Supporting Information

aza-Wittig Reaction with Nitriles: How Carbonyl Function Switches from Reacting to Activating

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General information

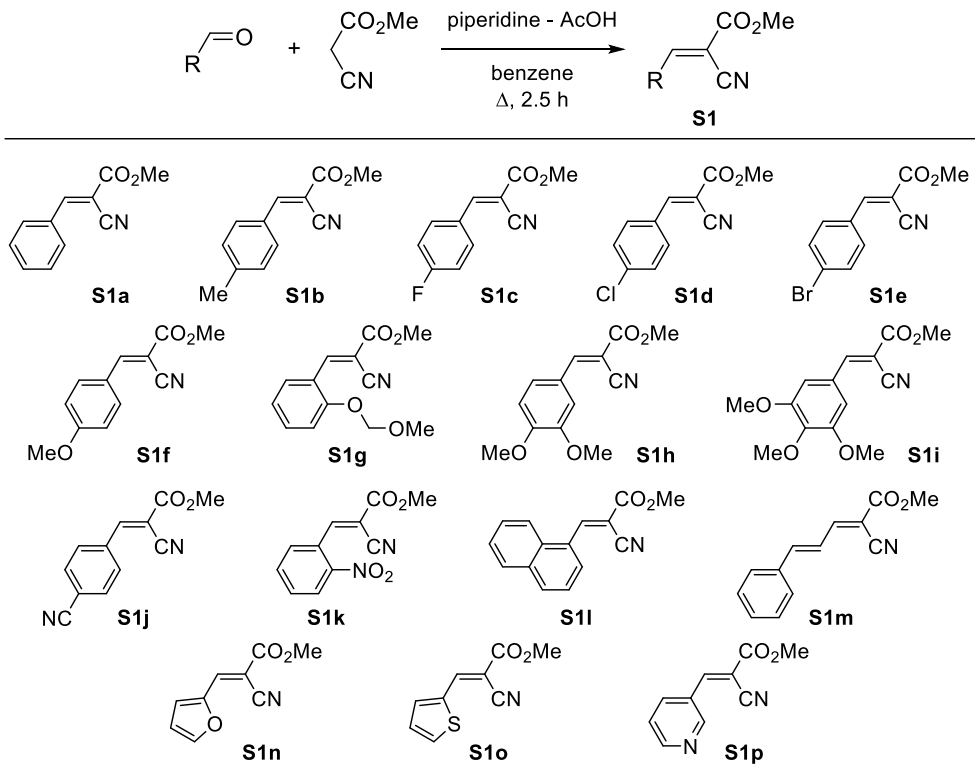
NMR spectra were acquired either on Bruker Avance 400 MHz or Bruker Avance 600 MHz spectrometers at room temperature; the chemical shifts δ were measured in ppm with respect to solvent (^{1}H: $CDCl_3$, δ = 7.27 ppm; DMSO-d_6, δ = 2.50 ppm; ^{13}C: $CDCl_3$, δ = 77.0 ppm; DMSO-d_6, δ = 39.5 ppm). Splitting patterns are designated as s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, double doublet. Coupling constants (*J*) are given in Hertz (Hz). The structures of compounds were elucidated with the aid of 1D NMR (^{1}H, ^{13}C) and 2D NMR (^{1}H-^{1}H COSY, ^{1}H-^{1}H NOESY, ^{1}H-^{13}C HSQC and HMBC) spectroscopy. IR spectra were recorded on Agilent FTIR Cary 630 spectrometers with ATR (Attenuated Total Reflectance) module. High resolution and accurate mass measurements were carried out using a BrukermicroTOF-Q^{TM} ESI-TOF (Electro Spray Ionization / Time of Flight) and Thermo Scientific^{TM} LTQ Orbitrap mass spectrometers. Elemental analyses were performed with Vario Micro Cube CHN/S elemental analyser instrument. Melting points (mp) were determined using Electrothermal IA 9100 capillary melting point apparatus. Single crystal X-Ray analysis was performed on Bruker SMART APEX II and Agilent XCalibur (Sapphire-3 CCD detector) diffractometers. Crystallographic data were collected using MoKα (λ = 0.71073 Å) and CuKα radiation (λ = 1.54186 Å) using a w-scan mode. Absorption corrections based on measurements of equivalent reflections were applied. For **S2c**, the X-ray single crystal data have been collected using CuKα radiation (λ = 1.54178 Å) on a Bruker D8Venture (Photon100 CMOS detector, IμS-microsource, focusing mirrors) diffractometer equipped with a Cryostream (Oxford Cryosystems) open-flow nitrogen cryostats at the temperature 120.0(2) K. All structures were solved by direct method and refined by full-matrix least squares on F2 for all data using Olex2[1] and SHELXTL[2] software. Analytical thin layer chromatography (TLC) was carried out with silica gel plates (silica gel 60, F_{254}, supported on aluminium) visualized with UV lamp (254 nm). Column chromatography was performed on silica gel 60 (230-400 mesh).

All the calculations reported in this paper have been performed within density functional theory (DFT),[3] using the hybrid functional B3LYP.[4,5] The standard def2-SVP basis set,[6] as implemented in the ORCA 3.0 suite of programs,[7] has been used in all cases together with the RIJCOSX approximation.[8] Frequency analysis was carried out to check whether optimized structures were local minima or transition states. No imaginary frequencies were found for local minima, and only one imaginary frequency was found for each transition state. All the energetic characteristics of reactions were computed assuming zero-point energy correction.

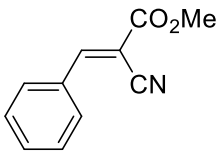
Synthesis of Cyanoacrylates S1

Alkenes **S1** were synthesized *via* Knoevenagel condensation under piperidinium acetate catalysis (Scheme S1). Mixture of the corresponding aldehyde (100 mmol), methyl cyanoacetate (9.90 g, 8.8 mL, 100 mmol), piperidine (0.85 g, 1 mL, 10 mmol) and acetic acid (1.20 g, 1.14 mL, 20 mmol) in benzene (40 mL) was heated under reflux with 20-mL Dean-Stark trap for 2.5 h. Reaction mixture was allowed to cool to ambient temperature, the precipitated alkene **S1** was filtered as a pure product. Spectral data for **S1a-f,h-p** are consistent with those reported previously.

Scheme S1. Synthesis of Knoevenagel alkenes **S1**



Methyl (*E*)-2-cyano-3-phenylacrylate[9] (S1a)

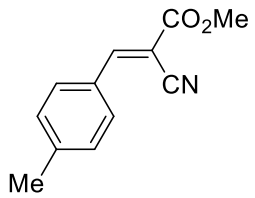


S1a was obtained from benzaldehyde (10.72 g, 101 mmol). Yield 18.66 g (99%); white solid, mp 83–84 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.95 (s, 3H, CH_3O), 7.51–7.53 (m, 2H, Ph), 7.57–7.59 (m, 1H, Ph), 8.00–8.01 (m, 2H, Ph), 8.28 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.4 (CH_3O), 102.6 (C=), 115.4 (CN), 129.3 (2×CH), 131.1 (2×CH), 131.4 (C), 133.4 (CH), 155.3 (CH=), 163.0 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(*p*-tolyl)acrylate[10] (S1b)

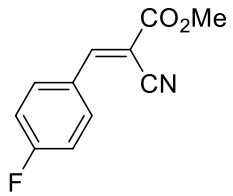


S1b was obtained from 4-methylbenzaldehyde (12.14 g, 101 mmol). Yield 20.10 g (99%); white solid, mp 111–112 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.43 (s, 3H, CH_3), 3.93 (s, 3H, CH_3O), 7.30–7.31 (m, 2H, Ar), 7.90–7.91 (m, 2H, Ar), 8.22 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 21.8 (CH_3), 53.2 (CH_3O), 101.0 (C=), 115.7 (CN), 128.8 (C), 130.0 (2×CH), 131.3 (2×CH), 144.8 (C), 155.2 (CH=), 163.2 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(4-fluorophenyl)acrylate[11] (S1c)

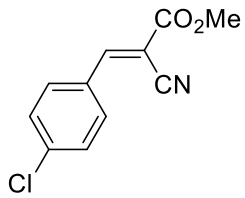


S1c was obtained from 4-fluorobenzaldehyde (24.82 g, 200 mmol). Yield 39.40 g (96%); yellow solid, mp 133–134 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.92 (s, 3H, CH_3O), 7.18 (dd, $^3J_{HH}$ = 9.0, $^3J_{HF}$ = 8.2 Hz, 2H, Ar), 8.01 (dd, $^3J_{HH}$ = 9.0, $^4J_{HF}$ = 5.3 Hz, 2H, Ar), 8.20 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.3 (CH_3O), 102.0 (C=), 115.3 (CN), 116.6 ($^2J_{CF}$ = 22 Hz, 2×CH), 127.7 ($^4J_{CF}$ = 3 Hz, C), 133.5 ($^3J_{CF}$ = 9 Hz, 2×CH), 153.6 (CH=), 162.8 (*C*O_2Me), 165.3 ($^1J_{CF}$ = 258 Hz, C).

Methyl (*E*)-3-(4-chlorophenyl)-2-cyanoacrylate[11] (S1d)

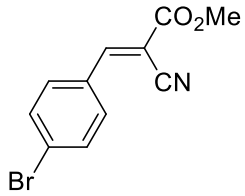


S1d was obtained from 4-chlorobenzaldehyde (28.11 g, 200 mmol). Yield 42.10 g (95%); white flaky crystals, mp 134–135 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.94 (s, 3H, CH_3O), 7.46–7.49 (m, 2H, Ar), 7.91–7.94 (m, 2H, Ar), 8.20 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.4 (CH_3O), 102.9 (C=), 115.1 (CN), 129.6 (2×CH), 129.7 (C), 132.2 (2×CH), 139.6 (C), 153.6 (CH=), 162.7 (*C*O_2Me).

Methyl (*E*)-3-(4-bromophenyl)-2-cyanoacrylate[11] (S1e)

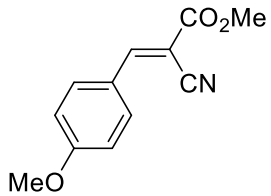


S1e was obtained from 4-bromobenzaldehyde (21.47 g, 116 mmol). Yield 29.31 g (95%); white solid, mp 132–133 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.94 (s, 3H, CH_3O), 7.63–7.66 (m, 2H, Ar), 7.84–7.86 (m, 2H, Ar), 8.19 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.5 (CH_3O), 103.1 (C=), 115.2 (CN), 128.4 (C), 130.2 (C), 132.2 (2×CH), 132.7 (2×CH), 153.7 (CH=), 162.7 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(4-methoxyphenyl)acrylate[9] (S1f)

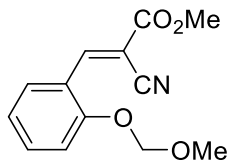


S1f was obtained from 4-methoxybenzaldehyde (13.62 g, 100 mmol). Yield 21.11 g (97%); white solid, mp 104–105 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.89 (s, 3H, CH_3O), 3.91 (s, 3H, CH_3O), 6.98–7.00 (m, 2H, Ar), 7.99–8.01 (m, 2H, Ar), 8.18 (s, 1H, CH).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.1 (CH_3O), 55.6 (CH_3O), 98.8 (C=), 114.7 (2×CH), 116.2 (CN), 124.3 (C), 133.7 (2×CH), 154.6 (CH=), 163.6 (C), 163.8 (C).

Methyl (*E*)-2-cyano-3-[2-(methoxymethoxy)phenyl]acrylate (S1g)



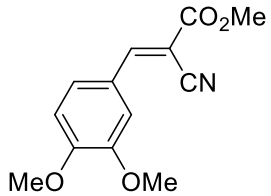
S1g was obtained from 2-(methoxymethoxy)benzaldehyde (3.02 g, 18 mmol). Yield 4.35 g (97%); yellowish solid, mp 74–75 °C. R_f = 0.62 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.49 (s, 3H, CH_3O), 3.92 (s, 3H, CH_3O), 5.26 (s, 2H, CH_3O), 7.08–7.12 (m, 1H, Ar), 7.21 (br.d, ^3J = 8.5 Hz, 1H, Ar), 7.46–7.50 (m, 1H, Ar), 8.28 (br.d, ^3J = 7.9 Hz, 1H, Ar), 8.76 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.1 ($^1J_{CH}$ = 148 Hz, CH_3O), 56.4 ($^1J_{CH}$ = 143 Hz, CH_3O), 94.6 ($^1J_{CH}$ = 167 Hz, OCH_2O), 102.1 (C=), 114.6 (CH), 115.6 (CN), 121.1 (C), 122.0 (CH), 129.1 (CH), 134.9 (CH), 149.8 (CH=), 157.1 (C), 163.1 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{13}H_{14}NO_4^+$ 248.0917; Found 248.0915.

Methyl (*E*)-2-cyano-3-(3,4-dimethoxyphenyl)acrylate[12] (S1h)

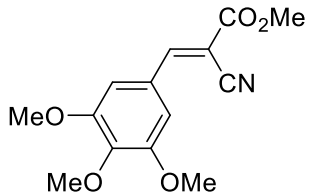


S1h was obtained from 3,4-dimethoxybenzaldehyde (16.62 g, 100 mmol). Yield 22.23 g (90%); white solid, mp 117–118 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.92 (s, 3H, CH_3O), 3.95 (s, 3H, CH_3O), 3.97 (s, 3H, CH_3O), 6.94 (d, ^3J = 8.4 Hz, 1H, Ar), 7.47 (dd, ^3J = 8.4, ^4J = 2.2 Hz, 1H, Ar), 7.80 (d, ^4J = 2.2 Hz, 1H, Ar) 8.16 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.2 (CH_3O), 56.0 (CH_3O), 56.1 (CH_3O), 98.9 (C=), 110.9 (CH), 111.6 (CH), 116.3 (CN), 124.5 (C), 128.0 (CH), 149.3 (C), 153.8 (C), 154.9 (CH=), 163.6 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(3,4,5-trimethoxyphenyl)acrylate[12] (S1i)

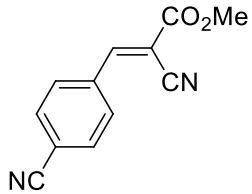


S1i was obtained from 3,4,5-trimethoxybenzaldehyde (9.81 g, 50 mmol). Yield 12.19 g (88%); white solid, mp 115–116 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.90 (s, 6H, 2×CH_3O), 3.91 (s, 3H, CH_3O), 3.94 (s, 3H, CH_3O), 7.28 (s, 2H, CH) 8.12 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.2 (CH_3O), 56.2 (2×CH_3O), 61.0 (CH_3O), 100.6 (C=), 108.5 (2×CH), 115.9 (CN), 126.4 (C), 142.8 (C), 153.2 (2×C), 155.0 (CH=), 163.1 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(4-cyanophenyl)acrylate[13] (S1j)

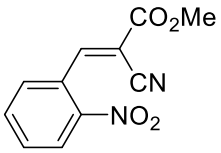


S1j was obtained from 4-cyanobenzaldehyde (13.11 g, 100 mmol). Yield 18.44 g (87%); yellow solid, mp 160–161 °C (with decomposition).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.95 (s, 3H, CH_3O), 7.78–7.80 (m, 2H, Ar), 8.04–8.06 (m, 2H, Ar), 8.25 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.7 (CH_3O), 106.3 (C=), 114.5 (C), 115.9 (C), 117.6 (C), 130.9 (2×CH), 132.8 (2×CH), 135.1 (C), 152.4 (CH=), 161.9 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(4-nitrophenyl)acrylate[14] (S1k)

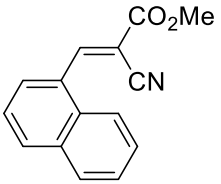


S1k was obtained from 2-nitrobenzaldehyde (3.02 g, 20 mmol). Yield 4.08 g (88%); yellow solid, mp 146–147 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.96 (s, 3H, CH_3O), 7.71–7.74 (m, 1H, Ar), 7.81–7.83 (m, 1H, Ar), 7.85–7.87 (m, 1H, Ar), 8.27–8.29 (m, 1H, Ar), 8.73 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.6 (CH_3O), 108.1 (C=), 113.8 (CN), 125.4 (CH), 127.9 (C), 130.5 (CH), 132.2 (CH), 134.5 (CH), 147.3 (C), 153.4 (CH=), 161.5 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(naphthen-1-yl)acrylate[15] (S1l)

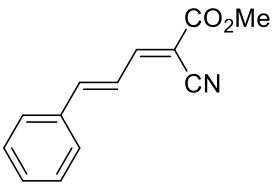


S1l was obtained from 1-naphthalenecarbaldehyde (15.62 g, 100 mmol). Yield 22.05 g (93%); white solid, mp 180–182 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 4.00 (s, 3H, CH_3O), 7.58–760 (m, 2H, Naph), 7.62–7.65 (m, 1H, Naph), 7.92 (d, ^3J = 8.0 Hz, 1H, Naph), 8.03–8.06 (m, 2H, Naph), 8.33 (d, ^3J = 7.3 Hz, 1H, Naph) 9.12 (s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.4 (CH_3O), 105.2 (C=), 115.3 (CN), 122.8 (CH), 125.3 (CH), 126.8 (CH), 127.8 (CH), 128.15 (C), 128.21 (CH), 129.1 (CH), 131.6 (C), 133.45 (C), 133.49 (CH), 152.9 (CH=), 162.8 (*C*O_2Me).

Methyl (2*E*,4*E*)-2-cyano-5-phenylpenta-2,4-dienoate[16] (S1m)

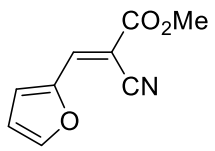


S1m was obtained from (*E*)-cinnamaldehyde (13.22 g, 100 mmol). Yield 20.27 g (95%); yellow solid, mp 135–139 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.88 (s, 3H, CH_3O), 7.27–7.28 (m, 2H, CH), 7.40–7.43 (m, 3H, CH), 7.57–7.59 (m, 2H, CH), 8.00–8.02 (m, 1H, CH).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 52.9 (CH_3O), 104.0 (C=), 114.4 (CN), 122.9 (CH=), 128.5 (2×CH), 129.1 (2×CH), 131.2 (CH), 134.6 (C), 149.0 (CH=), 155.5 (CH=), 162.7 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(furan-2-yl)acrylate[17,18] (S1n)

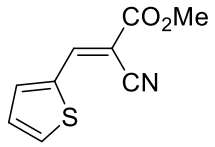


S1n was obtained from furfural (19.22 g, 200 mmol). Yield 33.71 g (95%); brown solid, mp 99–100 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.89 (s, 3H, CH_3O), 6.65–6.66 (m, 1H, Fu), 7.38 (d, ^3J = 3.5 Hz, 1H, Fu), 7.74–7.75 (m, 1H, Fu), 8.01 (br.s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.2 (CH_3O), 98.0 (C=), 113.8 (CH), 115.2 (CN), 121.9 (CH), 139.5 (CH), 148.3 (CH=), 148.6 (C), 163.0 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(thien-2-yl)acrylate[18] (S1o)

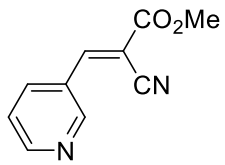


S1o was obtained from 2-thiophenecarbaldehyde (11.21 g, 100 mmol). Yield 17.37 g (90%); yellow solid, mp 107–108 °C.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.91 (s, 3H, CH_3O), 7.22 (dd, ^3J = 5.0, ^3J = 3.9 Hz, 1H, Th), 7.80 (ddd, ^3J = 5.0, ^4J = 1.2, ^4J = 0.9 Hz, 1H, Th), 7.83 (ddd, ^3J =3.9, ^4J = 1.2, ^5J = 0.6 Hz, 1H, Th), 8.35 (br.s, 1H, CH=).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.2 (CH_3O), 98.8 (C=), 115.6 (CN), 128.6 (CH), 135.3 (CH), 135.9 (C), 137.3 (CH), 146.8 (CH=), 163.1 (*C*O_2Me).

Methyl (*E*)-2-cyano-3-(pyridin-3-yl)acrylate[19] (S1p)



S1q was obtained from 3-pyridinecarbaldehyde (10.71 g, 100 mmol). Yield 17.26 g (92%); yellow solid, mp 124–125 °C.

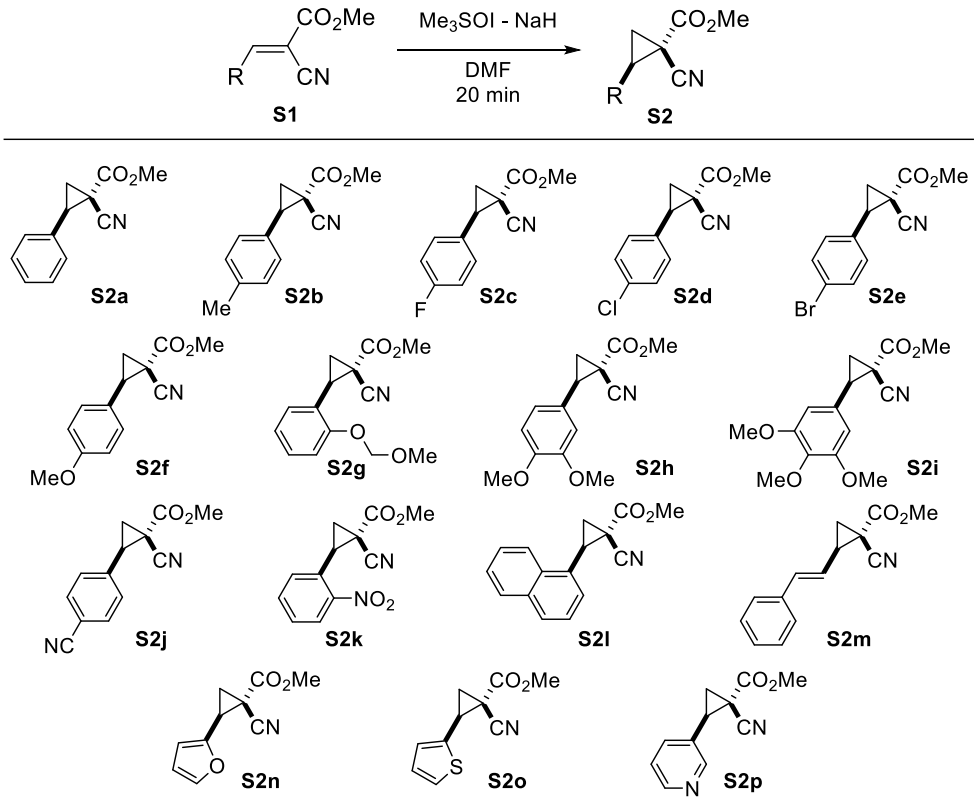
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 3.90 (s, 3H, CH_3O), 7.43 (dd, ^3J = 8.2, ^3J = 4.9 Hz, 1H, Py), 8.23 (br.s, 1H, CH=), 8.50–8.52 (m, 1H, Py), 8.71 (dd, ^3J = 4.9, ^4J = 1.6 Hz, 1H, Py), 7.83 (br.d, ^4J = 2.4 Hz, 1H, Py).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 53.5 (CH_3O), 105.0 (C=), 114.7 (CN), 123.9 (CH), 127.3 (C), 135.9 (CH), 151.4 (CH), 152.7 (CH), 153.3 (CH), 162.0 (*C*O_2Me).

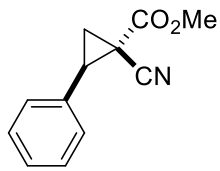
Synthesis of Cyclopropanes S2 under Corey-Chaykovsky Reaction Conditions

To suspension of NaH (29.4 mmol, 60% suspension in mineral oil) in dry DMF (76 mL) Me_3SOI (29.4 mmol) was added in one portion under inert atmosphere. After stirring for 20 min at rt, reaction mixture was cooled in ice-water bath and then alkene **S1** (26.7 mmol) was added in one portion under vigorous stirring. Cooling bath was taken away and the mixture was stirred for additional 20 min, quenched with ice water (100 mL) and extracted with EtOAc (3×100 mL). Combined organic fractions were washed with water (5×100 mL), dried with Na_2SO_4 and concentrated under reduced pressure. Residue was purified by column chromatography on silica gel (petroleum ether – ethyl acetate). Cyclopropanes **S2** were formed predominantly as *trans*-isomer (dr > 95:5) (Scheme S2).

Scheme S2. Synthesis of Cyclopropanes **S2** *via* Corey-Chaykovsky Reaction



Methyl (1*RS*,2*SR*)-1-cyano-2-phenylcyclopropane-1-carboxylate[20] (S2a)

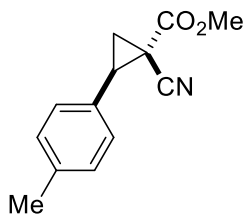


S2a was obtained from alkene **S1a** (5.00 g, 26.7 mmol). Yield 3.62 g (67%); yellow oil; R_f = 0.48 (petroleum ether – ethyl acetate 4:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.13 (dd, ^2J = 5.4, ^3J = 8.5 Hz, 1H, CH_2), 2.18 (dd, ^2J = 5.4, ^3J = 9.3 Hz, 1H, CH_2), 3.19 (dd, ^3J = 9.3, ^3J = 8.5 Hz, 1H, CH), 3.88 (s, 3H, CH_3O), 7.29–7.31 (m, 2H, Ph), 7.34–7.37 (m, 1H, Ph), 7.38–7.41 (m, 2H, Ph).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.7 (C), 22.8 ($^1J_{CH}$ = 165 Hz, CH_2), 35.5 ($^1J_{CH}$ = 169 Hz, CH), 53.6 ($^1J_{CH}$ = 148 Hz, CH_3O), 116.2 (CN), 128.3 (2×CH), 128.5 (CH), 128.7 (2×CH), 132.8 (C), 167.8 (*C*O_2Me).

Methyl (1*RS*,2*SR*)-1-cyano-2-(*p*-tolyl)cyclopropanecarboxylate[20] (S2b)

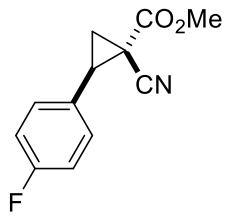


S2b was obtained from alkene **S1b** (5.00 g, 24.9 mmol). Yield 3.17 g (59%); white solid; mp 111–112 °C; R_f = 0.70 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.10 (dd, ^2J = 5.4, ^3J = 8.3 Hz, 1H, CH_2), 2.16 (dd, ^2J = 5.4, ^3J = 9.2 Hz, 1H, CH_2), 2.36 (s, 3H, CH_3), 3.16 (dd, ^3J = 9.2, ^3J = 8.3, Hz, 1H, CH), 3.87 (s, 3H, CH_3O), 7.17–7.21 (m, 4H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 21.1 (CH_3), 22.7 (C), 22.8 (CH_2), 35.4 (CH), 53.6 (CH_3O), 116.3 (CN), 128.1 (2×CH), 129.4 (2×CH), 129.7 (C), 138.3 (C), 167.8 (*C*O_2Me).

Methyl (1*RS*,2*SR*)-1-cyano-2-(4-fluorophenyl)cyclopropanecarboxylate (S2c)



S2c was obtained from alkene **S1c** (9.60 g, 46.8 mmol). Yield 4.81 g (47%); yellow solid; mp 80–81 °C; R_f = 0.30 (petroleum ether – ethyl acetate 4:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.05 (dd, ^2J = 5.4, ^3J = 8.4 Hz, 1H, CH_2), 2.14 (dd, ^2J = 5.4, ^3J = 9.3 Hz, 1H, CH_2), 3.14 (dd, ^3J = 9.3, ^3J = 8.4 Hz, 1H, CH), 3.82 (s, 3H, CH_3O), 7.03–7.07 (m, 2H, Ar), 7.24–7.26 (m, 2H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.5 (C), 22.7 ($^1J_{CH}$ = 171, $^1J_{CH}$ = 165 Hz, CH_2), 34.4 ($^1J_{CH}$ = 168 Hz, CH), 53.4 ($^1J_{CH}$ = 149 Hz, CH_3O), 115.5 ($^2J_{CF}$ = 22 Hz, 2×CH), 116.0 (CN), 128.6 ($^4J_{CF}$ = 3 Hz, C), 129.9 ($^3J_{CF}$ = 9 Hz, 2×CH), 162.4 ($^1J_{CF}$ = 248 Hz, C), 167.4 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{11}FNO_2^+$ 220.0768; Found 220.0767.

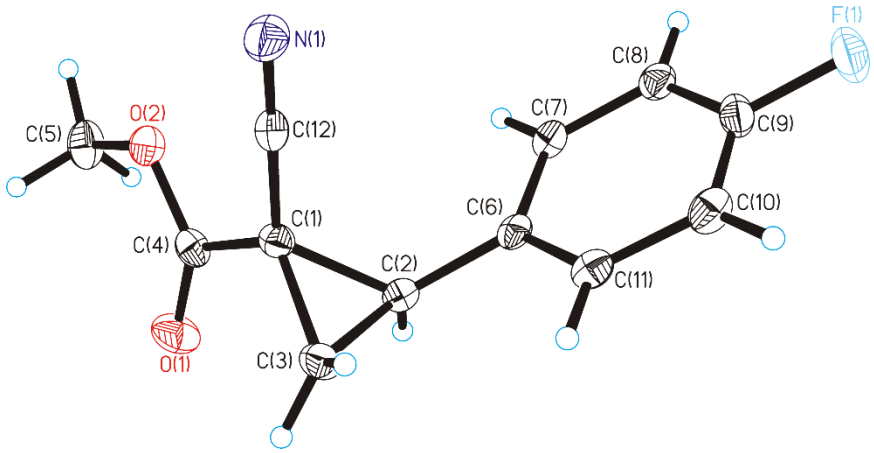
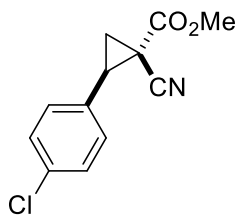


Figure S1. Molecular structure from single crystal X-ray study of **S2c** (thermal ellipsoids are drawn at the 50% probability level); CCDC 1865323.

Methyl (1*RS*,2*SR*)-2-(4-chlorophenyl)-1-cyanocyclopropanecarboxylate (S2d)



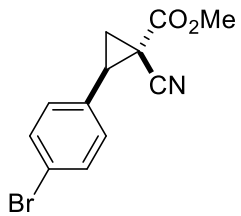
S2d was obtained from alkene **S1d** (7.14 g, 32.2 mmol); reaction was performed in DMSO. Yield 4.25 g (56%); white solid; mp 140–141 °C; R_f = 0.43 (petroleum ether – ethyl acetate 3:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.07 (dd, ^2J = 5.5, ^3J = 8.4 Hz, 1H, CH_2), 2.18 (dd, ^2J = 5.5, ^3J = 9.3 Hz, 1H, CH_2), 3.15 (dd, ^3J = 9.3, ^3J = 8.4 Hz, 1H, CH), 3.87 (s, 3H, CH_3O), 7.21–7.24 (m, 2H, Ar), 7.35–7.37 (m, 2H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.7 (C), 22.8 ($^1J_{CH}$ = 165 Hz, CH_2), 34.6 ($^1J_{CH}$ = 169 Hz, CH), 53.7 ($^1J_{CH}$ = 148 Hz, CH_3O), 116.0 (CN), 128.9 (2×CH), 129.6 (2×CH), 131.4 (C), 134.5 (C), 167.5 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{11}ClNO_2^+$ 236.0473; Found 236.0473.

Methyl (1*RS*,2*SR*)-2-(4-bromophenyl)-1-cyanocyclopropanecarboxylate[20] (S2e)

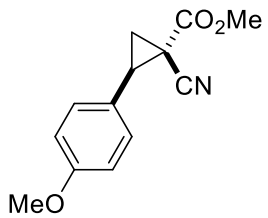


S2e was obtained from alkene **S1e** (5.00 g, 18.8 mmol). Yield 4.01 g (76%); yellow solid; mp 138–139 °C; R_f = 0.42 (petroleum ether – ethyl acetate 4:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.07 (dd, ^2J = 5.4, ^3J = 8.4 Hz, 1H, CH_2), 2.18 (dd, ^2J = 5.4, ^3J = 9.3 Hz, 1H, CH_2), 3.13 (dd, ^3J = 9.3, ^3J = 8.4 Hz, 1H, CH), 3.87 (s, 3H, CH_3O), 7.15–7.18 (m, 2H, Ar), 7.50–7.53 (m, 2H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.6 (C), 22.8 ($^1J_{CH}$ = 165 Hz, CH_2), 34.6 ($^1J_{CH}$ = 169 Hz, CH), 53.7 ($^1J_{CH}$ = 148 Hz, CH_3O), 116.0 (CN), 122.7 (C), 129.9 (2×CH), 131.91 (C), 131.92 (2×CH), 167.5 (*C*O_2Me).

Methyl (1*RS*,2*SR*)-1-cyano-2-(4-methoxyphenyl)cyclopropanecarboxylate (S2f)



S2f was obtained from alkene **S1f** (1.00 g, 4.6 mmol). Yield 0.70 g (66%); yellow solid, mp 68–69 ºC; R_f = 0.53 (petroleum ether – ethyl acetate 2:1).

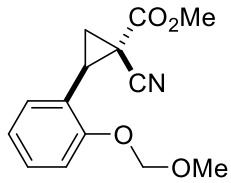
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.07 (dd, ^2J = 5.4, ^3J = 8.4 Hz, 1H, CH_2), 2.15 (dd, ^2J = 5.4, ^3J = 9.3 Hz, 1H, CH_2), 3.15 (dd, ^3J = 9.3, ^3J = 8.4 Hz, 1H, CH), 3.81 (s, 3H, CH_3O), 3.86 (s, 3H, CH_3O), 6.90–6.92 (m, 2H, Ar), 7.20–7.22 (m, 2H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.7 (C), 22.9 ($^1J_{CH}$ = 172, $^1J_{CH}$ = 164 Hz, CH_2), 35.3 ($^1J_{CH}$ = 168 Hz, CH), 53.5 ($^1J_{CH}$ = 149 Hz, CH_3O), 55.2 ($^1J_{CH}$ = 144 Hz, CH_3O), 114.1 (2×CH), 116.4 (CN), 124.6 (C), 129.4 (2×CH), 159.7 (C), 167.8 (*C*O_2Me).

IR (film) 2240, 1735, 1612, 1515, 1437, 1375, 1297, 1273, 1247, 1208, 1180, 1154, 1122, 1034, 967, 835, 738 cm^{-1}.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{13}H_{14}NO_3^+$ 232.0968; Found 232.0976.

Methyl (1*RS*,2*SR*)-1-cyano-2[2-(methoxymethoxy)phenyl]cyclopropanecarboxylate (S2g)



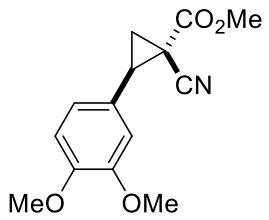
S2g was obtained from alkene **S1g** (6.06 g, 24.5 mmol). Yield 3.32 g (52%); yellow oil; R_f = 0.50 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.08 (dd, ^2J = 5.3, ^3J = 8.6 Hz, 1H, CH_2), 2.17 (dd, ^2J = 5.3, ^3J = 9.1 Hz, 1H, CH_2), 3.21 (dd, ^3J = 9.1, ^3J = 8.6 Hz, 1H, CH), 3.51 (s, 3H, CH_3O), 3.88 (s, 3H, CH_3O), 5.24 (d, ^2J = 6.6 Hz, 1H, OCH_2O), 5.25 (d, ^2J = 6.6 Hz, 1H, OCH_2O), 7.00–7.02 (m, 1H, Ar), 7.12–7.13 (m, 1H, Ar), 7.16 (dd, ^3J = 8.3, ^4J = 1.0 Hz, 1H, Ar), 7.30–7.33 (m, 1H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 21.6 (C), 22.2 ($^1J_{CH}$ = 170, $^1J_{CH}$ = 165 Hz, CH_2), 31.6 ($^1J_{CH}$ = 169 Hz, CH), 53.4 ($^1J_{CH}$ = 148 Hz, CH_3O), 56.1 ($^1J_{CH}$ = 143 Hz, CH_3O), 94.4 ($^1J_{CH}$ = 166 Hz, OCH_2O), 113.7 (CH), 116.6 (CN), 121.5 (CH), 122.4 (C), 128.3 (CH), 129.9 (CH), 156.6 (C), 168.2 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{15}NNaO_4^+$ 284.0893; Found 284.0892.

Methyl (1*RS*,2*SR*)-1-cyano-2-(3,4-dimethoxyphenyl)cyclopropanecarboxylate (S2h)



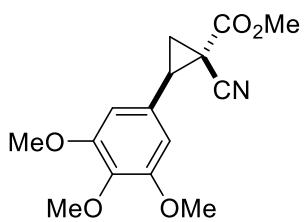
S2h was obtained from alkene **S1h** (5.00 g, 20.2 mmol). Yield 4.02 g (76%); yellow solid, mp 117–118 ºC; R_f = 0.68 (petroleum ether – ethyl acetate 1:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.05 (dd, ^2J = 5.4, ^3J = 8.5 Hz, 1H, CH_2), 2.11 (dd, ^2J = 5.4, ^3J = 9.2 Hz, 1H, CH_2), 3.11 (dd, ^3J = 9.2, ^3J = 8.5 Hz, 1H, CH), 3.82 (s, 3H, CH_3O), 3.83 (s, 3H, CH_3O), 3.86 (s, 3H, CH_3O), 6.77 (d, ^4J = 2.0 Hz, 1H, Ar), 6.78–6.80 (m, 1H, Ar), 6.82 (d, ^3J = 8.2 Hz, 1H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.6 (C), 22.9 ($^1J_{CH}$ = 168 Hz, CH_2), 35.4 ($^1J_{CH}$ = 168 Hz, CH), 53.4 ($^1J_{CH}$ = 148 Hz, CH_3O), 55.7 ($^1J_{CH}$ = 144 Hz, CH_3O), 55.8 ($^1J_{CH}$ = 144 Hz, CH_3O), 111.0 (CH), 111.5 (CH), 116.3 (CN), 120.3 (CH), 125.0 (C), 148.9 (C), 149.1 (C), 167.6 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{16}NO_4^+$ 262.1074; Found 262.1080.

Methyl (1*RS*,2*SR*)-1-cyano-2-(3,4,5-trimethoxyphenyl)cyclopropanecarboxylate (S2i)



S2i was obtained from alkene **S1i** (5.00 g, 18.0 mmol). Yield 2.53 g (48%); yellow oil; R_f = 0.31 (petroleum ether – ethyl acetate 2:1).

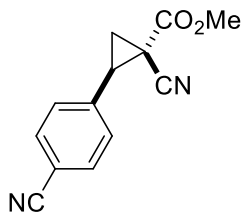
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.06 (dd, ^2J = 5.4, ^3J = 8.4 Hz, 1H, CH_2), 2.16 (dd, ^2J = 5.4, ^3J = 9.3 Hz, 1H, CH_2), 3.13 (ddd, ^3J = 9.3, ^3J = 8.4, ^4J =

0.6 Hz, 1H, CH), 3.84 (s, 3H, CH_3O), 3.87 (s, 6H, CH_3O), 3.88 (s, 3H, CH_3O), 6.49 (d, ^4J = 0.6 Hz, 2H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.6 (C), 23.3 (CH_2), 35.8 (CH), 53.7 (CH_3O), 56.2 (2×CH_3O), 60.8 (CH_3O), 105.5 (2×CH), 116.3 (CN), 128.2 (C), 138.3 (C), 153.3 (2×C), 167.7 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{18}NO_5^+$ 292.1179; Found 292.1185.

Methyl (1*RS*,2*SR*)-1-cyano-2-(4-cyanophenyl)cyclopropanecarboxylate (S2j)



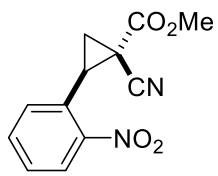
S1j was obtained from alkene **S1j** (4.24 g, 20.0 mmol). Yield 2.54 g (56%); yellow solid, mp 147–148 °C; R_f = 0.20 (petroleum ether – ethyl acetate 3:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.13 (dd, ^2J = 5.7, ^3J = 8.4 Hz, 1H, CH_2), 2.23 (dd, ^2J = 5.7, ^3J = 9.2 Hz, 1H, CH_2), 3.20 (dd, ^3J = 9.2, ^3J = 8.4 Hz, 1H, CH), 3.88 (s, 3H, CH_3O), 7.39–7.42 (m, 2H, Ar), 7.67–7.69 (m, 2H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 23.7 (CH_2), 22.9 (C), 34.4 (CH), 53.9 (CH_3O), 112.4 (C), 115.6 (CN), 118.2 (CN), 129.1 (CH), 132.4 (CH), 138.2 (C), 167.0 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{13}H_{11}N_2O_2^+$ 227.0815; Found 227.0808.

Methyl (1*RS*,2*SR*)-1-cyano-2-(2-nitrophenyl)cyclopropanecarboxylate (S2k)



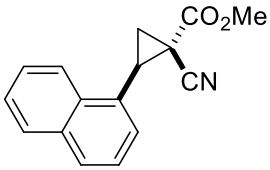
S2k was obtained from alkene **S1k** (2.83 g, 12.1 mmol). Reaction was performed at 40 °C for 5 h. Yield 1.88 g (63%); yellow solid, mp 111–112 °C; R_f = 0.48 (pethroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.15 (dd, ^2J = 5.8, ^3J = 8.4 Hz, 1H, CH_2), 2.30 (dd, ^2J = 5.8, ^3J = 8.7 Hz, 1H, CH_2), 3.54 (dd, ^3J = 8.7, ^3J = 8.4 Hz, 1H, CH), 3.92 (s, 3H, CH_3O), 7.43 (d, ^3J = 7.7 Hz, 1H, Ar), 7.57–7.60 (m, 1H, Ar), 7.68–7.71 (m, 1H, Ar), 8.22 (d, ^3J = 8.1 Hz, 1H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.2 (C), 23.0 (CH_2), 33.5 (CH), 53.9 (CH_3O), 116.0 (CN), 125.8 (CH), 129.3 (C), 129.9 (CH), 130.6 (CH), 134.0 (CH), 149.3 (C), 167.4 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{11}N_2O_4^+$ 247.0713; Found 247.0723.

Methyl (1*RS*,2*SR*)-1-cyano-2-(naphthen-1-yl)cyclopropanecarboxylate (S2l)



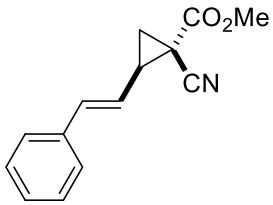
S2l was obtained from alkene **S1l** (5.00 g, 21.1 mmol). Yield 3.89 g (73%); white solid, mp 183–184 ºC; R_f = 0.53 (pethroleum ether – ethyl acetate 4:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.32–2.33 (m, 2H, CH_2), 3.61–3.64 (m, 1H, CH), 3.98 (s, 3H, CH_3O), 7.38–7.40 (m, 1H, Naph), 7.47–7.49 (m, 1H, Naph), 7.56–7.59 (m, 1H, Naph), 7.60–7.63 (m, 1H, Naph), 7.88–7.90 (m, 1H, Naph), 7.92–7.95 (m, 2H, Naph).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.3 (C), 22.9 ($^1J_{CH}$ 168 Hz, CH_2), 33.2 ($^1J_{CH}$ 168 Hz, CH), 53.9 ($^1J_{CH}$ 149 Hz, CH_3O), 116.1 (CN), 122.7 (CH), 125.2 (CH), 125.7 (CH), 126.3 (CH), 127.1 (CH), 129.0 (CH), 129.3 (C), 129.6 (CH), 132.6 (C), 133.7 (C), 168.1 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{16}H_{14}NO_2^+$ 252.1019; Found 252.1014.

Methyl (1*RS*,2*SR*)-1-cyano-2-((*E*)-styryl)cyclopropane-1-carboxylate (S2m)



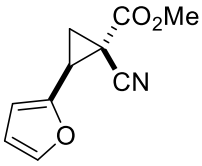
S2m was obtained from alkene **S1m** (5.00 g, 23.4 mmol). Yield 3.58 g (67%); yellow oil; R_f = 0.58 (pethroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.78 (dd, ^2J = 5.2, ^3J = 7.9 Hz, 1H, CH_2), 2.09 (dd, ^2J = 5.2, ^3J = 9.0 Hz, 1H, CH_2), 2.74 (ddd, ^3J = 9.0, ^3J = 8.8, ^3J = 7.9 Hz, 1H, CH), 3.85 (s, 3H, CH_3O), 5.96 (dd, ^3J = 15.7, ^3J = 8.8 Hz, 1H, CH), 6.77 (d, ^3J = 15.7 Hz, 1H, CH), 7.27–7.29 (m, 1H, Ph), 7.32–7.35 (m, 2H, Ph), 7.38–7.40 (m, 2H, Ph).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 21.2 (C), 24.5 ($^1J_{CH}$ = 168 Hz, CH_2), 34.2 ($^1J_{CH}$ = 161 Hz, CH), 53.6 ($^1J_{CH}$ = 148 Hz, CH_3O), 116.7 (CN), 123.2 (CH=), 126.4 (2×CH), 128.2 (CH), 128.6 (2×CH), 135.8 (C), 135.9 (CH=), 167.6 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{14}NO_2^+$ 228.1019; Found 228.1020.

Methyl (1*RS*,2*SR*)-1-cyano-2-(furan-2-yl)cyclopropanecarboxylate (S2n)



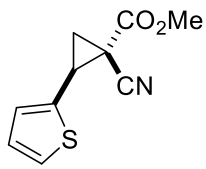
S2n was obtained from alkene **S1n** (9.40 g, 53.1 mmol). Yield 3.98 g (39%); yellow oil; R_f = 0.50 (petroleum ether – ethyl acetate 3:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.10–2.13 (m, 2H, CH_2), 3.10–3.13 (m, 1H, CH), 3.81 (s, 3H, CH_3O), 6.33–6.34 (m, 1H, Fu), 6.35–6.36 (m, 1H, Fu), 7.38–7.39 (m, 1H, Fu).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 21.8 ($^1J_{CH}$ = 170 Hz, CH_2), 21.9 (C), 28.5 ($^1J_{CH}$ = 172 Hz, CH), 53.5 ($^1J_{CH}$ = 149 Hz, CH_3O), 109.2 (CH), 110.6 (CH), 119.9 (CN), 143.1 (CH), 147.3 (C), 166.9 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{10}H_{10}NO_3^+$ 192.0655; Found 192.0655.

Methyl (1*RS*,2*SR*)-1-cyano-2-(thien-2-yl)cyclopropanecarboxylate (S2o)



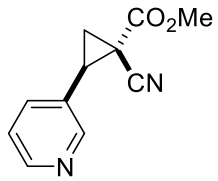
S2o was obtained from alkene **S1o** (5.00 g, 25.9 mmol). Yield 3.25 g (61%); white solid, mp 64–65 °C; R_f = 0.66 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.09 (dd, ^2J = 5.4, ^3J = 8.1 Hz, 1H, CH_2), 2.24 (dd, ^2J = 5.4, ^3J = 9.2 Hz, 1H, CH_2), 3.30 (dd, ^3J = 9.2, ^3J = 8.1 Hz, 1H, CH), 3.87 (s, 3H, CH_3O), 7.01–7.02 (m, 2H, Th), 7.30 (dd, ^3J = 4.4, ^4J = 1.9 Hz, 1H, Th).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 23.7 (C), 24.4 (CH_2), 30.5 (CH), 53.7 (CH_3O), 116.0 (CN), 126.1 (CH), 127.0 (CH), 127.3 (CH), 136.1 (C), 167.3 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{10}H_{10}NO_2S^+$ 208.0427; Found 208.0422.

Methyl (1*RS*,2*SR*)-1-cyano-2-(pyridin-3-yl)cyclopropanecarboxylate (S2p)



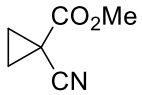
S2p was obtained from alkene **S1p** (5.00 g, 26.6 mmol). Yield 1.90 g (35%); yellow oil; R_f = 0.48 (ethyl acetate).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.04 (dd, ^2J = 5.5, ^3J = 8.4 Hz, 1H, CH_2), 2.13 (dd, ^2J = 5.5, ^3J = 9.3 Hz, 1H, CH_2), 3.09 (dd, ^3J = 9.3, ^3J = 8.4 Hz, 1H, CH), 3.77 (s, 3H, CH_3O), 7.23 (dd, ^3J = 8.0, ^3J = 4.9 Hz, 1H, Py), 7.48–7.50 (m, 1H, Py), 8.50 (dd, ^3J = 4.9, ^4J = 1.5 Hz, 1H, Py), 8.53 (d, ^4J = 2.2 Hz, 1H, Py).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.1 ($^1J_{CH}$ = 172, $^1J_{CH}$ = 165 Hz, CH_2), 22.3 (C), 32.1 ($^1J_{CH}$ = 168 Hz, CH), 53.5 ($^1J_{CH}$ = 149 Hz, CH_3O), 115.6 (CN), 123.1 (CH), 128.8 (C), 134.8 (CH), 149.4 (CH), 150.1 (CH), 167.0 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{11}H_{11}N_2O_2^+$ 203.0815; Found 203.0813.

Methyl 1-cyanocyclopropanecarboxylate[21] (S2q)



1,2-Dibromoethane (36.80 g, 17.0 mL, 196 mmol) was slowly added to a mixture of methyl cyanoacetate (15.00 g, 13.4 mL, 151 mmol) and powdered K_2CO_3 (52.40 g, 379 mmol) in dry acetone (110 mL) and the heterogeneous mixture was stirred at rt for 10 h. After completion, precipitate was filtered off and filtrate was concentrated under reduced pressure. Residue was distillated under reduced pressure. Yield 14.36 g (76%); colorless liquid, bp 98 °C/14 mm.

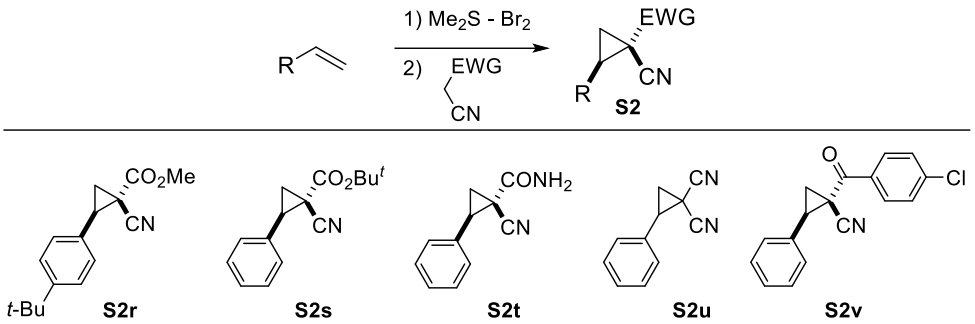
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.59–1.67 (m, 4H, CH_2), 3.78 (s, 3H, CH_3O).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 13.0 (C), 18.9 (2×CH_2), 53.4 (CH_3O), 118.4 (CN), 168.0 (*C*O_2Me).

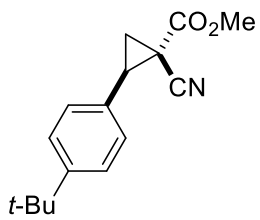
Synthesis of Cyclopropanes S2 *via* Bromosulfonium Bromides[22]

To a stirred solution of the corresponding styrene (0.10 mol) and dimethyl sulfide (31.00 g, 0.50 mol) in DCM (100 ml) at 0 °C a solution of bromine (16.00 g, 0.10 mol) in DCM (20 mL) was added dropwise and the resulting mixture was stirred at 0 °C for 30 min. White precipitate of bromodimethylsulfonium bromide was collected by vacuum filtration and washed with diethyl ether (yield *ca* 80%). To a stirred solution of bromodimethylsulfonium bromide (0.08 mol) in 50:50 %v/v DCM:H_2O mixture (160 mL) K_2CO_3 (33.12 g, 0.24 mol) and the corresponding methylene component (0.08 mol) was sequentially added. The resulting mixture was stirred at ambient temperature for 8 h. Organic layer was separated, water layer was washed with DCM (3×20 mL). Combined organic fractions were dried with Na_2SO_4 and concentrated under reduced pressure. Residue was purified by column chromatography on silica gel (petroleum ether – ethyl acetate). Cyclopropanes **S2** were formed predominantly as *E*-isomer (dr > 95:5) (Scheme S3).

Scheme S3. Synthesis of Cyclopropanes **S2** *via* Bromosulfonium Bromides



Methyl (1*RS*,2*SR*)-1-cyano-2-(4-*tert*-butylphenyl)cyclopropanecarboxylate (S2r)



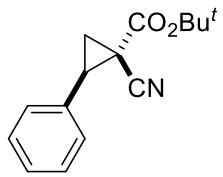
S2r was obtained from 4-*tert*-butylstyrene (3.36 g, 21.0 mmol) and methyl cyanoacetate (1.68 g, 17.0 mmol). Yield 3.83 g (88%); yellowish viscous oil; R_f = 0.64 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.34 (s, 9H, CH_3), 2.10 (dd, ^2J = 5.3, ^3J = 8.4 Hz, 1H, CH_2), 2.16 (dd, ^2J = 5.3, ^3J = 9.3 Hz, 1H, CH_2), 3.16 (dd, ^3J = 9.3, ^3J = 8.4, Hz, 1H, CH), 3.85 (s, 3H, CH_3O), 7.23–7.26 (m, 2H, Ar), 7.41–7.44 (m, 2H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.5 (C), 22.7 (CH_2), 31.0 (3×CH_3), 34.4 (C), 35.1 (CH), 53.4 (CH_3O), 116.2 (CN), 125.4 (2×CH), 127.8 (2×CH), 129.6 (C), 151.3 (C), 167.6 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{16}H_{20}NO_2^+$ 258.1489; Found 258.1494.

***tert*-Butyl (1*RS*,2*SR*)-1-cyano-2-phenylcyclopropanecarboxylate (S2s)**



S2s was obtained from styrene (5.00 g, 48.0 mmol) and *tert*-butyl cyanoacetate (5.36 g, 38.0 mmol). Yield 5.67 g (61%); yellow oil; R_f = 0.56 (petroleum ether – ethyl acetate 4:1); dr 83:17.

(1*RS*,2*SR*)-S2s: ^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.55 (s, 9H, CH_3), 2.01 (dd, ^2J = 5.3, ^3J = 8.3 Hz, 1H, CH_2), 2.07 (dd, ^2J = 5.3, ^3J = 9.3 Hz, 1H, CH_2), 3.10 (dd, ^3J = 9.3, ^3J = 8.3, Hz, 1H, CH), 7.29–7.30 (m, 2H, Ar), 7.32–7.35 (m, 1H, Ar), 7.37–7.40 (m, 2H, Ar).

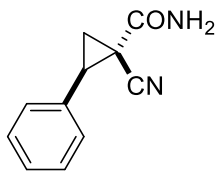
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.1 (CH_2), 23.4 (C), 27.6 (3×CH_3), 34.4 (CH), 83.7 (C), 116.3 (CN), 128.0 (3×CH), 128.4 (2×CH), 133.0 (C), 165.7 (*C*O_2Me).

(1*RS*,2*RS*)-S2s: ^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.19 (s, 9H, CH_3), 1.91 (dd, ^2J = 5.7, ^3J = 9.5 Hz, 1H, CH_2), 2.28 (dd, ^2J = 5.7, ^3J = 8.8 Hz, 1H, CH_2), 3.22 (dd, ^3J = 9.5, ^3J = 8.8, Hz, 1H, CH), 7.27–7.32 (m, 5H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 18.9 (CH_2), 21.5 (C), 27.2 (3×CH_3), 35.4 (CH), 83.1 (C), 119.1 (CN), 127.8 (CH), 127.9 (2×CH), 129.1 (2×CH), 132.2 (C), 162.6 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{18}NO_2^+$ 244.1332; Found 244.1333.

(1*RS*,2*SR*)-1-Cyano-2-phenylcyclopropanecarboxamide[23] (S2t)

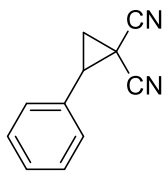


S2t was obtained from styrene (7.89 g, 75.88 mmol) and cyanoacetamide (5.10 g, 60.7 mmol). **S2t** was isolated in a pure form by filtration from its concentrated solution in DCM. Yield 9.56 g (85%); yellowish solid; mp 181–182 °C.

^{1}H NMR (DMSO-d_6, 600 MHz) δ = 2.00 (dd, ^2J = 5.4, ^3J = 9.2 Hz, 1H, CH_2), 2.22 (dd, ^2J = 5.4, ^3J = 8.1 Hz, 1H, CH_2), 3.05 (dd, ^3J = 9.2, ^3J = 8.1 Hz, 1H, CH), 7.31–7.34 (m, 1H, Ar), 7.35–7.40 (m, 4H, Ar), 7.60–7.70 (m, 2H, NH_2).

^{13}C NMR (DMSO-d_6, 150 MHz) δ = 20.0 (CH_2), 23.6 (C), 32.7 (CH), 117.9 (CN), 127.8 (CH), 128.33 (2×CH), 128.35 (2×CH), 134.3 (C), 166.3 (CO).

2-Phenylcyclopropane-1,1-dicarbonitrile[23] (S2u)

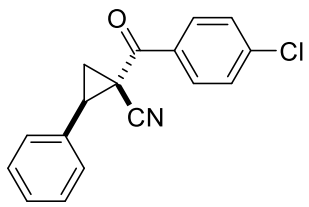


S2u was obtained from styrene (8.25 g, 125.0 mmol) and malononitrile (6.60 g, 100.0 mmol). Yield 11.45 g (68%); yellowish solid, mp 61–62 °C; R_f = 0.30 (petroleum ether – ethyl acetate; 3:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.24 (dd, ^2J = 6.4, ^3J = 9.4 Hz, 1H, CH_2), 2.26 (dd, ^2J = 6.4, ^3J = 8.7 Hz, 1H, CH_2), 3.30 (dd, ^3J = 9.4, ^3J = 8.7 Hz, 1H, CH), 7.30–7.32 (m, 2H, Ph), 7.42–7.46 (m, 3H, Ph).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 7.1 (C), 22.2 (CH_2), 35.0 (CH), 113.0 (CN), 115.2 (CN), 128.3 (2×CH), 129.0 (2×CH), 129.4 (CH), 130.6 (C).

(1*RS*,2*SR*)-1-(4-Chlorobenzoyl)-2-phenylcyclopropanecarbonitrile (S2v)



S2v was obtained from styrene (1.04 g, 10.0 mmol) and 3-(4-chlorophenyl)-3-oxopropanenitrile (1.44 g, 8.0 mmol). Yield 1.51 g (67%); yellow solid; mp 91–92 °C; R_f = 0.52 (petroleum ether – ethyl acetate 4:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.25 (dd, ^2J = 5.3, ^3J = 8.4 Hz, 1H, CH_2), 2.56 (dd, ^2J = 5.3, ^3J = 9.1 Hz, 1H, CH_2), 3.17 (dd, ^3J = 9.1, ^3J = 8.4 Hz, 1H, CH), 7.35–7.37 (m, 2H, Ar), 7.40–7.43 (m, 1H, Ar), 7.45–7.46 (m, 2H, Ar), 7.48–7.50 (m, 2H, Ar), 7.92–7.94 (m, 2H, Ar).

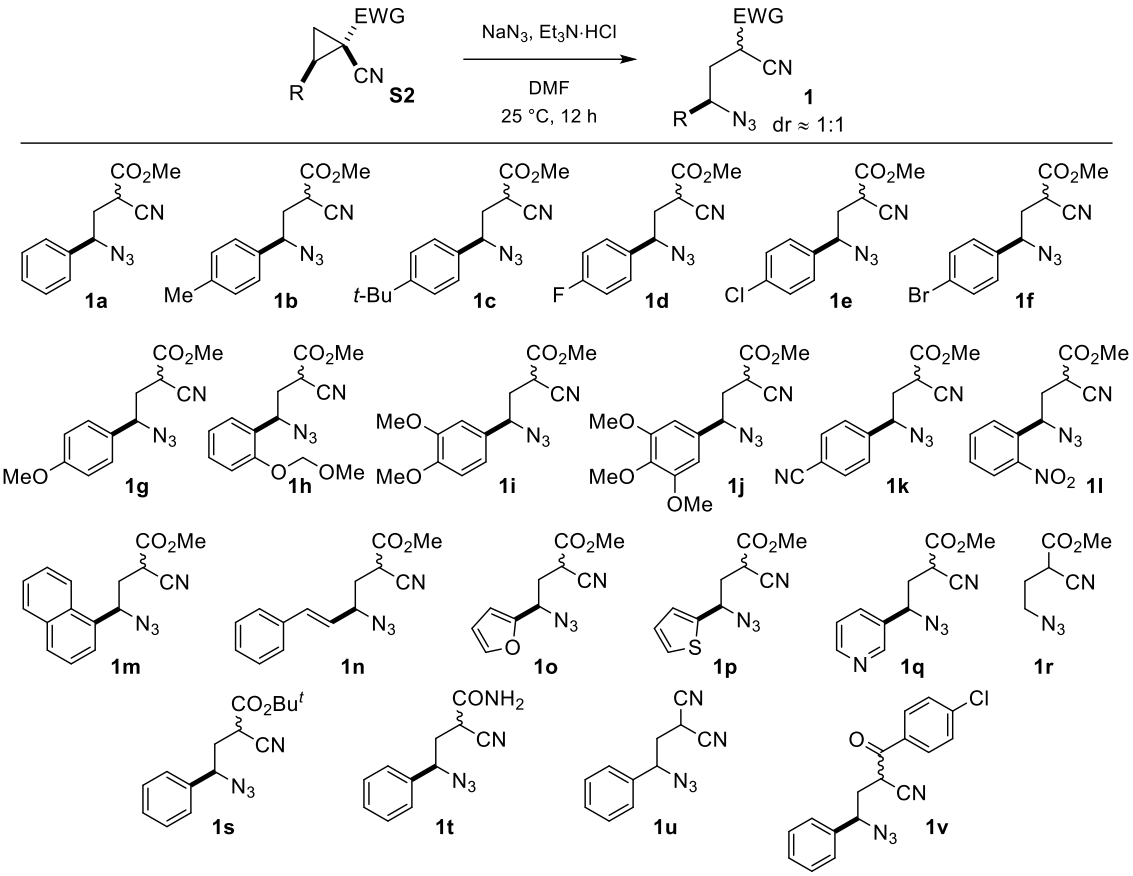
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.6 ($^1J_{CH}$ = 165, $^1J_{CH}$ = 172 Hz, CH_2), 28.6 (C), 38.2 ($^1J_{CH}$ = 167 Hz, CH), 118.4 (CN), 128.2 (2×CH), 128.8 (CH), 128.9 (2×CH), 129.0 (2×CH), 130.2 (2×CH), 132.9 (C), 133.8 (C), 140.3 (C), 190.5 (CO).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{17}H_{13}ClNO^+$ 282.0680; Found 282.0684.

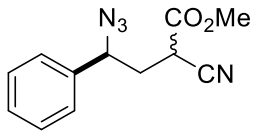
Synthesis of *γ*-Azidobutyronitriles 1

To a stirred solution of cyclopropane **S2** (18.0 mmol) in dry DMF (90 mL) NaN_3 (2.34 g, 36.0 mmol) and $Et_3N{\cdot}HCl$ (4.95 g, 36.0 mmol) were sequentially added (Scheme S4). Resulting suspension was stirred at ambient temperature for 12 h, diluted with brine (200 mL) and extracted with ethyl acetate (3×100 mL). Combined organic fractions were washed with water (3×100 mL), dried with Na_2SO_4 and concentrated under reduced pressure. Residue was purified by column chromatography on silica gel (petroleum ether – ethyl acetate).

Scheme S4. Synthesis of γ-Azidobutyronitriles **1**



Methyl 4-azido-2-cyano-4-phenylbutyrate (1a)



1a was obtained from cyclopropane **S2a** (3.62 g, 18.0 mmol). Yield 3.41 g (78%); dr **A**:**B** 57:43; yellow oil; R_f = 0.53 (petroleum ether – ethyl acetate 2:1).

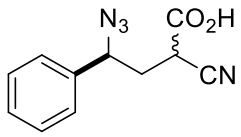
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.19 (ddd, ^2J = 14.1, ^3J = 10.3, ^3J = 4.3 Hz, 1H, CH_2, **A**), 2.35 (ddd, ^2J = 14.0, ^3J = 6.9, ^3J = 6.8 Hz, 1H, CH_2, **B**), 2.40 (ddd, ^2J = 14.0, ^3J = 8.5, ^3J = 7.0 Hz, 1H, CH_2, **B**), 2.41 (ddd, ^2J = 14.1, ^3J = 10.8, ^3J = 5.0 Hz, 1H, CH_2, **A**), 3.53 (dd, ^3J = 7.0, ^3J = 6.9, Hz, 1H, C^2H, **B**), 3.79 (s, 3H, CH_3O, **A**), 3.83 (s, 3H, CH_3O, **B**), 3.84 (dd, ^3J = 10.3, ^3J = 5.0, Hz, 1H, C^2H, **A**), 4.74 (dd, ^3J = 8.5, ^3J = 6.8 Hz, 1H, C^4H, **B**), 4.76 (dd, ^3J = 10.8 ^3J = 4.3 Hz, 1H, C^4H, **A**), 7.35–7.37 (m, 2H+2H, Ph, **A**, **B**), 7.37–7.41 (m, 1H+1H, Ph, **A**, **B**), 7.41–7.45 (m, 2H+2H, Ph, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.2 ($^1J_{CH}$ = 137 Hz, C^2H), 34.7 ($^1J_{CH}$ = 137 Hz, C^2H), 35.6 ($^1J_{CH}$ = 135 Hz, CH_2), 35.9 ($^1J_{CH}$ = 135 Hz, CH_2), 53.4 ($^1J_{CH}$ = 148 Hz, CH_3O), 53.5 ($^1J_{CH}$ = 148 Hz, CH_3O),

62.9 ($^1J_{CH}$ = 143 Hz, C^4H), 63.0 ($^1J_{CH}$ = 144 Hz, C^4H), 115.5 (2×CN), 126.8 (4×CH), 128.96 (CH), 129.01 (2×CH), 129.04 (CH), 129.1 (2×CH), 137.0 (C), 137.3 (C), 165.67 (*C*O_2Me), 165.69 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{13}N_4O_2^+$ 245.1033; Found 245.1031.

4-Azido-2-cyano-4-phenylbutyric acid (1a′)



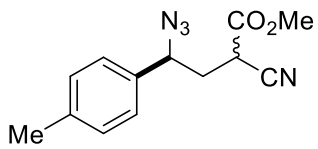
1a′ was obtained as a side product in a gram-scale synthesis of azidoester **1a** from cyclopropane **S2a** (4.38 g, 23.4 mmol). Yield 0.27 g (5%); dr **A**:**B** 56:44; yellow oil; R_f = 0.10 (petroleum ether – ethyl acetate 1:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.23 (ddd, ^2J = 14.0, ^3J = 10.3, ^3J = 4.1 Hz, 1H, CH_2, **A**), 2.37 (ddd, ^2J = 14.1, ^3J = 6.8, ^3J = 6.5 Hz, 1H, CH_2, **B**), 2.43 (ddd, ^2J = 14.0, ^3J = 10.8, ^3J = 5.0 Hz, 1H, CH_2, **A**), 2.44 (ddd, ^2J = 14.1, ^3J = 8.8, ^3J = 6.7 Hz, 1H, CH_2, **B**), 3.63 (dd, ^3J = 6.8, ^3J = 6.7, Hz, 1H, C^2H, **B**), 3.94 (dd, ^3J = 10.3, ^3J = 5.0, Hz, 1H, C^2H, **A**), 4.77 (dd, ^3J = 8.8, ^3J = 6.5 Hz, 1H, C^4H, **B**), 4.79 (dd, ^3J = 10.8 ^3J = 4.1 Hz, 1H, C^4H, **A**), 7.35–7.39 (m, 2H+2H, Ph, **A**, **B**), 7.39–7.46 (m, 3H+3H, Ph, **A**, **B**), 9.84 (br.s, 1H+1H, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.5 (C^2H), 34.9 (C^2H), 35.5 (CH_2), 35.9 (CH_2), 62.8 (C^4H), 62.9 (C^4H), 115.1 (CN), 115.2 (CN), 126.8 (4×CH), 129.1 (4×CH), 129.3 (2×CH), 136.9 (C), 137.1 (C), 169.9 (CO_2H), 170.0 (CO_2H).

HRMS (ESI) *m/z*: $[M - H]^-$ Calcd for $C_{11}H_9N_4O_2^-$ 229.0731; Found 229.0729.

Methyl 4-azido-2-cyano-4-(*p*-tolyl)butyrate (1b)



1b was obtained from cyclopropane **S2b** (2.60 g, 12.1 mmol). Yield 2.46 g (79%); dr **A**:**B** 56:44; yellow oil; R_f = 0.75 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.17 (ddd, ^2J = 14.3, ^3J = 10.2, ^3J = 4.3 Hz, 1H, CH_2, **A**), 2.33 (ddd, ^2J = 14.0, ^3J = 7.0, ^3J = 6.9 Hz, 1H, CH_2, **B**), 2.37 (s, 3H+3H, CH_3, **A**, **B**), 2.37–2.43 (m, 1H+1H, CH_2, **A**, **B**), 3.51 (dd, ^3J = 7.0, ^3J = 6.9 Hz, 1H, C^2H, **B**), 3.79 (s, 3H, CH_3O, **A**), 3.83 (s, 3H, CH_3O, **B**), 3.83

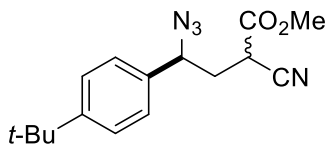
(dd, ^3J = 10.2, ^3J = 5.1 Hz, 1H, C^2H, **A**), 4.70 (dd, ^3J = 8.4, ^3J = 6.9 Hz, 1H, C^4H, **B**), 4.73 (dd, ^3J = 10.8, ^3J = 4.3 Hz, 1H, C^4H, **A**), 7.22–7.25 (m, 4H+4H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 21.0 (2×CH_3) 34.3 (CH), 34.8 (CH), 35.8 (CH_2), 36.1 (CH_2), 53.5 (2×CH_3O), 62.8 (CH), 62.9 (CH), 115.6 (2×CN), 126.8 (4×CH), 129.8 (2×CH), 129.9 (2×CH), 134.1 (C), 134.4 (C), 139.0 (C), 139.1 (C), 165.8 (2×*C*O_2Me).

IR (film) 2251, 2102, 1749, 1515, 1417, 1250, 1013, 819, 723 cm^{-1}.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{13}H_{15}N_4O_2^+$ 259.1190; Found 259.1196.

Methyl 4-azido-2-cyano-4-(4-*tert*-butylphenyl)butyrate (1c)



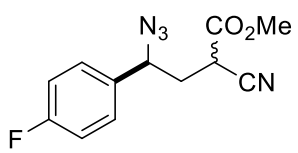
1c was obtained from cyclopropane **S2r** (0.62 g, 2.4 mmol). Yield 0.54 g (75%); dr **A**:**B** 57:43; yellow oil; R_f = 0.49 (petroleum ether – ethyl acetate 2:1).

^1H NMR ($CDCl_3$, 600 MHz) δ = 1.34 (s, 9H+9H, CH_3, **A**, **B**), 2.20 (ddd, ^2J = 14.0, ^3J = 10.1, ^3J = 4.3 Hz, 1H, CH_2, **A**), 2.36 (ddd, ^2J = 14.0, ^3J = 7.0, ^3J = 6.9 Hz, 1H, CH_2, **B**), 2.39–2.45 (m, 1H+1H, CH_2, **A**, **B**). 3.55 (dd, ^3J = 7.0, ^3J = 6.9 Hz, 1H, C^2H, **B**), 3.76 (s, 3H, CH_3O, **A**), 3.81 (s, 3H, CH_3O, **B**), 3.86 (dd, ^3J = 10.1, ^3J = 5.1 Hz, 1H, C^2H, **A**), 4.73 (dd, ^3J = 8.6, ^3J = 6.8 Hz, 1H, C^4H, **B**), 4.76 (dd, ^3J = 10.8, ^3J = 4.3 Hz, 1H, C^4H, **A**), 7.28–7.32 (m, 4H+4H, Ar, **A**, **B**), 7.43–7.47 (m, 4H+4H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 31.0 (6×CH_3) 34.2 (C^2H), 34.4 (2×C), 34.6 (C^2H), 35.4 (CH_2), 35.8 (CH_2), 53.3 (OCH_3), 53.4 (OCH_3), 62.5 (C^4H), 62.6 (C^4H), 115.6 (2×CN), 125.8 (2×CH), 125.9 (2×CH), 126.4 (4×CH), 133.9. (C), 134.2 (C), 151.8 (C), 151.9 (C), 165.7 (2×*C*O_2Me).

HRMS (ESI) *m/z*: $[M - H]^-$ Calcd for $C_{16}H_{19}N_4O_2^-$ 299.1513; Found 299.1511.

Methyl 4-azido-2-cyano-4-(4-fluorophenyl)butyrate (1d)



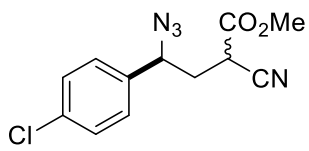
1d was obtained from cyclopropane **S2c** (2.97 g, 13.6 mmol). Yield 2.50 g (70%); dr **A**:**B** 58:42; yellow oil; R_f = 0.60 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.16 (ddd, ^2J = 14.1, ^3J = 10.3, ^3J = 4.2 Hz, 1H, CH_2, **A**), 2.31 (ddd, ^2J = 14.1, ^3J = 7.1, ^3J = 6.5 Hz, 1H, CH_2, **B**), 2.35–2.40 (m, 1H+1H, CH_2, **A**, **B**), 3.52–3.54 (m, 1H, C^2H, **B**), 3.80 (s, 3H, OCH_3, **A**), 3.83 (dd, ^3J = 10.4, ^3J = 5.0 Hz, 1H, C^2H, **A**), 3.85 (s, 3H, OCH_3, **B**), 4.74 (dd, ^3J = 8.8, ^3J = 6.4 Hz, 1H, C^4H, **B**), 4.75 (dd, ^3J = 10.9, ^3J = 4.3 Hz, 1H, C^4H, **A**), 7.10–7.14 (m, 2H+2H, Ar, **A**, **B**), 7.33–7.37 (m, 2H+2H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.1 (C^2H), 34.7 (C^2H), 35.8 (CH_2), 36.1 (CH_2), 53.66 (OCH_3), 53.71 (OCH_3), 62.2 (C^4H), 62.3 (C^4H), 115.5 (CN), 115.6 (CN), 116.2 ($^2J_{CF}$ = 22 Hz, 2×CH), 116.3 ($^2J_{CF}$ = 22 Hz, 2×CH), 128.7 ($^3J_{CF}$ = 8 Hz, 4×CH), 133.0 ($^3J_{CF}$ = 3 Hz, C), 133.3 ($^3J_{CF}$ = 3 Hz, C), 162.87 ($^1J_{CF}$ = 249 Hz, C), 162.92 ($^1J_{CF}$ = 249 Hz, C), 165.69 (CO_2Me), 165.70 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{12}FN_4O_2^+$ 263.0939; Found 263.0937.

Methyl 4-azido-4-(4-chlorophenyl)-2-cyanobutyrate (1e)



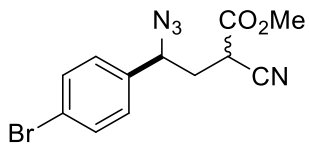
1e was obtained from cyclopropane **S2d** (1.56 g, 6.6 mmol). Yield 1.26 g (68%); dr **A**:**B** 56:44; yellow oil; R_f = 0.60 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.16 (ddd, ^2J = 14.3, ^3J = 10.3, ^3J = 4.1 Hz, 1H, CH_2, **A**), 2.30 (ddd, ^2J = 14.1, ^3J = 7.3, ^3J = 6.3 Hz, 1H, CH_2, **B**), 2.33–2.39 (m, 1H+1H, CH_2, **A**, **B**), 3.53–3.56 (m, 1H, C^2H, **B**), 3.79 (s, 3H, OCH_3, **A**), 3.829 (dd, ^3J = 10.3, ^3J = 5.0 Hz, 1H, C^2H, **A**), 3.833 (s, 3H, OCH_3, **B**), 4.73 (dd, ^3J = 8.9, ^3J = 6.3 Hz, 1H, C^4H, **B**), 4.74 (dd, ^3J = 11.0, ^3J = 4.2 Hz, 1H, C^4H, **A**), 7.29–7.31 (m, 2H+2H, Ar, **A**, **B**), 7.38–7.41 (m, 2H+2H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.1 (C^2H), 34.6 (C^2H), 35.6 (CH_2), 35.9 (CH_2), 53.6 (OCH_3), 53.7 (OCH_3), 62.2 (C^4H), 62.3 (C^4H), 115.46 (CN), 115.48 (CN), 128.18 (2×CH), 128.19 (2×CH), 129.3 (2×CH), 129.4 (2×CH), 134.8 (C), 134.9 (C), 135.7 (C), 135.9 (C), 165.6 (2×CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{12}ClN_4O_2^+$ 279.0643; Found 323.0143.

Methyl 4-azido-4-(4-bromophenyl)-2-cyanobutyrate (1f)



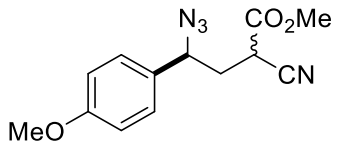
1f was obtained from cyclopropane **S2e** (4.00 g, 14.3 mmol). Yield 2.89 g (63%); dr **A**:**B** 55:45; yellow oil; R_f = 0.64 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.16 (ddd, ^2J = 14.1, ^3J = 10.4, ^3J = 4.1 Hz, 1H, CH_2, **A**), 2.33 (ddd, ^2J = 14.1, ^3J = 7.2, ^3J = 6.4 Hz, 1H, CH_2, **B**), 2.28–2.39 (m, 1H+1H, CH_2, **A**, **B**), 3.52–3.55 (m, 1H, C^{2}H, **B**), 3.81 (s, 3H, OCH_3, **A**), 3.83 (dd, ^3J = 10.4, ^3J = 4.9 Hz, 1H, C^{2}H, **A**), 3.86 (s, 3H, OCH_3, **B**), 4.72 (dd, ^3J = 8.8, ^3J = 6.4 Hz, 1H, C^{4}H, **B**), 4.74 (dd, ^3J = 11.0, ^3J = 4.1 Hz, 1H, C^{4}H, **A**), 7.24–7.28 (m, 2H+2H, Ar, **A**, **B**), 7.56–7.58 (m, 2H+2H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.3 (C^{2}H), 34.7 (C^{2}H), 35.7 (CH_2), 36.0 (CH_2), 53.8 (2×OCH_3), 62.3 (C^{4}H), 62.4 (C^{4}H), 115.5 (2×CN), 123.2 (C), 123.3 (C), 128.5 (4×CH), 132.4 (2×CH), 132.5 (2×CH), 136.2 (C), 136.5 (C), 165.7 (2×*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{12}BrN_4O_2^+$ 323.0138; Found 323.0143.

Methyl 4-azido-2-cyano-4-(4-methoxyphenyl)butyrate (1g)



1g was obtained from cyclopropane **S2f** (3.00 g, 13.0 mmol). Yield 1.87 g (53%); dr **A**:**B** 58:42; yellow oil; R_f = 0.51 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.16 (ddd, ^2J = 14.0, ^3J = 10.2, ^3J = 4.3 Hz, 1H, CH_2, **A**), 2.33 (m, 1H, CH_2, **B**), 2.39 (ddd, ^2J = 14.0, ^3J = 8.3, ^3J = 7.2 Hz, 1H, CH_2, **B**), 2.43 (ddd, ^2J = 14.0, ^3J = 10.8, ^3J = 5.1 Hz, 1H, CH_2, **A**), 3.49 (dd, ^3J = 7.2, ^3J = 6.9 Hz, 1H, C^{2}H, **B**), 3.80 (s, 3H, OCH_3, **A**), 3.81 (dd, ^3J = 10.2, ^3J = 5.1 Hz, 1H, C^{2}H, **A**), 3.83 (s, 3H+3H, OCH_3, **A, B**), 3.84 (s, 3H, OCH_3, **B**), 4.69 (dd ^3J = 8.3, ^3J = 7.2 Hz, 1H, C^{4}H, **B**), 4.71 (dd, ^3J = 10.8, ^3J = 4.3 Hz, 1H, C^{4}H, **A**), 6.94–6.96 (m, 2H+2H, Ar, **A**, **B**), 7.27–7.29 (m, 2H+2H, Ar, **A**, **B**).

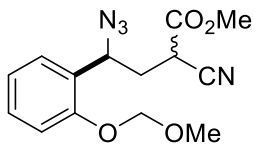
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.3 ($^1J_{CH}$ = 136 Hz, C^{2}H), 34.8 ($^1J_{CH}$ = 136 Hz, C^{2}H), 35.7 ($^1J_{CH}$ = 134 Hz, CH_2), 36.0 ($^1J_{CH}$ = 134 Hz, CH_2), 53.6 ($^1J_{CH}$ = 148 Hz, OCH_3), 53.7 ($^1J_{CH}$ = 148 Hz, OCH_3),

55.3 ($^1J_{CH}$ = 144 Hz, 2×OCH_3), 62.5 ($^1J_{CH}$ = 141 Hz, C^4H), 62.6 ($^1J_{CH}$ = 144 Hz, C^4H), 114.5 (2×CH), 114.6 (2×CH), 115.7 (2×CN), 128.3 (4×CH), 128.8 (C), 129.2 (C), 160.1 (2×C), 165.8 (*C*O_2Me), 165.9 (*C*O_2Me).

IR (film) 2249, 2099, 1744, 1610, 1585, 1512, 1437, 1245, 1209, 1175, 1029, 831 cm^{-1}.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{13}H_{15}N_4O_3^+$ 275.1139; Found 273.1146.

Methyl 4-azido-2-cyano-4-[2-(methoxymethoxy)phenyl]butyrate (1h)



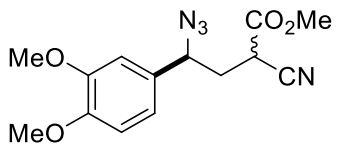
1h was obtained from cyclopropane **S2g** (0.52 g, 2.0 mmol); reaction time 48 h. Yield 0.45 g (74%); dr **A**:**B** 65:35; yellowish oil; R_f = 0.57 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.24 (ddd, ^2J = 14.2, ^3J = 10.4, ^3J = 4.0 Hz, 1H, CH_2, **A**), 2.37–2.45 (m, 2H, CH_2, **A**, **B**), 2.39 (ddd, ^2J = 14.0, ^3J = 10.7, ^3J = 4.9 Hz, 1H, CH_2, **B**), 2.43 (ddd, ^2J = 14.0, ^3J = 10.8, ^3J = 5.1 Hz, 1H, CH_2, **A**), 3.50 (s, 3H, OCH_3, **A**), 3.51 (s, 3H, OCH_3, **A**), 3.58–3.60 (m, 1H, C^2H, **B**), 3.78 (s, 3H, OCH_3, **A**), 3.83 (s, 3H, OCH_3, **B**), 3.84 (dd, ^3J = 10.4, ^3J = 4.9 Hz, 1H, C^2H, **A**), 5.22 (dd ^3J = 8.3, ^3J = 6.4 Hz, 1H, C^4H, **B**), 5.24–5.27 (m, 1H, C^4H, **A**), 5.25 (br.s, 2H+2H, OCH_2O, **A**, **B**), 7.05–7.09 (m, 1H+1H, Ar, **A**, **B**), 7.17–7.19 (m, 1H+1H, Ar, **A**, **B**), 7.30–7.33 (m, 1H+1H, Ar, **A**, **B**), 7.34–7.37 (m, 1H+1H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.4 ($^1J_{CH}$ = 136 Hz, C^2H), 34.6 ($^1J_{CH}$ = 135 Hz, CH_2), 34.7 ($^1J_{CH}$ = 135 Hz, CH_2), 34.8 ($^1J_{CH}$ = 136 Hz, C^2H), 53.46 ($^1J_{CH}$ = 148 Hz, OCH_3), 53.48 ($^1J_{CH}$ = 148 Hz, OCH_3), 56.22 ($^1J_{CH}$ = 143 Hz, OCH_3), 56.23 ($^1J_{CH}$ = 143 Hz, OCH_3), 57.08 ($^1J_{CH}$ = 144 Hz, C^4H), 57.12 ($^1J_{CH}$ = 144 Hz, C^4H), 94.39 ($^1J_{CH}$ = 166 Hz, OCH_2O), 94.41 ($^1J_{CH}$ = 166 Hz, OCH_2O), 114.18 (CH), 114.20 (CH), 115.7 (CN), 115.8 (CN), 122.0 (CH), 122.1 (CH), 125.8 (C), 126.2 (C), 127.0 (CH), 127.2 (CH), 129.9 (CH), 130.0 (CH), 154.3 (C), 154.4 (C), 165.9 (2×*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{17}N_4O_4^+$ 305.1244; Found 305.1243.

Methyl 4-azido-2-cyano-4-(3,4-dimethoxyphenyl)butyrate (1i)



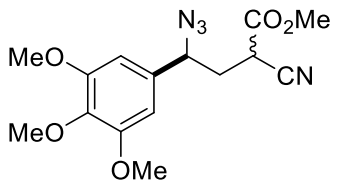
1i was obtained from cyclopropane **S2h** (3.00 g, 11.5 mmol). Yield 2.26 g (65%); dr **A**:**B** 53:47; yellow oil; R_f = 0.44 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.17 (ddd, ^2J = 14.1, ^3J = 10.2, ^3J = 4.3, Hz, 1H, CH_2, **A**), 2.32 (m, 1H, CH_2, **B**), 2.38 (ddd, ^2J = 14.0, ^3J = 8.2, ^3J = 7.3 Hz, 1H, CH_2, **B**), 2.39 (ddd, ^2J = 14.1, ^3J = 10.8, ^3J = 5.1 Hz, 1H, CH_2, **A**), 3.48 (dd, ^3J = 7.3, ^3J = 7.2 Hz, 1H, C^2H, **B**), 3.79 (s, 3H, OCH_3, **A**), 3.81 (dd, ^3J = 10.2, ^3J = 5.1 Hz, 1H, C^2H, **A**), 3.83 (s, 3H, OCH_3, **A**), 3.88 (s, 6H, 2×OCH_3, **B**), 3.90 (s, 6H, 2×OCH_3, **A**), 4.66 (dd, ^3J = 8.2, ^3J = 7.2 Hz, 1H, C^4H, **B**), 4.69 (dd, ^3J = 10.8, ^3J = 4.3 Hz, 1H, C^4H, **A**), 6.82–6.84 (m, 1H+1H, Ar, **A**, **B**), 6.87–6.91 (m, 2H+2H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.3 (C^2H), 34.7 (C^2H), 35.7 (CH_2), 36.0 (CH_2), 53.59 (OCH_3), 53.64 (OCH_3), 55.8 (OCH_3), 55.9 (OCH_3), 62.8 (C^4H), 62.9 (C^4H), 109.5 (CH), 109.6 (CH), 111.2 (CH), 111.3 (CH), 115.6 (2×CN), 119.5 (CH), 119.6 (CH), 129.3 (C), 129.6 (C), 149.4 (C), 149.5 (C), 149.57 (C), 149.63 (C), 165.77 (*C*O_2Me), 165.82 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{17}N_4O_4^+$ 305.1244; Found 305.1247.

Methyl 4-azido-2-cyano-4-(3,4,5-trimethoxyphenyl)butyrate (1j)



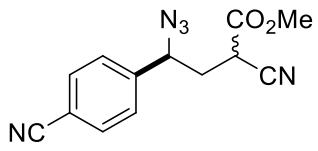
1j was obtained from cyclopropane **S2i** (2.50 g, 8.6 mmol). Yield 1.64 g (57%); dr **A**:**B** 55:45; yellow oil; R_f = 0.36 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.17 (ddd, ^2J = 14.1, ^3J = 10.3, ^3J = 4.2 Hz, 1H, CH_2, **A**), 2.28-2.33 (m, 1H, CH_2, **B**), 2.35 (ddd, ^2J = 14.1, ^3J = 10.9, ^3J = 4.9 Hz, 1H, CH_2, **A**), 2.37 (ddd, ^2J = 14.0, ^3J = 8.4, ^3J = 7.2Hz, 1H, CH_2, **B**), 3.50 (dd, ^3J = 7.2, ^3J = 7.0 Hz, 1H, C^2H, **B**), 3.80 (s, 3H, OCH_3, **A**), 3.83 (dd, ^3J = 10.3, ^3J = 4.9 Hz, 1H, C^2H, **A**), 3.84 (s, 9H, 3×OCH_3, **B**), 3.85 (s, 3H, OCH_3, **B**), 3.88 (s, 9H, 3×OCH_3, **A**), 4.66 (dd, ^3J = 8.4, ^3J = 6.9 Hz, 1H, C^4H, **B**), 4.68 (dd, ^3J = 10.9, ^3J = 4.2 Hz, 1H, C^4H, **A**), 6.54-6.55 (m, 2H+2H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.3 (C^2H), 34.8 (C^2H), 35.8 (CH_2), 36.2 (CH_2), 53.66 (OCH_3), 53.71 (OCH_3), 56.2 (4×OCH_3), 60.7 (2×OCH_3), 63.3 (C^4H), 63.4 (C^4H), 103.7 (2×CH), 103.8 (2×CH), 115.7 (2×CN), 132.6 (C), 133.0 (C), 138.3 (C), 138.4 (C), 153.7 (C), 153.8 (C), 165.77 (*C*O_2Me), 165.79 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{19}N_4O_5^+$ 335.1347; Found 335.1346.

Methyl 4-azido-2-cyano-4-(4-cyanophenyl)butyrate (1k)



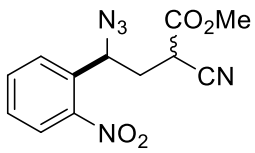
1k was obtained from cyclopropane **S2j** (1.81 g, 8.0 mmol). Yield 0.97 g (45%); dr **A**:**B** 57:43; yellow oil; R_f = 0.49 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.18 (ddd, ^2J = 14.2, ^3J = 10.5, ^3J = 3.8 Hz, 1H, CH_2, **A**), 2.30-2.39 (m, 1H+2H, CH_2, **A**, **B**), 3.61 (dd, ^3J = 7.3, ^3J = 6.2 Hz, 1H, C^2H, **B**), 3.84 (s, 3H, OCH_3, **A**), 3.86 (dd, ^3J = 10.5, ^3J = 4.8 Hz, 1H, C^2H, **A**), 3.87 (s, 3H, OCH_3, **B**), 4.83 (dd, ^3J = 8.8, ^3J = 6.0 Hz, 1H, C^4H, **B**), 4.84 (dd, ^3J = 11.2, ^3J = 3.8 Hz, 1H, C^4H, **A**), 7.49–7.51 (m, 2H+2H, Ar, **A**, **B**), 7.73–7.75 (m, 2H+2H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 33.9 (C^2H), 34.6 (C^2H), 35.7 (CH_2), 35.9 (CH_2), 53.8 (OCH_3), 53.9 (OCH_3), 62.4 (C^2H), 62.5 (C^2H), 113.11 (C), 113.15 (C), 115.4 (2×CN), 118.0 (2×CN), 127.6 (4×CH), 136.0 (4×CH), 142.7 (C), 142.8 (C), 165.5 (2×*C*O_2Me)

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{13}H_{12}N_5O_2^+$ 270.0986; Found 270.0983.

Methyl 4-azido-2-cyano-4-(2-nitrophenyl)butyrate (1l)

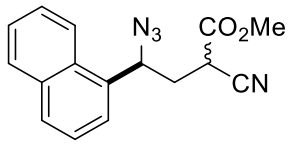


1l was obtained from cyclopropane **S2k** (1.21 g, 4.9 mmol). Yield 0.65 g (46%); dr **A**:**B** 53:47; yellow oil; R_f = 0.45 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.27 (ddd, ^2J = 14.3, ^3J = 10.2, ^3J = 4.7 Hz, 1H, CH_2, **B**), 2.30 (ddd, ^2J = 14.1, ^3J = 10.5, ^3J = 5.1 Hz, 1H, CH_2, **A**), 2.45 (ddd, ^2J = 14.1, ^3J = 10.2, ^3J = 3.6 Hz, 1H, CH_2, **A**), 2.56 (ddd, ^2J = 14.3, ^3J = 8.6, ^3J = 3.5 Hz, 1H, CH_2, **B**), 3.84 (s, 3H, OCH_3, **A**), 3.85 (dd, ^3J = 8.6, ^3J = 4.7 Hz, 1H, C^2H, **B**), 3.90 (dd, ^3J = 10.2, ^3J = 5.1 Hz, 1H, C^2H, **A**), 3.91 (s, 3H,

OCH_3, **B**), 5.48 (dd, ^3J = 3.5, ^3J = 10.2 Hz, 1H, C^4H, **B**), 5.52 (dd, ^3J = 10.5, ^3J = 3.6 Hz, 1H, C^4H, **A**), 7.54–7.58 (m, 1H+1H, Ar, **A**, **B**), 7.74–7.78 (m, 2H+2H, Ar, **A**, **B**), 8.04–8.06 (m, 1H+1H, Ar, **A**, **B**). ^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.4 (C^2H), 34.7 (C^2H), 36.1 (CH_2), 36.6 (CH_2), 53.77 (OCH_3), 53.84 (OCH_3), 58.6 (C^4H), 58.7 (C^4H), 115.1 (CN), 115.6 (CN), 125.2 (2×CH), 128.5 (2×CH), 129.7 (2×CH), 133.9 (C), 134.0 (C), 134.3 (2×CH), 134.4 (2×CH), 147.8 (C), 148.0 (C), 165.7 (2×*C*O_2Me) HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{12}N_5O_4^+$ 290.0884; Found 290.0886.

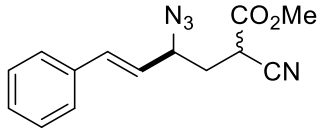
Methyl 4-azido-2-cyano-4-(naphthen-1-yl)butyrate (1m)



1m was obtained from cyclopropane **S2l** (2.01 g, 8.0 mmol). Yield 1.32 g (56%); dr **A**:**B** 53:47; yellow oil; R_f = 0.66 (petroleum ether – ethyl acetate 2:1).

^1H NMR ($CDCl_3$, 600 MHz) δ = 2,41 (ddd, ^2J = 14.3, ^3J = 10.7, ^3J = 3.6 Hz, 1H, CH_2, **A**), 2.49-2,57 (m, 1H+1H, CH_2, **A**, **B**), 2,60 (ddd, ^2J = 14.3, ^3J = 7.6, ^3J = 5.2 Hz, 1H, CH_2, **B**), 3.75 (dd, ^3J = 7.6, ^3J = 5.6 Hz, 1H, C^2H, **B**), 3.79 (s, 3H, OCH_3, **A**), 3.91 (s, 3H, OCH_3, **B**), 3.99 (dd, ^3J = 10.7, ^3J = 4.7 Hz, 1H, C^2H, **A**), 5.56 (dd, ^3J = 9.8, ^3J = 5.2 Hz, 1H, C^4H, **B**), 5.58 (dd, ^3J = 10.6, ^3J = 3.4 Hz, 1H, C^4H, **A**), 7.52–7.58 (m, 2H+2H, Ar, **A**, **B**),7.61–7.65 (m, 2H+2H, Ar, **A**, **B**), 7.89–7.92 (m, 1H+1H, Ar, **A**, **B**), 7.93–7.96 (m, 1H+1H, Ar, **A**, **B**), 8.14 (d, ^3J = 8.4 Hz, 1H, Ar, **A**), 8.19 (d, ^3J = 8.5 Hz, 1H, Ar, **B**). ^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.2 (C^2H), 35.1 (C^2H), 35.4 (CH_2), 35.7 (CH_2), 53.6 (OCH_3), 53.7 (OCH_3), 60.0 (C^4H), 60.2 (C^4H), 115.8 (2×CN), 122.3 (CH), 122.5 (CH), 124.5 (CH), 124.7 (CH), 125.3 (2×CH), 126.2 (2×CH), 127.03 (CH), 127.07 (CH), 129.2 (2×CH), 129.6 (CH), 129.7 (CH), 130.2 (C), 130.3 (C), 133.0 (C), 133.1 (C), 134.0 (C), 134.1 (C), 165.8 (*C*O_2Me), 166.0 (*C*O_2Me). HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{16}H_{15}N_4O_2^+$ 295.1190; Found 295.1194.

Methyl (*E*)-4-azido-2-cyano-6-phenylhex-5-enoate (1n)



1n was obtained from cyclopropane **S2m** (3.00 g, 13.2 mmol). Yield 2.59 g (73%); dr **A**:**B** 55:45; yellow oil; R_f = 0.55 (petroleum ether – ethyl acetate

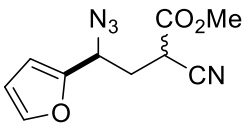
2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.16 (ddd, ^2J = 14.0, ^3J = 9.7, ^3J = 4.8 Hz, 1H, CH_2, **A**), 2.22-2.27 (m, 2H+1H, CH_2, **A**, **B**), 3.69 (dd, ^3J = 7.0, ^3J 6.8 Hz, 1H, C^2H, **B**), 3.80 (s, 3H, OCH_3, **A**), 3.82 (dd, ^3J = 9.7, ^3J = 5.1 Hz, 1H, C^2H, **A**), 3.85 (s, 3H, OCH_3, **B**), 4.32-4.38 (m, 1H+1H, C^4H, **A, B**), 6.10 (dd, ^3J = 15.8, ^3J = 8.5 Hz, 1H, CH, **B**), 6.11 (dd, ^3J = 15.8, ^3J = 8.4 Hz, 1H, CH, **A**), 6.76 (d, ^3J = 15.8 Hz, 1H+1H, CH, **A**, **B**), 7.31–7.34 (m, 1H+1H, Ar, **A**, **B**), 7.35–7.39 (m, 2H+2H, Ar, **A**, **B**), 7.42–7.45 (m, 2H+2H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 33.9 (C^2H), 34.2 (C^2H), 34.3 (CH_2), 34.4 (CH_2), 53.6 (OCH_3), 53.7 (OCH_3), 61.7 (C^4H), 61.8 (C^4H), 115.6 (CN), 115.7 (CN), 124.1 (CH), 124.3 (CH), 126.78 (2×CH), 126.82 (2×CH), 128.6 (2×CH), 128.7 (2×CH), 135.08 (C), 135.14 (C), 135.4 (CH), 135.7 (CH), 165.82 (CO_2Me), 165.86 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{15}N_4O_2^+$ 271.1190; Found 271.1191.

Methyl 4-azido-2-cyano-4-(furanyl-2-yl)butyrate (1o)



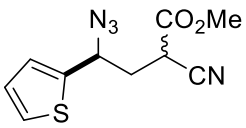
1o was obtained from cyclopropane **S2n** (1.38 g, 7.2 mmol). Yield 1.17 g (69%); dr **A**:**B** 57:43; yellow oil; R_f = 0.58 (pethroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.32 (ddd, ^2J = 14.3, ^3J = 10.1, ^3J = 4.6 Hz, 1H, CH_2, **A**), 2.45–2.56 (m, 1H+2H, CH_2, **A**, **B**), 3.61–3.63 (m, 1H, C^2H, **A**), 3.81 (dd, ^3J = 10.1, ^3J = 5.1 Hz, 1H, C^2H, **A**), 3.81 (s, 3H, OCH_3, **A**), 3.83 (s, 3H, OCH_3, **B**), 4.74 (dd, ^3J = 8.5, ^3J = 6.8 Hz, 1H, C^4H, **B**), 4.76 (dd, ^3J = 10.6, ^3J = 4.5 Hz, 1H, C^4H, **A**), 6.38–6.40 (m, 1H+1H, Fu, **A**, **B**), 6.41–6.42 (m, 1H, Fu, **A**), 6.42–6.43 (m, 1H, Fu, **B**), 7.44–7.46 (m, 1H+1H, Fu, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 32.3 ($^1J_{CH}$ = 136 Hz, CH_2), 32.4 ($^1J_{CH}$ = 136 Hz, CH_2), 33.8 ($^1J_{CH}$ = 136 Hz, C^2H), 34.3 ($^1J_{CH}$ = 136 Hz, C^2H), 53.61 ($^1J_{CH}$ = 149 Hz, OCH_3), 53.63 ($^1J_{CH}$ = 149 Hz, OCH_3), 55.6 ($^1J_{CH}$ = 145 Hz, C^4H), 55.7 ($^1J_{CH}$ = 145 Hz, C^4H), 109.0 (CH), 109.3 (CH), 110.3 (CH), 110.4 (CH), 115.37 (CN), 115.40 (CN), 143.5 (CH), 143.6 (CH), 149.4 (C), 149.6 (C), 165.6 (2×CO_2Me).

HRMS (ESI) *m/z*: $[M - H]^-$ Calcd for $C_{10}H_9N_4O_3^-$ 233.0680; Found 233.0686.

Methyl 4-azido-2-cyano-4-(thien-2-yl)butyrate (1p)



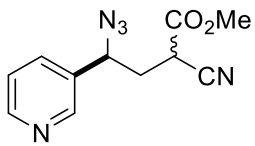
1p was obtained from cyclopropane **S2o** (2.70 g, 13.0 mmol). Yield 2.19 g (67%); dr **A**:**B** 52:48; yellow oil; R_f = 0.63 (pethroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.32 (ddd, ^2J = 14.0, ^3J = 10.2, ^3J = 4.3 Hz, 1H, CH_2, **A**), 2.43–2.49 (m, 2H, CH_2, **B**), 2.50 (ddd, ^2J = 14.0, ^3J = 10.8, ^3J = 5.1 Hz, 1H, CH_2, **A**), 3.61 (dd, ^3J = 7.1, ^3J = 7.0 Hz, 1H, C^2H, **B**), 3.83 (s, 3H, OCH_3, **A**), 3.84 (dd, ^3J = 10.2, ^3J = 5.1 Hz, 1H, C^2H, **A**), 3.86 (s, 3H, OCH_3, **B**), 5.01–5.05 (m, 1H+1H, C^4H, **A, B**), 7.04–7.06 (m, 1H+1H, Th, **A**, **B**), 7.12–7.14 (m, 1H+1H, Th, **A**, **B**), 7.37–7.39 (m, 1H+1H, Th, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.2 (C^2H), 34.6 (C^2H), 36.1 (CH_2), 36.2 (CH_2), 53.7 (OCH_3), 53.8 (OCH_3), 58.1 (C^4H), 58.3 (C^4H), 115.4 (2×CN), 126.5 (CH), 126.7 (2×CH), 126.9 (CH), 127.0 (CH), 127.1 (CH), 139.6 (C), 139.8 (C), 165.6 (2×CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{10}H_{11}N_4O_2S^+$ 251.0597; Found 251.0595.

Methyl 4-azido-2-cyano-4-(pyridin-3-yl)butyrate (1q)



1q was obtained from cyclopropane **S2p** (0.62 g, 3.1 mmol). Yield 0.41 g (54%); dr **A**:**B** 59:41; yellow oil; R_f = 0.56 (ethyl acetate).

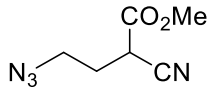
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.18 (ddd, ^2J = 14.3, ^3J = 10.4, ^3J = 4.1 Hz, 1H, CH_2, **A**), 2.33 (ddd, ^2J = 14.2, ^3J = 7.5, ^3J = 5.8 Hz, 1H, CH_2, **B**), 2.387 (ddd, ^2J = 14.2, ^3J = 11.1, ^3J = 4.9 Hz, 1H, CH_2, **A**), 2.391 (ddd, ^2J = 14.2, ^3J = 9.4, ^3J = 6.0 Hz, 1H, CH_2, **B**), 3.63 (dd, ^3J = 7.5, ^3J = 6.0 Hz, 1H, C^2H, **B**), 3.78 (s, 3H, CH_3, **A**), 3.84 (s, 3H, CH_3, **B**), 3.86 (dd, ^3J = 10.4, ^3J = 4.9 Hz, 1H, C^2H, **A**), 4.78 (dd, ^3J = 9.4, ^3J = 5.8 Hz, 1H, C^4H, **B**), 4.79 (dd, ^3J = 11.1, ^3J = 4.1 Hz, 1H, C^4H, **A**), 7.35–7.38 (m, 1H+1H, Py, **A**, **B**), 7.68–7.70 (m, 1H+1H, Py, **A**, **B**), 8.60–8.63 (m, 2H+2H, Ind, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.0 ($^1J_{CH}$ = 135 Hz, C^2H), 34.6 ($^1J_{CH}$ = 135 Hz, C^2H), 35.6 ($^1J_{CH}$ = 136 Hz, CH_2), 35.8 ($^1J_{CH}$ = 136 Hz, CH_2), 53.7 ($^1J_{CH}$ = 149 Hz, OCH_3), 53.8 ($^1J_{CH}$ = 149 Hz, OCH_3), 60.6 ($^1J_{CH}$ = 143 Hz, C^4H), 60.7 ($^1J_{CH}$ = 143 Hz, C^4H), 115.35 (CN), 115.37 (CN), 123.9 (CH), 124.0

(CH), 133.1 (C), 133.3 (C), 134.25 (CH), 134.31 (CH), 148.4 (2×CH), 150.5 (CH), 150.6 (CH), 165.5 (*C*O_2Me), 165.6 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{11}H_{12}N_5O_2^+$ 246.0986; Found 246.0982.

Methyl 4-azido-2-cyanobutyrate (1r)



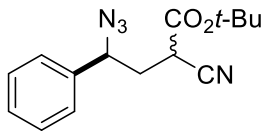
1r was obtained from cyclopropane **1q** (300 mg, 2.4 mmol). Yield 48 mg (12%); yellow oil; R_f = 0.45 (pethroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.10–2.26 (m, 2H, CH_2), 3.51–3.64 (m, 2H, CH_2), 3.71 (dd, ^3J = 8.1, ^3J = 6.1 Hz, 1H, C^{2}H), 3.83 (s, 3H, OCH_3).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 28.9 (CH_2), 34.4 (CH_2), 47.9 (C^{2}H), 53.6 (OCH_3), 115.5 (CN), 165.8 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_6H_9N_4O_2^+$ 169.0720; Found 169.0723.

***tert*-Butyl 4-azido-2-cyano-4-phenylbutyrate (1s)**



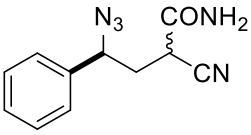
1s was obtained from cyclopropane **S2s** (4.69 g, 19.3 mmol). Yield 3.26 g (59%); dr **A**:**B** 54:46; yellow oil; R_f = 0.50 (petroleum ether – ethyl acetate 4:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.49 (s, 9H, CH_3, **A**), 1.52 (s, 9H, CH_3, **B**), 2.13 (ddd, ^2J = 14.1, ^3J = 10.3, ^3J = 4.1 Hz, 1H, CH_2, **A**), 2.29 (ddd, ^2J = 14.0, ^3J = 7.0, ^3J = 6.6 Hz, 1H, CH_2, **B**), 2.34 (ddd, ^2J = 14.1, ^3J = 11.0, ^3J = 5.1 Hz, 1H, CH_2, **A**), 2.41 (ddd, ^2J = 14.0, ^3J = 8.7, ^3J = 6.9 Hz, 1H, CH_2, **B**), 3.41 (dd, ^3J = 7.0, ^3J =6.9 Hz, 1H, C^{2}H, **B**), 3.70 (dd, ^3J = 10.3, ^3J = 5.1 Hz, 1H, C^{2}H, **A**) 4.72 (dd, ^3J = 11.0 ^3J = 4.1 Hz, 1H, C^{4}H, **A**), 4.75 (dd, ^3J = 8.7, ^3J = 6.6 Hz, 1H, C^{4}H, **B**), 7.3–7.36 (m, 2H+2H, Ph, **A**, **B**), 7.37–7.39 (m, 1H+1H, Ph, **A**, **B**), 7.40–7.43 (m, 2H+2H, Ph, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 27.5 (18×CH_3), 35.3 (C^{2}H), 35.5 (C^{2}H), 35.8 (CH_2), 35.9 (CH_2), 62.9 (C^{4}H), 63.0 (C^{4}H), 84.1 (C), 84.2 (C), 115.96 (CN), 116.01 (CN), 126.7 (4×CH), 128.8 (CH), 128.9 (CH), 128.96 (2×CH), 129.03 (2×CH), 137.2 (C), 137.5 (C), 163.97 (*C*O_2Me), 164.05 (*C*O_2Me).

HRMS (ESI) *m/z*: $[M - H]^-$ Calcd for $C_{15}H_{17}N_4O_2^-$ 285.1357; Found 285.1357.

4-Azido-2-cyano-4-phenylbutanamide (1t)



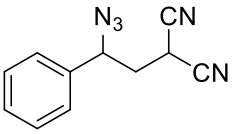
1t was obtained from cyclopropane **S2t** (1.86 g, 10.0 mmol). Yield 1.50 g (66%); dr **A**:**B** 52:48; yellow oil; R_f = 0.48 (petroleum ether – ethyl acetate 1:1).

^{1}H NMR (DMSO-d$_6$, 600 MHz) δ = 2.15 (ddd, ^2J = 14.0, ^3J = 9.3, ^3J = 4.7 Hz, 1H, CH$_2$, **A**), 2.27 (ddd, ^2J = 13.9, ^3J = 7.3, ^3J = 6.1 Hz, 1H, CH$_2$, **B**), 2.33 (ddd, ^2J = 13.9, ^3J = 8.8, ^3J = 7.6 Hz, 1H, CH$_2$, **B**), 2.35 (ddd, ^2J = 14.0, ^3J = 10.2, ^3J = 5.8 Hz, 1H, CH$_2$, **A**), 3.61 (dd, ^3J = 7.6, ^3J = 7.6 Hz, 1H, C^{2}H, **B**), 3.77 (dd, ^3J = 9.3, ^3J = 5.8 Hz, 1H, C^{2}H, **A**), 4.71 (dd, ^3J = 8.8, ^3J = 6.1 Hz, 1H, C^{4}H, **B**), 4.78 (dd, ^3J = 10.2, ^3J = 4.7 Hz, 1H, C^{4}H, **A**), 7.36–7.46 (m, 5H+5H, Ph, **A**, **B**), 7.55 (br.s, 1H, NH, **A**), 7.57 (br.s, 1H, NH, **B**), 7.85 (br.s, 1H, NH, **A**), 7.90 (br.s, 1H, NH, **B**).

^{13}C NMR (DMSO-d$_6$, 150 MHz) δ = 34.4 (C^{2}H), 34.5 (C^{2}H), 34.9 (CH$_2$), 35.0 (CH$_2$), 62.9 (C^{4}H), 63.0 (C^{4}H), 118.0 (CN), 118.2 (CN), 127.16 (2×CH), 127.18 (2×CH), 128.80 (CH), 128.83 (CH), 128.97 (2×CH), 129.00 (2×CH), 137.8 (C), 137.9 (C), 165.7 (CONH$_2$), 165.9 (CONH$_2$).

HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{11}H_{12}N_5O^+$ 230.1036; Found 230.1038.

2-(2-Azido-2-phenylethyl)malononitrile[24] (1u)

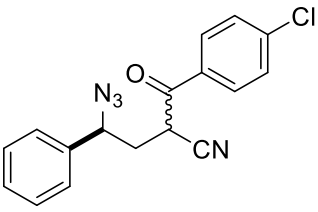


1u was obtained from cyclopropane **S2u** (0.20 g, 1.2 mmol). Yield 0.11 g (43%); colorless oil; R_f = 0.28 (diethyl ether – petroleum ether 1:1).

^{1}H NMR (600 MHz, CDCl$_3$) δ = 2.34 (ddd, ^2J = 13.9, ^3J = 9.3, ^3J = 4.8 Hz, 1H, CH$_2$), 2.42 (ddd, ^2J = 13.9, ^3J = 10.3, ^3J = 5.7 Hz, 1H, CH$_2$), 3.97 (dd, ^3J = 9.3, ^3J = 5.7 Hz, 1H, C^{2}H), 4.77 (dd, ^3J = 10.3, ^3J = 4.8 Hz, 1H, C^{4}H), 7.34–7.40 (m, 2H, Ph), 7.42–7.50 (m, 3H, Ph).

^{13}C NMR (150 MHz, CDCl$_3$) δ = 20.1 ($^1J_{CH}$ = 143 Hz, C^{2}H), 37.2 ($^1J_{CH}$ = 138 Hz, CH$_2$), 62.2 ($^1J_{CH}$ = 142 Hz, C^{4}H), 111.8 (CN), 111.9 (CN), 126.9 (2×CH, Ph), 129.6 (2×CH), 129.8 (CH), 136.1 (C).

4-Azido-2-(4-chlorobenzoyl)-4-phenylbutyronitrile (1v)



1v was obtained from cyclopropane **S2v** (0.75 g, 2.7 mmol). Yield 0.63 g (73%); dr **A**:**B** 63:37; yellow oil; R_f = 0.75 (pethroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.26 (ddd, ^2J = 14.3, ^3J = 10.5, ^3J = 3.6 Hz, 1H, CH_2, **A**), 2.35 (ddd, ^2J = 14.3, ^3J = 11.2, ^3J = 4.3 Hz, 1H, CH_2, **A**), 2.42 (ddd, ^2J = 14.0, ^3J = 8.2, ^3J = 7.2 Hz, 1H, CH_2, **B**), 2.49 (ddd, ^2J = 14.0, ^3J = 6.9, ^3J = 6.8 Hz, 1H, CH_2, **B**), 4.32 (dd, ^3J = 7.2, ^3J = 6.9 Hz, 1H, C^2H, **B**), 4.69 (dd, ^3J = 8.2, ^3J = 6.8 Hz, 1H, C^4H, **B**), 4.70 (dd, ^3J = 10.5, ^3J = 4.3 Hz, 1H, C^2H, **A**), 4.88 (dd, ^3J = 11.2 ^3J = 3.6 Hz, 1H, C^4H, **A**), 7.32–7.47 (m, 5H+7H, Ar, **A**, **B**), 7.49–7.51 (m, 2H, Ar, **A**) 7.82–7.85 (m, 2H, Ar, **B**), 7.90–7.95 (m, 2H, Ar, **A**).

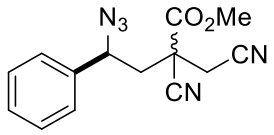
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 35.4 (CH_2), 35.9 (CH_2), 37.2 (2×C^2H), 62.9 (C^4H), 63.1 (C^4H), 116.3 (2×CN), 126.6 (2×CH), 126.7 (2×CH), 128.9 (CH), 129.00 (2×CH), 129.05 (CH), 129.11 (2×CH), 129.2 (2×CH), 129.3 (2×CH), 129.96 (2×CH), 130.04 (2×CH), 131.7 (C), 131.9 (C), 137.2 (C), 137.3 (C), 141.1 (2×C), 188.3 (COAr), 188.5 (COAr).

HRMS (ESI) *m/z*: $[M - H]^-$ Calcd for $C_{17}H_{12}ClN_4O^-$ 323.0705; Found 323.0710.

Synthesis of *γ*-Azidobutyronitriles 1w,x *via* 1a alkylation

To a cold (ice-water bath) stirred 1.0 M solution of **1a** (1 equiv) in dry DMF NaH (1.1 equiv, 60% suspension in oil) was added under argon. Cooling bath was removed. After 20 min at ambient temperature, a 1.0 M solution of the corresponding alkyl bromide (1.1-1.3 equiv) in dry DMF was added dropwise. Stirring was continued for 2 h, and then the reaction mixture was diluted with water and extracted with ethyl acetate. Combined organic fractions were washed with brine (4 times), dried with Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel.

Methyl 4-azido-2-cyano-2-(cyanomethyl)-4-phenylbutyrate (1w)



1w was obtained from **1a** (0.49 g, 2.0 mmol) and bromoacetonitrile (0.16 mL, 2.2 mmol). Yield 0.52 g (92%); dr **A**:**B** 56:44 [(2*RS*,4*RS*)-**1w**:(2*RS*,4*SR*)-**1w**]; yellowish oil; R_f = 0.37 (petroleum ether – ethyl acetate 3:1).

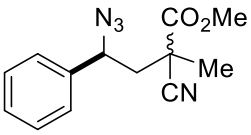
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.24 (dd, ^2J = 14.4, ^3J = 3.4 Hz, 1H, C^3H_2, **B**), 2.42 (dd, ^2J = 14.6, ^3J = 5.6 Hz, 1H, C^3H_2, **A**), 2.47 (dd, ^2J = 14.6, ^3J = 8.9 Hz, 1H, C^3H_2, **A**), 2.56 (dd, ^2J = 14.4, ^3J = 11.1

Hz, 1H, C^3H_2, **B**), 2.94 (d, ^2J = 16.9 Hz, 1H, CH_2, **B**), 3.02 (d, ^2J = 16.9 Hz, 1H, CH_2, **B**), 3.16 (d, ^2J = 16.9 Hz, 1H, CH_2, **A**), 3.20 (d, ^2J = 16.9 Hz, 1H, CH_2, **A**), 3.73 (s, 3H, CH_3O, **A**), 3.97 (s, 3H, CH_3O, **B**), 4.80 (dd, ^3J = 8.9, ^3J = 5.6, Hz, 1H, CH, **A**), 4.83 (dd, ^3J = 11.1, ^3J = 3.4 Hz, 1H, CH, **B**), 7.34–7.37 (m, 2H+2H, Ph, **A**, **B**), 7.39–7.42 (m, 1H+1H, Ph, **A**, **B**), 7.43–7.46 (m, 2H+2H, Ph, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 25.4 (CH_2), 26.3 (CH_2), 41.0 (CH_2), 42.3 (CH_2), 44.3 (C), 45.0 (C), 54.5 (CH_3O), 54.6 (CH_3O), 62.4 (CH), 62.6 (CH), 113.9 (CN), 114.2 (CN), 115.79 (CN), 115.81 (CN), 126.8 (2×CH), 127.1 (2×CH), 129.2 (2×CH), 129.3 (2×CH), 129.35 (CH), 129.41 (CH), 136.6 (C), 137.1 (C), 165.9 (CO_2Me), 166.5 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{14}N_5O_2^+$ 284.1142; Found 284.1145.

Methyl 4-azido-2-cyano-2-(methyl)-4-phenylbutyrate (1x)



1x was obtained from **1a** (1.47 g, 6.0 mmol) and methyl iodide (0.49 mL, 7.8 mmol). Yield 1.40 g (90%); dr **A**:**B** 57:43 [(2*RS*,4*SR*)-**1x**:(2*RS*,4*RS*)-**1x**]; colorless oil; R_f = 0.55 (petroleum ether – ethyl acetate 3:1).

^1H NMR ($CDCl_3$, 600 MHz) δ = 1.63 (s, 3H, CH_3, **B**), 1.67 (s, 3H, CH_3, **A**), 2.00 (dd, ^2J = 14.4, ^3J = 3.5 Hz, 1H, CH_2, **B**), 2.28 (dd, ^2J = 14.4, ^3J = 7.7 Hz, 1H, CH_2, **A**), 2.39 (dd, ^2J = 14.4, ^3J = 6.8 Hz, 1H, CH_2, **A**), 2.54 (dd, ^2J = 14.4, ^3J = 11.1 Hz, 1H, CH_2, **B**), 3.53 (s, 3H, CH_3O, **A**), 3.88 (s, 3H, CH_3O, **B**), 4.72 (dd, ^3J = 7.7, ^3J = 6.8, Hz, 1H, CH, **A**), 4.81 (dd, ^3J = 11.1, ^3J = 3.5 Hz, 1H, CH, **B**), 7.33–7.43 (m, 5H+5H, Ph, **A**, **B**).

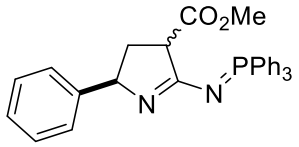
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 24.6 (CH_3), 24.7 (CH_3), 41.9 (C), 42.6 (C), 43.3 (CH_2), 44.1 (CH_2), 53.3 (CH_3O), 53.6 (CH_3O), 63.0 (CH), 63.2 (CH), 118.96 (CN), 119.00 (CN), 126.8 (2×CH), 127.3 (2×CH), 128.86 (2×CH), 128.89 (CH), 128.92 (CH), 129.02 (2×CH), 137.3 (C), 137.9 (C), 168.8 (CO_2Me), 169.5 (CO_2Me).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{13}H_{15}N_4O_2^+$ 259.1190; Found 259.1191.

Synthesis of Iminophosphazenes 3

To a stirred solution of azide **1** (2.05 mmol) in DCM (2 mL) PPh_3 (0.56 g, 2.15 mmol) was added in one portion. Resulting solution was stirred at ambient temperature for 48 h and concentrated under reduced pressure. Residue was purified by column chromatography on silica gel (ethyl acetate – methanol).

Methyl 2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3a)



3a was obtained from azide **1a** (0.500 g, 2.05 mmol). Yield 0.840 g (86%); dr **A**:**B** 54:46; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

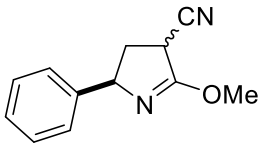
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.96 (dddd, ^2J = 12.8, ^3J = 9.4, ^3J = 5.0, ^5J = 1.2 Hz, 1H, CH_2, **B**), 2.03 (ddd, ^2J = 12.5, ^3J = 10.2, ^3J = 8.6 Hz, 1H, CH_2, **A**), 2.65 (dddd, ^2J = 12.5, ^3J = 8.7, ^3J = 7.1, ^5J = 2.3 Hz, 1H, CH_2, **A**), 2.79 (dddd, ^2J = 12.8, ^3J = 8.0, ^3J = 6.2, ^5J = 1.4 Hz, 1H, CH_2, **B**), 3.81 (s, 3H, CH_3O, **A**), 3.81-3.84 (m, 1H, C^4H, **B**), 3.83 (s, 3H, CH_3O, **B**), 3.91 (dddd, ^3J = 10.2, ^3J = 8.7, ^4J = 2.2, ^4J = 1.5 Hz, 1H, C^4H, **A**), 4.86-4.89 (m, 1H, C^2H, **A**), 5.11 (dd, ^3J = 8.0, ^3J = 5.0 Hz, 1H, C^2H, **B**), 6.86–6.89 (m, 2H+2H, Ph, **A**, **B**), 7.09–7.14 (m, 3H+3H, Ph, **A**, **B**), 7.44–7.48 (m, 6H+6H, PPh_3, **A**, **B**), 7.53–7.57 (m, 3H+3H, PPh_3, **A**, **B**), 7.84–7.88 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.6 ($^1J_{CH}$ = 133 Hz, CH_2), 39.1 ($^1J_{CH}$ = 133 Hz, CH_2), 51.7 ($^1J_{CH}$ = 147 Hz, CH_3O), 51.8 ($^1J_{CH}$ = 147 Hz, CH_3O), 54.8 ($^1J_{CH}$ = 135, $^3J_{CP}$ = 20 Hz, C^4H), 55.7 ($^1J_{CH}$ = 135, $^3J_{CP}$ 21 Hz, C^4H), 70.2 ($^1J_{CH}$ = 137 Hz, C^2H), 70.3 ($^1J_{CH}$ = 141 Hz, C^2H), 125.7 (CH), 125.8 (CH), 125.9 (2×CH), 126.3 (2×CH), 127.7 (4×CH), 128.32 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.4 ($^2J_{CP}$ = 12 Hz, 6×CH), 129.1 ($^1J_{CP}$ = 100 Hz, 3×C), 129.2 ($^1J_{CP}$ = 99 Hz, 3×C), 131.69 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.72 ($^4J_{CP}$ = 3 Hz, 3×CH), 133.1 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.2 ($^3J_{CP}$ = 10 Hz, 6×CH), 147.0 (C), 147.1 (C), 168.9 ($^2J_{CP}$ = 8 Hz, C), 169.1 ($^2J_{CP}$ = 8 Hz, C), 173.8 (*C*O_2Me), 174.0 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.4, 15.8.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{28}N_2O_2P^+$ 479.1883; Found 479.1882.

5-Methoxy-2-phenyl-3,4-dihydro-2*H*-pyrrole-4-carbonitrile (4a)



4a was obtained as a side product from azide **1a** (0.500 g, 2.05 mmol); reaction was performed in MeCN (2 mL) under reflux for 4 h. Yield 0.028 g (6%); dr **A**:**B** 57:43; colorless oil; R_f = 0.33 (petroleum ether – ethyl acetate 2:1).

A: ^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.25 (ddd, ^2J = 13.1, ^3J = 10.1, ^3J = 8.4 Hz, 1H, CH_2), 3.01 (ddd, ^2J = 13.1, ^3J = 9.2, ^3J = 7.1 Hz, 1H, CH_2), 3.82 (dd, ^3J = 10.4, ^3J = 9.2 Hz, 1H, C^4H), 4.01 (s, 3H, CH_3O), 4.95 (dd, ^3J = 8.4, ^3J = 7.1 Hz, 1H, C^2H), 7.27–7.31 (m, 3H, Ar), 7.34–7.39 (m, 2H, Ar).

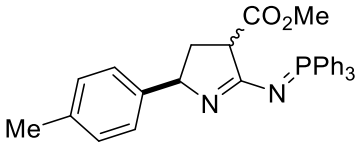
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.7 (C^4H), 39.1 (CH_2), 57.0 (CH_3O), 68.5 (C^2H), 117.0 (CN), 126.0 (2×CH), 127.6 (CH), 128.68 (2×CH), 142.5 (C), 165.3 (C=N).

B: ^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.37 (ddd, ^2J = 13.3, ^3J = 9.9, ^3J = 5.7 Hz, 1H, CH_2), 2.89 (ddd, ^2J = 13.3, ^3J = 7.8, ^3J = 5.9 Hz, 1H, CH_2), 3.79 (dd, ^3J = 9.9, ^3J = 5.9 Hz, 1H, C^4H), 4.02 (s, 3H, CH_3O), 5.23 (dd, ^3J = 7.8, ^3J = 5.7 Hz, 1H, C^2H), 7.21–7.23 (m, 2H, Ar), 7.27–7.31 (m, 1H, Ar), 7.34–7.39 (m, 2H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.1 (C^4H), 38.6 (CH_2), 57.1 (CH_3O), 68.5 (C^2H), 117.1 (CN), 125.8 (2×CH), 127.5 (CH), 128.67 (2×CH), 142.4 (C), 165.5 (C=N).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{13}N_2O^+$ 201.1022; Found 201.1023.

Methyl 2-(4-tolyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3b)



3b was obtained from azide **1b** (1.636 g, 6.33 mmol). Yield 2.897 g (93%); dr **A**:**B** 53:47; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.97 (dddd, ^2J = 12.7, ^3J = 9.3, ^3J = 5.0, ^5J = 1.2 Hz, 1H, CH_2, **B**), 2.05 (ddd, ^2J = 12.4, ^3J = 10.3, ^3J = 8.7 Hz, 1H, CH_2, **A**), 2.29 (s, 3H, CH_3, **B**), 2.31 (s, 3H, CH_3, **A**), 2.66 (dddd, ^2J = 12.4, ^3J = 8.7, ^3J = 7.0, ^5J = 2.3 Hz, 1H, CH_2, **A**), 2.79 (dddd, ^2J = 12.7, ^3J = 8.0, ^3J = 6.3, ^5J = 1.3 Hz, 1H, CH_2, **B**), 3.81–3.88 (m, 1H, C^4H, **B**), 3.82 (s, 3H, OCH_3, **A**), 3.84 (s, 3H, OCH_3,

B), 3.93 (dddd, ^3J = 10.3, ^3J = 8.7, ^4J = 2.1, ^4J = 1.4 Hz, 1H, C^4H, **A**), 4.83–4.87 (m, 1H, C^2H, **A**), 5.10 (dd, ^3J = 8.0, ^3J = 5.0 Hz, 1H, C^2H, **B**), 6.79–6.82 (m, 2H+2H, Ar, **A**, **B**), 6.95–6.97 (m, 2H+2H, Ar, **A**, **B**), 7.45–7.49 (m, 6H+6H, PPh_3, **A**, **B**), 7.54–7.57 (m, 3H+3H, PPh_3, **A**, **B**), 7.86–7.90 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 20.87 (CH_3), 20.91 (CH_3), 38.7 (CH_2), 39.3 (CH_2), 51.6 (CH_3O), 51.7 (CH_3O), 54.7 ($^3J_{CP}$ = 20 Hz, C^4H), 55.6 ($^3J_{CP}$ = 20 Hz, C^4H), 69.9 (C^2H), 70.0 (C^2H), 125.8 (2×CH), 126.1 (2×CH), 128.24 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.28 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.28 (4×CH), 129.0 ($^1J_{CP}$ = 100 Hz, 3×C), 129.1 ($^1J_{CP}$ = 99 Hz, 3×C), 131.6 ($^4J_{CP}$ = 2 Hz, 3×CH), 131.7 ($^4J_{CP}$ = 3 Hz, 3×CH), 133.06 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.13 ($^3J_{CP}$ = 10 Hz, 6×CH), 135.0 (C), 135.1 (C), 143.9 (C), 144.1 (C), 168.7 ($^2J_{CP}$ = 8 Hz, C), 168.9 ($^2J_{CP}$ = 8 Hz, C), 173.8 (*C*O_2Me), 173.9 (*C*O_2Me).

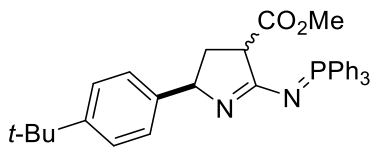
^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.3, 15.7.

IR (film) 1731, 1724, 1562, 1437, 1357, 1331, 1249, 1155, 1111 cm^{-1}.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{31}H_{30}N_2O_2P^+$ 493.2039; Found 493.2039.

Anal. calcd for $C_{31}H_{29}N_2O_2P$: C 75.59 H 5.93 N 5.69. Found: C 75.42, H 5.91, N 5.71.

Methyl 2-(4-*tert*-butylphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3c)



3c was obtained from azide **1c** (0.182 g, 0.61 mmol). Yield 0.262 g (81%); dr **A**:**B** 55:45; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

^1H NMR ($CDCl_3$, 600 MHz) δ = 1.34 (s, 9H, CH_3, **A**), 1.35 (s, 9H, CH_3, **B**), 2.02 (dddd, ^2J = 12.7, ^3J = 9.4, ^3J =5.4, ^5J = 1.1 Hz, 1H, CH_2, **B**), 2.12 (ddd, ^2J = 12.5, ^3J = 10.5, ^3J = 8.8 Hz, 1H, CH_2, **A**), 2.68 (dddd, ^2J = 12.5, ^3J = 8.7, ^3J = 6.9, ^5J = 2.3 Hz, 1H, CH_2, **A**), 2.82 (dddd, ^2J = 12.7, ^3J =8.1, ^3J =5.8, ^5J = 1.5 Hz, 1H, CH_2, **B**), 3.85 (s, 3H, OCH_3, **A**), 3.85 (s, 3H, OCH_3, **B**), 3.90 (dddd, ^3J = 9.4, ^3J = 5.8, ^4J = 1.8, ^4J = 0.9 Hz, 1H, C^4H, **B**), 3.96 (dddd, ^3J = 10.5, ^3J = 8.7, ^4J = 2.2, ^4J = 1.6 Hz, 1H, C^4H, **A**), 4.89 (dd, ^3J = 8.8, ^3J =6.9 Hz, 1H, C^2H, **A**), 5.15 (dd, ^3J = 8.1, ^3J = 5.4 Hz, 1H, C^2H, **B**), 6.90–6.93 (m,

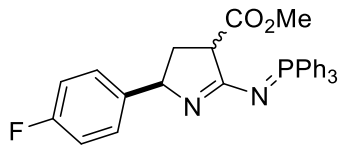
2H+2H, Ar, **A**, **B**), 7.20–7.22 (m, 2H+2H, Ar, **A**, **B**), 7.46–7.49 (m, 6H+6H, PPh_3, **A**, **B**), 7.54–7.58 (m, 3H+3H, PPh_3, **A**, **B**), 7.89–7.94 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 31.26 (3×CH_3), 31.28 (3×CH_3), 34.1 (2×C), 38.5 (CH_2), 39.1 (CH_2), 51.5 (CH_3O), 51.6 (CH_3O), 54.8 ($^3J_{CP}$ = 20 Hz, C^4H), 55.6 ($^3J_{CP}$ = 20 Hz, C^4H), 69.9 (C^2H), 70.0 (C^2H), 124.4 (4×CH), 125.5 (2×CH), 125.8 (2×CH), 128.2 ($^2J_{CP}$ = 12 Hz, 12×CH), 129.0 ($^1J_{CP}$ = 100 Hz, 3×C), 129.1 ($^1J_{CP}$ = 100 Hz, 3×C), 131.5 ($^4J_{CP}$ = 2 Hz, 6×CH), 133.0 ($^3J_{CP}$ = 9 Hz, 6×CH), 133.1 ($^3J_{CP}$ = 9 Hz, 6×CH), 143.9 (C), 144.0 (C), 148.2 (2×C), 168.6 ($^2J_{CP}$ = 8 Hz, C), 168.7 ($^2J_{CP}$ = 8 Hz, C), 173.7 (*C*O_2Me), 173.9 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.3, 15.9.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{34}H_{36}N_2O_2P^+$ 535.2509; Found 535.2509.

Methyl 2-(4-fluorophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3d)



3d was obtained from azide **1d** (0.570 g, 2.17 mmol). Yield 0.780 g (72%); dr **A**:**B** 56:44; colorless foam; R_f = 0.10 (ethyl acetate).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.92 (dddd, ^2J = 13.0, ^3J = 9.3, ^3J = 5.1, ^5J = 1.1 Hz, 1H, CH_2, **B**), 2.00 (ddd, ^2J = 12.6, ^3J = 10.1, ^3J = 8.5 Hz, 1H, CH_2, **A**), 2.65 (dddd, ^2J = 12.6, ^3J = 9.0, ^3J = 7.6, ^5J = 2.2 Hz, 1H, CH_2, **A**), 2.78 (dddd, ^2J = 13.0, ^3J = 7.8, ^3J = 6.2, ^5J = 1.3 Hz, 1H, CH_2, **B**), 3.81 (s, 3H, OCH_3, **A**), 3.82–3.84 (m, 1H, C^4H, **B**), 3.84 (s, 3H, OCH_3, **B**), 3.91-3.95 (m, 1H, C^4H, **A**), 4.84–4.87 (m, 1H, C^2H, **A**), 5.09 (dd, ^3J = 7.9, ^3J = 5.3 Hz, 1H, C^2H, **B**), 6.77–6.94 (m, 4H+4H, Ar, **A**, **B**), 7.43–7.47 (m, 6H+6H, PPh_3, **A**, **B**), 7.52–7.55 (m, 3H+3H, PPh_3, **A**, **B**), 7.84–7.89 (m, 6H+6H, PPh_3, **A**, **B**).

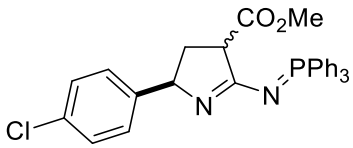
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.6 (CH_2), 39.0 (CH_2), 51.6 (CH_3O), 51.7 (CH_3O), 54.8 ($^3J_{CP}$ = 20 Hz, C^4H), 55.7 ($^3J_{CP}$ = 20 Hz, C^4H), 69.5 (C^2H), 69.7 (C^2H), 114.1 ($^2J_{CF}$ = 21 Hz, 2×CH), 114.2 ($^2J_{CF}$ = 21 Hz, 2×CH), 127.2 ($^3J_{CF}$ = 8 Hz, 2×CH), 127.6 ($^3J_{CF}$ = 8 Hz, 2×CH), 128.25 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.27 ($^2J_{CP}$ = 12 Hz, 6×CH), 129.07 ($^1J_{CP}$ = 99 Hz, 3×C), 129.12 ($^1J_{CP}$ = 99 Hz, 3×C), 131.64 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.67 ($^4J_{CP}$ = 3 Hz, 3×CH), 133.0 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.1 ($^3J_{CP}$ = 10 Hz,

6×CH), 142.7 ($^4J_{CF}$ = 3 Hz, C), 142.9 ($^4J_{CF}$ = 3 Hz, C), 169.0 ($^2J_{CP}$ = 8 Hz, C), 169.2 ($^2J_{CP}$ = 8 Hz, C), 161.1 ($^1J_{CF}$ = 243 Hz, C), 161.2 ($^1J_{CF}$ = 243 Hz, C), 173.7 (*C*O_2Me), 173.8 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.4, 15.8.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{27}FN_2O_2P^+$ 497.1789; Found 497.1785.

Methyl 2-(4-chlorophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3e)



3e was obtained from azide **1e** (0.557 g, 2.00 mmol). Yield 0.940 g (92%); dr **A**:**B** 55:45; yellowish foam; R_f = 0.10 (ethyl acetate).

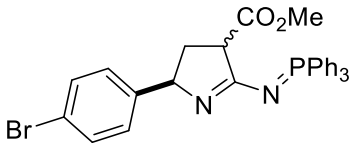
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.90 (dddd, ^2J = 13.0, ^3J = 9.4, ^3J = 5.1, ^5J = 1.0 Hz, 1H, CH_2, **B**), 1.98 (ddd, ^2J = 12.6, ^3J = 9.9, ^3J = 8.5 Hz, 1H, CH_2, **A**), 2.64 (dddd, ^2J = 12.6, ^3J = 9.0, ^3J = 7.4, ^5J = 2.0 Hz, 1H, CH_2, **A**), 2.78 (dddd, ^2J = 13.0, ^3J = 8.0, ^3J = 6.5, ^5J = 1.4 Hz, 1H, CH_2, **B**), 3.80 (s, 3H, OCH_3, **A**), 3.81–3.83 (m, 1H, C^4H, **B**), 3.83 (s, 3H, OCH_3, **B**), 3.90–3.94 (m, 1H, C^4H, **A**), 4.82–4.85 (m, 1H, C^2H, **A**), 5.08 (dd, ^3J = 8.0, ^3J = 5.1 Hz, 1H, C^2H, **B**), 6.76–6.80 (m, 2H+2H, Ar, **A**, **B**), 7.05–7.08 (m, 2H+2H, Ar, **A**, **B**), 7.42–7.46 (m, 6H+6H, PPh_3, **A**, **B**), 7.51–7.54 (m, 3H+3H, PPh_3, **A**, **B**), 7.83–7.88 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.4 (CH_2), 38.8 (CH_2), 51.6 (CH_3O), 51.7 (CH_3O), 54.8 ($^3J_{CP}$ = 20 Hz, C^4H), 55.6 ($^3J_{CP}$ = 20 Hz, C^4H), 69.5 (C^2H), 69.6 (C^2H), 127.2 (2×CH), 127.5 (4×CH), 127.6 (2×CH), 128.22 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.24 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.99 ($^1J_{CP}$ = 100 Hz, 3×C), 129.03 ($^1J_{CP}$ = 100 Hz, 3×C), 131.08 (C), 131.11 (C), 131.6 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.7 ($^4J_{CP}$ = 3 Hz, 3×CH), 132.95 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.00 ($^3J_{CP}$ = 10 Hz, 6×CH), 145.6 (C), 145.7 (C), 169.1 ($^2J_{CP}$ = 8 Hz, C), 169.3 ($^2J_{CP}$ = 8 Hz, C), 173.5 (*C*O_2Me), 173.6 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.4, 15.9.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{27}ClN_2O_2P^+$ 513.1493; Found 513.1491.

Methyl 2-(4-bromophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3f)



3f was obtained from azide **1f** (2.014 g, 6.23 mmol). Yield 3.121 g (90%); dr **A**:**B** 56:44; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

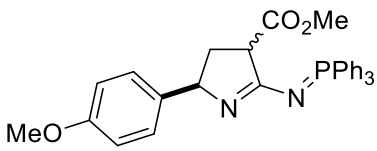
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.88 (dddd, ^2J = 12.8, ^3J = 9.4, ^3J = 5.0, ^5J = 1.0 Hz, 1H, CH_2, **B**), 1.96 (ddd, ^2J = 12.4, ^3J = 10.0, ^3J = 8.5 Hz, 1H, CH_2, **A**), 2.64 (dddd, ^2J = 12.4, ^3J = 8.8, ^3J = 7.2, ^5J = 2.2 Hz, 1H, CH_2, **A**), 2.76 (dddd, ^2J = 12.8, ^3J = 8.1, ^3J = 6.4, ^5J = 1.3 Hz, 1H, CH_2, **B**), 3.76–3.79 (m, 1H, C^{4}H, **B**), 3.80 (s, 3H, OCH_3, **A**), 3.83 (s, 3H, OCH_3, **B**), 3.88-3.91 (m, 1H, C^{4}H, **A**), 4.79–4.83 (m, 1H, C^{2}H, **A**), 5.04 (dd, ^3J = 8.0, ^3J = 5.0 Hz, 1H, C^{2}H, **B**), 6.68–6.71 (m, 2H+2H, Ar, **A**, **B**), 7.19–7.21 (m, 2H+2H, Ar, **A**, **B**), 7.44–7.47 (m, 6H+6H, PPh_3, **A**, **B**), 7.54–7.56 (m, 3H+3H, PPh_3, **A**, **B**), 7.81–7.85 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.4 (CH_2), 38.9 (CH_2), 51.8 (CH_3O), 51.9 (CH_3O), 54.9 ($^3J_{CP}$ = 20 Hz, C^{4}H), 55.7 ($^3J_{CP}$ = 20 Hz, C^{4}H), 69.6 (C^{2}H), 70.8 (C^{2}H), 119.3 (C), 119.4 (C), 127.8 (2×CH), 128.1 (2×CH), 128.3 ($^2J_{CP}$ = 11 Hz, 6×CH), 128.4 ($^2J_{CP}$ = 11 Hz, 6×CH), 129.07 ($^1J_{CP}$ = 100 Hz, 3×C), 129.14 ($^1J_{CP}$ = 100 Hz, 3×C), 130.6 (4×CH), 131.78 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.82 ($^4J_{CP}$ = 3 Hz, 3×CH), 133.1 ($^3J_{CP}$ = 9 Hz, 6×CH), 133.2 ($^3J_{CP}$ = 9 Hz, 6×CH), 146.2 (C), 146.4 (C), 169.3 ($^2J_{CP}$ = 8 Hz, C), 169.5 ($^2J_{CP}$ = 8 Hz, C), 173.7 (*C*O_2Me), 173.8 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.5, 15.9.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{27}BrN_2O_2P^+$ 557.0988; Found 557.1001.

Methyl 2-(4-methoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3g)



3g was obtained from azide **1g** (1.500 g, 5.47 mmol). Yield 2.123 g (76%); dr **A**:**B** 54:46; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

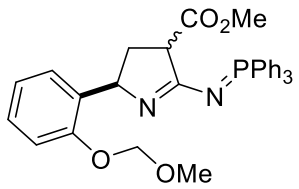
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.91 (dddd, ^2J = 12.6, ^3J = 9.4, ^3J = 4.9, ^5J = 1.3 Hz, 1H, CH_2, **B**), 1.99 (ddd, ^2J = 12.5, ^3J = 10.2, ^3J = 8.5 Hz, 1H, CH_2, **A**), 2.61 (dddd, ^2J = 12.5, ^3J = 8.8, ^3J = 6.9, ^5J = 2.3 Hz, 1H, CH_2, **A**), 2.74 (dddd, ^2J = 12.6, ^3J = 8.0, ^3J = 6.3, ^5J = 1.4 Hz, 1H, CH_2, **B**), 3.75 (s, 3H, OCH_3, **B**), 3.76 (s, 3H, OCH_3, **A**), 3.79–3.81 (m, 1H, C^4H, **B**), 3.80 (s, 3H, OCH_3, **A**), 3.82 (s, 1H, OCH_3, **B**), 3.89 (dddd, ^3J = 10.2, ^3J = 8.8, ^4J = 2.3, ^4J = 1.5 Hz, 1H, C^4H, **A**), 4.78–4.82 (m, 1H, C^2H, **A**), 5.05 (dd, ^3J = 8.0, ^3J = 4.9 Hz, 1H, C^2H, **B**), 6.64–6.67 (m, 2H+2H, Ar, **A**, **B**), 6.76–6.80 (m, 2H+2H, Ar, **A**, **B**), 7.43–7.46 (m, 6H+6H, PPh_3, **A**, **B**), 7.52–7.55 (m, 3H+3H, PPh_3, **A**, **B**), 7.82–7.86 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.9 (CH_2), 39.5 (CH_2), 51.8 (CH_3O), 51.9 (CH_3O), 55.0 ($^3J_{CP}$ = 20 Hz, C^4H), 55.2 (2×CH_3), 55.9 ($^3J_{CP}$ = 20 Hz, C^4H), 69.8 (2× C^2H), 113.1 (2×CH), 127.0 (CH), 127.3 (CH), 128.3 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.4 ($^2J_{CP}$ = 12 Hz, 6×CH), 129.3 ($^1J_{CP}$ = 100 Hz, 3×C), 129.4 ($^1J_{CP}$ = 99 Hz, 3×C), 131.7 ($^4J_{CP}$ = 3 Hz, 6×CH), 133.2 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.3 ($^3J_{CP}$ = 10 Hz, 6×CH), 139.4 (2×C), 157.7 (C), 157.8 (C), 168.8 ($^2J_{CP}$ = 7 Hz, C), 168.9 ($^2J_{CP}$ = 8 Hz, C), 174.0 (*C*O_2Me), 174.2 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.2, 15.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{31}H_{30}N_2O_3P^+$ 509.1989; Found 509.1990.

Methyl 2-(2-methoxymethoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3h)



3h was obtained from azide **1h** (0.324 g, 1.06 mmol). Yield 0.285 g (50%); dr **A**:**B** 51:49; yellowish oil; R_f = 0.10 (ethyl acetate).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.91–1.97 (m, 1H+1H, CH_2, **A**, **B**), 2.82–2.91 (m, 1H+1H, CH_2, **A**, **B**), 3.45 (s, 3H+3H, OCH_3, **A**, **B**), 3.77–3.80 (m, 1H, C^4H), 3.79 (s, 3H, OCH_3), 3.85 (s, 3H, OCH_3), 3.92–3.96 (m, 1H, C^4H), 5.159 (s, 2H, CH_2), 5.161 (s, 2H, CH_2), 5.17–5.21 (m, 1H, C^2H), 5.36 (dd, ^3J = 8.3, ^3J = 4.5 Hz, 1H, C^2H), 6.46–6.50 (m, 1H+1H, Ar, **A**, **B**), 6.61–

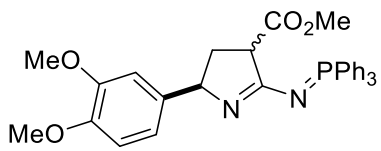
6.66 (m, 1H+1H, Ar, **A**, **B**), 6.95–6.98 (m, 1H+1H, Ar, **A**, **B**), 7.04–7.07 (m, 1H+1H, Ar, **A**, **B**), 7.45–7.49 (m, 6H+6H, PPh_3, **A**, **B**), 7.53–7.57 (m, 3H+3H, PPh_3, **A**, **B**), 7.86–7.90 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 37.1 (CH_2), 37.7 (CH_2), 51.6 (CH_3O), 51.7 (CH_3O), 54.6 ($^3J_{CP}$ = 20 Hz, C^4H), 55.6 ($^3J_{CP}$ = 20 Hz, C^4H), 55.8 (2×CH_3), 64.8 (C^2H), 65.5 (C^2H), 94.0 (OCH_2O), 94.1 (OCH_2O), 112.75 (CH), 112.84 (CH), 120.8 (CH), 121.2 (CH), 126.4 (CH), 126.5 (CH), 126.7 (CH), 127.2 (CH), 128.31 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.32 ($^2J_{CP}$ = 12 Hz, 6×CH), 129.29 ($^1J_{CP}$ = 100 Hz, 3×C), 129.33 ($^1J_{CP}$ = 99 Hz, 3×C), 131.6 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.7 ($^4J_{CP}$ = 3 Hz, 3×CH), 133.1 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.2 ($^3J_{CP}$ = 10 Hz, 6×CH), 135.8 (C), 136.1 (C), 153.6 (C), 153.8 (C), 168.6 ($^2J_{CP}$ = 7 Hz, C), 169.1 ($^2J_{CP}$ = 8 Hz, C), 173.9 (CO_2Me), 174.2 (CO_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.3, 15.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{32}H_{32}N_2O_4P^+$ 539.2094; Found 539.2089.

Methyl 2-(3,4-dimethoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3i)



3i was obtained from azide **1i** (1.510 g, 4.96 mmol). Yield 2.261 g (85%); dr **A**:**B** 51:49; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.94 (m, 1H, CH_2, **B**), 2.05 (ddd, ^2J = 12.4, ^3J = 10.3, ^3J = 8.8 Hz, 1H, CH_2, **A**), 2.63 (m, 1H, CH_2, **A**), 2.74 (dddd, ^2J = 12.5, ^3J = 8.0, ^3J = 6.1, ^5J = 1.2 Hz, 1H, CH_2, **B**), 3.63 (s, 3H, CH_3O, **B**), 3.65 (s, 3H, CH_3O, **A**), 3.81 (s, 6H+6H, CH_3O, **A**, **B**), 3.84-3.90 (m, 1H+1H, C^4H, **A**, **B**), 4.76–4.80 (m, 1H, C^2H, **A**), 5.04 (dd, ^3J = 8.0, ^3J = 5.2 Hz, 1H, C^2H, **B**), 6.48 (dd, ^3J = 8.2, ^4J = 1.6 Hz, 1H, Ar, **B**), 6.51 (dd, ^3J = 8.1, ^4J = 1.6 Hz, 1H, Ar, **A**), 6.54 (d, ^4J = 1.6 Hz, 1H, Ar, **B**), 6.64–6.67 (m, 2H+1H, Ar, **A**, **B**), 7.40–7.45 (m, 6H+6H, PPh_3, **A**, **B**), 7.49–7.53 (m, 3H+3H, PPh_3, **A**, **B**), 7.81–7.85 (m, 6H+6H, PPh_3, **A**, **B**).

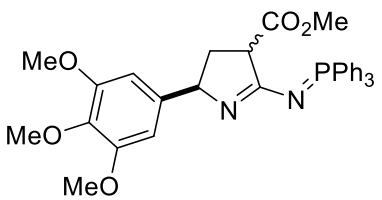
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.7 (CH_2), 39.1 (CH_2), 51.6 (CH_3), 51.7 (CH_3), 54.8 ($^3J_{CP}$ = 21 Hz, 2× C^4H), 55.5 (CH_3O), 55.6 (CH_3O), 55.7 (CH_3O), 55.8 (CH_3O), 69.9 (C^2H), 70.1 (C^2H), 109.2 (CH),

109.8 (CH), 110.5 (CH), 110.6 (CH), 117.8 (CH), 118.1 (CH), 128.1 ($^2J_{CP}$ = 11 Hz, 6×CH), 128.2 ($^2J_{CP}$ = 11 Hz, 6×CH), 128.8 ($^1J_{CP}$ = 99 Hz, 6×C), 131.6 ($^4J_{CP}$ = 2 Hz, 6×CH), 133.04 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.11 ($^3J_{CP}$ = 10 Hz, 6×CH), 139.7 (C), 139.8 (C), 147.0 (C), 147.1 (C), 148.4 (2×C), 168.5 ($^2J_{CP}$ = 7 Hz, C), 168.8 ($^2J_{CP}$ = 8 Hz, C), 173.8 (2×*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 14.7, 15.2.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{32}H_{22}N_2O_4P^+$ 539.2094; Found 539.2099.

Methyl 2-(3,4,5-trimethoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3j)



3j was obtained from azide **1j** (1.500 g, 4.49 mmol). Yield 2.159 g (85%); dr **A**:**B** 50:50; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

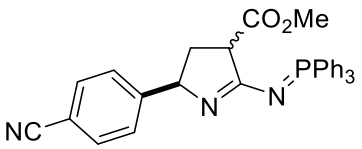
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.95 (ddd, ^2J = 12.5, ^3J = 9.7, ^3J = 5.3 Hz, 1H, CH_2, **B**), 2.09 (ddd, ^2J = 12.3, ^3J = 10.3, ^3J = 8.9 Hz, 1H, CH_2, **A**), 2.64 (m, 1H, CH_2, **A**), 2.74 (dddd, ^2J = 12.5, ^3J = 8.0, ^3J = 5.8, ^5J = 1.4 Hz, 1H, CH_2, **B**), 3.64 (s, 6H, CH_3O), 3.65 (s, 6H, CH_3O), 3.78 (s, 3H, CH_3O), 3.80 (s, 3H, CH_3O), 3.81 (s, 3H, CH_3O), 3.82 (s, 3H, CH_3O), 3.86–3.89 (m, 1H+1H, C^4H, **A**, **B**), 4.73–4.76 (m, 1H, C^2H, **A**), 5.01 (dd, ^3J = 8.0, ^3J = 5.3 Hz, 1H, C^2H, **B**), 6.26 (s, 1H+1H, Ar, **A**, **B**), 6.36 (s, 1H+1H, Ar, **A**, **B**), 7.40–7.44 (m, 6H+6H, PPh_3, **A**, **B**), 7.49–7.53 (m, 3H+3H, PPh_3, **A**, **B**), 7.80–7.84 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.7 (CH_2), 39.0 (CH_2), 51.7 (2×CH_3O), 54.9 ($^3J_{CP}$ = 21 Hz, C^4H), 55.8 ($^3J_{CP}$ = 21 Hz, C^4H), 55.86 (2×CH_3O), 55.93 (2×CH_3O), 60.7 (2×CH_3O), 70.5 (C^2H), 70.9 (C^2H), 102.8 (2×CH), 103.3 (2×CH), 128.2 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.3 ($^2J_{CP}$ = 12 Hz, 6×CH), 129.2 ($^1J_{CP}$ = 100 Hz, 6×C), 131.7 ($^4J_{CP}$ = 2 Hz, 6×CH), 133.1 ($^3J_{CP}$ = 9 Hz, 6×CH), 133.2 ($^3J_{CP}$ = 9 Hz, 6×CH), 136.0 (2×C), 142.9 (2×C), 152.7 (2×C), 152.8 (2×C), 168.8 ($^2J_{CP}$ = 7 Hz, C), 169.0 ($^2J_{CP}$ = 8 Hz, C), 173.9 (2×*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 14.5, 15.0.

HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{33}H_{34}N_2O_5P^+$ 569.2200; Found 569.2202.

Methyl 2-(4-cyanophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3k)



3k was obtained from azide **1k** (0.835 g, 3.10 mmol). Yield 1.157 g (74%); dr **A**:**B** 58:42; yellowish foam; R_f = 0.14 (ethyl acetate – methanol 10:1).

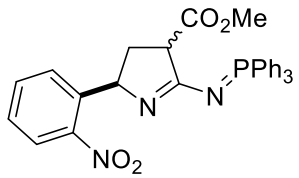
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.86 (dddd, ^2J = 12.8, ^3J = 9.4, ^3J = 5.3, ^5J = 0.9 Hz, 1H, CH_2, **B**), 1.95 (ddd, ^2J = 12.6, ^3J = 9.6, ^3J = 8.3 Hz, 1H, CH_2, **A**), 2.67 (dddd, ^2J = 12.6, ^3J = 9.0, ^3J = 7.4, ^5J 2.0 Hz, 1H, CH_2, **A**), 2.79 (dddd, ^2J = 12.8, ^3J = 8.2, ^3J = 5.8, ^5J = 1.4 Hz, 1H, CH_2, **B**), 3.75-3.78 (m, 1H, C^{4}H, **B**), 3.79 (s, 3H, CH_3O, **A**), 3.84 (s, 3H, CH_3O, **B**), 3.90-3.94 (m, 1H, C^{4}H, **A**), 4.90 (dd, ^3J = 8.3, ^3J = 7.4 Hz, 1H, C^{2}H, **A**), 5.11 (dd, ^3J = 8.2, ^3J = 5.3 Hz, 1H, C^{2}H, **B**), 6.87–6.89 (m, 2H+2H, Ar, **A**, **B**), 7.34–7.36 (m, 2H+2H, Ar, **A**, **B**), 7.44–7.48 (m, 6H+6H, PPh_3, **A**, **B**), 7.54–7.58 (m, 3H+3H, PPh_3, **A**, **B**), 7.80–7.85 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.1 (CH_2), 38.4 (CH_2), 51.8 (CH_3O), 51.9 (CH_3O), 54.9 ($^3J_{CP}$ = 21 Hz, C^{4}H), 55.6 ($^3J_{CP}$ = 20 Hz, C^{4}H), 69.9 (C^{2}H), 70.1 (C^{2}H), 109.3 (2×C), 119.3 (CN), 119.4 (CN), 126.7 (2×CH), 127.0 (2×CH), 128.4 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.5 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.9 ($^1J_{CP}$ = 100 Hz, 3×C), 129.0 ($^1J_{CP}$ = 99 Hz, 3×C), 131.6 (4×CH), 131.8 ($^4J_{CP}$ = 3 Hz, 6×CH), 133.0 ($^3J_{CP}$ = 9 Hz, 6×CH), 133.1 ($^3J_{CP}$ = 9 Hz, 6×CH), 152.9 (C), 153.0 (C), 169.8 ($^2J_{CP}$ = 8 Hz, C), 170.0 ($^2J_{CP}$ = 8 Hz, C), 173.6 (2×*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.7, 16.2.

HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{31}H_{27}N_3O_2P^+$ 504.1835; Found 504.1840.

Methyl 2-(2-nitrophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3l)



3l was obtained from azide **1l** (0.100 g, 0.34 mmol). Yield 0.119 g (66%); dr **A**:**B** 63:37; yellowish foam; R_f = 0.24 (ethyl acetate – methanol 10:1).

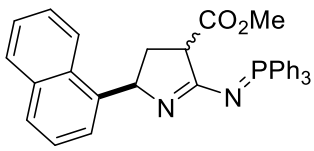
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.92–1.99 (m, 1H+1H, CH_2, **A**, **B**), 2.98 (dddd, ^2J = 12.9, ^3J = 9.5, ^3J = 7.4, ^5J = 1.9 Hz, 1H, CH_2, **A**), 3.03 (dddd, ^2J = 13.5, ^3J = 8.5, ^3J = 6.5, ^5J = 1.4 Hz, 1H, CH_2, **B**), 3.76-3.79 (m, 1H, C^{4}H, **B**), 3.79 (s, 3H, CH_3O, **A**), 3.84 (s, 3H, CH_3O, **B**), 3.93–3.96 (m, 1H, C^{4}H, **A**), 5.36–5.39 (m, 1H, C^{2}H, **A**), 5.56 (dd, ^3J = 8.5, ^3J = 4.8 Hz, 1H, C^{2}H, **B**), 6.70–6.72 (m, 1H, Ar, **B**), 6.73–6.75 (m, 1H, Ar, **A**), 7.13–7.16 (m, 1H+1H, Ar, **A**, **B**), 7.18–7.22 (m, 1H+1H, Ar, **A**, **B**), 7.45–7.49 (m, 6H+6H, PPh_3, **A**, **B**), 7.54–7.58 (m, 3H+3H, PPh_3, **A**, **B**), 7.79–7.81 (m, 1H, Ar, **A**), 7.82–7.86 (m, 6H+7H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 37.7 (CH_2), 39.4 (CH_2), 51.8 (CH_3O), 51.9 (CH_3O), 54.7 ($^3J_{CP}$ = 21 Hz, C^{4}H), 55.5 ($^3J_{CP}$ = 20 Hz, C^{4}H), 66.6 (C^{2}H), 67.1 (C^{2}H), 123.5 (CH), 124.0 (CH), 126.5 (CH), 126.6 (CH), 128.3 (CH), 128.5 ($^2J_{CP}$ = 12 Hz, 12×CH), 129.0 ($^1J_{CP}$ = 99 Hz, 6×C), 129.4 (CH), 131.8 ($^4J_{CP}$ = 3 Hz, 6×CH), 132.6 (CH), 132.8 (CH), 133.1 ($^3J_{CP}$ = 9 Hz, 6×CH), 133.2 ($^3J_{CP}$ = 9 Hz, 6×CH), 142.5 (C), 142.6 (C), 147.7 (2×C), 169.9 ($^2J_{CP}$ = 7 Hz, C), 170.6 ($^2J_{CP}$ = 8 Hz, C), 173.6 (*C*O_2Me), 173.8 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 16.6 (**A**), 17.1 (**B**).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{27}N_3O_4P^+$ 524.1734; Found 524.1736.

Methyl 2-(naphthalen-1-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3m)



3m was obtained from azide **1m** (1.320 g, 4.49 mmol). Yield 2.022 g (85%); dr **A**:**B** 44:56; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

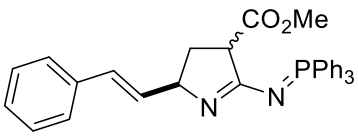
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.05 (dddd, ^2J = 12.7, ^3J = 9.4, ^3J = 4.5, ^5J = 1.4 Hz, 1H, CH_2, **B**), 2.07 (dddd, ^2J = 12.7, ^3J = 9.6, ^3J = 8.3 Hz, 1H, CH_2, **A**), 2.97 (dddd, ^2J = 12.7, ^3J = 9.1, ^3J = 7.3, ^5J = 2.1 Hz, 1H, CH_2, **A**), 3.04 (dddd, ^2J = 12.7, ^3J = 8.6, ^3J = 6.8, ^5J = 1.2 Hz, 1H, CH_2, **B**), 3.78 (s, 3H, CH_3O, **A**), 3.82 (dddd, ^3J = 9.4, ^3J = 6.8, ^4J = 2.0, ^4J = 1.0 Hz, 1H, C^4H, **B**), 3.88 (s, 3H, CH_3O, **B**), 4.03 (dddd, ^3J = 9.6, ^3J = 9.1, ^4J = 2.2, ^4J = 1.3 Hz, 1H, C^4H, **A**), 5.63 (dd, ^3J = 8.3, ^3J = 7.3 Hz, 1H, C^2H, **A**), 5.82 (dd, ^3J = 8.6, ^3J = 4.5 Hz, 1H, C^2H, **B**), 6.63 (d, ^3J = 7.2 Hz, 1H, Ar, **A**), 6.68 (d, ^3J = 7.2 Hz, 1H, Ar, **A**), 7.08 (dd, ^3J = 8.1, ^3J = 7.3 Hz, 1H, Ar, **B**), 7.10 (dd, ^3J = 8.0, ^3J = 7.3 Hz, 1H, Ar, **A**), 7.41–7.47 (m, 2H+2H, Ar, **A**, **B**), 7.47–7.50 (m, 6H+6H, PPh_3, **A**, **B**), 7.56–7.59 (m, 3H+3H, PPh_3, **A**, **B**), 7.59–7.62 (m, 1H+1H, Ar, **A**, **B**), 7.79–7.81 (m, 1H+1H, Ar, **A**, **B**), 7.89–7.93 (m, 6H+6H, PPh_3, **A**, **B**), 7.97–8.01 (m, 1H+1H, Ar, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 37.6 (CH_2), 38.3 (CH_2), 51.7 (CH_3O), 51.9 (CH_3O), 54.7 ($^3J_{CP}$ = 20 Hz, C^4H), 55.8 ($^3J_{CP}$ = 20 Hz, C^4H), 67.0 (CH), 67.2 (CH), 122.2 (CH), 123.1 (CH), 123.5 (CH), 123.6 (CH), 124.8 (CH), 124.9 (CH), 125.2 (2×CH), 125.4 (CH), 125.6 (CH), 126.1 (CH), 126.2 (CH), 128.4 (2×CH), 128.4 ($^2J_{CP}$ = 11 Hz, 12×CH), 129.3 ($^1J_{CP}$ = 100 Hz, 6×C), 130.7 (2×C), 131.7 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.8 ($^4J_{CP}$ = 3 Hz, 3×CH), 133.2 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.3 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.5 (C), 133.6 (C), 142.6 (C), 142.9 (C), 168.8 ($^2J_{CP}$ = 8 Hz, C), 169.3 ($^2J_{CP}$ = 8 Hz, C), 173.8 (CO_2Me), 174.1 (CO_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.4, 15.8.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{34}H_{30}N_2O_2P^+$ 529.2039; Found 529.2046.

Methyl (*E*)-2-styryl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3n)



3n was obtained from azide **1n** (1.509 g, 5.58 mmol). Yield 2.327 g (83%); dr **A**:**B** 45:55; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

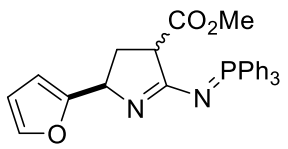
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.99 (dddd, ^2J = 12.6, ^3J = 9.0, ^3J = 5.5, ^5J = 1.7 Hz, 1H, CH_2, **B**), 2.04 (ddd, ^2J = 12.6, ^3J = 9.1, ^3J = 7.8 Hz, 1H, CH_2, **A**), 2.48 (dddd, ^2J = 12.6, ^3J = 9.2, ^3J = 7.3, ^5J = 2.1 Hz, 1H, CH_2, **A**), 2.60 (dddd, ^2J = 12.6, ^3J = 8.5, ^3J = 7.4, ^5J = 0.9 Hz, 1H, CH_2, **B**), 3.79–3.82 (m, 1H, C^4H, **B**), 3.80 (s, 3H, CH_3O, **A**), 3.83 (s, 3H, CH_3O, **B**), 3.84–3.87 (m, 1H, C^4H, **A**), 4.43–4.47 (m, 1H, C^2H, **A**), 4.63–4.66 (m, 1H, C^2H, **B**), 6.01 (dd, ^3J = 15.8, ^4J = 1.2 Hz, 1H, CH, **B**), 6.13–6.17 (m, 2H+1H, CH, **A**, **B**), 7.14–7.18 (m, 2H+2H, Ph, **A**, **B**), 7.20–7.22 (m, 1H+1H, Ph, **A**, **B**), 7.24–7.27 (m, 2H+2H, Ph, **A**, **B**), 7.44–7.48 (m, 6H+6H, PPh_3, **A**, **B**), 7.51–7.56 (m, 3H+3H, PPh_3, **A**, **B**), 7.81–7.86 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 35.7 (CH_2), 36.2 (CH_2), 51.8 (CH_3O), 51.9 (CH_3O), 54.2 ($^3J_{CP}$ = 21 Hz, C^4H), 55.3 ($^3J_{CP}$ = 21 Hz, C^4H), 68.1 (C^2H), 68.7 (C^2H), 126.1 (2×CH), 126.2 (2×CH), 126.56 (CH), 126.59 (CH), 127.1 (CH), 127.4 (CH), 128.2 (2×CH), 128.3 (2×CH), 128.4 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.5 ($^2J_{CP}$ = 12 Hz, 6×CH), 129.2 ($^1J_{CP}$ = 100 Hz, 3×C), 129.3 ($^1J_{CP}$ = 99 Hz, 3×C), 131.79 ($^4J_{CP}$ = 2 Hz, 3×CH), 131.84 ($^4J_{CP}$ = 3 Hz, 3×CH), 133.1 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.2 ($^3J_{CP}$ = 10 Hz, 6×CH), 134.6 (CH), 135.0 (CH), 138.0 (C), 138.1 (C), 168.4 ($^2J_{CP}$ = 7 Hz, C), 168.8 ($^2J_{CP}$ = 8 Hz, C), 174.0 (*C*O_2Me), 174.2 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 14.9, 15.0.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{32}H_{30}N_2O_2P^+$ 505.2039; Found 505.2042.

Methyl 2-(furan-2-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3o)



3o was obtained from azide **1o** (0.478 g, 2.04 mmol). Yield 0.658 g (69%); dr **A**:**B** 63:37; yellow oil; R_f = 0.10 (ethyl acetate).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.24 (dddd, ^2J = 12.4, ^3J = 9.0, ^3J = 3.2, ^5J = 2.0 Hz, 1H, CH_2, **A**), 2.29 (ddd, ^2J = 12.7, ^3J = 9.3, ^3J = 7.7 Hz, 1H, CH_2, **B**), 2.60 (dddd, ^2J = 12.6, ^3J = 9.4, ^3J = 7.4, ^5J = 2.0 Hz, 1H, CH_2, **B**), 2.68 (dddd, ^2J = 12.4, ^3J = 8.4, ^3J = 8.3, ^5J = 0.8 Hz, 1H, CH_2, **A**), 3.78 (s, 3H, CH_3O, **A**), 3.82 (s, 3H, CH_3O, **B**), 3.86–3.91 (m, 1H+1H, C^4H, **A**, **B**), 4.89 (dd,

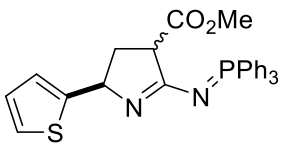
^3J = 7.7, ^3J = 7.4 Hz, 1H, C^{2}H, **B**), 5.05 (dd, ^3J = 8.3, ^3J = 3.2 Hz, 1H, C^{2}H, **A**), 5.54–5.55 (m, 1H, Ar, **A**), 5.58–5.59 (m, 1H, Ar, **B**), 6.13 (dd, ^3J = 3.2, ^3J = 1.9 Hz, 1H, Ar, **A**), 6.16 (dd, ^3J = 3.2, ^3J = 1.9 Hz, 1H, Ar, **B**), 7.22–7.23 (m, 1H+1H, Ar, **A**, **B**), 7.41–7.44 (m, 6H+6H, PPh_3, **A**, **B**), 7.49–7.52 (m, 3H+3H, PPh_3, **A**, **B**), 7.80–7.85 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 34.9 (CH_2), 35.2 (CH_2), 51.55 (CH_3O), 51.63 (CH_3O), 54.2 ($^3J_{CP}$ = 20 Hz, C^{4}H), 55.1 ($^3J_{CP}$ = 20 Hz, C^{4}H), 64.5 (C^{2}H), 64.6 (C^{2}H), 103.5 (CH), 103.7 (CH), 109.5 (CH), 109.7 (CH), 128.1 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.2 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.9 ($^1J_{CP}$ = 100 Hz, 3×C), 129.0 ($^1J_{CP}$ = 99 Hz, 3×C), 131.59 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.64 ($^4J_{CP}$ = 3 Hz, 3×CH), 132.9 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.0 ($^3J_{CP}$ = 10 Hz, 6×CH), 140.2 (CH), 140.5 (CH), 159.0 (C), 159.6 (C), 168.9 ($^2J_{CP}$ = 8 Hz, C), 169.7 ($^2J_{CP}$ = 8 Hz, C), 173.4 (*C*O_2Me), 173.8 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.4, 15.5.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{28}H_{26}N_2O_3P^+$ 469.1676; Found 469.1672.

