

# Adding Diversity to Diiron Aminocarbyne Complexes with Amine

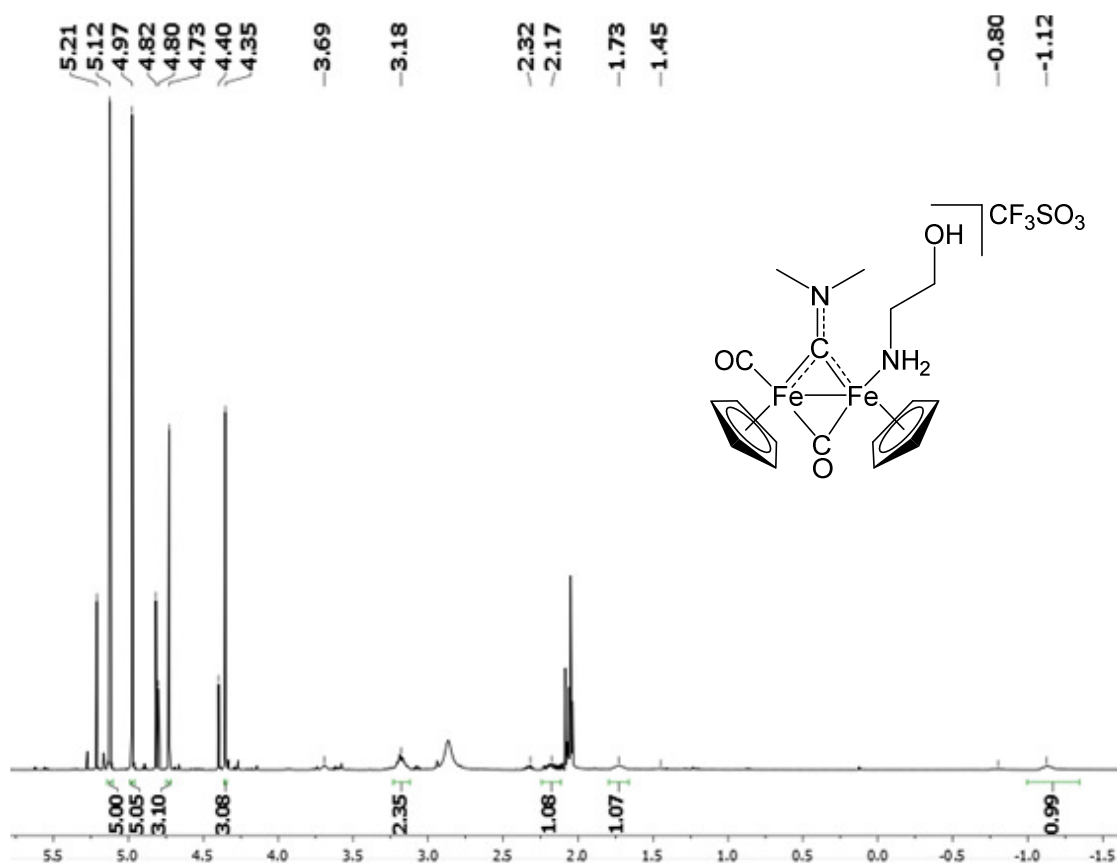
## Ligands

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# Supporting Information

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**Figure S1.**  $^1\text{H}$  NMR spectrum (401 MHz, acetone- $d_6$ ) of **2a** (integration refers to the major isomer)



