Selective Synthesis of
2,3-Disubstituted-2*H*-isoindol-1-ylphosphonate and
2,3-Disubstituted-1,2-dihydroisoquinolin-1-ylphosphonate
via Metal-tuned Reaction of α -amino
(2-alkynylphenyl)methylphosphonate

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Supporting Information

1. General procedure and characterization data for compound **1-3**. (S2-S17)
2. Copies of ¹H and ¹³C NMR spectra of compound **1-3**. (S18-S79).

General experimental method:

All reactions were performed in test tubes under air atmosphere at room temperature. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63 μm , standard grade). Analytical thin-layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated at ~20 Torr (house vacuum) at 25–35 $^{\circ}\text{C}$. Solvents were re-distilled prior to use in the reactions. Other commercial reagents were used as received. Nuclear magnetic resonance (NMR) spectra were recorded in parts per million from internal tetramethylsilane on the δ scale.

General Procedure for preparation of compound 1:

A mixture of 2-alkynyl benzaldehyde (3.0 mmol), amine (3.0 mmol), diethyl phosphite (3.0 mmol), and FeCl_3 (0.3 mmol, 10 mol%) in ethanol (3.0 mL) was stirred at $60\text{ }^{\circ}\text{C}$. After completion of the reaction as indicated by TLC, the solvent was removed under reduced pressure. The residue was diluted with EtOAc (5.0 mL), washed with water (5.0 mL). Evaporation of the solvent followed by purification on silica gel afforded 2-alkynyl α -amino benzylphosphonate **1**.

Diethyl (4-methoxyphenylamino)(2-(2-phenylethynyl)phenyl)methylphosphonate

(1a)

^1H NMR (400 MHz, CDCl_3) δ 1.06 (t, $J = 7.3$ Hz, 3H), 1.30 (t, $J = 7.3$ Hz, 3H), 3.60-3.65 (m, 1H), 3.66 (s, 3H), 3.86-3.93 (m, 1H), 4.18-4.24 (m, 2H), 4.80 (br, 1H), 5.49 (d, $J = 24.4$ Hz, 1H), 6.61 (d, $J = 8.8$ Hz, 2H), 6.68 (d, $J = 8.8$ Hz, 2H), 7.20-7.32 (m, 2H), 7.36-7.40 (m, 3H), 7.52-7.59 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.2, 16.6, 53.2, 54.7, 55.7, 63.4, 63.5, 87.2, 95.0, 114.9, 123.1, 123.4, 127.4, 127.7, 128.6, 128.7, 129.0, 131.6, 132.1, 138.4, 140.1, 140.3, 152.6. ^{31}P NMR (161 MHz, CDCl_3) δ 23.42. m/z 449 (M^+); Calcd for $\text{C}_{26}\text{H}_{28}\text{NO}_4\text{P}$: C 69.48, H 6.28, N 3.12; Found: C 69.20, H 6.17, N 3.07.

Diethyl (p-toluidino)(2-(2-phenylethynyl)phenyl)methylphosphonate (1b)

^1H NMR (400 MHz, CDCl_3) δ 1.05 (t, $J = 7.3$ Hz, 3H), 1.30 (t, $J = 7.3$ Hz, 3H), 2.16 (s, 3H), 3.56-3.65 (m, 1H), 3.84-3.93 (m, 1H), 4.17-4.24 (m, 2H), 4.89 (br, 1H), 5.52 (dd, $J = 24.4, 6.4$ Hz, 1H), 6.57 (d, $J = 8.0$ Hz, 2H), 6.90 (d, $J = 8.3$ Hz, 2H), 7.24 (t, $J = 7.3$ Hz, 1H), 7.30 (t, $J = 7.6$ Hz, 1H), 7.36-7.40 (m, 3H), 7.53-7.61 (m, 4H); ^{13}C

NMR (100 MHz, CDCl₃) δ 16.0, 16.4, 20.3, 52.6, 54.1, 63.2, 63.3, 87.2, 94.9, 113.7, 123.1, 123.3, 127.3, 127.4, 127.6, 128.4, 128.5, 128.9, 129.7, 131.5, 132.0, 138.4, 143.6. ³¹P NMR (161 MHz, CDCl₃) δ 23.37. *m/z* 433 (M⁺); Calcd for C₂₆H₂₈NO₃P: C 72.04, H 6.51, N 3.23; Found: C 72.15, H 6.52, N 3.14.

Diethyl (phenylamino)(2-(2-phenylethynyl)phenyl)methylphosphonate (1c)

¹H NMR (400 MHz, CDCl₃) δ 1.05 (t, *J* = 6.8 Hz, 3H), 1.30 (t, *J* = 6.8 Hz, 3H), 3.58-3.66 (m, 1H), 3.84-3.93 (m, 1H), 4.17-4.25 (m, 2H), 5.03 (br, 1H), 5.54 (dd, *J* = 24.9, 8.8 Hz, 1H), 6.65-6.69 (m, 3H), 7.10 (t, *J* = 8.4 Hz, 2H), 7.23-7.33 (m, 2H), 7.35-7.41 (m, 3H), 7.54-7.63 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 16.1, 16.4, 52.4, 53.9, 63.1, 63.4, 87.1, 95.0, 113.6, 118.2, 123.0, 123.3, 127.3, 127.6, 128.5, 128.6, 128.9, 129.2, 131.5, 132.0, 138.2, 146.1. ³¹P NMR (161 MHz, CDCl₃) δ 23.27. *m/z* 419 (M⁺); Calcd for C₂₅H₂₆NO₃P: C 71.59, H 6.25, N 3.34; Found: C 71.42, H 6.12, N 3.30.

