Supplementary Data and Figures.

Supplementary Figure S1. $[Re(CO)_3(H_2O)_3]OTf$ ESI-MS spectrometer: *m/z* 271 ($[Re(CO)_3]^+$, 90%), 289 ($[Re(CO)_3(H_2O)]^+$, 30%), 312 ($[Re(CO)_3(H_2O) + Na]^+$, 100%) and 330 ($[Re(CO)_3(H_2O)_2 + Na]^+$, 70%)

Supplementary Figure S2. $Re(CO)_3$D,L-DAPA IR (KBr, ν/cm^{-1}) spectrometer: 2026 (s) and 1895 (s)

Supplementary Figure S3. ^{1}H NMR spectrum of $Re(CO)_3$D,L-DAPA. ^{1}H NMR [δ (ppm), CD_3OD-D_2O]: 2.76 - 2.75 (m, 1H-methylene), 3.05 – 2.98 (m, 1H-methylene), 3.91 (s, 1H-methine)

Supplementary Figure S4. ^{13}C NMR spectrum of $Re(CO)_3$D,L-DAPA. ^{13}C NMR (CD_3OD): δ 197.9, 196.9 [*fac*-$Re(CO)_3$], 181.4 (C, COO^-), 59.9 (CH), 41.7 (CH_2)

Supplementary Figure S5. ^{13}C NMR spectrum of $Re(CO)_3$D,L-DAPA. DEPT-135

Supplementary Figure S6. ^{13}C NMR spectrum of $Re(CO)_3$D,L-DAPA. DEPT-90

Supplementary Figure S7. $Re(CO)_3$D,L-DAPA ESI-MS spectrometer: *m/z* 396.90 (100%, $M + Na)^+$

Supplementary Figure S8. $Re(CO)_3$L-Asp IR (KBr, ν/cm^{-1}) spectrometer: 2027 (s) and 1899 (s)

Supplementary Figure S9. ^{1}H NMR spectrum of $Re(CO)_3$L-Asp. ^{1}H NMR [δ (ppm), CD_3OD - D_2O]: 2.87-2.82 (m, 2H-methylene), 3.94 (s, 1H-methine)

Supplementary Figure S10. ^{13}C NMR spectrum of $Re(CO)_3$L-Asp. ^{13}C NMR (CD_3OD): δ 199.4, 198.5, 198.0 [*fac*-$Re(CO)_3$], 186.2 (C, α-COO), 176.9 (C, β-COO^-), 54.2 (CH), 40.9 (CH_2).

Supplementary Figure S11. ^{13}C NMR spectrum of $Re(CO)_3$L-Asp. DEPT-135

Supplementary Figure S12. ^{13}C NMR spectrum of $Re(CO)_3$L-Asp. DEPT-90

Supplementary Figure S13. $Re(CO)_3$L-Asp ESI-MS spectrometer: m/z 400.43 (100%, $M-H)^-$

Supplementary Figure S14. $Re(CO)_3$ D,L-Asp IR (KBr, ν/cm^{-1}) spectrometer: 2025 (s), 1905 (s), 1874 (s)

Supplementary Figure S15. ^{1}H NMR spectrum of $Re(CO)_3$ D,L-Asp. ^{1}H NMR [δ (ppm), D_2O]: 2.74 (s, 1H- methylene), 2.80 (d, 1H-methylene), 3.99-3.94 (b, 1H-methine).

Supplementary Figure S16. ^{13}C NMR spectrum of $Re(CO)_3$ D,L-Asp. ^{13}C NMR (D_2O): δ 198.0, 197.1, 196.3 [*fac*-$Re(CO)_3$], 185.8 (C, α-COO^-), 176.7 (C, β-COO^-), 52.4 (CH), 39.4 (CH_2).

Supplementary Figure S17. ^{13}C NMR spectrum of $Re(CO)_3$ D,L-Asp. DEPT-135

Supplementary Figure S18. ^{13}C NMR spectrum of $Re(CO)_3$ D,L-Asp. DEPT-90

Supplementary Figure S19. $Re(CO)_3$ D,L-Asp ESI-MS spectrometer: MS (ESI, -ve mode): m/z 400.32 (100%, $M-H)^-$.

Supplementary Figure S20. $[Et_3NH][Re(CO)_3$-(D,L-Asp)] dimeric complex IR (KBr, ν/cm^{-1}) spectrometer: IR (KBr, ν/cm^{-1}): 2011 (s), 1883 (s), 1856 (s).

Supplementary Figure S21. ^1H NMR spectrum of $[Et_3NH][Re(CO)_3$-(D,L-Asp)] dimeric complex. ^1H NMR [δ (ppm), CD_3OD]: δ 1.33 (t, 18H, CH_3-Triethylamine), 2.46-2.53, 2.75-2.94 (m, 4H, $2CH_2$), 3.22 (q, 12H, CH_2-Triethylamine), 3.35-3.41 (m, H, CH), 3.89-3.93 (m, H, CH).

Supplementary Figure S22. ^{13}C NMR spectrum of $[Et_3NH][Re(CO)_3$-(D,L-Asp)] dimeric complex. ^{13}C NMR [δ (ppm), CD_3OD]: δ 199.4, 199.2, 199.1, 198.5, 198.4 [2(*fac*-$Re(CO)_3$)], 186.2 (-COO^-), 183.9 (-COO^-), 177.7 (-COO^-), 177.0 (-COO^-), 57.2 (CH), 54.1 (CH), 48.0 (CH_2-triethylamine), 40.8 (CH_2), 40.3 (CH_2), 9.5 (CH_3-triethylamine).

Supplementary Figure S23. ^{13}C NMR spectrum of $[Et_3NH][Re(CO)_3$-(D,L-Asp)] dimeric complex. DEPT-135

Supplementary Figure S24. ^{13}C NMR spectrum of $[Et_3NH][Re(CO)_3$-(D,L-Asp)] dimeric complex. DEPT-90

Supplementary Figure S25. $[Et_3NH][Re(CO)_3$-(D,L-Asp)] dimeric complex. FAB(+) spectrometer: (mNBA) MS: m/z 1007.04 $[2M+2Et_3NH+H]^+$dimeric complex, 504.53 $[M+Et_3NH+H]^+$ monomeric complex.

Supplementary Figure S26. $Re(CO)_3$CysH. IR (KBr, ν/cm^{-1}) spectrometer: 2001 (s), 1896 (s).

Supplementary Figure S27. ^1H NMR spectrum of $Re(CO)_3$CysH. ^1H NMR [δ (ppm), D_2O]: 3.37-3.34 (m, 2H-methylene), 3.95-3.94 (m, 1H-methine).

Supplementary Figure S28. ^{13}C NMR spectrum of $Re(CO)_3$CysH. ^{13}C NMR (D_2O): δ 195.4 [*fac*-$Re(CO)_3$], 171.2 (C, α-COO^-), 58.0 (CH), 37.1 (CH_2).

