

Supporting Information

Engineering Ru(II) Schiff Base Complexes as Bio functional Materials: Cytotoxic and Cell Imaging Perspectives

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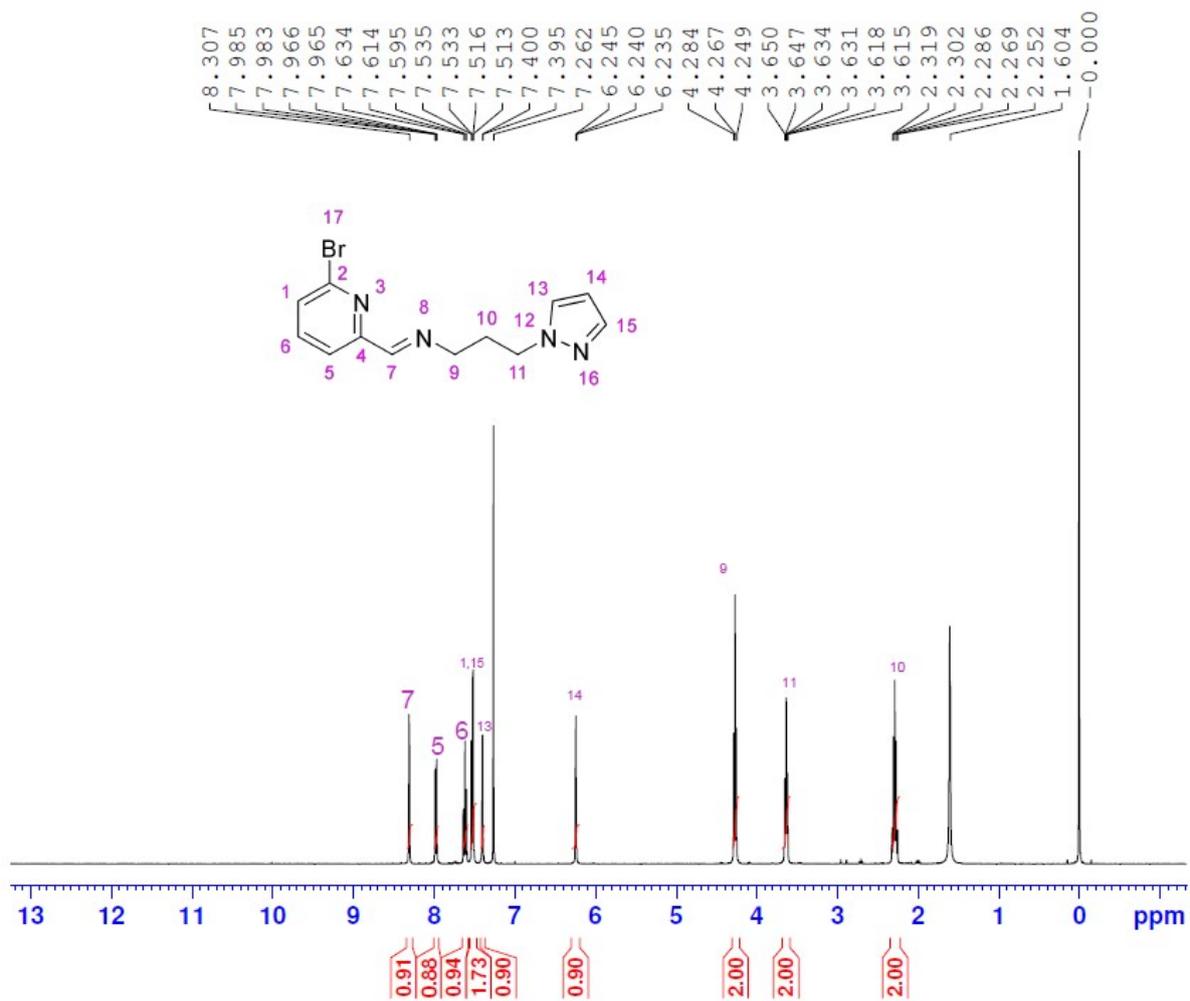


