Electronic Supplementary Information

The role of stereochemistry in the anticancer activity of Re(I) tricarbonyl complexes

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Analytical data

^{1}H and ^{13}C NMR spectra

Spectra of the ligands

5b

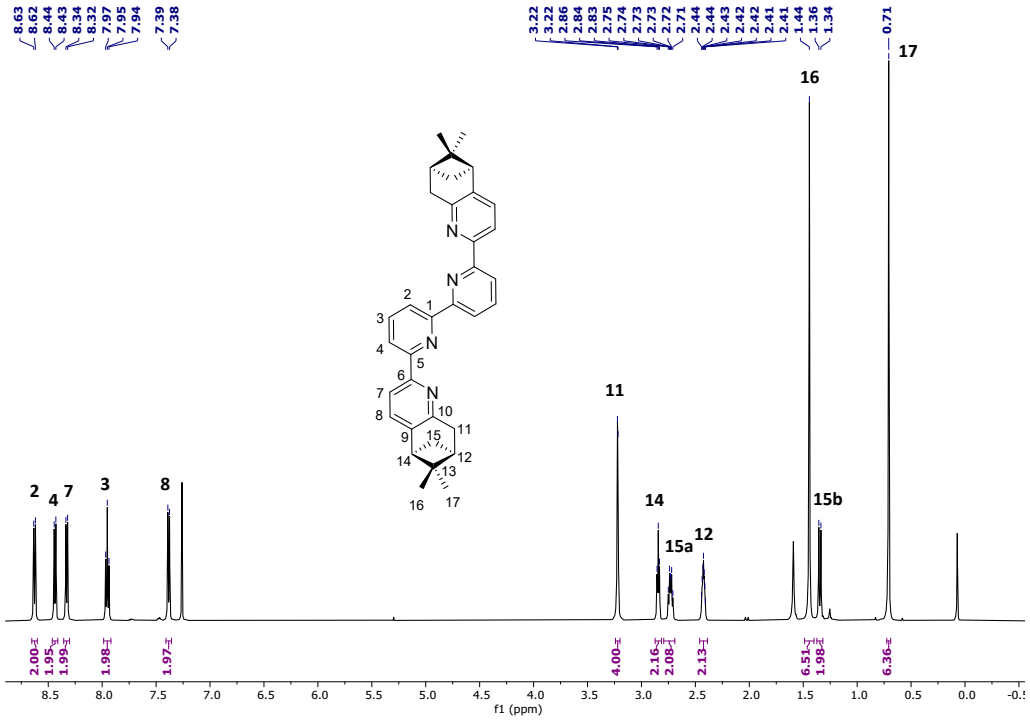

*Figure S1. ^{1}H-NMR spectrum of **5b** in $CDCl_3$*

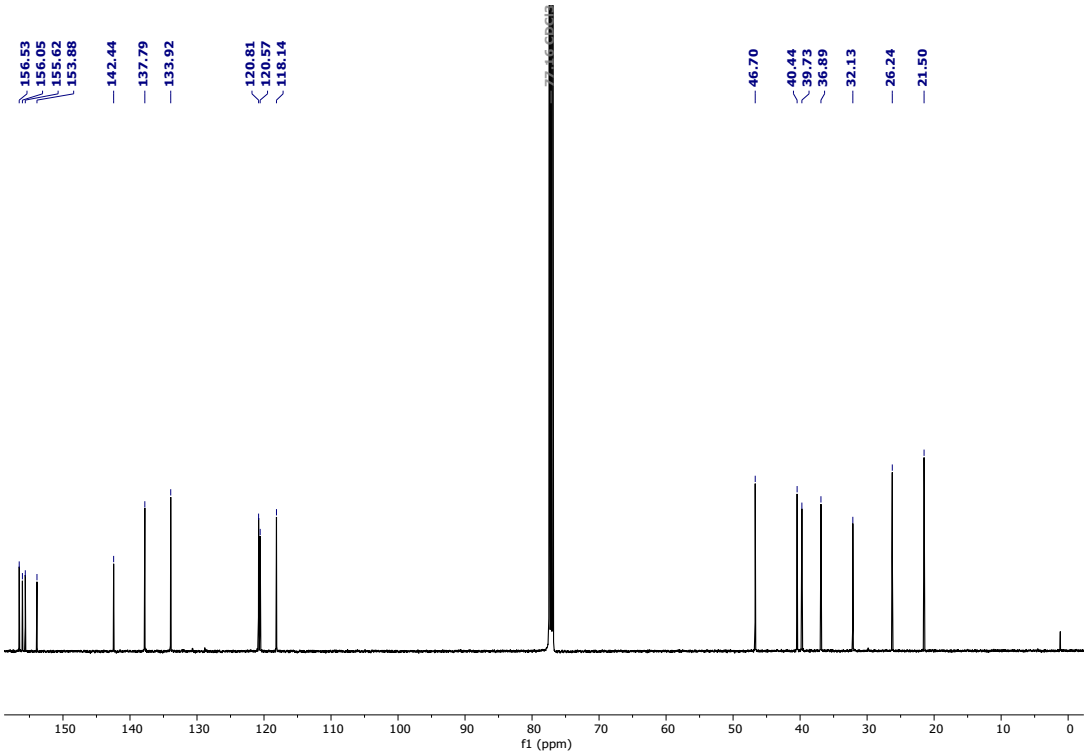

*Figure S2. ^{13}C-NMR spectrum of **5b** in $CDCl_3$*

*Figure S3. COSY spectrum of **5b** in $CDCl_3$*

6a

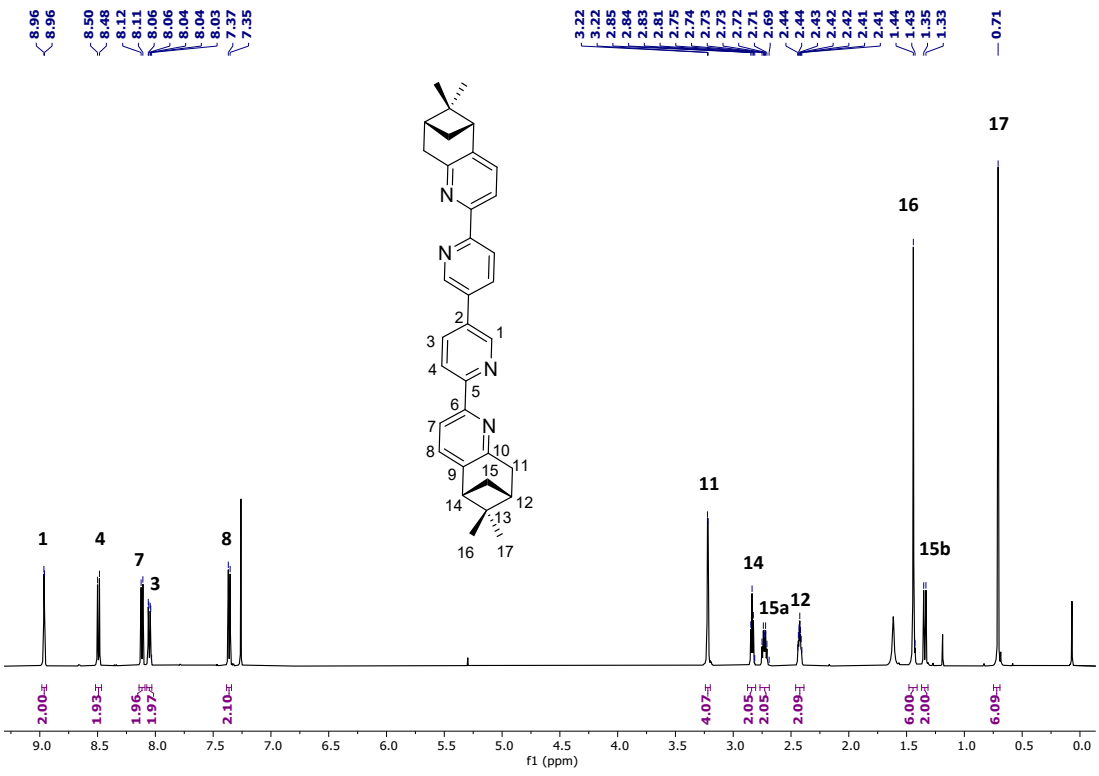

*Figure S4. ^{1}H-NMR spectrum of **6a** in $CDCl_3$*

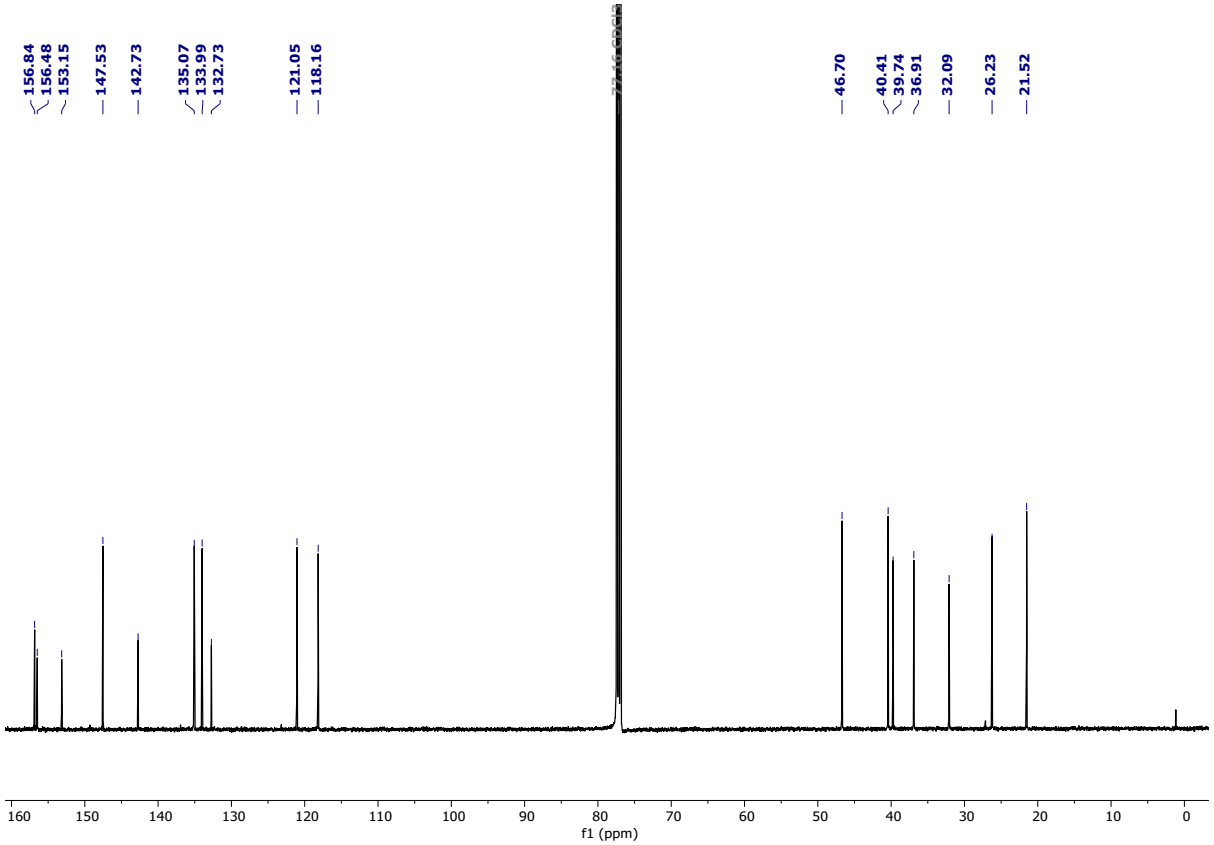

*Figure S5. ^{13}C-NMR spectrum of **6a** in $CDCl_3$*

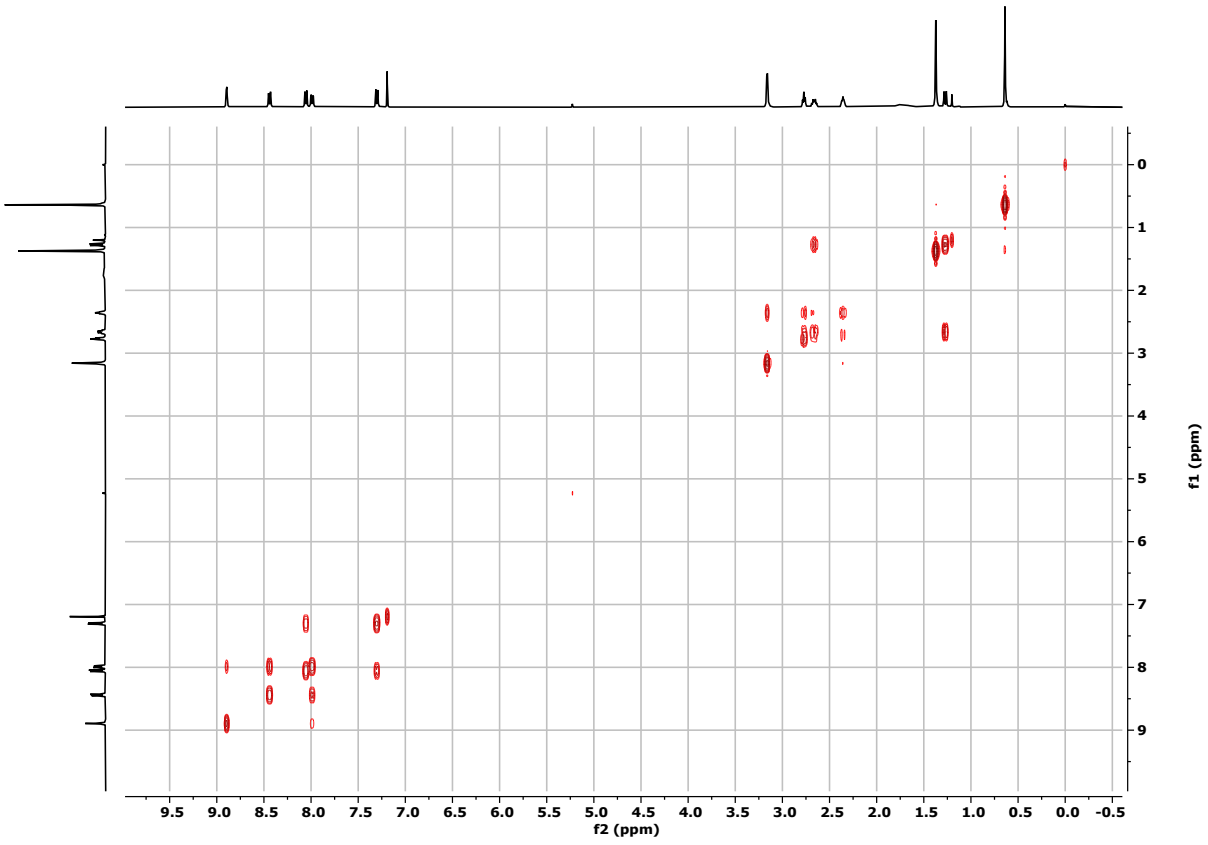

*Figure S 6. COSY spectrum of **6a** in $CDCl_3$*

6b

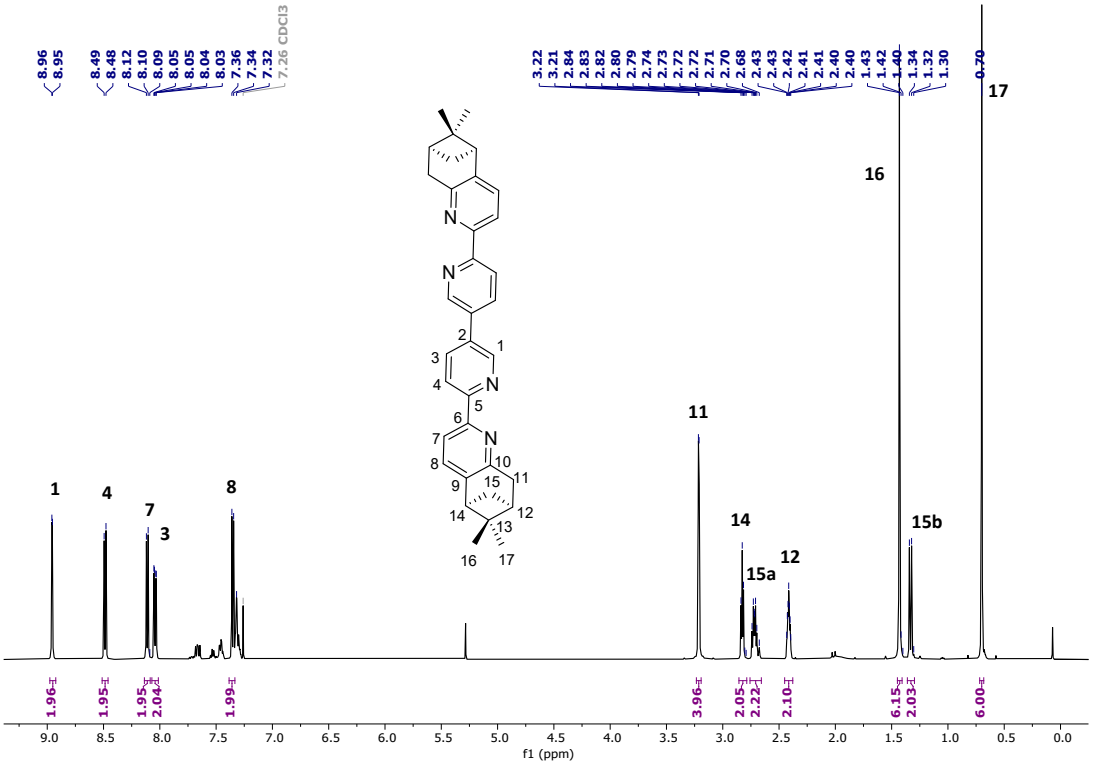

*Figure S7. ^{1}H-NMR spectrum of **6b** in $CDCl_3$*

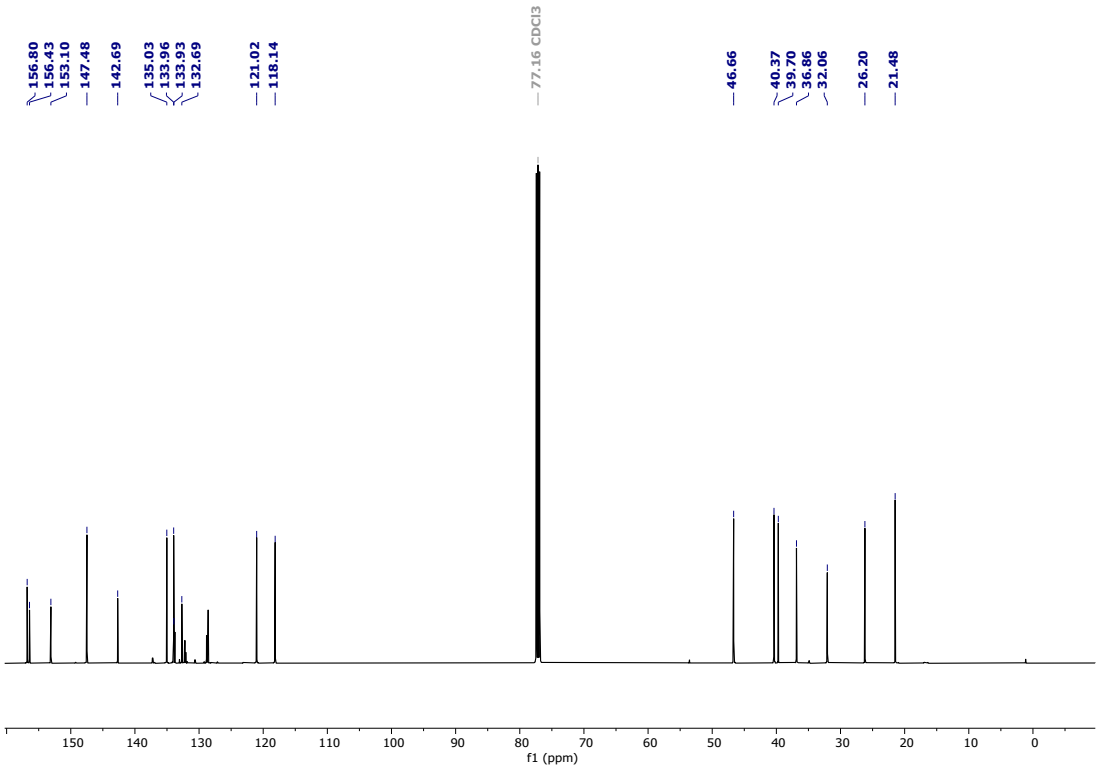

*Figure S8. ^{13}C-NMR spectrum of **6b** in $CDCl_3$*

d1-[Re_2(**5a**)$(CO)_6Cl_2$]

