

Supplementary Material

Chloro(η^2, η^2 -cycloocta-1,5-diene){1-[(2-[(*S*)-1-(hydroxymethyl)-3-methylbutyl]amino)-2-oxoethyl]-3-(1-naphthalenylmethyl)benzimidazol-2-ylidene}rhodium(I)

Satoshi Sakaguchi* and Shogo Matsuo

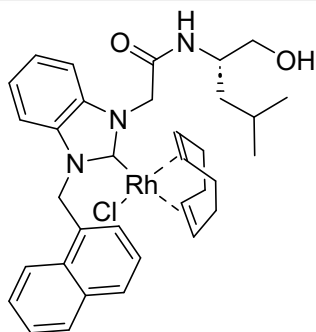
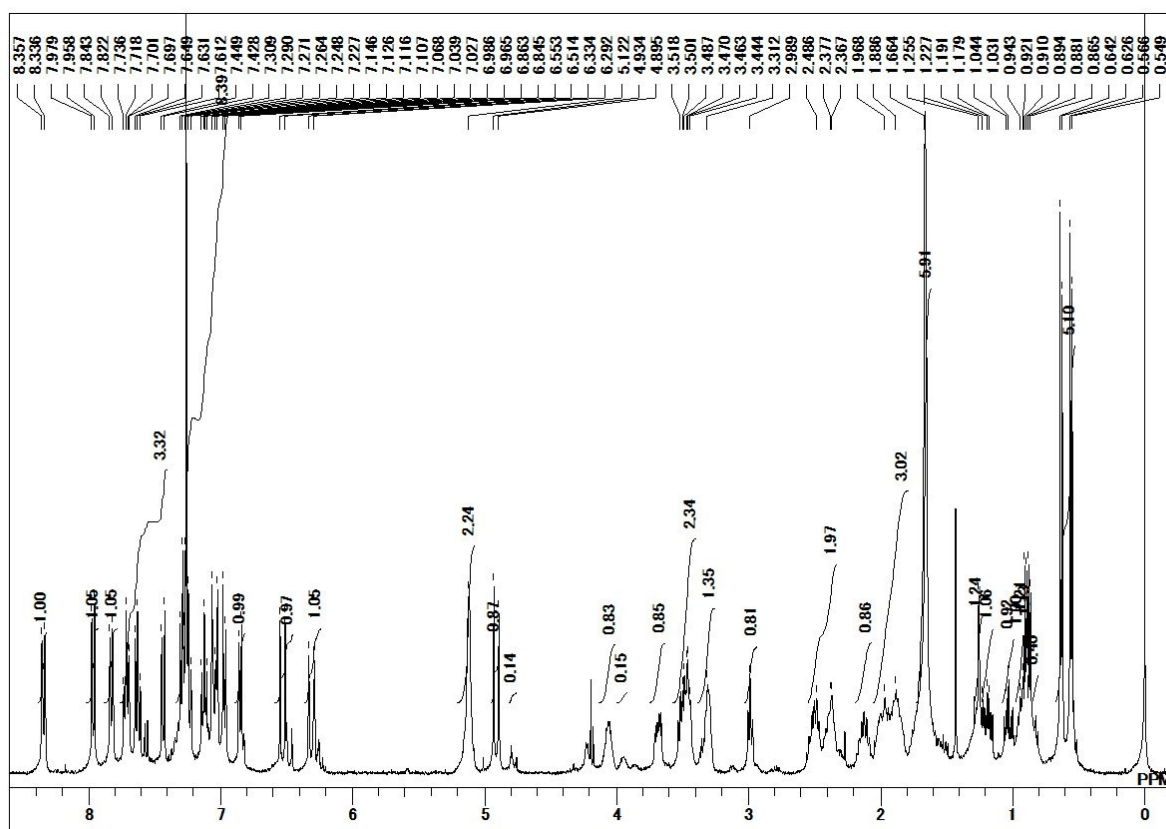
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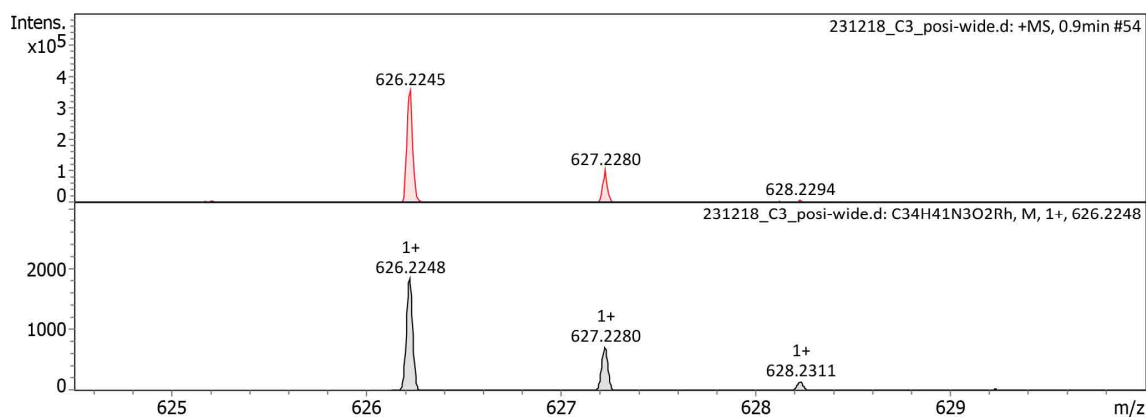
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Figure S1. ^1H NMR of compound 3



