

SUPPORTING INFORMATION

Aggregation Induced Emission characteristics of maleimide derivative

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Table of Contents

	Page(s)
1. Characterization data for 3a - 3e	S2
2. ¹ H, ¹³ C NMR and 2D NMR spectrum of 3a-3e	S3-S16
3. IR spectrum of 3a-3e	S17-21
4. Selected Crystallographic Data for 3a	S22

1-Phenyl-3-(phenylamino)-1H-pyrrole-2,5-dione (3a) Isolated yield 0.26 g (97%); Yellow solid; mp 229-231 °C, (230-232 °C lit)³³; ¹H NMR (300 MHz, DMSO-*d*₆) δ 5.82 (s, 1H), 7.12 (m, 1H), 7.36-7.50 (m, 9H), 9.86 (s, 1H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 89.3, 120.7, 124.8, 127.5, 128.3, 129.7, 130.2, 132.9, 140.2, 144.7, 167.4, 172.1.

1-(4-Methoxyphenyl)-3-(4-methoxyphenylamino)-1H-pyrrole-2,5-dione (3b) Isolated yield 0.32 g (98%); Yellow solid; mp 221-223 °C (221-223 °C lit)³³; ¹H NMR (300 MHz, DMSO-*d*₆) δ 2.51 (s, 3H), 2.54 (s, 3H), 4.36 (s, 1H), 5.73- 6.15 (m, 8H), 8.52 (s, 1H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 56.2, 56.3, 87.3, 115.0, 115.4, 122.3, 125.5, 129.0, 133.2, 145.1, 156.8, 159.2, 167.6, 172.3.

1-(4-Chlorophenyl)-3-(4-chlorophenylamino)-1H-pyrrole-2,5-dione (3c) Isolated yield 0.32 g (95%); Yellow solid; mp 247-249 °C, (249-251 °C lit)³³; ¹H NMR (300 MHz, DMSO-*d*₆) δ 5.86 (s, 1H), 7.31-7.55 (m, 8H), 9.99 (s, 1H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 89.8, 121.9, 128.2, 128.5, 129.2, 129.6, 131.3, 132.2, 138.7, 144.1, 166.6, 171.1.

1-(4-Bromophenyl)-3-(4-bromophenylamino)-1H-pyrrole-2,5-dione (3d) Isolated yield 0.41 g (97%); Yellow solid; mp 259-261 °C, (260-262 °C lit)³³; ¹H NMR (300 MHz, DMSO-*d*₆) δ 5.92 (s, 1H), 7.30-7.83 (m, 8H), 9.97 (s, 1H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 90.5, 118.5, 122.8, 125.7, 126.8, 130.9, 131.5, 133.7, 141.3, 143.7, 167.5, 170.7.

1-(4-Fluorophenyl)-3-(4-fluorophenylamino)-1H-pyrrole-2,5-dione (3e) Isolated yield 0.30 g (98%); Yellow solid; mp 274-276 °C, (274-276 °C lit)³³; ¹H NMR (300 MHz, DMSO-*d*₆) δ 5.80 (s, 1H), 7.24-7.52 (m, 8H), 9.95 (s, 1H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 88.4, 116.2, 122.2, 129.0, 136.1, 144.5, 157.4, 159.7, 160.6, 162.9, 166.8, 171.3.

