Supplementary Information

Investigation of Isomer Formation Upon Coordination of Bifunctional Histidine Analogues with $^{99m}Tc/Re(CO)_3$

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N^{α}-benzyl-L-histidine (6)

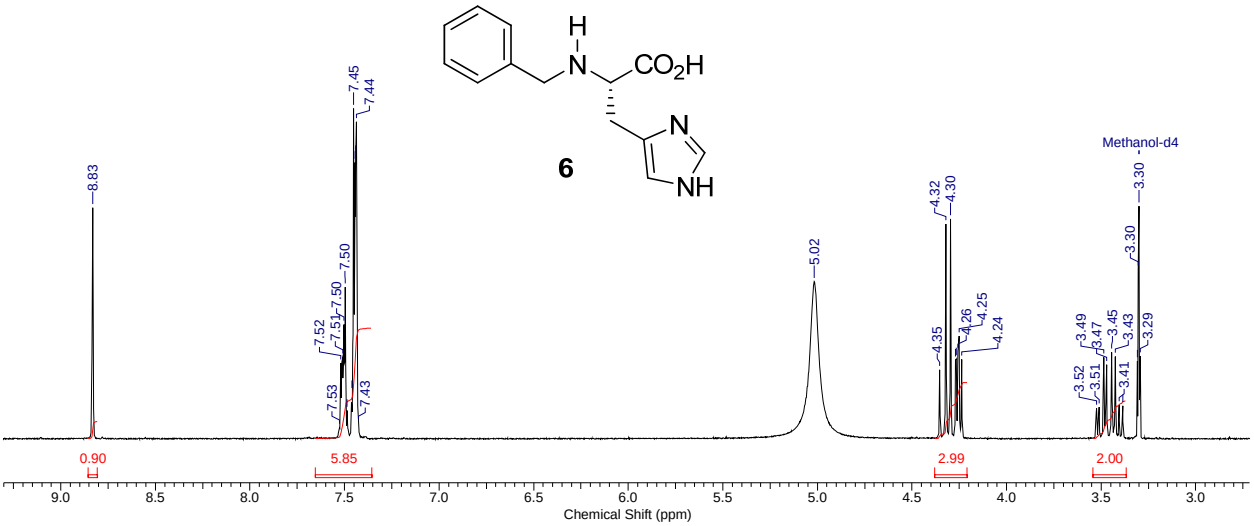


Fig. S1: ^{1}H NMR (400 MHz, $CDCl_3$) of **6**

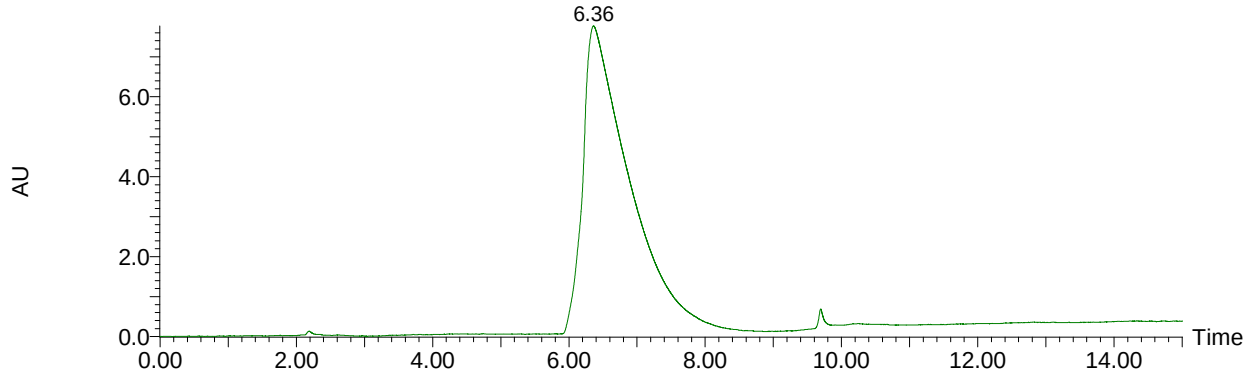


Fig. S2: Analytical HPLC trace, UV absorbance detected from 210-800 nm (RP-C18 4.6 x 250 mm, 5 µm), of **6**

Rhenium(I) tricarbonyl-N$^{\alpha}$-benzyl-L-histidine (1)

