

Supplementary Material

An eco-friendly approach for the synthesis of 1,2,5-trisubstituted and 4-amino-1,2,5-tetrasubstituted imidazoles *via* a multi-component condensation

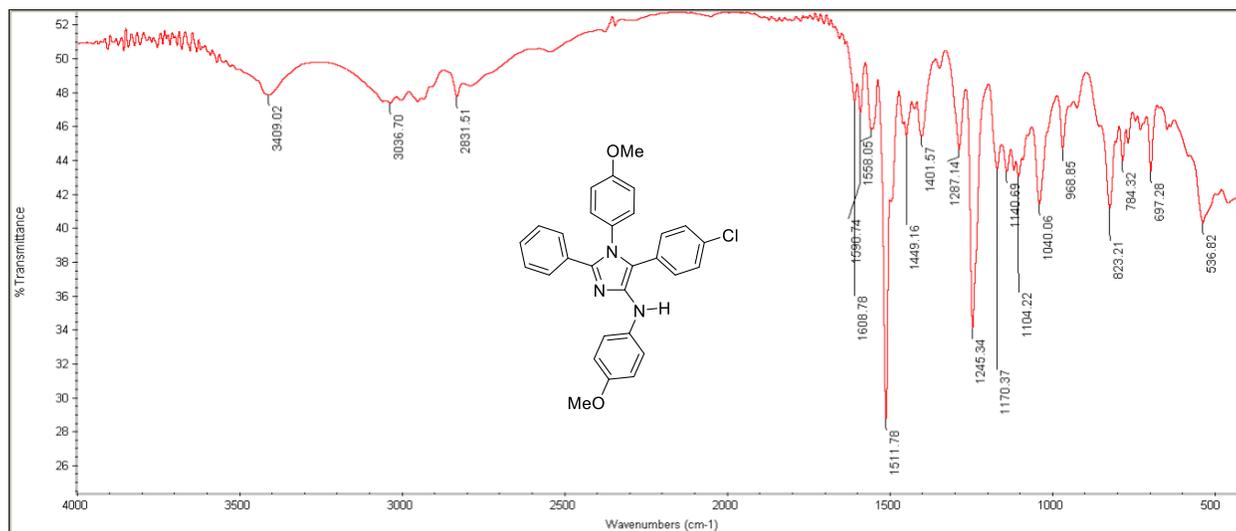
Hossein Mehrabi*, Farzaneh Alizadeh-Bami, Azam Meydani, and Soheila Besharat

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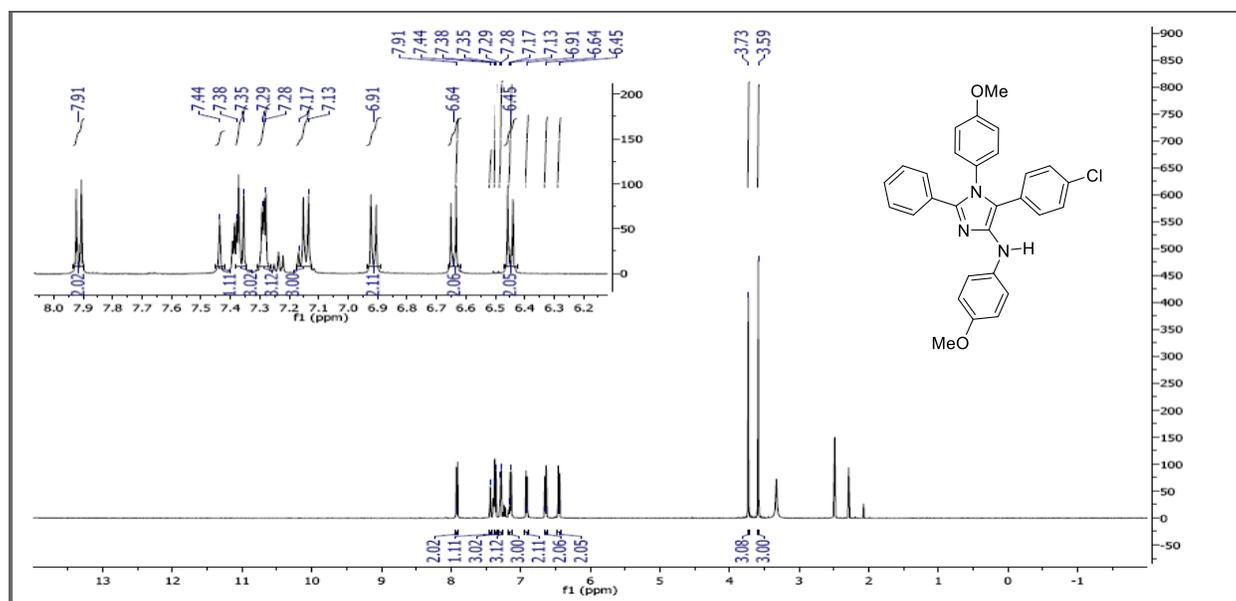
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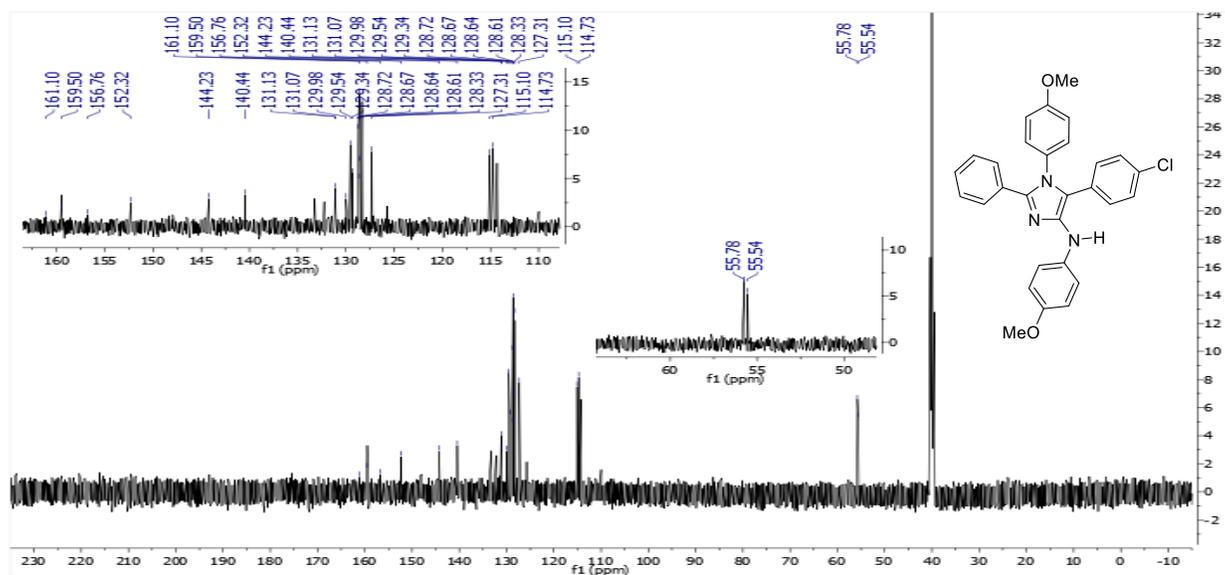
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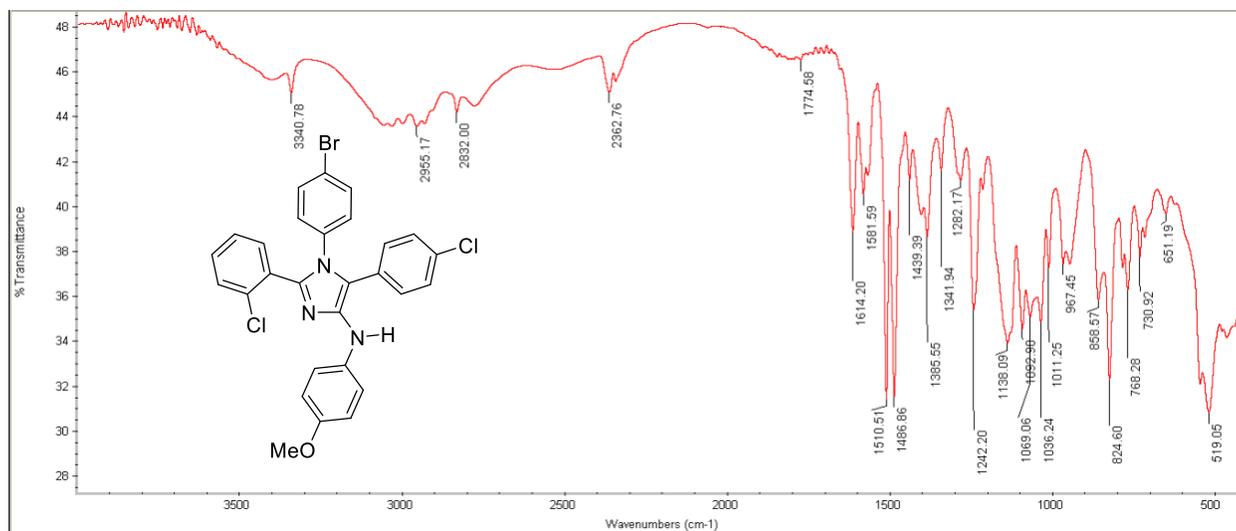
IR ν/cm^{-1} (KBr) for compound (**6a**): 3409 (NH), 1608 (C=N) cm^{-1} .



