

Supporting Information

for

**Phosphoryl- or phosphinoyl-functionalized benzo[de]isoquinolinones:  
Synthesis, experimental design, mechanism and biological activity**

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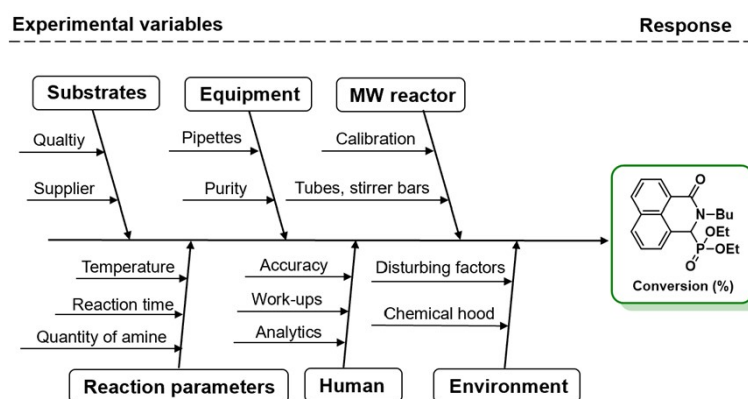
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## Experimental design



**Figure S1.** Ishikawa diagram for the synthesis of the diethyl (2-butyl-3-oxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-yl)phosphonate (**1**).

### <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>31</sup>P NMR data

#### Diethyl (2-butyl-3-oxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-yl)phosphonate (**1**)

Yield: 83% (0.31 g), yellow crystals; Mp: 81–83 °C; <sup>31</sup>P (CDCl<sub>3</sub>) δ 18.7; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 0.82 (t, *J*<sub>HH</sub> = 7.0, 3H), 0.92 (t, *J*<sub>HH</sub> = 7.3, 3H), 1.18 (t, *J*<sub>HH</sub> = 7.1, 3H), 1.28–1.43 (m, 2H), 1.59–1.73 (m, 2H), 3.18–3.37 (m, 2H), 3.50–3.66 (m, 1H), 3.92–4.07 (m, 2H), 4.49–4.64 (m, 1H), 5.23 (d, *J*<sub>HP</sub> = 15.8, 1H), 7.48–7.70 (m, 3H), 7.82–7.90 (m, 1H), 7.98 (m, 1H), 8.31–8.43 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 13.9, 16.0 (d, <sup>3</sup>*J*<sub>CP</sub> = 5.5), 16.4 (d, <sup>3</sup>*J*<sub>CP</sub> = 5.7), 20.2, 29.6, 47.4, 60.0 (d, <sup>1</sup>*J*<sub>CP</sub> = 150.0), 63.3 (d, <sup>2</sup>*J*<sub>CP</sub> = 8.0), 63.4 (d, <sup>2</sup>*J*<sub>CP</sub> = 7.5), 125.1 (d, *J*<sub>CP</sub> = 5.7), 125.5 (d, *J*<sub>CP</sub> = 7.8), 125.8 (d, *J*<sub>CP</sub> = 5.0), 125.8 (d, *J*<sub>CP</sub> = 3.7), 126.5 (d, *J*<sub>CP</sub> = 2.4), 126.6 (d, *J*<sub>CP</sub> = 3.0), 127.3 (d, *J*<sub>CP</sub> = 5.3), 129.1 (d, *J*<sub>CP</sub> = 4.0), 131.3 (d, *J*<sub>CP</sub> = 2.4), 132.2 (d, *J*<sub>CP</sub> = 3.7), 163.3; [M+H]<sup>+</sup><sub>found</sub> = 376.1677, C<sub>20</sub>H<sub>27</sub>NO<sub>4</sub>P requires 376.1599.

#### Diethyl (2-cyclohexyl-3-oxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-yl)phosphonate (**2**)

Yield: 62% (0.25 g), light yellow oil; <sup>31</sup>P (CDCl<sub>3</sub>) δ 18.8; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 0.88 (t, *J*<sub>HH</sub> = 7.0, 3H), 1.16 (t, *J*<sub>HH</sub> = 7.1, 3H), 1.22–1.45 (m, 4H), 1.84–1.92 (m, 2H), 1.98–2.04 (m, 1H), 2.10–2.17 (m, 2H), 2.37–2.47 (m, 1H), 3.30–3.40 (m, 1H), 3.54–3.64 (m, 1H), 3.69–3.77 (m, 1H), 3.89–3.98 (m, 2H), 5.24 (d, *J*<sub>HP</sub> = 16.8, 1H), 7.50–7.57 (m, 2H), 7.59–7.69 (m, 1H), 7.81–7.87 (m, 1H), 7.94–7.99 (m, 1H), 8.30–8.34 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) 16.0 (d, <sup>3</sup>*J*<sub>CP</sub> = 5.6), 16.3 (d, <sup>3</sup>*J*<sub>CP</sub> = 5.9), 25.6, 26.4, 26.6, 29.7, 30.6, 60.1 (d, <sup>1</sup>*J*<sub>CP</sub> = 152.0), 61.8, 63.25 (d, <sup>2</sup>*J*<sub>CP</sub> = 15.2), 63.34 (d, <sup>2</sup>*J*<sub>CP</sub> = 24.3), 125.4 (d, *J*<sub>CP</sub> = 5.7), 125.7 (d, *J*<sub>CP</sub> = 4.9), 125.8 (d, *J*<sub>CP</sub> = 5.3), 126.4 (d, *J*<sub>CP</sub> = 2.9), 126.6 (d, *J*<sub>CP</sub> = 2.2), 127.0 (d, *J*<sub>CP</sub> = 3.6), 127.1 (d, *J*<sub>CP</sub> = 5.3), 128.8 (d, *J*<sub>CP</sub> = 4.0),

131.1 (d,  $J_{CP} = 2.2$ ), 131.9 (d,  $J_{CP} = 4.1$ ), 163.6;  $[M+H]^+$ <sub>found</sub> = 402.1822, C<sub>22</sub>H<sub>29</sub>NO<sub>4</sub>P requires 402.1828.

### **Diethyl (2-benzyl-3-oxo-2,3-dihydro-1*H*-benzo[de]isoquinolin-1-yl)phosphonate (3)**

Yield: 81% (0.33 g), light yellow oil; <sup>31</sup>P (CDCl<sub>3</sub>) δ 18.9; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 0.86 (t,  $J_{HH} = 7.1$ , 3H), 1.20 (t,  $J_{HH} = 7.1$ , 3H), 3.29–3.38 (m, 1H), 3.56–3.66 (m, 1H), 3.97–4.05 (m, 2H), 4.50 (d,  $J_{HP} = 15.3$ , 1H), 5.14 (d,  $J_{HP} = 15.3$ , 1H), 6.01 (d,  $J_{HP} = 15.3$ , 1H), 7.22–7.30 (m, 5H), 7.40–7.44 (m, 1H), 7.46–7.51 (m, 1H), 7.61–7.67 (m, 1H), 7.82–7.86 (m, 1H), 7.97–8.03 (m, 1H), 8.40–8.47 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) 16.0 (d,  $^3J_{CP} = 5.4$ ), 16.4 (d,  $^3J_{CP} = 5.6$ ), 49.2, 58.2 (d,  $^1J_{CP} = 150.5$ ), 63.3 (d,  $^2J_{CP} = 2.3$ ), 63.4 (d,  $^2J_{CP} = 1.9$ ), 124.8 (d,  $J_{CP} = 5.8$ ), 125.4 (d,  $J_{CP} = 3.6$ ), 125.7 (d,  $J_{CP} = 8.1$ ), 125.8 (d,  $J_{CP} = 5.1$ ), 126.5 (d,  $J_{CP} = 2.3$ ), 127.1 (d,  $J_{CP} = 2.8$ ), 127.3 (d,  $J_{CP} = 5.2$ ), 127.6, 128.2, 128.8, 129.0 (d,  $J_{CP} = 3.8$ ), 131.7 (d,  $J_{CP} = 2.2$ ), 132.2 (d,  $J_{CP} = 3.7$ ), 136.6, 163.7;  $[M+H]^+$ <sub>found</sub> = 410.1535, C<sub>23</sub>H<sub>25</sub>NO<sub>4</sub>P requires 410.1521.