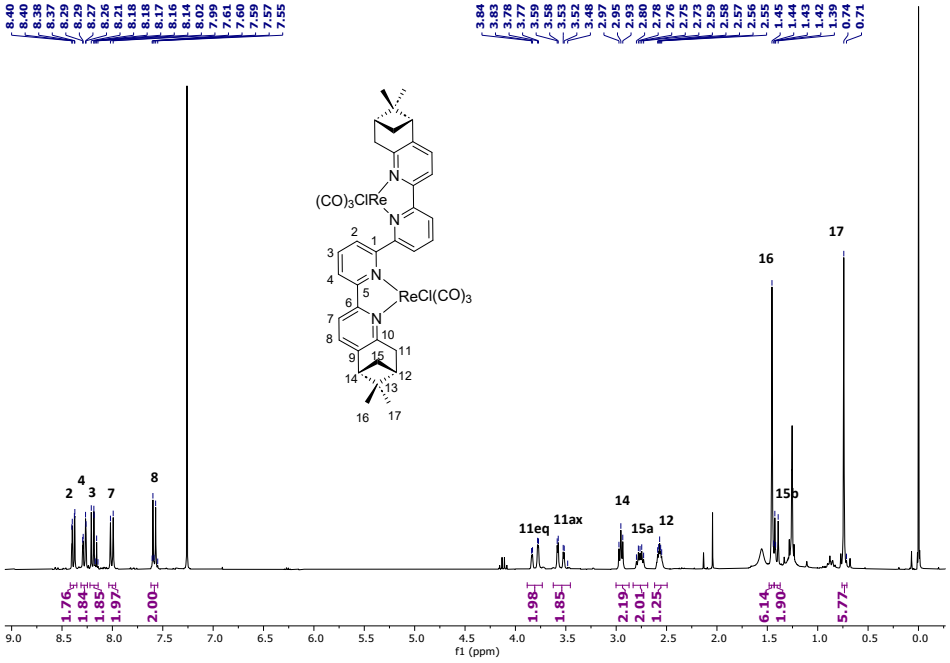

*Figure S9. ^{1}H-NMR spectrum of d1-[Re_2(**5a**)$(CO)_6Cl_2$] in $CDCl_3$*

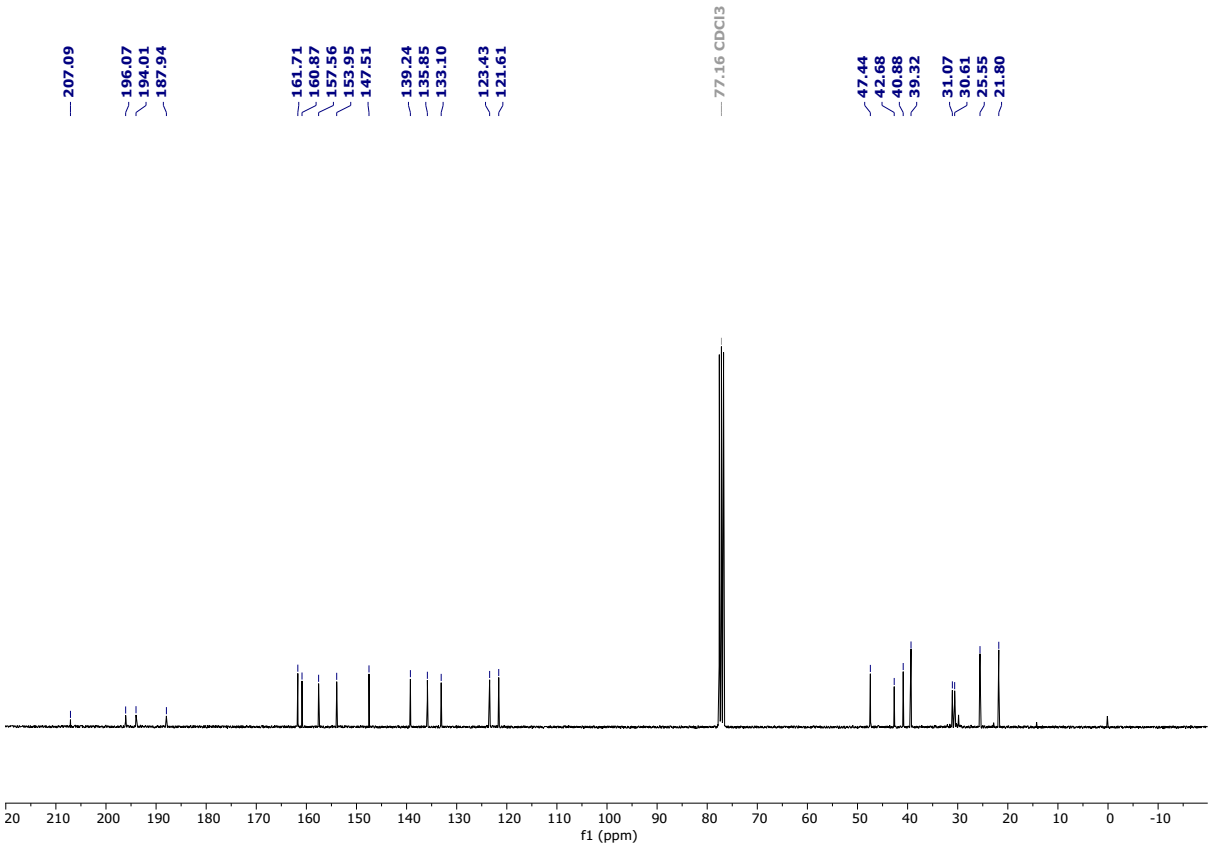

*Figure S10. ^{13}C-NMR spectrum of d1-[Re_2(**5a**)$(CO)_6Cl_2$] in $CDCl_3$*

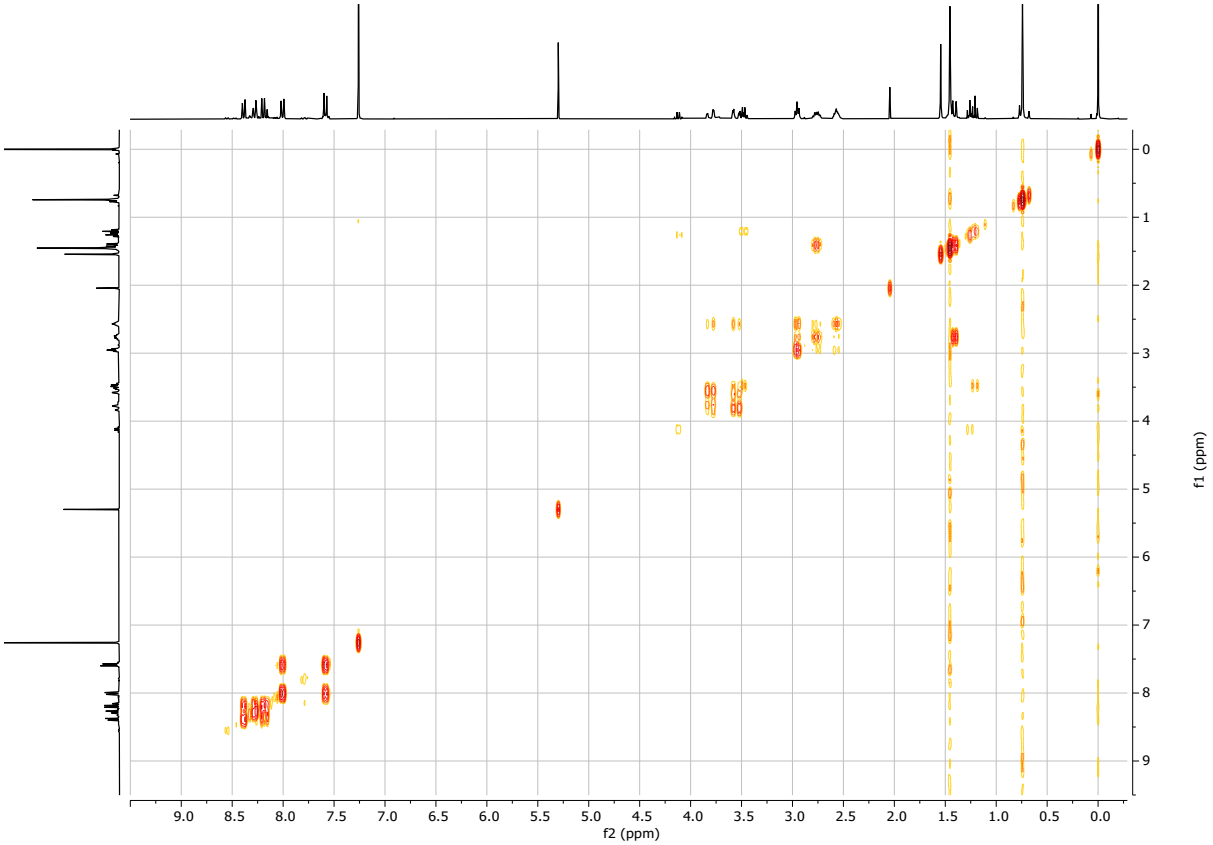

*Figure S11. COSY spectrum of d1-[Re_2(**5a**)$(CO)_6Cl_2$] in $CDCl_3$*

d2-[Re_2(**5a**)$(CO)_6Cl_2$]

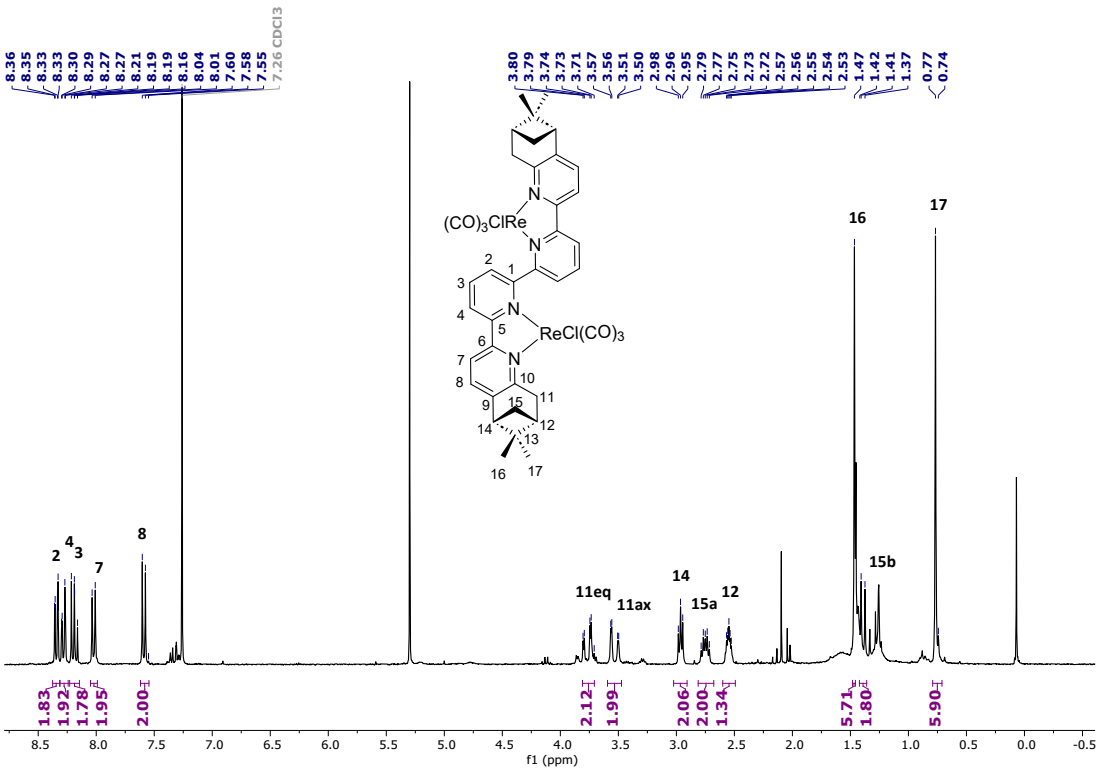

*Figure S12. ^{1}H-NMR spectrum of d2-[Re_2(**5a**)$(CO)_6Cl_2$] in $CDCl_3$*

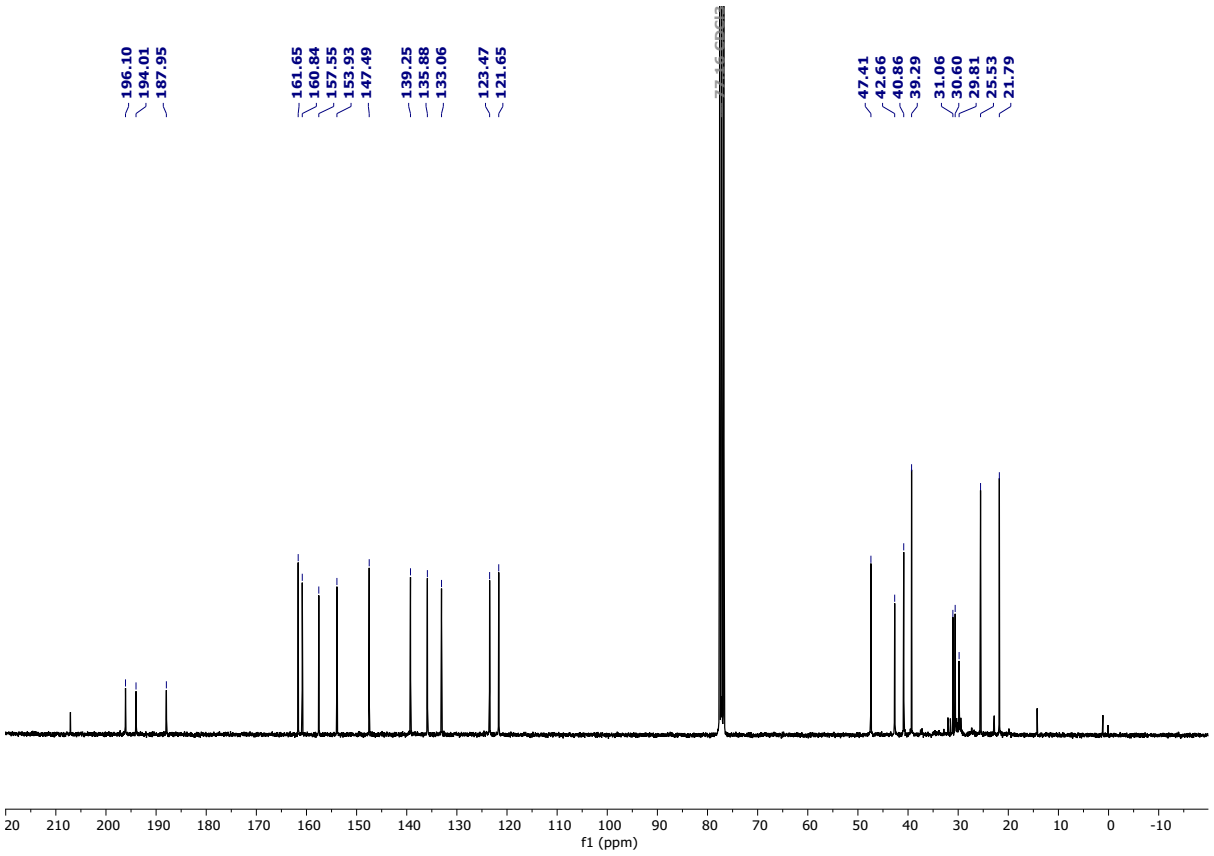

*Figure S13. ^{13}C-NMR spectrum of d2-[Re_2(**5a**)$(CO)_6Cl_2$] in $CDCl_3$*

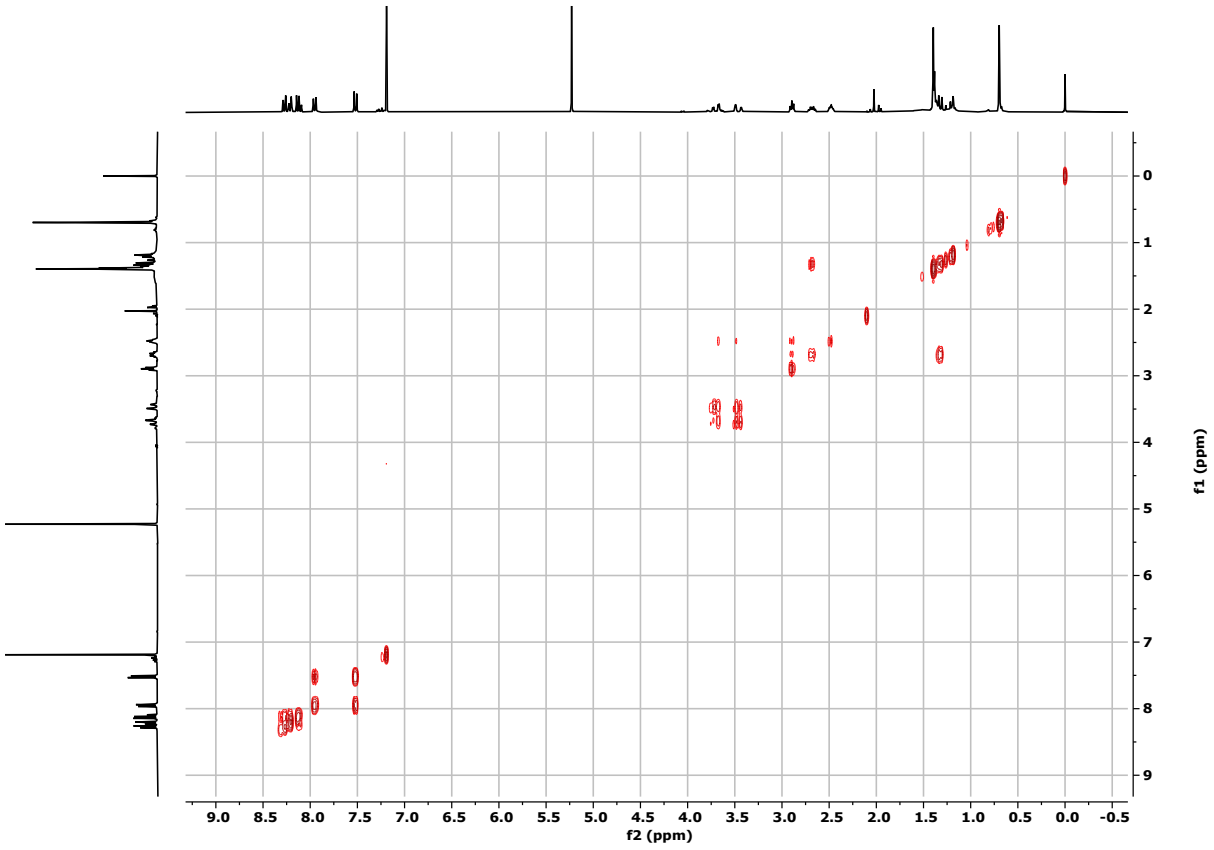

*Figure S 14. COSY spectrum of d2-[Re_2(**5a**)$(CO)_6Cl_2$] in $CDCl_3$*

d1-[Re_2(**5b**)$(CO)_6Cl_2$]

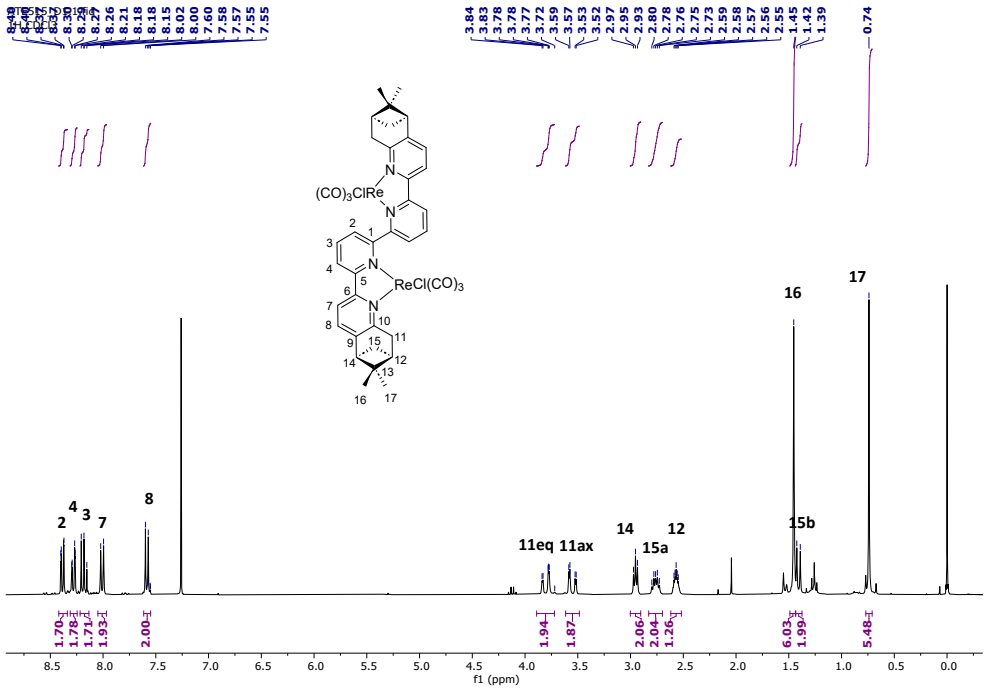

*Figure S15. ^{1}H-NMR spectrum of d1-[Re_2(**5b**)$(CO)_6Cl_2$] in $CDCl_3$*

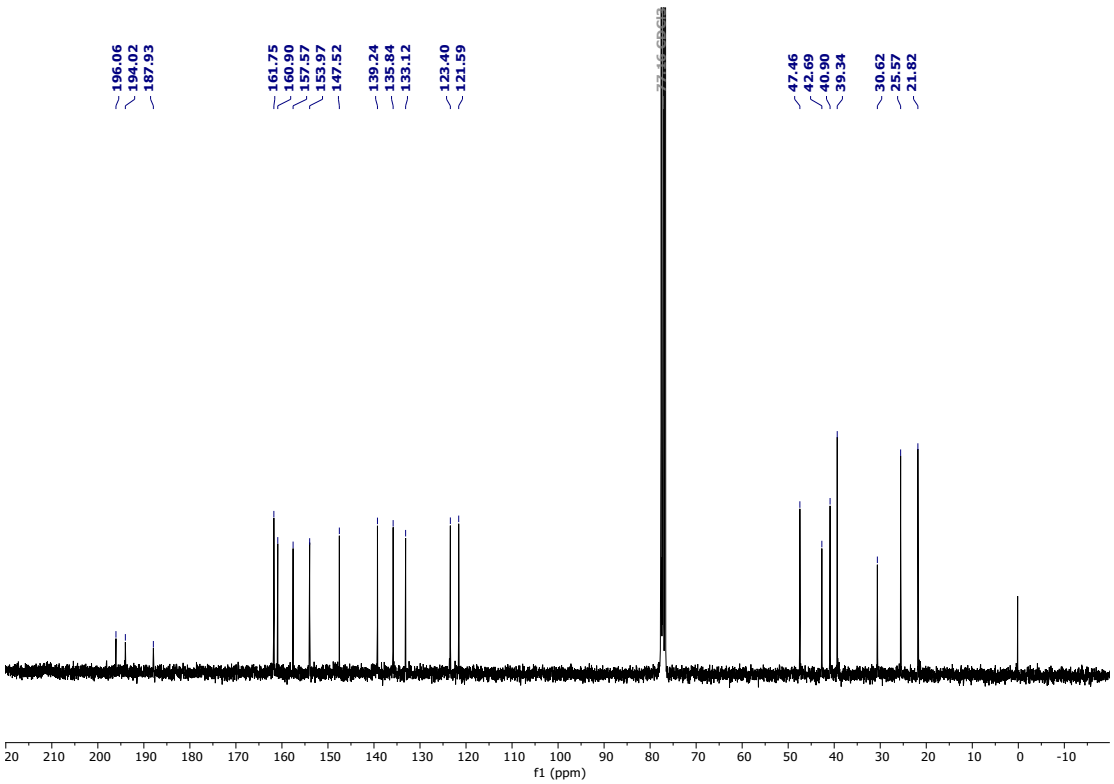

*Figure S16. ^{13}C-NMR spectrum of d1-[Re_2(**5b**)$(CO)_6Cl_2$] in $CDCl_3$*

d2-[Re_2(**5b**)$(CO)_6Cl_2$]

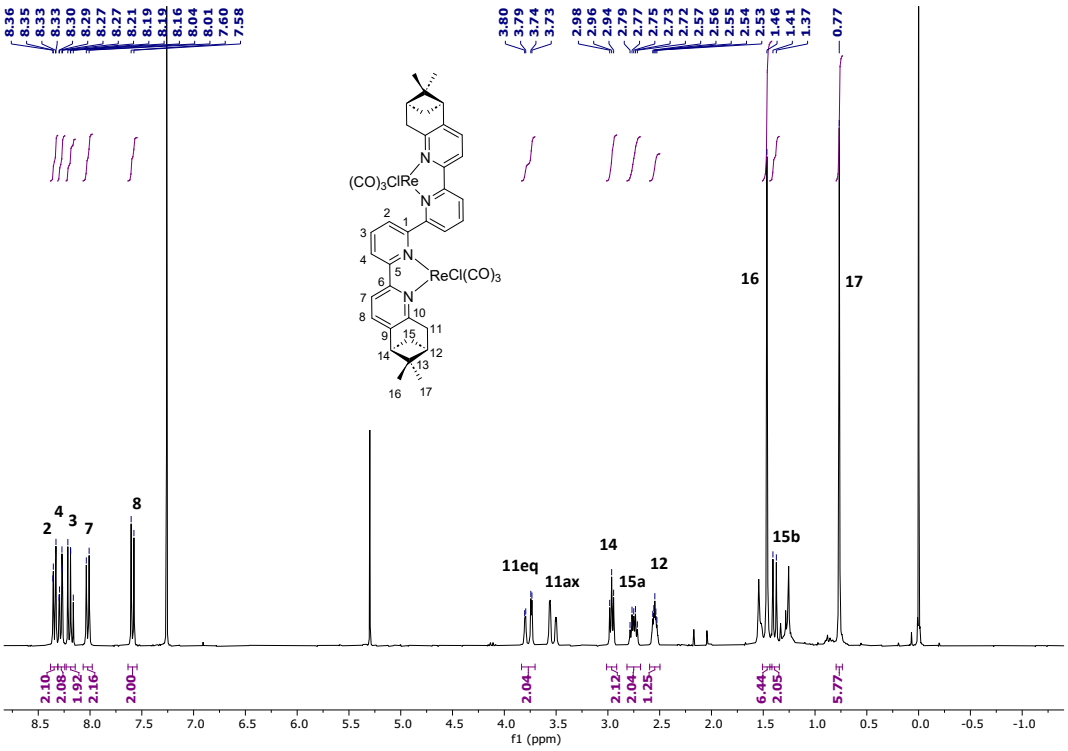

*Figure S17. ^{1}H-NMR spectrum of d2-[Re_2(**5b**)$(CO)_6Cl_2$] in $CDCl_3$*

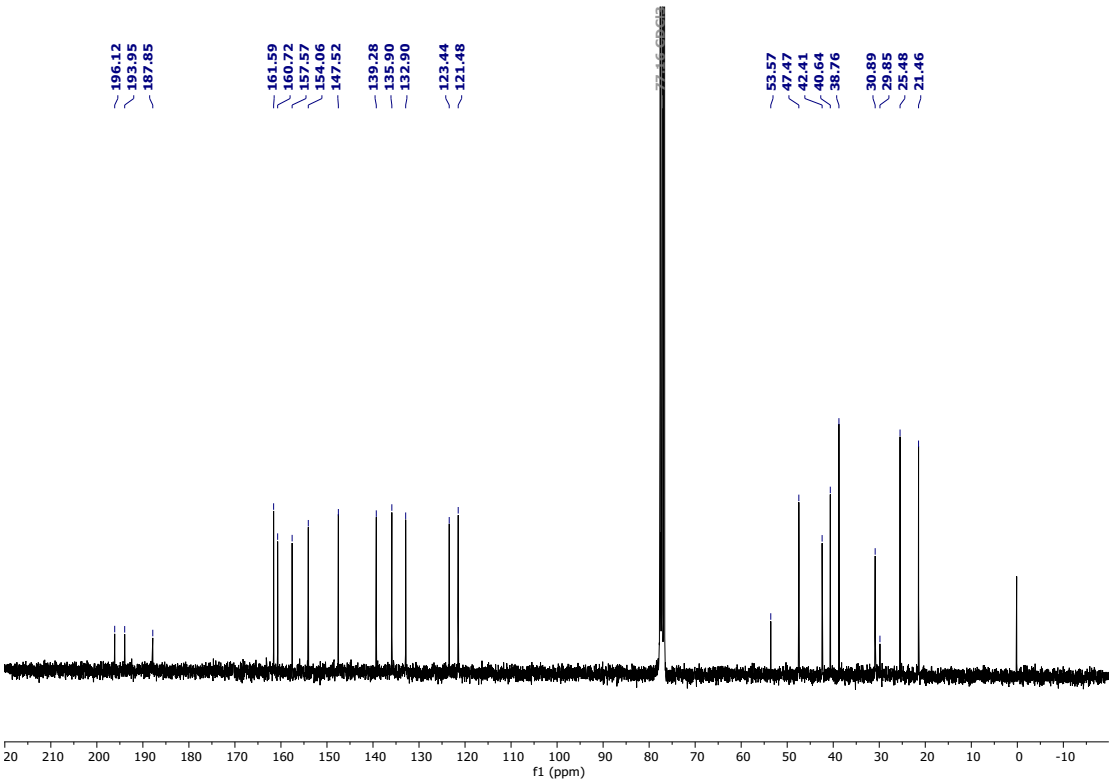

*Figure S18. ^{13}C-NMR spectrum of d2-[Re_2(**5b**)$(CO)_6Cl_2$] in $CDCl_3$*

d1-[Re_2(**6a**)$(CO)_6Cl_2$]