Supplementary Figure S29. ^{13}C NMR spectrum of $Re(CO)_3$CysH. DEPT-135

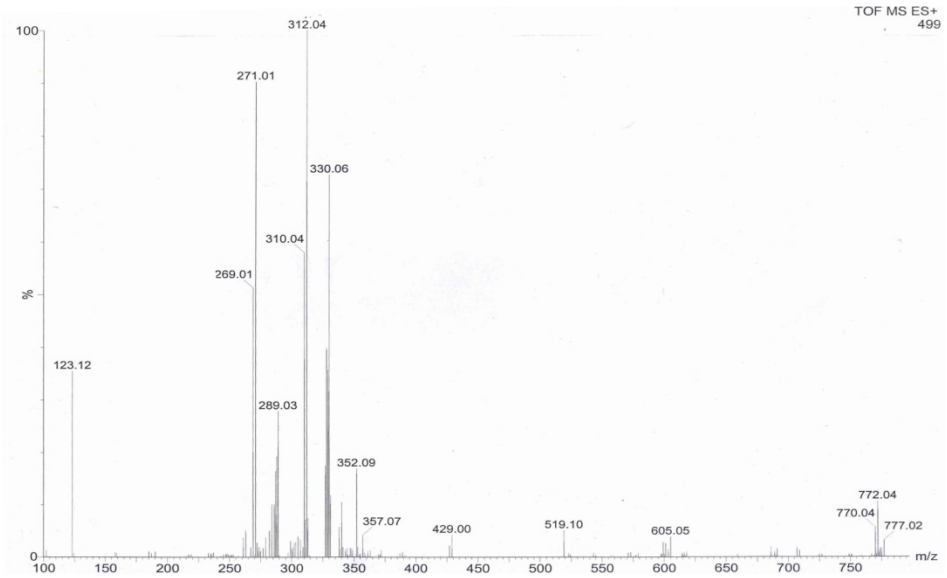
Supplementary Figure S30. ^{13}C NMR spectrum of $Re(CO)_3$CysH. DEPT-90

Supplementary Figure S31. $Re(CO)_3CysH$ ESI-MS spectrometer: m/z 391.91 [100%, $(M+H)^+$].

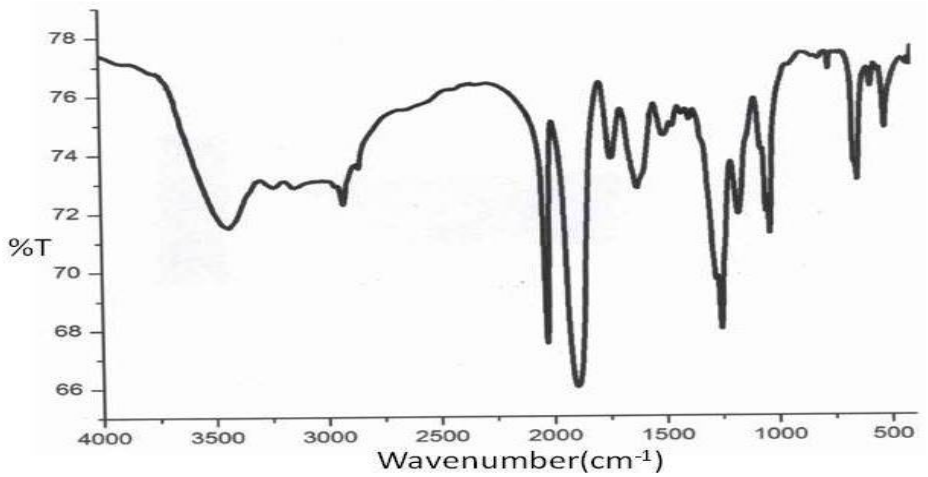
Supplementary Data S32. Bond lengths in [Å] of **$Re(CO)_3$-D,L-DAPA and $Re(CO)_3$-D,L-Asp.Et_3NH** crystal data in table.

Supplementary Data S33. Bond angle in Degree of **$Re(CO)_3$-D,L-DAPA and $Re(CO)_3$-D,L-Asp.Et_3NH** crystal data in table.

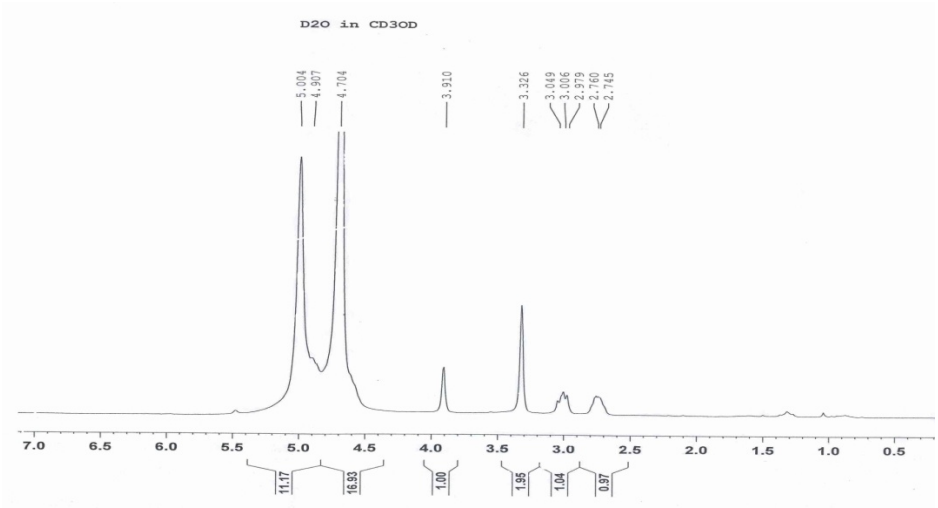
Supplementary Figure S34. Electrophoresis Fig. of tricarbonyltechnetium (I) complexes of amino acids. Electrophoresis done in 0.01M bicarbonate buffer pH 7 for 60 min at potential difference of 3kV and applied current of 10 mA for 1 h.



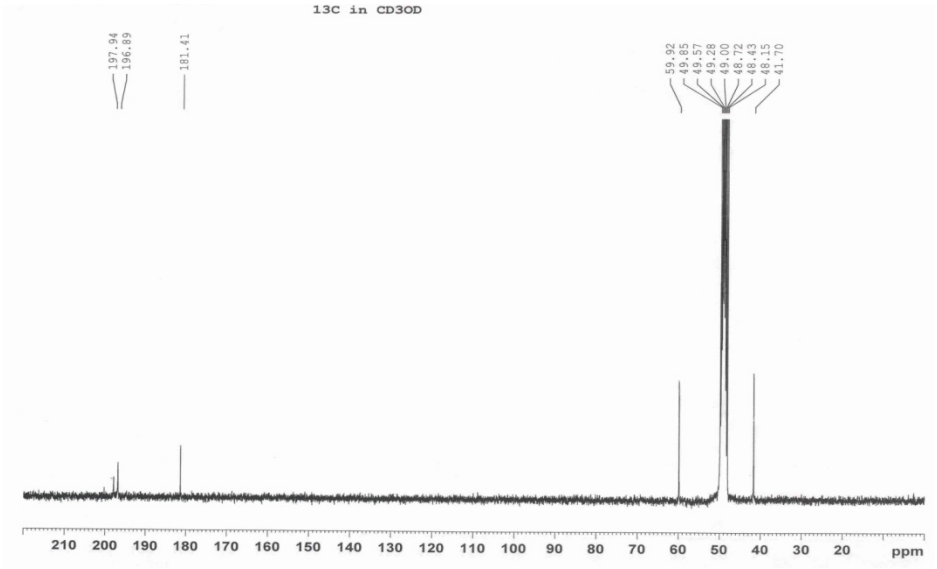
Supplementary Figure S1.



