

Supporting Information

The Preparation and Resolution of a Modular Class of Axially Chiral Quinazoline-Containing Ligands and their Application in Asymmetric Rhodium-Catalysed Olefin Hydroboration

^aDavid J. Connolly, ^aPatrick M. Lacey, ^aMary McCarthy, ^aCormac P. Saunders, ^aAnne-Marie Carroll, ^bRichard Goddard and ^aPatrick J. Guiry

^a*Centre for Synthesis and Chemical Biology, Conway Institute of Biomolecular and Biomedical Research, Department of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland*

^b*Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45466 Mülheim a. d. Ruhr, Germany*

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Preparation of Imidate Hydrochloride Salts 7b-7e

Benzimidic acid methyl ester 7b

Crystalline white solid (71%), m.p. 94-96 °C (lit.⁴⁶ m.p. 98-99°C); ν_{\max} (KBr) 3398, 2985, 2541, 1748, 1642, 1583, 1557, 1496, 1323 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ = 12.8 (1H, br. s), 12.1 (1H, br. s), 8.4 (2H, dd, J = 8.2, 1.5 Hz), 7.71 (1H, appt, J = 7.61 Hz), 7.57 (2H, t, J = 7.9 Hz), 4.57 (3H, s); ^{13}C NMR (75 MHz; CDCl_3) δ = 172.1, 136, 130, 129.5, 125.2, 61.6.

2-Phenyl-acetimidic acid methyl ester 7c

White solid (97%). m.p. 79-80°C (lit.⁴⁷ m.p. 74-75°C); ν_{\max} (KBr) 3352, 2995, 2111, 1665, 1583 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ = 12.7 (1H, br. s), 11.7 (1H, br. s), 7.44-7.28 (5H, m), 4.26 (3H, s), 4.08 (2H, s); ^{13}C NMR (75 MHz; CDCl_3) δ = 178.5, 131.3, 129.8, 129.4, 128.6, 61.3, 39.3.

Isobutyrimidic acid methyl ester 7d

White solid (94%), m.p. 102-105 °C (lit.⁴⁸ m.p.104-106°C); ν_{\max} (KBr) 3132, 2971, 2223, 1729, 1647, 1394 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ = 12.4 (1H, br. s), 11.6 (1H, br. s), 4.32 (3H, s), 3.24 (1H, sept, J = 6.7 Hz), 1.31 (6H, d, J = 7.0 Hz); ^{13}C NMR (75 MHz; CDCl_3) δ = 184, 61, 33.3, 19.2.

2,2-Dimethyl-propionimidic acid methyl ester 7e

Cream-coloured solid (85%). m.p. 152-155 °C; ν_{\max} (KBr) 3156, 2980, 2176, 1706, 1624, 1495 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ = 12.1 (1H, br. s), 11.8 (1H, br. s), 4.35 (3H, s), 1.42 (9H, s); ^{13}C NMR (75 MHz; CDCl_3) δ = 185, 61.6, 39, 27.6.

Preparation of 2-Substituted-4(3H)quinazolinones 9b-9e

2-Phenyl-4(3H)quinazolinone 9b

After 6 hours at reflux a considerable amount of crystallisation had occurred, the reaction mixture was allowed stand for an hour at room temperature to facilitate further precipitation. White needle-like crystals were obtained after filtration to give 2-phenyl-4(3H)quinazolinone (46%), m.p. 241-242°C (lit.⁵⁰ m.p. 242-243°C); ν_{\max} (KBr) 3560, 3155, 2979, 2945, 1620, 1521, 1399 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ = 8.33 (1H, ddd, J = 7.9, 1.17, 0.59 Hz), 8.29-8.22 (2H, m), 7.86-7.77 (2H, m), 7.62-

7.56 (3H, m), 7.51 (1H, dt, $J = 8.2, 6.74, 1.76$ Hz) ^{13}C NMR (75 MHz; CDCl_3) $\delta = 164.1, 153, 149.9, 135.1, 133, 131.9, 129.3, 128.3, 127.7, 127, 126, 121$.

2-Benzyl-4(3H)quinazolinone 9c

Transfer of the anthranilic acid solution to the free-based imidate in methanol resulted in instant precipitation of product, which appeared to increase during the 30 minute stirring period at room temperature. The reaction mixture including the initial precipitate was put to reflux for 6 h. The solution was cooled, filtered and vacuum dried to give 2-benzyl-4(3H)quinazolinone (65%) as a fine paper-like solid, m.p. 245-247°C (lit.⁵¹ m.p. 257-258°C); ν_{max} (KBr) 3710, 3169, 2896, 1688, 1482 cm^{-1} ; ^1H NMR (300 MHz; DMSO) $\delta = 8.1$ (1H, ddd, $J = 7.91, 1.46, 0.59$ Hz), 7.88 (1H, dt, $J = 8.79, 7.32, 1.76$ Hz), 7.62 (1H, ddd, $J = 8.2, 1.17, 0.59$ Hz), 7.47 (1H, dt, $J = 7.91, 7.03, 1.17$ Hz), 7.43-7.21 (5H, m) 3.98 (2H, s); ^{13}C NMR (75 MHz; CDCl_3) $\delta = 160.3, 156.7, 149.7, 137.3, 135.1, 135, 129.6, 129.2, 127.5, 126.9, 126.4, 121.4, 40.8$; EIMS m/z : 236 (M^+ , 49), 235 (100), 119 (23), 90 (26), 44 (32).

2-Isopropyl-4(3H)quinazolinone 9d

The reaction mixture was allowed stand at room temperature for 1 h to facilitate crystallisation. The needle-like crystals were filtered and dried under vacuum to give 2-isopropyl-4(3H)quinazolinone (47%) as fine white crystals, m.p. 212-214 °C (lit.⁵² m.p. 233°C); ν_{max} (KBr) 3408, 3189, 3024, 1946, 1840, 1680 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) $\delta = 10.98$ (1H, br. s), 8.29 (1H, ddd, $J = 8.2, 1.47, 0.88$ Hz), 7.74 (2H, m), 7.46 (1H, dt, $J = 8.2, 7.03, 1.17$ Hz), 3.05 (1H, sept., $J = 7.03$ Hz), 1.45 (6H, d, $J = 6.73$ Hz) ^{13}C NMR (75 MHz; CDCl_3) 164.4, 161, 149.7, 134.9, 127.7, 126.5, 126, 121, 35.1, 20.6; EIMS m/z : 188 (M^+ , 31), 173 (100), 160 (24), 119 (30), 90 (52), 63 (31).

2-tert-Butyl-4(3H)quinazolinone 9e

The addition of water (50 mL) to the reaction mixture produced a light cream-coloured precipitate which was filtered, washed with cold methanol (5 mL), then water (5 mL) and dried under vacuum to afford 2-tert-butyl-4(3H)quinazolinone (56%) as a cream-coloured solid, m.p. 184-186 °C (lit.⁵³ m.p. 185°C); ν_{max} (KBr) 3677, 3175, 2924, 1685, 1460 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) $\delta = 10.98$ (1H, br. s), 8.29 (1H, ddd, $J = 8.5, 2.3, 0.9$ Hz), 7.73 (2H, m), 7.45 (1H, ddd, $J = 8.5, 7.6, 1.7$ Hz), 1.49 (9H, s); ^{13}C NMR (75 MHz; CDCl_3) $\delta = 164.2, 162.5, 149.5, 134.7, 127.9, 126.5, 126.3, 120.8, 37.7, 28.5$; EIMS m/z : 202 (M^+ , 30), 187 (100), 160 (46), 119 (29), 90 (41).

Preparation of 2-Substituted-4-chloroquinazolines 8b-8e**4-Chloro-2-phenyl-quinazoline 8b**

Light yellow solid (84%), m.p. 122-123°C (lit.⁵⁵ m.p. 124-126°C); ν_{\max} (KBr) 3055, 2612, 1954, 1940, 1819, 1704, 1605, 1547, 1479, 740 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ = 8.62-8.56 (2H, m), 8.22 (1H, ddd, J = 8.05, 1.32, 0.59 Hz), 8.8 (1H, ddd, J = 8.5, 1.61, 0.44 Hz), 7.91 (1H, dt, J = 7.47, 6.88, 1.17 Hz), 7.63 (1H, dt, J = 7.32, 7.03, 1.17 Hz), 7.55-7.48 (3H, m); ^{13}C NMR (75 MHz; CDCl_3) δ = 162.5, 160.1, 151.9, 136.7, 134.8, 131.1, 128.9, 128.8, 128.7, 128.2, 125.8, 122.5.

2-Benzyl-4-chloroquinazoline 8c

Red powder (88%), m.p. 116-117 °C; ν_{\max} (KBr) 3415, 3065, 2947, 1631, 1555, 1477, 989 and 764 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ = 8.18 (1H, ddd, J = 8.35, 1.46, 0.59 Hz), 8.0 (1H, ddd, J = 8.49, 1.17, 0.59 Hz), 7.88 (1H, dt, J = 7.03, 6.88, 1.46 Hz), 7.62 (1H, dt, J = 8.2, 6.88, 1.17 Hz), 7.45 (2H, dd, J = 8.53, 1.13 Hz), 7.30 (2H, dt, J = 7.40, 1.54 Hz), 7.25-7.18 (1H, m), 4.39 (2H, s); ^{13}C NMR (75 MHz; CDCl_3) δ = 165.3, 163, 151.8, 137.9, 135, 134.9, 129.5, 128.7, 128.5, 126.9, 125.9, 122.4, 46.1; EIMS m/z : 254 (M^+ , 89), 237 (7), 219 (100), 190 (14), 116 (53). Anal. calcd for $\text{C}_{15}\text{H}_{11}\text{N}_2\text{Cl}$: C, 70.73%; H, 4.35%; N, 10.99%; Found: C, 70.61%; H, 4.34%; N, 10.83%.

4-Chloro-2-isopropyl-quinazoline 8d

Yellow powder (64%), m.p. 72-73°C (lit.⁵⁶ m.p. 68-70°C); ν_{\max} (KBr) 3052, 2710, 1960, 1832, 1714, 1609 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ = 8.22 (1H, ddd, J = 8.2, 1.46, 0.59 Hz), 8.0 (1H, ddd, J = 8.5, 1.5, 0.59 Hz), 7.9 (1H, dt, J = 8.2, 6.7, 1.46 Hz), 7.65 (1H, dt, J = 8.2, 6.7, 1.17 Hz), 3.3 (1H, sept, 6.73 Hz), 1.43 (6H, d, 7.03 Hz); ^{13}C NMR (75 MHz; CDCl_3) δ = 171.2, 162.5, 151.8, 134.7, 128.6, 128.1, 125.8, 122.1, 37.9, 26.6; EIMS m/z : 207 (M^+ , 4), 206 (7), 191 (30), 155 (31), 129 (80), 102 (73). Anal. calcd for $\text{C}_{11}\text{H}_{11}\text{N}_2\text{Cl}$: C, 63.93%; H, 5.36%; N, 13.55%; Found: C, 63.78%; H, 5.44%; N, 13.26%.

2-tert-Butyl-4-chloroquinazoline 8e

White solid (82%), m.p. 112-116 °C; ν_{\max} (KBr) 2953, 2611, 1833, 1803, 1710, 1557 cm^{-1} ; ^1H NMR (300 MHz; CDCl_3) δ = 8.20 (1H, d, J = 8.5 Hz), 8.01 (1H, d, J = 8.5 Hz), 7.89 (1H, t, J = 7.0 Hz), 7.61

(1H, t, J = 7.0 Hz) 1.49 (9H, s); ^{13}C NMR (75 MHz; CDCl_3) δ = 173.0, 162.1, 151.5, 134.4, 128.9, 128.0, 125.8, 122.1, 39.8, 26.6; EIMS m/z : 220 (M^+ , 18), 205 (100), 169 (30), 129 (74), 102 (52). Anal. calcd for $\text{C}_{12}\text{H}_{13}\text{N}_2\text{Cl}$: C, 65.30%; H, 5.94%; N, 12.69%; Found: C, 65.39%; H, 6.04%; N, 12.53%.

Preparation of 2-Substituted-4-(2-methoxy-naphthalen-1-yl)-quinazolines 11b-f

2-Methyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline 11b

Purified by silica gel column chromatography (2:1 petroleum ether / ethyl acetate) gave (79%) as a white solid, m.p. 200-202°C. ν_{max} (KBr) 1608, 1590, 1577, 1269, 1250, 858 and 815 cm^{-1} ; ^1H NMR (500 MHz): δ (CDCl_3) 8.05 (d, J = 8.6 Hz), 8.02 (1H, d, J = 8.9 Hz), 7.86 (1H, d, J = 8.0 Hz), 7.82 (1H, t, J = 7.7 Hz), 7.45 (1H, d, J = 8.3 Hz), 7.41 (1H, d, J = 9.2 Hz), 7.37-7.32 (2H, m), 7.28 (1H, t, J = 7.6 Hz), 7.07 (1H, d, J = 8.3 Hz), 3.77 (3H, s) and 3.00 (3H, s); ^{13}C NMR (125.7 MHz): δ (CDCl_3) 167.7, 164.5, 154.9, 151.0, 134.0, 133.2, 131.4, 129.3, 128.3, 128.2, 127.4, 127.2, 126.9, 124.5, 124.2, 123.6, 119.8, 113.5, 56.7 and 27.0; m/z (eims 70eV) 300 (M^+ , 96%), 299 (100), 285 (47), 284 (50), 269 (23), 150 (8), 102 (13) and 76 (24); Found: C, 79.9; H, 5.4; N, 9.3. $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}$ requires C, 80.0; H, 5.4; N, 9.3 %.

2-Benzyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline 11d

(79%) as a pale yellow solid. Alternatively, the crude product can be purified by silica gel column chromatography (2:1 petrol ether/ ethyl acetate). m.p. 153-155°C; ν_{max} (KBr) 3066, 3025, 2935, 2838, 1622, 1550, 1512, 1474, 1251, 1082, 807 and 768 cm^{-1} ; ^1H NMR (300 MHz): δ (CDCl_3) 8.08 (1H, d, J = 8.49 Hz), 8.01 (1H, d, J = 9.08 Hz), 7.85 (1H, d, J = 8.20 Hz), 7.81 (1H, dt, J = 8.49, 6.88, 1.61 Hz), 7.49 (1H, d, J = 8.49 Hz), 7.49-7.47 (1H, m), 7.43 (1H, dt, J = 7.47, 6.88, 1.17 Hz), 7.40 (1H, d, J = 9.08 Hz), 7.34 (1H, dt, J = 8.35, 6.30, 1.17 Hz), 7.30-7.28 (1H, m), 7.29 (1H, dt, J = 8.49, 7.03, 1.46 Hz), 7.26-7.24 (1H, m), 7.22-7.16 (2H, m), 7.01 (1H, d, J = 8.49 Hz), 4.57 (1H, d, J = 13.62 Hz), 4.55 (1H, d, J = 13.62 Hz) and 3.73 (3H, s); ^{13}C NMR (75 MHz): δ (CDCl_3) 167.9, 166.0, 155.0, 151.3, 139.2, 133.9, 133.3, 131.5, 129.5, 129.4, 128.7, 128.6, 128.3, 127.4, 127.2, 127.1, 126.5, 124.7, 124.2, 123.8, 120.1, 113.7, 56.9 and 46.7 ; m/z (eims 70eV) 376 (M^+ , 100%), 359 (74), 333 (9), 180 (26), 172 (32), 165 (57), 114 (12), 91 (86) and 65 (24). Anal. calcd for $\text{C}_{26}\text{H}_{20}\text{N}_2\text{O}$: C, 82.95; H, 5.36; N, 7.44 %; Found: C, 82.81; H, 5.43; N, 7.37 %

2-Isopropyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline 11e

Purified by stirring in diethylether for 15 minutes to give 2-isopropyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline as a white solid (93%). Alternatively, the crude reaction mixture can be purified by stirring in pentane for 1 h and filtering through silica gel (2:1 petroleum ether / ethyl acetate). m.p. 185-186°C. ν_{\max} (KBr) 2963, 2928, 2869, 1615, 1568, 1511 and 1280 cm^{-1} ; ^1H NMR (300 MHz): δ (CDCl_3) 8.08 (1H, d, J = 8.5 Hz), 8.02 (1H, d, J = 9.1 Hz), 7.87 (1H, d, J = 8.9 Hz), 7.82 (1H, dt, J = 8.31, 6.72, 1.58 Hz), 7.44 (1H, d, J = 8.3 Hz), 7.43 (1H, dt, J = 6.73, 6.13, 1.59 Hz), 7.42 (1H, d, J = 9.1 Hz), 7.33 (1H, dt, 8.11, 6.73, 1.37 Hz), 7.28 (1H, dt, J = 8.31, 6.92, 1.58 Hz), 7.10 (1H, d, J = 8.3 Hz), 3.77 (3H, s), 3.48 (1H, sept, J = 6.73 Hz), 1.5 (6H, d, J = 6.92 Hz); ^{13}C NMR (75 MHz) : δ (CDCl_3) 171.7, 167.4, 155, 151, 133.7, 133.3, 131.3, 129.4, 128.6, 128.3, 127.3, 127.1, 126.7, 124.6, 124.1, 123.9, 120.4, 114.2, 57, 38.3, 22.3; m/z (eims 70eV) 328 (M^+ , 87 %), 327 (77), 311 (47), 297 (55), 285 (30), 255 (8), 242 (10), Found: C, 80.22; H, 5.94; N, 8.44. $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}$ requires C, 80.46; H, 6.14; N, 8.53 %.

2-tert-Butyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline 11f

Purified by stirring in pentane for 2h and filtered through silica gel (CH_2Cl_2) to yield 2-tert-butyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline (87%) as a white powder. Alternatively, the crude reaction mixture can be purified by column chromatography (2:1 petroleum ether / ethyl acetate). m.p. 187-190°C. ν_{\max} (KBr) 3074, 2961, 2953, 2924, 1549, 1511, 1291 and 770 cm^{-1} ; ^1H NMR (300 MHz): δ (CDCl_3) 8.09 (1H, d, J = 8.49 Hz), 8.01 (1H, d, J = 9.08 Hz), 7.87 (1H, d, J = 7.91), 7.79 (1H, dt, J = 8.20, 6.44, 1.46 Hz), 7.43 (1H, d, J = 9.08 Hz), 7.42 (1H, d, J = 9.37 Hz), 7.35 (1H, dt, 7.91, 6.74, 1.17 Hz), 7.34 (1H, m), 7.27 (1H, dt, J = 8.49, 6.44, 1.76), 7.14 (1H, d, J = 8.5), 3.76 (3H, s), 1.56 (9H, s); ^{13}C NMR (75 MHz) : δ (CDCl_3) 173.5, 166.7, 155, 150.7, 133.4, 133.3, 131.2, 129.5, 128.9, 128.3, 127.2, 127, 126.6, 124.8, 124.2, 123.4, 121.1, 114.2, 57.2, 40, 29.9; m/z (eims 70eV) 342.3 (M^+ , 76 %), 327.3 (100), 311.2 (45), 285.2 (23), 255.2 (16), 192.1 (15), Found: C, 80.43; H, 6.32; N, 8.24. $\text{C}_{23}\text{H}_{22}\text{N}_2\text{O}$ requires C, 80.67; H, 6.48; N, 8.18 %.

Preparation of 1-(2-substituted-quinazolin-4-yl)-naphthalen-2-ols 12b-f**1-(2-Methylquinazolin-4-yl)naphthalen-2-ol 12b**

Purified by silica gel column chromatography (ethyl acetate) to give 1-(2-methylquinazolin-4-yl)naphthalen-2-ol as a yellow solid (71%), m.p. 260-262°C. ^1H NMR (270 MHz): δ (CDCl_3), 9.31

(br. s), 7.99 (1H, d, J = 8.1 Hz), 7.94 (1H, d, J = 8.8 Hz), 7.85 (1H, d, J = 7.1 Hz), 7.85 (1H, dt, J₁ = 7.4 Hz, J₂ = 1.6 Hz), 7.58 (1H, d, J = 8.4 Hz), 7.40-7.32 (3H, m), 7.27 (1H, dt, J₁ = 7.6 Hz, J₂ = 1.7 Hz), 7.21 (1H, d, J = 8.0 Hz) and 3.01 (3H, s); ¹³C NMR (75.4 MHz): δ (DMSO) 167.9, 164.3, 153.4, 151.0, 134.8, 133.6, 131.3, 128.8, 128.4, 127.7, 127.6, 127.4, 124.3, 123.6, 123.5, 118.9, 116.8 and 26.9; ν_{max} (KBr) 3026, 1620, 1567, 1514, 1206 and 772 (m) (Ar-H) cm⁻¹; HRMS calcd for C₁₉H₁₄N₂O: 286.111, found 286.113.

1-(2-Benzylquinazolin-4-yl)naphthalen-2-ol 12d

A mixture of 2-methoxy-1-(2-phenylmethylquinazolin-4-yl)naphthalene (0.50 g, 1.33 mmol), glacial acetic acid (2.40 mL) and 48% HBr (2.40 mL) was heated under reflux at 124°C for 22 h. The initial brown suspension became a black solution as reflux temperature was reached. The solution was cooled to room temperature and dichloromethane (~20 mL) and water (~20 mL) added. Sufficient 10% NaOH was added to adjust the pH of the solution to 14 and the aqueous layer went cloudy. The entire solution was then re-acidified by addition of 1M HCl until pH 1 was attained. The aqueous layer was seen to go clear again. The organic layer was isolated from the orange solution and the aqueous layer extracted twice with dichloromethane. The combined organic extracts were dried over anhydrous magnesium sulfate and the solvent reduced *in vacuo* to give a yellow-brown solid which was purified by silica gel column chromatography (2:1 petrol ether/ ethyl acetate) to give 1-(2-phenylmethylquinazolin-4-yl)naphthalen-2-ol (0.32 g, 67%) as a bright yellow solid; m.p. 182-184°C; ν_{max} (KBr) 3463, 3047, 2963, 1616, 1546, 1261, 1096 and 813 cm⁻¹; ¹H NMR (300 MHz): δ (CDCl₃) 9.28 (1H, br s), 7.95 (1H, d, J = 8.49 Hz), 7.80 (1H, d, J = 8.93 Hz), 7.77-7.71 (2H, m), 7.48 (1H, d, J = 8.49 Hz), 7.37-7.33 (1H, m), 7.35 (1H, dt, J = 8.79, 1.46 Hz), 7.29-7.14 (7H, m), 7.12 (1H, d, J = 8.20 Hz) and 4.37 (2H, s); ¹³C NMR (75 MHz): δ (CDCl₃) 165.6, 163.8, 153.7, 150.7, 137.1, 133.4, 131.6, 131.5, 128.3, 127.7, 127.7, 127.5, 127.3, 127.0, 125.9, 125.8, 125.7, 123.9, 122.6, 121.2, 118.3, 113.5 and 45.0 ; m/z (eims 70eV) 362 (M⁺, 81%), 361 (100), 219 (10), 180 (11), 165 (11), 115 (14), 91 (68) and 65 (24); m/z (MS ES⁺): 363 = M⁺+1; Found: C, 82.67; H, 4.98; N, 7.54. C₂₅H₁₈N₂O requires C, 82.85; H, 5.01; N, 7.73%.

1-(2-Isopropyl-quinazolin-4-yl)-naphthalen-2-ol 12e

1-(2-Isopropyl-quinazolin-4-yl)-naphthalen-2-ol was isolated as a light orange powder (93%) m.p. 194-195°C. ν_{\max} (KBr) 3620, 3047, 2977, 1621, 1562 and 1225 cm^{-1} ; ^1H NMR (300 MHz): δ (CDCl_3) 8.09 (1H, d, $J = 8.49$ Hz), 7.92 (1H, d, $J=9.08$ Hz), 7.88-7.82 (2H, m), 7.59 (1H, d, $J=8.5$ Hz), 7.38 (1H, dt, $J= 8.78, 1.46$ Hz), 7.37-7.28 (3H, m), 7.24 (1H, d, $J= 8.79$ Hz), 3.46 (1H, sept, $J= 6.98$), 1.51 (6H, d, $J= 6.77$); ^{13}C NMR (75 MHz): δ (CDCl_3) 170.4, 166.2, 155.3, 152.1, 134.4, 132.8, 132.7, 129.5, 128.9, 128.6, 128.2, 126.9, 126.7, 125.3, 123.8, 122.4, 119.4, 114.7, 38 and 22.3 ; m/z (eims 70eV) 314 (M^+ , 67 %), 313 (74), 299 (28), 297 (12), 271 (10), 243.2 (7), 155 (10) and 149 (13); Found: C, 80.11; H, 5.65; N, 8.78. $\text{C}_{21}\text{H}_{18}\text{N}_2\text{O}$ requires C, 80.23; H, 5.77; N, 8.91%.

1-(2-*tert*-Butyl-quinazolin-4-yl)-naphthalen-2-ol 12f

1-(2-*tert*-Butyl-quinazolin-4-yl)-naphthalen-2-ol was isolated as a light orange solid (97%) m.p. 197-199°C. ν_{\max} (KBr) 3502, 2956, 2915, 1611, 1482 and 1260 cm^{-1} ; ^1H NMR (300 MHz): δ (CDCl_3) 8.08 (1H, d, $J = 8.49$ Hz), 7.92 (1H, d, $J = 9.08$ Hz), 7.86-7.79 (2H, m), 7.57 (1H, d, $J = 8.5$ Hz), 7.38 (4H, m), 7.24 (1H, d, $J = 9.08$ Hz), 1.59 (9H, s); ^{13}C NMR (75 MHz): δ (CDCl_3) 172.1, 165.5, 155.6, 152.1, 134.1, 132.9, 132.7, 129.3, 129, 128.6, 128.2, 126.8, 126.6, 125.5, 123.8, 121.9, 119.4, 114.6, 39.8 and 29.9; m/z (eims 70eV) 328.3 (M^+ , 100 %), 313.2 (74), 286.2 (46), 271.2 (32), 243.2 (14), 156.4 (20), 129.1 (30) and 115.1 (20); Found: C, 80.13; H, 5.99; N, 8.41. $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}$ requires C, 80.46; H, 6.14; N, 8.53%.

Preparation of 1-(2-Substituted-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate 13b-f

1-(2-Methylquinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate 13b

Purified by silica gel column chromatography (petroleum ether / ethyl acetate 2:1) to give 1-(2-methylquinazolin-4-yl)-2-naphthyl(trifluoromethyl)sulfonate as a white solid (78%), m.p. 124-126°C. ν_{\max} (KBr) 3065, 1612, 1558, 1512, 1428, 1214 (s), 1140 (s) and 831 cm^{-1} ; ^1H NMR (500 MHz): δ (CDCl_3) 8.12 (1H, d, $J = 10.1$ Hz), 8.10 (1H, d, $J = 9.2$ Hz), 8.00 (1H, d, $J = 8.3$ Hz), 7.89 (1H, dt, $J_1 = 7.7$ Hz, $J_2 = 1.6$ Hz), 7.61 (1H, d, $J = 9.2$ Hz), 7.59 (1H, t, $J = 7.6$ Hz), 7.44-7.39 (3H, m), 7.27 (1H, d, $J = 8.6$ Hz) and 3.01 (3H, s); ^{13}C NMR (125.7 MHz): δ (CDCl_3) 164.6, 163.5, 151.3, 144.9, 134.6, 132.6, 132.5, 132.2, 128.6, 128.6, 128.5, 127.6, 127.5, 127.4, 126.6, 126.3, 122.9, 119.7, 118.4 (q, $J = 320.3$ Hz) and 26.6; m/z (eims 70eV) 418 (M^+ , 9%), 285 (100), 257 (53), 243 (12) and 69

(13); Found: C, 57.1; H, 3.2; N, 6.5; S, 8.1; F, 13.8. $C_{20}H_{13}N_2O_3SF_3$ requires C, 57.4; H, 3.1; N, 6.7; S, 7.7; F, 13.6 %.

1-(2-Phenylmethyl-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate 13d

(77%) as beige solid, m.p. 136-138°C; ν_{\max} (KBr) 3065, 2935, 1615, 1552, 1425, 1214, 1136, 950 and 834 cm^{-1} ; 1H NMR (300 MHz): δ ($CDCl_3$) 8.13 (1H, d, J = 8.55 Hz), 8.10 (1H, d, J = 8.95 Hz), 7.98 (1H, d, J = 8.15 Hz), 7.88 (1H, dt, J = 8.55, 6.56, 1.99 Hz), 7.60 (1H, d, J = 8.95 Hz), 7.57 (1H, dt, J = 8.15, 6.96, 1.19 Hz), 7.45 (1H, dt, J = 7.36, 1.39 Hz), 7.47-7.36 (4H, m), 7.31-7.19 (3H, m), 7.19 (1H, d, J = 8.35 Hz), 4.57 (1H, d, J = 13.91 Hz) and 4.56 (1H, d, J = 13.91 Hz); ^{13}C NMR (75 MHz): δ ($CDCl_3$) 166.1, 163.7, 151.5, 144.8, 138.7, 134.5, 132.7, 132.2, 129.5, 129.0, 128.6, 128.5, 128.4, 127.7, 127.6, 127.3, 126.6, 126.5, 126.4, 123.2, 119.7, 119.6 and 46.5; m/z (eims 70eV) 494 (M^+ , 10%), 361 (100), 180 (41), 165 (25), 114 (10), 91 (84) and 65 (17). Anal. calcd for $C_{26}H_{17}N_2O_3SF_3$: C, 63.15; H, 3.47; N, 5.67; S, 6.48; F, 11.53 %; Found: C, 62.83; H, 3.51; N, 5.53; S, 6.66; F, 11.14 %.

1-(2-Isopropyl-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate 13e

Purified by silica gel column chromatography (petroleum ether / ethyl acetate 2:1) to give 1-(2-isopropyl-quinazolin-4-yl)-2-naphthyl(trifluoromethyl)sulfonate as a yellow solid (97%), m.p. 117-118°C. ν_{\max} (KBr) 3059, 2978, 2929, 1616, 1491, 1434, 1229, 1135 and 847 cm^{-1} ; 1H NMR (300 MHz): δ ($CDCl_3$) 8.14 (1H, d, J = 8.49 Hz), 8.11 (1H, d, J = 8.78 Hz), 8.0 (1H, d, J = 8.2 Hz), 7.88 (1H, dt, J=8.5, 6.74, 1.78 Hz), 7.6 (1H, d, J = 9.08 Hz), 7.58 (1H, dt, J = 8.2, 7.03, 1.47 Hz), 7.44 (1H, dt, J= 8.49, 7.03, 1.17 Hz), 7.41-7.33 (2H, m) and 7.28 (1H, d, J = 8.5 Hz), 3.52 (1H, sept, J=7.03) and 1.50 (6H, d, J= 6.74 Hz); ^{13}C (75 MHz): δ ($CDCl_3$) 170.6, 162.1, 150, 143.6, 133, 131.5, 130.8, 127.7, 127.3, 127.2, 126.4, 126.3, 126.1, 125.2, 125.1, 122, 119.2, 118.5, 37.1, 20.6; m/z (eims 70eV) 446 (M^+ , 6%), 313 (39), 297 (14), 285 (9), 243 (5) and 214 (4); Found: C, 59.01; H, 3.76; N, 6.11. $C_{23}H_{19}F_3N_2O_3S$ requires C, 59.19; H, 3.84; N, 6.27%.

1-(2-tert-Butyl-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate 13f

Purified by column chromatography (silica gel, 2:1 petroleum ether / ethyl acetate) to give 1-(2-tert-butyl-quinazolin-4-yl)-2-naphthyl(trifluoromethyl)sulfonate as a yellow solid (86%), m.p. 115-117°C. ν_{\max} (KBr) 3070, 2963, 2921, 2885, 1612, 1559, 1420, 1280, 1140 and 875 cm^{-1} ; 1H NMR (300 MHz): δ ($CDCl_3$) 8.15 (1H, d, J = 8.49 Hz), 8.11 (1H, d, J = 9.1 Hz), 8.0 (1H, d, J = 8.5 Hz), 7.85 (1H, dt, J = 6.74, 1.78 Hz), 7.6 (1H, d, J = 9.08 Hz), 7.58 (1H, dt, J = 8.2, 1.78 Hz), 7.42 (1H, dt, J= 9.37, 1.17 Hz), 7.38-7.31 (2H, m), 7.28 (1H, d, J = 8.79 Hz) and 1.56 (9H, s); ^{13}C (75 MHz): δ ($CDCl_3$) 172.3,

161.5, 149.8, 143.5, 132.7, 131.6, 131.5, 130.6, 128, 127.3, 127, 126.7, 126.3, 126, 125.2, 124.9, 121.6, 118.5, 38.8, 28.5; m/z (eims 70eV) 460.2 (M^+ , 15%), 327.3 (100), 311.2 (46), 285.3 (11), 272.1 (14), 242.2 (14), 214.2 (8) and 189.2 (7); Found: C, 59.66; H, 4.00; N, 5.98. $C_{24}H_{21}F_3N_2O_3S$ requires C, 59.99; H, 4.16; N, 6.08%.

Preparation of (*R,S*)-Diphenyl(1-(2-substituted-quinazolin-4-yl)(2-naphthyl)phosphine 14b-f

(*R,S*)-Diphenyl[1-(2-methylquinazolin-4-yl)(2-naphthyl)]phosphine 14b

The product was purified by silica gel column chromatography (petroleum ether / ethyl acetate) to give (*R,S*)-diphenyl[1-(2-methylquinazolin-4-yl)(2-naphthyl)] phosphine as a white solid (63%), m.p. 195-197°C; ν_{max} (KBr) 3058, 1637, 1556, 1429, 743 and 696 cm^{-1} ; 1H NMR (500 MHz): δ ($CDCl_3$) 8.06 (d, 1H, $J = 8.5$ Hz), 7.93 (1H, d, $J = 8.5$ Hz), 7.91 (1H, d, $J = 8.5$ Hz), 7.81 (1H, t, $J = 7.5$ Hz), 7.51 (1H, t, $J = 7.6$ Hz), 7.43 (1H, dd, $J_{H,H} = 8.6$ Hz, $J_{P,H} = 3.2$ Hz), 7.34-7.17 (13H, m), 7.13 (1H, d, $J = 8.5$ Hz) and 2.82 (3H, s); ^{13}C NMR (125.7 MHz): δ ($CDCl_3$) 169.5, 164.1, 150.8, 141.8, 137.1, 137.0, 135.0, 134.1-133.7, 132.1, 130.1, 129.4, 128.8-128.6, 128.3, 128.3, 127.3, 127.2, 127.2, 126.9, 126.3, 123.6 and 26.6; ^{31}P NMR (101.3MHz): δ ($CDCl_3$) -12.6; m/z (eims 70eV) 454 (M^+ , 29%), 377 (100), 300 (19) and 77 (16); Found: C, 81.5; H, 5.1; N, 6.1. $C_{31}H_{23}N_2P$ requires C, 81.9; H, 5.1; N, 6.2 %

(*R,S*)-Diphenyl(1-(2-phenylmethyl-quinazolin-4-yl)(2-naphthyl)phosphine 14d

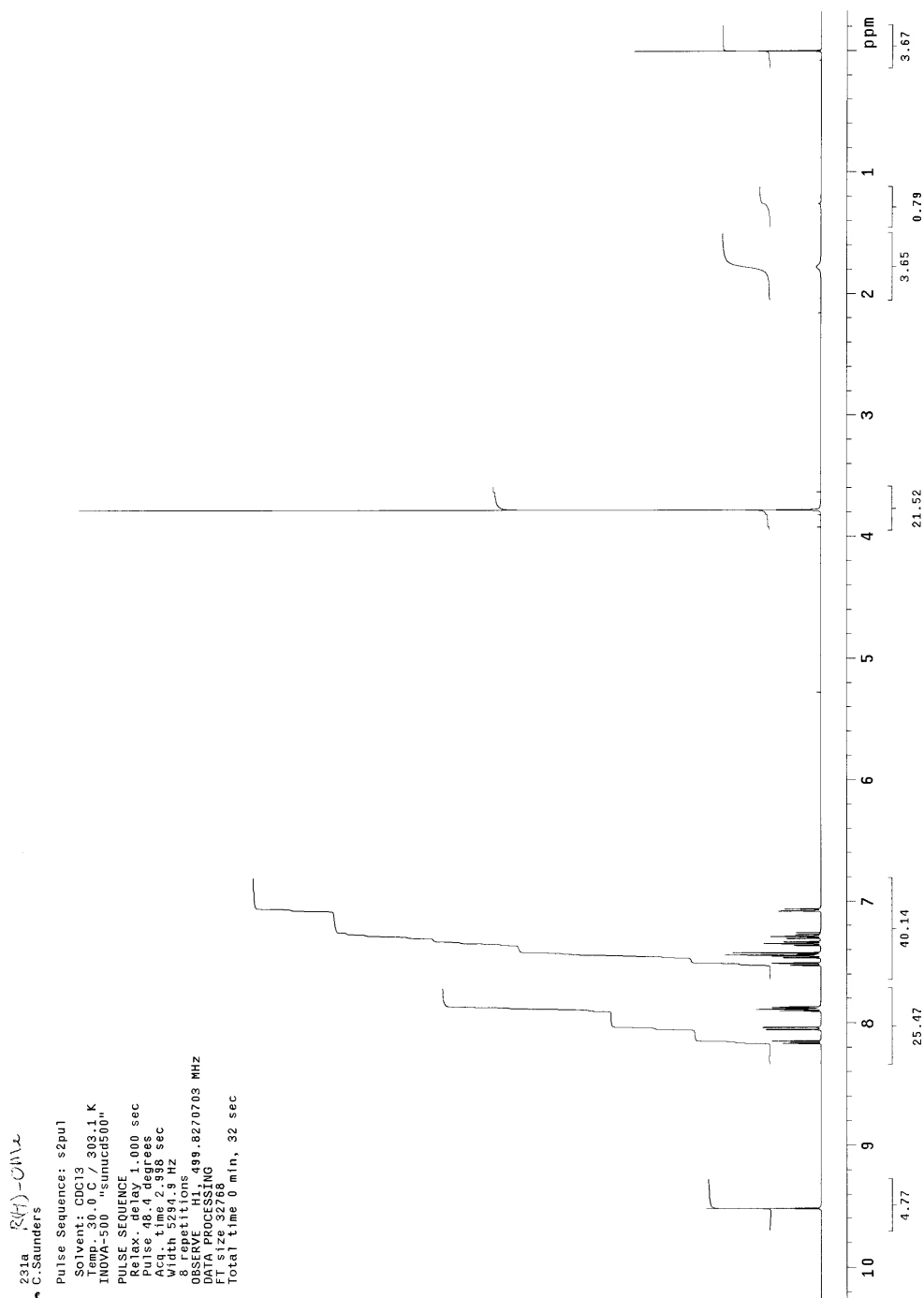
Purified by silica gel column chromatography (4:1 petrol ether/ ethyl acetate) to give (*R,S*)-diphenyl[1-(2-phenylmethylquinazolin-4-yl)(2-naphthyl)]phosphine (0.76 g, 80%) as a white solid, m.p. 218-220°C; ν_{max} (KBr) 3054, 2939, 1612, 1583, 1546, 1485, 1433, 746 and 693 cm^{-1} ; 1H NMR (300 MHz): δ ($CDCl_3$) 8.10 (1H, d, $J = 8.64$ Hz), 7.94 (1H, d, $J = 8.35$ Hz), 7.92 (1H, d, $J = 7.91$ Hz), 7.82 (1H, dt, $J = 8.49, 6.44, 1.90$ Hz), 7.53 (1H, dt, $J = 8.05, 6.88, 1.03$ Hz), 7.45 (1H, dd, $J = 8.49$ Hz, $J_{P-H} = 1.03$ Hz), 7.35-7.20 (16H, m), 7.15 (2H, dt $J = 7.18, 6.30, 1.90$ Hz), 7.10 (1H, d, $J = 8.49$ Hz), 4.44 (1H, d, $J = 13.76$ Hz) and 4.41 (1H, d, $J = 13.62$ Hz); ^{13}C NMR (75 MHz): δ ($CDCl_3$) 168.7, 164.4, 149.7, 140.9, 137.6, 135.9, 133.5, 132.7, 132.7, 132.5, 132.4, 132.4, 132.1, 130.8 (d, $J_{P-C} = 8.63$ Hz), 129.0, 128.2, 128.1, 127.5-127.0, 126.1, 125.9, 125.9, 125.8, 125.2, 125.2, 125.1, 122.7, 122.7 and 45.1; ^{31}P NMR (121 MHz): δ ($CDCl_3$) -12.9 ppm; m/z (eims 70eV) 494 (M^+ , 10%), 361 (100), 180 (41), 165 (25), 114 (10), 91 (84) and 65 (17). Found: C, 83.55; H, 5.24; N, 5.26; P, 5.64 % $C_{37}H_{27}PN_2$ requires C, 83.75; H, 5.13; N, 5.28; P, 5.84 %

(*R,S*)-Diphenyl(1-(2-isopropyl-quinazolin-4-yl)(2-naphthyl)phosphine 14e

Purified by chromatography (silica gel, 2:1 petrol ether / ethyl acetate) to give (*R,S*)-diphenyl(1-(2-isopropyl-quinazolin-4-yl)(2-naphthyl)phosphine as a white solid (67%). m.p. 220-221°C.; ν_{\max} (KBr) 3064, 2970, 2963, 1772, 1614, 1566 and 1470; ^1H NMR (300 MHz): δ (CDCl_3) 8.07 (1H, d, $J = 8.49$ Hz), 7.91 (1H, d, $J = 8.5$ Hz), 7.89, (1H, d, $J=7.32$ Hz), 7.8 (1H, dt, $J = 8.2, 6.44, 1.46$ Hz), 7.5 (1H, dt, $J=7.91, 6.73, 1.17$ Hz), 7.39 (1H, ddd, $J= 8.2, 1.17$ Hz), 7.36-7.19 (11H, m), 7.18 (2H, dt, 7.33, 5.57, 1.47 Hz), 7.10 (1H, d, $J= 8.79$ Hz), 3.28 (1H, sept, $J= 7.03$), 1.25 (6H, d, $J= 6.74$ Hz); ^{13}C (75 MHz): δ (CDCl_3) 172, 169, 150.8, 141.7, 138, 136.3, 133.9, 133.7, 133.5, 130.3, 129.3, 128.8, 128.6, 128.5, 128.3, 127.3-127, 126.9, 126.8, 126.5, 126.4-125.2, 125.1, 38.2, 22; ^{31}P NMR (121 MHz): δ (CDCl_3) -12.5 ppm; m/z (eims 70eV) 483 (M^+ , 8%), 482 (27), 405 (88), 334 (6), 258 (9) and 233 (25); HRMS 483.2000 $\text{C}_{33}\text{H}_{28}\text{N}_2\text{P}$ requires 483.1990.

(*R,S*)-Diphenyl(1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)phosphine 14f

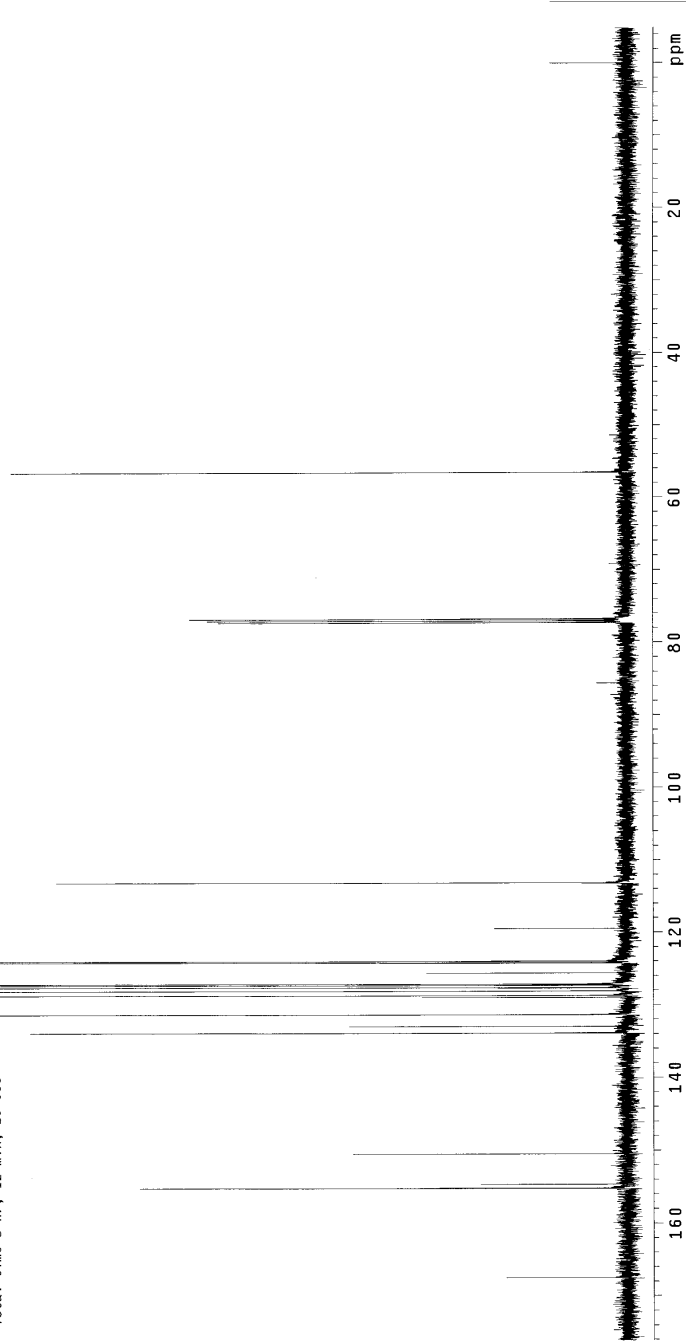
Purified by chromatography (silica gel, 2:1 petrol ether / ethyl acetate) to give (*R,S*)-diphenyl(1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)phosphine as a white solid (64%), m.p. 217-219°C; ν_{\max} (KBr) 3059, 2954, 2918, 1613, 1549, 1480 and 685; ^1H NMR (300 MHz): δ (CDCl_3) 8.08 (1H, d, $J = 8.2$ Hz), 7.89 (2H, app d, $J = 7.91$ Hz), 7.78 (1H, dt, $J = 8.49, 6.15, 1.78$ Hz), 7.49 (1H, dt, $J = 8.2, 5.86, 1.17$ Hz), 7.37 (1H, d, $J = 8.25$ Hz), 7.34-7.21 (11H, m), 7.18 (2H, dt, 8.79, 6.15, 1.47 Hz), 7.08 (1H, d, $J= 8.49$), 1.31 (9H, s); ^{13}C (75 MHz): δ (CDCl_3) 169, 160.3, 150.1, 150, 138, 137.7, 133.9, 133.6, 133.5, 133.4, 132.0, 131.0, 129.5, 129.3, 129.2, 129, 128.7-128.3, 127.5-127.1, 126.9, 126.8, 122, 120.1, 40, 29.6; ^{31}P NMR (121 MHz): δ (CDCl_3) -12.6 ppm; m/z (HRMS, ES) 497.2162 $\text{C}_{34}\text{H}_{30}\text{N}_2\text{P}$ requires 497.2147.