Methyl 2-(thien-2-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3p)



3p was obtained from azide **1p** (1.500 g, 6.00 mmol). Yield 2.487 g (86%); dr **A**:**B** 45:55; yellowish solid, mp 160–161 °C; R_f = 0.10 (ethyl acetate – methanol 10:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.13 (dddd, ^2J = 12.6, ^3J = 9.1, ^3J = 4.3, ^5J = 1.4 Hz, 1H, CH_2, **B**), 2.23 (ddd, ^2J = 12.4, ^3J = 10.2, ^3J = 8.4 Hz, 1H, CH_2, **A**), 2.67 (dddd, ^2J = 12.4, ^3J = 8.8, ^3J = 7.0, ^5J = 2.3 Hz, 1H, CH_2, **A**), 2.77 (dddd, ^2J = 12.6, ^3J = 8.1, ^3J = 7.0, ^5J = 1.1 Hz, 1H, CH_2, **B**), 3.80 (s, 3H, CH_3O, **A**), 3.81 (s, 3H, CH_3O, **B**), 3.86–3.91 (m, 1H+1H, C^{4}H, **A**, **B**), 5.05 (dd, ^3J = 8.4, ^3J = 7.0 Hz, 1H, C^{2}H, **A**), 5.27 (dd, ^3J = 8.1, ^3J = 4.3 Hz, 1H, C^{2}H, **B**), 6.56 (dd, ^3J = 3.4, ^4J = 1.2 Hz, 1H, Ar, **B**), 6.60 (dd, ^3J = 3.4, ^4J = 1.2 Hz, 1H, Ar, **A**), 6.81 (dd, ^3J = 5.0, ^3J = 3.4 Hz, 1H, Ar, **B**), 6.82 (dd, ^3J = 5.0, ^3J = 3.4 Hz, 1H, Ar, **A**), 7.01 (dd, ^3J = 5.0, ^4J = 1.2 Hz, 1H, Ar, **B**), 7.02 (dd, ^3J = 5.0, ^4J = 1.2 Hz,

1H, Ar, **A**), 7.42–7.48 (m, 6H+6H, PPh_3, **A**, **B**), 7.51–7.56 (m, 3H+3H, PPh_3, **A**, **B**), 7.81–7.84 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.8 (CH_2), 39.1 (CH_2), 51.8 (CH_3O), 51.9 (CH_3O), 54.8 ($^3J_{CP}$ = 21 Hz, C^4H), 55.9 ($^3J_{CP}$ = 21 Hz, C^4H), 66.3 (C^2H), 66.7 (C^2H), 121.6 (CH), 121.7 (CH), 122.7 (CH), 122.8 (CH), 126.1 (CH), 126.3 (CH), 128.4 ($^2J_{CP}$ = 11 Hz, 6×CH), 128.5 ($^2J_{CP}$ = 11 Hz, 6×CH), 129.1 ($^1J_{CP}$ = 100 Hz, 3×C), 129.2 ($^1J_{CP}$ = 99 Hz, 3×C), 131.78 ($^4J_{CP}$ = 2 Hz, 3×CH), 131.83 ($^4J_{CP}$ = 2 Hz, 3×CH), 133.2 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.3 ($^3J_{CP}$ = 10 Hz, 6×CH), 152.0 (C), 152.1 (C), 169.0 ($^2J_{CP}$ = 8 Hz, C), 169.4 ($^2J_{CP}$ = 8 Hz, C), 173.6 (CO_2Me), 173.9 (CO_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.3, 15.6.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{28}H_{26}N_2O_2PS^+$ 485.1447; Found 485.1445.

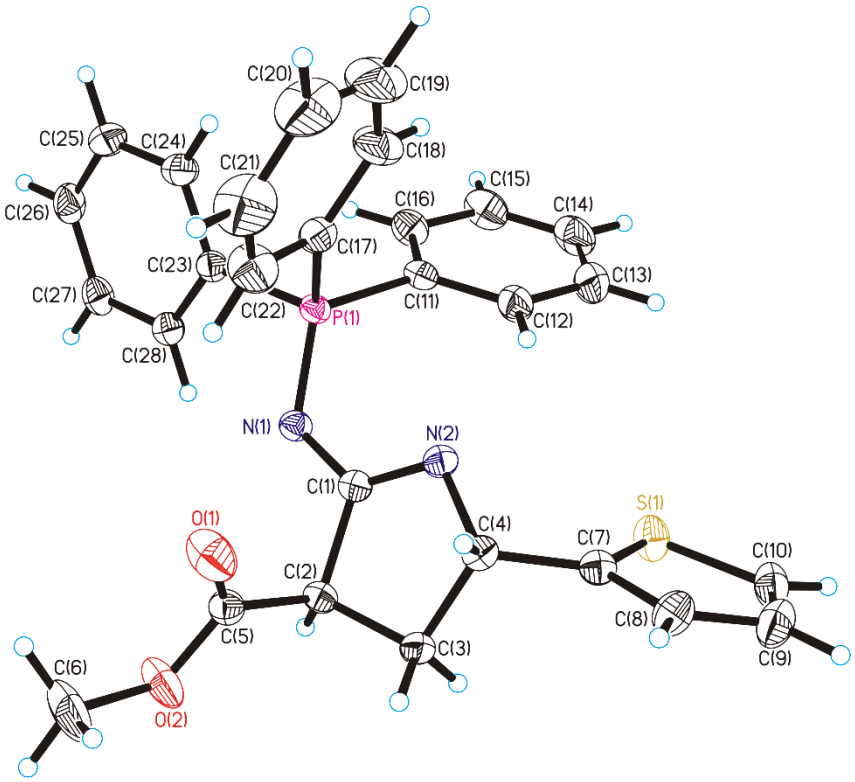
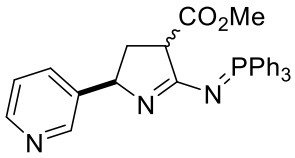


Figure S2. Molecular structure from single crystal X-ray study of *trans*-**3p** (thermal ellipsoids are drawn at the 50% probability level); CCDC 1838689.

Methyl 2-(pyridin-2-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3q)



3q was obtained from azide **1q** (0.360 g, 1.47 mmol). Yield 0.505 g (72%); dr **A**:**B** 57:43; white foam; R_f = 0.10 (ethyl acetate).

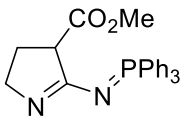
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.92 (dddd, ^2J = 12.8, ^3J = 9.4, ^3J = 5.4, ^5J = 1.2 Hz, 1H, CH_2, **B**), 2.00 (ddd, ^2J = 12.7, ^3J = 9.9, ^3J = 8.4 Hz, 1H, CH_2, **A**), 2.67 (dddd, ^2J = 12.7, ^3J = 9.1, ^3J = 7.2, ^5J = 2.2 Hz, 1H, CH_2, **A**), 2.79 (dddd, ^2J = 12.8, ^3J = 8.1, ^3J = 5.9, ^5J = 1.5 Hz, 1H, CH_2, **B**), 3.79 (s, 3H, CH_3O, **A**), 3.79–3.82 (m, 1H, C^4H, **B**), 3.83 (s, 3H, CH_3O, **B**), 3.92 (dddd, ^3J = 10.1, ^3J = 9.0, ^4J = 2.3, ^4J = 1.4 Hz, 1H, C^4H, **A**), 4.85–4.89 (m, 1H, C^2H, **A**), 5.10 (dd, ^3J = 8.1, ^3J = 5.4 Hz, 1H, C^2H, **B**), 6.97–7.00 (m, 1H+1H, Py, **A**, **B**), 7.03–7.06 (m, 1H+1H, Py, **A**, **B**), 7.44–7.48 (m, 6H+6H, PPh_3, **A**, **B**), 7.54–7.57 (m, 3H+3H, PPh_3, **A**, **B**), 7.80–7.84 (m, 6H+6H, PPh_3, **A**, **B**), 8.18–8.19 (m, 1H, Py, **B**), 8.19–8.20 (m, 1H, Py, **A**), 8.34 (dd, ^3J = 4.7, ^4J = 1.7 Hz, 1H, C^2H, **B**), 8.35 (dd, ^3J = 4.7, ^4J = 1.7 Hz, 1H, C^2H, **A**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.2 (CH_2), 38.6 (CH_2), 51.8 (CH_3O), 51.9 (CH_3O), 55.0 ($^3J_{CP}$ = 20 Hz, C^4H), 55.8 ($^3J_{CP}$ = 20 Hz, C^4H), 68.0 (C^2H), 68.2 (C^2H), 122.7 (CH), 122.9 (CH), 128.41 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.44 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.9 ($^1J_{CP}$ = 100 Hz, 3×C), 129.0 ($^1J_{CP}$ = 100 Hz, 3×C), 131.88 ($^4J_{CP}$ = 2 Hz, 3×CH), 131.91 ($^4J_{CP}$ = 2 Hz, 3×CH), 133.07 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.13 ($^3J_{CP}$ = 10 Hz, 6×CH), 142.1 (C), 142.3 (C), 147.3 (CH), 147.4 (CH), 148.1 (CH), 148.2 (CH), 169,6 ($^2J_{CP}$ = 8 Hz, C), 169.7 ($^2J_{CP}$ = 8 Hz, C), 173.6 (2×*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 15.6, 16.1.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{29}H_{27}N_3O_2P^+$ 480.1835; Found 480.1834.

Methyl 5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3r)



3r was obtained from azide **1r** (0.078 g, 0.46 mmol). Yield 0.157 g (84%); yellowish foam; R_f = 0.10 (ethyl acetate – methanol 2:1).

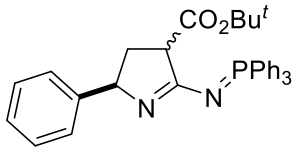
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.10–2.16 (m, 1H, CH_2), 2.20–2.27 (m, 1H, CH_2), 3.46–3.52 (m, 1H, CH_2), 3.62 (ddd, ^2J = 13.4, ^3J = 8.7, ^3J = 4.2, Hz, 1H, CH_2) 3.69–3.75 (m, 1H, CH), 3.73 (s, 3H, CH_3O), 7.37–7.40 (m, 6H, PPh_3), 7.45–7.48 (m, 3H, PPh_3), 7.72–7.76 (m, 6H, PPh_3).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 28.8 (CH_2), 51.5 (CH_3O), 54.7 ($^3J_{CP}$ = 20 Hz, C^4H), 55.7 (CH_2), 128.3 ($^2J_{CP}$ = 11 Hz, 6×CH), 129.1 ($^1J_{CP}$ = 100 Hz, 3×C), 131.6 ($^4J_{CP}$ = 3 Hz, 3×CH), 132.7 ($^3J_{CP}$ = 9 Hz, 6×CH), 168.0 ($^2J_{CP}$ = 7 Hz, C), 174.0 (CO_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 14.0.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{24}H_{24}N_2O_2P^+$ 403.1570; Found 403.1573.

***tetr*-Butyl 2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3s)**



3s was obtained from azide **1s** (0.275 g, 0.96 mmol). Reaction time 90 h. Yield 0.401 g (80%); dr **A**:**B** 54:46; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

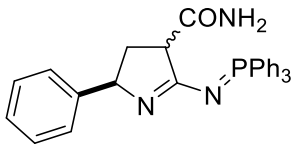
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.49 (s, 9H, CH_3, **A**), 1.56 (s, 9H, CH_3, **B**), 1.89–1.95 (m, 1H, CH_2, **B**), 1.98–2.05 (m, 1H, CH_2, **A**), 2.64–2.71 (m, 1H, CH_2, **A**), 2.76–2.81 (m, 1H, CH_2, **B**), 3.72 (dd, ^3J = 9.2, ^3J = 5.7 Hz, 1H, C^4H, **B**), 3.77–3.81 (m, 1H, C^4H, **A**), 4.86–4.89 (m, 1H, C^2H, **A**), 5.11–5.14 (m, 1H, C^2H, **B**), 6.90–6.95 (m, 2H+2H, Ph, **A**, **B**), 7.09–7.15 (m, 3H+3H, Ph, **A**, **B**), 7.44–7.50 (m, 6H+6H, PPh_3, **A**, **B**), 7.53–7.57 (m, 3H+3H, PPh_3, **A**, **B**), 7.88–7.93 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 28.0 (CH_3), 28.1 (CH_3), 38.6 (CH_2), 39.3 (CH_2), 56.3 ($^3J_{CP}$ = 20 Hz, C^4H), 57.2 ($^1J_{CH}$ = 135, $^3J_{CP}$ 21 Hz, C^4H), 70.4 (C^2H), 70.5 (C^2H), 125.5 (CH), 125.6 (CH), 125.9 (2×CH), 126.3 (2×CH), 127.5 (2×CH), 127.6 (2×CH), 128.2 ($^2J_{CP}$ = 13 Hz, 6×CH), 128.3 ($^2J_{CP}$ = 13 Hz, 6×CH), 129.3 ($^1J_{CP}$ = 99 Hz, 3×C), 129.4 ($^1J_{CP}$ = 100 Hz, 3×C), 131.5 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.6 ($^4J_{CP}$ = 3 Hz, 3×CH), 133.1 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.2 ($^3J_{CP}$ = 10 Hz, 6×CH), 147.4 (C), 147.6 (C), 169.4 ($^2J_{CP}$ = 8 Hz, 2×C), 172.6 (CO_2Me), 172.7 (CO_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 14.9, 15.1.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{33}H_{34}N_2O_2P^+$ 521.2352; Found 521.2358.

2-Phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxamide (3t)



3t was obtained from azide **1t** (0.229 g, 1.00 mmol). Yield 0.397 g (86%); dr **A**:**B** 44:56; yellowish foam; R_f = 0.10 (ethyl acetate – methanol 10:1).

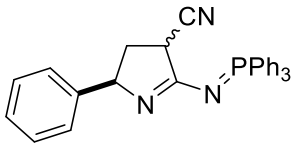
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.91 (ddd, ^2J = 13.0, ^3J = 10.2, ^3J = 6.2 Hz, 1H, CH_2, **B**), 2.03 (ddd, ^2J =13.0, ^3J =9.7, ^3J =8.3 Hz, 1H, CH_2, **A**), 2.81 (dddd, ^2J = 13.0, ^3J = 9.5, ^3J = 7.7, ^5J = 1.8 Hz, 1H, CH_2, **A**), 3.03 (dddd, ^2J = 13.0, ^3J = 7.9, ^3J = 5.0, ^5J = 1.6 Hz, 1H, CH_2, **B**), 3.75 (dd, ^3J = 10.2, ^3J = 5.0 Hz, 1H, C^4H, **B**), 3.81 (dd, ^3J = 9.7, ^3J = 9.5 Hz, 1H, C^4H, **A**), 4.79 (dd, ^3J = 8.3, ^3J = 7.7 Hz, 1H, C^2H, **A**), 4.94 (dd, ^3J = 7.9, ^3J = 6.2 Hz, 1H, C^2H, **B**), 6.18 (br.s, 1H, NH_2, **A**), 6.22 (br.s, 1H, NH_2, **B**), 6.82-6.84 (m, 2H+2H, Ph, **A**, **B**), 7.08–7.13 (m, 3H+3H, Ph, **A**, **B**), 7.46–7.50 (m, 6H+6H, PPh_3, **A**, **B**), 7.56–7.60 (m, 3H+3H, PPh_3, **A**, **B**), 7.81–7.85 (m, 6H+6H, PPh_3, **A**, **B**), 8.56 (br.s, 1H, NH_2, **B**), 9.18 (br.s, 1H, NH_2, **A**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 35.9 (CH_2), 36.6 (CH_2), 53.8 ($^3J_{CP}$ = 17 Hz, C^4H), 54.2 ($^3J_{CP}$ = 17 Hz, C^4H), 67.5 (C^2H), 69.1 (C^2H), 125.6 (2×CH), 125.87 (2×CH), 125.89 (2×CH), 127.57 (2×CH), 127.62 (2×CH), 128.5 ($^2J_{CP}$ = 12 Hz, 12×CH), 128.6 ($^1J_{CP}$ = 100 Hz, 6×C), 132.0 ($^4J_{CP}$ = 3 Hz, 6×CH), 133.0 ($^3J_{CP}$ = 10 Hz, 12×CH), 147.1 (C), 147.3 (C), 168.4 ($^2J_{CP}$ = 9 Hz, C), 168.8 ($^2J_{CP}$ = 8 Hz, C), 174.0 (*C*O_2Me), 174.6 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 18.7, 19.7.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{29}H_{27}N_3OP^+$ 464.1886; Found 464.1886.

2-Phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carbonitrile (3u)



3u was obtained from azide **1u** (0.106 g, 0.50 mmol). Reaction time 4 h. Yield 0.200 g (89%); dr **A**:**B** 55:45; yellowish foam; R_f = 0.26 (ethyl acetate).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.91–1.99 (m, 1H, CH_2, **A**), 2.12 (dddd, ^2J = 12.8, ^3J = 9.4, ^3J = 5.2, ^5J = 1.2 Hz, 1H, CH_2, **B**), 2.77 (dddd, ^2J = 12.8, ^3J = 7.6, ^3J = 6.6, ^5J = 1.2 Hz, 1H, CH_2, **B**), 2.81–2.88

(m, 1H, CH_2, **A**), 3.81 (dd, ^3J = 9.4, ^3J = 6.6 Hz, 1H, C^4H, **B**), 3.88–3.93 (m, 1H, C^4H, **A**), 4.88–4.92 (m, 1H, C^2H, **A**), 5.13 (dd, ^3J = 7.6, ^3J = 5.2 Hz, 1H, C^2H, **B**), 6.87–6.93 (m, 2H+2H, Ph, **A**, **B**), 7.16–7.20 (m, 3H+3H, Ph, **A**, **B**), 7.48–7.51 (m, 6H+6H, PPh_3, **A**, **B**), 7.57–7.60 (m, 3H+3H, PPh_3, **A**, **B**), 7.92–7.96 (m, 6H+6H, PPh_3, **A**, **B**).

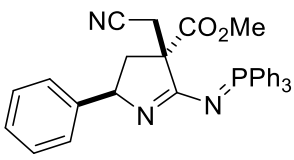
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 38.00 (CH_2), 38.01 ($^3J_{CP}$ = 22 Hz, C^4H), 39.6 (CH_2), 39.8 ($^3J_{CP}$ = 21 Hz, C^4H), 69.8 (C^2H), 70.0 (C^2H), 120.3 (CN), 120.4 (CN), 125.7 (2×CH), 125.8 (2×CH), 126.0 (CH), 126.1 (CH), 127.7 (2×CH), 127.8 (2×CH), 128.30 ($^1J_{CP}$ = 100 Hz, 6×C), 128.35 ($^2J_{CP}$ = 12 Hz, 12×CH), 131.88 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.93 ($^4J_{CP}$ = 3 Hz, 3×CH), 133.0 ($^3J_{CP}$ = 10 Hz, 6×CH), 133.1 ($^3J_{CP}$ = 10 Hz, 6×CH), 145.2 (C), 145.7 (C), 165.2 ($^2J_{CP}$ = 6 Hz, C), 165.5 ($^2J_{CP}$ = 7 Hz, C).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 16.9, 17.4.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{29}H_{25}N_3P^+$ 446.1781; Found 446.1782.

Methyl 4-(cyanomethyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3w)

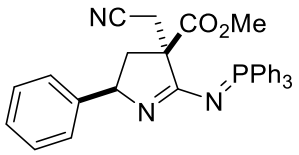
3w was obtained from azide **1w** (0.142 g, 0.50 mmol). Yield 0.195 g (75%); dr *trans*:*cis* 56:44. Diastereomers were separated by column chromatography.



trans-**3w:** colorless foam; R_f = 0.28 (ethyl acetate). ^1H NMR ($CDCl_3$, 600 MHz) δ = 1.87 (dd, ^2J = 13.2, ^3J = 7.6 Hz, 1H, CH_2), 2.96 (ddd, ^2J = 13.2, ^3J = 7.4, ^5J = 2.3 Hz, 1H, CH_2), 3.03 (d, ^2J = 16.7 Hz, 1H, CH_2), 3.17 (d, ^2J = 16.7 Hz, 1H, CH_2), 3.83 (s, 3H, CH_3O), 5.10 (dd, ^3J = 7.6, ^3J = 7.4 Hz, 1H, CH), 6.90–6.94 (m, 2H, Ph), 7.13–7.18 (m, 3H, Ph), 7.47–7.51 (m, 6H, PPh_3), 7.56–7.60 (m, 3H, PPh_3), 7.83–7.88 (m, 6H, PPh_3).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 24.4 (CH_2), 44.3 (CH_2), 52.5 (CH_3O), 60.4 ($^3J_{CP}$ = 20 Hz, C), 68.7 (CH), 118.5 (CN), 126.0 (CH), 126.1 (2×CH), 127.8 (2×CH), 128.4 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.8 ($^1J_{CP}$ = 100 Hz, 3×C), 131.9 ($^4J_{CP}$ = 2 Hz, 3×CH), 133.0 ($^3J_{CP}$ = 10 Hz, 6×CH), 146.6 (C), 168.0 ($^2J_{CP}$ = 7 Hz, C), 172.8 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 17.0.



cis-**3w:** colorless crystals, mp 143–144 °C; R_f = 0.42 (ethyl acetate). ^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.36 (dd, ^2J = 13.6, ^3J = 7.4 Hz, 1H, CH_2), 2.68 (ddd, ^2J = 13.6, ^3J = 7.7, ^5J = 2.2 Hz, 1H, CH_2), 3.01 (d, ^2J = 16.6 Hz, 1H, CH_2), 3.20 (d, ^2J = 16.6 Hz, 1H, CH_2), 3.67 (s, 3H, CH_3O), 5.07 (dd, ^3J = 7.7, ^3J = 7.4 Hz, 1H, CH), 6.86–6.89 (m, 2H, Ph), 7.12–7.15 (m, 3H, Ph), 7.46–7.50 (m, 6H, PPh_3), 7.56–7.59 (m, 3H, PPh_3), 7.80–7.85 (m, 6H, PPh_3).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 23.4 (CH_2), 43.7 (CH_2), 52.3 (CH_3O), 61.0 ($^3J_{CP}$ = 20 Hz, C), 69.3 (CH), 118.6 (CN), 125.9 (CH), 126.2 (2×CH), 127.7 (2×CH), 128.4 ($^2J_{CP}$ = 12 Hz, 6×CH), 128.8 ($^1J_{CP}$ = 100 Hz, 3×C), 131.9 ($^4J_{CP}$ = 2 Hz, 3×CH), 133.1 ($^3J_{CP}$ = 10 Hz, 6×CH), 146.6 (C), 168.7 ($^2J_{CP}$ = 7 Hz, C), 173.0 (CO_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 16.4.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{32}H_{29}N_3O_2P^+$ 518.1992; Found 518.1993.

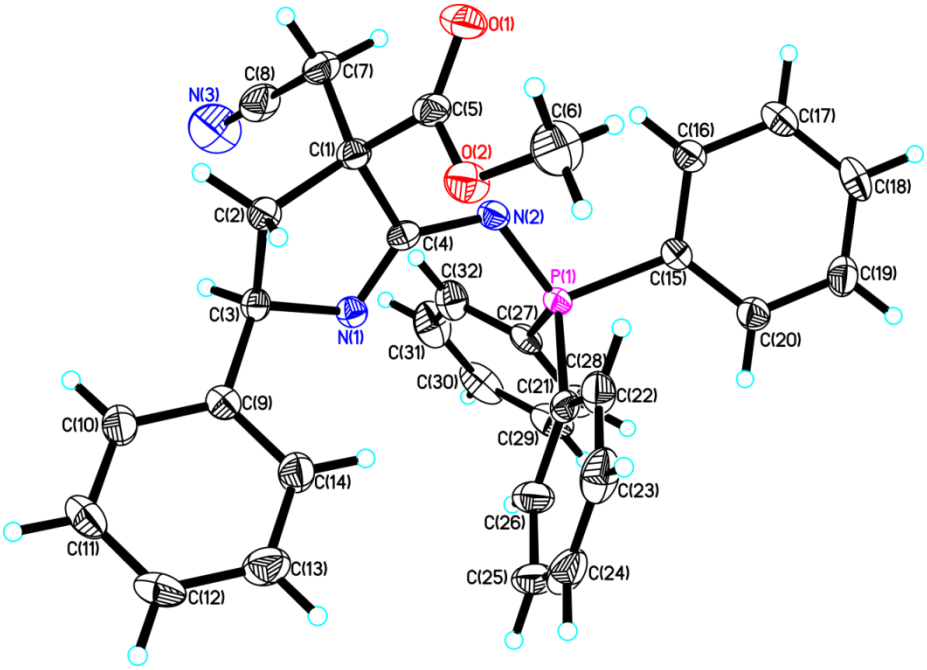
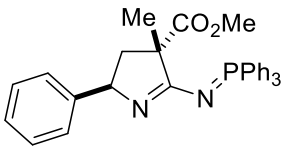


Figure S3. Molecular structure from single crystal X-ray study of **(2*RS*,4*SR*)-3w** (thermal ellipsoids are drawn at the 50% probability level); CCDC 1873067.

Methyl 4-(methyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3x)

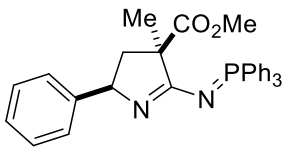
3x was obtained from azide **1x** (0.258 g, 1.00 mmol). Yield 0.376 g (76%); dr *trans*:*cis* 57:43. Diastereomers were separated by column chromatography.



trans-**3x:** colorless foam; R_f = 0.11 (ethyl acetate). ^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.49 (s, 3H, CH_3), 1.58 (ddd, ^2J = 12.8, ^3J = 6.7, ^5J = 0.8 Hz, 1H, CH_2), 2.93 (ddd, ^2J = 12.8, ^3J = 8.0, ^5J = 1.9 Hz, 1H, CH_2), 3.76 (s, 3H, CH_3O), 5.00 (dd, ^3J = 8.0, ^3J = 6.7 Hz, 1H, CH), 6.84–6.86 (m, 2H, Ph), 7.08–7.12 (m, 3H, Ph), 7.44–7.47 (m, 6H, PPh_3), 7.53–7.56 (m, 3H, PPh_3), 7.84–7.88 (m, 6H, PPh_3).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 22.7 (CH_3), 47.4 (CH_2), 51.9 (CH_3O), 58.9 ($^3J_{CP}$ = 19 Hz, C), 68.3 (CH), 125.6 (CH), 126.0 (2×CH), 127.7 (2×CH), 128.3 ($^2J_{CP}$ = 12 Hz, 6×CH), 129.7 ($^1J_{CP}$ = 99 Hz, 3×C), 131.6 ($^4J_{CP}$ = 2 Hz, 3×CH), 133.2 ($^3J_{CP}$ = 10 Hz, 6×CH), 148.0 (C), 172.4 ($^2J_{CP}$ = 8 Hz, C), 176.0 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 14.6.



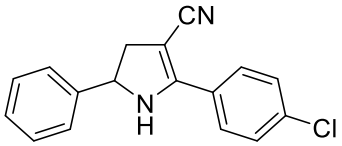
cis-**3x:** colorless foam; R_f = 0.23 (ethyl acetate). ^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.62 (s, 3H, CH_3), 2.27 (dd, ^2J = 12.4, ^3J = 8.3 Hz, 1H, CH_2), 2.33 (ddd, ^2J = 12.4, ^3J = 7.1, ^5J = 2.5 Hz, 1H, CH_2), 3.68 (s, 3H, CH_3O), 4.92 (dd, ^3J = 8.3, ^3J = 7.1 Hz, 1H, CH), 6.90–6.92 (m, 2H, Ph), 7.11–7.15 (m, 3H, Ph), 7.45–7.48 (m, 6H, PPh_3), 7.54–7.57 (m, 3H, PPh_3), 7.84–7.88 (m, 6H, PPh_3).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 20.3 (CH_3), 47.4 (CH_2), 51.6 (CH_3O), 59.3 ($^3J_{CP}$ = 19 Hz, C), 68.8 (CH), 125.6 (CH), 126.3 (2×CH), 127.6 (2×CH), 128.3 ($^2J_{CP}$ = 12 Hz, 6×CH), 129.7 ($^1J_{CP}$ = 99 Hz, 3×C), 131.6 ($^4J_{CP}$ = 2 Hz, 3×CH), 133.1 ($^3J_{CP}$ = 10 Hz, 6×CH), 147.4 (C), 173.3 ($^2J_{CP}$ = 8 Hz, C), 175.9 (*C*O_2Me).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 14.2.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{31}H_{30}N_2O_2P^+$ 493.2039; Found 493.2046.

2-(4-Chlorophenyl)-5-phenyl-4,5-dihydro-1*H*-pyrrole-3-carbonitrile (8)



8 was obtained from azide **1v** (0.200 g, 0.62 mmol). Yield 0.145 g (84%); white crystals; mp 141–142 °C; R_f = 0.71 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR (DMSO-d$_6$, 600 MHz) δ = 2.68 (dd, ^2J = 14.5, ^3J = 9.0 Hz, 1H, CH$_2$), 3.39 (dd, ^2J = 14.5, ^3J = 11.7 Hz, 1H, CH$_2$), 5.06 (ddd, ^3J = 11.7, ^3J = 9.0, ^3J = 1.6 Hz, 1H, CH), 7.29–7.32 (m, 1H, Ar), 7.37–7.40 (m, 4H, Ar), 7.57 (d, ^3J = 1.6 Hz, 1H, NH), 7.61–7.63 (m, 2H, Ar), 7.80–7.83 (m, 2H, Ar).

^{13}C NMR (DMSO-d$_6$, 150 MHz) δ = 39.6 (CH$_2$), 60.8 (CH), 70.2 (C), 120.5 (CN), 126.1 (2×CH), 127.4 (CH), 128.2 (C), 128.6 (2×CH), 128.7 (2×CH), 128.9 (2×CH), 135.2 (C), 143.7 (C), 160.0 (C).

HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{17}H_{14}ClN_2^+$ 281.0840; Found 281.0844.

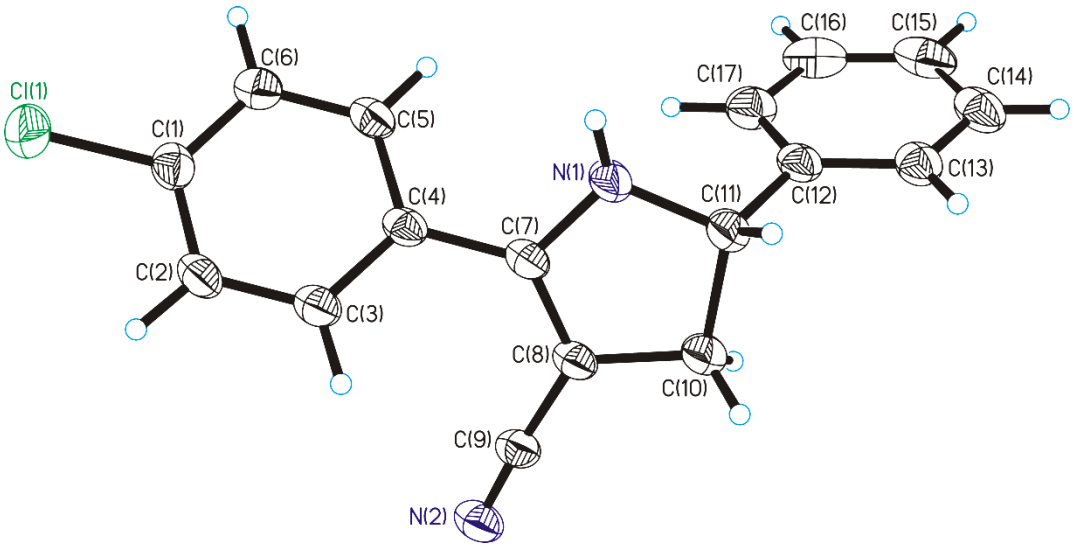
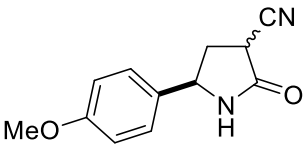


Figure S4. Molecular structure from single crystal X-ray study of **8** (thermal ellipsoids are drawn at the 50% probability level); CCDC 1852202.

5-(4-Methoxyphenyl)-2-oxopyrrolidine-3-carbonitrile (5b)



Mixture of azide **1g** (0.300 g, 1.09 mmol) and Pd/C 10% (0.044 g) in MeOH (11 mL) was stirred in a sealed reactor under H$_2$ (2 atm) at room temperature for 12 h. Resulting mixture was filtrated and concentrated under reduced pressure. Residue was purified by column chromatography on silica gel. Yield 0.137 g (58%); dr **A**:**B** 61:39; colorless crystals, mp 164–165 °C; R_f = 0.64 (ethyl acetate).

A: ^{1}H NMR (CD_2Cl_2, 600 MHz) δ = 2.23 (ddd, ^2J = 13.0, ^3J = 11.2, ^3J = 9.0 Hz, 1H, CH_2), 2.90 (dddd, ^2J = 13.0, ^3J = 8.8, ^3J = 6.5, ^5J = 0.8 Hz, 1H, CH_2), 3.63 (dd, ^3J = 11.2, ^3J = 8.8 Hz, 1H, C^3H), 3.80 (s, 3H, CH_3O), 4.68 (dd, ^3J = 9.0, ^3J = 6.5 Hz, 1H, C^5H), 6.58 (br.s, 1H, NH), 6.91–6.94 (m, 2H, Ar), 7.25–7.27 (m, 2H, Ar).

^{13}C NMR (CD_2Cl_2, 150 MHz) δ = 34.6 (C^3H), 37.0 (CH_2), 55.9 (CH_3O), 56.7 (C^5H), 114.9 (2×CH), 117.45 (CN), 127.9 (2×CH), 132.0 (C), 160.5 (C), 169.3 (C=O).

B: ^{1}H NMR (CD_2Cl_2, 600 MHz) δ = 2.36 (ddd, ^2J = 13.2, ^3J = 9.2, ^3J = 4.8 Hz, 1H, CH_2), 2.84 (ddd, ^2J = 13.2, ^3J = 7.8, ^3J = 7.4 Hz, 1H, CH_2), 3.61 (ddd, ^3J = 9.3, ^3J = 7.3, ^4J = 0.5 Hz, 1H, C^3H), 3.79 (s, 3H, CH_3O), 4.88 (dd, ^3J = 7.8, ^3J = 4.8 Hz, 1H, C^5H), 6.69 (br.s, 1H, NH), 6.90–6.93 (m, 2H, Ar), 7.17–7.20 (m, 2H, Ar).

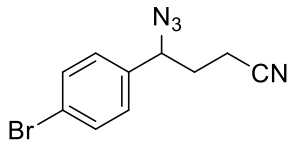
^{13}C NMR (CD_2Cl_2, 150 MHz) δ = 33.1 (C^3H), 36.2 (CH_2), 55.9 (CH_3O), 56.2 (C^5H), 115.0 (2×CH), 117.54 (CN), 127.3 (2×CH), 132.7 (C), 160.3 (C), 169.5 (C=O).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{13}N_2O_2^+$ 217.0972; Found 217.0970.

Synthesis of *γ*-Azidobutyronitriles 9 *via* Krapcho Dealkoxycarbonylation

Mixture of azide **1** (1 mmol), LiCl (0.255 g, 6 mmol), water (0.108 mL, 6 mmol) in DMF (0.5 M) was stirred under reflux for 5 h. The residue was diluted with DCM (50 mL), washed with water (3×20 mL) and brine (20 mL), then dried with Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether – ethyl acetate).

4-Azido-4-(4-bromophenyl)butyronitrile (9a)



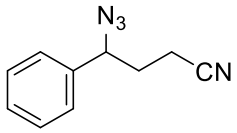
9a was obtained from azide **1f** (0.342 g, 1.06 mmol). Yield 0.072 g (26%); yellowish oil; R_f = 0.68 (petroleum ether – ethyl acetate 2:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.99 (dddd, ^2J = 14.0, ^3J = 7.8, ^3J = 7.1, ^3J = 5.6 Hz, 1H, CH_2), 2.07 (dddd, ^2J = 14.0, ^3J = 9.0, ^3J = 7.2, ^3J = 6.1 Hz, 1H, CH_2), 2.38 (ddd, ^2J = 17.1, ^3J = 7.1, ^3J = 6.1 Hz, 1H, CH_2), 2.50 (ddd, ^2J = 17.1, ^3J = 7.8, ^3J = 7.2 Hz, 1H, CH_2), 4.61 (dd, ^3J = 9.0, ^3J = 5.6 Hz, 1H, CH), 7.20–7.23 (m, 2H, Ar), 7.55–7.57 (m, 2H, Ar).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 14.2 (CH_2), 31.9 (CH_2), 63.6 (CH), 118.5 (CN), 122.9 (C), 128.4 (2×CH), 132.3 (2×CH), 136.8 (C).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{10}H_{10}BrN_4^+$ 265.0083; Found 265.0082.

4-Azido-4-phenylbutyronitrile (9b)



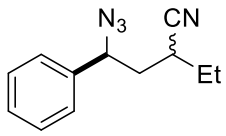
9b was obtained from azide **1a** (1.142 g, 4.68 mmol). Yield 0.358 g (41%); yellowish oil; R_f = 0.56 (petroleum ether – ethyl acetate 4:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.03 (dddd, ^2J = 13.5, ^3J = 7.7, ^3J = 7.5, ^3J = 5.8 Hz, 1H, CH_2), 2.10 (dddd, ^2J = 13.5, ^3J = 8.8, ^3J = 7.4, ^3J = 6.2 Hz, 1H, CH_2), 2.37 (ddd, ^2J = 17.1, ^3J = 7.5, ^3J = 6.2 Hz, 1H, CH_2), 2.47 (ddd, ^2J = 17.1, ^3J = 7.7, ^3J = 7.4 Hz, 1H, CH_2), 4.64 (dd, ^3J = 8.8, ^3J = 5.8 Hz, 1H, CH), 7.32–7.34 (m, 2H, Ph), 7.37–7.40 (m, 1H, Ph), 7.42–7.45 (m, 2H, Ph).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 14.1 (CH_2), 31.8 (CH_2), 64.2 (CH), 118.6 (CN), 126.7 (2×CH), 128.8 (CH), 129.0 (2×CH), 137.6 (C).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{10}H_{11}N_4^+$ 187.0978; Found 187.0971.

4-Azido-2-ethyl-4-phenylbutyronitrile (9c)



To a cold (ice-water bath) stirred solution of **1a** (1.47 g, 6.0 mmol) in dry DMF (6 mL) NaH (0.27 g, 6.6 mmol, 60% suspension in oil) was added under argon. Cooling bath was removed. After 20 min at ambient temperature, a solution of ethyl bromide (0.49 mL, 6.6 mmol) in dry DMF (6 mL) was added dropwise and resulting mixture was stirred for additional 3 h. Then NH_4Cl (0.10 g, 1.9 mmol), LiCl (0.70 g, 16.5 mmol) and water (0.7–0.8 mL) were sequentially added. The resulting mixture was stirred at 135 °C for 8 h, then cooled off, diluted with water and extracted with ethyl acetate. Combined organic fractions were washed with brine (3 times), dried with Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel. Yield 0.76 g (59%); dr **A**:**B** 54:46; colorless oil; R_f = 0.74 (petroleum ether – ethyl acetate 4:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.06 (t, ^3J = 7.5 Hz, 3H, CH_3, **B**), 1.12 (t, ^3J = 7.5 Hz, 3H, CH_3, **A**), 1.62–1.70 (m, 4H), 1.88–1.95 (m, 3H), 2.19 (ddd, ^2J = 13.7, ^3J = 9.8, ^3J = 6.6 Hz, 1H, CH_2, **B**), 2.27–2.32 (m, 1H, CH_2, **B**), 2.85 (ddd, ^2J = 13.9, ^3J = 9.6, ^3J = 6.0 Hz, 1H, CH_2, **A**), 4.67 (m, ^3J = 8.9, ^3J = 6.6, Hz, 1H, CH, **B**), 4.74–4.76 (m, 1H, CH, **A**), 7.34–7.45 (m, 10H, Ph).

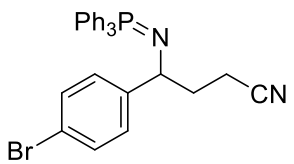
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 11.2 (CH_3), 11.4 (CH_3), 25.2 (CH_2), 25.6 (CH_2), 30.1 (CH), 30.7 (CH), 38.0 (CH_2), 39.0 (CH_2), 63.6 (CH), 64.0 (CH), 121.0 (CN), 121.1 (CN), 126.7 (2×CH), 127.0 (2×CH), 128.8 (CH), 129.0 (CH), 129.1 (2×CH), 129.2 (2×CH), 137.6 (C), 138.5 (C).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{15}N_4^+$ 215.1291; Found 215.1294.

Synthesis of Iminophosphazenes 10[24]

To a stirred 0.5 M solution of azide **1** (1 equiv) in DCM PPh_3 or PBu_3 (1.05 equiv) was added in one portion. Resulting solution was stirred at ambient temperature for 3 h and concentrated under reduced pressure. Iminophosphazenes **10** undergo rapid degradation on SiO_2.

4-(4-Bromophenyl)-4-[(triphenyl-λ^5-phosphanylidene)amino]butanenitrile (10a)



10a was obtained from azide **9a** (0.070 g, 0.26 mmol). Yield > 95% (according to ^{1}H NMR); yellow oil.

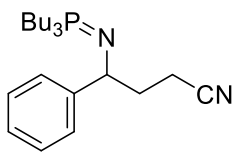
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 1.87–1.93 (m, 1H, C^3H_2), 1.98-2.05 (m, 1H, C^3H_2), 2.31 (ddd, ^2J = 16.7, ^3J = 8.0, ^3J = 5.8 Hz, 1H, C^2H_2), 2.54 (ddd, ^2J = 16.7, ^3J = 8.4, ^3J = 7.0 Hz, 1H, C^2H_2), 4.21 (ddd, $^3J_{HP}$ = 19.7, ^3J = 7.8, ^3J = 4.8 Hz, 1H, C^4H), 7.16–7.18 (m, 2H, Ar), 7.26–7.28 (m, 2H, Ar), 7.38–7.41 (m, 6H, PPh_3), 7.47–7.50 (m, 3H, PPh_3), 7.54–7.58 (m, 6H, PPh_3).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 13.9 (CH_2), 37.8 ($^3J_{CP}$ = 20 Hz, C^3H_2), 57.3 (CH), 119.5 (C), 120.6 (C), 128.3 ($^2J_{CP}$ = 11 Hz, 6×CH), 128.6 (2×CH), 130.8 (2×CH), 131.2 ($^4J_{CP}$ = 3 Hz, 3×CH), 131.5 ($^1J_{CP}$ = 97 Hz, 3×C), 132.3 ($^3J_{CP}$ = 9 Hz, 6×CH), 146.9 ($^3J_{CP}$ = 6 Hz, C).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 9.9.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{28}H_{25}BrN_2P^+$ 499.0933; Found 499.0922.

4-Phenyl-4-[(tributyl-λ^5-phosphanylidene)amino]butanenitrile (10b)



10b was obtained from azide **9b** (0.150 g, 0.81 mmol). Yield 0.034 g (12%); yellow oil; R_f = 0.16 (ethyl acetate – methanol 10:1).

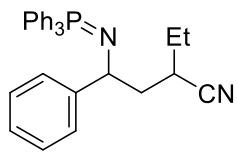
^{1}H NMR ($CDCl_3$, 600 MHz) δ = 0.87–0.90 (m, 9H, CH_3, PBu_3), 1.31–1.38 (m, 6H, CH_2, PBu_3), 1.38–1.46 (m, 6H, CH_2, PBu_3), 1.95–2.04 (m, 6H, CH_2, PBu_3), 2.06–2.12 (m, 1H, C^3H_2), 2.38 (ddd, ^2J = 17.5, ^3J = 5.3, ^3J = 5.0 Hz, 1H, C^3H_2), 2.53–2.59 (m, 1H, C^2H_2), 3.03 (ddd, ^2J = 17.4, ^3J = 10.3, ^3J = 5.0 Hz, 1H, C^2H_2), 4.07–4.13 (m, 1H, CH), 7.31–7.34 (m, 1H, Ph), 7.37–7.41 (m, 2H, Ph), 7.58–7.61 (m, 2H, Ph).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 13.3 (3×CH_3), 15.0 (CH_2), 21.8 ($^1J_{CP}$ = 58 Hz, 3×CH_2), 23.0 ($^2J_{CP}$ = 4 Hz, 3×CH_2), 23.7 ($^3J_{CP}$ = 16 Hz, 3×CH_2), 33.3 ($^3J_{CP}$ = 11 Hz, CH_2), 56.0 (CH), 119.5 (CN), 126.8 (2×CH), 128.6 (CH), 129.3 (2×CH), 142.4 (C).

^{31}P NMR ($CDCl_3$, 162 MHz) δ = 56.1.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{38}N_2P^+$ 361.2767; Found 361.2770.

2-Ethyl-4-phenyl-4-[(triphenyl-λ^5-phosphanylidene)amino]butanenitrile (10c)



10c was obtained from azide **9c** (0.110 g, 0.51 mmol). Yield > 95% (according to ^{1}H NMR); dr **A**:**B** 54:46; colorless oil.

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 0.90 (t, ^3J = 7.5 Hz, 3H, CH_3, **B**), 1.07 (t, ^3J = 7.5 Hz, 3H, CH_3, **A**), 1.29–1.39 (m, 2H, CH_2, **B**), 1.57–1.70 (m, 2H, CH_2, **A**), 1.87–1.94 (m, 1H+1H, C^3H_2, **A**, **B**), 2.02 (ddd, ^2J = 13.2, ^3J = 10.7, ^3J = 4.1 Hz, 1H, C^3H_2, **A**), 2.17 (ddd, ^2J = 13.4, ^3J = 8.2, ^3J = 7.2 Hz, 1H, C^3H_2, **B**), 2.44–2.49 (m, 1H, C^2H, **B**), 3.19 (dddd, ^3J = 11.0, ^3J = 8.9, ^3J = 5.2, ^3J = 4.1 Hz, 1H, C^2H, **A**), 4.20 (ddd, $^3J_{PH}$ = 20.7, ^3J = 7.3, ^3J = 7.2 Hz, 1H, C^4H, **B**), 4.31 (ddd, $^3J_{PH}$ = 18.2, ^3J = 10.7, ^3J = 3.2 Hz, 1H, C^4H, **A**), 7.07–7.10 (m, 1H, Ph, **A**), 7.11–7.16 (m, 2H+1H, Ph, **A**, **B**), 7.19–7.21 (m, 2H, Ph, **B**), 7.27–7.28 (m, 2H, Ph, **A**), 7.33–7.35 (m, 2H, Ph, **B**), 7.36–7.40 (m, 6H+6H, PPh_3, **A**, **B**), 7.44–7.48 (m, 3H+3H, PPh_3, **A**, **B**), 7.57–7.61 (m, 6H+6H, PPh_3, **A**, **B**).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 11.2 (CH_3), 11.5 (CH_3), 24.5 (CH_2), 25.8 (CH_2), 30.0 (C^2H), 30.9 (C^2H), 44.5 ($^3J_{CP}$ = 19 Hz, C^3H_2), 44.2 ($^3J_{CP}$ = 22 Hz, C^3H_2), 57.0 ($^2J_{CP}$ = 2 Hz, C^4H), 57.6 ($^2J_{CP}$ = 2 Hz, C^4H), 122.7 (CN), 122.8 (CN), 125.8 (CH), 126.0 (CH), 126.6 (2×CH), 126.8 (2×CH), 127.7 (2×CH), 127.9 (2×CH), 128.0 ($^2J_{CP}$ = 11 Hz, 6×CH), 128.1 ($^2J_{CP}$ = 11 Hz, 6×CH), 130.9 ($^4J_{CP}$ = 2 Hz, 3×CH), 131.0 ($^4J_{CP}$ = 2 Hz, 3×CH), 131.53 ($^1J_{CP}$ = 96 Hz, 3×C), 131.54 ($^1J_{CP}$ = 96 Hz, 3×C), 132.3 ($^3J_{CP}$ = 9 Hz, 6×CH), 132.4 ($^3J_{CP}$ = 9 Hz, 6×CH), 147.8 ($^3J_{CP}$ = 6 Hz, C), 148.5 ($^3J_{CP}$ = 3 Hz, C).

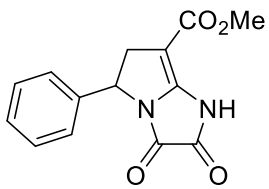
^{31}P NMR ($CDCl_3$, 162 MHz) δ = 9.8, 10.4.

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{30}H_{30}N_2P^+$ 449.2141; Found 449.2147.

Synthesis of Pyrrolo[1,2-*a*]imidazoles 11

Solution of iminophosphazene **3** (1.77 mmol) in DCM (9 mL) was added dropwise to a stirred solution of oxalyl chloride (0.167 mL, 1.95 mmol) in DCM (9 mL) at 0 °C. Resulting mixture was heated under reflux for 30 min, cooled down to ambient temperature and allowed to stay under this conditions for 48 h before precipitate was collected by vacuum filtration.

Methyl 2,3-dioxo-5-phenyl-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11a)



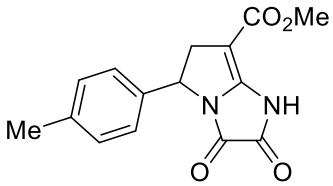
11a was synthesized from iminophosphazene **3a** (2.00 g, 4.18 mmol). Yield 0.737 g (65%); white solid, mp 245–246 °C (with decomposition).

^{1}H NMR (DMSO-d_6, 600 MHz) δ = 2.66 (dd, ^2J = 15.4, ^3J = 4.9 Hz, 1H, CH_2), 3.52 (dd, ^2J = 15.4, ^3J = 9.5 Hz, 1H, CH_2), 3.67 (s, 3H, OCH_3), 5.38 (dd, ^3J = 4.9, ^3J = 9.5 Hz, 1H, CH), 7.29–7.31 (m, 1H, Ph), 7.33–7.37 (m, 4H, Ph), 12.46 (s, 1H, NH).

^{13}C NMR (DMSO-d_6, 150 MHz) δ = 40.3 ($^1J_{CH}$ = 137 Hz, CH_2), 51.4 ($^1J_{CH}$ = 147 Hz, OCH_3), 57.7 ($^1J_{CH}$ = 149 Hz, CH), 89.2 (C^7), 126.3 ($^1J_{CH}$ = 159 Hz, 2×CH, Ph), 128.2 ($^1J_{CH}$ = 161 Hz, CH, Ph), 129.0 ($^1J_{CH}$ = 161 Hz, 2×CH, Ph), 139.4 (C, Ph), 144.1 (C^8), 153.2 (CO), 161.7 (CO), 163.9 (CO).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{13}N_2O_4^+$ 273.0870; Found 273.0871.

Methyl 2,3-dioxo-5-(*p*-tolyl)-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11b)



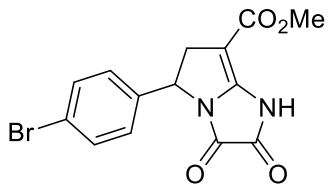
11b was synthesized from iminophosphazene **3b** (0.820 g, 1.66 mmol). Yield 0.276 g (58%); white solid, mp 220–221 °C (with decomposition).

^{1}H NMR (DMSO-d$_6$, 600 MHz) δ = 2.29 (s, 3H, CH$_3$), 2.65 (dd, ^2J = 15.4, ^3J = 4.9 Hz, 1H, CH$_2$), 3.49 (dd, ^2J = 15.4, ^3J = 9.5 Hz, 1H, CH$_2$), 3.68 (s, 3H, OCH$_3$), 5.34 (dd, ^3J = 9.5, ^3J = 4.9 Hz, 1H, CH), 7.17 (d, ^3J = 8.1 Hz, 2H, Ar), 7.24 (d, ^3J = 8.1 Hz, 2H, Ar), 12.41 (s, 1H, NH).

^{13}C NMR (DMSO-d$_6$, 150 MHz) δ = 20.7 ($^1J_{CH}$ = 127 Hz, CH$_3$), 40.1 ($^1J_{CH}$ = 140 Hz, CH$_2$), 51.1 ($^1J_{CH}$ = 147 Hz, OCH$_3$), 57.4 ($^1J_{CH}$ = 148 Hz, CH), 88.8 (C^7), 126.1 ($^1J_{CH}$ = 159 Hz, 2×CH), 129.3 ($^1J_{CH}$ = 158 Hz, 2×CH), 136.3 (C), 137.3 (C), 144.0 (C^8), 152.9 (CO), 161.5 (CO), 163.6 (CO).

HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{15}H_{15}N_2O_4^+$ 287.1026; Found 287.1026.

Methyl 5-(4-bromophenyl)-2,3-dioxo-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11c)



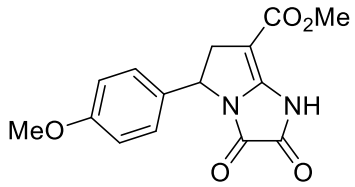
11c was synthesized from iminophosphazene **3f** (0.962 g, 1.73 mmol). Yield 0.473 g (78%); white solid, mp 250–251 °C (with decomposition).

^{1}H NMR (DMSO-d$_6$, 600 MHz) δ = 2.66 (dd, ^2J = 15.4, ^3J = 5.1 Hz, 1H, CH$_2$), 3.50 (dd, ^2J = 15.4, ^3J = 9.5 Hz, 1H, CH$_2$), 3.68 (s, 3H, OCH$_3$), 5.38 (dd, ^3J = 9.5, ^3J = 5.1 Hz, 1H, CH), 7.36 (d, ^3J = 8.4 Hz, 2H, Ar), 7.56 (d, ^3J = 8.4 Hz, 2H, Ar), 12.41 (s, 1H, NH).

^{13}C NMR (DMSO-d$_6$, 150 MHz) δ = 39.9 ($^1J_{CH}$ = 138 Hz, CH$_2$), 51.1 ($^1J_{CH}$ = 147 Hz, CH$_3$), 56.9 ($^1J_{CH}$ = 150 Hz, CH), 88.6 (C^7), 121.1 (C), 128.5 ($^1J_{CH}$ = 161 Hz, 2×CH), 131.6 ($^1J_{CH}$ = 166 Hz, 2×CH), 138.6 (C), 144.0 (C^8), 153.0 (CO), 161.4 (CO), 163.5 (CO).

HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{14}H_{12}BrN_2O_4^+$ 350.9975; Found 350.9955.

Methyl 5-(4-methoxyphenyl)-2,3-dioxo-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11d)



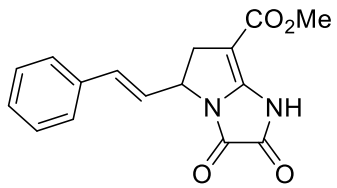
11d was synthesized from iminophosphazene **3g** (0.900 g, 1.77 mmol). Yield 0.339 g (63%); white solid, mp 210–211 °C (with decomposition).

^{1}H NMR (DMSO-d$_6$, 600 MHz) δ = 2.66 (dd, ^2J = 15.4, ^3J = 4.9 Hz, 1H, CH$_2$), 3.46 (dd, ^2J = 15.4, ^3J = 9.4 Hz, 1H, CH$_2$), 3.68 (s, 3H, OCH$_3$), 3.74 (s, 3H, OCH$_3$), 5.33 (dd, ^3J = 9.4, ^3J = 4.9 Hz, 1H, CH), 6.91 (d, ^3J = 8.8 Hz, 2H, Ar), 7.29 (d, ^3J = 8.8 Hz, 2H, Ar), 12.39 (s, 1H, NH).

^{13}C NMR (DMSO-d$_6$, 150 MHz) δ = 40.1 (CH$_2$), 51.0 (OCH$_3$), 55.1 (OCH$_3$), 57.1 (CH), 88.8 (C^7), 114.1 (2×CH**)**, 127.5 (2×CH), 131.1 (C), 143.9 (C^8), 152.9 (CO), 159.0 (C), 161.5 (CO), 163.6 (CO).

HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{15}H_{15}N_2O_5^+$ 303.0975; Found 303.0976.

Methyl (*E*)-2,3-dioxo-5-styryl-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11e)



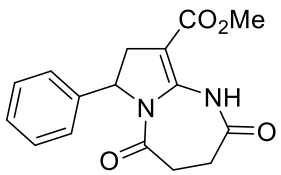
11e was synthesized from iminophosphazene **3n** (0.900 g, 1.78 mmol). Yield 0.112 g (21%); white solid, mp 181–182 °C (with decomposition).

^{1}H NMR (DMSO-d$_6$, 600 MHz) δ = 2.74 (dd, ^2J = 15.4, ^3J = 4.5 Hz, 1H, CH$_2$), 3.30 (dd, ^2J = 15.4, ^3J = 9.3 Hz, 1H, CH$_2$), 3.68 (s, 3H, CH$_3$), 5.01 (ddd, ^3J = 9.3, ^3J = 7.6, ^3J = 4.5 Hz, 1H, C^{5}H), 6.36 (dd, ^3J = 15.9, ^3J = 7.6 Hz, 1H, CH), 6.70 (d, ^3J = 15.9 Hz, 1H, CH), 7.25–7.28 (m, 1H, Ph), 7.33–7.35 (m, 2H, Ph), 7.45–7.46 (m, 2H, Ph), 12.33 (s, 1H, NH).

^{13}C NMR (DMSO-d$_6$, 150 MHz) δ = 37.1 (CH$_2$), 51.0 (OCH$_3$), 56.4 (CH), 89.0 (C^7), 126.3 (CH), 126.6 (2×CH, Ph**)**, 128.0 (CH, Ph), 128.6 (2×CH, Ph), 131.8 (CH), 135.8 (C, Ph), 143.8 (C^8), 153.2 (CO), 161.5 (CO), 163.6 (CO).

HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{16}H_{15}N_2O_4^+$ 299.1026; Found 299.1027.

Methyl 2,5-dioxo-7-phenyl-2,3,4,5,7,8-hexahydro-1*H*-pyrrolo[1,2-*a*][1,3]diazepine-9-carboxylate (12a)



Solution of iminophosphazene **3a** (0.500 g, 1.05 mmol) in DCE (5 mL) was added dropwise to a stirred solution of succinyl chloride (0.177 g, 1.26 mmol) in DCE (5 mL) at 0 °C. Resulting mixture was heated under reflux for 3.5 h, allowed to cool down to ambient temperature and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel. Yield 0.114 g (36%); colorless solid; R_f = 0.44 (petroleum ether – ethyl acetate 1:1).

^{1}H NMR (DMSO-d$_6$, 600 MHz) δ = 2.35 (dd, ^2J = 14.8, ^3J = 3.5 Hz, 1H, CH$_2$), 2.63–2.71 (m, 2H, CH$_2$), 2.98–3.07 (m, 2H, CH$_2$), 3.26 (dd, ^2J = 14.8, ^3J = 10.9 Hz, 1H, CH$_2$), 3.66 (s, 3H, CH$_3$O), 5.55 (dd, ^3J = 10.9, ^3J = 3.5 Hz, 1H, CH), 7.24–7.27 (m, 1H, Ph), 7.30–7.35 (m, 4H, Ph), 10.53 (s, 1H, NH).

^{13}C NMR (DMSO-d$_6$, 150 MHz) δ = 30.4 (CH$_2$), 30.8 (CH$_2$), 33.3 (CH$_2$), 51.3 (CH$_3$O), 59.9 (CH), 86.7 (C^7), 125.0 (2×CH), 127.3 (CH), 128.7 (2×CH), 142.7 (C), 145.7 (C^8), 167.5 (CO), 169.0 (CO), 170.4 (CO).

HRMS (ESI) *m/z*: [M + H]$^+$ Calcd for $C_{16}H_{17}N_2O_4^+$ 301.1183; Found 301.1188.

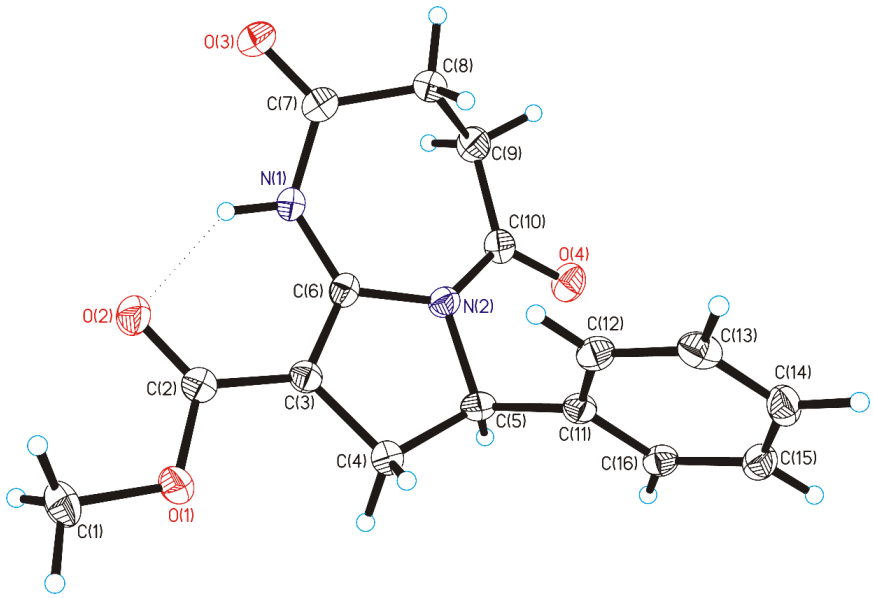
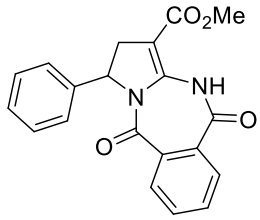


Figure S5. Molecular structure from single crystal X-ray study of **12a** (thermal ellipsoids are drawn at the 50% probability level); CCDC 1852209.

Synthesis of Pyrrolo[1,2-*b*][2,4]benzodiazepines 12b,c

To a solution of iminophosphazene **3** (1.77 mmol) in DCM (3 mL) at 0 °C a solution of *ortho*-phthaloyl chloride (0.281 mL, 1.95 mmol) in DCM (1.5 mL) was added dropwise. The resulting mixture was heated under reflux for 1 h, allowed to cool down to ambient temperature and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether – ethyl acetate).

Methyl 5,10-dioxo-1-phenyl-2,4,5,10-tetrahydro-1*H*-pyrrolo[1,2-*b*][2,4]benzodiazepine-3-carboxylate (12b)



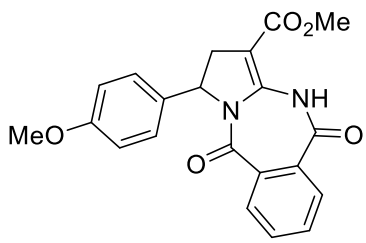
12b was synthesized from iminophosphazene **3a** (1.000 g, 2.09 mmol). Yield 0.229 g (31%); yellow solid, mp 208–209 °C (with decomposition); R_f = 0.73 (petroleum ether – ethyl acetate 1:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.70 (dd, ^2J = 15.0, ^3J = 3.5 Hz, 1H, CH_2), 3.36 (dd, ^2J = 15.0, ^3J = 10.6 Hz, 1H, CH_2), 3.78 (s, 3H, CH_3O), 3.79 (s, 3H, CH_3O), 5.78 (dd, ^3J = 10.6, ^3J = 3.5 Hz, 1H, CH), 7.26–7.29 (m, 1H, Ph), 7.34–7.36 (m, 4H, Ph), 7.64–7.69 (m, 2H, Ar), 8.31–8.34 (m, 1H, Ar), 8.43–8.46 (m, 1H, Ar), 11.27 (s, 1H, NH).

^{13}C NMR ($CDCl_3$, 150 MHz) δ = 33.0 (CH_2), 51.4 (CH_3O), 63.6 (CH), 87.8 (C^7), 125.3 (2×CH), 127.8 (CH), 128.2 (C), 128.8 (2×CH), 129.4 (C), 132.6 (CH), 132.8 (CH), 133.1 (CH), 133.5 (CH), 141.8 (C), 143.8 (C^8), 161.7 (CO), 162.2 (CO), 167.7 (CO).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{17}N_2O_4^+$ 349.1183; Found 349.1178.

Methyl 1-(4-methoxyphenyl)-5,10-dioxo-2,4,5,10-tetrahydro-1*H*-pyrrolo[1,2-*b*][2,4]benzo-diazepine-3-carboxylate (12c)



12c was synthesized from iminophosphazene **3g** (0.800 g, 1.57 mmol). Yield 0.190 g (32%); yellow solid, mp 132–133 °C (with decomposition); R_f = 0.46 (petroleum ether – ethyl acetate 1:1).

^{1}H NMR ($CDCl_3$, 400 MHz) δ = 2.70 (dd, ^{2}J = 15.0, ^{3}J = 3.4 Hz, 1H, CH_2), 3.33 (dd, ^{2}J = 15.0, ^{3}J = 10.5 Hz, 1H, CH_2), 3.78 (s, 3H, CH_3O), 3.79 (s, 3H, CH_3O), 5.74 (dd, ^{3}J = 10.5, ^{3}J = 3.4 Hz, 1H, CH), 6.85–6.89 (m, 2H, Ar), 7.28–7.32 (m, 2H, Ar), 7.63–7.70 (m, 2H, Ar), 8.31–8.35 (m, 1H, Ar), 8.41–8.46 (m, 1H, Ar), 11.26 (s, 1H, NH).

^{13}C NMR ($CDCl_3$, 100 MHz) δ = 33.1 (CH_2), 51.5 (CH_3O), 55.2 (CH_3O), 63.2 (CH), 87.9 (C^7), 114.2 (2×CH), 126.9 (2×CH), 128.2 (C), 129.5 (C), 132.6 (CH), 132.8 (CH), 133.1 (CH), 133.5 (CH), 134.0 (C), 143.8 (C^8), 159.2 (C), 161.7 (CO), 162.2 (CO), 167.8 (CO).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{19}N_2O_5^+$ 379.1288; Found 379.1297.

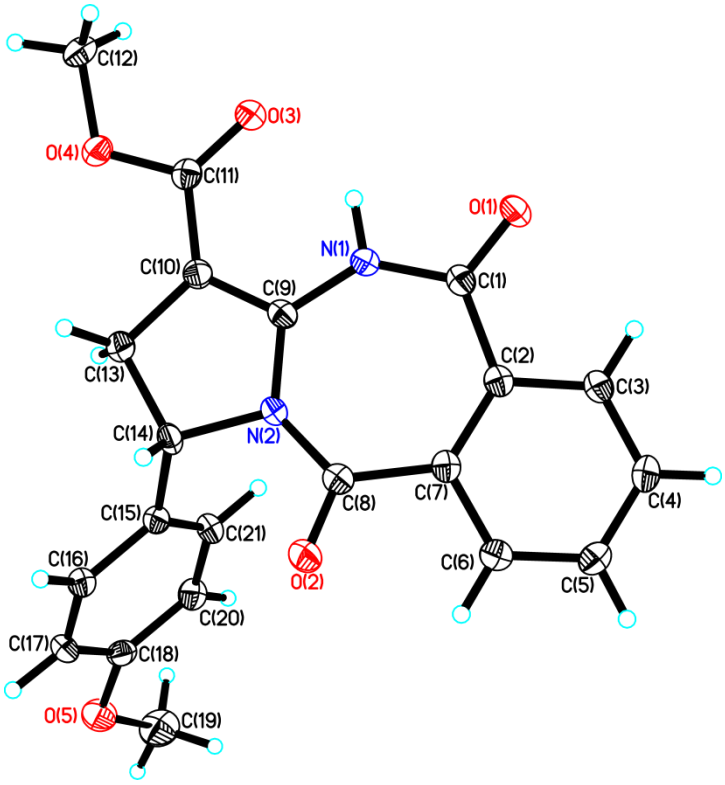
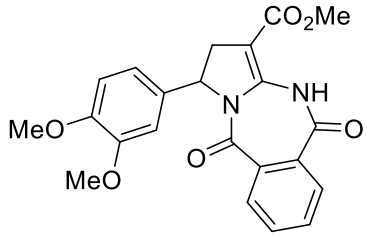


Figure S6. Molecular structure from single crystal X-ray study of **12c** (thermal ellipsoids are drawn at the 50% probability level); CCDC 1838688.

Methyl 1-(3,4-dimethoxyphenyl)-5,10-dioxo-2,4,5,10-tetrahydro-1*H*-pyrrolo[1,2-*b*][2,4]benzo-diazepine-3-carboxylate (12d)



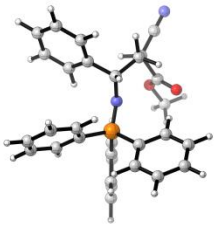
12d was synthesized from iminophosphazene **3i** (0.200 g, 0.37 mmol). Yield 0.044 g (29%); yellow solid, mp 204–205 °C (with decomposition); R_f = 0.62 (petroleum ether – ethyl acetate 1:1).

^{1}H NMR ($CDCl_3$, 600 MHz) δ = 2.70 (dd, ^2J = 15.0, ^3J = 3.6 Hz, 1H, CH_2), 3.34 (dd, ^2J = 15.0, ^3J = 10.6 Hz, 1H, CH_2), 3.78 (s, 3H, CH_3O), 3.84 (s, 3H, CH_3O), 3.87 (s, 3H, CH_3O), 5.73 (dd, ^3J = 10.5, ^3J = 3.6 Hz, 1H, CH), 6.81 (d, ^3J = 8.3 Hz, 1H, Ar), 6.87 (d, ^4J = 1.9 Hz, 1H, Ar), 6.89 (dd, ^3J = 8.3, ^4J = 1.9 Hz, 1H, Ar), 7.64–7.69 (m, 2H, Ar), 8.32–8.34 (m, 1H, Ar), 8.43–8.44 (m, 1H, Ar), 11.26 (s, 1H, NH).

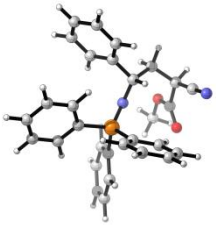
^{13}C NMR ($CDCl_3$, 150 MHz) δ = 33.1 (CH_2), 51.4 (CH_3O), 55.8 (CH_3O), 55.9 (CH_3O), 63.4 (CH), 87.8 (C^7), 109.1 (CH), 111.3 (CH), 117.4 (CH), 128.2 (C), 129.5 (C), 132.6 (CH), 132.8 (CH), 133.1 (CH), 133.5 (CH), 134.5 (C), 143.8 (C^8), 148.7 (C), 149.2 (C), 161.8 (CO), 162.2 (CO), 167.8 (CO).

HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{21}N_2O_6^+$ 409.1394; Found 409.1396.

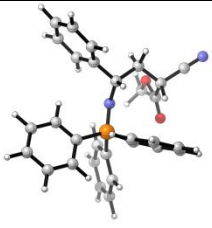
Results of DFT Calculations



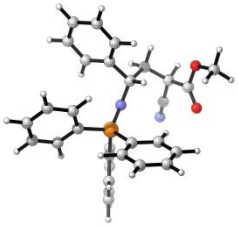
2a_i1: 0 (0)	**2a**_i2: 0.3	**2a**_i3: 0.8	**2a**_i4: 1.0



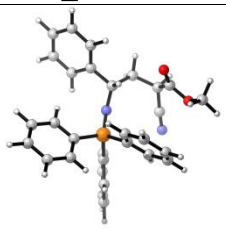
2a_i5: 1.3 (1.7)	**2a**_i6: 1.5	**2a**_i7: 1.5	**2a**_i8: 1.6



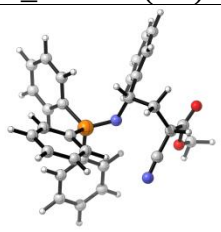
2a_i9: 2.0	**2a**_i10: 2.2	**2a**_i11: 2.4	**2a**_i12: 2.4 (4.3)



2a_i13: 2.7	**2a**_i14: 2.8	**2a**_i15: 2.9	**2a**_i16: 3.3



2a_i17: 3.3 (4.6)	**2a**_i18: 4.4	**2a**_i19: 4.6	**2a**_i20: 5.1



2a_i21: 5.8	**2a**_i22: 7.0

Figure S7. Selected isomers of phosphazene **2a**. Single point energies ΔE (and free energies ΔG_{298}) are given in kcal/mol relative to **2a**_i1.

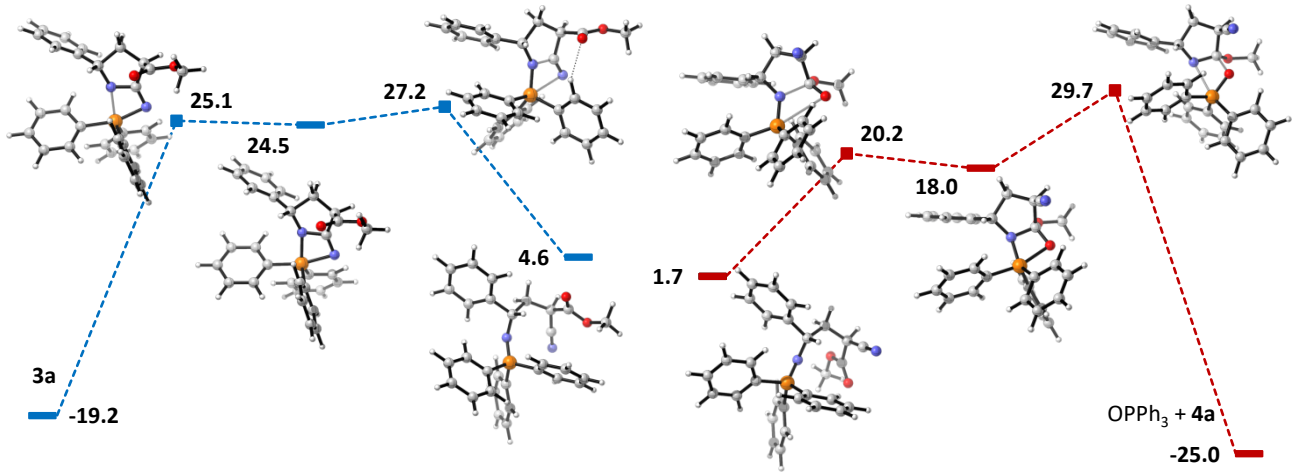
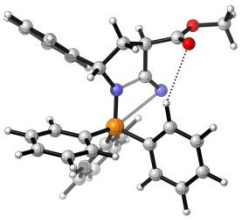
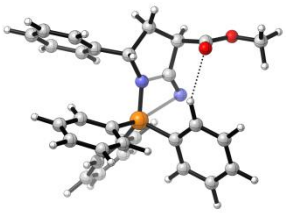
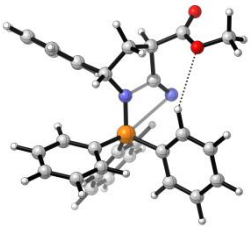
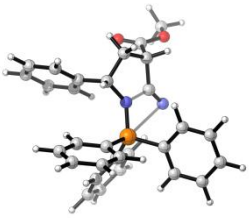
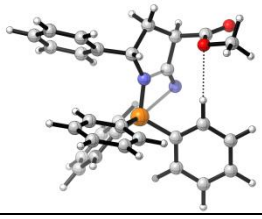
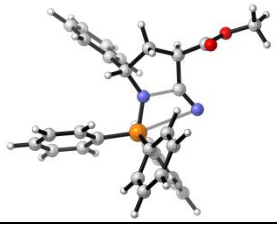
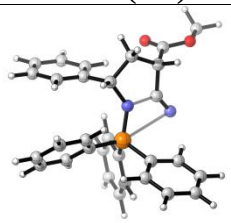
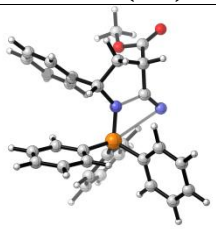


Figure S8. Key stationary points in *aza*-Wittig reactions for **2a**_i5 (red) and **2a**_i17 (blue) (ΔG_{298}, kcal/mol, relative to **2a**_i1). Geometries of **3a** and **4a** correspond to the conformers with the lowest relative energies (not to the reacting conformers).

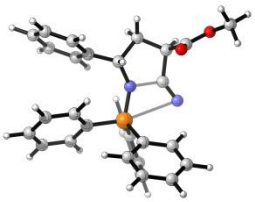
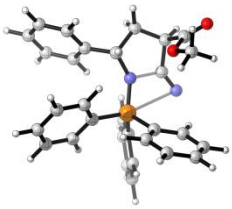
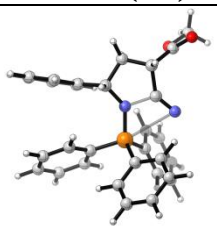
After preliminary geometry optimization for various conformers of **2a** (Figure S7), we chose two (**2a**_i5 and **2a**_i17) for further investigation. These are the reacting conformers in two different modes of intramolecular *aza*-Wittig reactions. For these conformers, we successfully calculated two sets of key stationary points that reflected the interaction of the phosphazene moiety with CN or CO_2Me groups, leading to **3a** or **4a**, respectively (Figure S8). Both energy diagrams qualitatively agree with the classical *aza*-Wittig reaction between phosphazene and aldehydes, including the formation of four-membered ring intermediates.[25–28] According to the obtained diagrams, both reactions proceed under kinetic control. Meanwhile, the rate-determining steps are different for these reactions, corresponding to [2+2]-cycloaddition *via* **TS1** for the CN-mode or [2+2]-cycloreversion *via* **TS2** for the CO-mode. Relying upon these results, we localized several isomeric **TS1** and **TS2** that differ in relative orientations of phenyl and EWG (*cis* and *trans* locations in isomers, axial and equatorial locations in conformers), as well as the relative orientations of the phenyl groups at the phosphorus atom (Figure S9). As a result, we determined **2a**_i12_TS1 and **2a**_i1_TS2 with the lowest relative ΔG_{298}. The energy diagrams for both *aza*-Wittig reactions of **2a** corresponding to these TS are given in the main text.

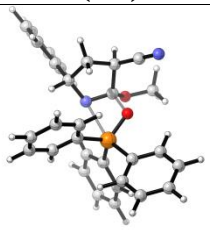
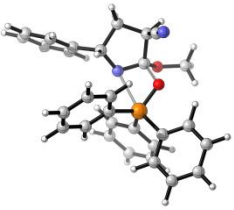
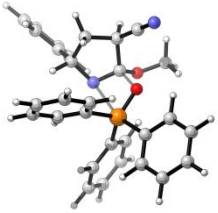
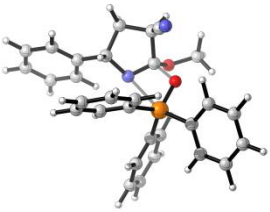
TS1_trans_e1 (**2a**_i12): -0.7 (-0.9)	**TS1**_trans_a1 (**2a**_i17): 0 (0)	**TS1**_trans_e1′: 1.1 (0.2)	**TS1**_cis_a1: 2.8 (2.4)

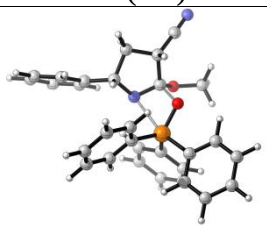
TS1_trans_a1′: 3.2 (2.2)	**TS1**_trans_e2: 3.3 (2.5)	**TS1**_cis_a2: 4.4 (3.6)	**TS1**_cis_a1′: 4.8 (4.4)

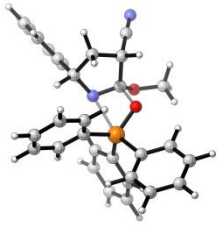
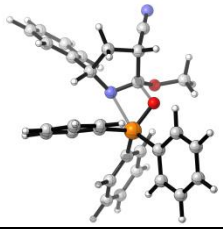




TS1_trans_a2: 4.9 (4.8)	**TS1**_trans_a2′: 5.3 (4.2)	**TS1**_cis_e2′: 5.6 (4.4)

TS2_trans_e1 (**2a**_i1): 2.9 (2.3)	**TS2**_trans_a1 (**2a**_i5): 3.5 (2.5)	**TS2**_trans_e2: 3.5 (3.6)	**TS2**_trans_a2: 4.5 (3.9)



TS2_cis_e1: 4.9 (4.1)	**TS2**_cis_e2: 5.2 (4.4)	**TS2**_cis_a1: 5.7 (4.8)	**TS2**_cis_a2: 8.2 (8.9)

Figure S9. Selected localized transition states of *aza*-Wittig reactions in **2a** isomers related to RDS: **TS1** (*via* CN) and **TS2** (*via* CO). Single point energies ΔE (and free energies ΔG_{298}) are given in kcal/mol relative to **2a**_i17_TS1.

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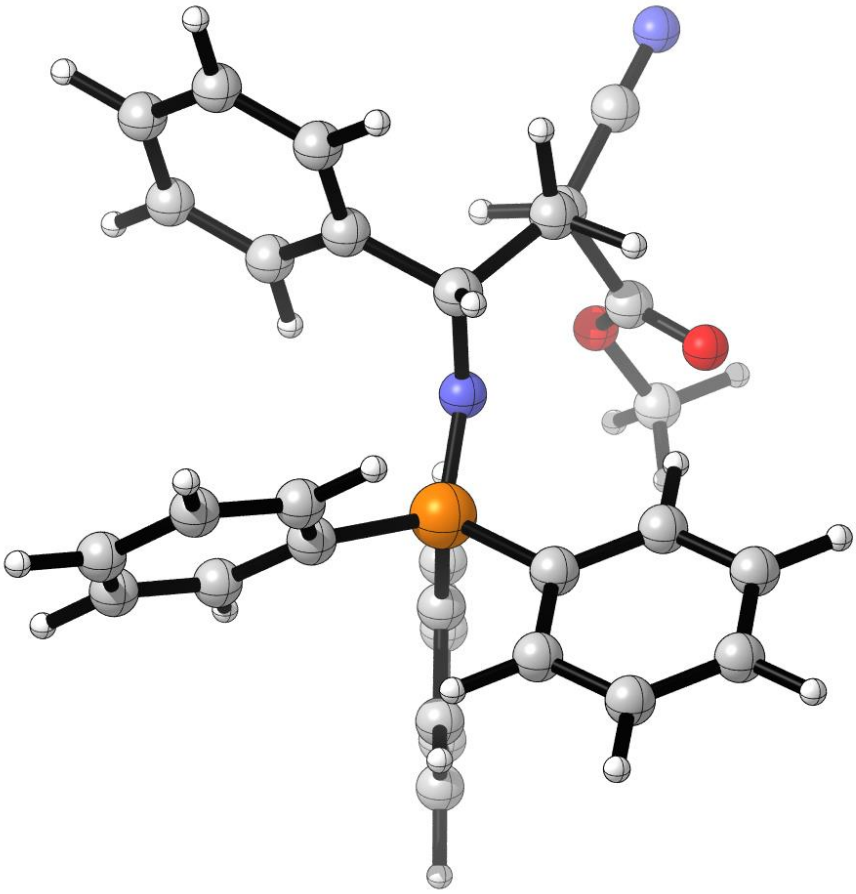
Cartesian Coordinates and Energies of Stationary Points

To Figure S7

2a_i1



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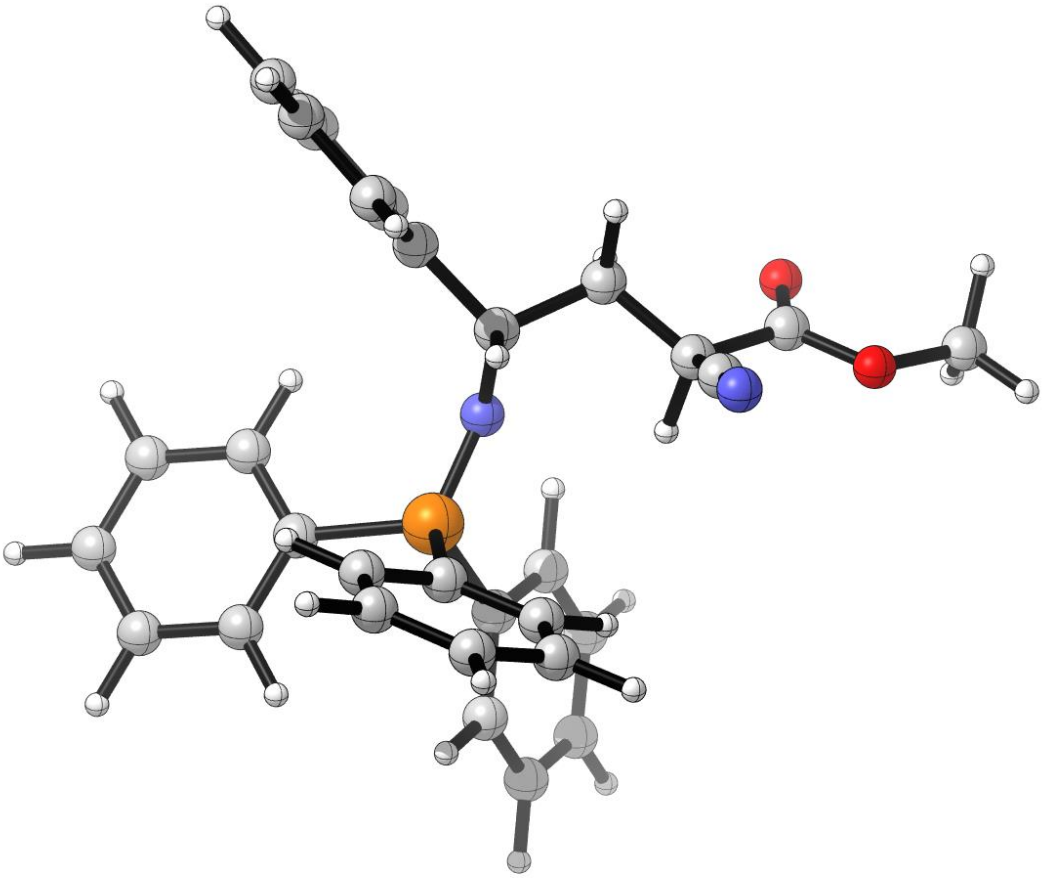
2a_i2



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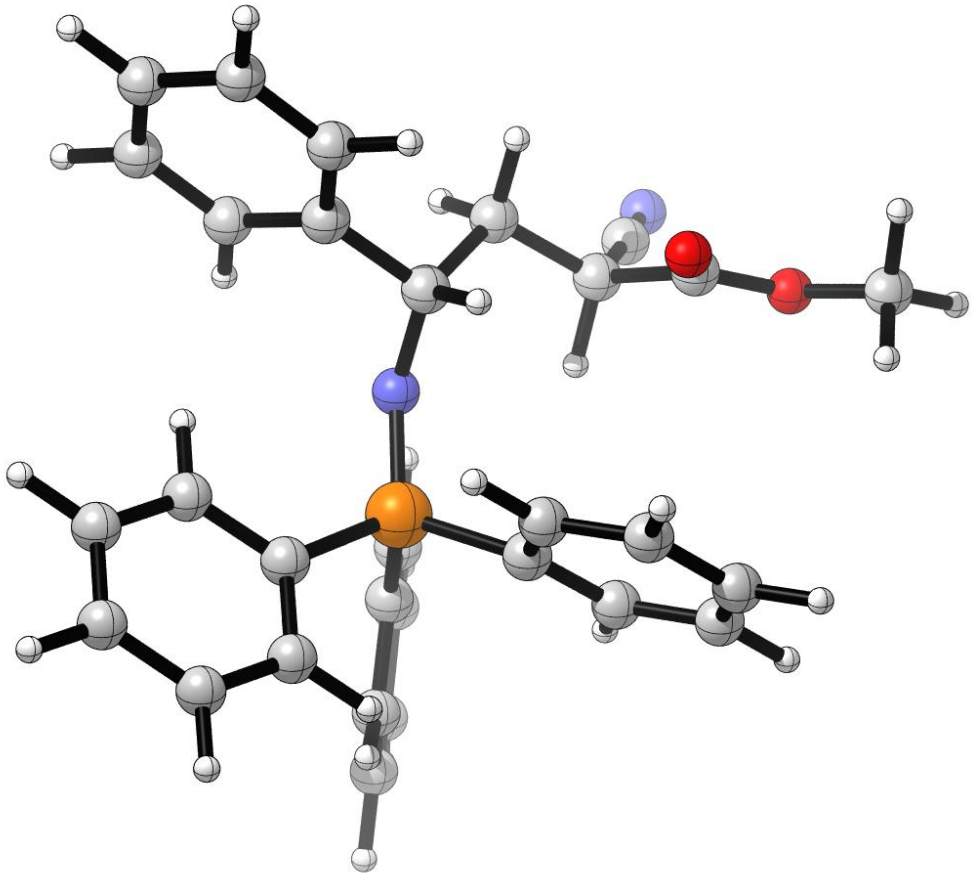
2a_i3



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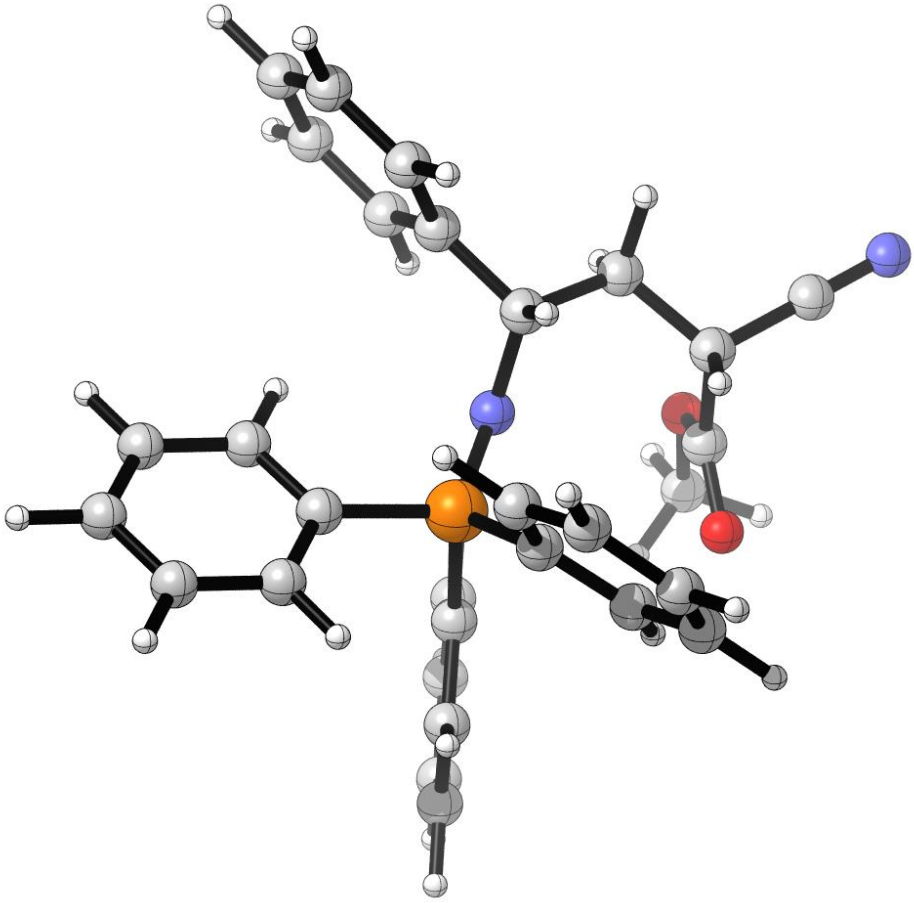
2a_i4



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6	1.399487000	1.894330000	11.107663000
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6	1.134192000	1.855446000	5.611326000
6	-0.038687000	2.537407000	5.983829000
6	-0.604590000	3.494771000	5.136451000

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6	4.293259000	-0.734250000	6.529185000
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1	-0.443938000	4.532262000	3.243944000
1	1.604909000	3.295126000	2.545430000
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6	-0.097613000	-2.349382000	4.899269000

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1	0.451618000	-3.272777000	5.133971000
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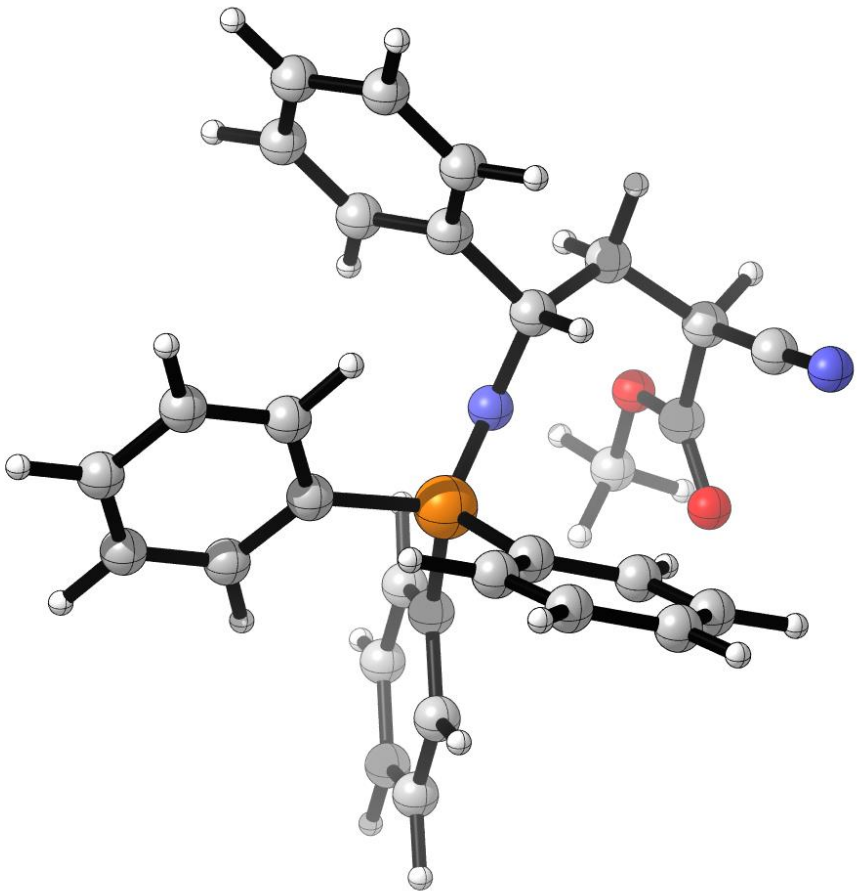

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6	3.631476000	2.641826000	9.771385000
15	1.765129000	1.058945000	6.488514000
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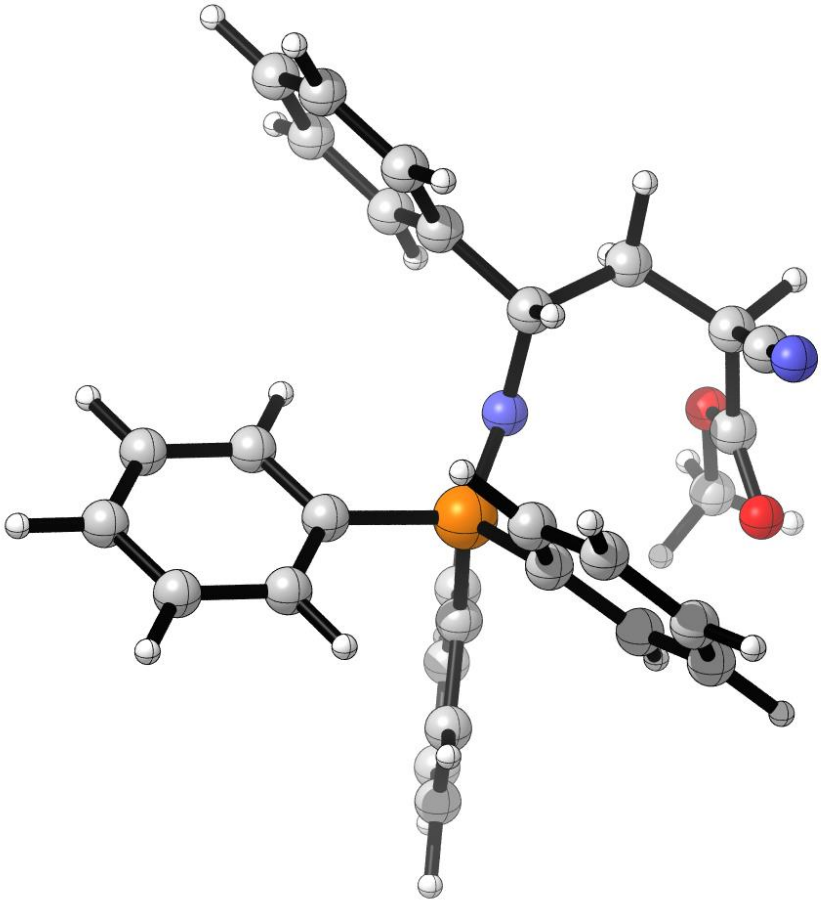

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6	1.282745000	0.540964000	10.726002000
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6	-0.511455000	3.466739000	4.972668000

6	0.169038000	3.778984000	3.792626000
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6	5.833324000	1.520172000	6.586961000
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1	-1.458824000	3.957771000	5.208867000
1	-0.243527000	4.517541000	3.100244000
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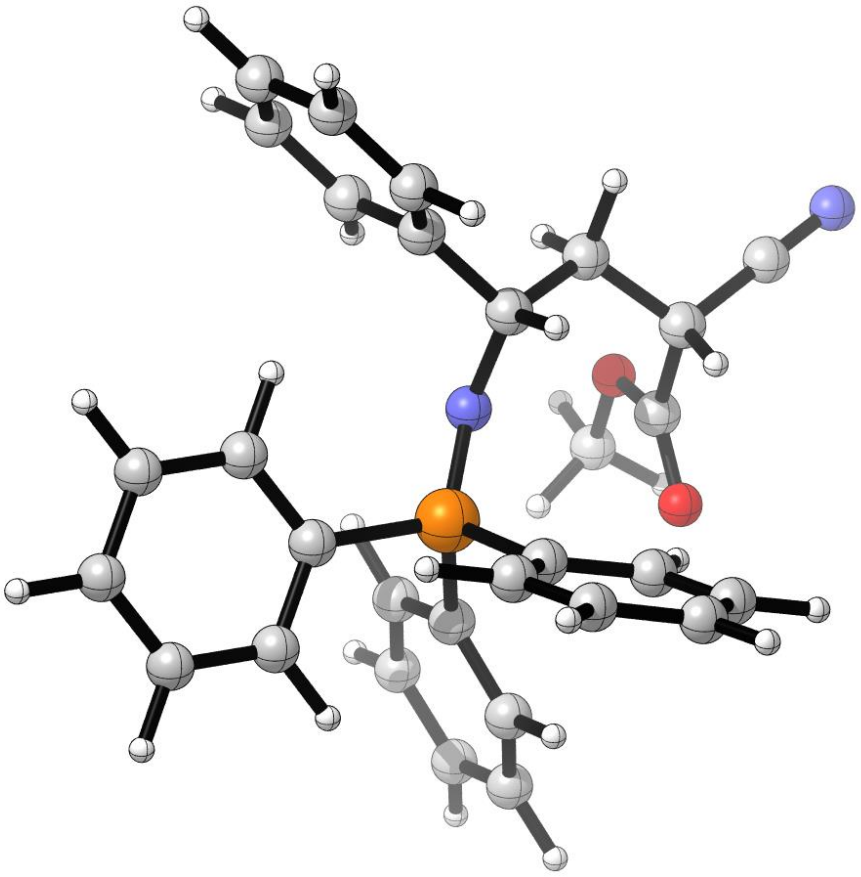

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6	0.355905000	2.846869000	3.094089000

6	0.225509000	1.803583000	2.174167000
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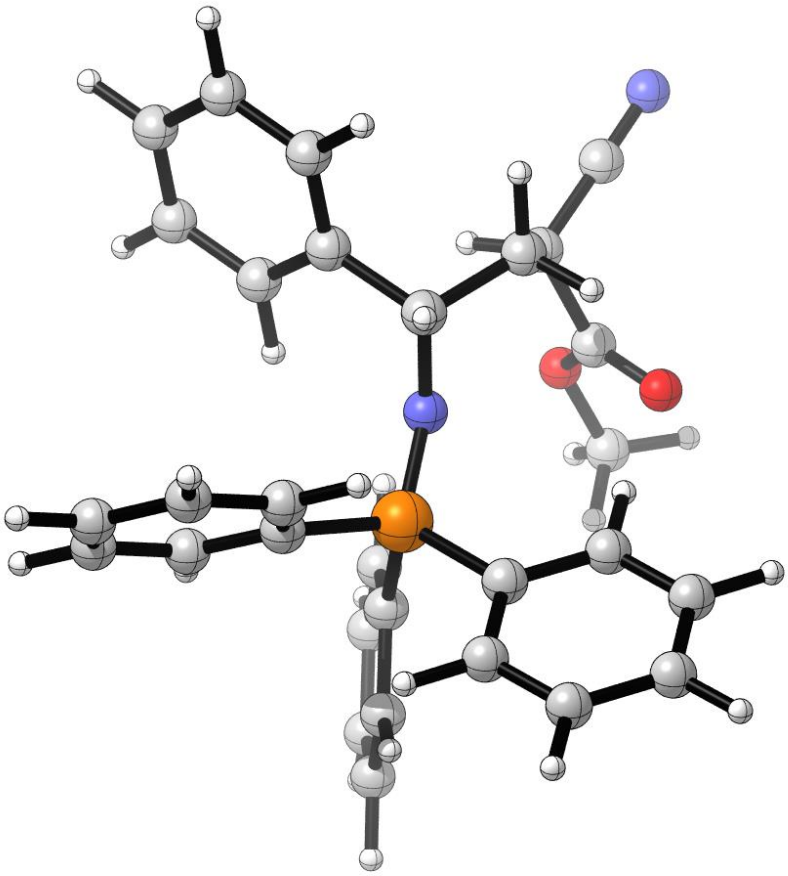

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6	4.020193000	-1.009876000	6.493621000
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1	1.450475000	-2.449124000	7.956832000
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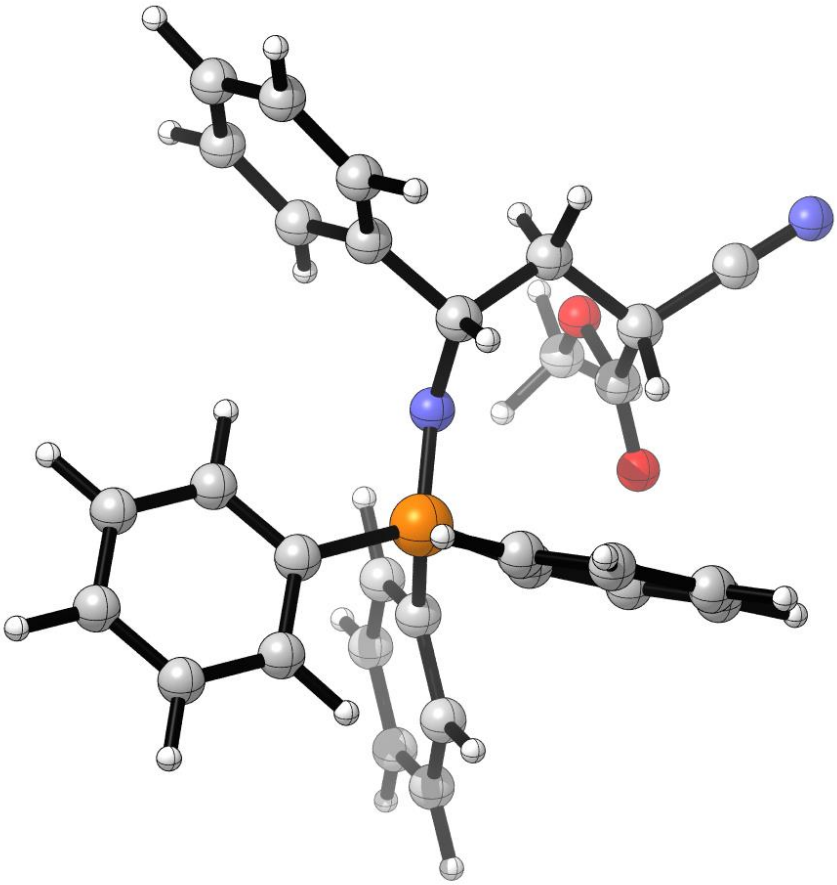

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6	0.685122000	3.558755000	5.093575000
6	1.952224000	3.880416000	5.588201000
6	2.517019000	3.109243000	6.609763000
15	-0.412465000	0.377413000	7.475638000
7	0.609210000	-0.639273000	8.148216000
6	-1.524490000	-0.393895000	6.229437000
6	-1.529132000	1.326741000	8.612432000
6	-1.233583000	1.308377000	9.983690000
6	-1.961072000	2.107238000	10.872499000

6	-2.992213000	2.924668000	10.402444000
6	-3.299607000	2.942327000	9.036214000
6	-2.569169000	2.152071000	8.146063000
6	-2.806923000	-0.844163000	6.588375000
6	-3.548546000	-1.645438000	5.712924000
6	-3.016665000	-2.001889000	4.470990000
6	-1.739135000	-1.559887000	4.105765000
1	-1.010130000	2.236114000	5.235389000
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1	2.501111000	4.730288000	5.174061000
1	3.505796000	3.362960000	7.000993000
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1	-1.711354000	2.093285000	11.937134000
1	-3.558321000	3.549008000	11.098587000
1	-4.107298000	3.577089000	8.661092000
1	-2.817329000	2.184485000	7.081901000
1	-3.230277000	-0.575079000	7.558880000
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6	-0.990489000	-0.767322000	4.979392000
1	2.255904000	1.402123000	7.927563000
6	1.454090000	-2.926737000	6.579064000
6	1.182597000	-3.043800000	8.096788000
1	2.147022000	-2.995321000	8.621198000

1	0.748133000	-4.032253000	8.313769000
6	0.226125000	-1.950395000	8.644710000
6	2.490268000	-1.851450000	6.213697000
8	2.385002000	-1.078360000	5.294662000
8	3.574541000	-1.951468000	6.992384000
6	4.654574000	-1.065029000	6.708848000
1	4.965091000	-1.156305000	5.656720000
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1	0.533130000	-2.655958000	6.040832000
6	1.923066000	-4.204935000	6.022627000
7	2.293580000	-5.210124000	5.580016000
6	0.250443000	-2.078832000	10.170958000
6	-0.641224000	-2.934079000	10.835243000
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6	0.466247000	-2.512063000	12.948708000
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1	-1.237220000	-3.826064000	12.714033000
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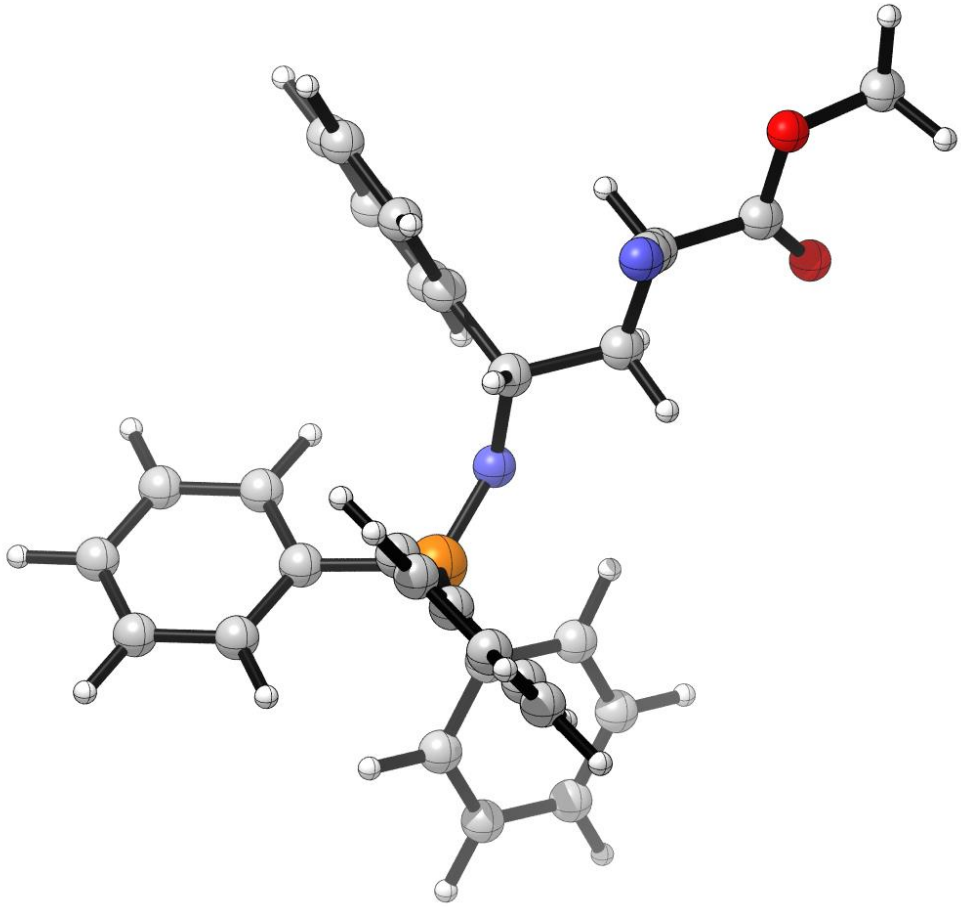
2a_i10



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6	-3.867960000	-8.810234000	5.657252000
6	-3.093547000	-8.345228000	4.590251000
15	-0.535862000	-5.609997000	6.307442000
7	0.016669000	-4.922989000	4.998606000
6	0.885573000	-6.491479000	7.061928000
6	-1.221447000	-4.464544000	7.576139000
6	-2.488019000	-3.895250000	7.344958000
6	-2.974148000	-2.885431000	8.178696000

6	-2.209689000	-2.442430000	9.262664000
6	-0.953164000	-3.006871000	9.504563000
6	-0.456810000	-4.006774000	8.662332000
6	2.173278000	-6.148920000	6.620283000
6	3.295835000	-6.762059000	7.183651000
6	3.142195000	-7.725642000	8.186252000
6	1.860317000	-8.080066000	8.620953000
1	-2.531021000	-6.927470000	8.167057000
1	-4.259803000	-8.663162000	7.781141000
1	-4.643812000	-9.561170000	5.483117000
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1	-3.100711000	-4.242829000	6.508359000
1	-3.951968000	-2.441024000	7.976752000
1	-2.591627000	-1.654005000	9.916654000
1	-0.351102000	-2.661471000	10.349217000
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1	4.293072000	-6.484564000	6.830378000
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1	-1.240916000	-3.205062000	4.807658000
6	0.709047000	-2.861827000	3.948591000

1	1.467094000	-3.431642000	3.390205000
1	1.172063000	-2.577229000	4.906094000
6	0.382972000	-1.595984000	3.134988000
6	-1.168333000	-4.239124000	2.938575000
6	-2.324521000	-3.604508000	2.460147000
6	-0.612937000	-5.280649000	2.175581000
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6	-2.358177000	-5.044630000	0.509098000
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1	0.275938000	-5.787392000	2.558910000
1	-3.819499000	-3.498419000	0.899519000
1	-0.755384000	-6.496104000	0.395585000
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1	3.037593000	1.400661000	2.157965000
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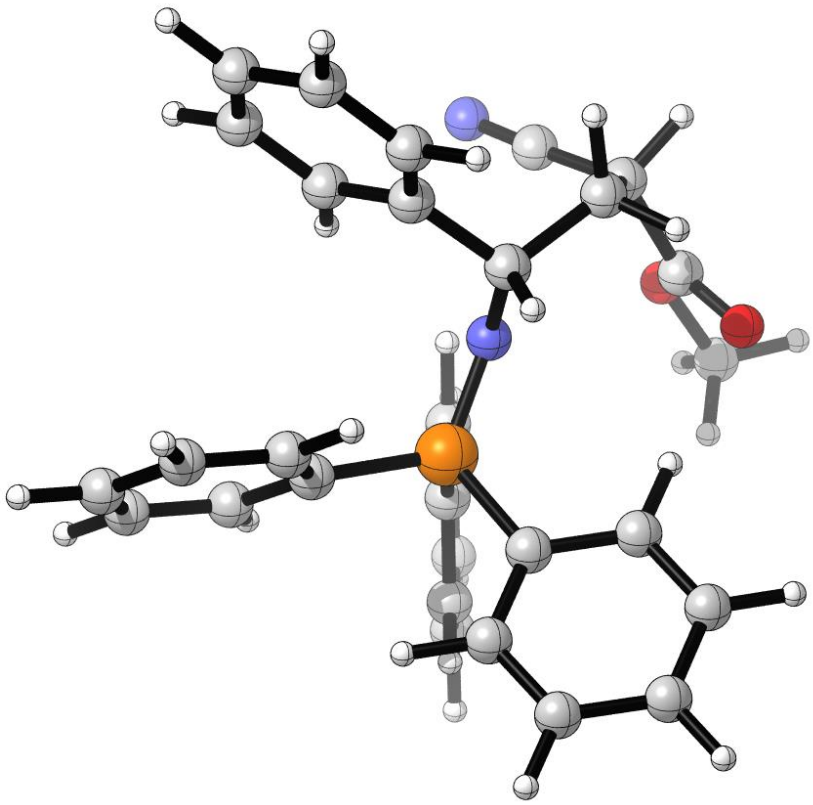

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6	2.963919000	3.880135000	10.413963000
6	3.622525000	2.652914000	10.298851000
15	1.797065000	0.969689000	6.967264000
7	0.337244000	0.366590000	7.077480000
6	2.935403000	-0.462554000	7.029233000
6	2.174664000	1.844899000	5.384071000
6	1.566056000	1.341389000	4.219568000
6	1.871337000	1.896300000	2.973283000

6	2.779100000	2.957077000	2.877127000
6	3.373050000	3.473854000	4.032759000
6	3.071658000	2.921894000	5.282616000
6	4.241308000	-0.385658000	6.517181000
6	5.076263000	-1.506325000	6.552153000
6	4.613720000	-2.709692000	7.095837000
6	3.316463000	-2.787327000	7.613195000
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1	3.024997000	3.387252000	1.902084000
1	4.072829000	4.311127000	3.961082000
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1	4.606468000	0.543310000	6.071929000
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1	1.460487000	-1.730718000	7.972996000
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1	-0.877775000	1.966082000	6.373837000
6	-1.997132000	0.149525000	6.353574000

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6	-2.918240000	3.061051000	9.632486000
6	-1.436416000	1.566276000	10.817530000
6	-2.427143000	2.552524000	10.840020000
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1	-3.690021000	3.836594000	9.635420000
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1	-2.817341000	2.928403000	11.790114000
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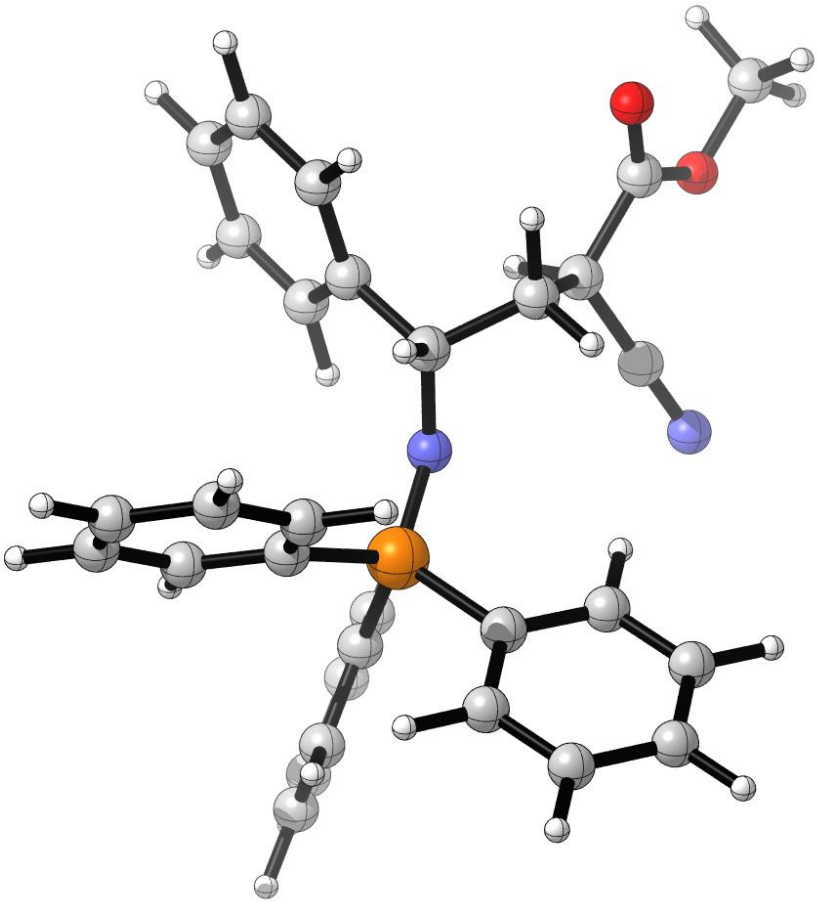

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6	-1.734320000	5.455962000	3.468081000
15	0.534396000	2.123785000	2.545001000
7	-0.102741000	0.797016000	3.122182000
6	1.920142000	2.624633000	3.634198000
6	1.323368000	1.983029000	0.874660000
6	1.786252000	0.713996000	0.487132000
6	2.451185000	0.549275000	-0.732451000

6	2.663296000	1.646475000	-1.572434000
6	2.212253000	2.914262000	-1.189907000
6	1.546474000	3.082904000	0.027906000
6	2.299021000	1.779407000	4.686894000
6	3.367879000	2.131274000	5.518416000
6	4.061283000	3.326684000	5.304830000
6	3.689507000	4.170295000	4.251304000
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1	-1.836020000	6.143614000	4.312547000
1	1.637050000	-0.143567000	1.148401000
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1	3.184502000	1.514679000	-2.524555000
1	2.382102000	3.775806000	-1.841765000
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1	1.752363000	0.845009000	4.828943000
1	3.663220000	1.463037000	6.331686000
1	4.895962000	3.601635000	5.955612000
1	4.231838000	5.103248000	4.076897000
1	2.351735000	4.482473000	2.591056000
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1	-2.033797000	0.974995000	2.223804000
6	-1.491640000	-1.072313000	2.245291000

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6	0.601695000	-2.357524000	2.776109000
7	1.722254000	-2.470065000	2.501258000
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6	-3.656761000	0.151489000	4.196582000
6	-1.628123000	0.390146000	5.473578000
6	-4.397701000	0.091906000	5.378970000
6	-2.365301000	0.318902000	6.661092000
6	-3.753574000	0.169959000	6.619183000
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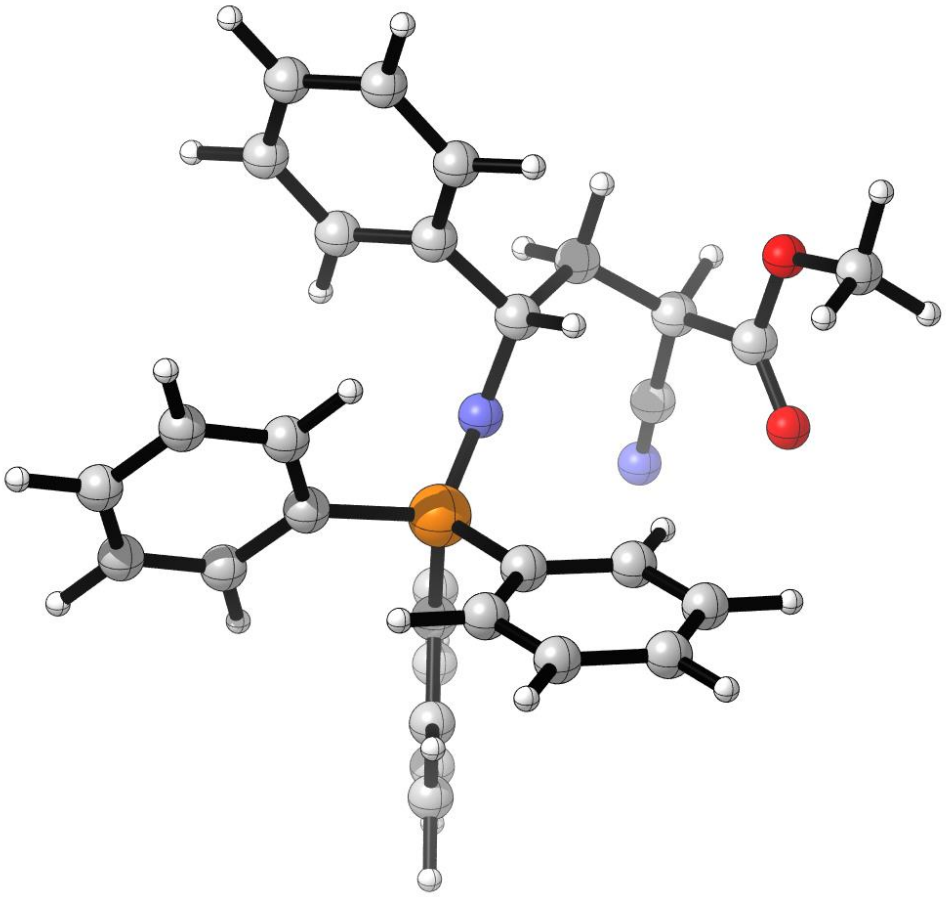

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6	-4.183787000	2.819462000	2.002150000
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7	-0.656976000	0.335400000	2.681148000
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6	0.639915000	2.029631000	0.651700000
6	0.022158000	2.686527000	-0.424959000
6	0.660793000	2.772886000	-1.666751000

6	1.920127000	2.196783000	-1.849761000
6	2.542207000	1.534471000	-0.785390000
6	1.907388000	1.450461000	0.455789000
6	0.556424000	2.520124000	4.842772000
6	1.284279000	3.199176000	5.822251000
6	2.301127000	4.087231000	5.453213000
6	2.592157000	4.289142000	4.099931000
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1	-5.130739000	2.277868000	1.937956000
1	-0.962773000	3.138520000	-0.295349000
1	0.169493000	3.293658000	-2.492935000
1	2.418778000	2.262808000	-2.820631000
1	3.523734000	1.074121000	-0.924526000
1	2.402166000	0.922302000	1.274497000
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1	2.866710000	4.624191000	6.219190000
1	3.384850000	4.982561000	3.804658000
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6	0.900802000	-1.549299000	2.062648000
6	2.103625000	-2.193072000	2.390341000
6	0.383568000	-1.714626000	0.769542000
6	2.770565000	-2.994573000	1.458334000
6	1.043603000	-2.519079000	-0.163737000
6	2.237207000	-3.164924000	0.176875000
1	2.520977000	-2.071361000	3.395507000
1	-0.543491000	-1.199664000	0.506236000
1	3.705801000	-3.489228000	1.735700000
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8	0.187099000	-1.730232000	6.517637000
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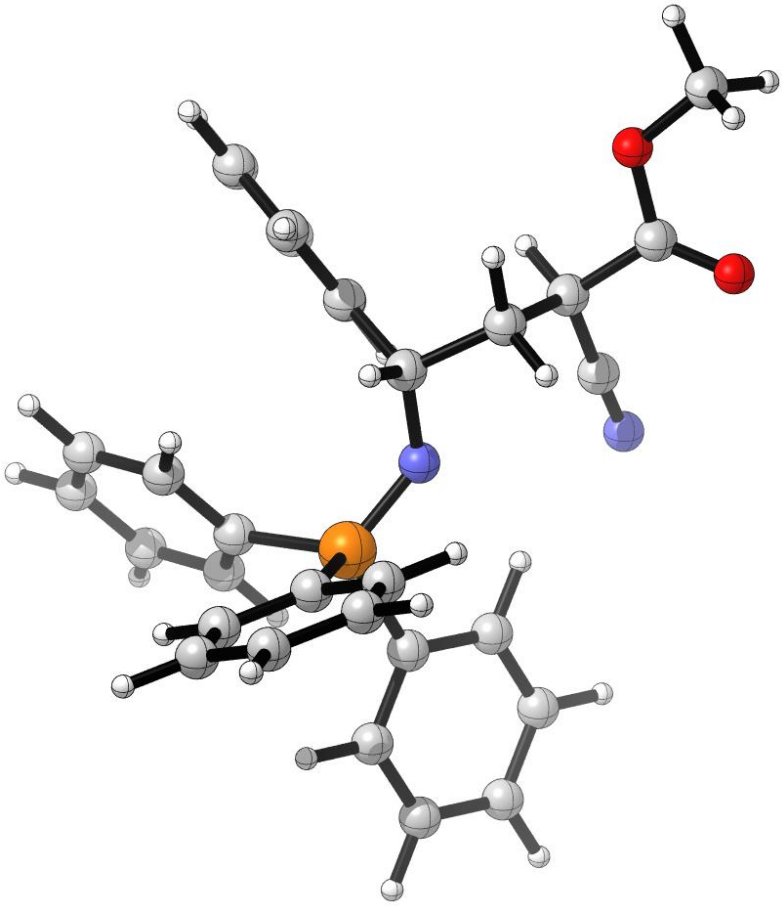
2a_i14



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6	0.999465000	2.319522000	8.359445000
6	2.365347000	2.570523000	8.525728000
6	3.188205000	2.696765000	7.403657000
15	0.588772000	1.941429000	4.268147000
7	0.343260000	0.411756000	3.935240000
6	1.790393000	2.574313000	3.047073000
6	-0.923437000	3.002626000	4.116847000
6	-1.840066000	2.642245000	3.111073000
6	-3.014534000	3.375879000	2.925212000

6	-3.291448000	4.474871000	3.746636000
6	-2.385671000	4.843836000	4.745961000
6	-1.206499000	4.112324000	4.931299000
6	2.488921000	1.659562000	2.244834000
6	3.411149000	2.124209000	1.300923000
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6	2.940049000	4.409375000	1.947045000
1	-0.604393000	1.980098000	6.963459000
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1	4.256077000	2.896112000	7.528209000
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1	-3.720162000	3.085995000	2.141781000
1	-4.213752000	5.044813000	3.606284000
1	-2.598171000	5.703157000	5.387829000
1	-0.507326000	4.408936000	5.716193000
1	2.301686000	0.589321000	2.352929000
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1	4.359485000	3.856818000	0.410798000
1	3.113471000	5.482453000	1.825989000
1	1.468353000	4.675345000	3.503725000
6	2.016307000	3.953133000	2.891993000
1	3.303772000	2.681506000	5.249322000
6	-0.637897000	-0.449112000	4.546079000
1	-1.595368000	0.083109000	4.740936000
6	-1.053882000	-1.564189000	3.547731000

1	-1.403347000	-1.085013000	2.619592000
1	-1.899447000	-2.121503000	3.981384000
6	0.023174000	-2.627518000	3.187164000
6	1.203391000	-2.112903000	2.482036000
7	2.161427000	-1.761910000	1.933303000
6	-0.225675000	-1.062873000	5.892644000
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6	1.460087000	-1.981910000	7.392817000
6	0.480998000	-2.254651000	8.353464000
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1	1.876442000	-1.151417000	5.432959000
1	-1.625730000	-2.133473000	8.833115000
1	2.504775000	-2.234819000	7.596764000
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8	-0.649178000	-3.783753000	1.145967000
8	-1.281740000	-4.592640000	3.149775000
6	-2.049336000	-5.607998000	2.498928000
1	-2.793508000	-5.159889000	1.822676000
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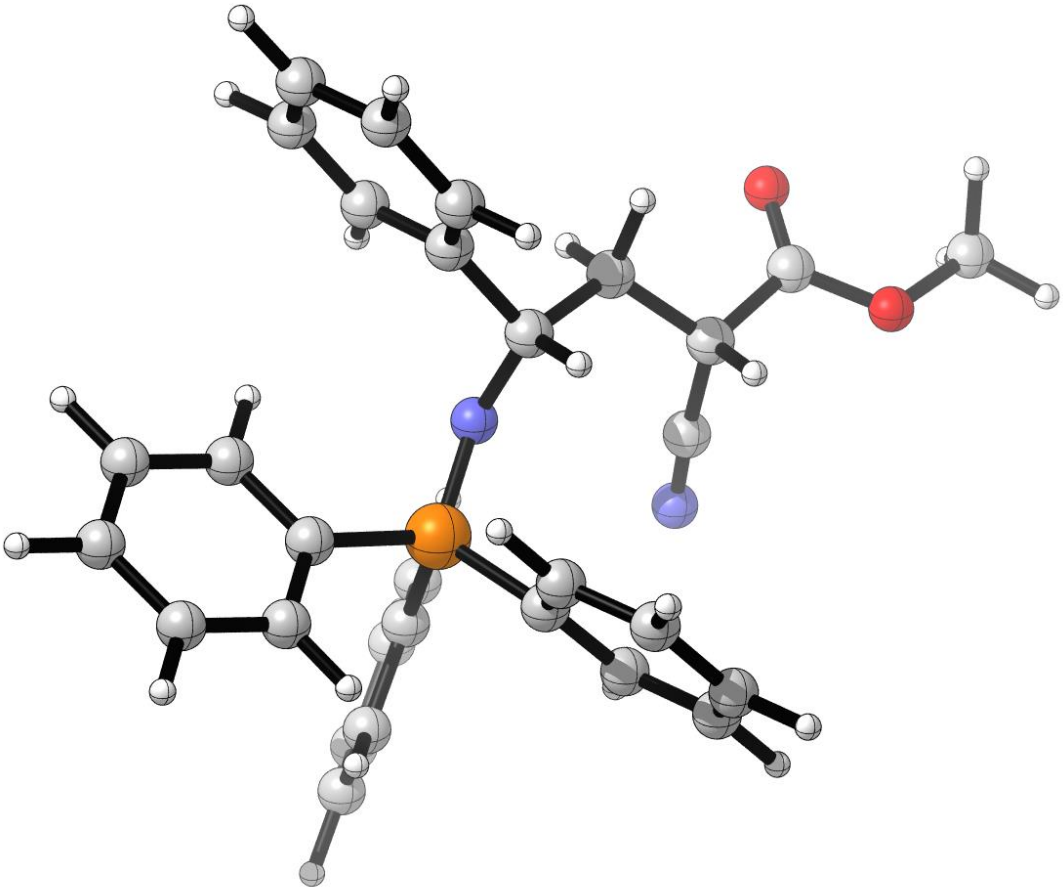
2a_i15



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6	-2.156420000	5.521940000	1.811284000
6	-2.813501000	5.855227000	2.999877000
6	-2.633340000	5.063962000	4.138688000
15	0.047401000	2.170464000	2.993120000
7	-0.267980000	1.035749000	4.055770000
6	1.636840000	2.941363000	3.461876000
6	0.217571000	1.557557000	1.264563000
6	-0.919038000	1.373971000	0.455636000
6	-0.811724000	0.728392000	-0.780479000

6	0.429234000	0.261014000	-1.222613000
6	1.563127000	0.429704000	-0.420794000
6	1.458596000	1.064966000	0.819516000
6	2.319850000	2.458393000	4.585773000
6	3.519371000	3.056454000	4.983346000
6	4.041940000	4.132833000	4.261359000
6	3.366336000	4.612348000	3.132487000
1	-0.804090000	4.161415000	0.828435000
1	-2.302416000	6.133465000	0.916345000
1	-3.466317000	6.731652000	3.038560000
1	-3.147545000	5.320538000	5.068746000
1	-1.894086000	1.738096000	0.789730000
1	-1.702129000	0.585190000	-1.398658000
1	0.513400000	-0.241257000	-2.189932000
1	2.532468000	0.055357000	-0.761070000
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1	1.897833000	1.611842000	5.127214000
1	4.051121000	2.669694000	5.856458000
1	4.978287000	4.600528000	4.577791000
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6	-1.263598000	-0.005551000	3.920325000
1	-1.483963000	-0.249834000	2.857832000
6	-0.761652000	-1.318229000	4.564510000

1	-1.592105000	-2.042073000	4.572514000
1	-0.487224000	-1.136852000	5.614528000
6	0.409952000	-2.014234000	3.846848000
1	0.156353000	-2.174019000	2.784033000
6	1.688741000	-1.285827000	3.864789000
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6	-2.606081000	0.356189000	4.566235000
6	-3.818205000	0.119781000	3.904452000
6	-2.646789000	0.910732000	5.855530000
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6	-3.864741000	1.233594000	6.456786000
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1	-3.804497000	-0.318663000	2.901443000
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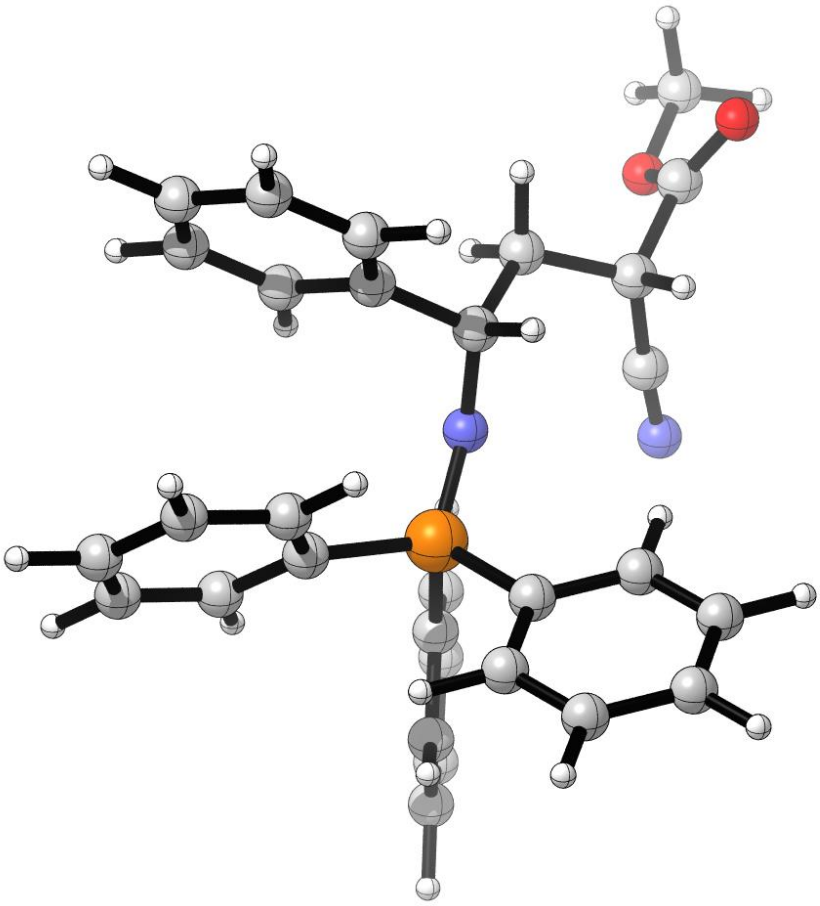
2a_i16



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6	2.958550000	1.289735000	-3.658306000
6	2.858578000	-0.029179000	-4.116240000
6	2.865961000	-1.087108000	-3.203415000
15	3.224527000	0.788394000	0.427375000
7	2.907461000	-0.594491000	1.128551000
6	2.041357000	2.167691000	0.775232000
6	4.898162000	1.532901000	0.694123000
6	5.929610000	1.313783000	-0.234264000
6	7.228288000	1.762902000	0.027104000

6	7.513474000	2.429992000	1.221799000
6	6.495192000	2.648542000	2.155361000
6	5.197190000	2.203263000	1.894660000
6	0.701893000	1.812469000	1.011379000
6	-0.268161000	2.799076000	1.202233000
6	0.088759000	4.151398000	1.161112000
6	1.419413000	4.513938000	0.933530000
1	3.136146000	2.583323000	-1.942949000
1	2.939926000	2.121220000	-4.367702000
1	2.761781000	-0.231883000	-5.186860000
1	2.767627000	-2.116815000	-3.557363000
1	5.719797000	0.784570000	-1.166317000
1	8.018773000	1.586196000	-0.707395000
1	8.527523000	2.782773000	1.429027000
1	6.714422000	3.165798000	3.092965000
1	4.415156000	2.379839000	2.637103000
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6	2.310592000	-2.363921000	2.687308000

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6	0.529974000	-2.407568000	0.859902000
7	0.230653000	-2.379038000	-0.259667000
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6	5.692388000	-0.217533000	5.064408000
6	6.640718000	-1.411701000	3.190267000
6	6.800988000	-0.786092000	4.432245000
1	3.570438000	0.181683000	4.953315000
1	5.264718000	-1.914464000	1.598367000
1	5.807936000	0.278605000	6.032008000
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1	7.787022000	-0.736770000	4.902586000
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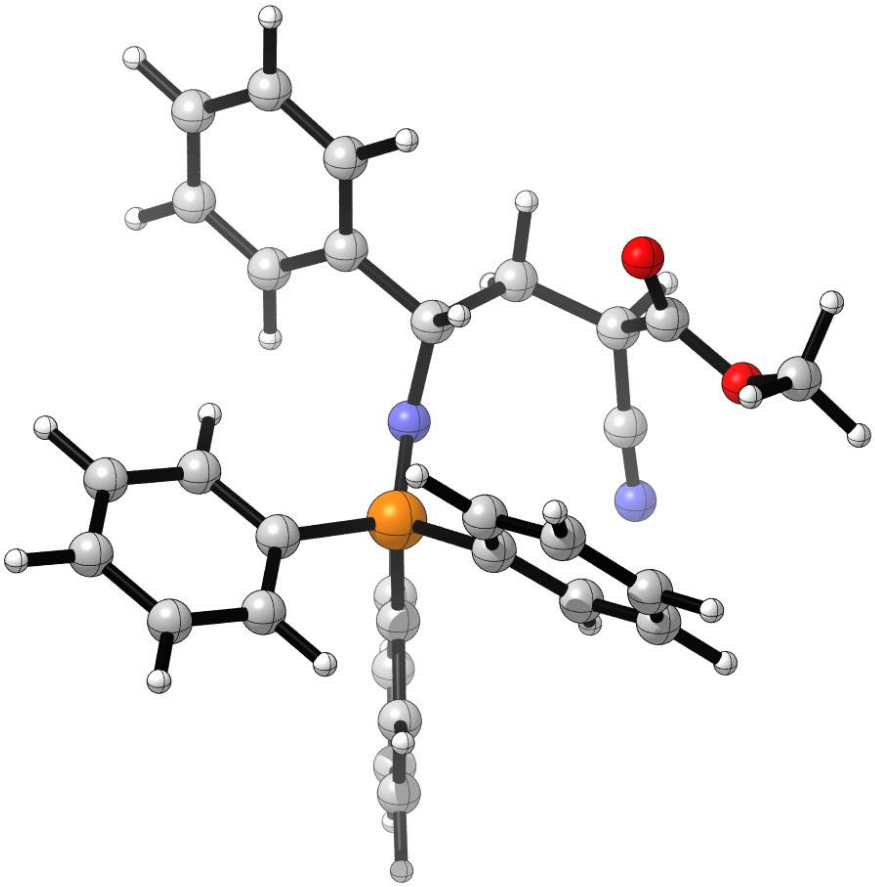
2a_i17



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6	-5.609630000	-5.735916000	0.116474000
6	-4.359122000	-6.157302000	0.574880000
15	-3.230472000	-3.254962000	3.282445000
7	-1.713467000	-3.654000000	3.465201000
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6	-3.613646000	-1.496545000	2.847774000
6	-3.699631000	-1.087189000	1.504071000
6	-3.949257000	0.250411000	1.181748000

6	-4.111669000	1.197164000	2.197671000
6	-3.997069000	0.805449000	3.535831000
6	-3.742379000	-0.529720000	3.861000000
6	-3.331231000	-4.267920000	5.876384000
6	-3.936703000	-4.579360000	7.097215000
6	-5.259472000	-4.201083000	7.343546000
6	-5.979536000	-3.507122000	6.365187000
1	-5.928741000	-2.872985000	1.935386000
1	-7.147912000	-4.218087000	0.260136000
1	-6.147799000	-6.323821000	-0.632233000
1	-3.908475000	-7.072502000	0.182008000
1	-3.592529000	-1.818247000	0.698999000
1	-4.030749000	0.551547000	0.133486000
1	-4.330673000	2.238363000	1.944361000
1	-4.114480000	1.540678000	4.336123000
1	-3.644531000	-0.820388000	4.909460000
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1	-2.687986000	-5.725523000	1.875765000
6	-0.553168000	-3.369192000	2.657932000
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6	0.608887000	-2.827235000	3.536335000

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6	0.354174000	-7.010369000	1.787255000
6	1.182482000	-6.840503000	0.673265000
1	1.050051000	-3.437841000	0.436025000
1	-0.862534000	-6.022539000	3.290083000
1	2.074132000	-5.402353000	-0.679749000
1	0.152102000	-8.013312000	2.175543000
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6	0.206902000	-0.311547000	3.236710000
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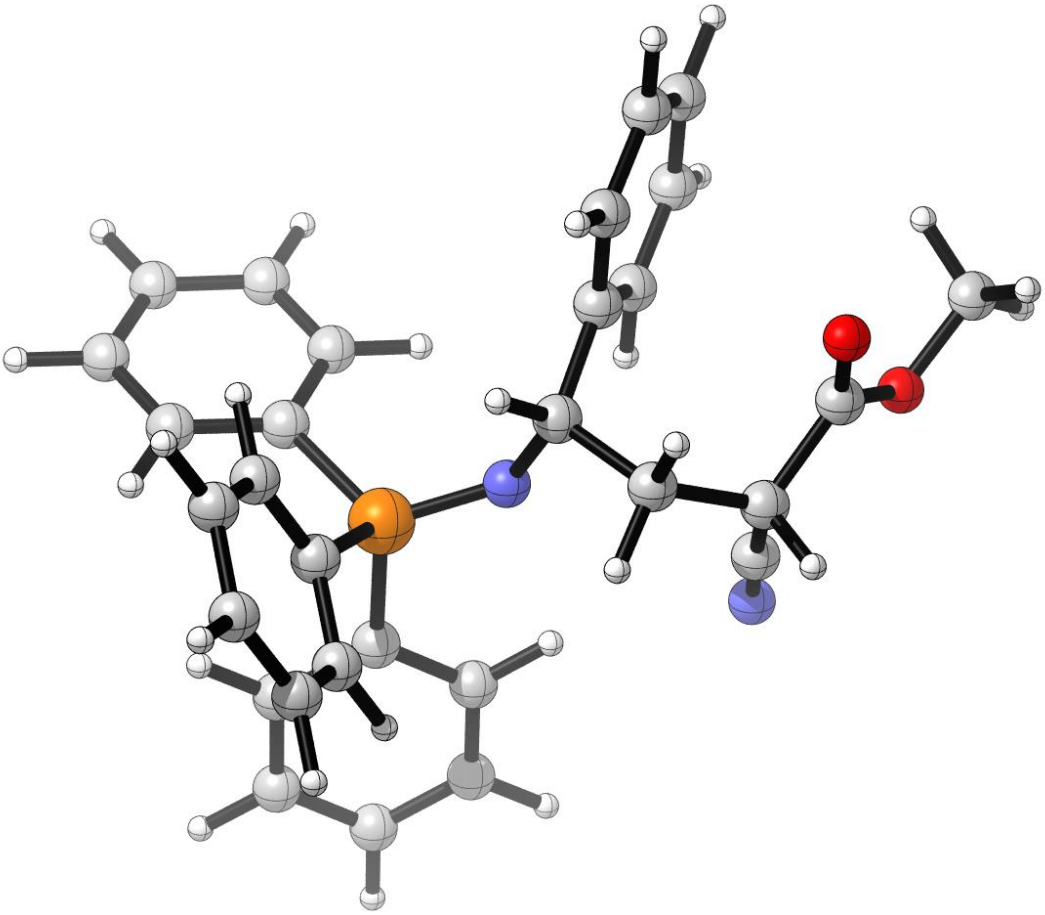

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6	-3.682745000	2.951125000	0.889317000
15	0.166661000	2.360756000	2.185295000
7	0.199293000	0.778310000	2.169665000
6	0.125930000	2.896195000	3.936902000
6	1.624471000	3.187457000	1.410577000
6	1.631402000	3.566674000	0.056785000
6	2.798129000	4.061837000	-0.535130000

6	3.973584000	4.173305000	0.212185000
6	3.982230000	3.782994000	1.556307000
6	2.817820000	3.290581000	2.150103000
6	0.140754000	1.916554000	4.940521000
6	0.115364000	2.297482000	6.286757000
6	0.080579000	3.649465000	6.638093000
6	0.063155000	4.629005000	5.638762000
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1	-4.654795000	4.728032000	0.120553000
1	-4.585908000	2.336728000	0.842807000
1	0.720036000	3.488453000	-0.540172000
1	2.785144000	4.369141000	-1.584007000
1	4.881598000	4.567365000	-0.252053000
1	4.898952000	3.867362000	2.146300000
1	2.832311000	2.986814000	3.200144000
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1	0.123575000	1.525413000	7.060599000
1	0.063670000	3.944910000	7.691292000
1	0.032279000	5.687793000	5.910616000
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6	-0.146740000	-1.304851000	-0.921846000
6	-1.467336000	-1.365280000	1.094241000
6	-1.064017000	-2.144569000	-1.556756000
6	-2.392801000	-2.203527000	0.459791000
6	-2.194560000	-2.598044000	-0.867523000
1	0.734425000	-0.957174000	-1.470301000
1	-1.621311000	-1.049185000	2.128595000
1	-0.892166000	-2.452951000	-2.591909000
1	-3.272908000	-2.551968000	1.008240000
1	-2.918072000	-3.251057000	-1.364093000
6	1.159648000	-3.346050000	1.751131000
8	1.555894000	-3.611823000	0.644907000
8	0.318385000	-4.107189000	2.455271000
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1	-0.863946000	-4.971638000	0.973423000
1	0.622535000	-5.879951000	1.382896000
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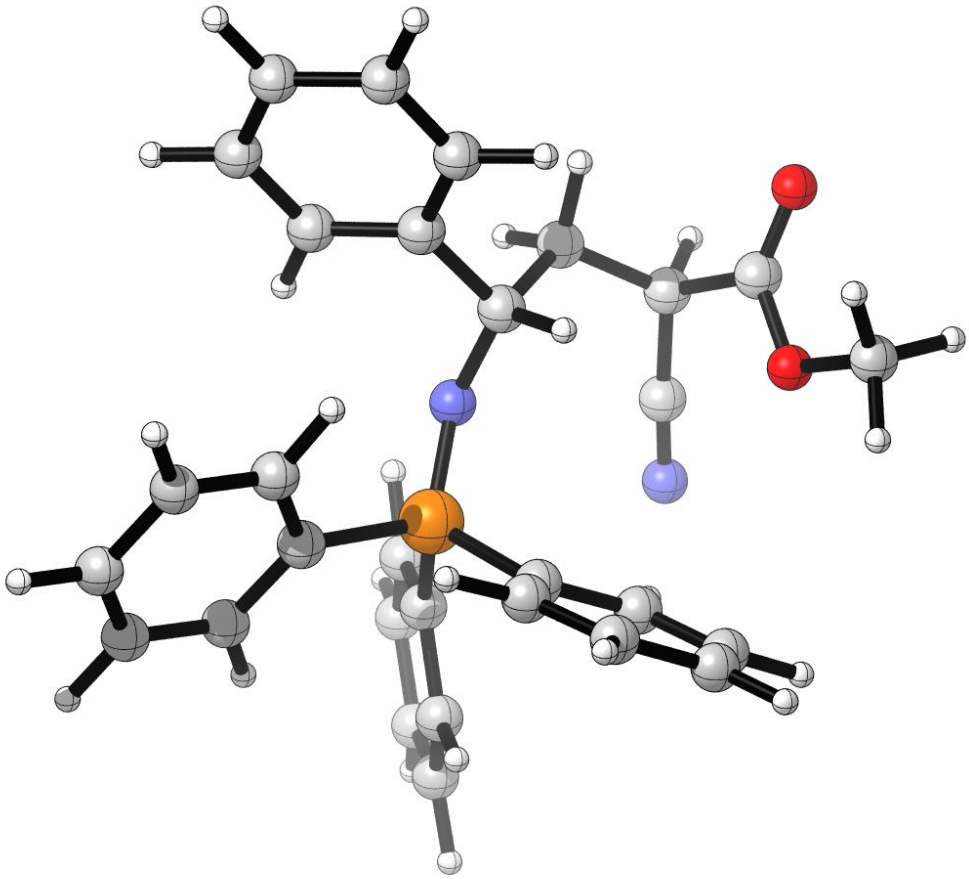
2a_i19



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6	-3.367622000	0.051186000	-0.805795000
6	-3.894229000	-0.206624000	0.463571000
15	-1.806824000	-3.490300000	1.744465000
7	-2.200178000	-3.136119000	3.233321000
6	0.002190000	-3.645634000	1.379189000
6	-2.559948000	-5.029893000	1.033705000
6	-3.301384000	-5.025606000	-0.159092000
6	-3.881788000	-6.203197000	-0.642511000

6	-3.723400000	-7.402969000	0.055840000
6	-2.994426000	-7.417913000	1.250041000
6	-2.428397000	-6.239352000	1.741866000
6	0.787827000	-2.476616000	1.405185000
6	2.168575000	-2.550010000	1.203685000
6	2.788053000	-3.788942000	1.003446000
6	2.019274000	-4.955561000	0.991511000
1	-1.106720000	-2.497105000	-0.993963000
1	-1.937684000	-0.562741000	-2.309541000
1	-3.734302000	0.900164000	-1.389046000
1	-4.669872000	0.442975000	0.877765000
1	-3.436721000	-4.097067000	-0.716395000
1	-4.457846000	-6.180213000	-1.571258000
1	-4.174297000	-8.322561000	-0.326925000
1	-2.870979000	-8.349024000	1.809549000
1	-1.894276000	-6.261965000	2.693890000
1	0.320123000	-1.504953000	1.577005000
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1	3.868795000	-3.845094000	0.844480000
1	2.497038000	-5.925152000	0.826066000
1	0.044731000	-5.802362000	1.123082000
6	0.633383000	-4.884665000	1.167769000
1	-3.787107000	-1.475241000	2.223053000
6	-1.653113000	-3.536484000	4.499747000
1	-0.567803000	-3.771504000	4.436009000
6	-1.806868000	-2.365818000	5.507585000

1	-1.642613000	-2.731093000	6.532826000
1	-2.844648000	-2.002961000	5.446250000
6	-0.846261000	-1.153404000	5.343423000
6	-0.878766000	-0.469021000	4.046130000
7	-0.876877000	0.156641000	3.070425000
6	-2.317664000	-4.774252000	5.125025000
6	-1.626301000	-5.540835000	6.077457000
6	-3.626476000	-5.146131000	4.789432000
6	-2.227552000	-6.647504000	6.685091000
6	-4.229496000	-6.256880000	5.389798000
6	-3.533789000	-7.011360000	6.340361000
1	-0.603633000	-5.262302000	6.352467000
1	-4.156421000	-4.559828000	4.035725000
1	-1.670777000	-7.233112000	7.422315000
1	-5.244843000	-6.543870000	5.100959000
1	-4.005622000	-7.878764000	6.809890000
1	-1.173097000	-0.408159000	6.088299000
6	0.567182000	-1.540070000	5.799238000
8	0.834341000	-1.743600000	6.956681000
8	1.437231000	-1.664456000	4.792129000
6	2.764637000	-2.077028000	5.138956000
1	3.296452000	-1.262120000	5.654281000
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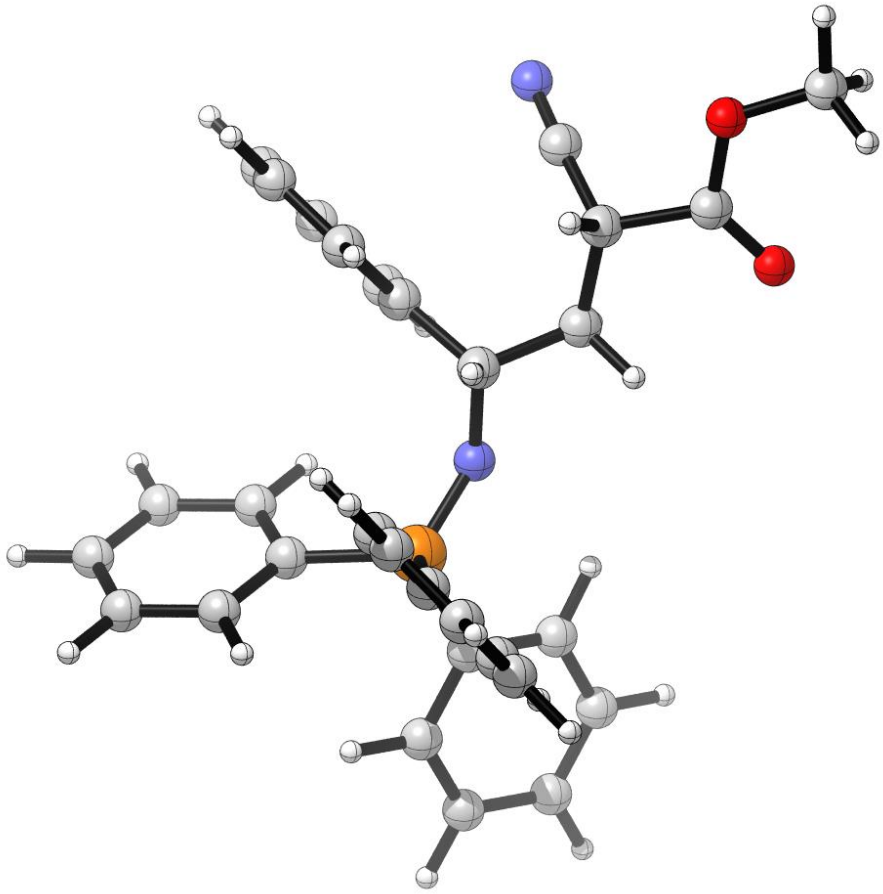
2a_i20



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6	-3.811524000	-8.007412000	6.695977000
6	-3.786917000	-8.741239000	5.505288000
6	-2.766445000	-8.521874000	4.573122000
15	-0.432270000	-5.588443000	6.263240000
7	0.211525000	-4.928941000	4.977714000
6	0.912256000	-6.522371000	7.079030000
6	-1.104170000	-4.391806000	7.497299000
6	-2.323471000	-3.741442000	7.227942000
6	-2.772341000	-2.703913000	8.049951000

6	-2.014513000	-2.306456000	9.156086000
6	-0.802447000	-2.947000000	9.432898000
6	-0.346521000	-3.978880000	8.606690000
6	2.235949000	-6.233036000	6.712786000
6	3.294902000	-6.905498000	7.328679000
6	3.039337000	-7.871441000	8.308687000
6	1.720386000	-8.169435000	8.669786000
1	-2.859215000	-6.478617000	7.883248000
1	-4.606687000	-8.175673000	7.427916000
1	-4.565541000	-9.481127000	5.299162000
1	-2.746796000	-9.085939000	3.637009000
1	-2.931274000	-4.050117000	6.373187000
1	-3.718650000	-2.205495000	7.823930000
1	-2.367732000	-1.497873000	9.801765000
1	-0.204636000	-2.639057000	10.294952000
1	0.607042000	-4.464243000	8.827320000
1	2.408621000	-5.486806000	5.934086000
1	4.322538000	-6.673650000	7.034441000
1	3.867394000	-8.399444000	8.788897000
1	1.514530000	-8.930519000	9.427496000
1	-0.368320000	-7.750856000	8.333877000
6	0.658324000	-7.499853000	8.054794000
1	-0.984801000	-7.390732000	4.099008000
6	-0.317364000	-3.858526000	4.161948000
1	-0.929464000	-3.142537000	4.753152000
6	0.895070000	-3.045771000	3.633680000

1	1.569332000	-3.717371000	3.079974000
1	1.461196000	-2.686860000	4.504491000
6	0.540737000	-1.819901000	2.766464000
6	-1.208606000	-4.351929000	3.020824000
6	-2.457194000	-3.767233000	2.769721000
6	-0.765424000	-5.377635000	2.169824000
6	-3.237770000	-4.179146000	1.682193000
6	-1.538931000	-5.791545000	1.085908000
6	-2.779173000	-5.190424000	0.836027000
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1	0.202236000	-5.845819000	2.368188000
1	-4.203567000	-3.702881000	1.492158000
1	-1.171405000	-6.580117000	0.423049000
1	-3.382661000	-5.510140000	-0.017604000
6	0.207253000	-2.138730000	1.369557000
1	-0.345019000	-1.314658000	3.196290000
6	1.648372000	-0.744930000	2.775914000
8	2.654127000	-0.786498000	3.434918000
8	1.315860000	0.268740000	1.966240000
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1	2.559485000	1.711565000	2.833736000
1	3.154649000	0.996069000	1.307051000
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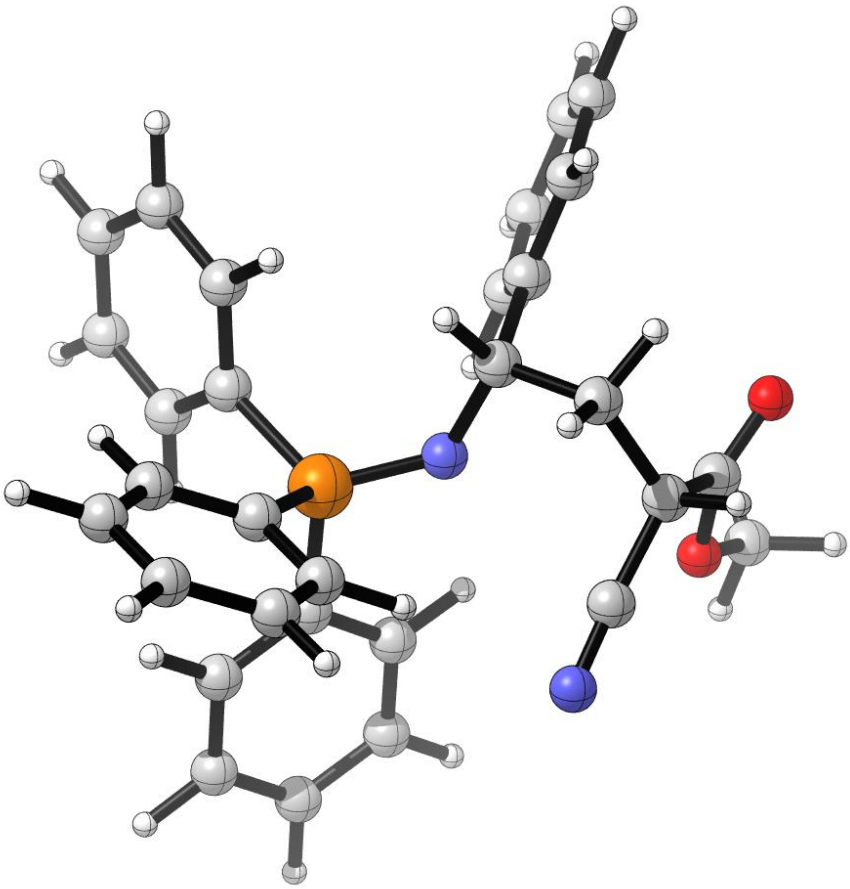
2a_i21



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6	-0.925367000	3.802774000	-0.118751000
6	0.017294000	4.291613000	-1.031038000
6	0.811634000	3.399367000	-1.755154000
15	-0.467774000	-0.289790000	-0.303775000
7	-0.173994000	-0.758423000	1.178799000
6	0.713757000	-1.180567000	-1.376725000
6	-2.136124000	-0.709895000	-0.983939000
6	-2.641665000	-1.986207000	-0.675056000
6	-3.869539000	-2.402254000	-1.194948000

6	-4.603730000	-1.554917000	-2.032437000
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6	-2.882725000	0.139879000	-1.817211000
6	1.848423000	-1.768252000	-0.796479000
6	2.746163000	-2.487638000	-1.590207000
6	2.513870000	-2.631824000	-2.961730000
6	1.378964000	-2.054556000	-3.542173000
1	-1.813673000	2.061234000	0.783597000
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1	1.551112000	3.778393000	-2.466061000
1	-2.056899000	-2.666434000	-0.050202000
1	-4.251795000	-3.395759000	-0.945802000
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1	-2.507830000	1.133865000	-2.069457000
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1	3.622269000	-2.951519000	-1.128929000
1	3.212068000	-3.203505000	-3.579282000
1	1.178319000	-2.186666000	-4.609067000
1	-0.411980000	-0.899157000	-3.213086000
6	0.481823000	-1.328936000	-2.753916000
1	1.293633000	1.332437000	-2.140210000
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6	-1.239644000	-1.598477000	3.234688000

1	-2.205697000	-1.962443000	2.850686000
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6	0.010967000	0.656586000	3.221411000
6	-0.540466000	1.249292000	4.370413000
6	1.290568000	1.057245000	2.819569000
6	0.167275000	2.206000000	5.100873000
6	2.003109000	2.020029000	3.545034000
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1	1.715216000	0.609910000	1.919524000
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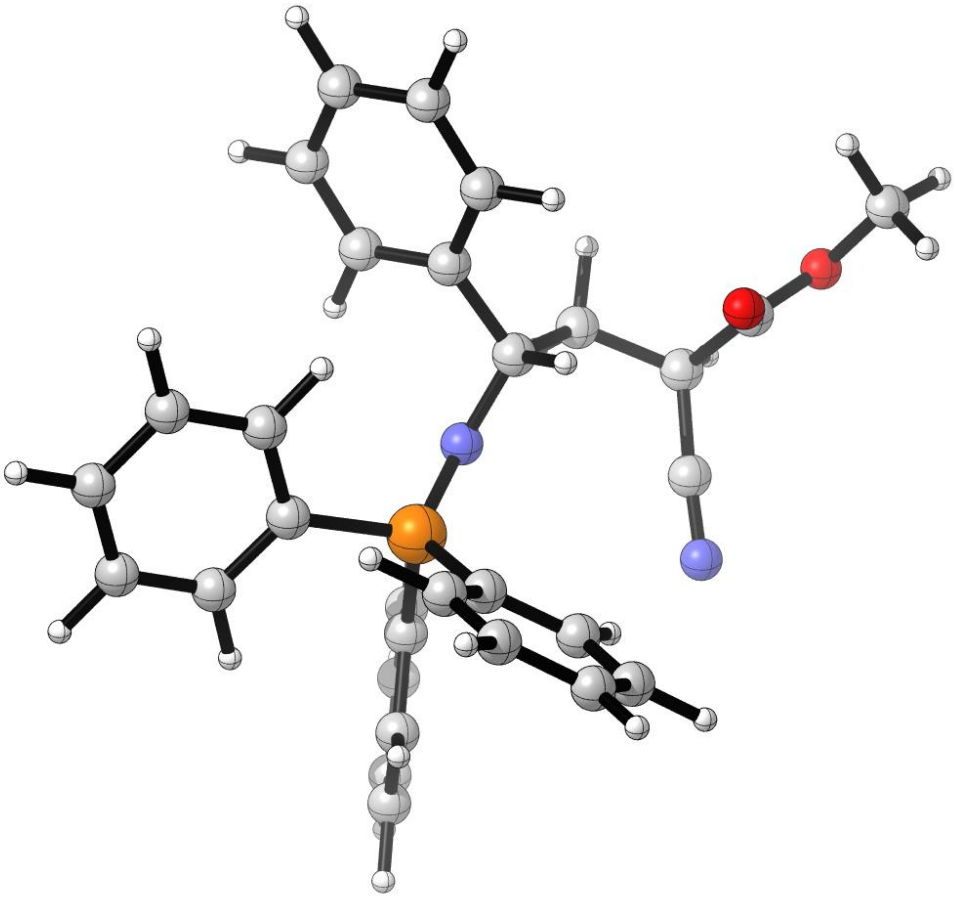
2a_i22



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6	-4.190279000	4.168513000	2.096190000
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15	-0.027227000	2.110202000	2.157942000
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6	1.064805000	3.204160000	3.179035000
6	0.648771000	2.332053000	0.441750000
6	0.155574000	3.302557000	-0.446904000
6	0.707624000	3.443607000	-1.723936000

6	1.757493000	2.615190000	-2.130918000
6	2.247945000	1.637584000	-1.259156000
6	1.696089000	1.494782000	0.017969000
6	0.657981000	3.528041000	4.487145000
6	1.432533000	4.385472000	5.272426000
6	2.621753000	4.923439000	4.768371000
6	3.042261000	4.592244000	3.477724000
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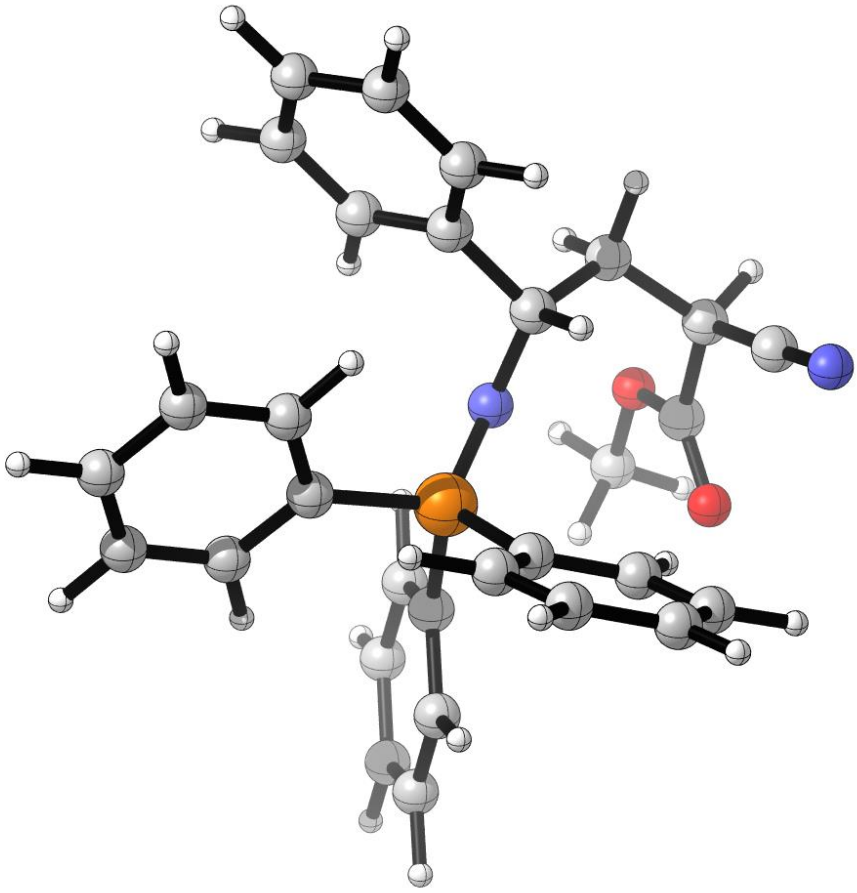
1	-3.126301000	6.048193000	2.215518000
1	-5.176835000	4.640292000	2.084497000
1	-4.972055000	2.152462000	2.003431000
1	-0.669612000	3.952528000	-0.149947000
1	0.311197000	4.201669000	-2.404918000
1	2.191390000	2.729496000	-3.127927000
1	3.061434000	0.978265000	-1.573945000
1	2.083003000	0.721861000	0.686027000
1	-0.267213000	3.116917000	4.896190000
1	1.095792000	4.644031000	6.279824000
1	3.223050000	5.598085000	5.384300000
1	3.970926000	5.007577000	3.077337000
1	2.601631000	3.498242000	1.674702000
6	2.267250000	3.738761000	2.685398000
1	-2.700752000	1.088874000	2.056136000
6	0.431830000	-0.456787000	3.178912000
1	1.208900000	-0.112850000	3.886954000
6	-0.559233000	-1.363756000	3.977798000