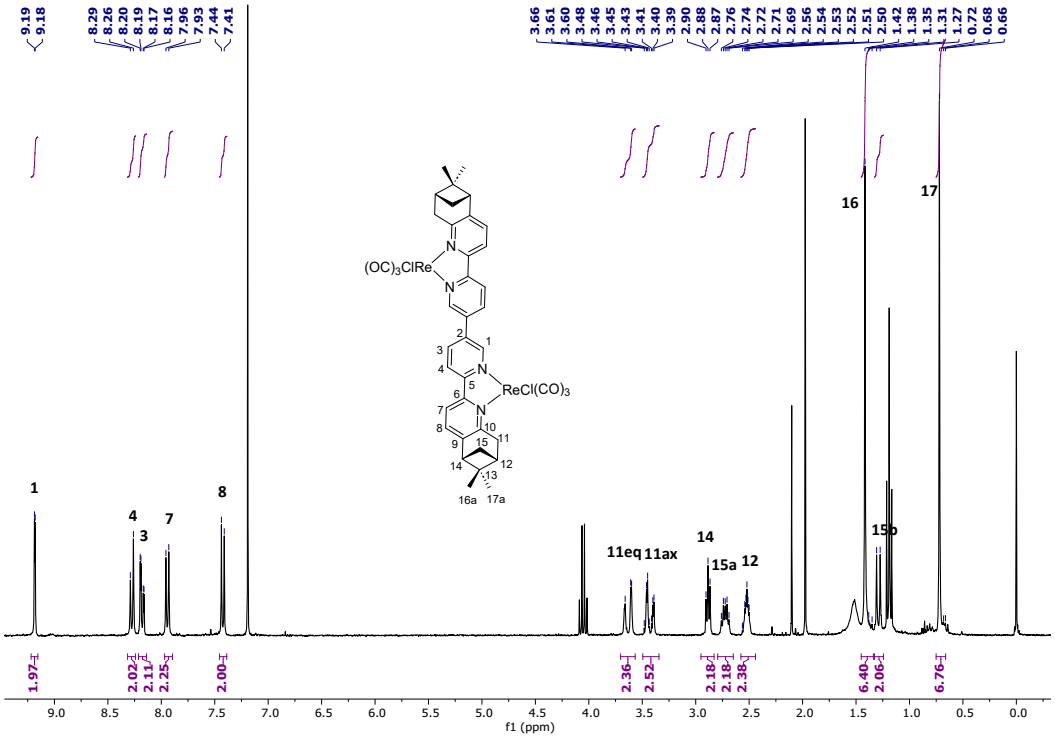

*Figure S19. ^{1}H-NMR spectrum of d1-[Re_2(**6a**)$(CO)_6Cl_2$] in $CDCl_3$*

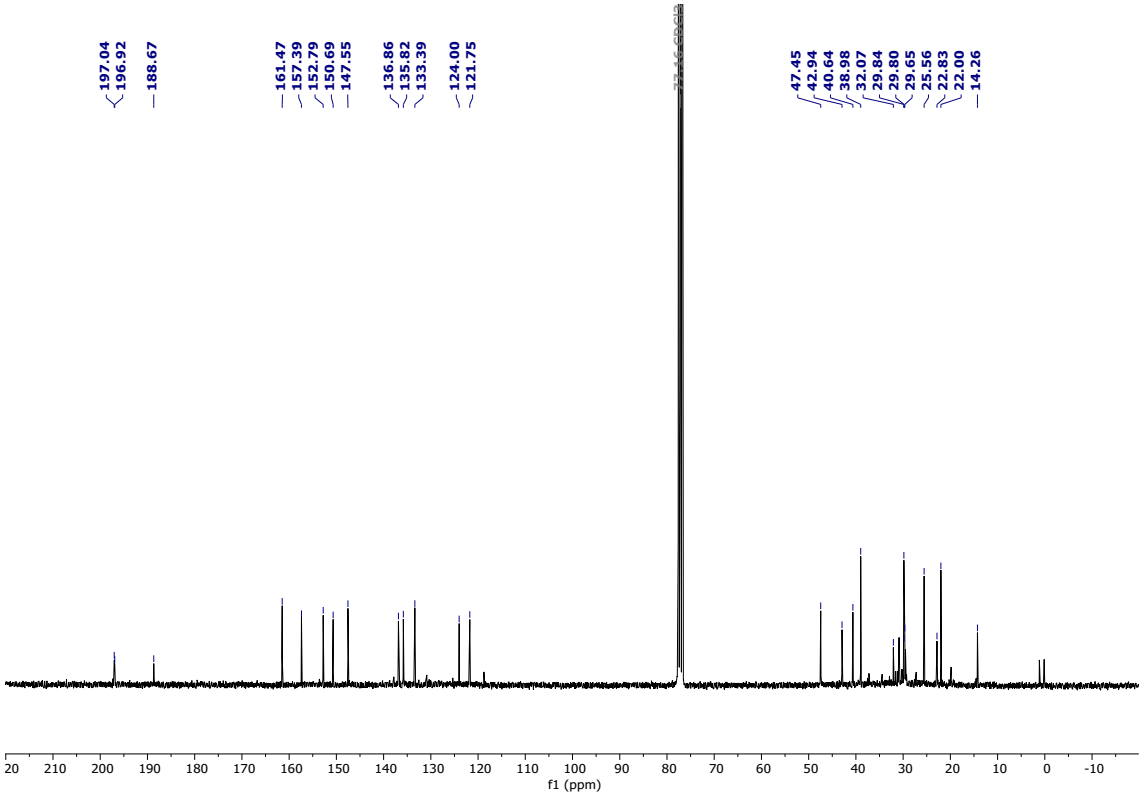

*Figure S20. ^{13}C-NMR spectrum of d1-[Re_2(**6a**)$(CO)_6Cl_2$] in $CDCl_3$*

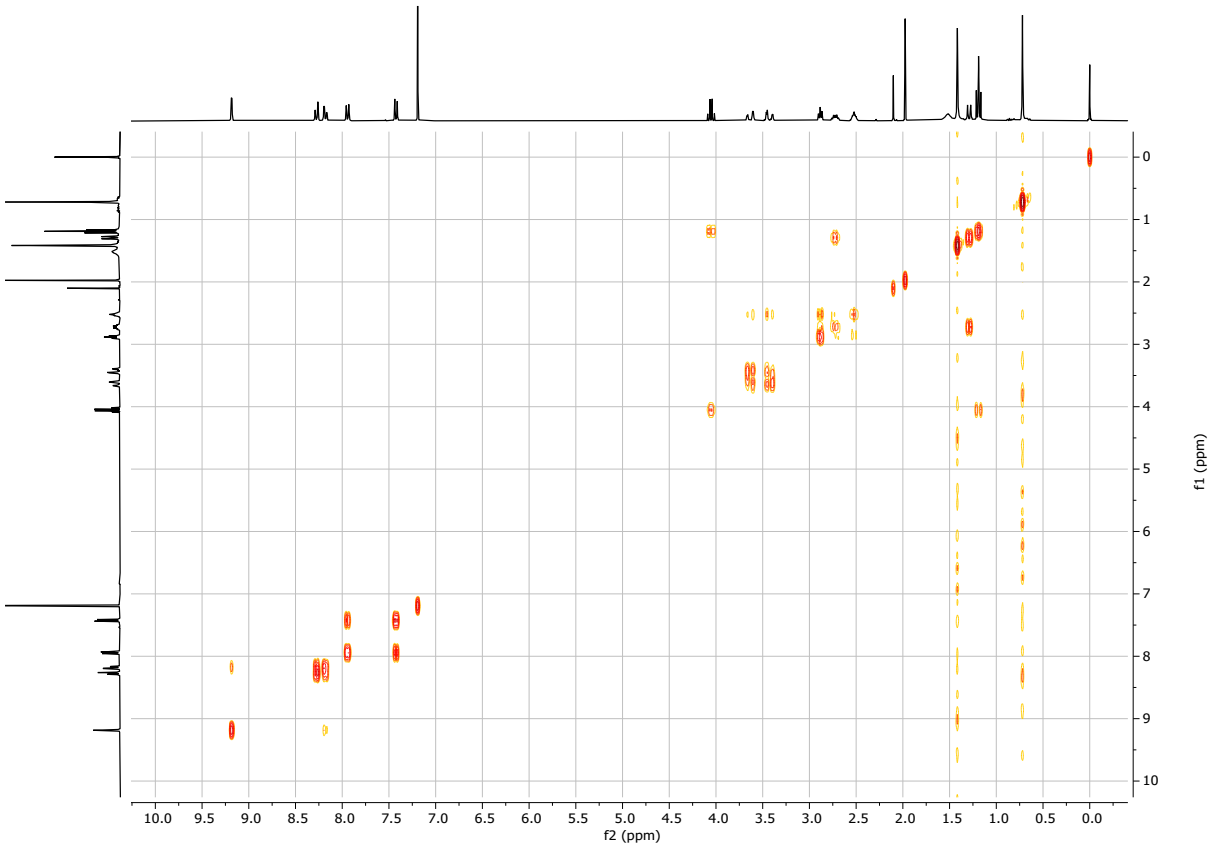

*Figure S21. COSY spectrum of d1-[Re_2(**6a**)$(CO)_6Cl_2$] in $CDCl_3$*

d2-[Re_2(**6a**)$(CO)_6Cl_2$]

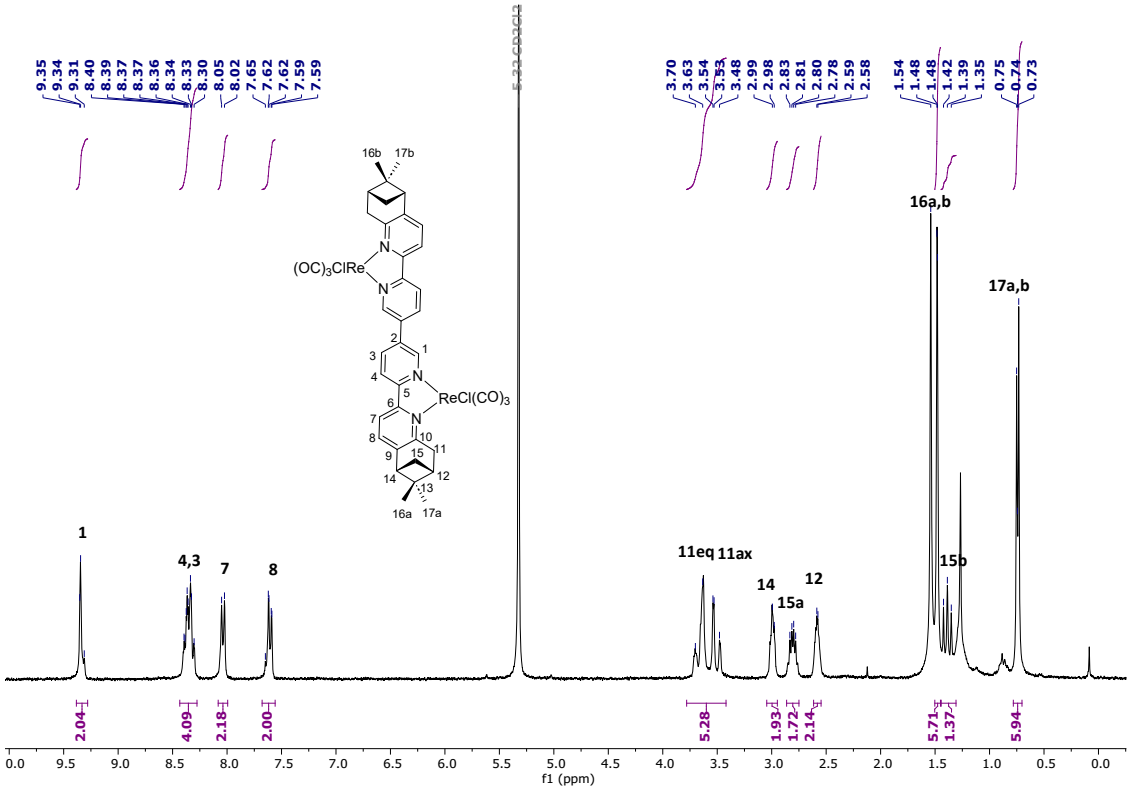

*Figure S22. ^{1}H-NMR spectrum of d2-[Re_2(**6a**)$(CO)_6Cl_2$] in CD_2Cl_2*

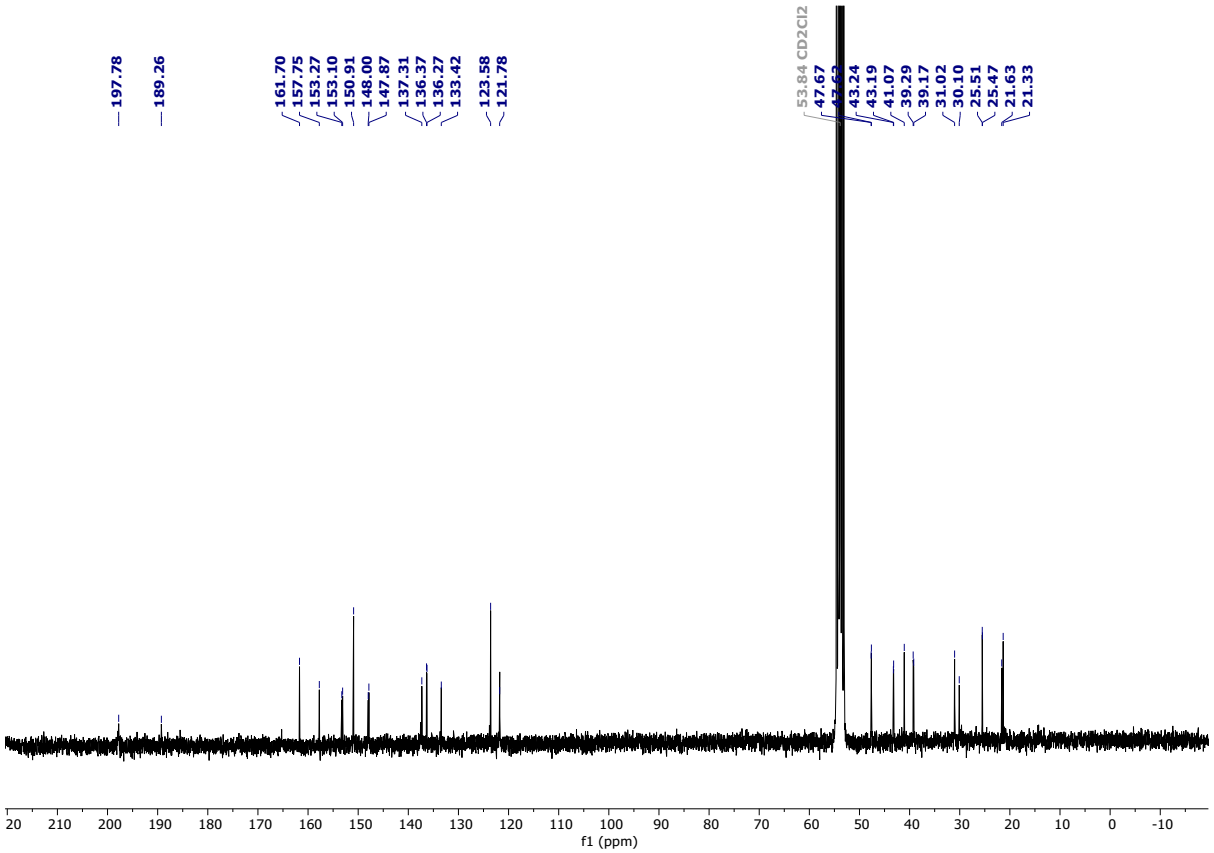

*Figure S23. ^{13}C-NMR spectrum of d2-[Re_2(**6a**)$(CO)_6Cl_2$] in CD_2Cl_2*

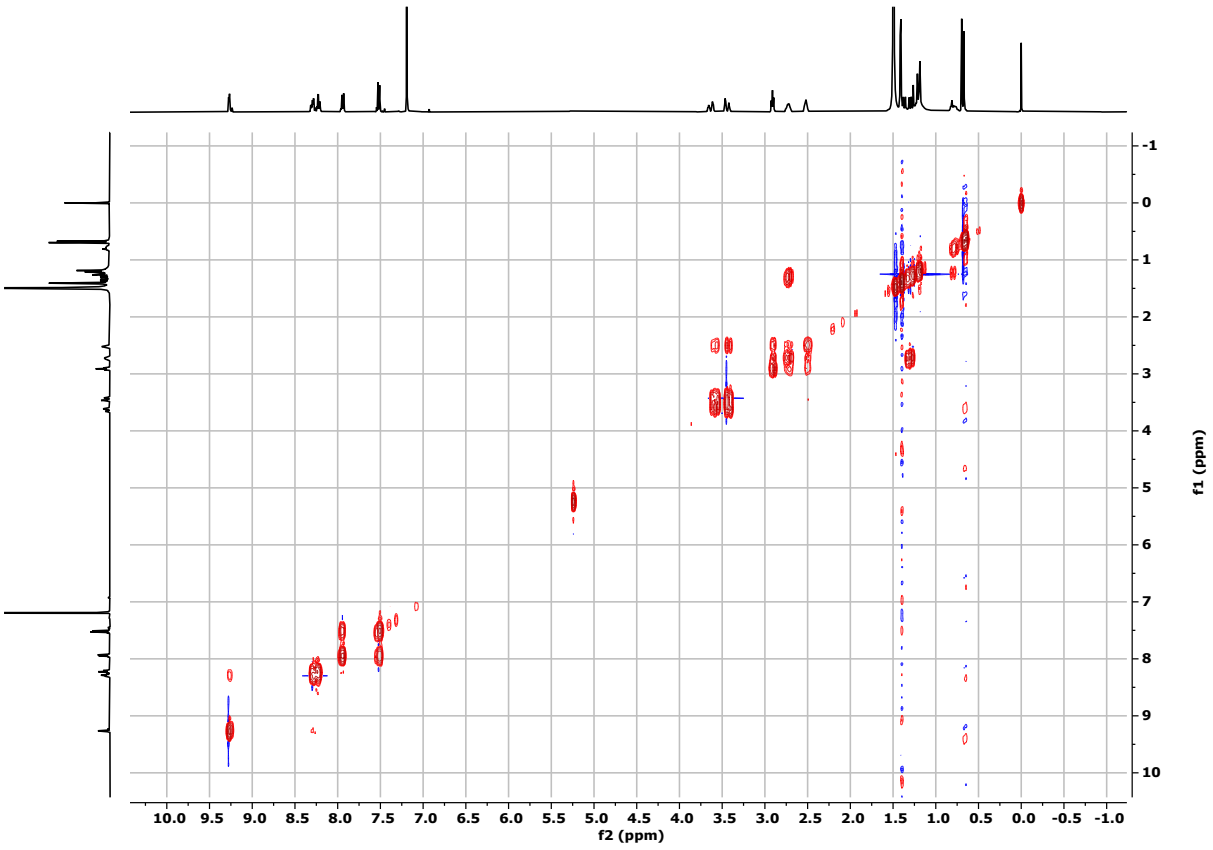

*Figure S24. COSY spectrum of d2-[Re_2(**6a**)$(CO)_6Cl_2$] in CD_2Cl_2*

*d1-[Re_2(**6b**)$(CO)_6Cl_2$]*

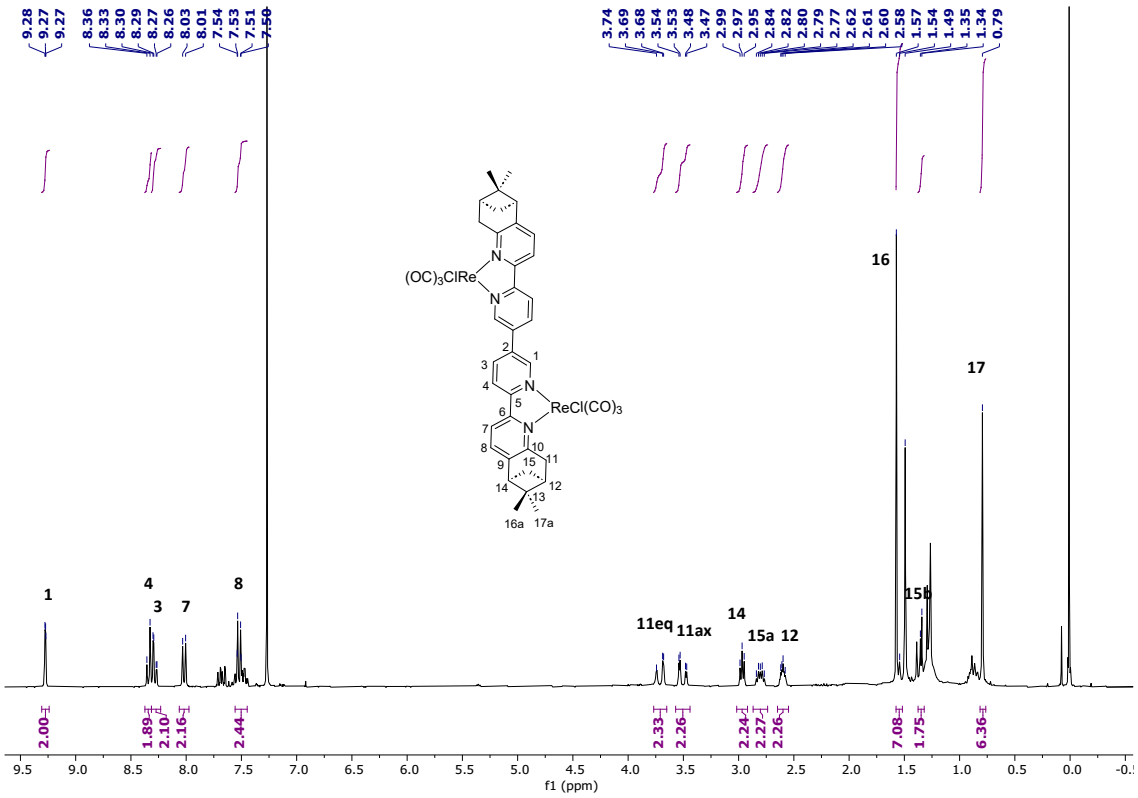

*Figure S26. ^{1}H-NMR spectrum of d1-[Re_2(**6b**)$(CO)_6Cl_2$] in $CDCl_3$*

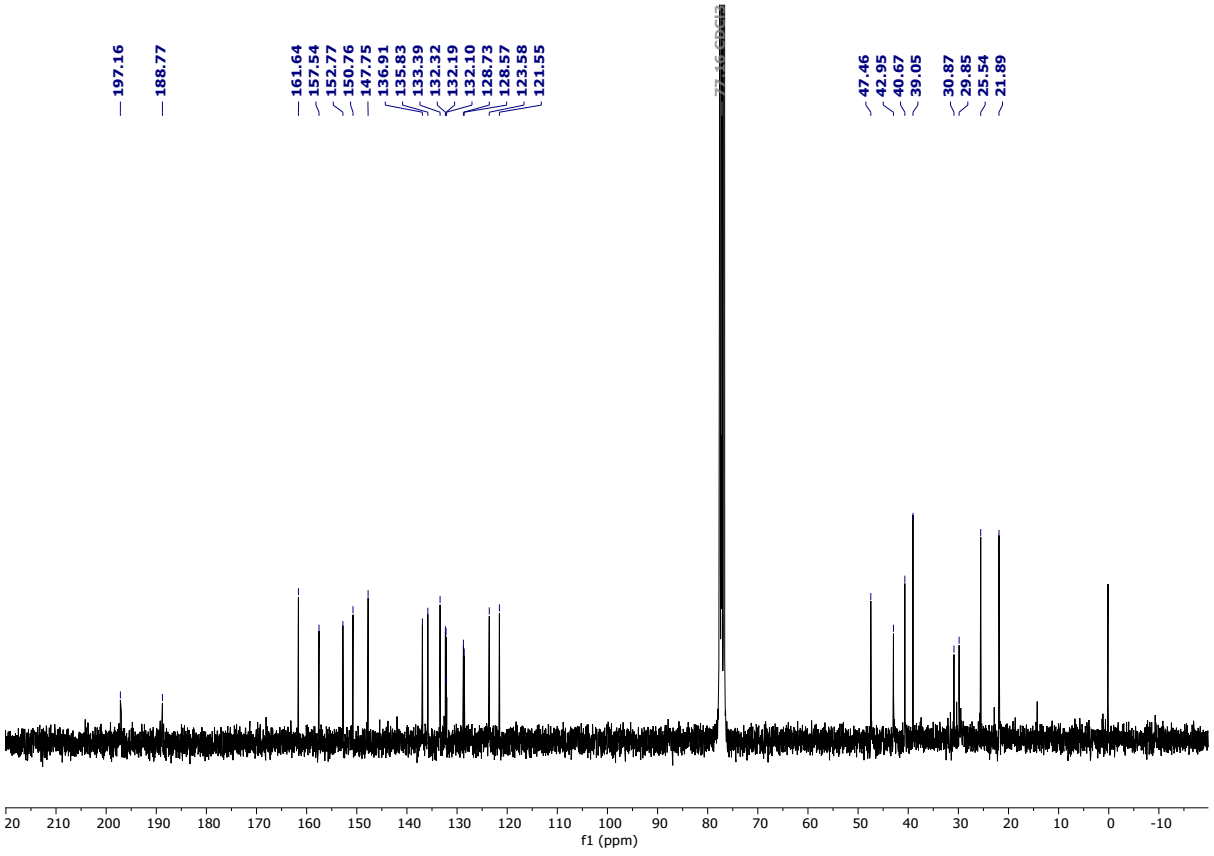

*Figure S27. ^{13}C-NMR spectrum of d1-[Re_2(**6b**)$(CO)_6Cl_2$] in $CDCl_3$*

d2-[Re_2(**6b**)$(CO)_6Cl_2$]