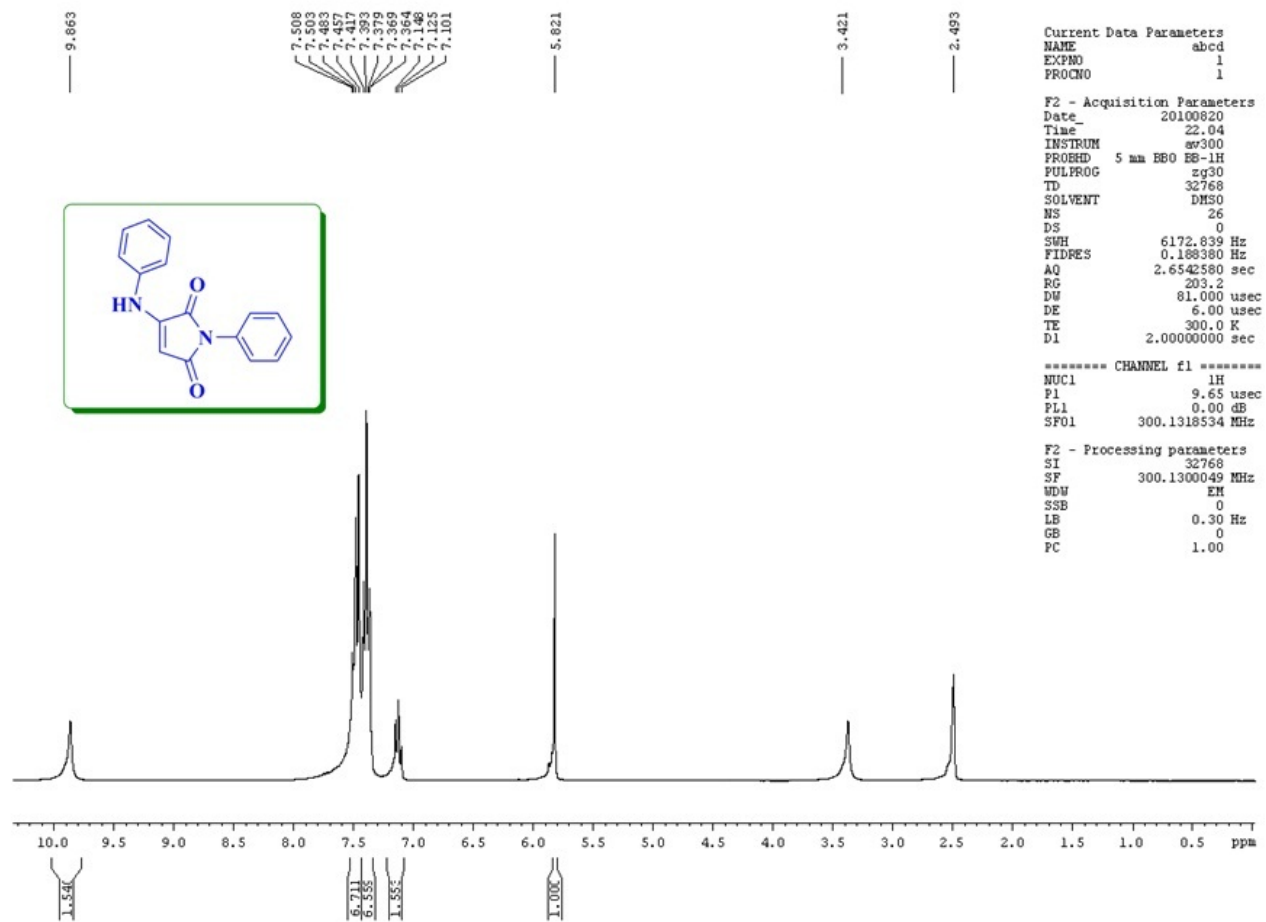


FIG 1: ¹H NMR spectrum of **3a**

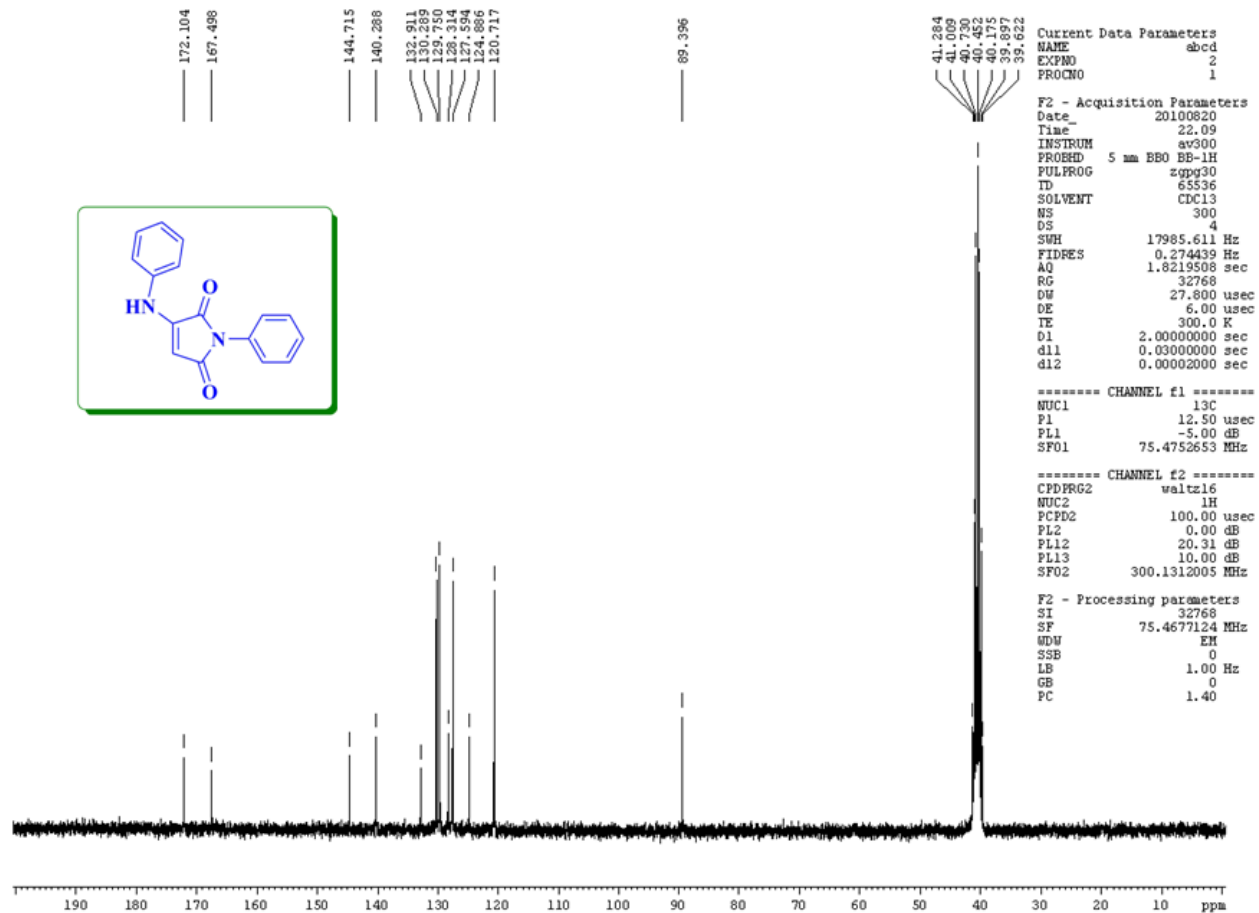


FIG 2: ^{13}C NMR spectrum of **3a**