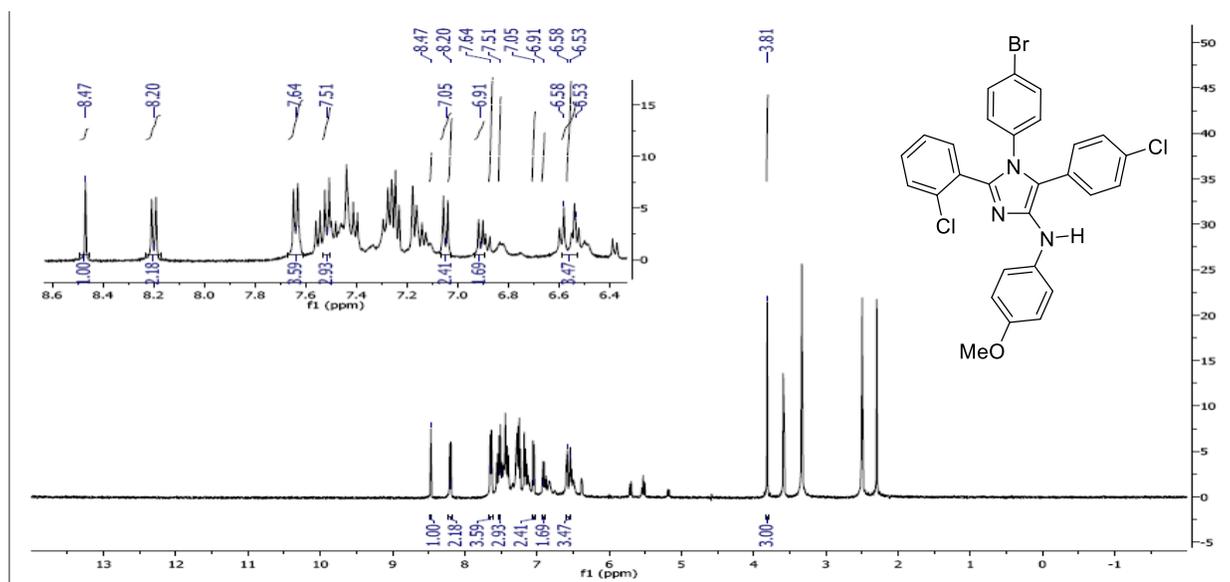
^1H NMR (500 MHz, $\text{DMSO}-d_6$) for compound (**6a**): δ_{H} 3.59 (s, 3H, OCH_3), 3.73 (s, 3H, OCH_3), 6.45 (d, J 9.0, 2H, ArH), 6.64 (d, J 9.0, 2H, ArH), 6.91 (d, J 9.0, 2H, ArH), 7.13-7.38 (m, 9H, ArH), 7.44 (bs, 1H, NH), 7.91 (d, J 9.0, 2H, ArH).



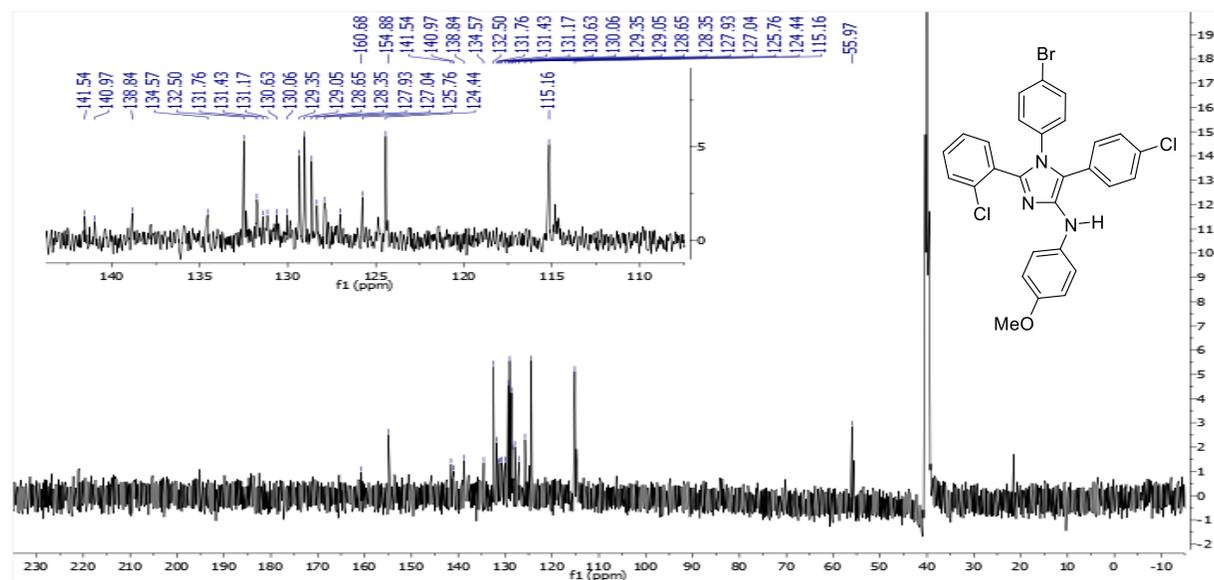
¹³C NMR (125 MHz, DMSO-*d*₆) for compound (6a): δ_c 55.5, 55.7, 114.7, 115.1, 127.1, 128.3, 128.6, 128.6, 128.6, 128.7, 129.3, 129.5, 129.9, 131.0, 131.1, 140.4, 144.2, 152.3, 156.7, 159.5, 161.1.



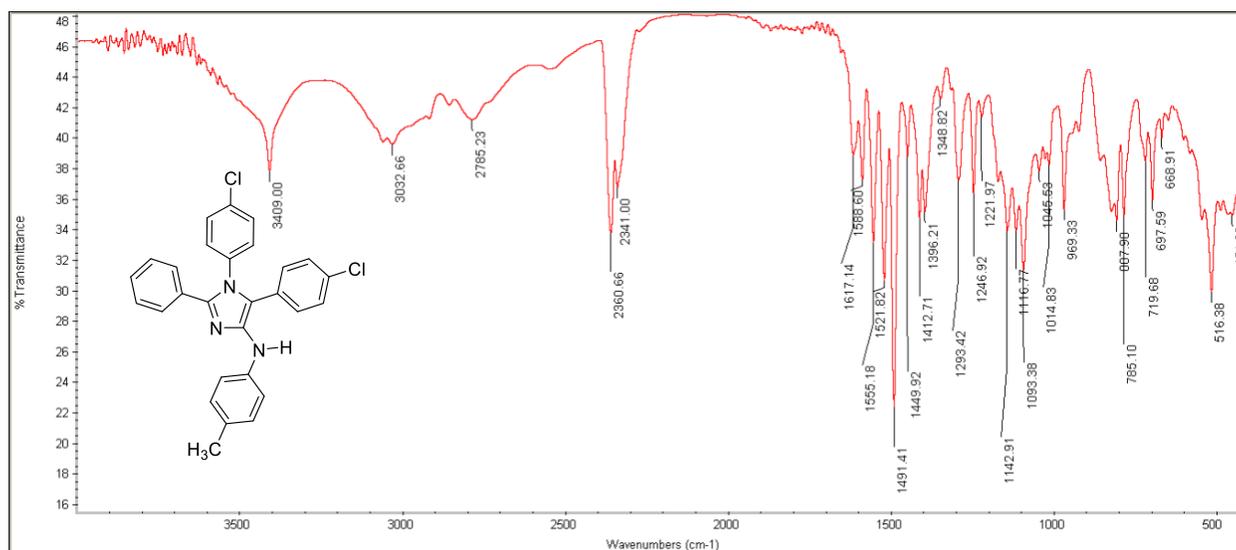
IR ν/cm^{-1} (KBr) for compound (6b): 3340 (NH), 1614 (C=N) cm^{-1} .



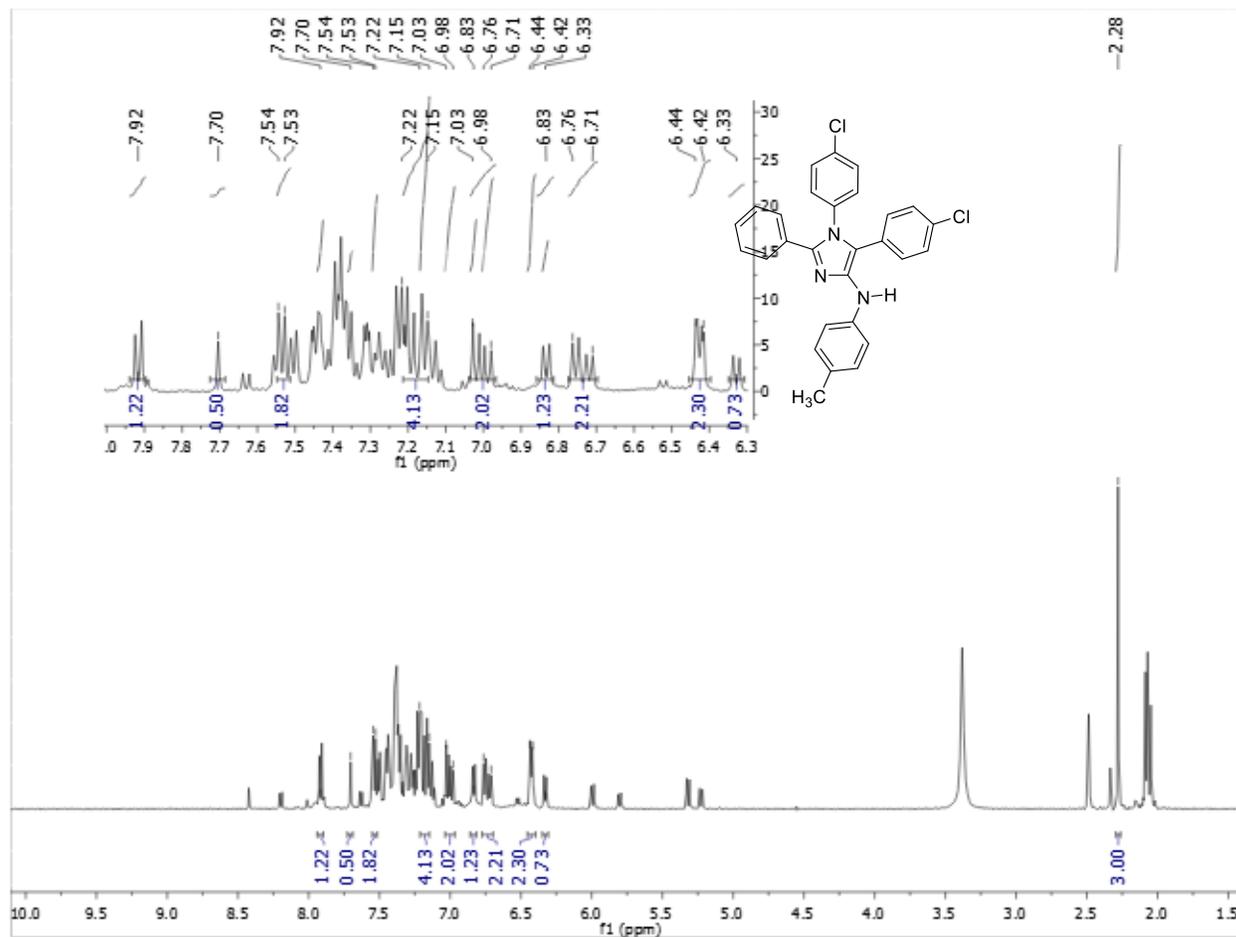
¹H NMR (500 MHz, DMSO-*d*₆) for compound (6b): δ_{H} 3.81 (s, 3H, OCH₃), 6.53-6.58 (m, 3H, ArH), 6.91 (d, 8.5, 2H, ArH), 7.06 (d, *J* 8.5, 2H, ArH), 7.51-7.64 (m, 7H, ArH), 8.20 (d, *J* 8.5, 2H, ArH), 8.47 (bs, 1H, NH).