Diethyl (4-fluorophenylamino)(2-(2-phenylethynyl)phenyl)methylphosphonate (1d)

^1H NMR (400 MHz, CDCl_3) δ 1.06 (t, J = 6.8 Hz, 3H), 1.31 (t, J = 7.3 Hz, 3H), 3.56-3.66 (m, 1H), 3.84-3.93 (m, 1H), 4.17-4.25 (m, 2H), 4.91 (t, J = 8.8 Hz, 1H), 5.48 (dd, J = 24.4, 8.8 Hz, 1H), 6.55-6.59 (m, 2H), 6.80 (t, J = 8.8 Hz, 2H), 7.24-7.33 (m, 2H), 7.37-7.41 (m, 3H), 7.55-7.60 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.1, 16.4, 53.0, 54.5, 63.1, 63.4, 87.0, 95.1, 114.5, 115.6, 122.9, 123.4, 127.2, 127.7, 128.5, 128.6, 128.9, 131.5, 132.1, 137.9, 142.3, 155.0, 157.4. ^{31}P NMR (161 MHz, CDCl_3) δ 23.14. m/z 437 (M^+); Calcd for $\text{C}_{25}\text{H}_{25}\text{FNO}_3\text{P}$: C 68.64, H 5.76, N 3.20; Found: C 68.74, H 5.68, N 3.13.

Diethyl (4-chlorophenylamino)(2-(2-phenylethynyl)phenyl)methylphosphonate (1e)

^1H NMR (400 MHz, CDCl_3) δ 1.05 (t, J = 6.8 Hz, 3H), 1.31 (t, J = 6.8 Hz, 3H), 3.56-3.65 (m, 1H), 3.84-3.93 (m, 1H), 4.17-4.24 (m, 2H), 5.03 (br, 1H), 5.48 (dd, J = 24.9, 8.3 Hz, 1H), 6.56 (d, J = 8.8 Hz, 2H), 7.04 (d, J = 8.8 Hz, 2H), 7.24-7.37 (m, 3H), 7.38-7.41 (m, 2H), 7.52-7.61 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.1, 16.4, 52.5, 54.0, 63.2, 63.5, 86.9, 95.2, 114.7, 122.9, 123.4, 127.3, 127.8, 128.5, 128.7, 128.9, 129.0, 129.1, 131.5, 132.1, 137.8, 144.7. ^{31}P NMR (161 MHz, CDCl_3) δ 22.79. m/z 453 (M^+); Calcd for $\text{C}_{25}\text{H}_{25}\text{ClNO}_3\text{P}$: C 66.15, H 5.55, N 3.09; Found: C 66.35, H 5.55, N 2.98.

Diethyl (3-nitrophenylamino)(2-(2-phenylethynyl)phenyl)methylphosphonate (1f)

^1H NMR (400 MHz, CDCl_3) δ 1.09 (t, $J = 6.8$ Hz, 3H), 1.33 (t, $J = 6.8$ Hz, 3H), 3.62-3.72 (m, 1H), 3.90-4.01 (m, 1H), 4.20-4.30 (m, 2H), 5.60 (dd, $J = 24.9, 8.8$ Hz, 1H), 6.08 (br, 1H), 6.93 (dd, $J = 8.0, 1.9$ Hz, 1H), 7.19 (t, $J = 8.0$ Hz, 1H), 7.27-7.33 (m, 2H), 7.38-7.42 (m, 3H), 7.47 (d, $J = 8.3$ Hz, 1H), 7.58-7.72 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.1, 16.4, 52.2, 53.7, 63.3, 63.8, 86.5, 95.4, 108.2, 112.6, 118.9, 122.8, 123.7, 127.4, 128.1, 128.5, 128.8, 129.0, 129.7, 131.6, 132.2, 137.2, 147.4, 149.3. ^{31}P NMR (161 MHz, CDCl_3) δ 22.38. m/z 464 (M^+); Calcd for $\text{C}_{25}\text{H}_{25}\text{N}_2\text{O}_5\text{P}$: C 64.65, H 5.43, N 6.03; Found: C 64.54, H 5.47, N 5.78.

Diethyl (2-(2-phenylethynyl)phenyl)(3-(trifluoromethyl)phenylamino)methylphosphonate (1g)

^1H NMR (400 MHz, CDCl_3) δ 1.06 (t, $J = 6.8$ Hz, 3H), 1.31 (t, $J = 6.8$ Hz, 3H), 3.58-3.68 (m, 1H), 3.86-3.95 (m, 1H), 4.18-4.26 (m, 2H), 5.53 (br, 1H), 5.56 (dd, $J = 24.9, 8.8$ Hz, 1H), 6.77 (dd, $J = 8.4, 2.0$ Hz, 1H), 6.89 (d, $J = 8.0$ Hz, 1H), 6.99 (s, 1H), 7.16 (t, $J = 7.8$ Hz, 1H), 7.25-7.33 (m, 2H), 7.36-7.40 (m, 3H), 7.56-7.60 (m,

3H), 7.65 (d, $J = 8.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.1, 16.4, 52.2, 53.7, 63.2, 63.6, 86.7, 95.2, 110.3, 114.6, 116.2, 122.8, 123.4, 125.5, 127.4, 127.9, 128.5, 128.7, 129.0, 129.6, 131.6, 132.1, 137.5, 146.5. ^{31}P NMR (161 MHz, CDCl_3) δ 22.73. m/z 487 (M^+); Calcd for $\text{C}_{26}\text{H}_{25}\text{F}_3\text{NO}_3\text{P}$: C 64.06, H 5.17, N 2.87; Found: C 63.99, H 5.13, N 2.84.

