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# Design, synthesis and biological evaluation of pyrazoline nucleus based homoleptic Ru(III) compounds

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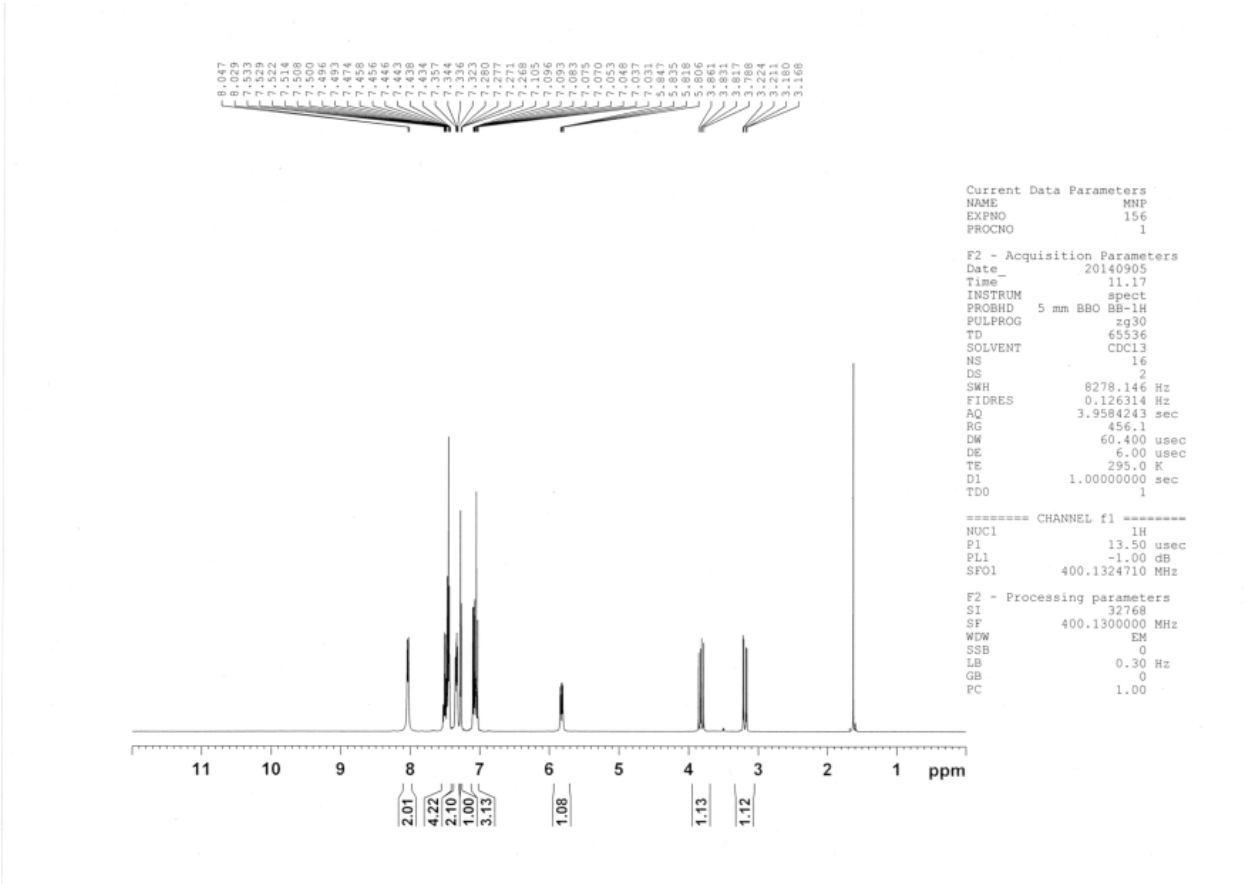
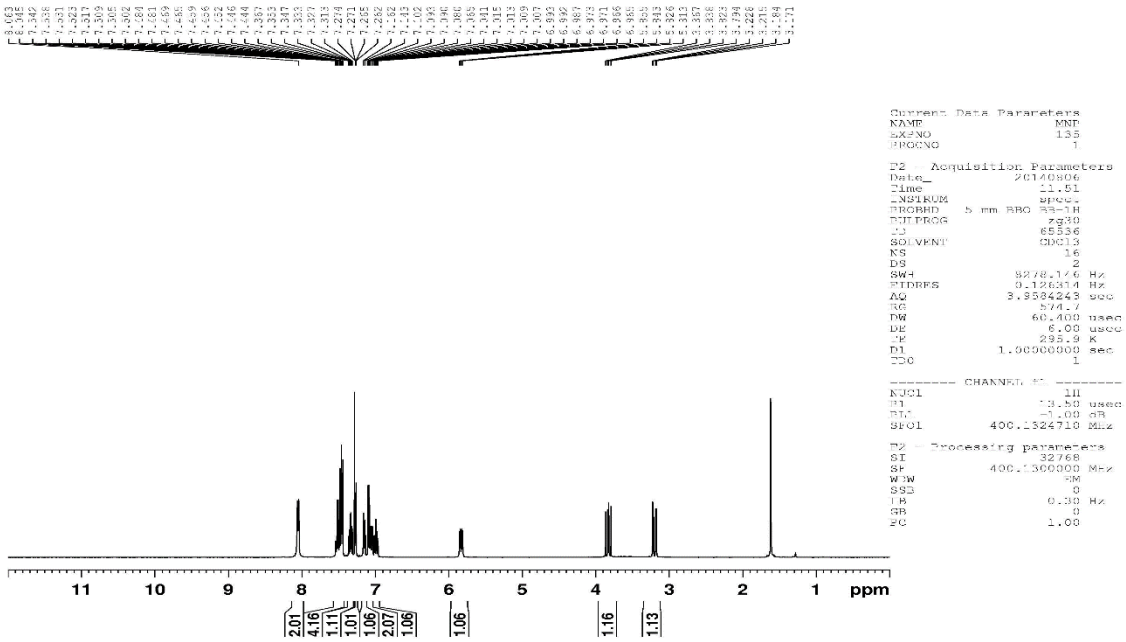
**Supplementary material 1:** $^{1}$H NMR spectra of ligands (5a–5g)

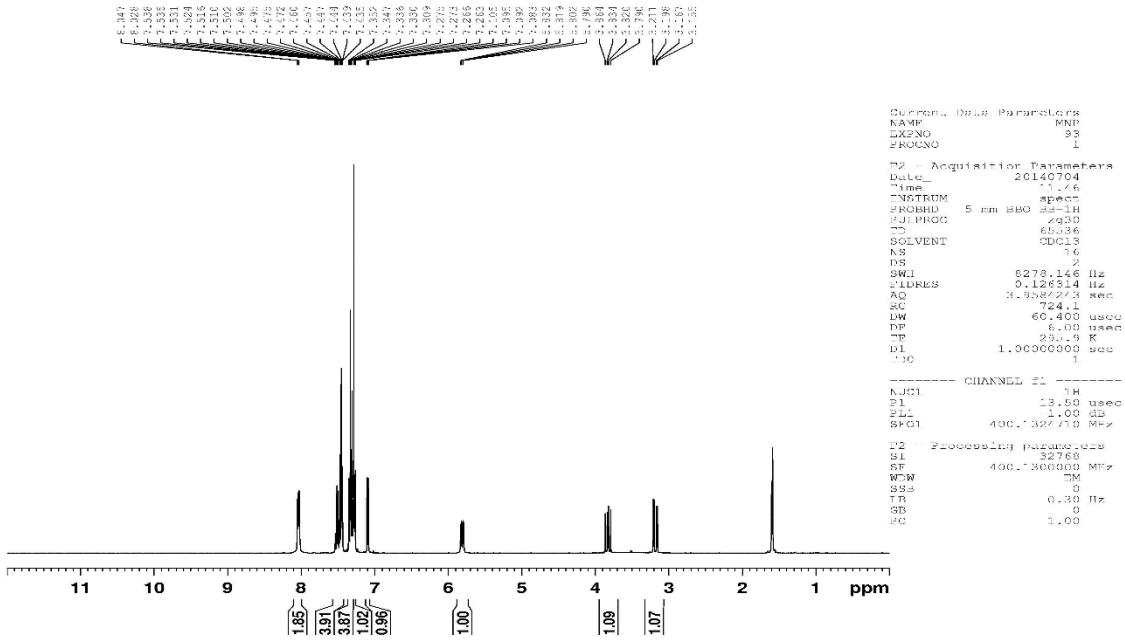
**1.** [5-(4-Fluorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5a)**



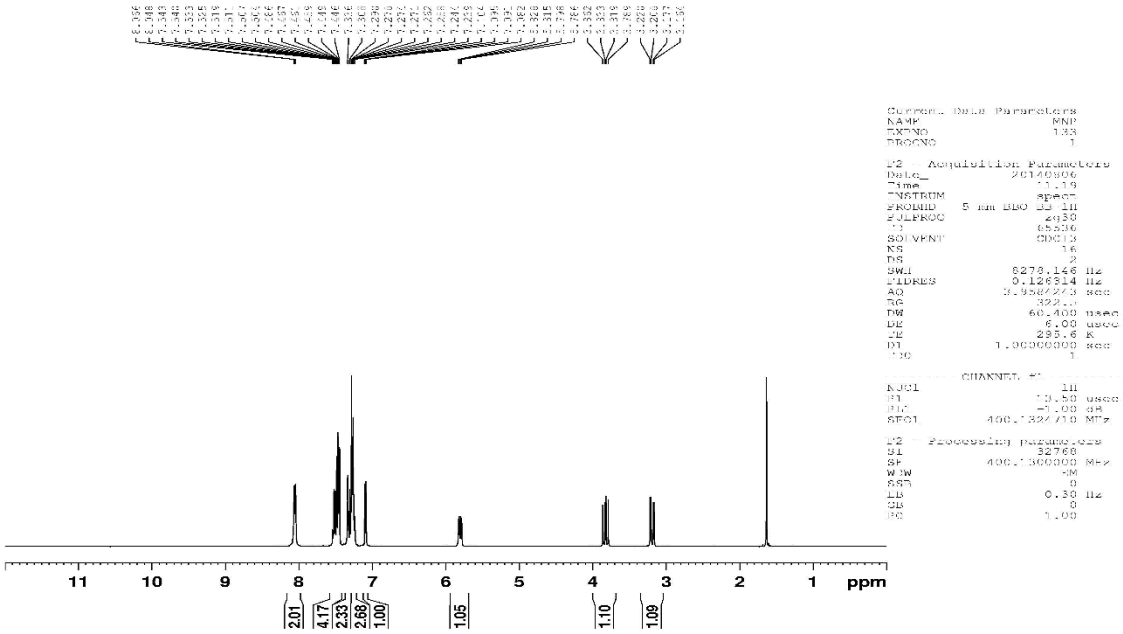
**2.** [5-(3-Fluorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5b)**



