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Supplementary Information

Niobium(V) Chloride as Catalyst in Diels-Alder Reaction of Furan Ring

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Characterization of desired products

The infrared (IR) spectroscopy analysis were carried out using a FTLA2000-102 device by BOMEM. The spectra were obtained with resolution set at 4 cm^{-1}, 16 scans, using Pike Technologies MIRacle Single Reflection ATR accessory, 45°, ZnSe, using atmosphere as blank. The reading range of the accessory was 550-4000 cm^{-1}. Nuclear magnetic resonance (NMR) spectra were recorded on a Varian 400 MHz spectrometer (400 MHz for ^{1}H and 100 MHz for ^{13}C); $CDCl_3$ was used as the solvent, and chemical shifts (δ) are presented in units of ppm relative to the standard reference tetramethylsilane (TMS).

Methyl 7-oxabicyclo[2.2.1]hept-5-ene-2-carboxylate (**3a**):

IR (film) n_{max}/cm^{-1} 2954, 1731, 1438, 1200, 1170, 1020; *Endo* adduct ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.42 (dd, 1H, *J* 5.9, 1.9 Hz), 6.23 (dd, 1H, *J* 5.9, 1.9 Hz), 5.17 (ddd, 1H, *J* 4.7, 1.6, 0.8 Hz), 5.02 (ddd, 1H, *J* 4.1, 1.7, 0.8 Hz), 3.65 (s, 3H), 3.13 (ddd, 1H, *J* 9.2, 4.9, 3.9 Hz), 2.11 (ddd, 1H, *J* 11.5, 9.2, 4.7 Hz), 1.58 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 137.0, 132.6, 79.0, 78.7, 51.8, 42.7, 28.5; *Exo* adduct ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.39 (dd, 1H, *J* 5.9, 1.7 Hz), 6.35 (dd, 1H, *J* 5.9, 1.7 Hz), 5.19 (dd, 1H, *J* 1.6, 0.8 Hz), 5.08 (dd, 1H, *J* 4.7, 0.8 Hz), 3.74 (s, 3H), 2.44 (dd, 1H, *J* 8.2, 3.9 Hz), 2.17 (dt, 1H, *J* 11.5, 4.1 Hz), 1.58 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 137.1, 134.7, 80.9, 78.0, 52.1, 42.7, 29.1.

7-oxabicyclo[2.2.1]hept-5-ene-2-carbonitrile (**3b**):

IR (film) ν/cm^{-1} 2961, 2242, 1665, 1020; *Endo* adduct ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.57 (dd, 1H, *J* 5.9, 1.9 Hz), 6.31 (dd, 1H, *J* 5.7, 1.7 Hz), 5.23 (ddd, 1H, *J* 4.7, 1.9, 0.8 Hz), 5.14 (dd, 1H, *J* 4.7, 1.4 Hz), 2.94 (dt, 1H, *J* 9.4, 3.9 Hz), 2.30 (ddd, 1H, *J* 11.4, 9.3, 4.3 Hz), 1.55 (dd, 1H, *J* 11.5, 3.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.6, 133.6, 121.7, 78.9, 78.8, 31.3, 26.2; *Exo* adduct ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.49 (dd, 1H, *J* 5.9, 1.6 Hz), 6.42 (dd, 1H, *J* 5.9, 1.9 Hz), 5.24 (dd, 1H, *J* 1.6, 0.8 Hz), 5.19 (dd, 1H, *J* 4.7, 1.6 Hz), 2.40 (dd, 1H, *J* 8.6, 3.9 Hz), 2.13 (dt, 1H, *J* 11.5, 4.0 Hz), 1.75 (dd, 1H, *J* 11.7, 8.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.4, 132.9, 120.4, 81.2, 78.0, 31.5, 27.6.

2-chloro-7-oxabicyclo[2.2.1]hept-5-ene-2-carbonitrile (**3d**):

IR (film) ν/cm^{-1} 2960, 1600, 1147, 700; *Endo* adduct ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.70 (dd, 1H, *J* 5.9, 1.6 Hz), 6.54 (dd, 1H, *J* 5.9, 1.6 Hz), 5.25 (ddd, 1H, *J* 4.3, 1.6, 0.8 Hz), 5.18 (dd, 1H, 1.6, 0.8 Hz), 2.52 (dd, 1H, *J* 13.3, 4.3 Hz), 2.37 (d, 1H, *J* 12.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 132.1, 120.1, 84.9, 79.6, 58.2, 45.7; *Exo* adduct ^{1}H RMN (400 MHz, $CDCl_3$) δ 6.64 (dd, 1H, *J* 5.7, 1.7 Hz), 6.43 (dd, 1H, *J* 5.7, 1.7 Hz), 5.33 (dd, 1H, *J* 1.6, 0.8 Hz), 5.21 (ddd, 1H, *J* 4.7, 1.6, 0.8 Hz), 2.88 (dd, 1H, *J* 12.5, 4.7 Hz), 1.84 (d, 1H, *J* 12.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 132.6, 118.4, 87.6, 79.4, 51.4, 44.3.

