Supporting Information for

Ruthenium complexes of sterically-hindered pentaarylcyclopentadienyl ligands

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TABLE OF CONTENTS

I. ^{1}H and ^{13}C NMR spectra of compound

1. CpOHAr2

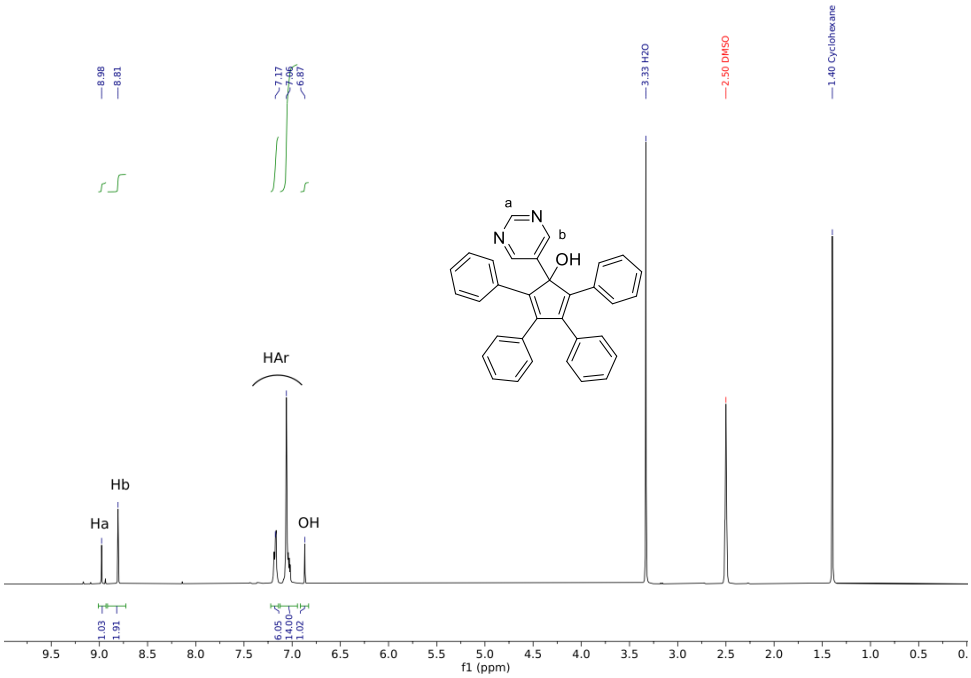


Fig. S1. ^{1}H NMR (300 MHz, $(CD_3)_2SO$, 25°C) of **CpOHAr2**

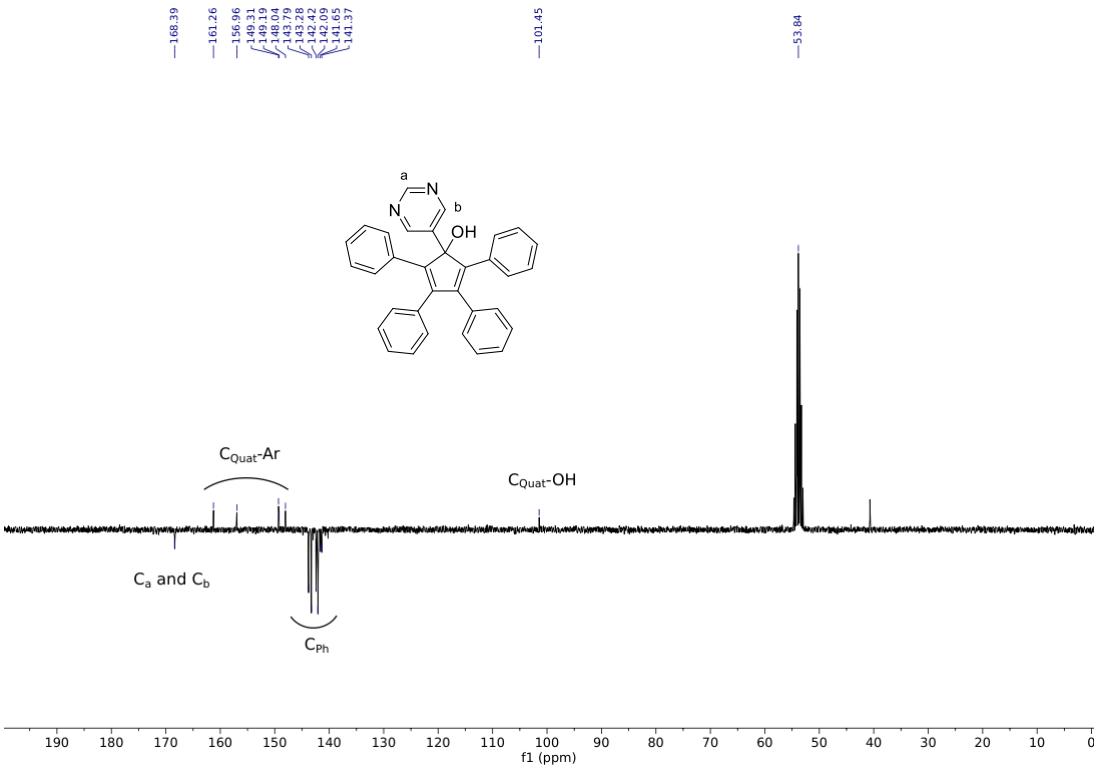


Fig. S2. ^{13}C-Jmod NMR (75 MHz, CD_2Cl_2, 25°C) of **CpOHAr2**

2. CpBrAr2

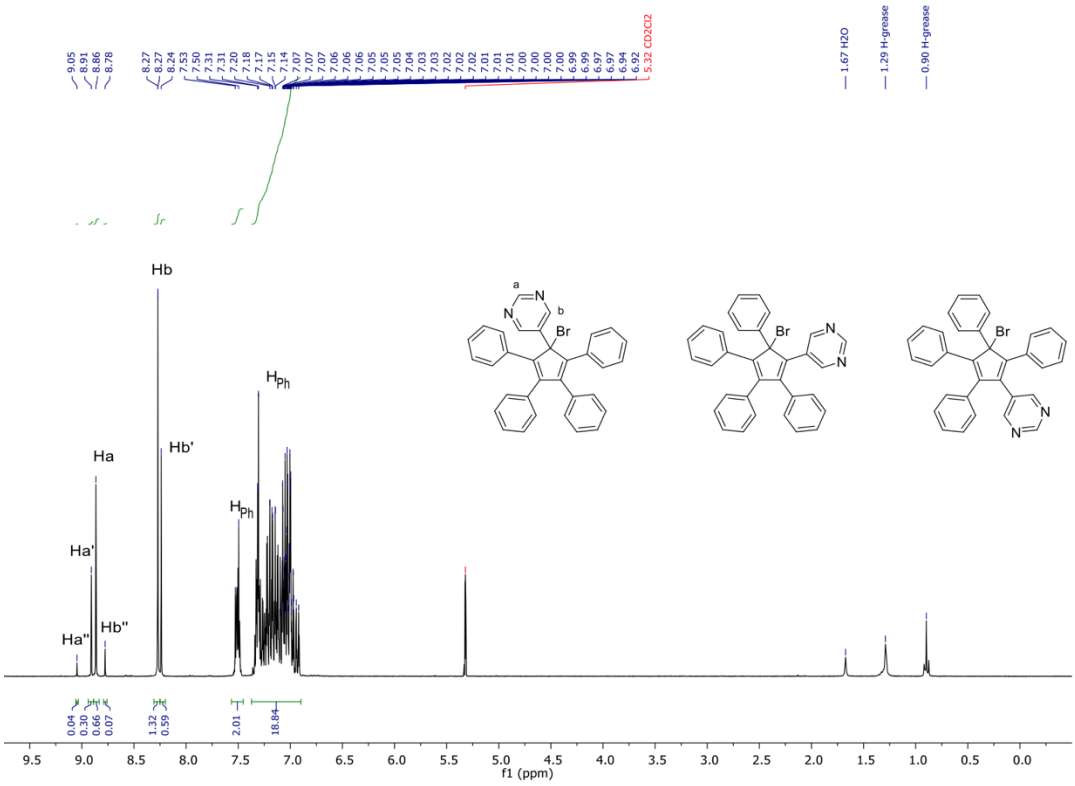


Fig. S3. ^{1}H-NMR (300 MHz, CD_2Cl_2, 25°C) of **CpBrAr2**, as a 66:30:4 mixture of three regioisomers

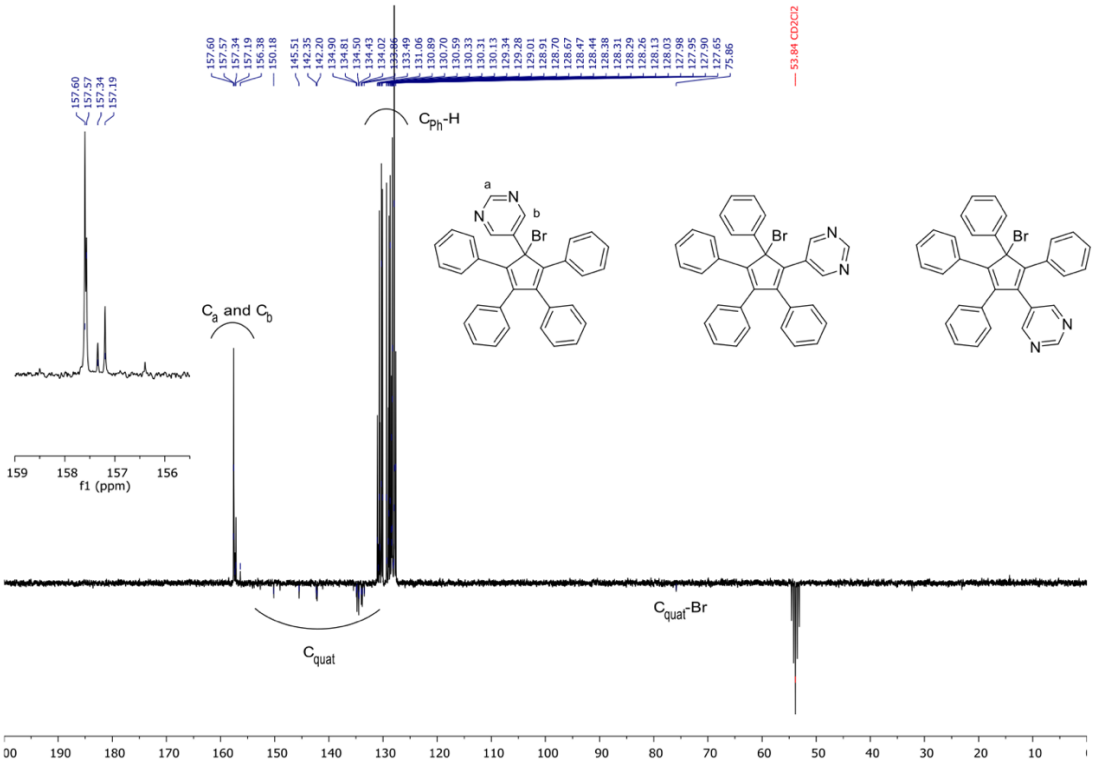


Fig. S4. ^{13}C-Jmod NMR (75 MHz, CD_2Cl_2, 25°C) of **CpBrAr2**, as a 66:30:4 mixture of three regioisomers

