Supporting Information

Accessing 2-(Hetero)Arylmethyl-, Allyl- and Propargyl-2,1-Borazaronaphthalenes: Palladium-Catalyzed Cross-Couplings of 2-Chloromethyl-2,1-Borazaronaphthalenes

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EXPERIMENTAL

General Considerations: CPME and THF were dried over activated alumina. Standard benchtop techniques were employed for handling air-sensitive reagents. Melting points (°C) are uncorrected. NMR spectra were recorded on a 400 or 500 MHz spectrometer. $^{11}$B NMR spectra were obtained on a spectrometer equipped with the appropriate decoupling accessories. All $^{11}$B NMR chemical shifts were referenced to external BF$_3$·OEt$_2$ (0.0 ppm) with a negative sign indicating an upfield shift. Data are presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad), coupling constant $J$ (Hz) and integration. Analytical thin-layer chromatography (TLC) was performed on TLC silica gel plates (0.25 mm) precoated with a fluorescent indicator. Visualization of the TLC plates was effected with ultraviolet light. Standard flash chromatography procedures were followed using 100-200 mesh silica gel. HRMS data were obtained by either ESI or CI using a TOF mass spectrometer.

Synthesis of 2-Chloromethyl-2,1-borazaronaphthalenes. 2-Chloromethyl-2,1-borazaronaphthalenes were synthesized according to the literature procedure.$^1$

High-Throughput Experimentation for optimization of the cross-coupling reaction of 2-chloromethyl-2,1-borazaronaphthalene with potassium (hetero)aryltrifluoroborates:

High Throughput Experimentation (HTE) was performed at the Penn/Merck Center for High Throughput Experimentation at the University of Pennsylvania. The screen was performed on a 10 μmol scale. After the reaction was complete, 1 μmol of 4,4'$-$di-tert-butylibiphenyl (500 μL of a 0.002 μM solution in acetonitrile) was added to each vial as an internal standard. The reaction
mixtures were then analyzed by HPLC. The product-to-internal standard (P/IS) ratios from the HPLC are shown in Figure S1.

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\text{Product} / \text{Internal Standard}
\]

**Figure S1. Product to Internal standard ratio of the cross coupling reaction of 1 with potassium phenyltrifluoroborate.**
In a further investigation, the reactivity of \( t\)-Bu\(_3\)P-Pd-G2 and Pd(OAc)\(_2\) was compared with that of Pd\(_2\)dba\(_3\) (Figure S2). In this comparison Pd\(_2\)dba\(_3\) as a catalyst and RuPhos as a ligand showed the best result.

![Chemical Structure](image1)

**Figure S2.** Product to Internal standard ratio of the cross coupling reaction of 1 with potassium phenyltrifluoroborates.

In Table S1 the effect of the changing the catalyst loading (entries 1 and 4), concentration (entries 1-3), amount of potassium phenyltrifluoroborate (entries 4-6), and temperature (entries 7-9) are shown.

| entry | compound 1 | Ph-BF\(_3\)K | Pd\(_2\)(dba)\(_3\) (mol %) | RuPhos (mol %) | concentration (M) | temperature (°C) | P/IS |
|-------|------------|--------------|---------------------------|---------------|------------------|-----------------|------|
| 1     | 1.0 equiv  | 1.10 equiv   | 2.5                       | 5.0           | 0.10             | 80              | 5.2  |
| 2     |            |              |                           |               | 0.25             |                 | 2.5  |
| 3     |            |              |                           |               | 0.50             |                 | 1.3  |
| 4     | 1.0 equiv  | 1.10 equiv   | 2.5                       | 5.0           | 0.10             |                 | 5.1  |
| 5     |            | 1.05 equiv   |                           |               |                  |                 | 4.8  |
| 6     |            | 1.00 equiv   |                           |               |                  |                 | 4.2  |
| 7     | 1.0 equiv  |              | 1.25                       | 2.5           | 0.10             | 100             | 4.9  |
| 8     |            |              |                           |               | 0.10             | 80              | 5.0  |
| 9     |            |              |                           |               |                  | 60              | 4.2  |
General procedure for the cross-coupling of 2-chloromethyl-2,1-borazaronaphthalene with potassium (hetero)aryltrifluoroborates. To an oven-dried Biotage microwave vial equipped with a stir bar were added 2-chloromethyl-2,1-borazaronaphthalene (177.4 mg, 1 mmol), the corresponding potassium (hetero)aryltrifluoroborate (1.1 mmol, 1.1 equiv), Pd$_2$dba$_3$ (11.4 mg, 12.5 µmol, 1.25 mol %), Ruphos (11.7 mg, 25 µmol, 2.5 mol %), and Cs$_2$CO$_3$ (651.6 mg, 2 mmol). The vial was sealed with a cap lined with a disposable Teflon septum, then evacuated under vacuum and purged with Ar three times. Anhydrous toluene (9.5 mL) and degassed H$_2$O (0.5 mL) were added by syringe under Ar. The resulting mixture was heated to 80 °C and vigorously stirred for 18 h. The reaction mixture was filtered through a plug of silica and flushed with 25-50% hexane/CH$_2$Cl$_2$. The solvent was removed under reduced pressure, and the crude material was purified by column chromatography to obtain the pure product.

![Structure](image)

2-(Benzyl)-2,1-borazaronaphthalene (2a). The title compound was obtained as a colorless oil in 90% yield (1 mmol scale, 197.2 mg). $^1$H NMR (500 MHz, CDCl$_3$): δ 7.92 (d, $J = 11.0$ Hz, 1H), 7.54 (d, $J = 8.0$ Hz, 1H), 7.31 (s, 1H), 7.31-7.27 (m, 3H), 7.17-7.14 (m, 3H), 7.10-7.07 (m, 1H), 7.02 (d, $J = 8.0$ Hz, 1H), 6.78 (dd, $J = 11.5$, 2.0 Hz, 1H), 2.82 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): δ 144.8, 141.9, 140.2, 129.6, 129.2, 129.0, 128.3, 125.5, 124.9, 121.1, 118.2; $^{11}$B NMR (128.38 MHz, CDCl$_3$): δ 36.4; FT-IR (neat): 3374, 1614, 1561, 1435, 756 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{15}$H$_{15}$BN [M+H]$^+$ 220.1298, found 220.1297.
**2-(4-Methylbenzyl)-2,1-borazaronaphthalene (2b).** The title compound was obtained as a white solid in 92% yield (1 mmol scale, 219.1 mg). mp 67-68 °C; \(^1\)H NMR (500 MHz, CDCl\(_3\)): δ 7.95 (d, \(J = 11.5\) Hz, 1H), 7.58 (d, \(J = 8.0\) Hz, 1H), 7.31 (s, 1H), 7.36-7.32 (m, 1H), 7.15-7.13 (m, 3H), 7.11-7.08 (m, 3H), 6.81 (dd, \(J = 11.5, 1.5\) Hz, 1H), 2.81 (s, 2H), 2.36 (s, 3H); \(^13\)C NMR (125.8 MHz, CDCl\(_3\)): δ 144.7, 140.2, 138.6, 134.2, 129.7, 129.5, 129.1, 128.2, 125.6, 121.0, 118.2, 21.3; \(^{11}\)B NMR (128.38 MHz, CDCl\(_3\)): δ 36.2; FT-IR (neat): 3368, 1613, 1560, 1511, 1438, 1272, 1253, 1162, 1032, 844 cm\(^{-1}\); HRMS (ES+) m/z calcd. for C\(_{16}\)H\(_{17}\)BN [M+H]\(^+\) 234.1454, found 234.1443.

**2-(3-Methoxybenzyl)-2,1-borazaronaphthalene (2c).** The title compound was obtained as a white solid in 85% yield (1 mmol scale, 211.7 mg). mp 73-74 °C; \(^1\)H NMR (500 MHz, CDCl\(_3\)): δ 7.93 (d, \(J = 11.0\) Hz, 1H), 7.55 (d, \(J = 8.0\) Hz, 1H), 7.42 (s, 1H), 7.32-7.29 (m, 1H), 7.22 (dd, \(J = 7.5, 7.5\) Hz, 1H), 7.11-7.05 (m, 2H), 6.80-6.71 (m, 4H), 3.78 (s, 3H), 2.81 (s, 2H); \(^13\)C NMR (125.8 MHz, CDCl\(_3\)): δ 160.2, 144.8, 143.6, 140.2, 129.9, 129.5, 128.3, 125.5, 121.6, 121.1, 118.2, 114.8, 110.3, 55.3; \(^{11}\)B NMR (128.38 MHz, CDCl\(_3\)): δ 36.3; FT-IR (neat): 3326, 1613, 1598, 1562, 1488, 1464, 1438, 1272, 1253, 1162, 1032, 844 cm\(^{-1}\); HRMS (ES+) m/z calcd. for C\(_{16}\)H\(_{17}\)BNO [M+H]\(^+\) 250.1403, found 250.1391.
**2-(4-Methoxybenzyl)-2,1-borazonaphthalene (2d).** The title compound was obtained as a solid in 89% yield (1 mmol scale, 224.2 mg). mp 65-66 °C; ¹H NMR (500 MHz, CDCl₃): δ 7.94 (d, J = 11.5 Hz, 1H), 7.57 (d, J = 7.5 Hz, 1H), 7.40 (s, 1H), 7.35-7.32 (m, 1H), 7.14-7.09 (m, 4H), 6.89-6.87 (m, 2H), 6.79 (dd, J = 11.5, 1.5 Hz, 1H), 3.82 (s, 3H), 2.78 (s, 2H); ¹³C NMR (125.8 MHz, CDCl₃): δ 157.3, 144.7, 140.2, 133.7, 130.0, 129.5, 128.3, 125.5, 121.1, 118.2, 114.4, 55.5; ¹¹B NMR (128.38 MHz, CDCl₃): δ 37.0; FT-IR (neat): 33 59, 1612, 1591, 1560, 1509, 1437, 1242, 1031, 765 cm⁻¹; HRMS (ES⁺) m/z calcd. for C₁₆H₁₇BNO [M+H]⁺ 250.1403, found 250.1411.

**2-(1-Naphthylmethyl)-2,1-borazonaphthalene (2e).** The title compound was obtained as a white solid in 91% yield (1 mmol scale, 247.6 mg). mp 64-65 °C; ¹H NMR (500 MHz, CDCl₃): δ 8.07-8.03 (m, 2H), 7.98 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.5 Hz, 1H), 7.64 (d, J = 7.5 Hz, 1H), 7.57-7.54 (m, 2H), 7.51-7.46 (m, 2H), 7.39 (s, 1H), 7.32 (dd, J = 7.5, 7.5 Hz, 1H), 7.17 (dd, J = 7.5, 7.5 Hz, 1H), 6.98-6.93 (m, 2H), 3.36 (s, 2H); ¹³C NMR (125.8 MHz, CDCl₃): δ 145.0, 140.2, 138.6, 134.4, 132.5, 129.5, 128.9, 128.2, 126.7, 126.2, 125.9, 125.8, 125.6, 125.1, 121.1, 118.2; ¹¹B NMR (128.38 MHz, CDCl₃): δ 37.0; FT-IR (neat): 3371, 1613, 1592, 1560, 1435, 1288, 1132, 776, 759 cm⁻¹; HRMS (CI⁺) m/z calcd. for C₁₉H₁₆BN [M⁺] 269.1376, found 269.1365.
2-(3-Methoxy-5-methylbenzyl)-2,1-borazaronaphthalene (2f). The title compound was obtained as a solid in 92% yield (1 mmol scale, 244.7 mg). mp 54-55 °C; $^1$H NMR (500 MHz, CDCl$_3$): δ 7.96 (d, $J = 11.5$ Hz, 1H), 7.59 (d, $J = 7.5$ Hz, 1H), 7.46 (s, 1H), 7.36-7.33 (m, 1H), 7.15-7.11 (m, 2H), 6.82 (dd, $J = 11.5$, 1.5 Hz, 1H), 6.62 (s, 1H), 6.57 (s, 2H), 3.80 (s, 3H), 2.80 (s, 2H), 2.34 (s, 3H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): δ 160.2, 144.7, 143.3, 140.2, 139.9, 129.5, 128.2, 125.5, 122.5, 121.0, 118.2, 111.7, 111.2, 55.3, 21.9; $^{11}$B NMR (128.38 MHz, CDCl$_3$): δ 36.6; FT-IR (neat): 3371, 1614, 1592, 1561, 1435, 1150, 1062, 758 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{17}$H$_{19}$BNO [M+H]$^+$ 264.1560, found 264.1548.

