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Supplementary material 1: $^1$H NMR & $^{13}$C NMR spectra
Figure S1: NMR
5'-(IH-Imidazol-1-yl)-3'-methyl-1',2-diphenyl-5-(pyridin-2-yl)-3,4-dihydro-J'H,2H-3,4'-bipyrazole (bpy-N) [4a]
3'-Methyl-5'-phenoxy-1',2-diphenyl-5-(pyridin-2-yl)-3,4-dihydro-1'H,2H-3,4'-bipyrazole (bpy-O) [4b]

Figure S3: $^1$H NMR
Figure S4: APT

4-(5-(1H-Imidazol-1-yl)-3-methyl-1-phenyl-1H-pyrazol-4-yl)-6-(pyridin-2-yl)pyrimidin-2-amine (pma-N) [5a]

Figure S5: $^1$H NMR
Figure S6: APT

4-(3-Methyl-5-phenoxy-1-phenyl-1H-pyrazol-4-yl)-6-(pyridin-2-yl)pyrimidin-2-amine (pma-O) [5b]

Figure S7: $^1$H NMR
7-(5-(1H-Imidazol-1-yl)-3-methyl-1-phenyl-1H-pyrazol-4-yl)-5-(pyridin-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidine (tpm-N) [6a]

Figure S9: $^1$H NMR
7-(3-Methyl-5-phenoxy-1-phenyl-1H-pyrazol-4-yl)-5-(pyridin-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidine (tpm-O) [6b]

Figure S11: $^1$H NMR
Figure S12: APT

$[(\eta^5-\text{C}_5\text{Me}_5)\text{Ir(bpy-N)}\text{Cl}]\text{Cl} \ [7a]$

Figure S13: $^1\text{H}$ NMR
Figure S14: APT

\[ (q^5\text{-C}_5\text{Me}_5)\text{Ir(bpy-O)}\text{Cl}]\text{Cl} [7b] 

Figure S15: $^1$H NMR
Figure S16: APT

\[ \text{APT}[\eta^5-C_5\text{Me}_5]\text{Ir}(\text{pma-N})\text{Cl}\text{Cl} \] [8a]

Figure S17: $^1$H NMR
Figure S18: APT

\[ \text{APT}[(\eta^5-\text{C}_5\text{Me}_5)\text{Ir(pma-O)}\text{Cl}]\text{Cl} [8b] \]

Figure S19: $^1$H NMR
Figure S20: APT

\[
[(\eta^5-C_5Me_5)Ir(tpm-N)Cl]Cl \quad [9a]
\]

Figure S21: \(^1\)H NMR
Figure S22: APT

\[(\eta^5{-}\text{CsMe}_5)\text{Ir}(\text{tpm-O})\text{Cl}]\text{Cl} \ [9b]\]

Figure S23: 'H NMR
Supplementary material 2: ESI-MS
Figure S25: Complex 7a
Supplementary material 3: Molecular docking

Figure S26: 4a

Figure S27: 4b

Figure S28: 5a
Supplementary material 4: DNA cleavage activity data presented with standard deviation for three independent experiments.

Table S34:

<table>
<thead>
<tr>
<th>Compounds</th>
<th>SC (µM)</th>
<th>L (µM)</th>
<th>NC (µM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNA control</td>
<td>$81 \pm 1.5$</td>
<td>$19 \pm 1.7$</td>
<td>-</td>
</tr>
<tr>
<td>Salt</td>
<td>$66 \pm 1.7$</td>
<td>$14 \pm 1.5$</td>
<td>$20 \pm 1.1$</td>
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<tr>
<td>4a</td>
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<td>$39 \pm 1.0$</td>
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<td>4b</td>
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<td>$49 \pm 2.0$</td>
<td>$30 \pm 1.5$</td>
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<td>5a</td>
<td>$23 \pm 1.1$</td>
<td>$43 \pm 1.1$</td>
<td>$34 \pm 1.1$</td>
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<td>5b</td>
<td>$25 \pm 2.0$</td>
<td>$40 \pm 1.2$</td>
<td>$35 \pm 2.0$</td>
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<tr>
<td>6a</td>
<td>$30 \pm 1.0$</td>
<td>$35 \pm 1.7$</td>
<td>$35 \pm 2.0$</td>
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<tr>
<td>6b</td>
<td>$23 \pm 1.5$</td>
<td>$41 \pm 1.5$</td>
<td>$36 \pm 1.5$</td>
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<tr>
<td>7a</td>
<td>$10 \pm 1.5$</td>
<td>$32 \pm 2.2$</td>
<td>$58 \pm 1.5$</td>
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<tr>
<td>7b</td>
<td>$19 \pm 2.0$</td>
<td>$29 \pm 1.2$</td>
<td>$52 \pm 1.0$</td>
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<td>8a</td>
<td>$20 \pm 2.0$</td>
<td>$39 \pm 0.9$</td>
<td>$41 \pm 2.0$</td>
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<tr>
<td>8b</td>
<td>$20 \pm 1.1$</td>
<td>$25 \pm 1.1$</td>
<td>$55 \pm 1.1$</td>
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<tr>
<td>9a</td>
<td>$21 \pm 1.5$</td>
<td>$28 \pm 1.6$</td>
<td>$51 \pm 1.5$</td>
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<tr>
<td>9b</td>
<td>$30 \pm 1.0$</td>
<td>$31 \pm 2.1$</td>
<td>$38 \pm 1.7$</td>
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</table>