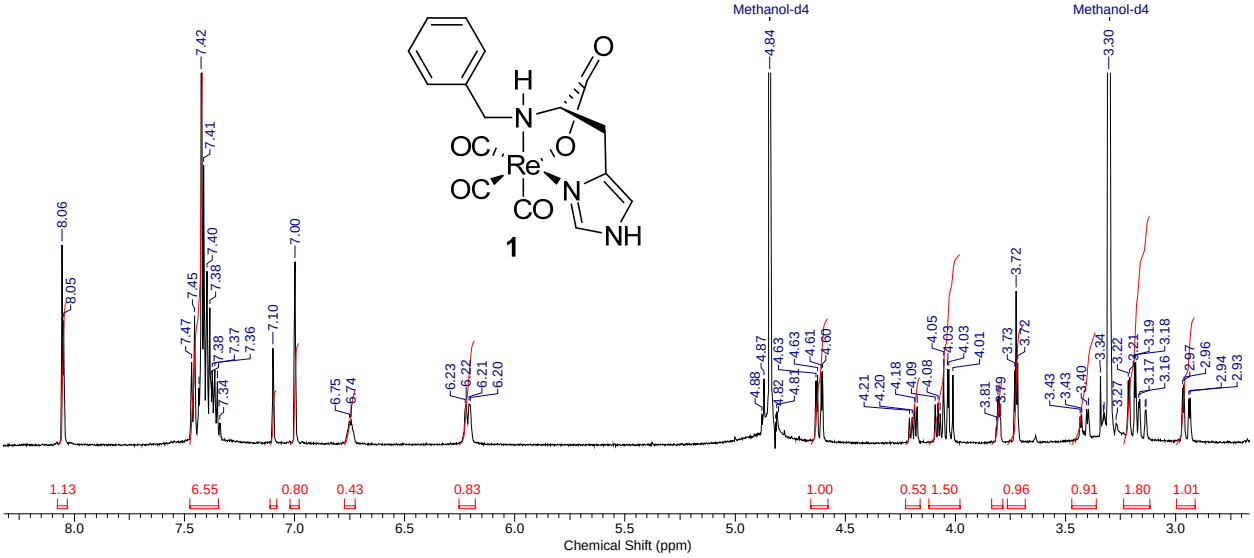


Fig. S3: ^{1}H NMR (400 MHz, MeOH-d4) of **1**

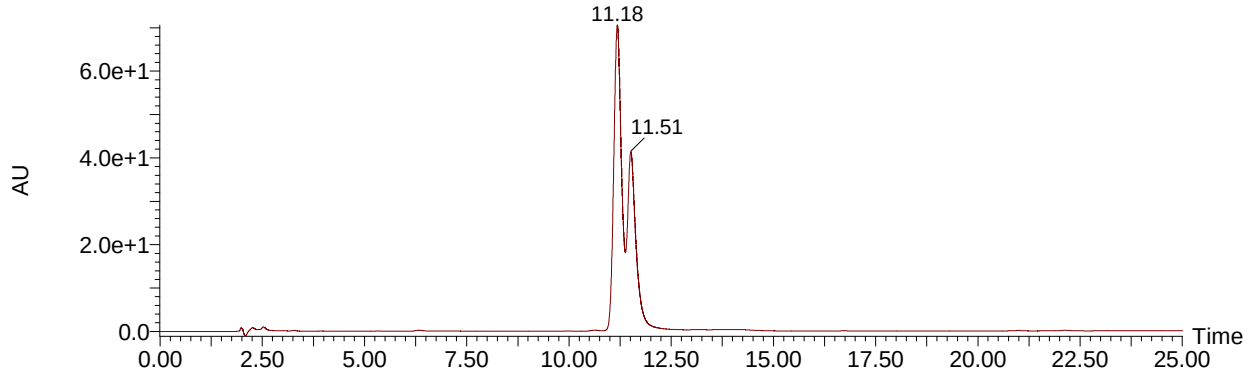


Fig. S4: Analytical HPLC trace, UV absorbance detected from 210-800 nm (RP-C18 4.6 x 250 mm, 5 µm), of **1**

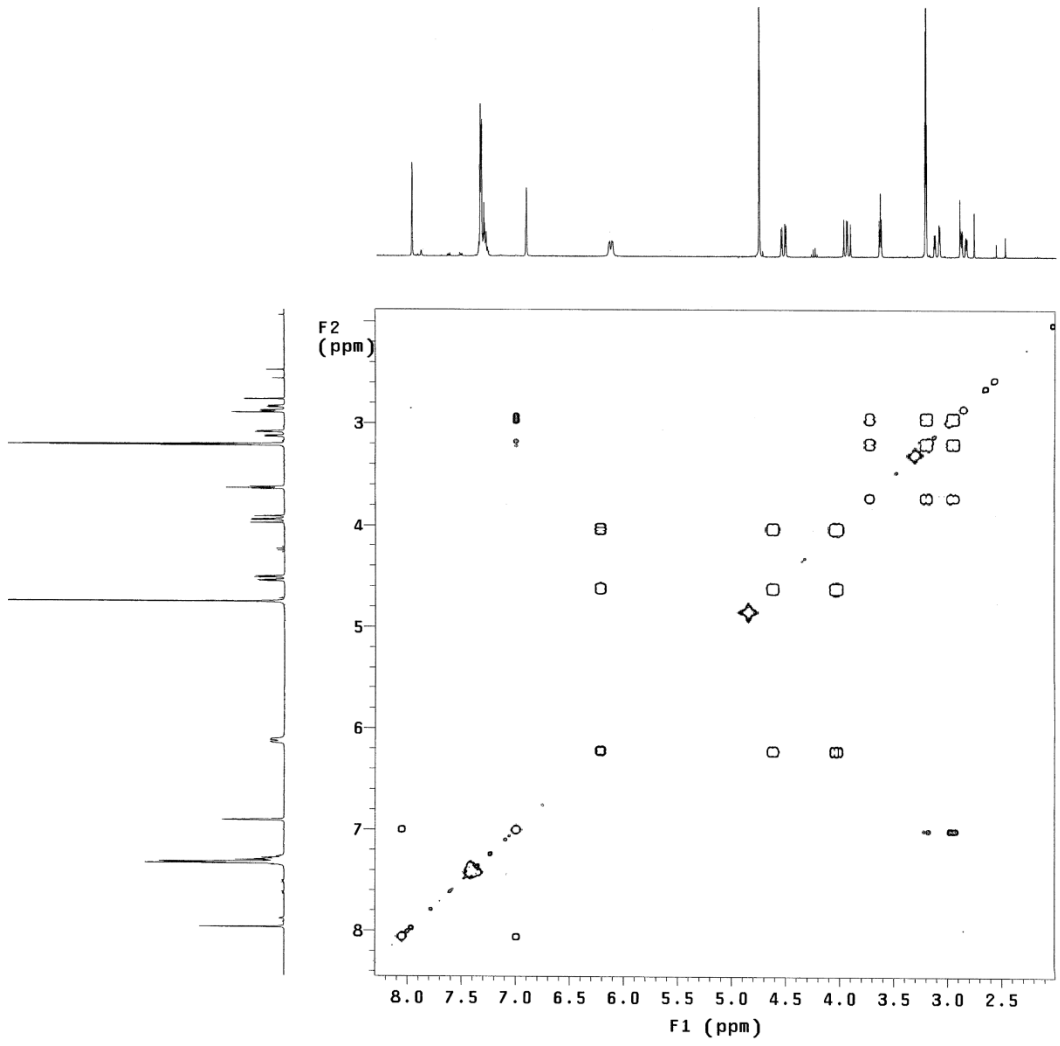


Fig. S5: gCOSY spectrum (400 MHz, MeOH-d4) of **1**

N^{α}-benzyl-L-histidine(Trt)-OMe (8)