2-(3-Vinylbenzyl)-2,1-borazaronaphthalene (2g). The title compound was obtained as an oil in 80% yield (1 mmol scale, 244.7 mg). $^1$H NMR (500 MHz, CDCl$_3$): δ 7.99 (d, $J = 11.5$ Hz, 1H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.44 (s, 1H), 7.38-7.28 (m, 4H), 7.18-7.10 (m, 3H), 6.85 (d, $J = 11.5$ Hz, 1H), 6.79-6.73 (m, 1H), 5.80 (d, $J = 17.5$ Hz, 1H), 5.28 (d, $J = 10.5$ Hz, 1H), 2.89 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): δ 144.8, 142.1, 140.2, 138.1, 137.4, 129.5, 129.1, 128.7, 128.3, 127.1, 125.5, 122.9, 121.1, 118.2, 113.9; $^{11}$B NMR (128.38 MHz, CDCl$_3$): δ 37.0; FT-IR (neat): 3372, 1614, 1594, 1561, 1435, 907, 758 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{17}$H$_{17}$BN [M+H]$^+$ 246.1454, found 246.1456.
2-(2,3-Dihydro-1,4-benzodioxin-6-ylmethyl)-2,1-borazaronaphthalene (2h). The title compound was obtained as an oil in 82% yield (1 mmol scale, 227.2 mg). $^1$H NMR (500 MHz, CDCl$_3$): δ 7.96 (d, $J = 11.5$ Hz, 1H), 7.58 (d, $J = 7.5$ Hz, 1H), 7.48 (s, 1H), 7.37-7.34 (m, 1H), 7.15-7.12 (m, 2H), 6.84-6.80 (m, 2H), 6.71 (d, $J = 1.5$ Hz, 1H), 6.66 (dd, $J = 8.0$, 2.0 Hz, 1H), 4.27 (s, 4H), 2.74 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): δ 144.7, 143.8, 141.1, 140.2, 135.0, 129.5, 128.2, 125.5, 122.0, 121.0, 118.2, 117.6, 117.6, 64.7, 64.5; $^{11}$B NMR (128.38 MHz, CDCl$_3$): δ 34.8; FT-IR (neat): 3367, 1614, 1561, 1504, 1436, 1305, 1281, 1255, 1068, 760 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{17}$H$_{17}$BNO$_2$ [M+H]$^+$ 278.1352, found 278.1342.

Methyl-3-(2-[2,1-borazaronaphthyl]methyl)benzoate (2i). The title compound was obtained as a white solid in 58% yield (1 mmol scale, 160.7 mg). mp: 76-77 °C; $^1$H NMR (500 MHz, CDCl$_3$): δ 7.97 (d, $J = 11.5$ Hz, 1H), 7.92 (s, 1H), 7.90-7.88 (m, 1H), 7.59 (d, $J = 7.5$ Hz, 1H), 7.47 (s, 1H), 7.40-7.39 (m, 2H), 7.37-7.34 (m, 1H), 7.16-7.11 (m, 2H), 6.80 (dd, $J = 11.5$, 1.0 Hz, 1H), 3.93 (s, 3H), 2.91 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): δ 167.6, 145.0, 142.4, 140.1, 133.8, 130.7, 130.1, 129.6, 128.9, 128.4, 126.3, 125.5, 121.2, 118.2, 52.3; $^{11}$B NMR (128.38 MHz, CDCl$_3$): δ 36.8; FT-IR (neat): 3347, 1714, 1614, 1564, 1439, 1431, 1305, 1289, 1199, 1100, 840, 759, 752 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{17}$H$_{17}$BNO$_2$ [M+H]$^+$ 278.1352, found 278.1350.
2-(3-Fluorobenzyl)-2,1-borazaronaphthalene (2j). The title compound was obtained as an oil in 61% yield (1 mmol scale, 144.5 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.97 (d, $J = 11.5$ Hz, 1H), 7.60 (d, $J = 7.5$ Hz, 1H), 7.42 (s, 1H), 7.38-7.35 (m, 1H), 7.31-7.26 (m, 1H), 7.17-7.12 (m, 2H), 6.97 (d, $J = 7.5$ Hz, 1H), 6.92-6.88 (m, 2H), 6.79 (d, $J = 11.5$ Hz, 1H), 2.86 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 163.5 (d, $J = 245.3$ Hz, 1C), 145.0, 144.7 (d, $J = 7.4$ Hz, 1C), 140.1, 130.3 (d, $J = 8.4$ Hz, 1C), 129.6, 128.4, 125.6, 124.8 (d, $J = 2.5$ Hz, 1C), 121.3, 118.2, 115.9 (d, $J = 20.5$ Hz, 1C), 111.8 (d, $J = 21.0$ Hz, 1C); $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.6; FT-IR (neat): 3377, 1613, 1592, 1562, 1435, 1136, 938, 757 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{15}$H$_{14}$BFN [M+H]$^+$ 238.1203, found 238.1214.

2-(2,4-Difluorobenzyl)-2,1-borazaronaphthalene (2k). The title compound was obtained as a white solid in 59% yield (1 mmol scale, 150.5 mg). mp: 44-45 °C; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.97 (d, $J = 11.5$ Hz, 1H), 7.59 (d, $J = 8.0$ Hz, 1H), 7.52 (s, 1H), 7.39-7.36 (m, 1H), 7.19-7.14 (m, 3H), 6.86-6.82 (m, 2H), 6.79-6.76 (m, 1H), 2.77 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 161.9 (dd, $J = 18.9$, 11.6 Hz, 1C), 159.9 (dd, $J = 19.5$, 11.8 Hz, 1C), 145.2, 140.1, 131.6 (dd, $J = 8.8$, 6.9 Hz, 1C), 129.7, 128.5, 125.6, 124.6 (dd, $J = 17.3$, 3.5 Hz, 1C), 121.3, 118.3, 111.4 (dd, $J = 20.6$, 3.6 Hz, 1C), 104.2-103.8 (m, 1C); $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.4; FT-IR (neat): 3357, 1613, 1561, 1502, 1436, 1277, 1131, 967, 844, 765 cm$^{-1}$; HRMS (CI+) m/z calcd. for C$_{15}$H$_{12}$BF$_2$ [M]$^+$ 255.1031, found 255.1029.
2-(4-Chlorobenzyl)-2,1-borazaronaphthalene (2l). The title compound was obtained as an oil in 45% yield (1 mmol scale, 114.1 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.96 (d, $J = 11.5$ Hz, 1H), 7.58 (d, $J = 7.5$ Hz, 1H), 7.37-7.34 (m, 2H), 7.29-7.27 (m, 2H), 7.15-7.11 (m, 4H), 6.77 (dd, $J = 11.5$, 1.5 Hz, 1H), 2.81 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 145.0, 140.4, 140.1, 130.7, 130.5, 129.6, 129.0, 128.4, 125.6, 121.3, 118.2; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.3; FT-IR (neat): 3370, 1613, 1561, 1435, 1132, 690 cm$^{-1}$; HRMS (ES$^+$) m/z calcd. for C$_{12}$H$_{14}$BNCl [M+H]$^+$ 254.0908, found 254.0898.

$N$-Benzyl-2-(3-methylbenzyl)-2,1-borazaronaphthalene (2m). The title compound was obtained as a solid in 79% yield (1 mmol scale, 255.3 mg). mp: 86-87°C; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.03 (d, $J = 11.5$ Hz, 1H), 7.70 (dd, $J = 8.0$, 1.0 Hz, 1H), 7.44-7.37 (m, 4H), 7.34-7.31 (m, 1H), 7.24-7.21 (m, 3H), 7.18-7.14 (m, 4H), 6.83 (d, $J = 11.5$ Hz, 1H), 5.47 (s, 2H), 2.91 (s, 2H), 2.42 (s, 3H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 145.1, 141.7, 139.1, 138.6, 134.0, 130.5, 129.4, 129.3, 129.0, 128.7, 127.2, 127.1, 126.0, 120.9, 116.3, 50.9, 21.2; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 38.4; FT-IR (neat): 1609, 1592, 1551, 1493, 1410, 1356, 1238, 1141, 993, 841, 761, 741 cm$^{-1}$; HRMS (CI$^+$) m/z calcd. for C$_{25}$H$_{22}$BN [M]$^+$ 323.1845, found 323.1838.
2-(3-Methylbenzyl)-6-methyl-2,1-borazaronaphthalene (2n). The title compound was obtained as a solid in 83% yield (1 mmol scale, 205.1 mg). mp 53-54 °C; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.86 (d, $J = 11.5$ Hz, 1H), 7.33 (s, 2H), 7.20-7.17 (m, 1H), 7.12 (d, $J = 8.5$ Hz, 1H), 7.98-7.95 (m, 4H), 6.75 (dd, $J = 11.5$, 1.5 Hz, 1H), 2.77 (s, 2H), 2.36 (s, 3H), 2.32 (s, 3H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 144.5, 141.9, 138.4, 138.2, 130.2, 130.0, 129.6, 129.3, 128.8, 126.2, 125.6, 125.5, 118.0, 21.8, 21.1; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.7; FT-IR (neat): 3361, 1566, 1438, 1281, 1135, 819, 790, 699 cm$^{-1}$; HRMS (Cl+) m/z calcd. for C$_{17}$H$_{18}$BN [M]$^+$ 247.1532, found 247.1543.

5-[(2,1-Borazaronaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (3a). The title compound was obtained as an oil in 90% yield (1 mmol scale, 322.4 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.11 (s, 1H), 7.96 (d, $J = 11.5$ Hz, 1H), 7.60-7.57 (m, 2H), 7.42 (s, 1H), 7.37 (s, 1H), 7.34-7.31 (m, 1H), 7.17-7.11 (m, 2H), 7.06 (d, $J = 8.0$ Hz, 1H), 6.84 (d, $J = 11.5$ Hz, 1H), 6.53 (d, $J = 3.5$ Hz, 1H), 2.95 (s, 2H), 1.70 (s, 9H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 150.1, 144.7, 140.2, 136.0, 133.3, 131.5, 129.5, 128.2, 126.2, 125.8, 125.5, 121.0, 120.8, 118.2, 115.5, 107.4, 83.6, 28.4; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.9; FT-IR (neat): 3370, 1730, 1614, 1561, 1466, 1436, 1370,
1345, 1162, 1128, 1023, 758, 727 cm\(^{-1}\); HRMS (ES-) m/z calcd. for C\(_{22}\)H\(_{22}\)BN\(_2\)O\(_2\) [M-H]\(^{-}\) 357.1774, found 357.1788.

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**2-(5-Methylfuran-2-yl)methyl-2,1-borazaronaphthalene (3b).** The title compound was obtained as an oil in 67% yield (1 mmol scale, 149.5 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 8.02 (d, \(J = 11.5\) Hz, 1H), 7.91 (s, 1H), 7.63 (d, \(J = 7.5\) Hz, 1H), 7.43-7.39 (m, 1H), 7.22-7.17 (m, 2H), 6.87 (dd, \(J = 11.5, 1.5\) Hz, 1H), 5.95-5.90 (m, 2H), 2.81 (s, 2H), 2.34 (s, 3H); \(^{13}\)C NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 154.0, 150.2, 145.1, 140.2, 129.6, 128.4, 125.7, 121.1, 118.3, 106.5, 105.5, 13.9; \(^{11}\)B NMR (128.38 MHz, CDCl\(_3\)): \(\delta\) 35.9; FT-IR (neat): 3370, 1615, 1561, 1437, 1217, 1018, 757 cm\(^{-1}\); HRMS (ES+) m/z calcd. for C\(_{14}\)H\(_{15}\)BNO [M+H]\(^{+}\) 224.1247, found 224.1251.

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\text{\includegraphics[width=0.2\textwidth]{image2.png}}
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**2-(2-Thiophenylmethyl)-2,1-borazaronaphthalene (3c).** The title compound was obtained as a white solid in 46% yield (1 mmol scale, 103.5 mg). mp: 41-42 °C; \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 8.04 (d, \(J = 11.5\) Hz, 1H), 7.12 (s, 1H), 7.65 (d, \(J = 7.5\) Hz, 1H), 7.41 (dd, \(J = 7.5, 7.5\) Hz, 1H), 7.21-7.16 (m, 3H), 7.05-7.04 (m, 1H), 6.89 (d, \(J = 11.5\) Hz, 1H), 6.84-6.83 (m, 1H), 3.10 (s, 2H); \(^{13}\)C NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 145.1, 143.9, 140.1, 129.6, 128.4, 127.6, 125.6, 124.5, 122.6, 121.2, 118.3; \(^{11}\)B NMR (128.38 MHz, CDCl\(_3\)): \(\delta\) 36.3; FT-IR (neat): 3363, 1613, 1561, 1436,
2-(3-Thiophenylmethyl)-2,1-borazaronaphthalene (3d). The title compound was obtained as an oil in 70% yield (1 mmol scale, 157.6 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.00 (d, $J = 11.5$ Hz, 1H), 7.62 (d, $J = 7.5$ Hz, 1H), 7.53 (s, 1H), 7.40-7.34 (m, 2H), 7.19-7.13 (m, 2H), 6.98-6.95 (m, 2H), 6.86 (d, $J = 11.5$ Hz, 1H), 2.89 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 144.9, 141.2, 140.2, 129.6, 129.6, 128.3, 125.9, 125.6, 121.7, 119.6, 118.2; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.7; FT-IR (neat): 3370, 1614, 1561, 1435, 1385, 1078, 757 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{13}$H$_{13}$BNS $[M+H]^+$ 226.0862, found 226.0871.

