Electronic Supplementary Material (ESI) for New Journal of Chemistry
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Kinetic Analysis of CO-releasing of a Diiron Hexacanbonyl Complex Promoted by Amino Acids

Limei Chen [1, 2], Xiujuan Jiang [2], Xiu Wang [2], Li Long [2], Jiayao, Zhang [2], Xiaoming Liu [1, 2]*

[1]School of Metallurgy and Chemical Engineering, Jiangxi University of Science and Technology

[2]College of Biological, Chemical Sciences and Engineering, Jiaxing University

Supporting information

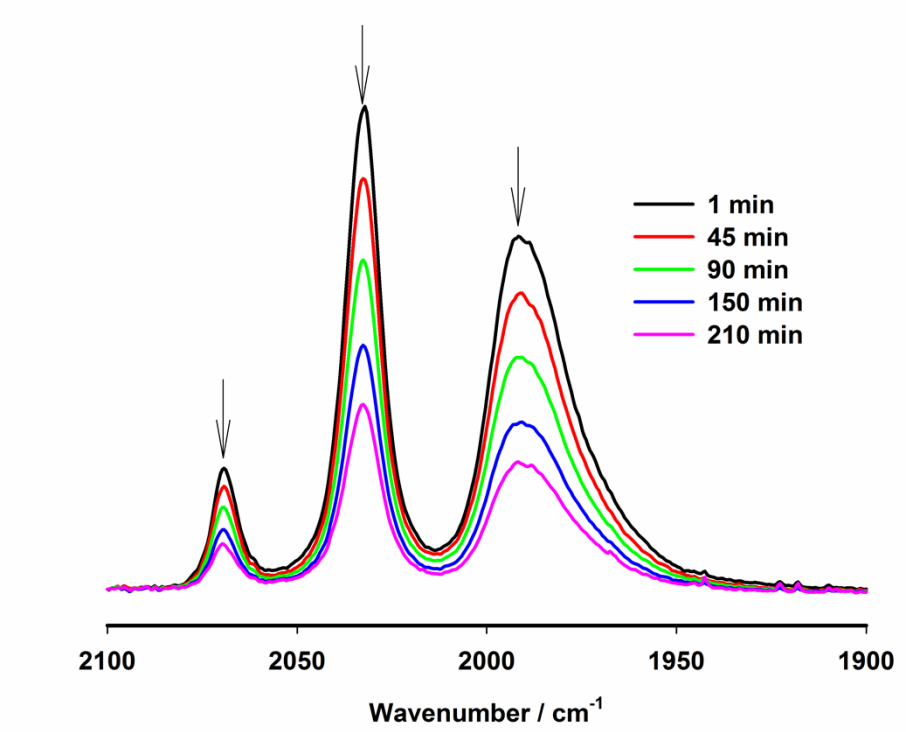


Fig. S1 Infrared spectral variation during the CO-releasing process ([**1**] = 0.0115 mol L^{-1} and [L-proline] = 0.0345 mol L^{-1}) in DMSO / H_2O mixture at 37 ℃ under open atmosphere.