1	-0.203291000	-2.405736000	3.977728000
1	-1.517908000	-1.350216000	3.439036000
6	-0.822814000	-1.017079000	5.467976000
6	-1.175205000	0.379921000	5.743874000
7	-1.469090000	1.463069000	6.031780000
6	1.132915000	-1.377826000	2.168093000
6	2.333665000	-2.016262000	2.517850000
6	0.544907000	-1.686544000	0.931910000
6	2.926032000	-2.951333000	1.662048000
6	1.131936000	-2.624813000	0.076948000
6	2.322955000	-3.263948000	0.439486000
1	2.801276000	-1.783733000	3.479532000
1	-0.376221000	-1.172765000	0.646399000
1	3.860782000	-3.439136000	1.953457000
1	0.655918000	-2.863376000	-0.878654000
1	2.780892000	-3.997155000	-0.230514000
1	-1.680980000	-1.619523000	5.805278000
6	0.376790000	-1.460716000	6.320597000
8	1.509209000	-1.071847000	6.186046000
8	0.005299000	-2.403487000	7.200810000
6	1.053835000	-2.986460000	7.982137000
1	1.771678000	-3.509845000	7.331166000
1	1.593613000	-2.214554000	8.550834000
1	0.565963000	-3.696186000	8.661831000

To Figure S8

2a_i5



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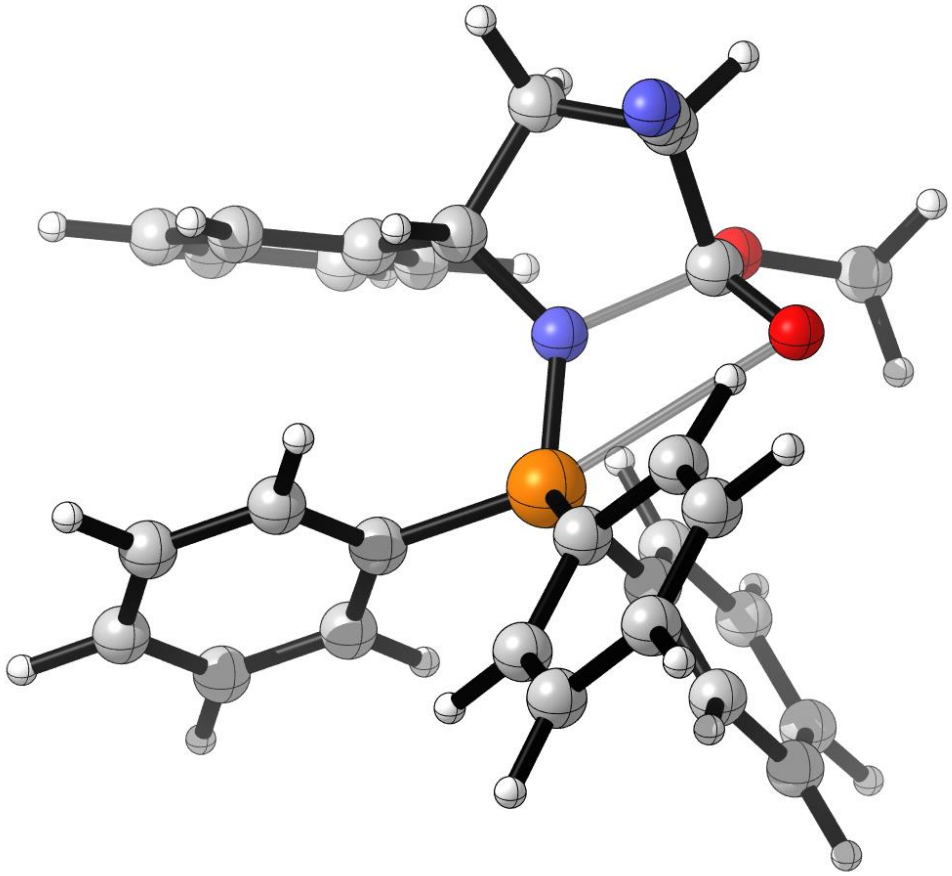
6	1.438288000	2.864699000	10.074404000
6	1.308517000	1.894947000	11.072838000
6	1.282745000	0.540964000	10.726002000
15	1.823038000	0.511991000	6.648236000
7	1.324615000	-0.953044000	6.286438000
6	3.653773000	0.448992000	6.572799000
6	1.232561000	1.874601000	5.566886000
6	0.014524000	2.518538000	5.853351000

6	-0.511455000	3.466739000	4.972668000
6	0.169038000	3.778984000	3.792626000
6	1.368188000	3.128137000	3.488837000
6	1.893394000	2.172847000	4.361840000
6	4.279747000	-0.806365000	6.619596000
6	5.674688000	-0.894403000	6.650764000
6	6.452914000	0.267311000	6.630596000
6	5.833324000	1.520172000	6.586961000
1	1.658481000	3.253014000	7.968333000
1	1.454588000	3.925545000	10.340134000
1	1.222717000	2.197616000	12.120290000
1	1.174822000	-0.221829000	11.501345000
1	-0.528136000	2.284286000	6.772406000
1	-1.458824000	3.957771000	5.208867000
1	-0.243527000	4.517541000	3.100244000
1	1.892747000	3.353105000	2.556959000
1	2.808461000	1.644128000	4.090267000
1	3.649932000	-1.698301000	6.626505000
1	6.158793000	-1.874405000	6.694415000
1	7.544152000	0.195159000	6.653166000
1	6.437467000	2.430820000	6.571461000
1	3.966865000	2.597429000	6.536844000
6	4.438932000	1.612564000	6.565830000
1	1.364188000	-0.902275000	9.115860000
6	-0.050198000	-1.382705000	6.110402000
1	-0.731120000	-0.544494000	5.854853000

6	-0.132017000	-2.386626000	4.938149000
1	-1.166789000	-2.755106000	4.851031000
1	0.505865000	-3.255081000	5.157228000
6	0.296356000	-1.837274000	3.553608000
6	-0.640510000	-2.059932000	7.353081000
6	-1.886745000	-1.674416000	7.864341000
6	0.047535000	-3.105929000	7.992417000
6	-2.434988000	-2.309521000	8.985513000
6	-0.501212000	-3.752647000	9.102717000
6	-1.745800000	-3.354553000	9.606176000
1	-2.435848000	-0.860950000	7.380963000
1	1.028810000	-3.404164000	7.614754000
1	-3.400625000	-1.978710000	9.377830000
1	0.047066000	-4.567426000	9.584422000
1	-2.174396000	-3.857462000	10.477280000
6	1.803185000	-1.620321000	3.368450000
8	2.321200000	-0.634558000	2.908792000
8	2.470817000	-2.742183000	3.672446000
6	3.882951000	-2.711163000	3.456014000
1	4.109694000	-2.546376000	2.391307000
1	4.349472000	-1.907510000	4.042532000
1	4.261698000	-3.689141000	3.779913000
6	-0.471962000	-0.650469000	3.157294000
7	-1.145303000	0.243521000	2.858785000
1	0.045099000	-2.624799000	2.818886000

2a_i5_TS1



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6	2.749430000	-0.006456000	8.075832000
6	3.890793000	0.632160000	8.587196000
6	4.356351000	0.313059000	9.865729000
6	3.689923000	-0.642904000	10.638943000
6	2.547892000	-1.273752000	10.135394000
15	2.080465000	0.391135000	6.423141000
7	1.446165000	-0.980774000	5.788188000
6	3.406738000	1.288070000	5.512095000
6	0.767395000	1.654735000	6.640796000
6	0.266718000	1.981881000	7.911287000
6	-0.712931000	2.971266000	8.047426000

6	-1.205038000	3.633759000	6.920365000
6	-0.714838000	3.308047000	5.650813000
6	0.269298000	2.327866000	5.510187000
6	4.316811000	0.601471000	4.690232000
6	5.358179000	1.297610000	4.067688000
6	5.523226000	2.667881000	4.281193000
6	4.635223000	3.352163000	5.119659000
1	4.431158000	1.363645000	7.983358000
1	5.250718000	0.806691000	10.253967000
1	4.068650000	-0.908150000	11.629691000
1	2.025703000	-2.024319000	10.734662000
1	0.645989000	1.471414000	8.798321000
1	-1.092264000	3.228764000	9.039940000
1	-1.969050000	4.407817000	7.033187000
1	-1.096738000	3.826094000	4.767602000
1	0.664234000	2.099974000	4.516902000
1	4.230919000	-0.481511000	4.584152000
1	6.048978000	0.750078000	3.421548000
1	6.344856000	3.205916000	3.800428000
1	4.770653000	4.420512000	5.309845000
1	2.886124000	3.225444000	6.366900000
6	3.574585000	2.672377000	5.723726000
1	1.204871000	-1.469293000	8.451714000
6	0.231923000	-1.155211000	4.981281000
1	0.187477000	-0.415187000	4.162078000
6	0.410988000	-2.568354000	4.337305000

1	-0.095911000	-2.620884000	3.363324000
1	-0.034890000	-3.326096000	4.993438000
6	1.914769000	-2.840354000	4.271303000
6	-1.087402000	-1.093409000	5.746631000
6	-2.157421000	-0.327035000	5.265338000
6	-1.289284000	-1.881813000	6.894383000
6	-3.401070000	-0.343159000	5.908296000
6	-2.528594000	-1.900370000	7.537872000
6	-3.591935000	-1.134358000	7.043697000
1	-2.018457000	0.288083000	4.371657000
1	-0.466082000	-2.502129000	7.259164000
1	-4.223003000	0.261998000	5.515512000
1	-2.672910000	-2.522485000	8.425748000
1	-4.564120000	-1.158589000	7.543673000
6	2.500250000	-2.346425000	5.658224000
8	3.701542000	-2.051381000	5.782010000
8	1.924451000	-3.226059000	6.645867000
6	2.865644000	-4.019489000	7.342896000
1	3.427114000	-4.691314000	6.666616000
1	3.599119000	-3.405828000	7.889329000
1	2.290354000	-4.633026000	8.053982000
6	2.558775000	-2.168899000	3.142256000
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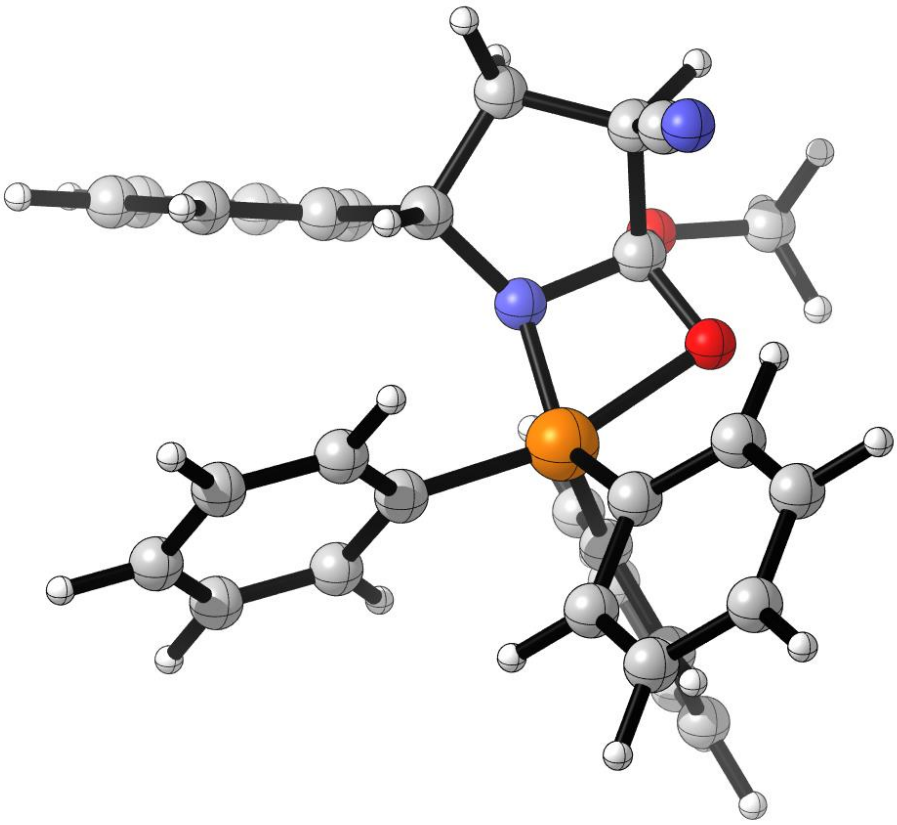
2a_i5_int



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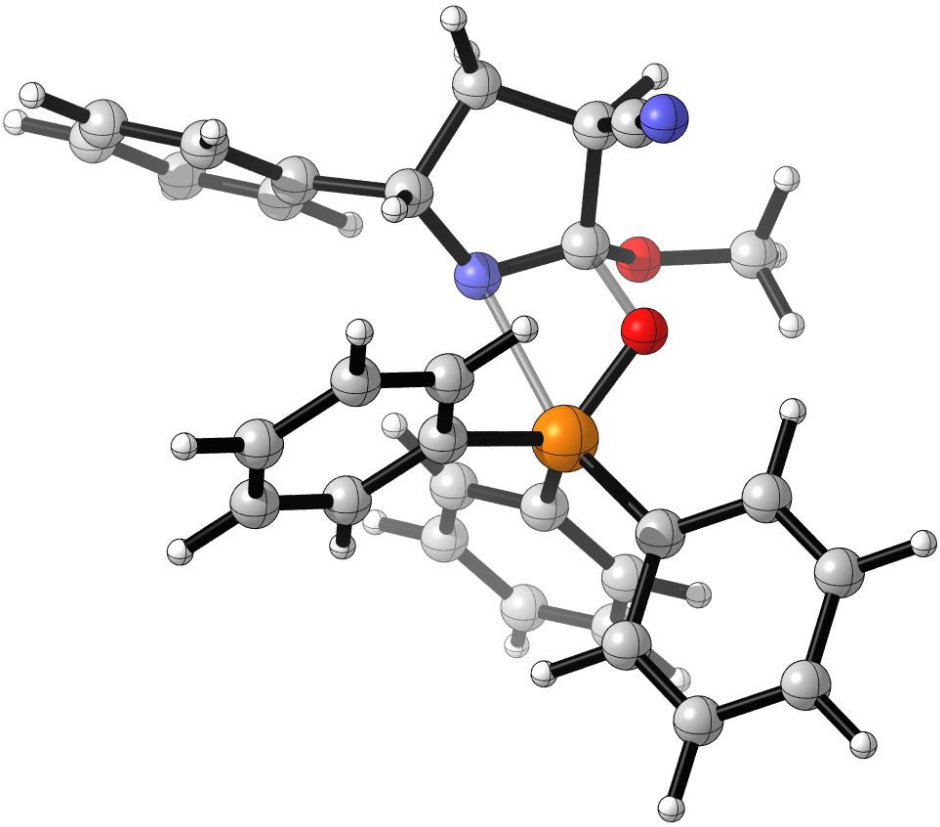
6	1.551508000	2.481868000	8.734706000
6	1.438288000	2.864699000	10.074404000
6	1.308517000	1.894947000	11.072838000
6	1.282745000	0.540964000	10.726002000
15	1.823038000	0.511991000	6.648236000
7	1.324615000	-0.953044000	6.286438000
6	3.653773000	0.448992000	6.572799000
6	1.232561000	1.874601000	5.566886000
6	0.014524000	2.518538000	5.853351000
6	-0.511455000	3.466739000	4.972668000

6	0.169038000	3.778984000	3.792626000
6	1.368188000	3.128137000	3.488837000
6	1.893394000	2.172847000	4.361840000
6	4.279747000	-0.806365000	6.619596000
6	5.674688000	-0.894403000	6.650764000
6	6.452914000	0.267311000	6.630596000
6	5.833324000	1.520172000	6.586961000
1	1.658481000	3.253014000	7.968333000
1	1.454588000	3.925545000	10.340134000
1	1.222717000	2.197616000	12.120290000
1	1.174822000	-0.221829000	11.501345000
1	-0.528136000	2.284286000	6.772406000
1	-1.458824000	3.957771000	5.208867000
1	-0.243527000	4.517541000	3.100244000
1	1.892747000	3.353105000	2.556959000
1	2.808461000	1.644128000	4.090267000
1	3.649932000	-1.698301000	6.626505000
1	6.158793000	-1.874405000	6.694415000
1	7.544152000	0.195159000	6.653166000
1	6.437467000	2.430820000	6.571461000
1	3.966865000	2.597429000	6.536844000
6	4.438932000	1.612564000	6.565830000
1	1.364188000	-0.902275000	9.115860000
6	-0.050198000	-1.382705000	6.110402000
1	-0.731120000	-0.544494000	5.854853000
6	-0.132017000	-2.386626000	4.938149000

1	-1.166789000	-2.755106000	4.851031000
1	0.505865000	-3.255081000	5.157228000
6	0.296356000	-1.837274000	3.553608000
6	-0.640510000	-2.059932000	7.353081000
6	-1.886745000	-1.674416000	7.864341000
6	0.047535000	-3.105929000	7.992417000
6	-2.434988000	-2.309521000	8.985513000
6	-0.501212000	-3.752647000	9.102717000
6	-1.745800000	-3.354553000	9.606176000
1	-2.435848000	-0.860950000	7.380963000
1	1.028810000	-3.404164000	7.614754000
1	-3.400625000	-1.978710000	9.377830000
1	0.047066000	-4.567426000	9.584422000
1	-2.174396000	-3.857462000	10.477280000
6	1.803185000	-1.620321000	3.368450000
8	2.321200000	-0.634558000	2.908792000
8	2.470817000	-2.742183000	3.672446000
6	3.882951000	-2.711163000	3.456014000
1	4.109694000	-2.546376000	2.391307000
1	4.349472000	-1.907510000	4.042532000
1	4.261698000	-3.689141000	3.779913000
6	-0.471962000	-0.650469000	3.157294000
7	-1.145303000	0.243521000	2.858785000
1	0.045099000	-2.624799000	2.818886000

2a_i5_TS2 (**TS2**_trans_a1)



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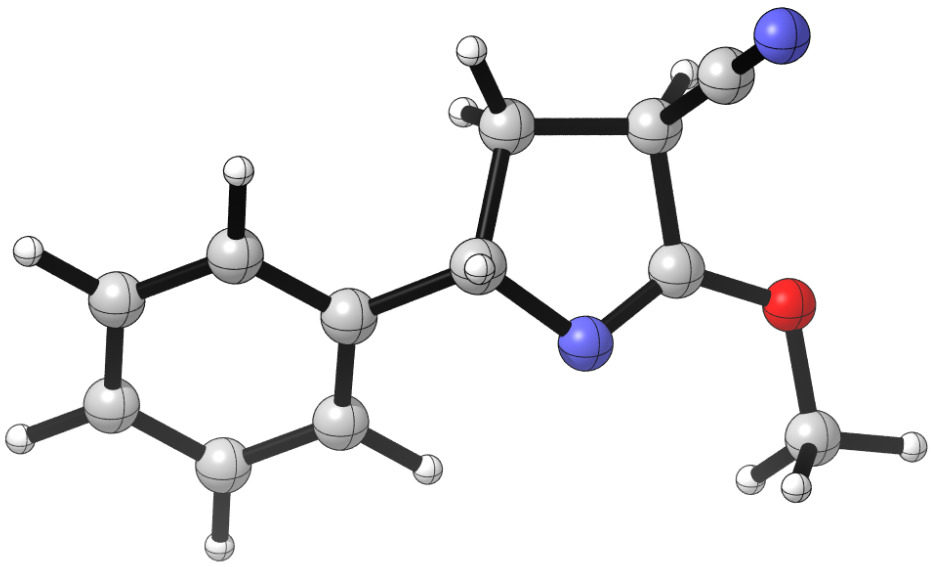
6	1.551508000	2.481868000	8.734706000
6	1.438288000	2.864699000	10.074404000
6	1.308517000	1.894947000	11.072838000
6	1.282745000	0.540964000	10.726002000
15	1.823038000	0.511991000	6.648236000
7	1.324615000	-0.953044000	6.286438000
6	3.653773000	0.448992000	6.572799000
6	1.232561000	1.874601000	5.566886000
6	0.014524000	2.518538000	5.853351000
6	-0.511455000	3.466739000	4.972668000

6	0.169038000	3.778984000	3.792626000
6	1.368188000	3.128137000	3.488837000
6	1.893394000	2.172847000	4.361840000
6	4.279747000	-0.806365000	6.619596000
6	5.674688000	-0.894403000	6.650764000
6	6.452914000	0.267311000	6.630596000
6	5.833324000	1.520172000	6.586961000
1	1.658481000	3.253014000	7.968333000
1	1.454588000	3.925545000	10.340134000
1	1.222717000	2.197616000	12.120290000
1	1.174822000	-0.221829000	11.501345000
1	-0.528136000	2.284286000	6.772406000
1	-1.458824000	3.957771000	5.208867000
1	-0.243527000	4.517541000	3.100244000
1	1.892747000	3.353105000	2.556959000
1	2.808461000	1.644128000	4.090267000
1	3.649932000	-1.698301000	6.626505000
1	6.158793000	-1.874405000	6.694415000
1	7.544152000	0.195159000	6.653166000
1	6.437467000	2.430820000	6.571461000
1	3.966865000	2.597429000	6.536844000
6	4.438932000	1.612564000	6.565830000
1	1.364188000	-0.902275000	9.115860000
6	-0.050198000	-1.382705000	6.110402000
1	-0.731120000	-0.544494000	5.854853000
6	-0.132017000	-2.386626000	4.938149000

1	-1.166789000	-2.755106000	4.851031000
1	0.505865000	-3.255081000	5.157228000
6	0.296356000	-1.837274000	3.553608000
6	-0.640510000	-2.059932000	7.353081000
6	-1.886745000	-1.674416000	7.864341000
6	0.047535000	-3.105929000	7.992417000
6	-2.434988000	-2.309521000	8.985513000
6	-0.501212000	-3.752647000	9.102717000
6	-1.745800000	-3.354553000	9.606176000
1	-2.435848000	-0.860950000	7.380963000
1	1.028810000	-3.404164000	7.614754000
1	-3.400625000	-1.978710000	9.377830000
1	0.047066000	-4.567426000	9.584422000
1	-2.174396000	-3.857462000	10.477280000
6	1.803185000	-1.620321000	3.368450000
8	2.321200000	-0.634558000	2.908792000
8	2.470817000	-2.742183000	3.672446000
6	3.882951000	-2.711163000	3.456014000
1	4.109694000	-2.546376000	2.391307000
1	4.349472000	-1.907510000	4.042532000
1	4.261698000	-3.689141000	3.779913000
6	-0.471962000	-0.650469000	3.157294000
7	-1.145303000	0.243521000	2.858785000
1	0.045099000	-2.624799000	2.818886000

4a



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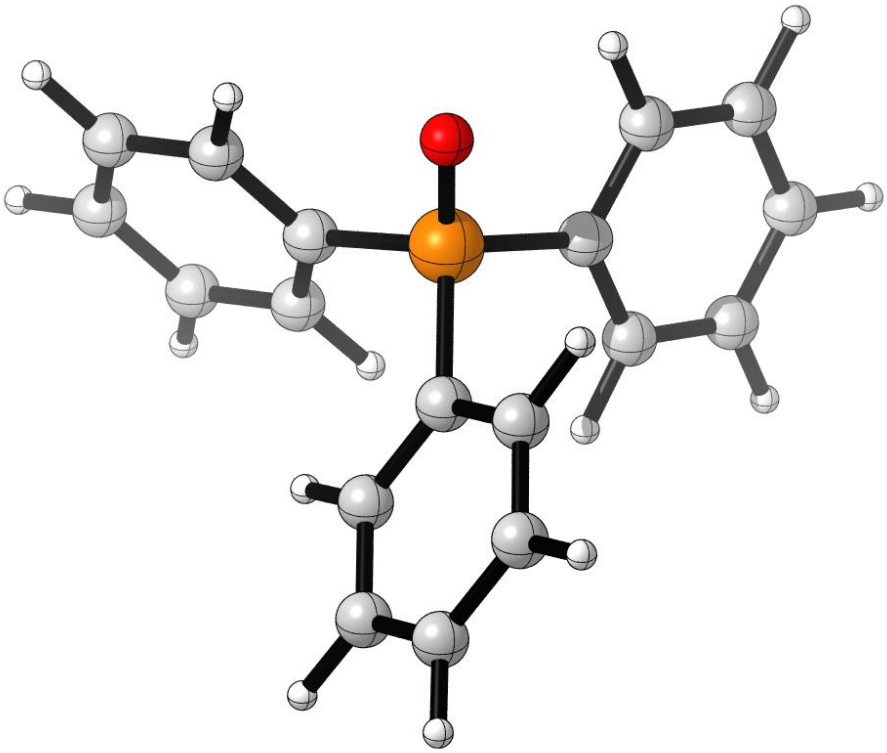
6	-0.002955955	-1.124462355	4.781516162
1	0.102857274	-1.325096162	3.696766075
6	-0.775679257	-2.309504501	5.443316801
1	-1.520011238	-2.777512641	4.784804384
1	-1.292741548	-1.949611412	6.345230146
6	0.358668978	-3.272441879	5.870097744
6	-0.691619944	0.222476133	4.936799250
6	-1.967573183	0.428231546	4.385559866
6	-0.079976913	1.276641308	5.629023524
6	-2.618703206	1.656024056	4.532391391
6	-0.731484401	2.505786954	5.776972725

6	-2.002401676	2.700321605	5.230523116
1	-2.459406759	-0.377936100	3.831919028
1	0.916779167	1.121887042	6.043989784
1	-3.610868960	1.799942832	4.096330694
1	-0.239662545	3.317112805	6.320874710
1	-2.512318935	3.660431772	5.347213474
6	1.523041817	-2.279244727	5.932487405
8	2.629343894	-2.688653919	6.541145476
6	3.743609391	-1.795101182	6.537186131
1	3.983115929	-1.475570917	5.511580188
1	3.521259453	-0.898062556	7.136293380
1	4.581323159	-2.350266287	6.977756625
6	0.638516378	-4.339298626	4.900045806
7	0.854882751	-5.163697640	4.114777198
1	0.187394924	-3.744277190	6.851314533

Ph_3PO



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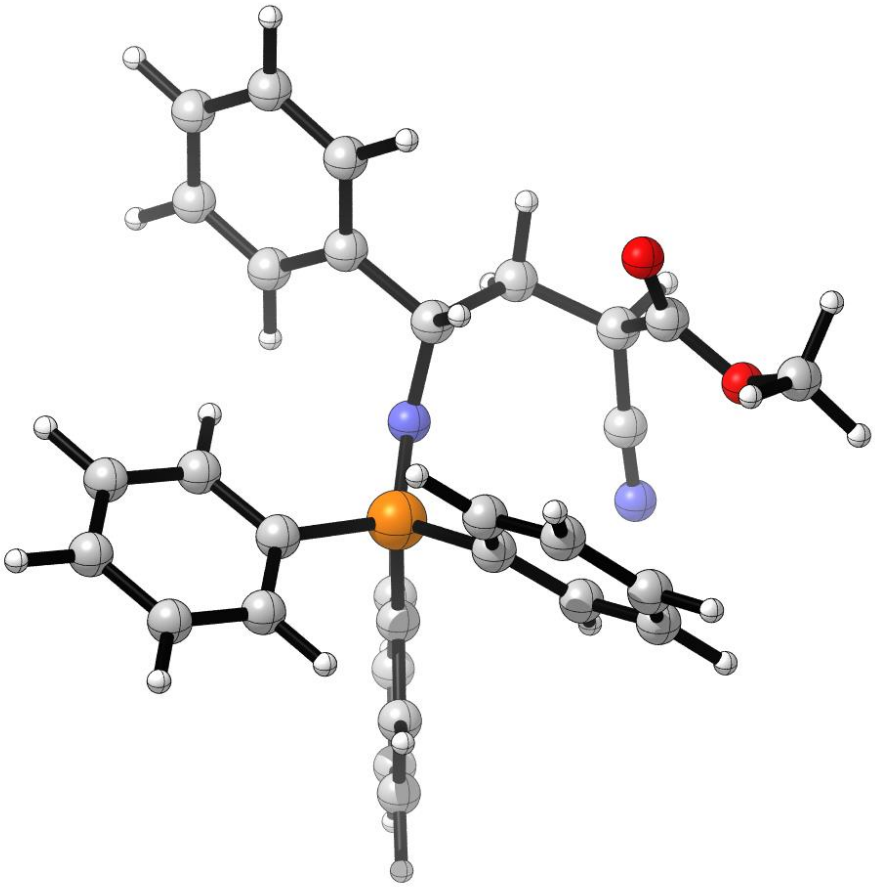
6	2.941927000	0.029708000	8.013225000
6	3.902502000	0.582134000	8.874341000
6	4.050317000	0.089533000	10.175685000
6	3.244029000	-0.960404000	10.622744000
6	2.286689000	-1.519849000	9.767961000
15	2.725143000	0.520219000	6.256626000
6	4.186717000	1.528218000	5.797455000
6	1.261900000	1.626772000	6.180198000
6	0.924596000	2.571648000	7.163117000
6	-0.195913000	3.392324000	6.992567000
6	-0.987938000	3.268987000	5.844832000

6	-0.664128000	2.318048000	4.870607000
6	0.452795000	1.494782000	5.038427000
6	5.066838000	0.940365000	4.875459000
6	6.215529000	1.624161000	4.466264000
6	6.493797000	2.895264000	4.978252000
6	5.616137000	3.488619000	5.892986000
1	4.555145000	1.387174000	8.530077000
1	4.805195000	0.522604000	10.837315000
1	3.370344000	-1.353896000	11.635078000
1	1.662737000	-2.348938000	10.113035000
1	1.524903000	2.660554000	8.073466000
1	-0.458741000	4.121876000	7.763586000
1	-1.866292000	3.906866000	5.713996000
1	-1.288299000	2.211577000	3.979116000
1	0.708642000	0.732632000	4.297949000
1	4.825861000	-0.050411000	4.482662000
1	6.896358000	1.162473000	3.745895000
1	7.391982000	3.429608000	4.657128000
1	5.831082000	4.483626000	6.291724000
1	3.767492000	3.298355000	6.988425000
6	4.460054000	2.813251000	6.294731000
1	1.419915000	-1.493162000	7.784833000
8	2.560709000	-0.665756000	5.341454000

2a_i17



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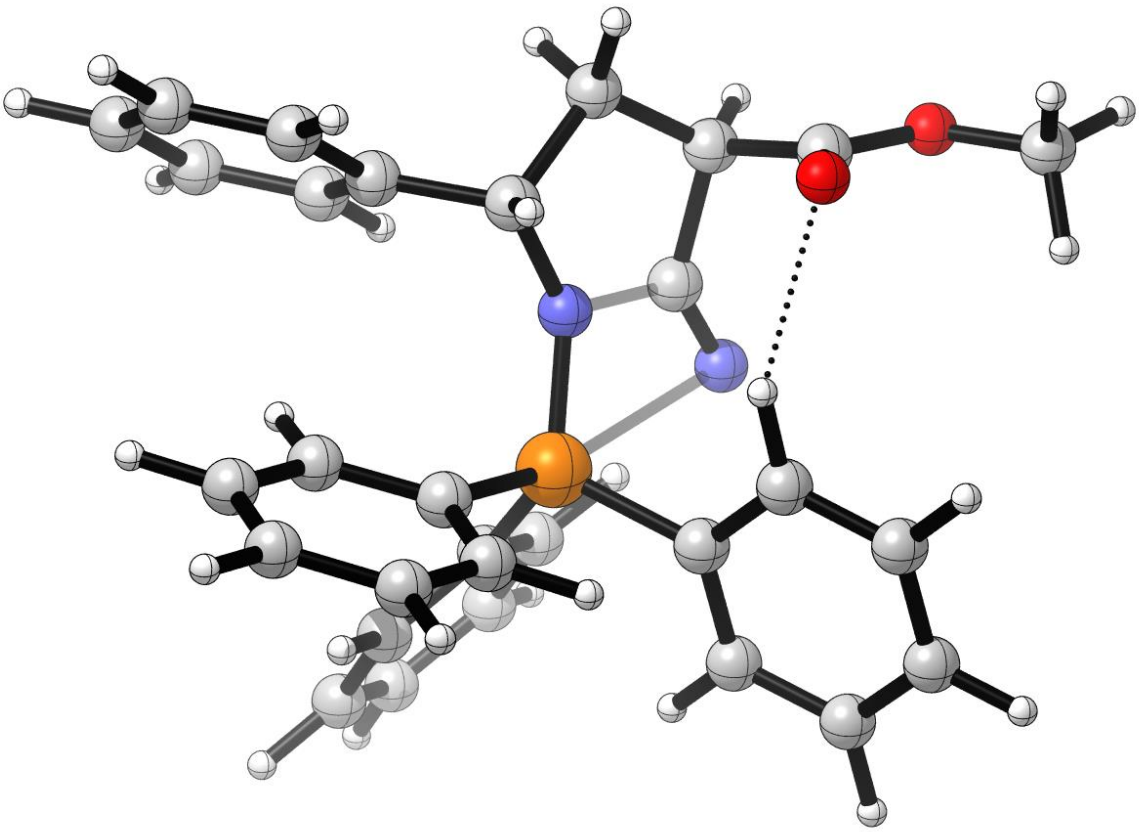
6	-5.481529000	-3.799248000	1.568127000
6	-6.173144000	-4.557927000	0.620303000
6	-5.609630000	-5.735916000	0.116474000
6	-4.359122000	-6.157302000	0.574880000
15	-3.230472000	-3.254962000	3.282445000
7	-1.713467000	-3.654000000	3.465201000
6	-4.054203000	-3.588718000	4.886001000
6	-3.613646000	-1.496545000	2.847774000
6	-3.699631000	-1.087189000	1.504071000
6	-3.949257000	0.250411000	1.181748000

6	-4.111669000	1.197164000	2.197671000
6	-3.997069000	0.805449000	3.535831000
6	-3.742379000	-0.529720000	3.861000000
6	-3.331231000	-4.267920000	5.876384000
6	-3.936703000	-4.579360000	7.097215000
6	-5.259472000	-4.201083000	7.343546000
6	-5.979536000	-3.507122000	6.365187000
1	-5.928741000	-2.872985000	1.935386000
1	-7.147912000	-4.218087000	0.260136000
1	-6.147799000	-6.323821000	-0.632233000
1	-3.908475000	-7.072502000	0.182008000
1	-3.592529000	-1.818247000	0.698999000
1	-4.030749000	0.551547000	0.133486000
1	-4.330673000	2.238363000	1.944361000
1	-4.114480000	1.540678000	4.336123000
1	-3.644531000	-0.820388000	4.909460000
1	-2.293907000	-4.535097000	5.669665000
1	-3.368085000	-5.111898000	7.864257000
1	-5.730024000	-4.444252000	8.300287000
1	-7.007910000	-3.191561000	6.560162000
1	-5.958514000	-2.670296000	4.380243000
6	-5.383572000	-3.210086000	5.136570000
1	-2.687986000	-5.725523000	1.875765000
6	-0.553168000	-3.369192000	2.657932000
1	-0.742125000	-2.608040000	1.877572000
6	0.608887000	-2.827235000	3.536335000

1	1.503040000	-2.723239000	2.905378000
1	0.838527000	-3.579474000	4.306638000
6	0.411706000	-1.463652000	4.234640000
6	0.012676000	-4.602747000	1.935643000
6	0.848423000	-4.443890000	0.818314000
6	-0.219644000	-5.899442000	2.415546000
6	1.430437000	-5.549909000	0.192239000
6	0.354174000	-7.010369000	1.787255000
6	1.182482000	-6.840503000	0.673265000
1	1.050051000	-3.437841000	0.436025000
1	-0.862534000	-6.022539000	3.290083000
1	2.074132000	-5.402353000	-0.679749000
1	0.152102000	-8.013312000	2.175543000
1	1.633797000	-7.706036000	0.180929000
6	-0.543597000	-1.449566000	5.350366000
1	1.382757000	-1.218464000	4.709339000
6	0.206902000	-0.311547000	3.236710000
8	0.542854000	-0.363396000	2.079815000
8	-0.310376000	0.771674000	3.823765000
6	-0.480361000	1.931516000	3.002664000
1	0.483020000	2.251088000	2.576600000
1	-1.180669000	1.722292000	2.182164000
1	-0.888172000	2.708066000	3.661247000
7	-1.224525000	-1.414569000	6.287487000

2a_i17_TS1 (**TS1**_trans_a1)



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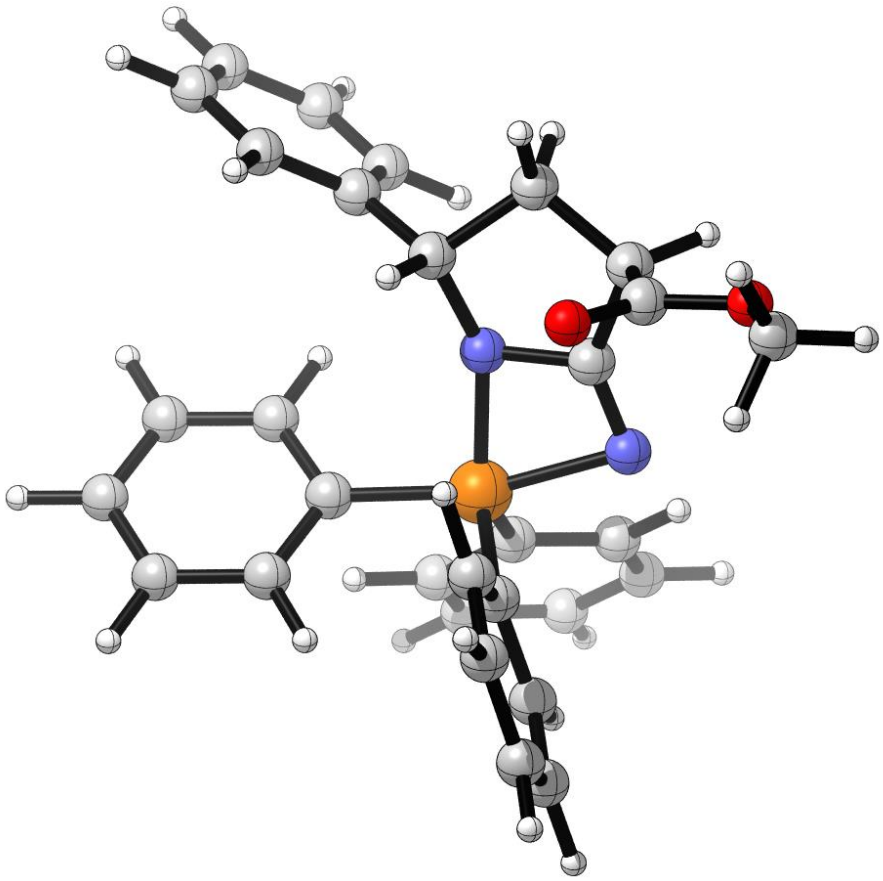
6	-4.599909000	-3.068507000	0.964490000
6	-5.119604000	-3.736990000	-0.149182000
6	-4.835710000	-5.088916000	-0.353728000
6	-4.032090000	-5.770973000	0.565470000
15	-3.106052000	-2.839449000	3.360879000
7	-1.438955000	-2.826863000	3.102399000
6	-3.770728000	-3.737817000	4.825107000
6	-3.848336000	-1.180406000	3.292439000
6	-3.338601000	-0.233460000	2.385975000
6	-3.912891000	1.036917000	2.310255000

6	-4.994796000	1.375456000	3.130333000
6	-5.504071000	0.432610000	4.029309000
6	-4.937757000	-0.841998000	4.112314000
6	-3.344506000	-3.391320000	6.122969000
6	-3.905691000	-4.025853000	7.233975000
6	-4.893984000	-5.002972000	7.072973000
6	-5.325745000	-5.346172000	5.788478000
1	-4.841211000	-2.015337000	1.109318000
1	-5.749296000	-3.192639000	-0.857893000
1	-5.242521000	-5.612653000	-1.222979000
1	-3.796243000	-6.827101000	0.412021000
1	-2.474969000	-0.467101000	1.760627000
1	-3.499120000	1.768829000	1.611184000
1	-5.440368000	2.371832000	3.070513000
1	-6.347287000	0.691011000	4.675547000
1	-5.335723000	-1.565051000	4.826593000
1	-2.591865000	-2.600600000	6.214103000
1	-3.565070000	-3.741756000	8.233689000
1	-5.333510000	-5.495048000	7.944986000
1	-6.103340000	-6.102088000	5.648747000
1	-5.133332000	-4.993897000	3.679222000
6	-4.769887000	-4.718785000	4.669458000
1	-2.901170000	-5.666881000	2.388199000
6	-0.530483000	-3.326655000	2.063919000
1	-0.842803000	-2.982058000	1.064790000
6	0.825886000	-2.625611000	2.452155000

1	1.361505000	-2.315380000	1.543784000
1	1.457358000	-3.354747000	2.980352000
6	0.515095000	-1.461646000	3.398315000
6	-0.350997000	-4.835745000	2.028033000
6	-0.192492000	-5.498753000	0.802838000
6	-0.279365000	-5.587193000	3.213835000
6	0.016644000	-6.881601000	0.757448000
6	-0.074703000	-6.968420000	3.171331000
6	0.070500000	-7.621903000	1.941568000
1	-0.245305000	-4.926929000	-0.128564000
1	-0.402574000	-5.083571000	4.176317000
1	0.138419000	-7.383228000	-0.206690000
1	-0.024956000	-7.538715000	4.103038000
1	0.235733000	-8.702242000	1.908095000
6	-0.877305000	-1.808219000	4.025693000
1	1.245353000	-1.344090000	4.208267000
6	0.352273000	-0.142382000	2.684932000
8	-0.177661000	0.002815000	1.600917000
8	0.826329000	0.878344000	3.415324000
6	0.579588000	2.196015000	2.930752000
1	0.881776000	2.293568000	1.876992000
1	-0.490448000	2.442497000	3.021145000
1	1.168495000	2.872237000	3.562303000
7	-1.546306000	-1.363366000	4.958202000

2a_i17_int



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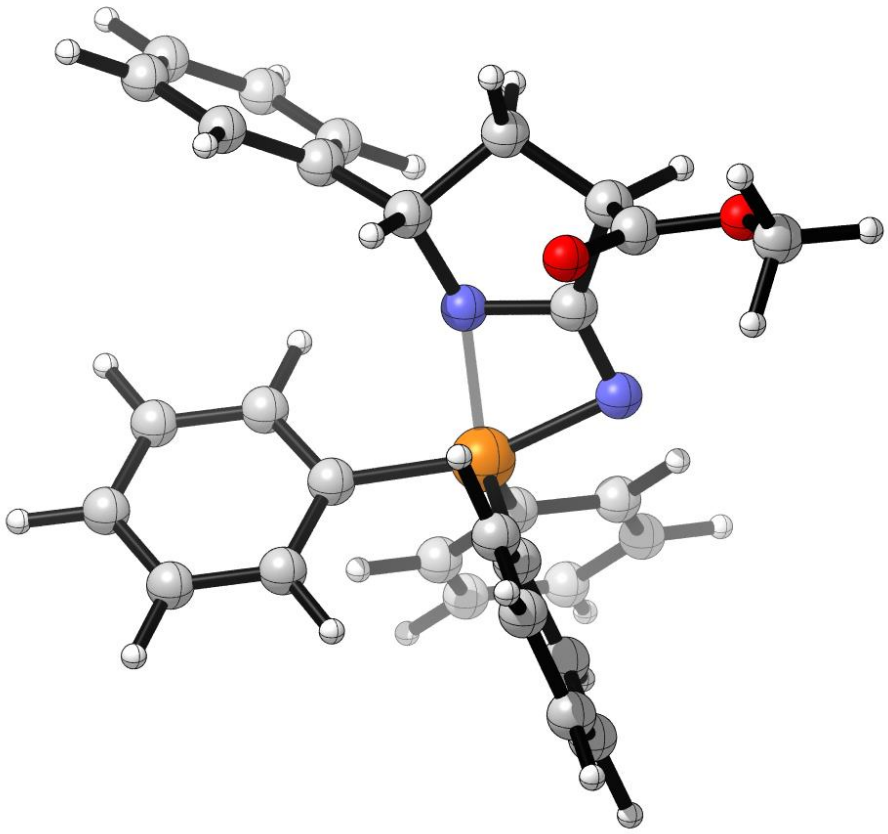
6	-3.852639000	-3.772022000	2.234868000
6	-4.875617000	-3.290443000	1.398011000
6	-5.393945000	-4.069992000	0.356893000
6	-4.900329000	-5.355504000	0.126947000
6	-3.896191000	-5.859482000	0.959748000
15	-3.112176000	-2.713195000	3.641679000
7	-1.381676000	-2.996622000	3.107473000
6	-3.936323000	-3.554528000	5.087101000
6	-3.940755000	-1.114421000	3.208532000
6	-3.451999000	-0.363282000	2.127693000
6	-4.049346000	0.853553000	1.791368000

6	-5.142737000	1.328718000	2.523669000
6	-5.622885000	0.589206000	3.608322000
6	-5.023370000	-0.627294000	3.954417000
6	-3.572863000	-3.193744000	6.401073000
6	-4.186574000	-3.800092000	7.500507000
6	-5.176218000	-4.770366000	7.313533000
6	-5.552250000	-5.129617000	6.016036000
1	-5.285465000	-2.292322000	1.549606000
1	-6.185752000	-3.662094000	-0.277903000
1	-5.298063000	-5.963485000	-0.690208000
1	-3.497003000	-6.863650000	0.793998000
1	-2.594344000	-0.715367000	1.549830000
1	-3.655190000	1.431749000	0.951284000
1	-5.616299000	2.275029000	2.249199000
1	-6.469962000	0.958931000	4.192889000
1	-5.404867000	-1.194232000	4.806731000
1	-2.809557000	-2.427969000	6.539789000
1	-3.884055000	-3.504029000	8.509208000
1	-5.656140000	-5.245517000	8.173569000
1	-6.328271000	-5.882906000	5.853806000
1	-5.247913000	-4.829247000	3.912330000
6	-4.936973000	-4.530004000	4.912843000
1	-2.622192000	-5.507775000	2.649175000
6	-0.388392000	-3.310001000	2.067285000
1	-0.616452000	-2.765967000	1.134896000
6	0.909411000	-2.707503000	2.719153000

1	1.615110000	-2.364073000	1.949416000
1	1.407798000	-3.496365000	3.302045000
6	0.458612000	-1.588147000	3.687386000
6	-0.178649000	-4.775731000	1.729809000
6	-0.029340000	-5.176358000	0.395496000
6	-0.050037000	-5.745828000	2.738340000
6	0.237096000	-6.511320000	0.070307000
6	0.210140000	-7.079590000	2.418256000
6	0.354550000	-7.468377000	1.080480000
1	-0.129288000	-4.434063000	-0.402041000
1	-0.168941000	-5.448339000	3.784433000
1	0.352819000	-6.805671000	-0.976789000
1	0.306280000	-7.821088000	3.216198000
1	0.565731000	-8.511069000	0.827573000
6	-0.968933000	-2.015074000	4.004070000
1	1.070029000	-1.514505000	4.596062000
6	0.433999000	-0.233721000	2.992933000
8	0.025327000	-0.055077000	1.867883000
8	0.937802000	0.740624000	3.761909000
6	0.962086000	2.053282000	3.194902000
1	1.634307000	2.086163000	2.323501000
1	-0.043378000	2.358650000	2.869767000
1	1.331743000	2.720083000	3.983935000
7	-1.913115000	-1.630517000	4.759888000

2a_i17_TS2



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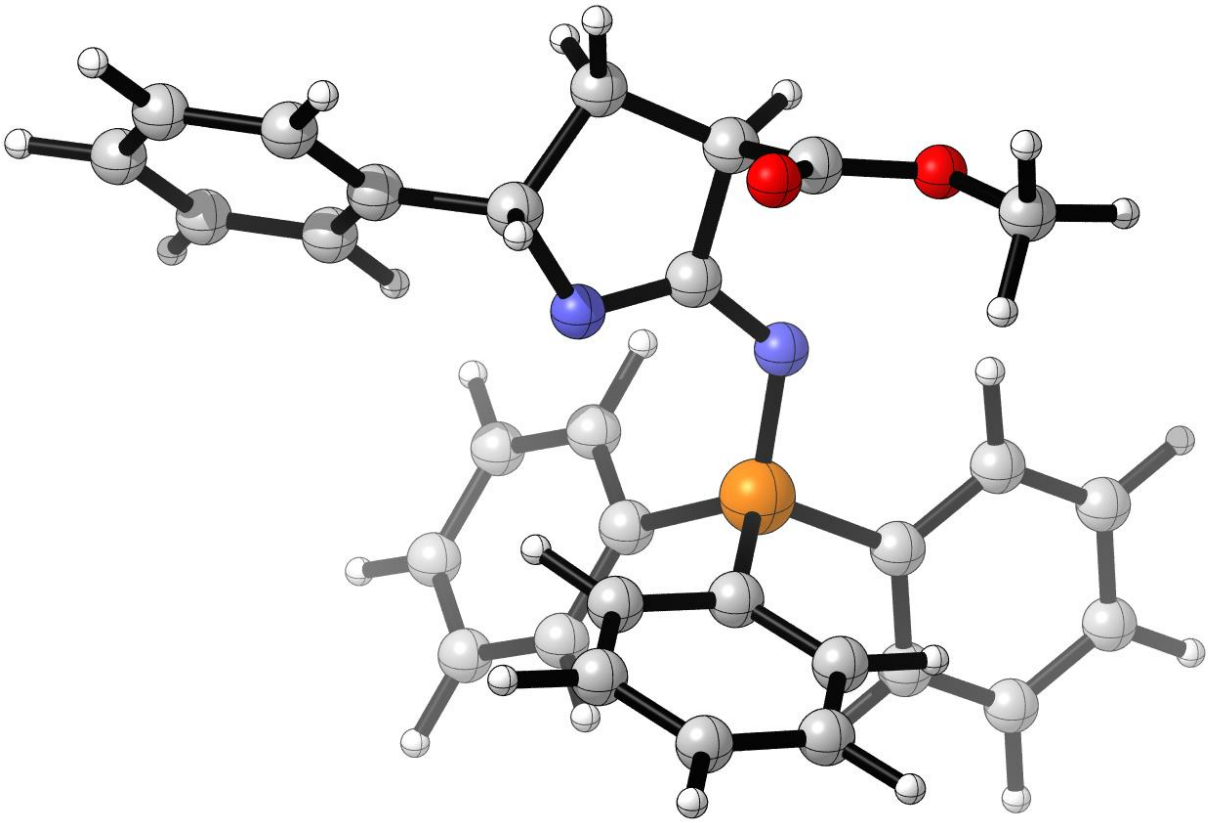
6	-3.366504000	-5.025175000	1.981291000
6	-3.891070000	-3.752713000	2.262661000
6	-4.975137000	-3.306789000	1.486352000
6	-5.493862000	-4.089659000	0.447678000
6	-4.941324000	-5.339997000	0.164797000
6	-3.876500000	-5.807827000	0.941721000
15	-3.150244000	-2.687439000	3.659172000
7	-1.346180000	-3.043733000	3.040747000
6	-3.964047000	-3.514729000	5.114317000
6	-4.010604000	-1.099491000	3.233853000
6	-3.538769000	-0.351348000	2.142625000
6	-4.143439000	0.862236000	1.809094000

6	-5.227839000	1.338000000	2.554831000
6	-5.691282000	0.602410000	3.649051000
6	-5.084074000	-0.611636000	3.992092000
6	-3.591812000	-3.135097000	6.420616000
6	-4.189985000	-3.734026000	7.532369000
6	-5.170193000	-4.717663000	7.364784000
6	-5.550956000	-5.098933000	6.074945000
1	-5.429125000	-2.335389000	1.680375000
1	-6.331632000	-3.710007000	-0.143977000
1	-5.338774000	-5.948931000	-0.651793000
1	-3.431553000	-6.784572000	0.734075000
1	-2.687681000	-0.704822000	1.555095000
1	-3.762170000	1.438270000	0.961592000
1	-5.706836000	2.282376000	2.283147000
1	-6.530966000	0.973159000	4.243628000
1	-5.452822000	-1.176343000	4.851446000
1	-2.829672000	-2.365163000	6.543202000
1	-3.881187000	-3.424107000	8.534991000
1	-5.637173000	-5.188545000	8.234267000
1	-6.316358000	-5.866189000	5.928704000
1	-5.261249000	-4.824291000	3.964203000
6	-4.951501000	-4.505868000	4.959506000
1	-2.544018000	-5.417485000	2.578878000
6	-0.324892000	-3.339322000	2.023419000
1	-0.537536000	-2.790861000	1.089104000
6	0.955557000	-2.731739000	2.701315000

1	1.676014000	-2.375799000	1.950621000
1	1.448964000	-3.517547000	3.292695000
6	0.464324000	-1.622239000	3.663505000
6	-0.106028000	-4.802112000	1.676513000
6	0.064331000	-5.192752000	0.341460000
6	0.000654000	-5.781677000	2.678544000
6	0.331466000	-6.525938000	0.009427000
6	0.261920000	-7.113753000	2.351734000
6	0.428287000	-7.491840000	1.013552000
1	-0.018890000	-4.443287000	-0.451418000
1	-0.136943000	-5.491801000	3.724529000
1	0.463893000	-6.812380000	-1.037920000
1	0.340580000	-7.862988000	3.144413000
1	0.640198000	-8.533013000	0.754858000
6	-0.964127000	-2.069728000	3.927352000
1	1.046971000	-1.547083000	4.590692000
6	0.446050000	-0.263708000	2.975616000
8	0.032803000	-0.075740000	1.854275000
8	0.967630000	0.701017000	3.745226000
6	1.014915000	2.013586000	3.179116000
1	1.693996000	2.036565000	2.312643000
1	0.016708000	2.333842000	2.846183000
1	1.389032000	2.674417000	3.971081000
7	-1.922825000	-1.674049000	4.676002000

3a



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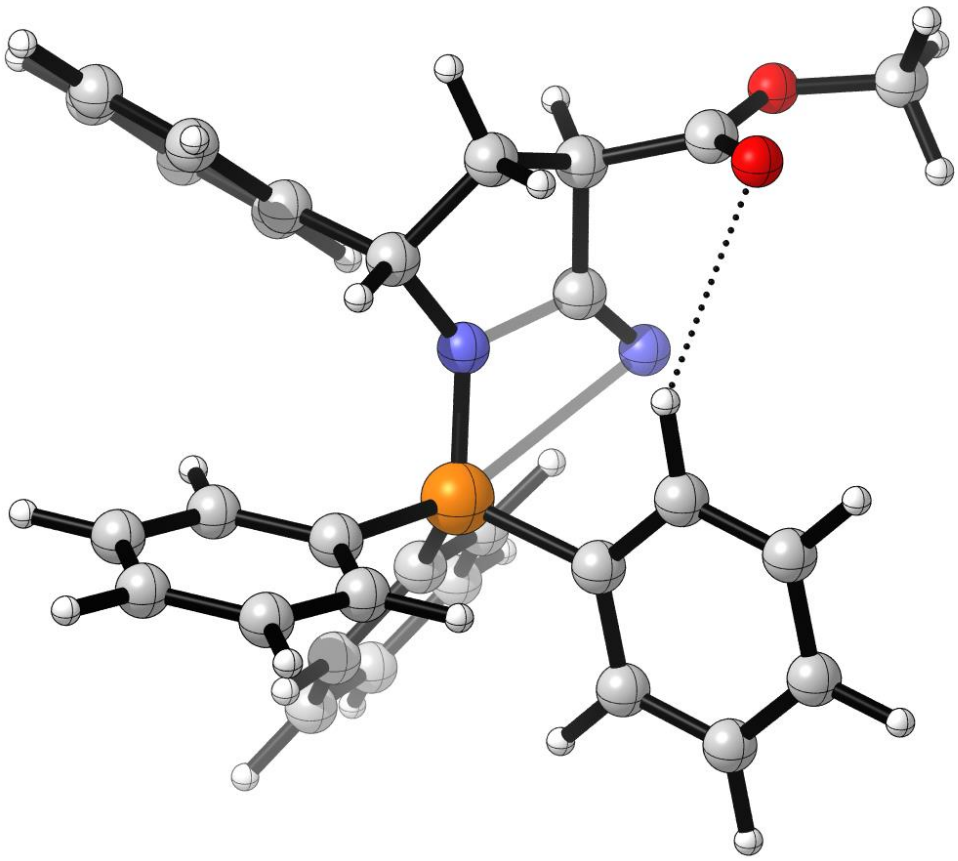
6	0.538975000	-2.898095000	-0.873133000
6	1.417999000	-2.877619000	-1.967633000
6	1.515367000	-3.989158000	-2.811684000
6	0.738673000	-5.125654000	-2.567084000
6	-0.144610000	-5.147443000	-1.480735000
15	0.342823000	-1.491358000	0.292953000
7	1.631605000	-3.337914000	2.279720000
6	-0.953917000	-0.415050000	-0.407661000
6	1.915788000	-0.551587000	0.271896000
6	3.139245000	-1.235531000	0.407374000
6	4.334002000	-0.517856000	0.502226000

6	4.321607000	0.880514000	0.478048000
6	3.107663000	1.564650000	0.363614000
6	1.908486000	0.854155000	0.261799000
6	-2.056838000	-0.059664000	0.384244000
6	-3.061486000	0.756997000	-0.145812000
6	-2.968050000	1.225618000	-1.460114000
6	-1.867330000	0.874395000	-2.250217000
1	2.043845000	-2.002172000	-2.158078000
1	2.207899000	-3.967914000	-3.657582000
1	0.830555000	-5.999241000	-3.218565000
1	-0.747229000	-6.037081000	-1.278174000
1	3.142017000	-2.324708000	0.473289000
1	5.278294000	-1.057824000	0.610780000
1	5.257812000	1.439472000	0.558842000
1	3.091846000	2.658060000	0.353709000
1	0.965859000	1.398795000	0.172767000
1	-2.106666000	-0.438230000	1.407180000
1	-3.919101000	1.031280000	0.474199000
1	-3.754046000	1.864794000	-1.871847000
1	-1.789017000	1.242995000	-3.276084000
1	-0.013164000	-0.219721000	-2.357731000
6	-0.864748000	0.053589000	-1.729272000
1	-0.918285000	-4.059499000	0.223807000
6	2.172259000	-3.999027000	3.465584000
1	2.983609000	-3.369880000	3.876302000
6	1.001723000	-4.010256000	4.495793000

1	1.352636000	-3.966926000	5.536691000
1	0.407416000	-4.928155000	4.361447000
6	0.163143000	-2.799218000	4.073487000
6	2.758470000	-5.369583000	3.180873000
6	3.681550000	-5.941728000	4.072205000
6	2.388453000	-6.096734000	2.040392000
6	4.221106000	-7.208652000	3.831941000
6	2.926952000	-7.364357000	1.796919000
6	3.847756000	-7.923572000	2.688461000
1	3.991690000	-5.382178000	4.960741000
1	1.687792000	-5.644124000	1.335828000
1	4.941332000	-7.635525000	4.536196000
1	2.628533000	-7.916017000	0.900545000
1	4.278289000	-8.909055000	2.490234000
6	0.557855000	-2.681769000	2.580685000
1	-0.924862000	-2.916809000	4.180750000
6	0.584171000	-1.502785000	4.742212000
8	1.686506000	-1.272708000	5.182965000
8	-0.409137000	-0.594293000	4.726552000
6	-0.057330000	0.730926000	5.120674000
1	-0.973550000	1.329407000	5.033922000
1	0.324146000	0.753591000	6.153513000
1	0.722057000	1.136543000	4.457288000
7	-0.187680000	-1.894785000	1.764419000

To Figure S9

TS1_trans_e1 (**2a**_i12_TS1)



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6	-0.974795000	3.525839000	0.942671000
6	-1.895242000	4.553260000	0.705994000
6	-2.521787000	5.197209000	1.776062000
6	-2.228100000	4.812022000	3.089540000
15	0.424943000	1.711248000	2.587248000
7	-0.566776000	0.498177000	3.124165000
6	1.719301000	2.289867000	3.754569000
6	1.239040000	1.280003000	1.014945000
6	0.711686000	0.266777000	0.196558000

6	1.315924000	-0.021586000	-1.027953000
6	2.440512000	0.697079000	-1.447935000
6	2.960088000	1.714223000	-0.641227000
6	2.366024000	2.004371000	0.590429000
6	2.535930000	1.337150000	4.394077000
6	3.532022000	1.762145000	5.277830000
6	3.735020000	3.124219000	5.521948000
6	2.943031000	4.072637000	4.868009000
1	-0.488637000	3.029339000	0.100813000
1	-2.123854000	4.853871000	-0.320082000
1	-3.238701000	6.000506000	1.585559000
1	-2.717478000	5.310211000	3.929721000
1	-0.144687000	-0.325406000	0.520332000
1	0.910657000	-0.825853000	-1.647093000
1	2.916754000	0.456510000	-2.402126000
1	3.838589000	2.278284000	-0.965276000
1	2.791138000	2.786407000	1.224414000
1	2.374843000	0.277386000	4.148405000
1	4.157617000	1.016810000	5.775283000
1	4.515130000	3.450684000	6.215852000
1	3.108341000	5.138819000	5.046613000
1	1.329895000	4.416133000	3.481977000
6	1.937111000	3.661912000	3.986409000
1	-1.106618000	3.478038000	4.360612000
6	-2.016508000	0.471091000	3.298443000
1	-2.522316000	1.183366000	2.628177000

6	-2.374353000	-0.977940000	2.838172000
1	-2.521609000	-0.985619000	1.746913000
1	-3.305596000	-1.324091000	3.308929000
6	-1.170615000	-1.854703000	3.174446000
6	0.098356000	-0.934286000	3.144472000
7	1.299421000	-1.116761000	3.082786000
6	-2.483734000	0.749967000	4.724459000
6	-3.825963000	1.098790000	4.949768000
6	-1.632519000	0.616714000	5.830081000
6	-4.309163000	1.297435000	6.245272000
6	-2.114367000	0.817586000	7.129244000
6	-3.453119000	1.155405000	7.342639000
1	-4.501996000	1.216985000	4.096612000
1	-0.586194000	0.349347000	5.668236000
1	-5.355526000	1.575375000	6.400546000
1	-1.437189000	0.701323000	7.979621000
1	-3.831216000	1.313410000	8.356552000
6	-0.926667000	-2.950040000	2.163796000
8	-1.196252000	-2.880396000	0.983200000
8	-0.309799000	-4.001595000	2.719443000
6	0.185861000	-4.988285000	1.817671000
1	-0.632736000	-5.448634000	1.242214000
1	0.900150000	-4.535589000	1.112661000
1	0.690965000	-5.742409000	2.435002000
1	-1.236365000	-2.300299000	4.178142000

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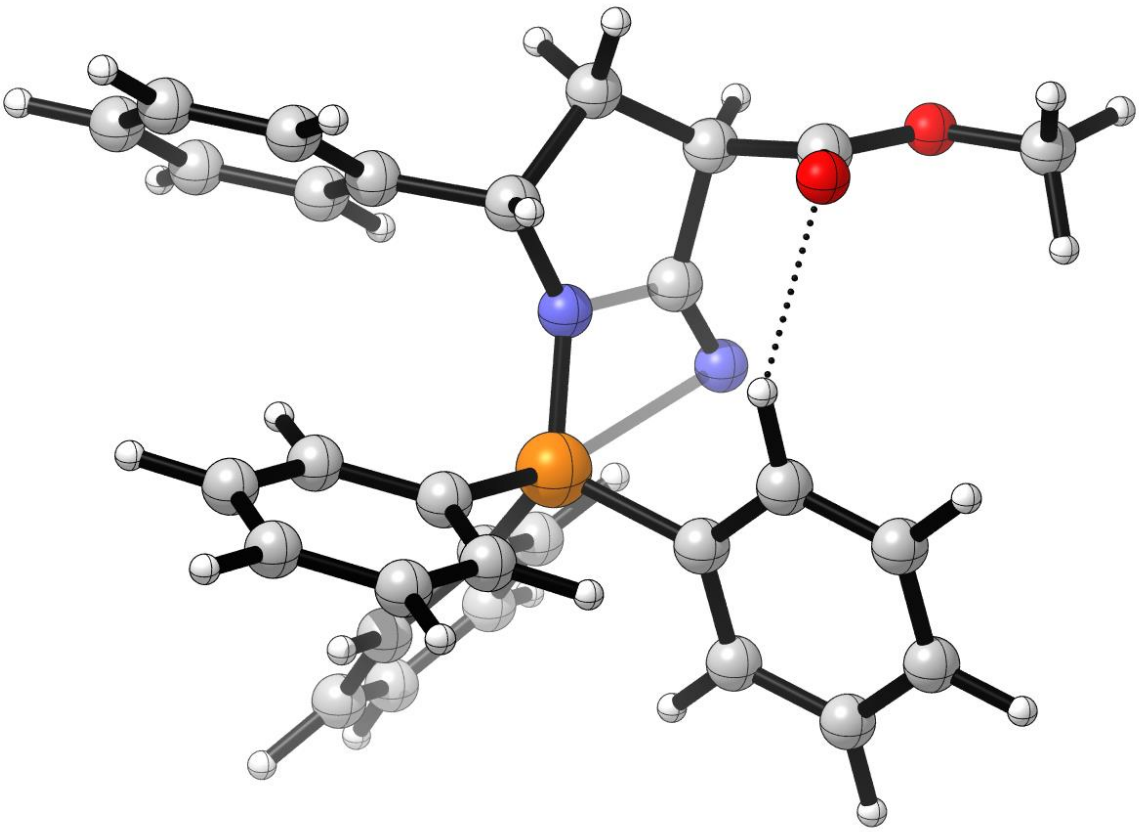

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6	-5.119604000	-3.736990000	-0.149182000
6	-4.835710000	-5.088916000	-0.353728000
6	-4.032090000	-5.770973000	0.565470000
15	-3.106052000	-2.839449000	3.360879000
7	-1.438955000	-2.826863000	3.102399000
6	-3.770728000	-3.737817000	4.825107000
6	-3.848336000	-1.180406000	3.292439000
6	-3.338601000	-0.233460000	2.385975000
6	-3.912891000	1.036917000	2.310255000

6	-4.994796000	1.375456000	3.130333000
6	-5.504071000	0.432610000	4.029309000
6	-4.937757000	-0.841998000	4.112314000
6	-3.344506000	-3.391320000	6.122969000
6	-3.905691000	-4.025853000	7.233975000
6	-4.893984000	-5.002972000	7.072973000
6	-5.325745000	-5.346172000	5.788478000
1	-4.841211000	-2.015337000	1.109318000
1	-5.749296000	-3.192639000	-0.857893000
1	-5.242521000	-5.612653000	-1.222979000
1	-3.796243000	-6.827101000	0.412021000
1	-2.474969000	-0.467101000	1.760627000
1	-3.499120000	1.768829000	1.611184000
1	-5.440368000	2.371832000	3.070513000
1	-6.347287000	0.691011000	4.675547000
1	-5.335723000	-1.565051000	4.826593000
1	-2.591865000	-2.600600000	6.214103000
1	-3.565070000	-3.741756000	8.233689000
1	-5.333510000	-5.495048000	7.944986000
1	-6.103340000	-6.102088000	5.648747000
1	-5.133332000	-4.993897000	3.679222000
6	-4.769887000	-4.718785000	4.669458000
1	-2.901170000	-5.666881000	2.388199000
6	-0.530483000	-3.326655000	2.063919000
1	-0.842803000	-2.982058000	1.064790000
6	0.825886000	-2.625611000	2.452155000

1	1.361505000	-2.315380000	1.543784000
1	1.457358000	-3.354747000	2.980352000
6	0.515095000	-1.461646000	3.398315000
6	-0.350997000	-4.835745000	2.028033000
6	-0.192492000	-5.498753000	0.802838000
6	-0.279365000	-5.587193000	3.213835000
6	0.016644000	-6.881601000	0.757448000
6	-0.074703000	-6.968420000	3.171331000
6	0.070500000	-7.621903000	1.941568000
1	-0.245305000	-4.926929000	-0.128564000
1	-0.402574000	-5.083571000	4.176317000
1	0.138419000	-7.383228000	-0.206690000
1	-0.024956000	-7.538715000	4.103038000
1	0.235733000	-8.702242000	1.908095000
6	-0.877305000	-1.808219000	4.025693000
1	1.245353000	-1.344090000	4.208267000
6	0.352273000	-0.142382000	2.684932000
8	-0.177661000	0.002815000	1.600917000
8	0.826329000	0.878344000	3.415324000
6	0.579588000	2.196015000	2.930752000
1	0.881776000	2.293568000	1.876992000
1	-0.490448000	2.442497000	3.021145000
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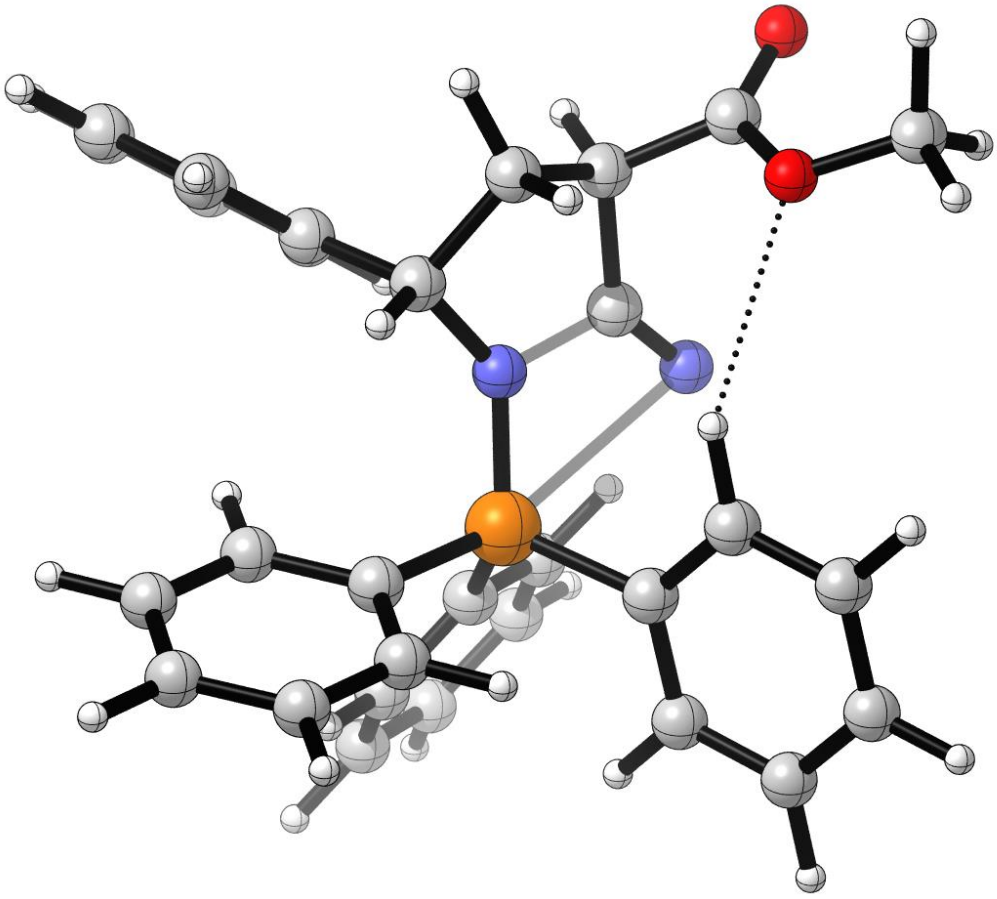

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6	-8.127167000	-1.353701000	4.445480000
6	-8.127990000	-0.660252000	5.658430000
6	-7.011966000	0.102805000	6.022565000
15	-4.468341000	-0.344566000	2.805827000
7	-3.202734000	-1.037089000	3.622819000
6	-4.362454000	1.442396000	2.382965000
6	-4.898708000	-1.245081000	1.283471000
6	-4.490820000	-2.575797000	1.088382000
6	-4.909553000	-3.266727000	-0.050260000

6	-5.740289000	-2.649918000	-0.993419000
6	-6.145700000	-1.326314000	-0.800909000
6	-5.725295000	-0.623328000	0.331707000
6	-3.247517000	1.931491000	1.672483000
6	-3.194473000	3.281662000	1.313618000
6	-4.240656000	4.148849000	1.644602000
6	-5.354993000	3.663568000	2.335770000
1	-7.044011000	-1.807318000	2.637685000
1	-8.990619000	-1.957224000	4.153512000
1	-8.994686000	-0.714121000	6.322930000
1	-6.999615000	0.639178000	6.974546000
1	-3.819810000	-3.057342000	1.801445000
1	-4.570609000	-4.293435000	-0.210523000
1	-6.067921000	-3.200053000	-1.879435000
1	-6.788595000	-0.834684000	-1.535940000
1	-6.044128000	0.412316000	0.469859000
1	-2.460513000	1.216107000	1.402691000
1	-2.328155000	3.656719000	0.761978000
1	-4.192844000	5.201426000	1.351626000
1	-6.181067000	4.332091000	2.592320000
1	-6.298987000	1.954479000	3.237087000
6	-5.418924000	2.316709000	2.704953000
1	-5.046157000	0.785101000	5.473926000
6	-3.083863000	-1.624052000	4.952499000
1	-4.029490000	-2.076613000	5.290701000
6	-2.042734000	-2.756050000	4.687862000

1	-2.570799000	-3.632214000	4.281679000
1	-1.532288000	-3.060608000	5.613752000
6	-1.089575000	-2.194560000	3.624499000
6	-1.957696000	-1.254791000	2.728755000
7	-1.858812000	-0.762194000	1.615086000
6	-2.603774000	-0.652799000	6.027582000
6	-2.822383000	-0.968642000	7.378304000
6	-1.899302000	0.521703000	5.719206000
6	-2.346706000	-0.141146000	8.398057000
6	-1.418033000	1.350325000	6.739355000
6	-1.638022000	1.023207000	8.080451000
1	-3.375677000	-1.877476000	7.635035000
1	-1.724215000	0.791176000	4.674932000
1	-2.533966000	-0.407664000	9.442521000
1	-0.865910000	2.257399000	6.478179000
1	-1.258848000	1.672623000	8.873367000
6	-0.394471000	-3.241780000	2.789920000
8	0.796623000	-3.333319000	2.629897000
8	-1.278090000	-4.099177000	2.222328000
6	-0.718951000	-5.078102000	1.350559000
1	-0.139428000	-4.597985000	0.547664000
1	-0.051483000	-5.759150000	1.902195000
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1	-0.291916000	-1.595336000	4.089602000

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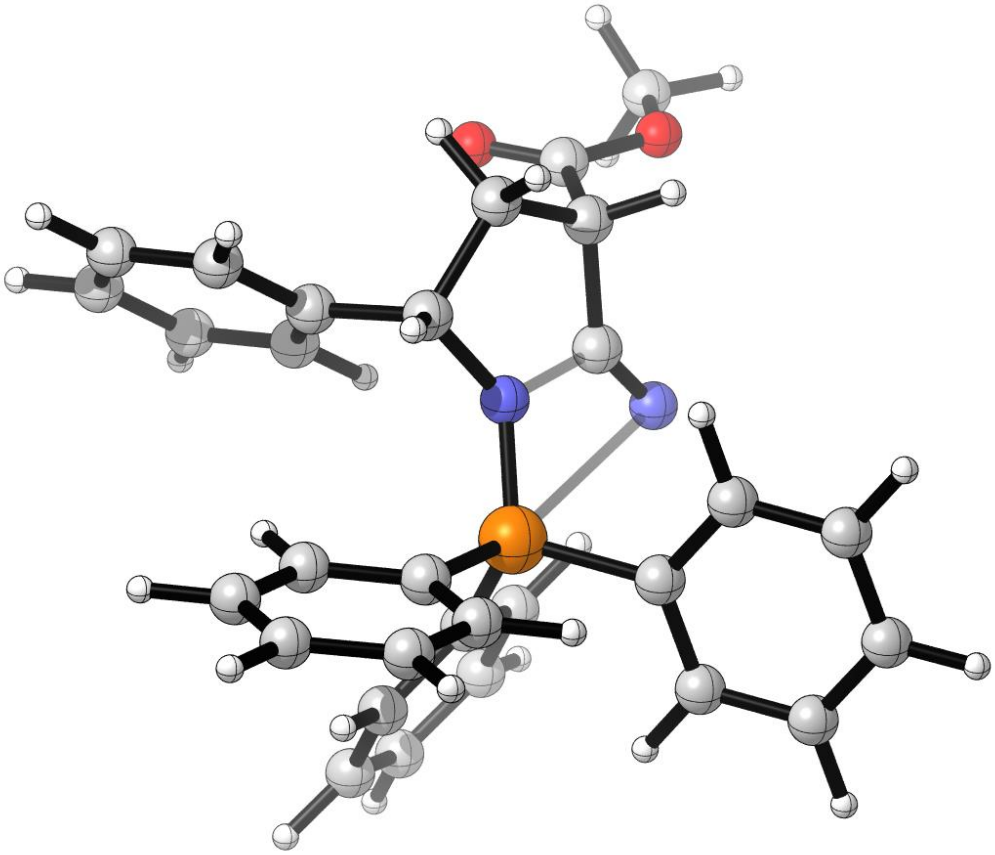

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6	-2.591363000	4.331320000	0.581724000
6	-3.313581000	4.887055000	1.640879000
6	-3.030605000	4.497079000	2.954707000
15	0.035024000	1.780132000	2.483272000
7	-0.692469000	0.405651000	3.036892000
6	1.266282000	2.588804000	3.581855000
6	0.863273000	1.433148000	0.897529000
6	0.358740000	0.419799000	0.065724000
6	0.952611000	0.168971000	-1.170465000

6	2.051592000	0.928020000	-1.589366000
6	2.544873000	1.949820000	-0.773030000
6	1.954375000	2.205498000	0.468729000
6	2.371401000	1.838938000	4.035925000
6	3.324117000	2.440069000	4.862714000
6	3.192087000	3.779421000	5.245497000
6	2.103673000	4.527312000	4.787638000
1	-1.011981000	2.981326000	-0.002546000
1	-2.813090000	4.631310000	-0.446011000
1	-4.098387000	5.621730000	1.441079000
1	-3.596602000	4.920722000	3.787677000
1	-0.483556000	-0.186923000	0.401377000
1	0.565201000	-0.632796000	-1.804422000
1	2.525830000	0.716023000	-2.551105000
1	3.401946000	2.545730000	-1.097391000
1	2.357880000	2.993253000	1.108881000
1	2.446784000	0.789192000	3.717925000
1	4.174387000	1.849912000	5.214759000
1	3.938102000	4.241460000	5.898453000
1	1.992756000	5.574078000	5.082723000
1	0.316723000	4.549907000	3.592820000
6	1.147039000	3.941428000	3.953100000
1	-1.828341000	3.256160000	4.240895000
6	-2.041354000	0.158172000	3.522968000
1	-2.791487000	0.651955000	2.883224000
6	-2.193253000	-1.397757000	3.336548000

1	-2.759888000	-1.587436000	2.411748000
1	-2.767343000	-1.819337000	4.172148000
6	-0.798302000	-2.025465000	3.225852000
1	-0.704534000	-2.678000000	2.346153000
6	0.255343000	-0.889051000	3.037126000
7	1.458544000	-0.839711000	2.893219000
6	-2.311571000	0.594063000	4.960418000
6	-3.633081000	0.856335000	5.358856000
6	-1.289767000	0.697789000	5.913975000
6	-3.929902000	1.210187000	6.677923000
6	-1.583888000	1.059084000	7.232674000
6	-2.902500000	1.313490000	7.620962000
1	-4.443839000	0.780847000	4.626386000
1	-0.260109000	0.485009000	5.621577000
1	-4.963682000	1.414911000	6.971869000
1	-0.774107000	1.137659000	7.962941000
1	-3.130952000	1.599013000	8.651589000
6	-0.381866000	-2.826354000	4.440215000
8	-0.709378000	-2.595519000	5.581677000
8	0.447971000	-3.825637000	4.095437000
6	1.045057000	-4.549105000	5.166957000
1	1.638667000	-3.876003000	5.805920000
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1	1.696157000	-5.301552000	4.702840000

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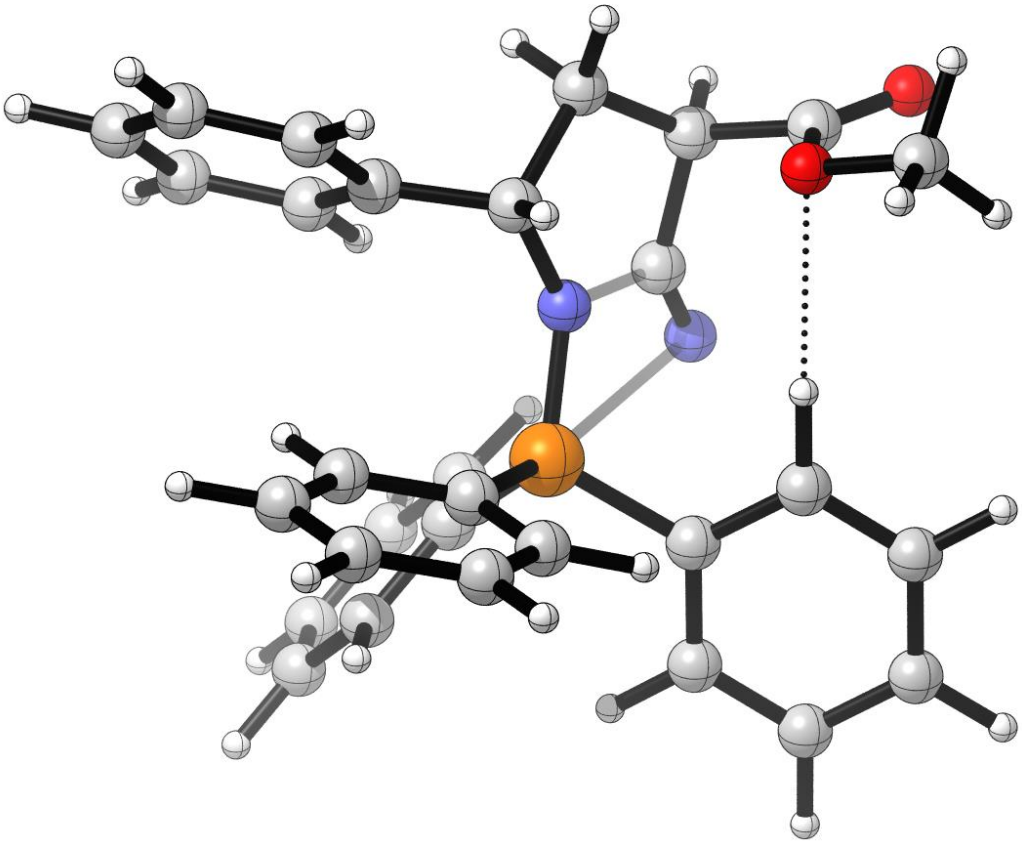

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6	3.467445000	-2.025902000	-0.940188000
6	4.741716000	-1.969579000	-1.513704000
6	5.711627000	-2.913421000	-1.163868000
6	5.404913000	-3.915665000	-0.236781000
15	1.489560000	-3.065606000	0.775232000
7	1.685221000	-2.433375000	2.304338000
6	0.920467000	-4.807817000	0.686093000
6	0.392849000	-2.066425000	-0.282897000
6	0.202625000	-0.696013000	-0.038261000
6	-0.639800000	0.046470000	-0.866174000

6	-1.280057000	-0.558538000	-1.955087000
6	-1.068021000	-1.914144000	-2.217885000
6	-0.236695000	-2.669295000	-1.385118000
6	-0.111586000	-5.241662000	1.540118000
6	-0.582025000	-6.554695000	1.447513000
6	-0.049580000	-7.434285000	0.499530000
6	0.963530000	-7.001911000	-0.361748000
1	2.712681000	-1.293559000	-1.232092000
1	4.974128000	-1.188971000	-2.242788000
1	6.705512000	-2.869456000	-1.616902000
1	6.158048000	-4.657138000	0.041973000
1	0.693993000	-0.222897000	0.811907000
1	-0.820462000	1.101449000	-0.642389000
1	-1.944138000	0.027732000	-2.595593000
1	-1.560718000	-2.396465000	-3.066164000
1	-0.093289000	-3.731810000	-1.592812000
1	-0.560515000	-4.511092000	2.221394000
1	-1.383845000	-6.885365000	2.113264000
1	-0.432764000	-8.455679000	0.423575000
1	1.378450000	-7.683118000	-1.109170000
1	2.241338000	-5.373707000	-0.950219000
6	1.451176000	-5.694798000	-0.269323000
1	3.915970000	-4.757451000	1.069573000
6	2.866257000	-2.122146000	3.110870000
1	3.503340000	-1.377513000	2.604799000
6	2.230072000	-1.475376000	4.397665000

1	2.866422000	-0.656774000	4.762084000
1	2.199004000	-2.238144000	5.189465000
6	0.793331000	-1.050627000	4.070209000
6	3.727072000	-3.305349000	3.526195000
6	5.109101000	-3.137607000	3.693295000
6	3.156614000	-4.546422000	3.858970000
6	5.904609000	-4.178202000	4.184583000
6	3.950329000	-5.591369000	4.339438000
6	5.328826000	-5.411111000	4.506361000
1	5.568797000	-2.178527000	3.434766000
1	2.079756000	-4.692019000	3.740768000
1	6.978150000	-4.020551000	4.322574000
1	3.486937000	-6.547995000	4.598005000
1	5.948134000	-6.225773000	4.890829000
6	0.341494000	-1.999603000	2.908174000
1	0.102598000	-1.208450000	4.907066000
6	0.647075000	0.402941000	3.687085000
8	-0.222590000	1.148065000	4.061878000
8	1.638572000	0.811504000	2.842011000
6	1.621031000	2.189853000	2.474853000
1	0.670510000	2.460796000	1.989923000
1	1.750305000	2.831757000	3.360365000
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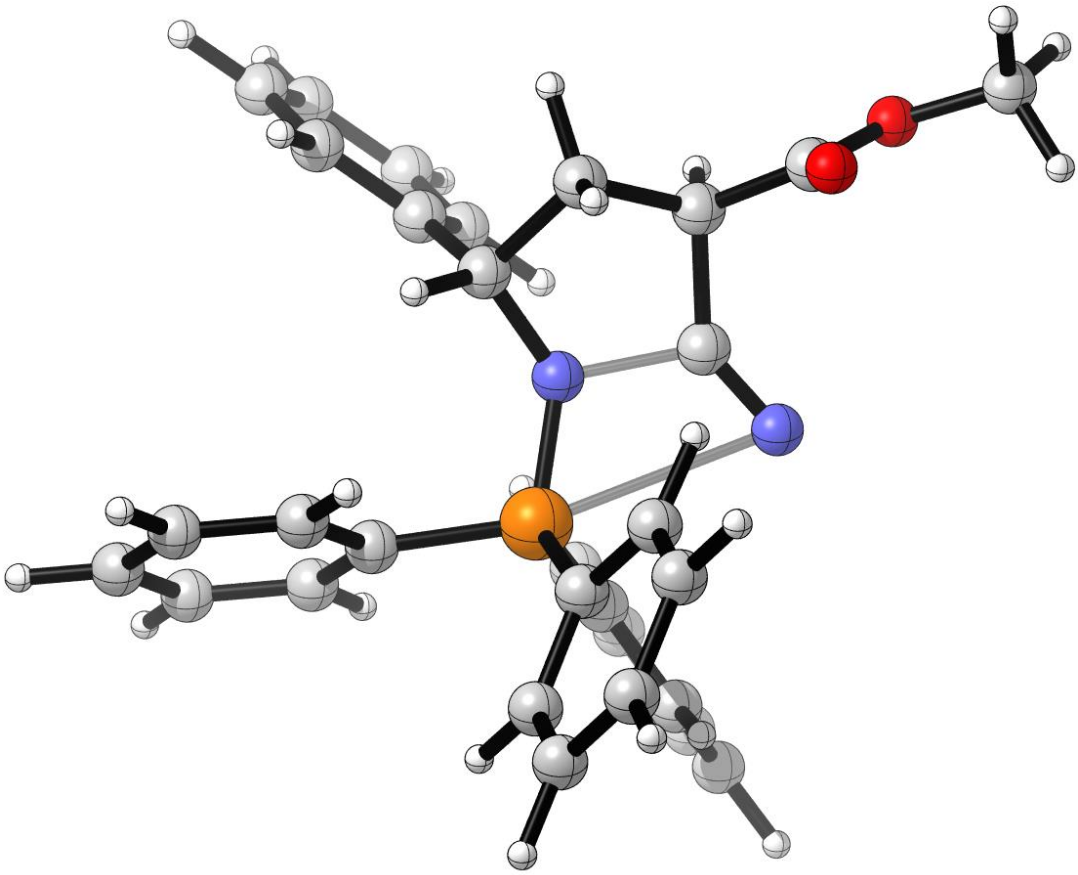
7	-0.727198000	-2.379693000	2.451976000

TS1_trans_e2



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6	-3.267934000	4.329148000	2.491021000
6	-4.090943000	3.612390000	1.614462000
6	-3.640667000	2.406417000	1.071267000
15	0.148584000	2.032632000	2.568317000
7	0.108415000	0.444012000	2.991645000
6	1.055490000	3.163674000	3.690023000
6	1.117306000	2.128861000	1.012734000
6	0.512241000	2.216141000	-0.252463000
6	1.291180000	2.221466000	-1.412804000

6	2.683630000	2.144108000	-1.328299000
6	3.296811000	2.072253000	-0.073306000
6	2.523136000	2.069145000	1.088726000
6	1.473102000	2.756537000	4.967361000
6	2.276979000	3.602407000	5.737855000
6	2.654572000	4.857487000	5.251559000
6	2.223463000	5.275668000	3.988291000
1	-1.370069000	4.408562000	3.512653000
1	-3.626247000	5.257487000	2.942852000
1	-5.083867000	3.991203000	1.358451000
1	-4.286274000	1.830045000	0.403066000
1	-0.572251000	2.289674000	-0.340516000
1	0.800240000	2.291474000	-2.386984000
1	3.291450000	2.146922000	-2.236540000
1	4.386454000	2.023400000	0.005224000
1	3.021623000	2.031810000	2.060487000
1	1.152139000	1.796721000	5.371540000
1	2.606385000	3.272846000	6.726289000
1	3.281814000	5.515222000	5.859646000
1	2.518514000	6.254691000	3.601754000
1	1.122230000	4.757245000	2.210330000
6	1.432751000	4.430553000	3.206265000
1	-2.036630000	0.966303000	0.981903000
6	1.030764000	-0.654368000	2.745342000
1	2.044137000	-0.304145000	2.486119000
6	1.086276000	-1.359585000	4.141289000

1	1.829970000	-0.856205000	4.778924000
1	1.378181000	-2.415420000	4.044545000
6	-0.299333000	-1.165269000	4.763429000
6	-0.705330000	0.285160000	4.412299000
7	-1.294452000	1.222683000	4.903587000
6	0.586130000	-1.622286000	1.649928000
6	1.550743000	-2.412907000	1.006080000
6	-0.762867000	-1.809310000	1.310849000
6	1.183276000	-3.365947000	0.051696000
6	-1.134893000	-2.766425000	0.358667000
6	-0.164654000	-3.547832000	-0.275382000
1	2.607292000	-2.282322000	1.262253000
1	-1.524799000	-1.200035000	1.801841000
1	1.952287000	-3.968448000	-0.438819000
1	-2.190898000	-2.905315000	0.108705000
1	-0.458264000	-4.293558000	-1.019438000
1	-1.033464000	-1.856267000	4.321755000
6	-0.325486000	-1.335540000	6.266234000
8	0.533666000	-0.959082000	7.028629000
8	-1.453162000	-1.954779000	6.659516000
6	-1.670859000	-2.062828000	8.064689000
1	-0.812259000	-2.536416000	8.564485000
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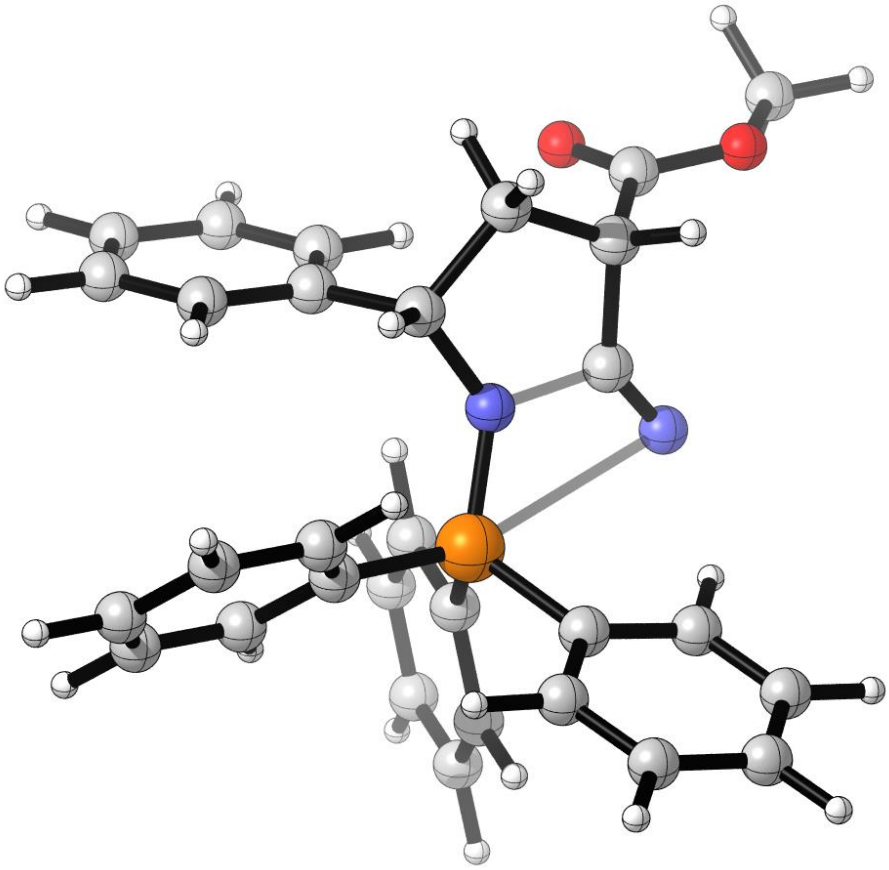

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6	-3.293936000	3.768850000	2.704523000
6	-4.057905000	2.984827000	1.833832000
6	-3.486035000	1.866028000	1.217329000
15	0.399325000	1.965506000	2.501467000
7	0.759618000	0.379425000	2.253008000
6	0.907020000	2.626377000	4.142481000
6	1.274183000	2.946537000	1.229053000
6	0.563840000	3.689926000	0.271313000
6	1.245181000	4.411692000	-0.714641000

6	2.641646000	4.403085000	-0.754493000
6	3.358251000	3.663283000	0.194232000
6	2.682553000	2.935904000	1.176276000
6	0.310689000	2.102998000	5.309411000
6	0.693029000	2.587003000	6.562986000
6	1.657970000	3.593046000	6.675389000
6	2.234319000	4.131565000	5.521732000
1	-1.364842000	4.064446000	3.625667000
1	-3.741016000	4.634815000	3.199688000
1	-5.099683000	3.248625000	1.631747000
1	-4.083463000	1.241232000	0.548233000
1	-0.527798000	3.701744000	0.287879000
1	0.675285000	4.979898000	-1.453982000
1	3.175829000	4.967790000	-1.523011000
1	4.451527000	3.651494000	0.166877000
1	3.256272000	2.362276000	1.908627000
1	-0.427047000	1.298348000	5.204867000
1	0.228007000	2.163477000	7.457285000
1	1.960755000	3.965369000	7.658349000
1	2.977181000	4.929985000	5.600105000
1	2.314223000	4.105079000	3.377925000
6	1.859557000	3.656766000	4.261036000
1	-1.710012000	0.654204000	0.990501000
6	1.548992000	-0.294781000	1.222526000
1	2.535868000	0.180945000	1.107346000
6	1.779195000	-1.733989000	1.826910000

1	2.827671000	-1.821231000	2.147948000
1	1.610678000	-2.489707000	1.048087000
6	0.855811000	-1.954572000	3.033836000
6	0.045032000	-0.663822000	3.325158000
7	-0.838925000	-0.340808000	4.079639000
6	0.919839000	-0.336444000	-0.169851000
6	1.532399000	0.335787000	-1.237772000
6	-0.241674000	-1.086242000	-0.431030000
6	1.008864000	0.263145000	-2.533958000
6	-0.762602000	-1.164146000	-1.725651000
6	-0.139076000	-0.492873000	-2.783353000
1	2.438684000	0.919724000	-1.055748000
1	-0.714923000	-1.656694000	0.370683000
1	1.507443000	0.793195000	-3.350080000
1	-1.655666000	-1.767543000	-1.911787000
1	-0.545870000	-0.566753000	-3.796001000
6	-0.143619000	-3.080008000	2.862520000
8	-0.771566000	-3.310886000	1.851737000
8	-0.290395000	-3.792247000	3.989471000
6	-1.331323000	-4.767889000	3.983744000
1	-2.309827000	-4.279851000	3.852672000
1	-1.187184000	-5.494978000	3.169891000
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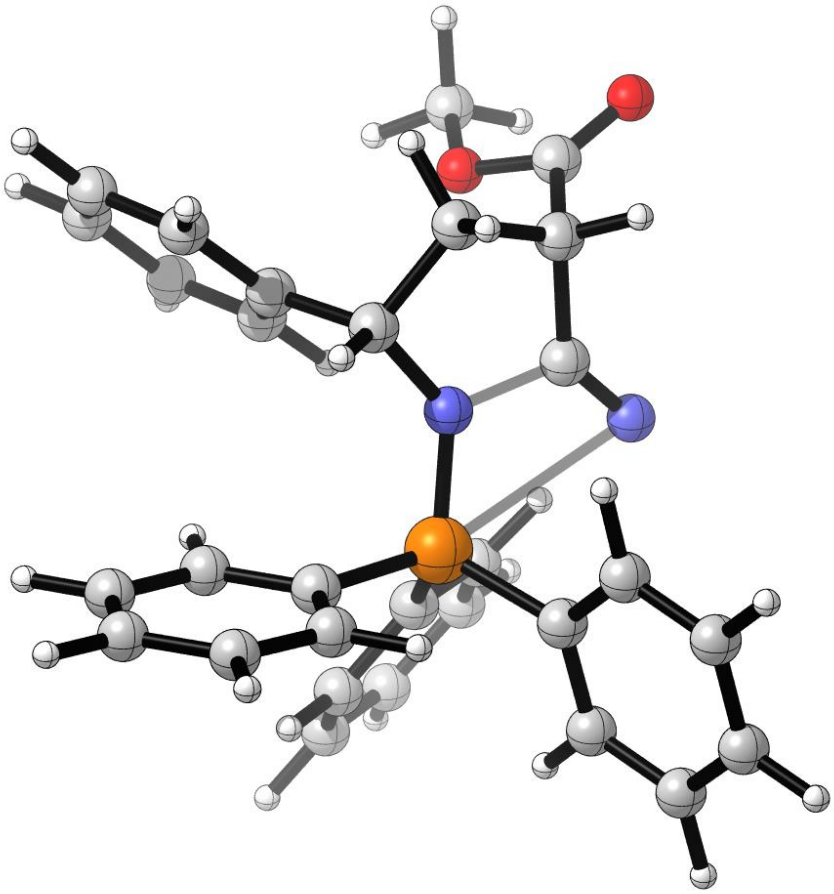

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6	-2.245660000	1.902830000	-0.556108000
6	-2.408754000	3.290846000	-0.590344000
6	-1.297751000	4.132353000	-0.494530000
6	-0.019229000	3.581728000	-0.355383000
15	-0.765204000	-0.471137000	-0.233215000
7	-0.587916000	-0.728312000	1.390923000
6	0.638075000	-0.985379000	-1.292863000
6	-2.269298000	-1.246978000	-0.909049000
6	-3.421314000	-1.375138000	-0.113805000
6	-4.606862000	-1.856657000	-0.671064000

6	-4.655590000	-2.218994000	-2.022601000
6	-3.509216000	-2.102198000	-2.813119000
6	-2.320713000	-1.615369000	-2.263408000
6	1.230125000	-2.244202000	-1.072027000
6	2.282148000	-2.666047000	-1.888939000
6	2.738945000	-1.859044000	-2.935518000
6	2.136653000	-0.619184000	-3.172320000
1	-3.121860000	1.258867000	-0.646808000
1	-3.409846000	3.715799000	-0.701633000
1	-1.428733000	5.217584000	-0.528317000
1	0.855166000	4.232038000	-0.274783000
1	-3.380490000	-1.116028000	0.945740000
1	-5.495245000	-1.963877000	-0.043273000
1	-5.581894000	-2.604571000	-2.456583000
1	-3.535352000	-2.400797000	-3.864155000
1	-1.430431000	-1.534266000	-2.889887000
1	0.810507000	-2.883829000	-0.286337000
1	2.740522000	-3.641297000	-1.705927000
1	3.560477000	-2.198323000	-3.572731000
1	2.482285000	0.013177000	-3.994297000
1	0.624761000	0.785706000	-2.560388000
6	1.089335000	-0.180806000	-2.356239000
1	1.151081000	1.785116000	-0.172711000
6	-0.455486000	0.214393000	2.492502000
1	-1.139969000	1.071715000	2.369621000
6	-0.961751000	-0.630117000	3.719680000

1	-2.022115000	-0.389307000	3.893234000
1	-0.411210000	-0.347558000	4.627984000
6	-0.840845000	-2.127437000	3.378631000
1	-1.725911000	-2.687092000	3.706982000
6	-0.755783000	-2.255203000	1.830656000
7	-0.797600000	-3.163582000	1.024770000
6	0.942326000	0.790073000	2.719621000
6	1.088900000	1.886091000	3.585802000
6	2.091922000	0.241471000	2.137410000
6	2.351824000	2.403520000	3.886678000
6	3.357771000	0.765060000	2.424409000
6	3.494417000	1.840220000	3.308624000
1	0.201518000	2.337492000	4.041055000
1	1.991882000	-0.621934000	1.478627000
1	2.446174000	3.251230000	4.571303000
1	4.241721000	0.317612000	1.960798000
1	4.483007000	2.241151000	3.549362000
6	0.336978000	-2.839022000	4.018546000
8	0.274072000	-3.851462000	4.670267000
8	1.500254000	-2.201852000	3.758785000
6	2.692538000	-2.794555000	4.262198000
1	2.724540000	-2.743212000	5.362644000
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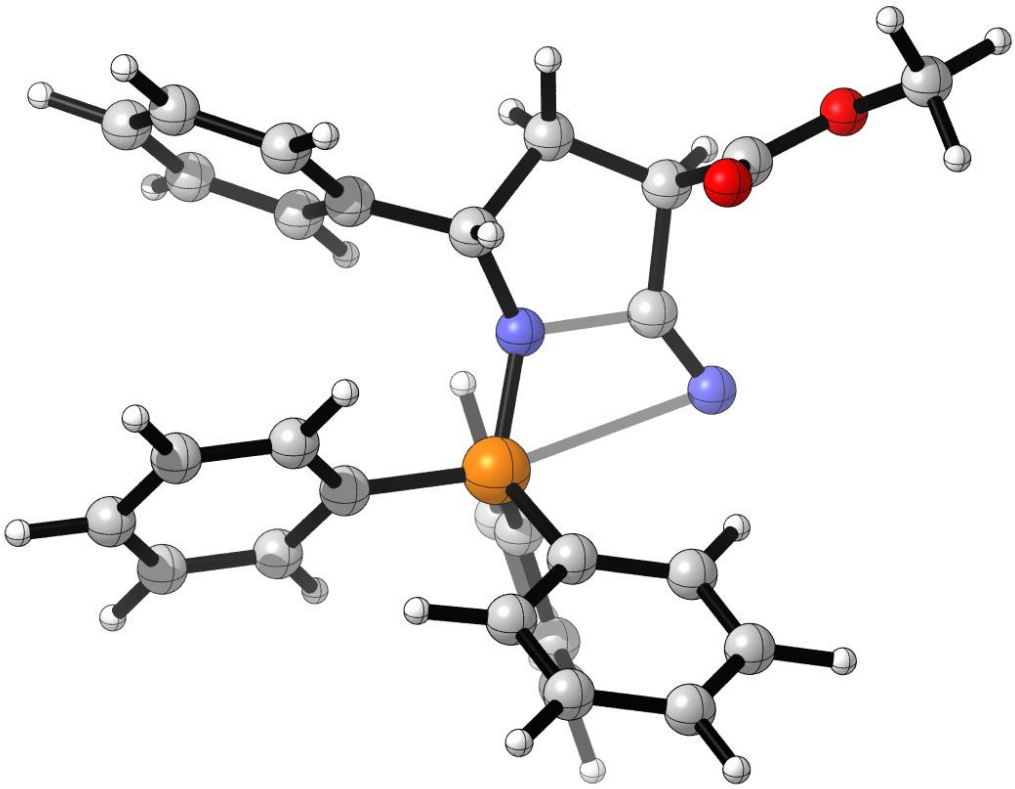

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6	-3.066333000	4.552381000	2.346337000
6	-4.076443000	3.711977000	1.870754000
6	-3.811085000	2.351255000	1.677800000
15	0.143821000	1.991793000	2.678265000
7	0.013547000	0.415977000	3.180475000
6	1.124071000	3.201661000	3.666945000
6	0.921175000	1.986942000	1.017488000
6	0.265675000	2.569313000	-0.080242000
6	0.858662000	2.562145000	-1.346518000

6	2.111386000	1.974407000	-1.533379000
6	2.777329000	1.401845000	-0.444561000
6	2.191225000	1.413215000	0.821991000
6	0.704695000	3.577690000	4.960624000
6	1.411391000	4.556689000	5.663751000
6	2.537715000	5.166846000	5.102129000
6	2.960481000	4.796359000	3.823389000
1	-1.019093000	4.710346000	3.005949000
1	-3.269671000	5.614147000	2.509250000
1	-5.067766000	4.116180000	1.648898000
1	-4.597145000	1.686425000	1.310665000
1	-0.714256000	3.029868000	0.048526000
1	0.333746000	3.019165000	-2.189137000
1	2.570958000	1.960490000	-2.525404000
1	3.754615000	0.933528000	-0.583387000
1	2.728892000	0.965755000	1.659815000
1	-0.177288000	3.086840000	5.383829000
1	1.067067000	4.851792000	6.658424000
1	3.085586000	5.931337000	5.660052000
1	3.834086000	5.272417000	3.370717000
1	2.590533000	3.572235000	2.100126000
6	2.255414000	3.826395000	3.105056000
1	-2.348037000	0.769335000	1.828252000
6	0.833527000	-0.780006000	2.996998000
1	1.841894000	-0.635715000	3.426976000
6	0.079936000	-1.817291000	3.888537000

1	0.757468000	-2.638453000	4.164406000
1	-0.739675000	-2.249045000	3.294009000
6	-0.512571000	-1.067299000	5.084708000
6	-0.756159000	0.391765000	4.631480000
7	-1.283565000	1.378598000	5.095635000
6	0.982732000	-1.363297000	1.598088000
6	2.184267000	-1.995078000	1.241124000
6	-0.085087000	-1.400171000	0.688350000
6	2.320836000	-2.640938000	0.007522000
6	0.043992000	-2.049175000	-0.542117000
6	1.249288000	-2.670840000	-0.888749000
1	3.025790000	-1.981090000	1.941558000
1	-1.025785000	-0.910799000	0.950424000
1	3.265316000	-3.125829000	-0.254911000
1	-0.802031000	-2.076331000	-1.235154000
1	1.351747000	-3.177364000	-1.852187000
1	-1.476642000	-1.487509000	5.397497000
6	0.423694000	-1.097613000	6.276701000
8	1.597182000	-0.801019000	6.252480000
8	-0.199512000	-1.543660000	7.383922000
6	0.600011000	-1.664895000	8.558369000
1	1.436660000	-2.360828000	8.390672000
1	1.018738000	-0.690873000	8.855110000
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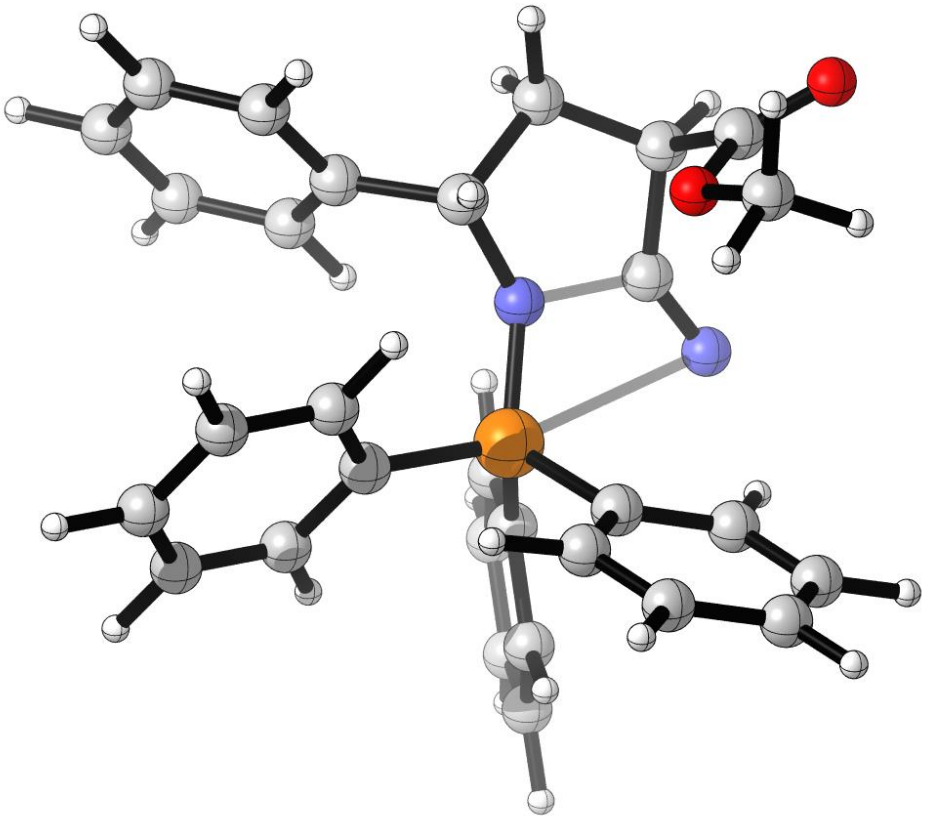

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6	1.231479000	-1.228618000	-1.564052000
6	0.061074000	-0.477686000	-1.704700000
6	-0.898405000	-0.485389000	-0.684370000
15	0.740588000	-3.042001000	2.084471000
7	-0.298936000	-2.635317000	3.310524000
6	2.553503000	-3.032408000	2.441715000
6	0.347354000	-4.764579000	1.586201000
6	0.012558000	-5.080892000	0.259278000
6	-0.250297000	-6.404193000	-0.110248000

6	-0.180886000	-7.427854000	0.836432000
6	0.148220000	-7.123065000	2.161374000
6	0.407969000	-5.804025000	2.534819000
6	3.237328000	-1.807458000	2.598564000
6	4.614994000	-1.802390000	2.830347000
6	5.329840000	-3.001100000	2.912127000
6	4.660685000	-4.217206000	2.754352000
1	2.363667000	-2.568849000	-0.306236000
1	1.988419000	-1.223012000	-2.353579000
1	-0.105345000	0.118098000	-2.606118000
1	-1.808469000	0.111444000	-0.785971000
1	-0.046470000	-4.293689000	-0.493933000
1	-0.518016000	-6.633420000	-1.145004000
1	-0.391178000	-8.460246000	0.543899000
1	0.199588000	-7.915923000	2.911829000
1	0.661912000	-5.587458000	3.574413000
1	2.661640000	-0.877748000	2.564463000
1	5.131540000	-0.847087000	2.955724000
1	6.406798000	-2.988246000	3.102356000
1	5.209826000	-5.160886000	2.810047000
1	2.794284000	-5.196598000	2.363587000
6	3.283561000	-4.235010000	2.513756000
1	-1.412170000	-1.203902000	1.289772000
6	-1.050093000	-3.432528000	4.277537000
1	-0.391810000	-4.130599000	4.823705000
6	-1.514747000	-2.341384000	5.294473000

1	-1.730304000	-2.794586000	6.274207000
1	-2.452050000	-1.899789000	4.921429000
6	-0.443061000	-1.246614000	5.315397000
6	0.110404000	-1.180477000	3.872535000
7	0.764533000	-0.403054000	3.207506000
6	-2.254344000	-4.203825000	3.760075000
6	-2.717737000	-5.319165000	4.475842000
6	-2.979339000	-3.783498000	2.636714000
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6	-4.586694000	-5.570687000	2.954710000
1	-2.165469000	-5.663079000	5.356156000
1	-2.626665000	-2.921647000	2.068685000
1	-4.221955000	-6.861038000	4.653544000
1	-4.684444000	-4.115271000	1.355624000
1	-5.488265000	-6.101425000	2.637834000
1	-0.855034000	-0.268122000	5.591864000
6	0.701039000	-1.503626000	6.278225000
8	1.033753000	-0.779453000	7.182089000
8	1.352584000	-2.660775000	5.991229000
6	2.523144000	-2.937912000	6.757474000
1	3.189914000	-2.063129000	6.777299000
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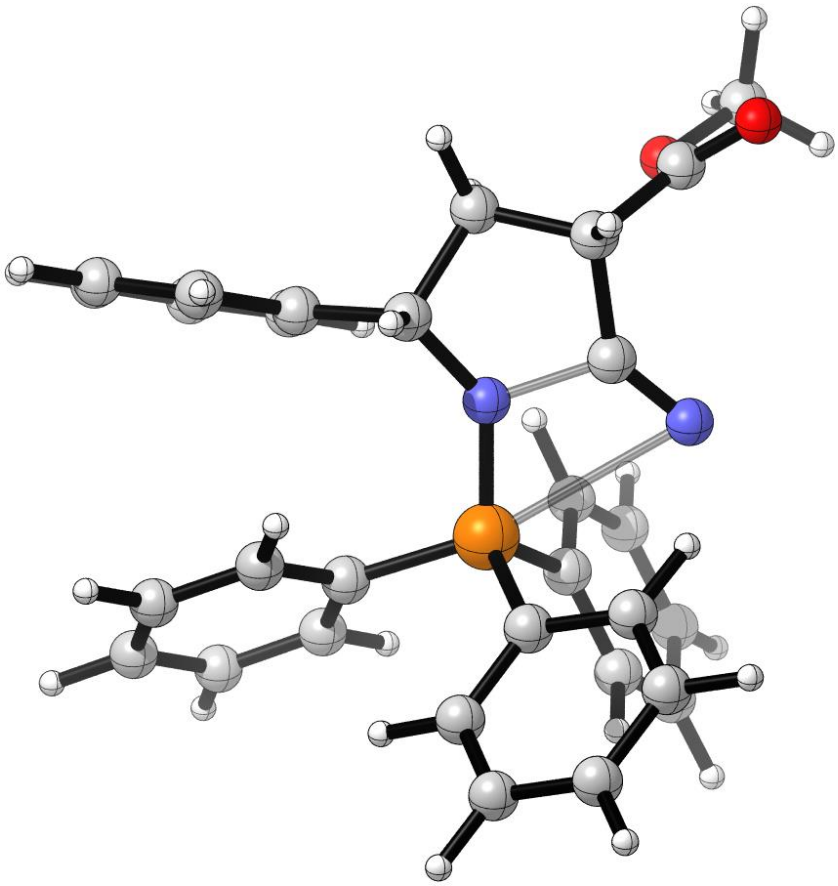

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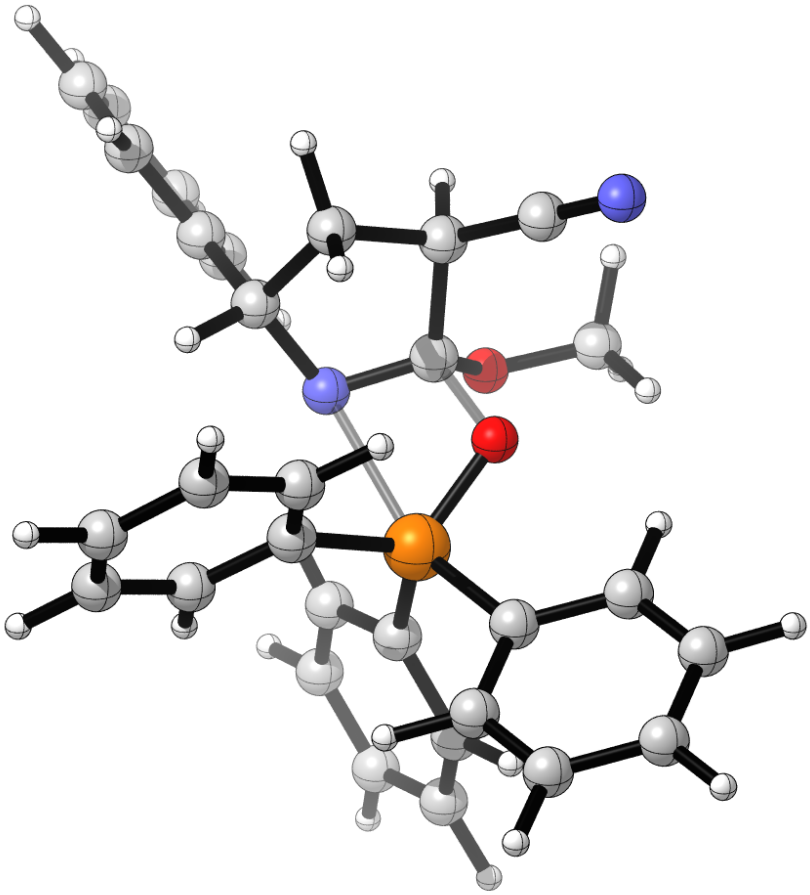
6	2.491378000	0.323839000	-3.367003000
6	2.939280000	-0.982152000	-3.583023000
6	3.308720000	-1.776886000	-2.491984000
15	2.804645000	0.731025000	0.707975000
7	2.552111000	-0.494560000	1.799394000
6	1.730089000	2.232393000	0.733975000
6	4.494471000	1.393820000	0.974975000
6	5.453441000	1.348811000	-0.050524000
6	6.719729000	1.913158000	0.138243000

6	7.042886000	2.524020000	1.351862000
6	6.092669000	2.577485000	2.377368000
6	4.825883000	2.023821000	2.189298000
6	0.325487000	2.122003000	0.671139000
6	-0.463248000	3.275436000	0.640413000
6	0.123201000	4.544209000	0.654500000
6	1.514936000	4.660897000	0.696559000
1	2.050721000	1.855135000	-1.912500000
1	2.188488000	0.947311000	-4.211786000
1	2.996423000	-1.385498000	-4.597915000
1	3.655614000	-2.800675000	-2.654501000
1	5.212065000	0.875503000	-1.003164000
1	7.452772000	1.876143000	-0.672126000
1	8.031463000	2.966183000	1.500573000
1	6.340426000	3.056803000	3.327517000
1	4.089658000	2.093557000	2.993505000
1	-0.117312000	1.123290000	0.612902000
1	-1.551083000	3.173605000	0.591661000
1	-0.501787000	5.440772000	0.622279000
1	1.989308000	5.646152000	0.692951000
1	3.397437000	3.636298000	0.759414000
6	2.314225000	3.515731000	0.737124000
1	3.492729000	-1.905836000	-0.343805000
6	3.021408000	-0.815773000	3.149185000
1	2.600754000	-0.100710000	3.884162000
6	2.343407000	-2.202042000	3.374643000

1	2.321602000	-2.456475000	4.445391000
1	2.940470000	-2.965703000	2.855311000
6	0.963227000	-2.112669000	2.727177000
6	1.117877000	-1.171415000	1.505581000
7	0.437327000	-0.845800000	0.553422000
6	4.516409000	-0.910457000	3.404137000
6	5.061620000	-0.341416000	4.564723000
6	5.368101000	-1.632930000	2.553129000
6	6.418783000	-0.485801000	4.872112000
6	6.722567000	-1.781767000	2.856593000
6	7.253986000	-1.212021000	4.019811000
1	4.413434000	0.225540000	5.240707000
1	4.964417000	-2.084320000	1.643572000
1	6.823454000	-0.030479000	5.780398000
1	7.369192000	-2.347617000	2.180275000
1	8.312079000	-1.341039000	4.263804000
6	0.339000000	-3.430292000	2.312239000
8	-0.794111000	-3.763611000	2.554060000
8	1.199768000	-4.206936000	1.614266000
6	0.664073000	-5.423116000	1.095995000
1	0.245405000	-6.046961000	1.901301000
1	-0.136645000	-5.215906000	0.369526000
1	1.496958000	-5.941433000	0.602246000
1	0.236834000	-1.638935000	3.406865000

TS2_trans_e1 (**2a**_i1_TS2)



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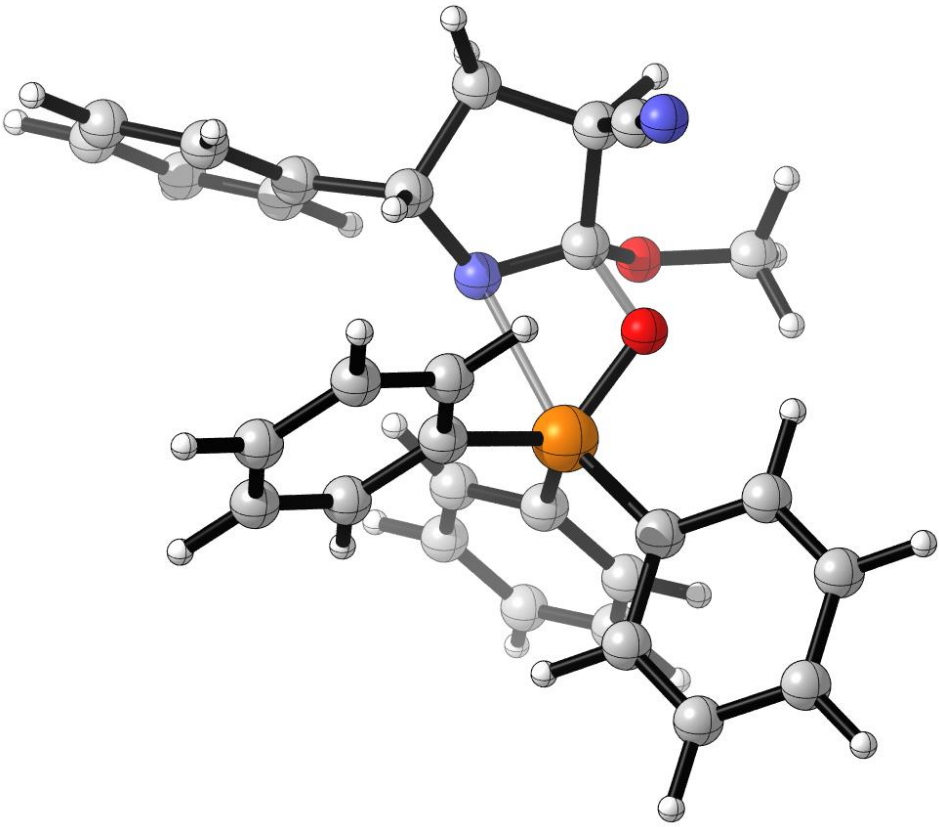
6	1.377575000	3.544517000	6.152262000
6	1.535192000	4.831970000	6.671505000
6	2.420300000	5.059867000	7.731263000
6	3.125682000	3.989120000	8.289527000
15	1.944167000	0.829775000	5.926895000
7	0.424585000	0.419368000	7.853965000
6	3.157860000	-0.383126000	6.580541000
6	2.499047000	1.206113000	4.202989000
6	1.844389000	0.640216000	3.094856000
6	2.244454000	0.967927000	1.795063000

6	3.296931000	1.863728000	1.585552000
6	3.955662000	2.429956000	2.682356000
6	3.559356000	2.104280000	3.981662000
6	4.191978000	-0.845475000	5.742060000
6	5.106928000	-1.794487000	6.206735000
6	5.003410000	-2.292323000	7.508857000
6	3.977482000	-1.839154000	8.343564000
1	0.712371000	3.380946000	5.300342000
1	0.972747000	5.660883000	6.233969000
1	2.559783000	6.069333000	8.127037000
1	3.810581000	4.160965000	9.123932000
1	1.001825000	-0.033094000	3.254969000
1	1.716371000	0.527250000	0.945645000
1	3.602781000	2.131924000	0.570330000
1	4.775623000	3.135404000	2.523904000
1	4.073397000	2.567904000	4.826555000
1	4.287492000	-0.474613000	4.721348000
1	5.897703000	-2.148952000	5.540723000
1	5.716798000	-3.038955000	7.869011000
1	3.879323000	-2.236998000	9.356873000
1	2.213298000	-0.559632000	8.499072000
6	3.055631000	-0.893966000	7.888157000
1	3.505333000	1.863824000	8.236555000
6	-0.436697000	1.354249000	8.550200000
1	0.130428000	2.261559000	8.834806000
6	-1.534293000	1.741012000	7.516852000

1	-1.156885000	2.524783000	6.843681000
1	-2.477889000	2.093177000	7.958765000
6	-1.702873000	0.423929000	6.732911000
6	-1.058908000	0.789337000	9.842720000
6	-1.905439000	1.585166000	10.635340000
6	-0.813541000	-0.528031000	10.253751000
6	-2.503547000	1.074395000	11.790509000
6	-1.401264000	-1.039746000	11.416886000
6	-2.253054000	-0.244300000	12.187718000
1	-2.111341000	2.619495000	10.340485000
1	-0.163535000	-1.148121000	9.632768000
1	-3.164542000	1.709553000	12.387773000
1	-1.186889000	-2.067893000	11.723865000
1	-2.719981000	-0.647073000	13.090863000
6	-0.255635000	-0.174821000	6.824892000
8	0.494317000	0.246731000	5.527500000
8	-0.184642000	-1.562518000	6.844101000
6	-0.785618000	-2.295353000	5.795073000
1	-1.888324000	-2.208515000	5.804249000
1	-0.414123000	-1.976531000	4.806450000
1	-0.518663000	-3.350447000	5.955915000
1	-2.359336000	-0.258707000	7.299806000
6	-2.256200000	0.577502000	5.390448000
7	-2.696840000	0.712809000	4.325715000

TS2_trans_a1 (**2a**_i5_TS2)



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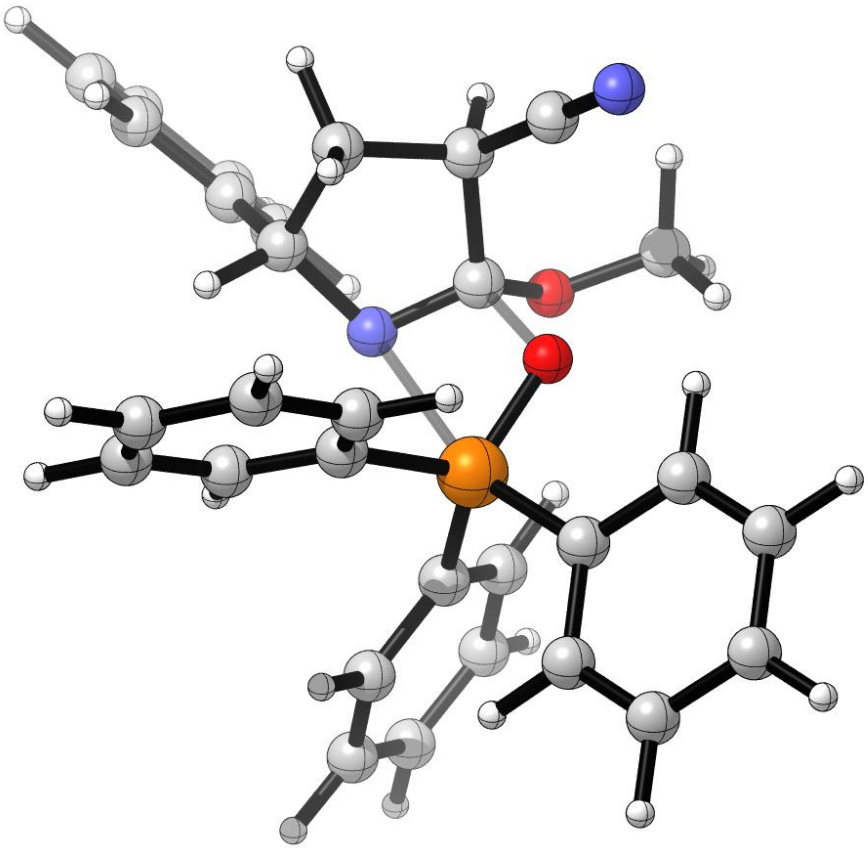
6	4.175062000	-0.042350000	8.579986000
6	4.442989000	-0.379342000	9.909560000
6	3.395441000	-0.696260000	10.776814000
6	2.079797000	-0.700790000	10.301863000
15	2.572084000	0.354787000	6.329419000
7	0.794572000	-1.338125000	6.357796000
6	4.040644000	1.382091000	5.872076000
6	1.213159000	1.519777000	6.015065000
6	0.552672000	2.193395000	7.055065000
6	-0.436455000	3.135775000	6.758523000

6	-0.774605000	3.411536000	5.429885000
6	-0.119486000	2.739140000	4.393605000
6	0.873876000	1.796365000	4.678127000
6	4.921671000	0.987853000	4.851584000
6	6.019238000	1.789308000	4.517727000
6	6.252278000	2.984537000	5.202166000
6	5.375710000	3.387343000	6.217017000
1	5.004154000	0.214815000	7.920058000
1	5.475640000	-0.389651000	10.268713000
1	3.606364000	-0.957958000	11.817358000
1	1.257048000	-0.969139000	10.968913000
1	0.811279000	1.989704000	8.095799000
1	-0.946472000	3.655754000	7.573125000
1	-1.549668000	4.147764000	5.200335000
1	-0.384935000	2.949956000	3.354034000
1	1.379424000	1.277476000	3.859476000
1	4.739072000	0.056280000	4.315795000
1	6.695159000	1.472052000	3.719088000
1	7.112395000	3.607282000	4.942438000
1	5.551058000	4.323183000	6.753685000
1	3.590102000	2.927626000	7.331564000
6	4.272809000	2.596128000	6.543788000
1	0.796530000	-0.485706000	8.571553000
6	-0.443717000	-1.330363000	5.601090000
1	-0.548269000	-0.423461000	4.963291000
6	-0.315708000	-2.559824000	4.661279000

1	-0.961540000	-2.515025000	3.772208000
1	-0.563499000	-3.471388000	5.226158000
6	1.192482000	-2.575387000	4.323236000
6	-1.707010000	-1.412941000	6.446343000
6	-2.900313000	-0.834166000	5.988285000
6	-1.731905000	-2.138492000	7.647651000
6	-4.096629000	-0.995929000	6.694494000
6	-2.926422000	-2.304148000	8.355804000
6	-4.114906000	-1.740030000	7.878509000
1	-2.891988000	-0.253740000	5.060317000
1	-0.797426000	-2.572870000	8.011506000
1	-5.015527000	-0.538828000	6.315606000
1	-2.931899000	-2.878034000	9.287146000
1	-5.048992000	-1.879730000	8.430123000
6	1.774577000	-1.970056000	5.656778000
8	2.821229000	-0.839958000	5.279224000
8	2.512269000	-2.865730000	6.424732000
6	3.732925000	-3.370039000	5.923836000
1	3.630029000	-3.813021000	4.914589000
1	4.509180000	-2.587670000	5.880171000
1	4.055426000	-4.160702000	6.616438000
6	1.500146000	-1.792763000	3.125800000
7	1.705788000	-1.172879000	2.167072000
1	1.570762000	-3.596411000	4.161669000

TS2_trans_e2



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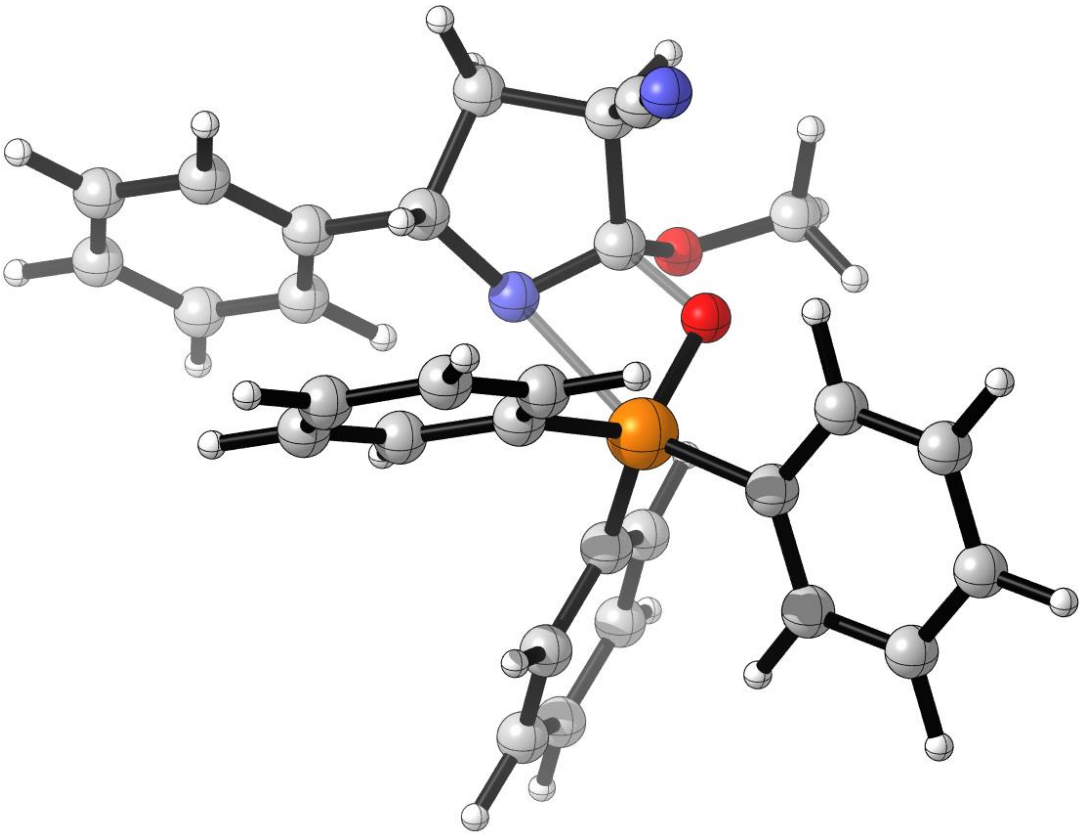
6	0.124206000	2.645592000	7.040582000
6	-0.524900000	3.253263000	8.118775000
6	-0.200625000	2.887668000	9.429030000
6	0.757116000	1.892485000	9.660137000
15	1.930846000	0.899630000	5.837971000
7	1.167197000	-1.335552000	6.799225000
6	3.598233000	0.314576000	6.286976000
6	2.207946000	2.325916000	4.696281000
6	1.459922000	2.453061000	3.511844000
6	1.660185000	3.549848000	2.665389000

6	2.604144000	4.528811000	2.988109000
6	3.351791000	4.409722000	4.165063000
6	3.154296000	3.317809000	5.013600000
6	4.147779000	-0.789602000	5.614396000
6	5.441956000	-1.216138000	5.918347000
6	6.195913000	-0.557872000	6.896072000
6	5.654268000	0.543013000	7.563802000
1	-0.118543000	2.958531000	6.022310000
1	-1.276529000	4.023919000	7.928843000
1	-0.698235000	3.377083000	10.270004000
1	1.009921000	1.593185000	10.680924000
1	0.722926000	1.690959000	3.253843000
1	1.075270000	3.632989000	1.745869000
1	2.762104000	5.381271000	2.321826000
1	4.095181000	5.168045000	4.425600000
1	3.755626000	3.242984000	5.920988000
1	3.543024000	-1.344091000	4.896463000
1	5.857927000	-2.082466000	5.397705000
1	7.198647000	-0.912257000	7.149290000
1	6.234469000	1.063295000	8.330321000
1	3.953638000	1.838760000	7.798447000
6	4.363059000	0.983765000	7.257713000
1	2.099521000	0.452593000	8.763483000
6	0.095271000	-1.637268000	7.719904000
1	0.153990000	-0.974693000	8.605666000
6	-1.221398000	-1.311578000	6.948980000

1	-1.464434000	-0.243986000	7.059625000
1	-2.094205000	-1.896195000	7.273501000
6	-0.833206000	-1.611840000	5.486853000
6	0.115893000	-3.072987000	8.268920000
6	-0.798658000	-3.467661000	9.261570000
6	1.051100000	-4.010719000	7.810639000
6	-0.791879000	-4.768526000	9.771577000
6	1.062541000	-5.314328000	8.320611000
6	0.140995000	-5.699461000	9.298990000
1	-1.522718000	-2.742624000	9.648531000
1	1.766184000	-3.690680000	7.050080000
1	-1.511340000	-5.057669000	10.543616000
1	1.797730000	-6.035004000	7.950257000
1	0.150871000	-6.716816000	9.700068000
6	0.731351000	-1.415586000	5.520174000
8	1.080312000	-0.020387000	4.845417000
8	1.427653000	-2.318588000	4.705091000
6	1.095332000	-2.398702000	3.330409000
1	0.048475000	-2.715573000	3.169554000
1	1.256469000	-1.437550000	2.813528000
1	1.754477000	-3.160102000	2.889951000
1	-1.012897000	-2.677539000	5.265152000
6	-1.554037000	-0.811445000	4.502517000
7	-2.132041000	-0.153146000	3.741559000

TS2_trans_a2



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6	3.301138000	2.893400000	6.986506000
6	3.669310000	3.890634000	7.894424000
6	3.831641000	3.580837000	9.247619000
6	3.626524000	2.269973000	9.691562000
15	2.656413000	0.266558000	6.251636000
7	0.456317000	0.031221000	7.633729000
6	4.226690000	-0.185671000	5.402416000
6	1.567690000	0.948987000	4.952565000
6	0.633007000	1.956690000	5.259784000
6	-0.164310000	2.507205000	4.255380000

6	-0.061323000	2.040038000	2.939847000
6	0.850491000	1.026965000	2.631390000
6	1.667678000	0.486727000	3.628225000
6	4.283931000	-1.396481000	4.681778000
6	5.466762000	-1.784021000	4.049620000
6	6.610935000	-0.982885000	4.138036000
6	6.564480000	0.211918000	4.859676000
1	3.175303000	3.151529000	5.932433000
1	3.830038000	4.911459000	7.537692000
1	4.114735000	4.362680000	9.956840000
1	3.749200000	2.022300000	10.749200000
1	0.516850000	2.291367000	6.291627000
1	-0.885557000	3.287746000	4.510886000
1	-0.697824000	2.461442000	2.157473000
1	0.931942000	0.645863000	1.610280000
1	2.378263000	-0.295400000	3.362100000
1	3.405789000	-2.044345000	4.625181000
1	5.497879000	-2.725974000	3.496293000
1	7.537263000	-1.298332000	3.650537000
1	7.455963000	0.838485000	4.948866000
1	5.365591000	1.544329000	6.053035000
6	5.378380000	0.612370000	5.485477000
1	3.038188000	0.262518000	9.153139000
6	-0.894459000	-0.073264000	7.117172000
1	-0.934037000	0.109755000	6.018702000
6	-1.299542000	-1.554355000	7.344634000

1	-2.085330000	-1.914834000	6.664927000
1	-1.640743000	-1.694637000	8.381666000
6	0.046768000	-2.290361000	7.169571000
6	-1.866424000	0.926234000	7.731568000
6	-3.106173000	1.180463000	7.120615000
6	-1.544273000	1.619610000	8.906446000
6	-4.003090000	2.099796000	7.671518000
6	-2.438050000	2.544829000	9.457011000
6	-3.670658000	2.788834000	8.843676000
1	-3.367486000	0.659383000	6.193274000
1	-0.573019000	1.420767000	9.363909000
1	-4.961802000	2.288791000	7.179705000
1	-2.167010000	3.081908000	10.370905000
1	-4.369241000	3.513403000	9.271685000
6	1.015278000	-1.188982000	7.749172000
8	2.360249000	-1.175655000	6.878166000
8	1.500642000	-1.512352000	9.025565000
6	2.290272000	-2.675456000	9.186484000
1	1.832847000	-3.565938000	8.718220000
1	3.298247000	-2.547755000	8.755546000
1	2.370313000	-2.858450000	10.268234000
6	0.347168000	-2.627148000	5.777409000
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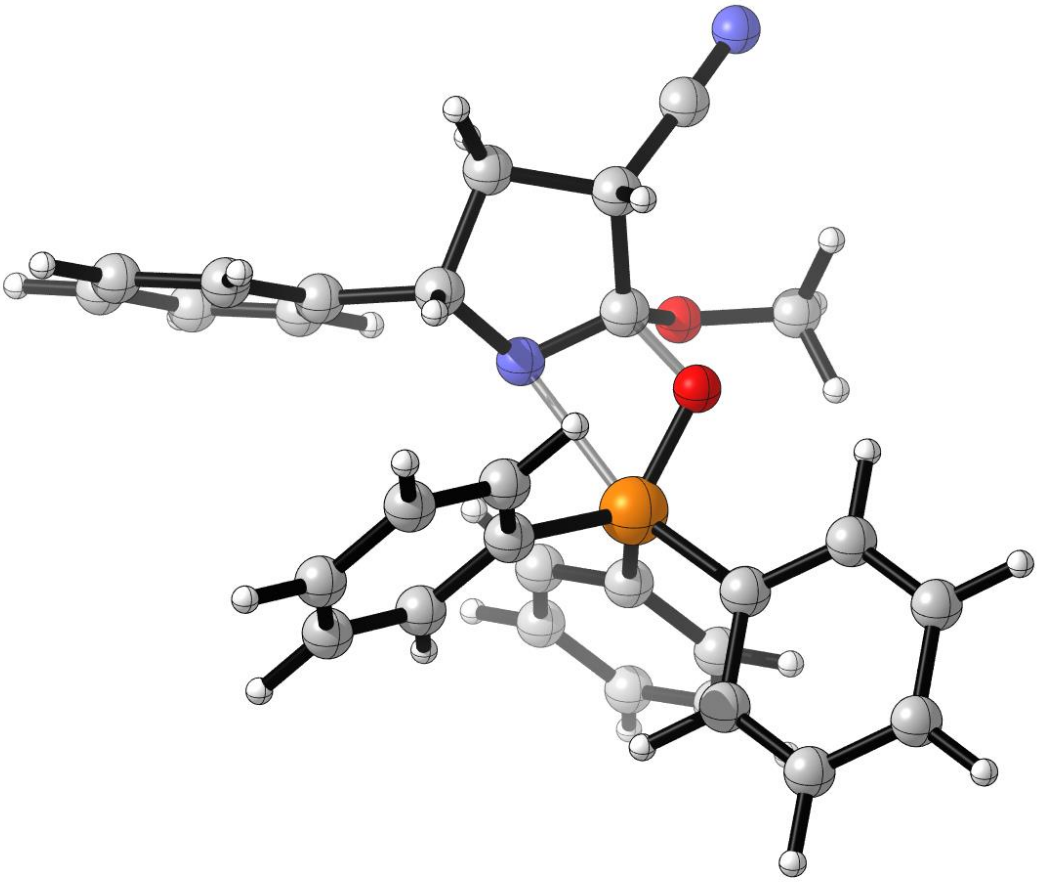
1	0.086444000	-3.224422000	7.749027000

TS2_cis_e1



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6	4.216373000	0.055135000	8.559509000
6	4.534064000	-0.255531000	9.884652000
6	3.544392000	-0.723911000	10.751793000
6	2.238087000	-0.898625000	10.282956000
15	2.541156000	0.272783000	6.323735000
7	0.798089000	-1.398276000	6.357323000
6	3.980645000	1.329680000	5.815607000
6	1.173973000	1.452720000	6.088784000
6	0.496628000	2.039941000	7.169466000
6	-0.502401000	2.989401000	6.934533000

6	-0.840524000	3.352691000	5.626992000
6	-0.173842000	2.762722000	4.548742000
6	0.833787000	1.819638000	4.775011000
6	4.924749000	0.884040000	4.875578000
6	6.003132000	1.698116000	4.510828000
6	6.158426000	2.960434000	5.088675000
6	5.223974000	3.413149000	6.027883000
1	5.000689000	0.427553000	7.900752000
1	5.559454000	-0.122990000	10.239493000
1	3.795074000	-0.967950000	11.787739000
1	1.462439000	-1.281755000	10.950517000
1	0.749971000	1.762384000	8.194292000
1	-1.022352000	3.445888000	7.780468000
1	-1.624155000	4.093330000	5.446118000
1	-0.439093000	3.043539000	3.525705000
1	1.363525000	1.374007000	3.928867000
1	4.806199000	-0.102419000	4.427720000
1	6.726016000	1.338619000	3.773373000
1	7.002203000	3.595202000	4.805478000
1	5.339163000	4.399330000	6.484900000
1	3.408991000	2.981807000	7.105065000
6	4.138647000	2.608531000	6.380860000
1	0.926556000	-0.826449000	8.555154000
6	-0.419974000	-1.340497000	5.568344000
1	-0.461466000	-0.440624000	4.912062000
6	-0.325899000	-2.580886000	4.642909000

1	-0.949311000	-2.511685000	3.739368000
1	-0.623598000	-3.481743000	5.201119000
6	1.182749000	-2.630663000	4.329263000
1	1.422078000	-1.915462000	3.526452000
6	1.651060000	-3.947048000	3.904084000
7	1.994771000	-4.993886000	3.542057000
6	-1.708852000	-1.346685000	6.377141000
6	-2.850283000	-0.693279000	5.888021000
6	-1.815305000	-2.077754000	7.570518000
6	-4.075799000	-0.788061000	6.555246000
6	-3.038728000	-2.175961000	8.240268000
6	-4.176079000	-1.539466000	7.730423000
1	-2.777289000	-0.106531000	4.966819000
1	-0.922556000	-2.574189000	7.958323000
1	-4.954145000	-0.274492000	6.153320000
1	-3.108549000	-2.755395000	9.165347000
1	-5.134056000	-1.627598000	8.250694000
6	1.778817000	-2.053229000	5.664132000
8	2.788177000	-0.903055000	5.240638000
8	2.519426000	-2.912521000	6.457762000
6	3.837723000	-3.287729000	6.088377000
1	3.907213000	-3.643768000	5.048110000
1	4.544119000	-2.453679000	6.233626000
1	4.119052000	-4.113763000	6.755842000

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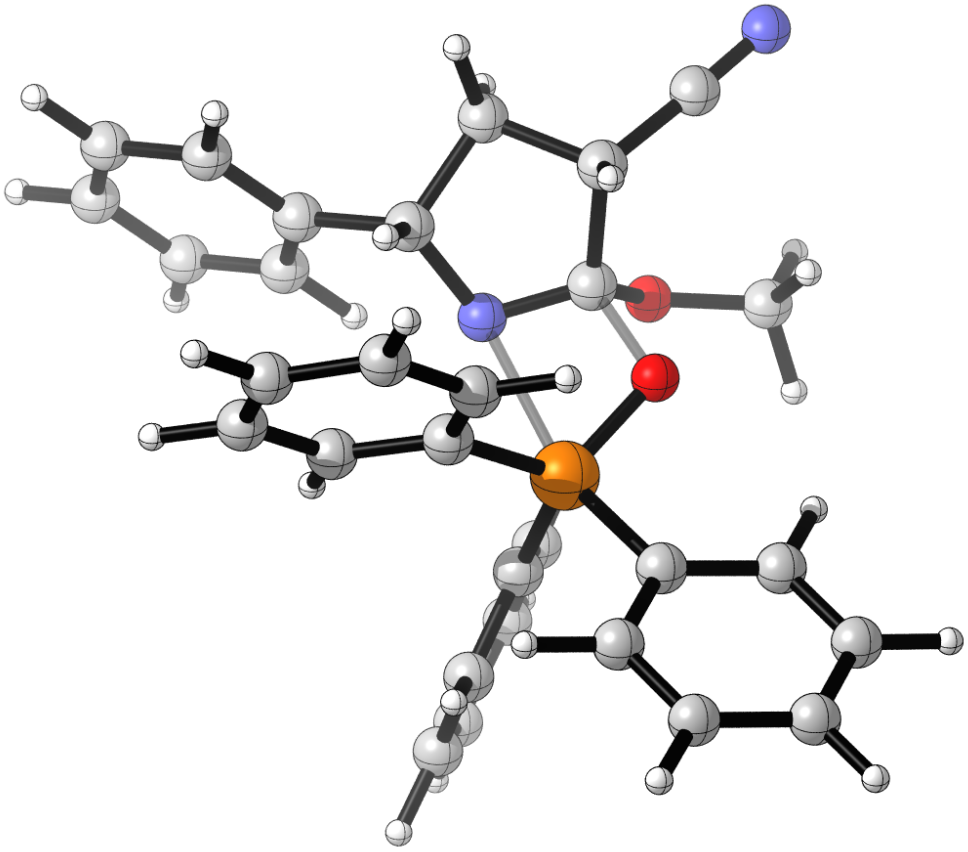

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6	3.762067000	2.595935000	7.175239000
6	4.215051000	3.517195000	8.123364000
6	4.050445000	3.255668000	9.486796000
6	3.420963000	2.076225000	9.897110000
15	2.597217000	0.195327000	6.325416000
7	0.463040000	-0.056977000	7.608495000
6	4.164207000	-0.121803000	5.394396000
6	1.504224000	0.925217000	5.069916000
6	0.810312000	2.123045000	5.303786000
6	-0.018192000	2.655732000	4.314162000

6	-0.182859000	1.985885000	3.096237000
6	0.482223000	0.776880000	2.870940000
6	1.328349000	0.248016000	3.850930000
6	4.986947000	-1.198513000	5.769998000
6	6.203605000	-1.420198000	5.119186000
6	6.615753000	-0.572341000	4.086300000
6	5.804012000	0.499097000	3.702641000
1	3.925608000	2.808361000	6.116278000
1	4.707802000	4.434405000	7.790271000
1	4.415199000	3.971102000	10.228070000
1	3.286914000	1.863405000	10.961414000
1	0.897935000	2.623608000	6.269747000
1	-0.554969000	3.587717000	4.506176000
1	-0.838791000	2.400196000	2.326179000
1	0.345569000	0.242168000	1.927530000
1	1.859305000	-0.688394000	3.659497000
1	4.662896000	-1.869280000	6.566467000
1	6.832536000	-2.261753000	5.421274000
1	7.566623000	-0.750272000	3.577232000
1	6.115343000	1.162892000	2.891516000
1	3.952726000	1.549998000	4.021292000
6	4.585137000	0.722158000	4.351028000
1	2.418342000	0.261378000	9.280559000
6	-0.871798000	-0.056318000	7.040188000
1	-0.856368000	0.157034000	5.947242000
6	-1.372795000	-1.512915000	7.207184000

1	-2.153558000	-1.799505000	6.487718000
1	-1.757946000	-1.672870000	8.225879000
6	-0.063201000	-2.304540000	7.014348000
6	-1.808306000	0.977155000	7.649431000
6	-2.987405000	1.343067000	6.978968000
6	-1.523793000	1.578331000	8.882650000
6	-3.863494000	2.282926000	7.528216000
6	-2.395045000	2.525361000	9.431353000
6	-3.568406000	2.880549000	8.758971000
1	-3.217677000	0.890889000	6.008226000
1	-0.599915000	1.293332000	9.389361000
1	-4.775365000	2.559039000	6.990865000
1	-2.151943000	2.992164000	10.390308000
1	-4.249811000	3.620770000	9.187616000
6	0.946033000	-1.316370000	7.695714000
8	2.308290000	-1.306903000	6.795252000
8	1.409998000	-1.686212000	8.950867000
6	2.313300000	-2.776156000	9.099004000
1	2.350649000	-3.422168000	8.211302000
1	3.329167000	-2.390174000	9.296781000
1	1.981043000	-3.378839000	9.957968000
1	0.192810000	-2.340129000	5.942352000
6	-0.130122000	-3.680068000	7.500480000
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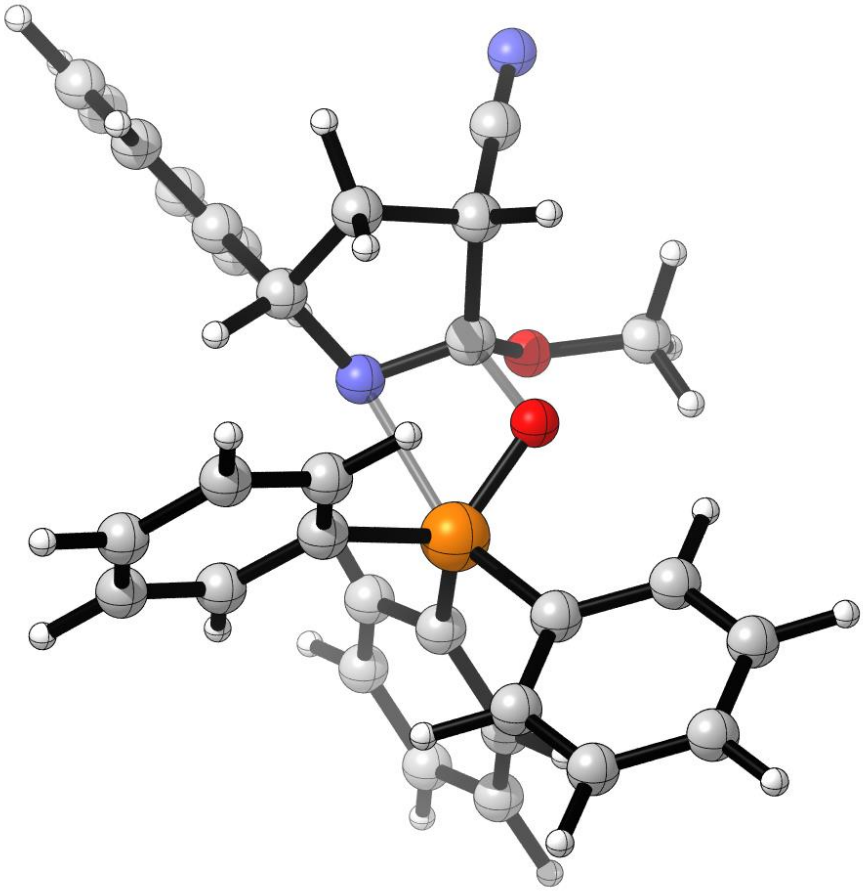

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6	1.331427000	3.531652000	6.192100000
6	1.490311000	4.813528000	6.724473000
6	2.375464000	5.028885000	7.786756000
6	3.078617000	3.951075000	8.333737000
15	1.886571000	0.815156000	5.942641000
7	0.373080000	0.378966000	7.815930000
6	3.090978000	-0.412324000	6.590677000
6	2.477938000	1.206955000	4.227046000
6	1.858041000	0.628536000	3.104645000
6	2.274005000	0.963597000	1.812190000

6	3.312089000	1.880482000	1.621896000
6	3.940189000	2.456345000	2.731181000
6	3.526129000	2.122572000	4.023557000
6	4.114606000	-0.887964000	5.746696000
6	5.023794000	-1.844342000	6.207784000
6	4.927332000	-2.334593000	7.513249000
6	3.913668000	-1.866722000	8.354723000
1	0.666590000	3.377661000	5.338154000
1	0.929025000	5.648038000	6.296063000
1	2.516307000	6.033807000	8.193316000
1	3.762865000	4.112757000	9.170655000
1	1.030481000	-0.066261000	3.250101000
1	1.772068000	0.510511000	0.953200000
1	3.631356000	2.154987000	0.612563000
1	4.750541000	3.176032000	2.588143000
1	4.017136000	2.594715000	4.877316000
1	4.207081000	-0.521476000	4.724167000
1	5.805087000	-2.209768000	5.536551000
1	5.636222000	-3.086646000	7.870938000
1	3.820561000	-2.257844000	9.371094000
1	2.162656000	-0.574406000	8.518877000
6	2.996240000	-0.916303000	7.901567000
1	3.455922000	1.826317000	8.258290000
6	-0.471680000	1.330144000	8.512342000
1	0.099730000	2.250599000	8.741292000
6	-1.603241000	1.687116000	7.501200000

1	-1.259675000	2.493007000	6.836208000
1	-2.546361000	2.007798000	7.966071000
6	-1.753960000	0.395879000	6.663747000
6	-1.025813000	0.812734000	9.852226000
6	-1.840960000	1.636772000	10.648374000
6	-0.744020000	-0.480941000	10.310039000
6	-2.375865000	1.174266000	11.853055000
6	-1.267468000	-0.943677000	11.522727000
6	-2.090494000	-0.122257000	12.296671000
1	-2.074041000	2.654234000	10.317132000
1	-0.122808000	-1.126657000	9.686246000
1	-3.016211000	1.829127000	12.451550000
1	-1.030562000	-1.956191000	11.862498000
1	-2.511442000	-0.488790000	13.237015000
6	-0.311549000	-0.213201000	6.792482000
8	0.442303000	0.260136000	5.485669000
8	-0.211772000	-1.592827000	6.775241000
6	-0.635912000	-2.308525000	5.629528000
1	-1.694091000	-2.117342000	5.377662000
1	-0.009035000	-2.072319000	4.753967000
1	-0.526806000	-3.375138000	5.873797000
6	-2.808805000	-0.499094000	7.149607000
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1	-1.978953000	0.616072000	5.609461000

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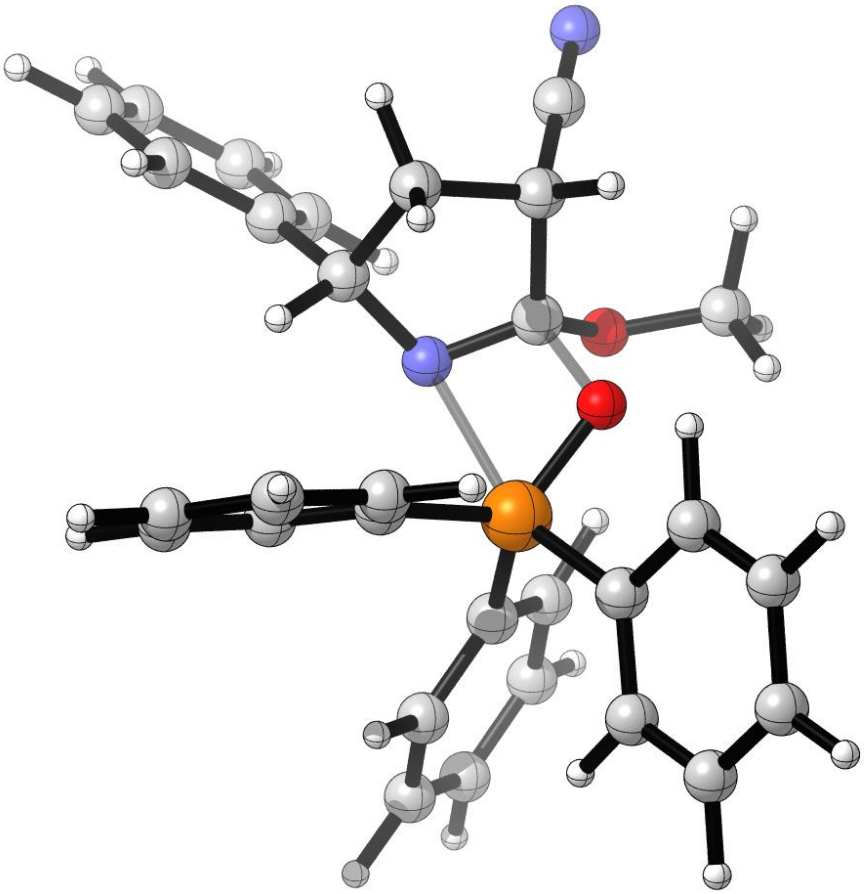

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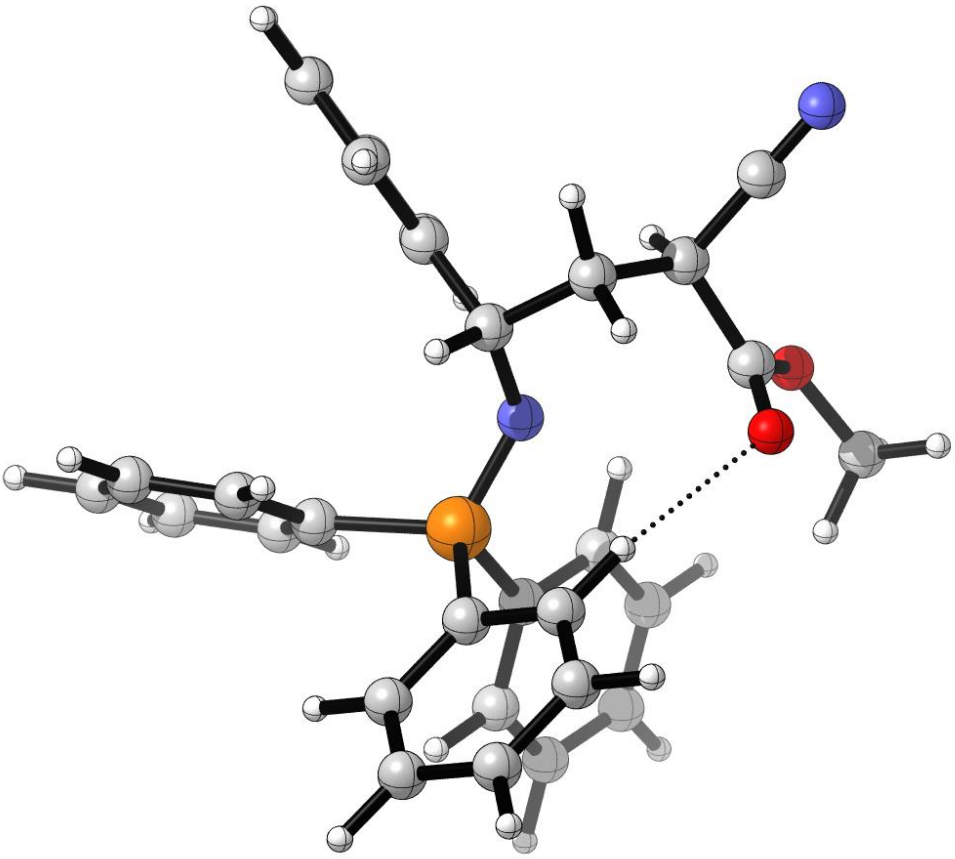
6	0.738860000	1.485577000	6.529627000
6	0.127041000	2.751946000	6.569656000
6	0.903325000	3.912514000	6.505792000
6	2.293943000	3.820938000	6.403431000
6	2.904019000	2.563702000	6.371759000
15	-0.286408000	-0.024183000	6.528151000
7	0.830041000	-0.721579000	8.619112000
6	-1.017774000	-0.104839000	4.821234000
6	-1.763296000	0.271293000	7.567525000
6	-1.673189000	1.098749000	8.702547000
6	-2.819198000	1.419528000	9.432965000

6	-4.061183000	0.889663000	9.066048000
6	-4.151918000	0.034184000	7.964137000
6	-3.012955000	-0.265292000	7.210587000
6	-1.452840000	-1.348987000	4.322031000
6	-2.063944000	-1.442728000	3.069742000
6	-2.243938000	-0.297687000	2.287426000
6	-1.803100000	0.938020000	2.764763000
1	-0.957129000	2.845328000	6.662048000
1	0.413870000	4.889488000	6.542170000
1	2.902071000	4.727942000	6.357171000
1	3.992613000	2.483375000	6.308510000
1	-0.700533000	1.485821000	9.010370000
1	-2.735532000	2.077311000	10.301985000
1	-4.954691000	1.144605000	9.641933000
1	-5.114812000	-0.391205000	7.669563000
1	-3.111036000	-0.899530000	6.328348000
1	-1.299121000	-2.251714000	4.914982000
1	-2.398597000	-2.415520000	2.698981000
1	-2.720894000	-0.371820000	1.306791000
1	-1.931112000	1.837434000	2.156737000
1	-0.842180000	2.008787000	4.362404000
6	-1.194642000	1.034889000	4.020761000
1	2.622771000	0.423821000	6.465448000
6	0.821922000	-3.121603000	8.297594000
6	-0.270715000	-2.743069000	9.318802000
1	-0.344556000	-3.452640000	10.155299000

1	-1.242063000	-2.724046000	8.800648000
6	0.118380000	-1.291990000	9.748249000
6	1.262740000	-1.702796000	7.783753000
8	0.453940000	-1.449755000	6.420707000
8	2.588148000	-1.605983000	7.375120000
6	3.031060000	-2.444832000	6.316733000
1	2.982786000	-3.513460000	6.588423000
1	2.441530000	-2.269316000	5.402220000
1	4.083673000	-2.187312000	6.131147000
1	0.427828000	-3.724834000	7.466229000
6	1.929068000	-3.874071000	8.898325000
7	2.789941000	-4.493256000	9.367359000
6	0.871179000	-1.229805000	11.081780000
6	0.153714000	-1.352393000	12.283745000
6	2.258083000	-1.047029000	11.147289000
6	0.802656000	-1.310817000	13.519728000
6	2.913108000	-1.013529000	12.383330000
6	2.190974000	-1.144134000	13.572840000
1	-0.934287000	-1.479484000	12.247732000
1	2.813334000	-0.919276000	10.215999000
1	0.224019000	-1.405320000	14.443204000
1	3.997642000	-0.874692000	12.417873000
1	2.706637000	-1.110202000	14.536760000
1	-0.821152000	-0.739033000	9.924592000

To Figure 1

2a_i1



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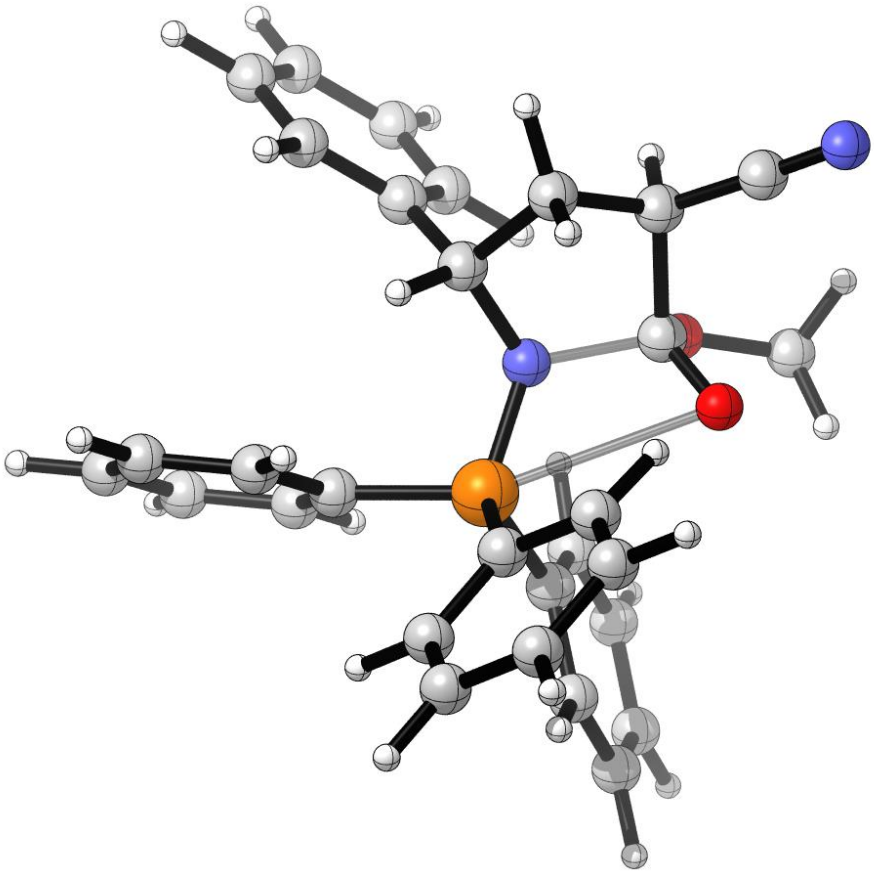
6	2.036987000	3.756152000	7.515388000
6	2.386623000	4.760475000	8.421523000
6	3.239734000	4.474487000	9.493315000
6	3.732195000	3.176622000	9.661833000
15	1.923186000	1.102334000	6.565689000
7	0.496383000	0.497770000	6.898827000
6	3.124914000	-0.270646000	6.689202000
6	2.124008000	1.768974000	4.853966000
6	1.322156000	1.192280000	3.852318000

6	1.466377000	1.598905000	2.521843000
6	2.408179000	2.575927000	2.179763000
6	3.206341000	3.154491000	3.171717000
6	3.064772000	2.754051000	4.504152000
6	4.458872000	-0.104347000	6.282350000
6	5.357709000	-1.170151000	6.367776000
6	4.929599000	-2.411037000	6.852804000
6	3.602372000	-2.579866000	7.259351000
1	1.375965000	3.997887000	6.678847000
1	1.988670000	5.769880000	8.286452000
1	3.518149000	5.262019000	10.198539000
1	4.396120000	2.942788000	10.498457000
1	0.595252000	0.417882000	4.115131000
1	0.838638000	1.146604000	1.749977000
1	2.519745000	2.894821000	1.139527000
1	3.938008000	3.923160000	2.907581000
1	3.687959000	3.218392000	5.271717000
1	4.800339000	0.853983000	5.883073000
1	6.391708000	-1.032868000	6.040467000
1	5.631917000	-3.246930000	6.911664000
1	3.261890000	-3.544400000	7.646100000
1	1.660702000	-1.632896000	7.490401000
6	2.700697000	-1.513799000	7.181671000
1	3.767446000	1.159197000	8.906233000
6	-0.724555000	1.258388000	7.061871000
1	-0.696325000	2.242105000	6.547686000