Figure S1 ¹H-NMR spectrum of ligand L1

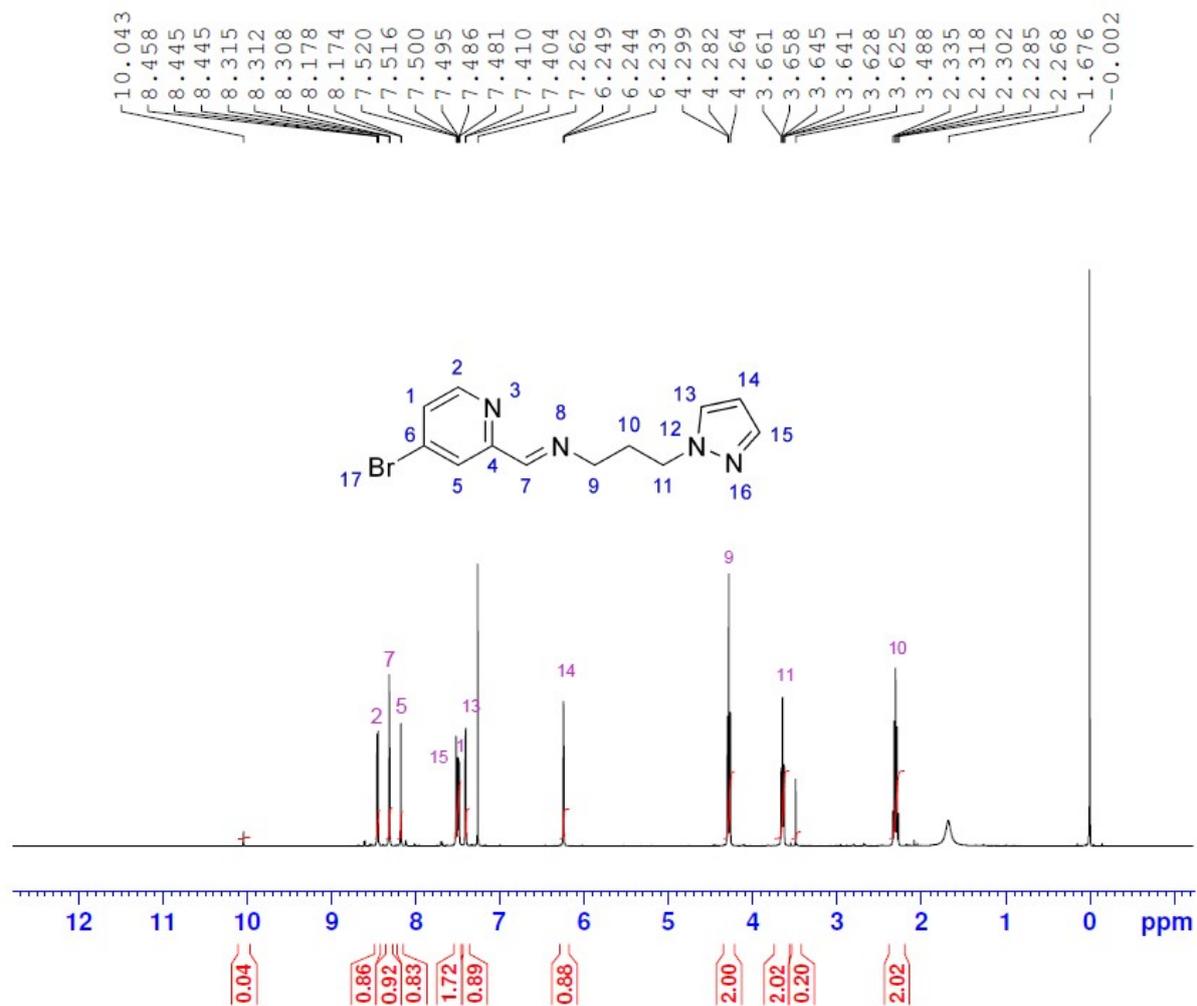


Figure S2 ¹H- NMR spectrum of ligand L2

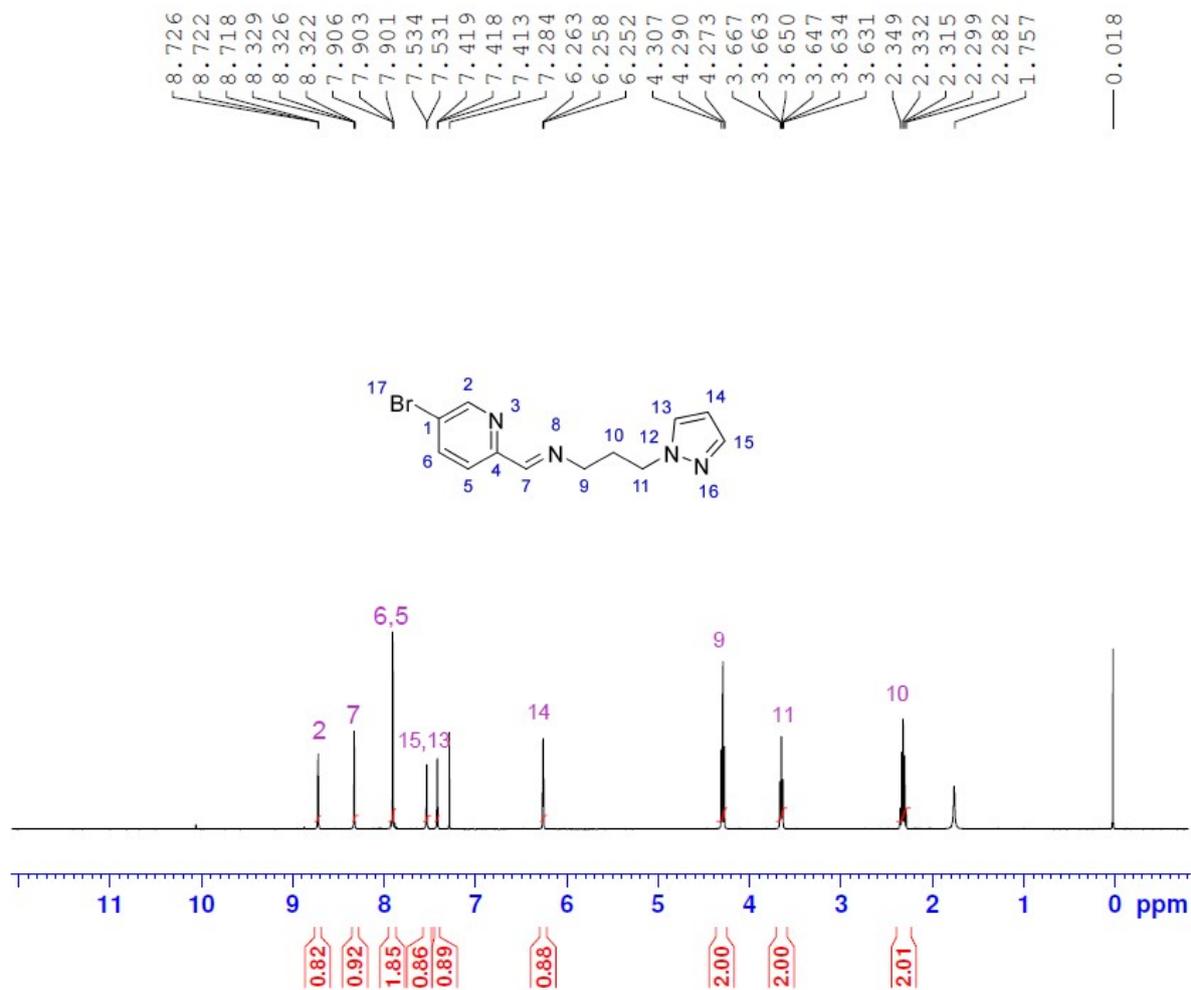


Figure S3 ¹H- NMR spectrum of ligand L3

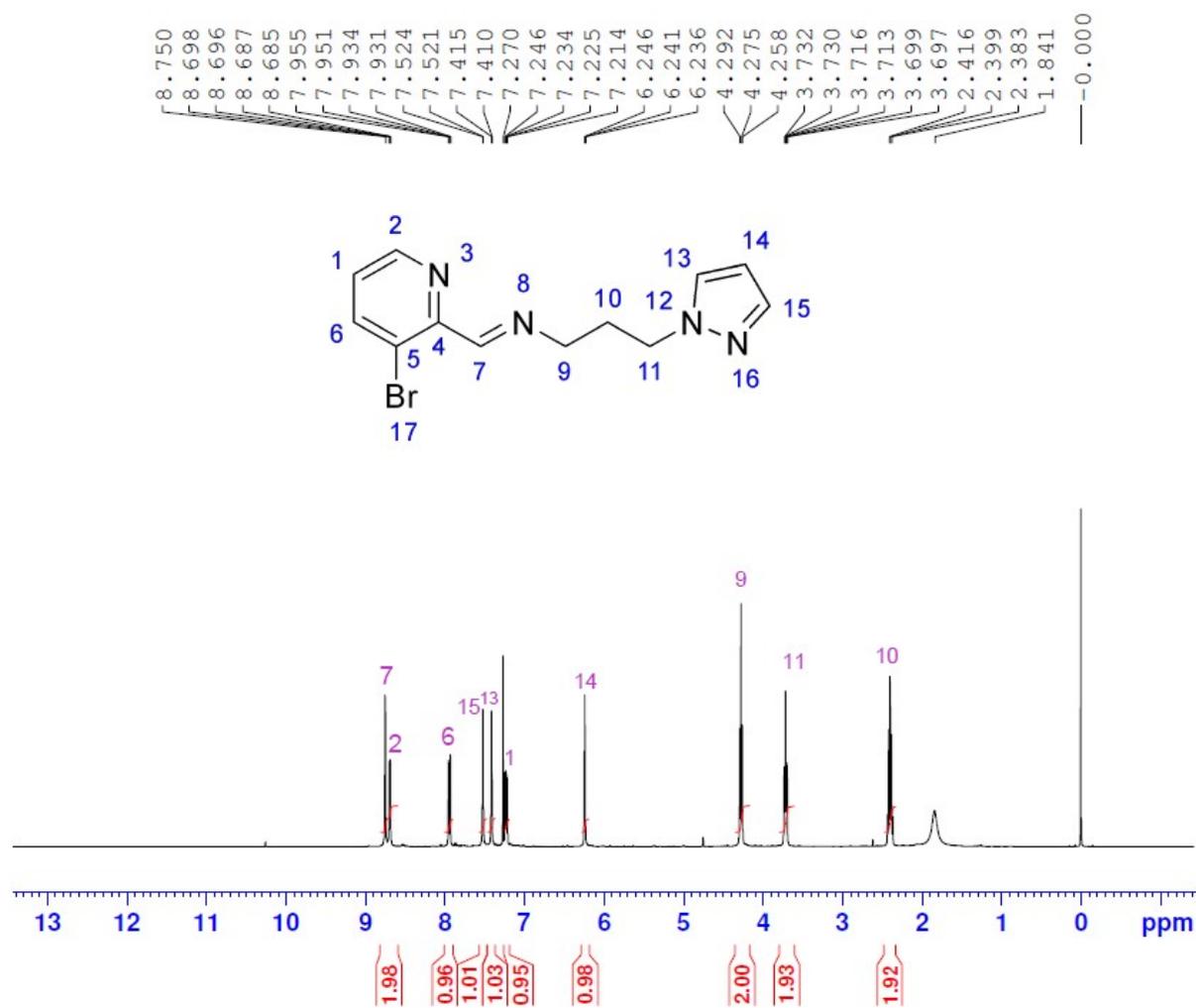


Figure S4 ¹H- NMR spectrum of ligand L4

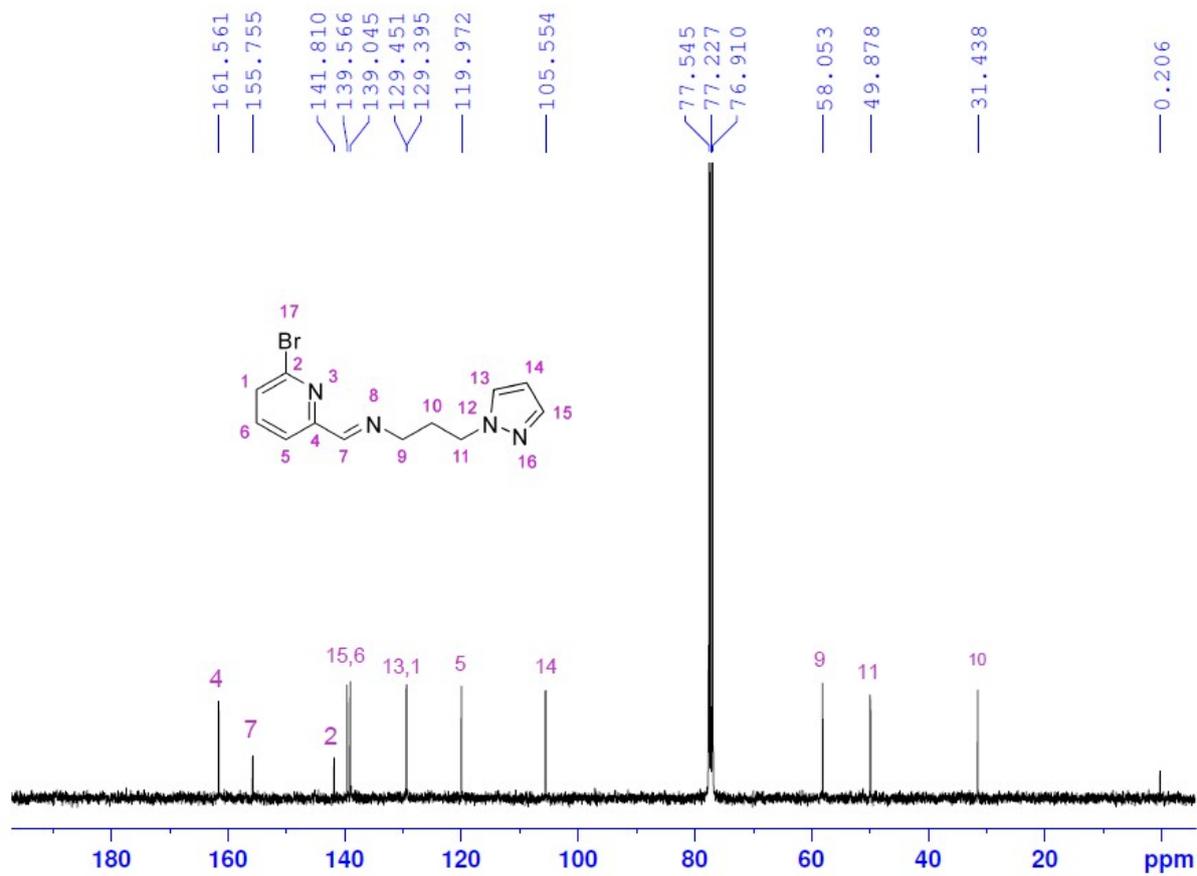


Figure S5 ^{13}C -NMR spectrum of ligand L1

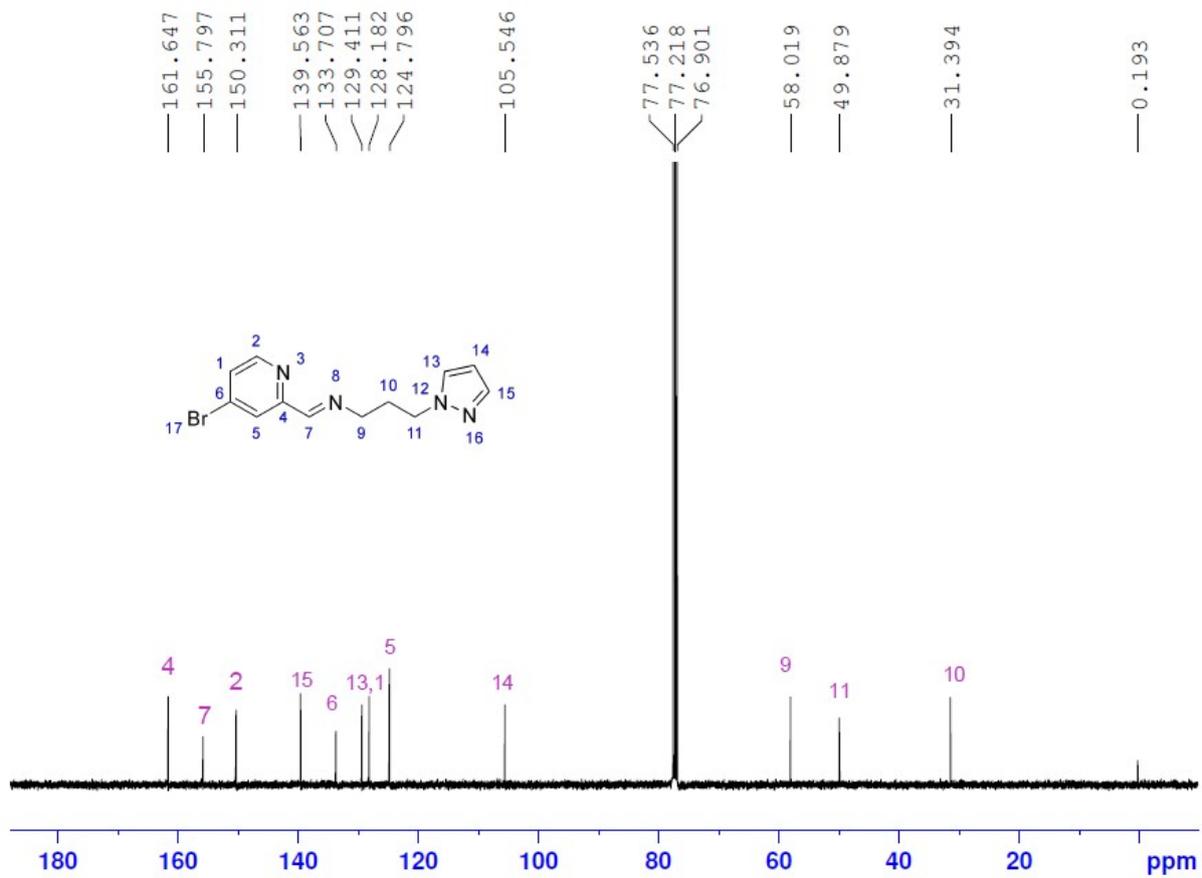


Figure S6 ^{13}C - NMR spectrum of ligand L2

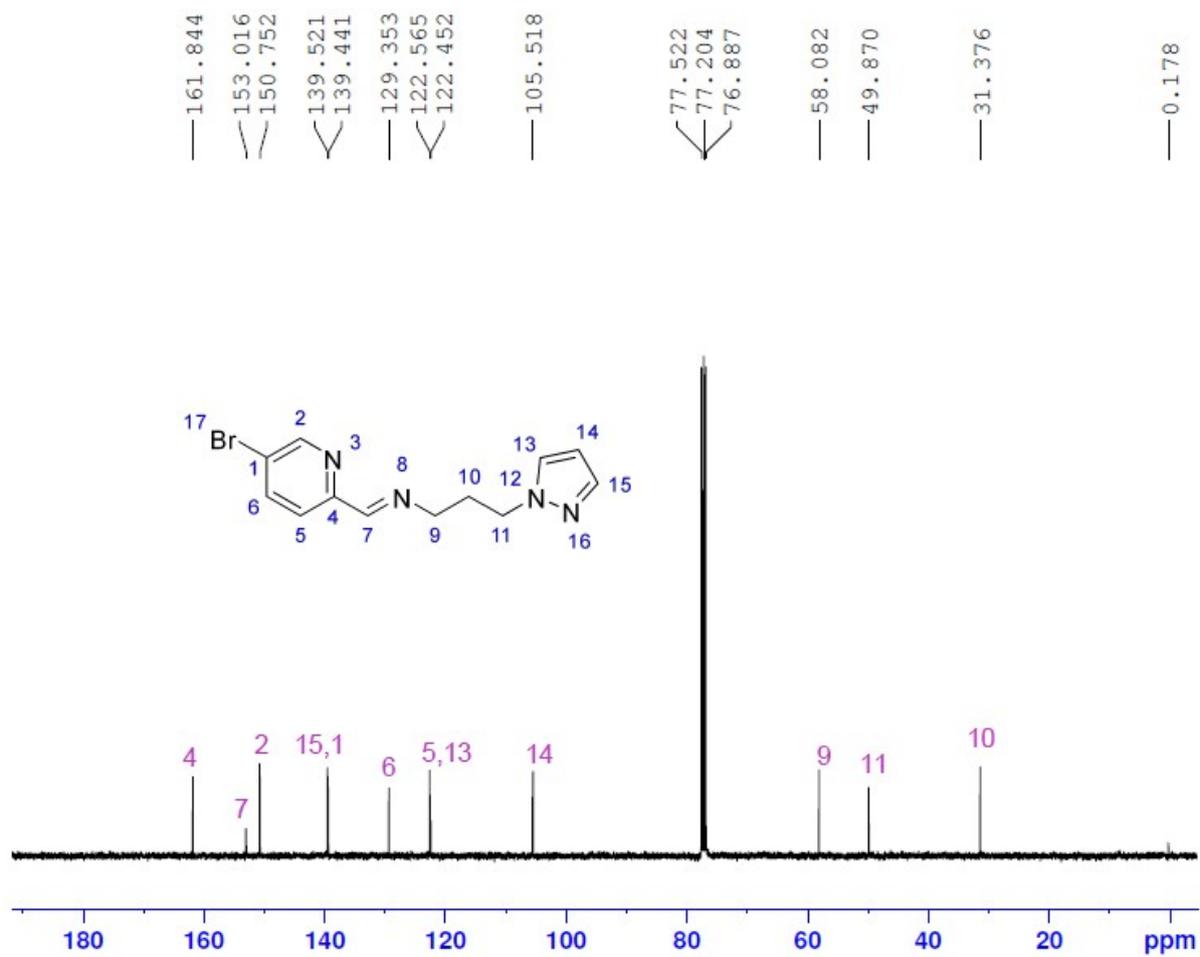


Figure S7 ¹³C- NMR spectrum of ligand L3

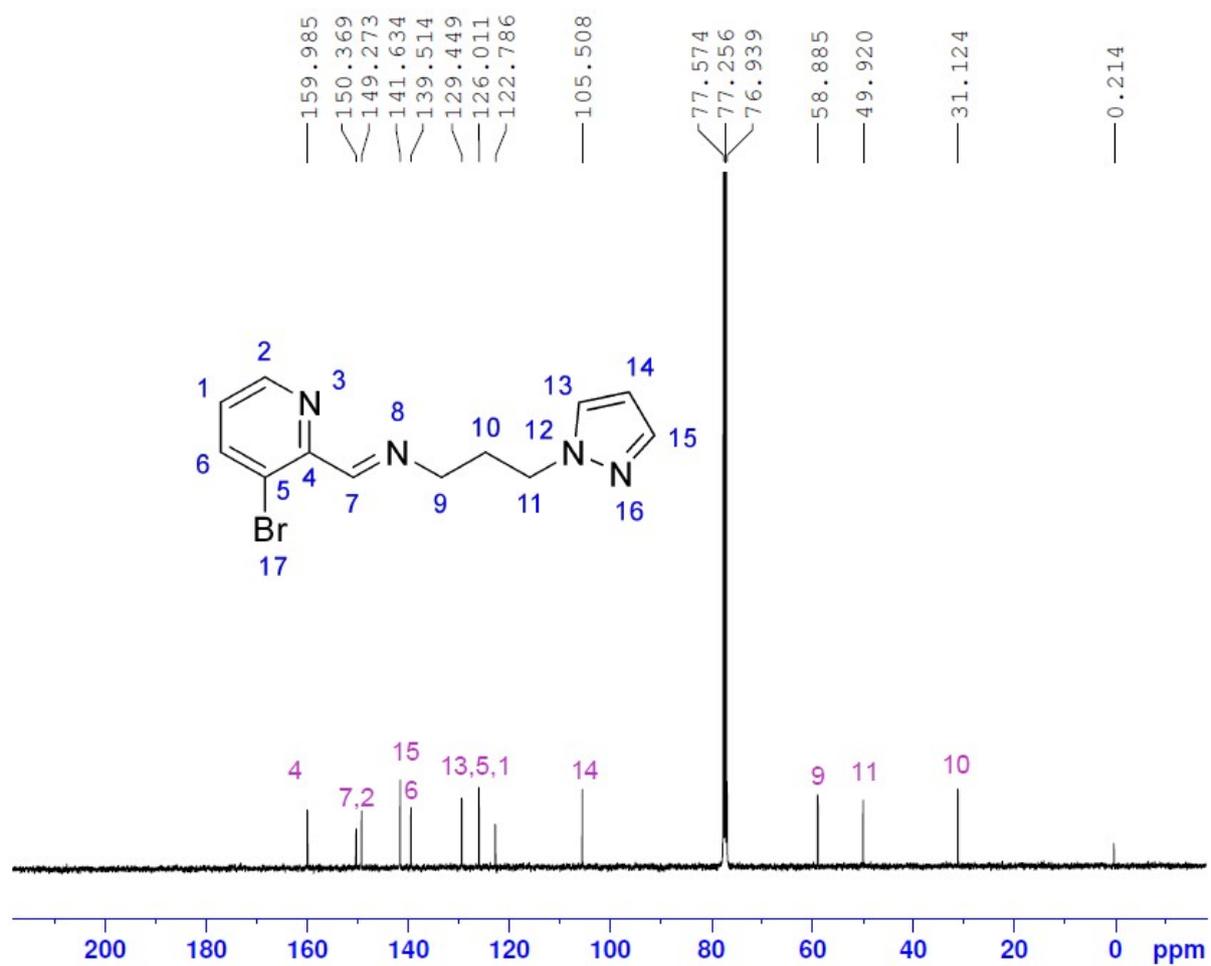


Figure S8 ¹³C- NMR spectrum of ligand L4