**<sup>1</sup>H NMR Spectrum (CDCl<sub>3</sub>)**

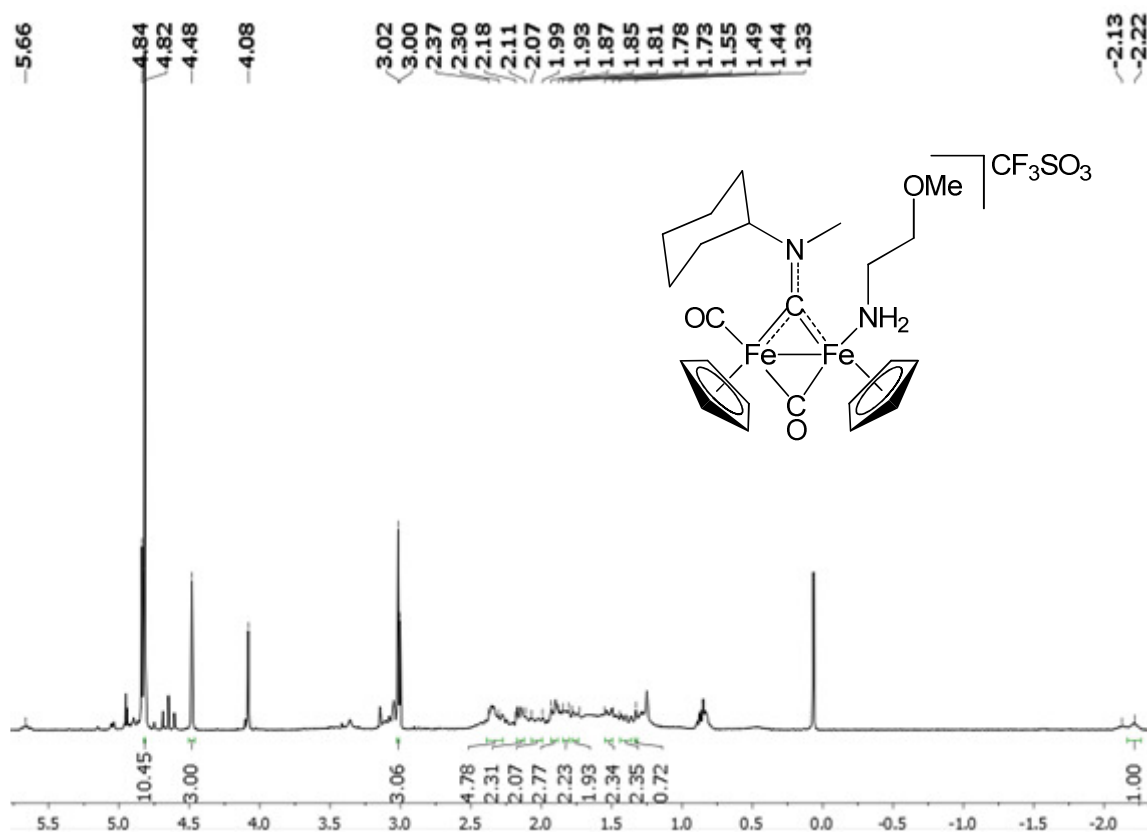
**Chemical Structure:** A ferrocene complex with two cyclopentadienyl rings sandwiching two iron atoms. The left ring is substituted with a cyclopropylmethyl group and a methoxy group (OC). The right ring is substituted with a 2-aminoethoxy group (NH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OH) and a triflate group (OTf, CF<sub>3</sub>SO<sub>3</sub><sup>-</sup>).