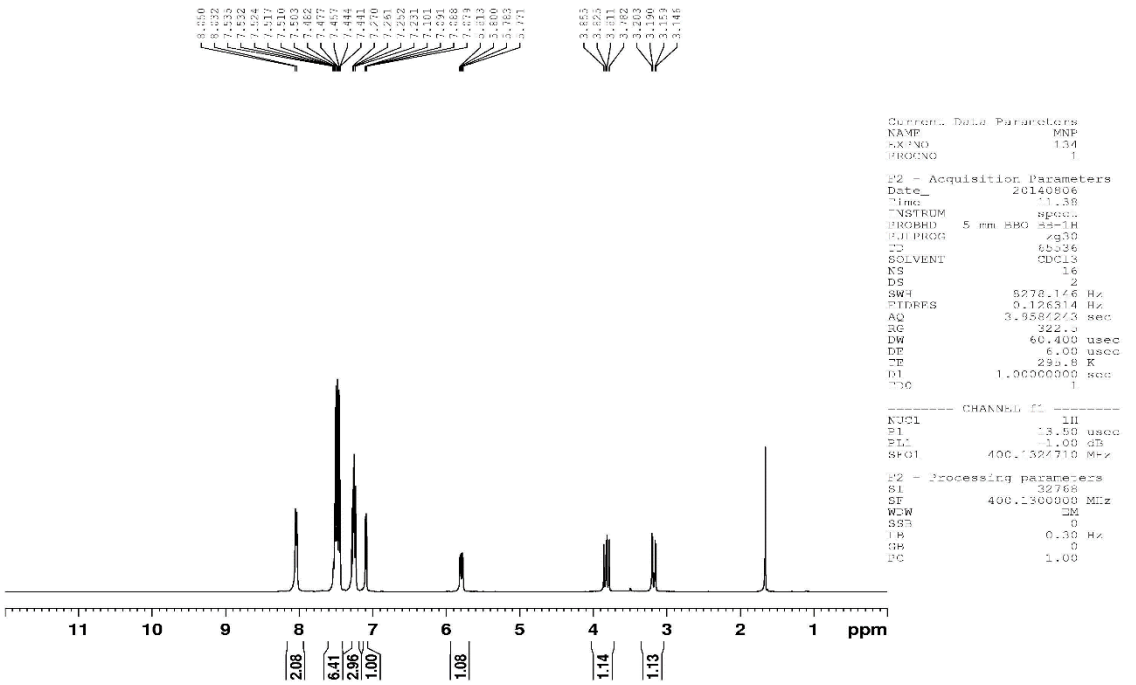

**3.** [5-(4-Chlorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5c)**



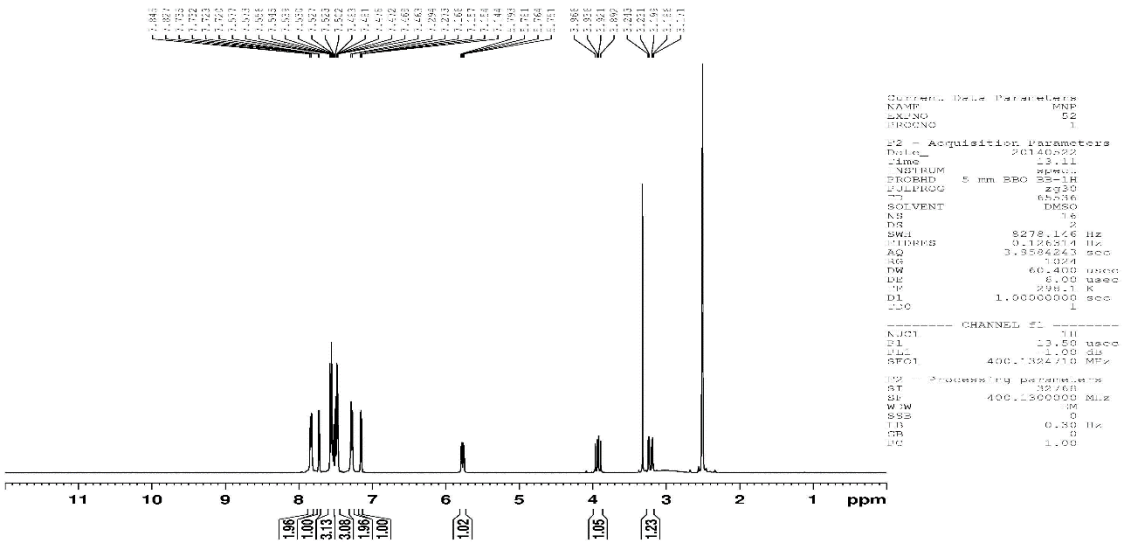
**4.** [5-(3-Chlorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5d)**