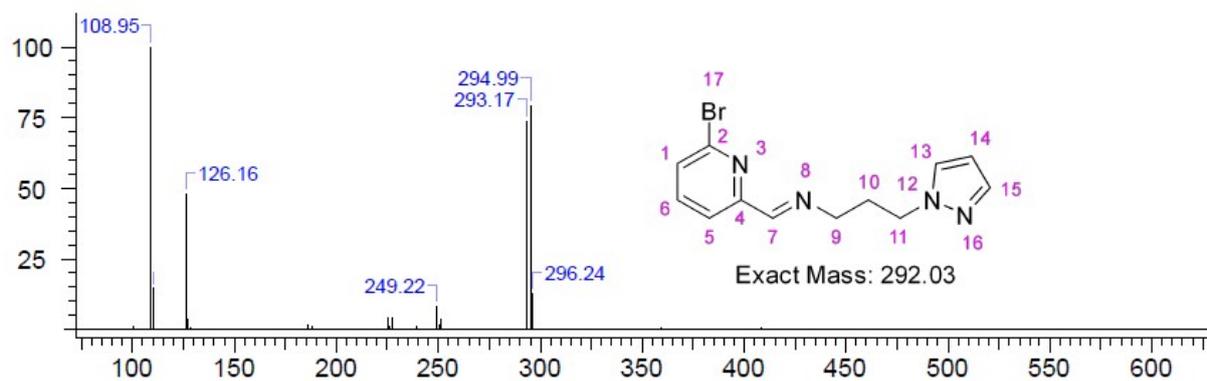


Figure S9 Mass spectrum of ligand L1

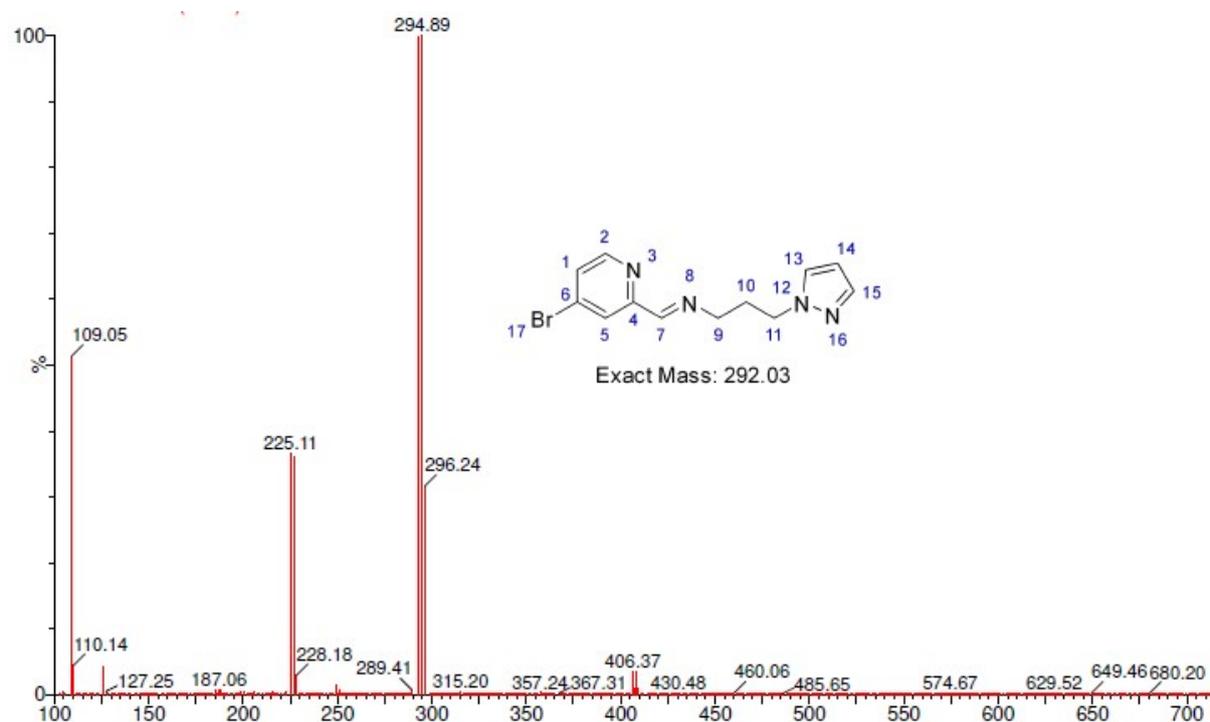


Figure S10 Mass spectrum of ligand L2

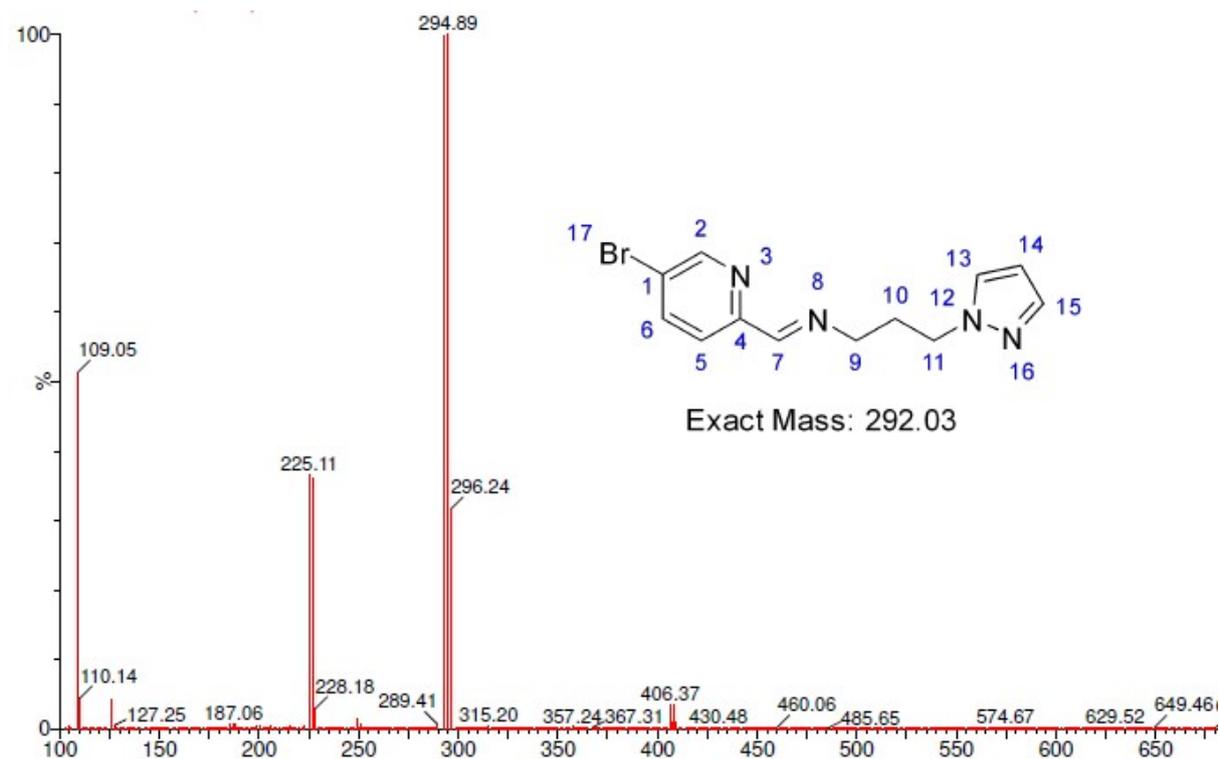


Figure S11 Mass spectrum of ligand L3

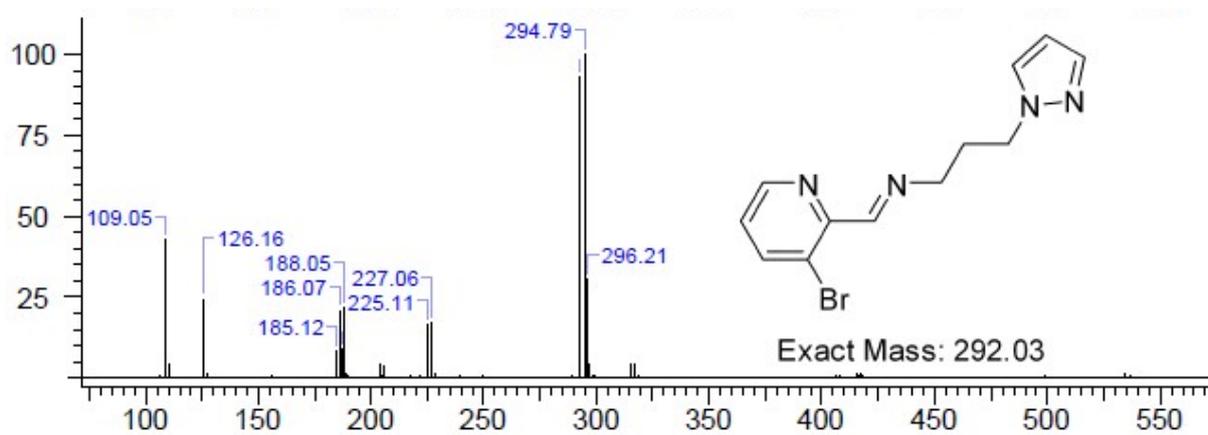


Figure S12 Mass spectrum of ligand L4

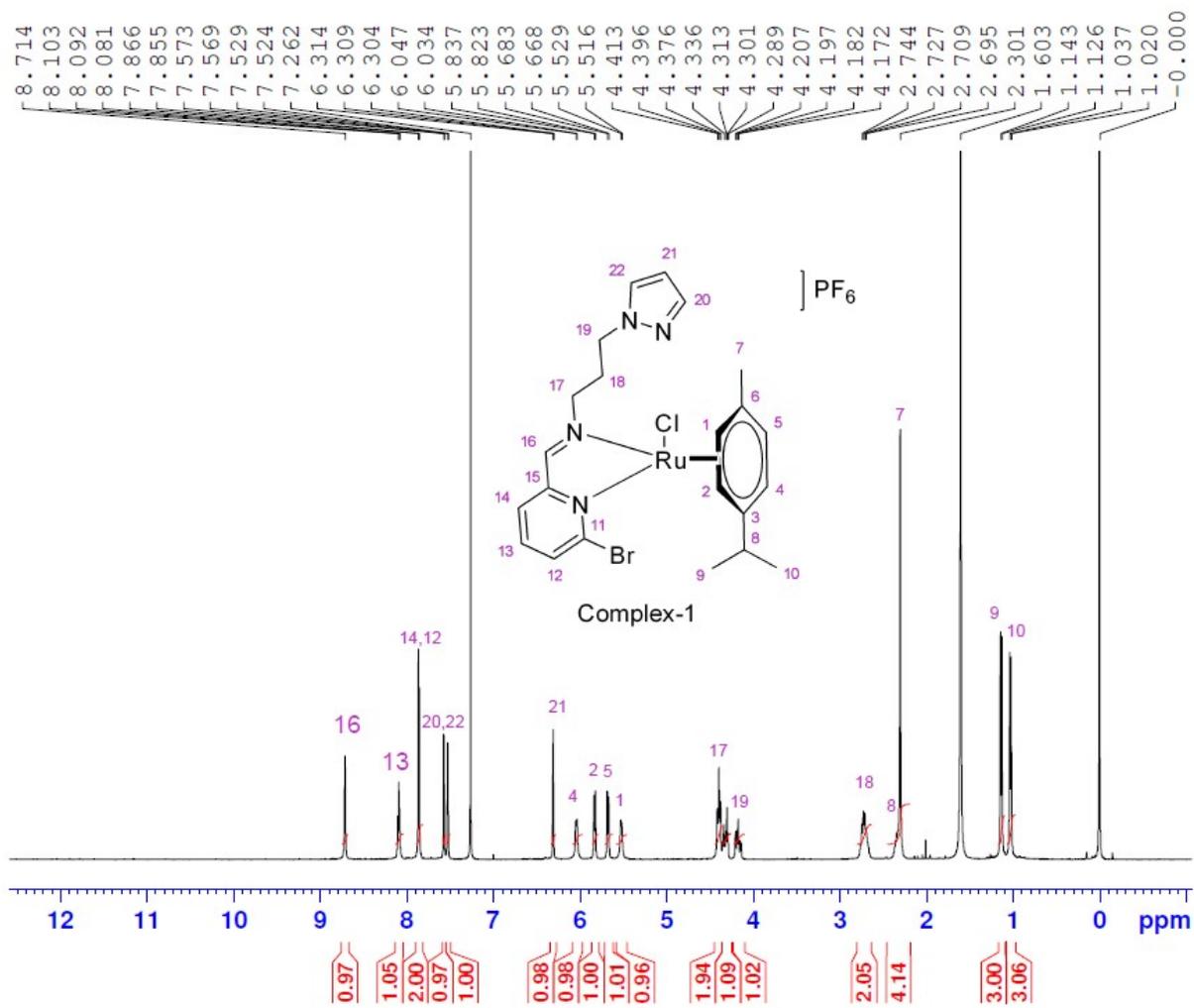


Figure S13 ¹H- NMR spectrum of complex 1

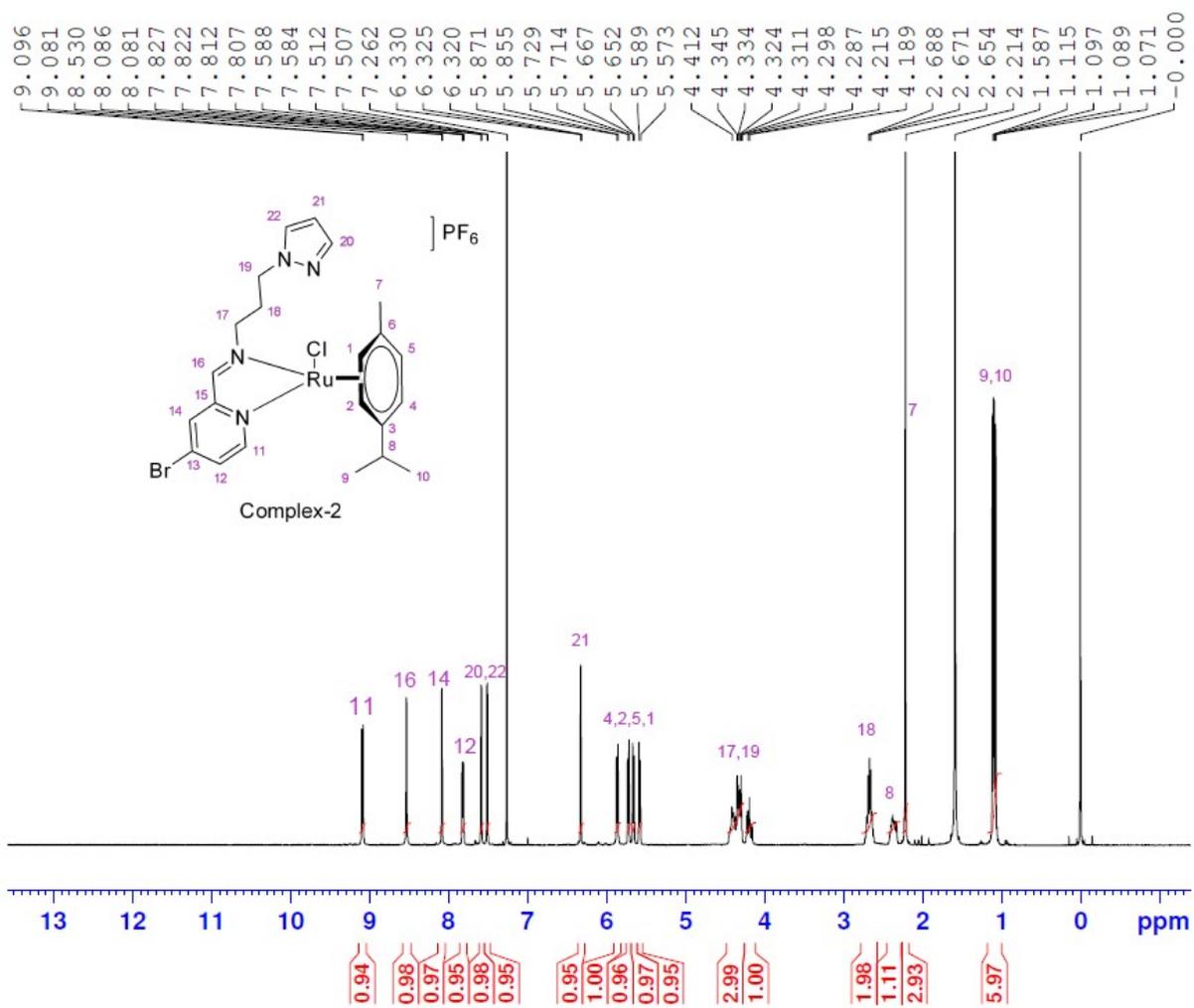


Figure S14 $^1\text{H-NMR}$ spectrum of complex 2

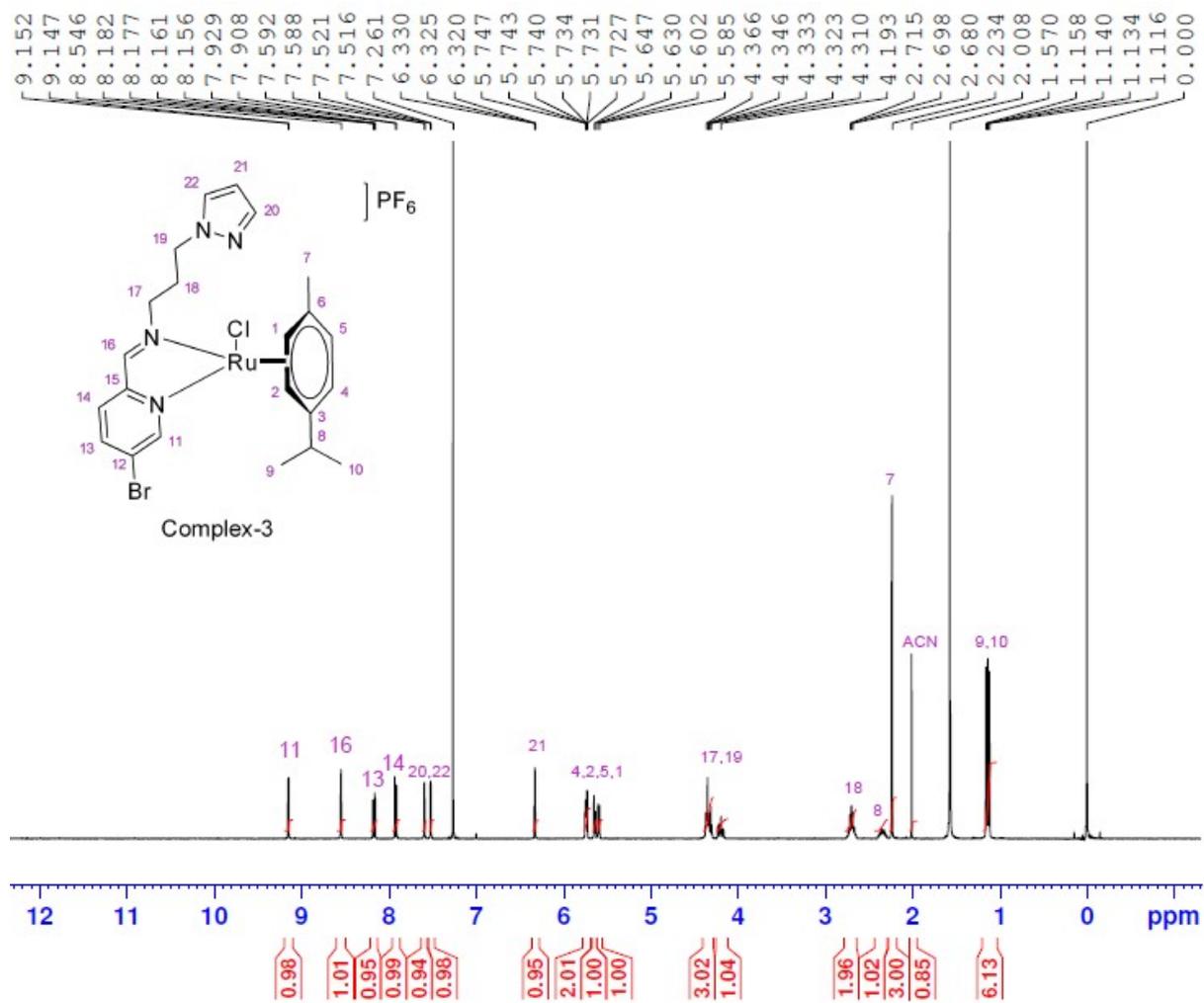


Figure S15 ¹H- NMR spectrum of complex 3

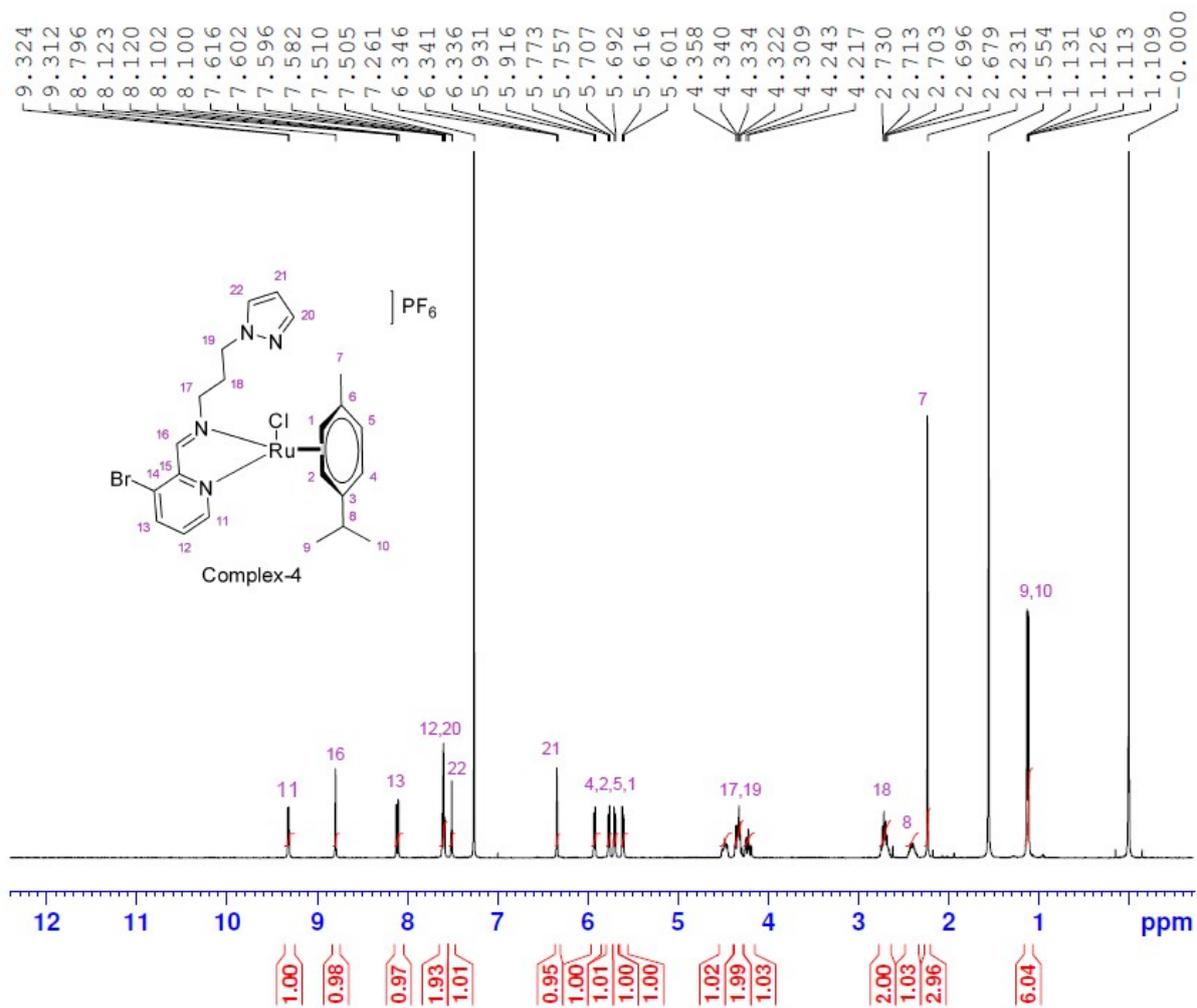


Figure S16 ¹H- NMR spectrum of complex 4