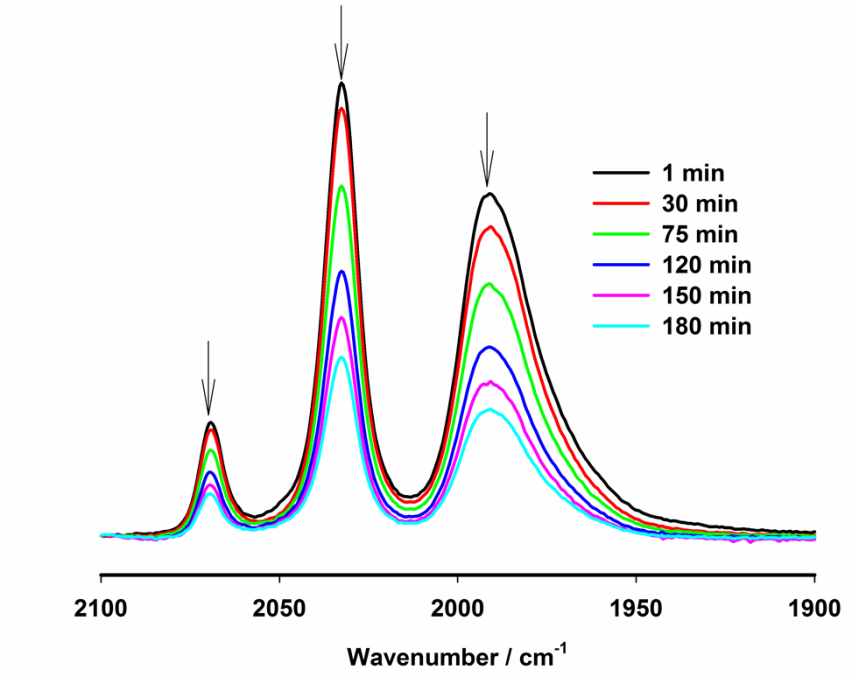


Fig. S2 Infrared spectral variation during the CO-releasing process ([**1**] = 0.0115 mol L^{-1} and [L-histidine] = 0.0345 mol L^{-1}) in DMSO / H_2O mixture at 37 ℃ under open atmosphere.

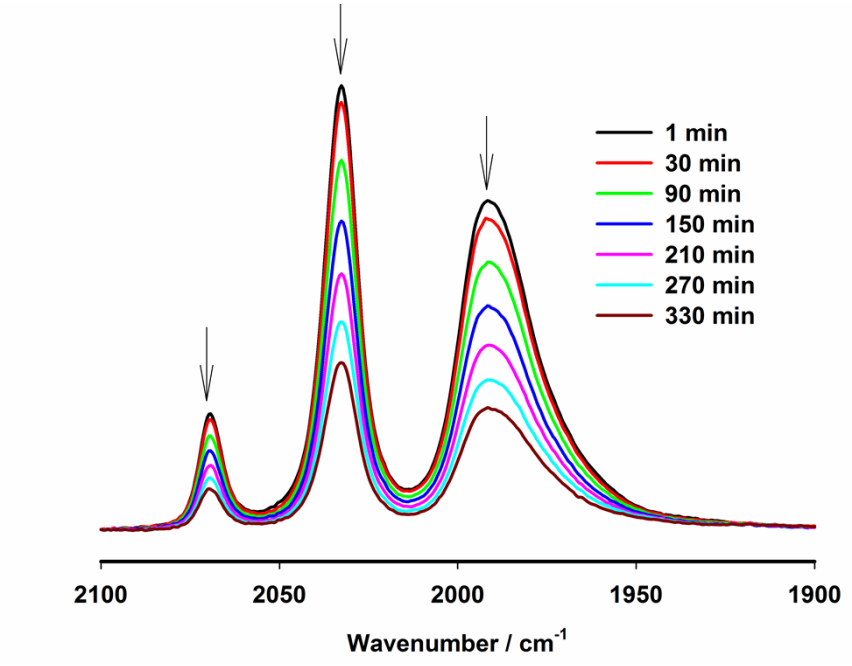


Fig. S3 Infrared spectral variation during the CO-releasing process ([**1**] = 0.0115 mol L^{-1} and [alanine] = 0.0345 mol L^{-1}) in DMSO / H_2O mixture at 37 ℃ under open atmosphere.

