

Supporting Information

Novel one-pot pseudo four component reaction: expeditious synthesis of functionalized imidazo[1,2-*a*]pyridines

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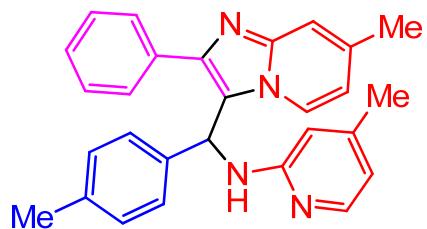
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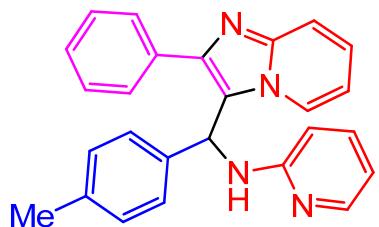
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4a

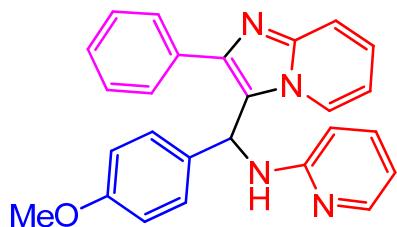
4-Methyl-N-((7-methyl-2-phenylH-imidazo[1,2-a]pyridin-3-yl)(*p*-tolyl)methyl)pyridin-2-amine (4a). Colorless crystal, mp 174-175 °C, 0.35 g, 85% yield, IR (KBr, cm⁻¹): 3250 (NH), 3053 (CH), 2908 (CH), 1438 & 1607 (CC of Ar). ¹H NMR (CDCl₃, 300 MHz): 1.97 (3 H, s, CH₃), 2.33 (3 H, s, CH₃), 2.36 (3 H, s, CH₃), 5.77 (1 H, s, NH), 6.04 (1 H, d, *J* = 5.9 Hz, CH of Ar), 6.21 (1 H, d, *J* = 6.8 Hz, CH of Ar), 6.31 (1 H, d, *J* = 5 Hz, CH of Ar), 6.45 (1 H, d, *J* = 5.9 Hz, CH of Ar), 7.14-7.67 (12 H, m, CHNH, CH of Ar). ¹³C NMR (CDCl₃, 100 MHz): δ = 22.2, 22.4, 52.6, 107.6, 115.50, 116.3, 117.2, 119.2, 125.4, 128.0, 129.1, 129.74, 130.0, 130.9, 135.7, 136.8, 138.8, 146.9, 148.7, 159.3. Anal. Calcd for C₂₈H₂₆N₄: C, 80.35; H, 6.26; N, 13.39. Found: C, 80.38; H, 6.23; N, 13.42.



4b

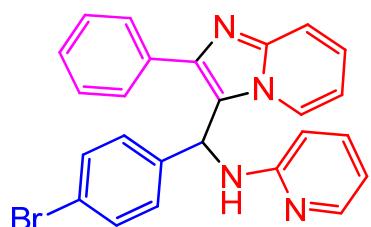
***N*-(2-phenylH-imidazo[1,2-a]pyridin-3-yl)(*p*-tolyl)methyl)pyridin-2-amine (4b).** White powder, mp 181-182 °C, 0.28 g, 73% yield, IR (KBr, cm⁻¹): 3254 (NH), 3025 (CH), 1602 and 1441 (CC of Ar). ¹H NMR (CDCl₃, 300 MHz): 2.33 (3 H, s, CH₃), 6.03 (1 H, d, *J* = 8

Hz, CH), 6.35-6.45 (3 H, m, CH of Ar, *CHNH*), 6.55 (1 H, d, *J* = 4.3 Hz, CH of Ar), 7.07-7.09 (14 H, m, CH of Ar). ^{13}C NMR (CDCl₃, 75 MHz): δ = 20.6, 51.1, 105.8, 111.4, 113.2, 117.1, 118.4, 124.08, 124.4, 126.4, 127.6, 128.1, 128.4, 129.3, 133.8, 135.0, 137.2, 137.2, 144.8, 147.5, 157.4. Anal. Calcd for C₂₆H₂₂N₄: C, 79.97; H, 5.68; N, 14.35. Found: C, 79.95; H, 5.67; N, 14.37.



4c

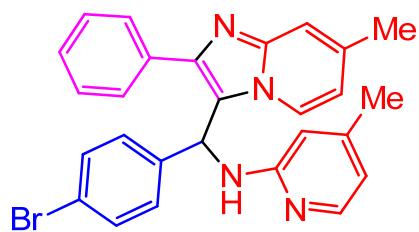
***N*-((4-methoxyphenyl)(2-phenyl*H*-imidazo[1,2-*a*]pyridin-3-yl)methyl)pyridin-2-amine(4c).** White powder, mp 188-189 °C, 0.30 g, 75% yield, IR (KBr): 3243 (NH), 3053 (CH), 2832 (CH), 1603 and 1441 (CC of Ar). ^1H NMR (Aceton-d₆, 300 MHz): δ = 3.80 (3H, s, CH₃), 6.56-8.14 (19 H, m, NH, *CHNH*, CH of Ar). ^{13}C NMR (Aceton-d₆, 75 MHz): δ = 50.3, 55.4, 109.3, 112.3, 113.8, 114.8, 114.9, 118.1, 121.1, 124.9, 126.4, 128.3, 128.4, 128.6, 129.0, 129.7, 130.5, 132.4, 136.1, 137.7, 148.6, 159.8. Anal. Calcd for C₂₆H₂₂N₄O: C, 76.83; H, 5.46; N, 13.78. Found: C, 76.85; H, 5.45; N, 13.79.



4d

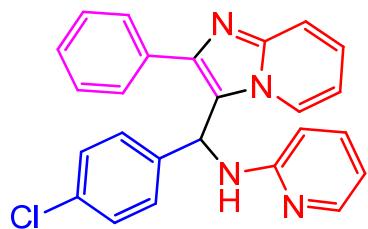
N-((4-bromophenyl)(2-phenyl*H*-imidazo[1,2-*a*]pyridin-3-yl)methyl)pyridin-2-amine(4d).

White powder, mp 190-191 °C, 0.31 g, 70% yield, IR (KBr): 3257(NH), 3049(CH), 1600 and 1441(CC of Ar). ¹H NMR (CDCl₃, 300 MHz): δ = 5.7 (1 H, s, NH), 6.16 (1H, s, CHNH), 6.59-6.65 (3 H, m, CH of Ar), 7.18-7.90 (14 H, m, CH of Ar). ¹³C NMR (CDCl₃, 75 MHz): δ = 51, 107.1, 112.4, 114.2, 117.9, 118.7, 121.7, 124.4, 124.8, 128.1, 128.5, 128.6, 128.8, 132.0, 134.0, 137.74, 137.9, 145.3, 145.4, 148.1, 157.4. Anal. Calcd for C₂₅H₁₉BrN₄: C, 65.94; H, 4.21; N, 12.30. Found: C, 65.95; H, 4.19; N, 12.32.



4e

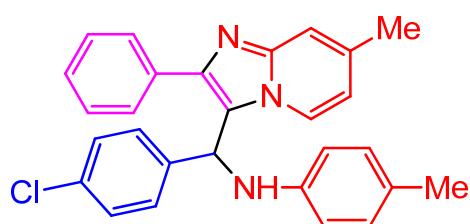
N-((2-(4-bromophenyl)-7-methyl*H*-imidazo[1,2-*a*]pyridin-3-yl)(phenyl)methyl)-4-methylpyridin-2-amine(4e). White powder, mp 170-171 °C, 0.37 g, 77% yield, IR (KBr): 3212(NH), 3086(CH), 2964(CH), 2910(CH), 1611 and 1448 (CC of Ar). ¹H NMR (CDCl₃, 300 MHz): δ = 2.00 (3 H, s, CH₃), 2.31 (3 H, s, CH₃), 5.83(1 H, s, NH), 6.13(1 H, s, CHNH), 6.33-6.49 (3 H, m, CH of Ar), 7.18-7.62(12 H, m, CH of Ar). ¹³C NMR (CDCl₃, 75 MHz): δ = 21.2, 51.0, 106.7, 114.3, 114.4, 115.4, 116.0, 117.5, 117.5, 123.7, 123.8, 128.7, 132.0, 132.0, 134.3, 134.3, 135.7, 135.7, 137.9, 144.6, 145.7, 147.4, 157.87. Anal. Calcd for C₂₇H₂₃BrN₄: C, 73.88; H, 5.28; N, 12.76. Found: C, 73.89; H, 5.25; N, 12.78.



4f

N-((4-chlorophenyl)(2-phenylH-imidazo[1,2-a]pyridin-3-yl)methyl)pyridin-2-amine(4f).

white powder, mp 199-200 °C, 0.32 g, 80 % yield, IR (KBr): 3255 (NH), 3114 (CH), 3050 (CH), 1601 and 1441 (CC of Ar). ¹H NMR (CDCl₃, 300 MHz): δ = 5.76 (1 H, s, NH), 6.15(1 H, d, *J* = 7.8 Hz, CH of Ar), 6.57-6.68 (3 H, m, CHNH, CH of Ar), 7.15-7.86(14 H, m, CH of Ar). ¹³C NMR (CDCl₃, 75 MHz): δ = 50.9, 107, 112.3, 114.2, 117.0, 118.7, 119.0, 124.4, 124.7, 128.1, 128.2, 128.6, 128.8, 129.1, 133.6, 134.0, 137.3, 137.7, 145.3, 148.1, 157.4. Anal. Calcd for C₂₅H₁₉ClN₄: C, 73.08; H, 4.66; N, 13.64. Found: C, 73.06; H, 4.68; N, 13.65.

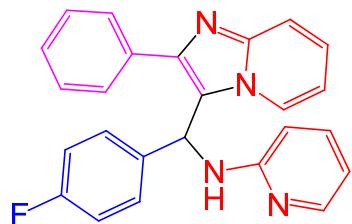


4g

N-((4-chlorophenyl)(7-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)methyl)-5-

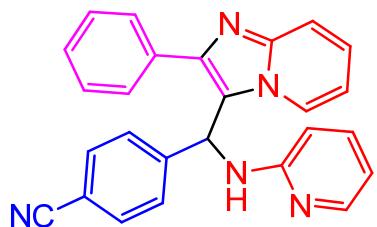
methylpyridin-2-amine (4g). White powder, mp 202-203 °C, 0.36 g, 83% yield, IR (KBr):

3212 (NH), 2965 (CH), 2910 (CH), 1610 and 1434 (CC of Ar). ^1H NMR (CDCl_3 , 300 MHz): δ = 2.04 (3 H, s, CH_3), 2.34 (3 H, s, CH_3), 5.85 (2 H, s, NH, CHNH), 6.30 (1 H, d, J = 6.7 Hz, CH of Ar), 6.39 (1 H, d, J = 4.7 Hz, CH of Ar), 6.54 (1 H, d, J = 5.8 Hz, CH of Ar), 7.27-7.68 (12 H, m, CH of Ar). ^{13}C NMR (CDCl_3 , 75 MHz): δ = 21.1, 21.3, 107.0, 114.8, 115.6, 116.2, 117.8, 123.7, 128.0, 128.3, 128.6, 128.8, 129.1, 133.6, 134.3, 135.8, 137.4, 145.2, 145.8, 147.6, 149.0, 157.7. Anal. Calcd for $\text{C}_{27}\text{H}_{23}\text{ClN}_4$: C, 73.88; H, 5.28; N, 12.76. Found: C, 73.85; H, 5.26; N, 12.78.



4h

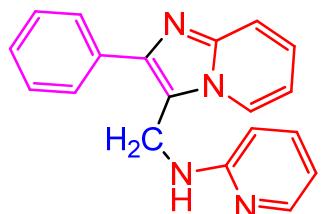
N-((4-fluorophenyl)(2-phenyl*H*-imidazo[1,2-*a*]pyridin-3-yl)methyl)pyridin-2-amine (4h).
White powder, mp 198-199 °C, 0.29 g, 75% yield, IR (KBr): 3251 (NH), 1602 and 1442 (CC of Ar). ^1H NMR (CDCl_3 , 300 MHz): δ = 5.59 (1 H, s, NH), 6.15 (1 H, d, J = 8.1 Hz, , CH of Ar), 6.62-6.69 (3 H, m, CHNH , CH of Ar), 7.00-7.96 (14 H, m, CH of Ar). ^{13}C NMR (CDCl_3 , 75 MHz): δ = 51.0, 76.6, 107.7, 112.3, 114.2, 115.7, 116.0, 117.9, 118.9, 119.0, 124.5, 124.7, 128.3 (d , $^2J_{\text{CF}}$ = 26.5 Hz), 128.6, 128.9, 134.2, 134.5, 137.8, 145.3, 148.1, 157.4, 162.6 (d , $^1J_{\text{CF}}$ = 257.0). Anal. Calcd for $\text{C}_{25}\text{H}_{19}\text{FN}_4$: C, 76.12; H, 4.86; N, 14.20. Found: C, 76.14; H, 4.85; N, 14.21.



4i

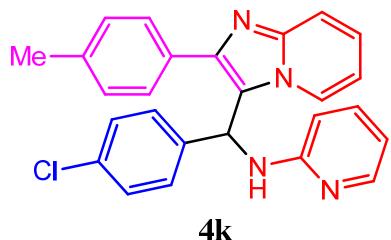
4-((2-phenylH-imidazo[1,2-a]pyridin-3-yl)(pyridin-2-ylamino)methyl)benzonitrile (4i).

Yellow powder, mp 199-200 °C, 0.39 g, 97% yield, IR (KBr): 3242 (NH), 3061 (CH), 3014 (CH), 1604 and 1474 (CC of Ar). ¹H NMR (CDCl₃, 300 MHz): δ = 5.55 (1 H, s, NH), 6.35 (1 H, s, CHNH), 6.66 (2 H, s, CH of Ar), 6.89 (1 H, s, CH of Ar), 7.18-8.01 (14 H, m, CH of Ar). ¹³C NMR (CDCl₃, 75 MHz): δ = 50.7, 107.9, 111.31, 112.7, 114.6, 118.0, 118.5, 124.0, 125.0, 127.6, 128.3, 128.5, 128.8, 132.5, 133.7, 137.7, 144.7, 145.2, 145.4, 148.2, 157.0. Anal. Calcd for C₂₆H₁₉N₅: C, 77.79; H, 4.77; N, 17.44. Found: C, 77.77; H, 4.75; N, 17.41.



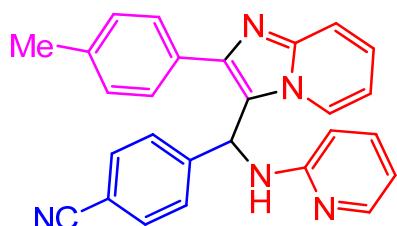
4j

N-((2-phenylH-imidazo[1,2-a]pyridin-3-yl)methyl)pyridin-2-amine(4j). White powder, mp 178-179 °C, 0.23 g, 78% yield, IR(KBr): 3248(NH), 3020(CH). ¹H NMR (CDCl₃, 400 MHz): δ = 4.62 (1 H, s, NH), 5.03 (2 H, s, CH₂NH), 6.35 (1H, d, *J* = 3.6 Hz, CH of Ar), 6.46 (1 H, s, CH), 6.67 (1 H, s, CH of Ar), 6.82 (1 H, s, CH of Ar), 6.95-8.42 (9 H, m, CH of Ar). ¹³C NMR (CDCl₃, 75 MHz): 35.5, 108.3, 112.4, 113.6, 117.0, 117.4, 124.3, 124.8, 127.9, 128.4, 128.7, 134.0, 137.4, 144.6, 145.1, 148.0, 158.1. Anal. Calcd for C₁₉H₁₆N₄: C, 75.98; H, 5.37; N, 18.65. Found: C, 75.96; H, 5.38; N, 18.63.



***N*-(4-chlorophenyl)(2-(*p*-tolyl)imidazo[1,2-a]pyridin-3-yl)methyl)pyridin-2-amine (4k).**

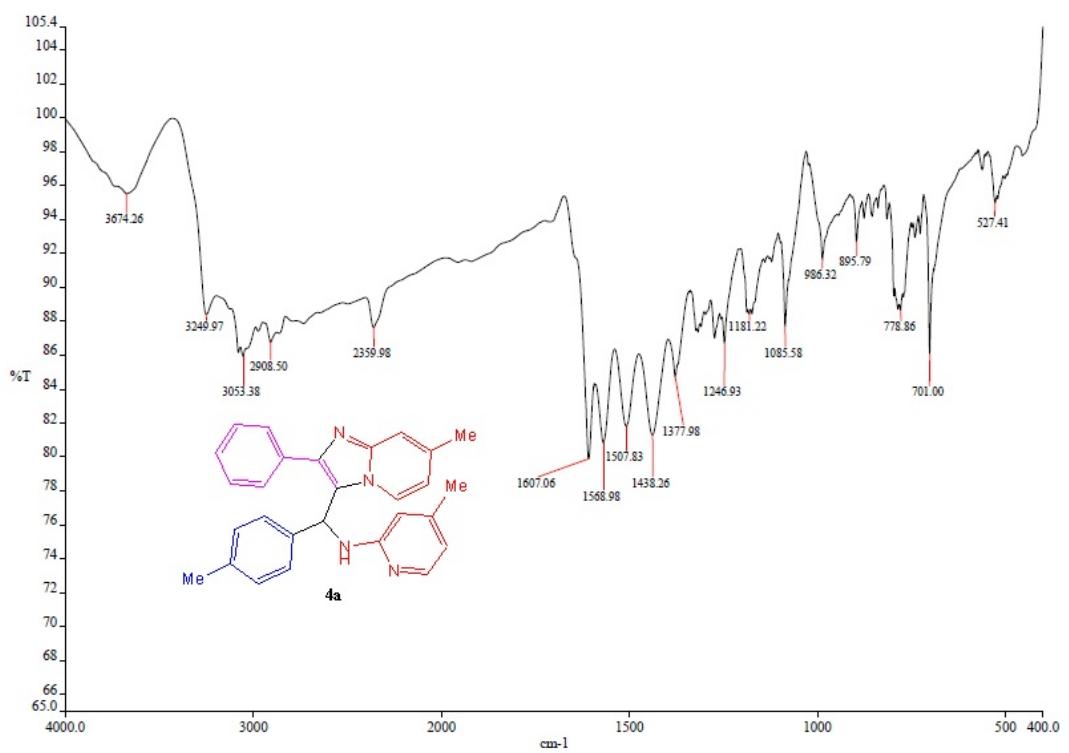
White powder, mp 170-171 °C, 0.35 g, 84 % yield, IR(KBr): 3244(NH), 3095(CH), 3029(CH), 1600 and 1478(CC of Ar). ¹H NMR (CDCl₃, 300 MHz): δ = 2.42 (3H, s, CH₃), 5.37 (1H, s, NH), 6.23(1H, s, CHNH), 6.68(2H, s, CH of Ar), 7.3-8.0 (14H, m, CH of Ar). ¹³C NMR (CDCl₃, 75 MHz): δ = 21.3, 51.0, 107.7, 112.7, 114.1, 117.7, 124.7, 125.2, 128.2, 128.7, 128.8, 129.3, 129.5, 130.7, 134.0, 137.3, 139.7, 143.0, 145.3, 148.8, 145.2, 148.0. Anal. Calcd for C₂₆H₂₁ClN₄: C, 73.49; H, 4.98; N, 13.19. Found: C, 73.47; H, 4.97; N, 13.17.



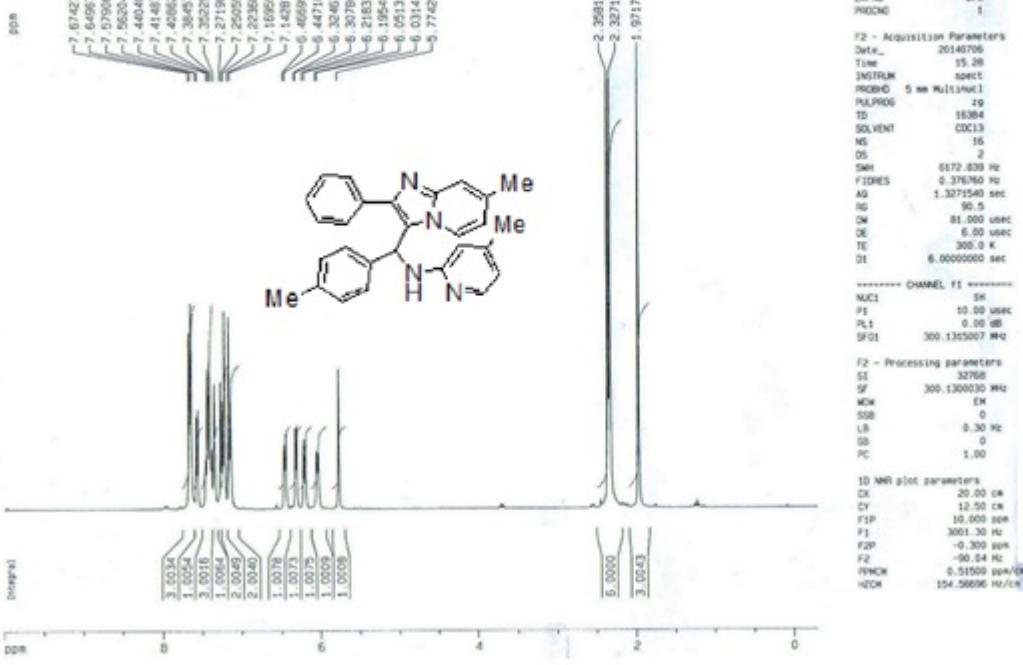
4l

4-((pyridin-2-ylamino)(2-(*p*-tolyl)imidazo[1,2-a]pyridin-3-yl)methyl)benzonitrile (4l).