4-[(2,1-Borazaronaphthyl)methyl]-3,5-dimethylisoxazole (3e). The title compound was obtained as a solid in 80% yield (1 mmol scale, 190.5 mg). mp: 106-107 °C; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.98 (d, $J = 11.5$ Hz, 1H), 7.61-7.60 (d, $J = 7.5$ Hz, 2H), 7.40-7.37 (m, 1H), 7.21 (d, $J = 8.0$ Hz, 1H), 7.18-7.15 (m, 1H), 6.77-6.75 (m, 1H), 2.38 (s, 2H), 2.29 (s, 3H), 2.13 (s, 3H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 164.1, 160.5, 145.3, 140.1, 129.6, 128.6, 125.7, 121.4, 118.2, 112.4, 11.3, 10.7; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.1; FT-IR (neat): 3234, 1614, 1566, 1455, 1442, 1282, 764 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{14}$H$_{16}$BN$_2$O $[M+H]^+$ 239.1356, found 239.1358.
**N-Benzyl-2-(5-methylfur-2-yl)methyl-2,1-borazaronaphthalene (3f).** The title compound was obtained as an oil in 70% yield (1 mmol scale, 219.2 mg). $^1$H NMR (500 MHz, CDCl$_3$): δ 7.94 (d, $J = 11.5$ Hz, 1H), 7.59-7.57 (m, 1H), 7.30-7.20 (m, 4H), 7.17-7.14 (m, 1H), 7.11-7.07 (m, 1H), 7.05 (d, $J = 8.0$ Hz, 2H), 6.81 (d, $J = 11$ Hz, 1H), 5.77 (d, $J = 2.5$ Hz, 1H), 5.71 (d, $J = 2.5$ Hz, 1H), 5.31 (s, 2H), 2.73 (s, 2H, 2.16 (s, 3H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): δ 153.7, 150.1, 145.4, 141.8, 138.5, 130.5, 129.0, 128.7, 127.3, 127.2, 126.0, 121.1, 116.4, 106.3, 105.9, 51.1, 13.8; $^{11}$B NMR (128.38 MHz, CDCl$_3$): δ 37.3; FT-IR (neat): 1610, 1593, 1552, 1493, 1418, 1357, 1296, 1217, 1003, 801, 758 cm$^{-1}$; HRMS (Cl$^+$) m/z calcd. for C$_{21}$H$_{20}$BNO $[M]^+$ 313.1638, found 313.1642.

**5-[(N-Benzyl-2,1-borazaronaphthalene-2-yl)methyl]-N-(tert-butoxycarbonyl)indole (3g).** The title compound was obtained as a solid in 84% yield (1 mmol scale, 376.6 mg). mp: 80-81 °C; $^1$H NMR (500 MHz, CDCl$_3$): δ 8.00 (s, 1H), 7.84 (d, $J = 11.5$ Hz, 1H), 7.52-7.51 (m, 2H), 7.27-7.20 (m, 5H), 7.16-7.13 (m, 1H), 7.08-7.03 (m, 4H), 6.65 (d, $J = 11.0$ Hz, 1H), 6.40 (d, $J = 3.0$ Hz, 1H), 5.30 (s, 2H), 2.86 (s, 2H), 1.60 (s, 9H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): δ 150.1, 145.0, 141.7, 138.6, 136.6, 133.2, 131.3, 130.4, 129.0, 128.8, 128.6, 127.2, 127.1, 126.3, 126.0,
121.2, 120.9, 116.3, 115.2, 107.4, 83.5, 50.9, 28.5; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 38.3; FT-IR (neat): 1731, 1609, 1551, 1466, 1370, 1346, 1163, 1127, 1081, 1023, 758, 729 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{29}$H$_{30}$BN$_2$O$_2$ [M+H]$^+$ 449.2400, found 449.2392.

**2-(5-Methylfuran-2-yl)methyl-6-methyl-2,1-borazaronaphthalene (3h).** The title compound was obtained as a white solid in 78% yield (1 mmol scale, 184.9 mg). mp: 44-45 °C; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.94 (d, $J$ = 11.5 Hz, 1H), 7.83 (s, 1H), 7.40 (s, 1H), 7.22 (d, $J$ = 8.0 Hz, 1H), 7.11 (d, $J$ = 8.5 Hz, 1H), 6.81 (dd, $J$ = 11.5, 1.5 Hz, 1H), 5.92-5.87 (m, 2H), 2.78 (s, 2H), 2.43 (s, 3H), 2.31 (s, 3H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 154.1, 150.1, 144.8, 138.2, 130.3, 129.7, 129.3, 125.5, 118.1, 106.4, 105.4, 21.1, 13.9; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 35.8; FT-IR (neat): 3360, 1617, 1566, 1437, 1234, 1215, 1021, 835, 822, 784, 703 cm$^{-1}$; HRMS (CI+) m/z calcd. for C$_{15}$H$_{16}$BNO [M]$^+$ 237.1325, found 237.1324.

**Optimization of the cross coupling reaction of 2-chloromethyl-2,1-borazaronaphthalene with potassium alkenyltrifluoroborates:** The cross-coupling reaction of 1 with potassium 2-trifluoroboratopropene serve as a model reaction to find optimal conditions for the cross-coupling with potassium alkenyltrifluoroborates. A variety of catalysts, ligands, bases, and solvents were screened (Table S2). The results of the screens can be illustrated in a heat map. The size of the circle corresponds to the product to internal standard ratios. The larger the circle, the more product formed during the reaction. Accordingly, the best conditions were the reaction...
in the presence of Pd\(_2\text{dba}_3\) as a catalyst, \(t\)-Bu\(_2\text{MeP} \cdot \text{HBF}_4\) as a ligand, and Cs\(_2\text{CO}_3\) in a mixture of toluene/H\(_2\text{O}\) as a solvent.

\[
\begin{array}{c}
\text{N} & \text{B} & \text{Cl} & \xrightarrow{\text{Pd catalyst (3 mol %)}} \xrightarrow{\text{ligand (6 mol %)}} \text{B} & \text{N} \\
& & & \xrightarrow{\text{Cs}_2\text{CO}_3 (3 equiv)}} & \text{solvent (0.1 M)}
\end{array}
\]

Table S2. Optimization of the cross coupling reaction with potassium 2-propenyltrifluoroborate.

| Temperature | Catalyst          | Base      | Ligands                  | Solvent 19:1         |
|-------------|-------------------|-----------|--------------------------|-----------------------|
| 80 °C       | Pd-G2-dimer       | Cs\(_2\text{CO}_3\) | RuPhos, PPh\(_3\), XPhos | toluene / H\(_2\text{O}\) dioxane / H\(_2\text{O}\) |
| 80 °C       | \((t\)-Bu\(_3\)P-Pd-G2 | Cs\(_2\text{CO}_3\) | -                        | toluene / H\(_2\text{O}\) dioxane / H\(_2\text{O}\) |
| 80 °C       | Pd\(_2\text{dba}_3\) | Cs\(_2\text{CO}_3\) | XPhos, RuPhos, A\(_{\mu}\)-Phos, CataCXium A t-Bu\(_3\)MeP-HBF\(_4\) | toluene / H\(_2\text{O}\) dioxane / H\(_2\text{O}\) |
| 80 °C       | Pd(OAc)\(_2\)     | Cs\(_2\text{CO}_3\) | XPhos, RuPhos, CataCXium A | toluene / H\(_2\text{O}\) |
| 80 °C       | RuPhos-Pd-G2      | Cs\(_2\text{CO}_3\) | -                        | toluene / H\(_2\text{O}\) |
| 80 °C       | XPhos-Pd-G2       | Cs\(_2\text{CO}_3\) | -                        | toluene / H\(_2\text{O}\) |
| 80 °C       | Pd(dppe)Cl\(_2\)  | Cs\(_2\text{CO}_3\) | -                        | toluene / H\(_2\text{O}\) |
To investigate the effect of the type of the base, catalyst loading, and the amount of the base, further optimization was completed. In the reaction of 1 with potassium 2-propenyltrifluoroborate various bases (entries 1-3) and different amounts of both base (entries 3-5) and the Pd catalyst (entries 4, 6 and 7) were used. The best conditions for the reaction were in the presence of 2 mol % of Pd3dba_3 and 2 equiv of K3PO4 (Table S3).
Table S3. Varying amounts of catalyst and base.

| entry | Pd_{2}dba_{3} (mol %) | t-Bu_{2}MeP-HBF_{4} (mol %) | base | product/starting compound |
|-------|----------------------|-----------------------------|------|--------------------------|
| 1     | 3.0                  | 6.0                         | Cs_{2}CO_{3} (3 equiv) | 41.1 |
| 2     | 3.0                  | 6.0                         | K_{3}PO_{4} (3 equiv)  | 44.0 |
| 3     | 3.0                  | 6.0                         | K_{2}CO_{3} (3 equiv)  | 39.7 |
| 4     | 3.0                  | 6.0                         | K_{3}PO_{4} (2 equiv)  | 43.9 |
| 5     | 3.0                  | 6.0                         | K_{3}PO_{4} (1 equiv)  | 21.2 |
| 6     | 2.0                  | 4.0                         | K_{3}PO_{4} (2 equiv)  | 48.1 |
| 7     | 1.5                  | 3.0                         | K_{3}PO_{4} (2 equiv)  | 40.7 |

General procedure for the cross coupling reaction of 2-chloromethyl-2,1-borazaronaphthalene with potassium alkenyltrifluoroborates. To an oven-dried Biotage microwave vial equipped with a stir bar were added 2-chloromethyl-2,1-borazaronaphthalene (177.4 mg, 1 mmol), the corresponding potassium alkenyltrifluoroborate (1.2 mmol, 1.2 equiv), Pd_{2}dba_{3} (18.3 mg, 20 µmol, 2 mol %), t-Bu_{2}MeP-HBF_{4} (9.9 mg, 40 µmol, 4 mol %), and K_{3}PO_{4} (460.6 mg, 2 mmol). The vial was sealed with a cap lined with a disposable Teflon septum, then evacuated under vacuum and purged with Ar three times. Anhydrous toluene (9.5 mL) and degassed H_{2}O (0.5 mL) were added by syringe under Ar. The resulting mixture was heated to 80 °C and vigorously stirred for 18 h. The reaction mixture was filtered through a plug of silica and flushed with 10-40% hexane/CH_{2}Cl_{2}. Then the solvent was removed under reduced pressure, and the crude extract was purified by column chromatography to obtain the pure product.

2-[(E)-2-Butenyl]-2,1-borazaronaphthalene (4a). The title compound was obtained as an oil in 90% yield (1 mmol scale, 168.4 mg). ^1H NMR (500 MHz, CDCl_{3}): δ 7.88 (d, J = 11.5 Hz, 1H), 7.58 (s, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.32-7.29 (m, 1H), 7.12-7.06 (m, 2H), 6.75 (dd, J = 11.5,
2.0 Hz, 1H), 5.67-5.60 (m, 1H), 5.47-5.40 (m, 1H), 2.10 (d, $J = 7.5$ Hz, 2H), 1.73-1.71 (m, 3H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 144.6, 140.3, 129.6, 129.2, 128.2, 125.6, 125.1, 120.9, 118.1, 18.5; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.4; FT-IR (neat): 3358, 1614, 1592, 1560, 1436, 1132, 962, 763, 752 cm$^{-1}$; HRMS (Cl$^+$) m/z calcd. for C$_{12}$H$_{14}$BN [M]$^+$ 183.1219, found 183.1223.

2-[(Z)-2-Butenyl]-2,1-borazonaphthalene (4b). The title compound was obtained as an oil in 82% yield (1 mmol scale, 150.1 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.92 (d, $J = 11.5$ Hz, 1H), 7.67 (s, 1H), 7.56 (d, $J = 7.5$ Hz, 1H), 7.36-7.33 (m, 1H), 7.18-7.15 (m, 1H), 7.12-7.09 (m, 1H), 6.80-6.78 (m, 1H), 5.75-5.69 (m, 1H), 5.69-5.58 (m, 1H), 2.20 (d, $J = 8.0$ Hz, 2H), 1.63-1.61 (m, 3H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 144.6, 140.3, 129.6, 128.4, 128.2, 125.6, 123.5, 121.0, 118.1, 13.0; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.1; FT-IR (neat): 3370, 1615, 1561, 1435, 1276, 837, 757, 733 cm$^{-1}$; HRMS (Cl$^+$) m/z calcd. for C$_{12}$H$_{14}$BN [M]$^+$ 183.1219, found 183.1207.

2-(2-Methylallyl)-2,1-borazonaphthalene (4c). The title compound was obtained as an oil in 80% yield (1 mmol scale, 146.4 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.92 (d, $J = 11.5$ Hz, 1H), 7.40 (s, 1H), 7.55 (d, $J = 8.0$ Hz, 1H), 7.35-7.31 (m, 1H), 7.15 (d, $J = 8.0$ Hz, 1H), 7.11-7.08 (m, 1H), 6.79 (dd, $J = 11.5$, 2.0 Hz, 1H), 4.83-4.7 (m, 2H), 2.21 (s, 2H), 1.75 (s, 3H); $^{13}$C NMR
(125.8 MHz, CDCl$_3$): $\delta$ 146.2, 144.7, 140.3, 129.6, 128.3, 125.7, 121.0, 118.2, 109.8, 25.1; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.3; FT-IR (neat): 3369, 1615, 1561, 1435, 875, 757 cm$^{-1}$; HRMS (Cl+) m/z calcd. for C$_{12}$H$_{15}$BN [M+H]$^+$ 184.1298, found 184.1289.

