Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2016

Supplementary material Antimicrobial activity of aroylhydrazone-based oxido vanadium(V)

complexes: *in-vitro* and *in silico* studies

S. Yousef Ebrahimipour*, Iran Sheikhshoaie, Jim Simpson, Hadi Ebrahimnejad, Michal Dusek,

Nima Kharazmi, Vaclav Eigner



Fig. S1. Overall packing for **HL** viewed along the *a* axis direction. Hydrogen bonds are drawn as dashed blue lines and a representative $\pi \dots \pi$ contact is shown as a dotted green line. Representative ring centroids are shown as red spheres.



Fig. S2. Overall packing for [VO(L)(MeOH)(OMe)] viewed along the *b* axis direction. Hydrogen bonds are drawn as dashed blue lines and representative $\pi \dots \pi$ and C—H $\dots \pi$ contacts are shown as green dotted lines.



Fig. S3. Overall packing for [VO(L)(OEt)] viewed along the *b* axis direction. Hydrogen bonds are drawn as dashed blue lines and representative C—H... π and V... π contacts are shown as dotted green lines. Representative ring centroids are shown as coloured spheres.



Fig. S4. Overall packing for [VO(L)(OPr)] viewed along the *b* axis direction. Hydrogen bonds are drawn as dashed blue lines and representative C—H... π and V... π contacts are shown as dotted green lines. Representative ring centroids are shown as coloured spheres.



Fig. S5. ¹H NMR spectrum of HL.



Fig. S6. ¹H NMR spectrum of [VO(L)(MeOH)(OMe)].



Fig. S7. ¹H NMR spectrum of [VO(L)(OEt)].



Fig. S8. ¹H NMR spectrum of [VO(L)(OPr)].



Fig. S9. FT-IR spectrum of $[H_2L]$.



Fig. S10. FT-IR spectrum of [VO(L)(MeOH)(OMe)].



Fig. S11. FT-IR spectrum of [VO(L)(OEt)].



Fig. S12. FT-IR spectrum of [VO(L)(OPr)].