¹H NMR of 2-Hydrogen-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11a)

¹³C NMR of 2-Hydrogen-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11a)

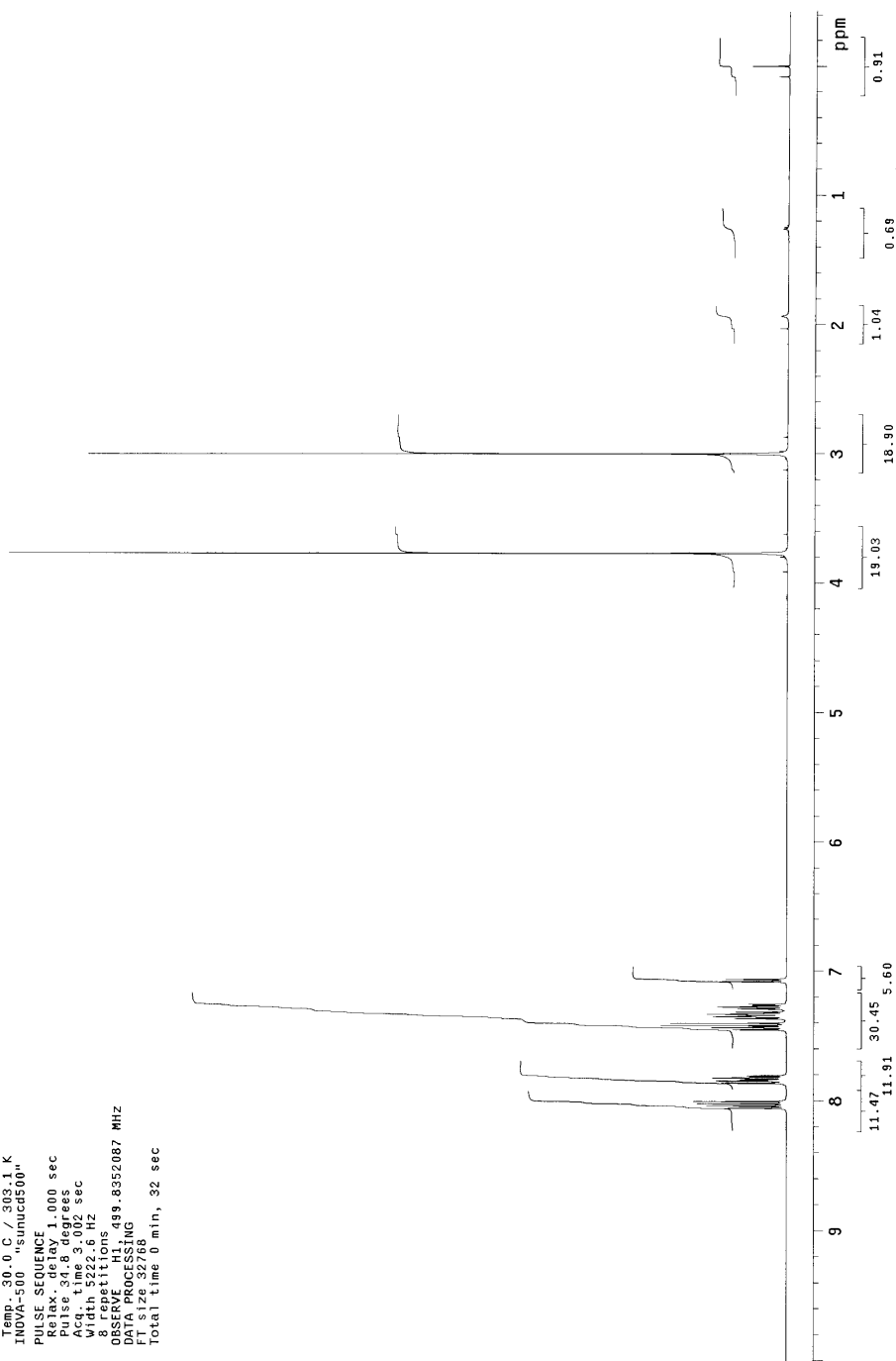
231a R(f)-ome
C.Saunders

Pulse Sequence: szpul
Solvent: CDCl₃
Temp. 30.0 C / 303.1 K
User: 1-14-87
INOVA-300 -smucd500"
PULSE SEQUENCE 1.000 sec
Pulse width 1.301 sec
Acq. time 1.301 sec
Width 22753.1 Hz
Pulse 54.8 degrees
Observer: J.L.P.
ORSERV: C13, 425.6816117 MHZ
DECOUPLE H1, 499.8235577 MHZ
Power 40 db
continuously on
during the run
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65636
Total time 3 hr, 12 min, 29 sec



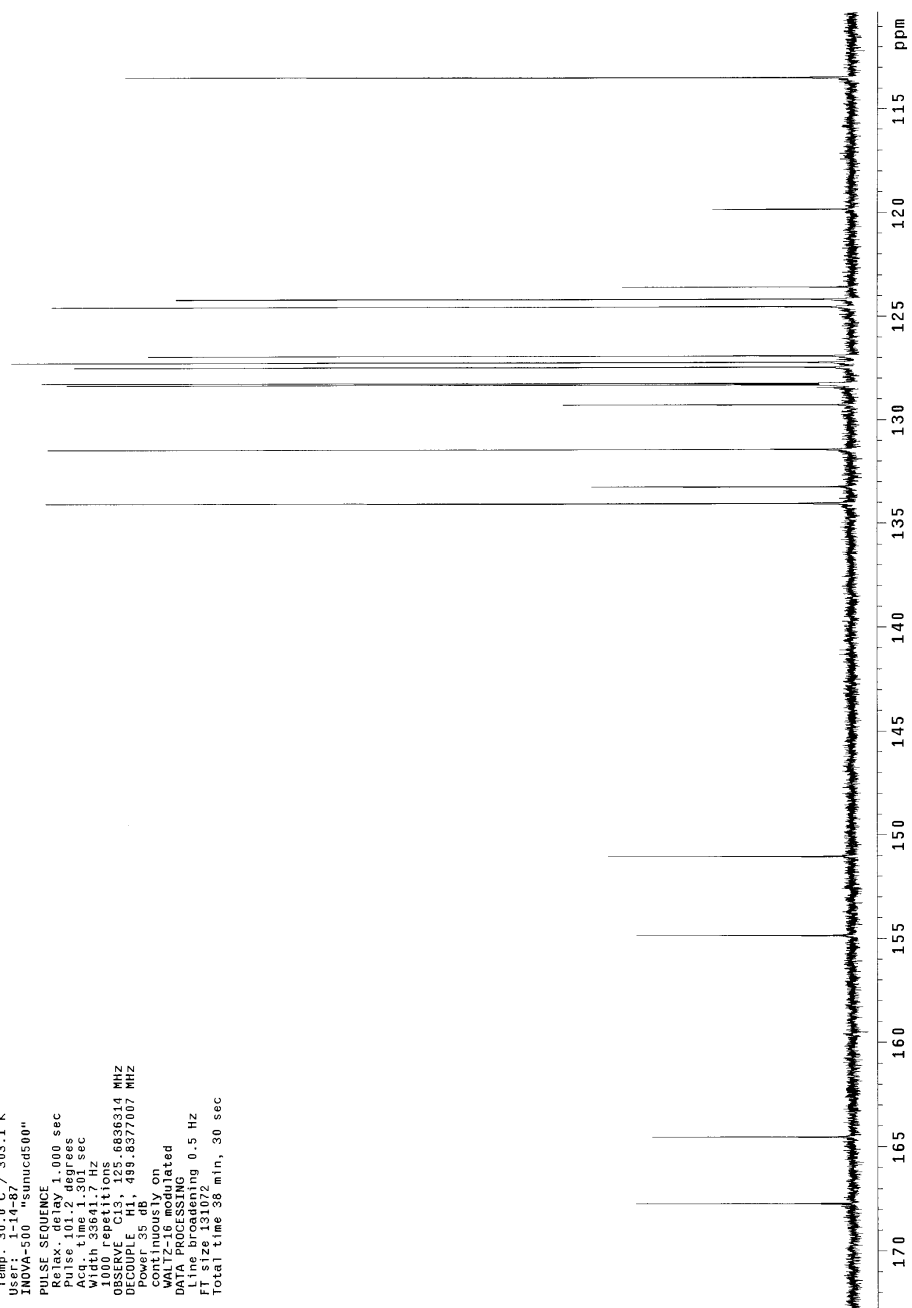
¹H NMR of 2-Methyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11b)

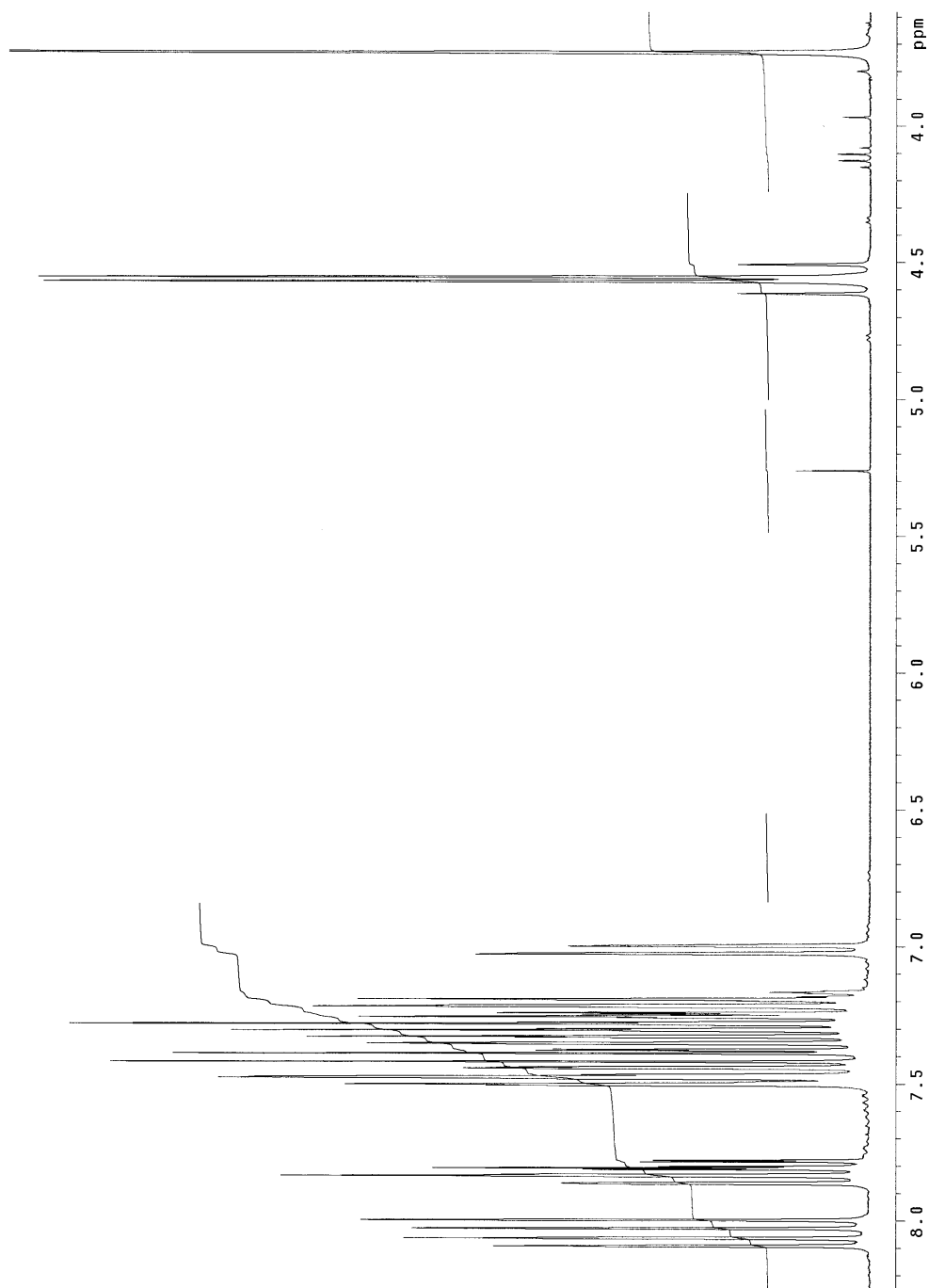
Patrick Lacey-2
Pulse Sequence: s2pul
Solvent: CDCl3
Temp: -30.0 C / 303.1 K
INQVA-500 "sumucd500"
PULSE_SEQUENCE 1.000 sec
Pulse: 3d 8 degrees
Acq: time 3.002 sec
Width 5222.6 Hz
8 repetitions
Oscillator 499.8352087 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 32 sec

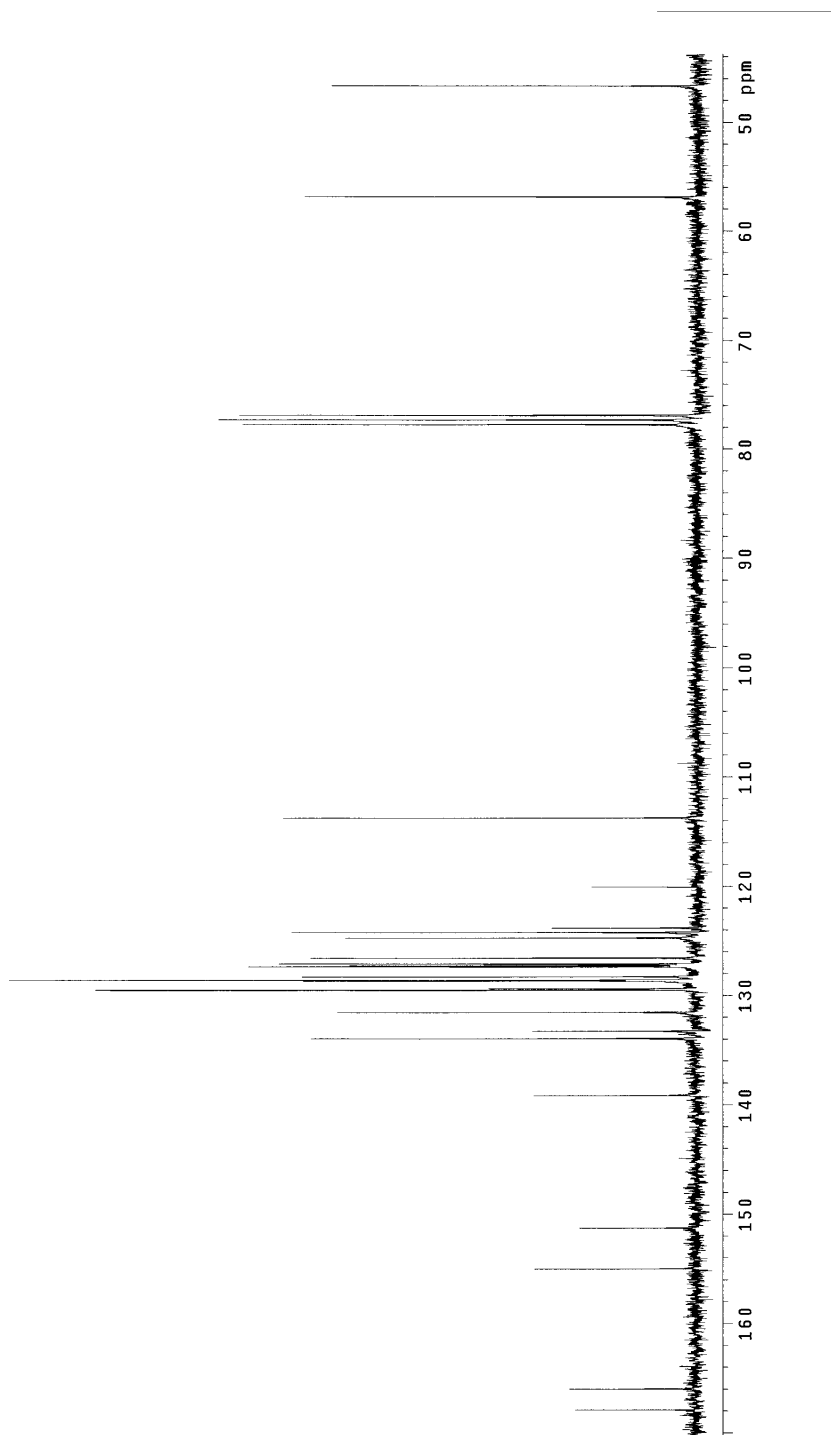


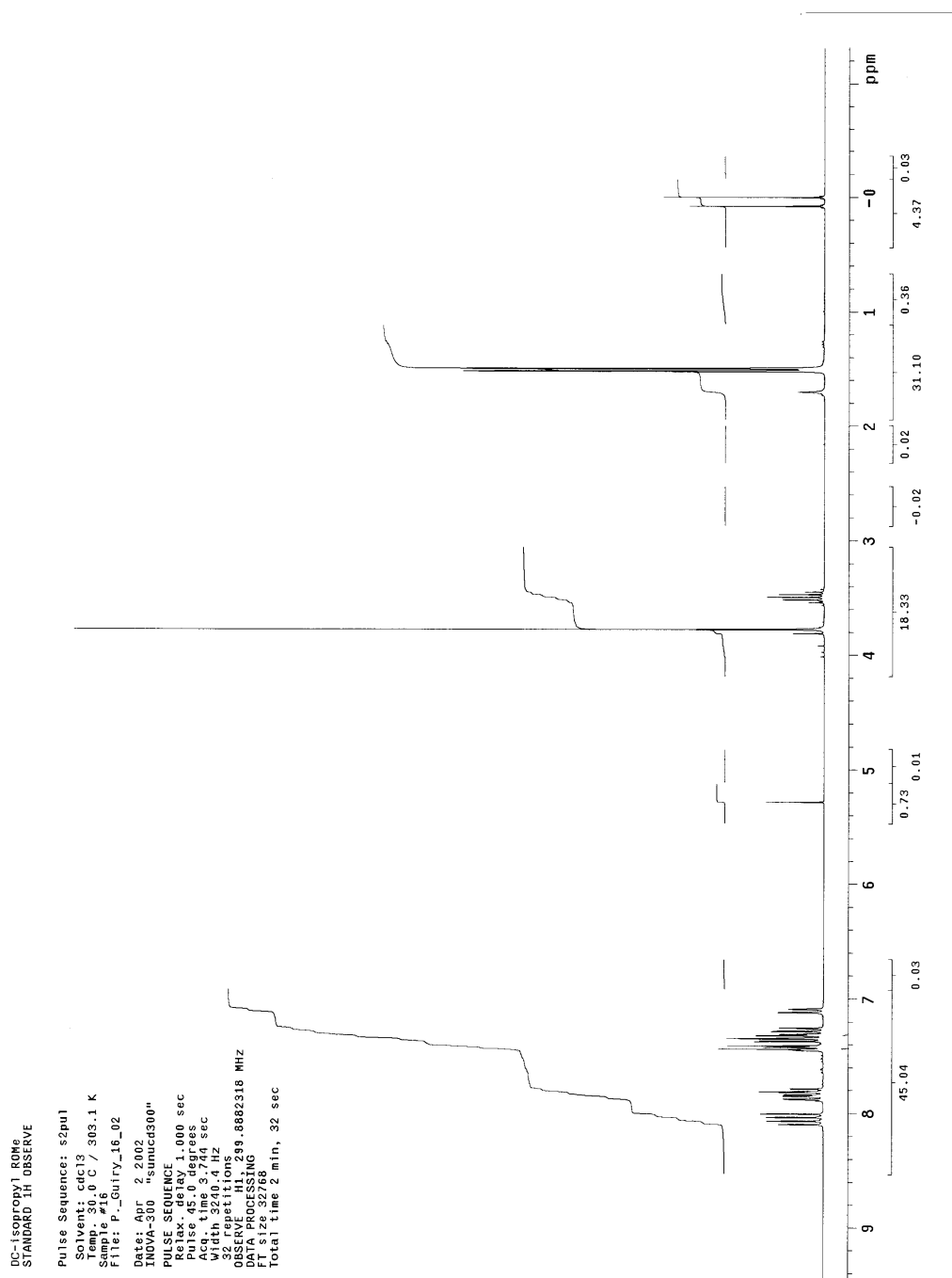
¹³C NMR of 2-Methyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11b)

Patrick Lacey-2
Pulse Sequence: zgpg30
Solvent: CDCl3
Temp: 30.0 C, 303.1 K
User: 1-14-87
INOVA-500 "sumucd500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Acq. time 1.301 sec
Width 33641.7 Hz
1000 repetitions
OBSERVE CH1, 6896314 MHZ
DECODE CH1, 439.8377007 MHZ
Power 35 dB,
continuously on
WALTZ-16 modulated
during irradiation
Line broadening 0.5 Hz
FT size 131072
Total time 38 min, 30 sec



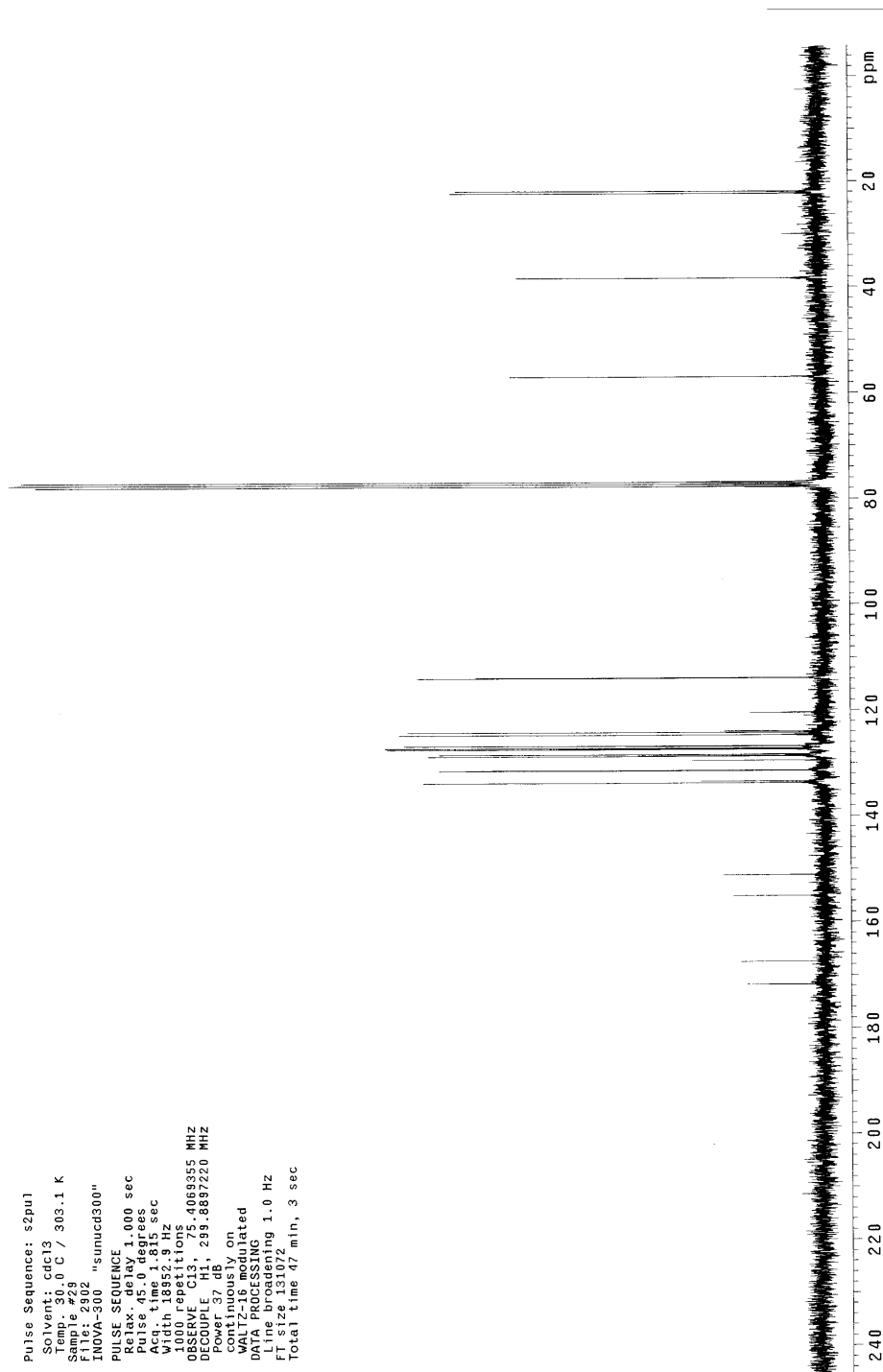
¹H NMR of 2-Benzyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11d)

^{13}C NMR of 2-Benzyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11d)

¹H NMR of 2-Isopropyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11e)

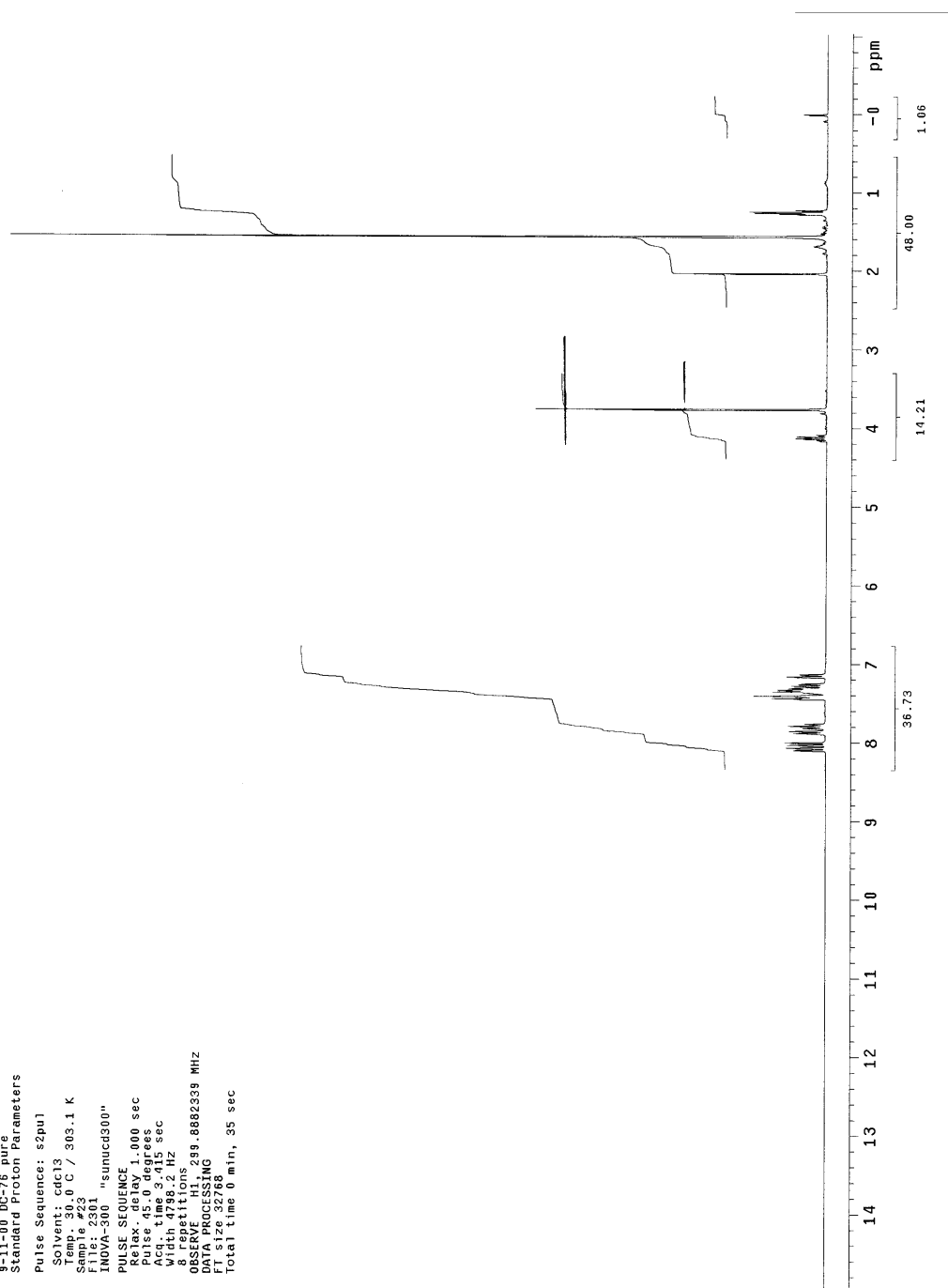
^{13}C NMR of 2-Isopropyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11e)

Pulse Sequence: s2pul
Solvent: cdcl3
Temp: 30.0 C / 303.1 K
Sample #29
File: 2902
INOVA-300 "sumucd300"
PULSE SEQUENCE
Relax. delay 1.000 sec
Acq. time 0.000 sec
Acq. time 1.835 sec
Width 18952.9 Hz
1000 repetitions
OBSERVE C13, 75.4069355 MHz
DECUPLE H1, 239.8697220 MHz
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
File size 172 min, 3 sec
Total time 47 min, 3 sec



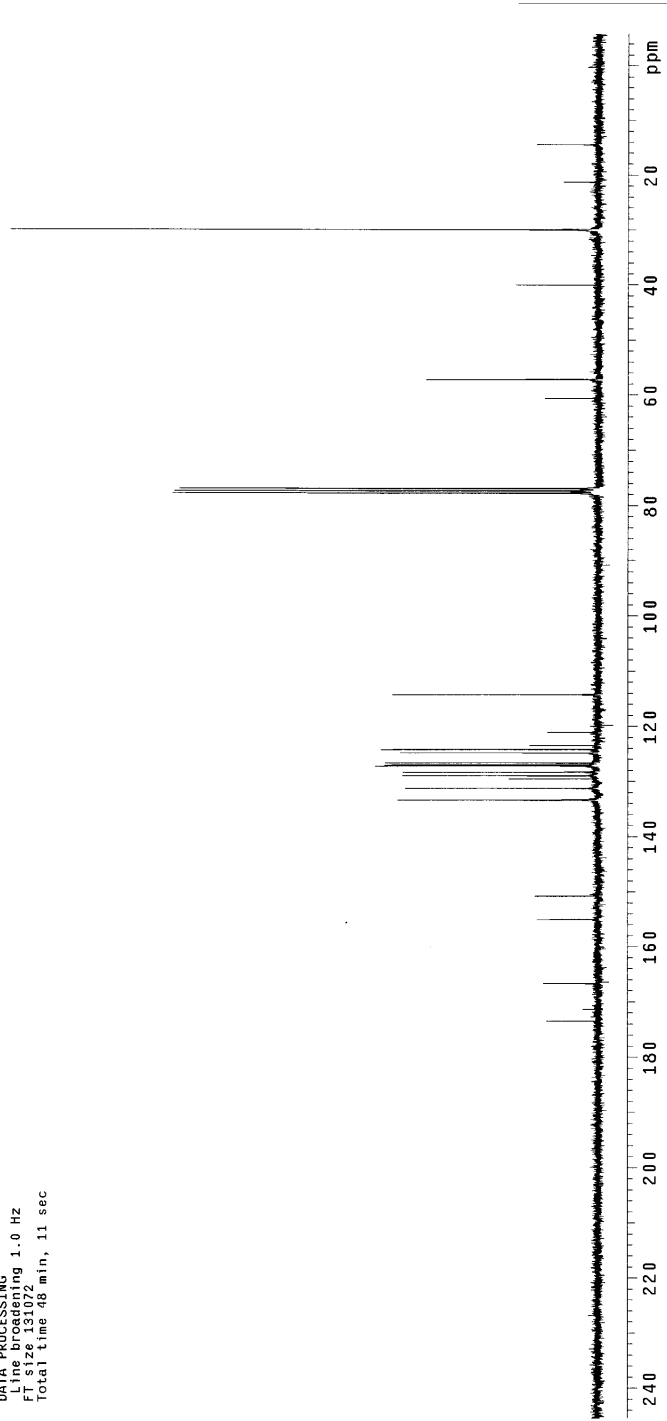
¹H NMR of 2-*tert*-Butyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11f)

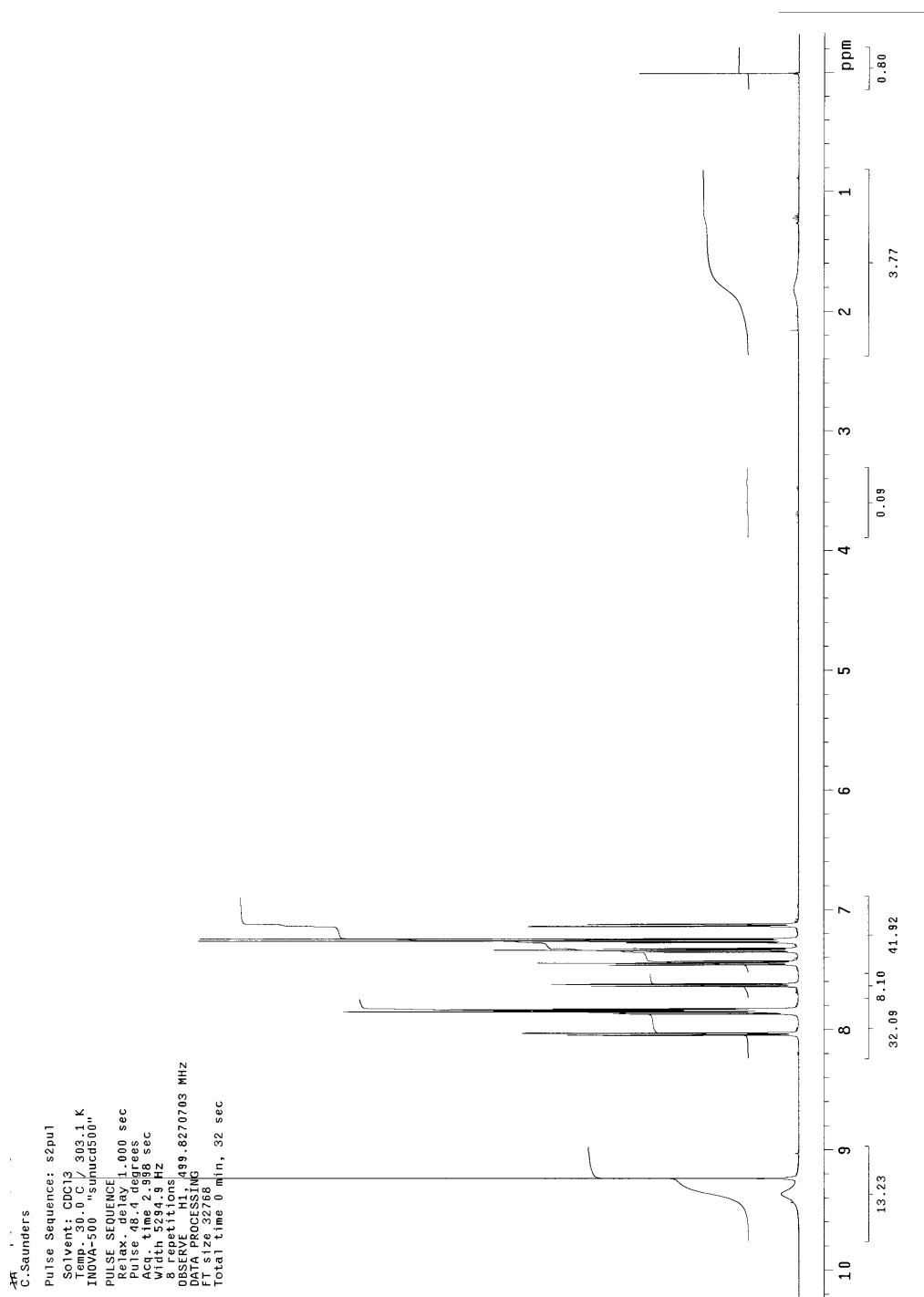
9-11-00 DC-76 pure
 Standard Proton Parameters
 Pulse Sequence: s2pu1
 Solvent: dcl3
 Temp: 30.0 C / 303.1 K
 Sample #23
 File: 2301
 INOVA-300 "sunucd30p"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Acq. time 3.415 sec
 Width 4788.2 Hz
 8 repetitions
 OBSERVED F1: 299.8862339 MHz
 OBSERVED F2: 100.6281100 MHz
 FT size 32768
 Total time 0 min, 35 sec

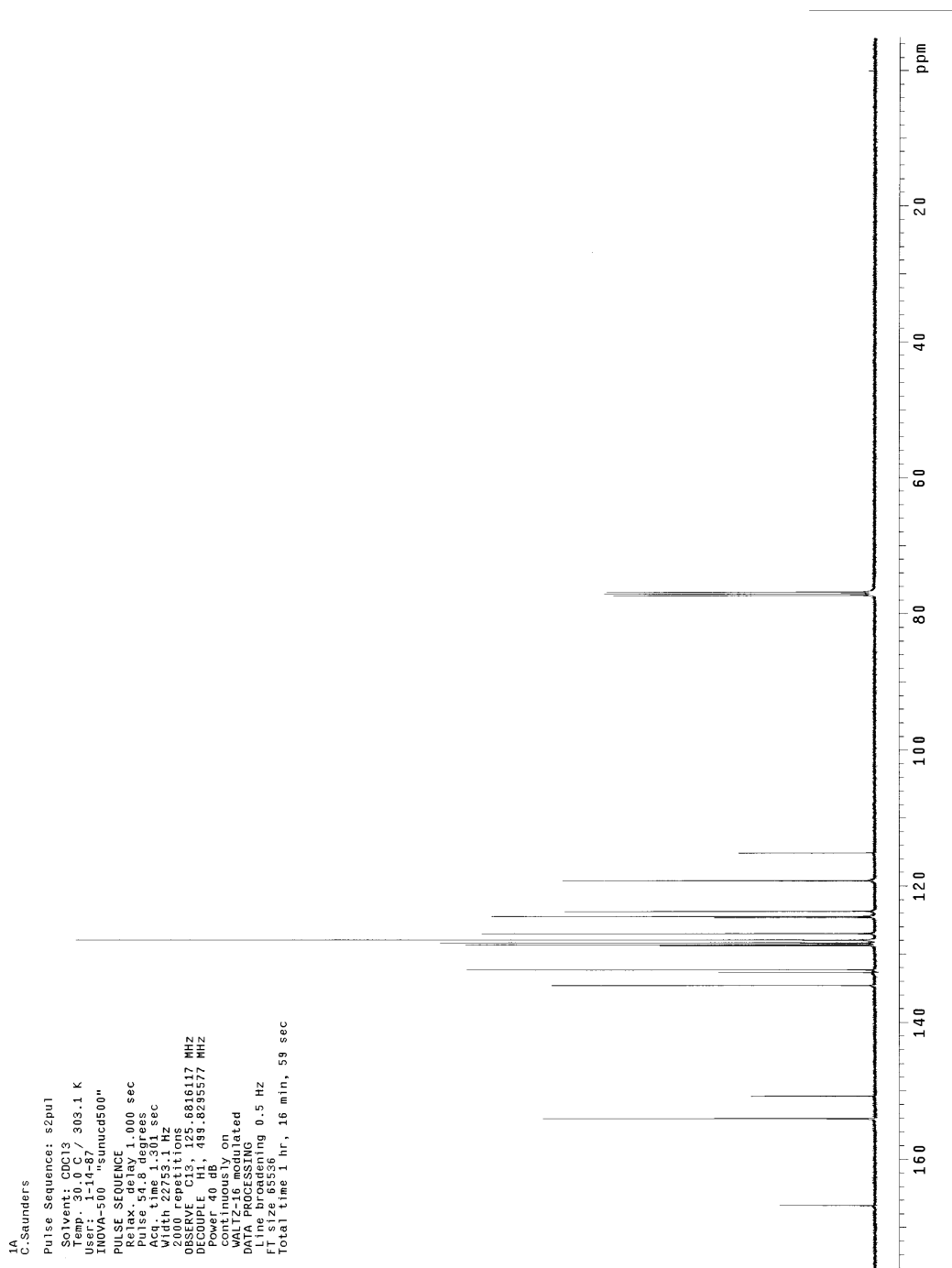


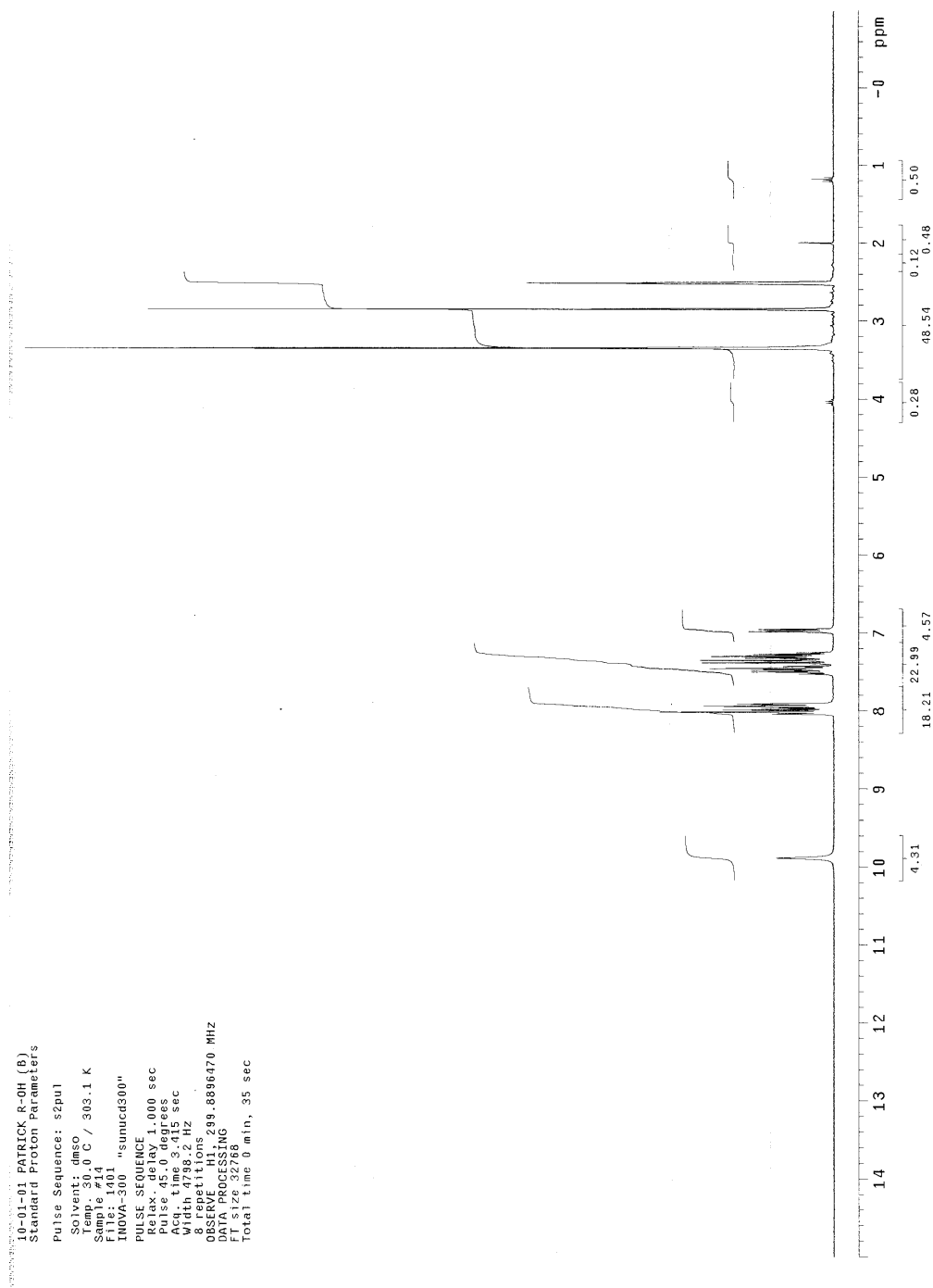
¹³C NMR of 2-*tert*-Butyl-4-(2-methoxy-naphthalen-1-yl)-quinazoline (11f)

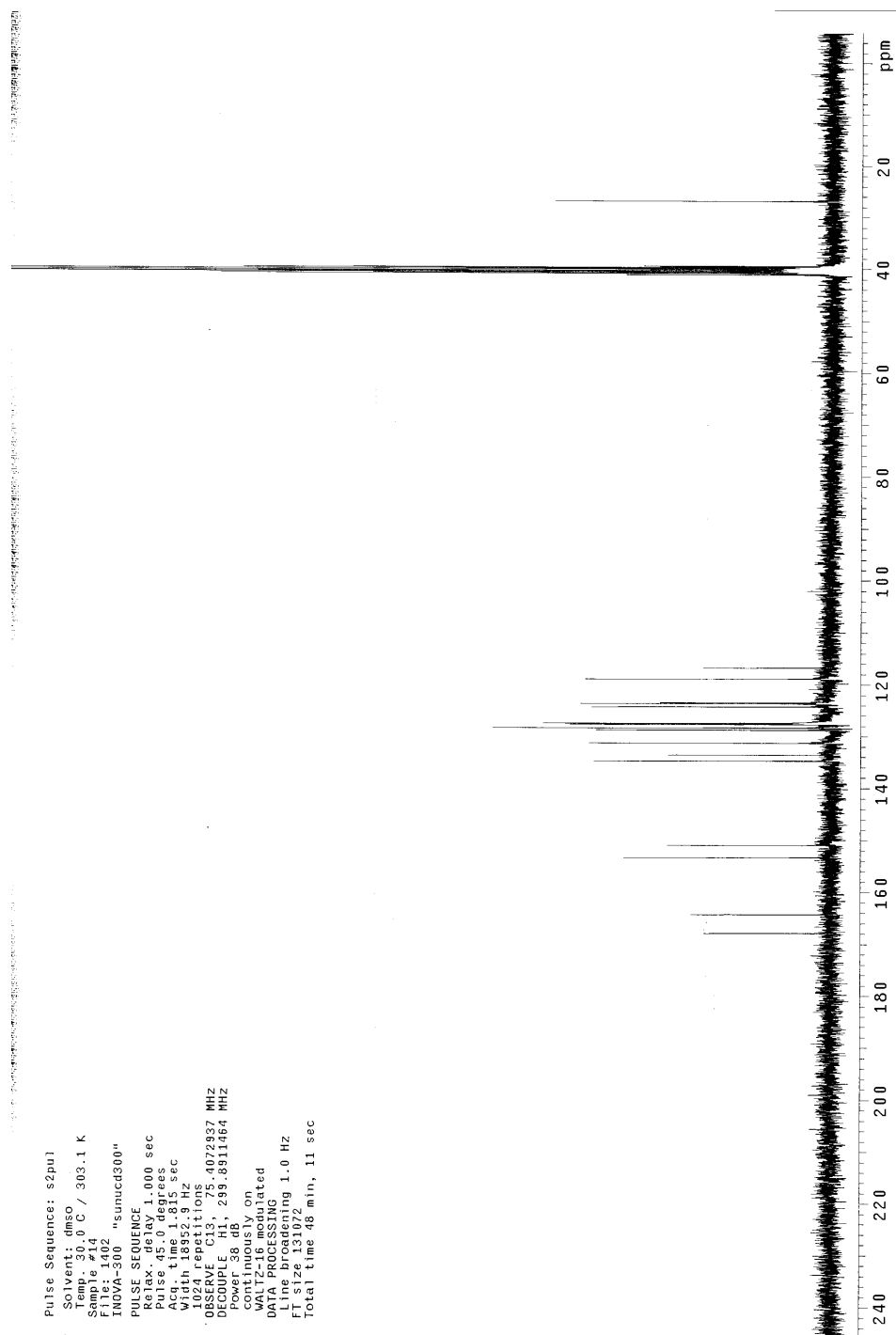
Pulse Sequence: s2pu1
 Solvent: CDCl3
 Sample: 223
 File: 2302
 INOVA-300 "sunucd300"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.815 sec
 Wdth 1024
 1024 F808110ms
 OBSERVE C13, 75.4069355 MHZ
 DECOUPLE H1, 299.8897220 MHZ
 Power 38 dB
 Continuously on
 gated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131072
 Total time 48 min, 11 sec

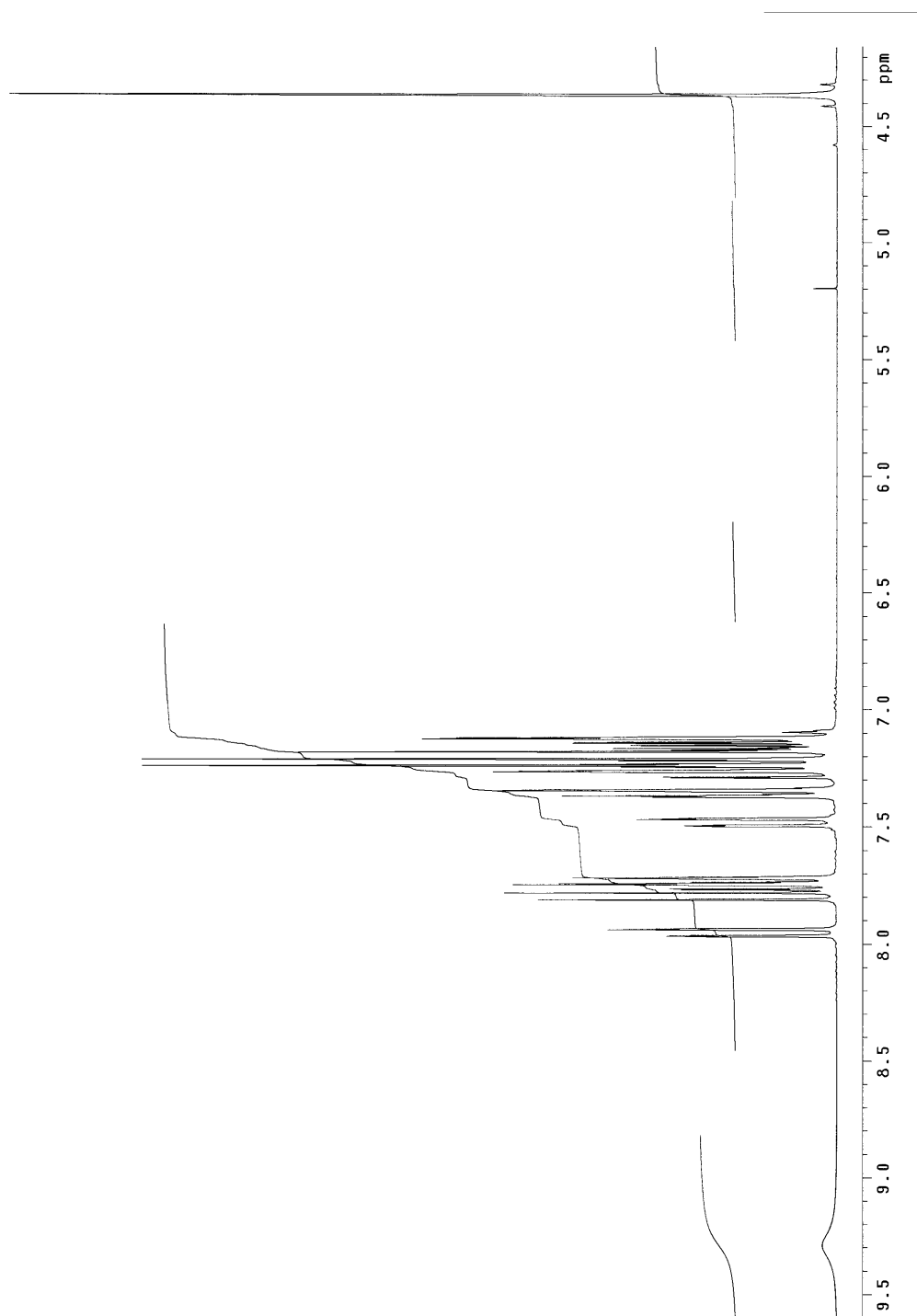


¹H NMR of 1-(Quinazolin-4-yl)naphthalen-2-ol (12a)

¹³C NMR of 1-(Quinazolin-4-yl)naphthalen-2-ol (12a)

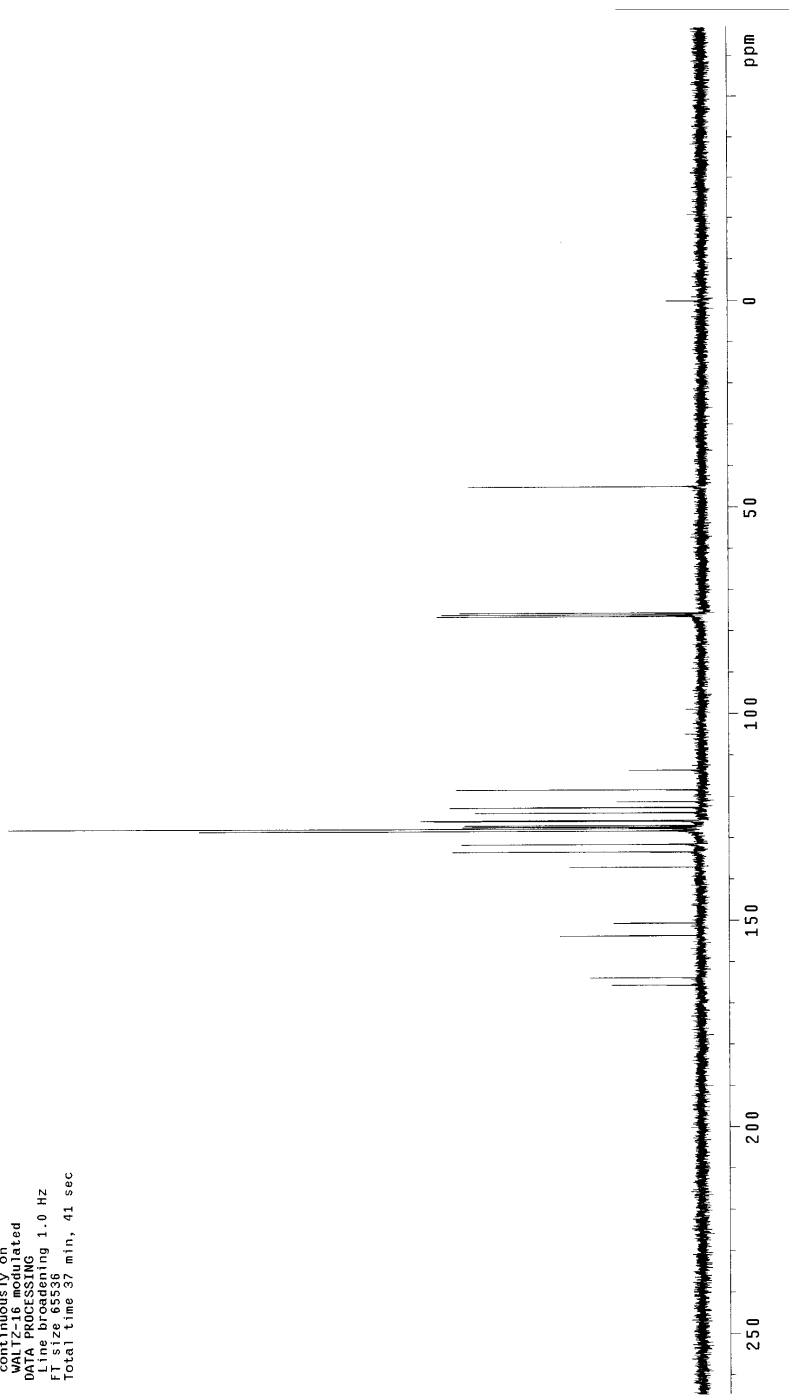
¹H NMR of 1-(2-Methylquinazolin-4-yl)naphthalen-2-ol (12b)