### **Dimethyl (2-butyl-3-oxo-2,3-dihydro-1*H*-benzo[de]isoquinolin-1-yl)phosphonate (4)**

Yield: 72% (0.25 g), light yellow crystals; Mp: 86–88 °C; <sup>31</sup>P (CDCl<sub>3</sub>) δ 21.0; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 0.92 (t,  $J_{HH} = 7.4$ , 3H), 1.30–1.44 (m, 2H), 1.59–1.73 (m, 2H), 3.14 (d,  $J_{HH} = 10.4$ , 3H), 3.21–3.31 (m, 1H), 3.62 (d,  $J_{HH} = 10.6$ , 3H), 4.50–4.62 (m, 1H), 5.26 (d,  $J_{HP} = 15.7$ , 1H), 7.51–7.60 (m, 2H), 7.61–7.67 (m, 1H), 7.82–7.90 (m, 1H), 7.95–8.02 (m, 1H), 8.33–8.41 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 13.9, 20.1, 29.6, 47.3, 53.6 (d,  $^2J_{CP} = 6.8$ ), 53.7 (d,  $^2J_{CP} = 6.5$ ), 59.6 (d,  $^1J_{CP} = 150.1$ ), 124.8 (d,  $J_{CP} = 5.7$ ), 125.50 (d,  $J_{CP} = 3.7$ ), 125.53 (d,  $J_{CP} = 8.2$ ), 125.8 (d,  $J_{CP} = 5.0$ ), 126.6 (d,  $J_{CP} = 2.3$ ), 126.8 (d,  $J_{CP} = 3.0$ ), 127.5 (d,  $J_{CP} = 5.3$ ), 128.9 (d,  $J_{CP} = 4.2$ ), 131.4 (d,  $J_{CP} = 2.3$ ), 132.2 (d,  $J_{CP} = 3.7$ ), 163.3;  $[M+H]^+$ <sub>found</sub> = 348.1363, C<sub>18</sub>H<sub>23</sub>NO<sub>4</sub>P requires 348.1364.

### **Dibutyl (2-butyl-3-oxo-2,3-dihydro-1*H*-benzo[de]isoquinolin-1-yl)phosphonate (5)**

Yield: 90% (0.39 g), light yellow oil; <sup>31</sup>P (CDCl<sub>3</sub>) δ 18.8; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 0.69 (t,  $J_{HH} = 7.3$ , 3H), 0.83 (t,  $J_{HH} = 7.4$ , 3H), 0.92 (t,  $J_{HH} = 7.3$ , 3H), 0.94–1.03 (m, 2H), 1.05–1.16 (m, 2H), 1.17–1.27 (m, 2H), 1.30–1.40 (m, 2H), 1.44–1.52 (m, 2H), 1.61–1.71 (m, 2H), 3.10–3.19 (m, 1H), 3.25–3.33 (m, 1H), 3.51–3.59 (m, 1H), 3.88–3.96 (m, 2H), 4.51–4.61 (m, 1H), 5.24 (d,  $J_{HP} = 15.8$ , 1H), 7.50–7.55 (m, 1H), 7.56–7.64 (m, 2H), 7.82–7.88 (m, 1H), 7.95–8.00 (m, 1H), 8.33–8.38 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 13.4, 13.5, 13.9, 18.3, 18.6, 20.2, 29.6, 32.1 (d,  $^3J_{CP} = 5.5$ ), 32.4 (d,  $^3J_{CP} = 5.8$ ), 47.4, 59.8 (d,  $^1J_{CP} = 150.1$ ), 66.9 (d,  $^2J_{CP} = 8.1$ ), 67.0 (d,  $^2J_{CP} = 7.7$ ), 125.1 (d,  $J_{CP} = 5.9$ ), 125.5 (d,  $J_{CP} = 7.9$ ), 125.7 (d,  $J_{CP} = 2.7$ ), 125.8 (d,  $J_{CP} = 1.4$ ), 126.5 (d,  $J_{CP} = 2.3$ ), 126.6 (d,  $J_{CP} = 2.9$ ), 127.2 (d,  $J_{CP} = 5.4$ ), 129.0 (d,  $J_{CP} = 4.1$ ), 131.3 (d,  $J_{CP} = 2.3$ ), 132.2 (d,  $J_{CP} = 3.7$ ), 163.3;  $[M+H]^+$ <sub>found</sub> = 432.2286, C<sub>24</sub>H<sub>35</sub>NO<sub>4</sub>P requires 432.2298.

### **Dibenzyl (2-butyl-3-oxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-yl)phosphonate (6)**

Yield: 93% (0.46 g), white crystals; Mp: 79–81 °C;  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  19.3;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  0.87 (t,  $J_{\text{HH}} = 7.3$ , 3H), 1.21–1.37 (m, 2H), 1.52–1.68 (m, 2H), 3.16–3.33 (m, 1H), 4.14–4.26 (m, 1H), 4.43–4.59 (m, 2H), 4.82 (d,  $J_{\text{HP}} = 8.1$ , 2H), 5.25 (d,  $J_{\text{HP}} = 15.5$ , 1H), 6.87–6.96 (m, 2H), 7.02–7.13 (m, 2H), 7.15–7.31 (m, 5H), 7.33–7.40 (m, 1H), 7.43–7.63 (m, 3H), 7.80–7.89 (m, 1H), 7.90–8.00 (m, 1H), 8.24–8.35 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  13.9, 20.1, 29.5, 47.4, 60.1 (d,  $^1J_{\text{CP}} = 149.5$ ), 68.59 (d,  $^2J_{\text{CP}} = 7.5$ ), 68.61 (d,  $^2J_{\text{CP}} = 7.9$ ), 124.8 (d,  $J_{\text{CP}} = 5.9$ ), 125.5 (d,  $J_{\text{CP}} = 5.2$ ), 125.6 (d,  $J_{\text{CP}} = 7.1$ ), 125.7 (d,  $J_{\text{CP}} = 5.0$ ), 126.6 (d,  $J_{\text{CP}} = 2.1$ ), 126.8 (d,  $J_{\text{CP}} = 2.9$ ), 127.4 (d,  $J_{\text{CP}} = 5.5$ ), 127.9, 128.0, 128.42, 128.49, 128.50, 128.52, 129.0 (d,  $J_{\text{CP}} = 3.9$ ), 131.4 (d,  $J_{\text{CP}} = 2.2$ ), 132.2 (d,  $J_{\text{CP}} = 3.6$ ), 135.4 (d,  $^3J_{\text{CP}} = 5.8$ ), 135.6 (d,  $^3J_{\text{CP}} = 5.9$ ), 163.3;  $[\text{M}+\text{H}]^+_{\text{found}} = 500.1988$ ,  $\text{C}_{30}\text{H}_{31}\text{NO}_4\text{P}$  requires 500.1990.

### **2-Butyl-3-hydroxy-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-one (8)**

Yield: 83% (0.21 g), white crystals; Mp: 130–132 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  0.85 (t,  $J_{\text{HH}} = 7.4$ , 3H), 1.24–1.33 (m, 2H), 1.54–1.64 (m, 2H), 3.39–3.49 (m, 1H), 3.82–3.91 (m, 1H), 6.03 (s, 1H), 7.24–7.34 (m, 1H), 7.48–7.54 (m, 1H), 7.60–7.66 (m, 1H), 7.76–7.85 (m, 2H), 7.89–7.95 (m, 1H),  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  13.9, 20.4, 30.0, 44.4, 80.9, 123.3, 126.2, 126.36, 126.39, 126.7, 127.4, 128.2, 130.8, 131.7, 131.8, 162.8;  $[\text{M}+\text{H}]^+_{\text{found}} = 256.1342$ ,  $\text{C}_{16}\text{H}_{18}\text{NO}_2$  requires 256.1337.

### **3-(Diphenylphosphoryl)-1*H*, 3*H*-benzo[*de*]isochromen-1-one (9)**

Yield: 30% (0.12 g), white crystals; Mp: 221–223 °C;  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  27.7;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.67 (d,  $J_{\text{HP}} = 9.3$ , 1H), 6.97–7.03 (m, 2H), 7.11–7.18 (m, 2H), 7.20–7.25 (m, 1H), 7.38–7.44 (m, 1H), 7.59–7.70 (m, 4H), 7.75–7.79 (m, 1H), 7.85–7.92 (m, 2H), 7.97–8.01 (m, 1H), 8.17–8.24 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  80.2 (d,  $^1J_{\text{CP}} = 75.8$ ), 119.2 (d,  $J_{\text{CP}} = 1.9$ ), 122.0 (d,  $J_{\text{CP}} = 3.2$ ), 125.5 (d,  $J_{\text{CP}} = 5.4$ ), 125.8 (d,  $J_{\text{CP}} = 1.4$ ), 126.5 (d,  $J_{\text{CP}} = 3.5$ ), 126.6 (d,  $J_{\text{CP}} = 35.8$ ), 126.7 (d,  $J_{\text{CP}} = 97.1$ ), 127.5 (d,  $J_{\text{CP}} = 3.7$ ), 127.8 (d,  $J_{\text{CP}} = 5.4$ ), 128.0 (d,  $J_{\text{CP}} = 11.8$ ), 128.4 (d,  $J_{\text{CP}} = 1.3$ ), 128.88 (d,  $J_{\text{CP}} = 3.2$ ), 128.98 (d,  $J_{\text{CP}} = 11.8$ ), 129.0 (d,  $J_{\text{CP}} = 99.0$ ), 129.8 (d,  $J_{\text{CP}} = 2.9$ ), 131.6 (d,  $J_{\text{CP}} = 2.3$ ), 132.3 (d,  $J_{\text{CP}} = 2.7$ ), 132.4 (d,  $J_{\text{CP}} = 2.2$ ), 132.5 (d,  $J_{\text{CP}} = 2.8$ ), 132.9 (d,  $J_{\text{CP}} = 2.9$ ), 133.5 (d,  $J_{\text{CP}} = 1.5$ ), 133.7 (d,  $J_{\text{CP}} = 1.4$ ), 162.3;  $[\text{M}+\text{H}]^+_{\text{found}} = 385.0995$ ,  $\text{C}_{24}\text{H}_{18}\text{O}_3\text{P}$  385.0993 requires.