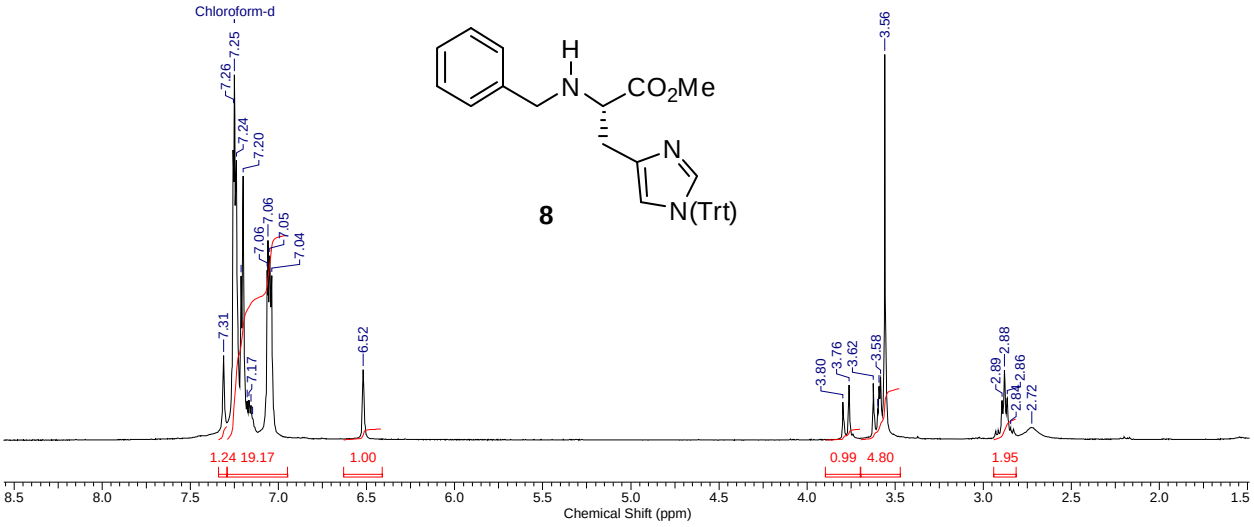


Fig. S6: ^{1}H NMR (400 MHz, $CDCl_3$) of **8**

Rhenium(I) tricarbonyl-N$^{\alpha}$-benzyl-L-histidine(Trt) (2)

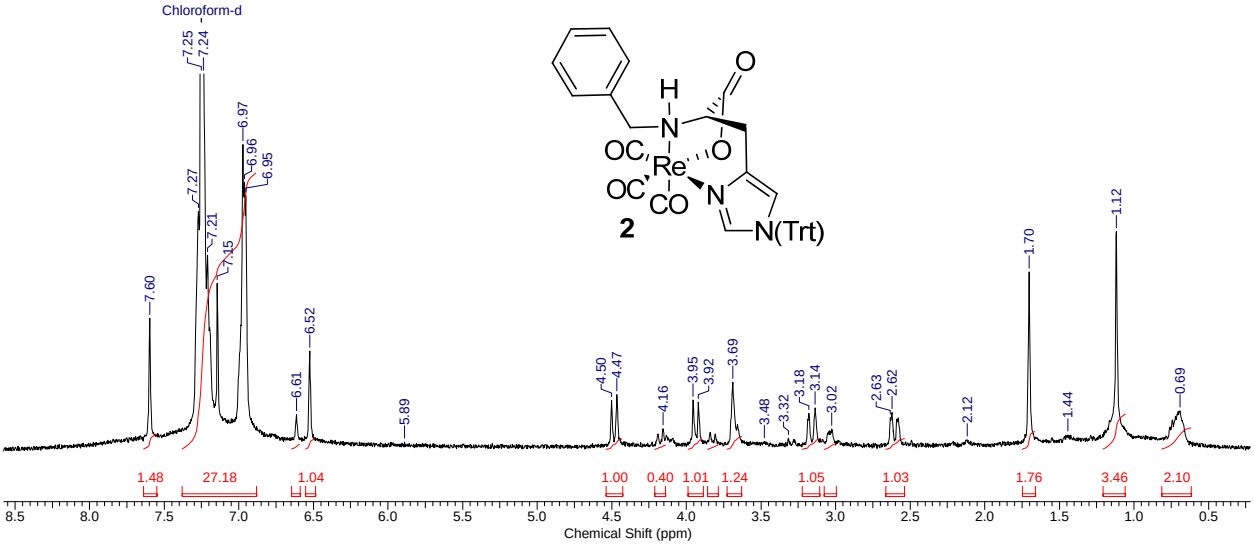


Fig. S7: ^{1}H NMR (400 MHz, MeOH-d4) of **2**

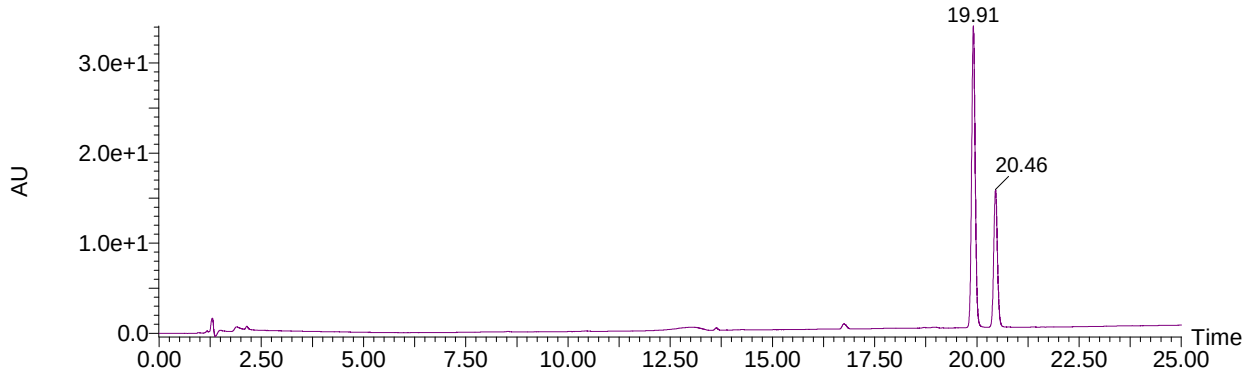


Fig. S8: Analytical HPLC trace, UV absorbance detected from 210-800 nm (RP-C18 4.6 x 250 mm, 5 µm), of **2**

N$^{\alpha}$-benzyl(methyl)-L-histidine (10)

