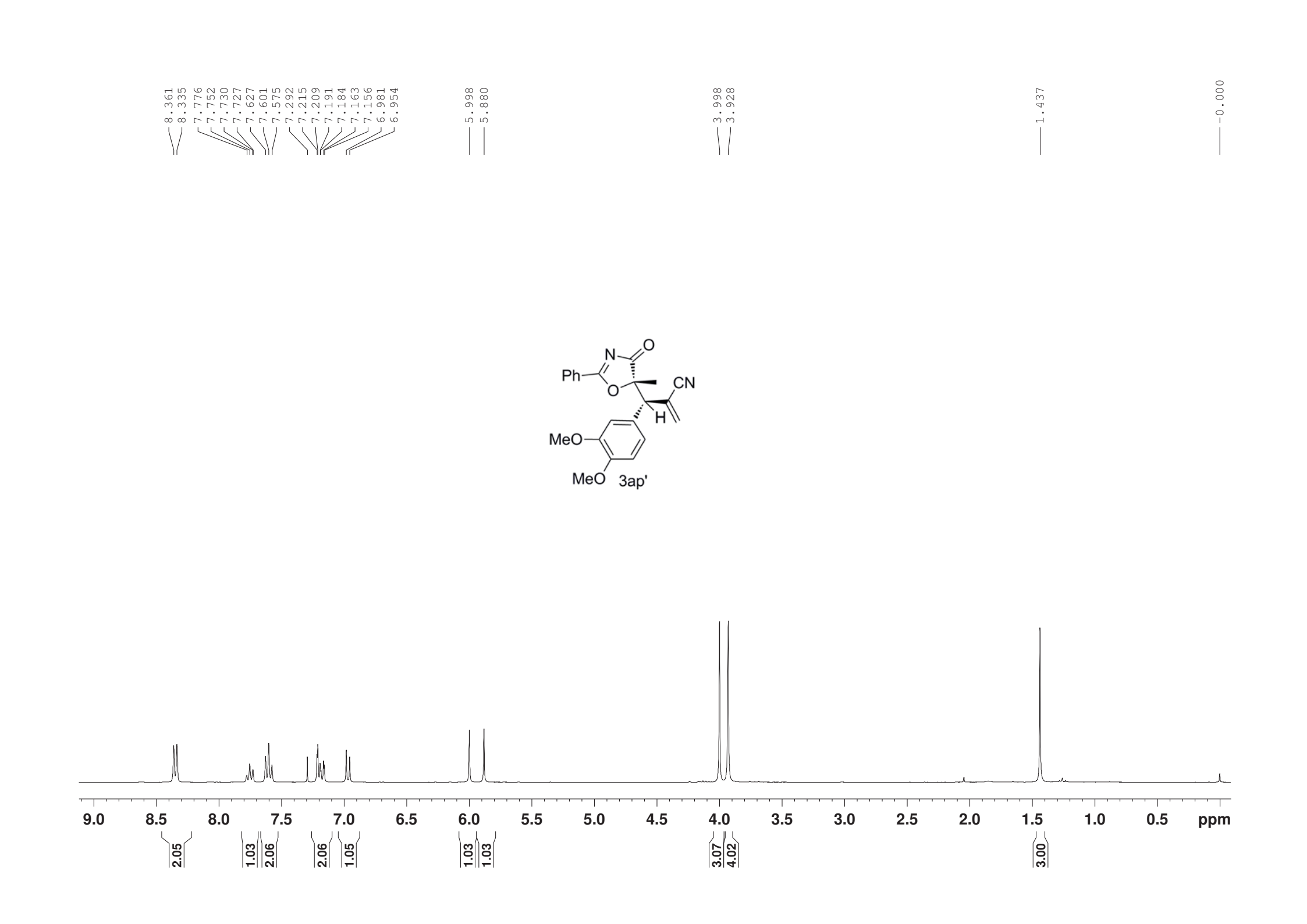
10
ppm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7.191
7.184
7.163
7.156
6.981
6.954
5.998
5.880
3.998
3.928
1.437
0.000
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O
Ph
O
CN
H
MeO
MeO
3ap'
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8.0
7.5
7.0
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6.0
5.5
5.0
4.5
4.0
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3.0
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1.0
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1.03
2.06
2.06
1.05
1.03
1.03
3.07
4.02
3.00

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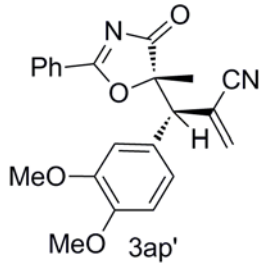

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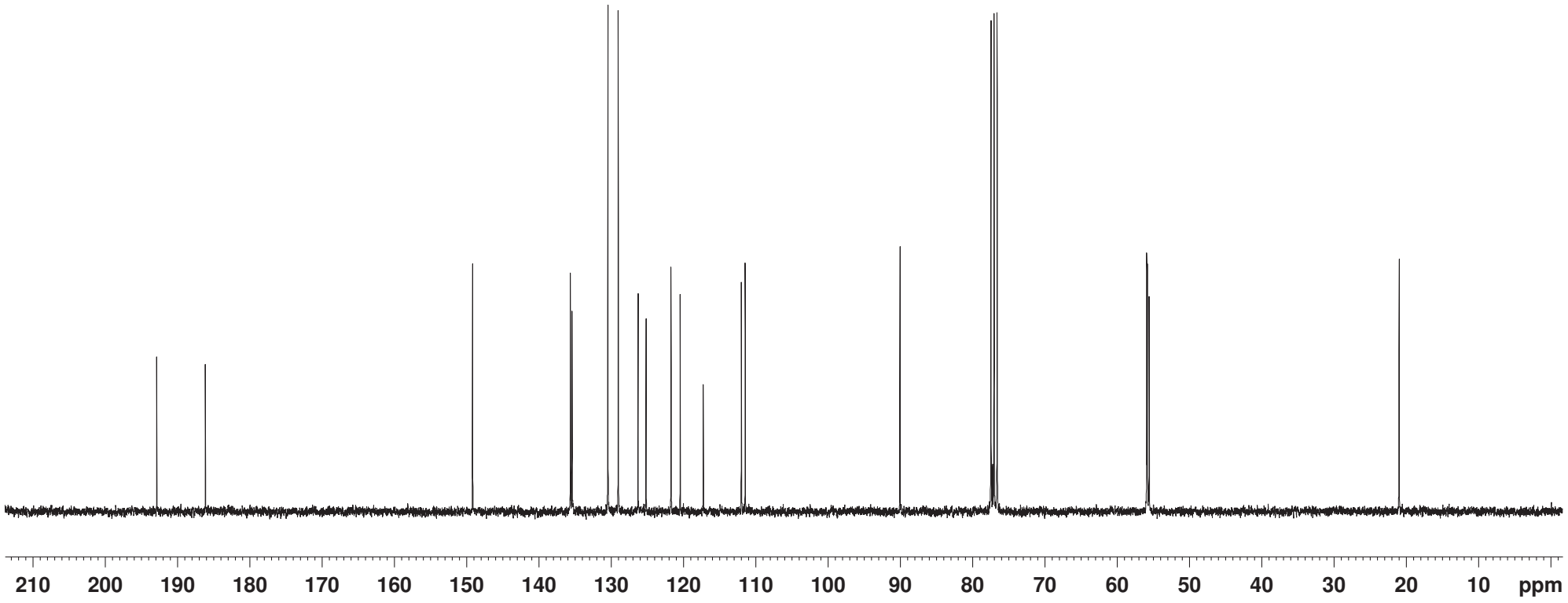

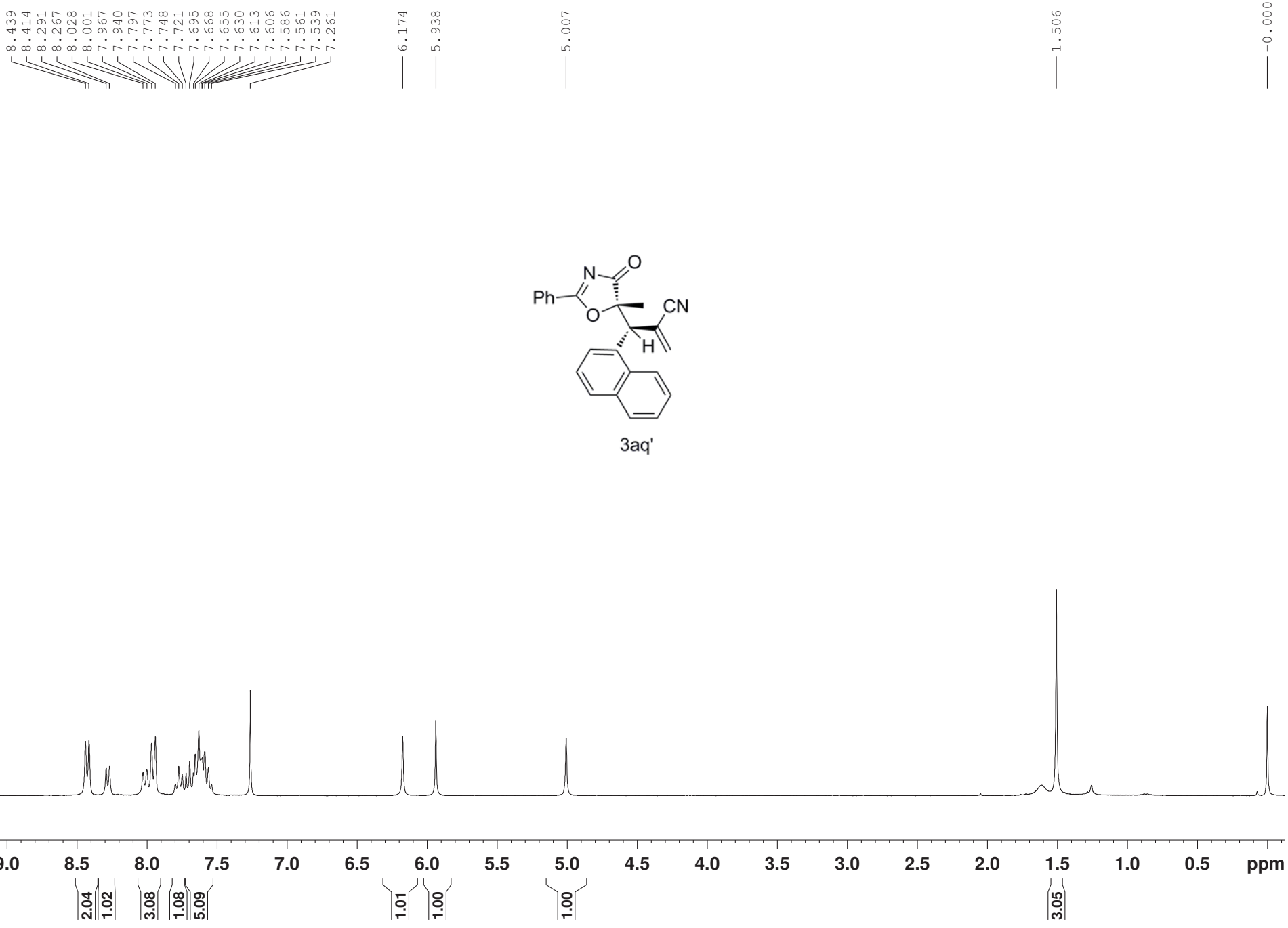
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7.773
7.748
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7.695
7.668
7.655
7.630
7.613
7.606
7.586
7.561
7.539
7.261
6.174
5.938
5.007
1.506
-0.000
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O
Ph
O
CN
H
3aq'
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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1.0
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1.02
3.08
1.08
5.09
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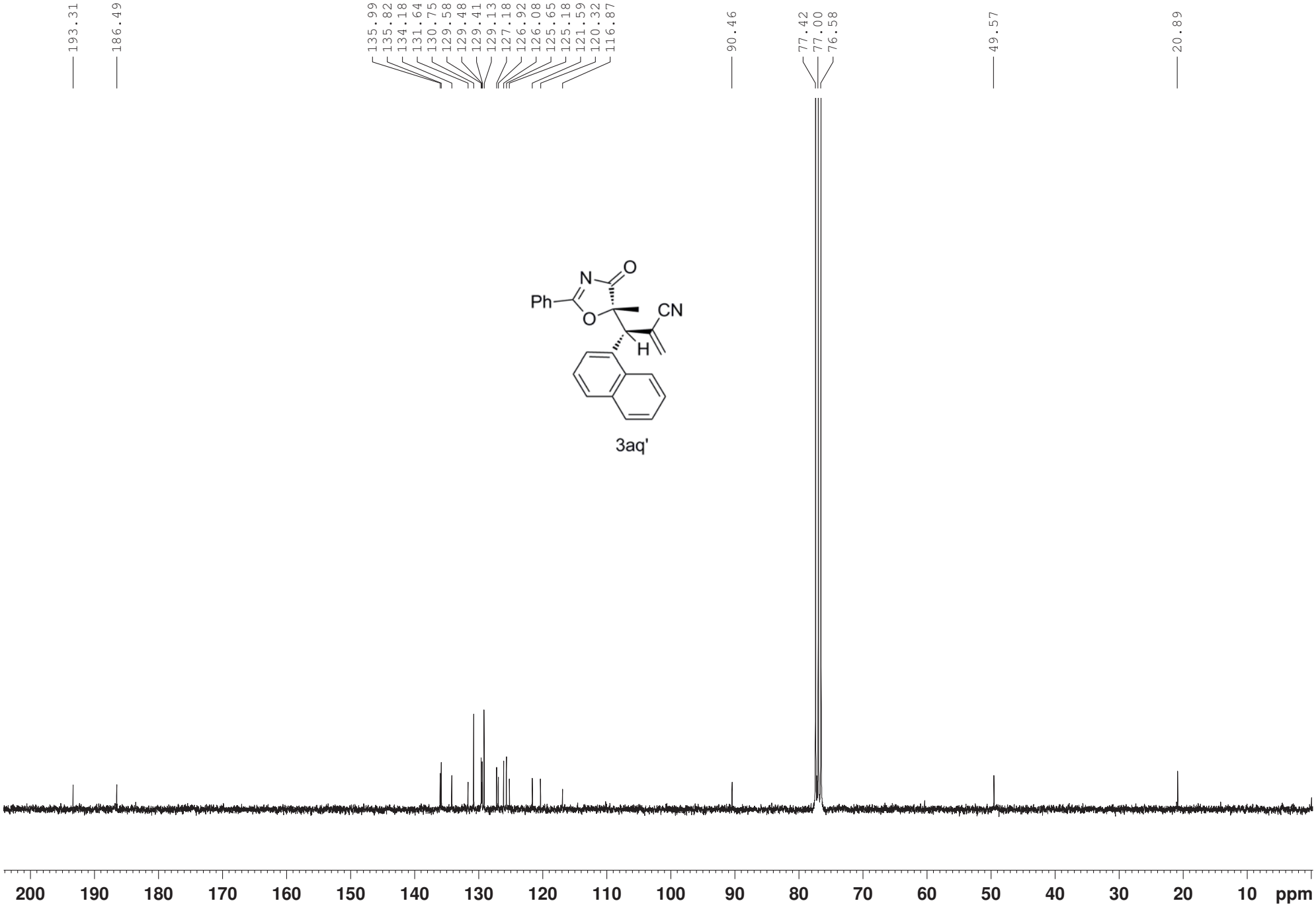
1.00
1.00
3.05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125.65
125.18
121.59
120.32
116.87
90.46
77.42
77.00
76.58
49.57
20.89
N
O
Ph
O
CN
H
3aq'
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150
140
130
120
110
100
90
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70
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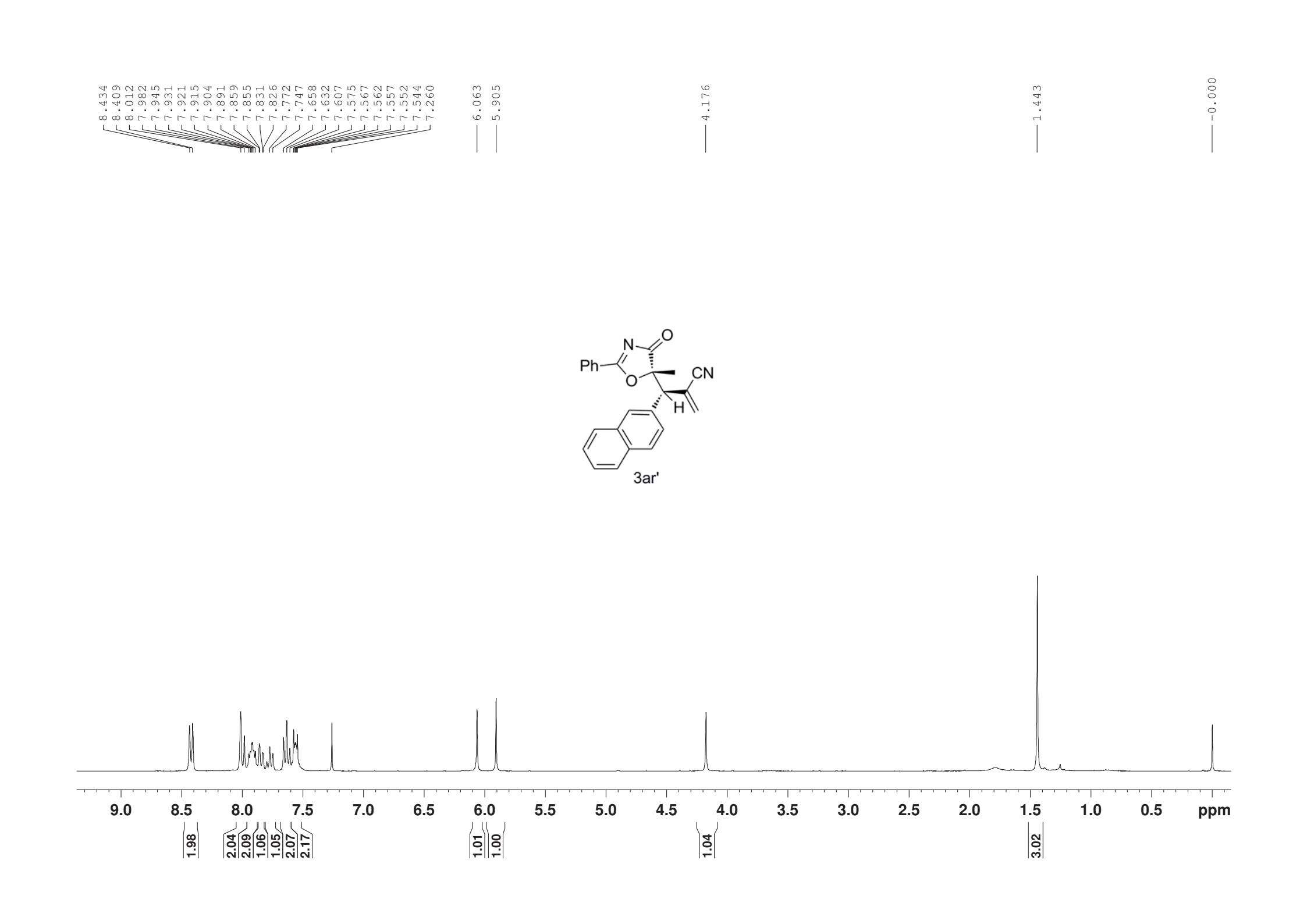
10
ppm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7.855
7.831
7.826
7.772
7.747
7.658
7.632
7.607
7.575
7.567
7.562
7.557
7.552
7.544
7.260
6.063
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0.000
Ph
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O
O
CN
H
3ar'
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7.0
6.5
6.0
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5.0
4.5
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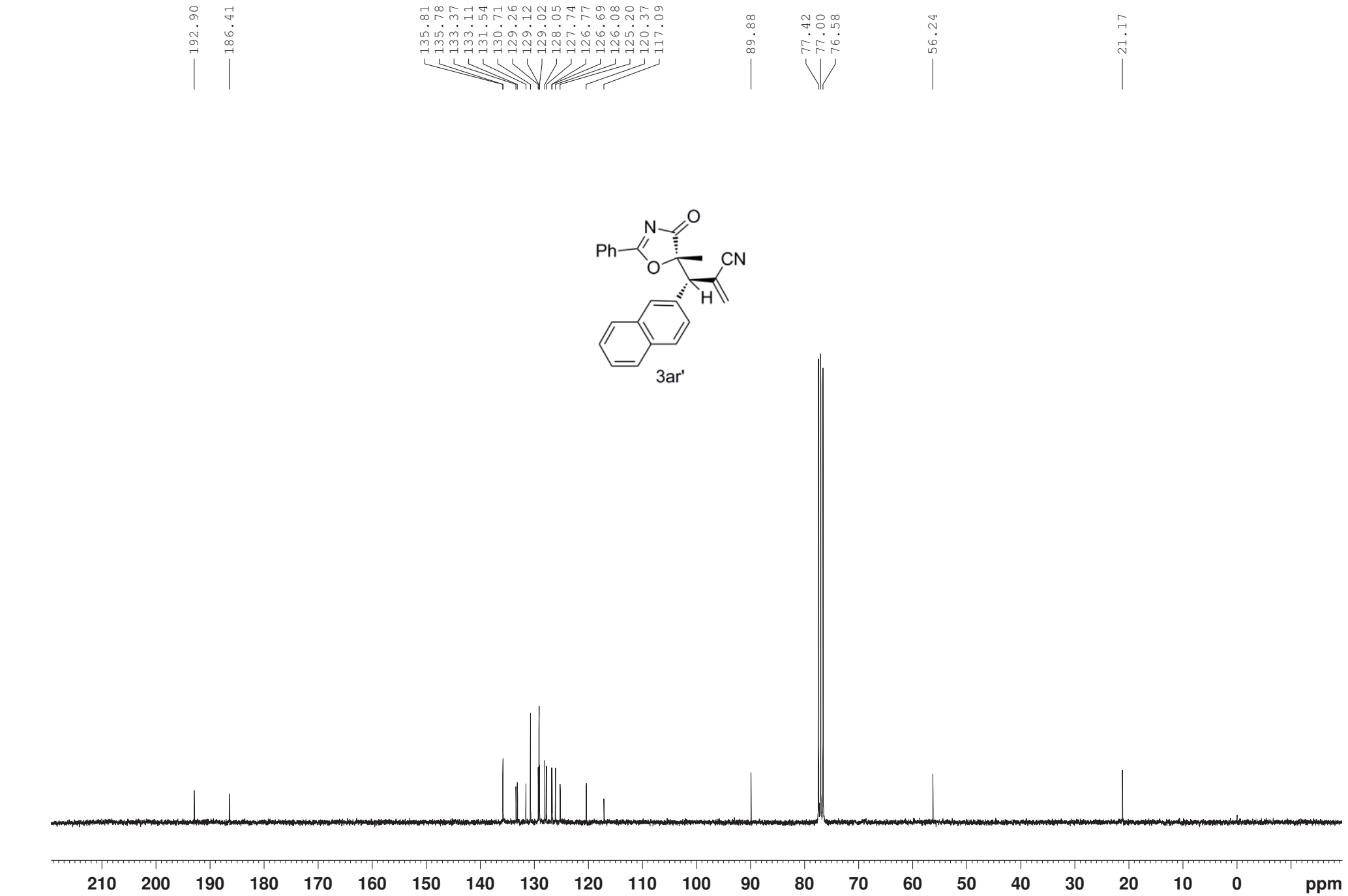
1.04
3.02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126.69
126.08
125.20
120.37
117.09
89.88
77.42
77.00
76.58
56.24
21.17
N
O
Ph
O
CN
H
3ar'
210
200
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130
120
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100
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60
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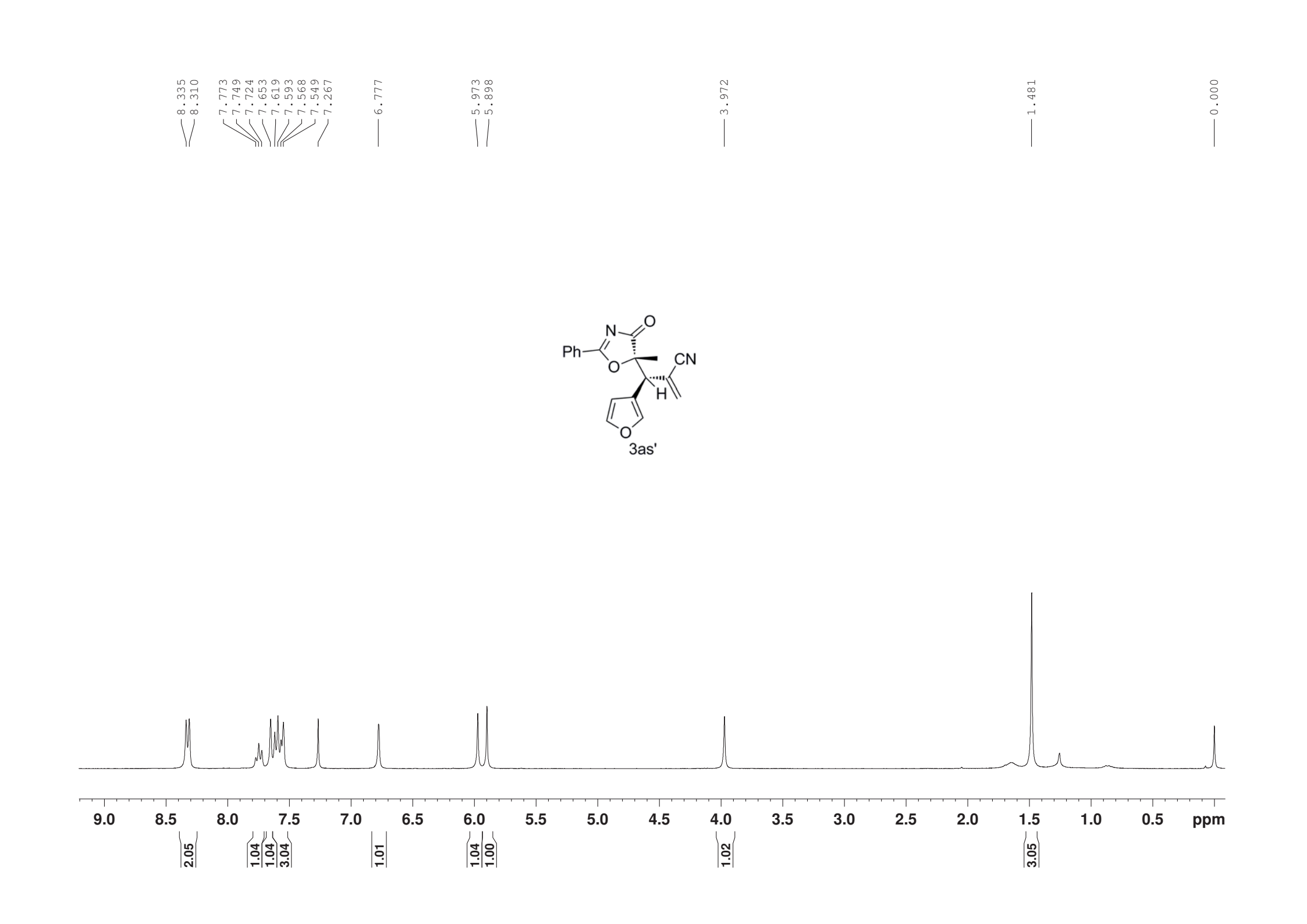
0
ppm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5.898
3.972
1.481
0.000
N
O
Ph
O
CN
H
O
3as'
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8.0
7.5
7.0
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6.0
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5.0
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4.0
3.5
3.0
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1.01
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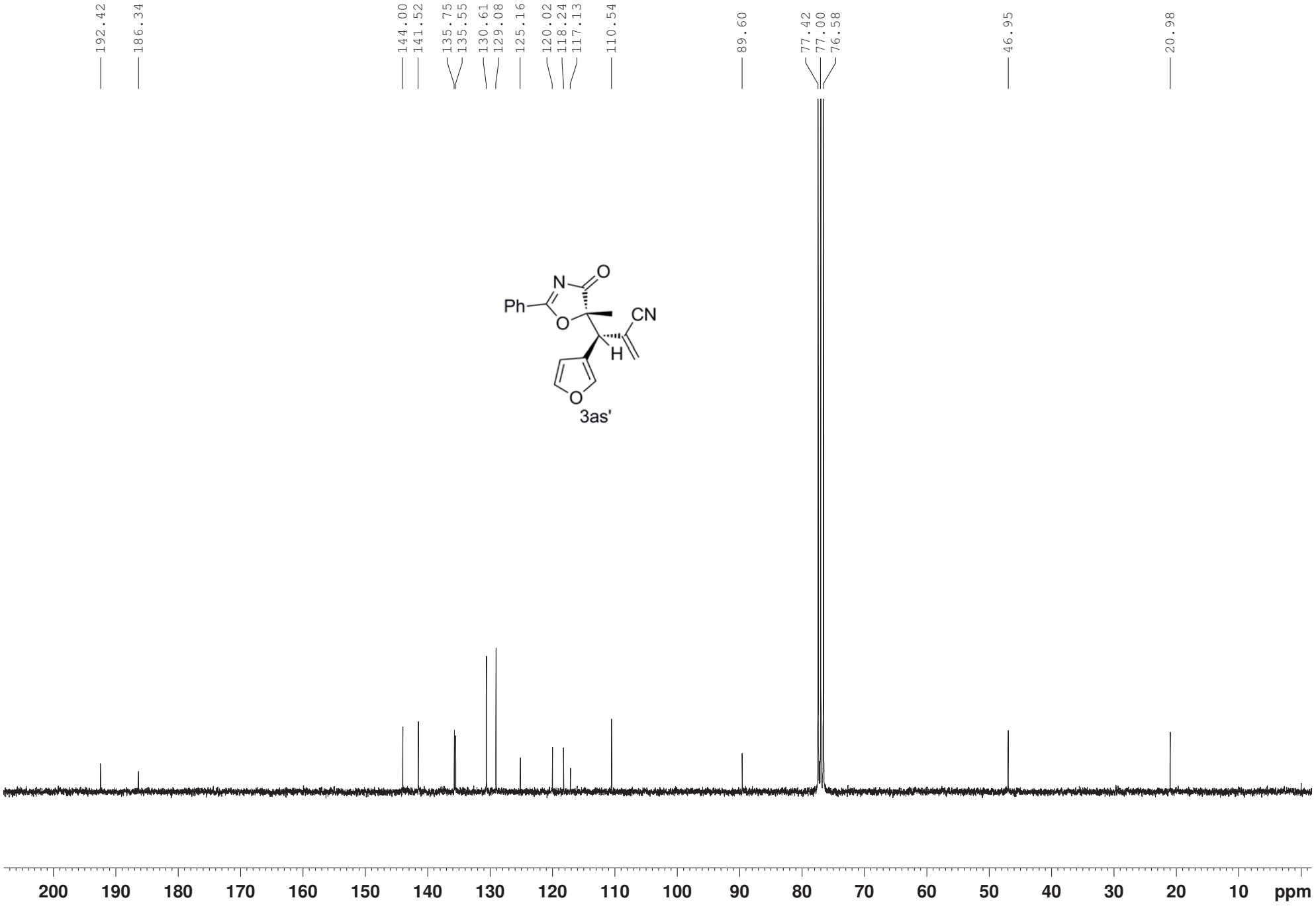
3.05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120.02
118.24
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110.54
89.60
77.42
77.00
76.58
46.95
20.98
N
O
Ph
O
CN
H
O
3as'
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140
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120
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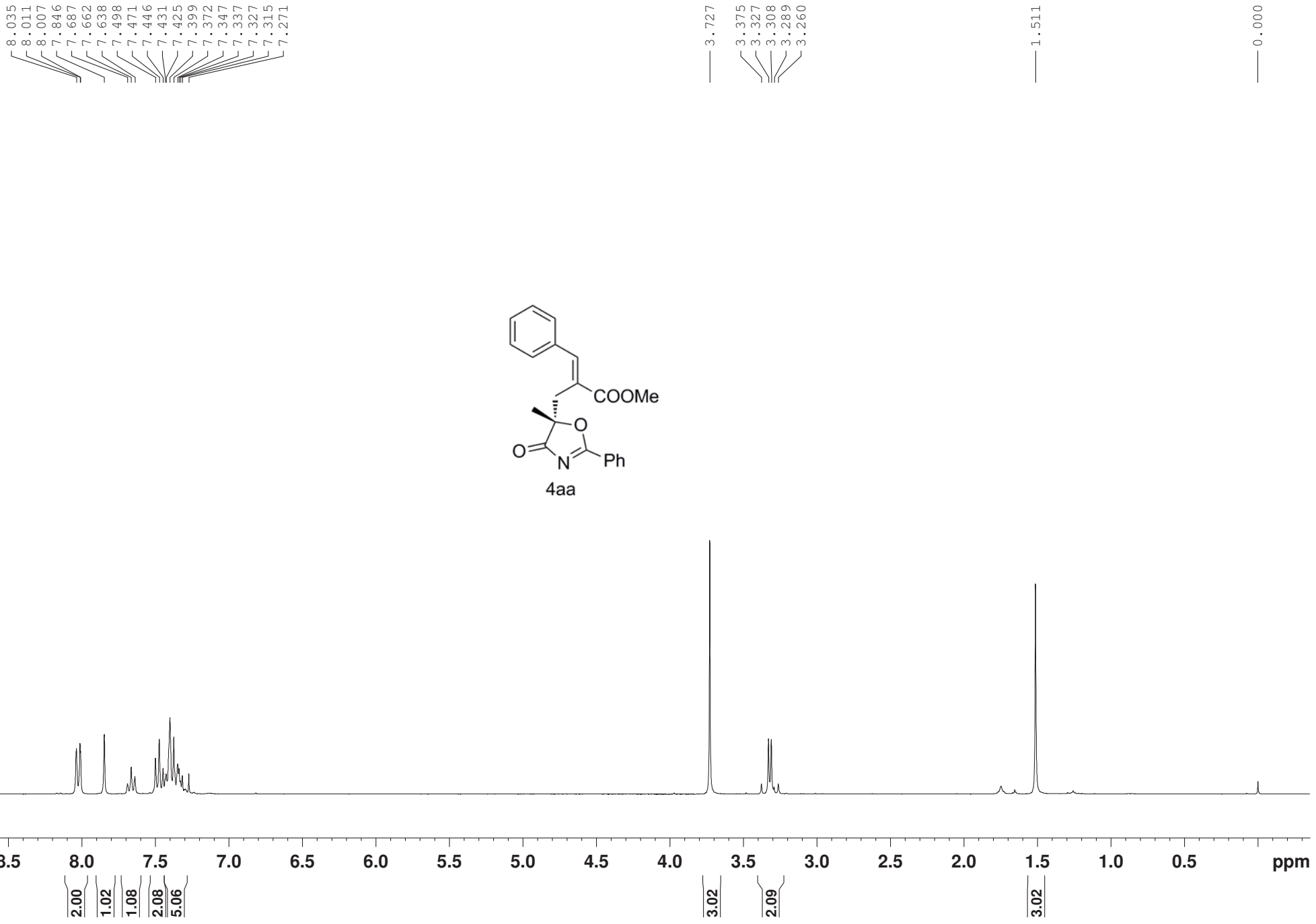
ppm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7.347
7.337
7.327
7.315
7.271
3.727
3.375
3.327
3.308
3.289
3.260
1.511
0.000
COOMe
O
O
N
Ph
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6.0
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4.0
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2.08
5.06
3.02
2.09
3.02