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Copy of the IR, ^{1}H NMR and ^{13}C NMR spectra of the desired products

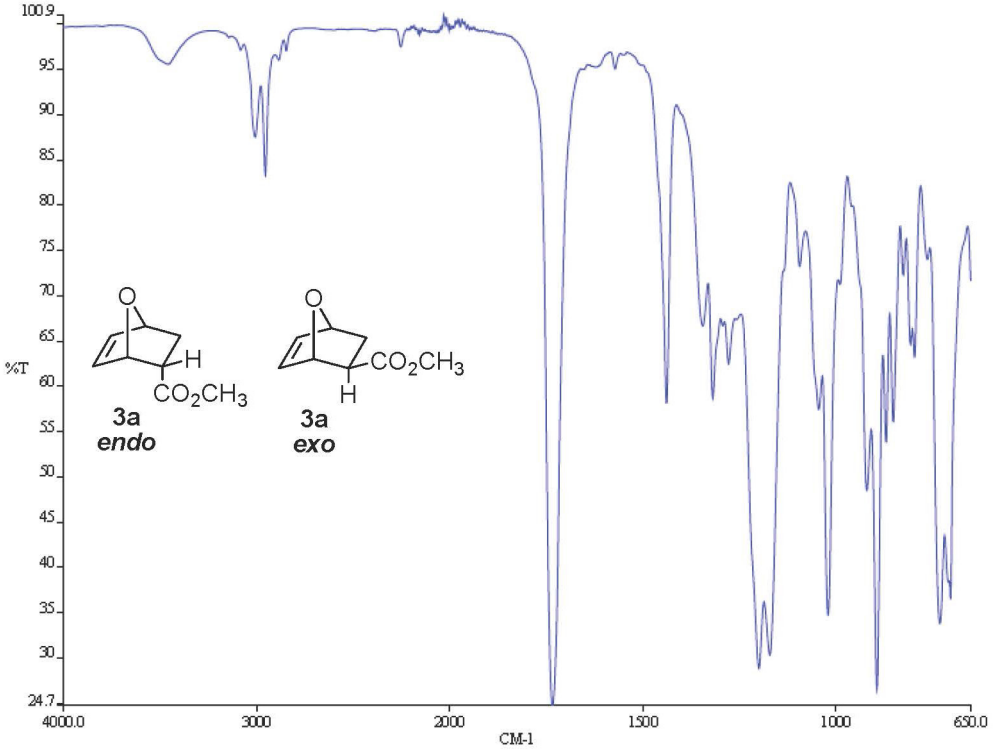

Figure S1. IR spectrum (film) of **3a**.

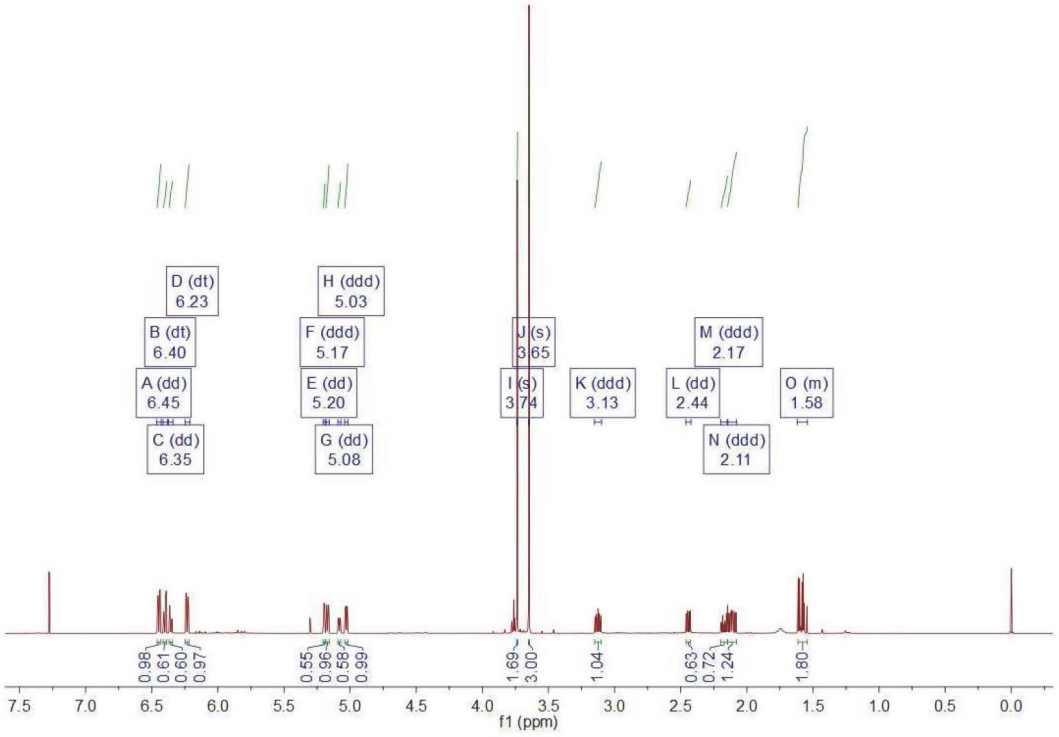

Figure S2. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3a**.