**Diphenyl (2-butyl-3-oxo-2,3-dihydro-1H-benzo[de]isoquinolin-1-yl)phosphine oxide (10)**

Yield: 80% (0.35 g), yellow crystals; Mp: 160–162 °C; <sup>31</sup>P (CDCl<sub>3</sub>) δ 30.7; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 0.86 (t, *J*<sub>HH</sub> = 7.5, 3H), 1.22–1.31 (m, 2H), 1.54–1.67 (m, 2H), 3.09–3.19 (m, 1H), 4.38–4.49 (m, 1H), 5.71 (d, *J*<sub>HP</sub> = 11.8, 1H), 7.06–7.13 (m, 1H), 7.15–7.24 (m, 2H), 7.25–7.37 (m, 5H), 7.38–7.47 (m, 3H), 7.51–7.60 (m, 2H), 7.70–7.76 (m, 1H), 7.77–7.84 (m, 1H), 7.90–8.00 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 13.9, 20.1, 29.6, 48.5, 65.2 (d, <sup>1</sup>*J*<sub>CP</sub> = 69.6), 125.02 (d, *J*<sub>CP</sub> = 1.8), 125.06 (d, *J*<sub>CP</sub> = 4.2), 125.08 (d, *J*<sub>CP</sub> = 2.1), 125.3 (d, *J*<sub>CP</sub> = 4.3), 125.6 (d, *J*<sub>CP</sub> = 3.2), 126.1 (d, *J*<sub>CP</sub> = 2.6), 126.4 (d, *J*<sub>CP</sub> = 1.4), 127.0 (d, *J*<sub>CP</sub> = 92.1), 127.1 (d, *J*<sub>CP</sub> = 4.7), 128.2 (d, *J*<sub>CP</sub> = 11.0), 128.3 (d, *J*<sub>CP</sub> = 11.3), 128.7 (d, *J*<sub>CP</sub> = 80.1), 129.4 (d, *J*<sub>CP</sub> = 3.1), 130.9 (d, *J*<sub>CP</sub> = 1.8), 131.9 (d, *J*<sub>CP</sub> = 8.8), 132.3 (d, *J*<sub>CP</sub> = 2.9), 132.4 (d, *J*<sub>CP</sub> = 3.0), 132.6 (d, *J*<sub>CP</sub> = 8.3), 163.1; [M+H]<sup>+</sup><sub>found</sub> = 440.1783, C<sub>28</sub>H<sub>27</sub>NO<sub>2</sub>P requires 440.1779.

**Bis(*p*-tolyl) (2-butyl-3-oxo-2,3-dihydro-1H-benzo[de]isoquinolin-1-yl)phosphine oxide (11)**

Yield: 90% (0.42 g), yellow crystals; Mp: 186–188 °C; <sup>31</sup>P (CDCl<sub>3</sub>) δ 31.8; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 0.86 (t, *J*<sub>HH</sub> = 7.4, 3H), 1.25–1.33 (m, 2H), 1.55–1.65 (m, 2H), 2.29 (s, 3H), 2.31 (s, 3H), 3.14–3.22 (m, 1H), 4.39–4.48 (m, 1H), 5.67 (d, *J*<sub>HP</sub> = 12.1, 1H), 6.94–7.00 (m, 2H), 7.05–7.10 (m, 3H), 7.14–7.20 (m, 2H), 7.28–7.32 (m, 1H), 7.37–7.44 (m, 3H), 7.70–7.74 (m, 1H), 7.77–7.81 (m, 1H), 7.88–7.92 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 13.9, 20.1, 21.49, 21.52, 29.7, 48.1, 65.1 (d, <sup>1</sup>*J*<sub>CP</sub> = 69.1), 123.6 (d, *J*<sub>CP</sub> = 95.0), 125.1 (d, *J*<sub>CP</sub> = 6.4), 125.2 (d, *J*<sub>CP</sub> = 4.3), 125.29 (d, *J*<sub>CP</sub> = 95.9), 125.32 (d, *J*<sub>CP</sub> = 1.7), 125.7 (d, *J*<sub>CP</sub> = 2.8), 125.9 (d, *J*<sub>CP</sub> = 2.4), 126.0 (d, *J*<sub>CP</sub> = 1.7), 126.9 (d, *J*<sub>CP</sub> = 5.3), 128.7 (d, *J*<sub>CP</sub> = 12.2), 128.90 (d, *J*<sub>CP</sub> = 11.6), 128.97 (d, *J*<sub>CP</sub> = 11.7), 129.7 (d, *J*<sub>CP</sub> = 11.8), 130.1 (d, *J*<sub>CP</sub> = 1.8), 131.9 (d, *J*<sub>CP</sub> = 8.9), 132.6 (d, *J*<sub>CP</sub> = 9.0), 142.8 (d, *J*<sub>CP</sub> = 2.9), 143.0 (d, *J*<sub>CP</sub> = 2.8), 163.1; [M+H]<sup>+</sup><sub>found</sub> = 468.2111, C<sub>30</sub>H<sub>31</sub>NO<sub>2</sub>P requires 468.2092.

**Bis(3,5-dimethylphenyl) (2-butyl-3-oxo-2,3-dihydro-1H-benzo[de]isoquinolin-1-yl)phosphine oxide (12)**

Yield: 92% (0.46 g), yellow crystals; Mp: 187–189 °C; <sup>31</sup>P (CDCl<sub>3</sub>) δ 32.1; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 0.87 (t, *J*<sub>HH</sub> = 7.4, 3H), 1.23–1.34 (m, 2H), 1.57–1.66 (m, 2H), 2.12 (s, 6H), 2.21 (s, 6H), 3.17–3.25 (m, 1H), 4.39–4.46 (m, 1H), 5.68 (d, *J*<sub>HP</sub> = 12.2, 1H), 6.85–6.90 (m, 2H), 6.97–7.03 (m, 2H), 7.06–7.11 (m, 3H), 7.29–7.34 (m, 1H), 7.38–7.43 (m, 1H), 7.70–7.75 (m, 1H), 7.80–7.85 (m, 1H), 7.95–7.98 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 13.9, 20.1, 21.05, 21.12, 29.6, 48.2, 65.1 (d, <sup>1</sup>*J*<sub>CP</sub> = 67.9), 125.20 (d, *J*<sub>CP</sub> = 1.4), 125.24 (d, *J*<sub>CP</sub> = 2.8), 125.4 (d, *J*<sub>CP</sub> = 1.5), 125.66 (d, *J*<sub>CP</sub> = 3.3), 125.73 (d, *J*<sub>CP</sub> = 2.4), 126.2 (d, *J*<sub>CP</sub> = 1.8), 126.87 (d, *J*<sub>CP</sub> = 4.7), 126.93 (d, *J*<sub>CP</sub> = 91.6), 128.2 (d, *J*<sub>CP</sub> = 92.1), 129.5 (d, *J*<sub>CP</sub> = 3.2), 129.7 (d, *J*<sub>CP</sub> = 8.7), 130.2 (d, *J*<sub>CP</sub> = 8.7), 130.6 (d,

$J_{CP} = 1.9$ ), 131.8 (d,  $J_{CP} = 2.9$ ), 133.9 (d,  $J_{CP} = 3.0$ ), 134.0 (d,  $J_{CP} = 3.1$ ), 137.8 (d,  $J_{CP} = 11.9$ ), 137.9 (d,  $J_{CP} = 12.0$ ), 163.0;  $[M+H]^+_{\text{found}} = 496.2416$ ,  $C_{32}H_{35}NO_2P$  requires 496.2405.

