Electronic Supplementary Material (ESI) for RSC Advances.

Diels-Alder Reactions of Pinacol Alkenylboronates: An experimental and theoretical study

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Supporting Information

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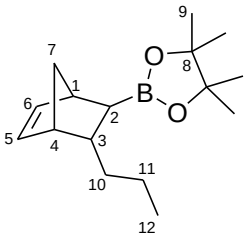
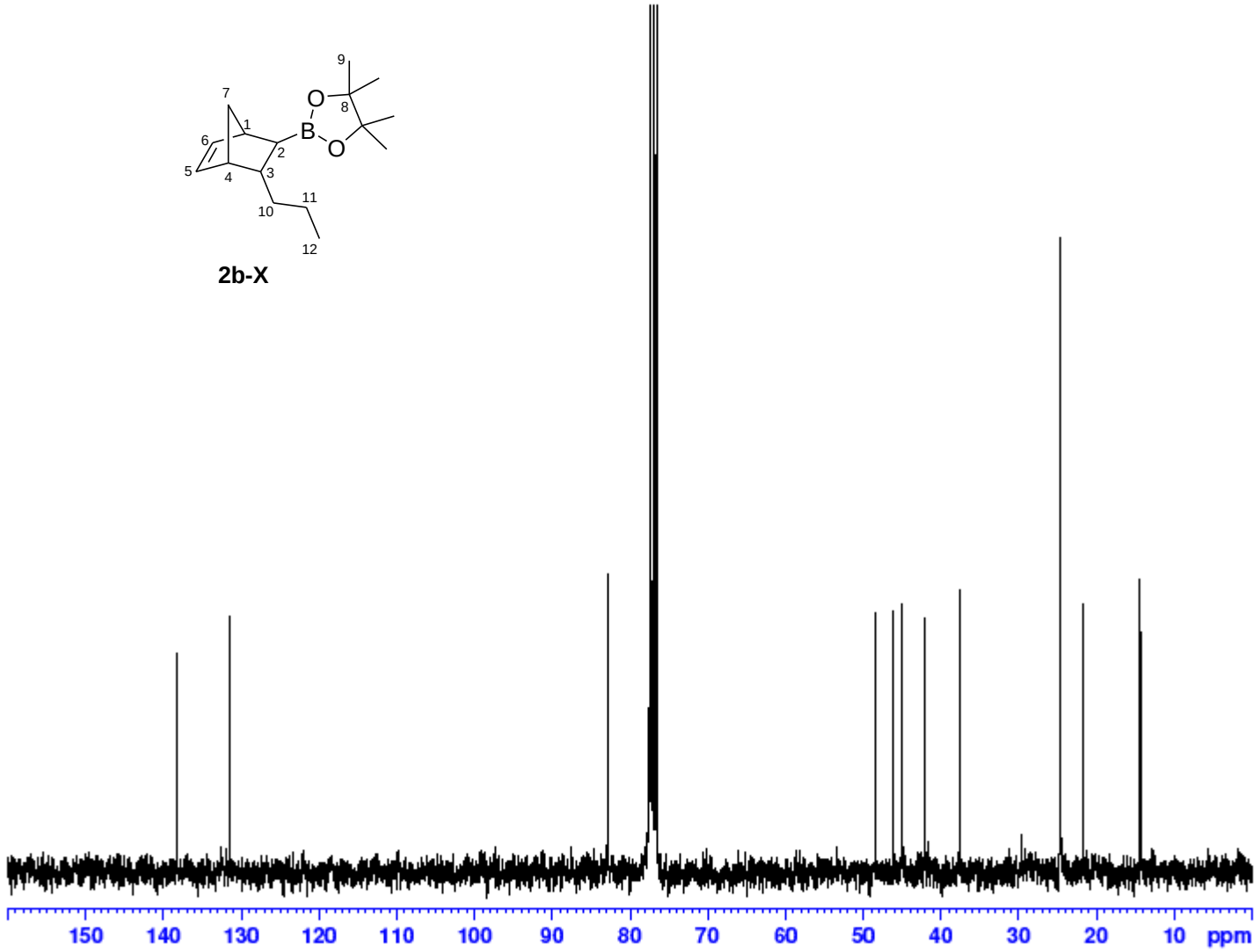


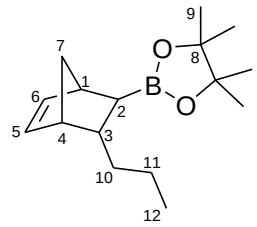
2b-X

^{1}H NMR spectra of **2b-X** at 300 MHz in $CDCl_3$

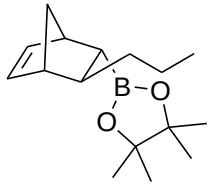


2b-X

^{13}C NMR spectra of **2b-X** at 75 MHz in $CDCl_3$

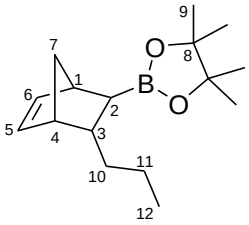


2b-X



2b-N

^{1}H NMR spectra of **2b-X**and **2b-N** at 300 MHz in $CDCl_3$



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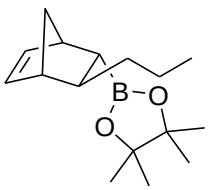

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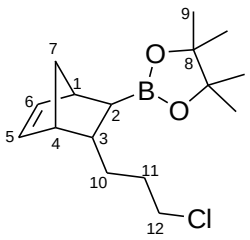
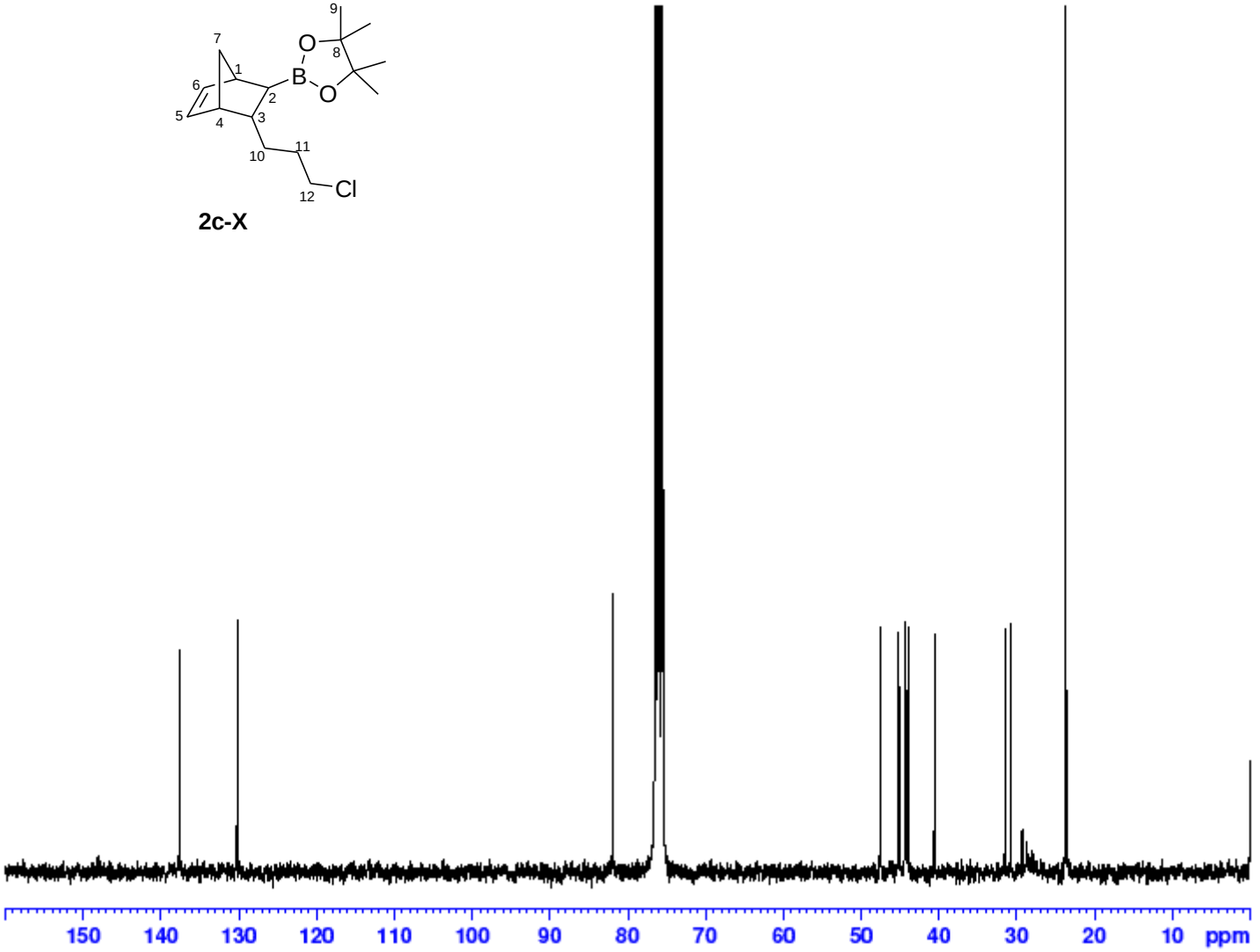


2c-X

^{1}H NMR spectra of **2c-X** at 300 MHz in $CDCl_3$



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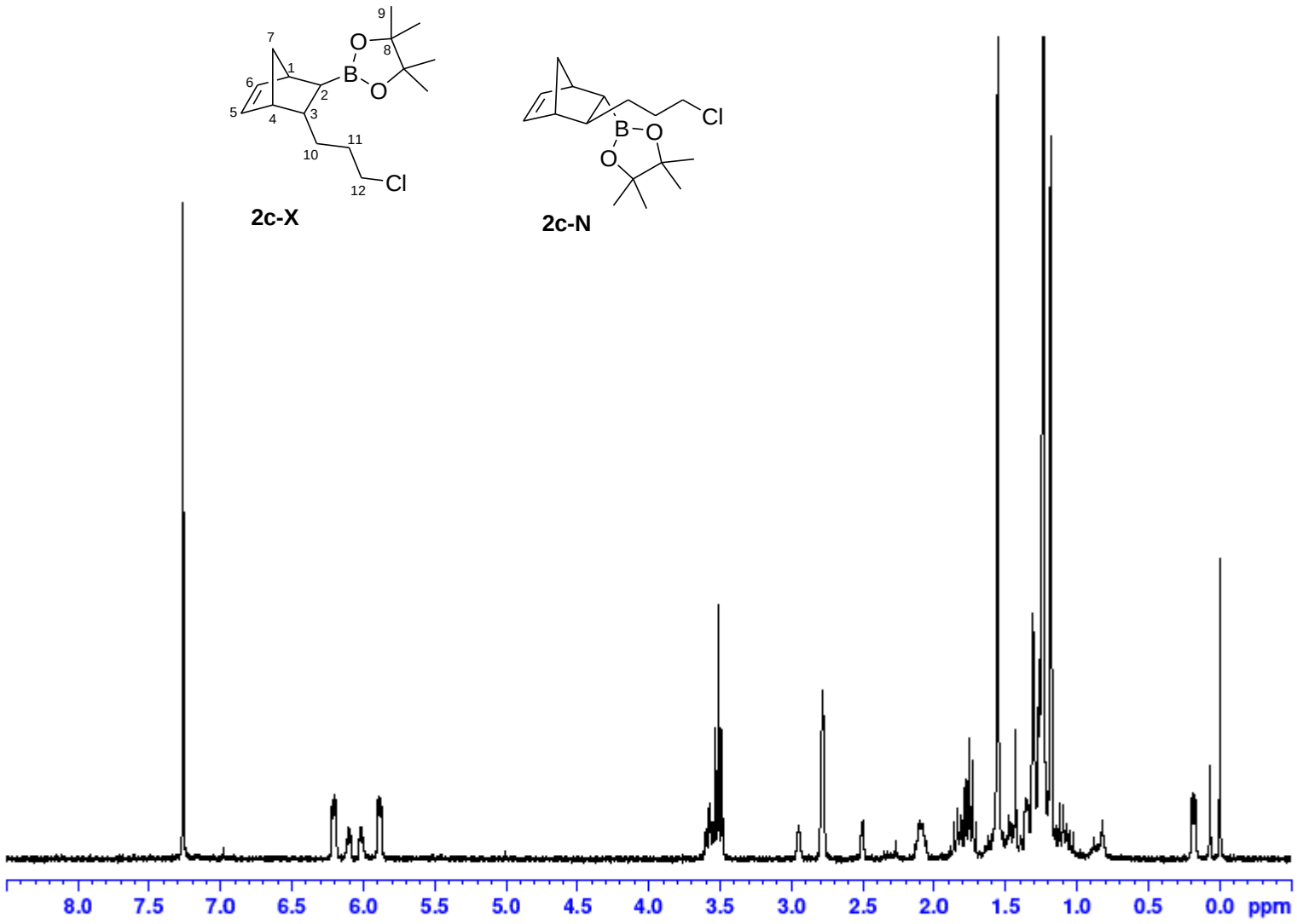