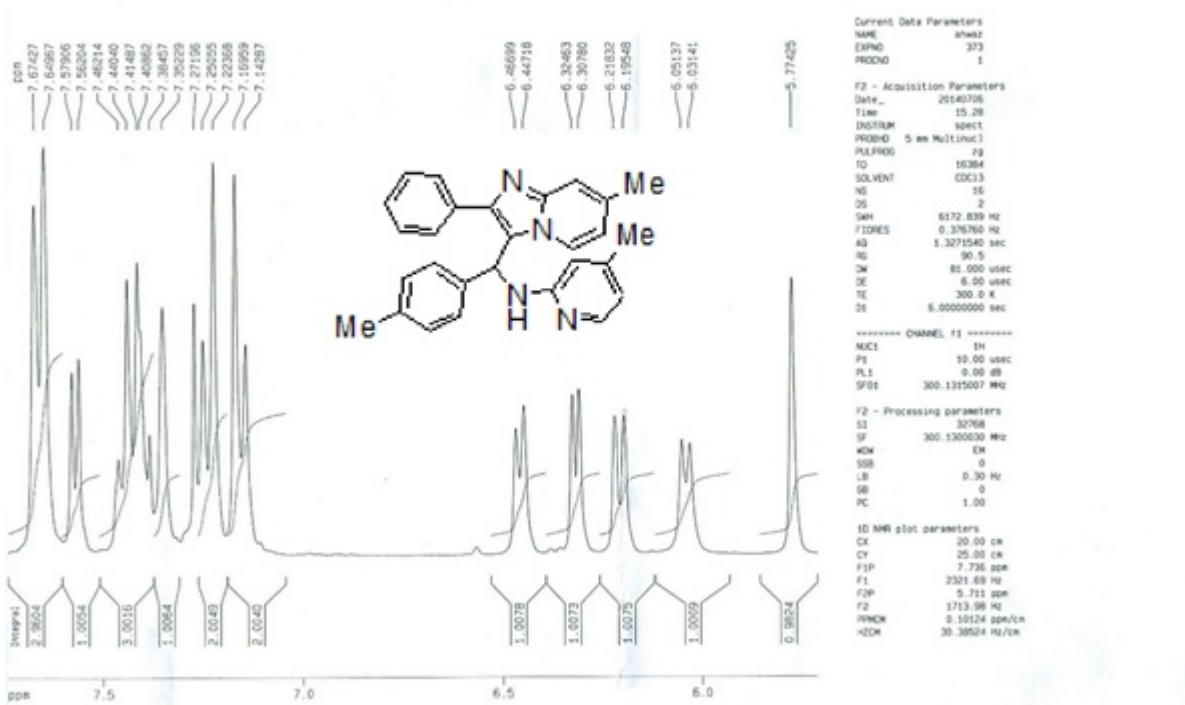
White powder, mp 187-188 °C, 0.41 g, 96% yield, IR (KBr): 3237(NH), 3088(CH), 3028(CH), 2225(CN), 1598 and 1474(CC of Ar). ¹H NMR (CDCl₃, 300 MHz): δ = 2.39 (3H, s, CH₃), 6.28 (2H, s, NH, CHNH), 6.44-8.05 (16H, m, CH of Ar). ¹³C NMR (CDCl₃, 75 MHz): δ = 21.3, 57.0, 114.1, 115.7, 119.8, 119.9, 122.0, 123.8, 124.4, 125.0, 126.4, 126.3, 126.6, 126.7, 133.4, 134.7, 136.6, 140.6, 141.7, 142.1, 143.7, 143.7, 153.0. Anal. Calcd for C₂₇H₂₁N₅: C, 78.05; H, 5.09; N, 16.86. Found: C, 78.06; H, 5.07; N, 16.84.



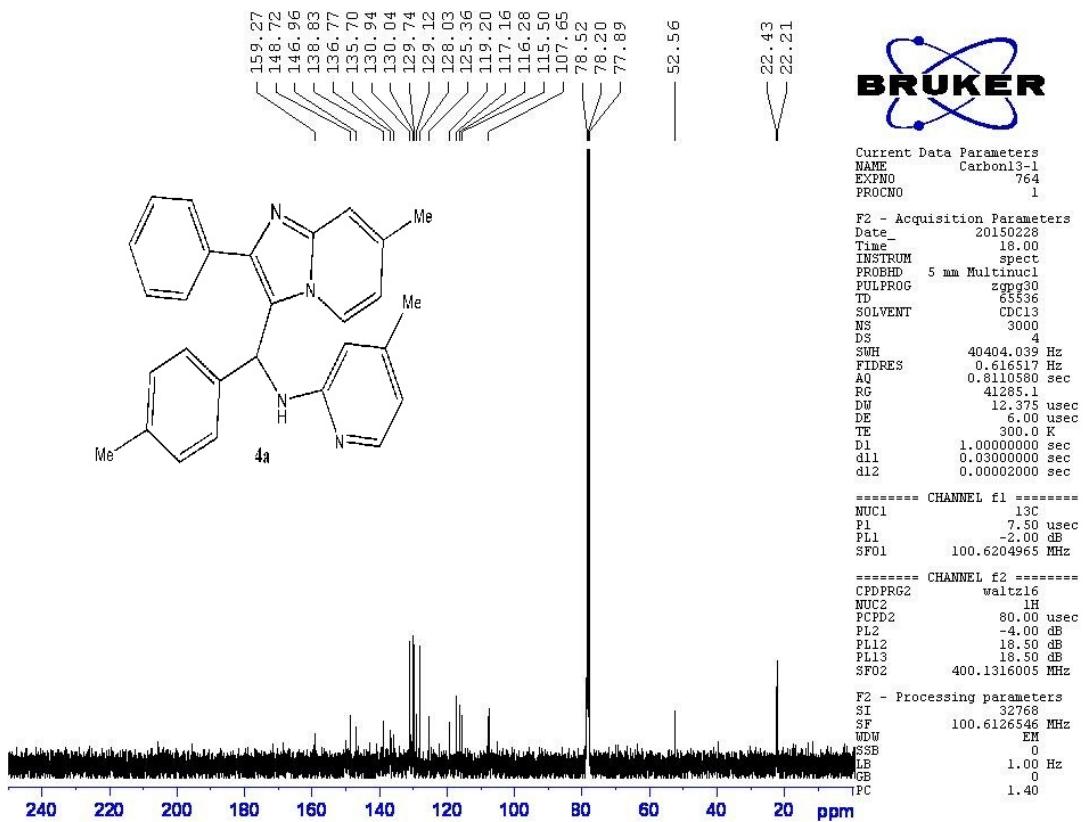
IR of **4a**



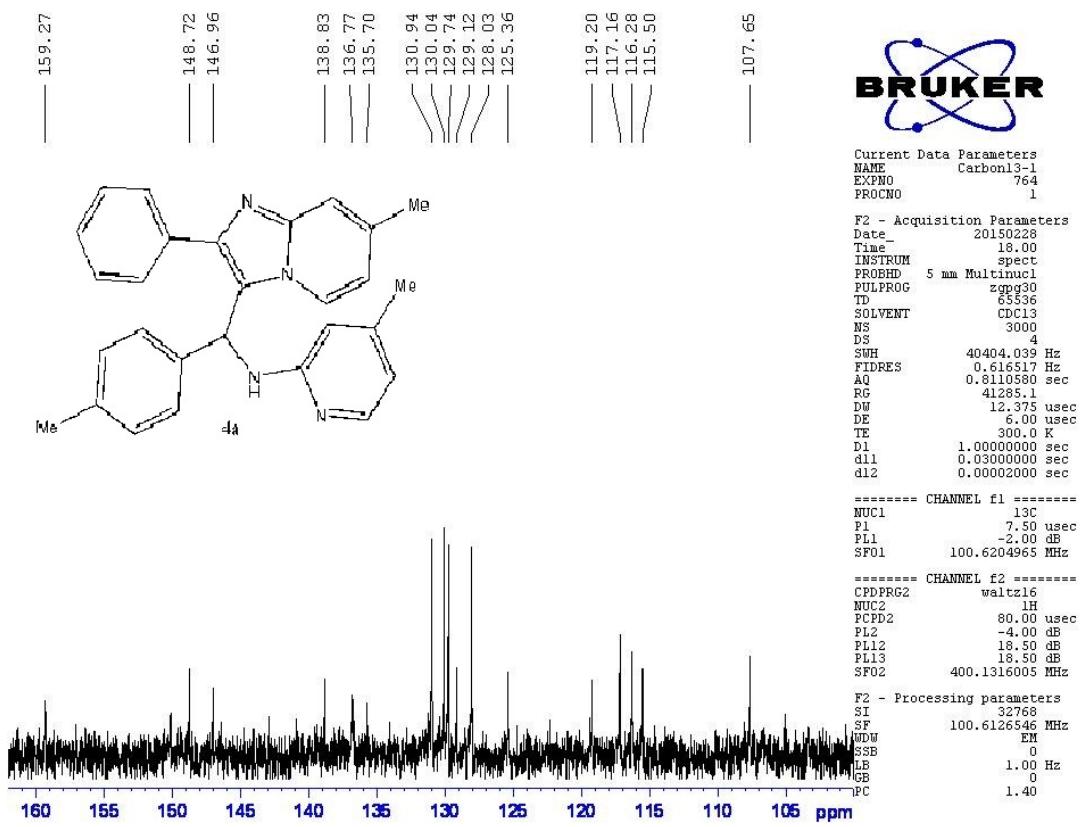
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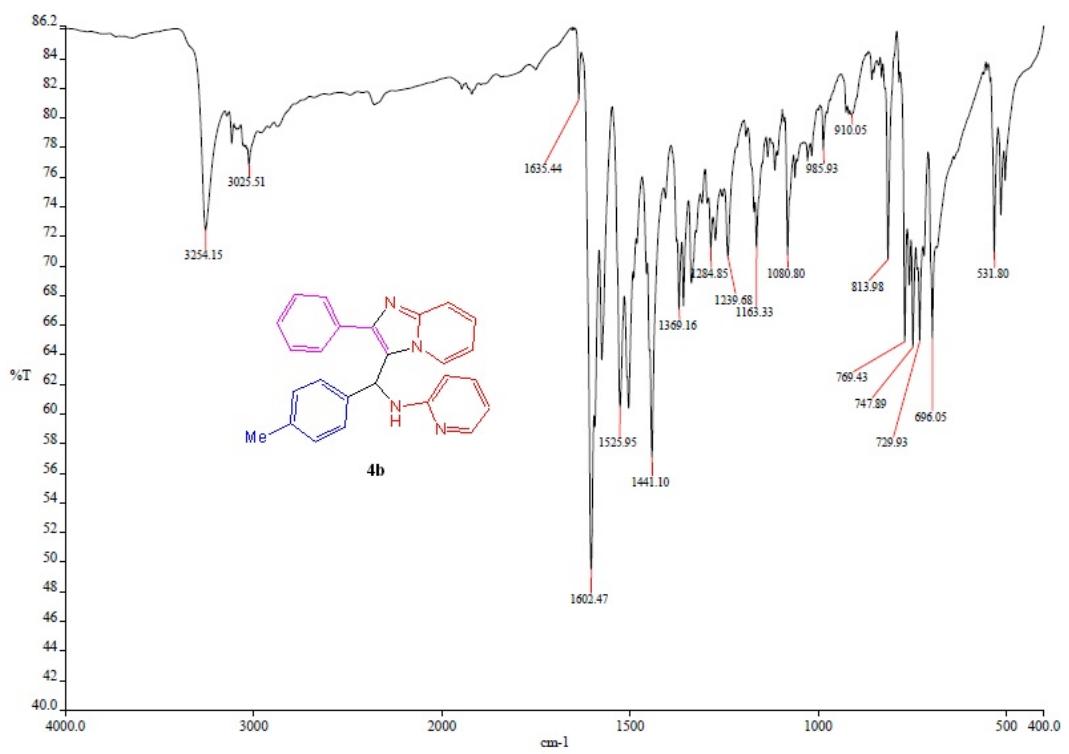
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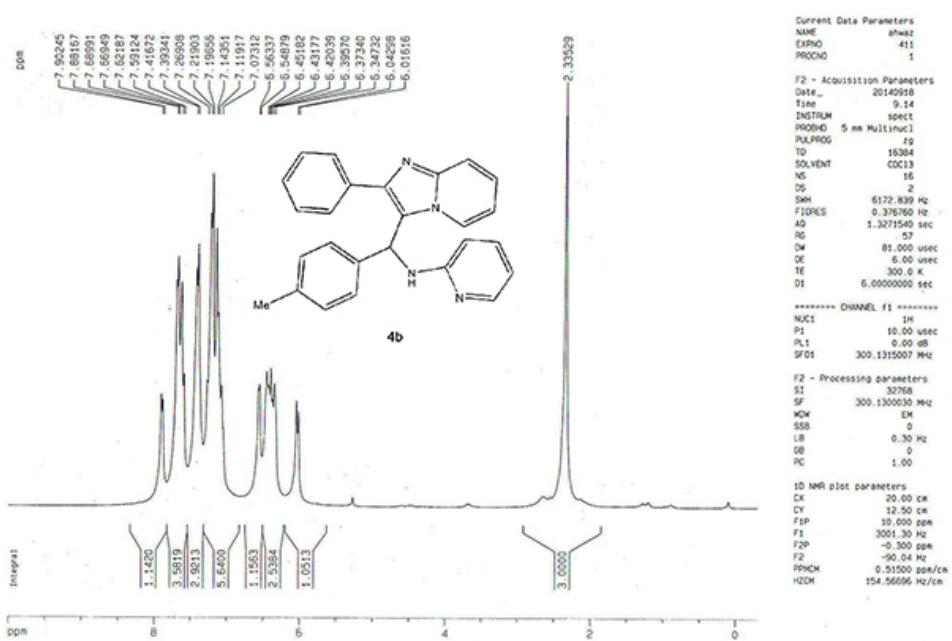
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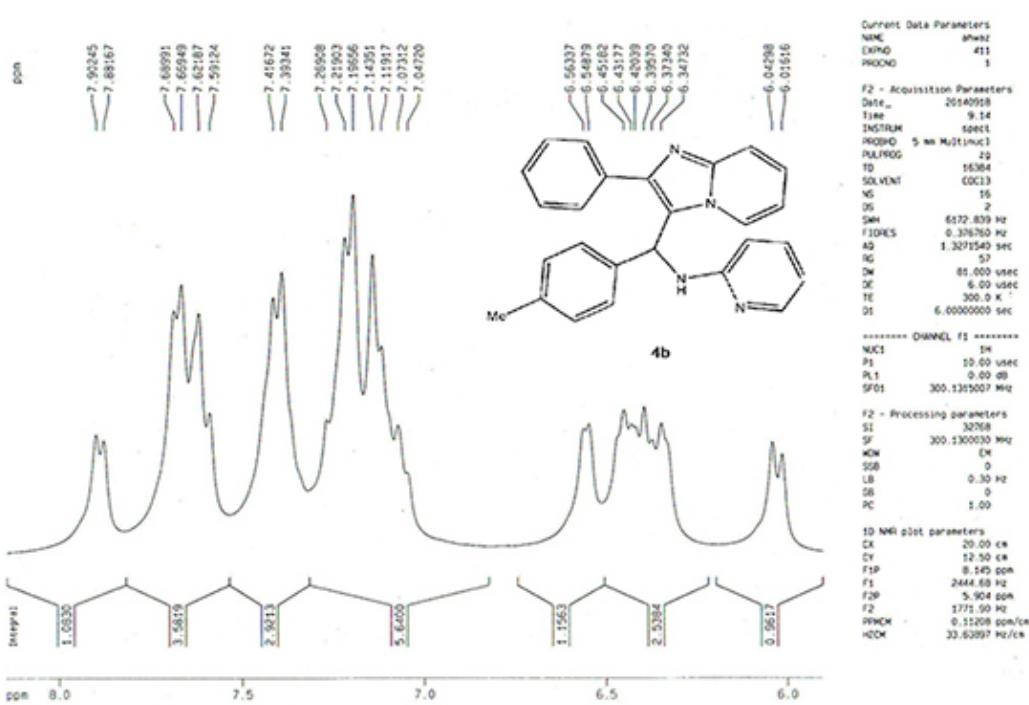
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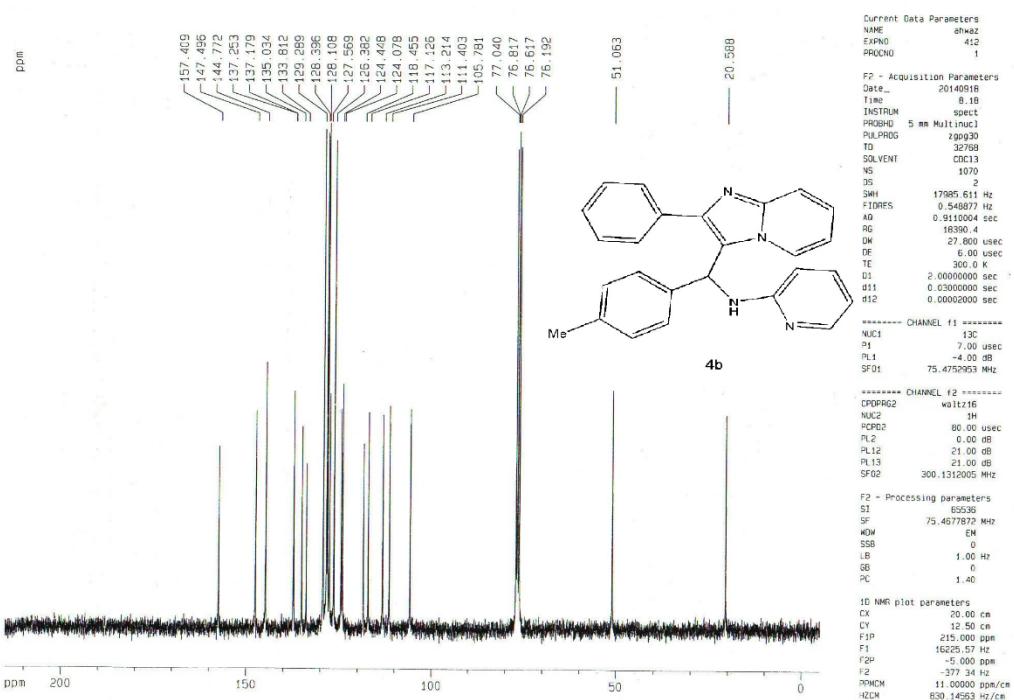
IR of **4b**