$\text{B}H\text{N}$

2-[(E)-Undec-2-enyl]-2,1-borazaronaphthalene (4d). The title compound was obtained as an oil in 89% yield (1 mmol scale, 253.1 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.99 (d, $J$ = 11.5 Hz, 1H), 7.72 (s, 1H), 7.63 (d, $J$ = 7.5 Hz, 1H), 7.43-7.40 (m, 1H), 7.23 (d, $J$ = 8.5 Hz, 1H), 7.18 (dd, $J$ = 7.5, 7.5 Hz, 1H), 6.83 (dd, $J$ = 11.5, 2.0 Hz, 1H), 5.74-5.68 (m, 1H), 5.55-5.50 (m, 1H), 2.21 (d, $J$ = 7.5 Hz, 2H), 2.15 (q, $J$ = 7.0 Hz, 2H), 1.51-1.32 (m, 12H), 0.97 (t, $J$ = 7.0 Hz, 3H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 144.6, 140.4, 131.2, 129.6, 128.2, 128.0, 125.7, 121.0, 118.1, 33.2, 32.2, 30.4, 29.9, 29.7, 29.6, 23.0, 14.4; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 36.6; FT-IR (neat): 3373, 1615, 1594, 1561, 1435, 1344, 1275, 967, 756 cm$^{-1}$; HRMS (Cl+) m/z calcd. for C$_{19}$H$_{29}$BN [M+H]$^+$ 282.2393, found 282.2393.

$\text{B}H\text{N}$

2-Cyclohexenylmethyl-2,1-borazaronaphthalene (4e). The title compound was obtained as an oil in 86% yield (1 mmol scale, 191.9 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 7.89 (d, $J$ = 11.0 Hz, 1H), 7.64 (s, 1H), 7.53 (d, $J$ = 7.5 Hz, 1H), 7.33-7.30 (m, 1H), 7.14-7.12 (m, 1H), 7.09-7.06 (m, 1H), 6.77 (dd, $J$ = 11.5, 1.5 Hz, 1H), 5.42 (s, 1H), 2.08-2.05 (m, 4H), 1.91-1.90 (m, 2H), 1.63-1.54 (m, 4H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 144.5, 140.4, 137.7, 129.6, 128.2, 125.7, 120.9,
120.7, 118.1, 31.0, 25.8, 23.7, 22.9; \(^{11}\)B NMR (128.38 MHz, CDCl\(_3\)): \(\delta\) 36.6; FT-IR (neat): 3370, 1614, 1594, 1560, 1435, 1343, 1279, 1136, 756 cm\(^{-1}\); HRMS (Cl\(^{+}\)) m/z calcd. for C\(_{15}\)H\(_{18}\)BN [M\(^{+}\)] 223.1532, found 223.1535.

![8-(2,1-Borazaronaphthyl)methyl-1,4-dioxaspiro[4.5]dec-7-ene (4f)](image)

8-(2,1-Borazaronaphthyl)methyl-1,4-dioxaspiro[4.5]dec-7-ene (4f). The title compound was obtained as a white solid in 84% yield (1 mmol scale, 236.2 mg). mp: 70-71 °C; \(^{1}\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 8.01 (s, 1H), 7.97 (d, \(J = 11.5\) Hz, 1H), 7.61 (d, \(J = 8.0\) Hz, 1H), 7.42-7.39 (m, 1H), 7.23 (d, \(J = 8.0\) Hz, 1H), 7.17-7.14 (m, 1H), 6.83 (dd, \(J = 11.5, 1.5\) Hz, 1H), 5.38 (t, \(J = 3.5\) Hz, 1H), 4.08-4.01 (m, 4H), 2.39 (s, 2H), 2.28-2.25 (m, 2H), 2.21 (s, 2H), 1.86-1.83 (m, 2H); \(^{13}\)C NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 144.5, 140.5, 137.6, 129.5, 128.1, 125.6, 120.8, 118.2, 117.9, 108.8, 64.6, 36.0, 31.5, 30.2; \(^{11}\)B NMR (128.38 MHz, CDCl\(_3\)): \(\delta\) 36.6; FT-IR (neat): 3322, 1611, 1564, 1446, 1293, 1133, 1011, 864, 756 cm\(^{-1}\); HRMS (ES\(^{+}\)) m/z calcd. for C\(_{17}\)H\(_{21}\)BNO\(_2\) [M+H\(^{+}\)] 282.1665, found 282.1654.

![2-(4,4-Difluorocyclohex-1-enyl)methyl-2,1-borazaronaphthalene (4g)](image)

2-(4,4-Difluorocyclohex-1-enyl)methyl-2,1-borazaronaphthalene (4g). The title compound was obtained as a solid in 75% yield (1 mmol scale, 202.1 mg). mp: 44-45 °C; \(^{1}\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 7.92 (d, \(J = 11.5\) Hz, 1H), 7.65 (s, 1H), 7.55 (d, \(J = 7.5\) Hz, 1H), 7.36-7.33 (m, 1H), 7.15 (d, \(J = 8.5\) Hz, 1H), 7.13-7.09 (m, 1H), 6.76 (dd, \(J = 11.5, 1.5\) Hz, 1H), 5.25 (s, 1H), 2.59-2.53 (m, 2H), 2.22-2.20 (m, 2H), 2.14 (s, 2H), 2.04-1.96 (m, 2H); \(^{13}\)C NMR (125.8 MHz,
CDCl₃: δ 144.9, 140.3, 137.4, 129.6, 128.4, 125.6, 123.6 (t, J = 239.3 Hz, 1C), 121.1, 118.2, 115.5 (t, J = 5.1 Hz, 1C), 35.0 (t, J = 26.2 Hz, 1C), 30.8 (t, J = 24.4 Hz, 1C), 29.2 (t, J = 5.3 Hz, 1C); ¹¹B NMR (128.38 MHz, CDCl₃): δ 36.2; FT-IR (neat): 3371, 1615, 1561, 1436, 1264, 1120, 1101, 1065, 886, 759 cm⁻¹; HRMS (Cl⁺) m/z calcd. for C₁₅H₁₆BNF₂ [M⁺] 259.1344, found 259.1354.

2-(3,6-Dihydro-2H-pyran-4-yl)methyl-2,1-borazonaphthalene (4h). The title compound was obtained as a white solid in 79% yield (1 mmol scale, 177.8 mg). mp: 74-75 °C; ¹H NMR (500 MHz, CDCl₃): δ 7.93 (d, J = 11.5 Hz, 1H), 7.72 (s, 1H), 7.56 (d, J = 7.5 Hz, 1H), 7.37-7.34 (m, 1H), 7.21-7.19 (m, 1H), 7.13-7.10 (m, 1H), 6.77 (dd, J = 11.5, 2.0 Hz, 1H), 5.44-5.43 (m, 1H), 4.18-4.17 (m, 2H), 3.78 (t, J = 5.5 Hz, 2H), 2.15 (s, 2H), 2.06-2.04 (m, 2H); ¹³C NMR (125.8 MHz, CDCl₃): δ 144.8, 140.3, 135.5, 129.6, 128.3, 125.7, 121.1, 119.4, 118.2, 66.0, 64.9, 31.0; ¹¹B NMR (128.38 MHz, CDCl₃): δ 36.3; FT-IR (neat): 3296, 1614, 1562, 1446, 1348, 1290, 1135, 1110, 843, 829, 763 cm⁻¹; HRMS (Cl⁺) m/z calcd. for C₁₄H₁₆BNO [M⁺] 225.1325, found 225.1320.

4-(2,1-Borazonaphthyl)methyl-1-(tert-butoxycarbonyl)-1,2,3,6-tetrahydropyridine (4i). The title compound was obtained as a solid in 83% yield (1 mmol scale, 269.1 mg). mp: 101-102 °C; ¹H NMR (500 MHz, CDCl₃): δ 7.96 (d, J = 11.5 Hz, 1H), 7.80 (s, 1H), 7.59 (d, J = 8.0 Hz, 1H), 7.54
7.40-7.37 (m, 1H), 7.23 (d, \( J = 8.0 \text{ Hz}, 1H \)), 7.16-7.13 (m, 1H), 6.80 (dd, \( J = 11.5, 2.0 \text{ Hz}, 1H \)), 5.41 (s, 1H), 3.96 (s, 2H), 3.54-3.51 (m, 2H), 2.18 (s, 2H), 2.08 (s, 2H), 1.50 (s, 9H); 13C NMR (125.8 MHz, CDCl3): \( \delta \) 155.2, 144.8, 140.2, 136.5, 129.8, 129.5, 128.2, 125.5, 121.0, 118.1, 79.5, 30.7, 29.3, 28.7, 28.4; 11B NMR (128.38 MHz, CDCl3): \( \delta \) 36.3; FT-IR (neat): 3303, 1675, 1614, 1566, 1450, 1418, 1365, 1284, 1238, 1169, 1117, 806, 761 cm\(^{-1}\); HRMS (ES+) m/z calcd. for C_{19}H_{25}BN_{2}O_{2}Na [M+Na]\(^+\) 347.1907, found 347.1921.

\[ \text{N-Benzyl-4-(2,1-borazaronaphthyl)methyl-1-(tetr-butoxycarbonyl)-1,2,3,6-tetrahydro pyridine (4j).} \]

The title compound was obtained as a white solid in 80\% yield (1 mmol scale, 331.4 mg). mp: 120°C; \(^1\)H NMR (500 MHz, CDCl3): \( \delta \) 8.00 (d, \( J = 11.5 \text{ Hz}, 1H \)), 7.64 (d, \( J = 7.5 \text{ Hz}, 1H \)), 7.33-7.27 (m, 4H), 7.24-7.21 (m, 1H), 7.17-7.14 (m, 1H), 7.08 (d, \( J = 7.5 \text{ Hz}, 2H \)), 6.88 (d, \( J = 11.5 \text{ Hz}, 1H \)), 5.34 (s, 2H), 5.31 (s, 1H), 3.84 (s, 2H), 3.48 (s, 2H), 2.22 (s, 2H), 2.07-2.05 (m, 2H), 1.49 (s, 9H); 13C NMR (125.8 MHz, CDCl3): \( \delta \) 155.2, 145.1, 141.8, 138.5, 136.4, 130.4, 128.9, 128.6, 127.1, 127.1, 125.9, 120.9, 117.9, 116.2, 79.5, 50.8, 31.8, 30.9, 29.8, 28.7; 11B NMR (128.38 MHz, CDCl3): \( \delta \) 38.1; FT-IR (neat): 1697, 1609, 1551, 1400, 1364, 1233, 1162, 1105, 762 cm\(^{-1}\); HRMS (ES+) m/z calcd. for C_{26}H_{32}BN_{2}O_{2} [M+H]\(^+\) 415.2557, found 415.2566.
N-Benzyl-8-(2,1-borazaronaphthyl)methyl-1,4-dioxaspiro[4.5]dec-7-ene (4k). The title compound was obtained as a pale-yellow solid in 90% yield (1 mmol scale, 337.9 mg). mp: 104-105 °C; ^1^H NMR (500 MHz, CDCl₃): δ 7.93 (d, J = 11.5 Hz, 1H), 7.55 (d, J = 7.5 Hz, 1H), 7.26-7.17 (m, 4H), 7.14-7.11 (m, 1H), 7.07-7.00 (m, 3H), 6.89 (dd, J = 11.5, 1.0 Hz, 1H), 5.25-5.22 (m, 3H), 3.91-3.85 (m, 4H), 2.20-2.15 (m, 6H), 1.71-1.68 (m, 2H); ^1^3^C NMR (125.8 MHz, CDCl₃): δ 144.8, 141.8, 138.6, 137.3, 130.3, 128.8, 128.4, 127.0, 127.0, 125.9, 120.7, 118.3, 116.1, 108.3, 64.4, 50.7, 36.0, 31.5, 30.2; ^1^B NMR (128.38 MHz, CDCl₃): δ 38.6; FT-IR (neat): 1608, 1592, 1551, 1492, 1411, 1350, 1233, 1114, 1057, 864, 757, 730 cm⁻¹; HRMS (CI⁺) m/z calcd. for C₂₄H₂₆BNO₂ [M]⁺ 371.2057, found 371.2067.

5-[(6-Methyl-2,1-borazaronaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (4l). The title compound was obtained as a solid in 78% yield (1 mmol scale, 273.9 mg). mp: 119-120 °C; ^1^H NMR (500 MHz, CDCl₃): δ 7.90 (d, J = 11.5 Hz, 1H), 7.77 (s, 1H), 7.37 (s, 1H), 7.21 (d, J = 8.5 Hz, 1H), 7.14 (d, J = 8.0 Hz, 1H), 6.77 (d, J = 11.5 Hz, 1H), 5.40 (s, 1H), 3.96 (s, 2H), 3.53 (s, 2H), 2.41 (s, 3H), 2.17 (s, 2H), 2.08 (s, 2H), 1.51 (s, 9H); ^1^3^C NMR (125.8 MHz, CDCl₃): δ 155.2, 144.5, 138.2, 136.6, 130.1, 129.5, 129.1, 125.4, 117.9, 117.4, 79.5, 30.6, 29.3, 28.6, 28.5, 20.9; ^1^B NMR (128.38 MHz, CDCl₃): δ 35.8; FT-IR (neat): 3302, 1673, 1570, 1415, 1366, 1114, 1057, 864, 757, 730 cm⁻¹; HRMS (CI⁺) m/z calcd. for C₂₄H₂₆BNO₂ [M]⁺ 371.2057, found 371.2067.
Optimization of the cross coupling reaction of 2-chloromethyl-2,1-borazaronaphthalene with alkynes: Optimization for the cross coupling reaction of 2-chloromethyl-2,1-borazaronaphthalene with alkynes was completed with phenylacetylene as a model alkyne. A variety of catalysts and ligands were screened (Figure S3). The ratios of product to internal standard from the HPLC are shown in Figure S3.