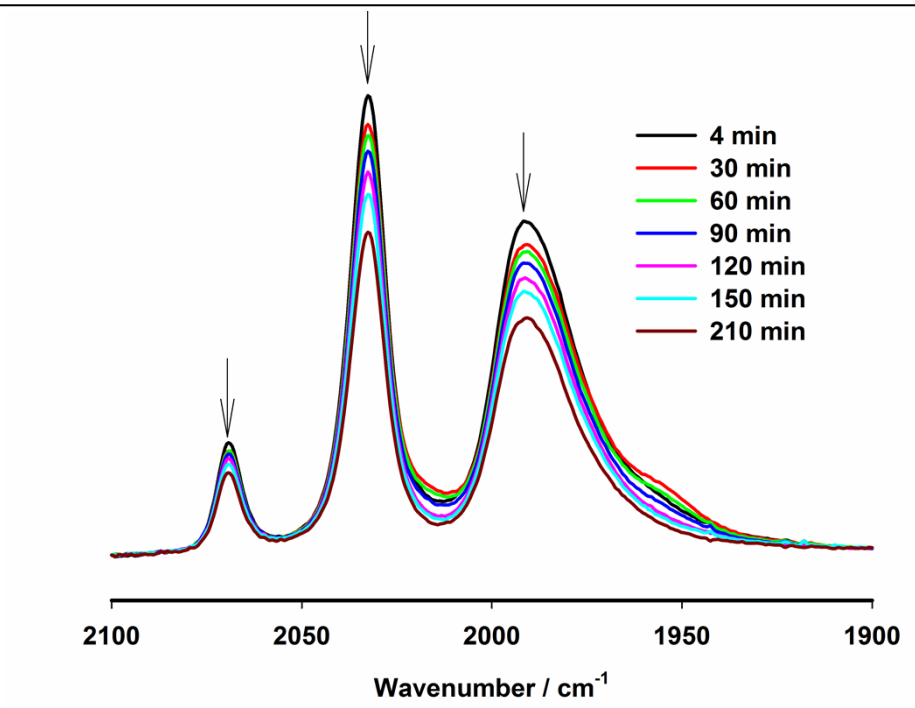
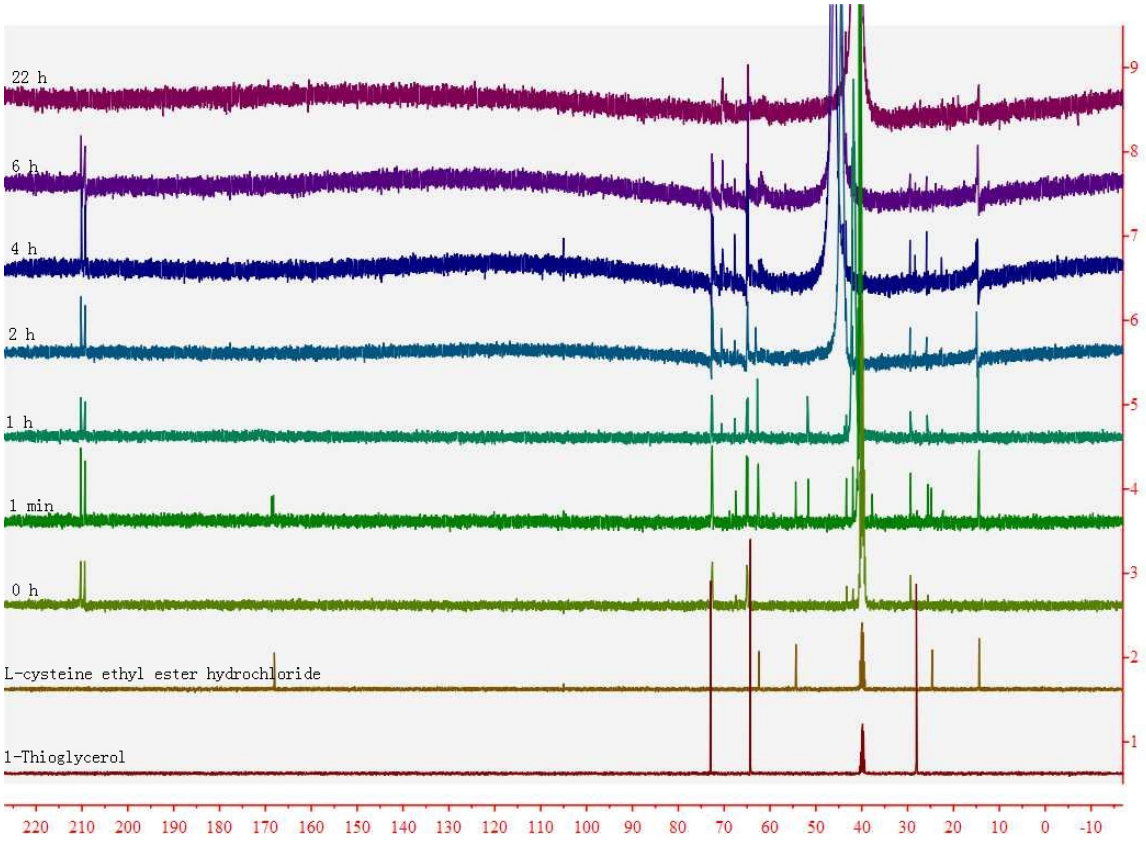


Fig. S4 Infrared spectral variation during the CO-releasing process ([**1**] = 0.0115 mol L^{-1} and [L-cysteine ethyl ester hydrochloride] = 0.0345 mol L^{-1}) in DMSO / H_2O mixture at 37 ℃ under open atmosphere.



