**ABSTRACT**

A new series of mercaptopyrimidineRu(III) complexes were synthesized and characterized using various spectral techniques like single‐crystal X‐ray diffraction, Fourier transform infrared and NMR spectroscopies, thermogravimetric analysis and energy‐dispersive X‐ray analysis. The complexes were evaluated for their pharmacological activities like *in vitro* antimicrobial, anticancer, antituberculosis and antioxidant activities. The DNA binding of the complexes was investigated by absorption and emission spectral measurements which indicated that the complexes bind to DNA *via* intercalation, with molecular docking studies validating the results. DNA cleavage studies of the complexes were carried out.