3.CpClAr1

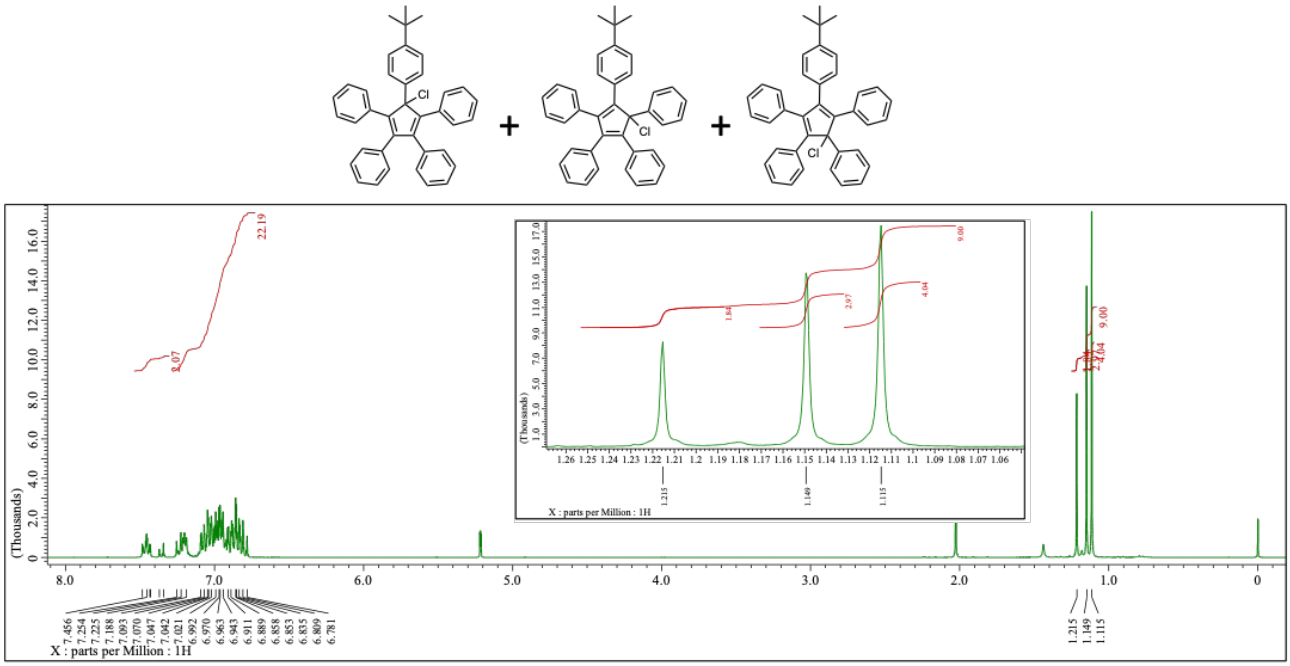


Fig. S5. ^{1}H-NMR (300 MHz, CD_2Cl_2, 25°C) of **CpClAr1** as a 46:34:20 mixture of three regioisomers

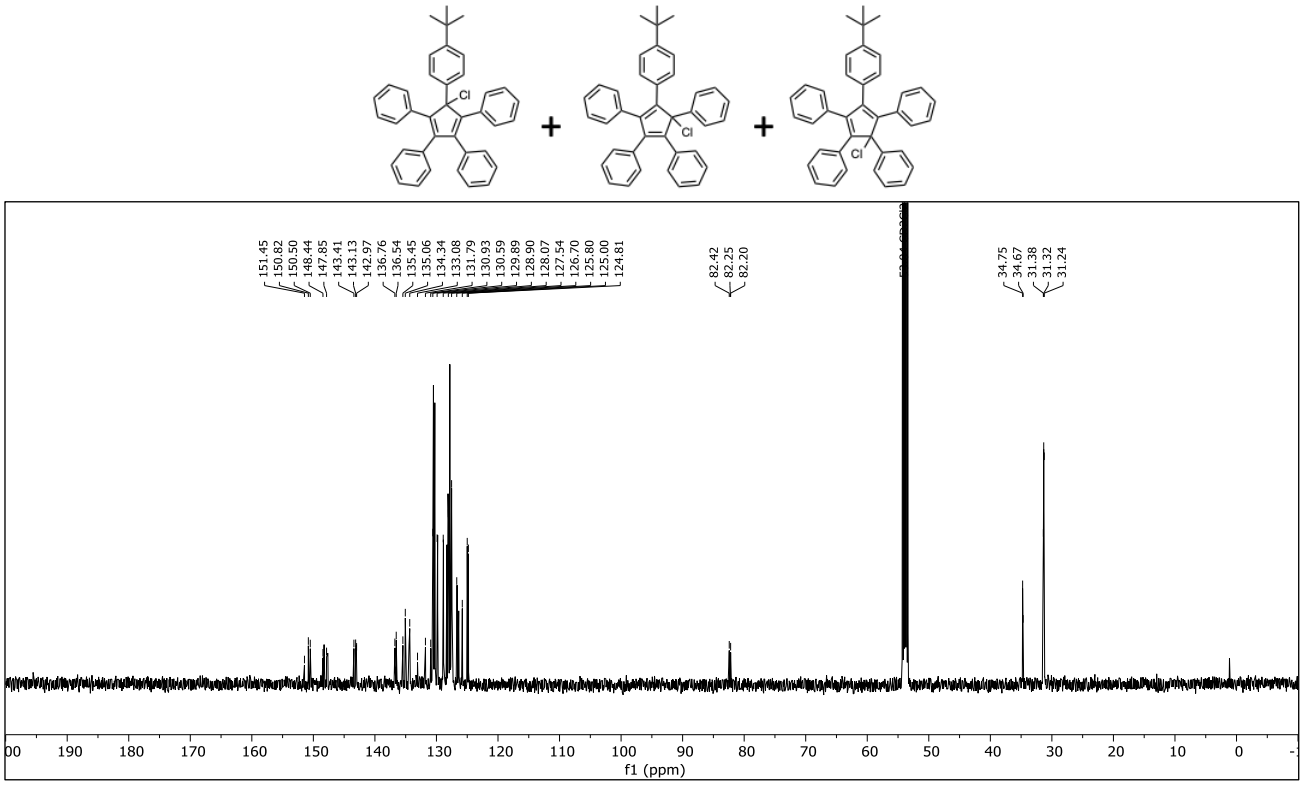


Fig. S6. $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2, 25°C) of **CpClAr1** as a 46:34:20 mixture of three regioisomers

4. CpClAr2

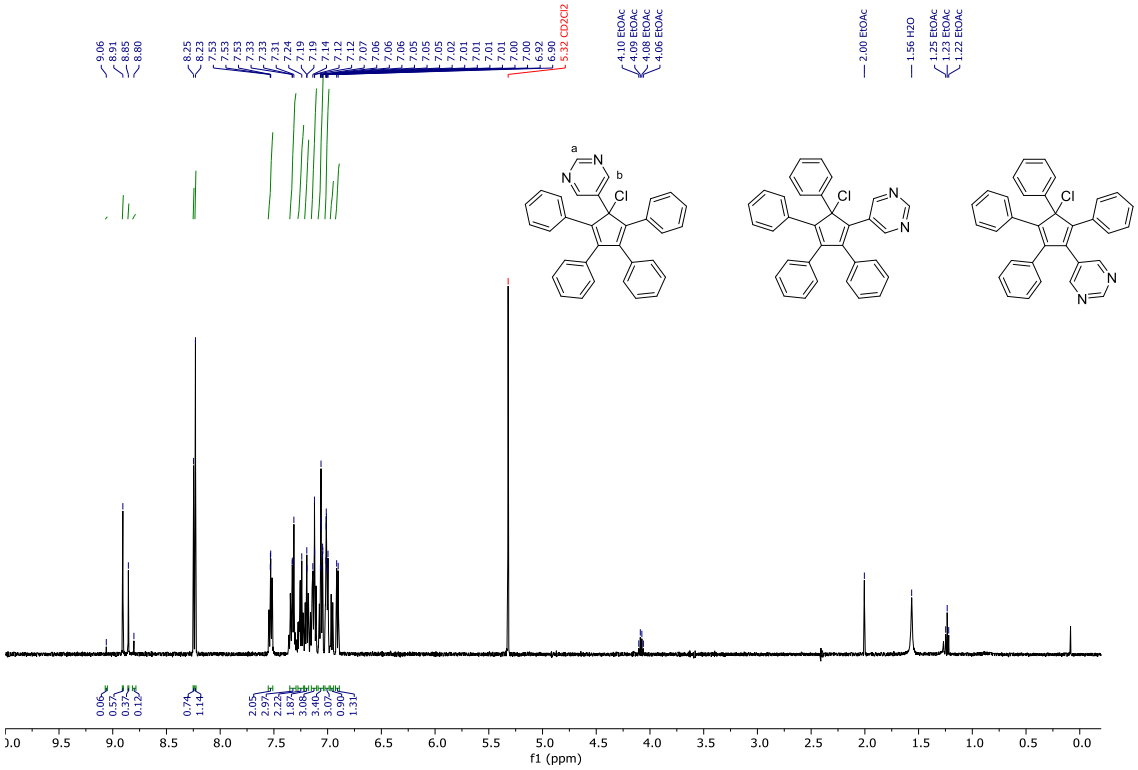


Fig. S7. ^{1}H NMR (500 MHz, CD_2Cl_2, 25°C) of **CpClAr2**, as a 57:37:6 mixture of three regioisomers