HRMS (ESI-TOF), m/z : calcd for $\text{C}_{34}\text{H}_{41}\text{N}_3\text{O}_2\text{Rh}$ $[\text{M}-\text{Cl}]^+$, 626.2248, found, 626.2245.



An 8:2 mixture of two NHC/Rh complexes

Major isomer: 6.53 ppm (d, $J = 15.4$ Hz, 1H, CH₂CO)

Minor isomer: 6.48 ppm (d, $J = 15.4$ Hz, 1H, CH₂CO)

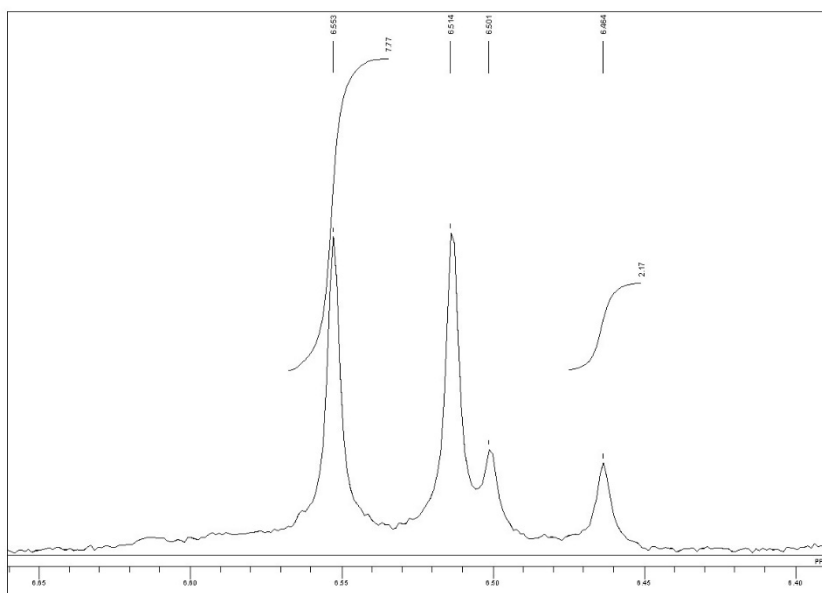
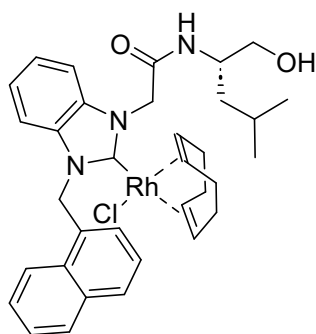
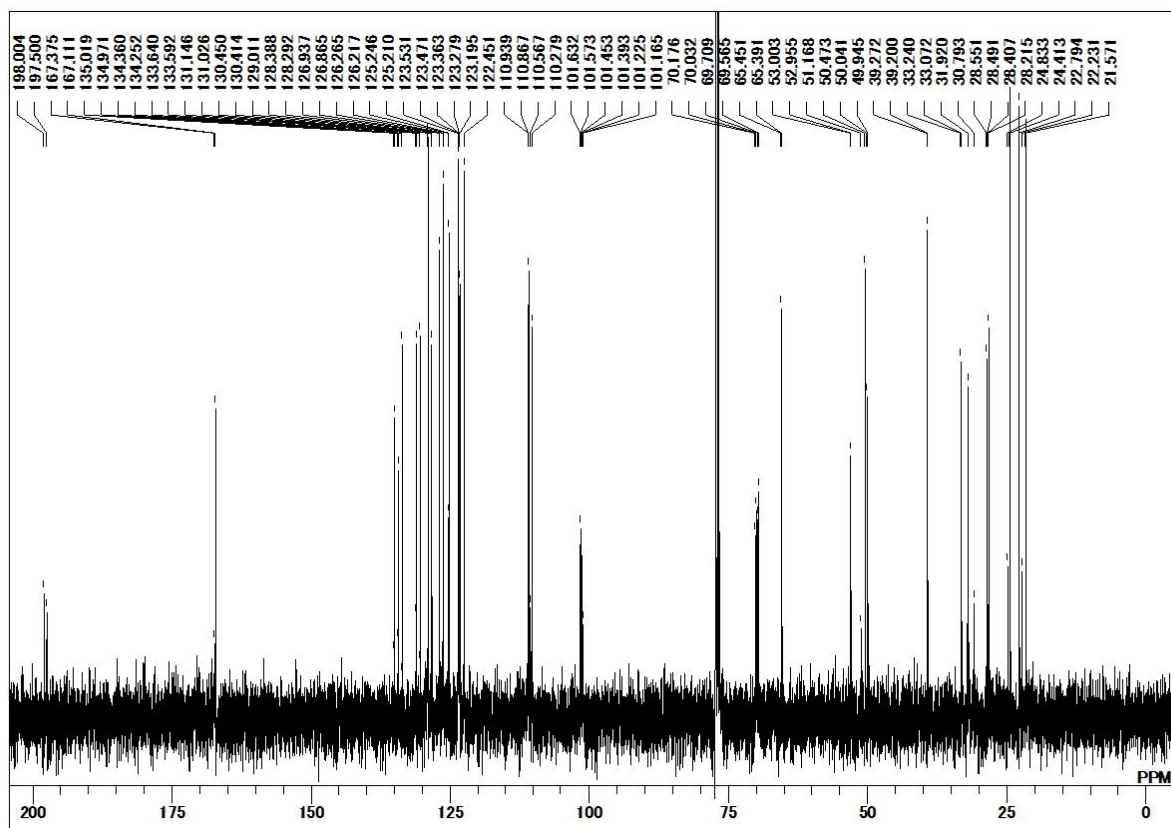
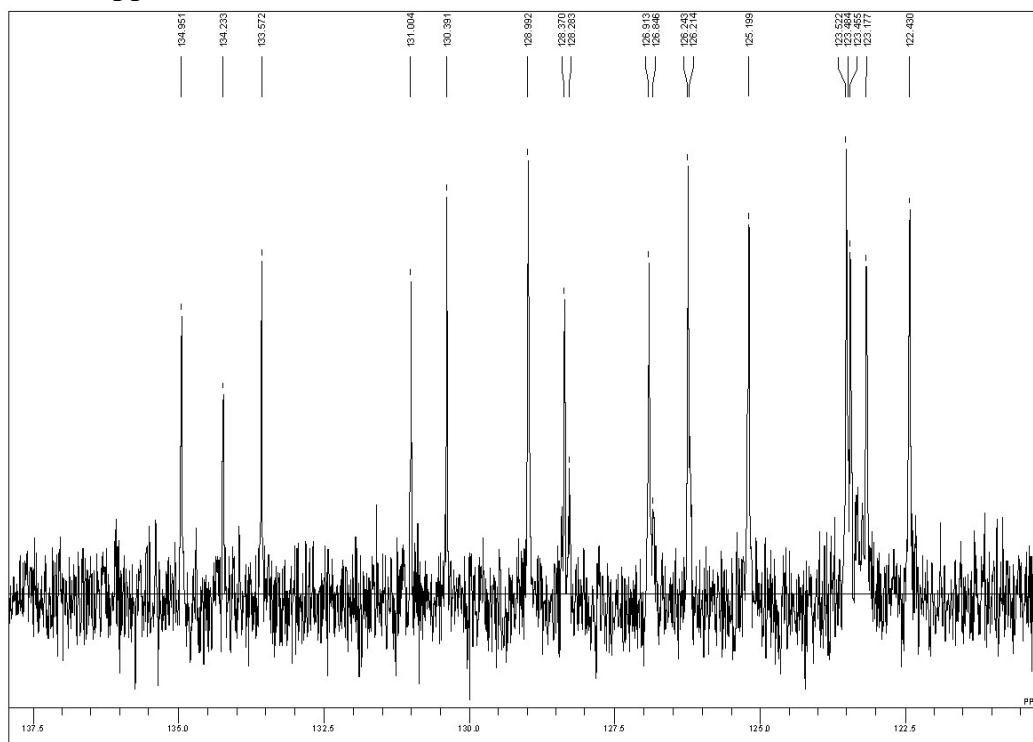