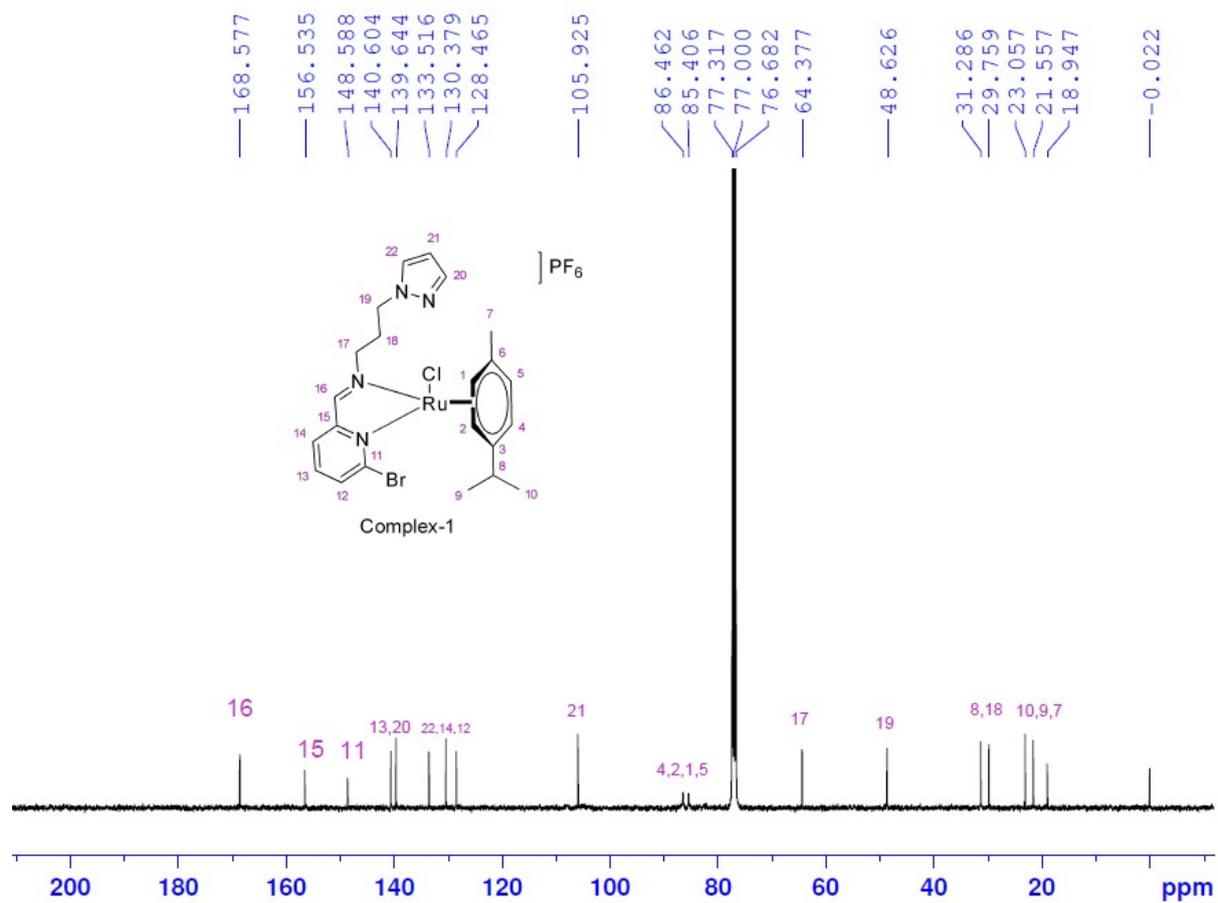


Figure S17 ^{13}C -NMR spectrum of complex 1

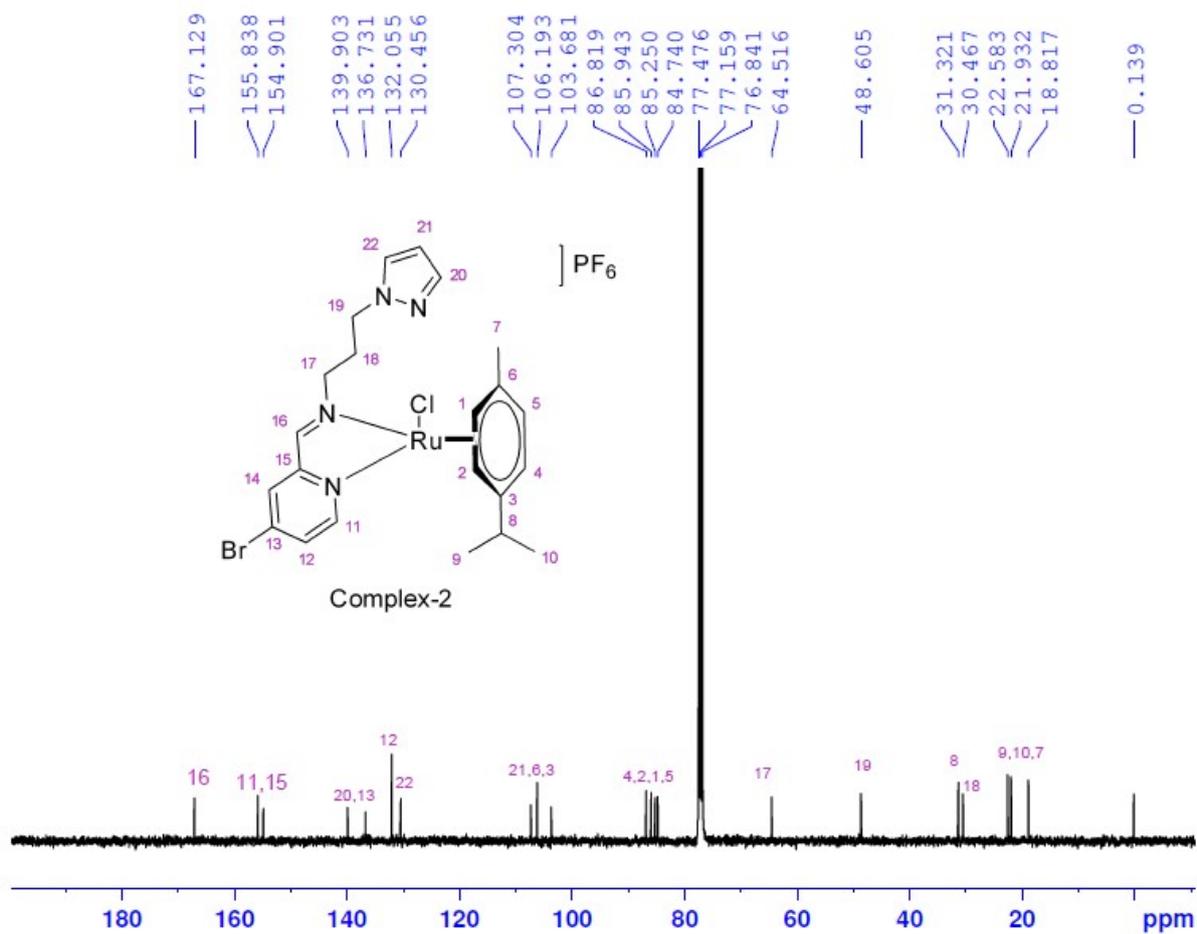


Figure S18 ^{13}C -NMR spectrum of complex 2

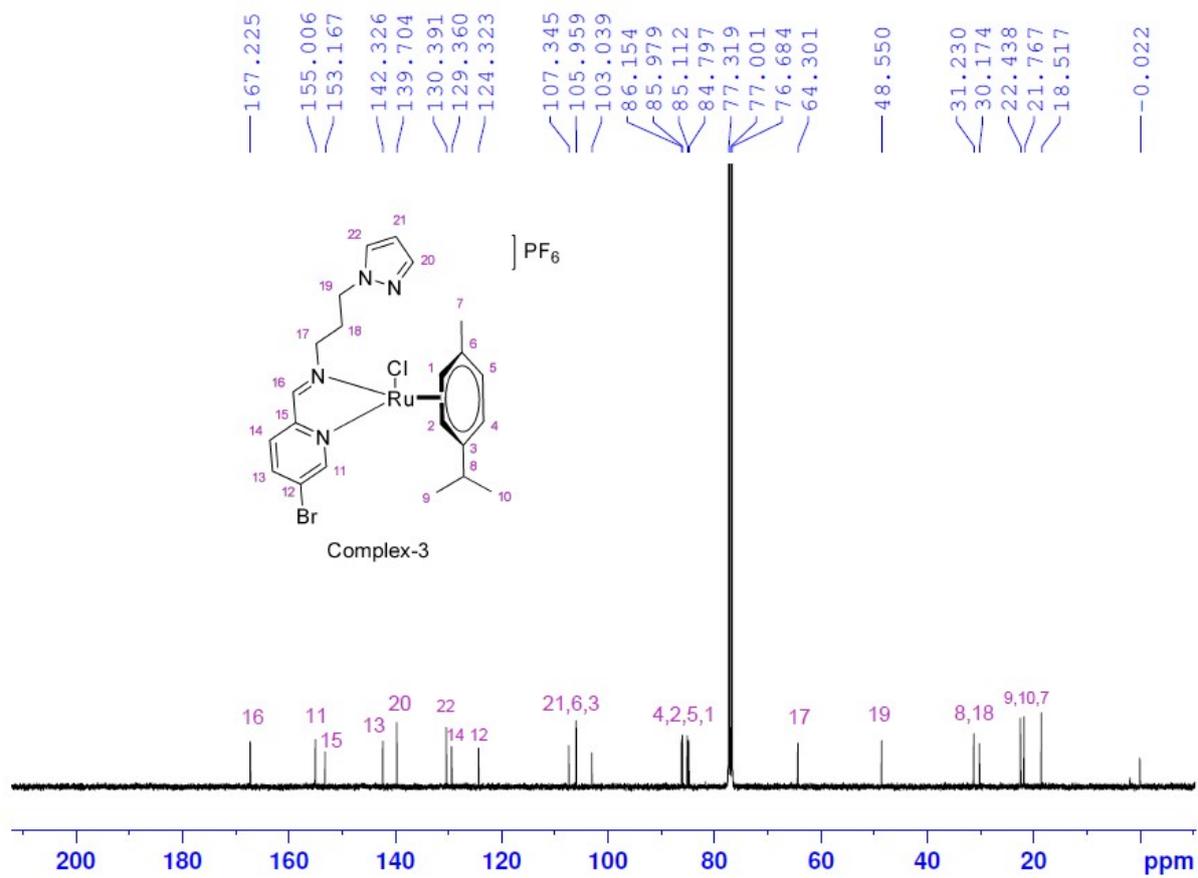


Figure S19 ^{13}C -NMR spectrum of complex 3

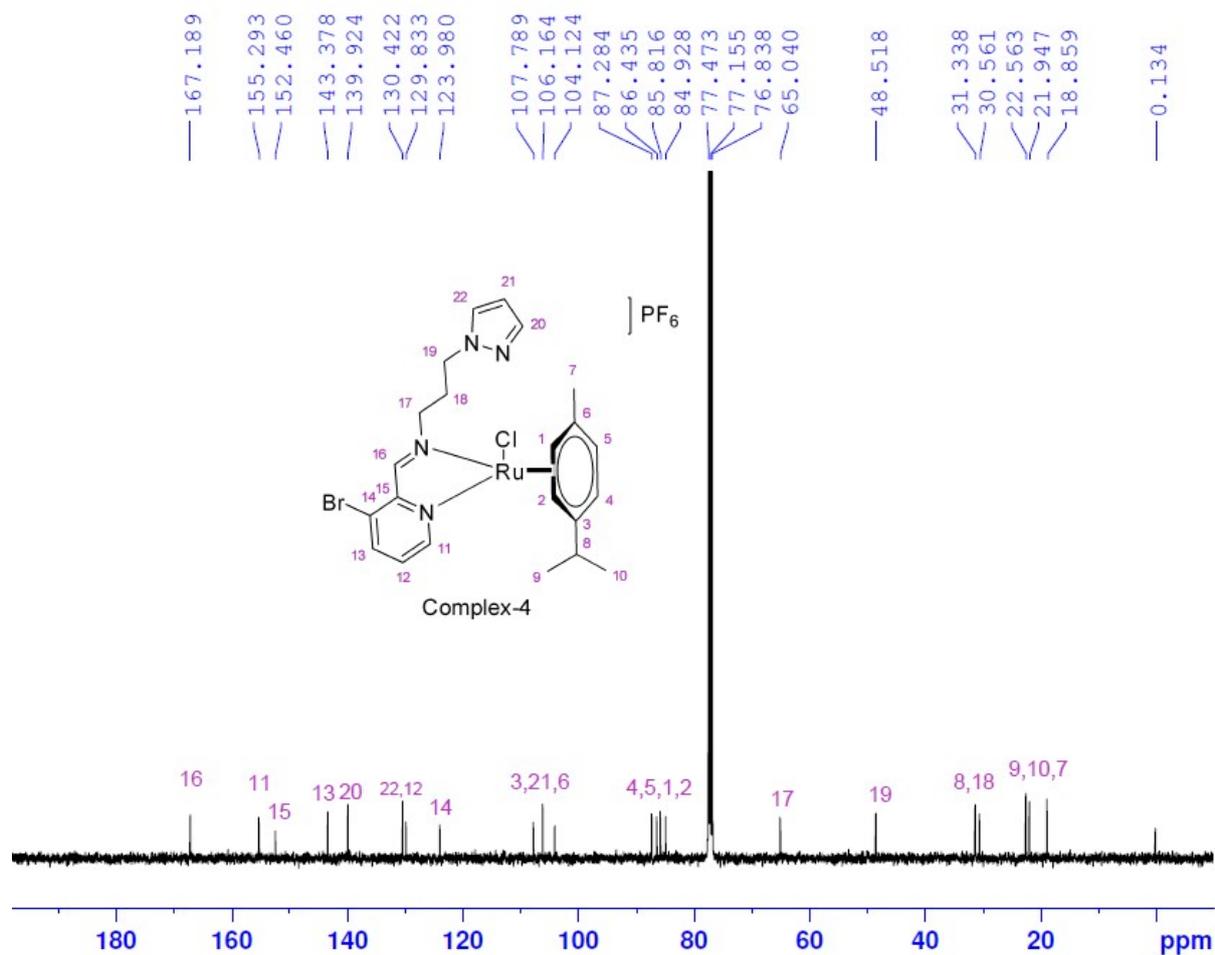


Figure S20 ^{13}C -NMR spectrum of complex 4

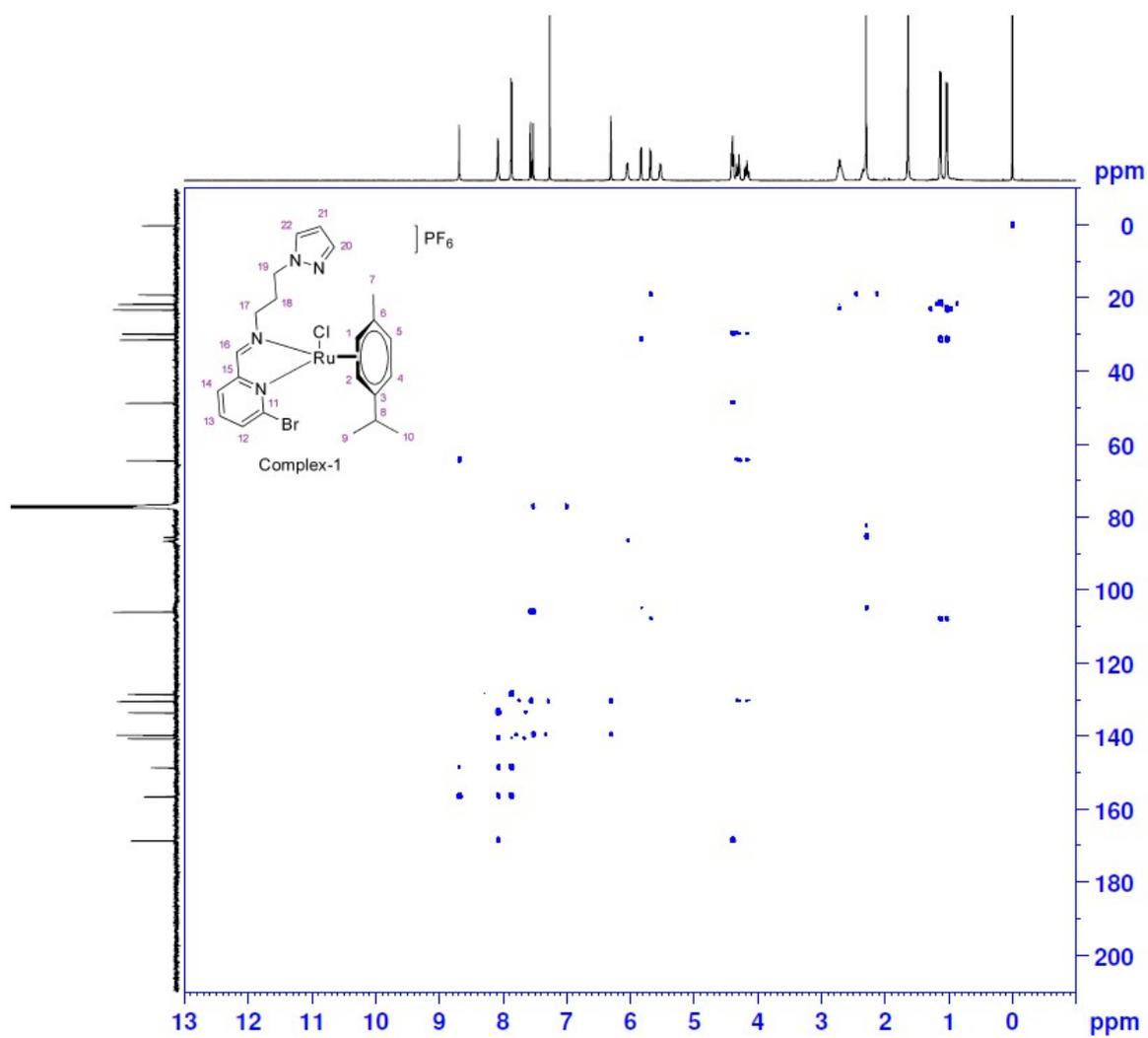


Figure S21 HMBC-NMR spectrum of complex 1

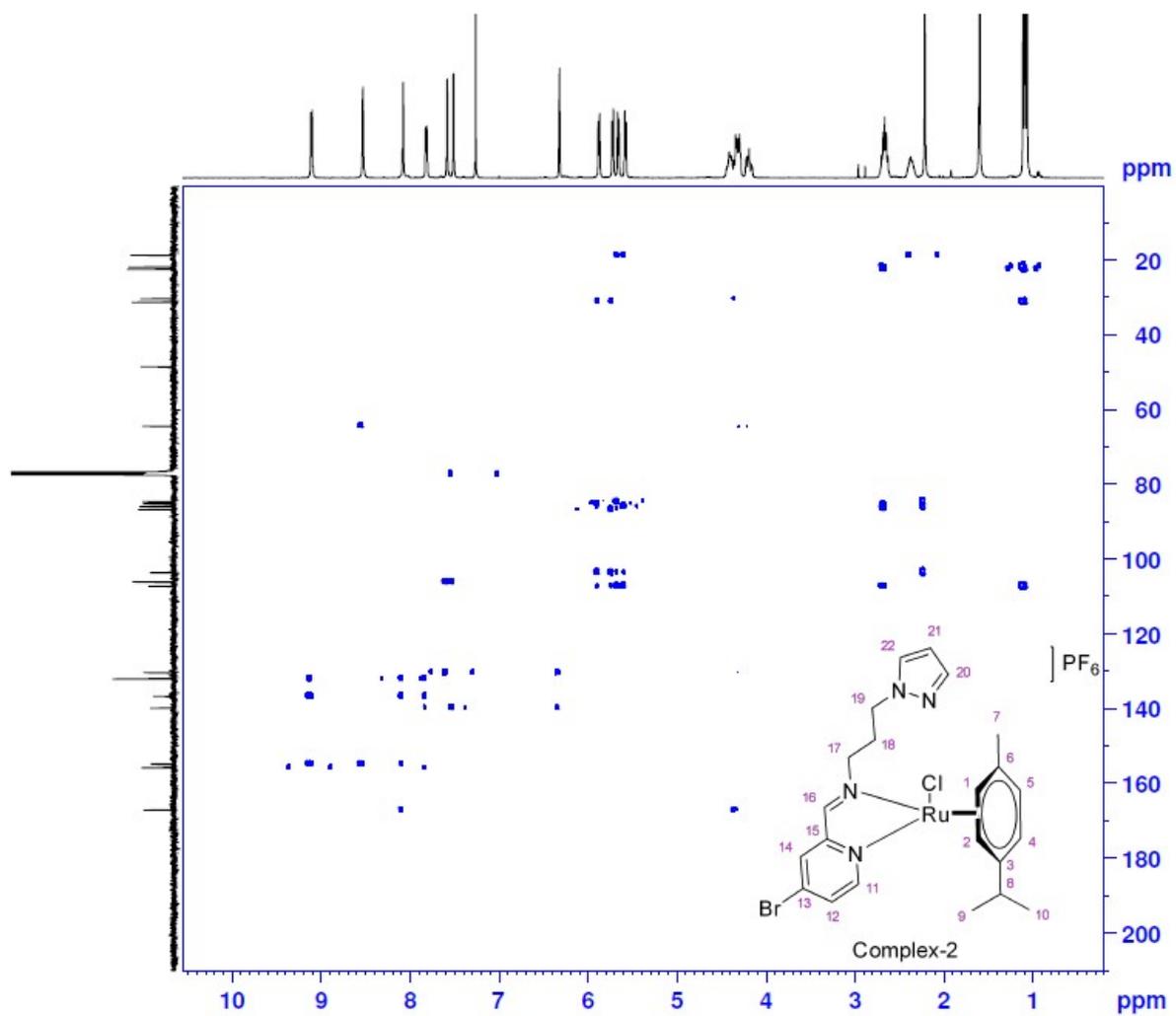


Figure S22 HMBC-NMR spectrum of complex 2

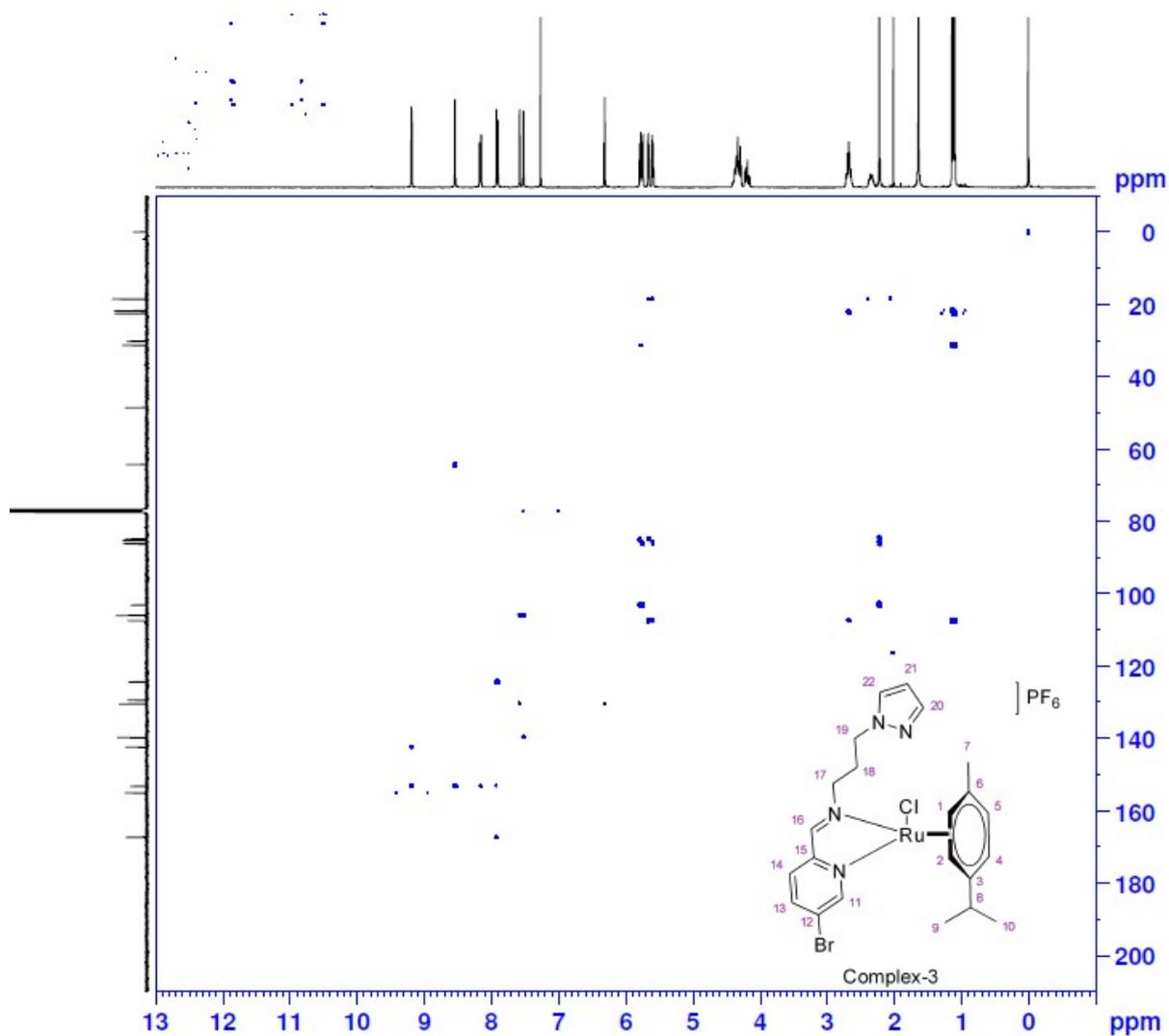


Figure S23 HMBC-NMR spectrum of complex 3

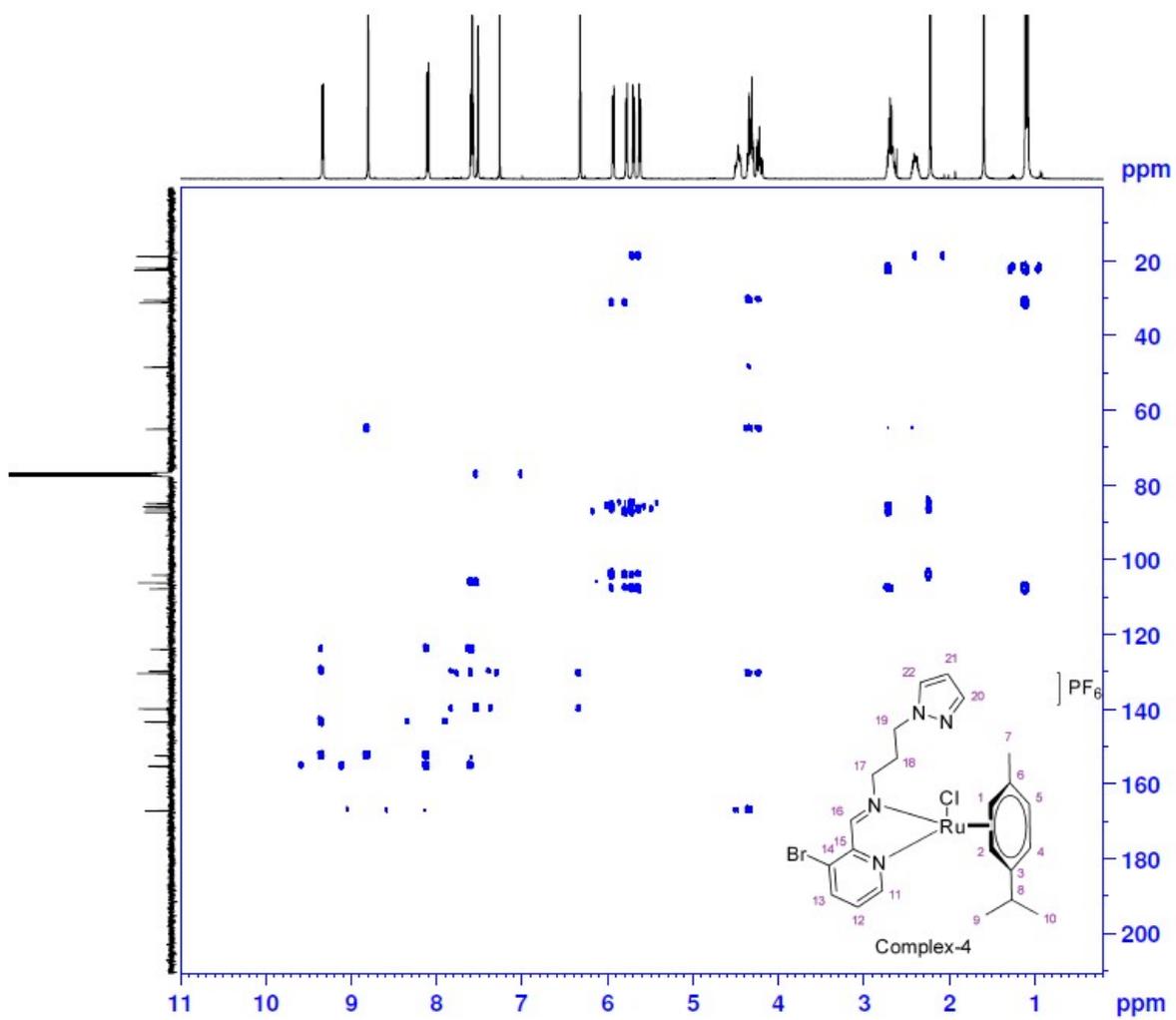