**Peak Data:**

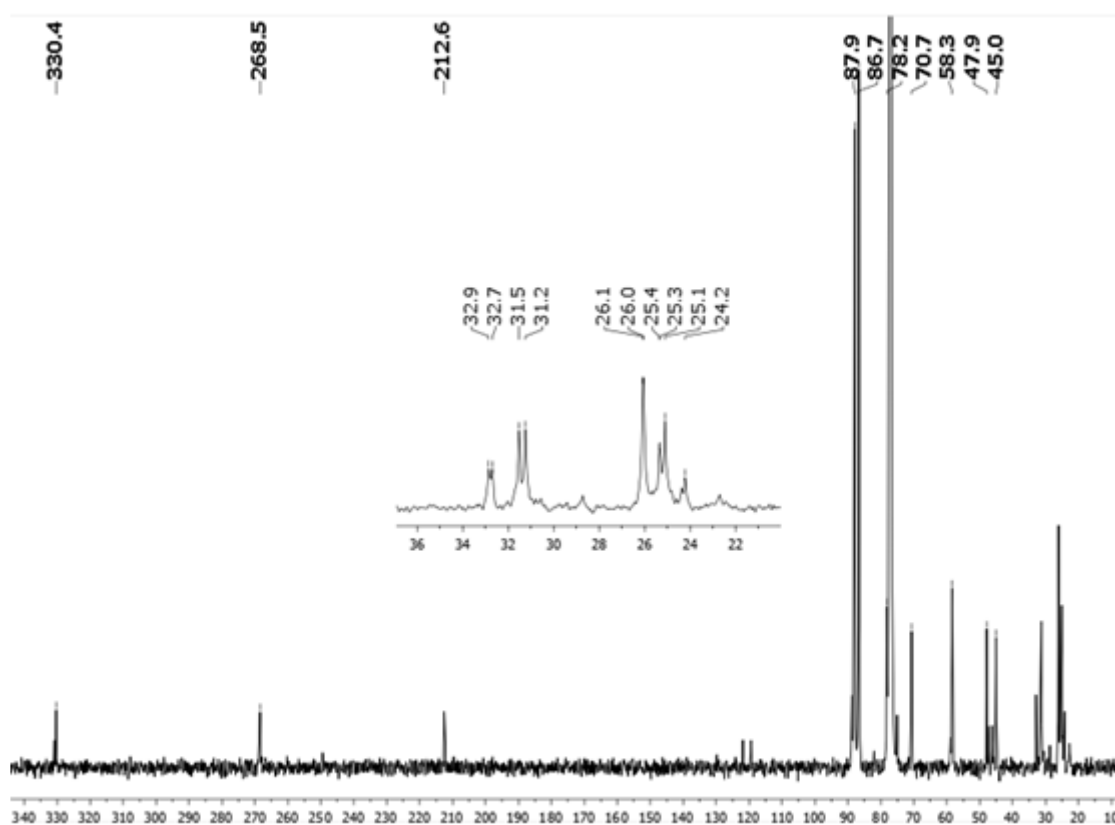
Chemical Shift (ppm)	Integration
-5.66	
-4.85	5.00
-4.83	5.00
-4.80	3.00
-4.79	
-4.50	
-4.09	
-3.60	1.06
-3.39	2.00
-3.32	1.71
-3.20	1.05
-3.13	
-2.84	
-2.43	2.01
-2.35	2.04
-2.31	4.97
-2.28	
-2.20	
-2.11	
-1.57	2.80
-1.45	5.04
-1.41	
-1.29	
-1.23	
-1.39	
-1.94	
-2.14	1.05

<sup>13</sup>C NMR spectrum of compound 1. The x-axis represents chemical shift in ppm, ranging from 0 to 340. The spectrum shows several sharp peaks. Key peaks are labeled with their chemical shift values: 330.46, 268.12, 212.59, 87.95, 86.73, 78.39, 75.35, 60.82, 50.68, 45.14, 32.99, 32.56, 31.82, 31.58, 31.13, 31.03, 30.81, 26.11, 26.03, 25.50, 25.31, 25.08, and 24.47. The peaks are distributed across the spectrum, with a cluster of peaks between 24 and 33 ppm and another cluster between 45 and 88 ppm.