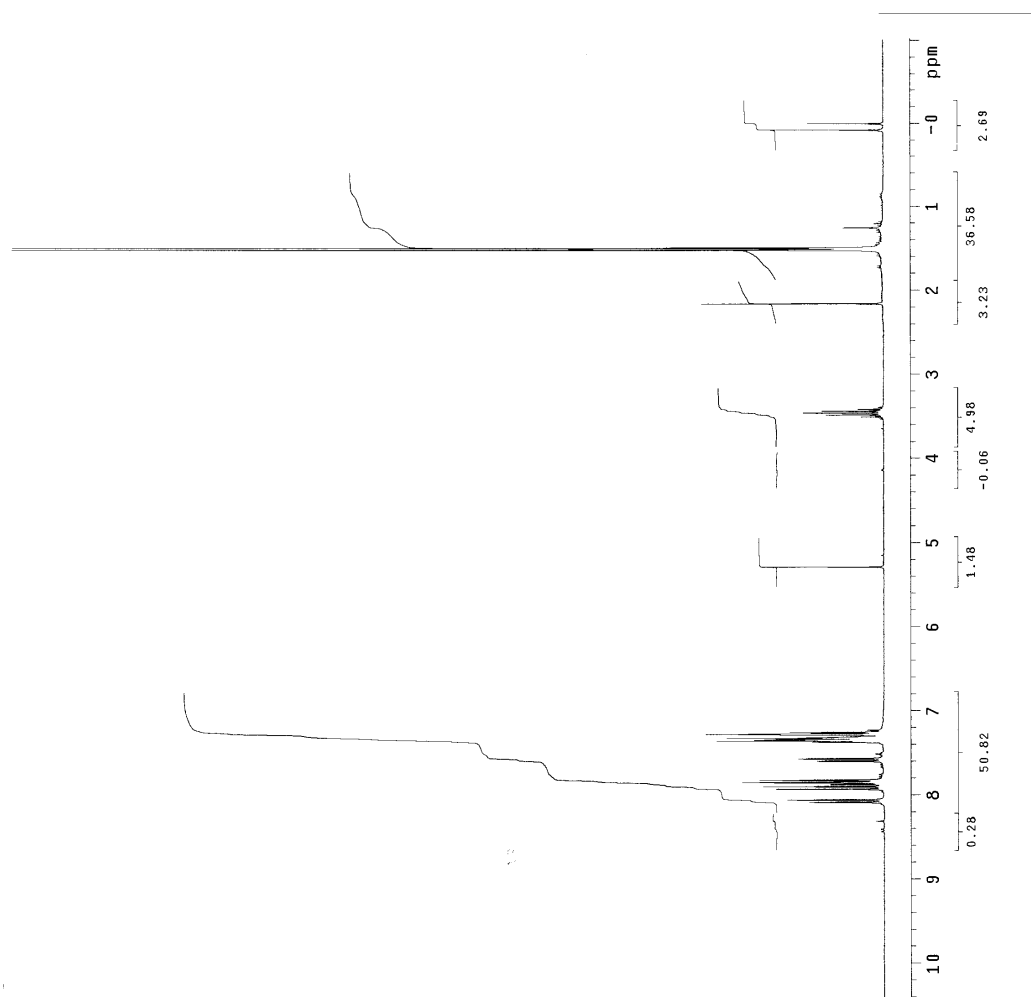
¹³C NMR of 1-(2-Methylquinazolin-4-yl)naphthalen-2-ol (12b)

¹H NMR of 1-(2-Benzylquinazolin-4-yl)naphthalen-2-ol (12d)

¹³C NMR of 1-(2-Benzylquinazolin-4-yl)naphthalen-2-ol (12d)

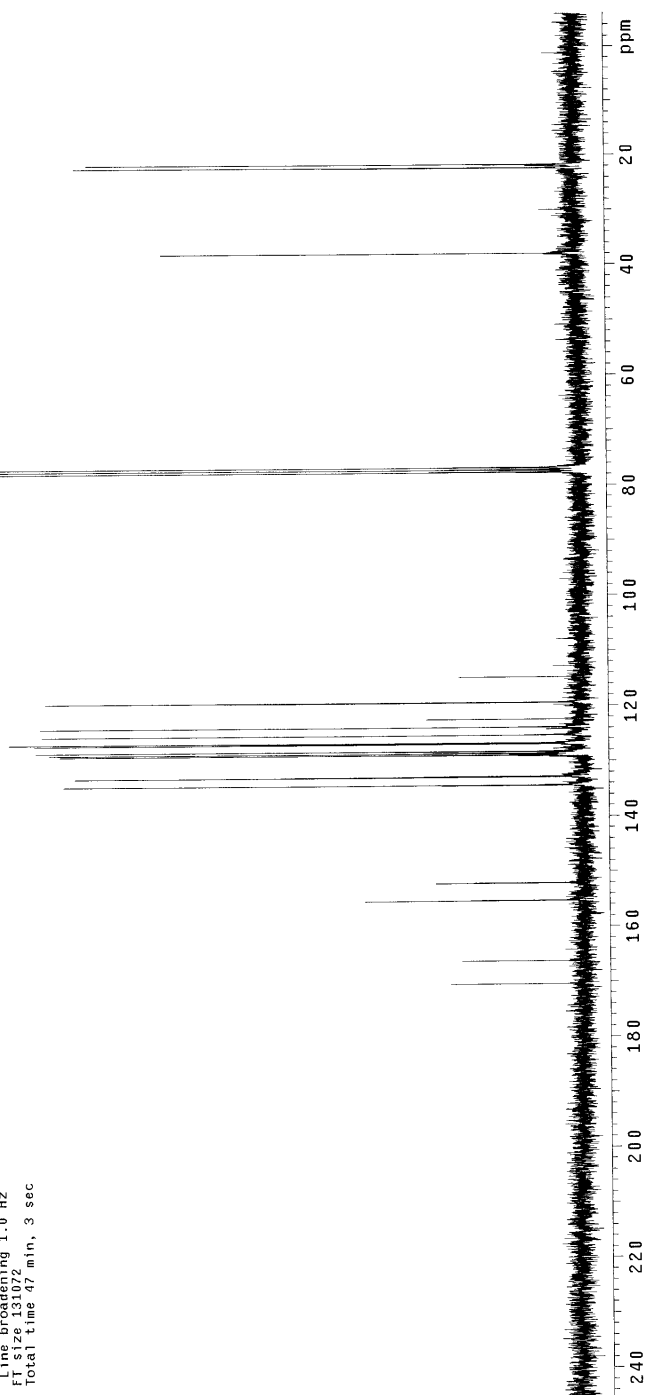
Pulse Sequence: s2pul
Solvent: cdcl3
Temp.: 30.0 C / 303.1 K
Sample #26
File: P_Guiry_26_03
Date: Nov 2, 2001
INOVA-300 "sunucd300"
PULSE SEQUENCE
Relax delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.195 sec
Width 25000.0 Hz
Sweep rate 107.5
OBSERVE C13, 25.4070323 MHz
DECOUPLE H1, 259.8897221 MHz
Power 38 dB
continuously on
WDW: EM
AQ: 600.000000
Line broadening 1.0 Hz
FT size 65536
Total time 37 min, 41 sec



¹H NMR of 1-(2-Isopropyl-quinazolin-4-yl)-naphthalen-2-ol (12e)

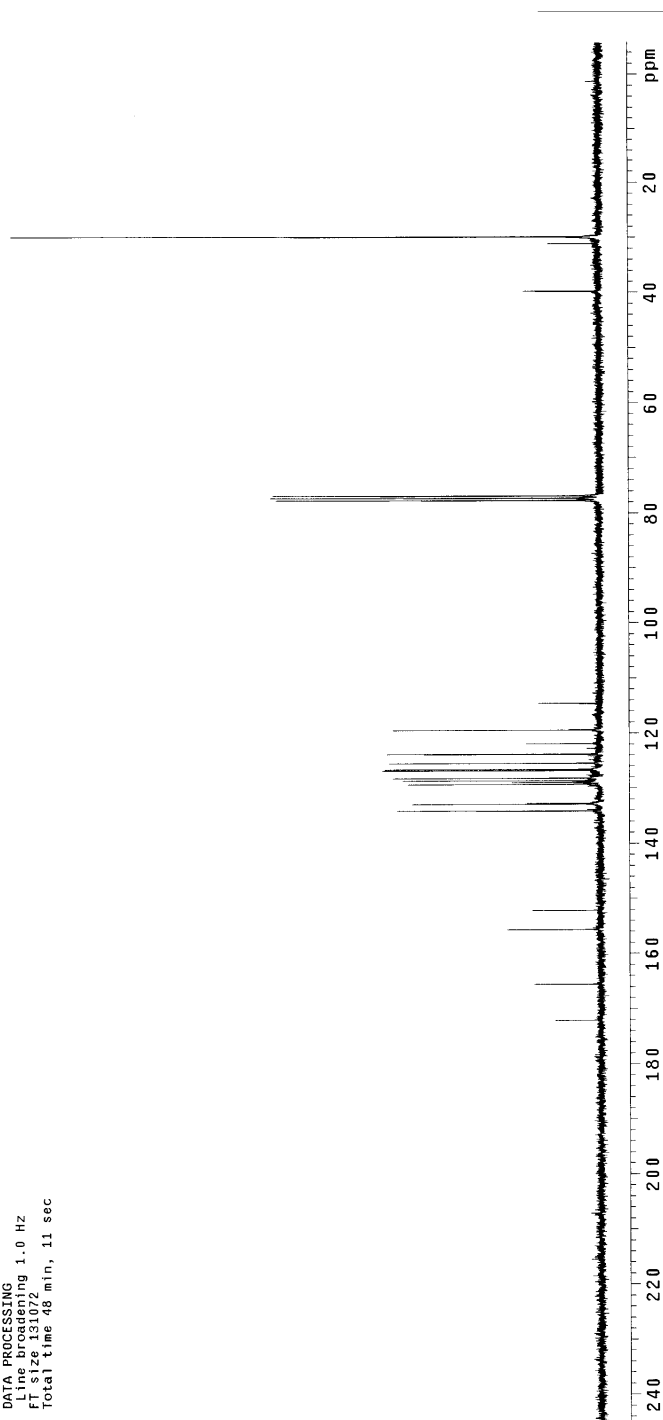
¹³C NMR of 1-(2-Isopropyl-quinazolin-4-yl)-naphthalen-2-ol (12e)

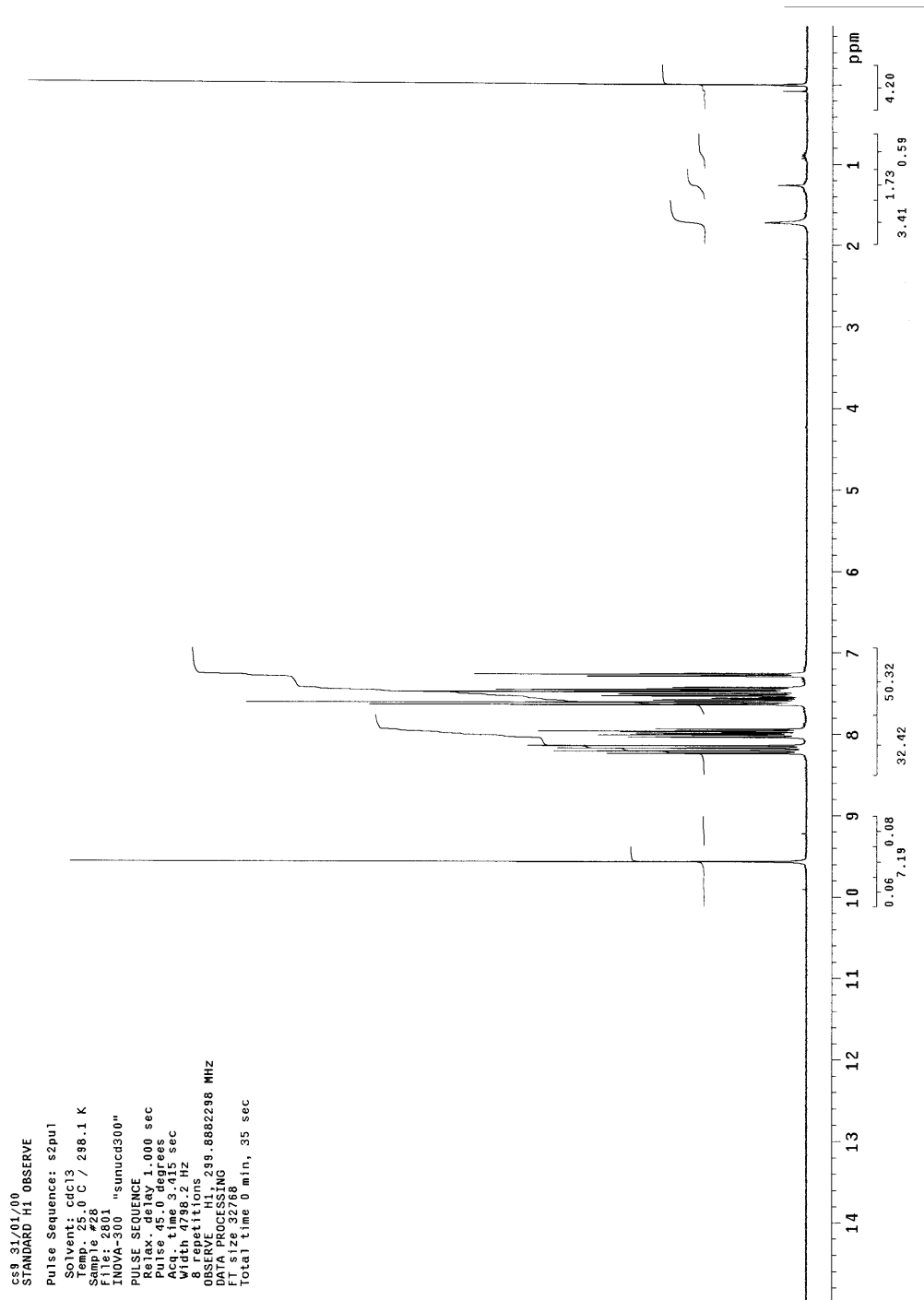
Pulse Sequence: s2pu1
Solvent: cdcl3
Temp: 300.2 K / 303.1 K
Sample #18
File: 1802
INDVA=300 "sunucd300"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.818 sec
Acq. time 1.852 sec
1000 repetitions
OBSERVE C13, 75.4064355 MHZ
DECOUPLE H1, 289.8897220 MHZ
Power 37 dB
Waltz16 on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 47 min, 3 sec

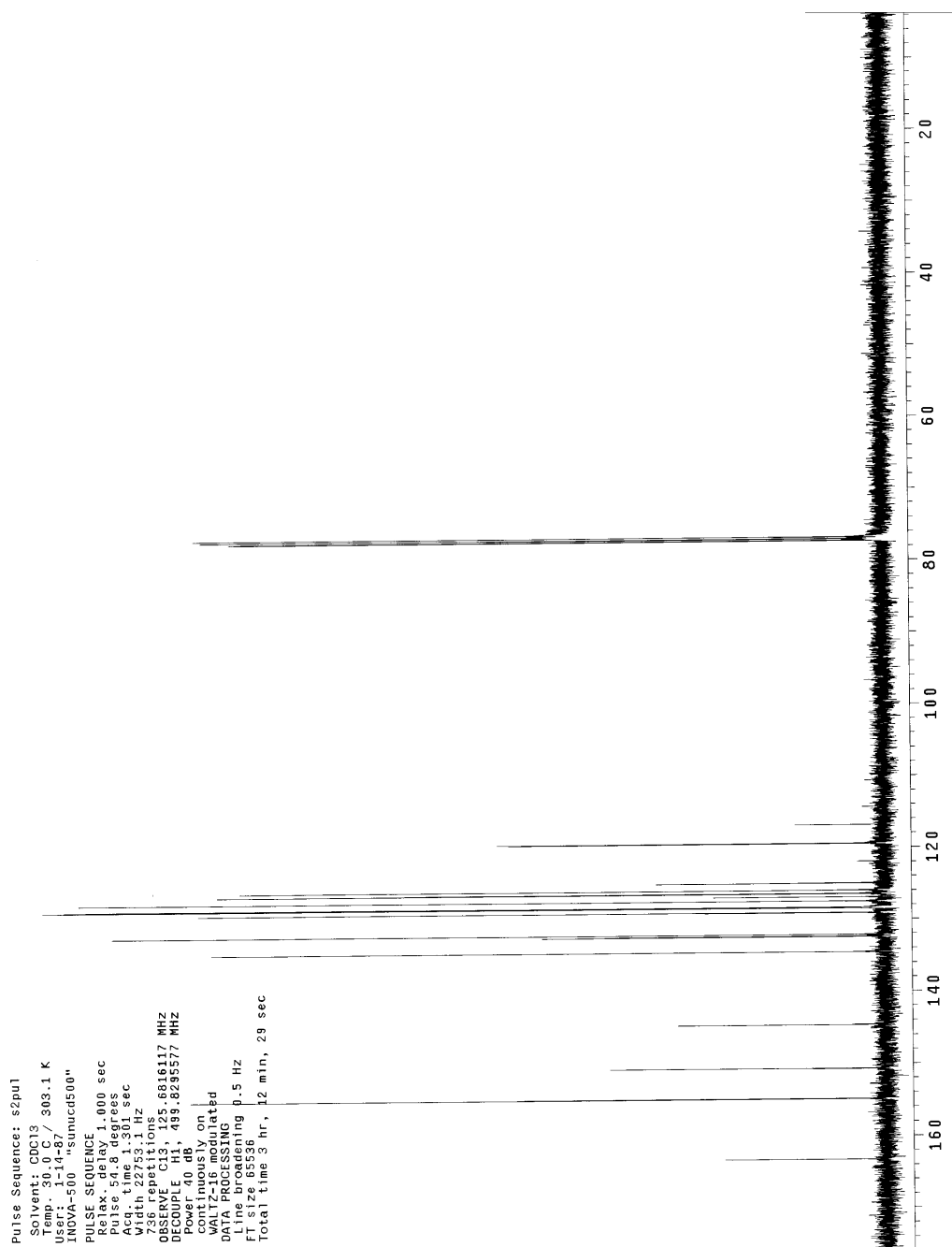


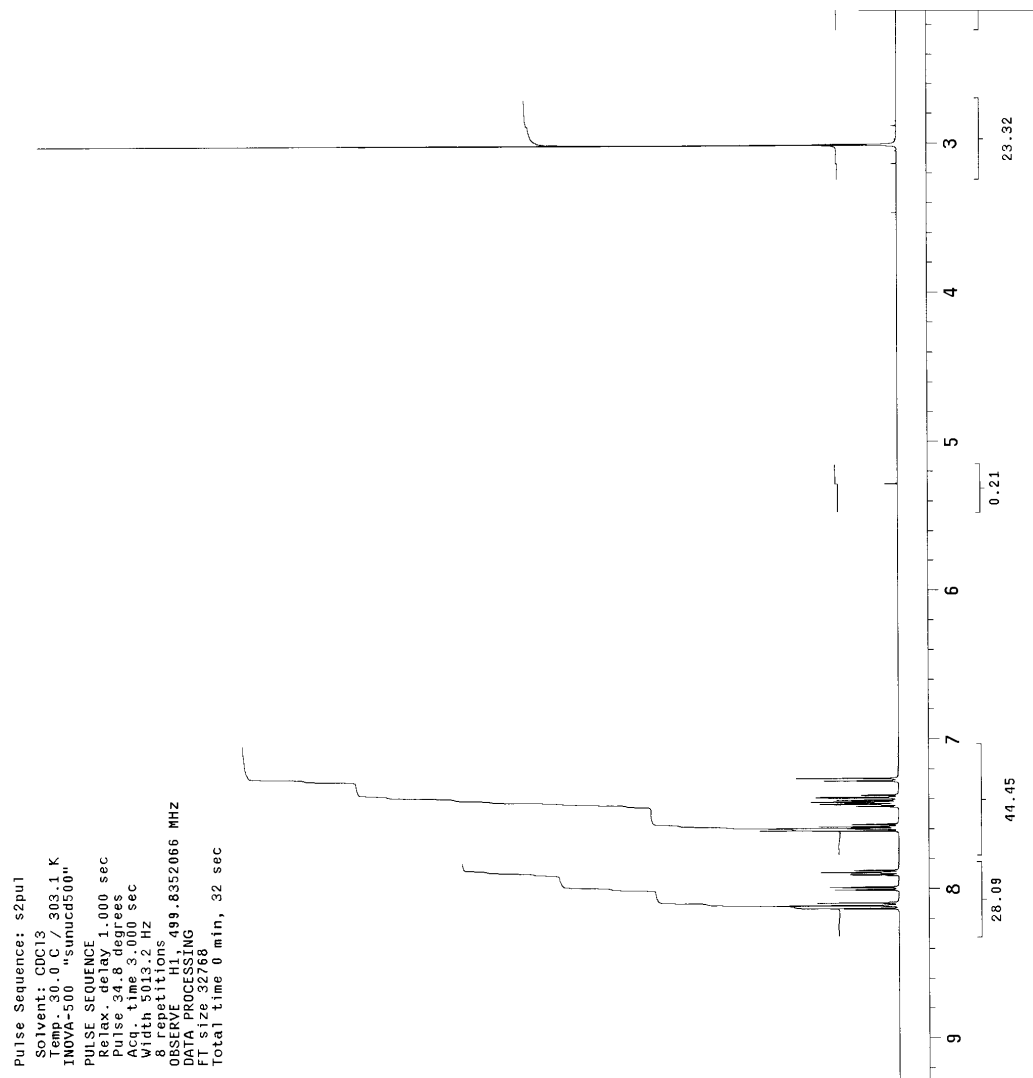
^{13}C NMR of 1-(2-*tert*-Butyl-quinazolin-4-yl)-naphthalen-2-ol (12f)

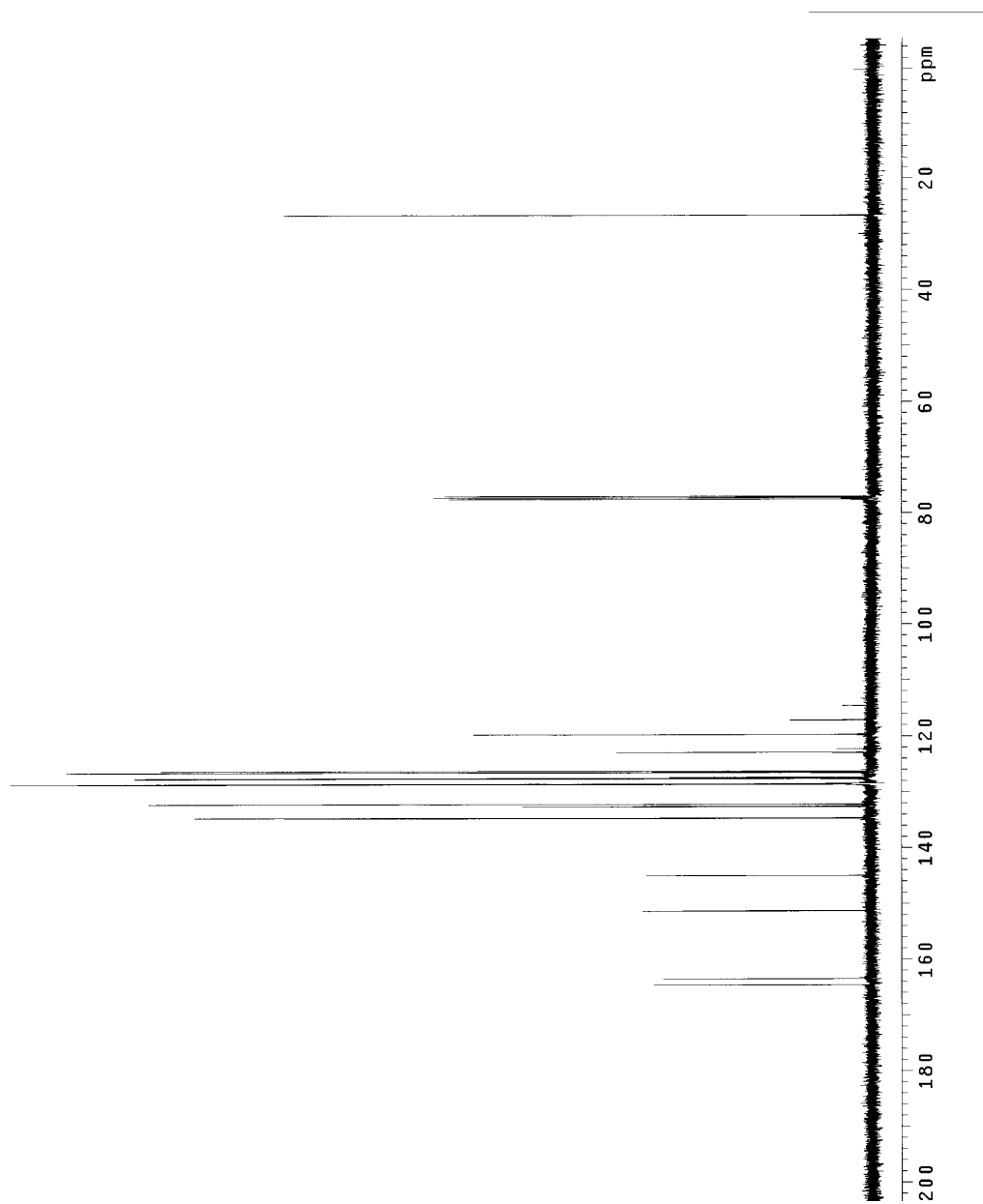
Pulse Sequence: s2pu1
Solvent: cdcl3
Temp: 30.0 C / 303.1 K
Sample: 722
INVA-300 "snuucd300"
PULSE SEQUENCE
Relax delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18952.9 Hz
OBSERVE CH: 13
DECOUPLE H1, 299.8897220 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
AQ: 0.0000000000000000
FI Size: 131072
Total time 48 min, 11 sec

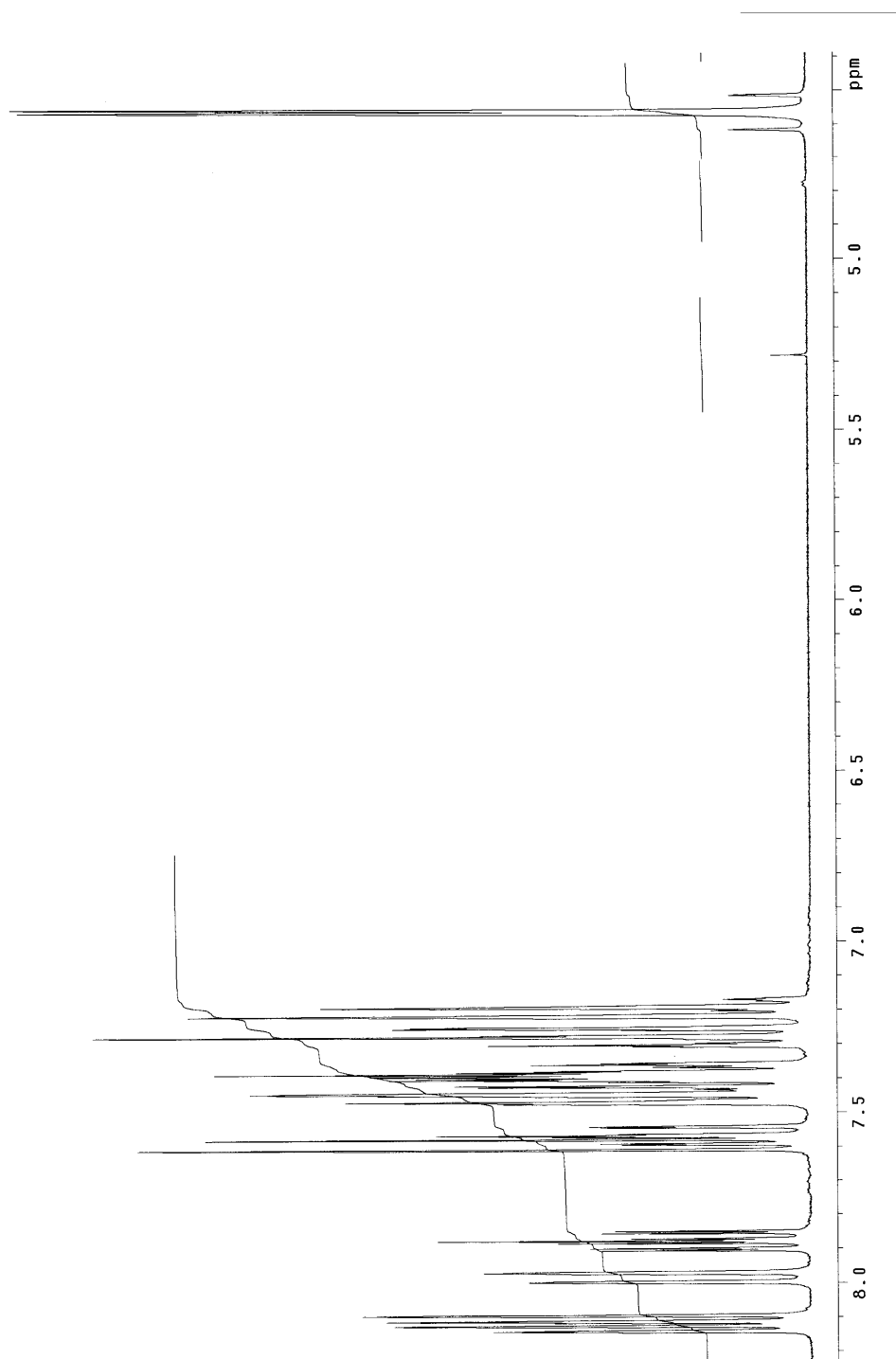


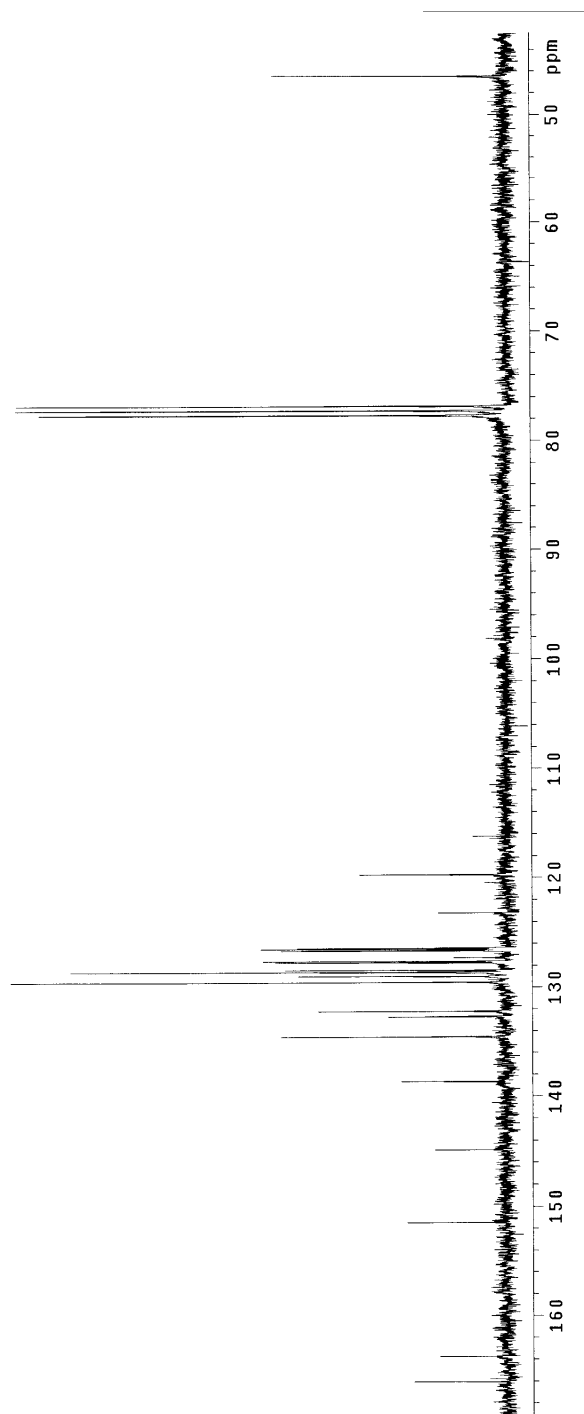
¹H NMR of 1-(Quinazolin-4-yl)-2-naphthyl(trifluoromethyl)sulfonate (13a)

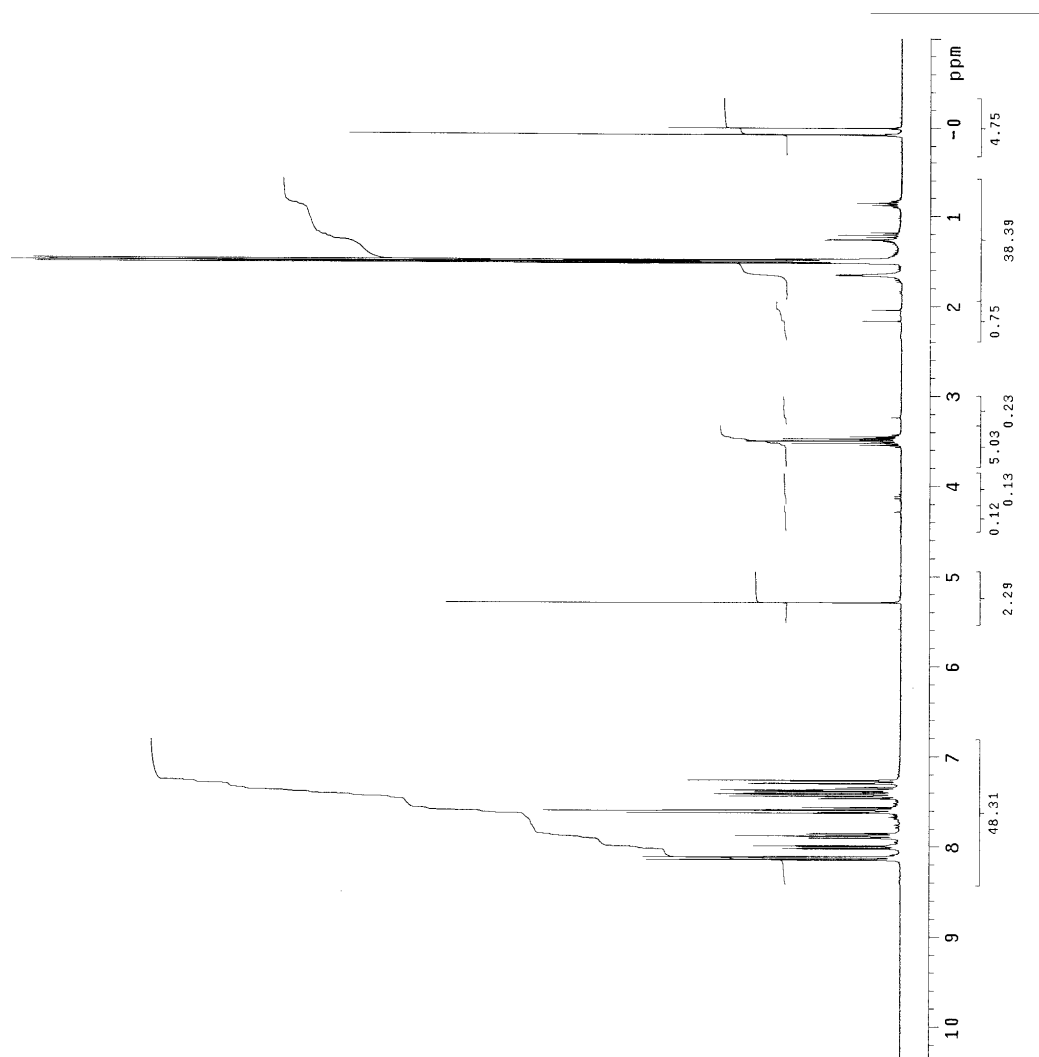
¹³C NMR of 1-(Quinazolin-4-yl)-2-naphthyl(trifluoromethyl)sulfonate (13a)

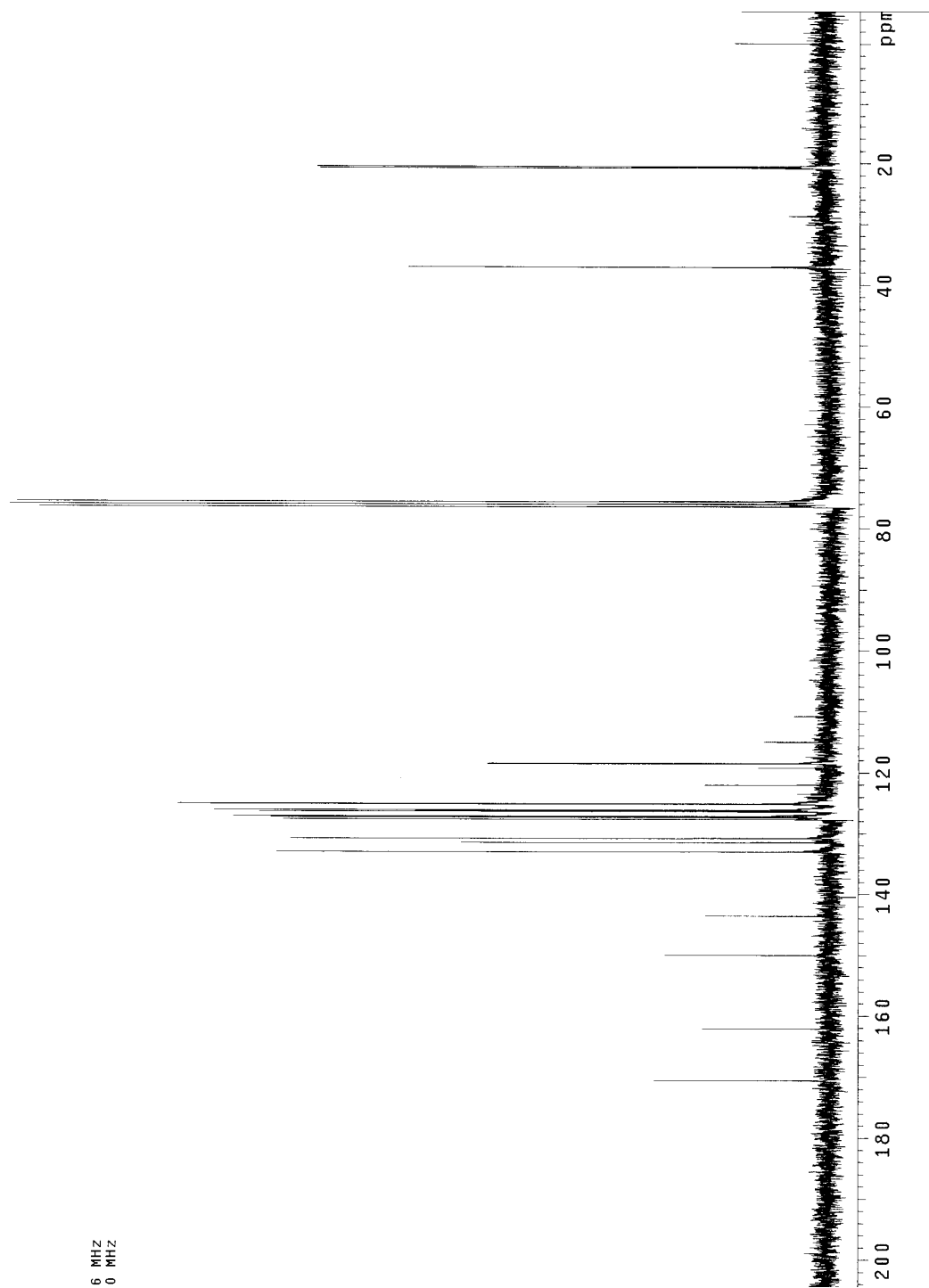
^1H NMR of 1-(2-Methylquinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate (13b)

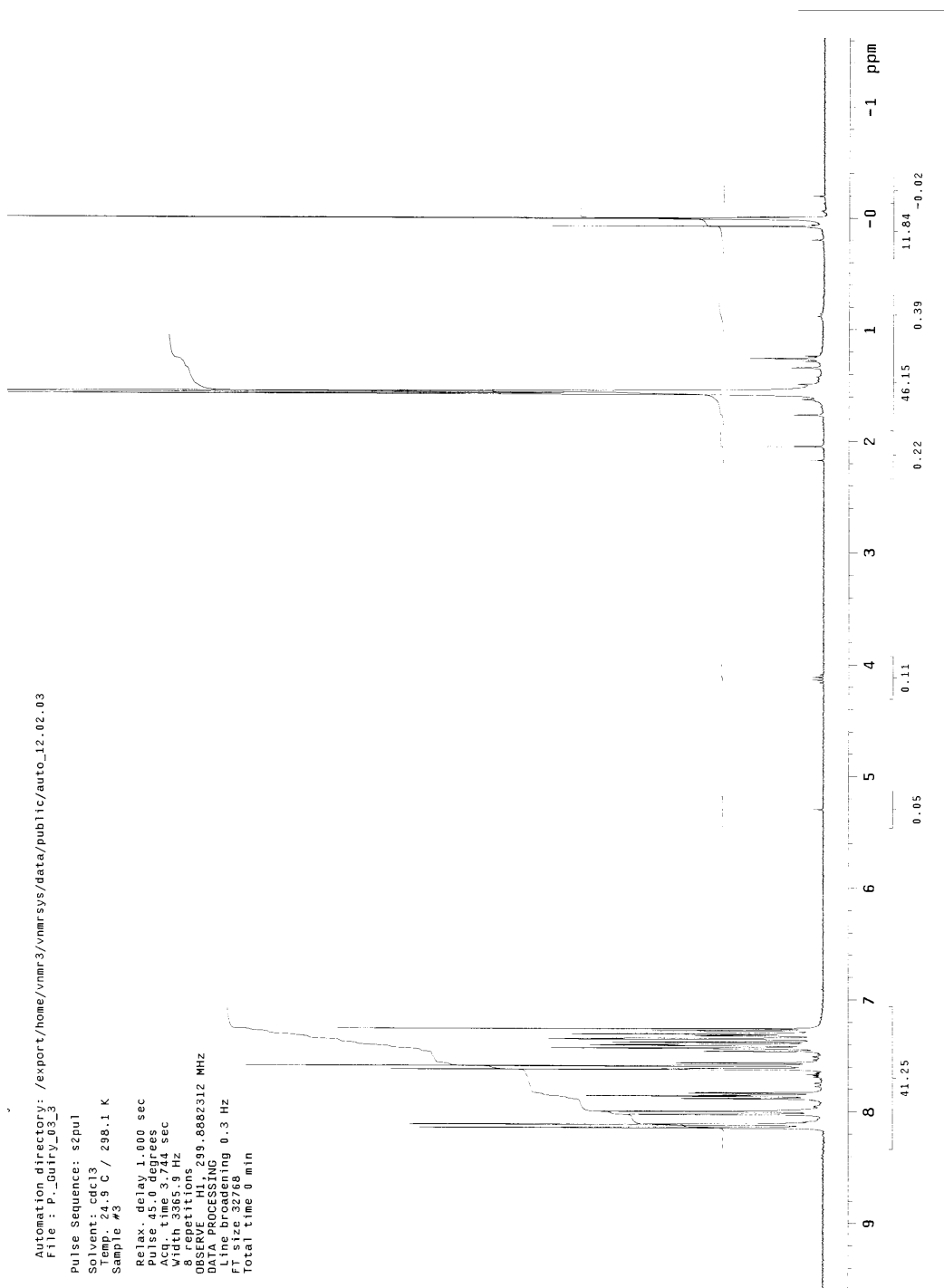
^{13}C NMR of 1-(2-Methylquinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate (13b)

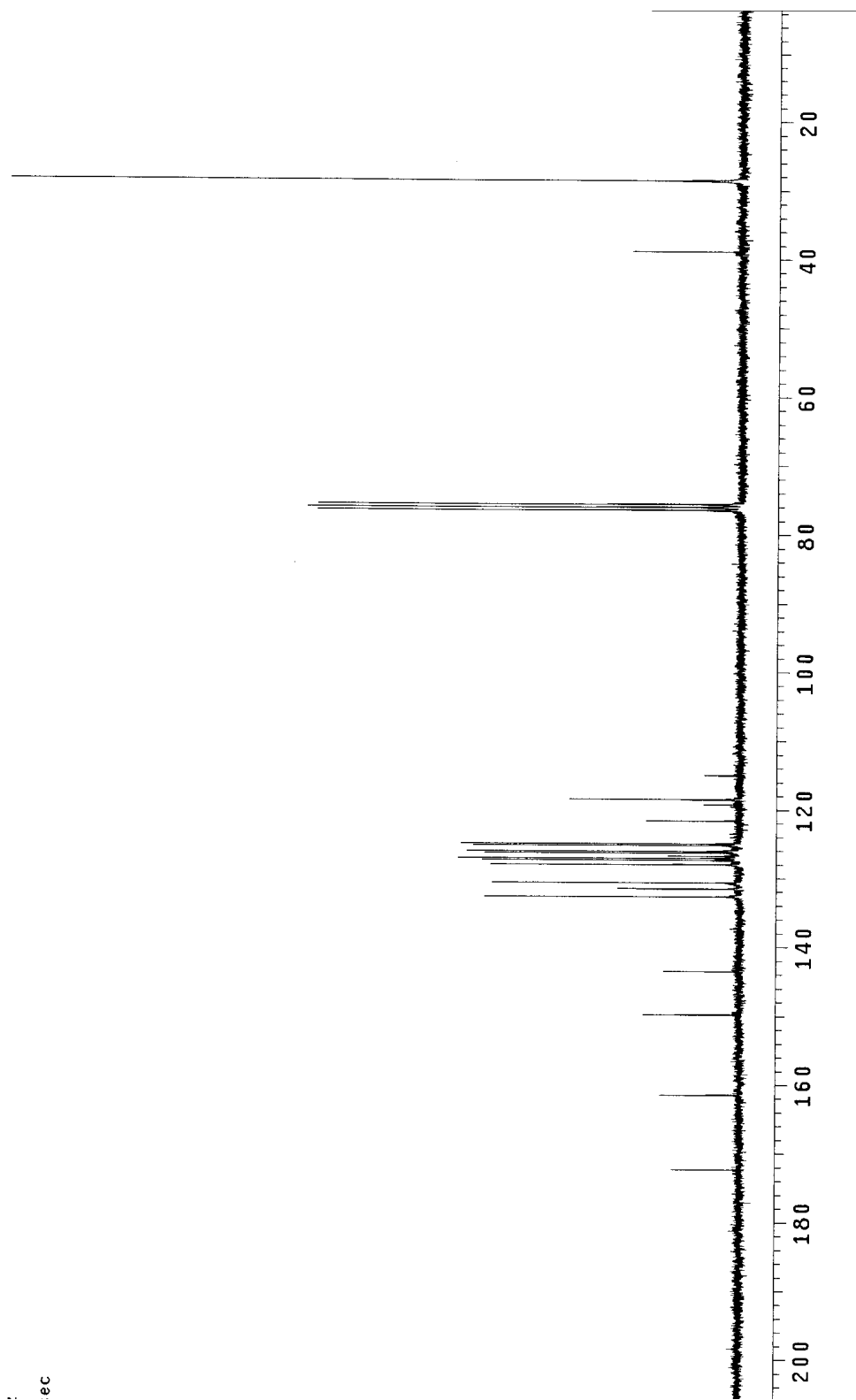
¹H NMR of 1-(2-Phenylmethyl-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate (13d)

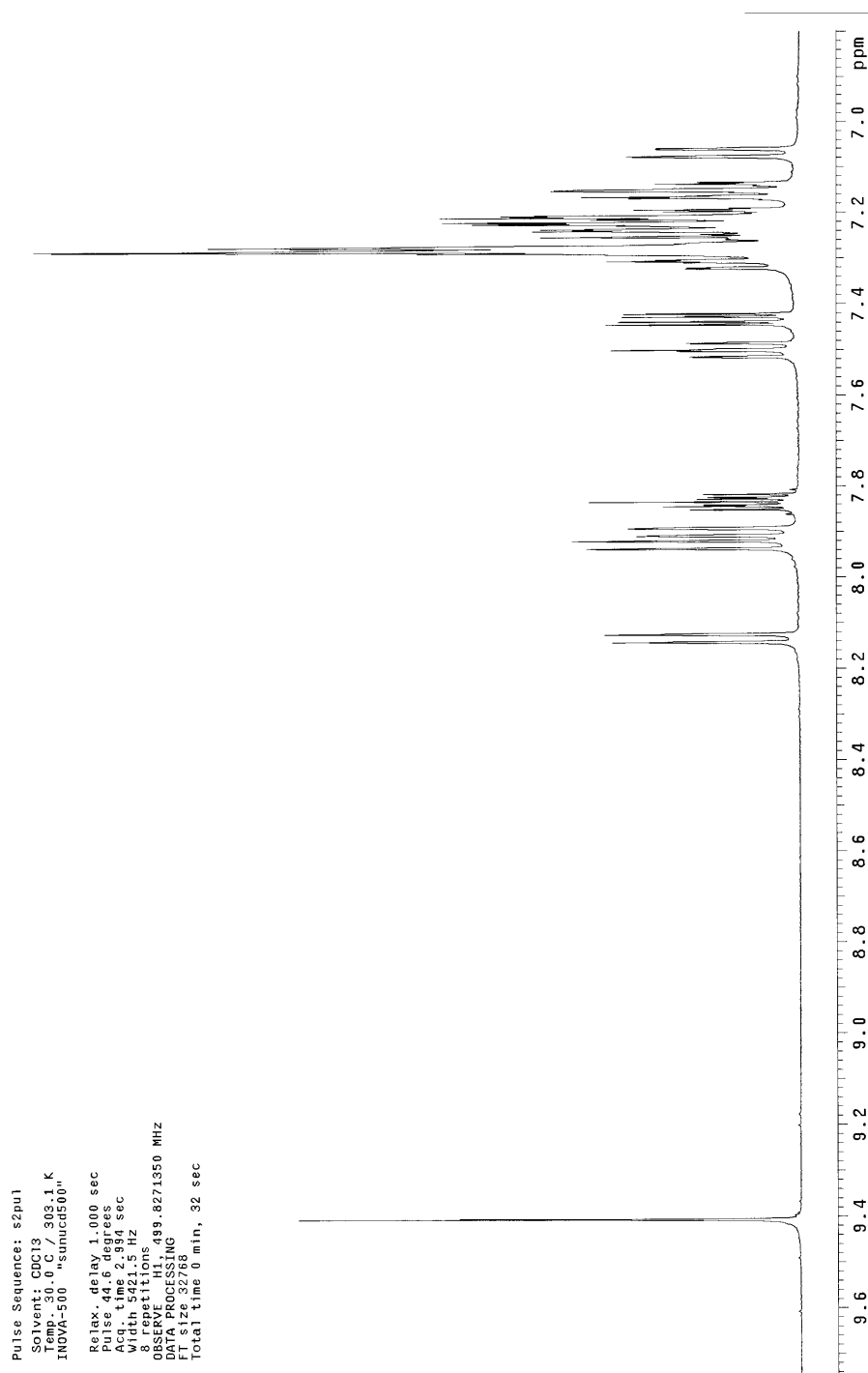
^{13}C NMR of 1-(2-Phenylmethyl-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate (13d)