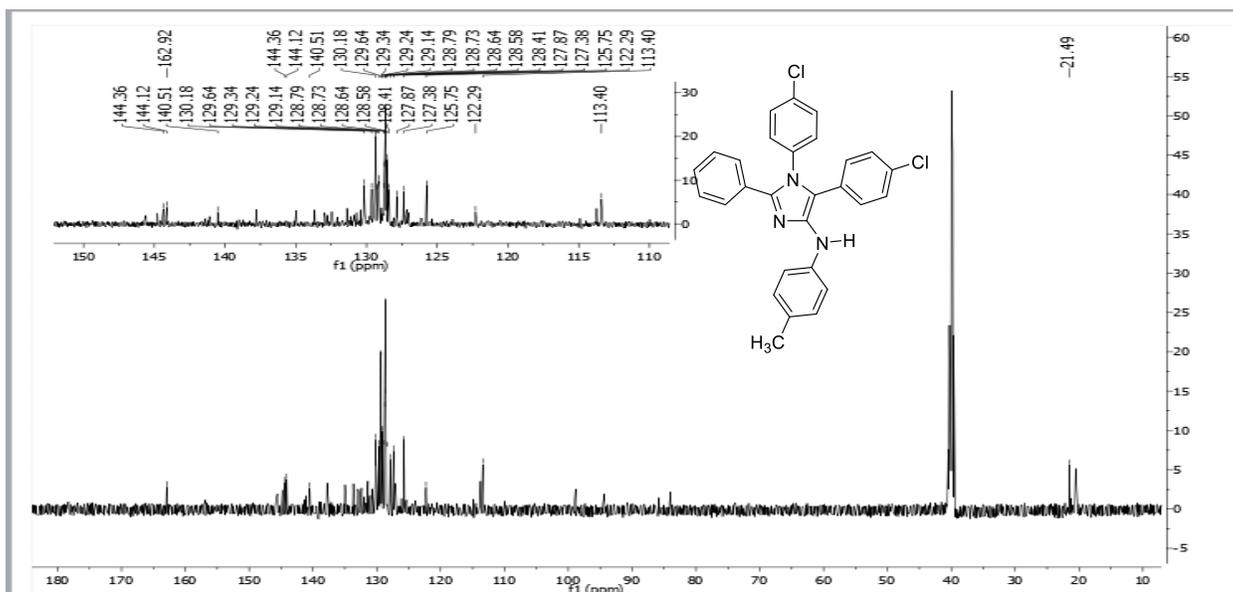
¹³C NMR (125 MHz, DMSO-*d*₆) for compound (6b): δ_{C} 55.9, 115.1, 124.4, 125.7, 127.0, 127.9, 128.3, 128.6, 129.0, 129.3, 130.0, 130.6, 131.1, 131.4, 131.7, 132.5, 134.5, 138.8, 140.9, 141.5, 154.8, 160.6.



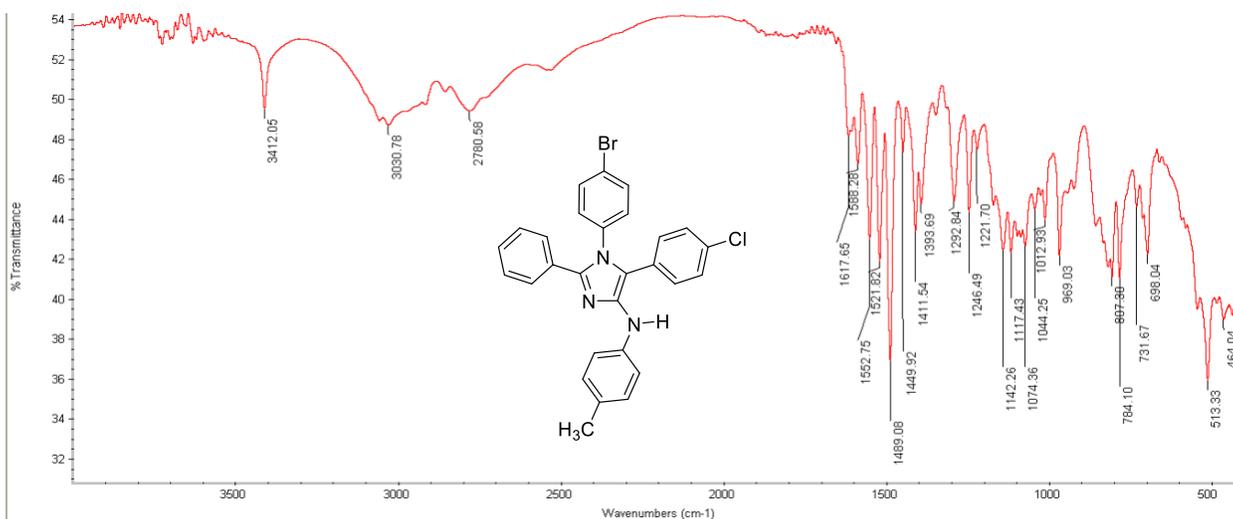
IR ν /cm⁻¹ (KBr) for compound (6c): 3409 (NH), 1617 (C=N) cm⁻¹.



¹H NMR (500 MHz, DMSO-*d*₆) for compound (6c): δ _H 2.28 (s, 3H, CH₃), 6.33 (d, *J* 8.5, 1H, ArH), 6.43 (d, *J* 8.5, 2H, ArH), 6.75 (d, *J* 8.5, 2H, ArH), 6.83 (d, *J* 8.5, 2H, ArH), 7.01 (d, *J* 8.5, 2H, ArH), 7.15-7.22 (m, 4H, ArH), 7.53 (d, *J* 8.5, 2H, ArH), 7.70 (bs, 1H, NH), 7.92 (d, *J* 8.5, 2H).

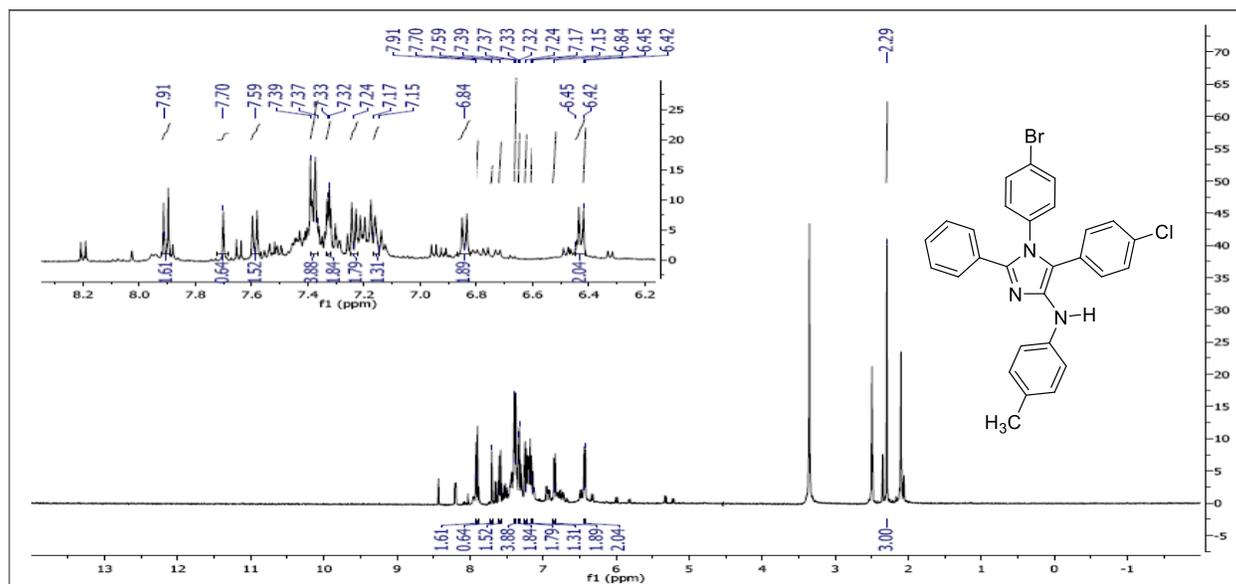


¹³C NMR (125 MHz, DMSO-*d*₆) for compound (6c): δ_C 21.4, 113.4, 122.2, 125.7, 127.3, 127.8, 128.4, 128.5, 128.6, 128.7, 128.7, 129.1, 129.2, 129.3, 129.6, 130.1, 140.5, 144.1, 144.3, 162.9.

