Coordination Modes of Multidentate Ligands in *fac*-[Re(CO)$_3$(polyaminocarboxylate)] Analogues of ^{99m}Tc Radiopharmaceuticals. Dependence on Aqueous Solution Reaction Conditions

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Supporting Information

Figure S1. ^{1}H NMR spectrum of complex **5**, [Re(CO)$_3$(DTGH)-NNO]$^+$, in D$_2$O, pH 4.8.
Figure S2. ^{1}H NMR spectrum of complex **9**, [Re(CO)$_3$(DTMH)-NNO], in D$_2$O, pH ~ 6.
Figure S3. ^{1}H NMR spectra of complex **10**, [Re(CO)$_3$(DTM-NNN)]$^-$:
A. in H$_2$O, pH ~ 9; spectrum with additional NH-coupling
B. in D$_2$O, pH 11.6; spectrum without NH-coupling

Table S1. Re-C Bond Distances (Å) and C-Re-C Bond Angles (º) of [Re(CO)$_3$(DTGH)-NNO]PF$_6$•H$_2$O (**5** PF$_6$•H$_2$O), [Re(CO)$_3$(DTG)-NNO]•H$_2$O (**6**•H$_2$O), [Re(CO)$_3$(UEDDAH)-NNO] (**8**), [Re(CO)$_3$(DTMH)-NNO]•2H$_2$O (**9**•2H$_2$O) and [Re(CO)$_3$(DTA)-NNN]•CH$_3$OH (**12**•CH$_3$OH).

Figure S1. ^{1}H NMR spectrum of complex **5**, $[Re(CO)_3(DTGH)\text{-}NNO]^+$, in D_2O, pH 4.8.

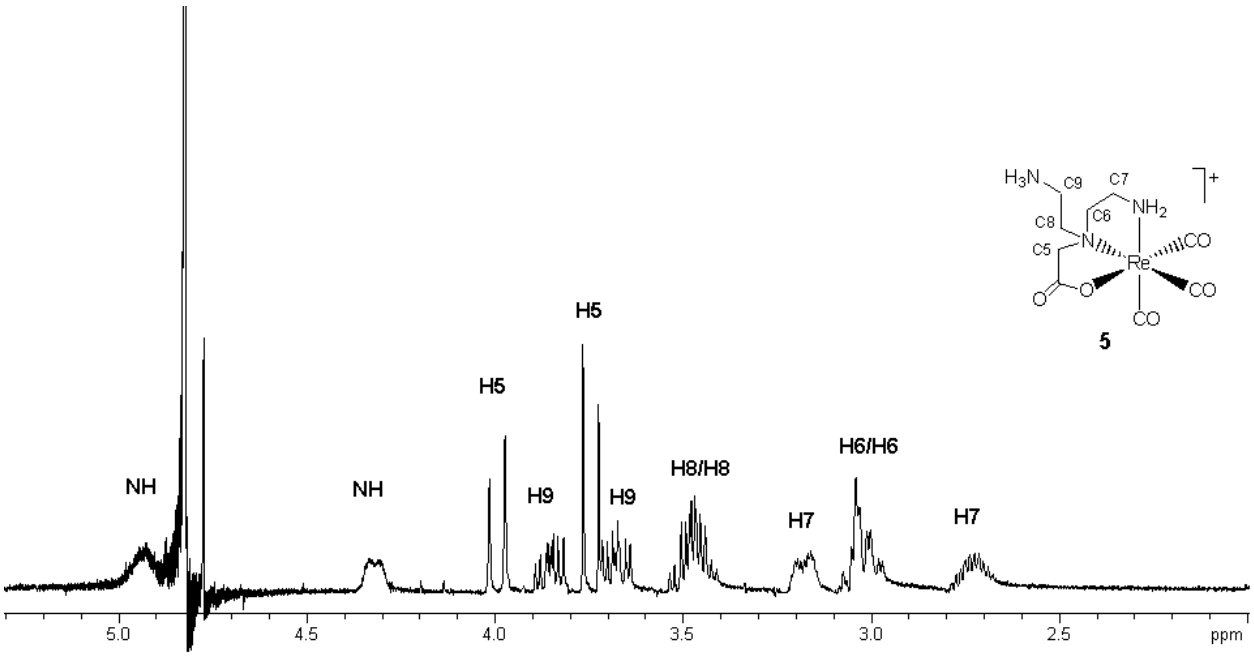


Figure S2. ^{1}H NMR spectrum of complex **9**, $[Re(CO)_3(DTMH)\text{-}NNO]$, in D_2O, pH 6.