**Bis(2-naphthyl) (2-butyl-3-oxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-yl)phosphine oxide (13)**

Yield: 80% (0.43 g), yellow crystals; Mp: 114–116 °C;  $^{31}P$  ( $CDCl_3$ )  $\delta$  31.9;  $^1H$  NMR ( $CDCl_3$ )  $\delta$  0.84 (t,  $J_{HH} = 7.4$ , 3H), 1.25–1.35 (m, 2H), 1.54–1.70 (m, 2H), 3.18–3.27 (m, 1H), 4.44–4.53 (m, 1H), 5.89 (d,  $J_{HP} = 11.6$ , 1H), 7.13–7.18 (m, 2H), 7.20–7.25 (m, 1H), 7.48–7.53 (m, 2H), 7.55–7.82 (m, 13H), 8.07–8.13 (m, 2H);  $^{13}C$  NMR ( $CDCl_3$ )  $\delta$  13.9, 20.2, 29.7, 48.6, 65.3 (d,  $^1J_{CP} = 69.5$ ), 124.4 (d,  $J_{CP} = 92.5$ ), 125.2 (d,  $J_{CP} = 6.1$ ), 125.3, 125.4 (d,  $J_{CP} = 4.1$ ), 125.47, 125.52 (d,  $J_{CP} = 2.4$ ), 125.8 (d,  $J_{CP} = 93.5$ ), 126.1 (d,  $J_{CP} = 17.6$ ), 126.2, 126.4 (d,  $J_{CP} = 8.6$ ), 126.7 (d,  $J_{CP} = 10.3$ ), 127.0 (d,  $J_{CP} = 11.8$ ), 127.1 (d,  $J_{CP} = 4.6$ ), 127.2, 127.7 (d,  $J_{CP} = 9.2$ ), 127.8 (d,  $J_{CP} = 10.9$ ), 128.03, 128.04 (d,  $J_{CP} = 11.1$ ), 128.6 (d,  $J_{CP} = 9.6$ ), 129.0 (d,  $J_{CP} = 13.5$ ), 129.8, 130.8, 131.9 (d,  $J_{CP} = 3.0$ ), 132.1 (d,  $J_{CP} = 3.3$ ), 132.2 (d,  $J_{CP} = 3.1$ ), 133.7, 134.4 (d,  $J_{CP} = 8.2$ ), 134.7 (d,  $J_{CP} = 2.3$ ), 134.8 (d,  $J_{CP} = 2.1$ ), 135.6 (d,  $J_{CP} = 8.1$ ), 163.1;  $[M+H]^+_{\text{found}} = 540.2110$ ,  $C_{36}H_{31}NO_2P$  requires 540.2092.

**Diphenyl (2-cyclohexyl-3-oxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-yl)phosphine oxide (14)**

Yield: 72% (0.33 g), yellow crystals; Mp: 188–190 °C;  $^{31}P$  ( $CDCl_3$ )  $\delta$  32.0;  $^1H$  NMR ( $CDCl_3$ )  $\delta$  1.15–1.28 (m, 3H), 1.62–1.87 (m, 5H), 1.88–1.98 (m, 1H), 2.24–2.35 (m, 1H), 3.55–3.64 (m, 1H), 5.69 (d,  $J_{HP} = 12.2$ , 1H), 7.09–7.18 (m, 3H), 7.26–7.34 (m, 2H), 7.35–7.42 (m, 1H), 7.46–7.61 (m, 5H), 7.68–7.74 (m, 1H), 7.78–7.83 (m, 1H), 7.84–7.90 (m, 1H), 8.02–8.08 (m, 1H), 8.30–8.39 (m, 1H);  $^{13}C$  NMR ( $CDCl_3$ )  $\delta$  25.6, 26.5, 26.6, 29.6, 30.9, 65.0, 65.8 (d,  $^1J_{CP} = 69.9$ ), 125.1 (d,  $J_{CP} = 6.9$ ), 125.2 (d,  $J_{CP} = 4.4$ ), 125.4 (d,  $J_{CP} = 2.8$ ), 126.0 (d,  $J_{CP} = 1.7$ ), 126.5 (d,  $J_{CP} = 12.0$ ), 126.9 (d,  $J_{CP} = 4.5$ ), 127.0 (d,  $J_{CP} = 3.1$ ), 127.1 (d,  $J_{CP} = 83.5$ ), 128.1 (d,  $J_{CP} = 11.1$ ), 128.3 (d,  $J_{CP} = 11.3$ ), 128.8 (d,  $J_{CP} = 1.7$ ), 128.9 (d,  $J_{CP} = 85.8$ ), 130.7 (d,  $J_{CP} = 1.4$ ), 131.7 (d,  $J_{CP} = 3.4$ ), 132.2 (d,  $J_{CP} = 8.7$ ), 132.26 (d,  $J_{CP} = 2.7$ ), 132.34 (d,  $J_{CP} = 2.4$ ), 132.6 (d,  $J_{CP} = 8.7$ ), 163.7;  $[M+H]^+_{\text{found}} = 466.1949$ ,  $C_{30}H_{29}NO_2P$  requires 466.1935.

**Bis(3,5-dimethylphenyl)(2-cyclohexyl-3-oxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-yl)phosphine oxide (15)**

Yield: 70% (0.37 g), yellow crystals; Mp: 188–190 °C;  $^{31}P$  ( $CDCl_3$ )  $\delta$  32.7;  $^1H$  NMR ( $CDCl_3$ )  $\delta$  1.09–1.38 (m, 4H), 1.72–1.97 (m, 4H), 2.09 (s, 6H), 2.23 (s, 6H), 2.31–2.47 (m, 2H), 3.64–3.72 (m, 1H), 5.69 (d,  $J_{HP} = 12.8$ , 1H), 6.75–6.81 (m, 2H), 6.93–6.98 (m, 2H), 7.03–7.06 (m, 1H), 7.08–7.13 (m, 2H), 7.23–7.26 (m, 1H), 7.39–7.44 (m, 1H), 7.69–7.73 (m, 1H), 7.80–7.84 (m,

1H), 7.90–7.94 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  21.1, 21.2, 25.6, 26.6, 26.7, 29.5, 30.8, 65.2, 66.2 (d,  $J_{\text{CP}} = 68.7$ ), 125.08 (d,  $J_{\text{CP}} = 2.3$ ), 125.13 (d,  $J_{\text{CP}} = 4.3$ ), 125.6 (d,  $J_{\text{CP}} = 2.3$ ), 126.1 (d,  $J_{\text{CP}} = 1.0$ ), 126.4 (d,  $J_{\text{CP}} = 1.8$ ), 126.7 (d,  $J_{\text{CP}} = 4.5$ ), 127.1 (d,  $J_{\text{CP}} = 3.0$ ), 127.2 (d,  $J_{\text{CP}} = 92.6$ ), 128.4 (d,  $J_{\text{CP}} = 92.8$ ), 129.4 (d,  $J_{\text{CP}} = 3.2$ ), 129.9 (d,  $J_{\text{CP}} = 8.3$ ), 130.33 (d,  $J_{\text{CP}} = 1.5$ ), 133.35 (d,  $J_{\text{CP}} = 8.6$ ), 131.7 (d,  $J_{\text{CP}} = 2.7$ ), 133.8 (d,  $J_{\text{CP}} = 2.8$ ), 133.9 (d,  $J_{\text{CP}} = 3.2$ ), 137.7 (d,  $J_{\text{CP}} = 11.9$ ), 137.9 (d,  $J_{\text{CP}} = 11.9$ ), 163.5;  $[\text{M}+\text{H}]^+_{\text{found}} = 522.2541$ ,  $\text{C}_{34}\text{H}_{37}\text{NO}_2\text{P}$  requires 522.2556.

**Diphenyl (2-benzyl-3-oxo-2,3-dihydro-1H-benzo[de]isoquinolin-1-yl)phosphine oxide (16)**

Yield: 85% (0.40 g), yellow crystals; Mp: 173–175 °C;  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  32.1;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  4.53 (d,  $J_{\text{HP}} = 15.5$ , 1H), 5.68 (d,  $J_{\text{HP}} = 10.8$ , 1H), 5.95 (d,  $J_{\text{HP}} = 15.4$ , 1H), 7.10–7.18 (m, 5H), 7.19–7.22 (m, 1H), 7.23–7.28 (m, 5H), 7.33–7.39 (m, 3H), 7.40–7.44 (m, 1H), 7.47–7.52 (m, 1H), 7.57–7.63 (m, 2H), 7.70–7.74 (m, 1H), 7.82–7.85 (m, 1H), 7.98–8.01 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  50.0, 63.0 (d,  $J_{\text{CP}} = 69.3$ ), 124.8 (d,  $J_{\text{CP}} = 1.4$ ), 125.1 (d,  $J_{\text{CP}} = 6.4$ ), 125.2 (d,  $J_{\text{CP}} = 4.5$ ), 126.4 (d,  $J_{\text{CP}} = 1.4$ ), 126.5 (d,  $J_{\text{CP}} = 92.9$ ), 126.6 (d,  $J_{\text{CP}} = 2.2$ ), 127.1 (d,  $J_{\text{CP}} = 4.7$ ), 127.5, 128.09 (d,  $J_{\text{CP}} = 11.1$ ), 128.10, 128.3 (d,  $J_{\text{CP}} = 3.8$ ), 128.5 (d,  $J_{\text{CP}} = 11.3$ ), 128.8, 129.0 (d,  $J_{\text{CP}} = 86.1$ ), 129.6 (d,  $J_{\text{CP}} = 3.3$ ), 131.2 (d,  $J_{\text{CP}} = 1.8$ ), 131.9 (d,  $J_{\text{CP}} = 2.9$ ), 132.0 (d,  $J_{\text{CP}} = 8.7$ ), 132.4 (d,  $J_{\text{CP}} = 2.8$ ), 132.5 (d,  $J_{\text{CP}} = 2.8$ ), 132.7 (d,  $J_{\text{CP}} = 8.6$ ), 136.9, 163.4;  $[\text{M}+\text{H}]^+_{\text{found}} = 474.1641$ ,  $\text{C}_{31}\text{H}_{25}\text{NO}_2\text{P}$  requires 474.1622.

