

SUPPLEMENTARY MATERIAL TO
**Synthesis of poly(itaconic acid) and its application for synthesis of
pyrrolinones as a reusable homogeneous catalyst**

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1,5-diphenyl-3-hydroxy-4-methoxycarbonyl-pyrrolin-2-one (1a)

White powder, MeOH (8 hours, yields: 90%), mp 182–183 °C (180–182 °C [21, 27–28]). FT-IR (KBr)(cm⁻¹): 3260 (OH), 2958, 1702 (C=O), 1680 (C=O), 1498, 1382, 1232, 1002. ¹H-NMR (400 MHz, DMSO-d₆): δ 3.60 (s, 3H, CH₃), 6.10 (s, 1H, CH), 7.07–7.62 (m, 10 H, Ar and OH); ¹³C NMR (100 MHz, DMSO-d₆): δ 50.55, 61.05, 112.35, 122.96, 125.80, 128.13, 128.38, 128.73, 129.13, 136.74, 137.00, 153.14, 162.96 (C=O), 164.49 (C=O). Anal. Calcd for C₁₈H₁₅NO₄: C (%), 69.89; H (%), 4.89; N (%), 4.53. Found: C (%), 69.92; H (%), 4.81; N (%), 4.48.

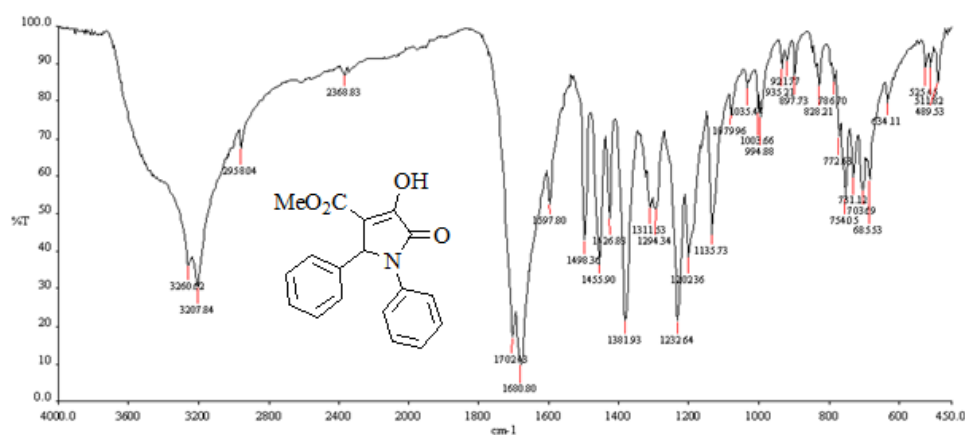
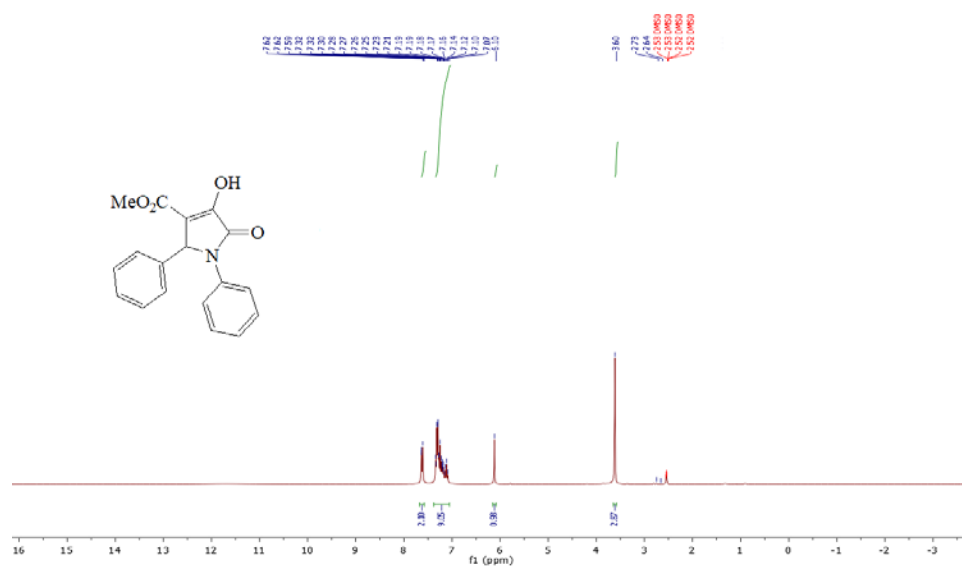


Fig. S-1. FT-IR (KBr, cm⁻¹) spectrum of compound 1a.

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1-(4-bromophenyl)-5-(4-bromophenyl)-3-hydroxy-4-methoxycarbonyl-3-pyrrolin-2-one (2a)

The white solid, MeOH (8 hours, yields: 92%), mp 217-219 °C (218-220 °C [21, 27]). FT-IR (KBr): $\nu_{\max}(\text{cm}^{-1})$: 3234 (OH), 2951, 1709 (C=O), 1684 (C=O), 1491, 1372, 1233, 1133; $^1\text{H-NMR}$ (400 MHz, DMSO- d_6) δH : 3.83 (s, 3H, OCH₃), 6.07 (s, 1H, CH), 7.24–8.63 (m, 8 H, Ar). $^{13}\text{C-NMR}$ (100 MHz, DMSO- d_6) δC : 51.35, 60.10, 110.15, 118.05, 121.43, 124.61, 130.40, 131.66, 132.04, 136.13, 137.17, 155.27, 163.26, 165.28 (C=O). Anal. Calcd for C₁₈H₁₃Br₂NO₄: C (%), 46.28; H (%), 2.81; N (%), 3.00. Found: C (%), 46.38; H (%), 2.75; N (%), 2.93.