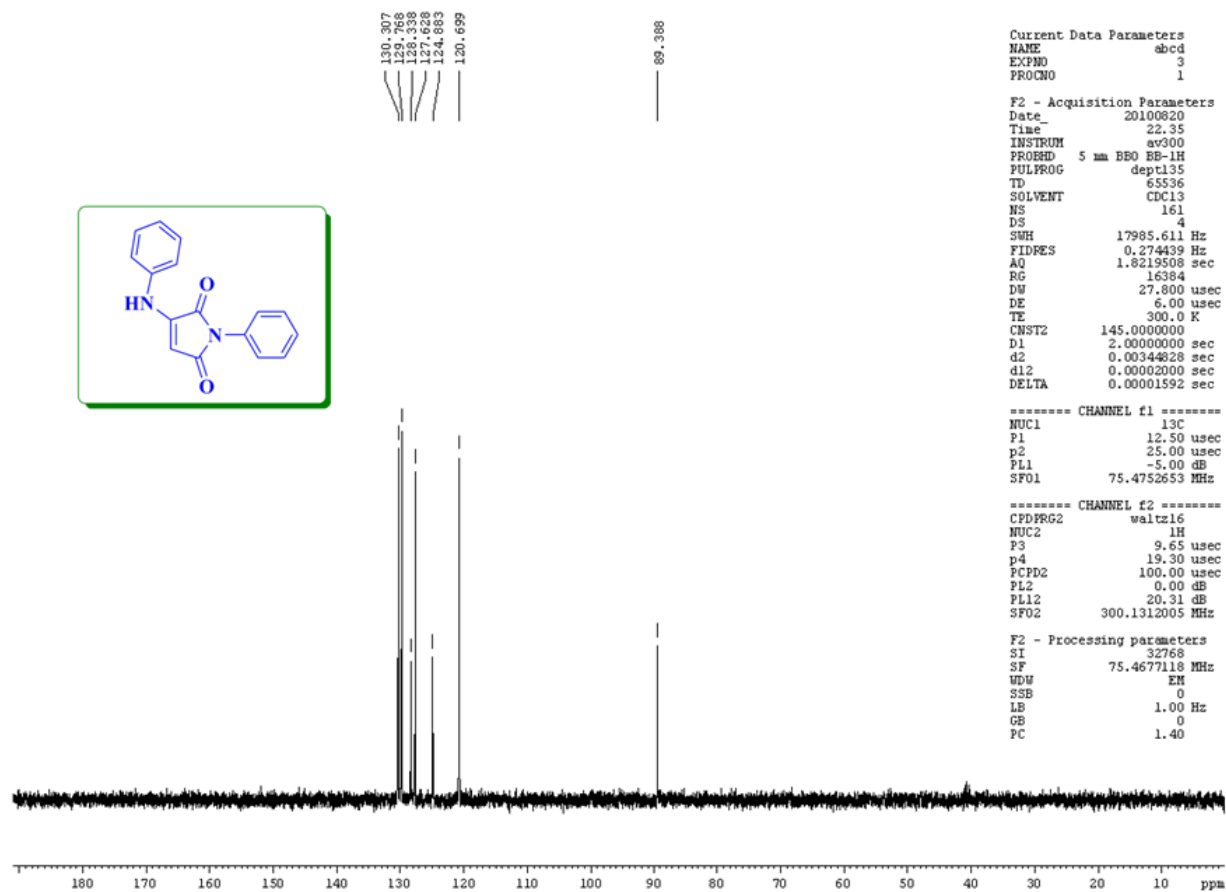


Fig. 3 DEPT Spectrum of 3a

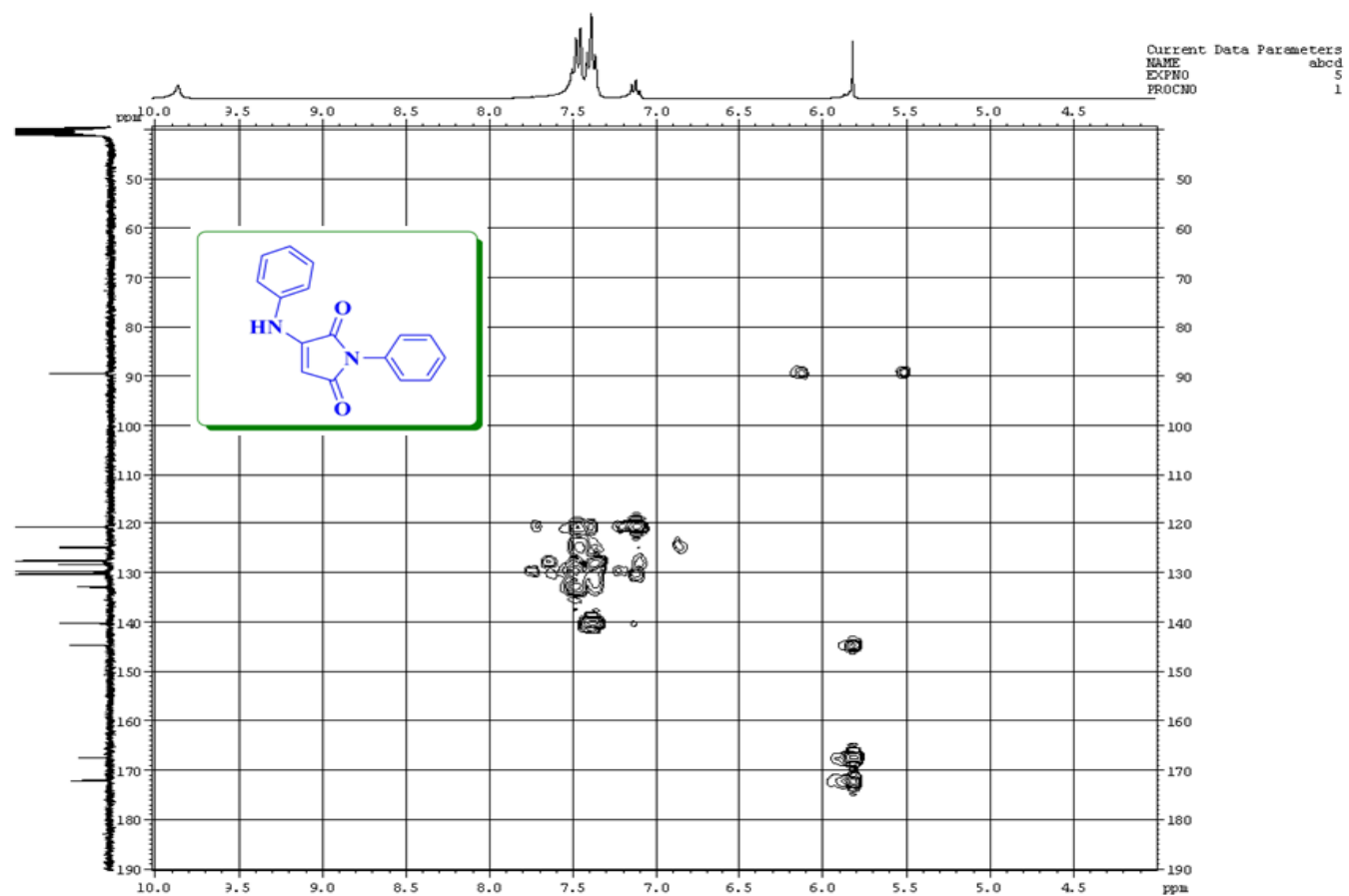


Fig. 4 HMBC Spectrum of **3a**