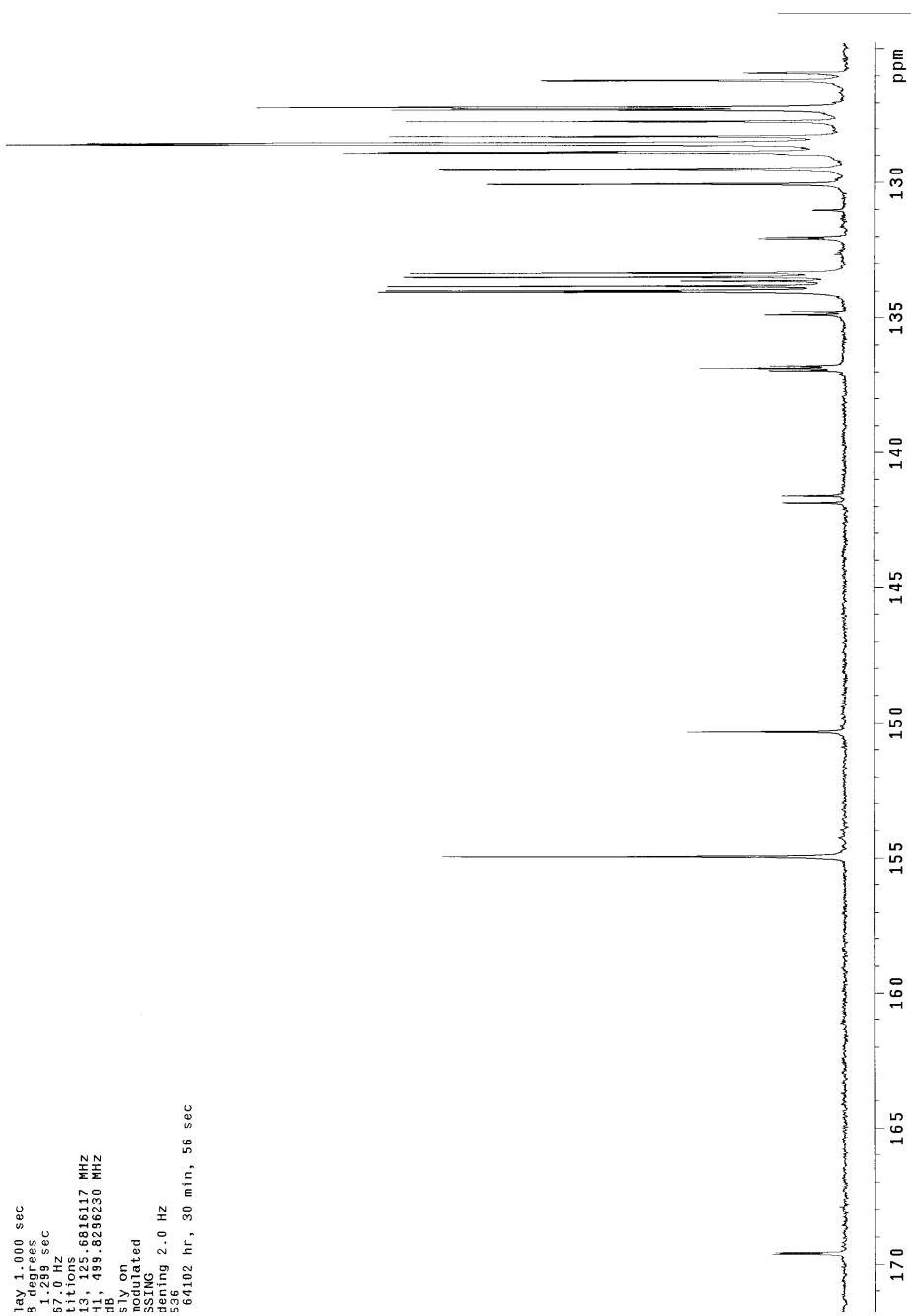
^1H NMR of 1-(2-Isopropyl-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate (13e)

^{13}C NMR of 1-(2-Isopropyl-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate (13e)

¹H NMR of 1-(2-*tert*-Butyl-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate (13f)

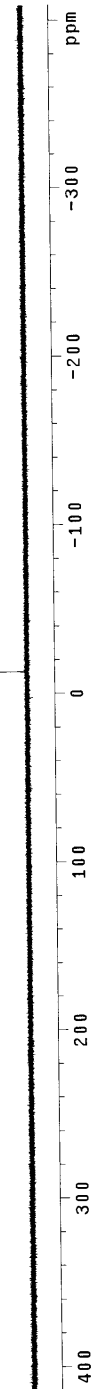
^{13}C NMR of 1-(2-*tert*-Butyl-quinazolin-4-yl)-2-naphthyl (trifluoromethyl)sulfonate (13f)

¹H NMR of (R,S)-Diphenyl[1-(quinazolin-4-yl)(2-naphthyl)]phosphine (14a)

^{13}C NMR of (*R,S*)-Diphenyl[1-(quinazolin-4-yl)(2-naphthyl)]phosphine (14a)

³¹P NMR of (*R,S*)-Diphenyl[1-(quinazolin-4-yl)(2-naphthyl)]phosphine (14a)

CS-7
Pulse Sequence: s2pul
Solvent: CDCl3
Acquisition Temperature: 300.15 K
INOVA-300 "sumncd300"
PULSE SEQUENCE
Pulse: 50.0 degrees
Acq. time 1.600 sec
Width 100.0 kHz
48 repetitions
OBSERVE P31, 221.366102 MHz
DETECT P31, 239.869720 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
File: 500028
Total time 44 hr, 41 min, 23 sec



¹H NMR of (R,S)-Diphenyl[1-(2-methylquinazolin-4-yl)(2-naphthyl)]phosphine (14b)

R(Me)PPH2
P. Lacey

Pulse Sequence: s2p1

Solvent: CDCl3

Temp: 30.0 C / 303.1 K

INOVA-500 "SunnuCD500"

Relax. delay: 1.000 sec

Acq. time: 2.997 sec

Width: 4813.6 Hz

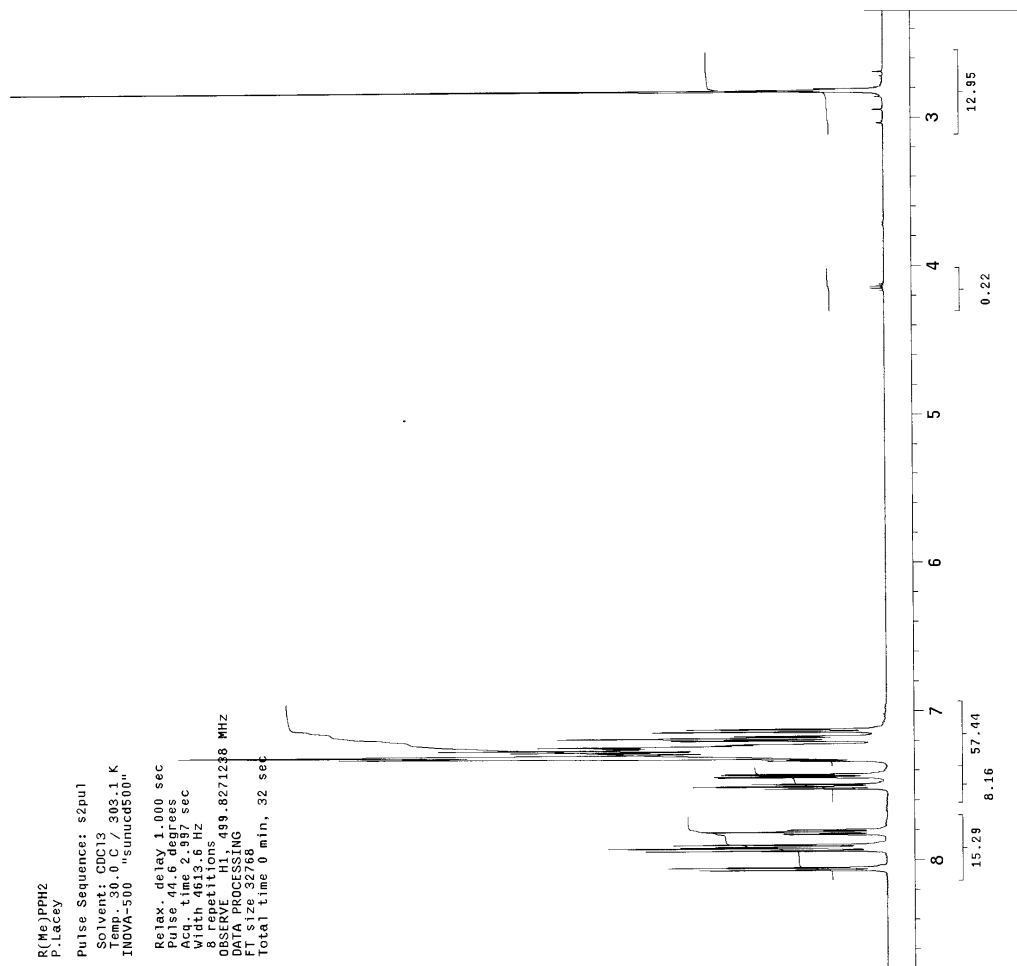
8 repetitions

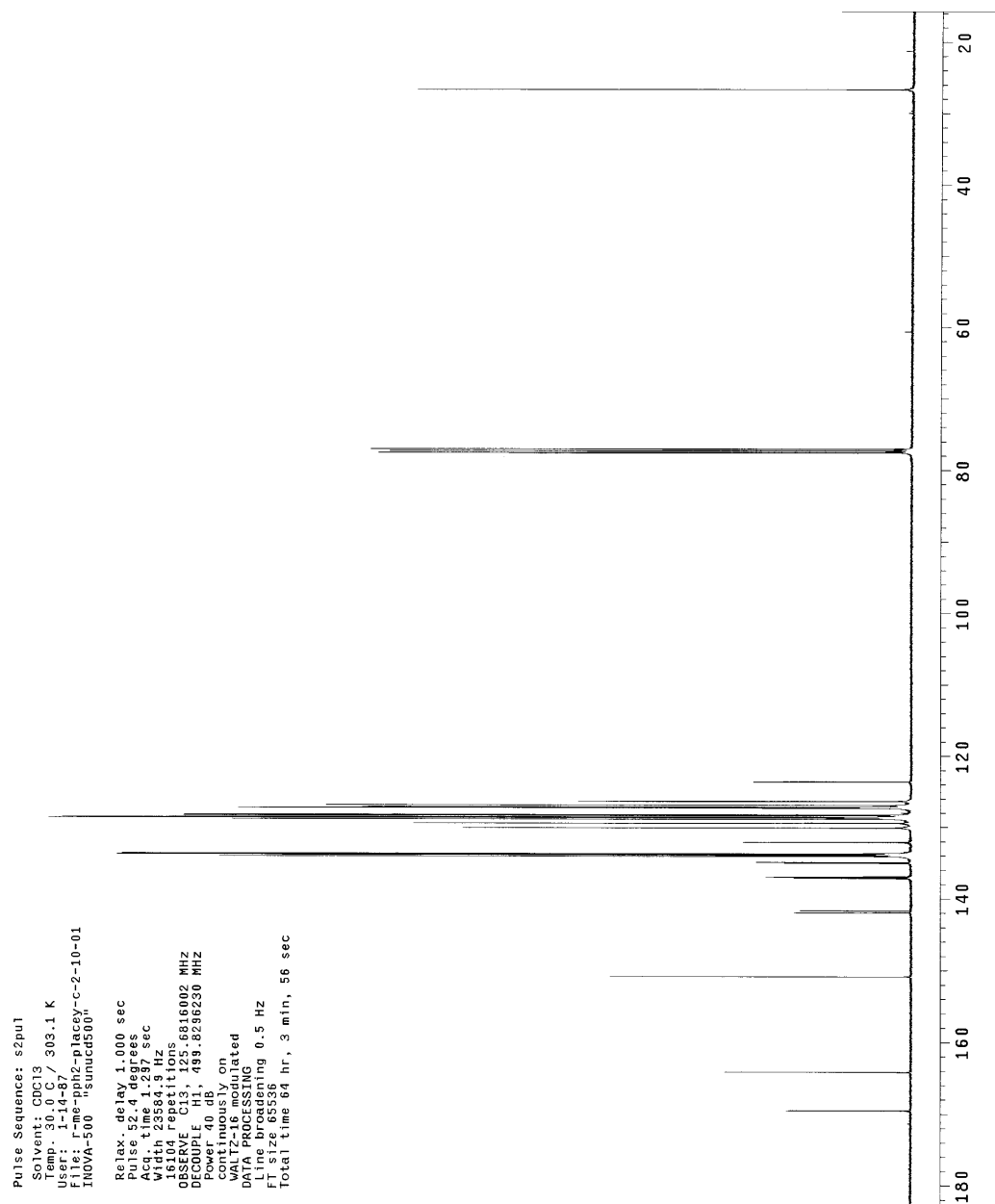
OBSERVE F1: 499.8271238 MHz

PROBHD: RUC3268

FT1: 3268

Total time: 0 min, 32 sec

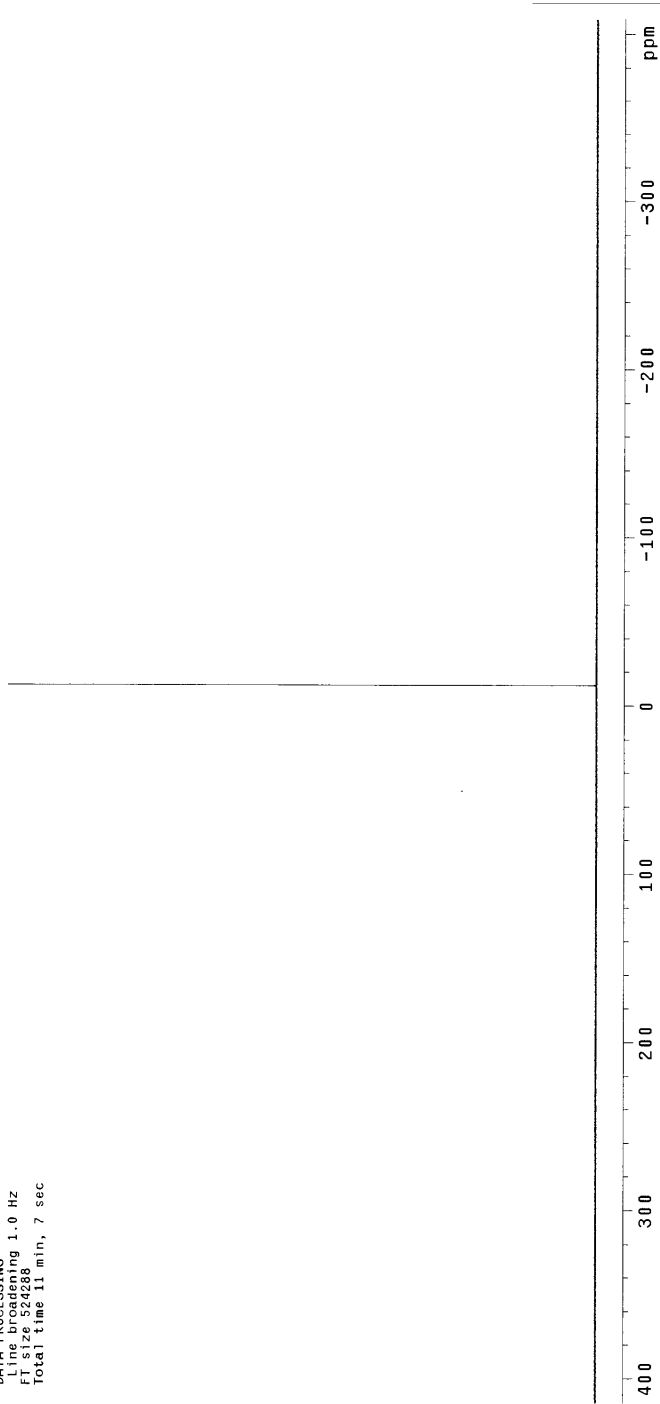


¹³C NMR of (R,S)-Diphenyl[1-(2-methylquinazolin-4-yl)(2-naphthyl)]phosphine (14b)

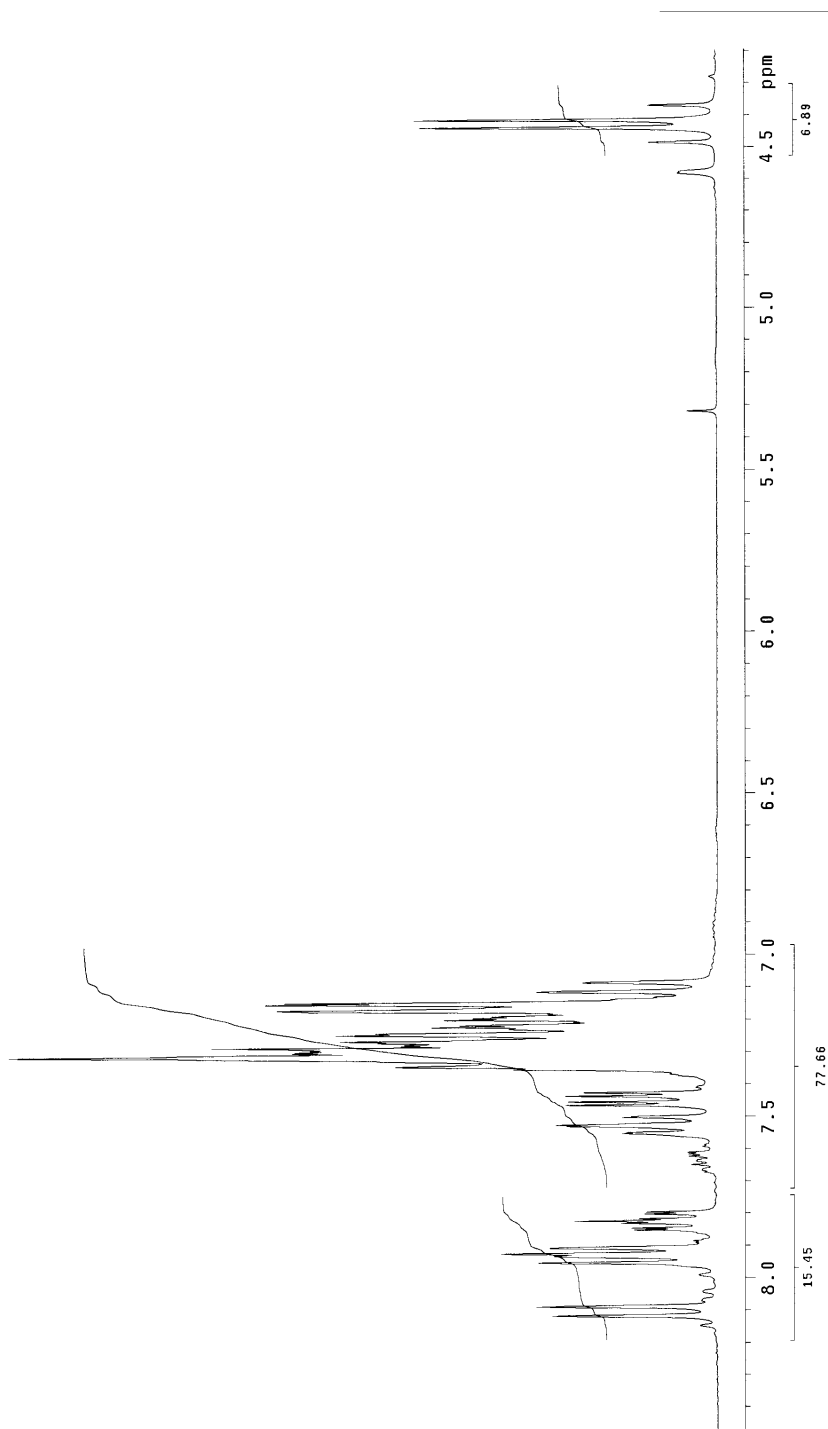
³¹P NMR of (R,S)-Diphenyl[1-(2-methylquinazolin-4-yl)(2-naphthyl)]phosphine (14b)

Pulse Sequence: s2pu1
 Solvent: cdcl3
 Temperature: 30.0 C / 303.1 K
 Sample #: 1
 File: 0202
 INOVA-300 "sunucd300"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 35.0 degrees
 Acq. time 1.000 sec
 Wdth 100.0 kHz
 256 Repetitions
 OBSERVE P31, 121.3968422 MHZ
 DECOUPLE H1, 299.8897220 MHZ
 Power 38 dB
 Channels On
 WAIT 116 seconds
 DATA PROCESSING
 Line broadening 1.0 Hz
 FI size 524288
 Total time 11 min, 7 sec

INDEX 1
 FREQUENCY PPM -1473.275
 HEIGHT 106.0

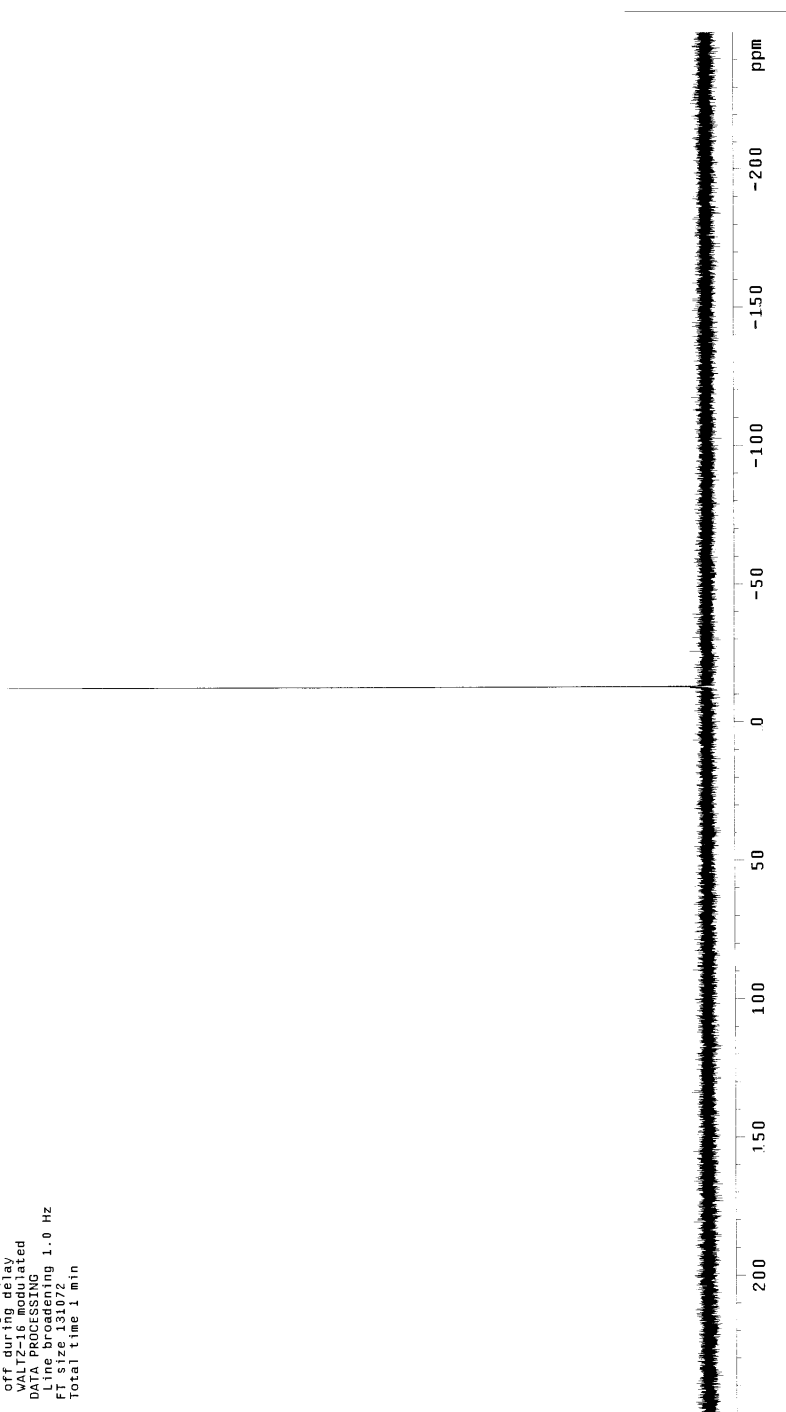


**^1H NMR of (*R,S*)-Diphenyl(1-(2-phenylmethyl-quinazolin-4-yl)
(2-naphthyl)phosphine (14d)**

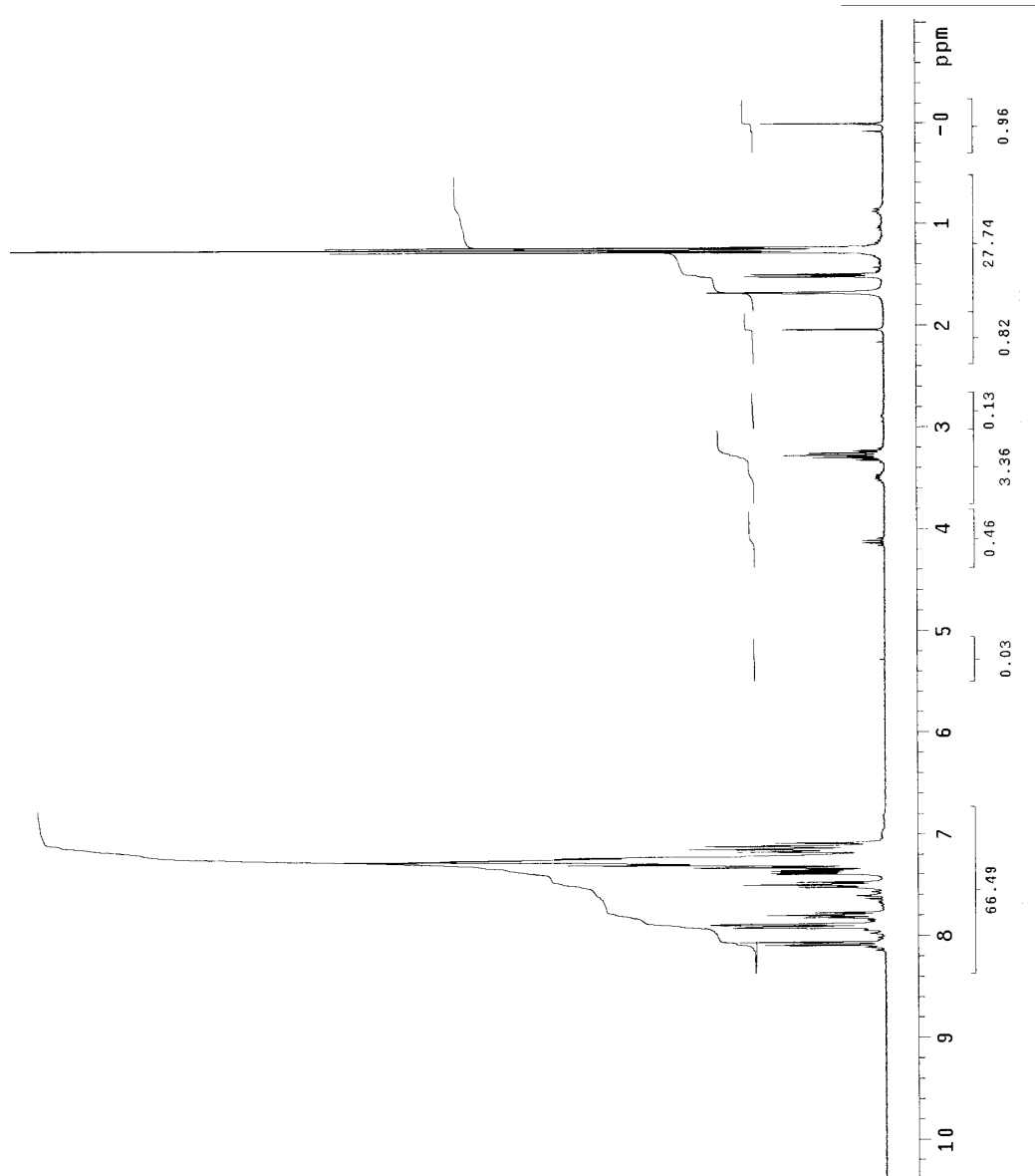


**^{31}P NMR of (*R,S*)-Diphenyl(1-(2-phenylmethyl-quinazolin-4-yl)
(2-naphthyl)phosphine (14d)**

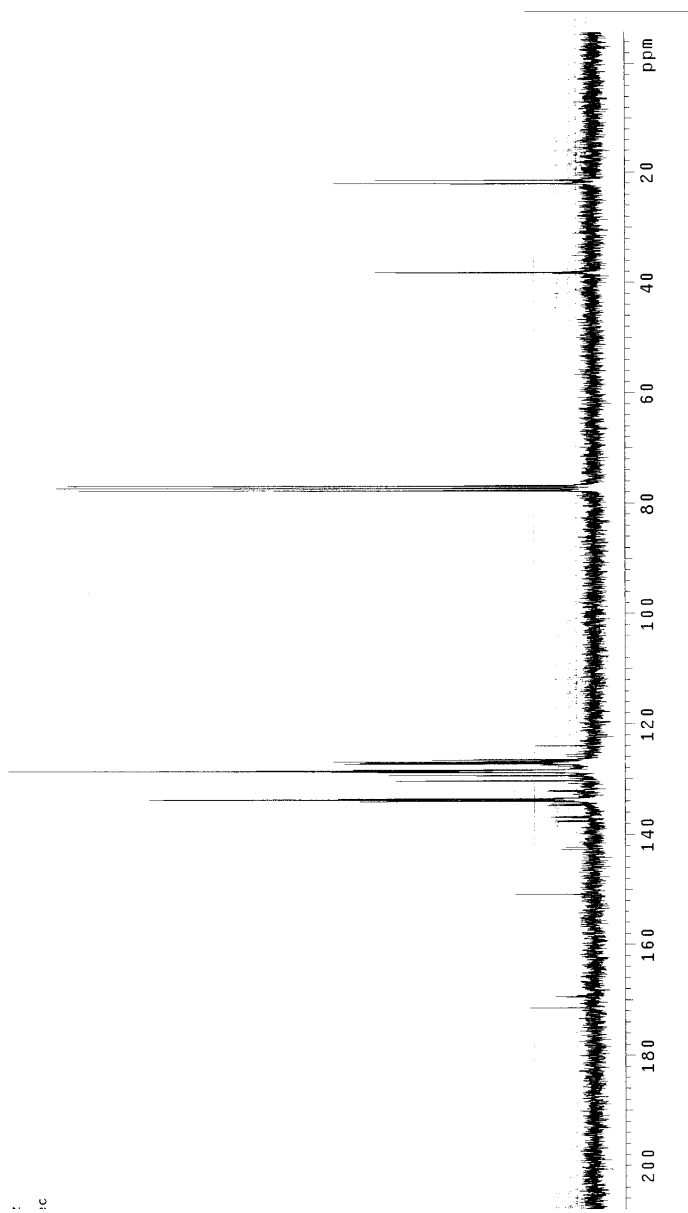
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 0.000 sec
Width 80698.0 Hz
64 repetitions
OBSERVE P31, 121.3968421 MHz
DECOUPLE H1, 299.8897221 MHz
Power 35.00 dB
during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 1 min



**¹H NMR of (*R,S*)-Diphenyl(1-(2-isopropyl-quinazolin-4-yl)
(2-naphthyl)phosphine (14e)**

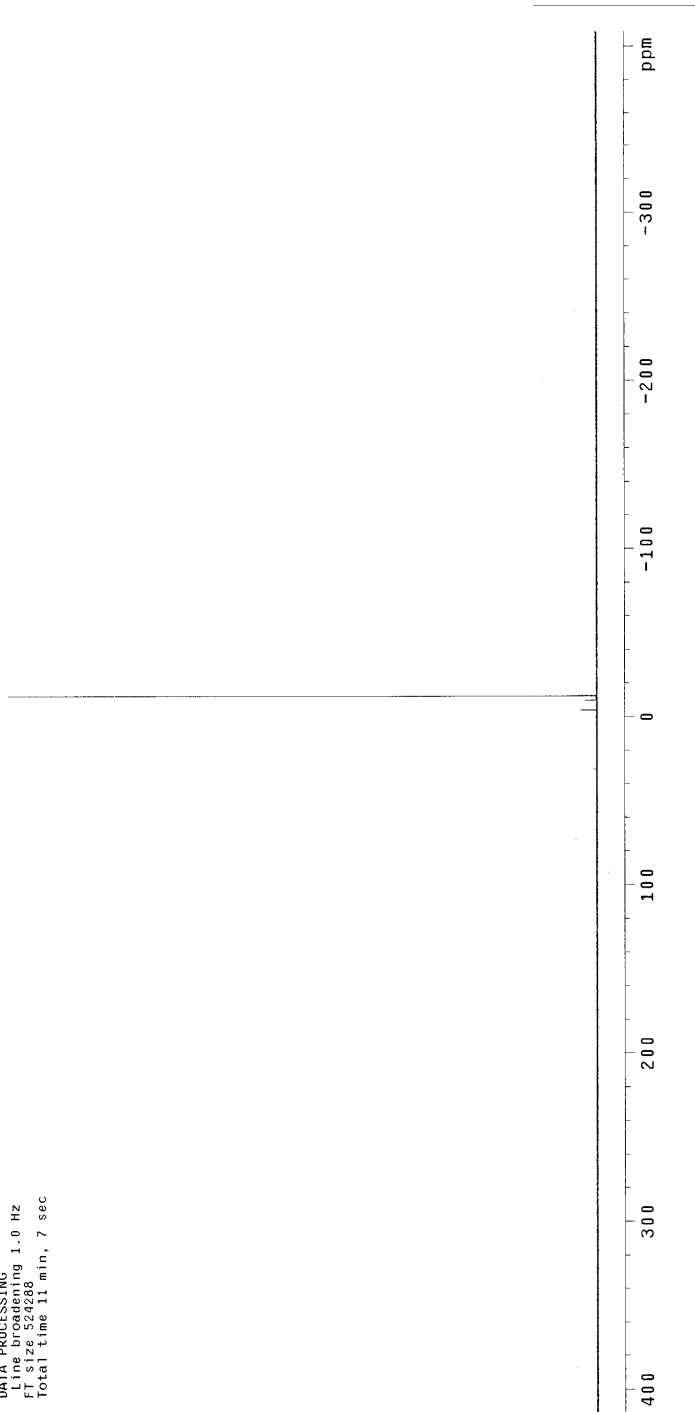


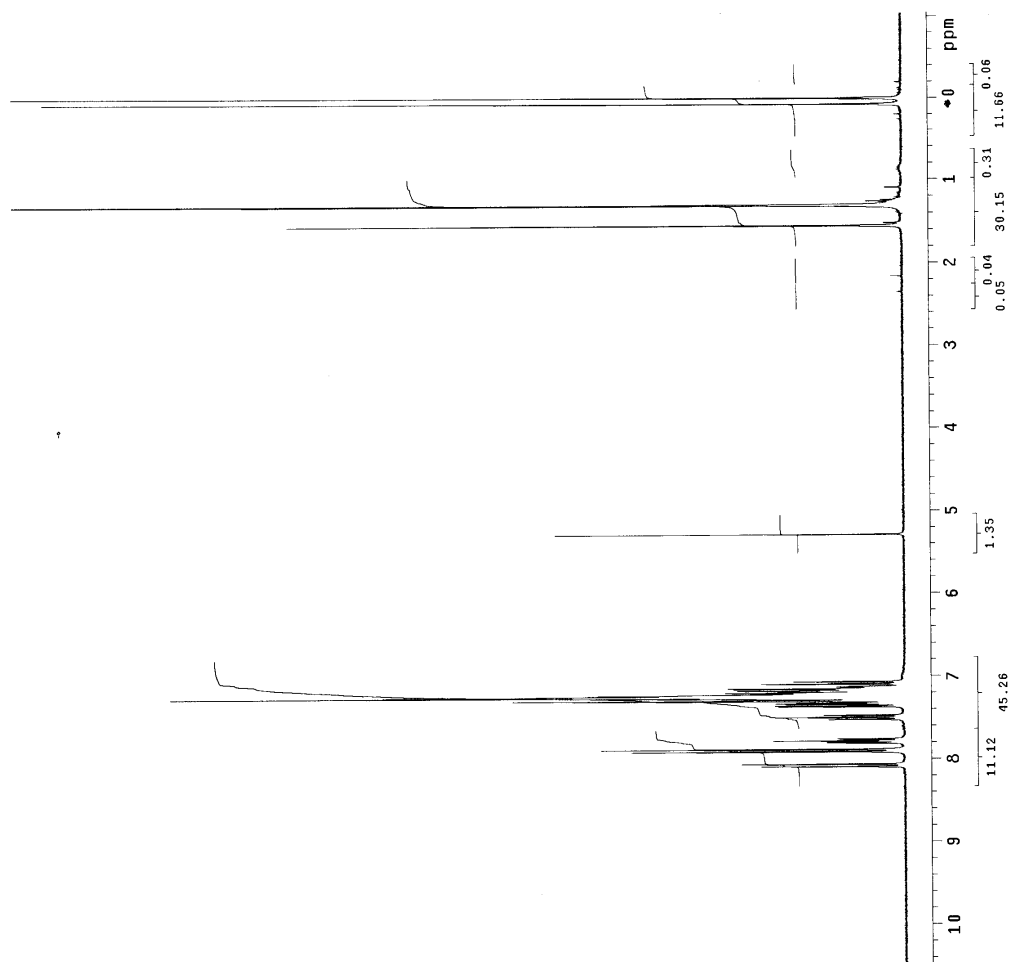
^{13}C NMR of (*R,S*)-Diphenyl(1-(2-isopropyl-quinazolin-4-yl)
(2-naphthyl)phosphine (14e)



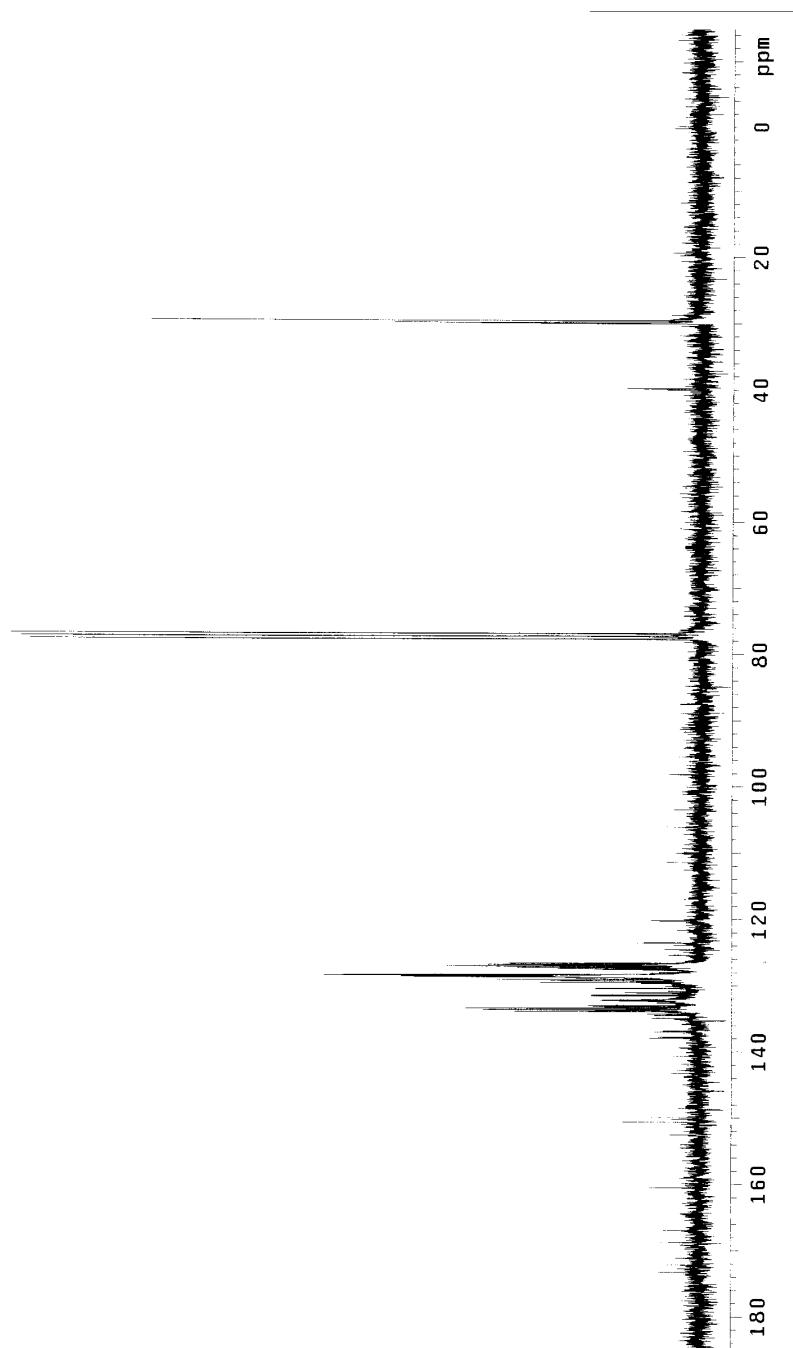
**³¹P NMR of (*R,S*)-Diphenyl(1-(2-isopropyl-quinazolin-4-yl)
(2-naphthyl)phosphine (14e)**

PULSE SEQUENCE
Pulse width 1.000 sec
Pulse delay 35.0 degrees
Acq. time 1.600 sec
Width 100.0 kHz
256 repetitions
DESCRIBE F31, 128, 3868492 MHZ
POWER 38 dB, 233.889720 MHZ
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT 56288
Total time 11 min, 7 sec



¹H NMR of (R,S)-Diphenyl(1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)phosphine (14f)

**^{13}C NMR of (*R,S*)-Diphenyl(1-(2-*tert*-butyl-quinazolin-4-yl)
(2-naphthyl)phosphine (14f)**

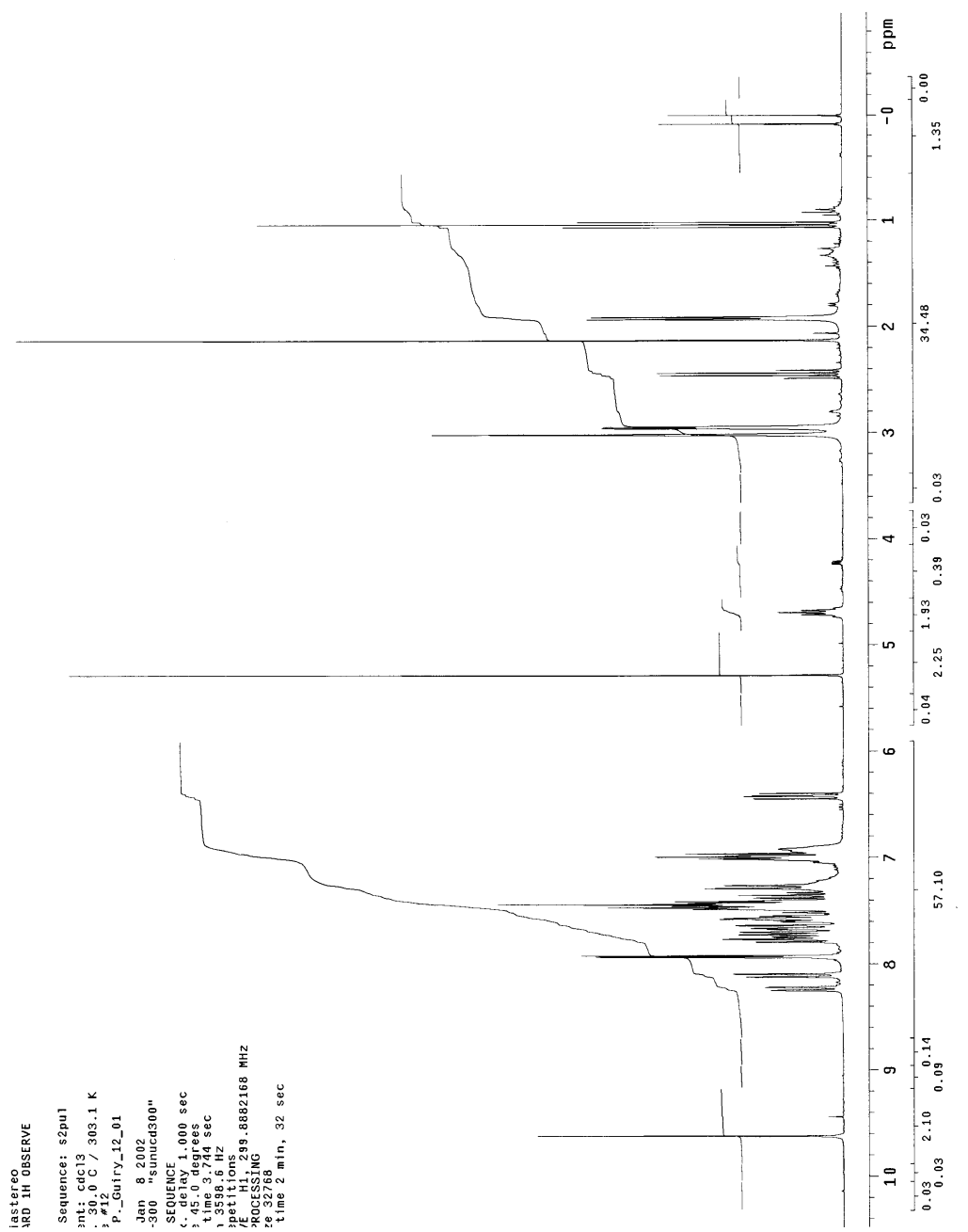


**³¹P NMR of (*R,S*)-Diphenyl(1-(2-*tert*-butyl-quinazolin-4-yl)
(2-naphthyl)phosphine (14f)**

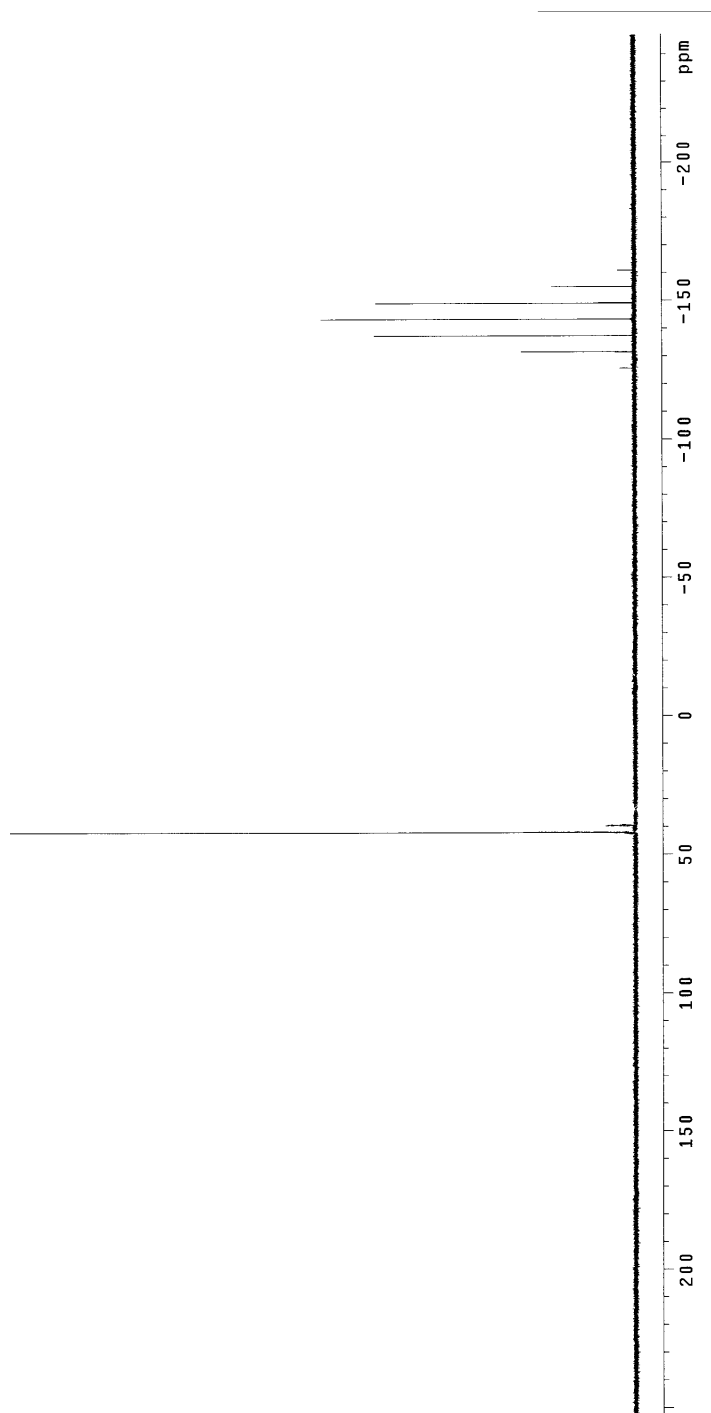
Acq. time 0.870 sec
Width 60698.0 Hz
256 repetitions
OBSERVE P21, 121.3968422 MHz
DECOUPLE H1, 299.8887221 MHz
Power 38 dB
C1 nucleus On
WALTZ16 decoupled
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 7 min, 43 sec