![Reaction Scheme](image)

**Figure S3. Ratios of product to internal standard.**
Furthermore, to determine the ideal amount of Cs$_2$CO$_3$ and also the ratio of the azaborine (1) to terminal alkyne, the reaction of 2-chloromethyl-2,1-borazonaphthalene with phenylacetylene was performed in the presence of different amounts of the base and different ratios of the starting materials (Table S4). The optimal conditions for the reaction were the presence of 1.05 equiv of the base and 1.3 equiv of the phenylacetylene.

**Table S4. Effects of the stoichiometry of Cs$_2$CO$_3$ and the ratio of the azaborine to phenylacetylene.**

| entry | compound 1 | Phenylacetylene | XPhos-Pd-G2 (mol %) | Cs$_2$CO$_3$ (equiv) | temperature (°C) | product/compound 1 |
|-------|------------|-----------------|---------------------|---------------------|------------------|-------------------|
| 1     | 1.0 equiv  | 1.3 equiv       |                     | 2                   | 80               | 123.8             |
| 2     |            | 1.3 equiv       |                     | 1.05                | 80               | 164.0             |
| 3     |            | 1.1 equiv       |                     | 1.05                | 80               | 156.8             |
| 4     |            | 1.3 equiv       |                     | 1.05                | 70               | 165.1             |
| 5     |            | 1.3 equiv       |                     | 1.05                | 60               | 149.0             |

**General procedure for the cross coupling reaction of 2-chloromethyl-2,1-borazonaphthalene with terminal alkynes.** To an oven-dried Biotage microwave vial equipped with a stir bar were added 2-chloromethyl-2,1-borazonaphthalene (177.4 mg, 1 mmol), XPhos-Pd-G2 (15.7 mg, 20 µmol, 2 mol %), and Cs$_2$CO$_3$ (342.1 mg, 1.05 mmol). The vial was sealed with a cap lined with a disposable Teflon septum, then evacuated under vacuum and purged with Ar three times. Anhydrous toluene (9.5 mL) and degassed H$_2$O (0.5 mL) were added by syringe under Ar followed by the corresponding terminal alkyne (1.3 mmol, 1.3 equiv). The resulting mixture was heated to 70 °C and vigorously stirred for 16 h. The reaction mixture was filtered through a plug of silica and flushed with hexane/CH$_2$Cl$_2$ (3:1). The solvent was then removed under reduced pressure, and the crude material was purified by column chromatography to obtain the pure product.
2-(3-Phenylprop-2-ynyl)-2,1-borazaronaphthalene (5a). The title compound was obtained as an oil in 84% yield (1 mmol scale, 204.2 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 8.25 (s, 1H), 8.03 (d, \(J = 11.0\) Hz, 1H), 7.64 (d, \(J = 7.5\) Hz, 1H), 7.53-7.51 (m, 2H), 7.45-7.42 (m, 1H), 7.37-7.30 (m, 4H), 7.21-7.18 (m, 1H), 6.84 (dd, \(J = 11.5, 1.5\) Hz, 1H), 2.59 (s, 2H); \(^13\)C NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 145.4, 140.1, 131.9, 129.7, 128.6, 128.6, 127.7, 125.8, 124.8, 121.4, 118.4, 89.6, 81.5; \(^11\)B NMR (128.38 MHz, CDCl\(_3\)): \(\delta\) 35.3; FT-IR (neat): 3367, 1615, 1562, 1435, 1386, 830, 754, 689 cm\(^{-1}\); HRMS (Cl\(^+\)) m/z calcd. for C\(_{17}\)H\(_{14}\)BN [M\(^+\)] 243.1219, found 243.1225.

2-(3-p-Tolylprop-2-ynyl)-2,1-borazaronaphthalene (5b). The title compound was obtained as an oil in 79% yield (1 mmol scale, 203.1 mg). mp: 72-73 °C; \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 8.18 (s, 1H), 7.94 (d, \(J = 11.5\) Hz, 1H), 7.56 (d, \(J = 8.0\) Hz, 1H), 7.36-7.33 (m, 3H), 7.21 (d, \(J = 8.0\) Hz, 1H), 7.13-7.08 (m, 3H), 6.77 (dd, \(J = 11.5, 2.0\) Hz, 1H), 2.51 (s, 2H), 2.31 (s, 3H); \(^13\)C NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 145.3, 140.1, 137.6, 131.7, 129.7, 129.3, 128.5, 125.8, 121.7, 121.3, 118.4, 88.7, 81.6, 21.7; \(^11\)B NMR (128.38 MHz, CDCl\(_3\)): \(\delta\) 34.6; FT-IR (neat): 3358, 1614, 562, 1508, 1438, 1212, 816, 763 cm\(^{-1}\); HRMS (ES\(^+\)) m/z calcd. for C\(_{18}\)H\(_{17}\)BN [M+H\(^+\)] 258.1454, found 258.1454.
2-(3-[4-Methoxyphenylprop-2-ynyl])-2,1-borazaronaphthalene (5c). The title compound was obtained as an oil in 81% yield (1 mmol scale, 221.2 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.26 (s, 1H), 8.02 (d, $J = 11.5$ Hz, 1H), 7.64 (d, $J = 8.0$ Hz, 1H), 7.46-7.41 (m, 3H), 7.30 (d, $J = 8.0$ Hz, 1H), 7.21-7.18 (m, 1H), 6.90-6.87 (m, 2H), 6.84 (dd, $J = 11.5$, 2.0 Hz, 1H), 3.83 (s, 3H), 2.57 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 159.2, 145.3, 140.1, 133.1, 129.6, 128.5, 125.8, 121.3, 118.4, 116.9, 114.2, 87.8, 81.2, 55.5; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 34.9; FT-IR (neat): 3365, 1614, 1562, 1508, 1436, 1290, 1172, 1032, 830, 758 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{18}$H$_{17}$BNO [M+H]$^+$ 274.1403, found 274.1390.

2-(3-[4-Tolylprop-2-ynyl])-2,1-borazaronaphthalene (5d). The title compound was obtained as a white solid in 70% yield (1 mmol scale, 182.7 mg). mp: 56-57 °C; $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.13 (s, 1H), 7.95 (d, $J = 11.5$ Hz, 1H), 7.57 (d, $J = 8.0$ Hz, 1H), 7.43-7.40 (m, 2H), 7.37-7.34 (m, 1H), 7.21 (d, $J = 8.0$ Hz, 1H), 7.13 (t, $J = 7.5$ Hz, 1H), 6.97 (t, $J = 8.5$ Hz, 2H), 6.79-6.76 (m, 1H), 2.50 (s, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 162.2 (d, $J = 248.1$ Hz, 1C), 145.4, 140.0, 133.6 (d, $J = 8.0$ Hz, 1C), 129.7, 128.5, 125.8, 121.4, 120.8 (d, $J = 3.5$ Hz, 1C), 118.4, 115.7 (d, $J = 21.9$ Hz, 1C), 89.3, 80.4; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 34.7; FT-IR (neat): 3371, 1613, 1560, 1504, 1435, 1221, 1208, 1129, 836, 758 cm$^{-1}$; HRMS (Cl+) m/z calcd. for C$_{17}$H$_{13}$BNF [M]$^+$ 261.1125, found 261.1128.
2-(3-Cyclohexenylprop-2-ynyl)-2,1-borazaronaphthalene (5e). The title compound was obtained as an oil in 74% yield (1 mmol scale, 185.3 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.20 (s, 1H), 7.98 (d, $J$ = 11.0 Hz, 1H), 7.62 (d, $J$ = 8.0 Hz, 1H), 7.43-7.40 (m, 1H), 7.29 (d, $J$ = 8.0 Hz, 1H), 7.19-7.16 (m, 1H), 6.78 (dd, $J$ = 11.5, 1.5 Hz, 1H), 6.11 (s, 1H), 2.45 (s, 2H), 2.23-2.21 (m, 2H), 2.13-2.12 (m, 2H), 1.71-1.67 (m, 2H), 1.64-1.60 (m, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 145.2, 140.2, 133.1, 129.7, 128.5, 125.8, 121.7, 121.3, 118.4, 86.3, 83.5, 30.4, 25.9, 22.8, 22.0; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 34.7; FT-IR (neat): 3387, 1614, 1564, 1437, 1341, 1186, 909, 800, 758, 731 cm$^{-1}$; HRMS (ES+) m/z calcd. for C$_{17}$H$_{18}$BN $[M]^{+}$ 247.1532, found 247.1530.

2-(3-Cyclopropylprop-2-ynyl)-2,1-borazaronaphthalene (5f). The title compound was obtained as an oil in 60% yield (1 mmol scale, 126.3 mg). $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ 8.17 (s, 1H), 7.96 (d, $J$ = 11.5 Hz, 1H), 7.61 (d, $J$ = 8.0 Hz, 1H), 7.43-7.40 (m, 1H), 7.29 (d, $J$ = 8.0 Hz, 1H), 7.18-7.15 (m, 1H), 6.74 (dd, $J$ = 11.5, 2.0 Hz, 1H), 2.27 (d, $J$ = 1.5 Hz, 2H), 1.36-1.30 (m, 1H), 0.80-0.76 (m, 2H), 0.71-0.67 (m, 2H); $^{13}$C NMR (125.8 MHz, CDCl$_3$): $\delta$ 145.1, 140.1, 129.6, 128.4, 125.8, 121.2, 118.3, 84.1, 74.5, 8.5, 0.1; $^{11}$B NMR (128.38 MHz, CDCl$_3$): $\delta$ 33.0; FT-IR (neat): 3366, 1614, 1562, 1436, 1278, 1187, 1030, 801, 756 cm$^{-1}$; HRMS (CI+) m/z calcd. for C$_{14}$H$_{14}$BN $[M]^{+}$ 207.1219, found 207.1220.
**N-Benzyl-2-(3-[4-methoxyphenylprop-2-ynyl])-2,1-borazonaphthalene (5g).** The title compound was obtained as a white solid in 78% yield (1 mmol scale, 286.9 mg). mp: 109-110°C; 
°C; \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 8.05 (d, \(J = 11.5\) Hz, 1H), 7.65 (d, \(J = 7.5\) Hz, 1H), 7.32-7.31 (m, 2H), 7.26-7.23 (m, 4H), 7.20-7.17 (m, 2H), 7.16-7.13 (m, 1H), 7.09 (d, \(J = 7.0\) Hz, 2H), 6.76 (dd, \(J = 7.0, 2.0\) Hz, 2H), 5.35 (s, 2H), 3.75 (s, 3H), 2.51 (s, 2H); \(^{13}\)C NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 159.0, 145.9, 141.6, 138.2, 133.0, 130.6, 129.0, 128.8, 127.3, 127.2, 126.0, 121.2, 117.1, 116.4, 114.0, 88.1, 80.3, 55.5, 50.9; \(^{11}\)B NMR (128.38 MHz, CDCl\(_3\)): \(\delta\) 36.6; FT-IR (neat): 1608, 1550, 1507, 1292, 1245, 1027, 757 cm\(^{-1}\); HRMS (CI+) m/z calcd. for C\(_{25}\)H\(_{22}\)BNO \([M]^+\) 363.1794, found 363.1795.

**2-(3-[4-Methoxyphenylprop-2-ynyl])-6-methyl-2,1-borazonaphthalene (5h).** The title compound was obtained as a white solid in 80% yield (1 mmol scale, 229.7 mg). mp: 46°C; 
\(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 8.14 (s, 1H), 7.89 (d, \(J = 11.0\) Hz, 1H), 7.39 (d, \(J = 8.0\) Hz, 2H), 7.35 (s, 1H), 7.18 (d, \(J = 8.0\) Hz, 1H), 7.13 (d, \(J = 8.0\) Hz, 1H), 6.81 (d, \(J = 8.5\) Hz, 2H), 6.75 (d, \(J = 11.5\) Hz, 1H), 3.75 (s, 3H), 2.49 (s, 2H), 2.37 (s, 3H); \(^{13}\)C NMR (125.8 MHz, CDCl\(_3\)): \(\delta\) 159.2, 145.0, 138.1, 133.1, 130.5, 129.8, 129.3, 125.7, 118.2, 116.9, 114.2, 88.0, 81.1, 55.5, 21.1; \(^{11}\)B NMR (128.38 MHz, CDCl\(_3\)): \(\delta\) 35.0; FT-IR (neat): 3367, 1603, 1566, 1505, 1438,
1240, 1171, 1034, 832, 820, 702 cm\(^{-1}\); HRMS (ES\(^{+}\)) m/z calcd. for C\(_{19}\)H\(_{19}\)BNO [M+H]\(^{+}\) \(288.1560\), found \(288.1553\).

References:

1) Molander, G. A.; Wisniewski, S. R.; Amani, J. *Org. Lett.* dx.doi.org/10.1021/ol502708z.