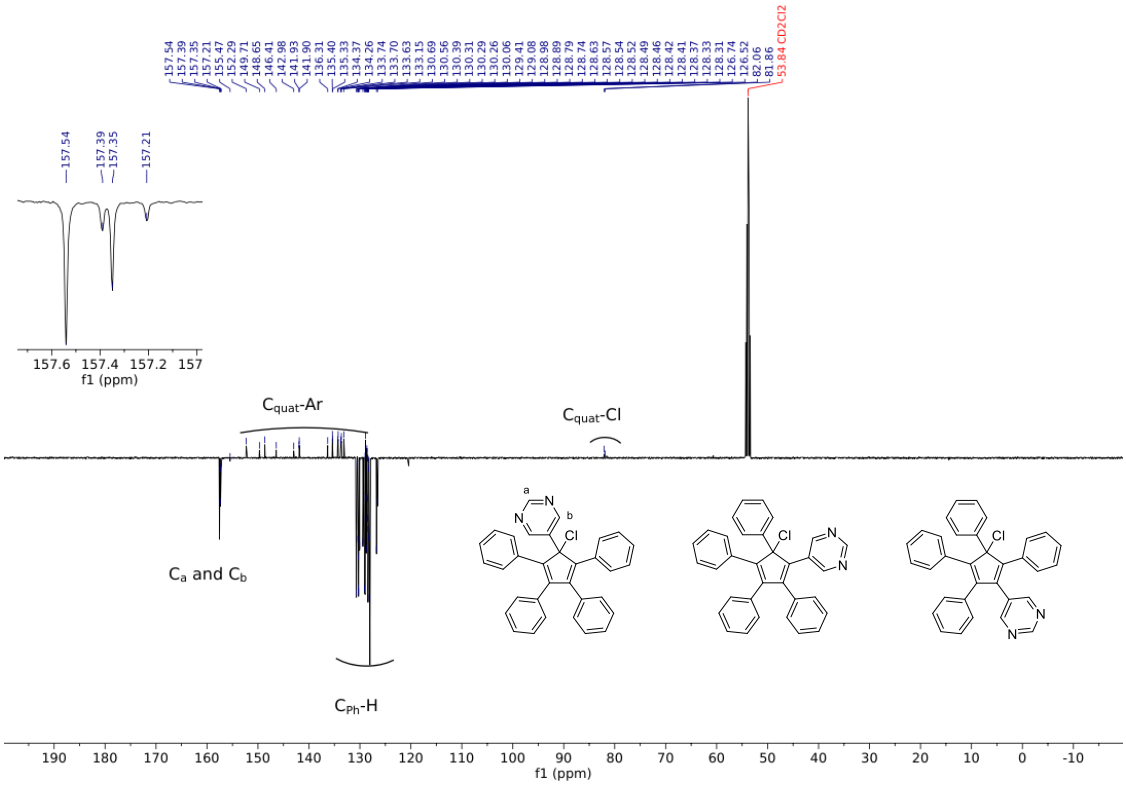


Fig. S8. ^{13}C-Jmod NMR (126 MHz, CD_2Cl_2, 25°C) of **CpClAr2**, as a 57:37:6 mixture of three regioisomers

5. CpClAr3

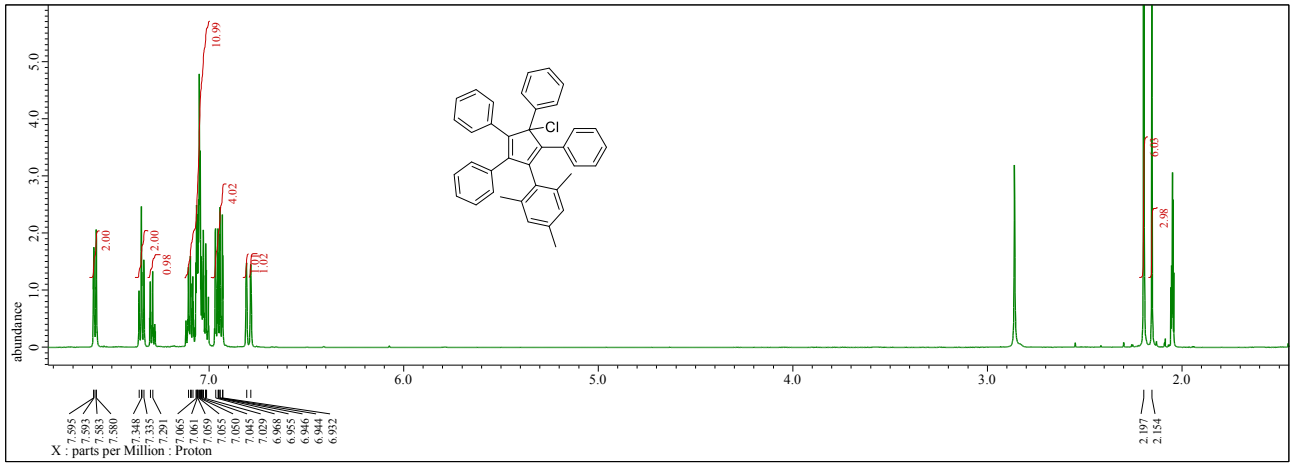


Fig. S9. ^{1}H NMR (600 MHz, $(CD_3)_2CO$, 25°C) of **CpClAr3**

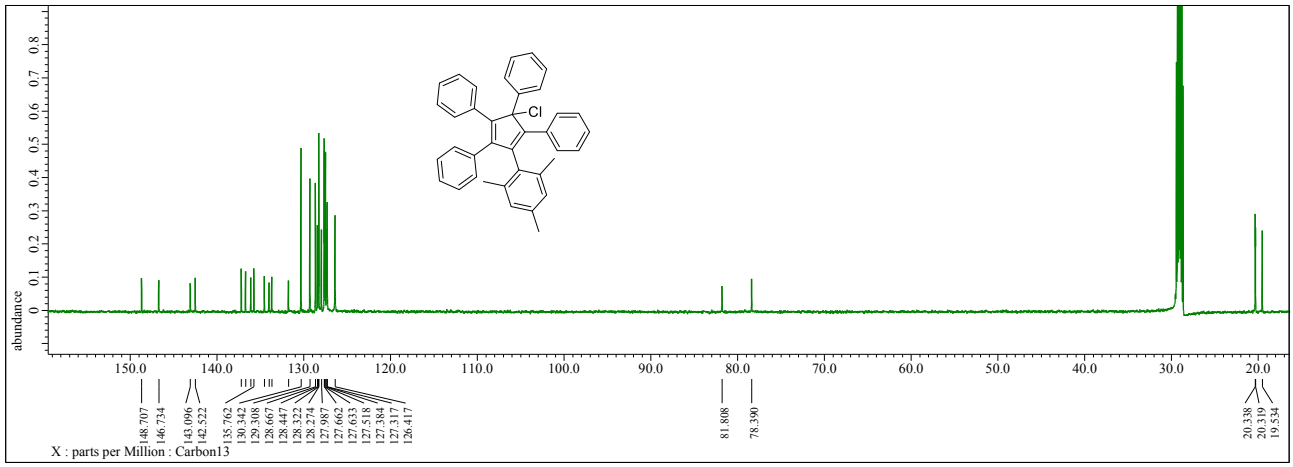


Fig. S10. $^{13}C\{^{1}H\}$ NMR (151 MHz, $(CD_3)_2CO$, 25°C) of **CpClAr3**
(signal at 78.4 ppm relates to chloroform traces)