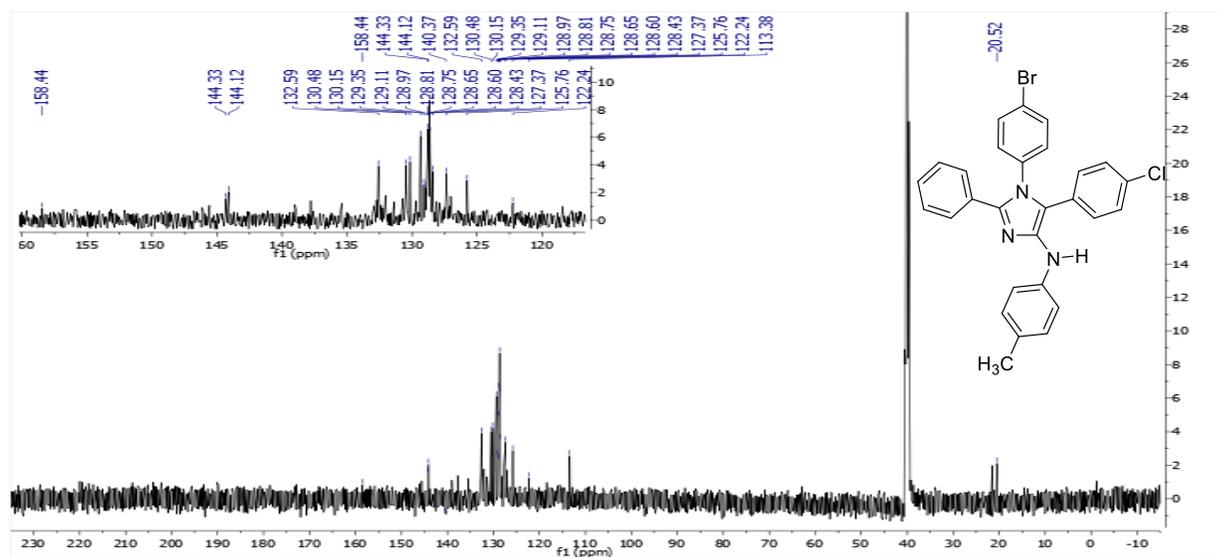


IR ν/cm⁻¹ (KBr) for compound (6d): 3412 (NH), 1617 (C=N) cm⁻¹.

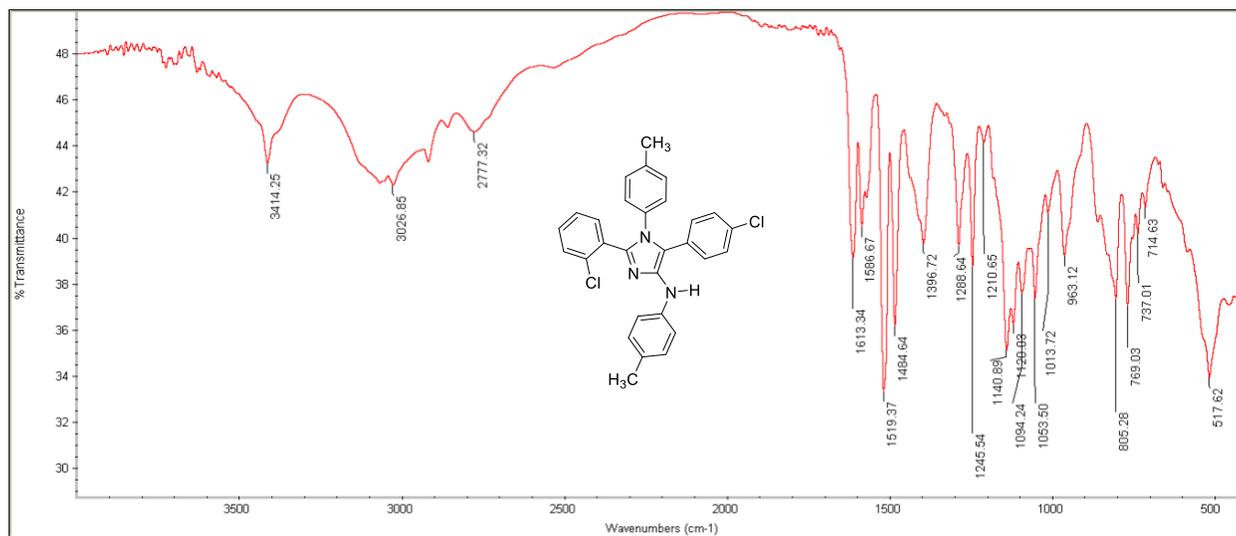




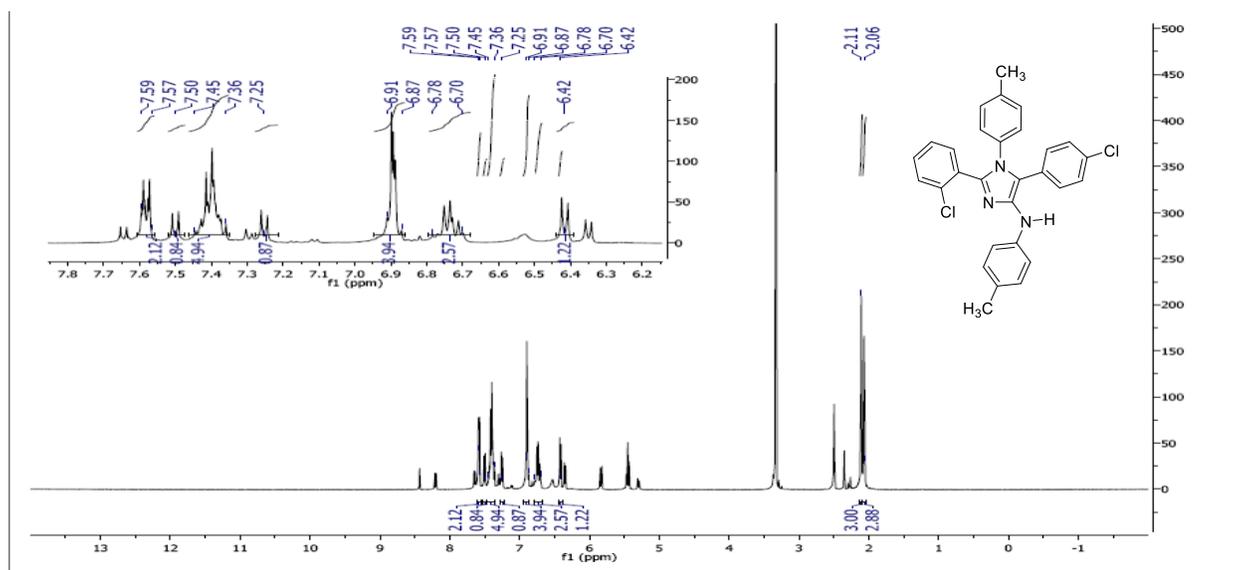
^1H NMR (500 MHz, $\text{DMSO}-d_6$) for compound (**6d**): δ_{H} 2.29 (s, 3H, CH_3), 6.43 (d, J 8.5, 2H, ArH), 6.84 (d, J 8.5, 2H, ArH), 7.15-7.39 (m, 9H, ArH), 7.59 (d, J 9.0, 2H, ArH), 7.70 (bs, 1H, NH), 7.91 (d, J 9.0, 2H, ArH).



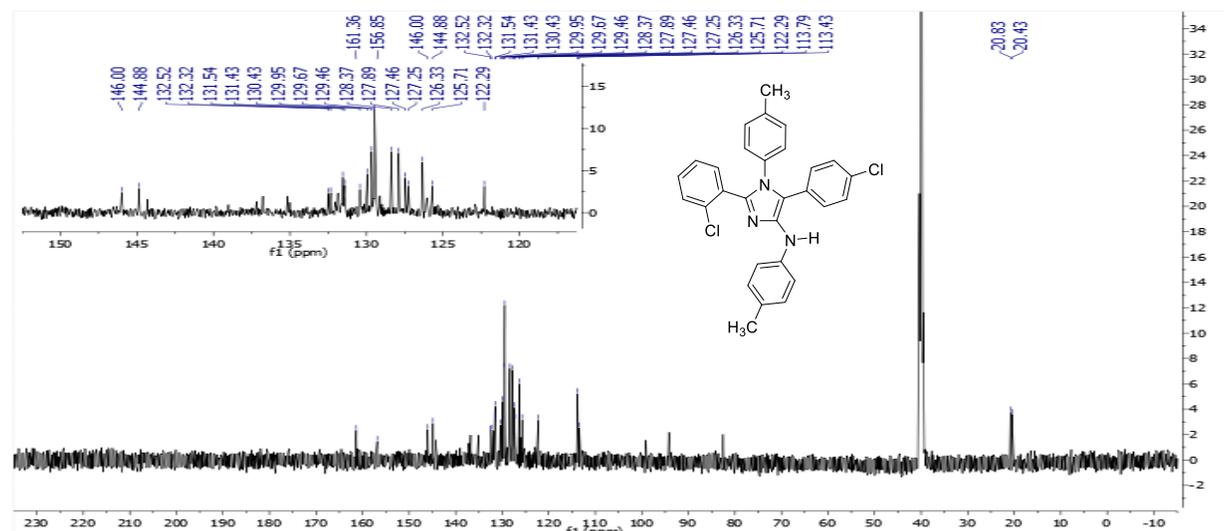
^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) for compound (**6d**): δ_{C} 20.5, 113.3, 122.2, 125.7, 127.3, 128.4, 128.6, 128.6, 128.7, 128.8, 128.9, 129.1, 129.3, 130.1, 130.4, 132.5, 140.3, 144.1, 144.3, 158.4.



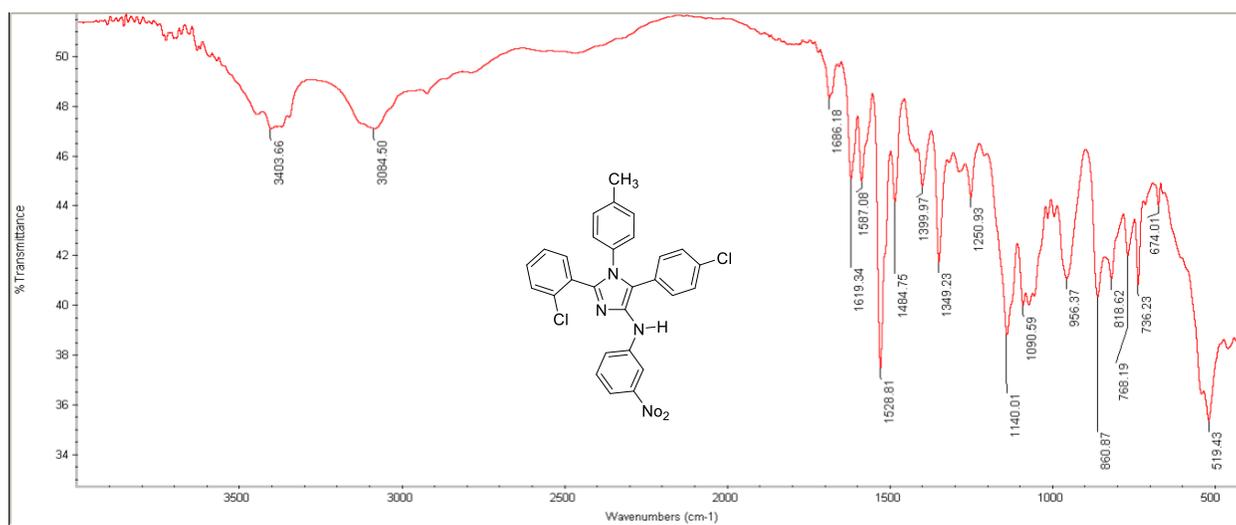
IR ν /cm⁻¹ (KBr) for compound (6e): 3414 (NH), 1613 (C=N) cm⁻¹.



