Supporting Information for:

Substituent Dependence of Imidazoline Derivatives on Capture and Release System of Carbon Dioxide

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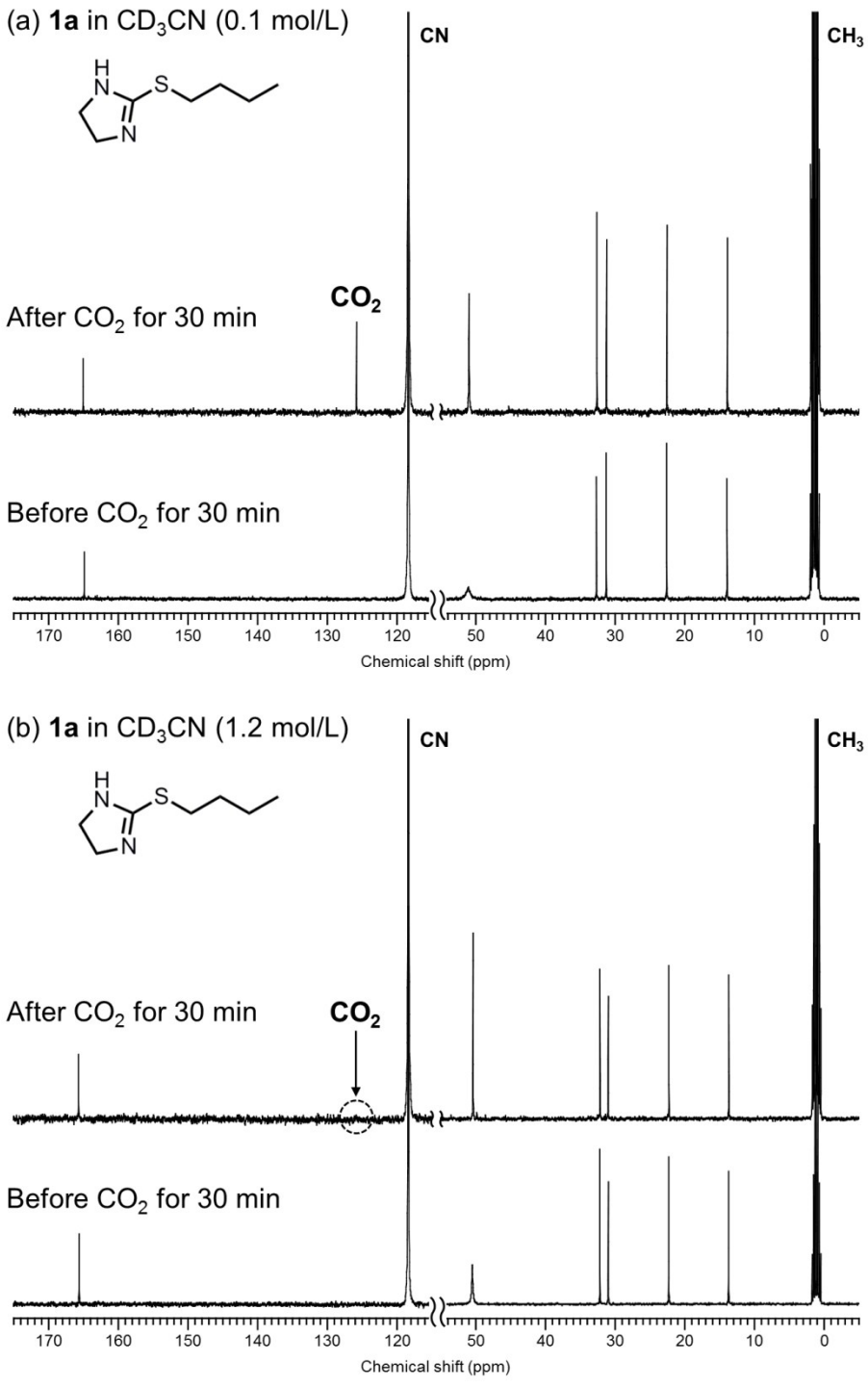

Fig 1S. ^{13}C NMR (100 MHz, 25 °C) spectra of a solution of **1a** in CD_3CN before and after bubbling CO_2 gas.