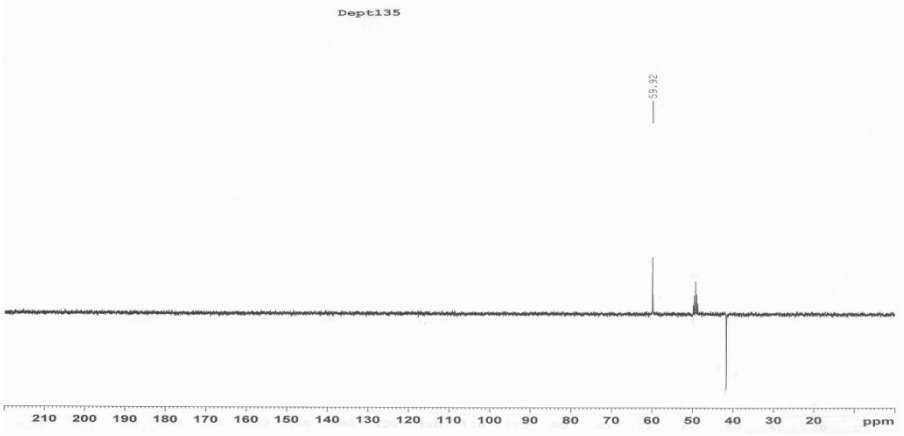
Supplementary Figure S2.



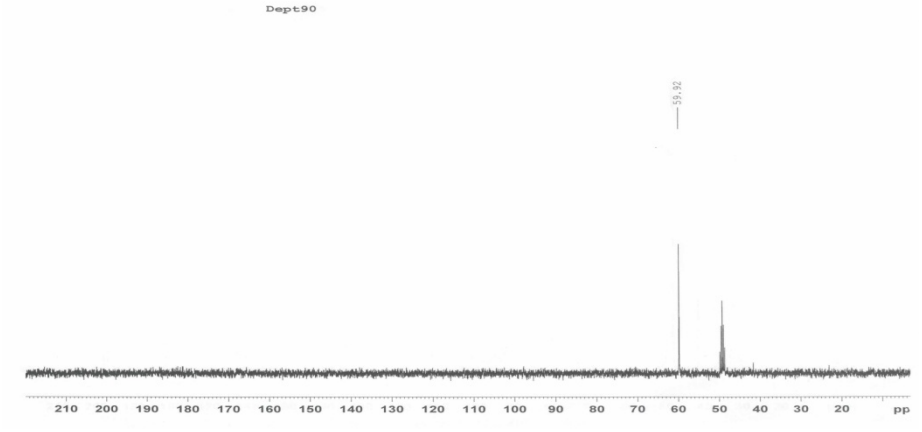
Supplementary Figure S3.



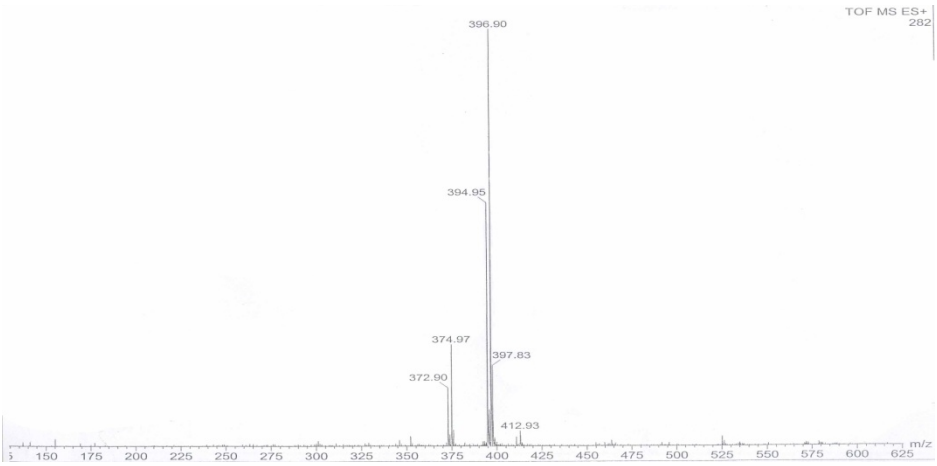
Supplementary Figure S4.



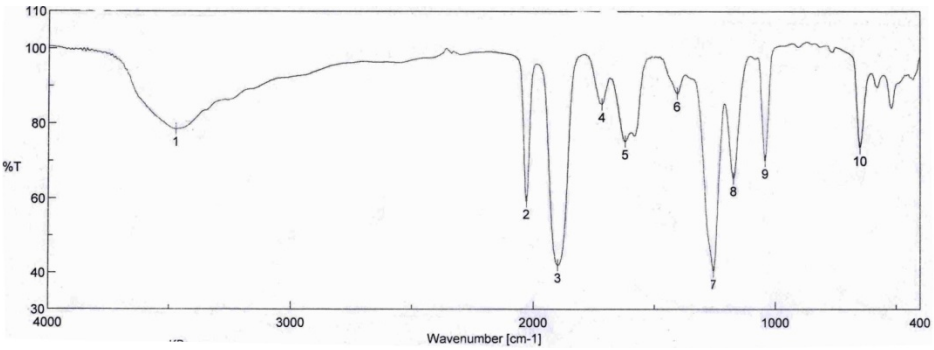
Supplementary Figure S5.



Supplementary Figure S6.



Supplementary Figure S7.



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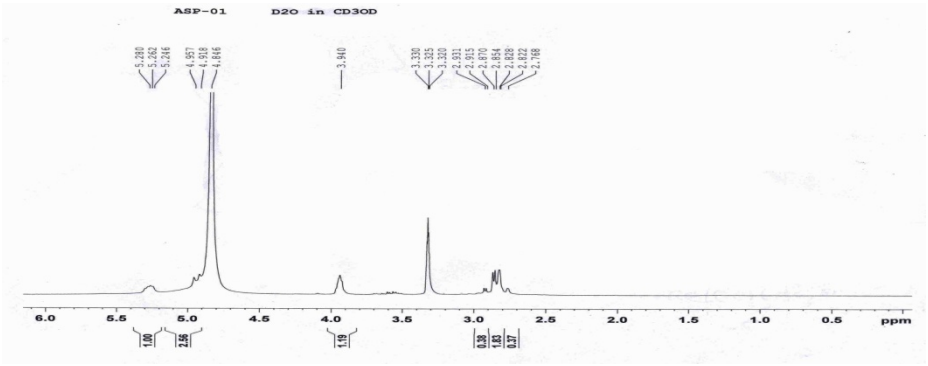
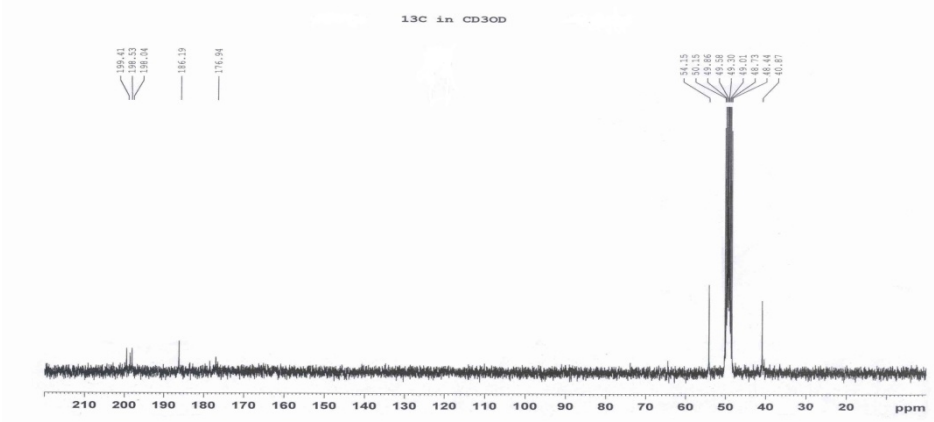
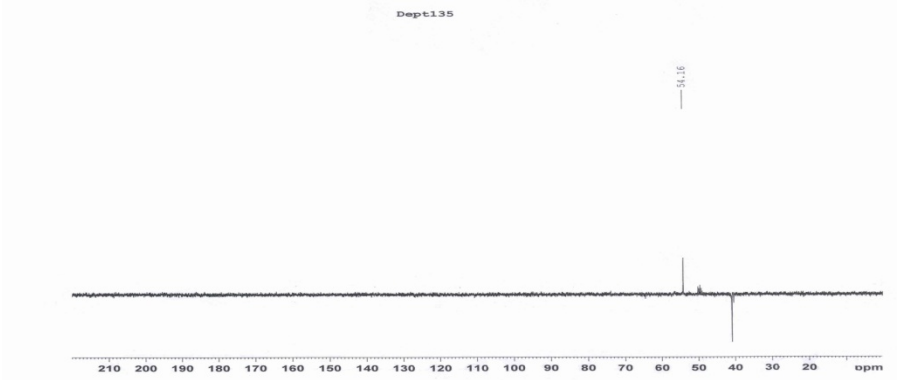