Figure S24 HMBC-NMR spectrum of complex 4

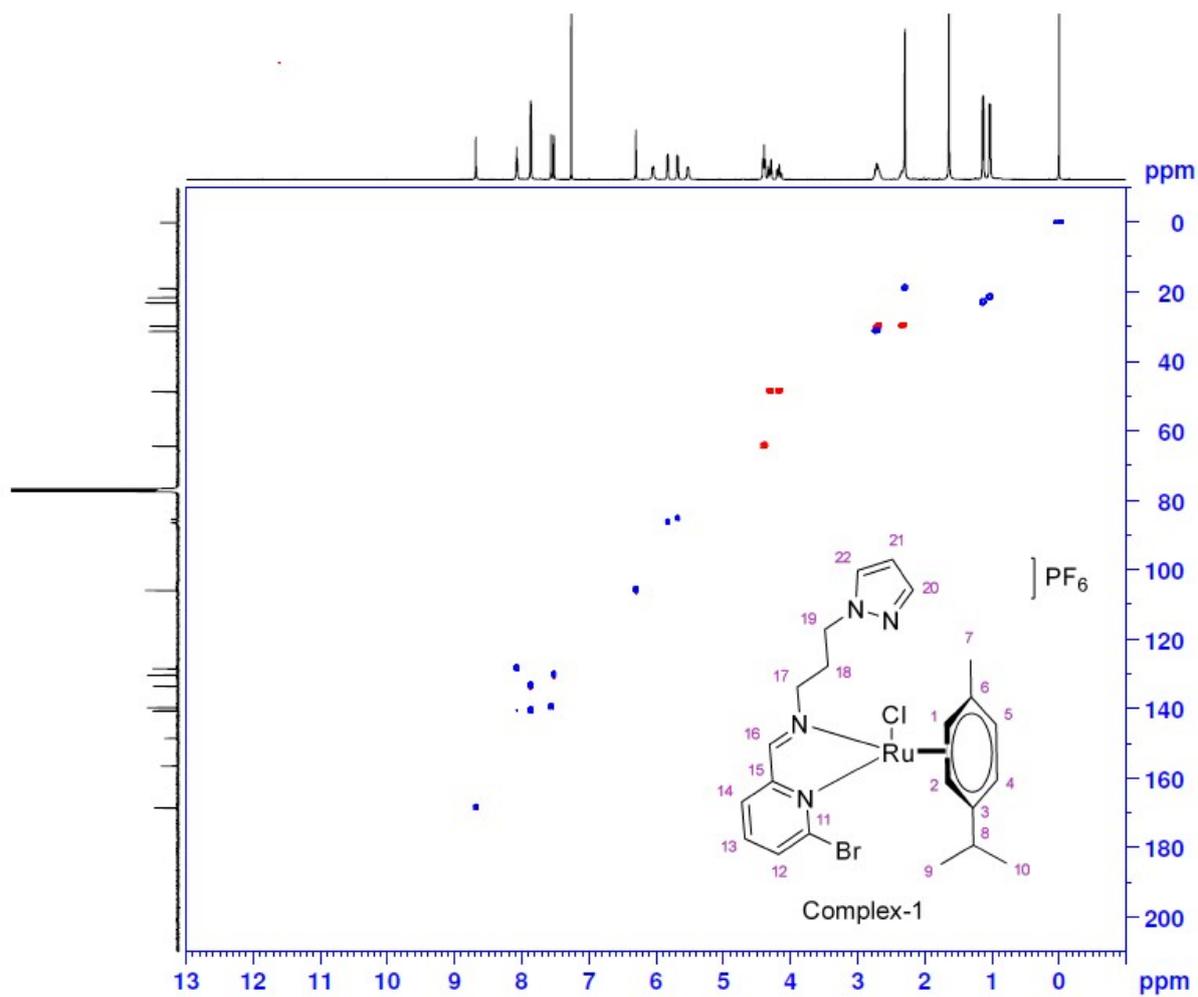


Figure S25 HSQC-NMR spectrum of complex 1

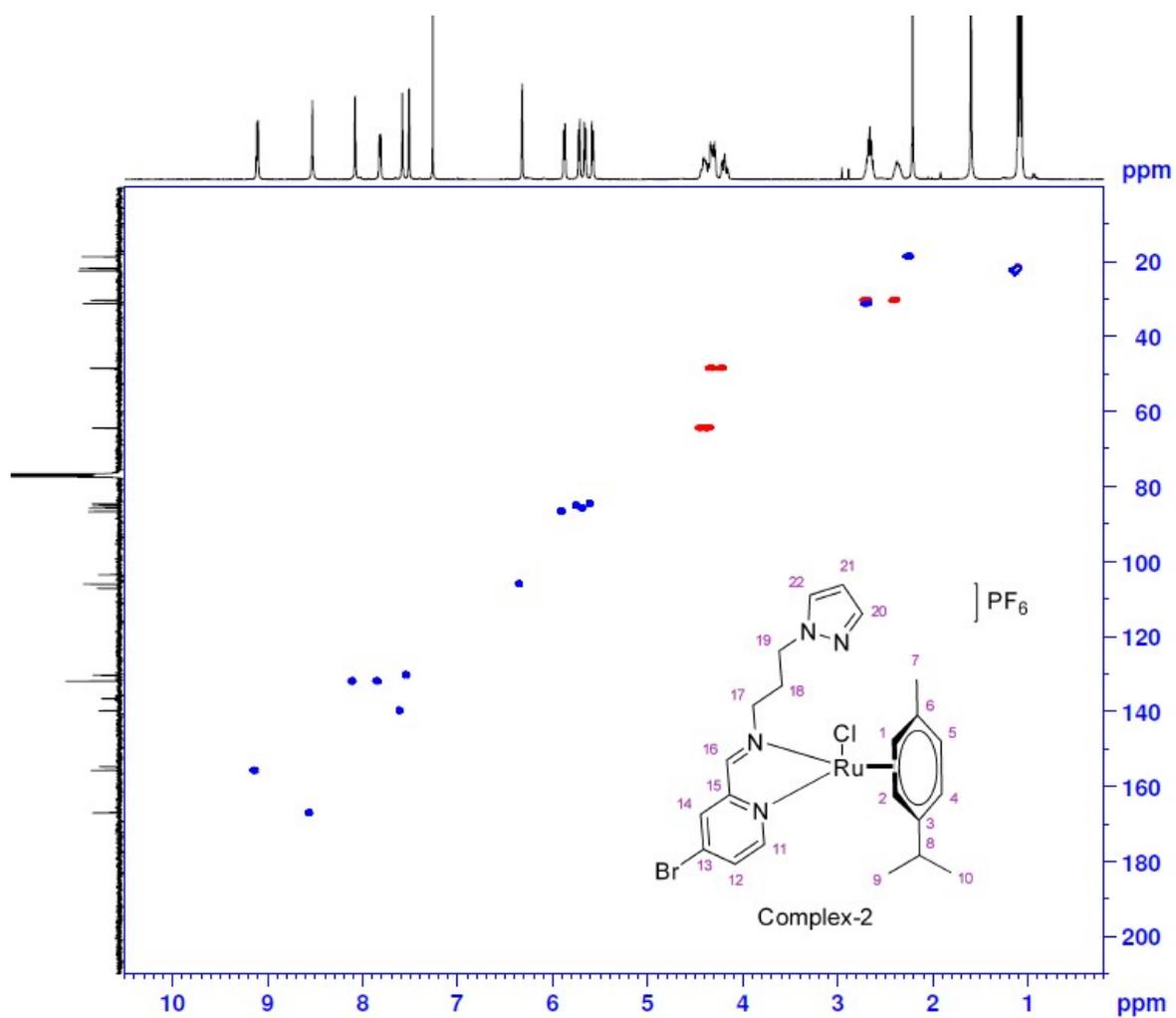


Figure S26 HSQC-NMR spectrum of complex 2

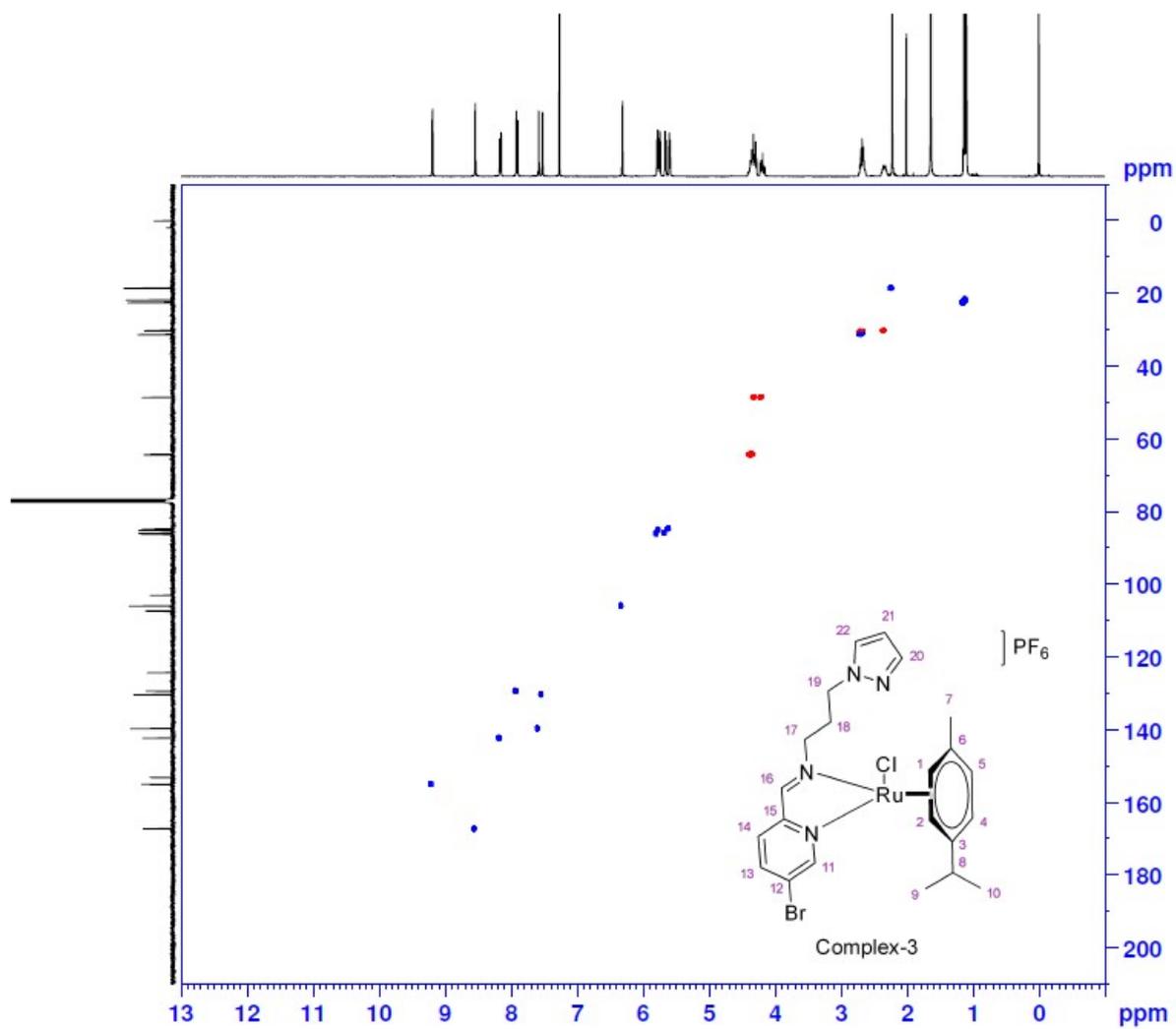


Figure S27 HSQC-NMR spectrum of complex 3

-70.401
-72.296

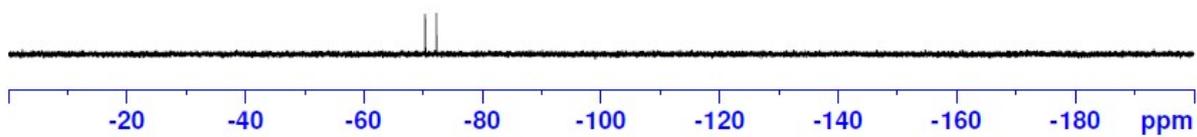
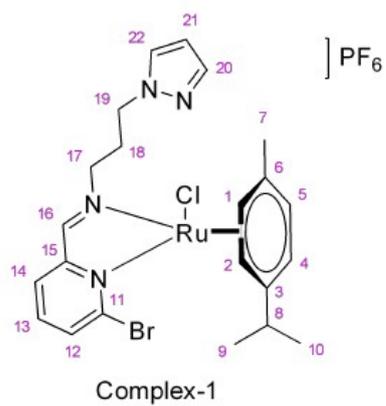


Figure S28 ¹⁹F- NMR spectrum of complex 1

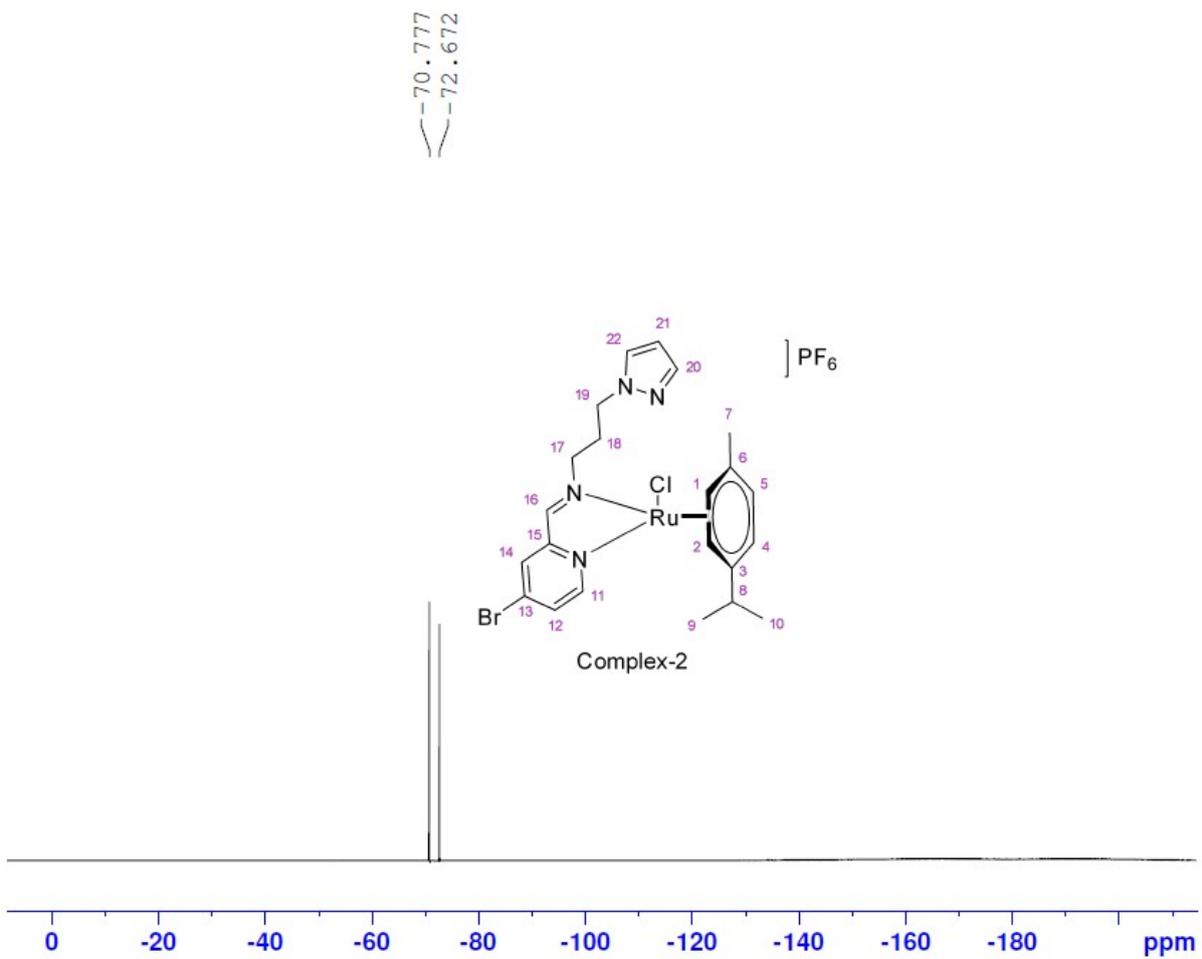


Figure S29 ^{19}F - NMR spectrum of complex 2

— -71.152
— -73.043

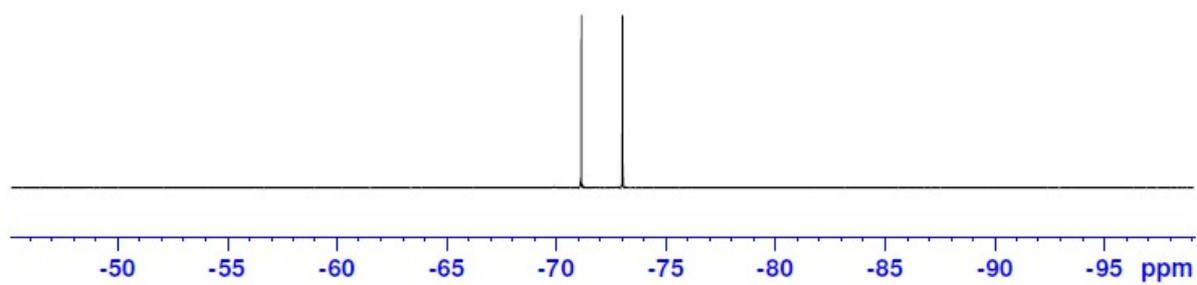
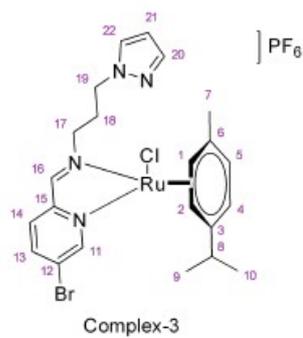