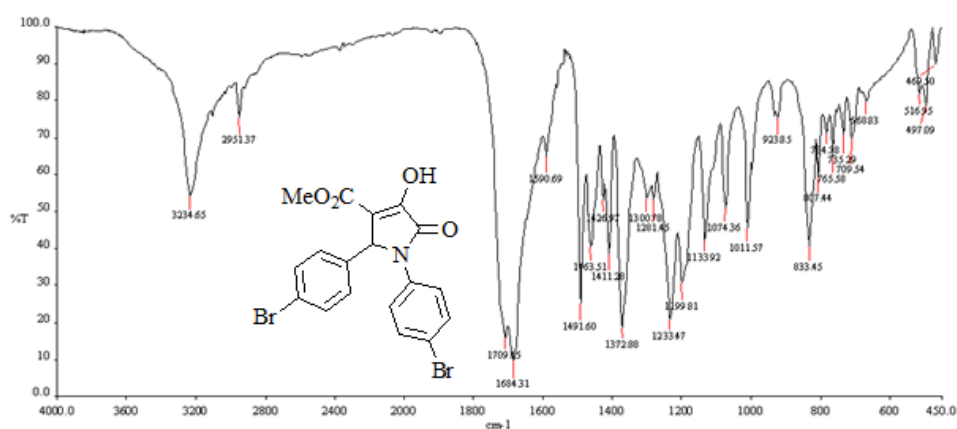
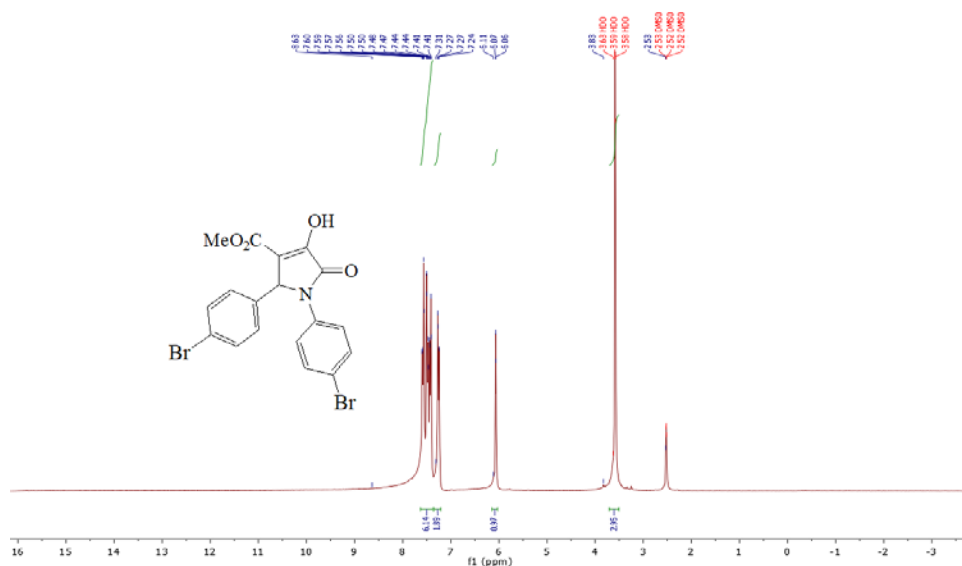
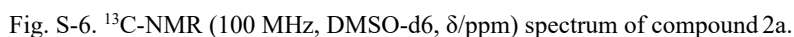
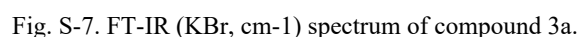


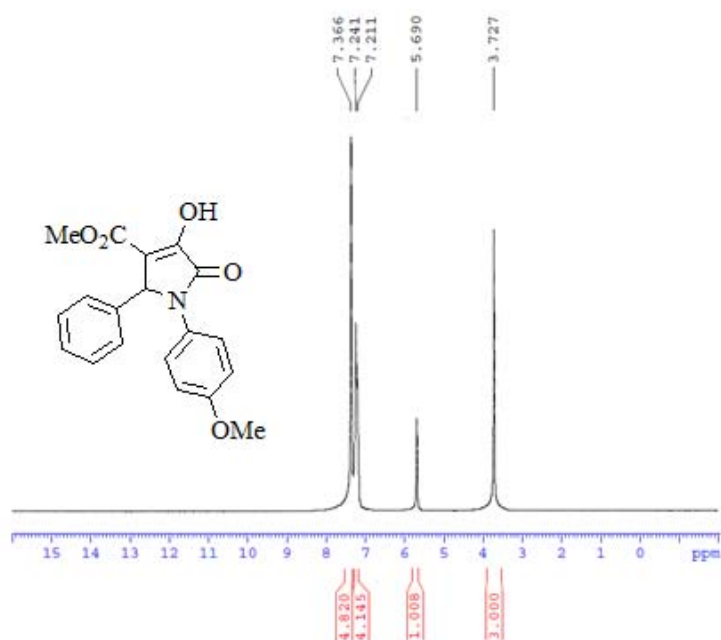
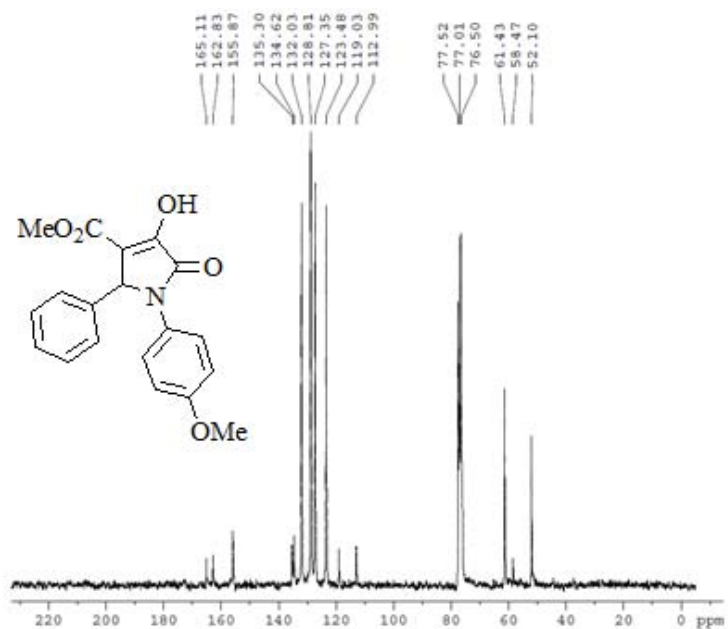
Fig. S-4. FT-IR (KBr, cm⁻¹) spectrum of compound 2a.