Diethyl (2-(hex-1-ynyl)phenyl)(4-methoxyphenylamino)methylphosphonate (1h)

^1H NMR (400 MHz, CDCl_3) δ 0.96 (t, $J = 7.3$ Hz, 3H), 1.04 (t, $J = 7.3$ Hz, 3H), 1.32 (t, $J = 7.3$ Hz, 3H), 1.50-1.58 (m, 2H), 1.62-1.68 (m, 2H), 2.52 (t, $J = 7.3$ Hz, 2H), 3.52-3.60 (m, 1H), 3.67 (s, 3H), 3.83-3.89 (m, 1H), 4.16-4.24 (m, 2H), 4.70 (t, $J = 7.3$ Hz, 1H), 4.71 (dd, $J = 24.9, 9.3$ Hz, 1H), 6.58 (d, $J = 9.3$ Hz, 2H), 6.68 (d, $J = 9.3$ Hz, 2H), 7.17 (t, $J = 7.3$ Hz, 1H), 7.23 (t, $J = 6.8$ Hz, 1H), 7.40 (d, $J = 8.0$ Hz, 1H), 7.52 (d, $J = 8.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.6, 16.1, 16.4, 19.3, 22.0, 30.8, 52.8, 54.3, 55.6, 63.0, 63.2, 78.4, 96.0, 114.7, 114.8, 124.3, 127.1, 127.4, 128.0, 132.0, 137.9, 140.2, 152.5. ^{31}P NMR (161 MHz, CDCl_3) δ 23.75. m/z 429 (M^+); Calcd for $\text{C}_{24}\text{H}_{32}\text{NO}_4\text{P}$: C 67.12, H 7.51, N 3.26; Found: C 67.32, H 7.45, N 3.13.

Diethyl (4-fluorophenylamino)(2-(hex-1-ynyl)phenyl)methylphosphonate (1i)

^1H NMR (400 MHz, CDCl_3) δ 0.97 (t, $J = 6.8$ Hz, 3H), 1.05 (t, $J = 6.8$ Hz, 3H), 1.33 (t, $J = 7.1$ Hz, 3H), 1.50-1.58 (m, 2H), 1.62-1.68 (m, 2H), 2.52 (t, $J = 7.1$ Hz, 2H), 3.51-3.60 (m, 1H), 3.83-3.91 (m, 1H), 4.16-4.24 (m, 2H), 4.87 (t, $J = 7.3$ Hz, 1H), 5.39 (dd, $J = 24.4, 8.8$ Hz, 1H), 6.51-6.58 (m, 2H), 6.80 (t, $J = 8.3$ Hz, 2H), 7.16-7.25 (m, 2H), 7.41 (d, $J = 7.3$ Hz, 1H), 7.52 (d, $J = 7.3$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.6, 16.0, 16.4, 19.3, 22.0, 30.8, 52.6, 54.1, 55.6, 63.0, 63.3, 78.3, 96.2, 114.5, 115.5, 124.3, 127.0, 127.6, 128.1, 132.0, 137.5, 142.4, 155.0, 157.3. ^{31}P NMR (161 MHz, CDCl_3) δ 23.46. m/z 417 (M^+); HRMS calcd for $\text{C}_{23}\text{H}_{29}\text{FNO}_3\text{P}$: 417.1869, found: 417.1872.

Diethyl (2-(hex-1-ynyl)phenyl)(3-nitrophenylamino)methylphosphonate (1j)

^1H NMR (400 MHz, CDCl_3) δ 0.96 (t, $J = 7.3$ Hz, 3H), 1.04 (t, $J = 7.3$ Hz, 3H), 1.34 (t, $J = 7.3$ Hz, 3H), 1.50-1.60 (m, 2H), 1.62-1.72 (m, 2H), 2.57 (t, $J = 6.8$ Hz, 2H), 3.53-3.62 (m, 1H), 3.85-3.93 (m, 1H), 4.18-4.26 (m, 2H), 5.51 (dd, $J = 25.4, 8.3$ Hz, 1H), 5.83 (br, 1H), 6.90 (d, $J = 8.3$ Hz, 1H), 7.13-7.26 (m, 3H), 7.44 (d, $J = 6.8$ Hz, 1H), 7.49 (dd, $J = 8.0, 2.0$ Hz, 1H), 7.54-7.62 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.6, 16.0, 16.4, 19.3, 22.0, 30.8, 51.8, 53.3, 63.1, 63.6, 78.0, 96.7, 107.9, 112.6, 119.2, 124.5, 127.2, 127.9, 128.1, 129.6, 132.1, 136.7, 147.4, 149.3. ^{31}P NMR (161

MHz, CDCl₃) δ 22.72. *m/z* 444 (M⁺); Calcd for C₂₃H₂₉N₂O₅P: C 62.15, H 6.58, N 6.30; Found: C 62.47, H 6.43, N 6.17.