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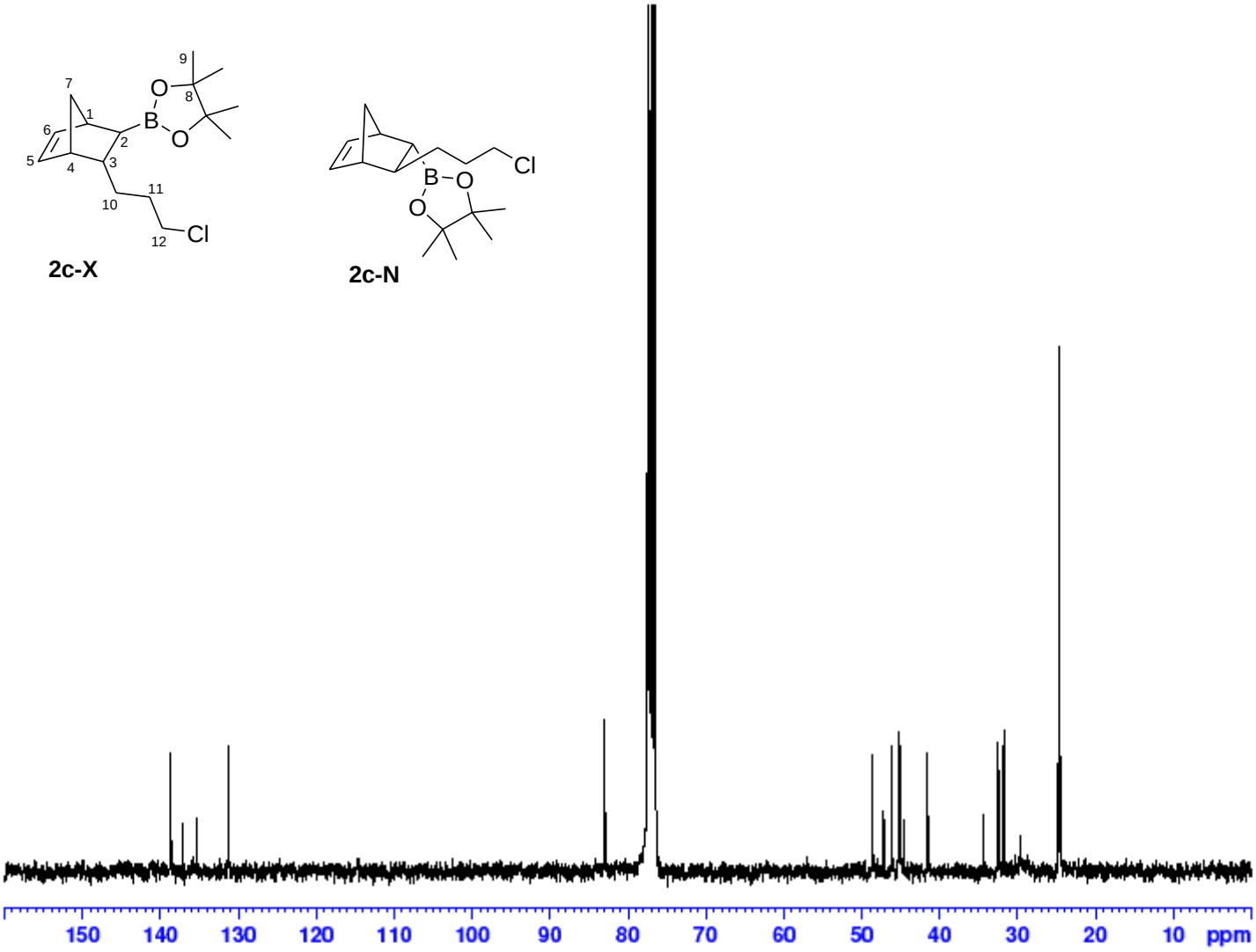

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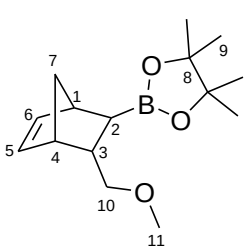
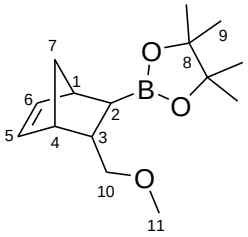


2d-X

^{1}H NMR spectra of **2d-X** at 300 MHz in $CDCl_3$



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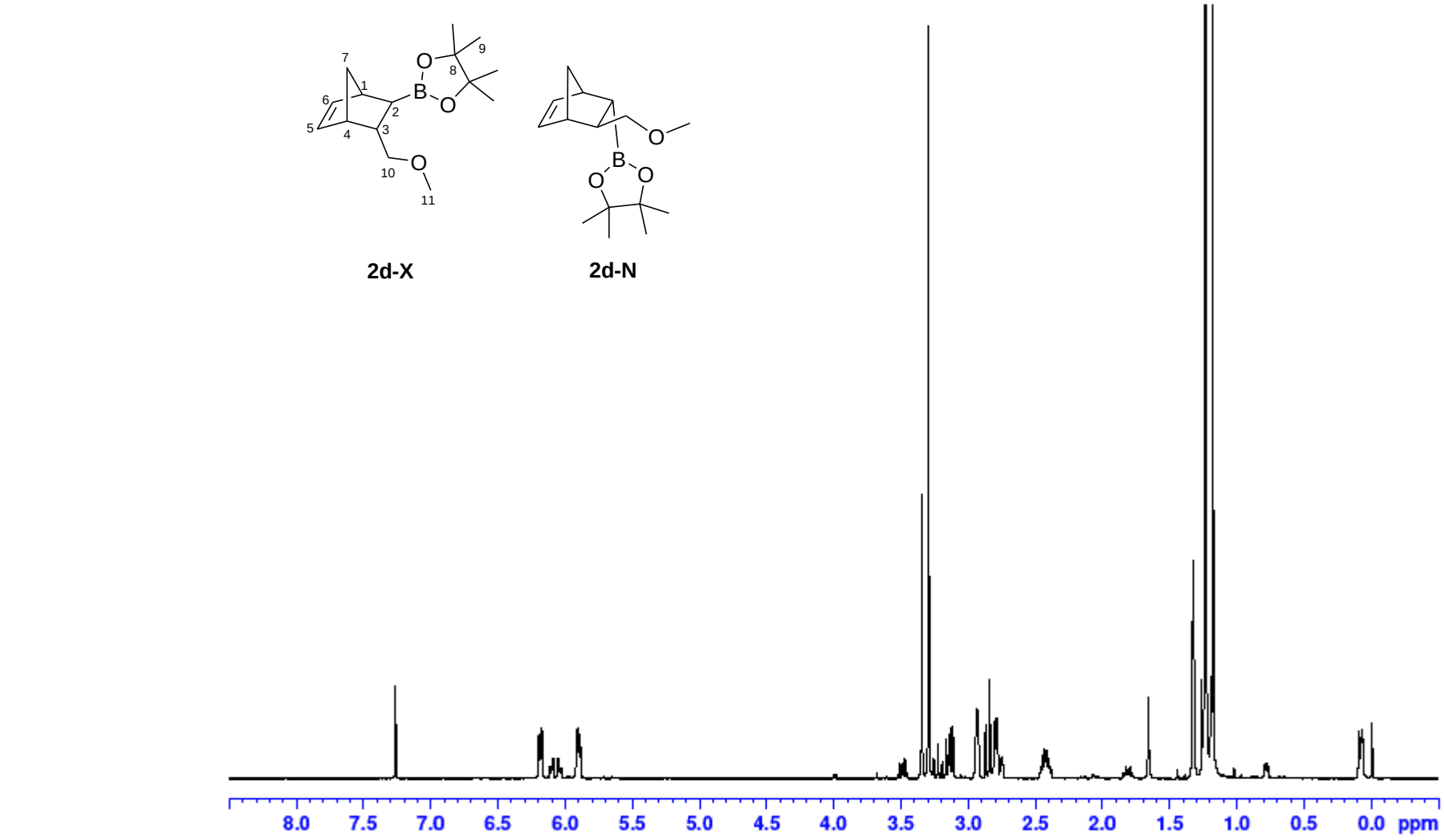

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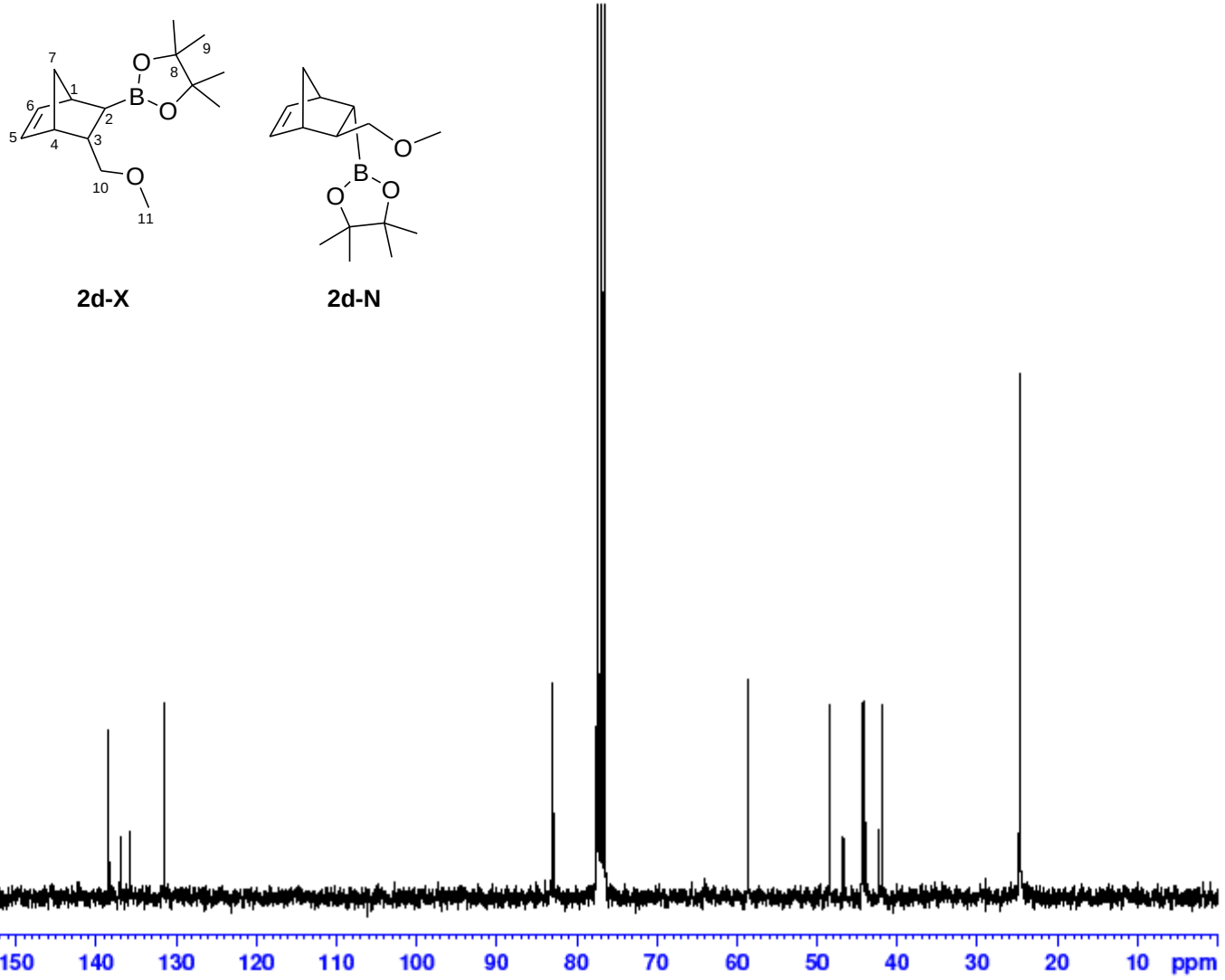

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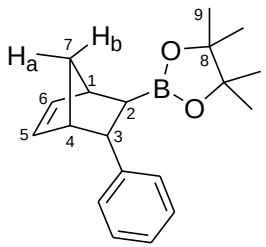
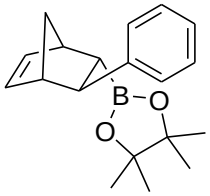


2e-X



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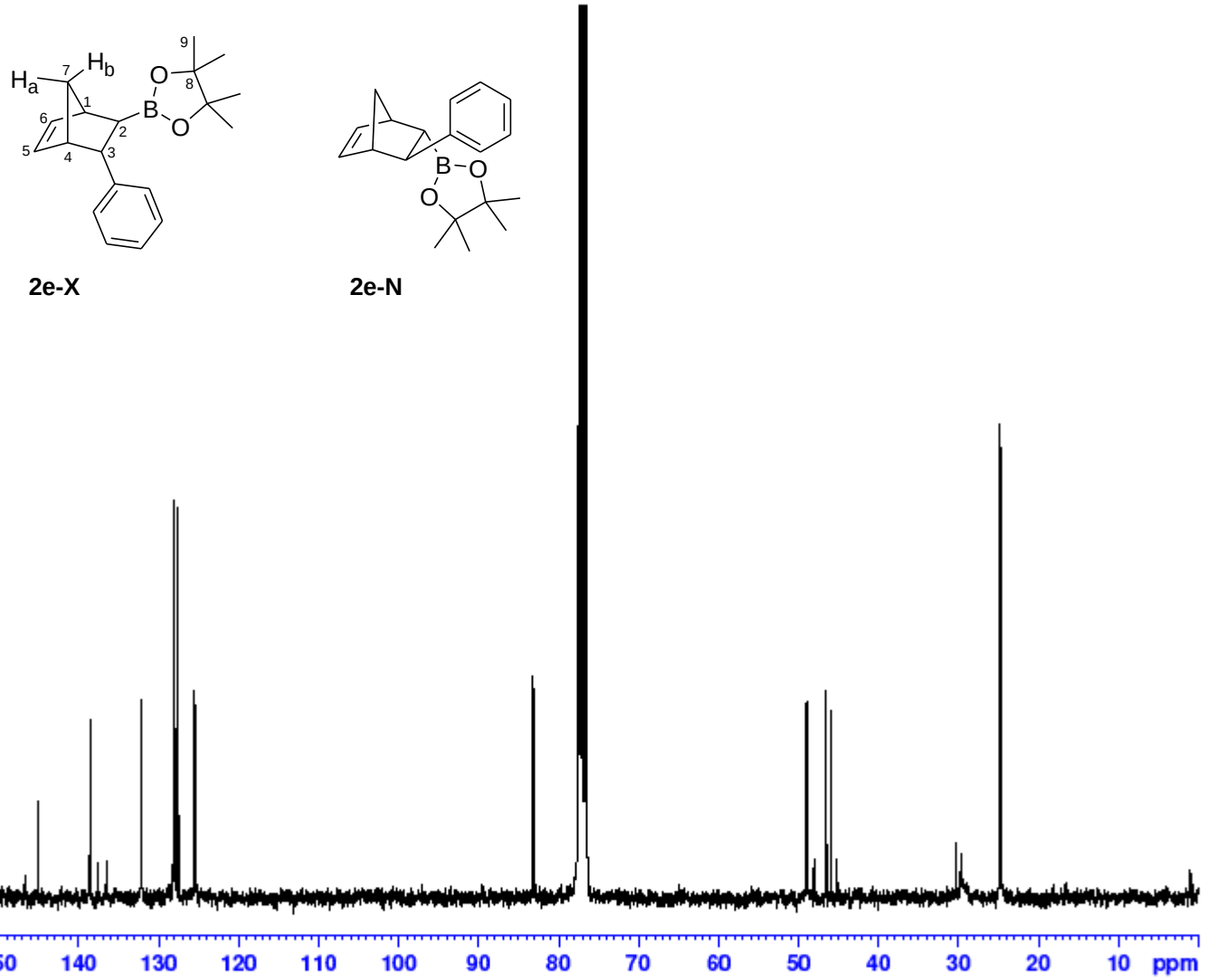

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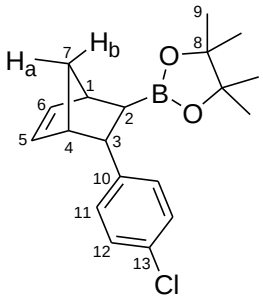