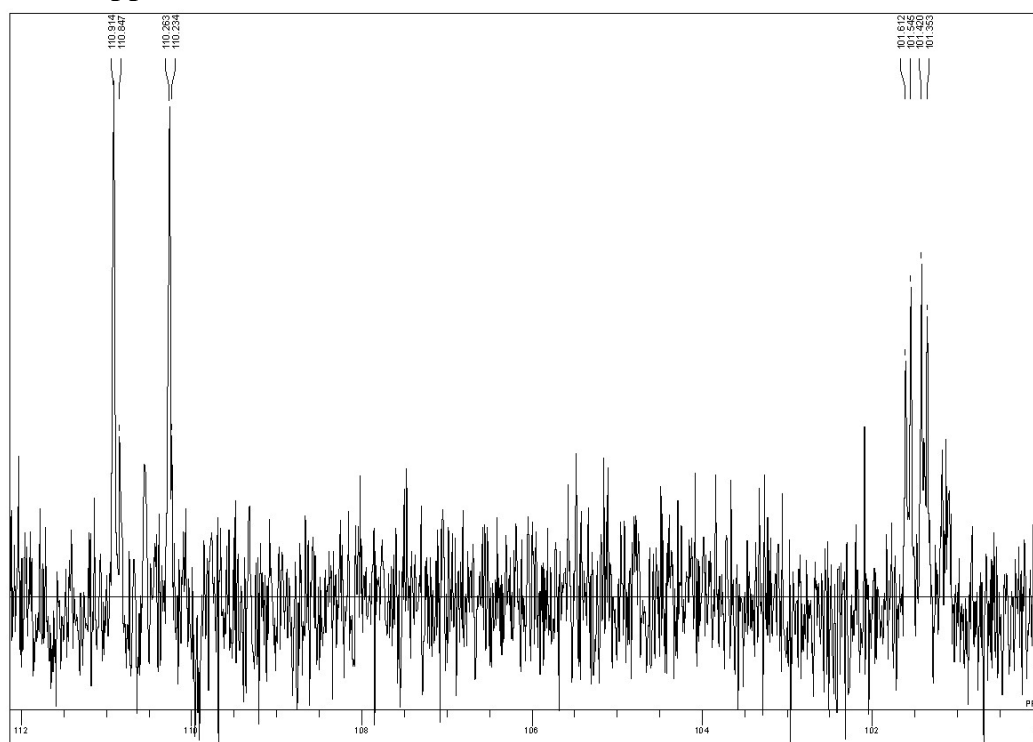
Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR of compound 3