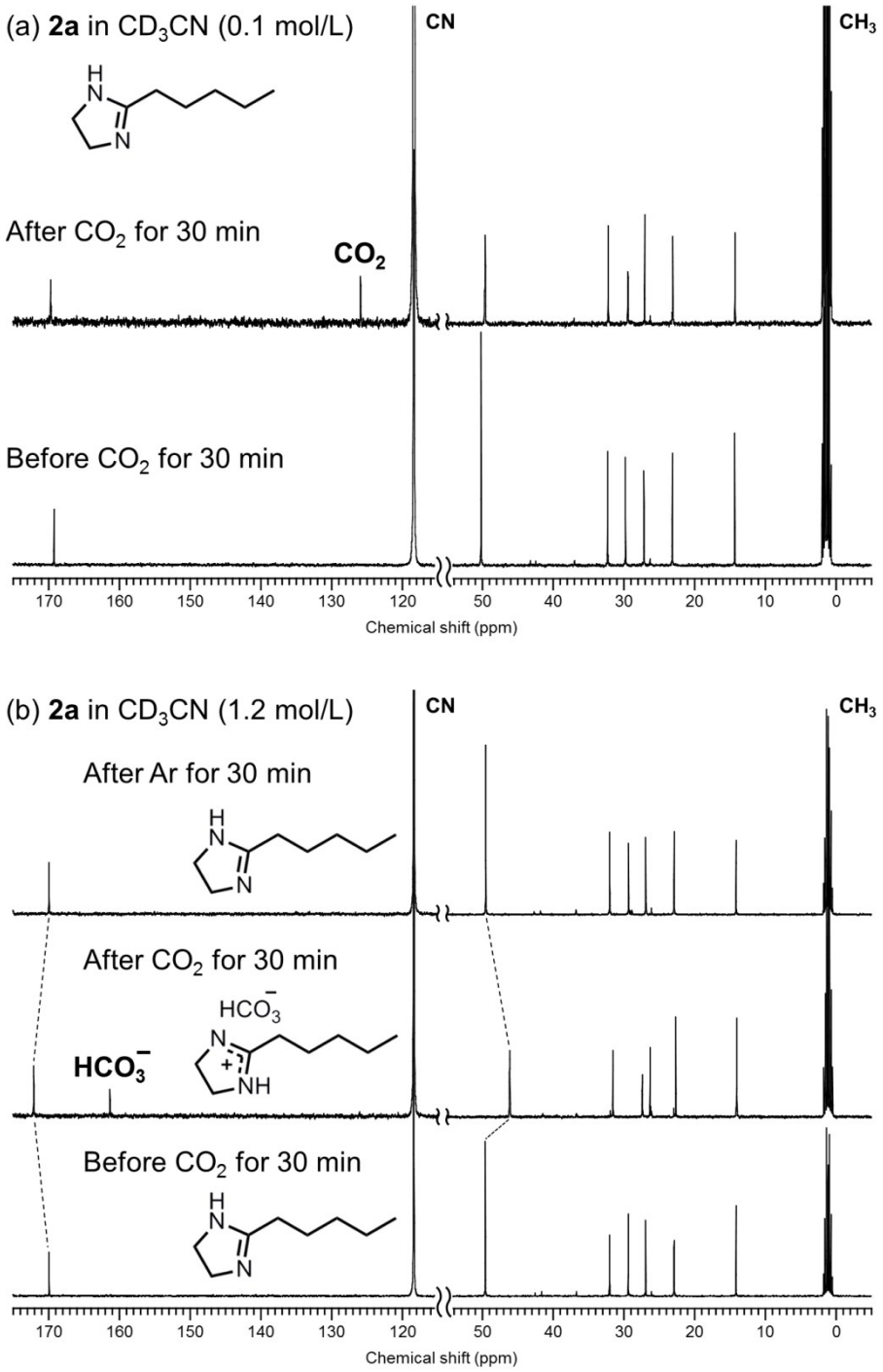

Fig 2S. ^{13}C NMR (100 MHz, 25 °C) spectra of a solution of **2a** in CD_3CN before and after bubbling CO_2 and Ar gas.