6	-1.896848000	0.501947000	6.378557000
1	-1.808285000	0.589917000	5.284881000
1	-2.853469000	0.958023000	6.672380000
6	-1.921443000	-1.003403000	6.723238000
6	-1.067994000	1.567960000	8.529556000
6	-2.024643000	2.553296000	8.829999000
6	-0.464129000	0.884566000	9.593580000
6	-2.374617000	2.843806000	10.150534000
6	-0.811846000	1.171070000	10.919626000
6	-1.767514000	2.150655000	11.204153000
1	-2.498331000	3.109451000	8.014921000
1	0.295390000	0.134285000	9.364735000
1	-3.118678000	3.617248000	10.362396000
1	-0.325885000	0.625590000	11.733488000
1	-2.040310000	2.381282000	12.238019000
6	-0.979410000	-1.815813000	5.820280000
8	-0.741908000	-1.560202000	4.667345000
8	-0.519810000	-2.903836000	6.457007000
6	0.266244000	-3.806335000	5.670606000
1	-0.360828000	-4.292382000	4.907268000
1	1.087228000	-3.273357000	5.171239000
1	0.661027000	-4.555924000	6.367657000
1	-1.613085000	-1.168182000	7.768325000
6	-3.269054000	-1.573290000	6.573716000
7	-4.330917000	-2.022914000	6.454385000

2a_i1_TS1



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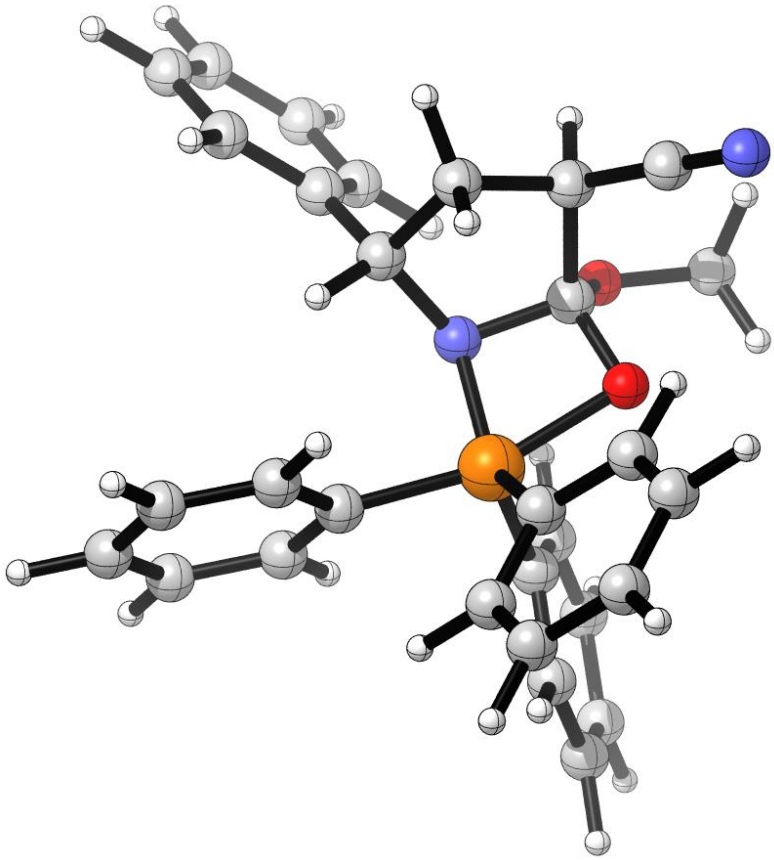
6	1.965955000	3.631241000	7.187441000
6	2.208235000	4.650860000	8.110732000
6	2.821109000	4.359549000	9.332937000
6	3.192561000	3.044132000	9.627382000
15	1.874103000	0.935219000	6.342638000
7	0.401543000	0.402608000	6.869798000
6	3.112897000	-0.388120000	6.492938000
6	1.985996000	1.633857000	4.648150000
6	1.127888000	1.155923000	3.640128000
6	1.242945000	1.657519000	2.339234000

6	2.211747000	2.616755000	2.029901000
6	3.076649000	3.083995000	3.026260000
6	2.965976000	2.597532000	4.331229000
6	4.192529000	-0.456374000	5.595523000
6	5.186489000	-1.423294000	5.770616000
6	5.110891000	-2.324604000	6.837638000
6	4.032883000	-2.262934000	7.727500000
1	1.484770000	3.878710000	6.239529000
1	1.908926000	5.674671000	7.870166000
1	3.011873000	5.157004000	10.055567000
1	3.673998000	2.807435000	10.579340000
1	0.421663000	0.354005000	3.885764000
1	0.573071000	1.280976000	1.561957000
1	2.300252000	3.003180000	1.010767000
1	3.837633000	3.831500000	2.786723000
1	3.646247000	2.972759000	5.098257000
1	4.256902000	0.229567000	4.748628000
1	6.019698000	-1.474366000	5.064673000
1	5.888392000	-3.081763000	6.973050000
1	3.959434000	-2.974398000	8.554469000
1	2.166025000	-1.287582000	8.219203000
6	3.033653000	-1.300852000	7.560089000
1	3.249129000	1.000793000	8.954232000
6	-0.662949000	1.360455000	7.217459000
1	-0.406819000	2.379776000	6.889818000
6	-1.865155000	0.883746000	6.366598000

1	-1.745045000	1.251695000	5.335033000
1	-2.822247000	1.259796000	6.756199000
6	-1.767235000	-0.644425000	6.378449000
6	-0.978424000	1.433246000	8.709651000
6	-1.458923000	2.636292000	9.252469000
6	-0.860875000	0.314513000	9.551155000
6	-1.825945000	2.722935000	10.598657000
6	-1.237368000	0.398817000	10.896034000
6	-1.721101000	1.599621000	11.424444000
1	-1.549405000	3.520441000	8.613233000
1	-0.477670000	-0.622700000	9.140945000
1	-2.200940000	3.667139000	11.004144000
1	-1.155400000	-0.484813000	11.535230000
1	-2.021774000	1.661043000	12.473912000
6	-0.206391000	-0.991121000	6.221084000
8	0.244139000	-1.224539000	5.072638000
8	0.124005000	-1.956932000	7.255689000
6	0.123867000	-3.295285000	6.799727000
1	-0.897622000	-3.655361000	6.566780000
1	0.737627000	-3.406667000	5.892572000
1	0.537480000	-3.914987000	7.610267000
1	-2.108371000	-1.027325000	7.352363000
6	-2.576126000	-1.281225000	5.344903000
7	-3.245996000	-1.774032000	4.536465000

2a_i1_int



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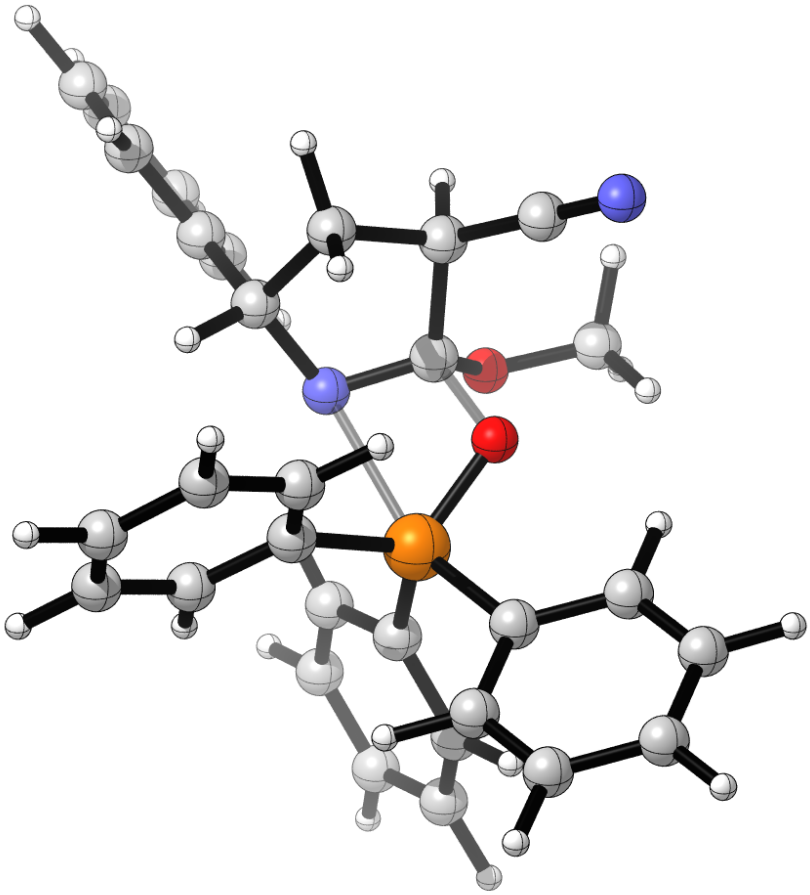
6	1.897802000	3.519005000	6.845250000
6	2.254616000	4.640152000	7.601107000
6	3.095494000	4.497681000	8.709637000
6	3.557477000	3.226621000	9.061044000
15	1.769759000	0.690058000	6.233338000
7	0.427789000	0.439289000	7.336244000
6	3.196401000	-0.436329000	6.543269000
6	1.874651000	1.379956000	4.500859000
6	1.028256000	0.934716000	3.467441000
6	1.178859000	1.421476000	2.164578000

6	2.187126000	2.339614000	1.861133000
6	3.042621000	2.782069000	2.874465000
6	2.880940000	2.317136000	4.182089000
6	4.412280000	-0.259010000	5.866076000
6	5.486114000	-1.122903000	6.104201000
6	5.361299000	-2.166005000	7.026127000
6	4.151599000	-2.344683000	7.704934000
1	1.250240000	3.659304000	5.975430000
1	1.873957000	5.625105000	7.315344000
1	3.388405000	5.371037000	9.298503000
1	4.208106000	3.099400000	9.930650000
1	0.264893000	0.190159000	3.681503000
1	0.502565000	1.064903000	1.383715000
1	2.310749000	2.712983000	0.840759000
1	3.836912000	3.498924000	2.649172000
1	3.552750000	2.691695000	4.953983000
1	4.533216000	0.545848000	5.139088000
1	6.424859000	-0.971177000	5.564709000
1	6.202400000	-2.838628000	7.215753000
1	4.038527000	-3.160243000	8.424787000
1	2.124569000	-1.652926000	7.977410000
6	3.073143000	-1.488657000	7.465028000
1	3.563092000	1.125195000	8.605617000
6	-0.579584000	1.431673000	7.729528000
1	-0.145050000	2.436058000	7.657331000
6	-1.670635000	1.261966000	6.634105000

1	-1.376624000	1.836746000	5.740620000
1	-2.662397000	1.613728000	6.953061000
6	-1.651180000	-0.252186000	6.311805000
6	-1.111410000	1.279965000	9.151157000
6	-1.748777000	2.382525000	9.746850000
6	-1.021631000	0.082805000	9.875993000
6	-2.297212000	2.289436000	11.027939000
6	-1.576974000	-0.012327000	11.157388000
6	-2.216001000	1.086235000	11.737624000
1	-1.812437000	3.329781000	9.200901000
1	-0.522853000	-0.779095000	9.430330000
1	-2.785550000	3.159329000	11.476041000
1	-1.506490000	-0.954958000	11.707457000
1	-2.648016000	1.008489000	12.738739000
6	-0.151321000	-0.689632000	6.612572000
8	0.714673000	-0.765008000	5.566454000
8	-0.143864000	-1.850605000	7.419996000
6	-0.358039000	-3.067543000	6.724889000
1	-1.384294000	-3.137051000	6.316702000
1	0.356025000	-3.178748000	5.894291000
1	-0.211934000	-3.878911000	7.452329000
1	-2.293784000	-0.786710000	7.028733000
6	-2.101559000	-0.577847000	4.963418000
7	-2.441615000	-0.819150000	3.881076000

2a_i1_TS2 (**TS2**_trans_e1)



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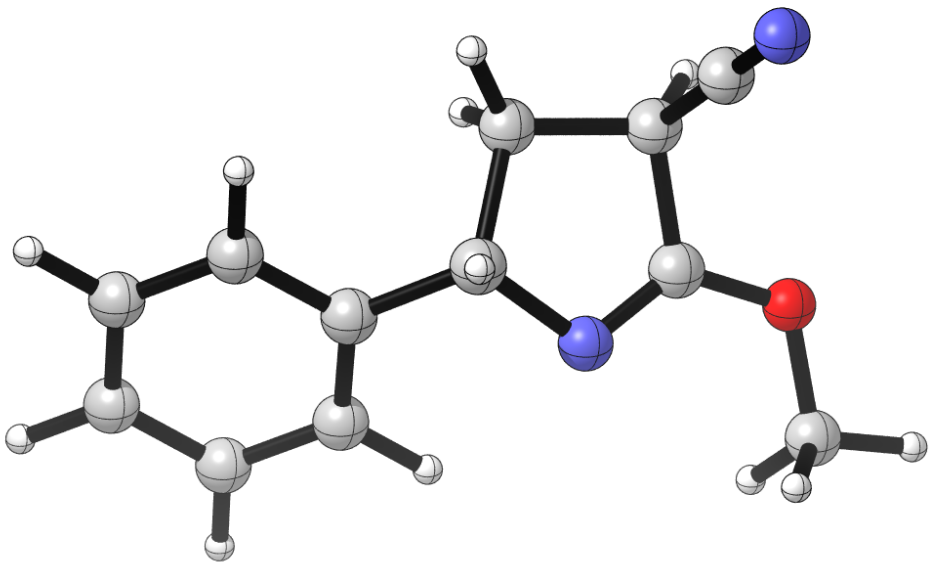
6	1.377575000	3.544517000	6.152262000
6	1.535192000	4.831970000	6.671505000
6	2.420300000	5.059867000	7.731263000
6	3.125682000	3.989120000	8.289527000
15	1.944167000	0.829775000	5.926895000
7	0.424585000	0.419368000	7.853965000
6	3.157860000	-0.383126000	6.580541000
6	2.499047000	1.206113000	4.202989000
6	1.844389000	0.640216000	3.094856000
6	2.244454000	0.967927000	1.795063000

6	3.296931000	1.863728000	1.585552000
6	3.955662000	2.429956000	2.682356000
6	3.559356000	2.104280000	3.981662000
6	4.191978000	-0.845475000	5.742060000
6	5.106928000	-1.794487000	6.206735000
6	5.003410000	-2.292323000	7.508857000
6	3.977482000	-1.839154000	8.343564000
1	0.712371000	3.380946000	5.300342000
1	0.972747000	5.660883000	6.233969000
1	2.559783000	6.069333000	8.127037000
1	3.810581000	4.160965000	9.123932000
1	1.001825000	-0.033094000	3.254969000
1	1.716371000	0.527250000	0.945645000
1	3.602781000	2.131924000	0.570330000
1	4.775623000	3.135404000	2.523904000
1	4.073397000	2.567904000	4.826555000
1	4.287492000	-0.474613000	4.721348000
1	5.897703000	-2.148952000	5.540723000
1	5.716798000	-3.038955000	7.869011000
1	3.879323000	-2.236998000	9.356873000
1	2.213298000	-0.559632000	8.499072000
6	3.055631000	-0.893966000	7.888157000
1	3.505333000	1.863824000	8.236555000
6	-0.436697000	1.354249000	8.550200000
1	0.130428000	2.261559000	8.834806000
6	-1.534293000	1.741012000	7.516852000

1	-1.156885000	2.524783000	6.843681000
1	-2.477889000	2.093177000	7.958765000
6	-1.702873000	0.423929000	6.732911000
6	-1.058908000	0.789337000	9.842720000
6	-1.905439000	1.585166000	10.635340000
6	-0.813541000	-0.528031000	10.253751000
6	-2.503547000	1.074395000	11.790509000
6	-1.401264000	-1.039746000	11.416886000
6	-2.253054000	-0.244300000	12.187718000
1	-2.111341000	2.619495000	10.340485000
1	-0.163535000	-1.148121000	9.632768000
1	-3.164542000	1.709553000	12.387773000
1	-1.186889000	-2.067893000	11.723865000
1	-2.719981000	-0.647073000	13.090863000
6	-0.255635000	-0.174821000	6.824892000
8	0.494317000	0.246731000	5.527500000
8	-0.184642000	-1.562518000	6.844101000
6	-0.785618000	-2.295353000	5.795073000
1	-1.888324000	-2.208515000	5.804249000
1	-0.414123000	-1.976531000	4.806450000
1	-0.518663000	-3.350447000	5.955915000
1	-2.359336000	-0.258707000	7.299806000
6	-2.256200000	0.577502000	5.390448000
7	-2.696840000	0.712809000	4.325715000

4a



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7	1.339075431	-1.155769542	5.368384376
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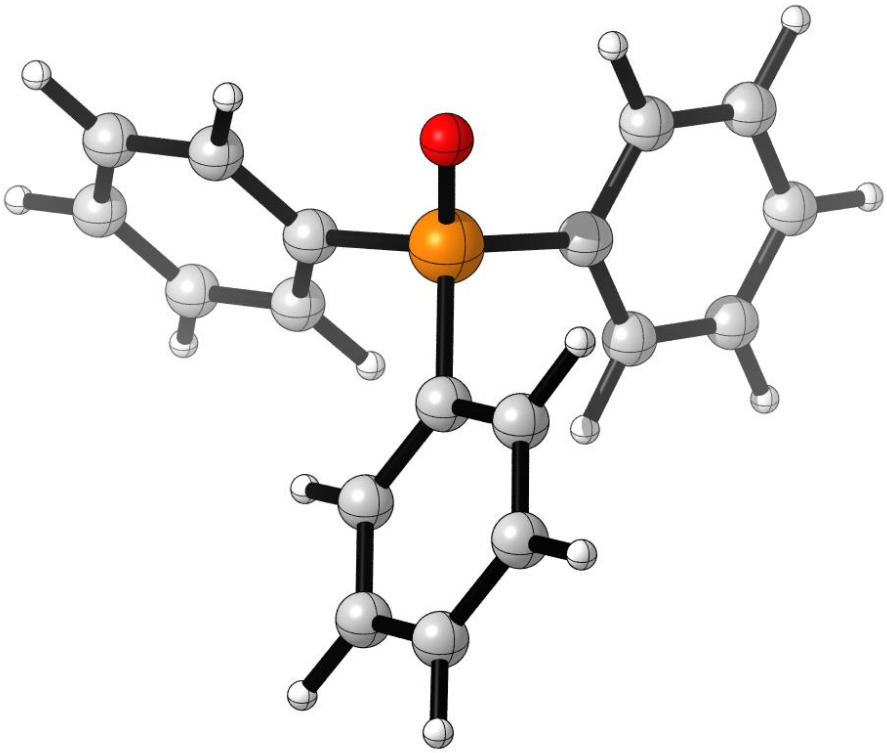
1	0.102857274	-1.325096162	3.696766075
6	-0.775679257	-2.309504501	5.443316801
1	-1.520011238	-2.777512641	4.784804384
1	-1.292741548	-1.949611412	6.345230146
6	0.358668978	-3.272441879	5.870097744
6	-0.691619944	0.222476133	4.936799250
6	-1.967573183	0.428231546	4.385559866
6	-0.079976913	1.276641308	5.629023524
6	-2.618703206	1.656024056	4.532391391
6	-0.731484401	2.505786954	5.776972725

6	-2.002401676	2.700321605	5.230523116
1	-2.459406759	-0.377936100	3.831919028
1	0.916779167	1.121887042	6.043989784
1	-3.610868960	1.799942832	4.096330694
1	-0.239662545	3.317112805	6.320874710
1	-2.512318935	3.660431772	5.347213474
6	1.523041817	-2.279244727	5.932487405
8	2.629343894	-2.688653919	6.541145476
6	3.743609391	-1.795101182	6.537186131
1	3.983115929	-1.475570917	5.511580188
1	3.521259453	-0.898062556	7.136293380
1	4.581323159	-2.350266287	6.977756625
6	0.638516378	-4.339298626	4.900045806
7	0.854882751	-5.163697640	4.114777198
1	0.187394924	-3.744277190	6.851314533

Ph_3PO



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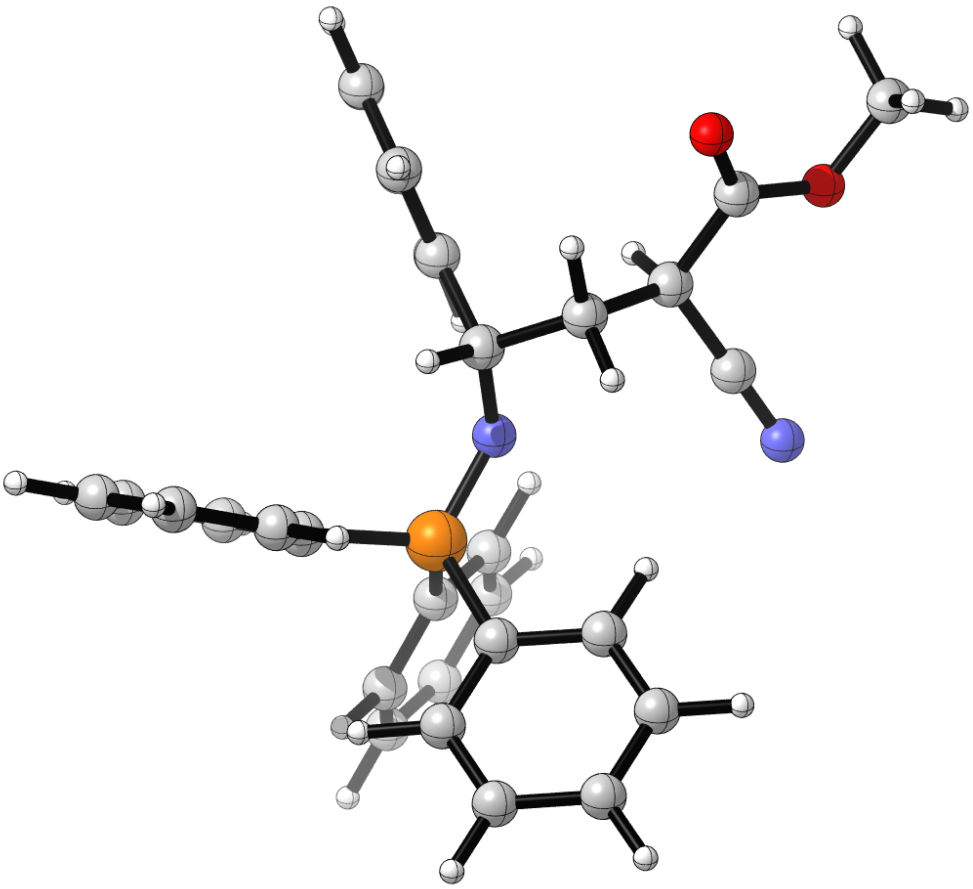
6	2.941927000	0.029708000	8.013225000
6	3.902502000	0.582134000	8.874341000
6	4.050317000	0.089533000	10.175685000
6	3.244029000	-0.960404000	10.622744000
6	2.286689000	-1.519849000	9.767961000
15	2.725143000	0.520219000	6.256626000
6	4.186717000	1.528218000	5.797455000
6	1.261900000	1.626772000	6.180198000
6	0.924596000	2.571648000	7.163117000
6	-0.195913000	3.392324000	6.992567000
6	-0.987938000	3.268987000	5.844832000

6	-0.664128000	2.318048000	4.870607000
6	0.452795000	1.494782000	5.038427000
6	5.066838000	0.940365000	4.875459000
6	6.215529000	1.624161000	4.466264000
6	6.493797000	2.895264000	4.978252000
6	5.616137000	3.488619000	5.892986000
1	4.555145000	1.387174000	8.530077000
1	4.805195000	0.522604000	10.837315000
1	3.370344000	-1.353896000	11.635078000
1	1.662737000	-2.348938000	10.113035000
1	1.524903000	2.660554000	8.073466000
1	-0.458741000	4.121876000	7.763586000
1	-1.866292000	3.906866000	5.713996000
1	-1.288299000	2.211577000	3.979116000
1	0.708642000	0.732632000	4.297949000
1	4.825861000	-0.050411000	4.482662000
1	6.896358000	1.162473000	3.745895000
1	7.391982000	3.429608000	4.657128000
1	5.831082000	4.483626000	6.291724000
1	3.767492000	3.298355000	6.988425000
6	4.460054000	2.813251000	6.294731000
1	1.419915000	-1.493162000	7.784833000
8	2.560709000	-0.665756000	5.341454000

2a_i12



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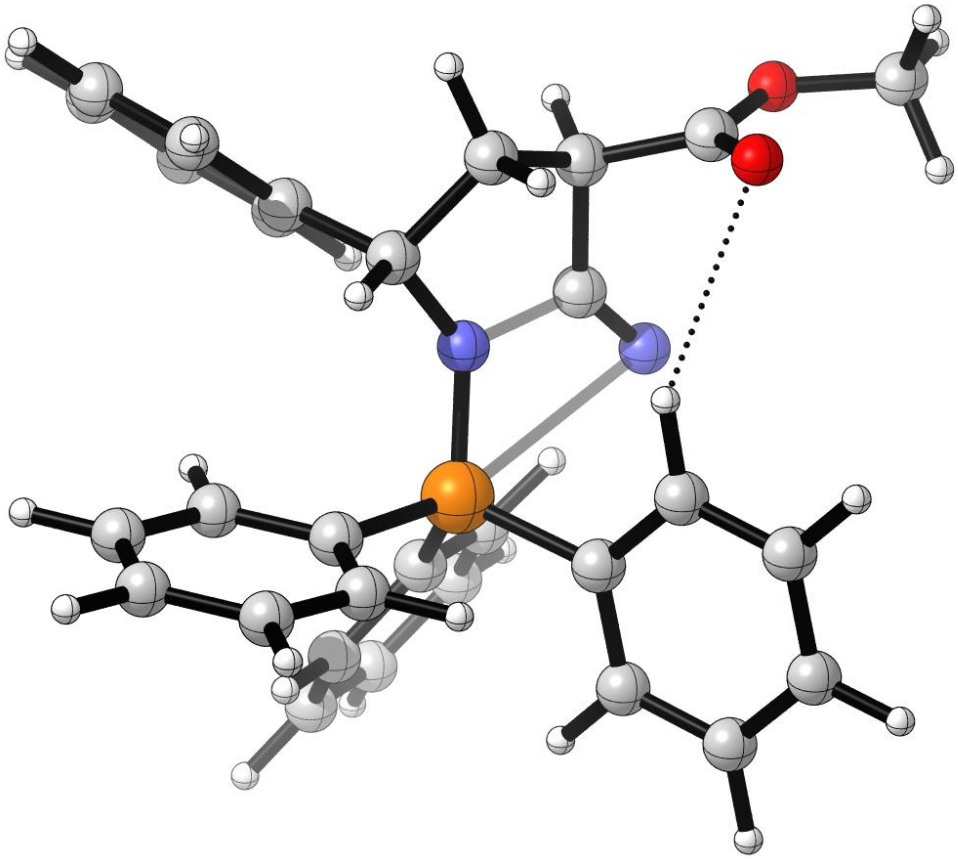
6	-0.608477000	3.567288000	2.420354000
6	-1.478759000	3.685260000	1.319536000
6	-2.459069000	4.682656000	1.292046000
6	-2.586534000	5.571495000	2.364234000
6	-1.734320000	5.455962000	3.468081000
15	0.534396000	2.123785000	2.545001000
7	-0.102741000	0.797016000	3.122182000
6	1.920142000	2.624633000	3.634198000
6	1.323368000	1.983029000	0.874660000
6	1.786252000	0.713996000	0.487132000
6	2.451185000	0.549275000	-0.732451000

6	2.663296000	1.646475000	-1.572434000
6	2.212253000	2.914262000	-1.189907000
6	1.546474000	3.082904000	0.027906000
6	2.299021000	1.779407000	4.686894000
6	3.367879000	2.131274000	5.518416000
6	4.061283000	3.326684000	5.304830000
6	3.689507000	4.170295000	4.251304000
1	-1.384681000	3.003128000	0.469858000
1	-3.122989000	4.768994000	0.427131000
1	-3.351767000	6.352571000	2.340814000
1	-1.836020000	6.143614000	4.312547000
1	1.637050000	-0.143567000	1.148401000
1	2.812278000	-0.440489000	-1.025133000
1	3.184502000	1.514679000	-2.524555000
1	2.382102000	3.775806000	-1.841765000
1	1.197218000	4.077974000	0.314884000
1	1.752363000	0.845009000	4.828943000
1	3.663220000	1.463037000	6.331686000
1	4.895962000	3.601635000	5.955612000
1	4.231838000	5.103248000	4.076897000
1	2.351735000	4.482473000	2.591056000
6	2.627713000	3.818708000	3.414562000
1	-0.101510000	4.373815000	4.371267000
6	-1.454436000	0.328654000	2.916476000
1	-2.033797000	0.974995000	2.223804000
6	-1.491640000	-1.072313000	2.245291000

1	-1.012727000	-1.007488000	1.255864000
1	-2.535766000	-1.374818000	2.083091000
6	-0.827262000	-2.200602000	3.069405000
6	0.601695000	-2.357524000	2.776109000
7	1.722254000	-2.470065000	2.501258000
6	-2.259499000	0.299128000	4.225466000
6	-3.656761000	0.151489000	4.196582000
6	-1.628123000	0.390146000	5.473578000
6	-4.397701000	0.091906000	5.378970000
6	-2.365301000	0.318902000	6.661092000
6	-3.753574000	0.169959000	6.619183000
1	-4.175947000	0.086703000	3.234714000
1	-0.547162000	0.535455000	5.493871000
1	-5.484864000	-0.019957000	5.331818000
1	-1.848360000	0.388574000	7.622738000
1	-4.333074000	0.117969000	7.544768000
6	-1.583933000	-3.539056000	2.946616000
8	-2.725511000	-3.643617000	2.577586000
8	-0.837901000	-4.565870000	3.371297000
6	-1.460499000	-5.853937000	3.371678000
1	-2.311015000	-5.873186000	4.070008000
1	-1.829818000	-6.109375000	2.367134000
1	-0.688344000	-6.564396000	3.691455000
1	-0.913898000	-1.944463000	4.143574000

2a_i12_TS1 (**TS1**_trans_e1)



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6	-0.974795000	3.525839000	0.942671000
6	-1.895242000	4.553260000	0.705994000
6	-2.521787000	5.197209000	1.776062000
6	-2.228100000	4.812022000	3.089540000
15	0.424943000	1.711248000	2.587248000
7	-0.566776000	0.498177000	3.124165000
6	1.719301000	2.289867000	3.754569000
6	1.239040000	1.280003000	1.014945000
6	0.711686000	0.266777000	0.196558000
6	1.315924000	-0.021586000	-1.027953000

6	2.440512000	0.697079000	-1.447935000
6	2.960088000	1.714223000	-0.641227000
6	2.366024000	2.004371000	0.590429000
6	2.535930000	1.337150000	4.394077000
6	3.532022000	1.762145000	5.277830000
6	3.735020000	3.124219000	5.521948000
6	2.943031000	4.072637000	4.868009000
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1	0.910657000	-0.825853000	-1.647093000
1	2.916754000	0.456510000	-2.402126000
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1	2.791138000	2.786407000	1.224414000
1	2.374843000	0.277386000	4.148405000
1	4.157617000	1.016810000	5.775283000
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1	-1.106618000	3.478038000	4.360612000
6	-2.016508000	0.471091000	3.298443000
1	-2.522316000	1.183366000	2.628177000
6	-2.374353000	-0.977940000	2.838172000

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1	-3.305596000	-1.324091000	3.308929000
6	-1.170615000	-1.854703000	3.174446000
6	0.098356000	-0.934286000	3.144472000
7	1.299421000	-1.116761000	3.082786000
6	-2.483734000	0.749967000	4.724459000
6	-3.825963000	1.098790000	4.949768000
6	-1.632519000	0.616714000	5.830081000
6	-4.309163000	1.297435000	6.245272000
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1	-4.501996000	1.216985000	4.096612000
1	-0.586194000	0.349347000	5.668236000
1	-5.355526000	1.575375000	6.400546000
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1	-3.831216000	1.313410000	8.356552000
6	-0.926667000	-2.950040000	2.163796000
8	-1.196252000	-2.880396000	0.983200000
8	-0.309799000	-4.001595000	2.719443000
6	0.185861000	-4.988285000	1.817671000
1	-0.632736000	-5.448634000	1.242214000
1	0.900150000	-4.535589000	1.112661000
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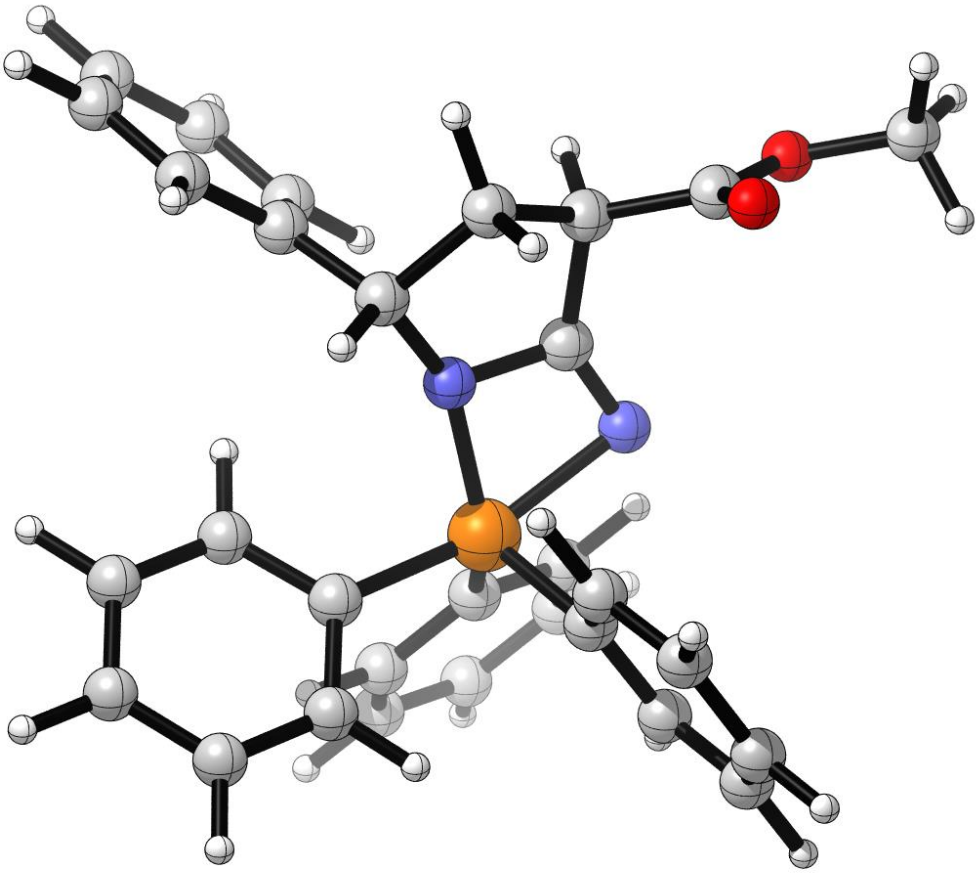

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6	-4.049548000	-3.533677000	5.034535000
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6	-5.110575000	1.400143000	2.454815000
6	-5.520169000	0.751271000	3.623445000
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6	-3.670898000	-3.118139000	6.327721000
6	-4.258815000	-3.693198000	7.457529000
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1	-5.755077000	-2.381529000	1.852049000
1	-6.787525000	-3.680083000	0.028358000
1	-5.774462000	-5.841980000	-0.710185000
1	-3.720543000	-6.689138000	0.433951000
1	-2.896739000	-0.919173000	1.296385000
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6	-0.768519000	-3.385072000	1.760668000
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6	0.323089000	-2.263135000	1.871140000

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1	1.298293000	-2.599829000	1.492278000
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6	-0.142056000	-4.773057000	1.844230000
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6	0.112009000	-5.397030000	3.075341000
6	0.974947000	-6.623368000	0.719380000
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1	0.778876000	1.813046000	5.117400000
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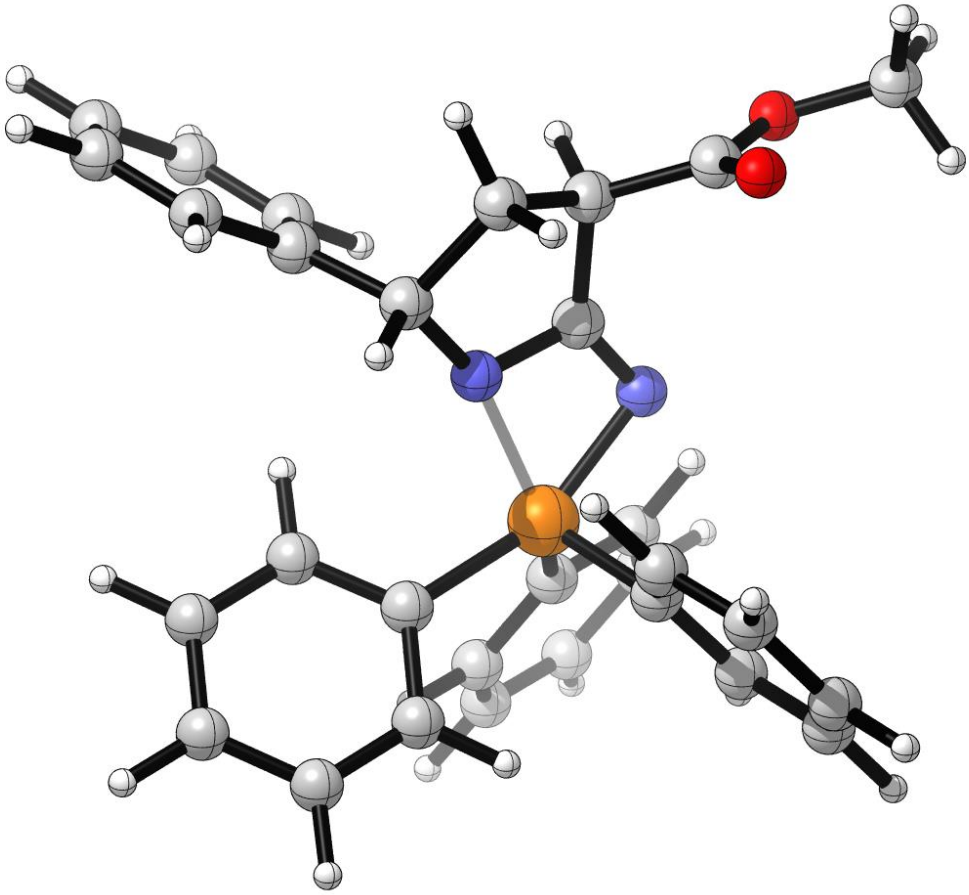

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6	-4.135898000	-5.848989000	0.915403000
15	-3.295319000	-2.740782000	3.608889000
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6	-4.150507000	-3.405613000	5.129791000
6	-4.046150000	-1.125427000	3.119761000
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6	-4.117966000	0.734645000	1.557268000

6	-5.097655000	1.359985000	2.336523000
6	-5.544654000	0.745122000	3.509038000
6	-5.016677000	-0.489173000	3.906119000
6	-3.752439000	-2.946534000	6.403140000
6	-4.363428000	-3.438625000	7.559175000
6	-5.376527000	-4.399186000	7.471058000
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1	-5.825433000	-2.531794000	2.007133000
1	-6.847871000	-3.902275000	0.226112000
1	-5.770012000	-6.039237000	-0.494841000
1	-3.655036000	-6.782072000	0.609199000
1	-2.845728000	-0.991204000	1.321436000
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1	-2.949504000	-2.211934000	6.464533000
1	-4.034804000	-3.068815000	8.534703000
1	-5.849787000	-4.791406000	8.375560000
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6	-5.169903000	-4.373215000	5.056528000
1	-2.624757000	-5.402267000	2.382428000
6	-0.636715000	-3.354504000	1.614595000
1	-1.123533000	-3.218152000	0.634223000
6	0.448533000	-2.242782000	1.827642000

1	0.171052000	-1.342858000	1.258414000
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6	0.446801000	-5.331065000	0.457125000
6	0.183111000	-5.441195000	2.851949000
6	1.120921000	-6.555443000	0.470000000
6	0.862742000	-6.663852000	2.869216000
6	1.339313000	-7.222667000	1.679904000
1	0.277724000	-4.813860000	-0.493118000
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1	1.025223000	-7.183530000	3.817774000
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1	1.043075000	-2.536120000	3.943500000
6	0.759371000	-0.442235000	3.632540000
8	0.705550000	0.462657000	2.835333000
8	1.170562000	-0.294429000	4.900608000
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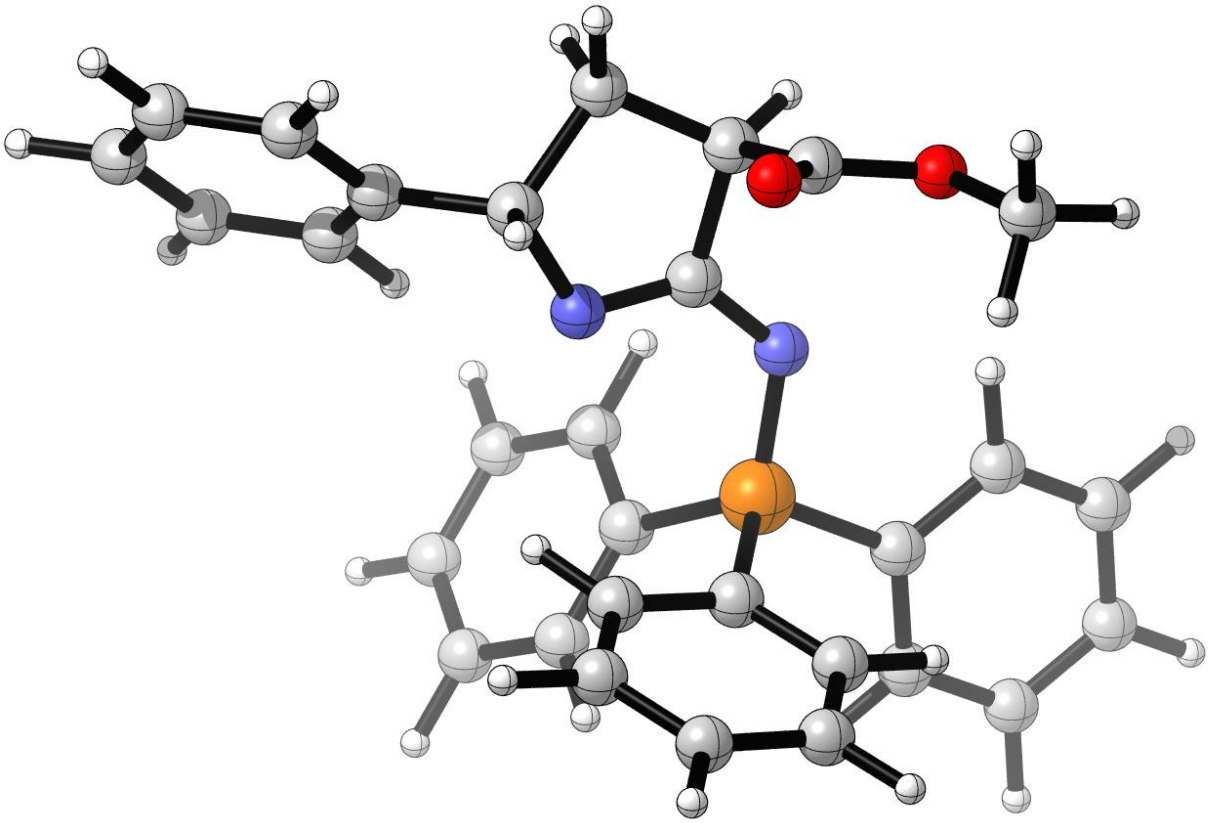
1	0.630923000	1.681792000	5.307072000
1	1.935387000	0.949470000	6.313831000
7	-1.920126000	-1.899454000	4.543057000

3a



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6	-0.144610000	-5.147443000	-1.480735000
15	0.342823000	-1.491358000	0.292953000
7	1.631605000	-3.337914000	2.279720000
6	-0.953917000	-0.415050000	-0.407661000
6	1.915788000	-0.551587000	0.271896000
6	3.139245000	-1.235531000	0.407374000
6	4.334002000	-0.517856000	0.502226000

6	4.321607000	0.880514000	0.478048000
6	3.107663000	1.564650000	0.363614000
6	1.908486000	0.854155000	0.261799000
6	-2.056838000	-0.059664000	0.384244000
6	-3.061486000	0.756997000	-0.145812000
6	-2.968050000	1.225618000	-1.460114000
6	-1.867330000	0.874395000	-2.250217000
1	2.043845000	-2.002172000	-2.158078000
1	2.207899000	-3.967914000	-3.657582000
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1	3.142017000	-2.324708000	0.473289000
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1	5.257812000	1.439472000	0.558842000
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6	1.001723000	-4.010256000	4.495793000

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6	2.758470000	-5.369583000	3.180873000
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6	2.926952000	-7.364357000	1.796919000
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1	4.941332000	-7.635525000	4.536196000
1	2.628533000	-7.916017000	0.900545000
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6	-0.057330000	0.730926000	5.120674000
1	-0.973550000	1.329407000	5.033922000
1	0.324146000	0.753591000	6.153513000
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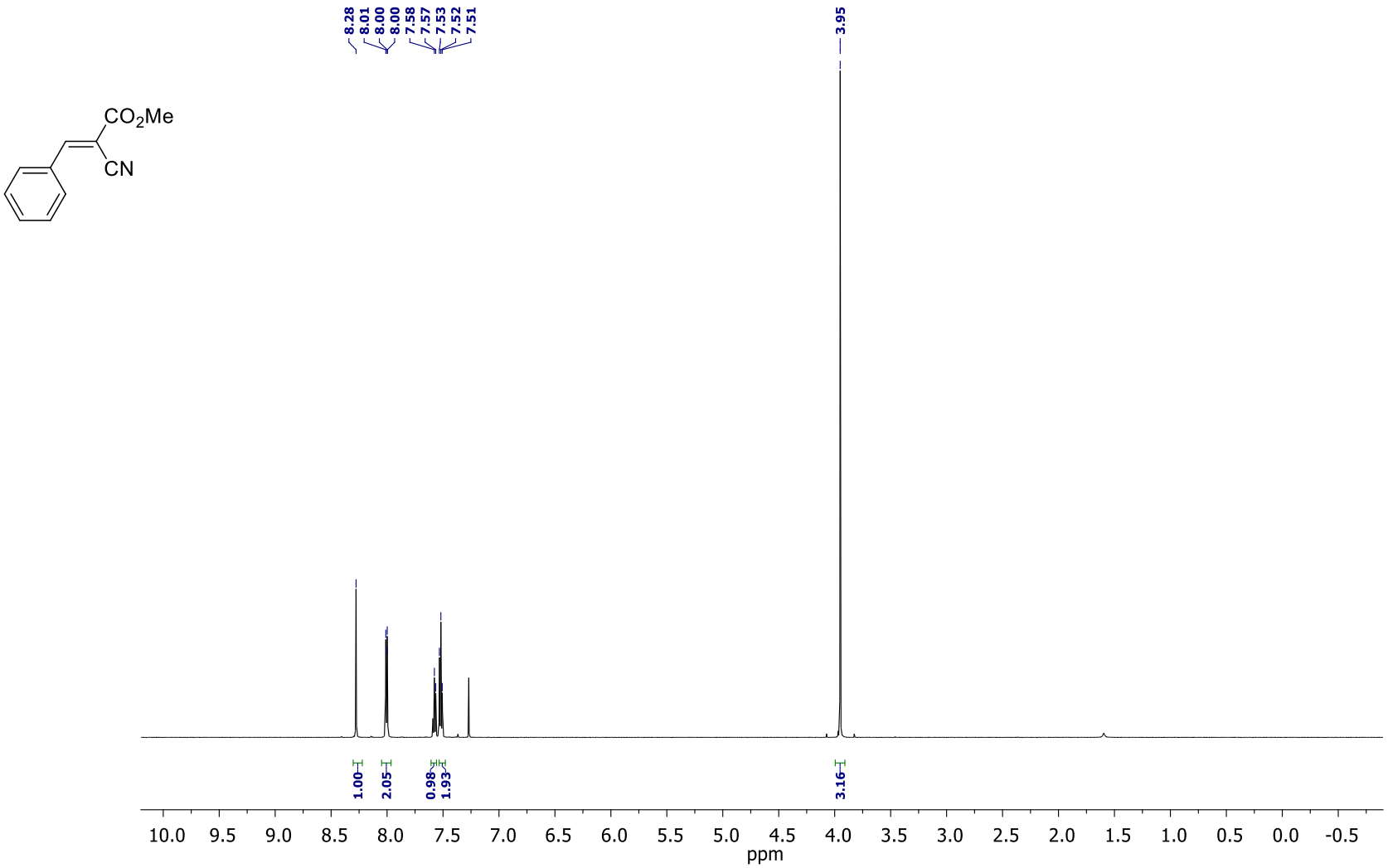
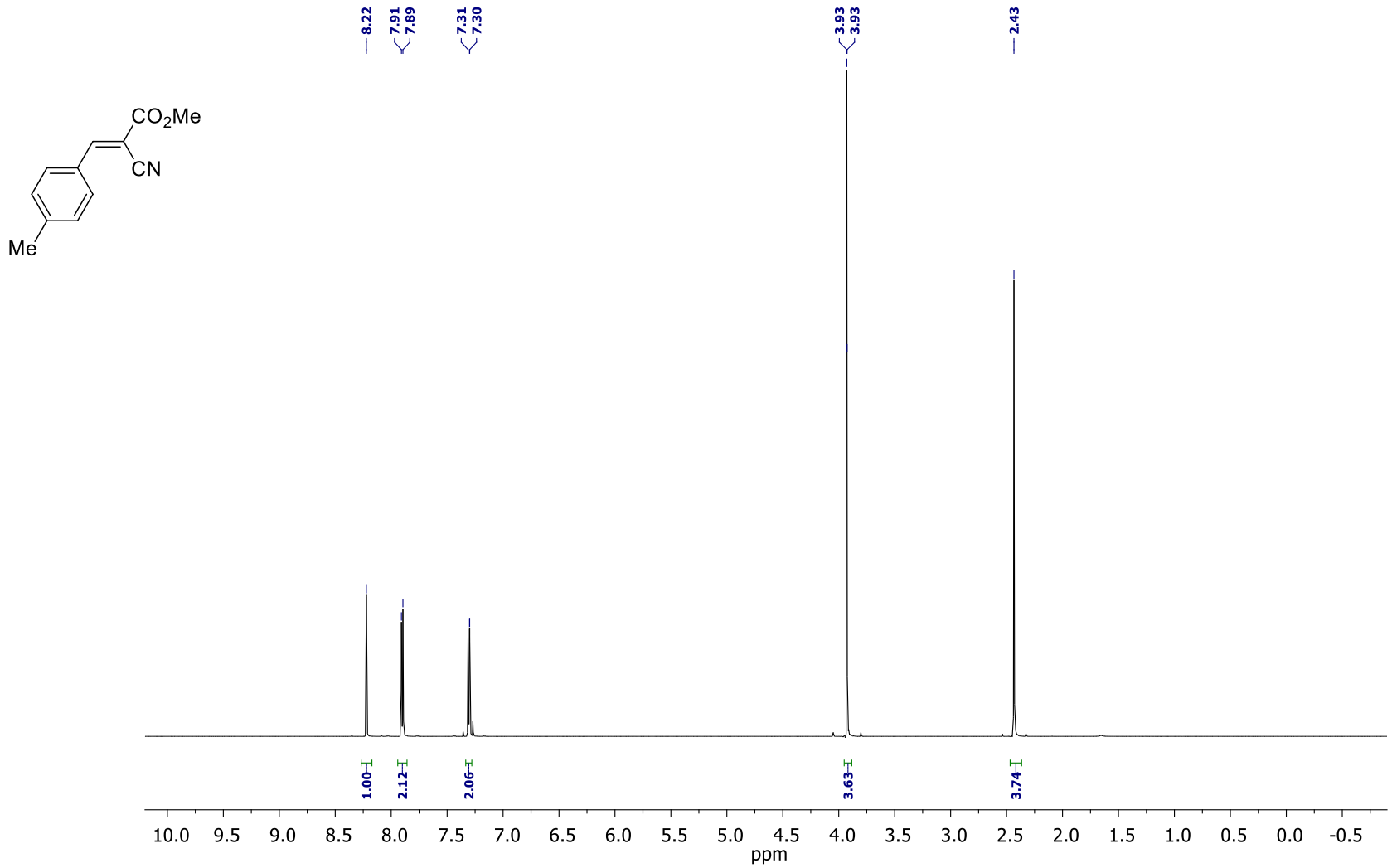
Methyl (*E*)-2-cyano-3-phenylacrylate (S1a)

^{1}H NMR ($CDCl_3$, 600 MHz)



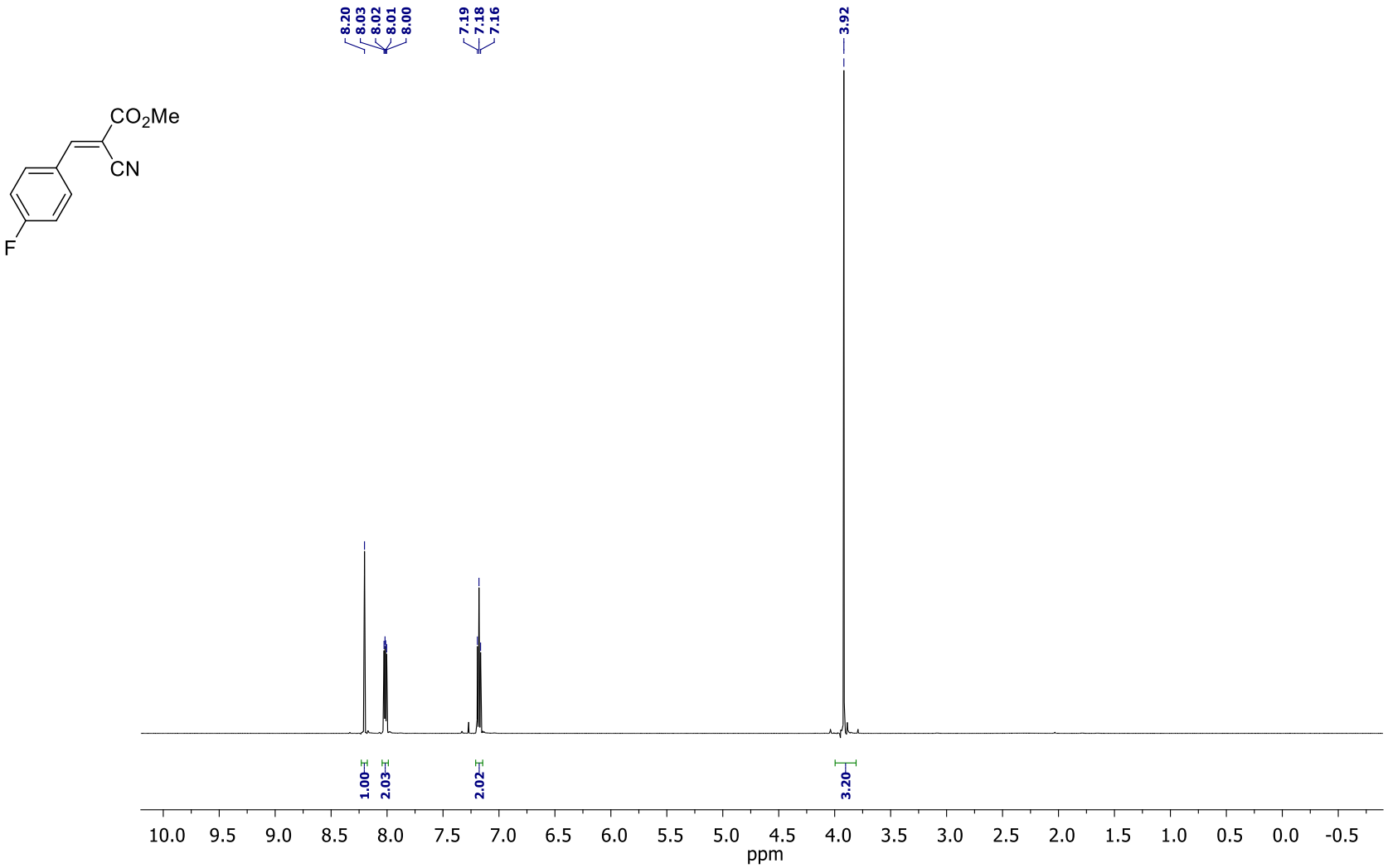
Methyl (*E*)-2-cyano-3-(*p*-tolyl)acrylate (S1b)

^{1}H NMR ($CDCl_3$, 600 MHz)



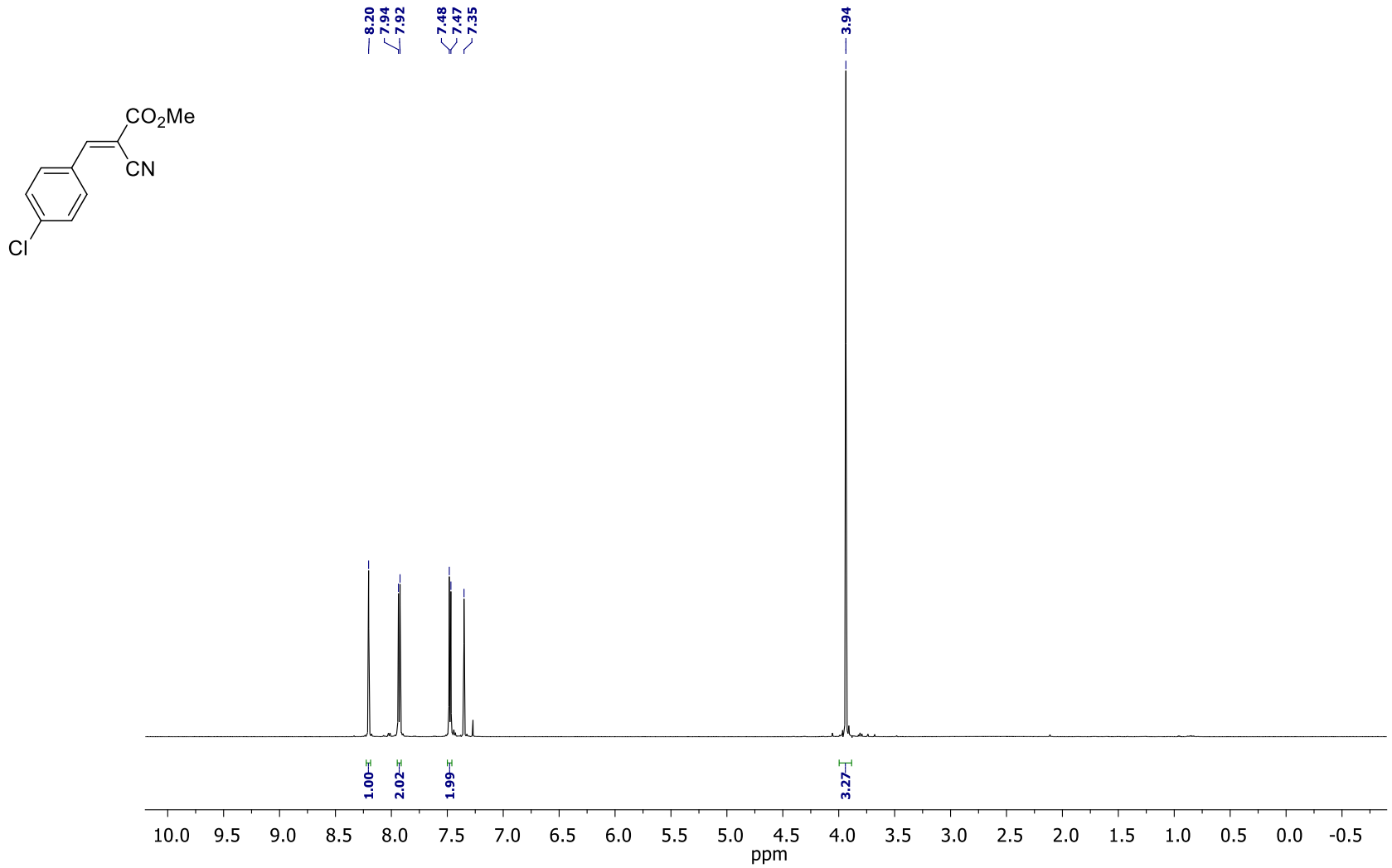
Methyl (*E*)-2-cyano-3-(4-fluorophenyl)acrylate (S1c)

^{1}H NMR ($CDCl_3$, 600 MHz)



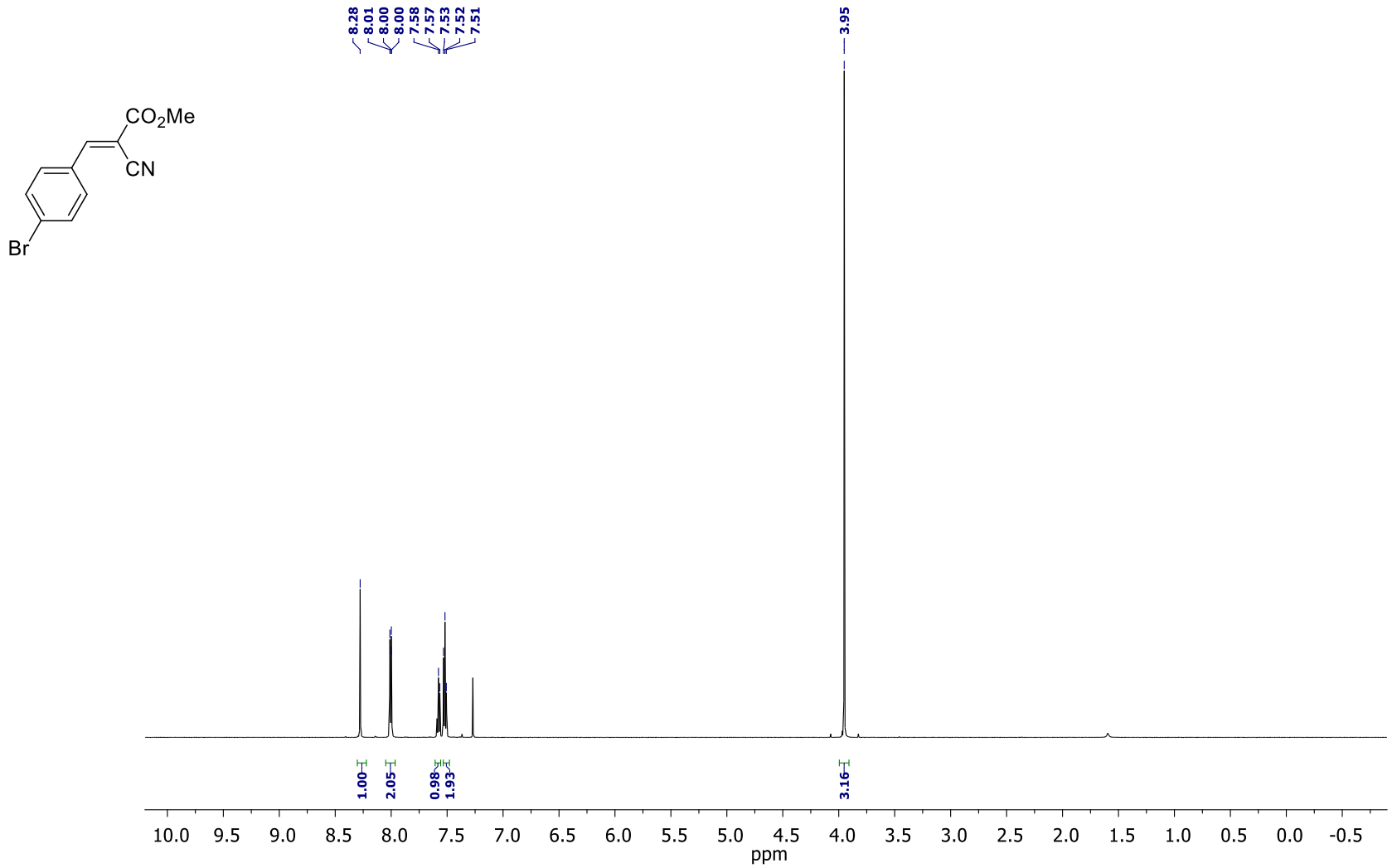
Methyl (*E*)-3-(4-chlorophenyl)-2-cyanoacrylate (S1d)

^{1}H NMR ($CDCl_3$, 600 MHz)



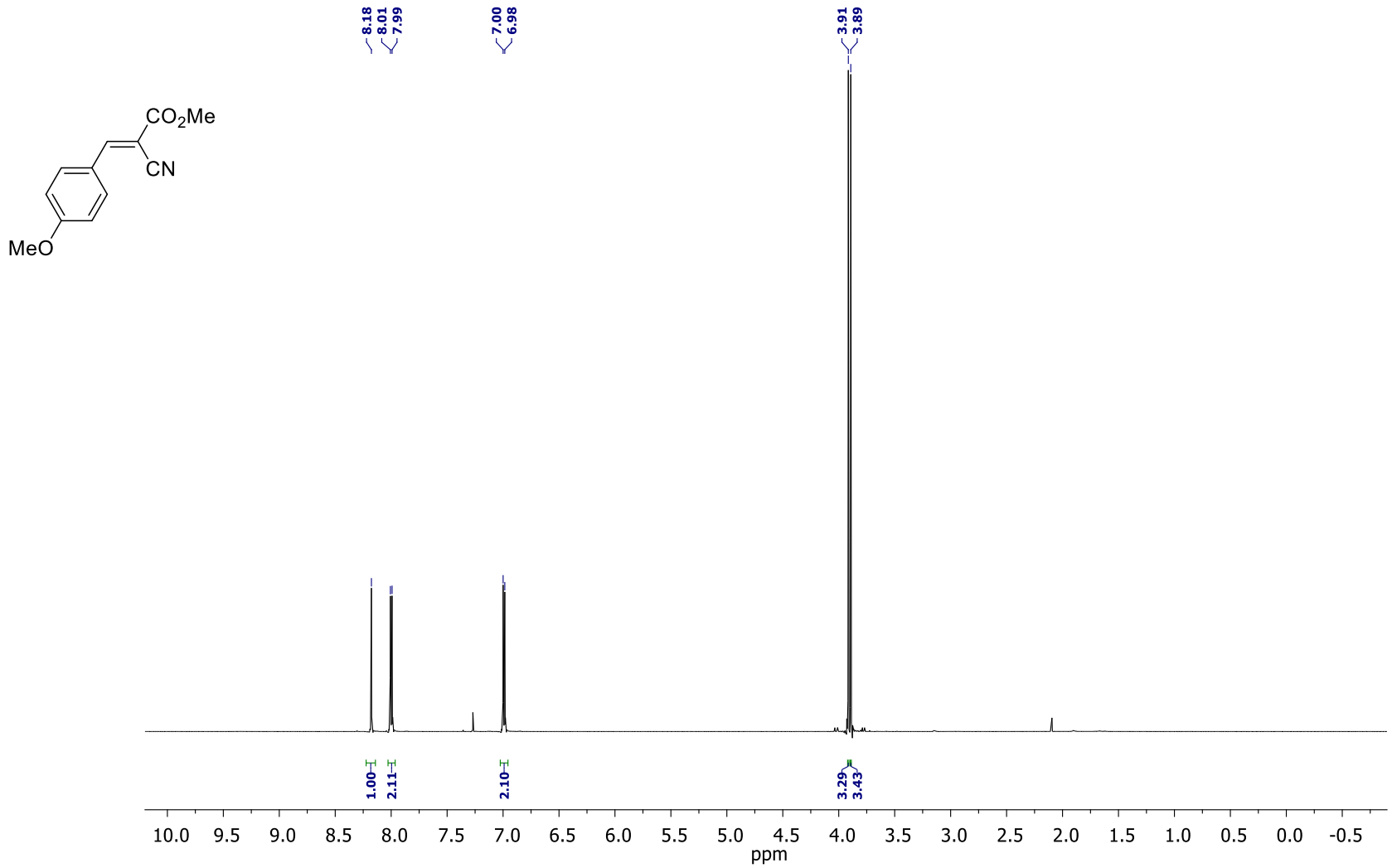
Methyl (*E*)-3-(4-bromophenyl)-2-cyanoacrylate (S1e)

^{1}H NMR ($CDCl_3$, 600 MHz)



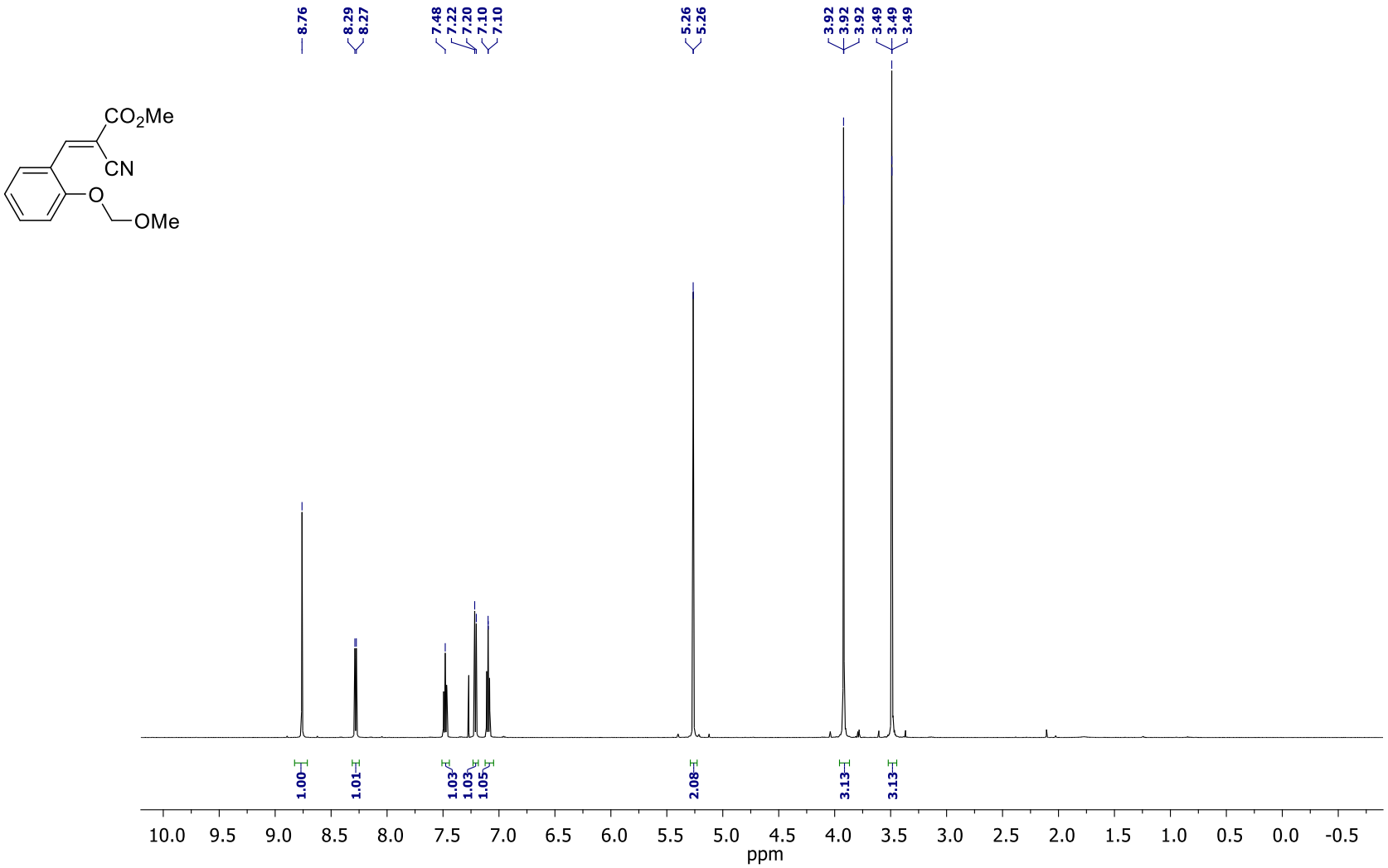
Methyl (*E*)-2-cyano-3-(4-methoxyphenyl)acrylate (S1f)

^{1}H NMR ($CDCl_3$, 600 MHz)



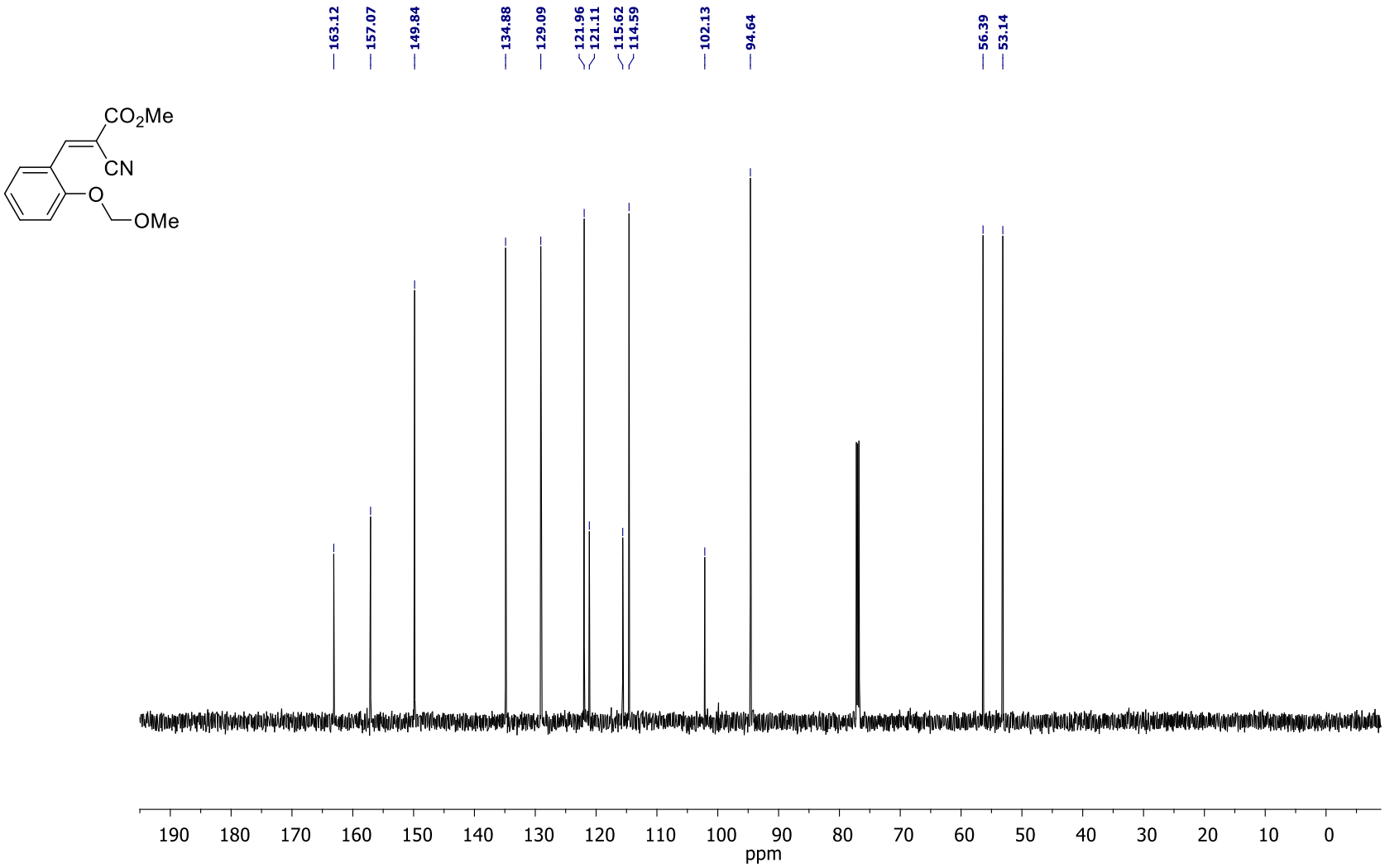
Methyl (*E*)-2-cyano-3-[2-(methoxymethoxy)phenyl]acrylate (S1g)

^{1}H NMR ($CDCl_3$, 600 MHz)



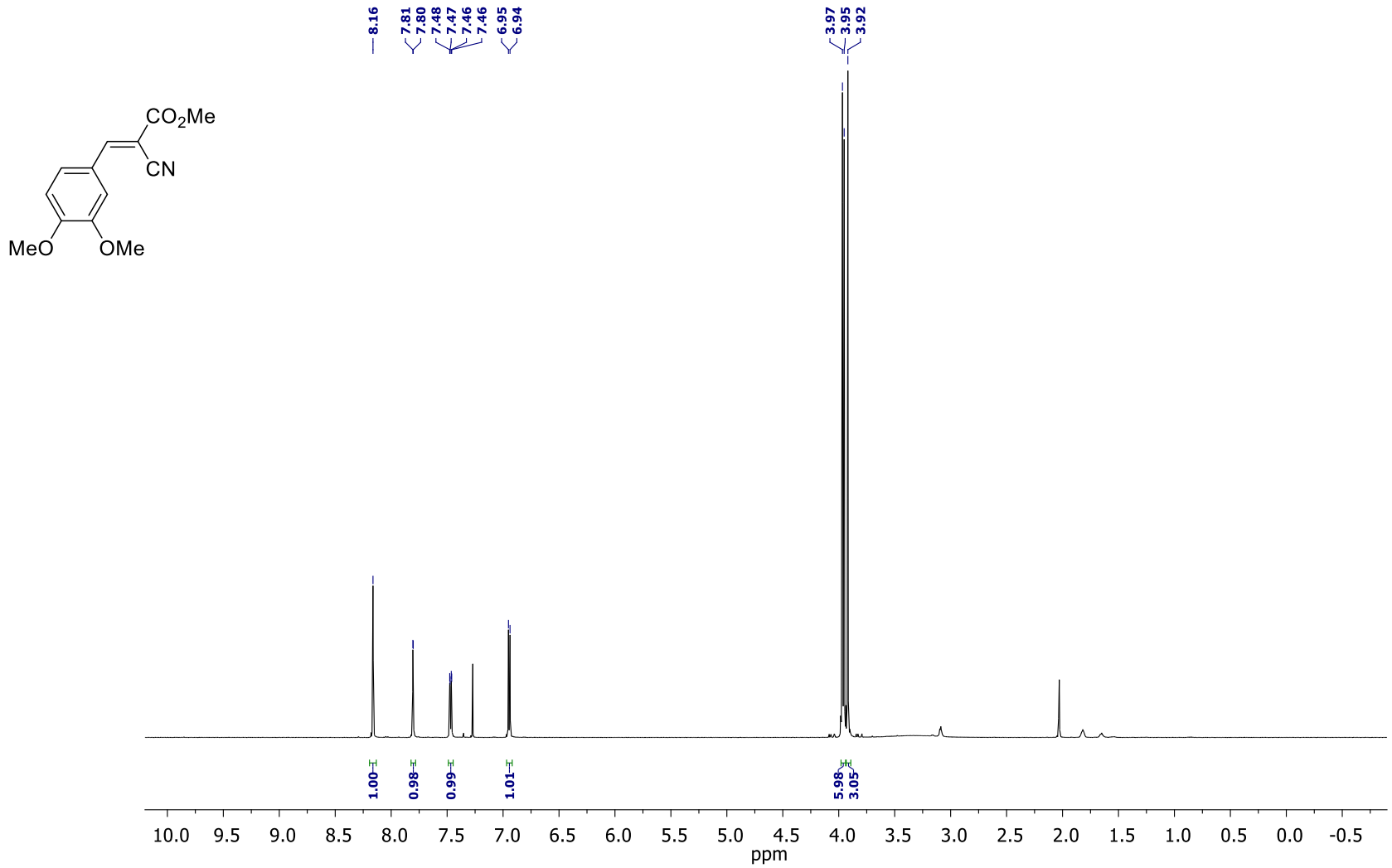
Methyl (*E*)-2-cyano-3-[2-(methoxymethoxy)phenyl]acrylate (S1g)

^{13}C NMR ($CDCl_3$, 150 MHz)



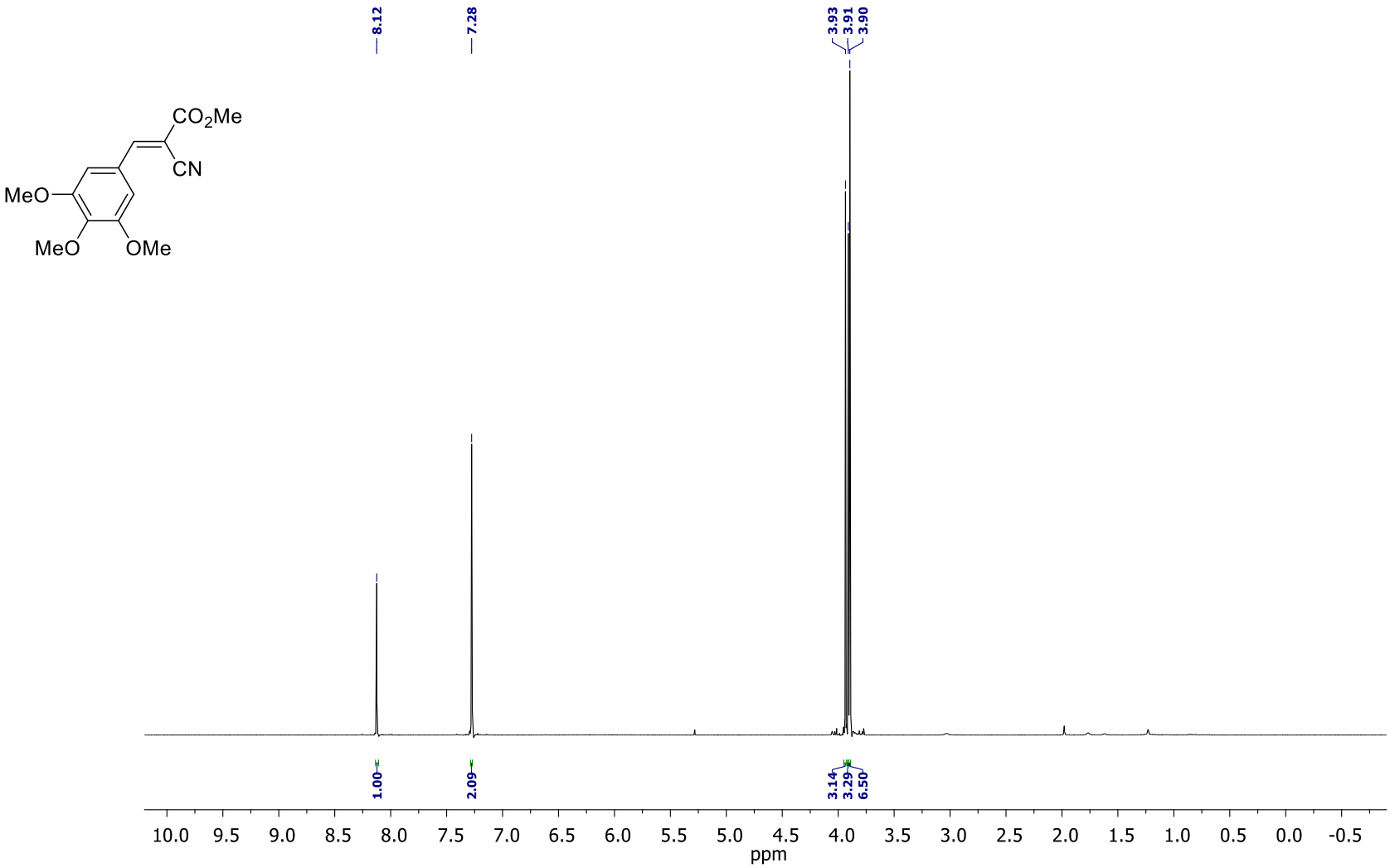
Methyl (*E*)-2-cyano-3-(3,4-dimethoxyphenyl)acrylate (S1h)

^{1}H NMR ($CDCl_3$, 600 MHz)



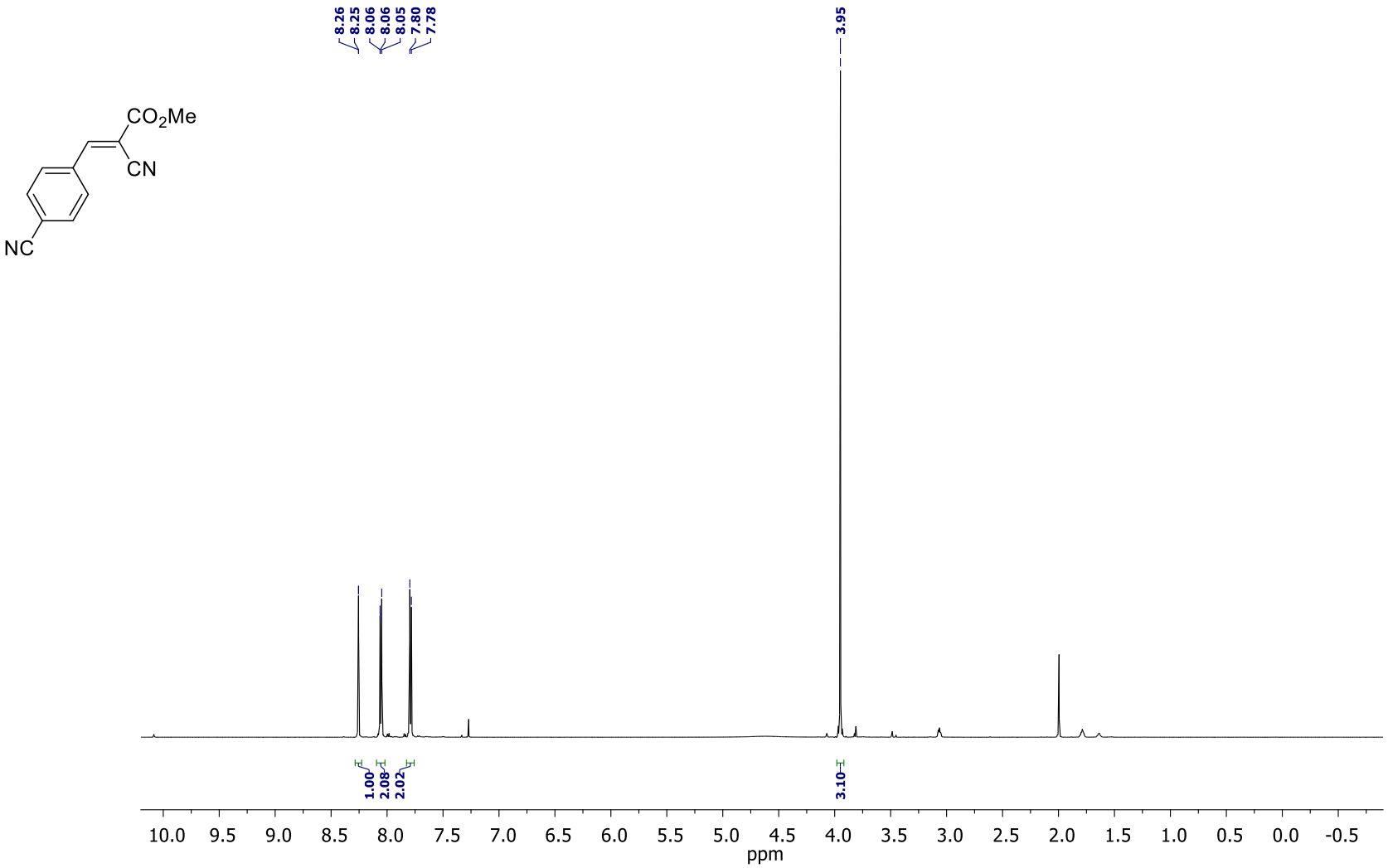
Methyl (*E*)-2-cyano-3-(3,4,5-trimethoxyphenyl)acrylate (S1i)

^{1}H NMR ($CDCl_3$, 600 MHz)



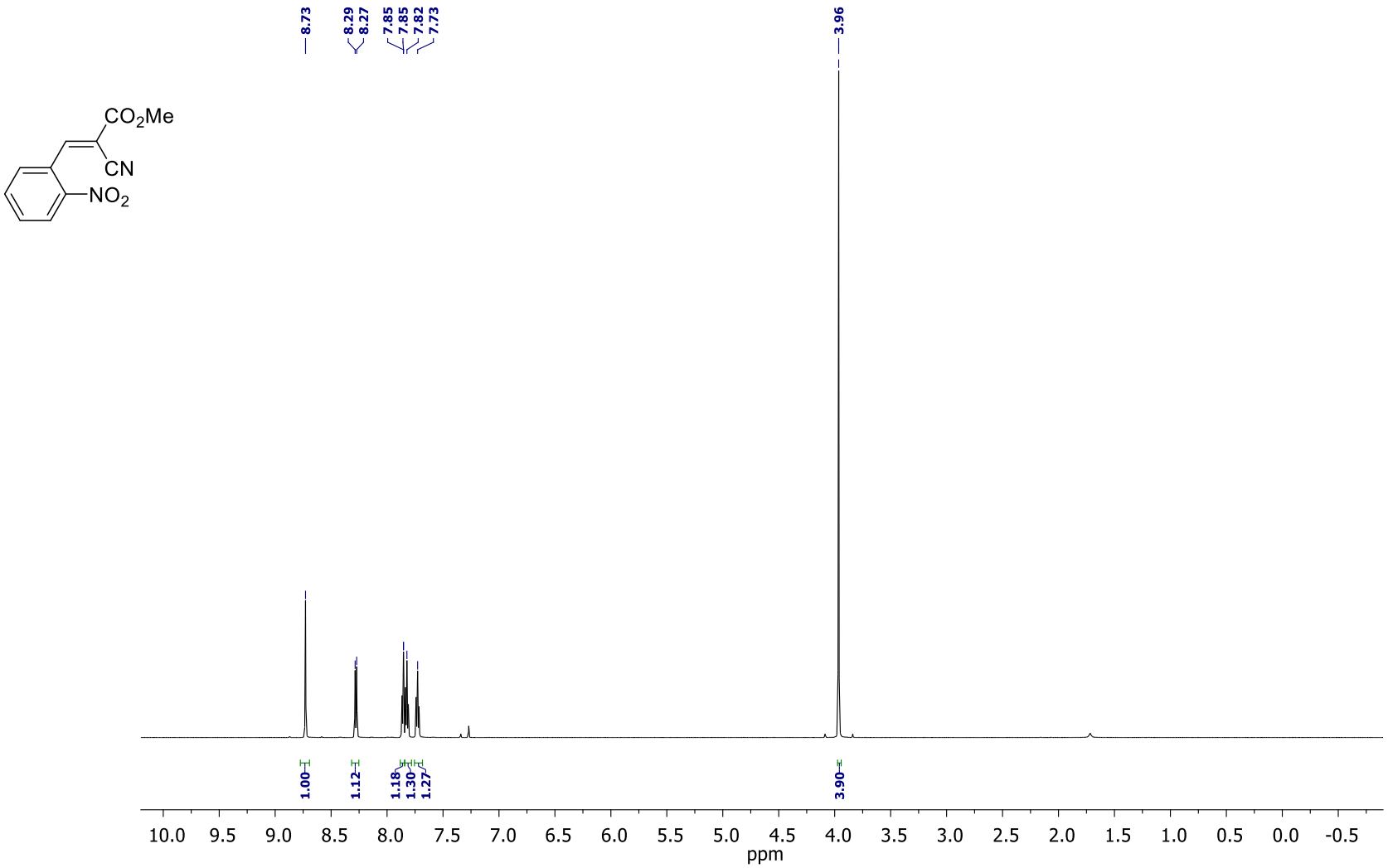
Methyl (*E*)-2-cyano-3-(4-cyanophenyl)acrylate (S1j)

^{1}H NMR ($CDCl_3$, 600 MHz)



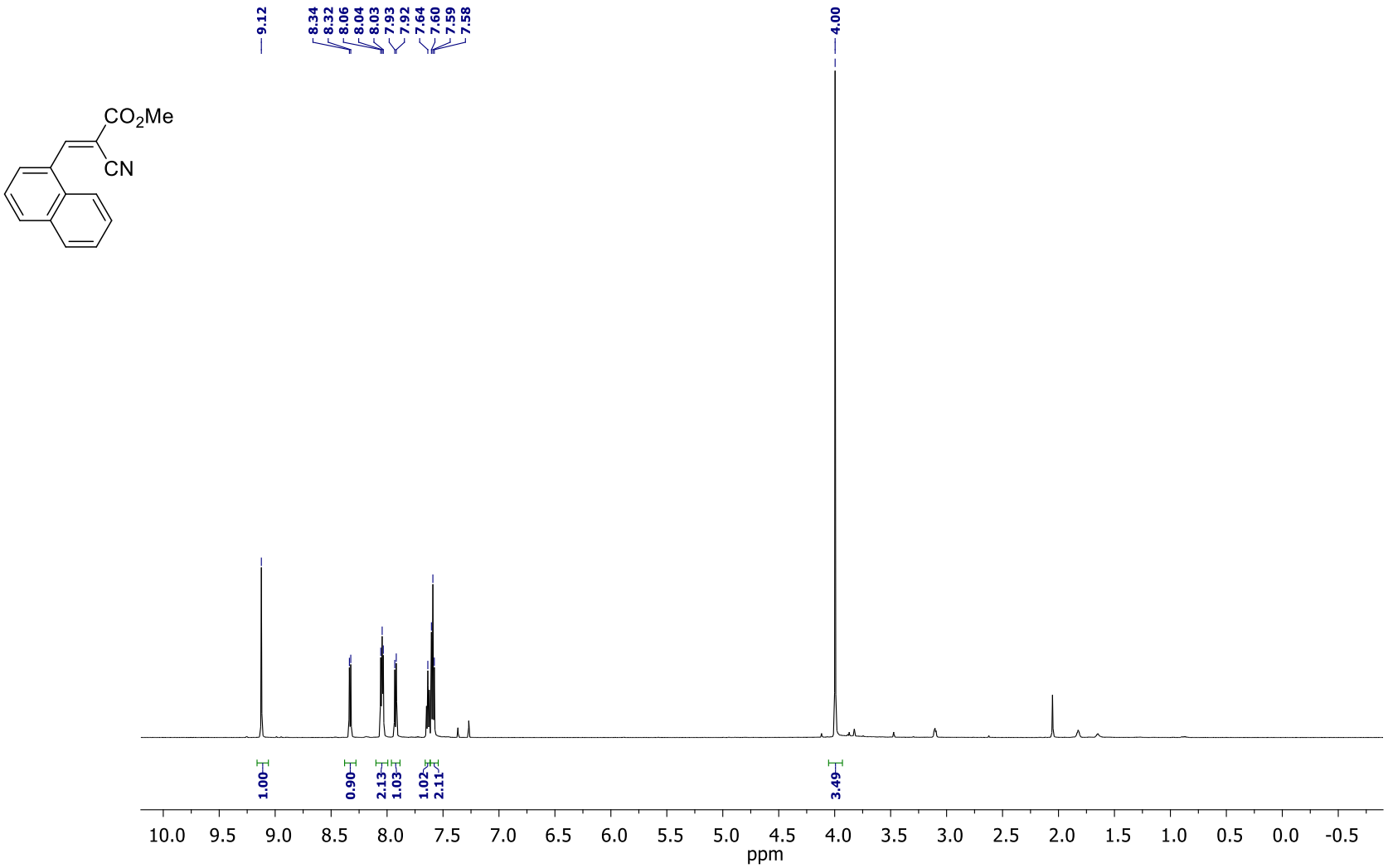
Methyl (*E*)-2-cyano-3-(4-nitrophenyl)acrylate (S1k)

^{1}H NMR ($CDCl_3$, 600 MHz)



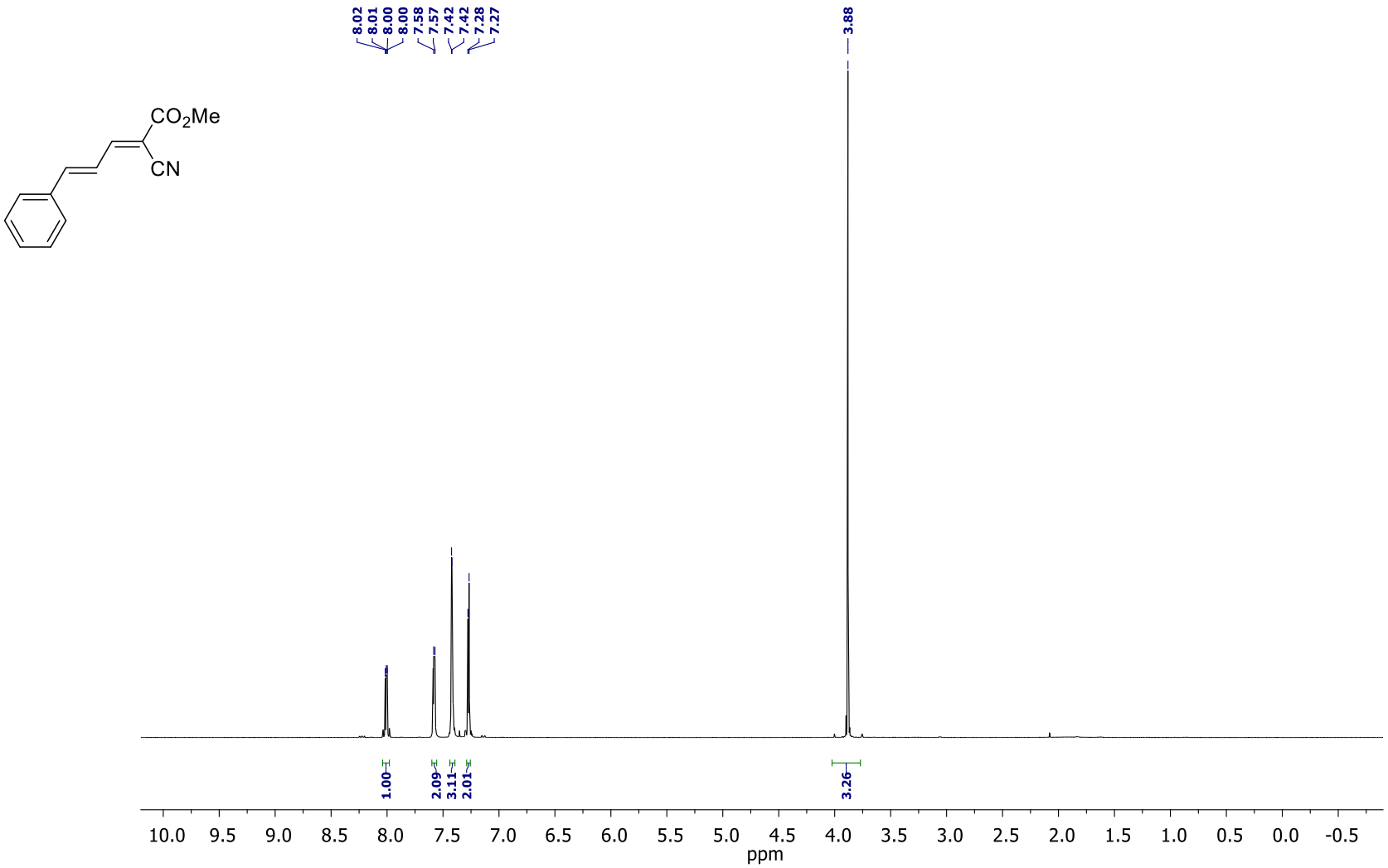
Methyl (*E*)-2-cyano-3-(naphthen-1-yl)acrylate (S1l)

^{1}H NMR ($CDCl_3$, 600 MHz)



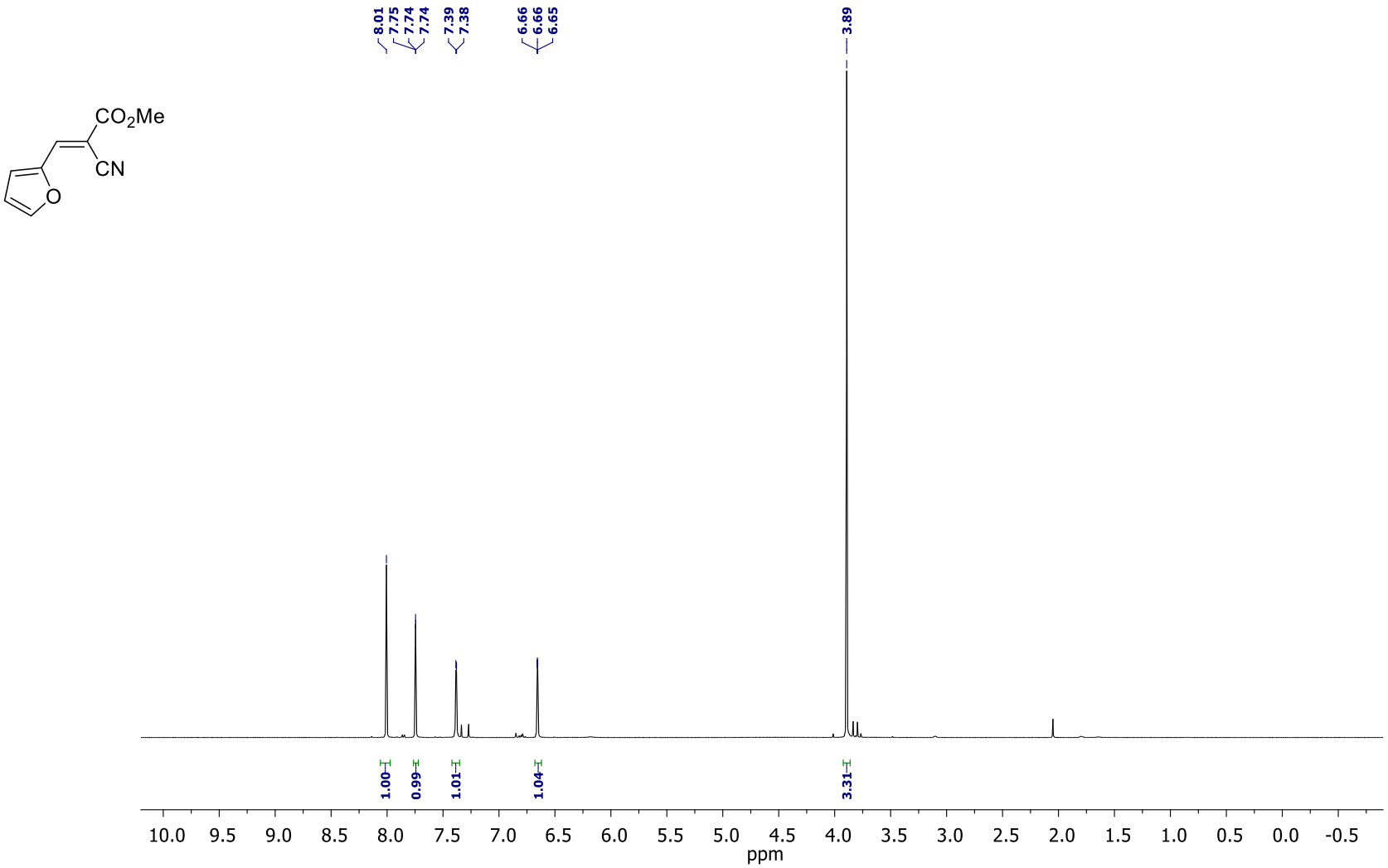
Methyl (2*E*,4*E*)-2-cyano-5-phenylpenta-2,4-dienoate (S1m)

^{1}H NMR ($CDCl_3$, 600 MHz)



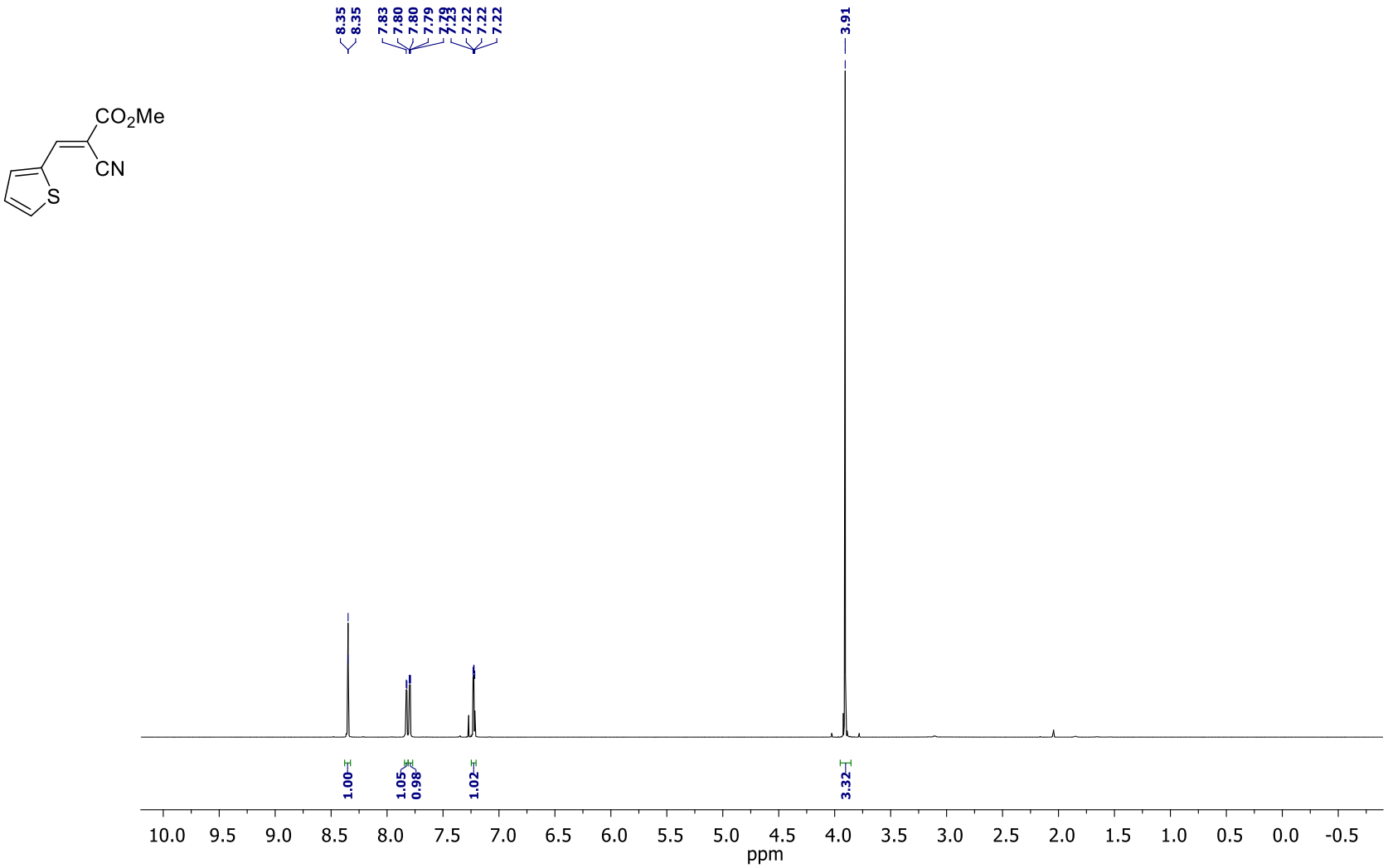
Methyl (*E*)-2-cyano-3-(furan-2-yl)acrylate (S1n)

^{1}H NMR ($CDCl_3$, 600 MHz)



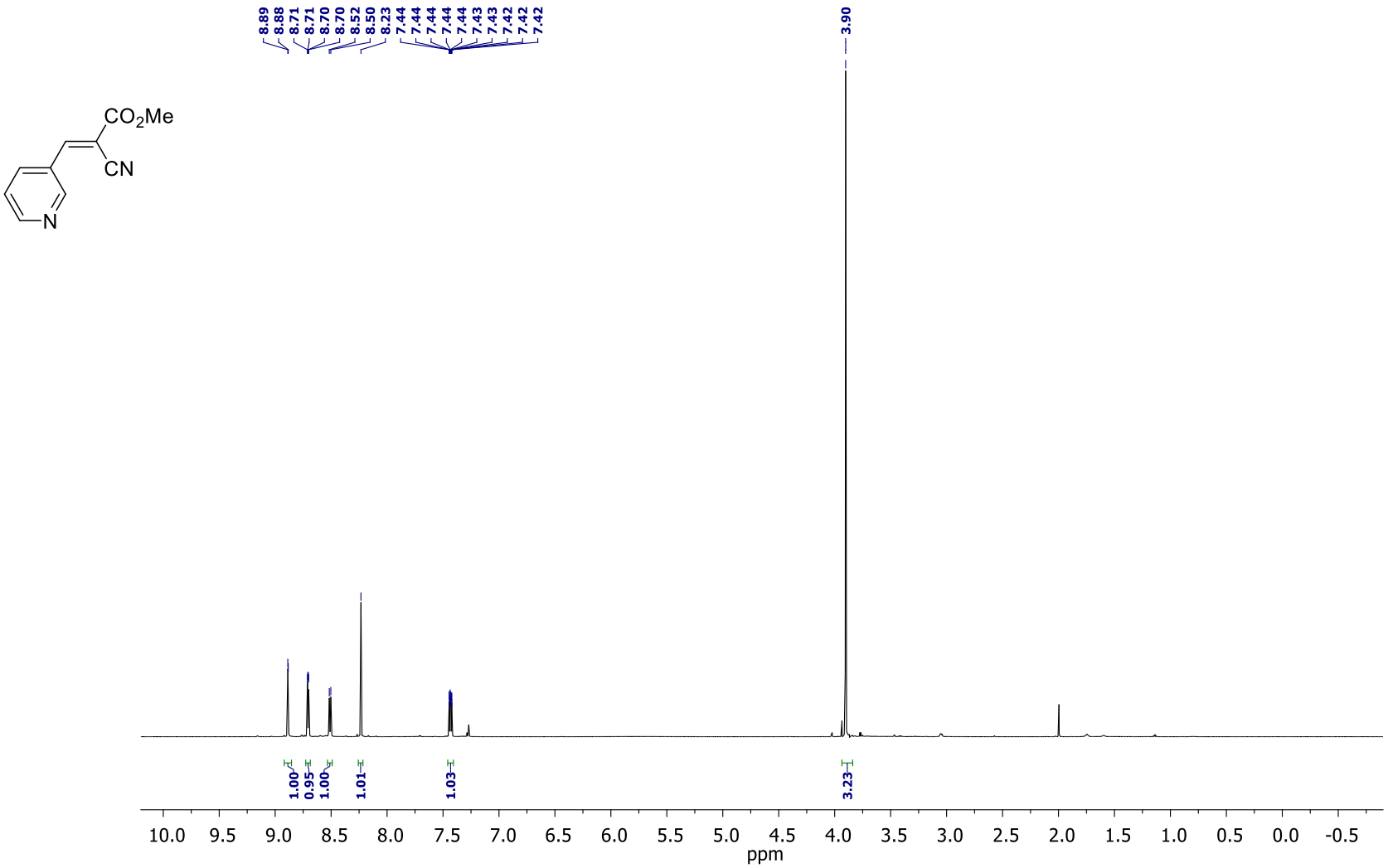
Methyl (*E*)-2-cyano-3-(thien-2-yl)acrylate (S1o)

^{1}H NMR ($CDCl_3$, 600 MHz)



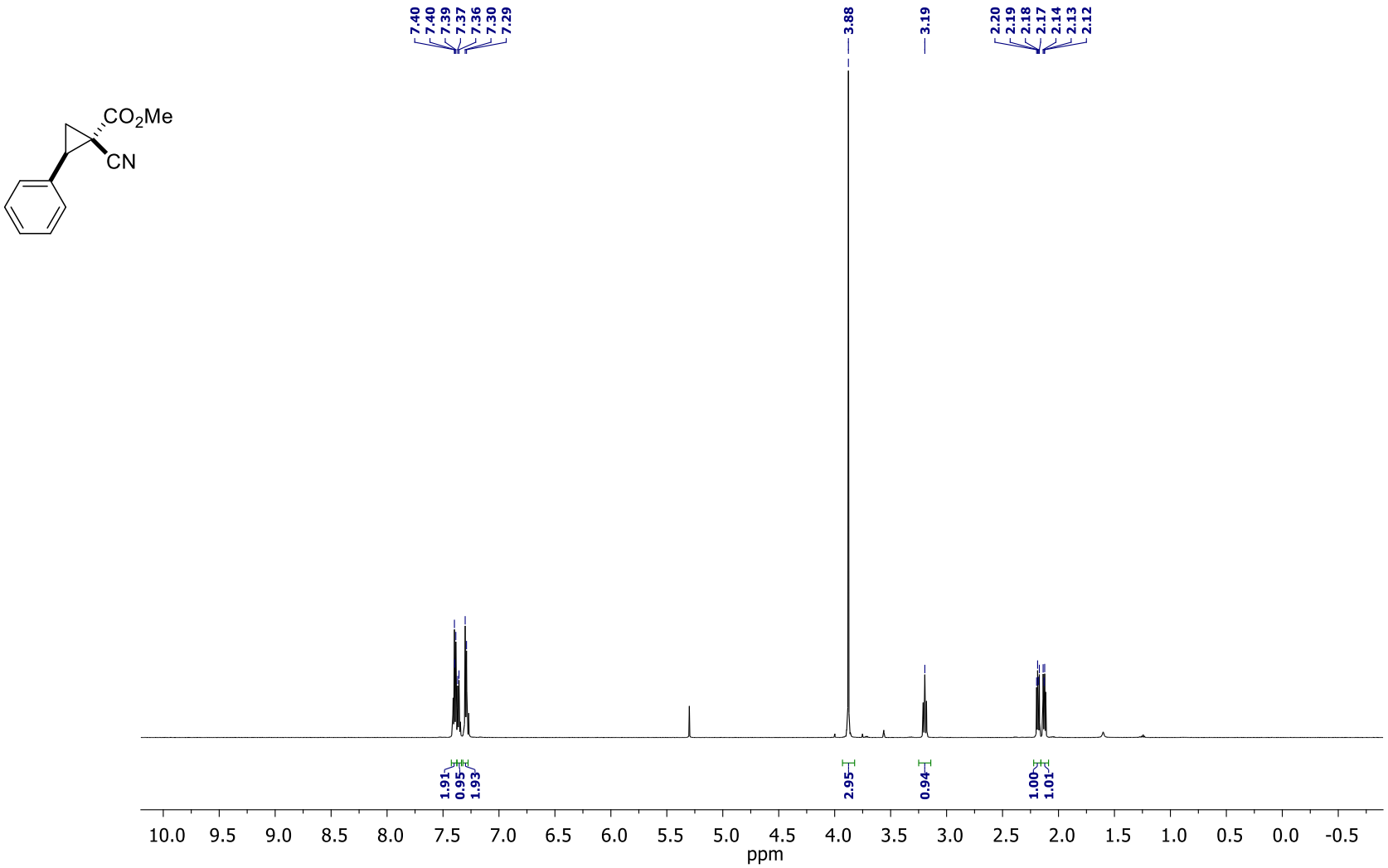
Methyl (*E*)-2-cyano-3-(pyridin-3-yl)acrylate (S1p)

^{1}H NMR ($CDCl_3$, 600 MHz)



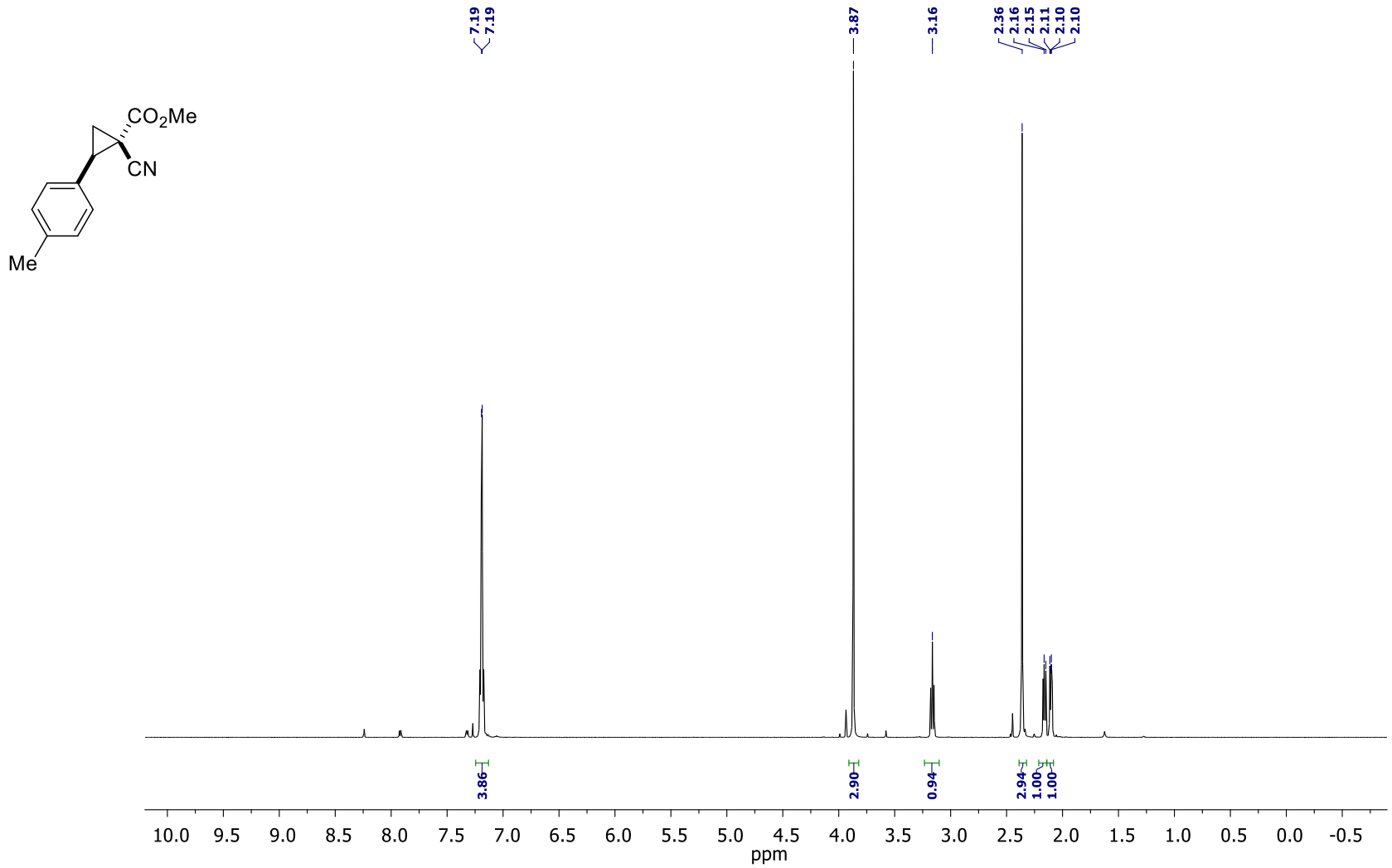
Methyl (1*RS*,2*SR*)-1-cyano-2-phenylcyclopropane-1-carboxylate (S2a)

^{1}H NMR ($CDCl_3$, 600 MHz)



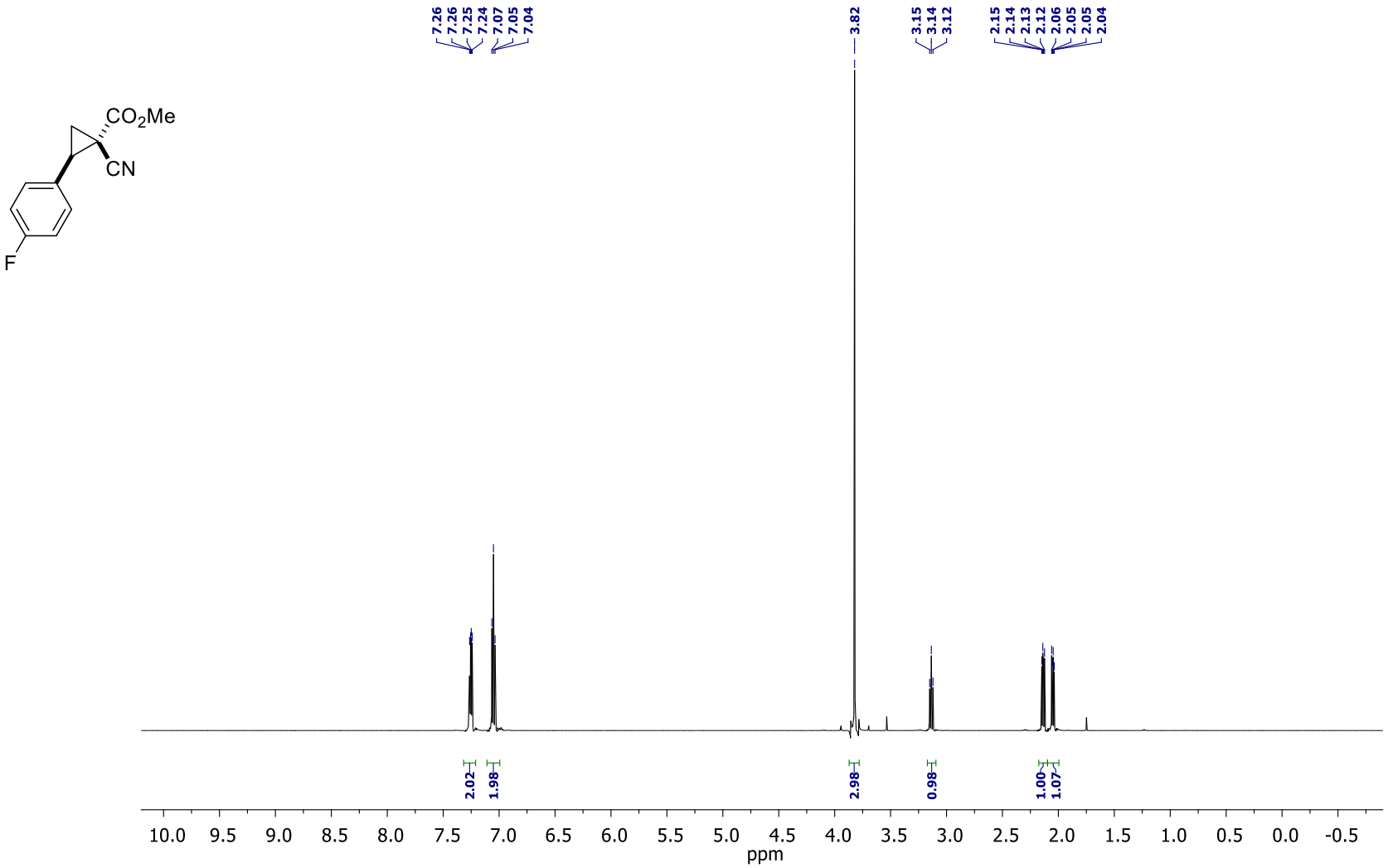
Methyl (1*RS*,2*SR*)-1-cyano-2-(*p*-tolyl)cyclopropanecarboxylate (S2b)

^{1}H NMR ($CDCl_3$, 600 MHz)



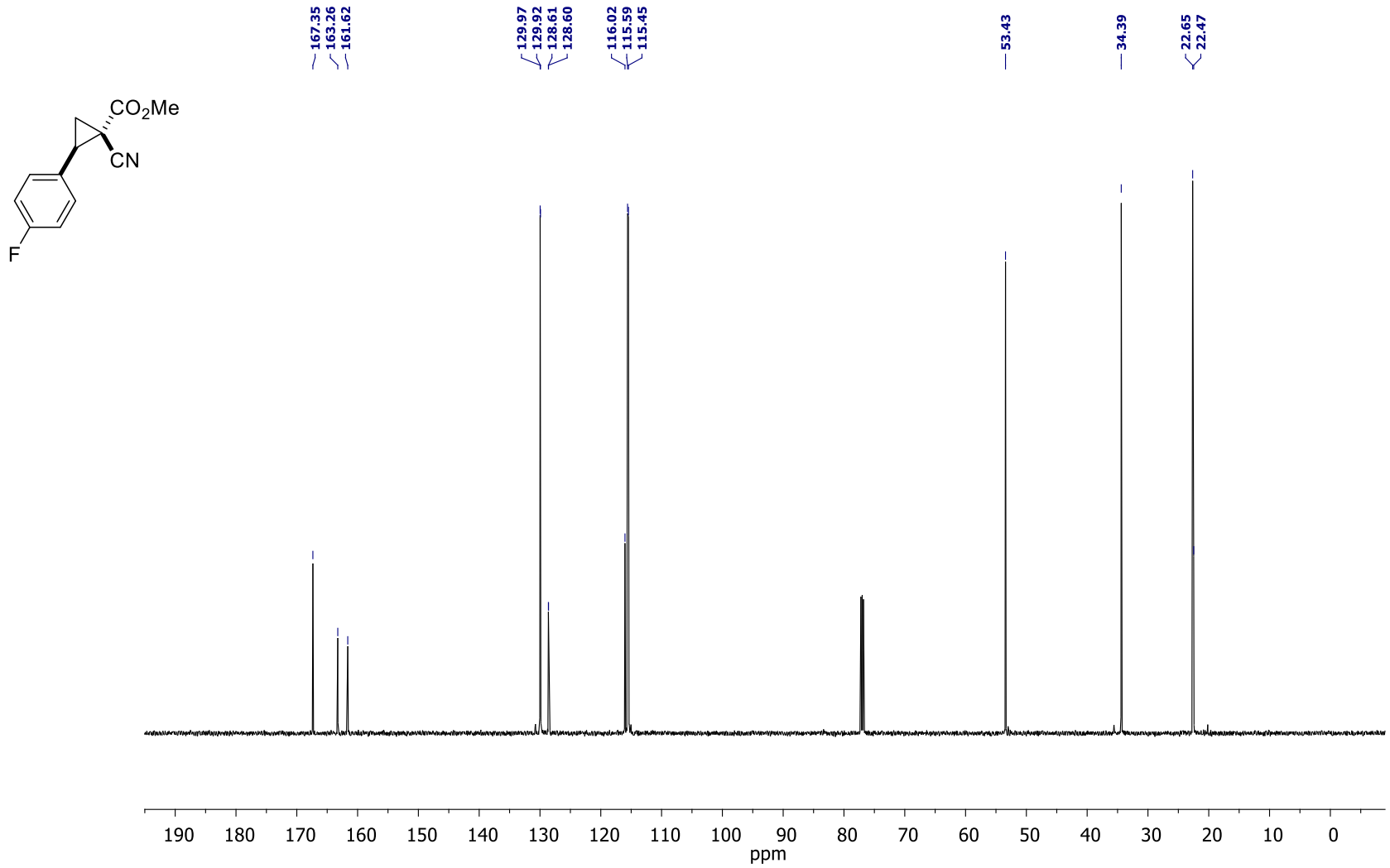
Methyl (1*RS*,2*SR*)-1-cyano-2-(4-fluorophenyl)cyclopropanecarboxylate (S2c)

^{1}H NMR ($CDCl_3$, 600 MHz)



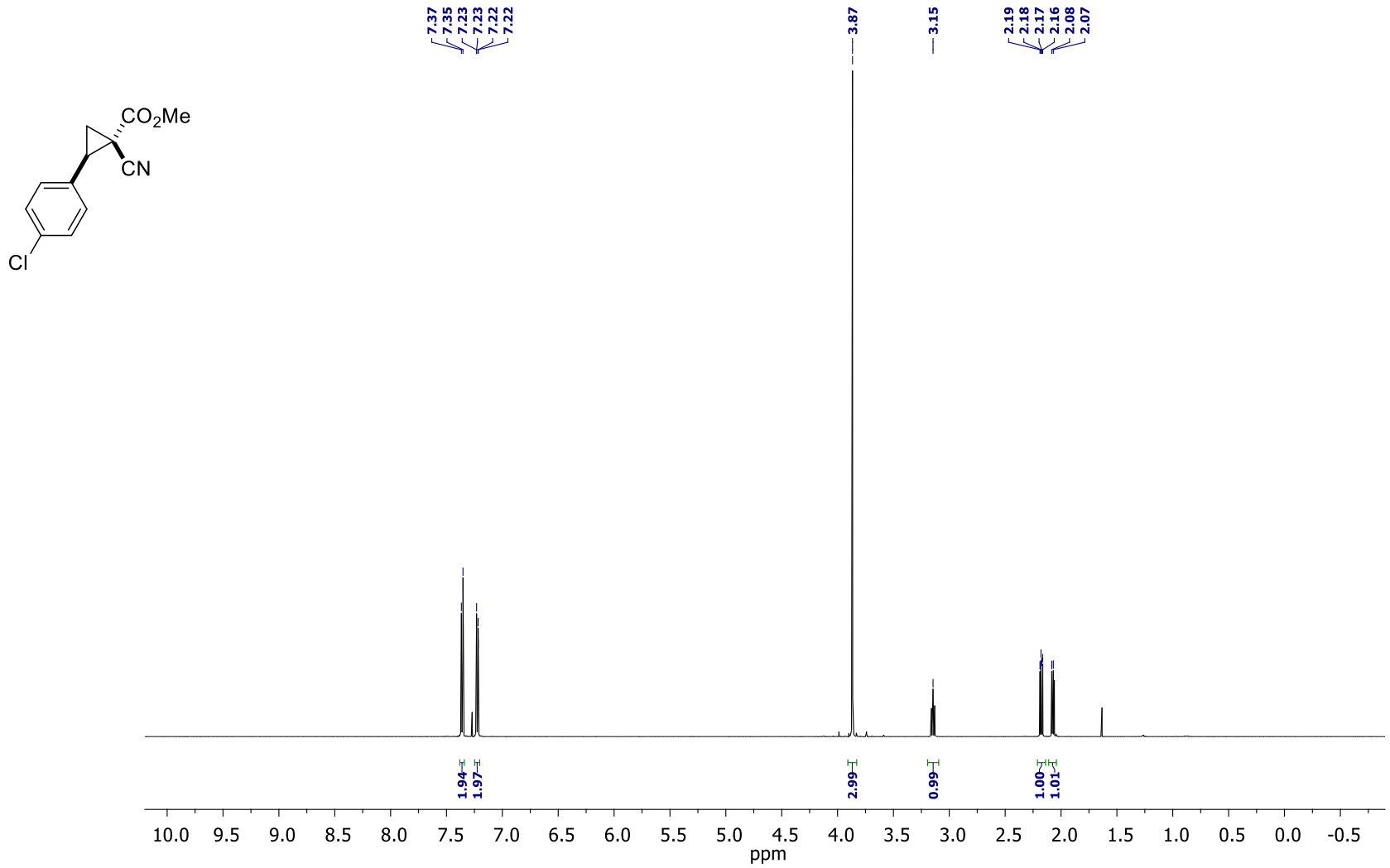
Methyl (1*RS*,2*SR*)-1-cyano-2-(4-fluorophenyl)cyclopropanecarboxylate (S2c)

^{13}C NMR ($CDCl_3$, 150 MHz)



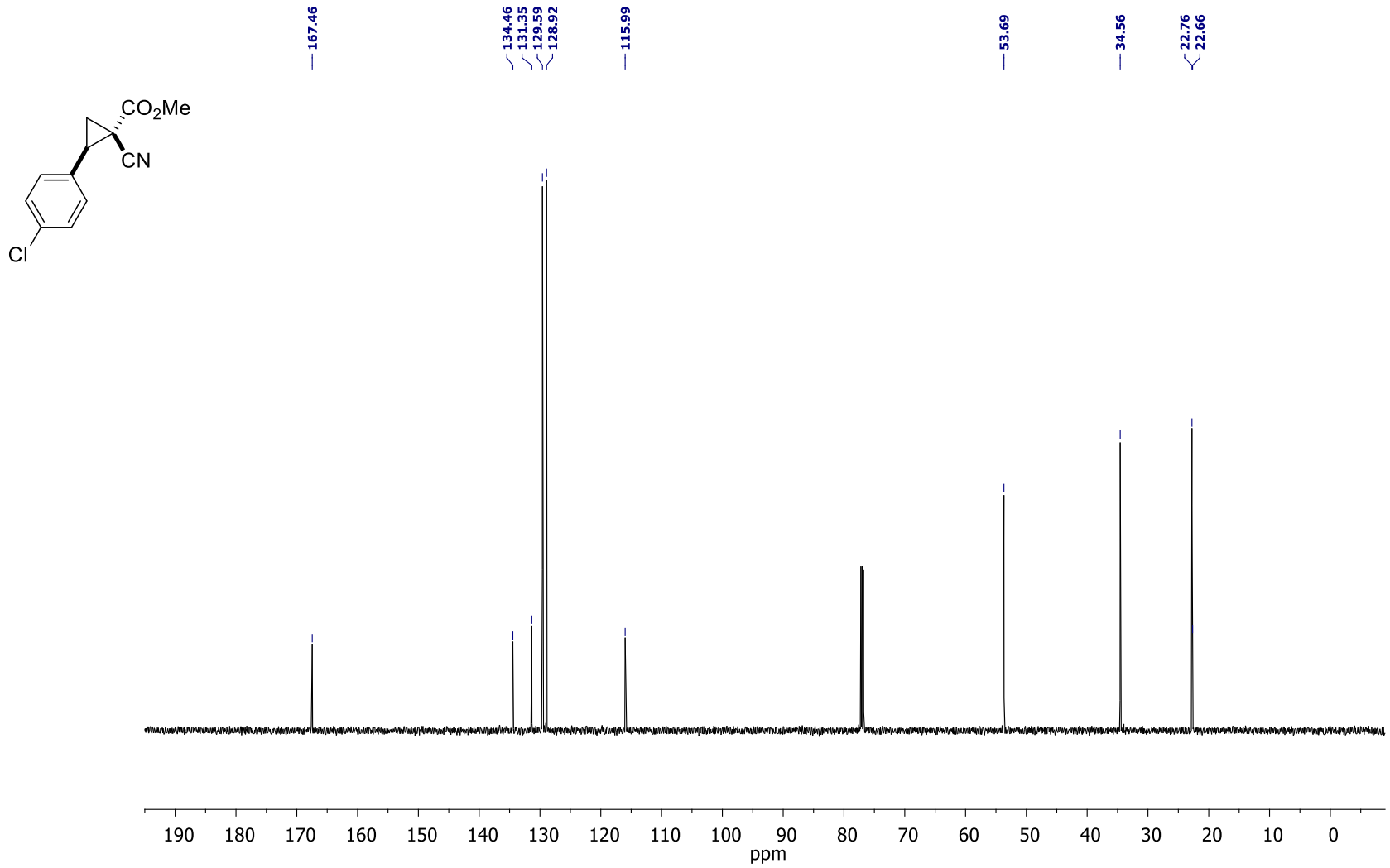
Methyl (1*RS*,2*SR*)-2-(4-chlorophenyl)-1-cyanocyclopropanecarboxylate (S2d)

^{1}H NMR ($CDCl_3$, 600 MHz)



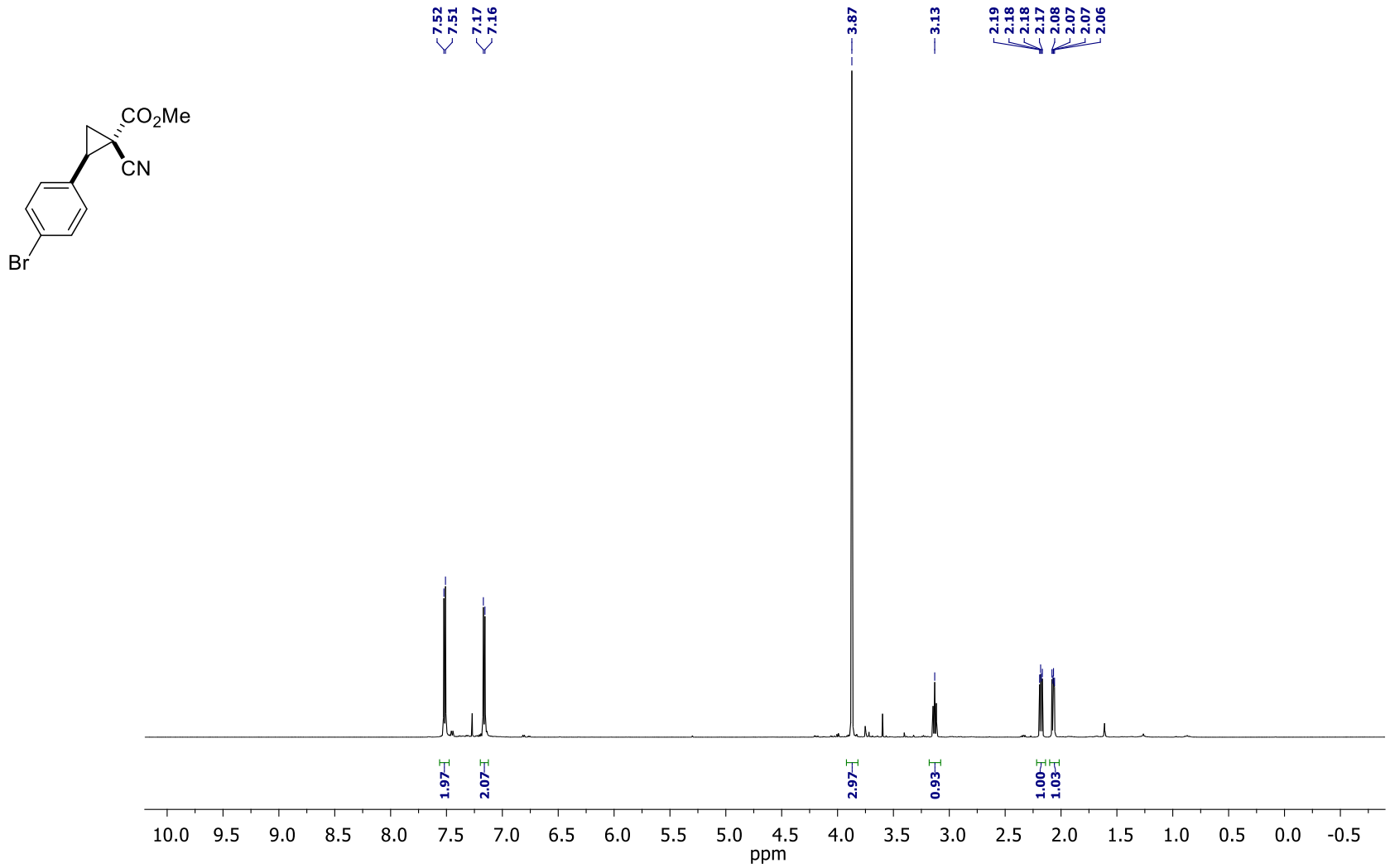
Methyl (1*RS*,2*SR*)-2-(4-chlorophenyl)-1-cyanocyclopropanecarboxylate (S2d)

^{13}C NMR ($CDCl_3$, 150 MHz)



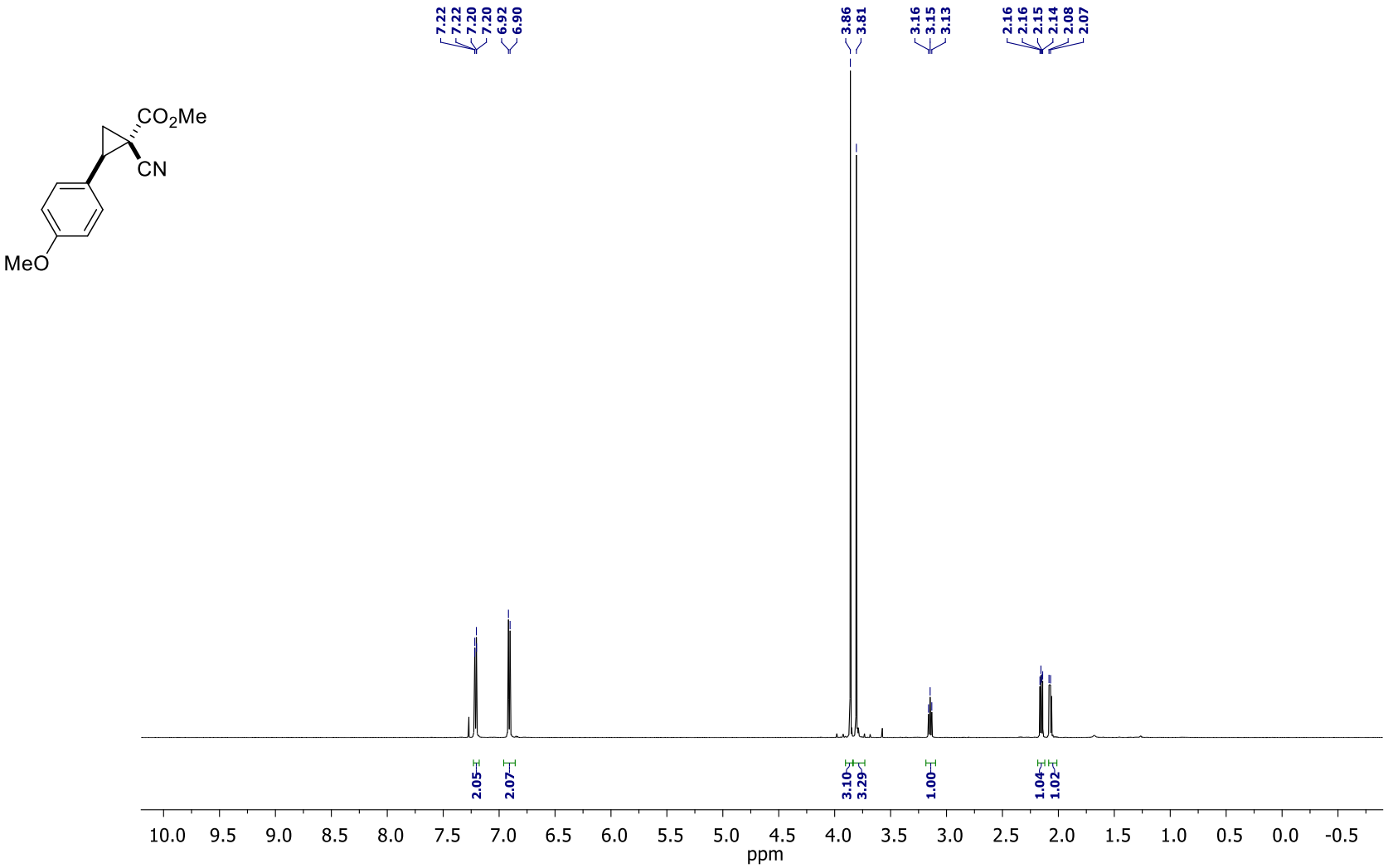
Methyl (1*RS*,2*SR*)-2-(4-bromophenyl)-1-cyanocyclopropanecarboxylate (S2e)

^{1}H NMR ($CDCl_3$, 600 MHz)



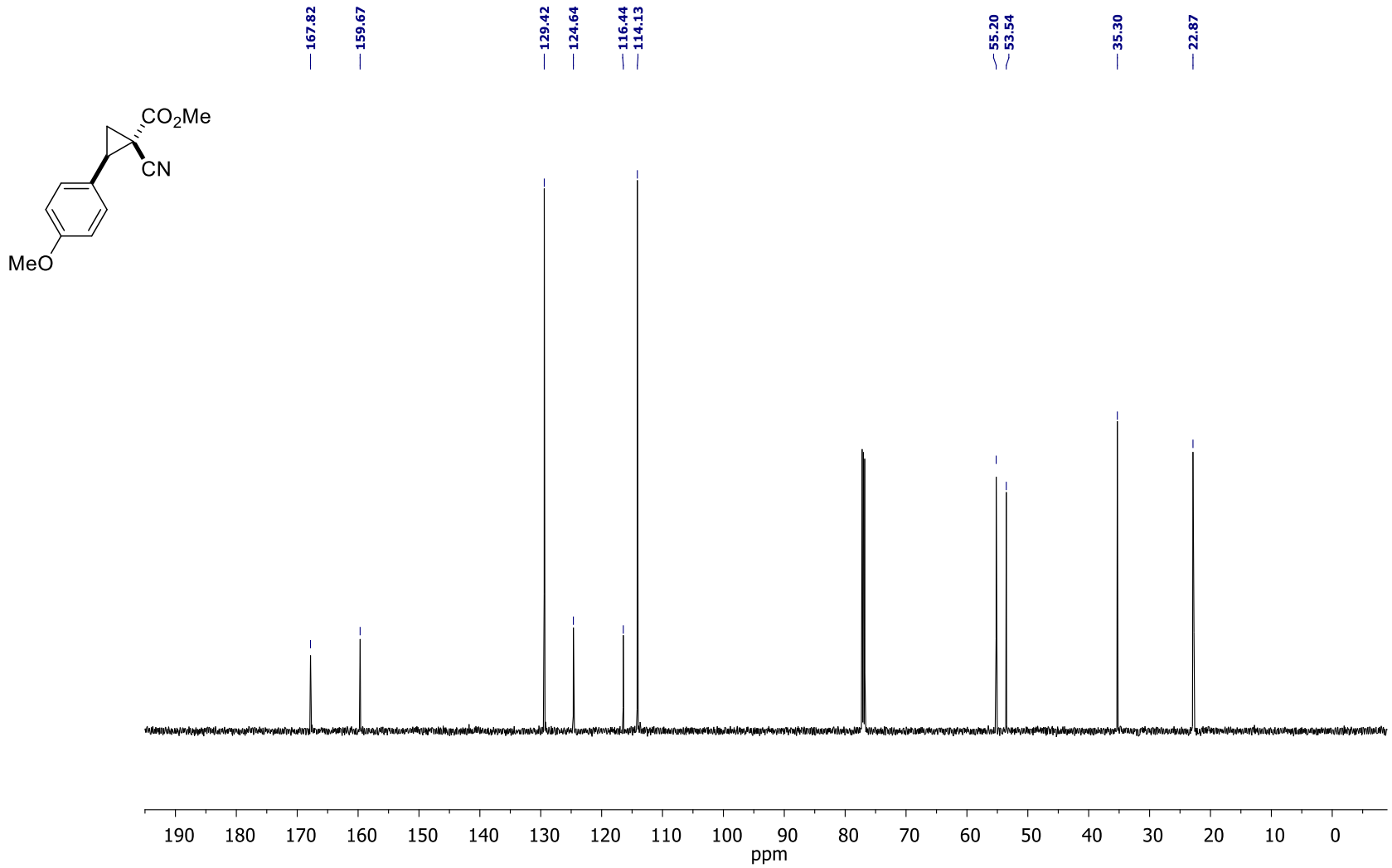
Methyl (1*RS*,2*SR*)-1-cyano-2-(4-methoxyphenyl)cyclopropanecarboxylate (S2f)

^{1}H NMR ($CDCl_3$, 600 MHz)



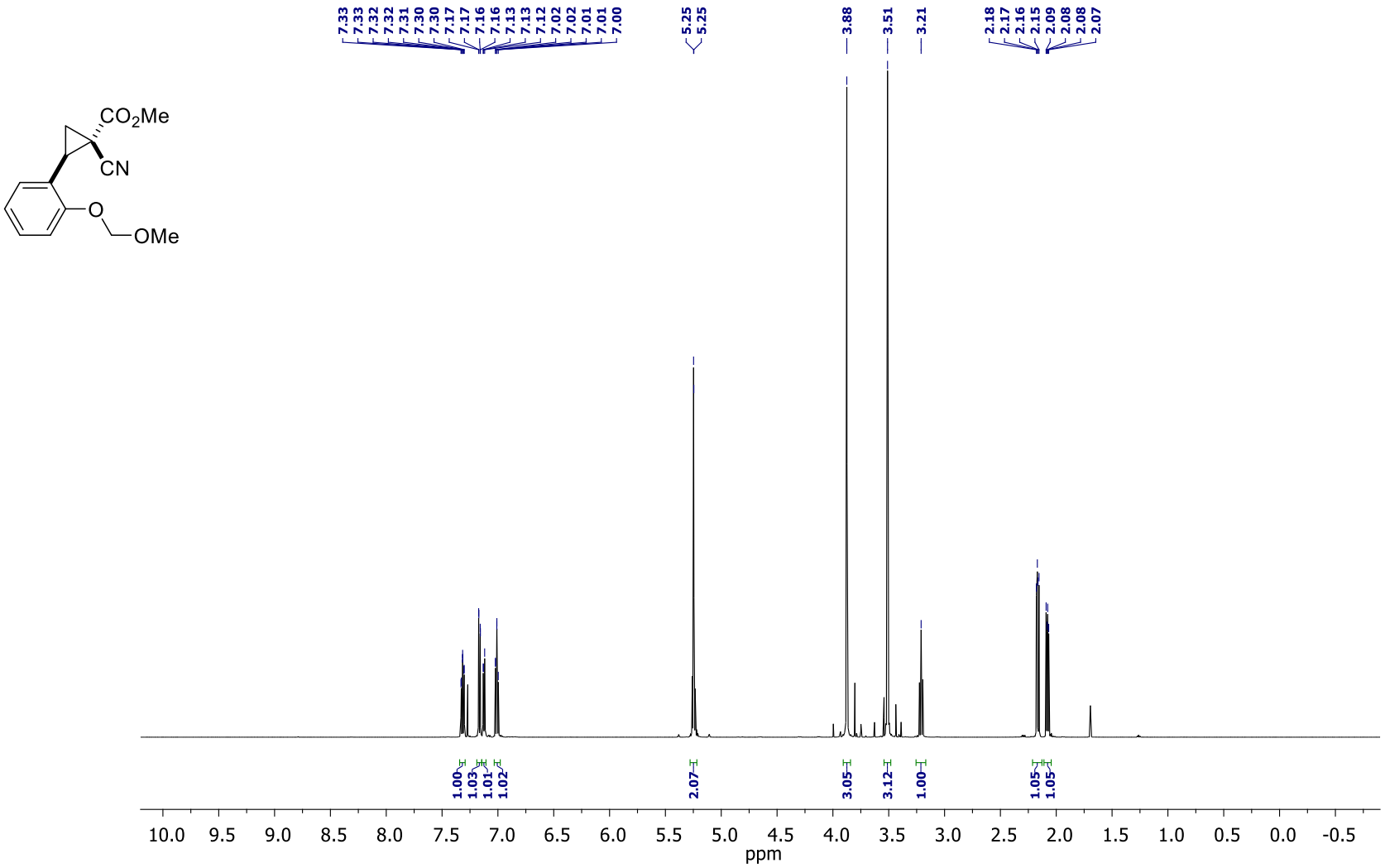
Methyl (1*RS*,2*SR*)-1-cyano-2-(4-methoxyphenyl)cyclopropanecarboxylate (S2f)

^{13}C NMR ($CDCl_3$, 150 MHz)



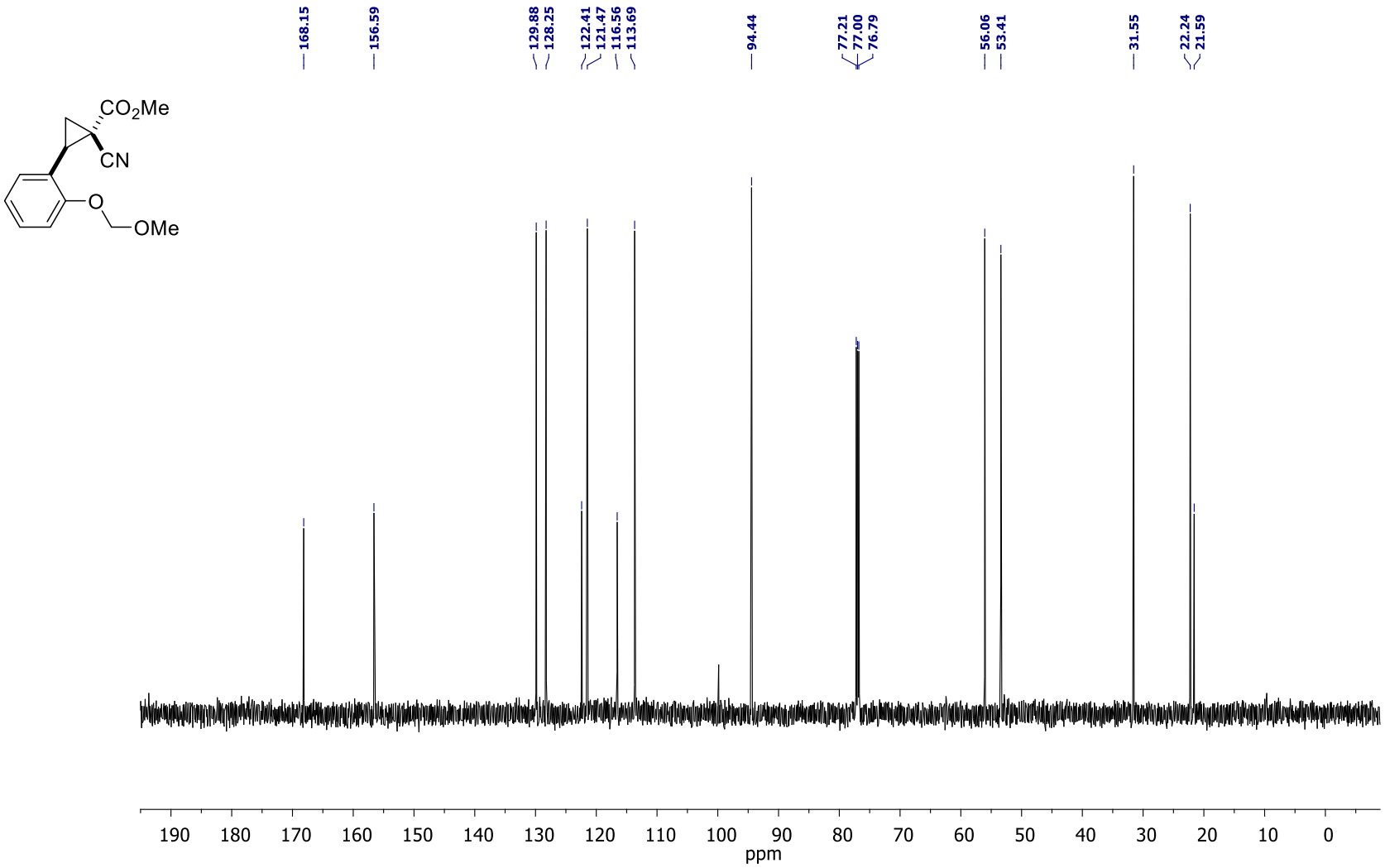
Methyl (1*RS*,2*SR*)-1-cyano-2[2-(methoxymethoxy)phenyl]cyclopropanecarboxylate (S2g)

^{1}H NMR ($CDCl_3$, 600 MHz)



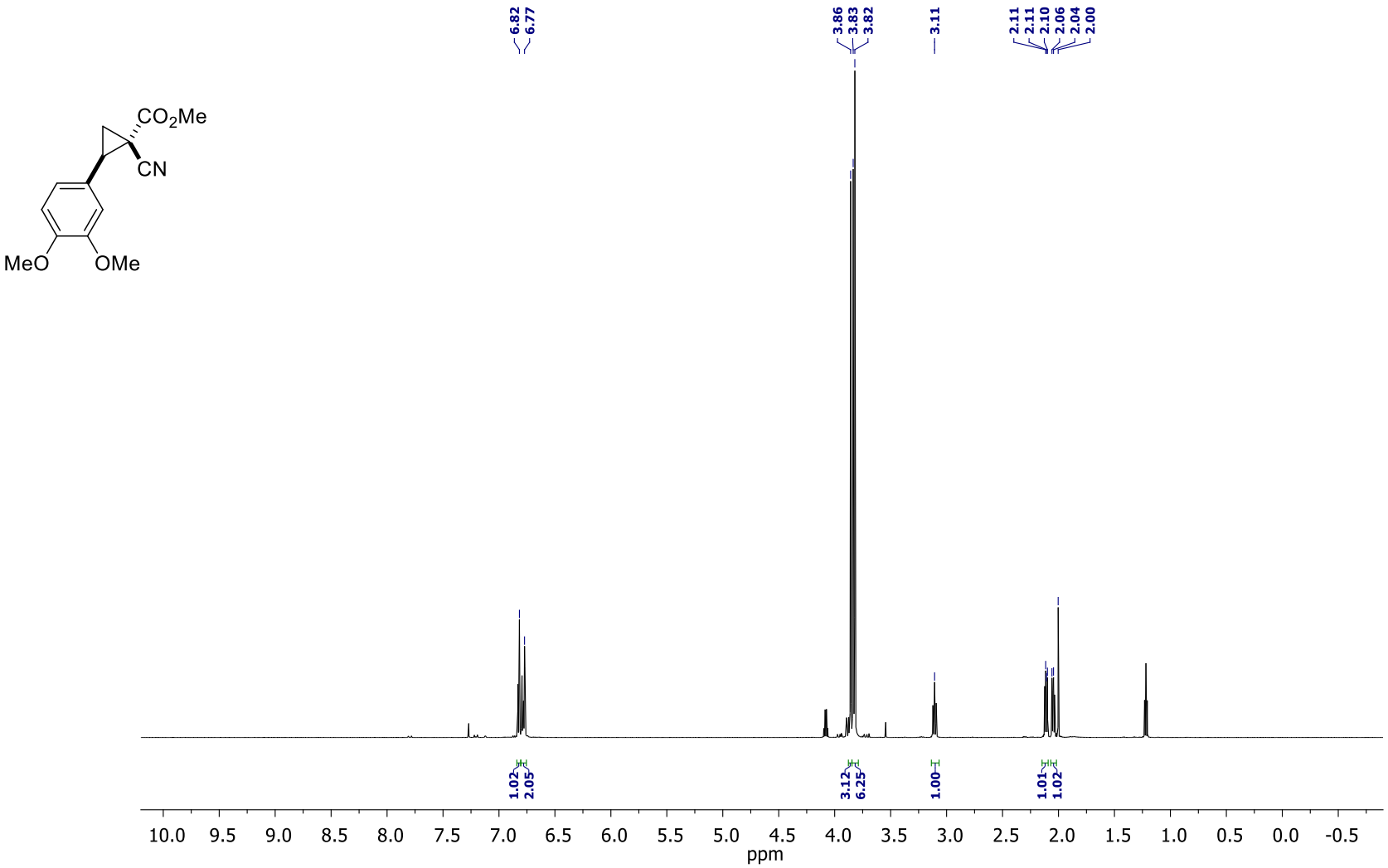
Methyl (1*RS*,2*SR*)-1-cyano-2[2-(methoxymethoxy)phenyl]cyclopropanecarboxylate (S2g)

^{13}C NMR ($CDCl_3$, 150 MHz)



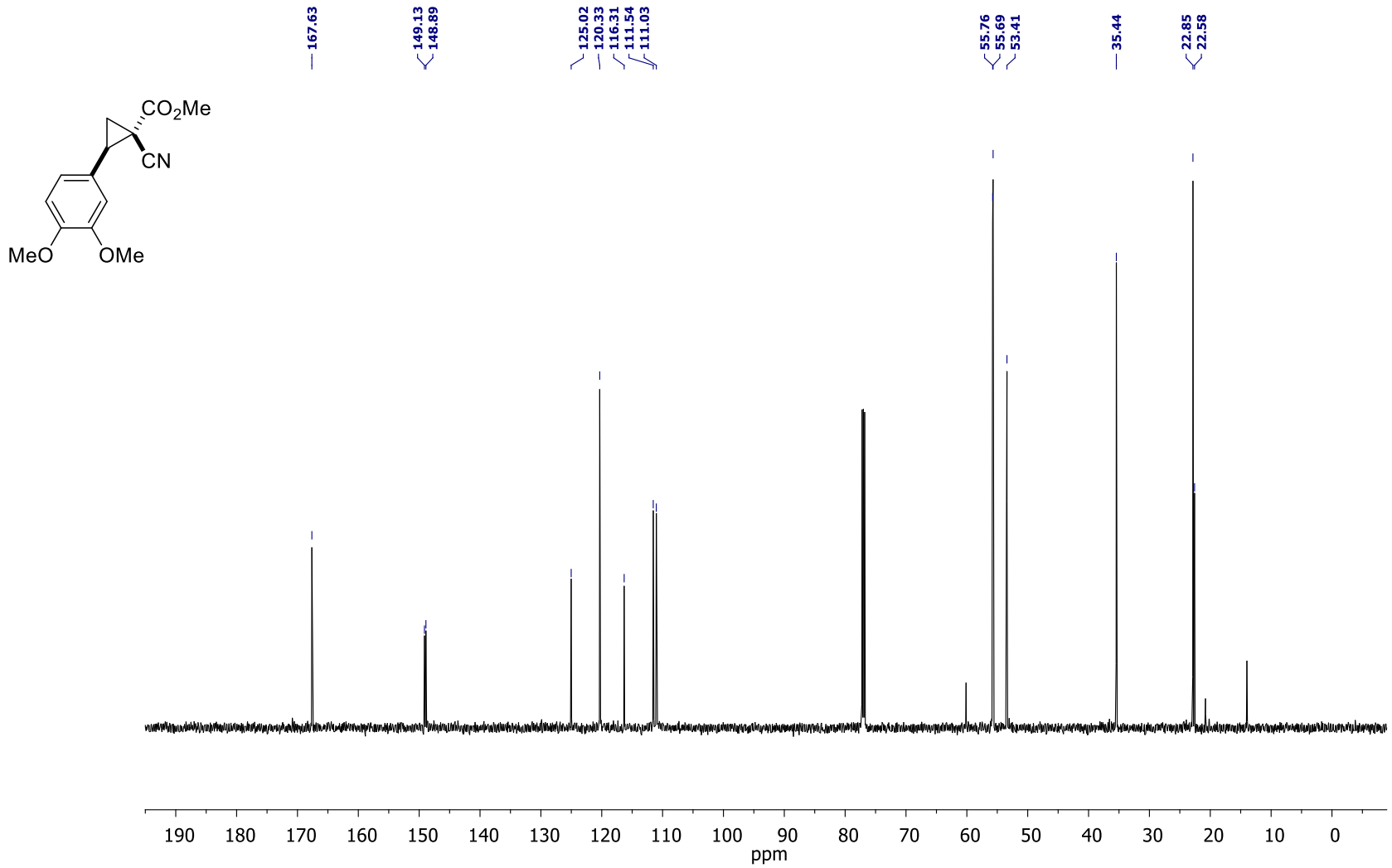
Methyl (1*RS*,2*SR*)-1-cyano-2-(3,4-dimethoxyphenyl)cyclopropanecarboxylate (S2h)

^{1}H NMR ($CDCl_3$, 600 MHz)



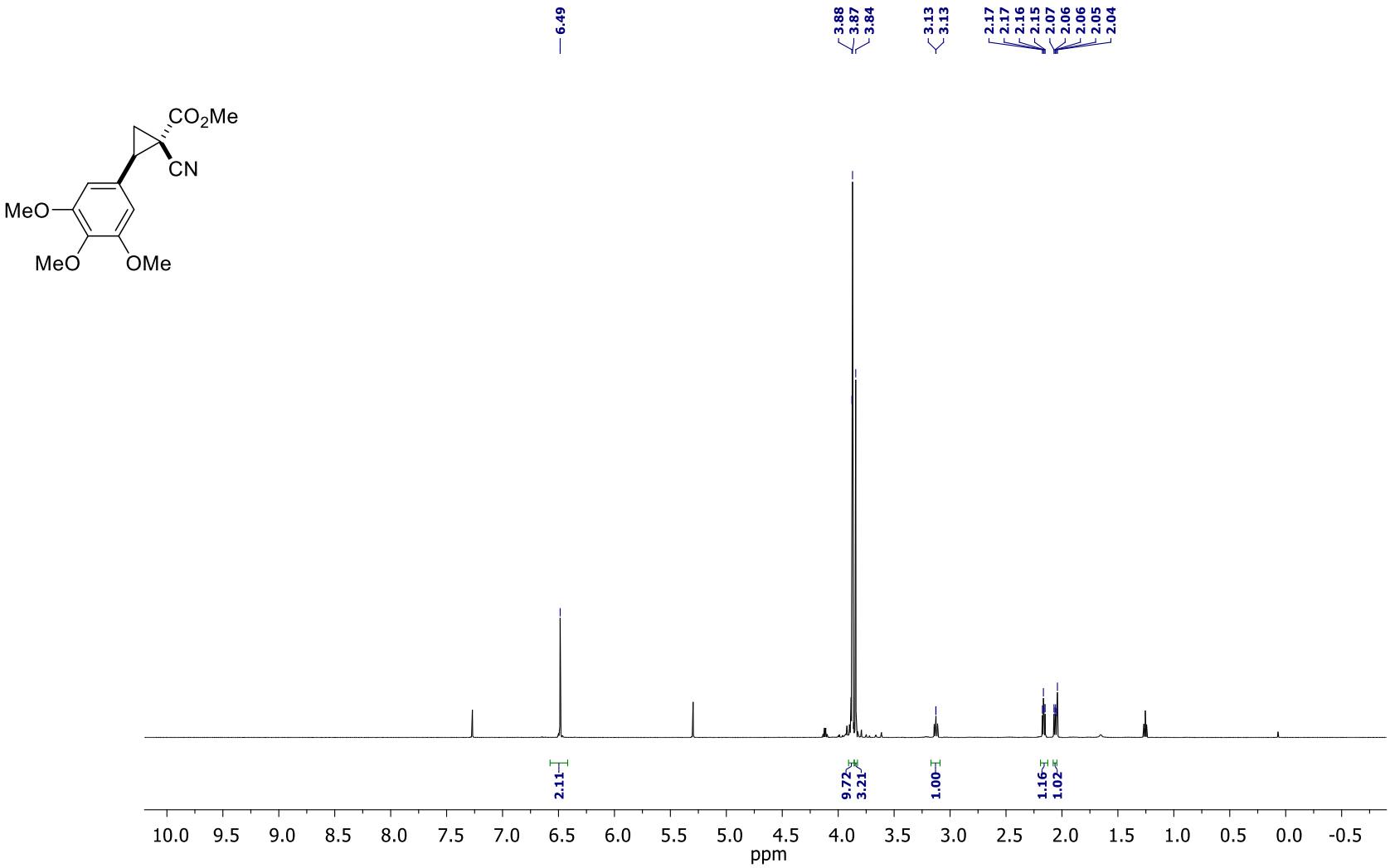
Methyl (1*RS*,2*SR*)-1-cyano-2-(3,4-dimethoxyphenyl)cyclopropanecarboxylate (S2h)

^{13}C NMR ($CDCl_3$, 150 MHz)



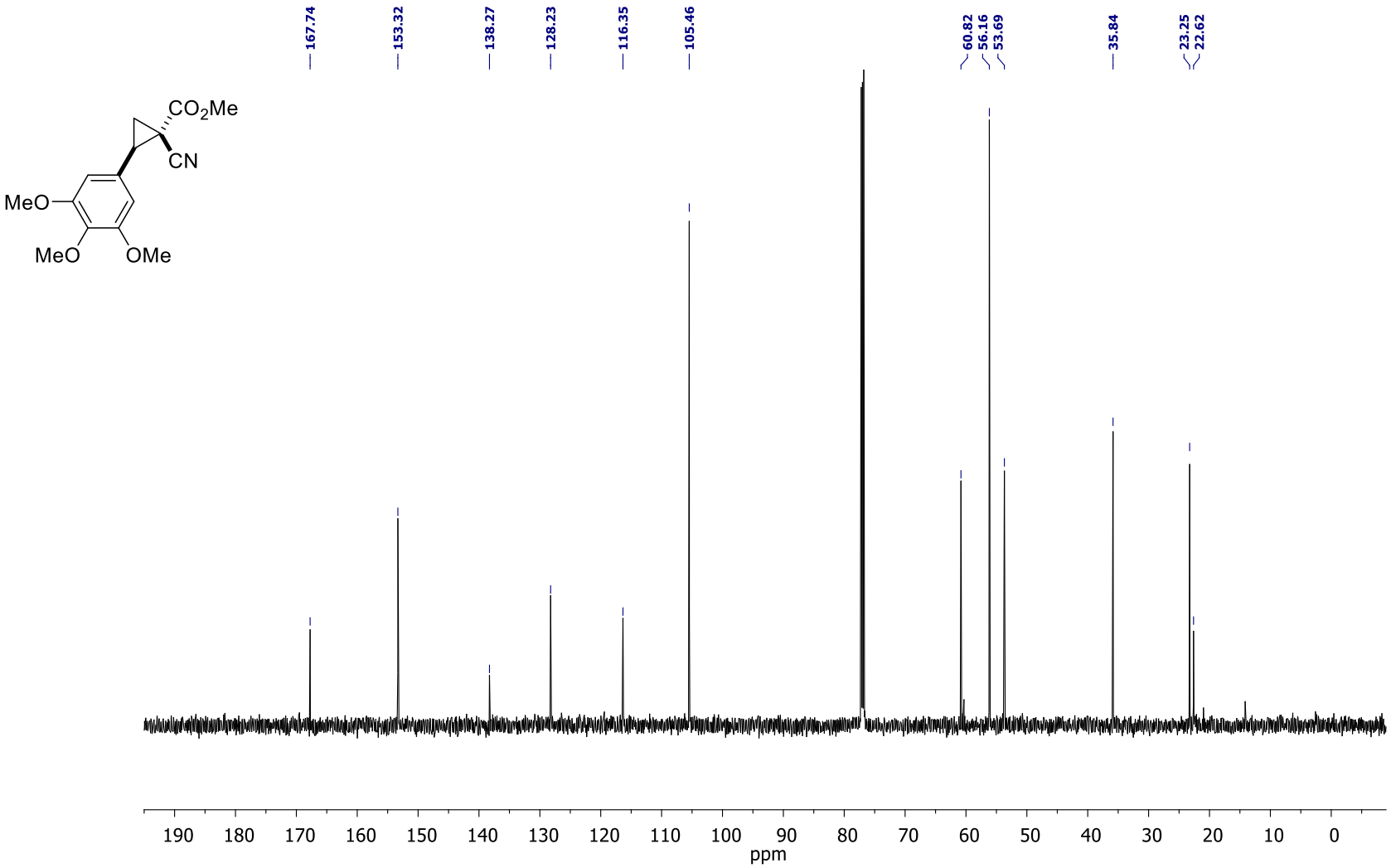
Methyl (1*RS*,2*SR*)-1-cyano-2-(3,4,5-trimethoxyphenyl)cyclopropanecarboxylate (S2i)