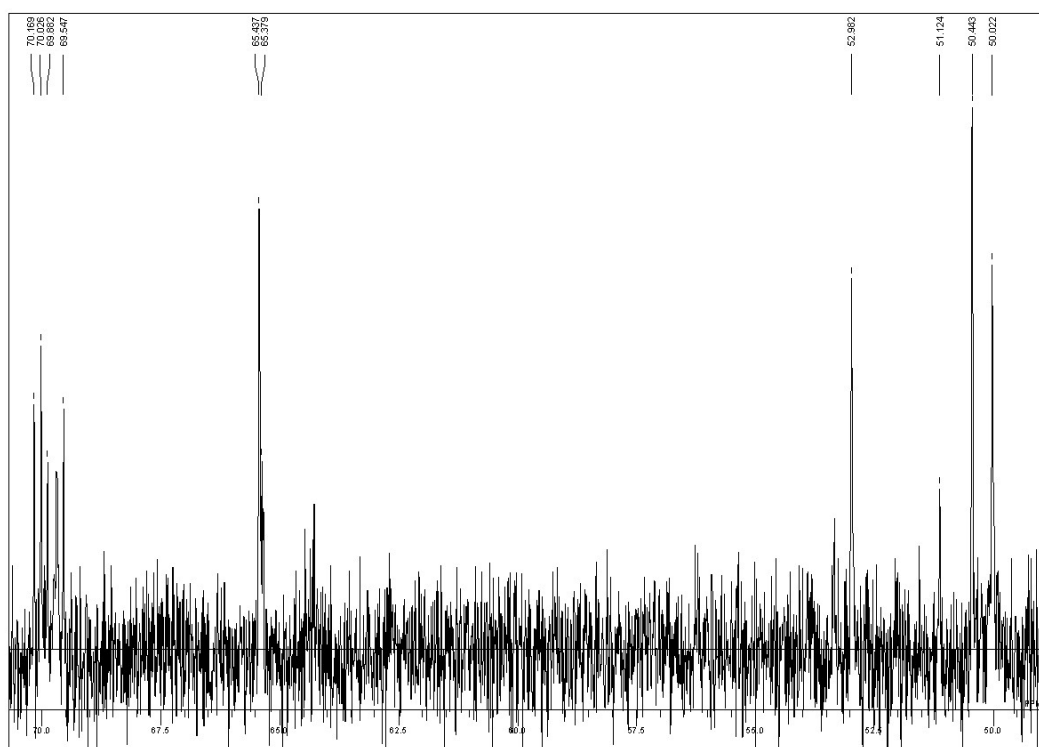
134.9-122.4 ppm



110.9-101.4 ppm