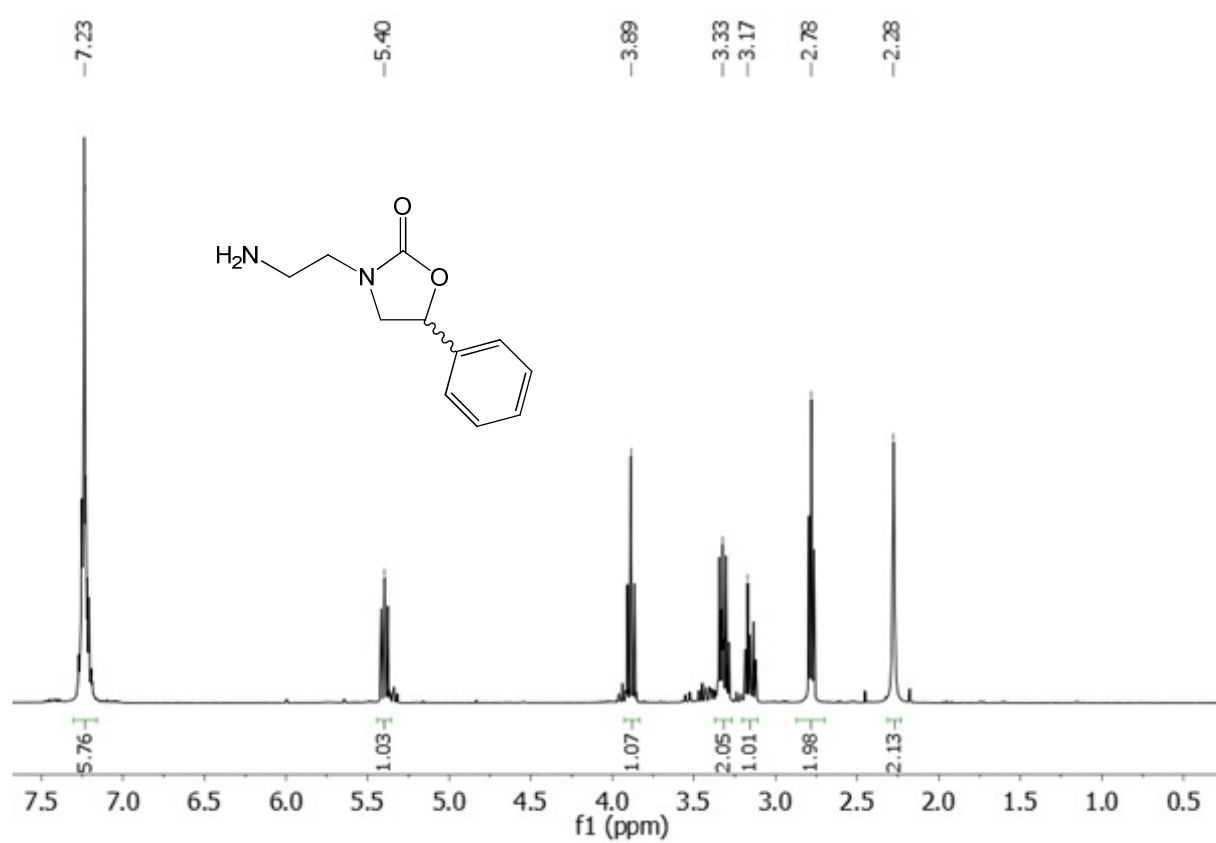
**Figure S5.**  $^1\text{H}$  NMR spectrum (401 MHz,  $\text{CDCl}_3$ ) of **2c** (integration refers to the major isomer)



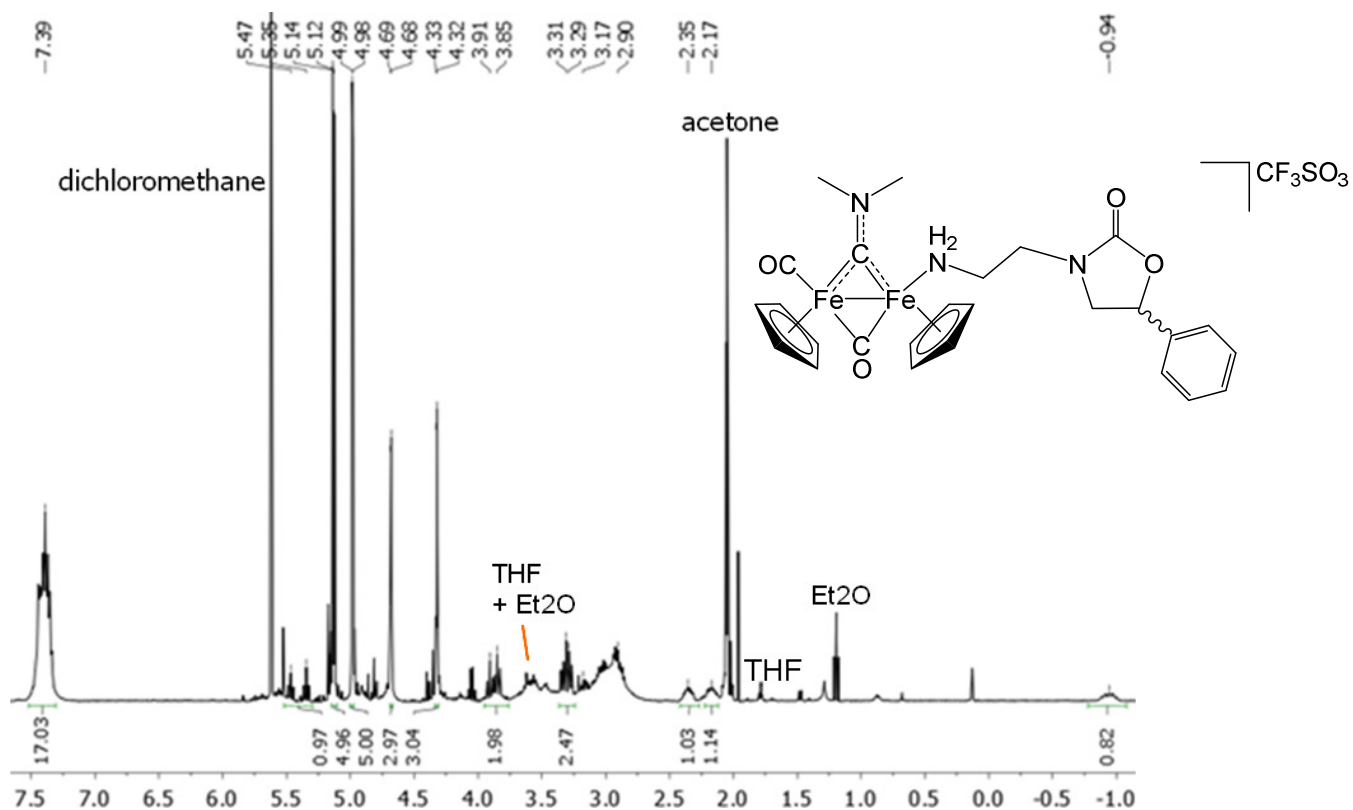
**Figure S6.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of **2c**