^{1}H NMR ($CDCl_3$, 600 MHz)



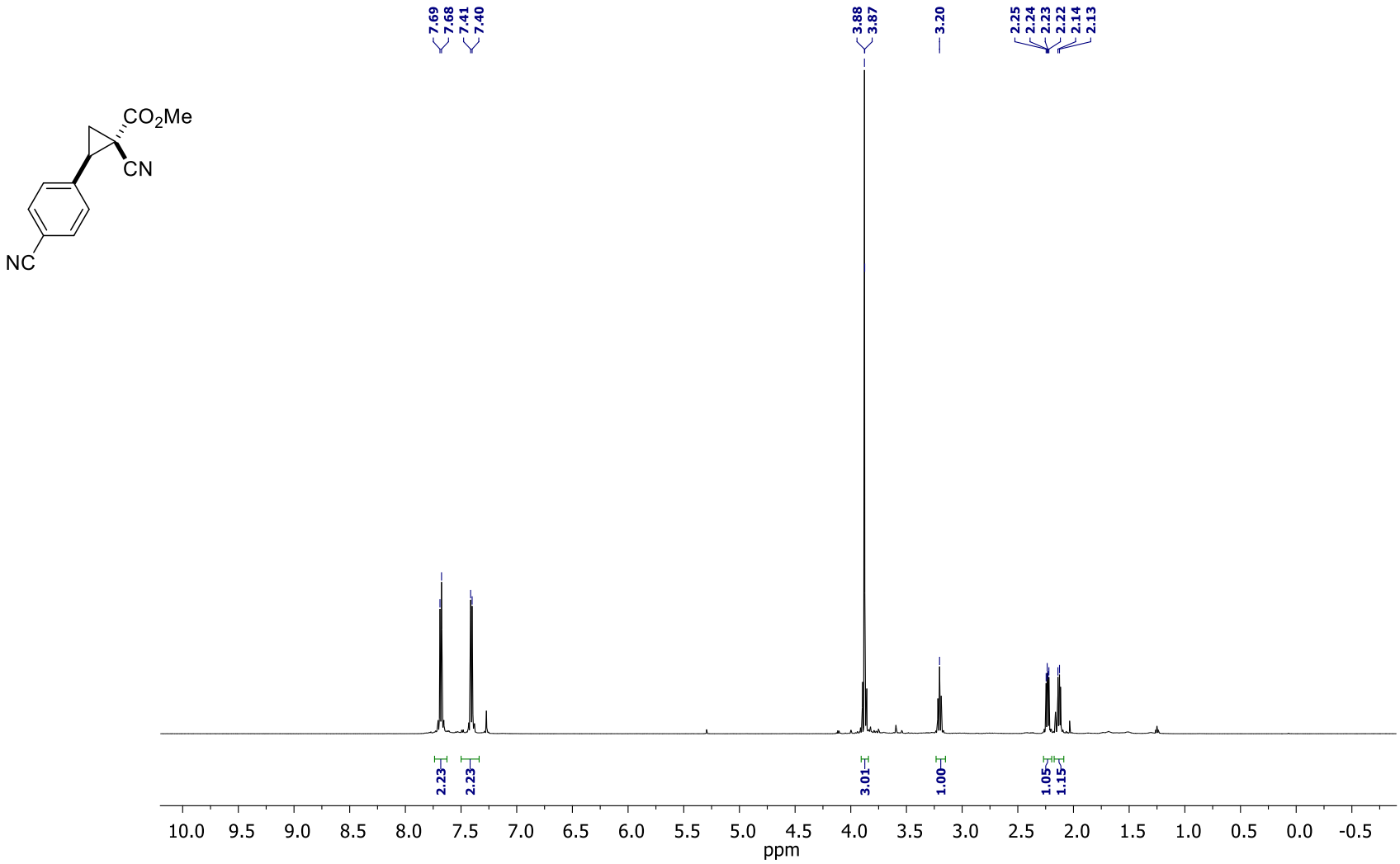
Methyl (1*RS*,2*SR*)-1-cyano-2-(3,4,5-trimethoxyphenyl)cyclopropanecarboxylate (S2i)

^{13}C NMR ($CDCl_3$, 150 MHz)



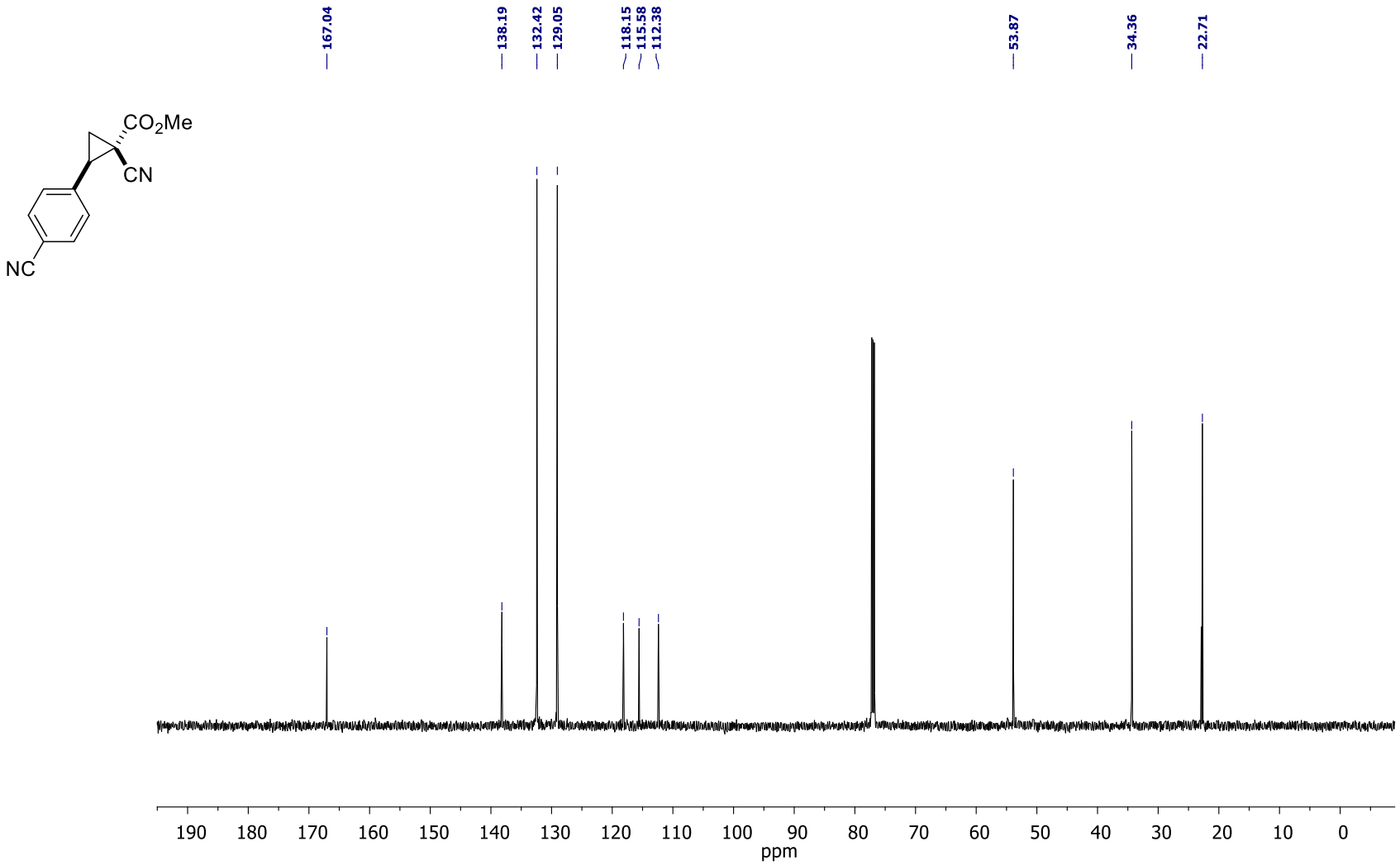
Methyl (1*RS*,2*SR*)-1-cyano-2-(4-cyanophenyl)cyclopropanecarboxylate (S2j)

^{1}H NMR ($CDCl_3$, 600 MHz)



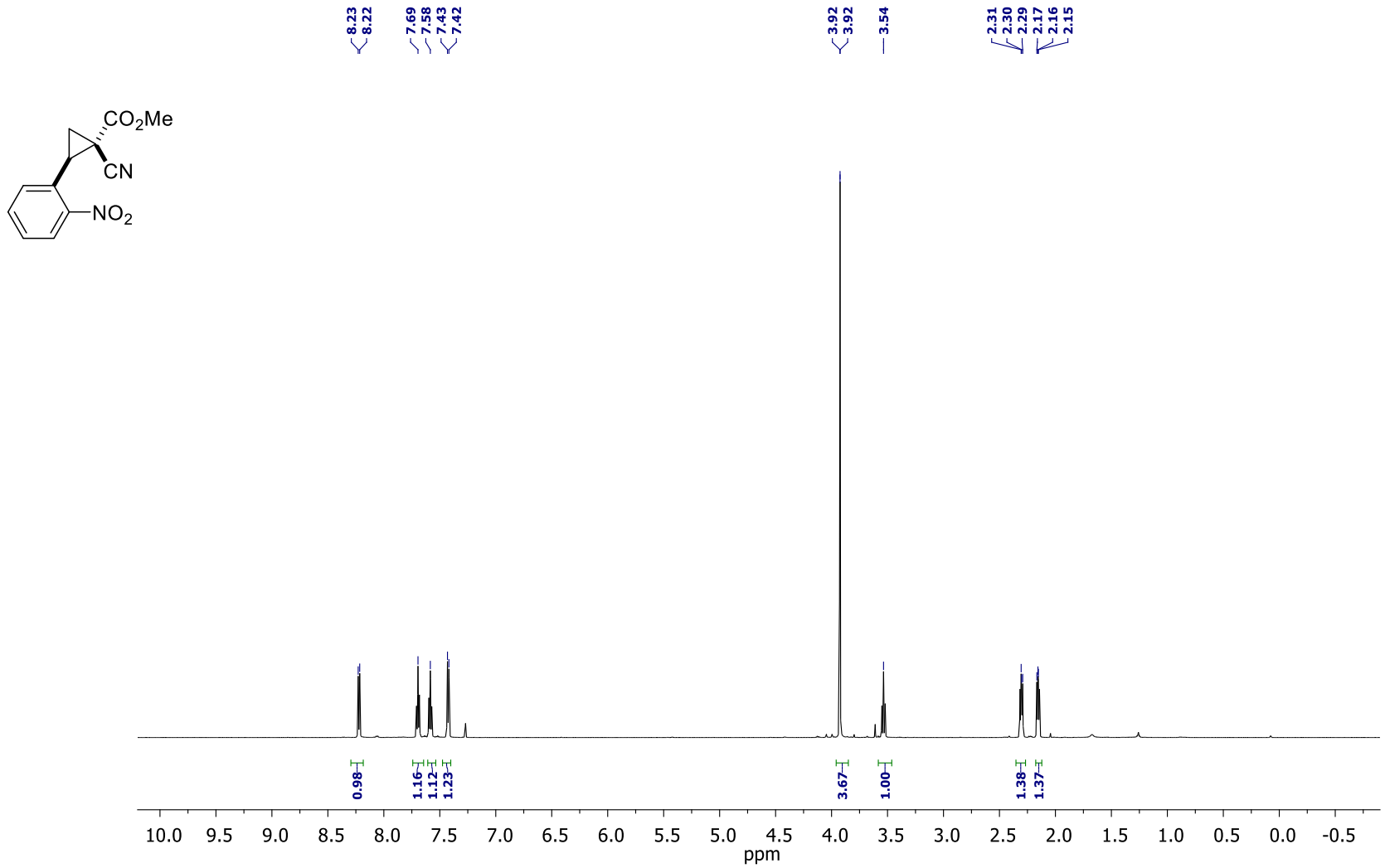
Methyl (1*RS*,2*SR*)-1-cyano-2-(4-cyanophenyl)cyclopropanecarboxylate (S2j)

^{13}C NMR ($CDCl_3$, 150 MHz)



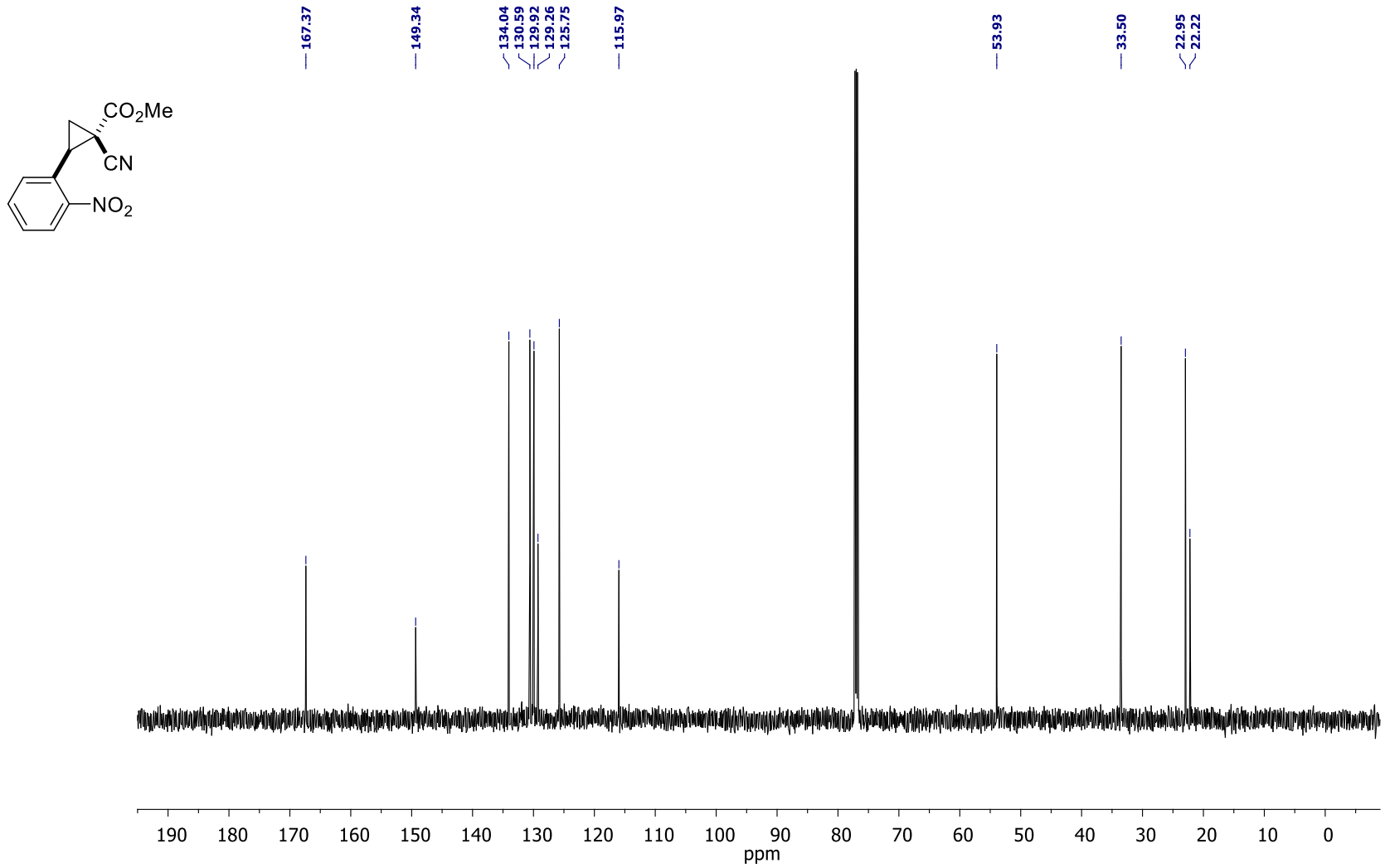
Methyl (1*RS*,2*SR*)-1-cyano-2-(2-nitrophenyl)cyclopropanecarboxylate (S2k)

^{1}H NMR ($CDCl_3$, 600 MHz)



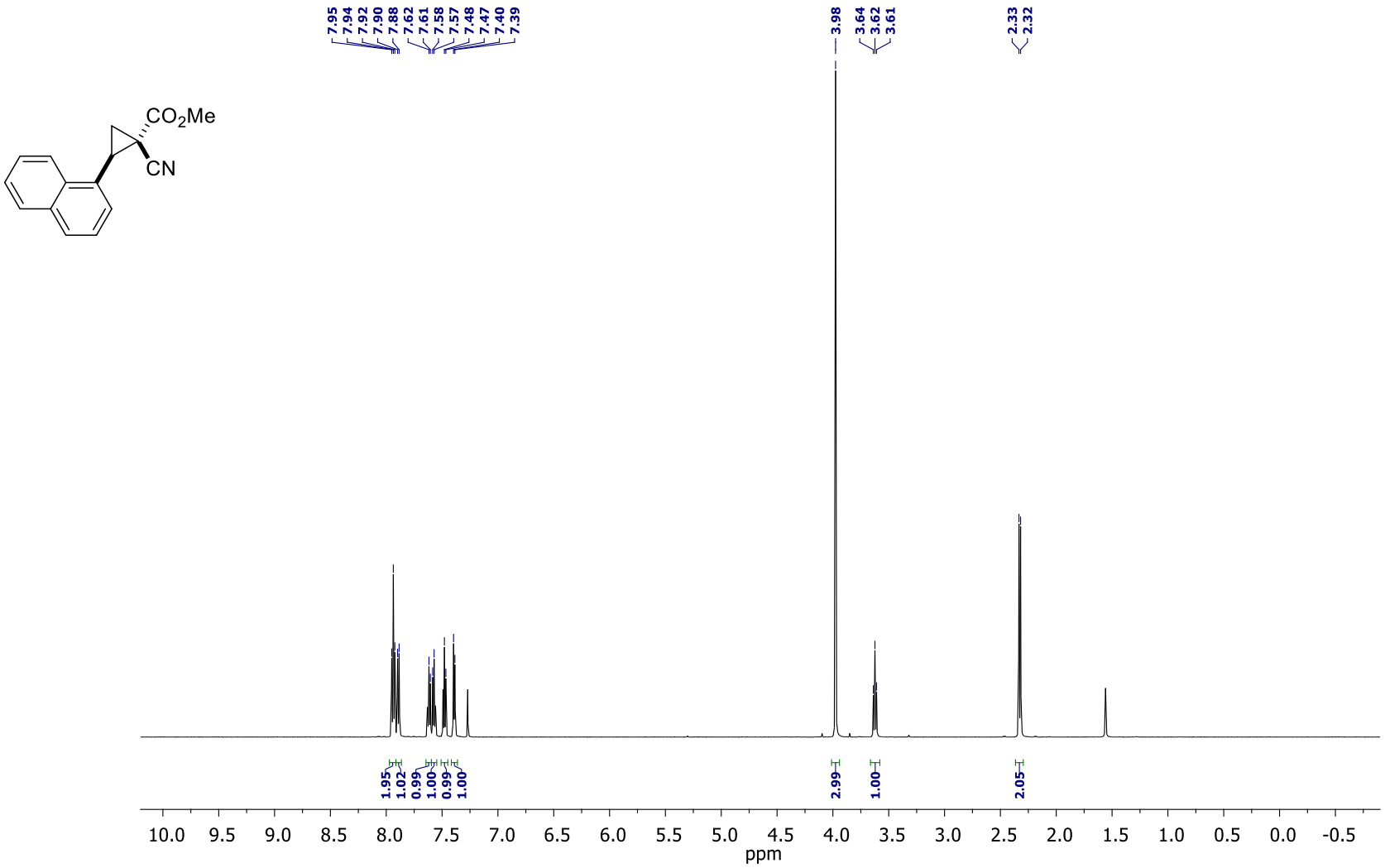
Methyl (1*RS*,2*SR*)-1-cyano-2-(2-nitrophenyl)cyclopropanecarboxylate (S2k)

^{13}C NMR ($CDCl_3$, 150 MHz)



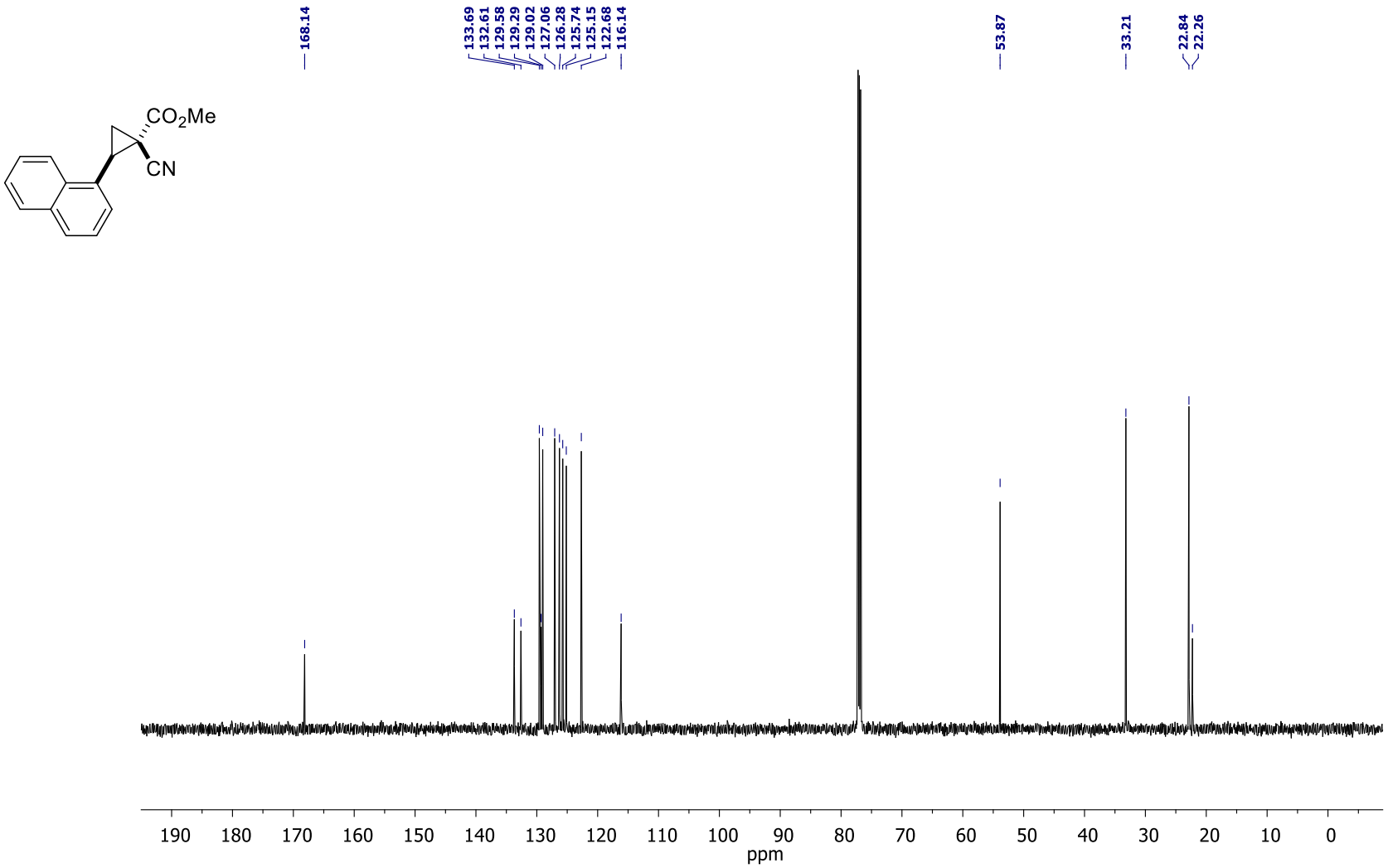
Methyl (1*RS*,2*SR*)-1-cyano-2-(naphthen-1-yl)cyclopropanecarboxylate (S2l)

^{1}H NMR ($CDCl_3$, 600 MHz)



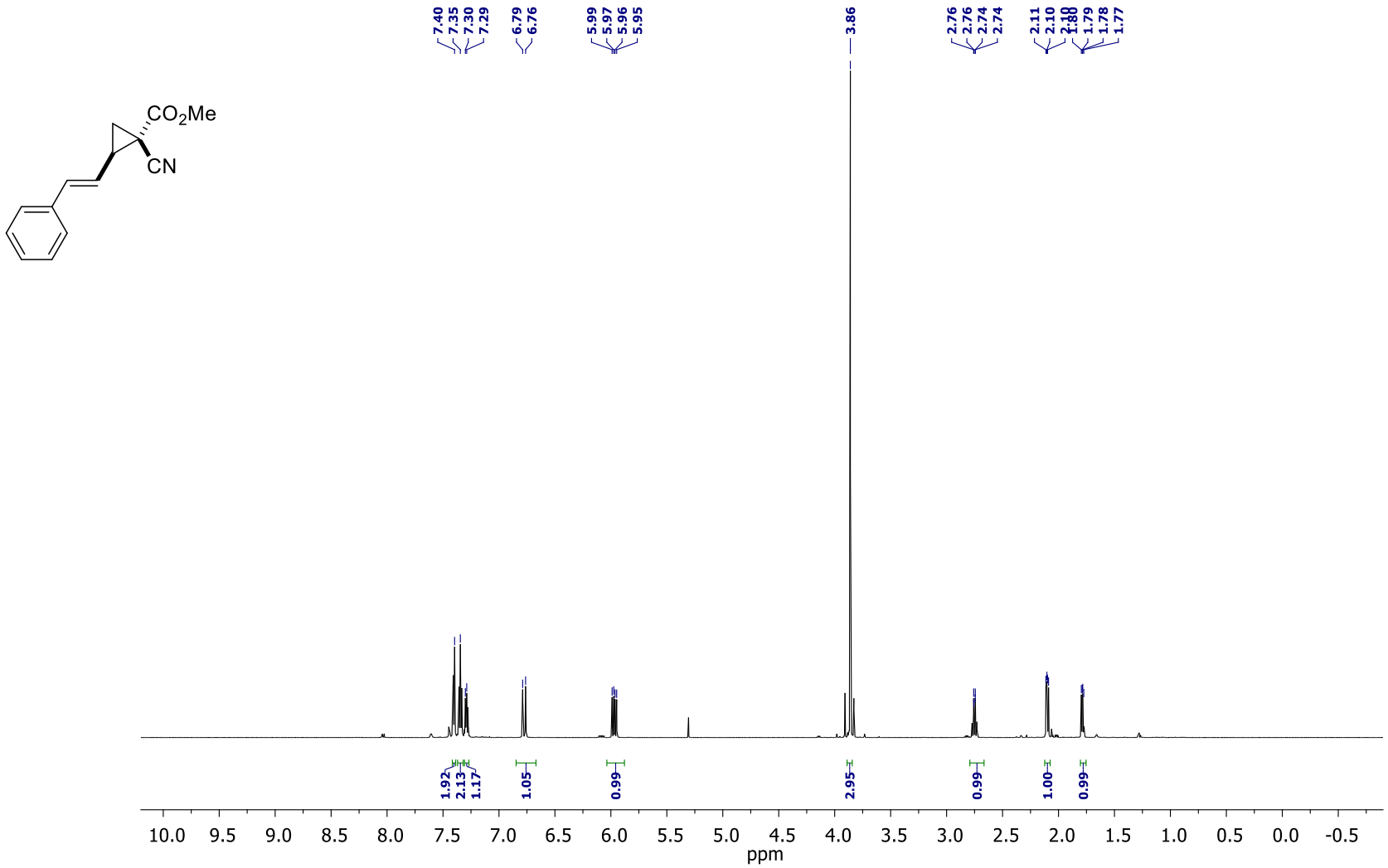
Methyl (1*RS*,2*SR*)-1-cyano-2-(naphthen-1-yl)cyclopropanecarboxylate (S2l)

^{13}C NMR ($CDCl_3$, 150 MHz)



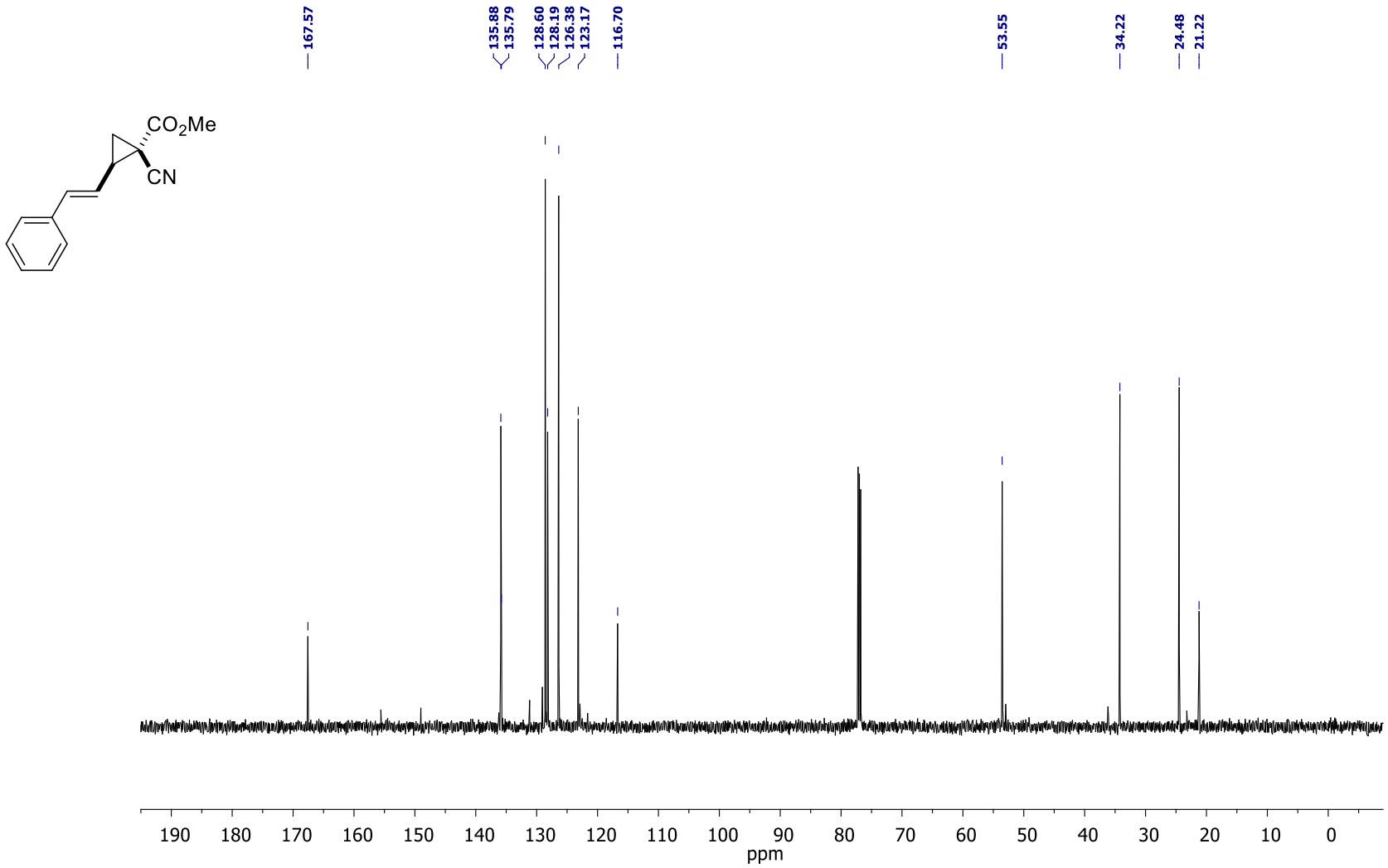
Methyl (1*RS*,2*SR*)-1-cyano-2-((*E*)-styryl)cyclopropane-1-carboxylate (S2m)

^{1}H NMR ($CDCl_3$, 600 MHz)



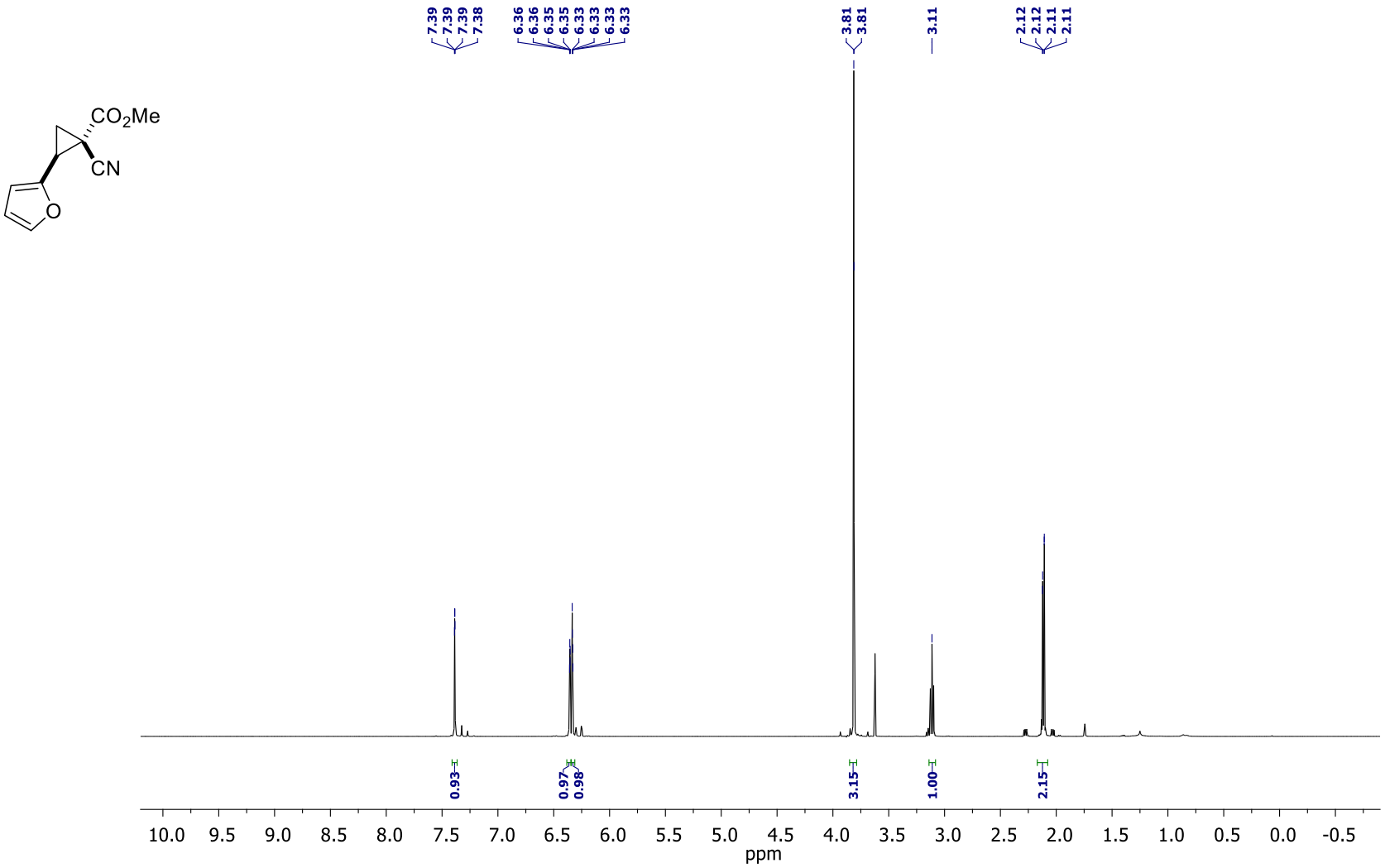
Methyl (1*RS*,2*SR*)-1-cyano-2-((*E*)-styryl)cyclopropane-1-carboxylate (S2m)

^{13}C NMR ($CDCl_3$, 150 MHz)



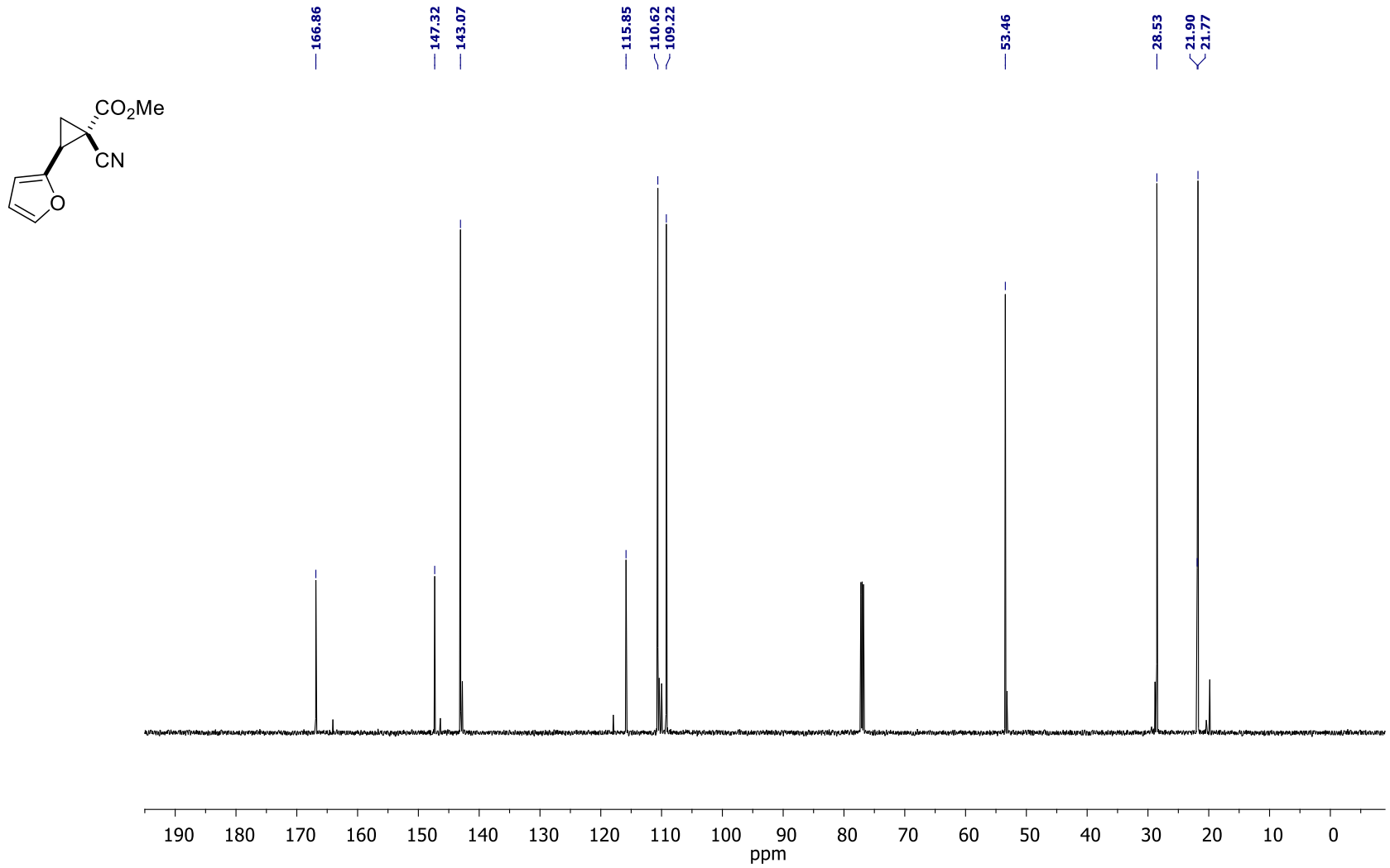
Methyl (1*RS*,2*SR*)-1-cyano-2-(furan-2-yl)cyclopropanecarboxylate (S2n)

^{1}H NMR ($CDCl_3$, 600 MHz)



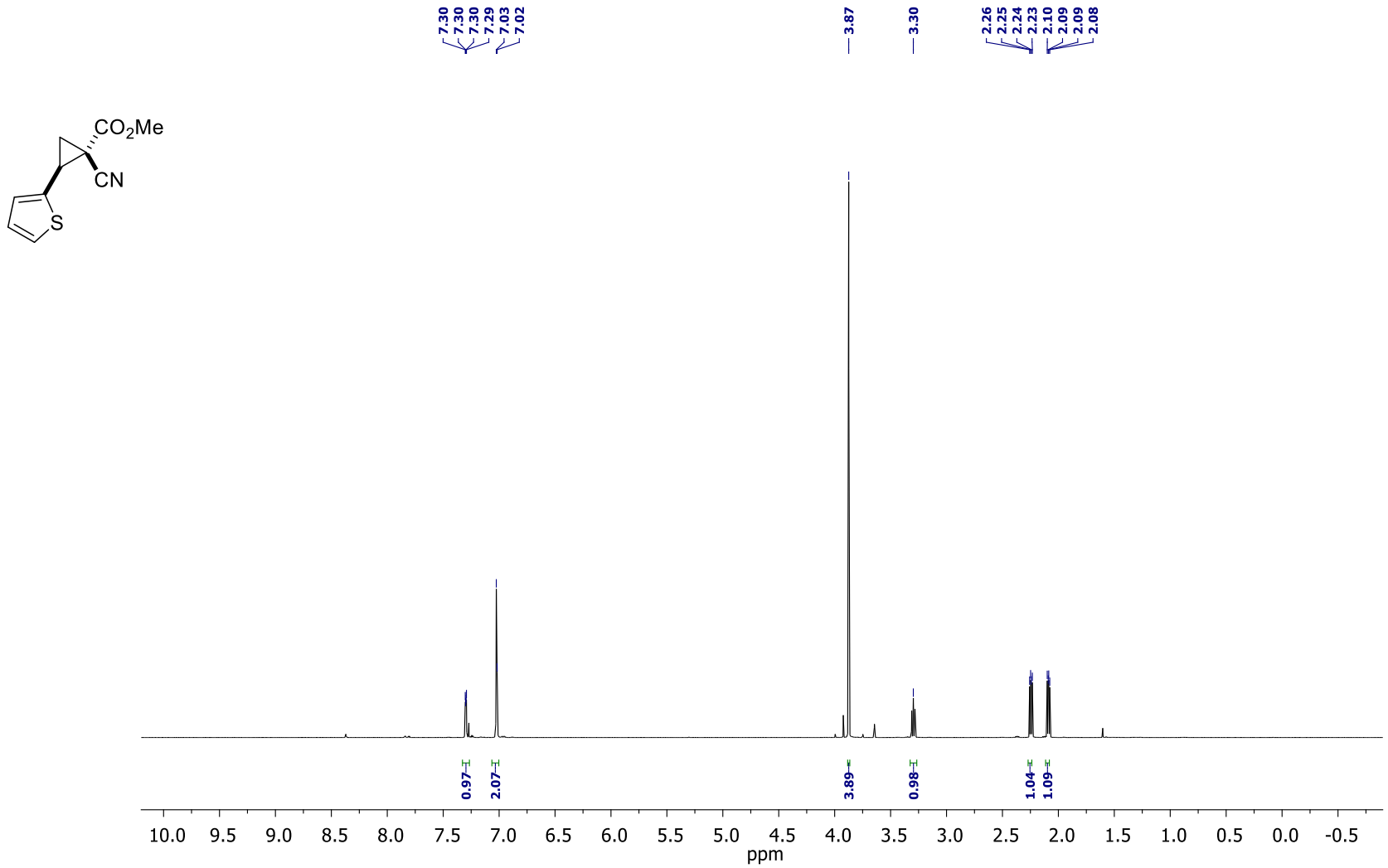
Methyl (1*RS*,2*SR*)-1-cyano-2-(furan-2-yl)cyclopropanecarboxylate (S2n)

^{13}C NMR ($CDCl_3$, 150 MHz)



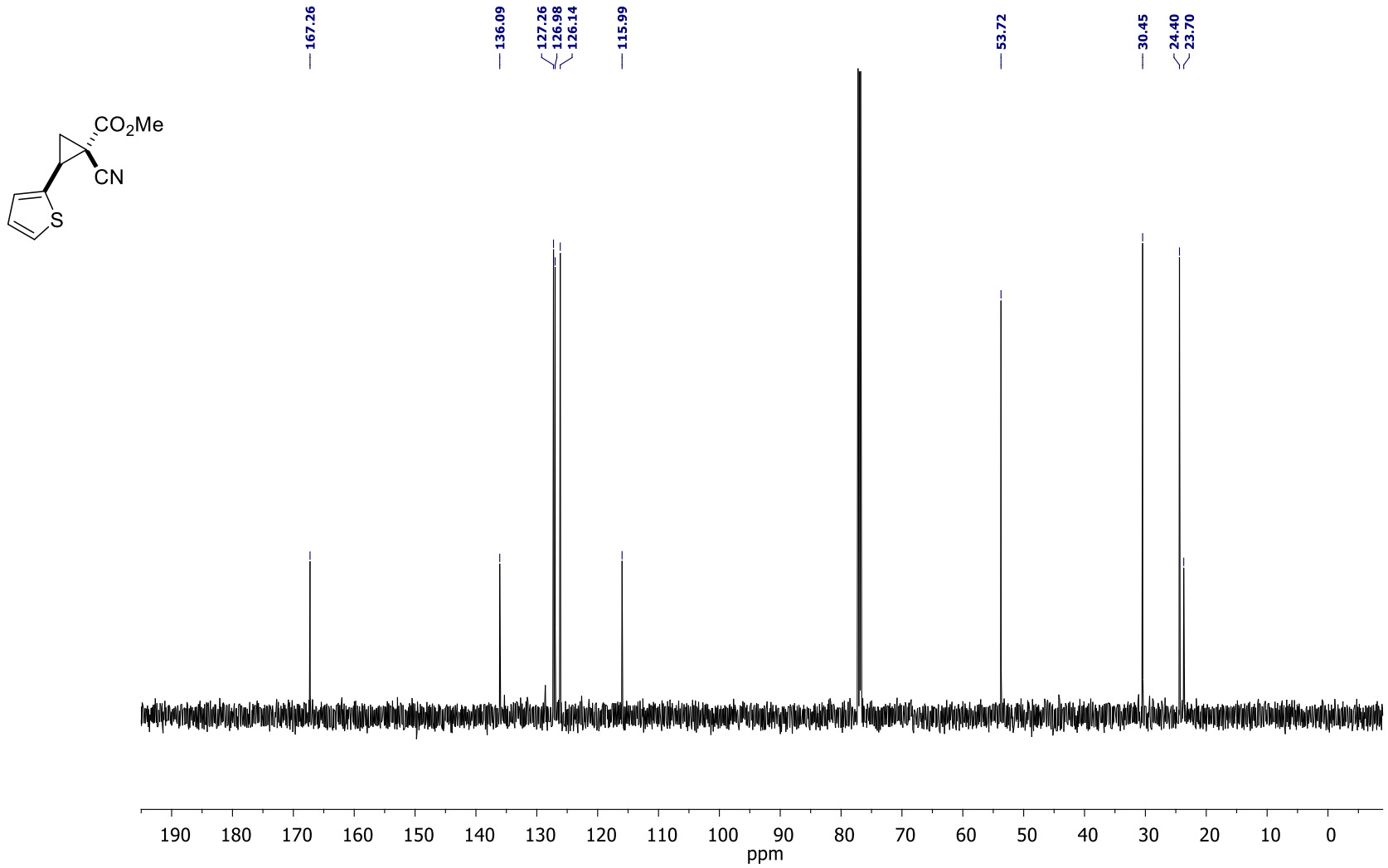
Methyl (1*RS*,2*SR*)-1-cyano-2-(thien-2-yl)cyclopropanecarboxylate (S2o)

^{1}H NMR ($CDCl_3$, 600 MHz)



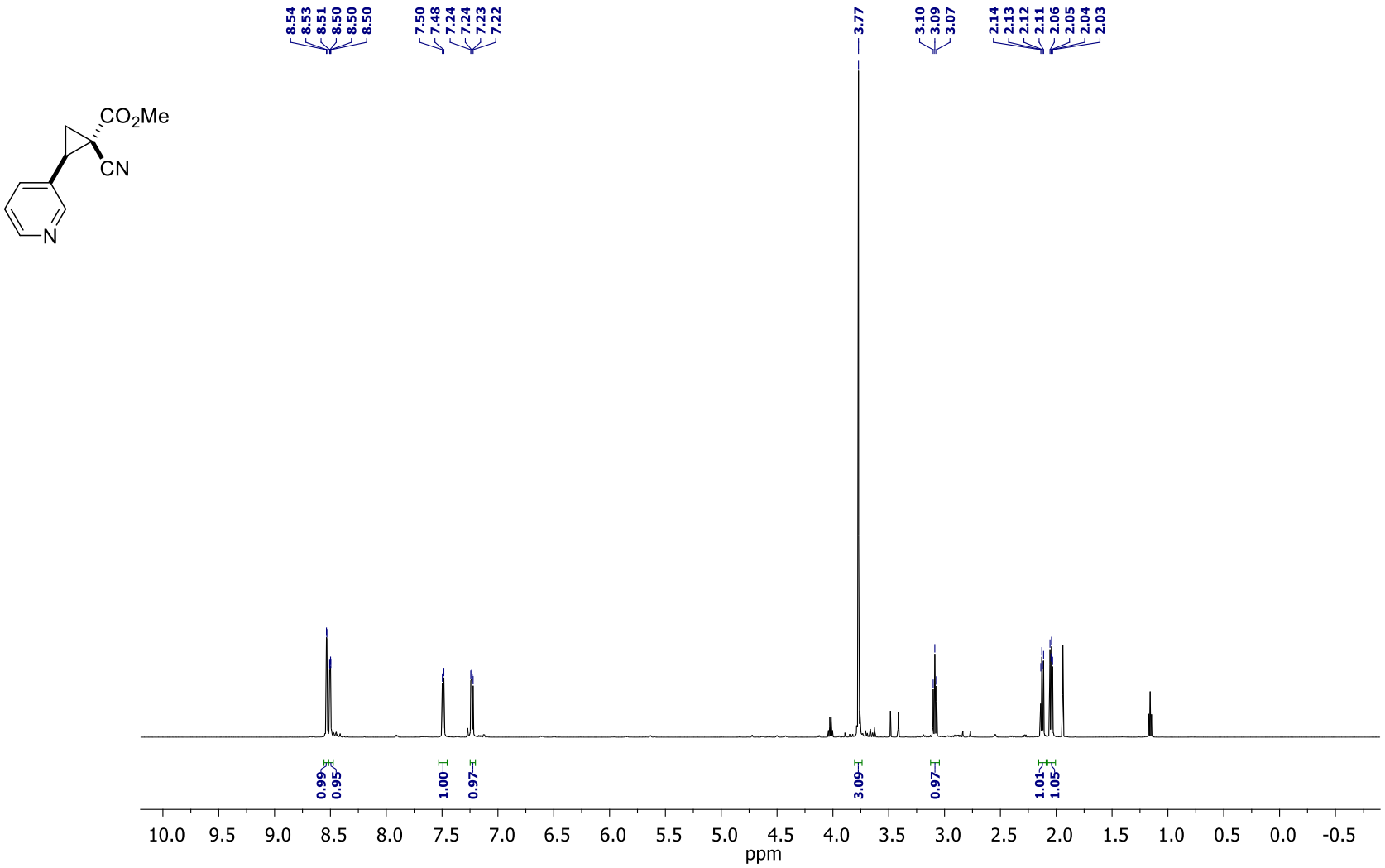
Methyl (1*RS*,2*SR*)-1-cyano-2-(thien-2-yl)cyclopropanecarboxylate (S2o)

^{13}C NMR ($CDCl_3$, 150 MHz)



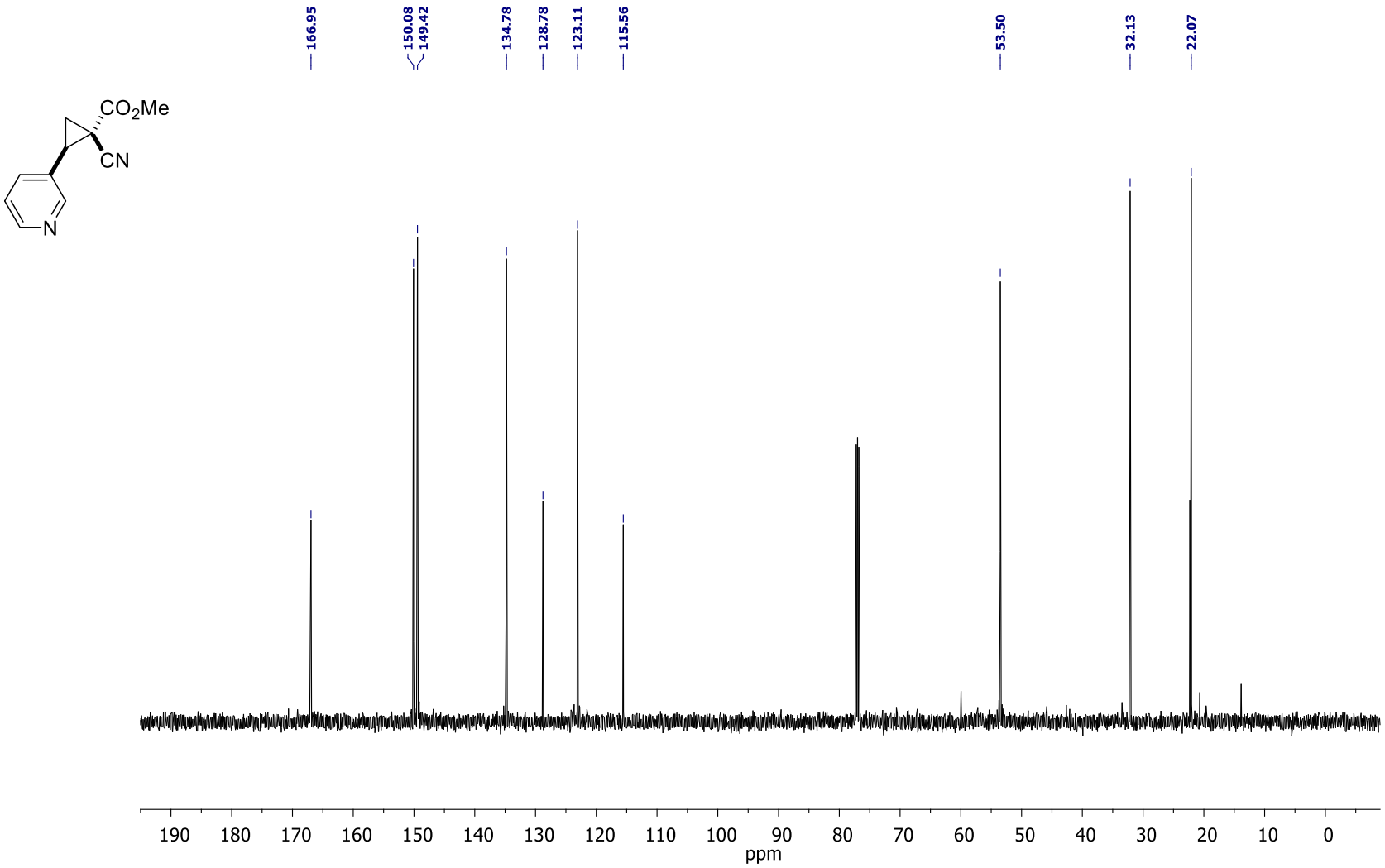
Methyl (1*RS*,2*SR*)-1-cyano-2-(pyridin-3-yl)cyclopropanecarboxylate (S2p)

^{1}H NMR ($CDCl_3$, 600 MHz)



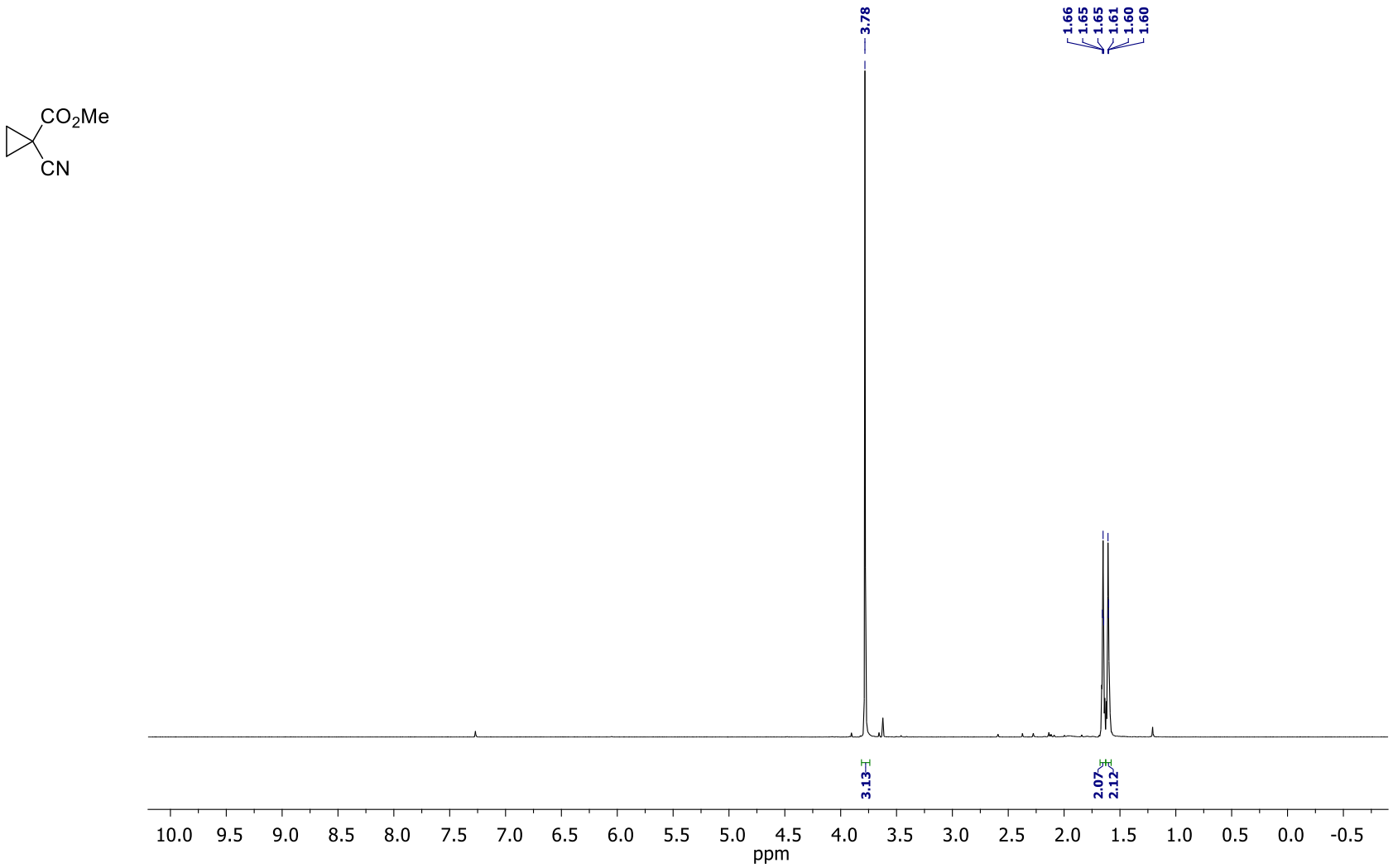
Methyl (1*RS*,2*SR*)-1-cyano-2-(pyridin-3-yl)cyclopropanecarboxylate (S2p)

^{13}C NMR ($CDCl_3$, 150 MHz)



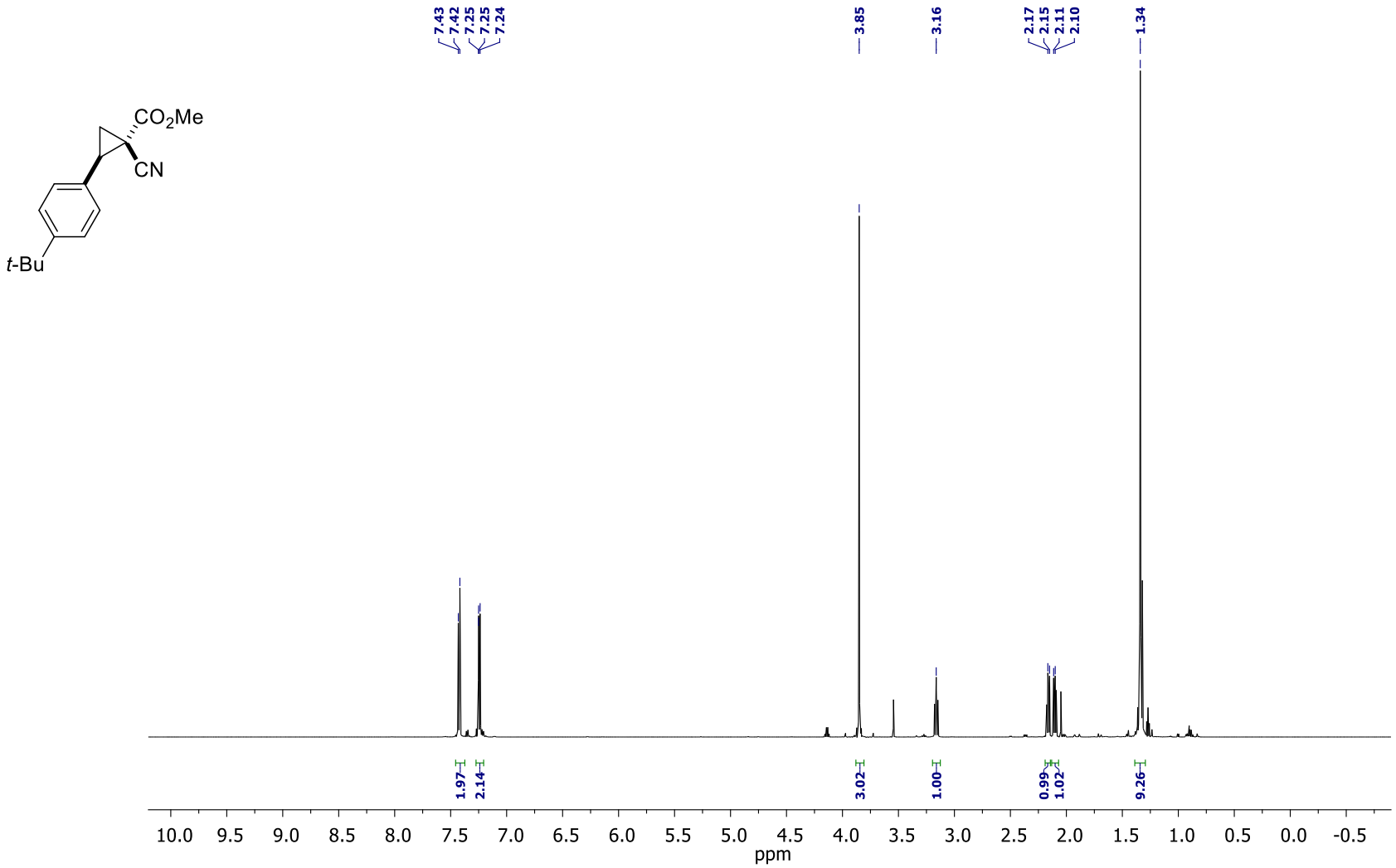
Methyl 1-cyanocyclopropanecarboxylate (S2q)

^{1}H NMR ($CDCl_3$, 600 MHz)



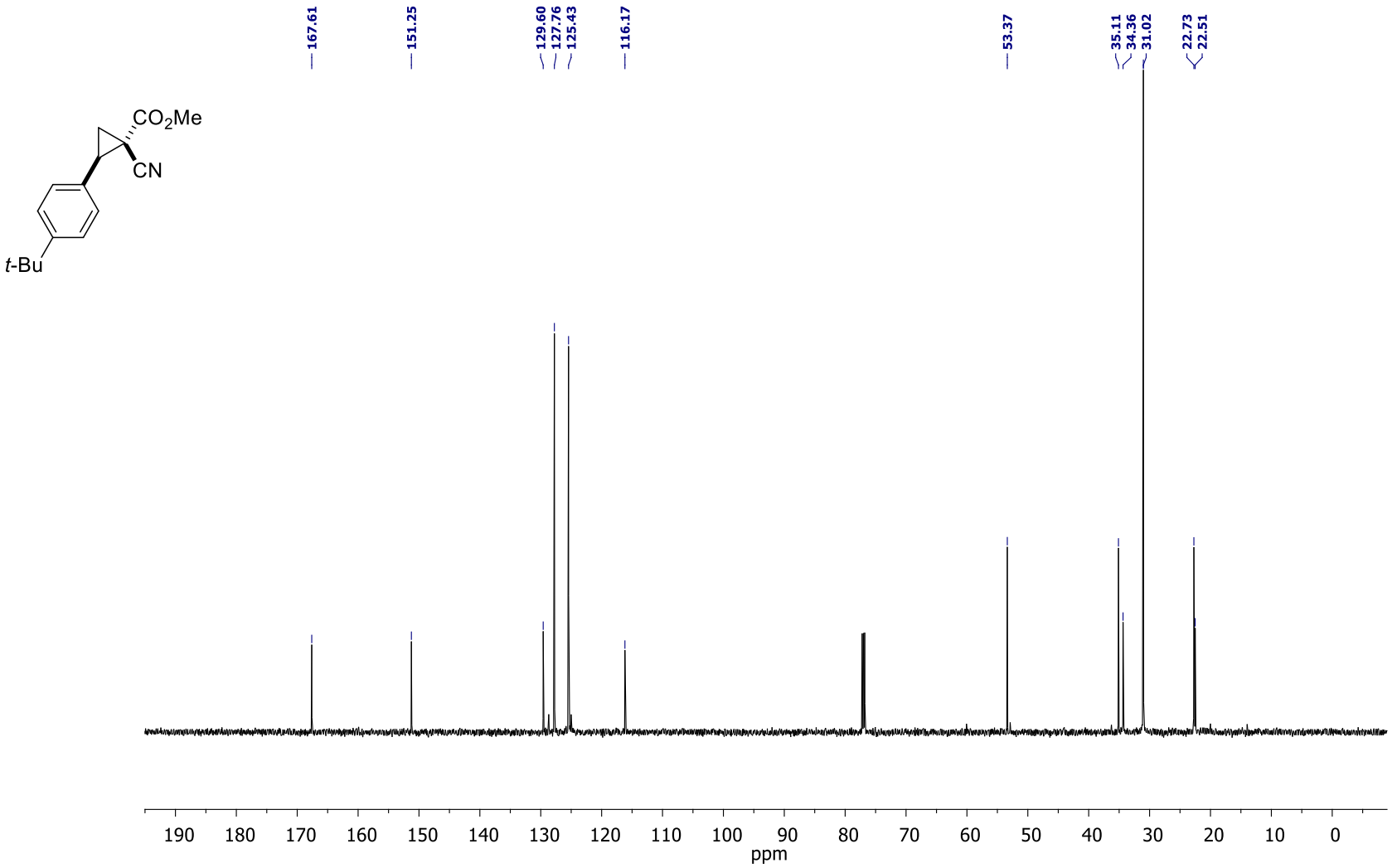
Methyl (1*RS*,2*SR*)-1-cyano-2-(4-*tert*-butylphenyl)cyclopropanecarboxylate (S2r)

^{1}H NMR ($CDCl_3$, 600 MHz)



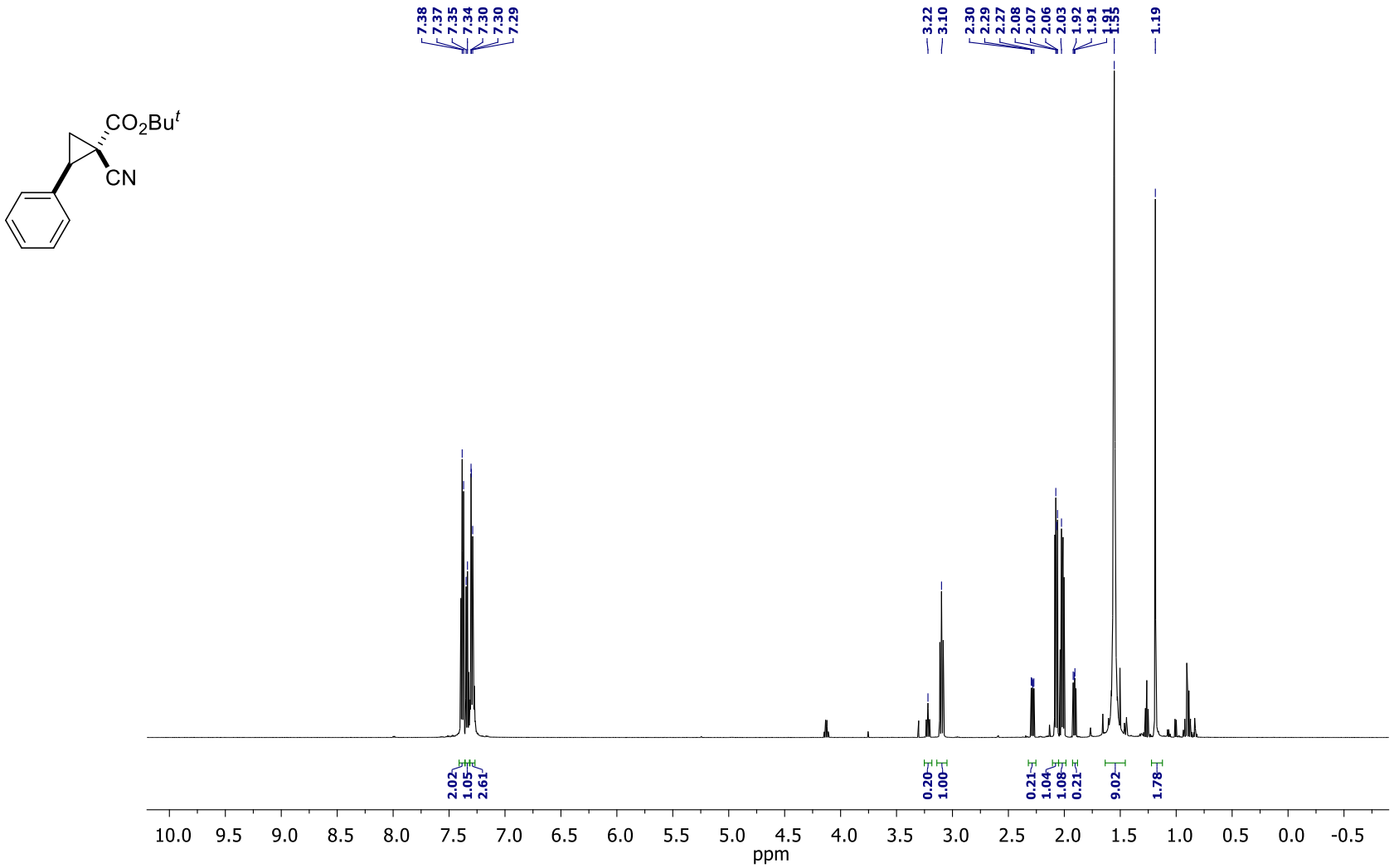
Methyl (1*RS*,2*SR*)-1-cyano-2-(4-*tert*-butylphenyl)cyclopropanecarboxylate (S2r)

^{13}C NMR ($CDCl_3$, 150 MHz)



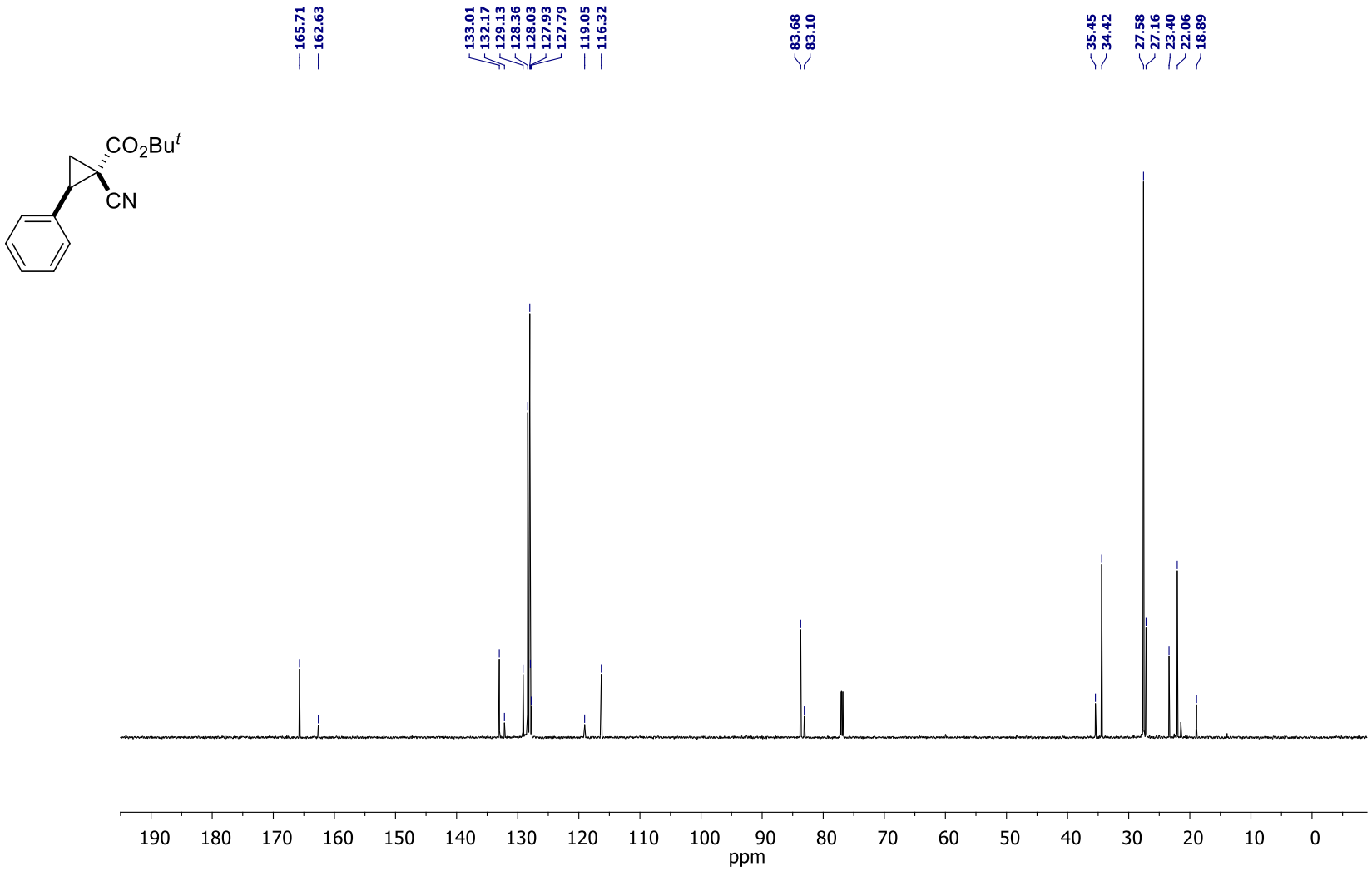
***tert*-Butyl (1*RS*,2*SR*)-1-cyano-2-phenylcyclopropanecarboxylate (S2s)**

^{1}H NMR ($CDCl_3$, 600 MHz)



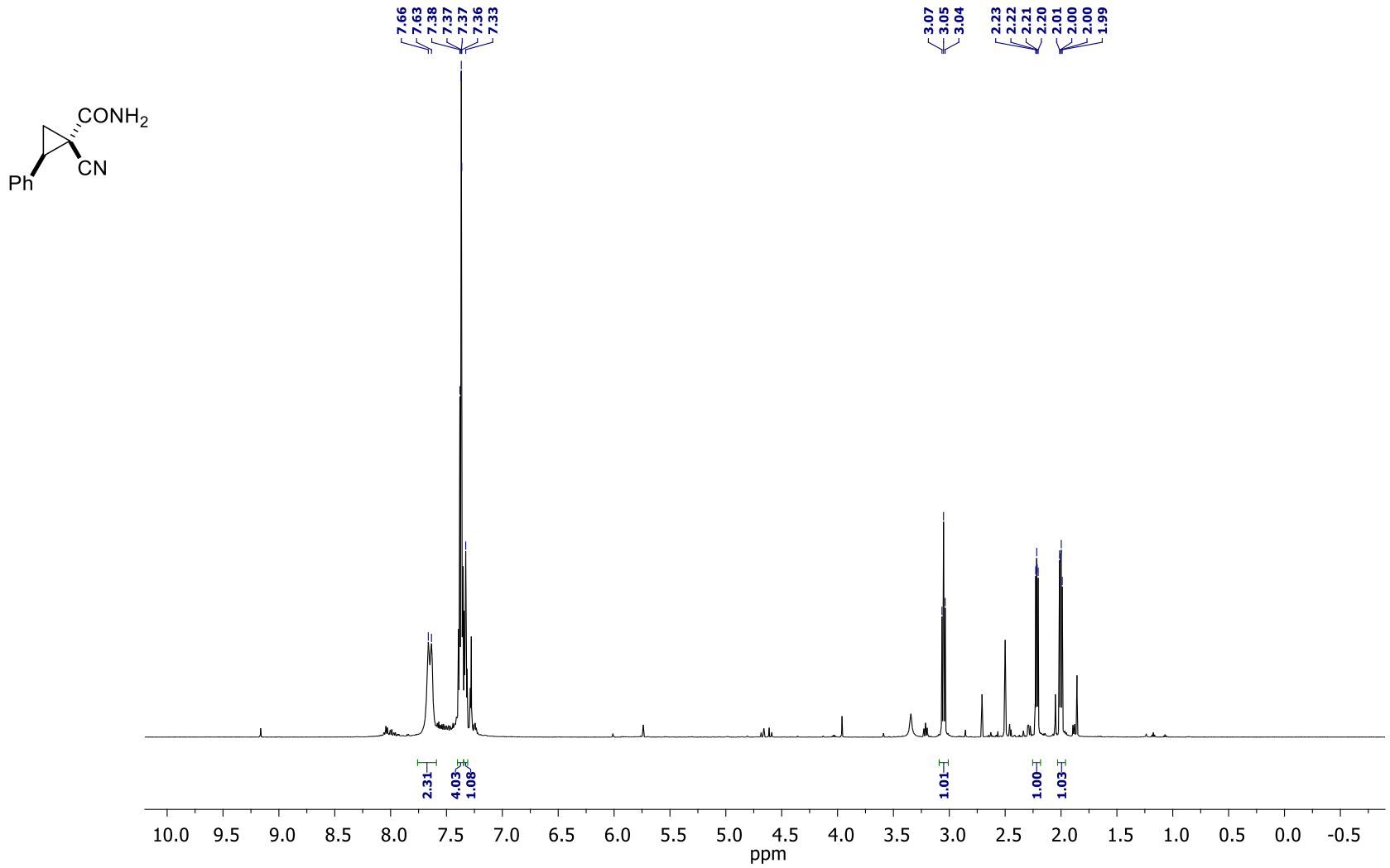
tert-Butyl (1_RS_,2_SR_)-1-cyano-2-phenylcyclopropanecarboxylate (S2s)

^{13}C NMR ($CDCl_3$, 150 MHz)



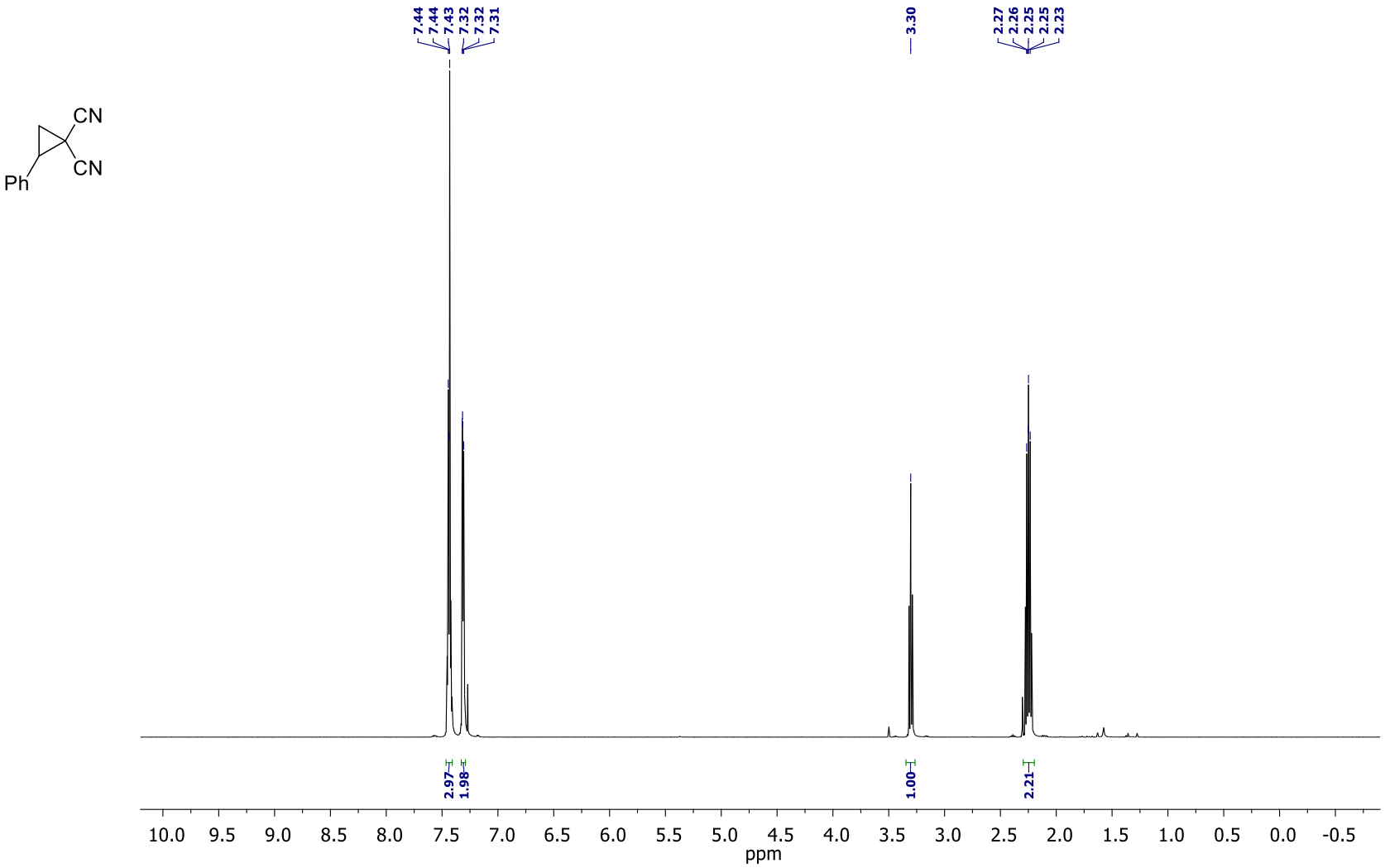
(1*RS*,2*SR*)-1-Cyano-2-phenylcyclopropanecarboxamide (S2t)

^{1}H NMR ($CDCl_3$, 600 MHz)



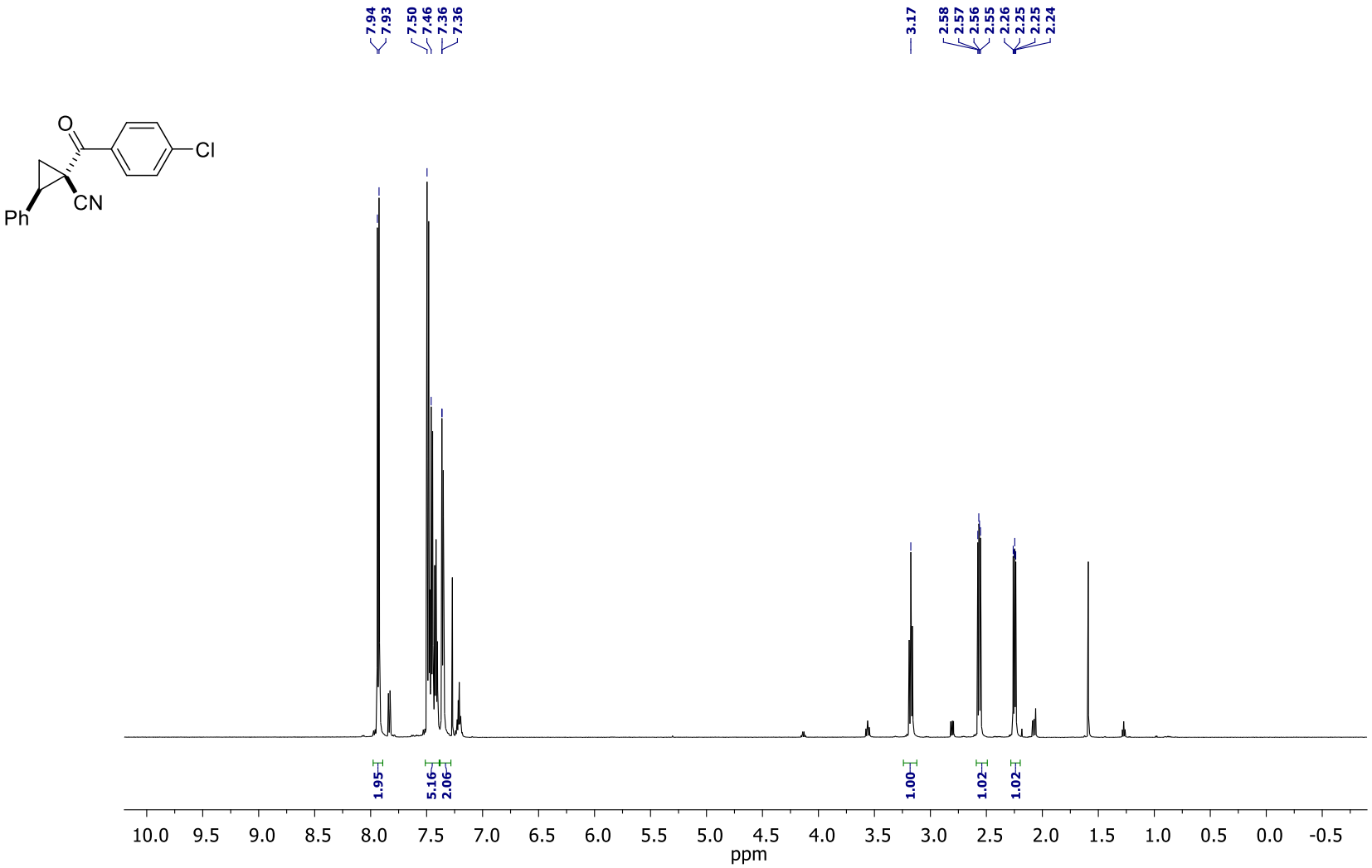
2-Phenylcyclopropane-1,1-dicarbonitrile (S2u)

^{1}H NMR ($CDCl_3$, 600 MHz)



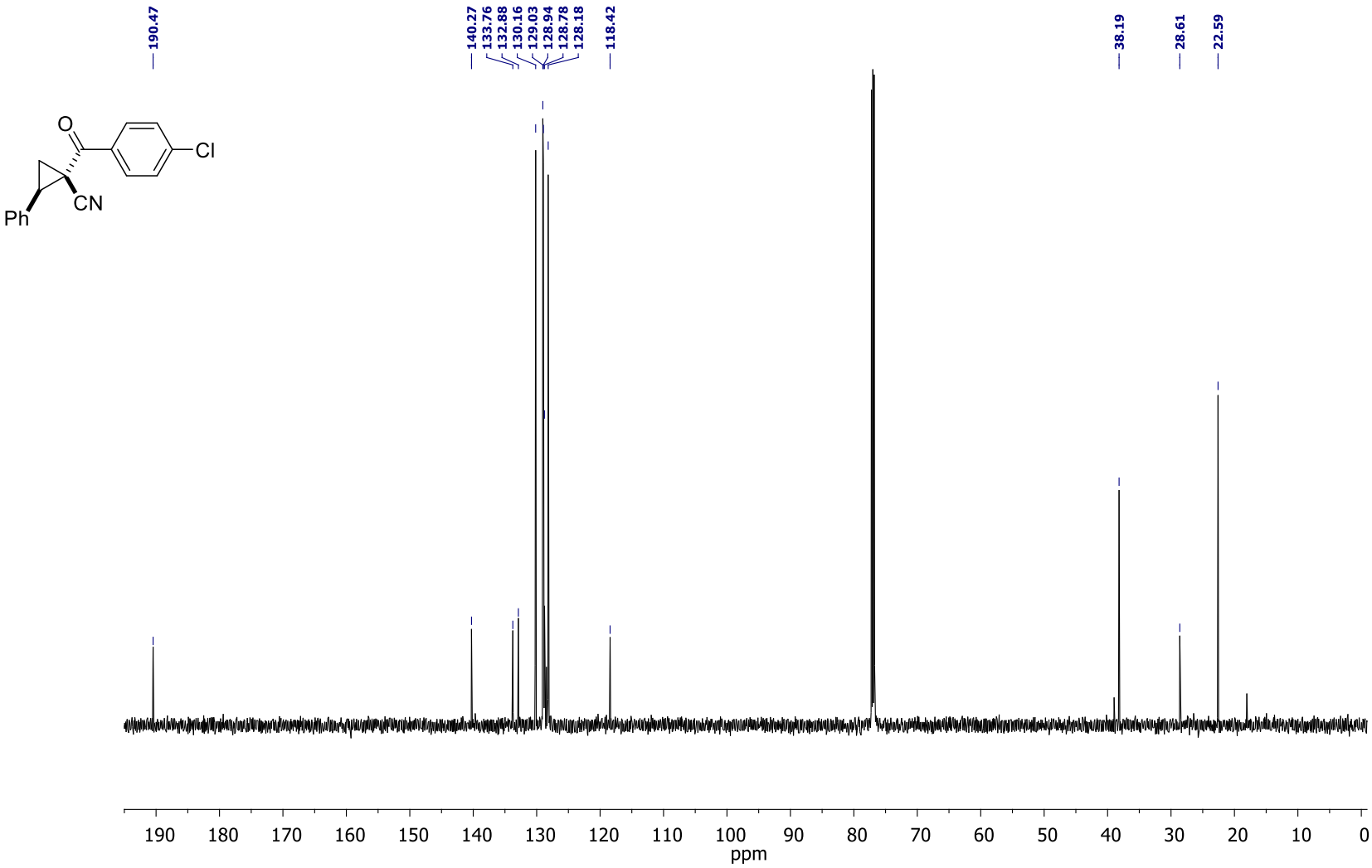
(1*RS*,2*SR*)-1-(4-Chlorobenzoyl)-2-phenylcyclopropanecarbonitrile (S2v)

^{1}H NMR ($CDCl_3$, 600 MHz)



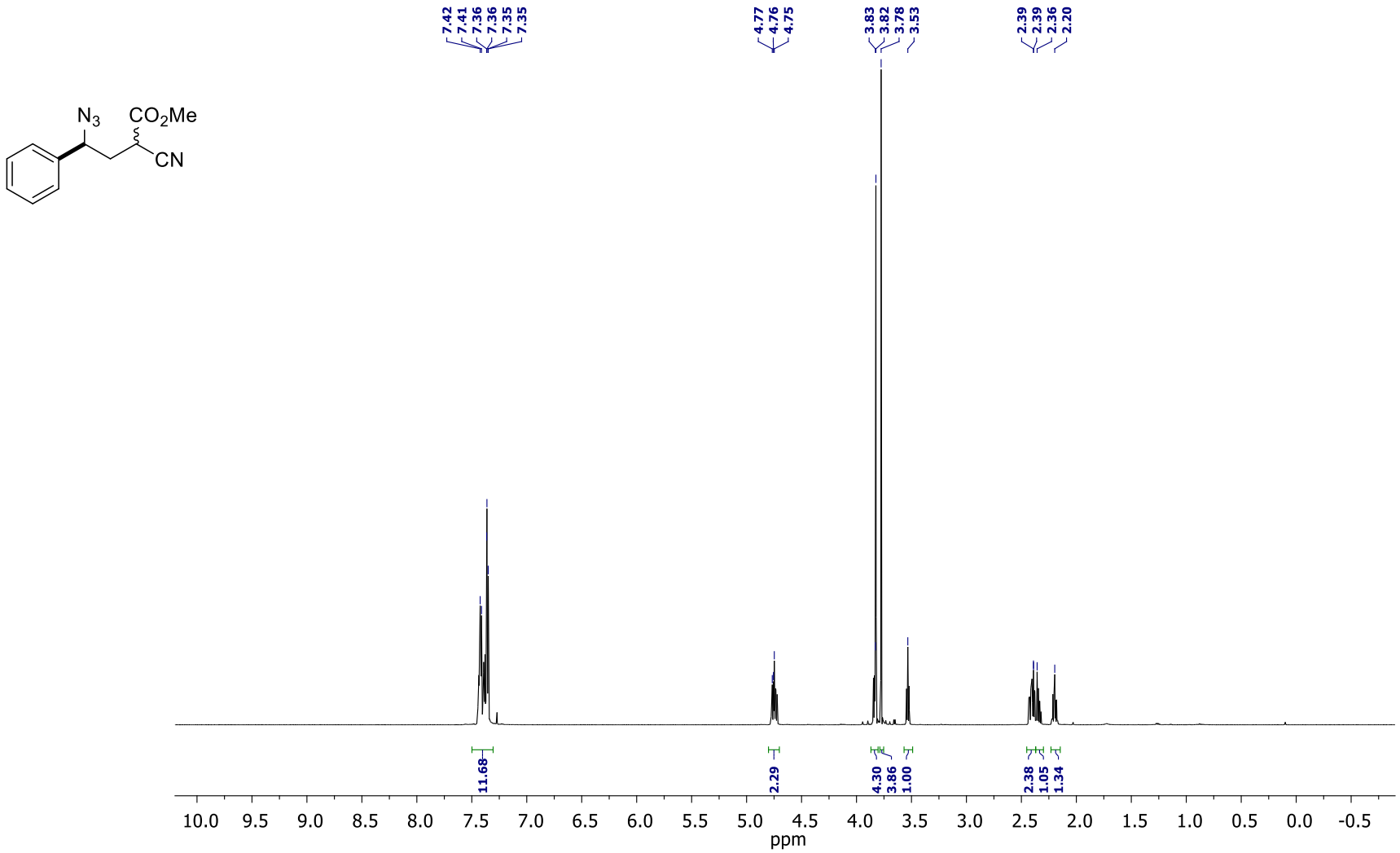
(1*RS*,2*SR*)-1-(4-Chlorobenzoyl)-2-phenylcyclopropanecarbonitrile (S2v)

^{13}C NMR ($CDCl_3$, 150 MHz)



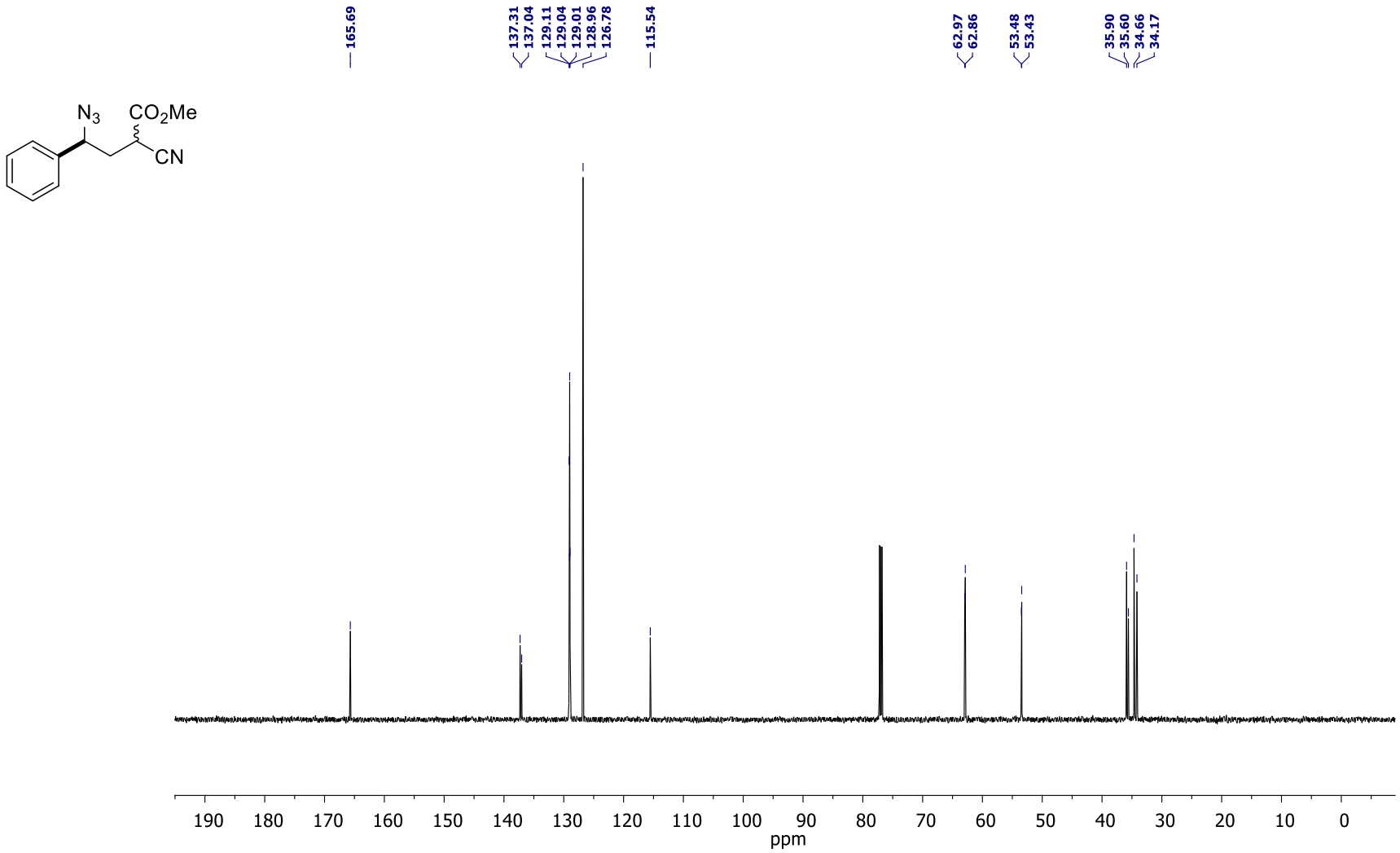
Methyl 4-azido-2-cyano-4-phenylbutyrate (1a)

^{1}H NMR ($CDCl_3$, 600 MHz)



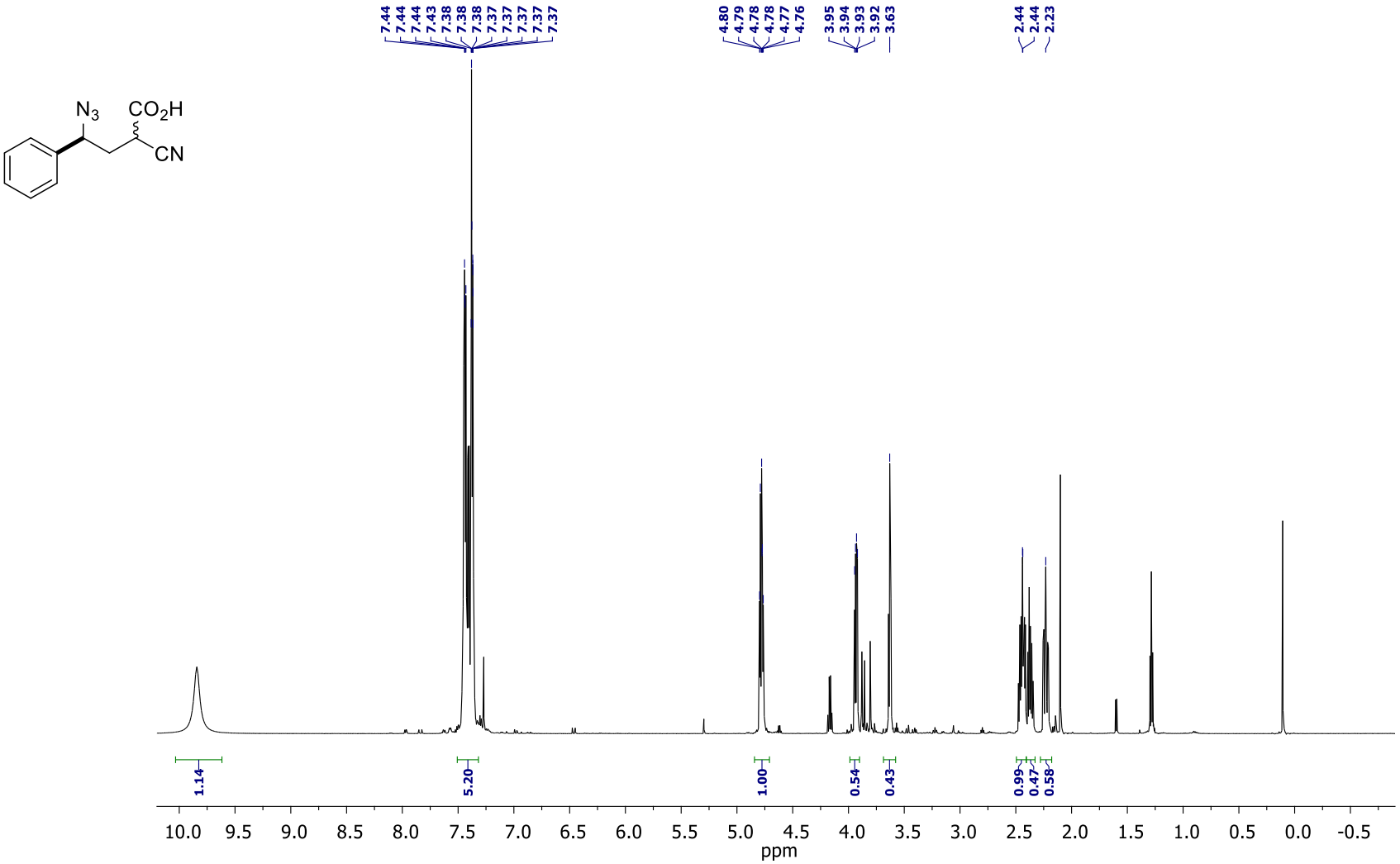
Methyl 4-azido-2-cyano-4-phenylbutyrate (1a)

^{13}C NMR ($CDCl_3$, 150 MHz)



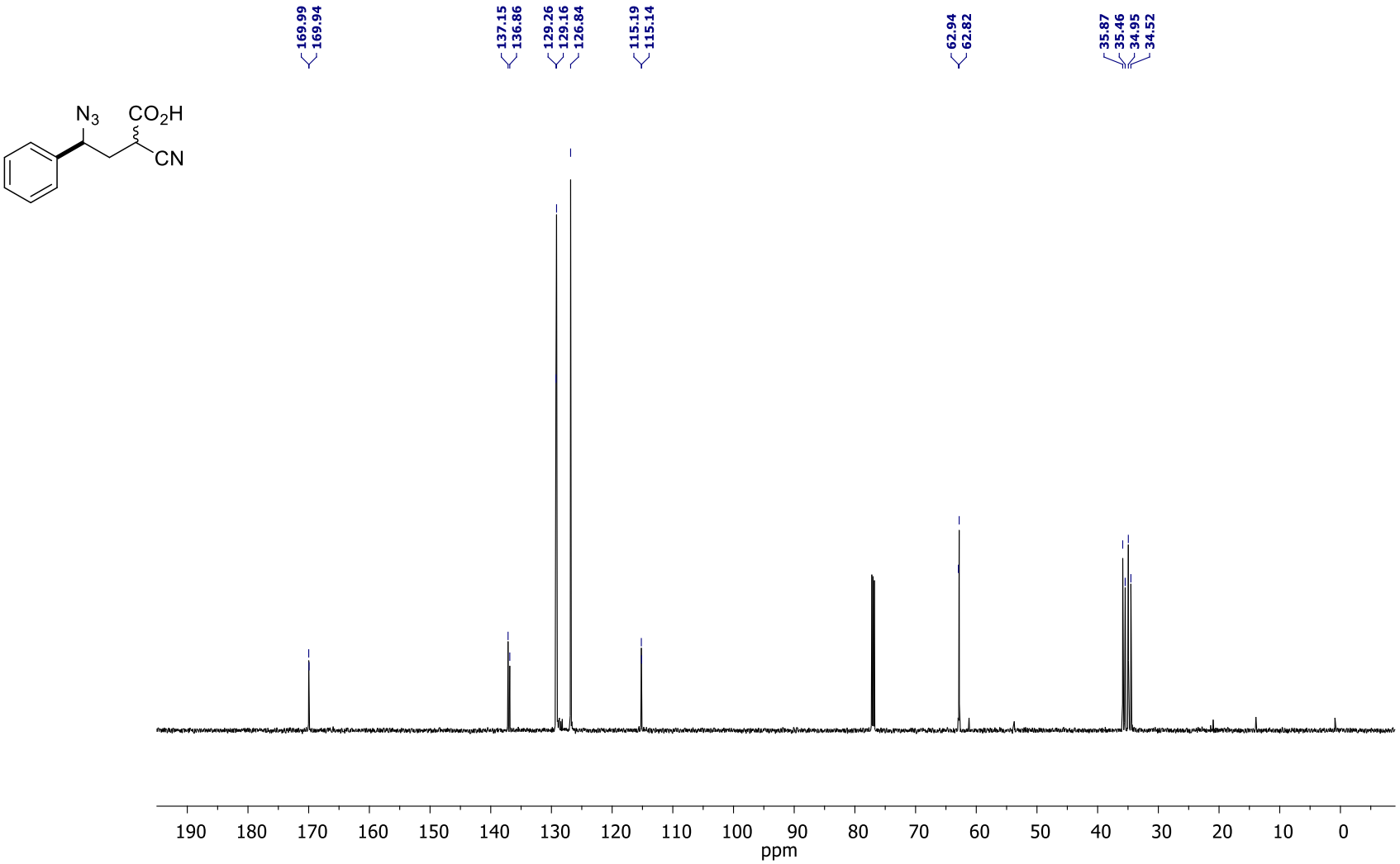
4-Azido-2-cyano-4-phenylbutyric acid (1a′)

^{1}H NMR ($CDCl_3$, 600 MHz)



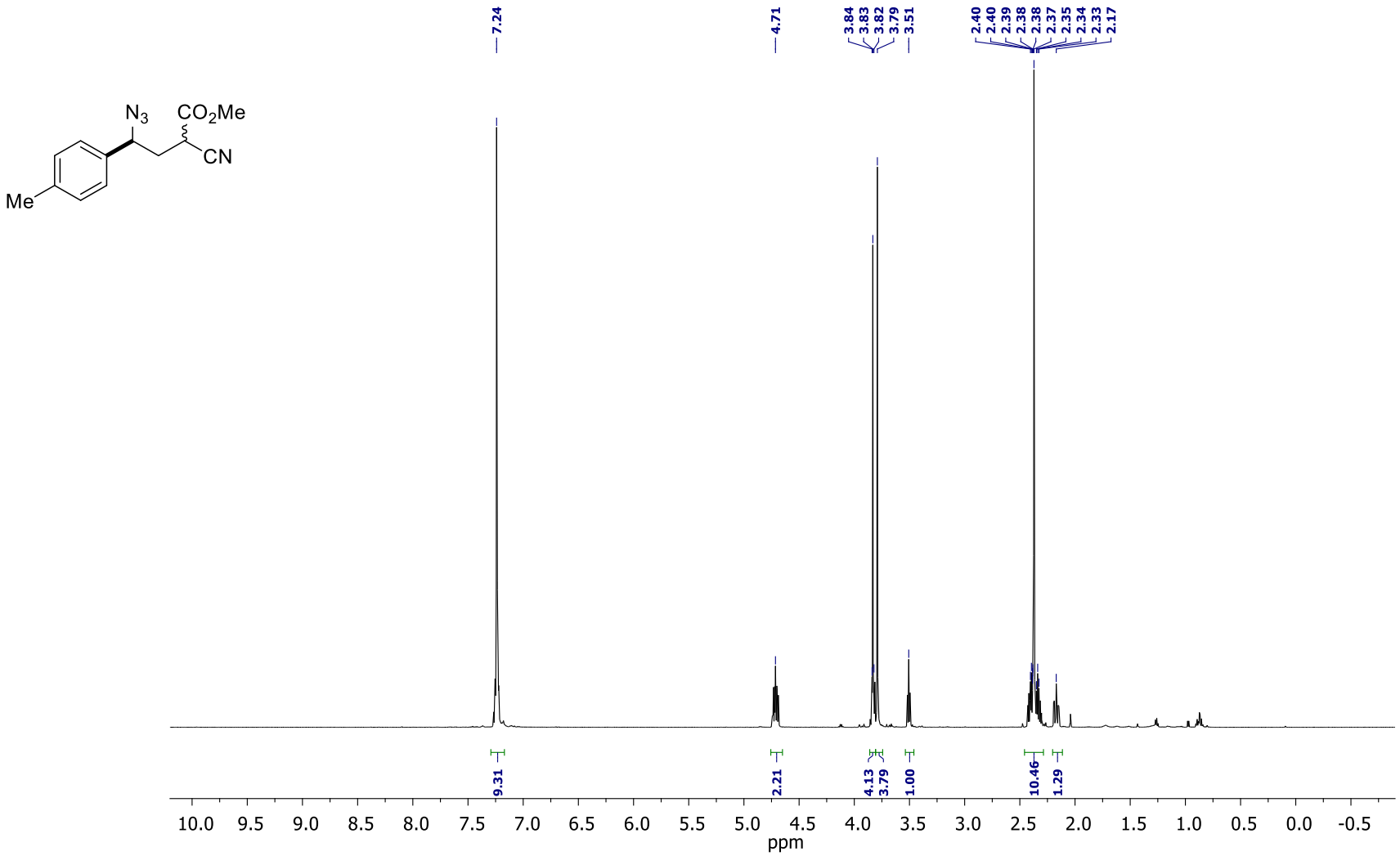
4-Azido-2-cyano-4-phenylbutyric acid (1a′)

^{13}C NMR ($CDCl_3$, 150 MHz)



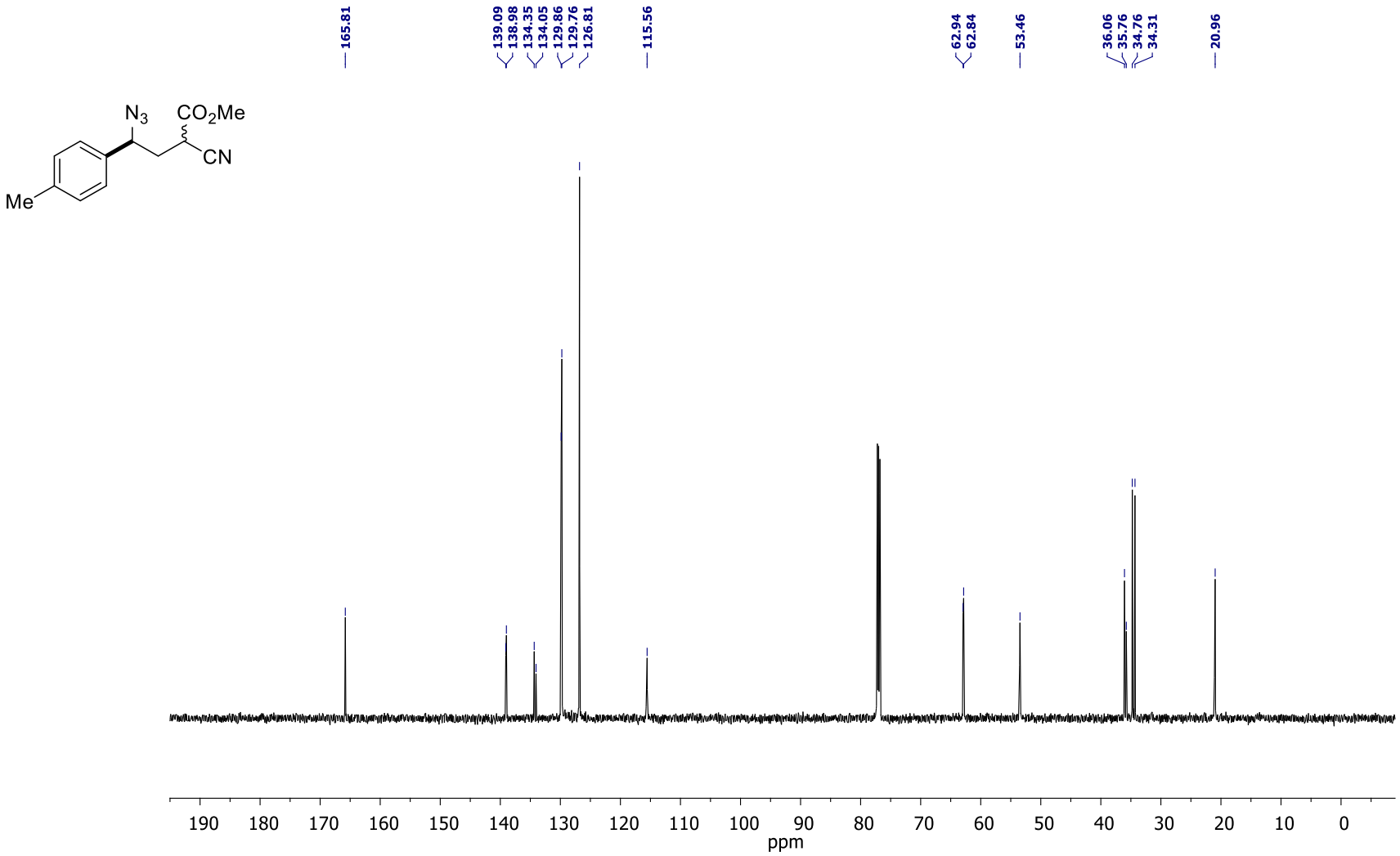
Methyl 4-azido-2-cyano-4-(*p*-tolyl)butyrate (1b)

^{1}H NMR ($CDCl_3$, 600 MHz)



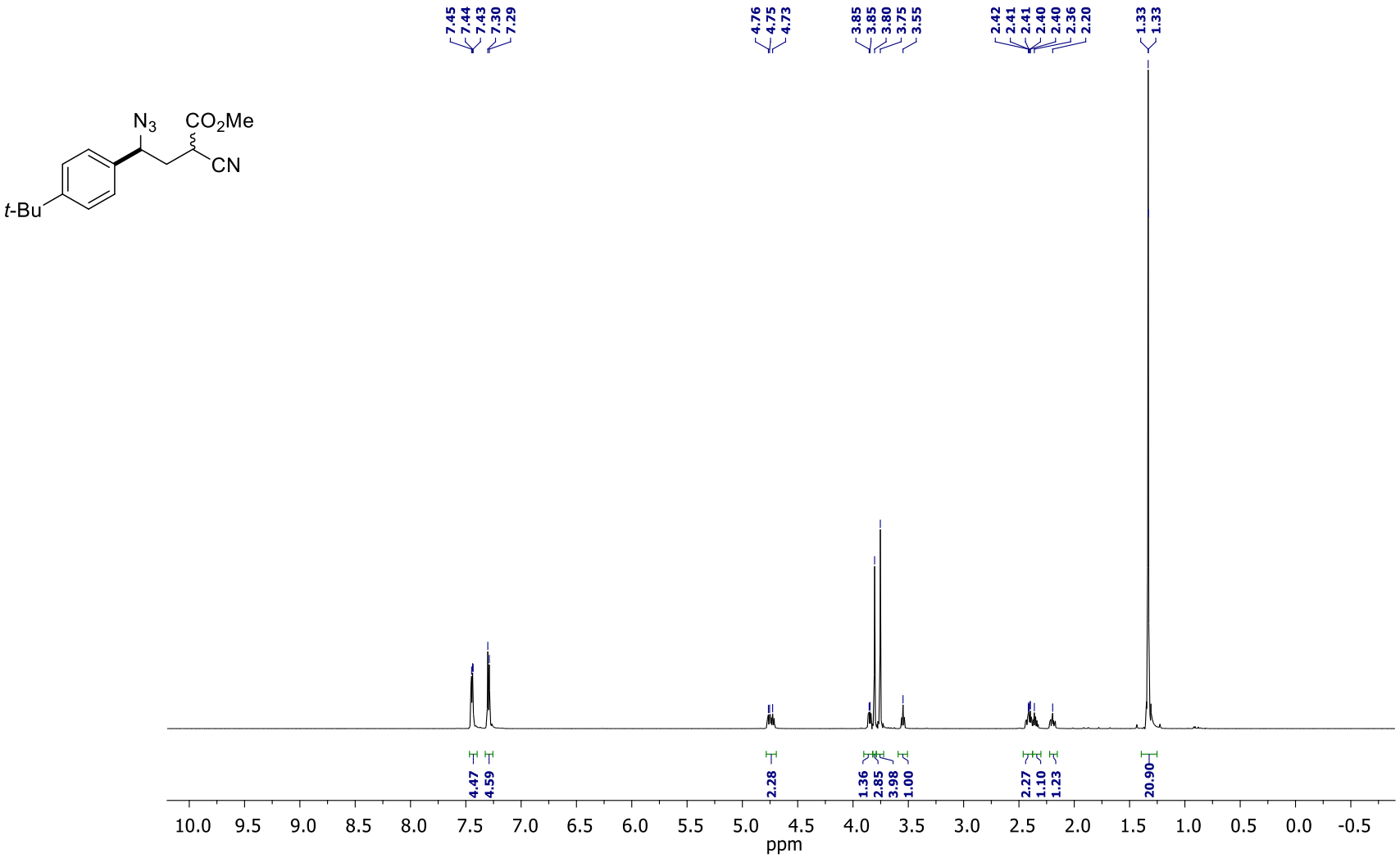
Methyl 4-azido-2-cyano-4-(*p*-tolyl)butyrate (1b)

^{13}C NMR ($CDCl_3$, 150 MHz)



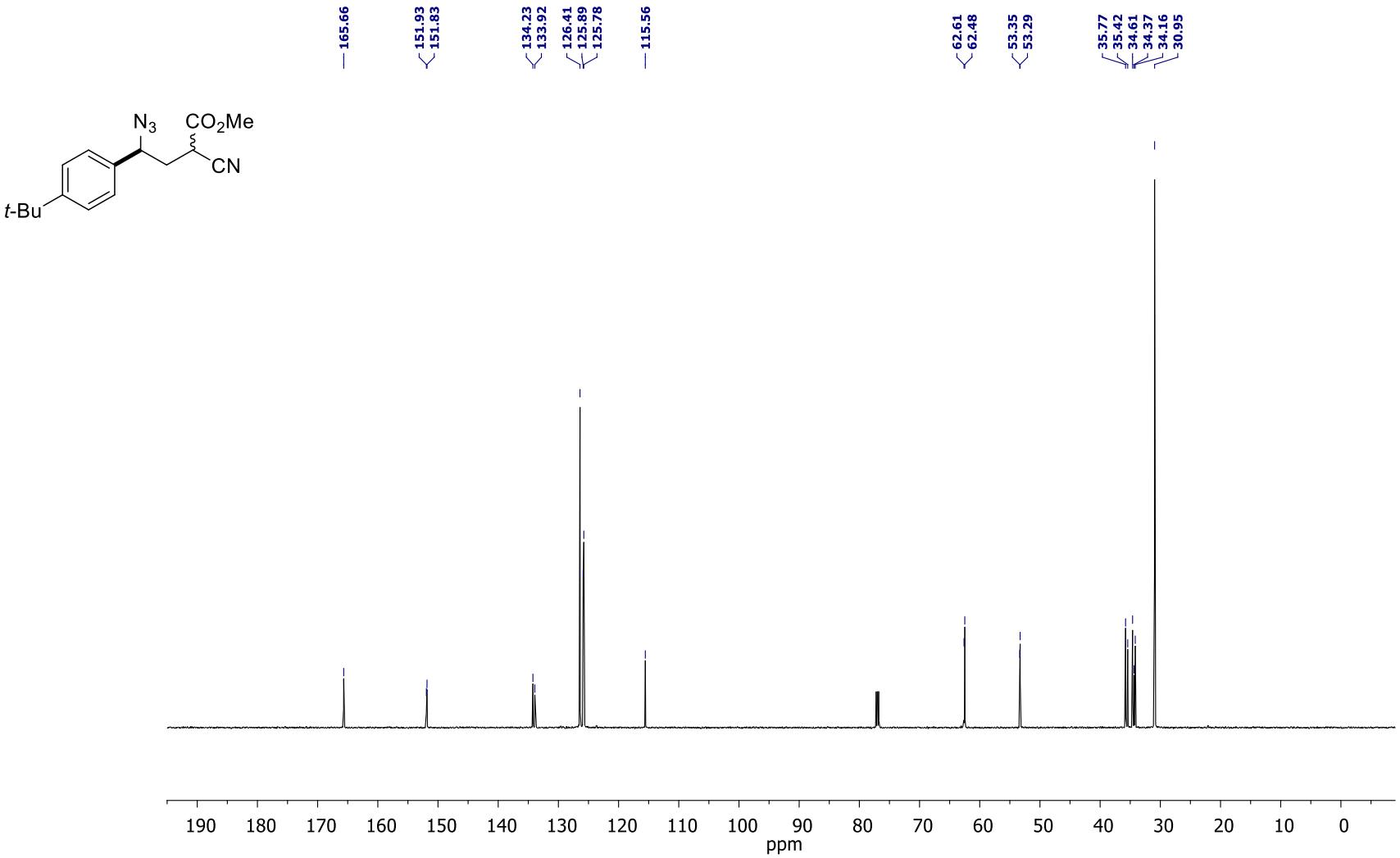
Methyl 4-azido-2-cyano-4-(4-*tert*-butylphenyl)butyrate (1c)

^{1}H NMR ($CDCl_3$, 600 MHz)



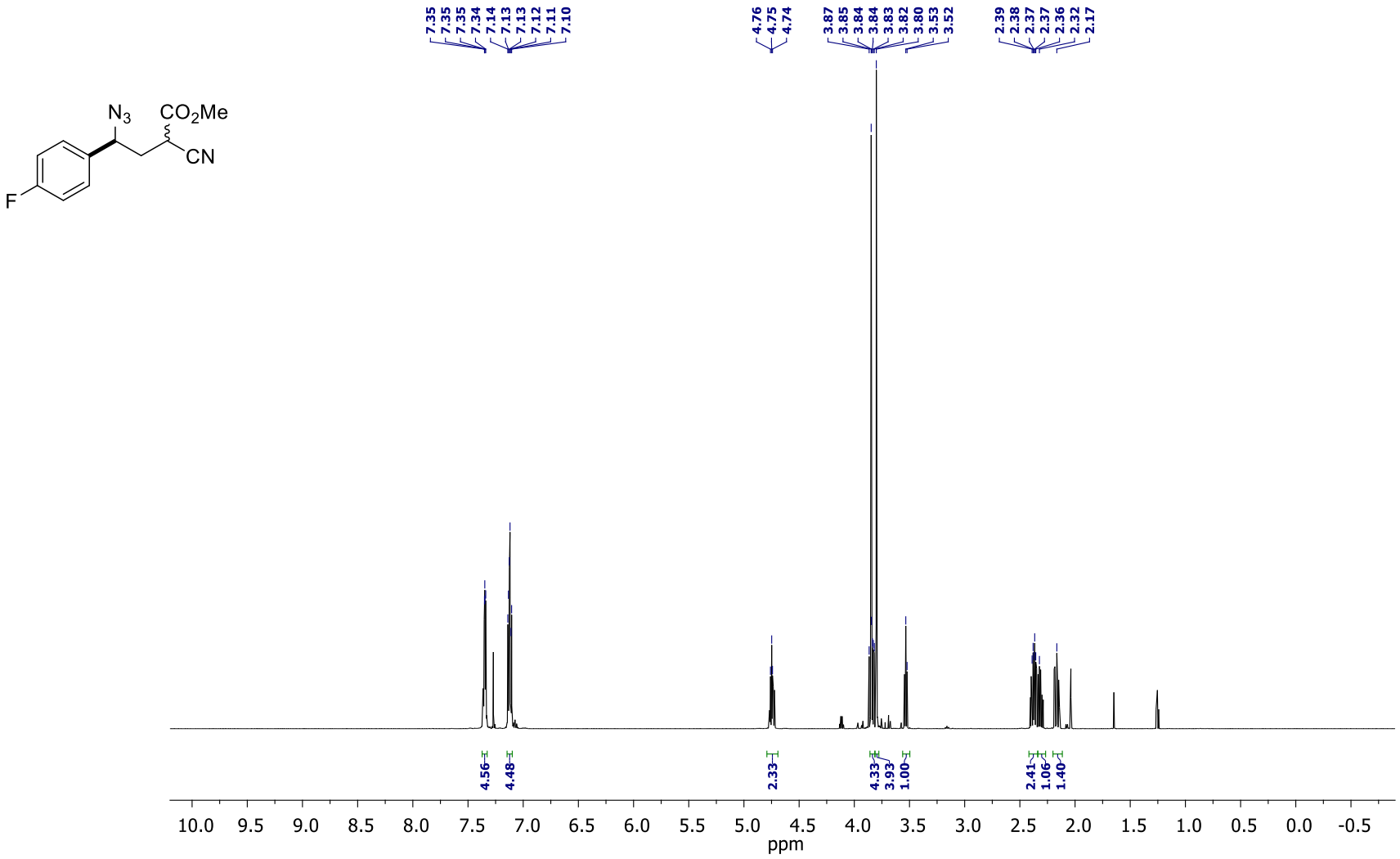
Methyl 4-azido-2-cyano-4-(4-*tert*-butylphenyl)butyrate (1c)

^{13}C NMR ($CDCl_3$, 150 MHz)



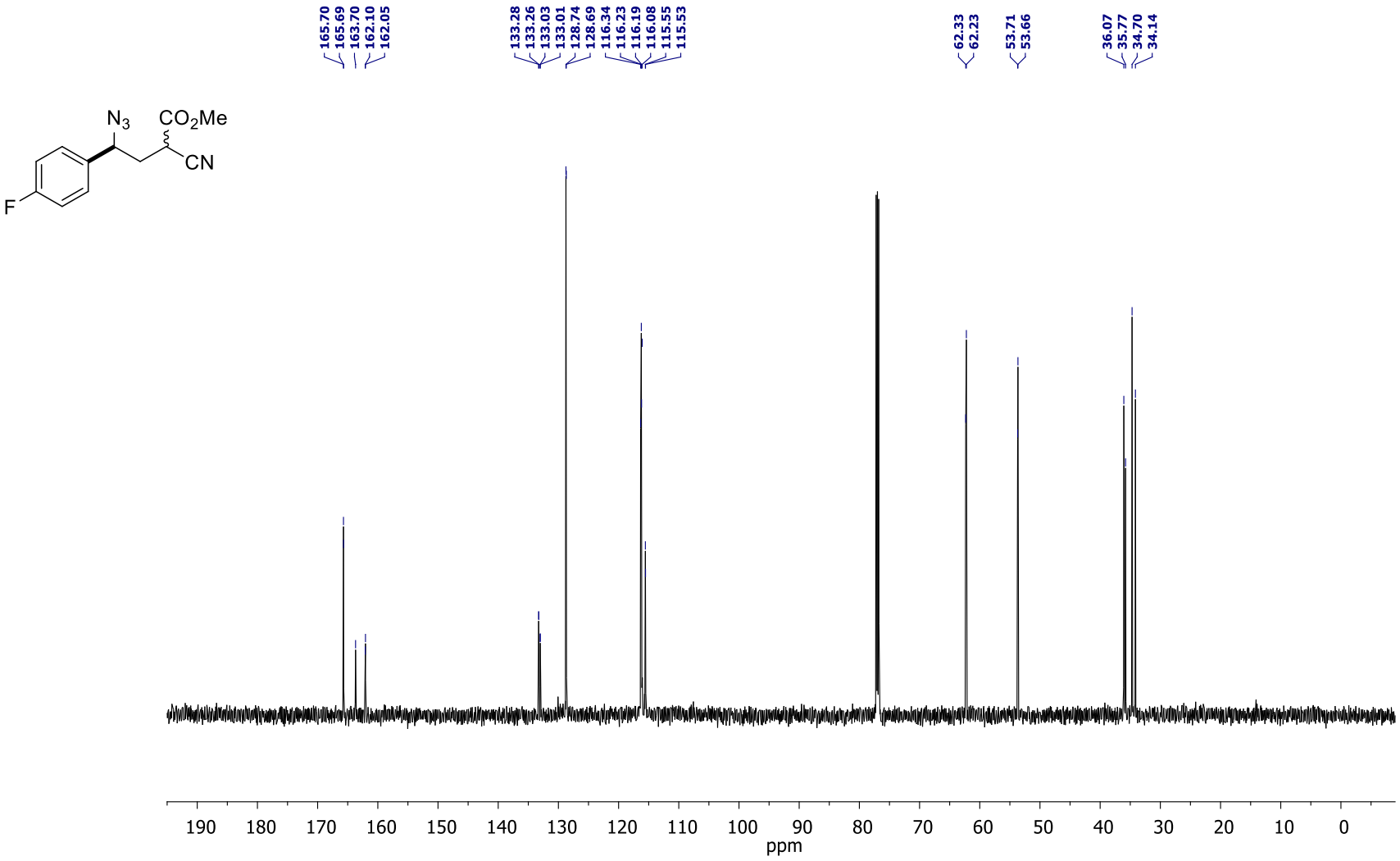
Methyl 4-azido-2-cyano-4-(4-fluorophenyl)butyrate (1d)

^{1}H NMR ($CDCl_3$, 600 MHz)



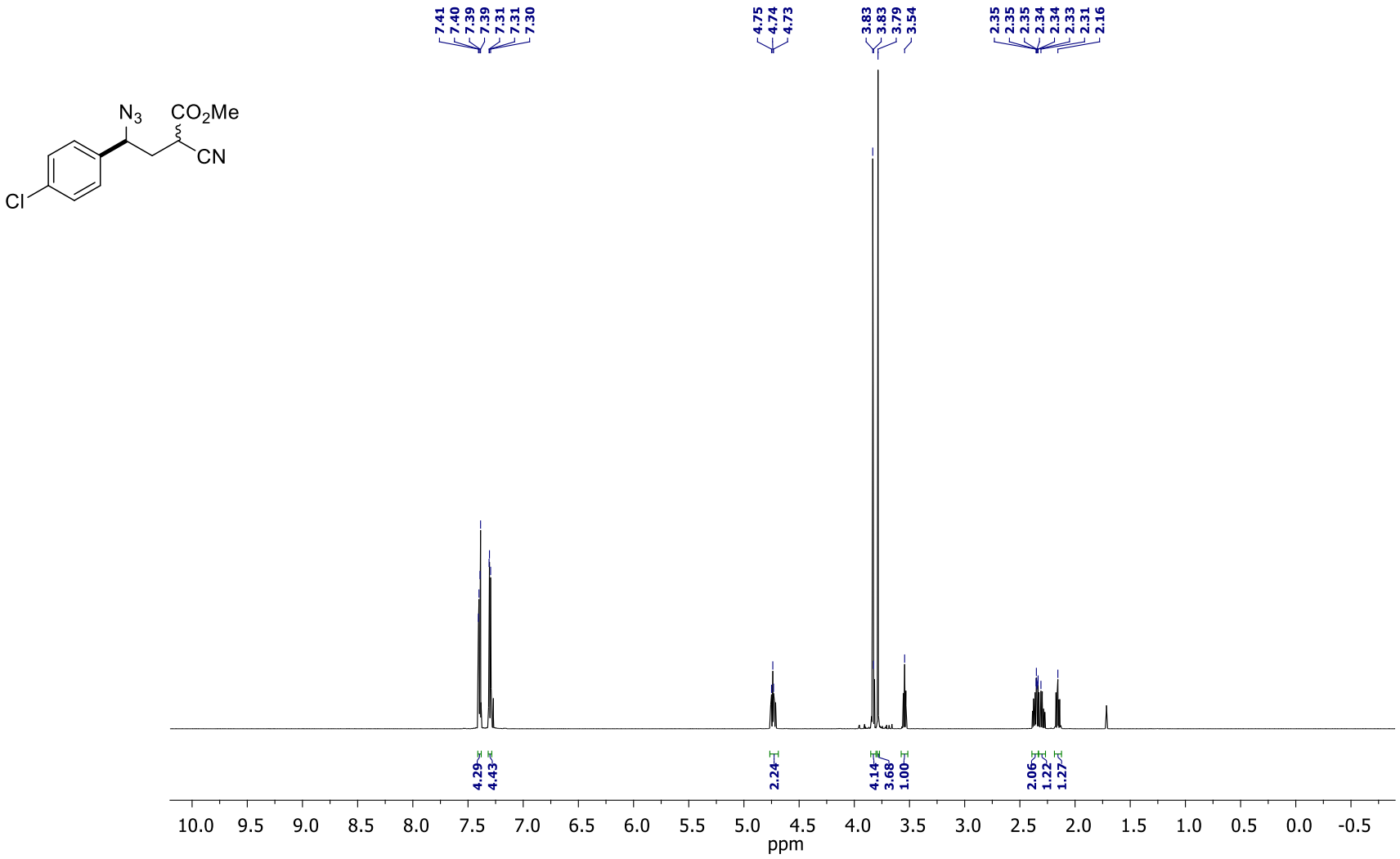
Methyl 4-azido-2-cyano-4-(4-fluorophenyl)butyrate (1d)

^{13}C NMR ($CDCl_3$, 150 MHz)



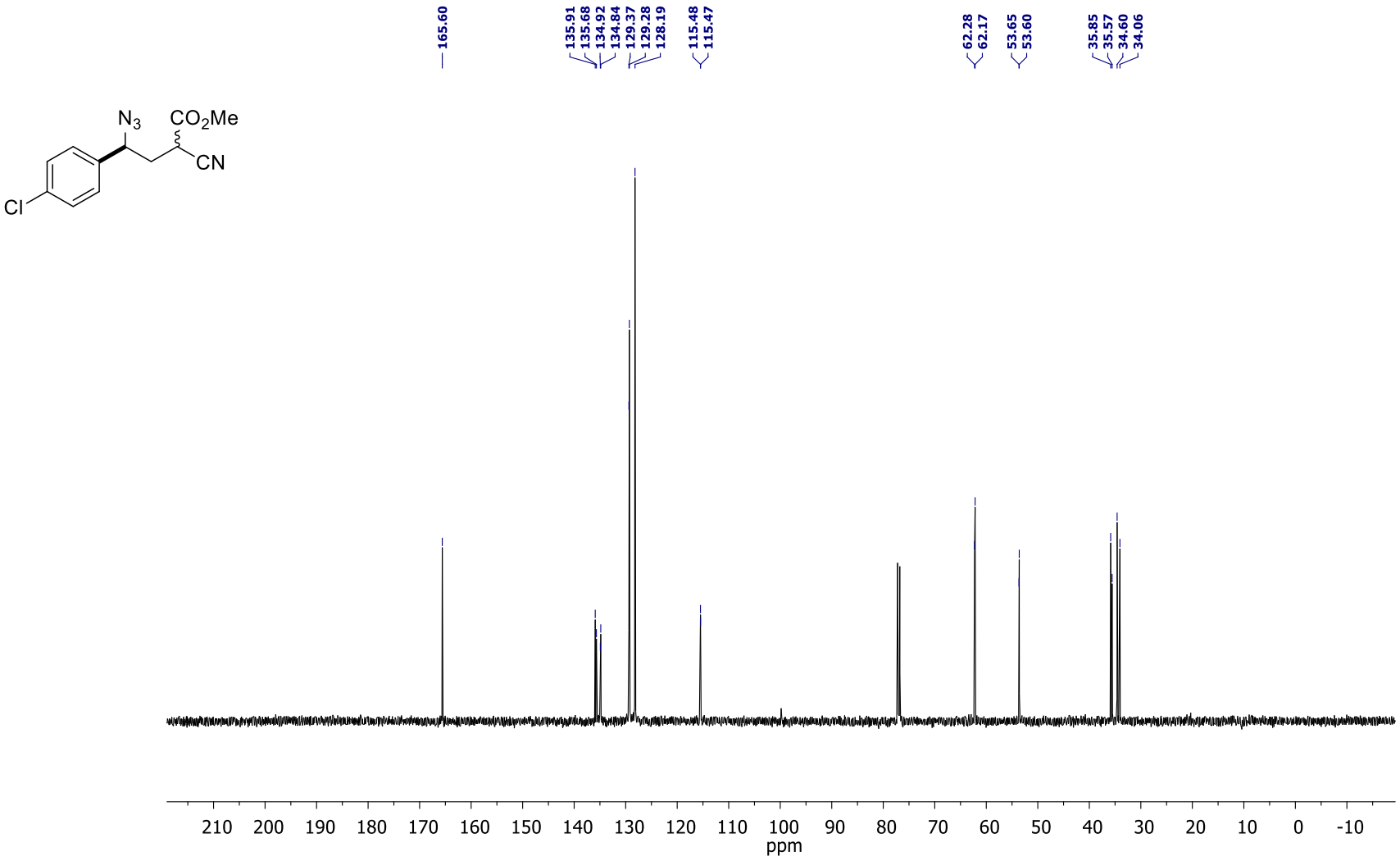
Methyl 4-azido-4-(4-chlorophenyl)-2-cyanobutyrate (1e)

^{1}H NMR ($CDCl_3$, 600 MHz)



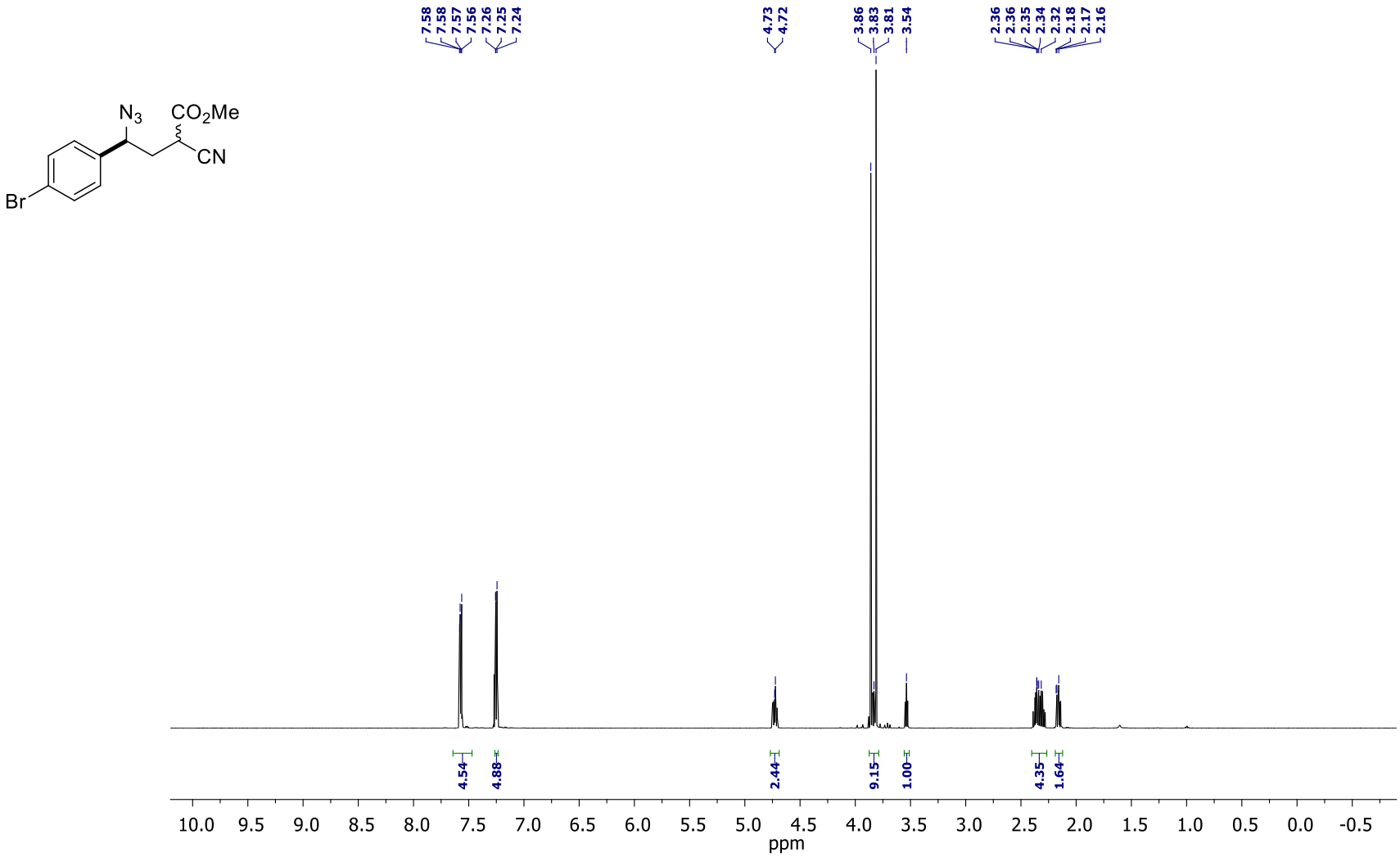
Methyl 4-azido-4-(4-chlorophenyl)-2-cyanobutyrate (1e)

^{13}C NMR ($CDCl_3$, 150 MHz)



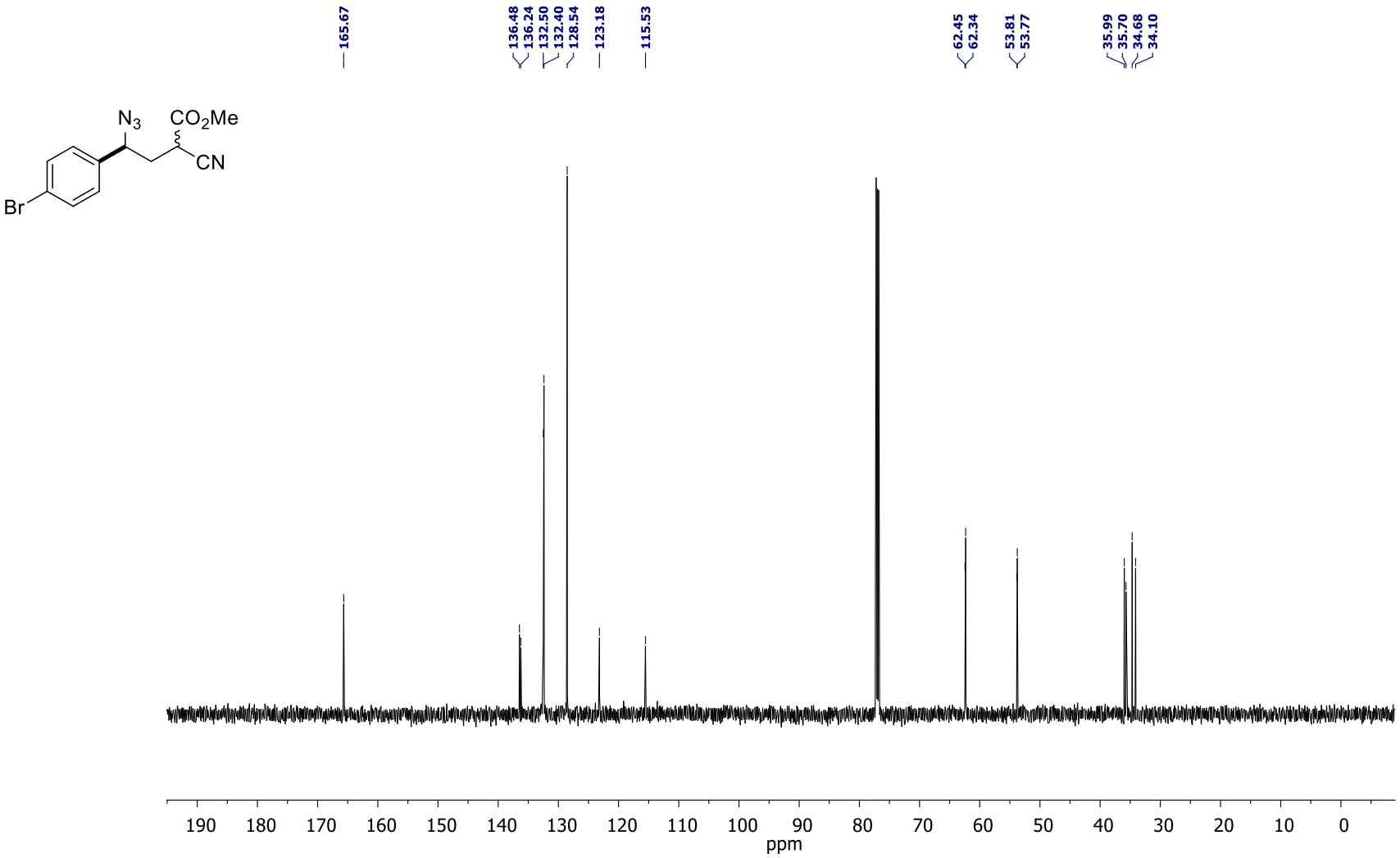
Methyl 4-azido-4-(4-bromophenyl)-2-cyanobutyrate (1f)

^{1}H NMR ($CDCl_3$, 600 MHz)



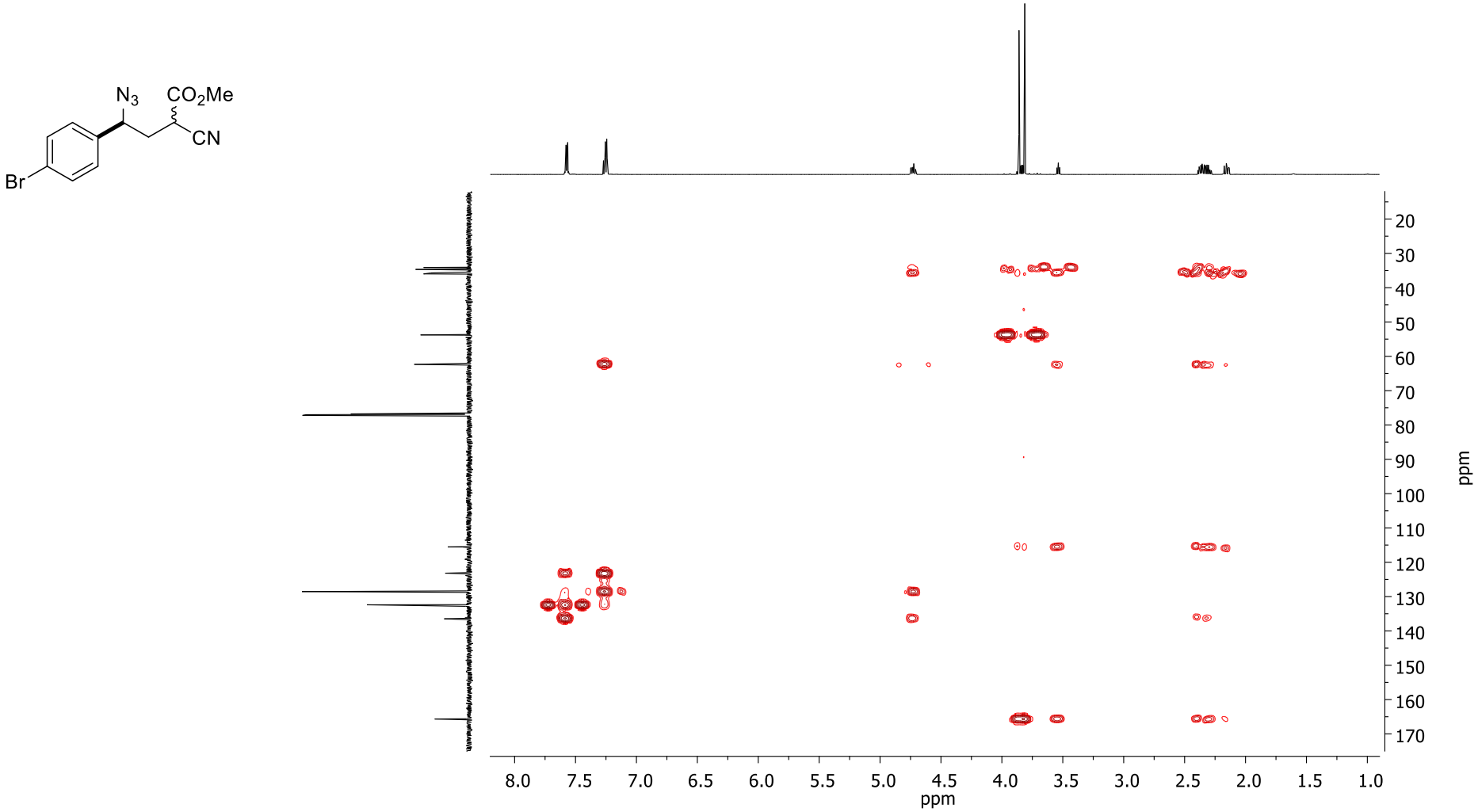
Methyl 4-azido-4-(4-bromophenyl)-2-cyanobutyrate (1f)

^{13}C NMR ($CDCl_3$, 150 MHz)



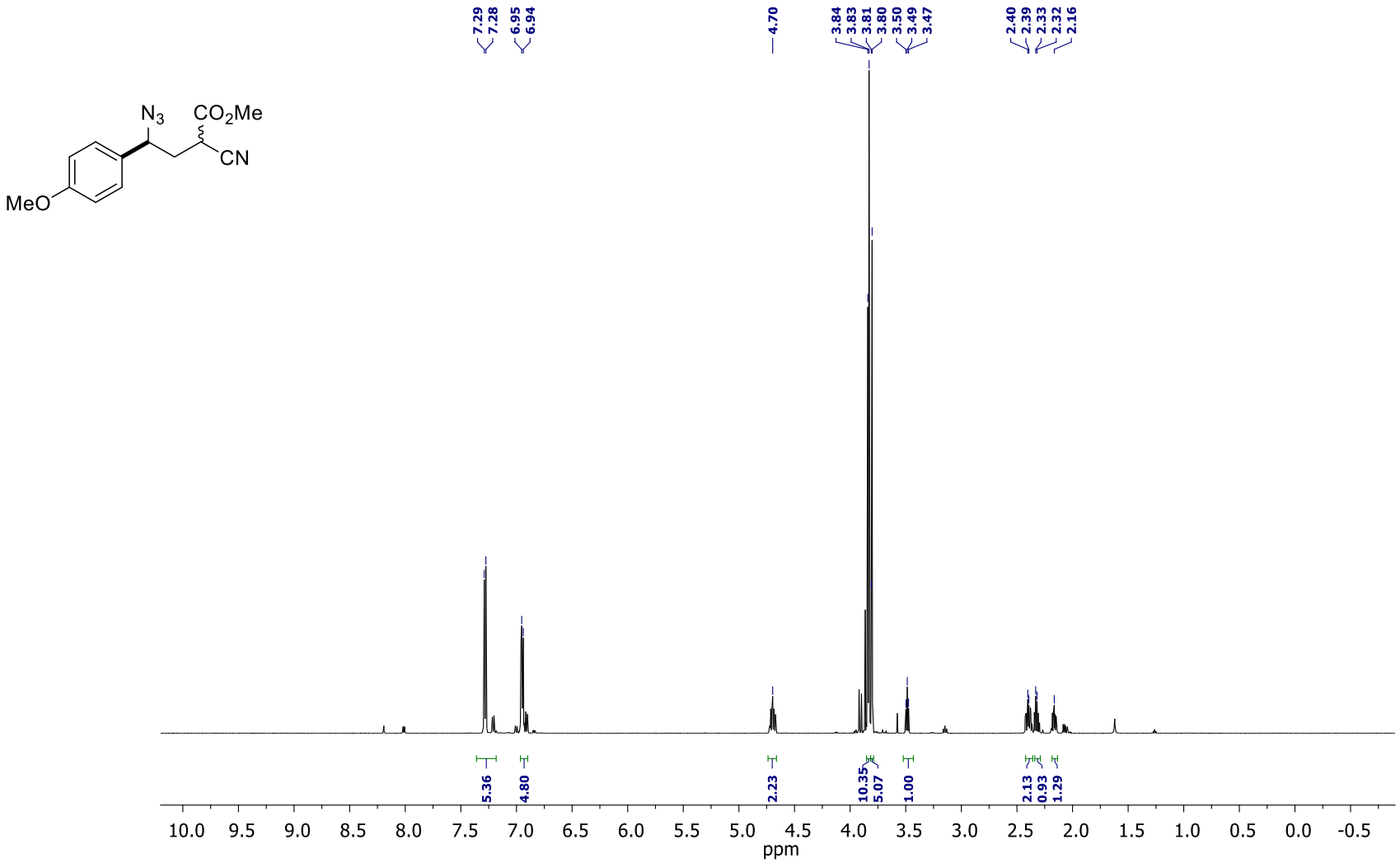
Methyl 4-azido-4-(4-bromophenyl)-2-cyanobutyrate (1f)

^{1}H-^{13}C HMBC ($CDCl_3$)



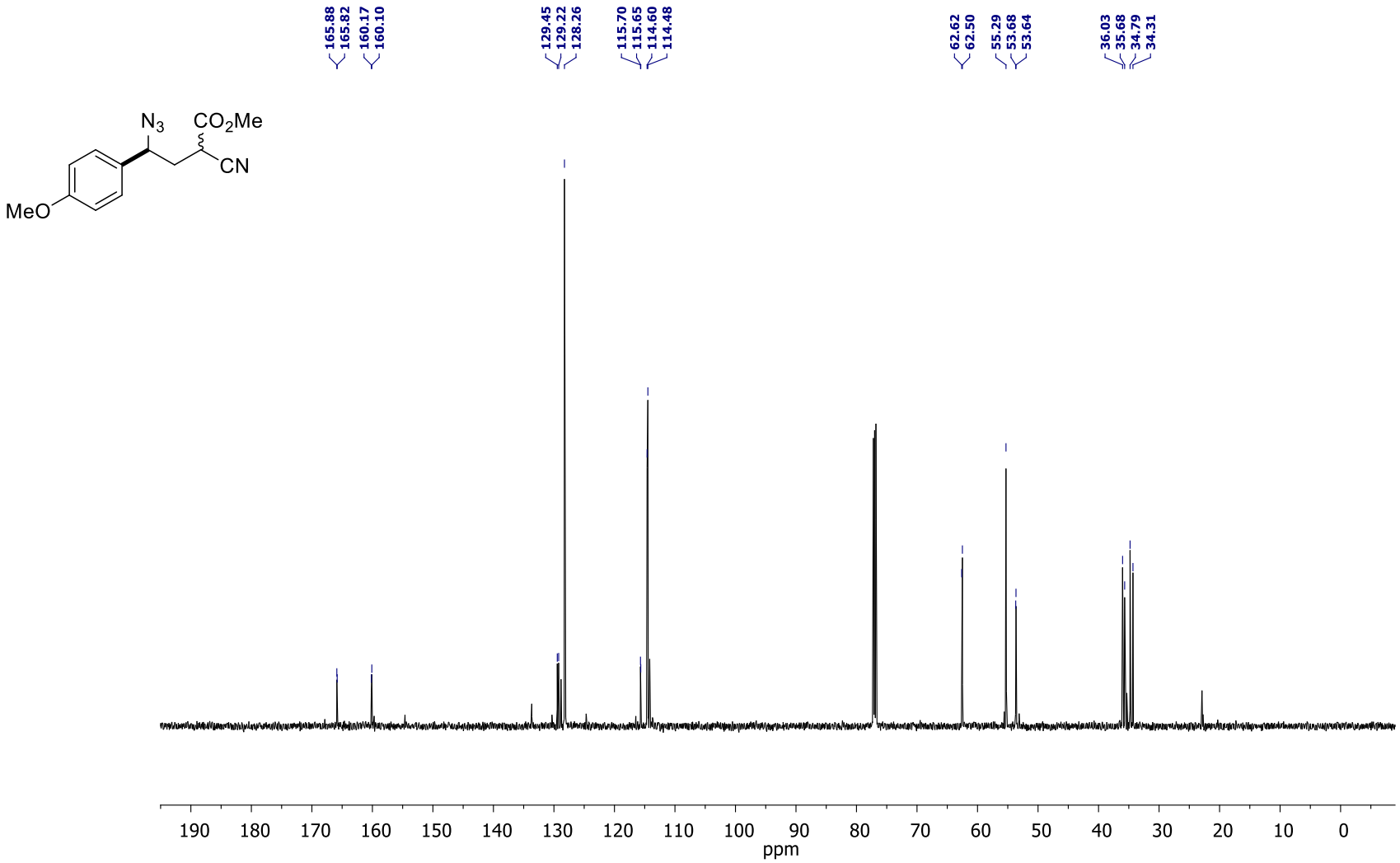
Methyl 4-azido-2-cyano-4-(4-methoxyphenyl)butyrate (1g)

^{1}H NMR (600 MHz, $CDCl_3$)



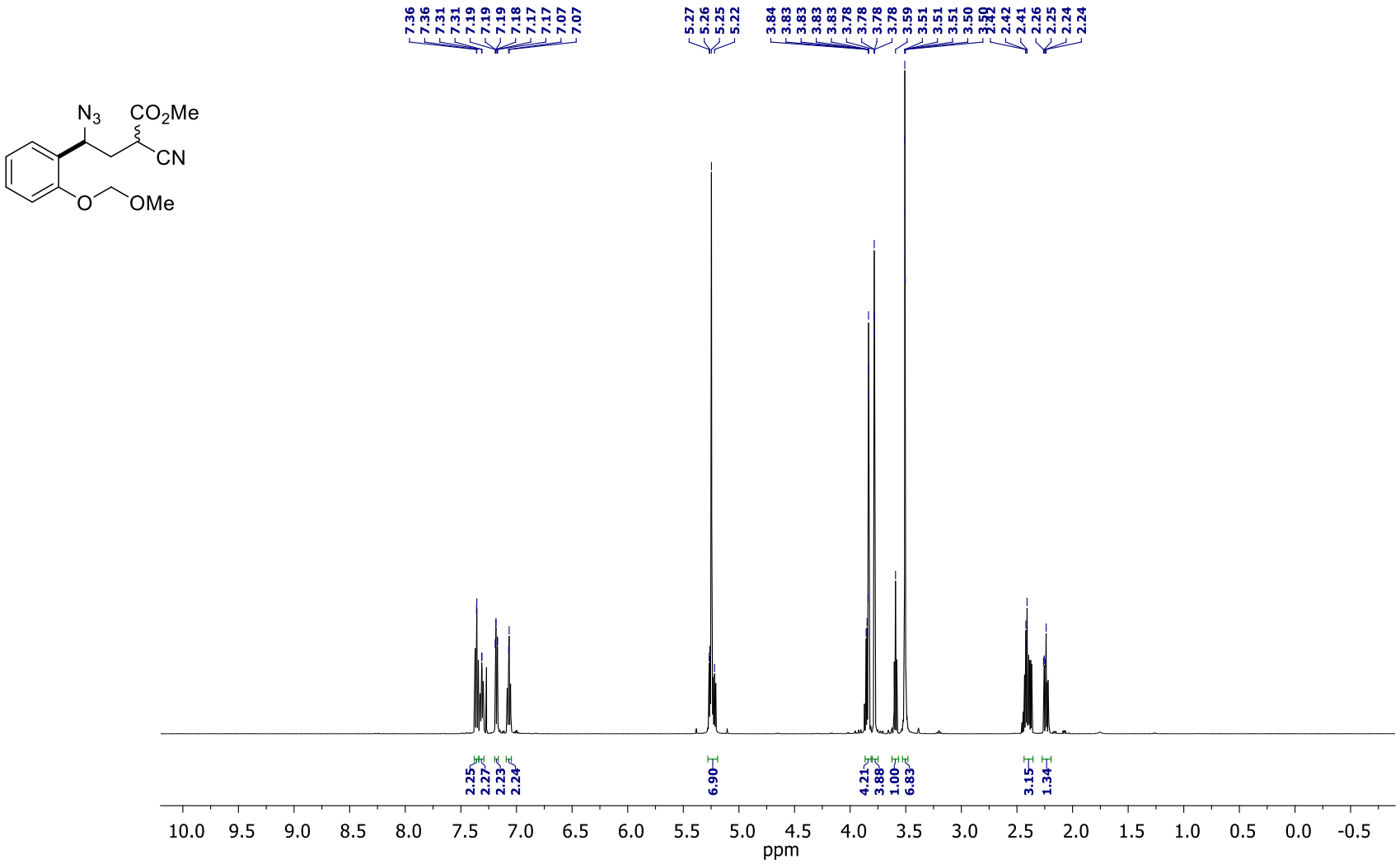
Methyl 4-azido-2-cyano-4-(4-methoxyphenyl)butyrate (1g)

^{13}C NMR (150 MHz, $CDCl_3$)



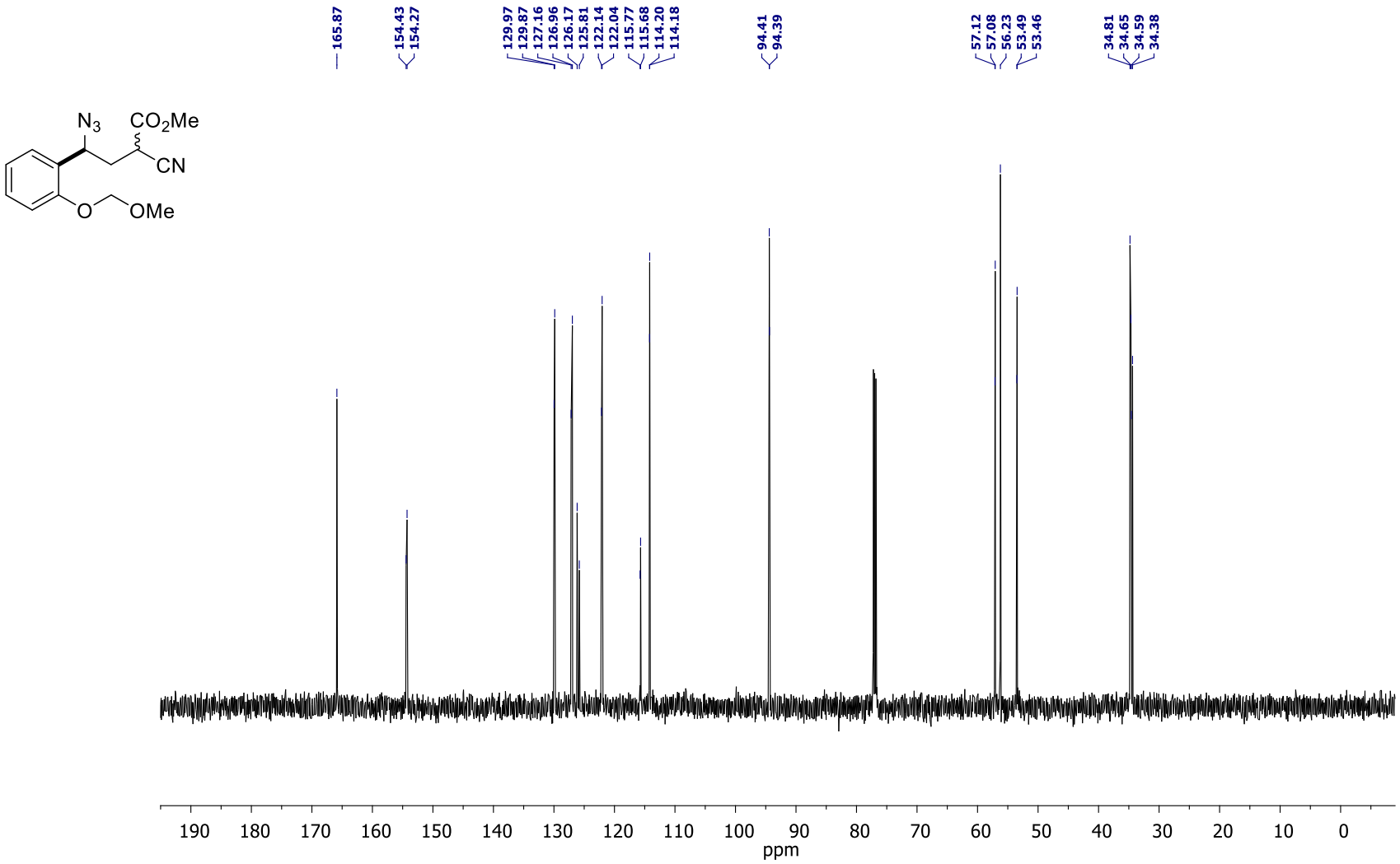
Methyl 4-azido-2-cyano-4-[2-(methoxymethoxy)phenyl]butyrate (1h)

^{1}H NMR (600 MHz, $CDCl_3$)



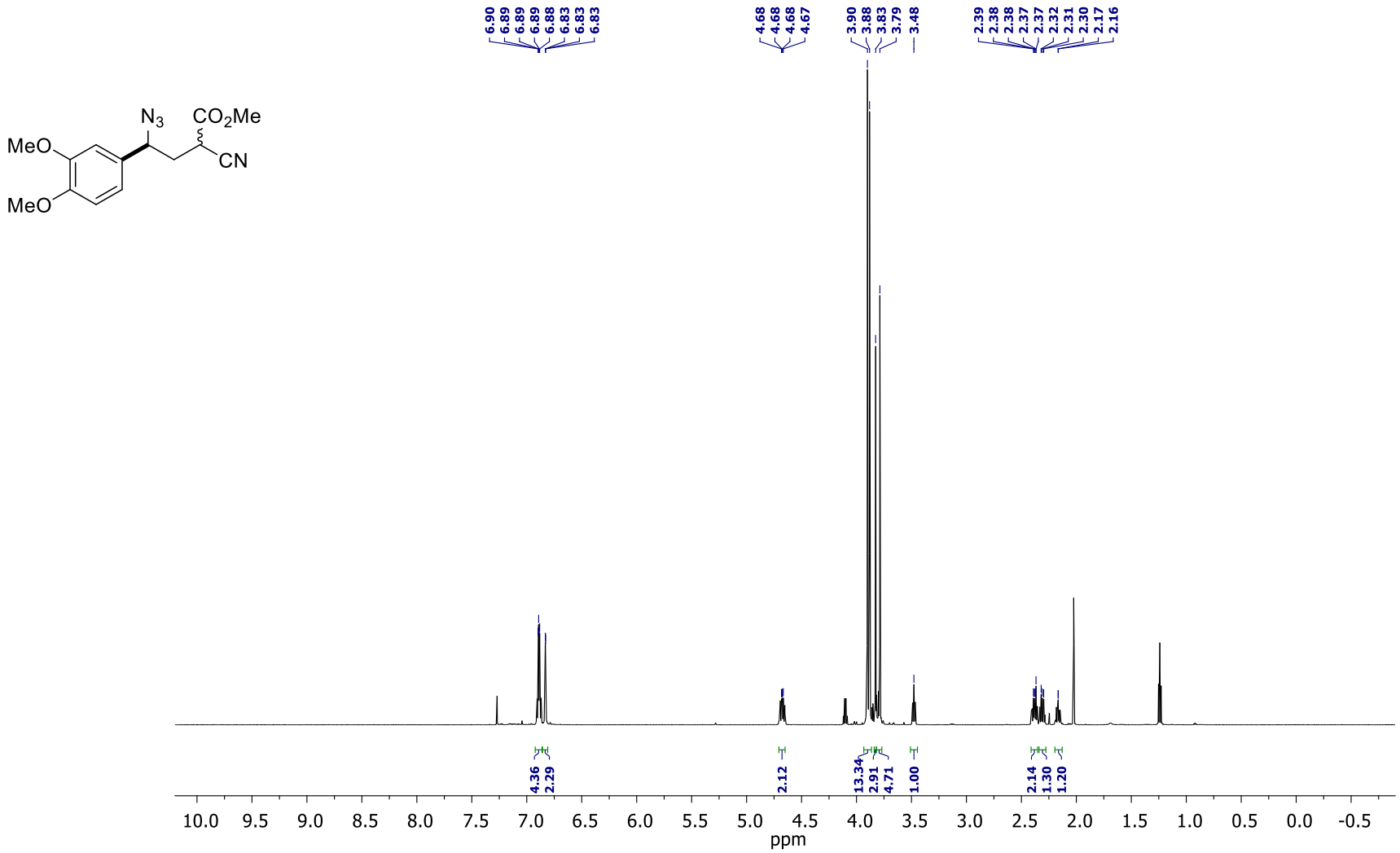
Methyl 4-azido-2-cyano-4-[2-(methoxymethoxy)phenyl]butyrate (1h)

^{13}C NMR (150 MHz, $CDCl_3$)