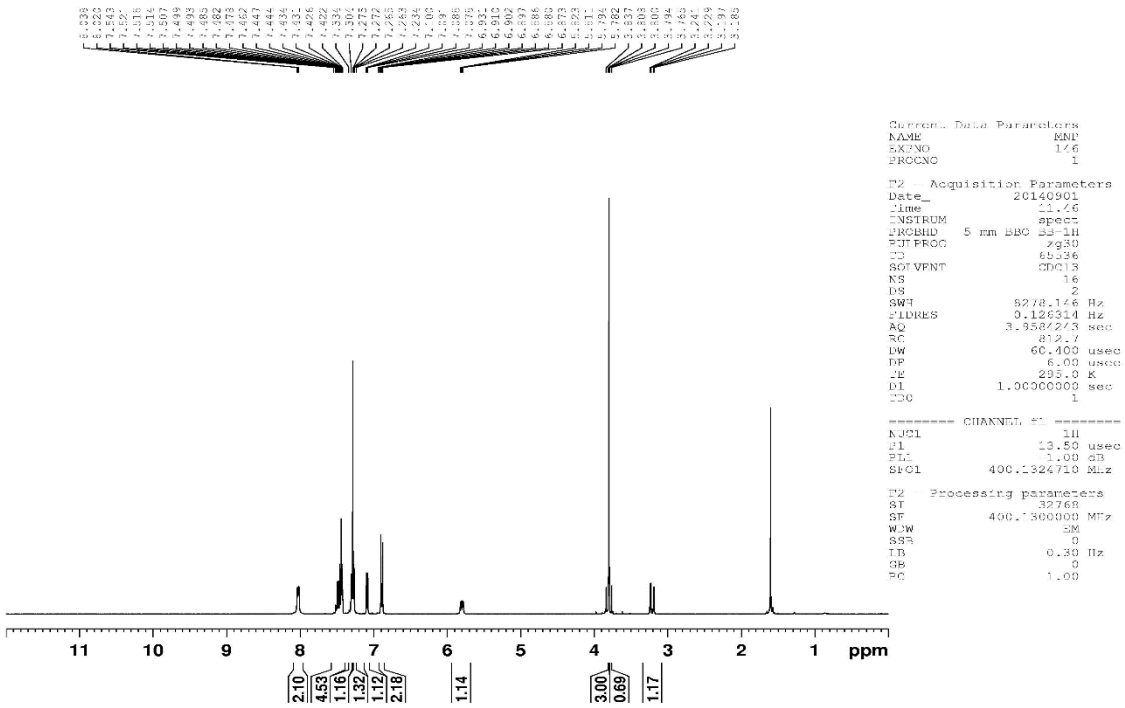

**5.** [5-(4-Bromophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5e)**



**6.** [5-(3-Bromophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5f)**

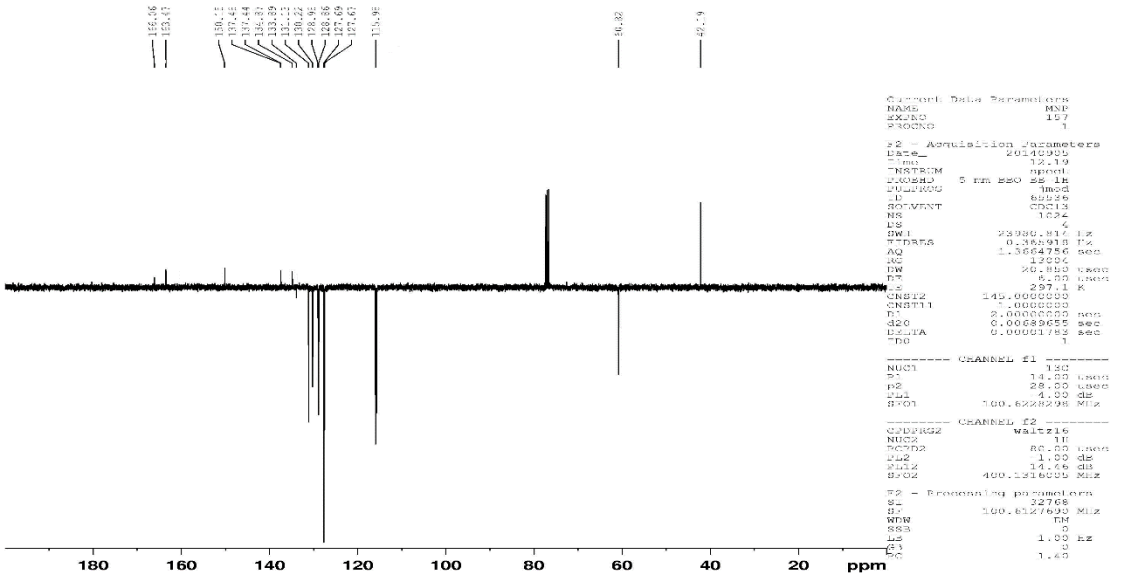


**7.** [5-(4-Methoxyphenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5g)**

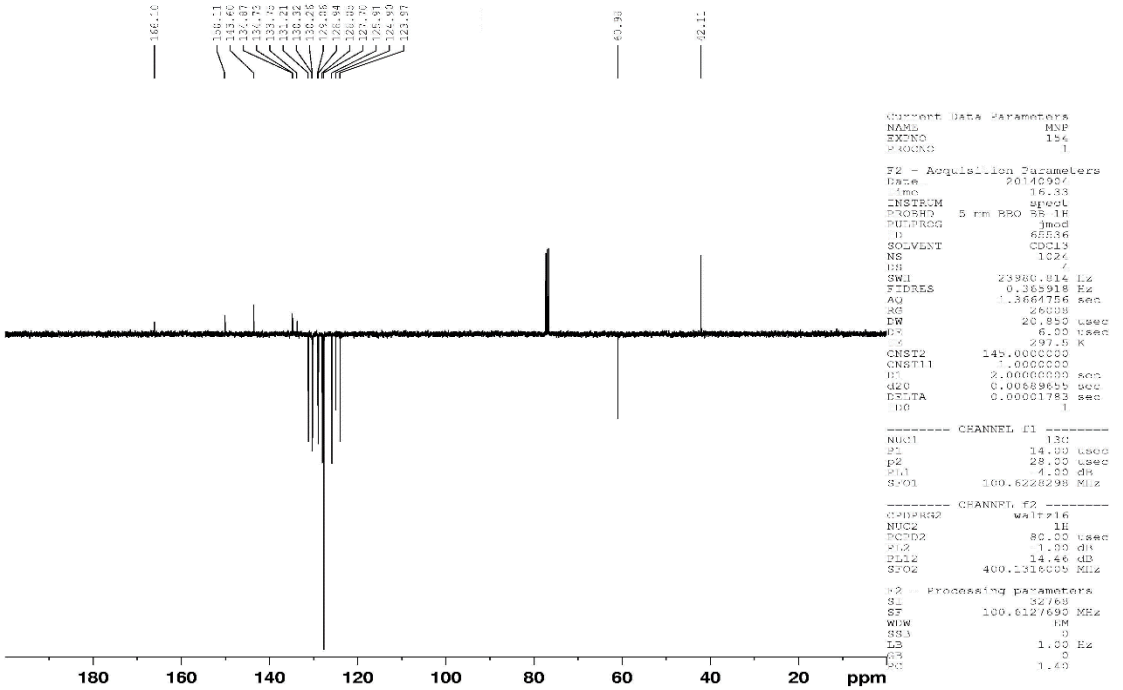


**Supplementary material 2:** $^{13}C$ NMR spectra of ligands (5a–5g)

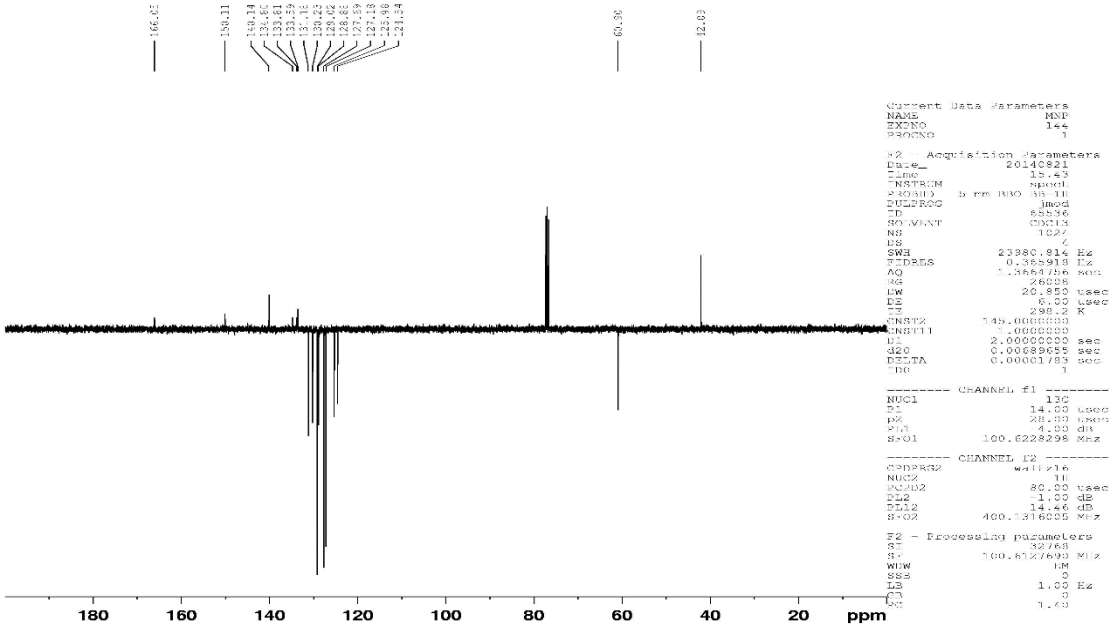
**1.** [5-(4-Fluorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5a)**



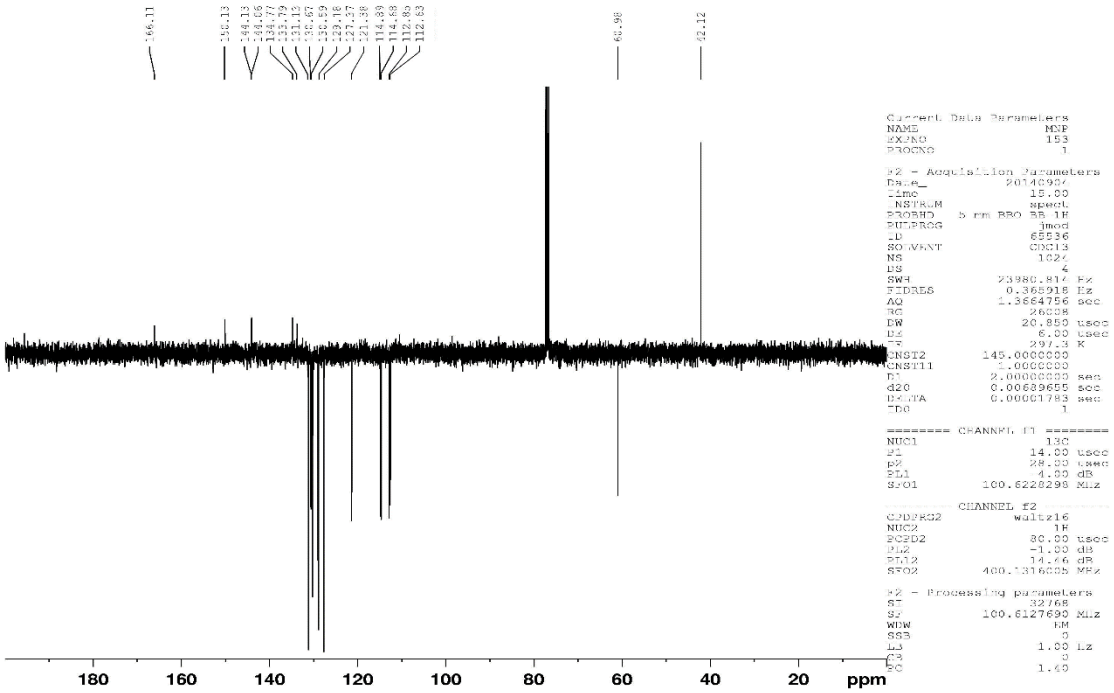

**2.** [5-(3-Fluorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5b)**



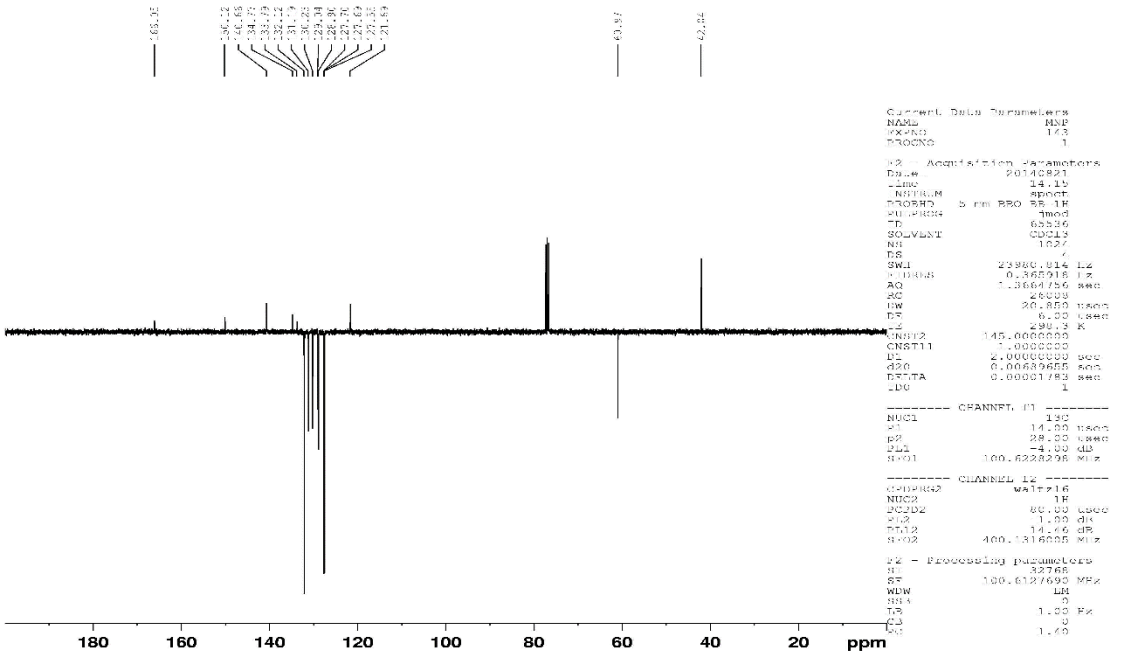
**3.** [5-(4-Chlorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5c)**



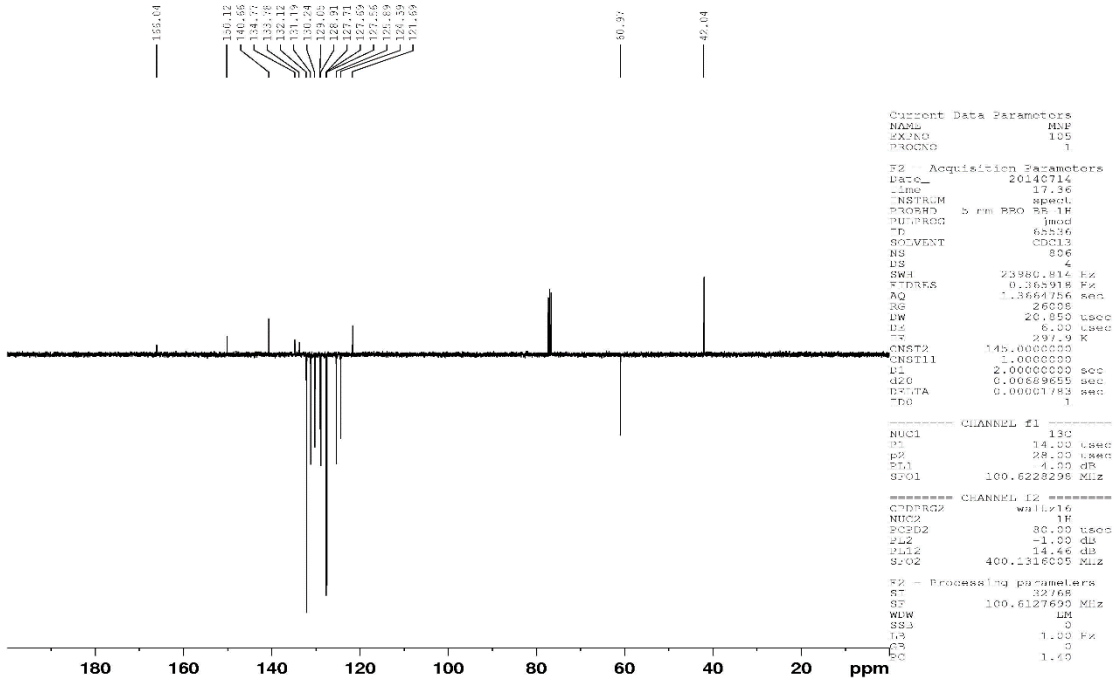

**4.** [5-(3-Chlorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5d)**



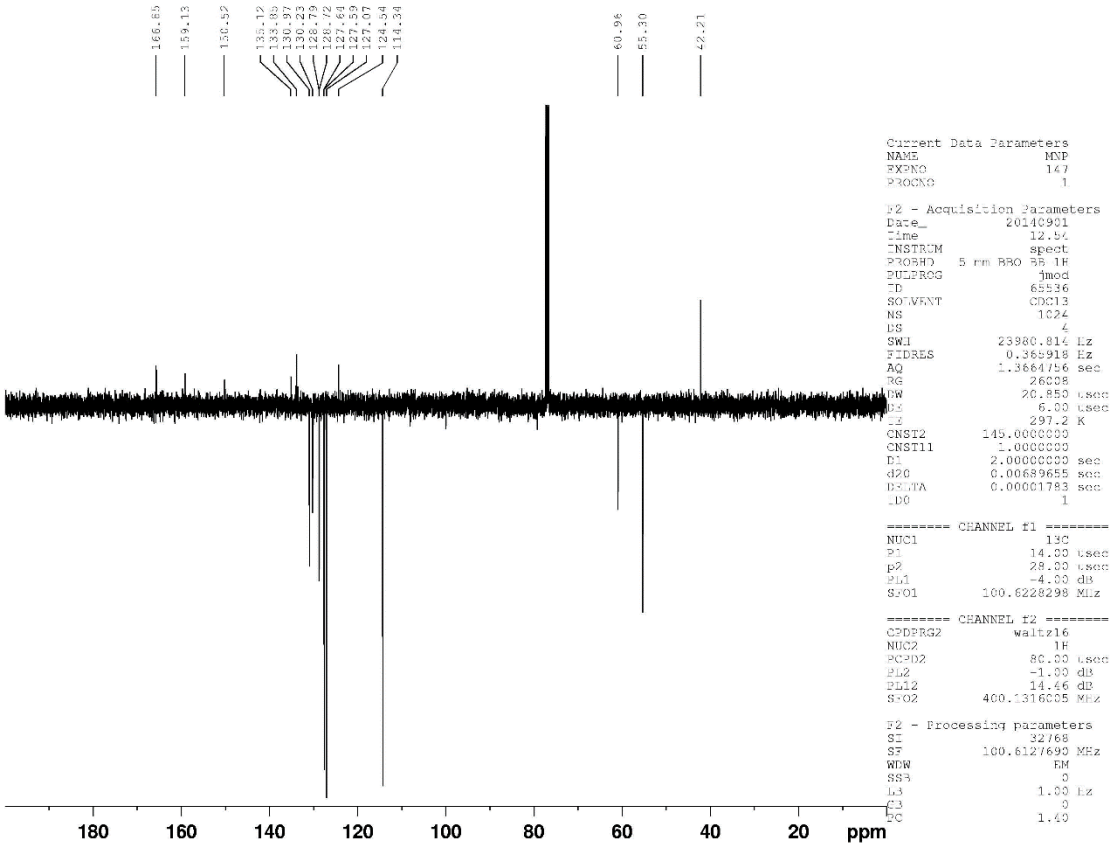
**5.** [5-(4-Bromophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5e)**