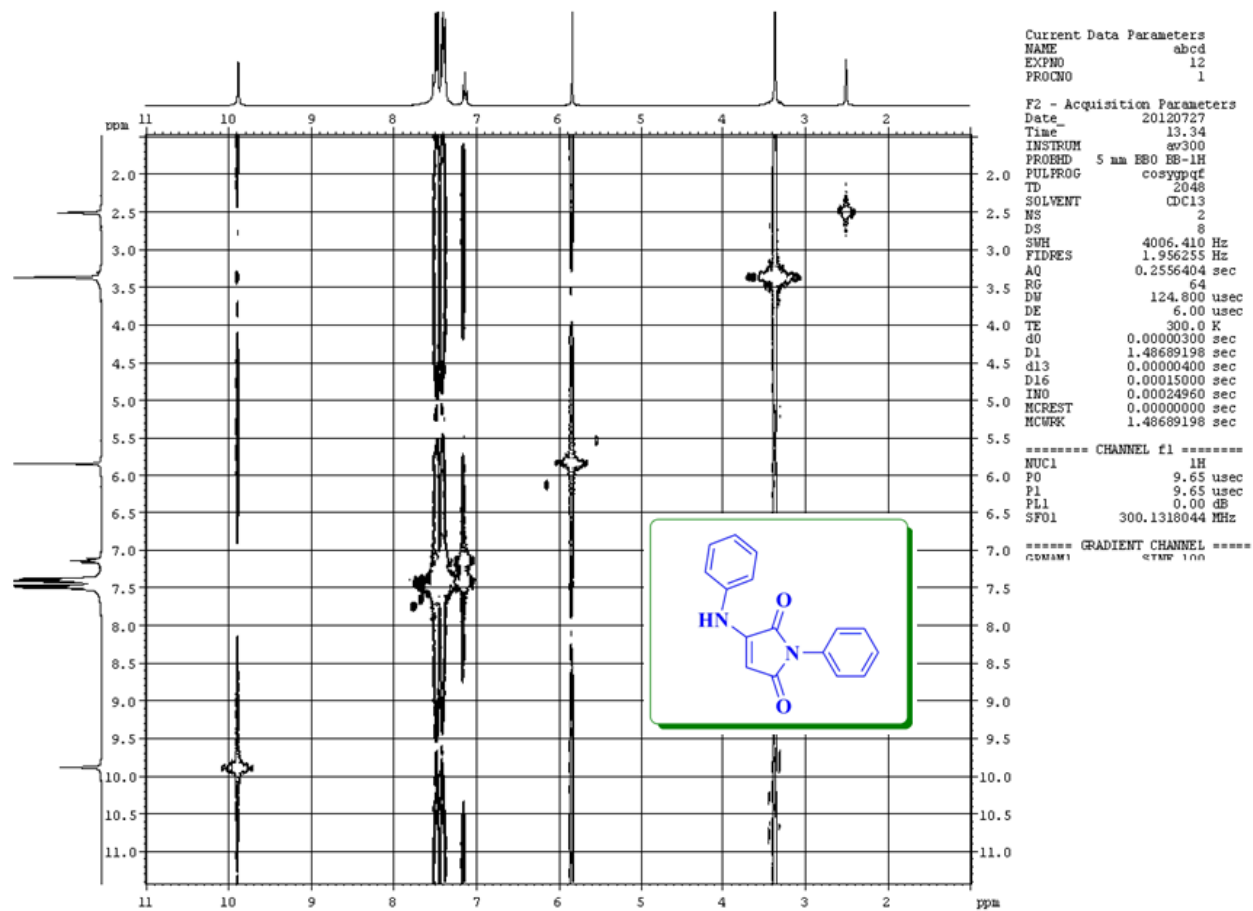


FIG 5: H-H COSY spectrum of **3a**

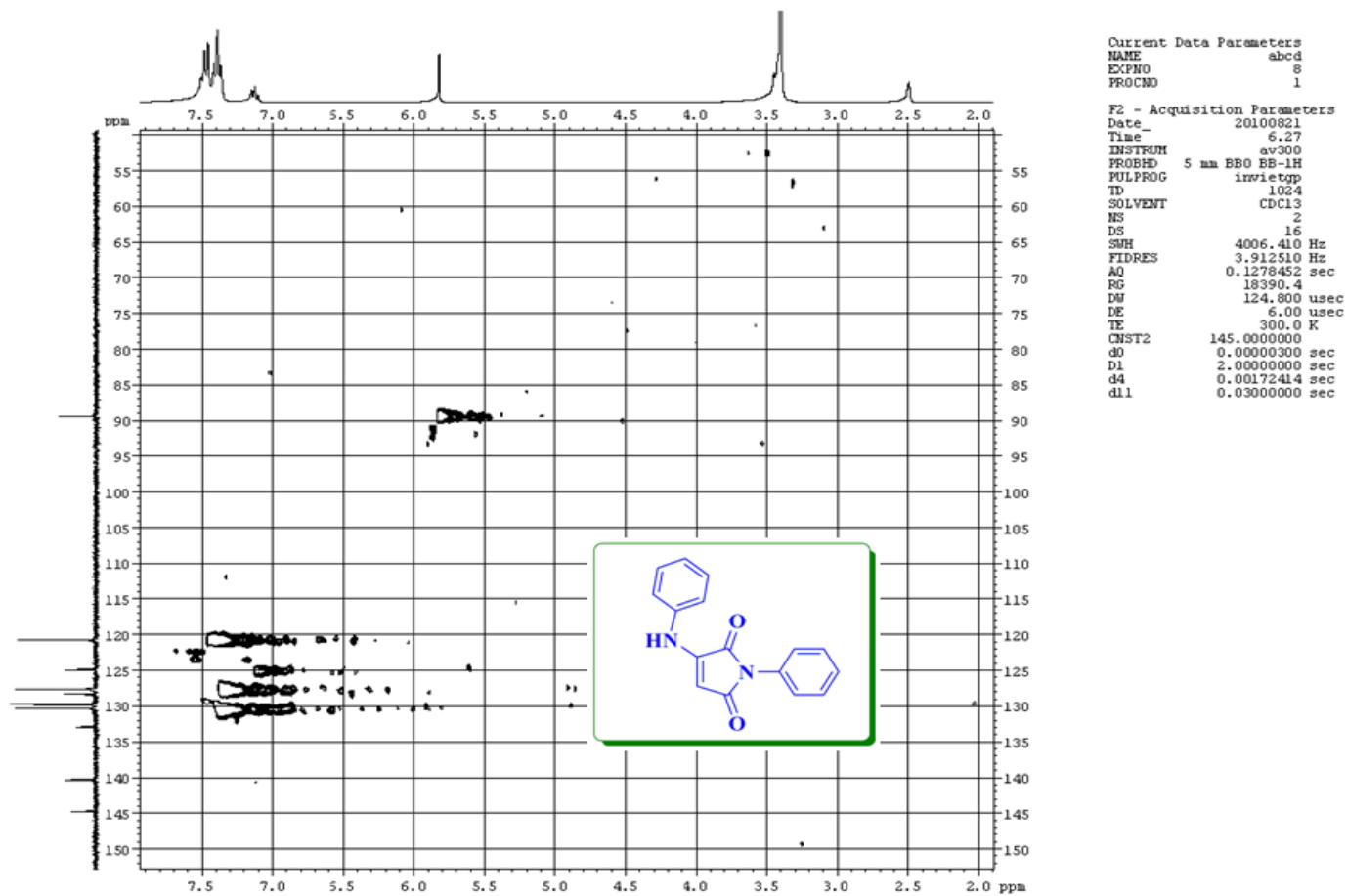