**Bis(3,5-dimethylphenyl) (2-benzyl-3-oxo-2,3-dihydro-1H-benzo[de]isoquinolin-1-yl)phosphine oxide (17)**

Yield: 76% (0.40 g), yellow crystals; Mp: 187–189 °C;  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  33.0;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  2.10 (s, 6H), 2.25 (s, 6H), 4.50 (d,  $J_{\text{HP}} = 15.6$ , 1H), 5.65 (d,  $J_{\text{HP}} = 10.9$ , 1H), 5.94 (d,  $J_{\text{HP}} = 15.5$ , 1H), 6.73–6.77 (m, 2H), 6.82–6.86 (m, 1H), 6.95–6.98 (m, 1H), 7.07–7.10 (m, 1H), 7.11–7.16 (m, 2H), 7.21–7.27 (m, 5H), 7.28–7.31 (m, 1H), 7.42–7.47 (m, 1H), 7.71–7.75 (m, 1H), 7.84–7.88 (m, 1H), 8.03–8.06 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  21.0, 21.2, 49.9, 62.9 (d,  $J_{\text{CP}} = 68.3$ ), 125.2 (d,  $J_{\text{CP}} = 1.6$ ), 125.25 (d,  $J_{\text{CP}} = 5.1$ ), 125.32 (d,  $J_{\text{CP}} = 6.0$ ), 126.3 (d,  $J_{\text{CP}} = 2.1$ ), 126.8 (d,  $J_{\text{CP}} = 92.3$ ), 126.9 (d,  $J_{\text{CP}} = 4.5$ ), 127.5, 128.1, 128.47 (d,  $J_{\text{CP}} = 92.4$ ), 128.48 (d,  $J_{\text{CP}} = 1.0$ ), 128.7, 129.0 (d,  $J_{\text{CP}} = 1.0$ ), 129.6 (d,  $J_{\text{CP}} = 3.0$ ), 129.7 (d,  $J_{\text{CP}} = 8.7$ ), 130.3 (d,  $J_{\text{CP}} = 8.7$ ), 130.9 (d,  $J_{\text{CP}} = 1.6$ ), 131.9 (d,  $J_{\text{CP}} = 2.8$ ), 134.08 (d,  $J_{\text{CP}} = 2.7$ ), 134.09 (d,  $J_{\text{CP}} = 3.2$ ), 137.0, 137.8 (d,  $J_{\text{CP}} = 11.8$ ), 138.2 (d,  $J_{\text{CP}} = 12.2$ ), 163.5;  $[\text{M}+\text{H}]^+_{\text{found}} = 530.2250$ ,  $\text{C}_{35}\text{H}_{33}\text{NO}_2\text{P}$  requires 530.2243.



**Diphenyl[2-(3-dimethylamino-propyl)-3-oxo-2,3-dihydro-1*H*-benzo[de]isoquinolin-1-yl]phosphine oxide (18)**

Yield: 80% (0.38 g), yellow oil;  $^{31}\text{P}$  (DMSO- $d_6$ )  $\delta$  31.4;  $^1\text{H}$  NMR (DMSO- $d_6$ )  $\delta$  1.56–1.66 (m, 1H), 1.67–1.76 (m, 1H), 1.98–2.04 (m, 1H), 2.14 (s, 6H), 2.19–2.24 (m, 1H), 3.02–3.09 (m, 1H), 4.08–4.15 (m, 1H), 6.44 (d,  $J_{\text{HP}} = 7.1$ , 1H), 7.12–7.20 (m, 5H), 7.34–7.40 (m, 1H), 7.41–7.49 (m, 3H), 7.55–7.60 (m, 1H), 7.71–7.78 (m, 3H), 7.85–7.89 (m, 2H), 7.96–7.99 (m, 1H);  $^{13}\text{C}$  NMR (DMSO- $d_6$ )  $\delta$  25.0, 44.7, 45.2, 55.3, 63.4 (d,  $^1J_{\text{CP}} = 67.2$ ), 124.4 (d,  $J_{\text{CP}} = 6.4$ ), 124.8 (d,  $J_{\text{CP}} = 4.5$ ), 125.0 (d,  $J_{\text{CP}} = 2.2$ ), 125.1 (d,  $J_{\text{CP}} = 2.5$ ), 125.6 (d,  $J_{\text{CP}} = 3.2$ ), 125.7 (d,  $J_{\text{CP}} = 1.3$ ), 126.4 (d,  $J_{\text{CP}} = 4.8$ ), 126.9 (d,  $J_{\text{CP}} = 92.4$ ), 127.6 (d,  $J_{\text{CP}} = 11.1$ ), 128.2 (d,  $J_{\text{CP}} = 11.3$ ), 129.1 (d,  $J_{\text{CP}} = 3.4$ ), 129.4 (d,  $J_{\text{CP}} = 91.3$ ), 130.5 (d,  $J_{\text{CP}} = 1.3$ ), 131.37 (d,  $J_{\text{CP}} = 9.1$ ), 131.39 (d,  $J_{\text{CP}} = 2.6$ ), 131.65 (d,  $J_{\text{CP}} = 8.5$ ), 131.72 (d,  $J_{\text{CP}} = 2.8$ ), 132.0 (d,  $J_{\text{CP}} = 2.8$ ), 162.4;  $[\text{M}+\text{H}]^+_{\text{found}} = 469.2043$ ,  $\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_2\text{P}$  requires 469.2039.

**Bis(*p*-tolyl)[2-(3-dimethylamino-propyl)-3-oxo-2,3-dihydro-1*H*-benzo[de]isoquinolin-1-yl]phosphine oxide (19)**

Yield: 85% (0.42 g), yellow oil;  $^{31}\text{P}$  (DMSO- $d_6$ )  $\delta$  30.9;  $^1\text{H}$  NMR (DMSO- $d_6$ )  $\delta$  1.29–1.37 (m, 1H), 1.72–1.78 (m, 1H), 1.83 (s, 6H), 1.85–1.89 (m, 1H), 2.02 (s, 3H), 2.15 (s, 3H), 2.26–2.28 (m, 1H), 2.58–2.65 (m, 1H), 3.70–3.78 (m, 1H), 6.23 (d,  $J_{\text{HP}} = 5.3$ , 1H), 6.67–6.71 (m, 1H), 6.80–6.89 (m, 4H), 6.96–7.01 (m, 1H), 7.12–7.16 (m, 2H), 7.28–7.33 (m, 1H), 7.47–7.52 (m, 2H), 7.55–7.58 (m, 1H), 7.64–7.67 (m, 1H), 7.74–7.78 (m, 1H);  $^{13}\text{C}$  NMR (DMSO- $d_6$ )  $\delta$  21.0, 21.1, 25.2, 45.0, 45.5, 56.0, 62.7 (d,  $^1J_{\text{CP}} = 67.0$ ), 124.7 (d,  $J_{\text{CP}} = 91.2$ ), 124.8 (d,  $J_{\text{CP}} = 6.8$ ), 125.1 (d,  $J_{\text{CP}} = 5.5$ ), 125.95 (d,  $J_{\text{CP}} = 2.4$ ), 126.01 (d,  $J_{\text{CP}} = 1.2$ ), 126.2 (d,  $J_{\text{CP}} = 3.1$ ), 126.4 (d,  $J_{\text{CP}} = 1.5$ ), 126.5 (d,  $J_{\text{CP}} = 4.8$ ), 126.6 (d,  $J_{\text{CP}} = 2.1$ ), 127.3 (d,  $J_{\text{CP}} = 1.1$ ), 127.5 (d,  $J_{\text{CP}} = 92.6$ ), 128.6 (d,  $J_{\text{CP}} = 11.4$ ), 129.3 (d,  $J_{\text{CP}} = 11.2$ ), 130.8 (d,  $J_{\text{CP}} = 1.2$ ), 131.6 (d,  $J_{\text{CP}} = 9.4$ ), 131.7 (d,  $J_{\text{CP}} = 9.1$ ), 142.1 (d,  $J_{\text{CP}} = 3.0$ ), 142.5 (d,  $J_{\text{CP}} = 2.8$ ), 162.7;  $[\text{M}+\text{H}]^+_{\text{found}} = 497.2353$ ,  $\text{C}_{31}\text{H}_{34}\text{N}_2\text{O}_2\text{P}$  requires 497.2352.