**X-ray Structure Determination of Compound 2c**

![Chemical structure of Compound 2c](image)

Compound 2c, C\(_{16}\)BH\(_{16}\)NO, crystallizes in the orthorhombic space group Pbca (systematic absences hk0: h=odd, 0kl: k=odd, and h0l: l=odd) with \(a=11.4325(8)\) Å, \(b=12.7583(8)\) Å, \(c=18.4625(11)\) Å, \(V=2692.9(3)\) Å\(^3\), \(Z=8\), and \(d_{\text{calc}}=1.229\) g/cm\(^3\). X-ray intensity data were collected on a Bruker APEXII CCD area detector employing graphite-monochromated Mo-K\(\alpha\) radiation (\(\lambda=0.71073\) Å) at a temperature of 100(1)K. Preliminary indexing was performed from a series of thirty-six 0.5° rotation frames with exposures of 10 seconds. A total of 2933 frames were collected with a crystal to detector distance of 37.6 mm, rotation widths of 0.5° and exposures of 15 seconds:

| scan type | 2\(\theta\) | \(\omega\) | \(\phi\) | \(\chi\) | frames |
|-----------|------------|----------|---------|----------|--------|
| \(\phi\)  | -13.00     | 344.60   | 342.59  | -39.24   | 739    |
| \(\omega\)| 14.50      | 282.56   | 54.11   | 21.36    | 202    |
Rotation frames were integrated using SAINT\textsuperscript{i}, producing a listing of unaveraged $F^2$ and $\sigma(F^2)$ values which were then passed to the SHELXTL\textsuperscript{ii} program package for further processing and structure solution. A total of 66539 reflections were measured over the ranges $2.21 \leq \theta \leq 25.37^\circ$, $-13 \leq h \leq 13$, $-15 \leq k \leq 15$, $-22 \leq l \leq 22$ yielding 2468 unique reflections ($R_{\text{int}} = 0.0242$). The intensity data were corrected for Lorentz and polarization effects and for absorption using SADABS\textsuperscript{iii} (minimum and maximum transmission 0.7049, 0.7452).

The structure was solved by direct methods (SHELXS-97\textsuperscript{iv}). Refinement was by full-matrix least squares based on $F^2$ using SHELXL-97.\textsuperscript{v} All reflections were used during refinement. The weighting scheme used was $w=1/[\sigma^2(F_o^2) + (0.0420P)^2 + 1.0532P]$ where $P = (F_o^2 + 2F_c^2)/3$. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model. Refinement converged to $R_1=0.0313$ and $wR_2=0.0827$ for 2236 observed reflections for which $F > 4\sigma(F)$ and $R_1=0.0346$ and $wR_2=0.0854$ and GOF =1.062 for all 2468 unique, non-zero reflections and 174 variables.\textsuperscript{vi} The maximum $\Delta/\sigma$ in the final cycle of least squares was 0.000 and the two most prominent peaks in the final difference Fourier were +0.216 and -0.171 e/Å$^3$.

Table 1. lists cell information, data collection parameters, and refinement data. Final positional and equivalent isotropic thermal parameters are given in Tables 2. and 3. Anisotropic thermal parameters are in Table 4. Tables 5. and 6. list bond distances and bond angles. Figure 1. is an ORTEP\textsuperscript{vii} representation of the molecule with 50% probability thermal ellipsoids displayed.
Figure 1. ORTEP drawing of the title compound with 50% probability thermal ellipsoids.

Table 1. Summary of Structure Determination of Compound 2c

| Property              | Value                        |
|-----------------------|------------------------------|
| Empirical formula     | C_{16}BH_{16}NO              |
| Formula weight        | 249.11                       |
| Temperature           | 100(1) K                     |
| Wavelength            | 0.71073 Å                    |
| Crystal system        | orthorhombic                 |
| Space group           | Pbca                         |
| Cell constants:       |                              |
| a                     | 11.4325(8) Å                 |
| b                     | 12.7583(8) Å                 |
| c                     | 18.4625(11) Å                |
| Volume                | 2692.9(3) Å³                 |
| Z                     | 8                            |
| Density (calculated)  | 1.229 Mg/m³                  |
Absorption coefficient 0.075 mm\(^{-1}\)

F(000) 1056

Crystal size 0.25 x 0.18 x 0.04 mm\(^3\)

Theta range for data collection 2.21 to 25.37°

Index ranges \(-13 \leq h \leq 13, -15 \leq k \leq 15, -22 \leq l \leq 22\)

Reflections collected 66539

Independent reflections 2468 \([R(int) = 0.0242]\)

Completeness to theta = 25.37° 99.9 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.7452 and 0.7049

Refinement method Full-matrix least-squares on F\(^2\)

Data / restraints / parameters 2468 / 0 / 174

Goodness-of-fit on F\(^2\) 1.062

Final R indices [I>2\(\sigma(I)\)] R1 = 0.0313, wR2 = 0.0827

R indices (all data) R1 = 0.0346, wR2 = 0.0854

Largest diff. peak and hole 0.216 and -0.171 e.Å\(^{-3}\)

Table 2. Refined Positional Parameters for Compound 2c

| Atom | x      | y      | z      | U\(_{eq}\), Å\(^2\) |
|------|--------|--------|--------|---------------------|
| C1   | 0.37297(9) | 0.78889(8) | 0.15075(6) | 0.0156(2) |
| C2   | 0.31772(9) | 0.85865(9) | 0.19848(6) | 0.0183(2) |
| C3   | 0.24832(10) | 0.93853(8) | 0.17236(6) | 0.0204(2) |
| C4   | 0.23277(10) | 0.95116(9) | 0.09753(6) | 0.0211(3) |
| C5   | 0.28668(9) | 0.88327(9) | 0.05020(6) | 0.0190(2) |
| Atom | x         | y         | z         | U_{iso}, Å² |
|------|-----------|-----------|-----------|-------------|
| C6   | 0.35784(9)| 0.80078(8)| 0.07519(6)| 0.0161(2)   |
| C7   | 0.41716(9)| 0.73048(8)| 0.02649(6)| 0.0175(2)   |
| C8   | 0.48689(9)| 0.65183(8)| 0.05007(6)| 0.0182(2)   |
| C9   | 0.56916(9)| 0.53937(9)| 0.16821(6)| 0.0194(2)   |
| C10  | 0.69673(9)| 0.53055(9)| 0.14709(6)| 0.0170(2)   |
| C11  | 0.77309(10)| 0.61368(8)| 0.15961(5)| 0.0166(2)   |
| C12  | 0.89157(10)| 0.60518(8)| 0.14245(5)| 0.0164(2)   |
| C13  | 0.93619(10)| 0.51392(9)| 0.11216(6)| 0.0205(3)   |
| C14  | 0.85953(10)| 0.43153(9)| 0.09895(6)| 0.0226(3)   |
| C15  | 0.74168(10)| 0.43933(8)| 0.11594(6)| 0.0197(2)   |
| C16  | 1.07876(10)| 0.69119(10)| 0.13608(7)| 0.0247(3)   |
| N1   | 0.44176(8) | 0.70757(7)| 0.17618(5)| 0.0167(2)   |
| O1   | 0.95800(7) | 0.69305(6)| 0.15776(4)| 0.0198(2)   |
| B1   | 0.50089(10)| 0.63407(10)| 0.13190(7)| 0.0174(3)   |

\[ U_{eq} = \frac{1}{3} \left[ U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos \gamma + 2U_{13}aa^*cc^*\cos \beta + 2U_{23}bb^*cc^*\cos \alpha \right] \]
Table 4. Refined Thermal Parameters (U’s) for Compound 2c

| Atom | U$_{11}$   | U$_{22}$   | U$_{33}$   | U$_{23}$   | U$_{13}$   | U$_{12}$   |
|------|------------|------------|------------|------------|------------|------------|
| C1   | 0.0129(5)  | 0.0158(5)  | 0.0182(5)  | 0.0006(4)  | -0.0006(4) | -0.0038(4) |
| C2   | 0.0175(5)  | 0.0210(6)  | 0.0162(5)  | -0.0016(4) | 0.0000(4)  | -0.0033(4) |
| C3   | 0.0172(5)  | 0.0192(6)  | 0.0248(6)  | -0.0044(4) | 0.0019(4)  | -0.0009(4) |
| C4   | 0.0166(5)  | 0.0189(5)  | 0.0277(6)  | 0.0024(5)  | -0.0015(5) | 0.0016(4)  |
| C5   | 0.0171(5)  | 0.0217(6)  | 0.0181(5)  | 0.0023(4)  | -0.0023(4) | -0.0027(4) |
| C6   | 0.0136(5)  | 0.0169(5)  | 0.0178(5)  | 0.0006(4)  | -0.0006(4) | -0.0042(4) |
| C7   | 0.0179(5)  | 0.0200(5)  | 0.0145(5)  | -0.0002(4) | -0.0002(4) | -0.0049(4) |
| C8   | 0.0172(5)  | 0.0176(5)  | 0.0197(5)  | -0.0027(4) | 0.0028(4)  | -0.0022(4) |
| C9   | 0.0176(6)  | 0.0192(6)  | 0.0215(6)  | 0.0024(4)  | 0.0009(4)  | -0.0010(4) |
| C10  | 0.0176(5)  | 0.0194(5)  | 0.0140(5)  | 0.0036(4)  | -0.0020(4) | 0.0012(4)  |
| C11  | 0.0200(6)  | 0.0160(5)  | 0.0140(5)  | 0.0004(4)  | 0.0000(4)  | 0.0023(4)  |
| C12  | 0.0186(5)  | 0.0181(5)  | 0.0124(5)  | 0.0025(4)  | -0.0024(4) | -0.0014(4) |
| C13  | 0.0162(5)  | 0.0236(6)  | 0.0216(6)  | 0.0003(5)  | 0.0004(4)  | 0.0028(5)  |
| C14  | 0.0241(6)  | 0.0190(6)  | 0.0247(6)  | -0.0036(5) | 0.0003(5)  | 0.0042(5)  |
| C15  | 0.0218(6)  | 0.0168(5)  | 0.0204(5)  | -0.0002(4) | -0.0030(4) | -0.0020(4) |
The form of the anisotropic displacement parameter is:
\[ \exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+2b^{*}c^{*}U_{23}kl+2a^{*}c^{*}U_{13}hl+2a^{*}b^{*}U_{12}hk)] \]

|       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|
| C16   | 0.0171(6) | 0.0273(6) | 0.0298(6) | 0.0024(5) | -0.0005(5) |
| N1    | 0.0171(5) | 0.0194(5) | 0.0135(4) | 0.0019(4) | -0.0014(3) |
| O1    | 0.0174(4) | 0.0207(4) | 0.0212(4) | -0.0016(3) | 0.0002(3) |
| B1    | 0.0125(6) | 0.0173(6) | 0.0225(6) | 0.0004(5) | -0.0039(5) |

Table 5. Bond Distances in Compound 2c, Å

| Bond           | Distance   |
|----------------|------------|
| C1-N1          | 1.3840(14) |
| C2-C3          | 1.3786(16) |
| C5-C6          | 1.4079(15) |
| C8-B1          | 1.5361(16) |
| C10-C11        | 1.3929(15) |
| C12-O1         | 1.3834(13) |
| C14-C15        | 1.3870(16) |

| Bond           | Distance   |
|----------------|------------|
| N1-C1-C2       | 121.22(10) |
| C3-C2-C1       | 120.55(10) |
| C4-C5-C6       | 121.41(10) |
| C1-C6-C7       | 119.46(10) |
| C10-C9-B1      | 114.94(9)  |
| C15-C10-C9     | 121.51(10) |
| O1-C12-C11     | 115.06(9)  |
| C15-C14-C13    | 121.24(10) |
| C12-O1-C16     | 117.19(9)  |
| C8-B1-C9       | 125.38(10) |

Table 6. Bond Angles in Compound 2c, °
Compound 2i, C$_{17}$BH$_{16}$NO$_2$, crystallizes in the monoclinic space group P2$_1$/n (systematic absences 0k0: k=odd and h0l: h+l=odd) with a=8.0214(3)Å, b=6.3023(2)Å, c=28.8463(10)Å, $\beta$=94.410(2)$^\circ$, V=1453.96(9)Å$^3$, Z=4, and $d_{calc}$=1.266 g/cm$^3$. X-ray intensity data were collected on a Bruker APEXII CCD area detector employing graphite-monochromated Mo-K$_\alpha$ radiation ($\lambda$=0.71073 Å) at a temperature of 100(1)K. Preliminary indexing was performed from a series of thirty-six 0.5° rotation frames with exposures of 10 seconds. A total of 1262 frames were collected with a crystal to detector distance of 37.9 mm, rotation widths of 0.5° and exposures of 5 seconds:

| scan type | 2$\theta$ | $\omega$ | $\phi$ | $\chi$ | frames |
|-----------|-----------|----------|--------|--------|--------|
| $\phi$    | 19.50     | 59.55    | 348.71 | -26.26` | 739    |
| $\omega$  | -10.50    | 345.67   | 80.80  | -60.33 | 122    |
| $\omega$  | -15.50    | 285.62   | 18.69  | 41.79  | 122    |
| $\phi$    | -23.00    | 328.34   | 44.17  | 79.39  | 279    |

Rotation frames were integrated using SAINT$^\text{viii}$, producing a listing of unaveraged F$^2$ and $\sigma$(F$^2$) values which were then passed to the SHELXTL$^\text{ix}$ program package for further processing and structure solution. A total of 15020 reflections were measured over the ranges $2.59 \leq \theta \leq 25.43^\circ$, -9 $\leq$ h $\leq$ 9, -7 $\leq$ k $\leq$ 7, -34 $\leq$ l $\leq$ 34 yielding 2678 unique reflections (R$_{int}$ = 0.0188). The intensity data were corrected for Lorentz and polarization effects and for absorption using SADABS$^x$ (minimum and maximum transmission 0.6886, 0.7452).
The structure was solved by direct methods (SHELXS-97\textsuperscript{iii}). Refinement was by full-matrix least squares based on $F^2$ using SHELXL-97.\textsuperscript{xii} All reflections were used during refinement. The weighting scheme used was $w=1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.4985P]$ where $P = (F_o^2 + 2F_c^2)/3$. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model. Refinement converged to $R1=0.0338$ and $wR2=0.0861$ for 2339 observed reflections for which $F > 4\sigma(F)$ and $R1=0.0393$ and $wR2=0.0904$ and GOF =1.043 for all 2678 unique, non-zero reflections and 192 variables.\textsuperscript{xiii} The maximum $\Delta/\sigma$ in the final cycle of least squares was 0.000 and the two most prominent peaks in the final difference Fourier were +0.191 and -0.197 e/Å$^3$.