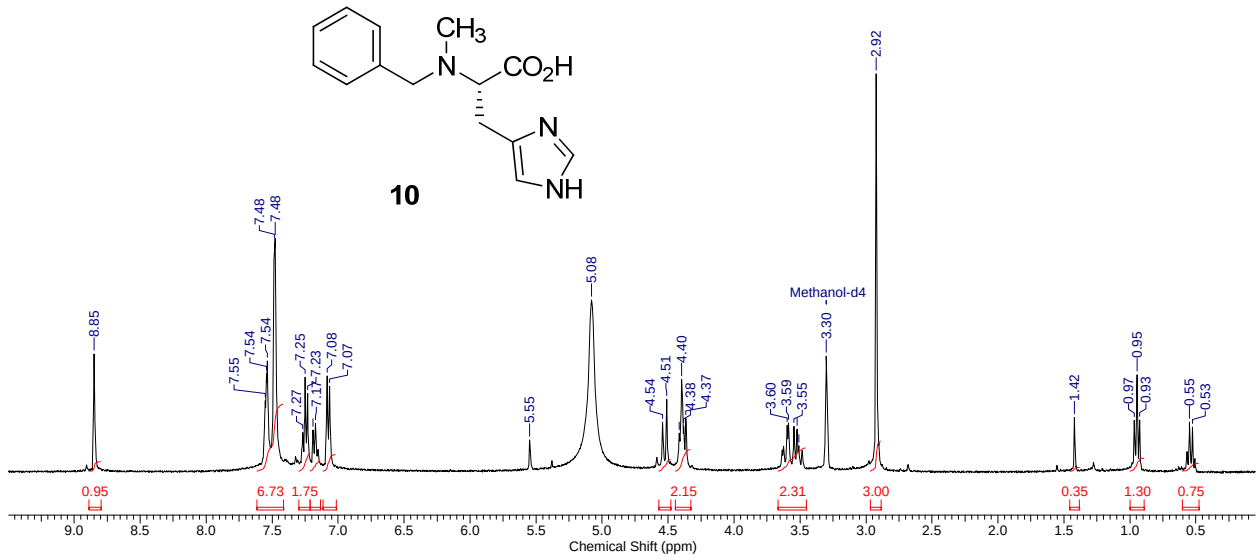


Fig. S9: ^{1}H NMR (400 MHz, MeOH-d4) of **10**

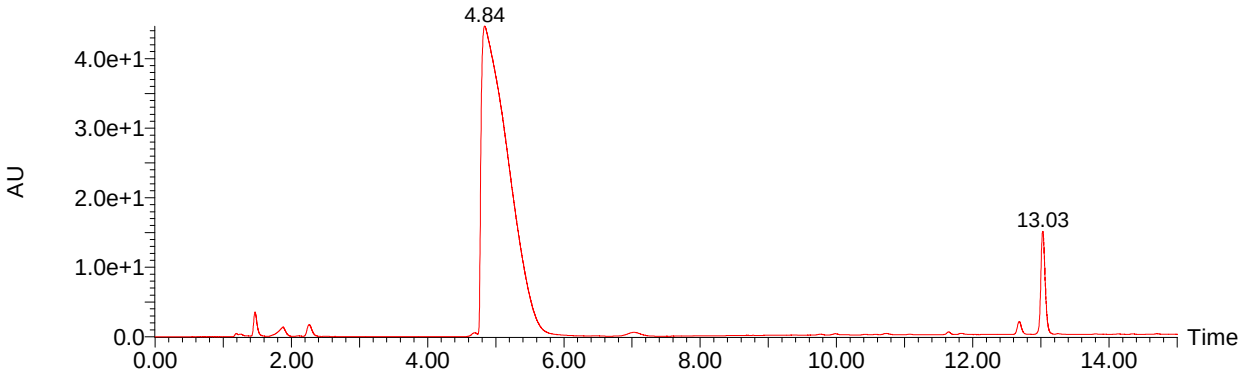


Fig. S10: Analytical HPLC trace, UV absorbance detected from 210-800 nm (RP-C18 4.6 x 250 mm, 5 µm), of **10**

Rhenium(I) tricarbonyl-N$^{\alpha}$-benzyl(methyl)-L-histidine (3)