6. RuCpBrAr1

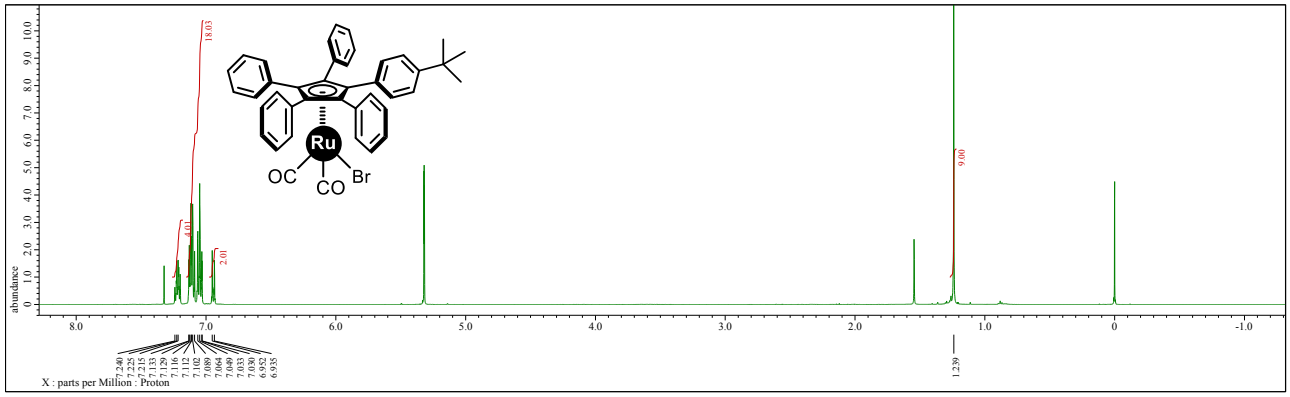


Fig. S11. ^{1}H NMR (600 MHz, CD_2Cl_2, 25°C) of **RuCpBrAr1**

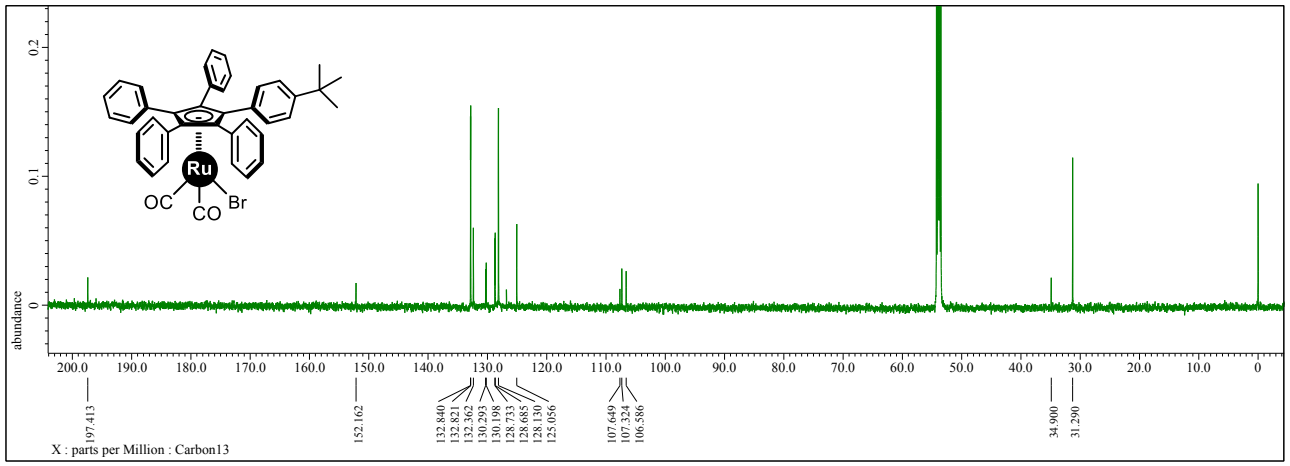


Fig. S12. $^{13}C\{^{1}H\}$ NMR (151 MHz, CD_2Cl_2, 25°C) of **RuCpBrAr1**

7. RuCpBrAr3

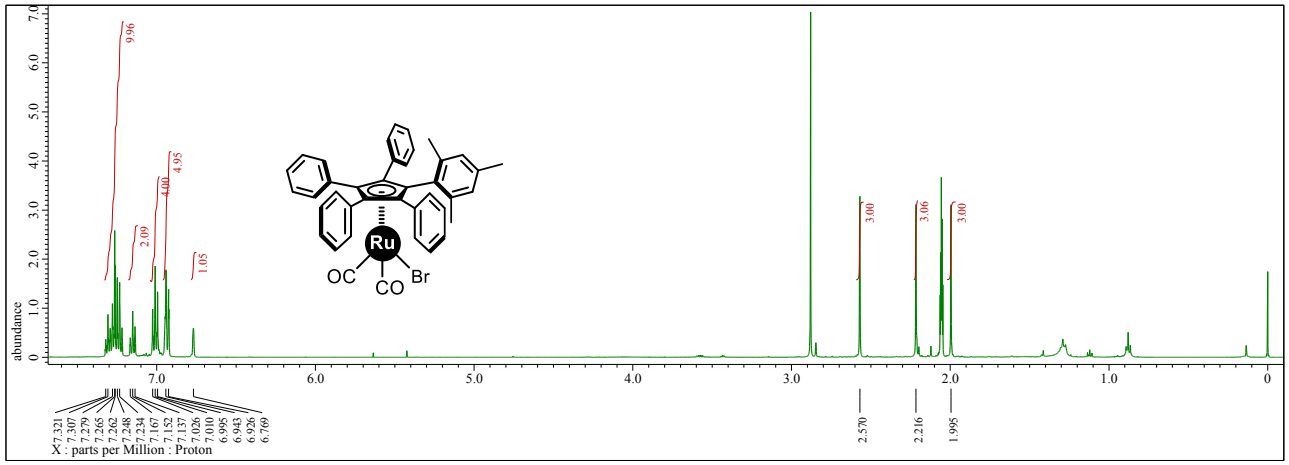


Fig. S13. ^{1}H NMR (500 MHz, $(CD_3)_2CO$, 25°C) of **RuCpBrAr3**

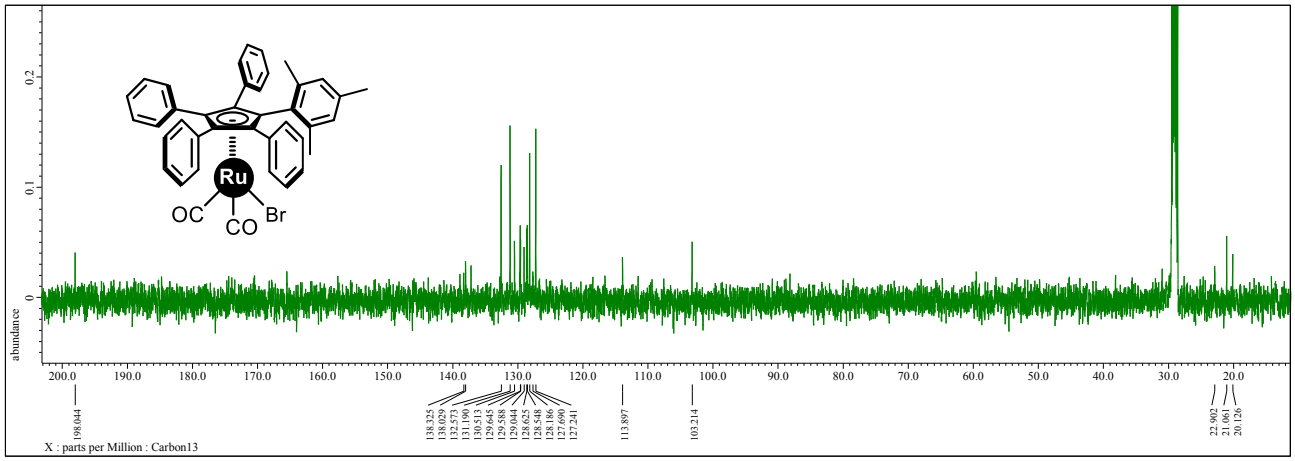


Fig. S14. $^{13}C\{^{1}H\}$ NMR (126 MHz, $(CD_3)_2CO$, 25°C) of **RuCpBrAr3**

8. RuCpClAr1

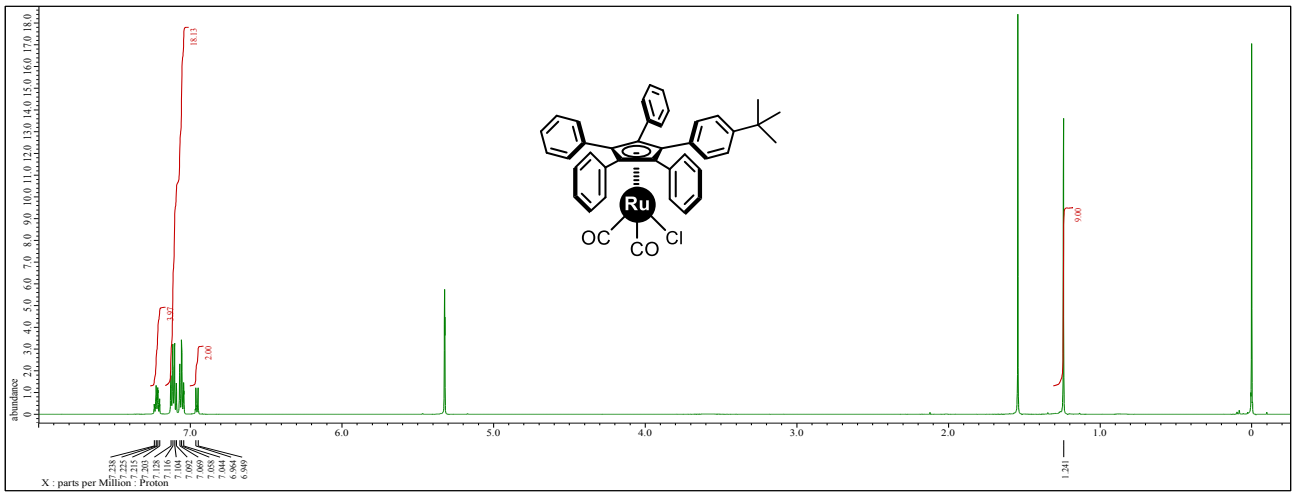


Fig. S15. ^{1}H-NMR (600 MHz, CD_2Cl_2, 25°C) of **RuCpClAr1**

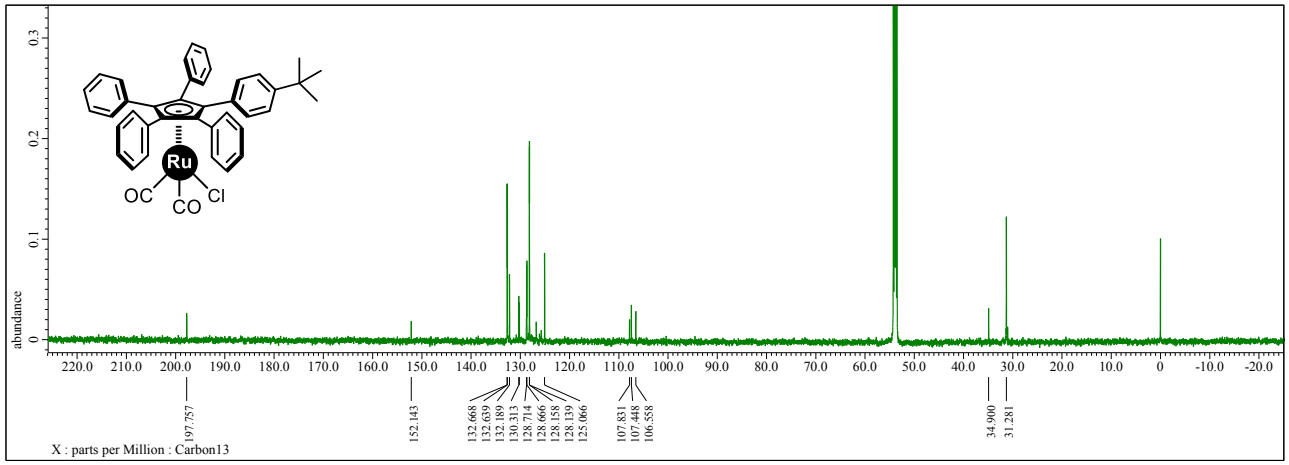


Fig. S16. $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2, 25°C) of **RuCpClAr1**