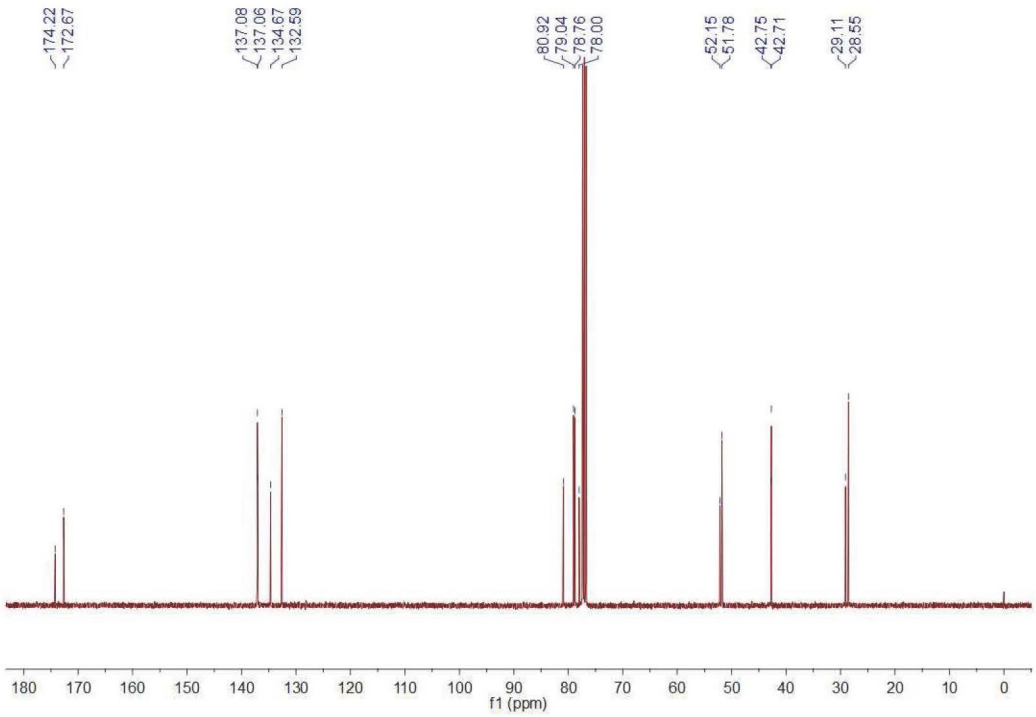

Figure S3. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **3a**.

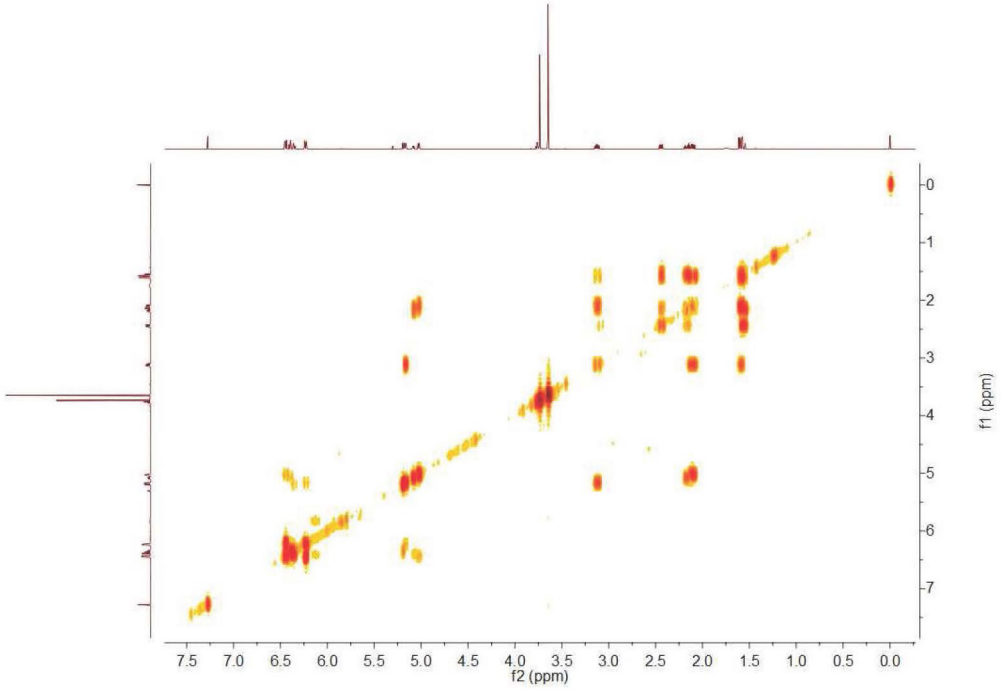

Figure S4. 2D NMR spectrum (^1H,^1H-COSY) of **3a**.