FIG 6: CH- COSY Spectrum of **3a**

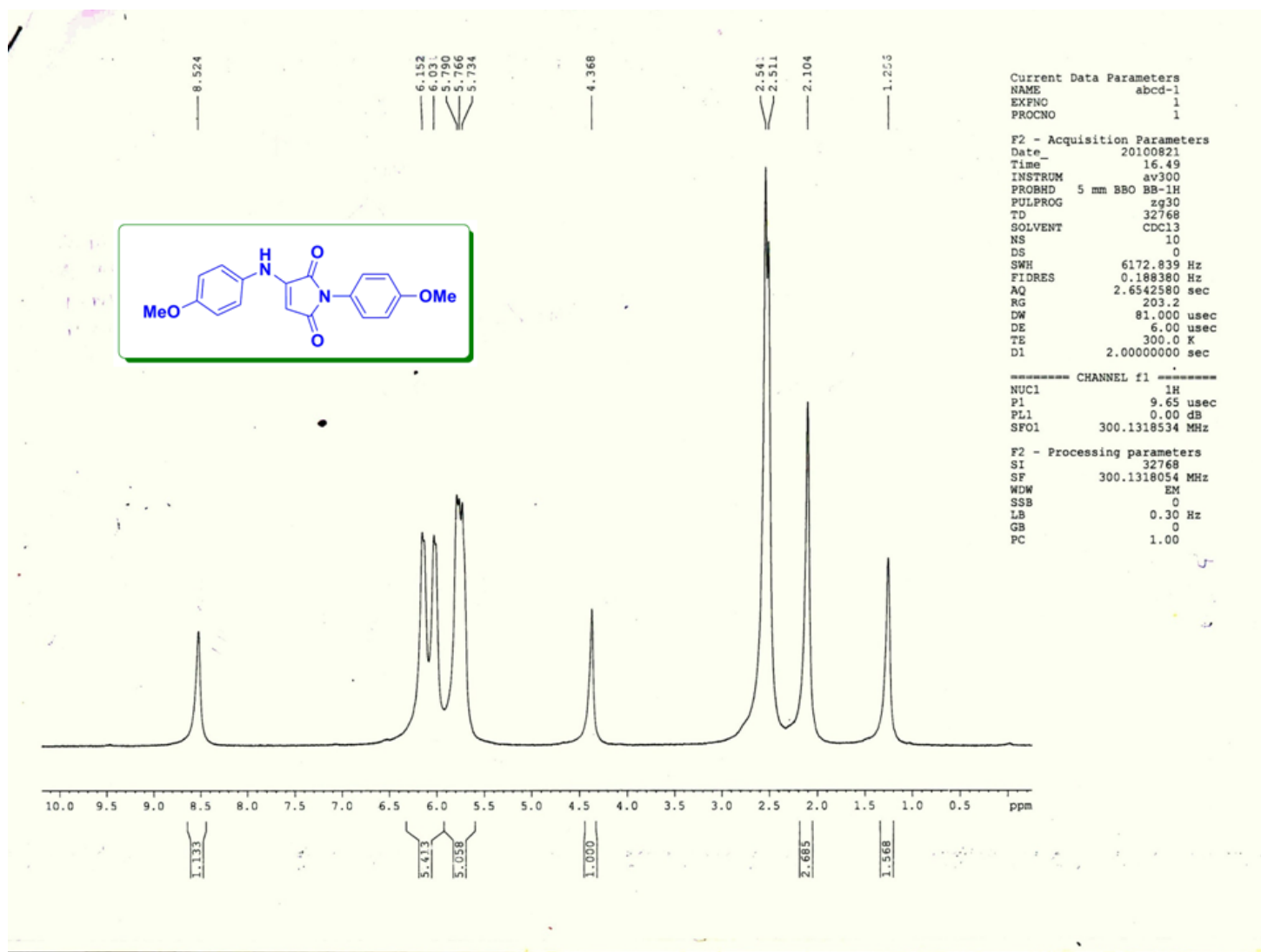


FIG 7: ^1H NMR spectrum of **3b**

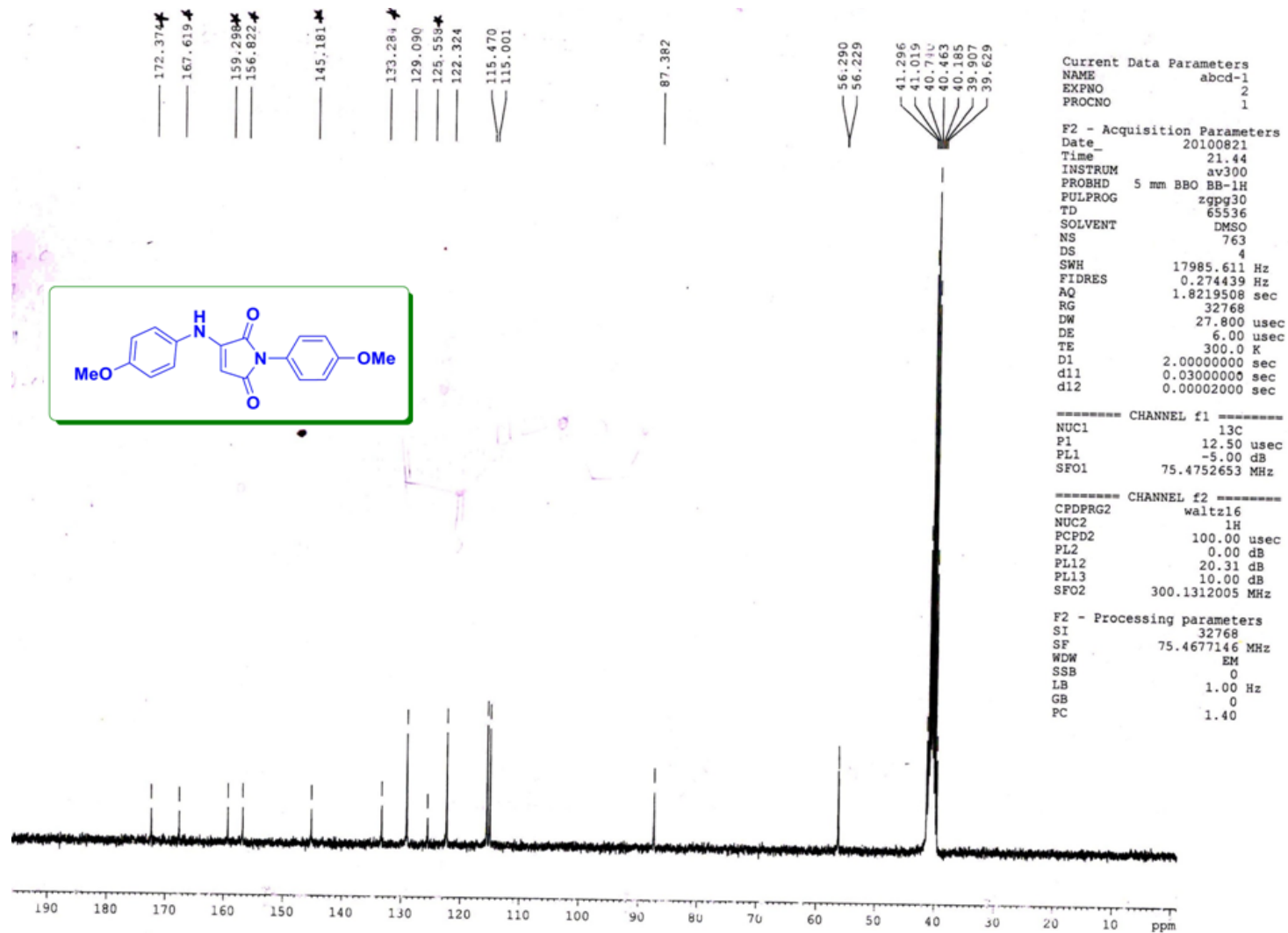


