Supporting Information For:

Unprecedented formation of organo-ruthenium(II) complexes containing 2hydroxy-1-naphthaldehyde S-benzyldithiocarbazate: Synthesis, X-ray crystal structure, DFT study and biological activities *in vitro*

Paranthaman Vijayan,^a Periasamy Viswanathamurthi,^{*a} Paramasivam Sugumar,^b Mondikalipudur Nanjappagounder Ponnuswamy,^b Manickam Dakshinamoorthi Balakumaran,^c Pudupalayam Thangavelu Kalaichelvan,^c Krishnaswamy Velmurugan,^d Raju Nandhakumar,^d Ray Jay Butcher,^e

^aDepartment of Chemistry, Periyar University, Salem-636 011, India.

^bCentre of Advanced Studies in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai- 600 025, India.

^cCentre for Advanced Studies in Botany, School of Life Sciences, University of Madras, Guindy Campus, Chennai - 600 025, Tamil Nadu, India.

^dDepartment of Chemistry, Karunya University, Karunya Nagar, Coimbatore - 641 114, India.

^eDepartment of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA.

*To whom correspondence should be addressed, e-mail:*viswanathamurthi72@gmail.com Fax:* +91 427 2345124

Table of Contents

1.	Molecular packing diagram of complexes	S1
2.	UV-vis and emission spectra of compounds	S2
3.	Representative ¹ H, ¹³ C and ³¹ P spectra of complexes	S3-S6
4.	Mass spectra of complex	S7
5.	Optimized structure of complexes 1, 2	



Fig. S1 Packing diagram of ruthenium complexes 1 and 2



Fig. S2 Absorption (A) and emission spectra (B) of compounds in DMSO solvent.



Fig. S3 ¹H NMR spectrum of complex 1



Fig. S4 ¹H NMR spectrum of complex 2



Fig. S5 ¹³C NMR spectrum of complex 2



Fig. S6 ³¹P NMR spectrum of complex 1



Fig. S7 ESI-MS spectrum of complex 1



Fig. S8 LANL2DZ and $6-31G^*$ (d, p) ground state optimized geometry of complexes 1, 2