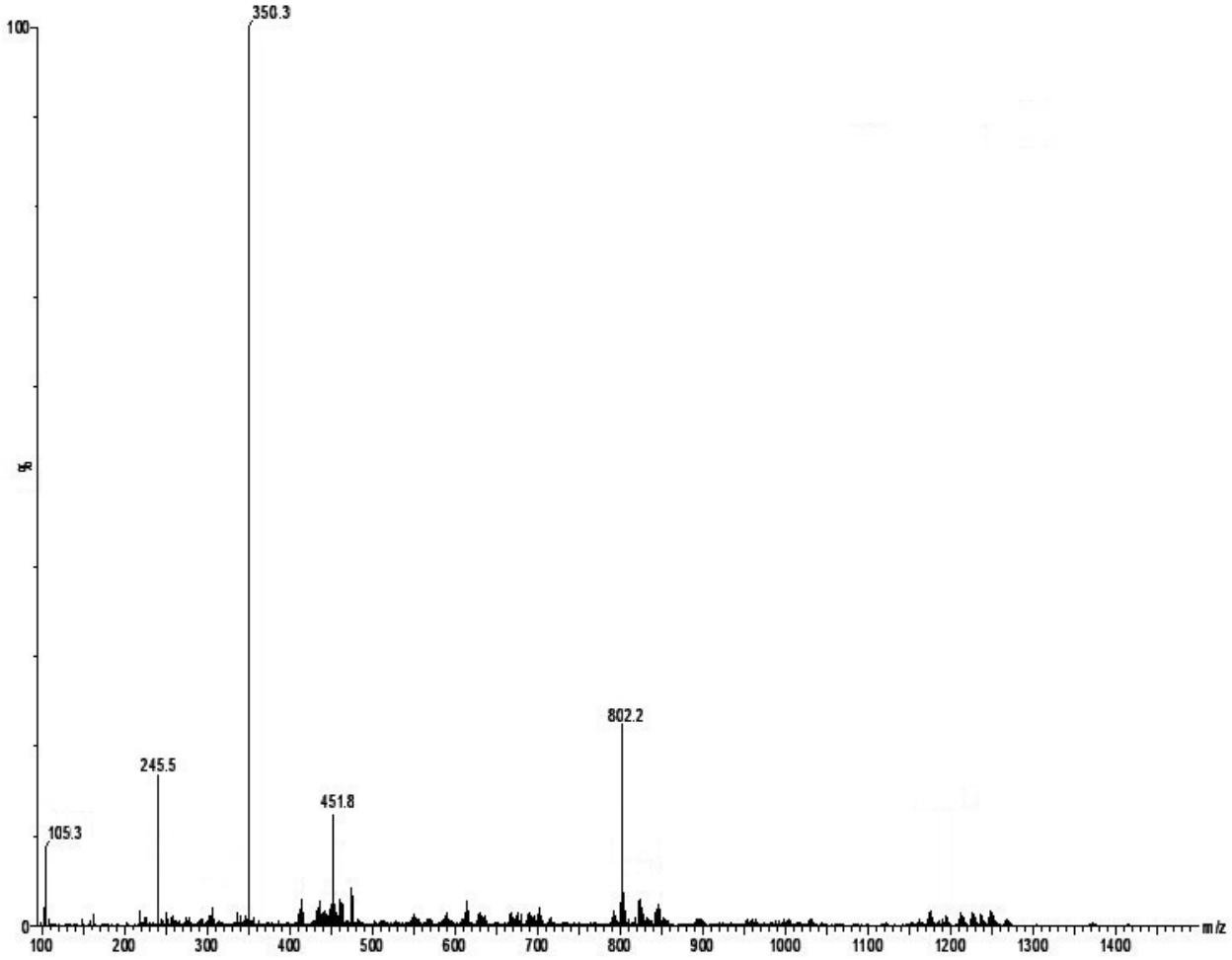

**6.** [5-(3-Bromophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5f)**



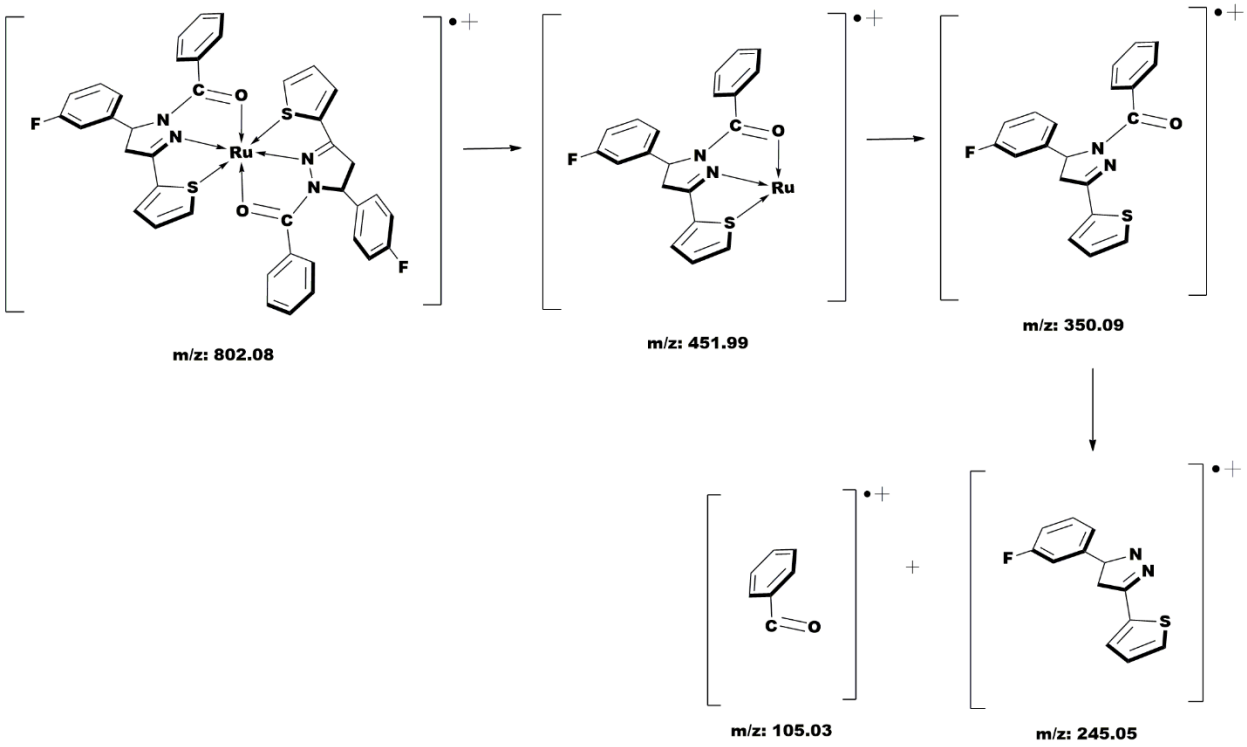
**7.** [5-(4-Methoxyphenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5g)**



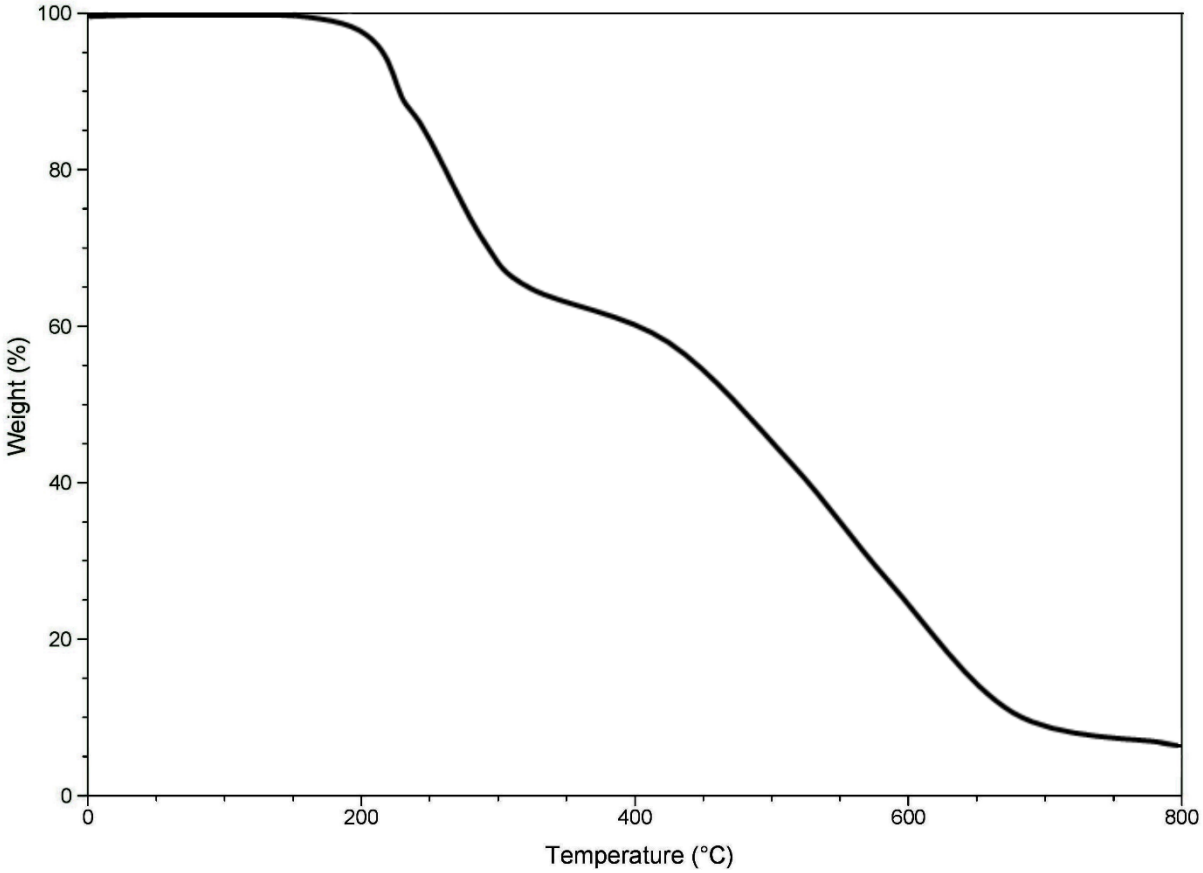
**Supplementary material 3:** LC-mass spectrum of complex **6a**