Figure S30 ^{19}F - NMR spectrum of complex 3

-71.171
-73.065

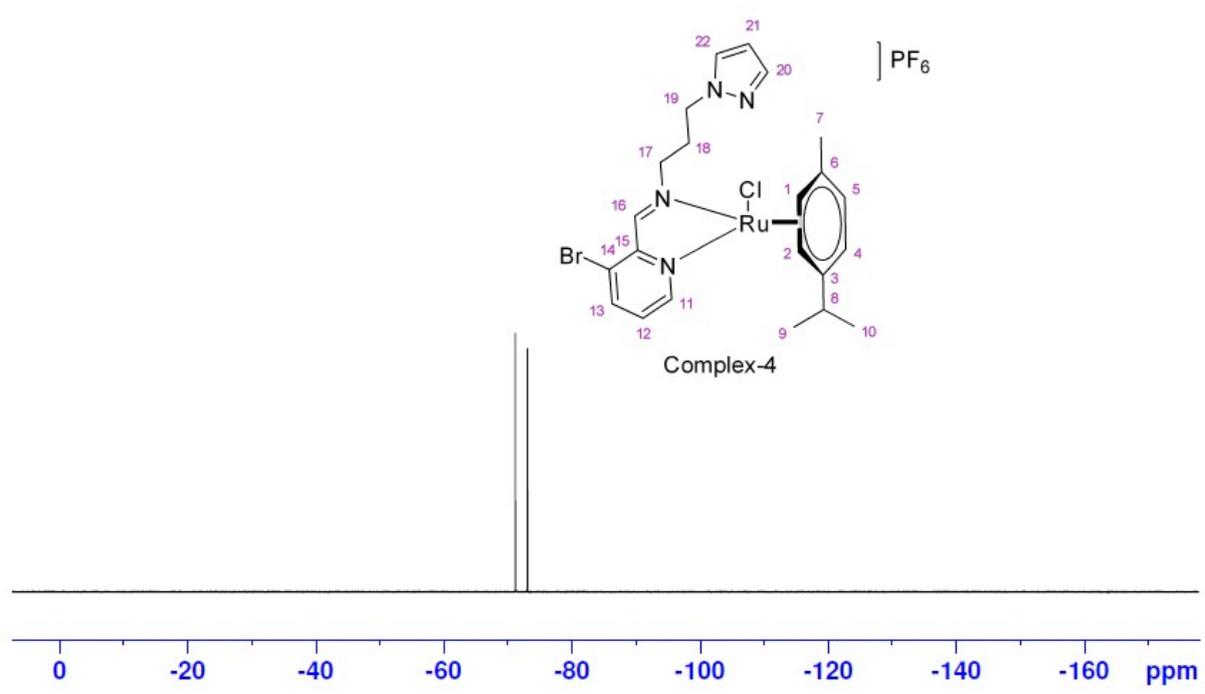


Figure S31 ¹⁹F- NMR spectrum of complex 4

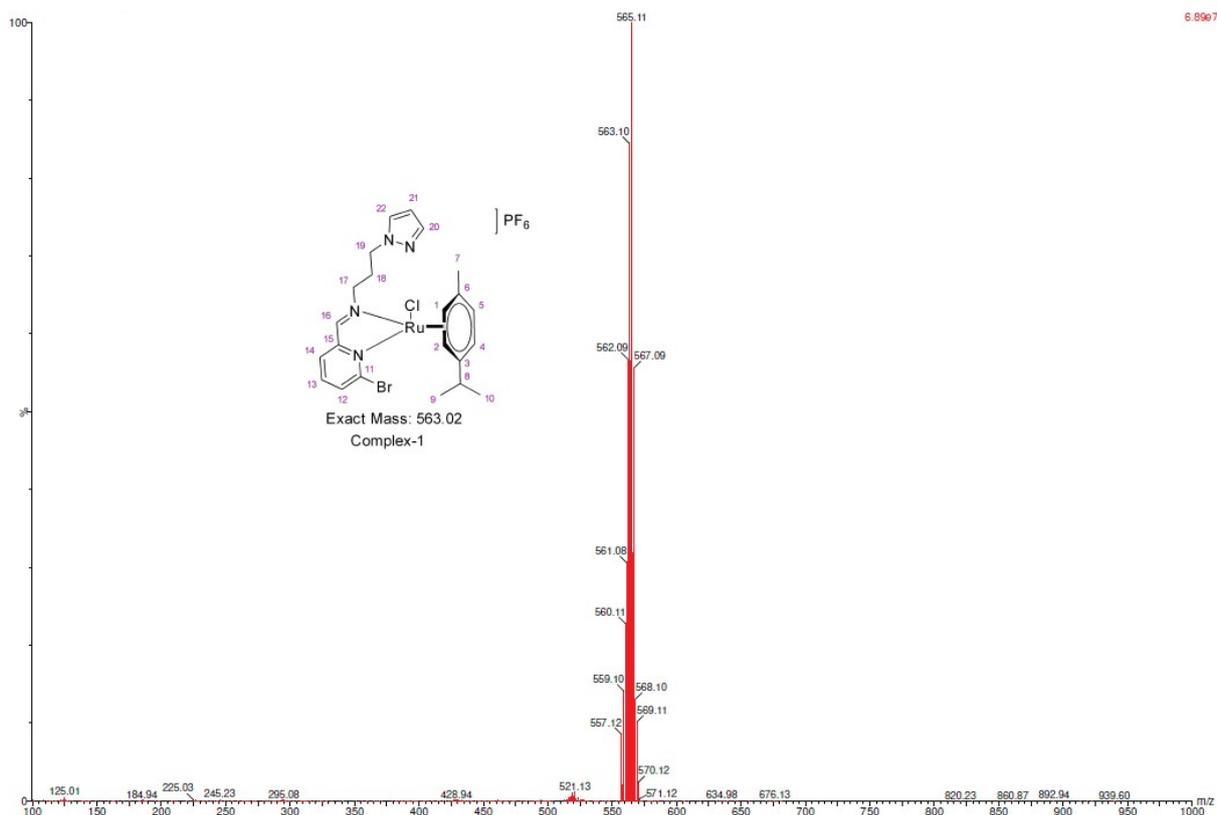


Figure S32 Mass spectrum of complex 1

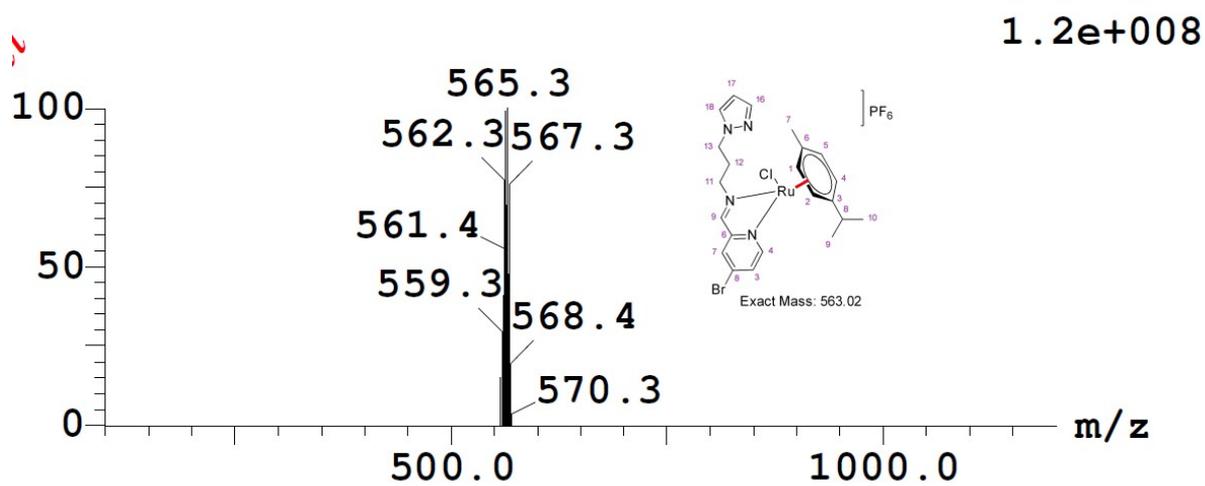


Figure S33 Mass spectrum of complex 2

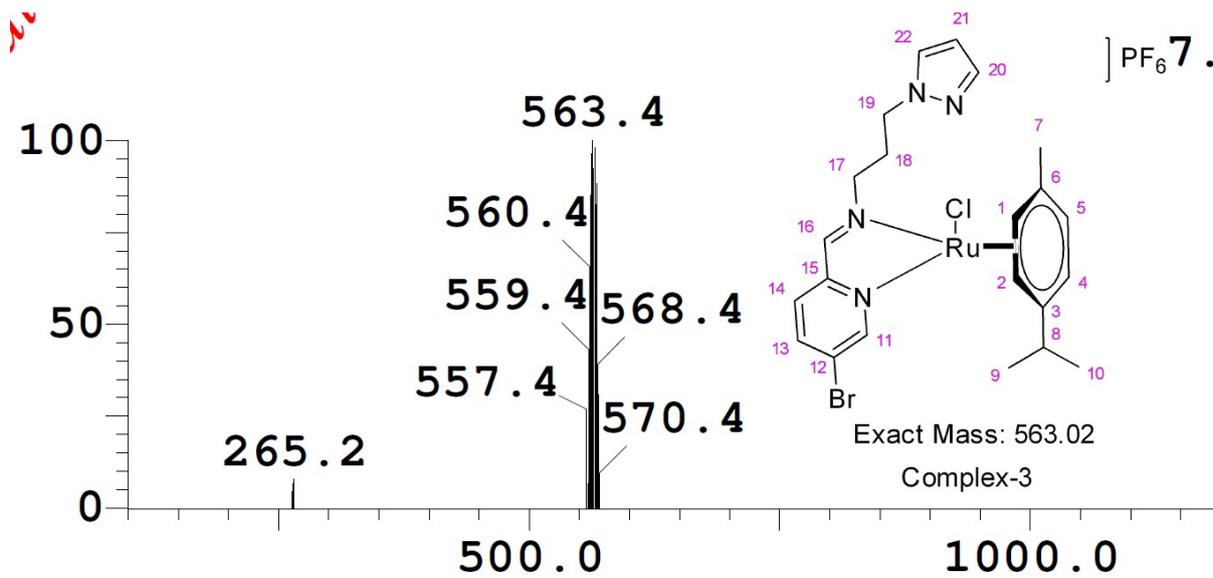


Figure S34 Mass spectrum of complex 3

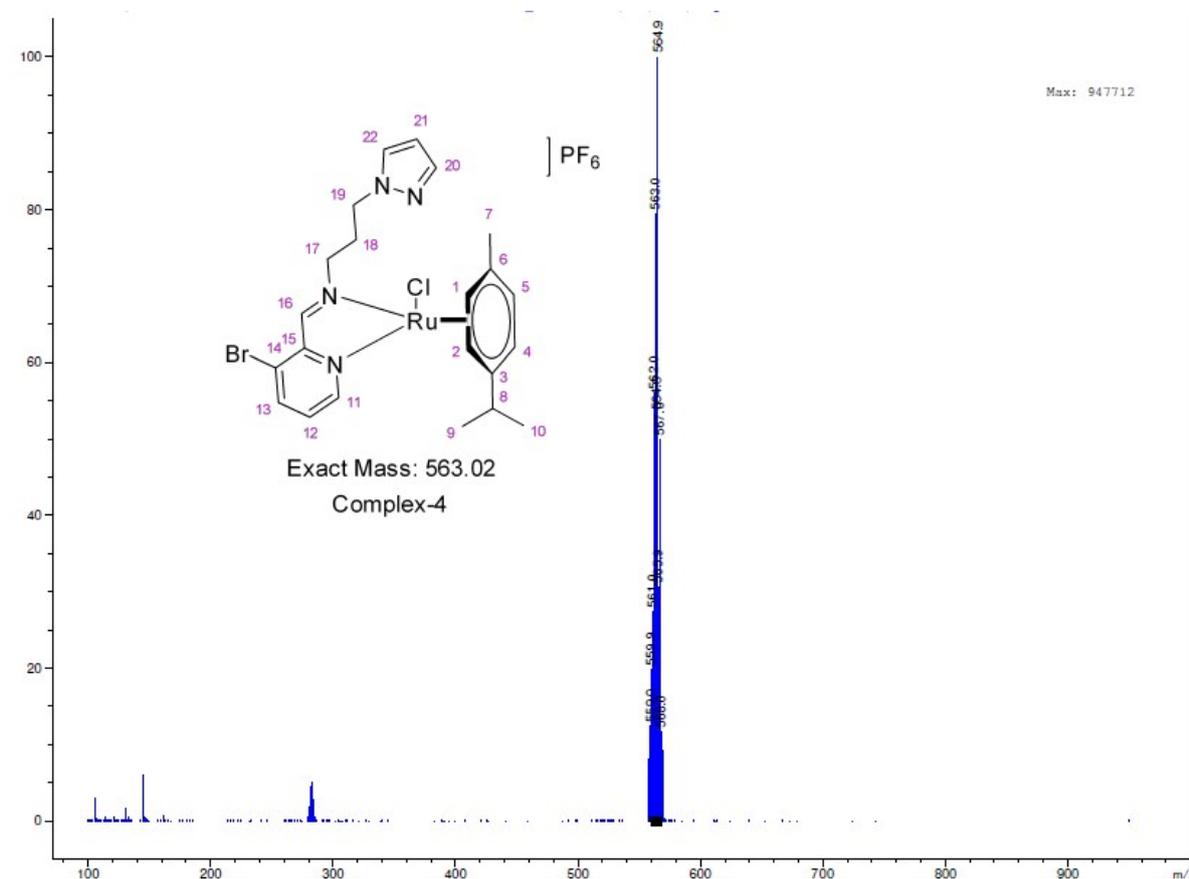


Figure S35 Mass spectrum of complex 4

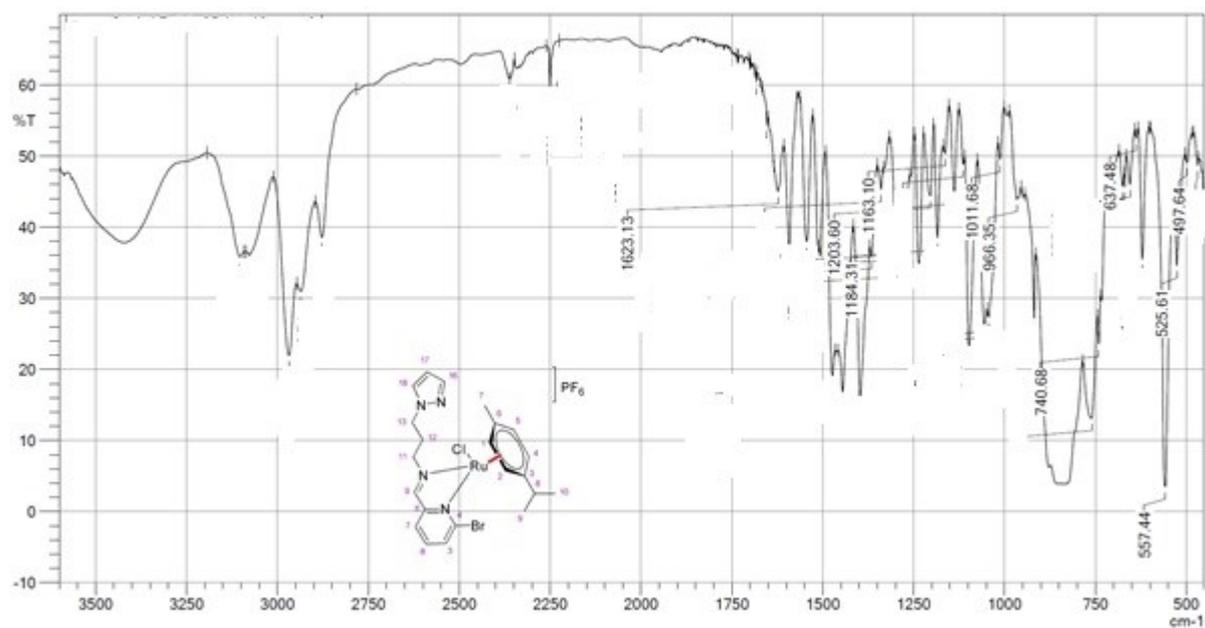


Figure S36 FTIR spectrum of complex 1

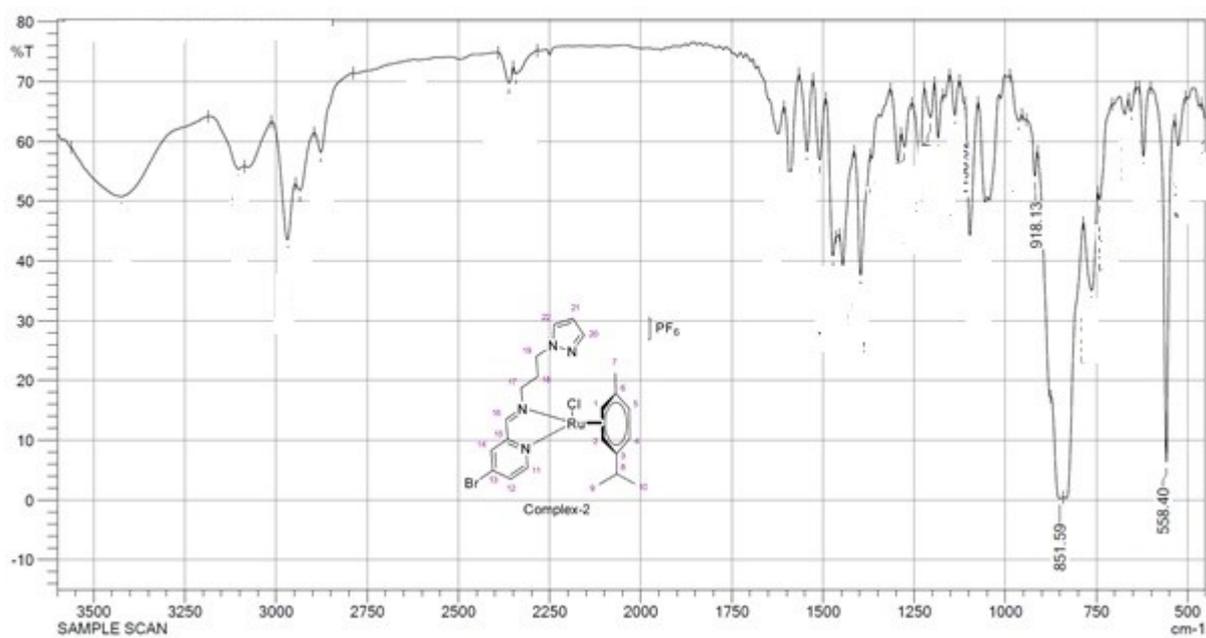


Figure S37 FTIR spectrum of complex 2

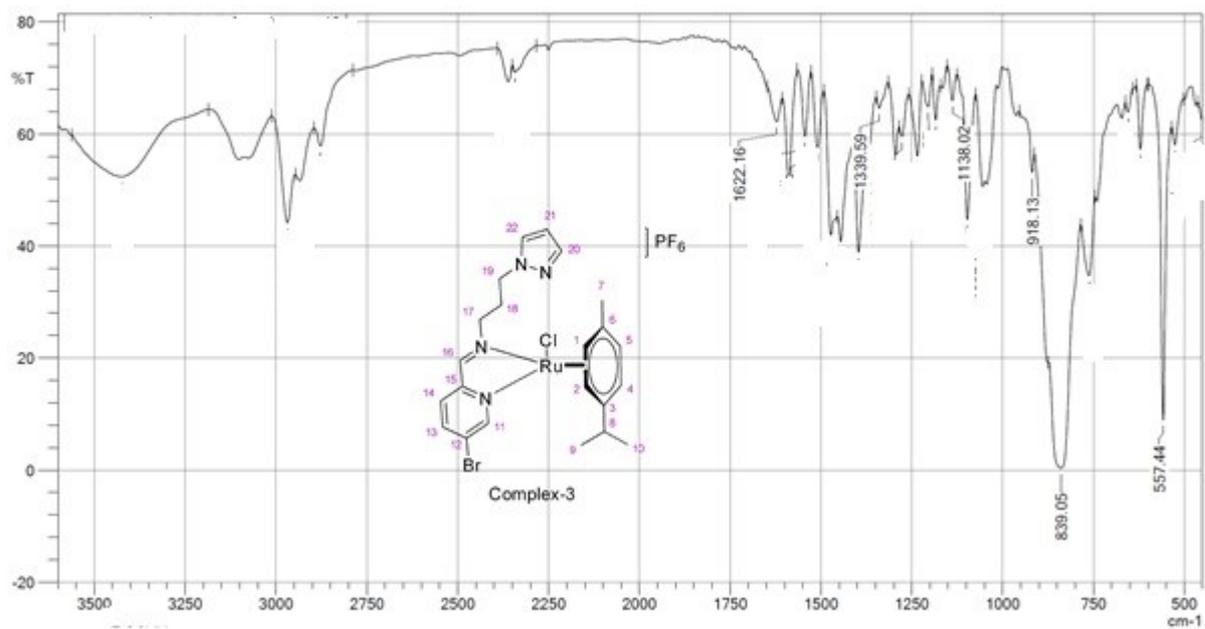


Figure S38 FTIR spectrum of complex 3

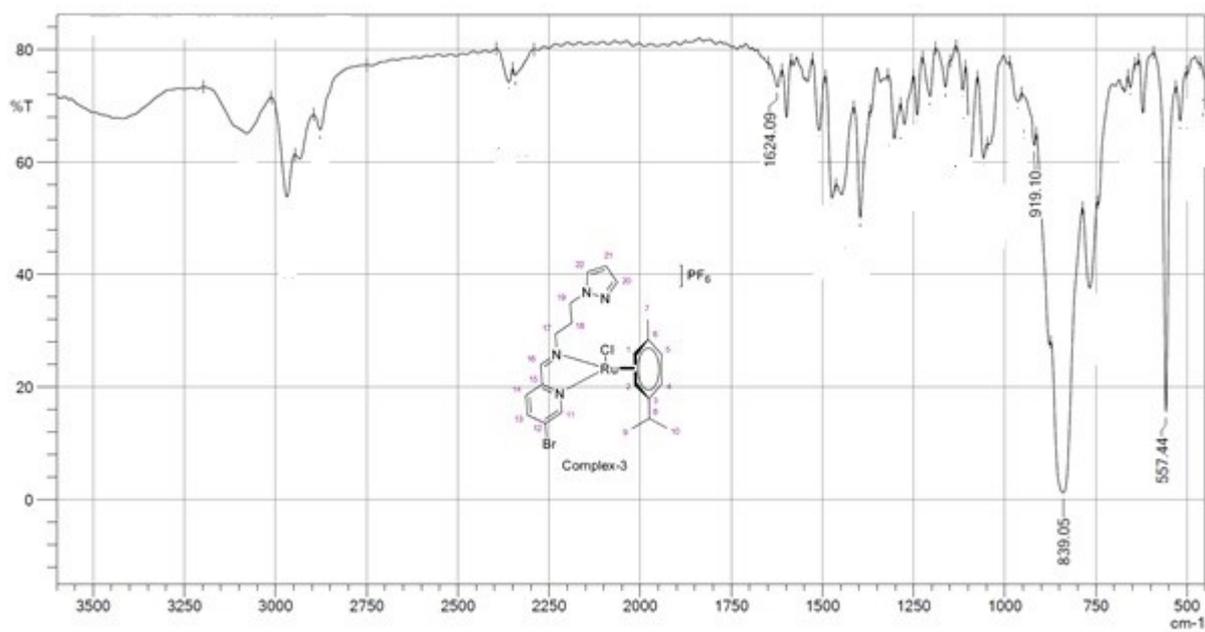


Figure S39 FTIR spectrum of complex 4

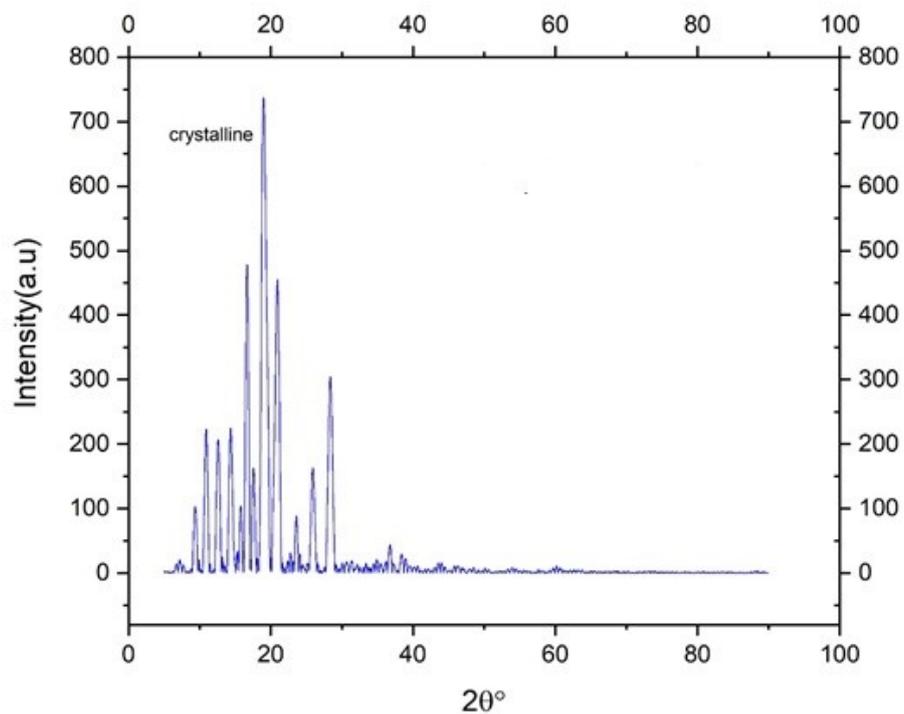


Figure S40 P-XRD spectrum of complex 2

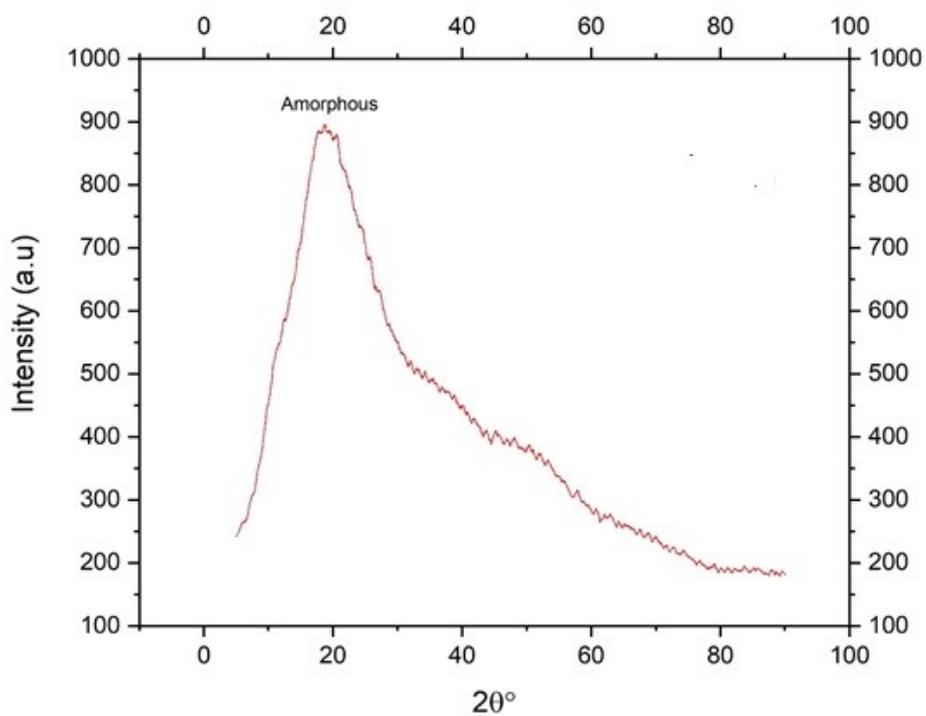


Figure S41 P-XRD spectrum of complex 4

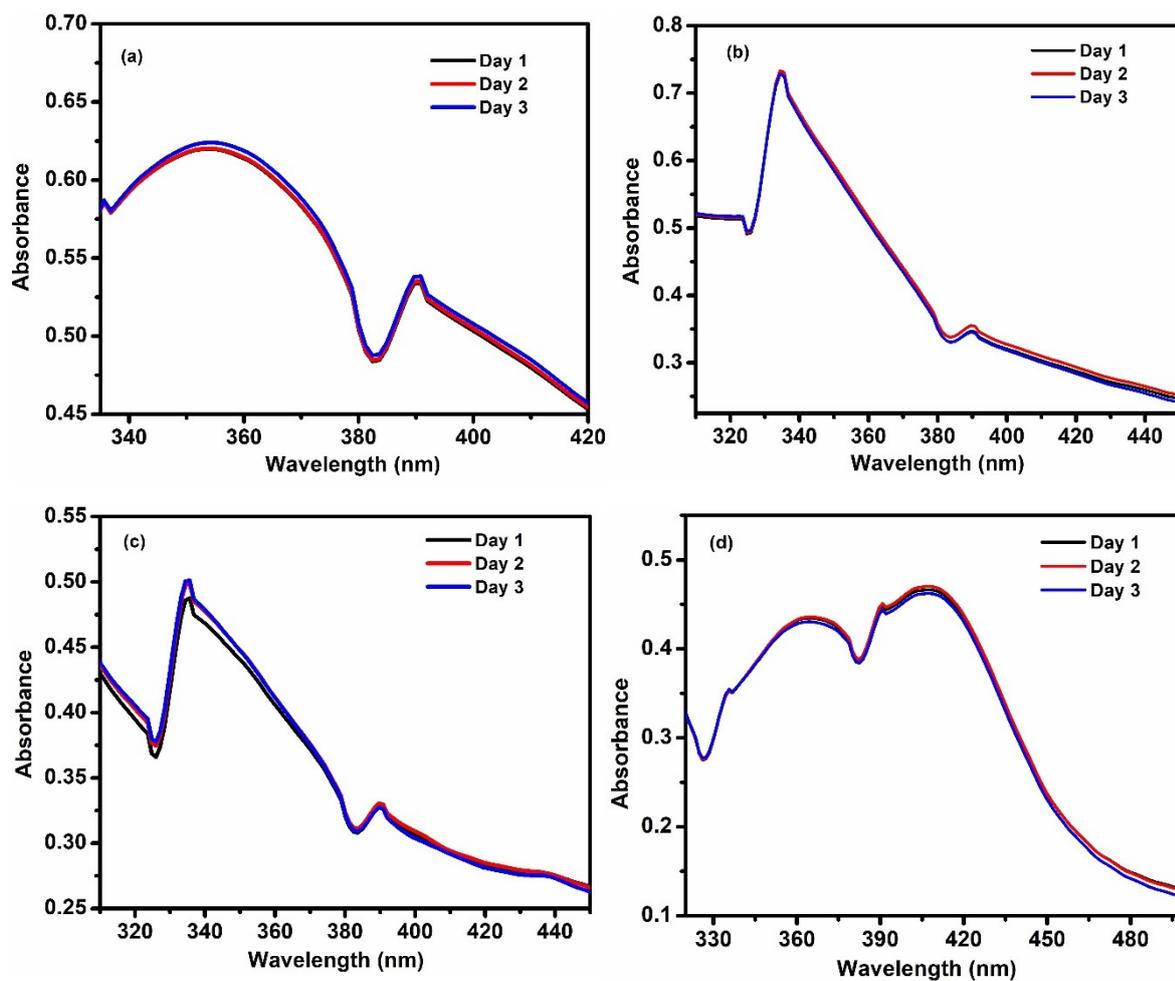


Figure S42 Solution stability using UV-Vis spectral studies of (a) complex 1 and (b) complex 2 (c) complex 3 (d) complex 4 over three successive days

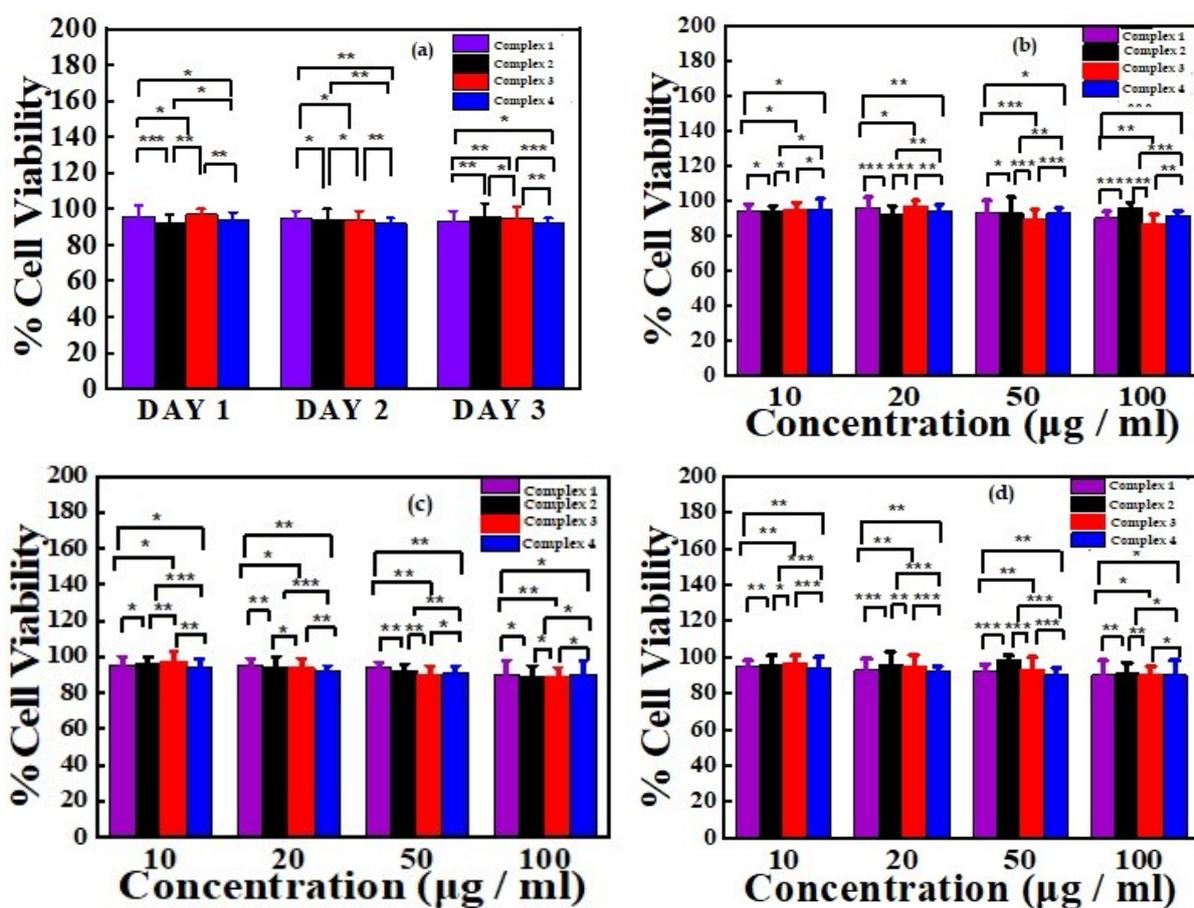


Figure S43 (a) Comparative study of cell viability between four samples at concentration 35.52 μM for day 1, 2 and 3 (b) to (d) Comparative study of cell viability between four samples at different concentration for Day 1, 2 and 3 respectively against 3T3-L1 normal cell line

Table S1: Refined atomic parameters of the complex 3

| Atom | Wyck. | Site | x/a | y/b | z/c | U [Å ²] |
|------|-------|------|-------------|-------------|-------------|---------------------|
| Ru01 | 2i | 1 | 0.26491(3) | 0.33327(3) | 0.32761(2) | |
| Br02 | 2i | 1 | -0.12220(6) | -0.06148(5) | 0.38788(4) | |
| Cl03 | 2i | 1 | 0.37910(12) | 0.19225(11) | 0.43141(8) | |
| P04 | 2i | 1 | 0.5748(2) | 0.76998(15) | 0.13334(11) | |
| N005 | 2i | 1 | 0.1854(3) | 0.1799(3) | 0.2878(2) | |
| N006 | 2i | 1 | 0.4116(3) | 0.2911(3) | 0.2074(2) | |
| N007 | 2i | 1 | 0.7887(4) | 0.1897(4) | 0.1844(3) | |
| N008 | 2i | 1 | 0.9089(4) | 0.2462(4) | 0.1527(4) | |
| C009 | 2i | 1 | 0.0736(4) | 0.1219(4) | 0.3372(3) | |
| H009 | 2i | 1 | 0.02020 | 0.15426 | 0.39041 | 0.0590 |
| C00A | 2i | 1 | 0.2644(4) | 0.1306(4) | 0.2122(3) | |
| C00B | 2i | 1 | 0.3886(4) | 0.1969(4) | 0.1691(3) | |
| H00B | 2i | 1 | 0.44925 | 0.17211 | 0.11554 | 0.0600 |
| C00C | 2i | 1 | 0.2298(6) | 0.0248(4) | 0.1819(4) | |
| H00C | 2i | 1 | 0.28411 | -0.00657 | 0.12855 | 0.0740 |
| C00D | 2i | 1 | 0.0354(5) | 0.0152(4) | 0.3112(3) | |
| C00E | 2i | 1 | 0.5388(5) | 0.3568(4) | 0.1676(4) | |
| H00A | 2i | 1 | 0.51724 | 0.44015 | 0.14824 | 0.0710 |
| H00D | 2i | 1 | 0.58448 | 0.32442 | 0.10783 | 0.0710 |
| C00F | 2i | 1 | 0.2720(4) | 0.5243(4) | 0.2726(4) | |