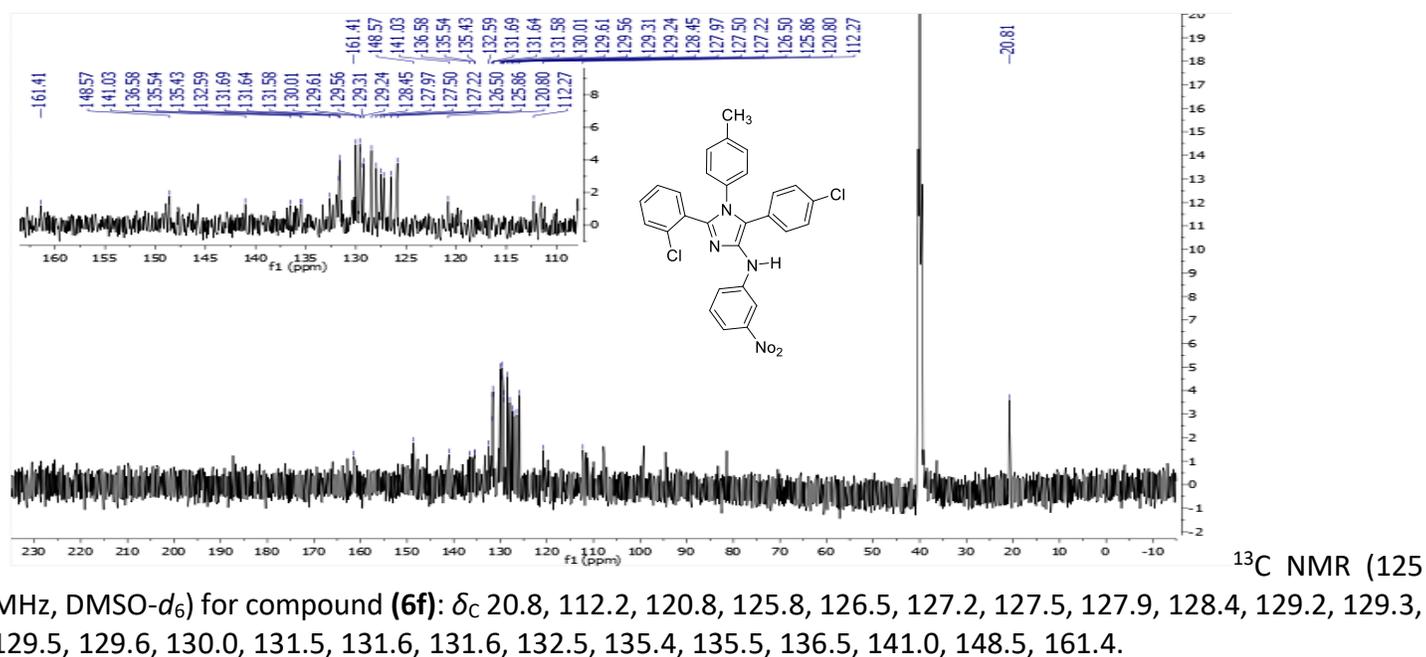
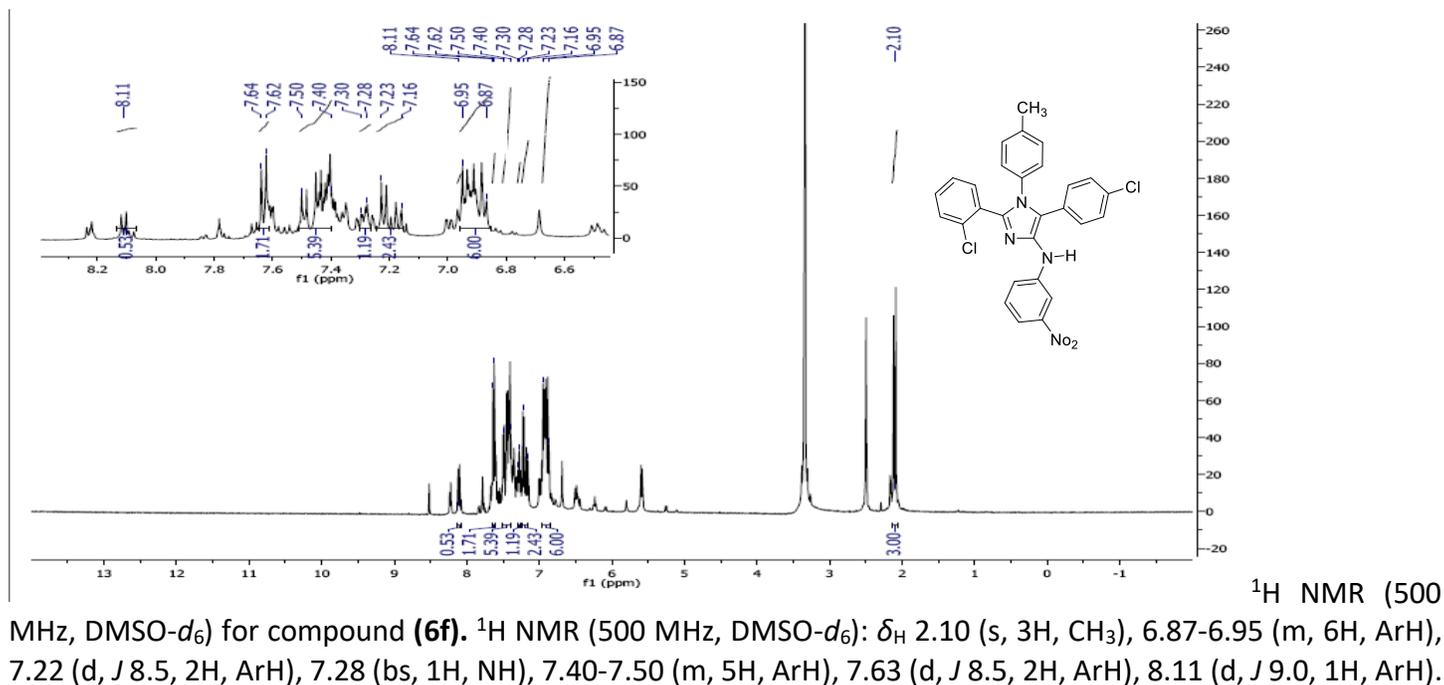
¹H NMR (500 MHz, DMSO-*d*₆) for compound (6e): δ_{H} 2.06 (s, 3H, CH₃), 2.11 (s, 3H, CH₃), 6.42 (d, *J* 9.0, 1H, ArH), 6.70-6.78 (m, 3H, ArH), 6.87-6.91 (m, 4H, ArH), 7.25 (d, *J* 9.0, 1H, ArH), 7.36-7.50 (m, 5H, ArH), 7.50 (bs, 1H, NH), 7.58 (d, *J* 8.5, 2H, ArH).

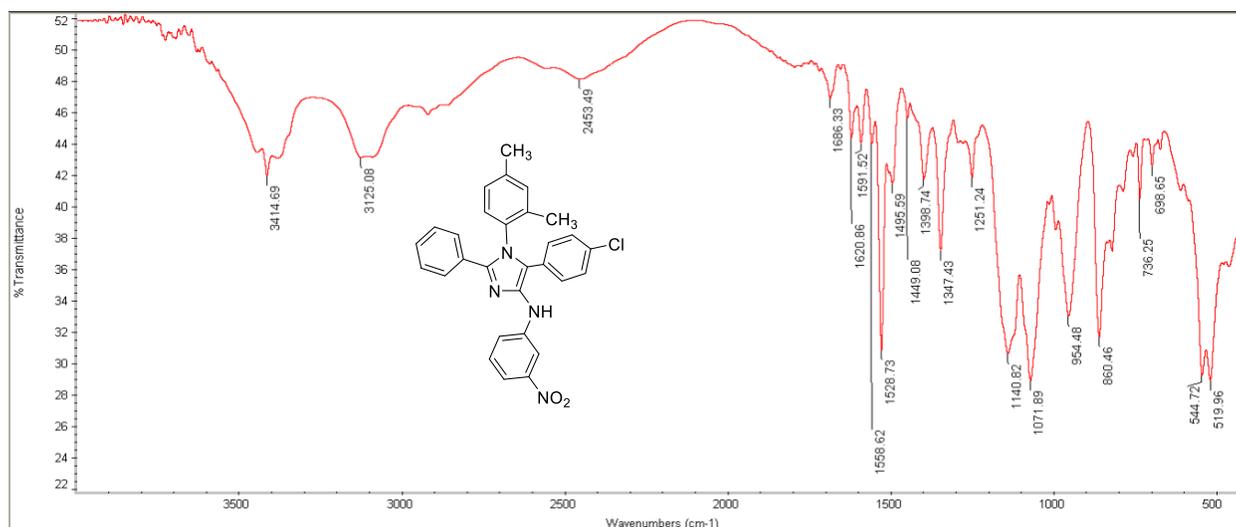


¹³C NMR (125 MHz, DMSO-*d*₆) for compound (6e): δ_c 20.4, 20.8, 113.4, 113.7, 122.2, 125.7, 126.3, 127.2, 127.4, 127.8, 128.3, 129.4, 129.6, 129.9, 130.4, 131.4, 131.5, 132.3, 132.5, 144.8, 146.0, 156.8, 161.3.