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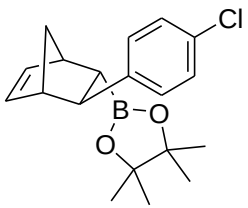

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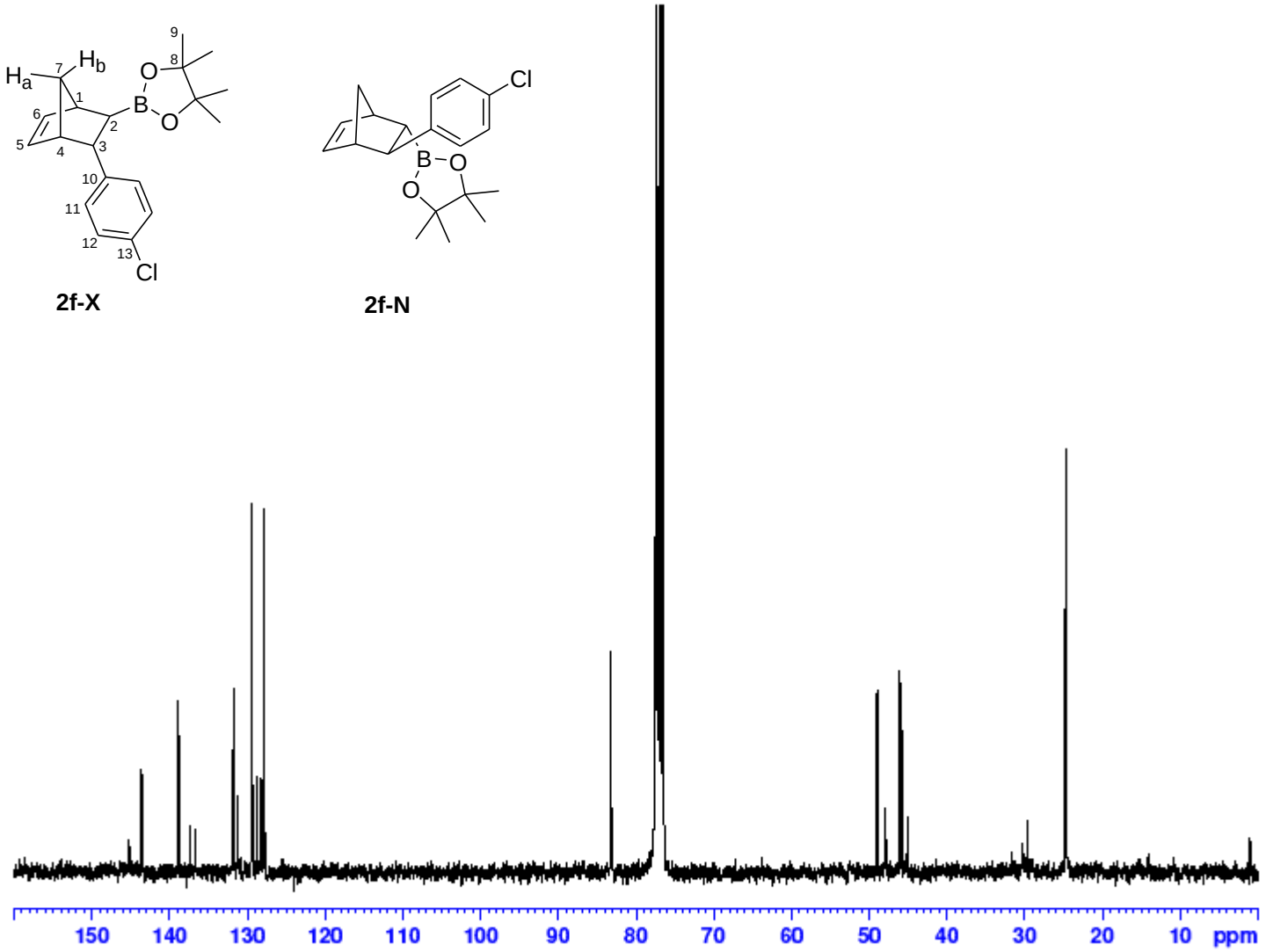

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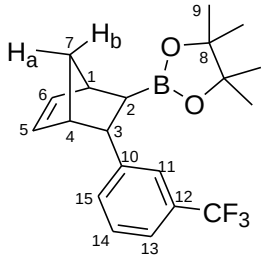
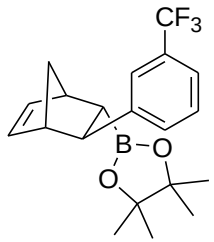
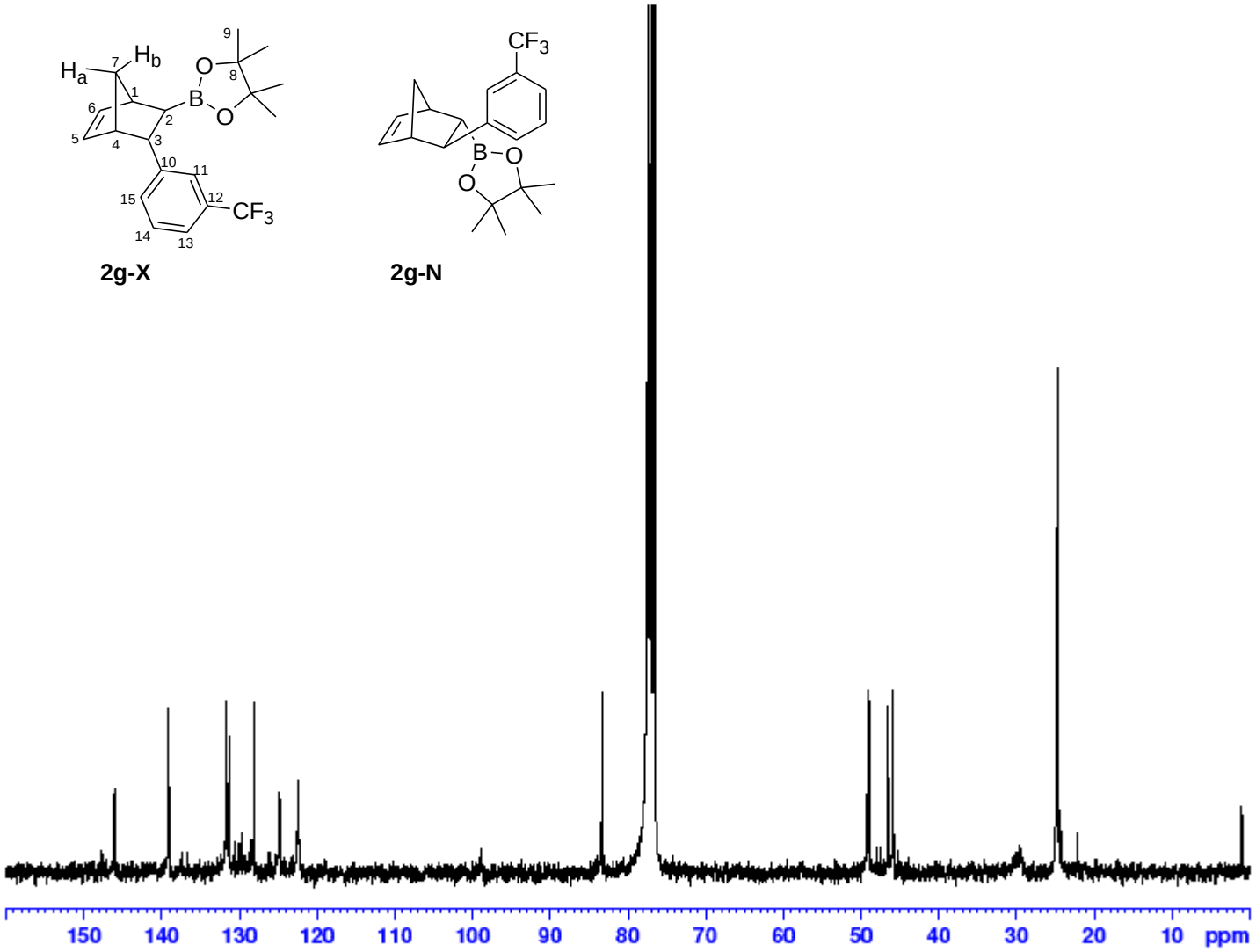