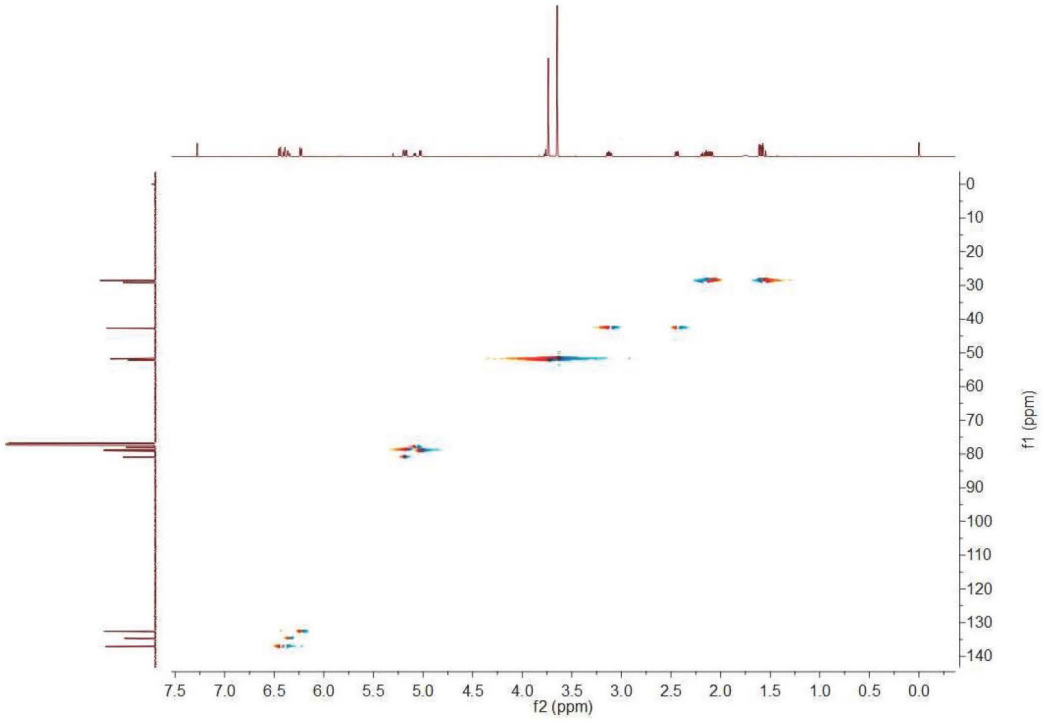

Figure S5. 2D NMR spectrum (^{1}H,^{13}C-HSQC) of **3a**.

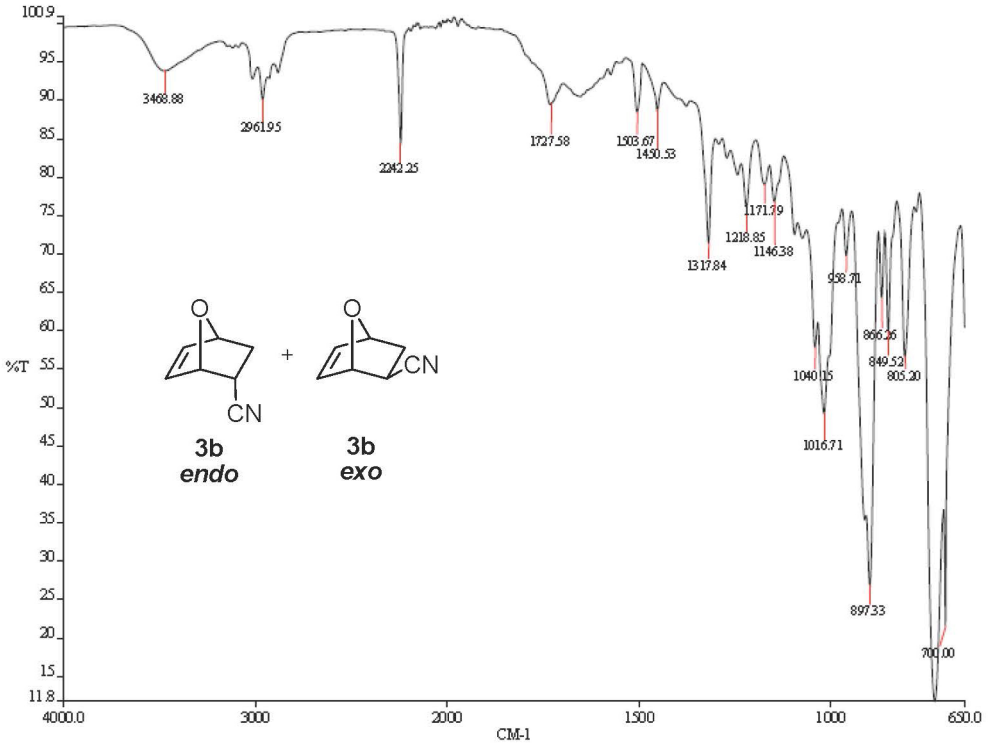

Figure S6. IR spectrum (film) of **3b**.