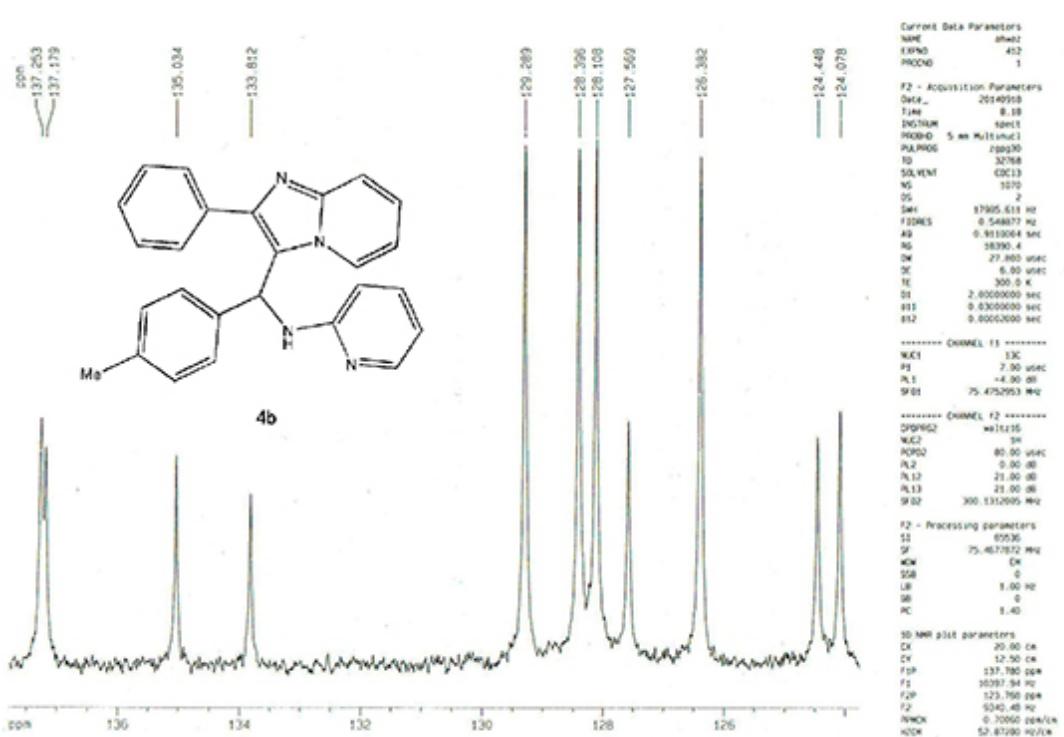
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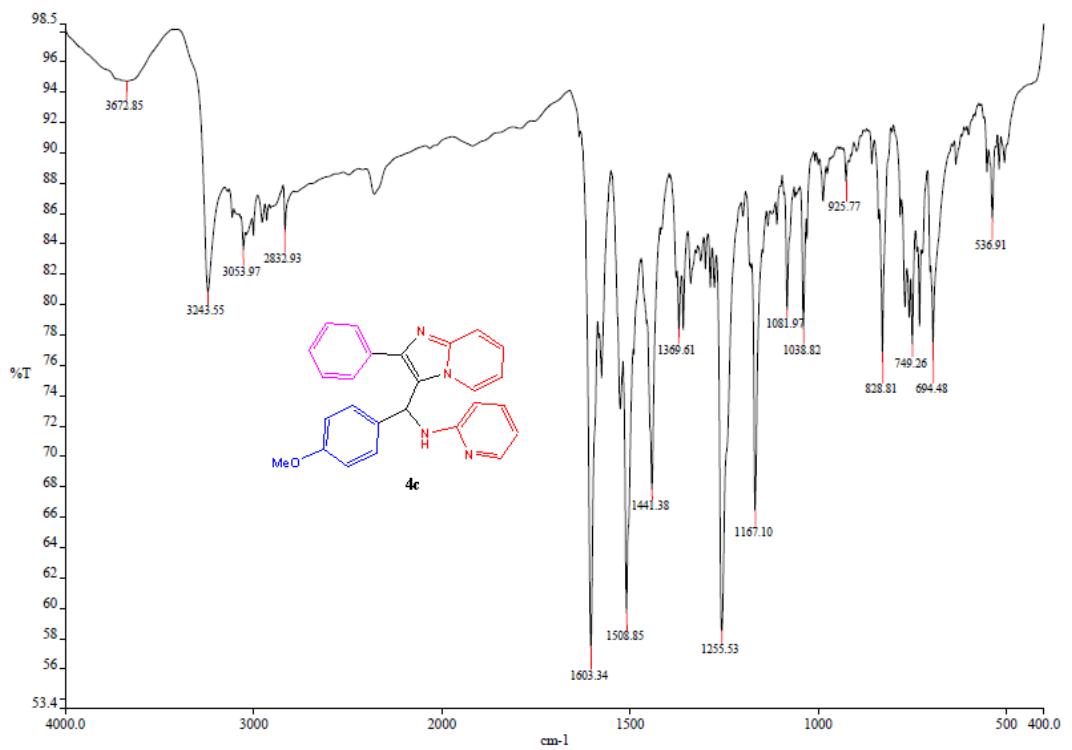
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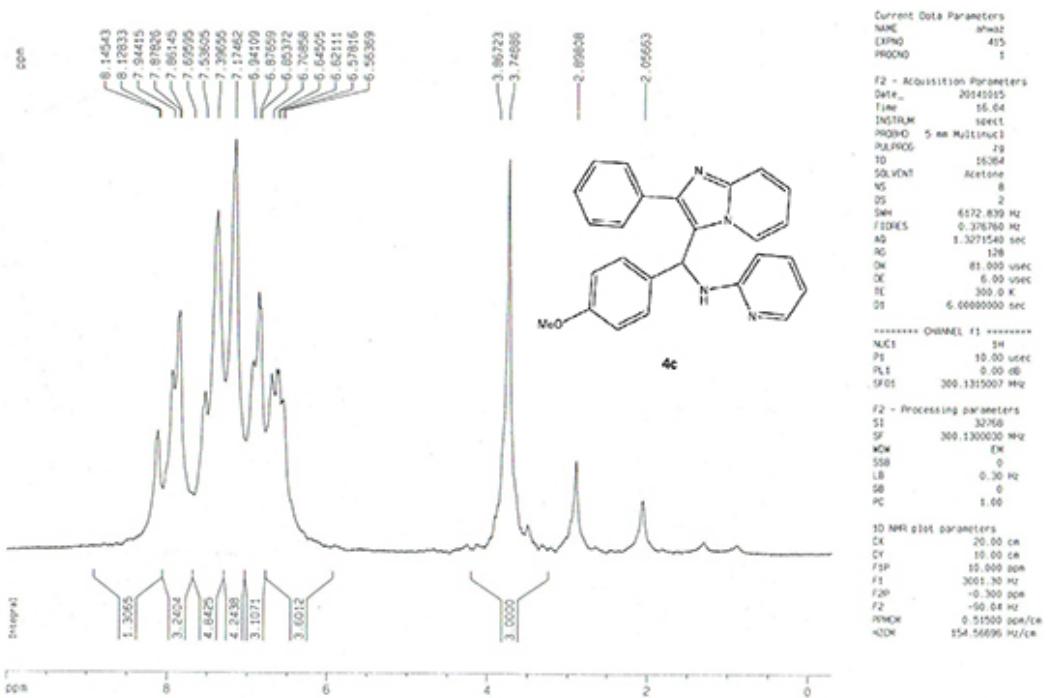
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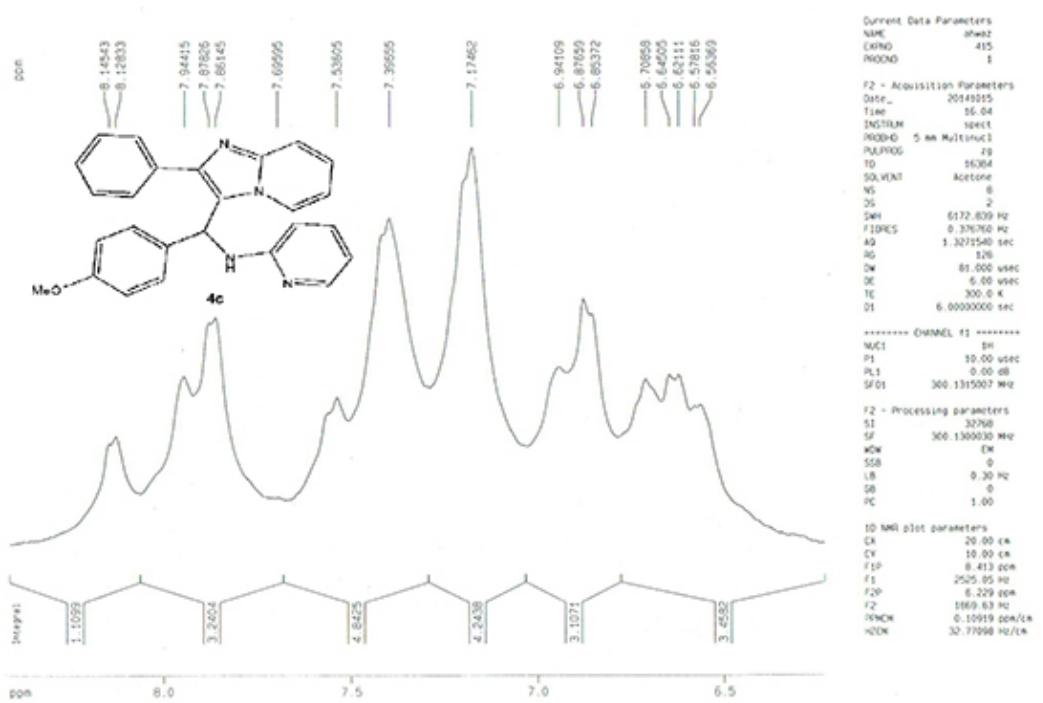
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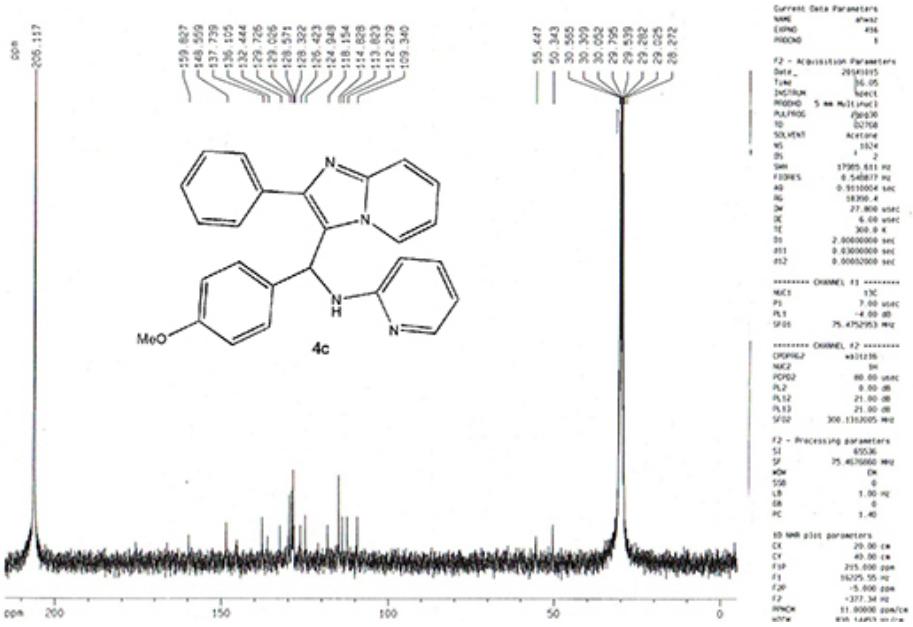
IR of **4c**



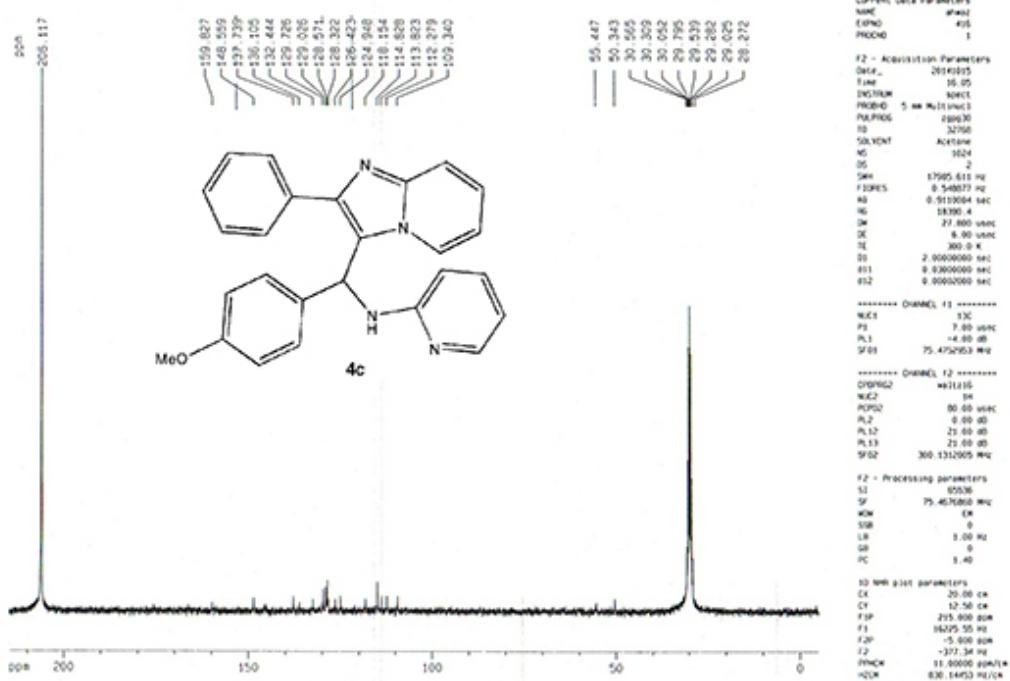
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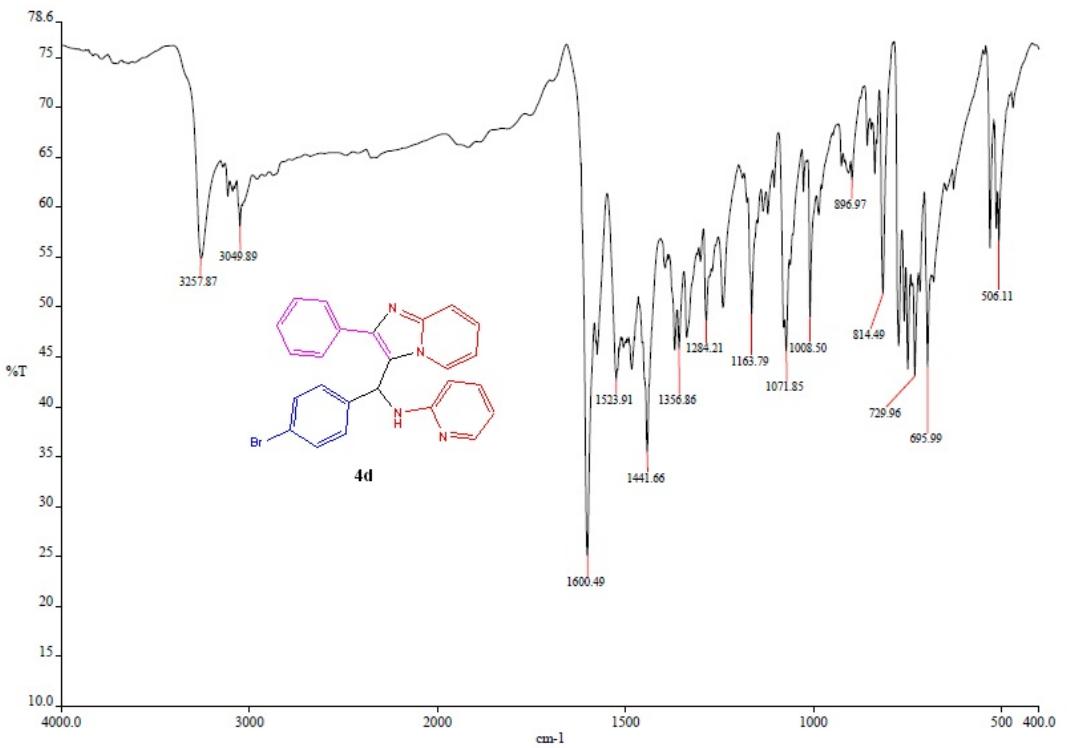
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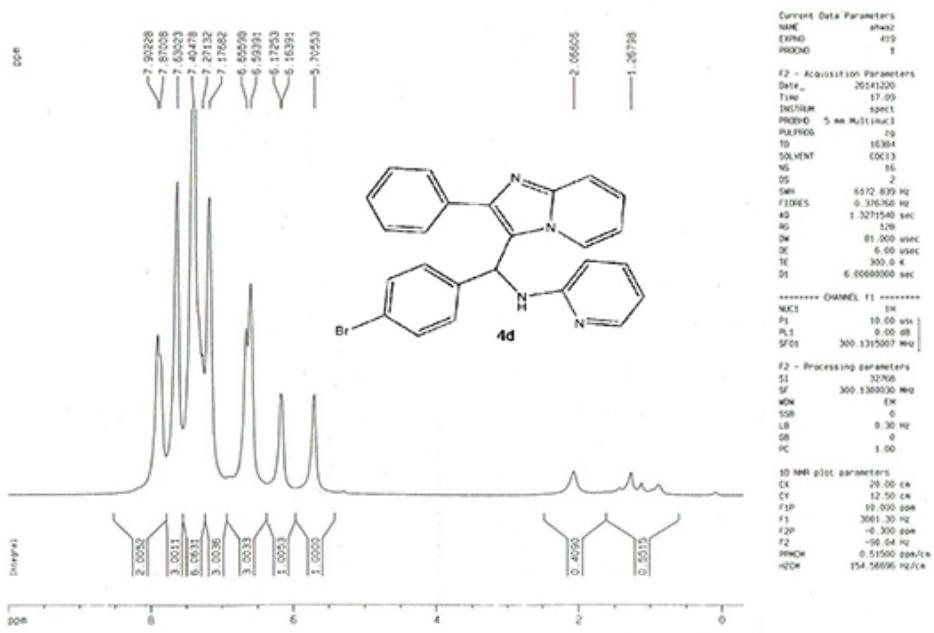
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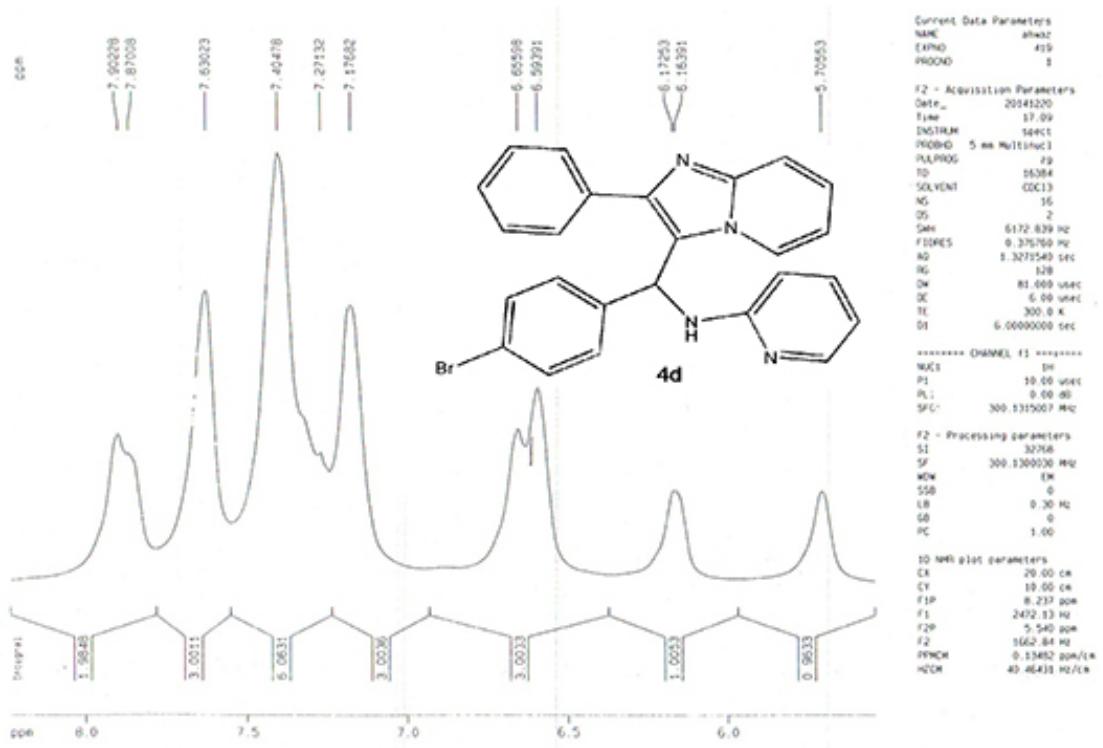
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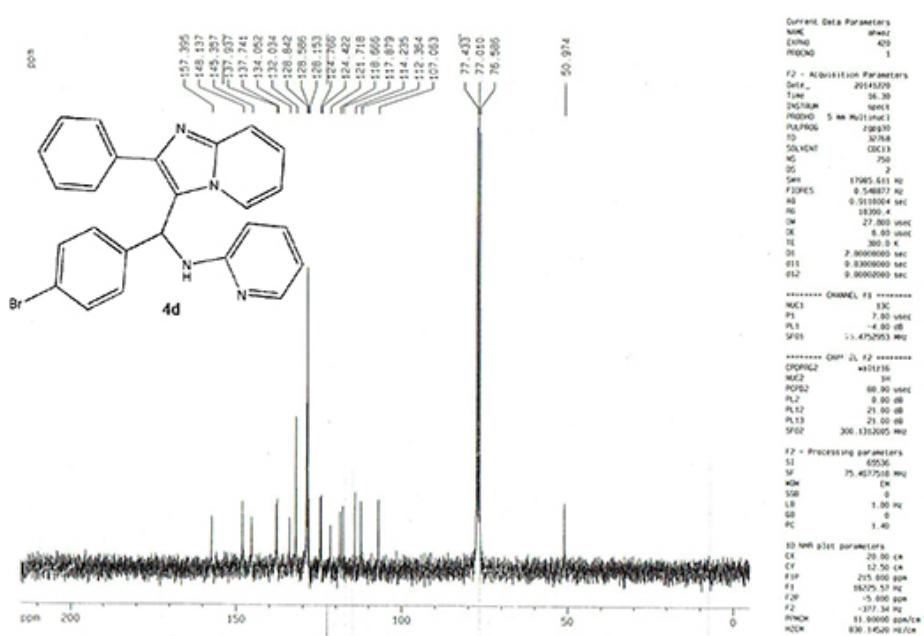
IR of **4d**