FIG 8: ^{13}C NMR spectrum of 3b

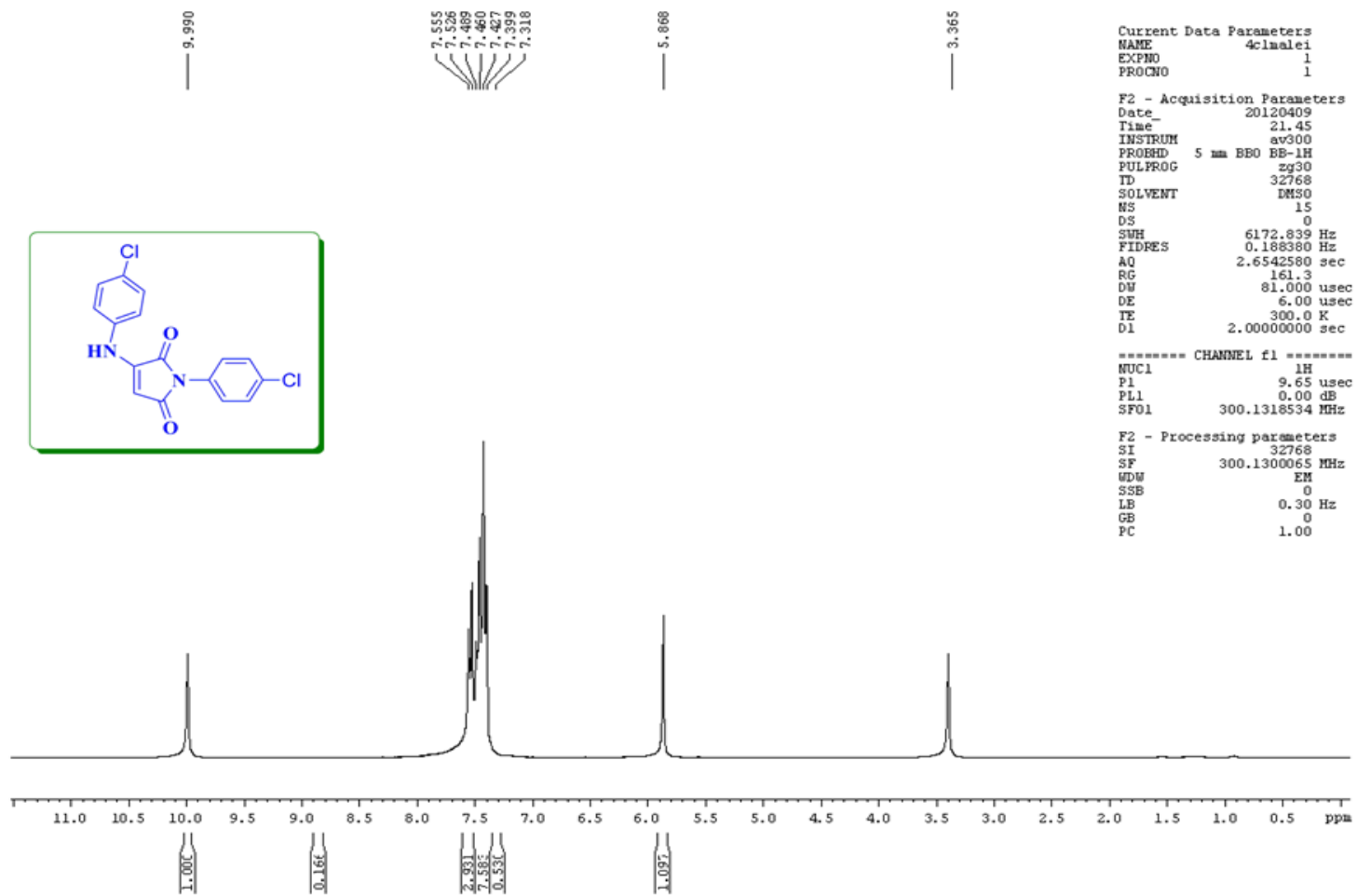


FIG 9: ^1H NMR spectrum of **3c**

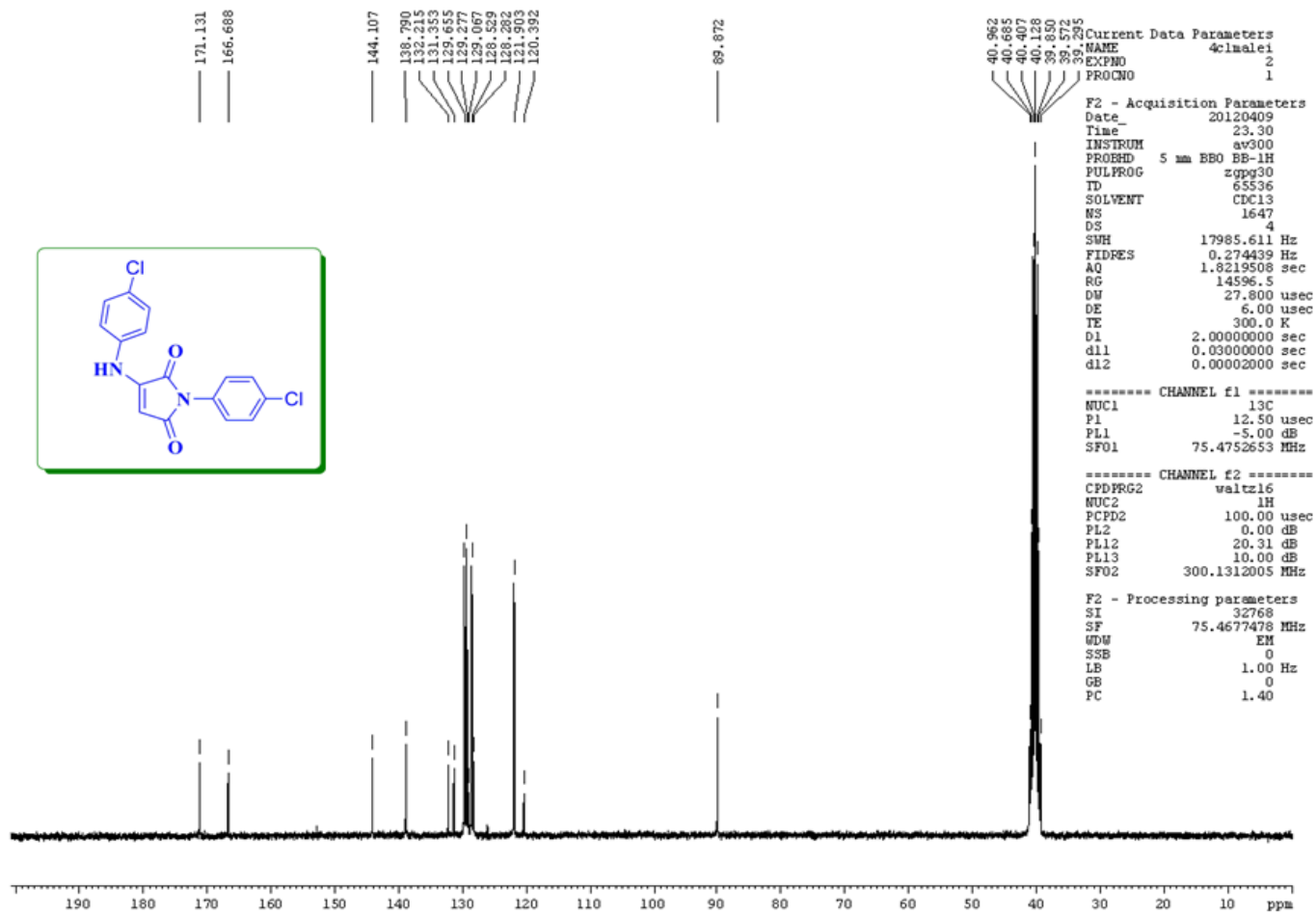