**Bis(3,5-dimethylphenyl)[2-(3-dimethylamino-propyl)-3-oxo-2,3-dihydro-1*H*-benzo[de]isoquinolin-1-yl]phosphine oxide (20)**

Yield: 81% (0.42 g), yellow oil;  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  32.6;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.71–1.80 (m, 1H), 1.81–1.90 (m, 1H), 2.11 (s, 6H), 2.13–2.18 (m, 1H), 2.23 (s, 6H), 2.24 (s, 6H), 2.31–2.37 (m, 1H), 3.37–3.45 (m, 1H), 4.34–4.41 (m, 1H), 6.24 (d,  $J_{\text{HP}} = 11.5$ , 1H), 6.79–6.85 (m, 2H), 6.94–6.98 (m, 1H), 7.02–7.08 (m, 2H), 7.12–7.18 (m, 2H), 7.28–7.33 (m, 1H), 7.37–7.42 (m, 1H),

7.70–7.74 (m, 1H), 7.79–7.84 (m, 1H), 7.92–7.96 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  21.1, 21.2, 25.4, 45.2, 46.1, 55.9, 64.8 (d,  $^1J_{\text{CP}} = 67.5$ ), 125.1 (d,  $J_{\text{CP}} = 6.4$ ), 125.3 (d,  $J_{\text{CP}} = 4.3$ ), 125.6 (d,  $J_{\text{CP}} = 2.3$ ), 125.7 (d,  $J_{\text{CP}} = 2.7$ ), 125.8 (d,  $J_{\text{CP}} = 1.7$ ), 126.2 (d,  $J_{\text{CP}} = 2.0$ ), 126.8 (d,  $J_{\text{CP}} = 4.7$ ), 127.0 (d,  $J_{\text{CP}} = 92.1$ ), 128.5 (d,  $J_{\text{CP}} = 92.6$ ), 129.7 (d,  $J_{\text{CP}} = 3.1$ ), 129.9 (d,  $J_{\text{CP}} = 8.7$ ), 130.3 (d,  $J_{\text{CP}} = 8.7$ ), 130.6 (d,  $J_{\text{CP}} = 1.8$ ), 131.9 (d,  $J_{\text{CP}} = 3.2$ ), 133.91 (d,  $J_{\text{CP}} = 3.6$ ), 133.94 (d,  $J_{\text{CP}} = 3.2$ ), 137.7 (d,  $J_{\text{CP}} = 11.8$ ), 138.01 (d,  $J_{\text{CP}} = 11.9$ ), 163.2;  $[\text{M}+\text{H}]^+_{\text{found}} = 525.2661$ ,  $\text{C}_{33}\text{H}_{38}\text{N}_2\text{O}_2\text{P}$  requires 525.2665.

**Diphenyl[2-(1-phenylethyl)-3-oxo-2,3-dihydro-1*H*-benzo[de]isoquinolin-1-yl]phosphine oxide (21)**

Yield: 84% (0.41 g), light yellow crystals; Mp: 196–198 °C; **Isomer A:**  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  31.6;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.88 (d,  $J_{\text{HP}} = 7.1$ , 3H), 5.54 (d,  $J_{\text{HP}} = 10.8$ , 1H), 5.93 (q,  $J_{\text{HH}} = 7.1$ , 1H), 6.56–6.61 (m, 1H), 6.91–6.97 (m, 2H), 7.03–7.06 (m, 2H), 7.15–7.21 (m, 1H), 7.32–7.33 (m, 1H), 7.34–7.35 (m, 1H), 7.35–7.36 (m, 1H), 7.36–7.39 (m, 4H), 7.39–7.42 (m, 1H), 7.43–7.44 (m, 1H), 7.48–7.50 (m, 1H), 7.55–7.60 (m, 1H), 7.65–7.73 (m, 2H), 7.82–7.86 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  18.4, 56.7, 61.7 (d,  $^1J_{\text{CP}} = 69.1$ ), 124.77 (d,  $J_{\text{CP}} = 4.3$ ), 125.10 (d,  $J_{\text{CP}} = 4.1$ ), 125.7 (d,  $J_{\text{CP}} = 93.6$ ), 126.2 (d,  $J_{\text{CP}} = 2.2$ ), 126.57 (d,  $J_{\text{CP}} = 2.1$ ), 126.64 (d,  $J_{\text{CP}} = 2.6$ ), 126.82, 127.01 (d,  $J_{\text{CP}} = 1.0$ ), 127.73, 127.74 (d,  $J_{\text{CP}} = 11.3$ ), 128.41, 128.44 (d,  $J_{\text{CP}} = 11.4$ ), 129.2 (d,  $J_{\text{CP}} = 93.5$ ), 129.4 (d,  $J_{\text{CP}} = 3.5$ ), 130.7 (d,  $J_{\text{CP}} = 1.7$ ), 131.78 (d,  $J_{\text{CP}} = 2.7$ ), 131.79 (d,  $J_{\text{CP}} = 8.5$ ), 131.87 (d,  $J_{\text{CP}} = 2.8$ ), 132.3 (d,  $J_{\text{CP}} = 2.8$ ), 132.4 (d,  $J_{\text{CP}} = 8.5$ ), 140.9, 163.4; **Isomer B:**  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  32.6;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  2.22 (d,  $J_{\text{HH}} = 6.9$ , 3H), 5.20 (q,  $J_{\text{HH}} = 6.8$ , 1H), 5.87 (d,  $J_{\text{HP}} = 11.9$ , 1H), 6.72–6.77 (m, 1H), 6.98–7.03 (m, 2H), 7.06–7.13 (m, 2H), 7.21–7.27 (m, 2H), 7.27–7.29 (m, 1H), 7.29–7.30 (m, 1H), 7.30–7.31 (m, 1H), 7.42–7.43 (m, 1H), 7.45–7.48 (m, 4H), 7.50–7.54 (m, 2H), 7.73–7.78 (m, 2H), 7.87–7.90 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  20.5, 65.0, 68.1 (d,  $^1J_{\text{CP}} = 69.7$ ), 124.82 (d,  $J_{\text{CP}} = 4.5$ ), 125.19 (d,  $J_{\text{CP}} = 4.2$ ), 126.3 (d,  $J_{\text{CP}} = 1.0$ ), 126.61 (d,  $J_{\text{CP}} = 1.8$ ), 126.78 (d,  $J_{\text{CP}} = 2.9$ ), 126.9, 127.04 (d,  $J_{\text{CP}} = 1.2$ ), 127.1 (d,  $J_{\text{CP}} = 93.7$ ), 127.74, 127.9 (d,  $J_{\text{CP}} = 11.4$ ), 128.58 (d,  $J_{\text{CP}} = 11.5$ ), 128.59, 129.5 (d,  $J_{\text{CP}} = 3.2$ ), 130.1 (d,  $J_{\text{CP}} = 92.6$ ), 131.0 (d,  $J_{\text{CP}} = 1.7$ ), 131.85 (d,  $J_{\text{CP}} = 2.8$ ), 132.1 (d,  $J_{\text{CP}} = 8.6$ ), 132.2 (d,  $J_{\text{CP}} = 2.8$ ), 132.5 (d,  $J_{\text{CP}} = 3.0$ ), 132.9 (d,  $J_{\text{CP}} = 8.6$ ), 141.7, 164.4;  $[\text{M}+\text{H}]^+_{\text{found}} = 488.1785$ ,  $\text{C}_{32}\text{H}_{27}\text{NO}_2\text{P}$  requires 488.1773.