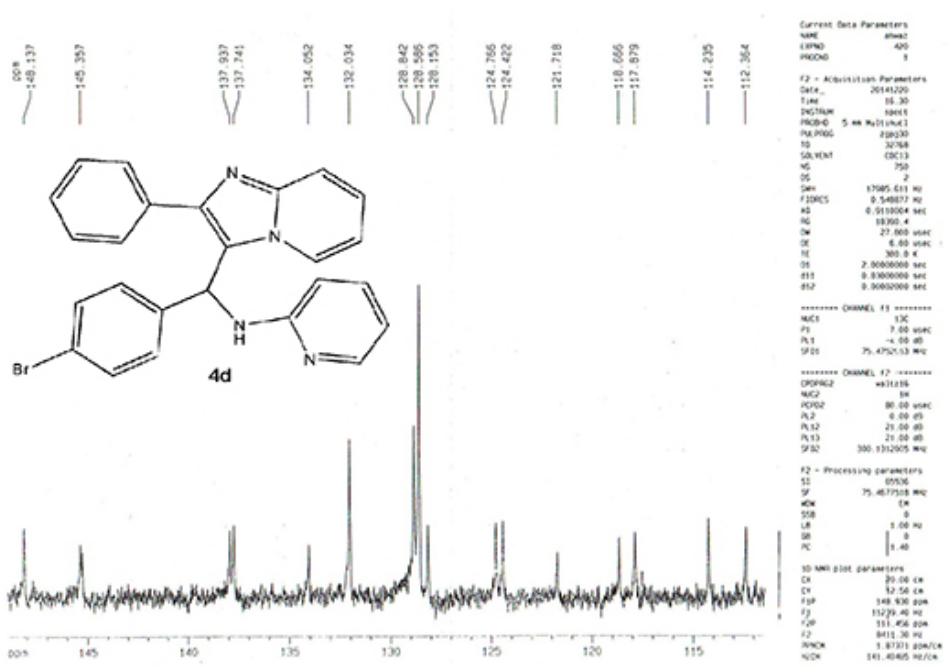
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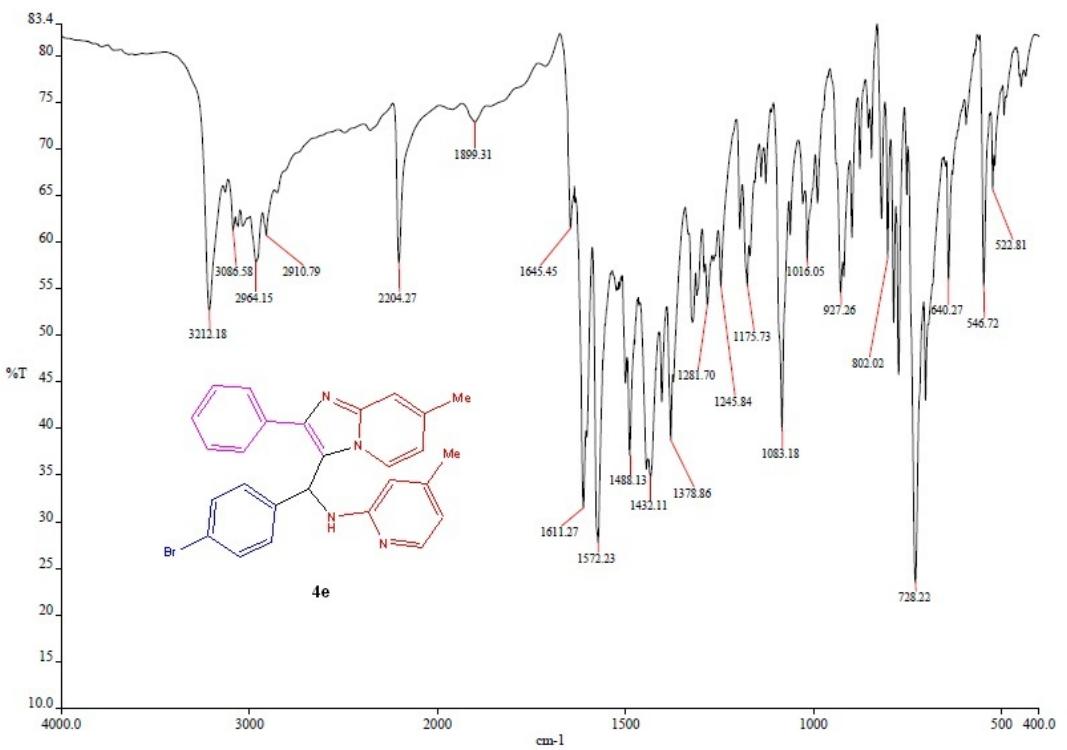
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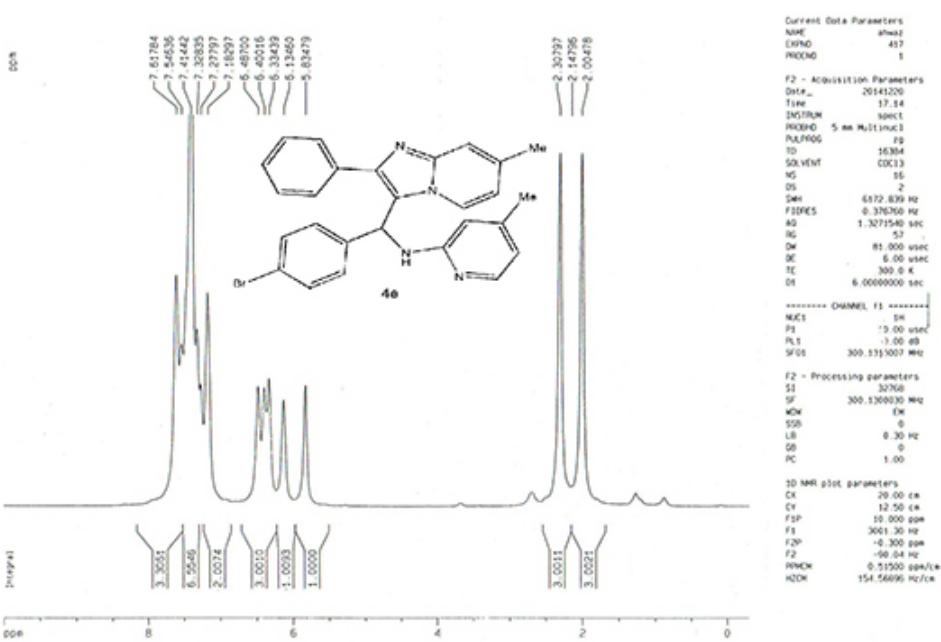
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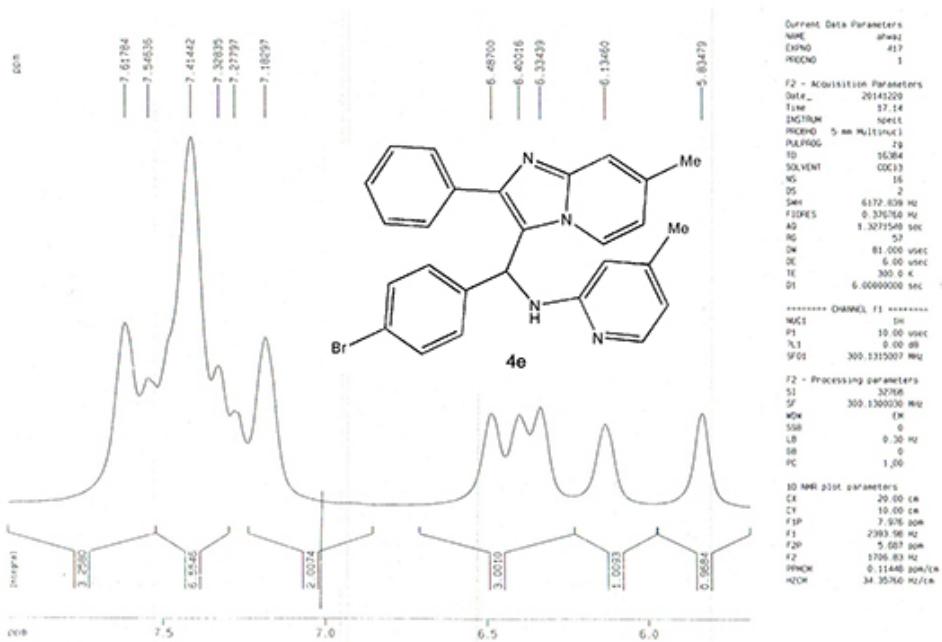
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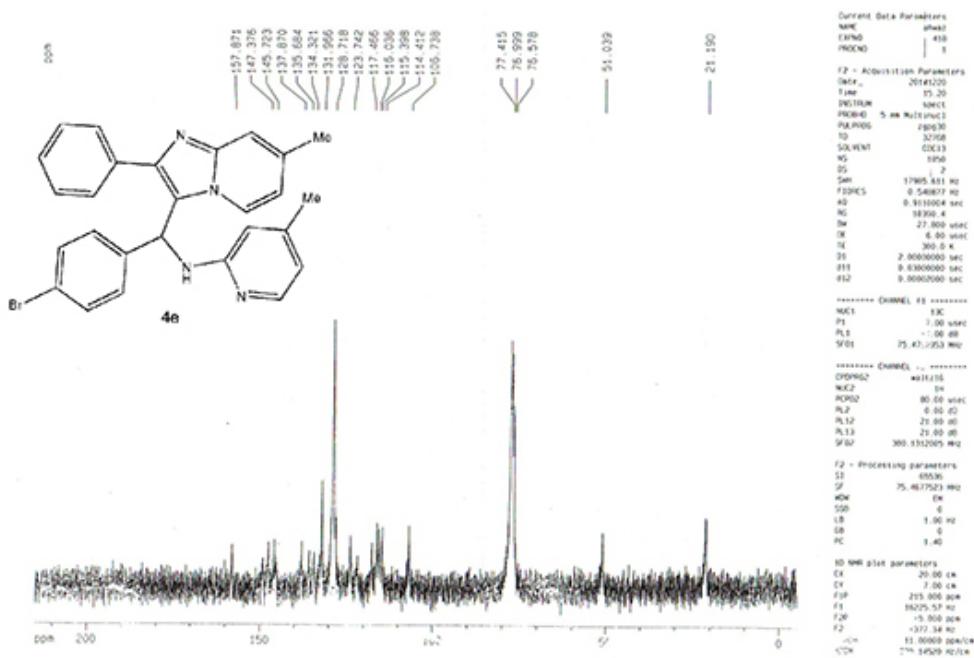
IR of **4e**



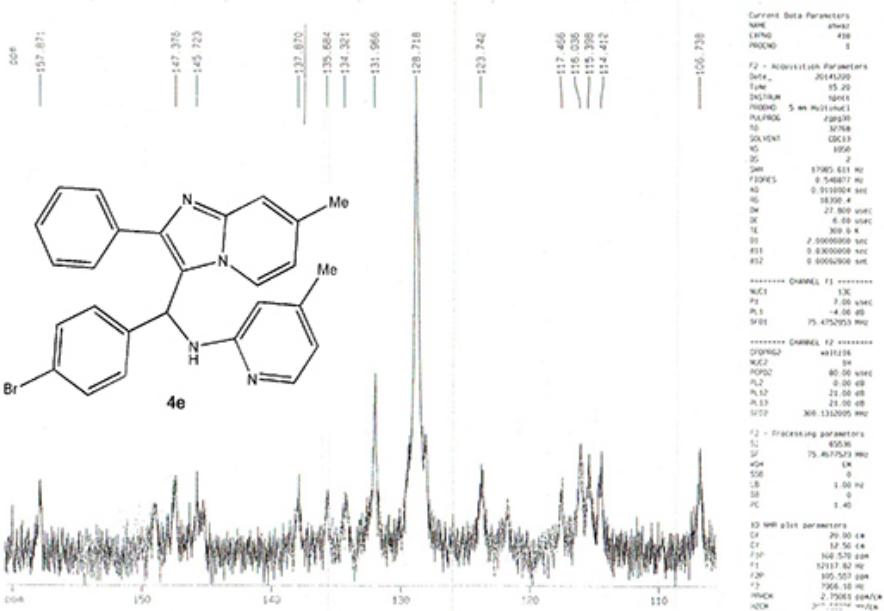
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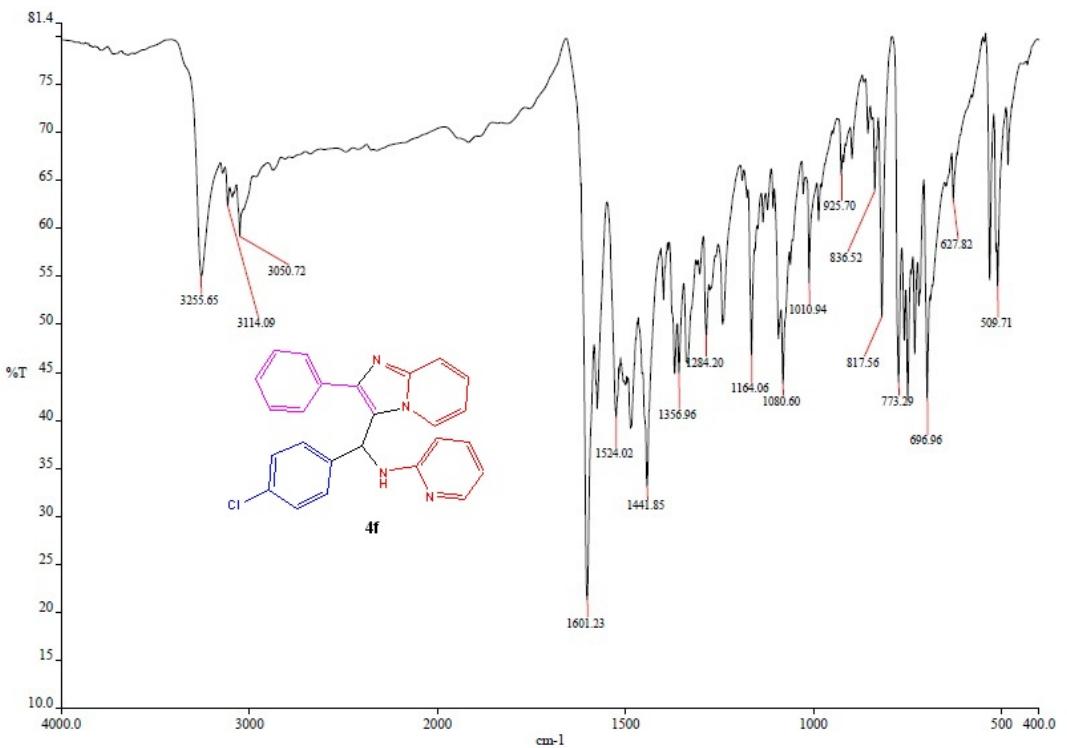
¹H-NMR of 4e