Diethyl (2-(hex-1-ynyl)phenyl)(phenylamino)methylphosphonate (1k)

¹H NMR (400 MHz, CDCl₃) δ 0.96 (t, *J* = 7.3 Hz, 3H), 1.04 (t, *J* = 7.3 Hz, 3H), 1.32 (t, *J* = 7.3 Hz, 3H), 1.50-1.58 (m, 2H), 1.62-1.68 (m, 2H), 2.52 (t, *J* = 7.2 Hz, 2H), 3.48-3.58 (m, 1H), 3.80-3.90 (m, 1H), 4.15-4.23 (m, 2H), 4.95 (t, *J* = 9.0 Hz, 1H), 5.45 (dd, *J* = 24.9, 8.8 Hz, 1H), 6.63 (d, *J* = 8.0 Hz, 2H), 6.66 (t, *J* = 7.8 Hz, 1H), 7.09 (t, *J* = 7.8 Hz, 2H), 7.17 (t, *J* = 7.8 Hz, 1H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.40 (d, *J* = 7.4 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 13.6, 16.0, 16.4, 19.3, 22.0, 30.8, 52.0, 53.5, 63.0, 63.3, 78.4, 96.1, 113.6, 118.1, 124.2, 127.1, 127.5, 128.1, 129.1, 132.0, 137.8, 146.1. ³¹P NMR (161 MHz, CDCl₃) δ 23.42. *m/z* 399 (M⁺); Calcd for C₂₃H₃₀NO₃P: C 69.15, H 7.57, N 3.51; Found: C 69.54, H 7.55, N 3.39.

General Procedure for synthesis of compound 2 using palladium(II) as catalyst

(method A):

The mixture of 2-alkynyl α -amino benzylphosphonate **1** (0.25 mmol) and $\text{Pd}(\text{PhCN})_2\text{Cl}_2$ (0.0125 mmol, 5 mol%) in CH_3CN (1.0 mL) was stirred at 60-70 °C under nitrogen atmosphere. After completion of the reaction as indicated by TLC, the reaction mixture was diluted with water (5.0 mL) and extracted with EtOAc (2×10 mL). The extracts were evaporated in vacuo, followed by purification on silica gel afforded the product 2,3-disubstituted-2*H*-isoindol-1-ylphosphonate **2**.

Diethyl 3-benzyl-2-(4-methoxyphenyl)-2*H*-isoindol-1-ylphosphonate **2a**

^1H NMR (400 MHz, CDCl_3) δ 1.16 (t, J = 7.0 Hz, 6H), 3.80-3.98 (m, 7H), 4.13 (s, 2 H), 6.84-6.88 (m, 4H), 7.03-7.08 (m, 3H), 7.12-7.22 (m, 4H), 7.56 (dd, J = 8.3, 1.0 Hz, 1H), 8.14 (d, J = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 15.9, 30.9, 55.2, 61.2, 106.5, 108.9, 113.1, 119.4, 120.4, 121.3, 122.9, 124.4, 126.0, 128.0, 128.1, 129.1, 130.6, 131.4, 132.4, 138.5, 159.6; ^{31}P NMR (161 MHz, CDCl_3) δ 10.34. m/z 449 (M^+); HRMS calcd for $\text{C}_{26}\text{H}_{28}\text{NO}_4\text{P}$: 449.1756, found: 449.1752.

Diethyl 3-benzyl-2-p-tolyl-2H-isoindol-1-ylphosphonate 2b

^1H NMR (400 MHz, CDCl_3) δ 1.15 (t, $J = 7.2$ Hz, 6H), 2.42 (s, 3H), 3.82-3.88 (m, 2H), 3.93-3.99 (m, 2 H), 4.12 (s, 2 H), 6.86 (d, $J = 7.6$ Hz, 2H), 7.01-7.07 (m, 3H), 7.13-7.25 (m, 6H), 7.54 (dd, $J = 8.4, 0.8$ Hz, 1H), 8.15 (d, $J = 8.8$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.2, 21.3, 31.1, 61.5, 106.5, 108.8, 119.7, 120.6, 121.5, 123.2, 124.7, 126.2, 128.1, 128.2, 128.3, 128.9, 131.4, 132.8, 135.5, 138.7, 139.1. ^{31}P NMR (161 MHz, CDCl_3) δ 10.25. m/z 433 (M^+); HRMS calcd for $\text{C}_{26}\text{H}_{28}\text{NO}_3\text{P}$: 433.1807, found: 433.1802.

Diethyl 3-benzyl-2-phenyl-2H-isoindol-1-ylphosphonate 2c

^1H NMR (400 MHz, CDCl_3) δ 1.12 (t, $J = 7.2$ Hz, 6H), 3.79-3.85 (m, 2H), 3.90-3.96 (m, 2H), 4.13 (s, 2 H), 6.82 (t, $J = 3.6$ Hz, 2H), 7.07 (t, $J = 7.2$ Hz, 1H), 7.12-7.23 (m, 6H), 7.37 (t, $J = 7.6$ Hz, 2H), 7.44 (d, $J = 7.2$ Hz, 1H), 7.57 (t, $J = 8.0$ Hz, 1H), 8.15 (d, $J = 8.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.1, 31.1, 61.6, 106.5, 108.9, 119.6, 120.6, 121.7, 123.3, 124.8, 126.3, 128.2, 128.3, 128.4, 128.5, 129.2, 131.4, 132.9, 138.1, 138.6. ^{31}P NMR (161 MHz, CDCl_3) δ 10.04. m/z 419 (M^+); HRMS calcd for $\text{C}_{25}\text{H}_{26}\text{NO}_3\text{P}$: 419.1650, found: 419.1653.