White solid, MeOH (8 hours, yields: 90%), 171-173 °C (170-171°C [30]). FT-IR (KBr): $\nu_{\text{max}}(\text{cm}^{-1})$: 3232 (OH), 2952, 1709 (C=O), 1679 (C=O), 1494, 1374, 1231, 1134; $^1\text{H-NMR}$ (250.13 MHz, CDCl_3) δH : 3.72 (s, 3H, OCH_3), 5.69 (s, 1H, CH), 7.21–7.36 (m, 9 H, Ar). The $^{13}\text{C-NMR}$ (62.90 MHz, CDCl_3) δC : 52.10, 58.47, 61.43, 112.99, 119.03, 123.48, 127.35, 128.81, 132.03, 134.62, 135.30, 155.87, 162.83 (C=O), 165.11 (C=O). Anal. Calcd for $\text{C}_{19}\text{H}_{17}\text{NO}_5$: C (%), 67.25; H (%), 5.05; N (%), 4.13. Found: C (%), 67.31; H (%), 4.98; N (%), 4.00.



Fig. S-8. ¹H-NMR (250 MHz, CDCl₃, δ/ppm) spectrum of compound 3a.Fig. S-9. ¹³C-NMR (62.90 MHz, CDCl₃, δ/ppm) spectrum of compound 3a.

1-(4-methoxyphenyl)-5-(2-chlorophenyl)-3-hydroxy-4-methoxycarbonyl-3-pyrrolin-2-one (4a)

The brown solid, MeOH (8 hours, yields: 90%), m.p. 191-193°C (192-194 °C [21]). FT-IR (KBr)(cm⁻¹): 3198 (OH), 2954, 1701 (C=O), 1684 (C=O), 1533, 1351, 1250, 1029. ¹H-NMR ((250.13 MHz, CDCl₃)) δ 3.62 (s, 3H, OCH₃), 3.71 (s, 3H, OCH₃), 6.37 (s, 1H, CH), 6.77–7.37 (m, 8 H, Ar), 9.11 (br s, 1H, OH). ¹³C-NMR (63 MHz, CDCl₃) δ 52.03, 55.30, 57.05, 112.40, 114.24, 123.77, 126.91, 127.44, 128.82, 129.77, 132.67, 134.96, 156.86, 157.60, 162.72 (C=O), 165.09 (C=O). Anal. Calcd. for C₁₉H₁₆ClNO₅ (373.79) C (%), 61.05; H (%), 4.31; Cl (%), 9.48; N (%), 3.75. Found: C (%), 61.15; H (%), 4.39; Cl (%), 9.37; N (%), 3.90.

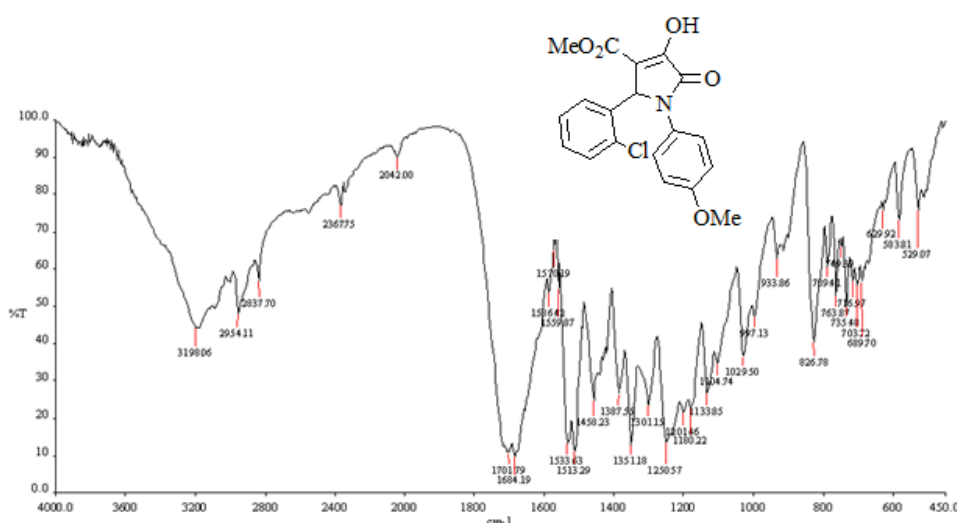
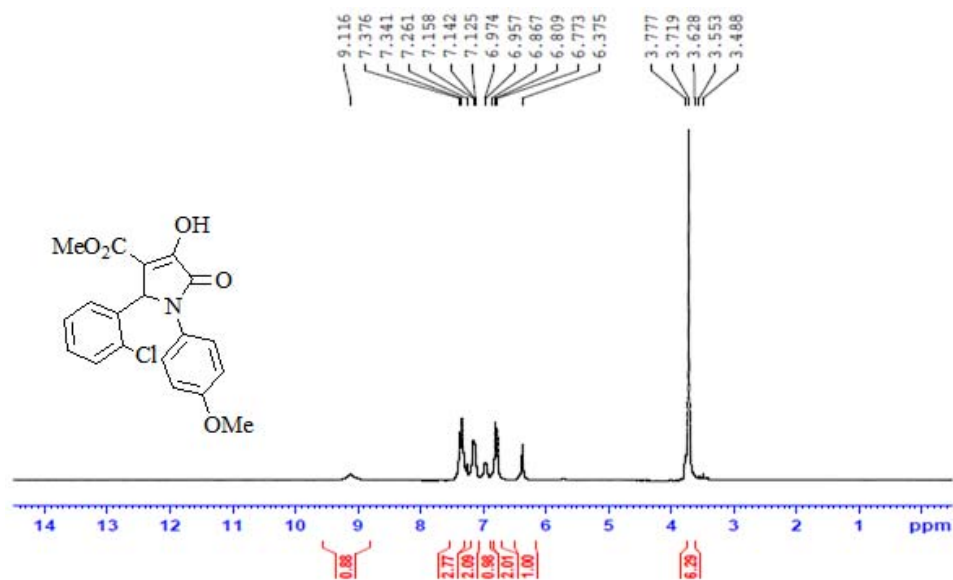
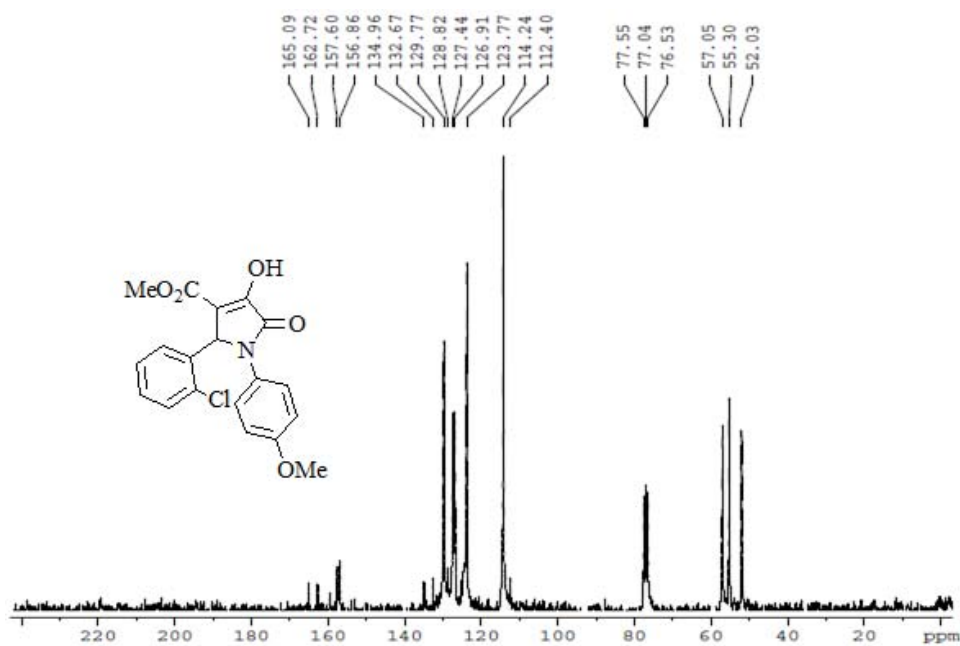