| H00F | 2i | 1 | 0.32715 | 0.56411 | 0.21648 | 0.0640 |
| C00G | 2i | 1 | 0.1126(6) | -0.0332(4) | 0.2327(4) | |
| H00G | 2i | 1 | 0.08640 | -0.10426 | 0.21385 | 0.0770 |
| C00H | 2i | 1 | 0.1425(4) | 0.4819(4) | 0.2629(3) | |
| C00I | 2i | 1 | 0.0652(4) | 0.4180(4) | 0.3489(4) | |
| H00I | 2i | 1 | -0.01746 | 0.38458 | 0.34377 | 0.0680 |
| C00J | 2i | 1 | 0.6962(5) | 0.2278(6) | 0.2676(4) | |
| H00E | 2i | 1 | 0.74480 | 0.22942 | 0.32335 | 0.0920 |
| H00H | 2i | 1 | 0.62339 | 0.16967 | 0.28877 | 0.0920 |
| F00K | 2i | 1 | 0.5184(8) | 0.6853(6) | 0.0681(4) | |
| C00L | 2i | 1 | 0.1101(5) | 0.4032(4) | 0.4427(4) | |
| H00L | 2i | 1 | 0.05529 | 0.36316 | 0.49888 | 0.0760 |
| C00M | 2i | 1 | 0.0860(5) | 0.5037(5) | 0.1652(4) | |
| H00M | 2i | 1 | 0.02903 | 0.43503 | 0.16256 | 0.0800 |
| C00N | 2i | 1 | 0.3185(5) | 0.5076(5) | 0.3645(4) | |
| H00N | 2i | 1 | 0.40436 | 0.53564 | 0.36833 | 0.0770 |
| C00O | 2i | 1 | 0.6343(5) | 0.3488(5) | 0.2437(4) | |
| H00J | 2i | 1 | 0.70779 | 0.40553 | 0.21877 | 0.0860 |
| H00K | 2i | 1 | 0.58435 | 0.37319 | 0.30561 | 0.0860 |
| F00P | 2i | 1 | 0.4187(6) | 0.7673(6) | 0.1943(5) | |
| C00Q | 2i | 1 | 0.2373(6) | 0.4487(5) | 0.4519(4) | |
| C00R | 2i | 1 | 0.2688(7) | 0.8016(6) | 0.4536(4) | |
| C00S | 2i | 1 | 0.9653(7) | 0.1934(8) | 0.0755(5) | |
| H00S | 2i | 1 | 1.05063 | 0.21340 | 0.03763 | 0.1190 |
| F00T | 2i | 1 | 0.5294(11) | 0.8755(6) | 0.0611(6) | |
| C00U | 2i | 1 | 0.1923(8) | 0.5171(7) | 0.0711(5) | |
| H00O | 2i | 1 | 0.24388 | 0.58855 | 0.06831 | 0.1550 |

| | | | | | | |
|------|----|---|-------------|------------|-----------|--------|
| H00P | 2i | 1 | 0.14816 | 0.52222 | 0.01330 | 0.1550 |
| H00Q | 2i | 1 | 0.25270 | 0.44899 | 0.07191 | 0.1550 |
| C00V | 2i | 1 | 0.3814(7) | 0.8771(6) | 0.4069(5) | |
| H00R | 2i | 1 | 0.39644 | 0.87507 | 0.33560 | 0.1270 |
| H00T | 2i | 1 | 0.46203 | 0.84923 | 0.43313 | 0.1270 |
| H00U | 2i | 1 | 0.36116 | 0.95767 | 0.42073 | 0.1270 |
| F00W | 2i | 1 | 0.7023(7) | 0.7867(10) | 0.0605(6) | |
| F00X | 2i | 1 | 0.6103(12) | 0.8553(9) | 0.1969(4) | |
| F00Y | 2i | 1 | 0.5871(9) | 0.6633(6) | 0.2100(6) | |
| C00Z | 2i | 1 | 0.7719(8) | 0.1055(6) | 0.1284(7) | |
| H00Z | 2i | 1 | 0.69671 | 0.05562 | 0.13697 | 0.1180 |
| C010 | 2i | 1 | -0.0059(10) | 0.6126(8) | 0.1691(6) | |
| H01A | 2i | 1 | 0.04672 | 0.68118 | 0.17365 | 0.1900 |
| H01B | 2i | 1 | -0.07700 | 0.59988 | 0.22681 | 0.1900 |
| H01C | 2i | 1 | -0.04603 | 0.62616 | 0.10920 | 0.1900 |
| N011 | 2i | 1 | 0.1805(8) | 0.7427(7) | 0.4903(6) | |
| C012 | 2i | 1 | 0.2883(8) | 0.4269(7) | 0.5506(5) | |
| H01D | 2i | 1 | 0.23499 | 0.36516 | 0.59419 | 0.1570 |
| H01E | 2i | 1 | 0.27997 | 0.49926 | 0.58134 | 0.1570 |
| H01F | 2i | 1 | 0.38251 | 0.40234 | 0.53917 | 0.1570 |
| C013 | 2i | 1 | 0.8842(11) | 0.1053(9) | 0.0567(7) | |
| H013 | 2i | 1 | 0.90252 | 0.05647 | 0.00592 | 0.1560 |