200 150 100 50 0 -50 -100 -150 -200 ppm

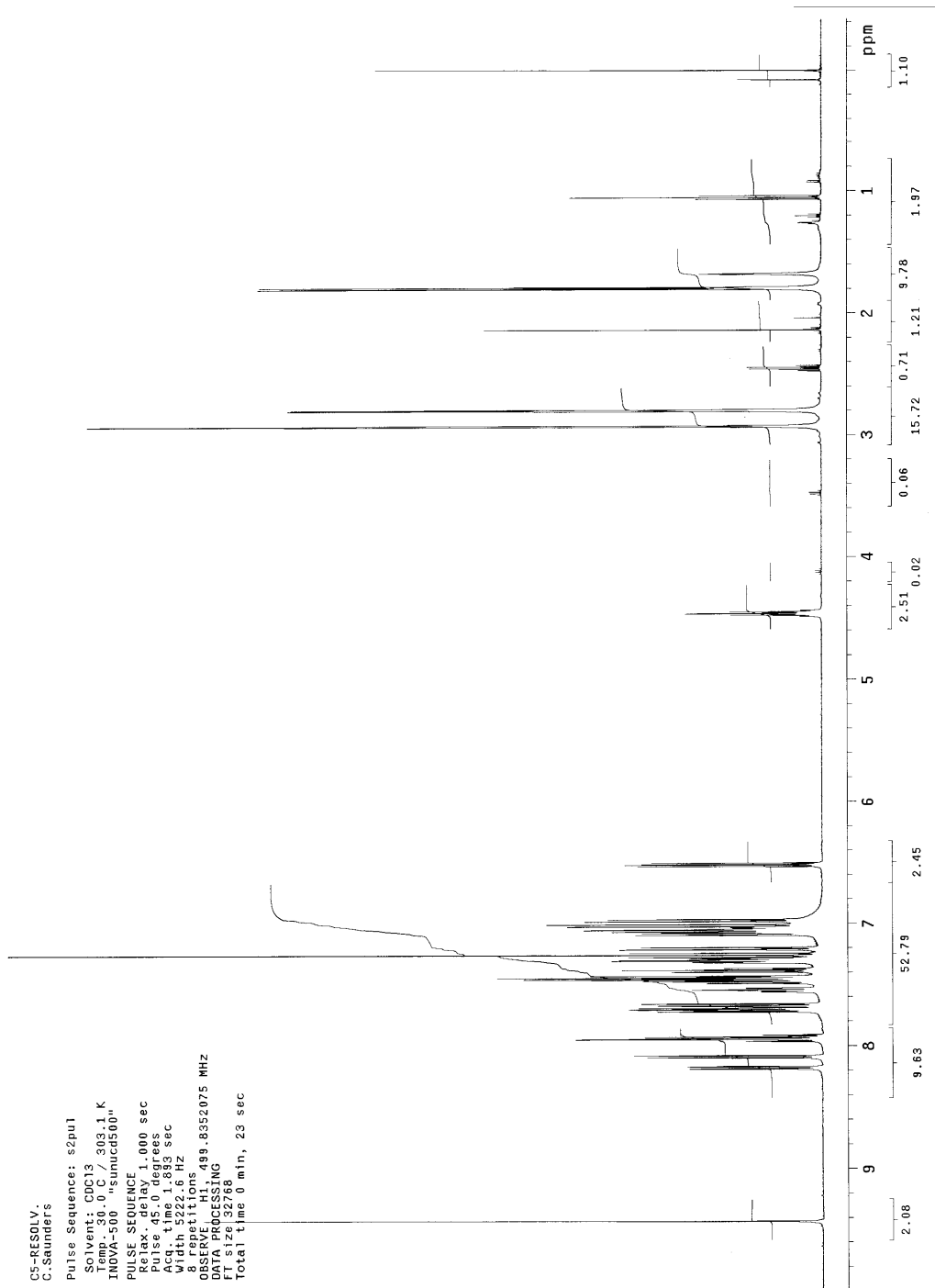
**¹H NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino-C₂,*N*]-
[1-(quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II) hexafluorophosphate (*R,R*)-(18a)**



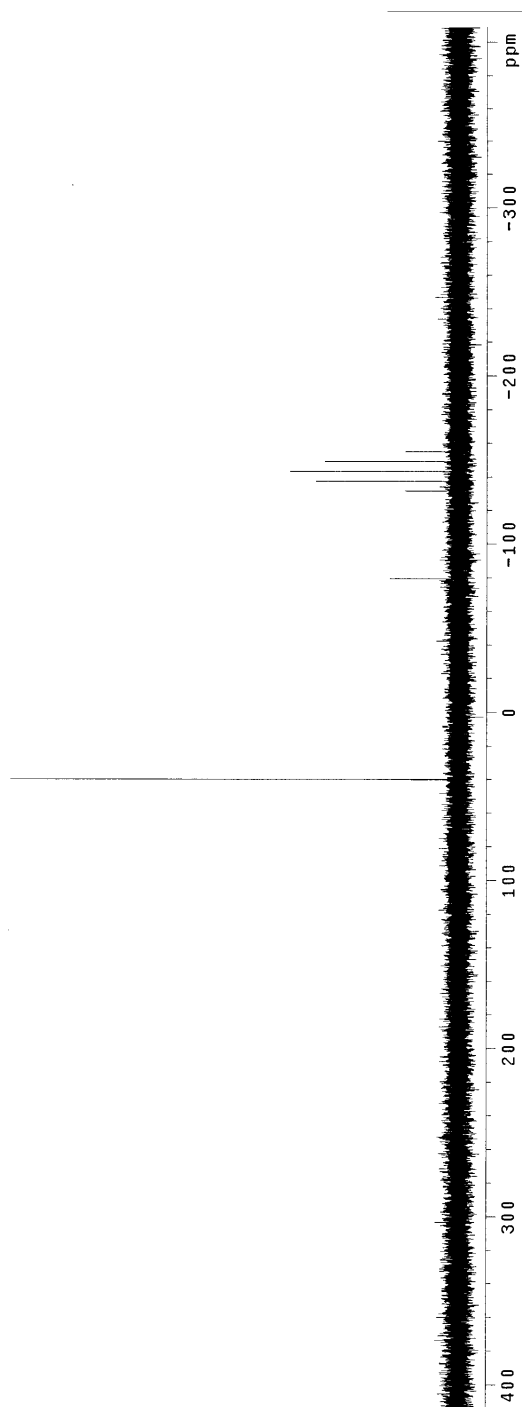
**^{31}P NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato- C_2,N]-
[1-(quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II) hexafluorophosphate (*R,R*)-(18a)**



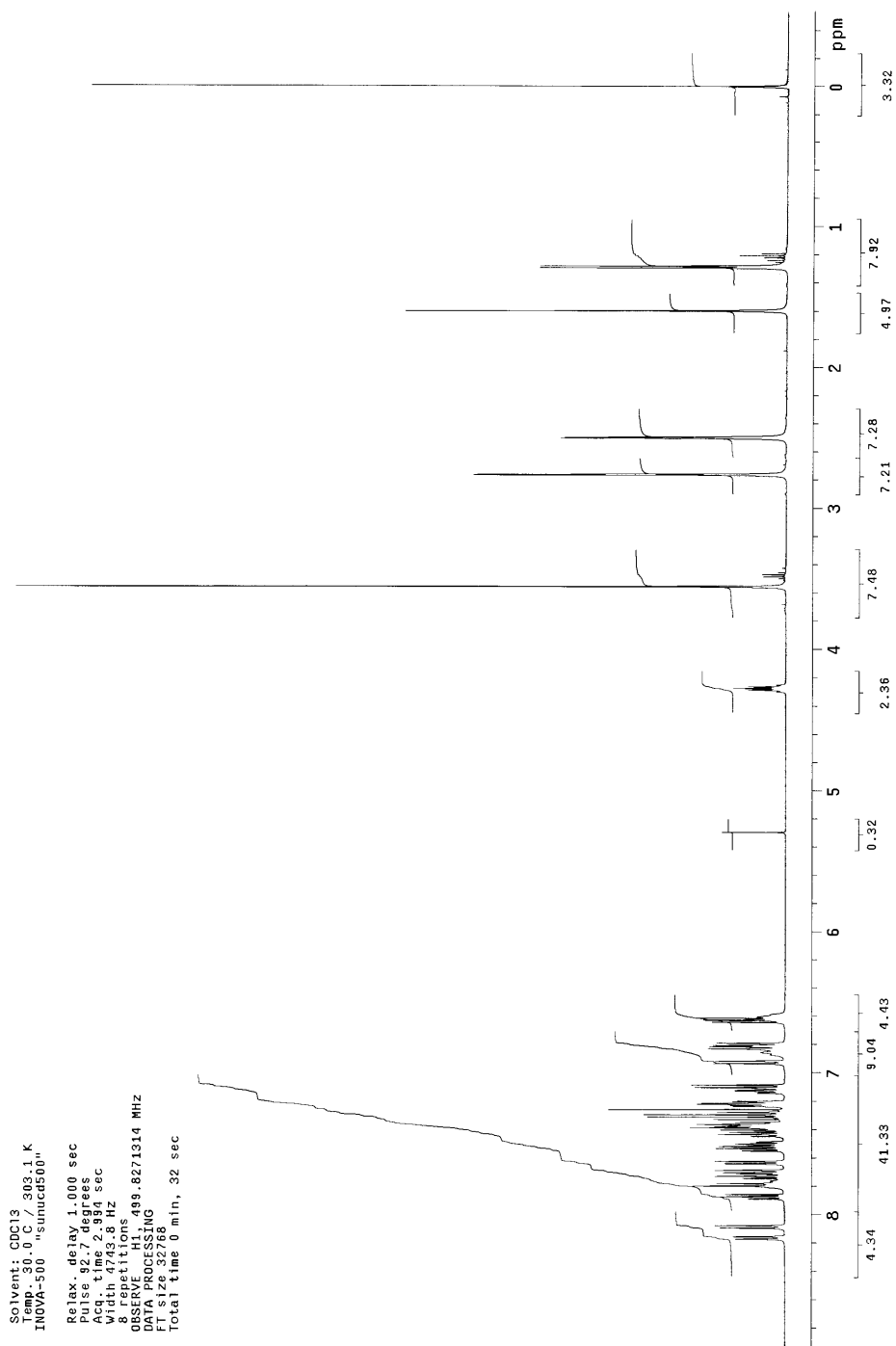
**¹H NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino-*C*₂,*N*]-
[1-(quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II) hexafluorophosphate (*S,R*)-(18a)**



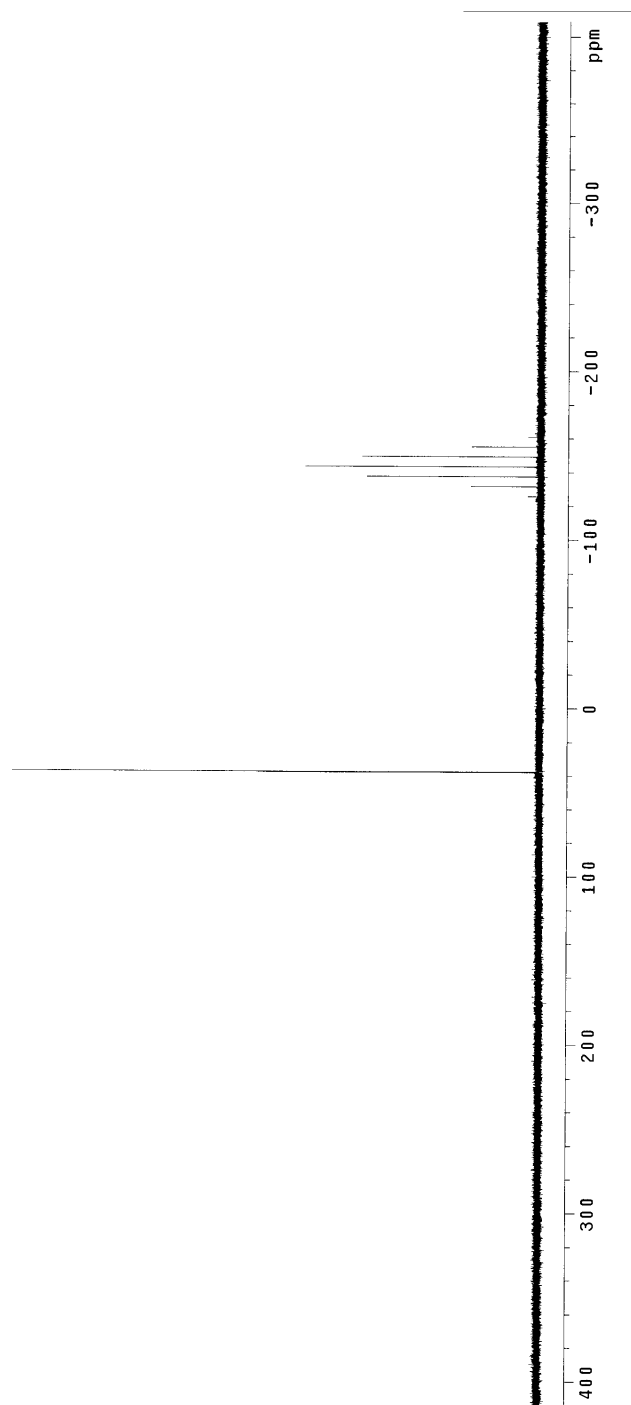
**^{31}P NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino- C_2N]-
[1-(quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II) hexafluorophosphate (*S,R*)-(18a)**



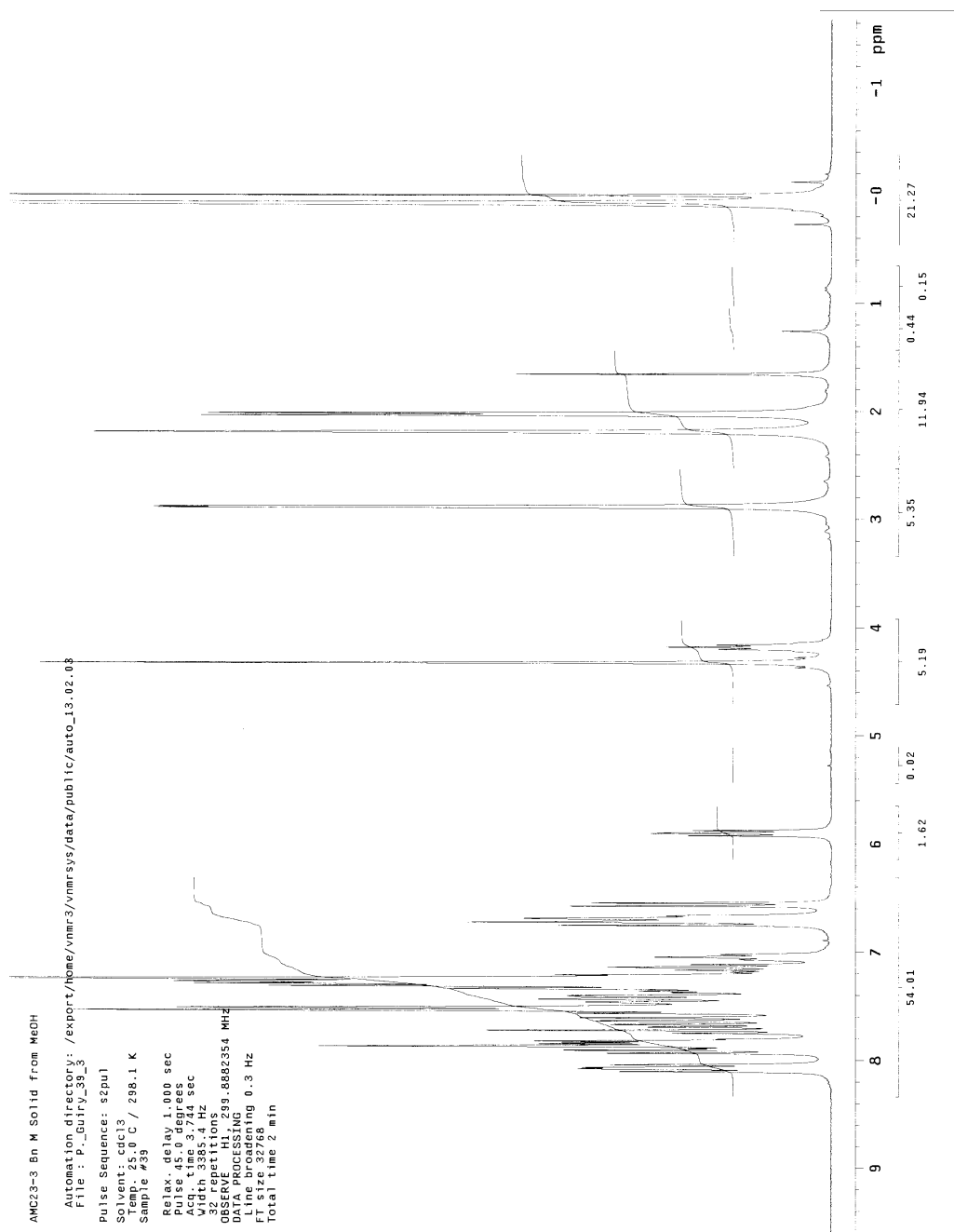
**^1H NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino- C_2,N]-
[diphenyl[1-(2-methylquinazolin-4-yl)(2-naphthyl)]phosphine]
palladium(II) hexafluorophosphate (*S,R*)-(18b)**



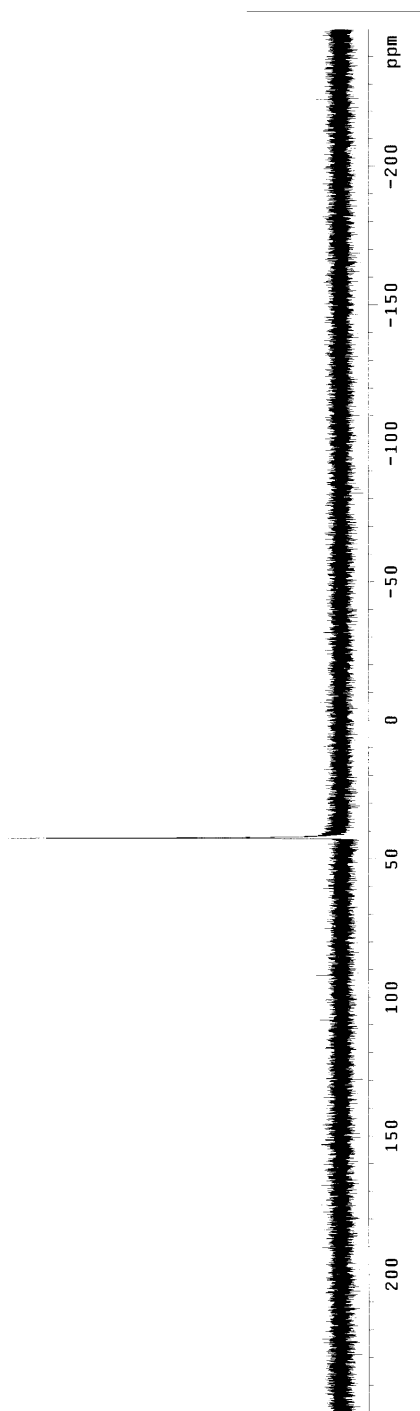
**^{31}P NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato- C_2,N]-
[diphenyl[1-(2-methylquinazolin-4-yl)(2-naphthyl)]phosphine]
palladium(II) hexafluorophosphate (*S,R*)-(18b)**



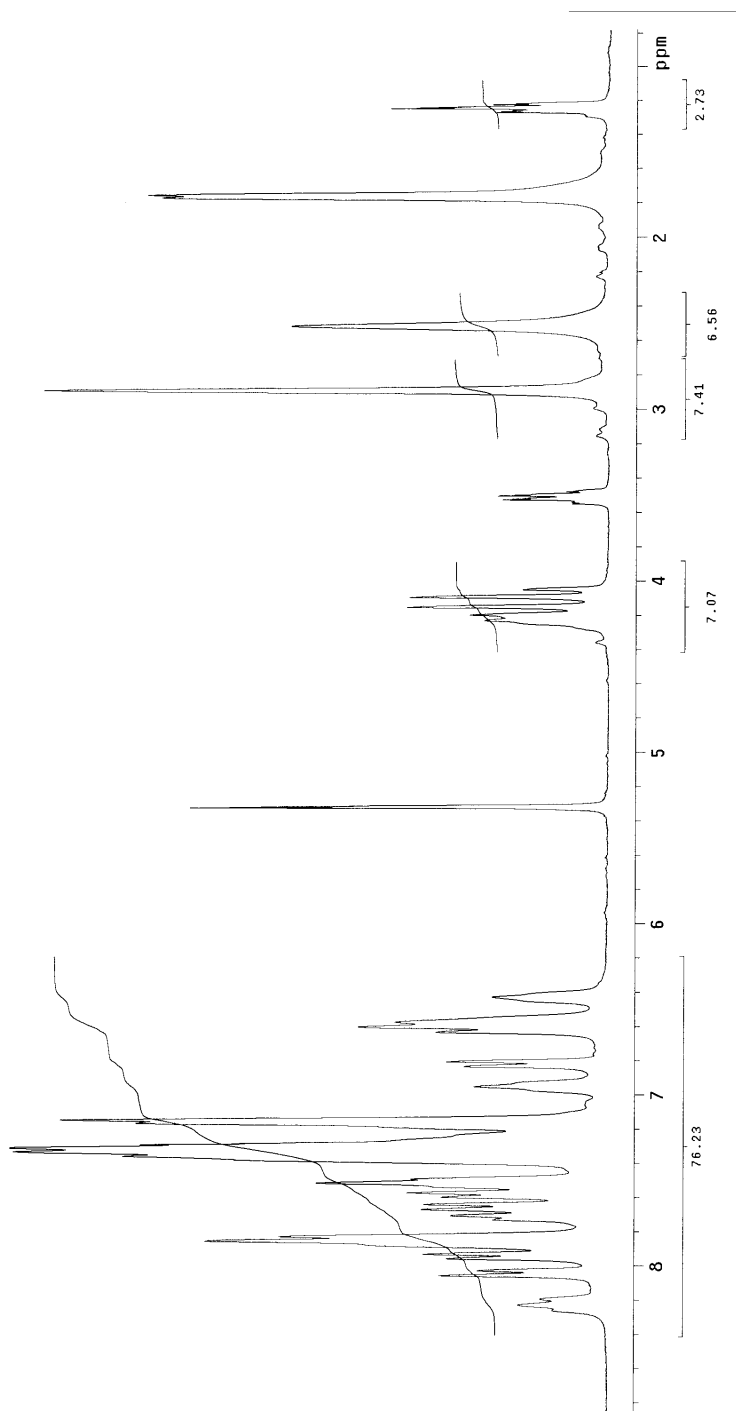
**¹H NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato-C₂,N]-
[1-(2-phenylmethylquinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*R,R*)-(17d)**



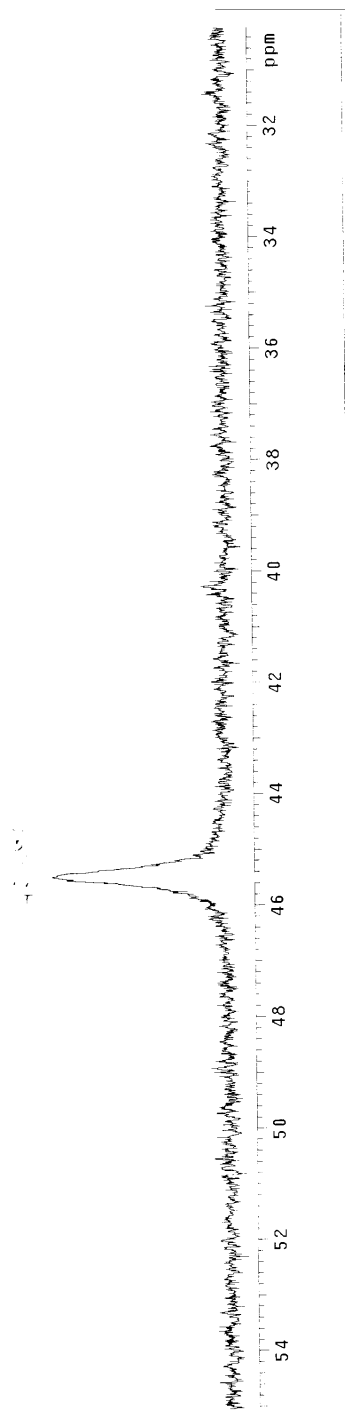
**^{31}P NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato- C_2,N]-
[1-(2-phenylmethylquinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*R,R*)-(17d)**



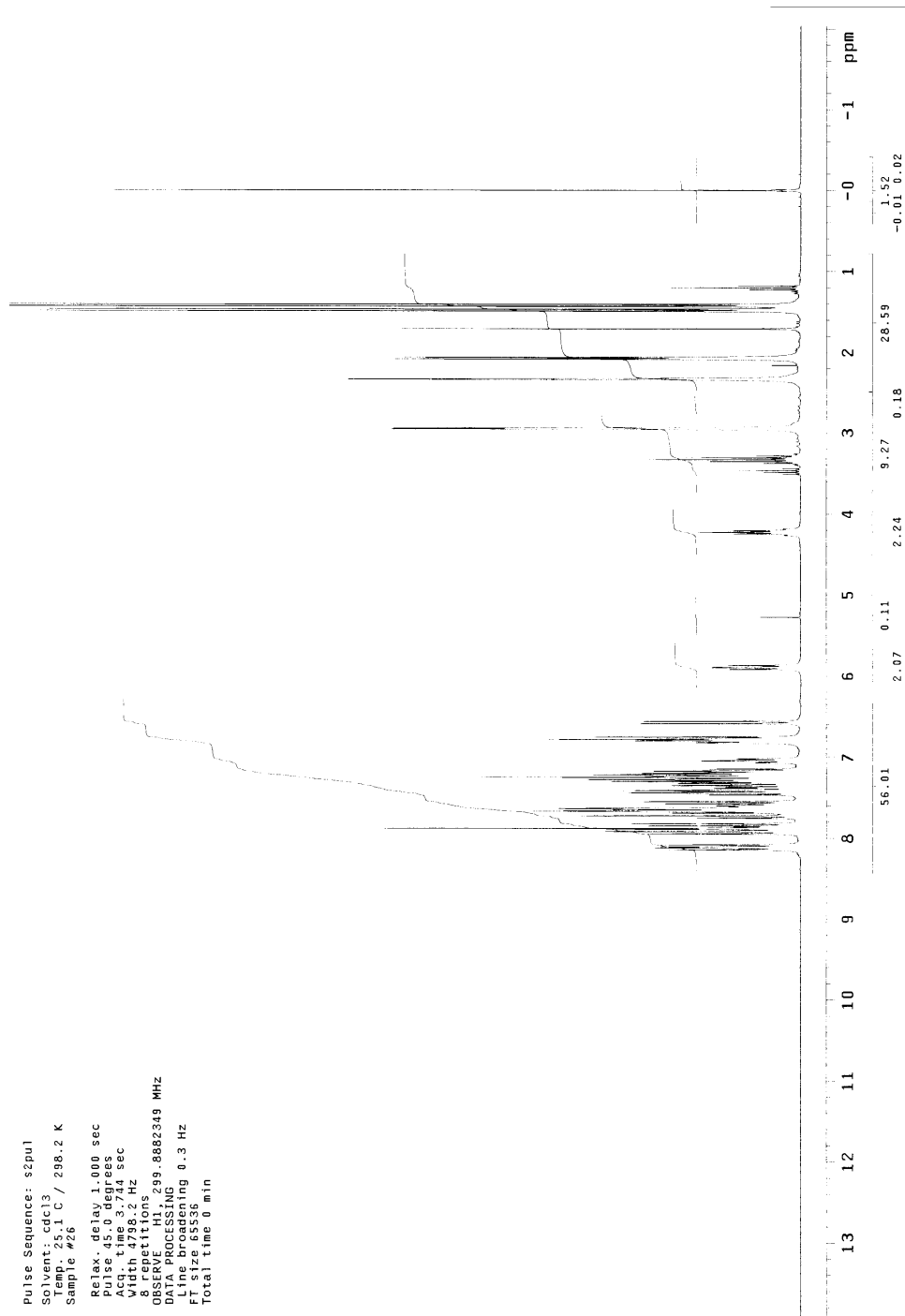
**¹H NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato-*C*₂,*N*]-
[1-(2-phenylmethylquinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*S,R*)-(17d)**



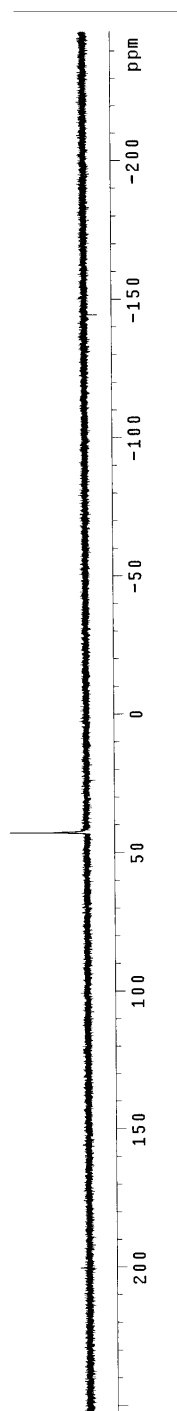
**^{31}P NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato- C_2,N]-
[1-(2-phenylmethylquinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*S,R*)-(17d)**



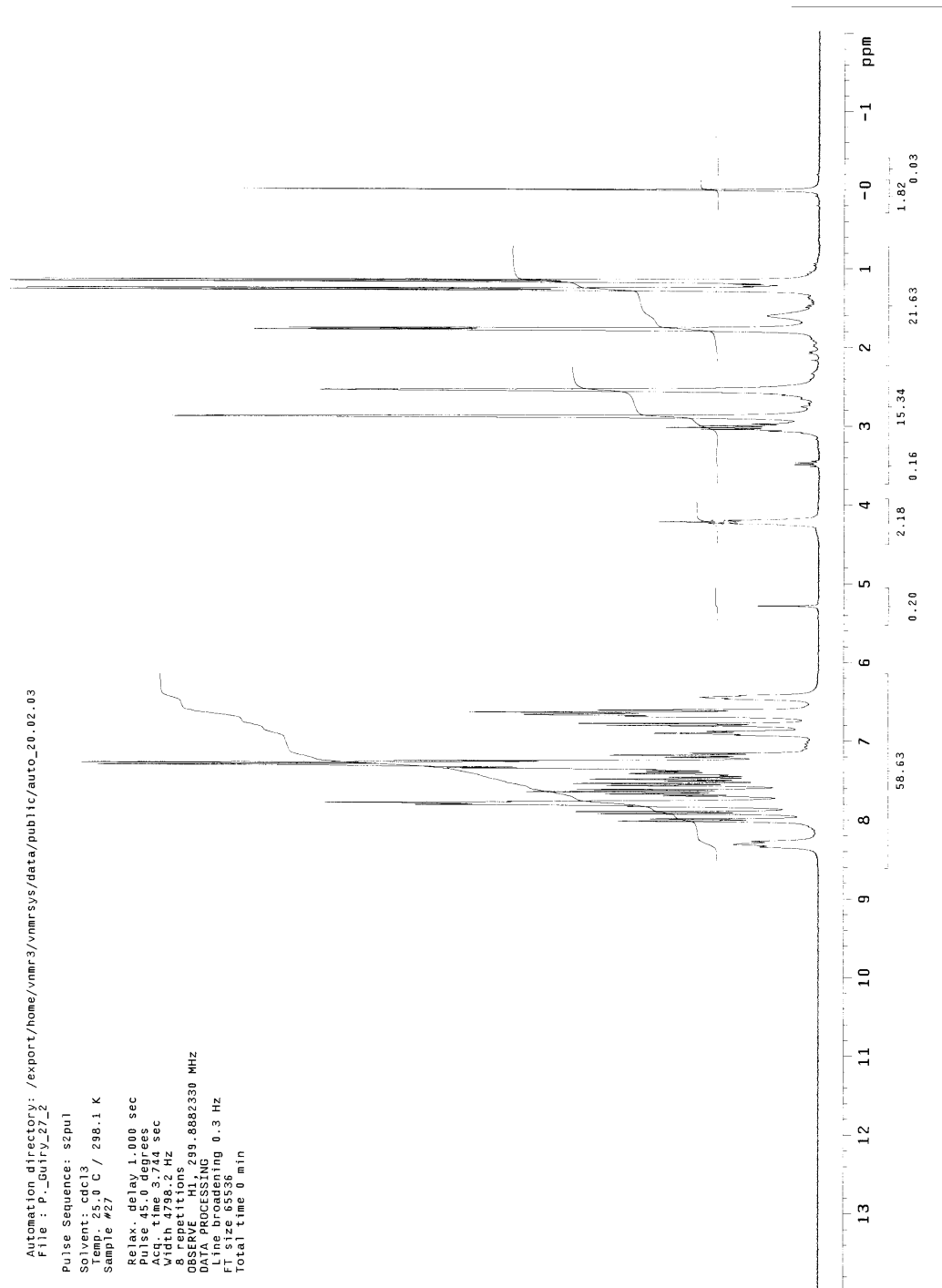
**^1H NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino- C_2,N]-
[1-(2-isopropyl-quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*R,R*)-(17e)**



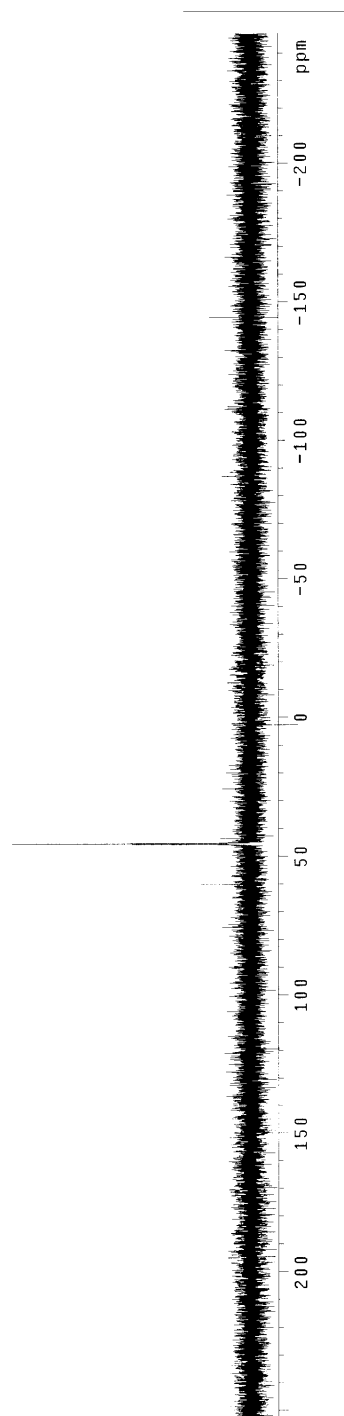
**^{31}P NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino- C_2,N]-
[1-(2-isopropyl-quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*R,R*)-(17e)**



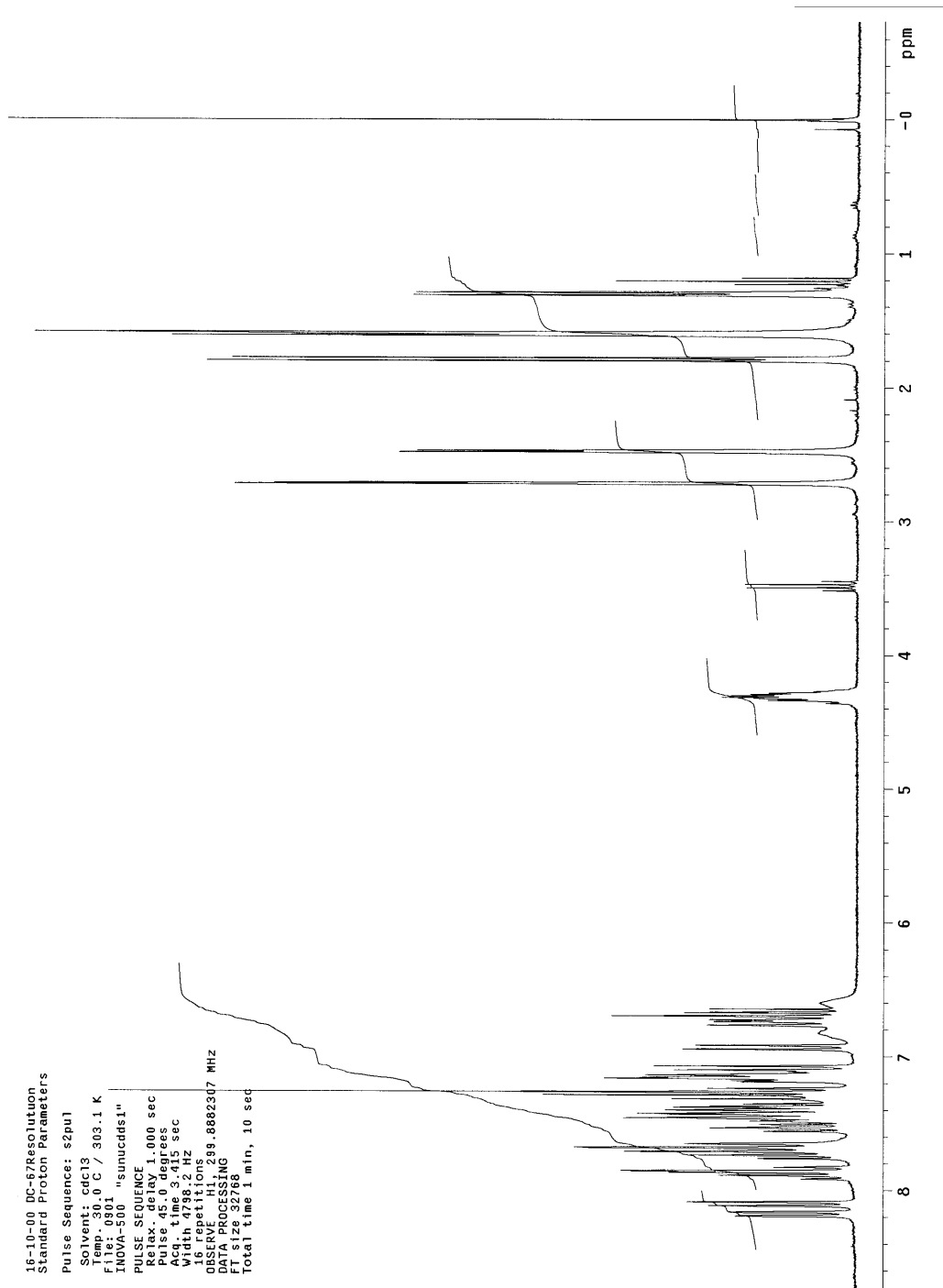
**^1H NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino- C_2,N]-
[1-(2-isopropyl-quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*S,R*)-(17e)**



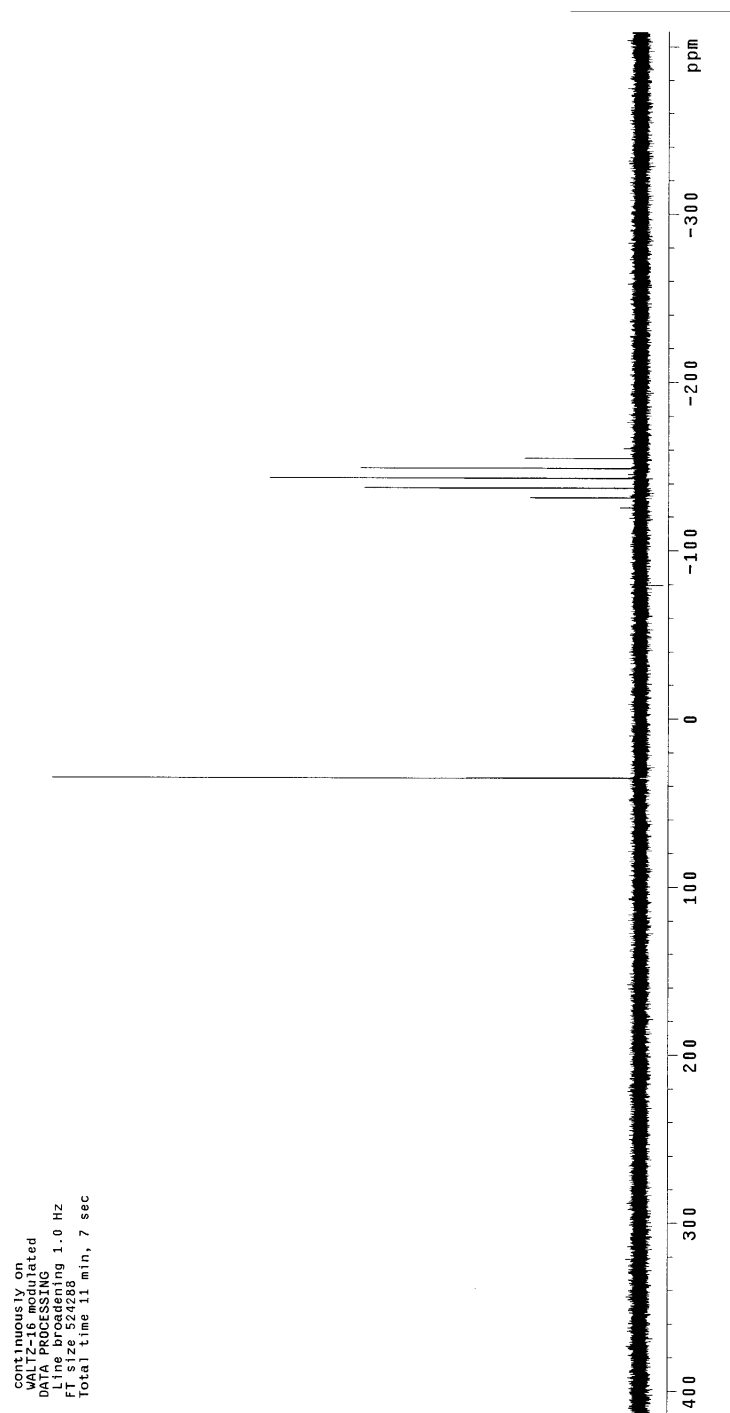
**^{31}P NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino- C_2N]-
[1-(2-isopropyl-quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*S,R*)-(17e)**



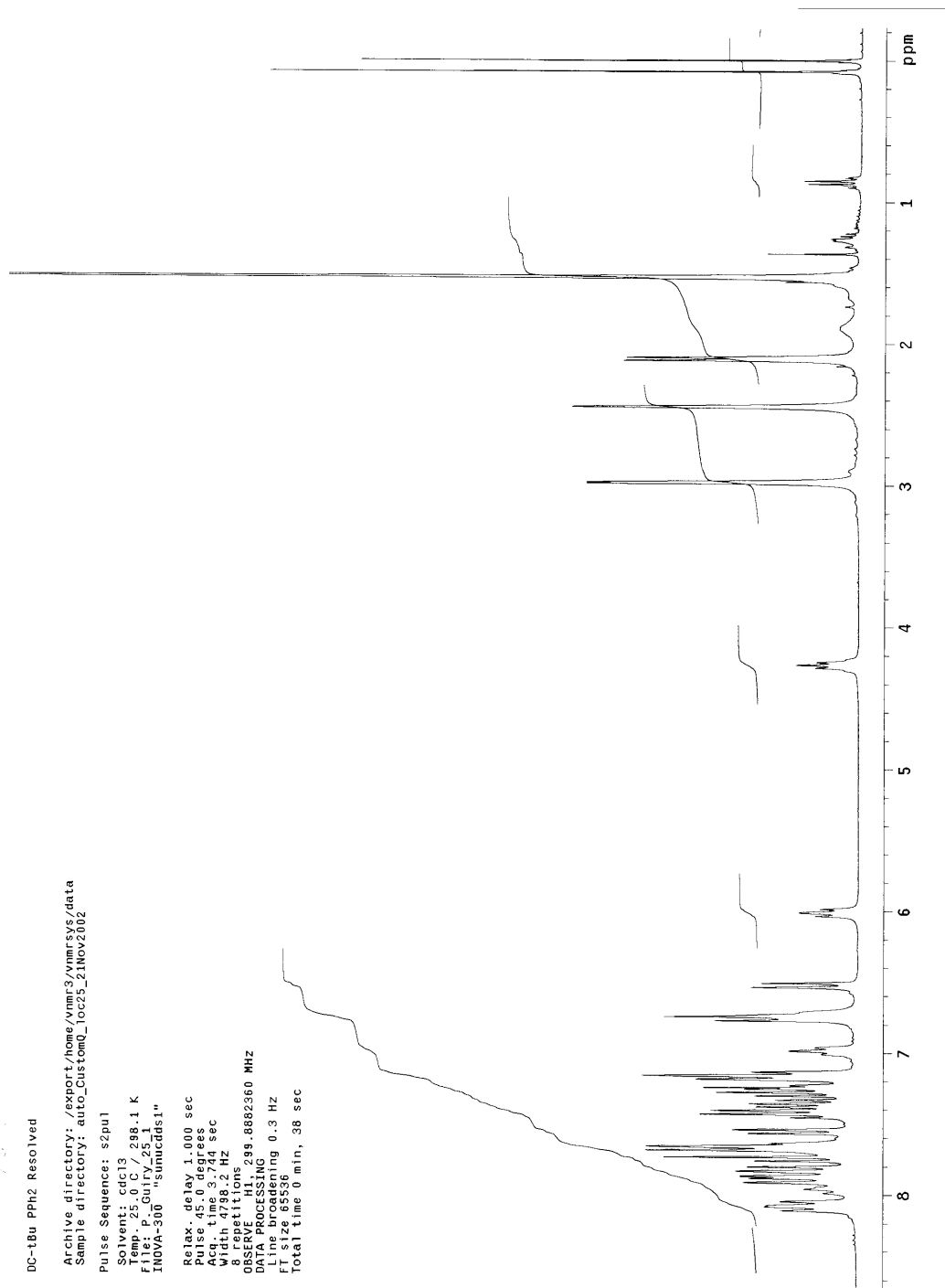
**¹H NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino-*C*₂,*N*]-
[1-(2-isopropyl-quinazolin-4-yl)(2-naphthyl)diphenyl phosphine]
palladium(II) hexafluorophosphate (*S,R*)-(18e)**



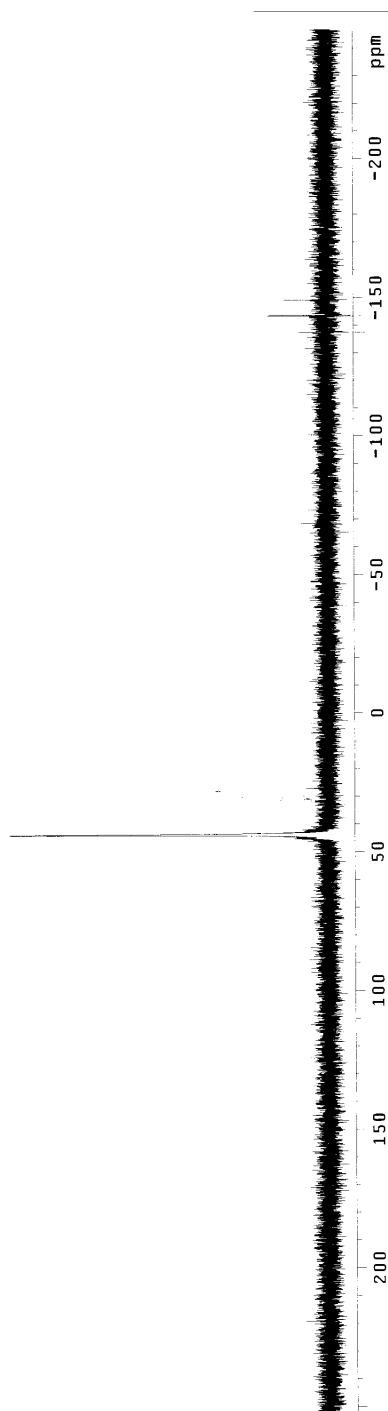
**³¹P NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino-*C*₂,*N*]-
[1-(2-isopropyl-quinazolin-4-yl)(2-naphthyl)diphenyl phosphine]
palladium(II) hexafluorophosphate (*S,R*)-(18e)**



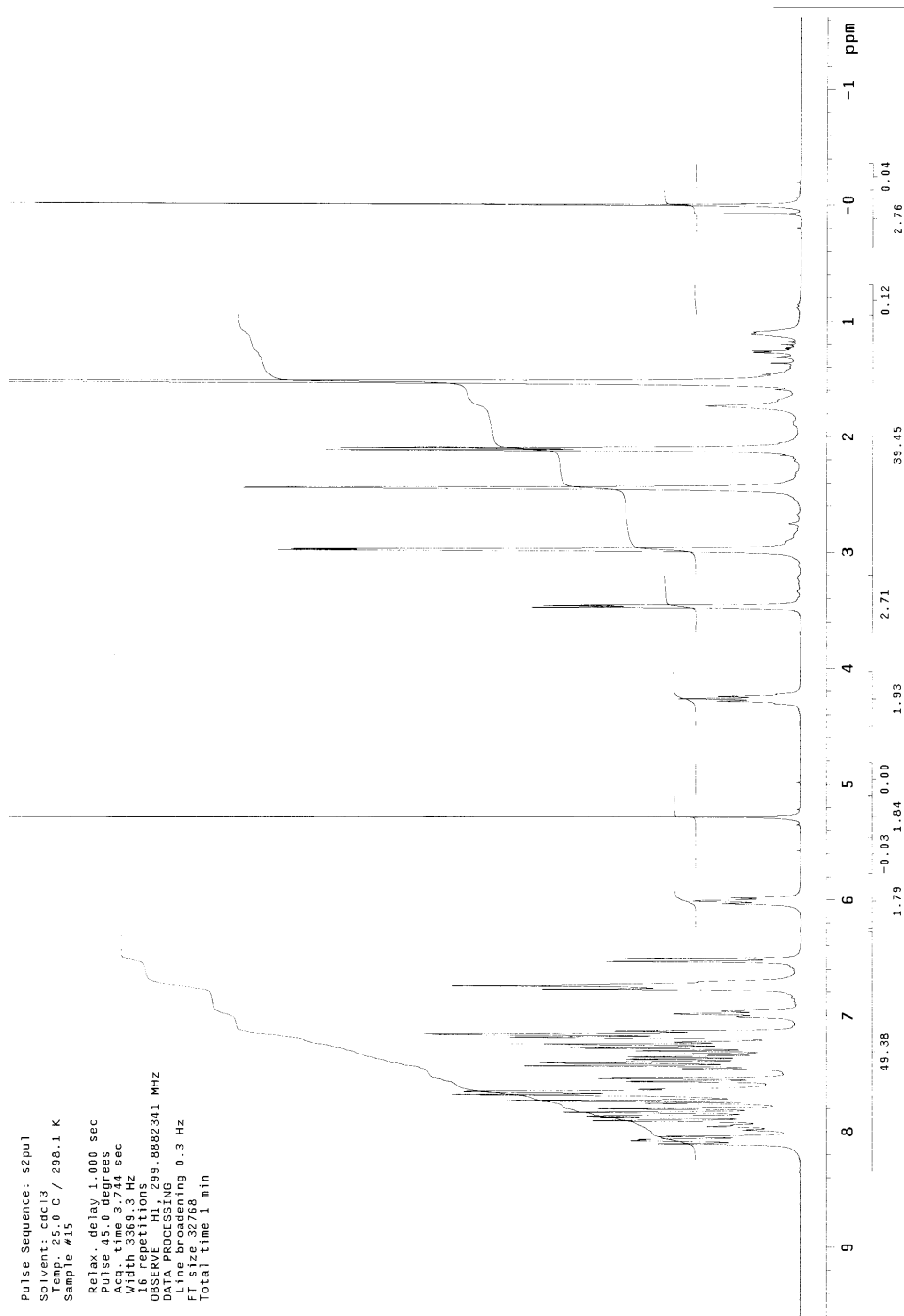
**¹H NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato-C₂,N]-
[1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*R,R*)-(17f)**