FIG 10: ¹³C NMR spectrum of 3c

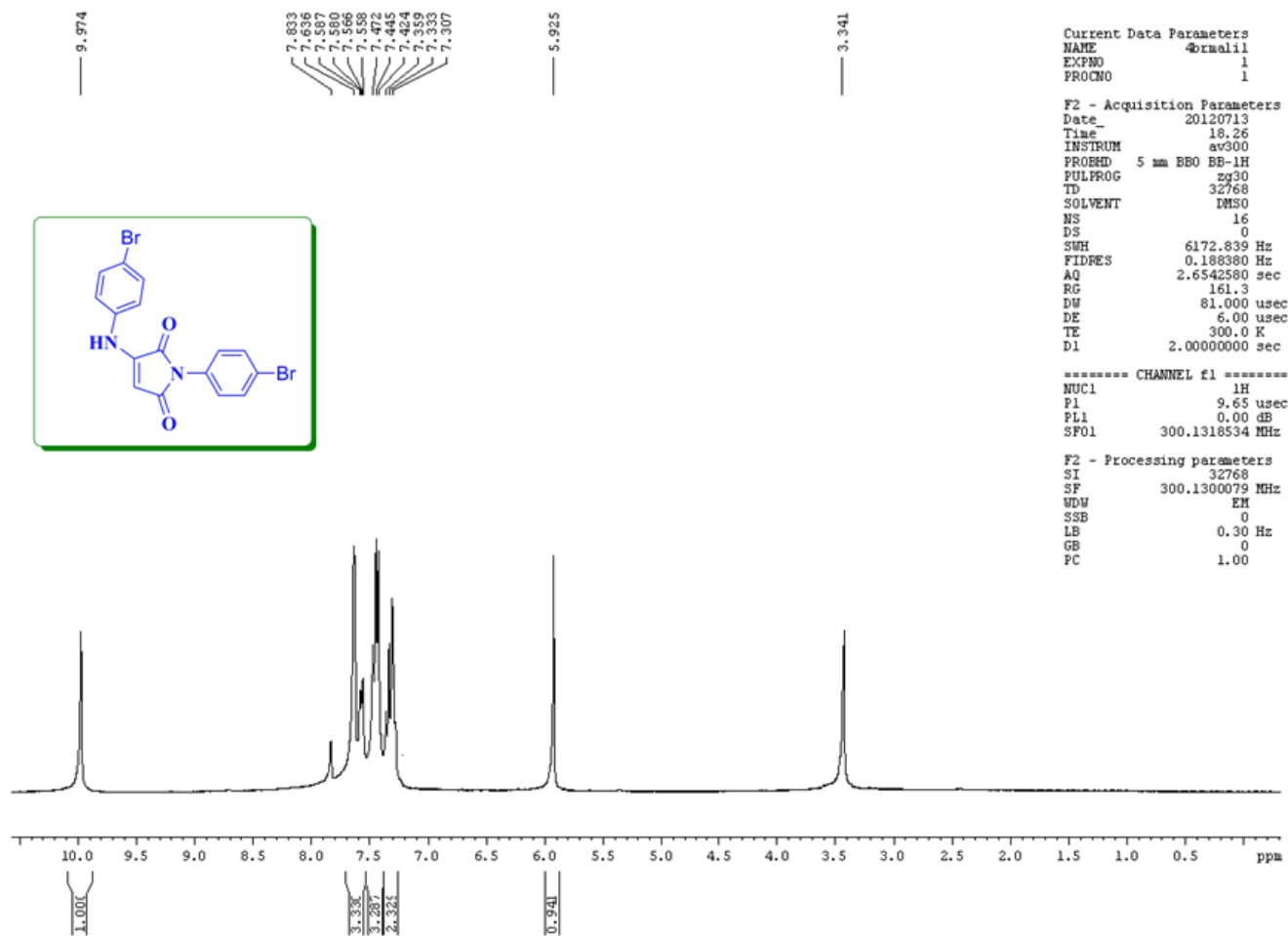


FIG 11: ¹H NMR spectrum of **3d**