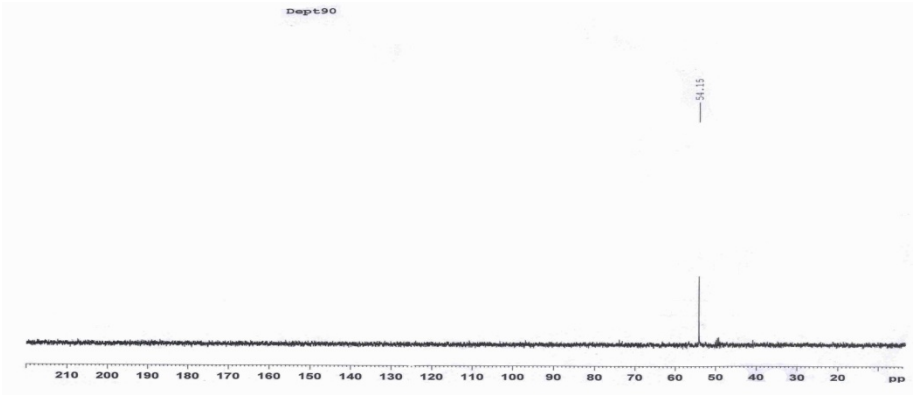
Supplementary Figure S9.



Supplementary Figure S10.



Supplementary Figure S11.



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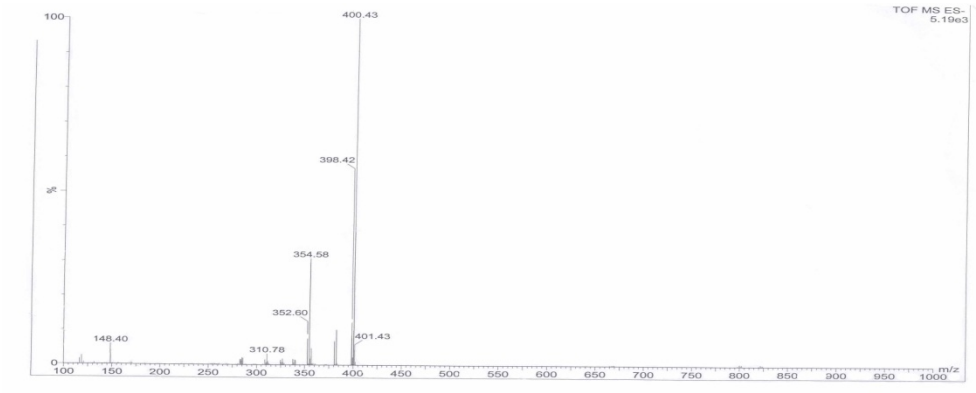

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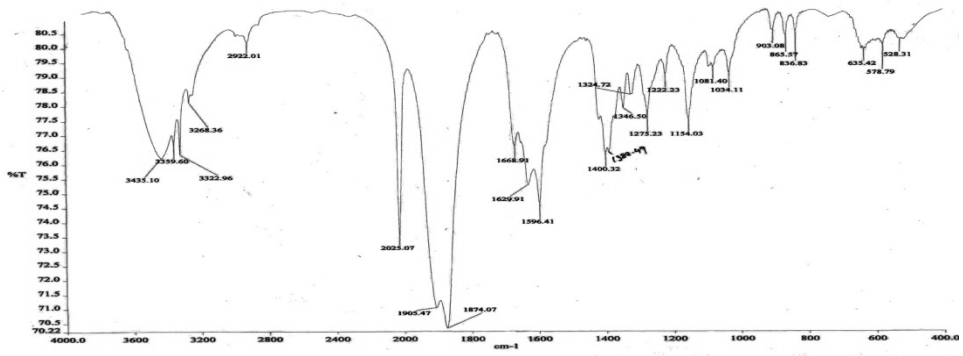
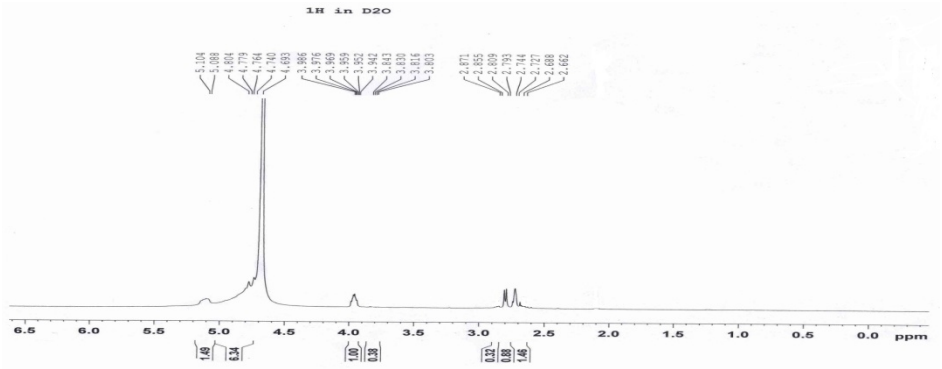
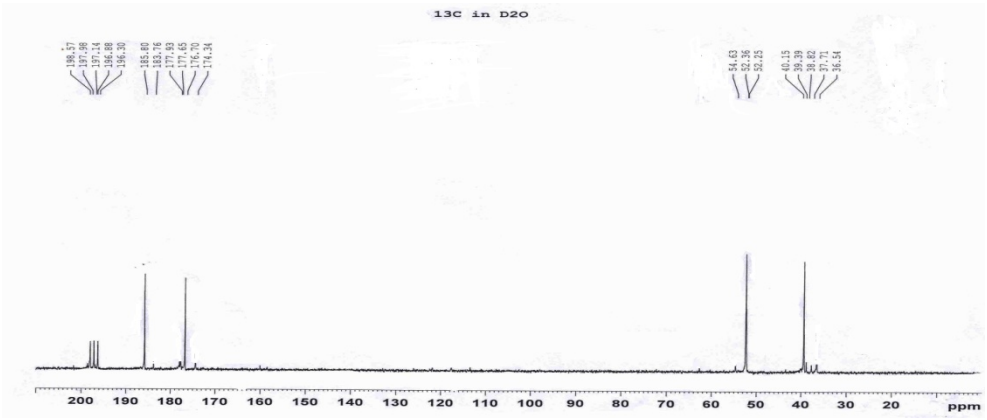