2g-X



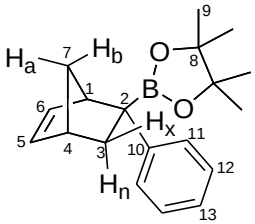
2g-N

^{1}H NMR spectra of **2g-X** and **2g-N** at 300 MHz in $CDCl_3$

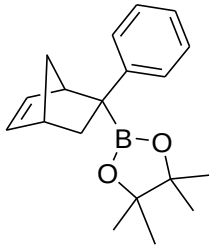


2g-X **2g-N**

^{13}C NMR spectra of **2g-X** and **2g-N** at 75 MHz in $CDCl_3$

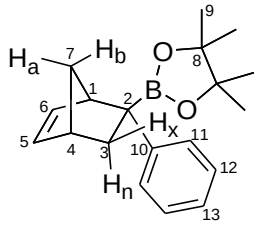


2h-X

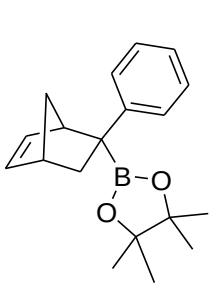


2h-N

^{1}H NMR spectra of **2h-X** and **2h-N** at 300 MHz in $CDCl_3$

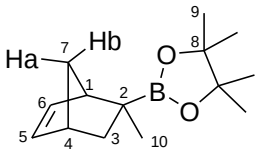


2h-X



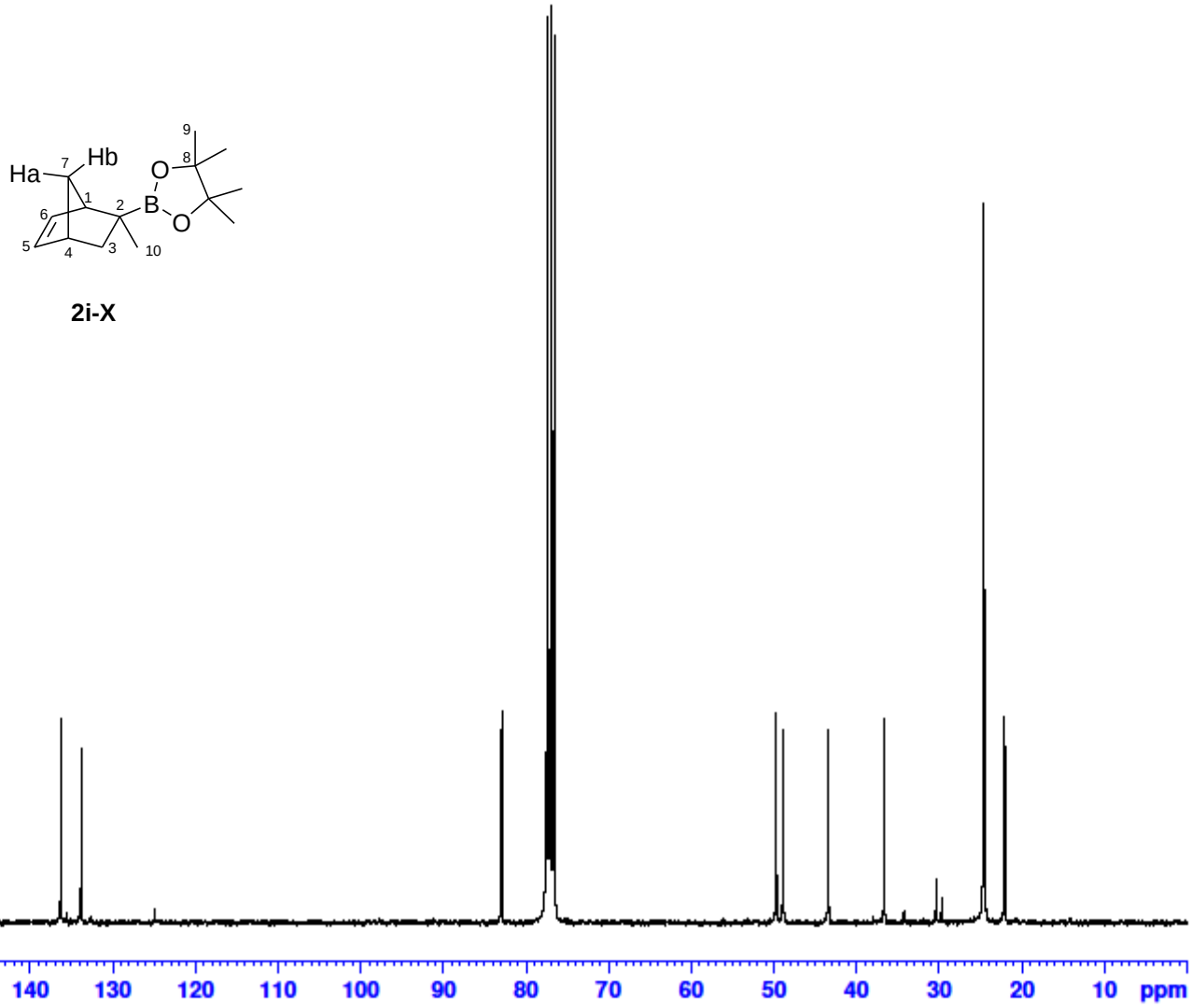
2h-N

^{13}C NMR spectra of **2h-X** and **2h-N** at 75 MHz in $CDCl_3$



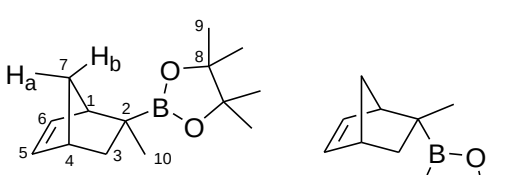
2i-X

^{1}H NMR spectra of **2i-X** at 300 MHz in $CDCl_3$



2i-X

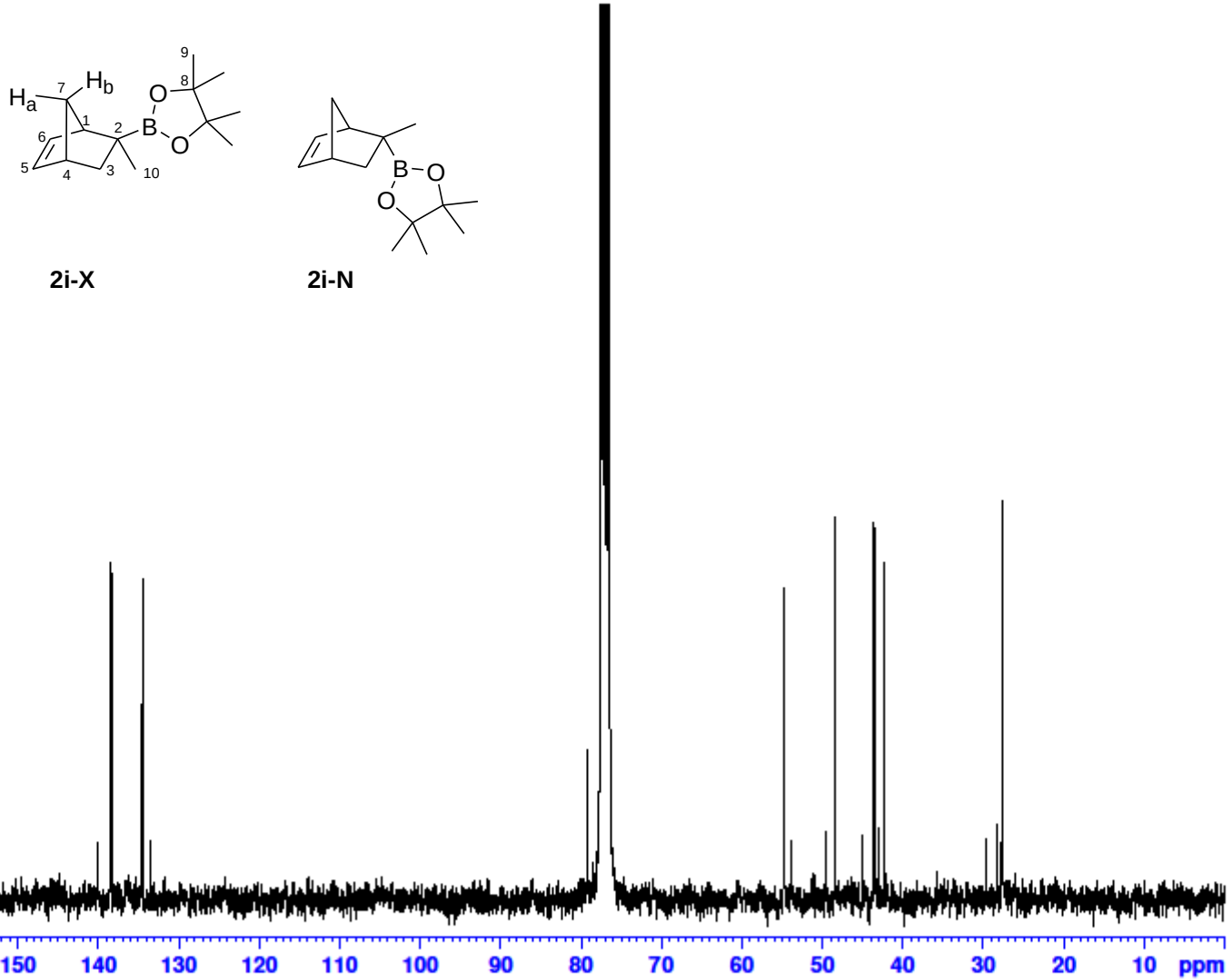
^{13}C NMR spectra of **2hi-X** at 75 MHz in $CDCl_3$



2i-X

2i-N

^{1}H NMR spectra of **2i-X** and **2i-N** at 300 MHz in $CDCl_3$



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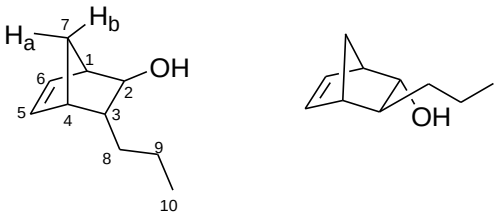
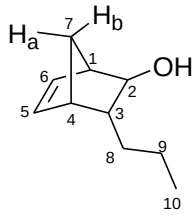


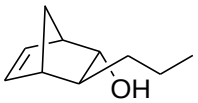
3b-X

3b-N

^{1}H NMR spectra of **3b-X** and **3b-N** at 300 MHz in $CDCl_3$



3b-X



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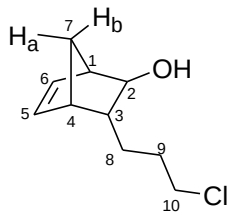
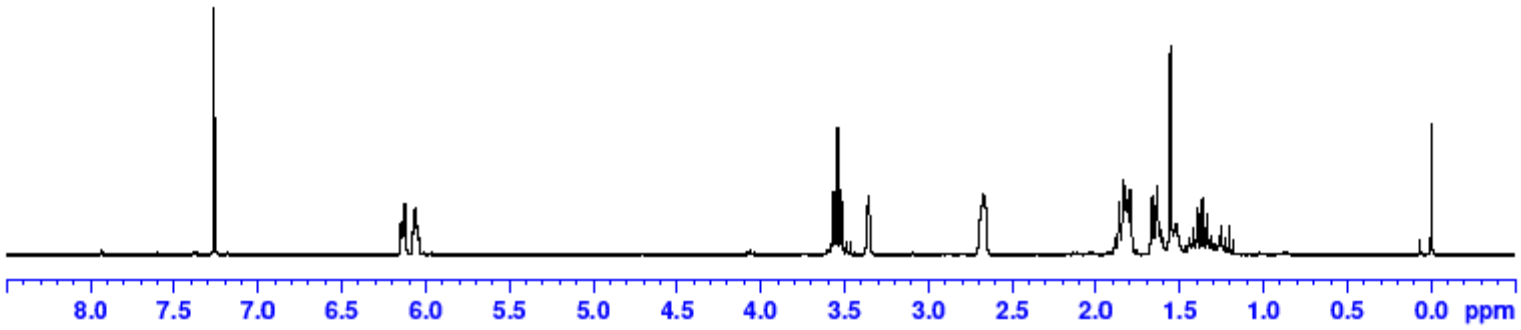


3c-X



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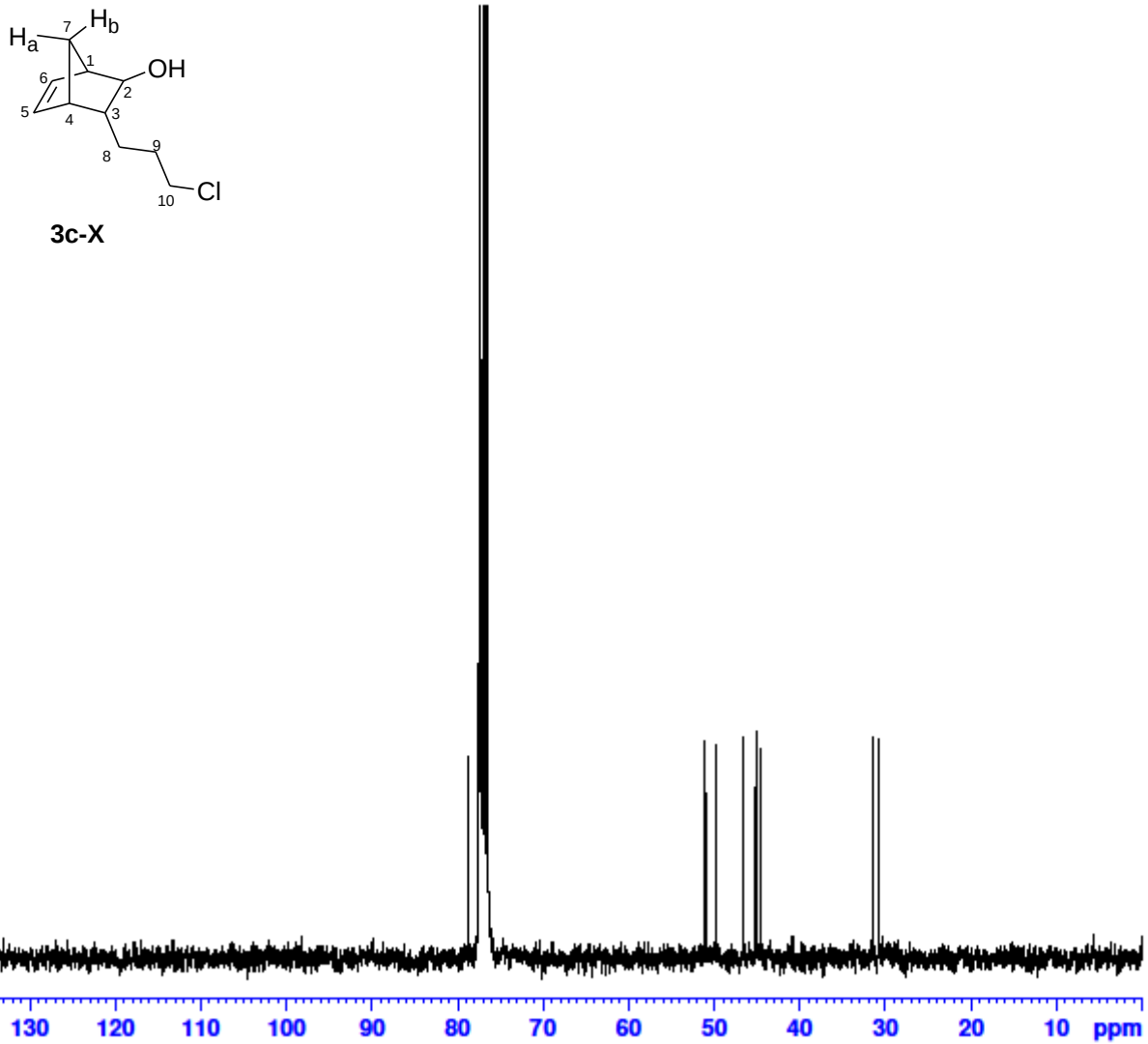

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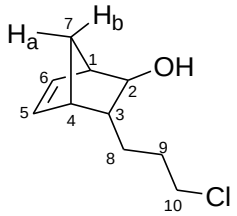

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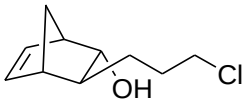

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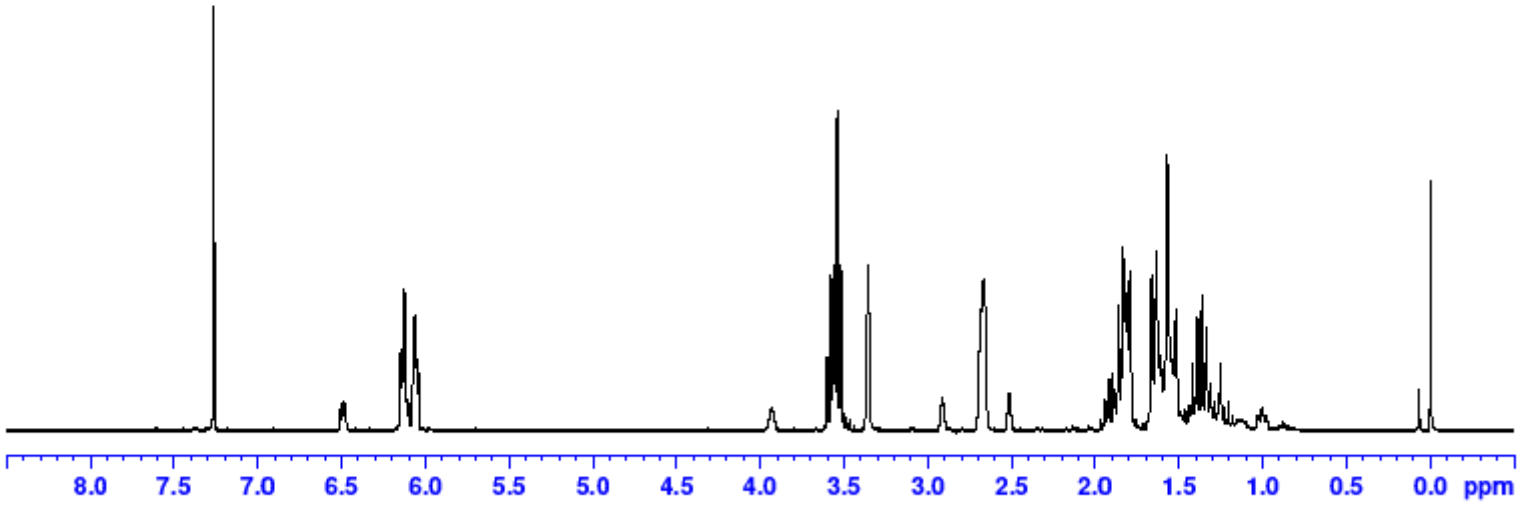

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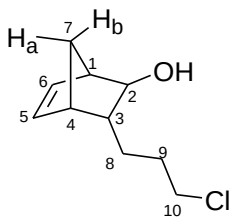

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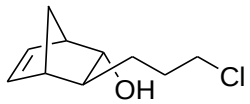

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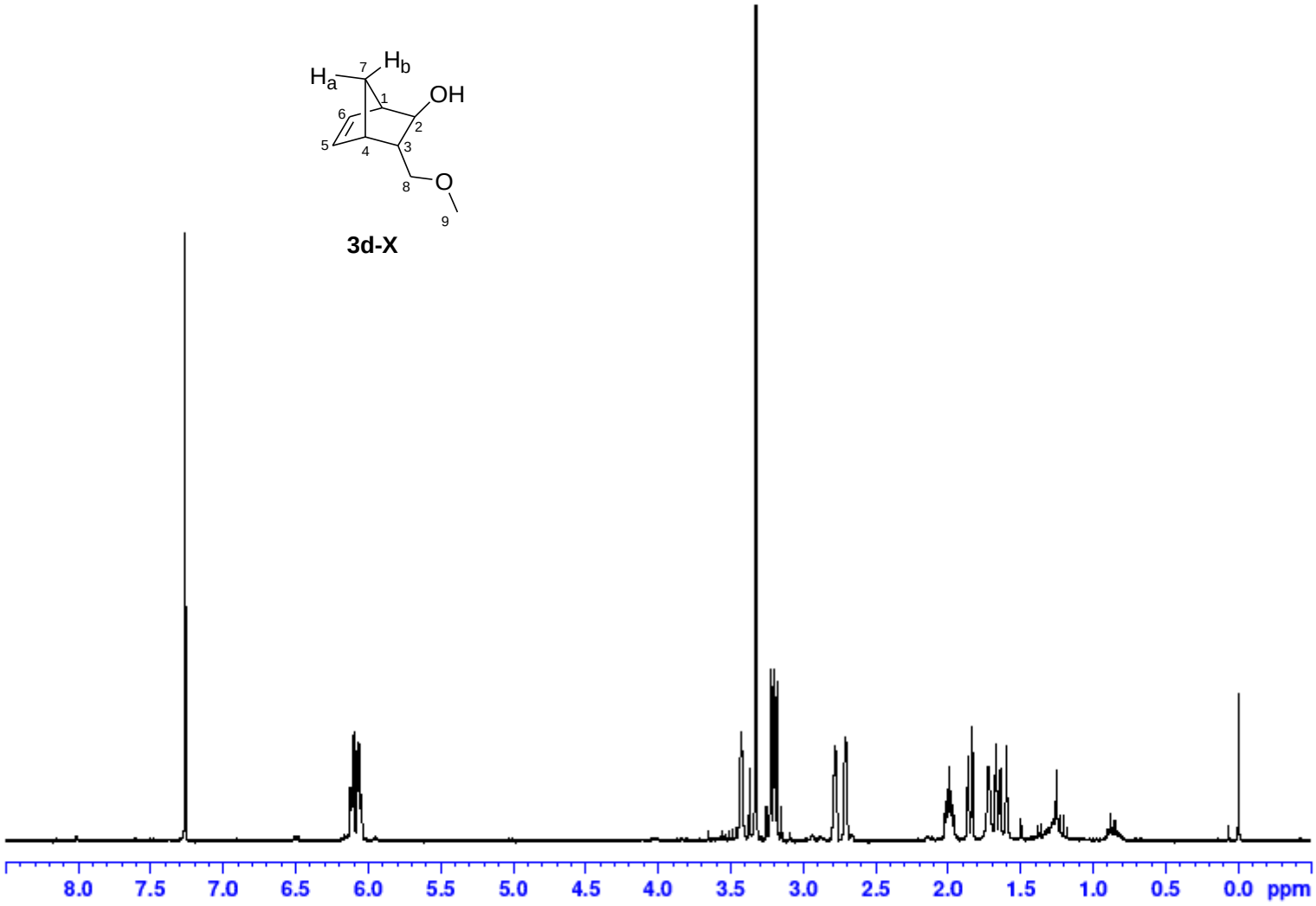