Fig. S-10. FT-IR (KBr, cm⁻¹) spectrum of compound 4a.

Fig. S-11. ¹H-NMR (250 MHz, CDCl₃, δ/ppm) spectrum of compound 4a.Fig. S-12. ¹³C-NMR (63 MHz, CDCl₃, δ/ppm) spectrum of compound 4a.

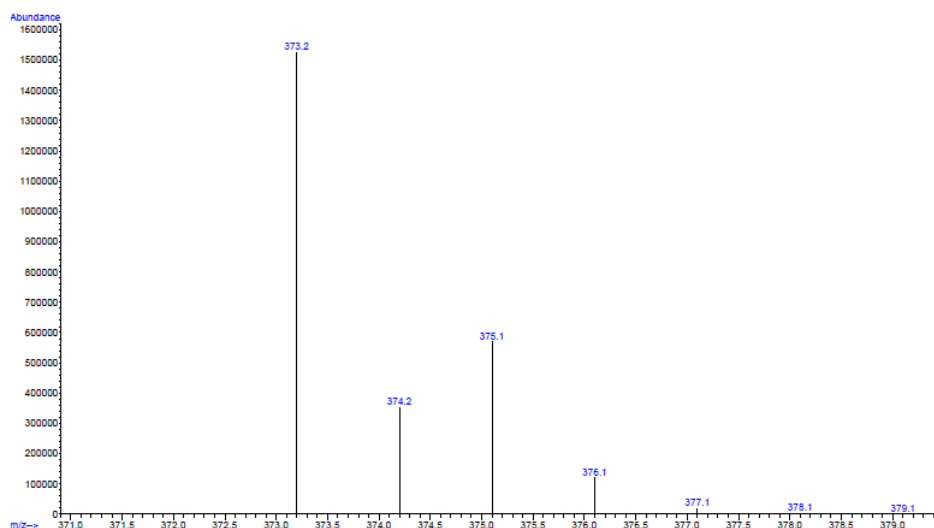
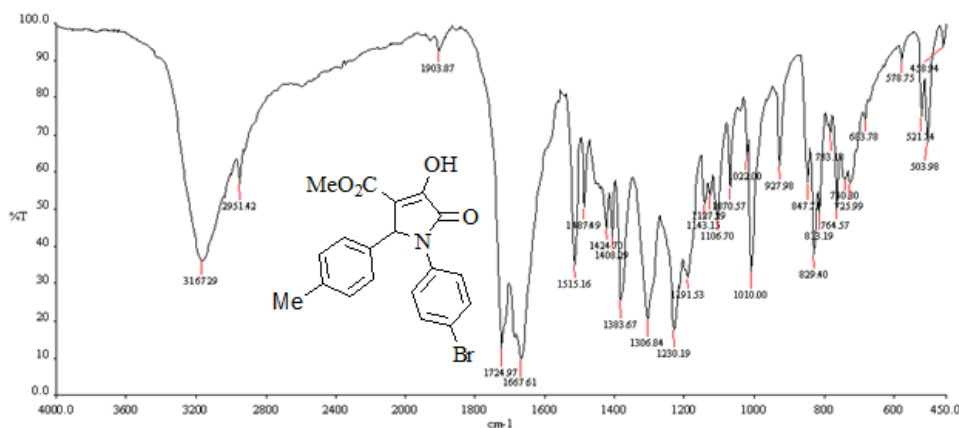
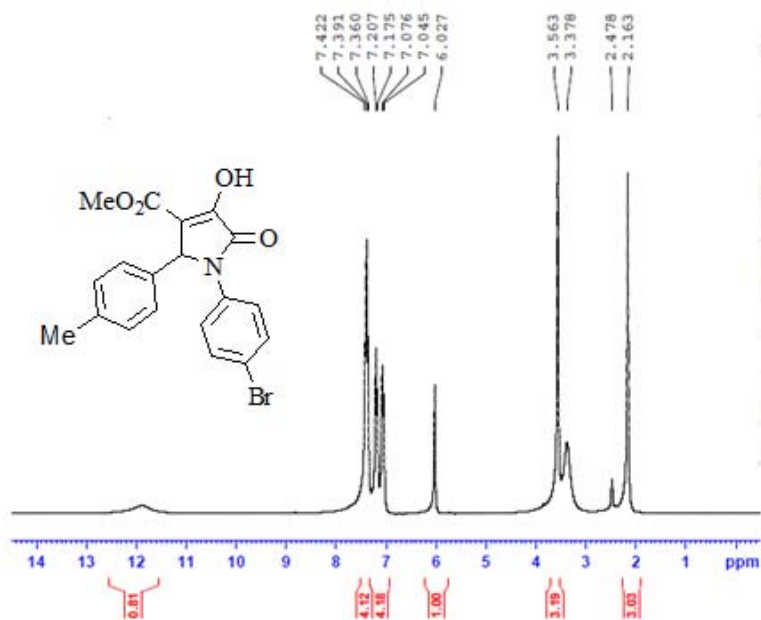
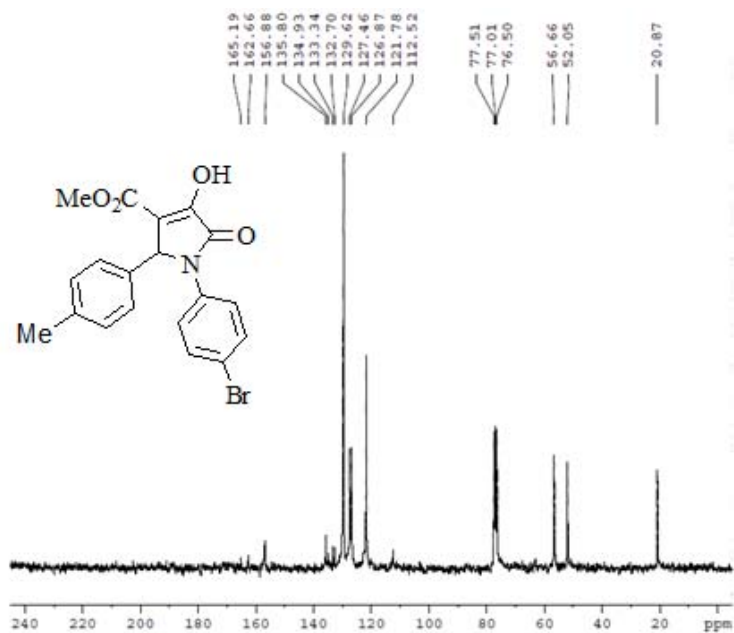