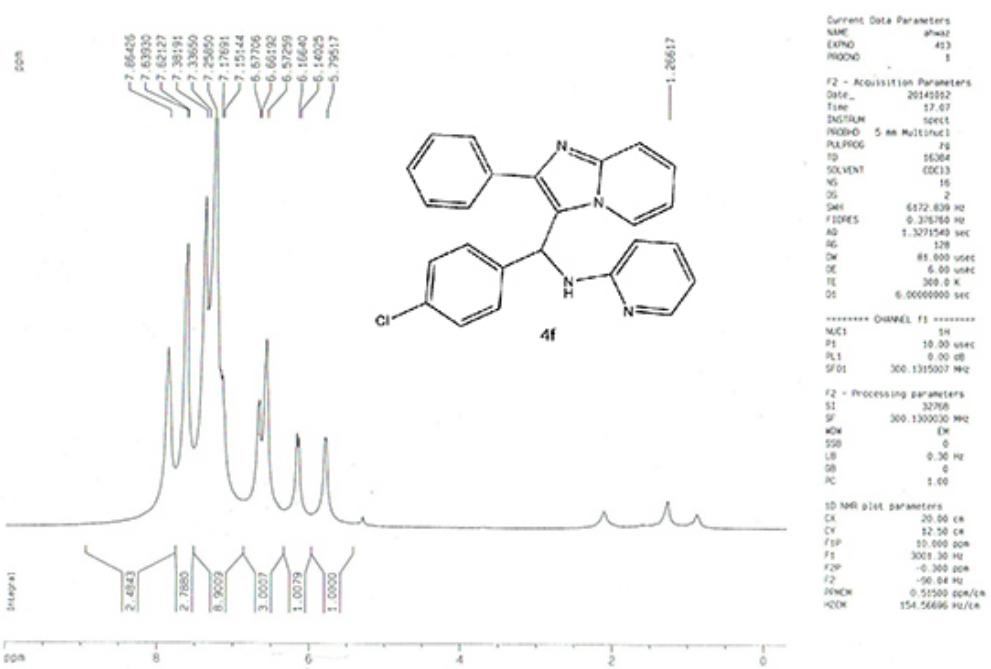
¹³C-NMR of 4e



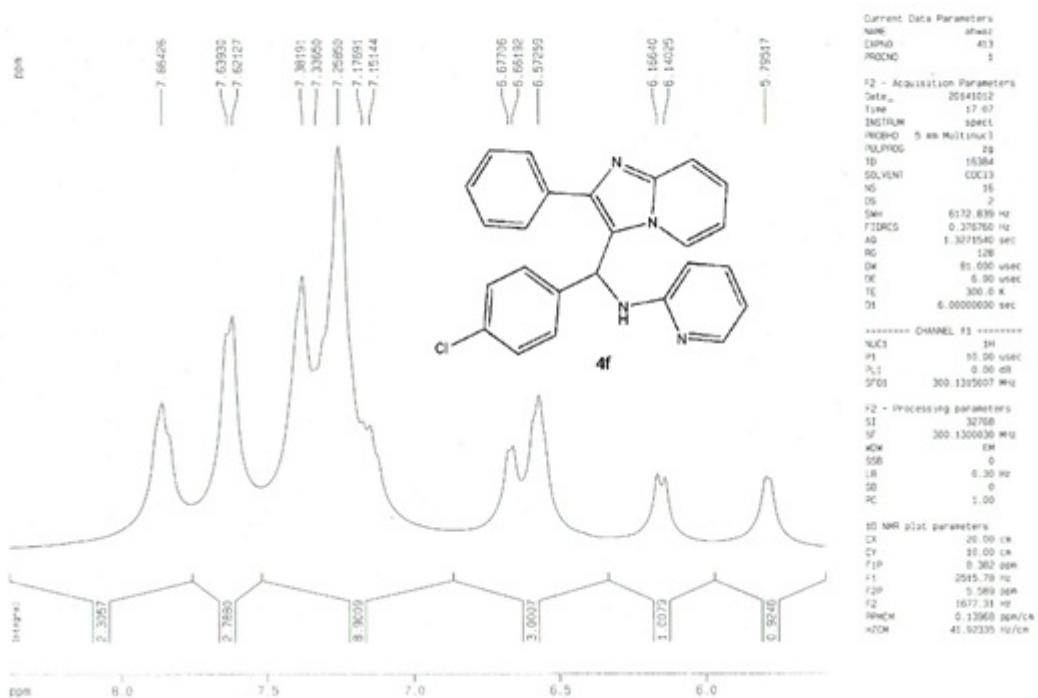
¹³C-NMR of 4e



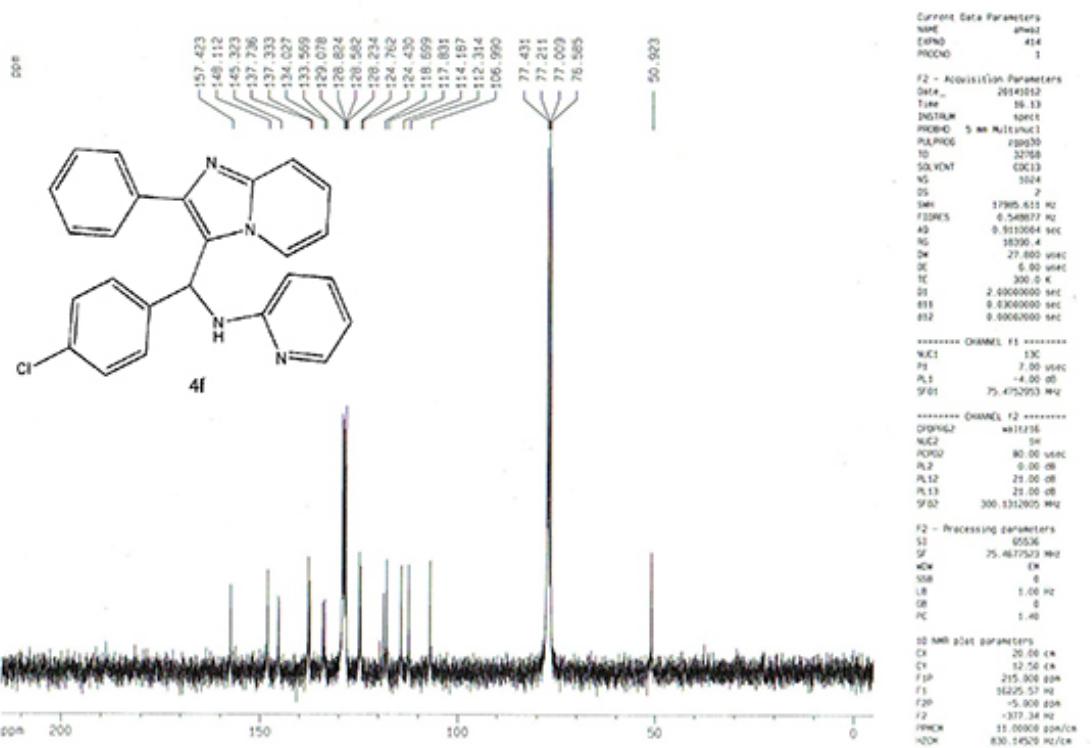
IR of **4f**



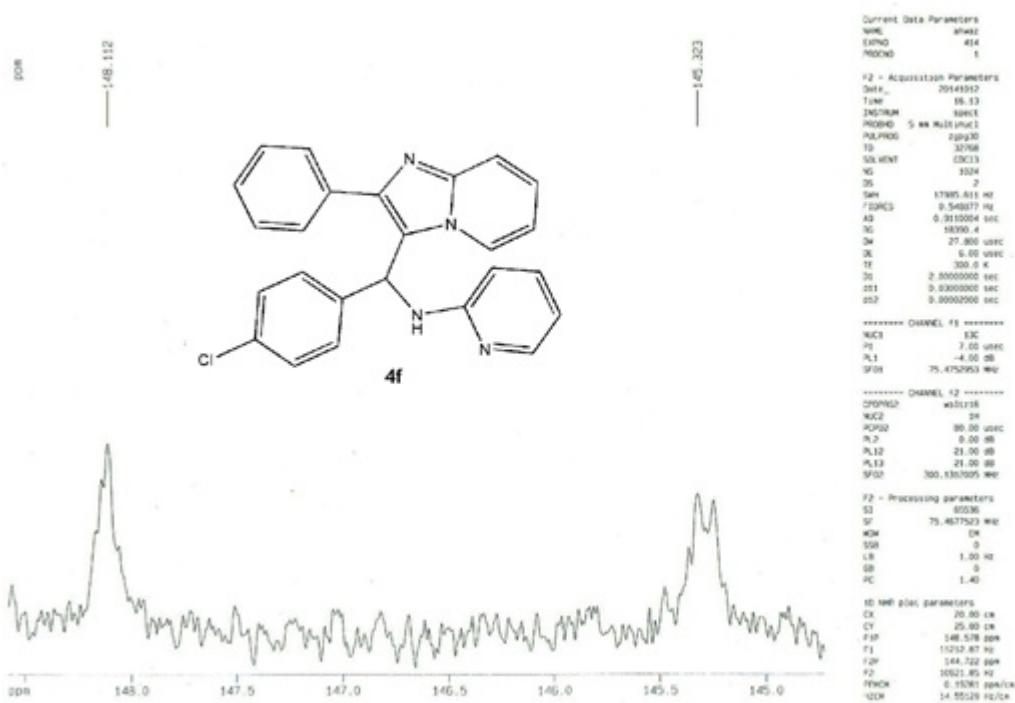
¹H-NMR of 4f



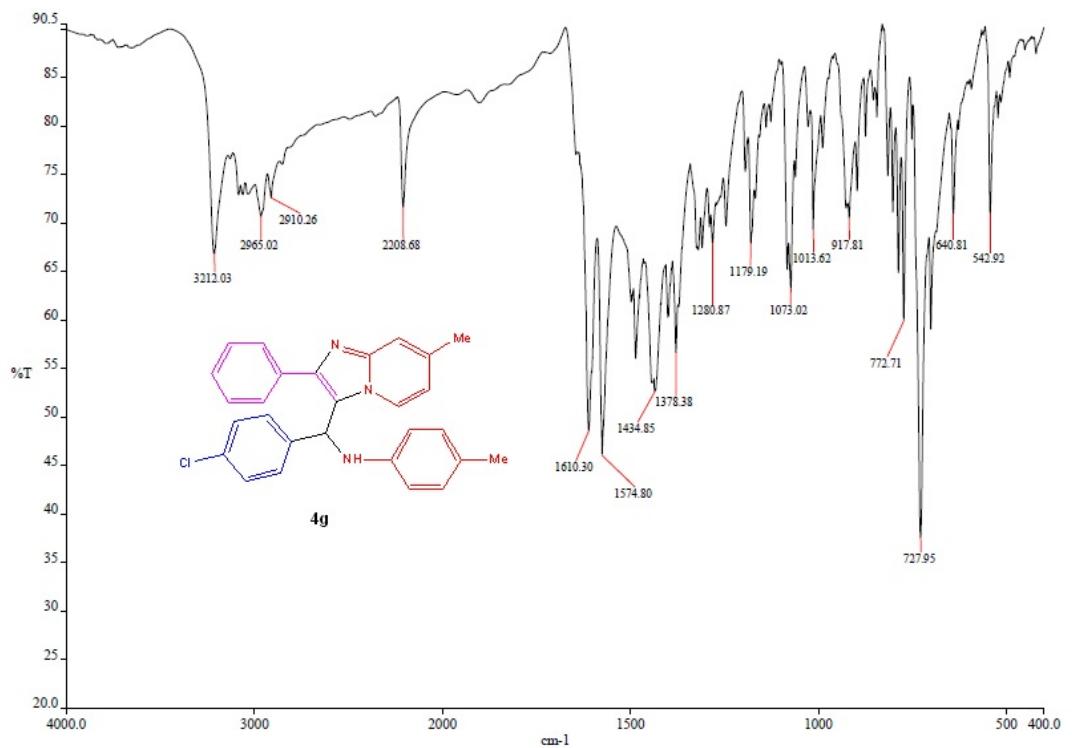
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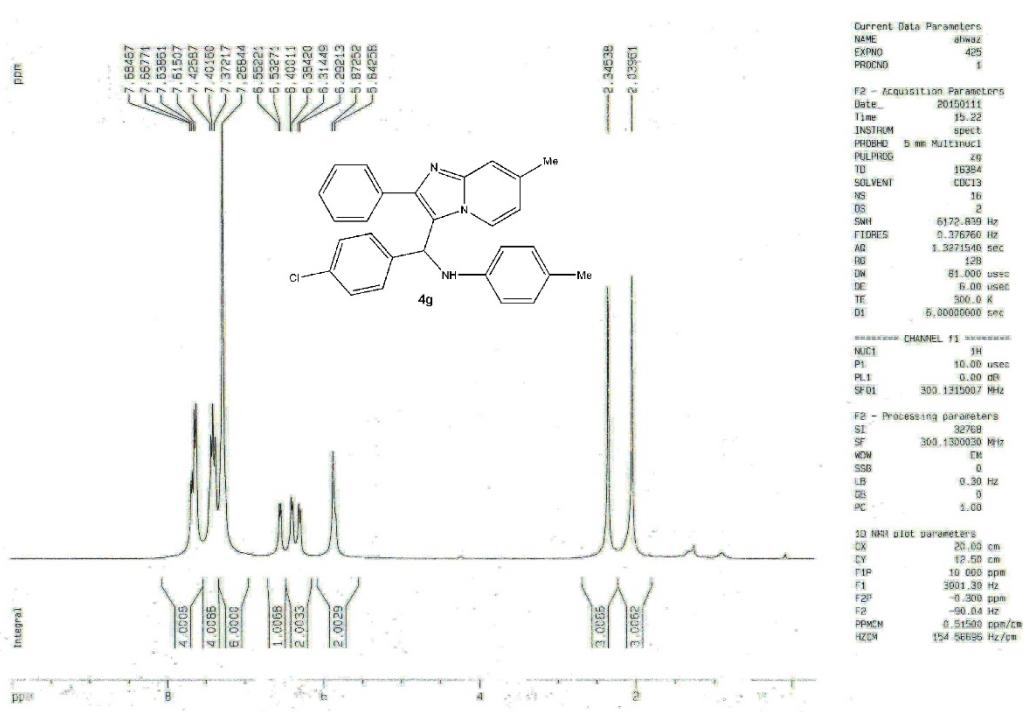
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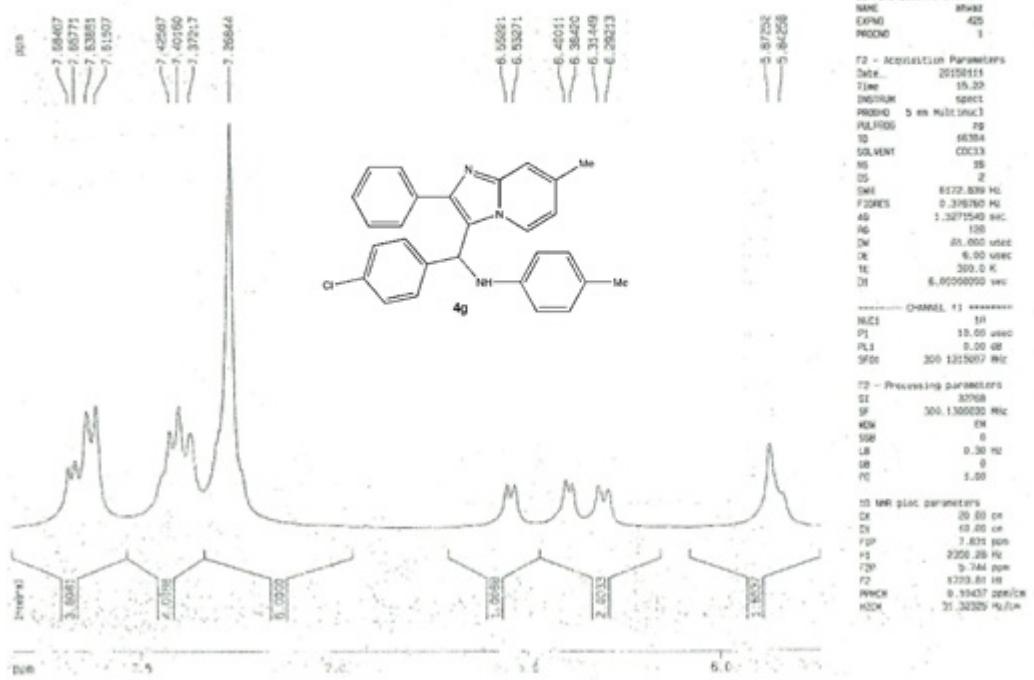
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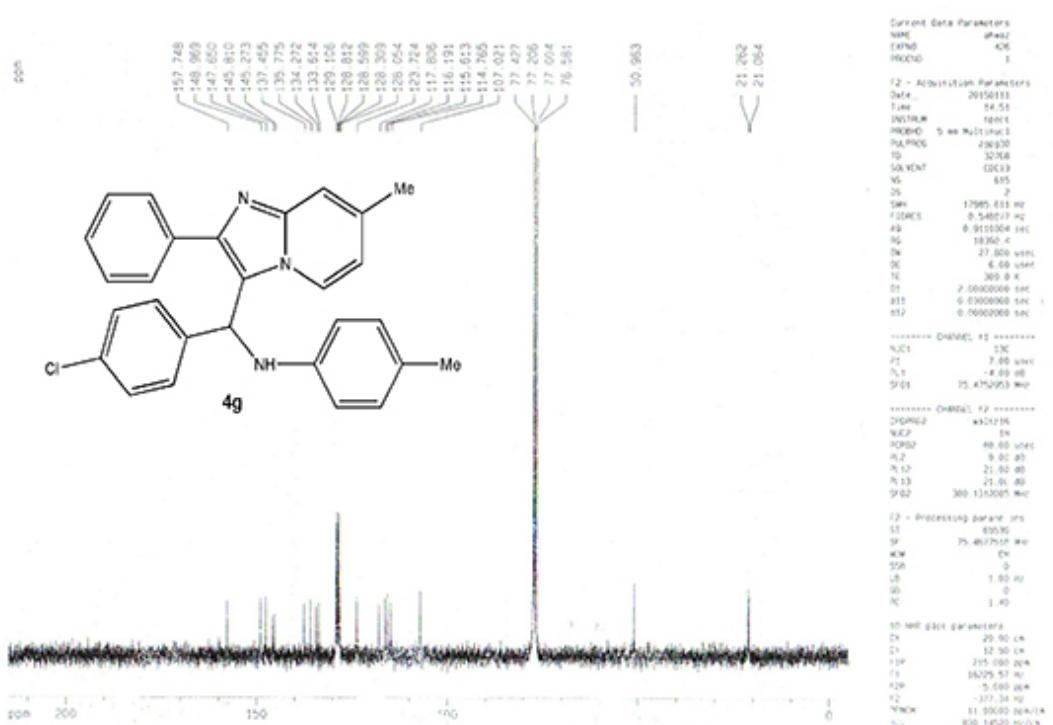
IR of **4g**



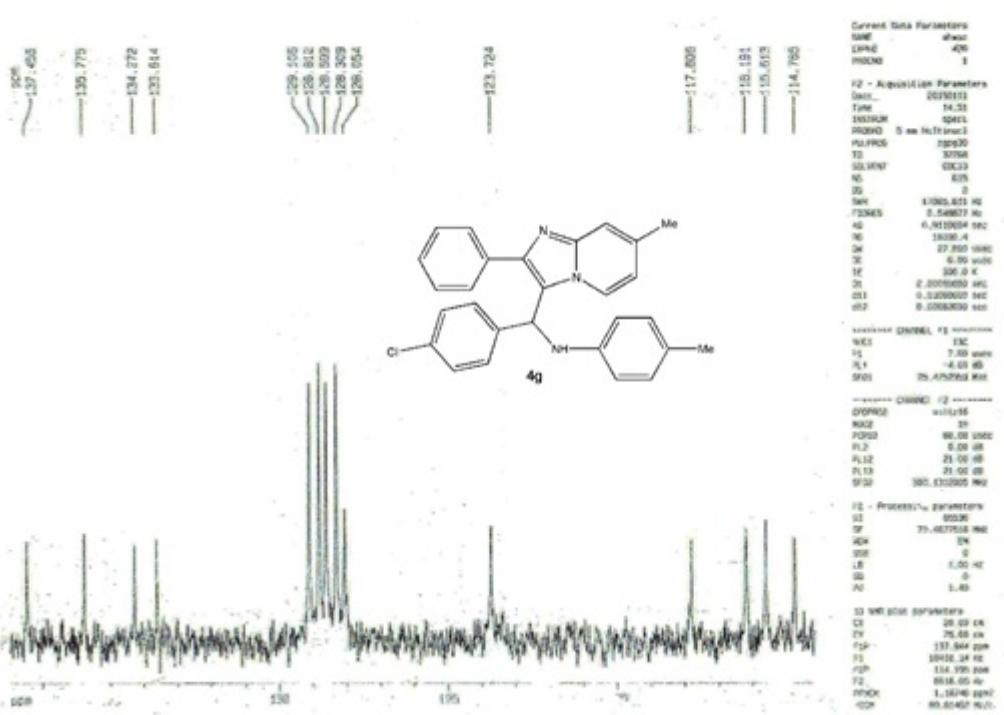
¹H-NMR of 4g



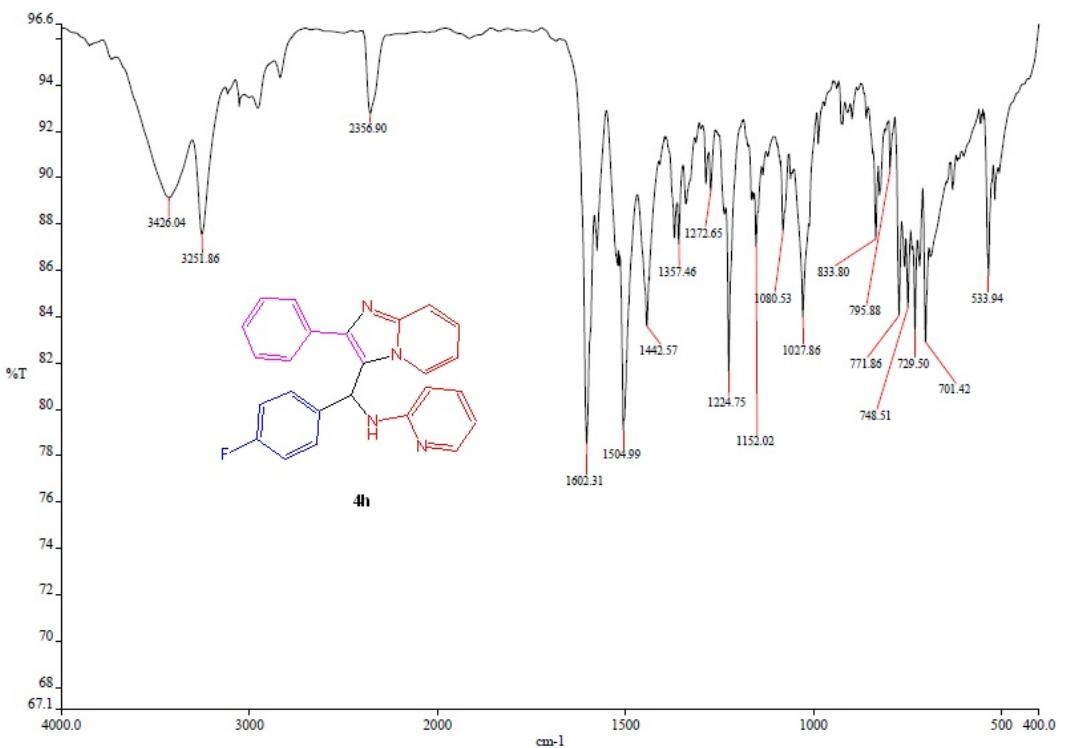
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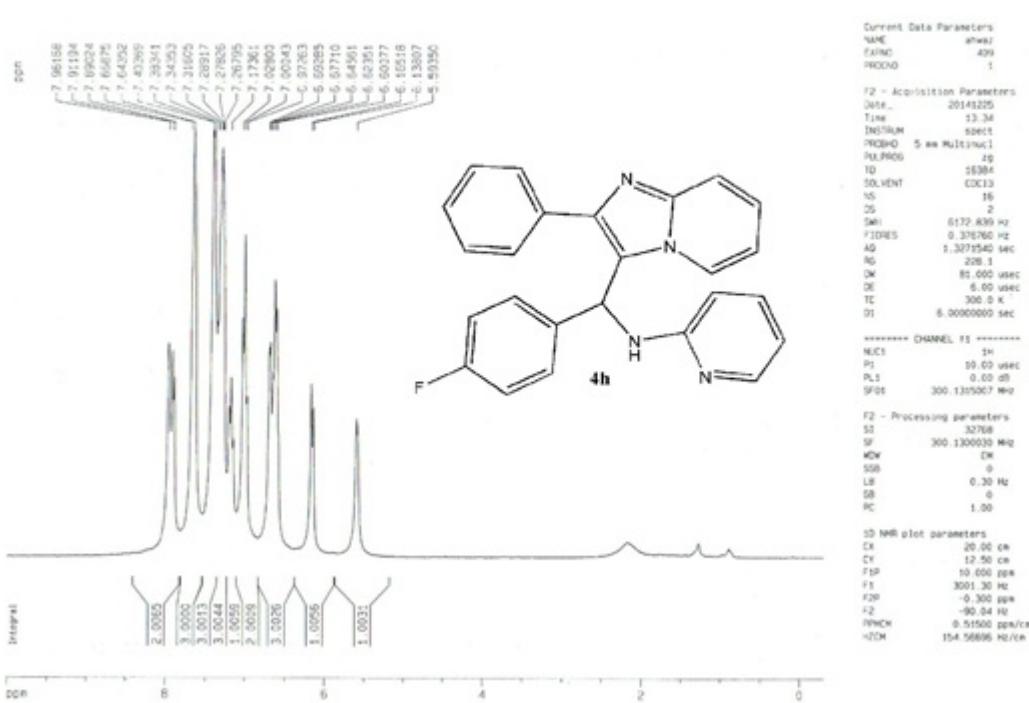
¹³C-NMR of 4g