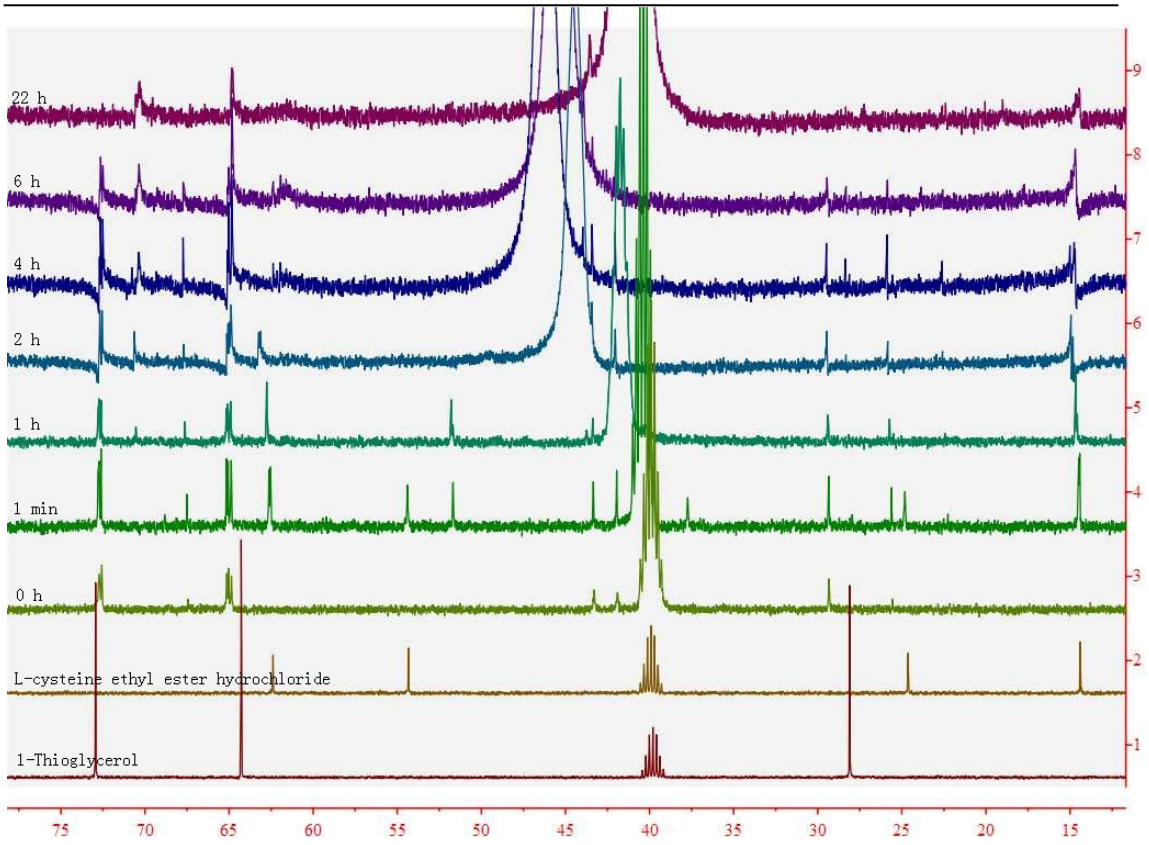


Fig. S5 ^{13}C NMR spectroscopic variation with reaction time of complex **1** under the substitution of L-cysteine ethyl ester hydrochloride (for comparison, the chemical shifts of free 1-thioglycerol, L-cysteine ethyl ester hydrochloride and complex **1** are also included).