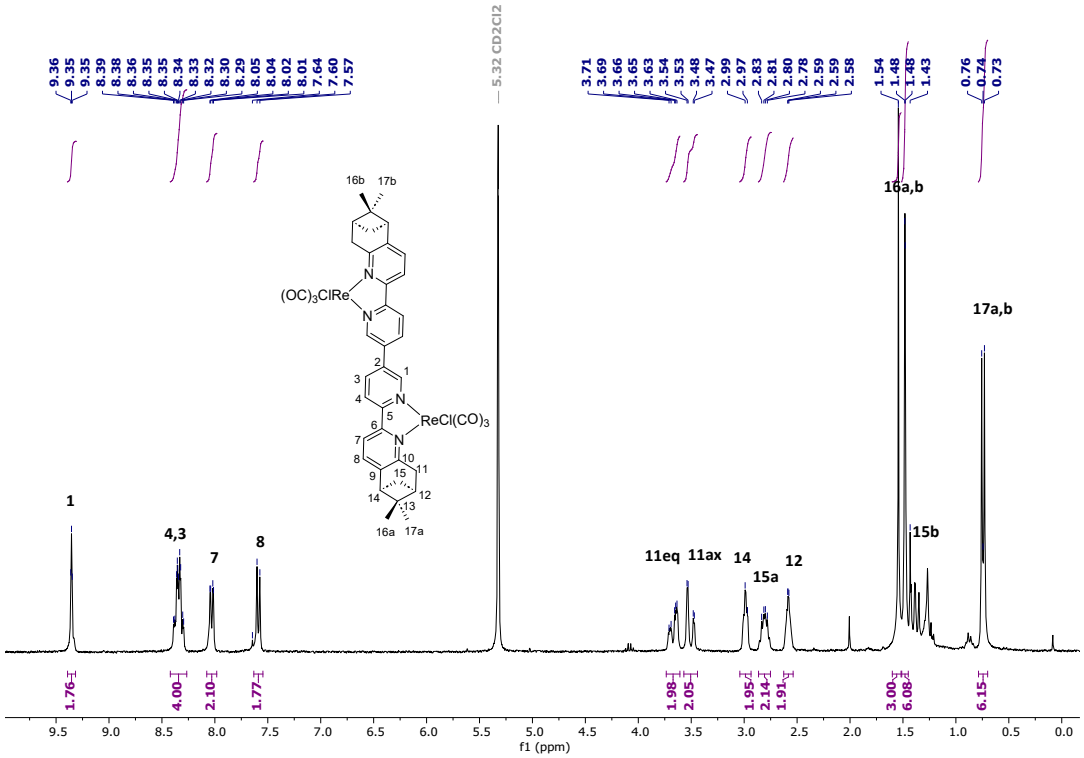

*Figure S28. ^{1}H-NMR spectrum of d2-[Re_2(**6b**)$(CO)_6Cl_2$] in CD_2Cl_2*

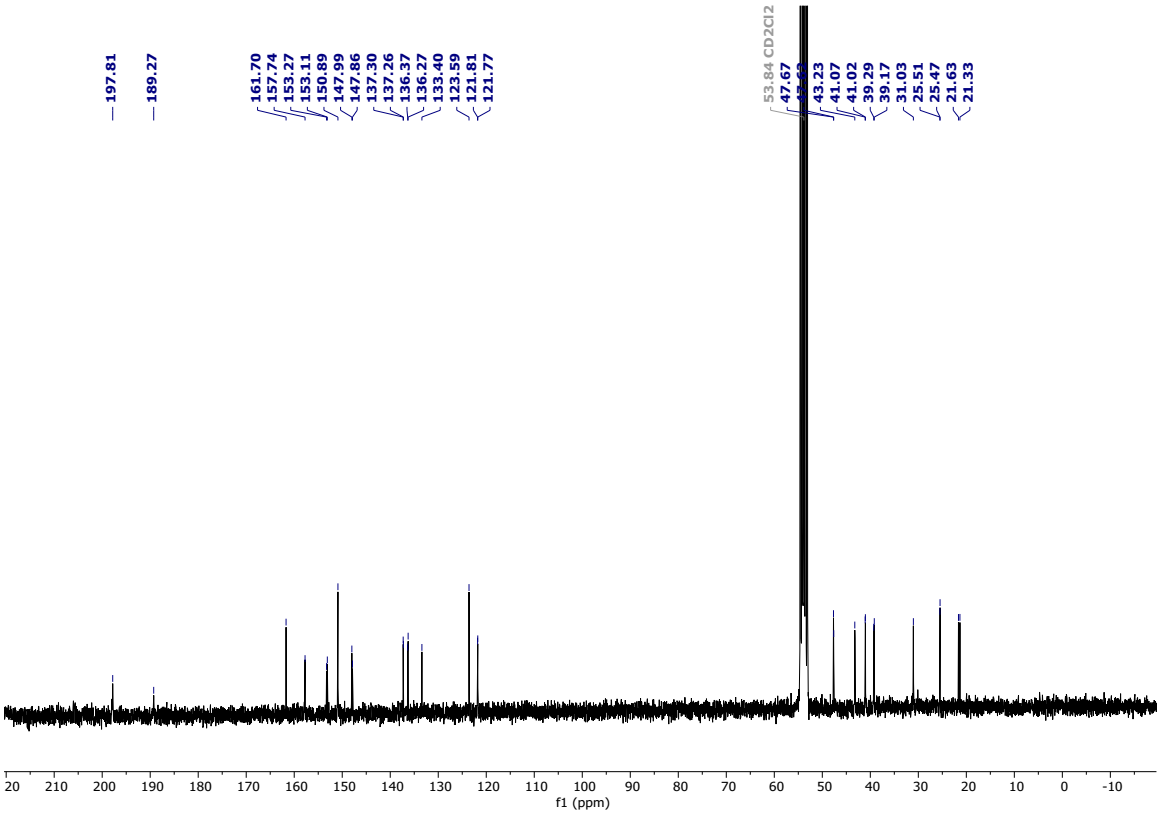

*Figure S29. ^{13}C-NMR spectrum of d2-[Re_2(**6b**)$(CO)_6Cl_2$] in CD_2Cl_2*

HRMS spectra

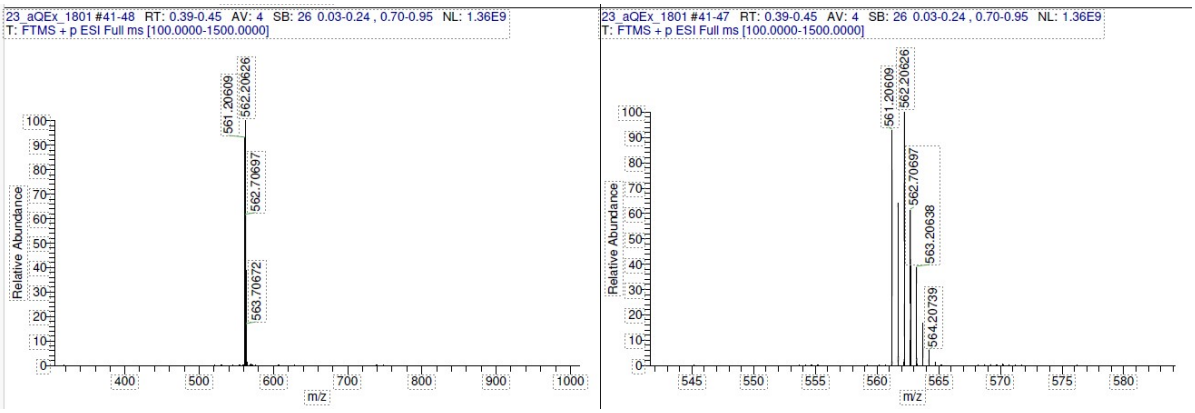

*Figure S30. HRMS spectrum of **5b***

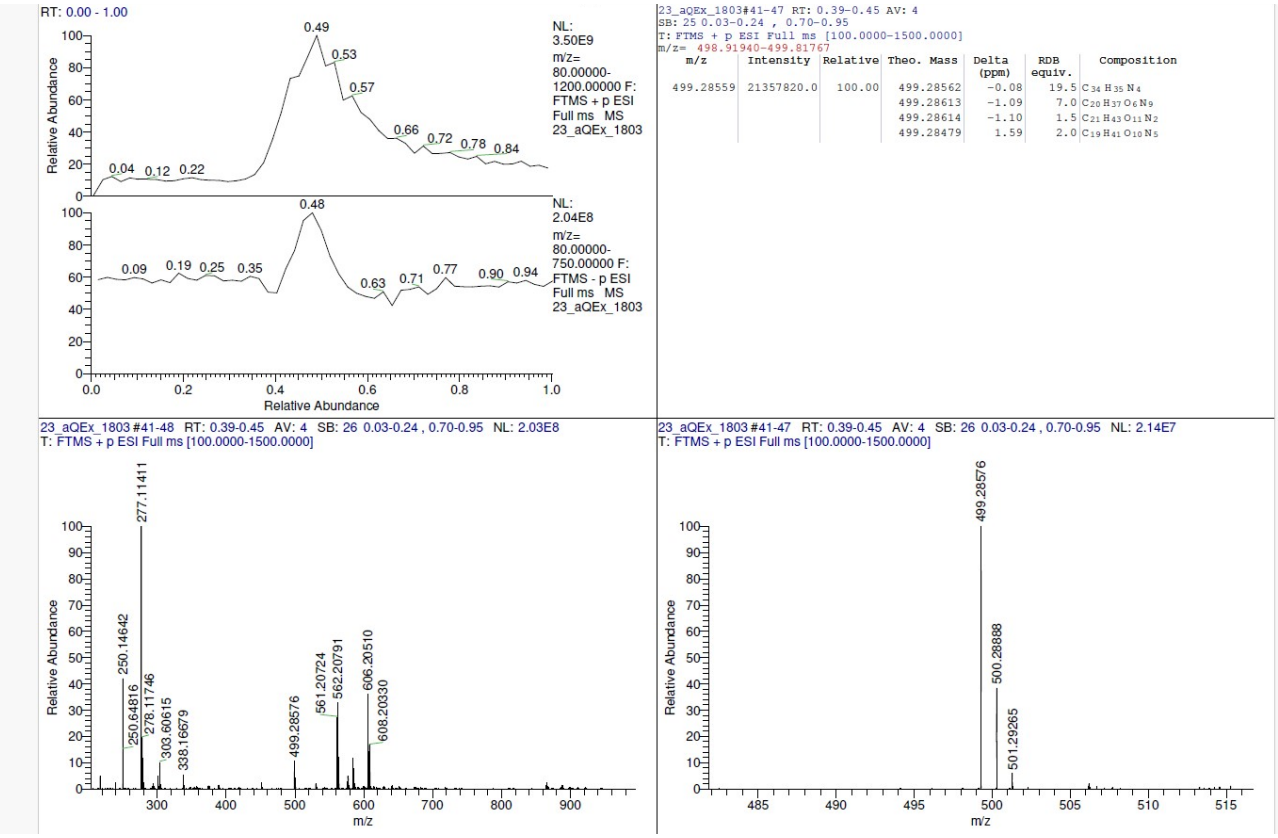

*Figure S31. HRMS spectrum of **6a***

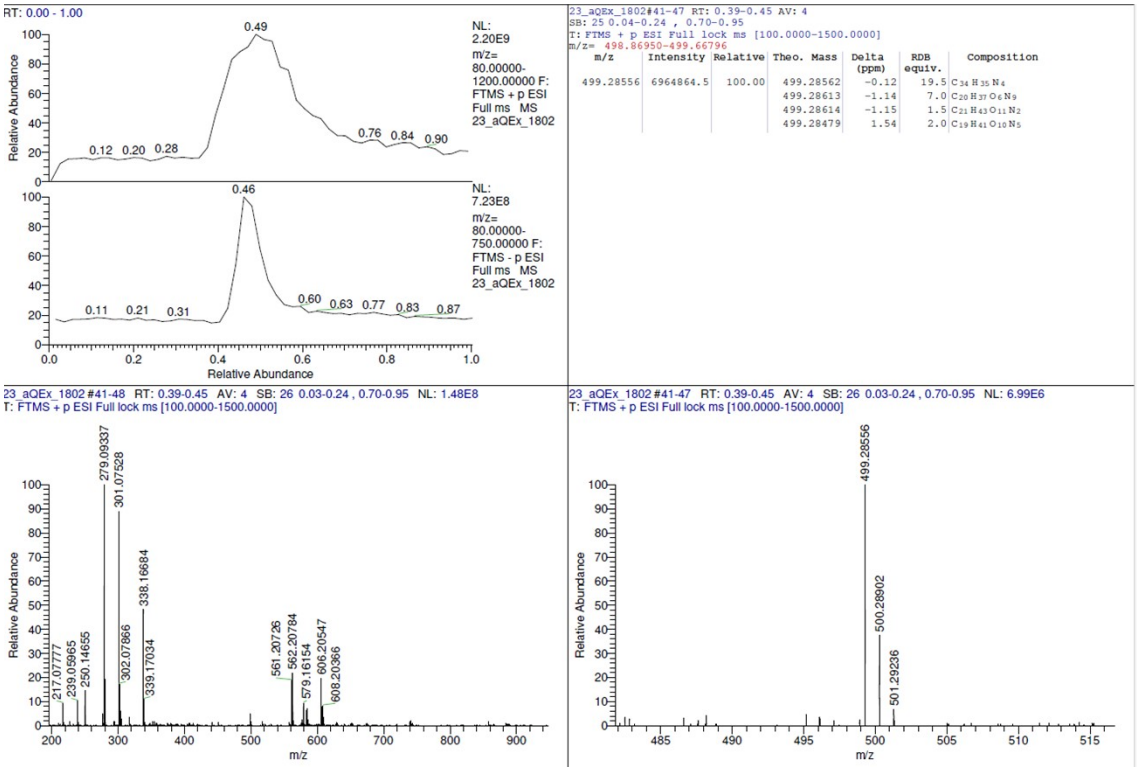

*Figure S32. HRMS spectrum of **6b***

d1-[Re_2(**5a**)$(CO)_6Cl_2$]

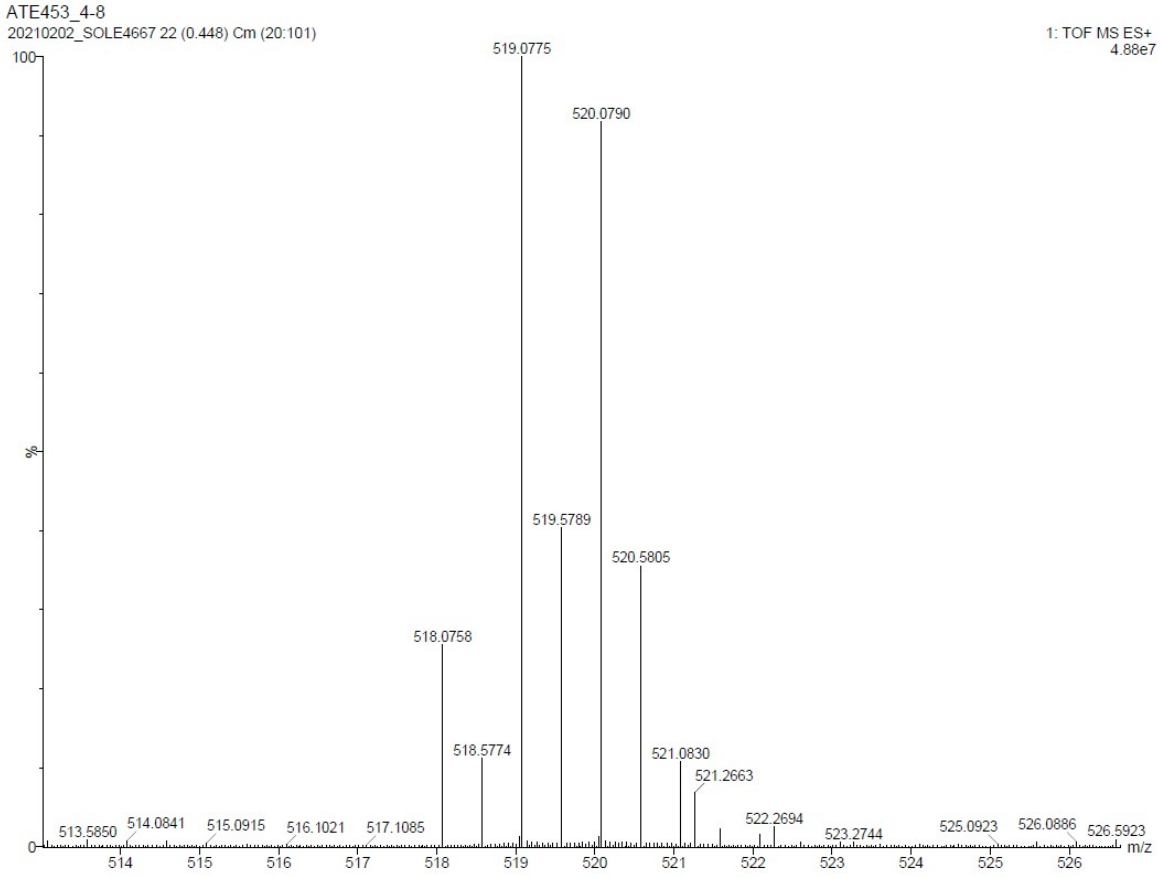

*Figure S33. HRMS spectrum of d1-[Re_2(**5a**)$(CO)_6Cl_2$]*

d2-[Re_2(**5a**)$(CO)_6Cl_2$]

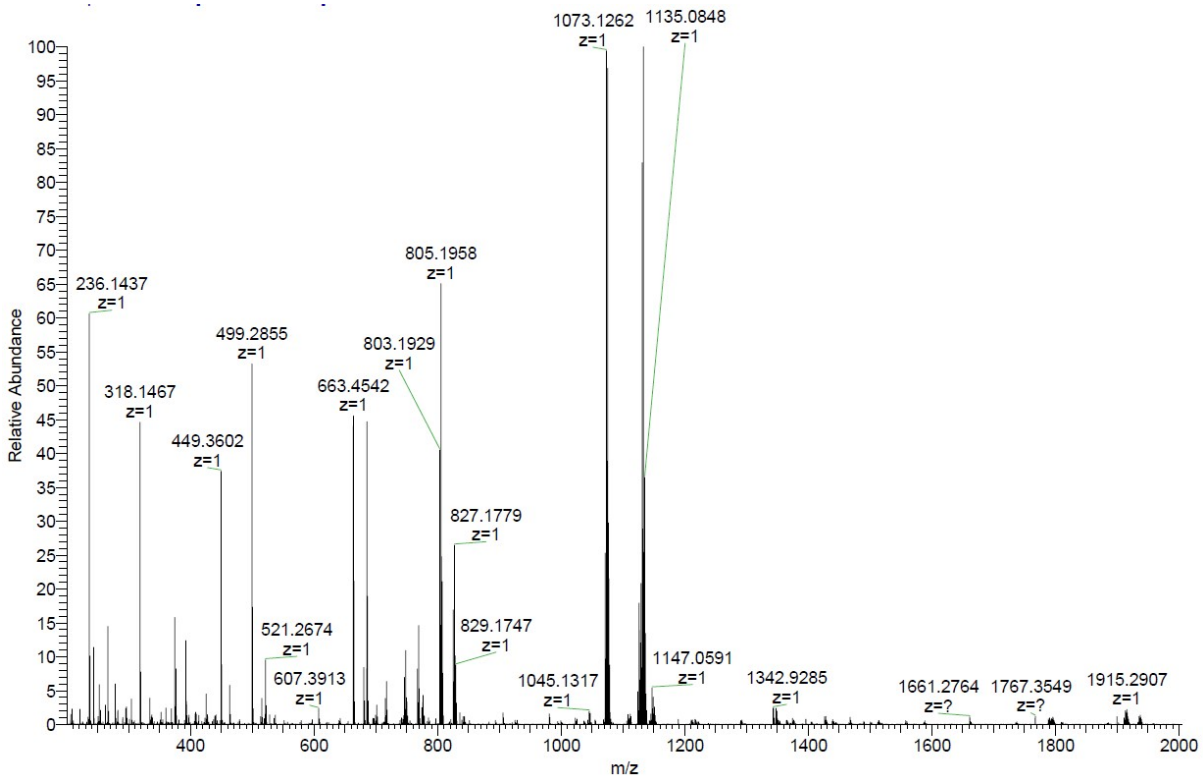

*Figure S34. HRMS spectrum of d2-[Re_2(**5a**)$(CO)_6Cl_2$]*

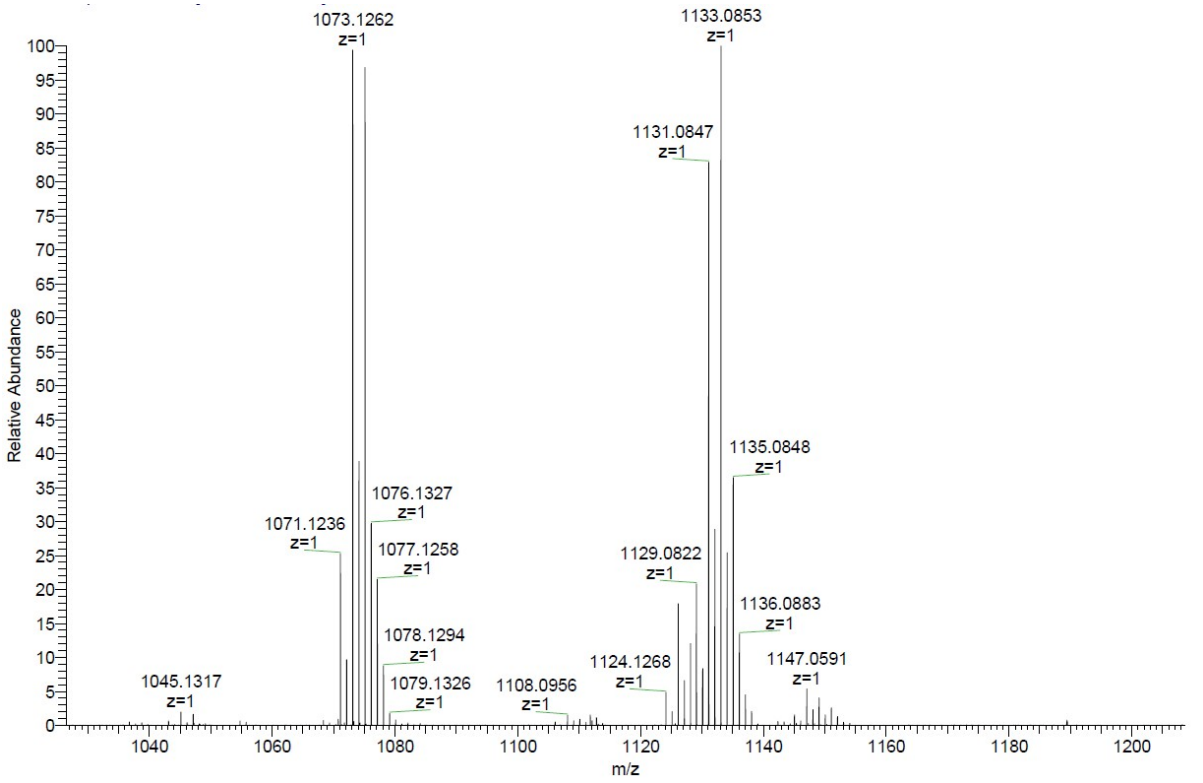

*Figure S35. HRMS spectrum of d2-[Re_2(**5a**)$(CO)_6Cl_2$]*

d1-[Re_2(**5b**)$(CO)_6Cl_2$]