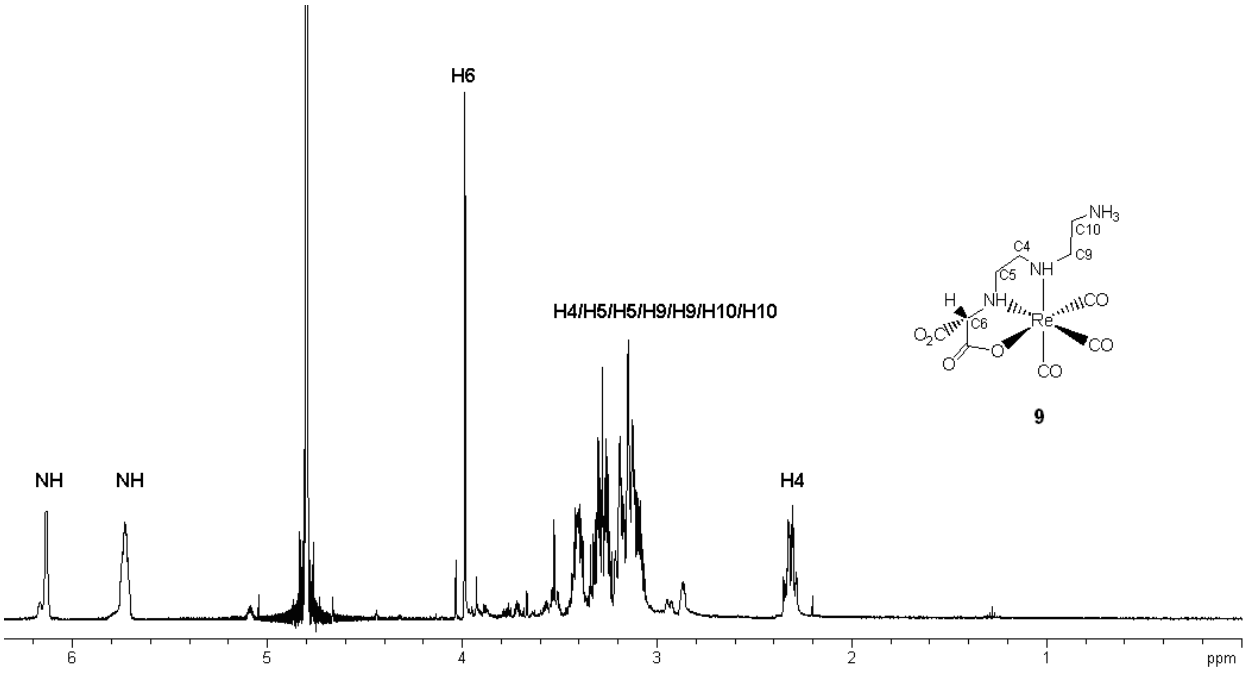
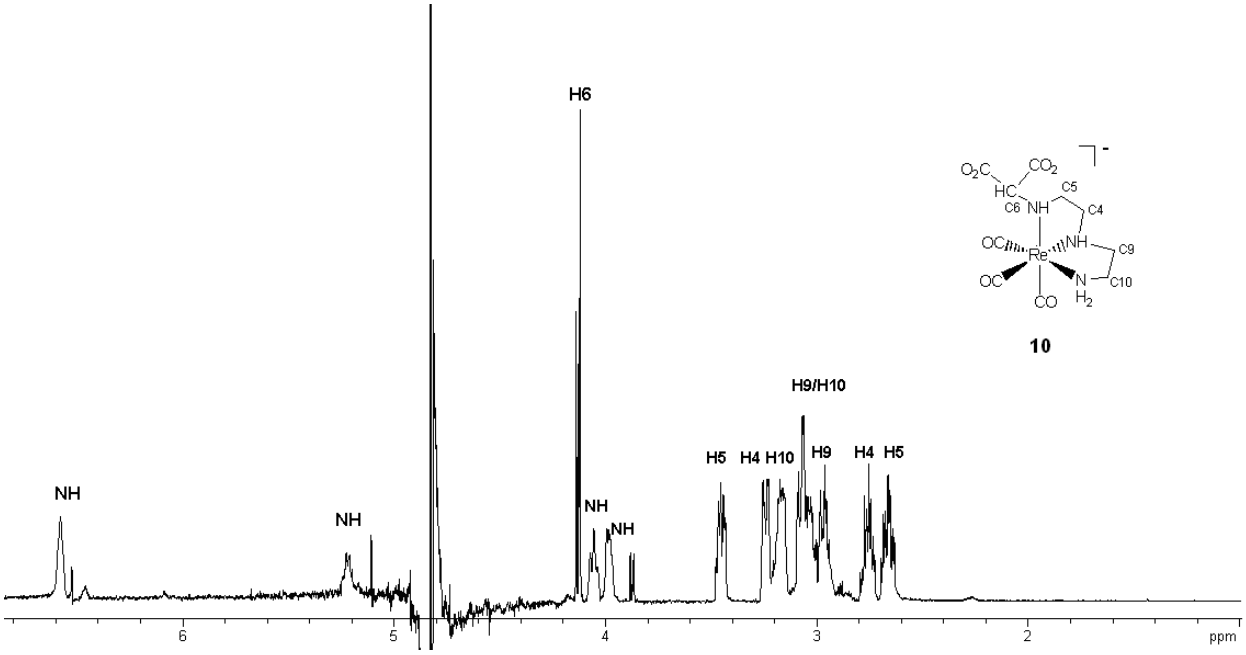
