

## SUPPORTING INFORMATION

### Selenium-Containing (Hetero)Aryl Hybrids as Potential Antileishmanial Drug Candidates: *In vitro* Screening Against *L. amazonensis*

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**TABLE S1: Cytotoxicity and selectivity index (SI) of selenium-compounds against different host cell lines and promastigote forms of *Leishmania amazonensis***

| Compound | CC50 NIH/3T3 (µM) | Selectivity Index (SI) | CC50 J774 (µM) | Selectivity Index (SI) | CC50 peritoneal cells (µM) | Selectivity Index (SI) |
|----------|-------------------|------------------------|----------------|------------------------|----------------------------|------------------------|
| 101      | > 200             | 6.57                   | > 200          | 6.57                   | > 200                      | 6.57                   |
| 102      | > 200             | 13.20                  | > 200          | 13.20                  | > 200                      | 13.20                  |
| 103      | > 200             | 12.92                  | > 200          | 12.92                  | > 200                      | 12.92                  |
| 104      | > 200             | 12.37                  | 126.7          | 7.84                   | > 200                      | 12.37                  |
| 105      | 87.85             | 7.22                   | 60.16          | 4.94                   | > 200                      | 16.43                  |
| 106      | > 200             | 50.53                  | > 200          | 50.53                  | > 200                      | 50.53                  |
| 107      | > 200             | 7.31                   | > 200          | 7.31                   | > 200                      | 7.31                   |
| 108      | > 200             | 47.31                  | > 200          | 47.31                  | > 200                      | 47.31                  |
| 111      | > 200             | 11.40                  | > 200          | 11.40                  | > 200                      | 11.40                  |
| 113      | > 200             | 4.88                   | > 200          | 4.88                   | > 200                      | 4.88                   |
| ANFB     | 19.26             | 2.05                   | 27.34          | 2.91                   | 25.15                      | 2.67                   |

The antileishmanial activity of selenium-compounds was evaluated against promastigote forms of *L. amazonensis* after 48 hours. The cytotoxicity was performed in NIH/3T3 cells, J774A.1 cells and peritoneal macrophages. Selectivity index (SI) was calculated as CC50/IC50 values for Abbreviations: CC50= half-maximal cytotoxic concentration; IC50 = half-maximal inhibitory concentration; SI = selectivity index. ANFB = amphotericin B used as reference drug for *L. amazonensis*.

**TABLE S2: Cytotoxicity and selectivity index (SI) of selenium-compounds against different host cell lines and intracellular amastigotes forms of *Leishmania amazonensis***

| Compound | CC50 NIH/3T3 (µM) | Selectivity Index (SI) | CC50 J774 (µM) | Selectivity Index (SI) | CC50 peritoneal cells (µM) | Selectivity Index (SI) |
|----------|-------------------|------------------------|----------------|------------------------|----------------------------|------------------------|
| 101      | > 200             | ind                    | > 200          | ind                    | > 200                      | ind                    |
| 102      | > 200             | ind                    | > 200          | ind                    | > 200                      | ind                    |
| 103      | > 200             | ind                    | > 200          | ind                    | > 200                      | ind                    |
| 104      | > 200             | ind                    | 126.7          | ind                    | > 200                      | ind                    |
| 105      | 87.85             | ind                    | 60.16          | ind                    | > 200                      | ind                    |
| 106      | > 200             | ind                    | > 200          | ind                    | > 200                      | ind                    |
| 107      | > 200             | 10.92                  | > 200          | 10.92                  | > 200                      | 10.92                  |
| 108      | > 200             | ind                    | > 200          | ind                    | > 200                      | ind                    |
| 111      | > 200             | ind                    | > 200          | ind                    | > 200                      | ind                    |
| 113      | > 200             | 12.55                  | > 200          | 12.55                  | 124.6                      | 12.55                  |
| ANFB     | 19.26             | 25.92                  | 27.34          | 28.19                  | 25.15                      | 25.93                  |

The antileishmanial activity of selenium-compounds was evaluated against intracellular amastigotes forms of *L. amazonensis* after 24 hours. The cytotoxicity was performed in NIH/3T3 cells, J774A.1 cells and peritoneal macrophages. Selectivity index (SI) was calculated as CC50/IC50 values for Abbreviations: CC50= half-maximal cytotoxic concentration; IC50 = half-maximal inhibitory concentration; SI = selectivity index. ANFB = amphotericin B used as reference drug for *L. amazonensis*. Ind = means indetermined results.