Supplementary material 5: Anticancer activity on A549 (lung) cancer cell line, IC$_{50}$ data presented with standard deviation for three independent experiments.

Table S35:

<table>
<thead>
<tr>
<th>Compounds</th>
<th>IC$_{50}$ (µM)</th>
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<tbody>
<tr>
<td>4a</td>
<td>$387 \pm 1.20$</td>
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<tr>
<td>4b</td>
<td>$220 \pm 0.82$</td>
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<tr>
<td>5a</td>
<td>$197 \pm 2.12$</td>
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<tr>
<td>5b</td>
<td>$88 \pm 0.98$</td>
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<tr>
<td>6a</td>
<td>$290 \pm 3.20$</td>
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<tr>
<td>6b</td>
<td>$170 \pm 1.65$</td>
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<tr>
<td>7a</td>
<td>$245 \pm 4.23$</td>
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<tr>
<td>7b</td>
<td>$89 \pm 0.79$</td>
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<td>8a</td>
<td>$96 \pm 1.72$</td>
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<td>8b</td>
<td>$74 \pm 2.78$</td>
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<tr>
<td>9a</td>
<td>$163 \pm 0.43$</td>
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<td>9b</td>
<td>$116 \pm 3.49$</td>
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**Supplementary material 6**: MIC values of ligands and complexes in µM presented with standard deviation for three independent experiments.

**Table S36**:

<table>
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<tr>
<th>Compounds</th>
<th>Gram positive (in µM)</th>
<th>Gram negative (in µM)</th>
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<tr>
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<td><em>S.aureus</em></td>
<td><em>B.subtilis</em></td>
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<tr>
<td>Salt</td>
<td>566 ± 12</td>
<td>572 ± 6</td>
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<tr>
<td>4a</td>
<td>303 ± 5</td>
<td>301 ± 5</td>
</tr>
<tr>
<td>4b</td>
<td>316 ± 6</td>
<td>317 ± 6</td>
</tr>
<tr>
<td>5a</td>
<td>341 ± 12</td>
<td>337 ± 12</td>
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<tr>
<td>5b</td>
<td>353 ± 4</td>
<td>353 ± 4</td>
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<tr>
<td>6a</td>
<td>283 ± 5</td>
<td>280 ± 8</td>
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<tr>
<td>6b</td>
<td>297 ± 8</td>
<td>292 ± 11</td>
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<tr>
<td>7a</td>
<td>103 ± 4</td>
<td>105 ± 6</td>
</tr>
<tr>
<td>7b</td>
<td>114 ± 5</td>
<td>117 ± 8</td>
</tr>
<tr>
<td>8a</td>
<td>109 ± 9</td>
<td>111 ± 9</td>
</tr>
<tr>
<td>8b</td>
<td>117 ± 4</td>
<td>120 ± 6</td>
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<tr>
<td>9a</td>
<td>93 ± 5</td>
<td>95 ± 5</td>
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<tr>
<td>9b</td>
<td>97 ± 2</td>
<td>99 ± 4</td>
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</table>

**Supplementary material 7**: Brine shrimp lethality bioassay data presented with standard deviation for three independent experiments.

**Table S37**:

<table>
<thead>
<tr>
<th>Compounds</th>
<th>LC50 (µg/mL)</th>
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<tbody>
<tr>
<td>4a</td>
<td>7.05 ± 0.074</td>
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<td>4b</td>
<td>7.53 ± 0.071</td>
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<tr>
<td>5a</td>
<td>7.80 ± 0.067</td>
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<tr>
<td>5b</td>
<td>8.49 ± 0.065</td>
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<tr>
<td>6a</td>
<td>5.00 ± 0.032</td>
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<tr>
<td>6b</td>
<td>5.34 ± 0.059</td>
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<tr>
<td>7a</td>
<td>6.33 ± 0.099</td>
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<tr>
<td>7b</td>
<td>6.63 ± 0.066</td>
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<tr>
<td>8a</td>
<td>6.12 ± 0.096</td>
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<tr>
<td>8b</td>
<td>7.77 ± 0.101</td>
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<tr>
<td>9a</td>
<td>2.91 ± 0.044</td>
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<tr>
<td>9b</td>
<td>4.83 ± 0.053</td>
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