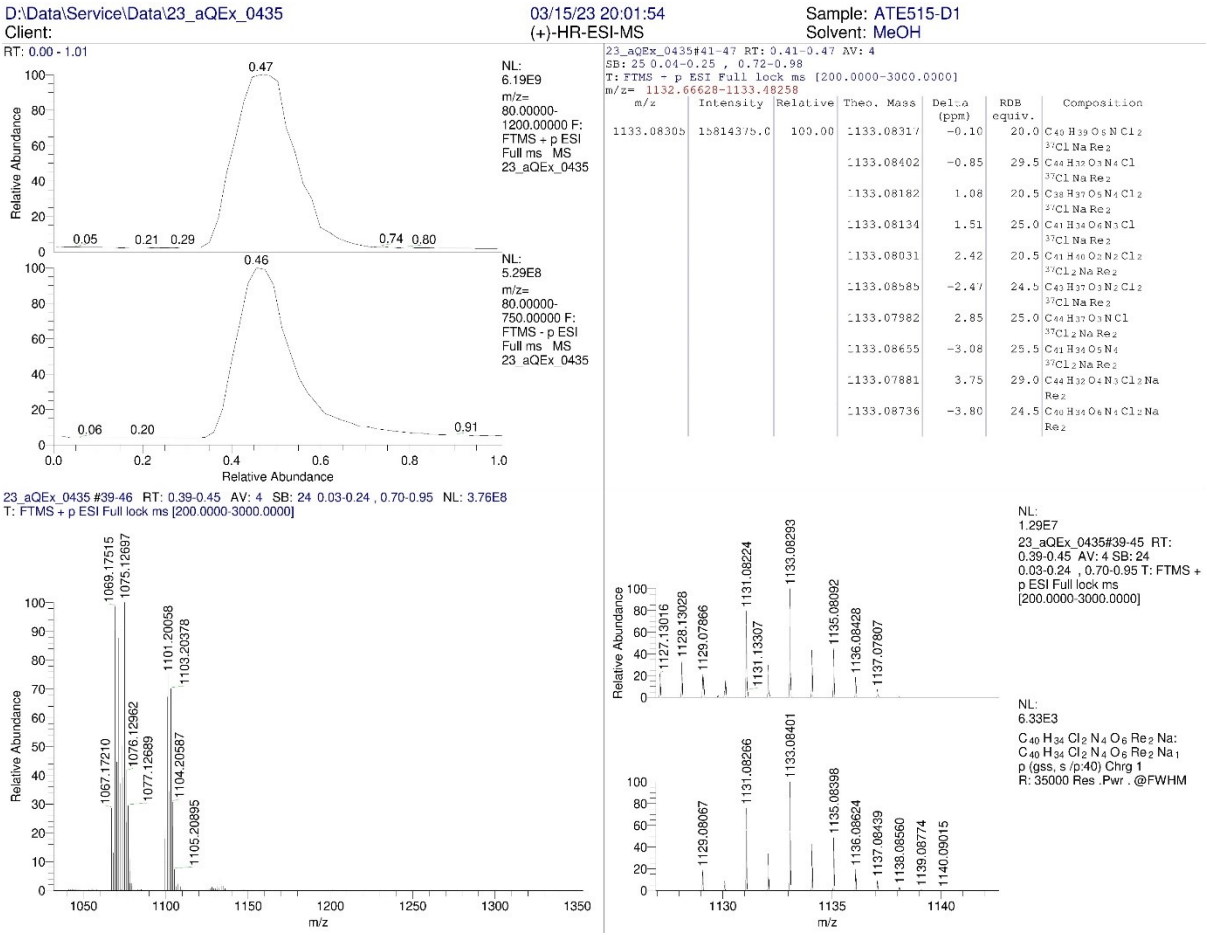

*Figure S36. HRMS spectrum of d1-[Re_2(**5b**)$(CO)_6Cl_2$]*

d2-[Re_2(**5b**)$(CO)_6Cl_2$]

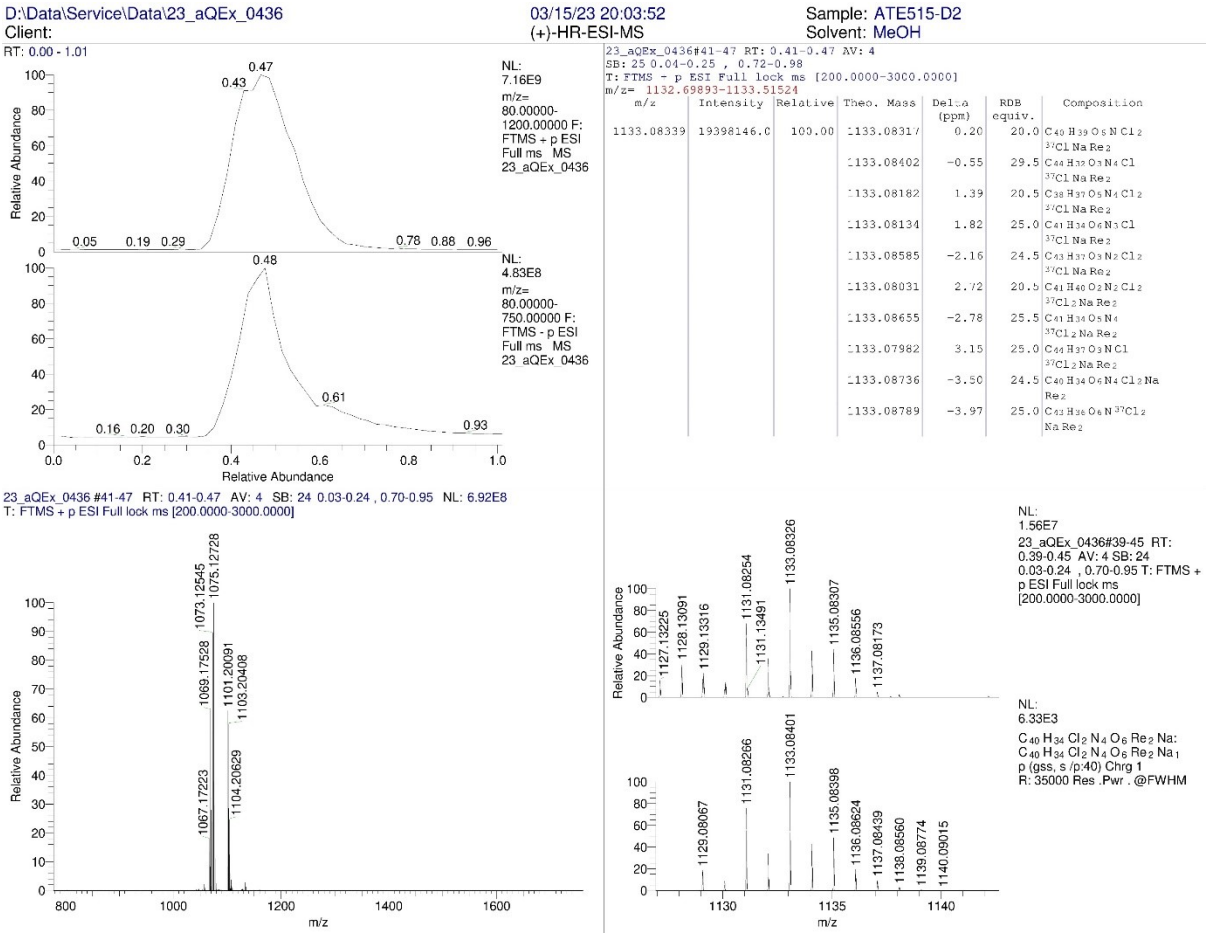

*Figure S37. HRMS spectrum of d2-[Re_2(**5b**)$(CO)_6Cl_2$]*

d1-[Re_2(**6a**)$(CO)_6Cl_2$]

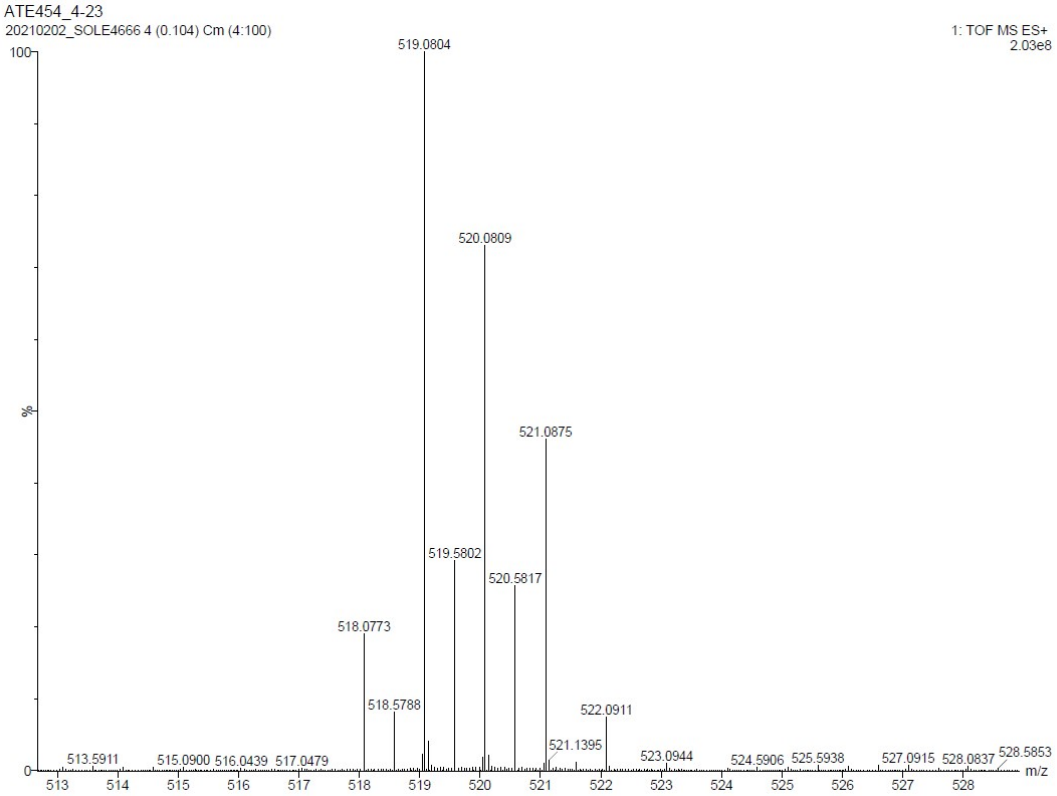

*Figure S38. HRMS spectrum of d1-[Re_2(**6a**)$(CO)_6Cl_2$]*

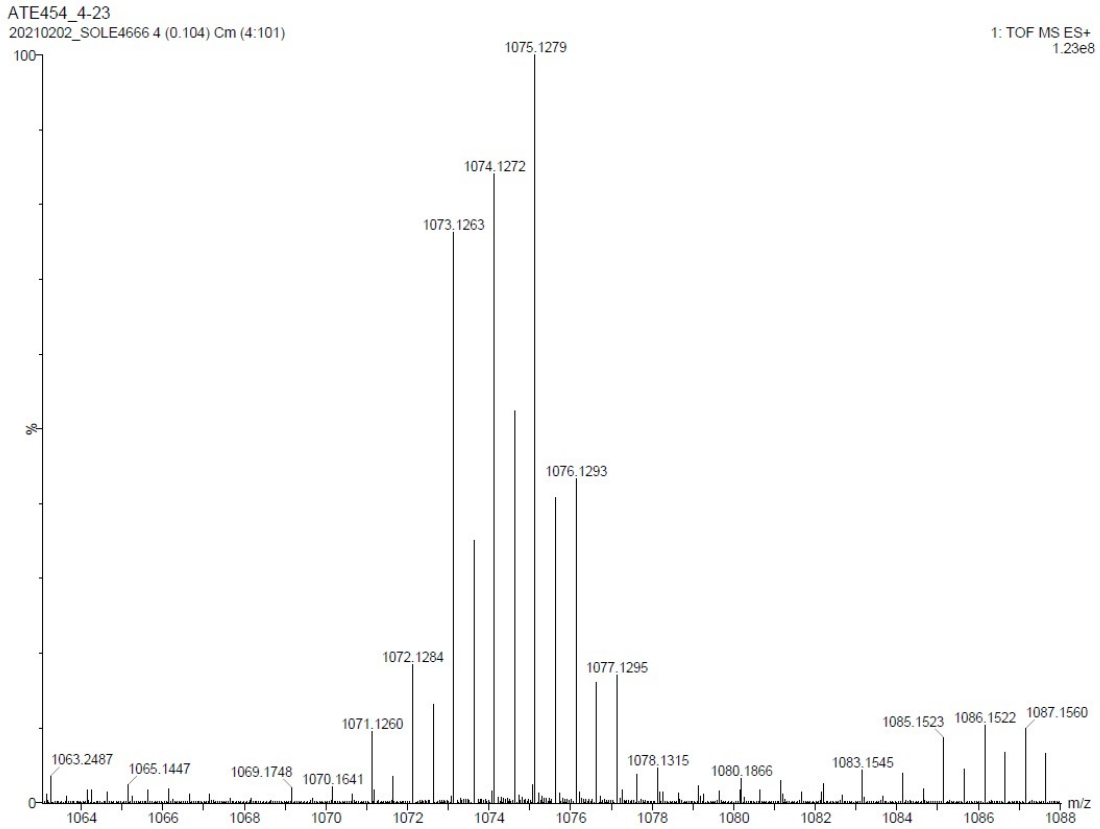

*Figure S39. HRMS spectrum of d1-[Re_2(**6a**)$(CO)_6Cl_2$]*

d2-[Re_2(**6a**)$(CO)_6Cl_2$]

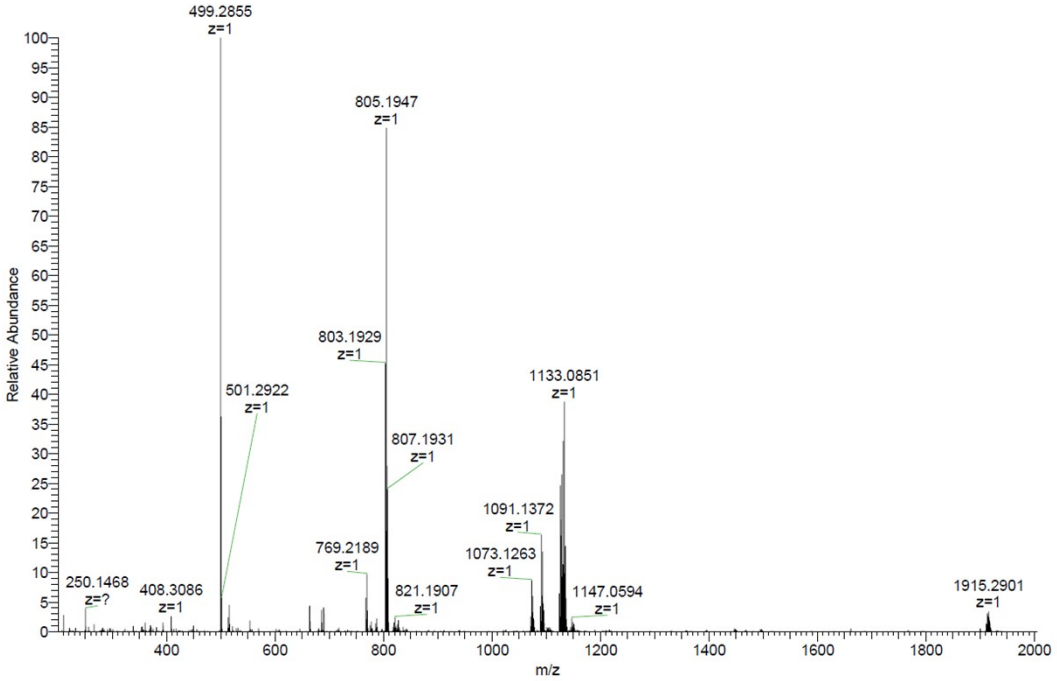

*Figure S40. HRMS spectrum of d2-[Re_2(**6a**)$(CO)_6Cl_2$]*

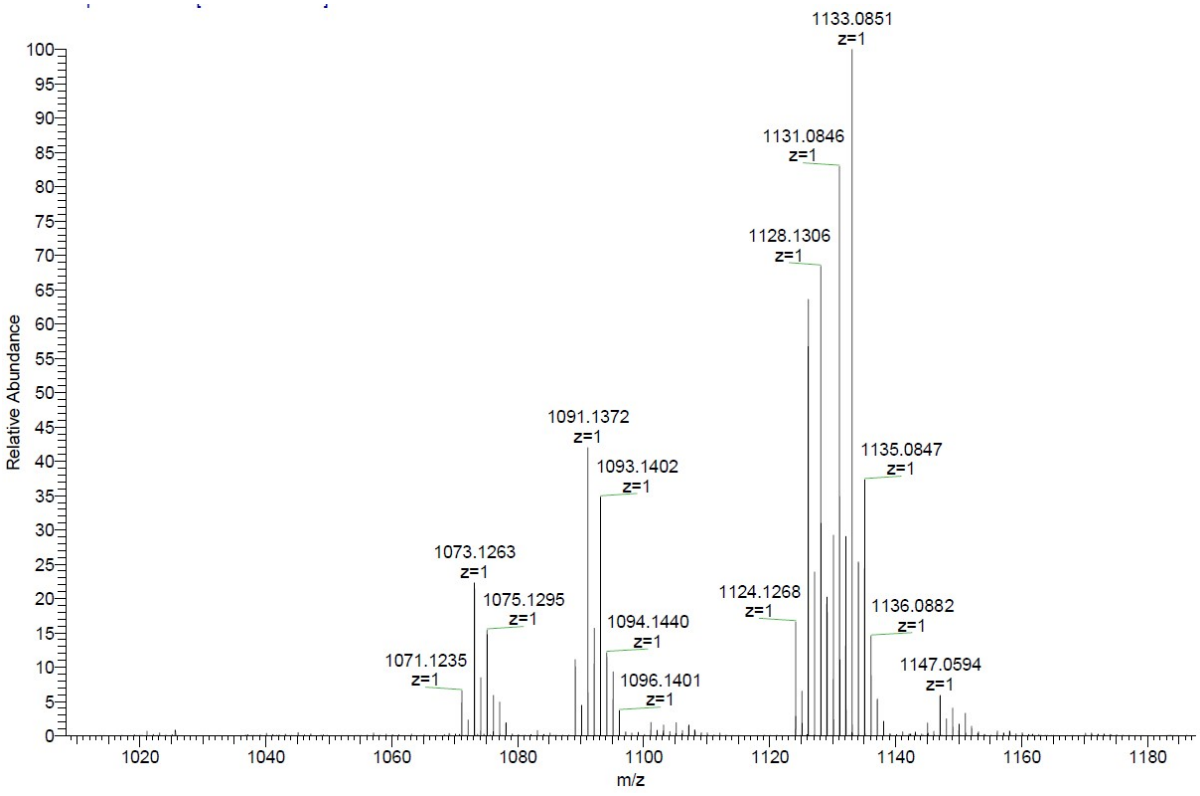

*Figure S41. HRMS spectrum of d2-[Re_2(**6a**)$(CO)_6Cl_2$]*

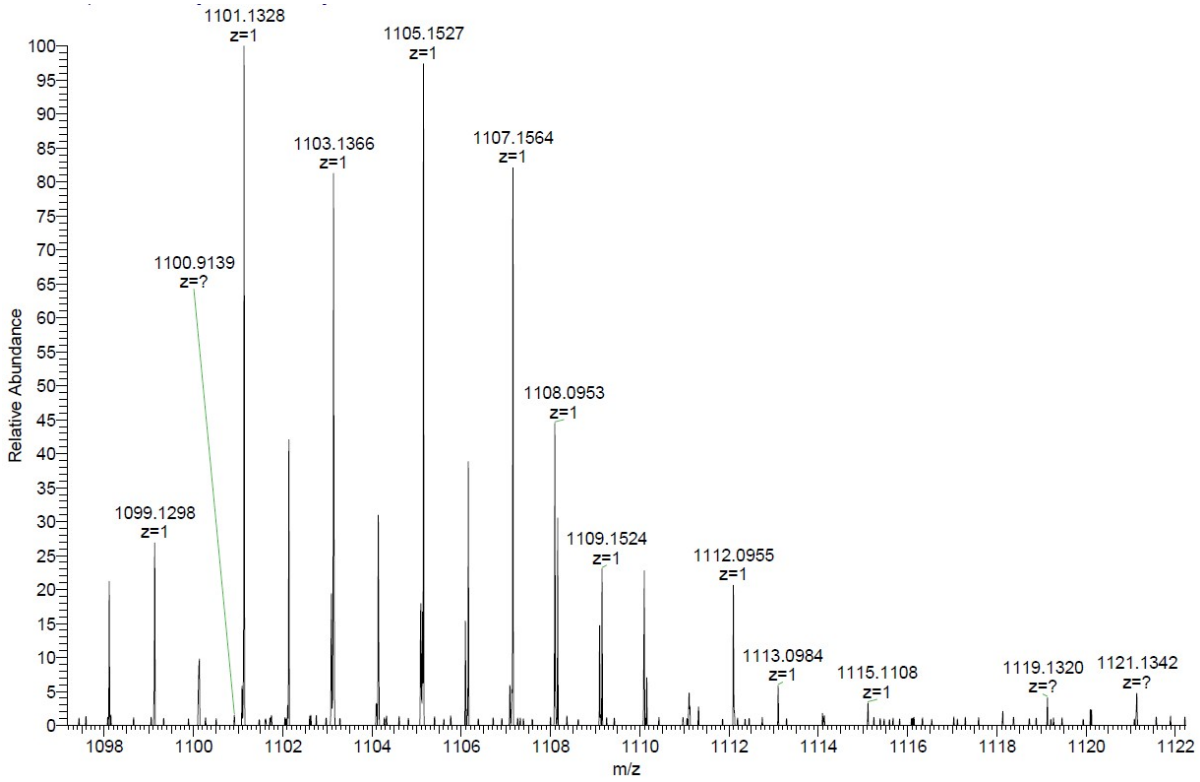

*Figure S42. HRMS spectrum of d2-[Re_2(**6a**)$(CO)_6Cl_2$]*

d1-[Re_2(**6b**)$(CO)_6Cl_2$]