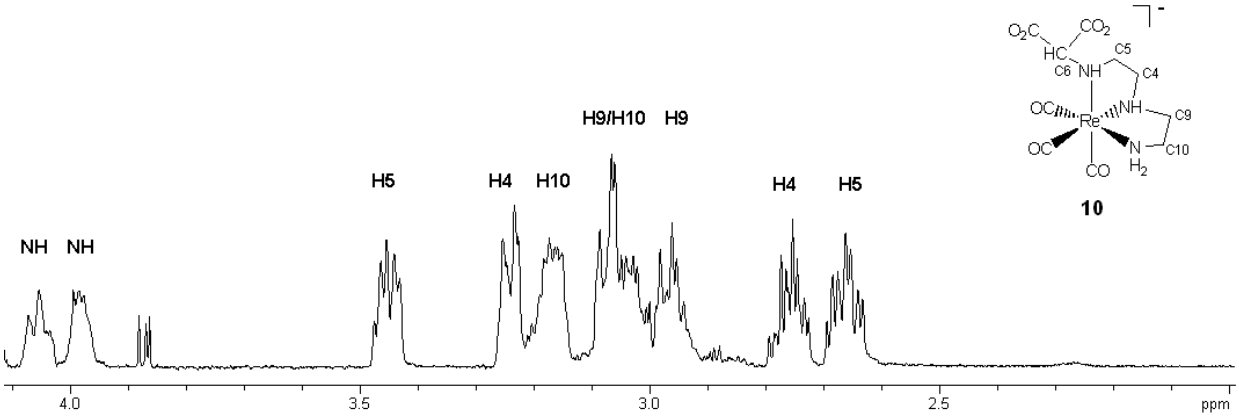