9. RuCpClAr3

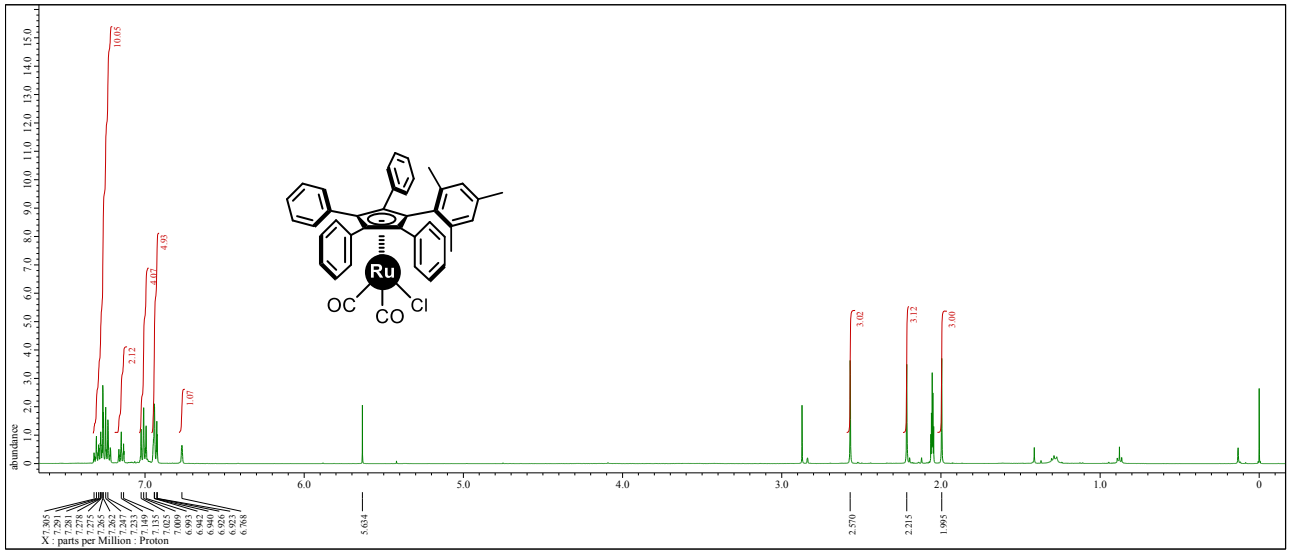


Fig. S17. ^{1}H NMR (500 MHz, $(CD_3)_2CO$, 25°C) of **RuCpClAr3**

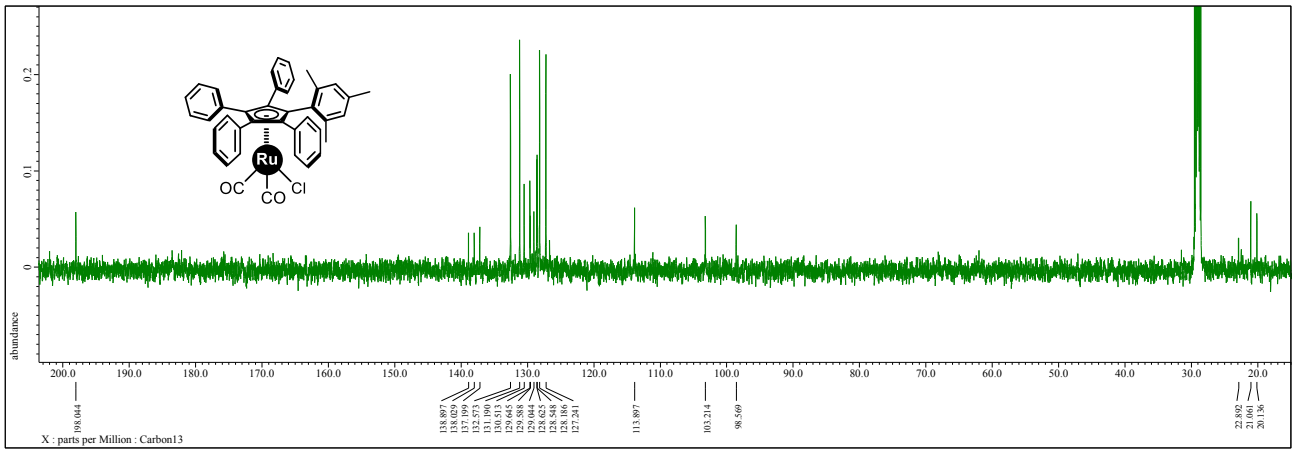
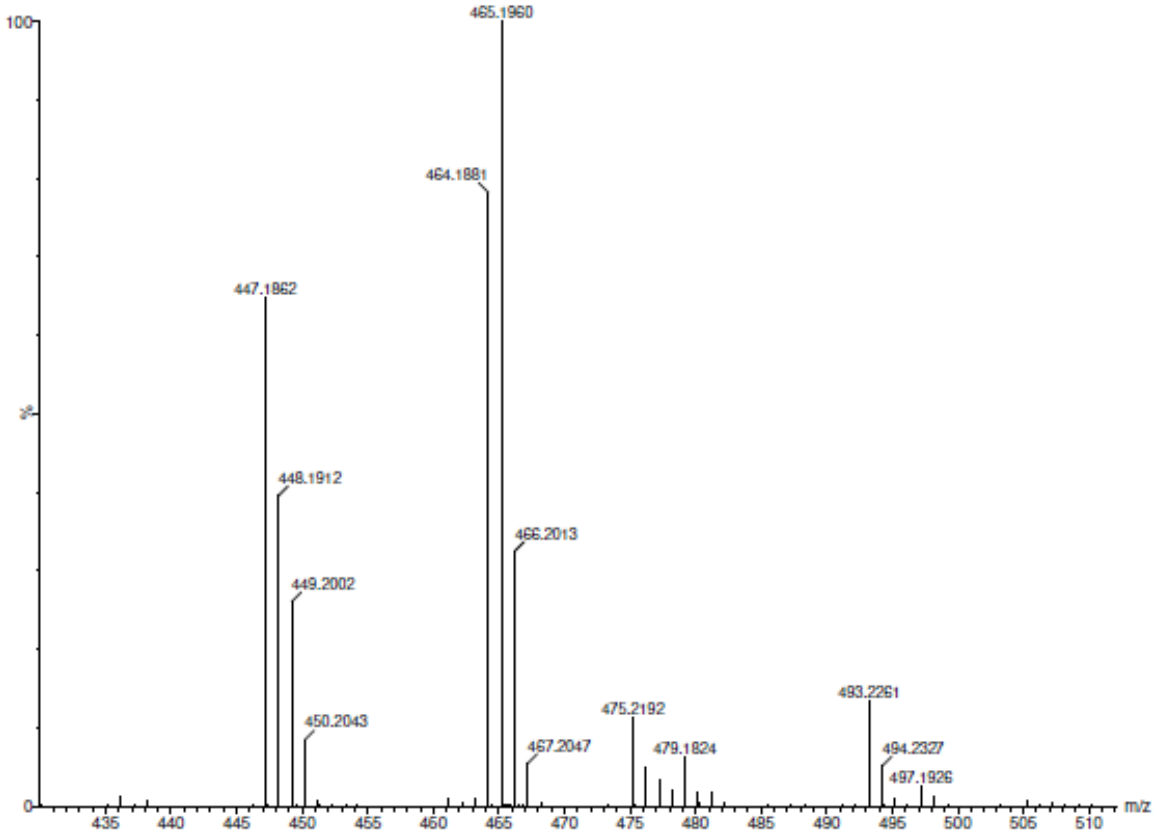
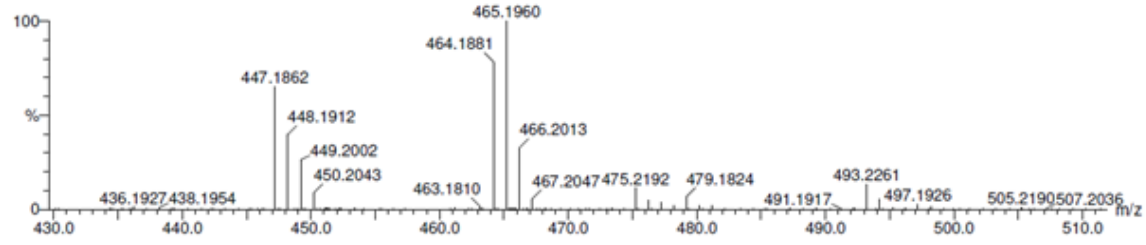


Fig. S18. $^{13}C\{^{1}H\}$ NMR (126 MHz, $(CD_3)_2CO$, 25°C) of **RuCpClAr3**

II. HR-MS OF

1. CpOHAr2

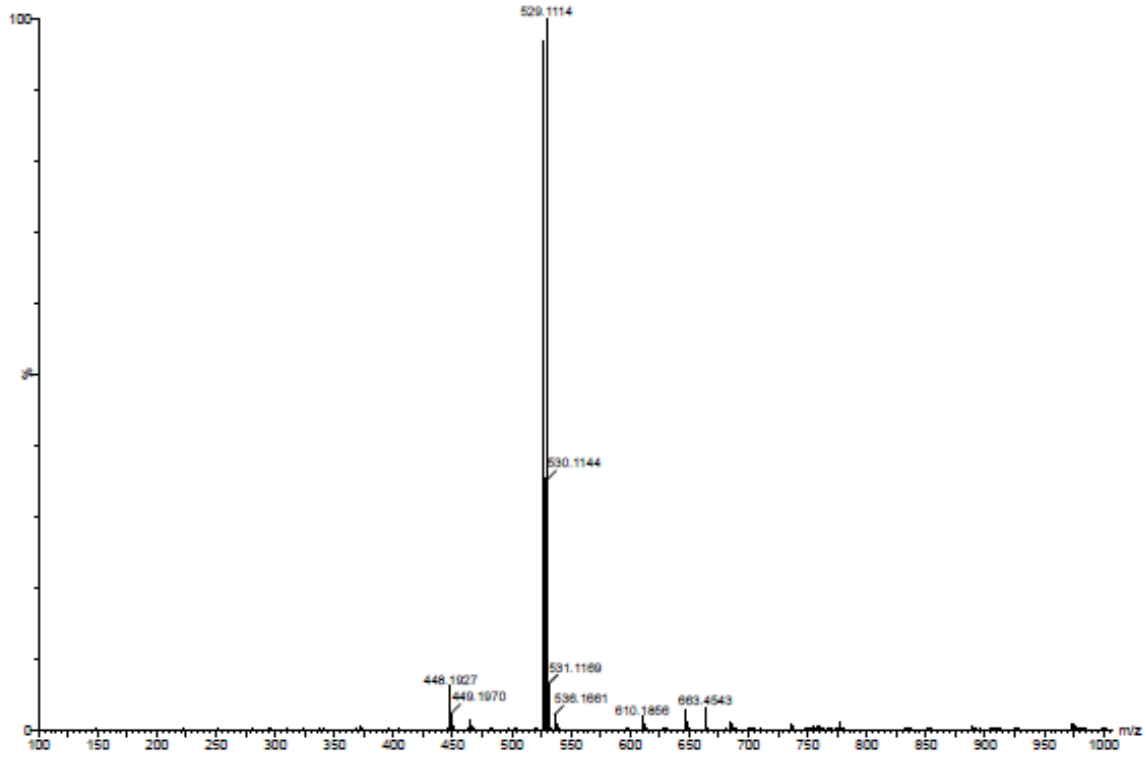


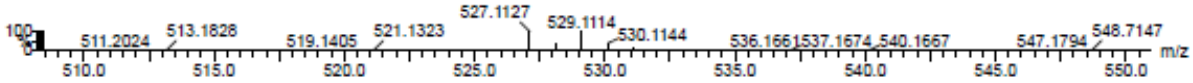


Minimum:				-1.5	
Maximum:		1.4	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
464.1881	464.1889	-0.8	-1.7	23.0	1449.5
	464.1875	0.6	1.3	23.5	1507.0
	464.1862	1.9	4.1	18.5	1578.0