**Bis(*p*-tolyl)[2-(1-phenylethyl)-3-oxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-yl)phosphine oxide (22)**

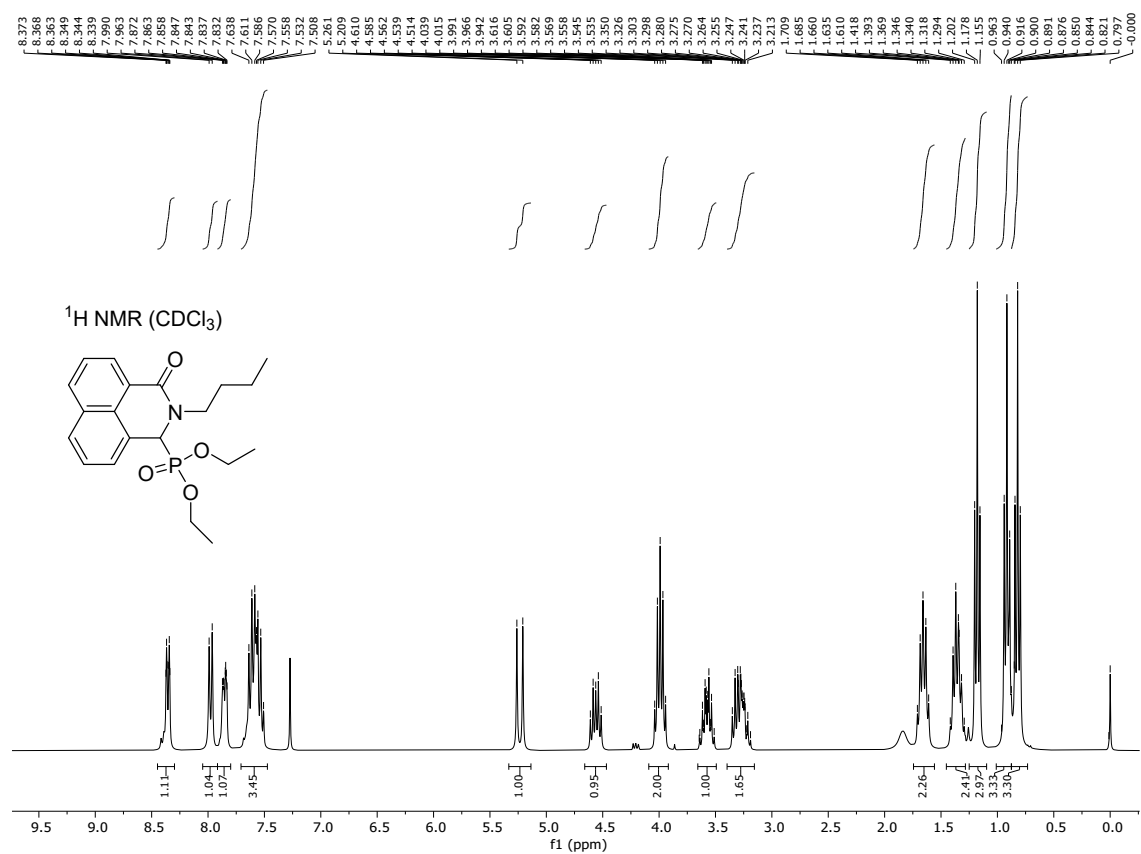
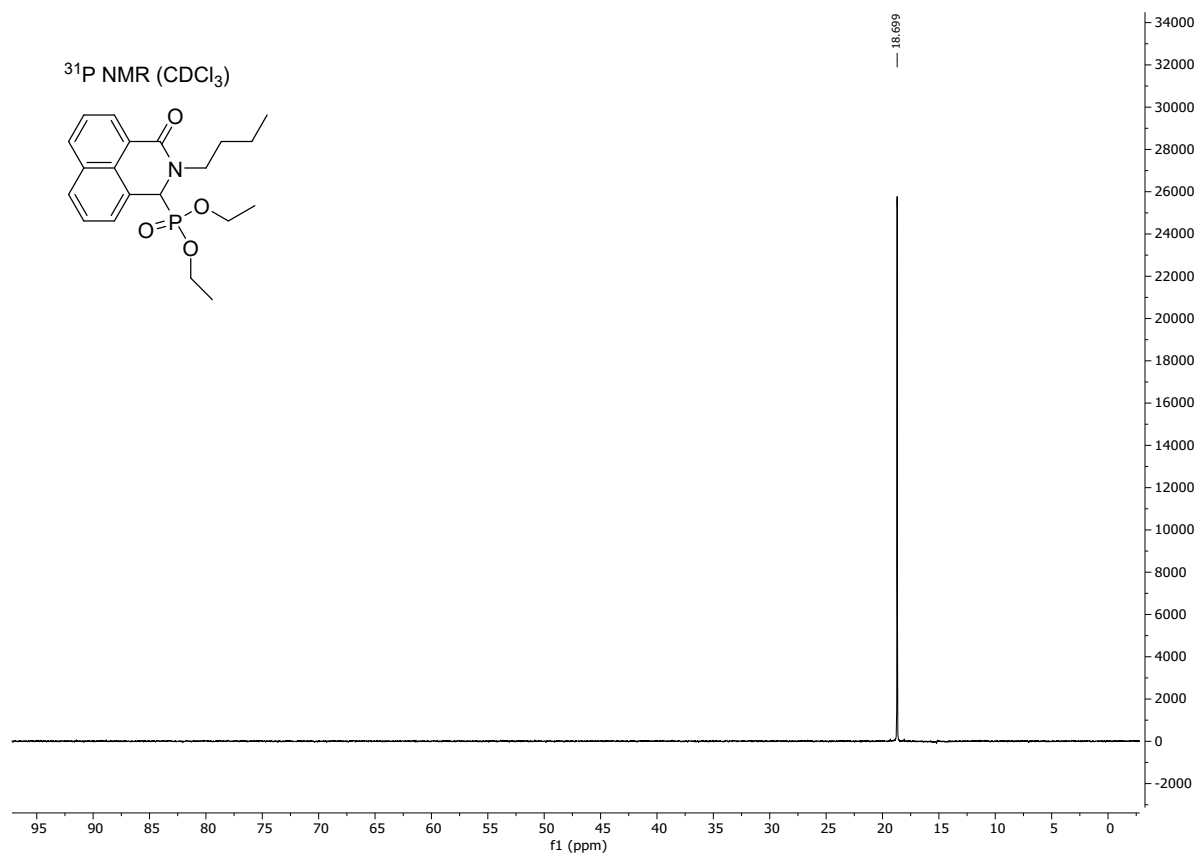
Yield: 81% (0.42 g), light yellow crystals; Mp: 200–202 °C; **Isomer A:**  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  32.1;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.89 (d,  $J_{\text{HH}} = 7.1$ , 3H), 2.21 (s, 3H), 2.36 (s, 3H), 5.49 (d,  $J_{\text{HP}} = 8.5$ , 1H), 5.89 (q,  $J_{\text{HH}} = 7.1$ , 1H), 6.56–6.60 (m, 1H), 6.77–6.82 (m, 3H), 7.08–7.15 (m, 4H), 7.28–7.29 (m, 1H), 7.29–7.34 (m, 5H), 7.40–7.42 (m, 1H), 7.51–7.56 (m, 1H), 7.64–7.68 (m, 1H), 7.79–7.83 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  18.6; 21.39, 21.59, 56.9, 61.8 (d,  $^1J_{\text{CP}} = 69.4$ ), 123.5 (d,  $J_{\text{CP}} = 96.0$ ), 124.81 (d,  $J_{\text{CP}} = 6.5$ ), 125.15 (d,  $J_{\text{CP}} = 4.0$ ), 126.0 (d,  $J_{\text{CP}} = 2.0$ ), 126.2 (d,  $J_{\text{CP}} = 1.3$ ), 126.5, 126.66 (d,  $J_{\text{CP}} = 2.3$ ), 126.68 (d,  $J_{\text{CP}} = 1.9$ ), 127.6, 128.4, 128.50 (d,  $J_{\text{CP}} = 11.2$ ), 129.1 (d,  $J_{\text{CP}} = 11.8$ ), 129.5 (d,  $J_{\text{CP}} = 3.1$ ), 130.9 (d,  $J_{\text{CP}} = 1.7$ ), 131.8 (d,  $J_{\text{CP}} = 8.9$ ), 132.5 (d,  $J_{\text{CP}} = 8.7$ ), 141.2, 142.4 (d,  $J_{\text{CP}} = 2.8$ ), 142.8 (d,  $J_{\text{CP}} = 3.0$ ), 164.3; **Isomer B:**  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  33.5;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  2.22 (s, 3H), 2.40 (d,  $J_{\text{HH}} = 8.5$ , 3H), 2.47 (s, 3H), 5.18 (q,  $J_{\text{HH}} = 8.5$ , 1H), 5.80 (d,  $J_{\text{HP}} = 12.1$ , 1H), 6.71–6.75 (m, 1H), 6.83–6.88 (m, 3H), 7.16–7.24 (m, 4H), 7.27–7.28 (m, 1H), 7.35–7.40 (m, 5H), 7.42–7.44 (m, 1H), 7.51–7.56 (m, 1H), 7.70–7.74 (m, 1H), 7.90–7.93 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  20.5, 21.41, 21.60, 65.1, 68.3 (d,  $^1J_{\text{CP}} = 70.1$ ), 124.82 (d,  $J_{\text{CP}} = 6.5$ ), 125.07 (d,  $J_{\text{CP}} = 4.5$ ), 125.4 (d,  $J_{\text{CP}} = 1.1$ ), 126.3 (d,  $J_{\text{CP}} = 2.2$ ), 126.6, 126.8 (d,  $J_{\text{CP}} = 95.5$ ), 126.9 (d,  $J_{\text{CP}} = 1.9$ ), 127.0 (d,  $J_{\text{CP}} = 2.4$ ), 127.6, 128.55, 128.6 (d,  $J_{\text{CP}} = 11.7$ ), 129.3 (d,  $J_{\text{CP}} = 11.8$ ), 129.6 (d,  $J_{\text{CP}} = 2.8$ ), 130.6 (d,  $J_{\text{CP}} = 1.7$ ), 132.1 (d,  $J_{\text{CP}} = 9.1$ ), 132.9 (d,  $J_{\text{CP}} = 8.7$ ), 141.9, 142.6 (d,  $J_{\text{CP}} = 3.0$ ), 143.1 (d,  $J_{\text{CP}} = 2.8$ ), 163.4;  $[\text{M}+\text{H}]^+$   $_{\text{found}} = 516.2091$ ,  $\text{C}_{34}\text{H}_{31}\text{NO}_2\text{P}$  requires 516.2086.