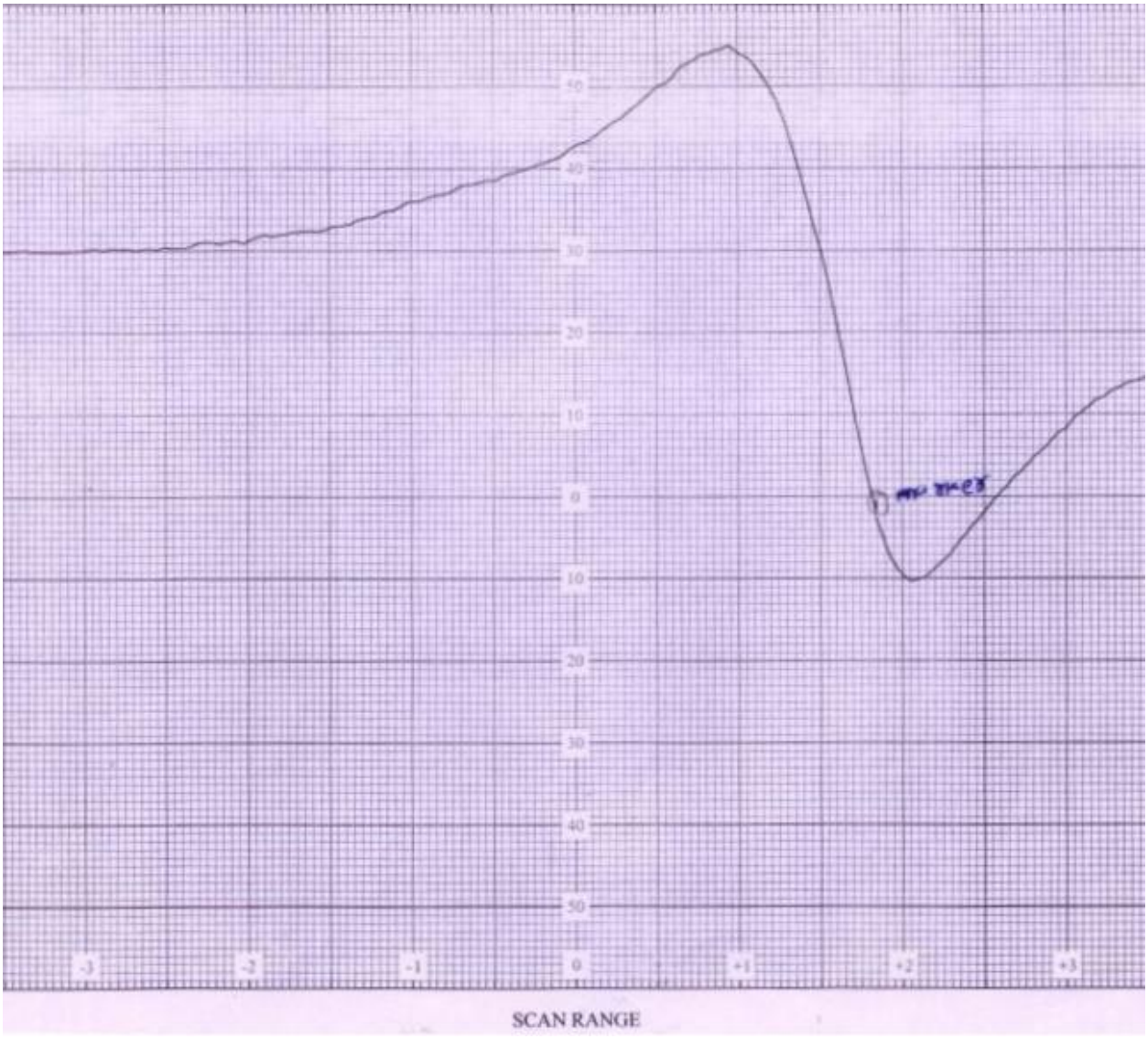
**Supplementary material 4:** Mass fragmentation pattern of complex **6a**



**Supplementary material 5:** Thermogravimetric analysis (TGA) of complex **6a**



**Supplementary material 6:** An electron paramagnetic resonance (EPR) spectrum of complex 6a



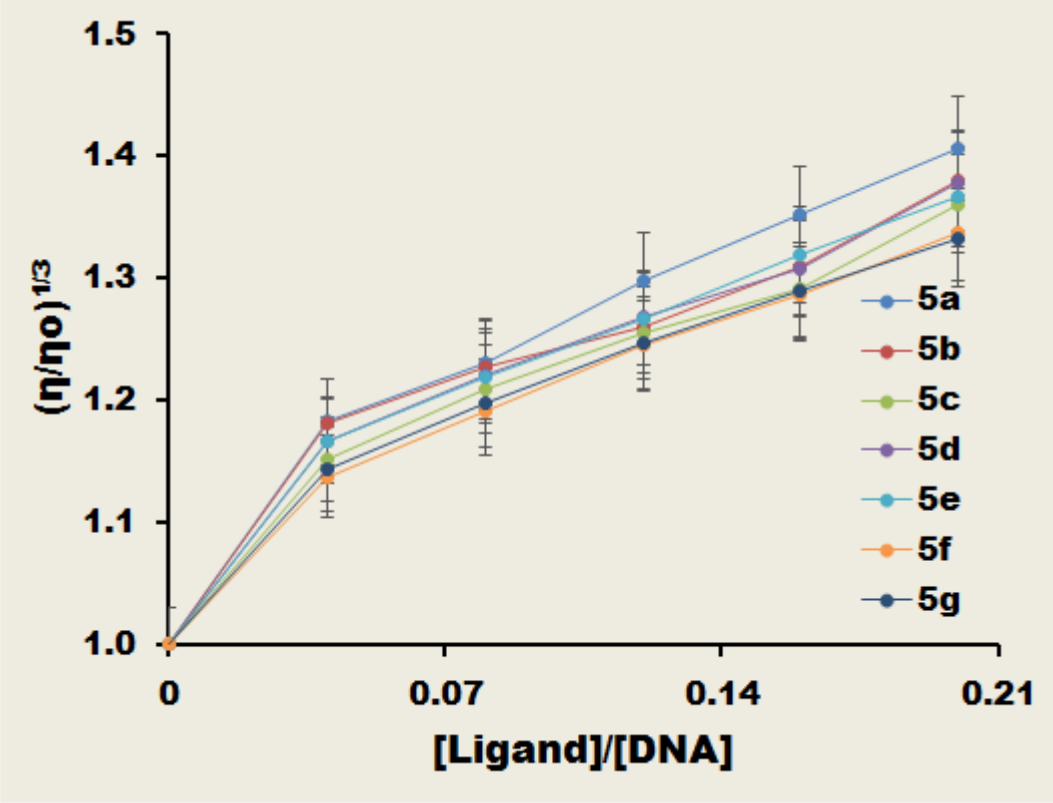
**Supplementary material 7:** Binding constant ($K_b$), percentage hypochromicity (%H), bathochromicity ($\Delta\lambda$), $IC_{50}$ (antimalarial) and $LC_{50}$ (*in vitro* cytotoxicity) values of free ligands and synthesized complexes with error uncertainty in the value ±5 %

| Compounds | $K_b$ (L mol$^{-1}$) | %H | $\Delta\lambda$ nm | $IC_{50}$(mg/L) | $LC_{50}$(mg/L) |
|---|---|---|---|---|---|
| 5a | 0.876±0.02 × $10^5$ | 21.31±0.55 | 2.9±0.08 | 1.12±0.03 | 71.614±2.15 |
| 5b | 0.825±0.02 × $10^5$ | 20.00±0.54 | 2.8±0.09 | 1.17±0.04 | 75.857±2.46 |
| 5c | 0.652±0.01 × $10^5$ | 18.53±0.61 | 2.9±0.10 | 1.22±0.04 | 80.909±2.70 |
| 5d | 0.552±0.01 × $10^5$ | 17.94±0.62 | 3.2±0.11 | 1.25±0.03 | 100.925±3.10 |
| 5e | 0.505±0.01 × $10^5$ | 18.71±0.60 | 3.7±0.10 | 1.24±0.03 | 99.311±3.03 |
| 5f | 0.476±0.01 × $10^5$ | 17.96±0.55 | 2.7±0.10 | 1.30±0.05 | 100.46±2.82 |
| 5g | 0.369±0.01 × $10^5$ | 18.70±0.56 | 2.9±0.10 | 1.50±0.06 | 119.124±3.56 |
| 6a | 5.02±0.13 × $10^5$ | 23.36±0.82 | 2.8±0.10 | 0.46±0.01 | 5.568±0.20 |
| 6b | 4.76±0.12 × $10^5$ | 22.02±0.59 | 2.8±0.09 | 0.50±0.01 | 5.680±0.19 |
| 6c | 3.84±0.12 × $10^5$ | 21.71±0.56 | 3.1±0.10 | 0.65±0.01 | 7.589±0.23 |
| 6d | 3.19±0.11 × $10^5$ | 20.80±0.62 | 3.6±0.12 | 0.76±0.01 | 7.908±0.24 |
| 6e | 3.29±0.11 × $10^5$ | 19.58±0.66 | 3.4±0.12 | 0.84±0.01 | 7.998±0.26 |
| 6f | 3.17±0.10 × $10^5$ | 19.32±0.58 | 2.9±0.10 | 0.88±0.01 | 7.852±0.25 |
| 6g | 2.80±0.09 × $10^5$ | 20.42±0.72 | 3.0±0.11 | 0.94±0.01 | 8.009±0.29 |

**Supplementary material 8:** Bacteriostatic concentration of ligands and synthesized complexes by broth dilution method in terms of MIC in µmol $L^{-1}$ with error uncertainty in the value ±5 %

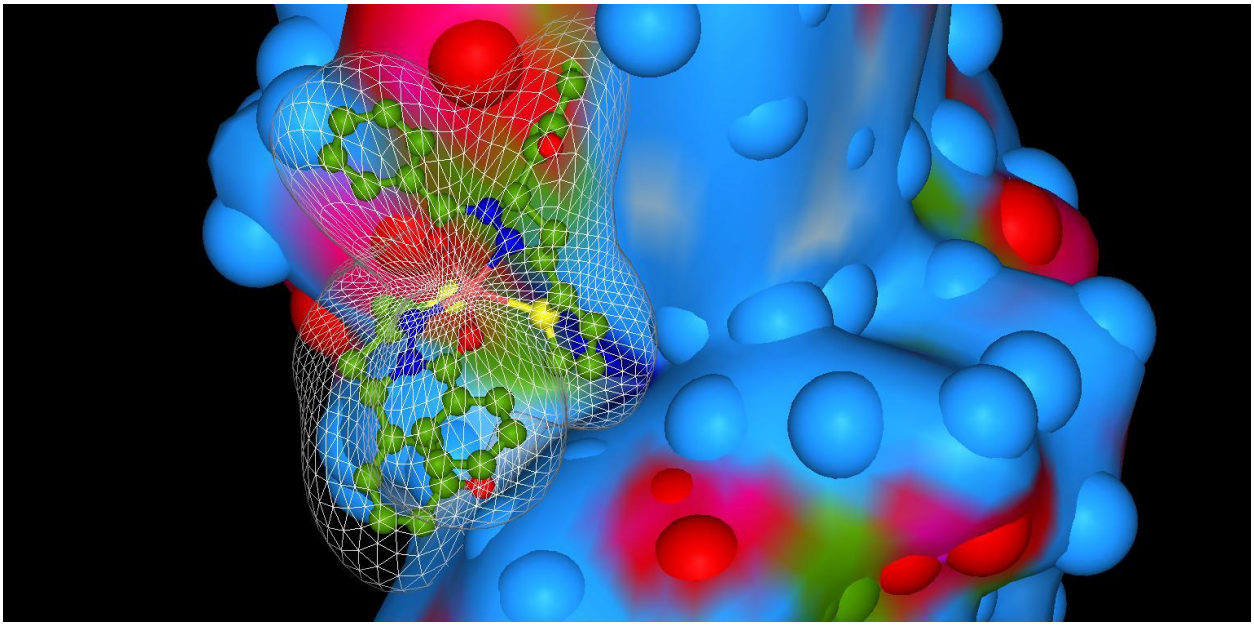
| Compounds | Gram(+ve) | | Gram(-ve) | | |
|---|---|---|---|---|---|
| | *S. Aureus* | *B. subtilis* | *S. marcescens* | *P. aeruginosa* | *E. coli* |
| 5a | 266±2 | 253±4 | 267±2 | 263±2 | 270±2 |
| 5b | 273±3 | 258±4 | 274±3 | 271±2 | 277±2 |
| 5c | 279±2 | 263±3 | 282±3 | 278±3 | 285±2 |
| 5d | 288±3 | 271±3 | 287±3 | 285±2 | 296±3 |
| 5e | 292±3 | 279±3 | 296±3 | 293±2 | 302±2 |
| 5f | 299±3 | 287±2 | 304±3 | 301±2 | 308±2 |
| 5g | 307±3 | 296±3 | 310±3 | 309±3 | 314±3 |
| 6a | 86±1 | 83±1 | 84±1 | 86±1 | 70±1 |
| 6b | 90±1 | 86±1 | 88±1 | 90±1 | 76±1 |
| 6c | 95±1 | 91±2 | 83±1 | 95±1 | 81±1 |
| 6d | 99±2 | 97±1 | 86±1 | 99±1 | 86±1 |
| 6e | 105±2 | 99±1 | 103±1 | 105±1 | 91±1 |
| 6f | 104±1 | 103±1 | 108±1 | 109±1 | 97±1 |
| 6g | 112±2 | 114±2 | 115±1 | 114±2 | 111±2 |