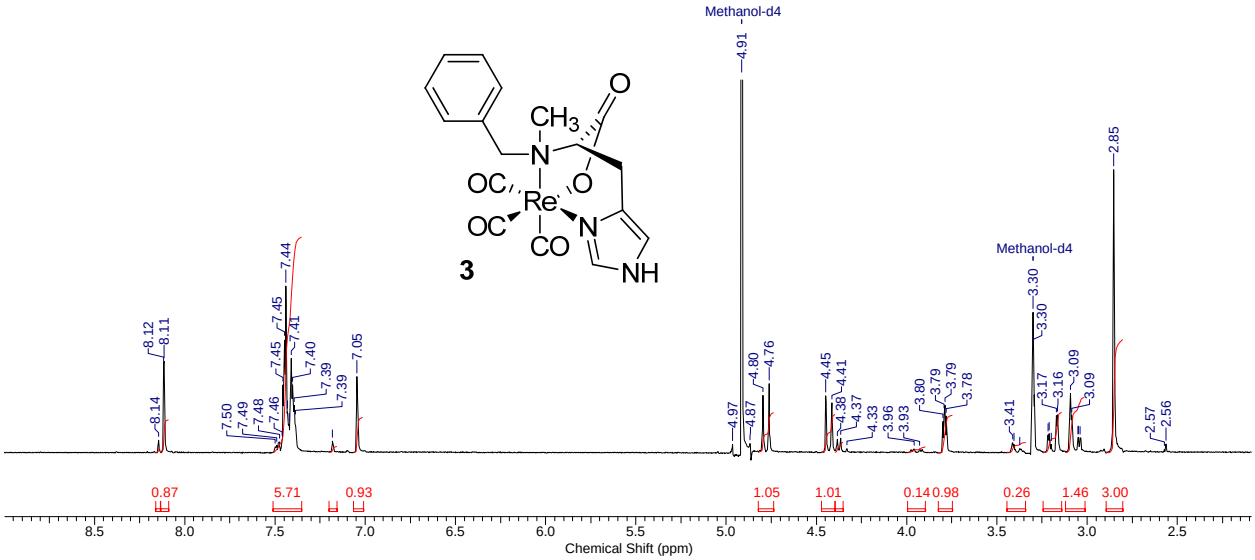


Fig. S11: ^{1}H NMR (400 MHz, MeOH-d4) of **3**

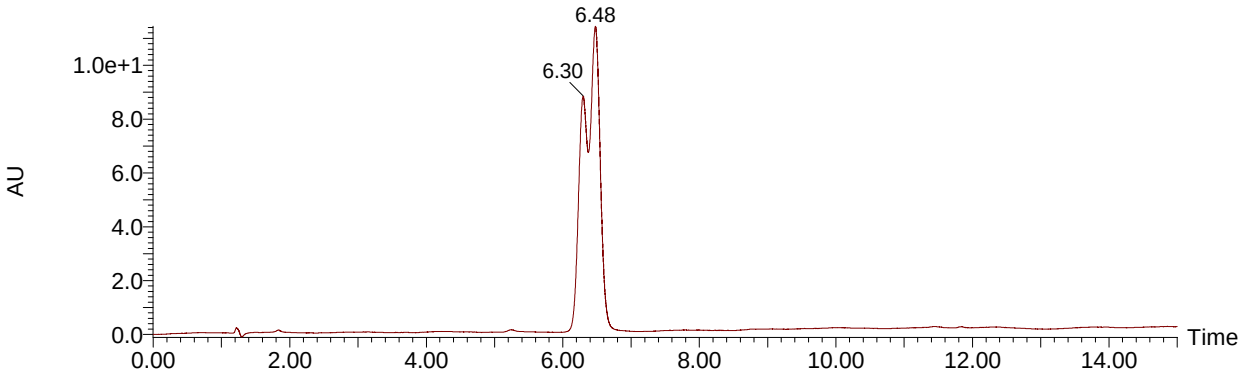


Fig. S12: Analytical HPLC trace, UV absorbance detected from 210-800 nm (RP-C18 4.6 x 250 mm, 5 µm), of **3**

