

Electronic Supplementary Information

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

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Analytical data

^1H and ^{13}C NMR spectra

Spectra of the ligands

5b

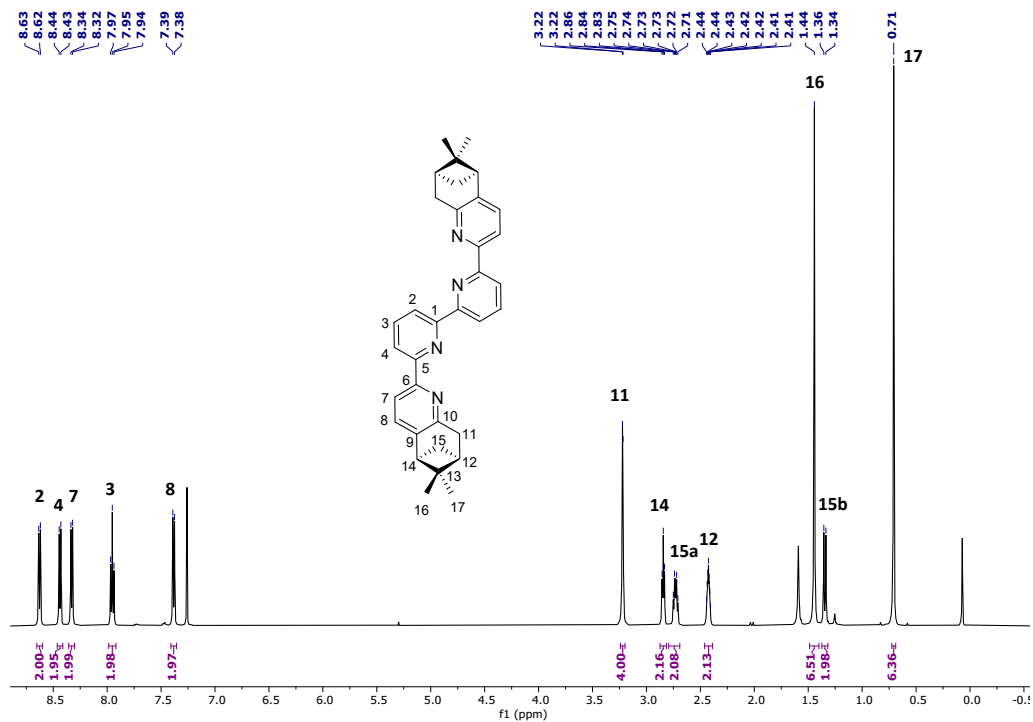


Figure S1. ^1H -NMR spectrum of **5b** in CDCl_3

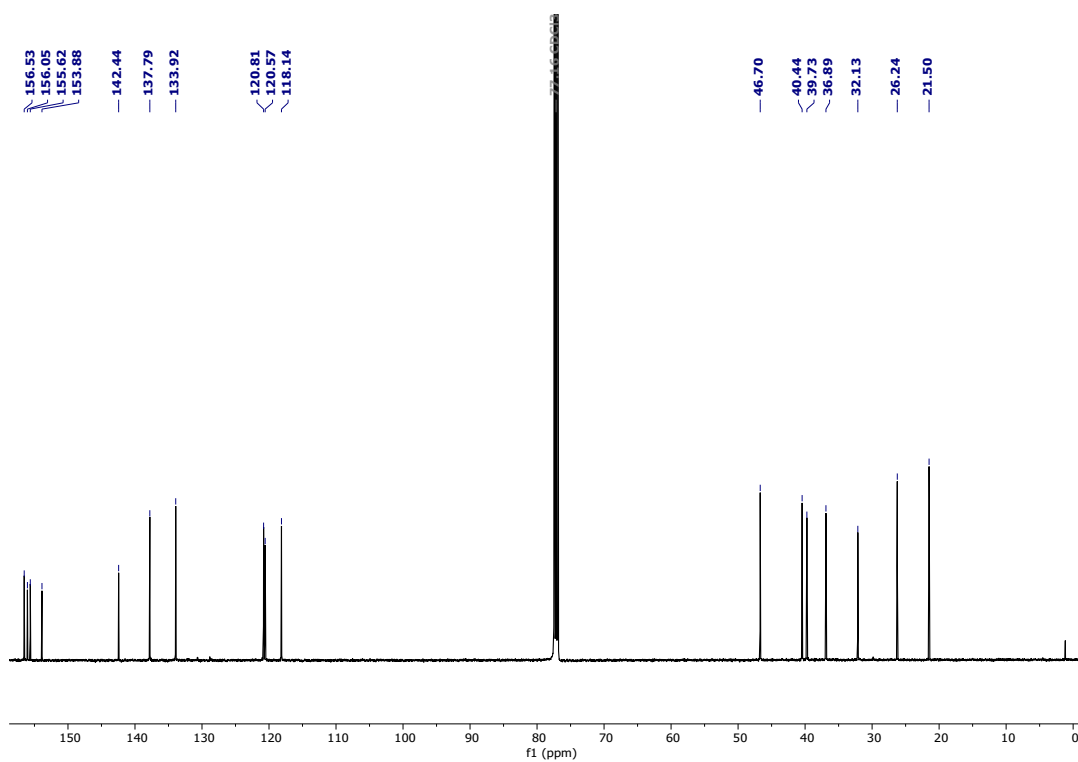


Figure S2. ^{13}C -NMR spectrum of **5b** in CDCl_3

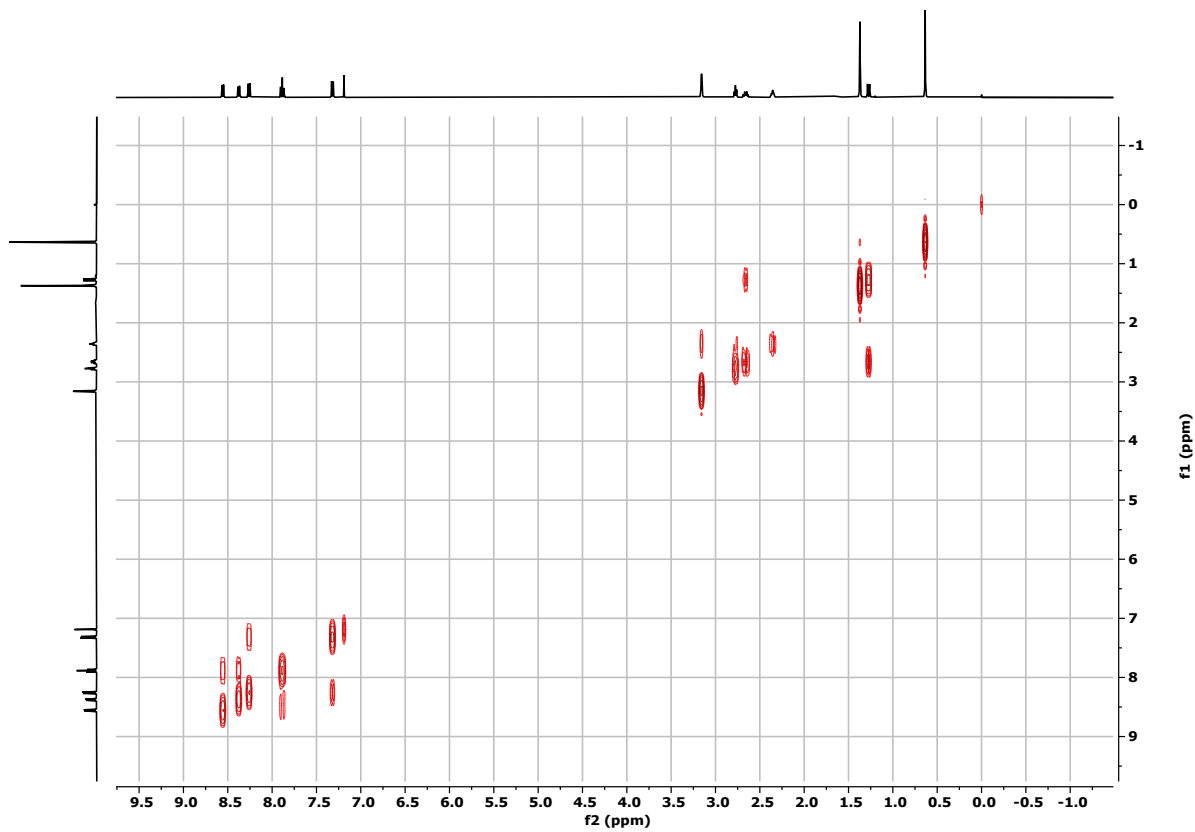


Figure S3. COSY spectrum of **5b** in $CDCl_3$

6a

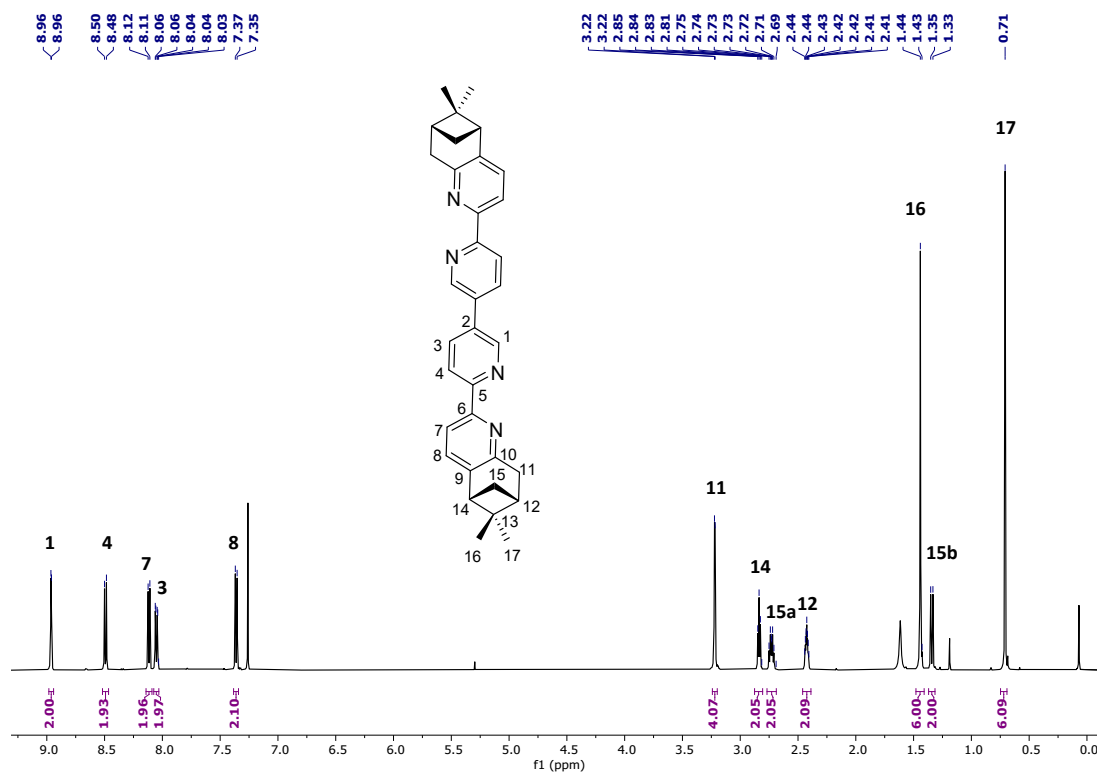


Figure S4. 1H -NMR spectrum of **6a** in $CDCl_3$

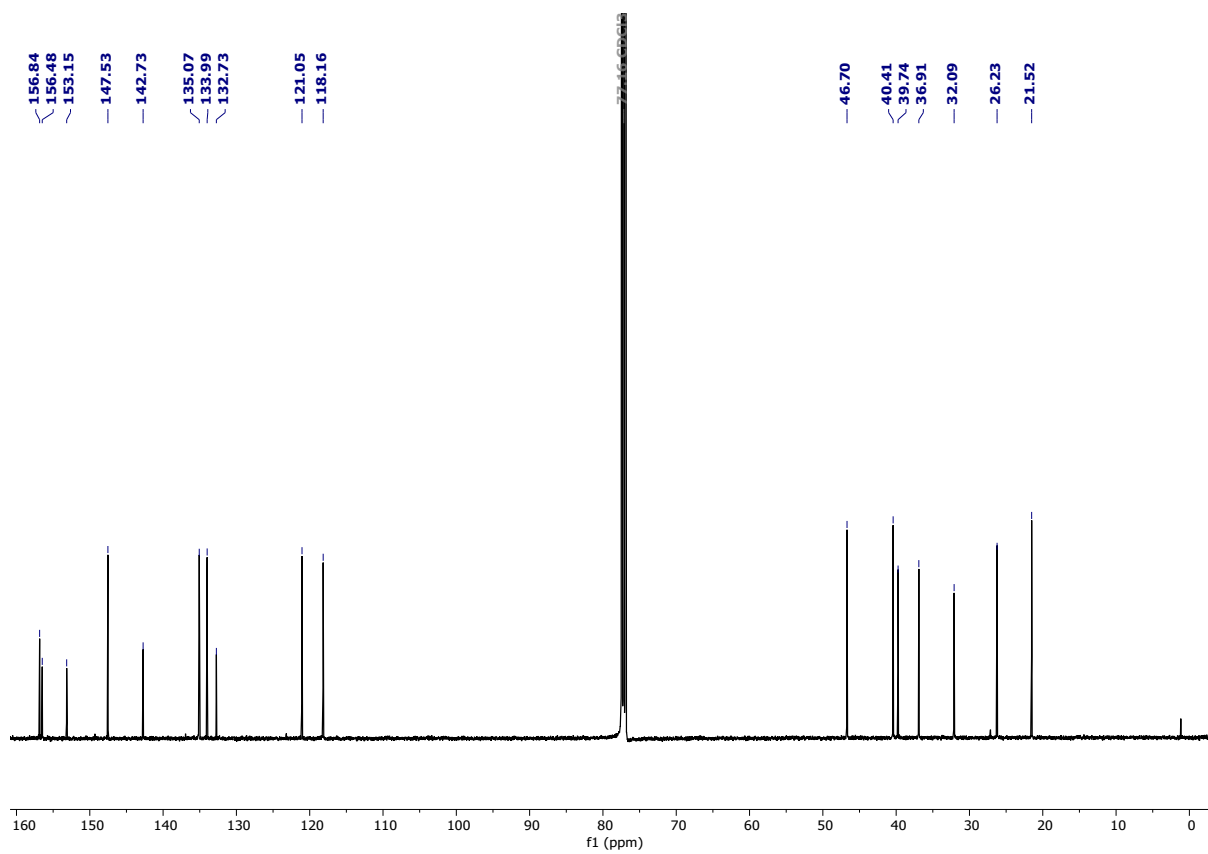


Figure S5. ^{13}C -NMR spectrum of **6a** in CDCl_3

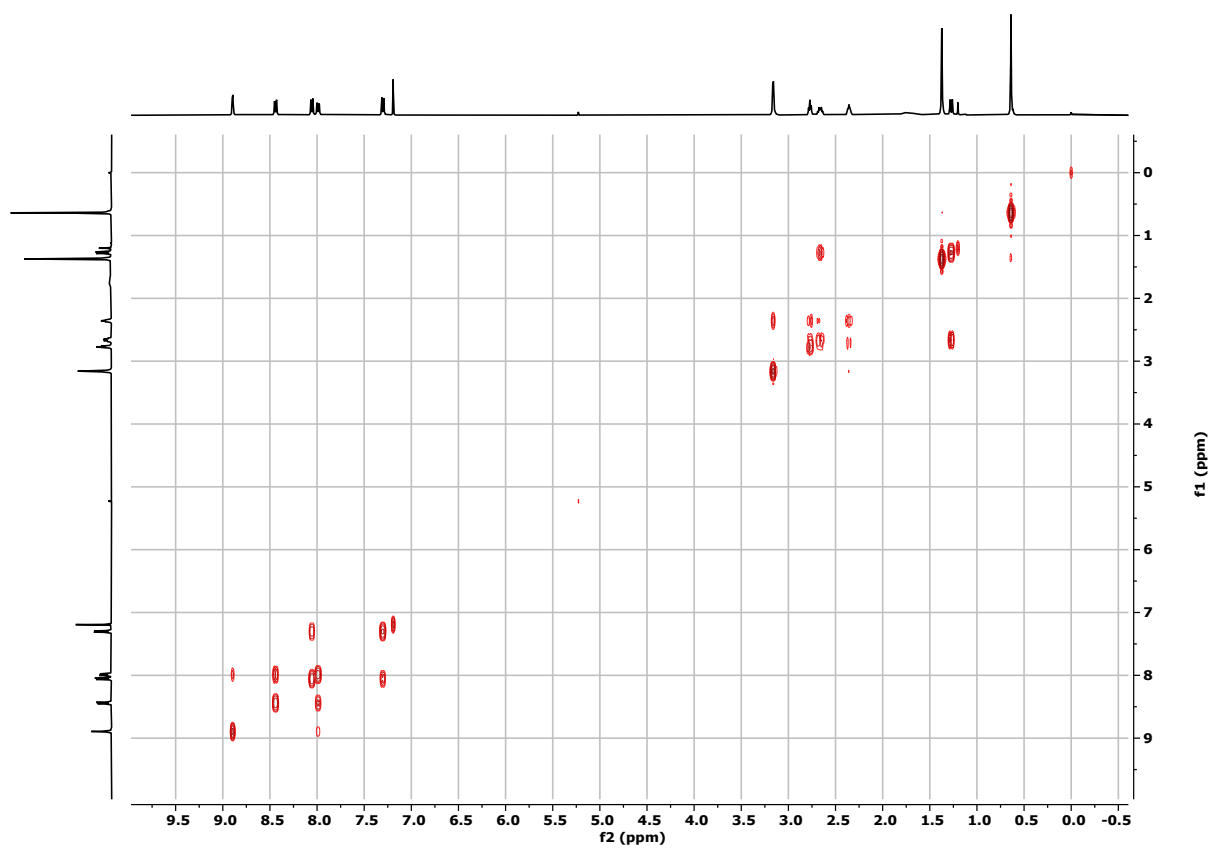


Figure S6. COSY spectrum of **6a** in CDCl_3

6b

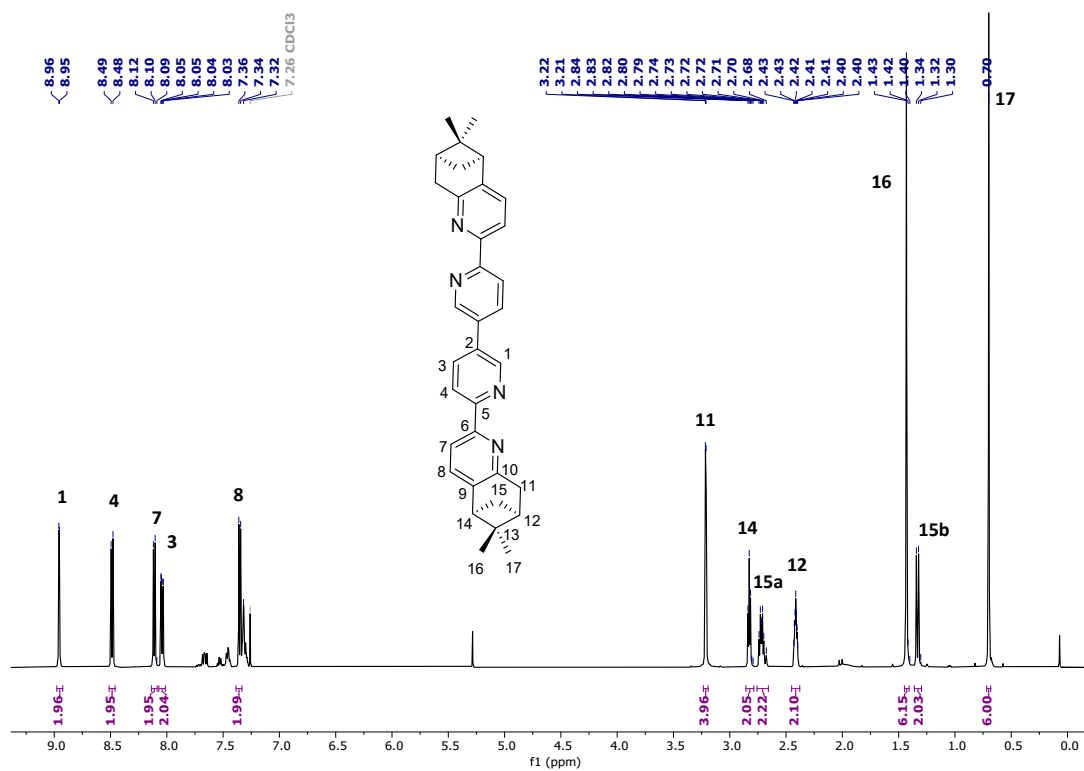


Figure S7. ¹H-NMR spectrum of 6b in CDCl₃

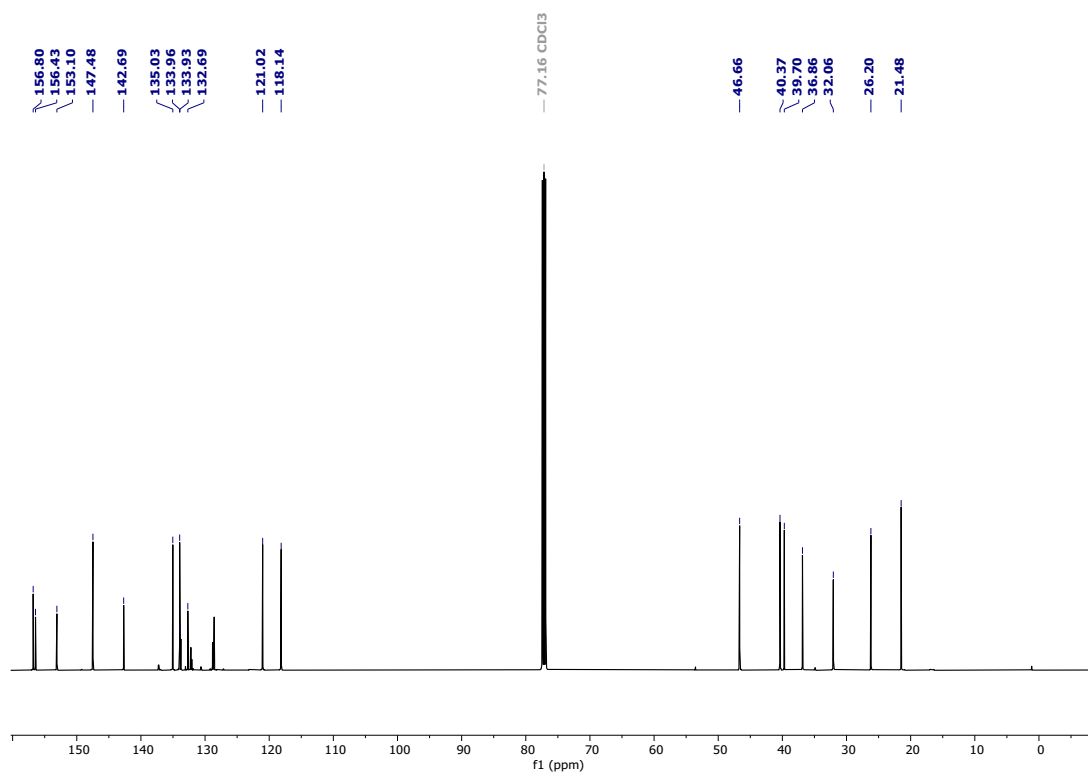


Figure S8. ¹³C-NMR spectrum of 6b in CDCl₃

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

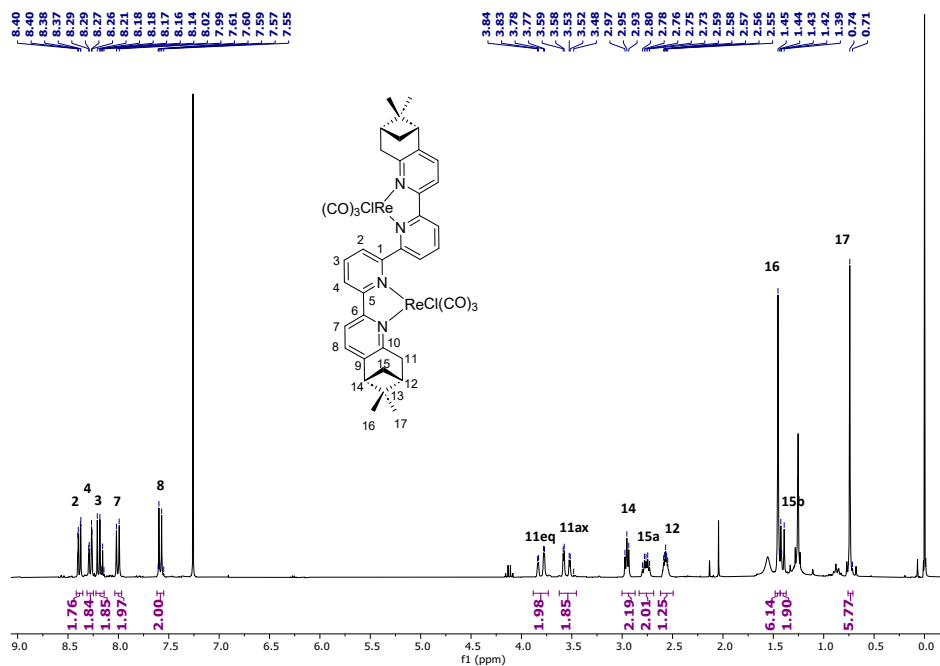