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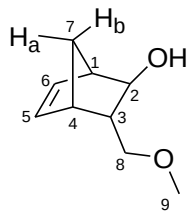

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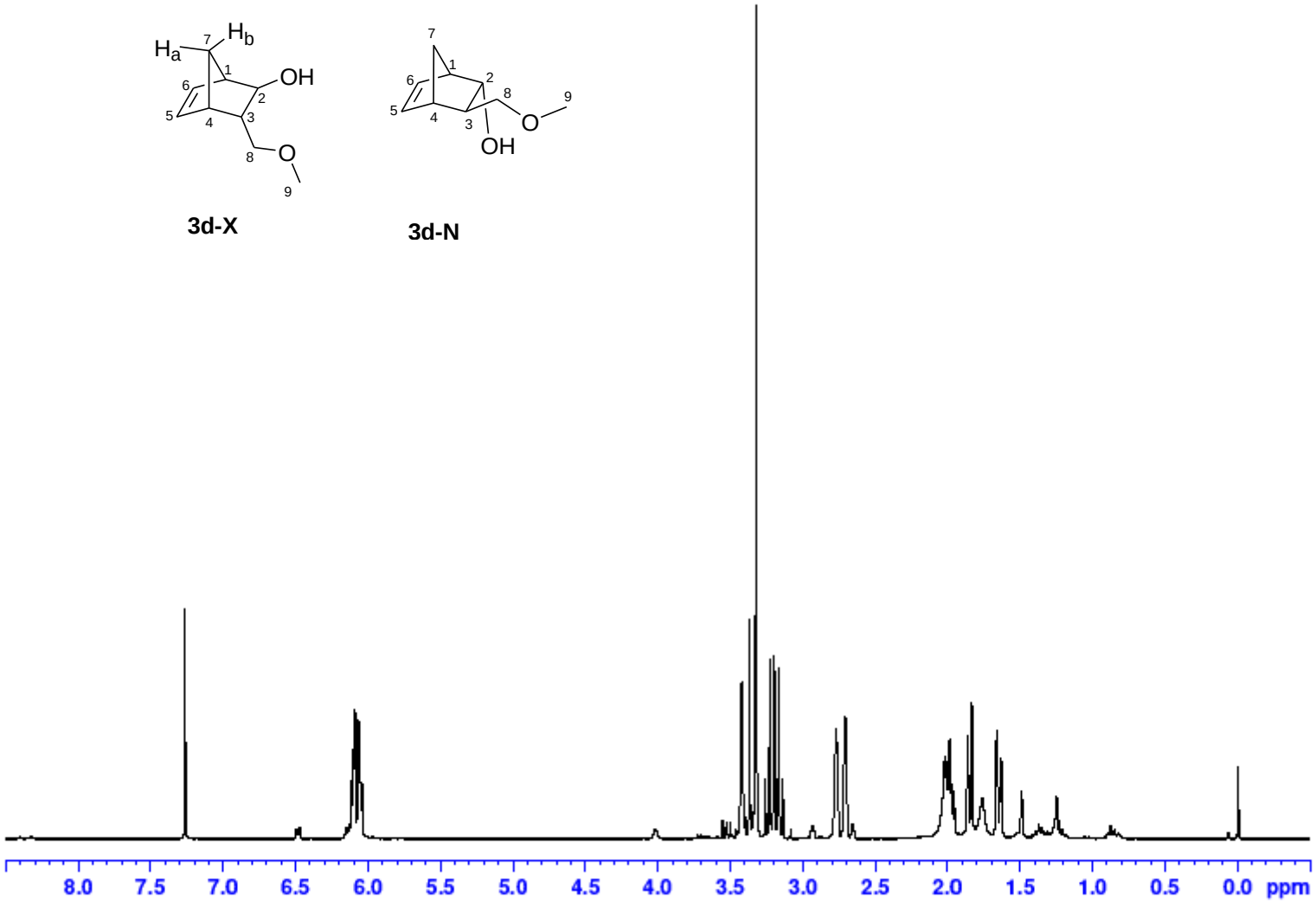

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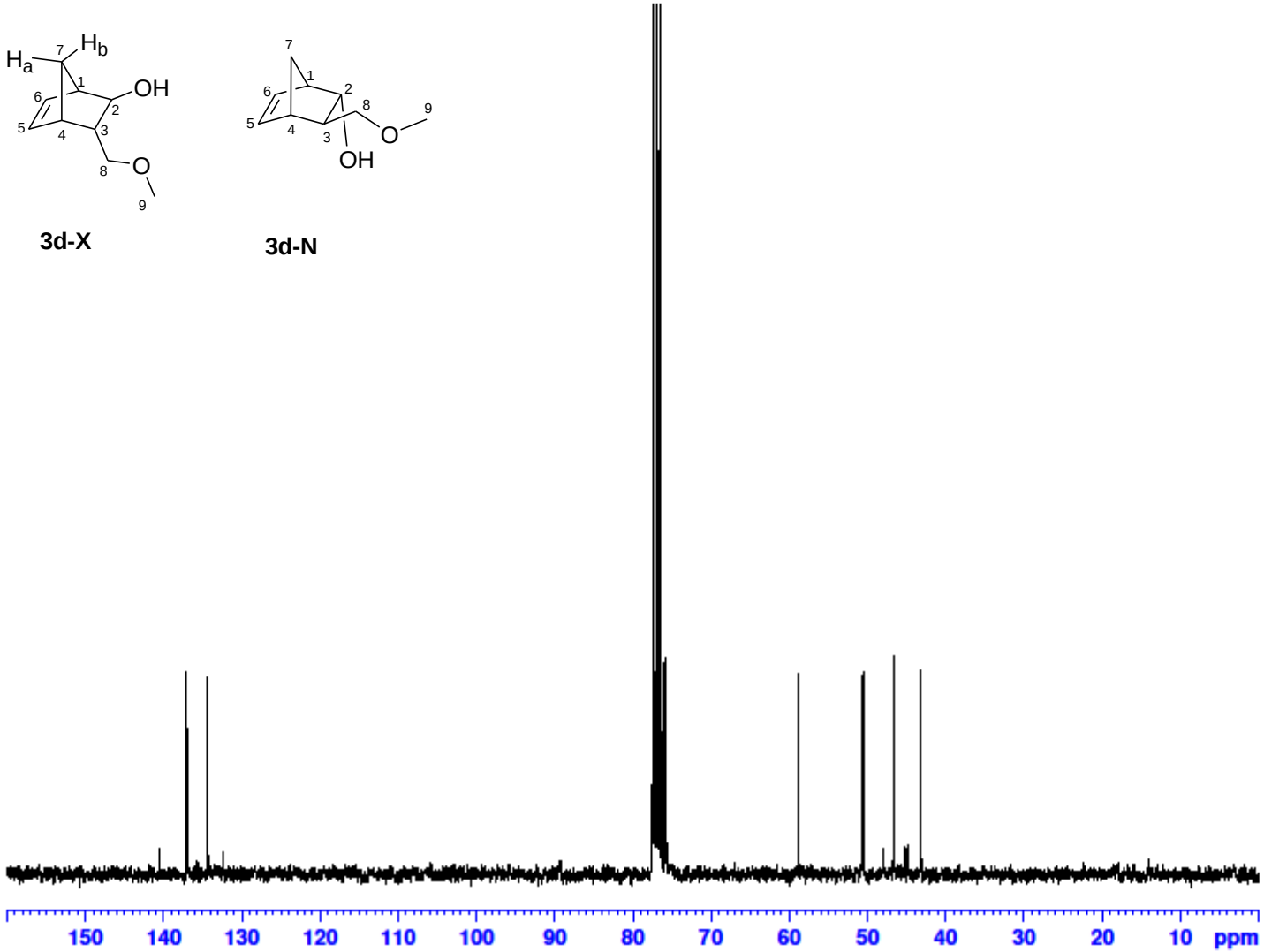

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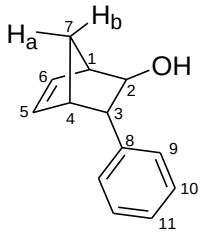
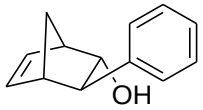


3e-X



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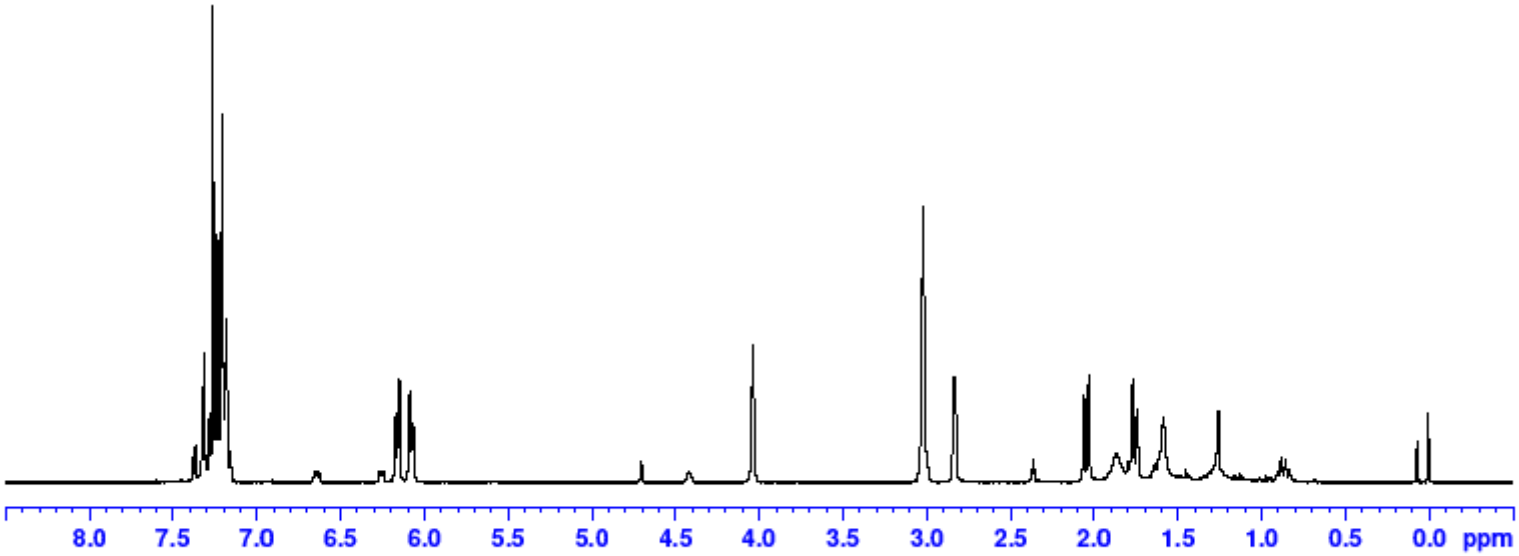

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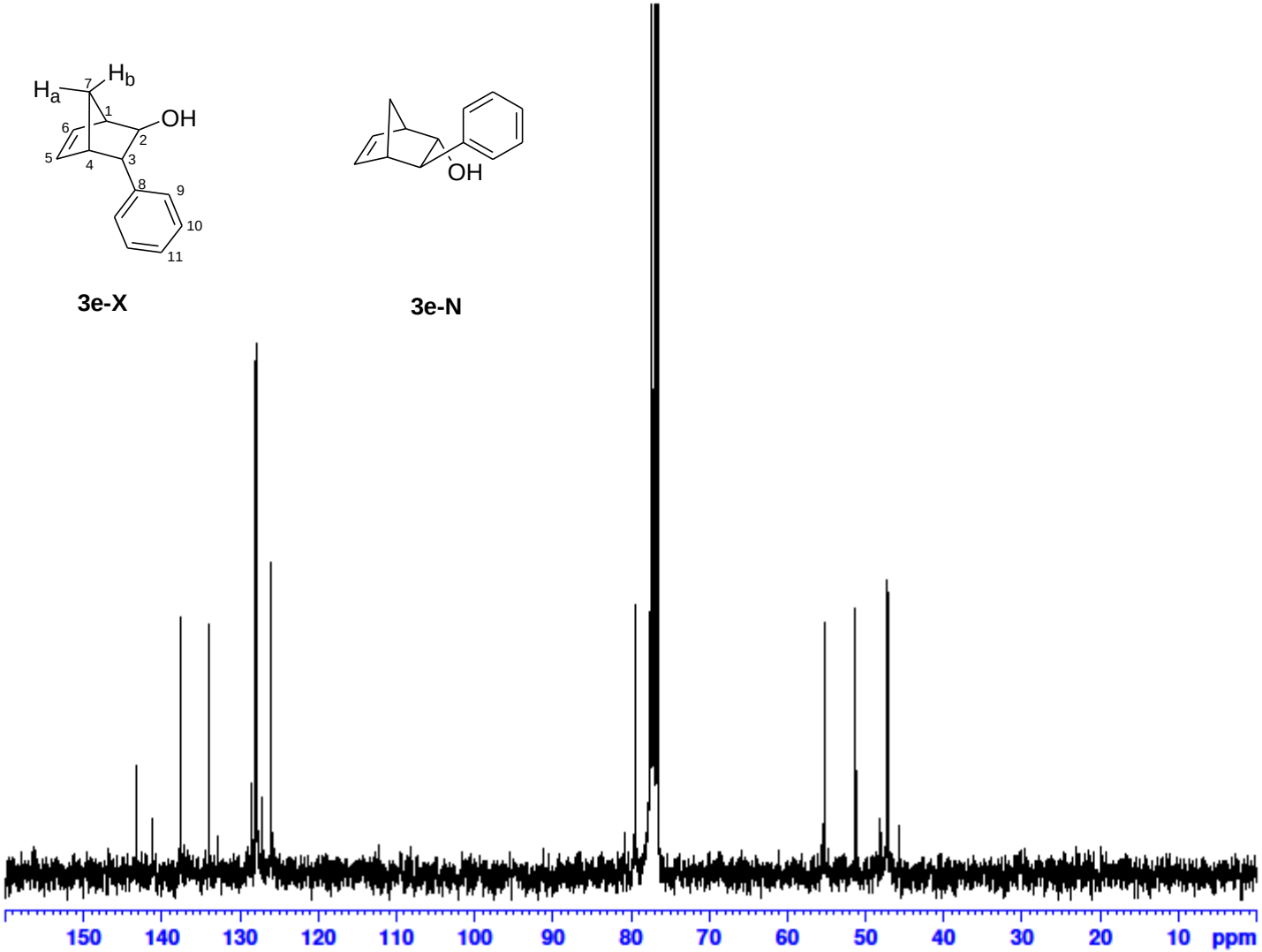