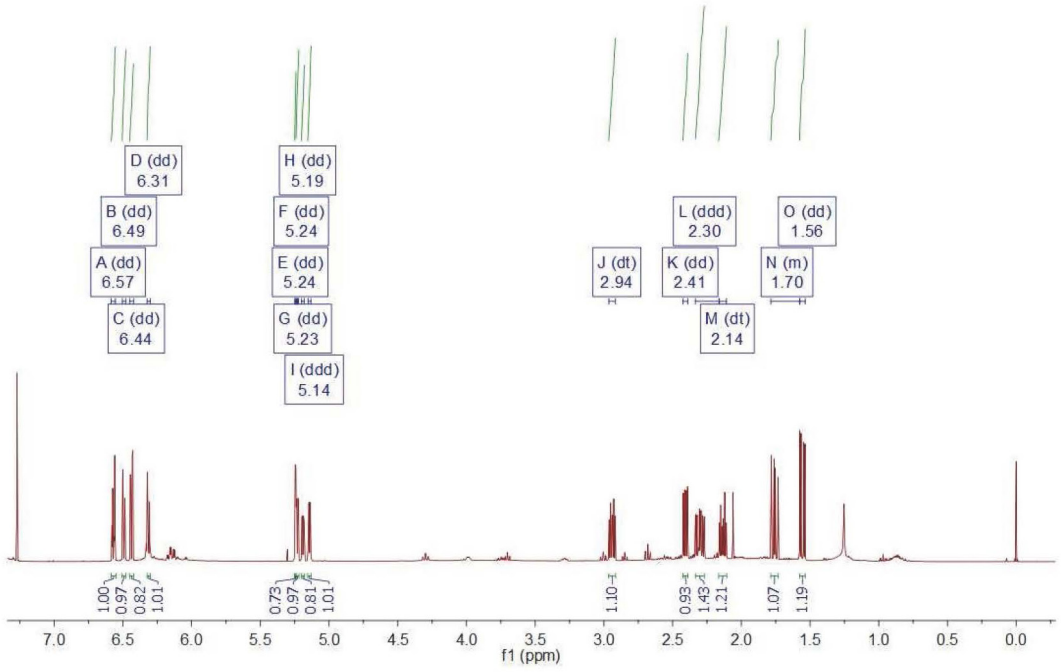

Figure S7. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3b**.

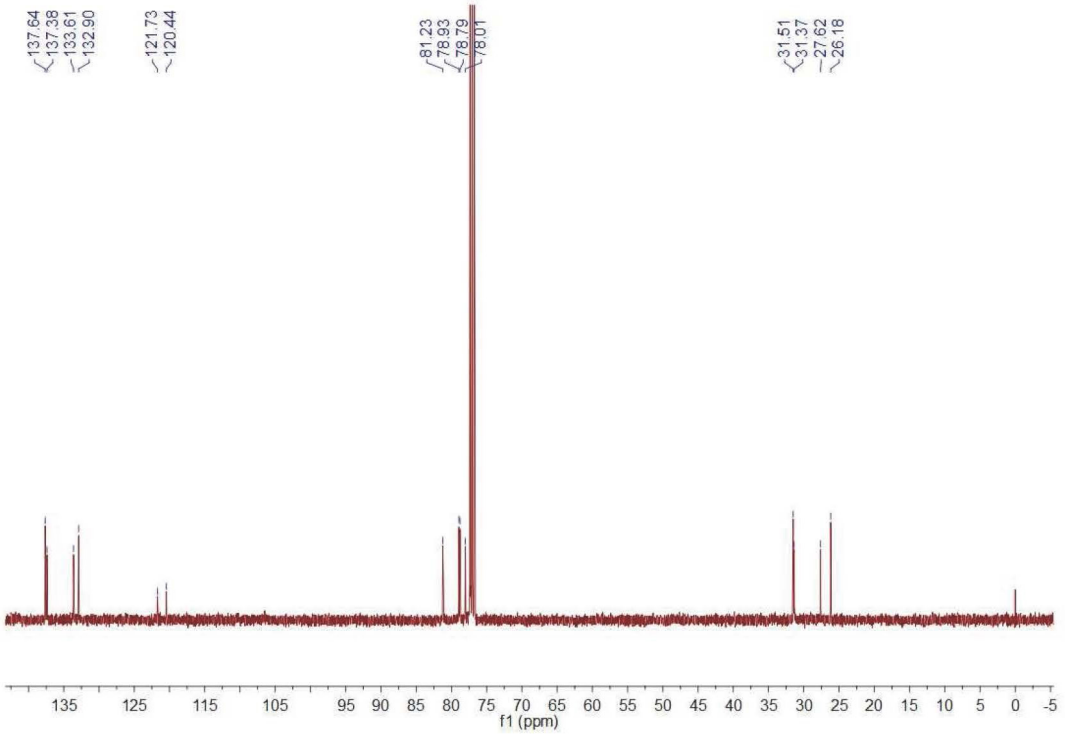

Figure S8. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **3b**.