Figure S9. 1H -NMR spectrum of $d1-[Re_2(5a)(CO)_6Cl_2]$ in $CDCl_3$

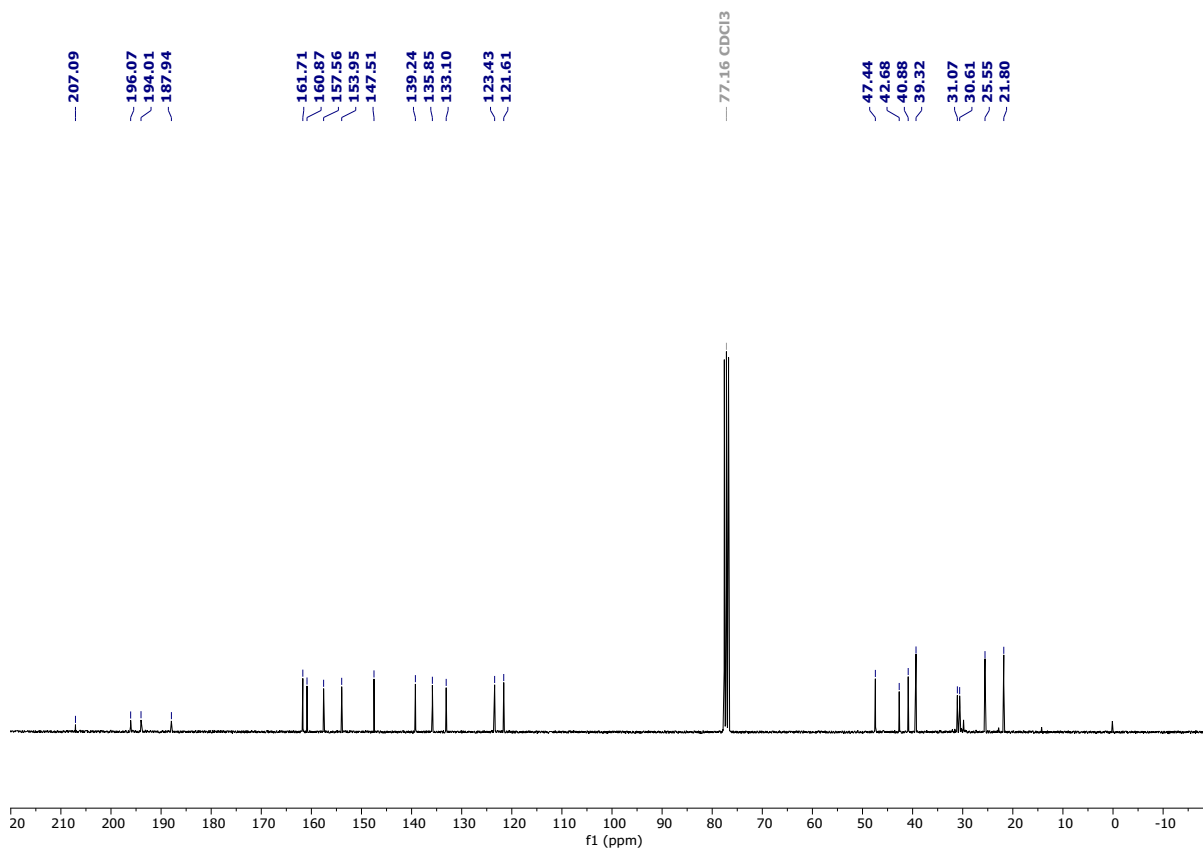


Figure S10. ^{13}C -NMR spectrum of $d1-[Re_2(5a)(CO)_6Cl_2]$ in $CDCl_3$

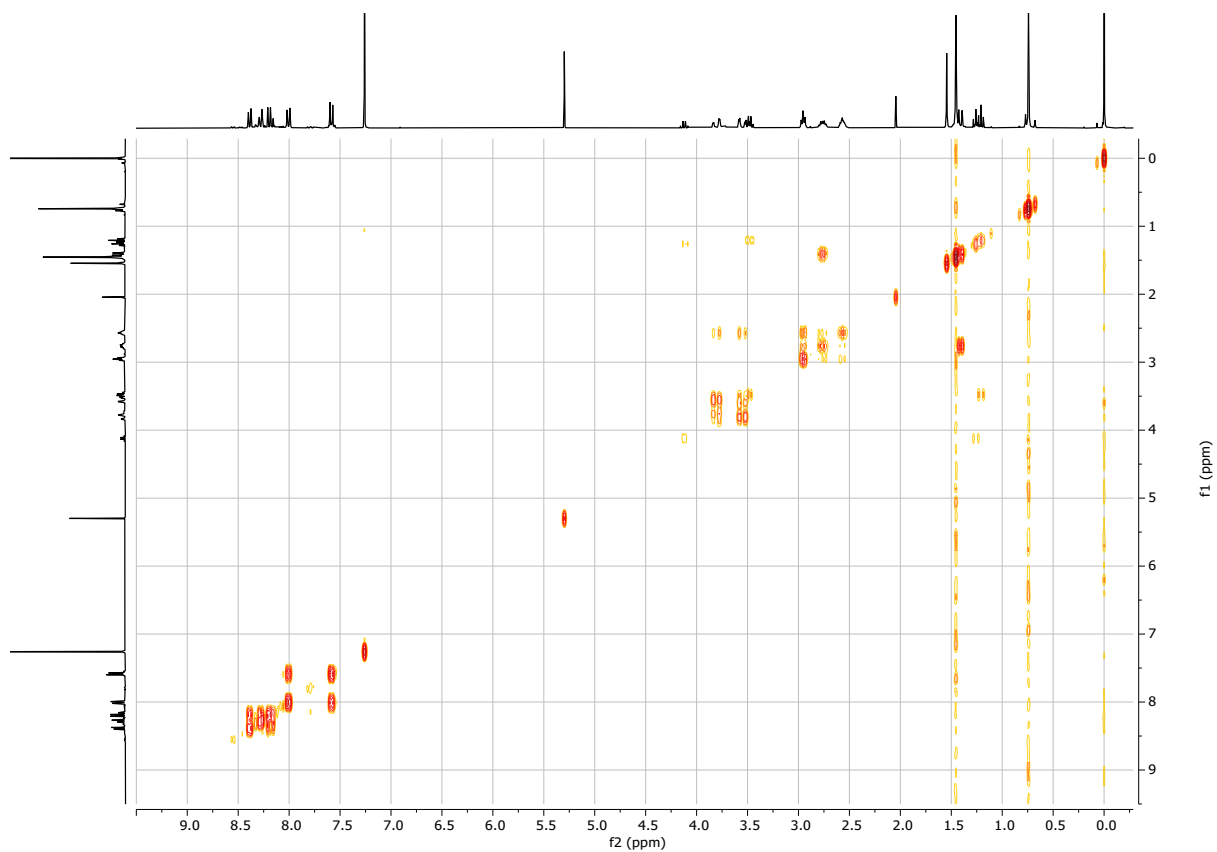


Figure S11. COSY spectrum of $d1\text{-}[\text{Re}_2(\mathbf{5a})(\text{CO})_6\text{Cl}_2]$ in CDCl_3

$d2\text{-}[\text{Re}_2(\mathbf{5a})(\text{CO})_6\text{Cl}_2]$

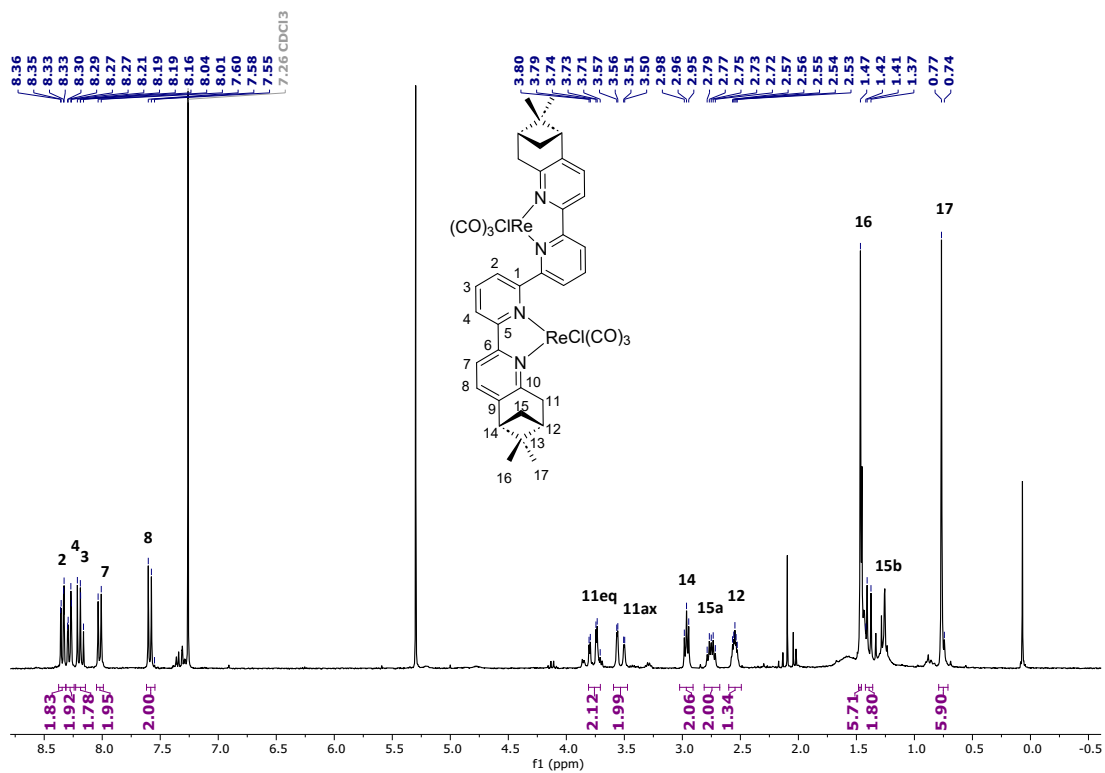


Figure S12. $^1\text{H-NMR}$ spectrum of $d2\text{-}[\text{Re}_2(\mathbf{5a})(\text{CO})_6\text{Cl}_2]$ in CDCl_3

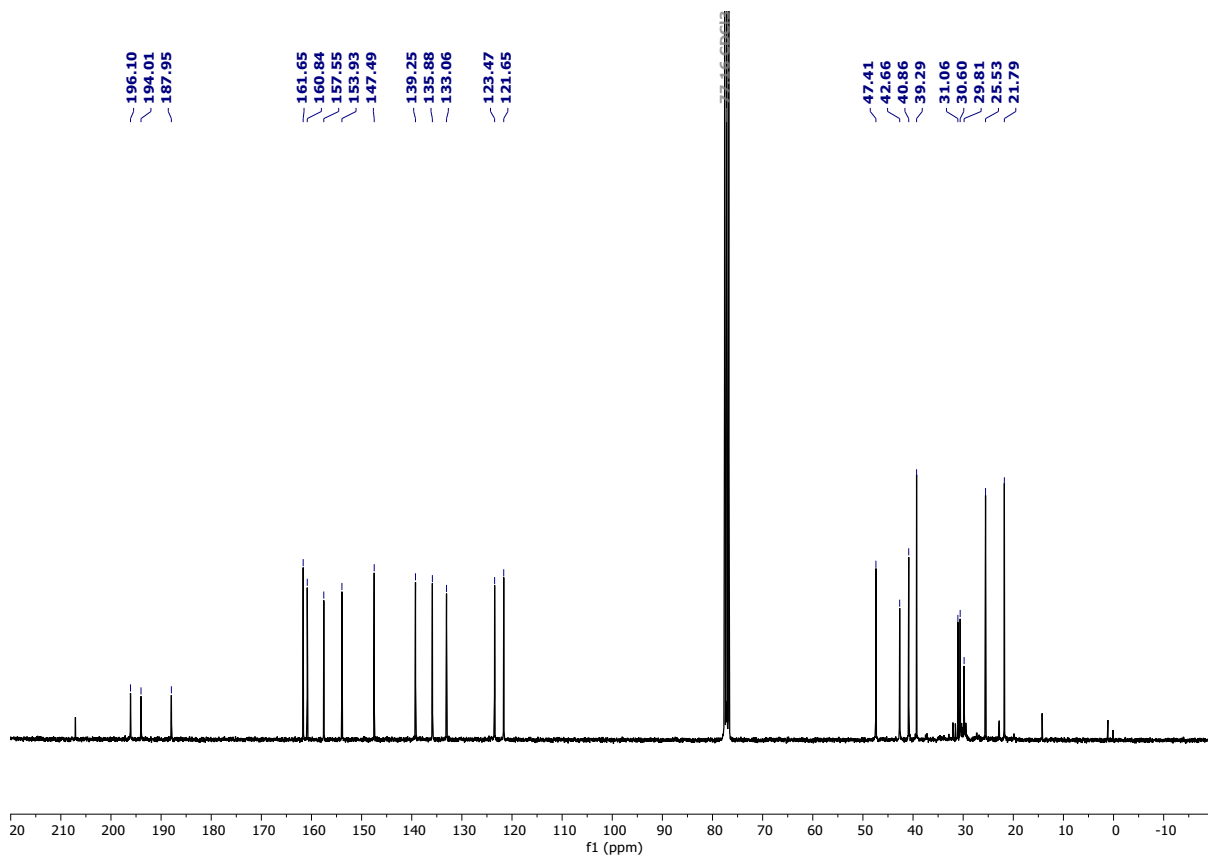


Figure S13. ^{13}C -NMR spectrum of d_2 - $[\text{Re}_2(\mathbf{5a})(\text{CO})_6\text{Cl}_2]$ in CDCl_3

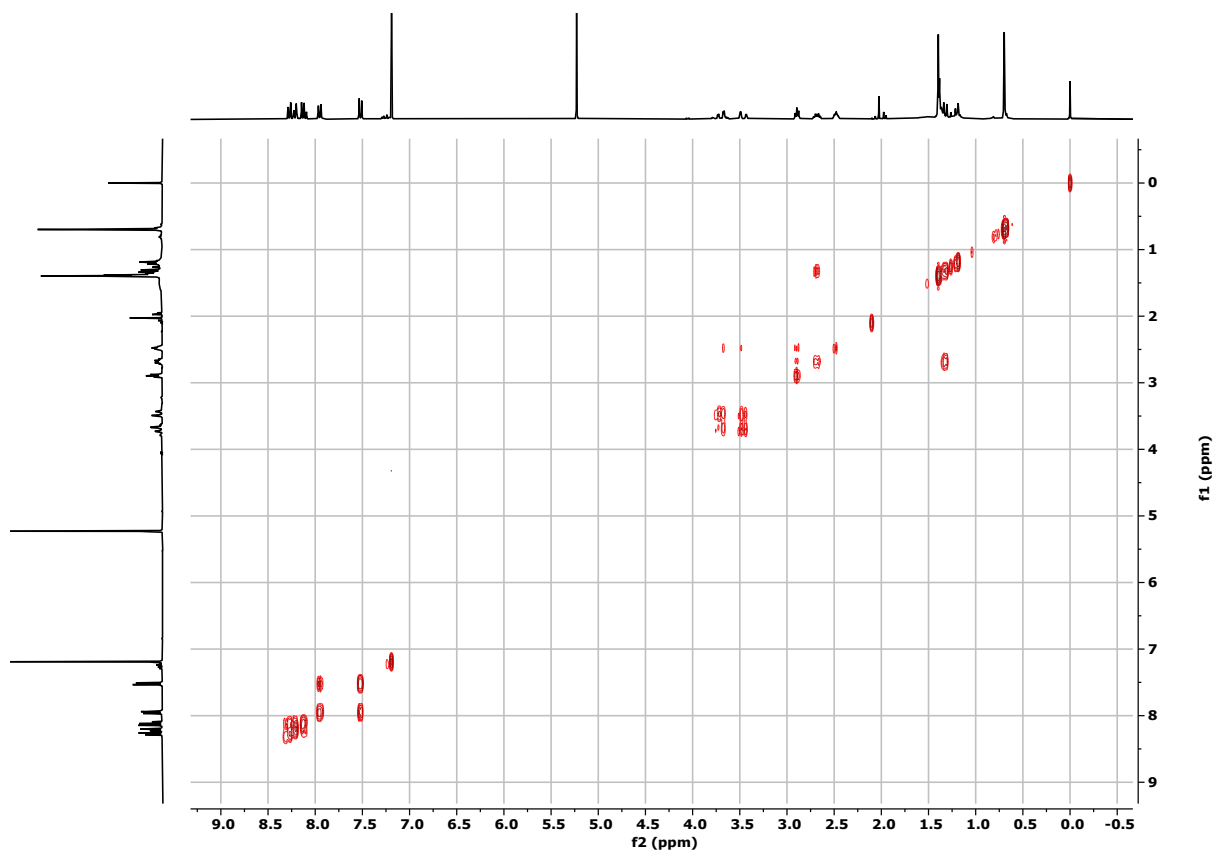


Figure S14. COSY spectrum of d_2 - $[\text{Re}_2(\mathbf{5a})(\text{CO})_6\text{Cl}_2]$ in CDCl_3

d1-[Re₂(**5b**)(CO)₆Cl₂]

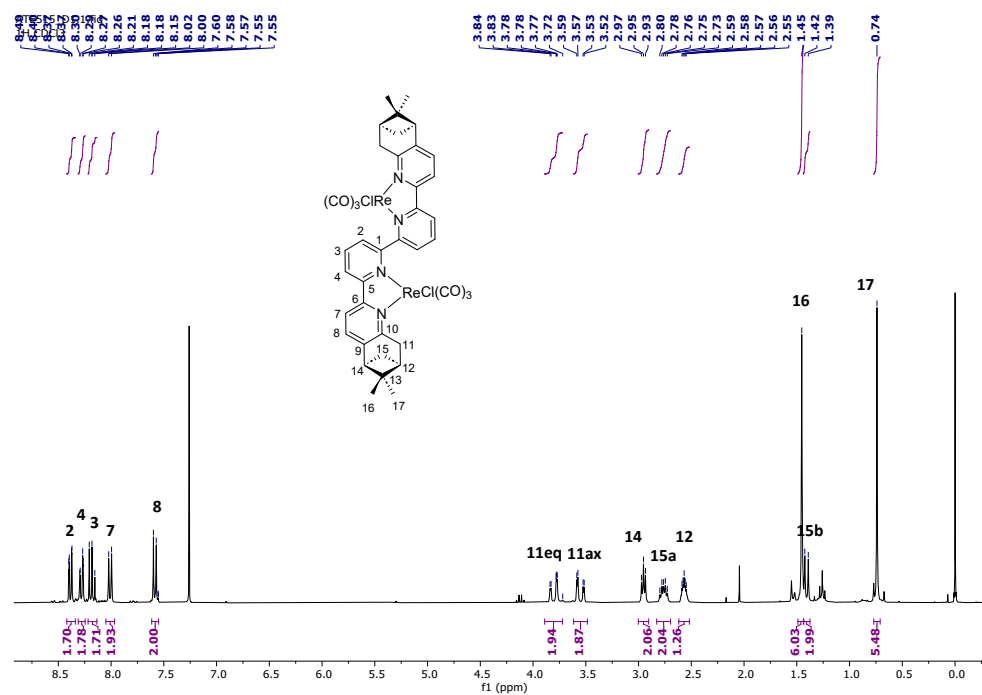


Figure S15. ¹H-NMR spectrum of d1-[Re₂(**5b**)(CO)₆Cl₂] in CDCl₃

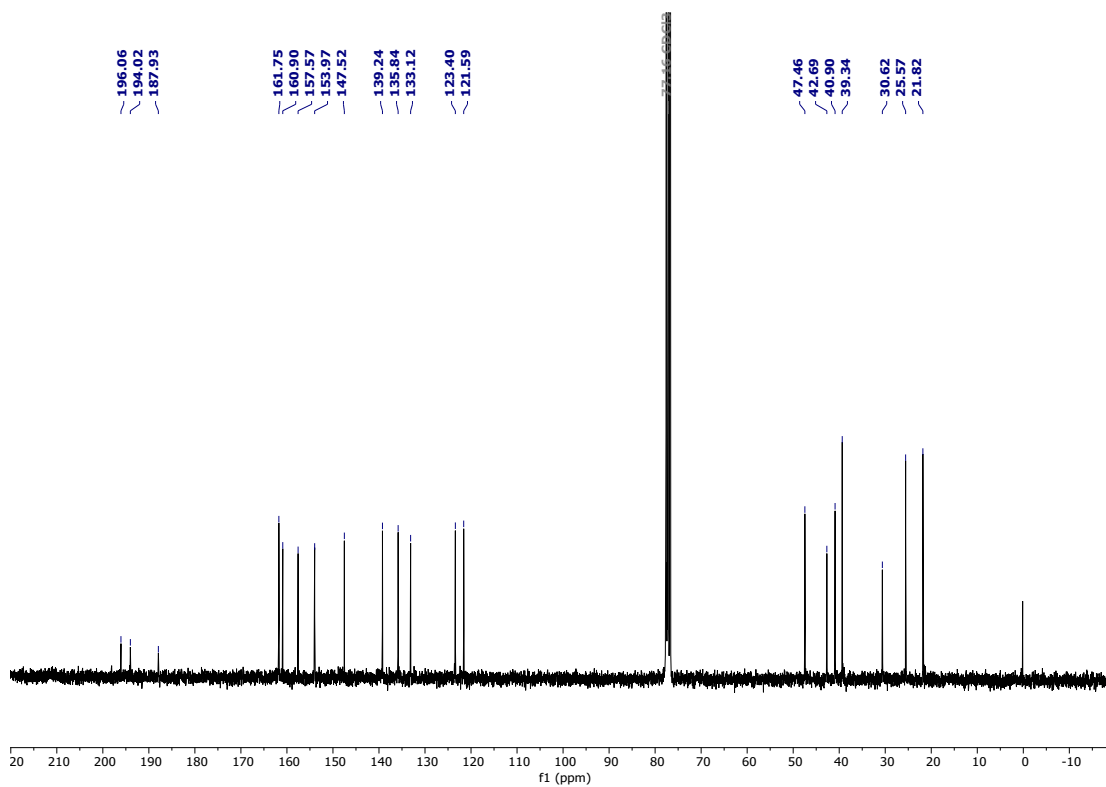


Figure S16. ¹³C-NMR spectrum of d1-[Re₂(**5b**)(CO)₆Cl₂] in CDCl₃

d_2 -[Re₂(**5b**)(CO)₆Cl₂]