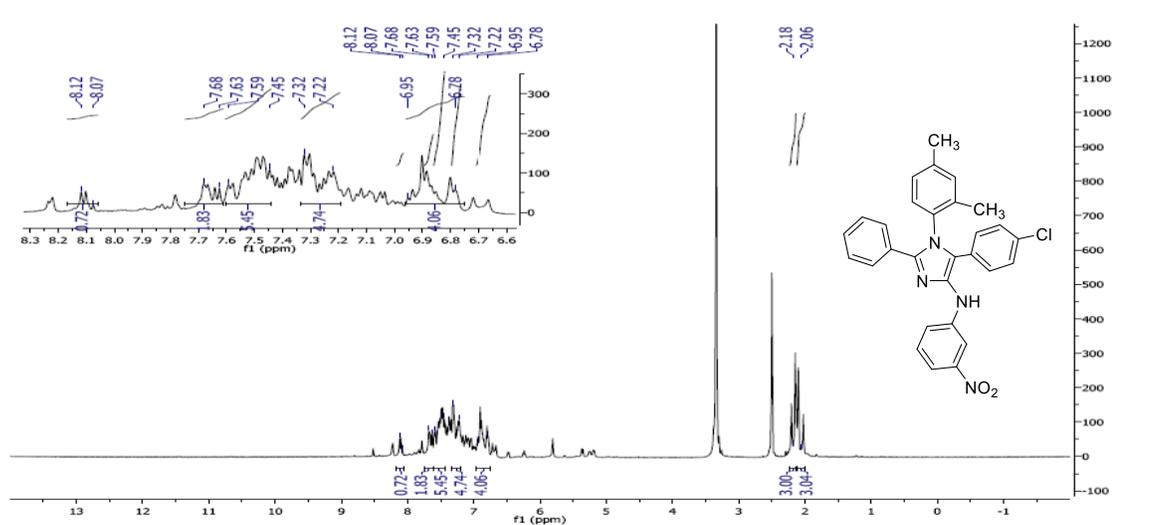


IR ν/cm⁻¹ (KBr) for compound (6f): 3403 (NH), 1619 (C=N) cm⁻¹.

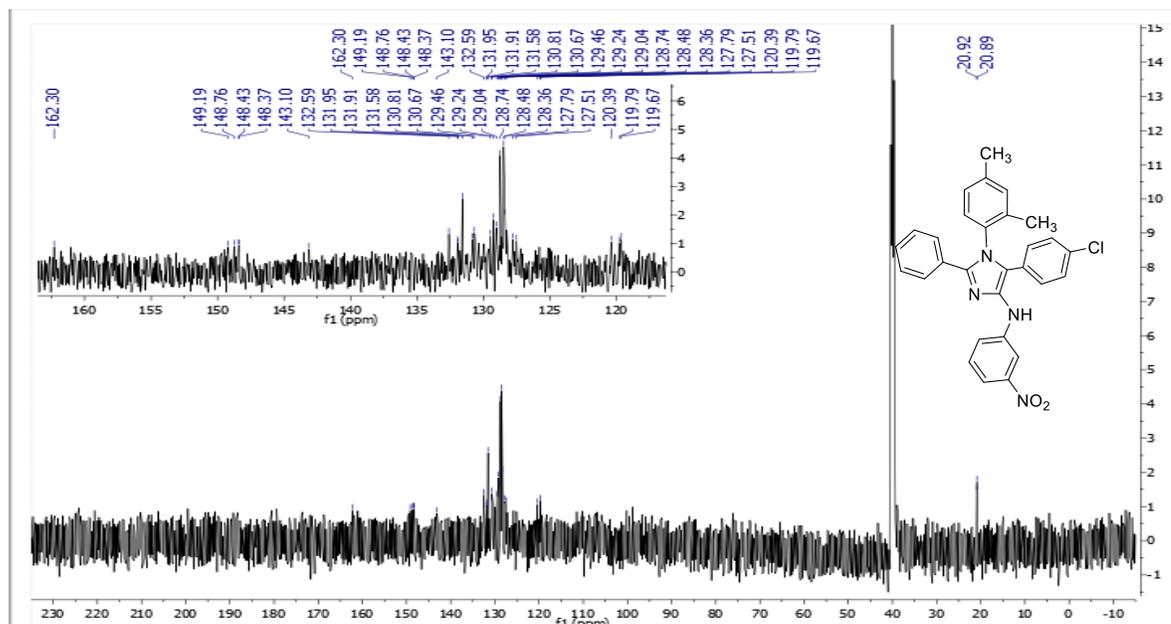




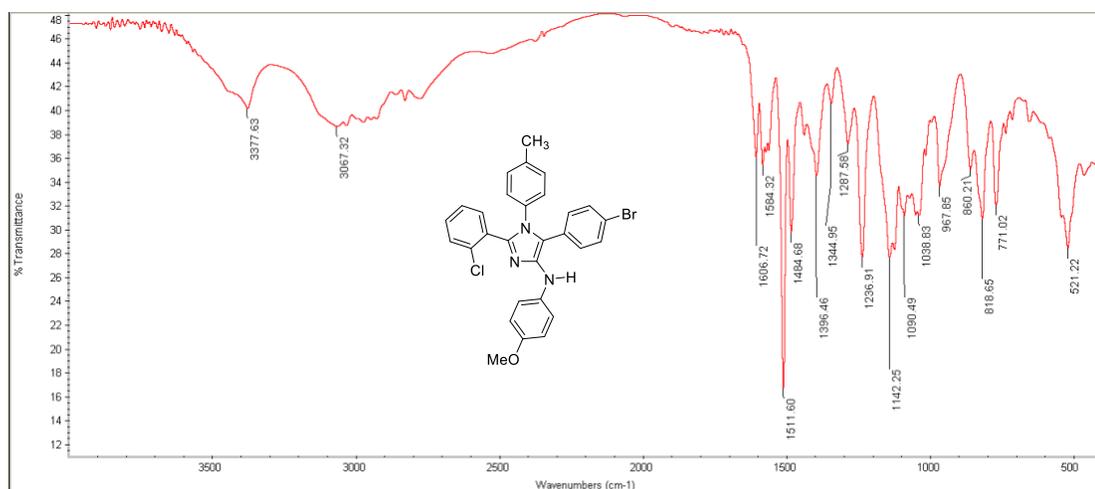
IR ν/cm^{-1} (KBr) for compound (**6g**): 3414 (NH), 1620 (C=N) cm^{-1} .



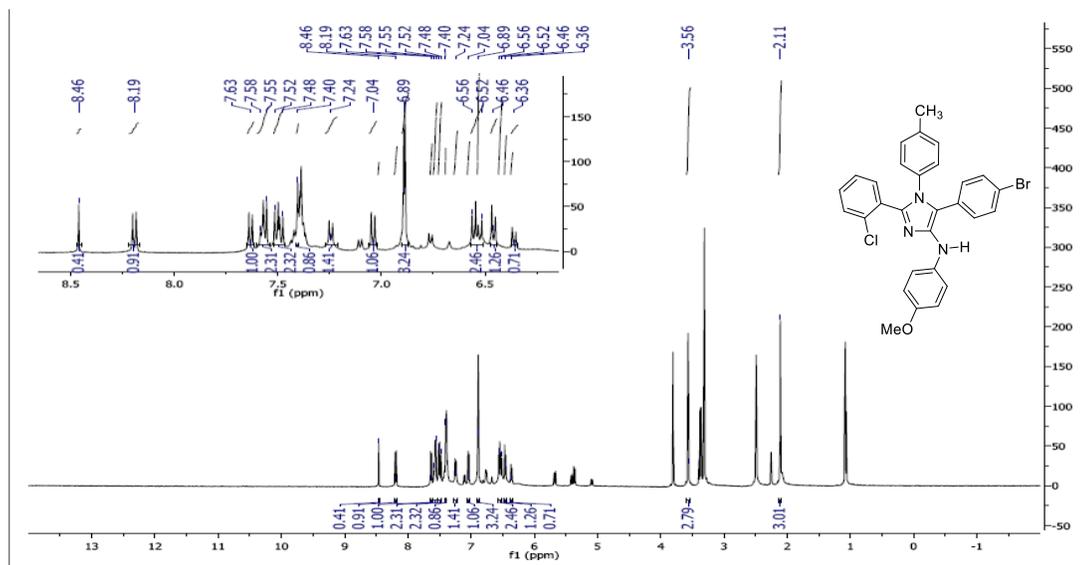
^1H NMR (500 MHz, $\text{DMSO}-d_6$) for compound (**6g**): δ_{H} 2.06 (s, 3H, CH_3), 2.18 (s, 3H, CH_3), 6.78-6.95 (m, 4H, ArH), 7.22-7.32 (m, 5H, ArH), 7.45-7.59 (m, 5H, ArH, NH), 7.68 (d, J 8.5, 2H, ArH), 8.11 (d, J 8.5, 1H, ArH).



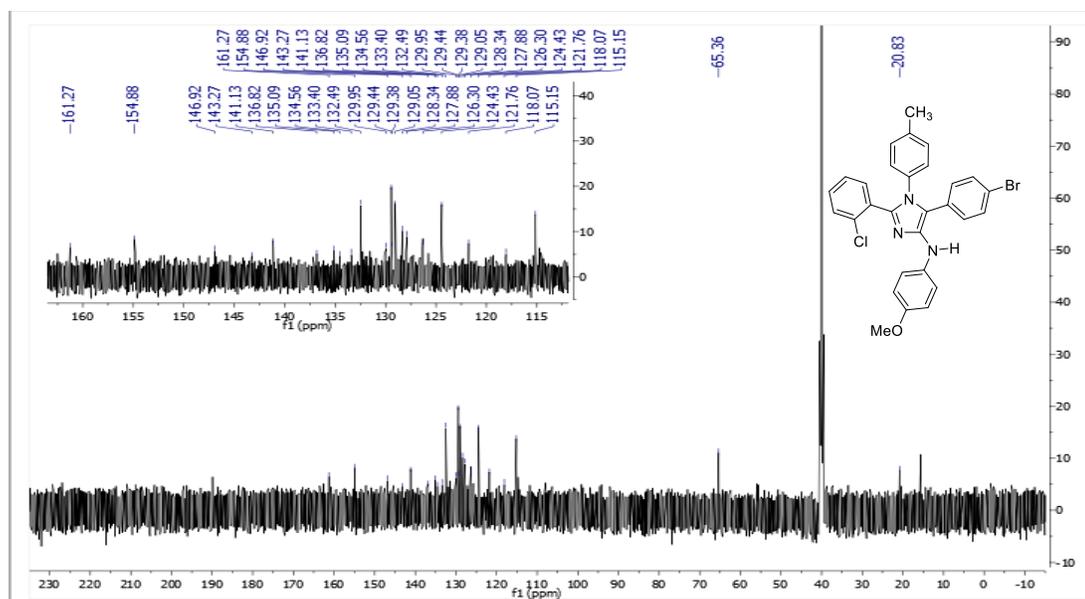
¹³C NMR (125 MHz, DMSO-*d*₆) for compound (**6g**): δ_c 20.8, 20.9, 119.6, 119.7, 120.3, 127.5, 127.7, 128.3, 128.4, 128.7, 129.0, 129.2, 129.4, 130.6, 130.8, 131.5, 131.9, 131.9, 132.5, 143.1, 148.3, 148.4, 148.7, 149.1, 162.3.