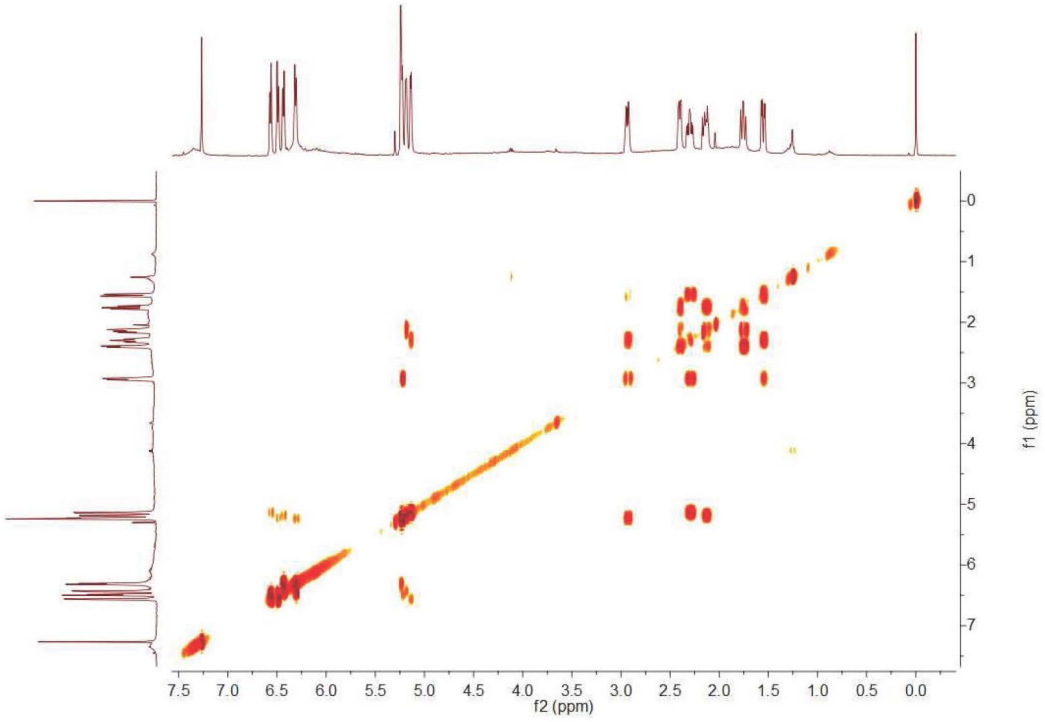

Figure S9. 2D NMR spectrum (^{1}H,^{1}H-COSY) of **3b**.

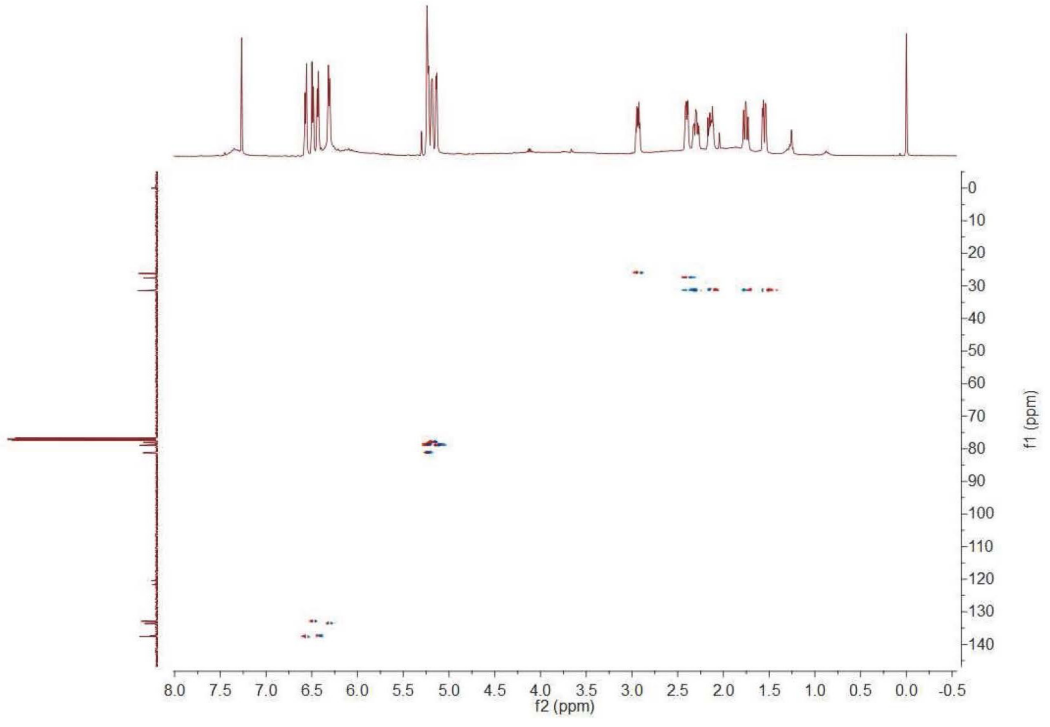

Figure S10. 2D NMR spectrum (^{1}H,^{13}C-HSQC) of **3b**.

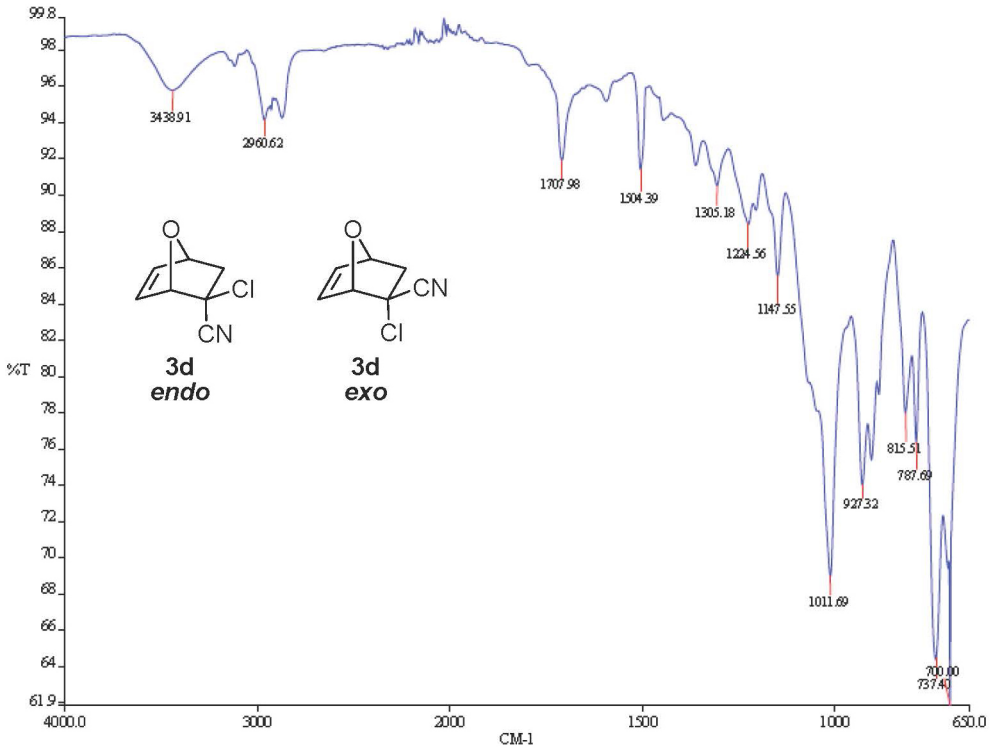

Figure S11. IR spectrum (film) of **3d**.