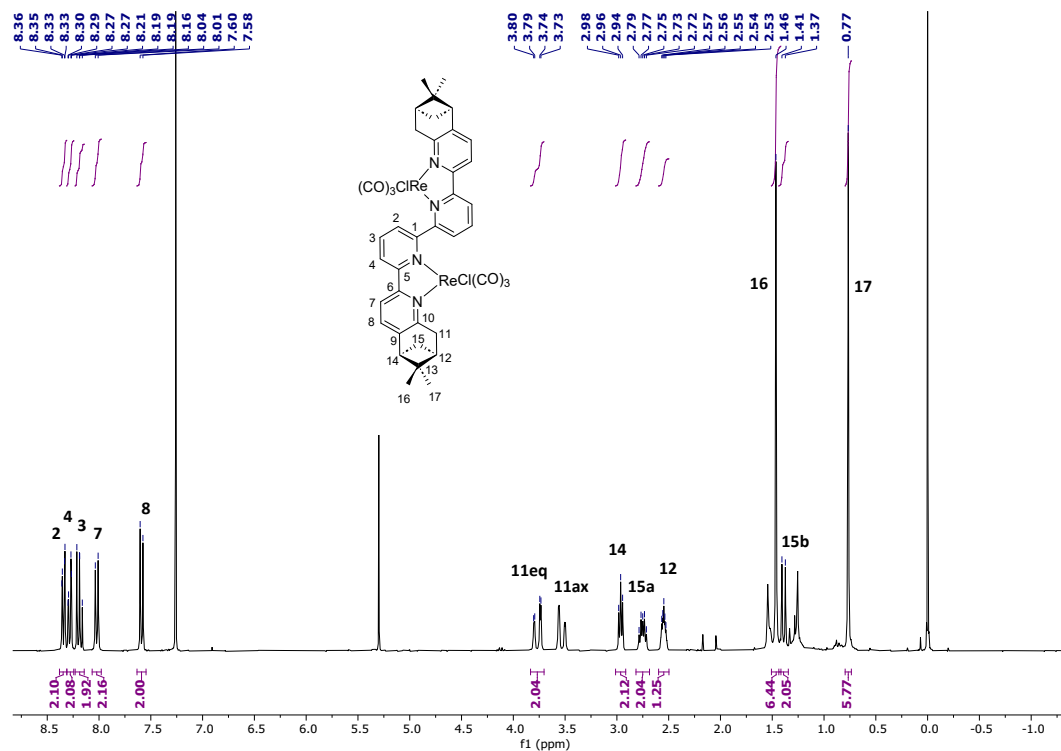


Figure S17. ¹H-NMR spectrum of d_2 -[Re₂(**5b**)(CO)₆Cl₂] in CDCl₃

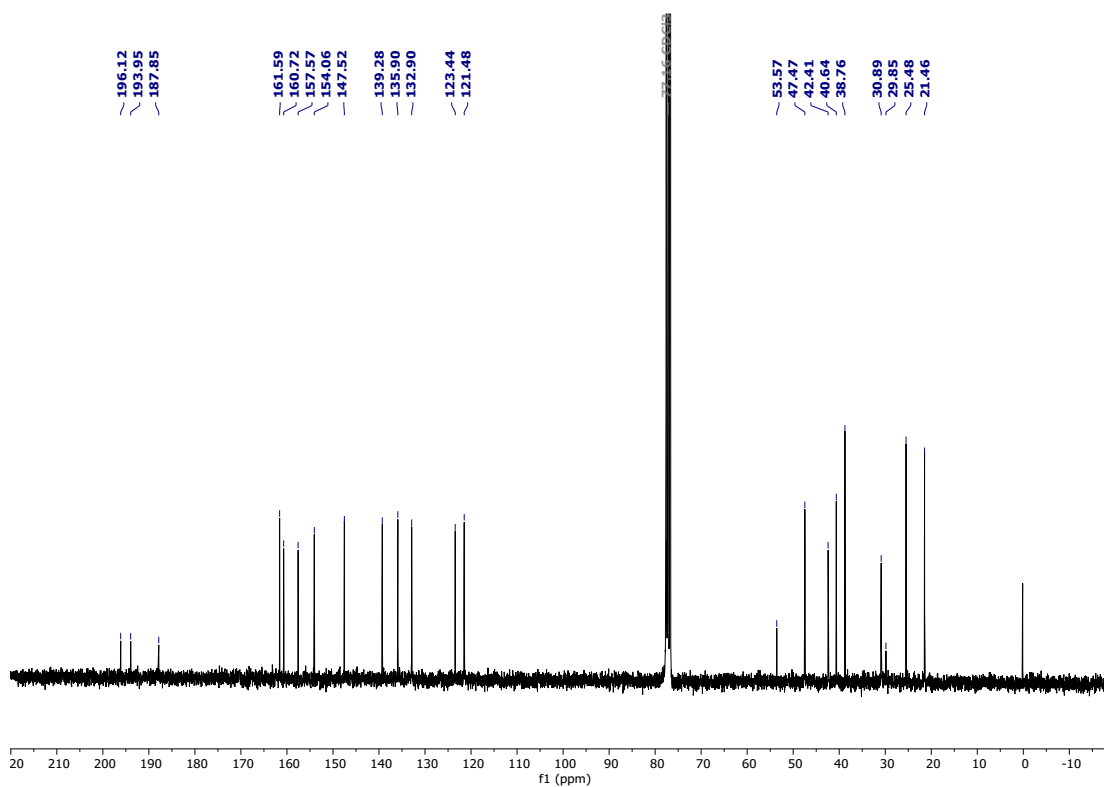


Figure S18. ¹³C-NMR spectrum of d_2 -[Re₂(**5b**)(CO)₆Cl₂] in CDCl₃

d1-[Re₂(**6a**)(CO)₆Cl₂]

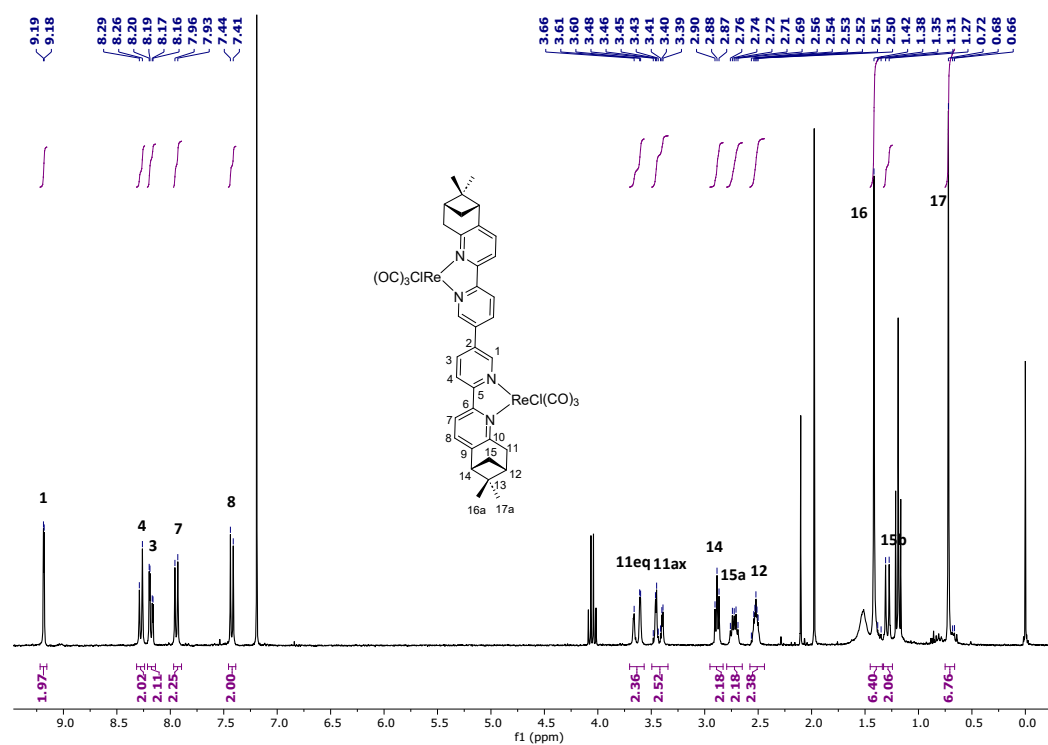


Figure S19. ¹H-NMR spectrum of d1-[Re₂(**6a**)(CO)₆Cl₂] in CDCl₃

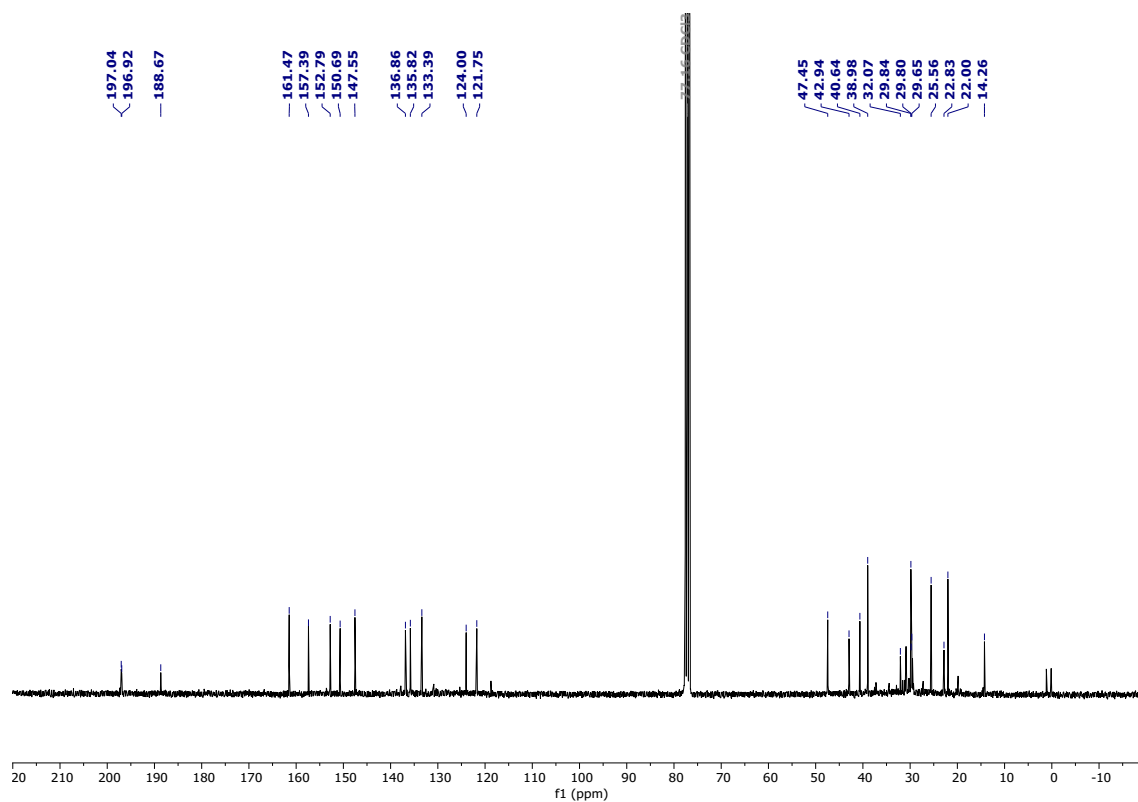


Figure S20. ^{13}C -NMR spectrum of d_1 - $[\text{Re}_2(\mathbf{6a})(\text{CO})_6\text{Cl}_2]$ in CDCl_3

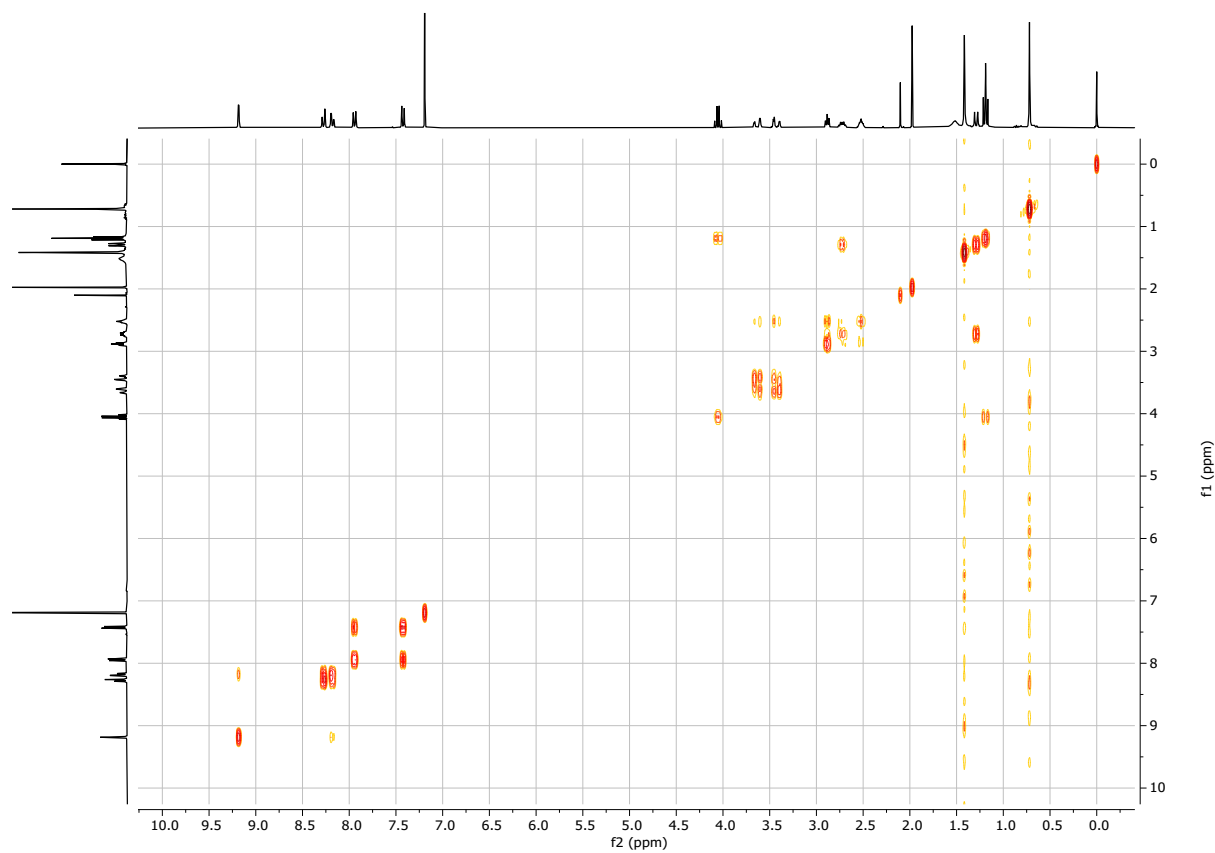


Figure S21. COSY spectrum of d_1 - $[\text{Re}_2(\mathbf{6a})(\text{CO})_6\text{Cl}_2]$ in CDCl_3

d_2 - $[\text{Re}_2(\mathbf{6a})(\text{CO})_6\text{Cl}_2]$

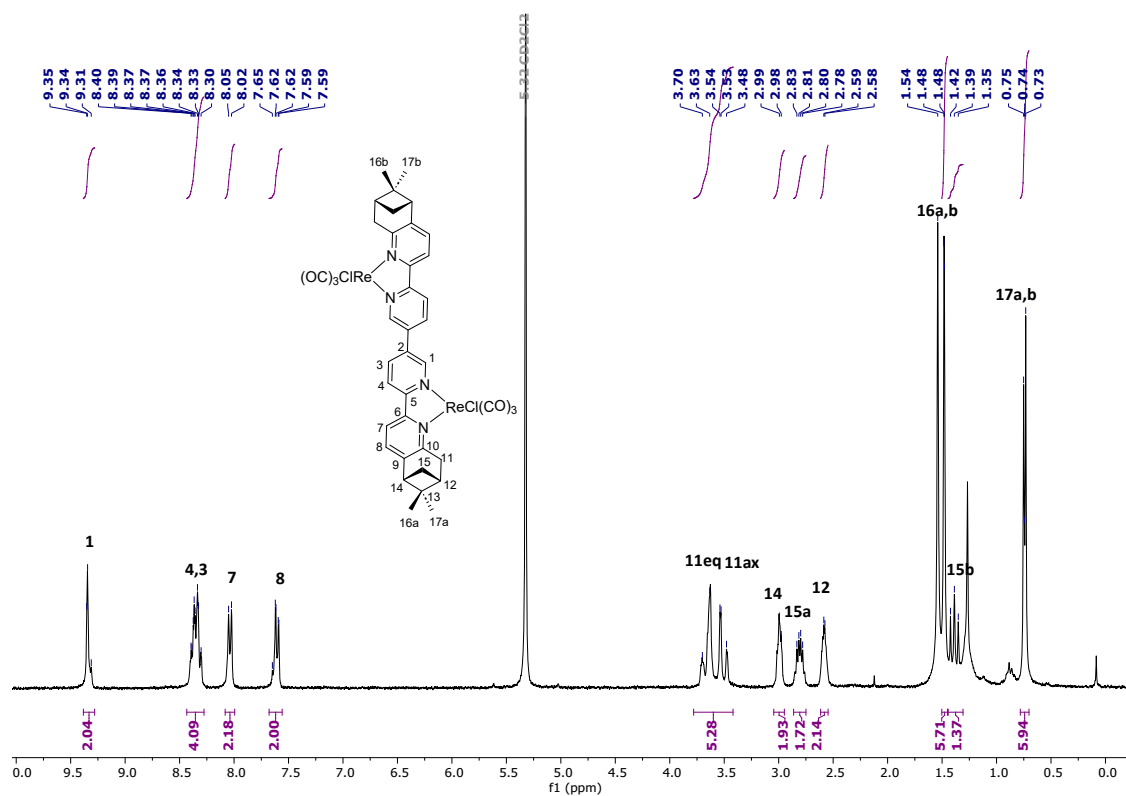


Figure S22. 1H -NMR spectrum of d_2 - $[Re_2(6a)(CO)_6Cl_2]$ in CD_2Cl_2

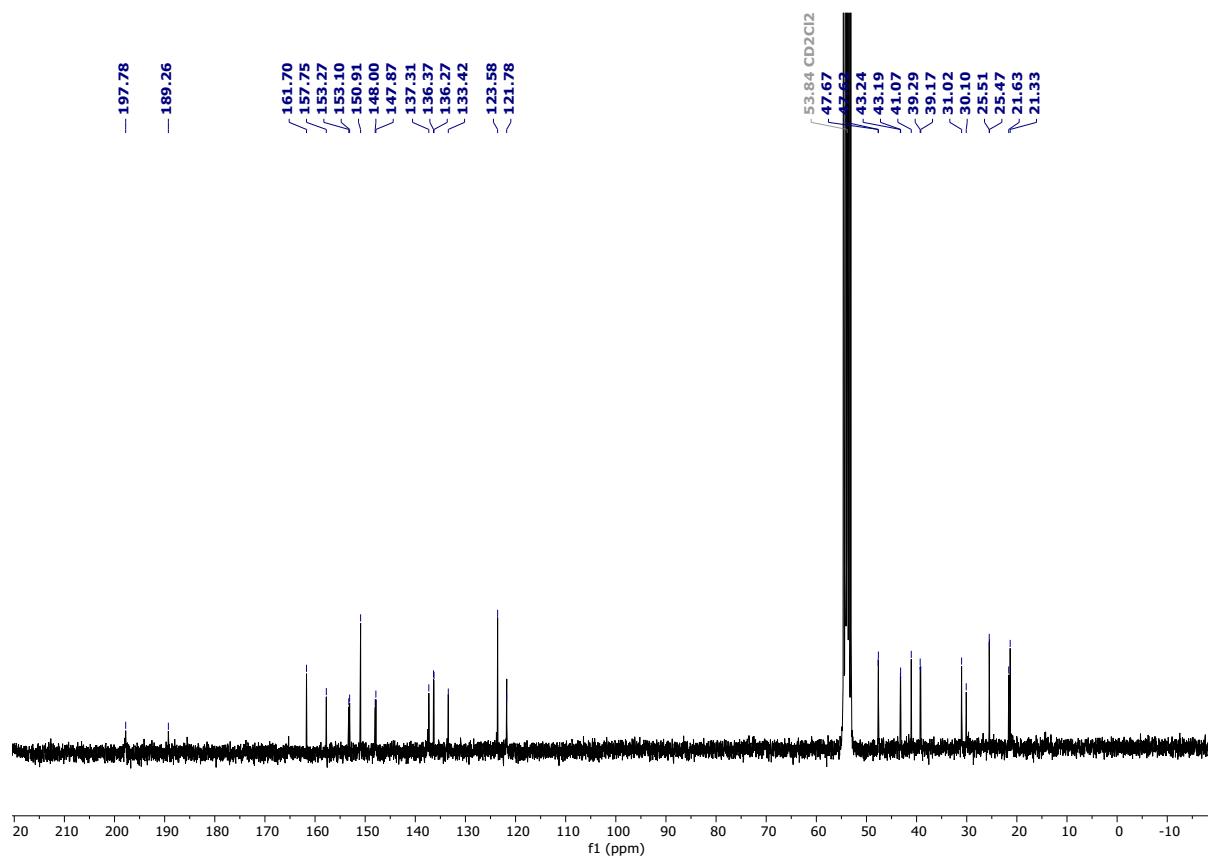


Figure S23. ^{13}C -NMR spectrum of d_2 - $[Re_2(6a)(CO)_6Cl_2]$ in CD_2Cl_2

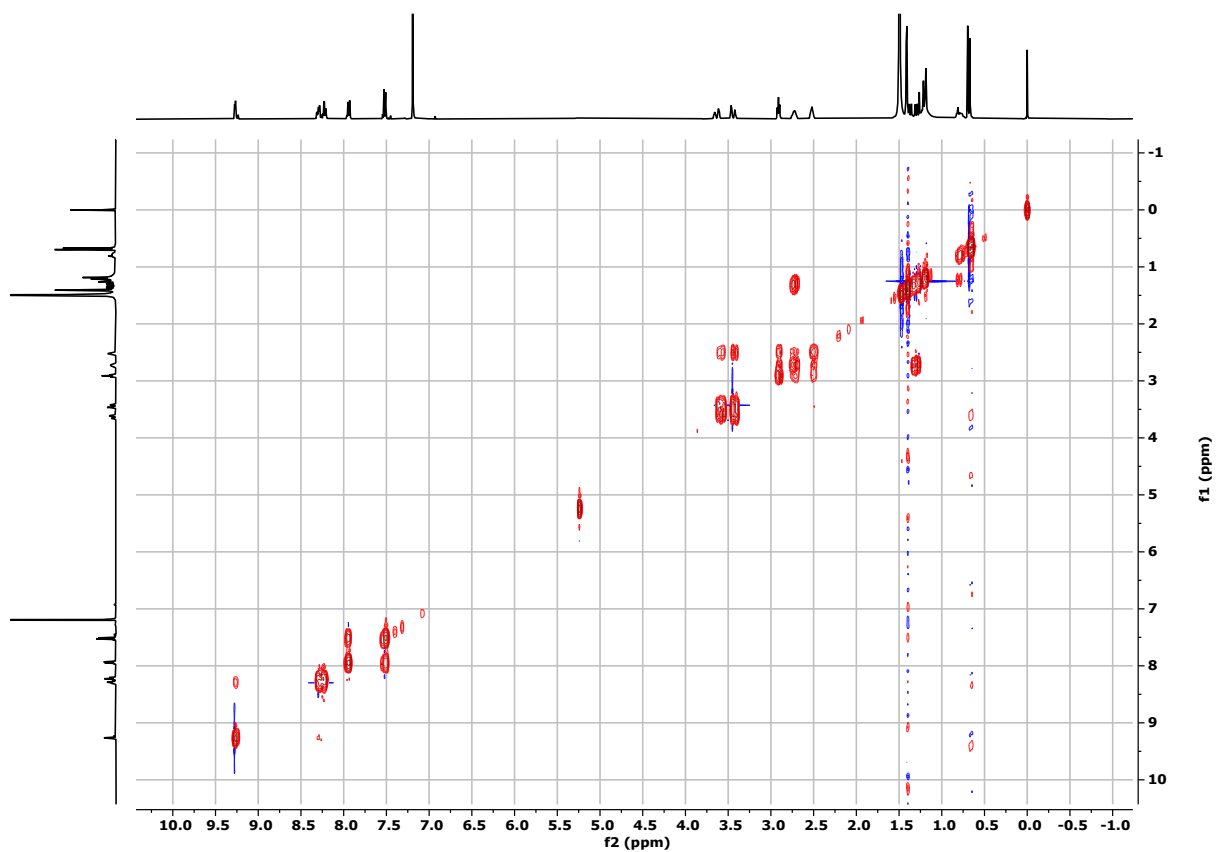


Figure S24. COSY spectrum of d_2 -[Re₂(**6a**)(CO)₆Cl₂] in CD₂Cl₂

d_1 -[Re₂(**6b**)(CO)₆Cl₂]

