

**A novel reversible chemosensor for discrimination of Hg(II) in aqueous solution based on isoxazolidine derivative and exhibiting pH sensing attendance.**

**NMR of the synthesized compound:**

NMR  $^1\text{H}$  (800 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{ppm}}$ : 0.65 (d, 3H,  $J = 6.4$  Hz,  $\text{CH}_3$ ), 0.80 (d, 3H,  $J = 6.4$  Hz,  $\text{CH}_3$ ), 0.82 (d, 3H,  $J = 6.4$  Hz,  $\text{CH}_3$ ), 0.83 (m, 1H), 1.09 (t, 1H,  $J = 11.2$  Hz), 1.21 (m, 1H), 1.28 (m, 1H), 1.36 (quin, 1H,  $J = 6.4$  Hz), 1.56 (m, 1H), 1.70 (m, 1H), 1.74 (m, 1H), 1.87 (m, 1H), 2.19 (s, 3H,  $\text{CH}_3$ ), 2.21 (ddd, 1H,  $J = 2.4, 8.0$  and  $12$  Hz, H4a), 2.61 (dd, 1H,  $J = 4.8$  and  $12$  Hz, H6), 2.65 (s, 3H,  $\text{NCH}_3$ ), 2.69 (ddd, 1H,  $J = 5.6, 8.0$  and  $12$  Hz, H4b), 3.01 (dd, 1H,  $J = 4.8$  and  $12$  Hz, H6), 3.88 (s, 3H,  $\text{OCH}_3$ ), 3.96 (m, 2H, H3 and H5), 7.17 (d, 1H,  $J = 1.6$  Hz,  $\text{H}_{\text{Ar}}$ ), 7.47 (d, 1H,  $J = 1.6$  Hz,  $\text{H}_{\text{Ar}}$ ), 10.75 (s, 1H, OH). NMR  $^{13}\text{C}$  (200 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{ppm}}$ : 18.3, 20.2, 21.8, 22.2, 24.0, 24.2, 25.9, 29.4, 32.5, 34.4, 38.5, 40.3, 47.9, 52.1, 66.2, 76.4, 89.7, 111.4, 126.1, 127.5, 127.9, 138.1, 157.4, 170.8, 172.6. Anal. Calcd. for  $\text{C}_{25}\text{H}_{36}\text{N}_2\text{O}_5$  (444.57): C, 67.54; H, 8.16; N, 6.30, Found: C, 67.77; H, 8.22; N, 6.39.