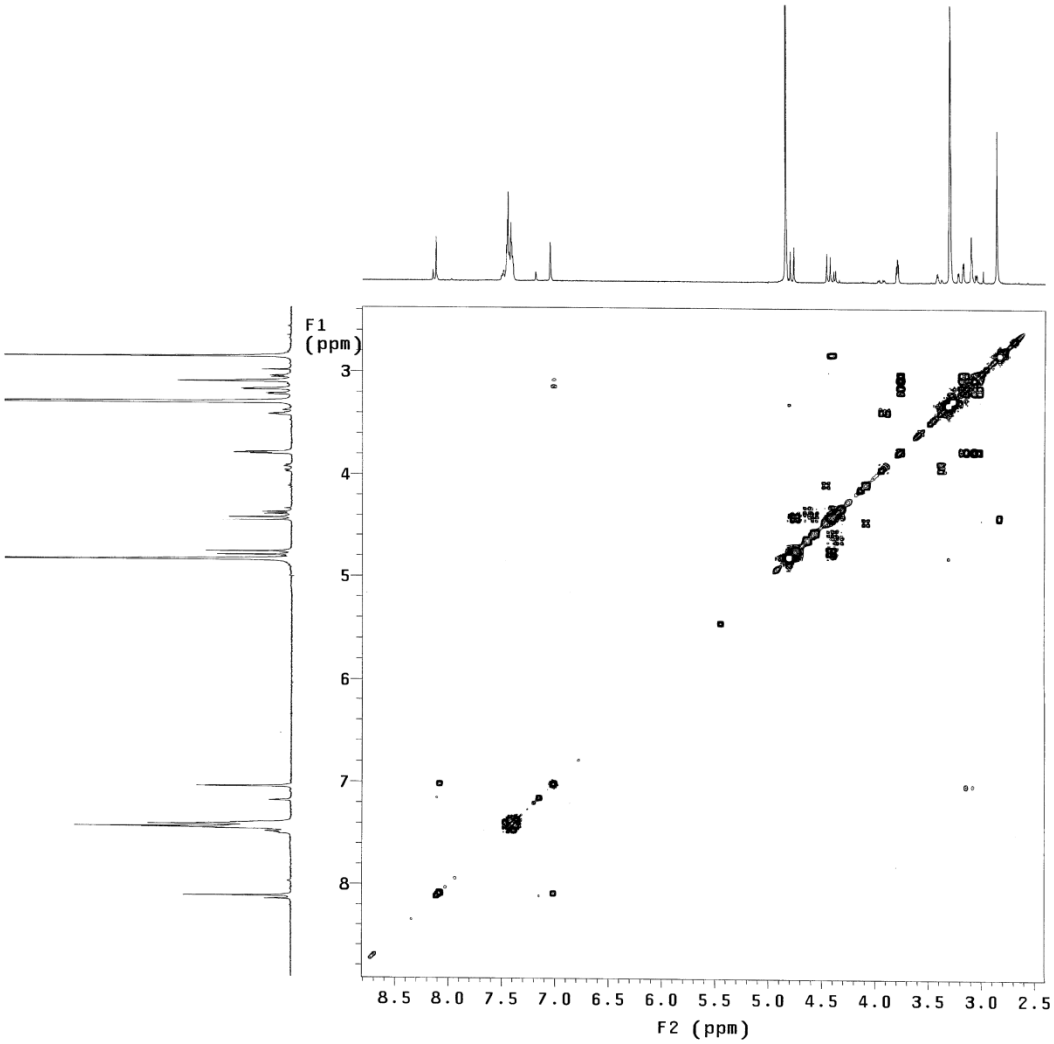


Fig. S13: gCOSY spectrum (400 MHz, MeOH-d4) of **3**

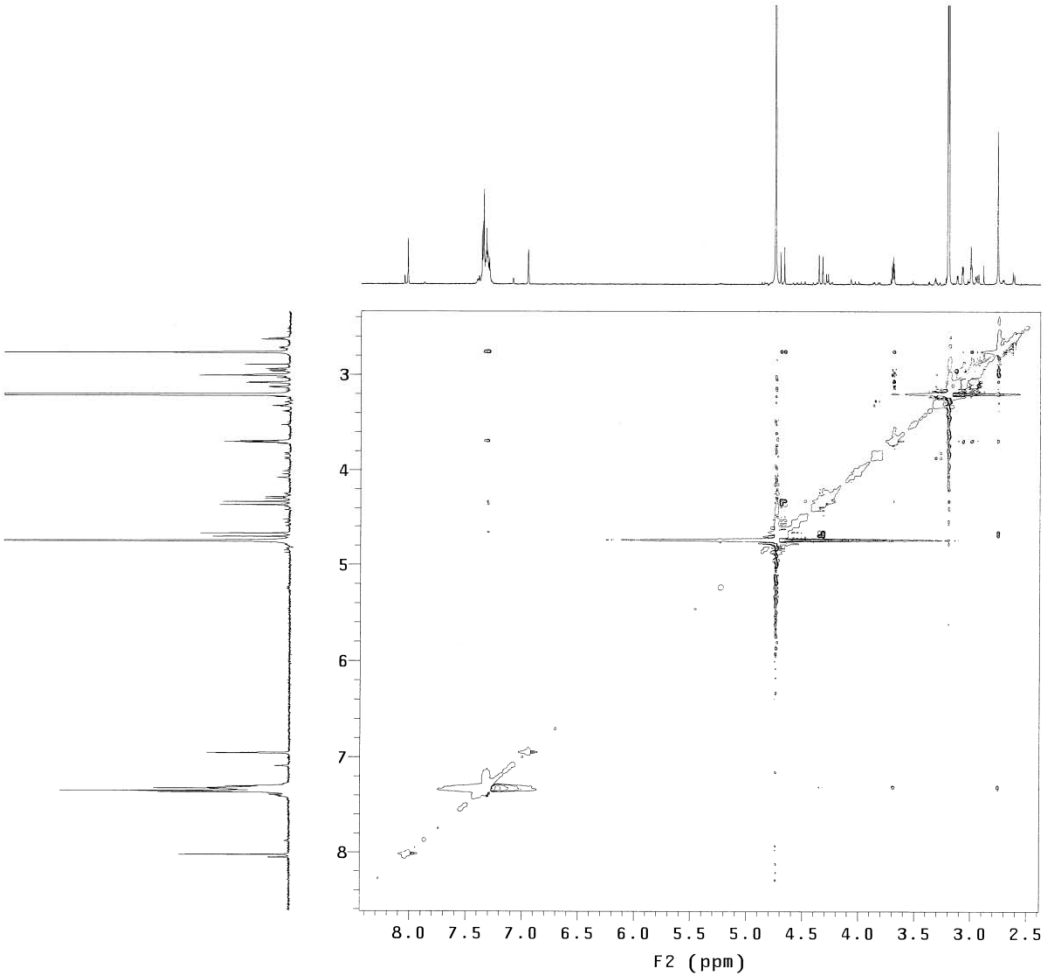
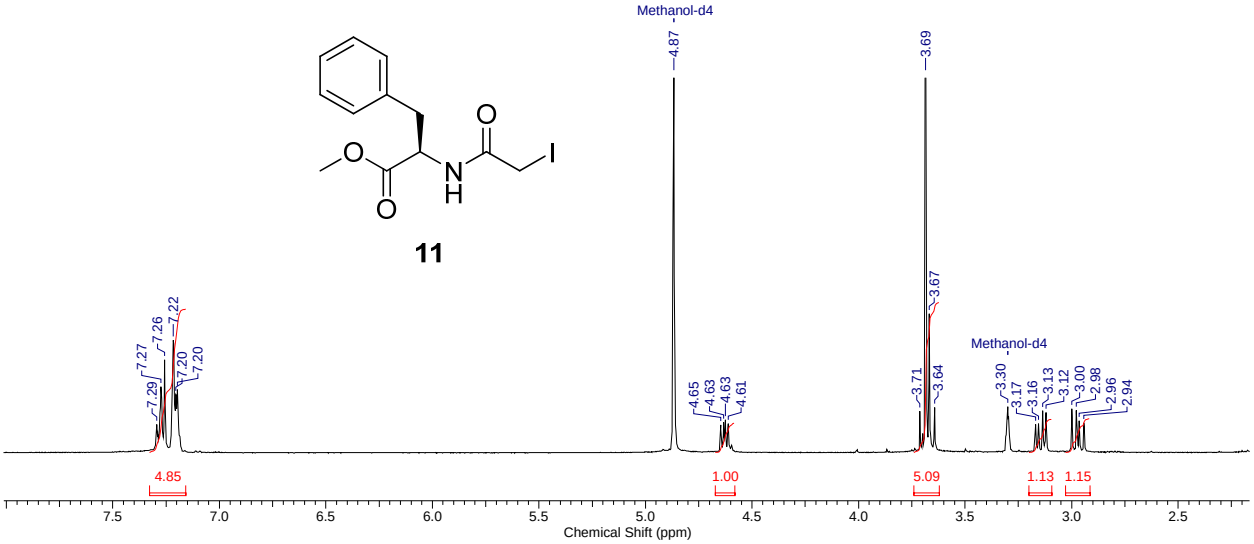


Fig. S14: NOESY spectrum (400 MHz, MeOH-d4) of **3**

N-iodocarbonyl-O-methyl phenylalanine (11)



11

Fig. S15: ^{1}H NMR (400 MHz, MeOH-d4) of **11**

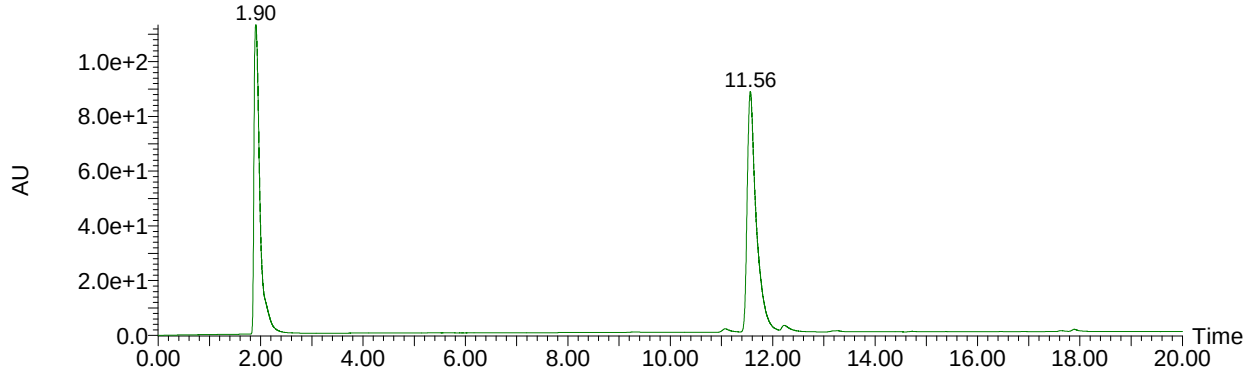


Fig. S16: Analytical HPLC trace, UV absorbance detected from 210-800 nm (RP-C18 4.6 x 250 mm, 5 µm), of **11**