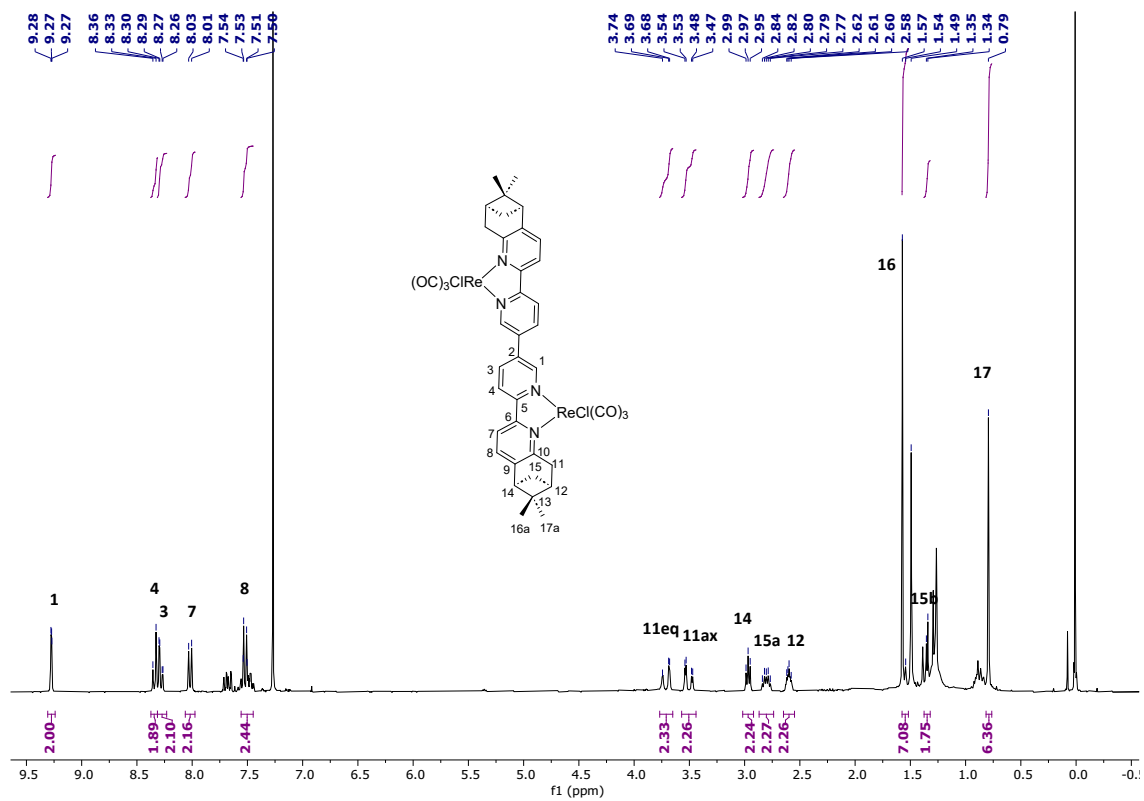


Figure S26. $^1\text{H-NMR}$ spectrum of d_1 - $[\text{Re}_2(\mathbf{6b})(\text{CO})_6\text{Cl}_2]$ in CDCl_3

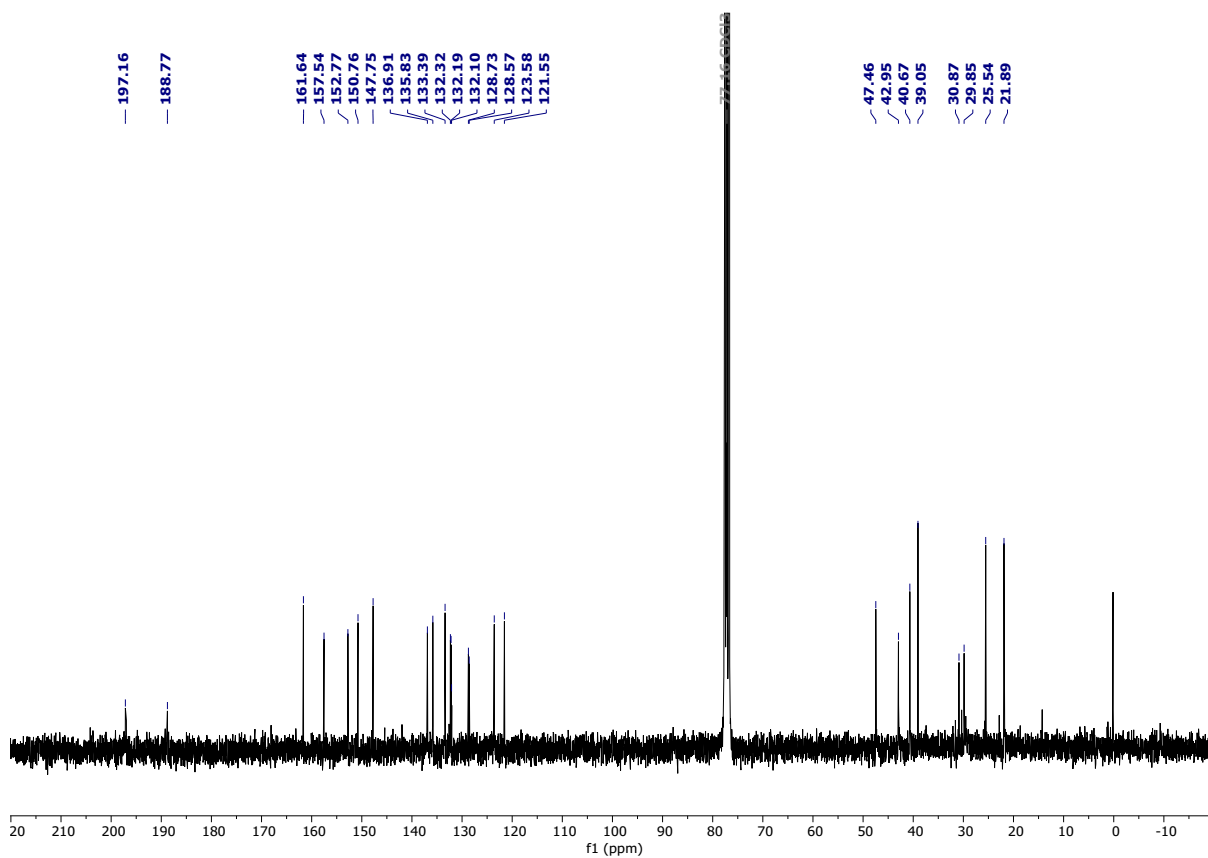


Figure S27. $^{13}\text{C-NMR}$ spectrum of d_1 - $[\text{Re}_2(\mathbf{6b})(\text{CO})_6\text{Cl}_2]$ in CDCl_3

d2-[Re₂(**6b**)(CO)₆Cl₂]

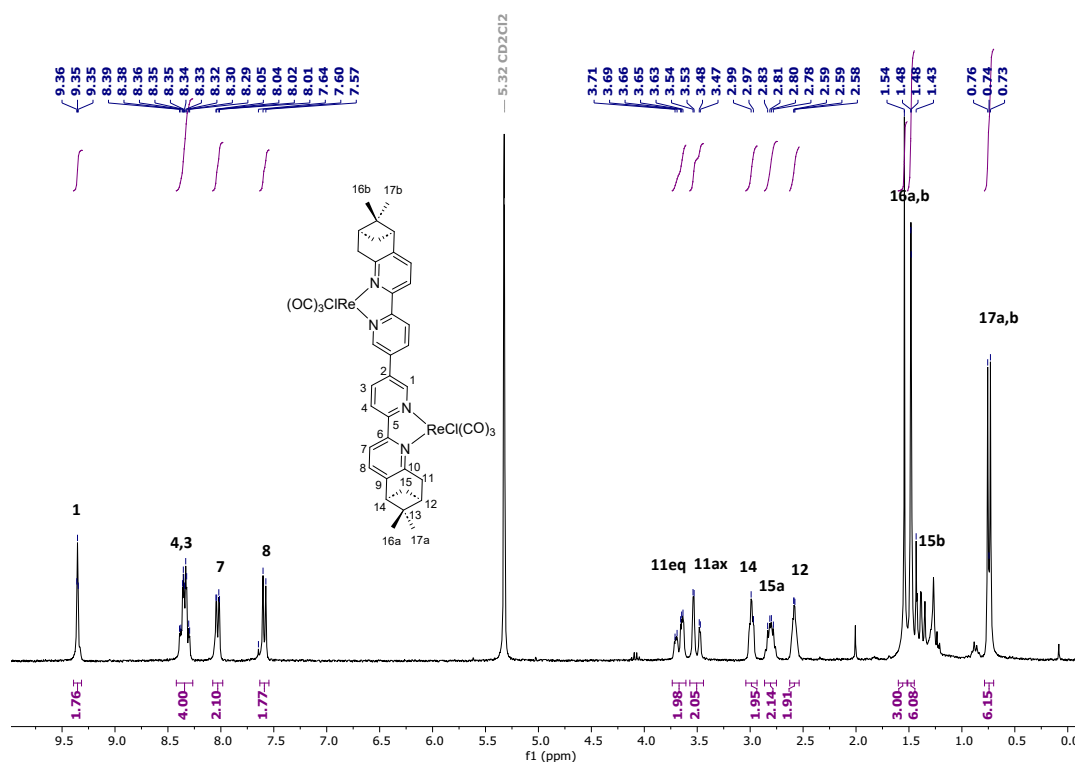


Figure S28. ¹H-NMR spectrum of d₂-[Re₂(**6b**)(CO)₆Cl₂] in CD₂Cl₂

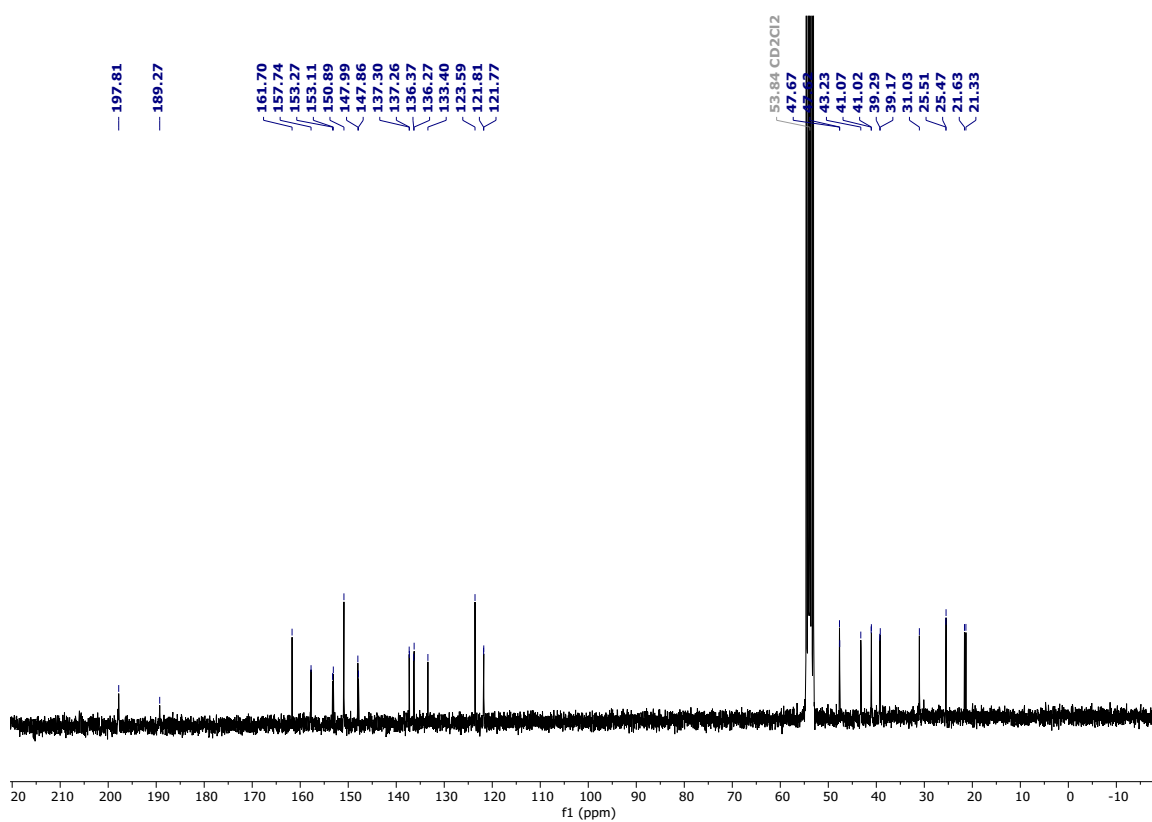


Figure S29. ¹³C-NMR spectrum of d₂-[Re₂(**6b**)(CO)₆Cl₂] in CD₂Cl₂

HRMS spectra

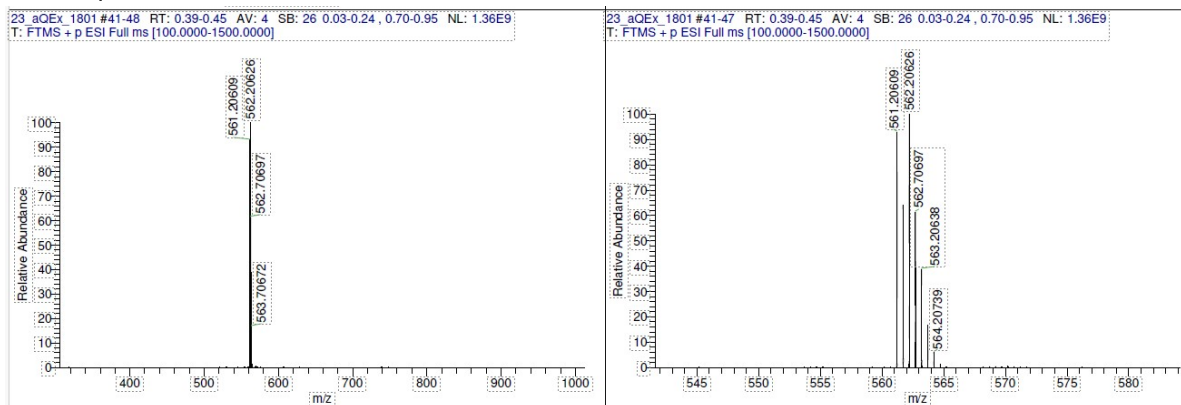


Figure S30. HRMS spectrum of **5b**

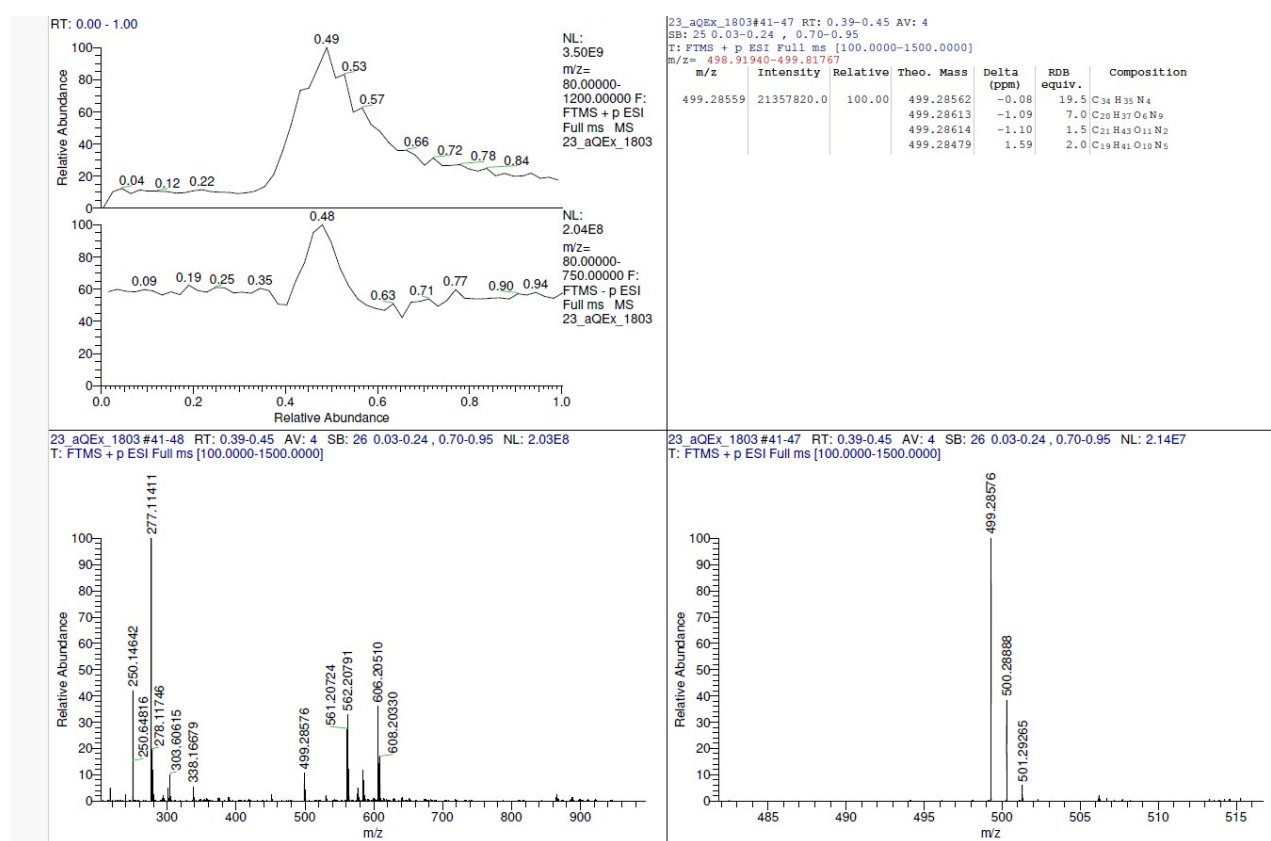


Figure S31. HRMS spectrum of **6a**

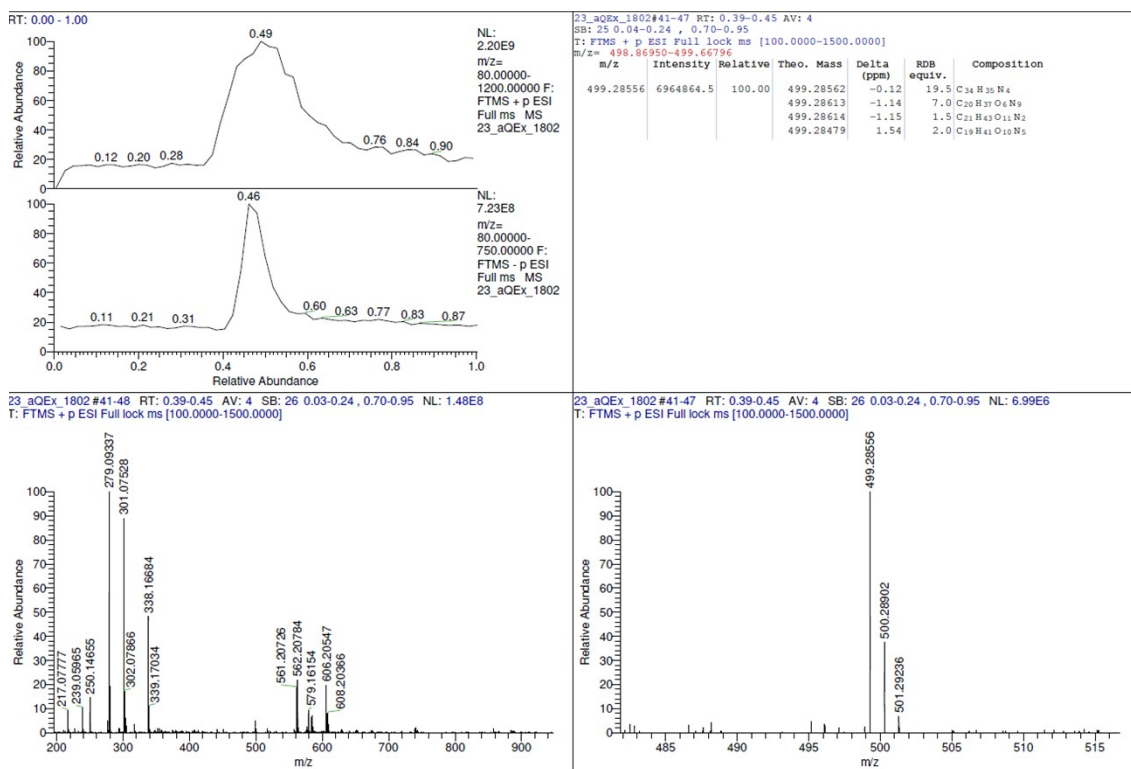


Figure S32. HRMS spectrum of **6b**

d1-[Re₂(5a**)(CO)₆Cl₂]**

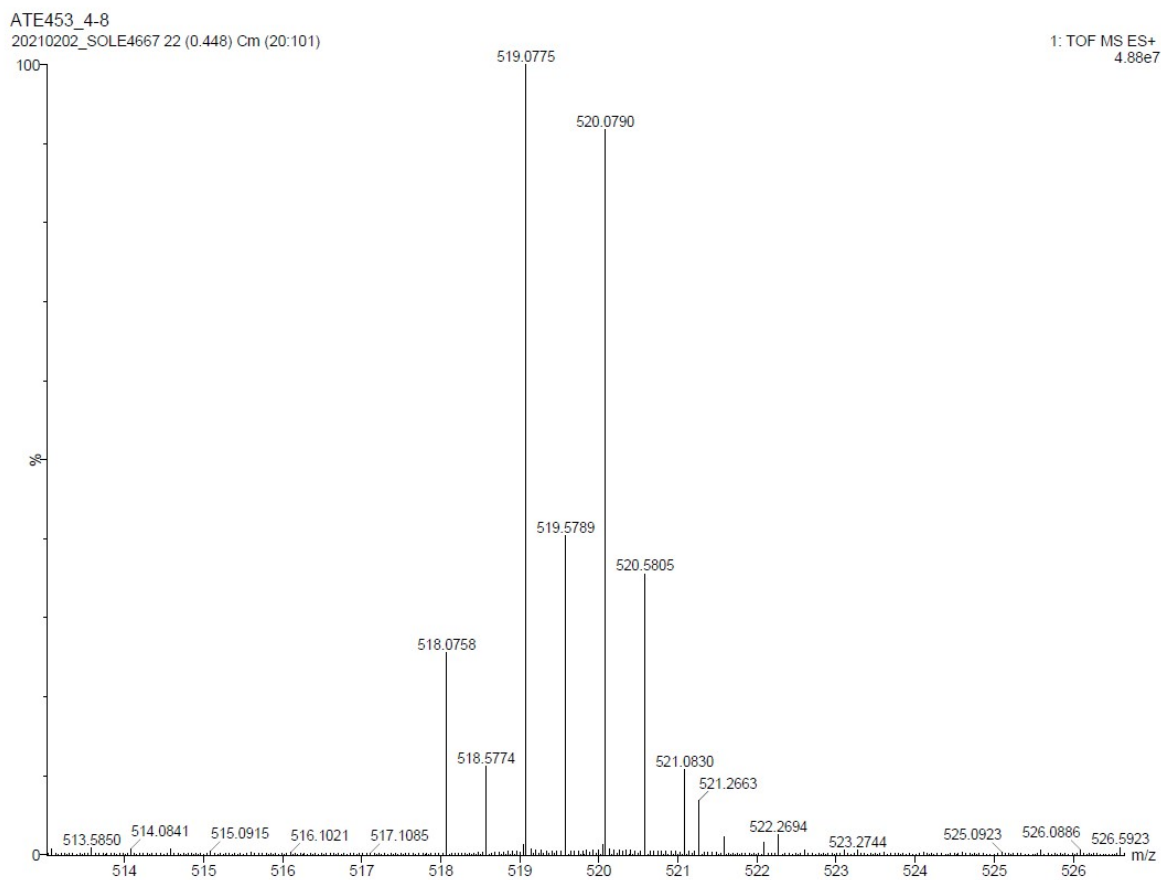


Figure S33. HRMS spectrum of **d1-[Re₂(**5a**)(CO)₆Cl₂]**

d₂-[Re₂(5a)(CO)₆Cl₂]