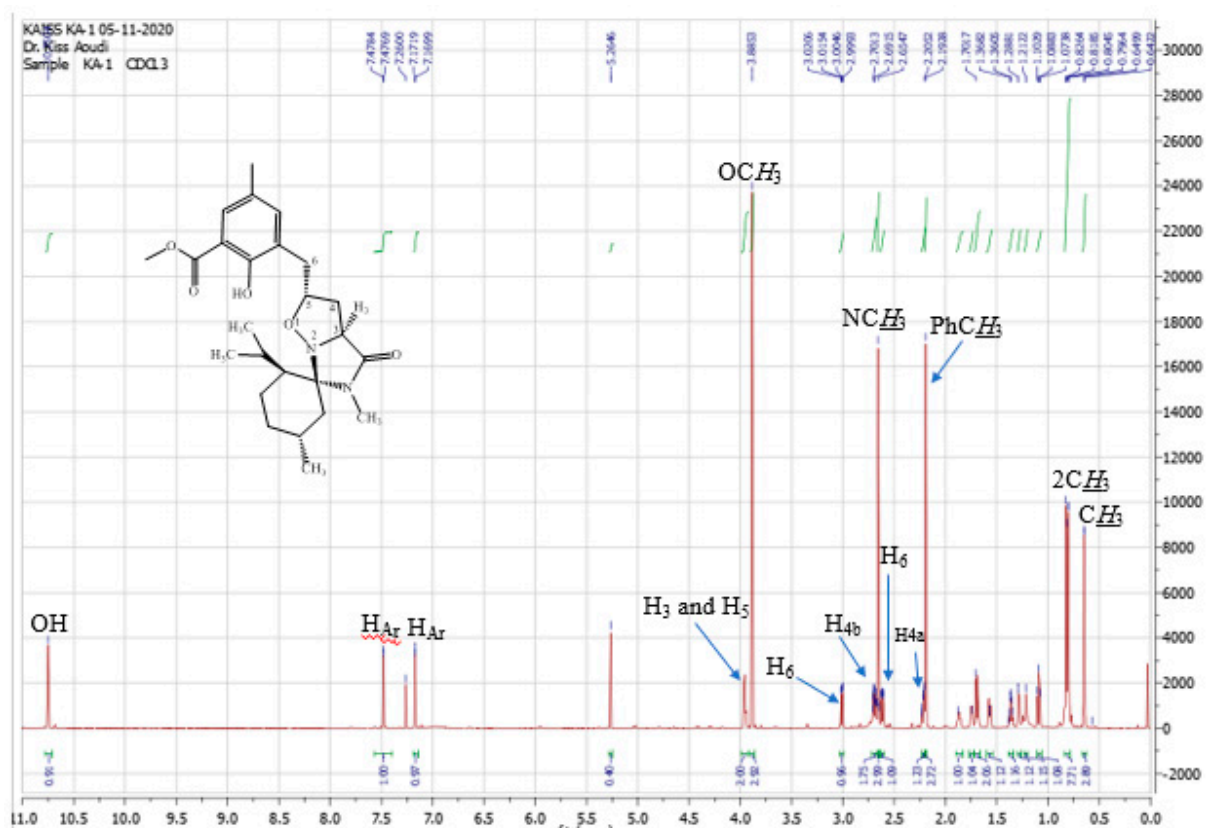


Figure S1. <sup>1</sup>H spectrum of the synthesized compound.

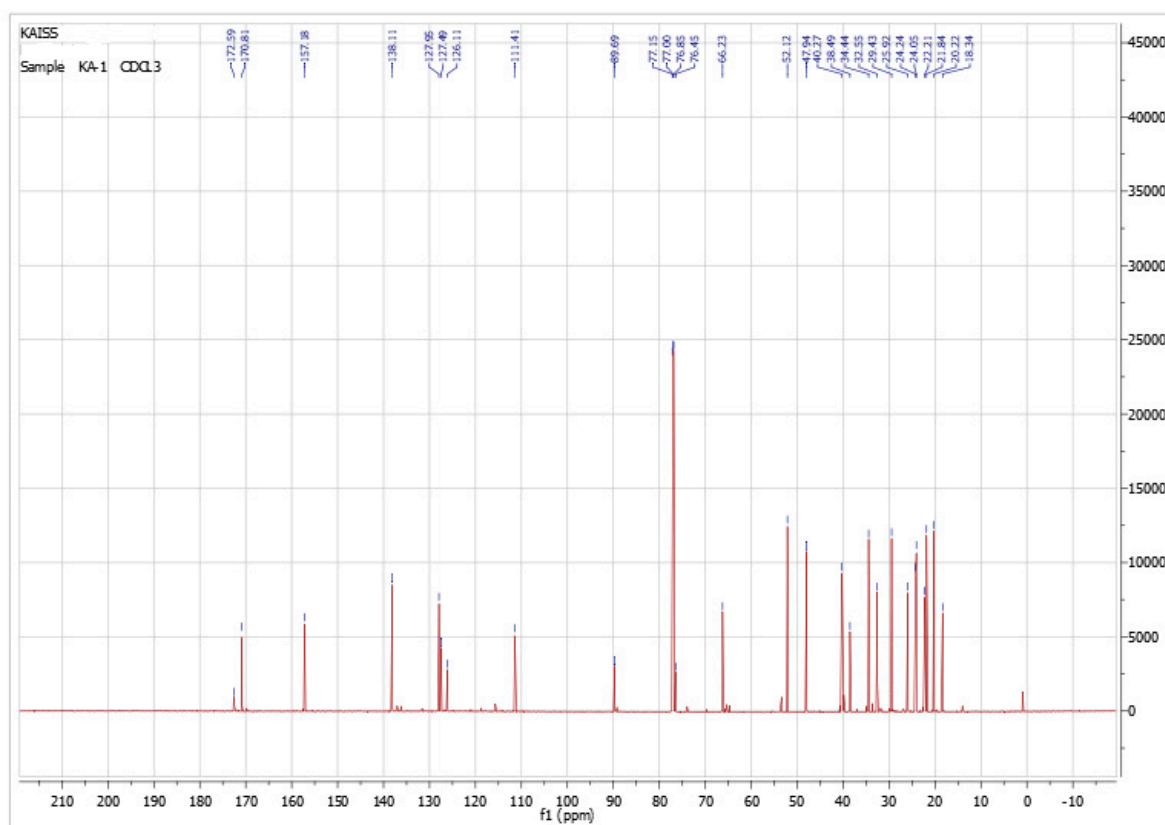


Figure S2.  $^{13}\text{C}$  spectrum of the synthesized compound.