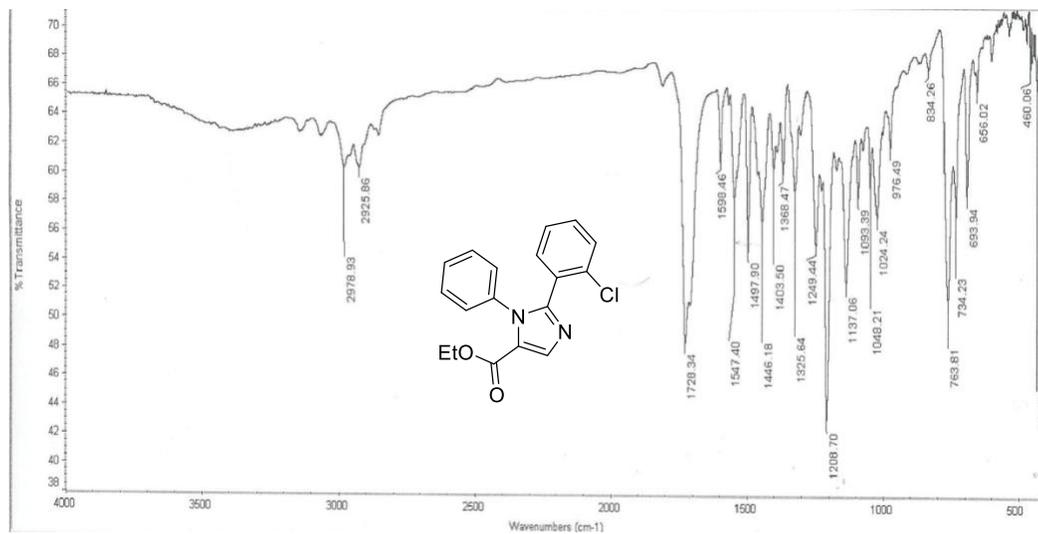
IR ν/cm^{-1} (KBr) for compound (**6h**): 3377 (NH), 1606 (C=N) cm^{-1} .



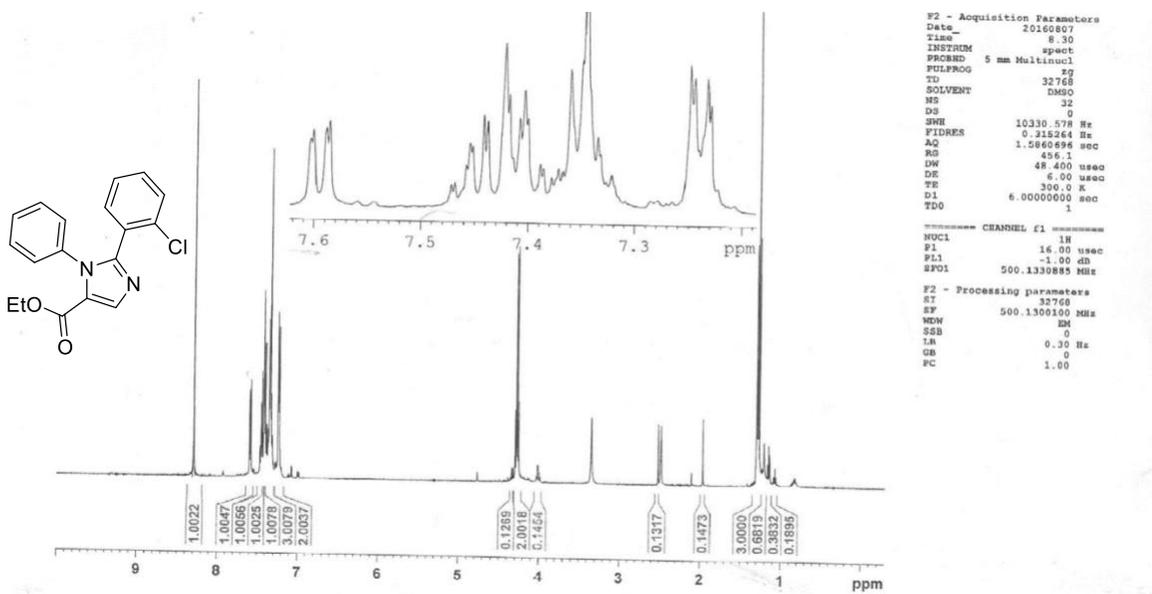
^1H NMR (500 MHz, $\text{DMSO}-d_6$) for compound (**6h**): δ_{H} 2.11 (s, 3H, CH_3), 3.56 (s, 3H, OCH_3), 6.46 (d, J 8.5, 2H, ArH), 6.55 (d, J 8.5, 2H, ArH), 6.84-6.89 (m, 4H, ArH), 7.04 (d, J 8.5, 1H, ArH), 7.25 (t, J 8.5, 1H, ArH), 7.40 (d, J 8.5, 2H, ArH), 7.56 (d, J 8.5, 2H, ArH), 7.62 (t, J 8.5, 1H, ArH), 8.19 (d, J 8.5, 1H, ArH), 8.46 (bs, 1H, NH).



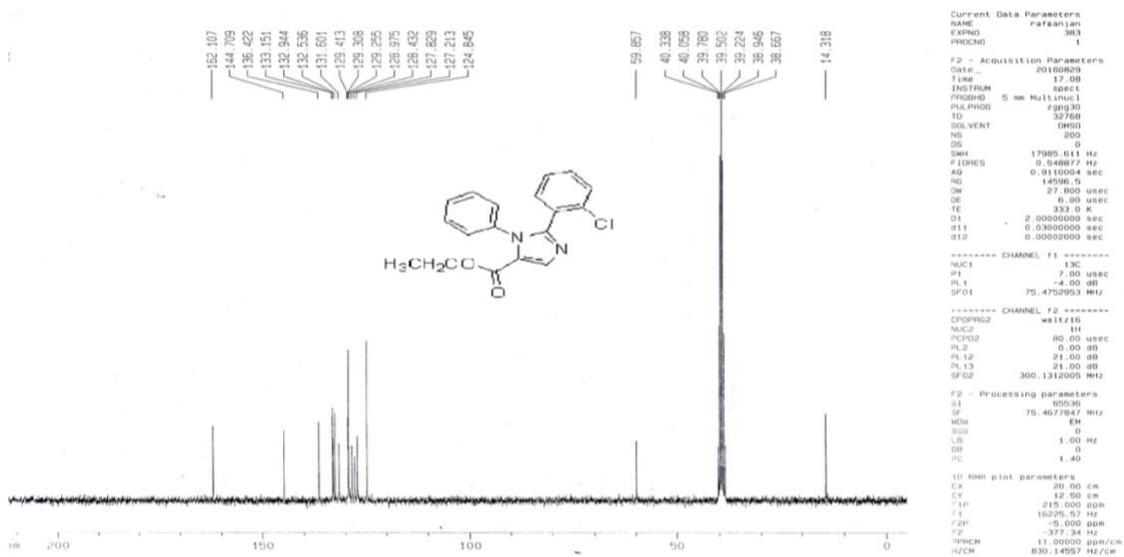
^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) for compound (**6h**): δ_{C} 20.8, 65.3, 115.1, 118.0, 121.7, 124.4, 126.3, 127.8, 128.3, 129.0, 129.3, 129.4, 129.9, 132.4, 133.4, 134.5, 135.0, 136.8, 141.1, 143.2, 146.9, 154.8, 161.2.



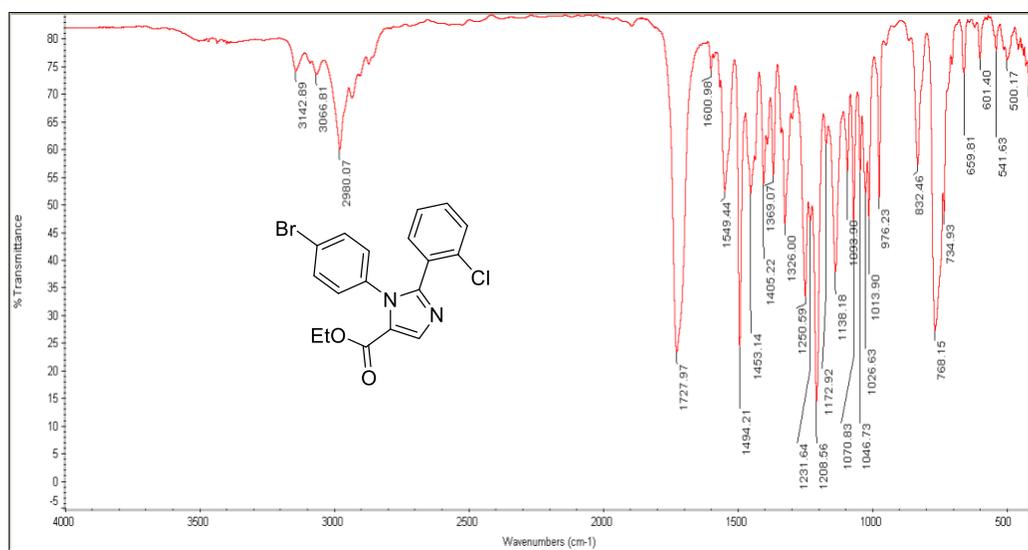
IR ν/cm^{-1} (KBr) for compound (**8a**): 1728 (C=O), 1598 (C=N) cm^{-1} .