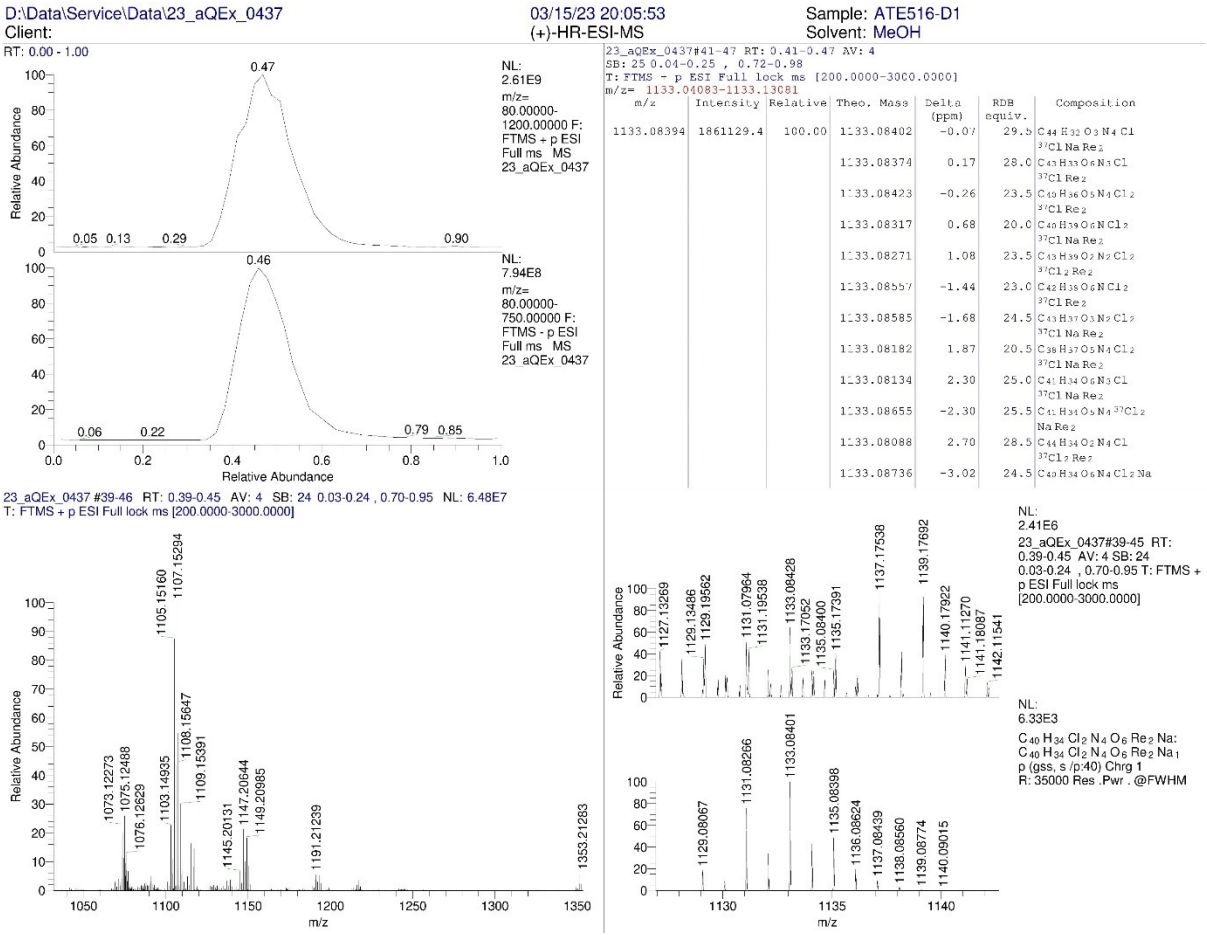

*Figure S43. HRMS spectrum of d1-[Re_2(**6b**)$(CO)_6Cl_2$]*

d2-[Re_2(**6b**)$(CO)_6Cl_2$]

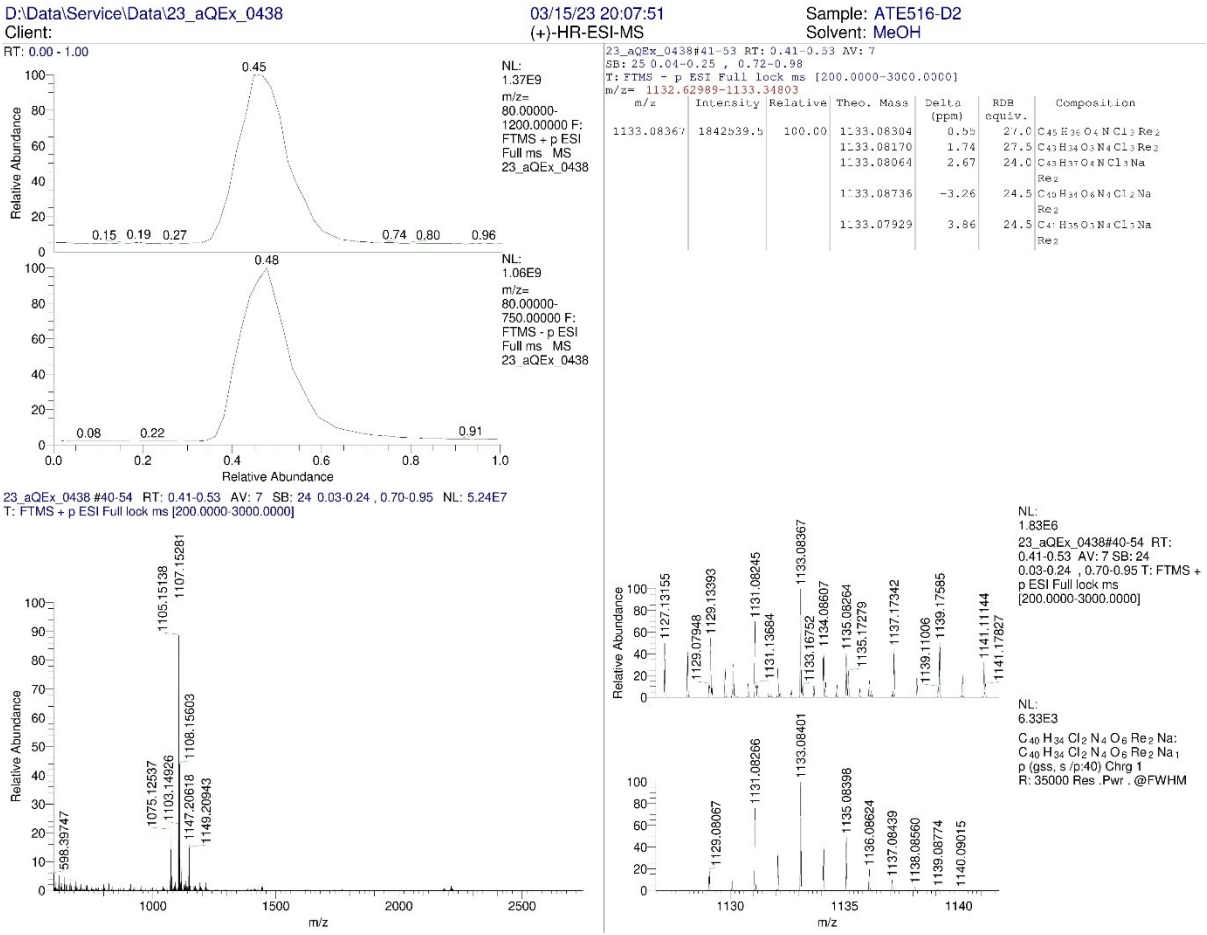

*Figure S44. HRMS spectrum of d2-[Re_2(**6b**)$(CO)_6Cl_2$]*

IR spectra

d1-[Re_2(**5a**)$(CO)_6Cl_2$]

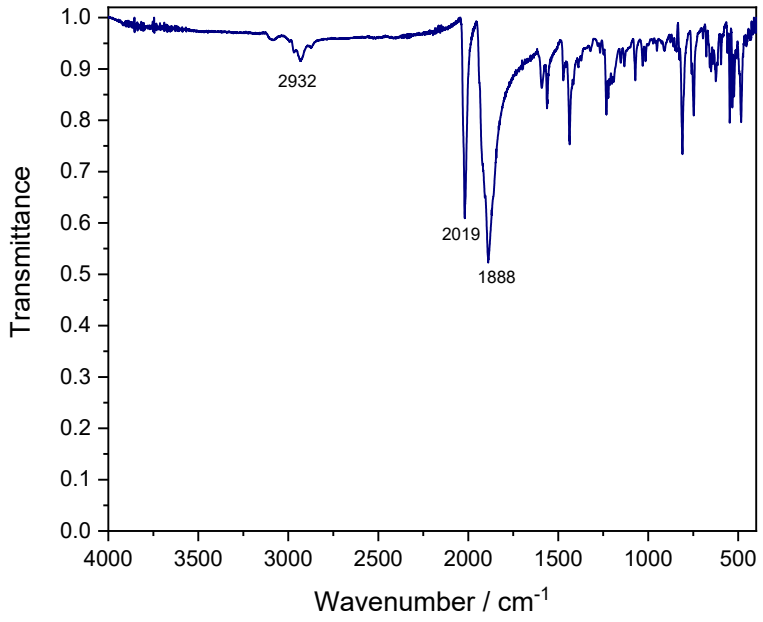

*Figure S45. IR spectrum of d1-[Re_2(**5a**)$(CO)_6Cl_2$]*

d2-[Re_2(**5a**)$(CO)_6Cl_2$]

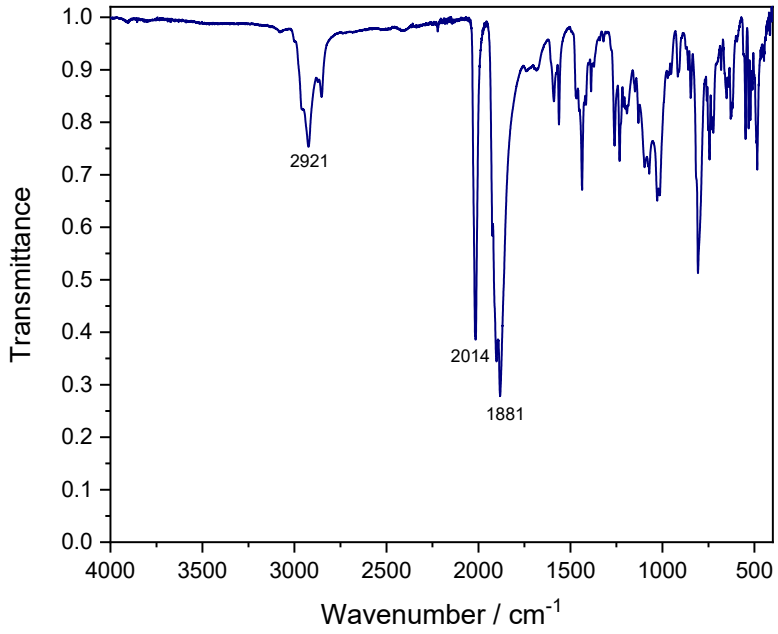

*Figure S46. IR spectrum of d2-[Re_2(**5a**)$(CO)_6Cl_2$]*

d1-[Re_2(**5b**)$(CO)_6Cl_2$]

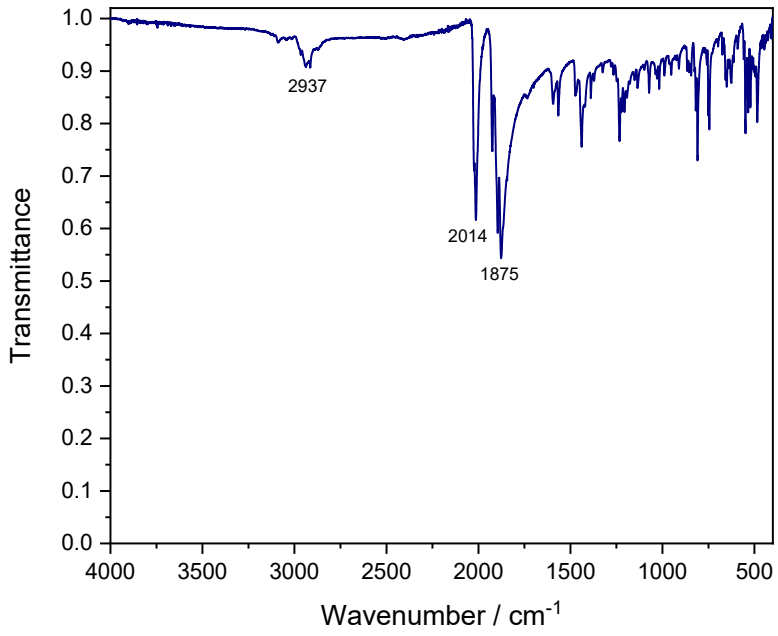

*Figure S47. IR spectrum of d1-[Re_2(**5b**)$(CO)_6Cl_2$]*

d2-[Re_2(**5b**)$(CO)_6Cl_2$]

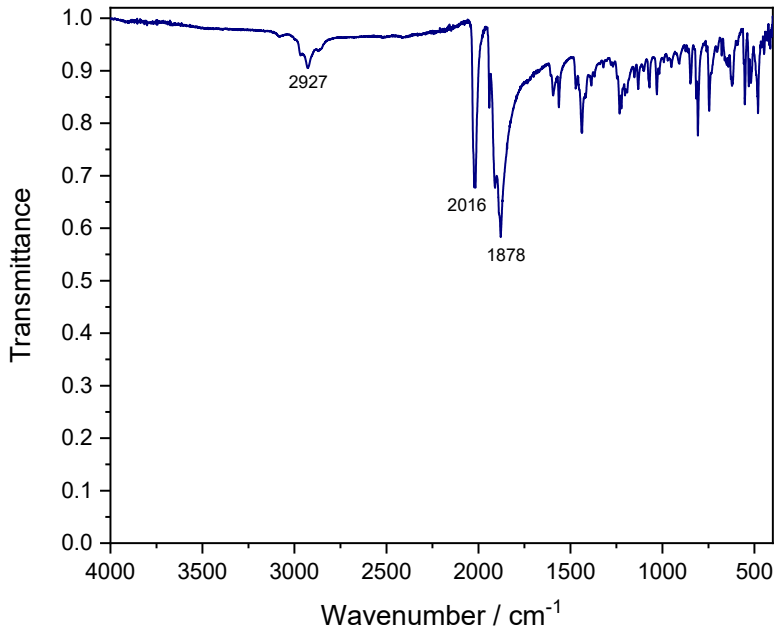

*Figure S48. IR spectrum of d2-[Re_2(**5b**)$(CO)_6Cl_2$]*

d1-[Re_2(**6a**)$(CO)_6Cl_2$]

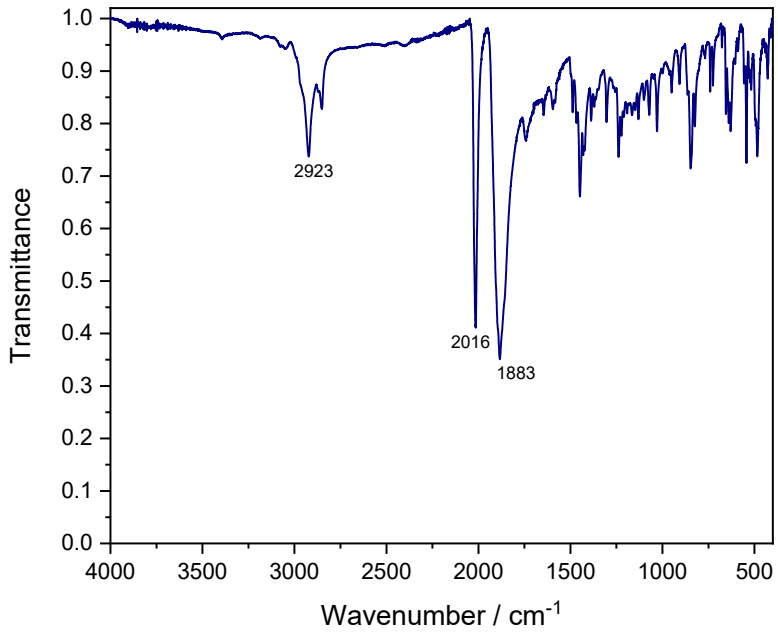

*Figure S49. IR spectrum of d1-[Re_2(**6a**)$(CO)_6Cl_2$]*

d2-[Re_2(**6a**)$(CO)_6Cl_2$]

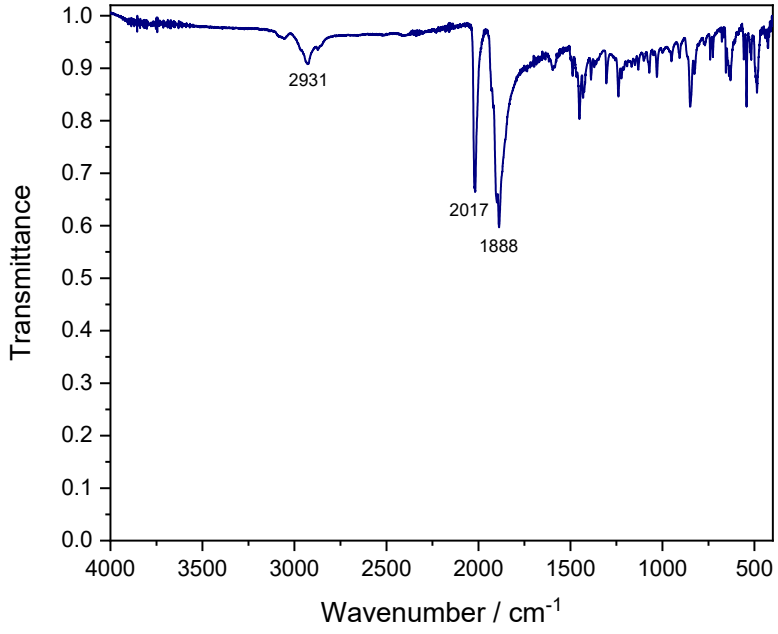

*Figure S50. IR spectrum of d2-[Re_2(**6a**)$(CO)_6Cl_2$]*

d1-[Re_2(**6b**)$(CO)_6Cl_2$]

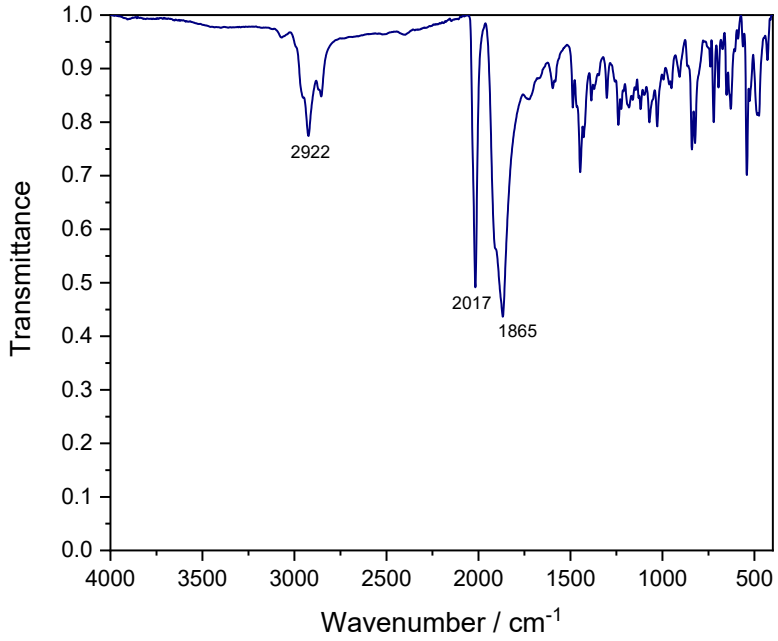

*Figure S51. IR spectrum of d1-[Re_2(**6b**)$(CO)_6Cl_2$]*

d2-[Re_2(**6b**)$(CO)_6Cl_2$]

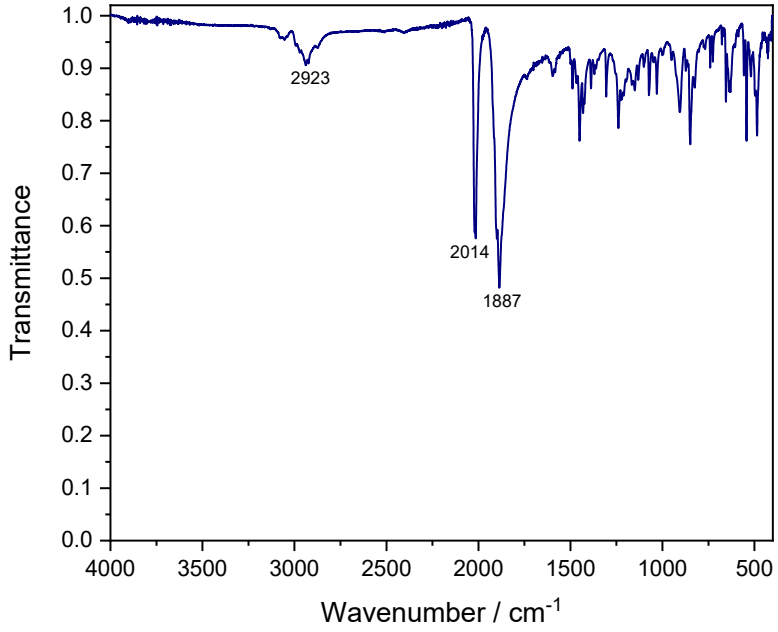

*Figure S52. IR spectrum of d2-[Re_2(**6b**)$(CO)_6Cl_2$]*

CD spectra

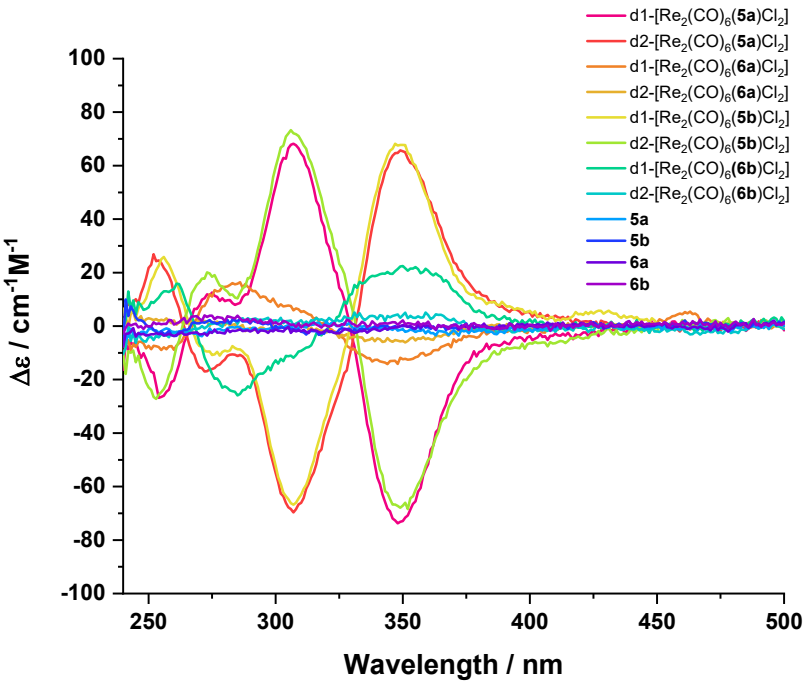

Figure S53. CD spectra of the ligands and different stereoisomers (0.005 mM in $CHCl_3$)

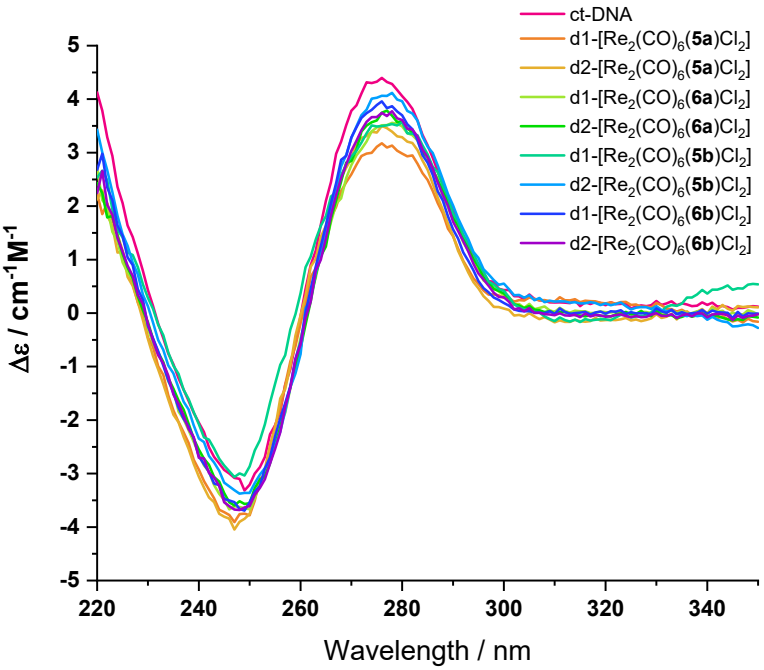

Figure S54. CD spectra of calf thymus DNA (100 µM) in the presence of different diastereomers (5 µM) in H_2O

Photophysical characterisation

d1-[Re_2(**5a**)$(CO)_6Cl_2$]