70.1-50.0 ppm



53.0-21.5 ppm

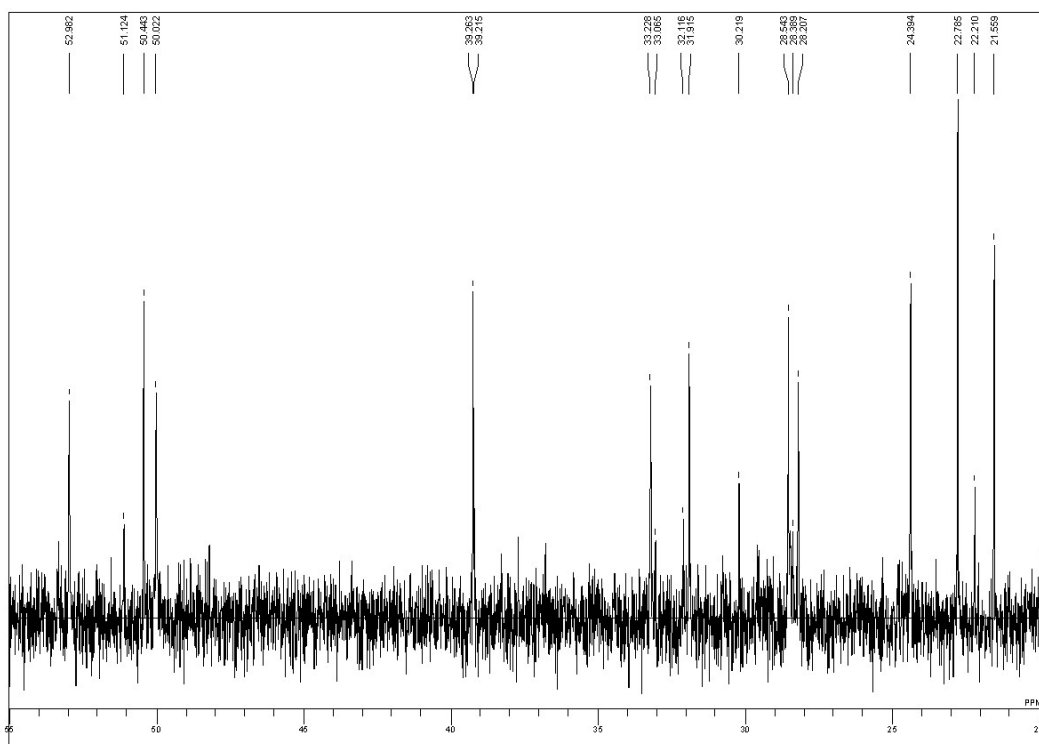