Fig. S-13. Mass spectrum of compound 4a.

1-(4-bromophenyl)-5-(4-methylphenyl)-3-hydroxy-4-methoxycarbonyl-3-pyrrolin-2-one (5a)

The cream powder; MeOH (8 hours, yields: 95%), m.p. 170-172 °C (170-172 °C [21]). FT-IR (KBr): $\nu_{\text{max}}(\text{cm}^{-1})$: 3167 (OH), 2951, 1724 (C=O), 1667 (C=O), 1515, 1383, 1230, 1010; $^1\text{H-NMR}$ (250.13 MHz, CDCl_3) δ H: 2.16 (s, 3H, CH_3), 3.56 (s, 3H, OCH_3), 6.02 (s, 1H, CH), 7.04–7.42 (m, 8 H, Ar), 11.90 (br s, 1H, OH). $^{13}\text{C-NMR}$ (62.90 MHz, CDCl_3) δ C: 20.85, 51.57, 60.39, 111.72, 121.46, 122.97, 129.65, 130.40, 131.65, 133.95, 136.66, 153.38, 162.88 (C=O), 164.16 (C=O). Mass (m/z): 403.1 ($\text{M}^+ + 2$), 401.1 (M^+), 369.1, 342.1, 267.0, 236.0, 208.0, 180.0, 157.1 (100%), 133.1, 115.1, 91.2, 65.2.). Anal. Calcd for $\text{C}_{19}\text{H}_{16}\text{BrNO}_4$: C (%), 56.73; H (%), 4.01; N (%), 3.48. Found: C (%), 56.55; H (%), 4.15; N (%), 3.60.

Fig. S-14. FT-IR (KBr, cm^{-1}) spectrum of compound 5a.

Fig. S-15. ¹H-NMR (250 MHz, CDCl₃, δ/ppm) spectrum of compound 5a.Fig. S-16. ¹³C-NMR (62.9 MHz, CDCl₃, δ/ppm) spectrum of compound 5a.

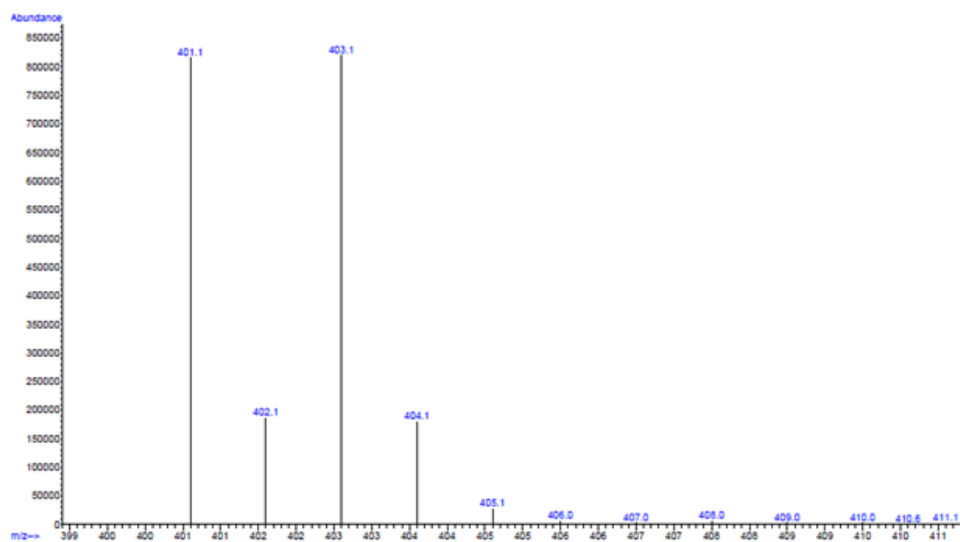


Fig. S-17. Mass spectrum of compound 5a.