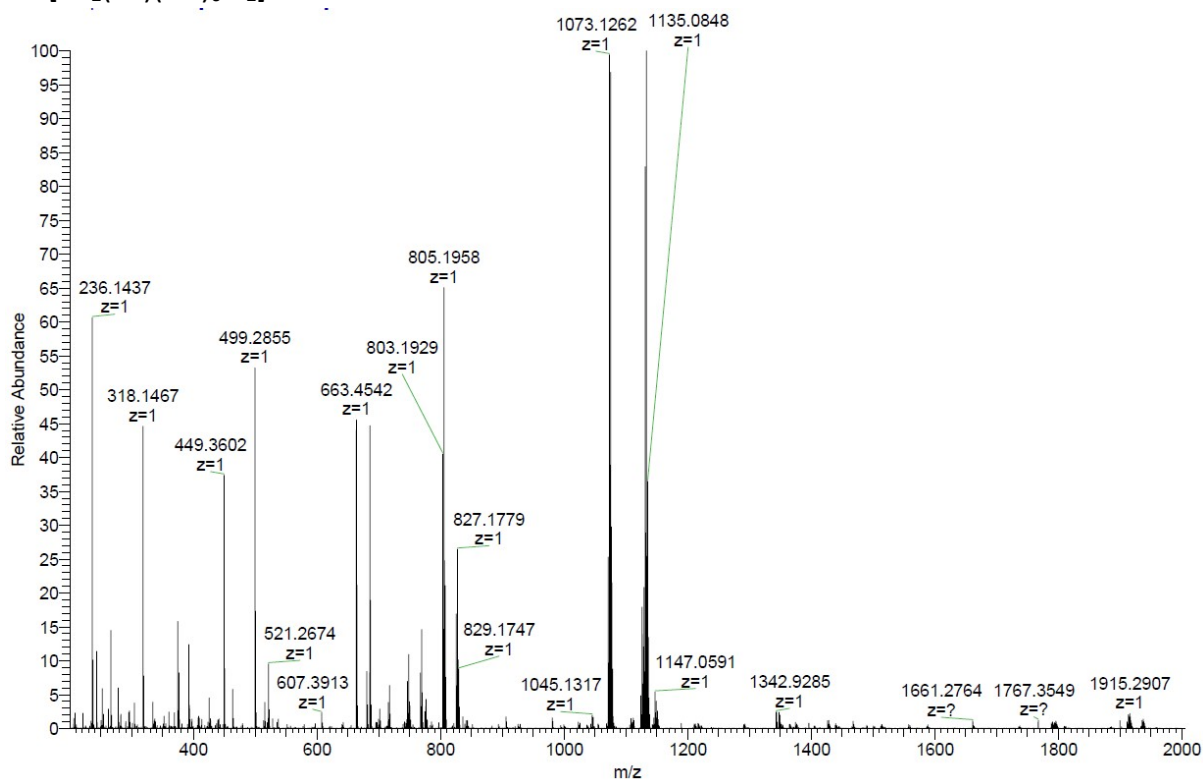


Figure S34. HRMS spectrum of d₂-[Re₂(5a)(CO)₆Cl₂]

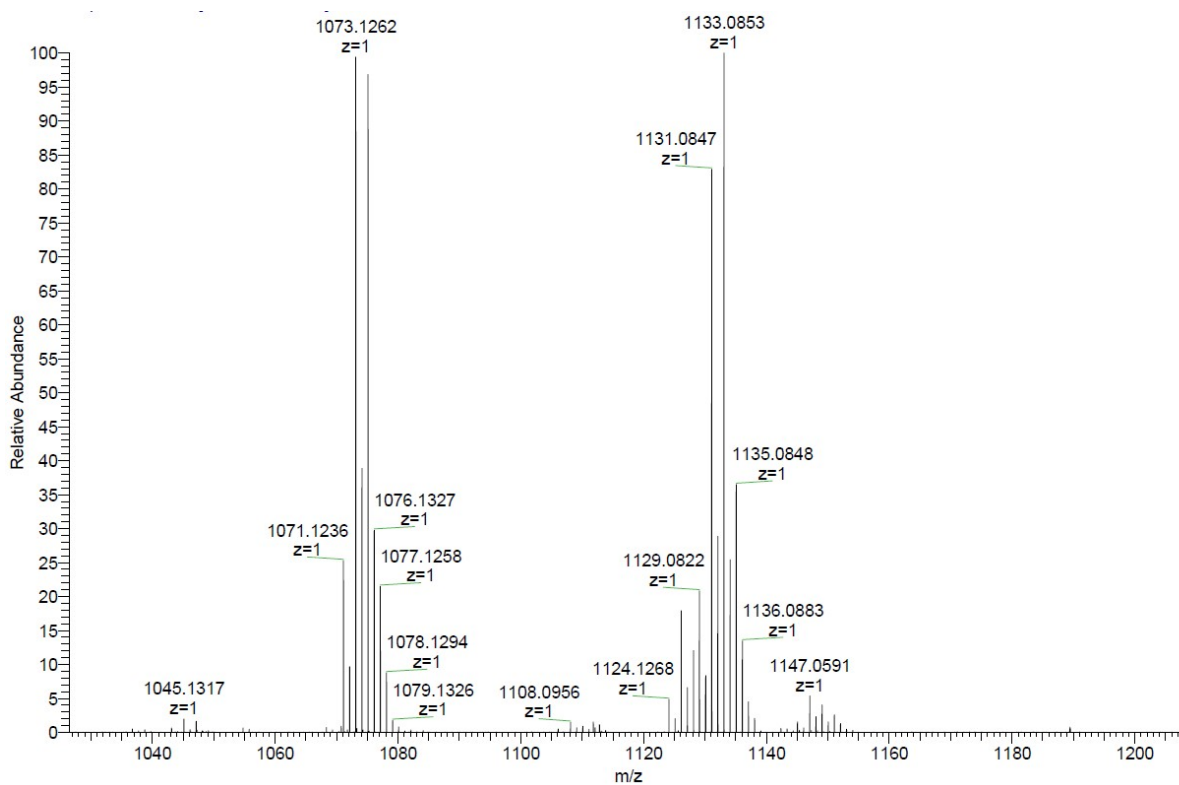


Figure S35. HRMS spectrum of d₂-[Re₂(5a)(CO)₆Cl₂]

d1-[Re₂(5b)(CO)₆Cl₂]

D:\Data\Service\Data\23_aQEx_0435

Client:

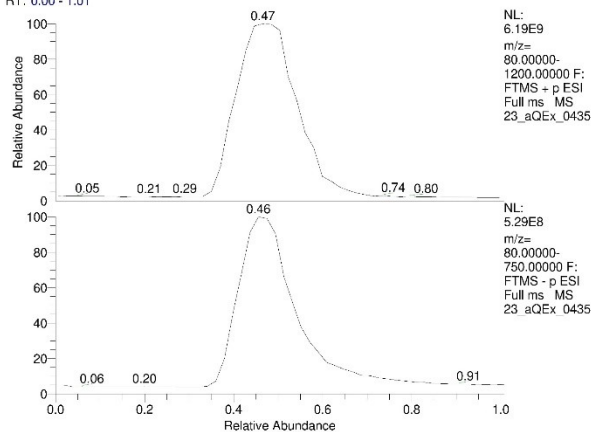
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(+)-HR-ESI-MS

Sample: ATE515-D1

Solvent: MeOH

RT: 0.00 - 1.01



23_aQEx_0435#41-47 RT: 0.41-0.47 AV: 4

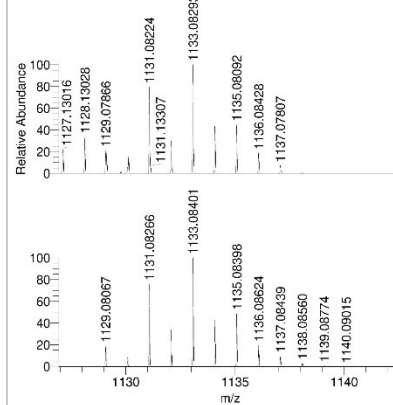
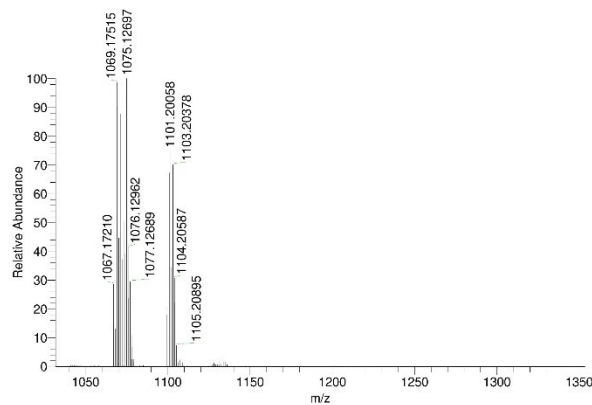
SB: 25 0.04-0.25 , 0.72-0.98

T: FTMS + p ESI Full lock ms [200.0000-3000.0000]

m/z= 1132.66628-1133.48258

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
1133.08305	158143/5.0	100.00	1133.08317	-0.10	20.0	C ₄₆ H ₃₄ O ₅ N ₄ Cl ₂ 37Cl ₂ Na ₂ Re ₂
			1133.08402	-0.85	29.5	C ₄₄ H ₃₂ O ₅ N ₄ Cl 37Cl ₂ Na ₂ Re ₂
			1133.08182	1.08	20.5	C ₃₈ H ₃₀ O ₅ N ₄ Cl ₂ 37Cl ₂ Na ₂ Re ₂
			1133.08134	1.51	25.0	C ₄₄ H ₃₄ O ₆ N ₃ Cl 37Cl ₂ Na ₂ Re ₂
			1133.08031	2.42	20.5	C ₄₁ H ₄₀ O ₅ N ₂ Cl ₂ 37Cl ₂ Na ₂ Re ₂
			1133.08585	-2.47	24.5	C ₄₃ H ₃₇ O ₅ N ₂ Cl ₂ 37Cl ₂ Na ₂ Re ₂
			1133.07982	2.85	25.0	C ₄₄ H ₃₇ O ₅ N ₃ Cl 37Cl ₂ Na ₂ Re ₂
			1133.08655	-3.08	25.5	C ₄₁ H ₃₄ O ₅ N ₄ 37Cl ₂ Na ₂ Re ₂
			1133.07881	3.75	29.0	C ₄₄ H ₃₂ O ₄ N ₃ Cl ₂ Na Re ₂
			1133.08736	-3.80	24.5	C ₄₀ H ₃₄ O ₆ N ₄ Cl ₂ Na Re ₂

23_aQEx_0435 #39-46 RT: 0.39-0.45 AV: 4 SB: 24 0.03-0.24 , 0.70-0.95 NL: 3.76E8
T: FTMS + p ESI Full lock ms [200.0000-3000.0000]



NL: 1.29E7
 23_aQEx_0435#39-45 RT:
 0.39-0.45 AV: 4 SB: 24
 0.03-0.24 , 0.70-0.95 T: FTMS +
 p ESI Full lock ms
 [200.0000-3000.0000]

NL: 6.33E3
 C₄₆H₃₄Cl₂N₄O₅Re₂Na:
 C₄₀H₃₄Cl₂N₄O₆Re₂Na₁
 p (gss, s /p:40) Chrg 1
 R: 35000 Res .Pwr . @FWHM

Figure S36. HRMS spectrum of d1-[Re₂(5b)(CO)₆Cl₂]

d2-[Re₂(5b)(CO)₆Cl₂]

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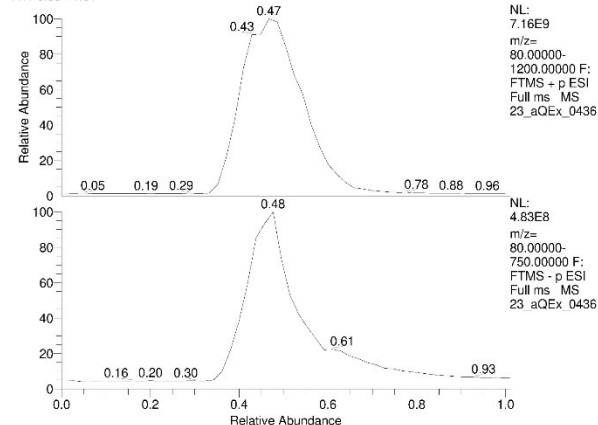
03/15/23 20:03:52

(+)-HR-ESI-MS

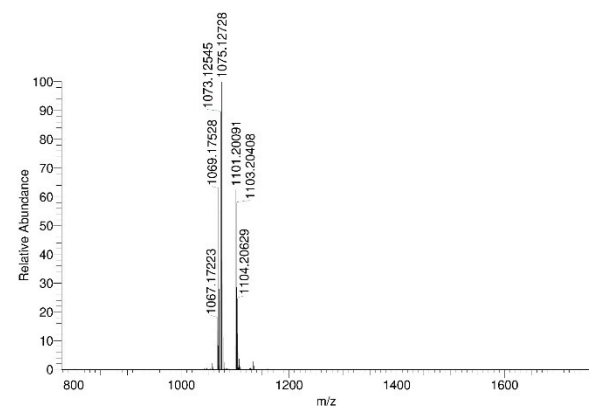
Sample: ATE515-D2

Solvent: MeOH

RT: 0.00 - 1.01



23_aQEx_0436 #41-47 RT: 0.41-0.47 AV: 4 SB: 24 0.03-0.24 , 0.70-0.95 NL: 6.92E8
 T: FTMS + p ESI Full lock ms [200.0000-3000.0000]



m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
1133.08339	19398146.0	100.00	1133.08317	0.20	20.0	C ₄₆ H ₃₄ O ₆ N ₄ Cl ₂ Re ₂
			1133.08402	-0.55	29.5	C ₄₄ H ₃₂ O ₆ N ₄ Cl
			1133.08182	1.39	20.5	C ₃₈ H ₃₇ O ₆ N ₄ Cl ₂ Re ₂
			1133.08134	1.82	25.0	C ₄₁ H ₃₄ O ₆ N ₃ Cl
			1133.08585	-2.16	24.5	C ₄₃ H ₃₇ O ₆ N ₂ Cl ₂ Re ₂
			1133.08031	2.72	20.5	C ₄₁ H ₄₀ O ₂ N ₂ Cl ₂ Re ₂
			1133.08655	-2.78	25.5	C ₄₁ H ₃₄ O ₆ N ₄
			1133.07982	3.15	25.0	C ₄₄ H ₃₇ O ₆ N ₃ Cl
			1133.08736	-3.50	24.5	C ₄₀ H ₃₄ O ₆ N ₄ Cl ₂ Na Re ₂
			1133.08789	-3.97	25.0	C ₄₂ H ₃₈ O ₆ N ₃ Cl ₂ Na Re ₂

m/z	Relative Abundance
1128.13091	~10
1129.13316	~10
1131.08254	~100
1131.13491	~10
1133.08320	~100
1135.08307	~10
1136.08556	~10
1137.08173	~10

m/z	Relative Abundance
1129.08067	~10
1131.08266	~100
1133.08401	~100
1135.08398	~10
1136.08624	~10
1137.08439	~10
1138.08560	~10
1139.08774	~10
1140.09015	~10

NL: 6.33E3
 C₄₆H₃₄Cl₂N₄O₆Re₂Na:
 C₄₆H₃₄Cl₂N₄O₆Re₂Na₁
 p (gss, s /p:40) Chrg 1
 R: 35000 Res .Pwr .@FWHM

Figure S37. HRMS spectrum of d2-[Re₂(5b)(CO)₆Cl₂]

d1-[Re₂(6a)(CO)₆Cl₂]

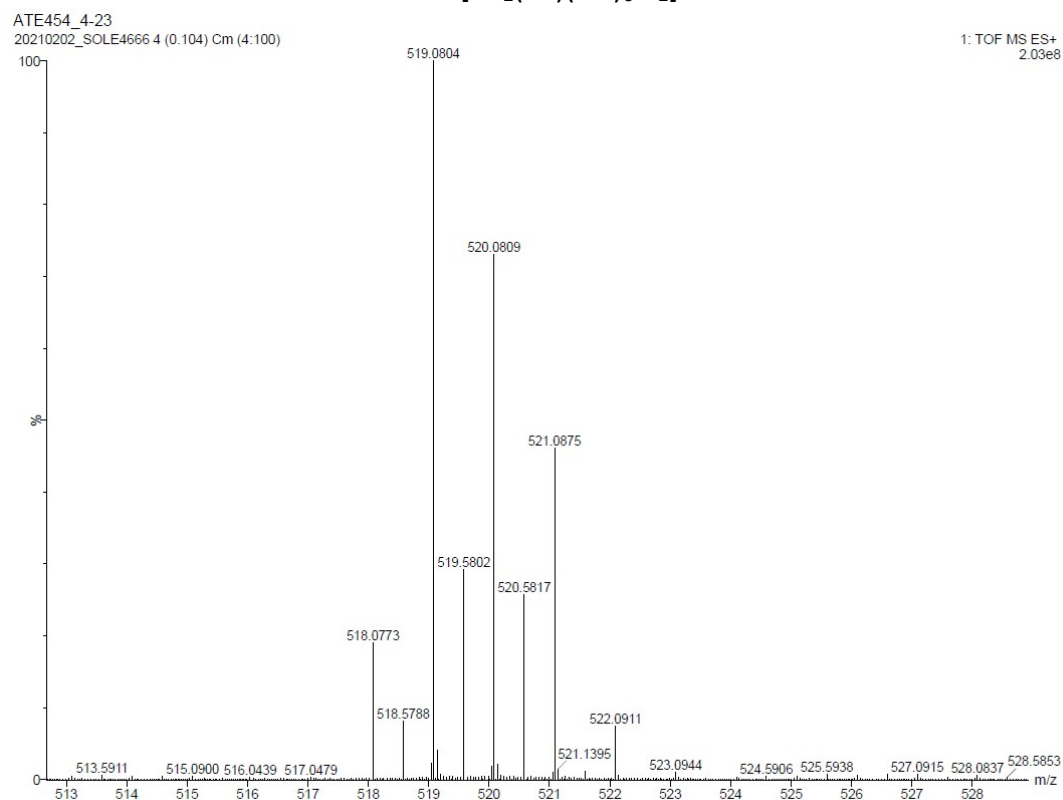


Figure S38. HRMS spectrum of d1-[Re₂(6a)(CO)₆Cl₂]

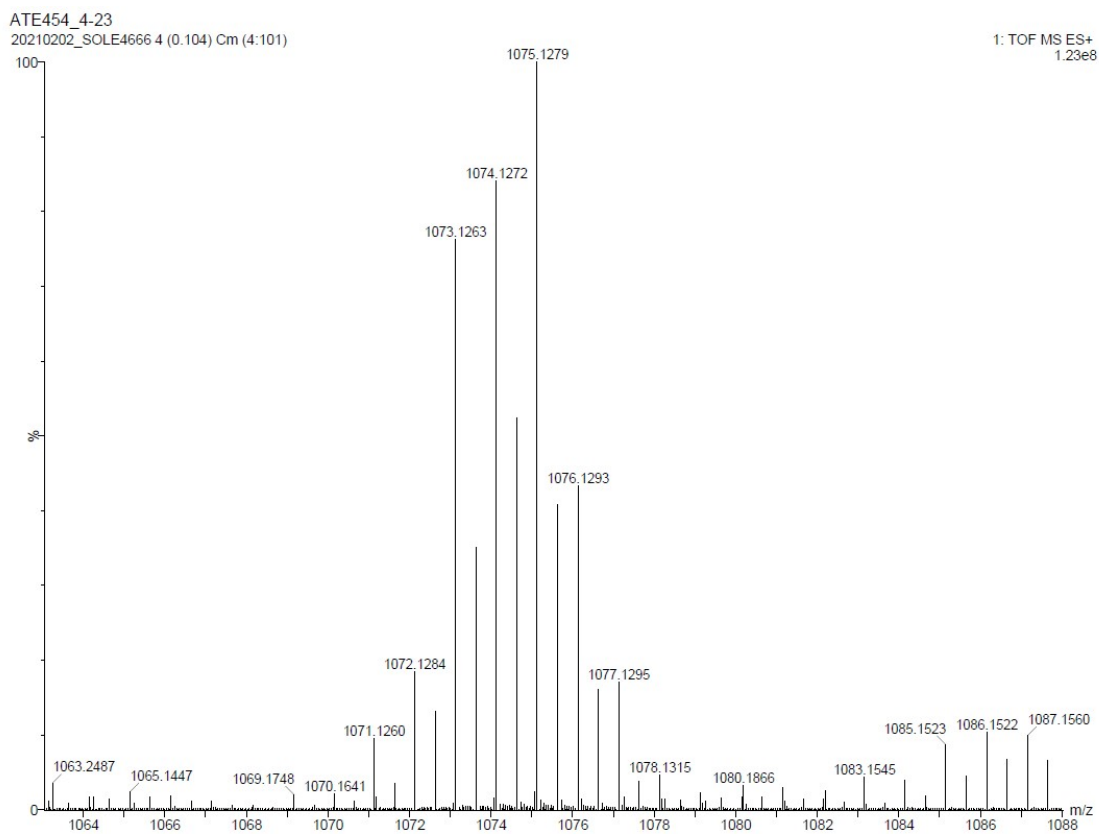


Figure S39. HRMS spectrum of d1-[Re₂(6a)(CO)₆Cl₂]

d2-[Re₂(6a)(CO)₆Cl₂]