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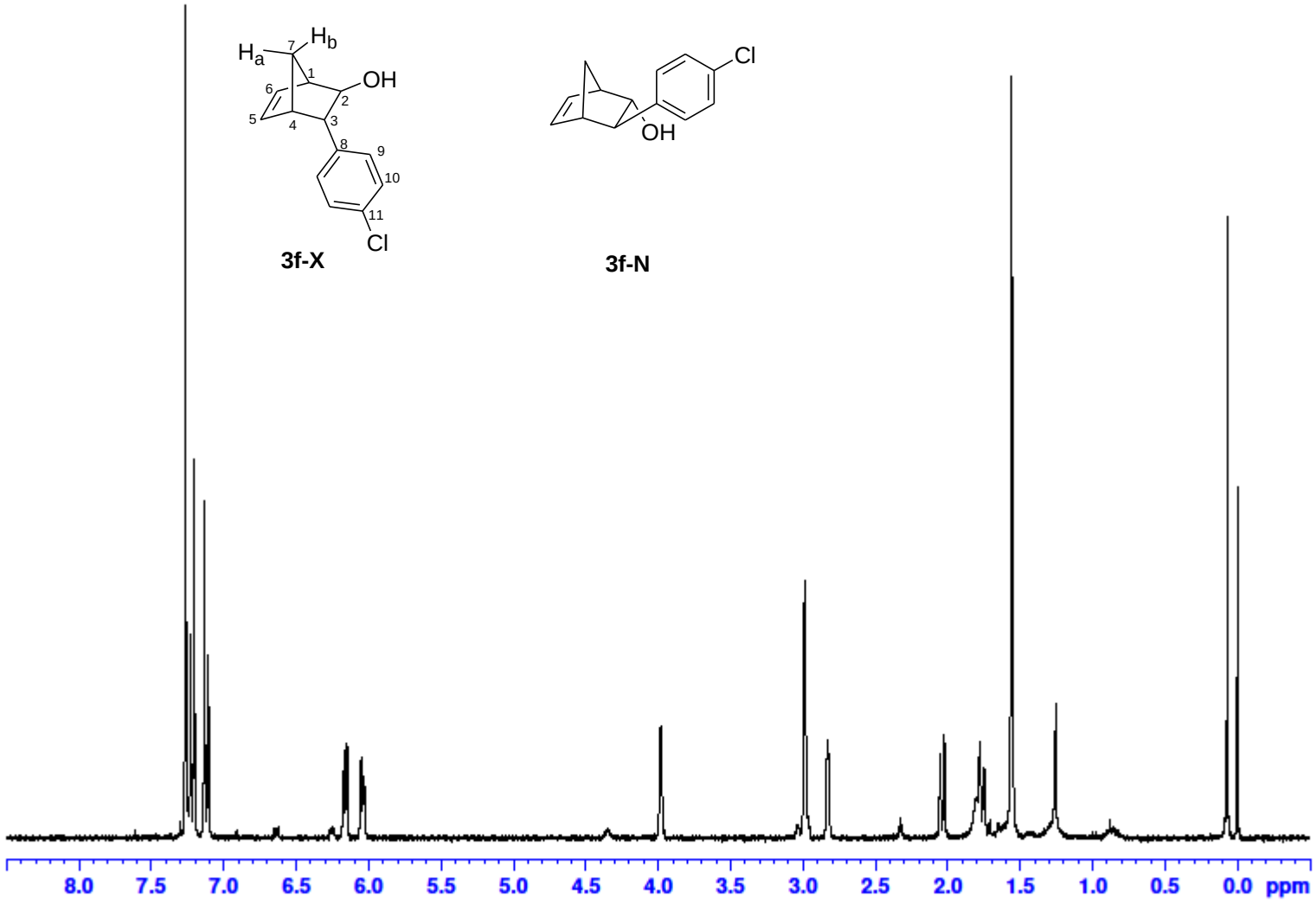
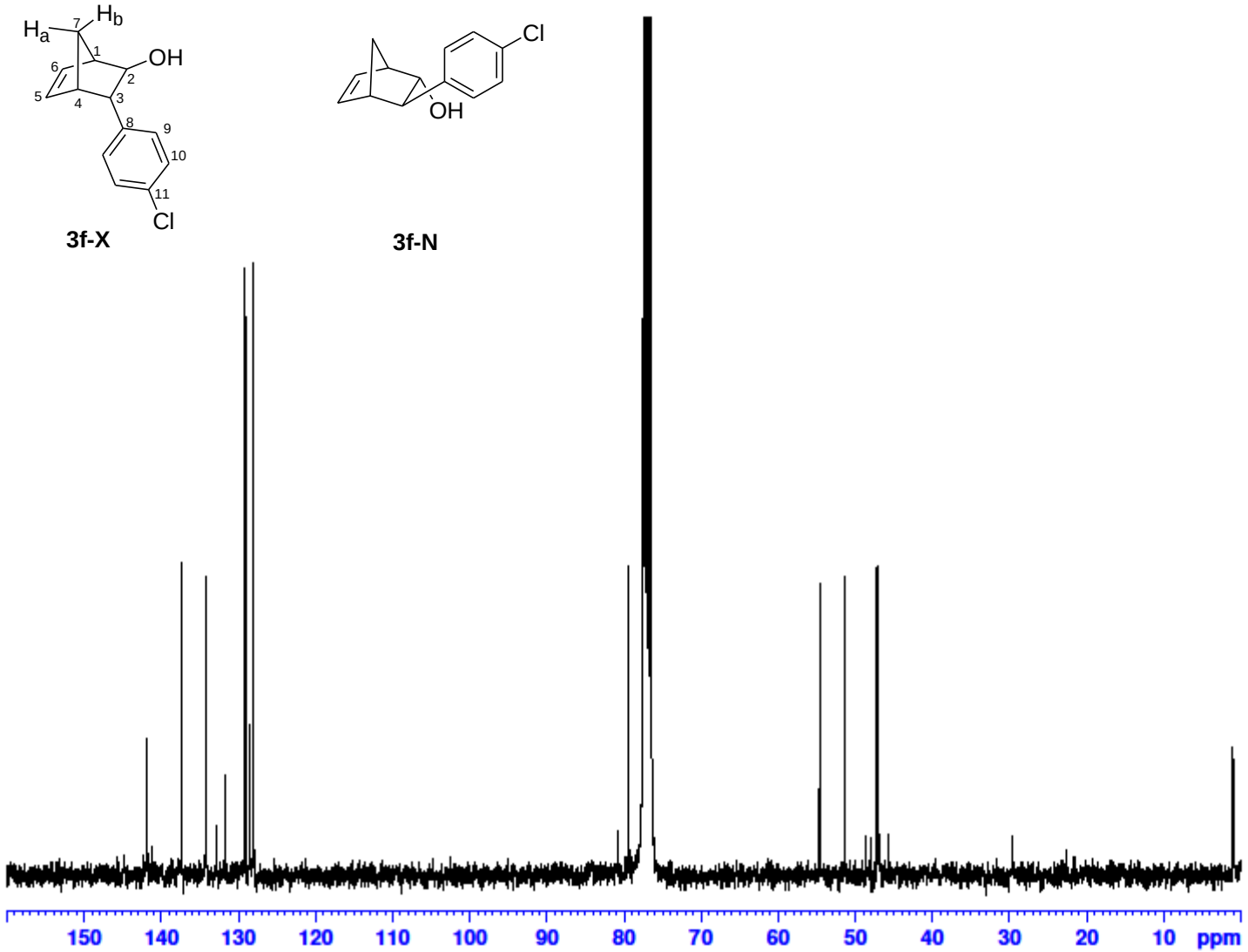
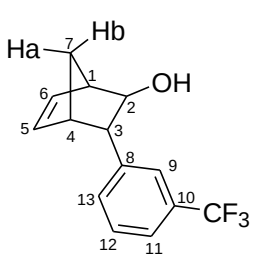


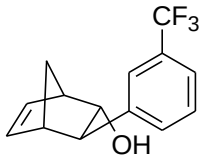
^{1}H NMR spectra of **3f-X** and **3f-N** at 300 MHz in $CDCl_3$



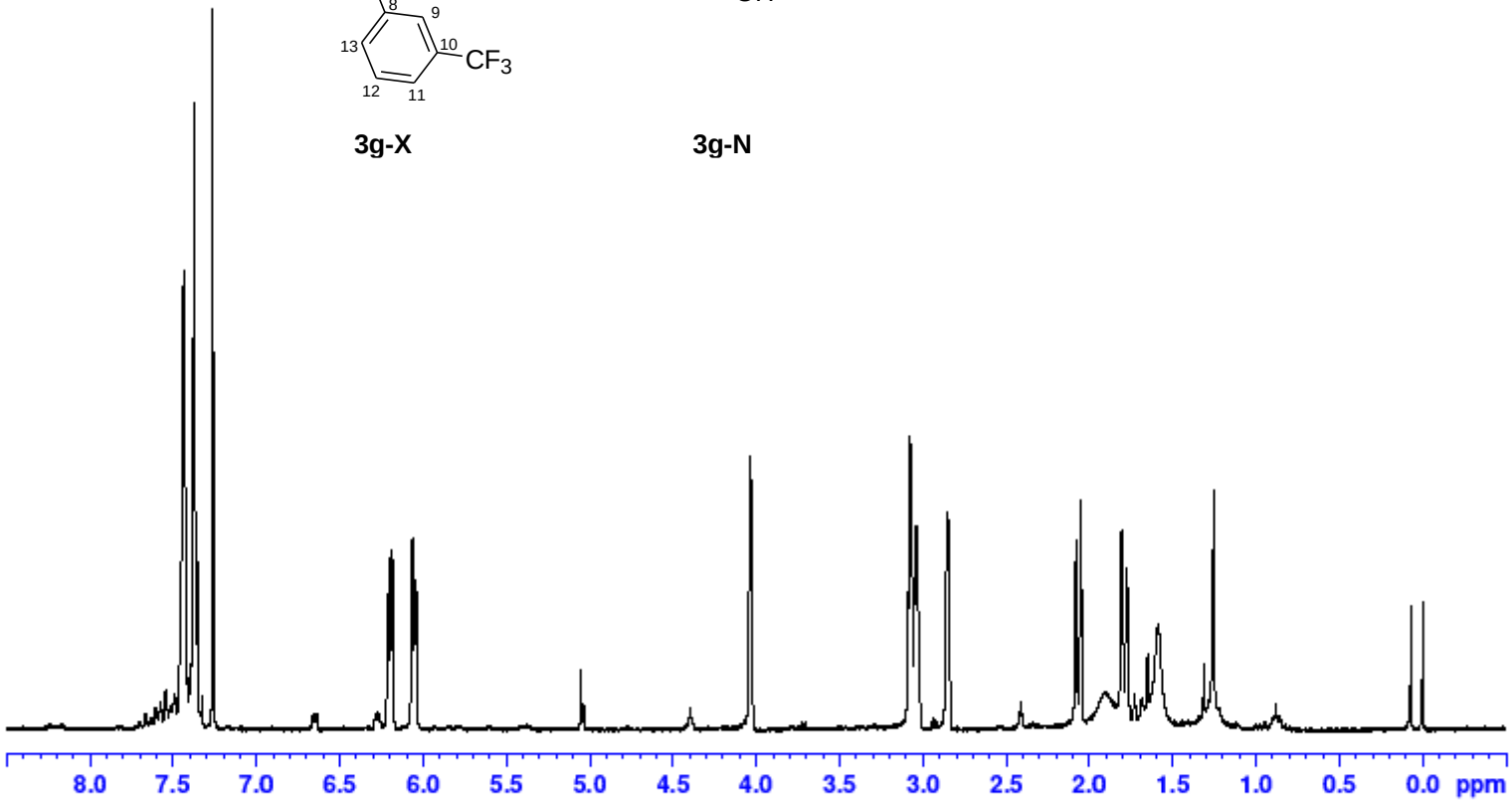
^{13}C NMR spectra of **3f-X** and **3f-N** at 75 MHz in $CDCl_3$