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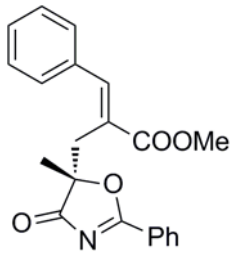

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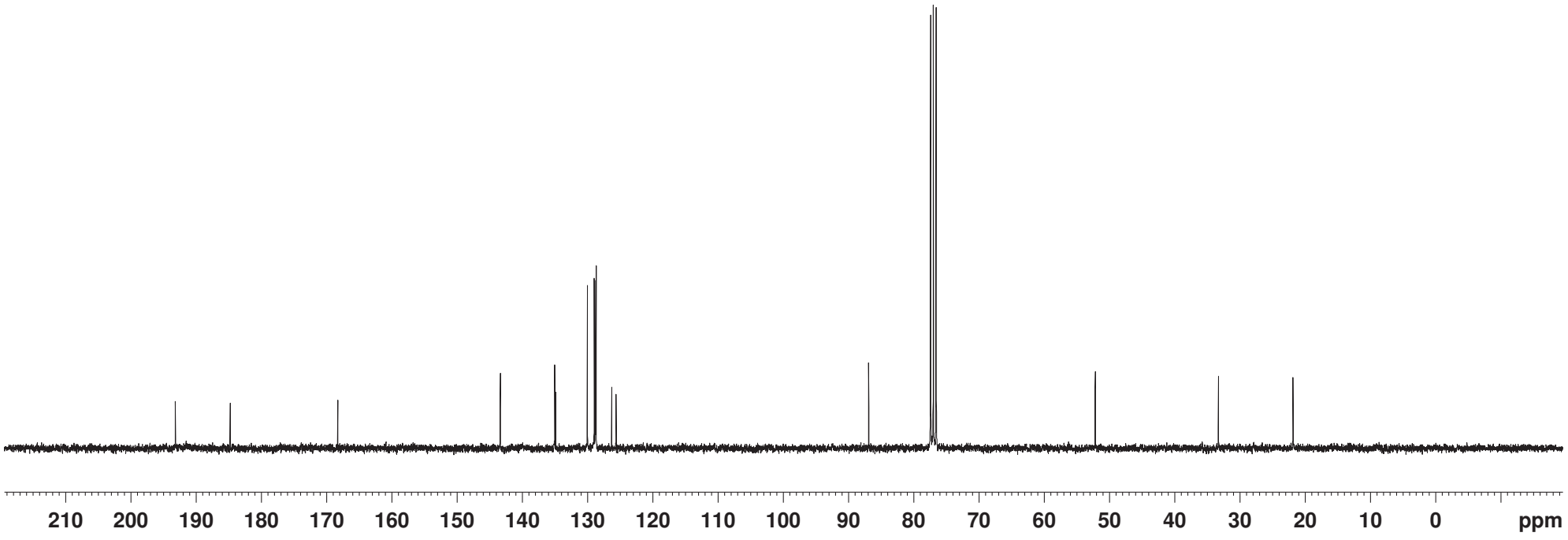

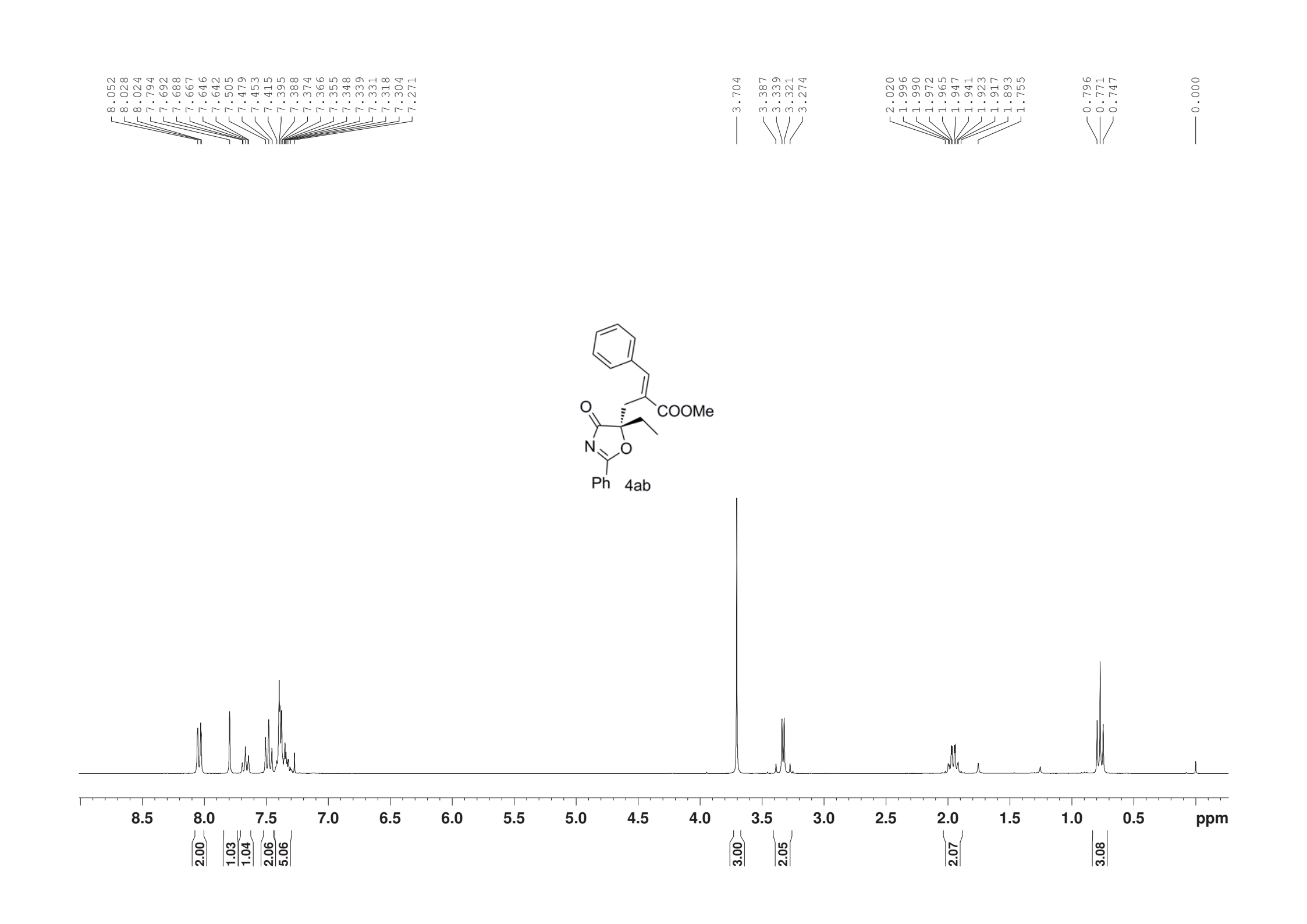
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1.947
1.941
1.923
1.917
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0.000
COOMe
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O
Ph
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5.06
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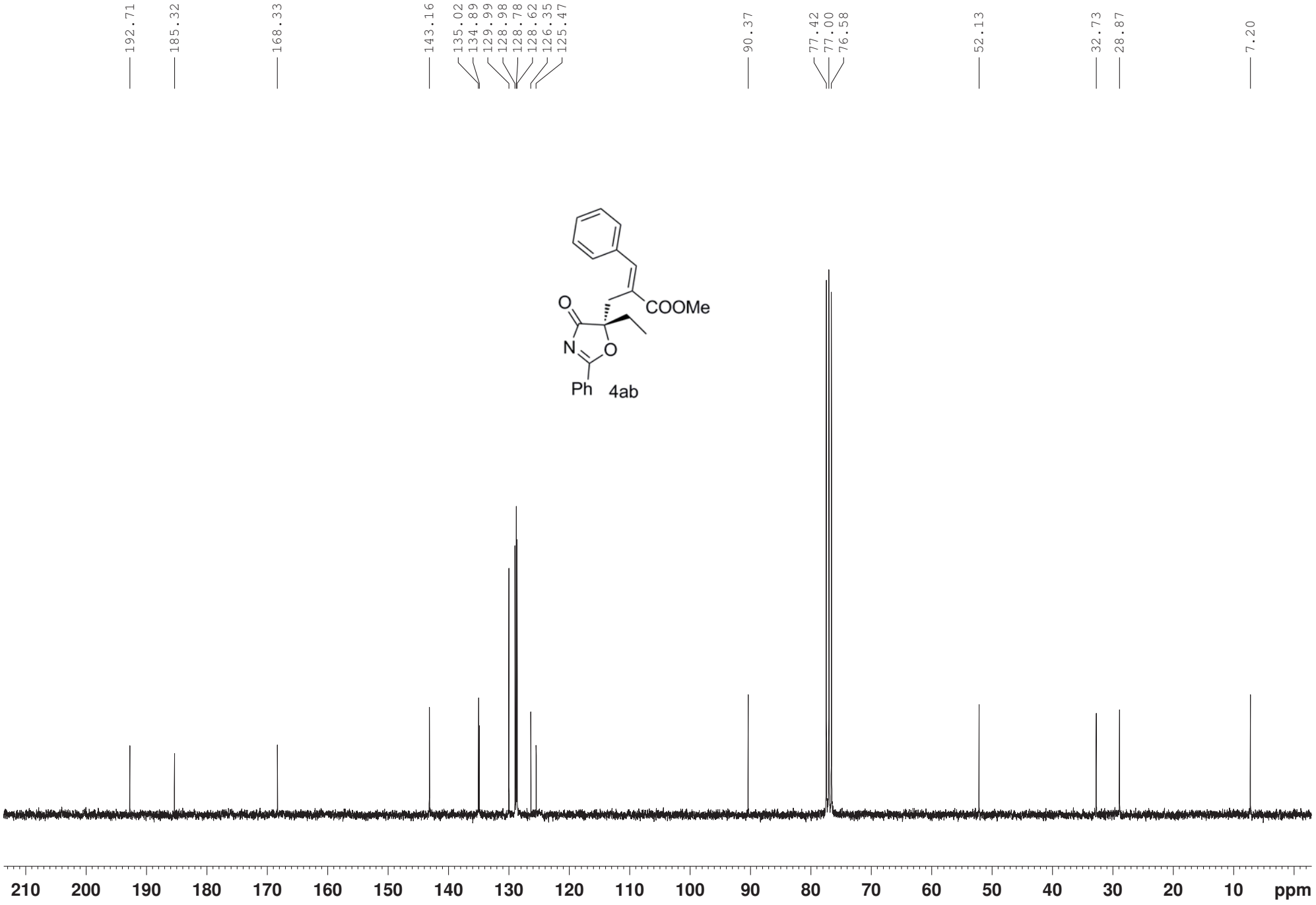
2.07
3.08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52.13
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7.20
O
COOMe
N
O
Ph
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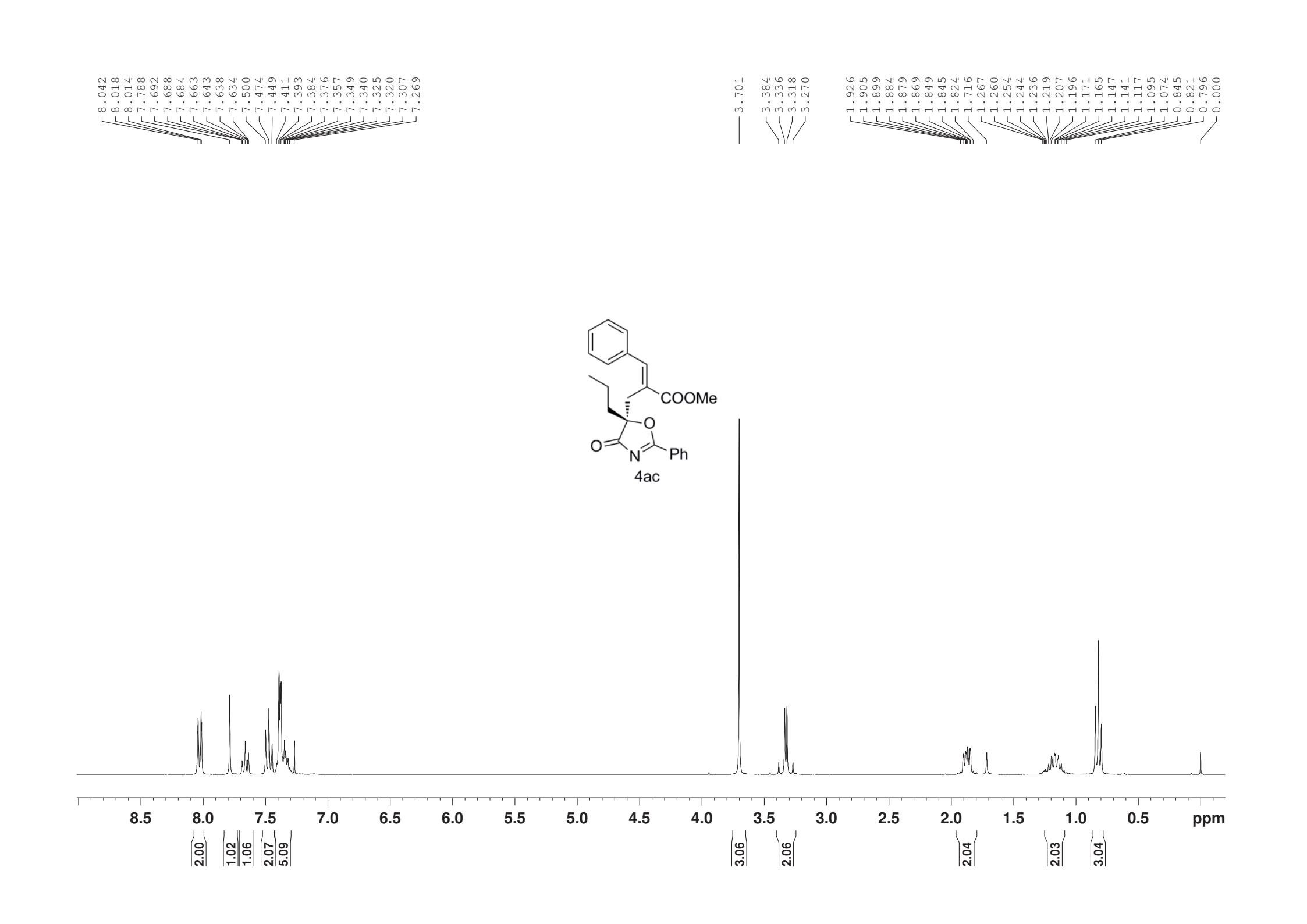
ppm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7.269
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3.270
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COOMe
O
O
N
Ph
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ppm
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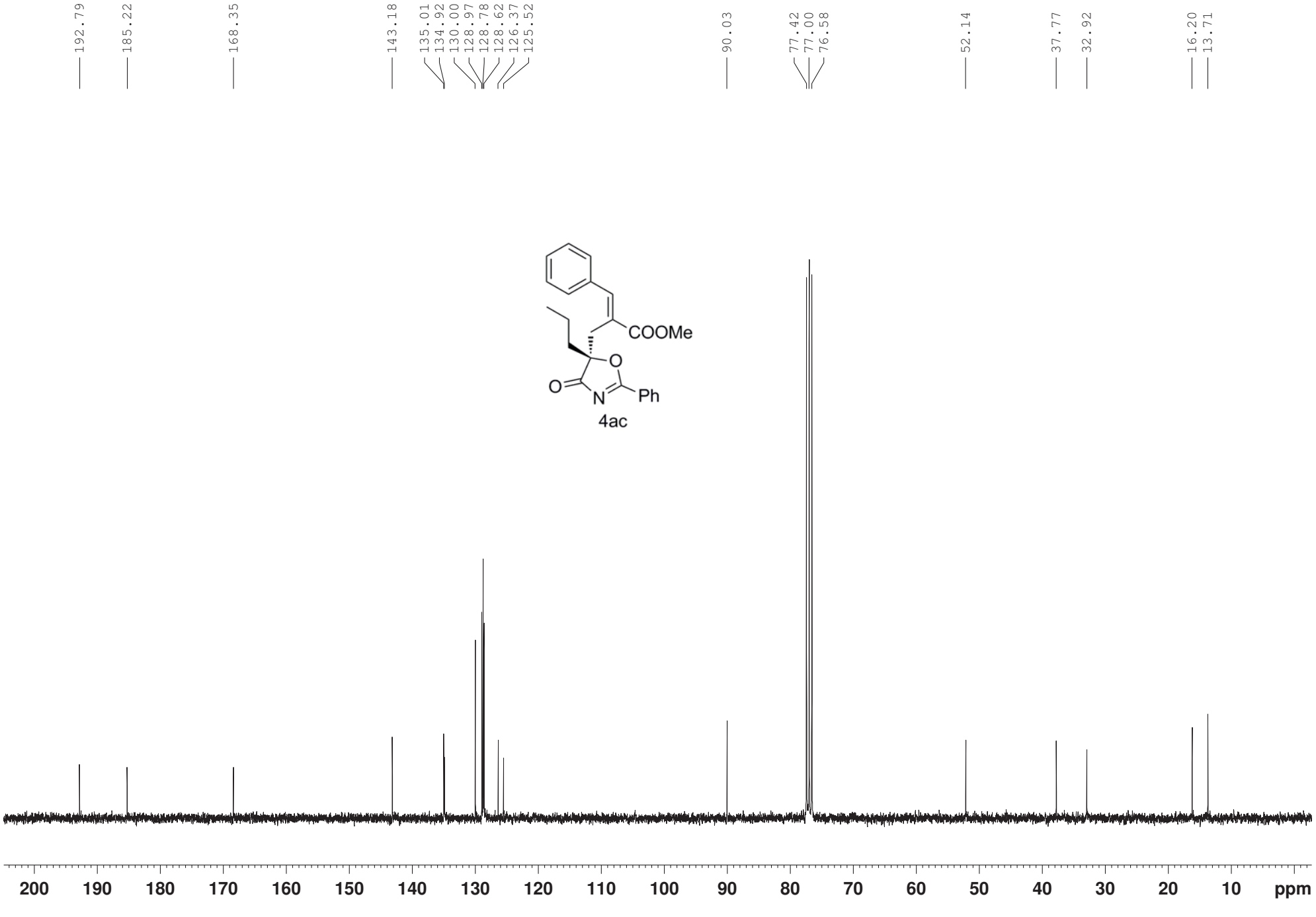
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77.00
76.58
52.14
37.77
32.92
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COOMe
O
O
N
Ph
4ac
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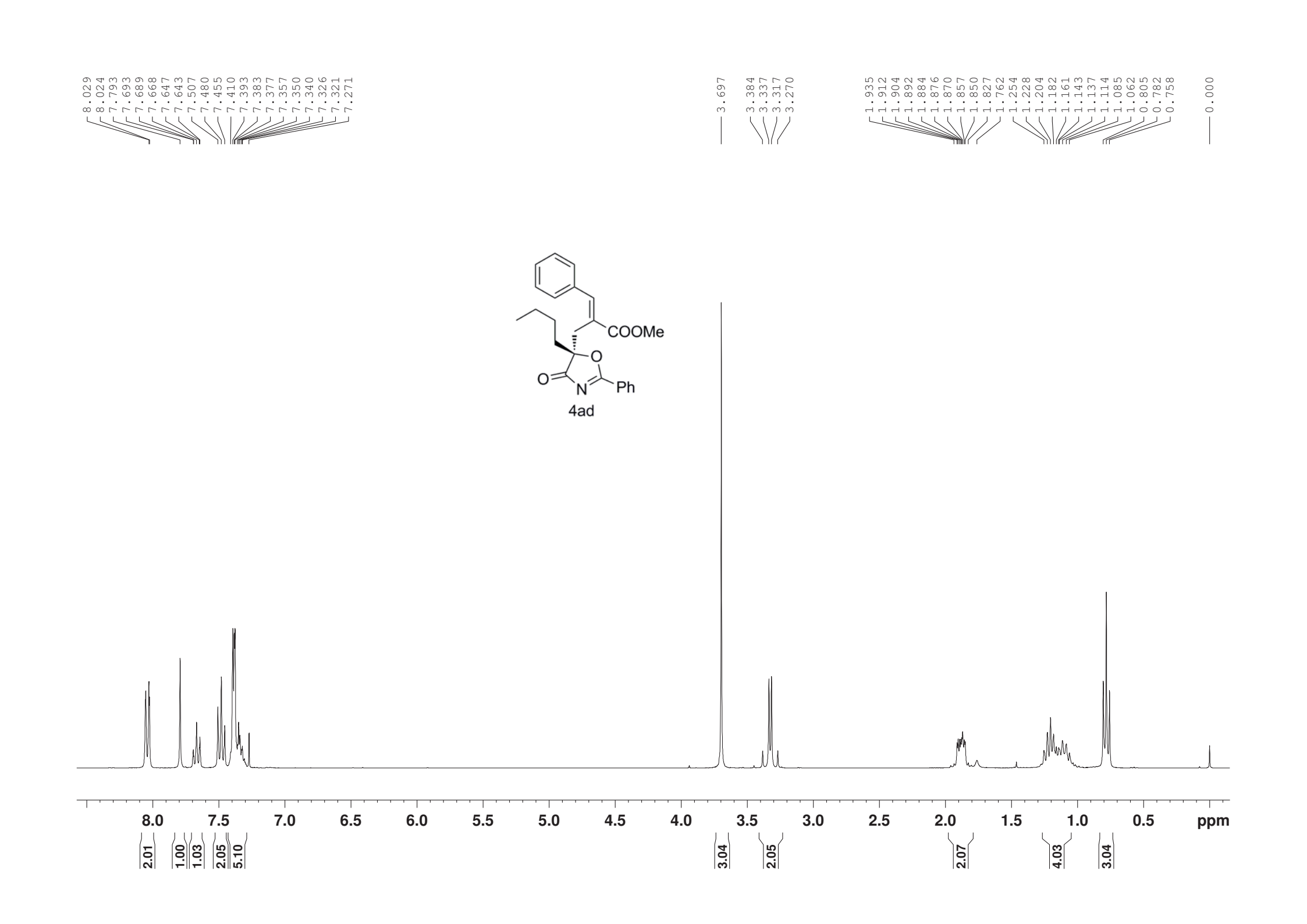
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3.317
3.270
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1.857
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1.161
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COOMe
O
O
N
Ph
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1.0
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2.05
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2.05
2.07
4.03
3.04

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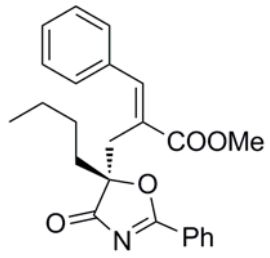

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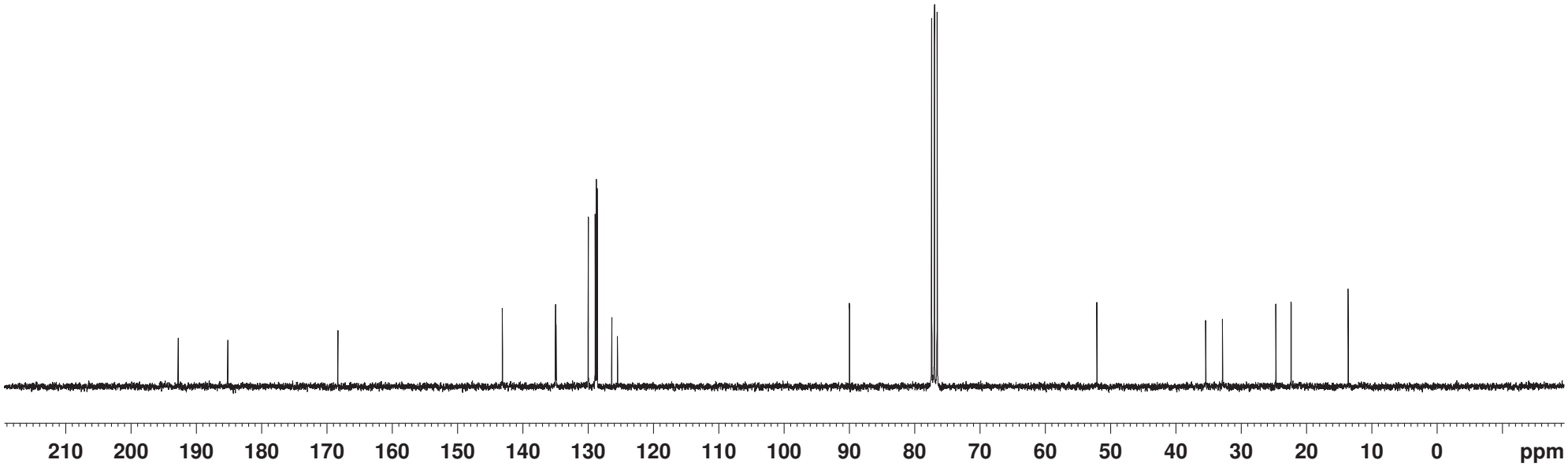