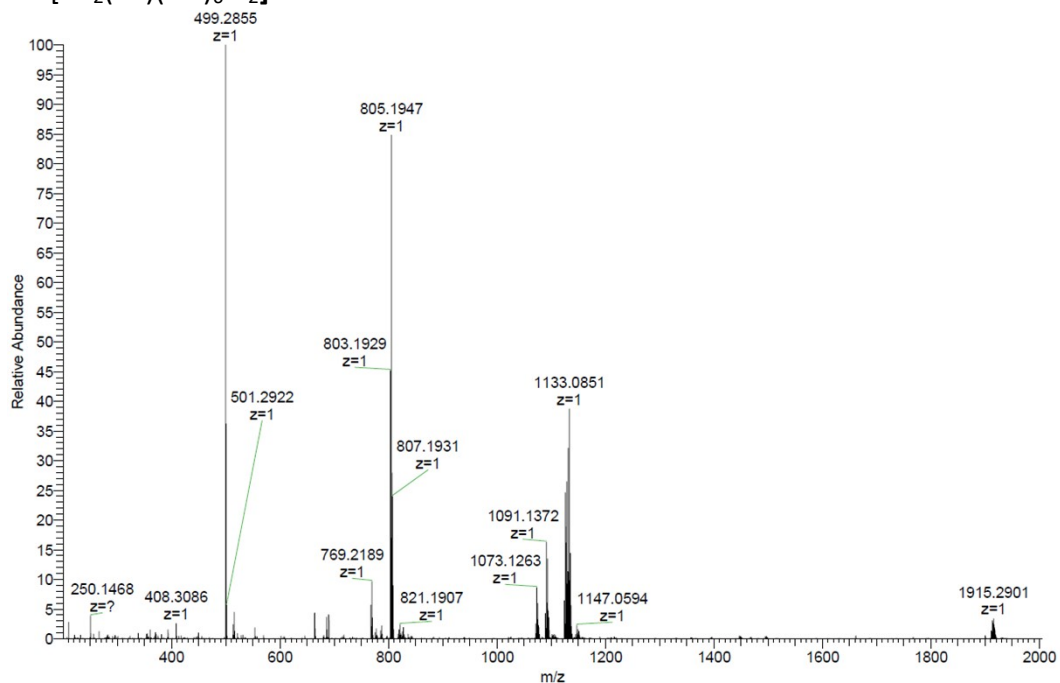


Figure S40. HRMS spectrum of d2-[Re₂(6a)(CO)₆Cl₂]

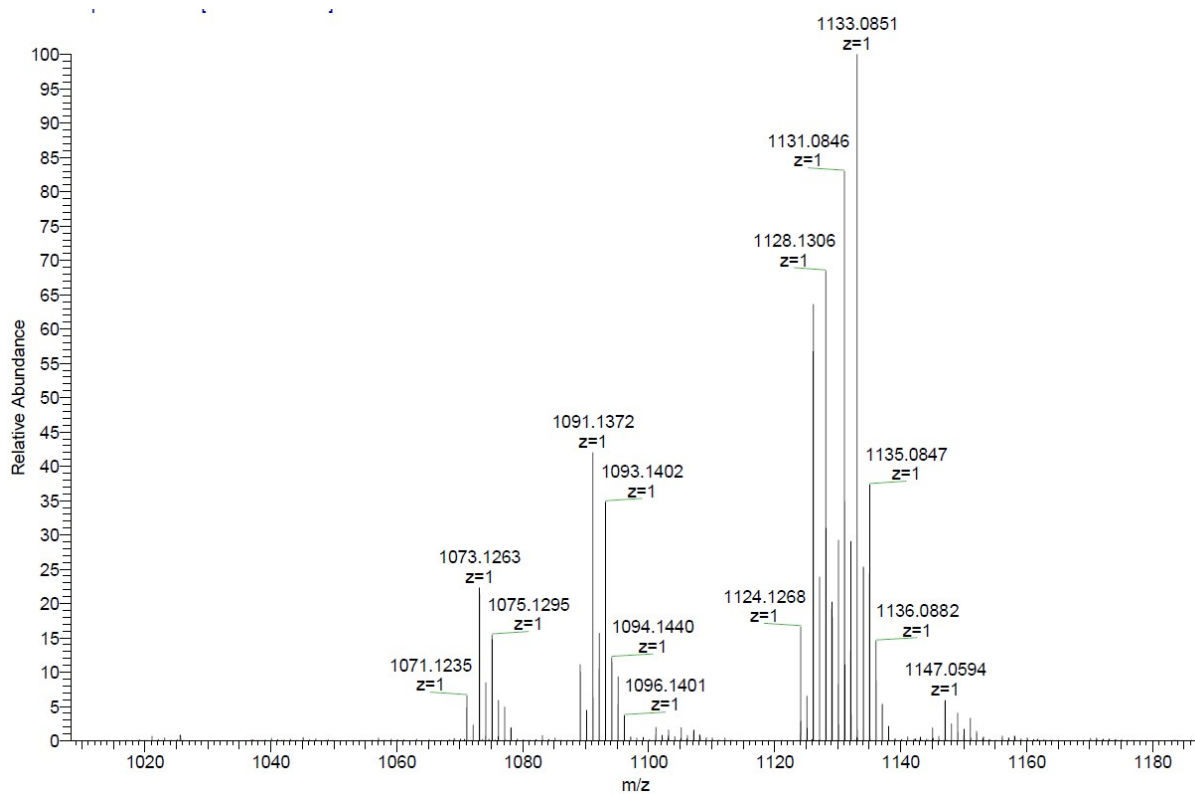


Figure S41. HRMS spectrum of d2-[Re₂(6a)(CO)₆Cl₂]

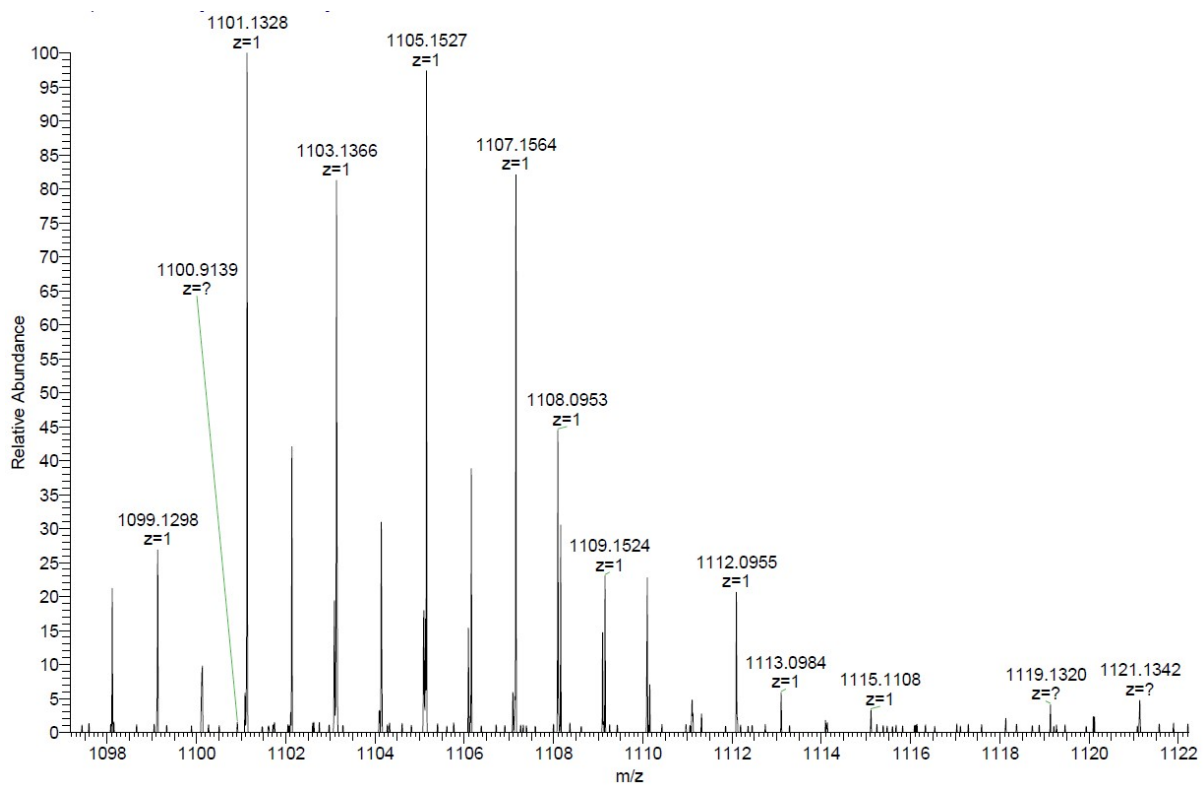


Figure S42. HRMS spectrum of d_2 -[$Re_2(6a)(CO)_6Cl_2$]

d1-[Re₂(6b)(CO)₆Cl₂]

D:\Data\Service\Data\23_aQEx_0437

Client:

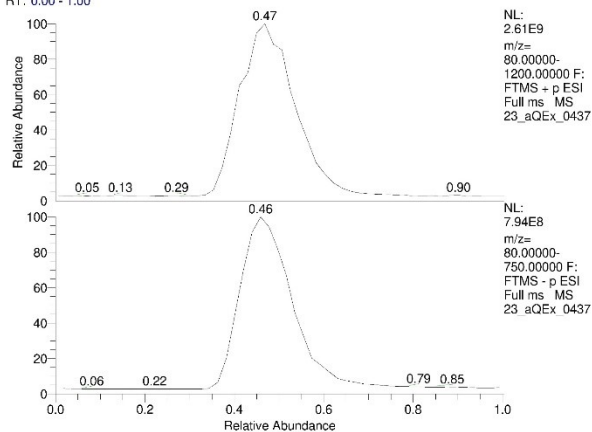
03/15/23 20:05:53

(+)-HR-ESI-MS

Sample: ATE516-D1

Solvent: MeOH

RT: 0.00 - 1.00



m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
1133.08394	1861129.4	100.00	1133.08402	-0.07	29.5	C ₄₄ H ₃₂ O ₃ N ₄ Cl ₁ ³⁷ Cl Na Re ₁
			1133.08374	0.17	28.0	C ₄₃ H ₃₃ O ₆ N ₅ Cl ₁ ³⁷ Cl Re ₂
			1133.08423	-0.26	23.5	C ₄₃ H ₃₆ O ₅ N ₄ Cl ₂ ³⁷ Cl Re ₂
			1133.08317	0.68	20.0	C ₄₃ H ₃₉ O ₆ N ₄ Cl ₂ ³⁷ Cl Na Re ₂
			1133.08271	1.08	23.5	C ₄₃ H ₃₉ O ₇ N ₂ Cl ₂ ³⁷ Cl ₂ Re ₂
			1133.08557	-1.44	23.0	C ₄₃ H ₃₈ O ₆ N ₄ Cl ₂ ³⁷ Cl Re ₂
			1133.08585	-1.68	24.5	C ₄₃ H ₃₇ O ₃ N ₂ Cl ₂ ³⁷ Cl Na Re ₂
			1133.08182	1.87	20.5	C ₃₈ H ₃₇ O ₅ N ₄ Cl ₂ ³⁷ Cl Na Re ₂
			1133.08134	2.30	25.0	C ₄₁ H ₃₄ O ₆ N ₃ Cl ₁ ³⁷ Cl Na Re ₂
			1133.08655	-2.30	25.5	C ₄₁ H ₃₅ O ₅ N ₄ ³⁷ Cl ₂ Na Re ₂
			1133.08088	2.70	28.5	C ₄₄ H ₃₄ O ₂ N ₄ Cl ₁ ³⁷ Cl ₂ Re ₂
			1133.08736	-3.02	24.5	C ₄₃ H ₃₄ O ₆ N ₄ Cl ₂ Na

23_aQEx_0437 #39-46 RT: 0.39-0.45 AV: 4 SB: 24 0.03-0.24 , 0.70-0.95 NL: 6.48E7
 T: FTMS + p ESI Full lock ms [200.0000-3000.0000]

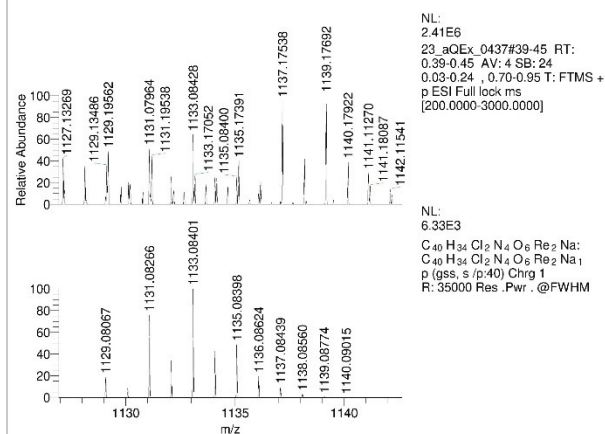
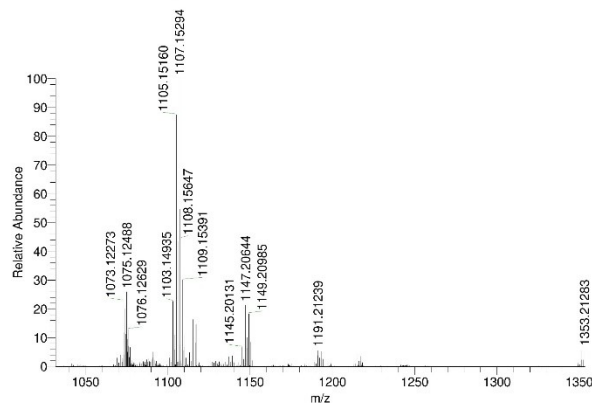


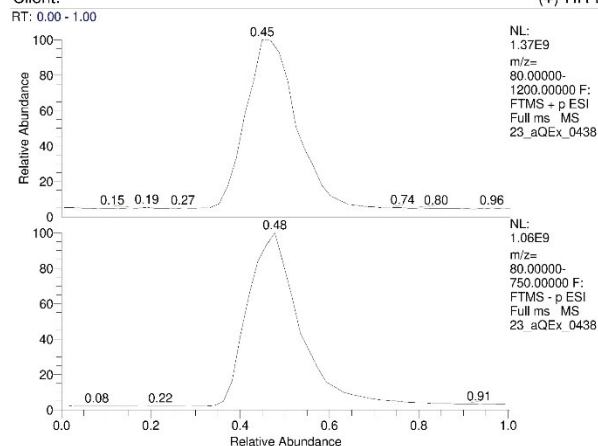
Figure S43. HRMS spectrum of d1-[Re₂(6b)(CO)₆Cl₂]

d2-[Re₂(6b)(CO)₆Cl₂]

D:\Data\Service\Data\23_aQEx_0438
Client:

03/15/23 20:07:51
(+)-HR-ESI-MS

Sample: ATE516-D2
Solvent: MeOH



23_aQEx_0438#41-53 RT: 0.41-0.53 AV: 7
SB: 25 0.04-0.25 , 0.72-0.98
T: FTMS - p ESI Full lock ms [200.0000-3000.0000]
m/z= 1132.62989-1133.34803

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
1133.08367	1842539.5	100.00	1133.08304	0.55	21.0	C ₄₅ H ₃₆ O ₄ NCl ₃ Re ₂
			1133.08170	1.74	27.5	C ₄₅ H ₃₄ O ₃ N ₂ Cl ₃ Re ₂
			1133.08064	2.67	24.0	C ₄₅ H ₃₇ O ₄ NCl ₃ Na Re ₂
			1133.08736	-3.26	24.5	C ₄₅ H ₃₄ O ₆ N ₄ Cl ₂ Na Re ₂
			1133.07929	3.86	24.5	C ₄₅ H ₃₅ O ₃ N ₄ Cl ₃ Na Re ₂

23_aQEx_0438 #40-54 RT: 0.41-0.53 AV: 7 SB: 24 0.03-0.24 , 0.70-0.95 NL: 5.24E7
T: FTMS + p ESI Full lock ms [200.0000-3000.0000]

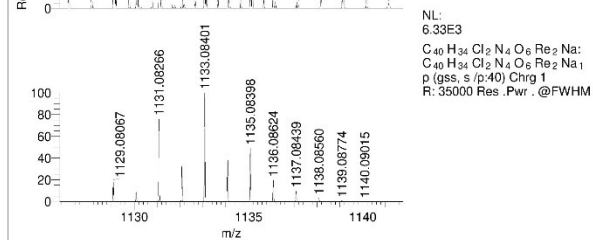
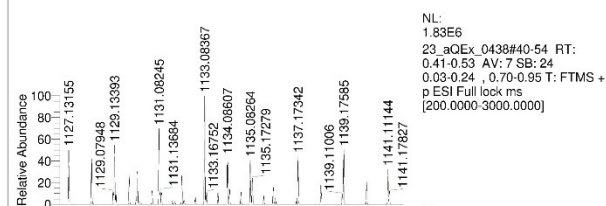
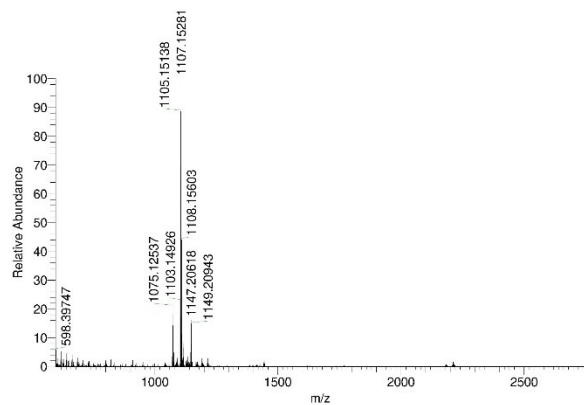


Figure S44. HRMS spectrum of d2-[Re₂(6b)(CO)₆Cl₂]

IR spectra

d1-[Re₂(5a)(CO)₆Cl₂]

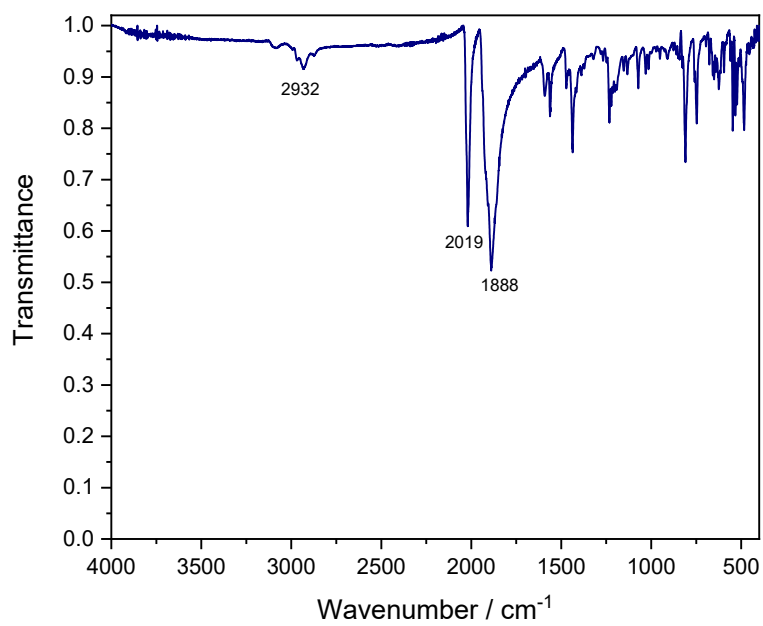


Figure S45. IR spectrum of d1-[Re₂(5a)(CO)₆Cl₂]

d2-[Re₂(5a)(CO)₆Cl₂]

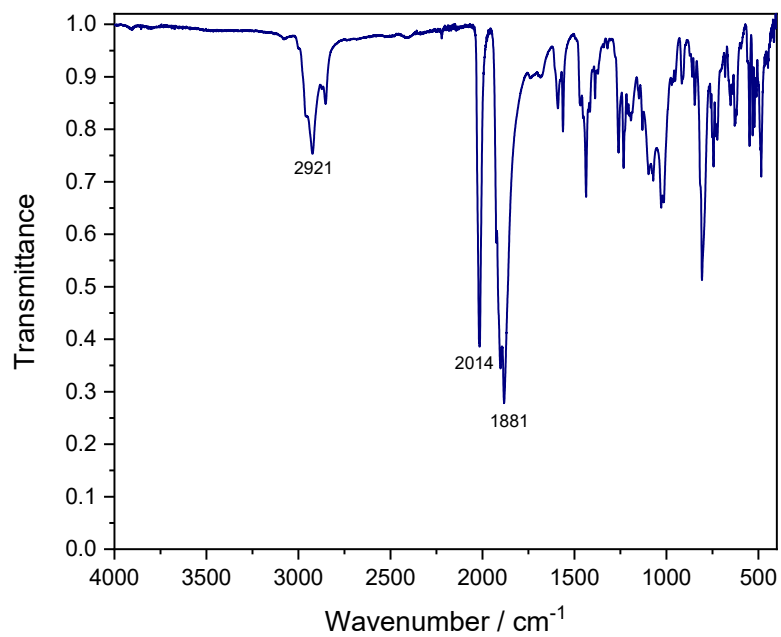


Figure S46. IR spectrum of d2-[Re₂(5a)(CO)₆Cl₂]

d1-[Re₂(**5b**)(CO)₆Cl₂]

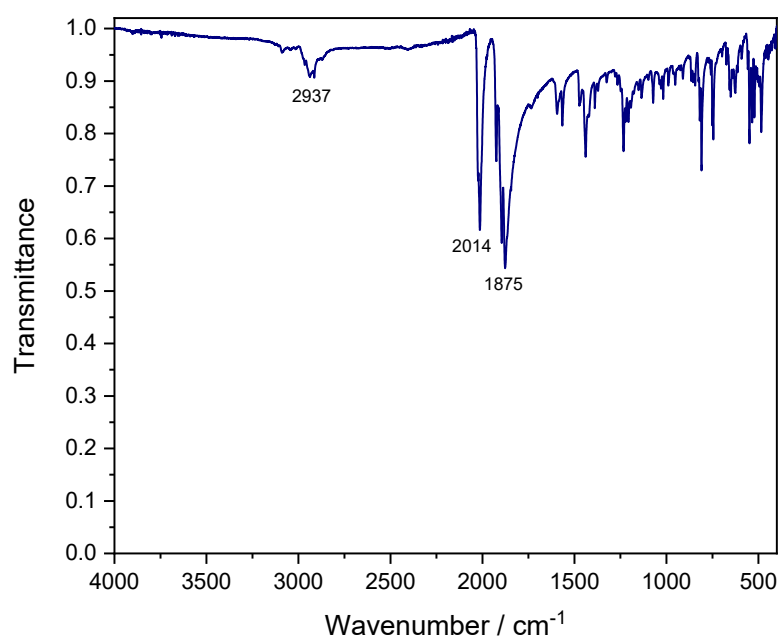


Figure S47. IR spectrum of d1-[Re₂(**5b**)(CO)₆Cl₂]

d2-[Re₂(**5b**)(CO)₆Cl₂]