Fig. S19. HR-MS (DCI-CH_4) data for compound **CpOHAr2**

2. CpBrAr2





Minimum:				-5.0			
Maximum:		1.0	3.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)
527.1127	527.1131	-0.4	-0.8	24.5	470.6	31.947	0.00
	527.1123	0.4	0.8	22.5	438.6	0.000	100.00
	527.1117	1.0	1.9	30.5	470.1	31.510	0.00
	527.1115	1.2	2.3	10.5	458.9	20.283	0.00
	527.1141	-1.4	-2.7	9.5	456.3	17.647	0.00

Fig. S20. HR-MS (ESI+) data for compound **CpBrAr2**

3. CpBrAr4

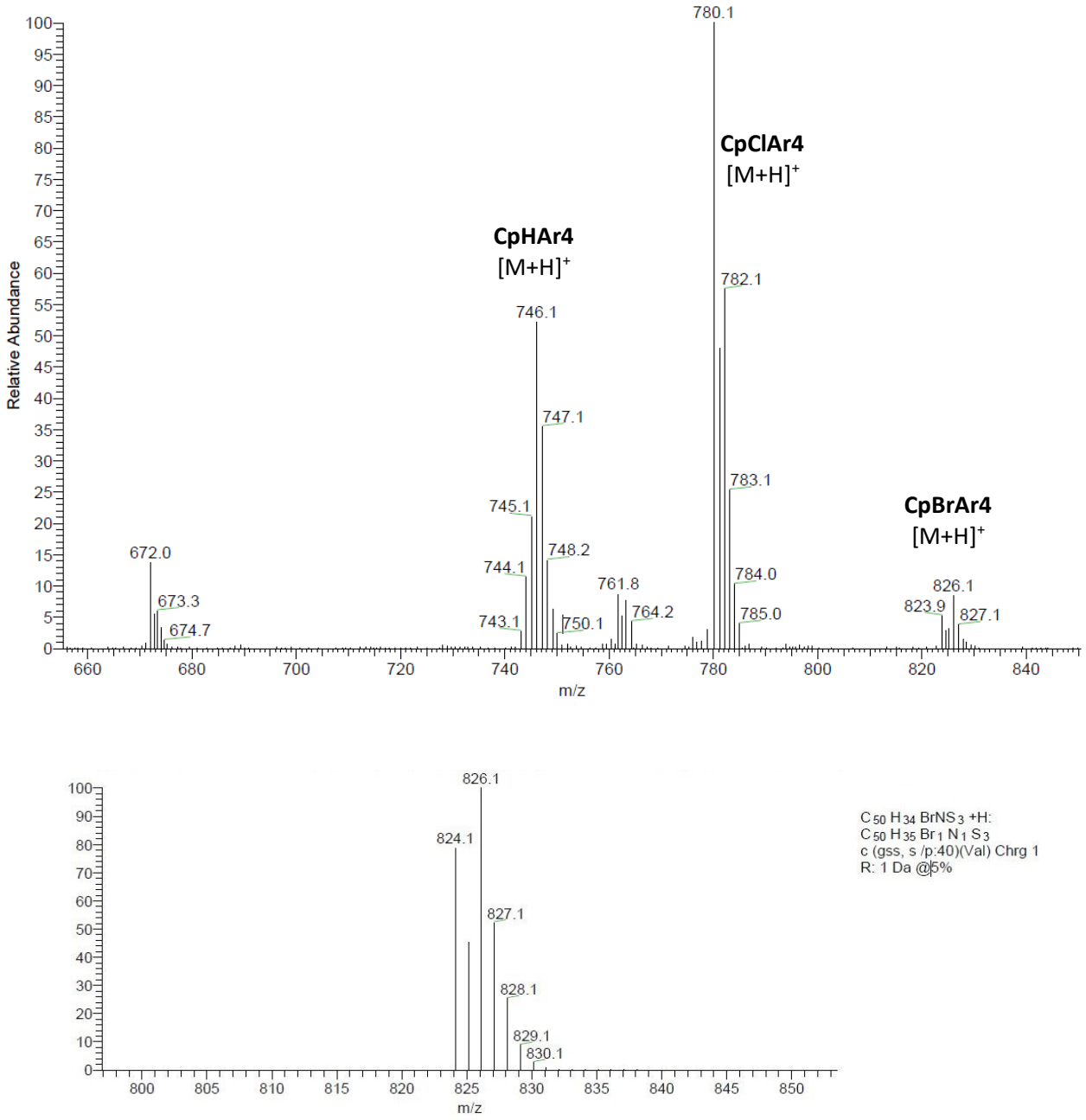
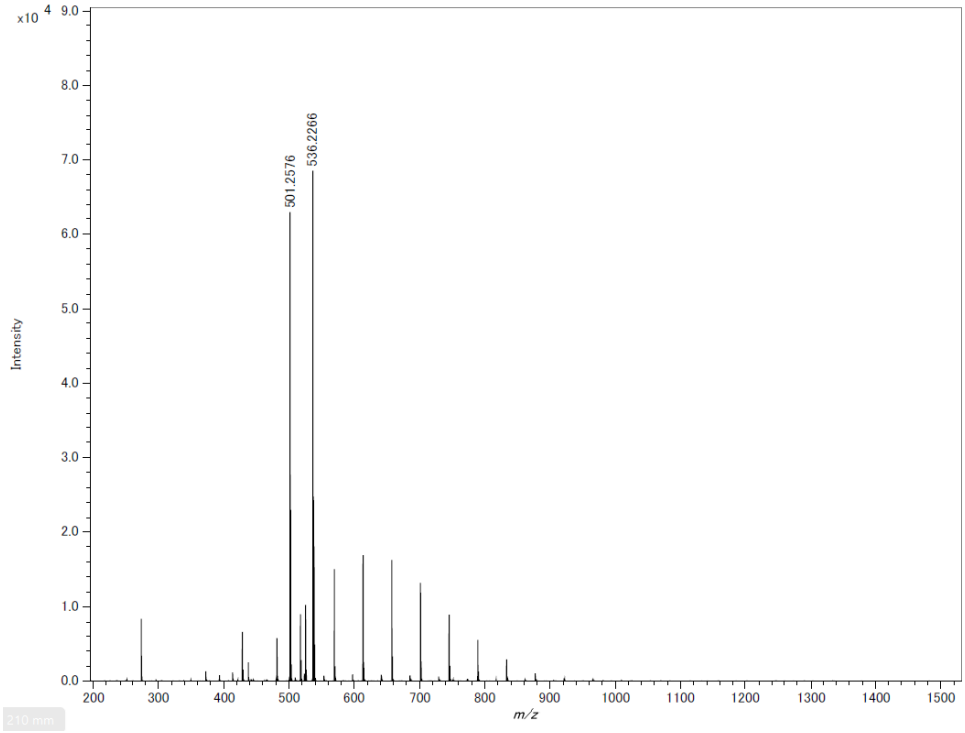
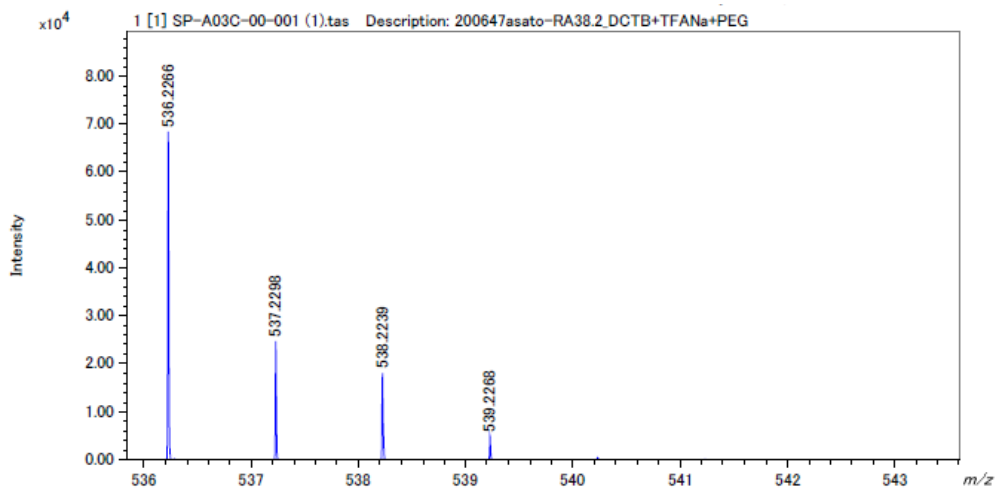


Fig. S21. MS (DCI-CH_4) data for compound **CpBrAr4**, obtained as a mixture with **CpClAr4** and **CpHAr4**

4. CpClAr1





Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
536.22656 ± 0.00268	5.0 ppm	Odd/Even	+1	-0.5 - 200.0	100