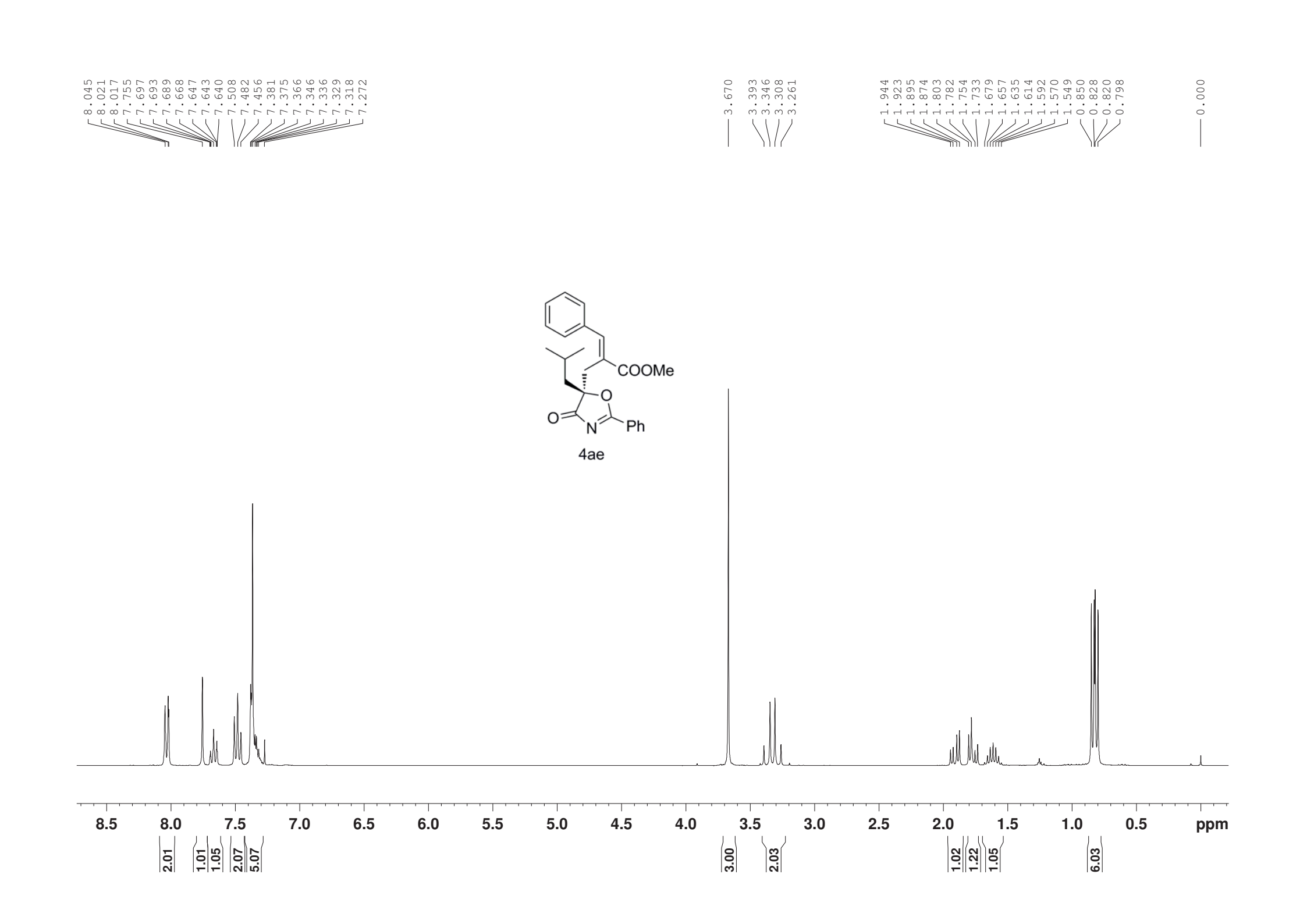
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COOMe
O
O
N
Ph
4ae
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7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
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1.0
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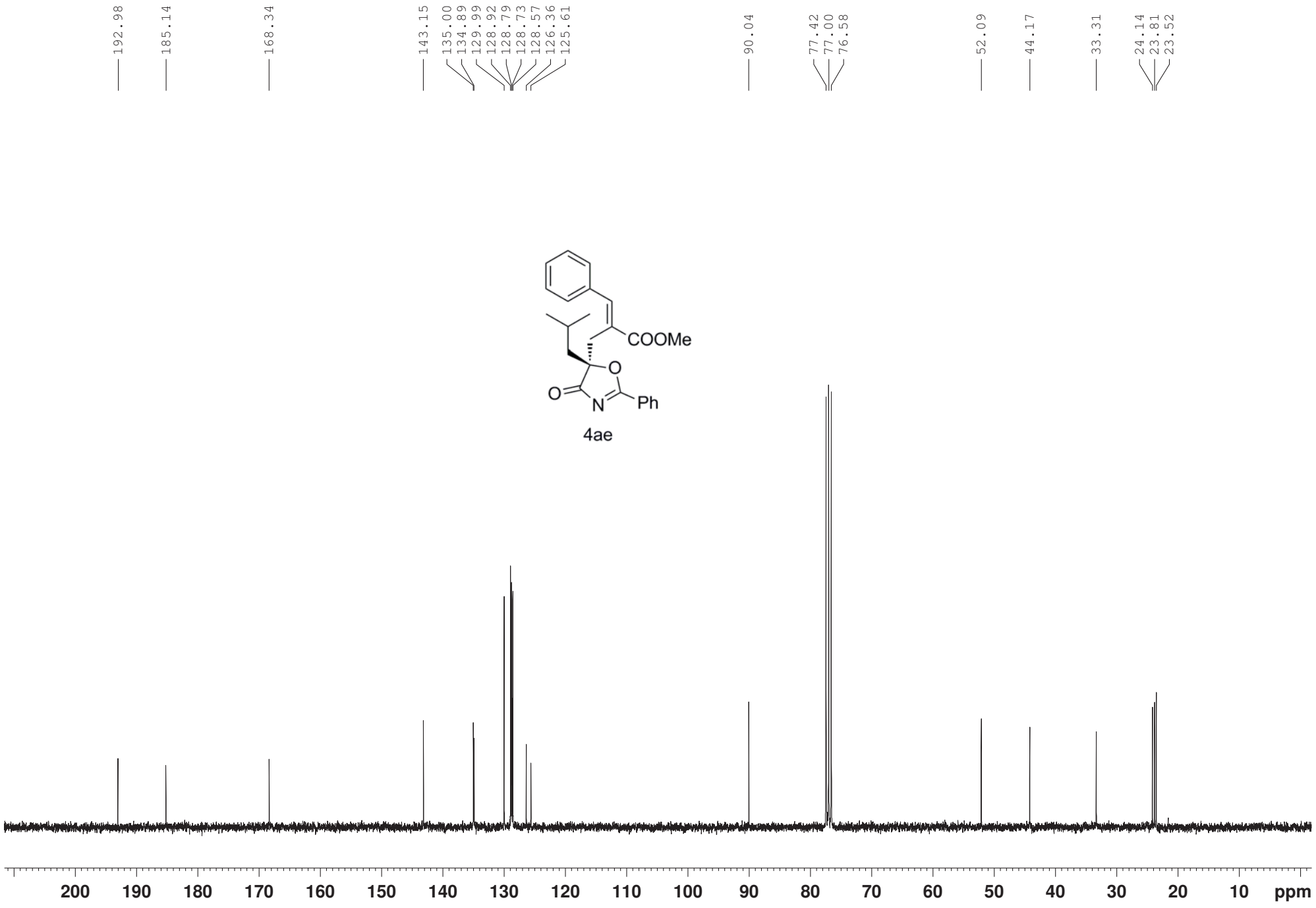
1.05
6.03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77.00
76.58
52.09
44.17
33.31
24.14
23.81
23.52
COOMe
O
O
N
Ph
4ae
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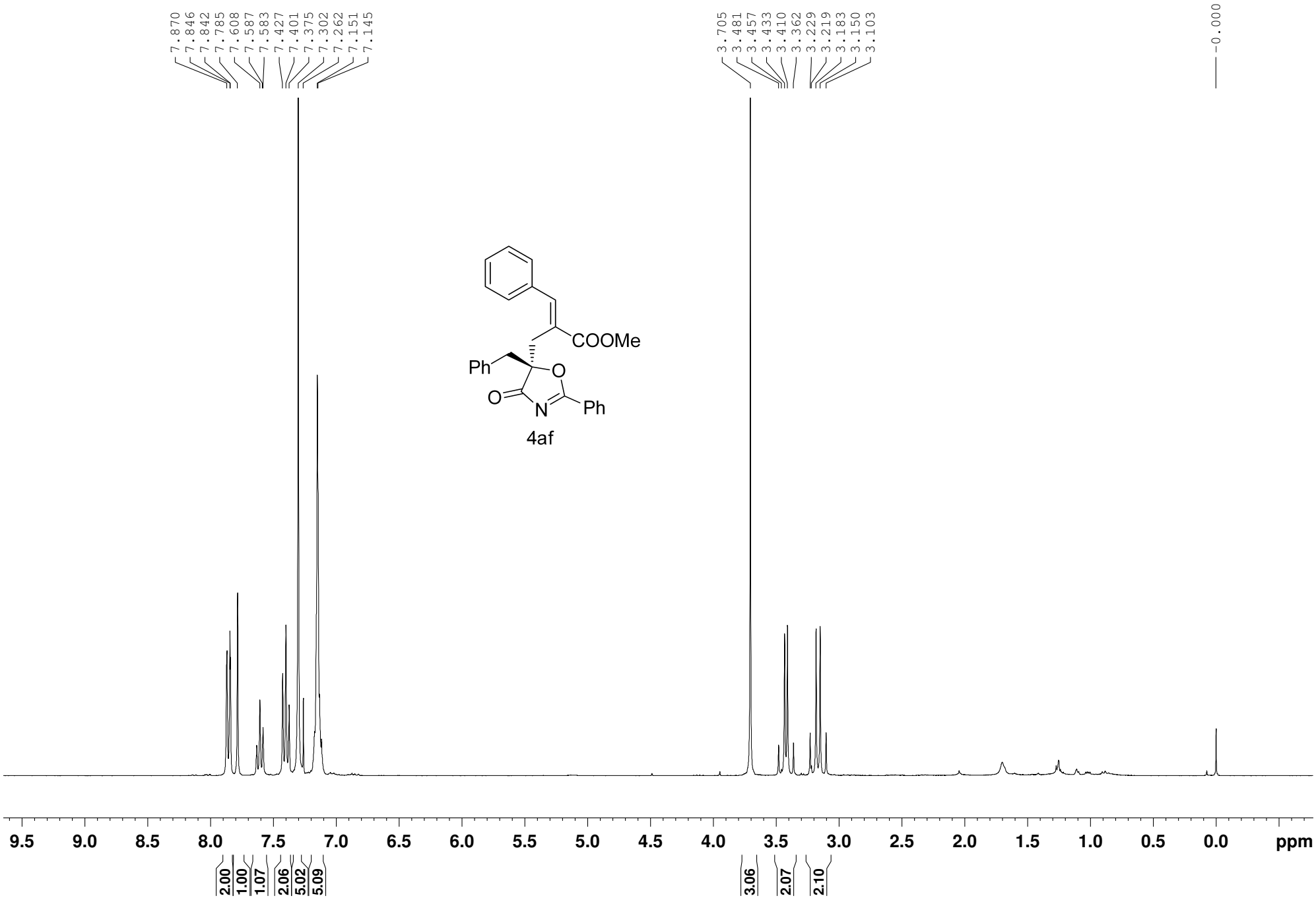
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7.145
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3.481
3.457
3.433
3.410
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3.229
3.219
3.183
3.150
3.103
0.000
COOMe
Ph
O
O
N
Ph
4af
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6.5
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4.0
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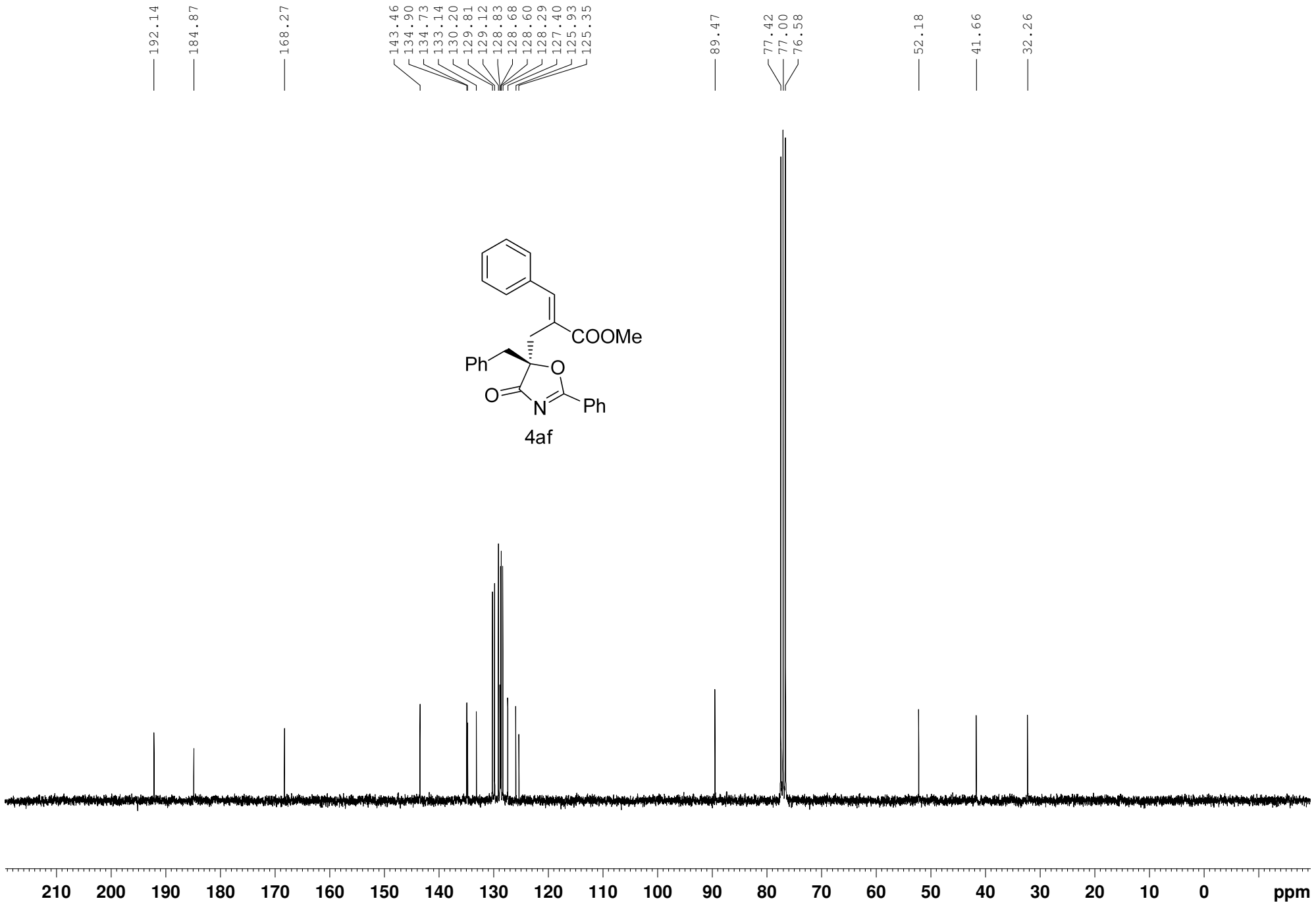
2.07
2.10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127.40
125.93
125.35
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77.00
76.58
52.18
41.66
32.26
COOMe
Ph
O
O
N
Ph
4af
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120
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80
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60
50
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20
10
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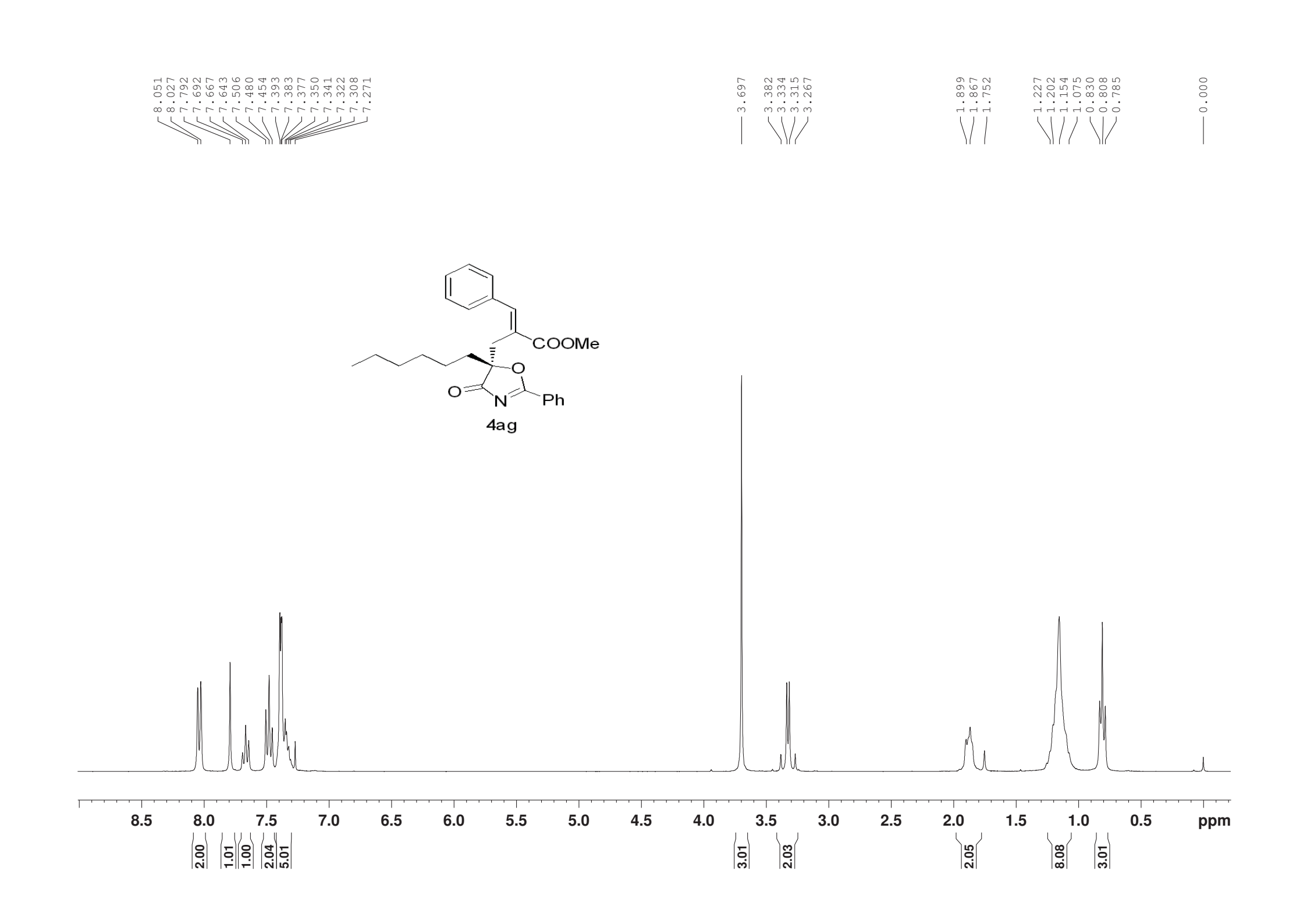
ppm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1.202
1.154
1.075
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0.808
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0.000
COOMe
O
O
N
Ph
4ag
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7.0
6.5
6.0
5.5
5.0
4.5
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3.01
2.03
2.05
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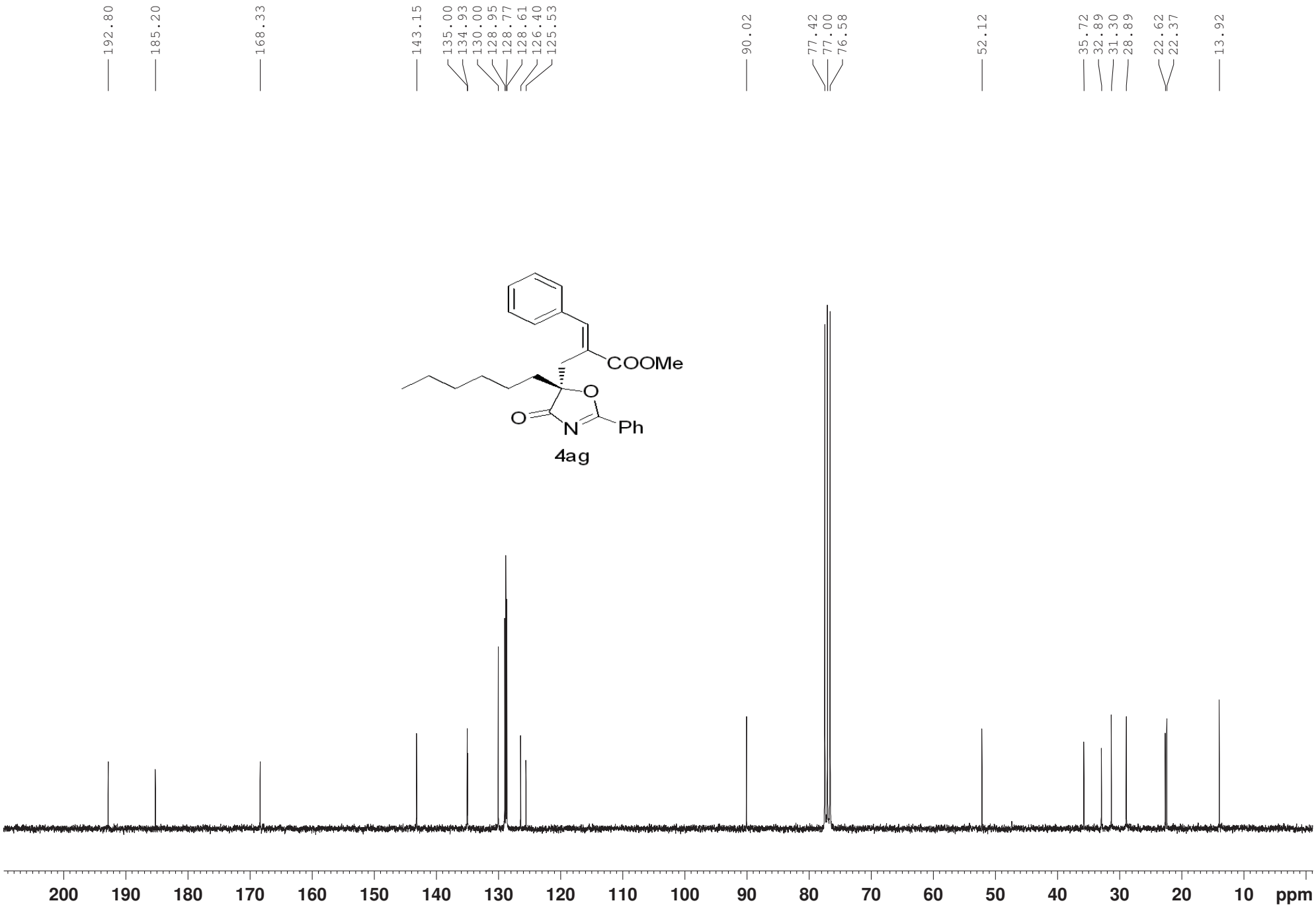
3.01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77.00
76.58
52.12
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22.62
22.37
13.92
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Ph
4ag
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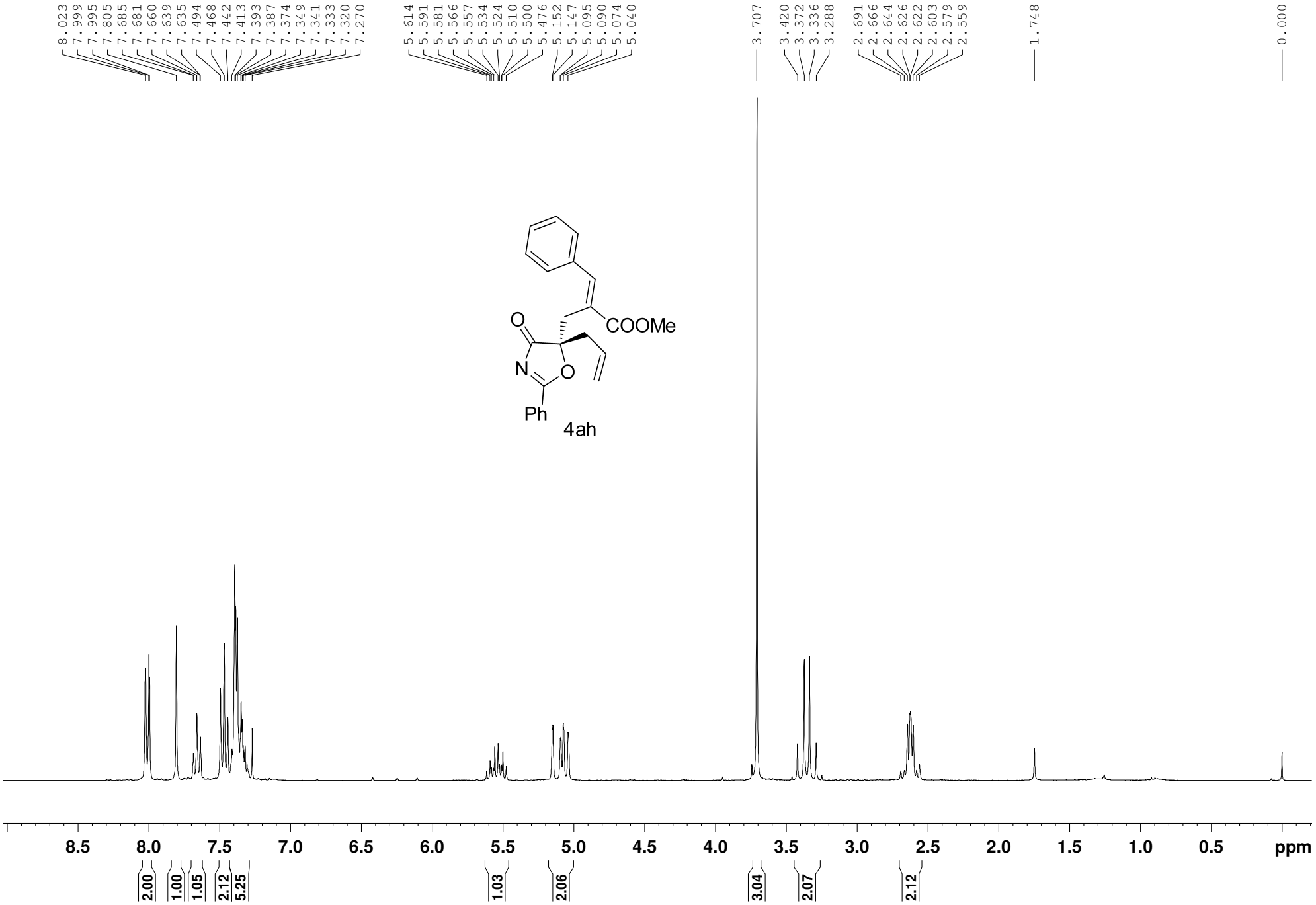
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7.341
7.333
7.320
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5.581
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5.557
5.534
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5.500
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COOMe
N
O
Ph
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7.0
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6.0
5.5
5.0
4.5
4.0
3.5
3.0
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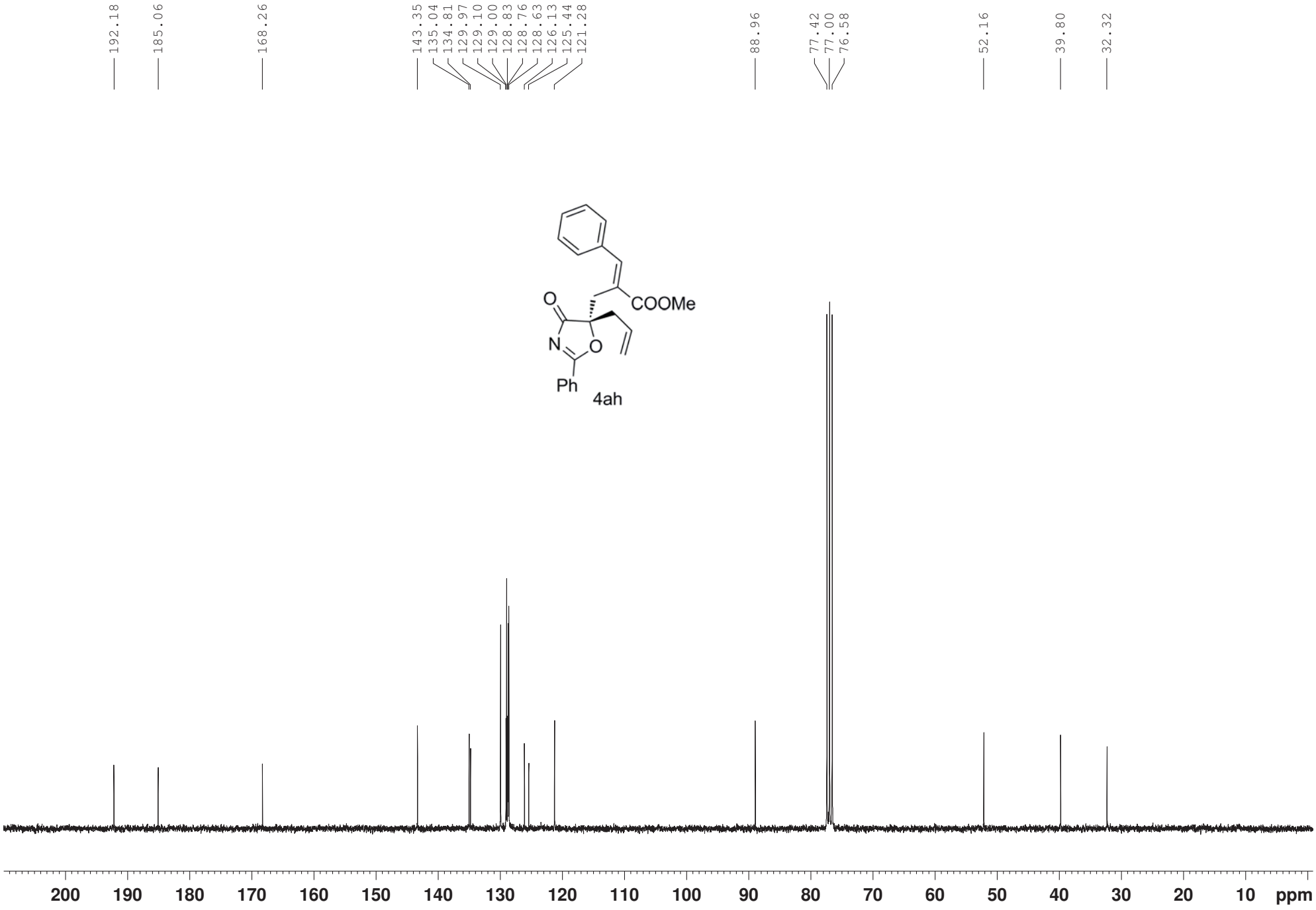
2.07
2.12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77.00
76.58
52.16
39.80
32.32
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COOMe
N
O
Ph
4ah
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150
140
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120
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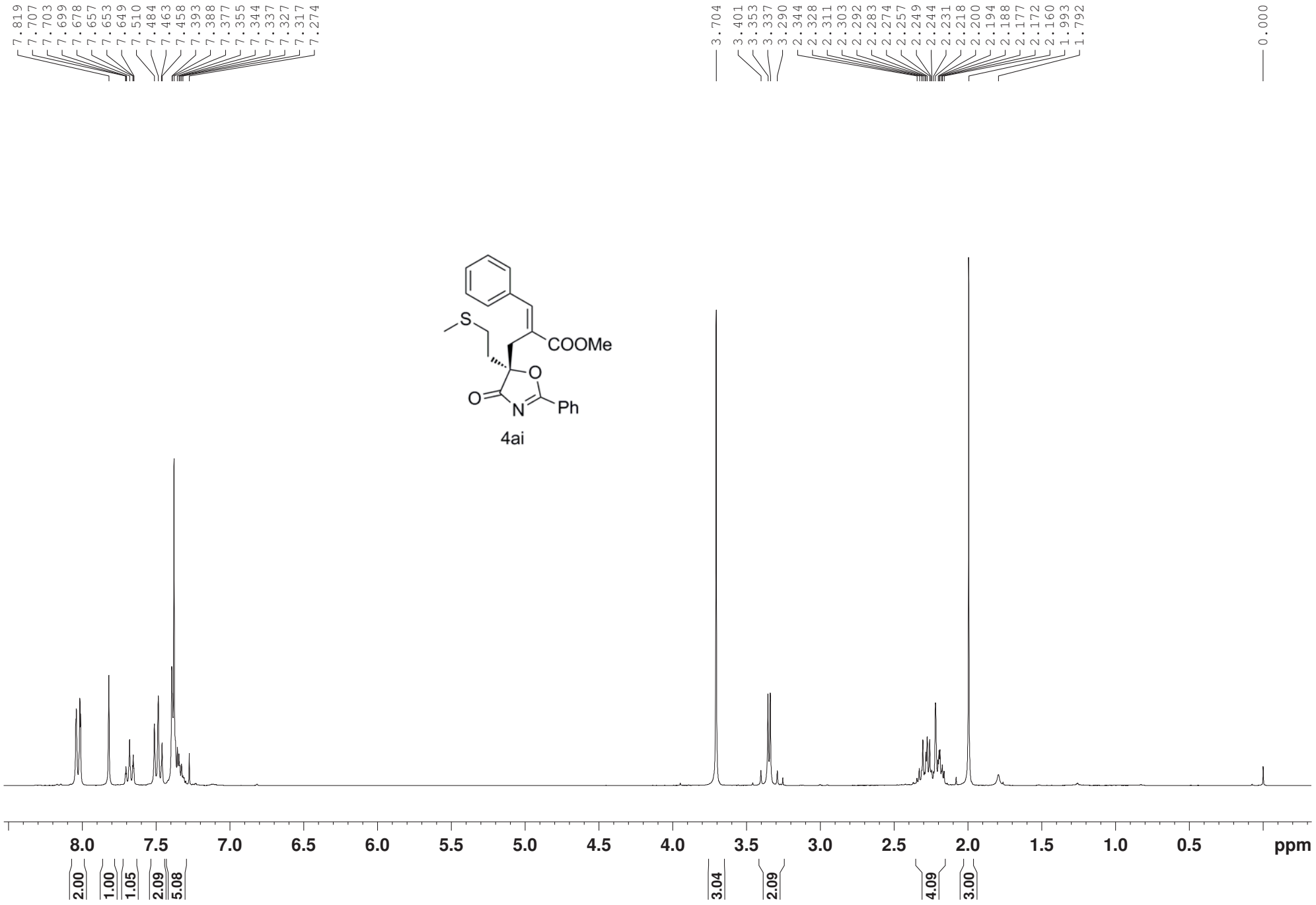
ppm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2.172
2.160
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COOMe
O
O
N
Ph
4ai