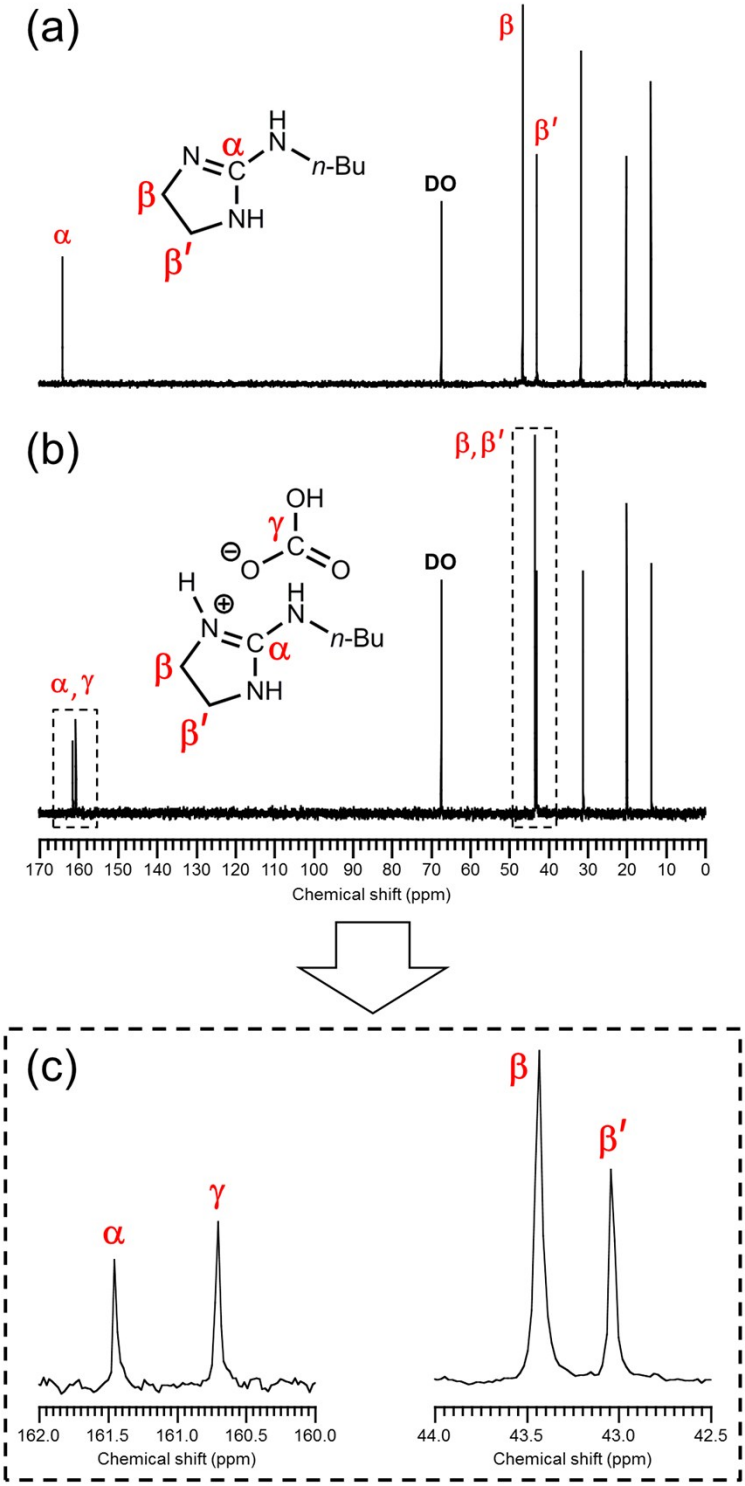

Fig 3S. ^{13}C NMR spectra observed in D_2O containing 1,4-dioxane (DO, 0.4%) of (a) **1c**, (b) **3c**, and (c) **3c** expanded at the range of 42.5-44.0 ppm and 160.0-162.0 ppm.

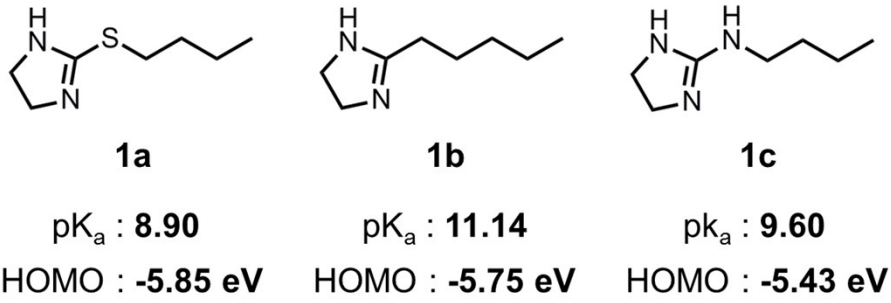

Fig 4S. Predicted pK$_a$ value and HOMO level (eV) of imidazoline derivatives by using Advanced Chemistry Development (ACD/Labs) Software V11.02 (c 1994-2017 ACD/Labs) for pK$_a$ and DFT calculation (B3LYP/6-31G*) for HOMO level.

Table S1. CO_2 fixation efficiency and adsorption capacity of **1c** with flows of CO_2 and Ar[a]

Time	CO_2 fixation efficiency (%)[b,c]					CO_2 adsorption capacity (mg/g)[b,c]				
(min)	1st		2nd		3rd	1st		2nd		3rd
	CO_2	Ar	CO_2	Ar	CO_2	CO_2	Ar	CO_2	Ar	CO_2
10	98.7	9.6	99.1	9.6	98.7	307.5	29.9	308.8	30.0	307.3
20	99.0	7.4	99.2	7.5	98.8	308.3	23.1	309.1	23.4	307.9
30	99.2	6.1	99.2	6.1	98.9	308.9	18.9	309.1	19.1	307.9
60	99.3	2.7	99.3	2.7	99.3	309.4	8.3	309.3	8.6	309.5

[a] Under CO_2 and Ar flows (0.2 L/min) at 25 °C and 60 °C in dry DMSO. [b] Calculated based on bicarbonate **3c**. [c] Estimated from weight change of the reaction mixture.