1-(4-methylphenyl)-5-(2-chlorophenyl)-3-hydroxy-4-methoxycarbonyl-3-pyrrolin-2-one (6a)

The white solid, MeOH (8 hours, yields: 90%), m.p. 192-194 °C (193-194 °C [21]). FT-IR (KBr): $\nu_{\max}(\text{cm}^{-1})$: 3310 (OH), 2954, 1706 (C=O), 1680 (C=O), 1516, 1374, 1222, 1009; $^1\text{H-NMR}$ (250.13 MHz, CDCl_3) δH : 2.23 (s, 3H, CH_3), 3.72 (s, 3H, OCH_3), 6.40 (s, 1H, CH), 6.96–7.38 (m, 8 H, Ar), 9.10 (br s, 1H, OH). $^{13}\text{C-NMR}$ (62.90 MHz, CDCl_3) δC : 20.87, 52.05, 56.66, 112.52, 121.78, 126.87, 127.46, 129.62, 132.70, 133.34, 135.80, 156.88, 162.66 (C=O), 165.19 (C=O). Mass (m/z): 359.2 ($\text{M}^+ + 2$), 357.2 (M^+), 325.1, 290.1, 262.1, 228.1, 164.1 (100%), 133.1, 115.1, 91.1, 65.1.). Anal. Calcd for $\text{C}_{19}\text{H}_{16}\text{ClNO}_4$: C (%), 63.78; H (%), 4.51; N (%), 3.91. Found: C (%), 63.59; H (%), 4.40; N (%), 3.77.

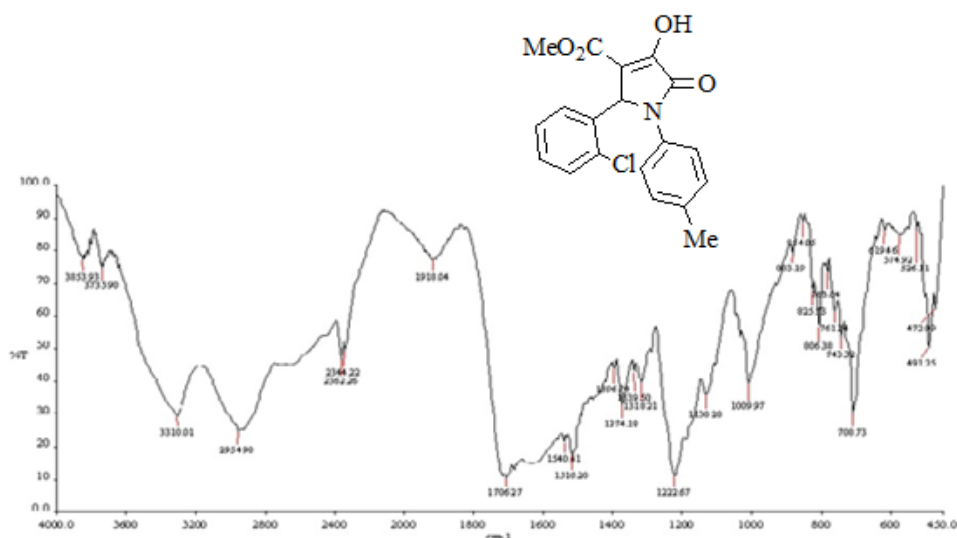
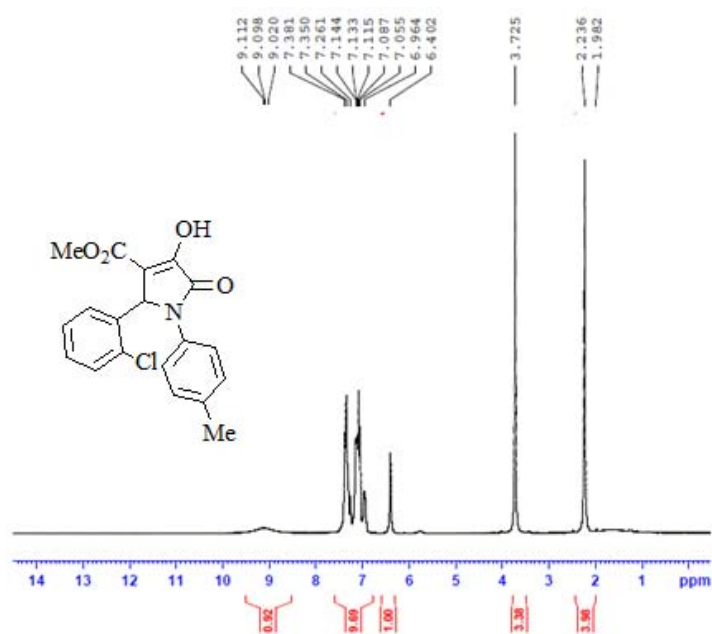
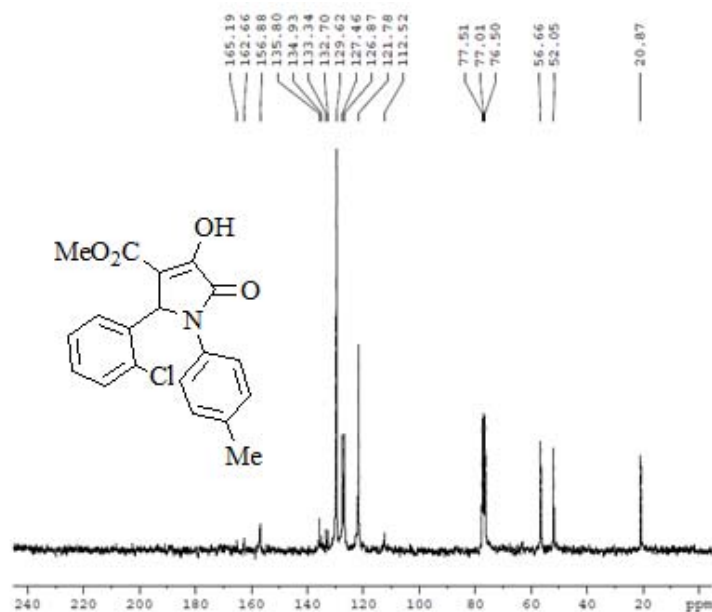


Fig. S-18. FT-IR (KBr, cm^{-1}) spectrum of compound 6a.