Diethyl 3-benzyl-2-(4-fluorophenyl)-2H-isoindol-1-ylphosphonate 2d

^1H NMR (400 MHz, CDCl_3) δ 1.16 (t, $J = 7.2$ Hz, 6H), 3.86-3.98 (m, 4H), 4.13 (s, 2H), 6.81 (d, $J = 4.0$ Hz, 2H), 7.02-7.10 (m, 5H), 7.13-7.15 (m, 3H), 7.21-7.25 (m, 1H), 7.59 (d, $J = 8.4$ Hz, 1H), 8.13 (d, $J = 8.8$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.2, 31.1, 61.6, 106.9, 109.3, 115.2, 119.6, 120.5, 121.9, 123.3, 125.0, 126.4, 128.2, 128.4, 130.2, 131.5, 132.7, 134.1, 138.4, 161.5, 163.9. ^{31}P NMR (161 MHz, CDCl_3) δ 9.98. m/z 437 (M^+); HRMS calcd for $\text{C}_{25}\text{H}_{25}\text{FNO}_3\text{P}$: 437.1556, found: 437.1560.

Diethyl 3-benzyl-2-(4-chlorophenyl)-2H-isoindol-1-ylphosphonate 2e

^1H NMR (400 MHz, CDCl_3) δ 1.16 (t, $J = 7.0$ Hz, 6H), 3.83-4.03 (m, 4H), 4.13 (s, 2H), 6.81-6.84 (m, 2H), 7.05 (d, $J = 8.8$ Hz, 2H), 7.06-7.10 (m, 1H), 7.14-7.16 (m, 3H), 7.20-7.25 (m, 1H), 7.33 (d, $J = 8.3$ Hz, 2H), 7.58 (d, $J = 8.0$ Hz, 1H), 8.12 (d, $J = 8.8$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.1, 30.9, 61.6, 107.0, 109.3, 119.5, 120.5, 121.8, 123.4, 124.9, 126.3, 128.1, 128.4, 129.7, 131.3, 132.6, 132.8, 135.1, 136.6, 138.3. ^{31}P NMR (161 MHz, CDCl_3) δ 9.88. m/z 453 (M^+); HRMS calcd for $\text{C}_{25}\text{H}_{25}\text{ClNO}_3\text{P}$: 453.1261, found: 453.1264.

Diethyl 3-benzyl-2-(3-nitrophenyl)-2H-isoindol-1-ylphosphonate 2f

^1H NMR (400 MHz, CDCl_3) δ 1.11 (t, $J = 7.2$ Hz, 3H), 1.19 (t, $J = 7.2$ Hz, 3H), 3.86-4.00 (m, 4H), 4.16 (s, 2 H), 6.75 (s, 2H), 7.11-7.15 (m, 4H), 7.26 (t, $J = 7.6$ Hz, 1H), 7.43 (d, $J = 7.6$ Hz, 1H), 7.54 (t, $J = 8.0$ Hz, 1H), 7.64 (d, $J = 8.8$ Hz, 1H), 7.93 (s, 1H), 8.11 (d, $J = 8.4$ Hz, 1H), 8.31 (d, $J = 8.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.1, 16.2, 31.1, 61.7, 61.9, 107.3, 109.7, 119.5, 120.4, 122.4, 123.7, 124.0, 125.4, 126.7, 128.0, 128.6, 129.0, 131.4, 132.7, 134.5, 137.9, 139.2, 147.6. ^{31}P NMR (161 MHz, CDCl_3) δ 9.44. m/z 464 (M^+); HRMS calcd for $\text{C}_{25}\text{H}_{25}\text{N}_2\text{O}_5\text{P}$: 464.1501, found: 464.1506.

Diethyl 3-benzyl-2-(3-(trifluoromethyl)phenyl)-2H-isoindol-1-ylphosphonate 2g

^1H NMR (400 MHz, CDCl_3) δ 1.07 (t, $J = 7.2$ Hz, 3H), 1.13 (t, $J = 7.2$ Hz, 3H), 3.78-3.96 (m, 4H), 4.13 (dd, $J = 29.2, 14.6$ Hz, 2H), 6.75 (t, $J = 3.2$ Hz, 2H), 7.09-7.16 (m, 4H), 7.23 (d, $J = 8.0$ Hz, 1H), 7.30-7.33 (m, 2H), 7.50 (t, $J = 8.0$ Hz, 1H), 7.63 (d, $J = 8.4$ Hz, 1H), 7.71 (d, $J = 7.6$ Hz, 1H), 8.16 (d, $J = 8.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.0, 31.1, 61.6, 61.8, 107.0, 109.3, 119.5, 120.6, 122.2,

123.5, 124.7, 125.8, 125.9, 126.5, 128.1, 128.5, 128.9, 130.8, 131.5, 131.8, 132.9, 138.1, 138.6. ^{31}P NMR (161 MHz, CDCl_3) δ 9.58. m/z 487 (M^+); HRMS calcd for $\text{C}_{26}\text{H}_{25}\text{F}_3\text{NO}_3\text{P}$: 487.1524, found: 487.1520.

Diethyl 2-(4-methoxyphenyl)-3-pentyl-2H-isoindol-1-ylphosphonate 2h

^1H NMR (400 MHz, CDCl_3) δ 0.80 (t, J = 6.4 Hz, 3H), 1.16-1.20 (m, 10H), 1.46-1.49 (m, 2H), 2.74 (t, J = 8.0 Hz, 2H), 3.84-3.87 (m, 2H), 3.89 (s, 3H), 3.94-4.00 (m, 2H), 6.98 (d, J = 8.8 Hz, 2H), 7.02 (t, J = 7.6 Hz, 1H), 7.12 (t, J = 8.4 Hz, 1H), 7.24 (d, J = 8.8 Hz, 2H), 7.60 (d, J = 7.6 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.8, 16.2, 22.2, 25.0, 29.6, 31.5, 55.5, 61.4, 105.6, 107.9, 113.4, 119.7, 120.4, 120.8, 122.3, 124.6, 129.3, 131.0, 132.8, 134.5, 159.8. ^{31}P NMR (161 MHz, CDCl_3) δ 10.71. m/z 429 (M^+); HRMS calcd for $\text{C}_{24}\text{H}_{32}\text{NO}_4\text{P}$: 429.2069, found: 429.2065.