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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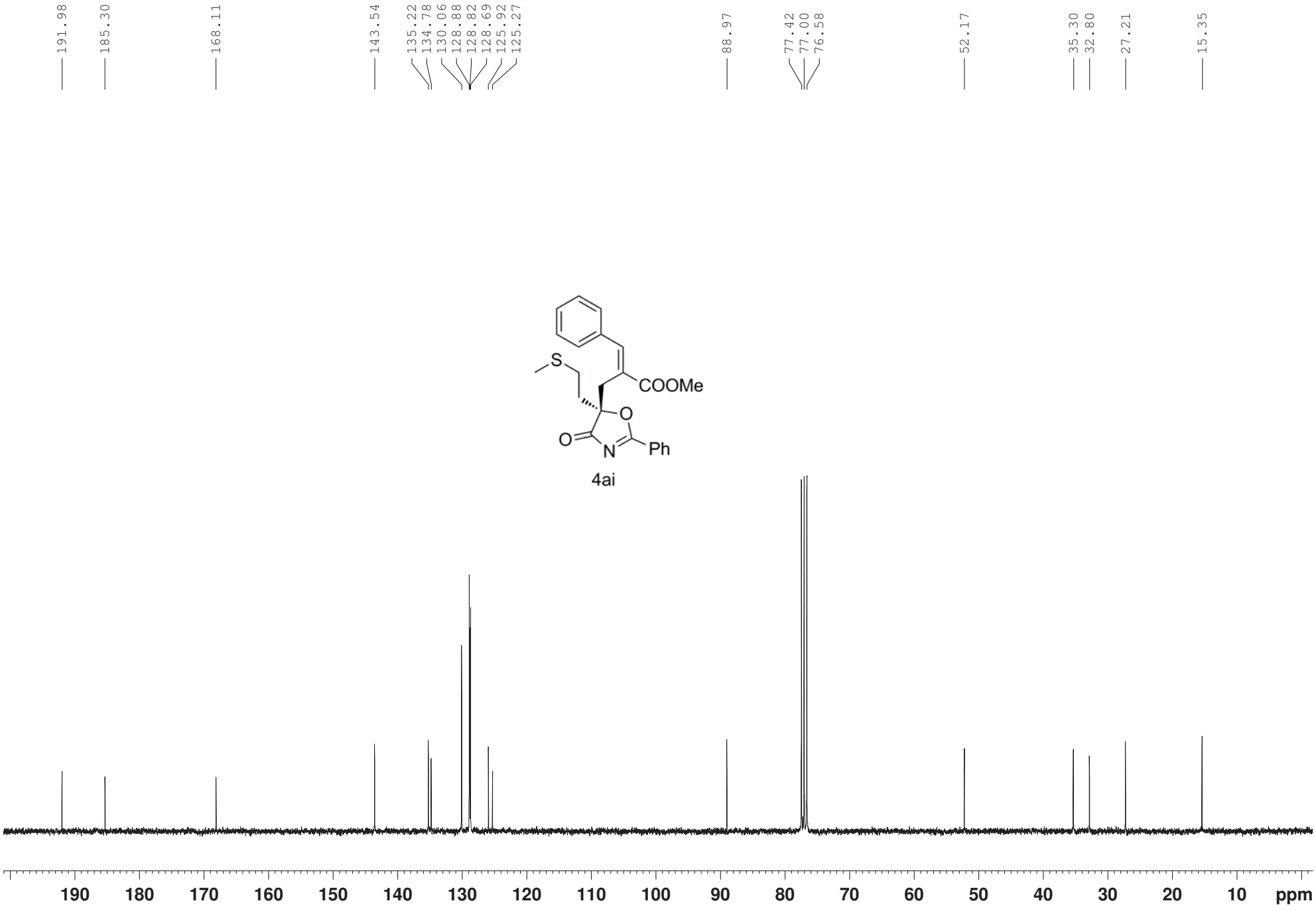
4.09
3.00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77.00
76.58
52.17
35.30
32.80
27.21
15.35
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COOMe
O
O
N
Ph
4ai
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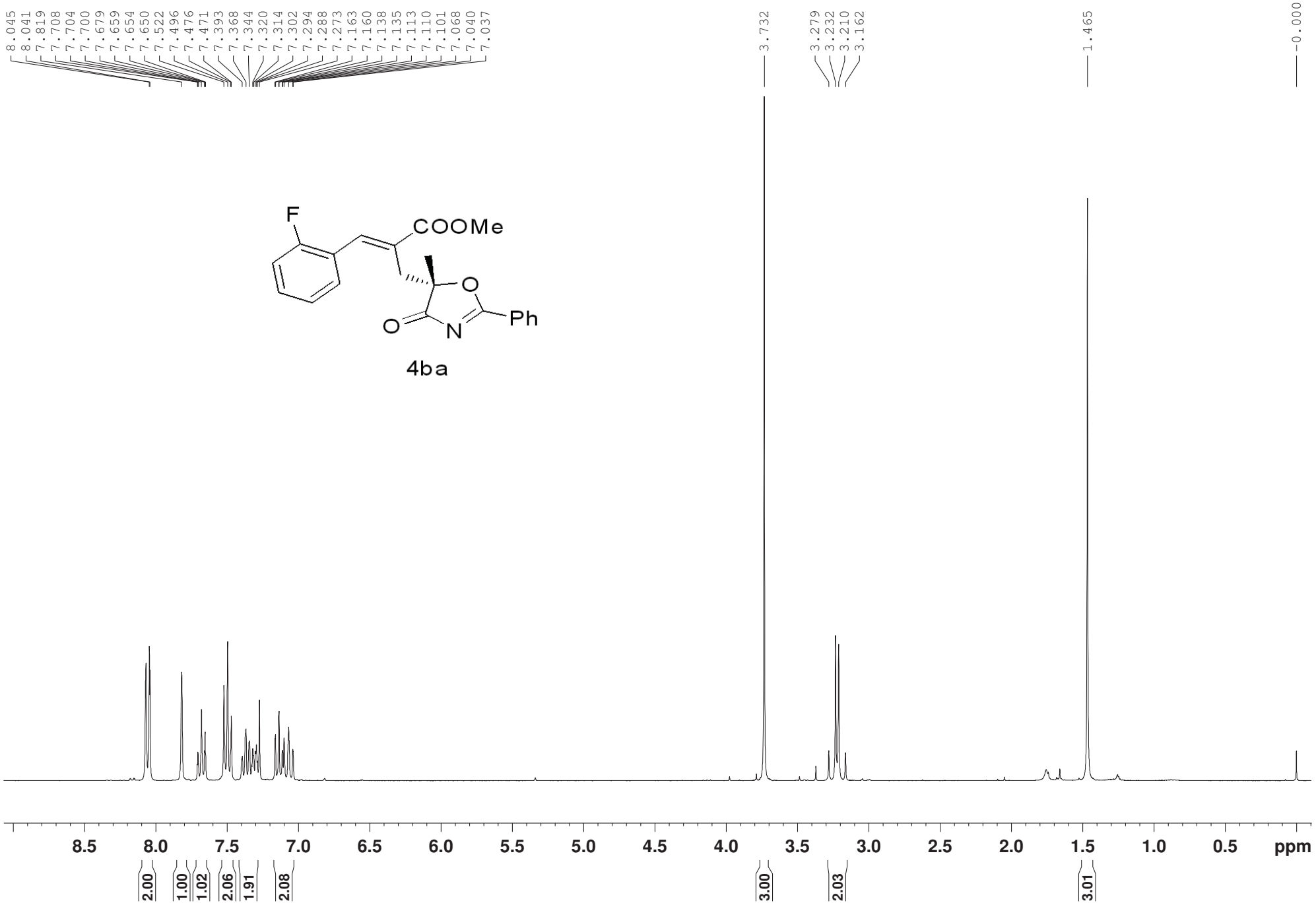
ppm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3.162
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O
O
N
Ph
4ba
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7.0
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6.0
5.5
5.0
4.5
4.0
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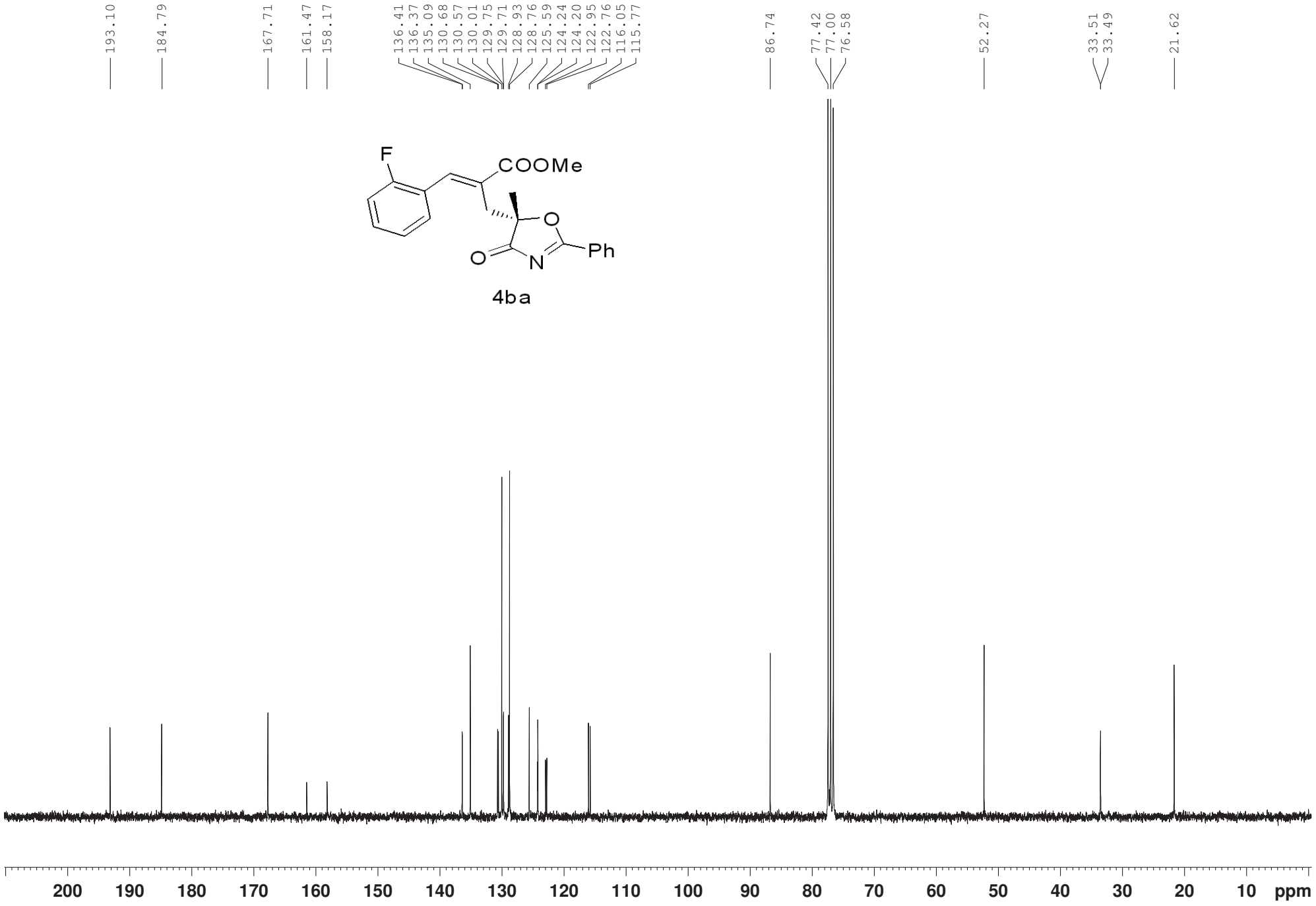
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128.76
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124.20
122.95
122.76
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86.74
77.42
77.00
76.58
52.27
33.51
33.49
21.62
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COOMe
O
O
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Ph
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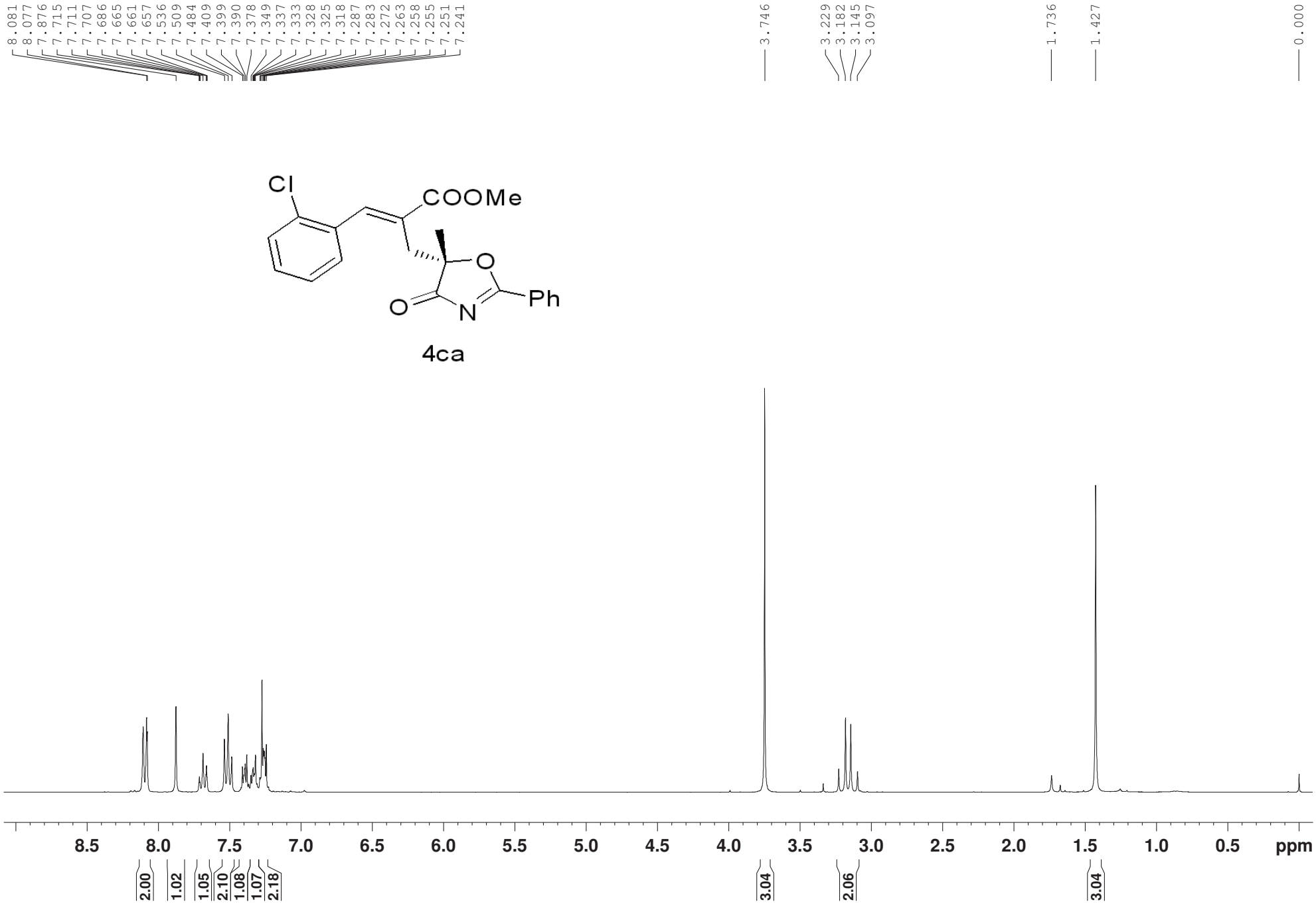
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7.409
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7.258
7.255
7.251
7.241
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3.229
3.182
3.145
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1.427
0.000
Cl
COOMe
O
O
N
Ph
4ca
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7.0
6.5
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5.5
5.0
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4.0
3.5
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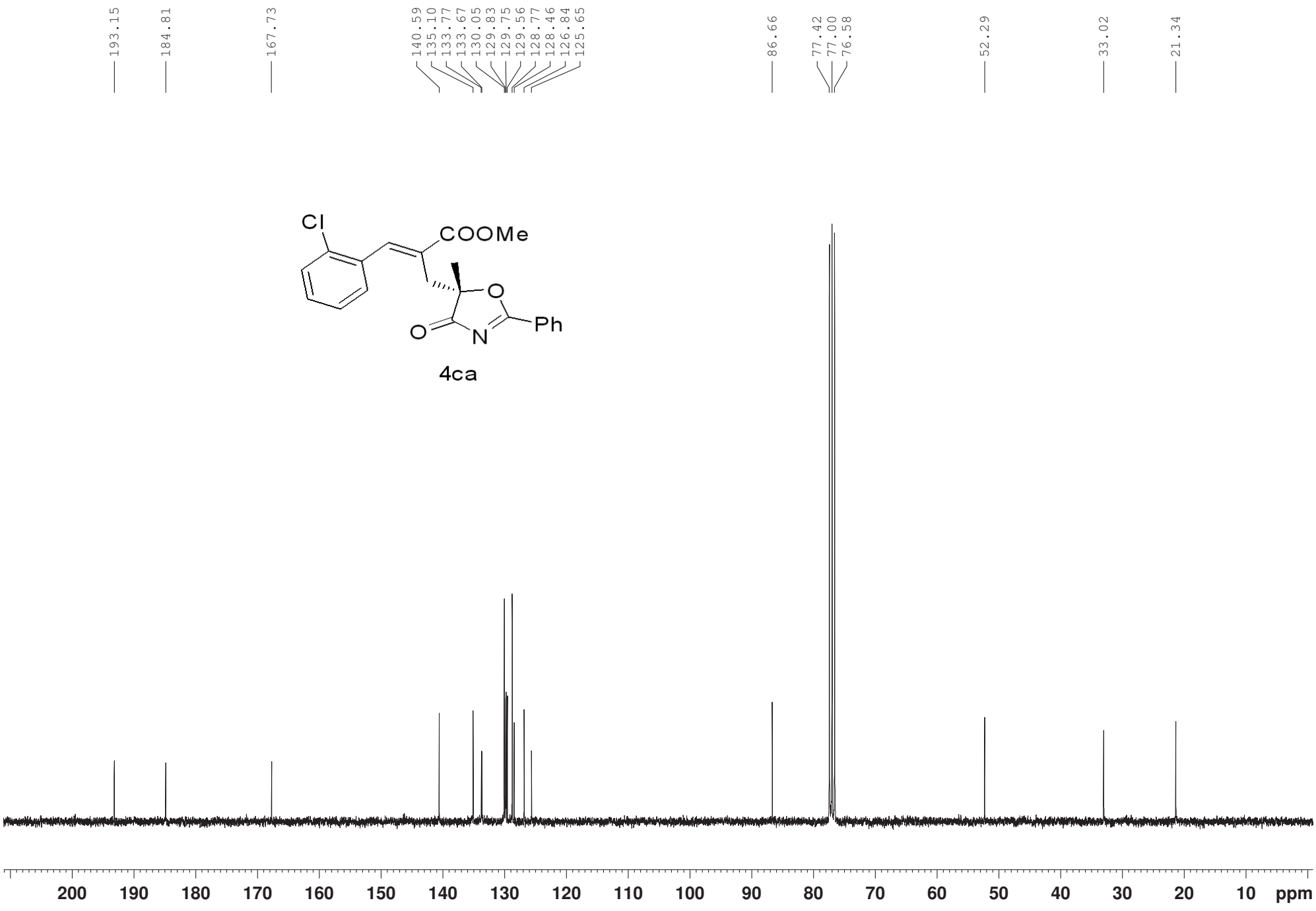
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86.66
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77.00
76.58
52.29
33.02
21.34
Cl
COOMe
O
O
N
Ph
4ca
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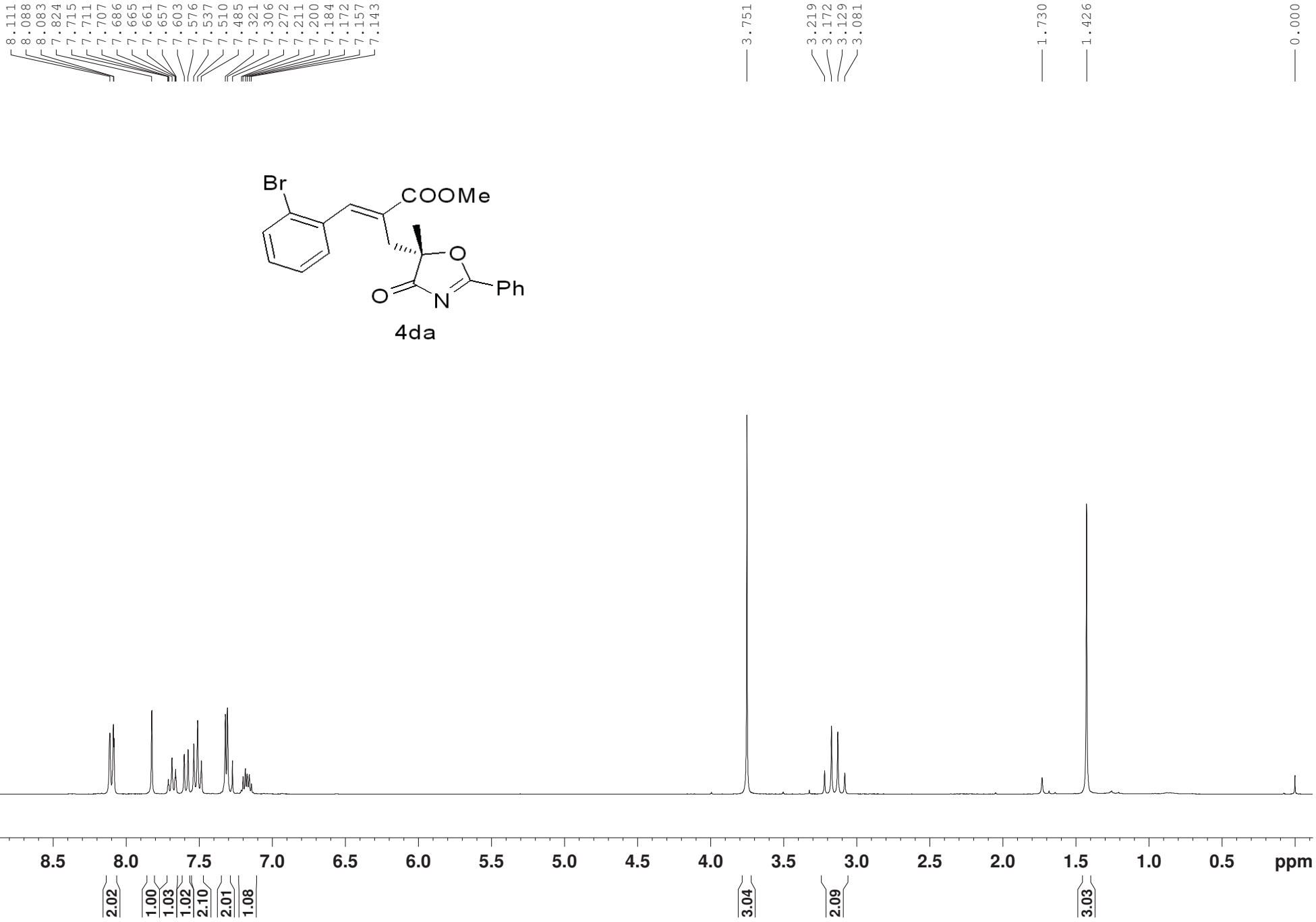
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7.537
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7.485
7.321
7.306
7.272
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7.172
7.157
7.143
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3.219
3.172
3.129
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Br
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O
N
Ph
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6.5
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5.0
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4.0
3.5
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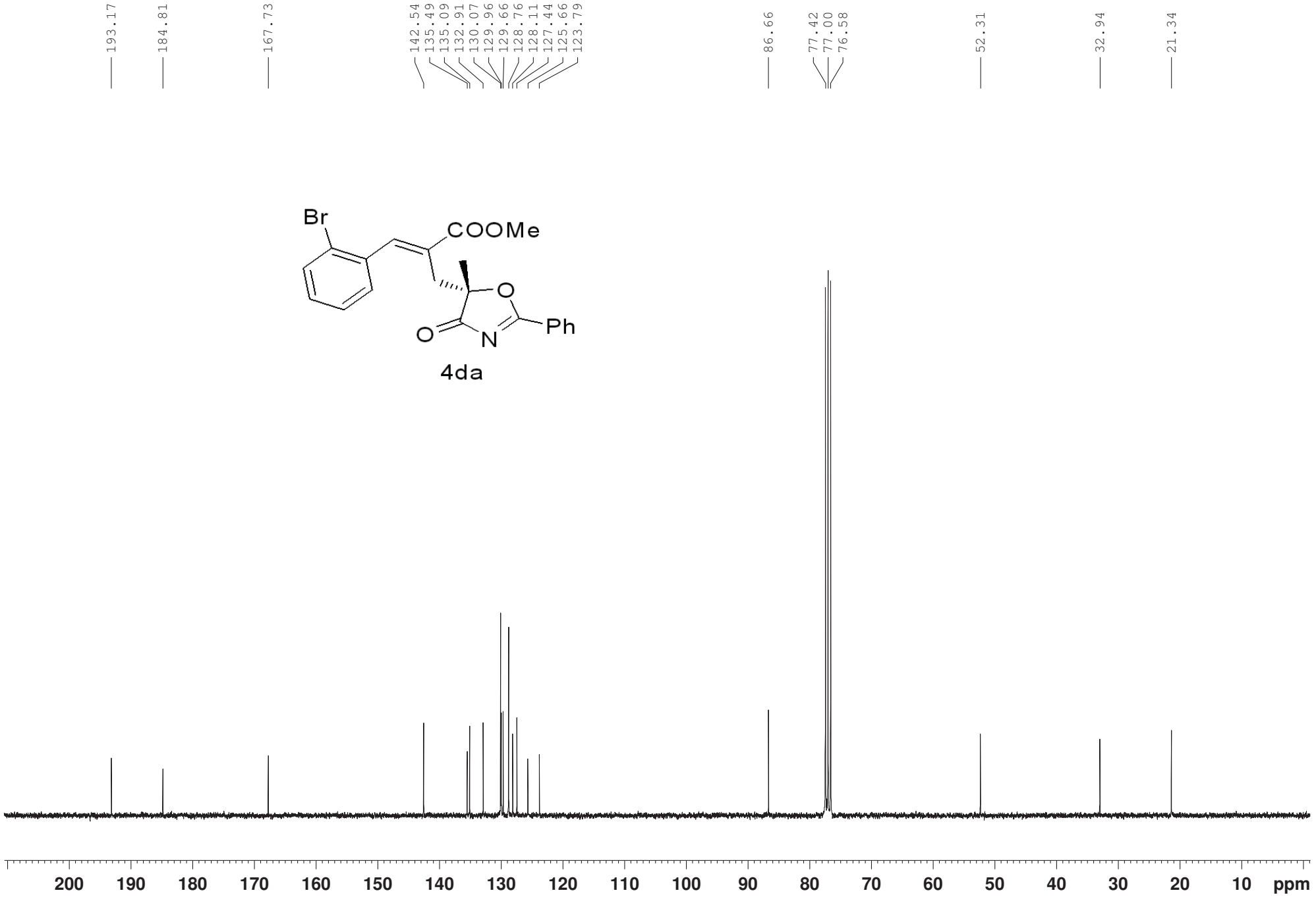
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Br
COOMe
O
O
N
Ph
4da
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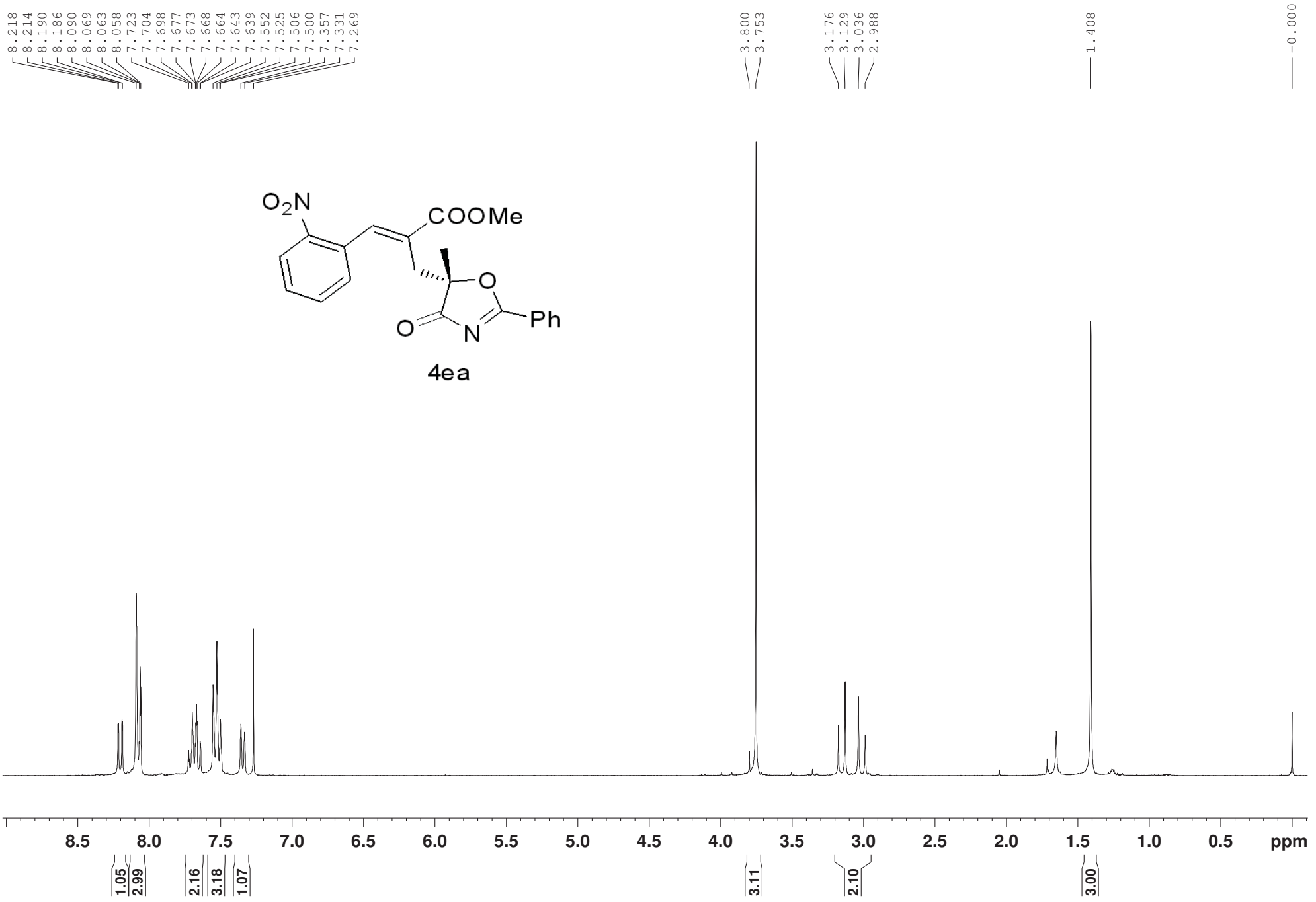
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7.500
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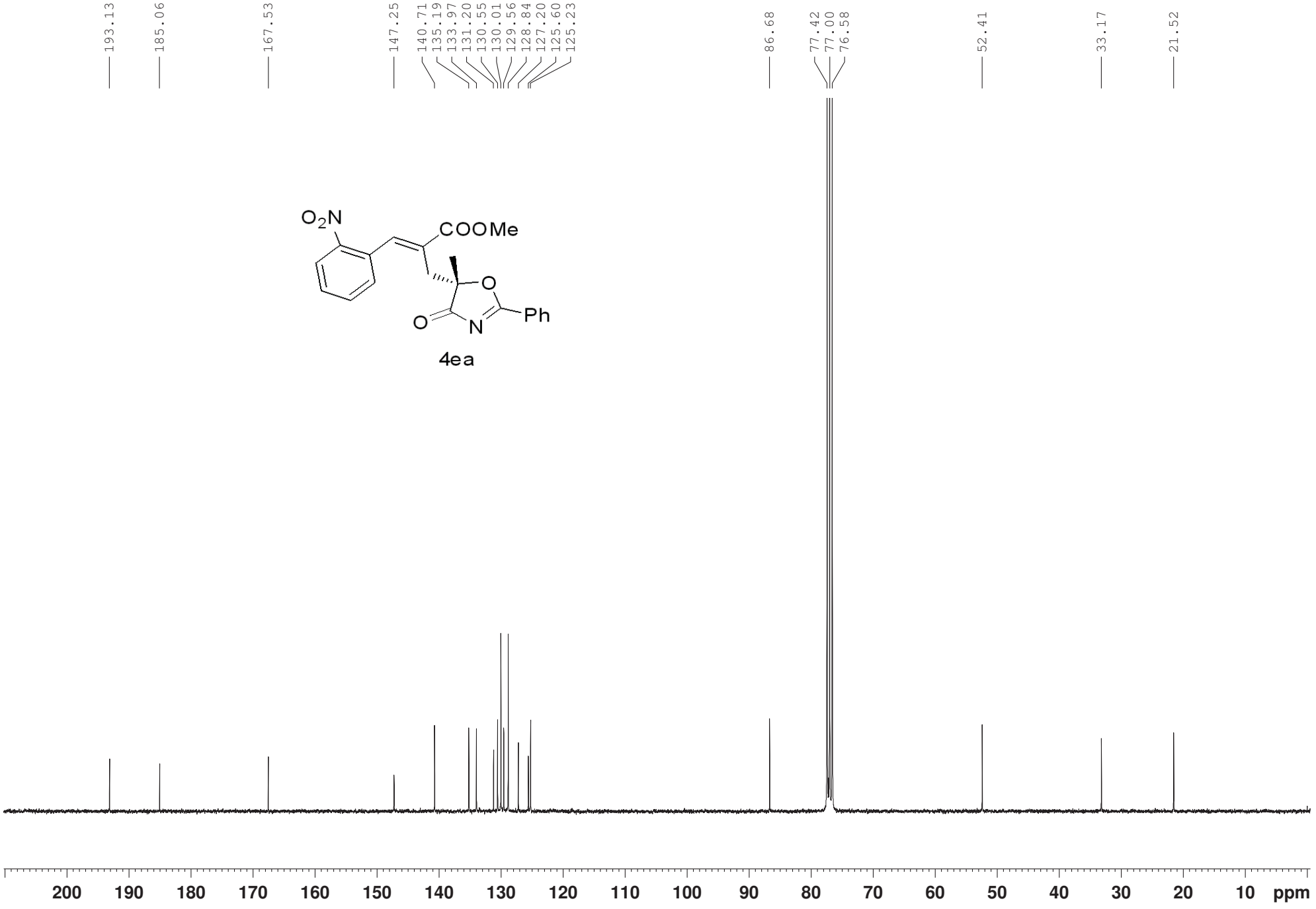
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125.23
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33.17
21.52
O2N
COOMe
O
O
N
Ph
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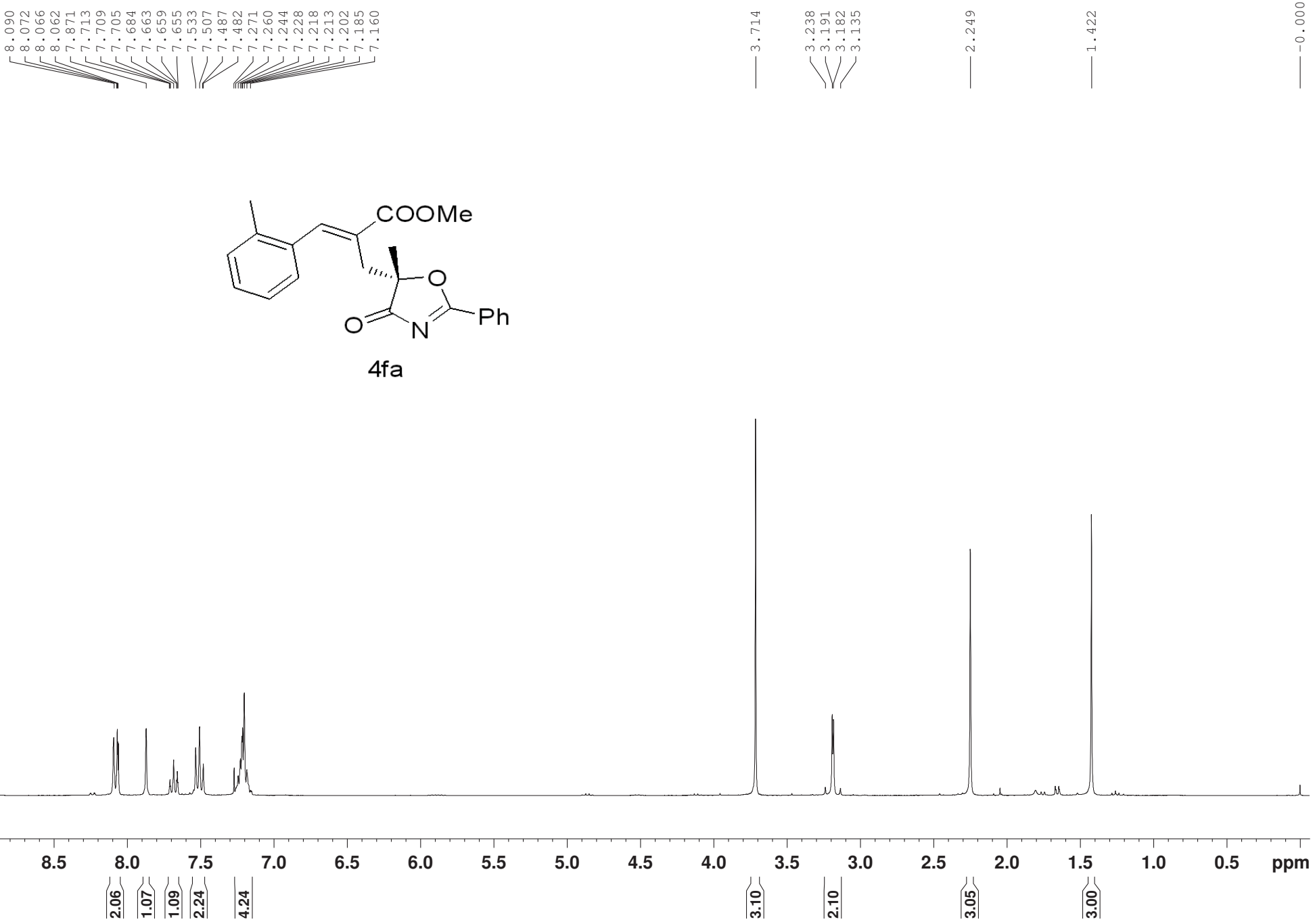
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7.228
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O
N
Ph
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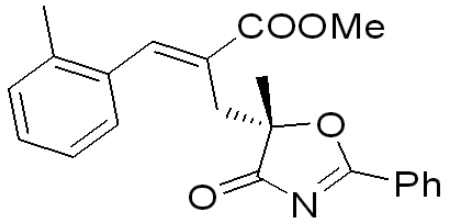