N$^{\alpha}$-histidinyl-acetyl-phenylalanine (12)

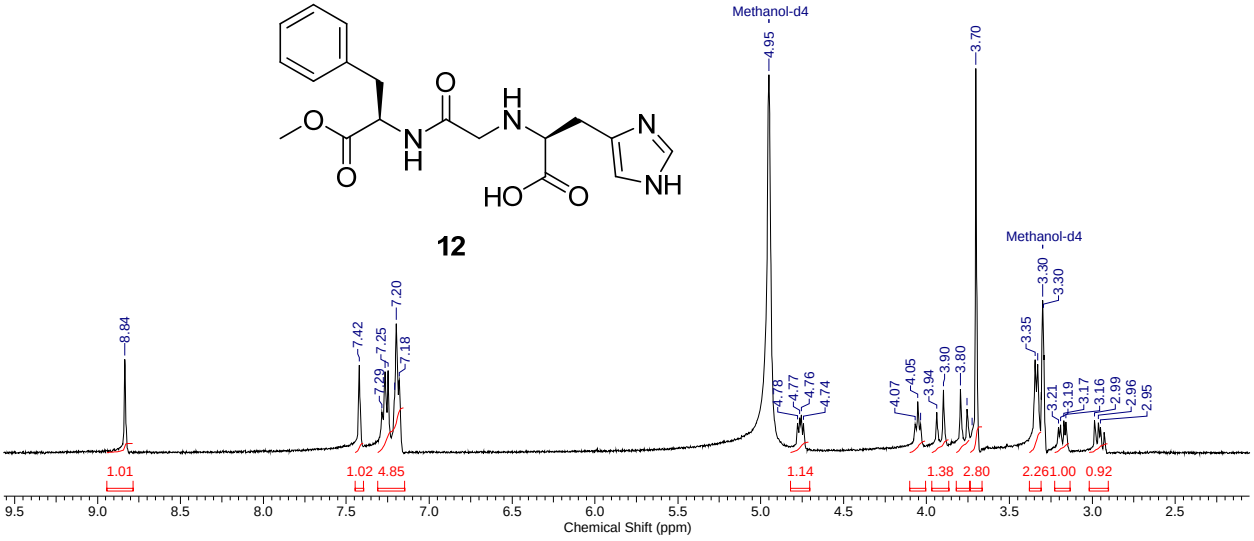


Fig. S17: ^{1}H NMR (400 MHz, MeOH-d4) of **12**

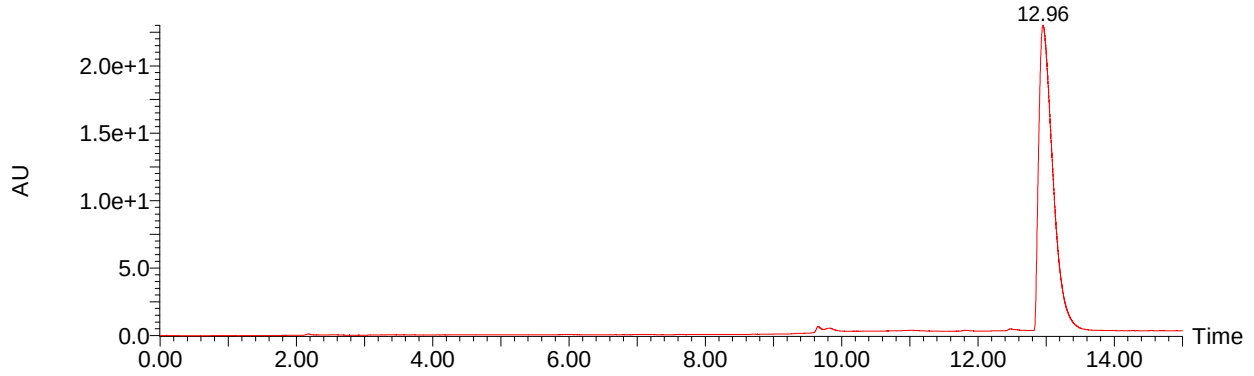


Fig. S18: Analytical HPLC trace, UV absorbance detected from 210-800 nm (RP-C18 4.6 x 250 mm, 5 µm), of **12**

Rhenium(I) tricarbonyl-N$^{\alpha}$-histidinyl-acetyl-phenylalanine (4)