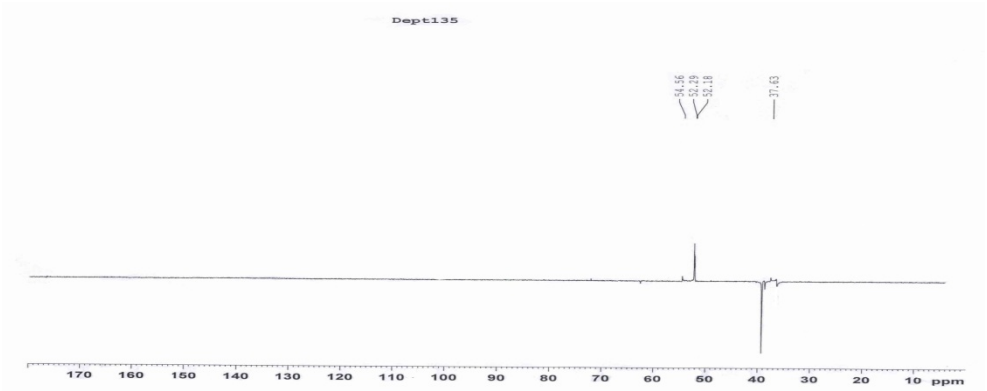
Supplementary Figure S14.



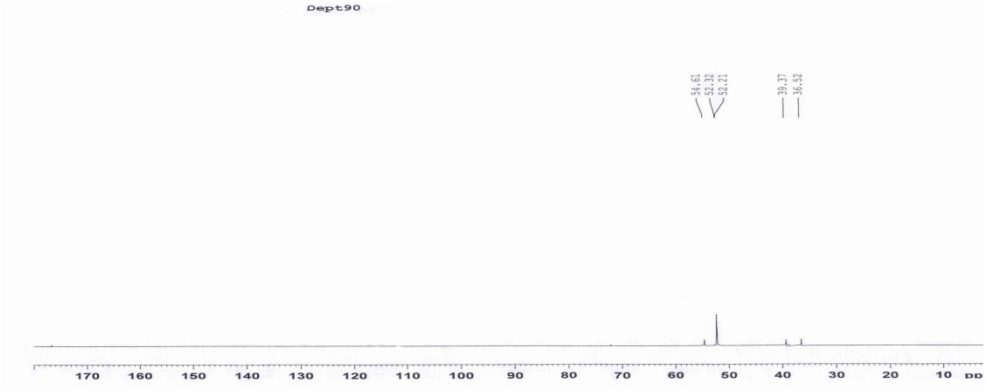
Supplementary Figure S15.



Supplementary Figure S16.



Supplementary Figure S17.



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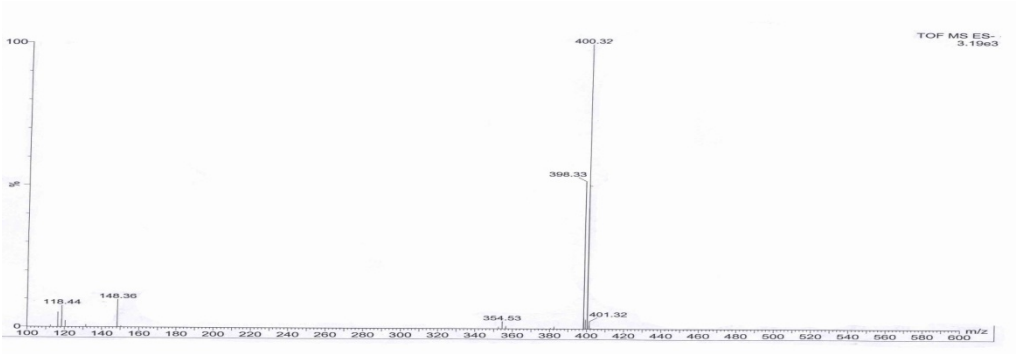
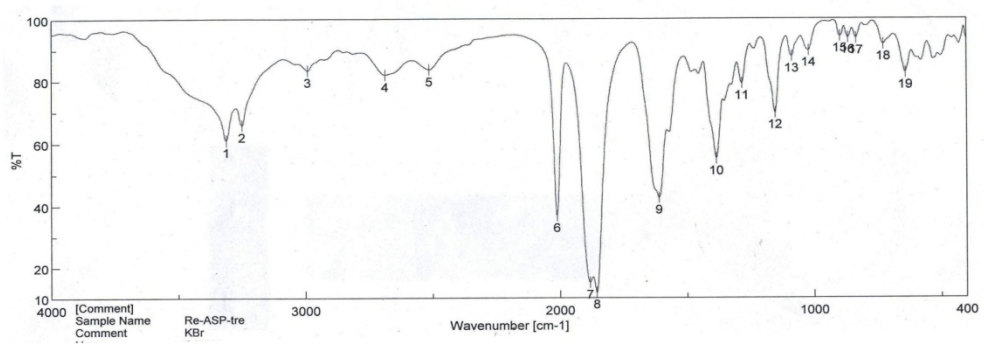
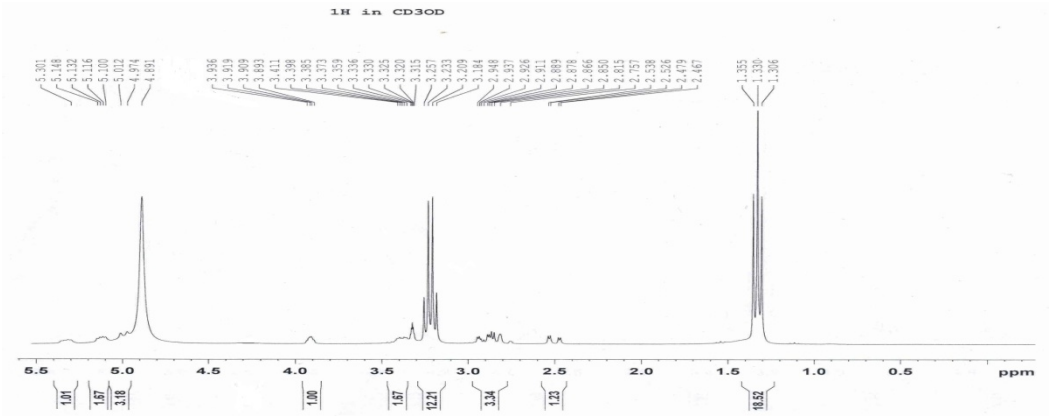


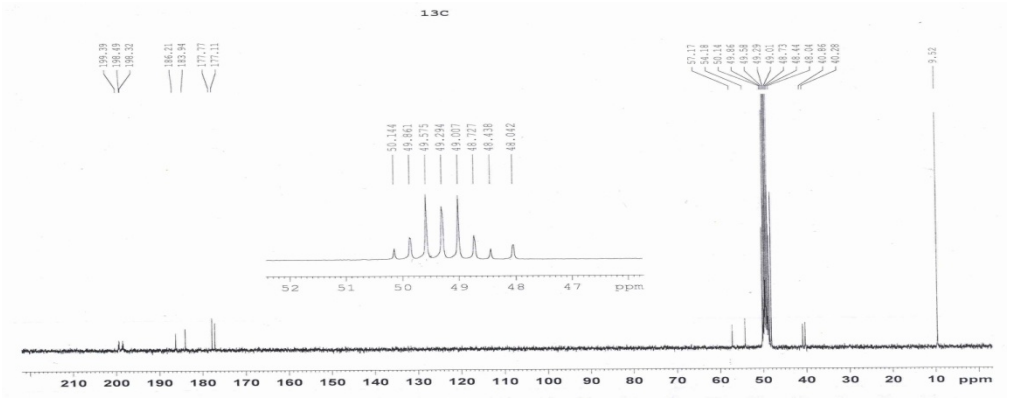
Supplementary Figure S19.