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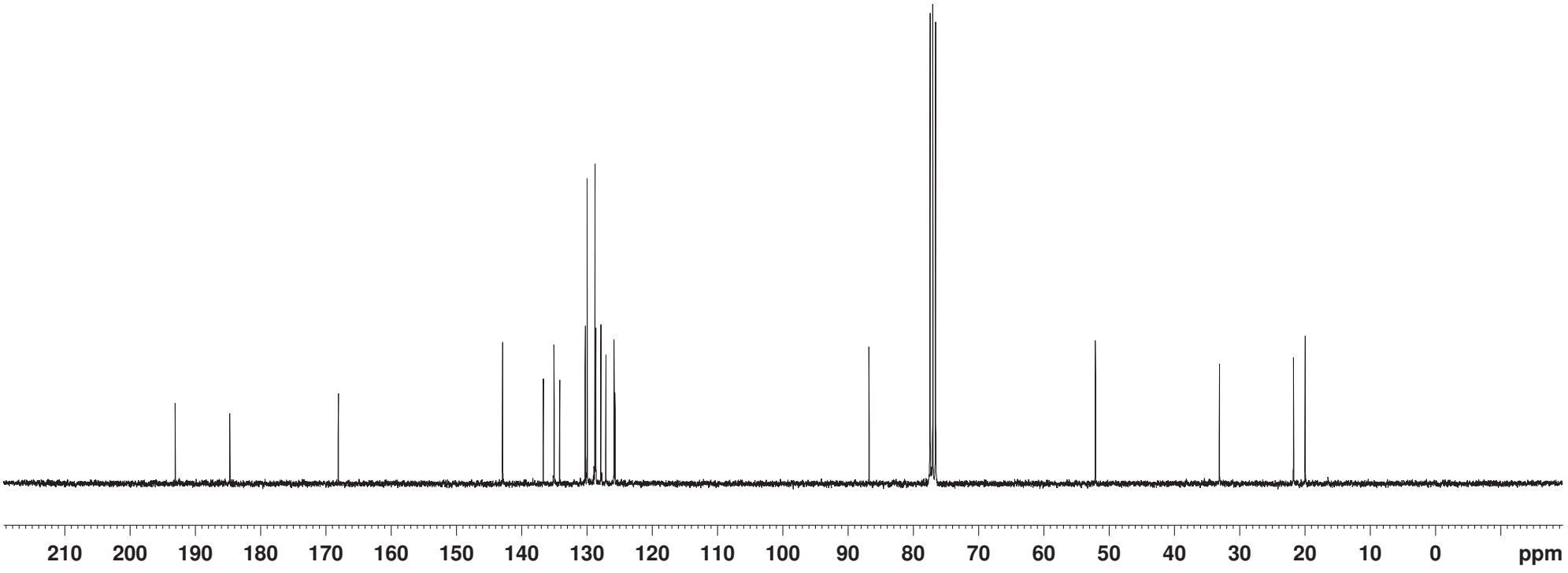