Figure S3. ^{1}H NMR spectra of complex **10**, $[Re(CO)_3(DTM\text{-}NNN)]^-$.

A: in H_2O, pH 9; spectrum with additional NH-coupling





B: in D_2O, pH 11.6; spectrum without NH-coupling

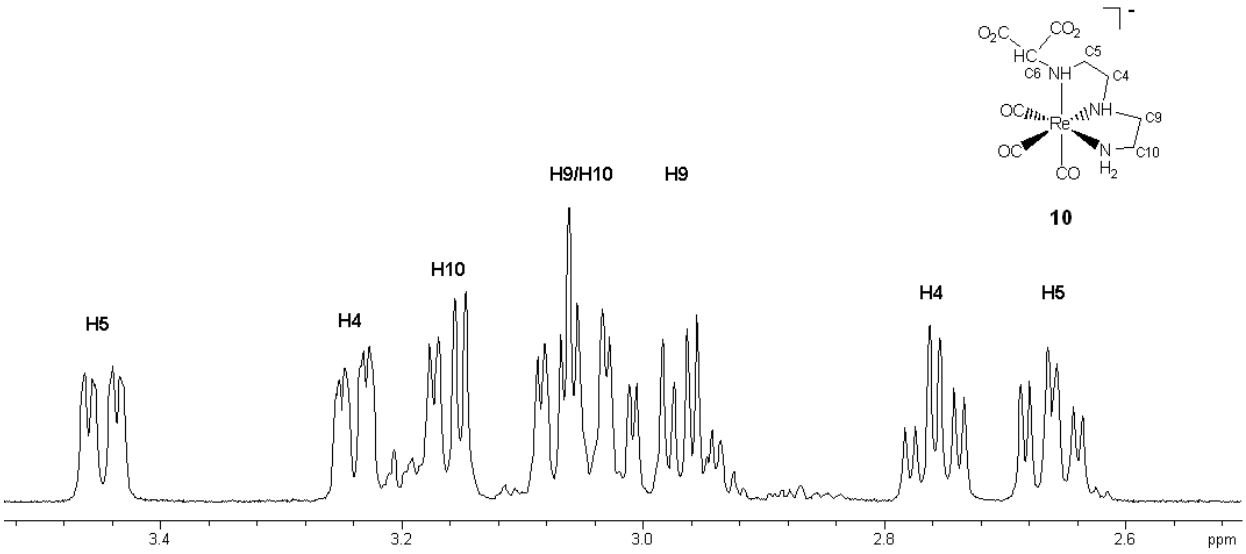


Table S1. Re-C Bond Distances (Å) and C-Re-C Bond Angles (º) of $[Re(CO)_3(DTGH)\text{-}NNO]PF_6 \bullet H_2O$ (**5** $PF_6 \bullet H_2O$), $[Re(CO)_3(DTG)\text{-}NNO] \bullet H_2O$ (**6**$\bullet H_2O$), $[Re(CO)_3(UEDDAH)\text{-}NNO]$ (**8**), $[Re(CO)_3(DTMH)\text{-}NNO] \bullet 2H_2O$ (**9**$\bullet 2H_2O$) and $[Re(CO)_3(DTA)\text{-}NNN] \bullet CH_3OH$ (**12**$\bullet CH_3OH$).

	5 $PF_6 \bullet H_2O$	**6**$\bullet H_2O$	**8**	**9**$\bullet 2H_2O$	**12**$\bullet CH_3OH$
Re(1)–C(1)	1.908(10)	1.924(13)	1.909(6)	1.90(4)	1.918(5)
Re(1)–C(2)	1.914(10)	1.904(12)	1.913(8)	1.90(3)	1.912(6)
Re(1)–C(3)	1.935(9)	1.934(14)	1.902(7)	1.90(3)	1.920(5)
C(1)–Re(1)–C(2)	88.6(4)	91.9(6)	87.8(2)	85.2(10)	86.9(2)
C(1)–Re(1)–C(3)	88.7(4)	88.8(6)	90.1(3)	89.2(12)	88.87(19)
C(2)–Re(1)–C(3)	91.6(4)	88.5(5)	85.0(3)	86.2(10)	90.6(2)