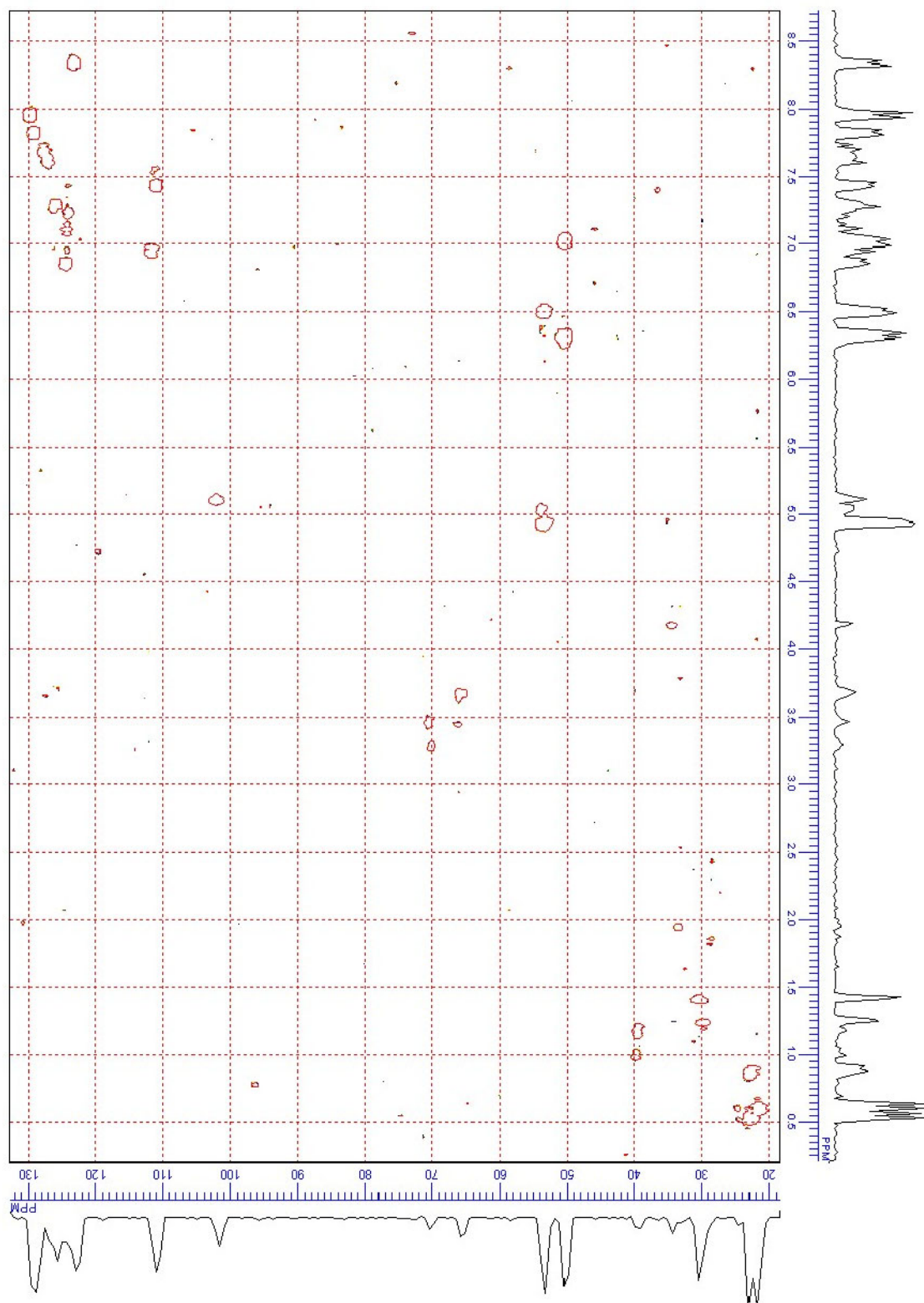
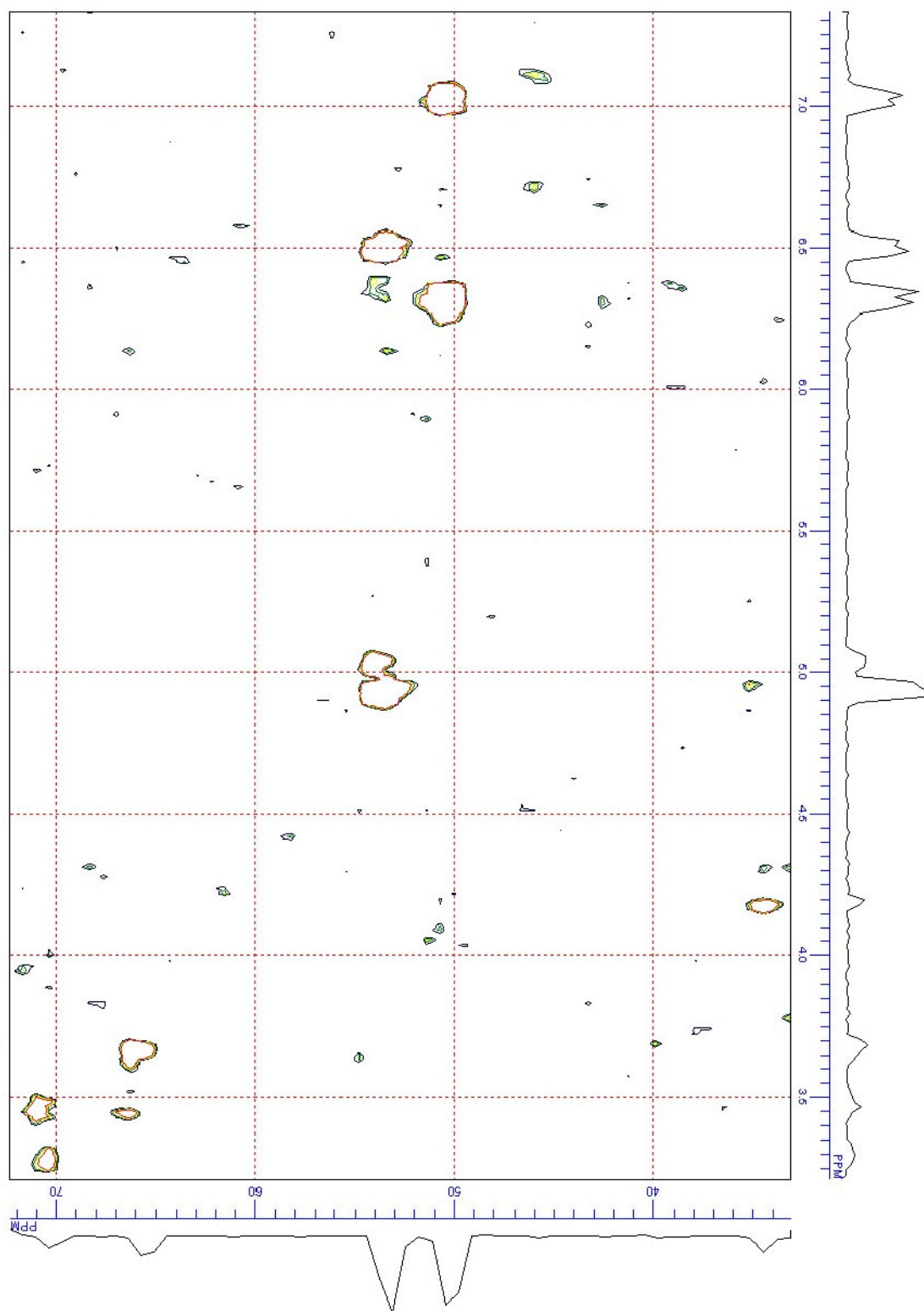