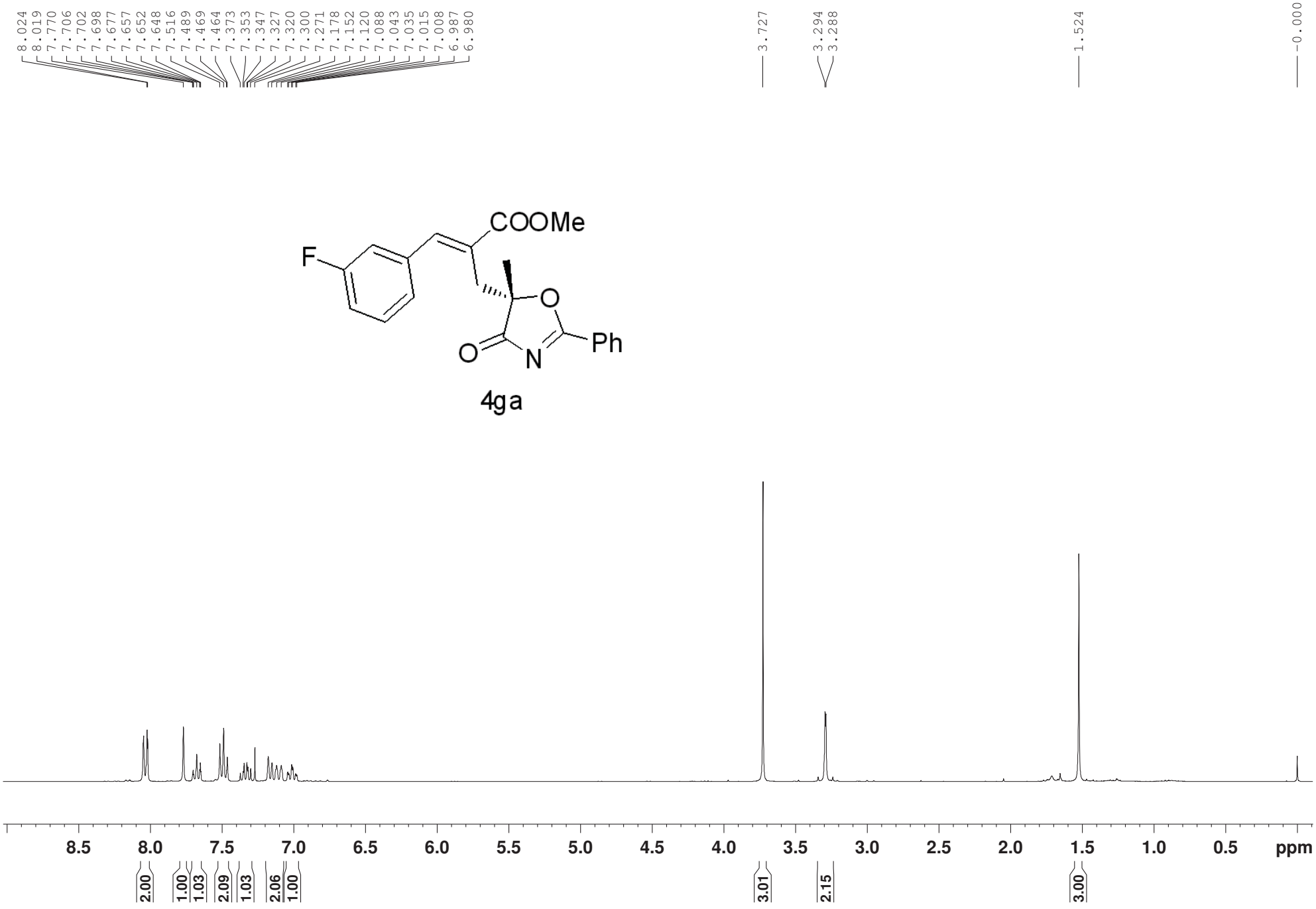
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7.320
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7.120
7.088
7.043
7.035
7.015
7.008
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6.980
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3.294
3.288
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COOMe
F
O
O
N
Ph
4ga
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
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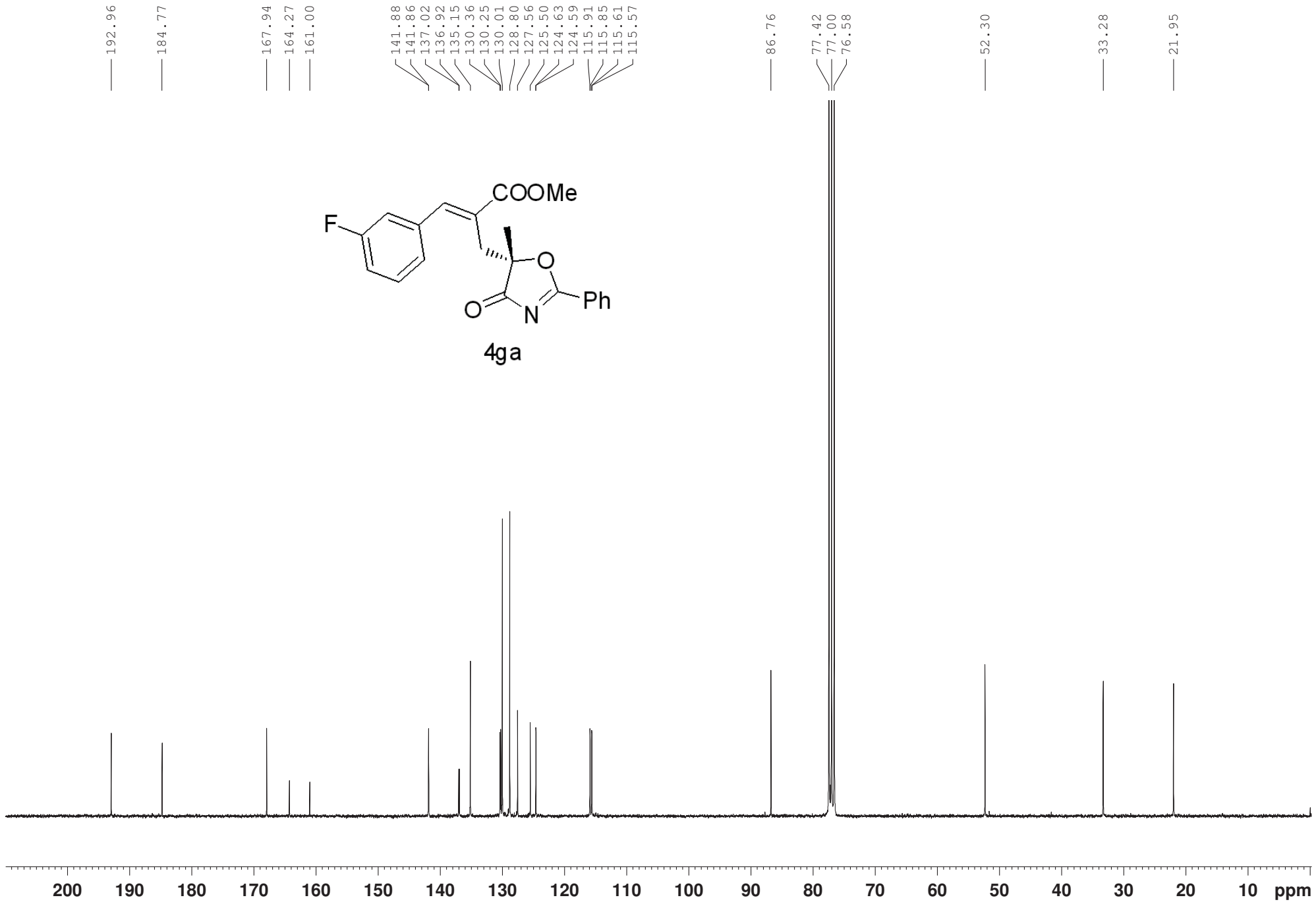
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124.59
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115.57
86.76
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COOMe
F
O
O
N
Ph
4ga
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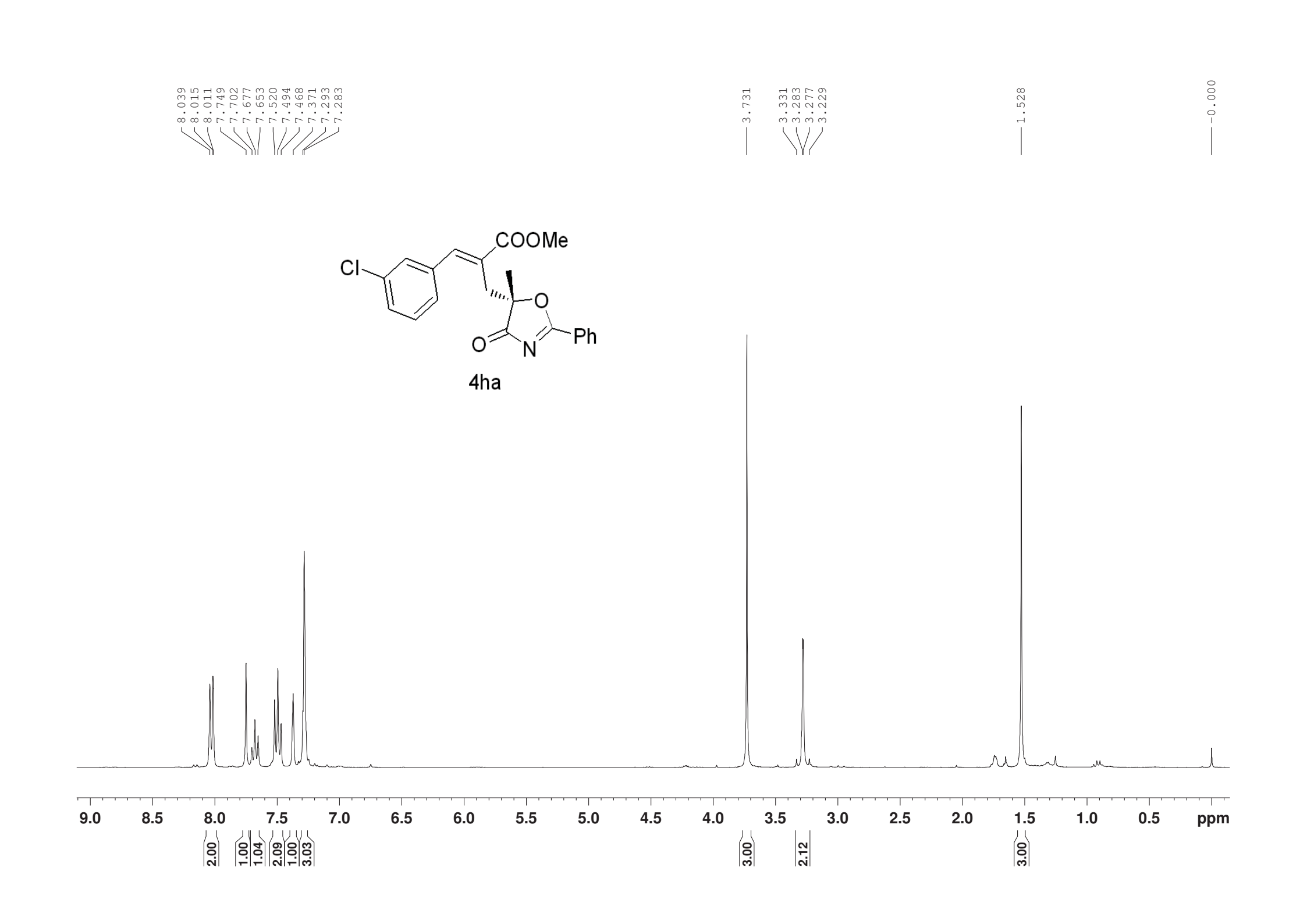
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7.520
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7.283
3.731
3.331
3.283
3.277
3.229
1.528
-0.000
COOMe
Cl
O
O
N
Ph
4ha
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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2.0
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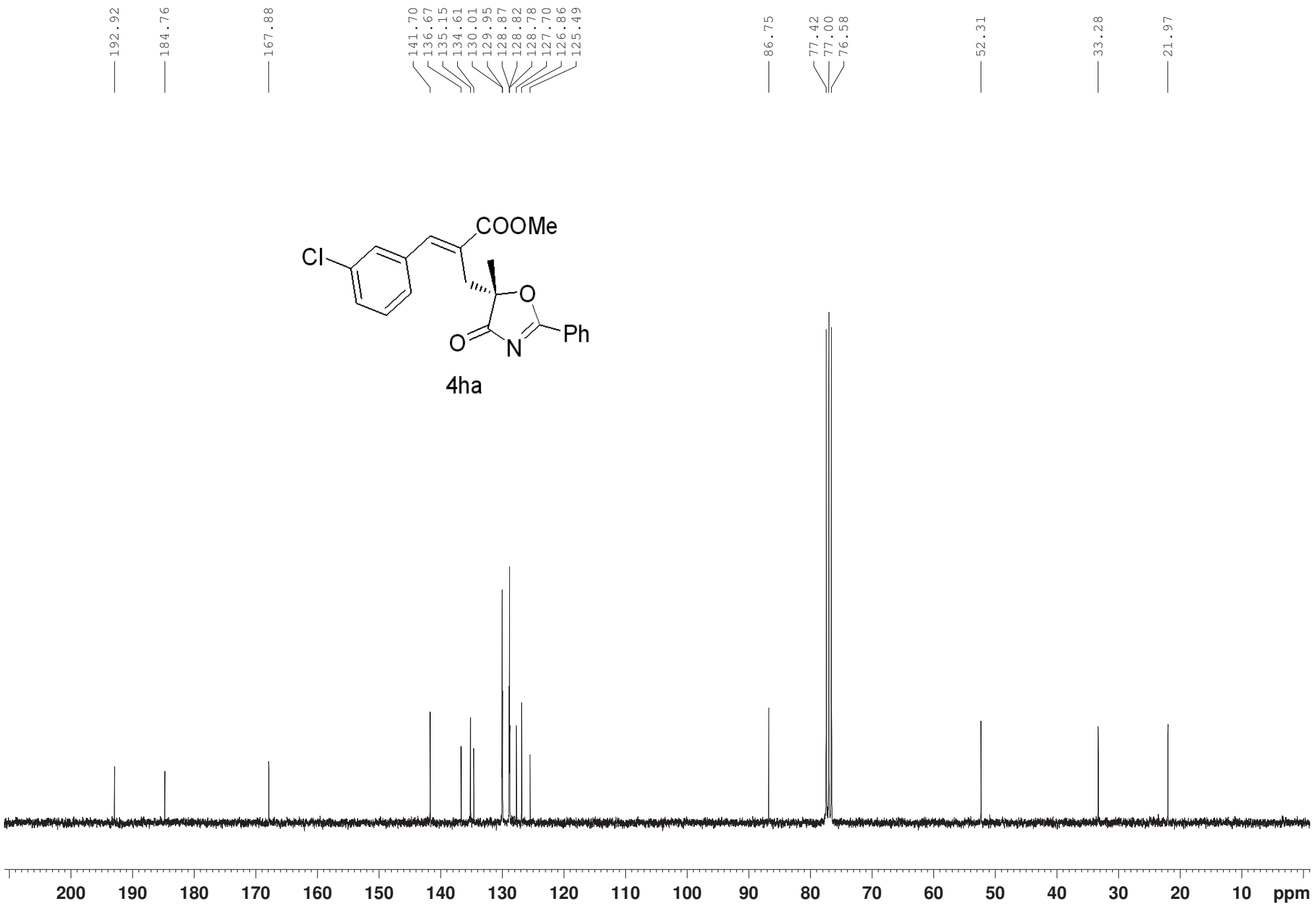
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125.49
86.75
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77.00
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52.31
33.28
21.97
COOMe
Cl
O
O
N
Ph
4ha
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100
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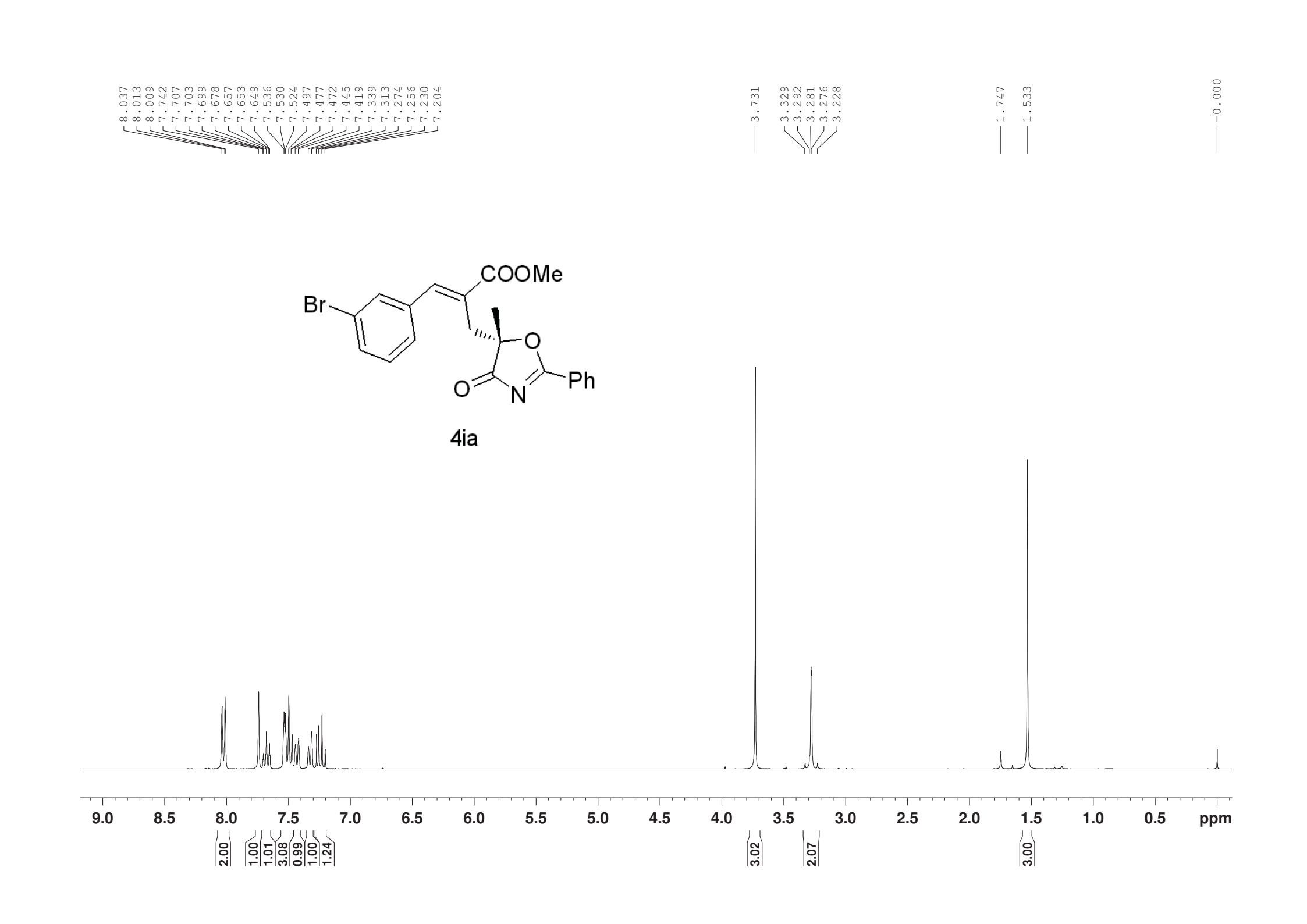
ppm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3.228
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O
N
Ph
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7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
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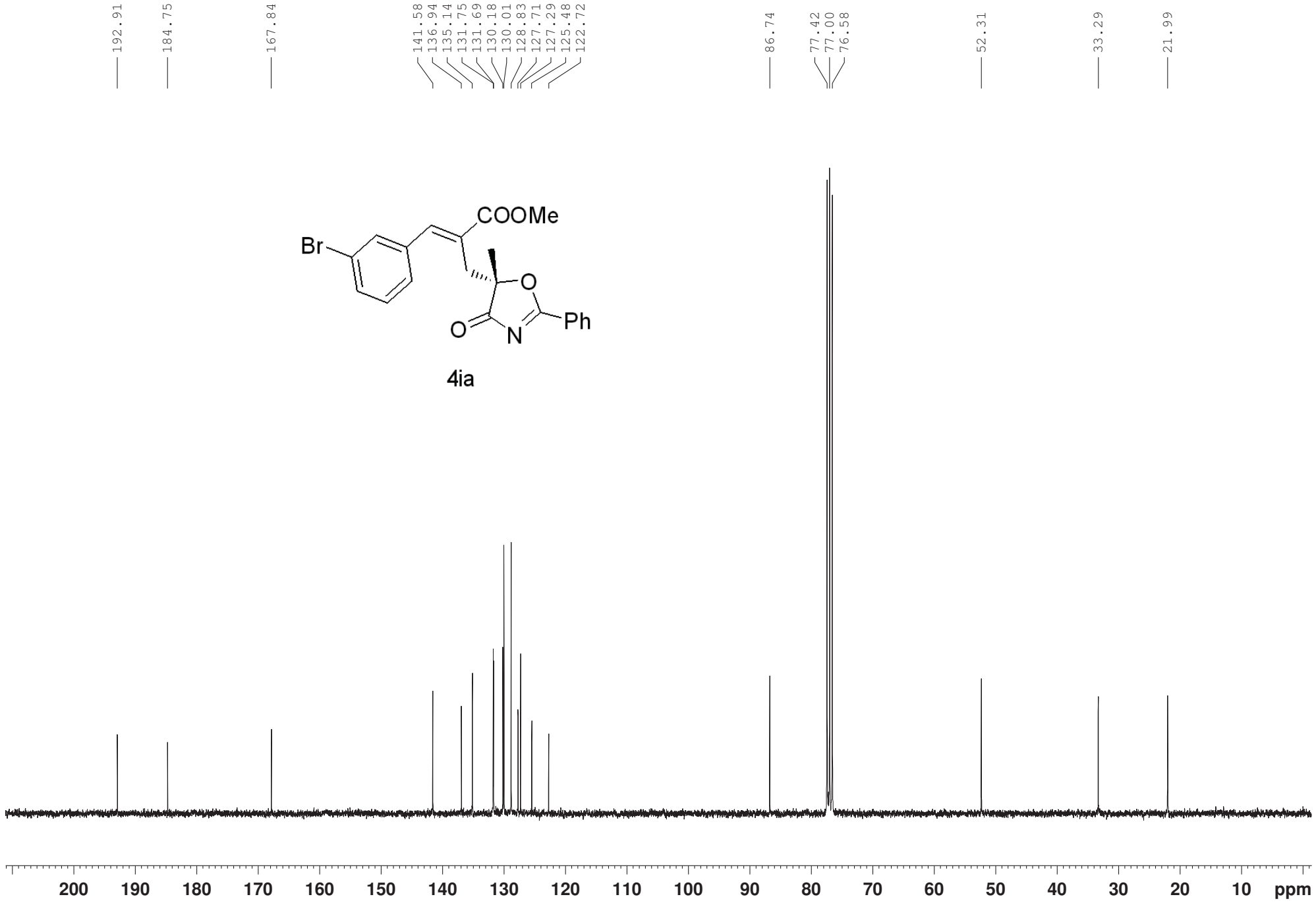
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77.00
76.58
52.31
33.29
21.99
COOMe
Br
O
O
N
Ph
4ia
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150
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130
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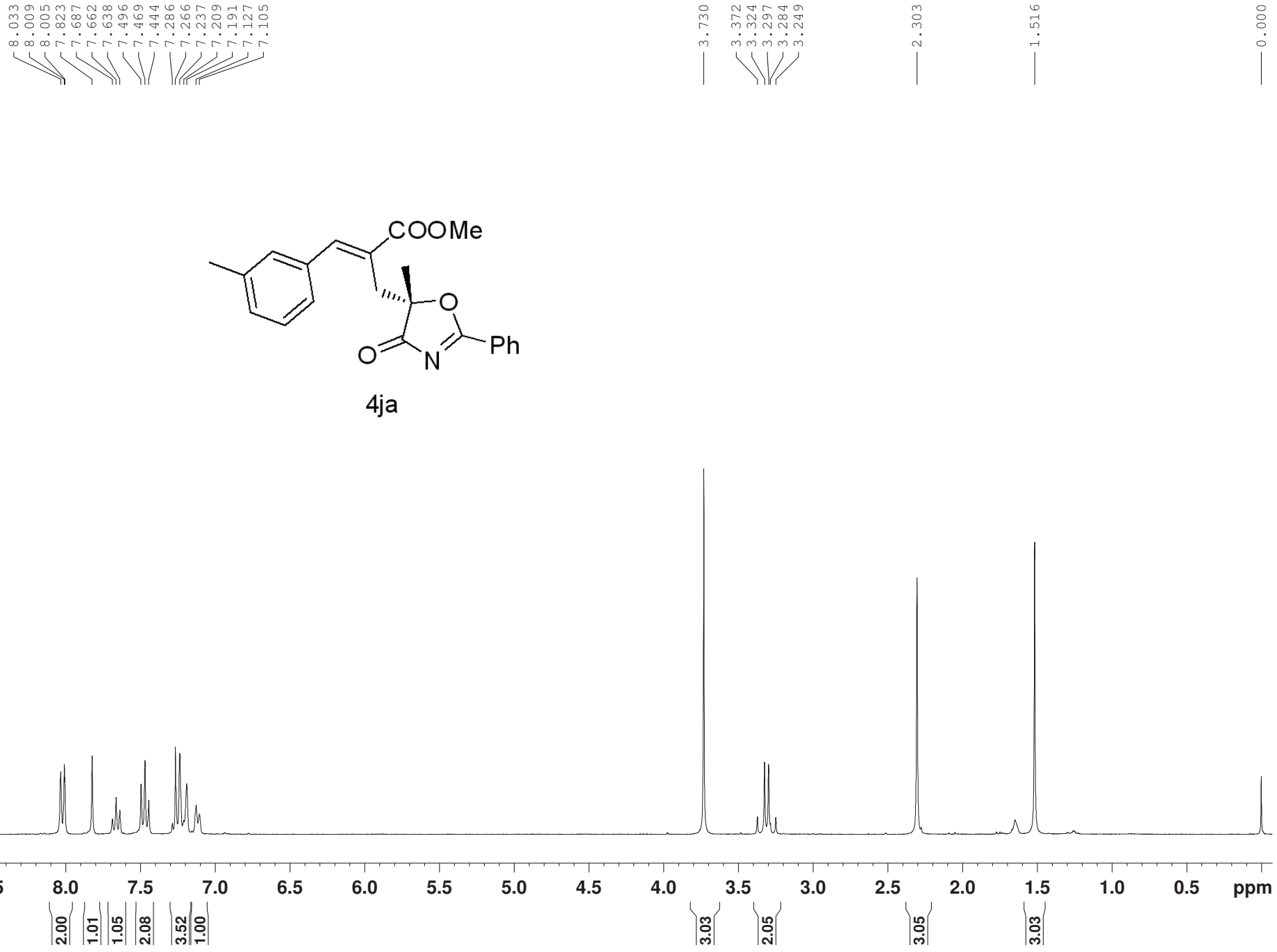
ppm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O
N
Ph
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8.0
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7.0
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6.0
5.5
5.0
4.5
4.0
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3.0
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2.0
1.5
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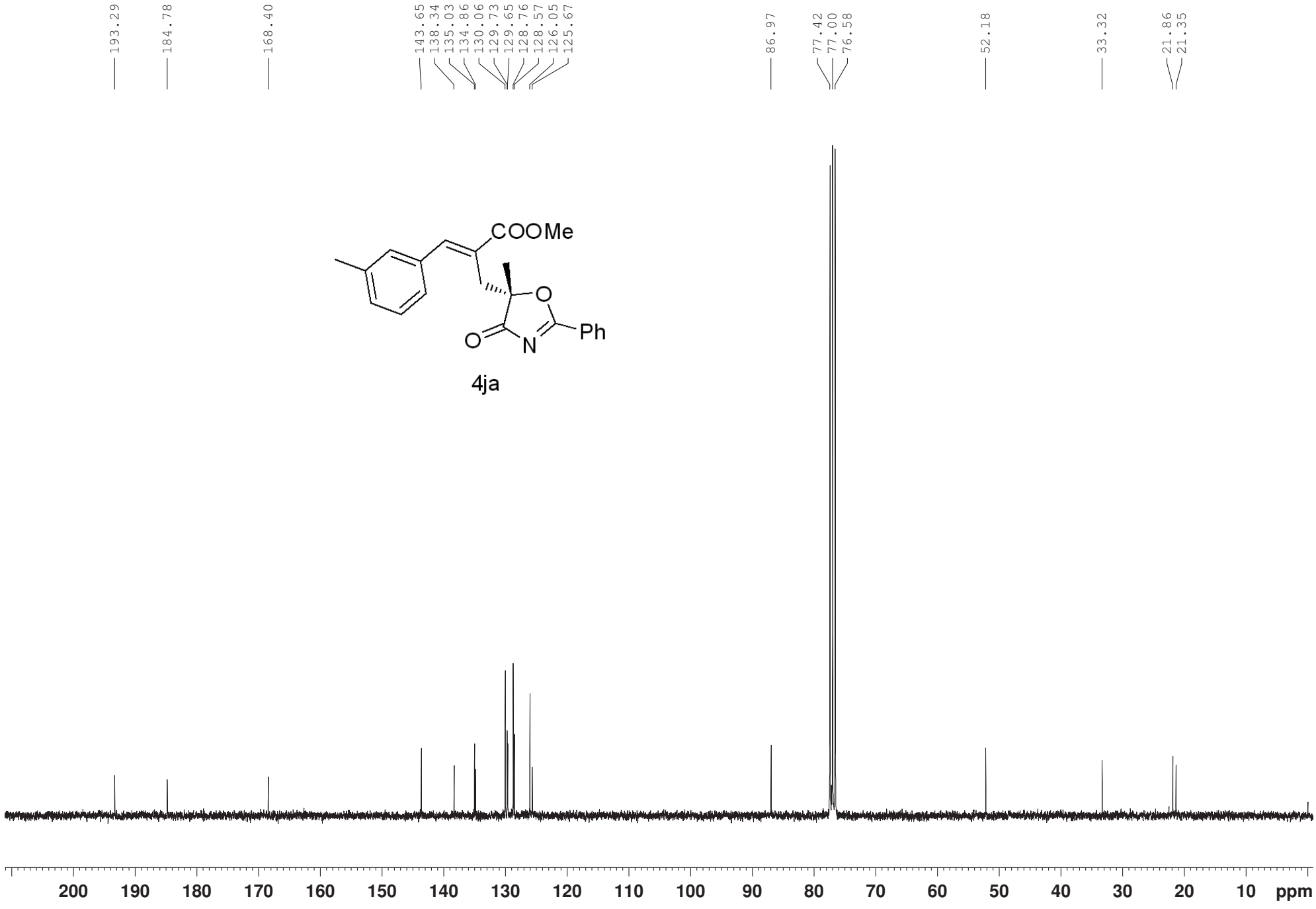
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77.42
77.00
76.58
52.18
33.32
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21.35
COOMe
O
O
N
Ph
4ja
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150
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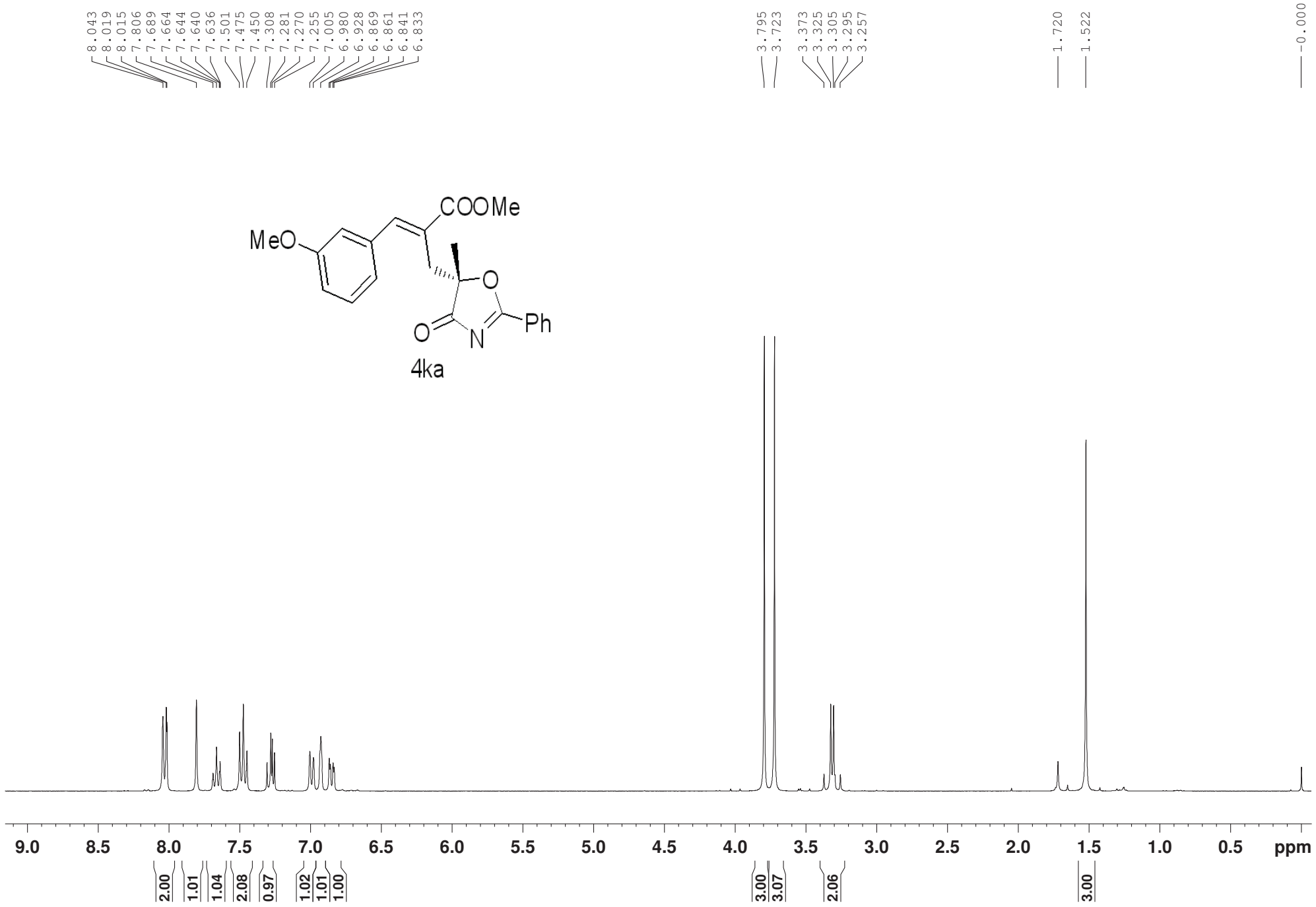
ppm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3.257
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1.522
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O
N
Ph
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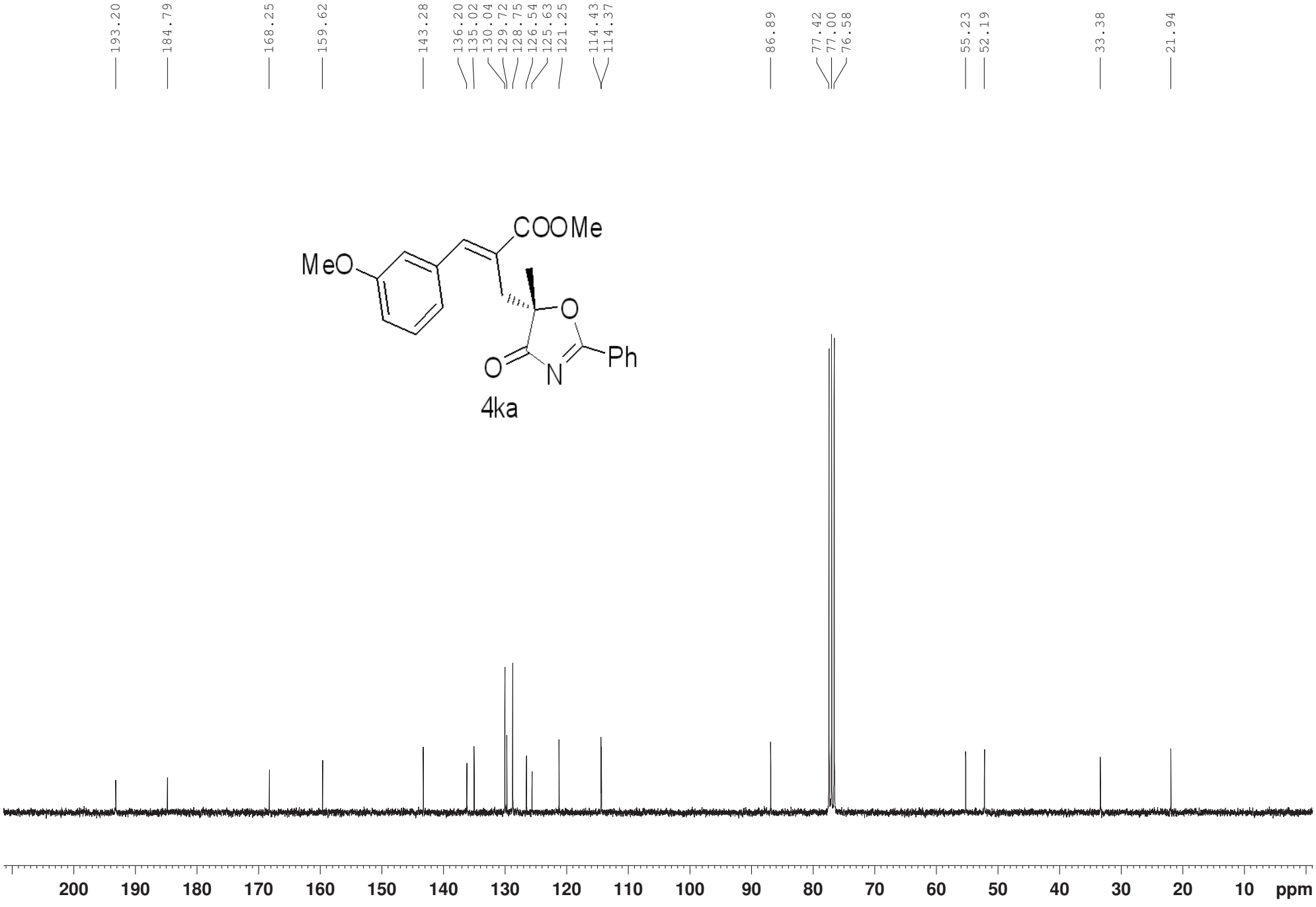
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114.37
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77.00
76.58
55.23
52.19
33.38
21.94
COOMe
MeO
O
O
N
Ph
4ka
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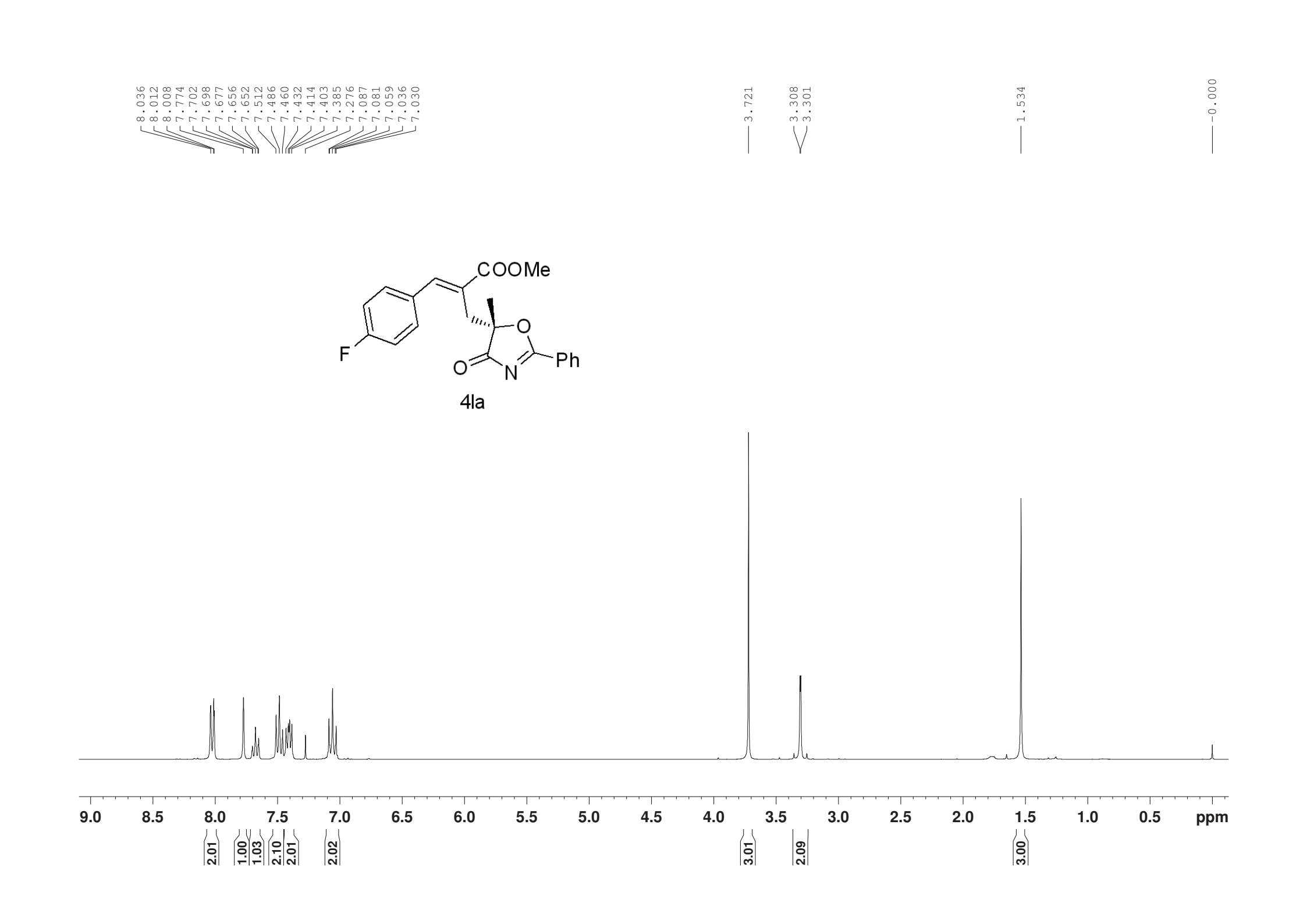
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7.030
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O
O
N
Ph
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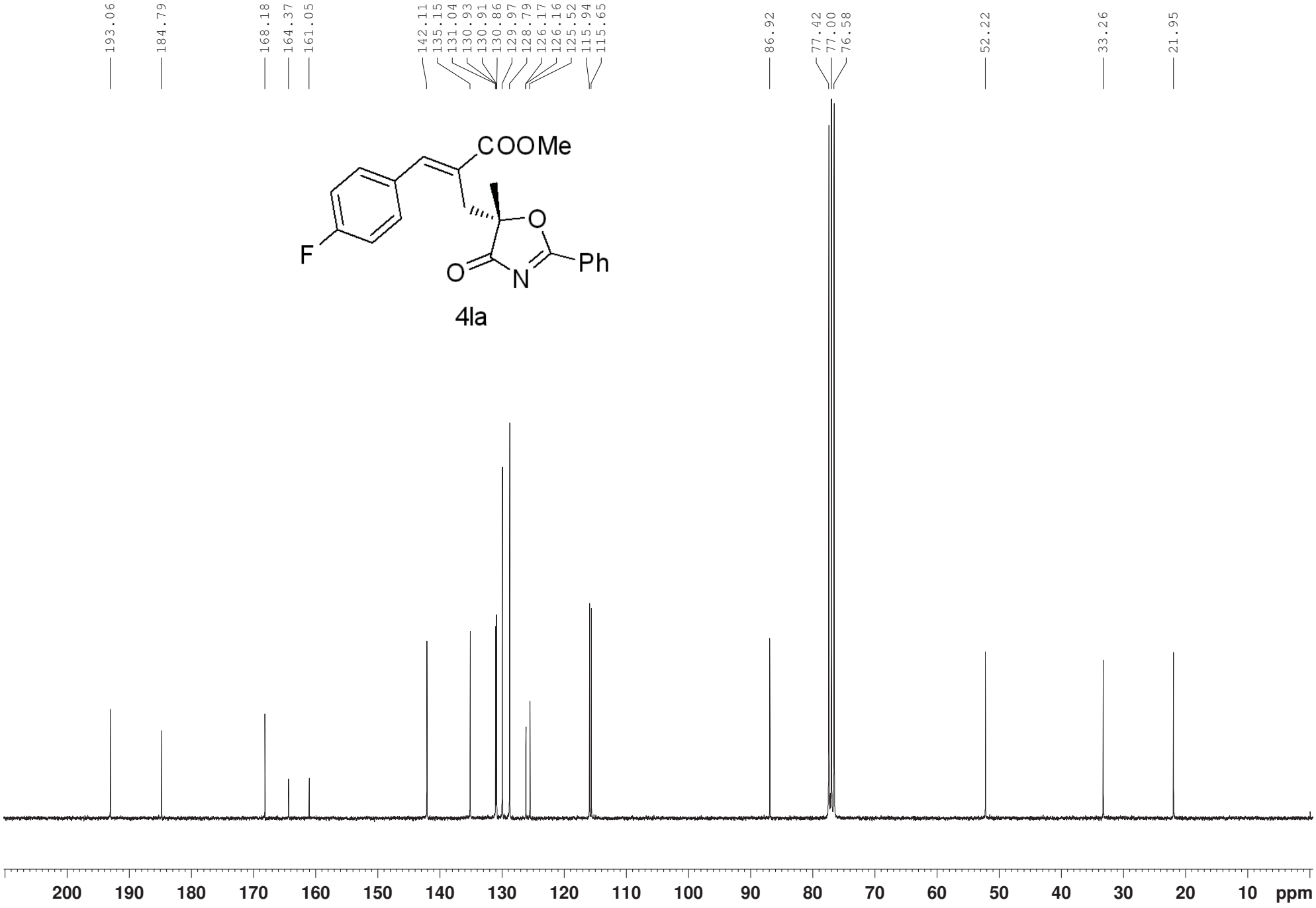
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126.16
125.52
115.94
115.65
86.92
77.42
77.00
76.58
52.22
33.26
21.95
COOMe
F
O
O
N
Ph
4la
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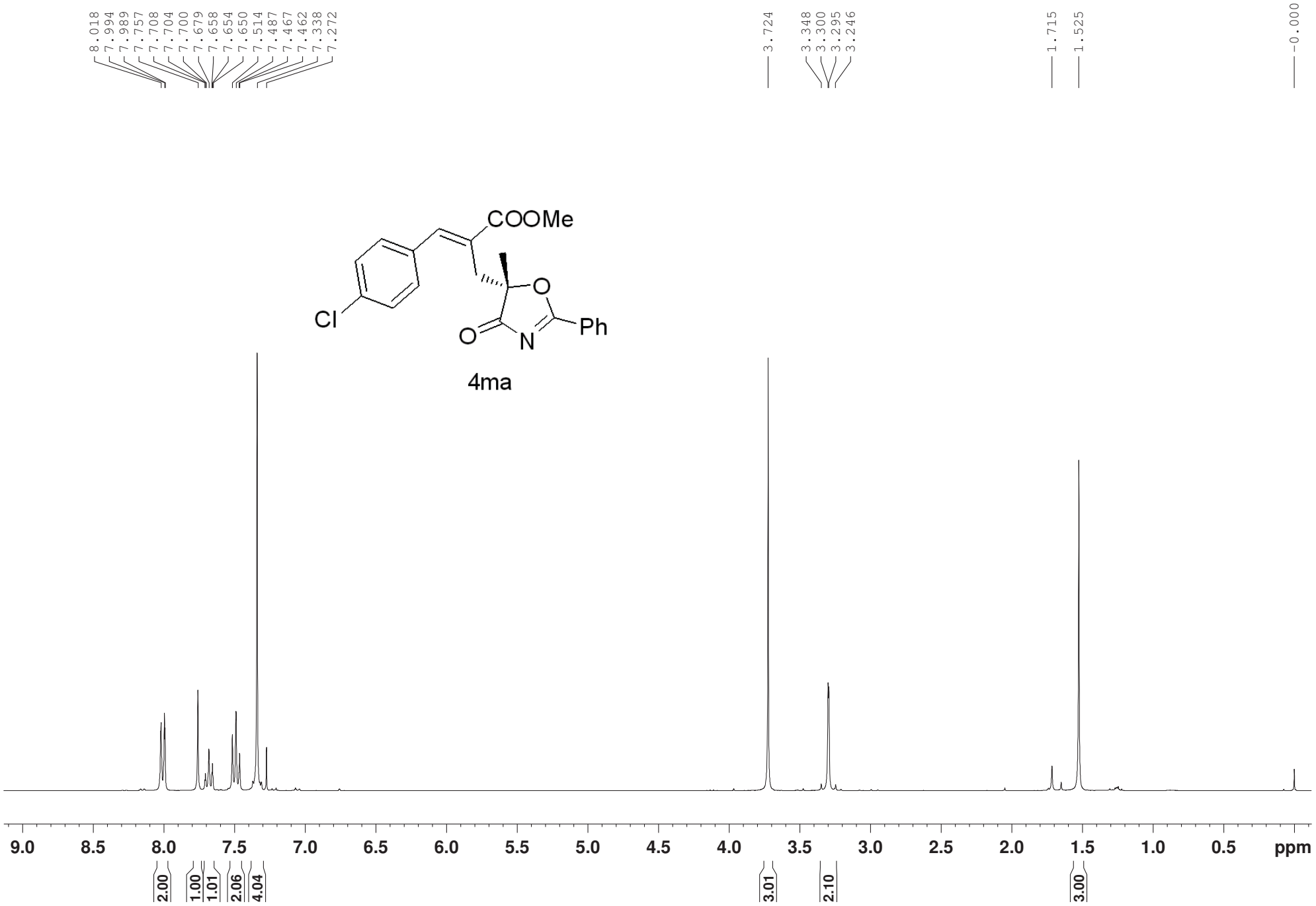
10
ppm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3.246
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1.525
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COOMe
Cl
O
O
N
Ph
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3.00