Diethyl 2-(4-fluorophenyl)-3-pentyl-2H-isoindol-1-ylphosphonate 2i

^1H NMR (400 MHz, CDCl_3) δ 0.80 (t, $J = 6.4$ Hz, 3H), 1.16-1.20 (m, 10H), 1.44-1.48 (m, 2H), 2.74 (t, $J = 8.0$ Hz, 2H), 3.84-3.90 (m, 2H), 3.92-4.00 (m, 2H), 7.06 (t, $J = 8.0$ Hz, 1H), 7.08-7.22 (m, 3H), 7.30-7.33 (m, 2H), 7.61 (d, $J = 8.4$ Hz, 1H), 8.08 (d, $J = 8.8$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.8, 16.2, 22.2, 25.0, 29.6, 31.5, 55.5, 61.6, 105.9, 108.2, 115.4, 119.7, 120.5, 121.1, 122.4, 124.9, 130.1, 132.8, 134.3, 161.5, 164.0. ^{31}P NMR (161 MHz, CDCl_3) δ 10.39. m/z 417 (M^+); HRMS calcd for $\text{C}_{23}\text{H}_{29}\text{FNO}_3\text{P}$: 417.1869, found: 417.1872.

Diethyl 2-(3-nitrophenyl)-3-pentyl-2H-isoindol-1-ylphosphonate 2j

^1H NMR (400 MHz, CDCl_3) δ 0.79 (t, $J = 6.4$ Hz, 3H), 1.13-1.22 (m, 10H), 1.45-1.50 (m, 2H), 2.77 (t, $J = 7.8$ Hz, 2H), 3.85-4.05 (m, 4H), 7.08 (d, $J = 8.3$ Hz, 1H), 7.23 (t, $J = 8.3$ Hz, 1H), 7.62 (d, $J = 7.8$ Hz, 1H), 7.71 (d, $J = 5.4$ Hz, 2H), 8.06 (d, $J = 8.3$ Hz, 1H), 8.25 (s, 1H), 8.41-8.43 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.7, 16.1, 16.2, 22.1, 25.0, 29.7, 31.4, 61.6, 61.8, 106.3, 108.6, 119.7, 120.3, 121.6, 122.7, 123.8, 124.1, 125.3, 129.2, 132.8, 134.0, 134.5, 139.6, 147.8. ^{31}P NMR (161 MHz, CDCl_3) δ 9.84. m/z 444 (M^+); HRMS calcd for $\text{C}_{23}\text{H}_{29}\text{N}_2\text{O}_5\text{P}$: 444.1814, found: 444.1818.

General Procedure for synthesis of compound 3 utilizing silver triflate as catalyst

(method B)

The mixture of 2-alkynyl α -amino benzylphosphonate **1** (0.5 mmol), AgOTf (0.025 mmol, 5 mol%) in CH₃CN (2.0 mL) was stirred at 60-70 °C under nitrogen atmosphere for overnight. After completion of the reaction as indicated by TLC, the reaction mixture was diluted with water (5.0 mL) and extracted with EtOAc (2×10 mL). The extracts were evaporated in vacuo and followed by purification on silica gel afforded the product 2,3-disubstituted-1,2-dihydroisoquinolin-1-ylphosphonate **3**.

Diethyl 2-(4-methoxyphenyl)-3-phenyl-1,2-dihydroisoquinolin-1-ylphosphonate

¹H NMR (400 MHz, CDCl₃) δ 1.22 (m, 6H), 3.65 (s, 3H), 3.90-4.12 (m, 4H), 5.33 (d, J = 19.0 Hz, 1H), 6.44 (s, 1H), 6.63 (d, J = 8.8 Hz, 2H), 7.05 (d, J = 8.8 Hz, 2H), 7.06-7.28 (m, 7H), 7.57 (d, J = 8.8 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 16.5, 55.3, 62.5, 62.6, 64.9, 111.1, 113.9, 124.1, 124.5, 125.0, 126.4, 127.3, 127.5, 127.8, 127.9, 128.2, 133.3, 137.5, 141.5, 142.6, 155.4; ³¹P NMR (161 MHz, CDCl₃) δ 21.25. MS (ESI) m/z 450.20 (M^+ +1); HRMS calcd for C₂₆H₂₈NO₄P: 449.1756, found: 449.1754.

Diethyl 2,3-diphenyl-1,2-dihydroisoquinolin-1-ylphosphonate

^1H NMR (400 MHz, CDCl_3) δ 1.21 (m, 6H), 3.90-4.10 (m, 4H), 5.45 (d, $J = 18.6$ Hz, 1H), 6.50 (s, 1H), 6.85 (m, 1H), 7.07-7.25 (m, 11H), 7.58 (d, $J = 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.4, 62.5, 62.7, 64.2, 112.2, 122.3, 122.6, 124.3, 125.6, 126.5, 127.1, 127.2, 127.6, 127.9, 128.2, 128.5, 133.0, 137.3, 142.0, 147.6; ^{31}P NMR (161 MHz, CDCl_3) δ 21.33. MS (ESI) m/z 420.20 (M^++1). HRMS calcd for $\text{C}_{25}\text{H}_{26}\text{NO}_3\text{P}$: 419.1650, found: 419.1654.