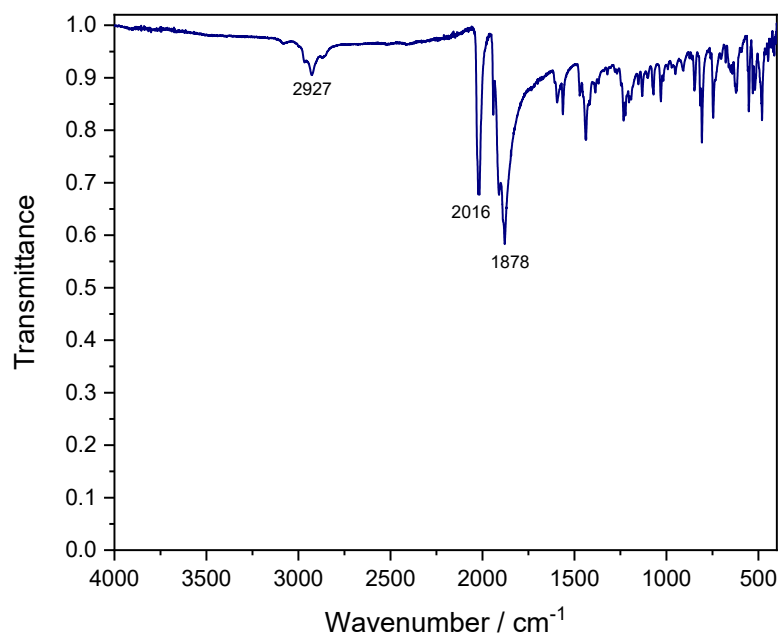


Figure S48. IR spectrum of d2-[Re₂(**5b**)(CO)₆Cl₂]

d1-[Re₂(**6a**)(CO)₆Cl₂]

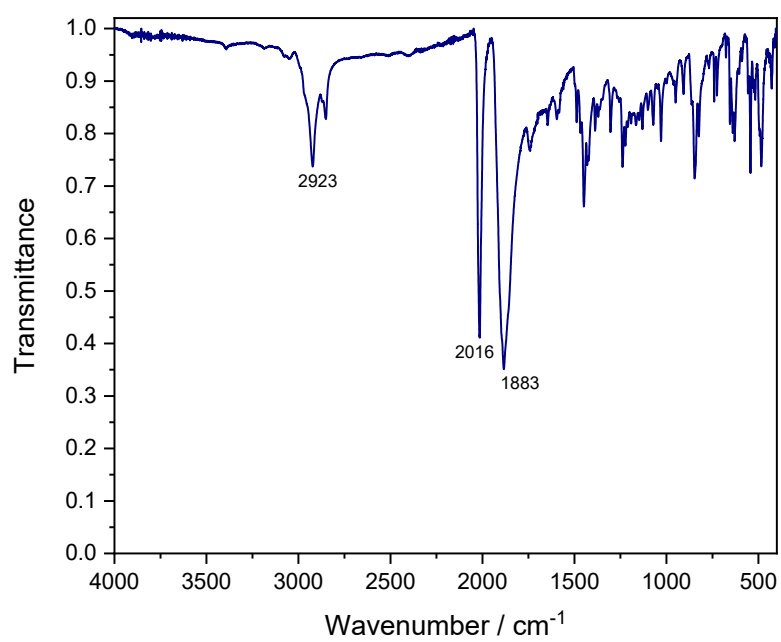


Figure S49. IR spectrum of d1-[Re₂(**6a**)(CO)₆Cl₂]

d2-[Re₂(**6a**)(CO)₆Cl₂]

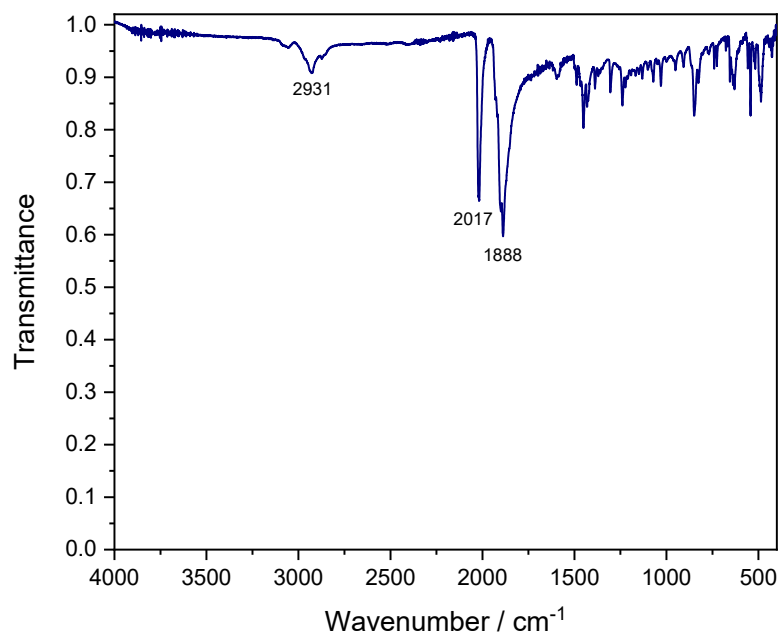


Figure S50. IR spectrum of d2-[Re₂(**6a**)(CO)₆Cl₂]

d1-[Re₂(**6b**)(CO)₆Cl₂]

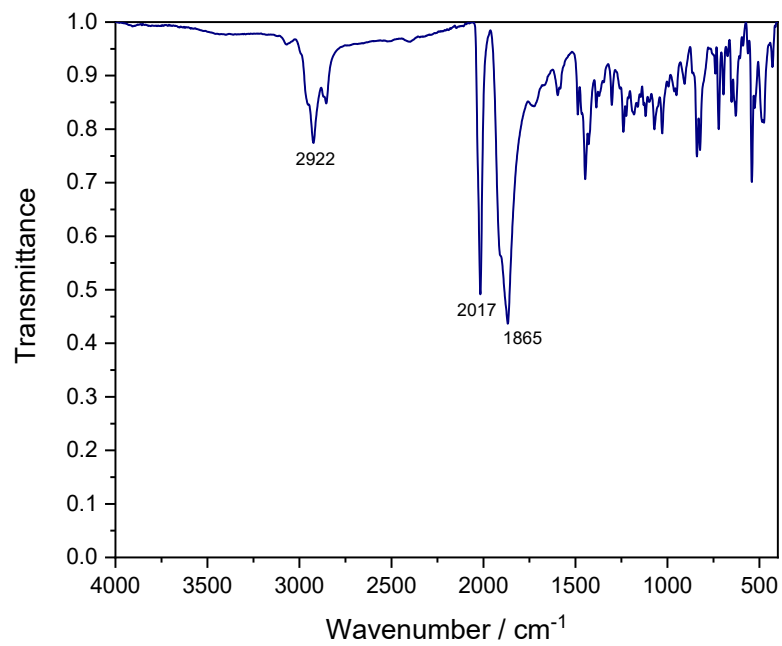


Figure S51. IR spectrum of d1-[Re₂(**6b**)(CO)₆Cl₂]

d2-[Re₂(**6b**)(CO)₆Cl₂]

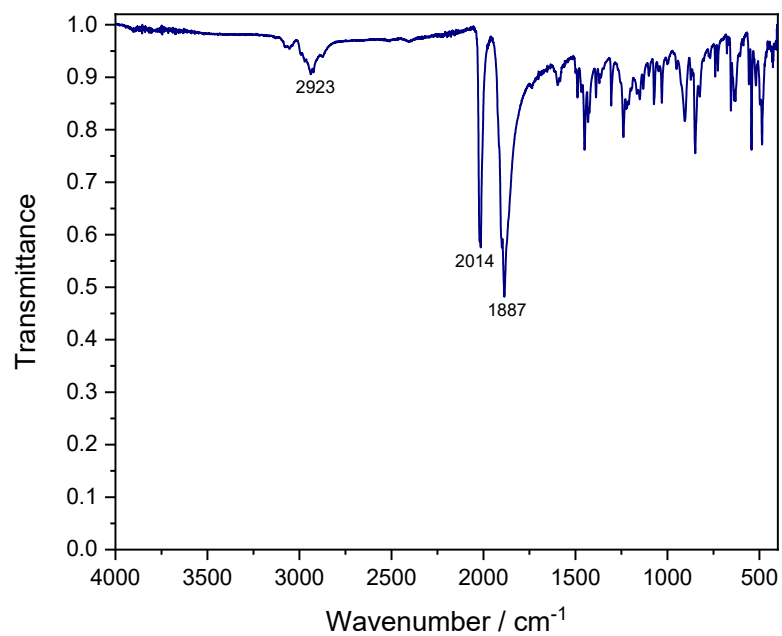


Figure S52. IR spectrum of d2-[Re₂(**6b**)(CO)₆Cl₂]

CD spectra

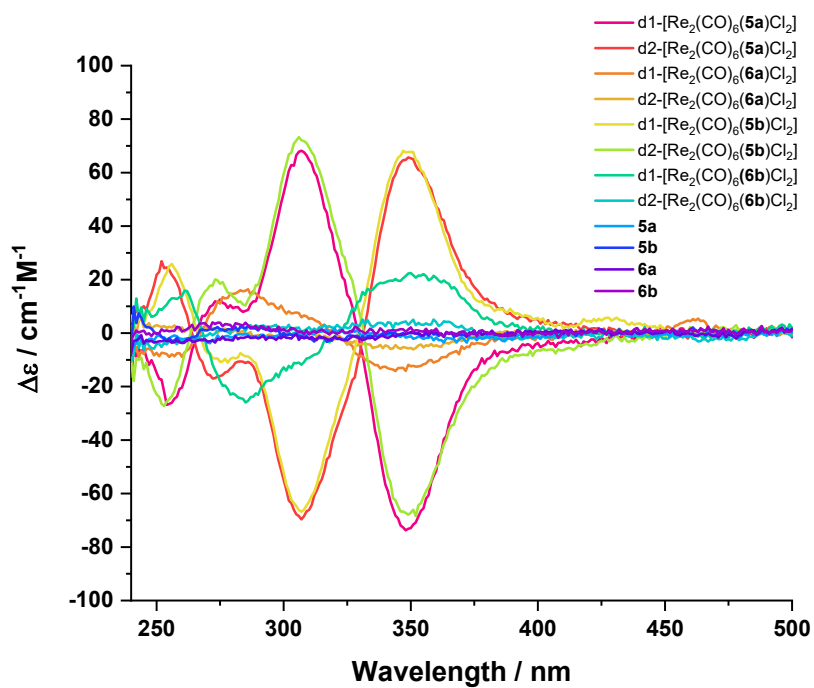


Figure S53. CD spectra of the ligands and different stereoisomers (0.005 mM in CHCl₃)

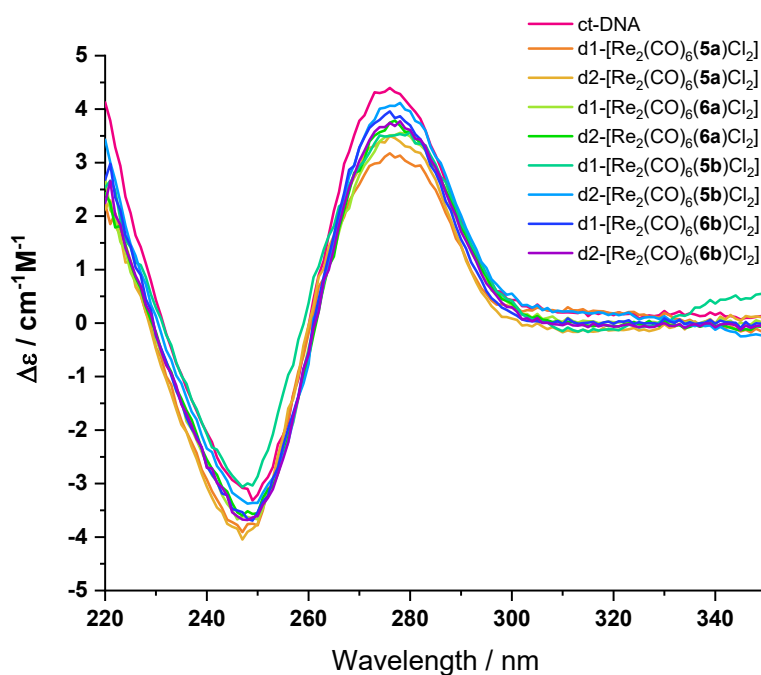


Figure S54. CD spectra of calf thymus DNA (100 μM) in the presence of different diastereomers (5 μM) in H₂O

Photophysical characterisation

d1-[Re₂(**5a**)(CO)₆Cl₂]

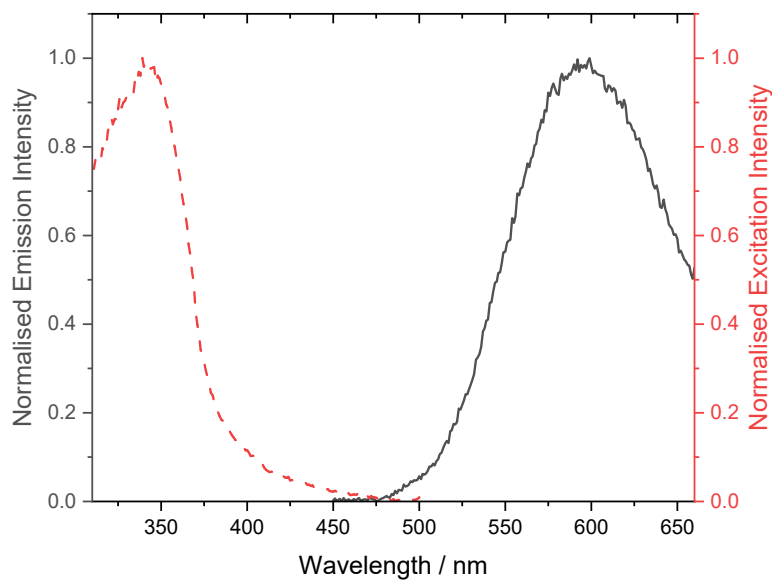


Figure S55. Emission (dark grey) and excitation spectra (red, dashed) of d1-[Re₂(**5a**)(CO)₆Cl₂] in CH₂Cl₂, c = 0.0025 mM, λ_{ex} = 342 nm

d2-[Re₂(**5a**)(CO)₆Cl₂]

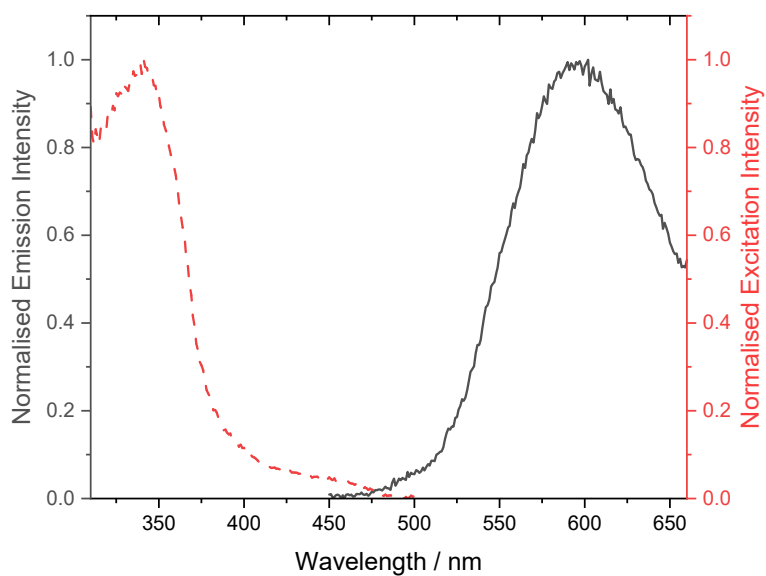


Figure S56. Emission (dark grey) and excitation spectra (red, dashed) of d2-[Re₂(**5a**)(CO)₆Cl₂] in CH₂Cl₂, c = 0.0025 mM, λ_{ex} = 342 nm

d1-[Re₂(**6a**)(CO)₆Cl₂]

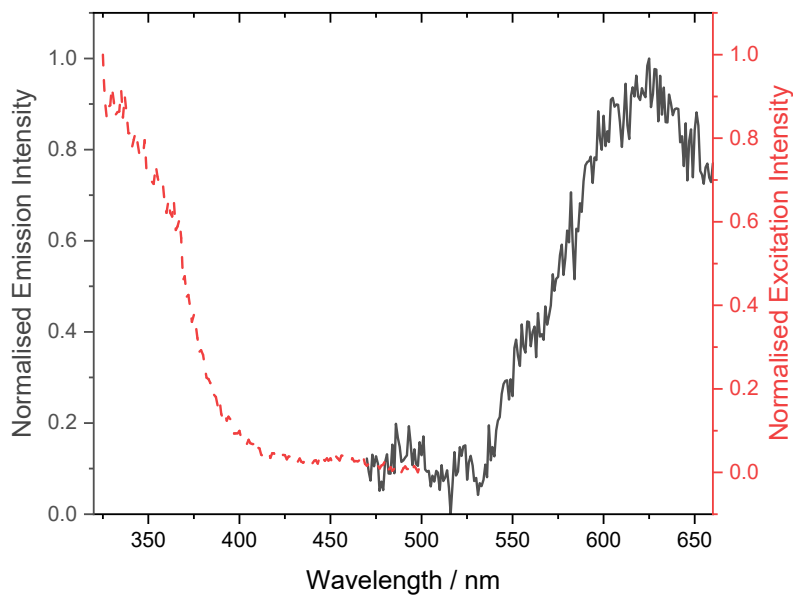


Figure S57. Emission (dark grey) and excitation spectra (red, dashed) of d1-[Re₂(**6a**)(CO)₆Cl₂] in CH₂Cl₂, c = 0.0025 mM, λ_{ex} = 350 nm

d2-[Re₂(**6a**)(CO)₆Cl₂]

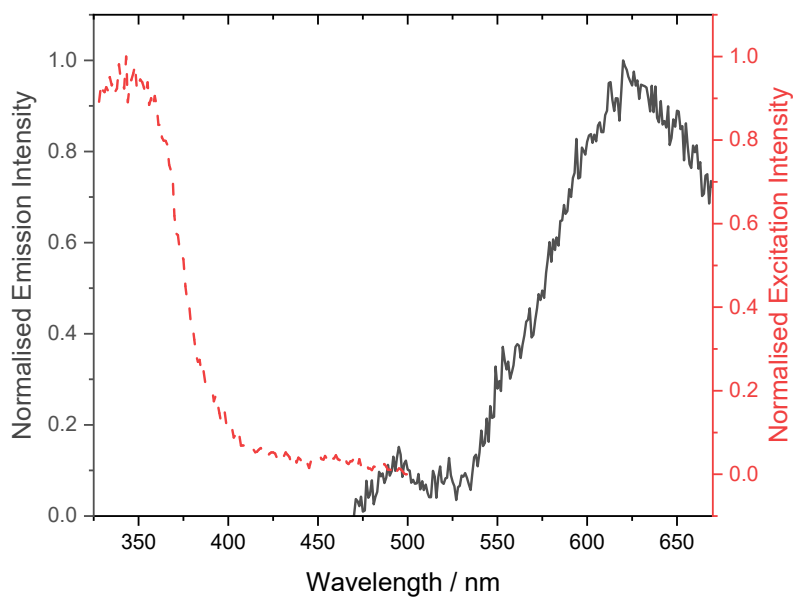


Figure S58. Emission (dark grey) and excitation spectra (red, dashed) of d2-[Re₂(**6a**)(CO)₆Cl₂] in CH₂Cl₂, c = 0.0025 mM, λ_{ex} = 350 nm

d1-[Re₂(**5b**)(CO)₆Cl₂]

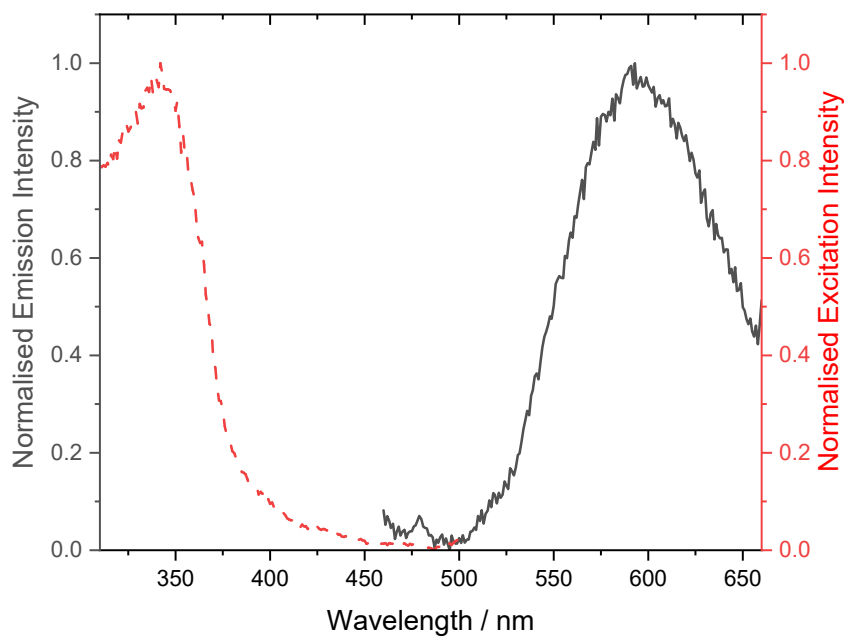


Figure S59. Emission (dark grey) and excitation spectra (red, dashed) of d1-[Re₂(**5b**)(CO)₆Cl₂] in CH₂Cl₂, c = 0.0025 mM, λ_{ex} = 342 nm

d2-[Re₂(**5b**)(CO)₆Cl₂]

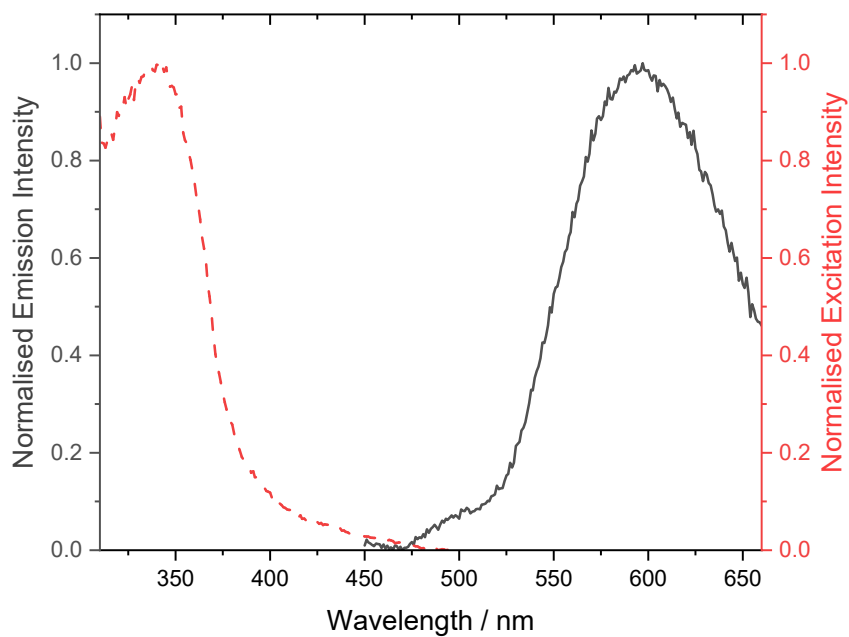


Figure S60. Emission (dark grey) and excitation spectra (red, dashed) of d2-[Re₂(**5b**)(CO)₆Cl₂] in CH₂Cl₂, c = 0.0025 mM, λ_{ex} = 342 nm

d1-[Re₂(**6b**)(CO)₆Cl₂]