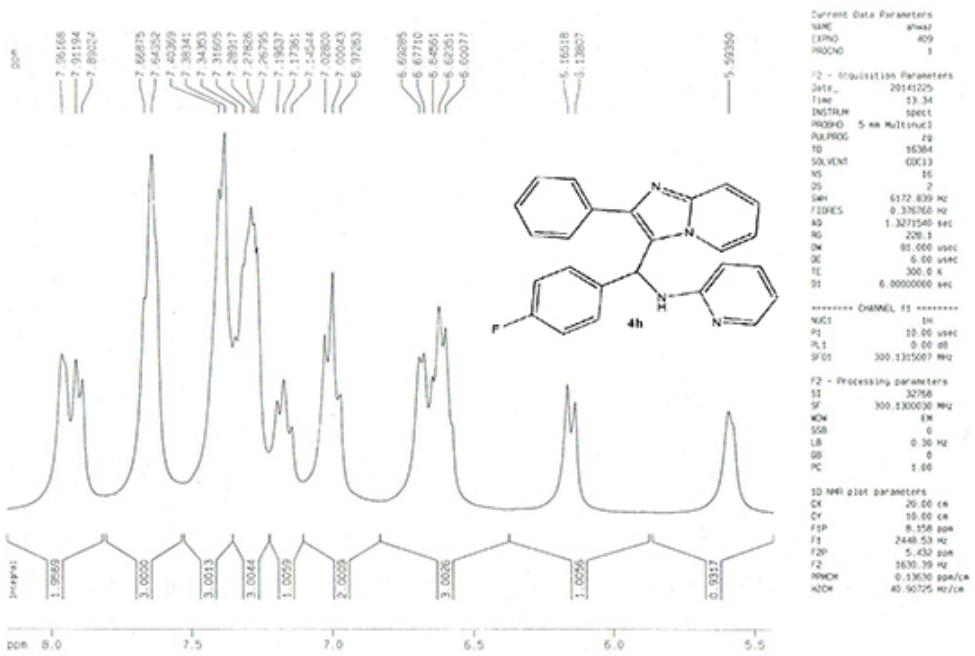
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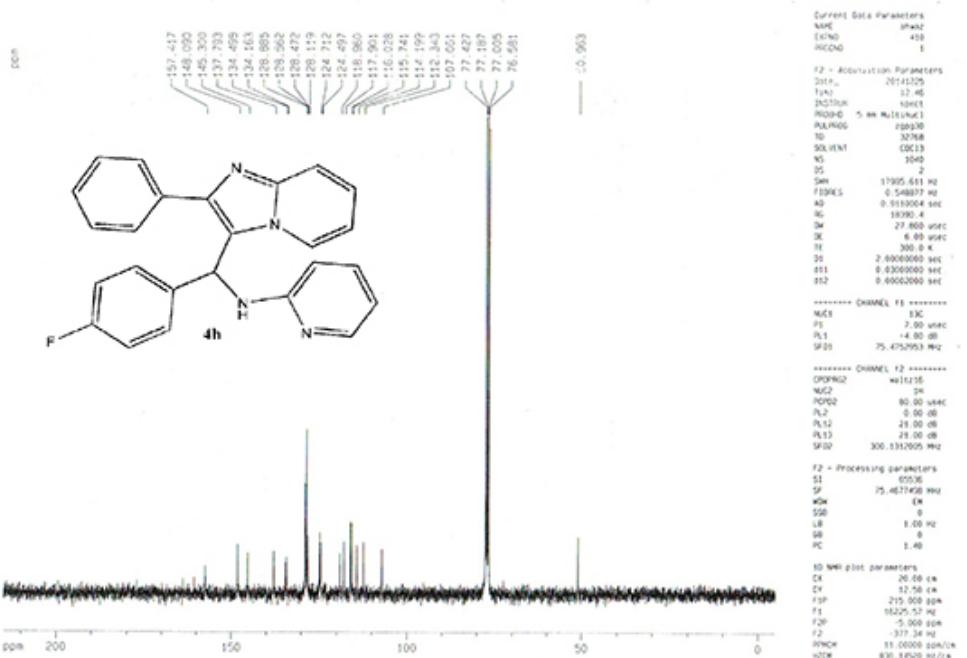
IR of **4h**



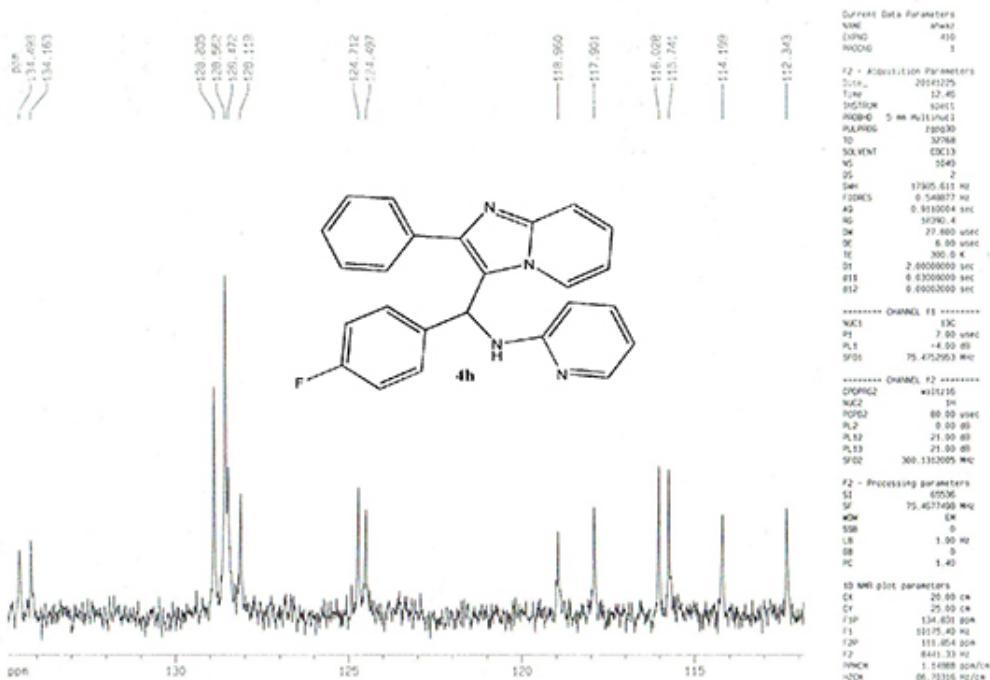
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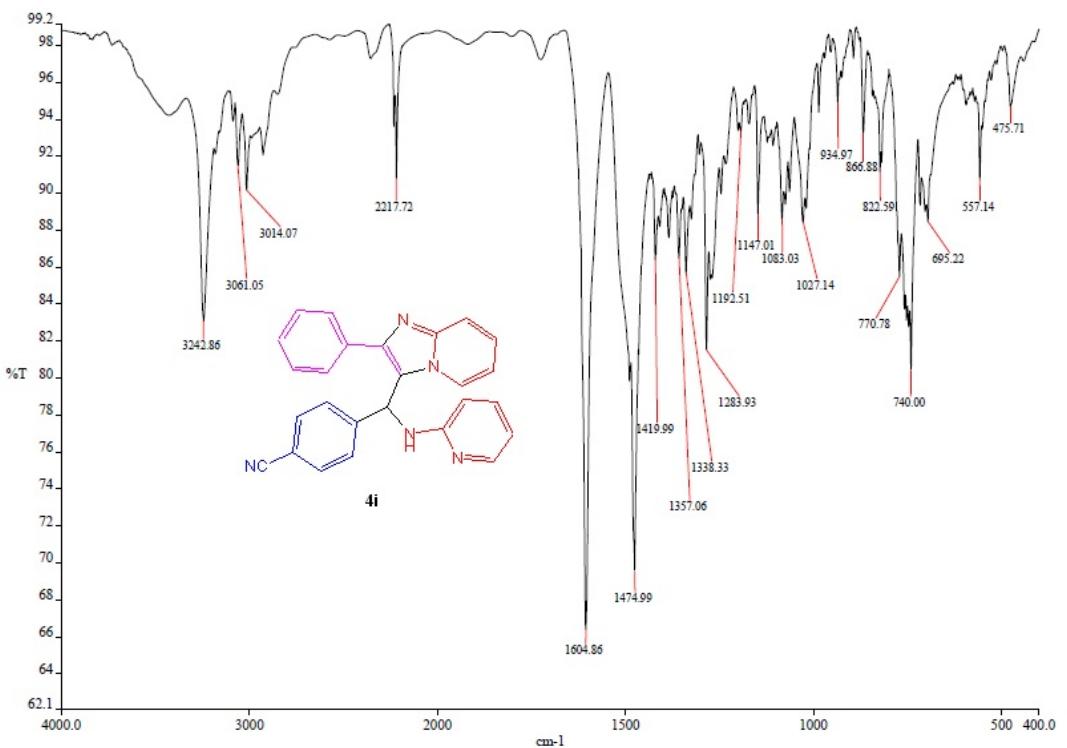
¹H-NMR of 4h



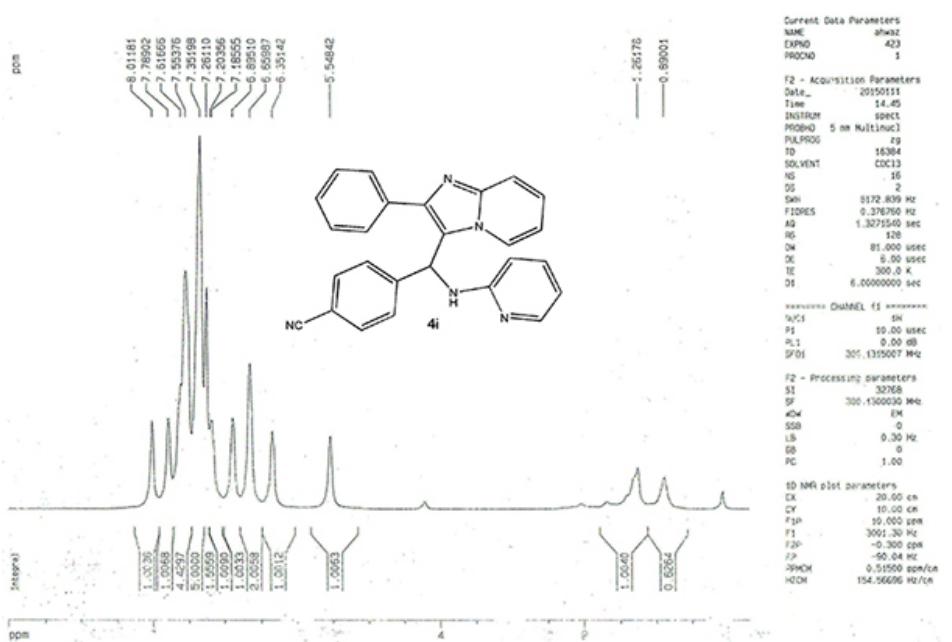
^{13}C -NMR of 4h



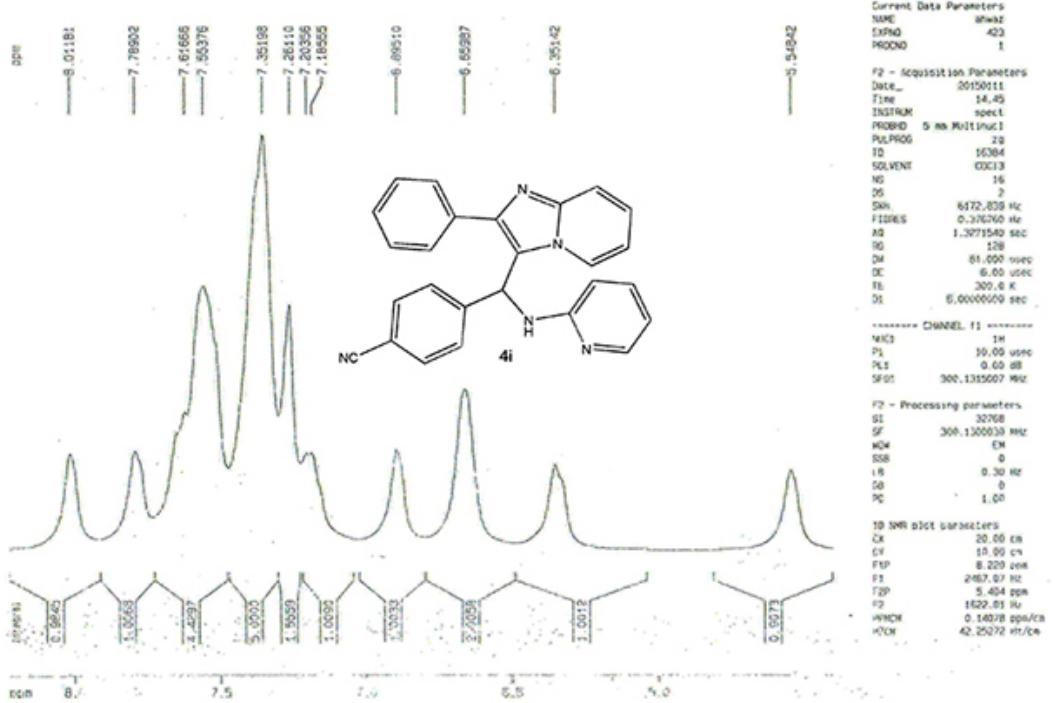
^{13}C -NMR of **4h**



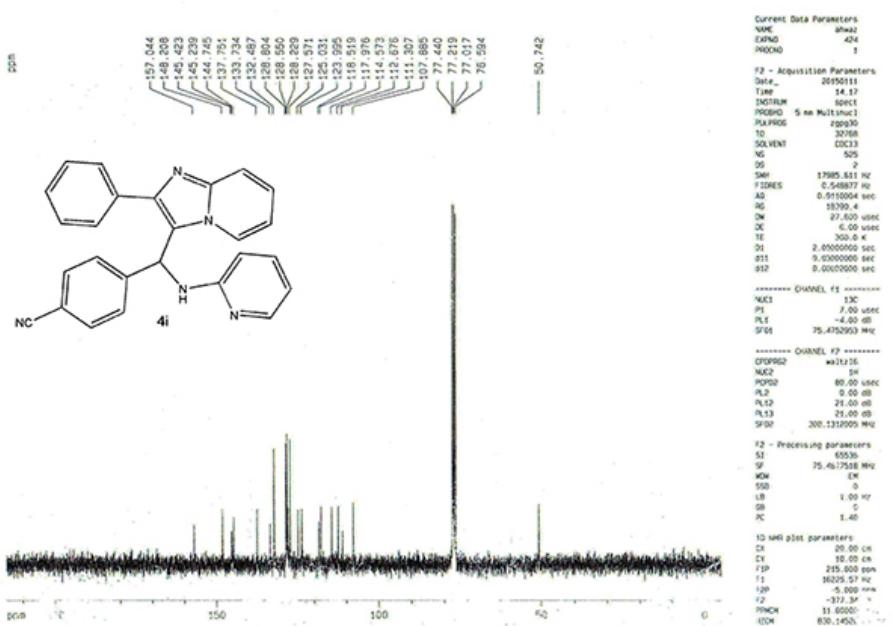
IR of **4i**



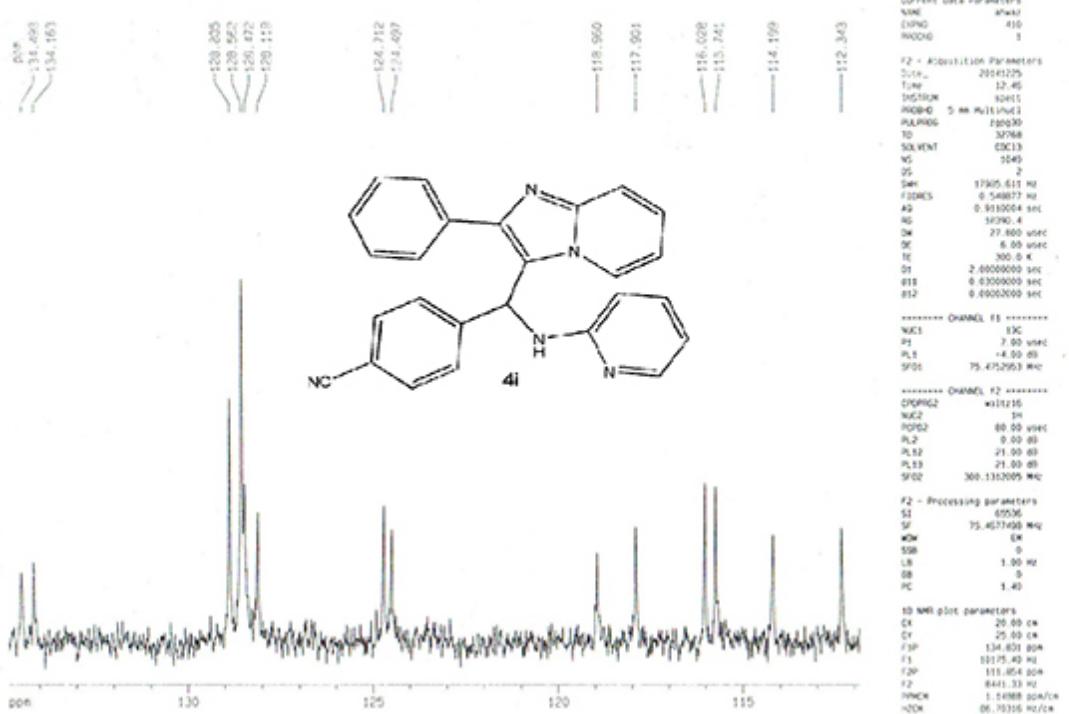
¹H-NMR of 4i



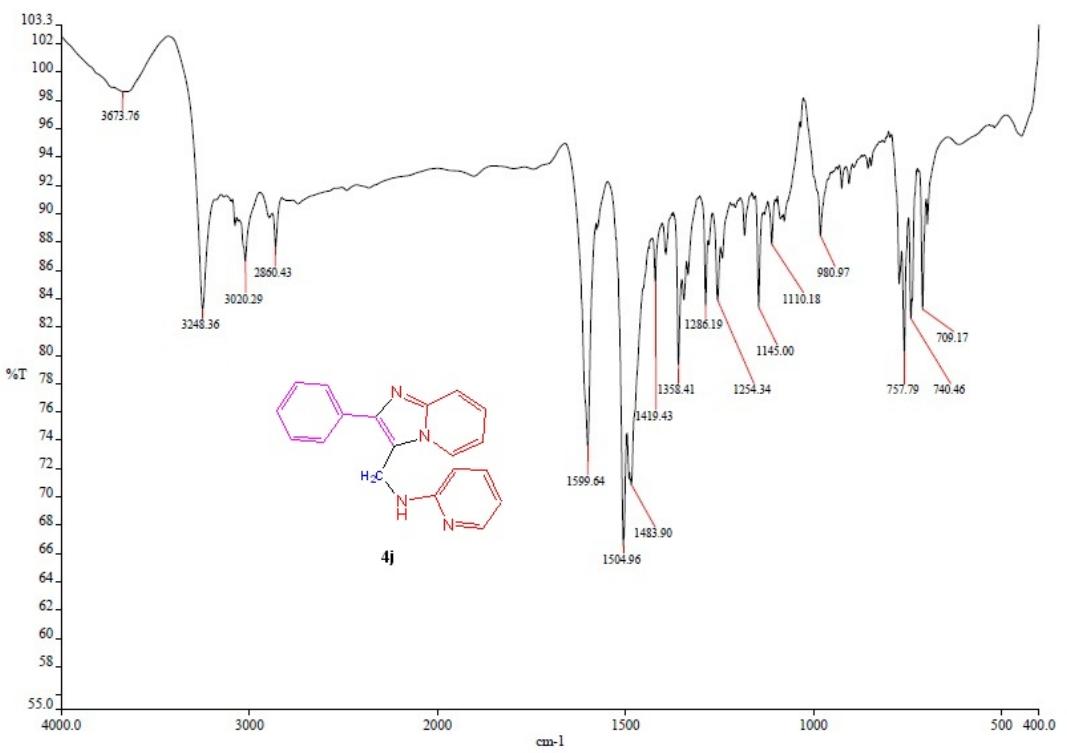
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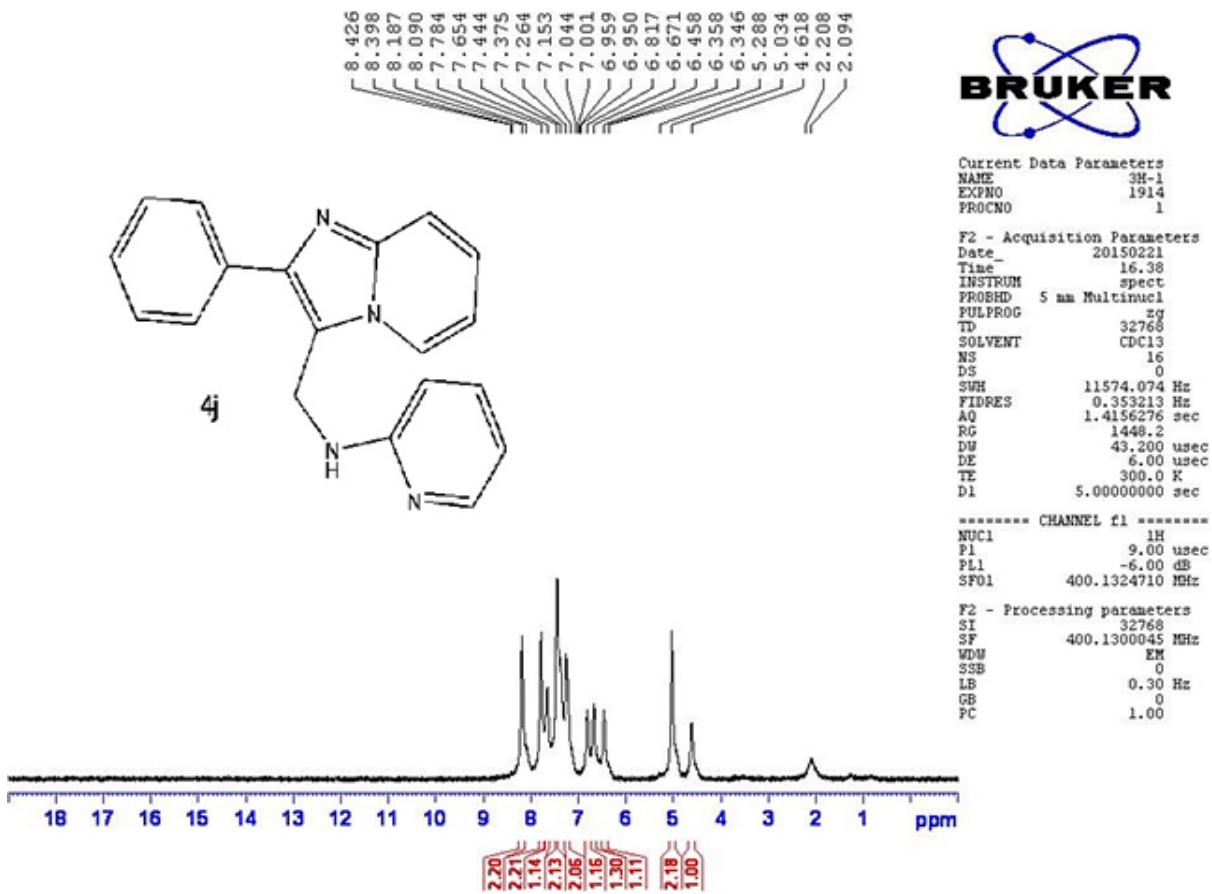
¹³C-NMR of 4i