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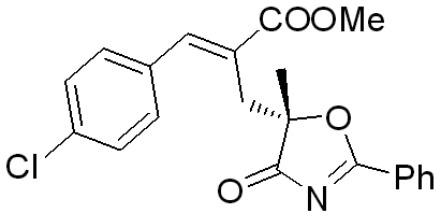

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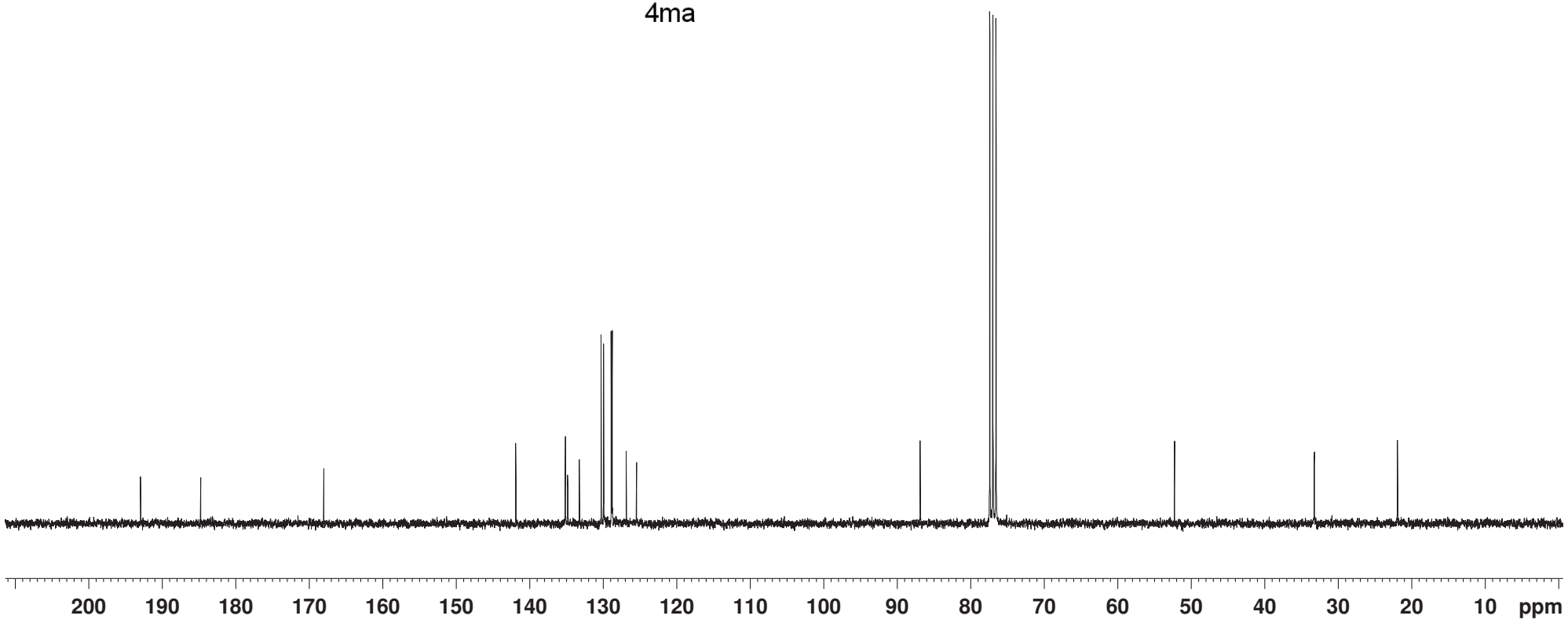

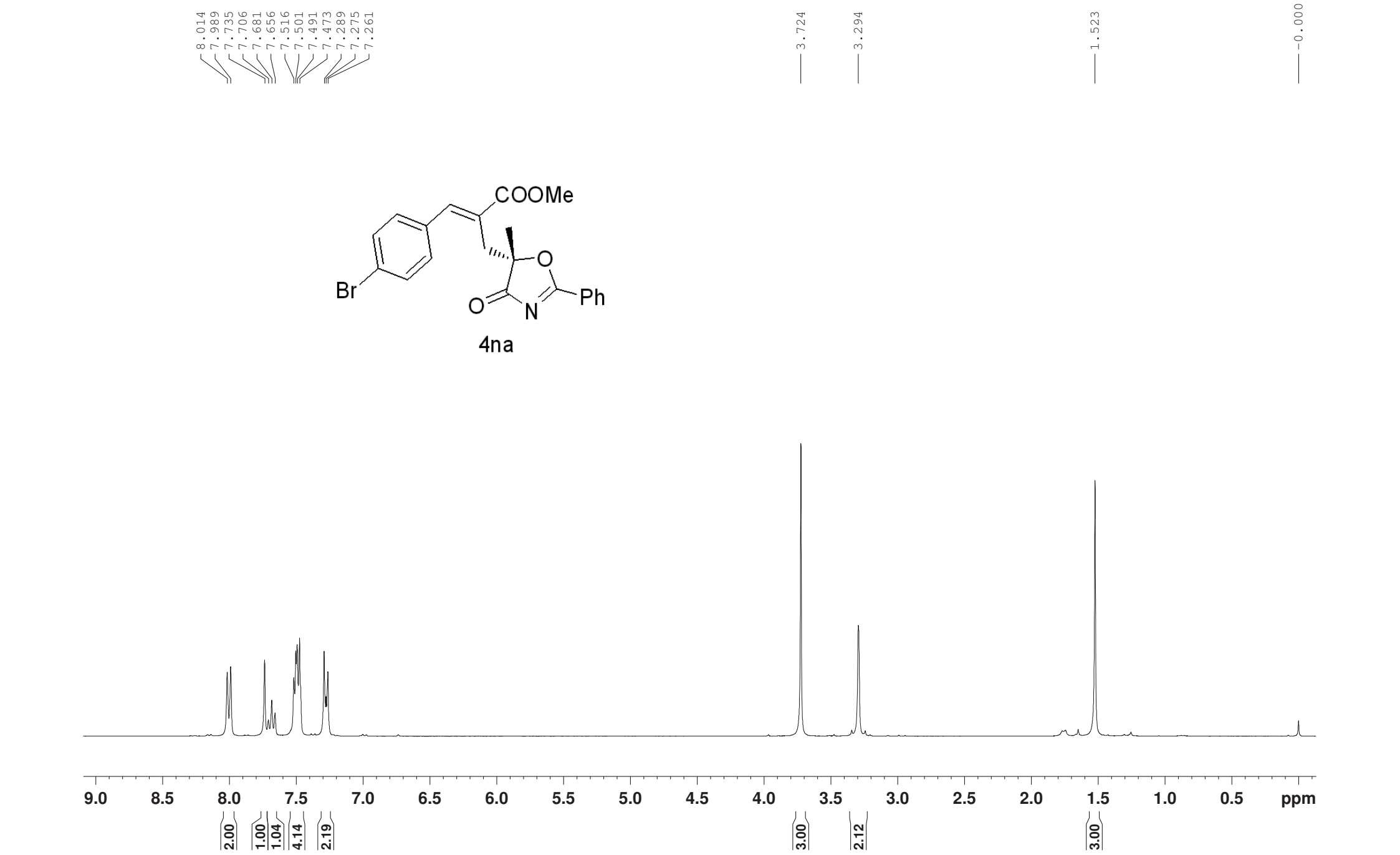
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3.294
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COOMe
Br
O
O
N
Ph
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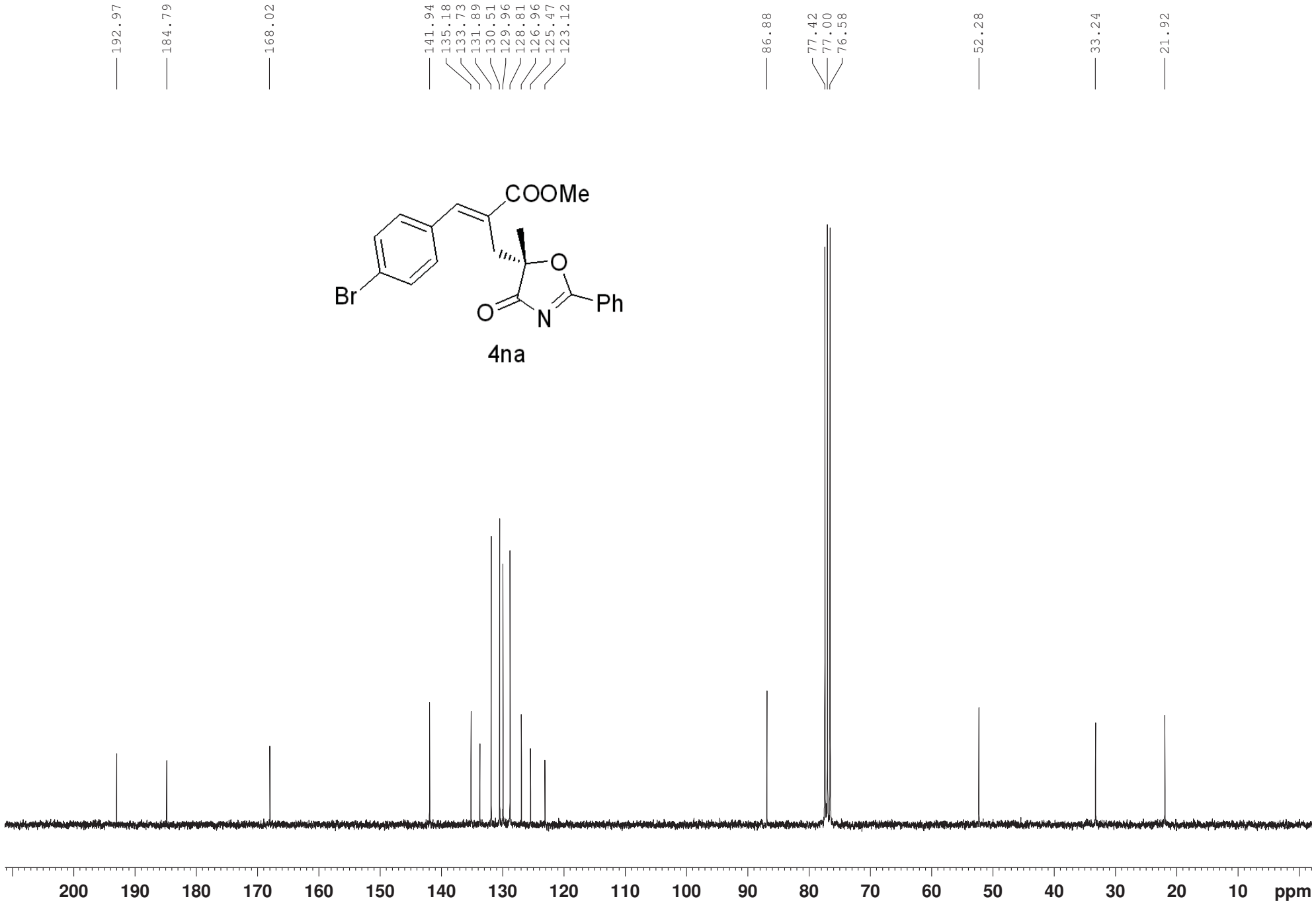
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77.42
77.00
76.58
52.28
33.24
21.92
COOMe
Br
O
O
N
Ph
4na
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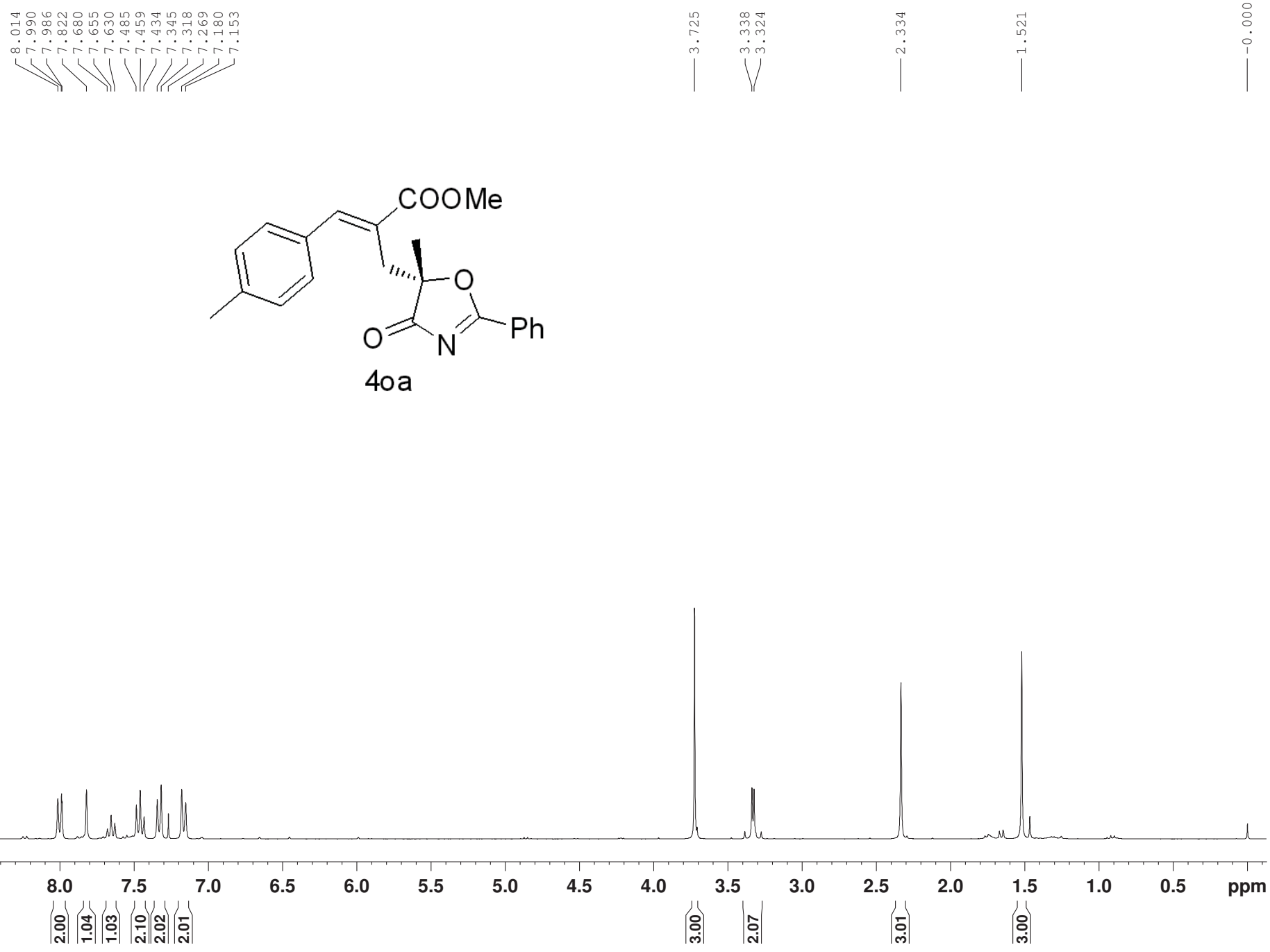
ppm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7.180
7.153
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O
O
N
Ph
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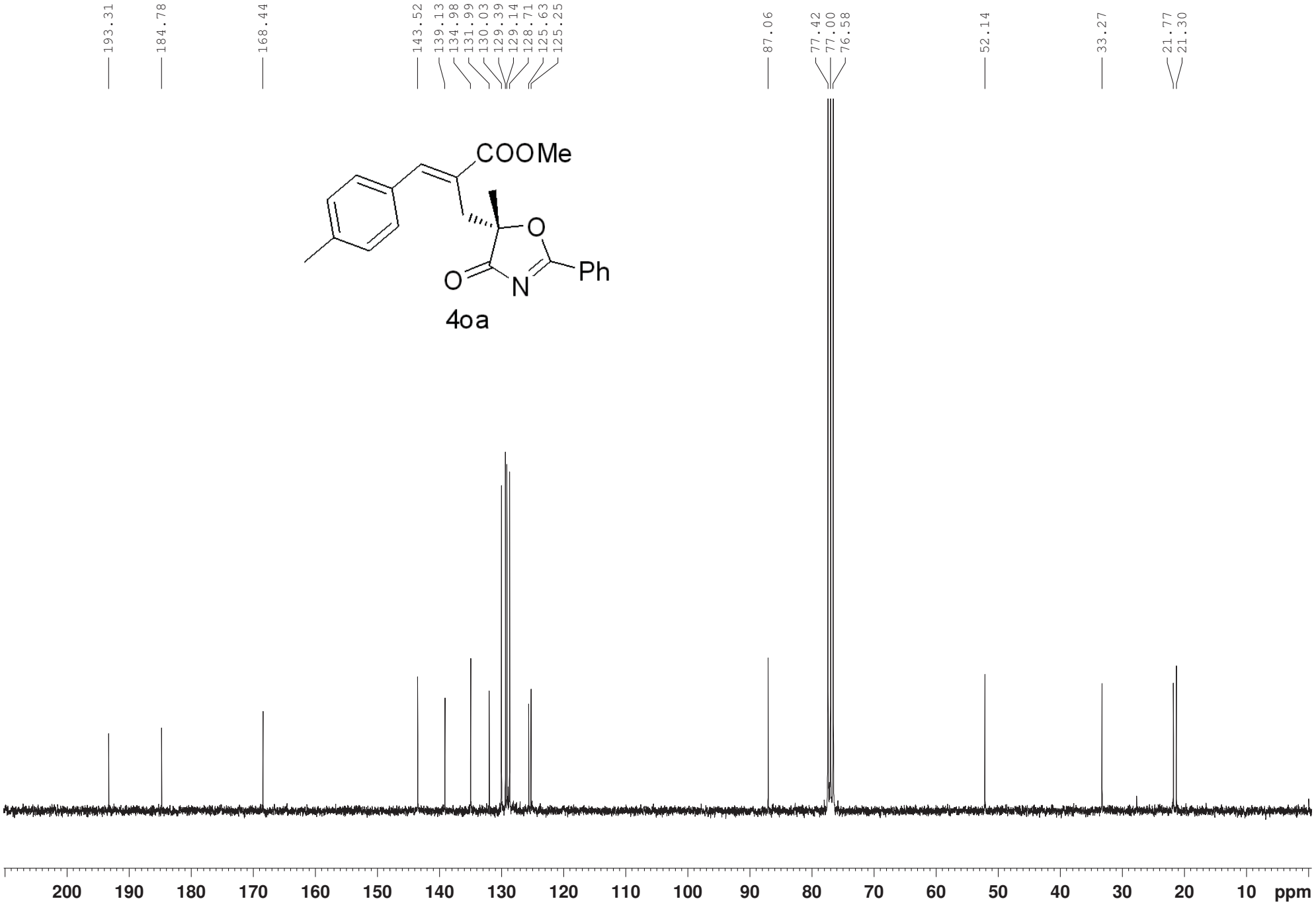
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O
O
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Ph
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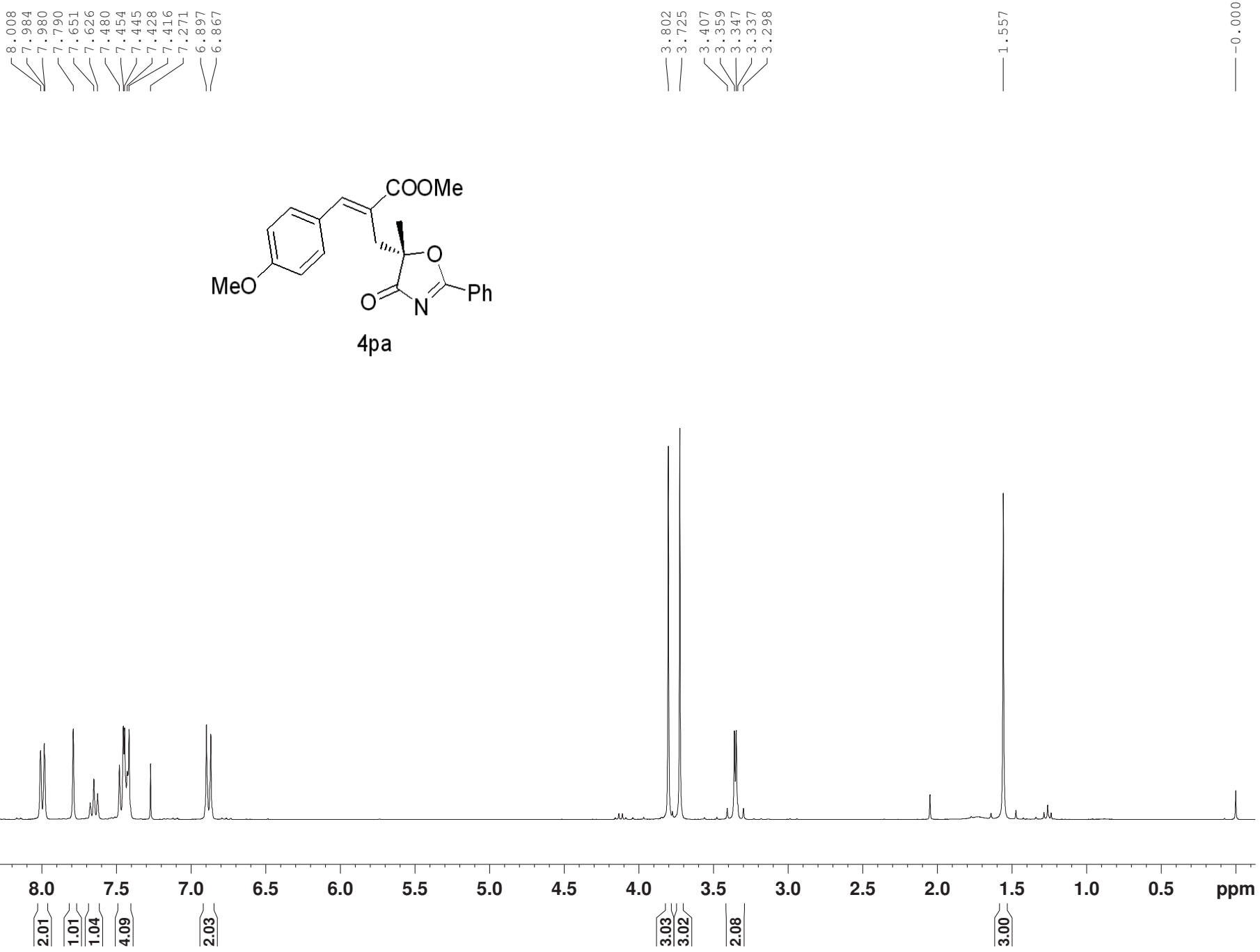
10
ppm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7.980
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7.651
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7.454
7.445
7.428
7.416
7.271
6.897
6.867
3.802
3.725
3.407
3.359
3.347
3.337
3.298
1.557
-0.000
COOMe
MeO
O
O
N
Ph
4pa
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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ppm
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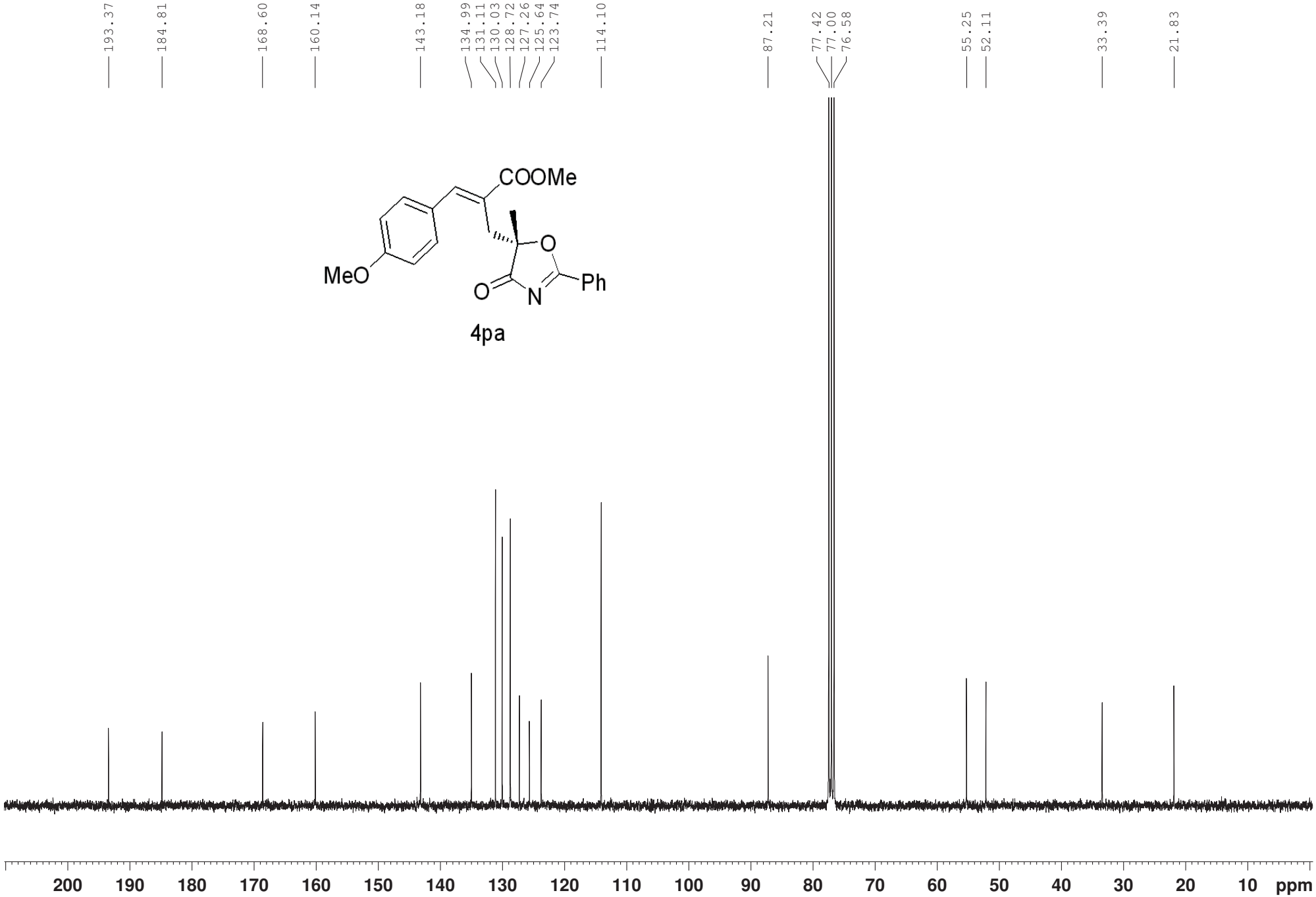
1.01
1.04
4.09
2.03
3.03
3.02
2.08
3.00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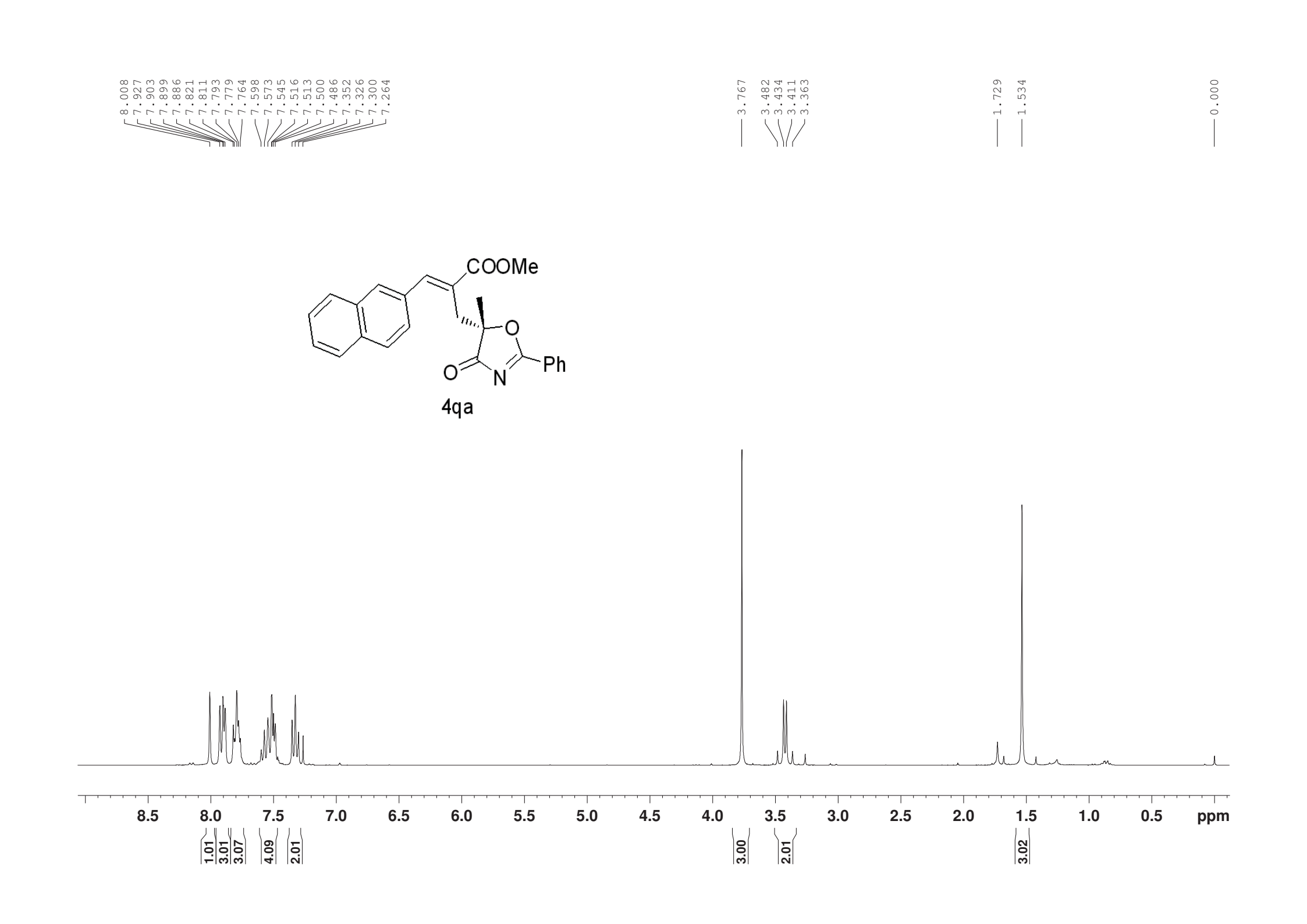
184.81
168.60
160.14
143.18
134.99
131.11
130.03
128.72
127.26
125.64
123.74
114.10
87.21
77.42
77.00
76.58
55.25
52.11
33.39
21.83
COOMe
MeO
O
O
N
Ph
4pa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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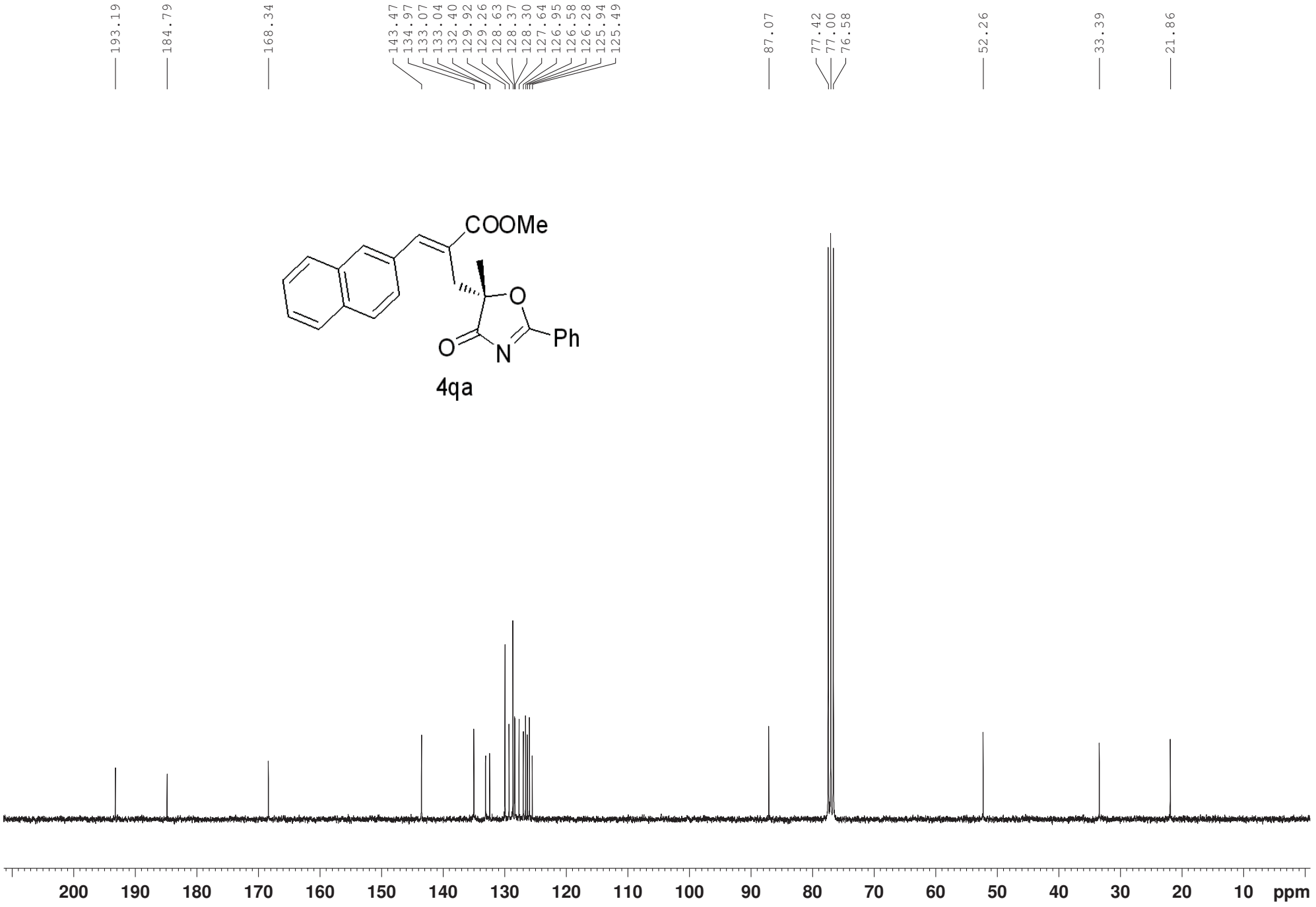
7.903
7.899
7.886
7.821
7.811
7.793
7.779
7.764
7.598
7.573
7.545
7.516
7.513
7.500
7.486
7.352
7.326
7.300
7.264
3.767
3.482
3.434
3.411
3.363
1.729
1.534
0.000
COOMe
O
O
N
Ph
4qa
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.01
3.01
3.07
4.09
2.01
3.00
2.01
3.02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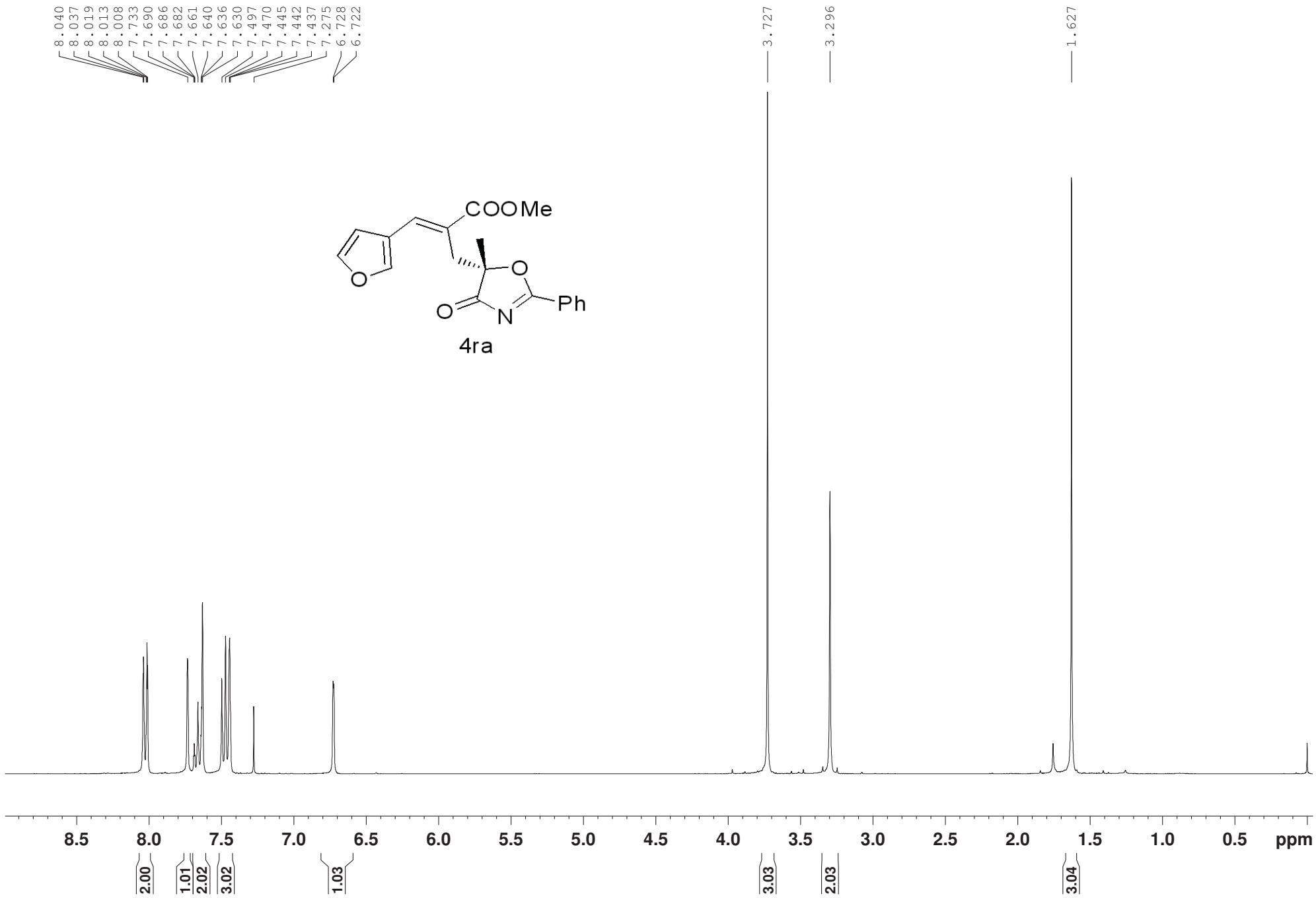
184.79
168.34
143.47
134.97
133.07
133.04
132.40
129.92
129.26
128.63
128.37
128.30
127.64
126.95
126.58
126.28
125.94
125.49
87.07
77.42
77.00
76.58
52.26
33.39
21.86
COOMe
O
O
N
Ph
4qa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.686
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7.661
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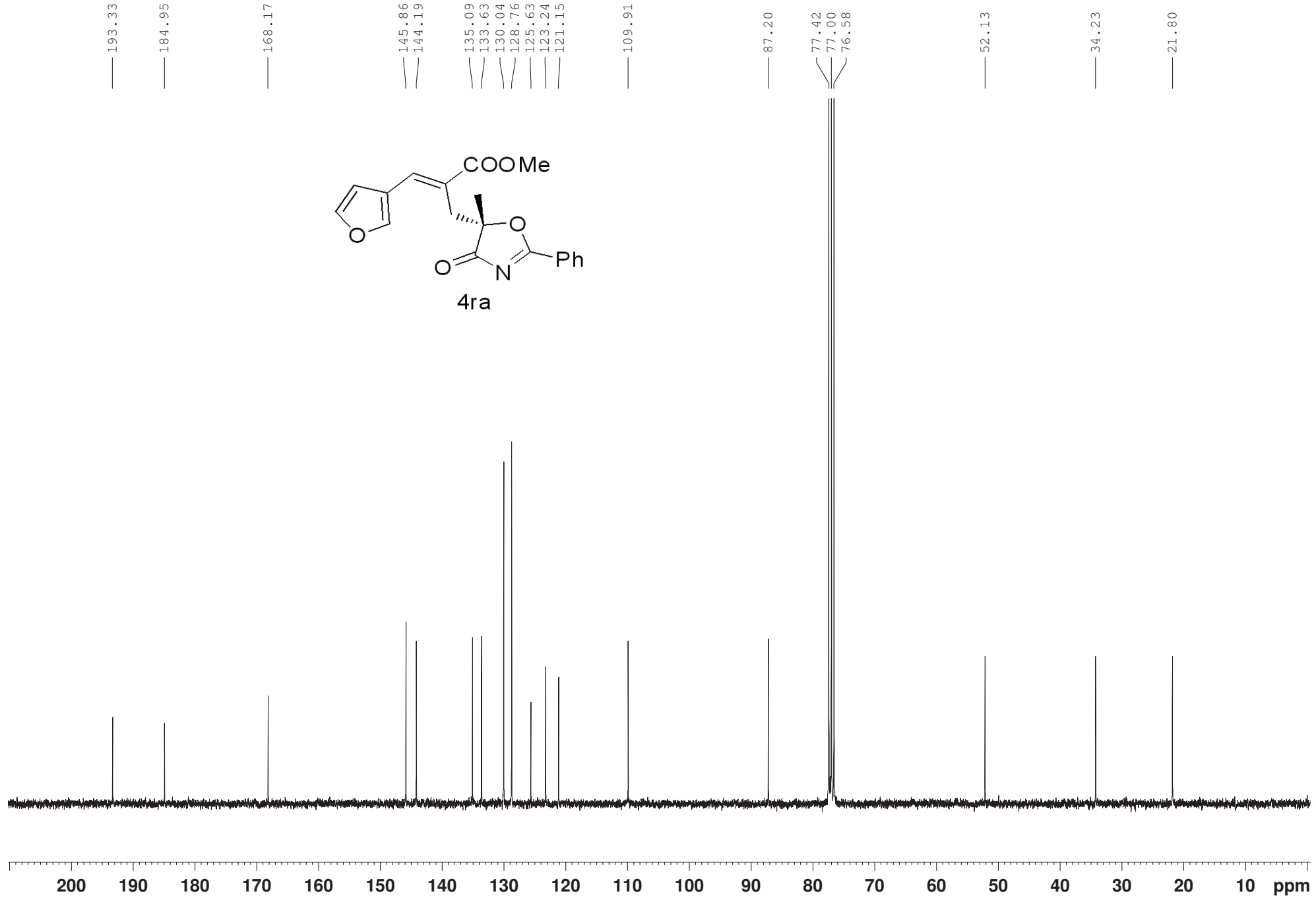
7.636
7.630
7.497
7.470
7.445
7.442
7.437
7.275
6.728
6.722
3.727
3.296
1.627
COOMe
O
O
O
N
Ph
4ra
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
1.01
2.02
3.02
1.03
3.03
2.03
3.04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168.17
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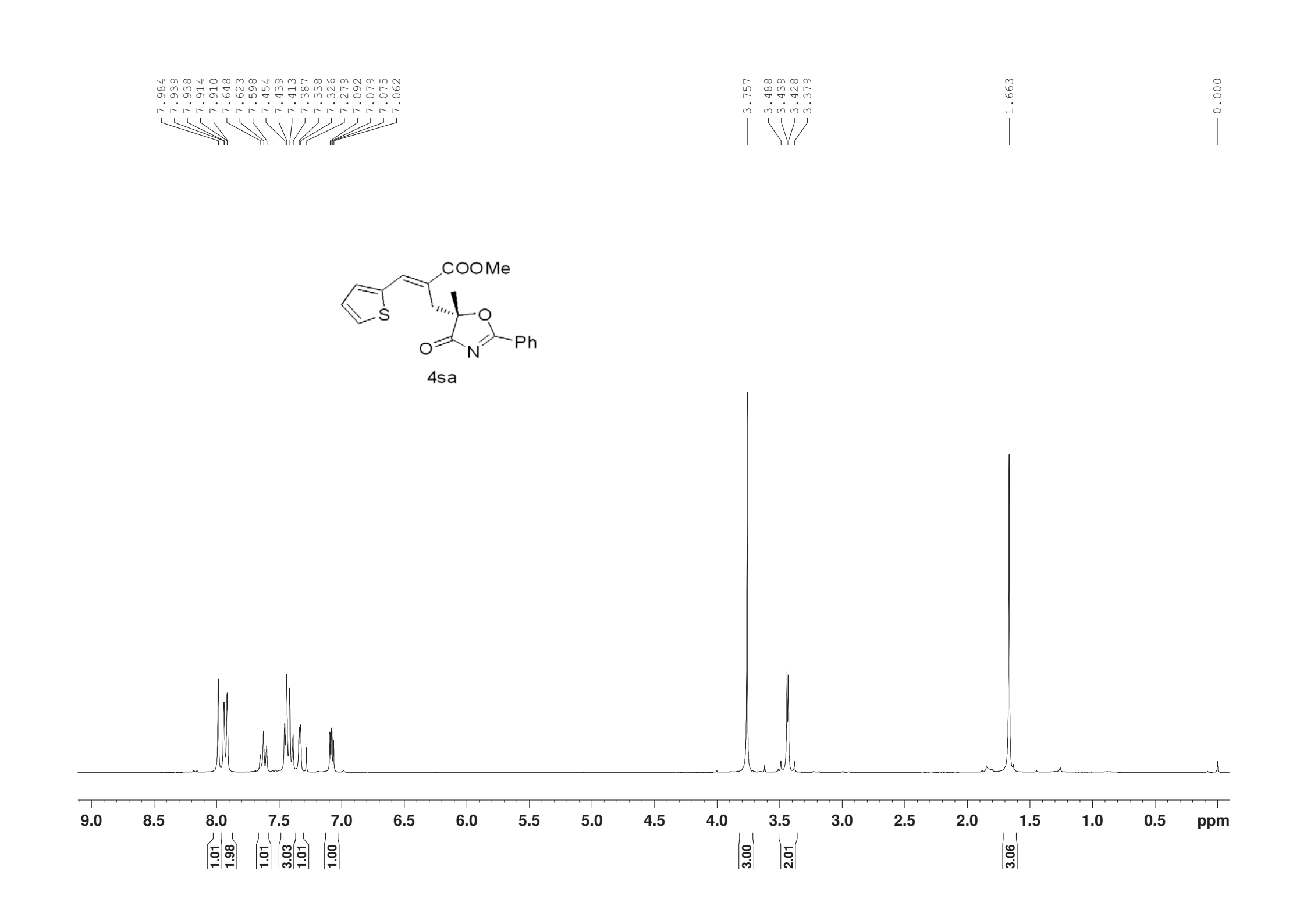
135.09
133.63
130.04
128.76
125.63
123.24
121.15
109.91
87.20
77.42
77.00
76.58
52.13
34.23
21.80
COOMe
O
O
O
N
Ph
4ra
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.939
7.938
7.914
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7.623
7.598
7.454
7.439
7.413
7.387
7.338
7.326
7.279
7.092
7.079
7.075
7.062
3.757
3.488
3.439
3.428
3.379
1.663
0.000
COOMe
S
O
O
N
Ph
4sa
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.01
1.98
1.01
3.03
1.01
1.00
3.00
2.01
3.06