Table 1. lists cell information, data collection parameters, and refinement data. Final positional and equivalent isotropic thermal parameters are given in Tables 2. and 3. Anisotropic thermal parameters are in Table 4. Tables 5. and 6. list bond distances and bond angles. Figure 1. is an ORTEP\textsuperscript{xiv} representation of the molecule with 50% probability thermal ellipsoids displayed.

![Figure 1. ORTEP drawing of the title compound with 50% probability thermal ellipsoids.](image-url)
Table 1. Summary of Structure Determination of Compound 2i

| Property                        | Value                                           |
|---------------------------------|-------------------------------------------------|
| Empirical formula               | C_{17}BH_{16}NO_{2}                              |
| Formula weight                  | 277.12                                          |
| Temperature                     | 100(1) K                                        |
| Wavelength                      | 0.71073 Å                                       |
| Crystal system                  | monoclinic                                      |
| Space group                     | P2_1/n                                          |
| Cell constants:                 |                                                 |
| \(a\)                           | 8.0214(3) Å                                     |
| \(b\)                           | 6.3023(2) Å                                     |
| \(c\)                           | 28.8463(10) Å                                   |
| \(\beta\)                       | 94.410(2)^\circ                                 |
| Volume                          | 1453.96(9) Å                                    |
| \(Z\)                           | 4                                               |
| Density (calculated)            | 1.266 Mg/m^3                                    |
| Absorption coefficient          | 0.082 mm^{-1}                                   |
| \(F(000)\)                      | 584                                             |
| Crystal size                    | 0.48 x 0.18 x 0.08 mm^3                         |
| Theta range for data collection | 2.59 to 25.43°                                  |
| Index ranges                    | -9 \(\leq\) h \leq 9, -7 \(\leq\) k \leq 7, -34 \(\leq\) l \leq 34 |
| Reflections collected           | 15020                                           |
| Independent reflections         | 2678 [R(int) = 0.0188]                           |
Completeness to theta = 25.43° 99.7 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7452 and 0.6886
Refinement method Full-matrix least-squares on F²
Data / restraints / parameters 2678 / 0 / 192
Goodness-of-fit on F² 1.043
Final R indices [I>2sigma(I)] R1 = 0.0338, wR2 = 0.0861
R indices (all data) R1 = 0.0393, wR2 = 0.0904
Largest diff. peak and hole 0.191 and -0.197 e.Å⁻³

| Atom | x      | y      | z      | Uₑₚ, Å² |
|------|--------|--------|--------|---------|
| C1   | 0.31914(14) | 0.16201(19) | 0.16220(4) | 0.0215(3) |
| C2   | 0.15698(14) | 0.1718(2) | 0.14056(4) | 0.0266(3) |
| C3   | 0.03719(16) | 0.0321(2) | 0.15313(5) | 0.0329(3) |
| C4   | 0.07437(17) | -0.1195(2) | 0.18742(5) | 0.0364(3) |
| C5   | 0.23212(17) | -0.1297(2) | 0.20914(4) | 0.0326(3) |
| C6   | 0.35821(15) | 0.01087(19) | 0.19733(4) | 0.0243(3) |
| C7   | 0.52255(15) | 0.0061(2) | 0.22070(4) | 0.0265(3) |
| C8   | 0.64353(14) | 0.1422(2) | 0.21014(4) | 0.0254(3) |
| C9   | 0.73650(14) | 0.4791(2) | 0.15759(4) | 0.0243(3) |
| C10  | 0.70459(13) | 0.58181(19) | 0.11067(4) | 0.0222(3) |
| C11  | 0.74402(13) | 0.47732(19) | 0.07036(4) | 0.0221(3) |
| C12  | 0.71506(14) | 0.5733(2) | 0.02699(4) | 0.0245(3) |
| C13  | 0.64759(15) | 0.7765(2) | 0.02373(5) | 0.0304(3) |
\[ U_{eq} = \frac{1}{3} (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos \gamma + 2U_{13}aa^*cc^*\cos \beta + 2U_{23}bb^*cc^*\cos \alpha) \]

Table 3. Positional Parameters for Hydrogens in Compound 2l

| Atom | x     | y     | z     | Uiso, Å² |
|------|-------|-------|-------|----------|
| H2   | 0.1305| 0.2729| 0.1177| 0.035    |
| H3   | -0.0702| 0.0388| 0.1385| 0.044    |
| H4   | -0.0077| -0.2137| 0.1956| 0.048    |
| H5   | 0.2562| -0.2313| 0.2321| 0.043    |
| H7   | 0.5464| -0.0943| 0.2439| 0.035    |
| H8   | 0.7488| 0.1361| 0.2260| 0.034    |
| H9a  | 0.7416| 0.5902| 0.1809| 0.032    |
| H9b  | 0.8459| 0.4128| 0.1588| 0.032    |
| H11  | 0.7902| 0.3420| 0.0724| 0.029    |
| H13  | 0.6294| 0.8420| -0.0051| 0.040    |
| H14  | 0.5627| 1.0164| 0.0614| 0.043    |
| H15  | 0.6051| 0.8537| 0.1328| 0.037    |
| H17a | 0.7681| 0.1465| -0.0707| 0.058    |
| H17b | 0.9160| 0.0306| -0.0424| 0.058    |
| H17c | 0.9474| 0.2469| -0.0671| 0.058    |
| Atom | $U_{11}$  | $U_{22}$  | $U_{33}$  | $U_{23}$  | $U_{13}$  | $U_{12}$  |
|------|----------|----------|----------|----------|----------|----------|
| C1   | 0.0233(6)| 0.0231(6)| 0.0187(6)| -0.0040(5)| 0.0062(4)| -0.0027(5)|
| C2   | 0.0236(6)| 0.0315(7)| 0.0250(6)| -0.0009(5)| 0.0038(5)| -0.0030(5)|
| C3   | 0.0241(6)| 0.0416(8)| 0.0334(7)| -0.0052(6)| 0.0054(5)| -0.0080(6)|
| C4   | 0.0347(7)| 0.0377(8)| 0.0380(8)| -0.0023(6)| 0.0117(6)| -0.0171(6)|
| C5   | 0.0414(7)| 0.0289(7)| 0.0284(7)| 0.0022(5)  | 0.0088(5)| -0.0082(6)|
| C6   | 0.0297(6)| 0.0237(6)| 0.0203(6)| -0.0018(5)| 0.0075(5)| -0.0028(5)|
| C7   | 0.0344(7)| 0.0265(6)| 0.0187(6)| 0.0029(5)  | 0.0033(5)| 0.0019(5)  |
| C8   | 0.0248(6)| 0.0326(7)| 0.0186(6)| -0.0014(5)| -0.0007(4)| 0.0001(5)  |
| C9   | 0.0228(6)| 0.0302(7)| 0.0195(6)| -0.0021(5)| -0.0008(4)| -0.0045(5)|
| C10  | 0.0165(5)| 0.0258(6)| 0.0241(6)| 0.0003(5)  | -0.0004(4)| -0.0085(5)|
| C11  | 0.0191(5)| 0.0235(6)| 0.0233(6)| 0.0024(5)  | -0.0008(4)| -0.0051(4)|
| C12  | 0.0199(5)| 0.0297(7)| 0.0234(6)| 0.0051(5)  | -0.0013(4)| -0.0084(5)|
| C13  | 0.0263(6)| 0.0318(7)| 0.0318(7)| 0.0124(6)  | -0.0067(5)| -0.0072(5)|
| C14  | 0.0273(6)| 0.0244(7)| 0.0439(8)| 0.0033(6)  | -0.0054(5)| -0.0017(5)|
| C15  | 0.0230(6)| 0.0279(7)| 0.0331(7)| -0.0042(5)| -0.0002(5)| -0.0050(5)|
| C16  | 0.0224(6)| 0.0375(7)| 0.0235(6)| 0.0056(5)  | -0.0004(5)| -0.0103(5)|
| C17  | 0.0372(7)| 0.0538(9)| 0.0255(7)| -0.0093(6)| 0.0069(5)| -0.0056(7)|
| N1   | 0.0224(5)| 0.0227(5)| 0.0179(5)| 0.0022(4)  | 0.0028(4)| -0.0026(4)|
| O1   | 0.0381(5)| 0.0560(7)| 0.0202(5)| 0.0099(4)  | -0.0021(4)| -0.0099(5)|
| O2   | 0.0371(5)| 0.0415(6)| 0.0209(4)| -0.0020(4)| 0.0039(4)| -0.0012(4)|
| B1   | 0.0235(6)| 0.0263(7)| 0.0166(6)| -0.0050(5)| 0.0031(5)| -0.0012(5)|

The form of the anisotropic displacement parameter is:

$$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+2b^{*}c^{*}U_{23}kl+2a^{*}c^{*}U_{13}hl+2a^{*}b^{*}U_{12}hk)]$$
Table 5. Bond Distances in Compound 2i, Å

| Bond          | Distance (Å) |
|---------------|--------------|
| C1-N1         | 1.3847(14)   |
| C1-C2         | 1.4002(16)   |
| C1-C6         | 1.4084(17)   |
| C2-C3         | 1.3727(18)   |
| C3-C4         | 1.391(2)     |
| C4-C5         | 1.3478(17)   |
| C5-C6         | 1.4084(17)   |
| C2-C3         | 1.3727(18)   |
| C3-C4         | 1.391(2)     |
| C4-C5         | 1.3697(19)   |
| C5-C6         | 1.4061(17)   |
| C6-C7         | 1.4339(17)   |
| C7-C8         | 1.3478(17)   |
| C8-B1         | 1.5284(18)   |
| C9-C10        | 1.5043(16)   |
| C10-C15       | 1.3886(18)   |
| C10-C11       | 1.3938(17)   |
| C11-C12       | 1.3933(16)   |
| C12-C13       | 1.3906(18)   |
| C12-C16       | 1.4843(18)   |
| C14-C15       | 1.3832(18)   |
| C15-C10       | 1.2100(15)   |
| C16-O1        | 1.4128(16)   |
| C16-O2        | 1.3363(16)   |
| C17-O2        | 1.4473(16)   |
| N1-B1         | 1.4128(16)   |

