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> Electronic Supplementary Information (ESI) to RSC Advance Mononuclear manganese (III) complexes of bidentate NO donor Schiff base ligands: synthesis, structural characterization, magnetic and catecholase studies

> Arpan Dutta, Surajit Biswas, Malay Dolai, Bikash Kumar Shaw, Abhishake Mondal, Shyamal Kumar Saha and Mahammad Ali

# <sup>1</sup>H and <sup>13</sup>C NMR spectroscopic characterization of four ligandsin CDCl<sub>3</sub>:



Fig. S2: The<sup>13</sup>C NMR spectra of HL<sup>1</sup>

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Fig. S4: The<sup>13</sup>C NMR spectra of HL<sup>2</sup>

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Fig. S8: The<sup>13</sup>C NMR spectra of HL<sup>4</sup>

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Supramolecular assemblies in complexes 2-4:



**Fig. S9**: The supramolecular interactions: H-bonding and Br $\cdots\pi$  (orange dotted line), CH $\cdots\pi$ (phenyl)(magenta dotted line) as well as  $\pi$ (phenyl) $\cdots\pi$ (phenyl)(violet dotted line) are combined to form 2D framework along crystallographic *ab*plane in **2**.



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**Fig. S10**: The supramolecular interactions: H-bonding (orange dotted line), CH··· $\pi$ (phenyl)(blue dotted line) as well as Br··· $\pi$ (phenyl)(violet dotted line) are combined to form 2D framework along crystallographic *bc*plane in **3**.



Fig. S11: The supramolecular interactions: H-bondings (green dotted line), CH··· $\pi$  (phenyl)(blue dotted line) are combined to form 2D framework along crystallographic *ac* plane in **4**.



## Catecholase activities and their corresponding spectra of complexes 3 and 4:

Fig. S12. Time-resolved spectra for the reaction of 3 with 3, 5-DTBC.

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Fig. S13. Time-resolved spectra for the reaction of 4 with 3, 5-DTBC.



Fig. S14. Lineweaver–Burk Plot for complexes 1-4.

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Fig.S15: M vs. H plots collectedat 2, 4 and 5 K for complex 3.Solid lines represent the theoretical curve and the points are the experimental data.



Fig. S16: M vs. H plots collected t 2, 4 and 5 K for complex 4. Solid lines represent the theoretical curve and the points are the experimental data.

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