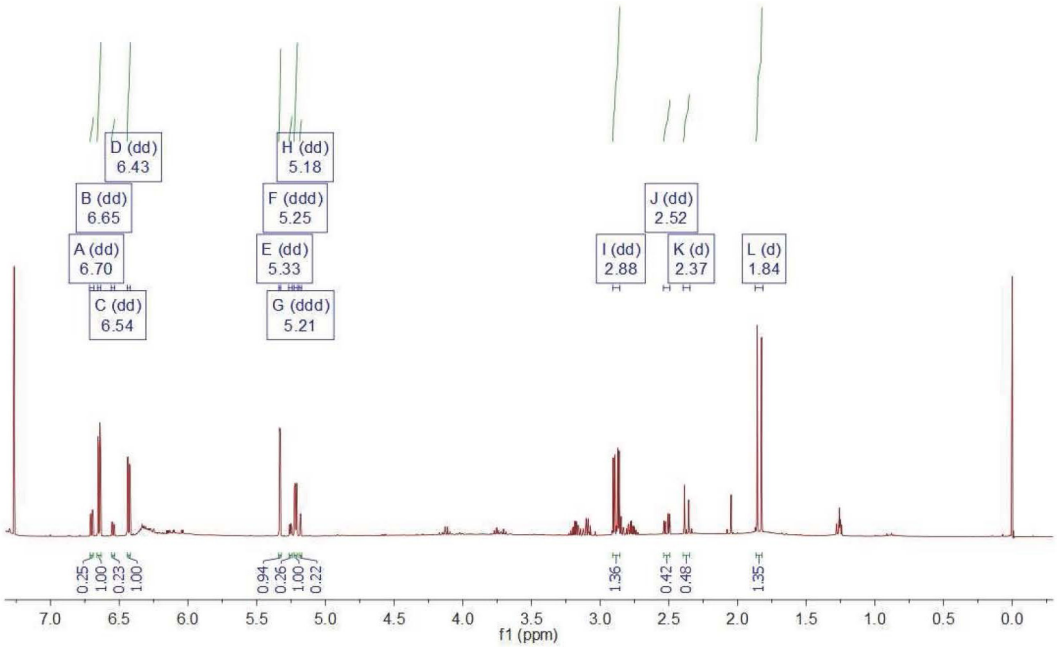

Figure S12. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3d**.

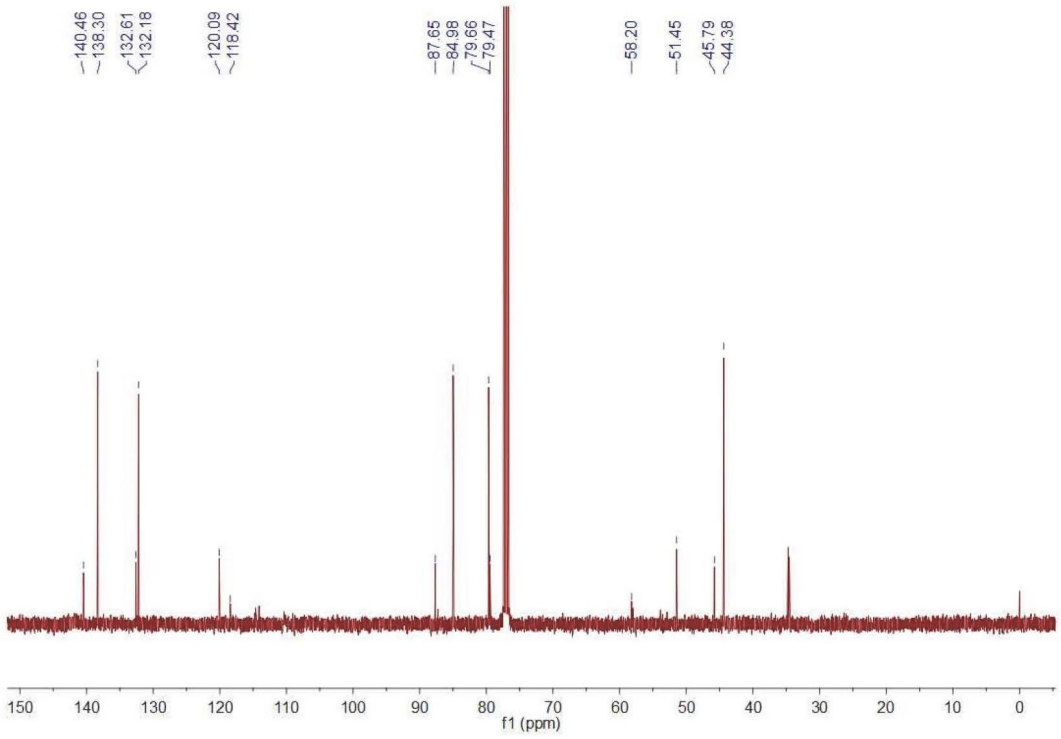

Figure S13. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **3d**.