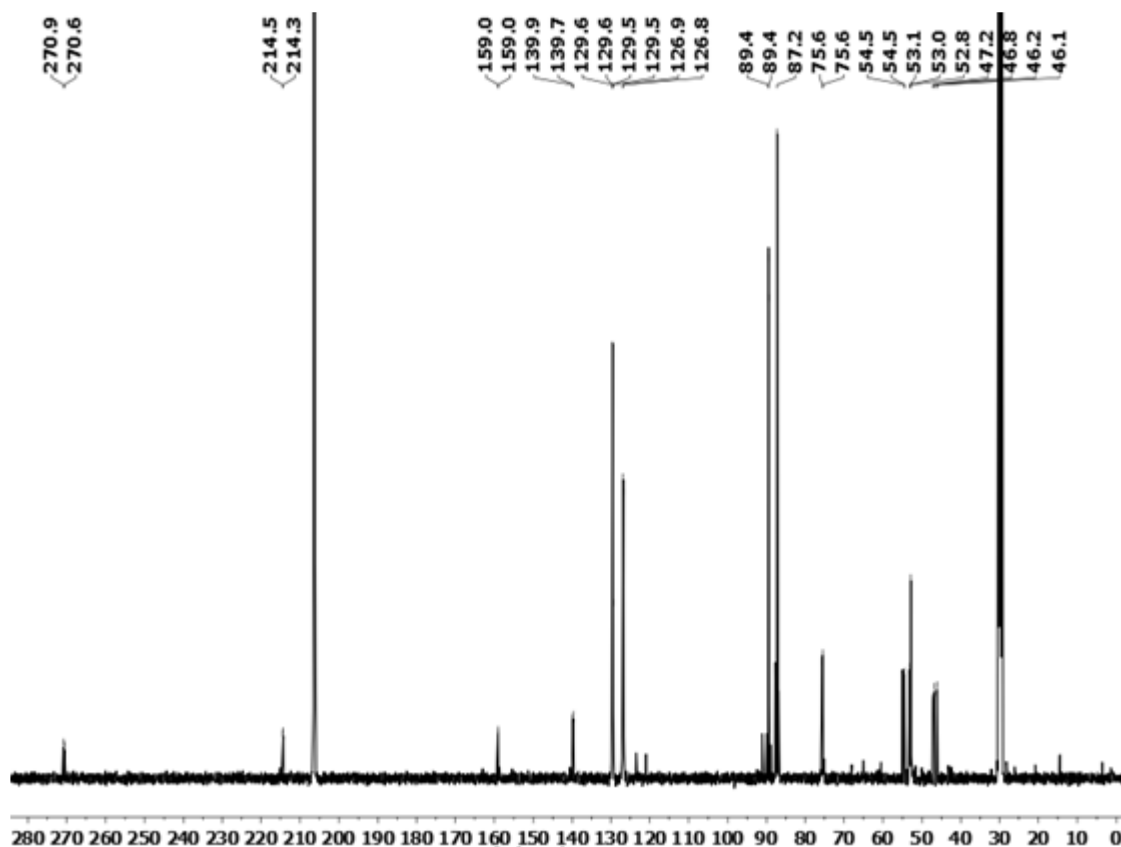
**Figure S7.**  $^1\text{H}$  NMR spectrum (401 MHz,  $\text{CDCl}_3$ ) of  $\text{NH}_2^{\text{ox}}$