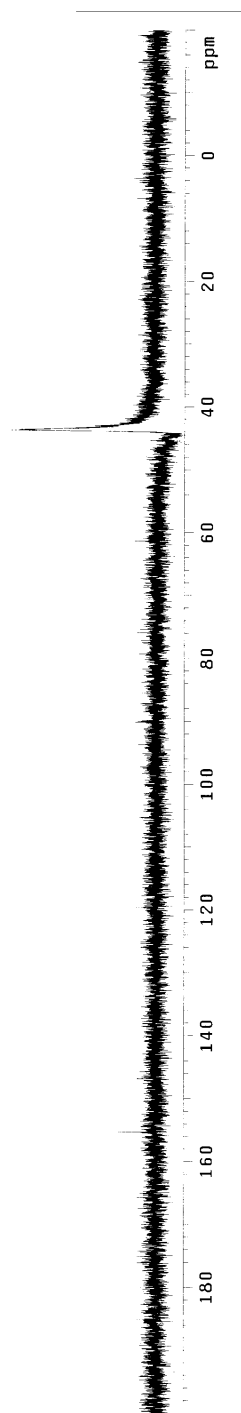
**³¹P NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino-*C*₂,*N*]-
[1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)diphenylphosphine]
palladium(II)chloride (*R,R*)-(17f)**



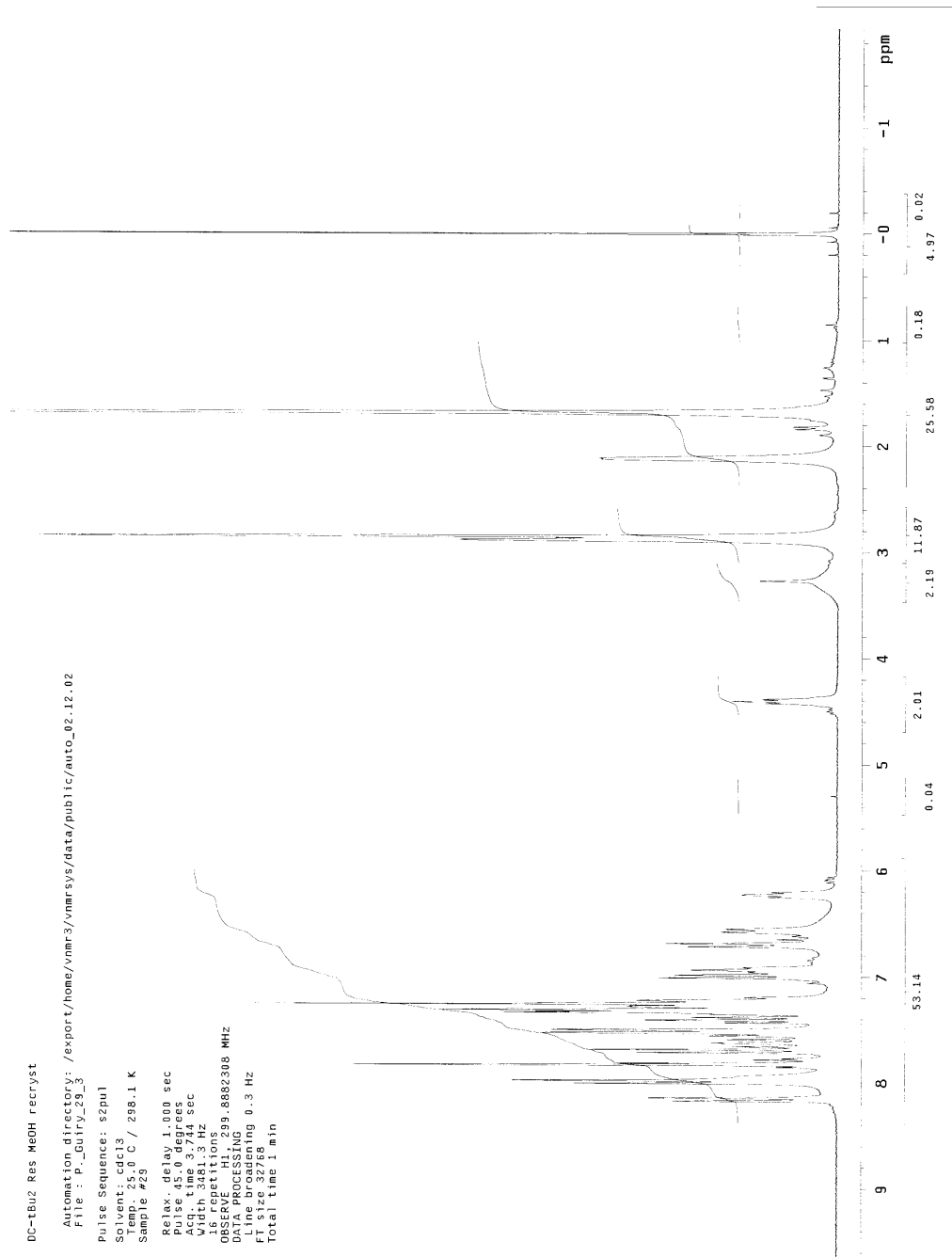
**¹H NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino-*C*₂,*N*]-
[1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)diphenyl phosphine]
palladium(II) hexafluorophosphate (*R,R*)-(18f)**



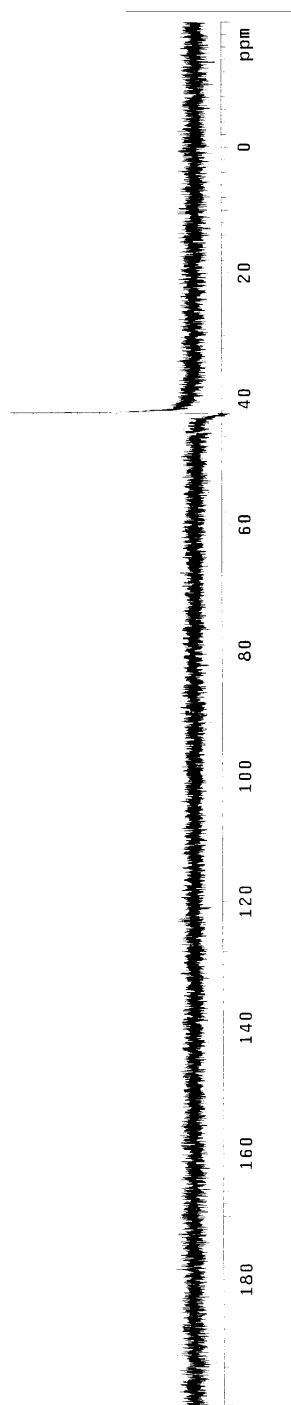
**^{31}P NMR of (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino- C_2,N]-
[1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)diphenyl phosphine]
palladium(II) hexafluorophosphate (*R,R*)-(18f)**



**¹H NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino-*C*₂,*N*]-
[1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)diphenyl phosphine]
palladium(II) hexafluorophosphate (*S,R*)-(18f)**



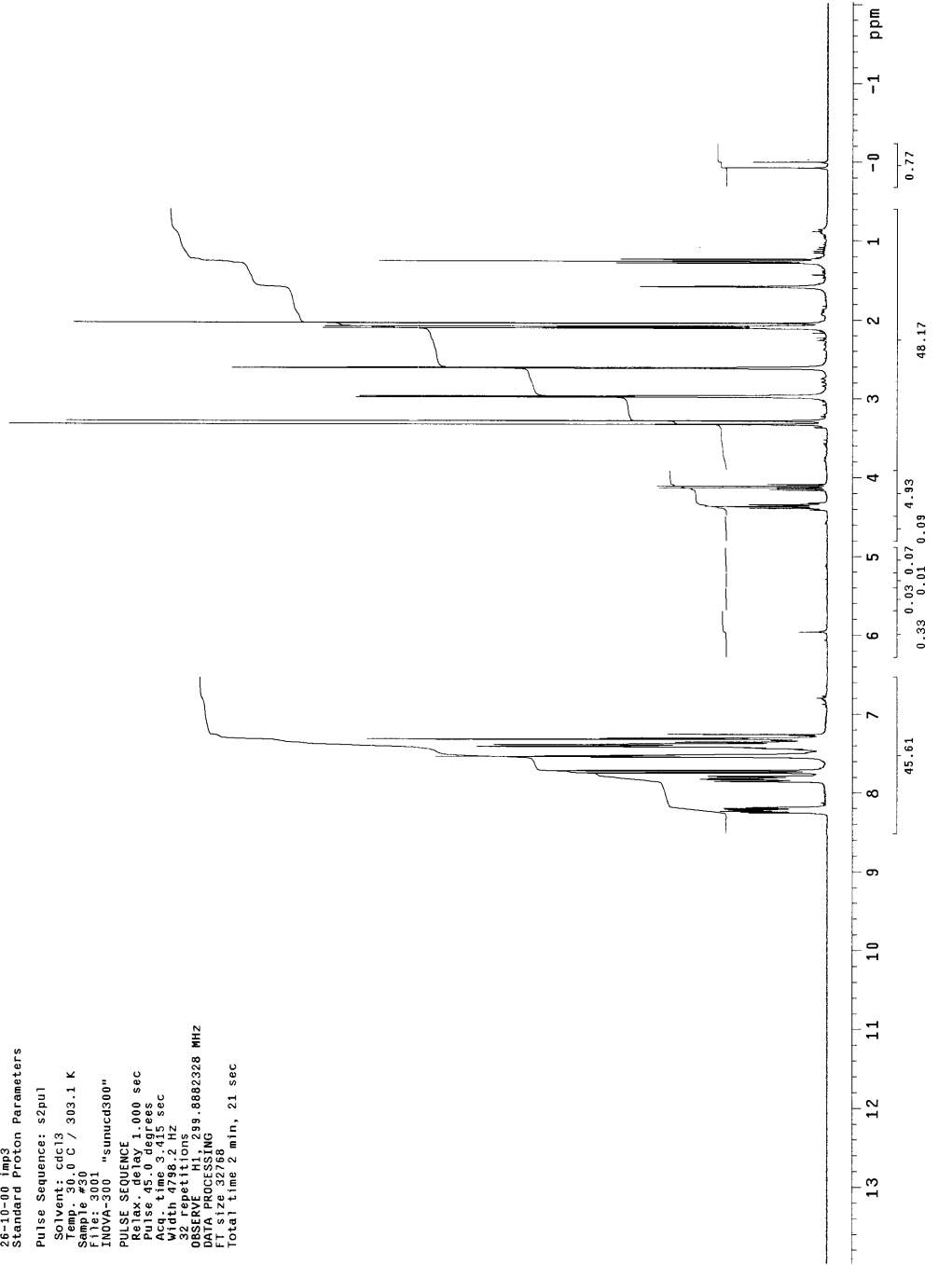
**^{31}P NMR of (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)amino- C_2N]-
[1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)diphenyl phosphine]
palladium(II) hexafluorophosphate (*S,R*)-(18f)**



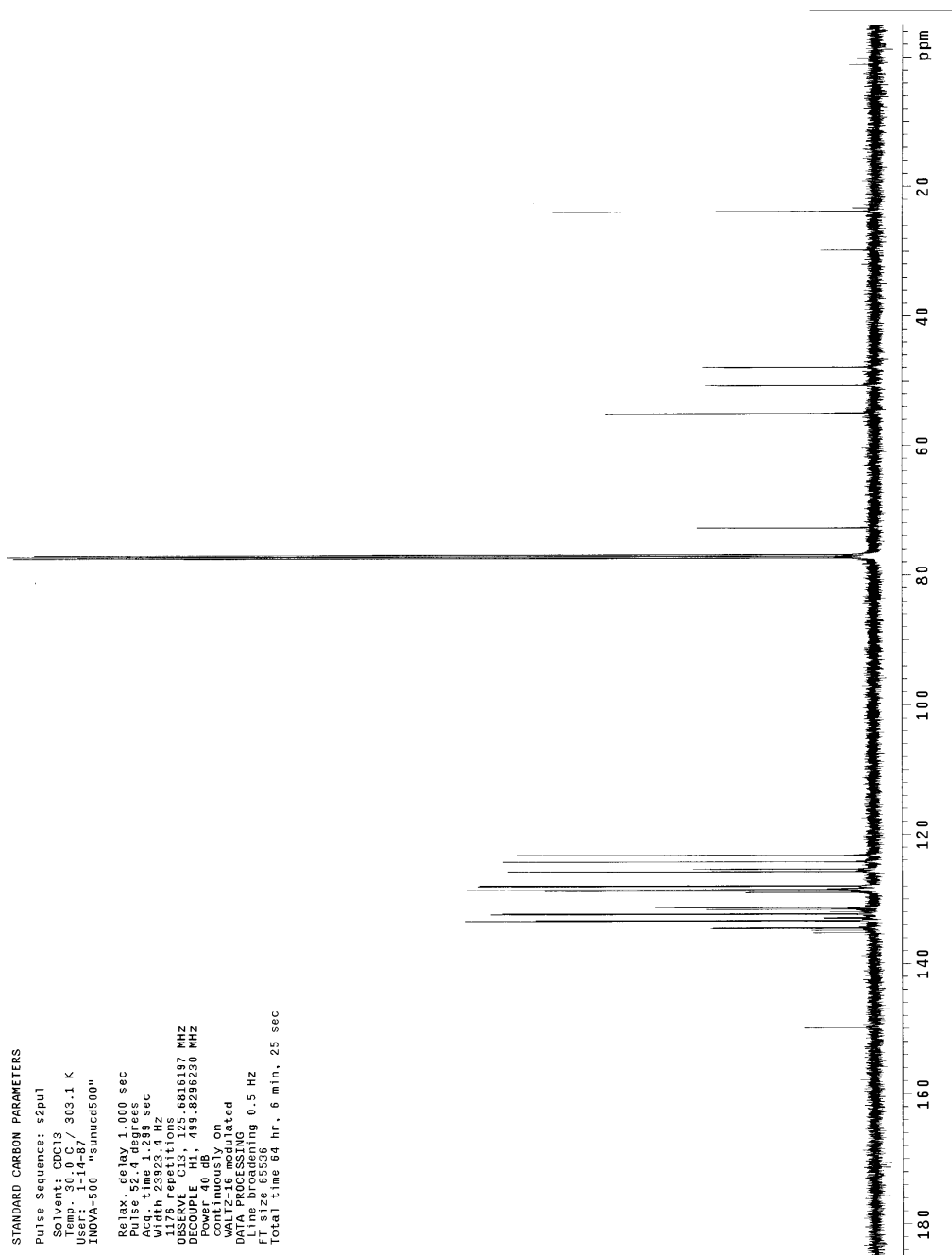
¹H NMR of (R)-[dimethyl(1-(1-naphthyl)ethyl)amino-C₂,N]-
[methyl(diphenyl)phosphite]palladium (II)chloride (19)

26-10-00_1m3
Standard Proton Parameters

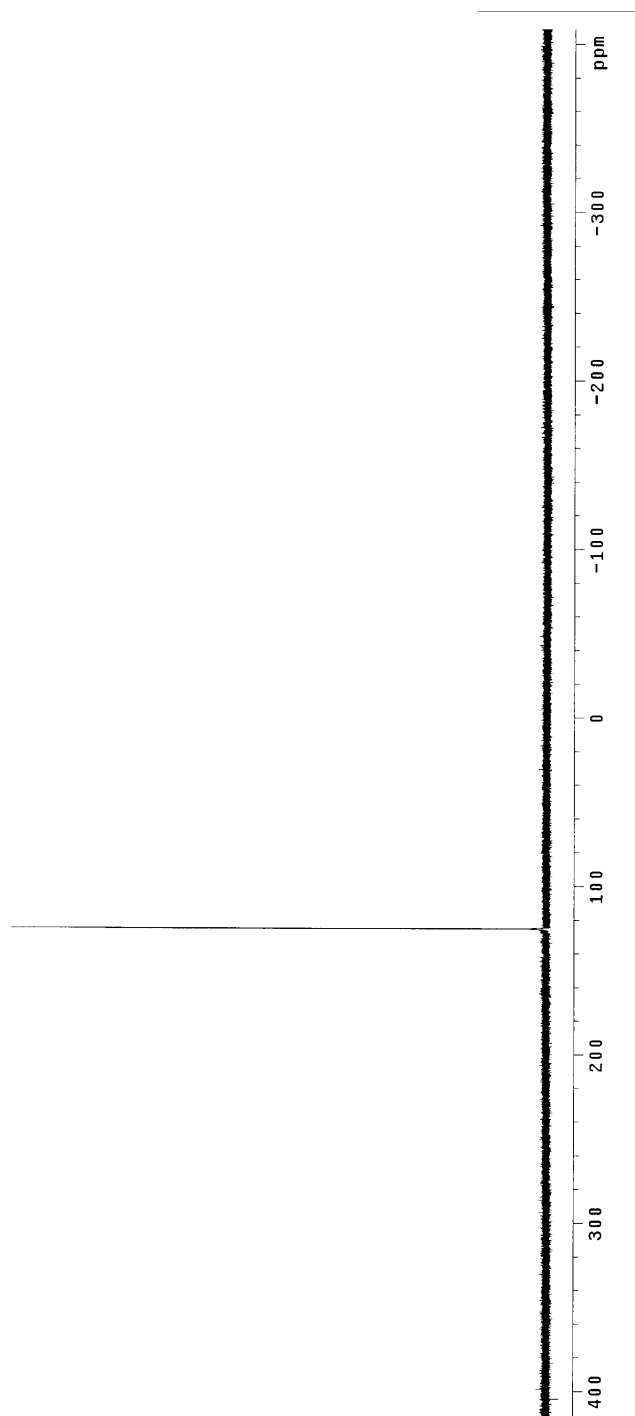
Pulse Sequence: s2pu1
Solvent: cdcl3
Temp.: 30.0 C / 303.1 K
Sample: 19
INSTR: spect
INVA: 300 "sunucd300"
PULSE SEQUENCE
Relax. delay: 1.000 sec
Pulse: 45.0 degrees
Acq. time: 3.415 sec
Date_ time: 12/21/00
320 MHz
OBSERVE: H1, 299.8882328 MHZ
DATA PROCESSING
FT size 32768
Total time 2 min, 21 sec



**¹³C NMR of (*R*)-[dimethyl(1-(1-naphthyl)ethyl)amino-C₂N]-
[methyl(diphenyl)phosphite]palladium (II)chloride (19)**



**^{31}P NMR of (*R*)-[dimethyl(1-(1-naphthyl)ethyl)aminato- C_2,N]-
[methyl(diphenyl)phosphite]palladium (II)chloride (19)**



Crystallographic Data for (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato-*C*₂,*N*]-[1-(2-phenylmethylquinazolin-4-yl)(2-naphthyl)diphenylphosphine]palladium(II)chloride
(*S,R*)-(17d)

Table 1. Crystal data and structure refinement.

Identification code	(<i>S,R</i>)-17d	
Empirical formula	C₅₁ H₄₃ Cl N₃ P Pd	
Color	yellow	
Formula weight	870.70 g · mol ⁻¹	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2₁2₁2₁, (no. 19)	
Unit cell dimensions	a = 10.62430(10) Å	α = 90°.
	b = 16.1488(2) Å	β = 90°.
	c = 23.9876(4) Å	γ = 90°.
Volume	4115.55(9) Å ³	
Z	4	
Density (calculated)	1.405 Mg · m ⁻³	
Absorption coefficient	0.595 mm ⁻¹	
F(000)	1792 e	
Crystal size	0.11 x 0.11 x 0.10 mm ³	
θ range for data collection	3.40 to 33.19°.	
Index ranges	-15 ≤ h ≤ 16, -24 ≤ k ≤ 22, -20 ≤ l ≤ 36	
Reflections collected	37966	
Independent reflections	15577 [R _{int} = 0.0859]	
Reflections with I > 2σ(I)	11181	
Completeness to θ = 33.19°	99.4 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.95 and 0.94	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	15577 / 0 / 514	
Goodness-of-fit on F ²	1.059	
Final R indices [I > 2σ(I)]	R ₁ = 0.0605	wR ² = 0.1304
R indices (all data)	R ₁ = 0.0977	wR ² = 0.1503
Absolute structure parameter	-0.01(3)	
Largest diff. peak and hole	0.827 and -1.249 e · Å ⁻³	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2).

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.2687(4)	0.4999(2)	0.0257(2)	0.016(1)
C(2)	0.2838(3)	0.5359(2)	0.0777(2)	0.017(1)
C(3)	0.4085(4)	0.5528(3)	0.0973(2)	0.022(1)
C(4)	0.5116(4)	0.5326(2)	0.0661(2)	0.021(1)
C(5)	0.4989(5)	0.4965(2)	0.0130(2)	0.019(1)
C(6)	0.6054(4)	0.4764(3)	-0.0203(2)	0.022(1)
C(7)	0.5914(4)	0.4452(3)	-0.0727(2)	0.024(1)
C(8)	0.4703(4)	0.4315(3)	-0.0940(2)	0.027(1)
C(9)	0.3649(4)	0.4481(3)	-0.0630(2)	0.022(1)
C(10)	0.3749(4)	0.4807(2)	-0.0083(2)	0.018(1)
C(11)	0.1418(4)	0.4819(2)	0.0016(2)	0.017(1)
C(12)	-0.0349(4)	0.5299(3)	-0.0426(2)	0.022(1)
C(13)	-0.0139(4)	0.3890(2)	-0.0371(2)	0.021(1)
C(14)	-0.0569(4)	0.3092(3)	-0.0500(2)	0.025(1)
C(15)	0.0082(5)	0.2408(3)	-0.0317(2)	0.029(1)
C(16)	0.1194(4)	0.2500(3)	-0.0005(2)	0.024(1)
C(17)	0.1657(4)	0.3270(2)	0.0119(2)	0.021(1)
C(18)	0.0999(4)	0.3984(2)	-0.0064(2)	0.019(1)
C(19)	-0.1051(4)	0.6060(3)	-0.0614(2)	0.029(1)
C(20)	-0.0306(4)	0.6498(3)	-0.1065(2)	0.028(1)
C(21)	0.0276(5)	0.7260(3)	-0.0954(2)	0.035(1)
C(22)	0.1054(6)	0.7644(4)	-0.1341(3)	0.050(2)
C(23)	0.1260(7)	0.7264(4)	-0.1848(3)	0.061(2)
C(24)	0.0683(9)	0.6517(5)	-0.1980(3)	0.072(3)
C(25)	-0.0093(8)	0.6132(4)	-0.1588(2)	0.053(2)
C(26)	0.0966(4)	0.6612(2)	0.1000(2)	0.021(1)
C(27)	-0.0028(5)	0.6979(2)	0.1287(2)	0.026(1)
C(28)	-0.0453(5)	0.7762(3)	0.1150(2)	0.033(1)
C(29)	0.0140(5)	0.8196(3)	0.0721(2)	0.033(1)
C(30)	0.1134(5)	0.7848(3)	0.0435(2)	0.030(1)
C(31)	0.1551(4)	0.7049(3)	0.0578(2)	0.024(1)
C(32)	0.2162(4)	0.5832(2)	0.1913(2)	0.019(1)
C(33)	0.2050(4)	0.5268(3)	0.2351(2)	0.022(1)
C(34)	0.2583(4)	0.5450(3)	0.2870(2)	0.029(1)
C(35)	0.3220(4)	0.6199(3)	0.2954(2)	0.032(1)

C(36)	0.3337(4)	0.6757(3)	0.2517(2)	0.028(1)
C(37)	0.2799(4)	0.6591(3)	0.1999(2)	0.022(1)
C(38)	0.1184(4)	0.3694(3)	0.1560(2)	0.020(1)
C(39)	0.2505(4)	0.3628(3)	0.1493(2)	0.020(1)
C(40)	0.3153(4)	0.2915(3)	0.1617(2)	0.024(1)
C(41)	0.2525(4)	0.2228(2)	0.1848(2)	0.022(1)
C(42)	0.3168(5)	0.1479(3)	0.1974(2)	0.030(1)
C(43)	0.2574(5)	0.0833(3)	0.2239(2)	0.033(1)
C(44)	0.1290(5)	0.0917(3)	0.2382(2)	0.027(1)
C(45)	0.0621(4)	0.1623(3)	0.2247(2)	0.025(1)
C(46)	0.1209(4)	0.2285(2)	0.1967(2)	0.020(1)
C(47)	0.0556(4)	0.3026(3)	0.1808(2)	0.021(1)
C(48)	-0.0829(4)	0.3125(3)	0.1916(2)	0.023(1)
C(49)	-0.1047(5)	0.3502(3)	0.2481(2)	0.028(1)
C(50)	-0.2664(4)	0.3899(3)	0.1560(2)	0.028(1)
C(51)	-0.1400(5)	0.3102(3)	0.0934(2)	0.029(1)
Cl	-0.1564(1)	0.5422(1)	0.0857(1)	0.025(1)
N(1)	0.0767(3)	0.5456(2)	-0.0158(1)	0.021(1)
N(2)	-0.0811(3)	0.4565(2)	-0.0552(1)	0.023(1)
N(3)	-0.1350(3)	0.3624(2)	0.1441(2)	0.023(1)
P	0.1486(1)	0.5590(1)	0.1225(1)	0.017(1)
Pd	0.0004(1)	0.4586(1)	0.1283(1)	0.018(1)

Table 3. Bond lengths [Å] and angles [°].

C(1)-C(2)	1.386(5)	C(1)-C(10)	1.427(5)
C(1)-C(11)	1.495(5)	C(2)-C(3)	1.433(5)
C(2)-P	1.831(4)	C(3)-C(4)	1.366(6)
C(4)-C(5)	1.408(5)	C(5)-C(6)	1.422(6)
C(5)-C(10)	1.436(6)	C(6)-C(7)	1.362(6)
C(7)-C(8)	1.402(6)	C(8)-C(9)	1.370(6)
C(9)-C(10)	1.417(6)	C(11)-N(1)	1.307(5)
C(11)-C(18)	1.434(5)	C(12)-N(2)	1.318(6)
C(12)-N(1)	1.372(5)	C(12)-C(19)	1.507(6)
C(13)-N(2)	1.373(5)	C(13)-C(14)	1.402(6)
C(13)-C(18)	1.424(6)	C(14)-C(15)	1.375(7)
C(15)-C(16)	1.406(7)	C(16)-C(17)	1.369(6)
C(17)-C(18)	1.417(6)	C(19)-C(20)	1.515(7)
C(20)-C(21)	1.402(7)	C(20)-C(25)	1.405(7)
C(21)-C(22)	1.389(8)	C(22)-C(23)	1.379(10)
C(23)-C(24)	1.390(11)	C(24)-C(25)	1.397(10)
C(26)-C(31)	1.383(6)	C(26)-C(27)	1.393(6)
C(26)-P	1.821(4)	C(27)-C(28)	1.383(6)
C(28)-C(29)	1.396(7)	C(29)-C(30)	1.379(7)
C(30)-C(31)	1.406(6)	C(32)-C(33)	1.395(6)
C(32)-C(37)	1.415(5)	C(32)-P	1.844(4)
C(33)-C(34)	1.398(6)	C(34)-C(35)	1.401(7)
C(35)-C(36)	1.388(7)	C(36)-C(37)	1.394(6)
C(38)-C(47)	1.400(6)	C(38)-C(39)	1.416(6)
C(38)-Pd	2.023(4)	C(39)-C(40)	1.374(6)
C(40)-C(41)	1.408(6)	C(41)-C(42)	1.421(6)
C(41)-C(46)	1.431(6)	C(42)-C(43)	1.375(7)
C(43)-C(44)	1.414(7)	C(44)-C(45)	1.381(6)
C(45)-C(46)	1.409(6)	C(46)-C(47)	1.435(6)
C(47)-C(48)	1.503(6)	C(48)-N(3)	1.501(6)
C(48)-C(49)	1.505(7)	C(50)-N(3)	1.492(5)
C(51)-N(3)	1.481(6)	Cl-Pd	2.3742(10)
N(3)-Pd	2.151(4)	P-Pd	2.2642(10)
C(2)-C(1)-C(10)	121.0(4)	C(2)-C(1)-C(11)	122.2(3)
C(10)-C(1)-C(11)	116.7(3)	C(1)-C(2)-C(3)	118.8(3)
C(1)-C(2)-P	121.5(3)	C(3)-C(2)-P	119.7(3)
C(4)-C(3)-C(5)	121.2(4)	C(3)-C(4)-C(5)	121.2(4)

C(4)-C(5)-C(6)	121.7(4)	C(4)-C(5)-C(10)	119.0(4)
C(6)-C(5)-C(10)	119.3(4)	C(7)-C(6)-C(5)	121.0(4)
C(6)-C(7)-C(8)	119.7(4)	C(9)-C(8)-C(7)	121.4(4)
C(8)-C(9)-C(10)	120.9(4)	C(9)-C(10)-C(1)	123.4(4)
C(9)-C(10)-C(5)	117.7(4)	C(1)-C(10)-C(5)	118.9(4)
N(1)-C(11)-C(18)	122.2(4)	N(1)-C(11)-C(1)	116.6(3)
C(18)-C(11)-C(1)	120.9(3)	N(2)-C(12)-N(1)	126.5(4)
N(2)-C(12)-C(19)	118.7(4)	N(1)-C(12)-C(19)	114.7(4)
N(2)-C(13)-C(14)	119.5(4)	N(2)-C(13)-C(18)	121.4(4)
C(14)-C(13)-C(18)	119.1(4)	C(15)-C(14)-C(13)	120.3(4)
C(14)-C(15)-C(16)	120.5(4)	C(17)-C(16)-C(15)	120.8(4)
C(16)-C(17)-C(18)	119.6(4)	C(17)-C(18)-C(13)	119.5(4)
C(17)-C(18)-C(11)	124.8(4)	C(13)-C(18)-C(11)	115.6(4)
C(12)-C(19)-C(20)	109.7(4)	C(21)-C(20)-C(25)	117.8(5)
C(21)-C(20)-C(19)	120.3(4)	C(25)-C(20)-C(19)	121.7(5)
C(22)-C(21)-C(20)	121.9(5)	C(23)-C(22)-C(21)	119.0(6)
C(22)-C(23)-C(24)	121.2(6)	C(23)-C(24)-C(25)	119.5(6)
C(24)-C(25)-C(20)	120.6(6)	C(31)-C(26)-C(27)	119.0(4)
C(31)-C(26)-P	122.9(3)	C(27)-C(26)-P	118.0(3)
C(28)-C(27)-C(26)	121.3(4)	C(27)-C(28)-C(29)	119.2(5)
C(30)-C(29)-C(28)	120.5(4)	C(29)-C(30)-C(31)	119.6(4)
C(26)-C(31)-C(30)	120.4(4)	C(33)-C(32)-C(37)	119.9(4)
C(33)-C(32)-P	120.2(3)	C(37)-C(32)-P	119.9(3)
C(32)-C(33)-C(34)	119.8(4)	C(33)-C(34)-C(35)	120.4(4)
C(36)-C(35)-C(34)	119.7(4)	C(35)-C(36)-C(37)	120.8(4)
C(36)-C(37)-C(32)	119.4(4)	C(47)-C(38)-C(39)	117.6(4)
C(47)-C(38)-Pd	113.1(3)	C(39)-C(38)-Pd	129.0(3)
C(40)-C(39)-C(38)	122.3(4)	C(39)-C(40)-C(41)	120.5(4)
C(40)-C(41)-C(42)	121.8(4)	C(40)-C(41)-C(46)	119.3(4)
C(42)-C(41)-C(46)	118.9(4)	C(43)-C(42)-C(41)	121.6(5)
C(42)-C(43)-C(44)	118.8(4)	C(45)-C(44)-C(43)	121.3(4)
C(44)-C(45)-C(46)	120.7(4)	C(45)-C(46)-C(41)	118.6(4)
C(45)-C(46)-C(47)	123.1(4)	C(41)-C(46)-C(47)	118.3(4)
C(38)-C(47)-C(46)	121.7(4)	C(38)-C(47)-C(48)	117.3(4)
C(46)-C(47)-C(48)	121.0(4)	N(3)-C(48)-C(47)	106.7(4)
N(3)-C(48)-C(49)	114.2(4)	C(47)-C(48)-C(49)	110.4(4)
C(11)-N(1)-C(12)	117.5(4)	C(12)-N(2)-C(13)	116.6(3)
C(51)-N(3)-C(50)	107.0(4)	C(51)-N(3)-C(48)	109.3(3)
C(50)-N(3)-C(48)	111.1(4)	C(51)-N(3)-Pd	106.9(3)
C(50)-N(3)-Pd	116.4(3)	C(48)-N(3)-Pd	106.0(3)

C(26)-P-C(2)	104.44(19)	C(26)-P-C(32)	101.06(19)
C(2)-P-C(32)	105.20(17)	C(26)-P-Pd	117.13(14)
C(2)-P-Pd	115.80(13)	C(32)-P-Pd	111.56(13)
C(38)-Pd-N(3)	80.91(14)	C(38)-Pd-P	95.70(12)
N(3)-Pd-P	173.22(11)	C(38)-Pd-Cl	168.89(12)
N(3)-Pd-Cl	90.98(10)	P-Pd-Cl	93.11(4)

Table 4. Anisotropic displacement parameters (\AA^2).

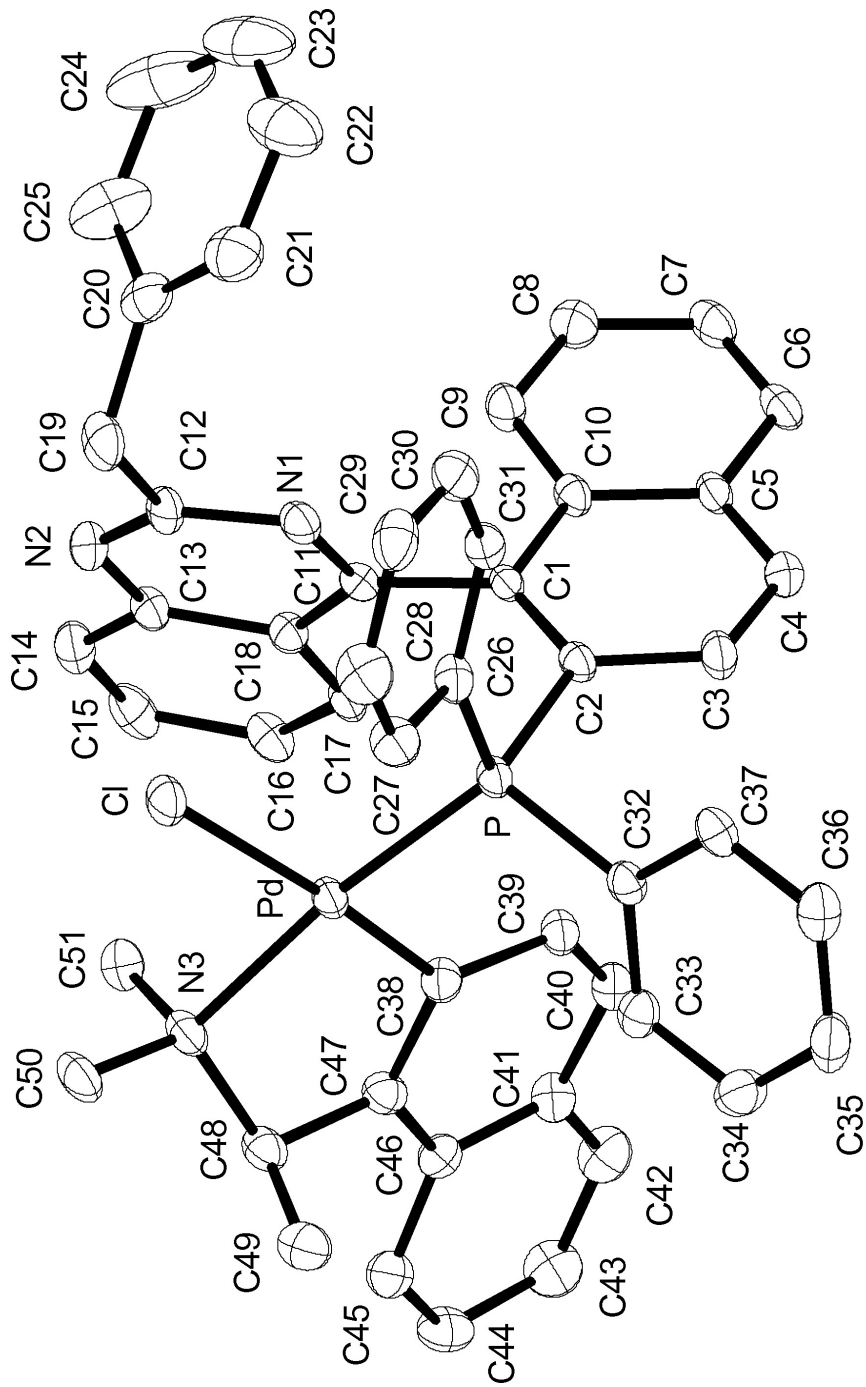
The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}].$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	0.011(1)	0.016(2)	0.020(2)	0.006(1)	0.000(1)	-0.001(1)
C(2)	0.012(1)	0.018(2)	0.022(2)	0.004(2)	0.001(1)	0.001(1)
C(3)	0.014(2)	0.025(2)	0.027(2)	0.001(2)	-0.003(1)	-0.002(1)
C(4)	0.016(2)	0.025(2)	0.022(2)	0.001(1)	-0.001(2)	0.000(2)
C(5)	0.013(1)	0.018(1)	0.025(2)	0.005(1)	-0.001(2)	-0.003(2)
C(6)	0.014(2)	0.021(2)	0.032(2)	0.006(2)	0.004(2)	-0.001(1)
C(7)	0.015(2)	0.026(2)	0.032(2)	0.003(2)	0.006(2)	0.003(2)
C(8)	0.024(2)	0.034(2)	0.024(2)	-0.002(2)	0.002(2)	-0.001(2)
C(9)	0.015(2)	0.026(2)	0.025(2)	-0.001(2)	0.000(2)	0.000(2)
C(10)	0.013(2)	0.017(2)	0.024(2)	0.004(1)	0.000(1)	0.001(1)
C(11)	0.015(2)	0.018(2)	0.018(2)	0.000(1)	0.002(1)	-0.001(1)
C(12)	0.012(2)	0.027(2)	0.027(2)	0.003(2)	-0.001(1)	0.002(1)
C(13)	0.015(2)	0.026(2)	0.022(2)	0.000(1)	0.001(2)	-0.002(2)
C(14)	0.018(2)	0.030(2)	0.027(2)	-0.005(2)	-0.001(2)	-0.003(2)
C(15)	0.025(2)	0.025(2)	0.037(2)	-0.007(2)	0.006(2)	-0.009(2)
C(16)	0.019(2)	0.019(2)	0.033(2)	0.000(2)	0.004(2)	0.000(1)
C(17)	0.014(2)	0.021(2)	0.028(2)	0.003(2)	0.000(2)	-0.003(1)
C(18)	0.016(2)	0.023(2)	0.018(2)	-0.001(2)	0.001(1)	-0.001(1)
C(19)	0.015(2)	0.028(2)	0.044(3)	0.006(2)	-0.004(2)	0.004(2)
C(20)	0.026(2)	0.033(2)	0.026(2)	0.003(2)	-0.002(2)	0.011(2)
C(21)	0.036(3)	0.034(2)	0.036(2)	0.005(2)	-0.001(2)	0.005(2)
C(22)	0.044(3)	0.044(3)	0.063(4)	0.021(3)	0.014(3)	0.008(2)
C(23)	0.065(5)	0.062(4)	0.055(4)	0.035(3)	0.023(3)	0.027(4)
C(24)	0.108(7)	0.076(5)	0.034(3)	0.012(3)	0.023(4)	0.046(5)
C(25)	0.078(5)	0.046(3)	0.034(2)	0.001(2)	-0.002(4)	0.009(4)
C(26)	0.017(2)	0.016(2)	0.029(2)	0.002(2)	-0.004(2)	-0.001(1)
C(27)	0.025(2)	0.020(1)	0.033(2)	0.004(2)	0.000(3)	0.003(2)
C(28)	0.030(2)	0.026(2)	0.044(3)	0.001(2)	0.000(2)	0.009(2)
C(29)	0.030(3)	0.023(2)	0.044(2)	0.004(2)	-0.013(2)	-0.001(2)
C(30)	0.030(2)	0.025(2)	0.034(2)	0.007(2)	-0.006(2)	-0.010(2)
C(31)	0.020(2)	0.026(2)	0.027(2)	0.004(2)	-0.003(2)	-0.004(2)
C(32)	0.015(2)	0.022(2)	0.020(2)	-0.003(2)	0.002(1)	0.000(1)
C(33)	0.018(2)	0.024(2)	0.024(2)	-0.002(2)	-0.001(2)	0.004(1)
C(34)	0.030(2)	0.035(2)	0.022(2)	0.002(2)	0.000(2)	0.002(2)

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C(35)	0.019(2)	0.050(3)	0.028(2)	-0.010(2)	-0.004(2)	-0.001(2)
C(36)	0.021(2)	0.032(2)	0.033(2)	-0.006(2)	-0.003(2)	0.001(2)
C(37)	0.016(2)	0.022(2)	0.028(2)	-0.003(2)	0.004(2)	-0.001(1)
C(38)	0.019(2)	0.019(2)	0.023(2)	0.001(2)	-0.002(2)	-0.001(2)
C(39)	0.016(2)	0.020(2)	0.024(2)	0.001(2)	-0.002(2)	-0.001(2)
C(40)	0.020(2)	0.028(2)	0.026(2)	0.003(2)	-0.003(2)	-0.002(2)
C(41)	0.021(2)	0.017(2)	0.027(2)	-0.001(2)	-0.002(2)	0.002(2)
C(42)	0.029(2)	0.029(2)	0.032(2)	-0.002(2)	-0.001(2)	0.008(2)
C(43)	0.035(3)	0.022(2)	0.040(3)	0.004(2)	-0.001(2)	0.006(2)
C(44)	0.036(3)	0.019(2)	0.027(2)	0.003(2)	0.003(2)	-0.003(2)
C(45)	0.023(2)	0.026(2)	0.025(2)	0.002(2)	0.000(2)	0.001(2)
C(46)	0.022(2)	0.020(2)	0.019(2)	-0.001(1)	-0.001(2)	0.001(2)
C(47)	0.023(2)	0.020(2)	0.021(2)	0.000(2)	0.001(2)	-0.003(2)
C(48)	0.020(2)	0.019(2)	0.029(2)	0.005(2)	0.002(2)	-0.002(2)
C(49)	0.028(2)	0.027(2)	0.030(2)	0.004(2)	0.004(2)	0.001(2)
C(50)	0.014(2)	0.031(2)	0.040(3)	0.010(2)	0.004(2)	0.000(2)
C(51)	0.024(2)	0.033(2)	0.029(2)	0.001(2)	-0.004(2)	-0.008(2)
Cl	0.016(1)	0.026(1)	0.034(1)	0.007(1)	-0.003(1)	0.001(1)
N(1)	0.014(1)	0.024(2)	0.025(2)	0.005(2)	0.002(1)	0.001(1)
N(2)	0.015(1)	0.028(2)	0.026(2)	0.001(2)	-0.003(1)	0.000(2)
N(3)	0.015(2)	0.021(2)	0.032(2)	0.007(1)	0.002(1)	-0.002(1)
P	0.013(1)	0.018(1)	0.020(1)	0.001(1)	-0.001(1)	0.000(1)
Pd	0.013(1)	0.019(1)	0.022(1)	0.003(1)	0.000(1)	-0.001(1)



Crystallographic Data for (*R,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato-*C*₂,*N*]-[1-(2-*tert*-butyl-quinazolin-4-yl)(2-naphthyl)diphenylphosphine]palladium(II)chloride (*R,R*)-(17f)

Table 1. Crystal data and structure refinement.

Identification code	<i>(R,R)</i> -17f	
Empirical formula	C ₄₈ H ₄₅ ClN ₃ PPd	
Color	pale yellow	
Formula weight	836.69 g · mol ⁻¹	
Temperature	293 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2₁2₁2₁, (no. 19)	
Unit cell dimensions	a = 13.2921(1) Å	α = 90°.
	b = 14.3043(2) Å	β = 90°.
	c = 21.8897(2) Å	γ = 90°.
Volume	4161.98(8) Å ³	
Z	4	
Density (calculated)	1.335 Mg · m ⁻³	
Absorption coefficient	0.585 mm ⁻¹	
F(000)	1728 e	
Crystal size	0.26 x 0.24 x 0.19 mm ³	
θ range for data collection	4.15 to 28.28°.	
Index ranges	-17 ≤ h ≤ 16, -14 ≤ k ≤ 19, -26 ≤ l ≤ 29	
Reflections collected	27470	
Independent reflections	10281 [R _{int} = 0.0373]	
Reflections with I > 2σ(I)	9106	
Completeness to θ = 28.28°	99.5 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.91 and 0.88	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10281 / 0 / 487	
Goodness-of-fit on F ²	1.031	
Final R indices [I > 2σ(I)]	R ₁ = 0.0312	wR ² = 0.0715
R indices (all data)	R ₁ = 0.0394	wR ² = 0.0750
Absolute structure parameter	-0.037(16)	
Largest diff. peak and hole	0.443 and -0.300 e · Å ⁻³	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2).

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.5645(2)	0.4228(2)	0.9159(1)	0.035(1)
C(2)	0.5165(2)	0.3716(2)	0.8712(1)	0.035(1)
C(3)	0.5744(2)	0.3238(2)	0.8273(1)	0.044(1)
C(4)	0.6766(2)	0.3231(2)	0.8282(1)	0.047(1)
C(5)	0.7285(2)	0.3714(2)	0.8749(1)	0.045(1)
C(6)	0.8346(3)	0.3693(2)	0.8789(2)	0.064(1)
C(7)	0.8835(3)	0.4142(3)	0.9250(2)	0.075(1)
C(8)	0.8292(3)	0.4648(2)	0.9680(2)	0.068(1)
C(9)	0.7266(2)	0.4700(2)	0.9654(2)	0.055(1)
C(10)	0.6722(2)	0.4224(2)	0.9190(1)	0.039(1)
C(11)	0.5115(2)	0.4833(2)	0.9620(1)	0.039(1)
C(12)	0.4533(3)	0.6281(2)	0.9883(2)	0.069(1)
C(13)	0.4453(2)	0.5159(3)	1.0611(1)	0.068(1)
C(14)	0.4195(3)	0.4869(5)	1.1210(2)	0.097(2)
C(15)	0.4397(3)	0.4001(5)	1.1389(2)	0.109(2)
C(16)	0.4845(3)	0.3327(4)	1.1003(2)	0.087(1)
C(17)	0.5083(2)	0.3581(2)	1.0412(1)	0.059(1)
C(18)	0.4891(2)	0.4491(2)	1.0212(1)	0.046(1)
C(19)	0.4406(4)	0.7301(3)	0.9690(3)	0.112(2)
C(20)	0.5161(8)	0.7828(5)	0.9888(7)	0.340(10)
C(21)	0.3994(14)	0.7384(4)	0.9121(6)	0.414(14)
C(22)	0.3510(11)	0.7691(6)	1.0084(12)	0.450(16)
C(23)	0.3677(2)	0.4410(2)	0.7936(1)	0.039(1)
C(24)	0.3926(2)	0.5352(2)	0.8015(1)	0.047(1)
C(25)	0.3819(3)	0.5968(2)	0.7539(2)	0.062(1)
C(26)	0.3505(3)	0.5661(2)	0.6971(2)	0.065(1)
C(27)	0.3304(3)	0.4735(2)	0.6879(1)	0.063(1)
C(28)	0.3387(2)	0.4105(2)	0.7361(1)	0.050(1)
C(29)	0.3057(2)	0.4001(2)	0.9209(1)	0.035(1)
C(30)	0.2601(2)	0.4868(2)	0.9242(1)	0.045(1)
C(31)	0.1953(2)	0.5084(2)	0.9715(1)	0.056(1)
C(32)	0.1747(3)	0.4437(2)	1.0161(1)	0.062(1)
C(33)	0.2202(3)	0.3574(2)	1.0140(1)	0.062(1)
C(34)	0.2852(2)	0.3352(2)	0.9669(1)	0.050(1)
C(35)	0.2104(2)	0.2404(2)	0.7943(1)	0.039(1)

C(36)	0.1498(2)	0.3216(2)	0.8010(1)	0.045(1)
C(37)	0.0602(2)	0.3309(2)	0.7710(1)	0.053(1)
C(38)	0.0222(2)	0.2579(2)	0.7346(1)	0.055(1)
C(39)	-0.0736(3)	0.2627(3)	0.7061(2)	0.078(1)
C(40)	-0.1100(3)	0.1905(3)	0.6726(2)	0.100(2)
C(41)	-0.0538(3)	0.1095(3)	0.6660(2)	0.094(1)
C(42)	0.0396(3)	0.1013(3)	0.6914(2)	0.068(1)
C(43)	0.0789(2)	0.1745(2)	0.7278(1)	0.050(1)
C(44)	0.1743(2)	0.1682(2)	0.7590(1)	0.043(1)
C(45)	0.2409(2)	0.0833(2)	0.7526(1)	0.049(1)
C(46)	0.3150(3)	0.0974(2)	0.7002(2)	0.070(1)
C(47)	0.2194(2)	0.0361(2)	0.8583(2)	0.060(1)
C(48)	0.3751(2)	0.0010(2)	0.8094(2)	0.063(1)
Cl	0.4651(1)	0.1537(1)	0.9073(1)	0.053(1)
N(1)	0.4950(2)	0.5698(2)	0.9454(1)	0.050(1)
N(2)	0.4286(2)	0.6050(3)	1.0433(2)	0.081(1)
N(3)	0.2921(2)	0.0706(1)	0.8130(1)	0.045(1)
P	0.3808(1)	0.3584(1)	0.8568(1)	0.033(1)
Pd	0.3377(1)	0.2087(1)	0.8391(1)	0.036(1)

Table 3. Bond lengths [Å] and angles [°].

