Identifying inhibitors of the *Leishmania* inositol phosphorylceramide synthase with antiprotozoal activity using a yeast-based assay and ultra-high throughput screening platform

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Supplementary Information

SI Table 1

Data from analyses of the clustered 211 hits. Structure – chemical structure (where available); Cmpd Number – compound reference number; PFI - Property Forecast Index; A'ring – number of aromatics ring; pIC50 LmjIPCS – -logIC_{50} mol against *α ade⁻.lys⁻.leu⁻.Δaur1⁻*.pESC-LEU_*Lmj*IPCS; pIC50 AUR1 – -logIC_{50} mol against *α ade⁻.lys⁻.leu⁻.Δaur1⁻*.pESC-LEU_AUR1; pIC50 axenic – -logIC_{50} mol against *L. donovani* (MHOM/SD/62/1S-CL2D, LdBOB) axenic amastigotes; pIC50 axenic ≥5 **TRUE** or **FALSE**; pIC50 HepG2 – -logIC_{50} mol against HepG2 cells; pSI v HepG2 – logSI (Selectivity Index) of compounds for axenic amastigotes over HepG2 cells; pSI v HepG2≥1, PFI≤8, A'ring≤4 **TRUE** or **FALSE**; pIC50 InMac – -logIC_{50} mol against intramacrophage *L. donovani*; pIC50 THP-1 – -logIC_{50} mol against THP-1 macrophages; pSI v THP-1 - logSI (Selectivity Index) of compounds for axenic amastigotes over THP-1 macrophages; InMac ≥5, pSI v THP1 ≥ 1 **TRUE** or **FALSE**; Hit Ref – Hit reference number in article

pIC50 of 4 (4.3 for iMac and THP-1 assay) are the minimum values obtainable from the assays, therefore actual pSI values could be higher.

SI Figure 1

The activity of compound **1** against wild type *Leishmania major* (red; -logIC_{50} mol [pIC_{50}] 5.5; 95% CI: 5.9-5.0) and the mutant, *Δlcb2* (blue; pIC_{50} 5.5; 95% CI: 5.7-5.2). Values are from 3 independent experiments.