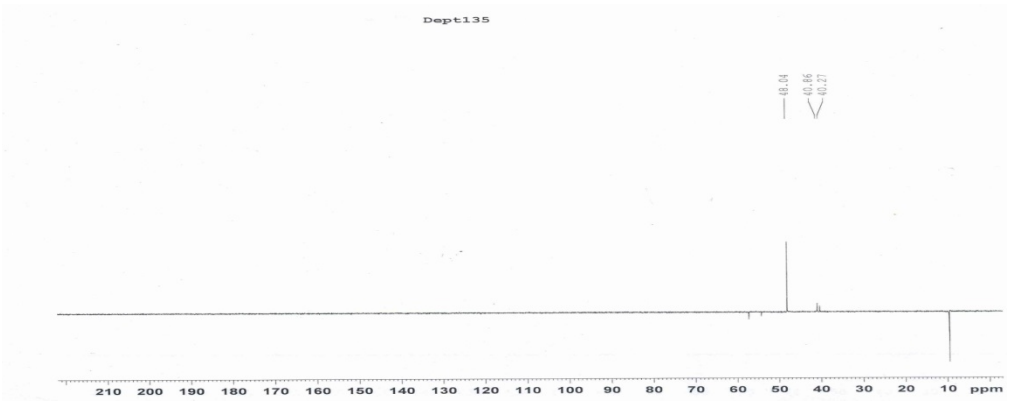
Supplementary Figure S20.



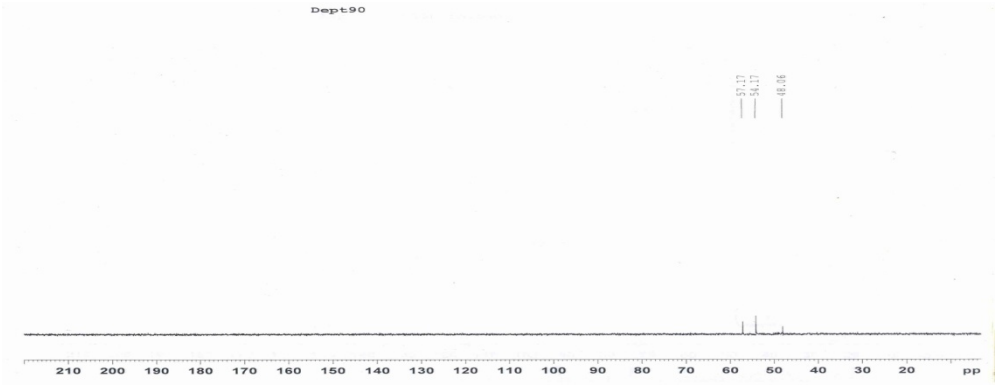
Supplementary Figure S21.



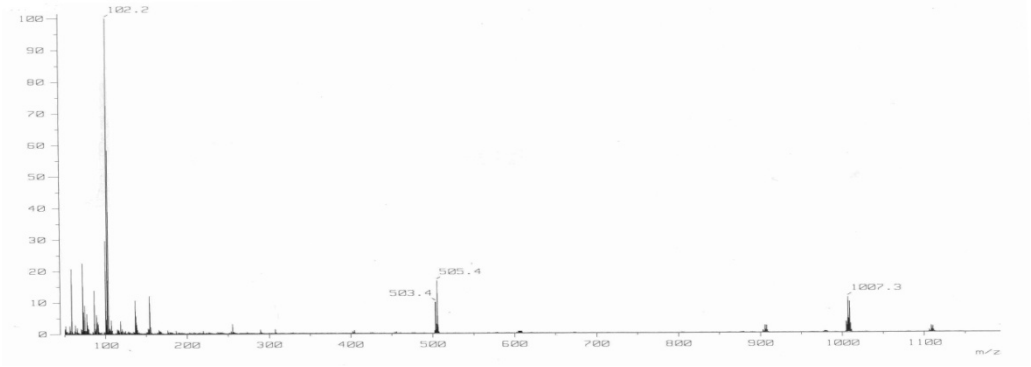
Supplementary Figure S22.



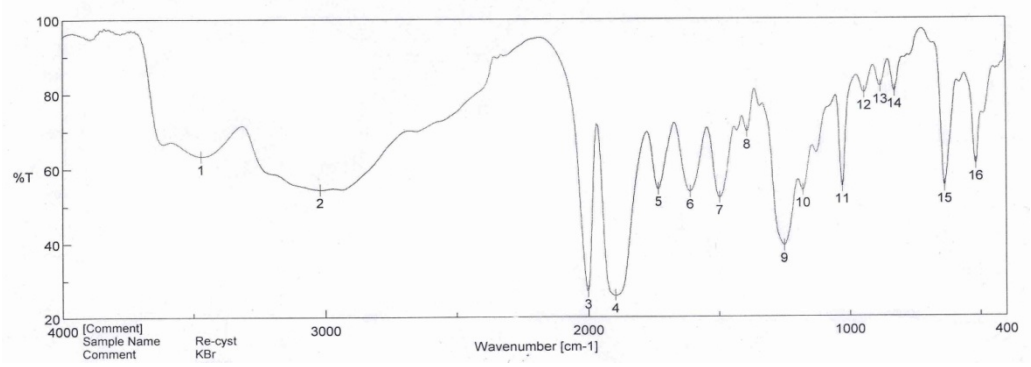
Supplementary Figure S23.



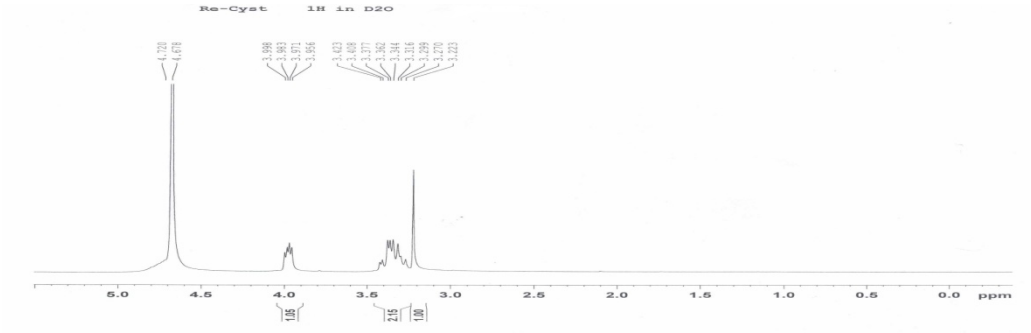
Supplementary Figure S24.