**Supplementary material 9:** Effect on relative viscosity of HS DNA under the influence of increasing amounts of pyrazolines ligands at 27 (±0.1) °C in phosphate buffer at pH=7.2 with error uncertainty in the value ±5 %

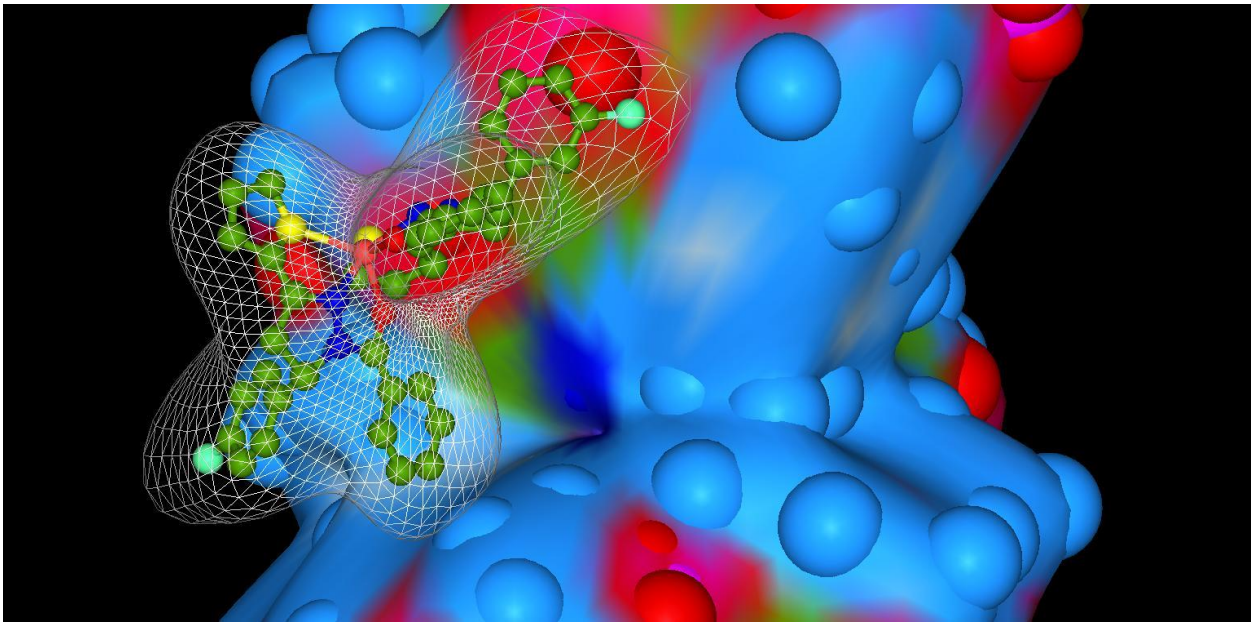


**Supplementary material 10:** Molecular docking of the complexes 6b–6g and pyrazolines ligands (5a-5g) (ball and stick) with the DNA duplex (VDW spheres) of sequence d(ACCGACGTCGGT)$_2$. The complex is docked in to the DNA showing intercalation between the DNA base pairs.