Elements

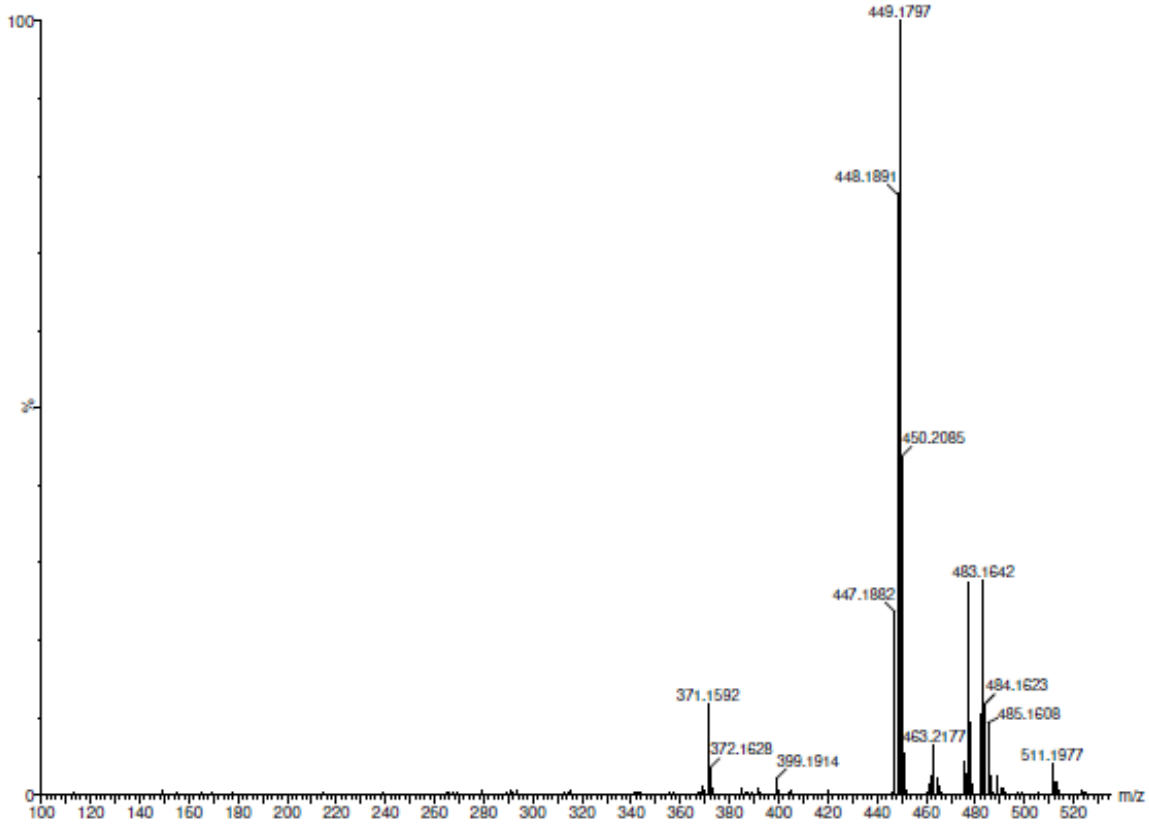
C 0 - 40 H 0 - 40 Cl 0 - 1

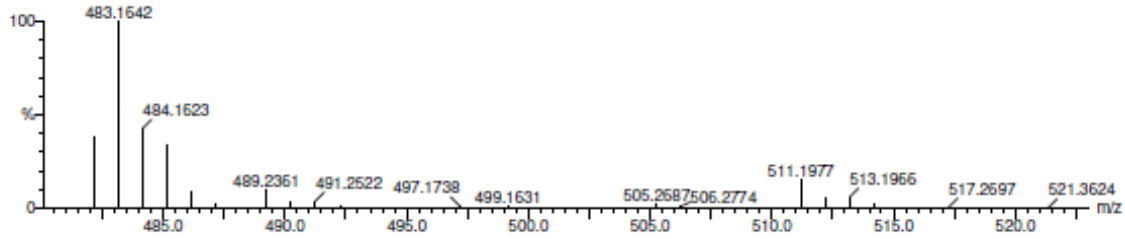
Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C39 H33 Cl	536.22653	23.0	0.00003	0.00003	0.05

Fig. S22. HR-MS (Spiral-TOF) DCTB+TFANa+PEG data for compound **CpClAr1**

5. CpClAr2





Minimum:				-1.5	
Maximum:		1.3	5.0	80.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT
483.1642	483.1628	1.4	2.9	22.5	376.8

Fig. S23. HR-MS (DCI-CH_4) data for compound **CpClAr2**

6. CpClAr3

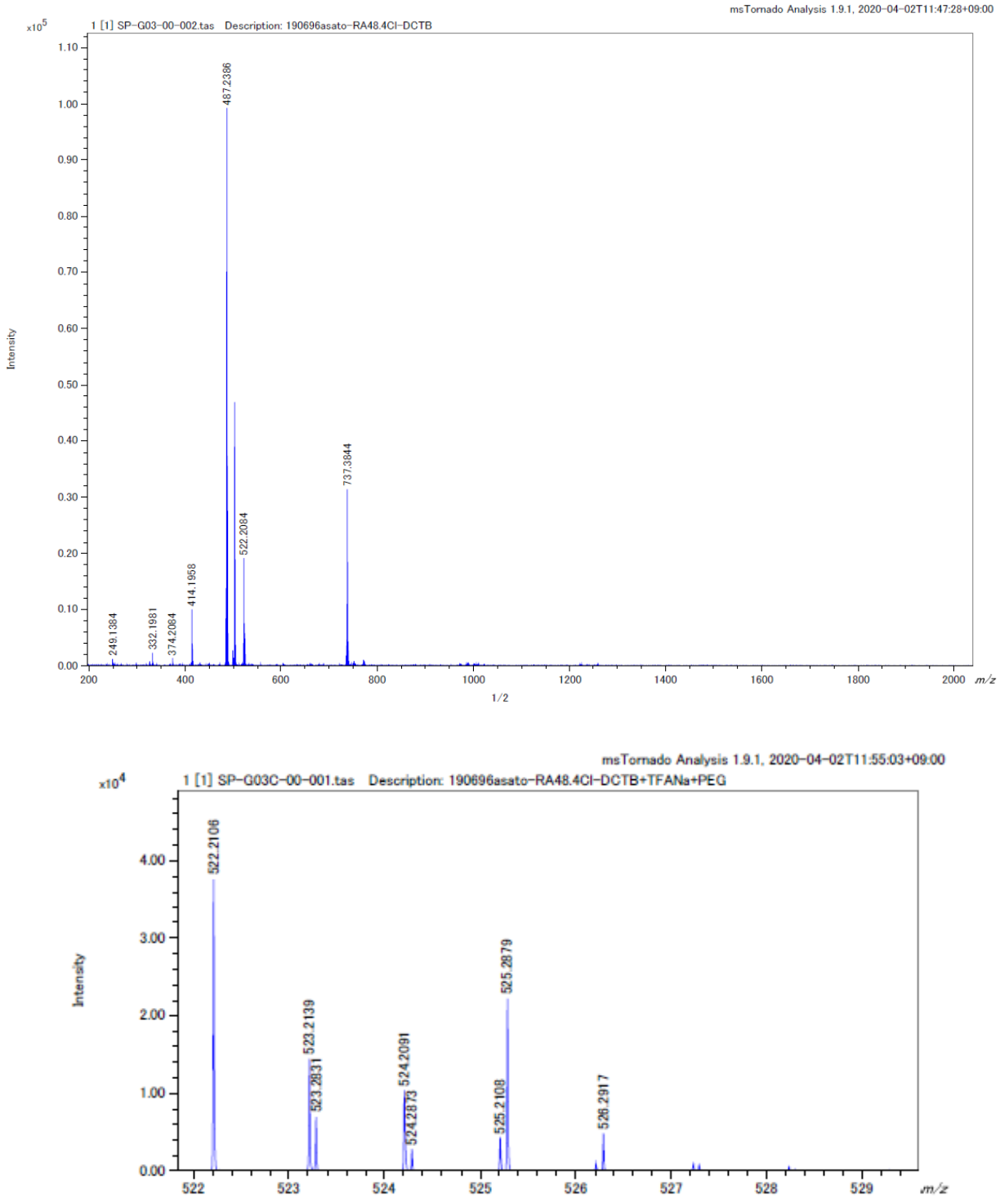


Fig. S24. HR-MS (MALDI-TOF) DCTB+TFANa (with PEG for the HR) data for compound **CpClAr3**