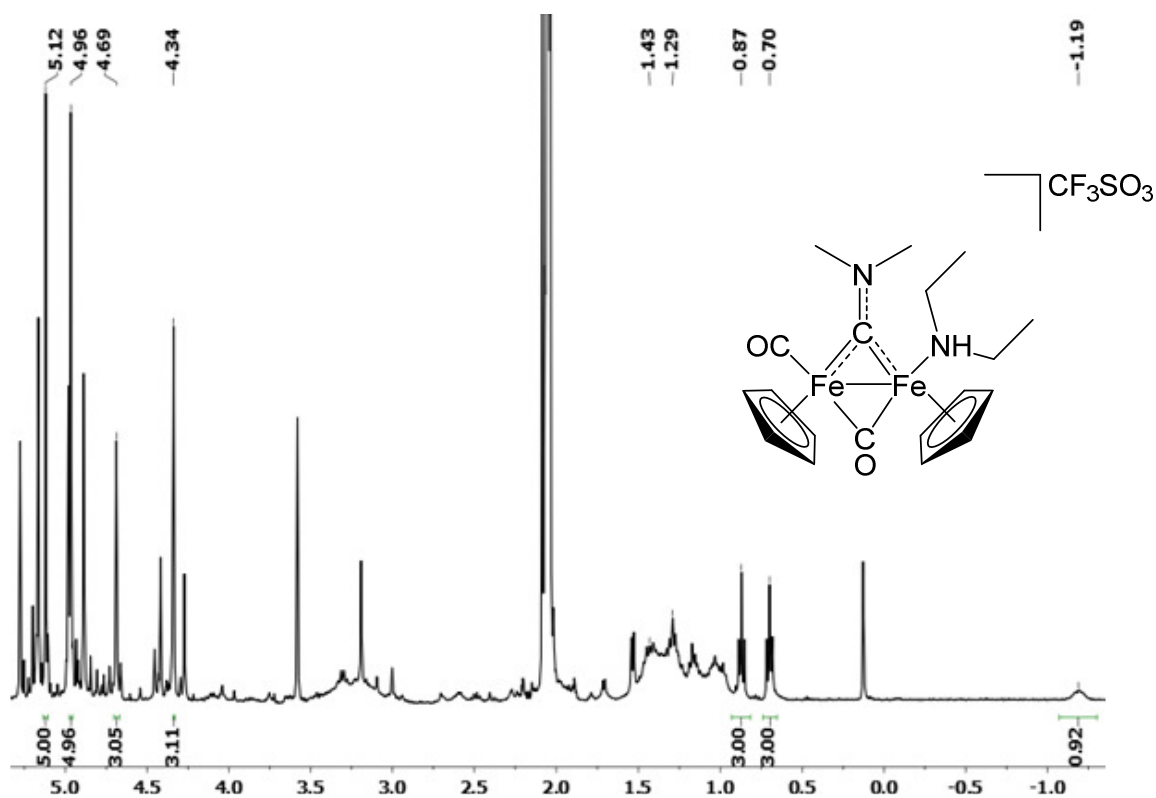
**Figure S8.**  $^1\text{H}$  NMR spectrum (401 MHz, acetone- $d_6$ ) of **3**



**Figure S9.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum (101 MHz, acetone- $d_6$ ) of **3**



**Figure S10.**  $^1\text{H}$  NMR spectrum (401 MHz, acetone- $d_6$ ) of **4a** (integration refers to the major isomer)



**Figure S11.**  $^1\text{H}$  NMR spectrum (401 MHz,  $\text{CDCl}_3$ ) of **4b** (integration refers to the major isomer)