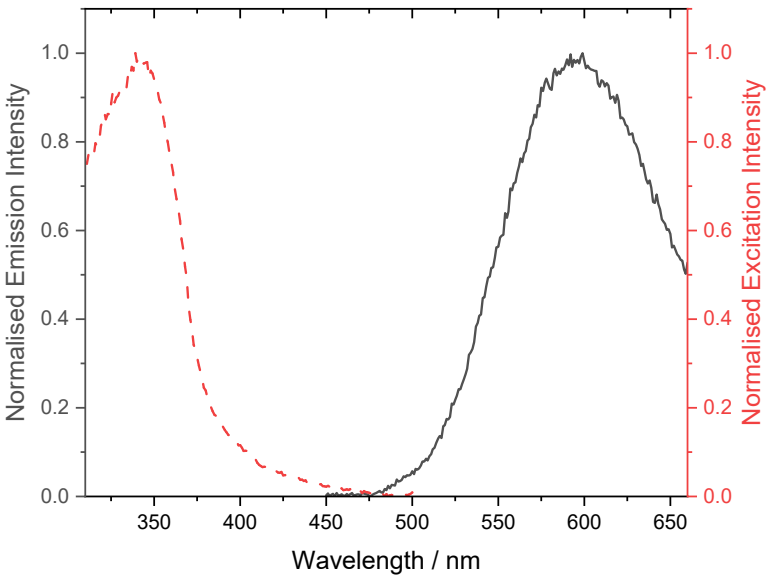

*Figure S55. Emission (dark grey) and excitation spectra (red, dashed) of d1-[Re_2(**5a**)$(CO)_6Cl_2$] in CH_2Cl_2, c = 0.0025 mM, λ_{ex} = 342 nm*

d2-[Re_2(**5a**)$(CO)_6Cl_2$]

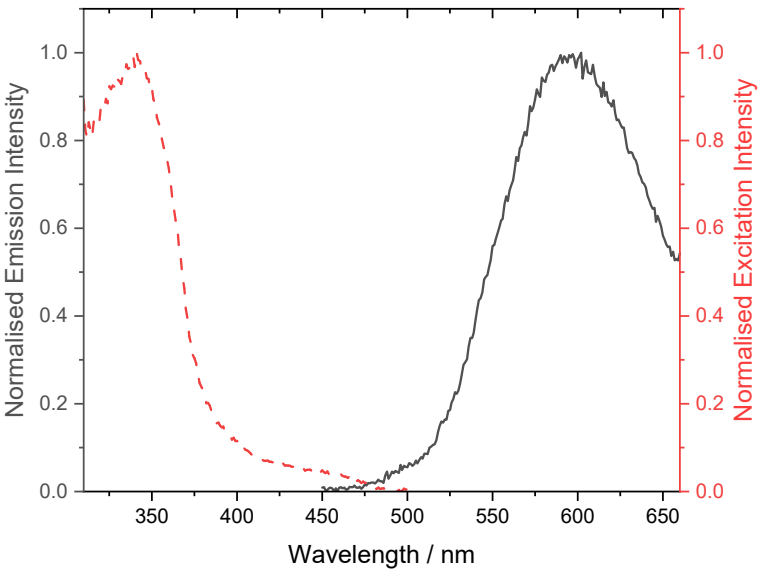

*Figure S56. Emission (dark grey) and excitation spectra (red, dashed) of d2-[Re_2(**5a**)$(CO)_6Cl_2$] in CH_2Cl_2, c = 0.0025 mM, λ_{ex} = 342 nm*

d1-[Re_2(**6a**)$(CO)_6Cl_2$]

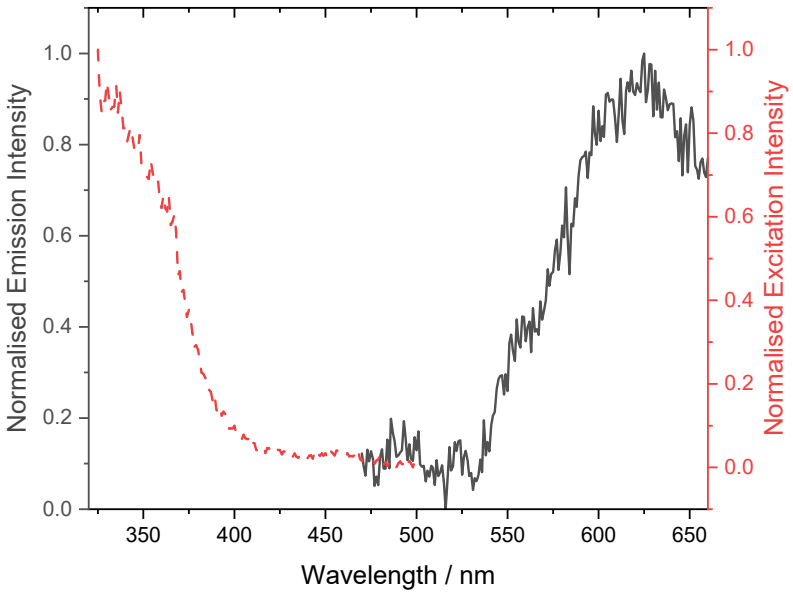

*Figure S57. Emission (dark grey) and excitation spectra (red, dashed) of d1-[Re_2(**6a**)$(CO)_6Cl_2$] in CH_2Cl_2, c = 0.0025 mM, λ_{ex} = 350 nm*

d2-[Re_2(**6a**)$(CO)_6Cl_2$]

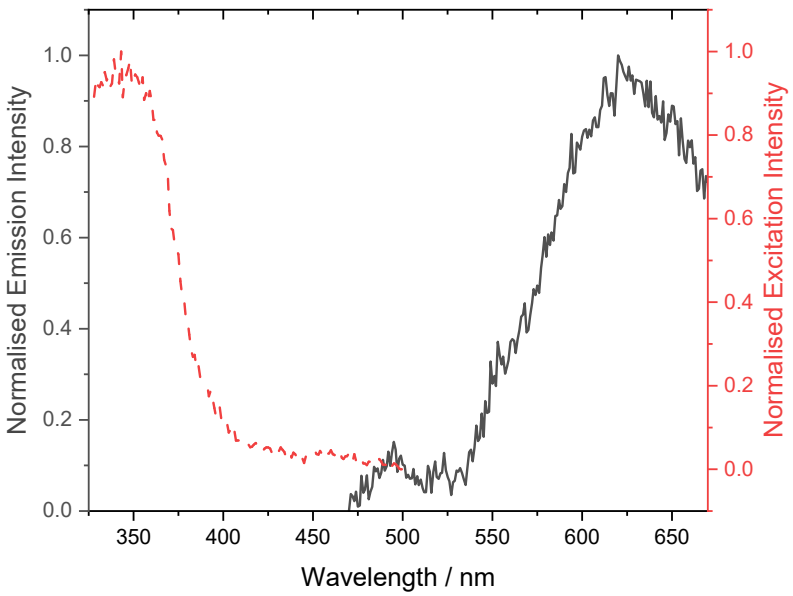

*Figure S58. Emission (dark grey) and excitation spectra (red, dashed) of d2-[Re_2(**6a**)$(CO)_6Cl_2$] in CH_2Cl_2, c = 0.0025 mM, λ_{ex} = 350 nm*

d1-[Re_2(**5b**)$(CO)_6Cl_2$]

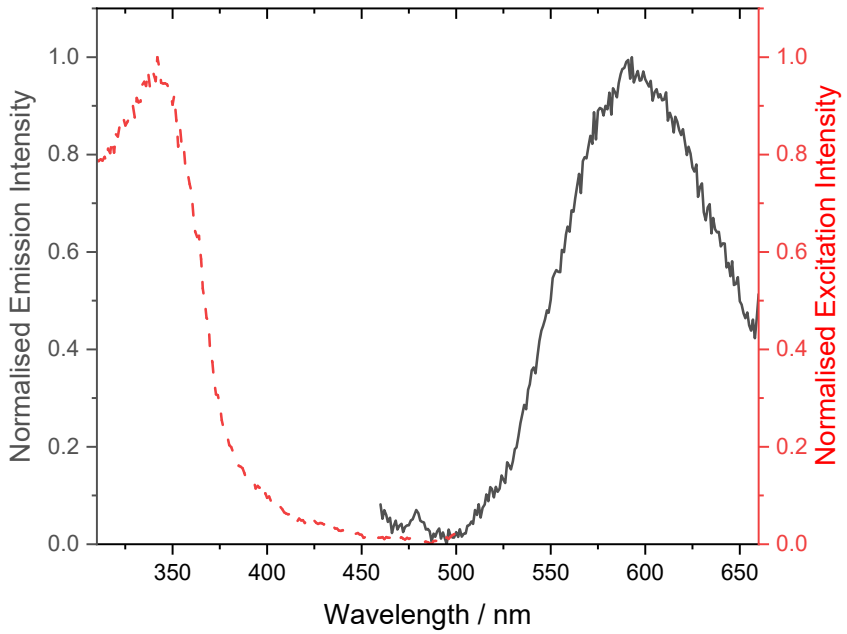

*Figure S59. Emission (dark grey) and excitation spectra (red, dashed) of d1-[Re_2(**5b**)$(CO)_6Cl_2$] in CH_2Cl_2, c = 0.0025 mM, λ_{ex} = 342 nm*

d2-[Re_2(**5b**)$(CO)_6Cl_2$]

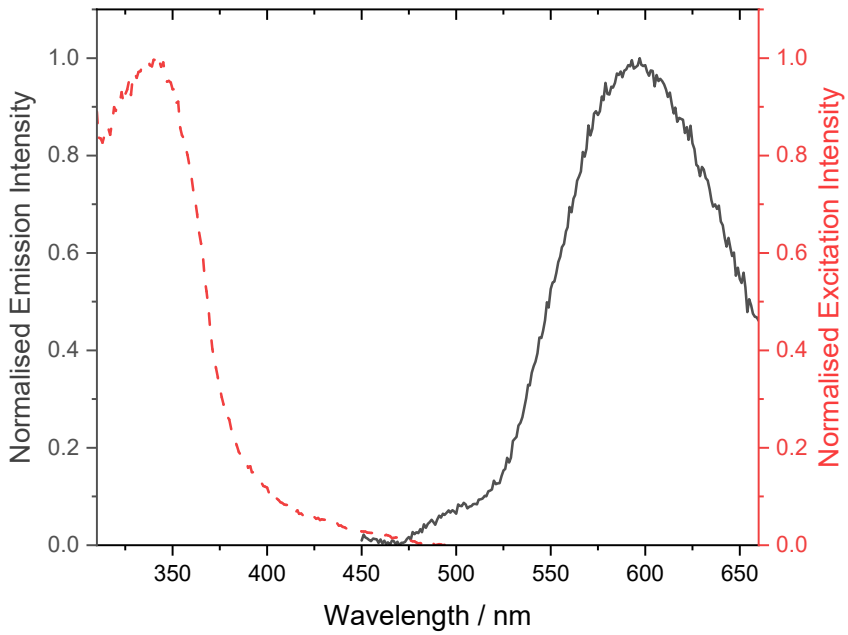

*Figure S60. Emission (dark grey) and excitation spectra (red, dashed) of d2-[Re_2(**5b**)$(CO)_6Cl_2$] in CH_2Cl_2, c = 0.0025 mM, λ_{ex} = 342 nm*

d1-[Re_2(**6b**)$(CO)_6Cl_2$]

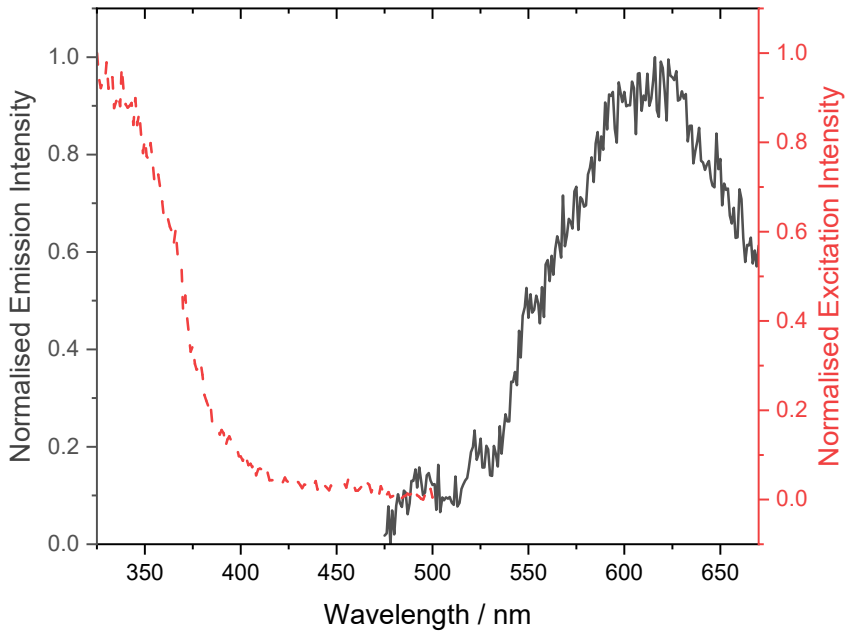

*Figure S61. Emission (dark grey) and excitation spectra (red, dashed) of d1-[Re_2(**6b**)$(CO)_6Cl_2$] in CH_2Cl_2, c = 0.0025 mM, λ_{ex} = 350 nm*

d2-[Re_2(**6b**)$(CO)_6Cl_2$]

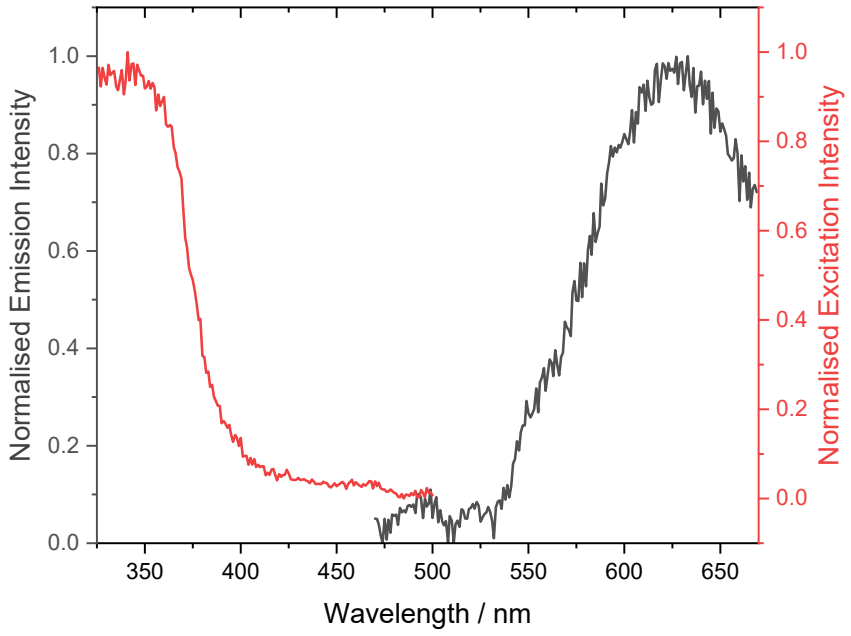

*Figure S62. Emission (dark grey) and excitation spectra (red, dashed) of d2-[Re_2(**6b**)$(CO)_6Cl_2$] in CH_2Cl_2, c = 0.0025 mM, λ_{ex} = 350 nm*

Table S1. Quantum yield values for the complexes, in CH_2Cl_2

Compound	QY (%)
d1-[Re_2(**5a**)$(CO)_6Cl_2$]	3.7
d2-[Re_2(**5a**)$(CO)_6Cl_2$]	5.4
d1-[Re_2(**6a**)$(CO)_6Cl_2$]	0.6
d2-[Re_2(**6a**)$(CO)_6Cl_2$]	0.6
d1-[Re_2(**5b**)$(CO)_6Cl_2$]	3.2
d2-[Re_2(**5b**)$(CO)_6Cl_2$]	5.2
d1-[Re_2(**6b**)$(CO)_6Cl_2$]	0.6
d2-[Re_2(**6b**)$(CO)_6Cl_2$]	0.6

Docking calculations

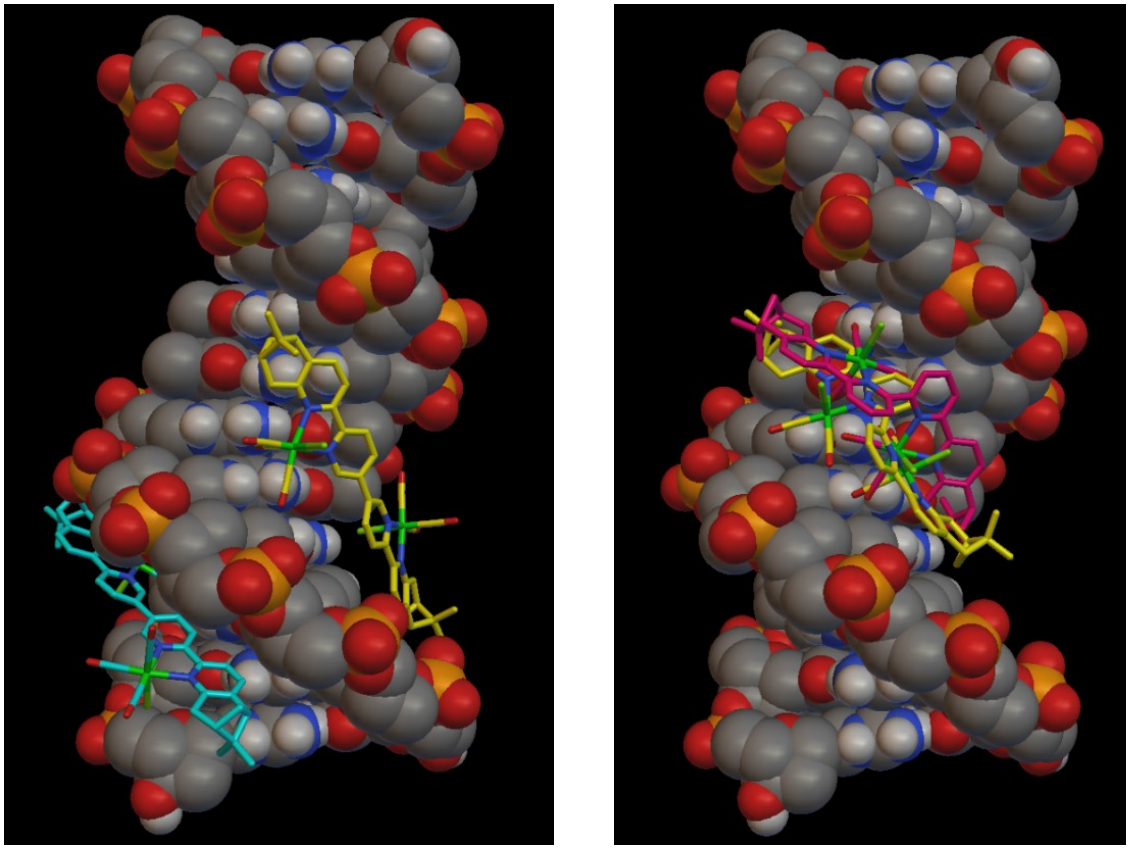

*Figure S63. Lowest calculated energy poses of d1- and d2-[Re_2(**6a**)$(CO)_6Cl_2$] (left) and d1- and d2-[Re_2(**5a**)$(CO)_6Cl_2$] with double stranded (d(CpGpCpGpApApTpTpCpGpCpG) dodecamer.*

Biological data

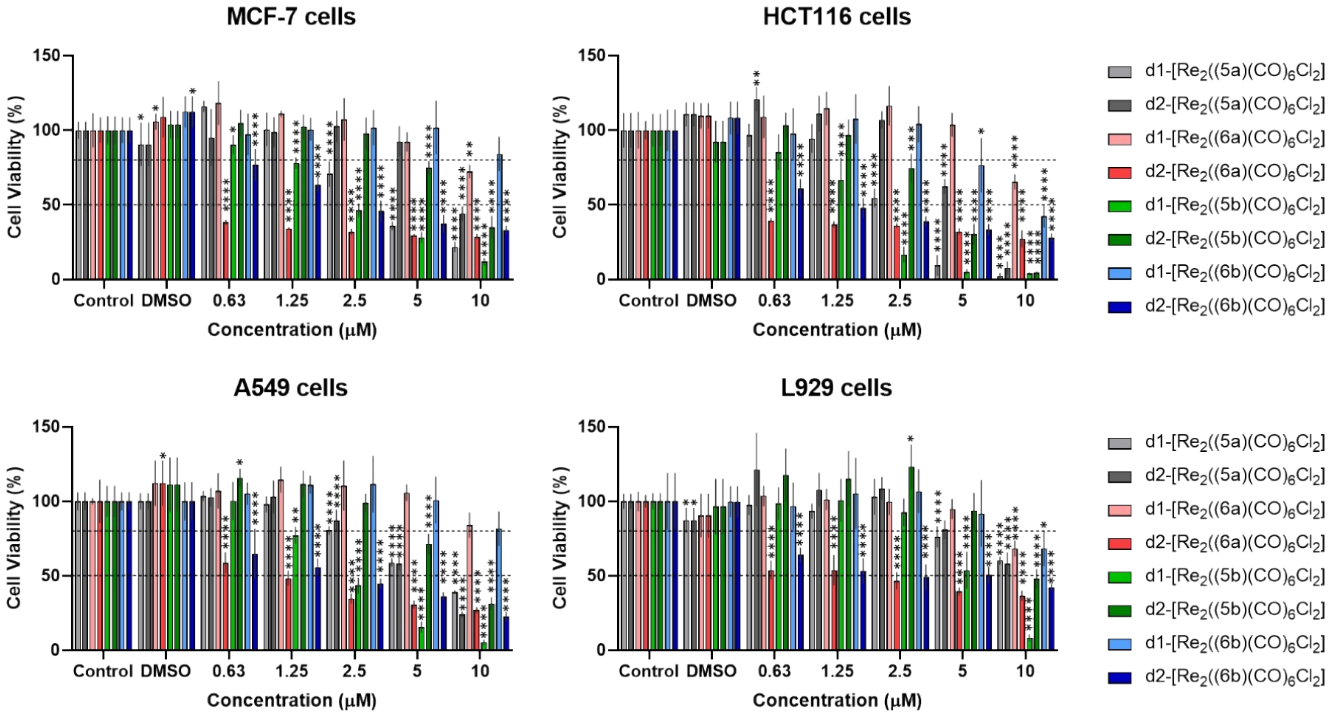

Figure S64. Cytotoxicity graphs of the complexes on MCF-7, HCT116, A549 and L929 cells.