Figure S3. HMQC-NMR of compound 3





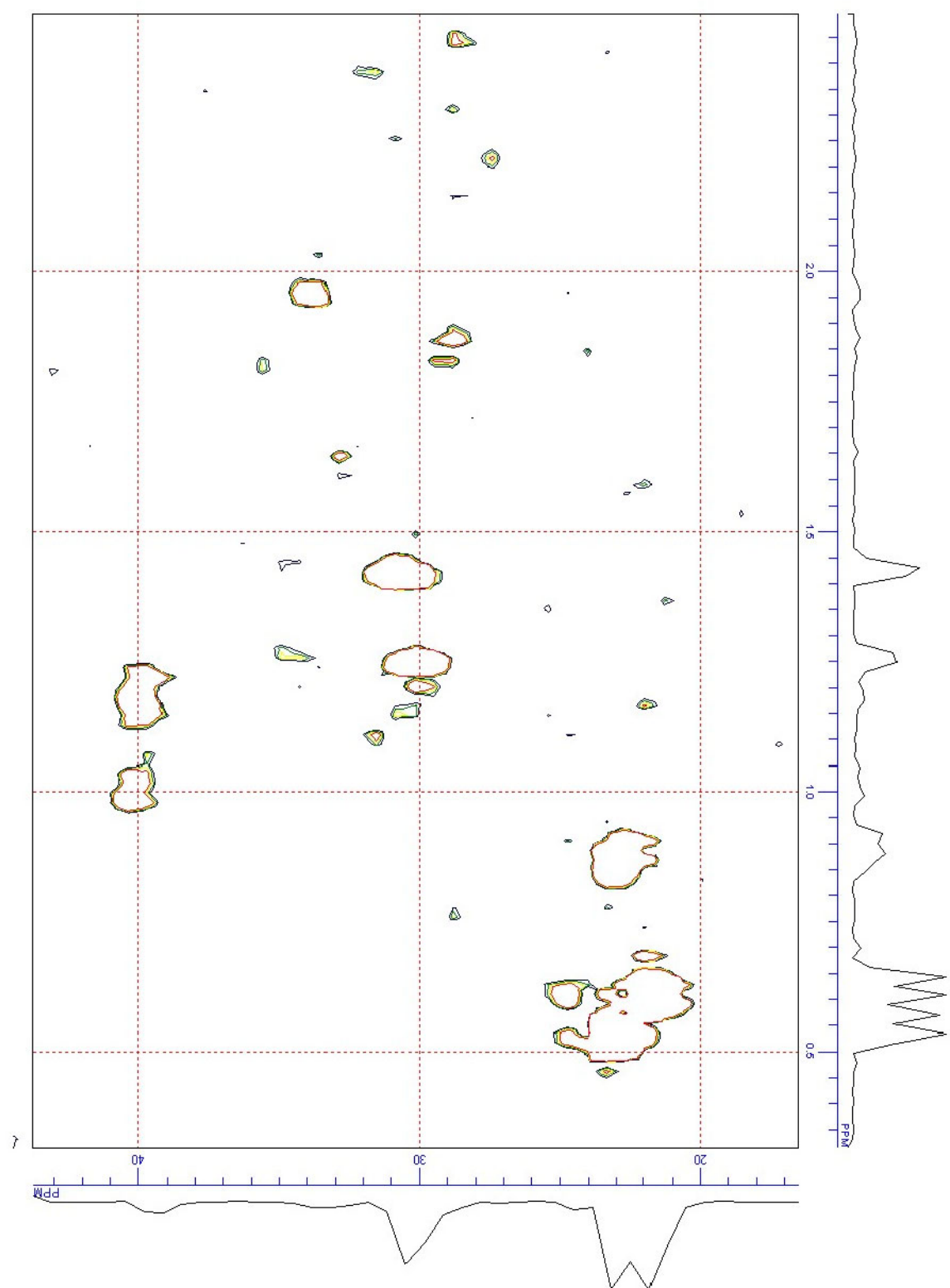
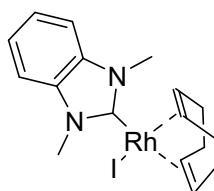
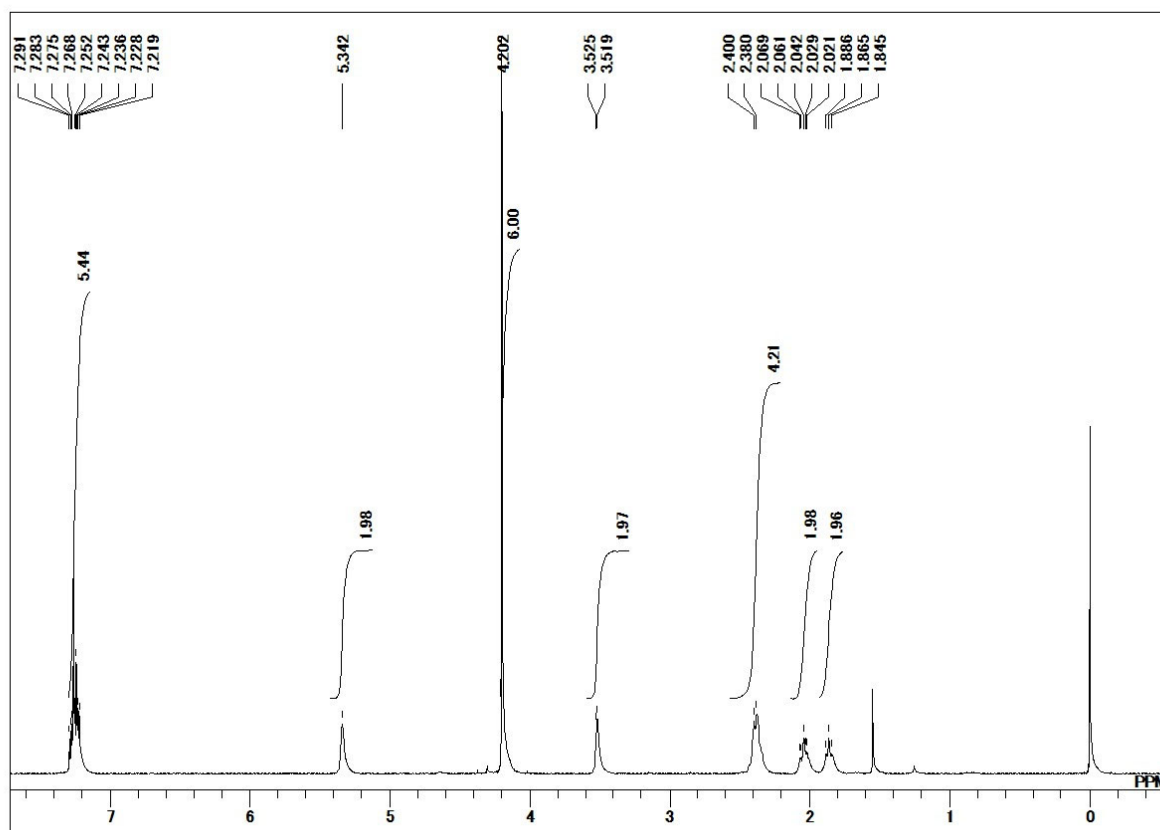