Fig. S-19. ¹H-NMR (250 MHz, CDCl₃, δ/ppm) spectrum of compound 6a.Fig. S-20. ¹³C-NMR (62.9 MHz, CDCl₃, δ/ppm) spectrum of compound 6a.

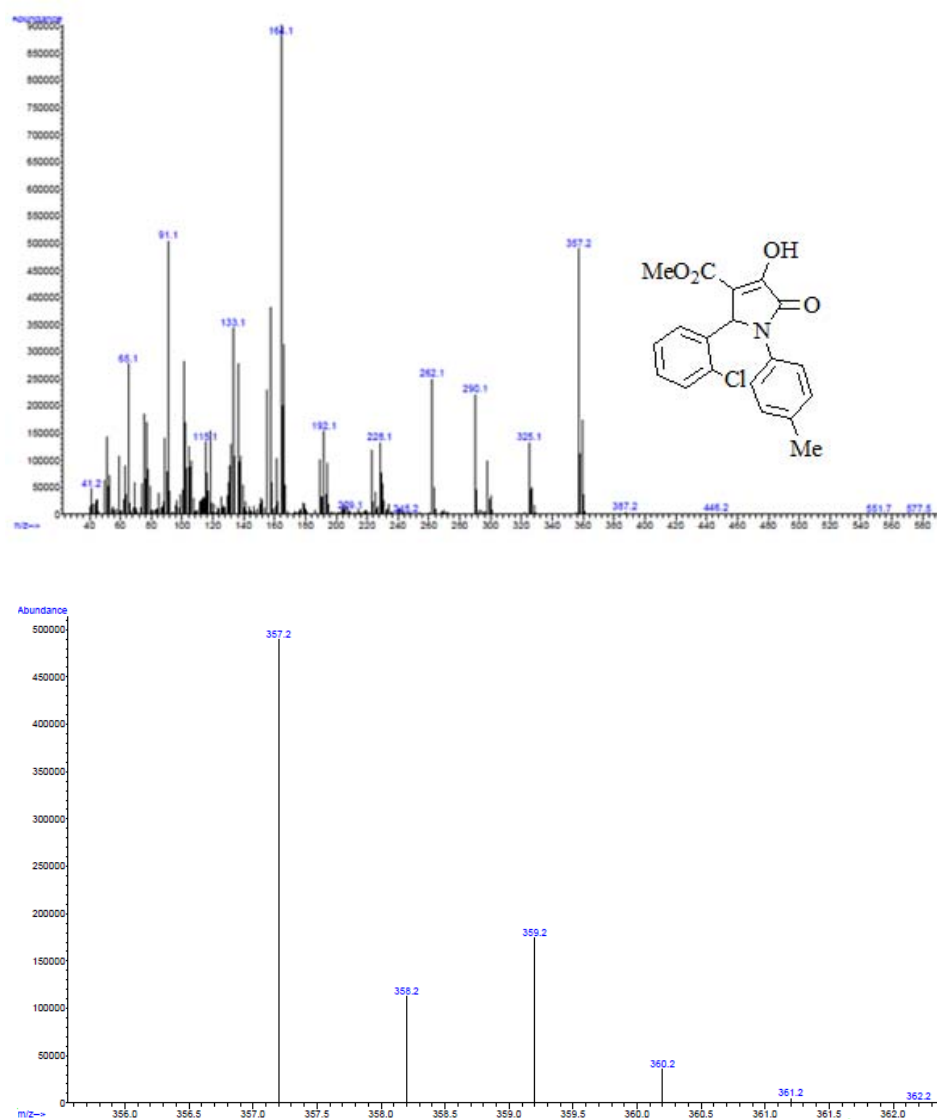


Fig. S-21. Mass spectrum of compound 6a.

1-(4-methoxyphenyl)-5-(3-bromophenyl)-3-hydroxy-4-methoxycarbonyl-3-pyrrolin-2-one (7a)

The cream solid, MeOH (8 hours, yields: 94%), 170-171 °C (170-171 °C [21]). FT-IR (KBr): $\nu_{\max}(\text{cm}^{-1})$: 3198 (OH), 2954, 1707 (C=O), 1683 (C=O), 1514, 1385, 1254, 1132; $^1\text{H-NMR}$ (250.13 MHz, CDCl_3) δH : 3.72 (s, 3H, OCH_3), 3.74 (s, 3H, OCH_3), 5.59 (s, 1H, CH), 6.78–7.36 (m, 8H, Ar). $^{13}\text{C-NMR}$ (62.90 MHz, CDCl_3) δC : 52.10, 55.34, 61.56, 112.17, 114.37, 122.59, 124.44, 126.28, 128.62, 130.22, 130.46, 131.78, 137.53, 156.22, 157.80, 162.77 (C=O), 164.83 (C=O). Mass (m/z): 419.1 ($\text{M}^+ + 2$), 417.1 (M^+), 387.1, 208.0, 149.2 (100%), 101.1, 77.2. Anal. Calcd for $\text{C}_{19}\text{H}_{16}\text{BrNO}_5$: C (%), 54.56; H (%), 3.86; N (%), 3.35. Found: C (%), 54.45; H (%), 3.98; N (%), 3.48.

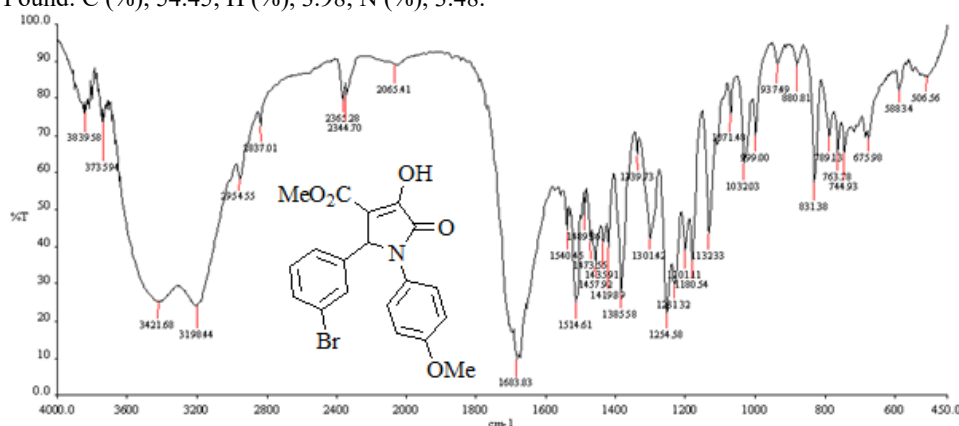


Fig. S-22. FT-IR (KBr, cm^{-1}) spectrum of compound 7a.