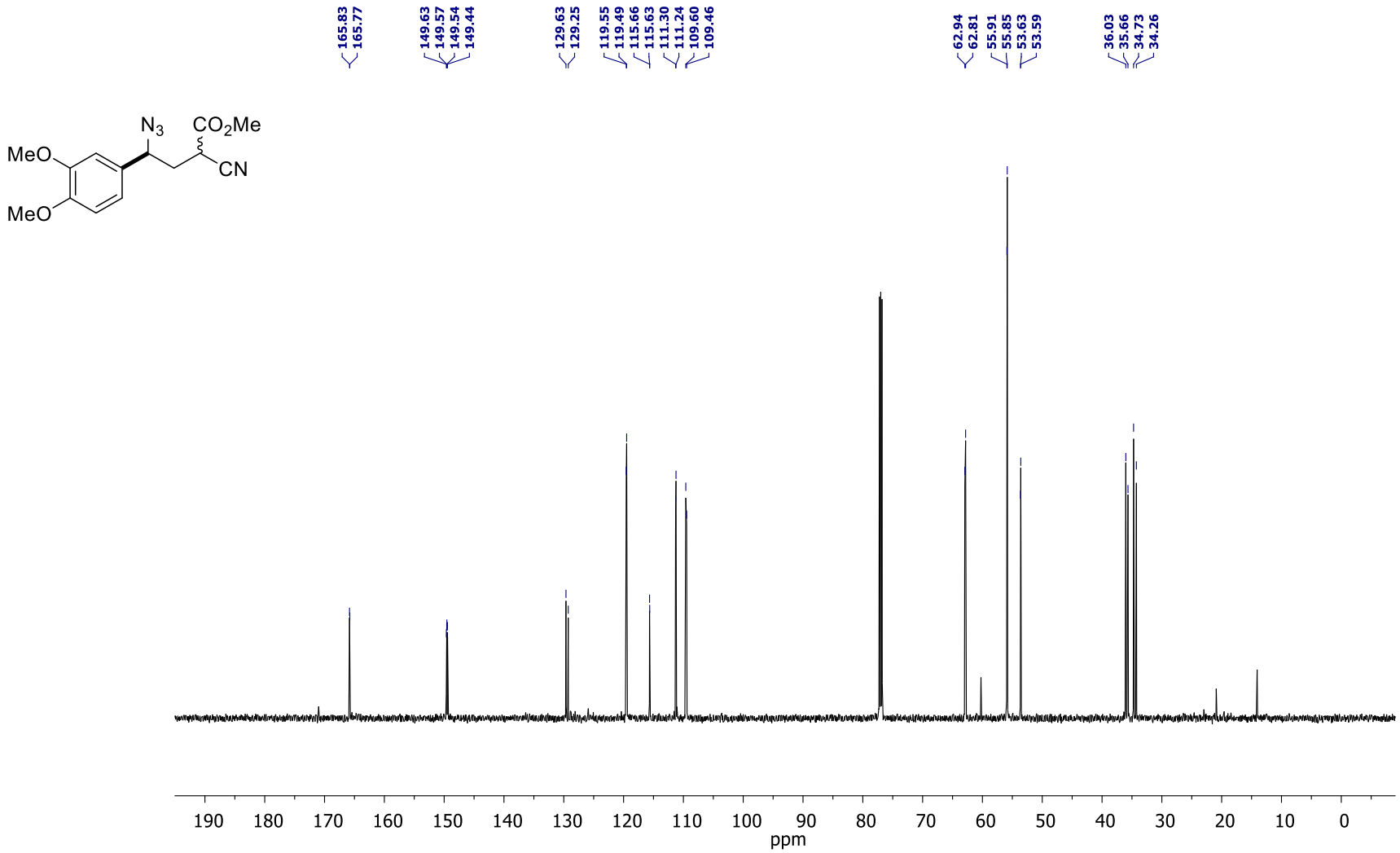
Methyl 4-azido-2-cyano-4-(3,4-dimethoxyphenyl)butyrate (1i)

^{1}H NMR (600 MHz, $CDCl_3$)



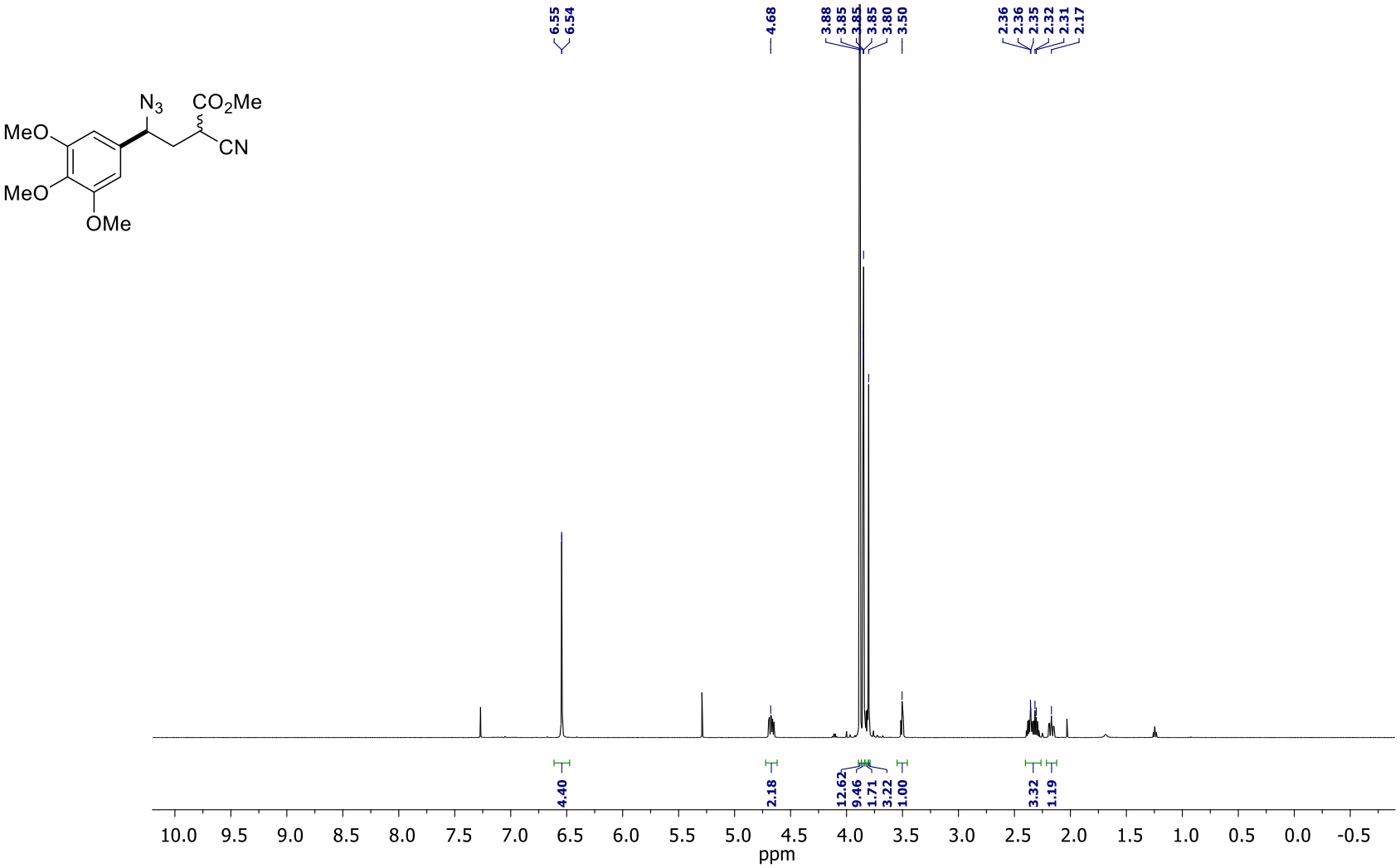
Methyl 4-azido-2-cyano-4-(3,4-dimethoxyphenyl)butyrate (1i)

^{13}C NMR (150 MHz, $CDCl_3$)



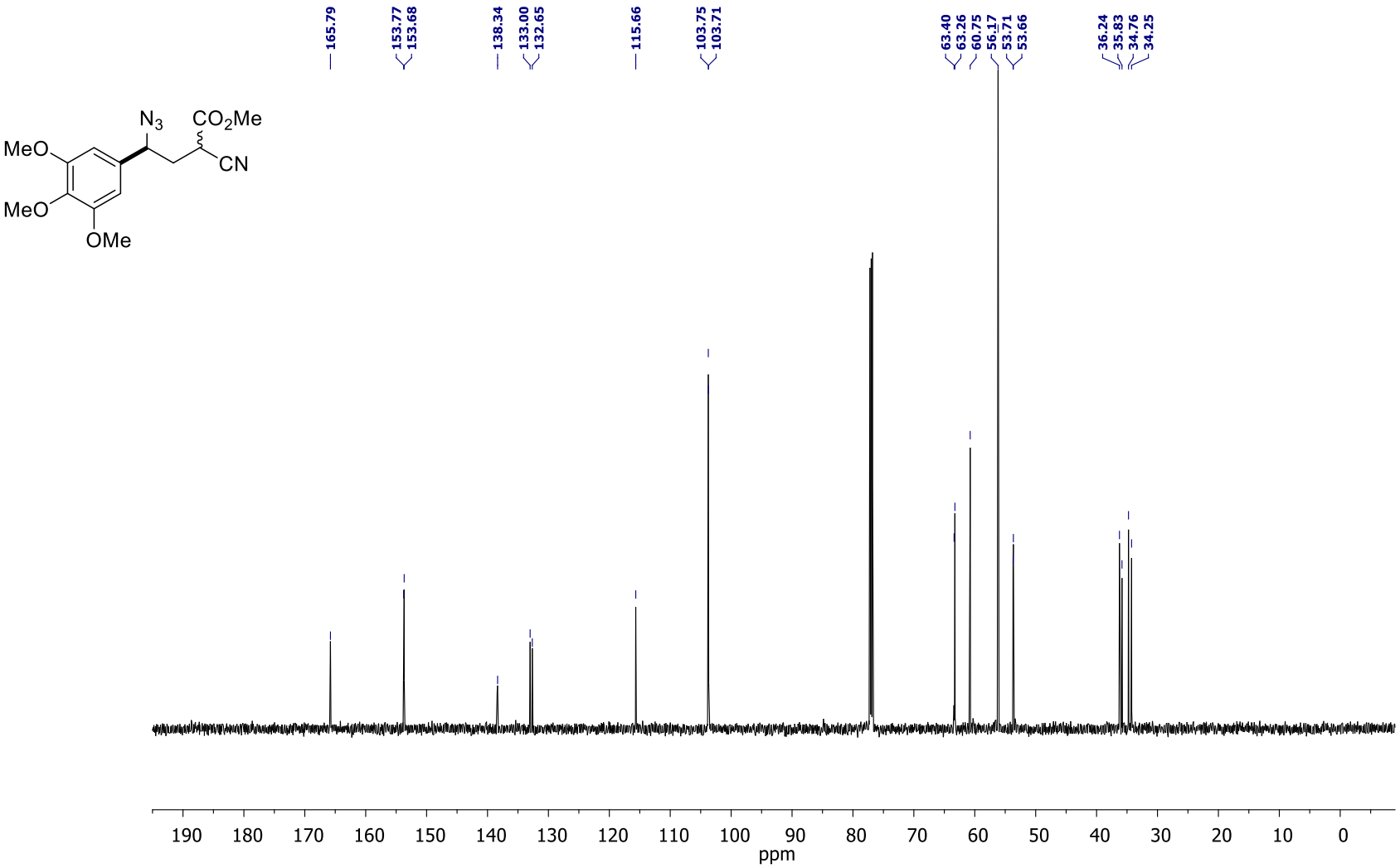
Methyl 4-azido-2-cyano-4-(3,4,5-trimethoxyphenyl)butyrate (1j)

^{1}H NMR (600 MHz, $CDCl_3$)



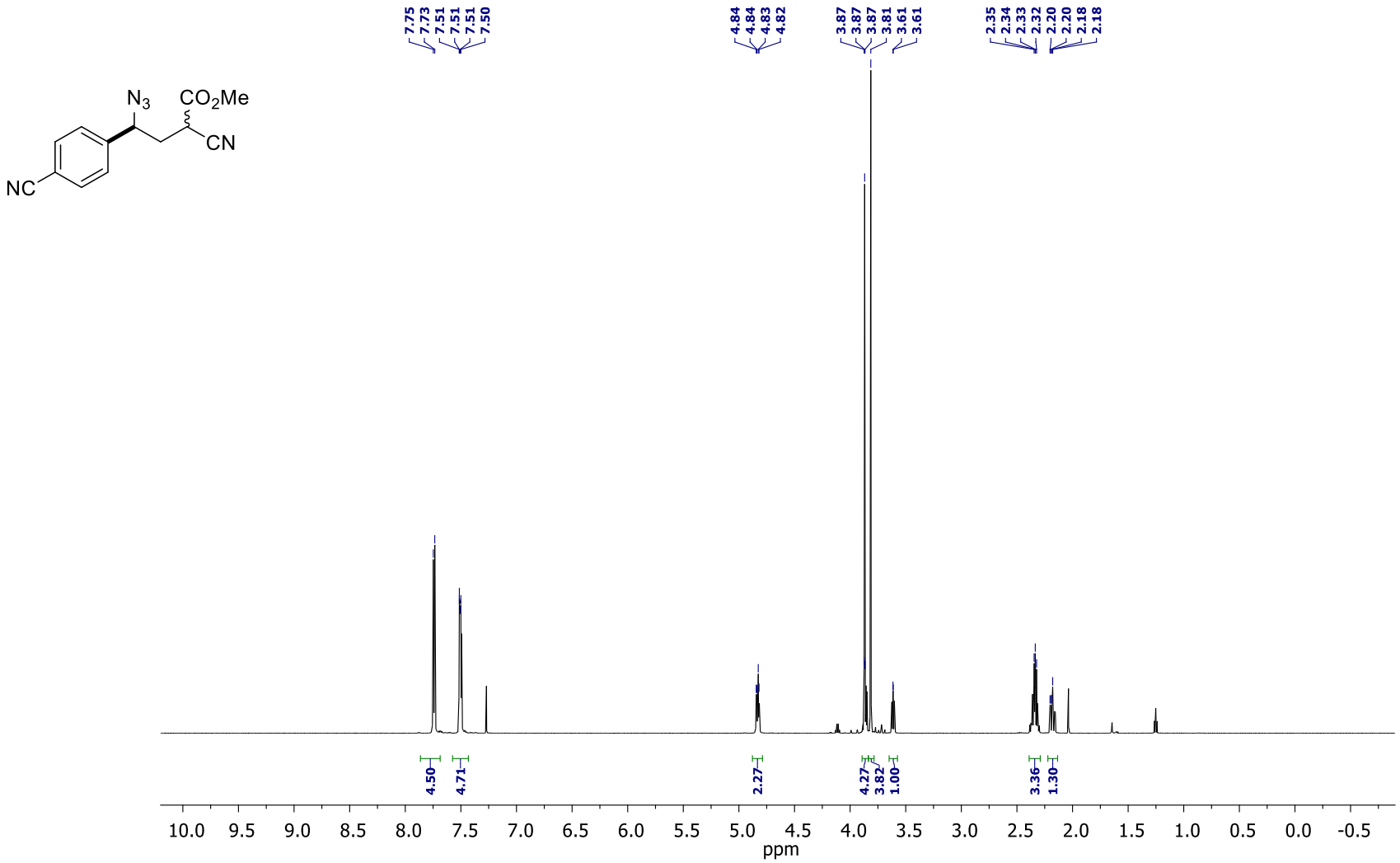
Methyl 4-azido-2-cyano-4-(3,4,5-trimethoxyphenyl)butyrate (1j)

^{13}C NMR (150 MHz, $CDCl_3$)



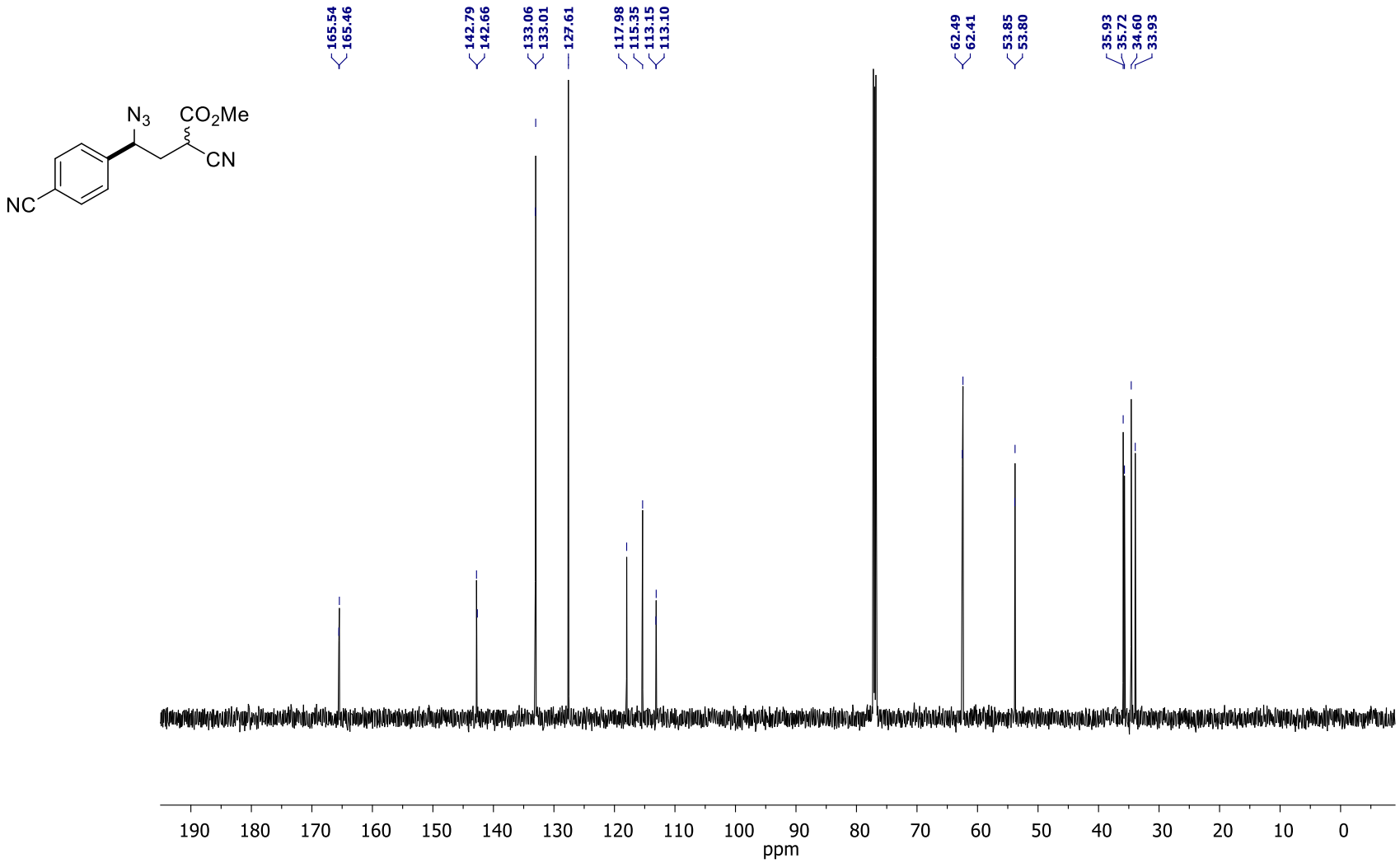
Methyl 4-azido-2-cyano-4-(4-cyanophenyl)butyrate (1k)

^{1}H NMR (600 MHz, $CDCl_3$)



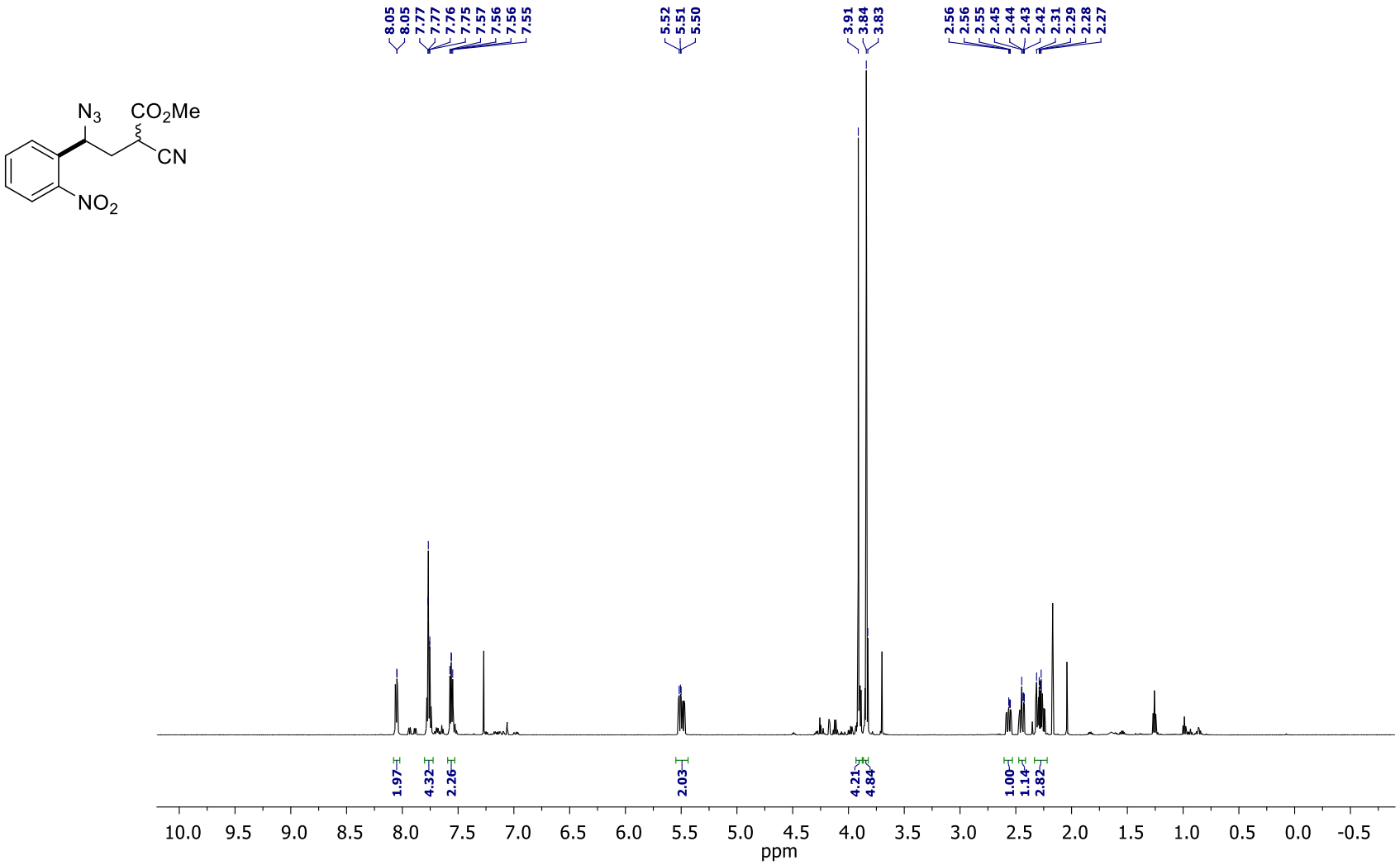
Methyl 4-azido-2-cyano-4-(4-cyanophenyl)butyrate (1k)

^{13}C NMR (150 MHz, $CDCl_3$)



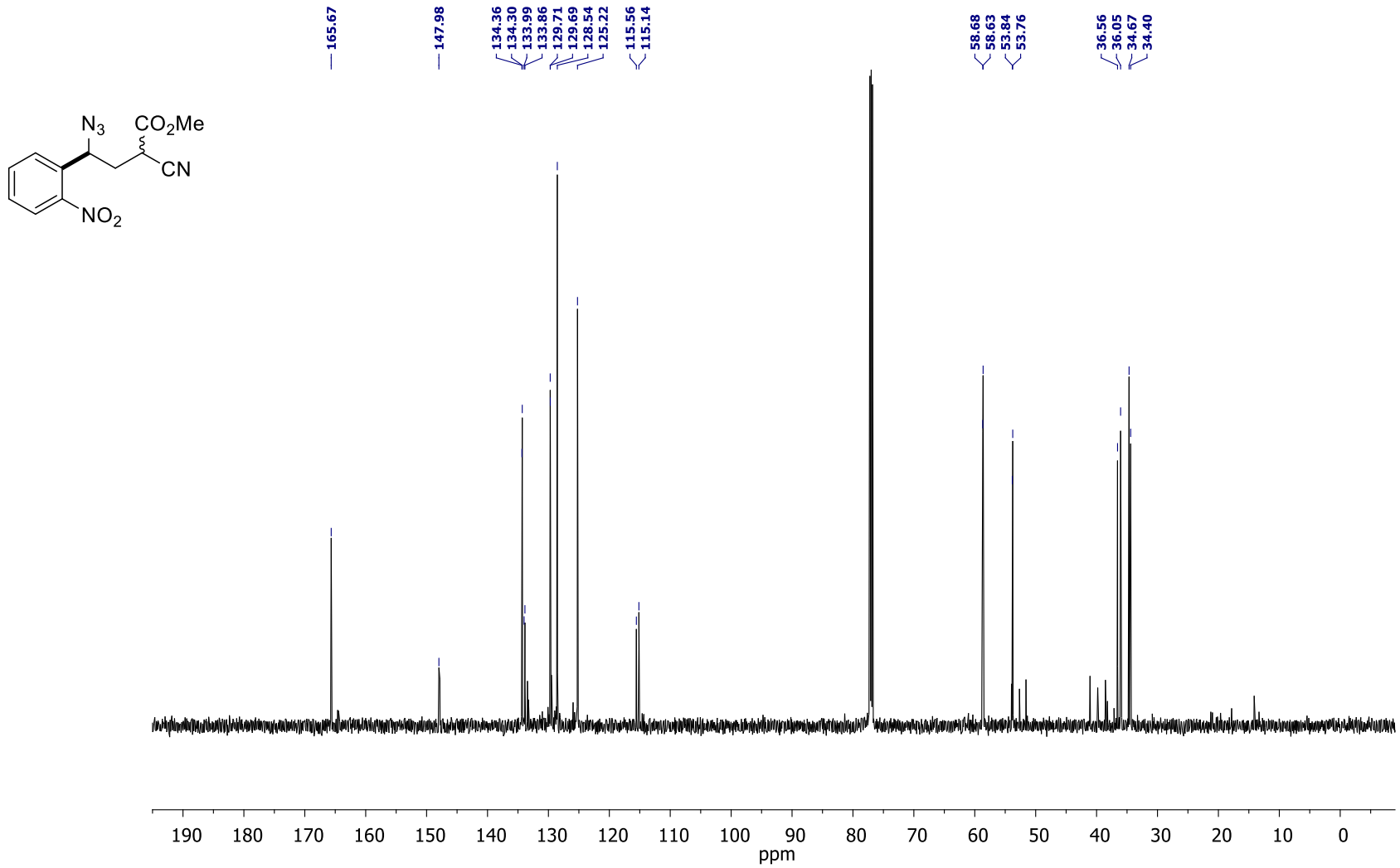
Methyl 4-azido-2-cyano-4-(2-nitrophenyl)butyrate (1l)

^{1}H NMR (600 MHz, $CDCl_3$)



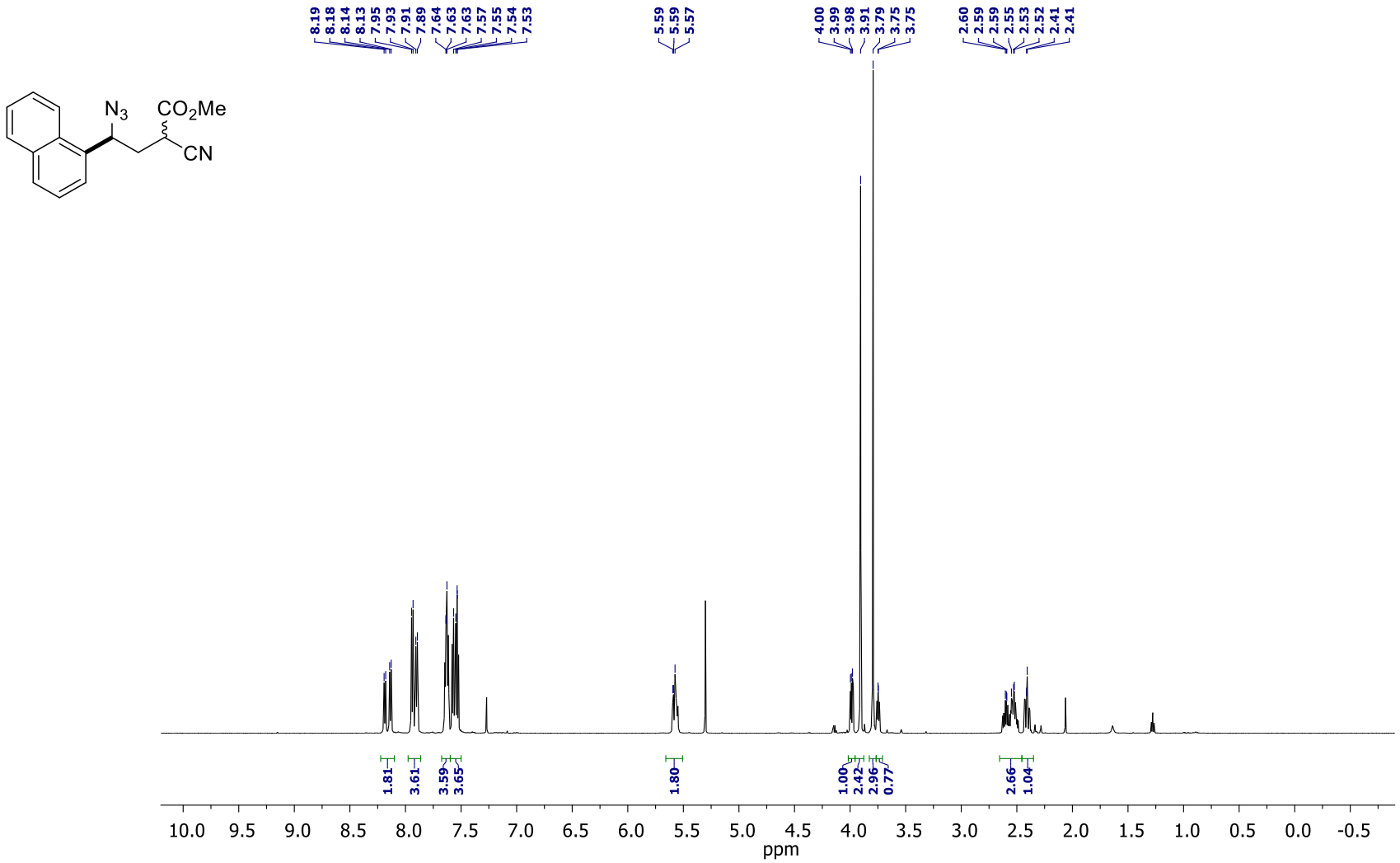
Methyl 4-azido-2-cyano-4-(2-nitrophenyl)butyrate (1l)

^{13}C NMR (150 MHz, $CDCl_3$)



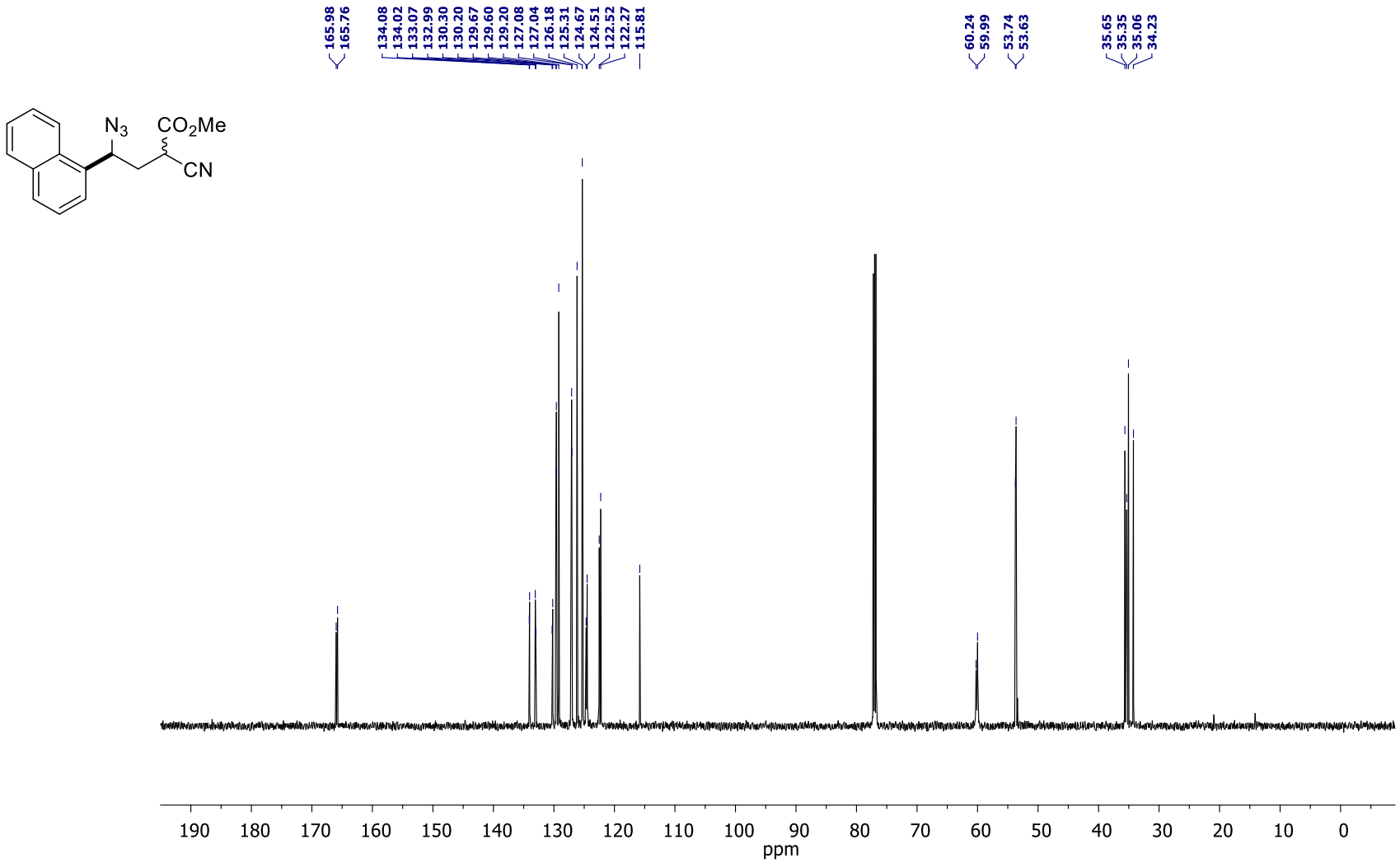
Methyl 4-azido-2-cyano-4-(naphthen-1-yl)butyrate (1m)

^{1}H NMR (600 MHz, $CDCl_3$)



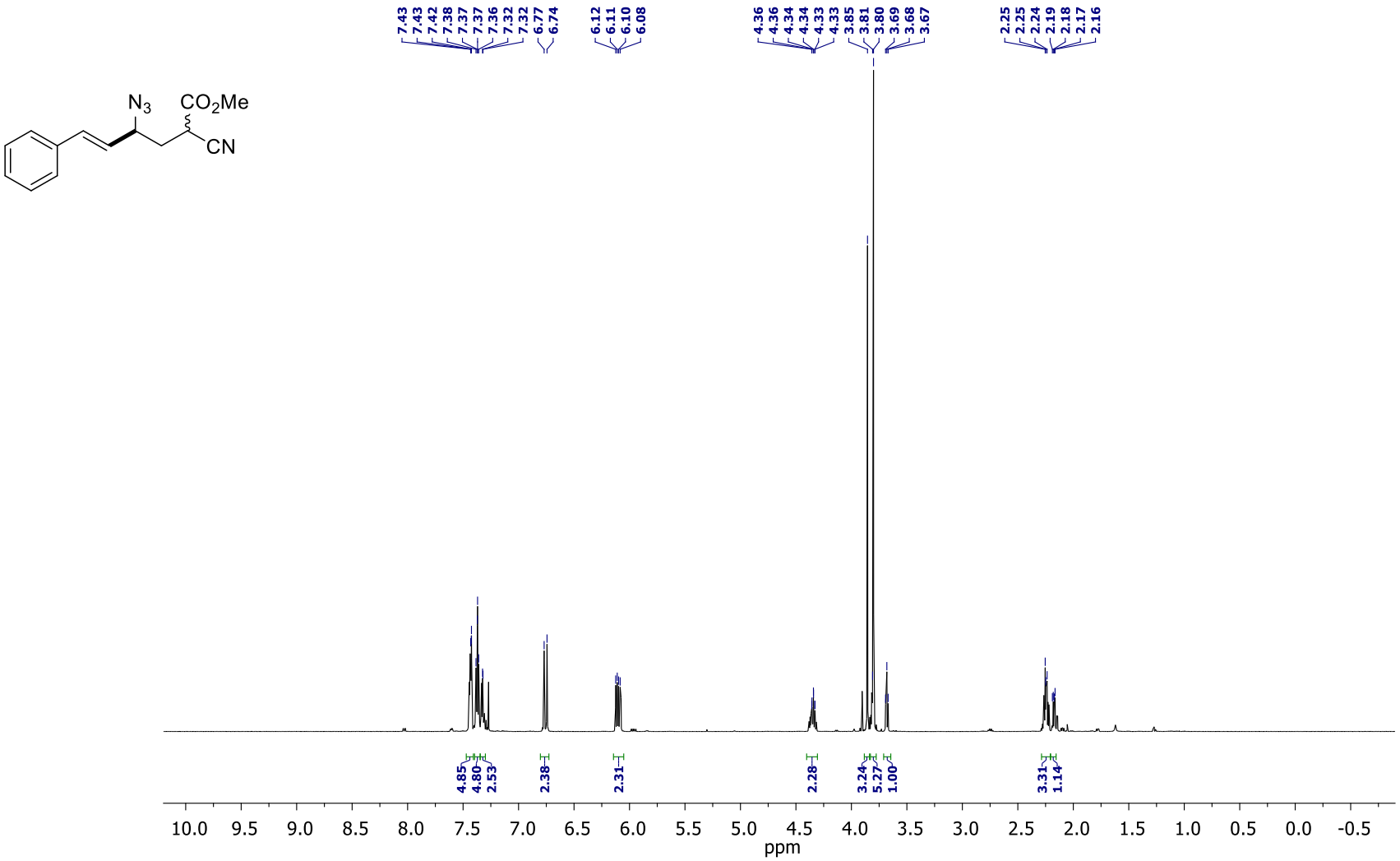
Methyl 4-azido-2-cyano-4-(naphthen-1-yl)butyrate (1m)

^{13}C NMR (150 MHz, $CDCl_3$)



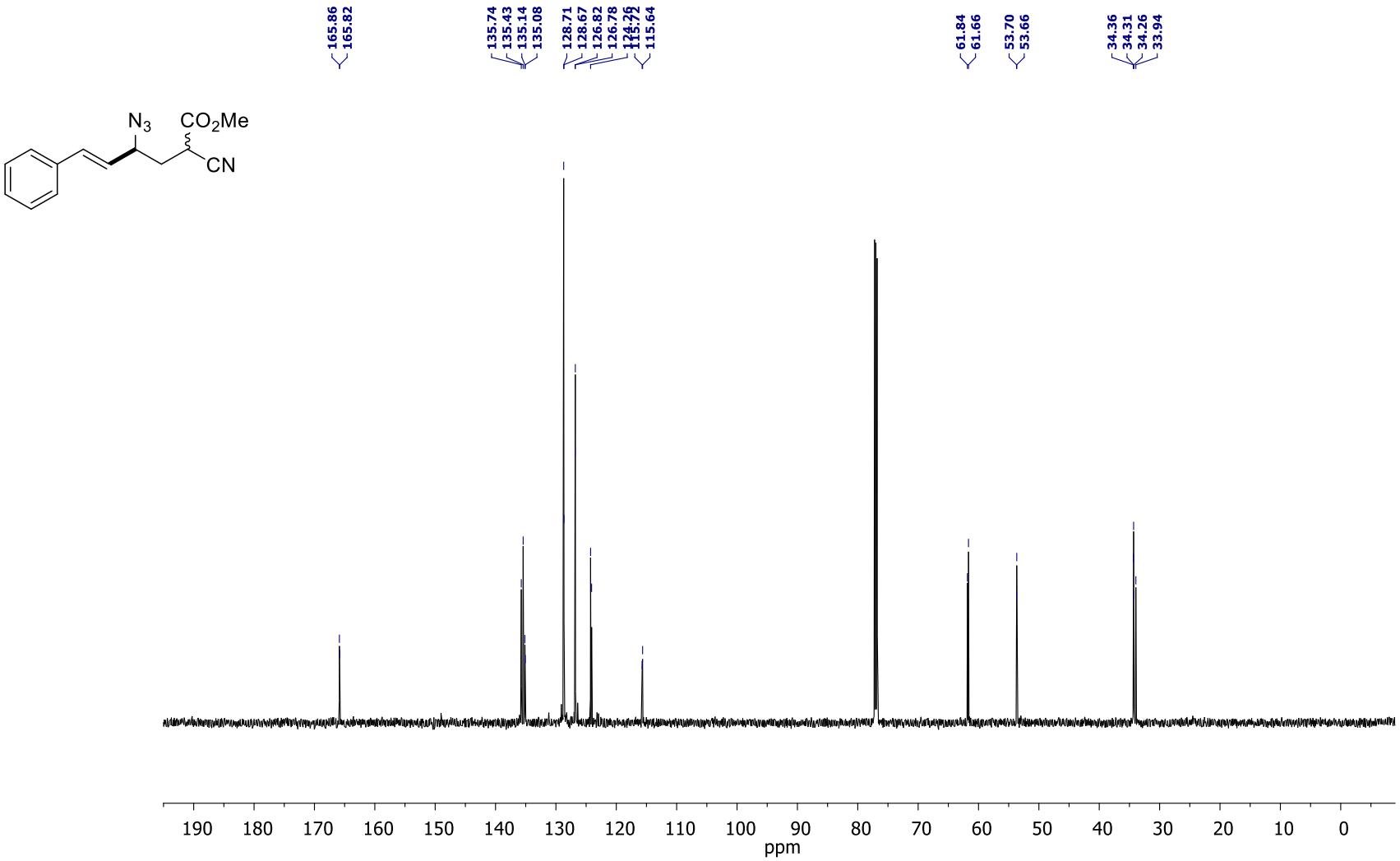
Methyl (*E*)-4-azido-2-cyano-6-phenylhex-5-enoate (1n)

^{1}H NMR (600 MHz, $CDCl_3$)



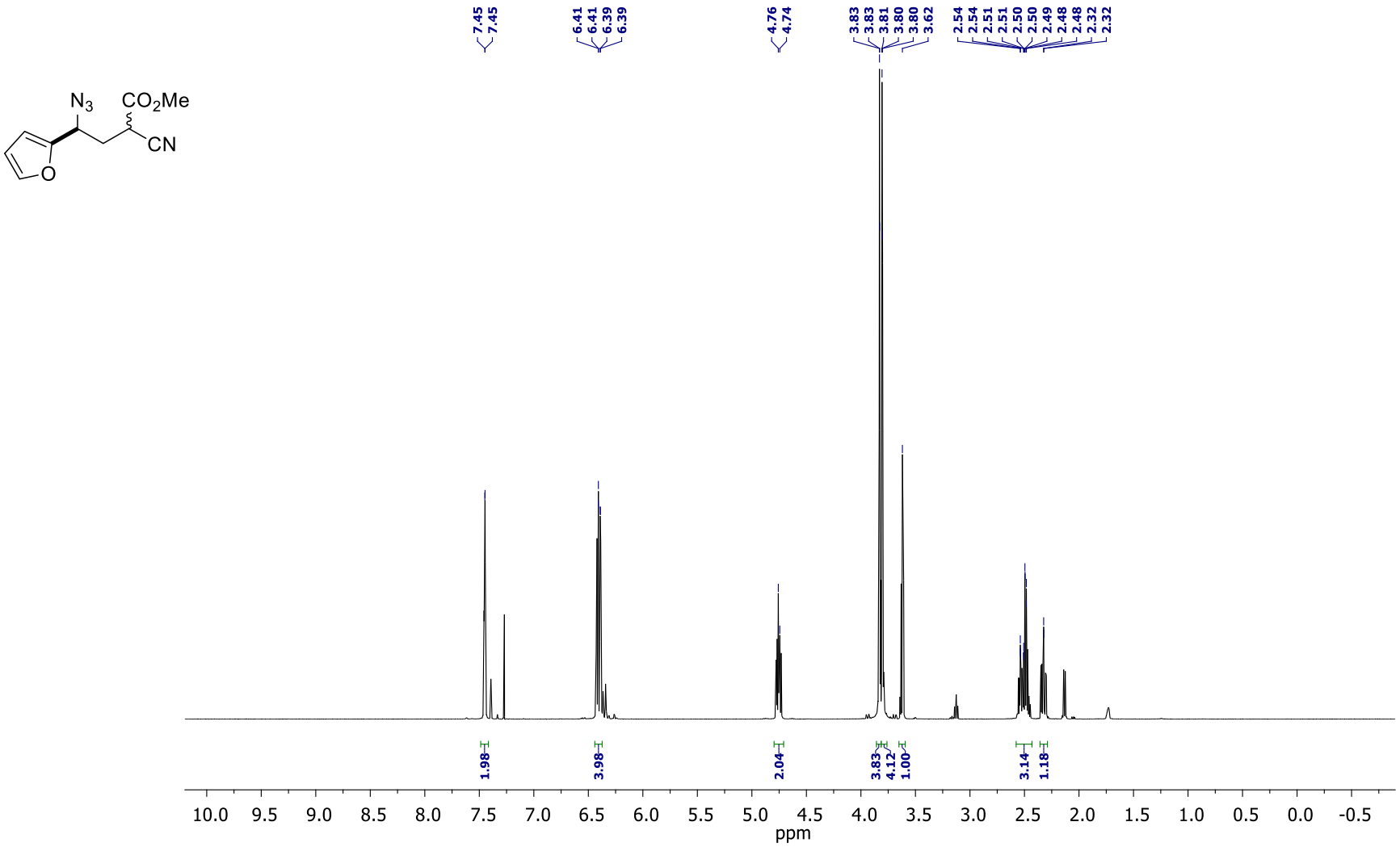
Methyl (*E*)-4-azido-2-cyano-6-phenylhex-5-enoate (1n)

^{13}C NMR (150 MHz, $CDCl_3$)



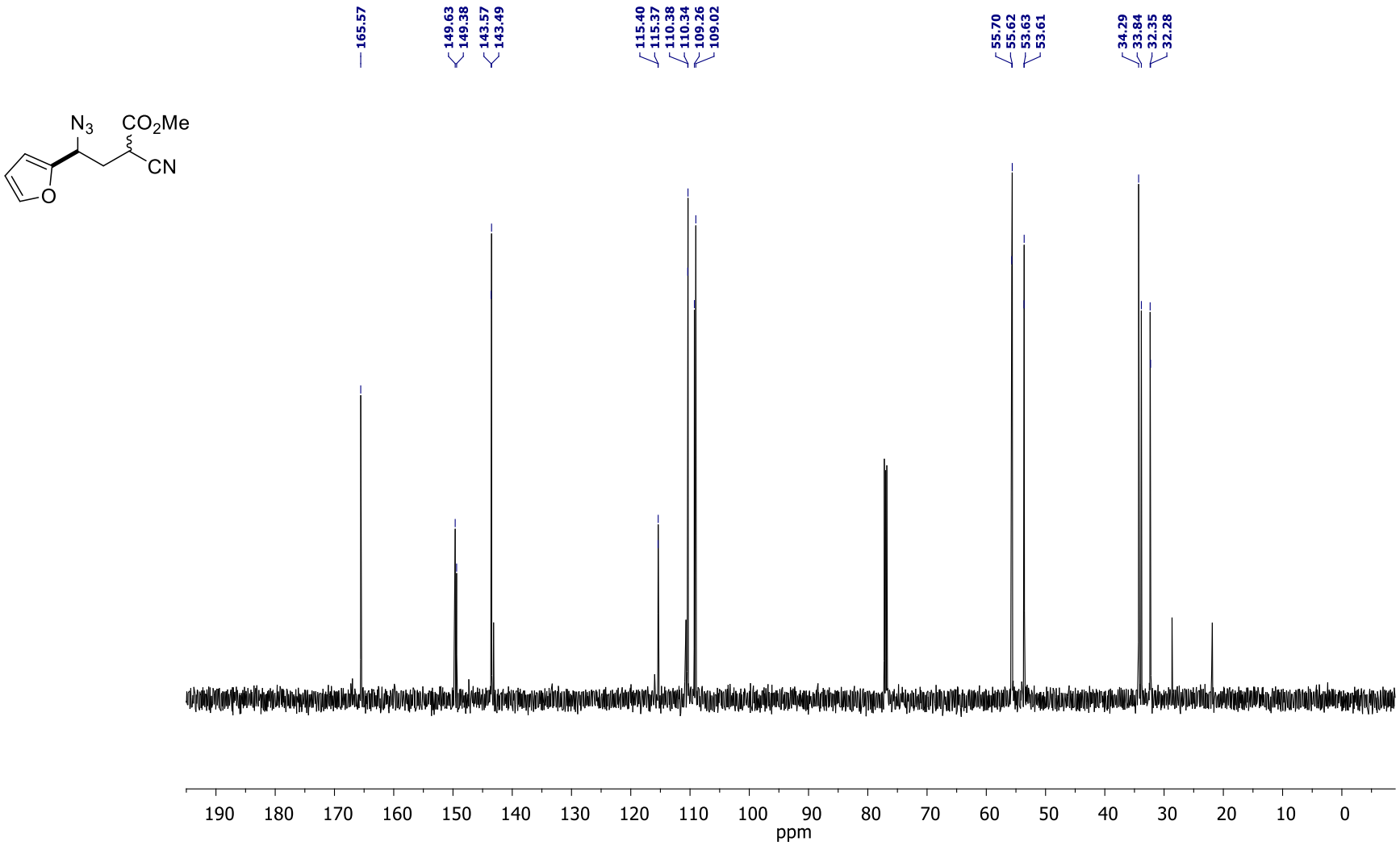
Methyl 4-azido-2-cyano-4-(furanyl-2-yl)butyrate (1o)

^{1}H NMR (600 MHz, $CDCl_3$)



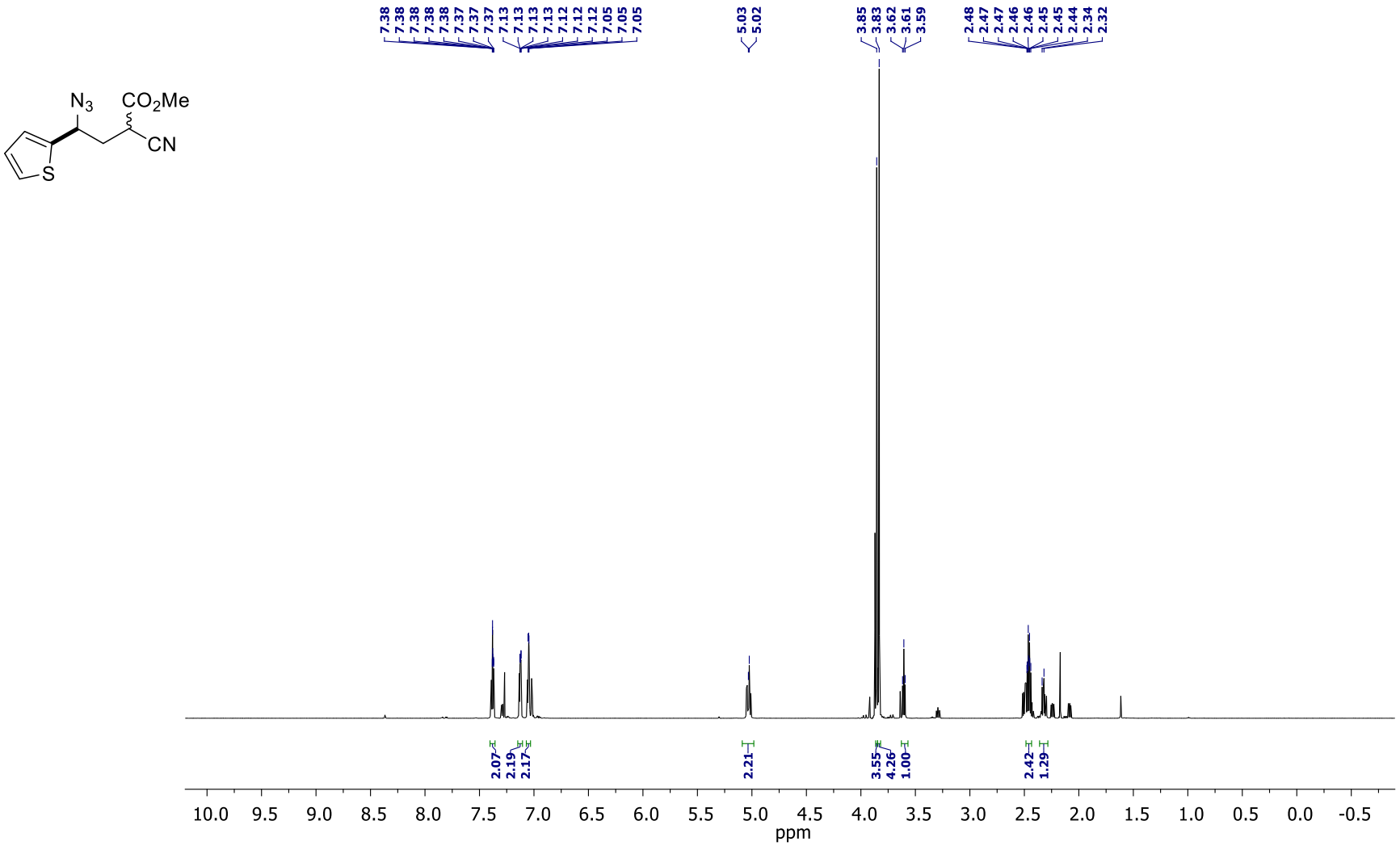
Methyl 4-azido-2-cyano-4-(furanyl-2-yl)butyrate (1o)

^{13}C NMR (150 MHz, $CDCl_3$)



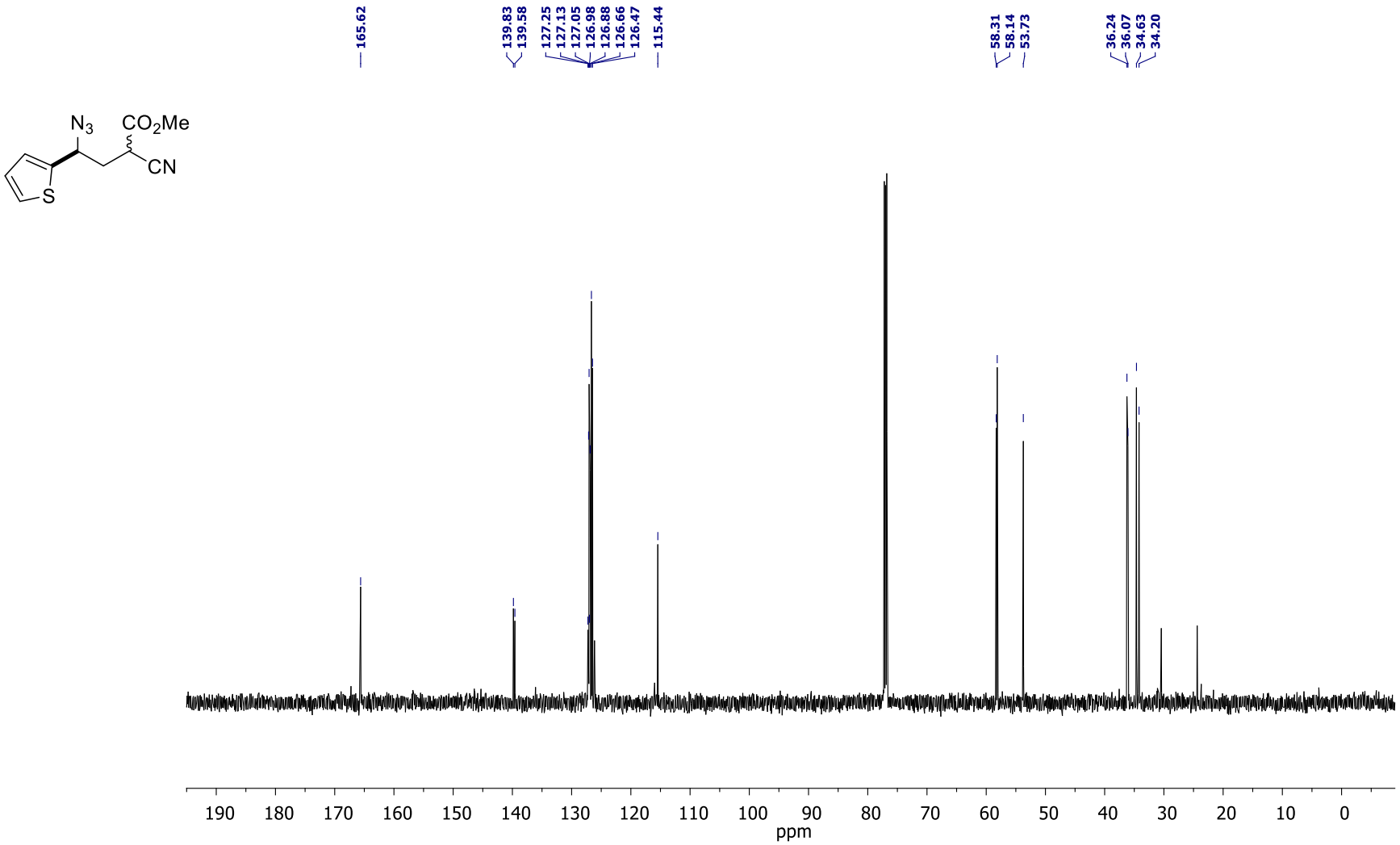
Methyl 4-azido-2-cyano-4-(thien-2-yl)butyrate (1p)

^{1}H NMR (600 MHz, $CDCl_3$)



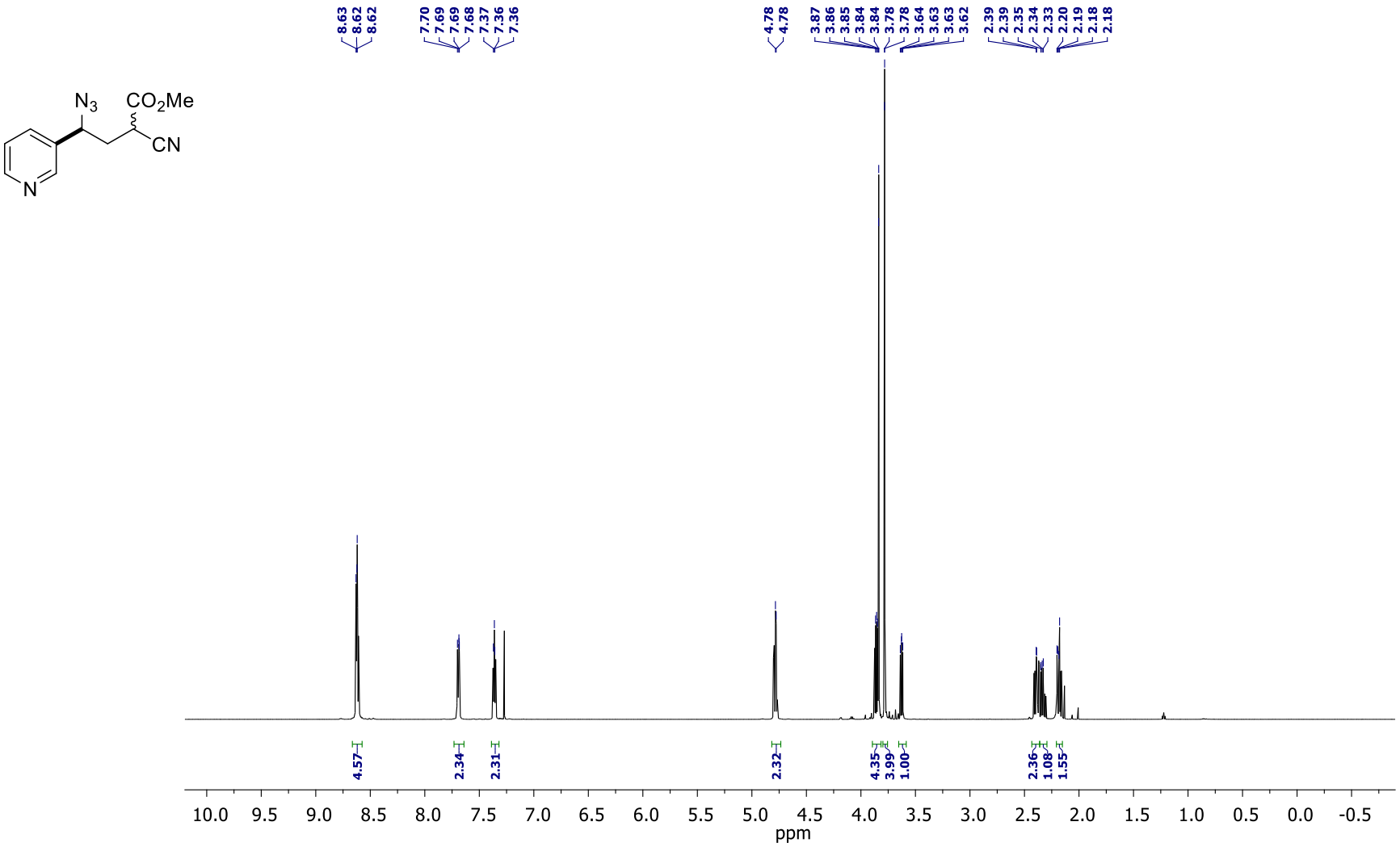
Methyl 4-azido-2-cyano-4-(thien-2-yl)butyrate (1p)

^{13}C NMR (150 MHz, $CDCl_3$)



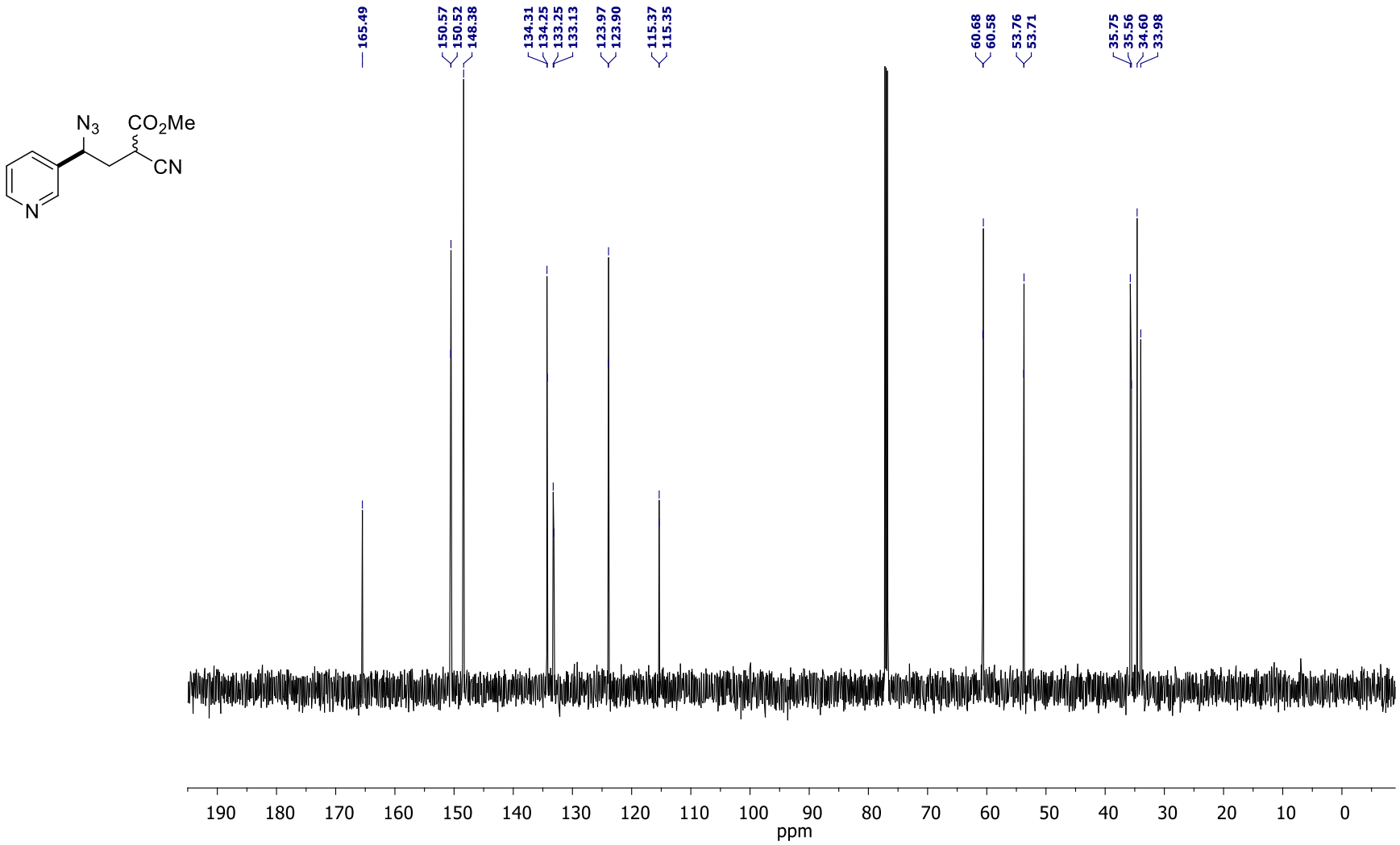
Methyl 4-azido-2-cyano-4-(pyridin-3-yl)butyrate (1q)

^{1}H NMR (600 MHz, $CDCl_3$)



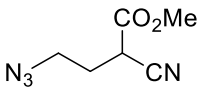
Methyl 4-azido-2-cyano-4-(pyridin-3-yl)butyrate (1q)

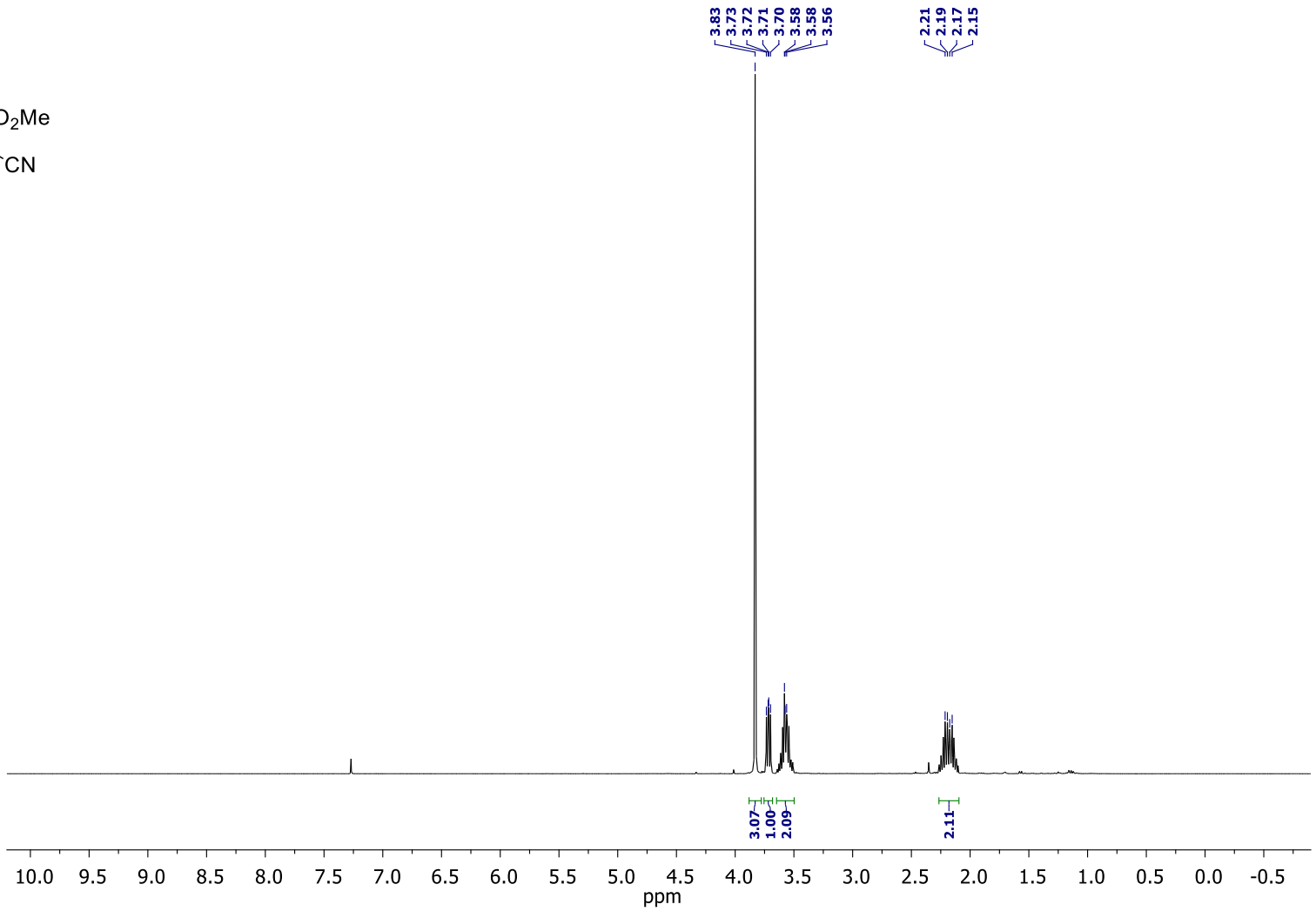
^{13}C NMR (150 MHz, $CDCl_3$)



Methyl 4-azido-2-cyanobutyrate (1r)

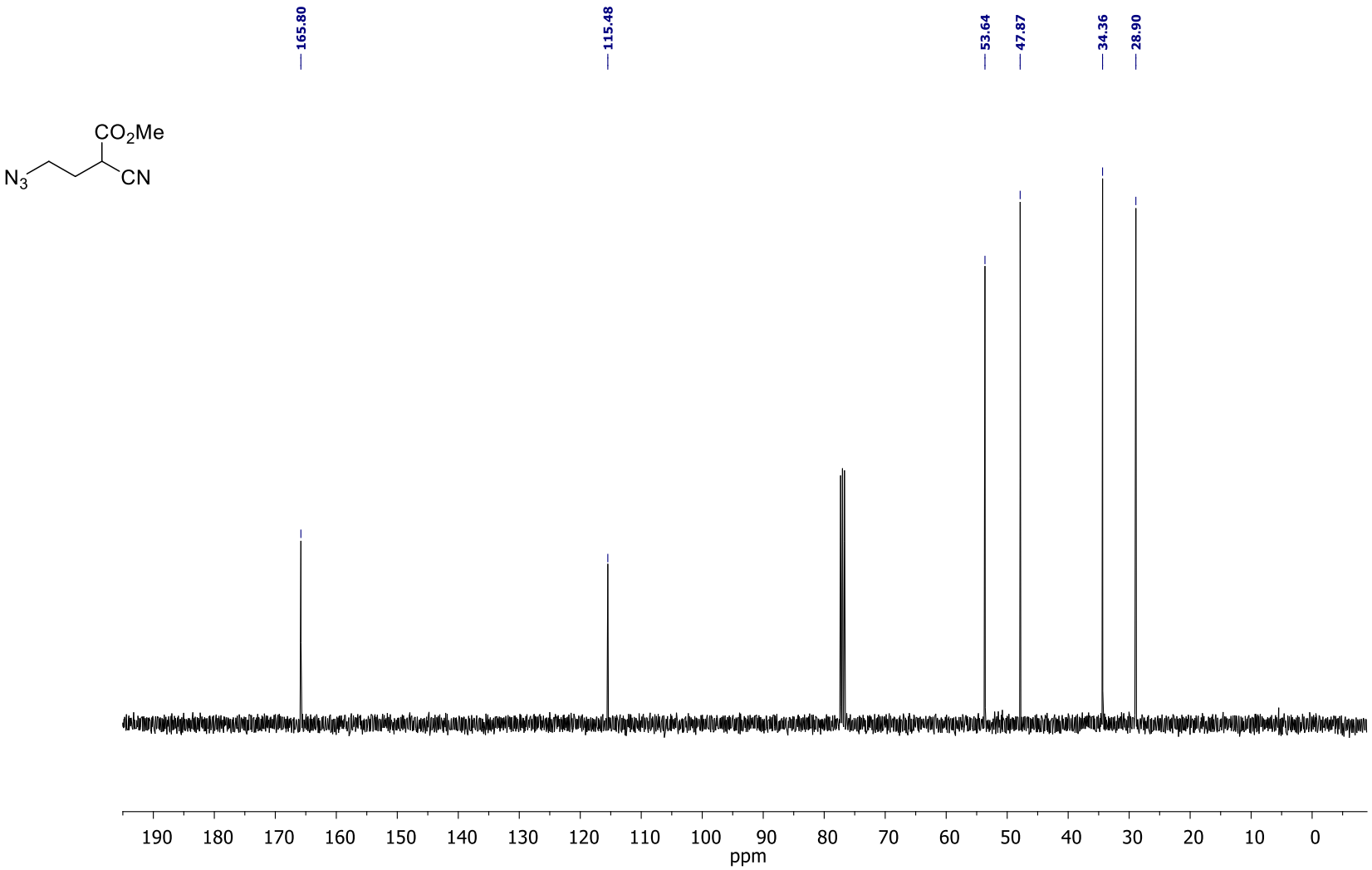
^{1}H NMR (600 MHz, $CDCl_3$)





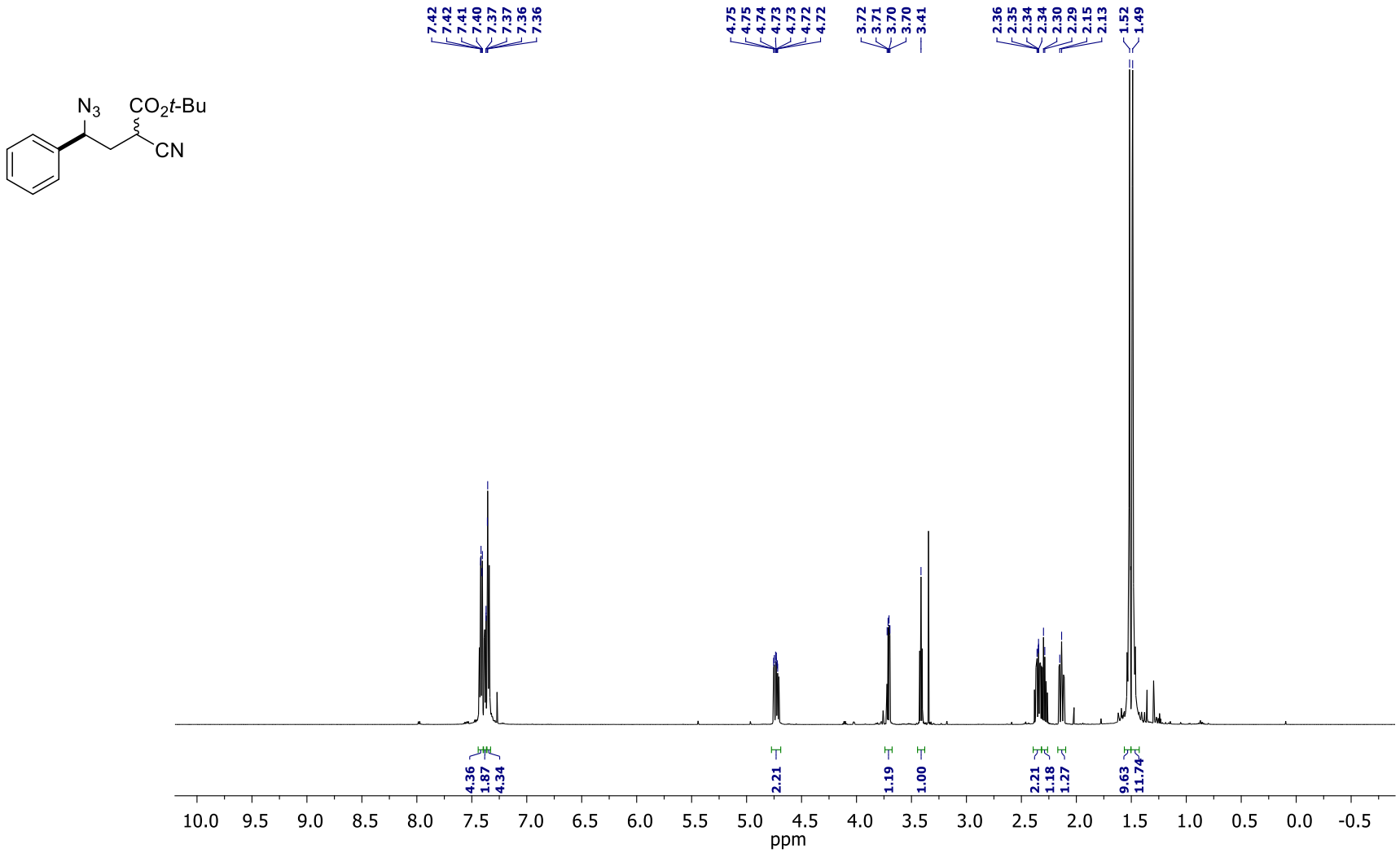
Methyl 4-azido-2-cyanobutyrate (1r)

^{13}C NMR (150 MHz, $CDCl_3$)



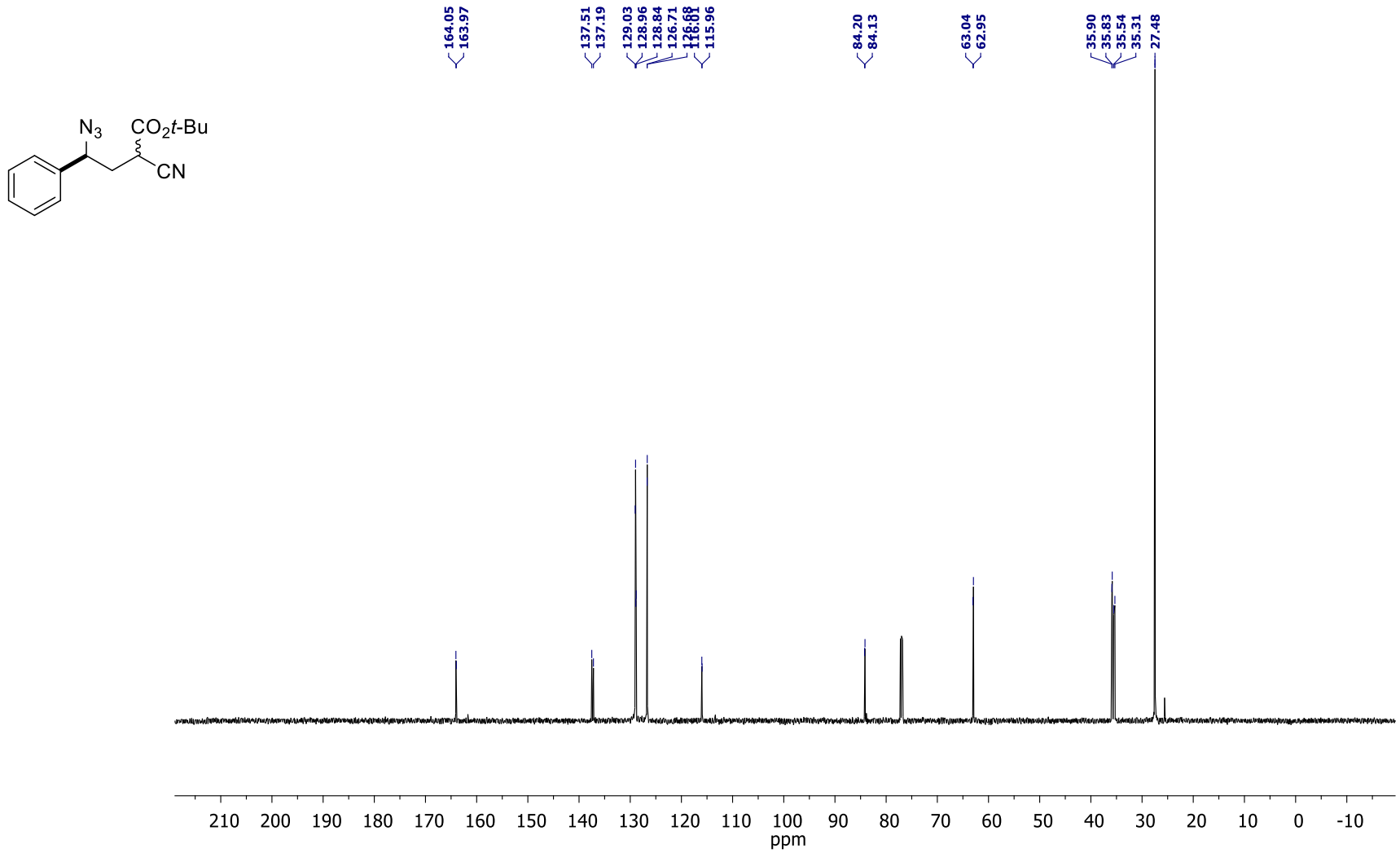
tert-Butyl 4-azido-2-cyano-4-phenylbutyrate (1s)

^{1}H NMR (600 MHz, $CDCl_3$)



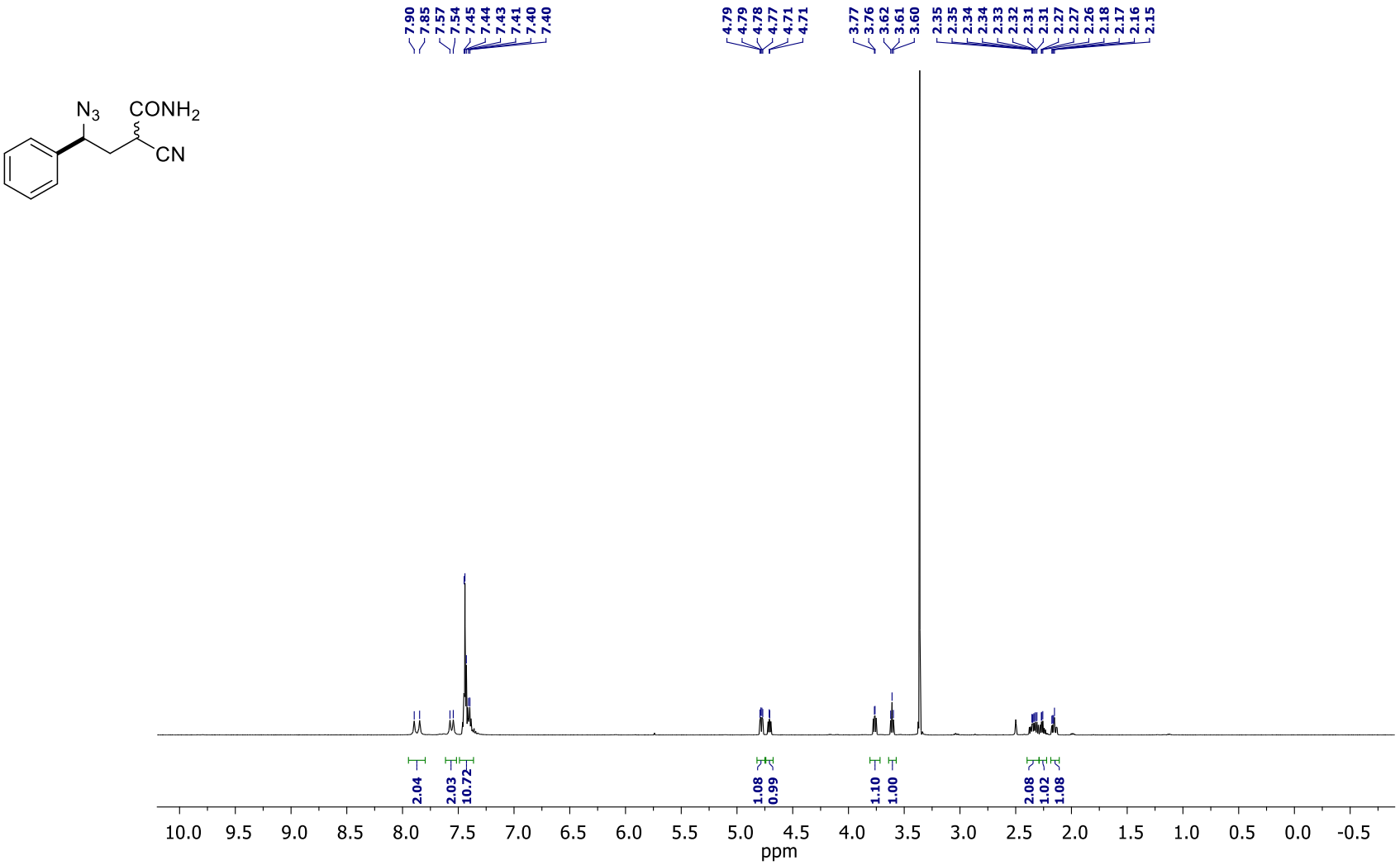
tert-Butyl 4-azido-2-cyano-4-phenylbutyrate (1s)

^{13}C NMR (150 MHz, $CDCl_3$)



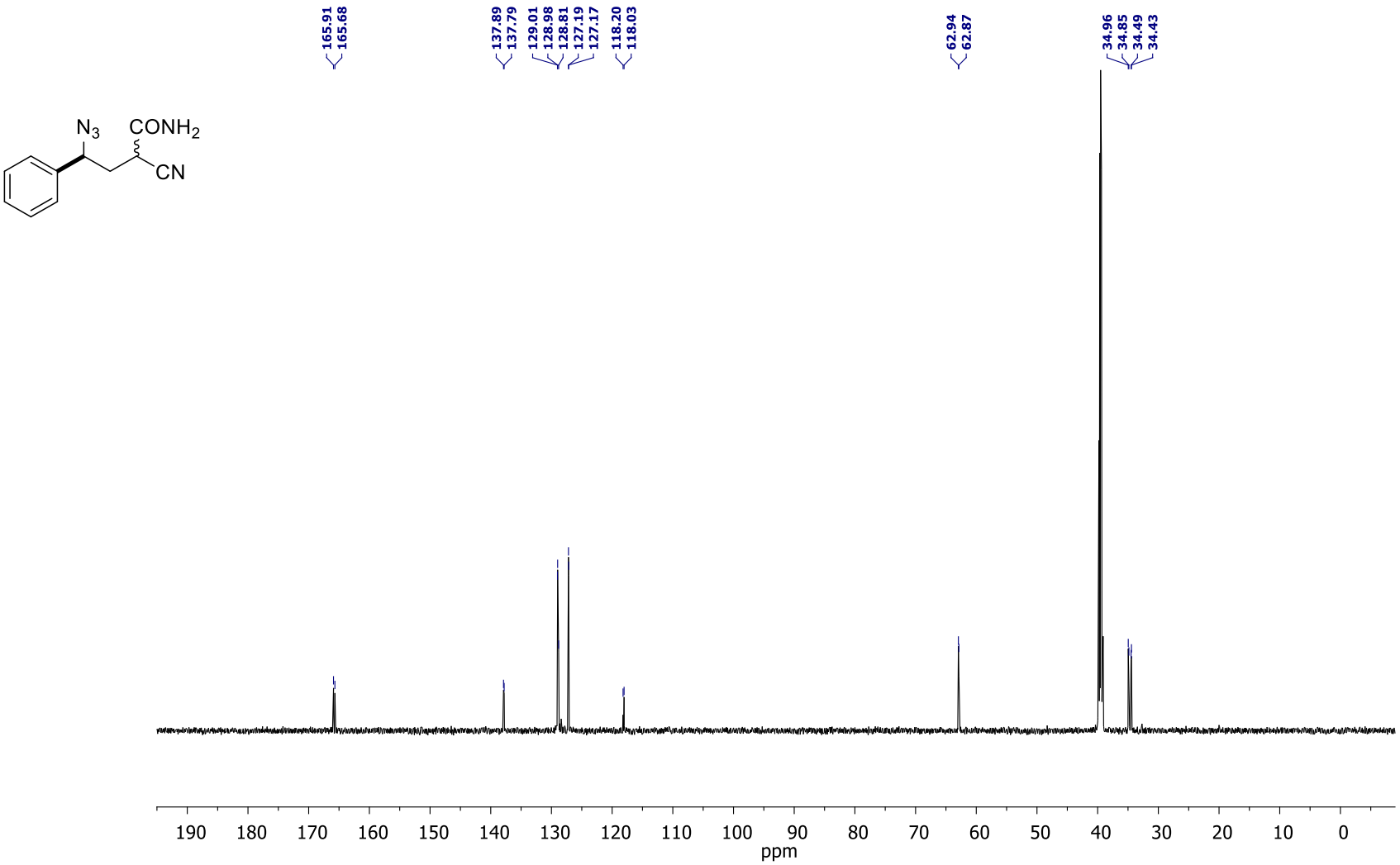
4-Azido-2-cyano-4-phenylbutanamide (1t)

^{1}H NMR (600 MHz, DMSO-d$_6$)



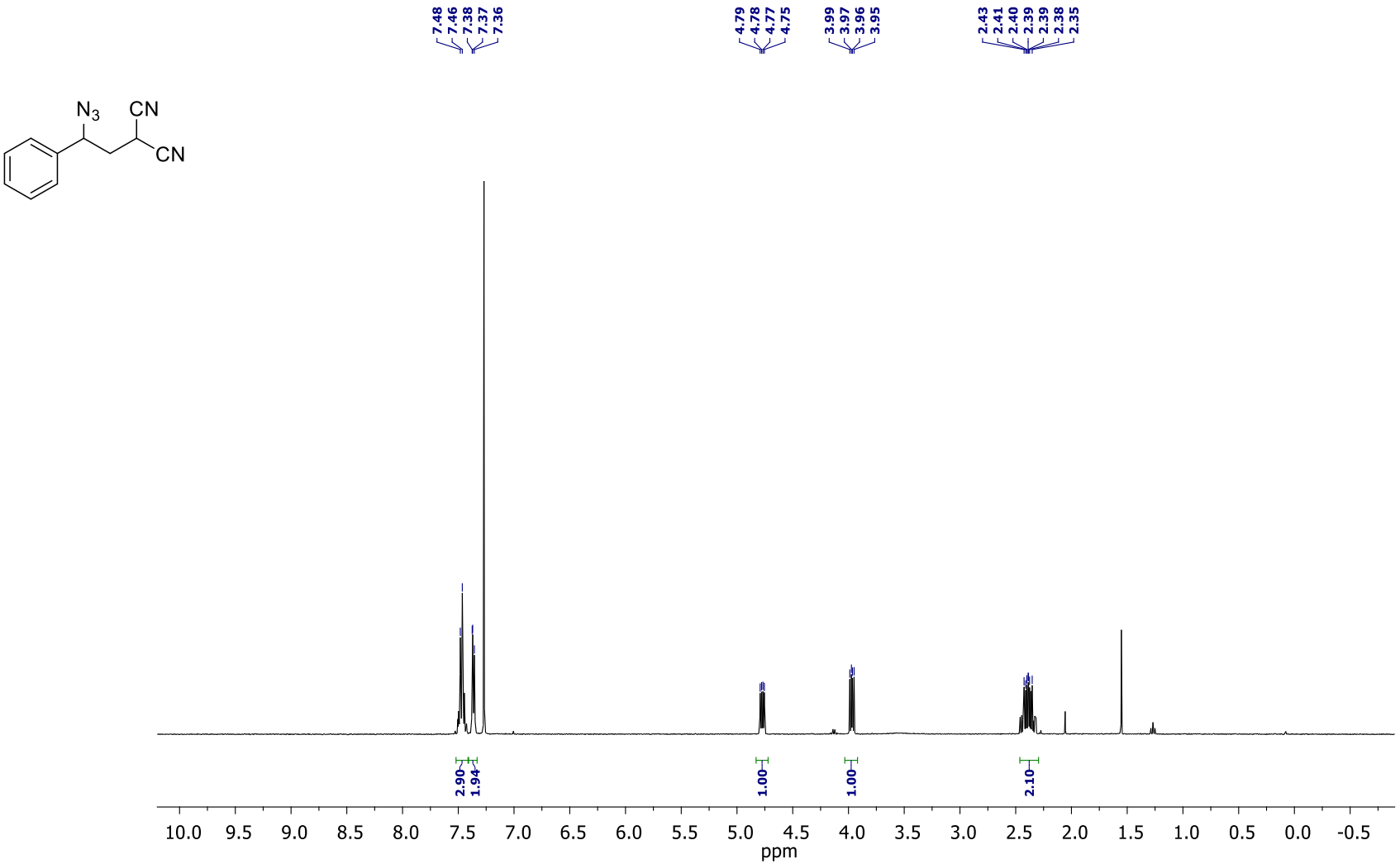
4-Azido-2-cyano-4-phenylbutanamide (1t)

^{13}C NMR (150 MHz, DMSO-d$_6$)



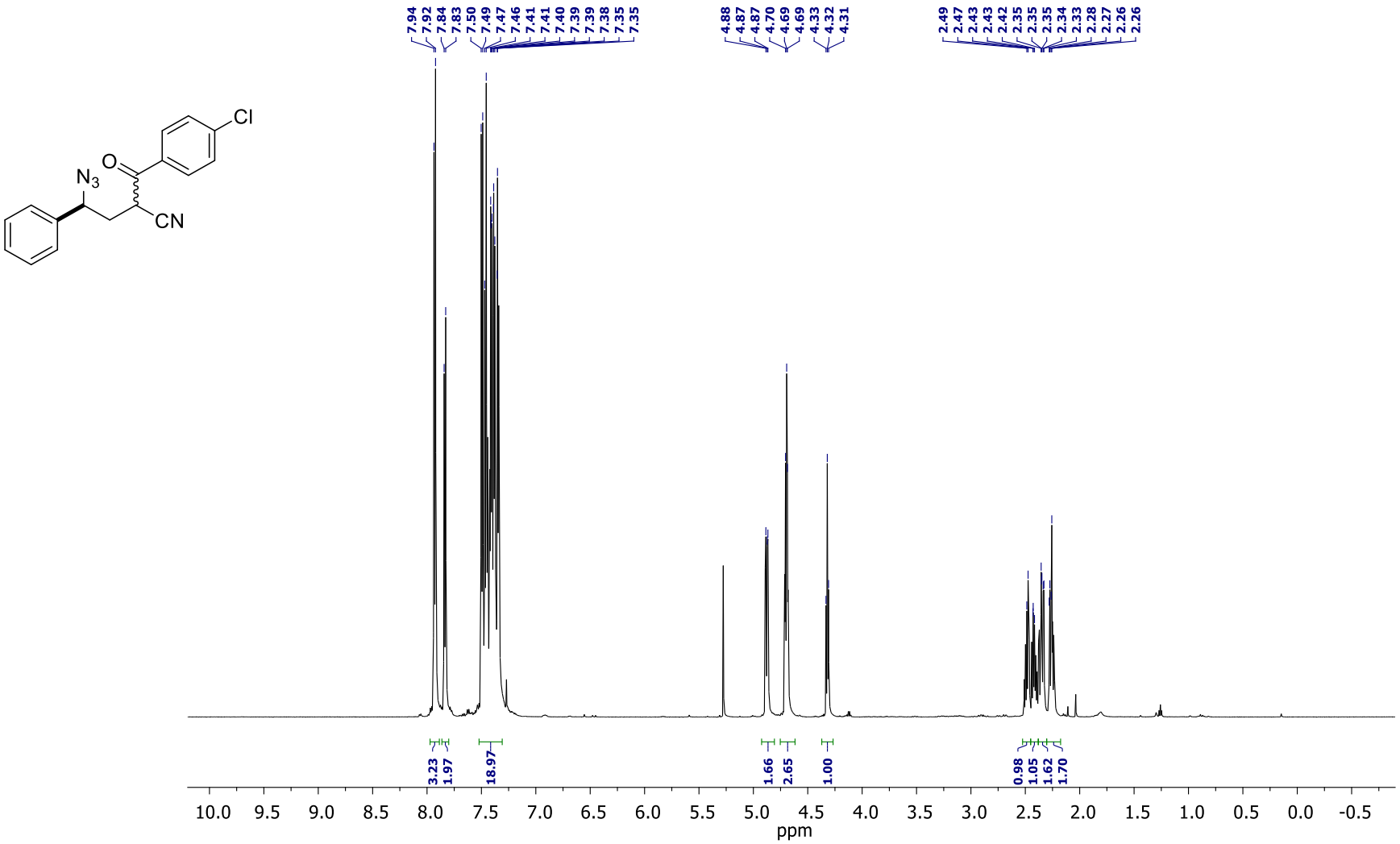
2-(2-Azido-2-phenylethyl)malononitrile (1u)

^{1}H NMR (600 MHz, $CDCl_3$)



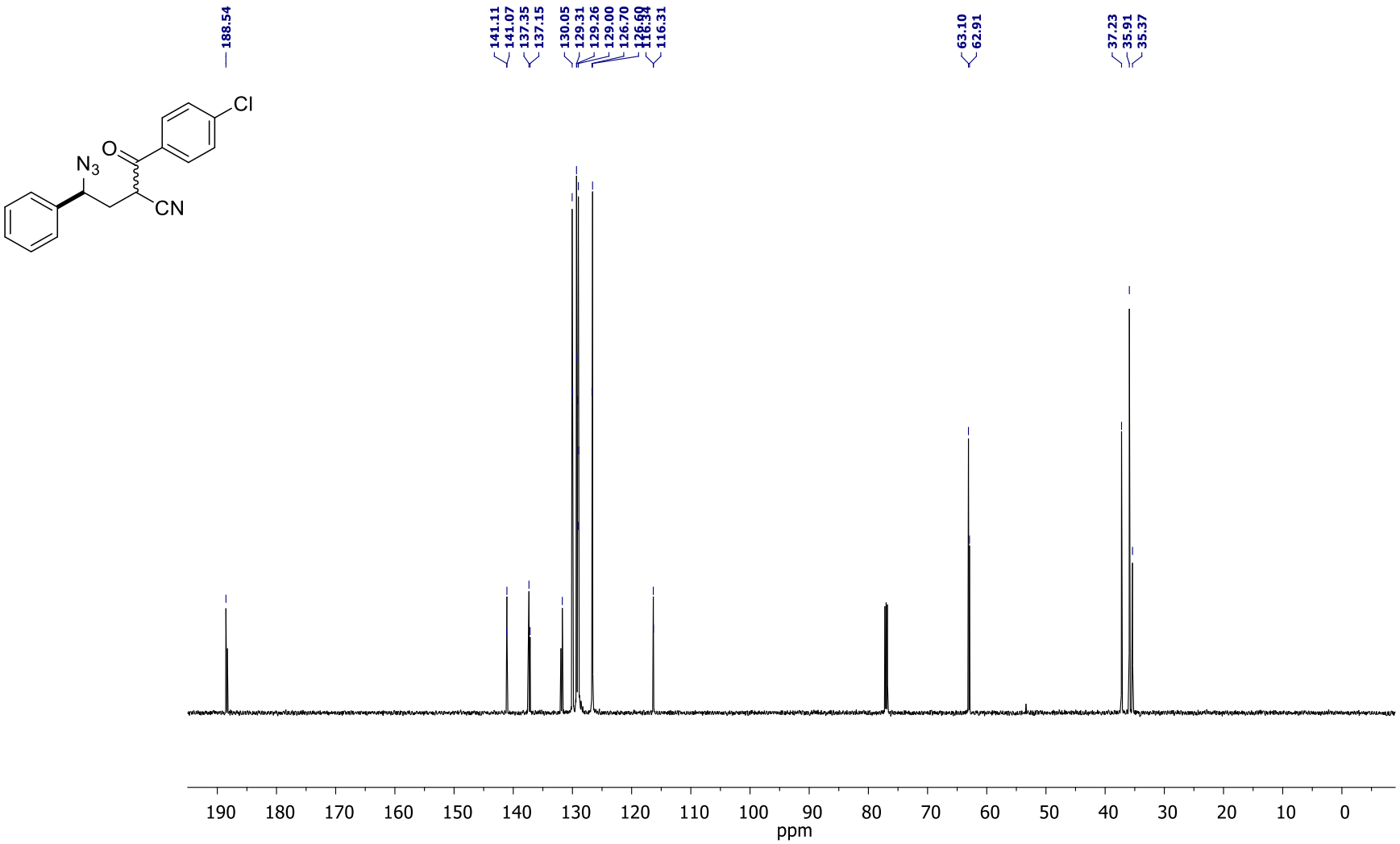
4-Azido-2-(4-chlorobenzoyl)-4-phenylbutyronitrile (1v)

^{1}H NMR (600 MHz, $CDCl_3$)



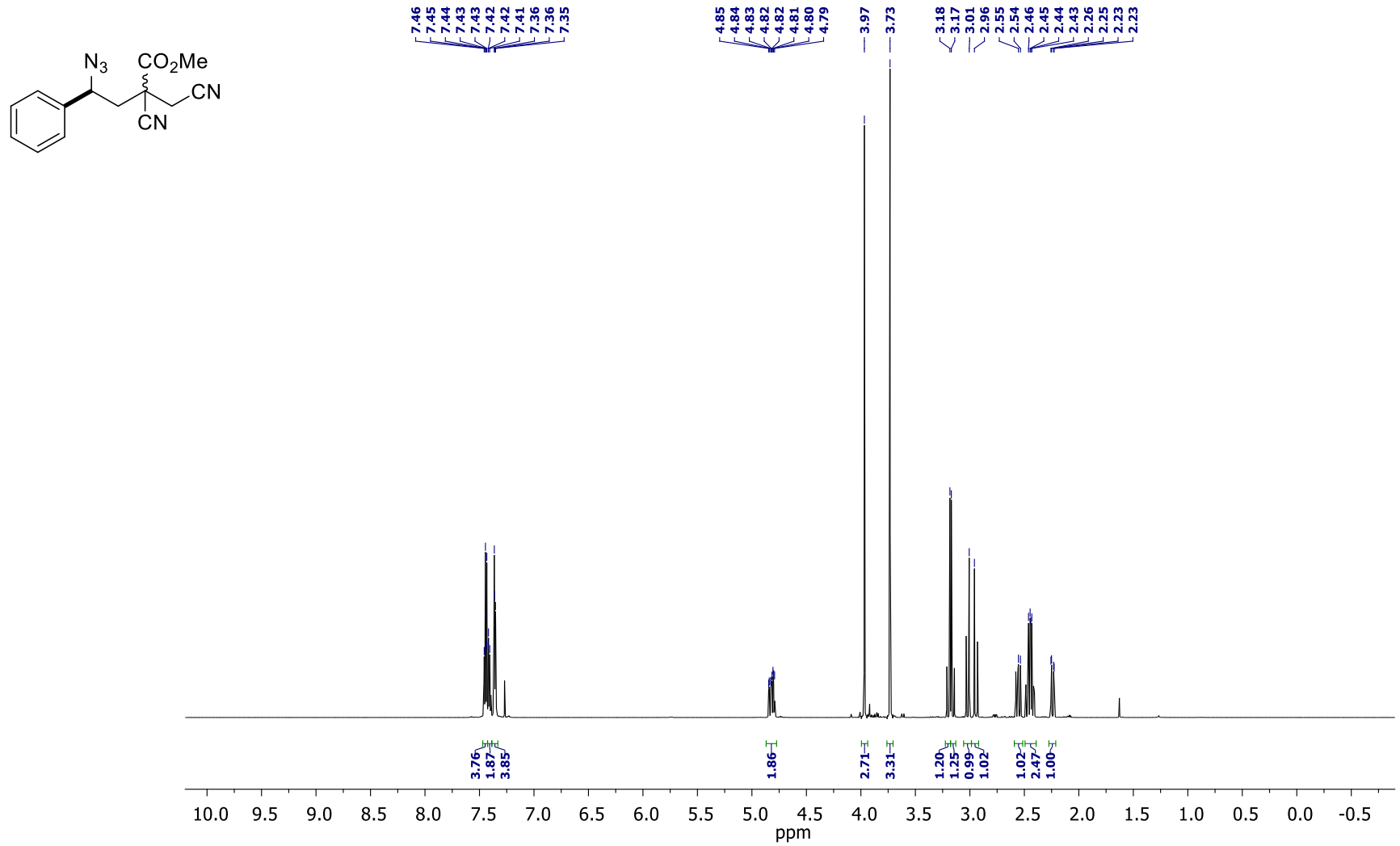
4-Azido-2-(4-chlorobenzoyl)-4-phenylbutyronitrile (1v)

^{13}C NMR (150 MHz, $CDCl_3$)



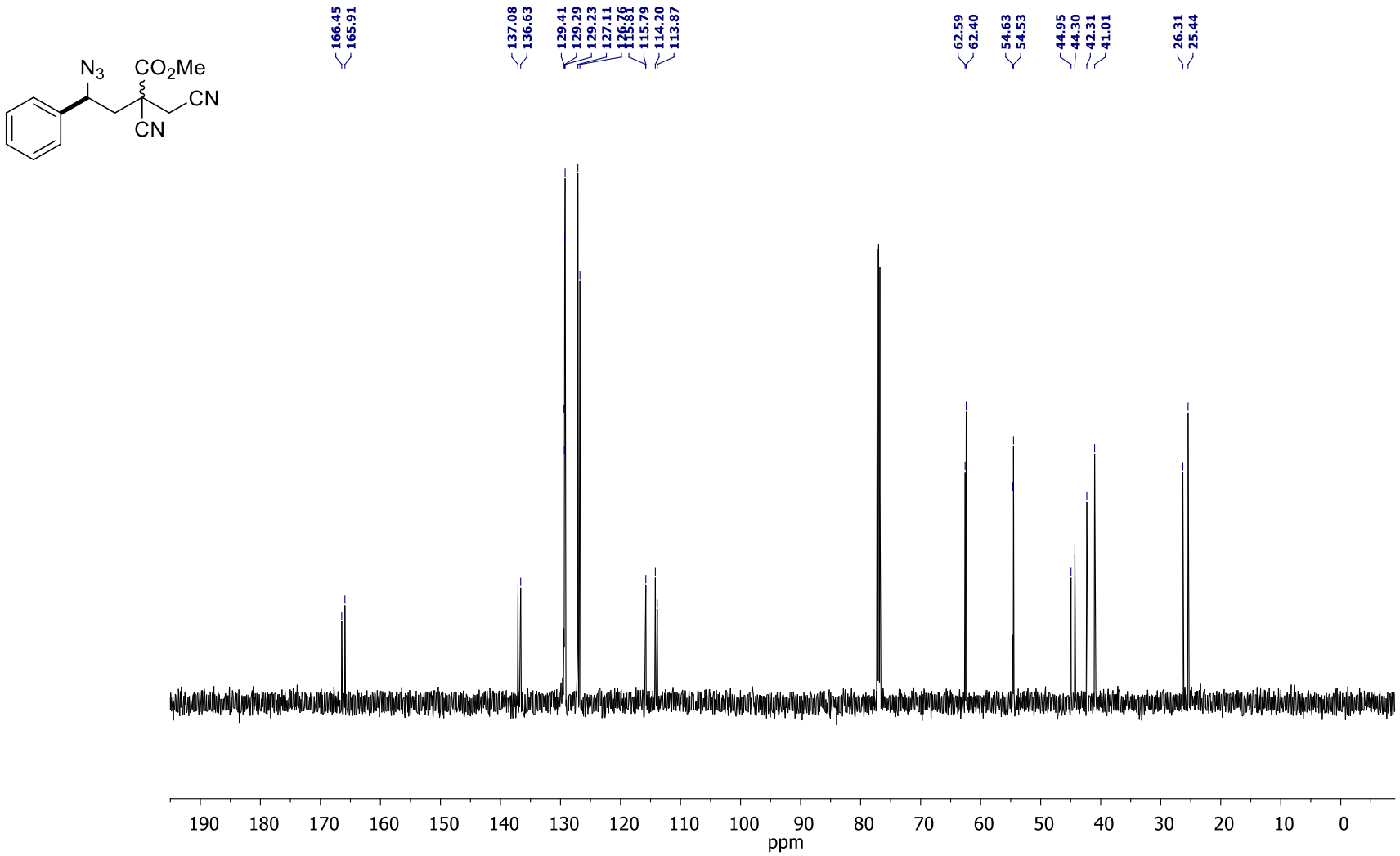
Methyl 4-azido-2-cyano-2-(cyanomethyl)-4-phenylbutanoate (1w)

^{1}H NMR (600 MHz, $CDCl_3$)



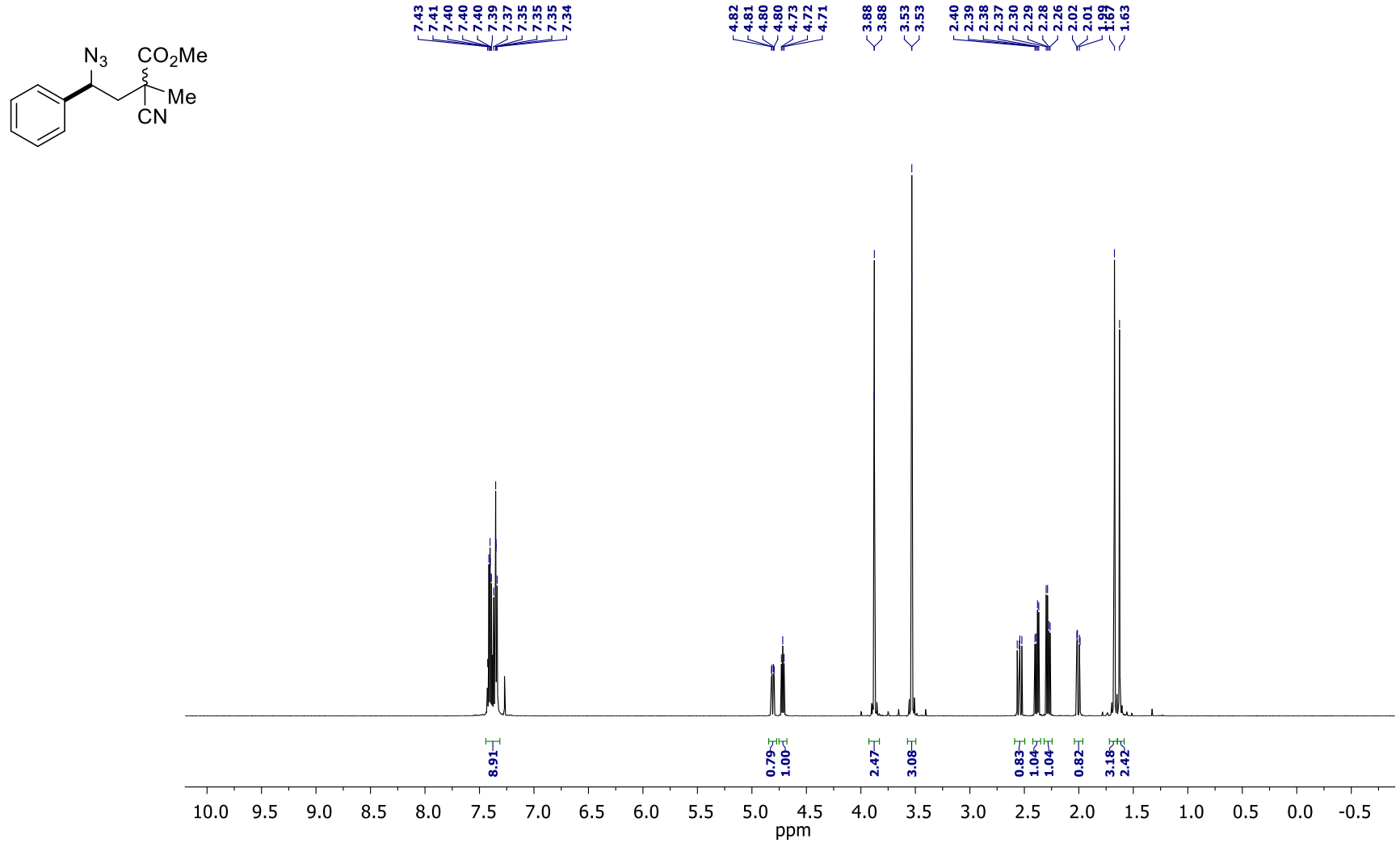
Methyl 4-azido-2-cyano-2-(cyanomethyl)-4-phenylbutanoate (1w)

^{13}C NMR (150 MHz, $CDCl_3$)



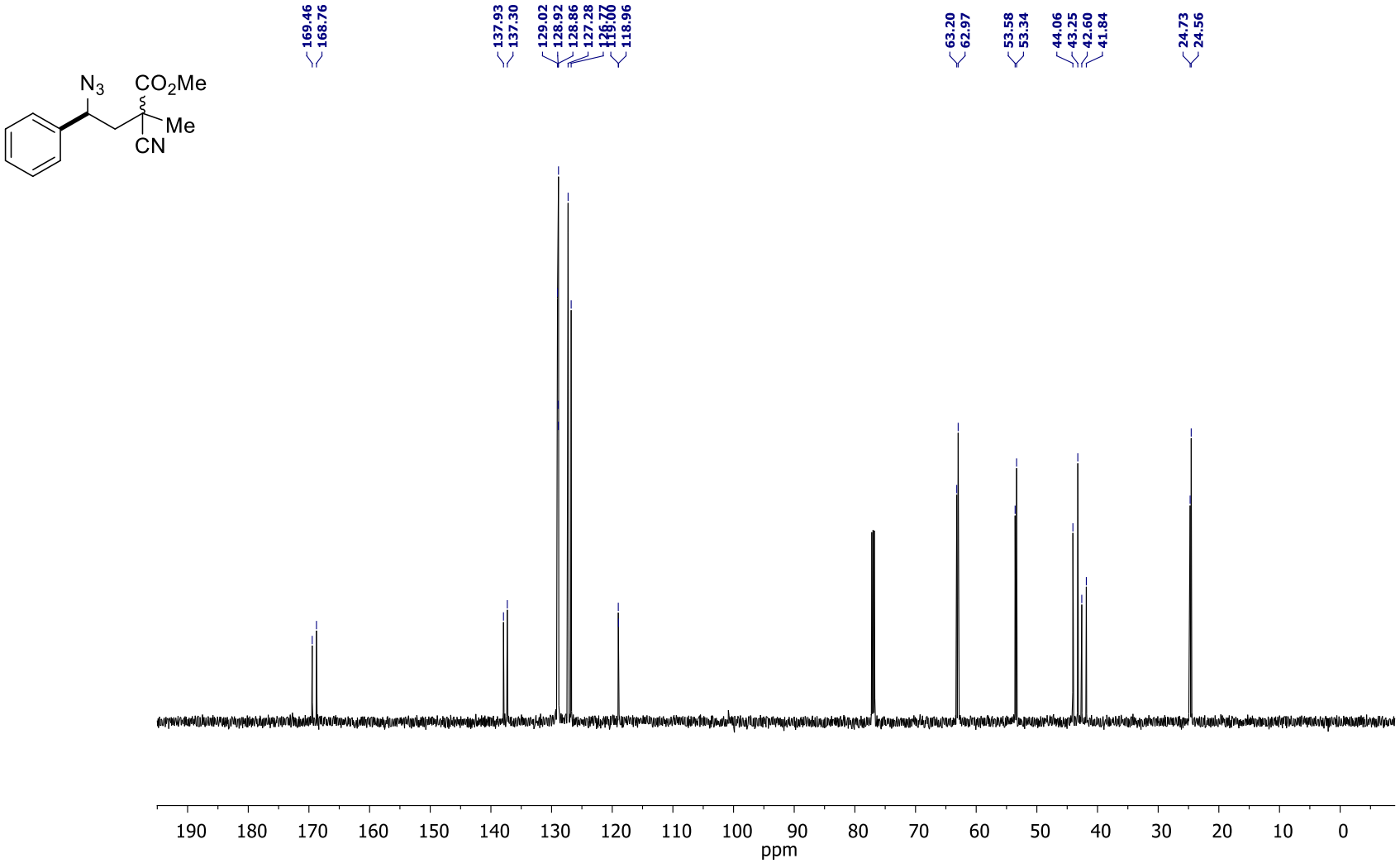
Methyl 4-azido-2-cyano-2-(methyl)-4-phenylbutyrate (1x)

^{1}H NMR (600 MHz, $CDCl_3$)



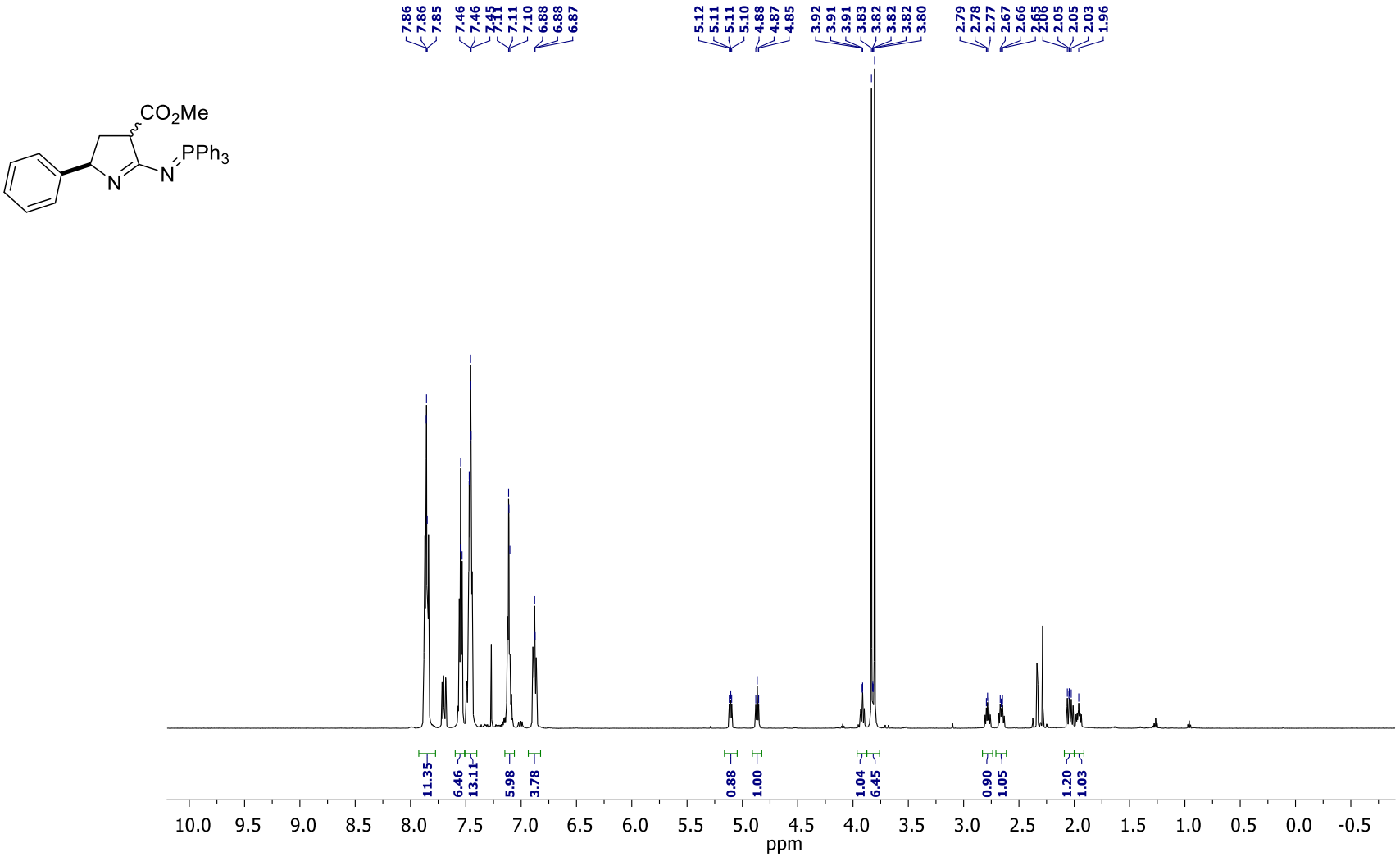
Methyl 4-azido-2-cyano-2-(methyl)-4-phenylbutyrate (1x)

^{13}C NMR (150 MHz, $CDCl_3$)



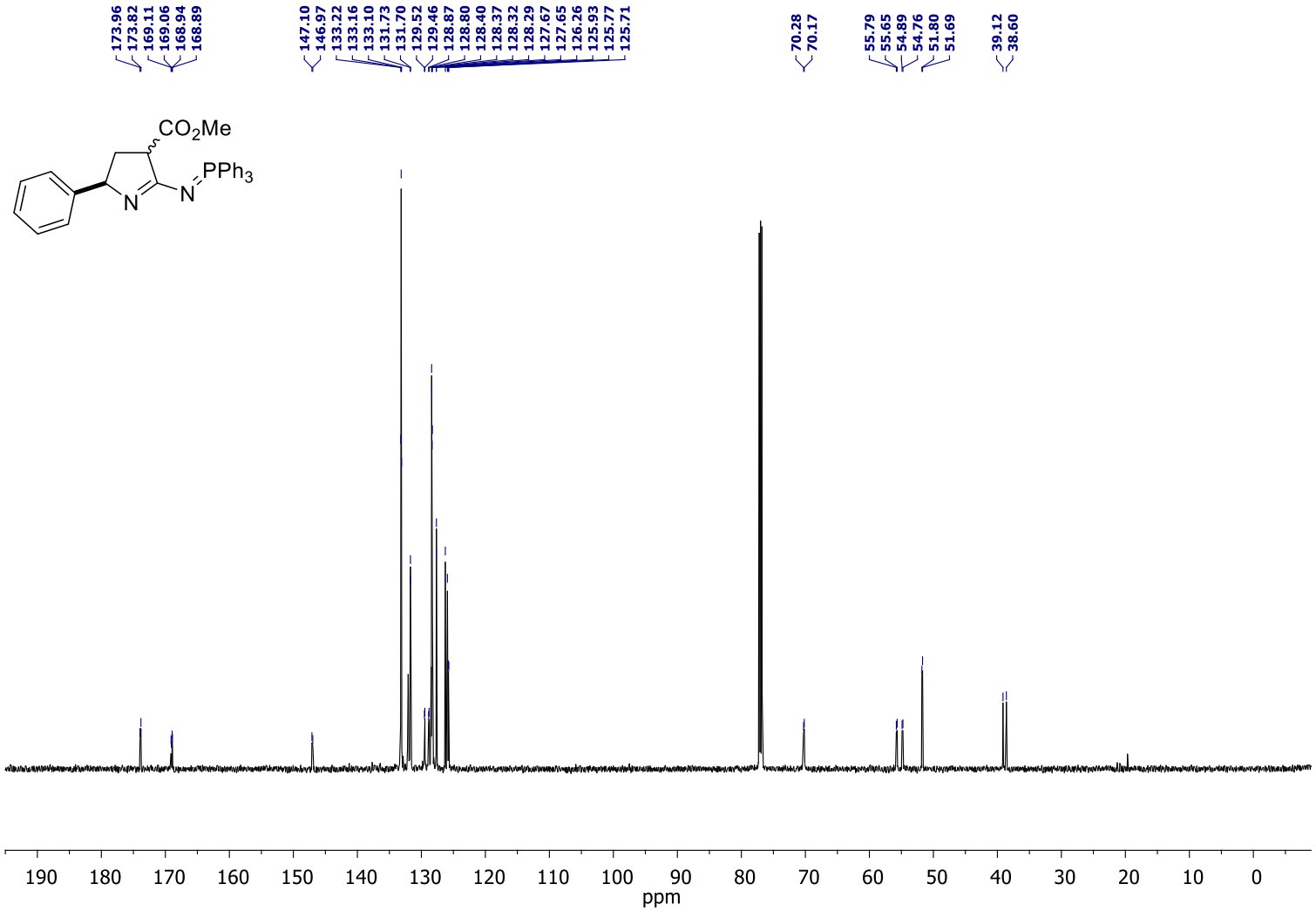
Methyl 2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3a)

^{1}H NMR (600 MHz, $CDCl_3$)

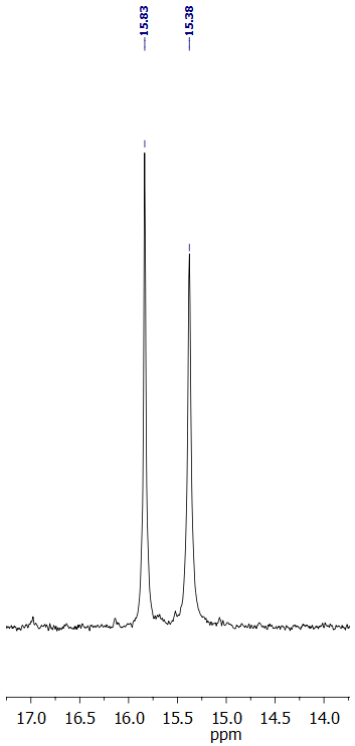


Methyl 2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3a)

^{13}C NMR (150 MHz, $CDCl_3$)

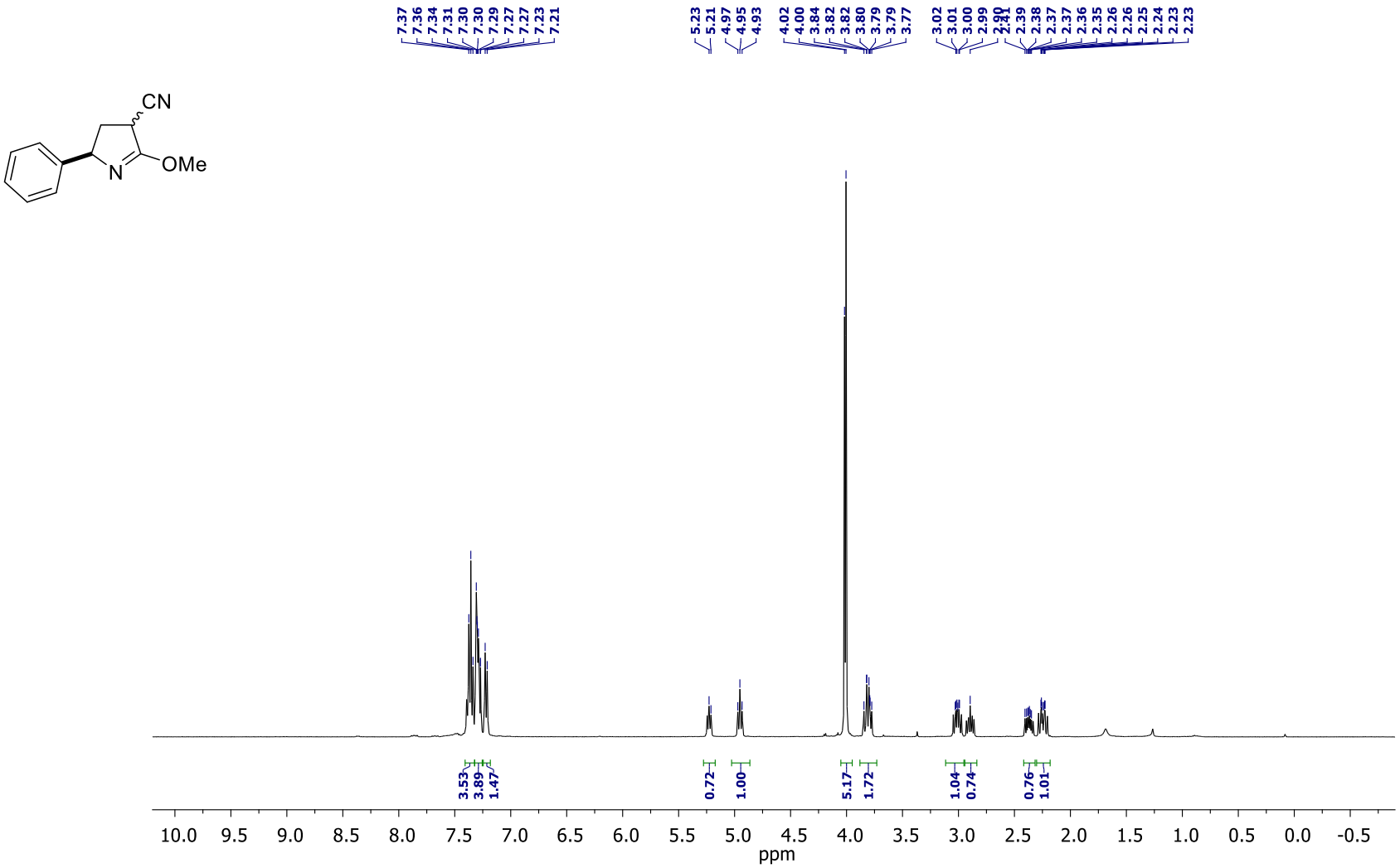


^{31}P NMR ($CDCl_3$, 162 MHz)



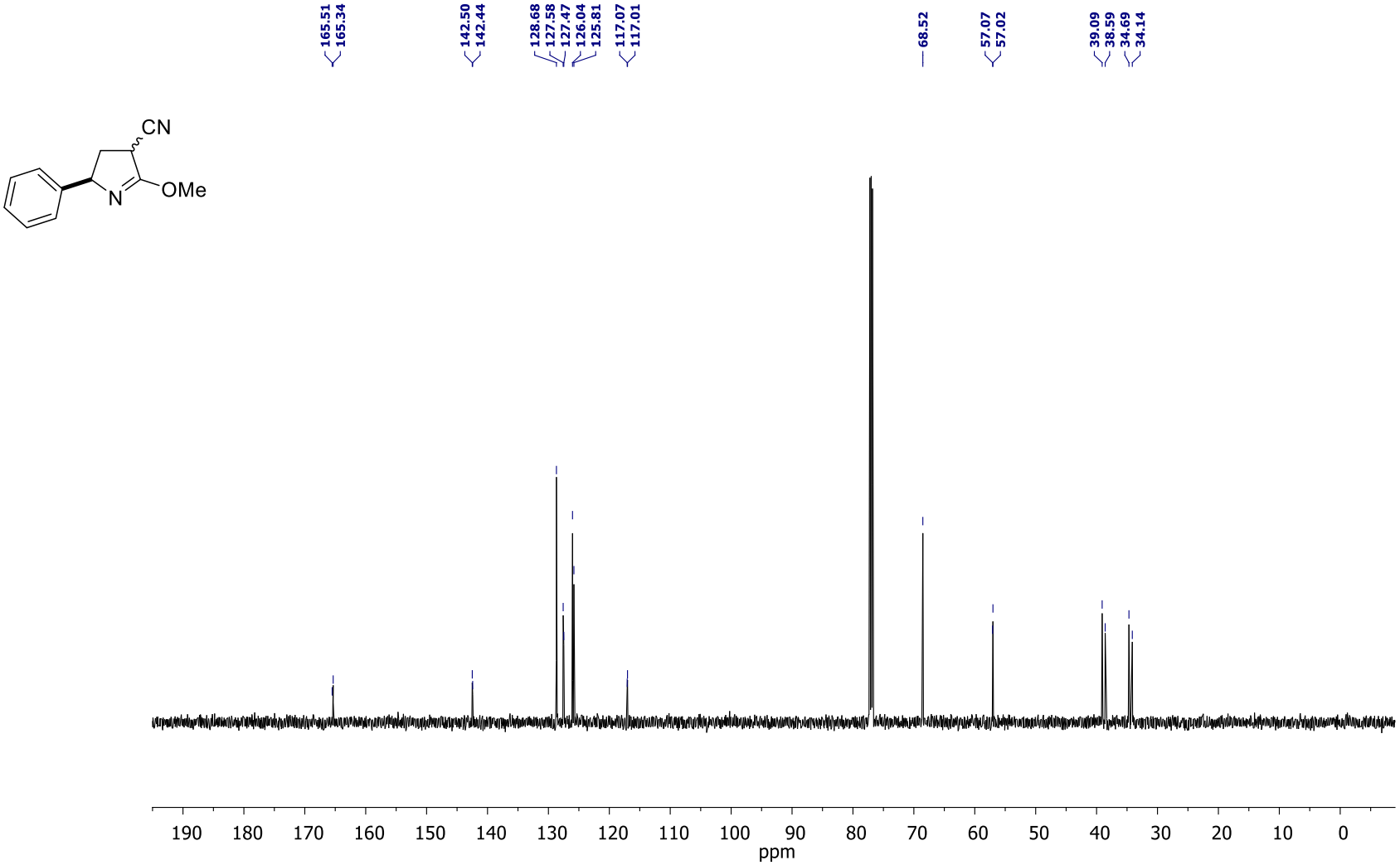
5-Methoxy-2-phenyl-3,4-dihydro-2*H*-pyrrole-4-carbonitrile (4a)

^{1}H NMR (600 MHz, $CDCl_3$)



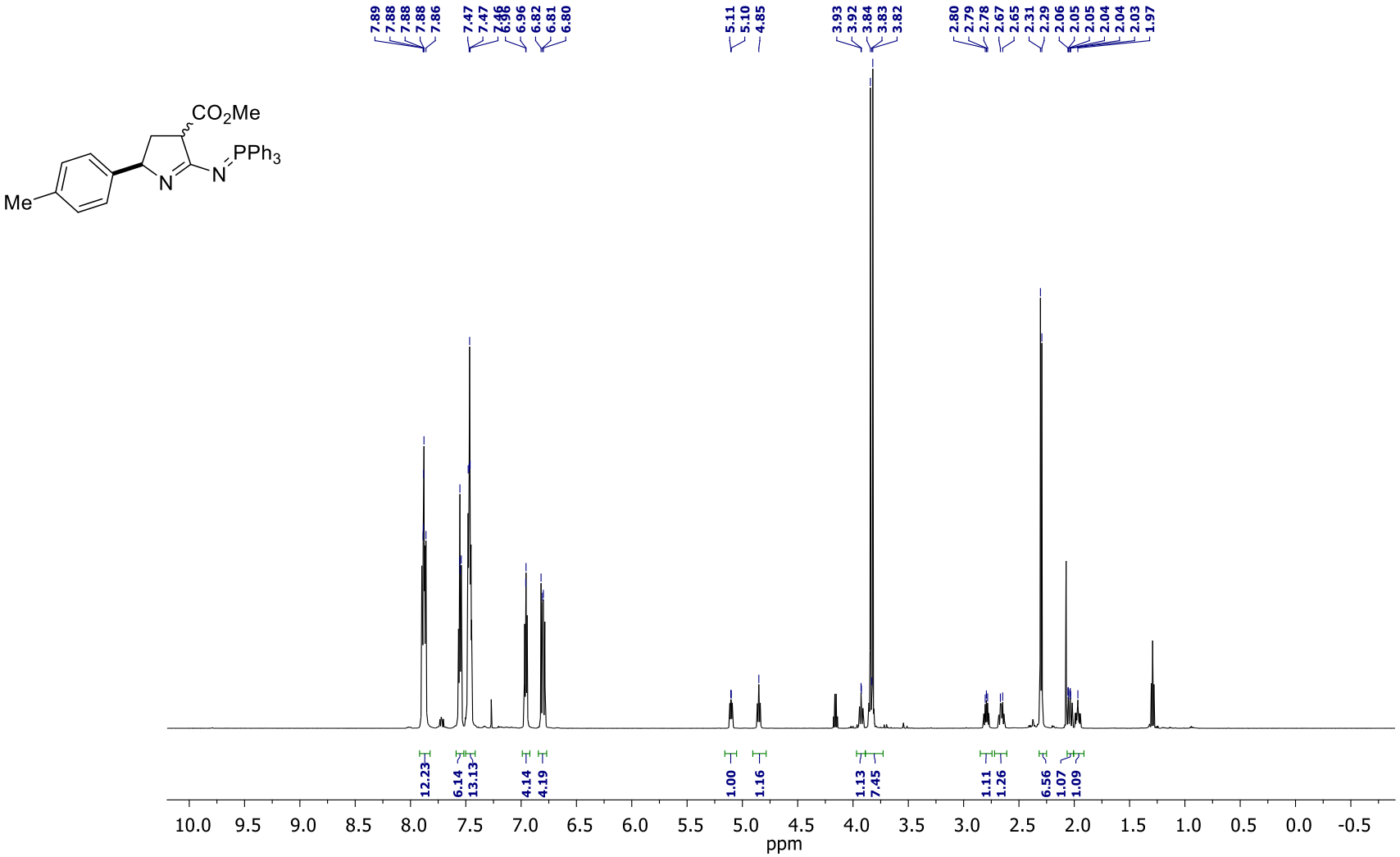
5-Methoxy-2-phenyl-3,4-dihydro-2*H*-pyrrole-4-carbonitrile (4a)

^{13}C NMR (150 MHz, $CDCl_3$)



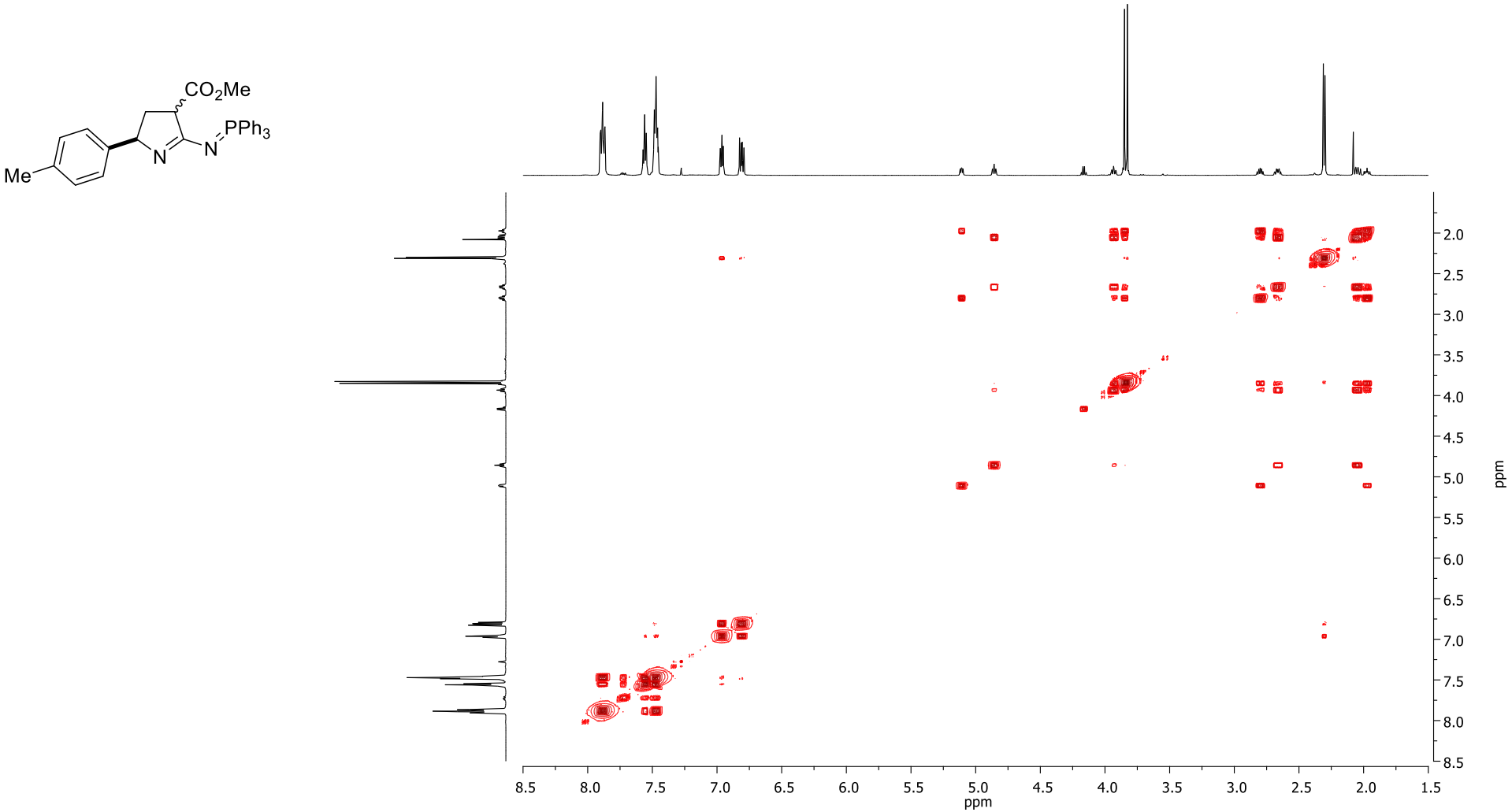
Methyl 2-(4-tolyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3b)

^{1}H NMR (600 MHz, $CDCl_3$)



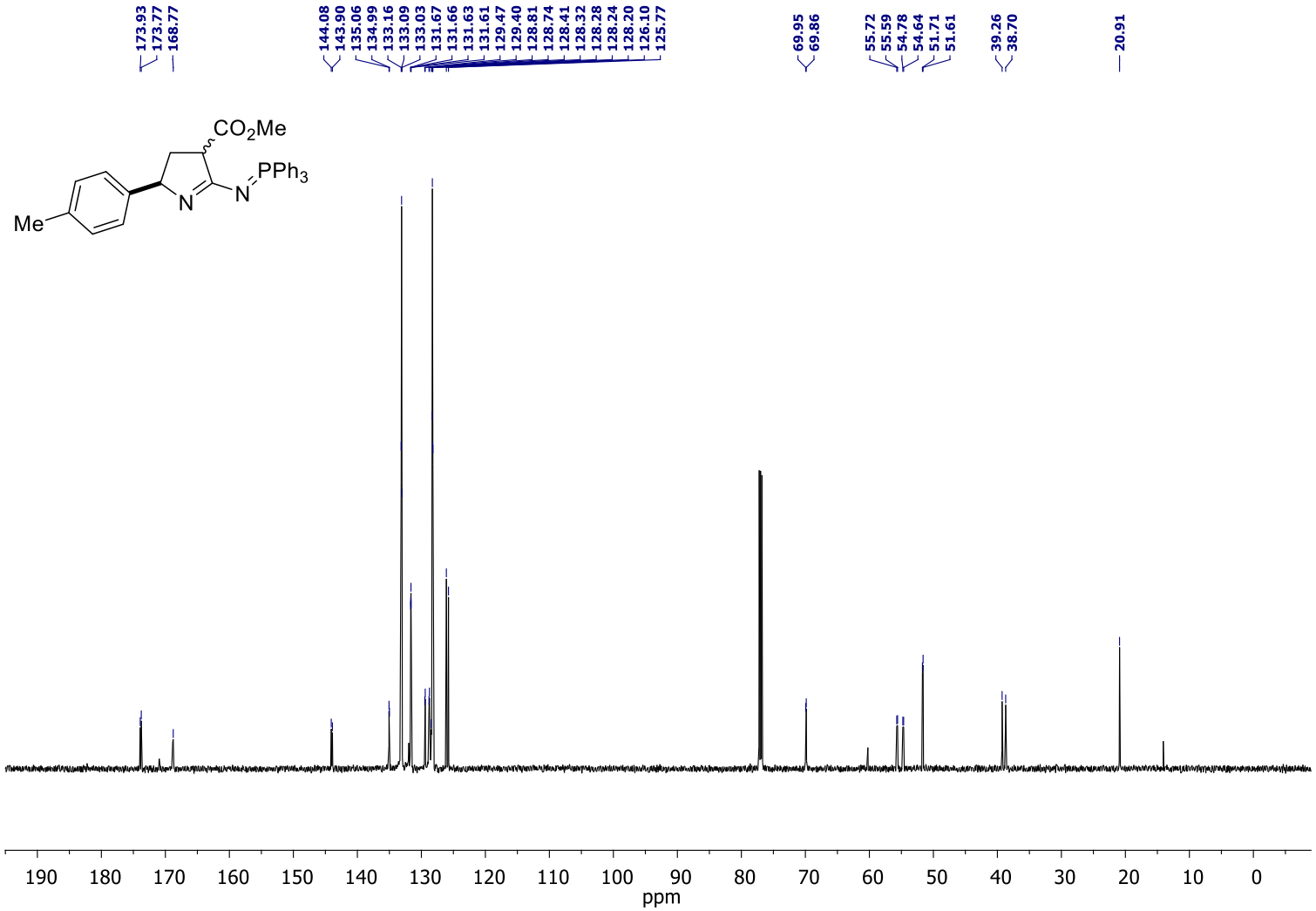
Methyl 2-(4-tolyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3b)

^{1}H-^{1}H COSY ($CDCl_3$)

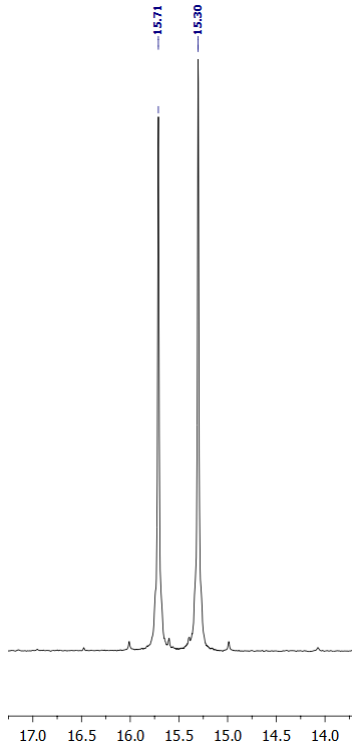


Methyl 2-(4-tolyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3b)

^{13}C NMR (150 MHz, $CDCl_3$)

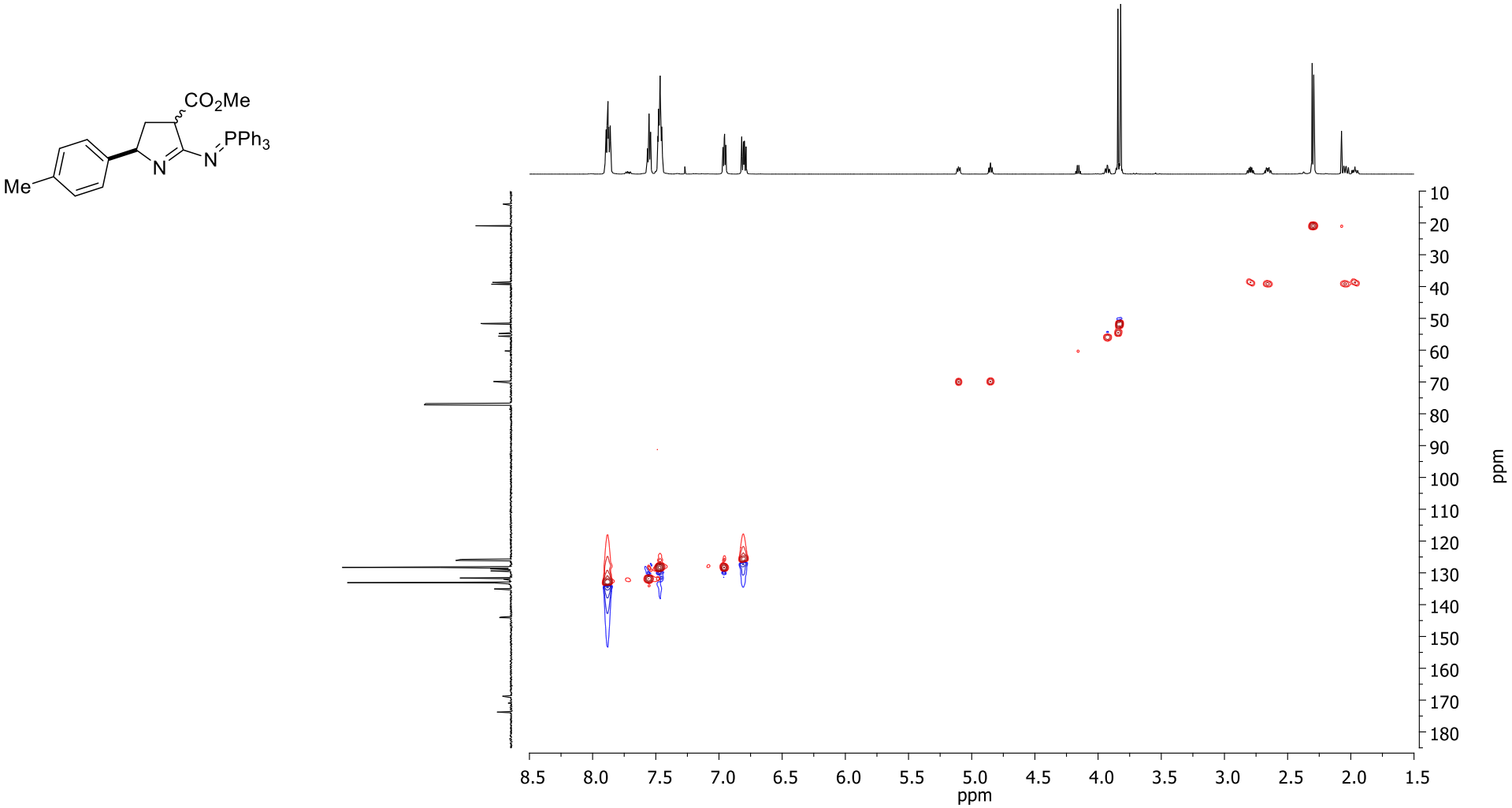


^{31}P NMR ($CDCl_3$, 162 MHz)



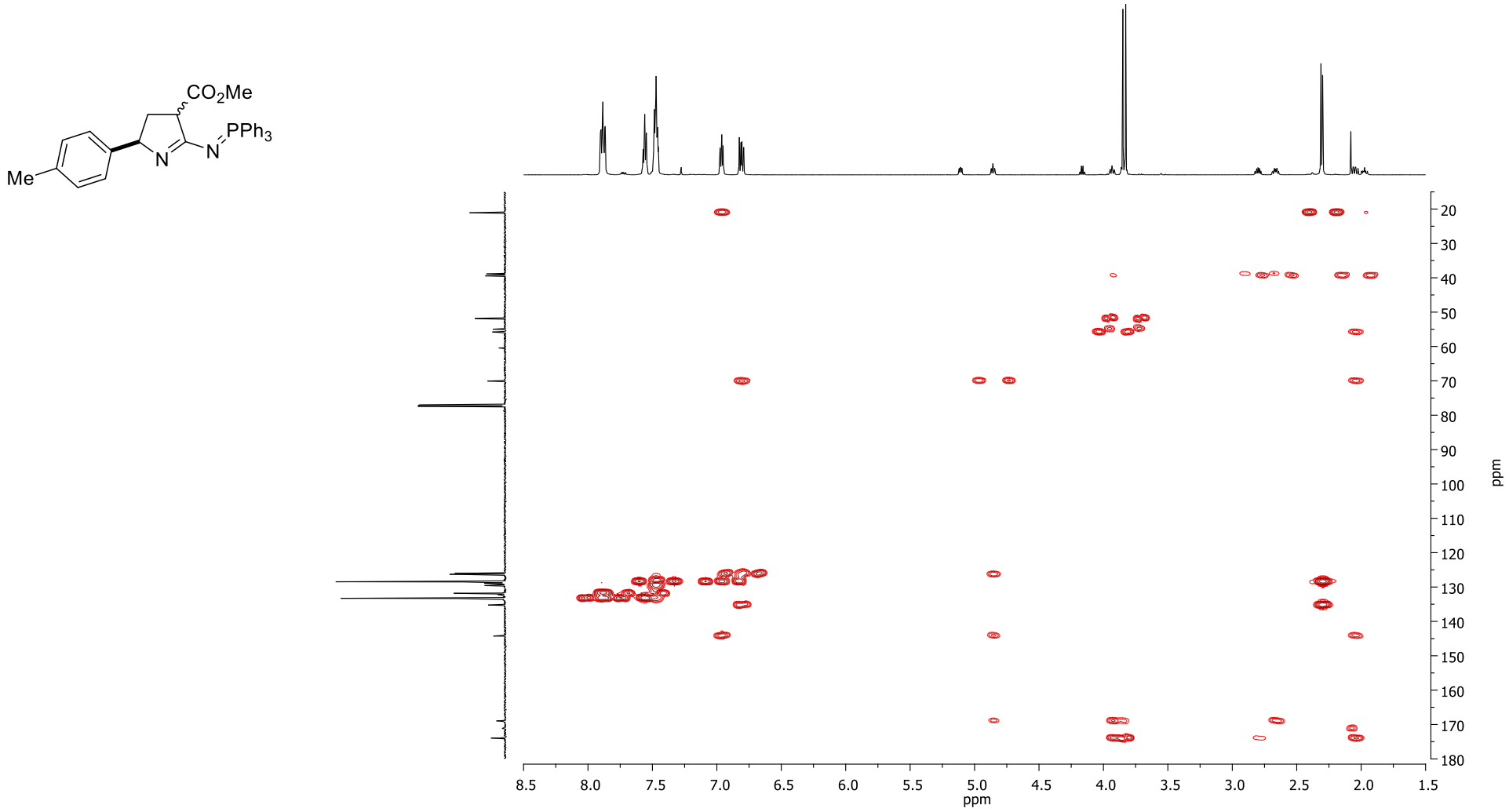
Methyl 2-(4-tolyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3b)

^{1}H-^{13}C HSQC ($CDCl_3$)



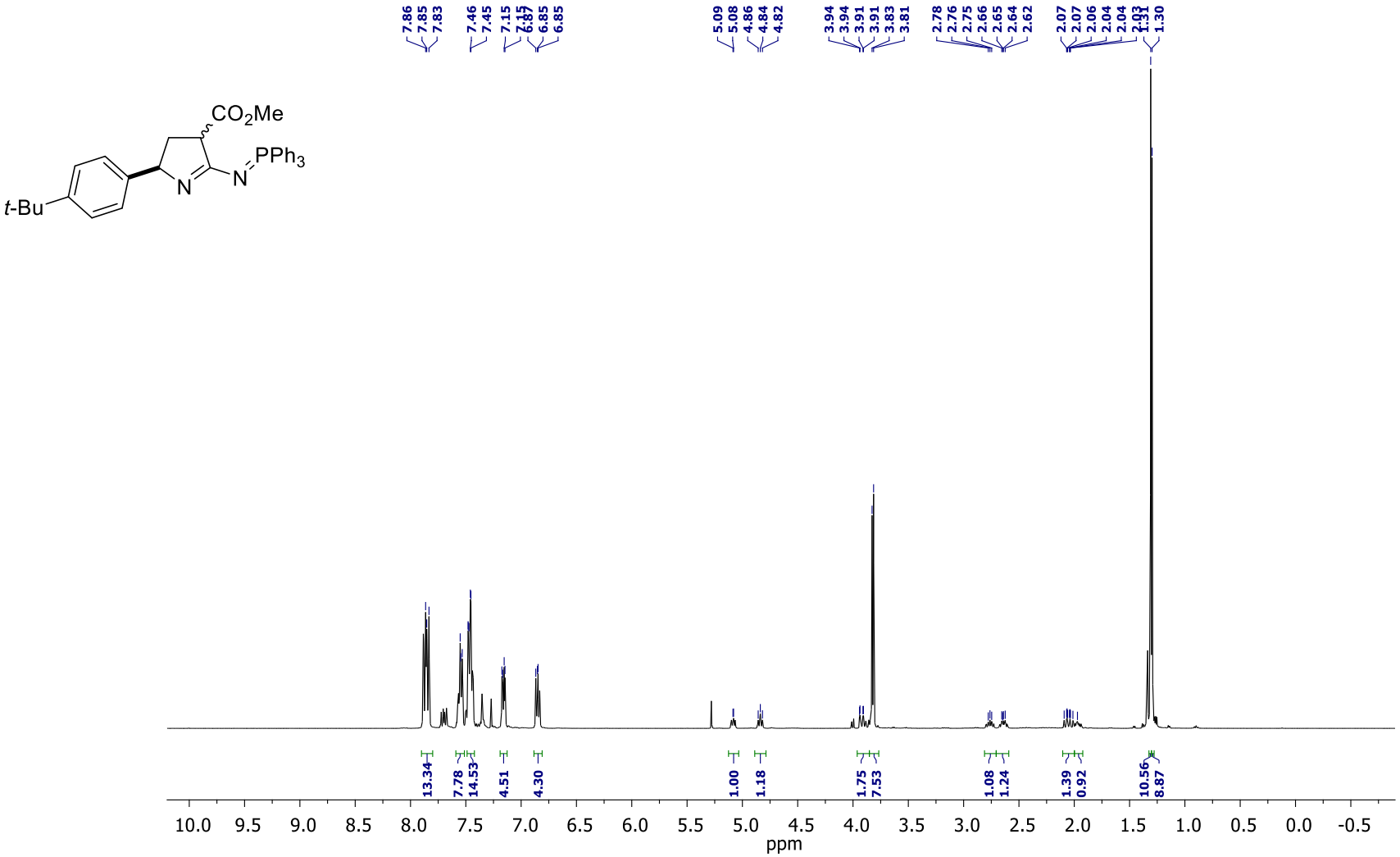
Methyl 2-(4-tolyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3b)

^{1}H-^{13}C HMBC ($CDCl_3$)



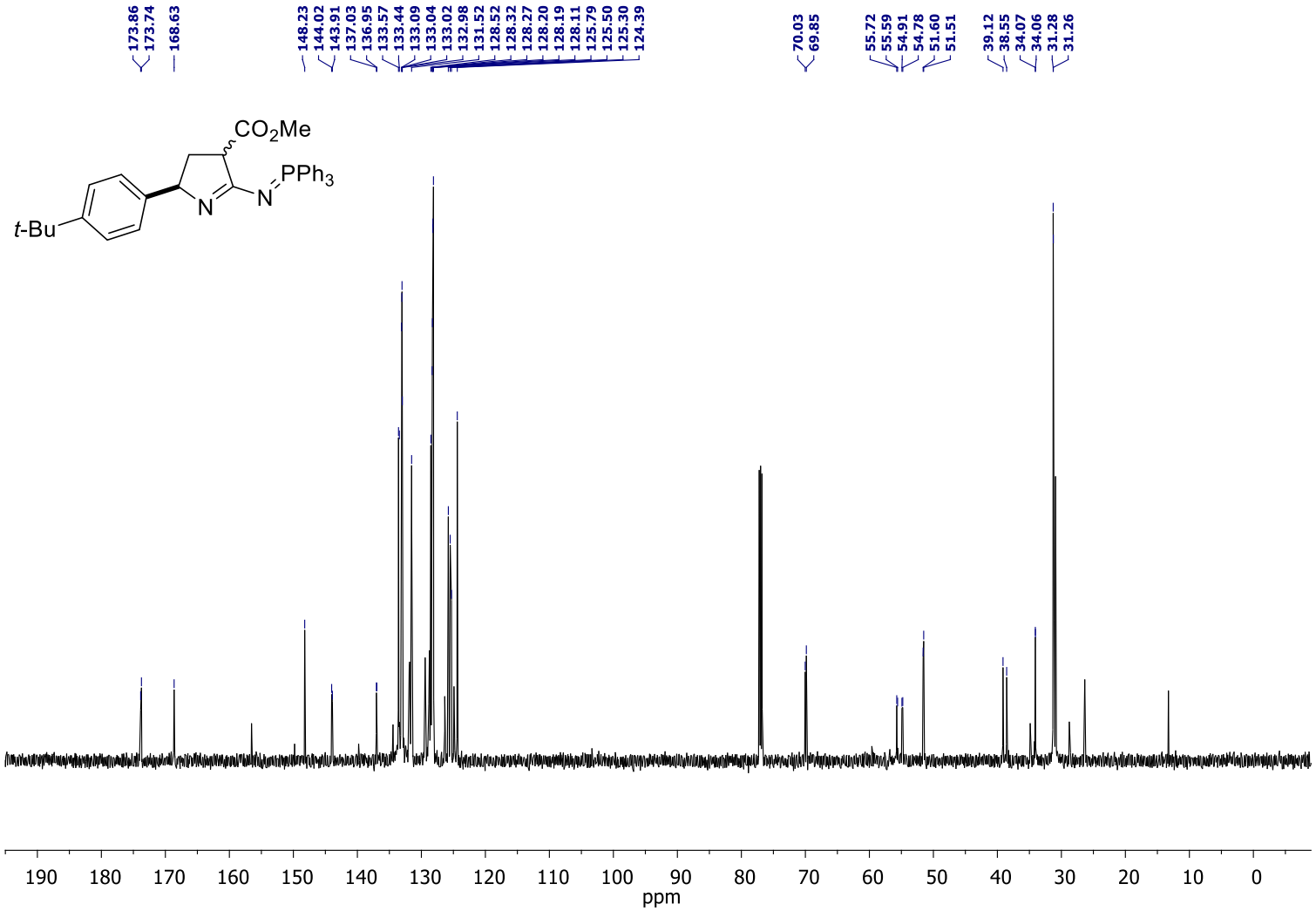
Methyl 2-(4-*tert*-butylphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3c)

^{1}H NMR (600 MHz, $CDCl_3$)

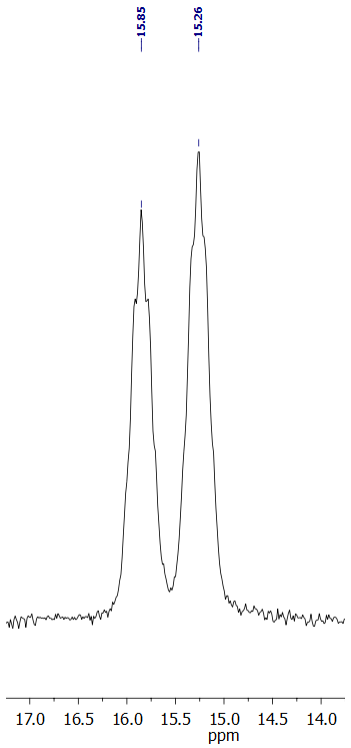


Methyl 2-(4-*tert*-butylphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3c)

^{13}C NMR (150 MHz, $CDCl_3$)

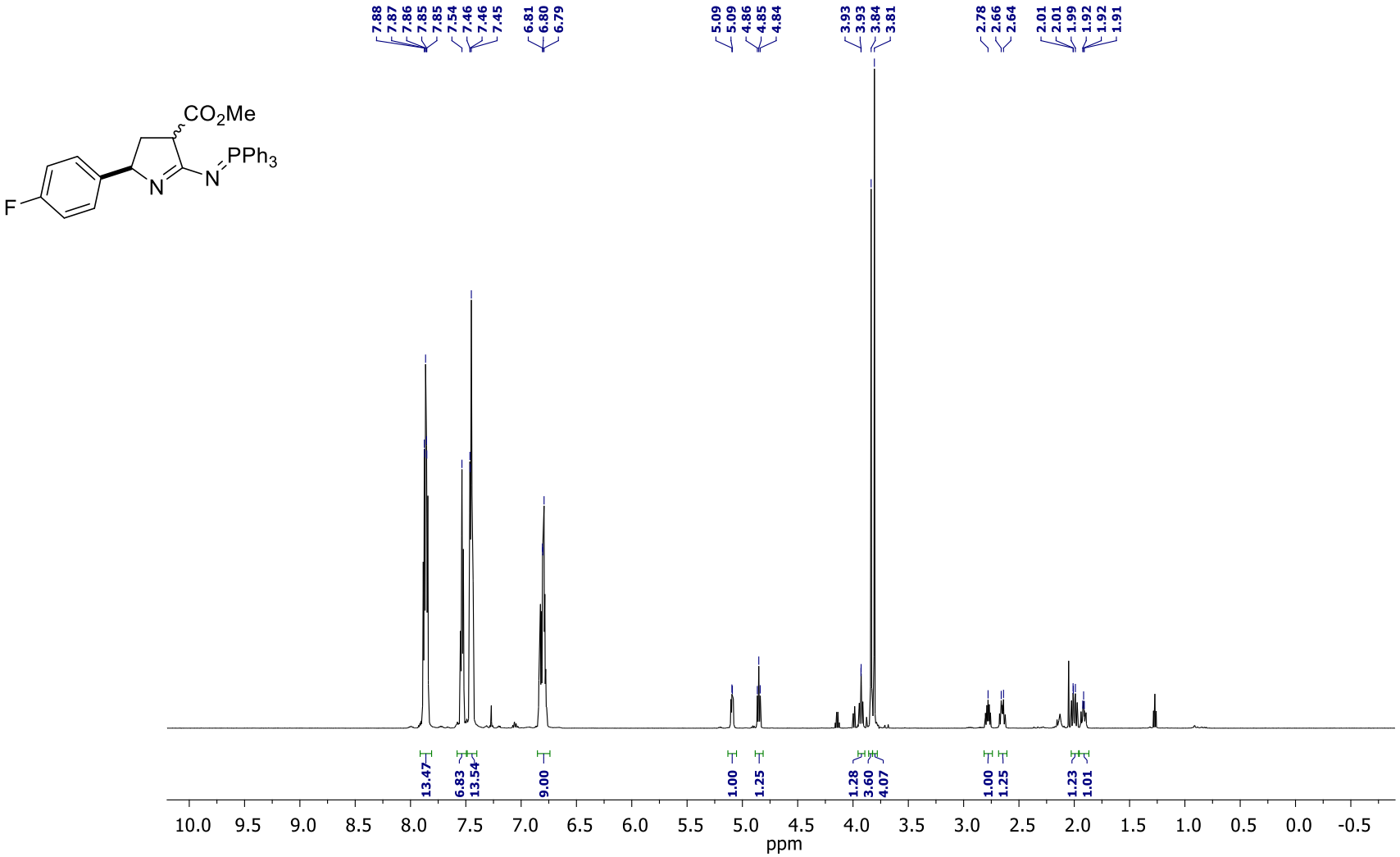


^{31}P NMR ($CDCl_3$, 162 MHz)



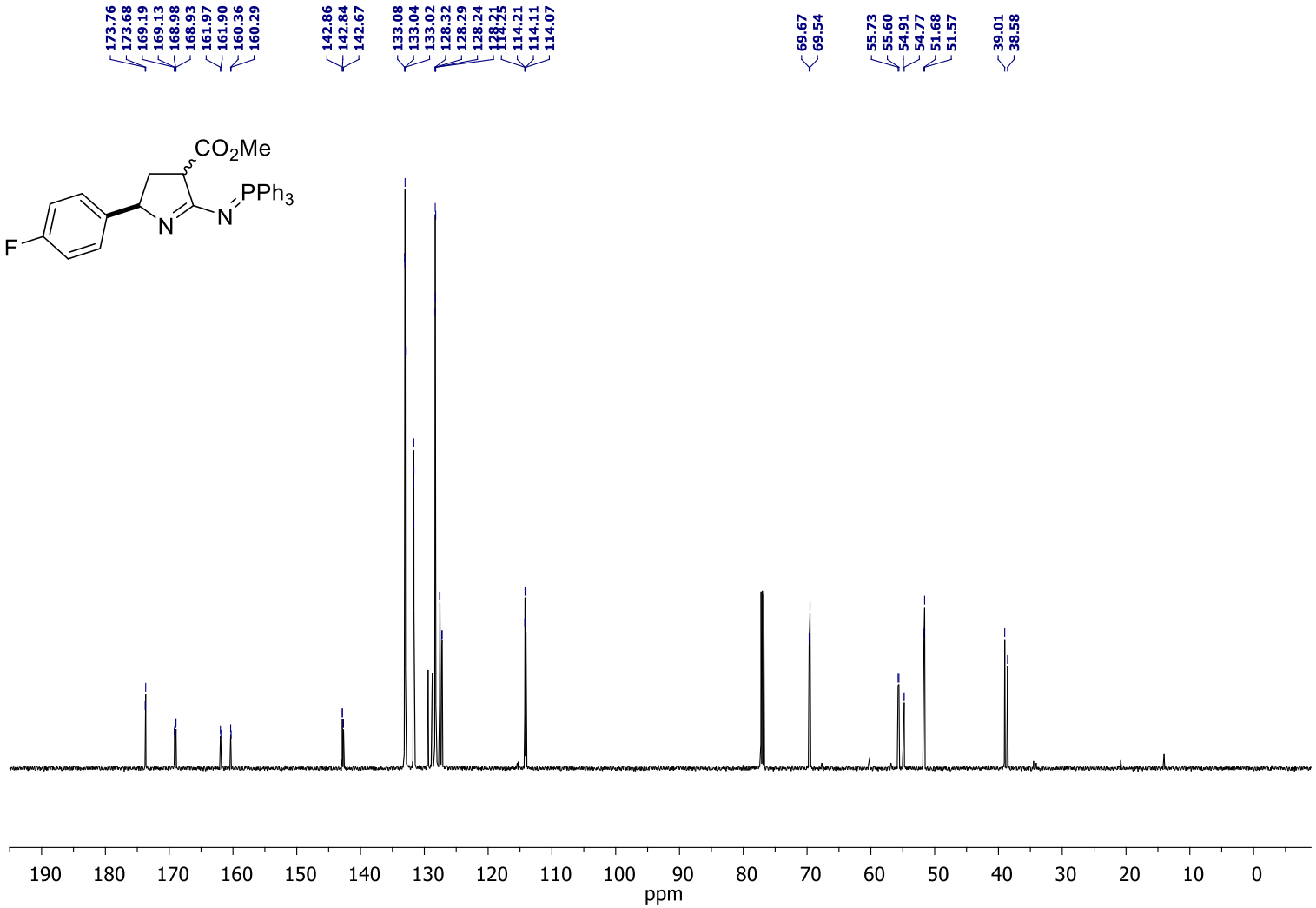
Methyl 2-(4-fluorophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3d)