193.14
184.86
168.12
137.47
136.14
134.91
134.05
130.00
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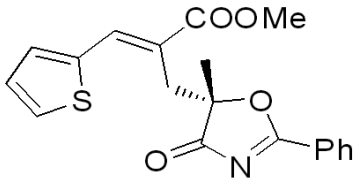
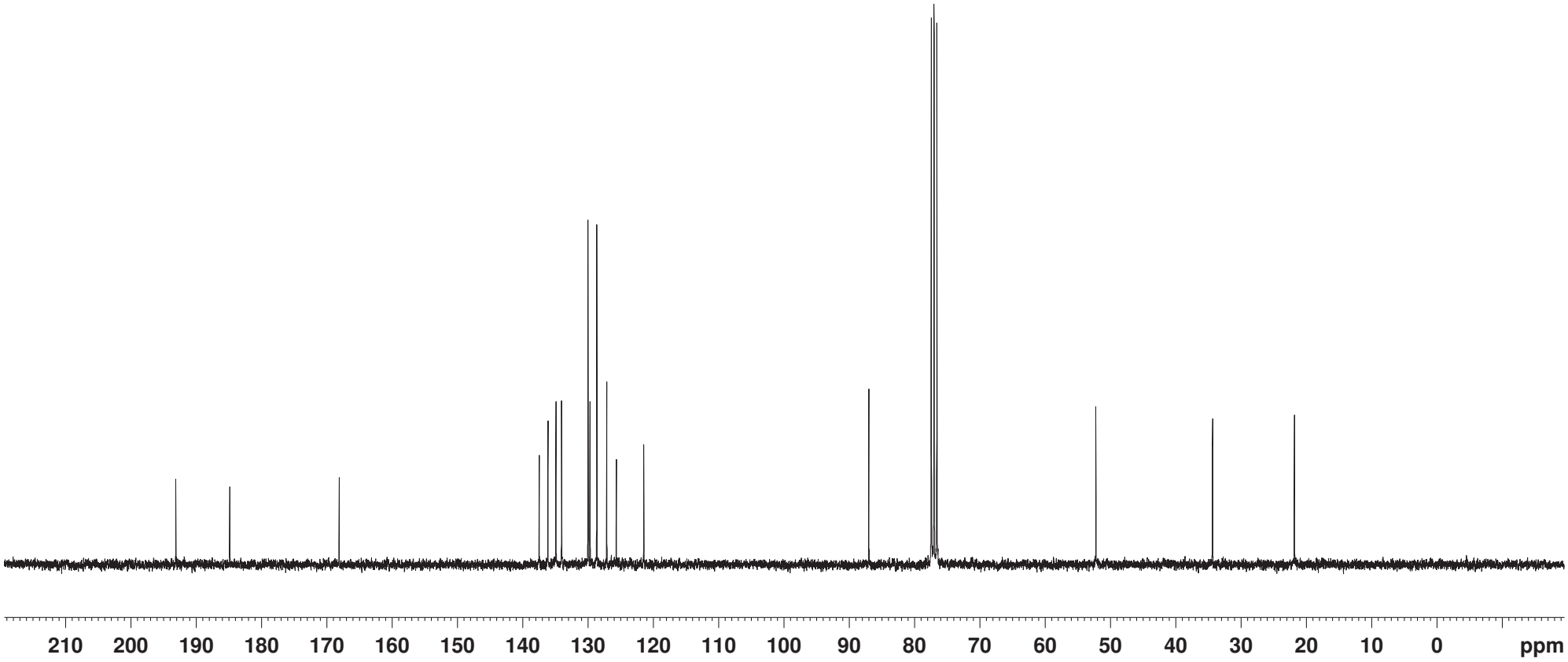
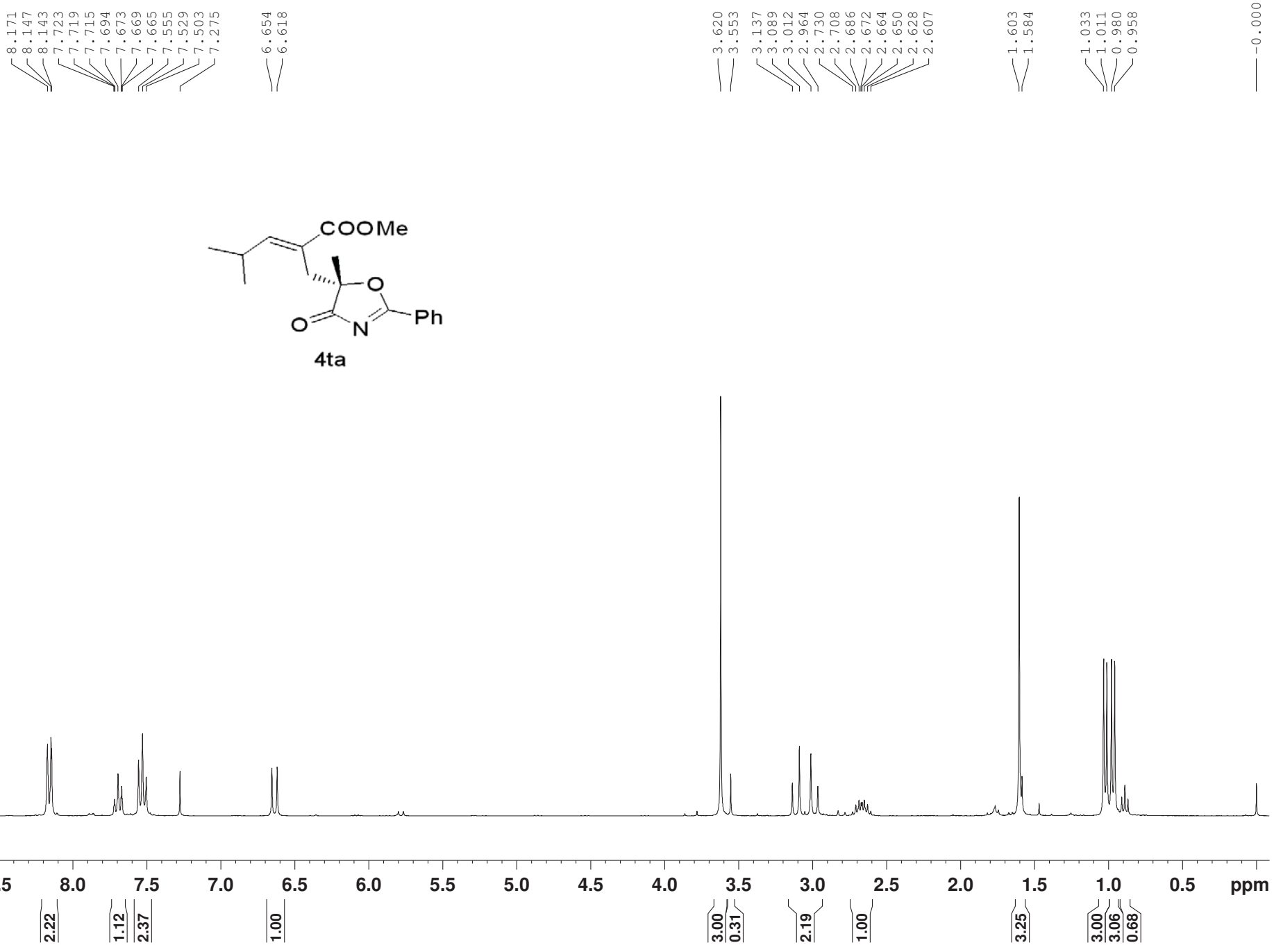
128.66
127.12
125.67
121.47
86.98
77.42
77.00
76.58
52.22
34.35
21.81



4sa

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8.143
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7.694
7.673
7.669
7.665
7.555
7.529
7.503
7.275
6.654
6.618
3.620
3.553
3.137
3.089
3.012
2.964
2.730
2.708
2.686
2.672
2.664
2.650
2.628
2.607
1.603
1.584
1.033
1.011
0.980
0.958
-0.000
COOMe
O
O
N
Ph
4ta
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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1.00
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1.00
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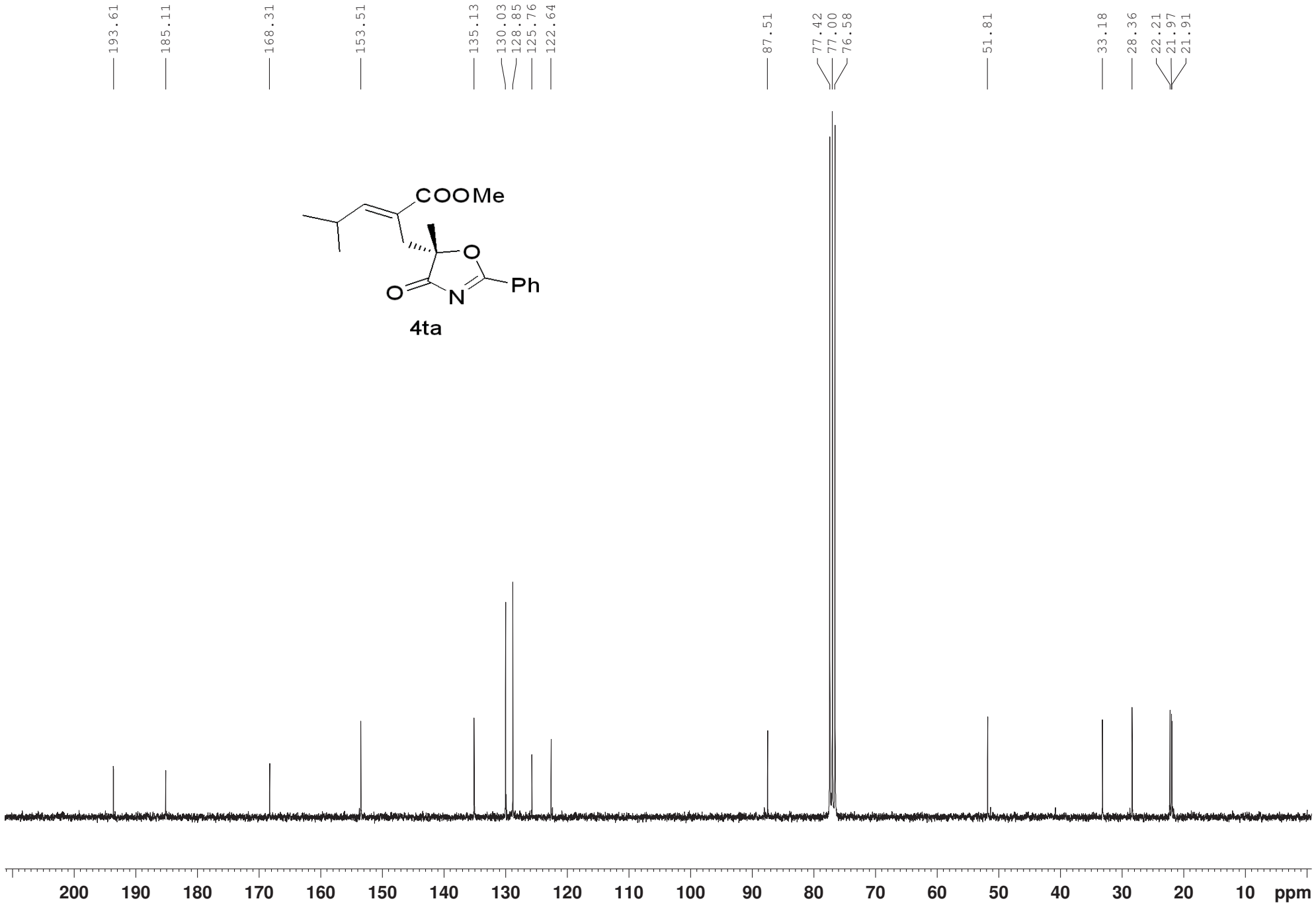
3.00
3.06
0.68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130.03
128.85
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122.64
87.51
77.42
77.00
76.58
51.81
33.18
28.36
22.21
21.97
21.91
COOMe
O
O
N
Ph
4ta
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm