

# Supporting Information

## Mechanism of Anti-Trypanosoma cruzi Action of Gold(I) Compounds: A Theoretical and Experimental Approach

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**Table S1:** Natural Bond Orbital (NBO) results for [AuCl(HL2)] (**2**) compound

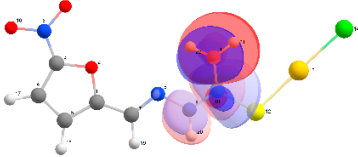
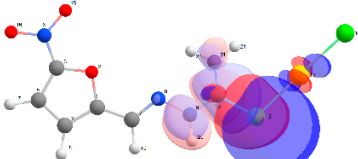
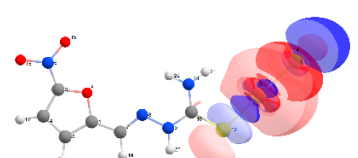
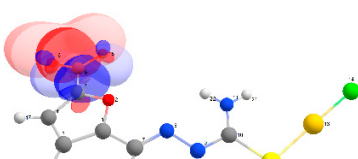
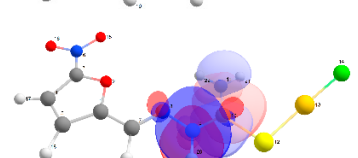
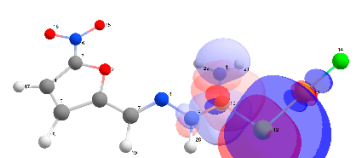
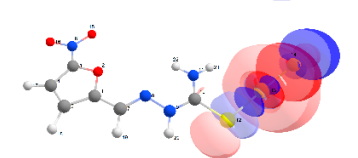
Spin	Donor (L) NBO		Acceptor (NL) NBO		E(2) kcal/mol
$\alpha$	33.	LP (1) N 11	97.	BD*(2) N 9 – C10	79.66
$\alpha$	75.	BD (1) S 12 – Au 13	97.	BD*(2) N 9 – C10	9.05
$\alpha$	44.	LP (4) Cl 21	103.	BD*(1) S 12 – Au 13	73.31
$\beta$	31.	LP (1) N 6	103.	BD*(1) O 15 – O 16	1065.04
$\beta$	33.	LP (1) N 9	98.	BD*(2) C 10–N 11	64.60
$\beta$	73.	BD (1) S 12 – Au 13	98.	BD*(2) C 10 – N 11	9.67
$\beta$	44.	LP (4) Cl 14	102.	BD*(1) S 12 – Au 13	73.43

**Table S2:** Natural Bond Orbital (NBO) results for [AuCl(HL3)] (**3**) compound

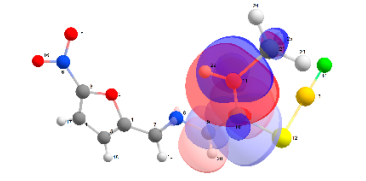
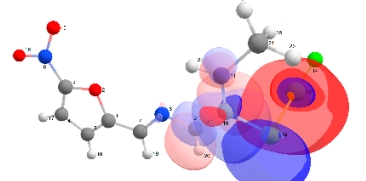
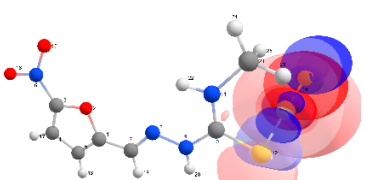
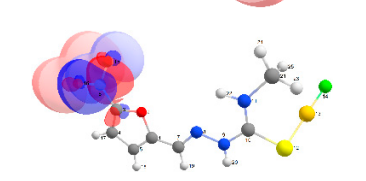
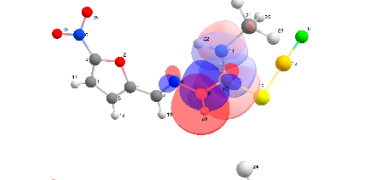
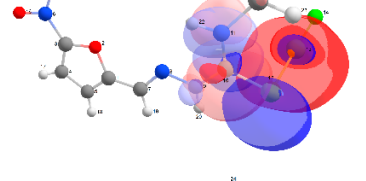
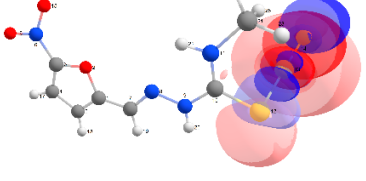
Spin	Donor (L) NBO		Acceptor (NL) NBO		E(2) kcal/mol
$\alpha$	34.	LP (1) N 11	101.	BD*(2) N 9 – C 10	80.40
$\alpha$	76.	BD (1) S 12 – Au 13	101.	BD*(2) N 9 – C 10	7.90
$\alpha$	45.	LP (4) Cl 14	107.	BD*(1) S 12 – Au 13	73.09
$\beta$	32.	LP (1) N 6	107.	BD*(1) O 15 – O 16	1066.05
$\beta$	34.	LP (1) N 9	102.	BD*(2) C 10–N 11	62.91
$\beta$	74.	BD (1) S 12 – Au 13	102.	BD*(2) C 10–N 11	8.39
$\beta$	45.	LP (4) Cl 14	106.	BD*(1) S 12 – Au 13	73.23

**Table S3:** Natural Bond Orbital (NBO) results for [AuCl(HL4)] (**4**) compound

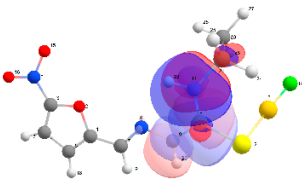
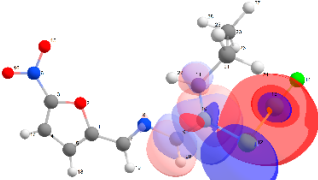
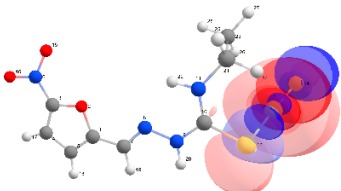
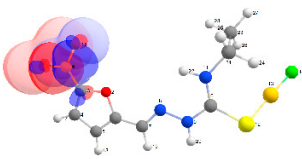
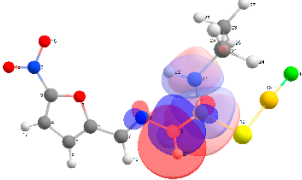
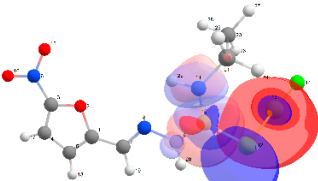
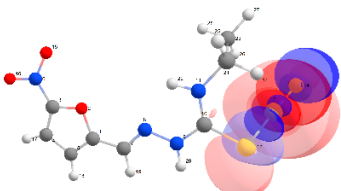
Spin	Donor (L) NBO		Acceptor (NL) NBO		E(2) kcal/mol
$\alpha$	38.	LP (1) N 11	113.	BD*(2) N 9 – C 10	70.25
$\alpha$	40.	LP (2) S 12	113.	BD*(2) N 9 – C 10	21.79
$\beta$	36.	LP (1) N 6	119.	BD*(1) O 15 – O 16	1044.90
$\beta$	38.	LP (1) N 11	112.	BD*(2) N 9 – C 10	75.62
$\beta$	40.	LP (2) S 12	112.	BD*(2) N 9 – C 10	22.81
$\beta$	49.	LP (4) Cl 14	118.	BD*(1) S 12 – Au 13	73.14

Spin	D – A NBO	E(2) kcal/mol
$\alpha$	32. – 93. 	73.13
$\alpha$	34. – 93 	33.07
$\alpha$	43. – 99. 	75.17
$\beta$	30. – 99. 	1075.57
$\beta$	32. – 93. 	68.87
$\beta$	34. – 93. 	35.94
$\beta$	43. – 98. 	75.13

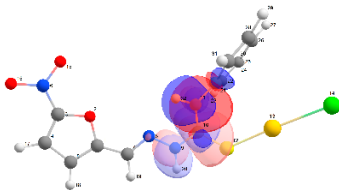
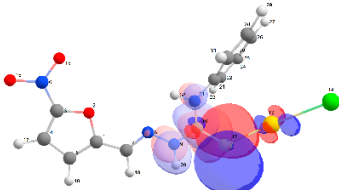
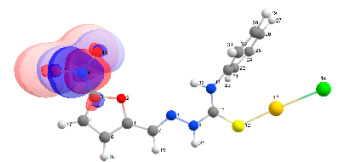
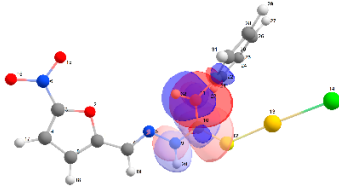
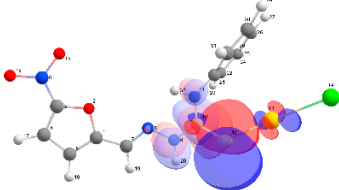
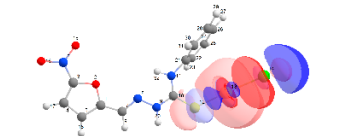
**Figure S1:** Natural Bond Orbital (NBO) selected bond for [AuCl(HL1)] (1) compound

Spin	D – A NBO		E(2) kcal/mol
$\alpha$	33. – 97.		79.66
$\alpha$	75. – 97.		9.05
$\alpha$	44. – 103.		73.31
$\beta$	31. – 103.		1065.04
$\beta$	33. – 98.		64.60
$\beta$	73. – 98.		9.67
$\beta$	44. – 102.		73.43

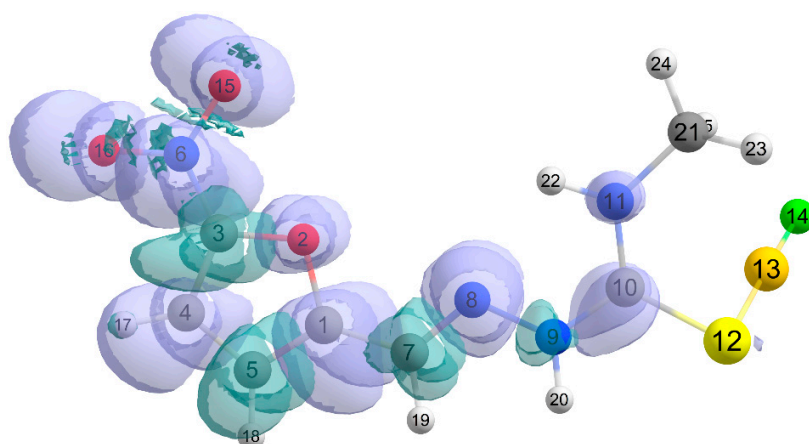
**Figure S2:** Natural Bond Orbital (NBO) selected bond for [AuCl(HL2)] (**2**) compound

Spin	D – A NBO	E(2) kcal/mol
$\alpha$	34. – 101. 	80.40
$\alpha$	76. – 101. 	7.90
$\alpha$	45. – 107. 	73.09
$\beta$	32. – 107. 	1066.05
$\beta$	34. – 102. 	62.91
$\beta$	74. – 102. 	8.39
$\beta$	45. – 106. 	73.23

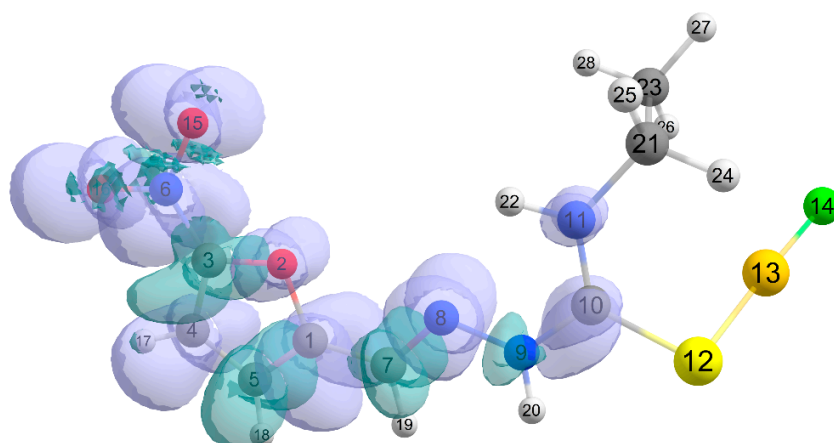
**Figure S3:** Natural Bond Orbital (NBO) selected bond for [AuCl(HL3)] (**3**) compound

Spin	D – A NBO	E(2) kcal/mol
$\alpha$	38. – 113. 	70.25
$\alpha$	40. – 113. 	21.79
$\beta$	36. – 119. 	1044.90
$\beta$	38. – 112. 	75.62
$\beta$	40. – 112. 	22.81
$\beta$	49. – 118. 	73.14

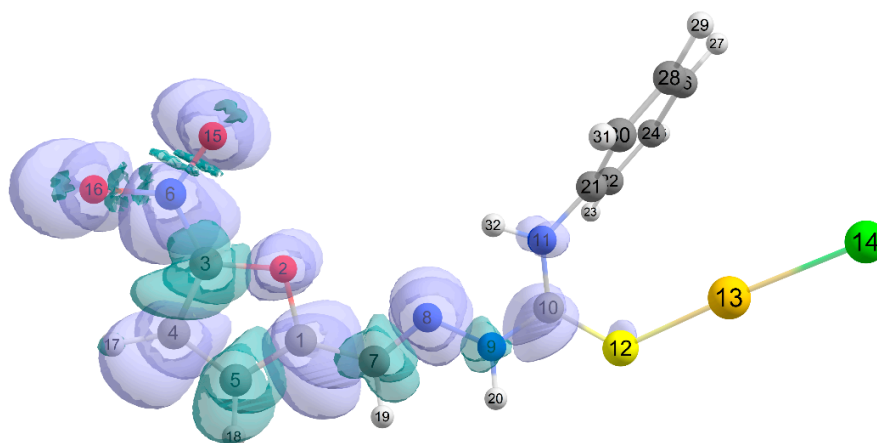
**Figure S4:** Natural Bond Orbital (NBO) selected bond for [AuCl(HL4)] (**4**) compound



**Figure S5:** Spin density calculated for  $[\text{AuCl}(\text{HL2})]$  (**2**) compound



**Figure S6:** Spin density calculated for  $[\text{AuCl}(\text{HL3})]$  (**3**) compound

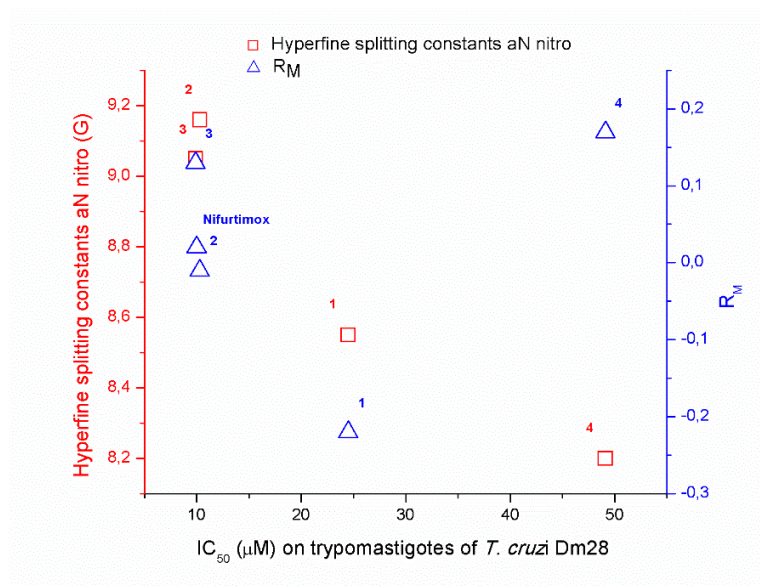


**Figure S7:** Spin density calculated for  $[\text{AuCl}(\text{HL4})]$  (**4**) compound

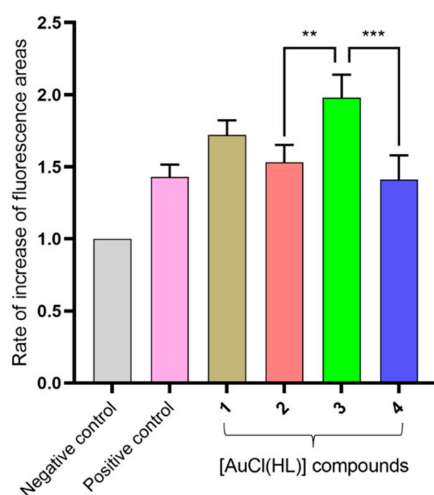
**Table S4:** Spin density calculated by ORCA for [AuCl(HL)] compounds