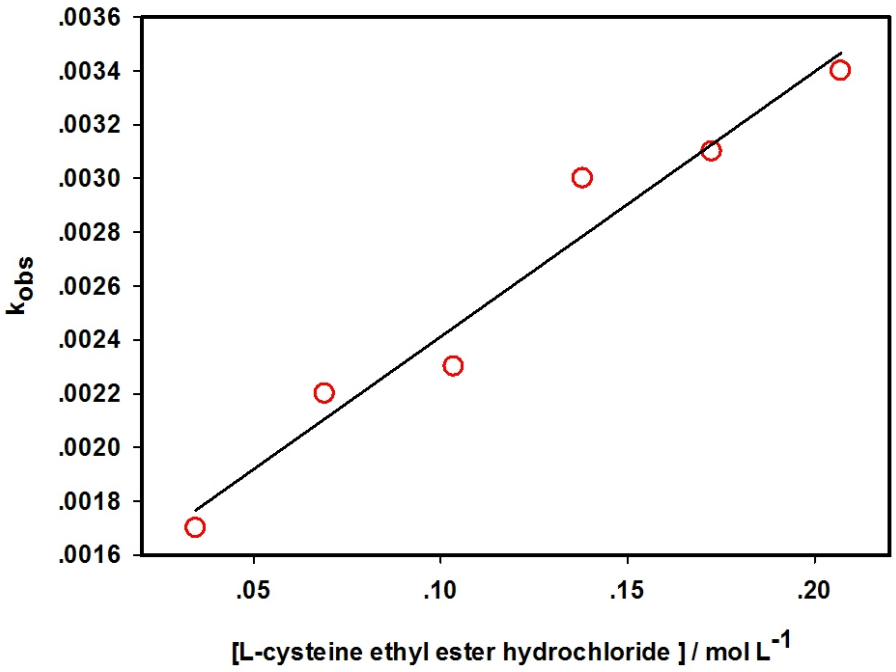


Fig. S6 Plot of k_{obs} *versus* the concentration of L-cysteine ethyl ester hydrochloride in which the concentration of complex **1** was kept at 0.0115 mol L^{-1}.

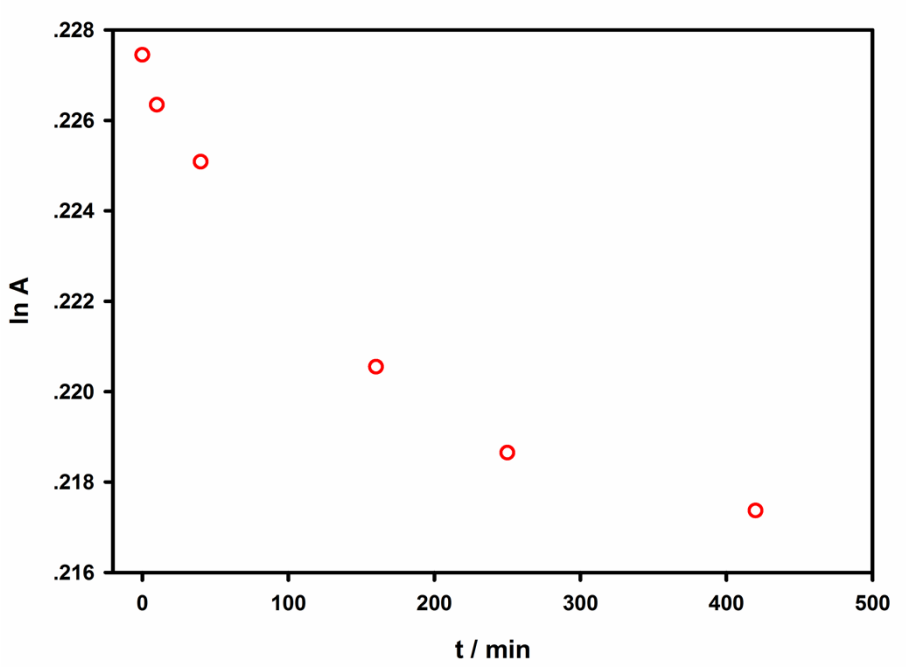


Fig. S7 The logarithmic plots of concentrations of complex **1** against reaction time in the presence of pyridine in DMSO / H_2O mixture (4:1) at 37 ℃ under open

atmosphere ([**1**] = 0.0115 mol L^{-1}, the absorbance used for the kinetic analysis was used at 2032 cm^{-1}).