^{1}H NMR (600 MHz, $CDCl_3$)

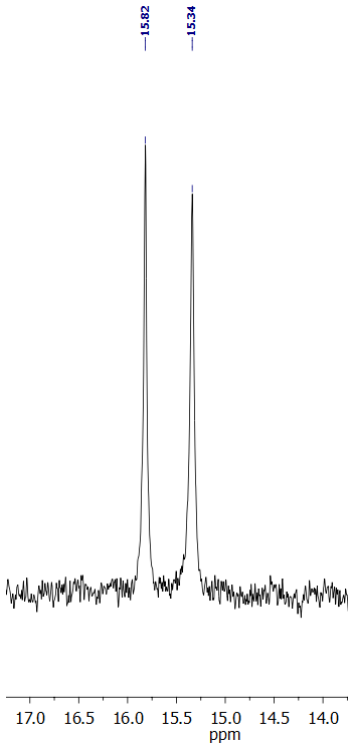


Methyl 2-(4-fluorophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3d)

^{13}C NMR (150 MHz, $CDCl_3$)

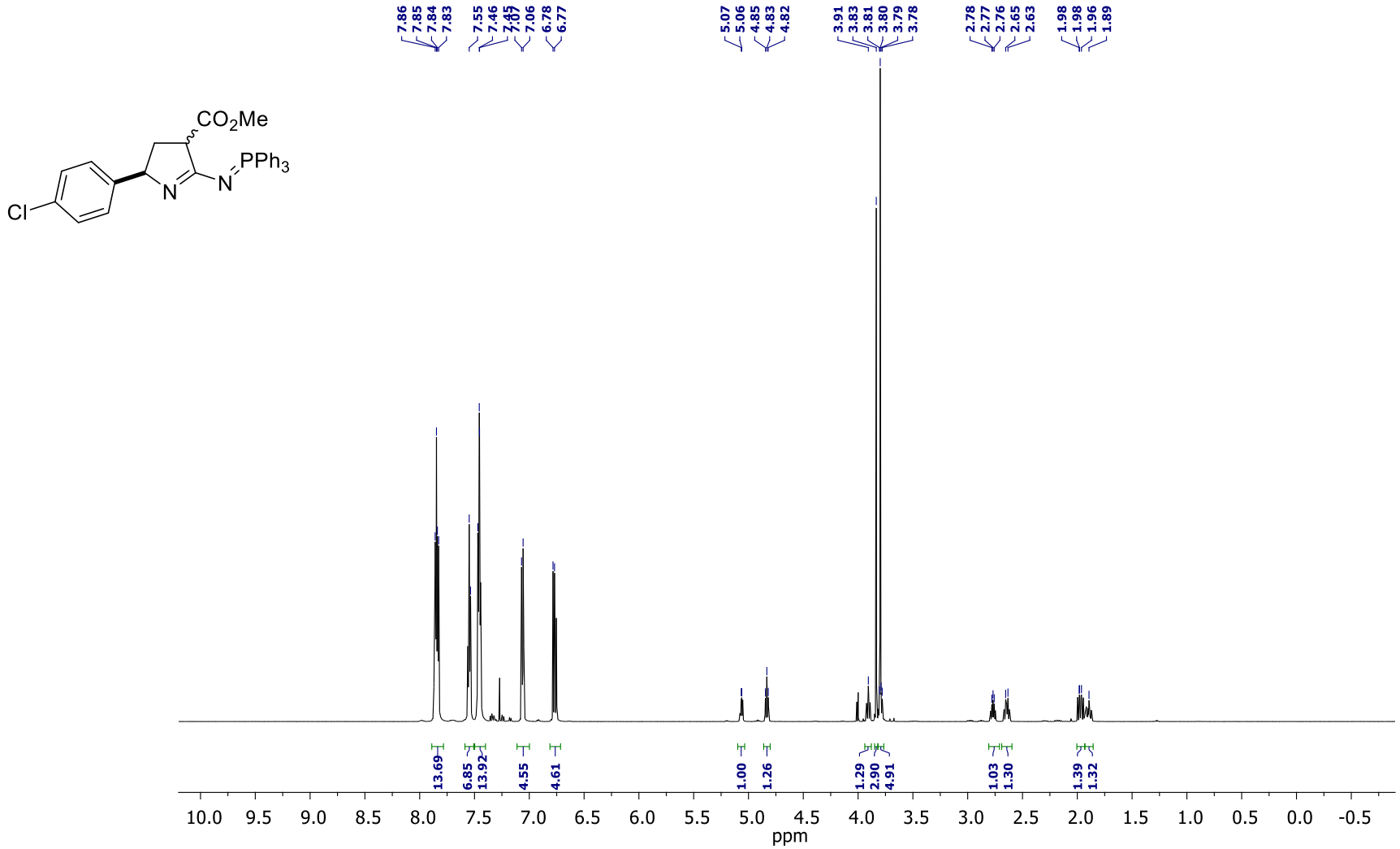


^{31}P NMR ($CDCl_3$, 162 MHz)



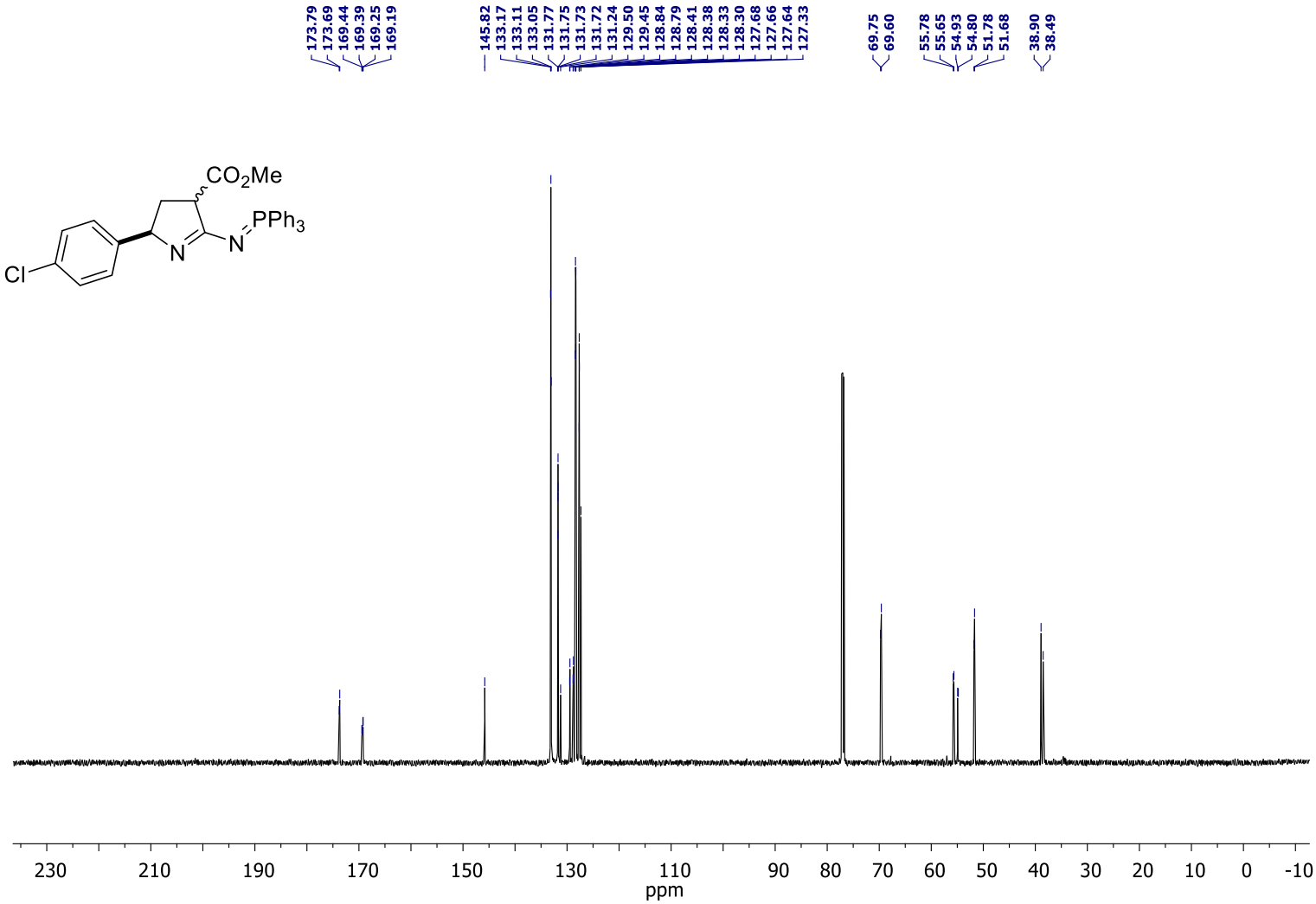
Methyl 2-(4-chlorophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3e)

^{1}H NMR (600 MHz, $CDCl_3$)

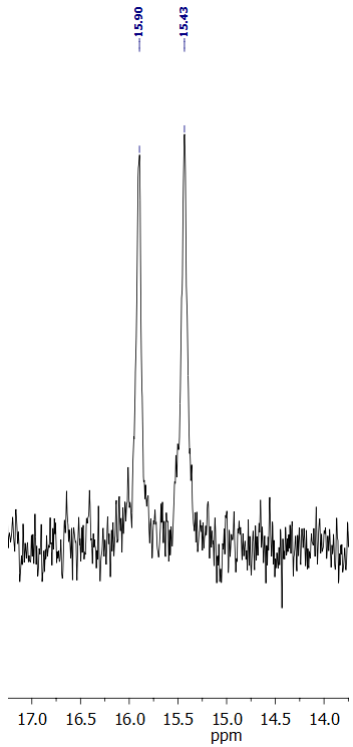


Methyl 2-(4-chlorophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3e)

^{13}C NMR (150 MHz, $CDCl_3$)

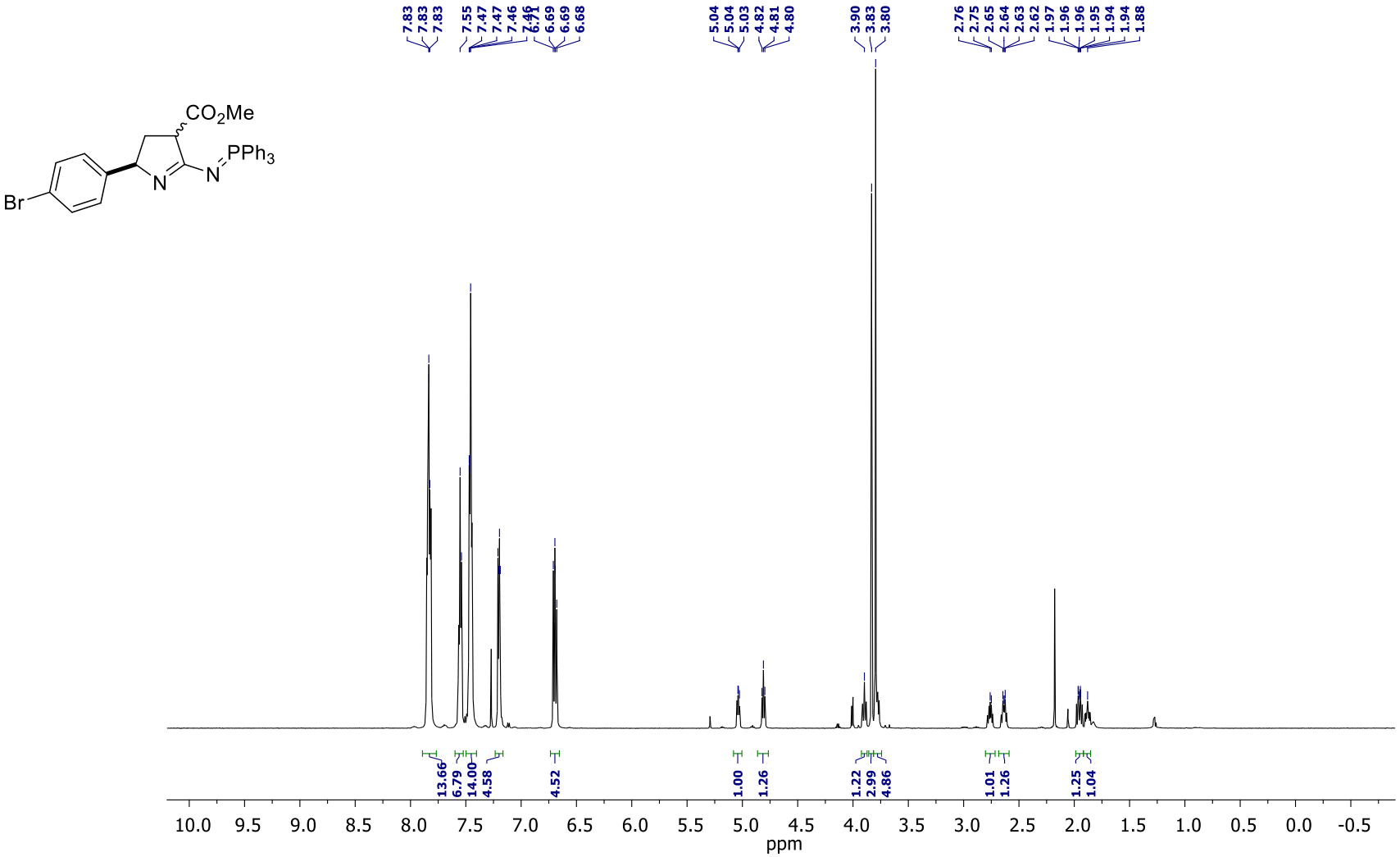


^{31}P NMR ($CDCl_3$, 162 MHz)



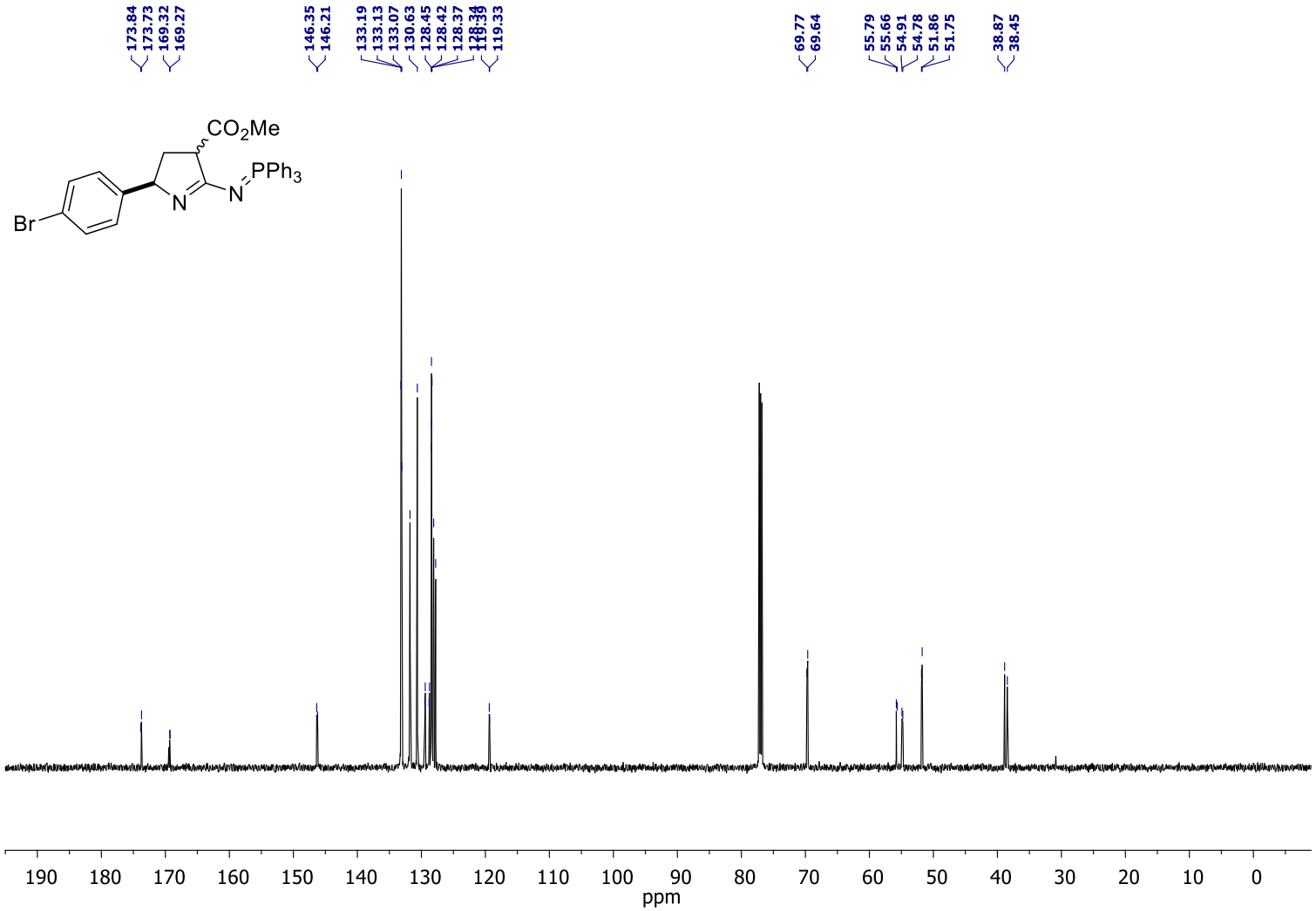
Methyl 2-(4-bromophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3f)

^{1}H NMR (600 MHz, $CDCl_3$)

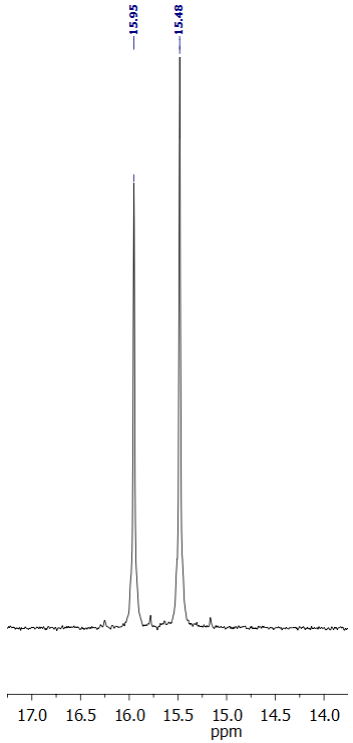


Methyl 2-(4-bromophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3f)

^{13}C NMR (150 MHz, $CDCl_3$)

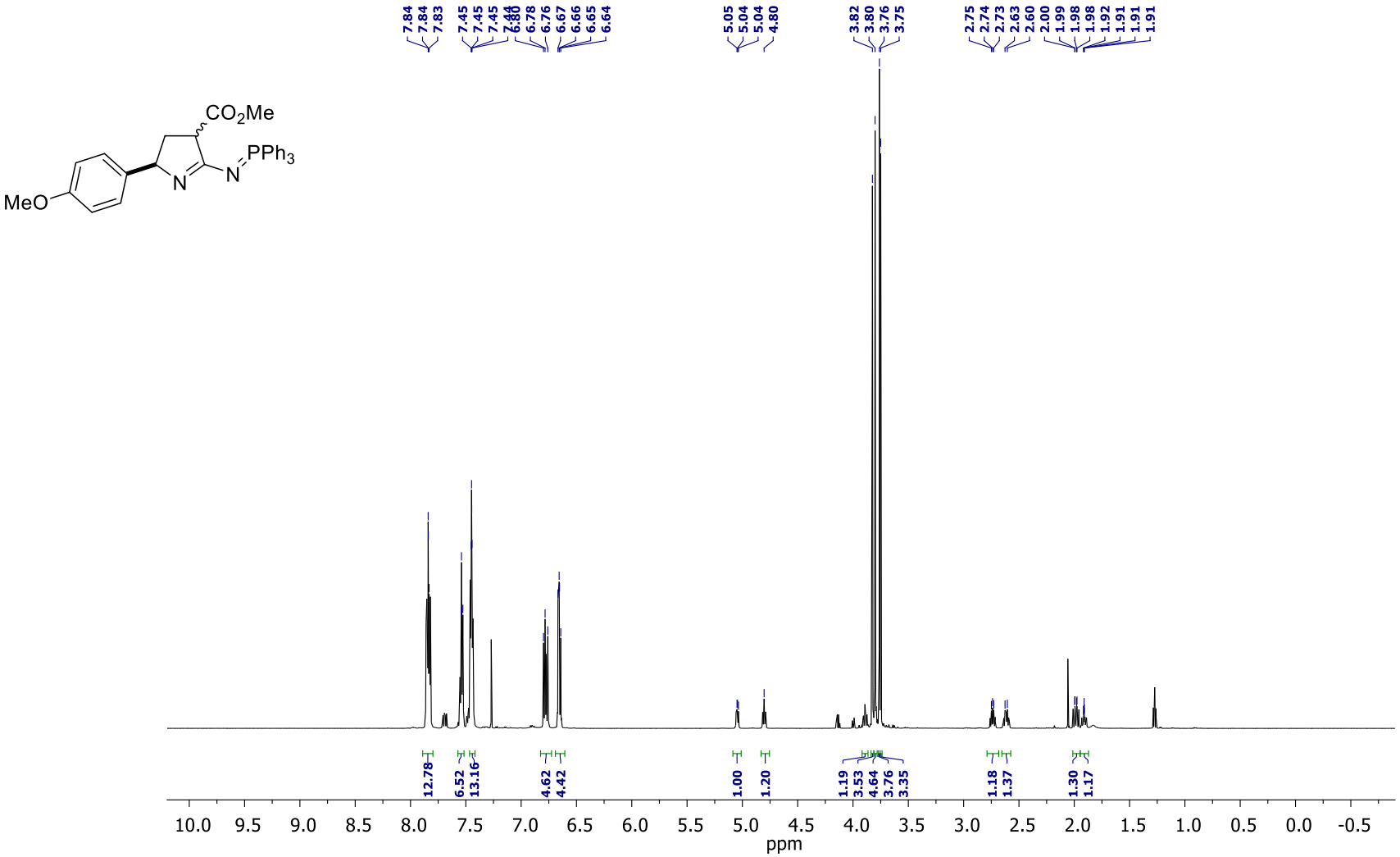


^{31}P NMR ($CDCl_3$, 162 MHz)



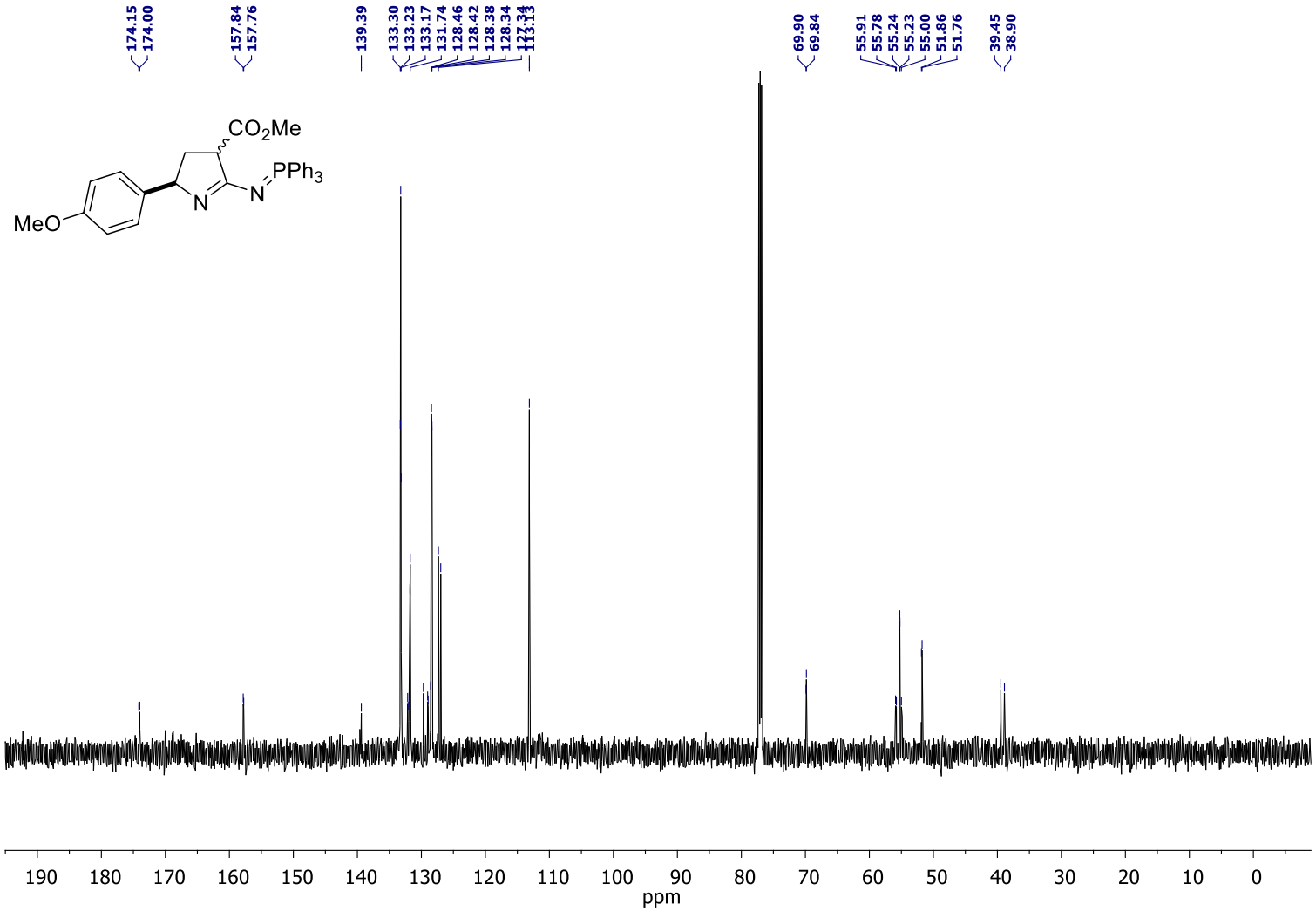
Methyl 2-(4-methoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3g)

^{1}H NMR (600 MHz, $CDCl_3$)

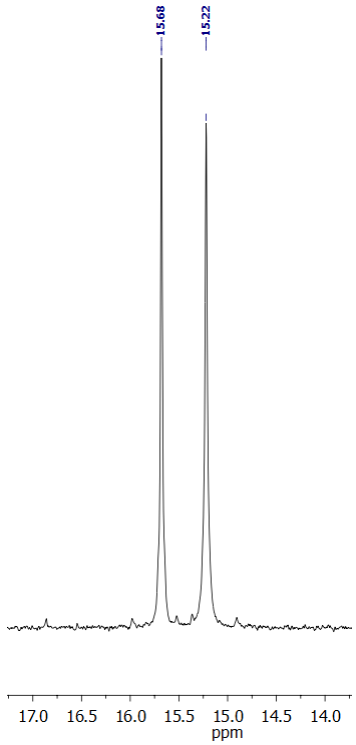


Methyl 2-(4-methoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3g)

^{13}C NMR (150 MHz, $CDCl_3$)

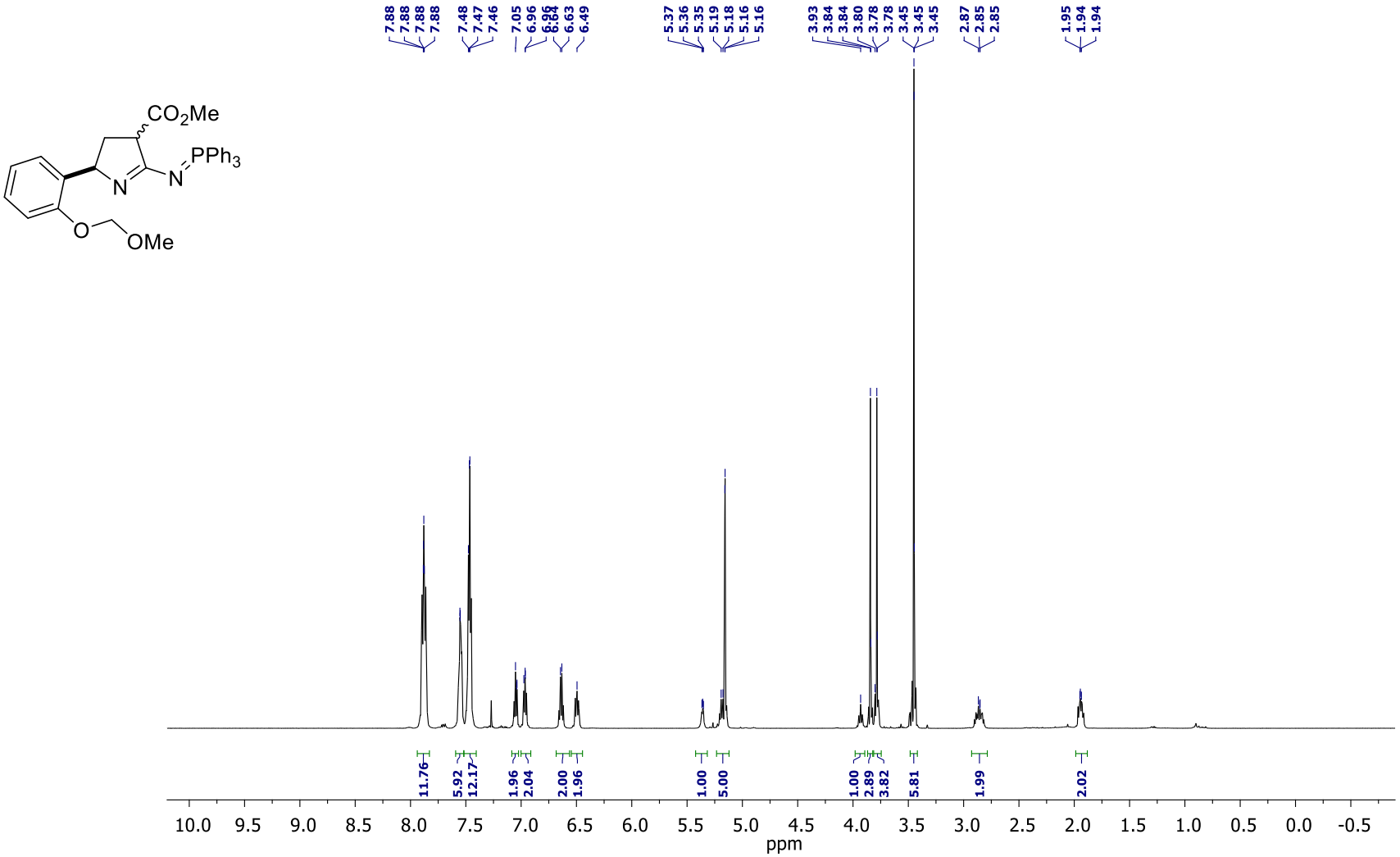


^{31}P NMR ($CDCl_3$, 162 MHz)



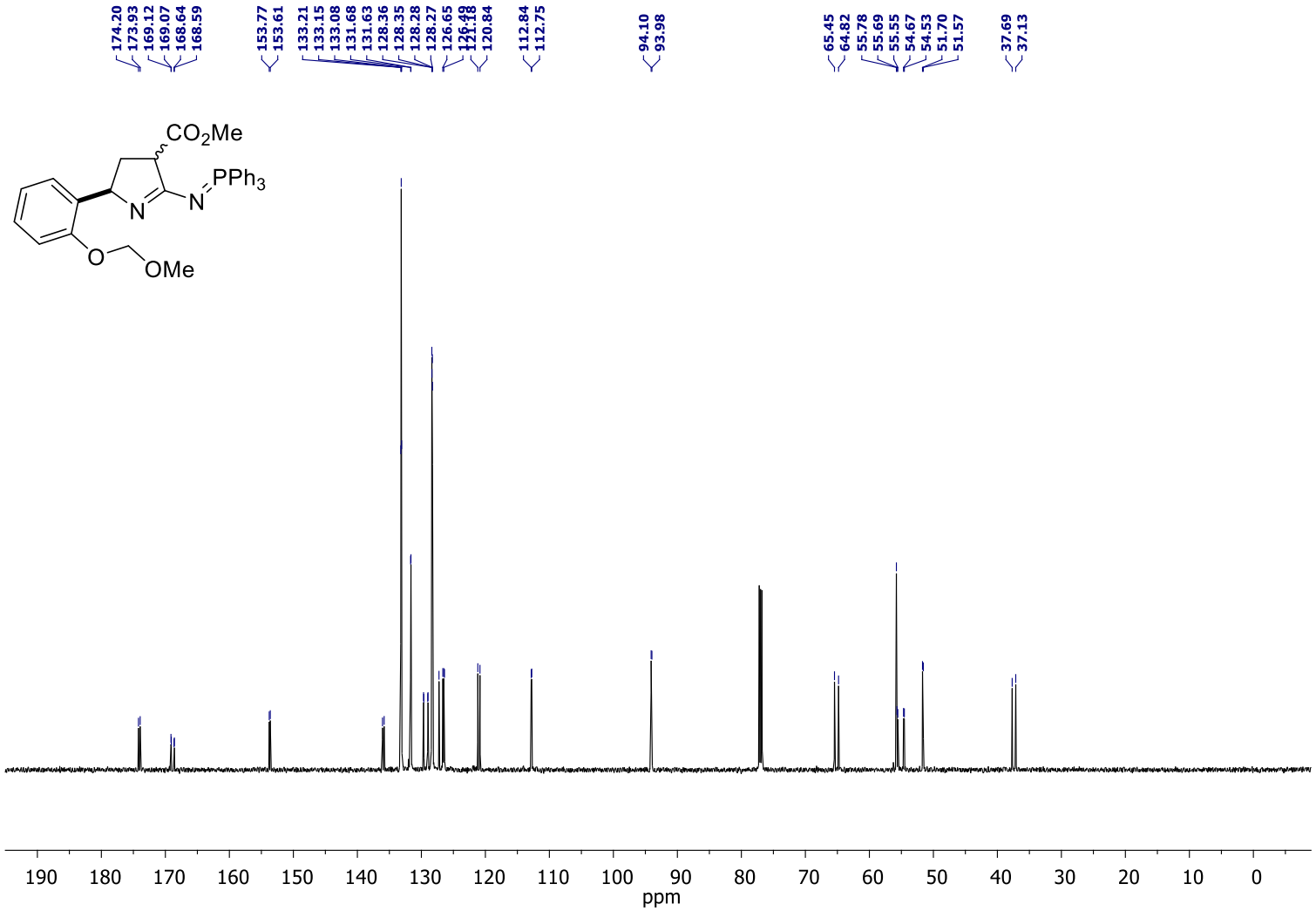
Methyl 2-(2-methoxymethoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3h)

^{1}H NMR (600 MHz, $CDCl_3$)

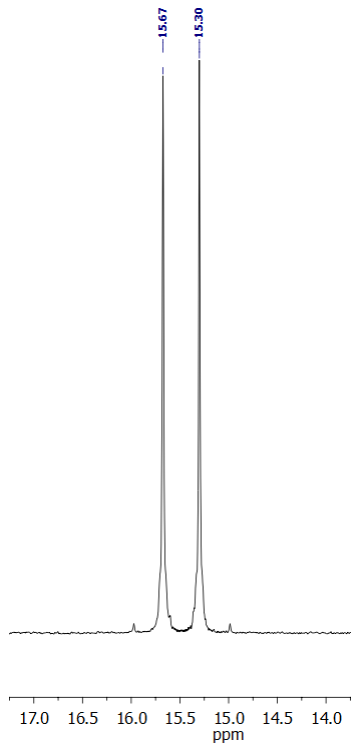


Methyl 2-(2-methoxymethoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3h)

^{13}C NMR (150 MHz, $CDCl_3$)

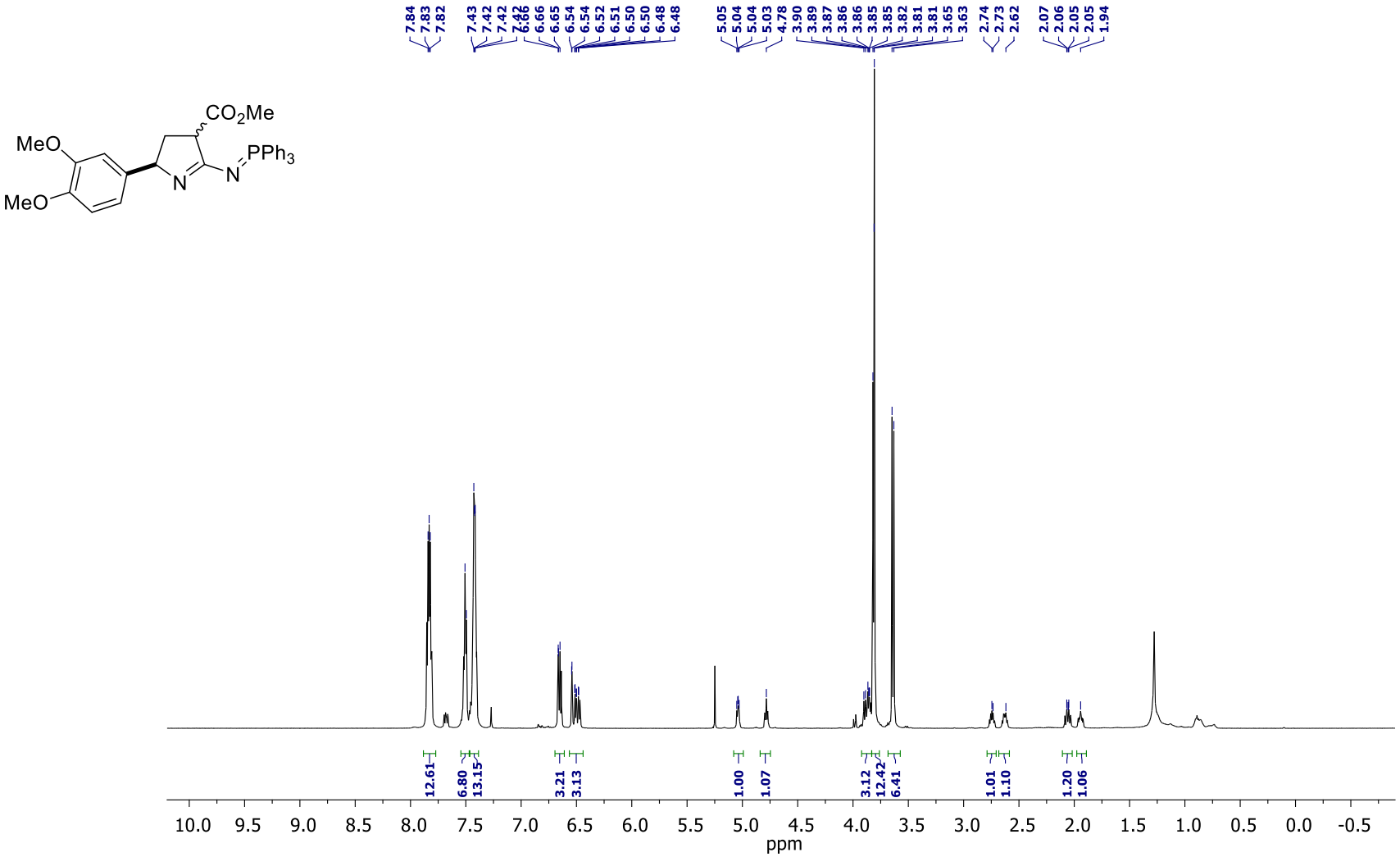


^{31}P NMR ($CDCl_3$, 162 MHz)



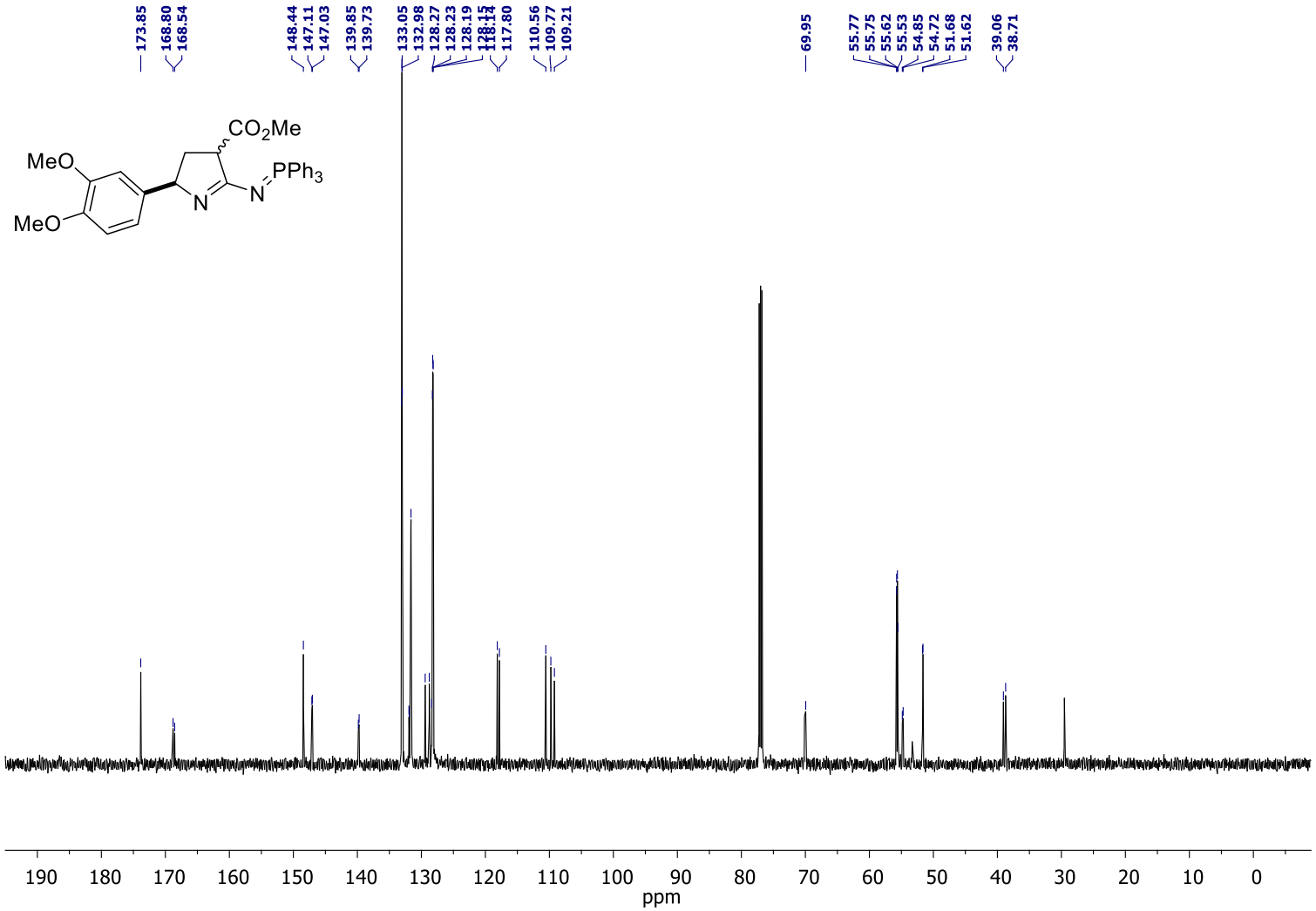
Methyl 2-(3,4-dimethoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3i)

^{1}H NMR (600 MHz, $CDCl_3$)

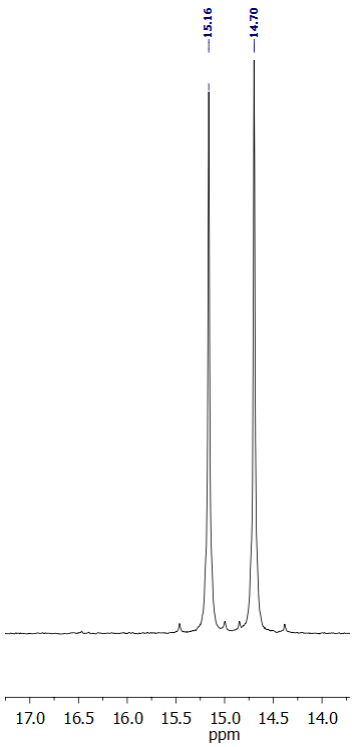


Methyl 2-(3,4-dimethoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3i)

^{13}C NMR (150 MHz, $CDCl_3$)

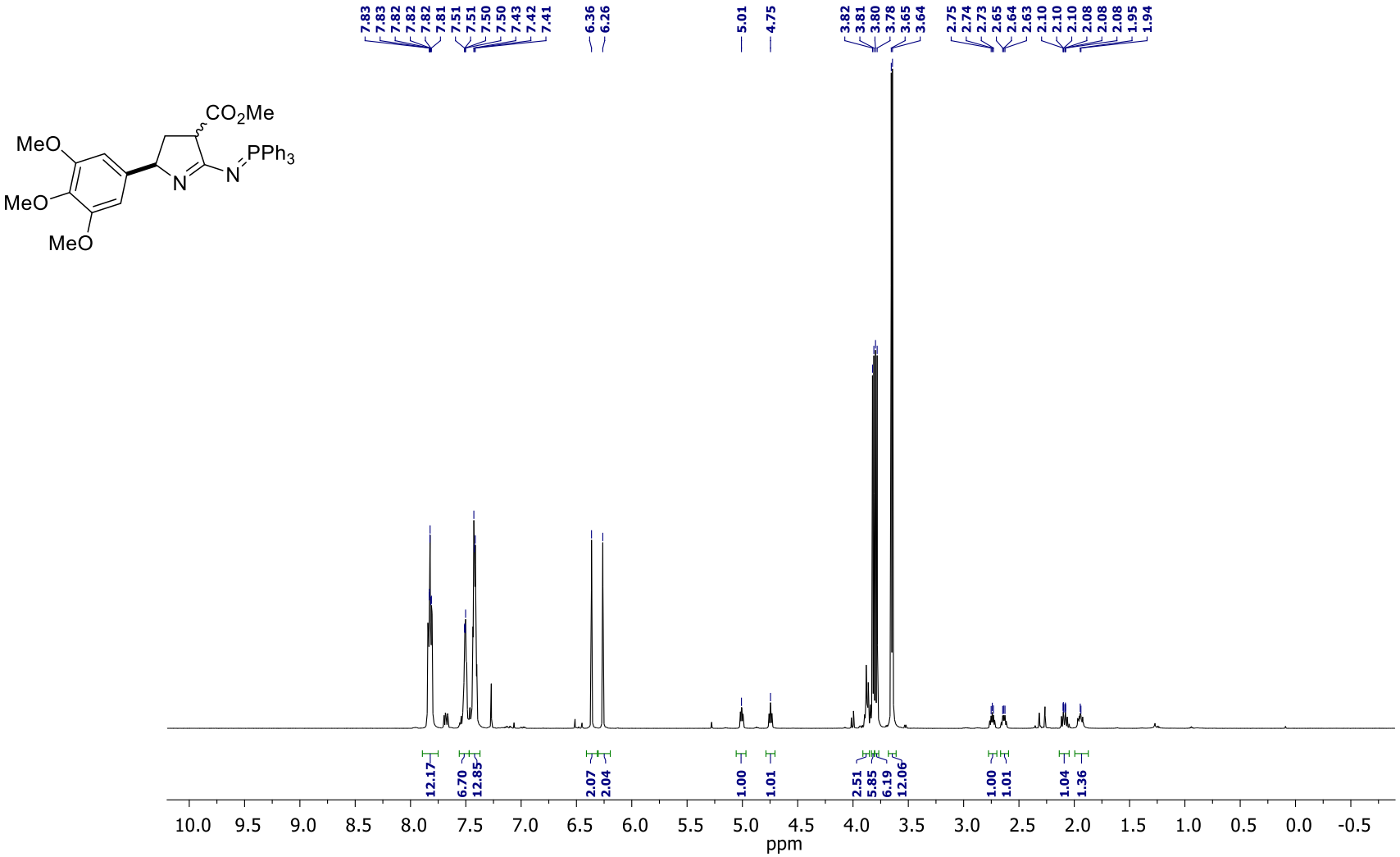


^{31}P NMR ($CDCl_3$, 162 MHz)



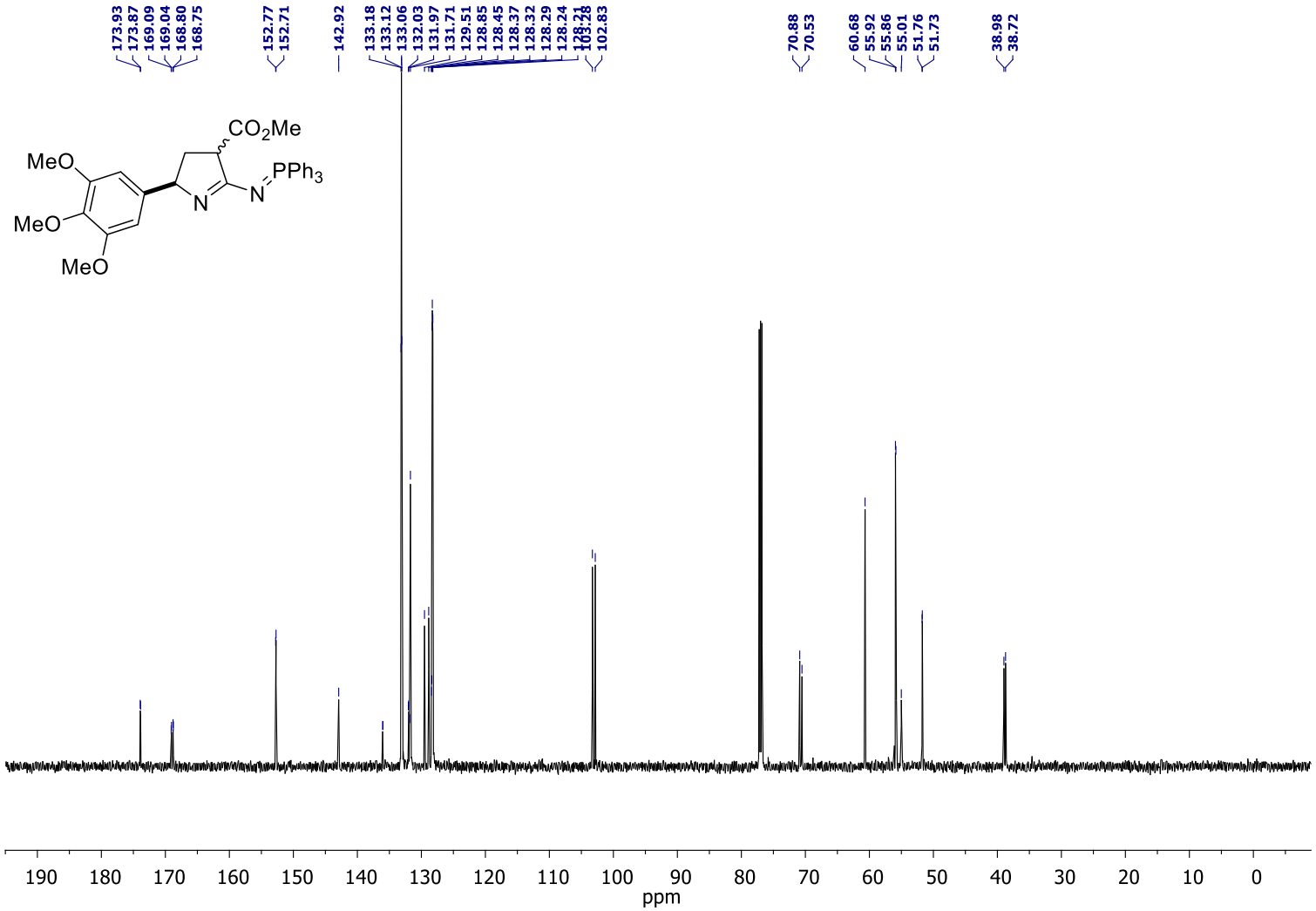
Methyl 2-(3,4,5-trimethoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3j)

^{1}H NMR (600 MHz, $CDCl_3$)

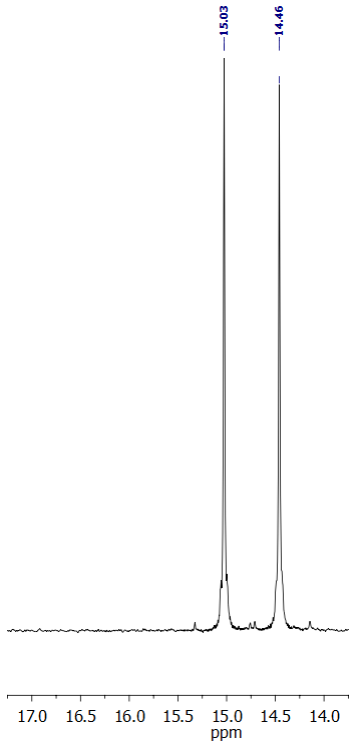


Methyl 2-(3,4,5-trimethoxyphenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3j)

^{13}C NMR (150 MHz, $CDCl_3$)

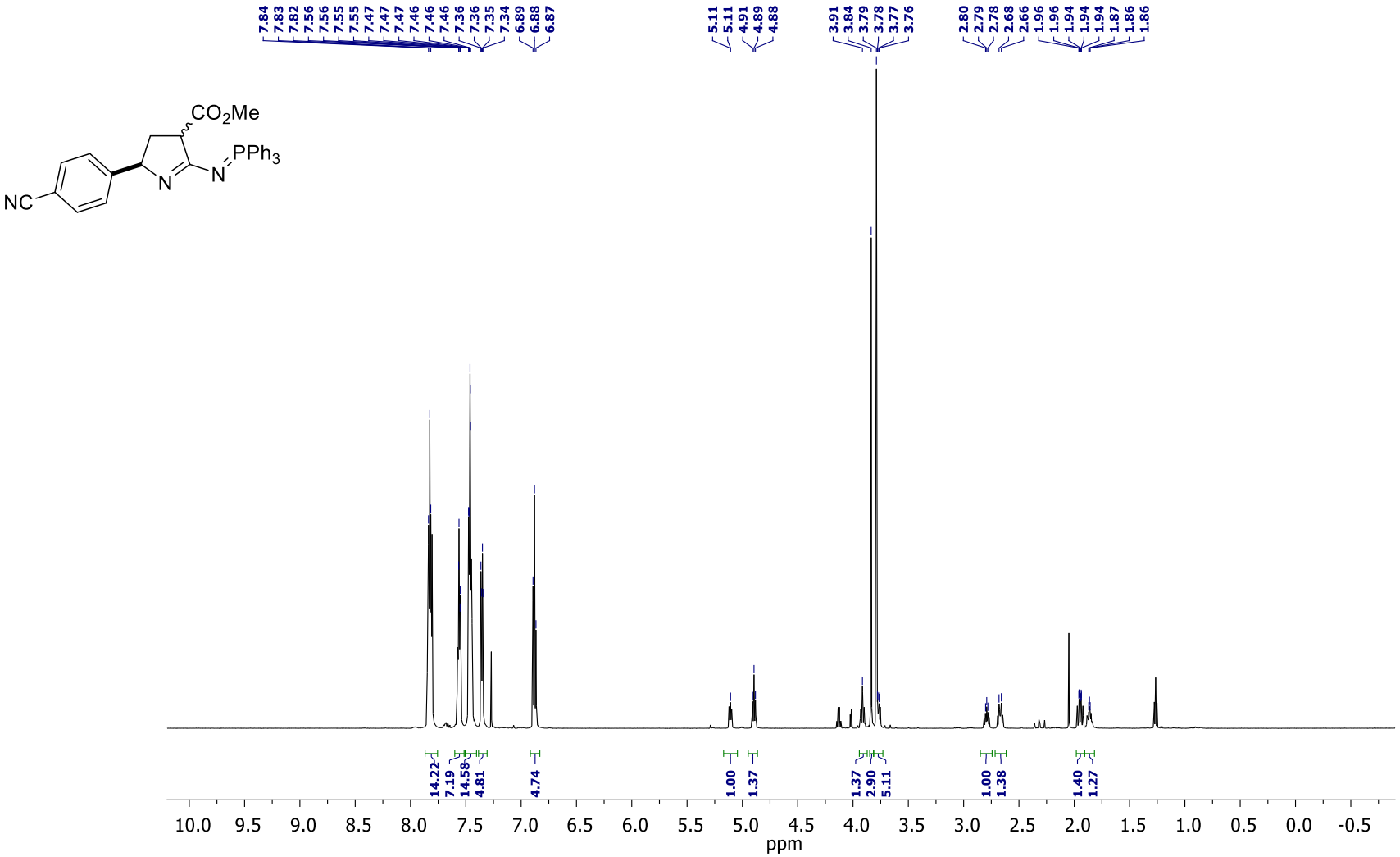


^{31}P NMR ($CDCl_3$, 162 MHz)



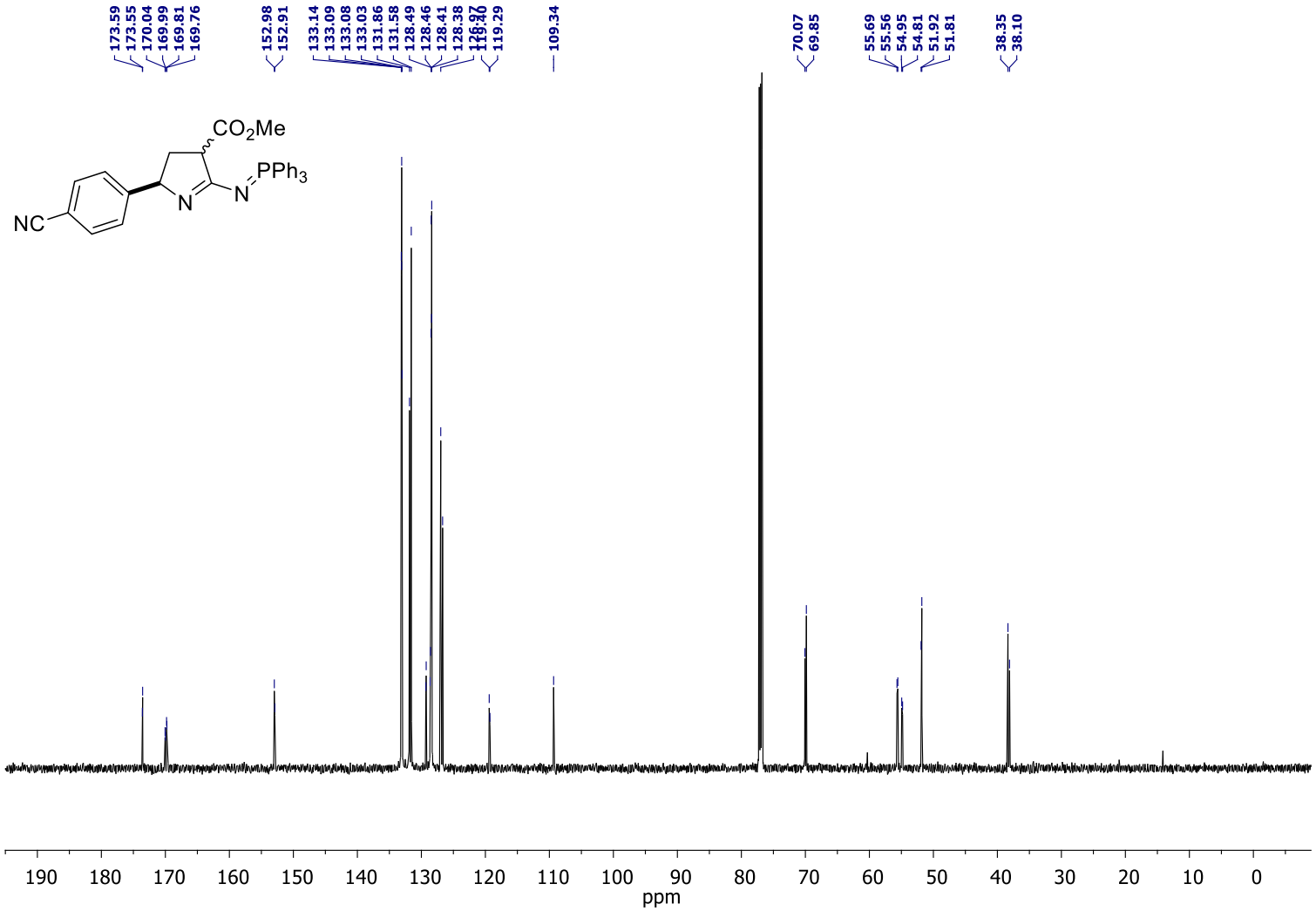
Methyl 2-(4-cyanophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3k)

^{1}H NMR (600 MHz, $CDCl_3$)

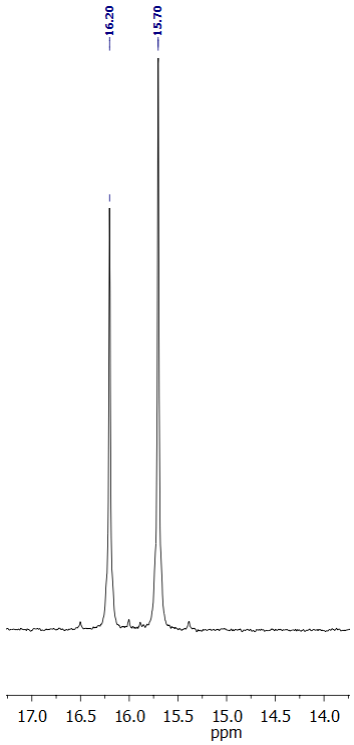


Methyl 2-(4-cyanophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3k)

^{13}C NMR (150 MHz, $CDCl_3$)

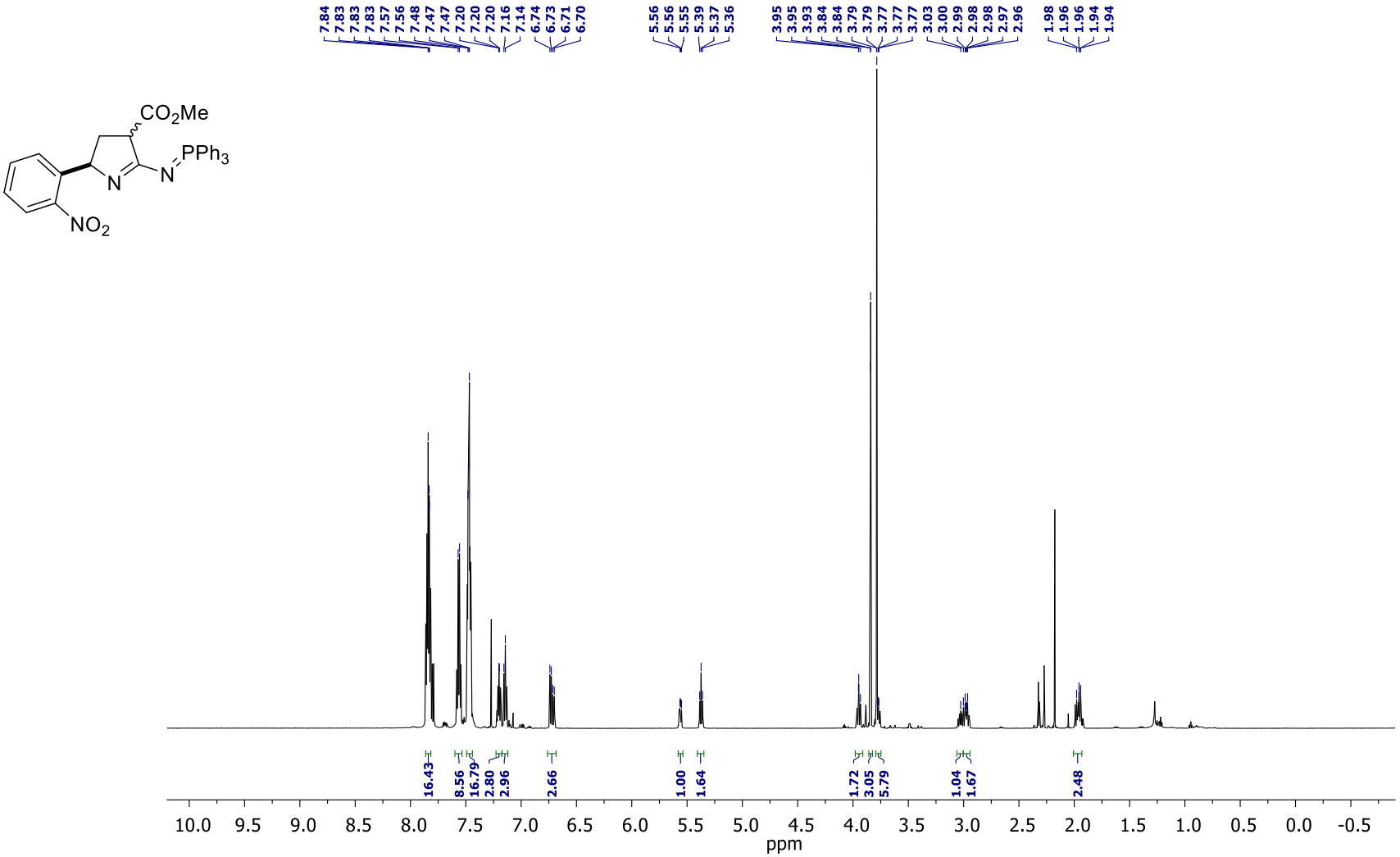


^{31}P NMR ($CDCl_3$, 162 MHz)



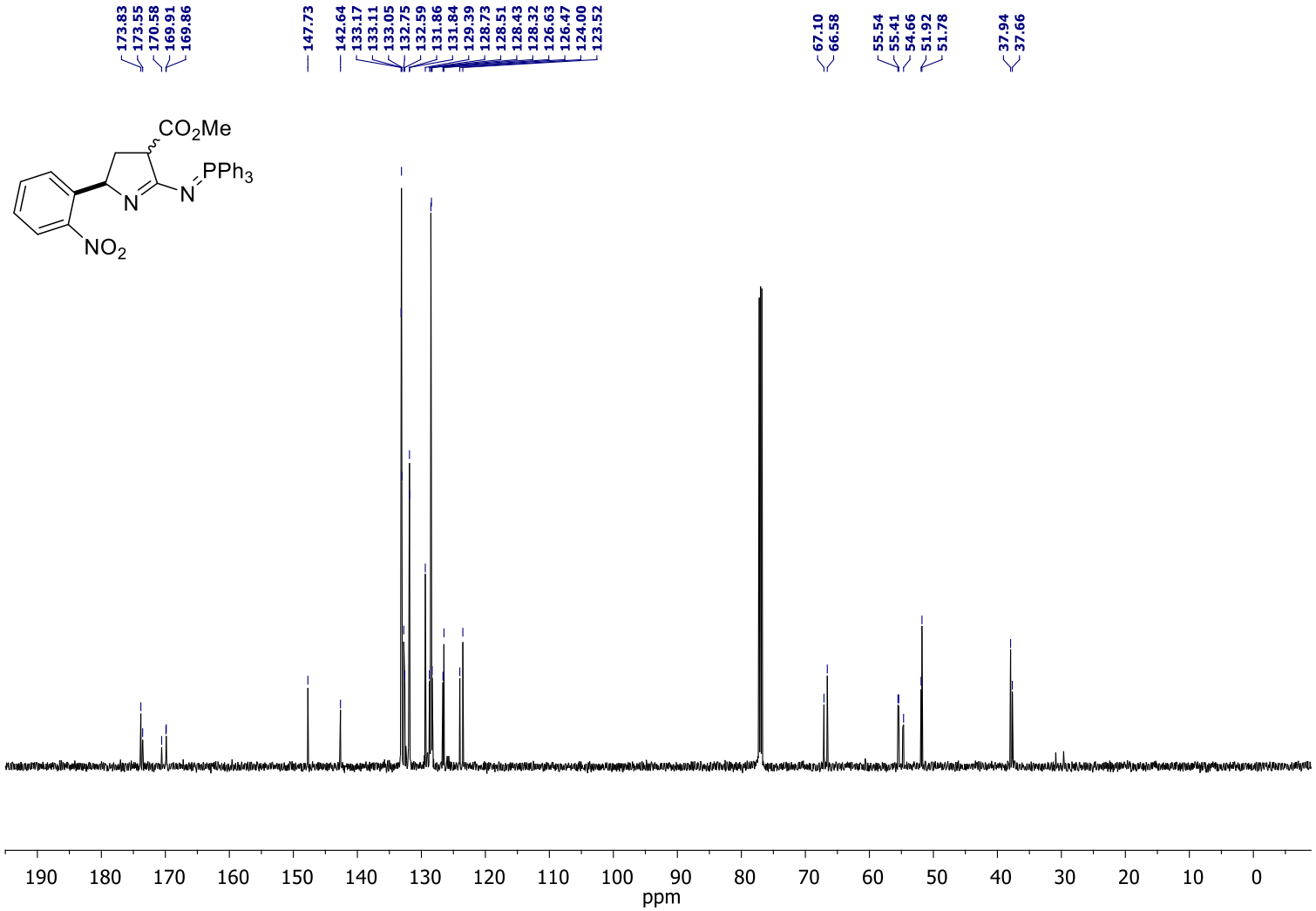
Methyl 2-(2-nitrophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3l)

^{1}H NMR (600 MHz, $CDCl_3$)

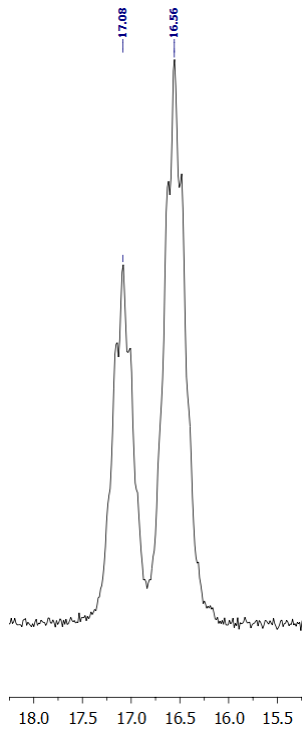


Methyl 2-(2-nitrophenyl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3l)

^{13}C NMR (150 MHz, $CDCl_3$)

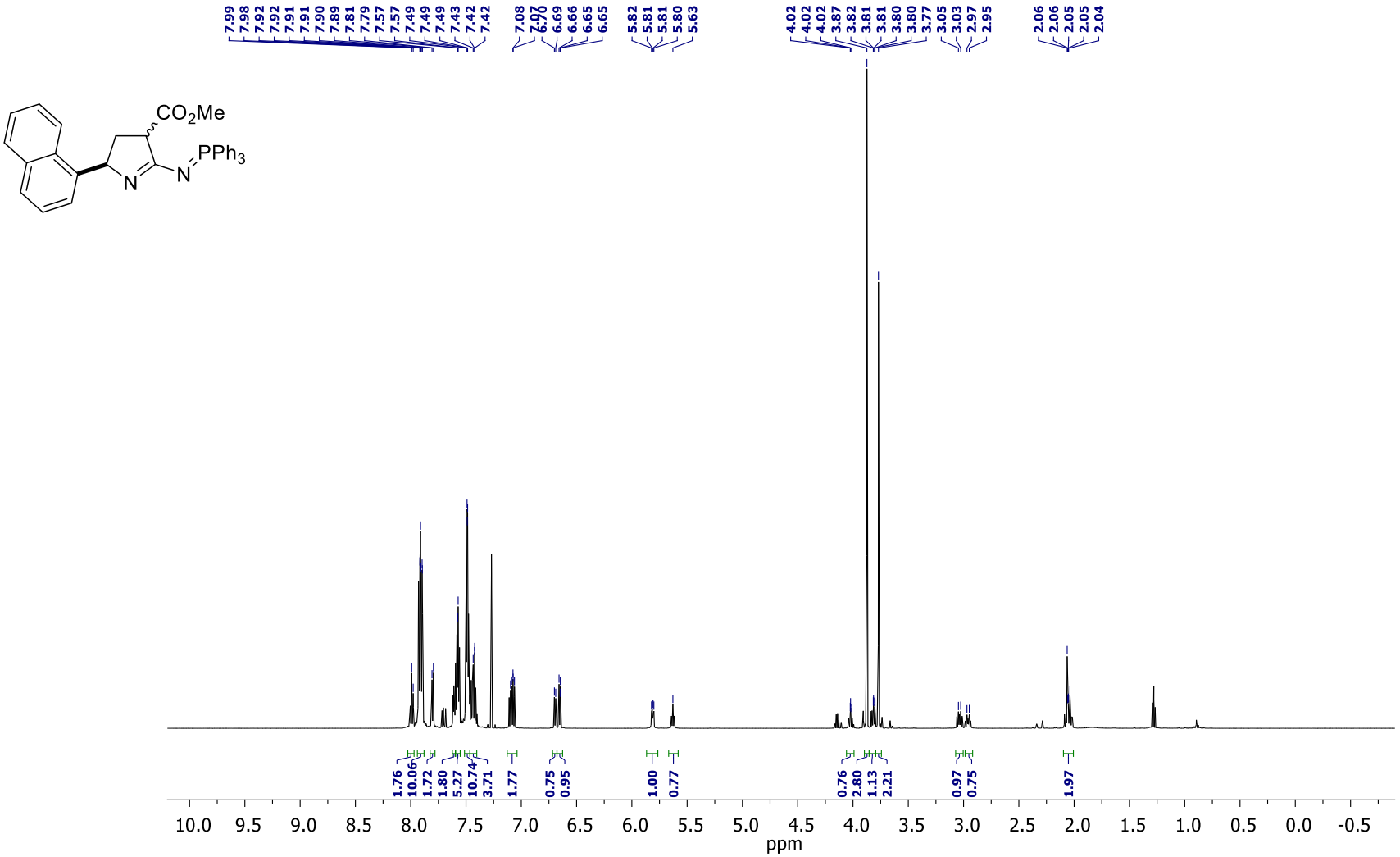


^{31}P NMR ($CDCl_3$, 162 MHz)



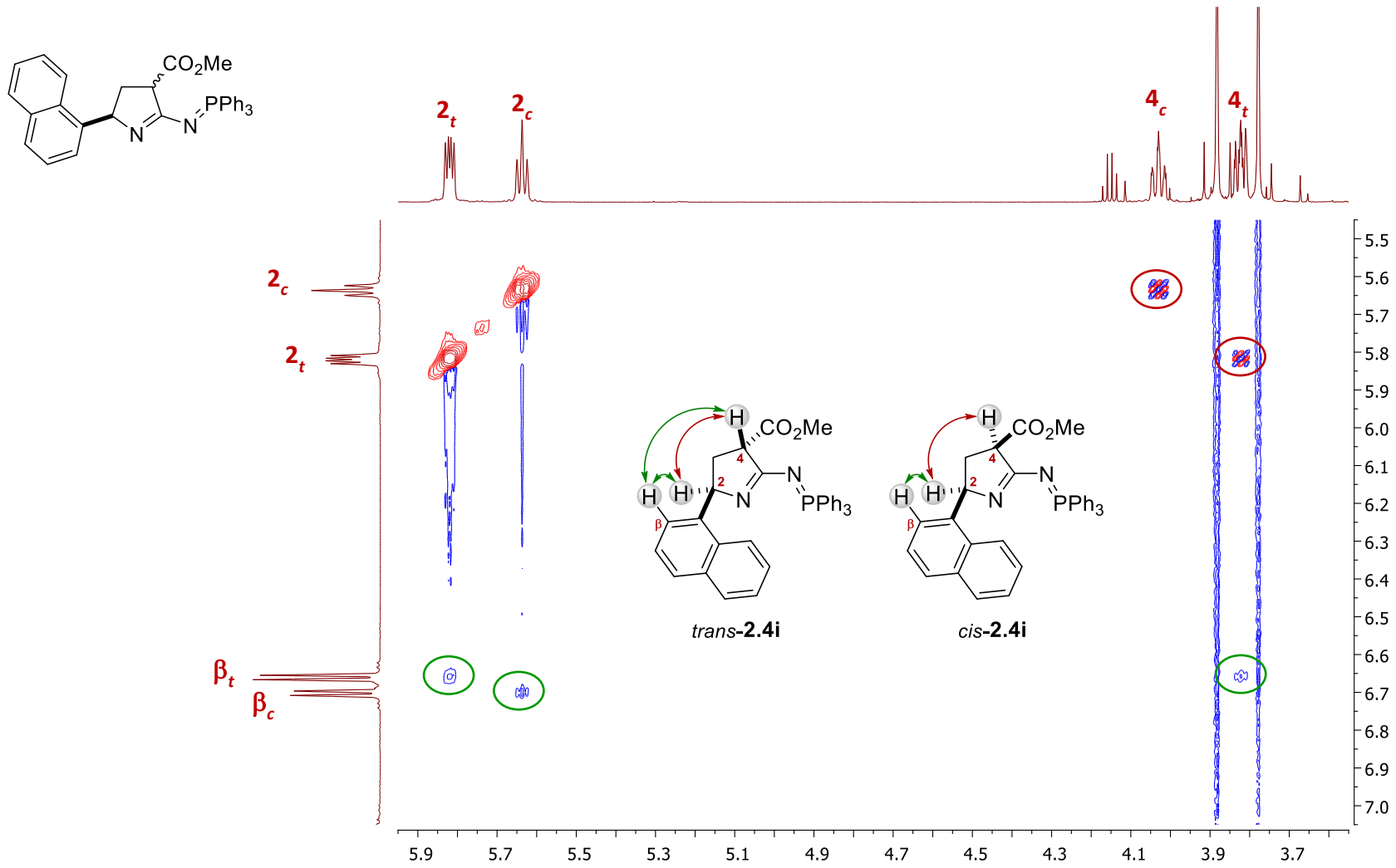
Methyl 2-(naphthalen-1-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3m)

^{1}H NMR (600 MHz, $CDCl_3$)



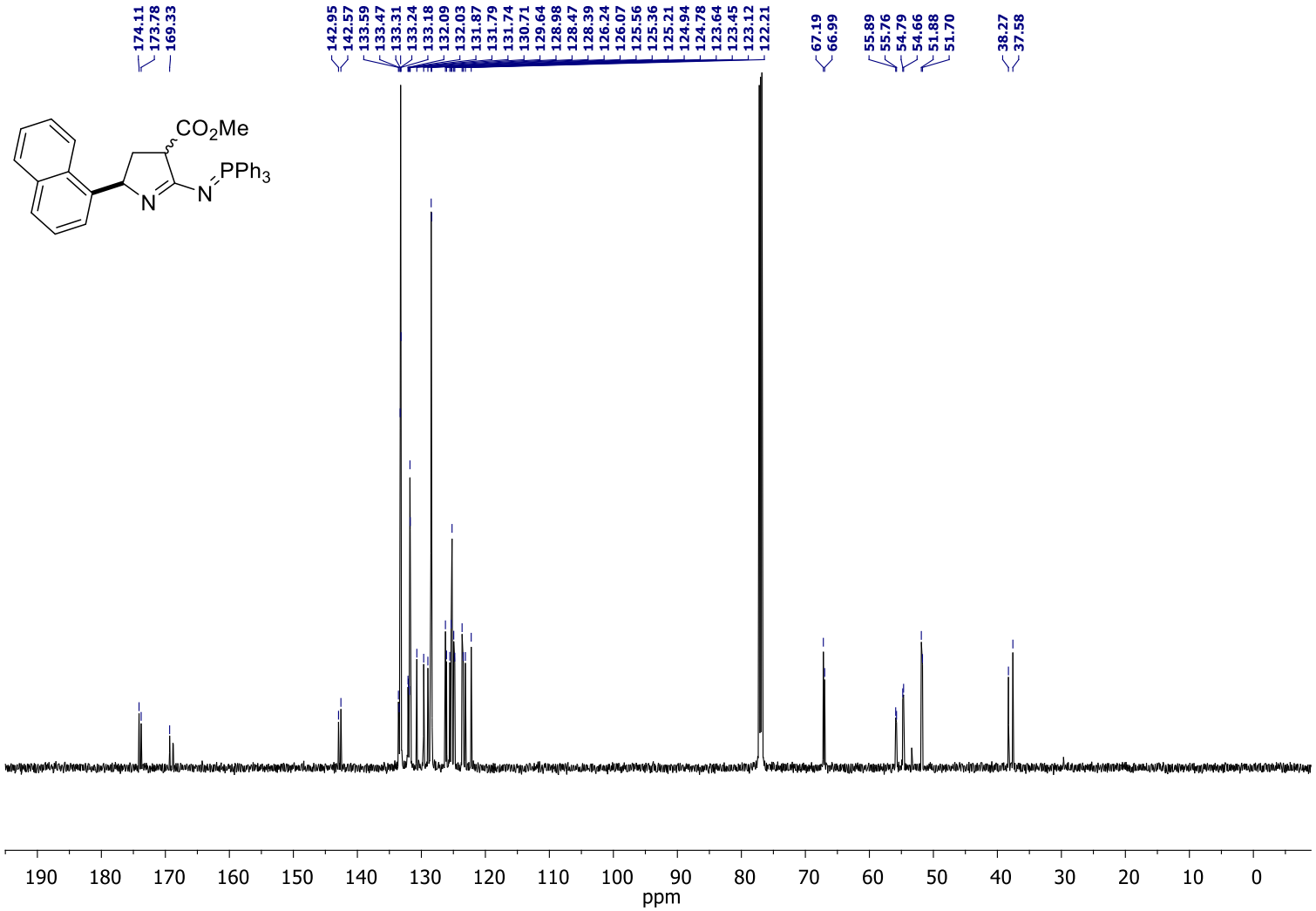
Methyl 2-(naphthalen-1-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3m)

^{1}H-^{1}H NOESY ($CDCl_3$)

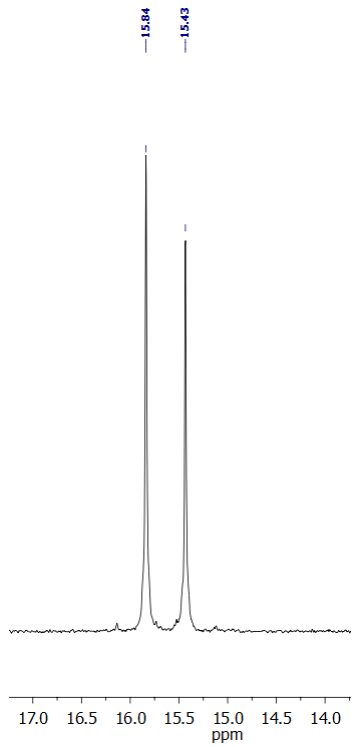


Methyl 2-(naphthalen-1-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3m)

^{13}C NMR (150 MHz, $CDCl_3$)

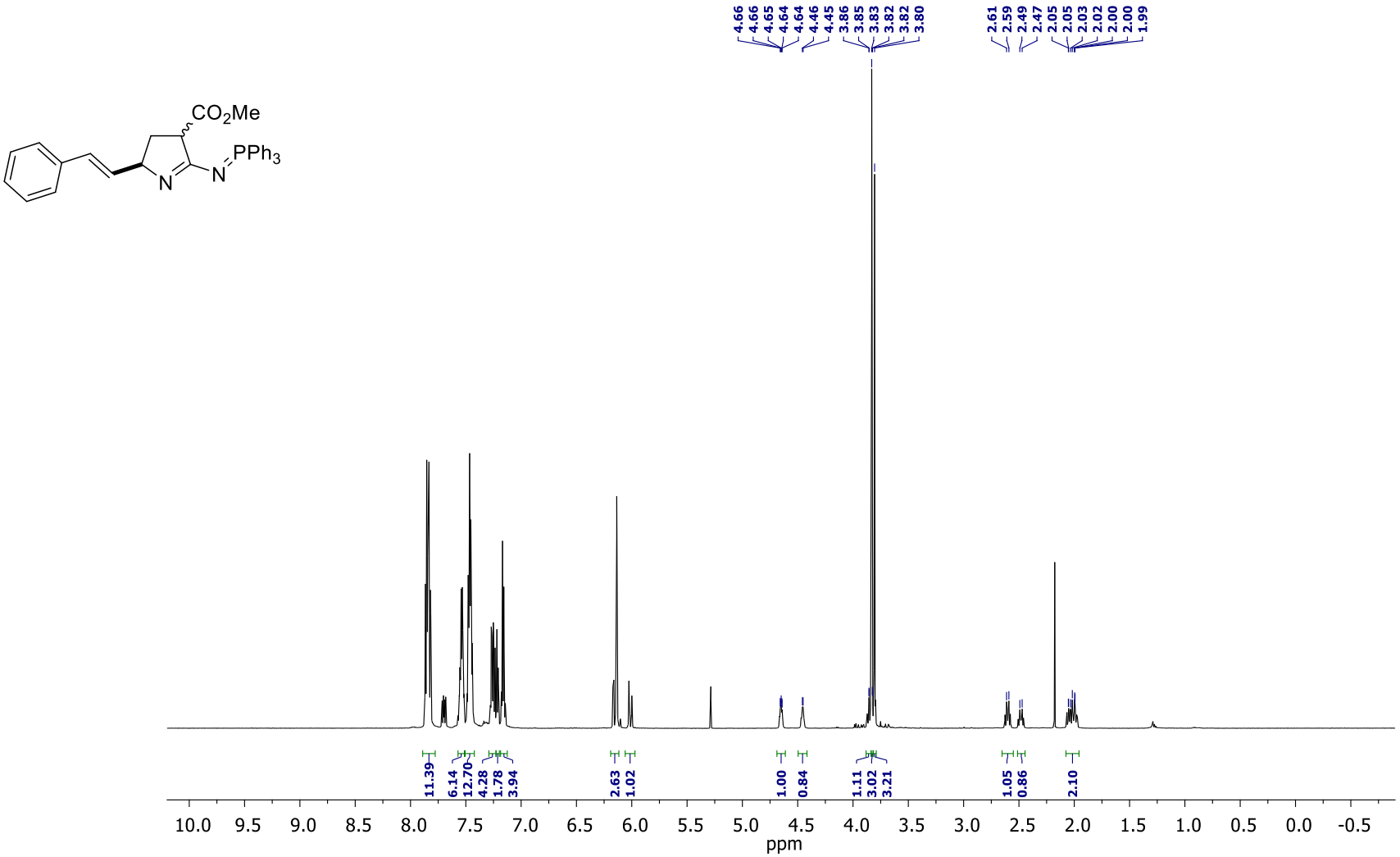


^{31}P NMR ($CDCl_3$, 162 MHz)



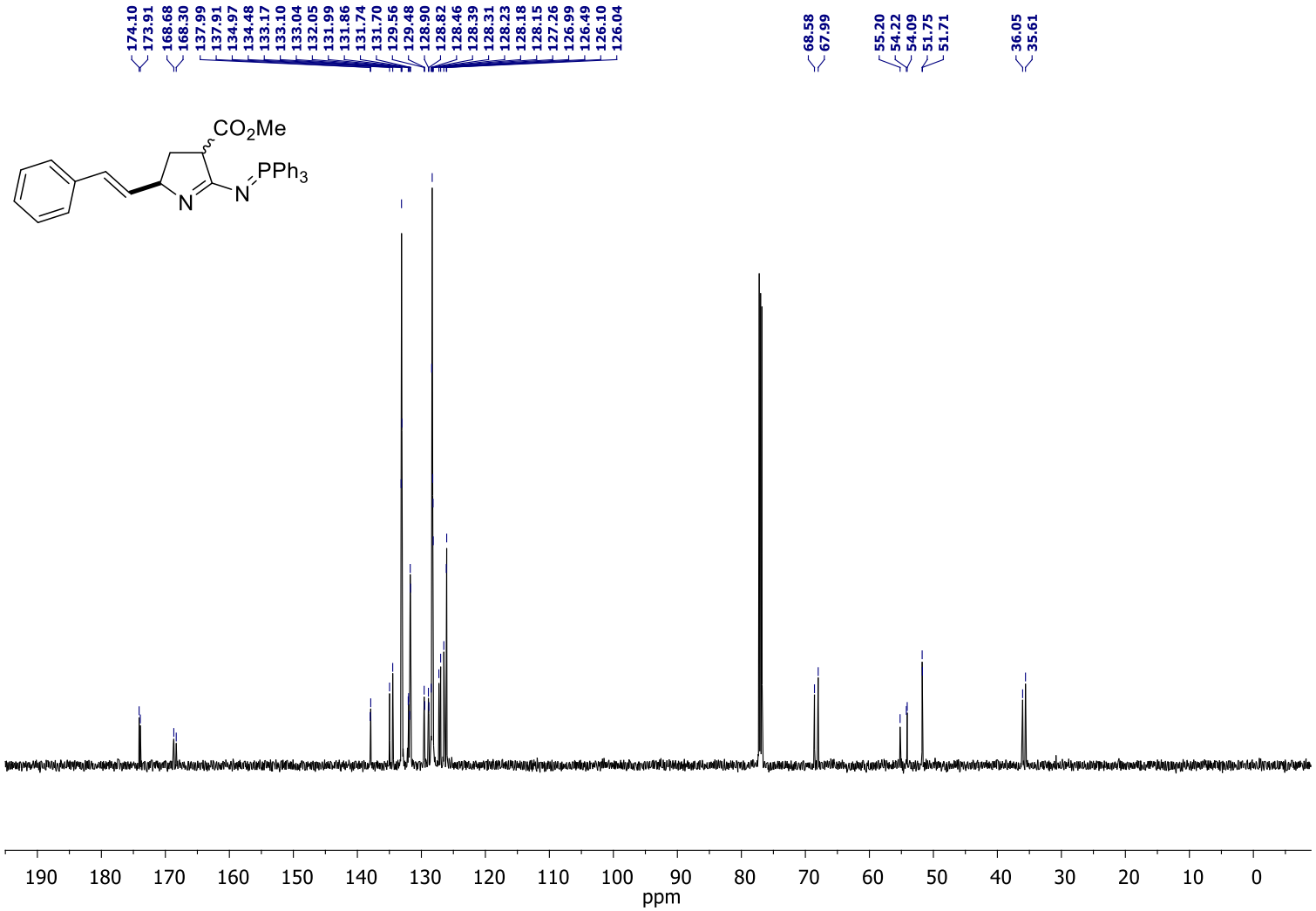
Methyl (*E*)-2-styryl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3n)

^{1}H NMR (600 MHz, $CDCl_3$)

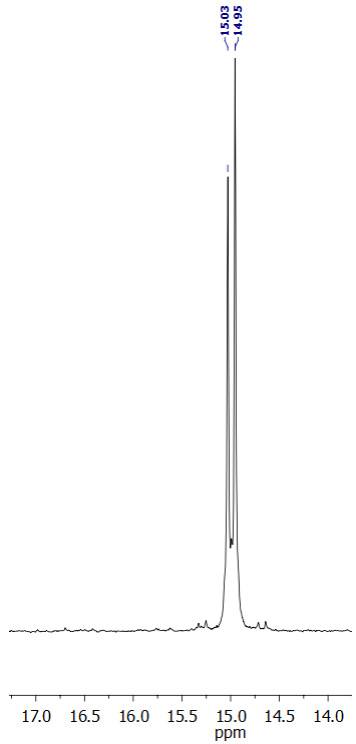


Methyl (*E*)-2-styryl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3n)

^{13}C NMR (150 MHz, $CDCl_3$)

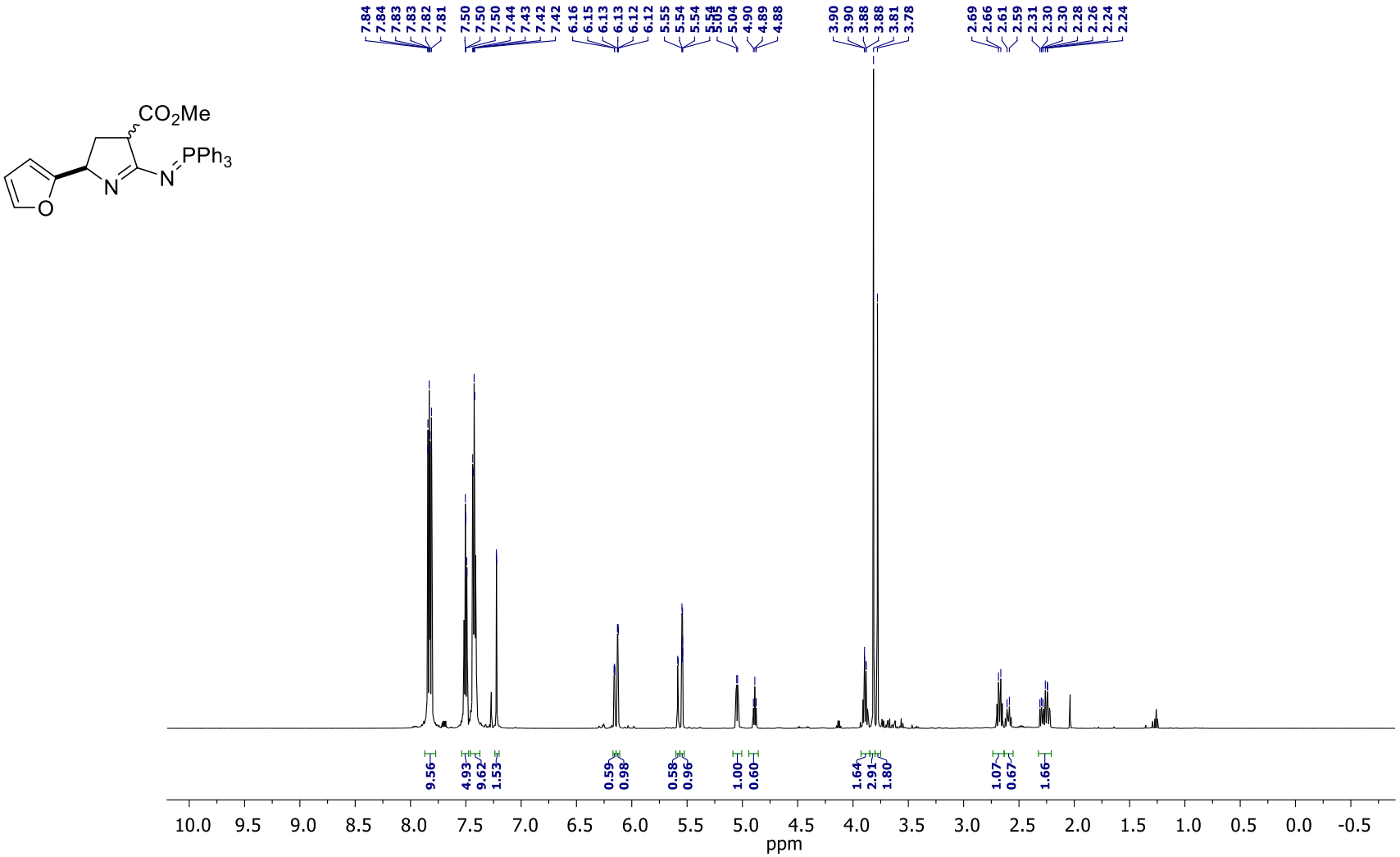


^{31}P NMR ($CDCl_3$, 162 MHz)



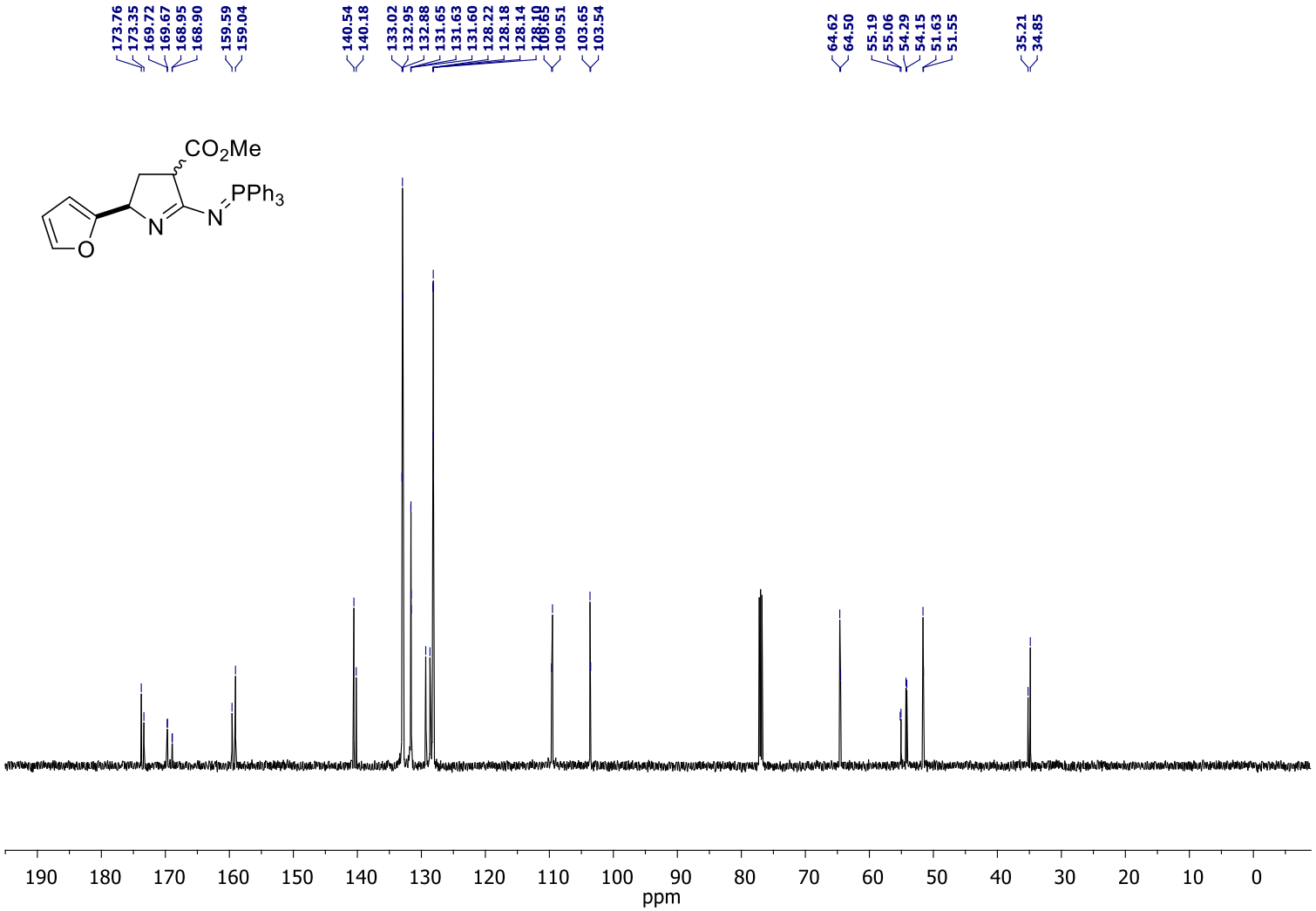
Methyl 2-(furan-2-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3o)

^{1}H NMR (600 MHz, $CDCl_3$)

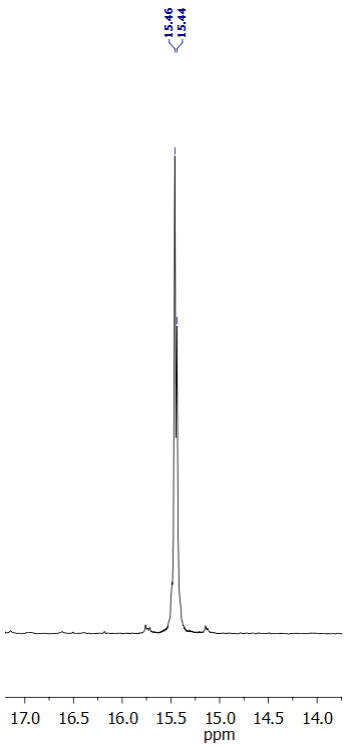


Methyl 2-(furan-2-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3o)

^{13}C NMR (150 MHz, $CDCl_3$)

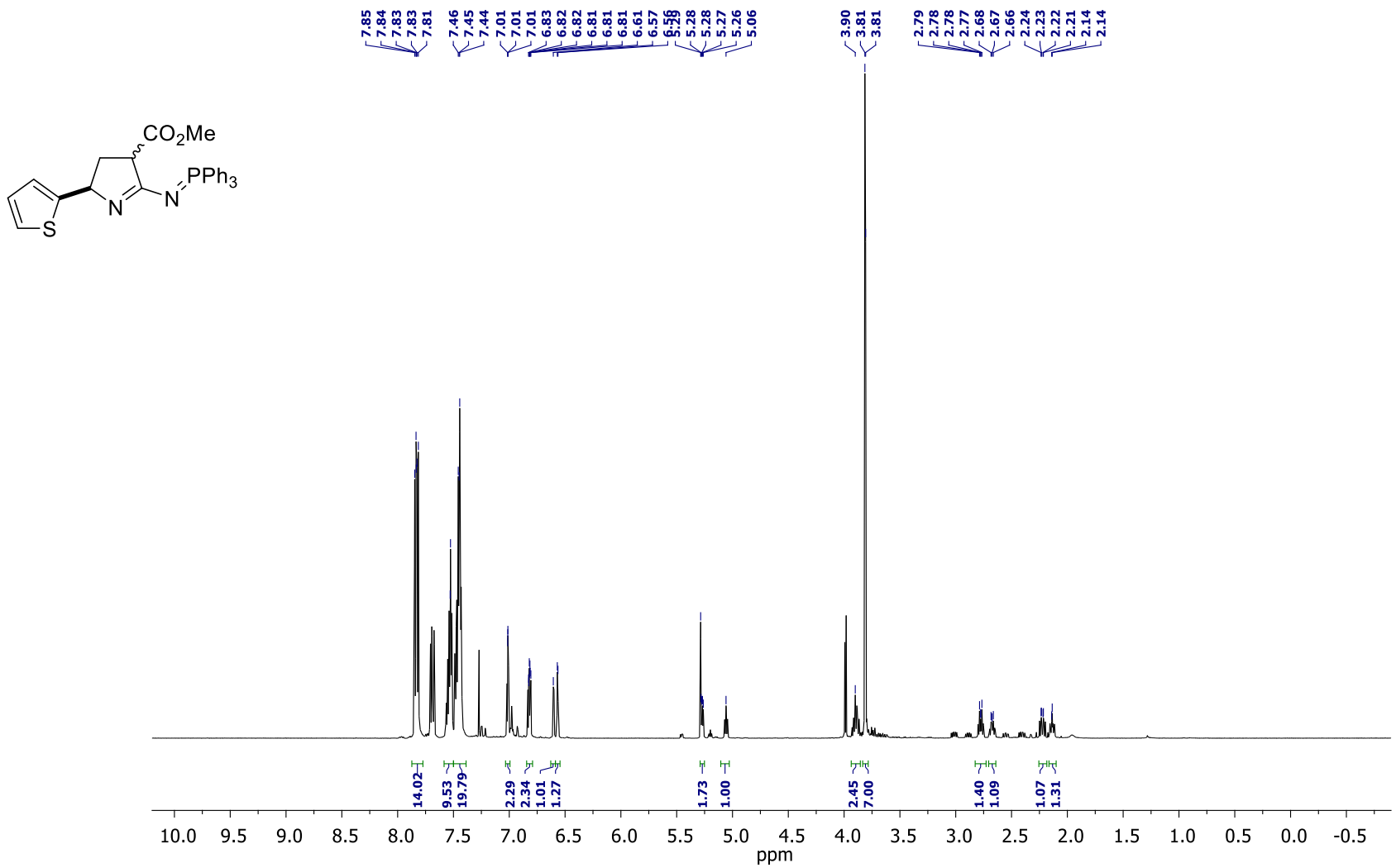


^{31}P NMR ($CDCl_3$, 162 MHz)



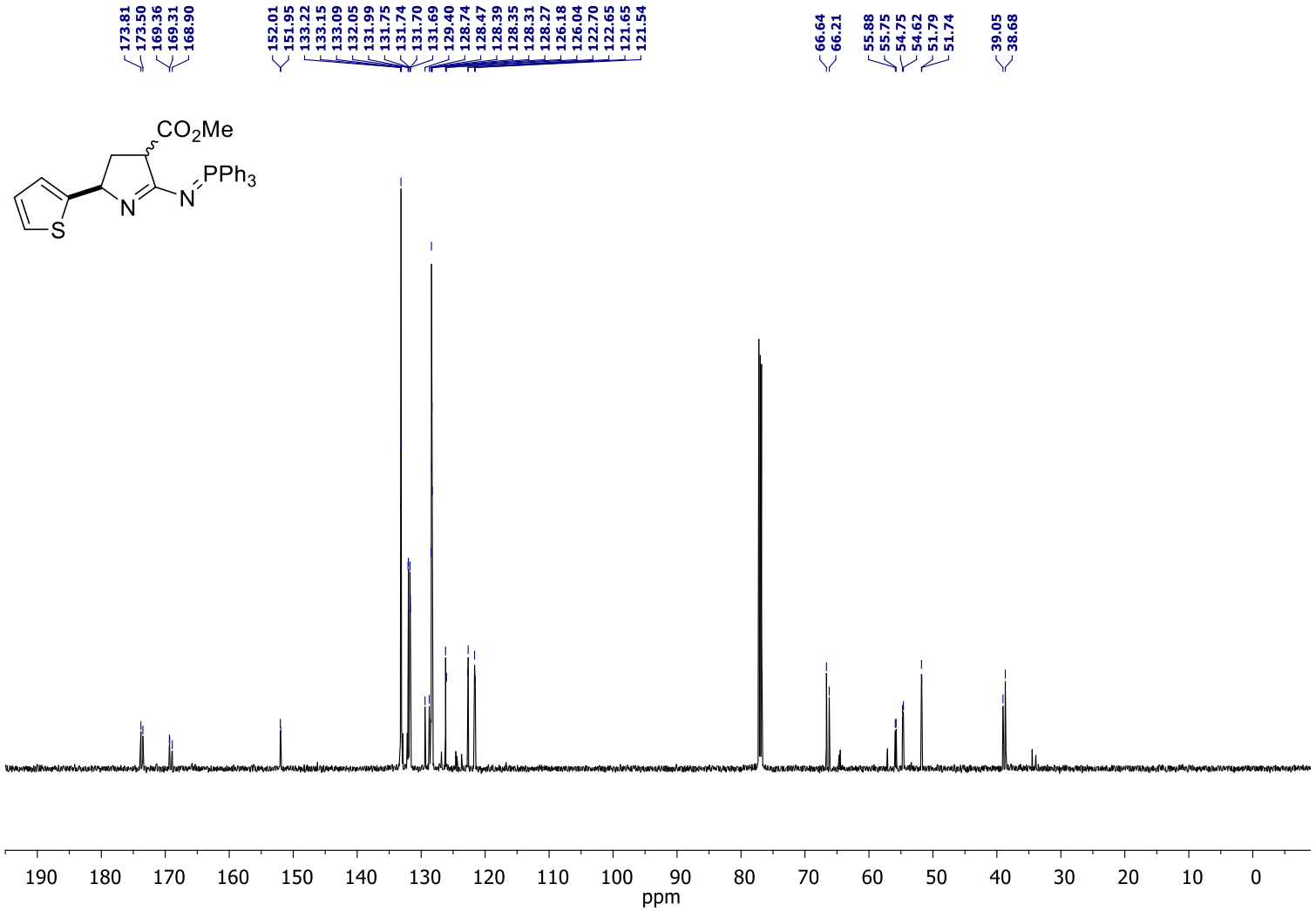
Methyl 2-(thien-2-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3p)

^{1}H NMR (600 MHz, $CDCl_3$)

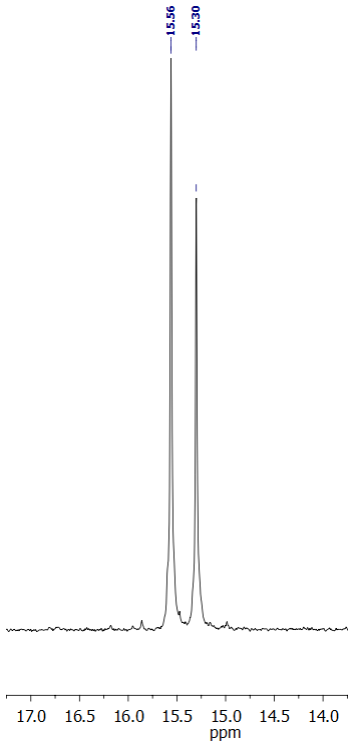


Methyl 2-(thien-2-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3p)

^{13}C NMR (150 MHz, $CDCl_3$)

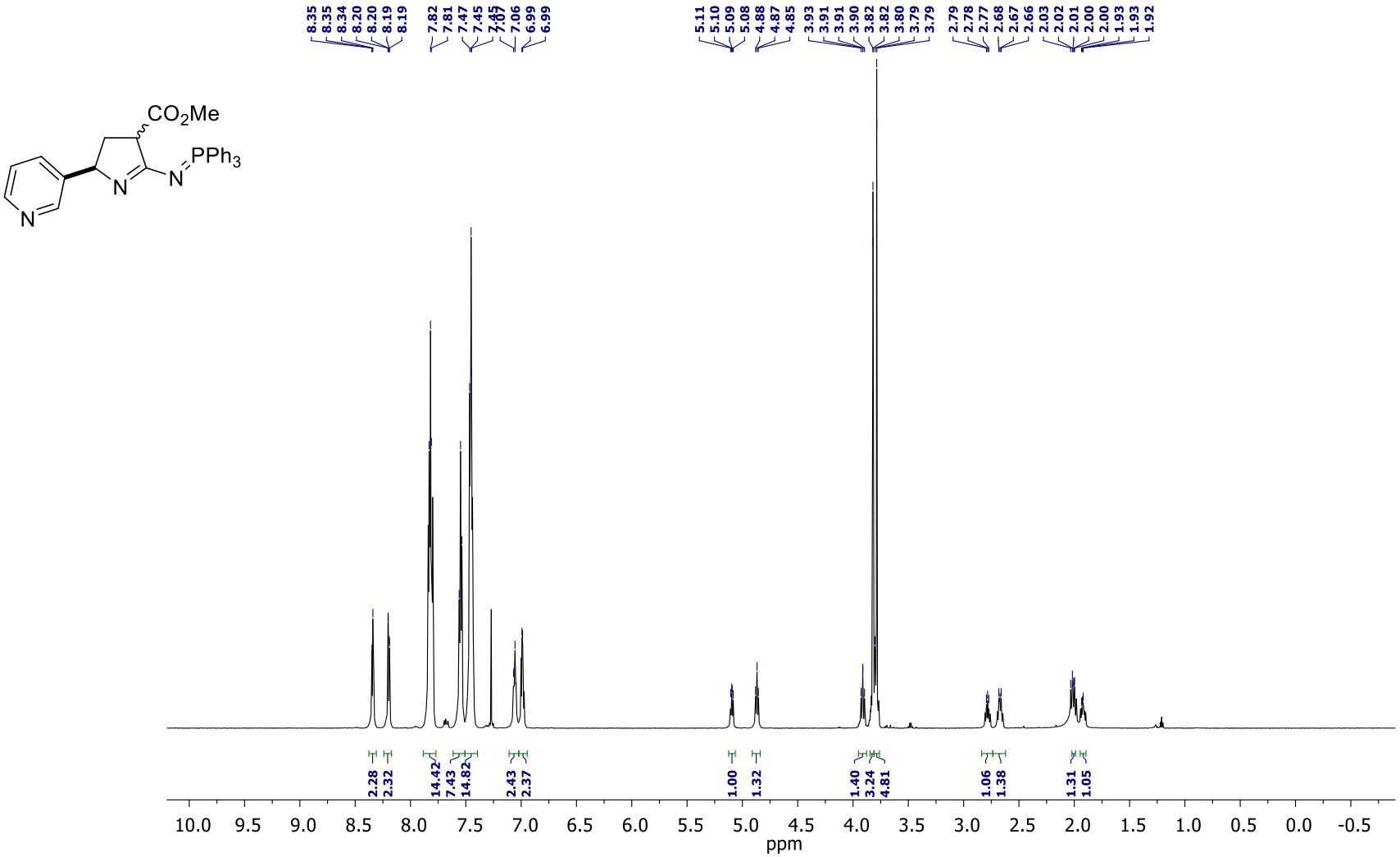


^{31}P NMR ($CDCl_3$, 162 MHz)



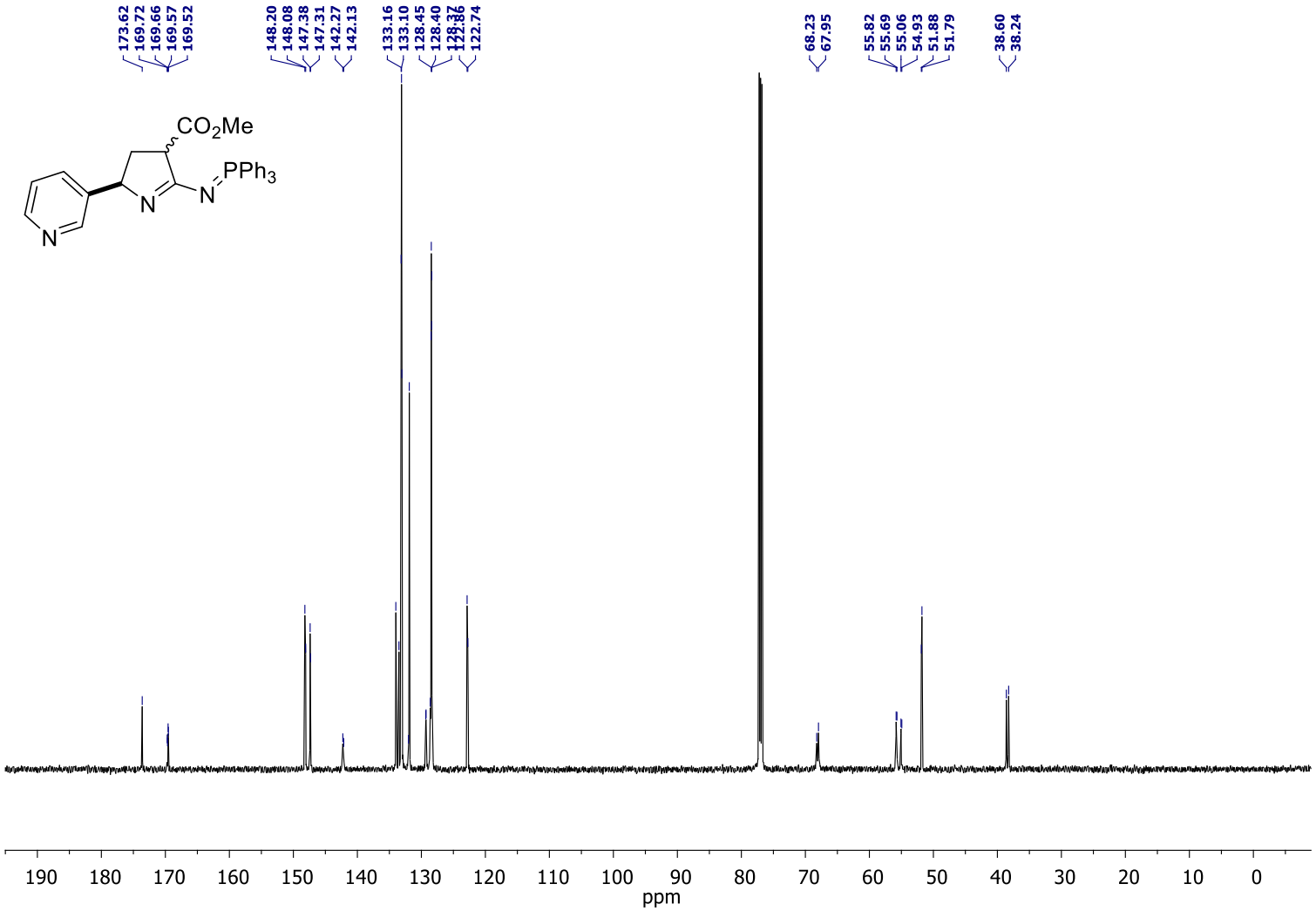
Methyl 2-(pyridin-2-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3q)

^{1}H NMR (600 MHz, $CDCl_3$)

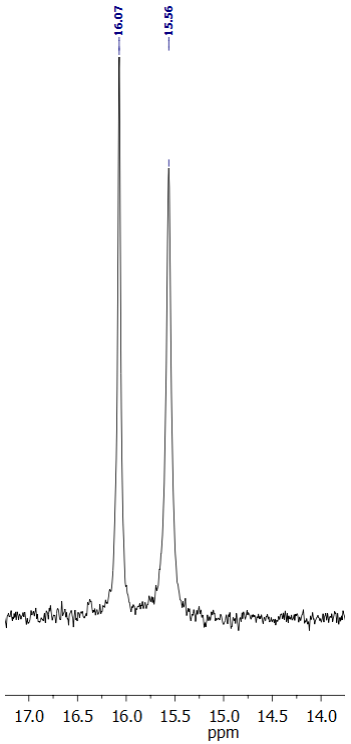


Methyl 2-(pyridin-2-yl)-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3q)

^{13}C NMR (150 MHz, $CDCl_3$)

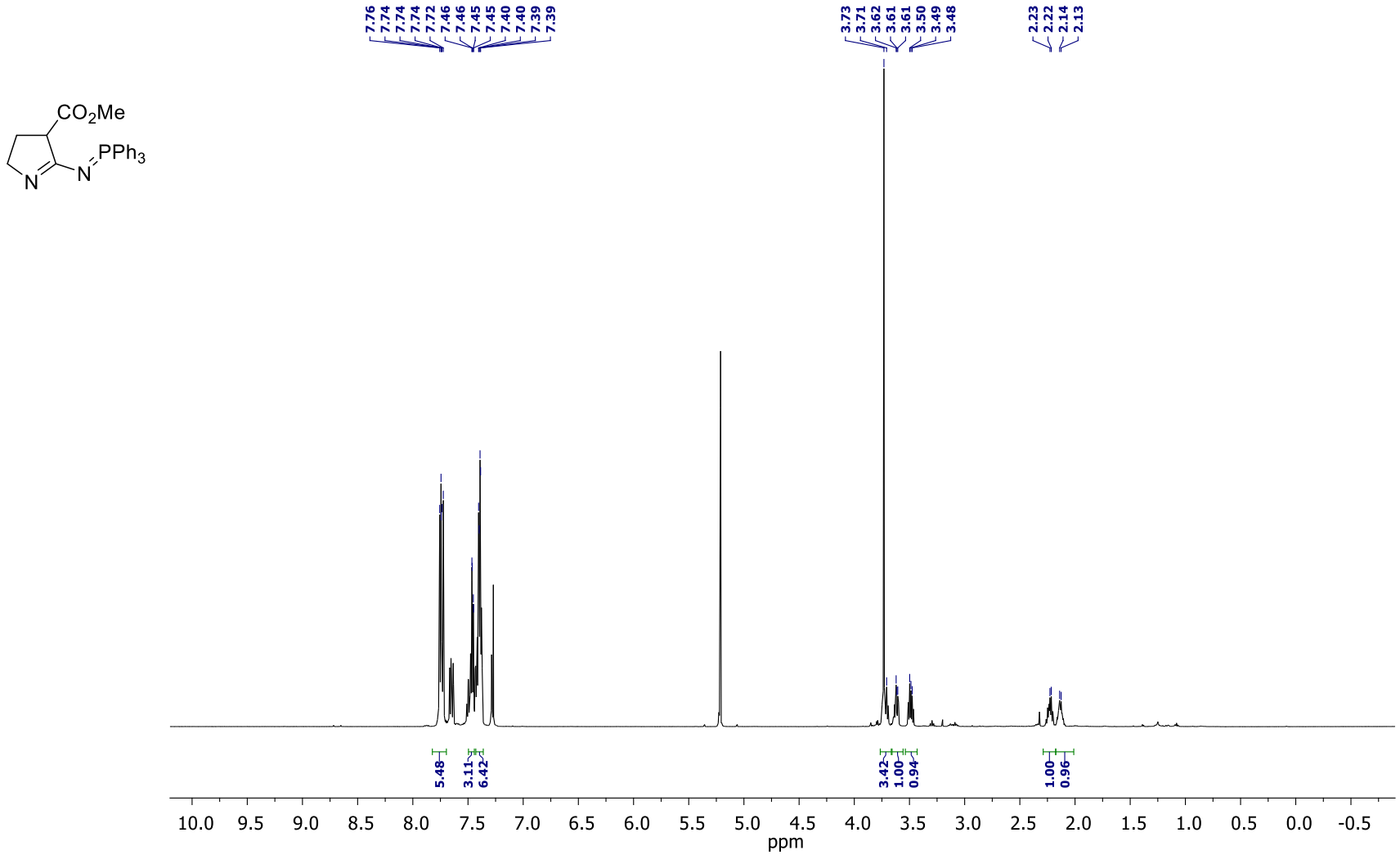


^{31}P NMR ($CDCl_3$, 162 MHz)



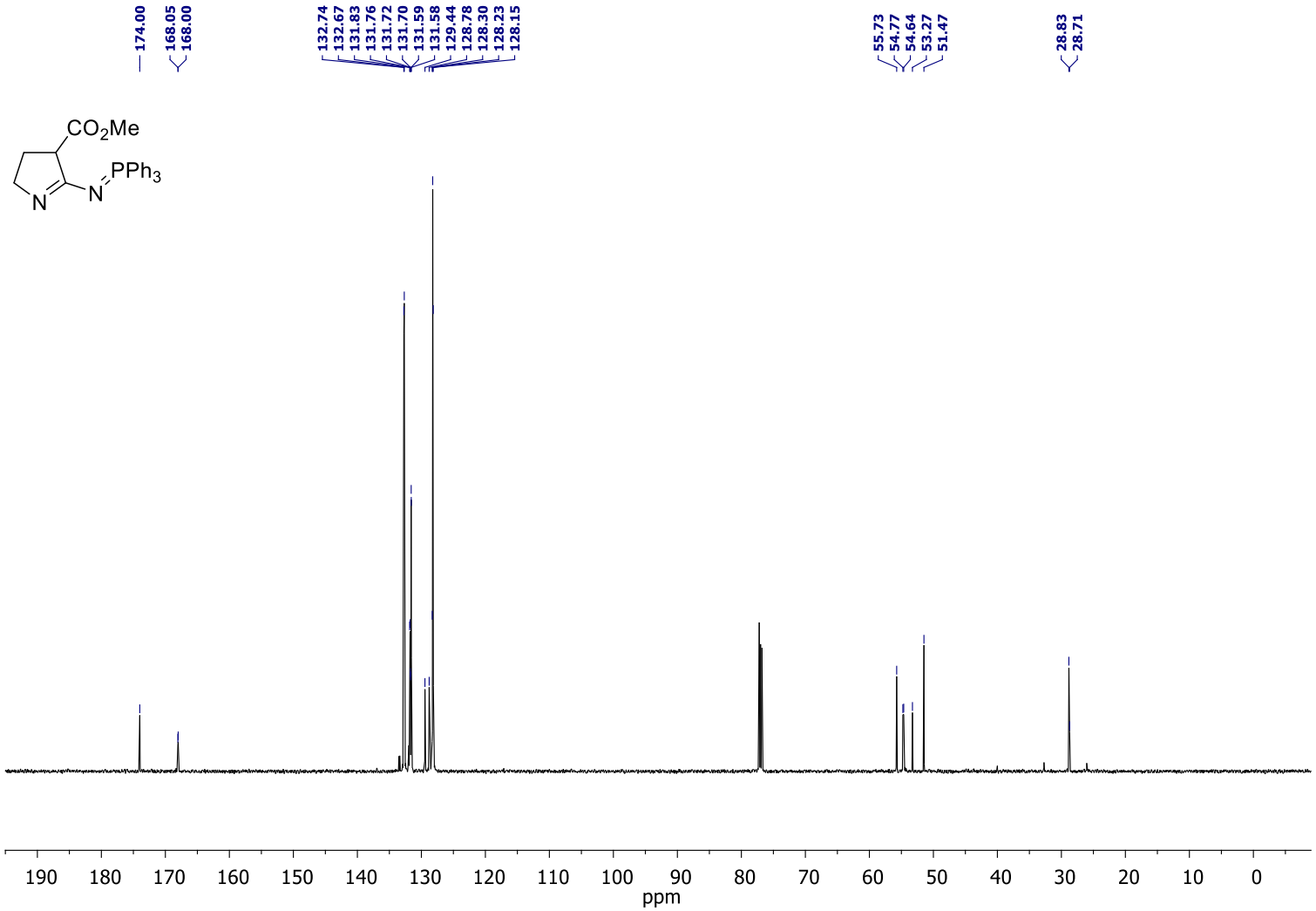
Methyl 5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3r)

^{1}H NMR (600 MHz, $CDCl_3$)

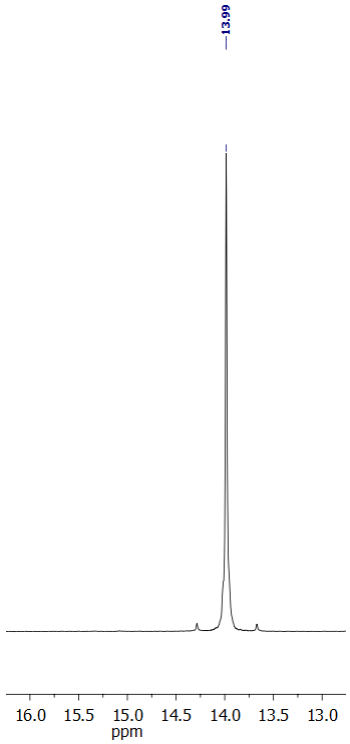


Methyl 5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3r)

^{13}C NMR (150 MHz, $CDCl_3$)

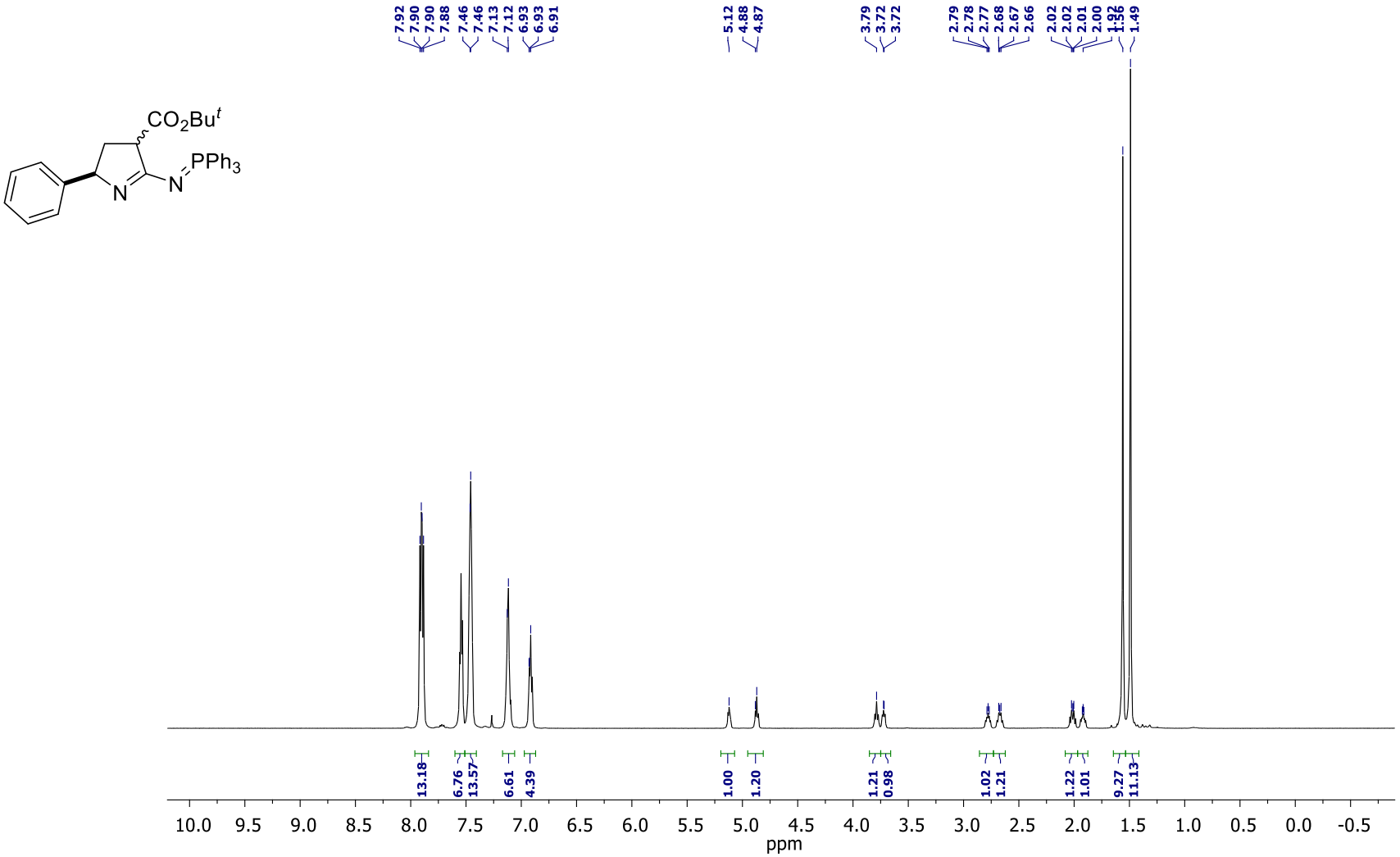


^{31}P NMR ($CDCl_3$, 162 MHz)



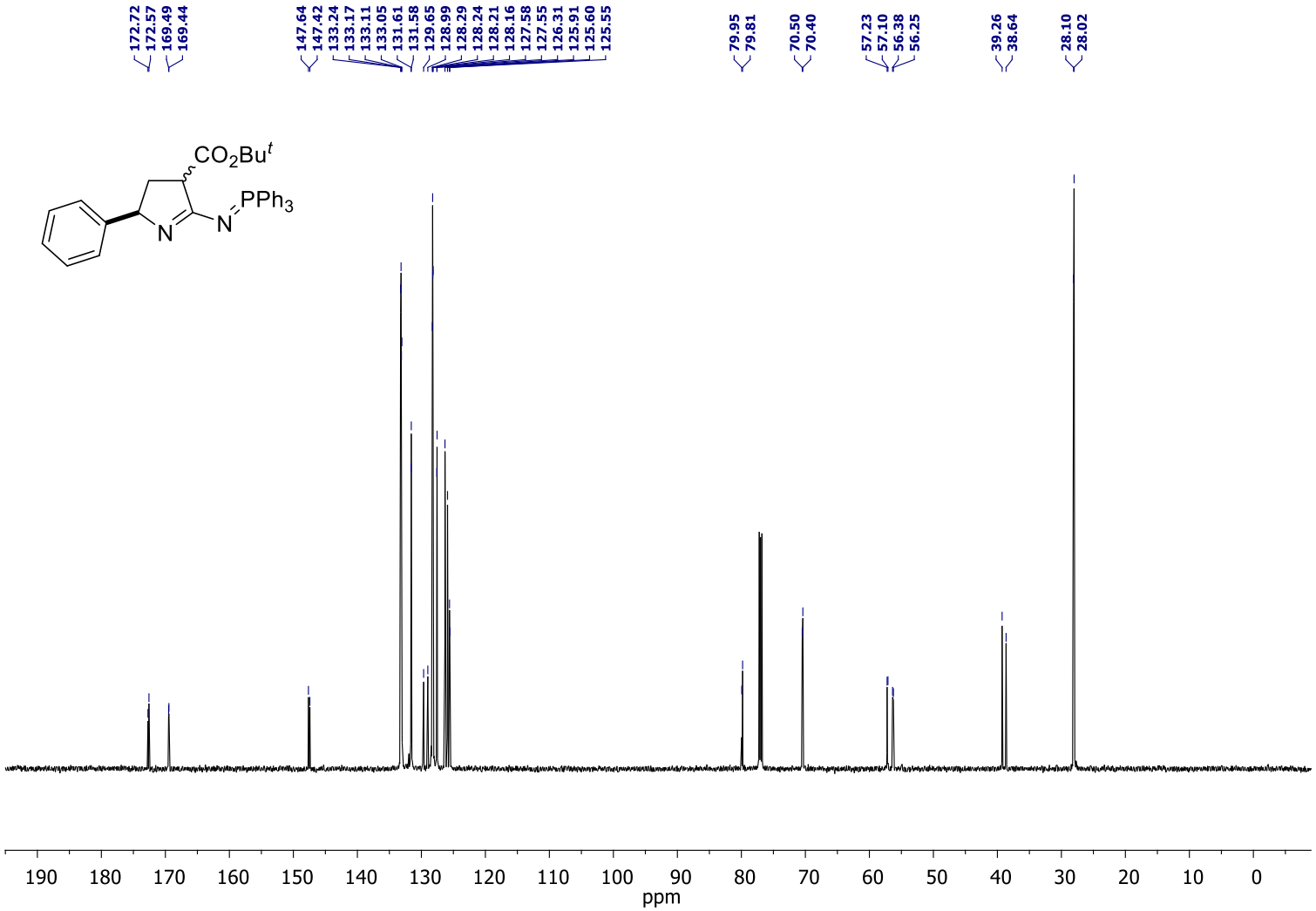
***tetr*-Butyl 2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (3s)**

^{1}H NMR (600 MHz, $CDCl_3$)

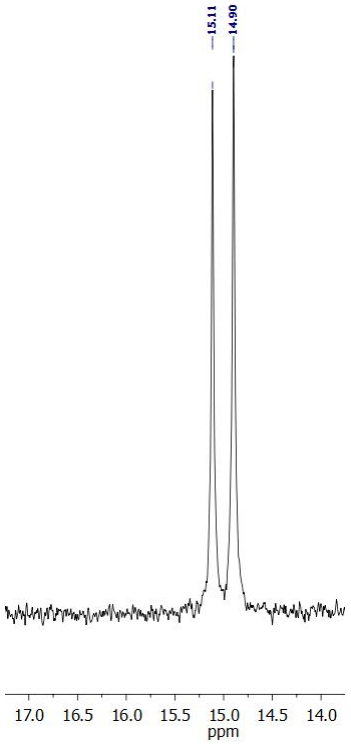


tetr-Butyl 2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2_H_-pyrrole-4-carboxylate (3s)

^{13}C NMR (150 MHz, $CDCl_3$)

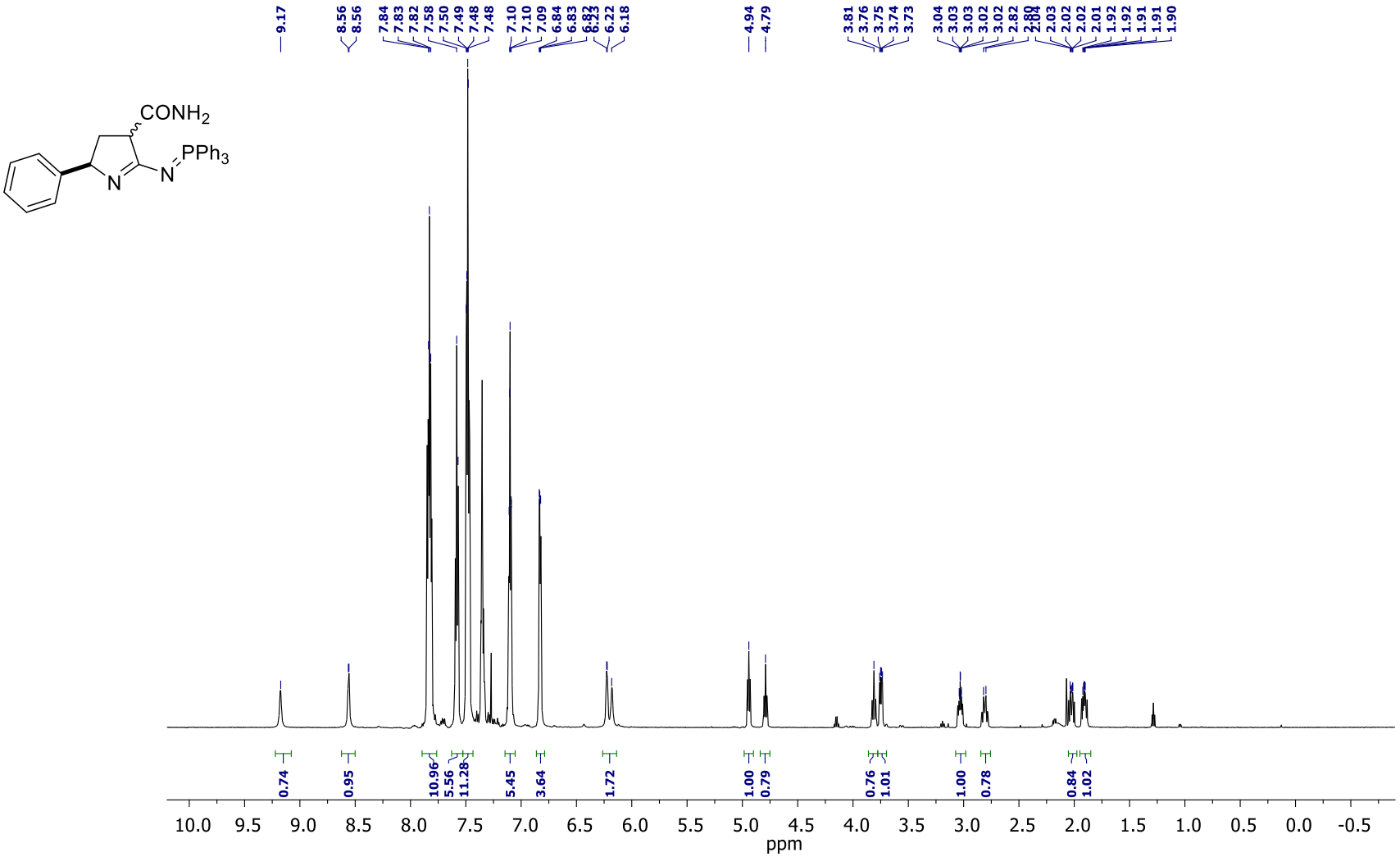


^{31}P NMR ($CDCl_3$, 162 MHz)



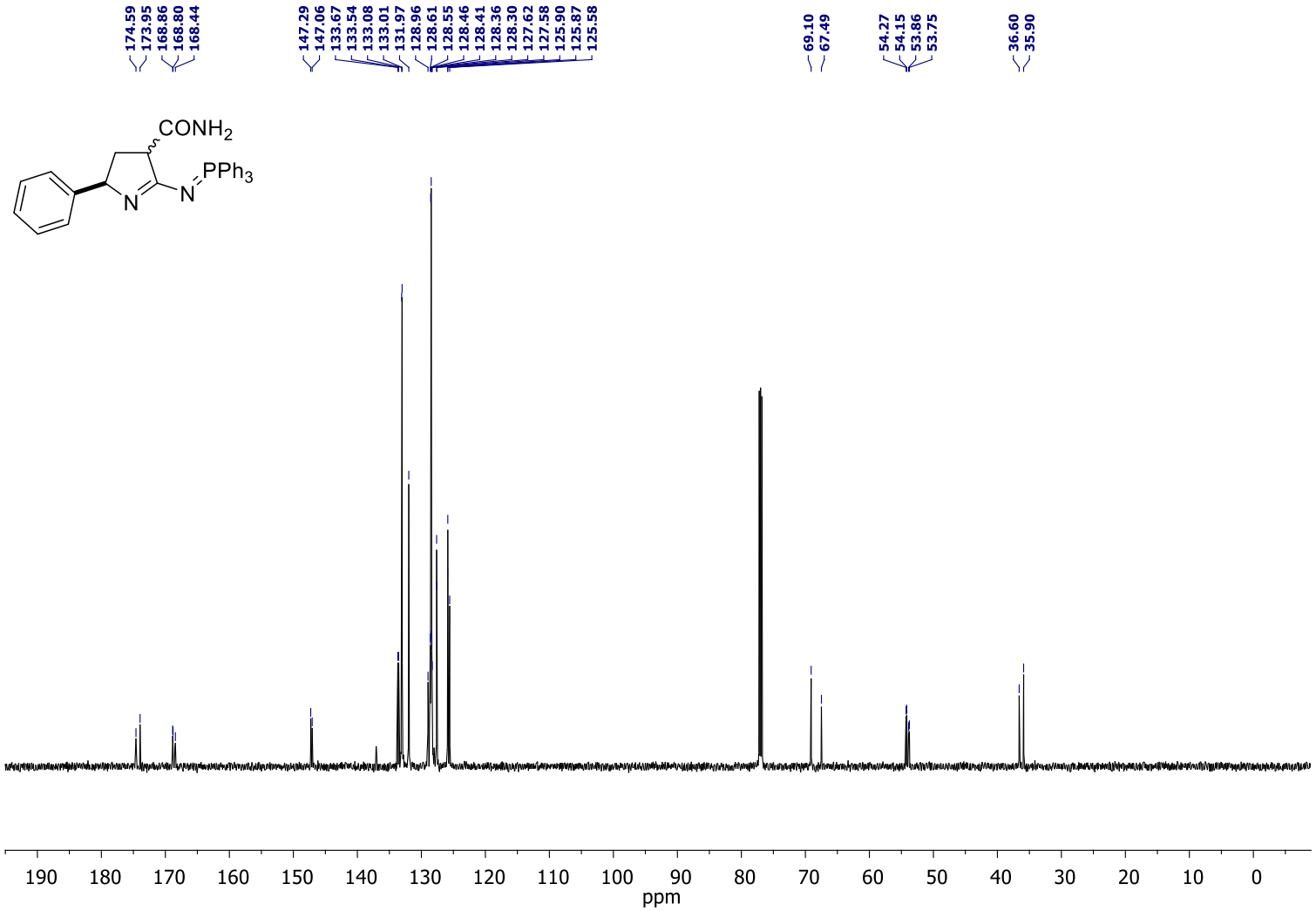
2-Phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxamide (3t)

^{1}H NMR (600 MHz, $CDCl_3$)

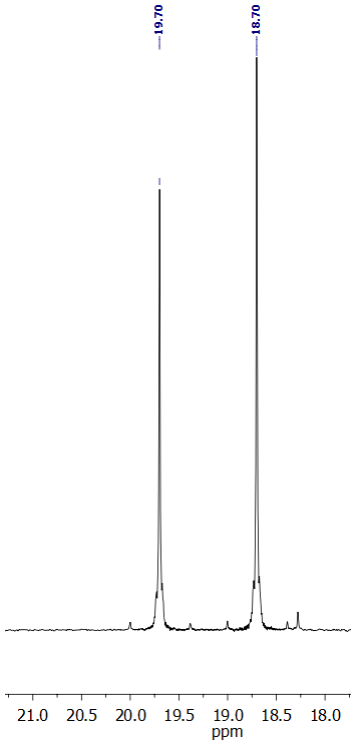


2-Phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxamide (3t)

^{13}C NMR (150 MHz, $CDCl_3$)

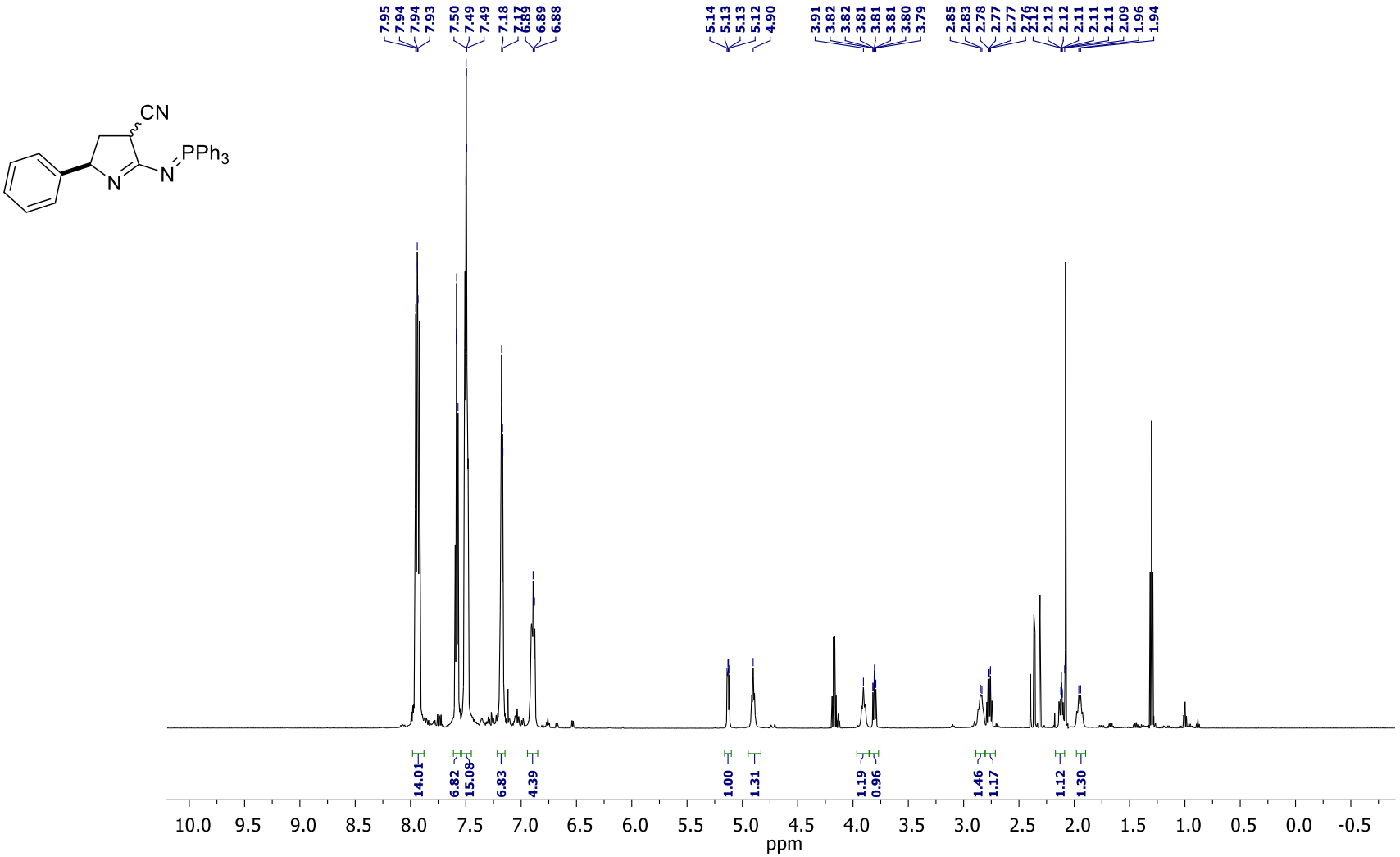


^{31}P NMR ($CDCl_3$, 162 MHz)



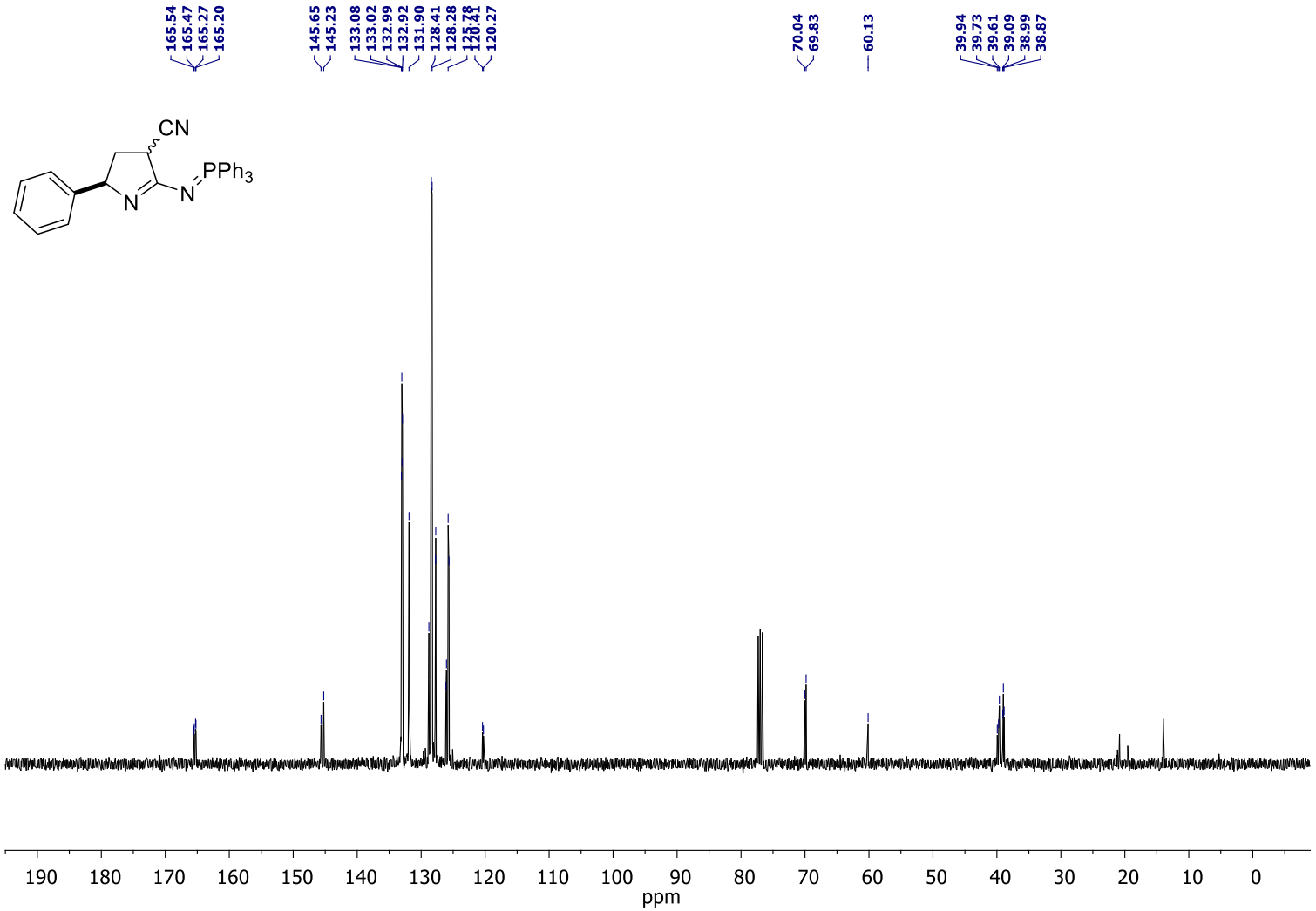
2-Phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carbonitrile (3u)

^{1}H NMR (600 MHz, $CDCl_3$)

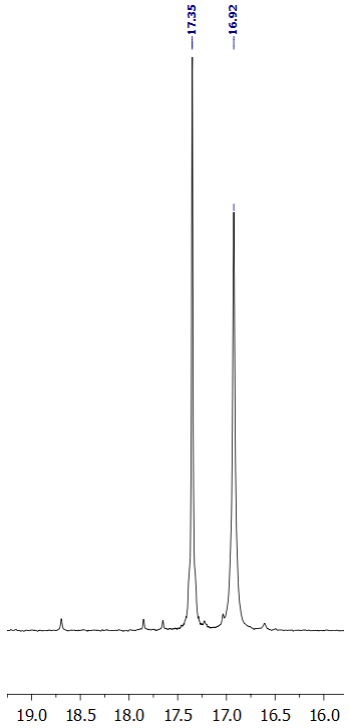


2-Phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carbonitrile (3u)

^{13}C NMR (150 MHz, $CDCl_3$)

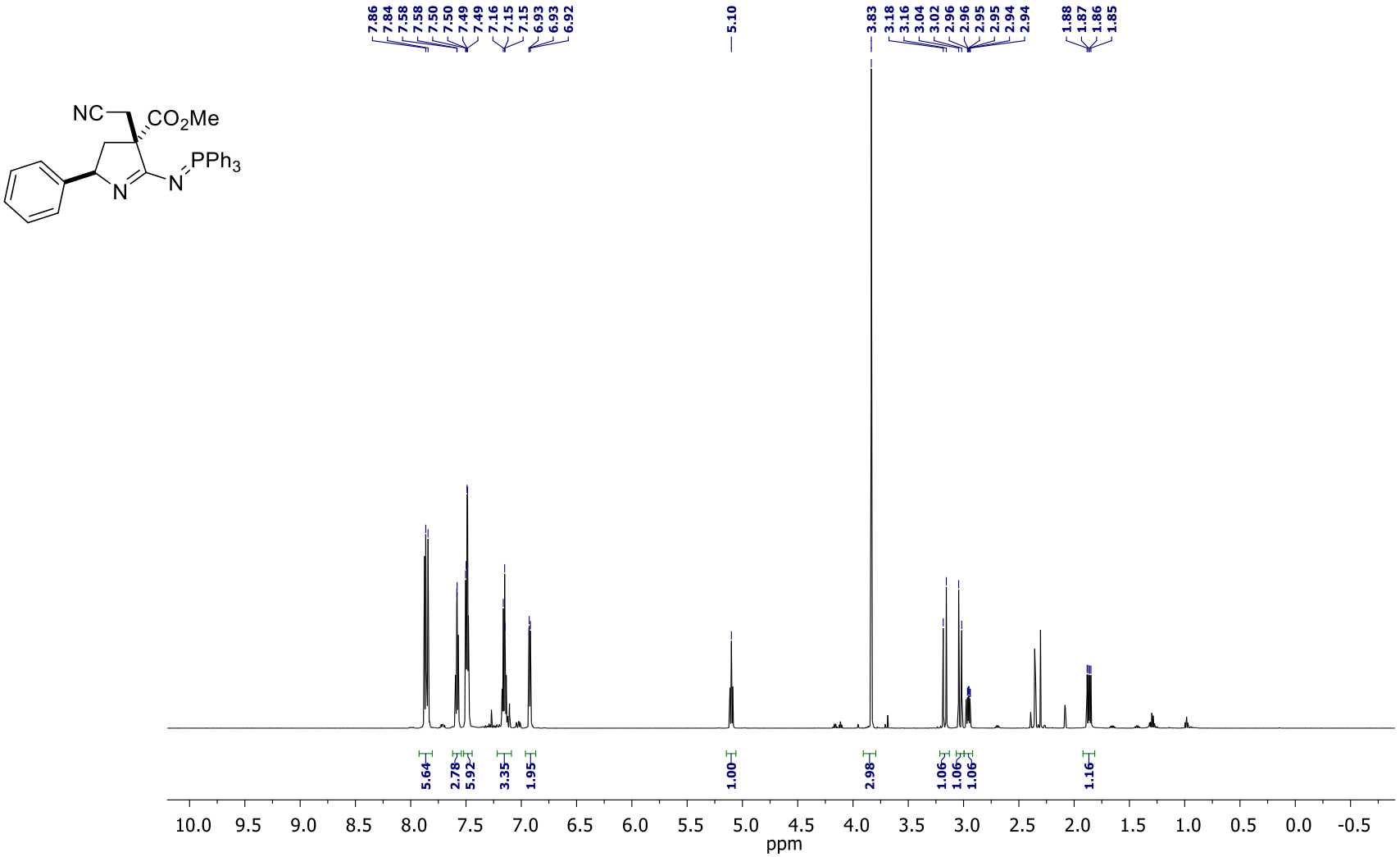


^{31}P NMR ($CDCl_3$, 162 MHz)



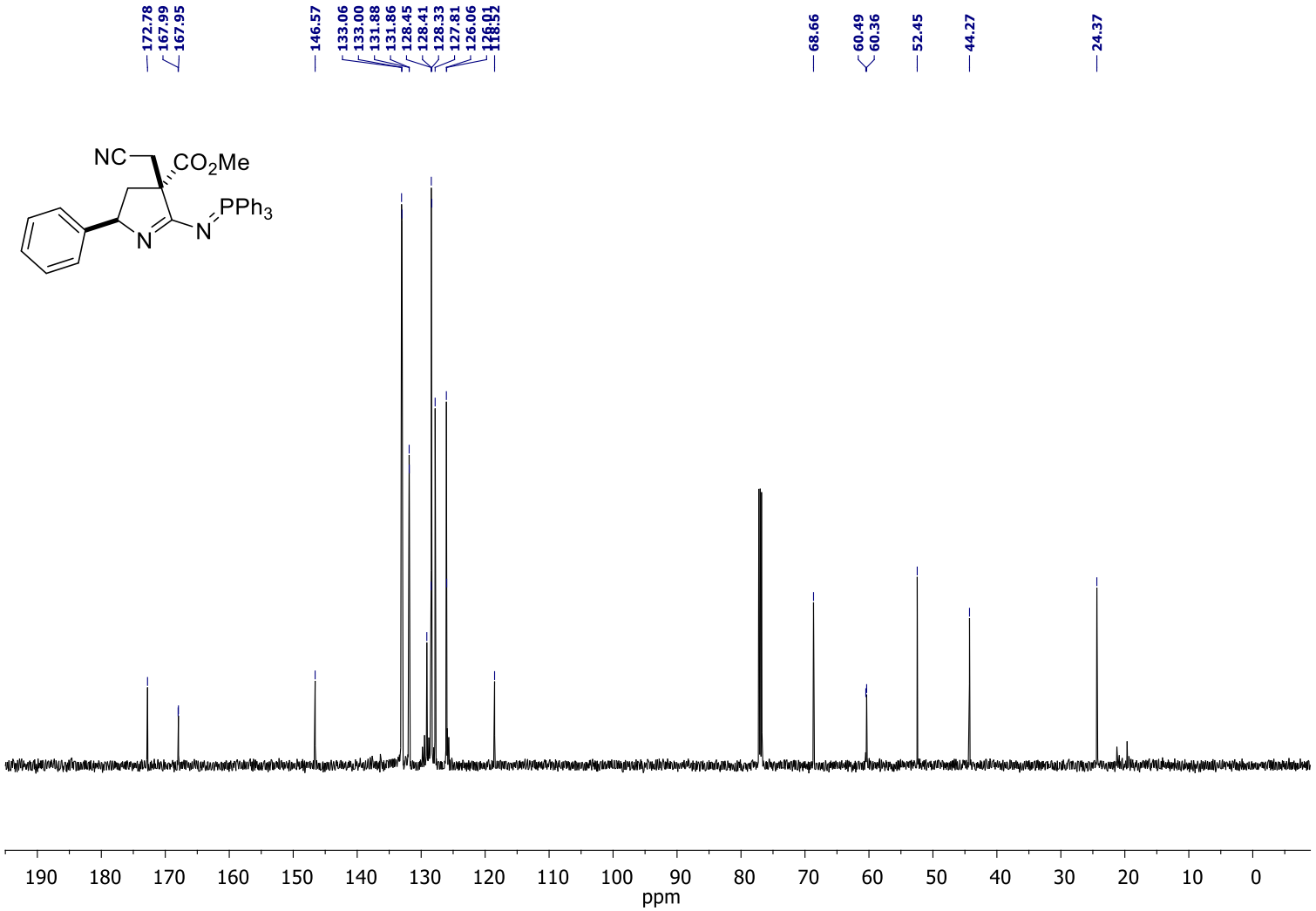
Methyl (2*RS*,4*RS*)-4-(cyanomethyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*trans*-3w)

^{1}H NMR (600 MHz, $CDCl_3$)

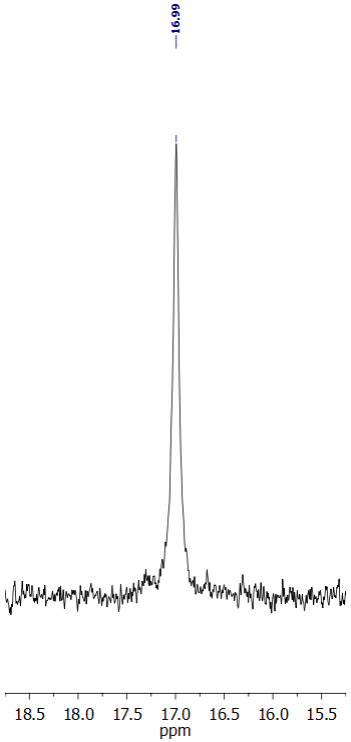


Methyl (2*RS*,4*RS*)-4-(cyanomethyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*trans*-3w)

^{13}C NMR (150 MHz, $CDCl_3$)

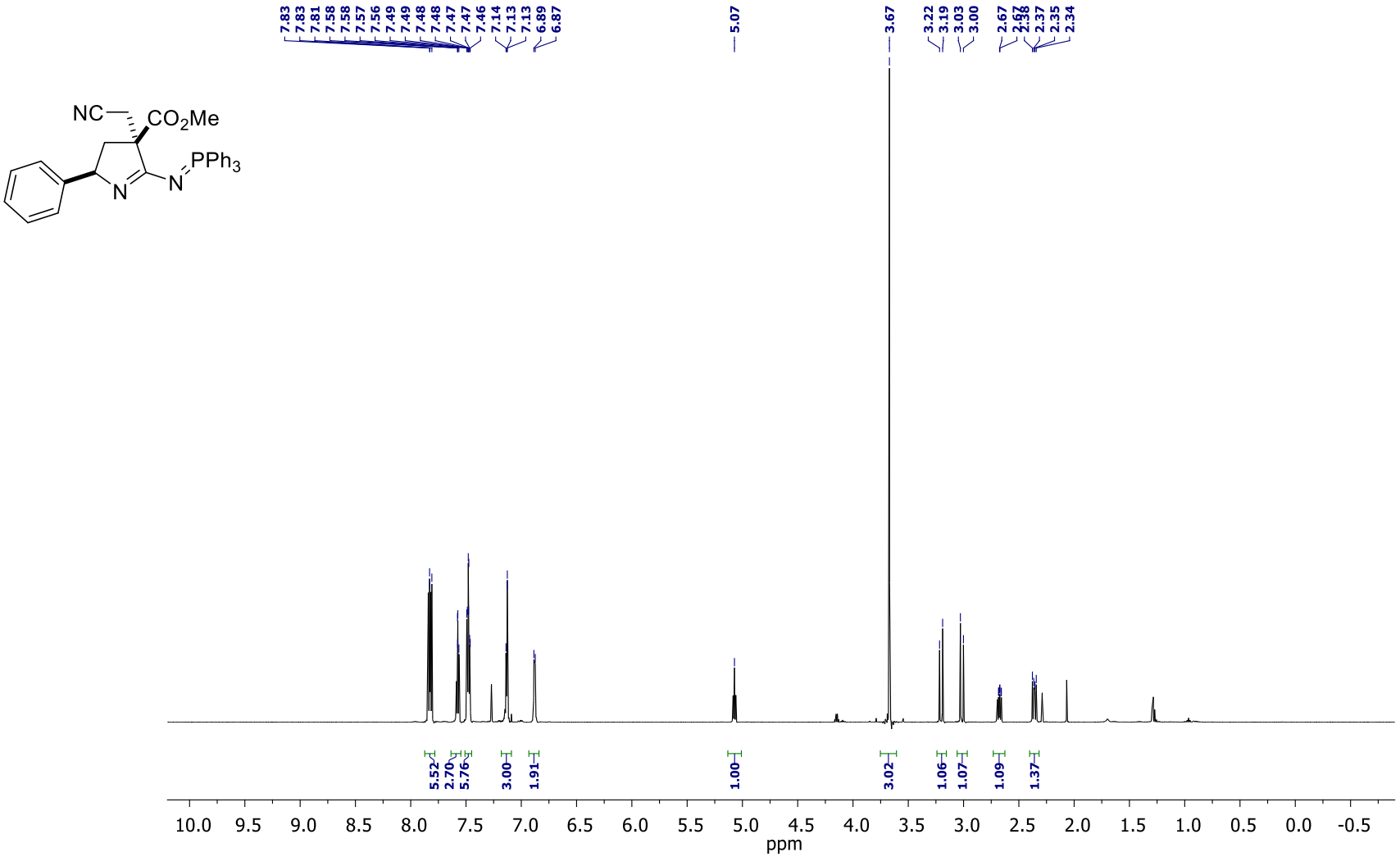


^{31}P NMR ($CDCl_3$, 162 MHz)



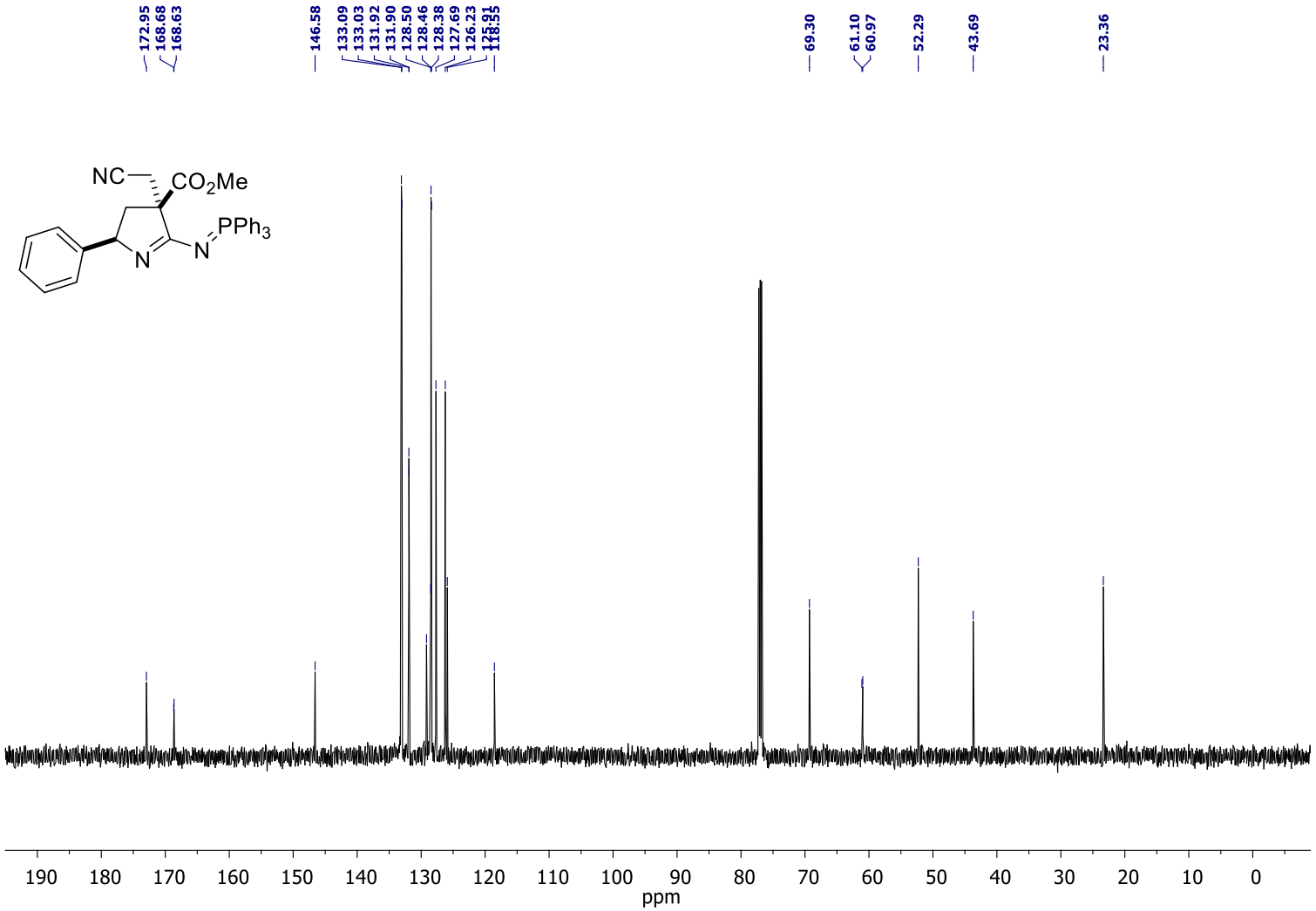
Methyl (2*RS*,4*RS*)-4-(cyanomethyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*cis*-3w)

^{1}H NMR (600 MHz, $CDCl_3$)

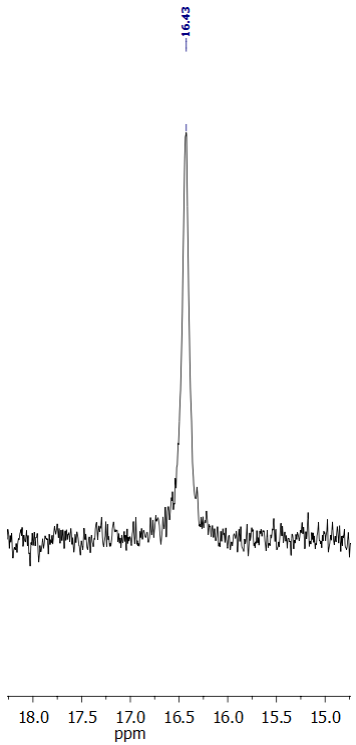


Methyl (2*RS*,4*RS*)-4-(cyanomethyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*cis*-3w)

^{13}C NMR (150 MHz, $CDCl_3$)