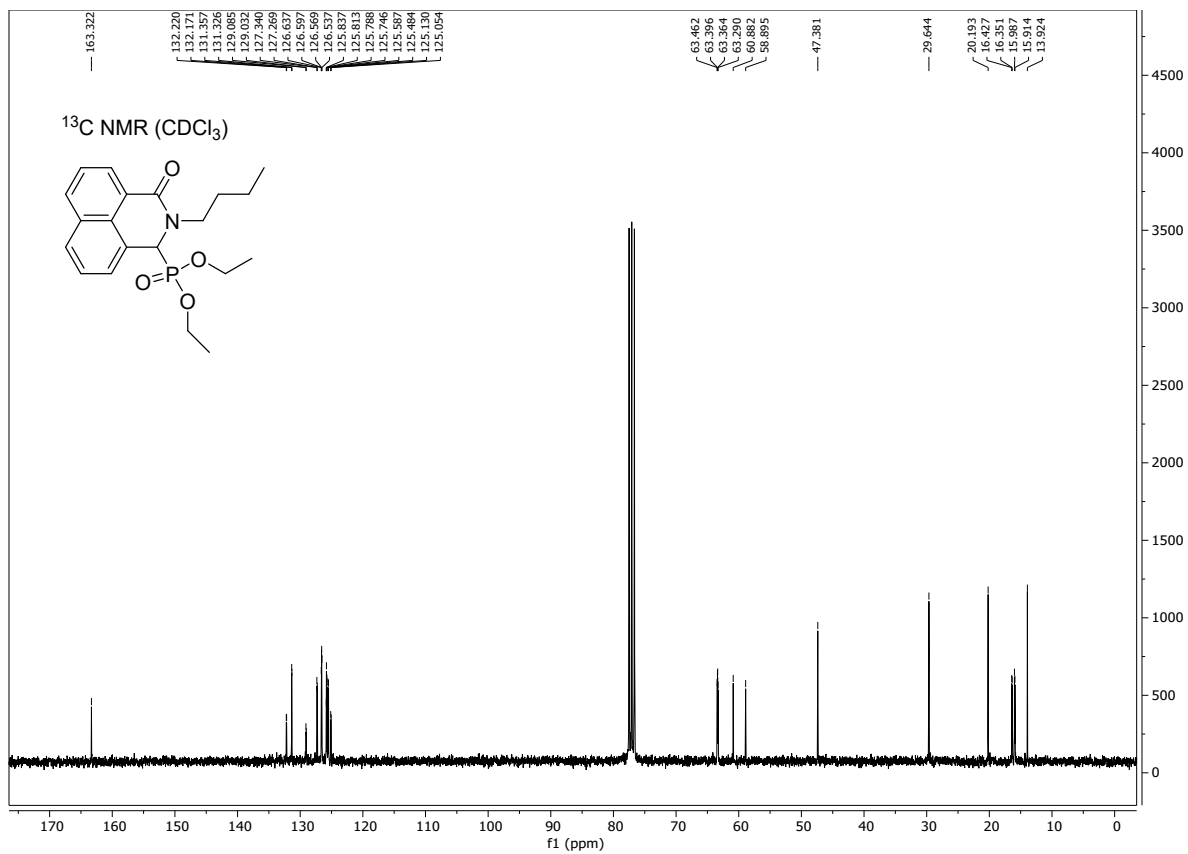
**Bis(3,5-dimethylphenyl)[2-(1-phenylethyl)-3-oxo-2,3-dihydro-1*H*-benzo[*de*]isoquinolin-1-yl)phosphine oxide (23)**

Yield: 90% (0.49 g), light yellow crystals; Mp: 192–194 °C; **Isomer A:**  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  32.5;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.84 (d,  $J_{\text{HH}} = 7.2$ , 3H), 2.01 (s, 6H), 2.27 (s, 6H), 5.47 (d,  $J_{\text{HP}} = 10.4$ , 1H), 5.90 (q,  $J_{\text{HH}} = 7.1$ , 1H), 6.43–6.48 (m, 2H), 6.54–6.57 (m, 1H), 6.82–6.85 (m, 1H), 6.99–7.04 (m, 2H), 7.19–7.24 (m, 2H), 7.30–7.32 (m, 1H), 7.32–7.40 (m, 5H), 7.63–7.67 (m, 1H), 7.82–7.85 (m, 1H), 8.02–8.05 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  18.2, 20.9, 21.3, 56.6, 61.6 (d,  $^1J_{\text{CP}} = 68.0$ ), 124.8 (d,  $J_{\text{CP}} = 6.5$ ), 125.05 (d,  $J_{\text{CP}} = 4.6$ ), 125.67 (d,  $J_{\text{CP}} = 93.6$ ), 126.3 (d,  $J_{\text{CP}} = 2.1$ ), 126.54 (d,  $J_{\text{CP}} = 1.4$ ), 126.6 (d,  $J_{\text{CP}} = 4.4$ ), 126.65, 127.28 (d,  $J_{\text{CP}} = 87.7$ ), 127.6, 128.4, 129.55 (d,  $J_{\text{CP}} = 8.6$ ), 129.6 (d,  $J_{\text{CP}} = 3.3$ ), 130.0 (d,  $J_{\text{CP}} = 8.7$ ), 130.65 (d,  $J_{\text{CP}} = 1.7$ ), 131.82 (d,  $J_{\text{CP}} = 3.0$ ), 133.5 (d,  $J_{\text{CP}} = 3.0$ ), 133.8 (d,  $J_{\text{CP}} = 2.9$ ), 137.3 (d,  $J_{\text{CP}} = 12.0$ ), 138.1 (d,  $J_{\text{CP}} = 12.0$ ), 140.9, 164.4; **Isomer B:**  $^{31}\text{P}$  ( $\text{CDCl}_3$ )  $\delta$  33.6;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  2.01 (s, 6H), 2.19 (d,  $J_{\text{HH}} = 6.8$ , 3H), 2.29 (s, 6H), 5.21 (q,  $J_{\text{HH}} = 6.8$ , 1H), 5.81 (d,  $J_{\text{HP}} = 12.5$ , 1H), 6.57–6.59 (m, 2H), 6.70–6.73

(m, 1H), 6.88–6.91 (m, 1H), 7.07–7.10 (m, 2H), 7.13–7.19 (m, 2H), 7.27–7.29 (m, 1H), 7.41–7.48 (m, 5H), 7.73–7.77 (m, 1H), 7.85–7.87 (m, 1H), 7.89–7.93 (m, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  20.4, 21.0, 21.3, 64.8, 68.3 (d,  $^1J_{\text{CP}} = 68.6$ ), 125.0 (d,  $J_{\text{CP}} = 6.4$ ), 125.1 (d,  $J_{\text{CP}} = 4.0$ ), 125.68 (d,  $J_{\text{CP}} = 92.8$ ), 125.9 (d,  $J_{\text{CP}} = 1.6$ ), 126.50 (d,  $J_{\text{CP}} = 1.5$ ), 126.75, 126.82 (d,  $J_{\text{CP}} = 3.4$ ), 127.29 (d,  $J_{\text{CP}} = 93.1$ ), 129.3, 129.52, 129.7 (d,  $J_{\text{CP}} = 8.5$ ), 129.8 (d,  $J_{\text{CP}} = 9.3$ ), 130.5 (d,  $J_{\text{CP}} = 8.5$ ), 131.77 (d,  $J_{\text{CP}} = 2.7$ ), 134.0 (d,  $J_{\text{CP}} = 2.8$ ), 134.1 (d,  $J_{\text{CP}} = 3.0$ ), 137.5 (d,  $J_{\text{CP}} = 11.8$ ), 138.2 (d,  $J_{\text{CP}} = 12.2$ ), 141.9, 163.3;  $[\text{M}+\text{H}]^+_{\text{found}} = 544.2391$ ,  $\text{C}_{36}\text{H}_{35}\text{NO}_2\text{P}$  requires 544.2399.

### <sup>31</sup>P NMR, <sup>1</sup>H NMR, <sup>13</sup>C NMR spectra





<sup>31</sup>P NMR (CDCl<sub>3</sub>)

