Supplementary material

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**Exploratory Study of Guanidine Derivatives as Novel Anti *Trypanosoma cruzi* Scaffolds**

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# Analysis of LQOF-G29

# NMR measurements

H13, H14, H18

21

H17, H20, H21

H15, H16, H19

NH1

H2

H11

NH2

**Figure S1.** 1H NMR spectrum of **LQOF-G29**.

21

C15, C16, C19

C5

C6

C12

C9

C8

C2C3

C11

C17, C20,

C4 C13, C14, C21

C18

C1 C10

C7

**Figure S2.** 13C NMR spectrum of **LQOF-G29**.

# EI-MS analysis

**Figure. S3.** EI-MS (70 eV) spectrum of compound **LQOF-G29**.

# 1.3. HRESIMS and HPLC-UV analysis of LQOF-G29.



**Figure. S4.** HPLC-UV (254 nm) analysis of **LQOF-G29**.



**Figure. S5.** HRESI-(+) MS analysis of **LQOF-G29**.



**Figure. S6.** HRESI-(+) MS/MS analysis of **LQOF-G29**.

# Structural data of LQOF-G29

***N-((adamantanemethylamine))((4-bromophenyl)amino)methylene)benzamide*** (**LQOF-G29**). White solid. Yield 62%. Recrystallized with hexane. **LC-UV/MS**: 99.73%; **ESI(+)-MS** *m/z* found 466.1489, *m/z* calculated for [C25H27BrN3O + H]+: 466.1489; **ESI(+)-MS/MS**: [M + H – C7H5ONH2]+ *m/z* 345.0959, [M + H – C14H10BrN2O]+ *m/z* 166.1589, [M + H – C14H11BrN3O]+ *m/z* 149.1325. **1H NMR** (400.13 MHz, CDCl3) δ = 12.19 (s, 1H), 8.28 (d, *J* = 4.0 Hz, 2H), 7.61 (d, *J* = 4.8 Hz, 2H), 7.52 (t, *J* = 4.0 Hz, 1H), 7.47 (t, 4.2 Hz, 2H), 7.20 (d, 4.8 Hz, 2H), 4.97 (t, *J* = 3.5 Hz, 1H), 3.32 (d, *J* = 3.5 Hz, 2H), 1.99 (m, 3H), 1.75 (m, 6H), 1.49 (m, 6H); **13C NMR** (100.61 MHz, CDCl3) δ = 177.3 (C=O), 158.6 (C=N), 138.7 (C), 134.7 (C-Br), 133.1 (CH), 131.2 (CH), 128.8 (2CH), 127.9 (2CH), 127.1 (2CH), 120.3 (C), 52.3 (CH2), 40.1 (3CH2), 36.5 (3CH2), 33.9 (C), 27.7 (3CH).