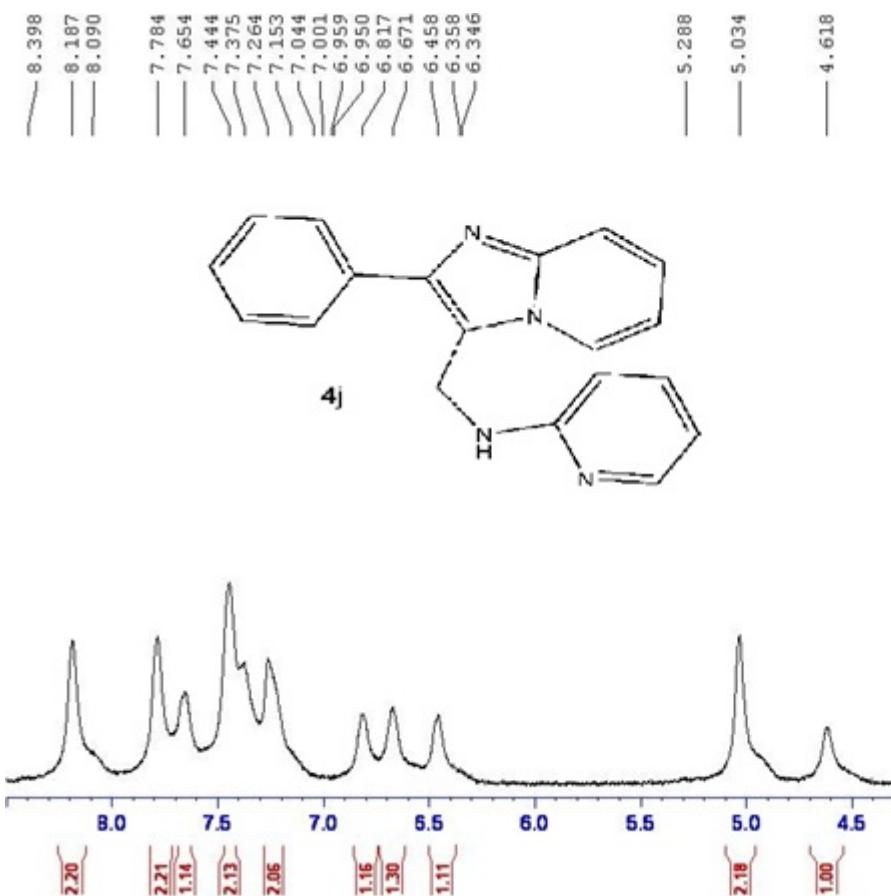
¹³C-NMR of 4i



IR of **4j**



¹H-NMR of 4j



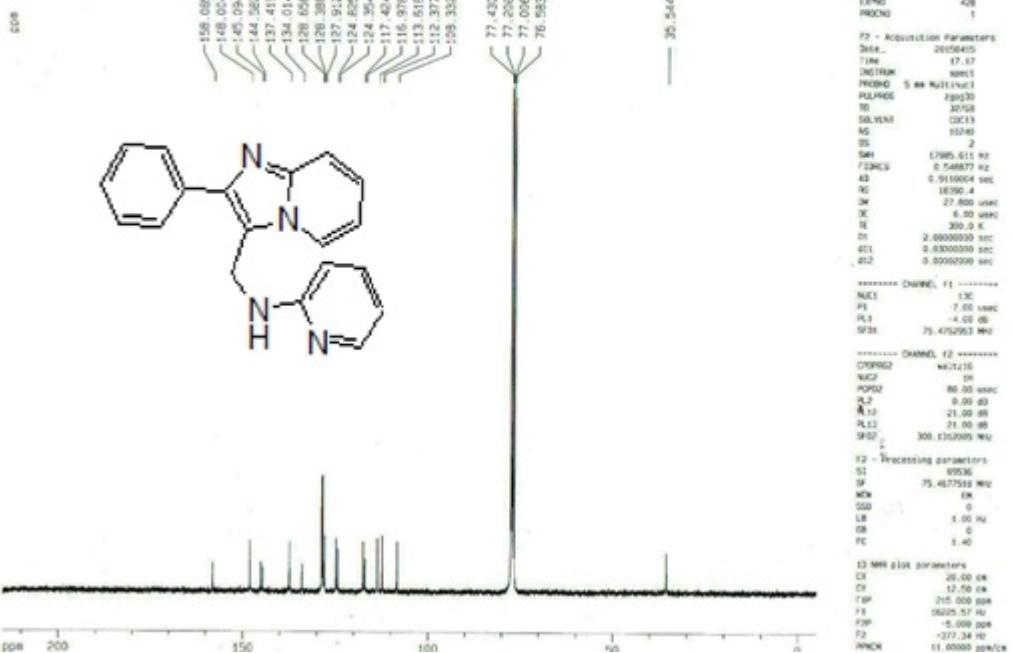
Current Data Parameters
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EXPNO 1914
PROCNO 1

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PULPROG zg3
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 11574.074 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 1448.2
DW 43.200 usec
DE 6.00 usec
TE 300.0 K
D1 5.0000000 sec

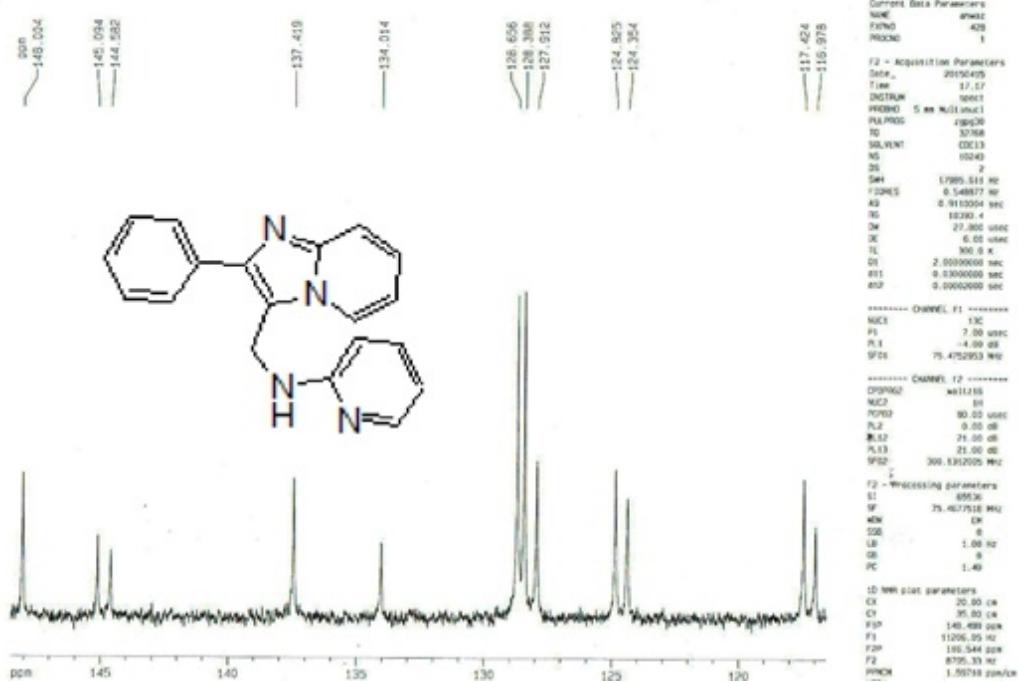
***** CHANNEL f1 *****
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P1 9.00 usec
PL1 -6.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
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SF 400.1300045 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

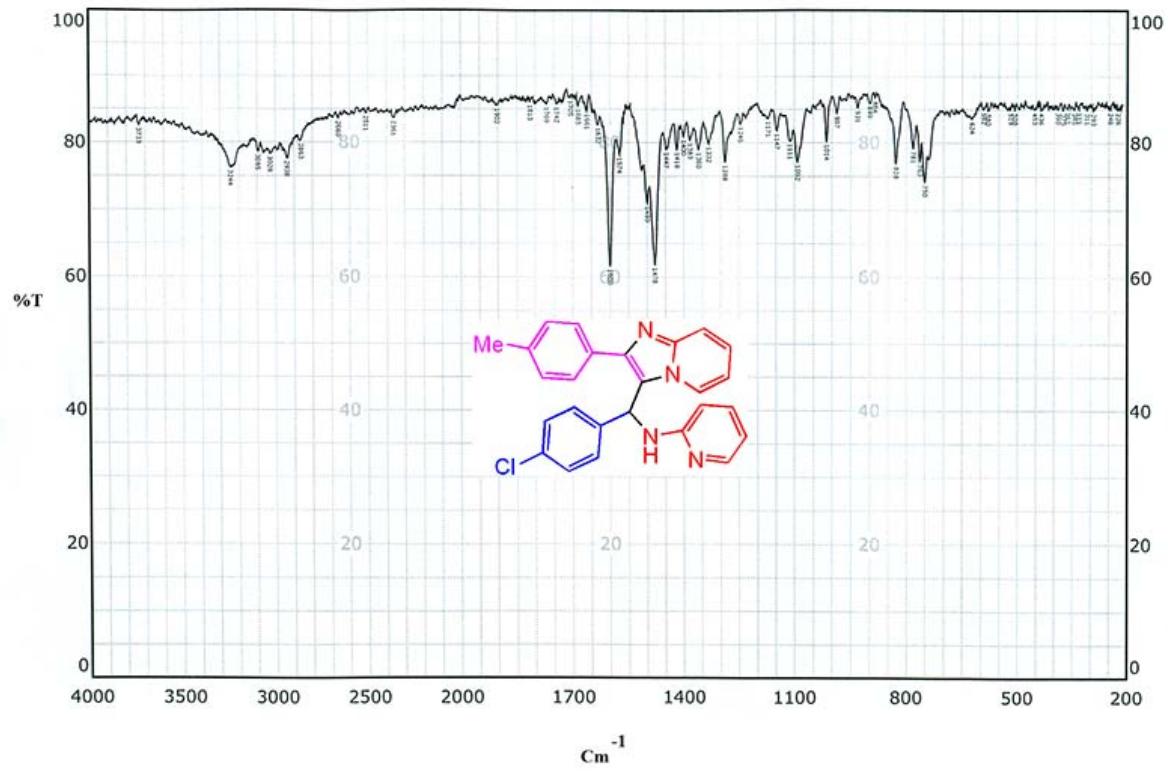
¹H-NMR of 4j



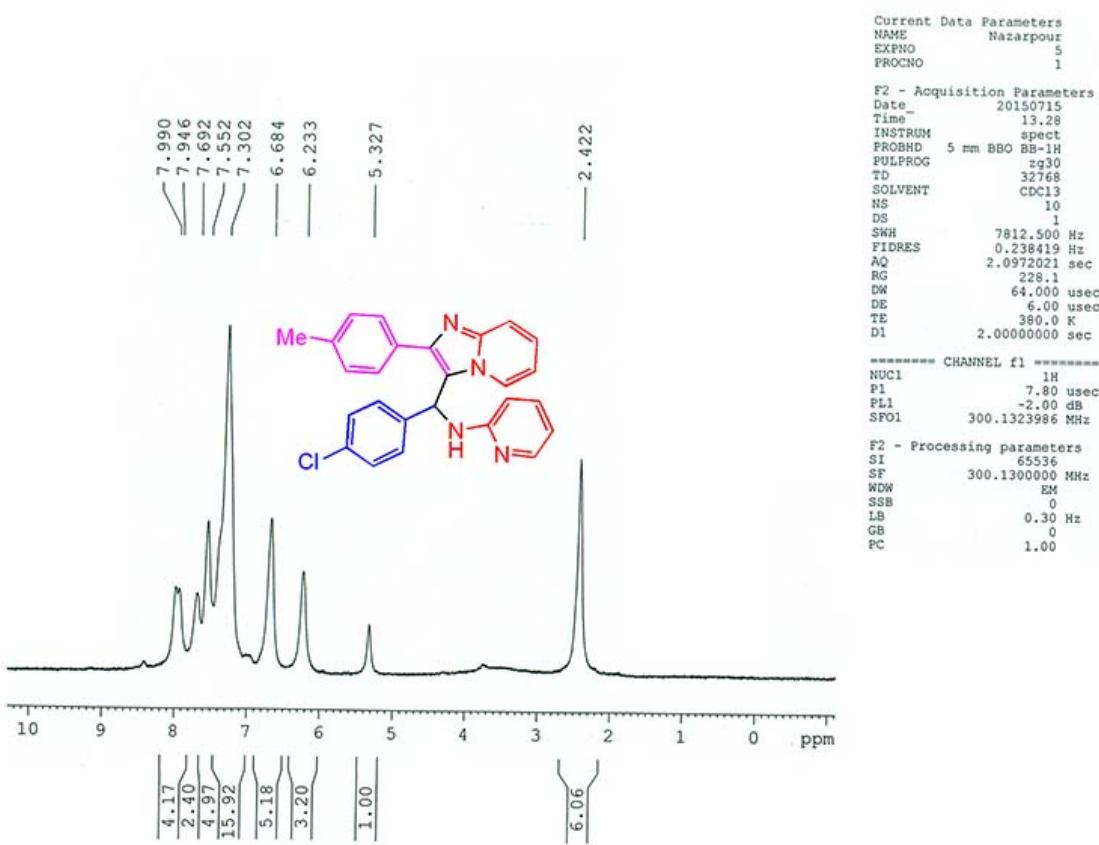
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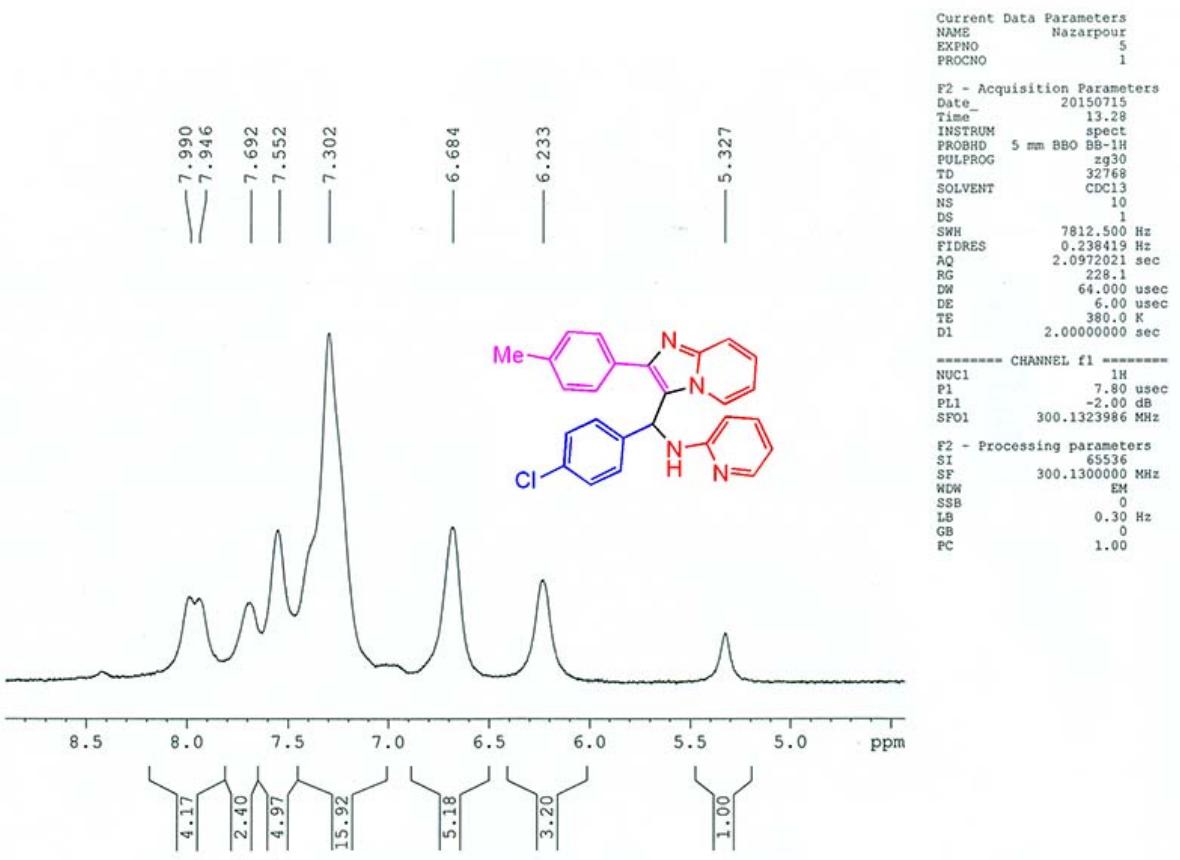
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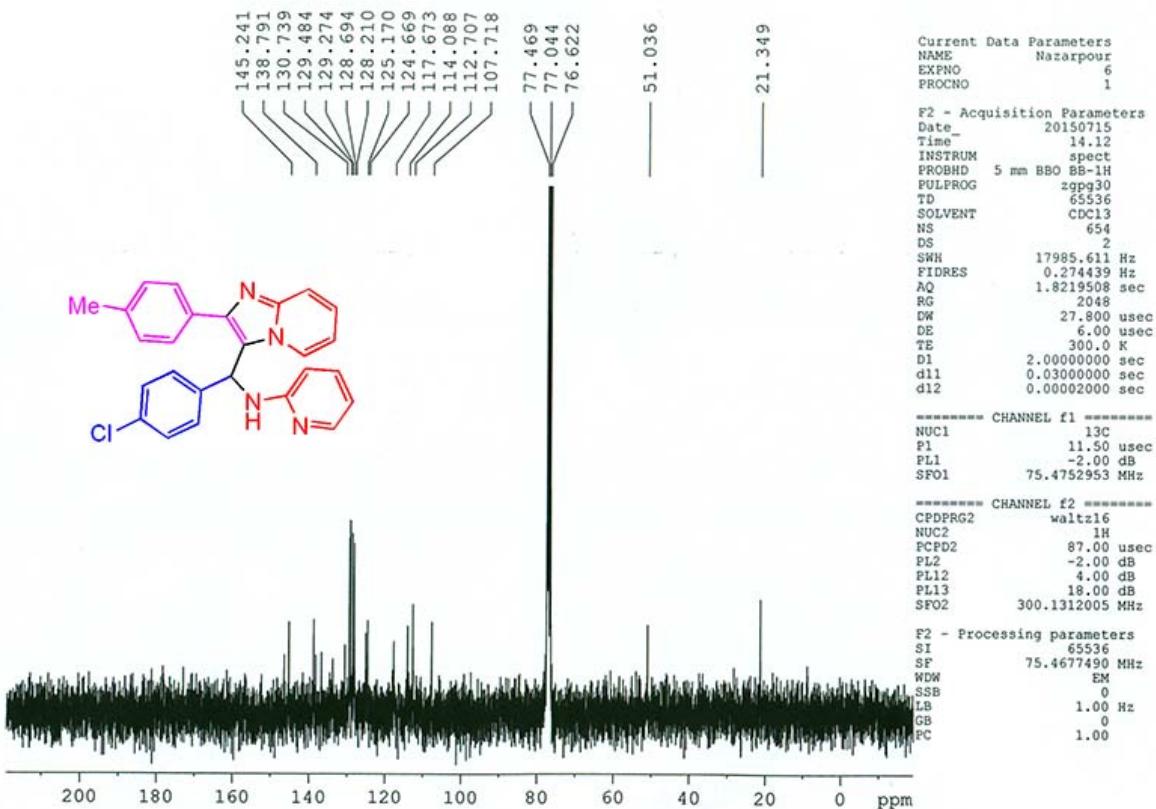