Figure S4. ^1H NMR of compound 4



HRMS (ESI-TOF), m/z : calcd for $\text{C}_{17}\text{H}_{22}\text{N}_2\text{Rh}$ $[\text{M}-\text{I}]^+$, 357.0832, found, 357.0832.

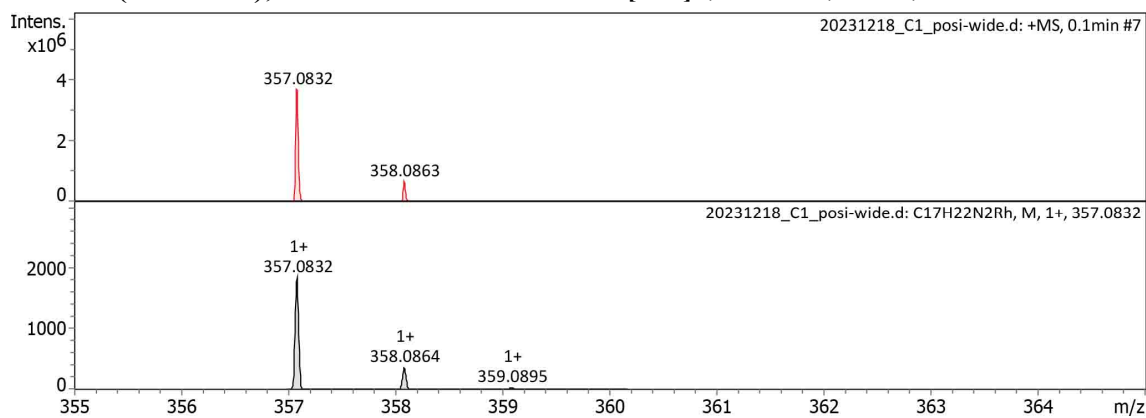


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR of compound 4