C(1)-C(2)	1.379(3)	C(1)-C(10)	1.433(3)
C(1)-C(11)	1.504(3)	C(2)-C(3)	1.409(3)
C(2)-P	1.840(2)	C(3)-C(4)	1.358(4)
C(4)-C(5)	1.414(4)	C(5)-C(6)	1.414(4)
C(5)-C(10)	1.423(4)	C(6)-C(7)	1.361(5)
C(7)-C(8)	1.389(5)	C(8)-C(9)	1.367(5)
C(9)-C(10)	1.420(4)	C(11)-N(1)	1.308(3)
C(11)-C(18)	1.416(4)	C(12)-N(2)	1.290(5)
C(12)-N(1)	1.373(4)	C(12)-C(19)	1.528(6)
C(13)-N(2)	1.350(5)	C(13)-C(14)	1.418(6)
C(13)-C(18)	1.420(4)	C(14)-C(15)	1.329(7)
C(15)-C(16)	1.413(7)	C(16)-C(17)	1.380(4)
C(17)-C(18)	1.397(4)	C(19)-C(20)	1.327(7)
C(19)-C(21)	1.366(9)	C(19)-C(22)	1.571(14)
C(23)-C(28)	1.386(4)	C(23)-C(24)	1.399(4)
C(23)-P	1.827(2)	C(24)-C(25)	1.373(4)
C(25)-C(26)	1.383(5)	C(26)-C(27)	1.367(5)
C(27)-C(28)	1.392(4)	C(29)-C(30)	1.382(3)
C(29)-C(34)	1.396(4)	C(29)-P	1.823(2)
C(30)-C(31)	1.382(4)	C(31)-C(32)	1.374(4)
C(32)-C(33)	1.375(5)	C(33)-C(34)	1.383(4)
C(35)-C(44)	1.376(3)	C(35)-C(36)	1.421(4)
C(35)-Pd	2.007(2)	C(36)-C(37)	1.365(4)
C(37)-C(38)	1.407(4)	C(38)-C(43)	1.420(4)
C(38)-C(39)	1.420(4)	C(39)-C(40)	1.354(5)
C(40)-C(41)	1.387(6)	C(41)-C(42)	1.365(5)
C(42)-C(43)	1.416(4)	C(43)-C(44)	1.443(4)
C(44)-C(45)	1.509(4)	C(45)-N(3)	1.498(4)
C(45)-C(46)	1.525(4)	C(47)-N(3)	1.469(4)
C(48)-N(3)	1.488(4)	Cl-Pd	2.3901(7)
N(3)-Pd	2.145(2)	P-Pd	2.2495(6)
C(2)-C(1)-C(10)	119.6(2)	C(2)-C(1)-C(11)	124.4(2)
C(10)-C(1)-C(11)	116.0(2)	C(1)-C(2)-C(3)	119.3(2)
C(1)-C(2)-P	129.01(19)	C(3)-C(2)-P	111.61(18)
C(4)-C(3)-C(2)	122.6(2)	C(3)-C(4)-C(5)	119.7(2)
C(6)-C(5)-C(4)	121.4(3)	C(6)-C(5)-C(10)	119.6(3)
C(4)-C(5)-C(10)	118.9(2)	C(7)-C(6)-C(5)	120.8(3)

C(6)-C(7)-C(8)	120.0(3)	C(9)-C(8)-C(7)	121.2(3)
C(8)-C(9)-C(10)	120.8(3)	C(9)-C(10)-C(5)	117.5(3)
C(9)-C(10)-C(1)	122.7(2)	C(5)-C(10)-C(1)	119.7(2)
N(1)-C(11)-C(18)	123.1(2)	N(1)-C(11)-C(1)	115.9(2)
C(18)-C(11)-C(1)	120.8(2)	N(2)-C(12)-N(1)	125.8(3)
N(2)-C(12)-C(19)	118.3(4)	N(1)-C(12)-C(19)	115.8(4)
N(2)-C(13)-C(14)	120.2(4)	N(2)-C(13)-C(18)	121.7(3)
C(14)-C(13)-C(18)	118.1(4)	C(15)-C(14)-C(13)	119.8(4)
C(14)-C(15)-C(16)	123.1(4)	C(17)-C(16)-C(15)	118.5(4)
C(16)-C(17)-C(18)	119.8(4)	C(17)-C(18)-C(11)	124.8(3)
C(17)-C(18)-C(13)	120.6(3)	C(11)-C(18)-C(13)	114.6(3)
C(20)-C(19)-C(21)	123.4(10)	C(20)-C(19)-C(12)	111.7(5)
C(21)-C(19)-C(12)	112.3(4)	C(20)-C(19)-C(22)	101.1(10)
C(21)-C(19)-C(22)	99.5(11)	C(12)-C(19)-C(22)	105.7(6)
C(28)-C(23)-C(24)	118.8(2)	C(28)-C(23)-P	120.7(2)
C(24)-C(23)-P	120.4(2)	C(25)-C(24)-C(23)	120.0(3)
C(24)-C(25)-C(26)	120.6(3)	C(27)-C(26)-C(25)	120.0(3)
C(26)-C(27)-C(28)	120.0(3)	C(23)-C(28)-C(27)	120.4(3)
C(30)-C(29)-C(34)	118.2(2)	C(30)-C(29)-P	125.03(19)
C(34)-C(29)-P	116.40(18)	C(31)-C(30)-C(29)	120.9(3)
C(32)-C(31)-C(30)	120.4(3)	C(33)-C(32)-C(31)	119.5(3)
C(32)-C(33)-C(34)	120.4(3)	C(33)-C(34)-C(29)	120.5(3)
C(44)-C(35)-C(36)	118.3(2)	C(44)-C(35)-Pd	113.45(19)
C(36)-C(35)-Pd	127.79(19)	C(37)-C(36)-C(35)	121.6(3)
C(36)-C(37)-C(38)	120.9(3)	C(37)-C(38)-C(43)	119.5(3)
C(37)-C(38)-C(39)	122.4(3)	C(43)-C(38)-C(39)	118.1(3)
C(40)-C(39)-C(38)	121.4(4)	C(39)-C(40)-C(41)	120.1(3)
C(42)-C(41)-C(40)	121.2(4)	C(41)-C(42)-C(43)	120.1(4)
C(42)-C(43)-C(38)	119.0(3)	C(42)-C(43)-C(44)	123.0(3)
C(38)-C(43)-C(44)	118.0(2)	C(35)-C(44)-C(43)	121.7(3)
C(35)-C(44)-C(45)	116.9(2)	C(43)-C(44)-C(45)	121.4(2)
N(3)-C(45)-C(44)	106.4(2)	N(3)-C(45)-C(46)	112.7(2)
C(44)-C(45)-C(46)	110.1(2)	C(11)-N(1)-C(12)	116.9(3)
C(12)-N(2)-C(13)	118.0(3)	C(47)-N(3)-C(48)	107.4(2)
C(47)-N(3)-C(45)	109.7(2)	C(48)-N(3)-C(45)	111.9(2)
C(47)-N(3)-Pd	108.33(17)	C(48)-N(3)-Pd	114.90(17)
C(45)-N(3)-Pd	104.55(16)	C(29)-P-C(23)	108.60(11)
C(29)-P-C(2)	111.77(11)	C(23)-P-C(2)	99.01(11)
C(29)-P-Pd	107.71(8)	C(23)-P-Pd	117.45(8)
C(2)-P-Pd	112.16(8)	C(35)-Pd-N(3)	80.79(9)

C(35)-Pd-P	94.80(7)	N(3)-Pd-P	174.07(6)
C(35)-Pd-Cl	167.52(7)	N(3)-Pd-Cl	93.62(6) P-
Pd-Cl	91.46(2)		

Table 4. Anisotropic displacement parameters (\AA^2).

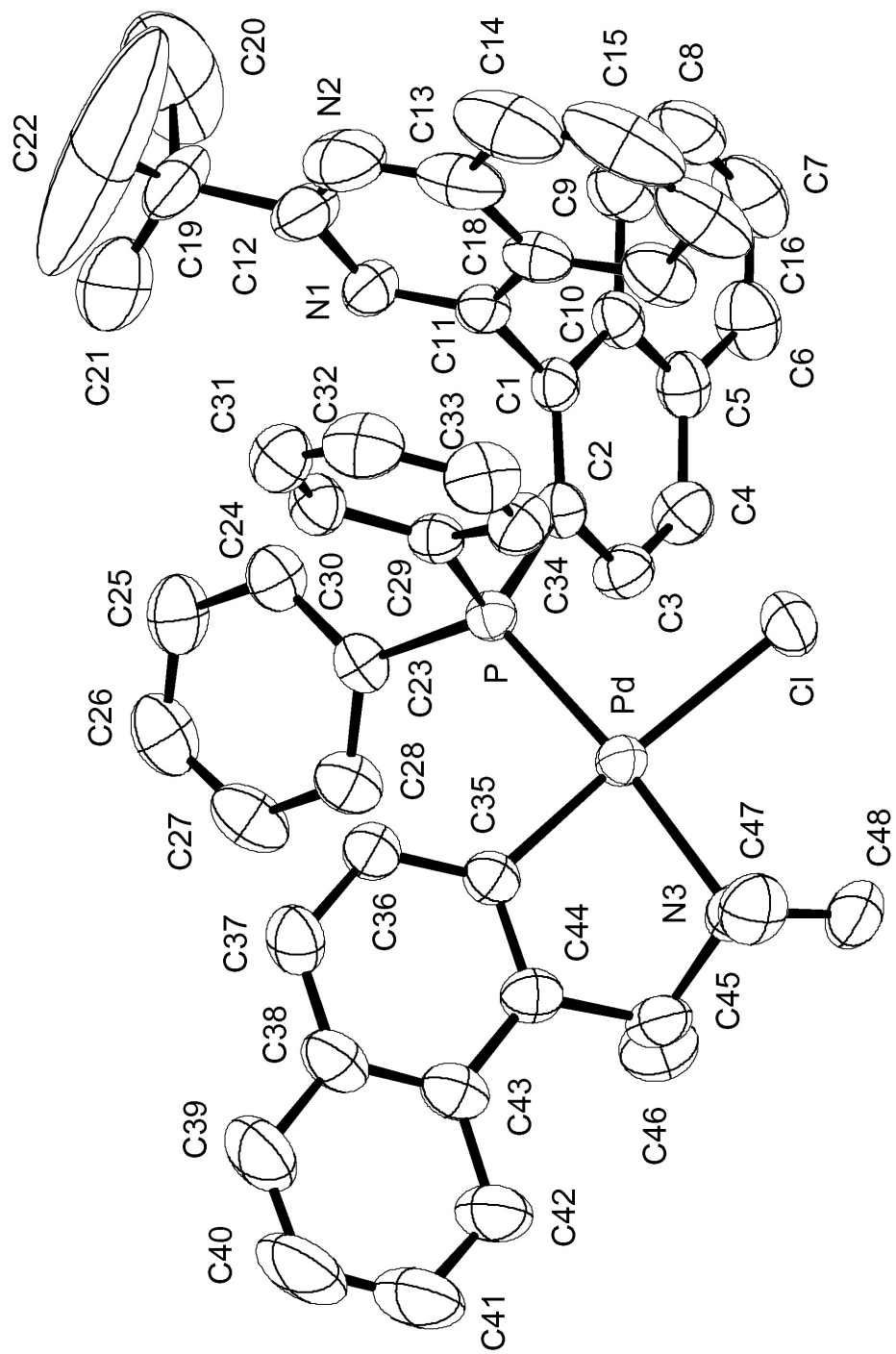
The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}].$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	0.037(1)	0.030(1)	0.037(1)	0.005(1)	-0.002(1)	0.000(1)
C(2)	0.032(1)	0.036(1)	0.038(1)	0.003(1)	0.002(1)	0.001(1)
C(3)	0.043(1)	0.045(1)	0.044(2)	-0.009(1)	0.002(1)	0.000(1)
C(4)	0.042(2)	0.048(1)	0.050(2)	-0.004(1)	0.008(1)	0.002(1)
C(5)	0.038(1)	0.042(1)	0.055(2)	0.010(1)	0.003(1)	0.001(1)
C(6)	0.040(2)	0.070(2)	0.080(2)	0.010(2)	0.004(2)	0.005(2)
C(7)	0.034(2)	0.096(3)	0.094(3)	0.019(2)	-0.008(2)	-0.005(2)
C(8)	0.047(2)	0.081(2)	0.077(2)	0.001(2)	-0.019(2)	-0.013(2)
C(9)	0.048(2)	0.061(2)	0.058(2)	0.004(1)	-0.009(1)	-0.009(1)
C(10)	0.038(1)	0.038(1)	0.041(1)	0.008(1)	-0.003(1)	-0.002(1)
C(11)	0.034(1)	0.038(1)	0.044(1)	-0.006(1)	-0.006(1)	-0.002(1)
C(12)	0.061(2)	0.054(2)	0.093(3)	-0.032(2)	-0.020(2)	0.008(2)
C(13)	0.045(2)	0.111(3)	0.048(2)	-0.027(2)	-0.003(1)	0.000(2)
C(14)	0.062(2)	0.182(5)	0.048(2)	-0.026(3)	0.006(2)	0.003(3)
C(15)	0.057(2)	0.229(7)	0.041(2)	0.016(3)	0.004(2)	-0.027(3)
C(16)	0.062(2)	0.138(4)	0.062(2)	0.038(2)	-0.012(2)	-0.034(2)
C(17)	0.056(2)	0.072(2)	0.049(2)	0.013(2)	-0.007(1)	-0.015(2)
C(18)	0.035(1)	0.063(2)	0.040(1)	-0.008(1)	-0.002(1)	-0.006(1)
C(19)	0.119(4)	0.045(2)	0.174(5)	-0.044(3)	-0.055(4)	0.022(2)
C(20)	0.322(13)	0.096(4)	0.60(2)	0.126(9)	-0.331(15)	-0.117(7)
C(21)	0.77(3)	0.040(3)	0.431(17)	-0.011(5)	-0.46(2)	0.057(7)
C(22)	0.279(15)	0.097(6)	0.97(5)	-0.028(13)	0.26(2)	0.062(8)
C(23)	0.034(1)	0.045(1)	0.039(1)	0.007(1)	0.001(1)	0.000(1)
C(24)	0.048(2)	0.049(2)	0.046(2)	0.011(1)	0.004(1)	-0.003(1)
C(25)	0.068(2)	0.050(2)	0.069(2)	0.022(1)	0.007(2)	-0.002(2)
C(26)	0.065(2)	0.075(2)	0.056(2)	0.031(2)	0.005(2)	0.000(2)
C(27)	0.060(2)	0.092(2)	0.037(1)	0.014(1)	-0.004(2)	-0.005(2)
C(28)	0.049(1)	0.061(2)	0.041(1)	0.006(1)	0.002(1)	-0.006(1)
C(29)	0.031(1)	0.040(1)	0.035(1)	-0.004(1)	0.000(1)	-0.002(1)
C(30)	0.043(1)	0.048(2)	0.044(2)	0.000(1)	0.002(1)	0.006(1)
C(31)	0.053(2)	0.059(2)	0.056(2)	-0.008(1)	0.007(1)	0.014(1)
C(32)	0.053(2)	0.085(2)	0.047(2)	-0.014(2)	0.014(2)	-0.002(2)
C(33)	0.069(2)	0.070(2)	0.048(2)	0.006(2)	0.013(2)	-0.012(2)
C(34)	0.062(2)	0.046(1)	0.042(1)	0.000(1)	0.007(1)	-0.001(1)

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C(35)	0.034(1)	0.042(1)	0.041(1)	0.000(1)	-0.002(1)	-0.003(1)
C(36)	0.040(1)	0.044(1)	0.053(1)	-0.003(1)	-0.005(1)	0.000(1)
C(37)	0.038(1)	0.055(2)	0.066(2)	0.005(1)	-0.002(1)	0.006(1)
C(38)	0.042(2)	0.067(2)	0.056(2)	0.008(1)	-0.013(1)	-0.006(1)
C(39)	0.054(2)	0.089(3)	0.093(3)	0.010(2)	-0.028(2)	0.005(2)
C(40)	0.071(2)	0.123(4)	0.107(3)	0.010(3)	-0.053(3)	-0.017(3)
C(41)	0.088(3)	0.103(3)	0.092(3)	-0.008(3)	-0.044(3)	-0.022(2)
C(42)	0.068(2)	0.070(2)	0.066(2)	-0.007(2)	-0.021(2)	-0.015(2)
C(43)	0.046(2)	0.059(2)	0.045(2)	0.002(1)	-0.006(1)	-0.010(1)
C(44)	0.041(1)	0.044(1)	0.043(1)	-0.001(1)	0.000(1)	-0.008(1)
C(45)	0.048(2)	0.046(1)	0.052(2)	-0.014(1)	-0.004(1)	-0.006(1)
C(46)	0.083(3)	0.077(2)	0.050(2)	-0.016(2)	0.008(2)	0.006(2)
C(47)	0.060(2)	0.052(2)	0.068(2)	0.005(1)	0.004(2)	-0.009(1)
C(48)	0.062(2)	0.043(2)	0.084(2)	-0.012(2)	-0.008(2)	0.011(1)
Cl	0.047(1)	0.052(1)	0.060(1)	0.006(1)	-0.012(1)	0.006(1)
N(1)	0.048(1)	0.036(1)	0.067(2)	-0.009(1)	-0.012(1)	0.001(1)
N(2)	0.067(2)	0.093(2)	0.083(2)	-0.047(2)	-0.010(2)	0.019(2)
N(3)	0.045(1)	0.036(1)	0.054(1)	-0.004(1)	-0.002(1)	-0.001(1)
P	0.032(1)	0.033(1)	0.033(1)	-0.001(1)	0.000(1)	-0.001(1)
Pd	0.033(1)	0.033(1)	0.041(1)	-0.004(1)	-0.002(1)	0.000(1)



Crystallographic Data for (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato-*C*₂,*N*]-[1-(quinazolin-4-yl)(2-naphthyl)diphenylphosphine]palladium(II) hexafluorophosphate
(*S,R*)-(18a)

Table 1. Crystal data and structure refinement.

Identification code	(<i>S,R</i>)-18a	
Empirical formula	C ₄₆ H ₃₉ Cl ₆ F ₆ N ₃ P ₂ Pd	
Color	pale yellow	
Formula weight	1128.84 g · mol ⁻¹	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2₁2₁2₁, (no. 19)	
Unit cell dimensions	a = 13.2070(7) Å	α = 90°.
	b = 13.9716(8) Å	β = 90°.
	c = 25.6685(14) Å	γ = 90°.
Volume	4736.4(5) Å ³	
Z	4	
Density (calculated)	1.583 Mg · m ⁻³	
Absorption coefficient	0.859 mm ⁻¹	
F(000)	2272 e	
Crystal size	0.26 x 0.16 x 0.09 mm ³	
θ range for data collection	1.59 to 27.48°.	
Index ranges	-17 ≤ h ≤ 13, -18 ≤ k ≤ 13, -33 ≤ l ≤ 30	
Reflections collected	42281	
Independent reflections	10666 [R _{int} = 0.1477]	
Reflections with I > 2σ(I)	6413	
Completeness to θ = 27.48°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.92044 and 0.87353	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10666 / 0 / 577	
Goodness-of-fit on F ²	0.997	
Final R indices [I > 2σ(I)]	R ₁ = 0.0600	wR ² = 0.0990
R indices (all data)	R ₁ = 0.1287	wR ² = 0.1149
Absolute structure parameter	-0.05(3)	
Largest diff. peak and hole	0.906 and -0.546 e · Å ⁻³	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2).

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.7514(4)	1.0681(5)	0.9077(3)	0.022(2)
C(2)	0.7387(5)	1.0689(5)	0.8179(3)	0.022(2)
C(3)	0.7225(4)	1.2129(4)	0.8588(3)	0.023(2)
C(4)	0.7049(4)	1.3118(5)	0.8563(3)	0.031(2)
C(5)	0.7076(5)	1.3657(5)	0.9000(3)	0.036(2)
C(6)	0.7294(5)	1.3242(5)	0.9486(3)	0.033(2)
C(7)	0.7435(5)	1.2282(5)	0.9532(2)	0.024(2)
C(8)	0.7393(5)	1.1689(4)	0.9079(2)	0.020(2)
C(9)	0.7690(5)	1.0171(5)	0.9582(2)	0.020(2)
C(10)	0.8613(4)	0.9724(4)	0.9678(2)	0.022(2)
C(11)	0.8835(5)	0.9407(4)	1.0193(2)	0.022(2)
C(12)	0.8144(5)	0.9502(5)	1.0583(2)	0.026(2)
C(13)	0.7166(5)	0.9833(5)	1.0483(2)	0.024(2)
C(14)	0.6393(5)	0.9842(5)	1.0859(2)	0.031(2)
C(15)	0.5437(5)	1.0129(5)	1.0755(3)	0.031(2)
C(16)	0.5188(5)	1.0440(5)	1.0248(3)	0.030(2)
C(17)	0.5926(5)	1.0481(5)	0.9869(3)	0.027(2)
C(18)	0.6922(5)	1.0185(4)	0.9972(2)	0.021(2)
C(19)	0.9965(4)	1.0651(4)	0.8969(2)	0.021(2)
C(20)	0.9972(4)	1.0949(4)	0.8449(2)	0.022(2)
C(21)	1.0235(5)	1.1881(5)	0.8324(2)	0.027(2)
C(22)	1.0488(5)	1.2510(5)	0.8714(2)	0.032(2)
C(23)	1.0519(5)	1.2232(5)	0.9228(3)	0.030(2)
C(24)	1.0249(4)	1.1284(4)	0.9346(2)	0.020(1)
C(25)	1.0453(5)	0.8760(5)	0.9416(2)	0.022(1)
C(26)	1.1429(5)	0.9087(5)	0.9502(2)	0.029(2)
C(27)	1.2126(5)	0.8486(6)	0.9734(3)	0.043(2)
C(28)	1.1851(7)	0.7572(6)	0.9891(3)	0.044(2)
C(29)	1.0884(6)	0.7242(5)	0.9803(3)	0.040(2)
C(30)	1.0203(5)	0.7835(5)	0.9564(2)	0.029(2)
C(31)	0.9233(5)	0.7716(4)	0.8347(2)	0.023(2)
C(32)	1.0313(4)	0.7709(5)	0.8281(2)	0.020(1)
C(33)	1.0776(5)	0.6907(4)	0.8103(2)	0.021(2)
C(34)	1.0236(4)	0.6057(5)	0.8006(2)	0.019(1)
C(35)	1.0712(5)	0.5197(5)	0.7849(2)	0.021(2)

C(36)	1.0173(5)	0.4395(5)	0.7749(2)	0.024(2)
C(37)	0.9119(5)	0.4385(5)	0.7803(2)	0.024(2)
C(38)	0.8628(5)	0.5200(4)	0.7953(2)	0.023(2)
C(39)	0.9160(4)	0.6055(5)	0.8055(2)	0.019(1)
C(40)	0.8680(5)	0.6935(5)	0.8215(2)	0.023(2)
C(41)	0.7547(5)	0.7016(4)	0.8277(2)	0.019(2)
C(42)	0.7211(5)	0.6731(5)	0.8812(2)	0.029(2)
C(43)	0.6237(4)	0.8300(5)	0.8300(3)	0.030(2)
C(44)	0.7320(5)	0.8126(5)	0.7559(2)	0.025(2)
C(45)	1.0796(5)	0.7199(5)	1.3827(3)	0.029(2)
C(46)	1.3550(6)	0.9523(6)	0.8301(3)	0.045(2)
Cl(1)	1.0344(1)	0.8066(1)	1.3389(1)	0.038(1)
Cl(2)	1.2112(2)	0.7116(2)	1.3806(1)	0.058(1)
Cl(3)	1.0405(2)	0.7455(2)	1.4467(1)	0.048(1)
Cl(4)	1.3291(2)	0.8359(2)	0.8086(1)	0.068(1)
Cl(5)	1.4143(2)	0.9497(2)	0.8922(1)	0.055(1)
Cl(6)	1.2420(1)	1.0197(2)	0.8334(1)	0.048(1)
F(1)	0.9974(3)	0.9971(3)	1.1398(2)	0.045(1)
F(2)	1.1007(3)	0.9789(3)	1.2093(2)	0.043(1)
F(3)	0.9831(3)	0.8665(3)	1.1904(2)	0.057(1)
F(4)	0.9779(3)	1.0899(3)	1.2107(2)	0.037(1)
F(5)	0.9631(3)	0.9599(3)	1.2617(1)	0.040(1)
F(6)	0.8593(3)	0.9788(3)	1.1922(1)	0.041(1)
N(1)	0.7553(3)	1.0194(4)	0.8635(2)	0.021(1)
N(2)	0.7222(4)	1.1593(4)	0.8135(2)	0.026(1)
N(3)	0.7281(4)	0.8032(4)	0.8137(2)	0.020(1)
P(1)	0.9467(1)	0.9491(1)	0.9129(1)	0.021(1)
P(2)	0.9802(1)	0.9774(1)	1.2006(1)	0.028(1)
Pd	0.8393(1)	0.8856(1)	0.8539(1)	0.019(1)

Table 3. Bond lengths [Å] and angles [°].

C(1)-N(1)	1.323(8)	C(1)-C(8)	1.418(8)
C(1)-C(9)	1.497(9)	C(2)-N(2)	1.286(8)
C(2)-N(1)	1.379(8)	C(3)-N(2)	1.382(8)
C(3)-C(4)	1.402(8)	C(3)-C(8)	1.420(9)
C(4)-C(5)	1.353(9)	C(5)-C(6)	1.405(9)
C(6)-C(7)	1.359(9)	C(7)-C(8)	1.428(9)
C(9)-C(10)	1.392(8)	C(9)-C(18)	1.426(8)
C(10)-C(11)	1.424(8)	C(10)-P(1)	1.835(6)
C(11)-C(12)	1.361(8)	C(12)-C(13)	1.396(9)
C(13)-C(14)	1.404(8)	C(13)-C(18)	1.437(8)
C(14)-C(15)	1.351(9)	C(15)-C(16)	1.412(9)
C(16)-C(17)	1.377(9)	C(17)-C(18)	1.404(9)
C(19)-C(24)	1.362(8)	C(19)-C(20)	1.399(8)
C(19)-P(1)	1.797(6)	C(20)-C(21)	1.386(9)
C(21)-C(22)	1.374(9)	C(22)-C(23)	1.376(9)
C(23)-C(24)	1.405(9)	C(25)-C(26)	1.385(8)
C(25)-C(30)	1.387(9)	C(25)-P(1)	1.811(6)
C(26)-C(27)	1.382(9)	C(27)-C(28)	1.388(11)
C(28)-C(29)	1.377(11)	C(29)-C(30)	1.369(9)
C(31)-C(40)	1.355(9)	C(31)-C(32)	1.437(9)
C(31)-Pd	2.002(6)	C(32)-C(33)	1.356(9)
C(33)-C(34)	1.408(9)	C(34)-C(35)	1.415(9)
C(34)-C(39)	1.427(8)	C(35)-C(36)	1.352(9)
C(36)-C(37)	1.399(8)	C(37)-C(38)	1.366(8)
C(38)-C(39)	1.410(9)	C(39)-C(40)	1.443(9)
C(40)-C(41)	1.510(9)	C(41)-C(42)	1.497(8)
C(41)-N(3)	1.506(8)	C(43)-N(3)	1.488(7)
C(44)-N(3)	1.491(7)	C(45)-Cl(2)	1.743(7)
C(45)-Cl(1)	1.757(7)	C(45)-Cl(3)	1.758(7)
C(46)-Cl(4)	1.752(8)	C(46)-Cl(6)	1.767(8)
C(46)-Cl(5)	1.778(7)	F(1)-P(2)	1.602(4) F(2)-
P(2)	1.608(4)	F(3)-P(2)	1.571(4) F(4)-
P(2)	1.594(4)	F(5)-P(2)	1.602(4) F(6)-
P(2)	1.611(4)	N(1)-Pd	2.189(5)
N(3)-Pd	2.132(5)	P(1)-Pd	2.2564(17)
N(1)-C(1)-C(8)	121.1(6)	N(1)-C(1)-C(9)	119.4(6)
C(8)-C(1)-C(9)	119.2(6)	N(2)-C(2)-N(1)	126.4(7)

N(2)-C(3)-C(4)	119.7(6)	N(2)-C(3)-C(8)	120.8(5)
C(4)-C(3)-C(8)	119.5(7)	C(5)-C(4)-C(3)	120.4(7)
C(4)-C(5)-C(6)	120.8(6)	C(7)-C(6)-C(5)	120.8(6)
C(6)-C(7)-C(8)	119.8(6)	C(1)-C(8)-C(3)	116.4(6)
C(1)-C(8)-C(7)	125.0(6)	C(3)-C(8)-C(7)	118.5(6)
C(10)-C(9)-C(18)	120.3(5)	C(10)-C(9)-C(1)	120.2(5)
C(18)-C(9)-C(1)	119.4(5)	C(9)-C(10)-C(11)	119.0(5)
C(9)-C(10)-P(1)	118.8(4)	C(11)-C(10)-P(1)	122.1(5)
C(12)-C(11)-C(10)	120.9(6)	C(11)-C(12)-C(13)	121.2(6)
C(12)-C(13)-C(14)	123.3(6)	C(12)-C(13)-C(18)	119.3(6)
C(14)-C(13)-C(18)	117.5(6)	C(15)-C(14)-C(13)	123.1(6)
C(14)-C(15)-C(16)	119.4(6)	C(17)-C(16)-C(15)	119.9(7)
C(16)-C(17)-C(18)	121.2(6)	C(17)-C(18)-C(9)	122.6(6)
C(17)-C(18)-C(13)	118.8(6)	C(9)-C(18)-C(13)	118.5(6)
C(24)-C(19)-C(20)	118.8(6)	C(24)-C(19)-P(1)	121.7(5)
C(20)-C(19)-P(1)	119.2(5)	C(21)-C(20)-C(19)	120.2(6)
C(22)-C(21)-C(20)	119.5(6)	C(21)-C(22)-C(23)	121.8(6)
C(22)-C(23)-C(24)	117.7(6)	C(19)-C(24)-C(23)	121.9(6)
C(26)-C(25)-C(30)	119.0(6)	C(26)-C(25)-P(1)	123.2(5)
C(30)-C(25)-P(1)	117.7(5)	C(27)-C(26)-C(25)	119.2(7)
C(26)-C(27)-C(28)	120.7(7)	C(29)-C(28)-C(27)	120.2(7)
C(30)-C(29)-C(28)	118.7(7)	C(29)-C(30)-C(25)	122.1(7)
C(40)-C(31)-C(32)	119.9(6)	C(40)-C(31)-Pd	113.8(5)
C(32)-C(31)-Pd	125.8(5)	C(33)-C(32)-C(31)	119.6(6)
C(32)-C(33)-C(34)	121.9(6)	C(33)-C(34)-C(35)	122.8(5)
C(33)-C(34)-C(39)	119.4(6)	C(35)-C(34)-C(39)	117.8(6)
C(36)-C(35)-C(34)	121.6(6)	C(35)-C(36)-C(37)	120.9(6)
C(38)-C(37)-C(36)	119.4(6)	C(37)-C(38)-C(39)	121.5(6)
C(38)-C(39)-C(34)	118.8(6)	C(38)-C(39)-C(40)	123.8(5)
C(34)-C(39)-C(40)	117.4(6)	C(31)-C(40)-C(39)	121.4(6)
C(31)-C(40)-C(41)	116.6(6)	C(39)-C(40)-C(41)	121.9(6)
C(42)-C(41)-N(3)	113.5(5)	C(42)-C(41)-C(40)	111.8(5)
N(3)-C(41)-C(40)	106.1(5)	Cl(2)-C(45)-Cl(1)	111.4(4)
Cl(2)-C(45)-Cl(3)	109.6(4)	Cl(1)-C(45)-Cl(3)	110.9(4)
Cl(4)-C(46)-Cl(6)	110.2(4)	Cl(4)-C(46)-Cl(5)	110.4(4)
Cl(6)-C(46)-Cl(5)	109.9(4)	C(1)-N(1)-C(2)	117.7(6)
C(1)-N(1)-Pd	123.7(4)	C(2)-N(1)-Pd	114.4(4)
C(2)-N(2)-C(3)	117.3(6)	C(43)-N(3)-C(44)	106.8(5)
C(43)-N(3)-C(41)	112.8(5)	C(44)-N(3)-C(41)	108.2(5)
C(43)-N(3)-Pd	111.5(4)	C(44)-N(3)-Pd	114.2(4)

C(41)-N(3)-Pd	103.5(4)	C(19)-P(1)-C(25)	109.7(3)	
C(19)-P(1)-C(10)	103.9(3)	C(25)-P(1)-C(10)	103.2(3)	
C(19)-P(1)-Pd	115.6(2)	C(25)-P(1)-Pd	120.2(2)	
C(10)-P(1)-Pd	101.49(19)	F(3)-P(2)-F(4)	179.6(3)	F(3)-
P(2)-F(5)	91.0(2)	F(4)-P(2)-F(5)	89.3(2)	F(3)-
P(2)-F(1)	90.2(2)	F(4)-P(2)-F(1)	89.5(2)	F(5)-
P(2)-F(1)	178.9(2)	F(3)-P(2)-F(2)	90.7(2)	F(4)-
P(2)-F(2)	89.0(2)	F(5)-P(2)-F(2)	90.3(2)	F(1)-
P(2)-F(2)	89.6(2)	F(3)-P(2)-F(6)	90.8(2)	F(4)-
P(2)-F(6)	89.5(2)	F(5)-P(2)-F(6)	89.6(2)	F(1)-
P(2)-F(6)	90.4(2)	F(2)-P(2)-F(6)	178.5(3)	
C(31)-Pd-N(3)	80.4(2)	C(31)-Pd-N(1)	171.2(2)	
N(3)-Pd-N(1)	99.61(18)	C(31)-Pd-P(1)	97.45(18)	
N(3)-Pd-P(1)	165.91(15)	N(1)-Pd-P(1)	84.65(14)	

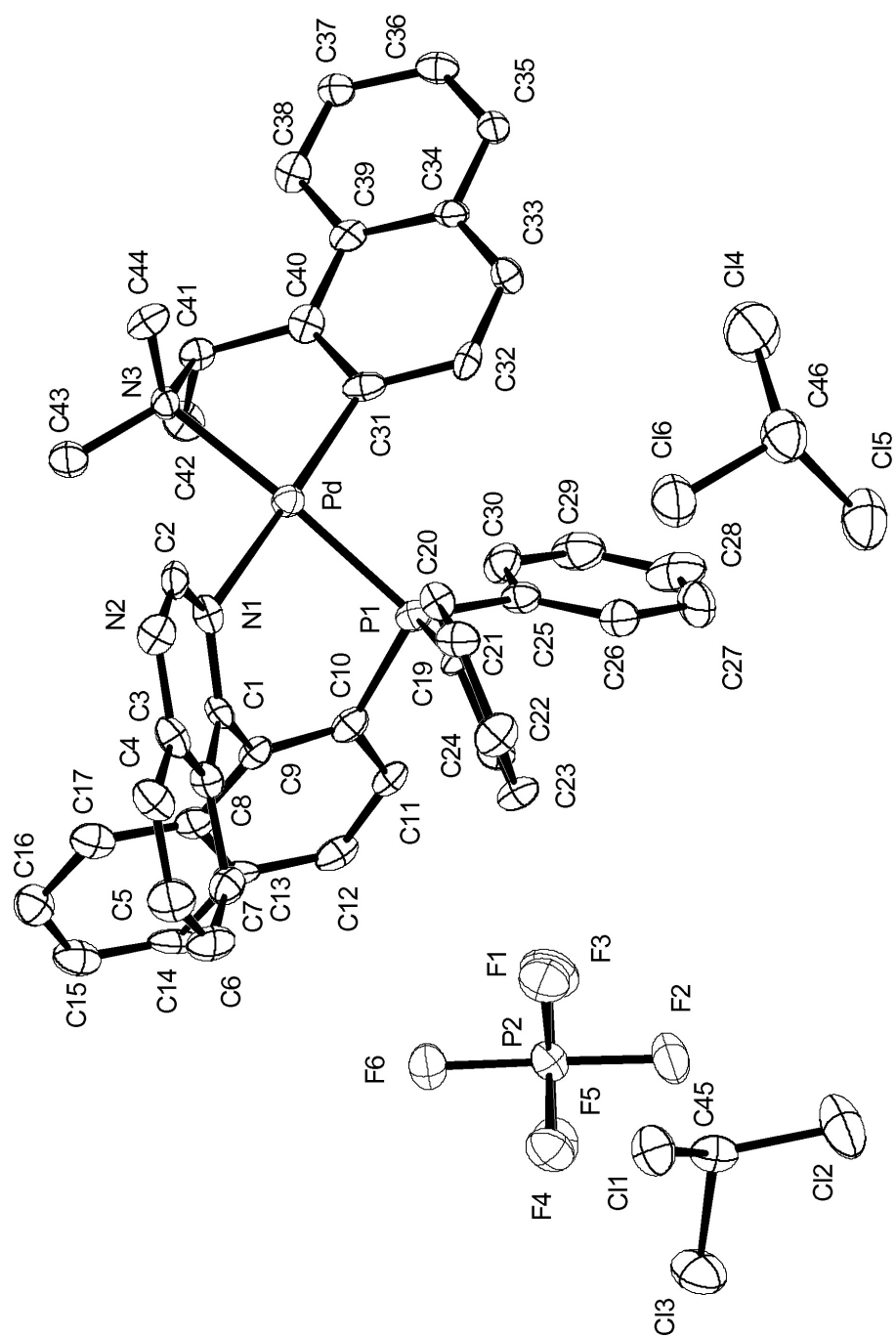
Table 4. Anisotropic displacement parameters (\AA^2).

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}].$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	0.013(3)	0.027(4)	0.025(4)	-0.005(3)	0.006(3)	0.001(3)
C(2)	0.013(3)	0.031(4)	0.022(4)	0.001(3)	0.000(3)	-0.002(3)
C(3)	0.020(3)	0.021(3)	0.030(4)	0.007(3)	0.006(3)	0.004(3)
C(4)	0.029(4)	0.026(4)	0.037(4)	0.002(4)	0.009(4)	0.002(3)
C(5)	0.041(4)	0.019(4)	0.048(5)	-0.003(4)	0.000(3)	-0.001(3)
C(6)	0.043(5)	0.020(4)	0.035(4)	-0.008(3)	0.000(3)	-0.005(3)
C(7)	0.024(4)	0.027(4)	0.022(4)	0.001(3)	-0.001(3)	-0.005(3)
C(8)	0.020(4)	0.013(3)	0.026(4)	0.004(3)	0.000(3)	0.002(3)
C(9)	0.022(4)	0.018(3)	0.021(4)	-0.002(3)	-0.004(3)	-0.003(3)
C(10)	0.027(4)	0.017(3)	0.023(3)	0.000(3)	-0.005(3)	-0.006(3)
C(11)	0.026(4)	0.021(4)	0.018(3)	0.000(3)	-0.008(3)	-0.003(3)
C(12)	0.036(4)	0.026(4)	0.016(3)	0.000(3)	-0.003(3)	-0.010(3)
C(13)	0.040(4)	0.018(3)	0.013(3)	-0.005(3)	-0.001(3)	0.002(3)
C(14)	0.049(5)	0.025(4)	0.018(3)	-0.009(3)	0.015(3)	-0.008(4)
C(15)	0.038(5)	0.027(4)	0.028(4)	-0.003(3)	0.013(3)	-0.007(4)
C(16)	0.029(4)	0.029(4)	0.032(4)	0.001(3)	0.003(3)	-0.002(3)
C(17)	0.034(4)	0.018(4)	0.029(4)	-0.001(3)	0.008(3)	-0.005(3)
C(18)	0.029(4)	0.010(3)	0.025(4)	-0.002(3)	-0.001(3)	0.000(3)
C(19)	0.017(3)	0.020(3)	0.026(4)	-0.008(3)	-0.005(3)	-0.004(3)
C(20)	0.022(3)	0.021(4)	0.022(4)	0.006(3)	0.002(3)	0.002(3)
C(21)	0.037(4)	0.021(4)	0.022(4)	0.002(3)	-0.002(3)	0.007(3)
C(22)	0.036(4)	0.027(4)	0.033(4)	0.003(3)	-0.003(3)	-0.005(3)
C(23)	0.033(4)	0.028(4)	0.029(4)	-0.011(3)	-0.004(3)	-0.005(3)
C(24)	0.025(3)	0.019(4)	0.017(3)	0.002(3)	0.003(3)	-0.001(3)
C(25)	0.030(4)	0.016(3)	0.021(3)	-0.001(3)	-0.002(3)	0.003(3)
C(26)	0.029(4)	0.031(4)	0.027(4)	-0.004(3)	0.001(3)	-0.001(3)
C(27)	0.031(4)	0.061(6)	0.039(4)	-0.007(4)	-0.012(4)	0.022(4)
C(28)	0.073(7)	0.034(5)	0.025(4)	-0.001(4)	-0.014(4)	0.014(4)
C(29)	0.056(5)	0.029(4)	0.034(4)	-0.006(4)	-0.007(4)	0.010(4)
C(30)	0.029(4)	0.030(4)	0.027(4)	0.000(3)	-0.009(3)	0.002(3)
C(31)	0.036(4)	0.020(4)	0.013(3)	-0.001(3)	-0.002(3)	0.001(3)
C(32)	0.016(3)	0.026(4)	0.019(3)	0.004(3)	-0.004(3)	-0.007(3)
C(33)	0.018(3)	0.021(4)	0.025(4)	0.002(3)	0.003(3)	0.000(3)
C(34)	0.024(3)	0.019(3)	0.014(3)	-0.003(3)	-0.002(2)	0.005(3)

C(35)	0.019(4)	0.034(4)	0.010(3)	0.001(3)	0.001(3)	0.003(3)
C(36)	0.034(4)	0.017(4)	0.023(4)	-0.002(3)	0.002(3)	0.002(3)
C(37)	0.025(4)	0.022(4)	0.025(4)	-0.005(3)	0.001(3)	0.000(3)
C(38)	0.025(4)	0.018(3)	0.026(4)	0.007(3)	-0.004(3)	0.000(3)
C(39)	0.026(3)	0.025(4)	0.006(3)	0.005(3)	0.000(2)	-0.002(3)
C(40)	0.024(4)	0.022(4)	0.022(3)	0.005(3)	-0.001(3)	-0.002(3)
C(41)	0.023(4)	0.015(3)	0.020(3)	0.001(3)	0.001(3)	-0.003(3)
C(42)	0.031(4)	0.029(4)	0.029(4)	0.002(3)	0.003(3)	0.000(3)
C(43)	0.028(4)	0.020(4)	0.042(4)	-0.010(3)	-0.001(3)	0.001(3)
C(44)	0.035(4)	0.020(4)	0.022(4)	-0.001(3)	-0.007(3)	-0.004(3)
C(45)	0.041(4)	0.016(4)	0.030(4)	0.001(3)	0.006(3)	-0.004(3)
C(46)	0.040(5)	0.054(5)	0.042(4)	0.007(4)	-0.002(4)	0.006(4)
Cl(1)	0.036(1)	0.037(1)	0.041(1)	0.009(1)	-0.001(1)	0.004(1)
Cl(2)	0.036(1)	0.092(2)	0.044(1)	0.019(1)	0.006(1)	0.021(1)
Cl(3)	0.054(1)	0.058(1)	0.031(1)	-0.002(1)	0.011(1)	0.007(1)
Cl(4)	0.054(1)	0.050(1)	0.099(2)	-0.014(1)	0.005(1)	-0.010(1)
Cl(5)	0.038(1)	0.076(2)	0.050(1)	0.011(1)	-0.005(1)	0.003(1)
Cl(6)	0.036(1)	0.066(1)	0.041(1)	0.001(1)	-0.001(1)	0.005(1)
F(1)	0.045(2)	0.057(3)	0.032(2)	-0.004(2)	0.008(2)	-0.001(2)
F(2)	0.024(2)	0.050(3)	0.054(3)	-0.002(2)	0.002(2)	0.005(2)
F(3)	0.060(3)	0.027(3)	0.084(3)	-0.016(2)	0.010(2)	0.004(2)
F(4)	0.041(2)	0.026(2)	0.045(2)	-0.001(2)	0.005(2)	0.004(2)
F(5)	0.040(2)	0.041(3)	0.037(2)	0.014(2)	0.003(2)	-0.003(2)
F(6)	0.026(2)	0.059(3)	0.039(2)	-0.007(2)	-0.001(2)	0.003(2)
N(1)	0.016(3)	0.022(3)	0.026(3)	0.004(3)	0.002(2)	0.002(2)
N(2)	0.028(3)	0.024(3)	0.028(3)	0.003(3)	-0.003(3)	-0.002(3)
N(3)	0.015(3)	0.018(3)	0.028(3)	-0.004(2)	-0.002(2)	0.002(2)
P(1)	0.025(1)	0.018(1)	0.020(1)	-0.002(1)	-0.001(1)	0.000(1)
P(2)	0.025(1)	0.027(1)	0.031(1)	0.000(1)	0.002(1)	0.004(1)
Pd	0.020(1)	0.017(1)	0.021(1)	-0.001(1)	-0.002(1)	0.000(1)



Crystallographic Data for (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato-*C*₂,*N*]-
[diphenyl[1-(2-methylquinazolin-4-yl)(2-naphthyl)]phosphine]palladium(II)
hexafluorophosphate (*S,R*)-(18b)

Table 1. Crystal data and structure refinement.

Identification code	(<i>S,R</i>)-18b	
Empirical formula	C ₄₅ H ₃₉ F ₆ N ₃ P ₂ Pd · 0.2(H ₂ O)	
Color	colourless	
Formula weight	907.74 g · mol ⁻¹	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 2₁ 2₁ 2₁, (no. 19)	
Unit cell dimensions	a = 11.4972(1) Å	α = 90°.
	b = 15.6101(1) Å	β = 90°.
	c = 21.7615(2) Å	γ = 90°.
Volume	3905.59(6) Å ³	
Z	4	
Density (calculated)	1.544 Mg · m ⁻³	
Absorption coefficient	0.624 mm ⁻¹	
F(000)	1848 e	
Crystal size	0.25 x 0.10 x 0.07 mm ³	
θ range for data collection	3.78 to 33.15°.	
Index ranges	-17 ≤ h ≤ 13, -23 ≤ k ≤ 24, -33 ≤ l ≤ 23	
Reflections collected	31043	
Independent reflections	14658 [R _{int} = 0.0621]	
Reflections with I > 2σ(I)	12379	
Completeness to θ = 33.15°	99.5 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.96590 and 0.88590	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	14658 / 0 / 536	
Goodness-of-fit on F ²	1.014	
Final R indices [I > 2σ(I)]	R ₁ = 0.0428	wR ² = 0.0879
R indices (all data)	R ₁ = 0.0571	wR ² = 0.0943
Absolute structure parameter	-0.048(17)	
Largest diff. peak and hole	0.955 and -0.619 e · Å ⁻³	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2).

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.7567(2)	0.5153(1)	0.8900(1)	0.015(1)
C(2)	0.7974(2)	0.5781(2)	0.9845(1)	0.019(1)
C(3)	0.6408(2)	0.4892(2)	0.9799(1)	0.018(1)
C(4)	0.5495(3)	0.4467(2)	1.0103(1)	0.023(1)
C(5)	0.4806(3)	0.3911(2)	0.9794(1)	0.027(1)
C(6)	0.5003(3)	0.3746(2)	0.9166(1)	0.026(1)
C(7)	0.5875(2)	0.4142(2)	0.8857(1)	0.021(1)
C(8)	0.6601(2)	0.4738(2)	0.9165(1)	0.017(1)
C(9)	0.8744(3)	0.6356(2)	1.0207(1)	0.029(1)
C(10)	0.7936(2)	0.4999(1)	0.8251(1)	0.016(1)
C(11)	0.9030(2)	0.4654(1)	0.8138(1)	0.016(1)
C(12)	0.9405(2)	0.4522(2)	0.7527(1)	0.019(1)
C(13)	0.8694(3)	0.4724(2)	0.7048(1)	0.020(1)
C(14)	0.7569(2)	0.5057(2)	0.7143(1)	0.019(1)
C(15)	0.6813(3)	0.5237(2)	0.6645(1)	0.022(1)
C(16)	0.5735(3)	0.5561(2)	0.6748(1)	0.025(1)
C(17)	0.5357(2)	0.5739(2)	0.7350(1)	0.023(1)
C(18)	0.6067(2)	0.5575(2)	0.7839(1)	0.021(1)
C(19)	0.7182(2)	0.5211(2)	0.7756(1)	0.017(1)
C(20)	1.1240(2)	0.3876(2)	0.8476(1)	0.018(1)
C(21)	1.2077(2)	0.4279(2)	0.8119(1)	0.023(1)
C(22)	1.2943(3)	0.3807(2)	0.7842(1)	0.028(1)
C(23)	1.3000(3)	0.2930(2)	0.7926(1)	0.028(1)
C(24)	1.2169(3)	0.2527(2)	0.8288(1)	0.026(1)
C(25)	1.1292(3)	0.2991(2)	0.8558(1)	0.022(1)
C(26)	0.9261(2)	0.3785(2)	0.9295(1)	0.018(1)
C(27)	0.8490(2)	0.3182(2)	0.9060(1)	0.020(1)
C(28)	0.7813(3)	0.2693(2)	0.9447(1)	0.026(1)
C(29)	0.7913(3)	0.2790(2)	1.0074(1)	0.030(1)
C(30)	0.8705(3)	0.3360(2)	1.0309(1)	0.033(1)
C(31)	0.9382(3)	0.3868(2)	0.9926(1)	0.025(1)
C(32)	1.1742(2)	0.6128(1)	0.8891(1)	0.018(1)
C(33)	1.2638(2)	0.5713(2)	0.9221(1)	0.022(1)
C(34)	1.3740(3)	0.6034(2)	0.9221(1)	0.026(1)
C(35)	1.4023(2)	0.6763(2)	0.8868(1)	0.022(1)

C(36)	1.5163(3)	0.7117(2)	0.8872(1)	0.028(1)
C(37)	1.5419(3)	0.7828(2)	0.8531(2)	0.034(1)
C(38)	1.4565(3)	0.8211(2)	0.8166(2)	0.033(1)
C(39)	1.3461(3)	0.7894(2)	0.8153(1)	0.026(1)
C(40)	1.3150(2)	0.7168(2)	0.8512(1)	0.020(1)
C(41)	1.1994(2)	0.6854(2)	0.8555(1)	0.019(1)
C(42)	1.0961(2)	0.7307(2)	0.8275(1)	0.021(1)
C(43)	1.0635(3)	0.6920(2)	0.7656(1)	0.029(1)
C(44)	0.8861(3)	0.7489(2)	0.8497(2)	0.032(1)
C(45)	1.0297(3)	0.7836(2)	0.9255(1)	0.026(1)
F(1)	0.8743(2)	1.0982(1)	0.8808(1)	0.043(1)
F(2)	0.6693(2)	0.9625(1)	0.8695(1)	0.063(1)
F(3A)	0.8614(6)	0.9602(4)	0.8938(4)	0.042(1)
F(3B)	0.8696(6)	0.9656(4)	0.8534(3)	0.040(1)
F(3C)	0.8259(7)	0.9820(5)	0.8215(4)	0.051(2)
F(4A)	0.8072(7)	1.0221(5)	0.8026(3)	0.050(2)
F(4B)	0.7473(7)	1.0572(5)	0.8037(3)	0.048(2)
F(4C)	0.7046(6)	1.0959(5)	0.8397(3)	0.041(2)
F(5A)	0.6856(5)	1.1103(3)	0.8583(3)	0.024(1)
F(5B)	0.6688(7)	1.0950(5)	0.8939(4)	0.063(2)
F(5C)	0.7099(8)	1.0641(5)	0.9387(4)	0.050(2)
F(6A)	0.7495(6)	1.0561(4)	0.9473(3)	0.026(1)
F(6B)	0.7867(8)	1.0077(5)	0.9410(4)	0.062(2)
F(6C)	0.8339(6)	0.9553(4)	0.9242(3)	0.034(1)
N(1)	0.8249(2)	0.5657(1)	0.9236(1)	0.015(1)
N(2)	0.7094(2)	0.5433(1)	1.0124(1)	0.019(1)
N(3)	1.0012(2)	0.7242(1)	0.8750(1)	0.020(1)
O	1.2159(12)	0.6834(8)	1.0347(6)	0.043(3)
P(1)	1.0042(1)	0.4495(1)	0.8783(1)	0.015(1)
P(2)	0.7717(1)	1.0302(1)	0.8759(1)	0.034(1)
Pd	1.0058(1)	0.5905(1)	0.8981(1)	0.015(1)

Table 3. Bond lengths [Å] and angles [°].