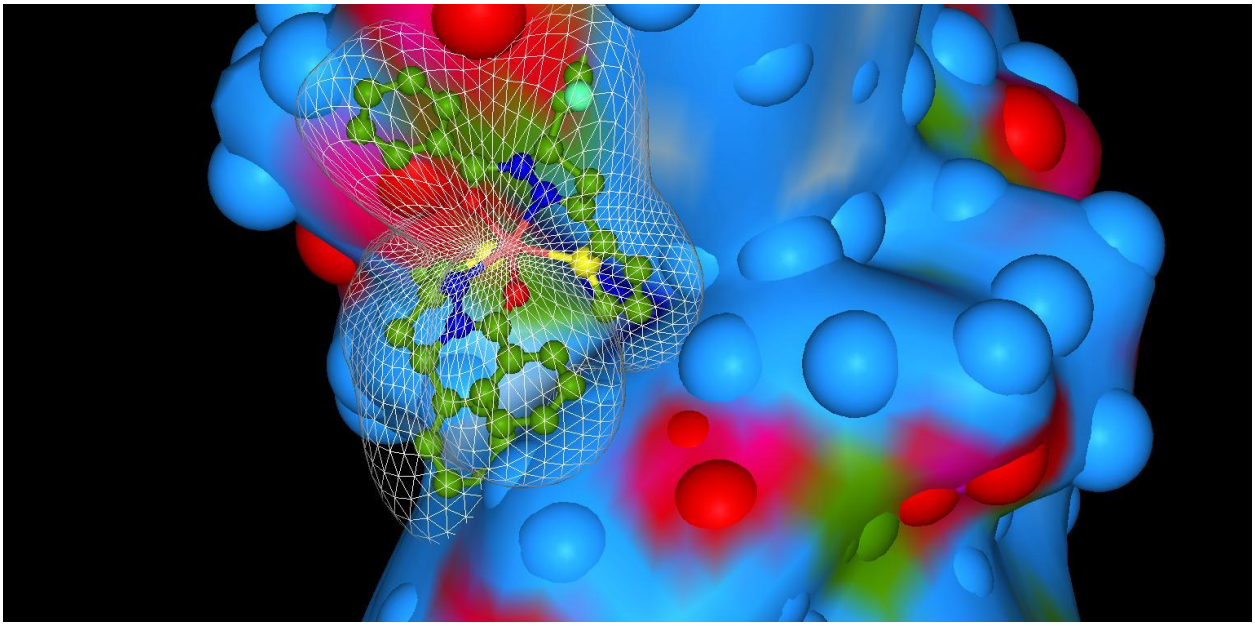
**1.** $Ru^{III}$ Complex **(6b)**



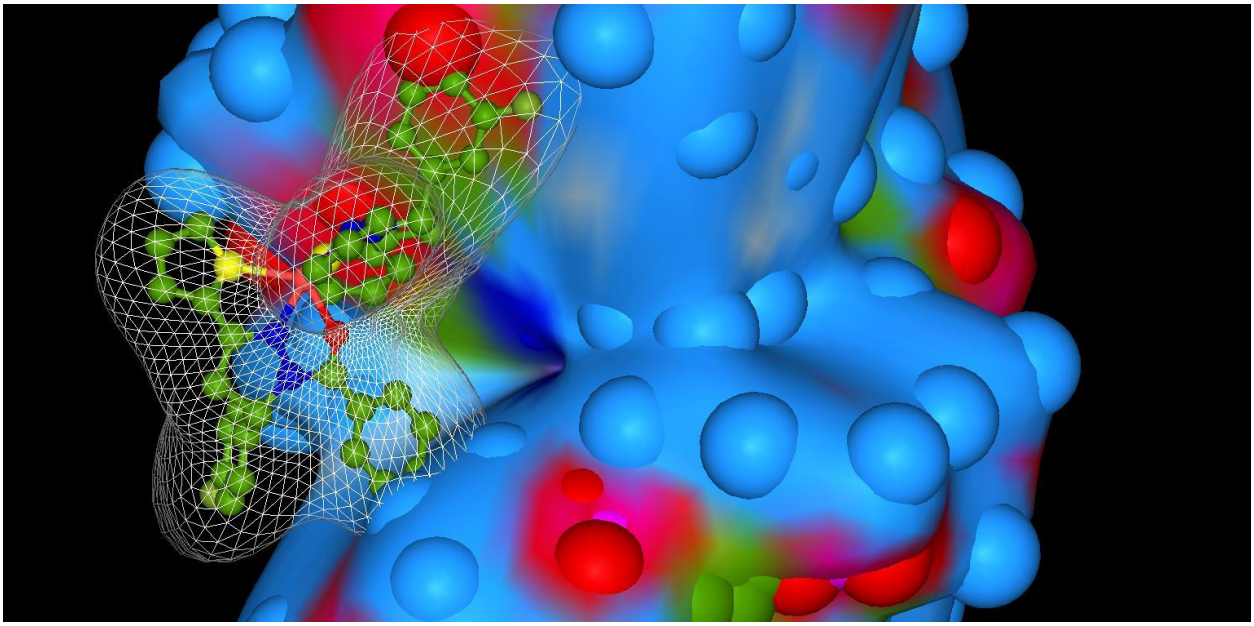
**2.** $Ru^{III}$ Complex **(6c)**



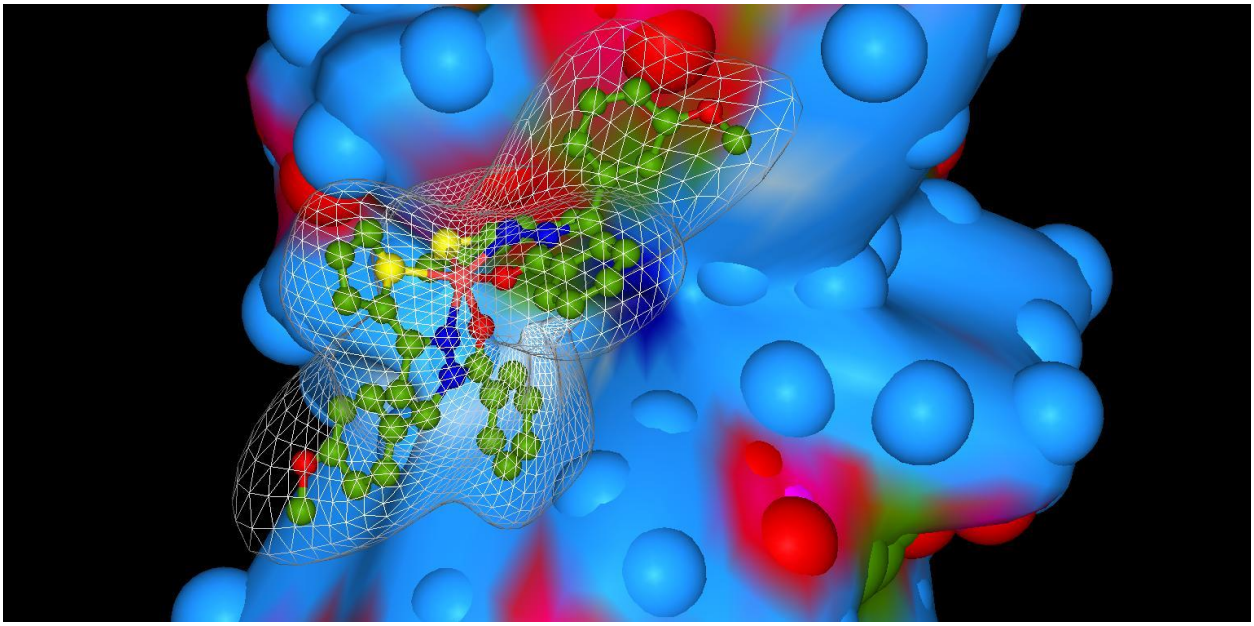
**3.** $Ru^{III}$ Complex **(6d)**



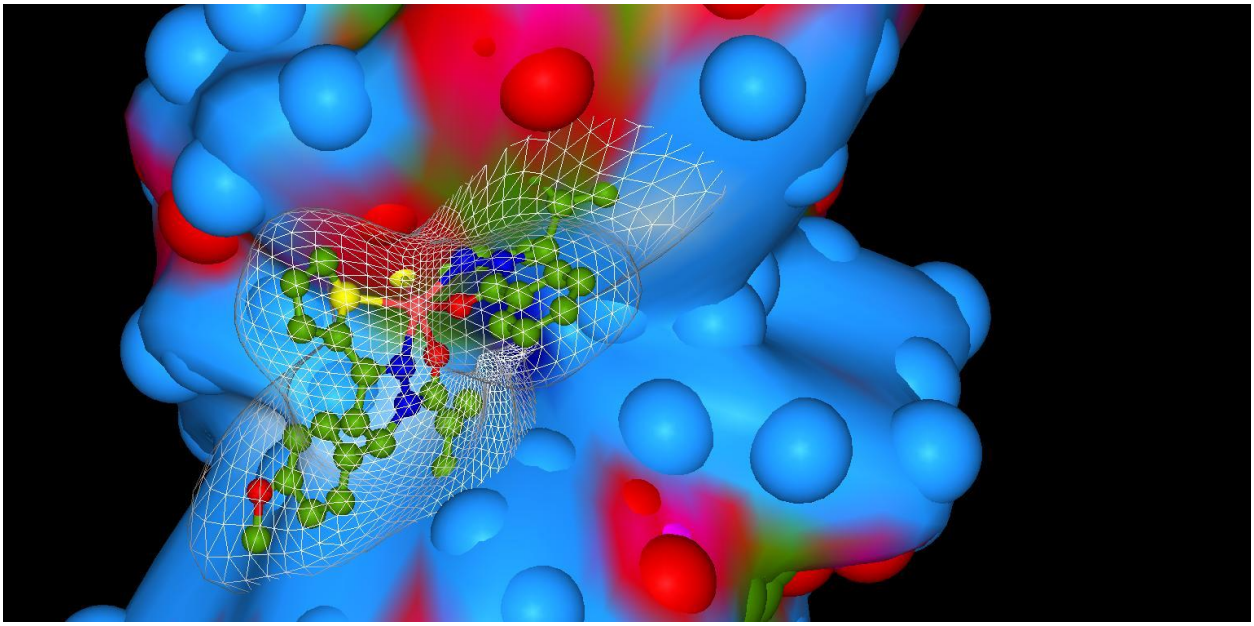
**4.** $Ru^{III}$ Complex **(6e)**



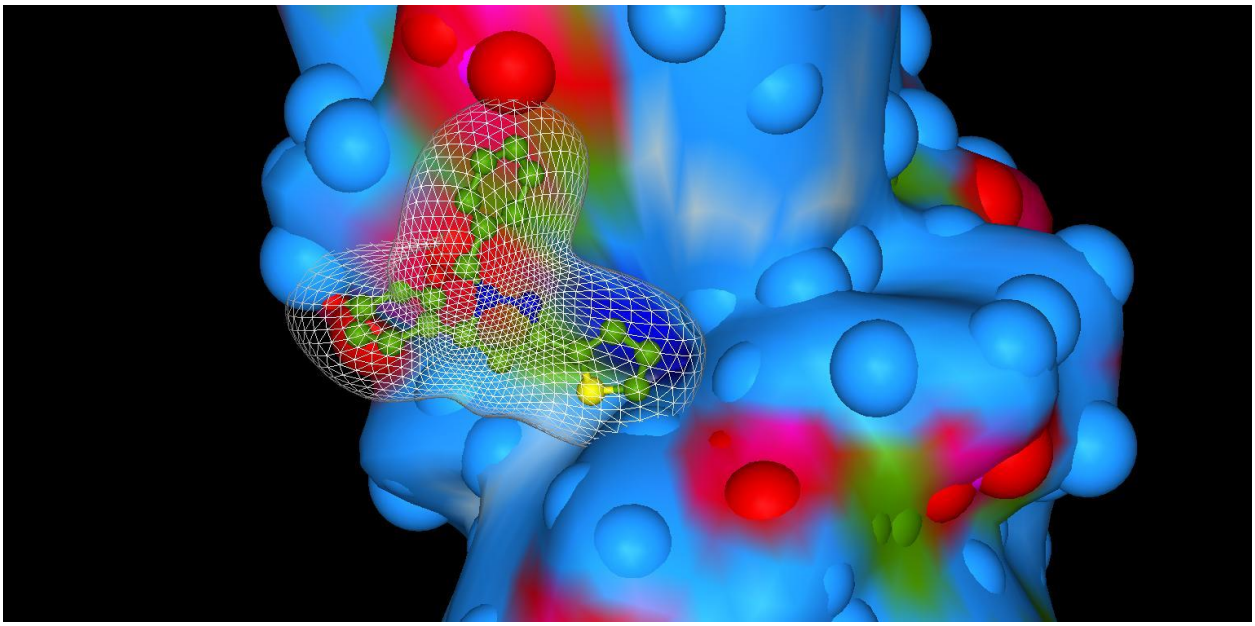
**5.** $Ru^{III}$ Complex **(6f)**



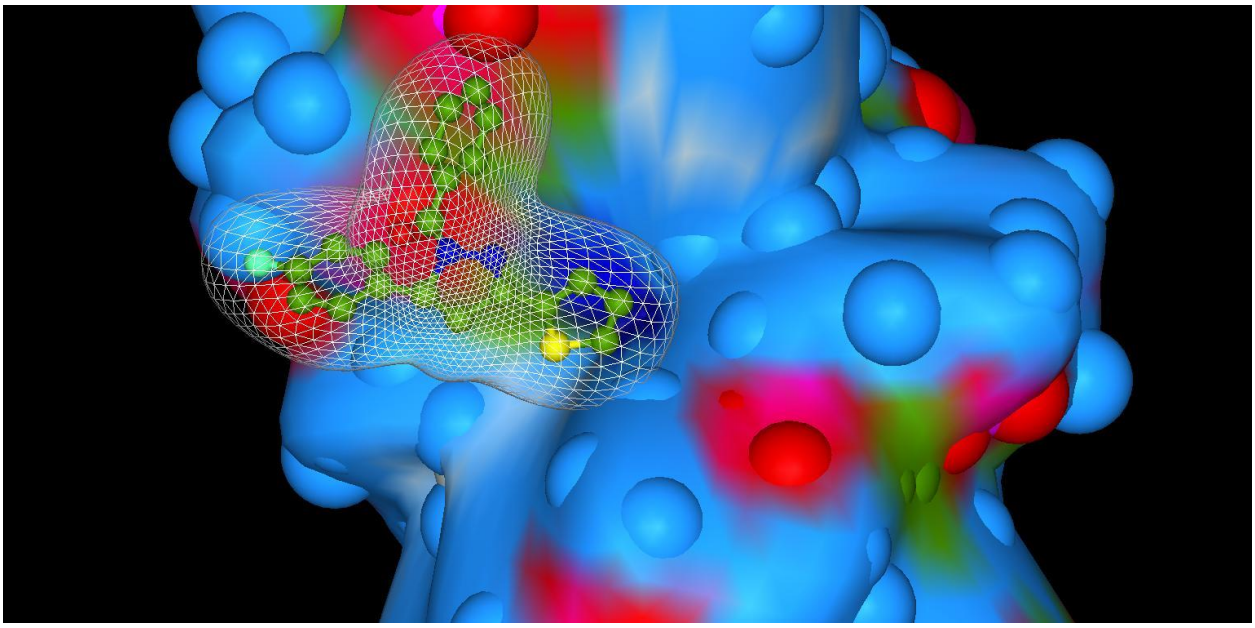
**6.** $Ru^{III}$ Complex **(6g)**



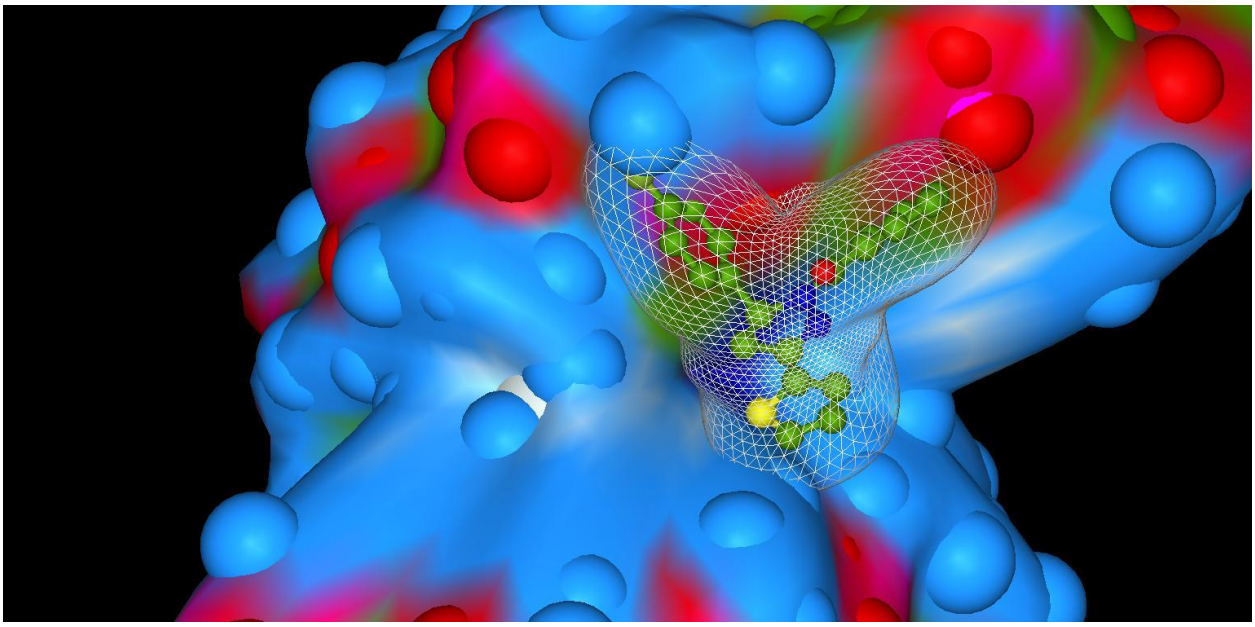
**7.** [5-(4-Fluorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5a)**