7. RuCpBrAr1

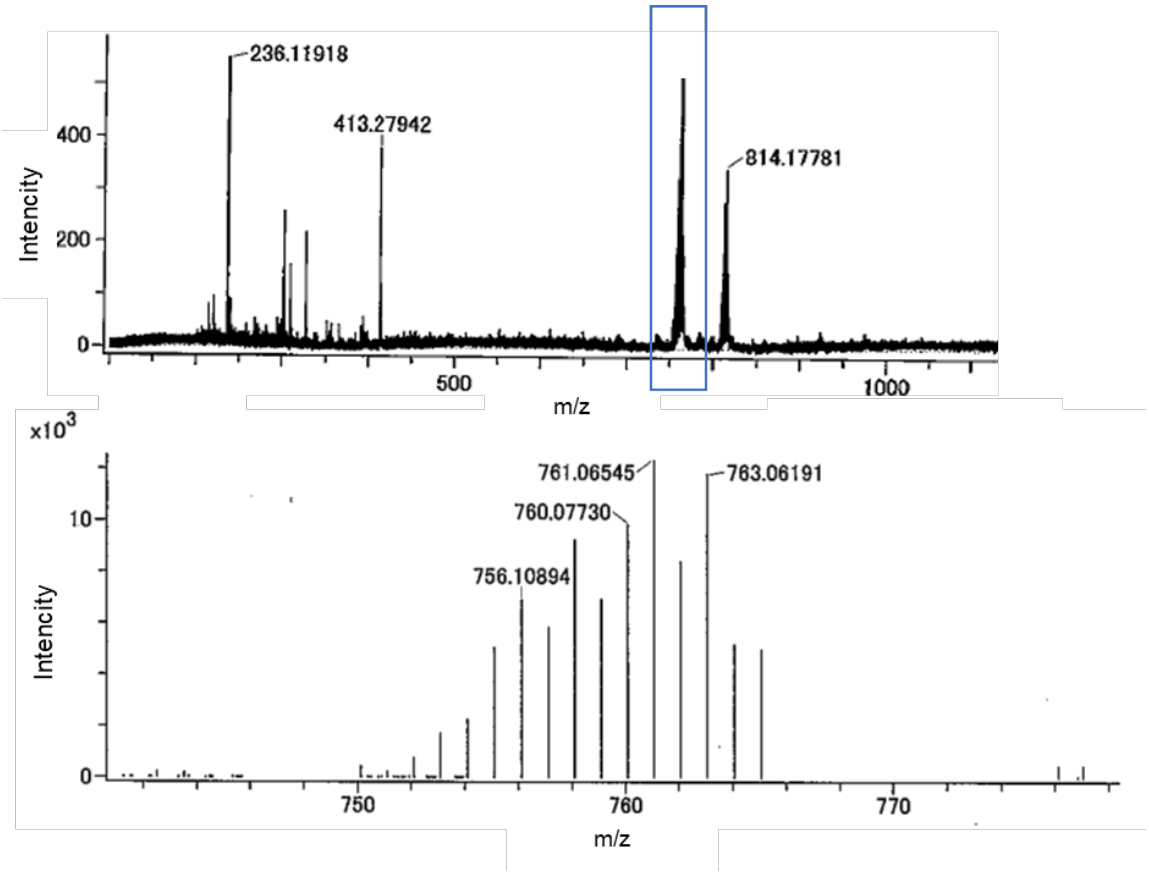


Fig. S25. HR-MS (ESI$^+$) data for compound **RuCpBrAr1**

8. RuCpBrAr3

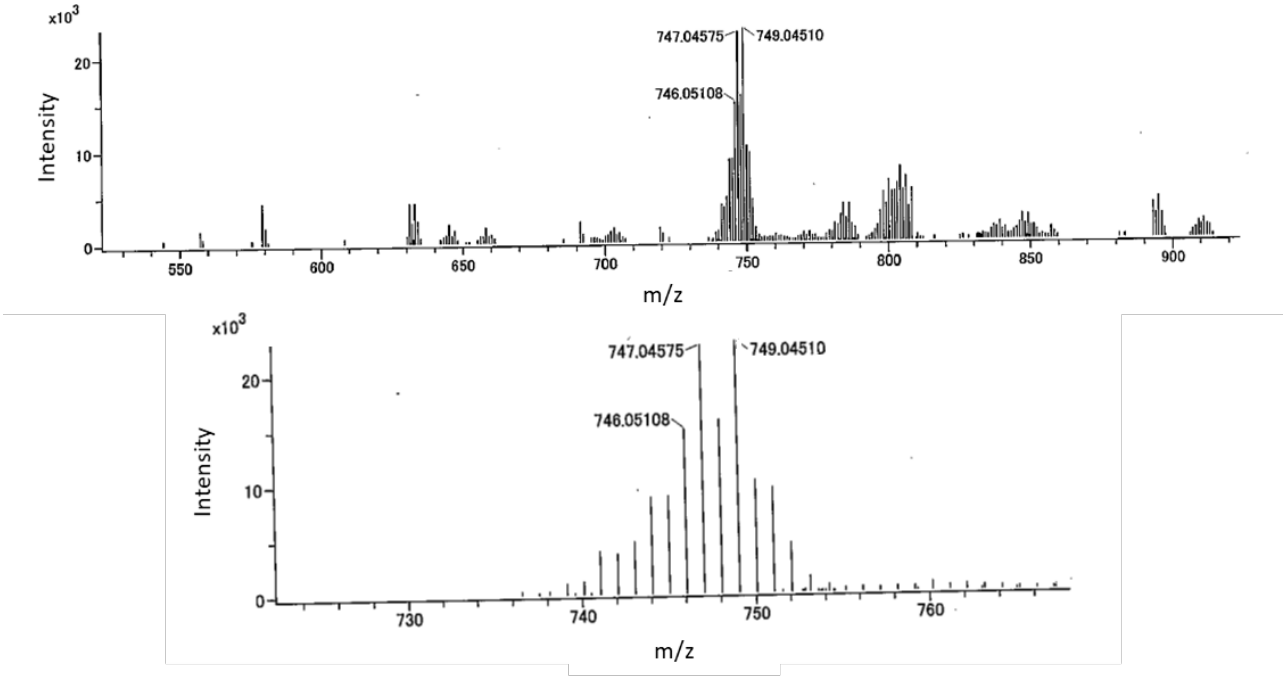


Fig. S26. HR-MS (ESI^+) data for compound **RuCpBrAr3**

9. RuCpClAr1

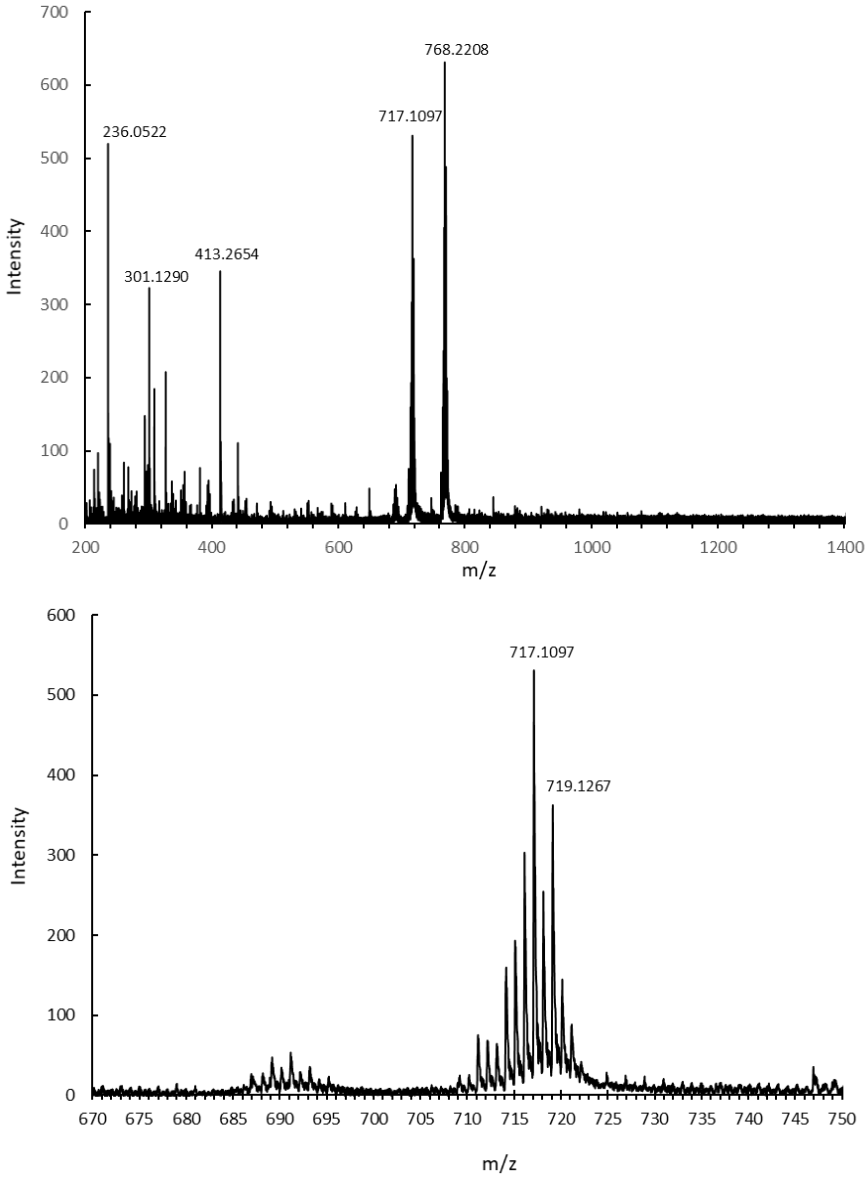


Fig. S27. HR-MS (ESI$^+$) data for compound **RuCpClAr1**

10. RuCpClAr3

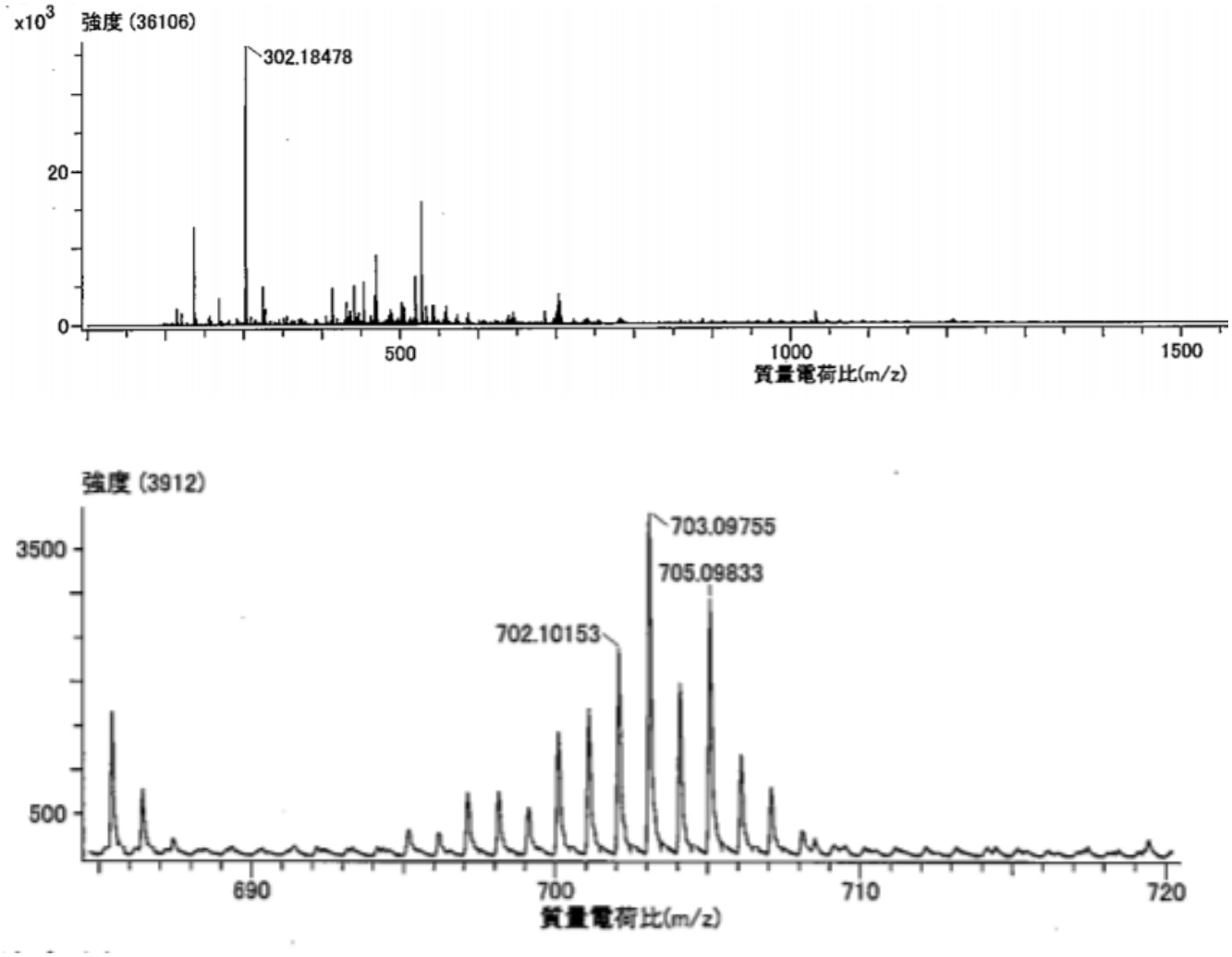


Fig. S28. HR-MS (ESI^+) data for compound **RuCpClAr3**