C(1)-N(1)	1.328(3)	C(1)-C(8)	1.408(3)
C(1)-C(10)	1.495(3)	C(2)-N(2)	1.299(3)
C(2)-N(1)	1.377(3)	C(2)-C(9)	1.486(4)
C(3)-N(2)	1.353(3)	C(3)-C(4)	1.407(4)
C(3)-C(8)	1.420(3)	C(4)-C(5)	1.353(4)
C(5)-C(6)	1.408(4)	C(6)-C(7)	1.357(4)
C(7)-C(8)	1.418(3)	C(10)-C(11)	1.390(4)
C(10)-C(19)	1.421(3)	C(11)-C(12)	1.413(3)
C(11)-P(1)	1.840(3)	C(12)-C(13)	1.361(4)
C(13)-C(14)	1.410(4)	C(14)-C(15)	1.417(4)
C(14)-C(19)	1.426(4)	C(15)-C(16)	1.357(4)
C(16)-C(17)	1.407(4)	C(17)-C(18)	1.365(4)
C(18)-C(19)	1.414(4)	C(20)-C(21)	1.388(4)
C(20)-C(25)	1.393(3)	C(20)-P(1)	1.811(3)
C(21)-C(22)	1.378(4)	C(22)-C(23)	1.384(4)
C(23)-C(24)	1.388(4)	C(24)-C(25)	1.375(4)
C(26)-C(31)	1.388(4)	C(26)-C(27)	1.391(4)
C(26)-P(1)	1.809(3)	C(27)-C(28)	1.379(4)
C(28)-C(29)	1.376(4)	C(29)-C(30)	1.373(5)
C(30)-C(31)	1.388(4)	C(32)-C(41)	1.379(3)
C(32)-C(33)	1.412(4)	C(32)-Pd	1.978(3)
C(33)-C(34)	1.363(4)	C(34)-C(35)	1.411(4)
C(35)-C(40)	1.417(4)	C(35)-C(36)	1.422(4)
C(36)-C(37)	1.366(4)	C(37)-C(38)	1.398(5)
C(38)-C(39)	1.362(4)	C(39)-C(40)	1.423(4)
C(40)-C(41)	1.420(4)	C(41)-C(42)	1.511(4)
C(42)-N(3)	1.507(4)	C(42)-C(43)	1.523(4)
C(44)-N(3)	1.485(4)	C(45)-N(3)	1.475(3) F(1)-
P(2)	1.591(2)	F(2)-P(2)	1.587(2)
F(3A)-F(6C)	0.738(7)	F(3A)-F(3B)	0.888(8)
F(3A)-F(6B)	1.531(11)	F(3A)-P(2)	1.552(7)
F(3A)-F(3C)	1.659(10)	F(3B)-F(3C)	0.893(8)
F(3B)-F(4A)	1.585(10)	F(3B)-P(2)	1.588(6)
F(3B)-F(6C)	1.604(8)	F(3C)-F(4A)	0.780(9)
F(3C)-F(4B)	1.531(11)	F(3C)-P(2)	1.533(7)
F(4A)-F(4B)	0.879(9)	F(4A)-P(2)	1.650(7)
F(4B)-F(4C)	1.105(9)	F(4B)-F(5A)	1.614(9)
F(4B)-P(2)	1.650(7)	F(4C)-F(5A)	0.512(8)

F(4C)-F(5B)	1.250(10)	F(4C)-P(2)	1.506(7)
F(5A)-F(5B)	0.833(8)	F(5A)-P(2)	1.640(6)
F(5B)-F(5C)	1.186(10)	F(5B)-F(6A)	1.605(10)
F(5B)-P(2)	1.605(8)	F(5C)-F(6A)	0.507(10)
F(5C)-F(6B)	1.247(12)	F(5C)-P(2)	1.629(8)
F(6A)-F(6B)	0.879(9)	F(6A)-P(2)	1.626(6)
F(6B)-F(6C)	1.048(9)	F(6B)-P(2)	1.471(8)
F(6C)-P(2)	1.728(6)	N(1)-Pd	2.187(2)
N(3)-Pd	2.1472(17)	P(1)-Pd	2.2423(5)
N(1)-C(1)-C(8)	120.9(2)	N(1)-C(1)-C(10)	116.6(2)
C(8)-C(1)-C(10)	122.4(2)	N(2)-C(2)-N(1)	124.7(2)
N(2)-C(2)-C(9)	118.0(2)	N(1)-C(2)-C(9)	117.3(2)
N(2)-C(3)-C(4)	119.0(2)	N(2)-C(3)-C(8)	121.5(2)
C(4)-C(3)-C(8)	119.6(2)	C(5)-C(4)-C(3)	120.4(2)
C(4)-C(5)-C(6)	120.3(3)	C(7)-C(6)-C(5)	121.1(3)
C(6)-C(7)-C(8)	120.0(2)	C(1)-C(8)-C(7)	125.0(2)
C(1)-C(8)-C(3)	116.3(2)	C(7)-C(8)-C(3)	118.6(2)
C(11)-C(10)-C(19)	120.5(2)	C(11)-C(10)-C(1)	119.1(2)
C(19)-C(10)-C(1)	120.4(2)	C(10)-C(11)-C(12)	120.0(2)
C(10)-C(11)-P(1)	119.28(18)	C(12)-C(11)-P(1)	120.4(2)
C(13)-C(12)-C(11)	120.2(2)	C(12)-C(13)-C(14)	121.6(2)
C(13)-C(14)-C(15)	121.6(2)	C(13)-C(14)-C(19)	119.1(2)
C(15)-C(14)-C(19)	119.3(3)	C(16)-C(15)-C(14)	120.5(3)
C(15)-C(16)-C(17)	120.6(3)	C(18)-C(17)-C(16)	120.2(3)
C(17)-C(18)-C(19)	121.2(2)	C(18)-C(19)-C(10)	123.4(2)
C(18)-C(19)-C(14)	118.0(2)	C(10)-C(19)-C(14)	118.6(2)
C(21)-C(20)-C(25)	119.4(2)	C(21)-C(20)-P(1)	119.44(19)
C(25)-C(20)-P(1)	121.0(2)	C(22)-C(21)-C(20)	120.3(3)
C(21)-C(22)-C(23)	120.3(3)	C(22)-C(23)-C(24)	119.5(3)
C(25)-C(24)-C(23)	120.5(3)	C(24)-C(25)-C(20)	120.0(3)
C(31)-C(26)-C(27)	119.4(2)	C(31)-C(26)-P(1)	120.2(2)
C(27)-C(26)-P(1)	120.29(19)	C(28)-C(27)-C(26)	120.6(3)
C(29)-C(28)-C(27)	119.9(3)	C(30)-C(29)-C(28)	119.7(3)
C(29)-C(30)-C(31)	121.3(3)	C(26)-C(31)-C(30)	119.0(3)
C(41)-C(32)-C(33)	119.5(2)	C(41)-C(32)-Pd	113.71(19)
C(33)-C(32)-Pd	125.72(19)	C(34)-C(33)-C(32)	120.7(2)
C(33)-C(34)-C(35)	120.7(3)	C(34)-C(35)-C(40)	119.6(2)
C(34)-C(35)-C(36)	121.5(3)	C(40)-C(35)-C(36)	118.9(2)
C(37)-C(36)-C(35)	120.7(3)	C(36)-C(37)-C(38)	120.3(3)

C(39)-C(38)-C(37)	120.7(3)	C(38)-C(39)-C(40)	120.8(3)
C(35)-C(40)-C(41)	118.3(2)	C(35)-C(40)-C(39)	118.5(3)
C(41)-C(40)-C(39)	123.2(3)	C(32)-C(41)-C(40)	121.0(2)
C(32)-C(41)-C(42)	115.7(2)	C(40)-C(41)-C(42)	123.2(2)
N(3)-C(42)-C(41)	105.1(2)	N(3)-C(42)-C(43)	113.7(2)
C(41)-C(42)-C(43)	111.4(2)	F(6C)-F(3A)-F(3B)	160.8(13)
F(6C)-F(3A)-F(6B)	37.6(7)	F(3B)-F(3A)-F(6B)	132.7(8)
F(6C)-F(3A)-P(2)	90.8(8)	F(3B)-F(3A)-P(2)	75.8(6)
F(6B)-F(3A)-P(2)	57.0(4)	F(6C)-F(3A)-F(3C)	140.0(10)
F(3B)-F(3A)-F(3C)	21.4(6)	F(6B)-F(3A)-F(3C)	113.5(6) P(2)-
F(3A)-F(3C)	56.9(3)	F(3A)-F(3B)-F(3C)	137.3(11)
F(3A)-F(3B)-F(4A)	134.0(8)	F(3C)-F(3B)-F(4A)	17.3(6)
F(3A)-F(3B)-P(2)	71.3(6)	F(3C)-F(3B)-P(2)	70.0(6)
F(4A)-F(3B)-P(2)	62.7(4)	F(3A)-F(3B)-F(6C)	8.7(6)
F(3C)-F(3B)-F(6C)	129.1(8)	F(4A)-F(3B)-F(6C)	127.6(5) P(2)-
F(3B)-F(6C)	65.5(3)	F(4A)-F(3C)-F(3B)	142.7(13)
F(4A)-F(3C)-F(4B)	24.2(8)	F(3B)-F(3C)-F(4B)	138.5(9)
F(4A)-F(3C)-P(2)	84.3(9)	F(3B)-F(3C)-P(2)	76.8(7)
F(4B)-F(3C)-P(2)	65.2(4)	F(4A)-F(3C)-F(3A)	137.2(10)
F(3B)-F(3C)-F(3A)	21.3(6)	F(4B)-F(3C)-F(3A)	122.9(6) P(2)-
F(3C)-F(3A)	58.0(4)	F(3C)-F(4A)-F(4B)	134.6(13)
F(3C)-F(4A)-F(3B)	20.0(7)	F(4B)-F(4A)-F(3B)	133.0(9)
F(3C)-F(4A)-P(2)	67.6(8)	F(4B)-F(4A)-P(2)	74.5(7)
F(3B)-F(4A)-P(2)	58.8(3)	F(4A)-F(4B)-F(4C)	135.0(10)
F(4A)-F(4B)-F(3C)	21.3(6)	F(4C)-F(4B)-F(3C)	120.1(7)
F(4A)-F(4B)-F(5A)	133.1(9)	F(4C)-F(4B)-F(5A)	2.5(5)
F(3C)-F(4B)-F(5A)	117.8(5)	F(4A)-F(4B)-P(2)	74.6(7)
F(4C)-F(4B)-P(2)	62.6(5)	F(3C)-F(4B)-P(2)	57.5(4)
F(5A)-F(4B)-P(2)	60.3(3)	F(5A)-F(4C)-F(4B)	172.1(15)
F(5A)-F(4C)-F(5B)	28.0(10)	F(4B)-F(4C)-F(5B)	144.1(8)
F(5A)-F(4C)-P(2)	95.9(12)	F(4B)-F(4C)-P(2)	76.7(6)
F(5B)-F(4C)-P(2)	70.6(5)	F(4C)-F(5A)-F(5B)	135.2(16)
F(4C)-F(5A)-F(4B)	5.4(11)	F(5B)-F(5A)-F(4B)	129.8(8)
F(4C)-F(5A)-P(2)	66.0(11)	F(5B)-F(5A)-P(2)	72.8(7)
F(4B)-F(5A)-P(2)	60.9(3)	F(5A)-F(5B)-F(5C)	142.1(12)
F(5A)-F(5B)-F(4C)	16.8(6)	F(5C)-F(5B)-F(4C)	130.5(9)
F(5A)-F(5B)-F(6A)	130.3(10)	F(5C)-F(5B)-F(6A)	11.9(5)
F(4C)-F(5B)-F(6A)	119.8(7)	F(5A)-F(5B)-P(2)	77.4(7)
F(5C)-F(5B)-P(2)	69.6(6)	F(4C)-F(5B)-P(2)	62.2(5)
F(6A)-F(5B)-P(2)	60.9(4)	F(6A)-F(5C)-F(5B)	139.4(17)

F(6A)-F(5C)-F(6B)	34.6(12)	F(5B)-F(5C)-F(6B)	127.0(9)
F(6A)-F(5C)-P(2)	80.7(14)	F(5B)-F(5C)-P(2)	67.4(5)
F(6B)-F(5C)-P(2)	59.8(5)	F(5C)-F(6A)-F(6B)	126.2(17)
F(5C)-F(6A)-F(5B)	28.7(12)	F(6B)-F(6A)-F(5B)	119.6(8)
F(5C)-F(6A)-P(2)	81.4(13)	F(6B)-F(6A)-P(2)	64.0(6)
F(5B)-F(6A)-P(2)	59.6(4)	F(6A)-F(6B)-F(6C)	167.9(11)
F(6A)-F(6B)-F(5C)	19.1(7)	F(6C)-F(6B)-F(5C)	154.6(10)
F(6A)-F(6B)-P(2)	83.5(7)	F(6C)-F(6B)-P(2)	84.9(6)
F(5C)-F(6B)-P(2)	73.2(5)	F(6A)-F(6B)-F(3A)	142.5(9)
F(6C)-F(6B)-F(3A)	25.4(5)	F(5C)-F(6B)-F(3A)	135.4(7) P(2)-
F(6B)-F(3A)	62.2(4)	F(3A)-F(6C)-F(6B)	117.0(10)
F(3A)-F(6C)-F(3B)	10.5(7)	F(6B)-F(6C)-F(3B)	112.9(7)
F(3A)-F(6C)-P(2)	63.9(7)	F(6B)-F(6C)-P(2)	58.0(5)
F(3B)-F(6C)-P(2)	56.8(3)	C(1)-N(1)-C(2)	118.5(2)
C(1)-N(1)-Pd	121.78(16)	C(2)-N(1)-Pd	115.91(17)
C(2)-N(2)-C(3)	118.1(2)	C(45)-N(3)-C(44)	108.1(2)
C(45)-N(3)-C(42)	108.0(2)	C(44)-N(3)-C(42)	111.9(2)
C(45)-N(3)-Pd	115.49(15)	C(44)-N(3)-Pd	111.19(18)
C(42)-N(3)-Pd	102.03(15)	C(26)-P(1)-C(20)	106.07(12)
C(26)-P(1)-C(11)	103.82(12)	C(20)-P(1)-C(11)	105.76(11)
C(26)-P(1)-Pd	119.15(8)	C(20)-P(1)-Pd	126.06(9)
C(11)-P(1)-Pd	91.12(7)	F(6B)-P(2)-F(4C)	136.6(5)
F(6B)-P(2)-F(3C)	125.3(5)	F(4C)-P(2)-F(3C)	98.0(4)
F(6B)-P(2)-F(3A)	60.8(4)	F(4C)-P(2)-F(3A)	162.1(4)
F(3C)-P(2)-F(3A)	65.1(4)	F(6B)-P(2)-F(2)	90.7(3)
F(4C)-P(2)-F(2)	91.6(3)	F(3C)-P(2)-F(2)	84.7(3)
F(3A)-P(2)-F(2)	92.6(3)	F(6B)-P(2)-F(3B)	93.6(4)
F(4C)-P(2)-F(3B)	129.4(4)	F(3C)-P(2)-F(3B)	33.2(3)
F(3A)-P(2)-F(3B)	32.8(3)	F(2)-P(2)-F(3B)	94.4(3)
F(6B)-P(2)-F(1)	90.4(3)	F(4C)-P(2)-F(1)	87.7(3)
F(3C)-P(2)-F(1)	94.5(3)	F(3A)-P(2)-F(1)	87.7(3) F(2)-
P(2)-F(1)	178.88(15)	F(3B)-P(2)-F(1)	85.3(3)
F(6B)-P(2)-F(5B)	90.0(5)	F(4C)-P(2)-F(5B)	47.2(4)
F(3C)-P(2)-F(5B)	142.9(5)	F(3A)-P(2)-F(5B)	150.7(4) F(2)-
P(2)-F(5B)	83.9(3)	F(3B)-P(2)-F(5B)	176.0(4) F(1)-
P(2)-F(5B)	96.2(3)	F(6B)-P(2)-F(6A)	32.5(3)
F(4C)-P(2)-F(6A)	104.4(4)	F(3C)-P(2)-F(6A)	157.3(4)
F(3A)-P(2)-F(6A)	92.3(4)	F(2)-P(2)-F(6A)	97.6(3)
F(3B)-P(2)-F(6A)	124.3(4)	F(1)-P(2)-F(6A)	83.4(2)
F(5B)-P(2)-F(6A)	59.6(4)	F(6B)-P(2)-F(5C)	47.1(4)

F(4C)-P(2)-F(5C)	89.7(4)	F(3C)-P(2)-F(5C)	169.6(4)
F(3A)-P(2)-F(5C)	107.9(4)	F(2)-P(2)-F(5C)	88.1(3)
F(3B)-P(2)-F(5C)	140.7(4)	F(1)-P(2)-F(5C)	92.8(3)
F(5B)-P(2)-F(5C)	43.0(4)	F(6A)-P(2)-F(5C)	17.9(3)
F(6B)-P(2)-F(5A)	118.5(4)	F(4C)-P(2)-F(5A)	18.1(3)
F(3C)-P(2)-F(5A)	116.1(4)	F(3A)-P(2)-F(5A)	175.1(3) F(2)-
P(2)-F(5A)	92.2(2)	F(3B)-P(2)-F(5A)	147.1(4) F(1)-
P(2)-F(5A)	87.4(2)	F(5B)-P(2)-F(5A)	29.7(3)
F(6A)-P(2)-F(5A)	86.5(3)	F(5C)-P(2)-F(5A)	71.6(4)
F(6B)-P(2)-F(4A)	152.1(5)	F(4C)-P(2)-F(4A)	71.0(4)
F(3C)-P(2)-F(4A)	28.0(3)	F(3A)-P(2)-F(4A)	91.4(4) F(2)-
P(2)-F(4A)	92.8(3)	F(3B)-P(2)-F(4A)	58.6(4) F(1)-
P(2)-F(4A)	86.2(3)	F(5B)-P(2)-F(4A)	117.8(4)
F(6A)-P(2)-F(4A)	168.8(3)	F(5C)-P(2)-F(4A)	160.6(4)
F(5A)-P(2)-F(4A)	89.0(4)	C(32)-Pd-N(3)	80.21(10)
C(32)-Pd-N(1)	171.00(9)	N(3)-Pd-N(1)	102.03(9)
C(32)-Pd-P(1)	99.30(7)	N(3)-Pd-P(1)	155.30(5)
N(1)-Pd-P(1)	82.34(6)		

Table 4. Anisotropic displacement parameters (\AA^2).

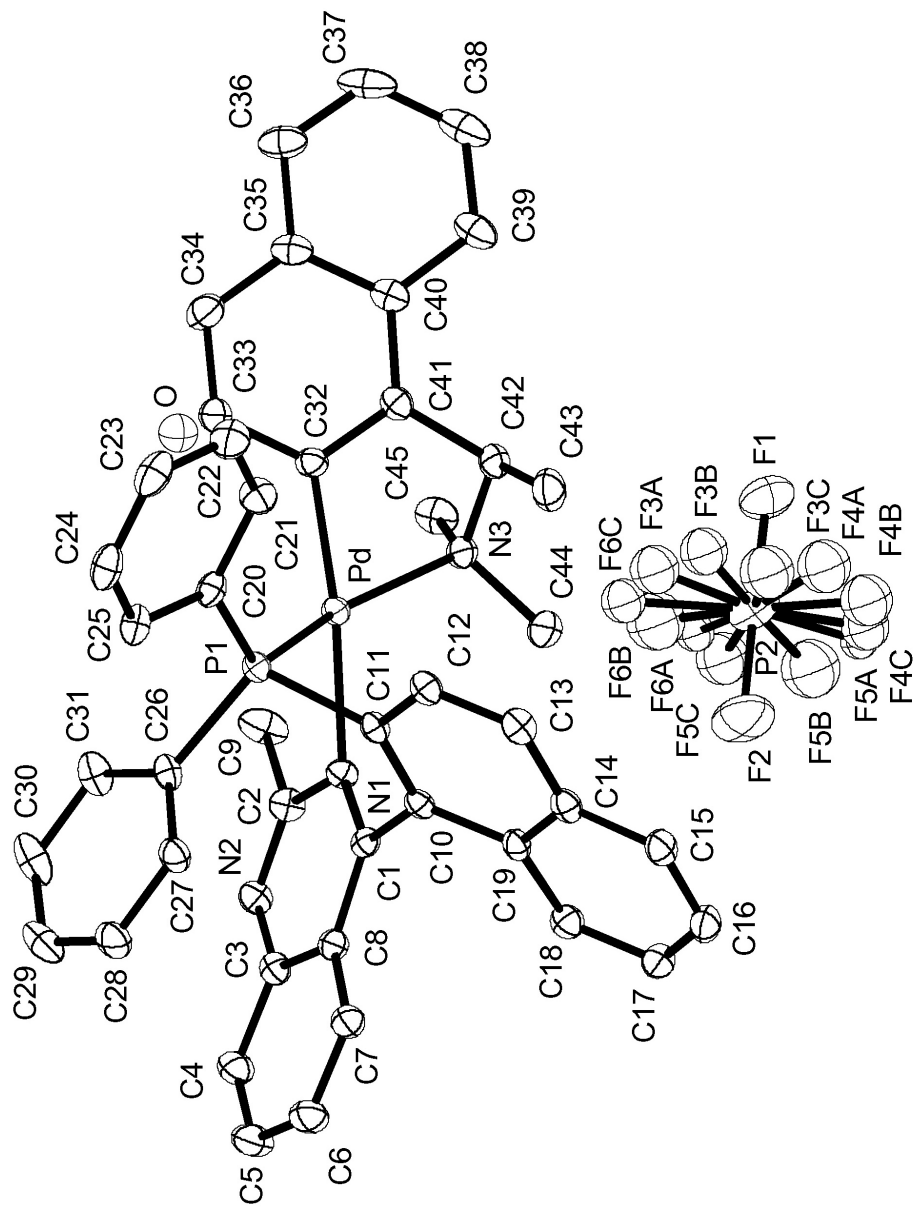
The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}].$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	0.015(1)	0.013(1)	0.019(1)	-0.001(1)	-0.002(1)	0.002(1)
C(2)	0.021(1)	0.018(1)	0.018(1)	-0.004(1)	0.002(1)	-0.001(1)
C(3)	0.019(1)	0.017(1)	0.018(1)	0.000(1)	0.001(1)	0.002(1)
C(4)	0.022(1)	0.028(1)	0.019(1)	0.002(1)	0.003(1)	-0.003(1)
C(5)	0.024(2)	0.032(1)	0.026(1)	0.001(1)	0.004(1)	-0.008(1)
C(6)	0.024(1)	0.026(1)	0.027(1)	0.000(1)	-0.003(1)	-0.009(1)
C(7)	0.022(1)	0.022(1)	0.020(1)	0.000(1)	-0.002(1)	-0.003(1)
C(8)	0.017(1)	0.016(1)	0.018(1)	0.000(1)	0.000(1)	0.001(1)
C(9)	0.035(2)	0.033(1)	0.021(1)	-0.010(1)	0.005(1)	-0.015(1)
C(10)	0.019(1)	0.012(1)	0.016(1)	0.000(1)	0.001(1)	-0.003(1)
C(11)	0.019(1)	0.013(1)	0.015(1)	0.001(1)	0.001(1)	-0.001(1)
C(12)	0.022(1)	0.015(1)	0.019(1)	0.000(1)	0.002(1)	0.000(1)
C(13)	0.026(1)	0.018(1)	0.016(1)	-0.003(1)	0.002(1)	-0.002(1)
C(14)	0.024(1)	0.013(1)	0.018(1)	0.000(1)	-0.001(1)	-0.003(1)
C(15)	0.027(1)	0.023(1)	0.015(1)	0.001(1)	-0.004(1)	-0.005(1)
C(16)	0.026(1)	0.024(1)	0.024(1)	0.005(1)	-0.008(1)	-0.002(1)
C(17)	0.021(1)	0.022(1)	0.027(1)	0.003(1)	-0.003(1)	0.000(1)
C(18)	0.022(1)	0.021(1)	0.020(1)	0.000(1)	0.002(1)	0.000(1)
C(19)	0.020(1)	0.013(1)	0.017(1)	0.002(1)	-0.002(1)	-0.002(1)
C(20)	0.018(1)	0.020(1)	0.017(1)	-0.001(1)	-0.002(1)	0.005(1)
C(21)	0.023(1)	0.023(1)	0.024(1)	-0.001(1)	0.004(1)	0.003(1)
C(22)	0.025(1)	0.034(1)	0.024(1)	-0.001(1)	0.005(1)	0.006(1)
C(23)	0.026(1)	0.037(2)	0.022(1)	-0.007(1)	-0.002(1)	0.015(1)
C(24)	0.032(2)	0.021(1)	0.027(1)	-0.002(1)	-0.007(1)	0.010(1)
C(25)	0.025(1)	0.022(1)	0.019(1)	0.001(1)	-0.003(1)	0.006(1)
C(26)	0.024(1)	0.014(1)	0.015(1)	0.001(1)	0.002(1)	0.003(1)
C(27)	0.024(1)	0.015(1)	0.022(1)	0.002(1)	0.000(1)	-0.001(1)
C(28)	0.026(1)	0.016(1)	0.037(2)	0.006(1)	0.003(1)	0.000(1)
C(29)	0.038(2)	0.020(1)	0.033(2)	0.007(1)	0.016(1)	0.001(1)
C(30)	0.056(2)	0.022(1)	0.020(1)	0.003(1)	0.010(1)	0.003(1)
C(31)	0.038(2)	0.018(1)	0.019(1)	-0.001(1)	0.000(1)	0.000(1)
C(32)	0.016(1)	0.015(1)	0.022(1)	0.000(1)	0.000(1)	-0.001(1)
C(33)	0.020(1)	0.018(1)	0.029(1)	0.004(1)	0.000(1)	0.002(1)
C(34)	0.020(1)	0.024(1)	0.033(1)	-0.001(1)	-0.004(1)	0.002(1)

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C(35)	0.019(1)	0.019(1)	0.027(1)	-0.006(1)	0.005(1)	-0.001(1)
C(36)	0.020(1)	0.025(1)	0.038(1)	-0.010(1)	0.005(1)	-0.002(1)
C(37)	0.022(1)	0.026(1)	0.054(2)	-0.016(1)	0.017(1)	-0.008(1)
C(38)	0.034(2)	0.021(1)	0.044(2)	-0.003(1)	0.022(1)	-0.004(1)
C(39)	0.029(2)	0.019(1)	0.031(2)	-0.001(1)	0.012(1)	-0.001(1)
C(40)	0.022(1)	0.015(1)	0.023(1)	-0.005(1)	0.006(1)	0.000(1)
C(41)	0.022(1)	0.015(1)	0.021(1)	-0.001(1)	0.001(1)	0.000(1)
C(42)	0.022(1)	0.016(1)	0.025(1)	0.004(1)	-0.002(1)	0.000(1)
C(43)	0.034(2)	0.028(1)	0.023(1)	0.005(1)	-0.006(1)	-0.002(1)
C(44)	0.022(1)	0.028(1)	0.048(2)	0.015(1)	-0.004(1)	0.002(1)
C(45)	0.026(2)	0.017(1)	0.035(1)	-0.005(1)	0.006(1)	0.000(1)
F(1)	0.033(1)	0.053(1)	0.044(1)	-0.010(1)	-0.007(1)	-0.007(1)
F(2)	0.045(1)	0.041(1)	0.103(2)	-0.004(1)	-0.018(1)	-0.015(1)
N(1)	0.017(1)	0.014(1)	0.015(1)	-0.002(1)	0.000(1)	-0.002(1)
N(2)	0.021(1)	0.019(1)	0.016(1)	-0.001(1)	0.002(1)	0.000(1)
N(3)	0.018(1)	0.014(1)	0.027(1)	0.003(1)	-0.002(1)	0.001(1)
O	0.043(8)	0.043(6)	0.043(7)	-0.005(6)	-0.001(6)	0.010(6)
P(1)	0.017(1)	0.013(1)	0.015(1)	0.000(1)	0.001(1)	0.001(1)
P(2)	0.027(1)	0.034(1)	0.040(1)	-0.015(1)	-0.006(1)	0.004(1)
Pd	0.015(1)	0.012(1)	0.017(1)	0.000(1)	0.000(1)	0.000(1)



Crystallographic Data for (*S,R*)-*cis*-[dimethyl(1-(1-naphthyl)ethyl)aminato-*C*₂,*N*]-[1-(2-isopropyl-quinazolin-4-yl)(2-naphthyl)diphenyl phosphine] palladium(II) hexafluorophosphate (*S,R*)-(18e)

Table 1. Crystal data and structure refinement.

Identification code	<i>(S,R)</i> - 18e	
Empirical formula	C ₄₇ H ₄₃ F ₆ N ₃ P ₂ Pd	
Color	yellow-green	
Formula weight	932.18 g · mol ⁻¹	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2₁, (no. 4)	
Unit cell dimensions	a = 11.2498(12) Å	α = 90°.
	b = 16.1672(17) Å	β = 92.273(2)°.
	c = 11.3790(12) Å	γ = 90°.
Volume	2068.0(4) Å ³	
Z	2	
Density (calculated)	1.497 Mg · m ⁻³	
Absorption coefficient	0.591 mm ⁻¹	
F(000)	952 e	
Crystal size	0.17 x 0.13 x 0.08 mm ³	
θ range for data collection	1.79 to 23.26°.	
Index ranges	-12 ≤ h ≤ 12, -17 ≤ k ≤ 14, -12 ≤ l ≤ 12	
Reflections collected	8039	
Independent reflections	4573 [R _{int} = 0.0537]	
Reflections with I > 2σ(I)	3976	
Completeness to θ = 23.26°	99.3 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.95613 and 0.90701	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4573 / 1 / 532	
Goodness-of-fit on F ²	1.054	
Final R indices [I > 2σ(I)]	R ₁ = 0.0416	wR ² = 0.0820
R indices (all data)	R ₁ = 0.0545	wR ² = 0.0868
Absolute structure parameter	-0.05(3)	
Largest diff. peak and hole	0.434 and -0.467 e · Å ⁻³	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2).

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.2509(6)	0.6872(5)	0.2718(5)	0.017(2)
C(2)	0.4240(5)	0.7616(6)	0.2349(4)	0.015(1)
C(3)	0.4336(6)	0.6703(4)	0.3877(6)	0.022(2)
C(4)	0.5003(6)	0.6324(5)	0.4795(6)	0.026(2)
C(5)	0.4475(7)	0.5726(5)	0.5465(6)	0.028(2)
C(6)	0.3268(6)	0.5499(5)	0.5253(6)	0.028(2)
C(7)	0.2608(6)	0.5869(5)	0.4387(7)	0.023(2)
C(8)	0.3102(6)	0.6480(4)	0.3662(6)	0.018(2)
C(9)	0.4819(6)	0.8271(5)	0.1621(6)	0.022(2)
C(10)	0.5005(7)	0.9060(5)	0.2364(6)	0.028(2)
C(11)	0.5998(6)	0.7966(4)	0.1121(6)	0.023(2)
C(12)	0.1239(5)	0.6691(4)	0.2337(6)	0.016(2)
C(13)	0.0997(6)	0.6367(5)	0.1233(7)	0.016(2)
C(14)	-0.0204(6)	0.6246(4)	0.0833(6)	0.018(2)
C(15)	-0.1122(6)	0.6457(4)	0.1549(6)	0.021(2)
C(16)	-0.0895(6)	0.6797(4)	0.2682(6)	0.019(2)
C(17)	-0.1829(6)	0.7023(5)	0.3421(6)	0.023(2)
C(18)	-0.1595(6)	0.7377(4)	0.4486(6)	0.023(2)
C(19)	-0.0409(5)	0.7530(6)	0.4880(5)	0.024(2)
C(20)	0.0495(6)	0.7305(4)	0.4212(5)	0.022(2)
C(21)	0.0296(6)	0.6925(4)	0.3084(5)	0.016(2)
C(22)	0.3259(6)	0.5583(4)	0.0950(6)	0.014(2)
C(23)	0.4458(6)	0.5814(5)	0.1017(6)	0.023(2)
C(24)	0.5254(7)	0.5372(5)	0.1722(7)	0.033(2)
C(25)	0.4890(7)	0.4682(5)	0.2321(7)	0.038(2)
C(26)	0.3725(7)	0.4418(5)	0.2237(7)	0.031(2)
C(27)	0.2906(6)	0.4889(5)	0.1562(6)	0.024(2)
C(28)	0.1621(6)	0.5700(4)	-0.1094(6)	0.017(2)
C(29)	0.1997(6)	0.4893(4)	-0.1332(6)	0.019(2)
C(30)	0.1564(6)	0.4488(5)	-0.2350(6)	0.024(2)
C(31)	0.0767(6)	0.4868(4)	-0.3105(6)	0.020(2)
C(32)	0.0402(6)	0.5663(5)	-0.2885(6)	0.024(2)
C(33)	0.0819(6)	0.6087(4)	-0.1897(6)	0.018(2)
C(34)	0.2354(5)	0.7833(4)	-0.1523(5)	0.016(2)
C(35)	0.3095(5)	0.7430(4)	-0.2343(5)	0.019(2)

C(36)	0.3194(6)	0.7765(5)	-0.3433(5)	0.023(2)
C(37)	0.2562(6)	0.8483(5)	-0.3791(6)	0.021(2)
C(38)	0.2702(7)	0.8864(5)	-0.4900(6)	0.033(2)
C(39)	0.2141(8)	0.9564(6)	-0.5219(7)	0.035(2)
C(40)	0.1370(8)	0.9940(5)	-0.4433(7)	0.037(2)
C(41)	0.1174(7)	0.9600(4)	-0.3369(6)	0.025(2)
C(42)	0.1775(6)	0.8866(5)	-0.3001(6)	0.021(2)
C(43)	0.1706(6)	0.8511(4)	-0.1832(5)	0.014(2)
C(44)	0.1022(6)	0.8894(5)	-0.0876(6)	0.019(2)
C(45)	-0.0150(6)	0.8456(5)	-0.0693(6)	0.028(2)
C(46)	0.2796(6)	0.9519(5)	0.0040(6)	0.026(2)
C(47)	0.1229(7)	0.9096(5)	0.1297(7)	0.026(2)
F(1)	0.2958(5)	0.1034(4)	0.2983(5)	0.079(2)
F(2)	0.2086(4)	0.1267(3)	0.1230(4)	0.066(2)
F(3)	0.1722(4)	0.2123(3)	0.2701(4)	0.052(1)
F(4)	0.2819(4)	0.2563(5)	0.1248(4)	0.063(1)
F(5)	0.3687(4)	0.2329(3)	0.3036(4)	0.064(2)
F(6)	0.4068(5)	0.1478(4)	0.1531(5)	0.079(2)
N(1)	0.3062(4)	0.7436(3)	0.2045(4)	0.014(2)
N(2)	0.4873(5)	0.7284(3)	0.3213(4)	0.018(1)
N(3)	0.1853(5)	0.8892(4)	0.0224(6)	0.018(2)
P(1)	0.2201(2)	0.6257(1)	0.0185(2)	0.016(1)
P(2)	0.2905(2)	0.1789(1)	0.2115(2)	0.028(1)
Pd	0.2480(1)	0.7628(1)	0.0204(1)	0.015(1)

Table 3. Bond lengths [Å] and angles [°].

C(1)-N(1)	1.357(8)	C(1)-C(8)	1.394(9)
C(1)-C(12)	1.505(9)	C(2)-N(2)	1.307(7)
C(2)-N(1)	1.387(7)	C(2)-C(9)	1.508(10)
C(3)-N(2)	1.361(8)	C(3)-C(4)	1.402(10)
C(3)-C(8)	1.446(9)	C(4)-C(5)	1.381(10)
C(5)-C(6)	1.418(10)	C(6)-C(7)	1.351(10)
C(7)-C(8)	1.414(10)	C(9)-C(10)	1.540(10)
C(9)-C(11)	1.545(9)	C(12)-C(13)	1.378(10)
C(12)-C(21)	1.437(9)	C(13)-C(14)	1.422(9)
C(13)-P(1)	1.849(8)	C(14)-C(15)	1.383(9)
C(15)-C(16)	1.416(9)	C(16)-C(21)	1.413(9)
C(16)-C(17)	1.420(9)	C(17)-C(18)	1.355(9)
C(18)-C(19)	1.413(9)	C(19)-C(20)	1.343(9)
C(20)-C(21)	1.433(9)	C(22)-C(27)	1.387(10)
C(22)-C(23)	1.398(9)	C(22)-P(1)	1.811(7)
C(23)-C(24)	1.378(10)	C(24)-C(25)	1.379(11)
C(25)-C(26)	1.378(11)	C(26)-C(27)	1.400(10)
C(28)-C(29)	1.401(10)	C(28)-C(33)	1.406(9)
C(28)-P(1)	1.811(7)	C(29)-C(30)	1.401(9)
C(30)-C(31)	1.363(9)	C(31)-C(32)	1.375(10)
C(32)-C(33)	1.383(9)	C(34)-C(43)	1.355(9)
C(34)-C(35)	1.432(8)	C(34)-Pd	1.993(6)
C(35)-C(36)	1.362(9)	C(36)-C(37)	1.414(10)
C(37)-C(38)	1.418(10)	C(37)-C(42)	1.427(10)
C(38)-C(39)	1.339(12)	C(39)-C(40)	1.409(11)
C(40)-C(41)	1.354(10)	C(41)-C(42)	1.422(10)
C(42)-C(43)	1.453(9)	C(43)-C(44)	1.491(9)
C(44)-C(45)	1.518(9)	C(44)-N(3)	1.533(9)
C(46)-N(3)	1.488(9)	C(47)-N(3)	1.469(9) F(1)-
P(2)	1.570(5)	F(2)-P(2)	1.582(5) F(3)-
P(2)	1.605(5)	F(4)-P(2)	1.594(6) F(5)-
P(2)	1.601(5)	F(6)-P(2)	1.574(5)
N(1)-Pd	2.192(5)	N(3)-Pd	2.164(6) P(1)-
Pd	2.238(2)		
N(1)-C(1)-C(8)	121.6(6)	N(1)-C(1)-C(12)	114.8(6)
C(8)-C(1)-C(12)	123.6(6)	N(2)-C(2)-N(1)	126.0(7)
N(2)-C(2)-C(9)	117.9(6)	N(1)-C(2)-C(9)	116.1(6)

N(2)-C(3)-C(4)	118.6(6)	N(2)-C(3)-C(8)	121.4(6)
C(4)-C(3)-C(8)	120.0(6)	C(5)-C(4)-C(3)	119.2(7)
C(4)-C(5)-C(6)	121.1(7)	C(7)-C(6)-C(5)	120.3(7)
C(6)-C(7)-C(8)	121.2(7)	C(1)-C(8)-C(7)	125.4(7)
C(1)-C(8)-C(3)	116.4(6)	C(7)-C(8)-C(3)	118.2(6)
C(2)-C(9)-C(10)	109.4(6)	C(2)-C(9)-C(11)	112.0(6)
C(10)-C(9)-C(11)	111.5(6)	C(13)-C(12)-C(21)	121.0(6)
C(13)-C(12)-C(1)	119.2(6)	C(21)-C(12)-C(1)	119.6(6)
C(12)-C(13)-C(14)	119.7(7)	C(12)-C(13)-P(1)	120.0(5)
C(14)-C(13)-P(1)	119.5(6)	C(15)-C(14)-C(13)	120.0(7)
C(14)-C(15)-C(16)	121.4(6)	C(21)-C(16)-C(15)	119.1(6)
C(21)-C(16)-C(17)	119.0(6)	C(15)-C(16)-C(17)	121.9(6)
C(18)-C(17)-C(16)	121.0(7)	C(17)-C(18)-C(19)	120.3(6)
C(20)-C(19)-C(18)	120.0(7)	C(19)-C(20)-C(21)	121.8(6)
C(16)-C(21)-C(20)	117.7(6)	C(16)-C(21)-C(12)	118.9(6)
C(20)-C(21)-C(12)	123.4(6)	C(27)-C(22)-C(23)	118.9(6)
C(27)-C(22)-P(1)	122.1(5)	C(23)-C(22)-P(1)	118.6(5)
C(24)-C(23)-C(22)	119.7(7)	C(23)-C(24)-C(25)	120.6(8)
C(26)-C(25)-C(24)	121.1(7)	C(25)-C(26)-C(27)	118.2(8)
C(22)-C(27)-C(26)	121.3(7)	C(29)-C(28)-C(33)	118.7(7)
C(29)-C(28)-P(1)	121.1(5)	C(33)-C(28)-P(1)	120.2(5)
C(30)-C(29)-C(28)	119.8(7)	C(31)-C(30)-C(29)	120.6(7)
C(30)-C(31)-C(32)	120.0(7)	C(31)-C(32)-C(33)	121.2(7)
C(32)-C(33)-C(28)	119.7(7)	C(43)-C(34)-C(35)	121.3(6)
C(43)-C(34)-Pd	114.0(5)	C(35)-C(34)-Pd	123.1(5)
C(36)-C(35)-C(34)	118.9(7)	C(35)-C(36)-C(37)	122.0(7)
C(36)-C(37)-C(38)	122.7(7)	C(36)-C(37)-C(42)	119.4(6)
C(38)-C(37)-C(42)	117.8(7)	C(39)-C(38)-C(37)	122.7(8)
C(38)-C(39)-C(40)	119.2(8)	C(41)-C(40)-C(39)	121.3(8)
C(40)-C(41)-C(42)	120.6(7)	C(41)-C(42)-C(37)	118.4(6)
C(41)-C(42)-C(43)	123.9(7)	C(37)-C(42)-C(43)	117.6(7)
C(34)-C(43)-C(42)	120.6(6)	C(34)-C(43)-C(44)	115.7(6)
C(42)-C(43)-C(44)	123.5(6)	C(43)-C(44)-C(45)	112.5(6)
C(43)-C(44)-N(3)	106.2(5)	C(45)-C(44)-N(3)	113.1(6)
C(1)-N(1)-C(2)	117.1(5)	C(1)-N(1)-Pd	120.5(4)
C(2)-N(1)-Pd	117.0(4)	C(2)-N(2)-C(3)	117.5(6)
C(47)-N(3)-C(46)	109.4(6)	C(47)-N(3)-C(44)	112.5(6)
C(46)-N(3)-C(44)	107.4(6)	C(47)-N(3)-Pd	112.8(5)
C(46)-N(3)-Pd	114.1(5)	C(44)-N(3)-Pd	100.4(4)
C(22)-P(1)-C(28)	107.2(3)	C(22)-P(1)-C(13)	103.4(3)

C(28)-P(1)-C(13)	108.4(3)	C(22)-P(1)-Pd	120.1(2)	
C(28)-P(1)-Pd	123.1(2)	C(13)-P(1)-Pd	90.3(2)	F(1)-
P(2)-F(6)	90.4(4)	F(1)-P(2)-F(2)	89.6(3)	F(6)-
P(2)-F(2)	91.9(3)	F(1)-P(2)-F(4)	178.5(3)	F(6)-
P(2)-F(4)	91.1(3)	F(2)-P(2)-F(4)	90.3(3)	F(1)-
P(2)-F(5)	90.4(3)	F(6)-P(2)-F(5)	90.3(3)	F(2)-
P(2)-F(5)	177.8(3)	F(4)-P(2)-F(5)	89.7(3)	F(1)-
P(2)-F(3)	90.7(3)	F(6)-P(2)-F(3)	178.9(3)	F(2)-
P(2)-F(3)	88.4(3)	F(4)-P(2)-F(3)	87.8(3)	F(5)-
P(2)-F(3)	89.3(3)	C(34)-Pd-N(3)	80.9(2)	
C(34)-Pd-N(1)	166.7(2)	N(3)-Pd-N(1)	102.0(2)	
C(34)-Pd-P(1)	98.70(19)	N(3)-Pd-P(1)	152.93(16)	
N(1)-Pd-P(1)	84.56(15)			

Table 4. Anisotropic displacement parameters (\AA^2).

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}].$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	0.021(4)	0.012(4)	0.017(4)	-0.007(4)	-0.003(3)	0.001(4)
C(2)	0.021(3)	0.011(3)	0.012(3)	0.001(5)	0.003(3)	0.007(5)
C(3)	0.025(4)	0.024(5)	0.017(4)	-0.001(3)	0.006(3)	0.006(4)
C(4)	0.010(4)	0.040(5)	0.026(4)	0.002(4)	-0.002(3)	0.004(4)
C(5)	0.037(5)	0.027(5)	0.020(4)	0.013(4)	0.000(4)	0.002(4)
C(6)	0.022(4)	0.036(6)	0.026(5)	0.011(4)	0.000(3)	0.000(4)
C(7)	0.018(4)	0.027(5)	0.025(5)	0.011(4)	-0.002(4)	-0.006(4)
C(8)	0.023(4)	0.015(4)	0.017(4)	-0.002(3)	-0.003(3)	0.001(3)
C(9)	0.014(4)	0.027(5)	0.027(4)	0.002(4)	0.002(3)	0.002(3)
C(10)	0.038(5)	0.023(5)	0.023(4)	-0.004(4)	0.004(4)	-0.011(4)
C(11)	0.027(4)	0.018(4)	0.025(4)	0.002(3)	0.016(3)	-0.011(3)
C(12)	0.012(4)	0.015(4)	0.021(4)	-0.001(3)	0.002(3)	0.000(3)
C(13)	0.020(4)	0.008(4)	0.021(5)	0.002(4)	0.001(3)	-0.006(3)
C(14)	0.024(4)	0.014(4)	0.015(4)	0.002(3)	-0.006(3)	-0.002(4)
C(15)	0.018(4)	0.013(4)	0.031(5)	0.006(4)	-0.005(3)	-0.004(3)
C(16)	0.026(4)	0.012(4)	0.018(4)	0.003(3)	0.004(3)	0.003(3)
C(17)	0.019(4)	0.024(5)	0.026(4)	0.006(4)	0.000(3)	0.005(4)
C(18)	0.030(4)	0.023(6)	0.018(4)	-0.001(3)	0.011(3)	-0.001(3)
C(19)	0.027(4)	0.026(5)	0.020(3)	0.003(5)	0.000(3)	-0.004(5)
C(20)	0.022(4)	0.028(5)	0.018(4)	-0.002(3)	0.003(3)	-0.002(3)
C(21)	0.021(4)	0.007(4)	0.019(4)	0.001(4)	0.000(3)	-0.002(3)
C(22)	0.023(4)	0.008(4)	0.011(4)	0.000(3)	-0.007(3)	0.005(3)
C(23)	0.017(4)	0.024(5)	0.028(4)	-0.012(4)	-0.003(3)	0.009(4)
C(24)	0.023(5)	0.039(6)	0.037(5)	-0.017(4)	-0.008(4)	0.016(4)
C(25)	0.043(6)	0.036(6)	0.034(5)	0.003(4)	-0.010(4)	0.022(5)
C(26)	0.040(5)	0.023(5)	0.031(5)	-0.001(4)	0.007(4)	0.008(4)
C(27)	0.025(4)	0.020(5)	0.027(4)	0.005(4)	-0.004(3)	0.004(4)
C(28)	0.014(4)	0.017(5)	0.020(4)	0.006(3)	0.002(3)	0.003(3)
C(29)	0.019(4)	0.013(4)	0.024(4)	-0.004(4)	0.004(3)	-0.001(3)
C(30)	0.028(4)	0.018(5)	0.027(4)	-0.009(4)	0.009(4)	-0.004(4)
C(31)	0.026(4)	0.018(5)	0.017(4)	-0.001(3)	0.002(3)	-0.001(4)
C(32)	0.025(4)	0.023(5)	0.023(4)	-0.001(4)	-0.003(4)	-0.008(4)
C(33)	0.014(4)	0.015(4)	0.024(4)	-0.004(4)	0.001(3)	-0.005(3)
C(34)	0.018(4)	0.011(6)	0.021(4)	-0.001(3)	0.002(3)	-0.003(3)

C(35)	0.024(4)	0.007(5)	0.026(4)	-0.003(3)	-0.001(3)	0.003(3)
C(36)	0.028(4)	0.031(6)	0.011(3)	-0.002(4)	0.001(3)	-0.003(4)
C(37)	0.030(5)	0.022(5)	0.010(4)	-0.003(3)	-0.010(3)	-0.009(4)
C(38)	0.043(5)	0.033(5)	0.023(5)	-0.001(4)	0.006(4)	-0.008(4)
C(39)	0.061(6)	0.026(6)	0.017(5)	0.011(4)	-0.020(4)	-0.025(5)
C(40)	0.065(6)	0.015(5)	0.028(5)	0.006(4)	-0.017(4)	-0.011(4)
C(41)	0.038(5)	0.015(5)	0.020(4)	0.000(4)	-0.005(4)	0.000(4)
C(42)	0.024(4)	0.018(5)	0.019(4)	0.002(3)	-0.008(3)	-0.008(4)
C(43)	0.020(4)	0.010(4)	0.011(4)	-0.003(3)	0.002(3)	-0.006(3)
C(44)	0.025(4)	0.014(4)	0.018(4)	0.007(3)	-0.011(3)	0.003(4)
C(45)	0.026(5)	0.033(5)	0.026(5)	-0.006(4)	-0.004(4)	0.014(4)
C(46)	0.039(5)	0.012(4)	0.027(5)	-0.002(4)	0.005(4)	-0.004(4)
C(47)	0.048(5)	0.014(5)	0.016(5)	0.000(4)	0.005(4)	0.011(4)
F(1)	0.069(4)	0.062(4)	0.104(5)	0.061(4)	-0.037(3)	-0.022(3)
F(2)	0.053(3)	0.070(4)	0.073(4)	-0.044(3)	-0.035(3)	0.018(3)
F(3)	0.049(3)	0.066(4)	0.044(3)	-0.008(3)	0.016(2)	0.003(3)
F(4)	0.069(3)	0.067(4)	0.053(3)	0.039(4)	0.008(2)	-0.008(4)
F(5)	0.066(3)	0.059(4)	0.064(3)	0.006(3)	-0.030(3)	-0.027(3)
F(6)	0.046(3)	0.094(5)	0.098(5)	-0.019(4)	0.018(3)	0.018(3)
N(1)	0.016(3)	0.010(4)	0.015(3)	0.004(3)	0.000(2)	0.000(3)
N(2)	0.027(3)	0.016(3)	0.012(3)	0.000(3)	-0.003(3)	-0.002(3)
N(3)	0.024(4)	0.013(4)	0.018(4)	-0.001(3)	0.004(3)	0.002(3)
P(1)	0.018(1)	0.016(1)	0.013(1)	-0.001(1)	0.001(1)	-0.001(1)
P(2)	0.027(1)	0.031(1)	0.024(1)	0.003(1)	-0.004(1)	-0.005(1)
Pd	0.020(1)	0.013(1)	0.014(1)	0.001(1)	0.001(1)	-0.001(1)