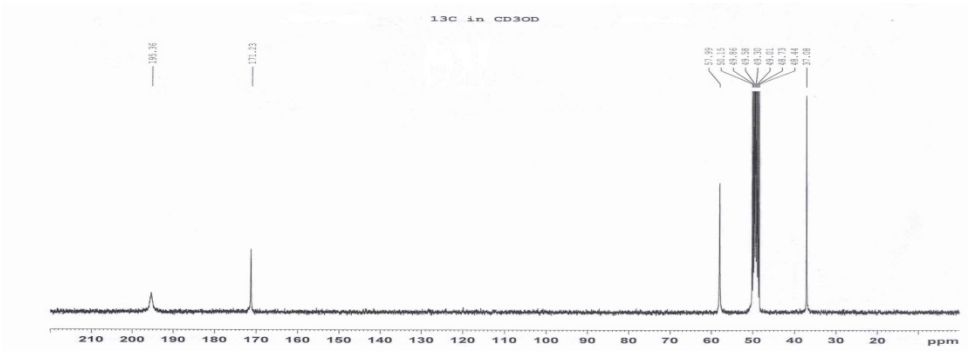
Supplementary Figure S25.



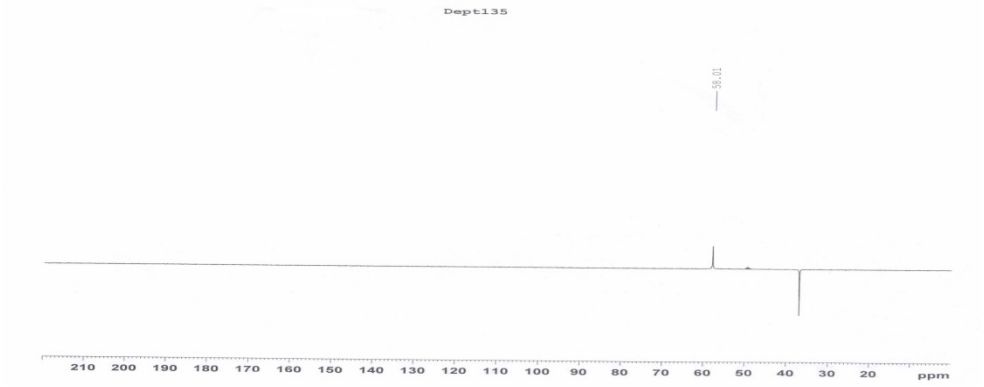
Supplementary Figure S26.



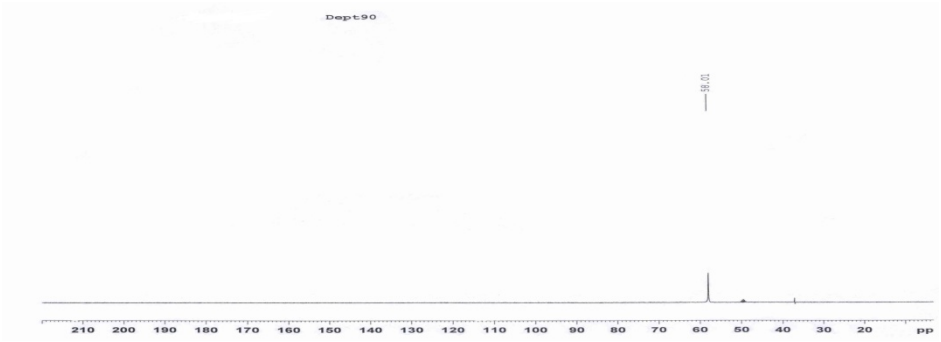
Supplementary Figure S27.



Supplementary Figure S28.



Supplementary Figure S29.



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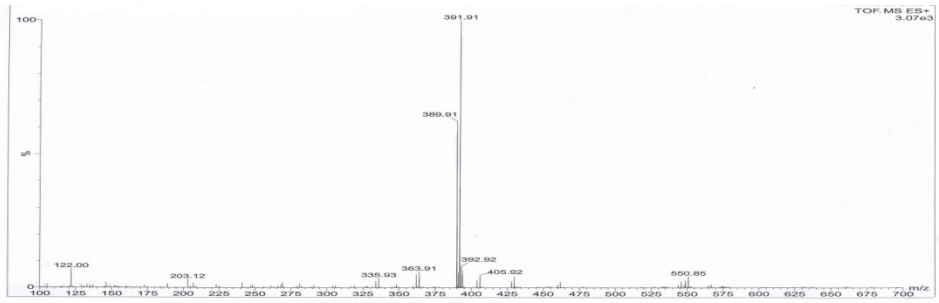


Supplementary Figure S31.

Bond lengths in [Å] of **$Re(CO)_3$-D,L-DAPA and $Re(CO)_3$-D,L-Asp.Et_3NH** crystal data.

$Re(CO)_3$-D,L-DAPA	Bond lengths [Å]	**$Re(CO)_3$-D,L-Asp.Et_3NH**	Bond lengths [Å]
Re(1)-C(1)	1.899(10)	Re(1)-C(2)	1.892(7)
Re(1)-C(3)	1.924(10)	Re(1)-C(1)	1.894(8)
Re(1)-C(2)	1.946(11)	Re(1)-C(3)	1.922(7)
Re(1)-O(4)	2.182(7)	Re(1)-O(6)	2.145(4)
Re(1)-N(1)	2.208(9)	Re(1)-O(4)	2.150(4)
Re(1)-N(2)	2.223(8)	Re(1)-N(1)	2.200(5)
N(2)-C(6)	1.467(14)	C(1)-O(1)	1.160(8)
C(4)-O(3)	1.242(14)	C(2)-O(2)	1.152(8)
C(4)-O(4)	1.267(13)	C(3)-O(5)	1.149(8)
C(4)-C(5)	1.522(16)	C(4)-O(3)	1.219(7)
N(1)-C(5)	1.492(14)	C(4)-O(4)	1.284(7)
C(1)-O(1)	1.152(13)	C(4)-C(5)	1.529(8)
C(5)-C(6)	1.505(16)	C(5)-N(1)	1.493(7)
C(3)-O(5)	1.139(13)	C(5)-C(7)	1.525(8)

C(2)-O(2)	1.102(14)	C(6)-O(7)	1.241(7)
		C(6)-O(6)	1.289(7)
		C(6)-C(7)#1	1.511(8)
		C(7)-C(6)#1	1.511(8)
		N(2)-C(12)	1.443(12)
		N(2)-C(8)	1.462(14)
		N(2)-C(10)	1.531(12)
		C(8)-C(9)	1.404(15)
		C(11)-C(10)	1.442(15)
		C(12)-C(13)	1.487(15)