Table S2: Anisotropic displacement parameters, in Å² of the complex 3

| Atom | U ₁₁ | U ₂₂ | U ₃₃ | U ₁₂ | U ₁₃ | U ₂₃ |
|------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Ru01 | 0.04094(19) | 0.0409(2) | 0.04050(19) | -0.00021(12) | -0.00449(12) | -0.00695(13) |
| Br02 | 0.0720(3) | 0.0583(3) | 0.0875(4) | -0.0190(2) | -0.0133(3) | 0.0046(3) |
| Cl03 | 0.0601(6) | 0.0662(7) | 0.0503(6) | 0.0052(5) | -0.0149(5) | 0.0004(5) |
| P04 | 0.1090(13) | 0.0732(10) | 0.0617(8) | -0.0240(9) | 0.0055(8) | -0.0081(7) |
| N005 | 0.0458(17) | 0.0395(17) | 0.0405(16) | 0.0023(13) | -0.0094(13) | -0.0058(13) |
| N006 | 0.0431(17) | 0.050(2) | 0.0406(17) | 0.0024(14) | -0.0013(13) | -0.0030(15) |
| N007 | 0.047(2) | 0.057(2) | 0.070(2) | -0.0027(17) | -0.0120(17) | -0.0039(19) |
| N008 | 0.054(2) | 0.065(3) | 0.088(3) | -0.0015(19) | -0.004(2) | 0.003(2) |
| C009 | 0.054(2) | 0.041(2) | 0.054(2) | 0.0004(18) | -0.0123(18) | -0.0035(18) |
| C00A | 0.053(2) | 0.048(2) | 0.042(2) | 0.0031(17) | -0.0138(17) | -0.0065(17) |
| C00B | 0.053(2) | 0.056(3) | 0.040(2) | 0.0084(19) | -0.0051(17) | -0.0095(18) |
| C00C | 0.080(3) | 0.054(3) | 0.053(3) | 0.004(2) | -0.013(2) | -0.020(2) |
| C00D | 0.061(3) | 0.046(2) | 0.059(3) | -0.0063(19) | -0.019(2) | 0.0002(19) |
| C00E | 0.052(2) | 0.058(3) | 0.060(3) | -0.003(2) | 0.008(2) | -0.001(2) |
| C00F | 0.056(2) | 0.035(2) | 0.067(3) | -0.0043(17) | -0.002(2) | -0.0098(19) |
| C00G | 0.081(3) | 0.050(3) | 0.067(3) | -0.009(2) | -0.024(3) | -0.011(2) |
| C00H | 0.056(2) | 0.036(2) | 0.062(3) | 0.0015(17) | -0.0117(19) | -0.0081(18) |
| C00I | 0.043(2) | 0.046(2) | 0.077(3) | 0.0067(17) | -0.002(2) | -0.009(2) |
| C00J | 0.053(3) | 0.106(5) | 0.067(3) | 0.002(3) | -0.006(2) | 0.001(3) |
| F00K | 0.255(7) | 0.179(5) | 0.103(3) | -0.082(5) | -0.020(4) | -0.031(3) |
| C00L | 0.065(3) | 0.056(3) | 0.063(3) | 0.008(2) | 0.012(2) | -0.014(2) |
| C00M | 0.071(3) | 0.055(3) | 0.076(3) | 0.001(2) | -0.027(3) | 0.003(2) |
| C00N | 0.064(3) | 0.060(3) | 0.073(3) | -0.003(2) | -0.014(2) | -0.026(2) |
| C00O | 0.047(2) | 0.087(4) | 0.084(4) | -0.007(2) | 0.001(2) | -0.033(3) |
| F00P | 0.157(5) | 0.142(5) | 0.203(6) | -0.040(4) | 0.048(4) | -0.059(4) |

| | | | | | | |
|------|-----------|-----------|----------|------------|-----------|-----------|
| C00Q | 0.081(3) | 0.061(3) | 0.056(3) | 0.007(2) | -0.004(2) | -0.026(2) |
| C00R | 0.092(4) | 0.070(4) | 0.066(3) | 0.009(3) | -0.001(3) | -0.014(3) |
| C00S | 0.081(4) | 0.118(6) | 0.077(4) | 0.048(4) | 0.014(3) | 0.019(4) |
| F00T | 0.319(11) | 0.131(5) | 0.204(7) | 0.065(6) | -0.017(7) | 0.022(5) |
| C00U | 0.121(6) | 0.126(6) | 0.070(4) | 0.033(5) | -0.031(4) | -0.024(4) |
| C00V | 0.088(4) | 0.089(4) | 0.079(4) | 0.006(3) | -0.024(3) | -0.005(3) |
| F00W | 0.122(5) | 0.387(12) | 0.230(7) | -0.094(6) | 0.089(5) | -0.127(8) |
| F00X | 0.517(15) | 0.326(10) | 0.111(4) | -0.343(11) | 0.070(6) | -0.084(5) |
| F00Y | 0.30(1) | 0.165(6) | 0.204(7) | -0.077(6) | -0.145(7) | 0.085(5) |
| C00Z | 0.086(4) | 0.072(4) | 0.156(7) | 0.013(3) | -0.050(5) | -0.045(4) |
| C010 | 0.146(7) | 0.124(6) | 0.104(5) | 0.071(6) | -0.037(5) | 0.012(5) |
| N011 | 0.121(5) | 0.113(5) | 0.128(5) | -0.028(4) | 0.033(4) | -0.023(4) |
| C012 | 0.144(6) | 0.116(6) | 0.065(4) | 0.007(5) | -0.025(4) | -0.045(4) |
| C013 | 0.136(7) | 0.148(8) | 0.133(7) | 0.088(7) | -0.067(6) | -0.076(6) |

Table S3: Selected bond lengths of the complex 3

| Atoms 1,2 | d 1,2 [Å] | Atoms 1,2 | d 1,2 [Å] |
|-----------|------------|-----------|-----------|
| Ru01—C103 | 2.3802(11) | C00G—H00G | 0.9300 |
| Ru01—N005 | 2.093(3) | C00H—C00I | 1.407(6) |
| Ru01—N006 | 2.089(3) | C00H—C00M | 1.519(7) |
| Ru01—C00F | 2.184(4) | C00I—H00I | 0.9300 |
| Ru01—C00H | 2.219(4) | C00I—C00L | 1.413(7) |
| Ru01—C00I | 2.165(4) | C00J—H00E | 0.9700 |
| Ru01—C00L | 2.205(4) | C00J—H00H | 0.9700 |
| Ru01—C00N | 2.193(5) | C00J—C00O | 1.499(8) |
| Ru01—C00Q | 2.242(4) | C00L—H00L | 0.9300 |
| Br02—C00D | 1.888(5) | C00L—C00Q | 1.407(7) |
| P04—F00K | 1.561(6) | C00M—H00M | 0.9800 |
| P04—F00P | 1.626(6) | C00M—C00U | 1.507(9) |
| P04—F00T | 1.549(7) | C00M—C010 | 1.509(8) |
| P04—F00W | 1.467(5) | C00N—H00N | 0.9300 |
| P04—F00X | 1.463(5) | C00N—C00Q | 1.414(7) |
| P04—F00Y | 1.502(6) | C00O—H00J | 0.9700 |
| N005—C009 | 1.335(5) | C00O—H00K | 0.9700 |
| N005—C00A | 1.352(5) | C00Q—C012 | 1.504(8) |
| N006—C00B | 1.285(5) | C00R—C00V | 1.431(9) |
| N006—C00E | 1.467(5) | C00R—N011 | 1.120(8) |
| N007—N008 | 1.346(5) | C00S—H00S | 0.9300 |
| N007—C00J | 1.434(7) | C00S—C013 | 1.373(12) |
| N007—C00Z | 1.323(7) | C00U—H00O | 0.9600 |
| N008—C00S | 1.309(8) | C00U—H00P | 0.9600 |
| C009—H009 | 0.9300 | C00U—H00Q | 0.9600 |
| C009—C00D | 1.379(6) | C00V—H00R | 0.9600 |
| C00A—C00B | 1.454(6) | C00V—H00T | 0.9600 |
| C00A—C00C | 1.383(6) | C00V—H00U | 0.9600 |
| C00B—H00B | 0.9300 | C00Z—H00Z | 0.9300 |
| C00C—H00C | 0.9300 | C00Z—C013 | 1.350(12) |
| C00C—C00G | 1.382(7) | C010—H01A | 0.9600 |
| C00D—C00G | 1.368(7) | C010—H01B | 0.9600 |

| | | | |
|-----------|----------|-----------|--------|
| C00E—H00A | 0.9700 | C010—H01C | 0.9600 |
| C00E—H00D | 0.9700 | C012—H01D | 0.9600 |
| C00E—C00O | 1.514(7) | C012—H01E | 0.9600 |
| C00F—H00F | 0.9300 | C012—H01F | 0.9600 |
| C00F—C00H | 1.418(6) | C013—H013 | 0.9300 |
| C00F—C00N | 1.395(7) | | |

Table S4: Selected bond angles of the complex 3

| Atoms 1,2,3 | Angle 1,2,3 [°] | Atoms 1,2,3 | Angle 1,2,3 [°] |
|----------------|-----------------|----------------|-----------------|
| N005—Ru01—Cl03 | 83.55(9) | C00N—C00F—C00H | 121.4(4) |
| N005—Ru01—C00F | 136.46(15) | C00C—C00G—H00G | 120.400 |
| N005—Ru01—C00H | 103.97(14) | C00D—C00G—C00C | 119.2(4) |
| N005—Ru01—C00I | 91.91(15) | C00D—C00G—H00G | 120.400 |
| N005—Ru01—C00L | 107.94(16) | C00F—C00H—Ru01 | 69.9(2) |
| N005—Ru01—C00N | 171.08(16) | C00F—C00H—C00M | 122.7(4) |
| N005—Ru01—C00Q | 141.01(17) | C00I—C00H—Ru01 | 69.3(2) |
| N006—Ru01—Cl03 | 86.55(9) | C00I—C00H—C00F | 117.2(4) |
| N006—Ru01—N005 | 76.93(13) | C00I—C00H—C00M | 120.1(4) |
| N006—Ru01—C00F | 92.87(15) | C00M—C00H—Ru01 | 132.4(3) |
| N006—Ru01—C00H | 105.26(15) | Ru01—C00I—H00I | 126.800 |
| N006—Ru01—C00I | 137.53(16) | C00H—C00I—Ru01 | 73.3(2) |
| N006—Ru01—C00L | 171.97(16) | C00H—C00I—H00I | 119.200 |
| N006—Ru01—C00N | 107.56(17) | C00H—C00I—C00L | 121.6(4) |
| N006—Ru01—C00Q | 140.41(17) | C00L—C00I—Ru01 | 72.7(3) |
| C00F—Ru01—Cl03 | 138.71(12) | C00L—C00I—H00I | 119.200 |
| C00F—Ru01—C00H | 37.58(16) | N007—C00J—H00E | 108.900 |
| C00F—Ru01—C00L | 79.20(18) | N007—C00J—H00H | 108.900 |
| C00F—Ru01—C00N | 37.18(18) | N007—C00J—C00O | 113.4(4) |
| C00F—Ru01—C00Q | 67.10(18) | H00E—C00J—H00H | 107.700 |
| C00H—Ru01—Cl03 | 167.07(12) | C00O—C00J—H00E | 108.900 |
| C00H—Ru01—C00Q | 79.93(18) | C00O—C00J—H00H | 108.900 |
| C00I—Ru01—Cl03 | 133.40(13) | Ru01—C00L—H00L | 130.200 |
| C00I—Ru01—C00F | 67.33(17) | C00I—C00L—Ru01 | 69.6(2) |
| C00I—Ru01—C00H | 37.40(17) | C00I—C00L—H00L | 119.800 |
| C00I—Ru01—C00L | 37.71(19) | C00Q—C00L—Ru01 | 73.0(3) |
| C00I—Ru01—C00N | 79.58(18) | C00Q—C00L—C00I | 120.5(4) |
| C00I—Ru01—C00Q | 67.47(19) | C00Q—C00L—H00L | 119.800 |
| C00L—Ru01—Cl03 | 100.21(14) | C00H—C00M—H00M | 107.600 |
| C00L—Ru01—C00H | 67.63(18) | C00U—C00M—C00H | 115.0(5) |
| C00L—Ru01—C00Q | 36.89(19) | C00U—C00M—H00M | 107.600 |
| C00N—Ru01—Cl03 | 104.21(14) | C00U—C00M—C010 | 110.8(5) |
| C00N—Ru01—C00H | 67.59(18) | C010—C00M—C00H | 108.0(5) |
| C00N—Ru01—C00L | 66.75(19) | C010—C00M—H00M | 107.600 |
| C00N—Ru01—C00Q | 37.18(19) | Ru01—C00N—H00N | 128.500 |
| C00Q—Ru01—Cl03 | 87.62(14) | C00F—C00N—Ru01 | 71.1(3) |
| F00K—P04—F00P | 84.1(4) | C00F—C00N—H00N | 119.400 |
| F00T—P04—F00K | 86.9(5) | C00F—C00N—C00Q | 121.1(5) |
| F00T—P04—F00P | 87.1(5) | C00Q—C00N—Ru01 | 73.3(3) |

| | | | |
|----------------|----------|----------------|----------|
| F00W—P04—F00K | 91.1(4) | C00Q—C00N—H00N | 119.400 |
| F00W—P04—F00P | 167.5(5) | C00E—C00O—H00J | 108.400 |
| F00W—P04—F00T | 81.1(6) | C00E—C00O—H00K | 108.400 |
| F00W—P04—F00Y | 110.2(6) | C00J—C00O—C00E | 115.4(5) |
| F00X—P04—F00K | 172.9(6) | C00J—C00O—H00J | 108.400 |
| F00X—P04—F00P | 89.6(5) | C00J—C00O—H00K | 108.400 |
| F00X—P04—F00T | 89.5(6) | H00J—C00O—H00K | 107.500 |
| F00X—P04—F00W | 94.5(5) | C00L—C00Q—Ru01 | 70.1(3) |
| F00X—P04—F00Y | 93.7(5) | C00L—C00Q—C00N | 118.0(5) |
| F00Y—P04—F00K | 88.6(4) | C00L—C00Q—C012 | 120.3(5) |
| F00Y—P04—F00P | 81.3(4) | C00N—C00Q—Ru01 | 69.5(3) |
| F00Y—P04—F00T | 167.9(5) | C00N—C00Q—C012 | 121.5(5) |
| C009—N005—Ru01 | 125.4(3) | C012—C00Q—Ru01 | 128.4(4) |
| C009—N005—C00A | 118.8(3) | N011—C00R—C00V | 179.8(8) |
| C00A—N005—Ru01 | 115.3(3) | N008—C00S—H00S | 123.800 |
| C00B—N006—Ru01 | 116.0(3) | N008—C00S—C013 | 112.4(7) |
| C00B—N006—C00E | 118.6(3) | C013—C00S—H00S | 123.800 |
| C00E—N006—Ru01 | 125.3(3) | C00M—C00U—H00O | 109.500 |
| N008—N007—C00J | 119.2(4) | C00M—C00U—H00P | 109.500 |
| C00Z—N007—N008 | 111.9(5) | C00M—C00U—H00Q | 109.500 |
| C00Z—N007—C00J | 128.8(5) | H00O—C00U—H00P | 109.500 |
| C00S—N008—N007 | 103.8(6) | H00O—C00U—H00Q | 109.500 |
| N005—C009—H009 | 119.200 | H00P—C00U—H00Q | 109.500 |
| N005—C009—C00D | 121.6(4) | C00R—C00V—H00R | 109.500 |
| C00D—C009—H009 | 119.200 | C00R—C00V—H00T | 109.500 |
| N005—C00A—C00B | 113.9(4) | C00R—C00V—H00U | 109.500 |
| N005—C00A—C00C | 122.0(4) | H00R—C00V—H00T | 109.500 |
| C00C—C00A—C00B | 124.0(4) | H00R—C00V—H00U | 109.500 |
| N006—C00B—C00A | 117.7(4) | H00T—C00V—H00U | 109.500 |
| N006—C00B—H00B | 121.100 | N007—C00Z—H00Z | 126.300 |
| C00A—C00B—H00B | 121.100 | N007—C00Z—C013 | 107.4(7) |
| C00A—C00C—H00C | 120.800 | C013—C00Z—H00Z | 126.300 |
| C00G—C00C—C00A | 118.4(4) | C00M—C010—H01A | 109.500 |
| C00G—C00C—H00C | 120.800 | C00M—C010—H01B | 109.500 |
| C009—C00D—Br02 | 118.2(4) | C00M—C010—H01C | 109.500 |
| C00G—C00D—Br02 | 121.9(4) | H01A—C010—H01B | 109.500 |
| C00G—C00D—C009 | 119.9(4) | H01A—C010—H01C | 109.500 |
| N006—C00E—H00A | 109.200 | H01B—C010—H01C | 109.500 |
| N006—C00E—H00D | 109.200 | C00Q—C012—H01D | 109.500 |
| N006—C00E—C00O | 112.0(4) | C00Q—C012—H01E | 109.500 |
| H00A—C00E—H00D | 107.900 | C00Q—C012—H01F | 109.500 |
| C00O—C00E—H00A | 109.200 | H01D—C012—H01E | 109.500 |
| C00O—C00E—H00D | 109.200 | H01D—C012—H01F | 109.500 |
| Ru01—C00F—H00F | 128.800 | H01E—C012—H01F | 109.500 |
| C00H—C00F—Ru01 | 72.5(2) | C00S—C013—H013 | 127.700 |
| C00H—C00F—H00F | 119.300 | C00Z—C013—C00S | 104.5(7) |
| C00N—C00F—Ru01 | 71.8(3) | C00Z—C013—H013 | 127.700 |
| C00N—C00F—H00F | 119.300 | | |

Table S5: Selected torsional bond angles of the complex 3

| Atoms 1,2,3,4 | Tors. an. 1,2,3,4 [°] | Atoms 1,2,3,4 | Tors. an. 1,2,3,4 [°] |
|---------------------|--------------------------|---------------------|--------------------------|
| Ru01—N005—C009—C00D | -173.9(3) | C00A—N005—C009—C00D | -1.7(6) |
| Ru01—N005—C00A—C00B | -2.6(4) | C00A—C00C—C00G—C00D | -0.3(7) |
| Ru01—N005—C00A—C00C | 175.8(3) | C00B—N006—C00E—C00O | -112.6(5) |
| Ru01—N006—C00B—C00A | 0.3(5) | C00B—C00A—C00C—C00G | 176.4(4) |
| Ru01—N006—C00E—C00O | 64.6(5) | C00C—C00A—C00B—N006 | -176.8(4) |
| Ru01—C00F—C00H—C00I | 52.2(3) | C00E—N006—C00B—C00A | 177.7(4) |
| Ru01—C00F—C00H—C00M | -128.2(4) | C00F—C00H—C00I—Ru01 | -52.5(3) |
| Ru01—C00F—C00N—C00Q | -55.8(4) | C00F—C00H—C00I—C00L | 4.1(6) |
| Ru01—C00H—C00I—C00L | 56.7(4) | C00F—C00H—C00M—C00U | 28.5(7) |
| Ru01—C00H—C00M—C00U | -63.4(7) | C00F—C00H—C00M—C010 | -95.8(6) |
| Ru01—C00H—C00M—C010 | 172.3(5) | C00F—C00N—C00Q—Ru01 | 54.8(4) |
| Ru01—C00I—C00L—C00Q | 54.5(4) | C00F—C00N—C00Q—C00L | 2.4(7) |
| Ru01—C00L—C00Q—C00N | 52.1(4) | C00F—C00N—C00Q—C012 | 178.1(5) |
| Ru01—C00L—C00Q—C012 | -123.7(5) | C00H—C00F—C00N—Ru01 | 55.1(4) |
| Ru01—C00N—C00Q—C00L | -52.4(4) | C00H—C00F—C00N—C00Q | -0.7(7) |
| Ru01—C00N—C00Q—C012 | 123.3(5) | C00H—C00I—C00L—Ru01 | -57.0(4) |
| Br02—C00D—C00G—C00C | -177.5(4) | C00H—C00I—C00L—C00Q | -2.5(7) |
| N005—C009—C00D—Br02 | 178.6(3) | C00I—C00H—C00M—C00U | -152.0(5) |
| N005—C009—C00D—C00G | -0.3(6) | C00I—C00H—C00M—C010 | 83.7(6) |
| N005—C00A—C00B—N006 | 1.6(5) | C00I—C00L—C00Q—Ru01 | -52.9(4) |
| N005—C00A—C00C—C00G | -1.8(7) | C00I—C00L—C00Q—C00N | -0.8(7) |
| N006—C00E—C00O—C00J | 69.0(5) | C00I—C00L—C00Q—C012 | -176.6(5) |
| N007—N008—C00S—C013 | 0.3(7) | C00J—N007—N008—C00S | -178.0(5) |
| N007—C00J—C00O—C00E | 66.6(6) | C00J—N007—C00Z—C013 | 177.5(6) |
| N007—C00Z—C013—C00S | 0.3(8) | C00M—C00H—C00I—Ru01 | 127.9(4) |

| | | | |
|-------------------------|-----------|-------------------------|-----------|
| N008—N007—C00J— C00O | 69.0(6) | C00M—C00H—C00I—C00L | -175.5(4) |
| N008—N007—C00Z— C013 | -0.1(8) | C00N—C00F—C00H—Ru01 | -54.8(4) |
| N008—C00S—C013— C00Z | -0.4(9) | C00N—C00F—C00H—C00I | -2.5(6) |
| C009—N005—C00A— C00B | -175.5(3) | C00N—C00F—C00H— C00M | 177.0(4) |
| C009—N005—C00A— C00C | 2.8(6) | C00Z—N007—N008—C00S | -0.1(6) |
| C009—C00D—C00G— C00C | 1.4(7) | C00Z—N007—C00J—C00O | -108.4(7) |