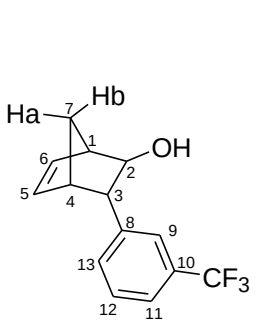
3g-X



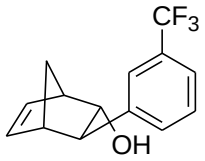
3g-N



^{1}H NMR spectra of **3g-X** and **3g-N** at 300 MHz in $CDCl_3$

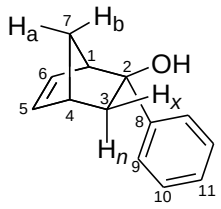


3g-X

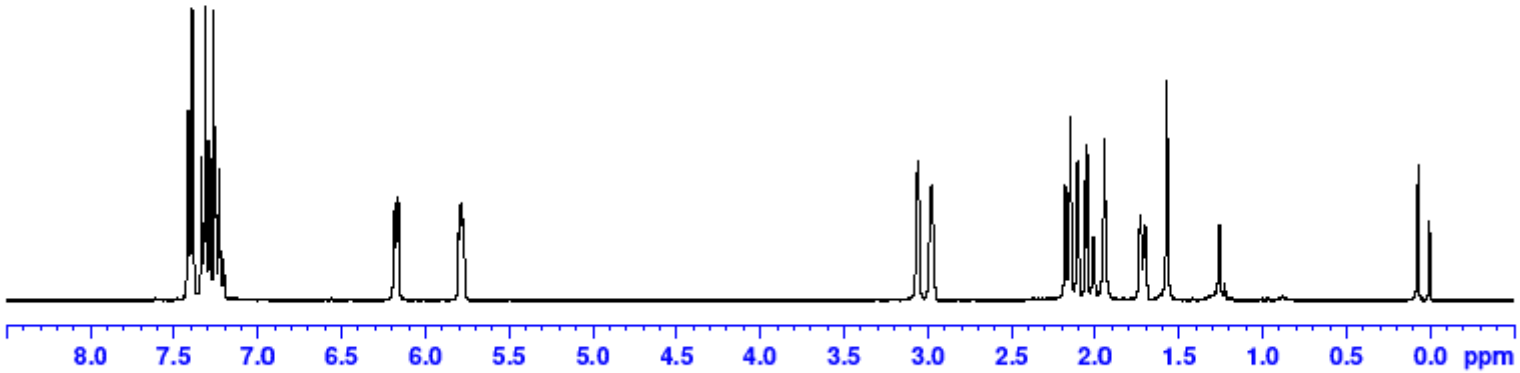


3g-N

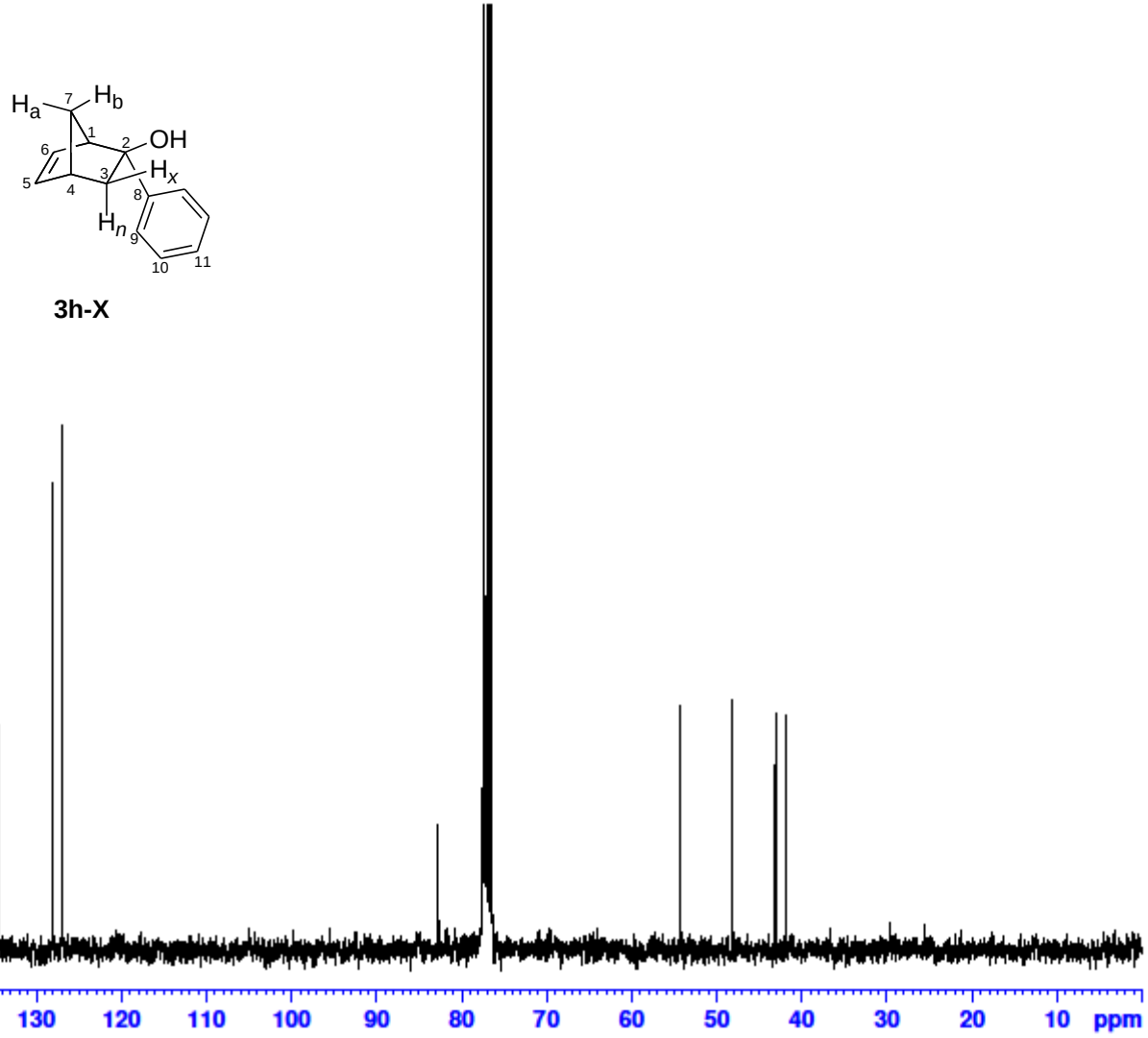
^{13}C NMR spectra of **3g-X** and **3g-N** at 75 MHz in $CDCl_3$



3h-X

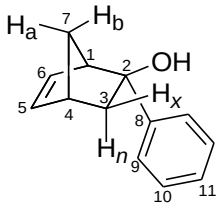


^{1}H NMR spectra of **3h-X** at 300 MHz in $CDCl_3$

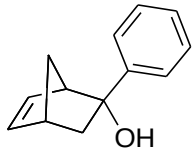


3h-X

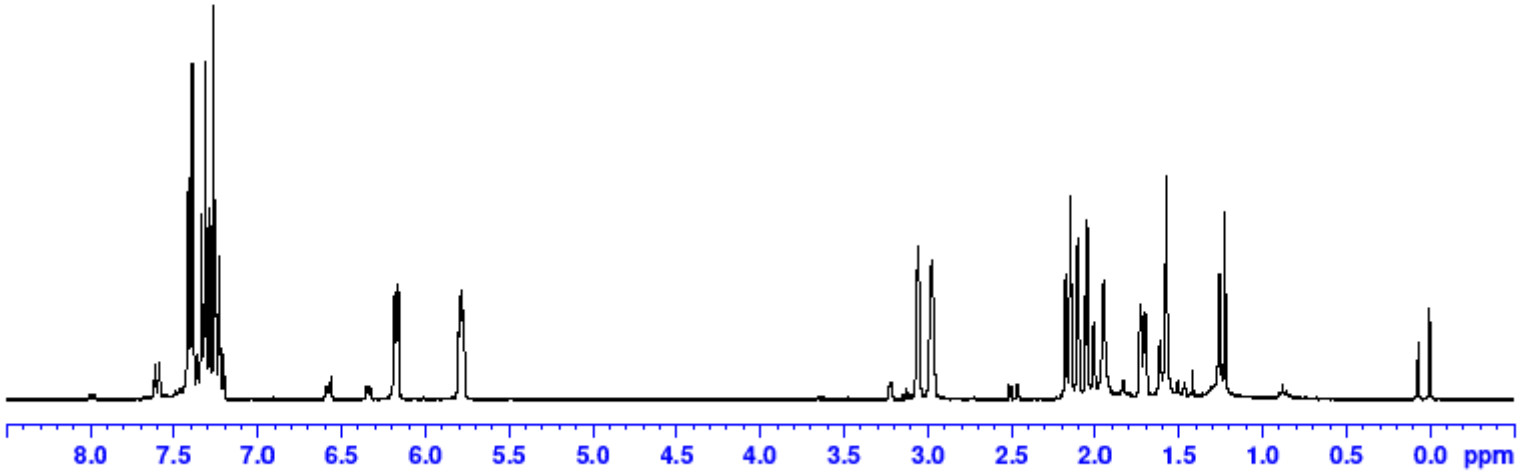
^{13}C NMR spectra of **3h-X** at 75 MHz in $CDCl_3$