[AuCl(HL1)]		[AuCl(HL2)]		[AuCl(HL3)]		[AuCl(HL4)]	
<b>C1</b>	0,110249	<b>C1</b>	0,109644	<b>C1</b>	0,109588	<b>C1</b>	0,107825
<b>O2</b>	0,06127	<b>O2</b>	0,061964	<b>O2</b>	0,06184	<b>O2</b>	0,062917
<b>C3</b>	0,007067	<b>C3</b>	0,007871	<b>C3</b>	0,007686	<b>C3</b>	0,010055
<b>C4</b>	0,095429	<b>C4</b>	0,093705	<b>C4</b>	0,093971	<b>C4</b>	0,090157
<b>C5</b>	-0,062236	<b>C5</b>	-0,061893	<b>C5</b>	-0,061881	<b>C5</b>	-0,06049
<b>N6</b>	0,202404	<b>N6</b>	0,199949	<b>N6</b>	0,200306	<b>N6</b>	0,196242
<b>C7</b>	0,011783	<b>C7</b>	0,013145	<b>C7</b>	0,013038	<b>C7</b>	0,017251
<b>N8</b>	0,149215	<b>N8</b>	0,15112	<b>N8</b>	0,150759	<b>N8</b>	0,152195
<b>N9</b>	0,003226	<b>N9</b>	0,002067	<b>N9</b>	0,002081	<b>N9</b>	0,000466
<b>C10</b>	0,019612	<b>C10</b>	0,020673	<b>C10</b>	0,020842	<b>C10</b>	0,022055
<b>N11</b>	0,0088	<b>N11</b>	0,012168	<b>N11</b>	0,012004	<b>N11</b>	0,00945
<b>S12</b>	0,010499	<b>S12</b>	0,006895	<b>S12</b>	0,006579	<b>S12</b>	0,010702
<b>Au13</b>	0,001745	<b>Au13</b>	0,001728	<b>Au13</b>	0,001637	<b>Au13</b>	0,001868
<b>Cl14</b>	0,000122	<b>Cl14</b>	0,000416	<b>Cl14</b>	0,000475	<b>Cl14</b>	0,000287
<b>O15</b>	0,194452	<b>O15</b>	0,193022	<b>O15</b>	0,193296	<b>O15</b>	0,191827
<b>O16</b>	0,186368	<b>O16</b>	0,185708	<b>O16</b>	0,185822	<b>O16</b>	0,184761
<b>H17</b>	0,000468	<b>H17</b>	0,000456	<b>H17</b>	0,000462	<b>H17</b>	0,00043
<b>H18</b>	-0,000346	<b>H18</b>	-0,000343	<b>H18</b>	-0,000348	<b>H18</b>	-0,000338
<b>H19</b>	-0,000119	<b>H19</b>	-0,000103	<b>H19</b>	-0,000107	<b>H19</b>	-8,70E-05
<b>H20</b>	-5,10E-05	<b>H20</b>	-3,10E-05	<b>H20</b>	-3,40E-05	<b>H20</b>	-6,10E-05
<b>H21</b>	0,000103	<b>C21</b>	0,000931	<b>C21</b>	0,000904	<b>C21</b>	0,00017
<b>H22</b>	-6,10E-05	<b>H22</b>	-3,00E-06	<b>H22</b>	-1,20E-05	<b>C22</b>	9,81E-04
		<b>H23</b>	0,000246	<b>C23</b>	0,000617	<b>H23</b>	2,60E-05
		<b>H24</b>	5,80E-05	<b>H24</b>	-1,70E-05	<b>C24</b>	-3,26E-04
		<b>H25</b>	0,000607	<b>H25</b>	0,00034	<b>H25</b>	7,00E-06
				<b>H26</b>	2,50E-05	<b>C26</b>	8,64E-04
				<b>H27</b>	9,10E-05	<b>H27</b>	2,00E-06
				<b>H28</b>	3,60E-05	<b>C28</b>	-3,20E-04
						<b>H29</b>	3,00E-06
						<b>C30</b>	0,001059
						<b>H31</b>	3,80E-05
						<b>H32</b>	-1,30E-05





**Figure S8:** Correlation between the anti-*T. cruzi* activity and the hyperfine splitting constant on the nitrogen atom (N6) and  $R_M$  values of the  $[\text{AuCl}(\text{HL})]$  compounds



**Figure S9:** Rate of increase in areas of fluorescence spectra concerning compound **3**. One-way analysis of variance (ANOVA) compared to compound 3 rate was performed with subsequent Dunnett's test (\*\* $p < 0.01$ ; \*\*\* $p < 0.001$ ; \*\*\*\* $p < 0.0001$ ).