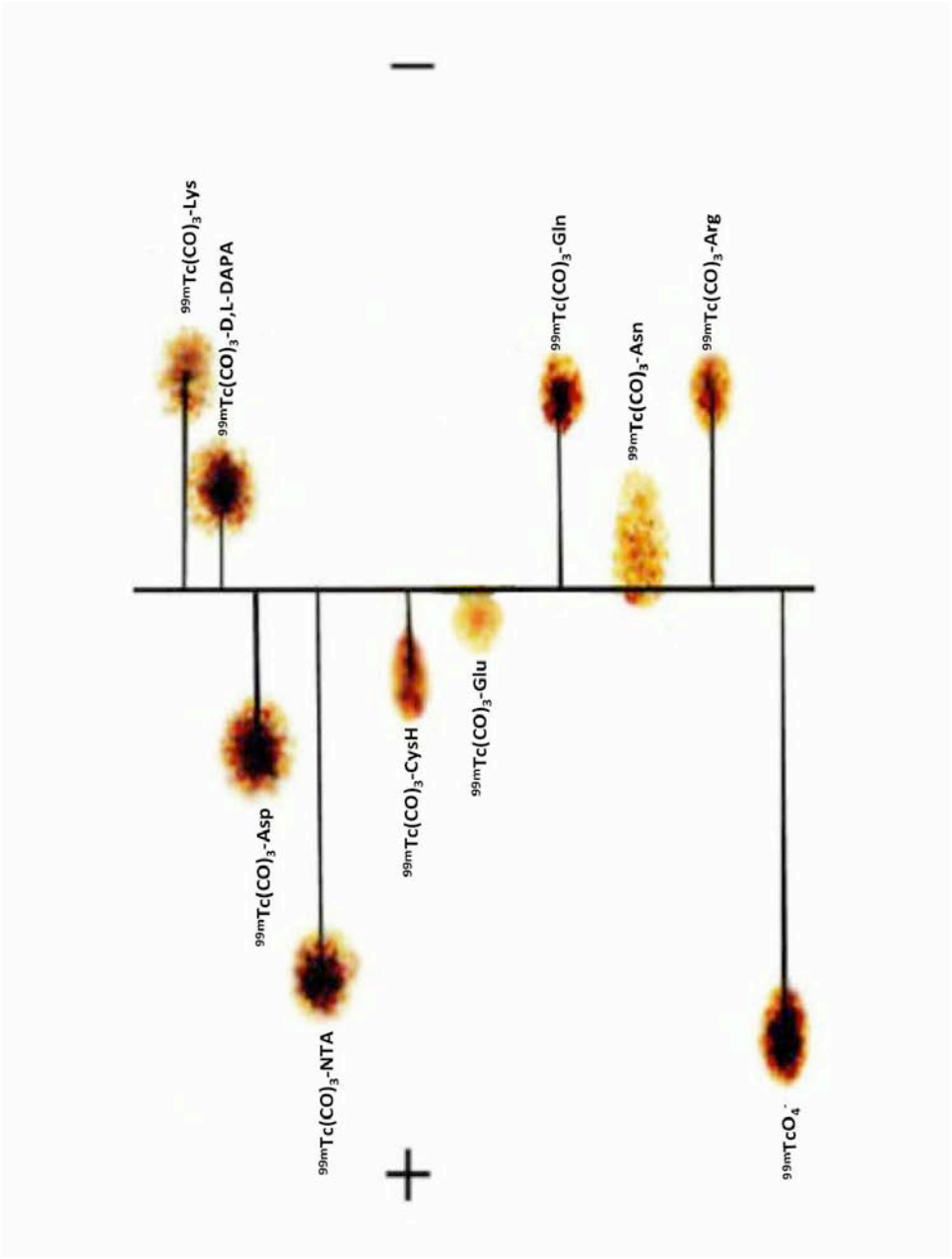
Supplementary Data S32.

Bond angle in Degree of **$Re(CO)_3$-D,L-DAPA and $Re(CO)_3$-D,L-Asp.Et_3NH** crystal data.

$Re(CO)_3$-D,L-DAPA	Angle	**$Re(CO)_3$-D,L-Asp.Et_3NH**	Angle
C(1)-Re(1)-C(3)	88.7(5)	C(2)-Re(1)-C(1)	88.6(3)
C(1)-Re(1)-C(2)	88.1(5)	C(2)-Re(1)-C(3)	88.4(3)
C(3)-Re(1)-C(2)	89.7(5)	C(1)-Re(1)-C(3)	88.3(3)
C(1)-Re(1)-O(4)	171.2(4)	C(2)-Re(1)-O(6)	172.9(3)
C(3)-Re(1)-O(4)	98.6(4)	C(1)-Re(1)-O(6)	95.1(2)
C(2)-Re(1)-O(4)	96.7(4)	C(3)-Re(1)-O(6)	97.8(2)
C(1)-Re(1)-N(1)	98.0(4)	C(2)-Re(1)-O(4)	96.5(3)
C(3)-Re(1)-N(1)	171.2(4)	C(1)-Re(1)-O(4)	172.3(2)
C(2)-Re(1)-N(1)	96.2(4)	C(3)-Re(1)-O(4)	97.6(2)
O(4)-Re(1)-N(1)	74.2(3)	O(6)-Re(1)-O(4)	79.24(17)
C(1)-Re(1)-N(2)	97.7(4)	C(2)-Re(1)-N(1)	93.3(3)
C(3)-Re(1)-N(2)	96.5(4)	C(1)-Re(1)-N(1)	99.1(2)
C(2)-Re(1)-N(2)	171.6(4)	C(3)-Re(1)-N(1)	172.4(2)
O(4)-Re(1)-N(2)	76.8(3)	O(6)-Re(1)-N(1)	80.15(17)

N(1)-Re(1)-N(2)	77.1(3)	O(4)-Re(1)-N(1)	74.88(17)
C(6)-N(2)-Re(1)	111.0(6)	O(1)-C(1)-Re(1)	178.4(7)
O(3)-C(4)-O(4)	123.2(10)	O(2)-C(2)-Re(1)	179.2(8)
O(3)-C(4)-C(5)	120.2(10)	O(5)-C(3)-Re(1)	177.5(6)
O(4)-C(4)-C(5)	116.6(9)	O(3)-C(4)-O(4)	123.8(6)
C(4)-O(4)-Re(1)	113.9(6)	O(3)-C(4)-C(5)	120.7(6)
C(5)-N(1)-Re(1)	101.6(6)	O(4)-C(4)-C(5)	115.5(5)
O(1)-C(1)-Re(1)	178.2(9)	C(4)-O(4)-Re(1)	118.5(4)
N(1)-C(5)-C(6)	106.9(9)	N(1)-C(5)-C(7)	115.0(5)
N(1)-C(5)-C(4)	105.5(9)	N(1)-C(5)-C(4)	108.0(4)
C(6)-C(5)-C(4)	109.0(9)	C(7)-C(5)-C(4)	113.5(5)
N(2)-C(6)-C(5)	109.2(9)	O(7)-C(6)-O(6)	125.1(6)
O(5)-C(3)-Re(1)	179.2(11)	O(7)-C(6)-C(7)#1	118.7(5)
O(2)-C(2)-Re(1)	178.8(12)	O(6)-C(6)-C(7)#1	116.2(5)
		C(6)-O(6)-Re(1)	126.3(4)
		C(5)-N(1)-Re(1)	107.8(3)
		C(6)#1-C(7)-C(5)	115.8(5)
		C(12)-N(2)-C(8)	109.4(10)
		C(12)-N(2)-C(10)	113.5(9)
		C(8)-N(2)-C(10)	105.7(9)
		C(9)-C(8)-N(2)	119.3(12)
		C(11)-C(10)-N(2)	113.4(9)
		N(2)-C(12)-C(13)	115.4(10)

Supplementary Data S33.



Supplementary Figure S34.