Diethyl 2-(4-fluorophenyl)-3-phenyl-1,2-dihydroisoquinolin-1-ylphosphonate

^1H NMR (400 MHz, CDCl_3) δ 1.21 (m, 6H), 3.90-4.12 (m, 4H), 5.34 (d, $J = 18.6$ Hz, 1H), 6.47 (s, 1H), 6.78 (t, $J = 10.6$ Hz, 2H), 7.04-7.28 (m, 9H), 7.56 (d, $J = 8.0$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 16.4, 62.6, 64.5, 111.8, 115.2, 124.3, 124.4, 125.2, 126.6, 127.1, 127.2, 127.7, 128.0, 128.3, 133.0, 137.1, 142.1, 143.9, 157.3, 159.7; ^{31}P NMR (161 MHz, CDCl_3) δ 20.92. MS (ESI) m/z 438.20 (M^++1). HRMS calcd for $\text{C}_{25}\text{H}_{25}\text{FNO}_3\text{P}$: 437.1556, found: 437.1561.

Diethyl 3-butyl-2-(4-methoxyphenyl)-1,2-dihydroisoquinolin-1-ylphosphonate

^1H NMR (400 MHz, CDCl_3) δ 0.83 (t, $J = 7.2$ Hz, 3H), 1.20-1.38 (m, 8H), 1.50 (m, 2H), 2.09 (m, 1H), 2.26 (m, 1H), 3.77 (s, 3H), 4.01-3.87 (m, 4H), 5.03 (d, $J = 18.6$ Hz, 1H), 5.93 (s, 1H), 6.79 (d, $J = 8.0$ Hz, 2H), 6.99 (d, $J = 8.0$ Hz, 2H), 7.05 (t, $J = 7.6$ Hz, 1H), 7.15 (m, 1H), 7.18 (d, $J = 8.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.8, 16.4, 22.3, 30.2, 33.0, 55.4, 62.2, 62.6, 65.03, 107.8, 113.9, 123.0, 125.4, 126.0, 127.0, 128.0, 129.7, 133.4, 140.6, 144.7, 156.3; ^{31}P NMR (161 MHz, CDCl_3) δ 21.02. MS (ESI): m/z 428.30 ($\text{M}^+ - 1$). HRMS calcd for $\text{C}_{24}\text{H}_{32}\text{NO}_4\text{P}$: 429.2069, found: 429.2065.

Diethyl 3-butyl-2-phenyl-1,2-dihydroisoquinolin-1-ylphosphonate

^1H NMR (400 MHz, CDCl_3) δ 0.84 (t, $J = 7.2$ Hz, 3H), 1.22-1.28 (m, 8H), 1.56 (m, 2H), 2.17 (m, 1H), 2.33 (m, 1H), 3.86-4.02 (m, 4H), 5.15 (d, $J = 19.0$ Hz, 1H), 6.04 (s, 1H), 6.97-7.06 (m, 4H), 7.18-7.26 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.8, 16.4, 22.4, 30.3, 32.9, 62.2, 62.7, 64.6, 109.8, 123.2, 123.3, 123.6, 123.7, 125.6, 127.0, 128.1, 128.7, 133.2, 144.0, 147.2; ^{31}P NMR (161 MHz, CDCl_3) δ 20.91. MS (ESI): m/z 400.20 ($\text{M}^+ + 1$); HRMS calcd for $\text{C}_{23}\text{H}_{30}\text{NO}_3\text{P}$: 399.1963, found 399.1967.

Diethyl 3-butyl-2-(4-fluorophenyl)-1,2-dihydroisoquinolin-1-ylphosphonate

^1H NMR (400 MHz, CDCl_3) δ 0.84 (t, $J = 7.2$ Hz, 3H), 1.20-1.38 (m, 8H), 1.52 (m, 2H), 2.12 (m, 1H), 2.26 (m, 1H), 3.88-4.05 (m, 4H), 5.04 (d, $J = 18.6$ Hz, 1H), 5.99 (s, 1H), 6.95 (t, $J = 8.0$ Hz, 2H), 7.00 (d, $J = 8.0$ Hz, 2H), 7.08 (t, $J = 7.6$ Hz, 1H), 7.20 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.8, 16.4, 22.3, 30.1, 32.9, 62.3, 62.7, 64.8, 109.1, 115.4, 123.2, 125.6, 125.8, 125.9, 127.0, 128.1, 133.1, 143.3, 144.0, 159.1, 160.6; ^{31}P NMR (161 MHz, CDCl_3) δ 20.70. MS (ESI): m/z 416.20 ($\text{M}^+ - 1$); HRMS calcd for $\text{C}_{23}\text{H}_{29}\text{FNO}_3\text{P}$: 417.1869, found 417.1864.

Year	Percentage (%)
1990	45
1991	48
1992	50
1993	52
1994	54
1995	50
1996	52
1997	54
1998	58
1999	56
2000	60

c1ccc(cc1)C#Cc2ccccc2
1c

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Current Data Parameters
NAME 070205-108
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070205
Time 9.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 443
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 90.5
DW 20.800 usec
DE 6.00 usec
TE 296.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

CHANNEL f1
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
SFO1 100.628258 MHz

CHANNEL f2
waltz16
CPDPRG2
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 12.98 dB
PL13 15.00 dB
SFO2 400.1315805 MHz

F2 - Processing parameters
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
NAME 070205-107
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070205
Time 14.40
INSTRUM spect
PROBHD 5 mm F400 BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 159
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.363188 sec
RG 90.5
DW 20.800 usec
DE 6.00 usec
TE 297.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 12.98 dB
PL13 15.00 dB
SFO2 400.1315925 MHz