ICP-MS measurements

Table S2. Re amount found in the cells, as determined by ICP-MS

Sample name	Re, ng/mg	RSD, %
d1-[$Re_2(CO)_6$(**6a**)Cl_2]	11.14	2.9%
d2-[$Re_2(CO)_6$(**6a**)Cl_2]	200.45	2.6%
d1-[$Re_2(CO)_6$(**6b**)Cl_2]	7.43	3.2%
d2-[$Re_2(CO)_6$(**6b**)Cl_2]	192.81	2.00%
control	2.00	13.4%

Crystallographic data

Inter-and intramolecular interactions in the solid state

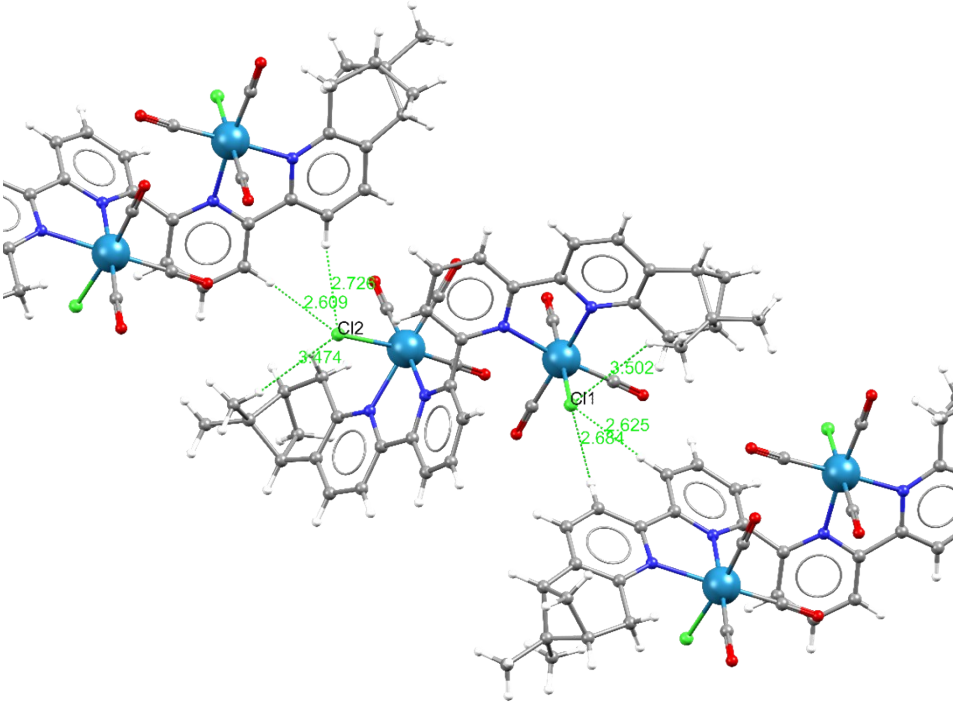

*Figure S65. Intra-and intermolecular interactions in the single crystal structure of d1-[Re_2(**5a**)$(CO)_6Cl_2$]*

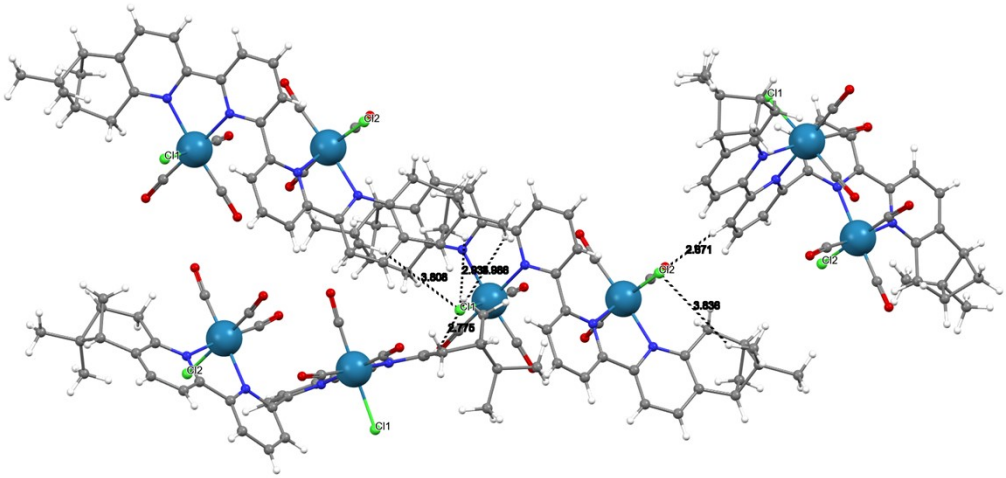

*Figure S66. Intra-and intermolecular interactions in the single crystal structure of d1-[Re_2(**5b**)$(CO)_6Cl_2$]*

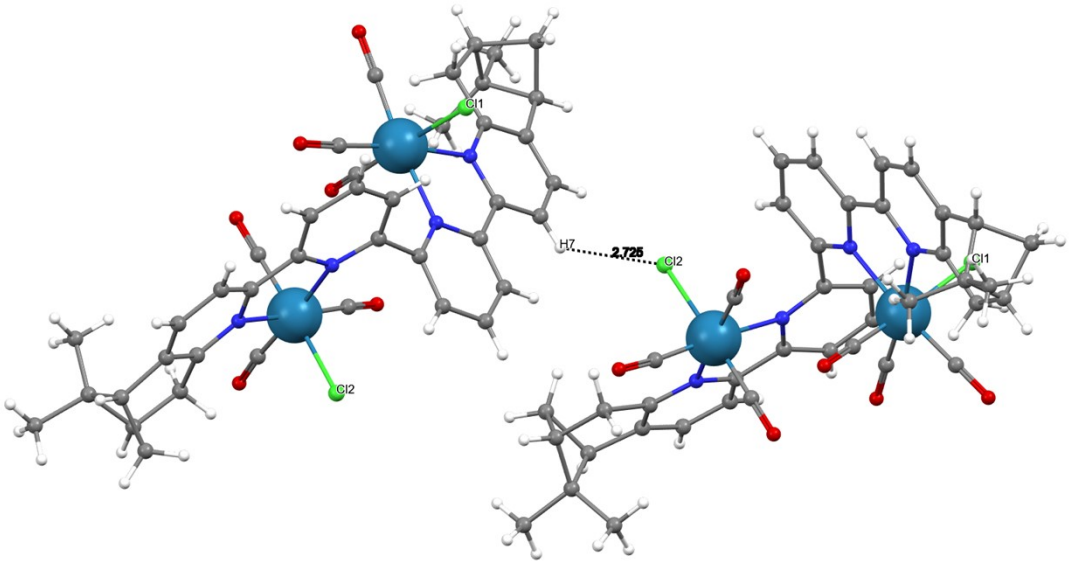

*Figure S67. Intermolecular interactions in the single crystal structure of d2-[Re_2(**5a**)$(CO)_6Cl_2$]*

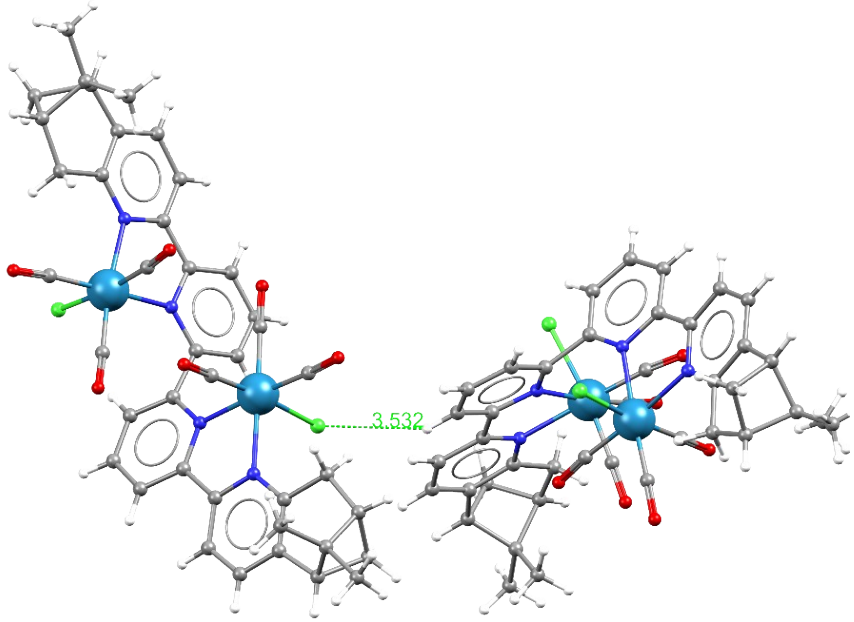

*Figure S68. Intermolecular interactions in the single crystal structure of d2-[Re_2(**5b**)$(CO)_6Cl_2$]*

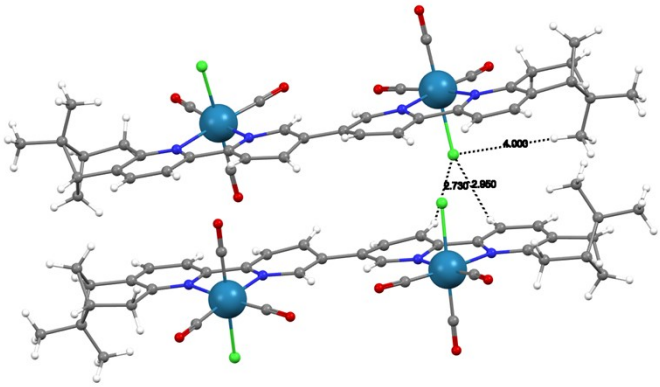

*Figure S69. Intermolecular interactions in the single crystal structure of d1-[Re_2(**6a**)$(CO)_6Cl_2$]*

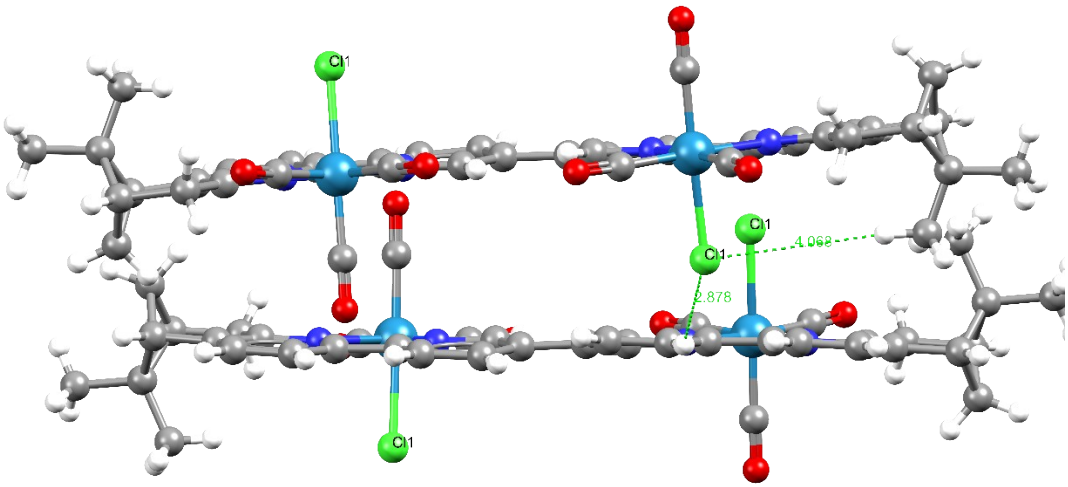

*Figure S70. Intermolecular interactions in the single crystal structure of d1-[Re_2(**6b**)$(CO)_6Cl_2$]*

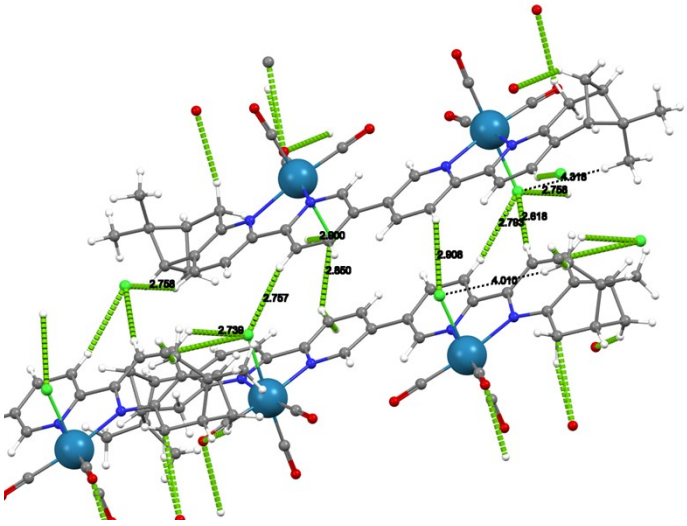

*Figure S71. Intra-and intermolecular interactions in the single crystal structure of d2-[Re_2(**6a**)$(CO)_6Cl_2$]*

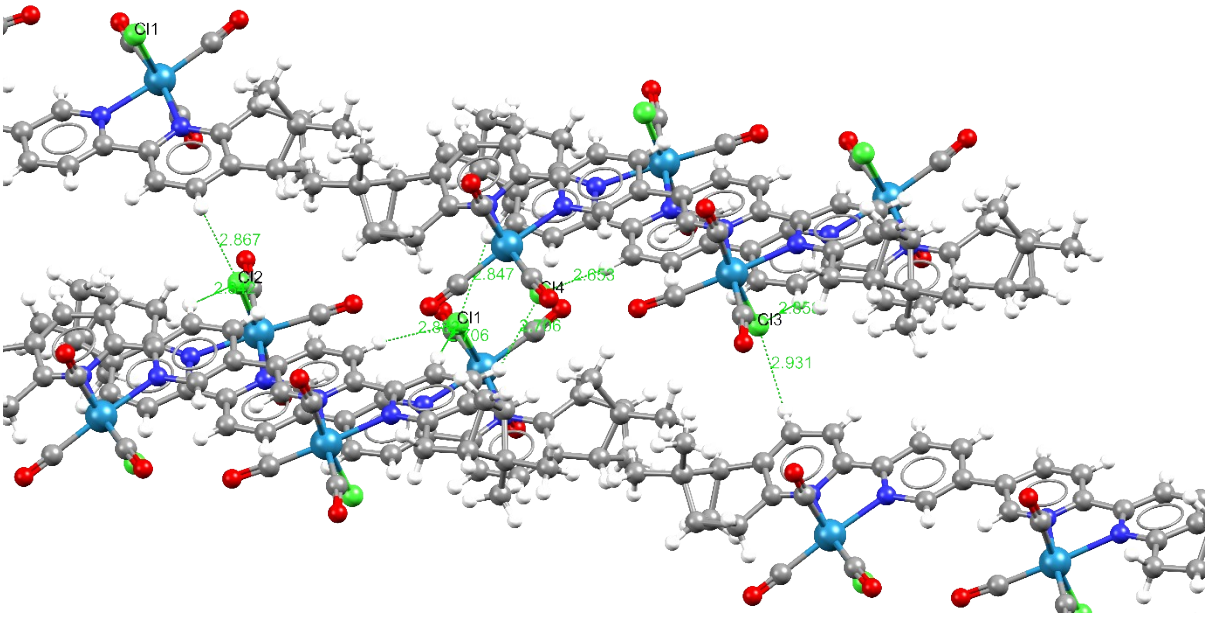

*Figure S72. Intra-and intermolecular interactions in the single crystal structure of d2-[Re_2(**6b**)$(CO)_6Cl_2$]*

X-Ray tables

6a/b

Identification code	**6a**	**6b**
Empirical formula	$C_{34}H_{34}N_4$	$C_{34}H_{34}N_4$
CCDC number	2310572	2366457
Formula weight	498.65	498.65
Temperature/K	200(2)	250(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$
a/Å	14.2664(9)	14.2355(4)
b/Å	6.1555(3)	6.17310(10)
c/Å	15.5307(10)	15.5568(4)
α/°	90	90
β/°	100.364(5)	100.451(2)
γ/°	90	90
Volume/Å^3	1341.60(14)	1344.41(6)
Z	2	2
ρ_{calc}g/cm^3	1.234	1.232
μ/mm^{-1}	0.562	0.561
F(000)	532.0	532.0
Crystal size/mm^3	0.34 × 0.16 × 0.06	0.36 × 0.15 × 0.03
Radiation	CuKα (λ = 1.54186)	CuKα (λ = 1.54186)
2Θ range for data collection/°	6.298 to 135.884	9.304 to 138.714
Index ranges	-17 ≤ h ≤ 16, -6 ≤ k ≤ 6, -18 ≤ l ≤ 18	-16 ≤ h ≤ 17, -7 ≤ k ≤ 5, -18 ≤ l ≤ 18
Reflections collected	18057	28983
Independent reflections	4689 [R_{int} = 0.0534, R_{sigma} = 0.0325]	3648 [R_{int} = 0.0602, R_{sigma} = 0.0322]
Data/restraints/parameters	4689/1/348	3648/1/347
Goodness-of-fit on F^2	1.077	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0943, wR_2 = 0.2092	R_1 = 0.0642, wR_2 = 0.1642
Final R indexes [all data]	R_1 = 0.1484, wR_2 = 0.2695	R_1 = 0.0670, wR_2 = 0.1692
Largest diff. peak/hole / e Å^{-3}	0.34/-0.38	0.36/-0.21
Flack parameter	0.1(10)	0.8(6)

$[Re_2(\mathbf{5a})(CO)_6Cl_2]$

Identification code	d1-$[Re_2(\mathbf{5a})(CO)_6Cl_2]$	d2-$[Re_2(\mathbf{5a})(CO)_6Cl_2]$

CCDC number	2310573	2310577
Empirical formula	$C_{41}Cl_4H_{36}N_4O_6Re_2$	$C_{40}H_{34}Cl_2N_4O_6Re_2$
Formula weight	1194.94	1110.01
Temperature/K	200(2)	200(2)
Crystal system	orthorhombic	monoclinic
Space group	$P2_12_12_1$	$P2_1$
a/Å	13.6887(2)	9.60080(10)
b/Å	15.7230(3)	16.6361(2)
c/Å	20.3145(3)	14.24960(10)
α/°	90	90
β/°	90	102.6440(10)
γ/°	90	90
Volume/Å^3	4372.24(12)	2220.75(4)
Z	4	2
ρ_{calc}g/cm^3	1.815	1.660
μ/mm^{-1}	13.319	11.979
F(000)	2304.0	1068.0
Crystal size/mm^3	0.21 × 0.12 × 0.06	0.3 × 0.2 × 0.1
Radiation	Cu Kα (λ = 1.54186)	Cu Kα (λ = 1.54186)
2Θ range for data collection/°	7.11 to 135.072	8.288 to 130.208
Index ranges	-5 ≤ h ≤ 15, -18 ≤ k ≤ 18, -23 ≤ l ≤ 23	-7 ≤ h ≤ 11, -18 ≤ k ≤ 19, -15 ≤ l ≤ 16
Reflections collected	53947	79563
Independent reflections	7515 [R_{int} = 0.0550, R_{sigma} = 0.0293]	7200 [R_{int} = 0.0425, R_{sigma} = 0.0133]
Data/restraints/parameters	7515/0/492	7200/1/492
Goodness-of-fit on F^2	1.081	1.075
Final R indexes [I>=2σ (I)]	R_1 = 0.0381, wR_2 = 0.0914	R_1 = 0.0339, wR_2 = 0.0887
Final R indexes [all data]	R_1 = 0.0438, wR_2 = 0.0947	R_1 = 0.0339, wR_2 = 0.0887
Largest diff. peak/hole / e Å^{-3}	1.45/-0.46	1.00/-0.70
Flack parameter	0.05(2)	0.056(16)

$[Re_2(\mathbf{5b})(CO)_6Cl_2]$

Identification code	d1-$[Re_2(\mathbf{5b})(CO)_6Cl_2]$	d2-$[Re_2(\mathbf{5b})(CO)_6Cl_2]$
CCDC number	2310574	2310578
Empirical formula	$C_{40}H_{34}Cl_2N_4O_6Re_2$	$C_{40}H_{34}Cl_2N_4O_6Re_2$
Formula weight	1110.01	1110.01
Temperature/K	250	250
Crystal system	orthorhombic	monoclinic
Space group	$P2_12_12_1$	$P2_1$
a/Å	13.8365(2)	9.62135(21)
b/Å	16.5716(4)	16.6058(5)
c/Å	17.2135(3)	14.2479(4)
α/°	90.00	90.00
β/°	90.00	102.679(2)
γ/°	90.00	90.00
Volume/Å^3	3946.93(13)	2220.87(10)
Z	4	2
ρ_{calc}g/cm^3	1.868	1.660
μ/mm^{-1}	3.390	3.012
F(000)	2136.0	1068.0
Crystal size/mm^3	0.56 × 0.363 × 0.19	0.44 × 0.3 × 0.16
Radiation	Ag Kα (λ = 0.56083)	Ag Kα (λ = 0.56083)
2Θ range for data collection/°	4.522 to 53.134	4.51 to 53.314
Index ranges	-21 ≤ h ≤ 21, -26 ≤ k ≤ 25, -27 ≤ l ≤ 26	-13 ≤ h ≤ 15, -26 ≤ k ≤ 25, -21 ≤ l ≤ 22
Reflections collected	73000	45516
Independent reflections	14577 [R_{int} = 0.0911, R_{sigma} = 0.0575]	15275 [R_{int} = 0.0583, R_{sigma} = 0.0488]
Data/restraints/parameters	14577/31/491	15275/1/491
Goodness-of-fit on F^2	1.024	0.957
Final R indexes [I>=2σ (I)]	R_1 = 0.0362, wR_2 = 0.0737	R_1 = 0.0319, wR_2 = 0.0672
Final R indexes [all data]	R_1 = 0.0504, wR_2 = 0.0768	R_1 = 0.0403, wR_2 = 0.0692
Largest diff. peak/hole / e Å^{-3}	1.32/-1.16	0.76/-0.85
Flack parameter	0.002(8)	0.017(8)

$[Re_2(\mathbf{6a})(CO)_6Cl_2]$

Identification code	d1-$[Re_2(\mathbf{6a})(CO)_6Cl_2]$	d2-$[Re_2(\mathbf{6a})(CO)_6Cl_2]$
CCDC number	2310575	2310579
Empirical formula	$C_{40}H_{34}Cl_2N_4O_6Re_2$	$C_{80}H_{68}Cl_4N_8O_{12}Re_4$
Formula weight	1110.01	2220.02
Temperature/K	200(2)	200(2)
Crystal system	orthorhombic	triclinic
Space group	$C222_1$	P1
a/Å	19.7136(5)	12.0572(2)
b/Å	25.7034(7)	14.1674(2)
c/Å	8.5965(2)	14.4880(3)
α/°	90	115.3320(10)
β/°	90	94.9130(10)
γ/°	90	93.3450(10)
Volume/Å^3	4355.90(19)	2216.20(7)
Z	4	1
ρ_{calc}g/cm^3	1.693	1.663
μ/mm^{-1}	12.215	12.004
F(000)	2136.0	1068.0
Crystal size/mm^3	0.18 × 0.133 × 0.08	0.06 × 0.05 × 0.03
Radiation	Cu Kα (λ = 1.54186)	Cu Kα (λ = 1.54186)
2Θ range for data collection/°	8.972 to 134.89	7.306 to 135.708
Index ranges	-14 ≤ h ≤ 23, -28 ≤ k ≤ 30, -8 ≤ l ≤ 10	-14 ≤ h ≤ 14, -16 ≤ k ≤ 14, -17 ≤ l ≤ 16
Reflections collected	14971	9052
Independent reflections	3789 [R_{int} = 0.0250, R_{sigma} = 0.0172]	9052 [R_{int} = ?, R_{sigma} = 0.0263]
Data/restraints/parameters	3789/0/246	9052/4/814
Goodness-of-fit on F^2	1.049	1.109
Final R indexes [I>=2σ (I)]	R_1 = 0.0398, wR_2 = 0.1087	R_1 = 0.0479, wR_2 = 0.1391
Final R indexes [all data]	R_1 = 0.0400, wR_2 = 0.1089	R_1 = 0.0493, wR_2 = 0.1401
Largest diff. peak/hole / e Å^{-3}	1.72/-1.22	2.76/-2.19
Flack parameter	0.03(3)	-0.008(12)

$[Re_2(\mathbf{6b})(CO)_6Cl_2]$

Identification code	d1-$[Re_2(\mathbf{6b})(CO)_6Cl_2]$	d2-$[Re_2(\mathbf{6b})(CO)_6Cl_2]$
CCDC number	2310576	2310580
Empirical formula	$C_{40}H_{34}Cl_2N_4O_6Re_2$	$C_{44}H_{46}Cl_2N_4O_8Re_2$
Formula weight	1110.01	1202.15
Temperature/K	250	250(2)
Crystal system	orthorhombic	triclinic
Space group	$C222_1$	P1
a/Å	19.8460(3)	12.0797(3)
b/Å	25.9024(4)	14.3295(3)
c/Å	8.63570(10)	14.5093(3)
α/°	90.00	116.153(2)
β/°	90.00	95.311(2)
γ/°	90.00	91.952(2)
Volume/Å^3	4439.26(11)	2236.81(9)
Z	4	2
ρ_{calc}g/cm^3	1.661	1.785
μ/mm^{-1}	3.014	11.980
F(000)	2136.0	1172.0
Crystal size/mm^3	0.45 × 0.27 × 0.14	0.11 × 0.093 × 0.07
Radiation	AgKα (λ = 0.56083)	Cu Kα (λ = 1.54186)
2Θ range for data collection/°	4.474 to 53.106	10.158 to 138.264
Index ranges	-30 ≤ h ≤ 27, -41 ≤ k ≤ 35, -13 ≤ l ≤ 13	-14 ≤ h ≤ 10, -16 ≤ k ≤ 17, -17 ≤ l ≤ 17
Reflections collected	70371	64439
Independent reflections	8594 [R_{int} = 0.0714, R_{sigma} = 0.0417]	11433 [R_{int} = 0.0525, R_{sigma} = 0.0333]
Data/restraints/parameters	8594/0/246	11433/168/794
Goodness-of-fit on F^2	1.010	1.077
Final R indexes [I>=2σ (I)]	R_1 = 0.0354, wR_2 = 0.0897	R_1 = 0.0666, wR_2 = 0.1903
Final R indexes [all data]	R_1 = 0.0513, wR_2 = 0.0938	R_1 = 0.0697, wR_2 = 0.1954
Largest diff. peak/hole / e Å^{-3}	1.84/-0.56	3.04/-1.53
Flack parameter	-0.013(11)	0.17(2)