Table 6. Bond Angles in Compound 2i, °

| Bond Angle         | Angle (°) |
|--------------------|-----------|
| N1-C1-C2           | 121.10(11)|
| N1-C1-C6           | 119.01(10)|
| C2-C1-C6           | 119.89(11)|
| C3-C2-C1           | 119.94(12)|
| C2-C3-C4           | 120.83(12)|
| C5-C4-C3           | 119.84(12)|
| C4-C5-C6           | 121.07(12)|
| C6-C7              | 118.43(11)|
| C5-C6-C7           | 121.68(11)|
| C1-C6-C7           | 119.88(11)|
| C8-C7-C6           | 122.16(11)|
| C7-C8-B1           | 119.43(11)|
| C10-C9-B1          | 117.30(9) |
| C15-C10-C11        | 118.18(11)|
| C15-C10-C9         | 120.93(11)|
| C11-C10-C9         | 120.89(11)|
| C12-C11-C10        | 120.74(11)|
| C13-C12-C11        | 119.85(12)|
| C13-C12-C16        | 117.85(11)|
| C11-C12-C16        | 122.30(12)|
| C14-C13-C12        | 119.70(12)|
| C13-C14-C15        | 120.15(12)|
| C14-C15-C10        | 121.35(12)|
| O1-C16-O2          | 123.17(12)|
| O2-C16-C12         | 112.90(10)|
| C16-O2-C17         | 115.23(10)|
| N1-B1-C8           | 115.23(10)|
| N1-B1-C9           | 120.92(11)|
| C8-B1-C9           | 123.84(10)|
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(Benzyl)-2,1-borazaronaphthalene (2a)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(Benzyl)-2,1-borazonaphthalene (2a)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(Benzyl)-2,1-borazaronaphthalene (2a)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(4-Methylbenzyl)-2,1-borazaronaphthalene (2b)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(4-Methylbenzyl)-2,1-borazaronaphthalene (2b)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(4-Methylbenzyl)-2,1-borazaronaphthalene (2b)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-Methoxybenzyl)-2,1-borazonaphthalene (2c)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-Methoxybenzyl)-2,1-borazonaphthalene (2c)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-Methoxybenzyl)-2,1-borazonaphthalene (2c)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(4-Methoxybenzyl)-2,1-borazonaphthalene (2d)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(4-Methoxybenzyl)-2,1-borazonaphthalene (2d)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(4-Methoxybenzyl)-2,1-borazonaphthalene (2d)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(1-Naphthylmethyl)-2,1-borazonaphthalene (2e)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(1-Naphthylmethyl)-2,1-borazonaphthalene (2e)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(1-Naphthylmethyl)-2,1-borazonaphthalene (2e)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-Methoxy-5-methylbenzyl)-2,1-borazonaphthalene (2f)
13C NMR (125.8 MHz, CDCl3) Spectrum of 2-(3-Methoxy-5-methylbenzyl)-2,1-borazonaphthalene (2f)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-Methoxy-5-methylbenzyl)-2,1-borazonaphthalene (2f)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-Vinylbenzyl)-2,1-borazonaphthalene (2g)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-Vinylbenzyl)-2,1-borazonaphthalene (2g)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-Vinylbenzyl)-2,1-borazaronaphthalene (2g)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(2,3-Dihydro-1,4-benzodioxin-6-ylmethyl)-2,1-borazonaphthalene (2h)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(2,3-Dihydro-1,4-benzodioxin-6-ylmethyl)-2,1-borazaronaphthalene (2h)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(2,3-Dihydro-1,4-benzodioxin-6-ylmethyl)-2,1-borazonaphthalene (2h)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of Methyl-3-(2-[1,2-borazaronaphthyl]methyl)benzoate (2i)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of Methyl-3-(2-[2,1-borazaronaphthyl]methyl)benzoate (2i)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of Methyl-3-[(2-[1,2-borazaronaphthyl]methyl)benzoate (2i)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-fluorobenzyl)-2,1-borazonaphthalene (2j)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-fluorobenzyl)-2,1-borazaronaphthalene (2j)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-fluorobenzyl)-2,1-borazonaphthalene (2j)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(2,4-Difluorobenzyl)-2,1-borazonaphthalene (2k)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(2,4-Difluorobenzyl)-2,1-borazaronaphthalene (2k)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(2,4-Difluorobenzyl)-2,1-borazonaphthalene (2k)
$^{1}$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(4-Chlorobenzyl)-2,1-borazonaphthalene (2l)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(4-Chlorobenzyl)-2,1-borazonaphthalene (2l)
$^{11}\text{B NMR (128.38 MHz, CDCl}_3\text{) Spectrum of 2-}(4\text{-Chlorobenzyl})\text{-2,1-borazonaphthalene (2l)}$
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of N-Benzyl-2-(4-methylbenzyl)-2,1-borazonaphthalene (2m)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of N-Benzyl-2-(4-methylbenzyl)-2,1-borazonaphthalene (2m)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of N-Benzyl-2-(4-methylbenzyl)-2,1-borazonaphthalene (2m)
$^1\text{H NMR (500 MHz, CDCl}_3\text{) Spectrum of 2-(3-Methylbenzyl)-6-methyl-2,1-borazaronaphthalene (2n)}$
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-Methylbenzyl)-6-methyl-2,1-borazonaphthalene (2n)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-Methylbenzyl)-6-methyl-2,1-borazonaphthalene (2n)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 5-[(2,1-Borazaronaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (3a)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 5-[(2,1-Borazaronaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (3a)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 5-[(2,1-Borazaronaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (3a)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(5-Methylfuran-2-yl)methyl-2,1-borazaronaphthalene (3b)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(5-Methylfuran-2-yl)methyl-2,1-borazaronaphthalene (3b)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(5-Methylfuran-2-yl)methyl-2,1-borazonaphthalene (3b)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(2-Thiophenylmethyl)-2,1-borazaronaphthalene (3c)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(2-Thiophenylmethyl)-2,1-borazonaphthalene (3c)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(2-Thiophenylmethyl)-2,1-borazonaphthalene (3c)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-Thiophenethyl)-2,1-borazonaphthalene (3d)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-Thiophenylmethyl)-2,1-borazonaphthalene (3d)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-Thiophenylmethyl)-2,1-borazaronaphthalene (3d)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 4-[(2,1-Borazaronaphthyl)methyl]-3,5-dimethylisoxazole (3e)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 4-[(2,1-Borazaronaphthyl)methyl]-3,5-dimethylisoxazole (3e)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 4-[(2,1-Borazonaphthyl)methyl]-3,5-dimethylisoxazole (3e)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of $N$-Benzyl-2-(5-methylfuran-2-yl)methyl-2,1-borazonaphthalene (3f)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of $N$-Benzyl-2-(5-methylfuran-2-yl)methyl-2,1-borazaronaphthalene (3f)
$^{11}\!\!\!\!\!\!\text{B NMR (128.38 MHz, CDCl}_3\text{) Spectrum of N-Benzyl-2-\!(5-methylfuran-2-yl)methyl-2,1-borazonaphthalene (3f)}}$
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 5-[(N-Benzyl-2,1-borazonaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (3g)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 5-[(N-Benzyl-2,1-borazaronaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (3g)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 5-[(N-Benzyl-2,1-borazonaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (3g)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(5-Methylfuran-2-yl)methyl-6-methyl-2,1-borazonaphthalene (3h)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(5-Methylfuran-2-yl)methyl-6-methyl-2,1-borazaronaphthalene (3h)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(5-Methylfuran-2-yl)methyl-6-methyl-2,1-borazonaphthalene (3h)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-[(E)-2-Butenyl]-2,1-borazonaphthalene (4a)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-[(E)-2-Butenyl]-2,1-borazaronaphthalene (4a)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-[(E)-2-Butenyl]-2,1-borazonaphthalene (4a)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-[(Z)-2-Butenyl]-2,1-borazonaphthalene (4b)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-[(Z)-2-Butenyl]-2,1-borazonaphthalene (4b)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-[(Z)-2-Butenyl]-2,1-borazonaphthalene (4b)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(2-Methylallyl)-2,1-borazonaphthalene (4c)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(2-Methylallyl)-2,1-borazonaphthalene (4c)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(2-Methylallyl)-2,1-borazaronaphthalene (4c)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-[(E)-Undec-2-enyl]-2,1-borazonaphthalene (4d)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-[(E)-Undec-2-enyl]-2,1-borazonaphthalene (4d)
$^{11}\text{B} \text{ NMR (128.38 MHz, CDCl}_3\text{)}$ Spectrum of 2-[(E)-Undec-2-enyl]-2,1-borazonaphthalene (4d)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-Cyclohexenylmethyl-2,1-borazonaphthalene (4e)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-Cyclohexenylmethyl-2,1-borazaronaphthalene (4e)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-Cyclohexenylmethyl-2,1-borazonaphthalene (4e)
$^1$H NMR (500 MHz, CDCl₃) Spectrum of (2,1-Borazaronaphthy)methyl-1,4-dioxa$spiro[4.5]$dec-7-ene (4f)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of (2,1-Borazaronaphthyl)methyl-1,4-dioxaspiro[4.5]dec-7-ene (4f)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of (2,1-Borazonaphthyl)methyl-1,4-dioxaspiro[4.5]dec-7-ene (4f)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(4,4-Difluorocyclohex-1-enyl)methyl-2,1-borazaronaphthalene (4g)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(4,4-Difluorocyclohex-1-enyl)methyl-2,1-borazonaphthalene (4g)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(4,4-Difluorocyclohex-1-enyl)methyl-2,1-borazaronaphthalene (4g)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3,6-Dihydro-2H-pyran-4-yl)methyl-2,1-borazonaphthalene (4h)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3,6-Dihydro-2H-pyran-4-yl)methyl-2,1-borazonaphthalene (4h)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3,6-Dihydro-2H-pyran-4-yl)methyl-2,1-borazaronaphthalene (4h)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 4-(2,1-Borazaronaphthyl)methyl-1-(tert-butoxycarbonyl)-1,2,3,6-tetrahydropyridine (4i)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 4-(2,1-Borazaronaphthyl)methyl-1-(tert-butoxycarbonyl)-1,2,3,6-tetrahydropyridine (4i)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 4-(2,1-Borazaronaphthyl)methyl-1-(tert-butoxycarbonyl)-1,2,3,6-tetrahydropyridine (4i)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of N-Benzyl-4-(2,1-borazaronaphthyl)methyl-1-(tert-butoxycarbonyl)-1,2,3,6-tetrahydropyridine (4j)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of $N$-Benzyl-4-(2,1-borazonaphthyl)methyl-1-(tert-butoxycarbonyl)-1,2,3,6-tetrahydropyridine (4j)
\[^{11}\text{B} \text{NMR (128.38 MHz, CDCl}_3\text{)} \text{ Spectrum of N-Benzyl-4-(2,1-borazonaphthyl)methyl-1-(tert-butoxycarbonyl)-1,2,3,6-tetrahydropyridine (4j)}\]
\(^1\)H NMR (500 MHz, CDCl\textsubscript{3}) Spectrum of N-Benzyl-8-(2,1-borazonaphthyl)methyl-1,4-dioxaspiro[4.5]dec-7-ene (4k)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of N-Benzyl-8-(2,1-borazaronaphthyl)methyl-1,4-dioxa[4.5]dec-7-ene (4k)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of N-Benzyl-8-(2,1-borazonaphthyl)methyl-1,4-dioxaspiro[4.5]dec-7-ene (4k)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 5-[(6-methyl-2,1-borazaronaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (4l)
$^{13}$C NMR (125.8 MHz, CDCl₃) Spectrum of 5-[(6-methyl-2,1-borazaronaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (4l)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 5-[(6-methyl-2,1-borazonaphthyl)methyl]-N-(tert-butoxycarbonyl)indole (4l)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-Phenylprop-2-ynyl)-2,1-borazaronaphthalene (5a)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-Phenylprop-2-ynyl)-2,1-borazonaphthalene (5a)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-Phenylprop-2-ynyl)-2,1-borazonaphthalene (5a)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-$p$-Tolylprop-2-ynyl)-2,1-borazaronaphthalene (5b)
${^13}\text{C NMR (125.8 MHz, CDCl}_3\text{) Spectrum of 2-(3-p-Tolyprop-2-ynyl)-2,1-borazonaphthalene (5b)}}$
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-p-Tolylprop-2-ynyl)-2,1-borazonaphthalene (5b)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-[4-Methoxyphenylprop-2-ynyl])-2,1-borazonaphthalene (5c)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-[4-Methoxyphenylprop-2-ynyl])-2,1-borazonaphthalene (5c)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-[4-Methoxyphenylprop-2-ynyl])-2,1-borazonaphthalene (5c)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-[4-Tolylprop-2-ynyl])-2,1-borazaronaphthalene (5d)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-[4-Tolylprop-2-ynyl])-2,1-borazonaphthalene (5d)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-[4-Tolylprop-2-ynyl])-2,1-borazonaphthalene (5d)
\(^1\)H NMR (500 MHz, CDCl\(_3\)) Spectrum of 2-(3-Cyclohexenylprop-2-ynyl)-2,1-borazonaphthalene (5e)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-Cyclohexenylprop-2-ynyl)-2,1-borazonaphthalene (5e)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-Cyclohexenylprop-2-ynyl)-2,1-borazonaphthalene (5e)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-Cyclopropylprop-2-ynyl)-2,1-borazonaphthalene (5f)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-Cyclopropylprop-2-ynyl)-2,1-borazonaphthalene (5f)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-Cyclopropylprop-2-ynyl)-2,1-borazaronaphthalene (5f)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of N-Benzyl-2-(3-[4-methoxyphenylprop-2-ynyl])-2,1-borazaronaphthalene (5g)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of N-Benzyl-2-(3-[4-methoxyphenylprop-2-ynyl])-2,1-borazonaphthalene (5g)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of $N$-Benzyl-2-(3-[4-methoxyphenylprop-2-ynyl])-2,1-borazonaphthalene (5g)
$^1$H NMR (500 MHz, CDCl$_3$) Spectrum of 2-(3-[4-Methoxyphenylprop-2-ynyl])-6-methyl-2,1-borazaronaphthalene (5h)
$^{13}$C NMR (125.8 MHz, CDCl$_3$) Spectrum of 2-(3-[4-Methoxyphenylprop-2-ynyl])-6-methyl-2,1-borazaronaphthalene (5h)
$^{11}$B NMR (128.38 MHz, CDCl$_3$) Spectrum of 2-(3-[4-Methoxyphenylprop-2-ynyl])-6-methyl-2,1-borazonaphthalene (5h)
\[
R1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|}
\]

\[
wR2 = \left( \frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right)^{1/2}
\]

\[
GOF = \left( \frac{\sum w(F_o^2 - F_c^2)^2/(n - p)}{\sum w(F_o^2)^2} \right)^{1/2}
\]

where \( n \) = the number of reflections and \( p \) = the number of parameters refined.
Sheldrick, G.M. (2007) SADABS. University of Gottingen, Germany.

Sheldrick, G.M. (2008) Acta Cryst. A64,112-122.

\[ R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|} \]

\[ wR^2 = \left( \frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right)^{1/2} \]

\[ GOF = \left[ \frac{\sum w(F_o^2 - F_c^2)^2}{(n - p)} \right]^{1/2} \]

where \( n \) = the number of reflections and \( p \) = the number of parameters refined.

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