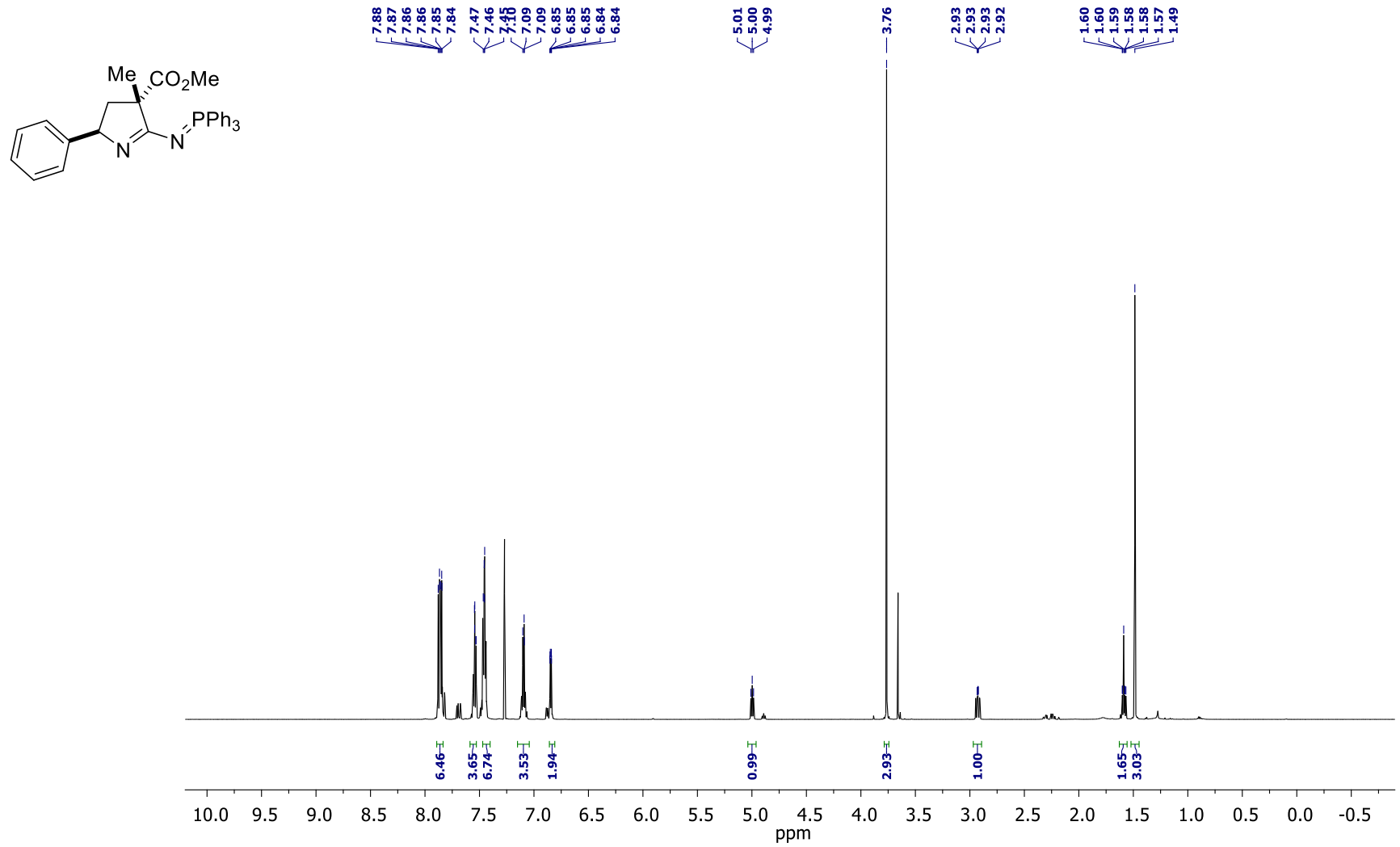


^{31}P NMR ($CDCl_3$, 162 MHz)



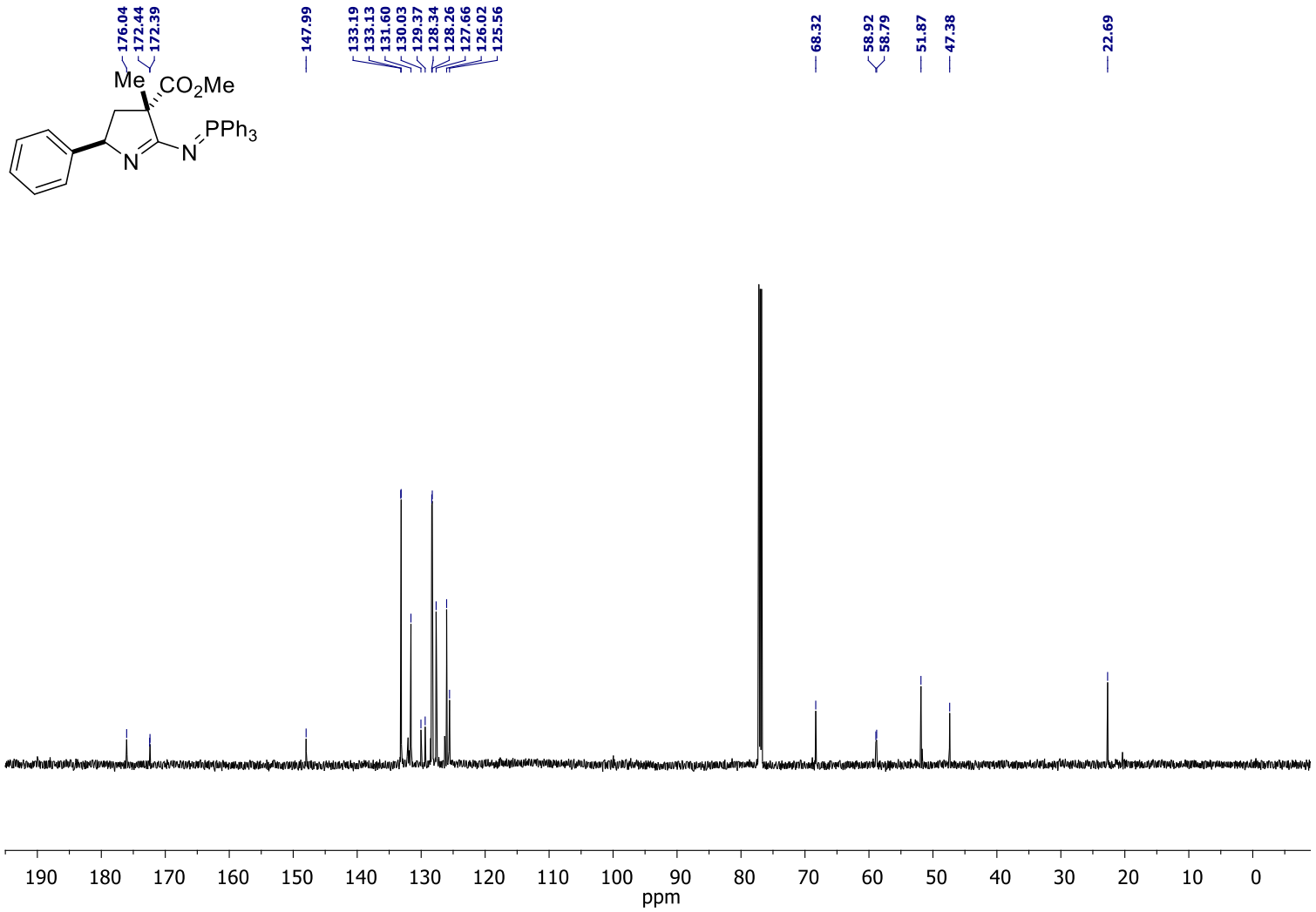
Methyl (2*RS*,4*SR*)-4-(methyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*trans*-3x)

^{1}H NMR (600 MHz, $CDCl_3$)

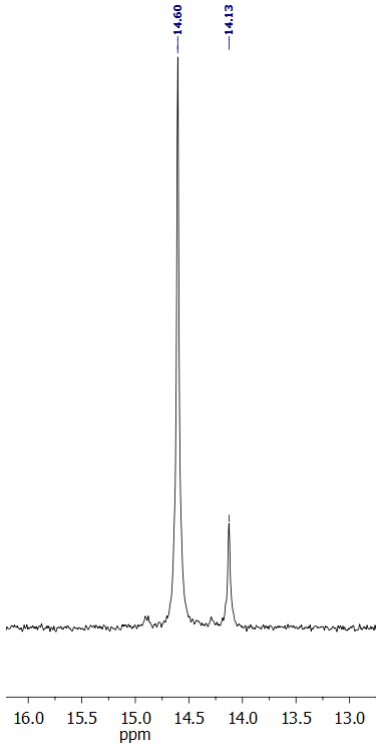


Methyl (2*RS*,4*SR*)-4-(methyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*trans*-3x)

^{13}C NMR (150 MHz, $CDCl_3$)

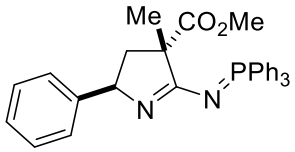


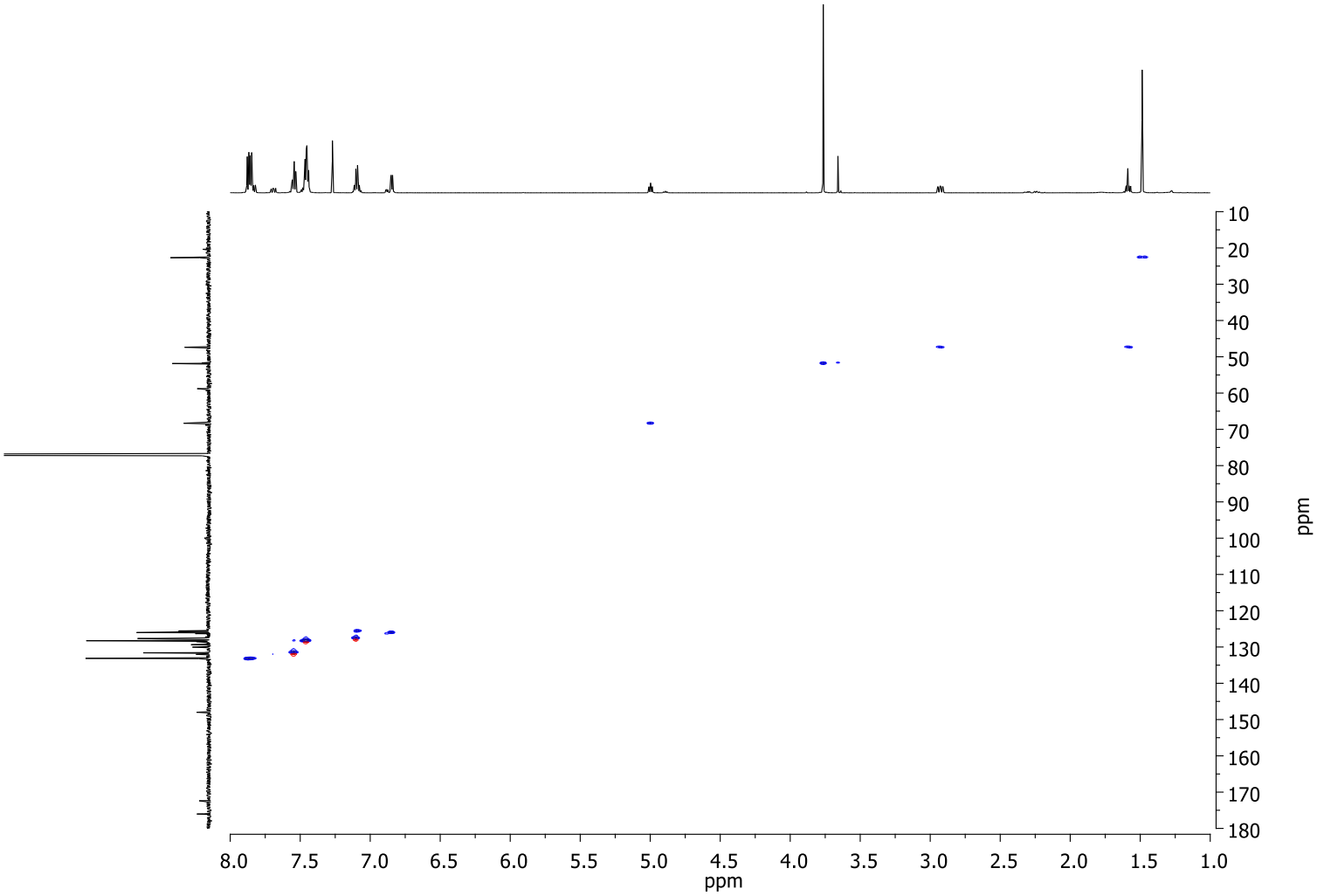
^{31}P NMR ($CDCl_3$, 162 MHz)



Methyl (2*RS*,4*SR*)-4-(methyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*trans*-3x)

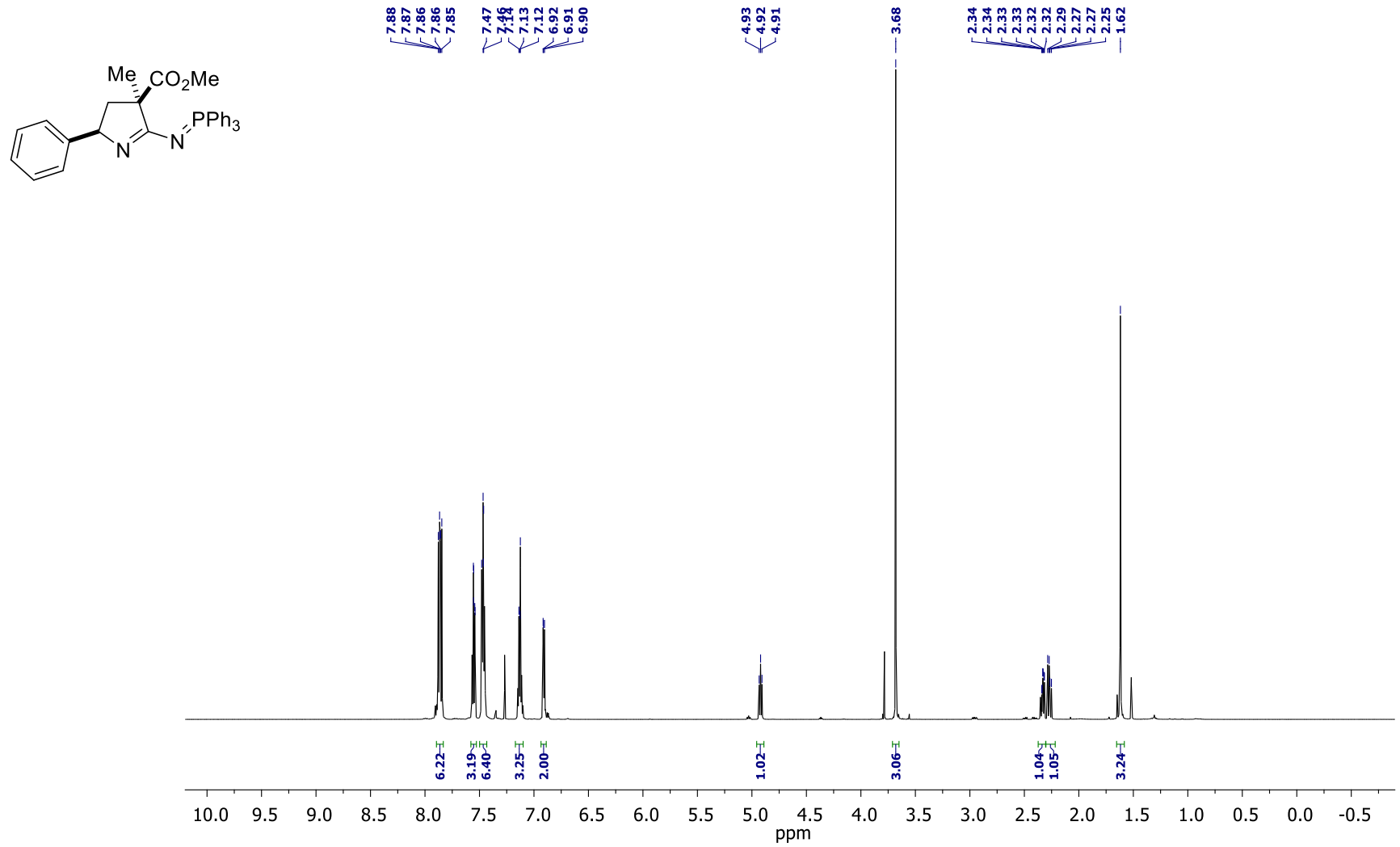
^{1}H-^{13}C HSQC ($CDCl_3$)





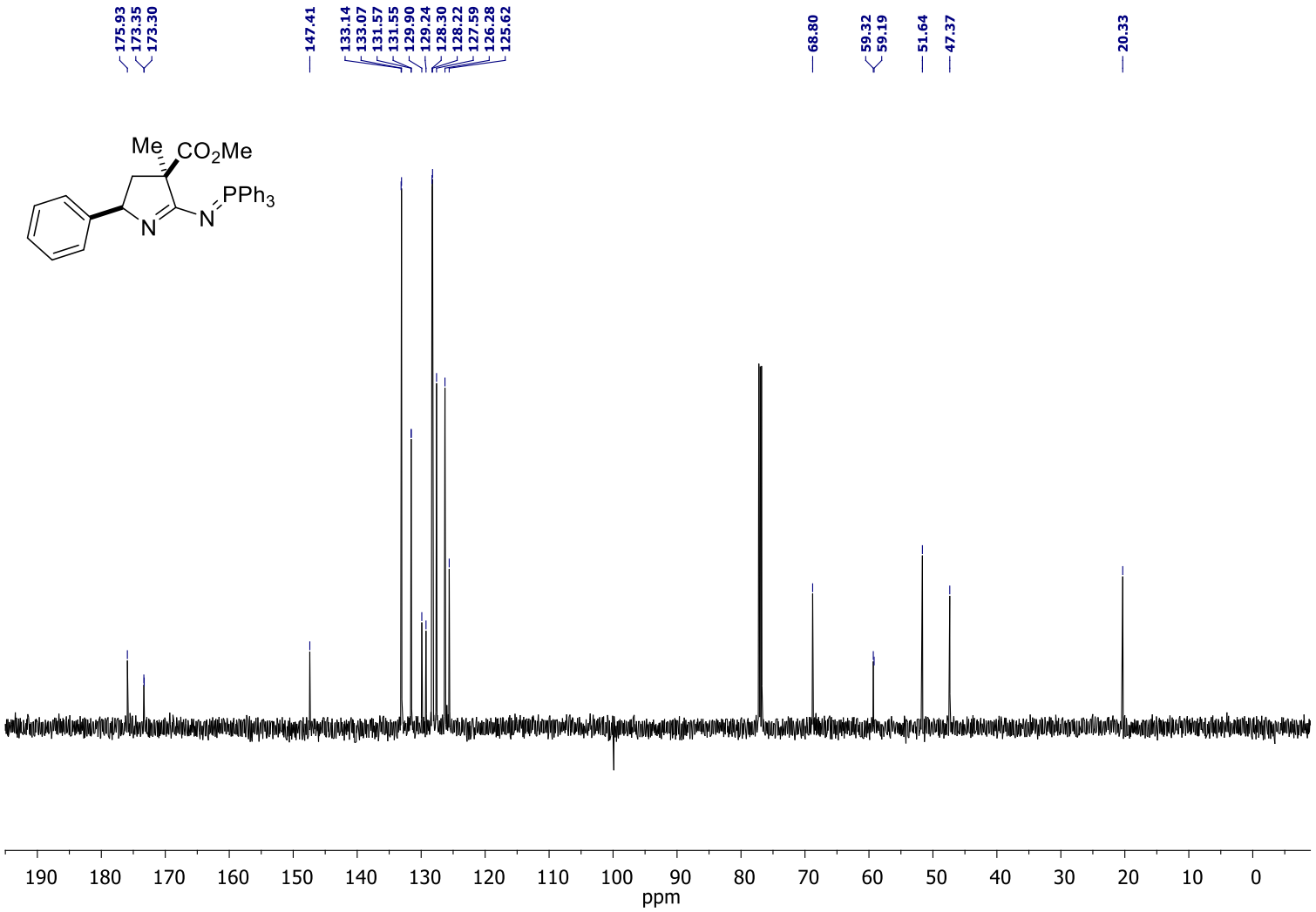
Methyl (2*RS*,4*RS*)-4-(methyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*cis*-3x)

^{1}H NMR (600 MHz, $CDCl_3$)

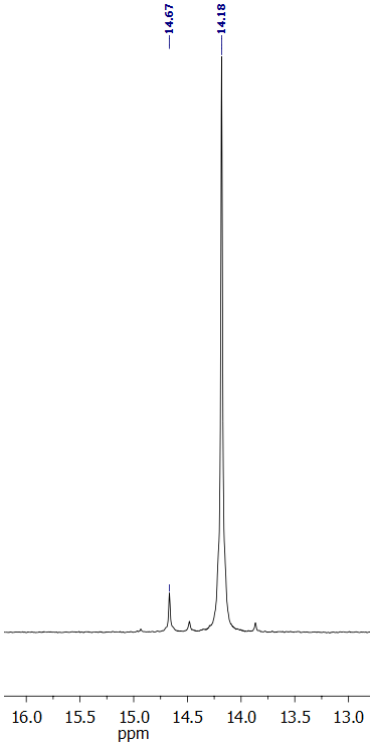


Methyl (2*RS*,4*RS*)-4-(methyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*cis*-3x)

^{13}C NMR (150 MHz, $CDCl_3$)

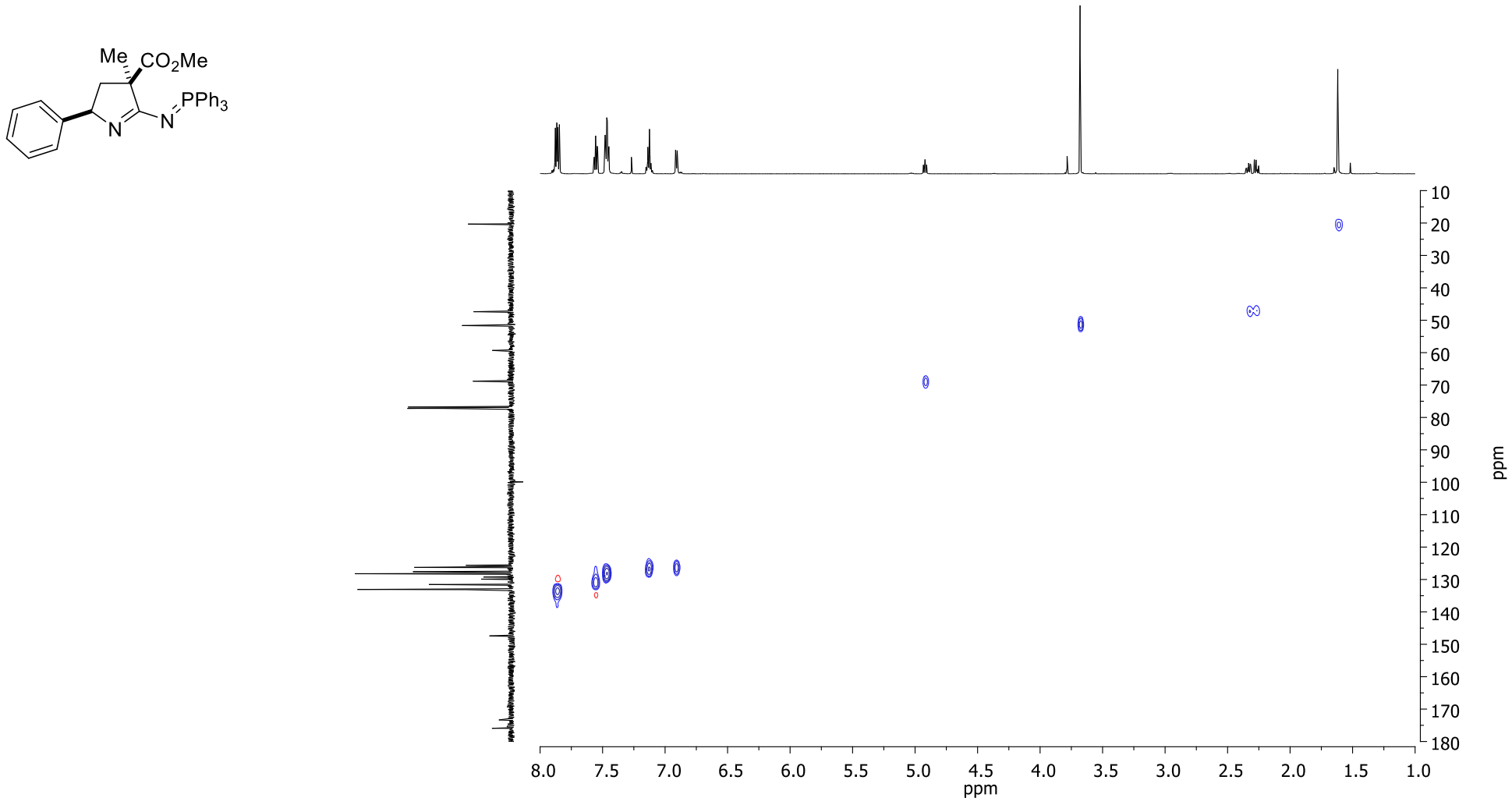


^{31}P NMR ($CDCl_3$, 162 MHz)



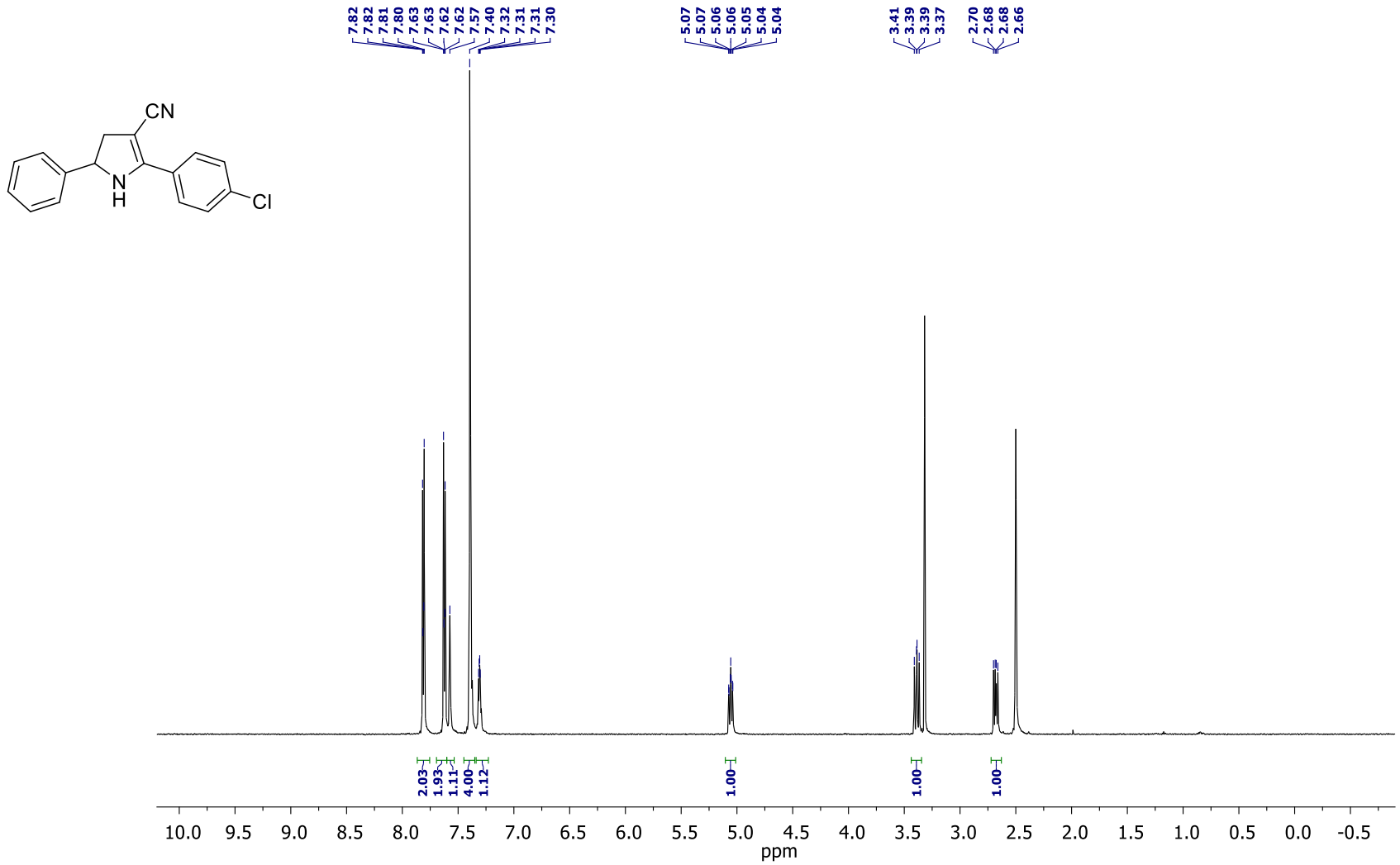
Methyl (2*RS*,4*RS*)-4-(methyl)-2-phenyl-5-[(triphenyl-λ^5-phosphanylidene)amino]-3,4-dihydro-2*H*-pyrrole-4-carboxylate (*cis*-3x)

^{1}H-^{13}C HSQC ($CDCl_3$)



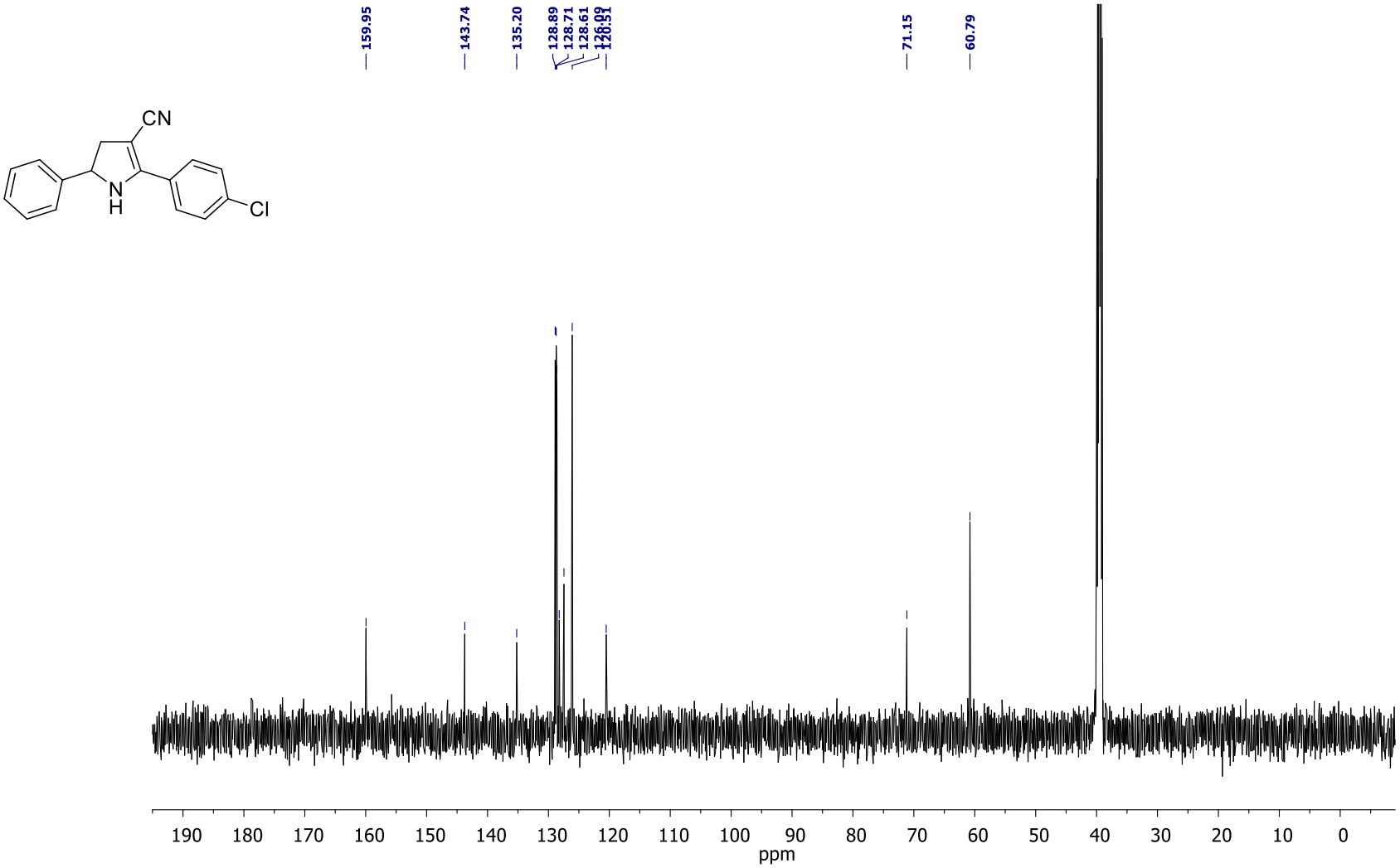
2-(4-Chlorophenyl)-5-phenyl-4,5-dihydro-1*H*-pyrrole-3-carbonitrile (8)

^{1}H NMR (600 MHz, DMSO-d$_6$)



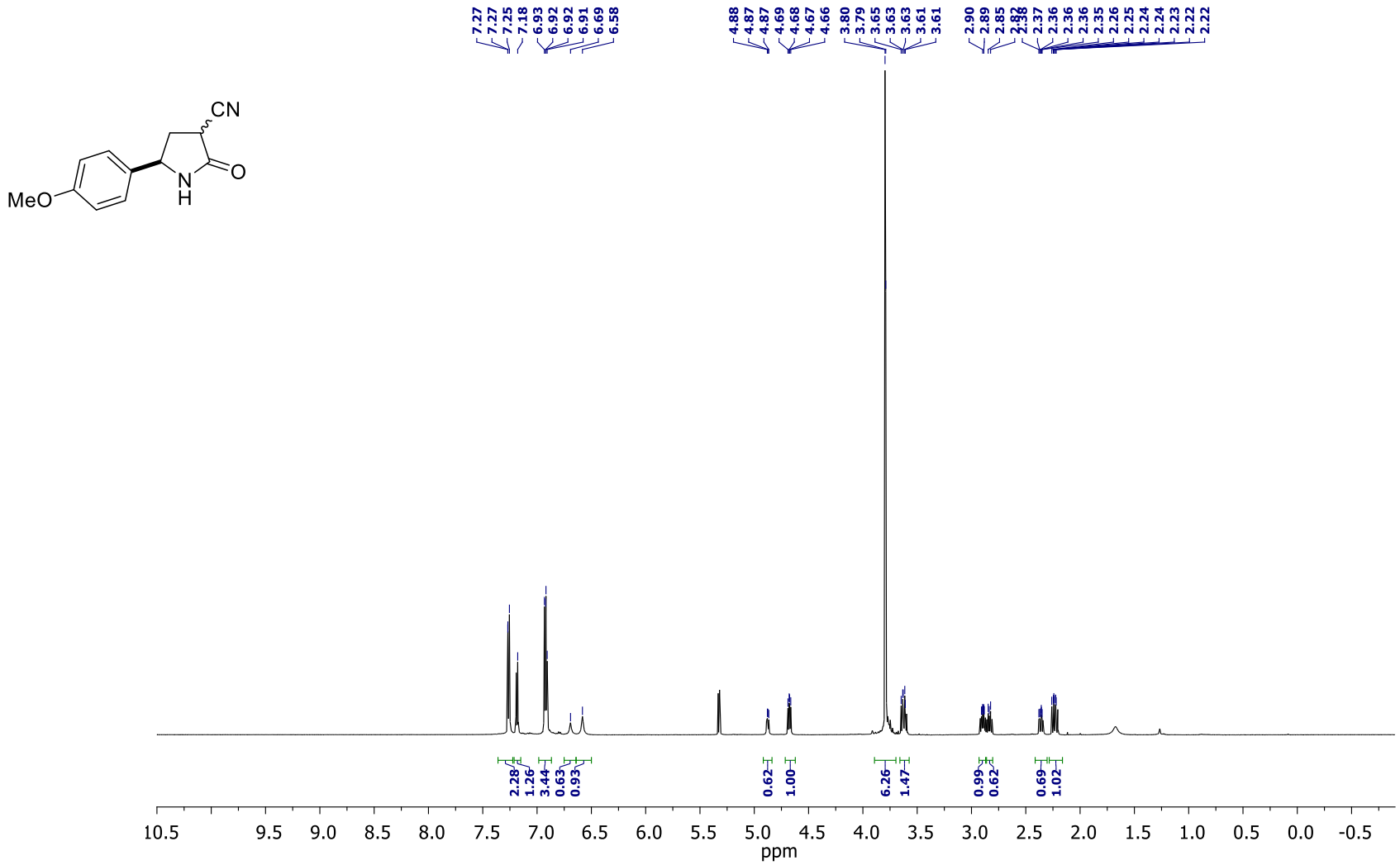
2-(4-Chlorophenyl)-5-phenyl-4,5-dihydro-1*H*-pyrrole-3-carbonitrile (8)

^{13}C NMR (150 MHz, DMSO-d$_6$)



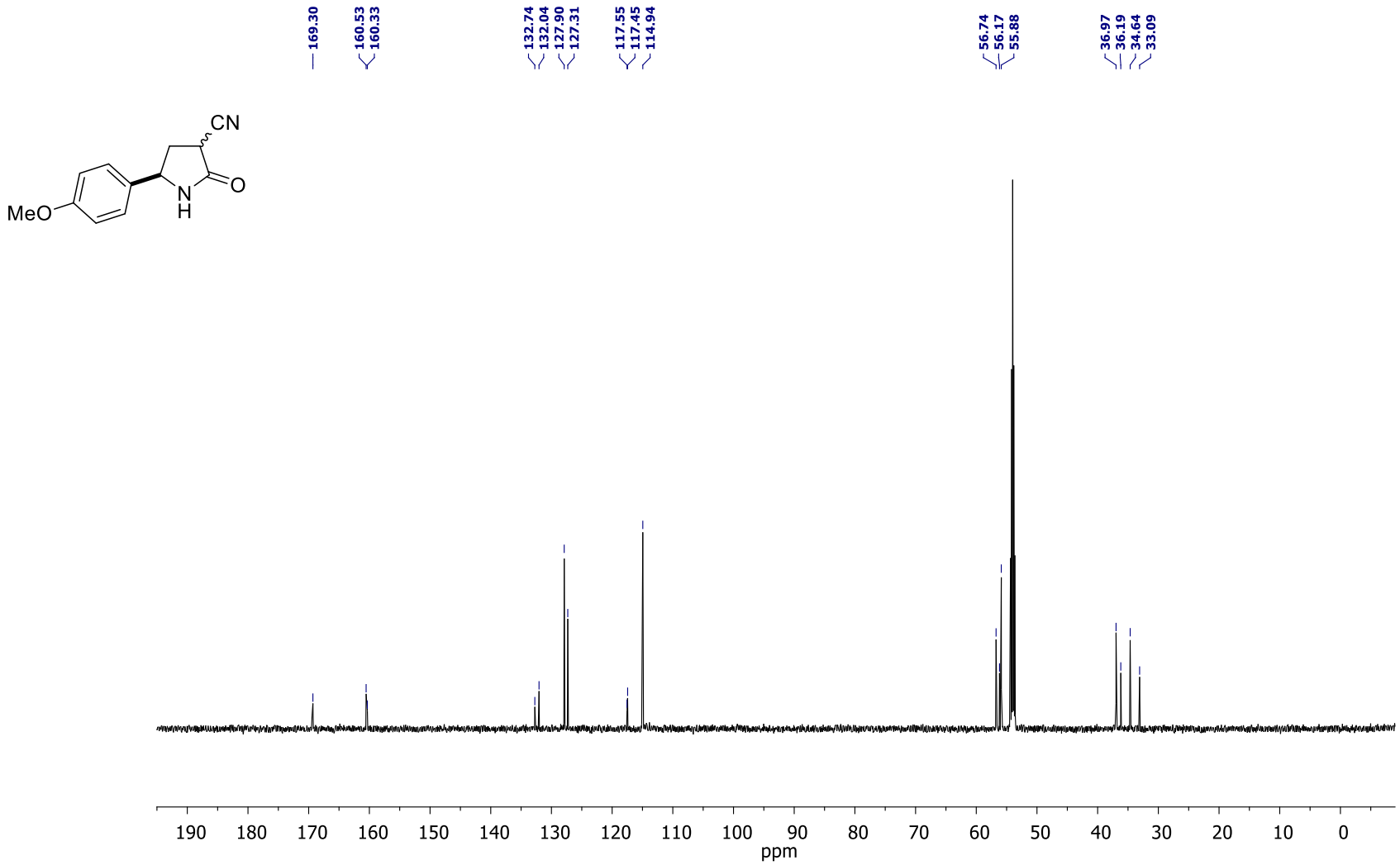
5-(4-Methoxyphenyl)-2-oxopyrrolidine-3-carbonitrile (5b)

^{1}H NMR (600 MHz, $CDCl_3$)



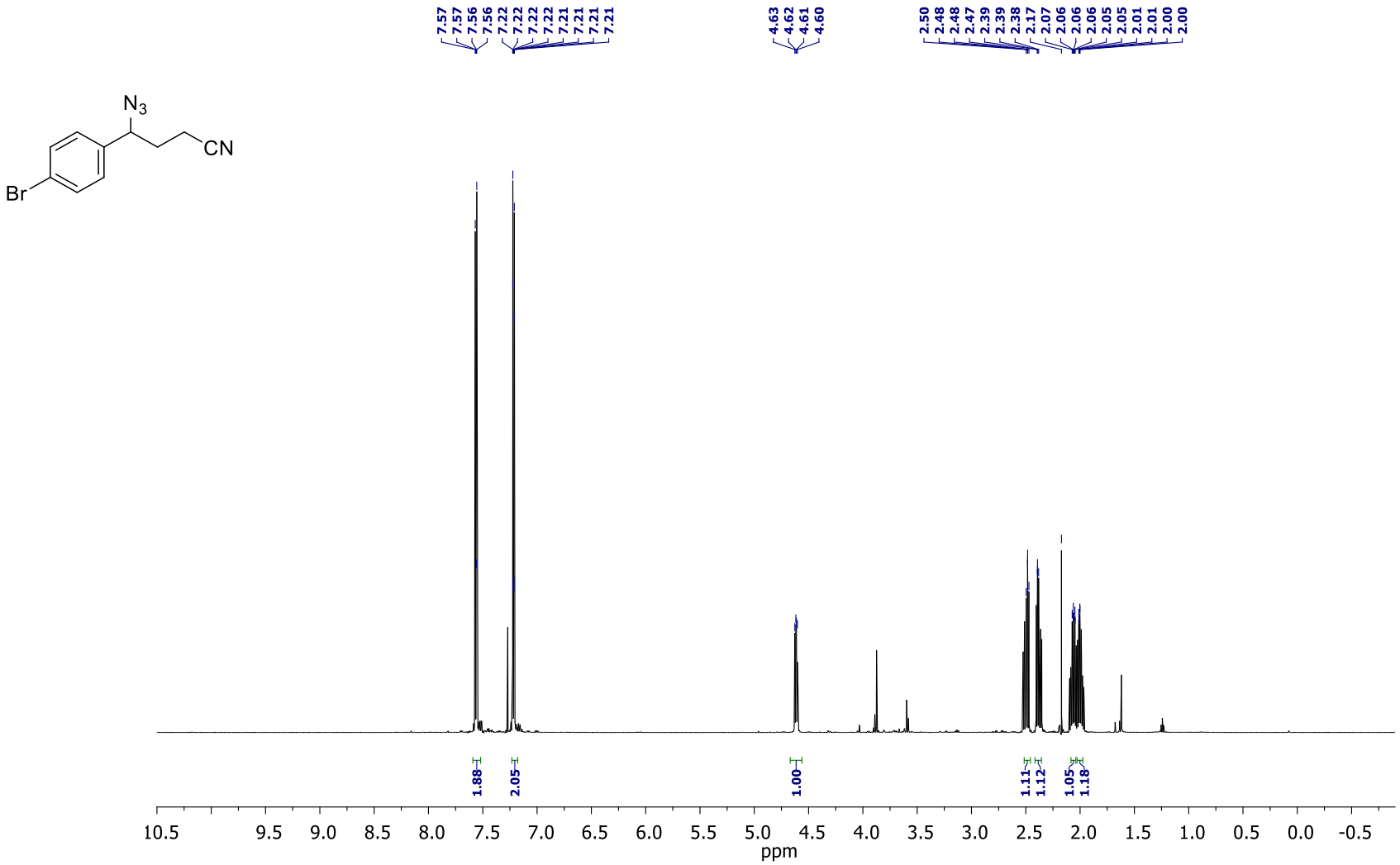
5-(4-Methoxyphenyl)-2-oxopyrrolidine-3-carbonitrile (5b)

^{13}C NMR (150 MHz, $CDCl_3$)



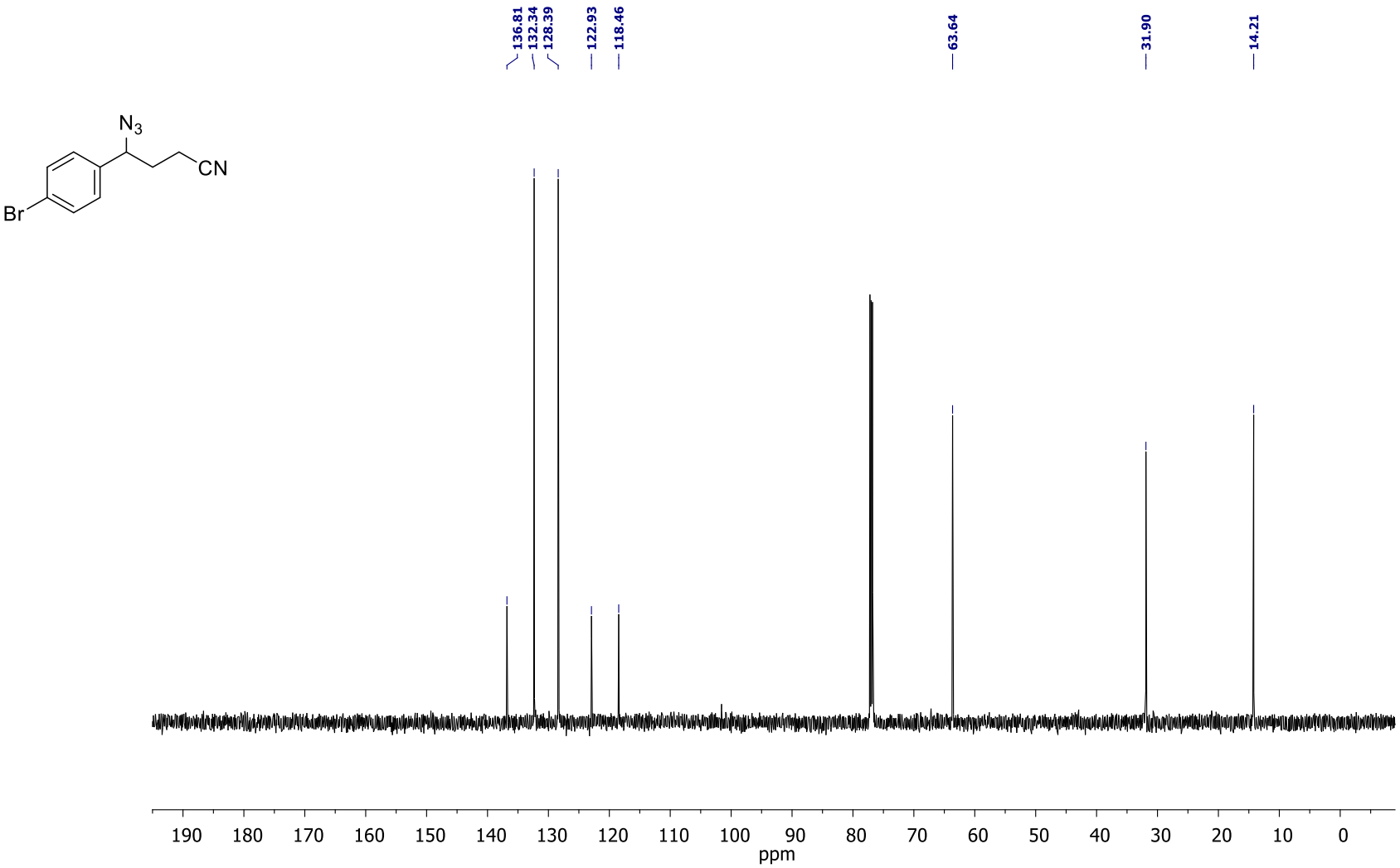
4-Azido-4-(4-bromophenyl)butyronitrile (9a)

^{1}H NMR (600 MHz, $CDCl_3$)



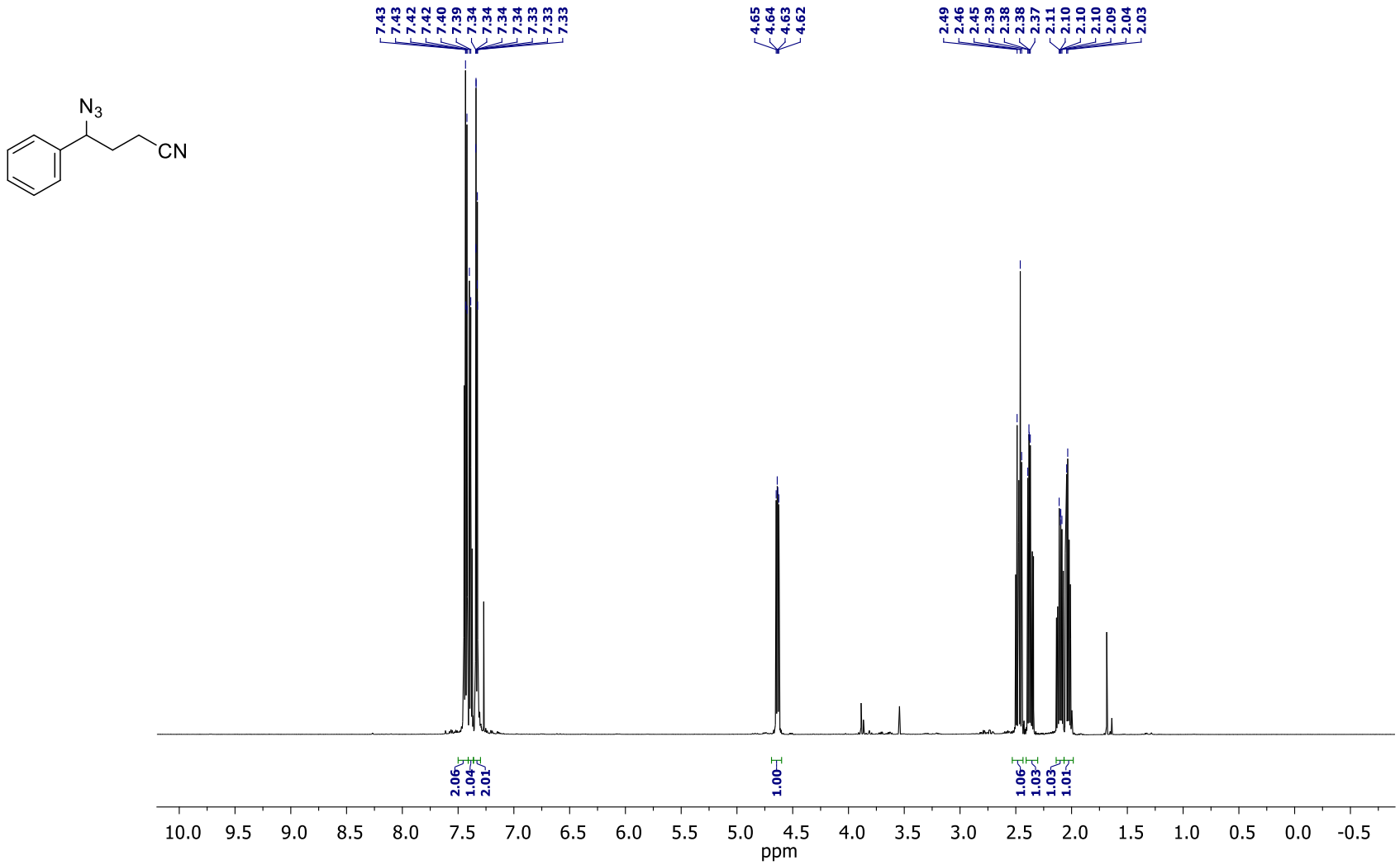
4-Azido-4-(4-bromophenyl)butyronitrile (9a)

^{13}C NMR (150 MHz, $CDCl_3$)



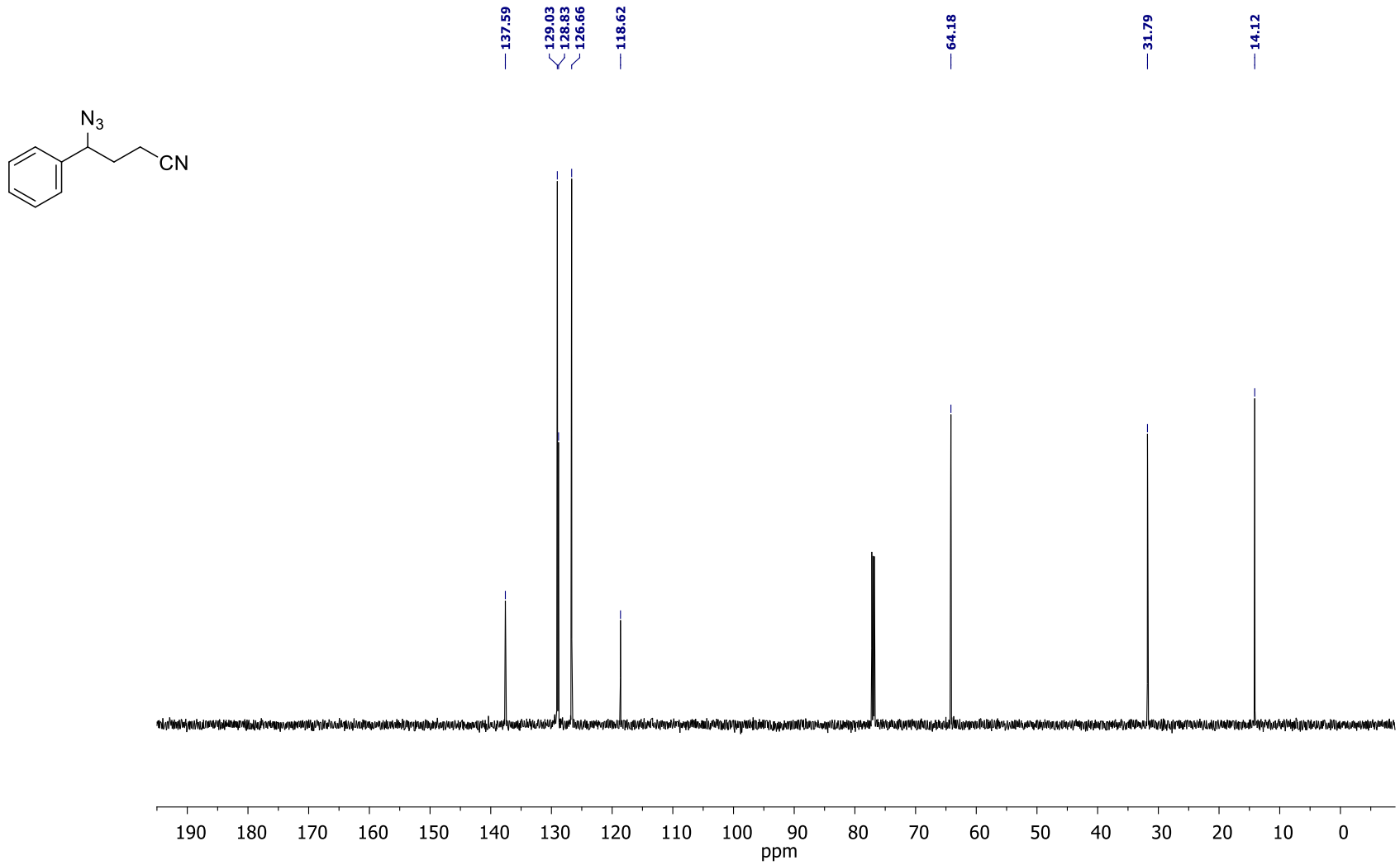
4-Azido-4-phenylbutyronitrile (9b)

^{1}H NMR (600 MHz, $CDCl_3$)



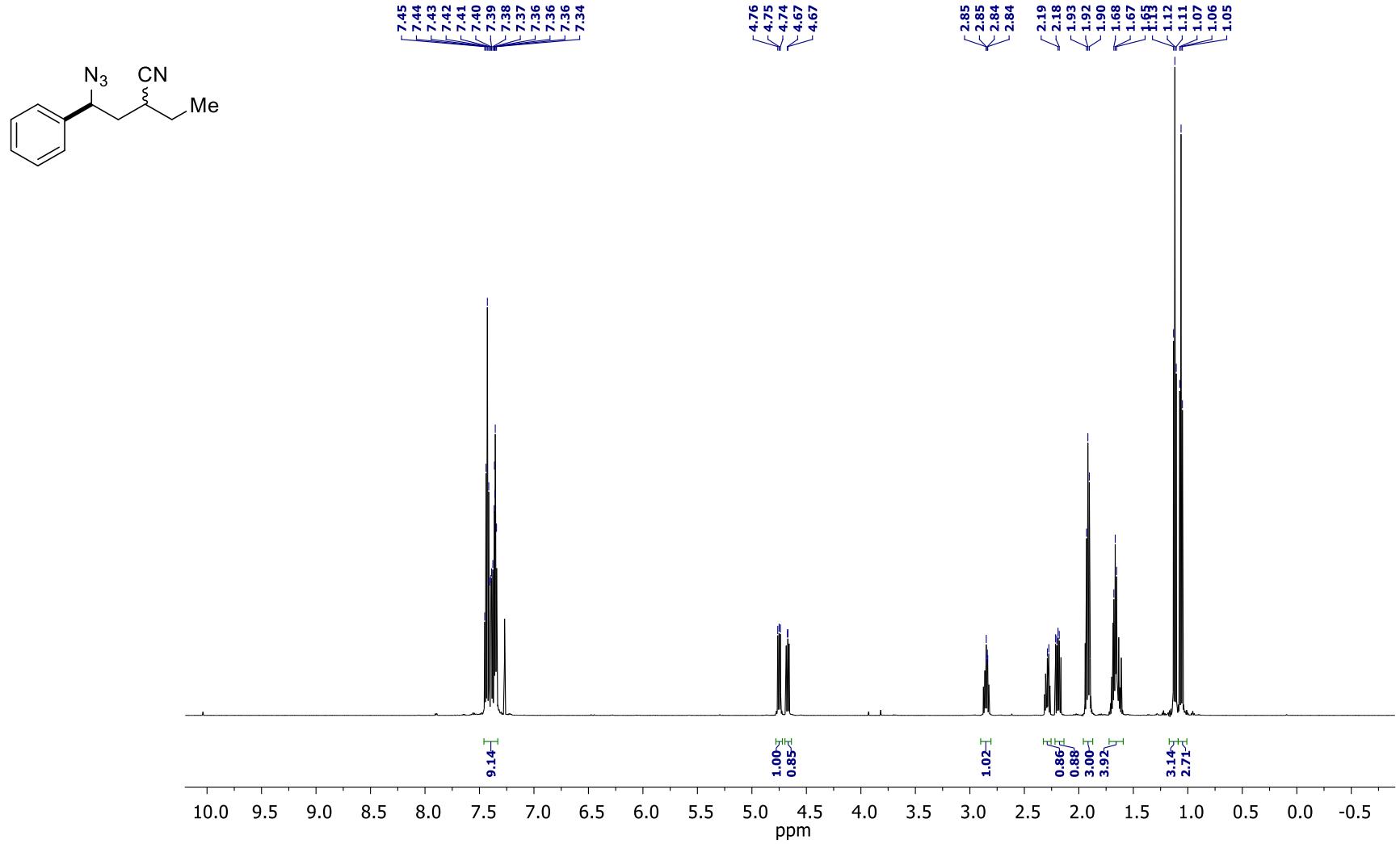
4-Azido-4-phenylbutyronitrile (9b)

^{13}C NMR (150 MHz, $CDCl_3$)



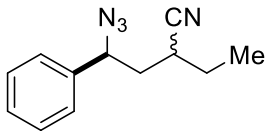
4-Azido-2-ethyl-4-phenylbutyronitrile (9c)

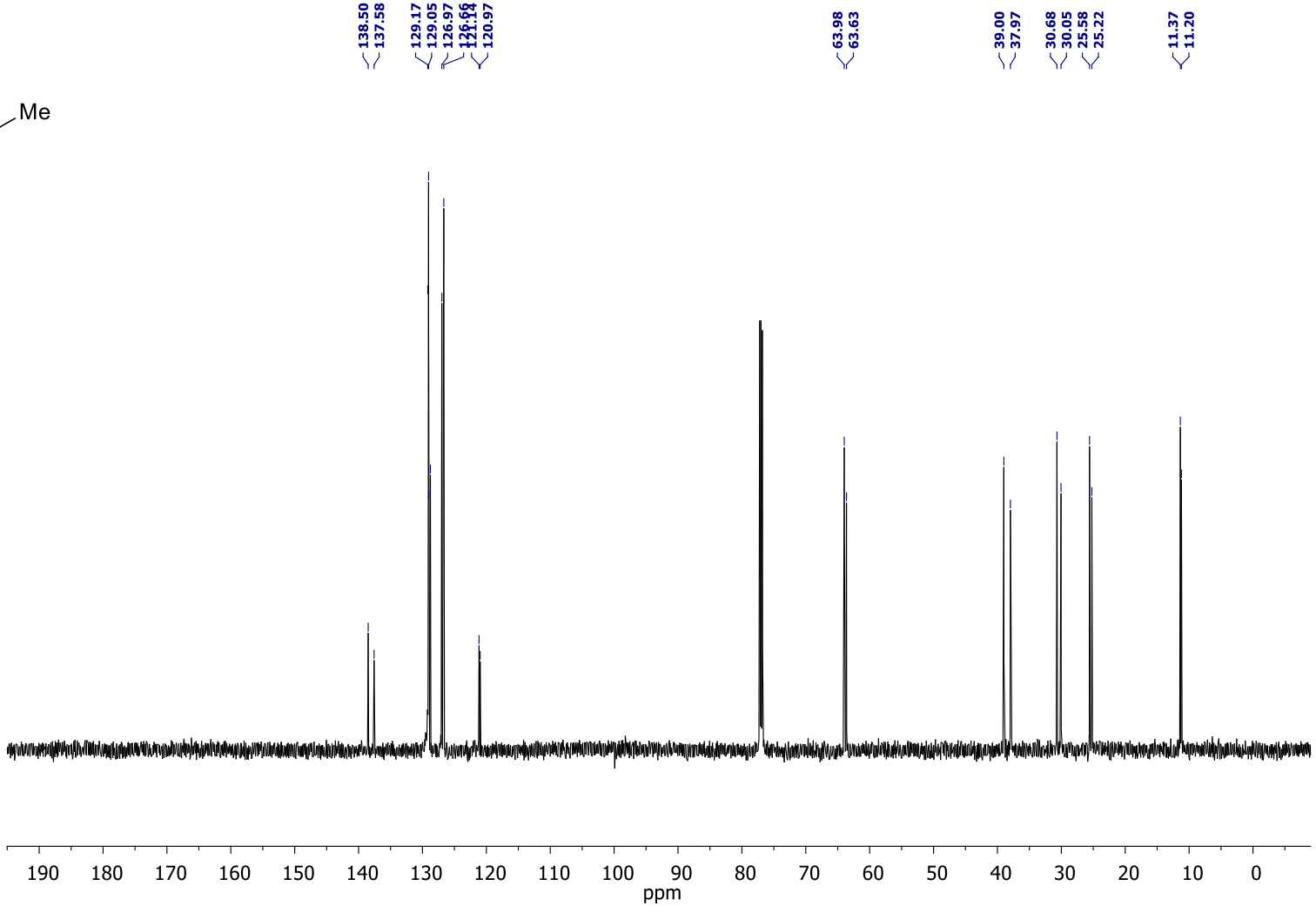
^{1}H NMR (600 MHz, $CDCl_3$)



4-Azido-2-ethyl-4-phenylbutyronitrile (9c)

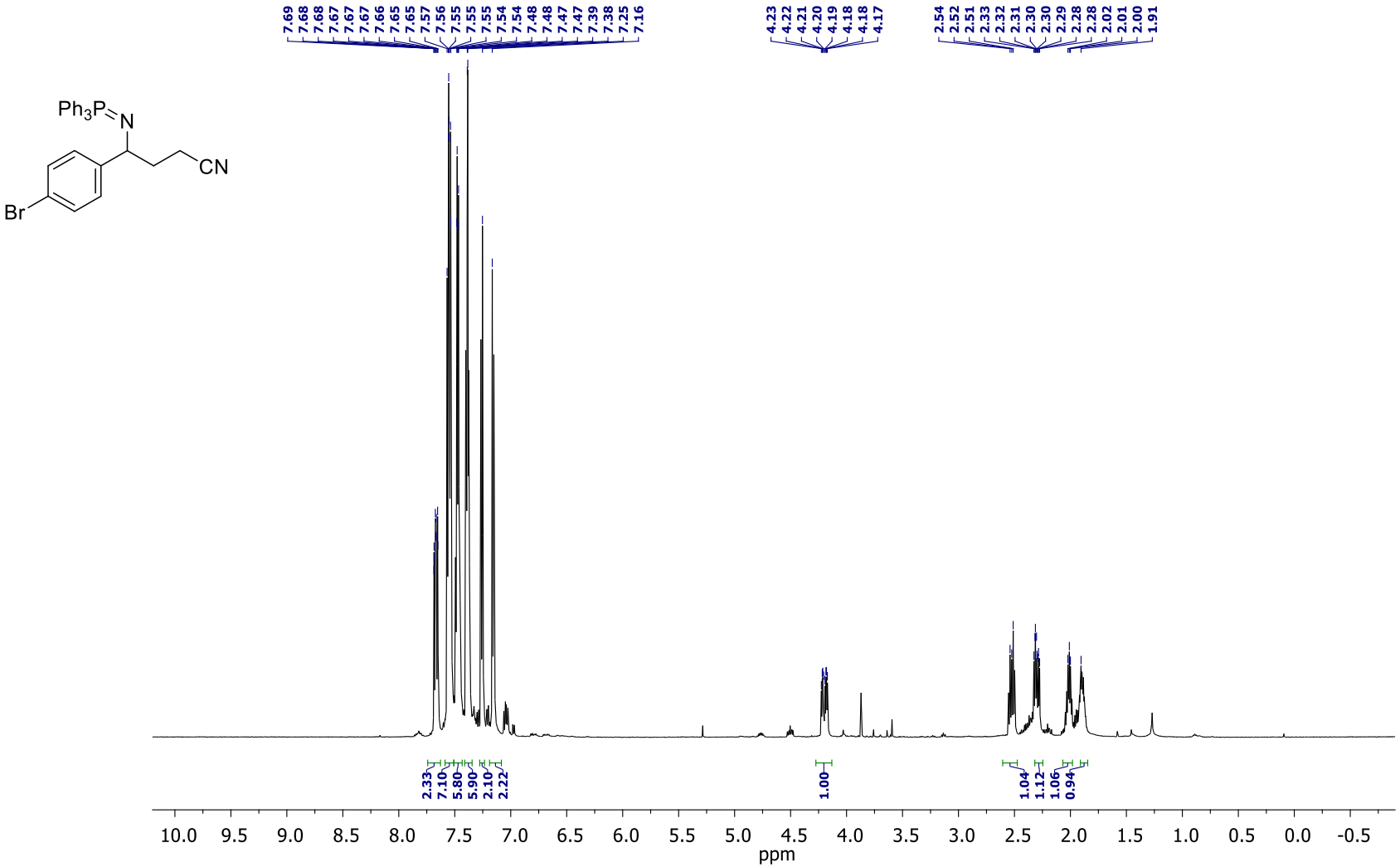
^{13}C NMR (150 MHz, $CDCl_3$)





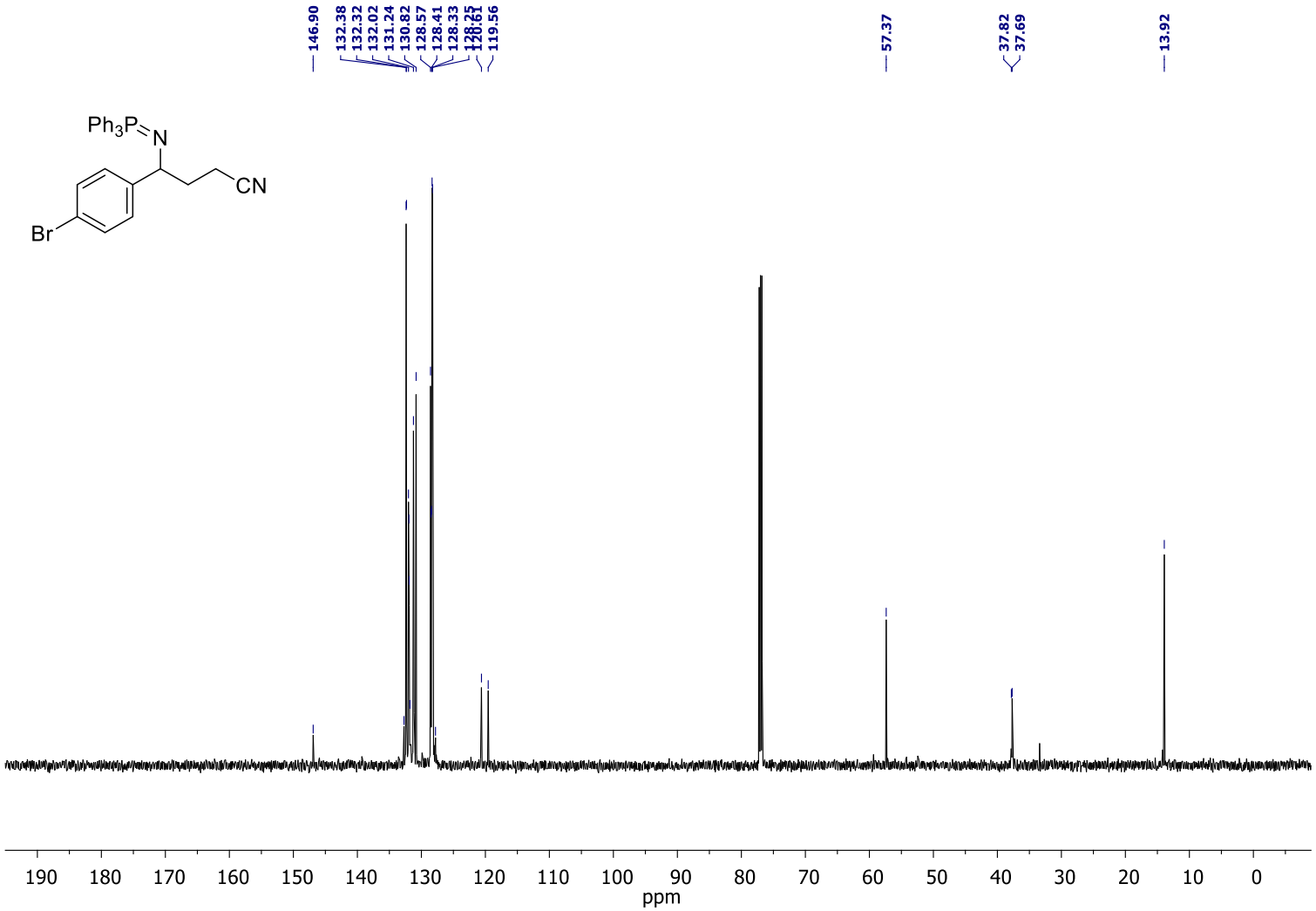
4-(4-Bromophenyl)-4-[(triphenyl-λ^5-phosphanylidene)amino]butyronitrile (10a)

^{1}H NMR (600 MHz, $CDCl_3$)

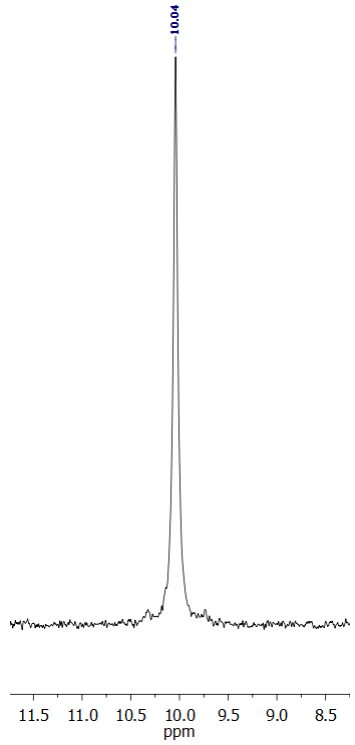


4-(4-Bromophenyl)-4-[(triphenyl-λ^5-phosphanylidene)amino]butyronitrile (10a)

^{13}C NMR (150 MHz, $CDCl_3$)

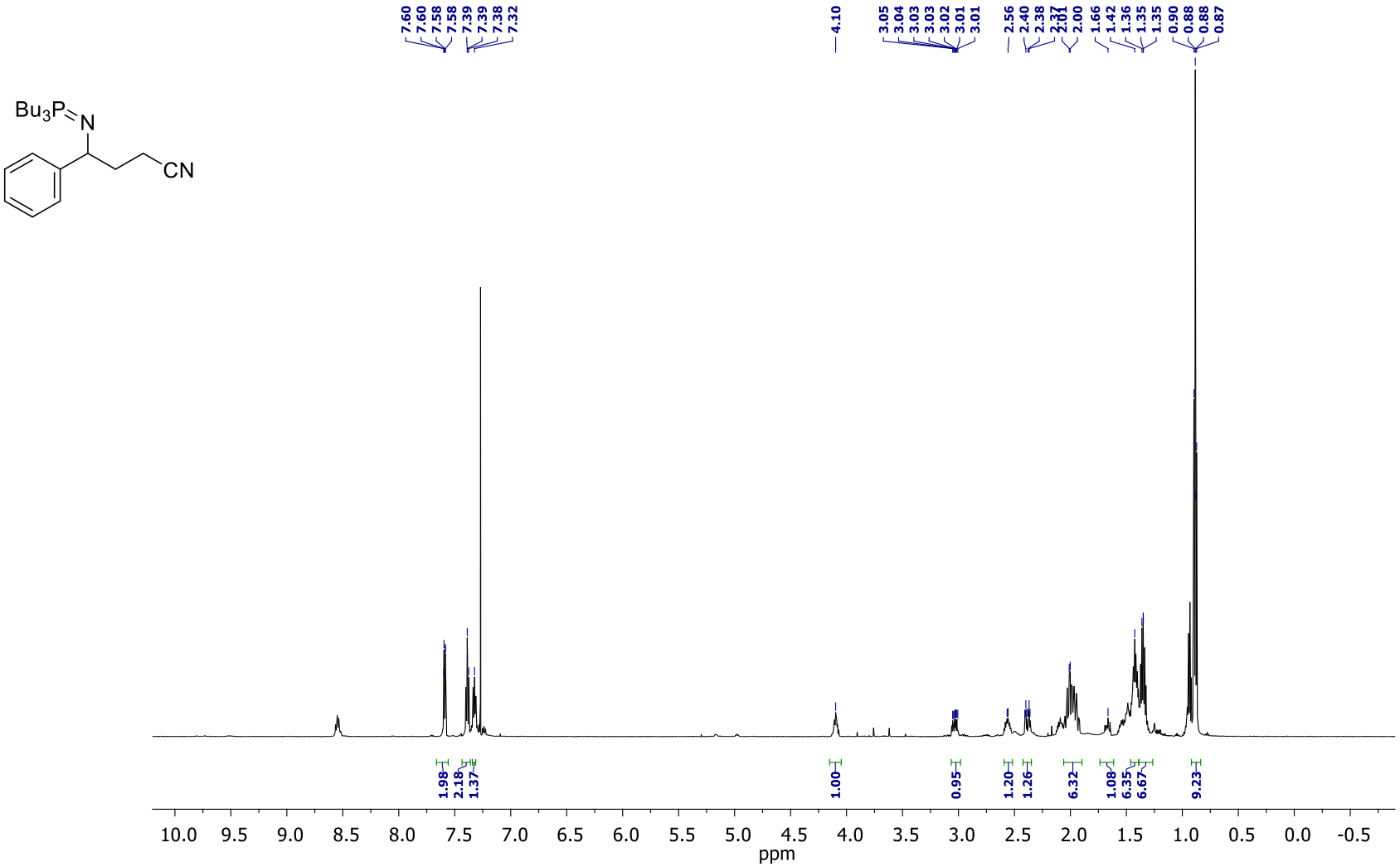


^{31}P NMR ($CDCl_3$, 162 MHz)



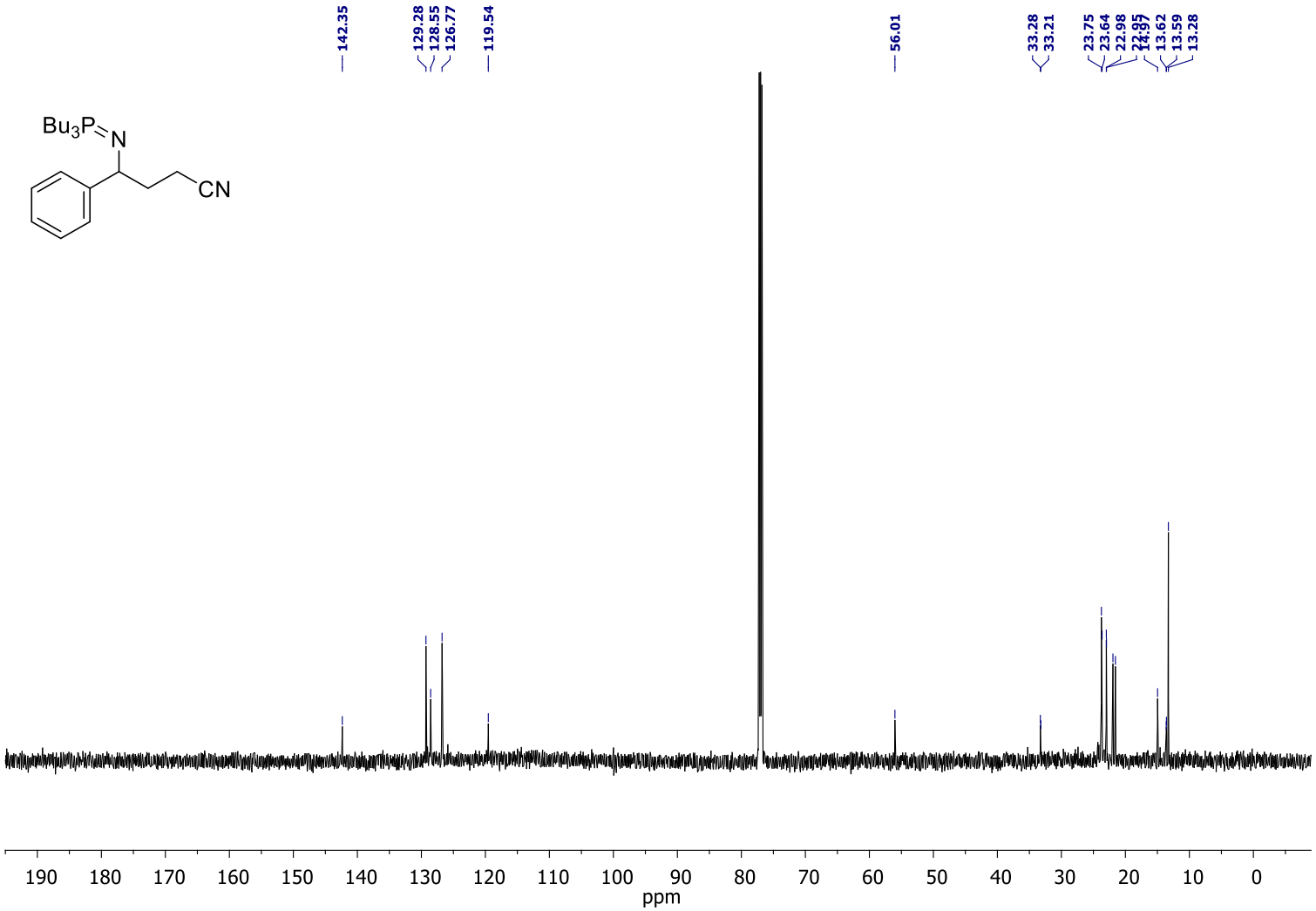
4-Phenyl-4-[(tributyl-λ^5-phosphanylidene)amino]butyronitrile (10b)

^{1}H NMR (600 MHz, $CDCl_3$)

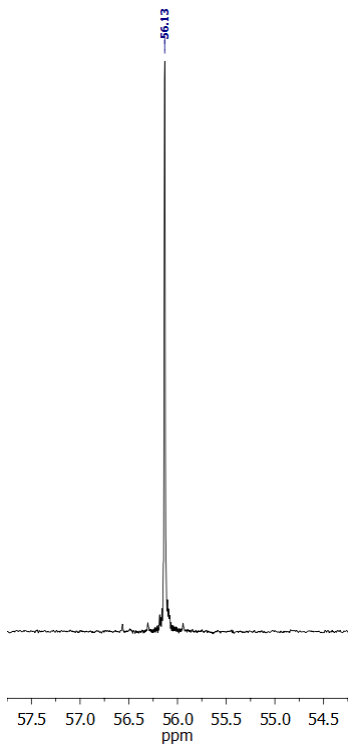


4-Phenyl-4-[(tributyl-λ^5-phosphanylidene)amino]butyronitrile (10b)

^{13}C NMR (150 MHz, $CDCl_3$)

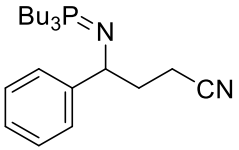


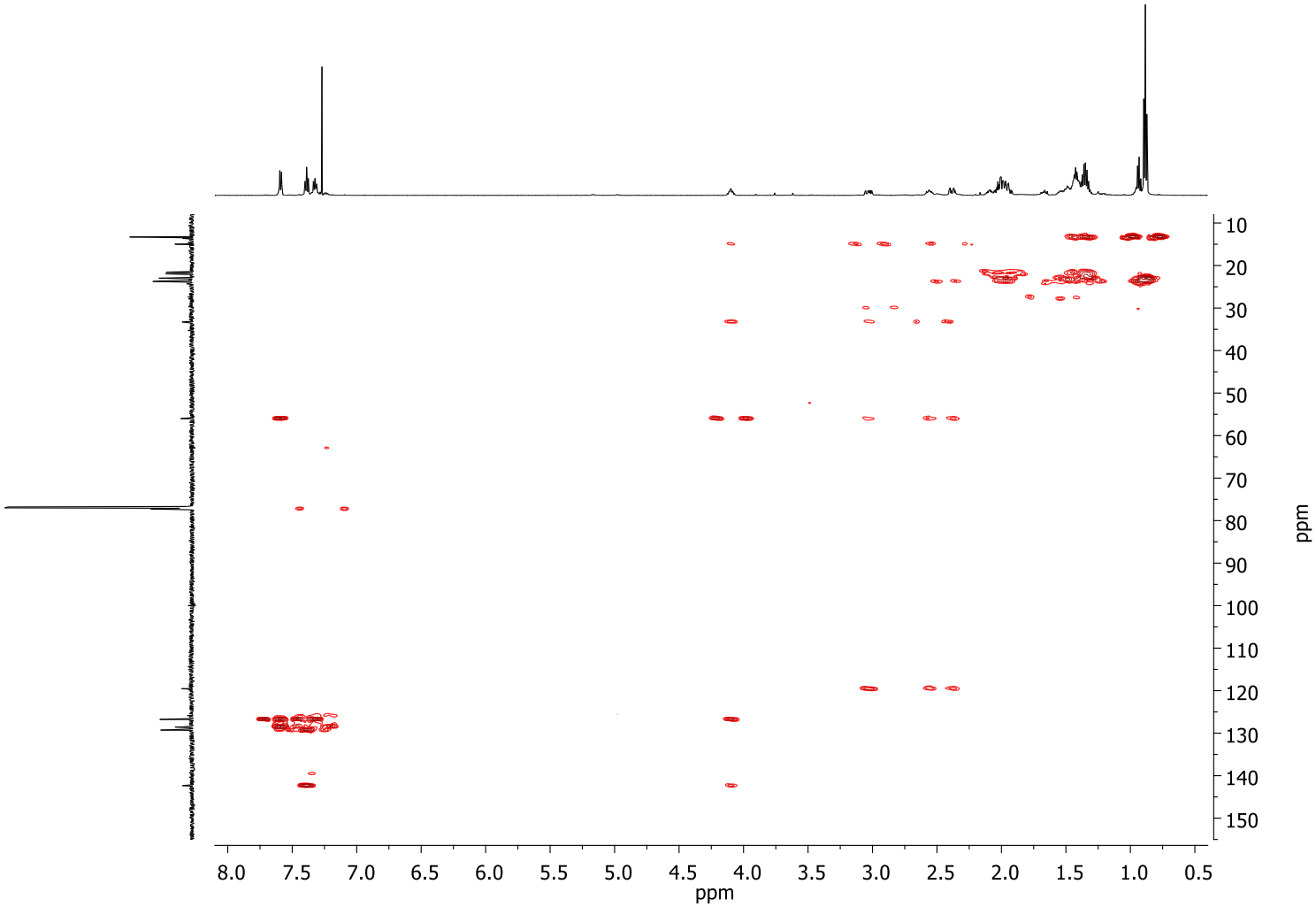
^{31}P NMR ($CDCl_3$, 162 MHz)



4-Phenyl-4-[(tributyl-λ^5-phosphanylidene)amino]butyronitrile (10b)

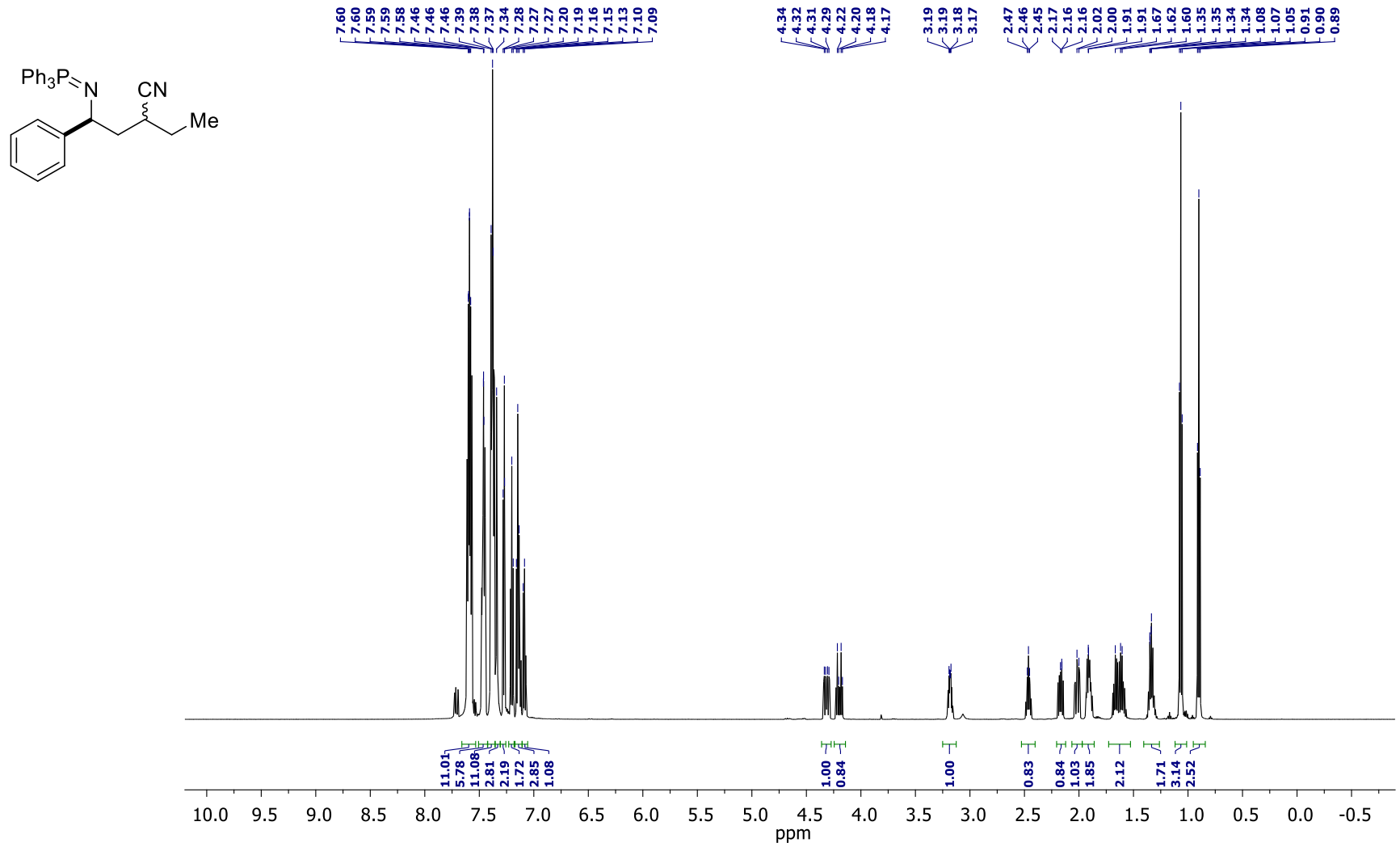
^{1}H-^{13}C HMBC ($CDCl_3$)





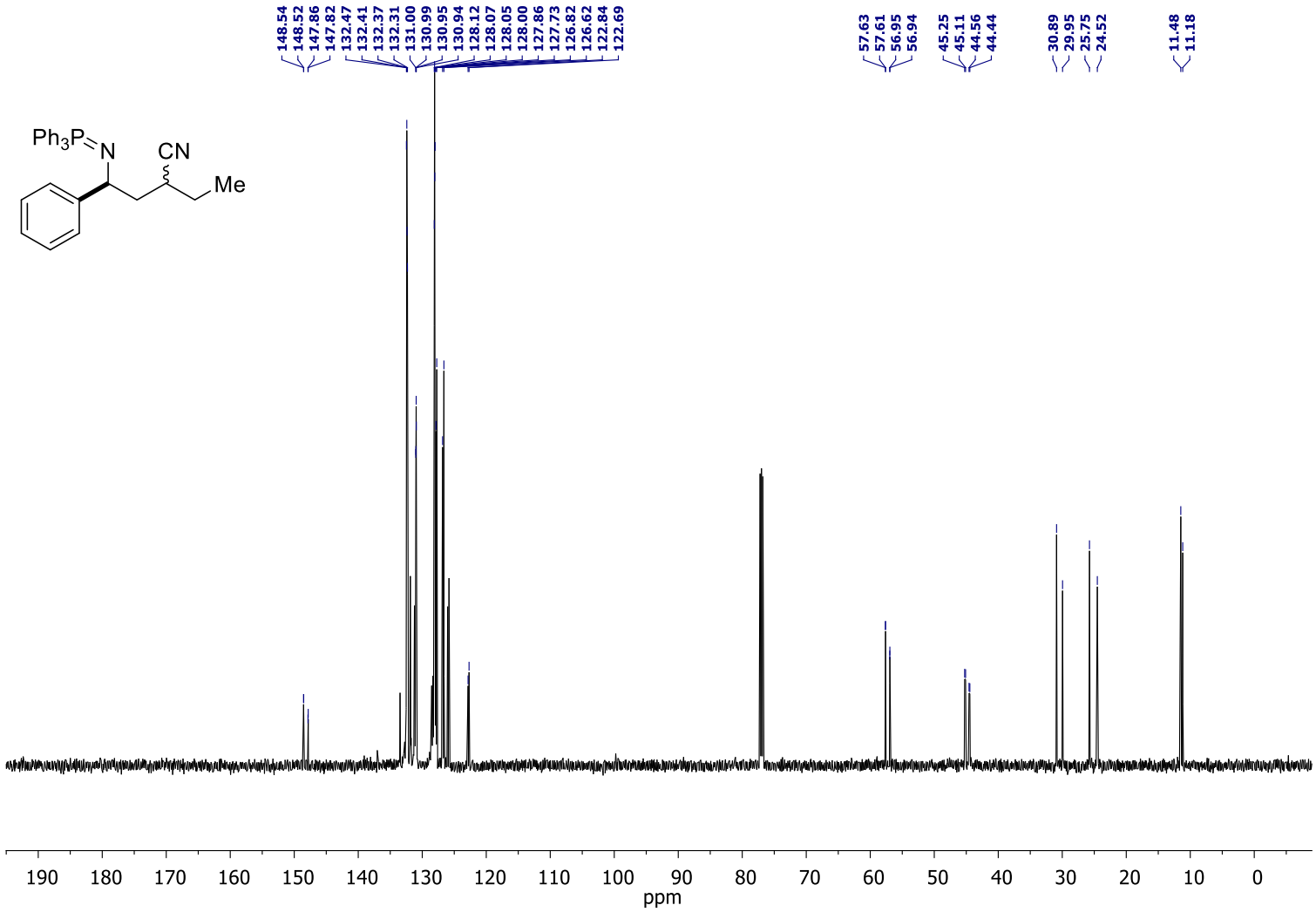
2-Ethyl-4-phenyl-4-[(triphenyl-λ^5-phosphanylidene)amino]butanenitrile (10c)

^{1}H NMR (600 MHz, $CDCl_3$)

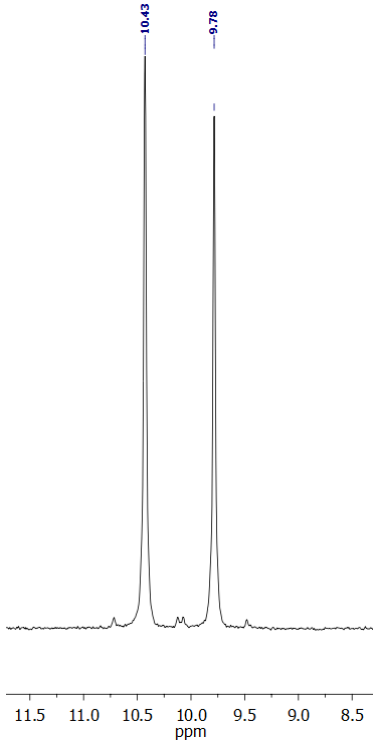


2-Ethyl-4-phenyl-4-[(triphenyl-λ^5-phosphanylidene)amino]butanenitrile (10c)

^{13}C NMR (150 MHz, $CDCl_3$)

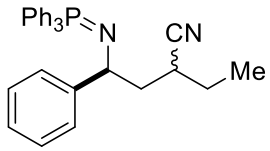


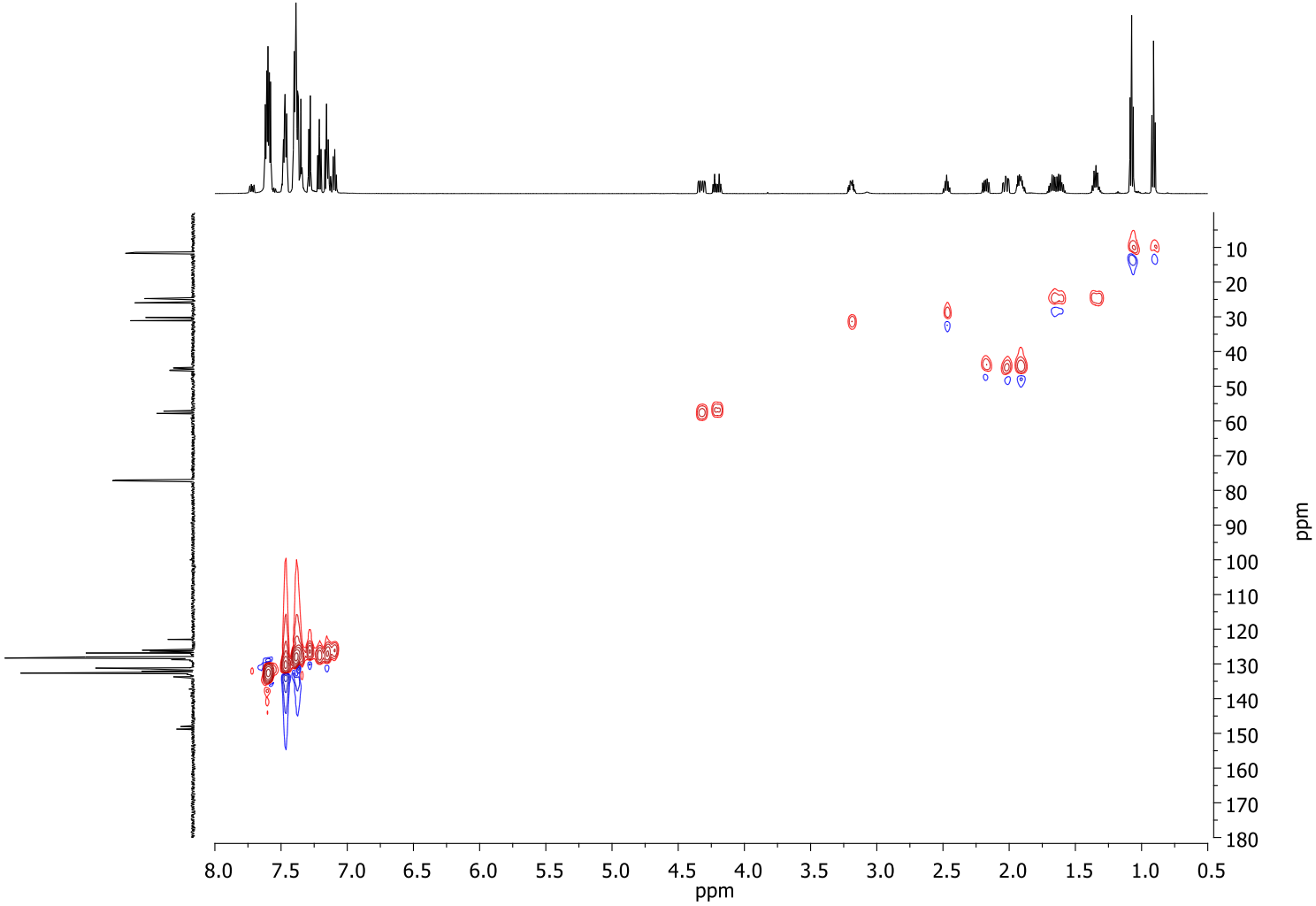
^{31}P NMR ($CDCl_3$, 162 MHz)



2-Ethyl-4-phenyl-4-[(triphenyl-λ^5-phosphanylidene)amino]butanenitrile (10c)

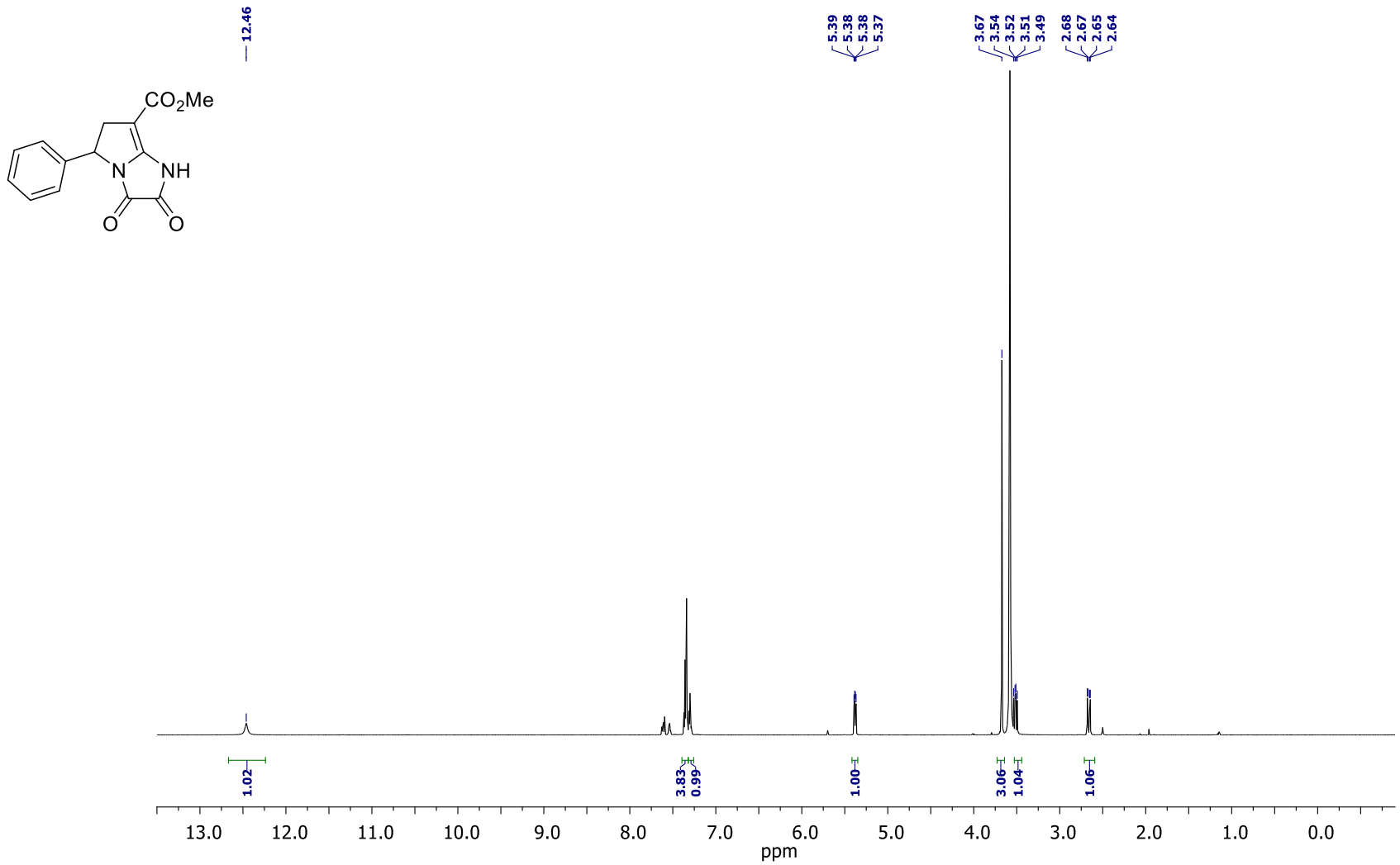
^{1}H-^{13}C HSQC ($CDCl_3$)





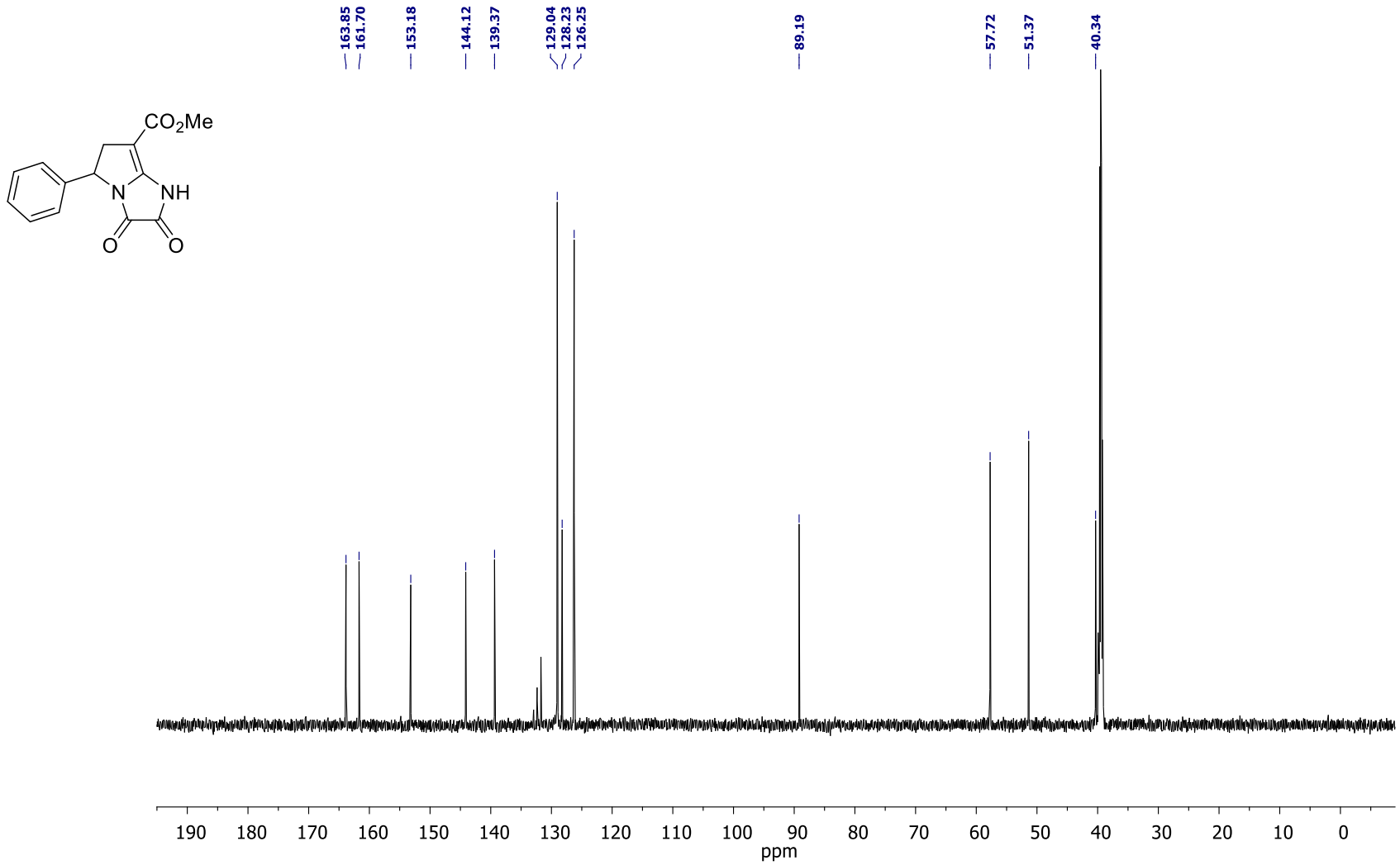
Methyl 2,3-dioxo-5-phenyl-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11a)

^{1}H NMR (600 MHz, DMSO-d$_6$)



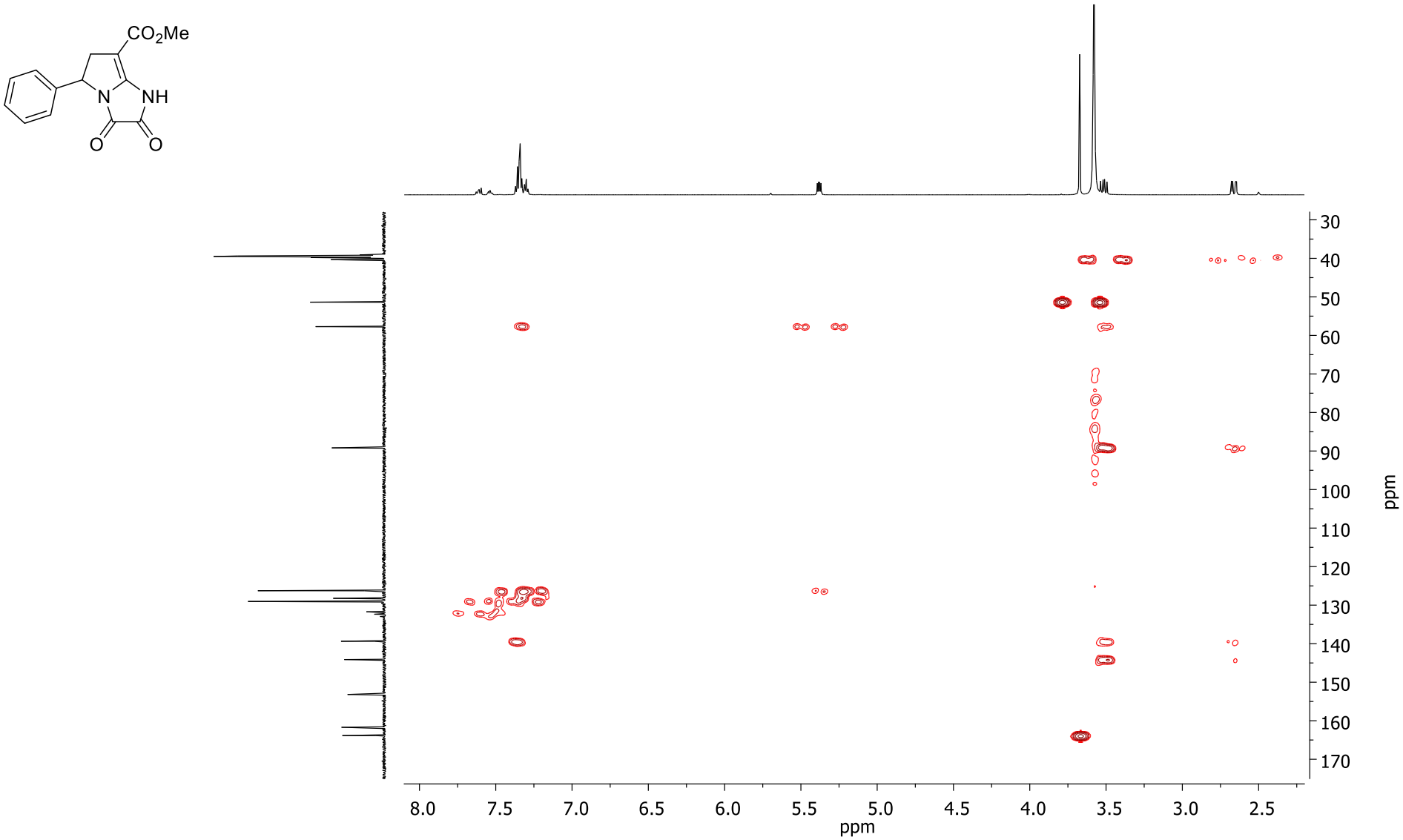
Methyl 2,3-dioxo-5-phenyl-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11a)

^{13}C NMR (150 MHz, DMSO-d$_6$)



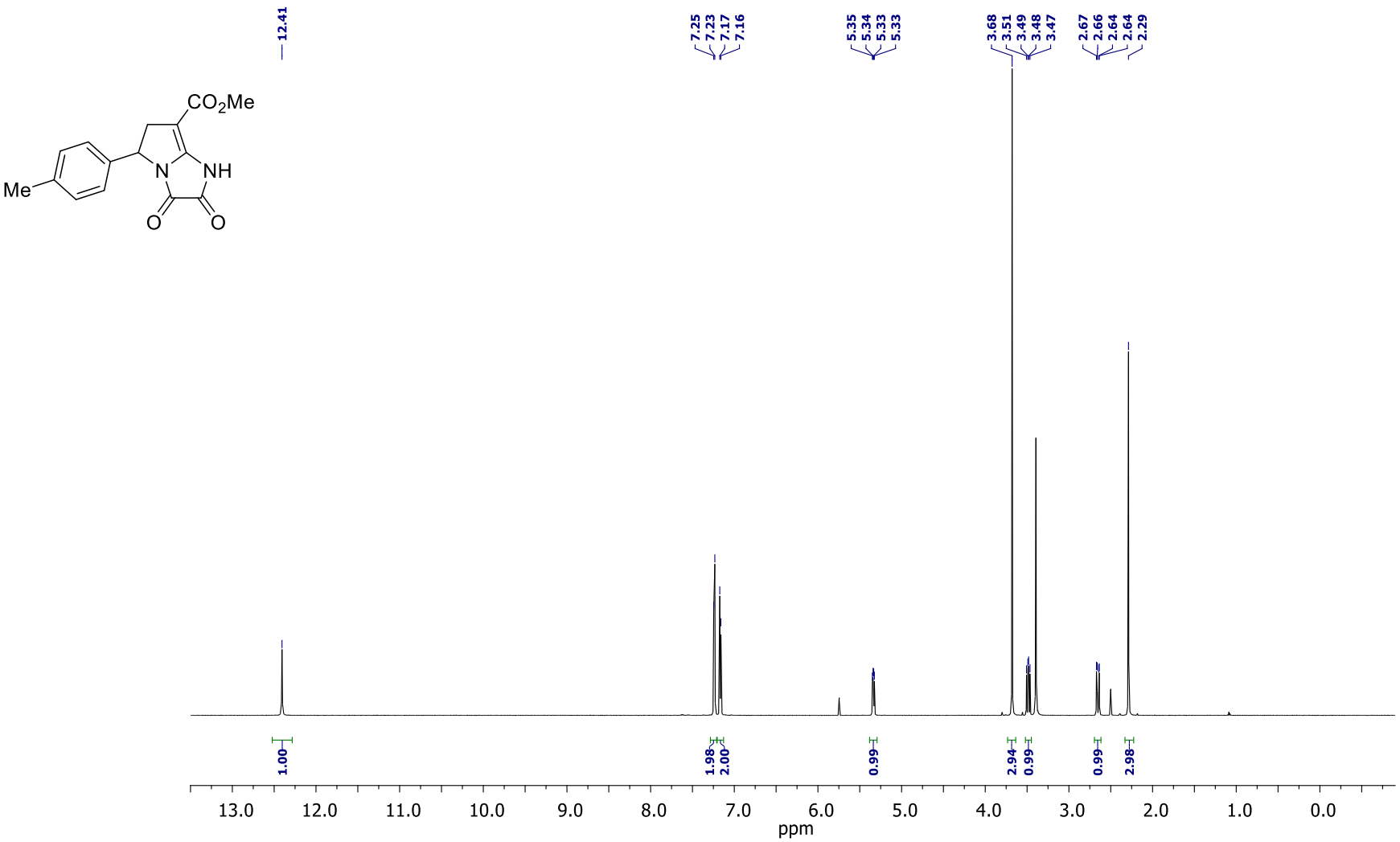
Methyl 2,3-dioxo-5-phenyl-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11a)

^{1}H-^{13}C HMBC (DMSO-d_6)



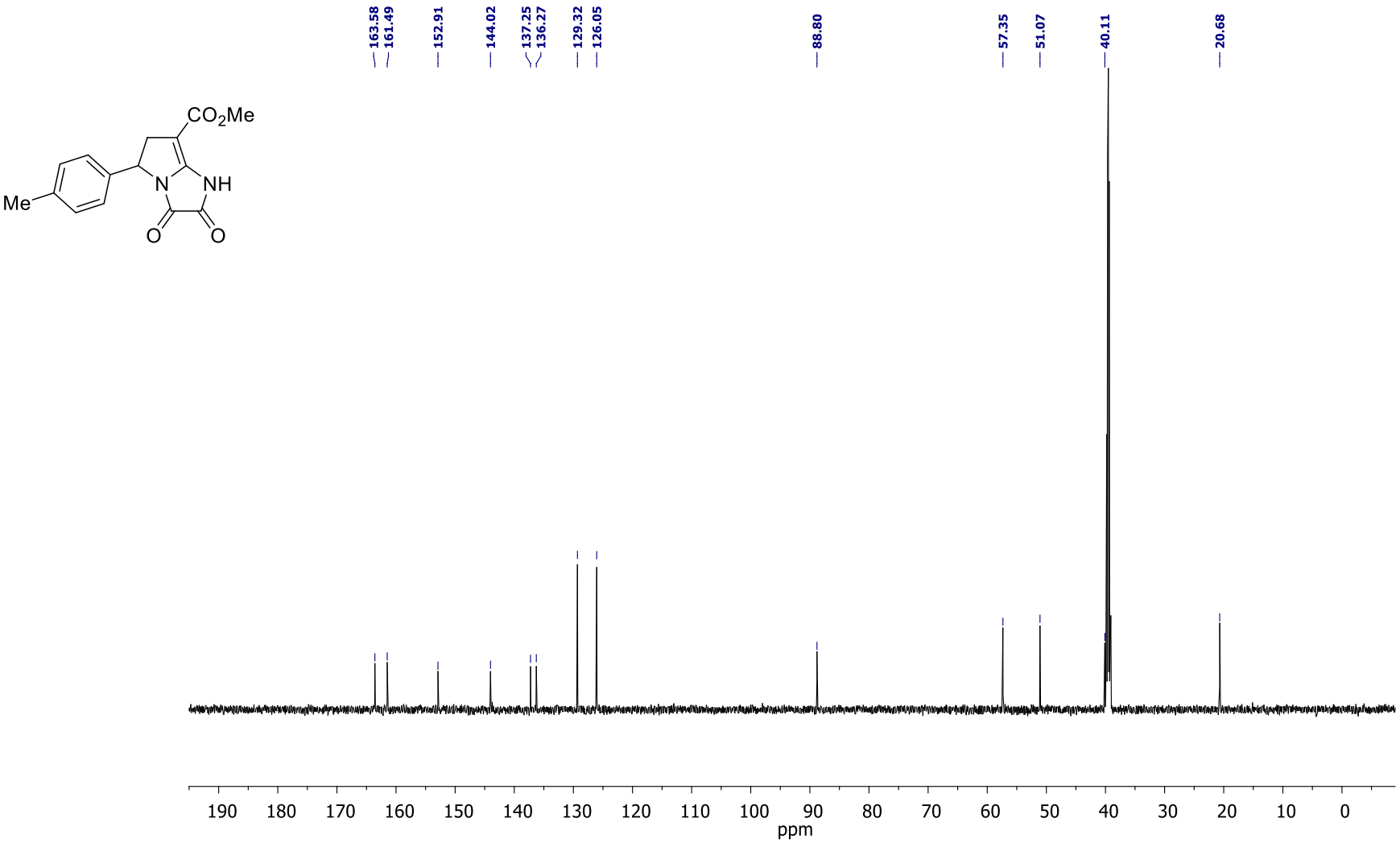
Methyl 2,3-dioxo-5-(*p*-tolyl)-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11b)

^{1}H NMR (600 MHz, DMSO-d$_6$)



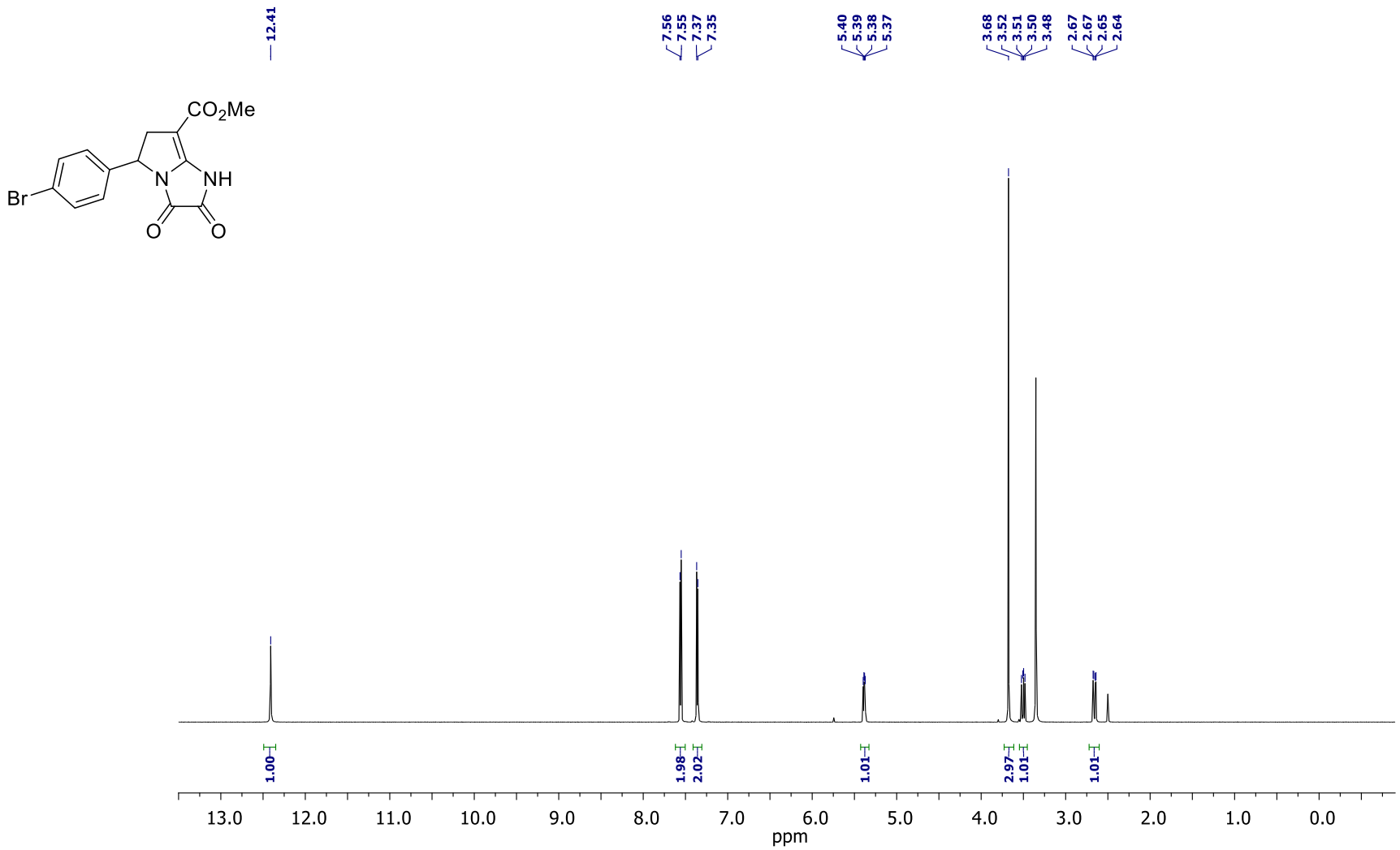
Methyl 2,3-dioxo-5-(*p*-tolyl)-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11b)

^{13}C NMR (150 MHz, DMSO-d$_6$)



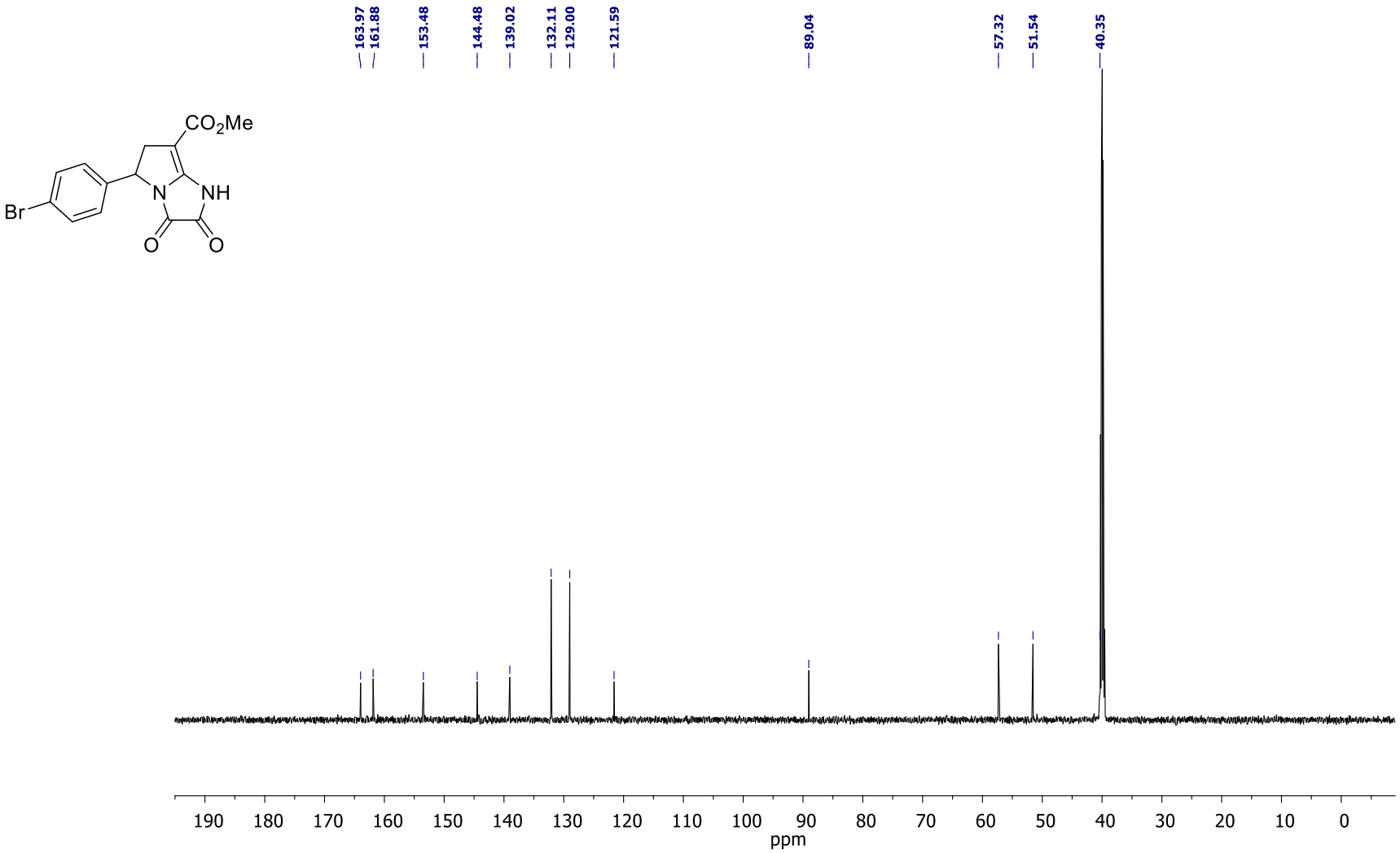
Methyl 5-(4-bromophenyl)-2,3-dioxo-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11c)

^{1}H NMR (600 MHz, DMSO-d$_6$)



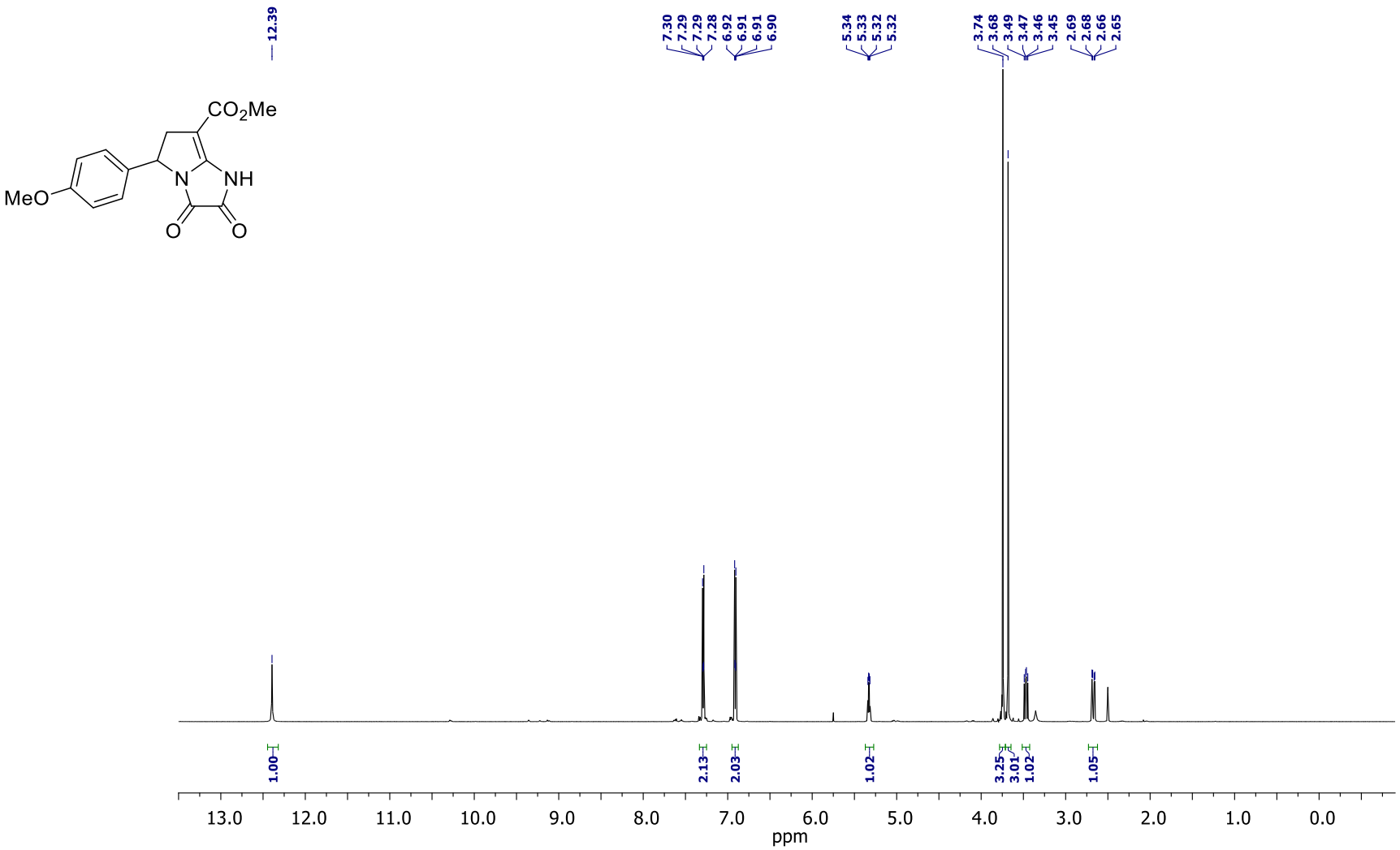
Methyl 5-(4-bromophenyl)-2,3-dioxo-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11c)

^{13}C NMR (150 MHz, DMSO-d$_6$)



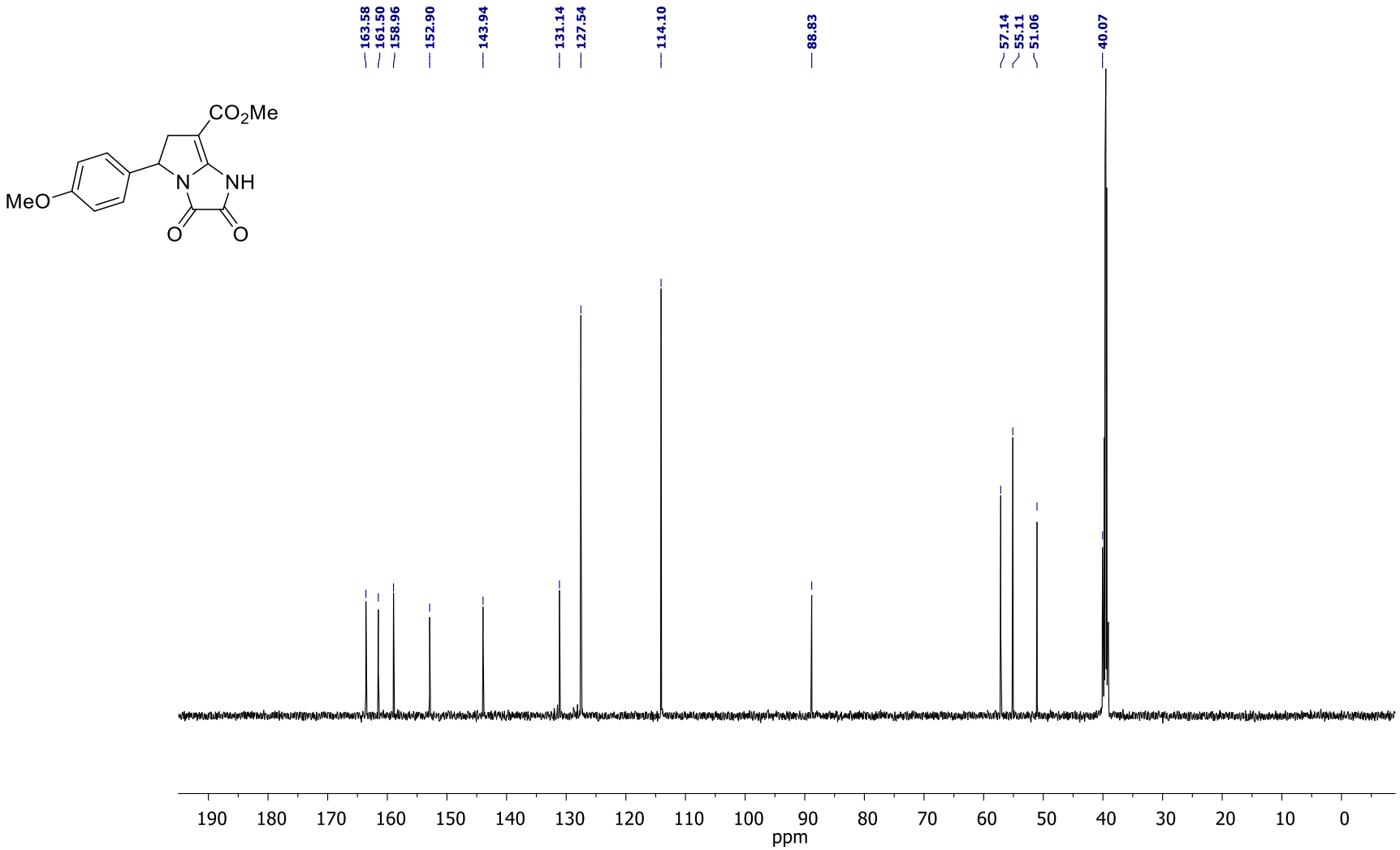
Methyl 5-(4-methoxyphenyl)-2,3-dioxo-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11d)

^{1}H NMR (600 MHz, DMSO-d$_6$)



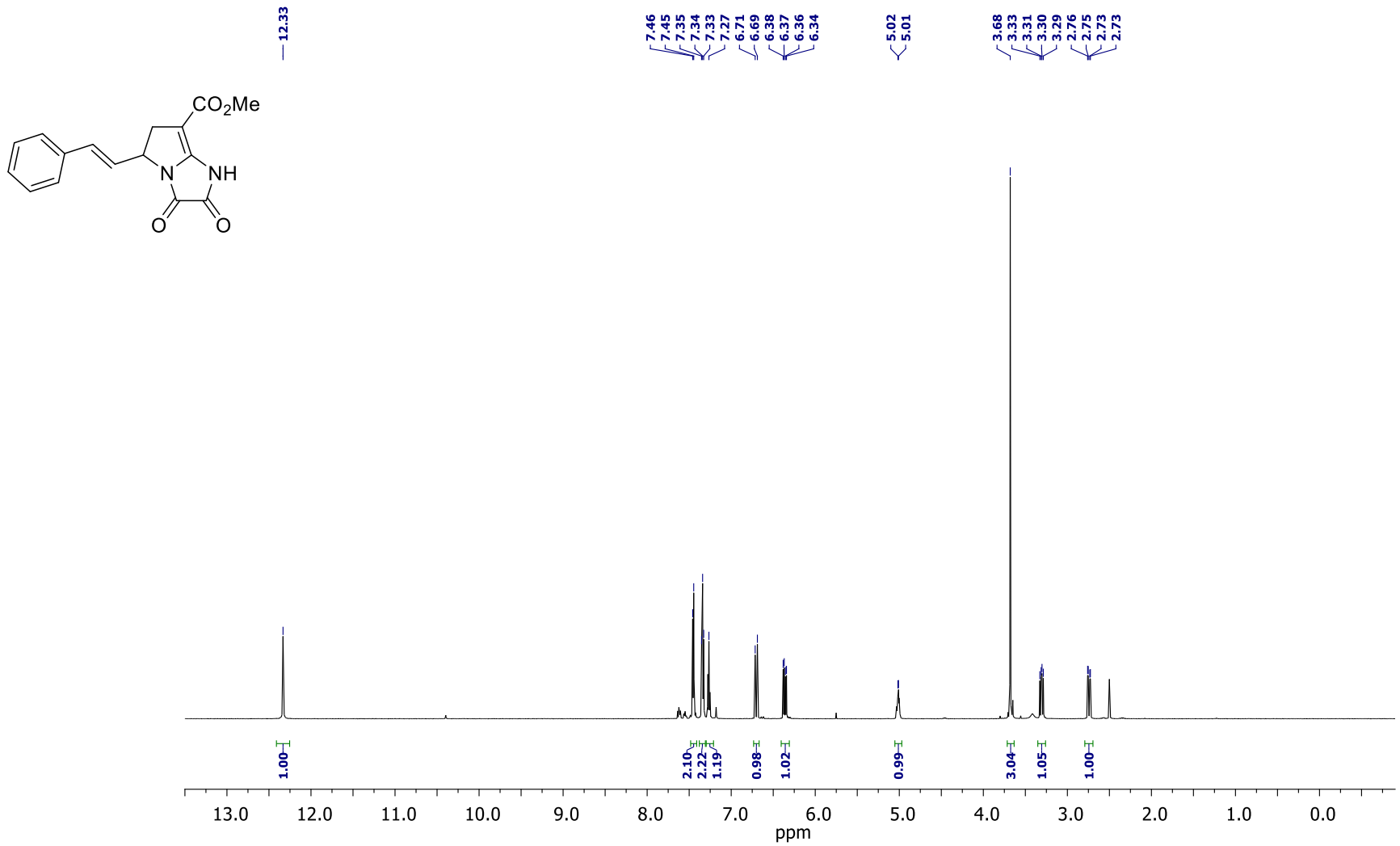
Methyl 5-(4-methoxyphenyl)-2,3-dioxo-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11d)

^{13}C NMR (150 MHz, DMSO-d$_6$)



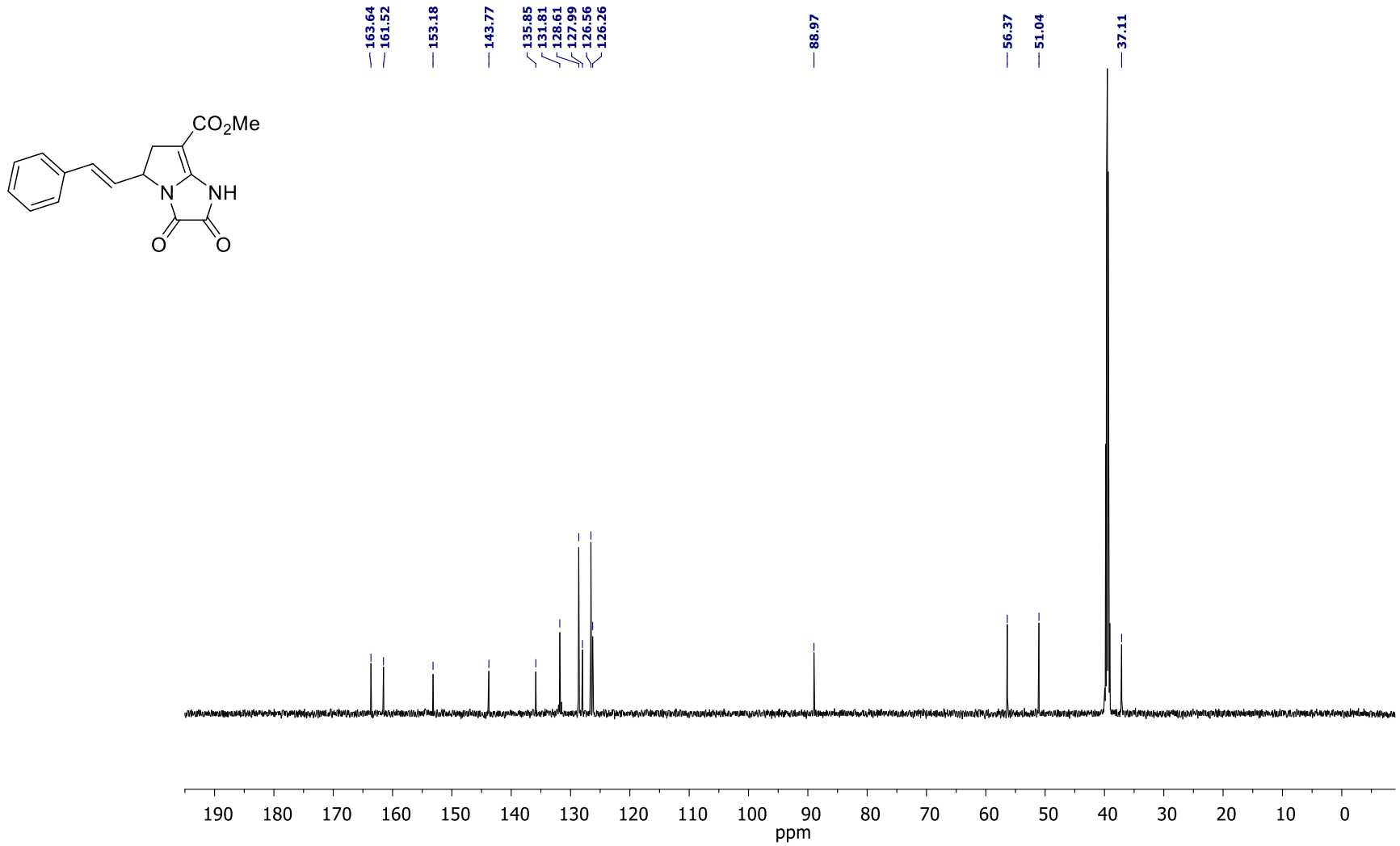
Methyl (*E*)-2,3-dioxo-5-styryl-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11e)

^{1}H NMR (600 MHz, DMSO-d$_6$)



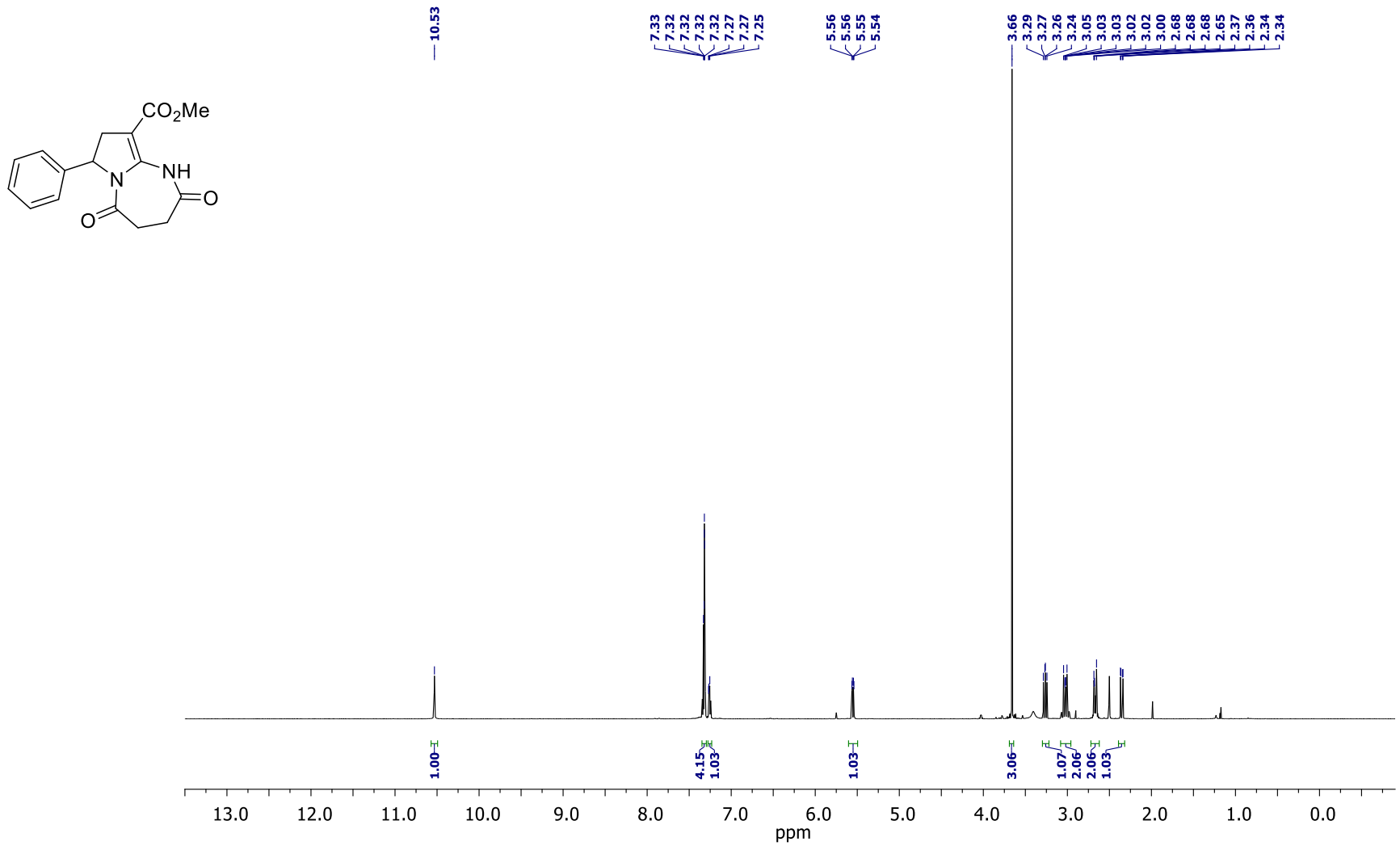
Methyl (*E*)-2,3-dioxo-5-styryl-2,3,5,6-tetrahydro-1*H*-pyrrolo[1,2-*a*]imidazole-7-carboxylate (11e)

^{13}C NMR (150 MHz, DMSO-d$_6$)



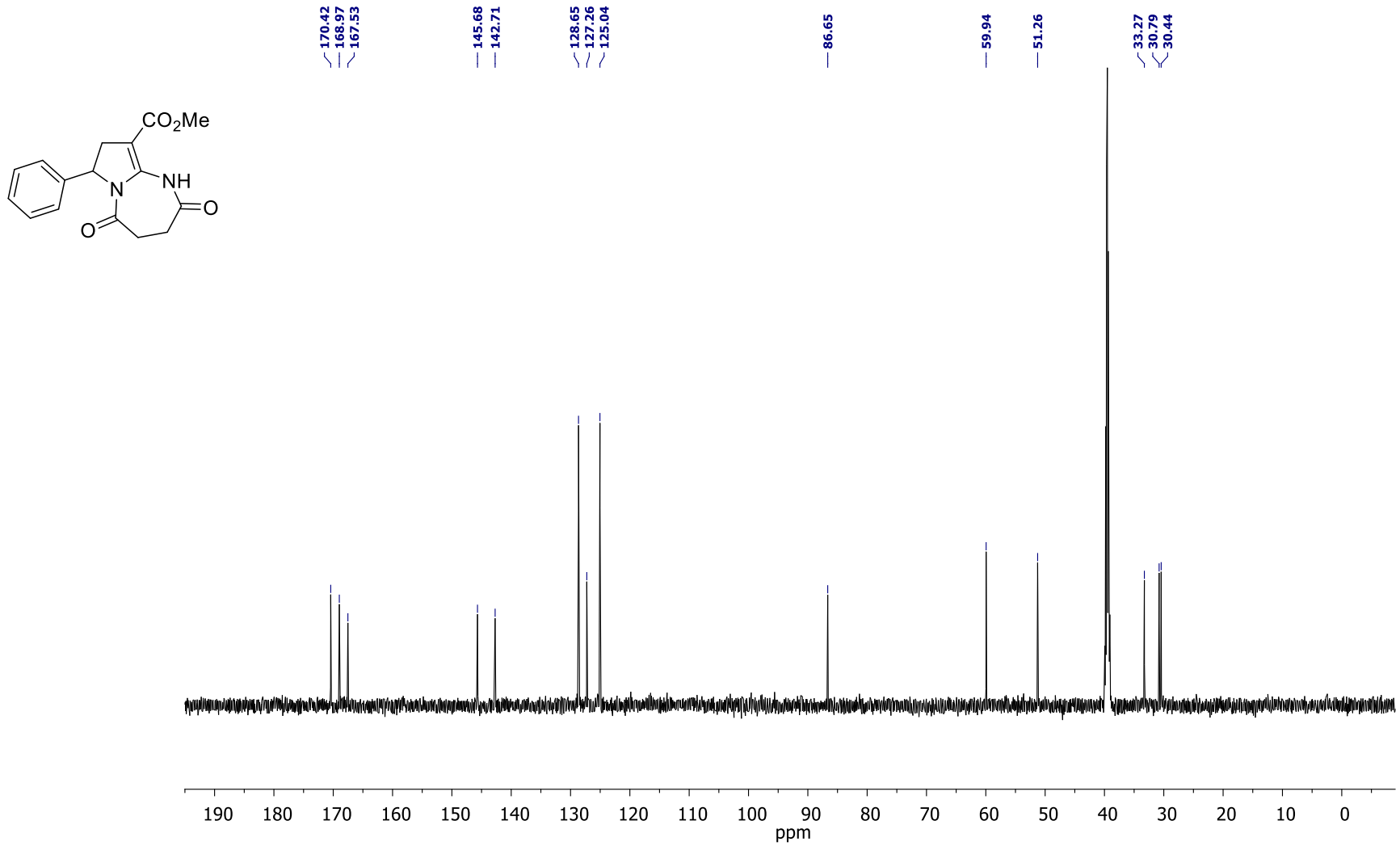
Methyl 2,5-dioxo-7-phenyl-2,3,4,5,7,8-hexahydro-1*H*-pyrrolo[1,2-*a*][1,3]diazepine-9-carboxylate (12a)

^{1}H NMR (600 MHz, DMSO-d$_6$)



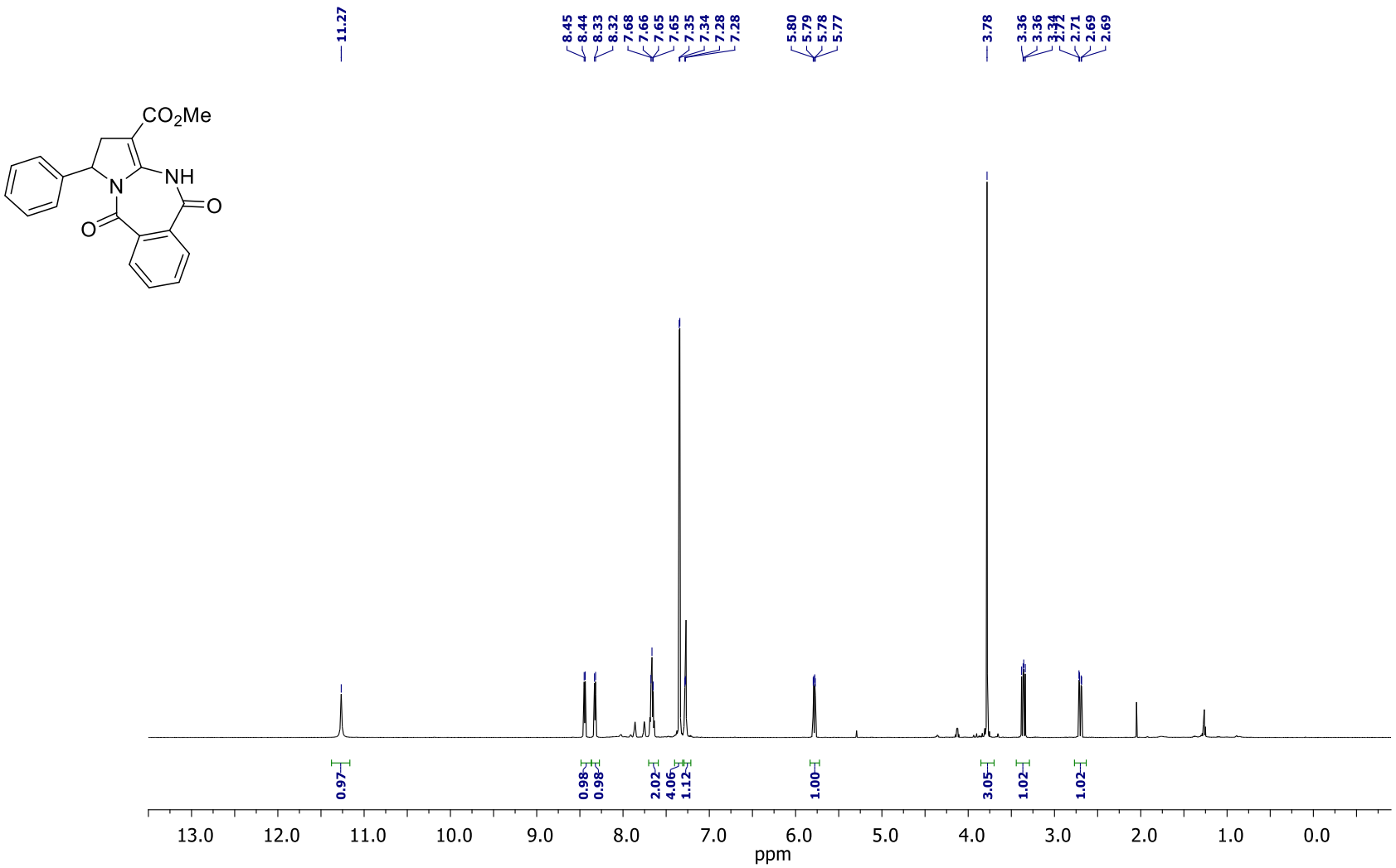
Methyl 2,5-dioxo-7-phenyl-2,3,4,5,7,8-hexahydro-1*H*-pyrrolo[1,2-*a*][1,3]diazepine-9-carboxylate (12a)

^{13}C NMR (150 MHz, DMSO-d$_6$)



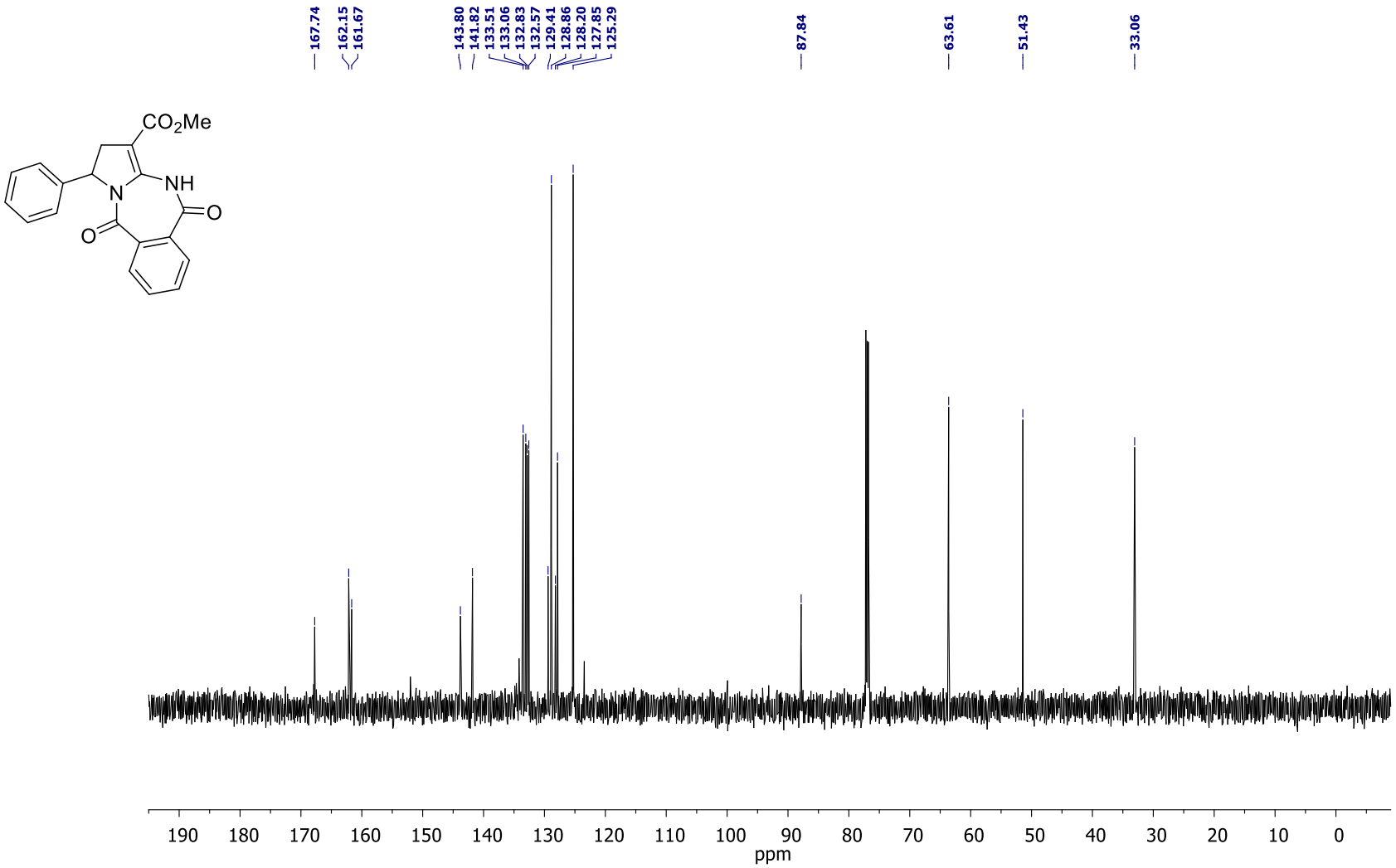
Methyl 5,10-dioxo-1-phenyl-2,4,5,10-tetrahydro-1*H*-pyrrolo[1,2-*b*][2,4]benzodiazepine-3-carboxylate (12b)

^{1}H NMR (600 MHz, $CDCl_3$)



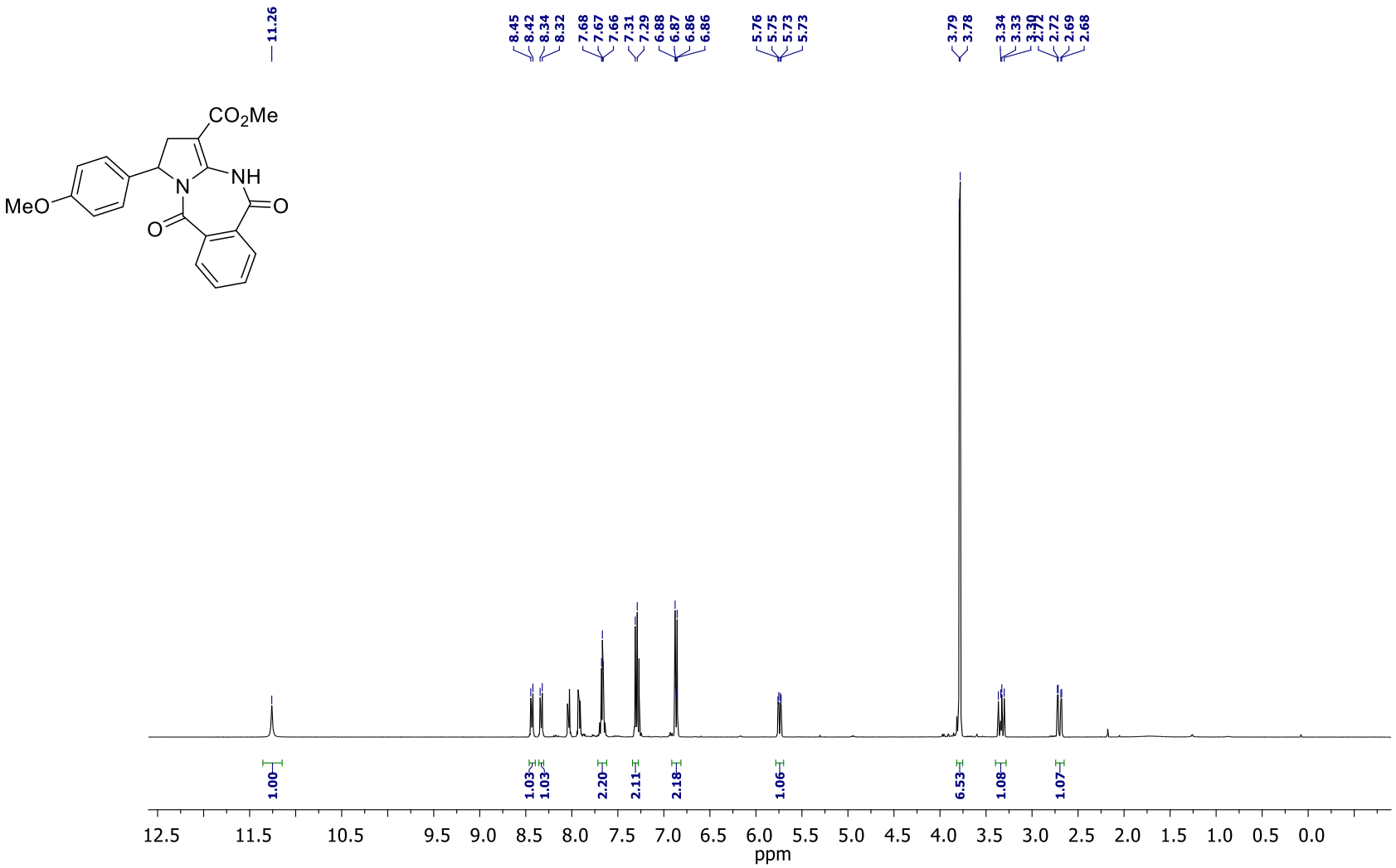
Methyl 5,10-dioxo-1-phenyl-2,4,5,10-tetrahydro-1*H*-pyrrolo[1,2-*b*][2,4]benzodiazepine-3-carboxylate (12b)

^{13}C NMR (150 MHz, $CDCl_3$)



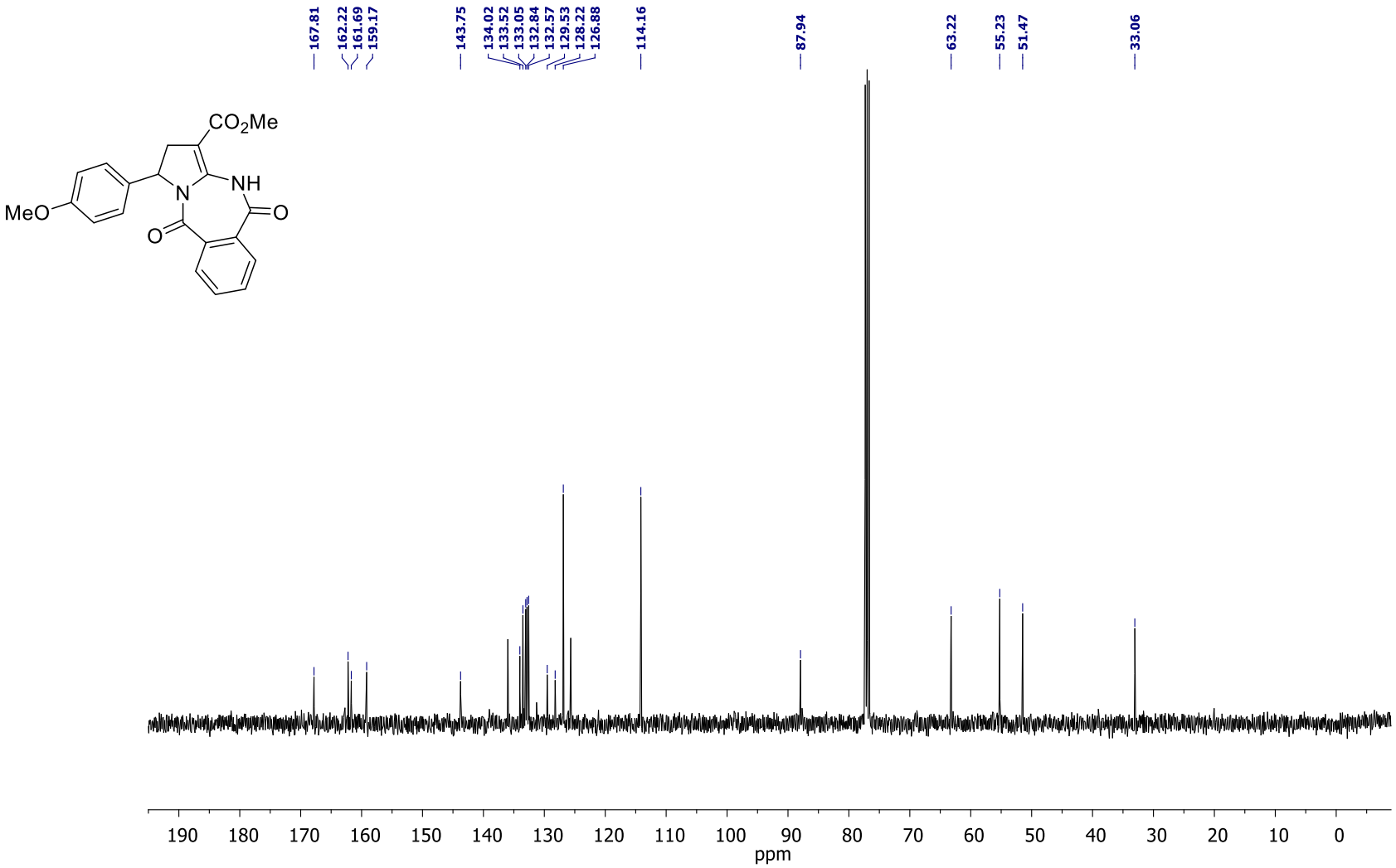
Methyl 1-(4-methoxyphenyl)-5,10-dioxo-2,4,5,10-tetrahydro-1*H*-pyrrolo[1,2-*b*][2,4]benzodiazepine-3-carboxylate (12c)

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



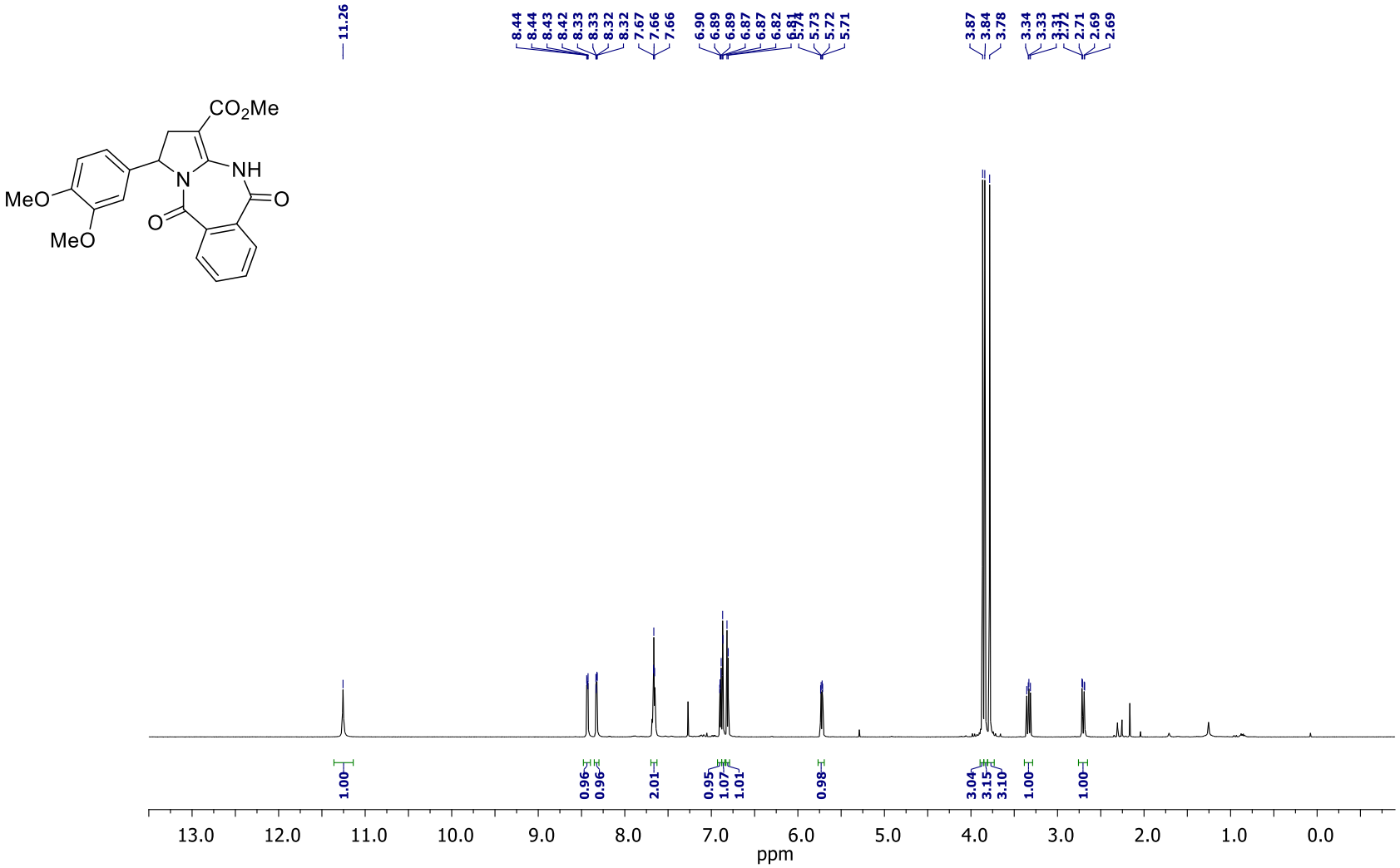
Methyl 1-(4-methoxyphenyl)-5,10-dioxo-2,4,5,10-tetrahydro-1*H*-pyrrolo[1,2-*b*][2,4]benzodiazepine-3-carboxylate (12c)

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



Methyl 1-(3,4-dimethoxyphenyl)-5,10-dioxo-2,4,5,10-tetrahydro-1*H*-pyrrolo[1,2-*b*][2,4]benzodiazepine-3-carboxylate (12d)

^{1}H NMR (600 MHz, $CDCl_3$)



Methyl 1-(3,4-dimethoxyphenyl)-5,10-dioxo-2,4,5,10-tetrahydro-1*H*-pyrrolo[1,2-*b*][2,4]benzodiazepine-3-carboxylate (12d)

^{13}C NMR (150 MHz, $CDCl_3$)