IR of 4k

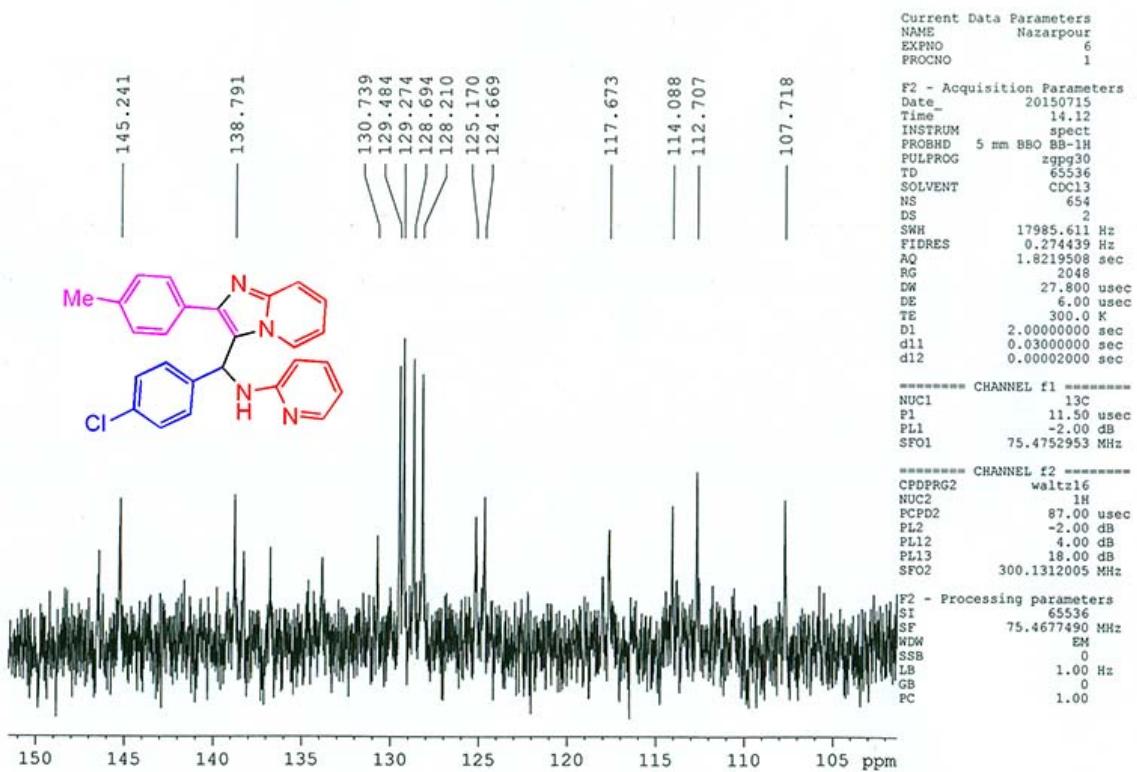


¹H-NMR of 4k

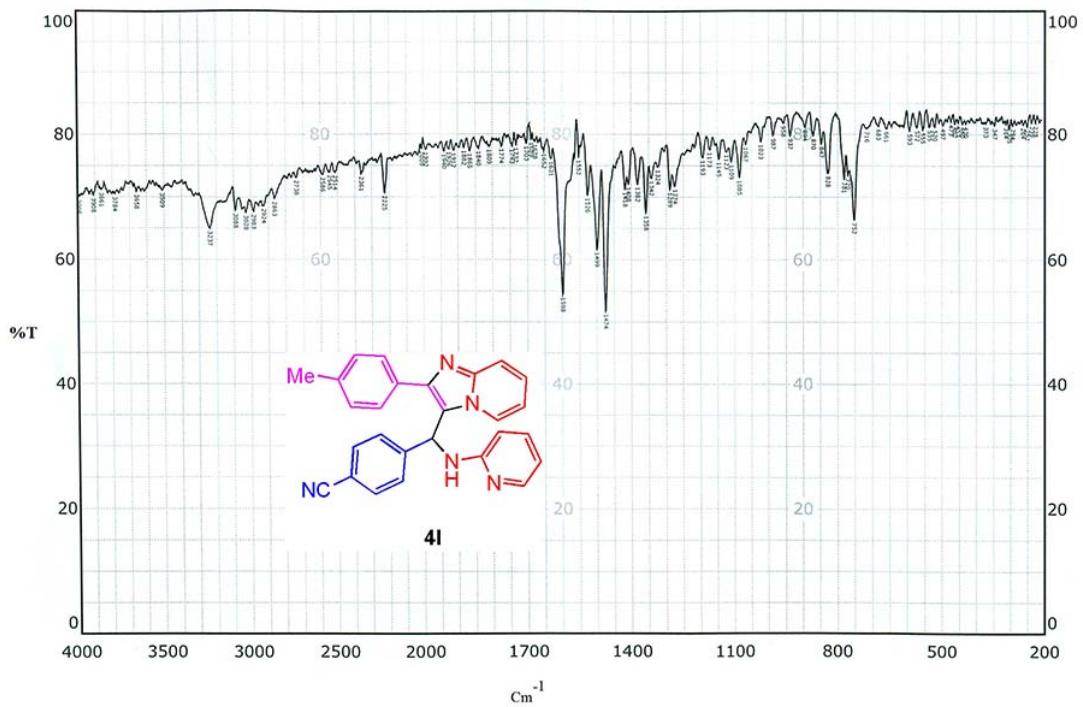




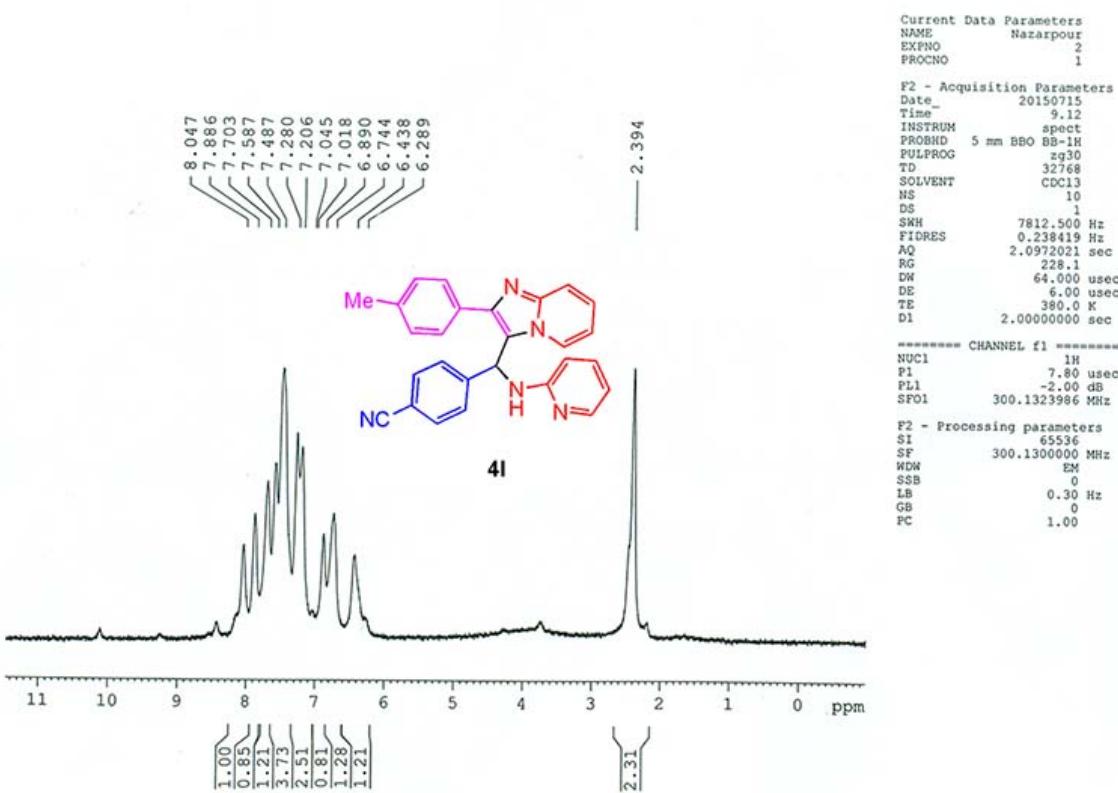
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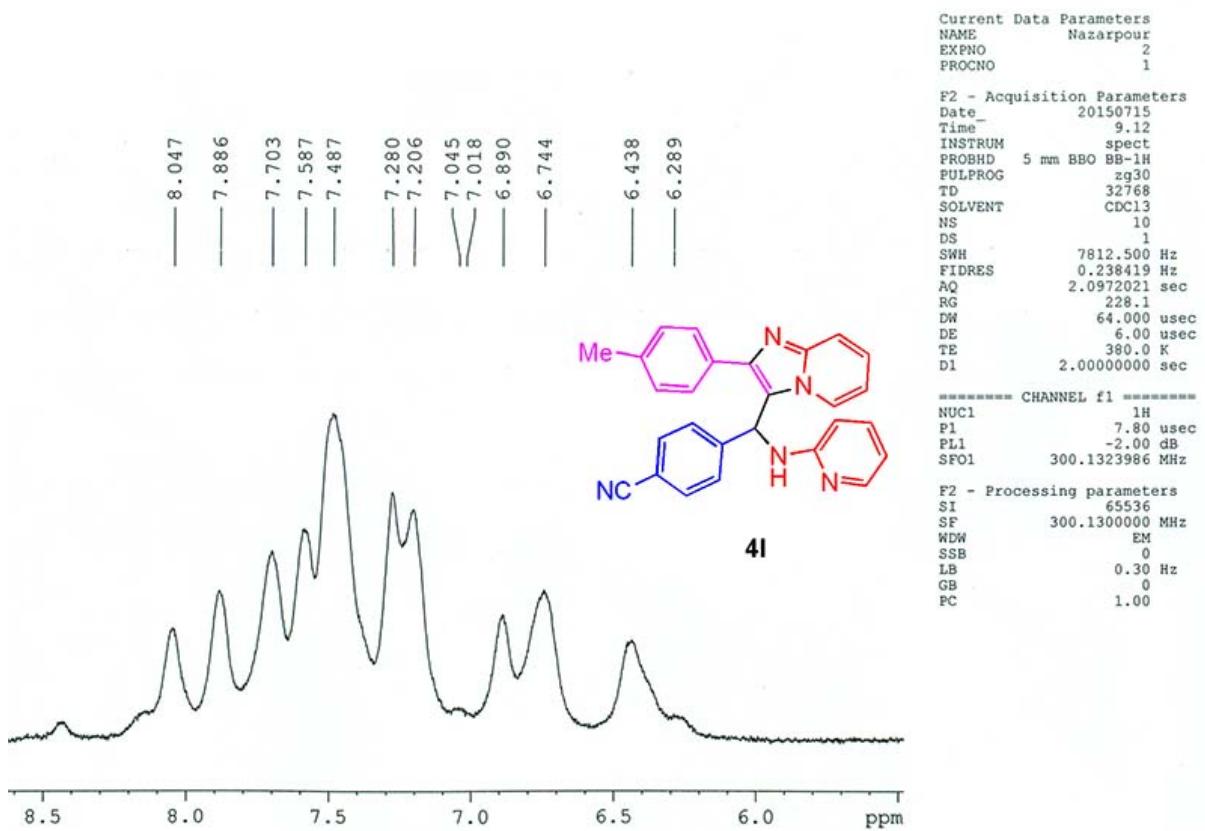
¹³C-NMR of 4k



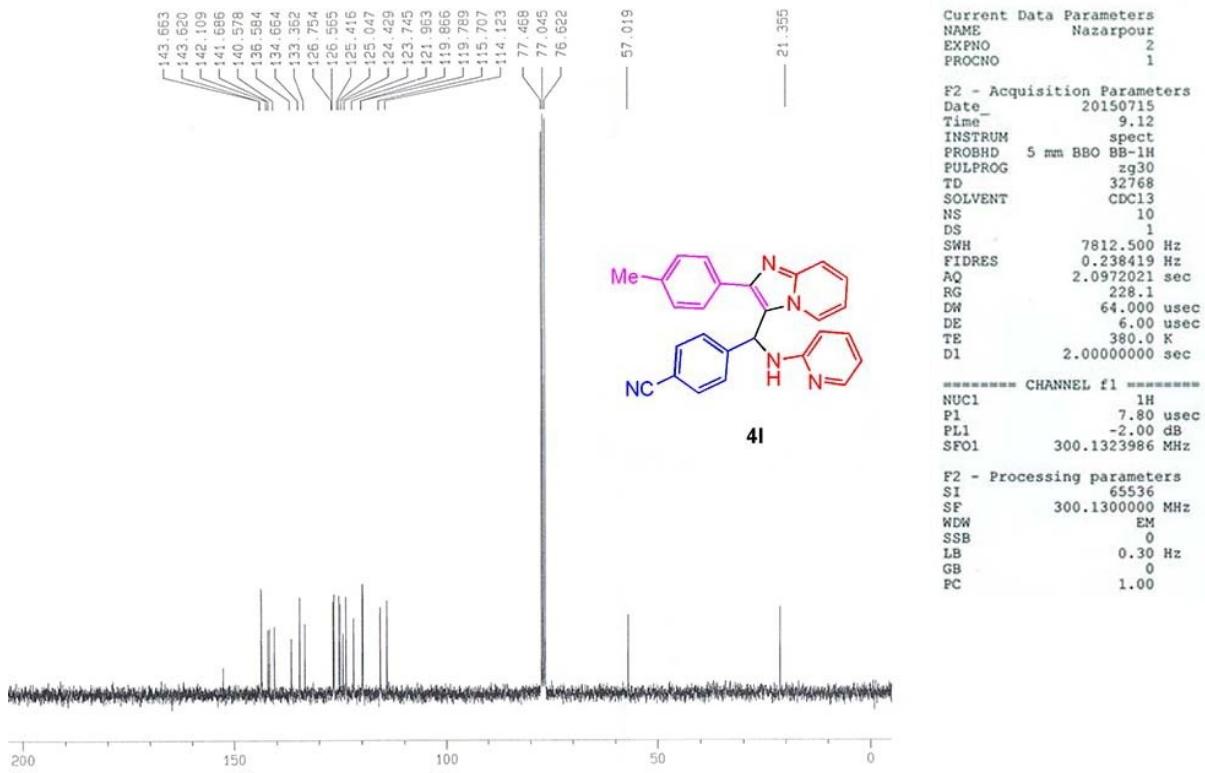
IR of **4l**



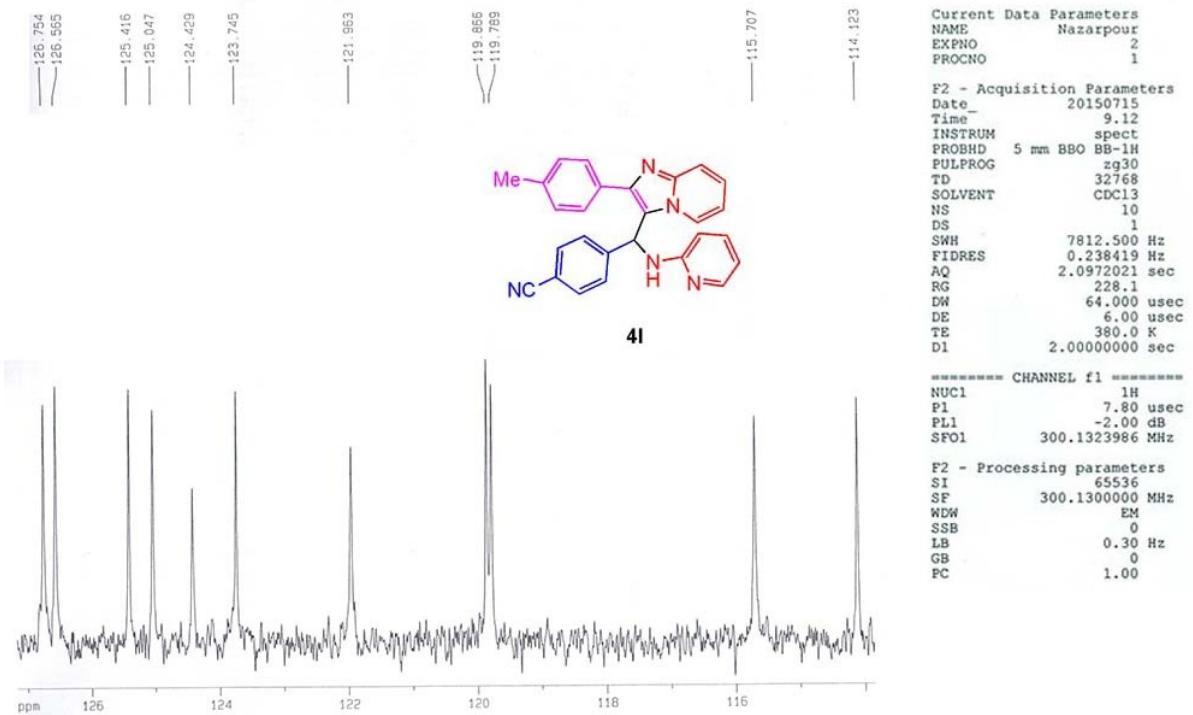
¹H-NMR of 4l



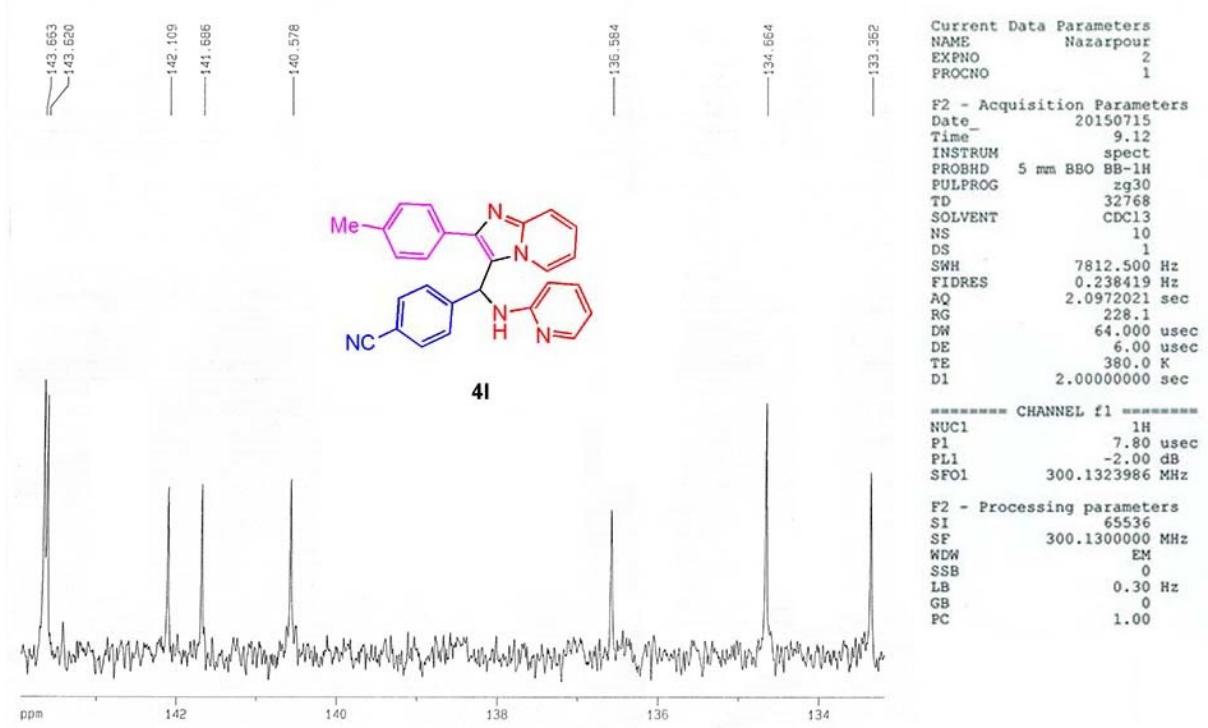
¹H-NMR of 4l



¹³C-NMR of 4l



¹³C-NMR of 4l



¹³C-NMR of 4l