F2 - Processing parameters
SI 32768
SF 100.6127722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
 NAME 070205-106
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070205
 Time 9:37
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 320
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.363198 sec
 RG 90.5
 DW 20.800 usec
 DE 6.00 usec
 TE 296.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 15.00 dB
 SFO2 400.1317686 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME 070205-117
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070205
 Time_ 14.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.363198 sec
 RG 90.5
 DW 20.800 usec
 DE 6.00 usec
 TE 296.8 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.8999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SF01 100.6228298 MHz

===== CHANNEL f2 =====
 CFBPRG2 waitz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 15.00 dB
 SF02 400.1316245 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127722 MHz
 NRG 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

CCOP(=O)(OC)C1=CC=C(C#CC2=CC=CC=C2)C(=C1)N

Current Data Parameters
 NAME 070205-104
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070205
 Time 10.19

INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 486
 DS 4
 SWH 24030.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 90.5
 DW 20.800 usec
 DE 6.00 usec
 TE 295.7 K
 D1 2.00000000 sec
 d11 0.63000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SFO1 100.628298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 15.00 dB
 SFO2 400.1315125 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127722 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME 070203-102
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070203
 Time 13.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 790
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631088 sec
 RG 50.8
 DM 20.800 usec
 DE 6.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SF01 100.628298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 13.00 dB
 SP02 400.1315845 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127722 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME 070108-11
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070108
 Time 11.10
 INSTRUM spect
 PROBHD 5 mm FAHQ BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 300
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.363198 sec
 RG 50.8
 DW 20.800 usec
 DE 6.00 usec
 TE 295.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

CHANNEL f1
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SFO1 100.628298 MHz

CHANNEL f2
 waitz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 15.00 dB
 SFO2 400.1318566 MHz

F2 - Processing parameters
 SI 32768
 SF 100.612736 MHz
 MDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 EC 1.40

Current Data Parameters
 NAME 070203-642
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070203
 Time_ 14.32
 INSTRUM spect
 PROBHD 5 mm PARBO BB-
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 851
 DS 4
 SNH 24038.461 Hz
 FIDRES 0.365798 Hz
 AQ 1.3631988 sec
 RG 50.8
 DW 20.800 usec
 DE 6.00 usec
 TE 295.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 15.00 dB
 SFO2 400.131605 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127722 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME 070313-113
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070313
 Time 15:54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1038
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 101
 DW 20.800 usec
 DE 6.00 usec
 TE 295.7 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SFO1 100.628298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 15.00 dB
 SFO2 400.1317446 MHz

F2 - Processing parameters
 SI 32768
 SF 100.612722 MHz
 MDW EN
 SSB 0
 LB 1.00 Hz
 GB 0
 EC 1.40

Current Data Parameters
 NAME 061117-100
 EXNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061117
 Time_ 9.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 230
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 64
 DW 20.800 usec
 DE 6.00 usec
 TE 299.9 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999999 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SFO1 100.628298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.88 dB
 PL13 13.00 dB
 SFO2 400.1317286 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 NDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

Current Data Parameters
 NAME 061206-40-1
 EXFNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061206
 Time_ 15.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 311
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 30.5
 DW 20.800 usec
 DE 5.00 usec
 TE 297.3 K
 DL 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SFO1 100.628298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 12.45 dB
 PL13 15.00 dB
 SFO2 400.1317006 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127758 MHz
 SFO 100.6127758 MHz
 GB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

Current Data Parameters
 NAME 061206-40-2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061206
 Time_ 16:20
 INSTRUM spect
 PROBHD 5 mm PABBO SBC
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 312
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631998 sec
 RG 114
 DW 20.800 usec
 DE 6.00 usec
 TE 297.7 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

CHANNEL F1
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SF01 100.628298 MHz

CHANNEL F2
 NUC2 1H
 P2 80.00 usec
 PL2 -3.00 dB
 PL12 12.46 dB
 PL13 15.00 dB
 SF02 400.1317670 MHz

F2 - Processing Parameters
 SI 32768
 SF 100.6127758 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

Current Data Parameters
 NAME 061220-47-3
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061220
 Time 10.16
 INSTRUM spect
 PROBHD 5 mm FBBBO BB-
 PULPROG zgpg30
 TO 65336
 SOLVENT CDCl3
 NS 475
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 80.6
 DW 20.800 usec
 DE 6.00 usec
 TE 294.7 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TLO 1

===== CHANNEL f1 =====
 NUC1 13C
 PL 9.00 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 15.00 dB
 SFO2 400.1316805 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127758 MHz
 NW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
NAME 061220-47-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061220
Time 9.41
INSTRUM spect
PROBHD 5 mm F400 BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 322
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 80.6
DW 20.800 usec
DE 6.00 usec
TE 295.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
SFO1 100.628298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 12.98 dB
PL13 15.00 dB
SFO2 400.1316805 MHz

F2 - Processing parameters
SI 32768
SF 100.6127758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
 NAME 061220-47-1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061220
 Time 9.41
 INSTRUM spect
 PROBHD 5 mm F400 BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 322
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 80.6
 DW 20.800 usec
 DE 6.00 usec
 TE 295.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SF01 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 15.00 dB
 SF02 400.1316805 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127758 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME 061220-47-4
 EXNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061220
 Time_ 10.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 483
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 80.6
 DW 20.800 usec
 DE 6.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -2.00 dB
 SF01 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 12.98 dB
 PL13 15.00 dB
 SFO2 400.1316805 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127758 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40