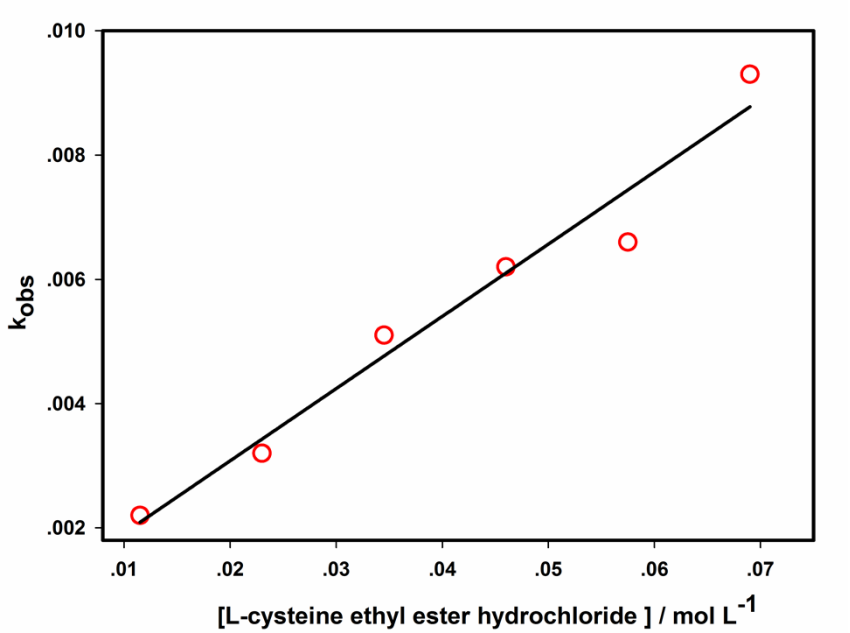


Fig. S8 Plot of k_{obs} *versus* the concentration of L-cysteine ethyl ester hydrochloride in the second stage ([**1**] = 0.0115 mol L^{-1} in D_2O).

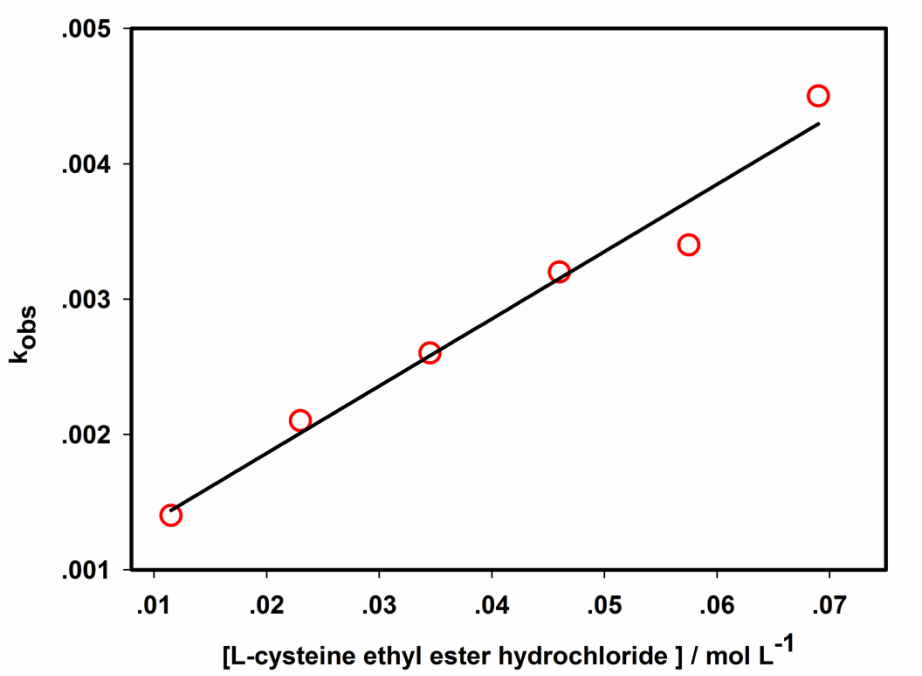


Fig. S9 Plot of k_{obs} *versus* the concentration of L-cysteine ethyl ester hydrochloride in the second stage ([**1**] = 0.0115 mol L^{-1} in physiological saline).

Table S1 The kinetic data of the decomposition of complex **1** in D_2O and physiological saline at 37℃ in the second stage, respectively ([**1**] = 0.0115 mol L^{-1}, [L-cysteine ethyl ester hydrochloride] / [**1**] = 3, 6, 9, 12, 15 and 18, respectively).

k_{obs} × 10 $^{-3}$ (D_2O)	2.2	3.2	5.1	6.2	6.6	9.3
$t_{1/2}$ (min) (D_2O)	315	217	136	112	105	75
k_{obs} ×10 $^{-3}$ (physiological saline)	1.4	2.1	2.6	3.2	3.4	4.5
$t_{1/2}$ (min) (physiological saline)	495	330	267	217	204	154