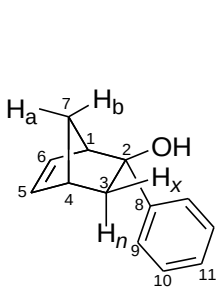
3h-X



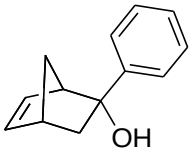
3h-N



^{1}H NMR spectra of **3h-X** and **3h-N** at 300 MHz in $CDCl_3$

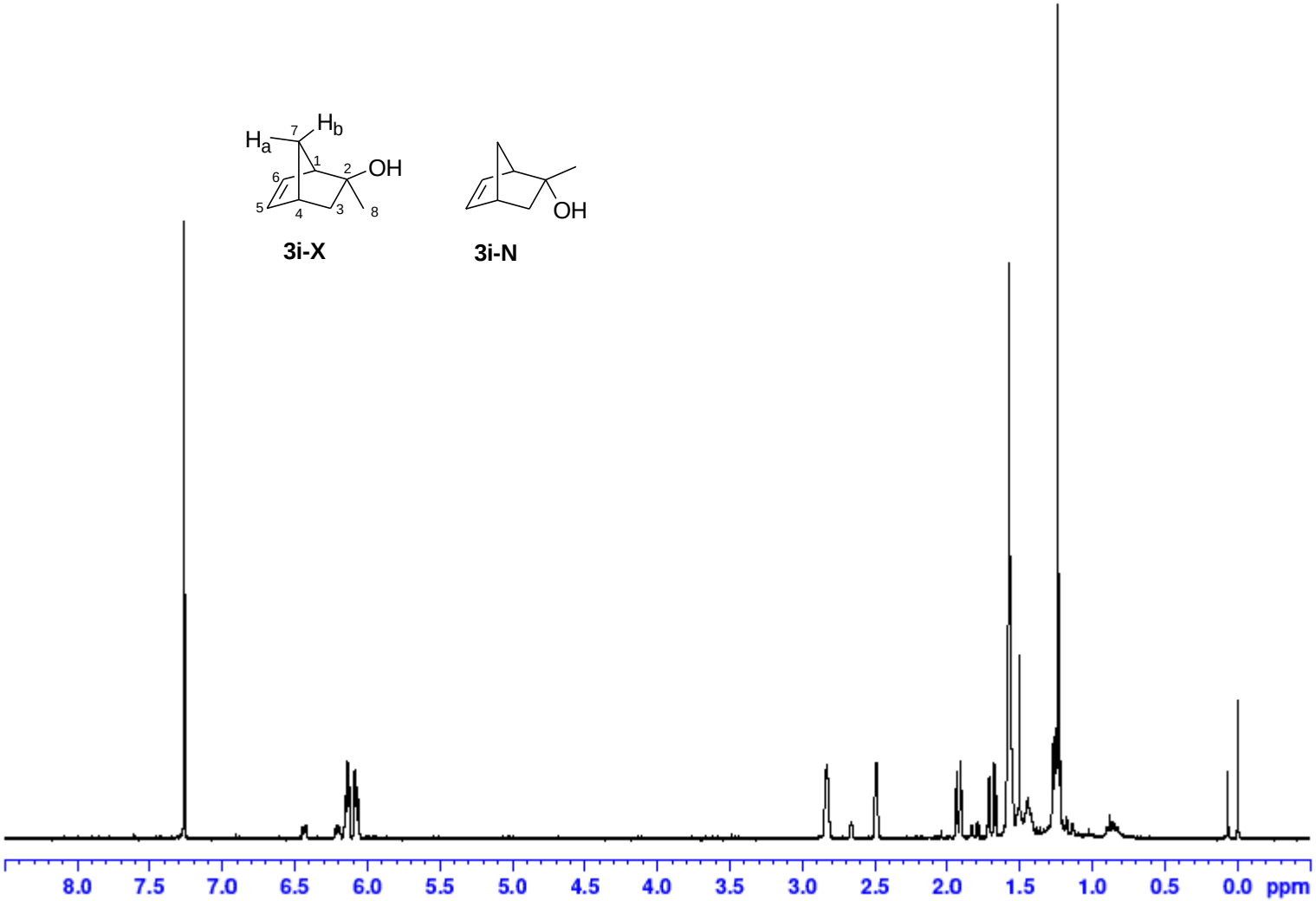


3h-X

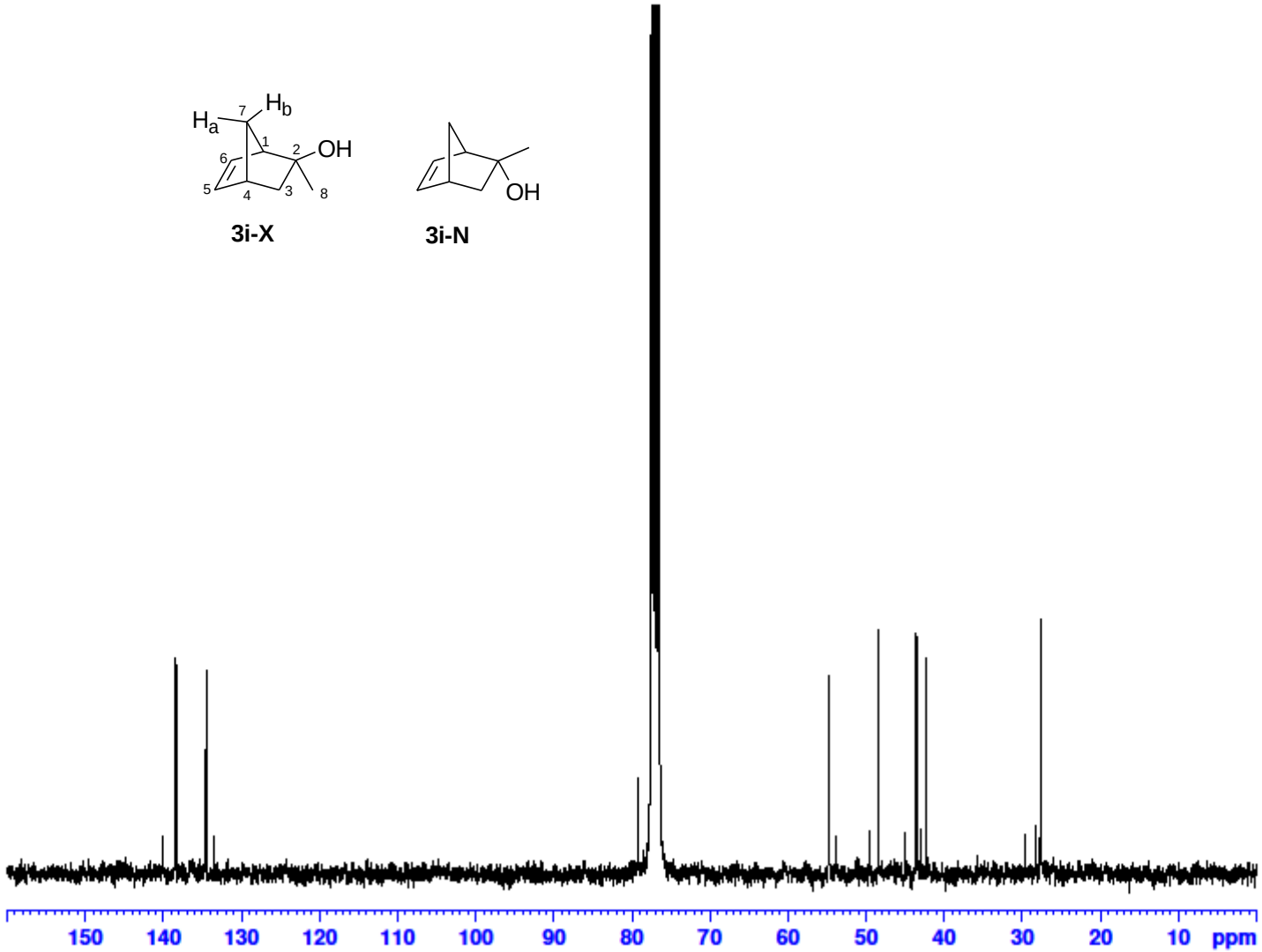


3h-N

^{13}C NMR spectra of **3h-X** and **3h-N** at 75 MHz in $CDCl_3$



^{1}H NMR spectra of **3i-X** and **3i-N** at 300 MHz in $CDCl_3$



^{13}C NMR spectra of **3i-X** and **3i-N** at 75 MHz in $CDCl_3$

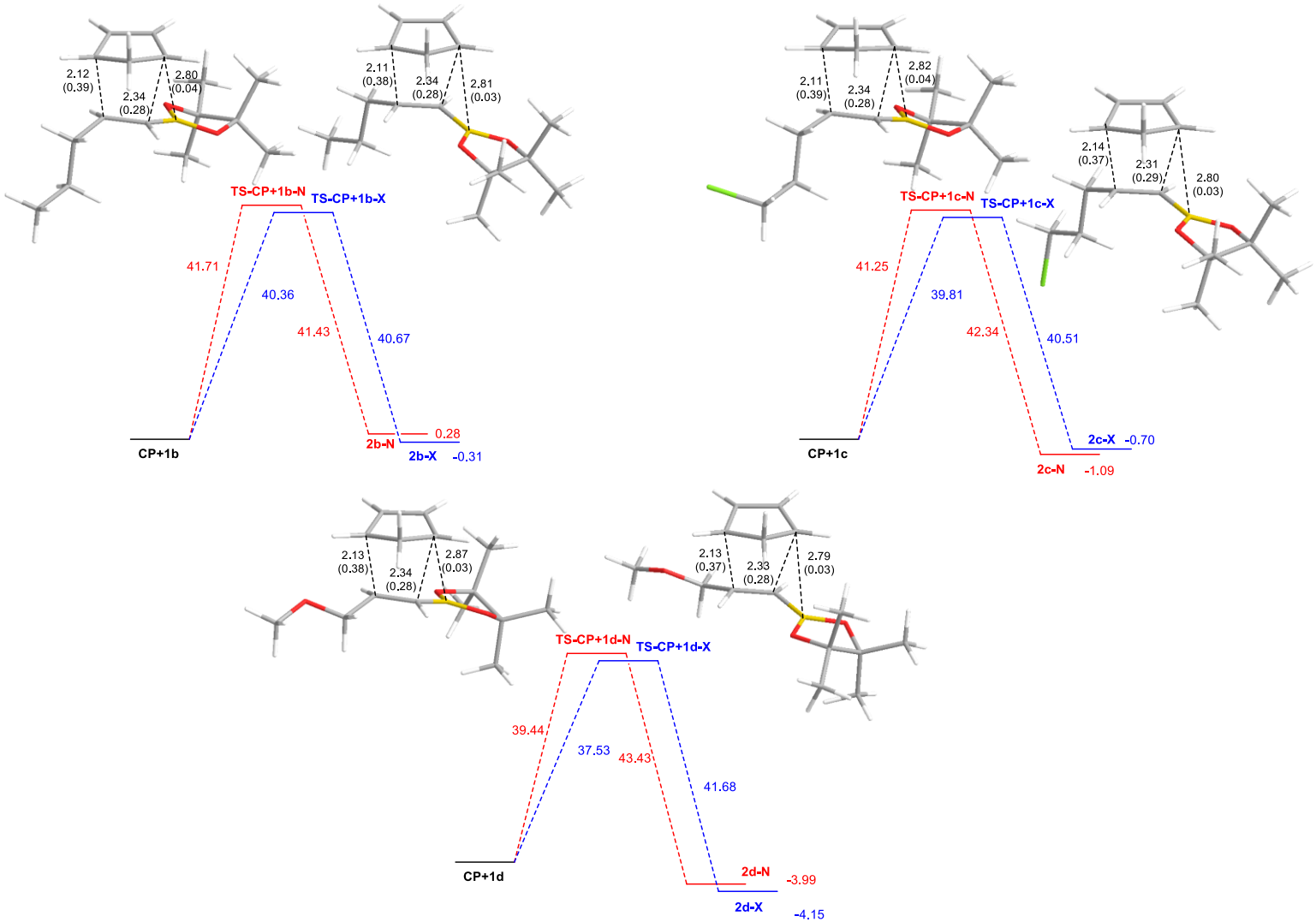


Figure S1. MPWB1K/6-311G* free energy profiles for the Diels-Alder reactions of aliphatic pinacol alkenylboronates **1b** (top left), **1c** (top right) and **1d** (bottom) with cyclopentadiene (free activation energies in toluene at 170 ºC for the direct and reverse reaction, in kcal/mol). The optimized geometries in toluene for the transition structures with selected distances in Å and Wiberg bond indexes in parentheses are also shown.

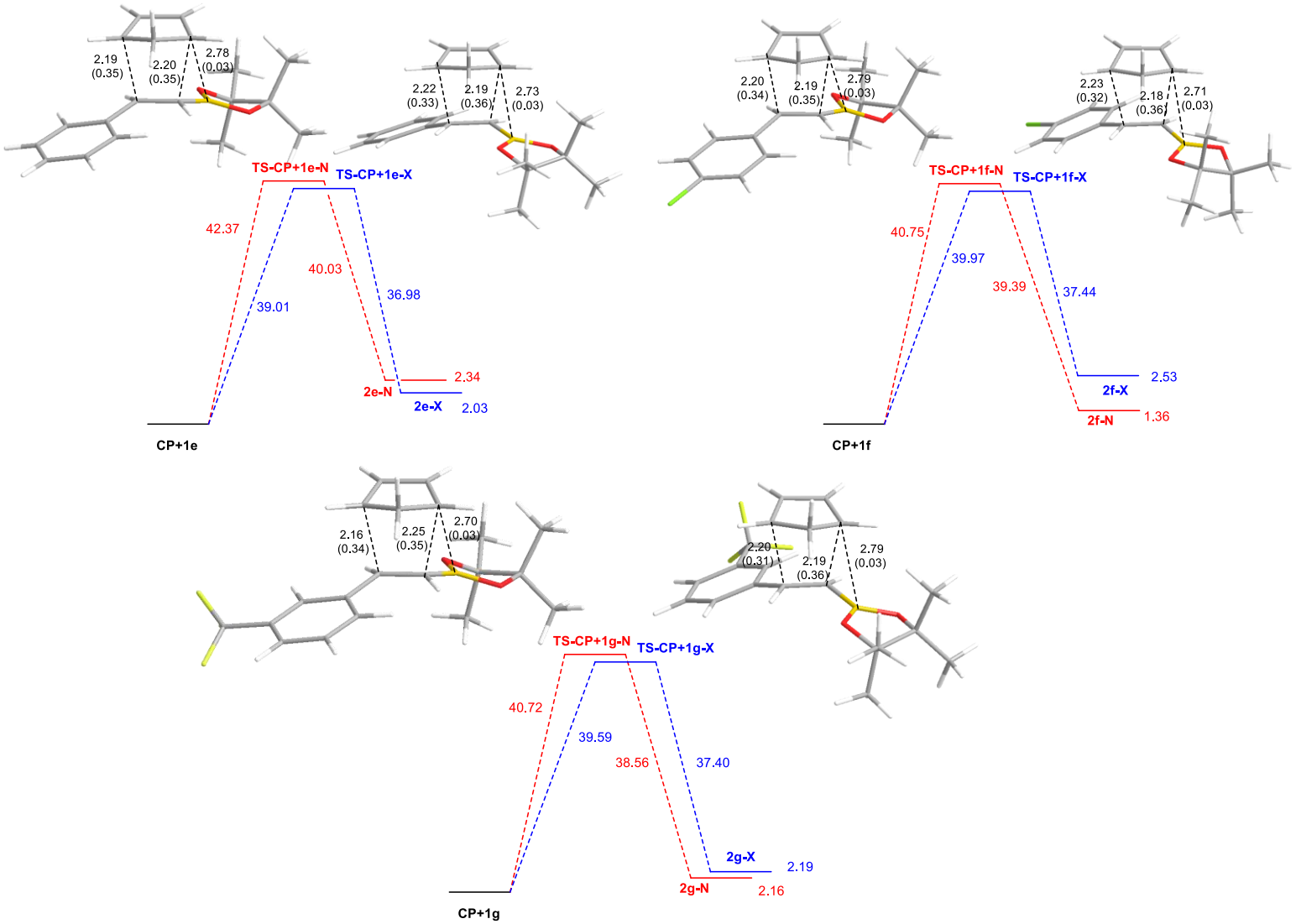


Figure S2. MPWB1K/6-311G* free energy profiles for the Diels-Alder reactions of aromatic pinacol alkenylboronates **1e** (top left), **1f** (top right) and **1g** (bottom) with cyclopentadiene (free activation energies in toluene at 170 ºC for the direct and reverse reaction, in kcal/mol). The optimized geometries in toluene for the transition structures with selected distances in Å and Wiberg bond indexes in parentheses are also shown.

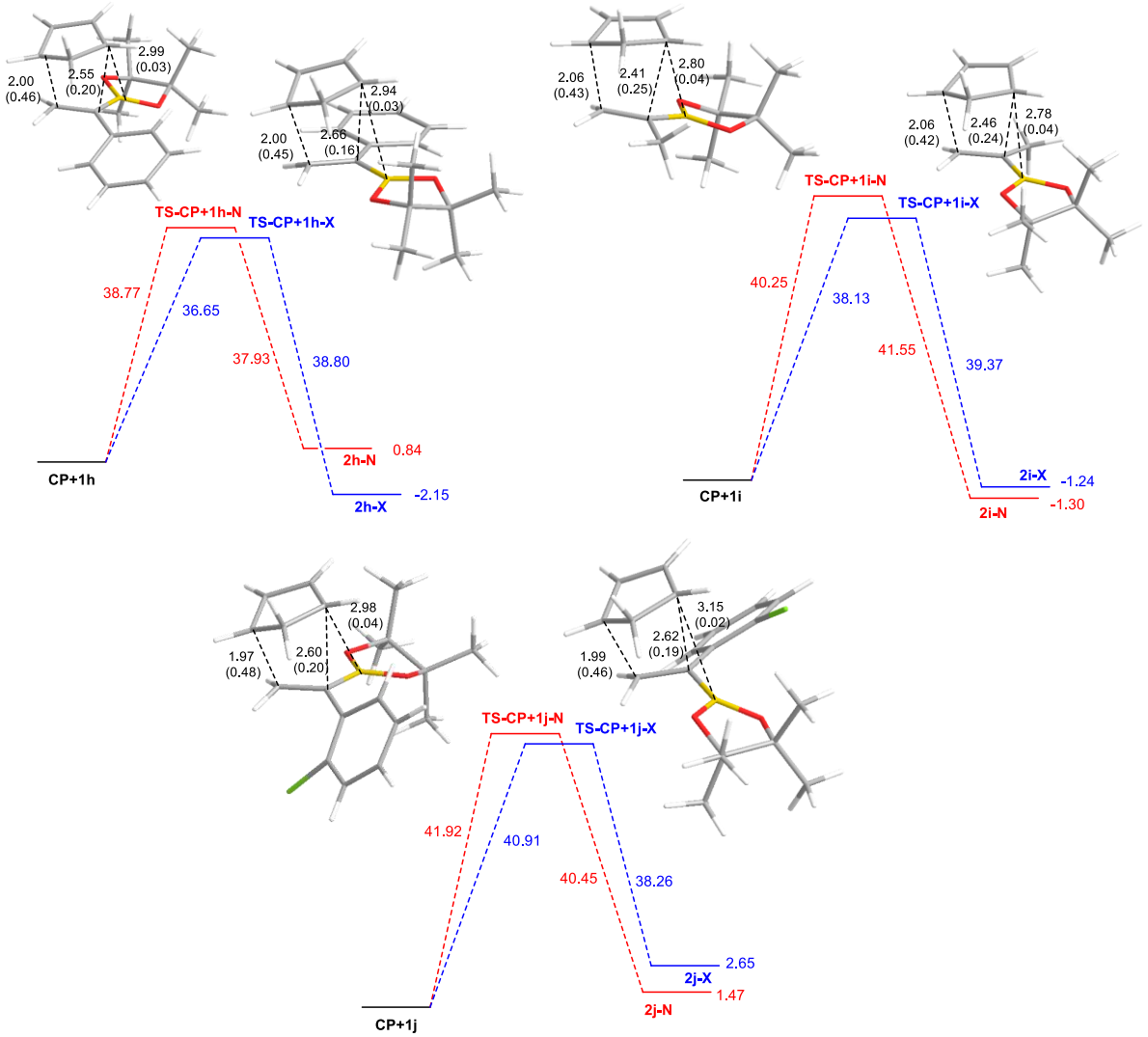


Figure S3. MPWB1K/6-311G*free energy profiles for the Diels-Alder reactions of 1-substituted pinacol alkenylboronates **1h** (top left), **1i** (top right) and **1j** (bottom) with cyclopentadiene (free activation energies in toluene at 170 ºC for the direct and reverse reaction, in kcal/mol). The optimized geometries in toluene for the transition structures with selected distances in Å and Wiberg bond indexes in parentheses are also shown.