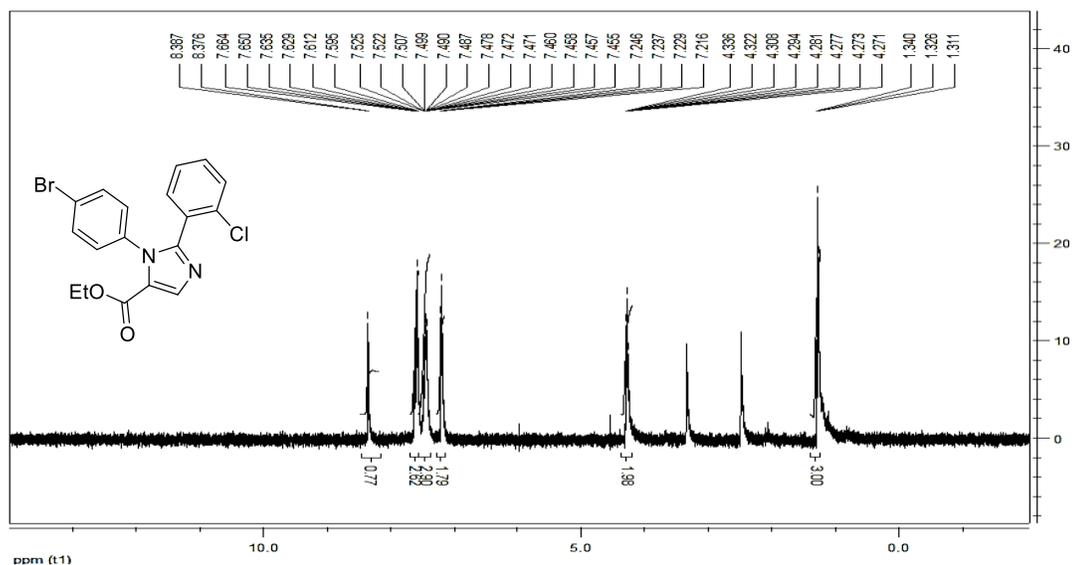


^1H NMR (500 MHz, $\text{DMSO}-d_6$) for compound (**8a**): δ_{H} 1.32 (t, J 5.6, 3H, CH_3), 4.36 (q, J 5.6, 2H, CH_2), 7.23-7.48 (m, 7H, ArH), 7.59 (d, J 8.5, 2H, ArH), 8.33 (s, 1H, CH).

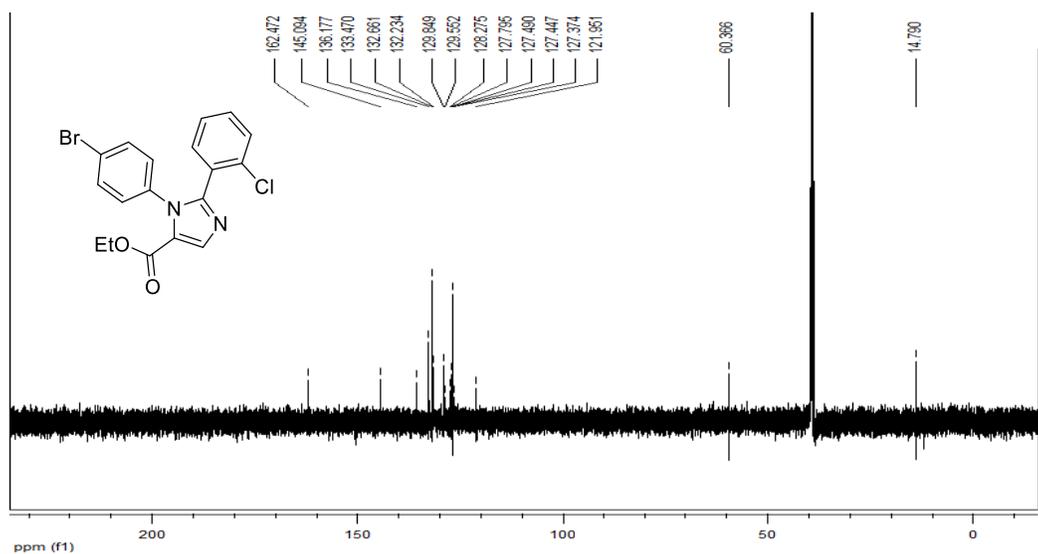


^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) for compound (**8a**): δ_{C} 14.3, 59.8, 124.8, 127.2, 127.8, 128.9, 129.2, 129.4, 131.6, 132.5, 132.9, 133.1, 134.5, 136.4, 144.7, 162.1.

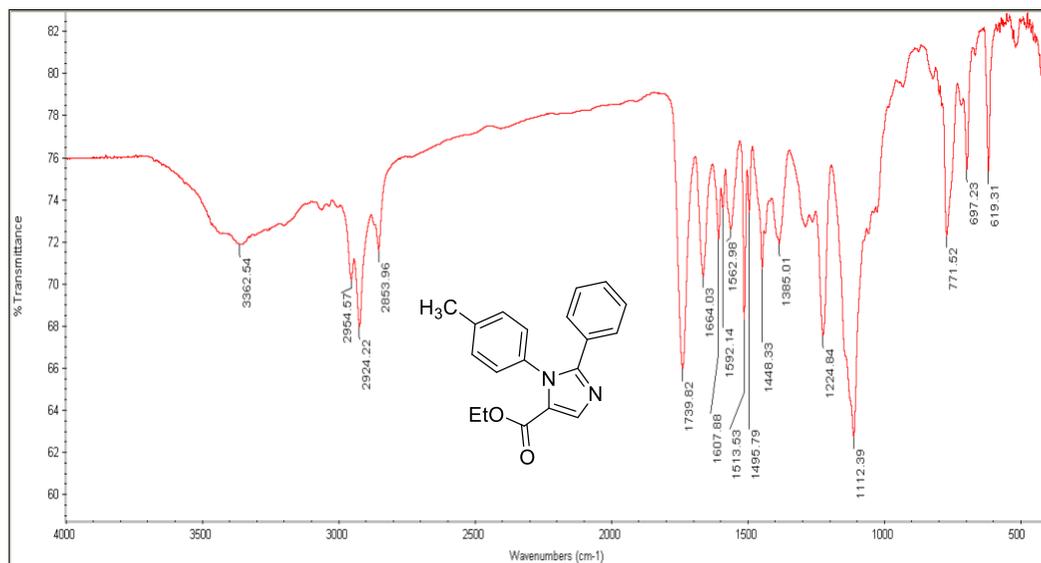




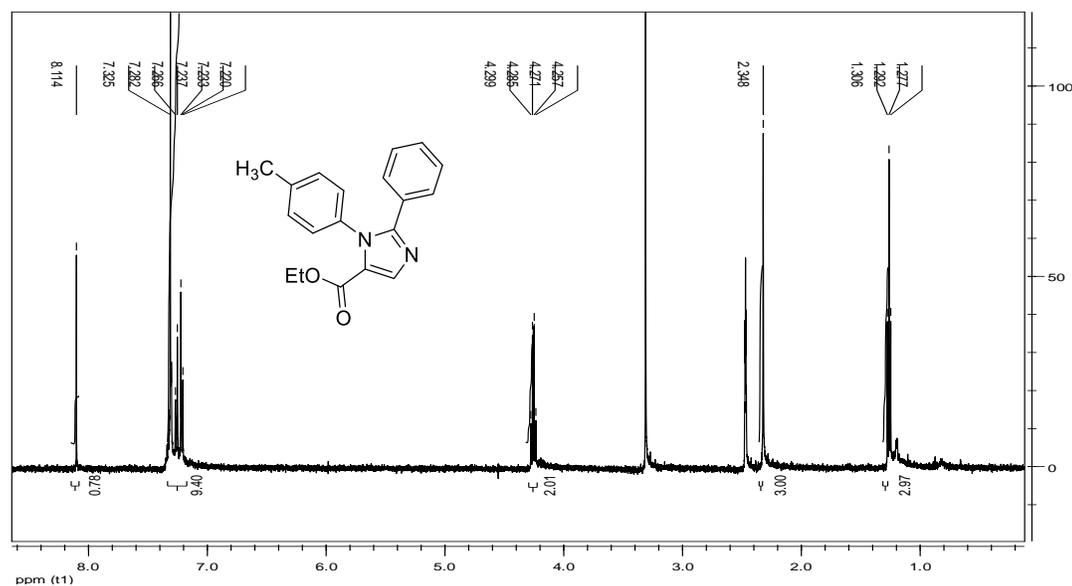
¹H NMR (500 MHz, DMSO-*d*₆) for compound **(8b)**: δ _H 1.32 (t, *J* 5.6, 3H, CH₃), 4.28 (q, *J* 5.6, 2H, CH₂), 7.22 (d, *J* 8.5, 2H, ArH), 7.45-7.49 (m, 3H, ArH), 7.53 (d, *J* 8.5, 2H, ArH), 7.65 (d, *J* 9.0, 1H, ArH), 8.38 (s, 1H, CH).



¹³C NMR (125 MHz, DMSO-*d*₆) for compound **(8b)**: δ _C 14.7, 60.3, 121.9, 127.3, 127.4, 127.5, 127.7, 128.3, 129.6, 129.8, 132.2, 132.7, 133.5, 136.2, 145.1, 162.4.



IR ν /cm⁻¹ (KBr) for compound **(8d)**: 1739 (C=O), 1592 (C=N) cm⁻¹.



¹H NMR (500 MHz, DMSO-*d*₆) for compound **(8d)**: δ _H 1.29 (t, *J* 5.6, 3H, CH₃), 2.34 (s, 3H, CH₃), 4.27 (q, *J* 5.6, 2H, CH₂), 7.22 (d, *J* 8.5, 2H, ArH), 7.27 (d, *J* 8.5, 2H, ArH), 7.32-7.37 (m, 5H, ArH), 8.11 (s, 1H, CH).