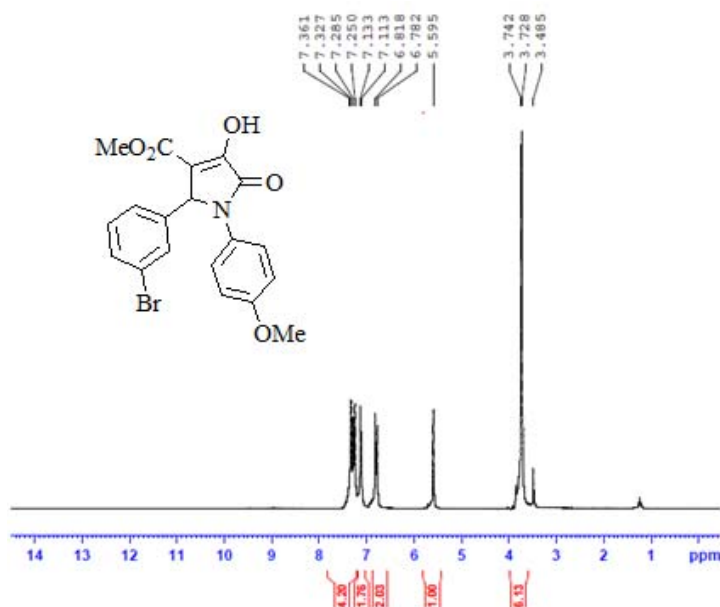


Fig. S-23. $^1\text{H-NMR}$ (250 MHz, CDCl_3 , δ/ppm) spectrum of compound 7a.

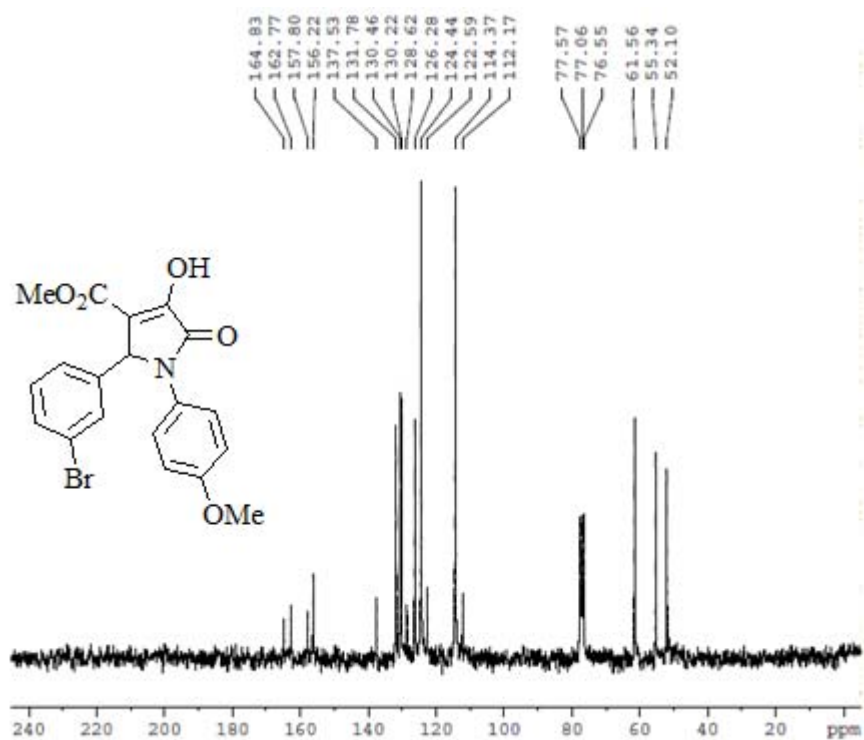
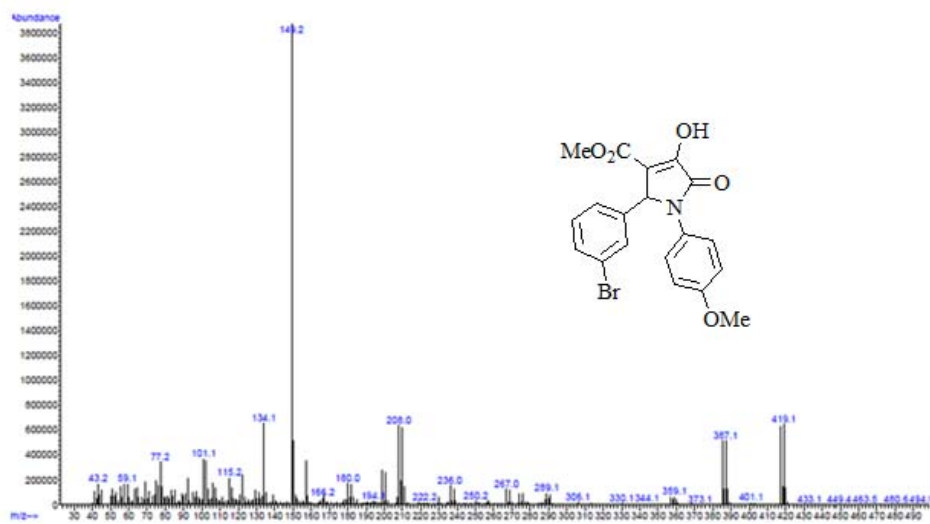
Fig. S-24. ^{13}C -NMR (62.9 MHz, CDCl_3 , δ/ppm) spectrum of compound 7a.

Fig. S-25. Mass spectrum of compound 7a.