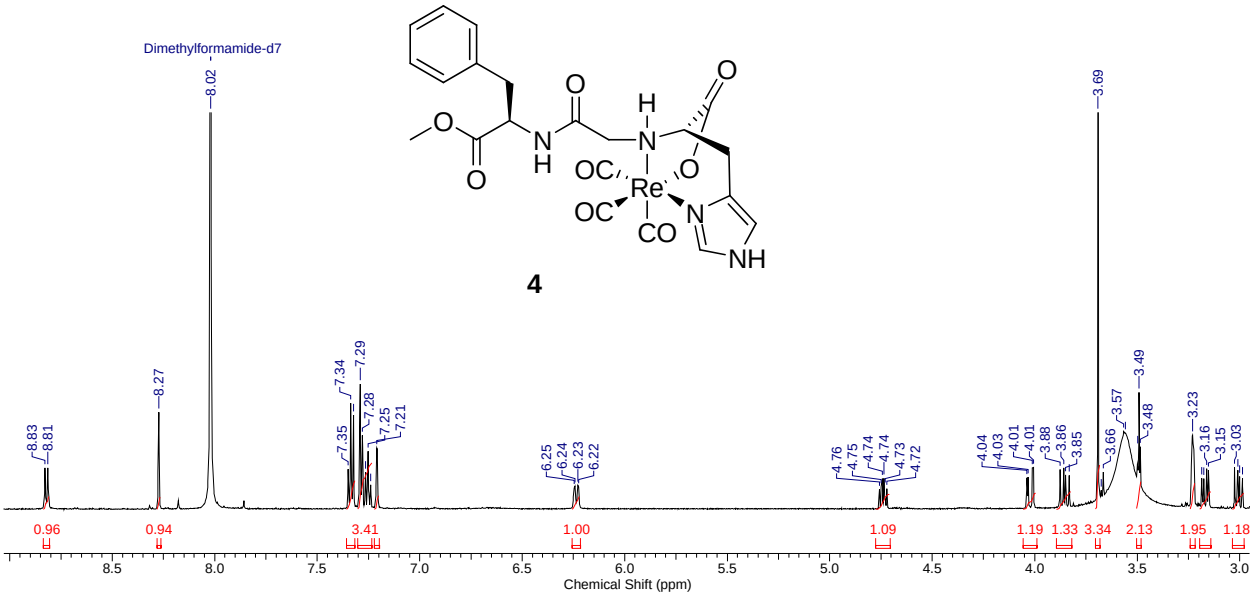


Fig. S19: ^{1}H NMR (600 MHz, DMF-d7) of **4**

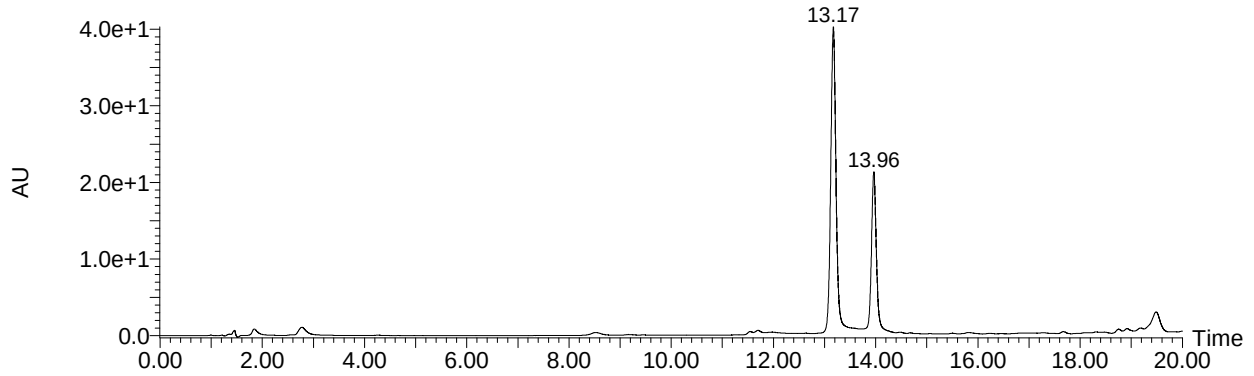


Fig. S20: Analytical HPLC trace, UV absorbance detected from 210-800 nm (RP-C18 4.6 x 250 mm, 5 µm), of **4**

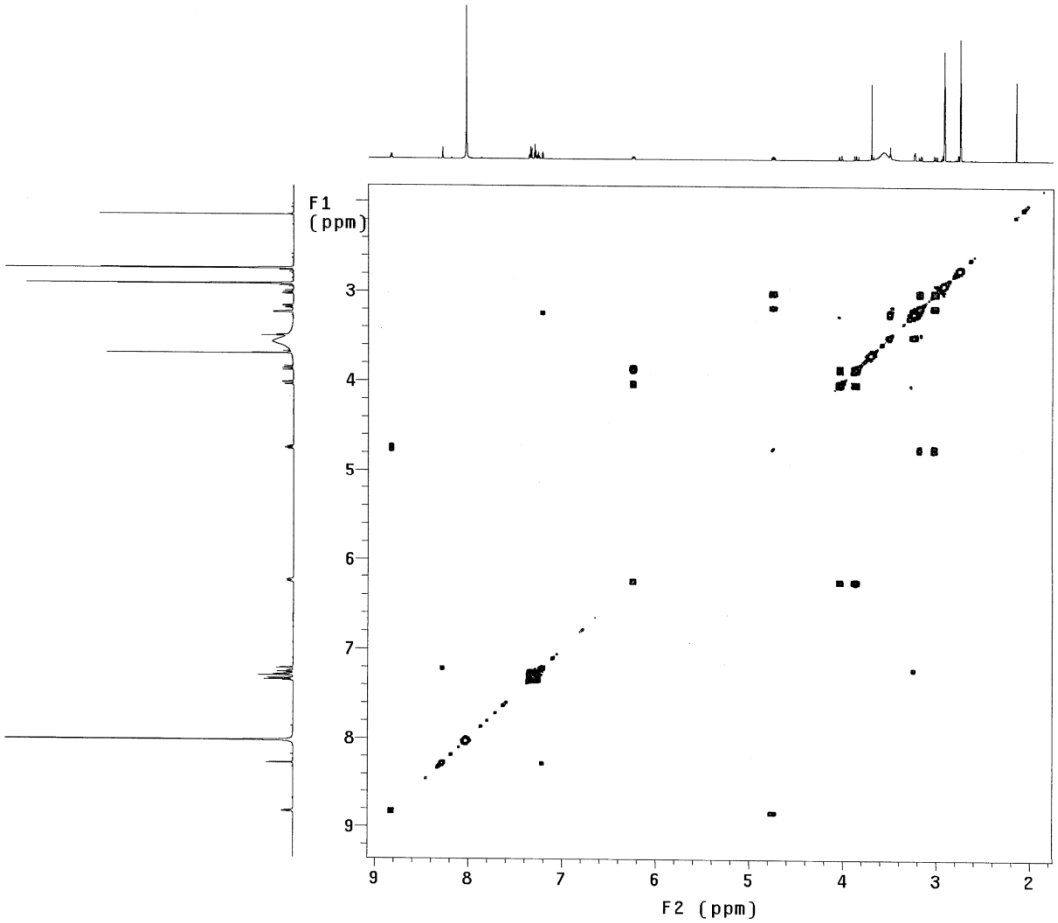


Fig. S21: gCOSY spectrum (600 MHz, DMF-d7) of **4**