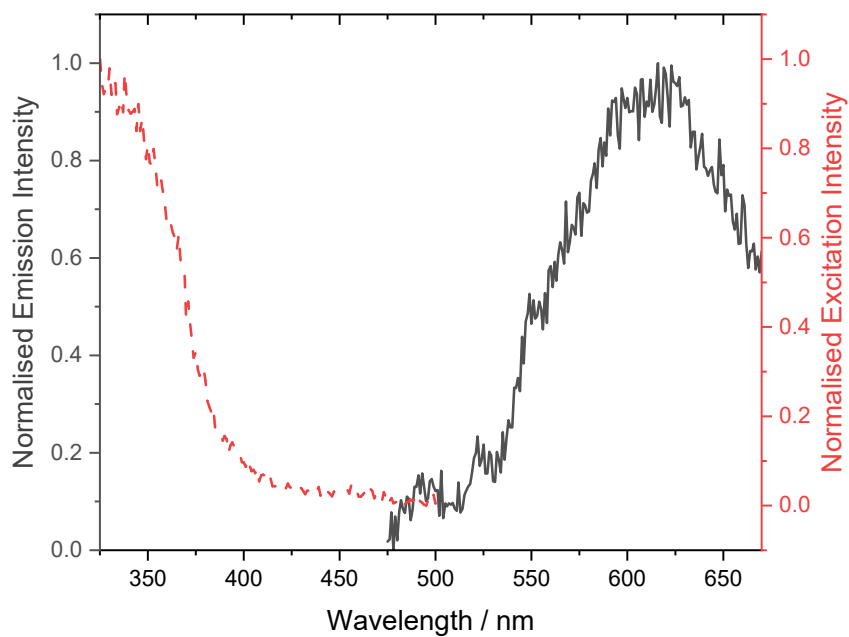


Figure S61. Emission (dark grey) and excitation spectra (red, dashed) of d1-[Re₂(**6b**)(CO)₆Cl₂] in CH₂Cl₂, c = 0.0025 mM, λ_{ex} = 350 nm

d2-[Re₂(**6b**)(CO)₆Cl₂]

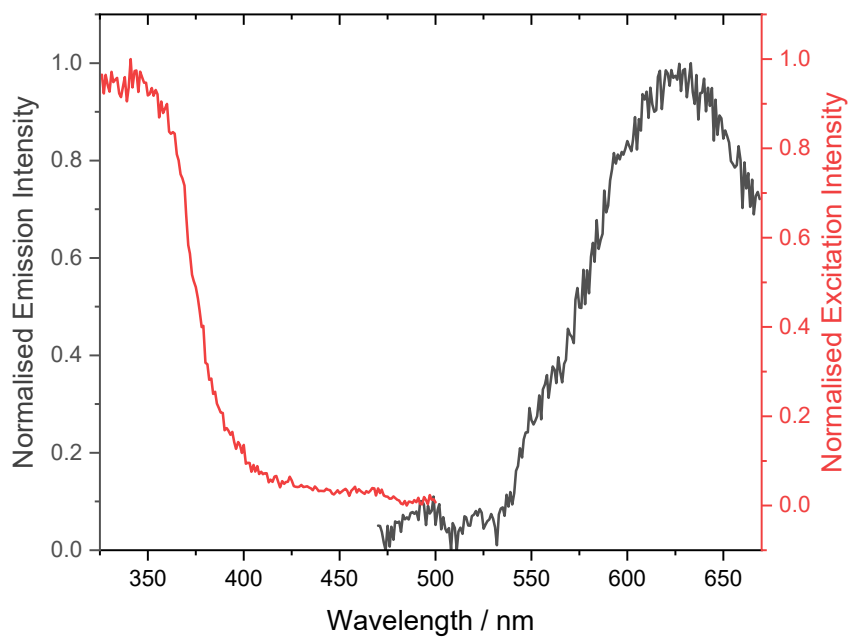


Figure S62. Emission (dark grey) and excitation spectra (red, dashed) of d2-[Re₂(**6b**)(CO)₆Cl₂] in CH₂Cl₂, c = 0.0025 mM, λ_{ex} = 350 nm

Table S1. Quantum yield values for the complexes, in CH₂Cl₂

Compound	QY (%)
d1-[Re ₂ (5a)(CO) ₆ Cl ₂]	3.7
d2-[Re ₂ (5a)(CO) ₆ Cl ₂]	5.4
d1-[Re ₂ (6a)(CO) ₆ Cl ₂]	0.6
d2-[Re ₂ (6a)(CO) ₆ Cl ₂]	0.6
d1-[Re ₂ (5b)(CO) ₆ Cl ₂]	3.2
d2-[Re ₂ (5b)(CO) ₆ Cl ₂]	5.2
d1-[Re ₂ (6b)(CO) ₆ Cl ₂]	0.6
d2-[Re ₂ (6b)(CO) ₆ Cl ₂]	0.6

Docking calculations

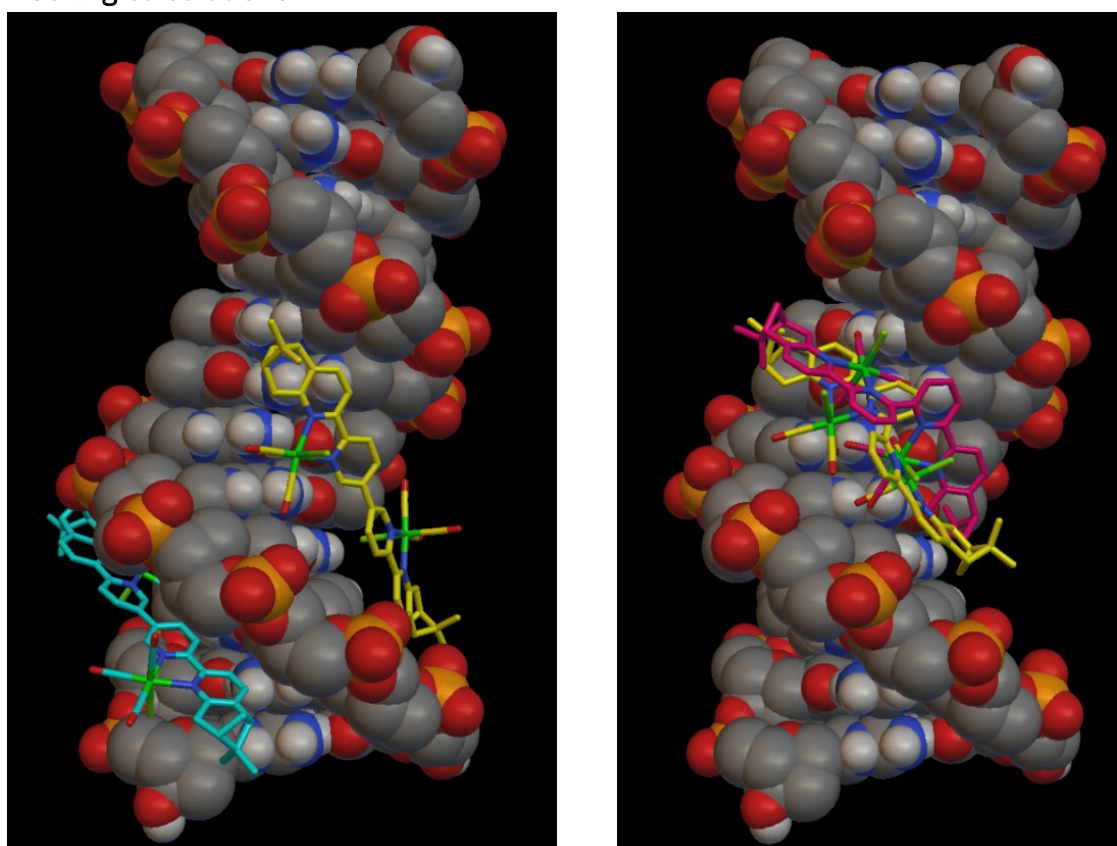


Figure S63. Lowest calculated energy poses of d1- and d2-[Re₂(**6a**)(CO)₆Cl₂] (left) and d1- and d2-[Re₂(**5a**)(CO)₆Cl₂] with double stranded (d(CpGpCpGpApApTpTpCpGpCpG) dodecamer.

Biological data

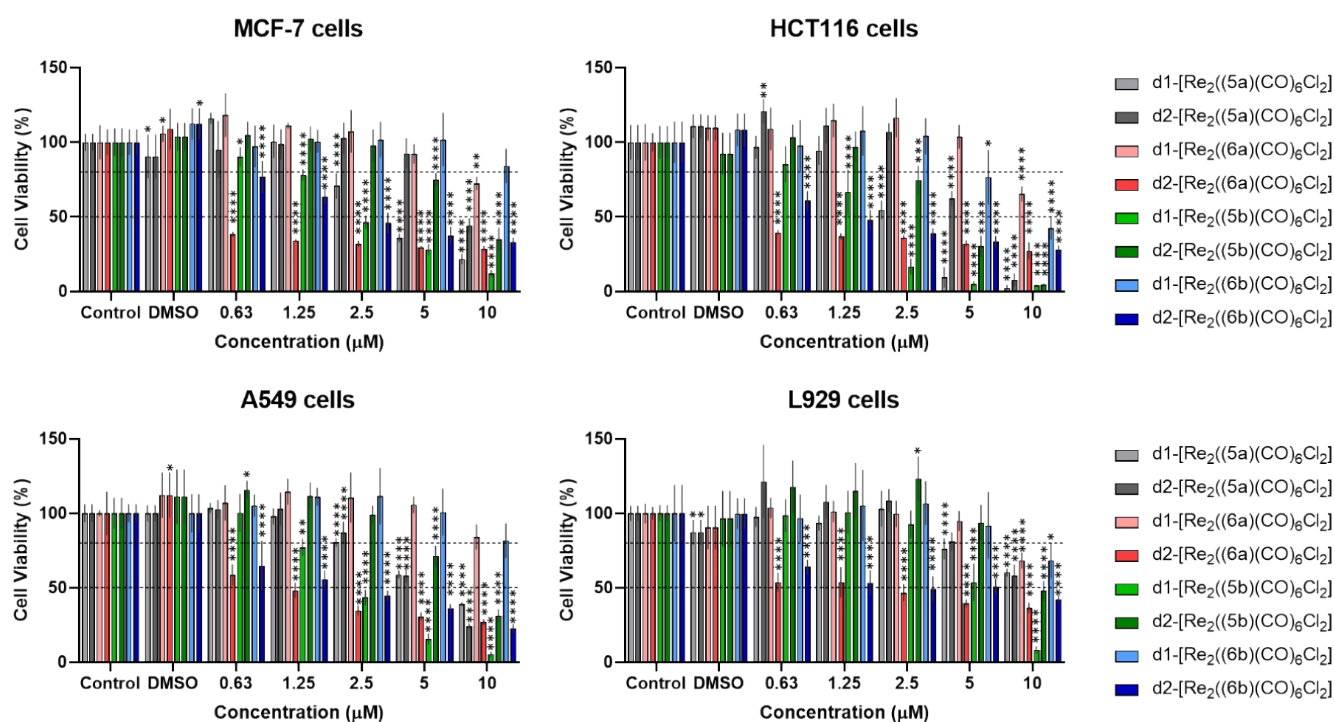


Figure S64. Cytotoxicity graphs of the complexes on MCF-7, HCT116, A549 and L929 cells.

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

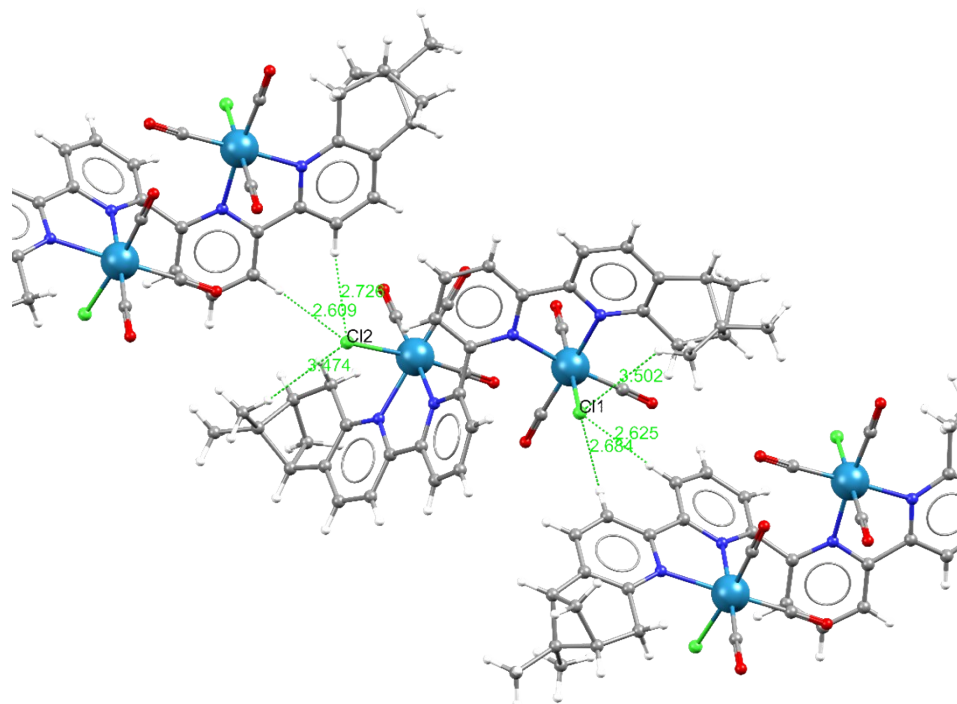


Figure S65. Intra-and intermolecular interactions in the single crystal structure of $d1\text{-[Re}_2(5a)(\text{CO})_6\text{Cl}_2]$

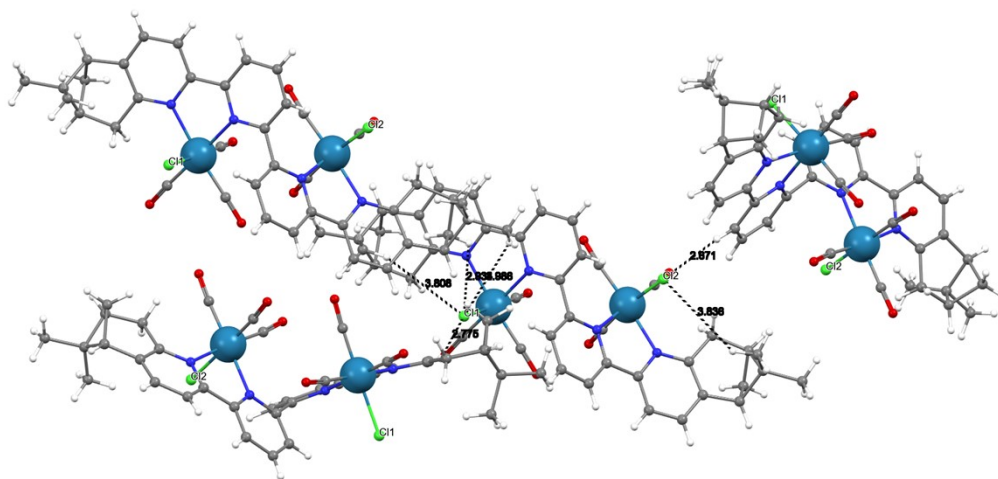


Figure S66. Intra-and intermolecular interactions in the single crystal structure of $d1\text{-[Re}_2(5b)(\text{CO})_6\text{Cl}_2]$

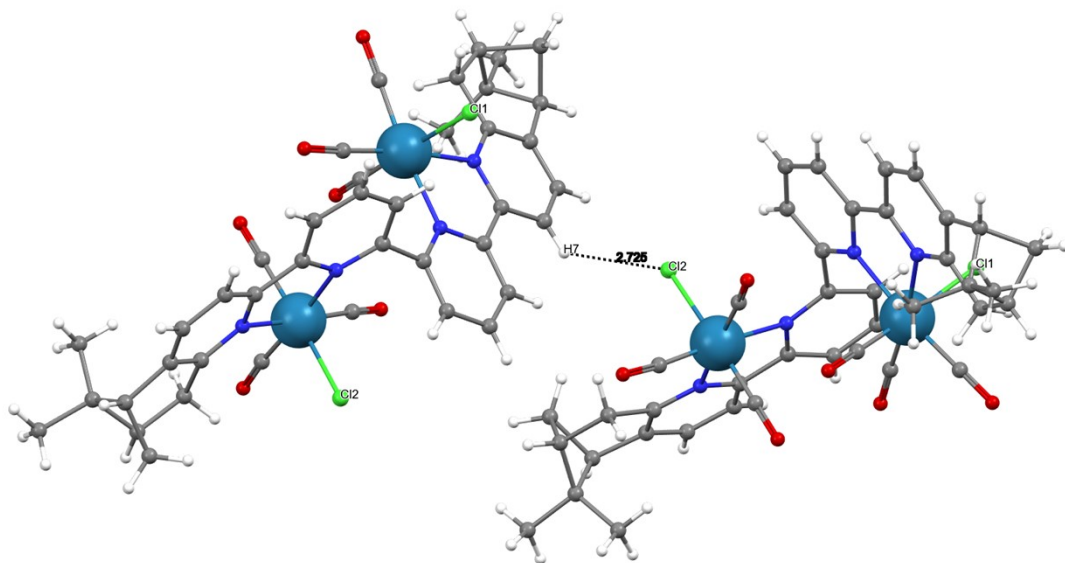


Figure S67. Intermolecular interactions in the single crystal structure of $d2\text{-[Re}_2\text{(5a)(CO)}_6\text{Cl}_2\text{]}$

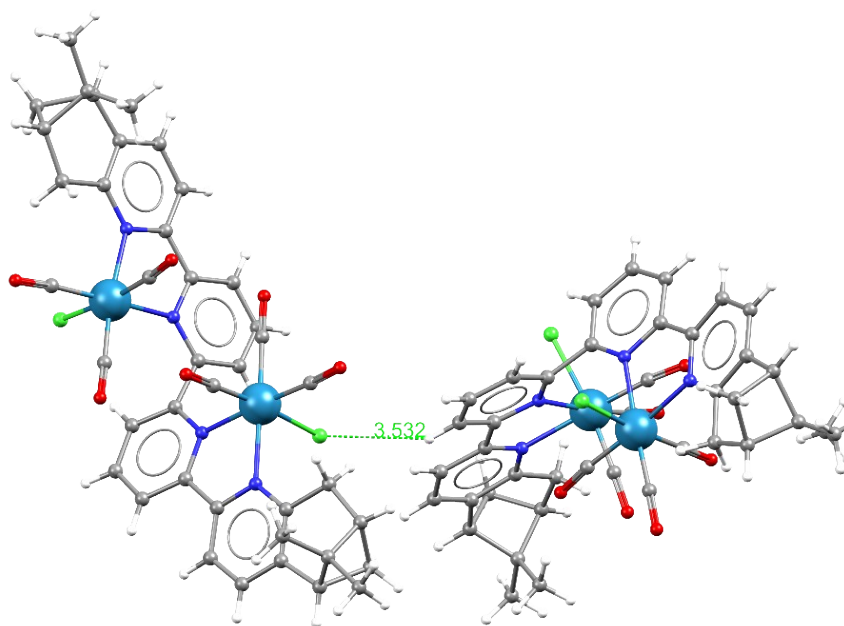


Figure S68. Intermolecular interactions in the single crystal structure of $d2\text{-[Re}_2\text{(5b)(CO)}_6\text{Cl}_2\text{]}$

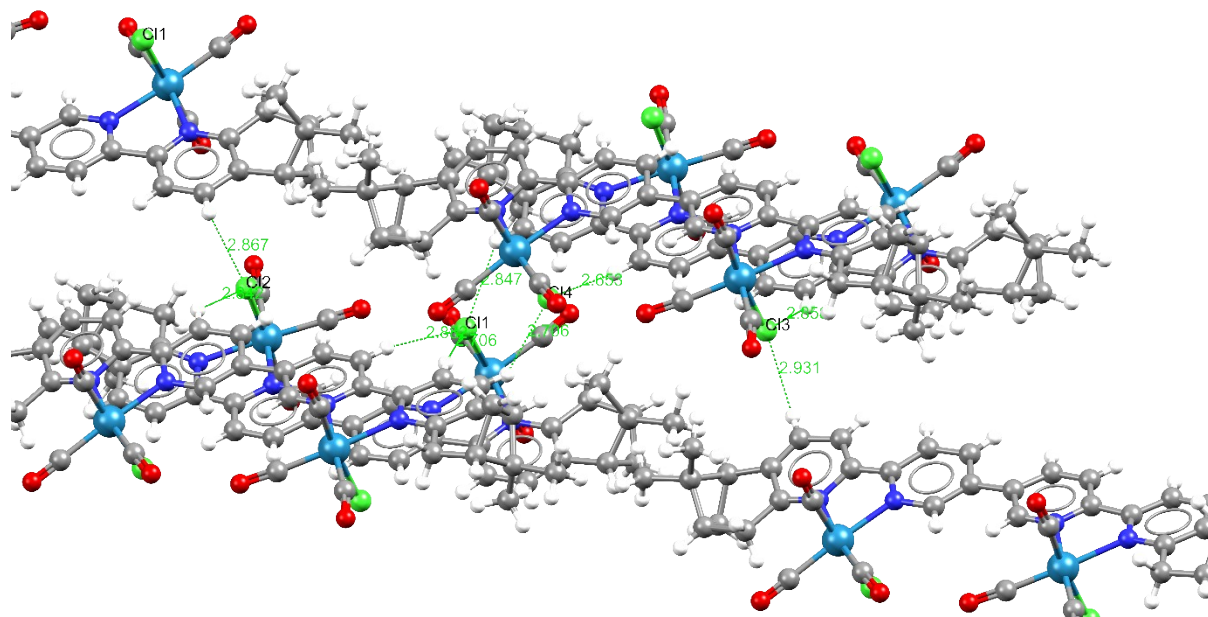


Figure S72. Intra- and intermolecular interactions in the single crystal structure of d₂-[Re₂(6b)(CO)₆Cl₂]

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)

[Re₂(5a)(CO)₆Cl₂]

Identification code	d1-[Re ₂ (5a)(CO) ₆ Cl ₂]	d2-[Re ₂ (5a)(CO) ₆ Cl ₂]
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CCDC number	2310573	2310577
Empirical formula	C ₄₁ Cl ₄ H ₃₆ N ₄ O ₆ Re ₂	C ₄₀ H ₃₄ Cl ₂ N ₄ O ₆ Re ₂
Formula weight	1194.94	1110.01
Temperature/K	200(2)	200(2)
Crystal system	orthorhombic	monoclinic
Space group	P2 ₁ 2 ₁ 2 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} /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)

[Re₂(**5b**)(CO)₆Cl₂]

Identification code	d1-[Re ₂ (5b)(CO) ₆ Cl ₂]	d2-[Re ₂ (5b)(CO) ₆ Cl ₂]
CCDC number	2310574	2310578
Empirical formula	C ₄₀ H ₃₄ Cl ₂ N ₄ O ₆ Re ₂	C ₄₀ H ₃₄ Cl ₂ N ₄ O ₆ Re ₂
Formula weight	1110.01	1110.01
Temperature/K	250	250
Crystal system	orthorhombic	monoclinic
Space group	P2 ₁ 2 ₁ 2 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} /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)

[Re₂(**6a**)(CO)₆Cl₂]

Identification code	d1-[Re ₂ (6a)(CO) ₆ Cl ₂]	d2-[Re ₂ (6a)(CO) ₆ Cl ₂]
CCDC number	2310575	2310579
Empirical formula	C ₄₀ H ₃₄ Cl ₂ N ₄ O ₆ Re ₂	C ₈₀ H ₆₈ Cl ₄ N ₈ O 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} /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)

[Re₂(**6b**)(CO)₆Cl₂]

Identification code	d1-[Re ₂ (6b)(CO) ₆ Cl ₂]	d2-[Re ₂ (6b)(CO) ₆ Cl ₂]
CCDC number	2310576	2310580
Empirical formula	C ₄₀ H ₃₄ Cl ₂ N ₄ O ₆ Re ₂	C ₄₄ H ₄₆ Cl ₂ N ₄ O ₈ Re 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} /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)