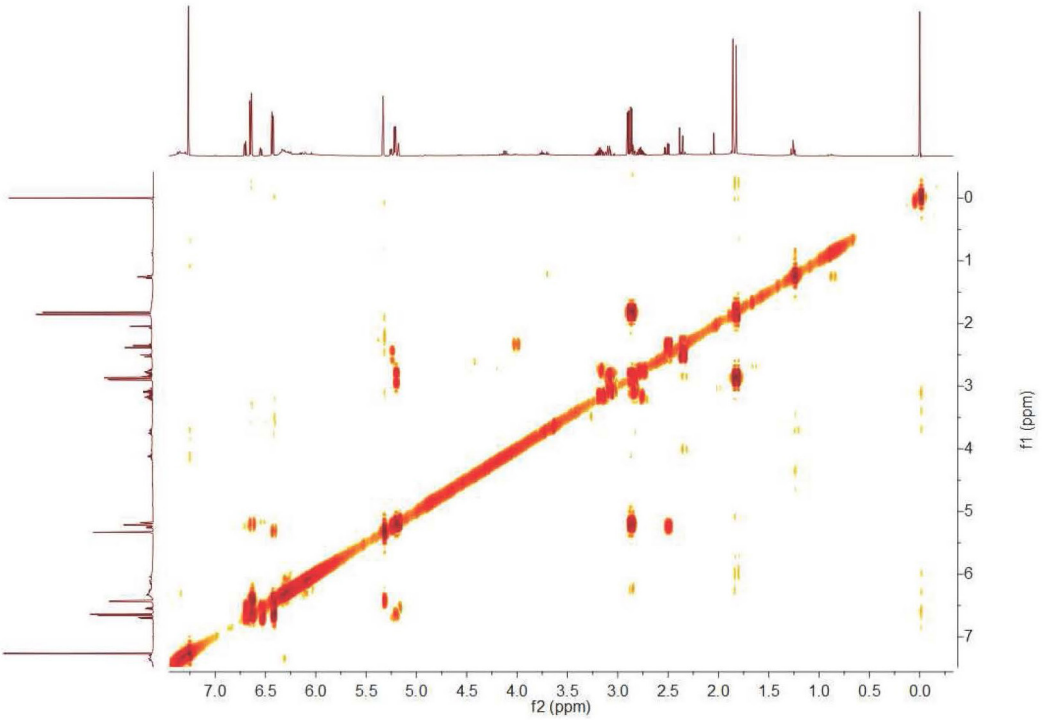

Figure S14. 2D NMR spectrum (^1H,^1H-COSY) of **3d**.

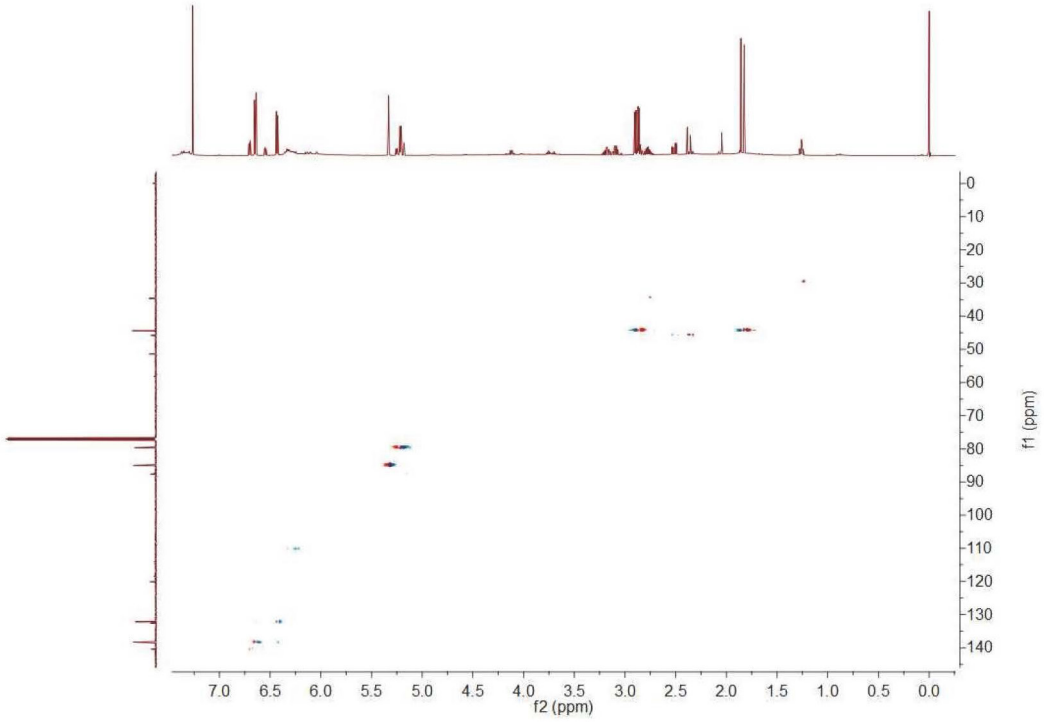

Figure S15. 2D NMR spectrum (^{1}H,^{13}C-HSQC) of **3d**.