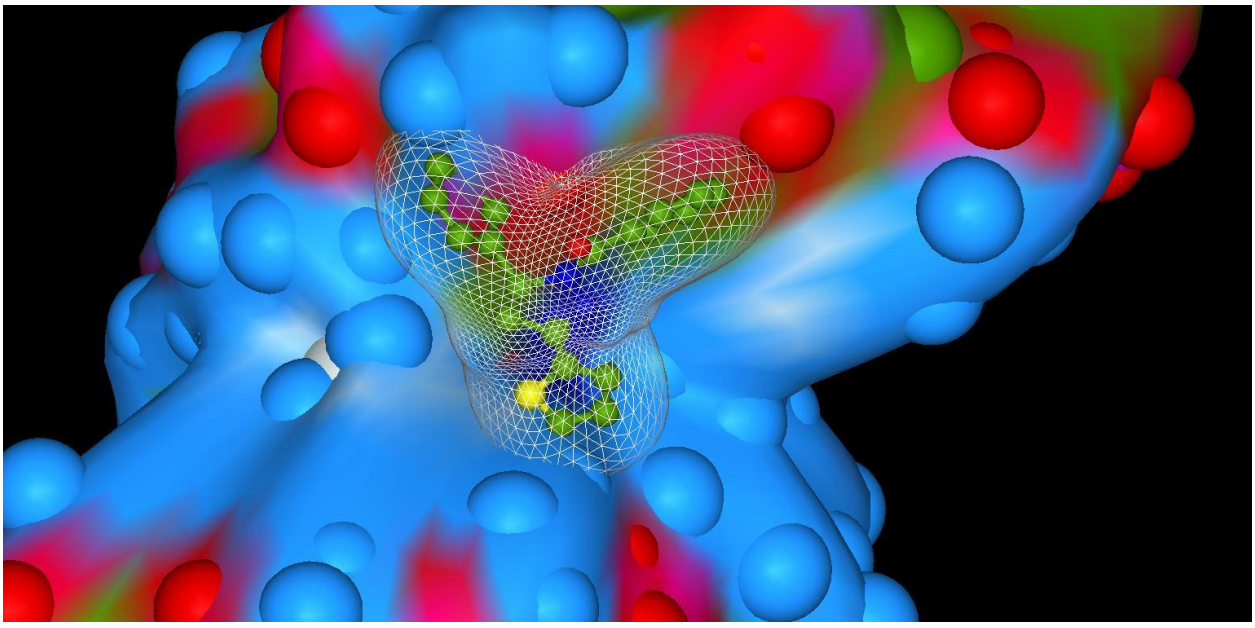
**8.** [5-(3-Fluorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5b)**



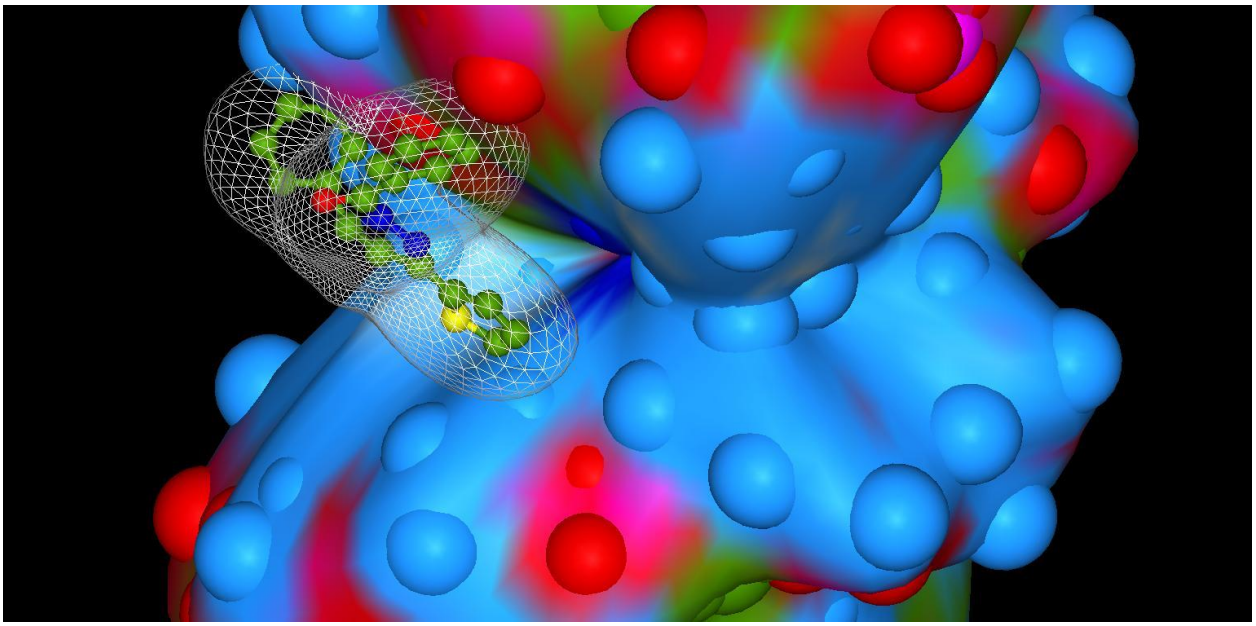
**9.** [5-(4-Chlorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5c)**



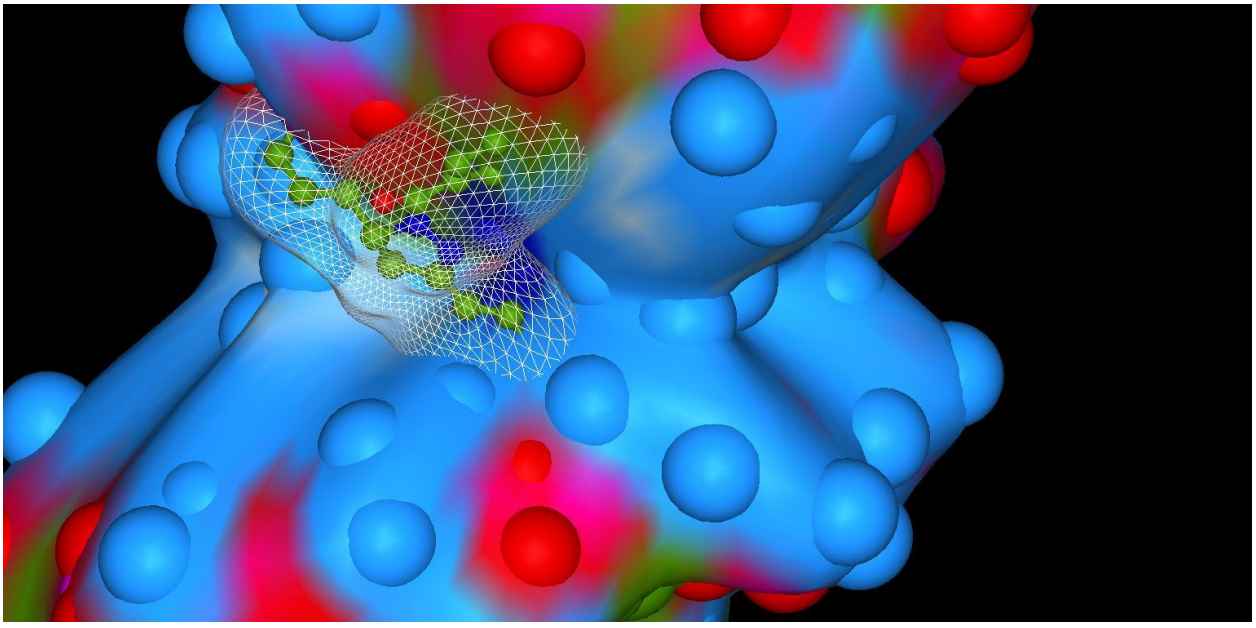
**10.** [5-(3-Chlorophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5d)**



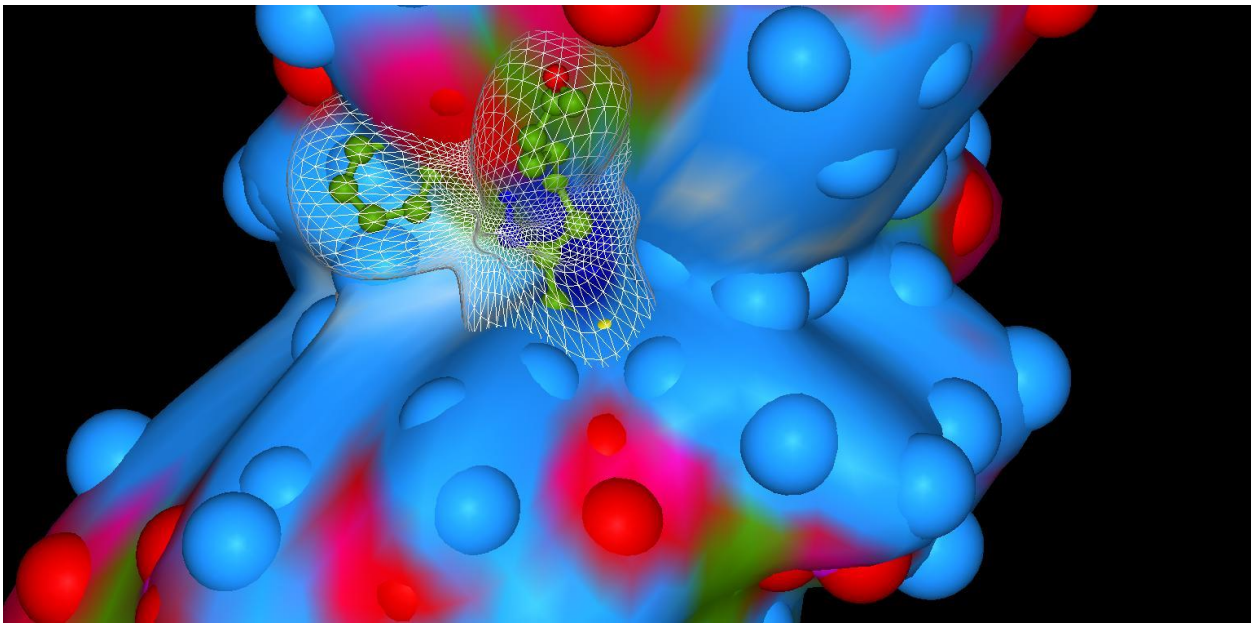
**11.** [5-(4-Bromophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5e)**



**12.** [5-(3-Bromophenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5f)**



**13.** [5-(4-Methoxyphenyl)-3-(thiophen-2-yl)-4, 5-dihydro-1H-pyrazol-1-yl]-phenyl methanone **(5g)**



**Supplementary material 11:** Complex mediated DNA cleavage data by agarose gel electrophoresis with error uncertainty in the value ±5 %

| Lane No. | Compound | Form I | Form II | Form III | % Cleavage |
|---|---|---|---|---|---|
| 1 | 5a | 48±1 | 30±1 | 22±1 | 45.45±.1.0 |
| 2 | 5b | 48±1 | 32±1 | 20±1 | 45.45±0.9 |
| 3 | 5c | 49±1 | 32±1 | 19±1 | 44.31±0.8 |
| 4 | 5d | 50±1 | 34±1 | 16±1 | 43.18±0.8 |
| 5 | 5e | 51±1 | 32±1 | 17±1 | 42.04±0.8 |
| 6 | 5f | 51±1 | 34±1 | 15±1 | 42.04±0.7 |
| 7 | 5g | 52±1 | 33±1 | 15±1 | 40.90±0.7 |
| 8 | DNA Control | 88±2 | 12±1 | – | – |
| 9 | $RuCl_3 \cdot 3H_2O$ | 81±2 | 19±1 | – | 7.95±0.21 |
| 10 | 6a | 21±1 | 53±1 | 26±1 | 76.13±2.2 |
| 11 | 6b | 23±1 | 43±1 | 34±1 | 73.86±2.0 |
| 12 | 6c | 25±1 | 40±1 | 35±1 | 71.59±1.8 |
| 13 | 6d | 26±1 | 42±1 | 32±1 | 70.45±1.7 |
| 14 | 6e | 27±1 | 44±1 | 29±1 | 69.31±1.6 |
| 15 | 6f | 28±1 | 44±1 | 28±1 | 68.18±1.6 |
| 16 | 6g | 29±1 | 40±1 | 31±1 | 67.04±1.5 |