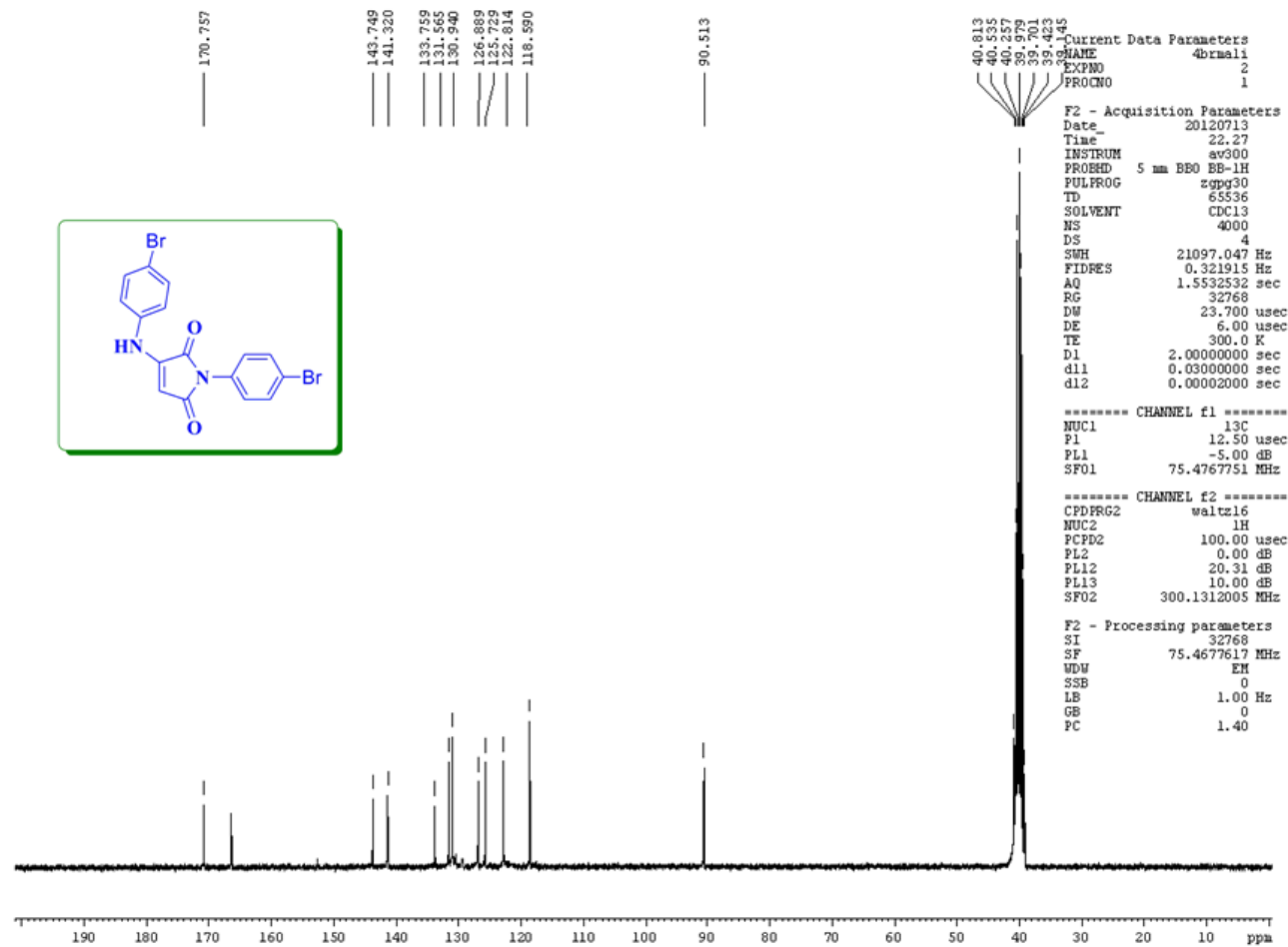


FIG 12: ^{13}C NMR spectrum of **3d**

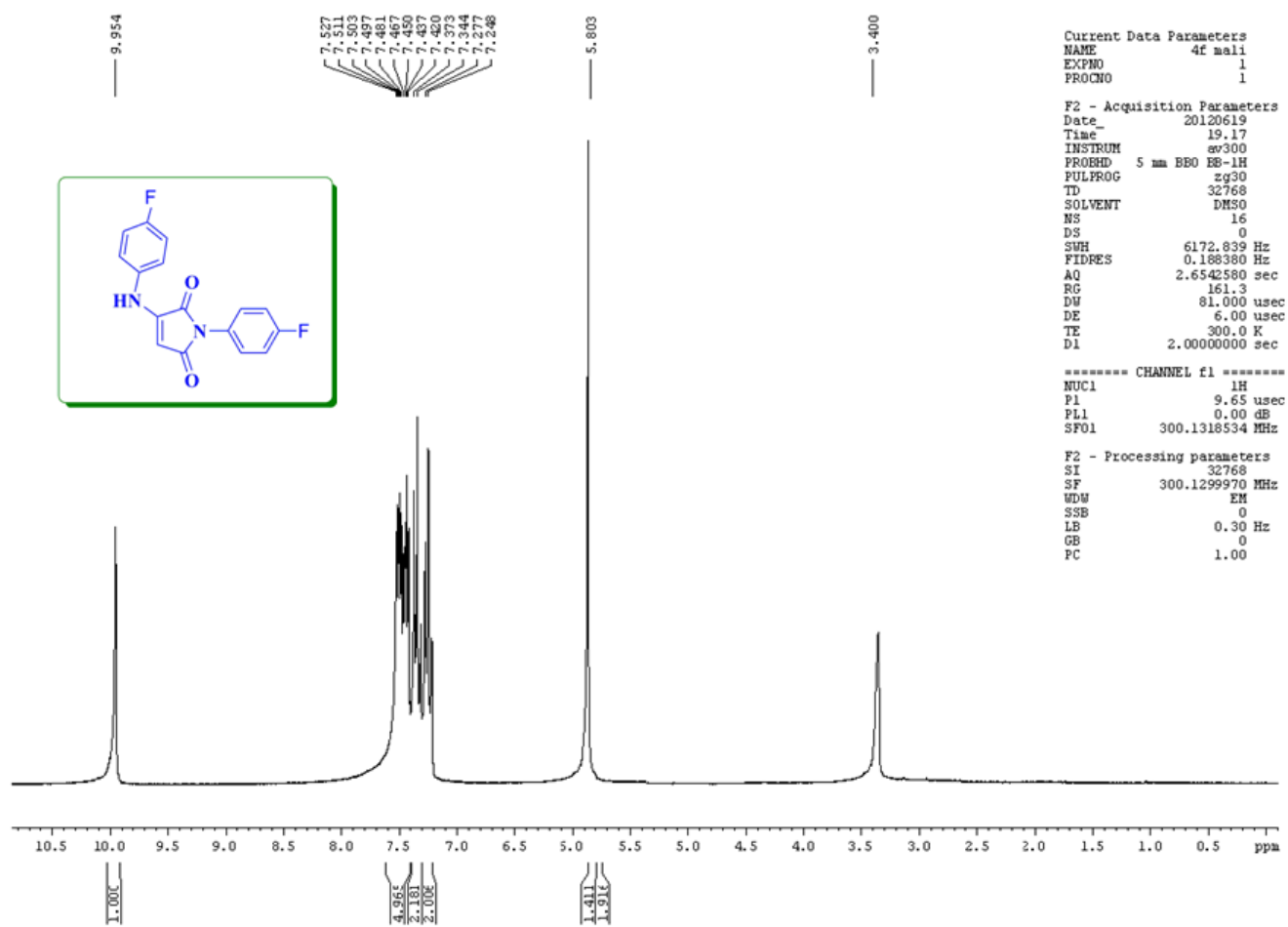


FIG 13: ^1H NMR spectrum of **3e**

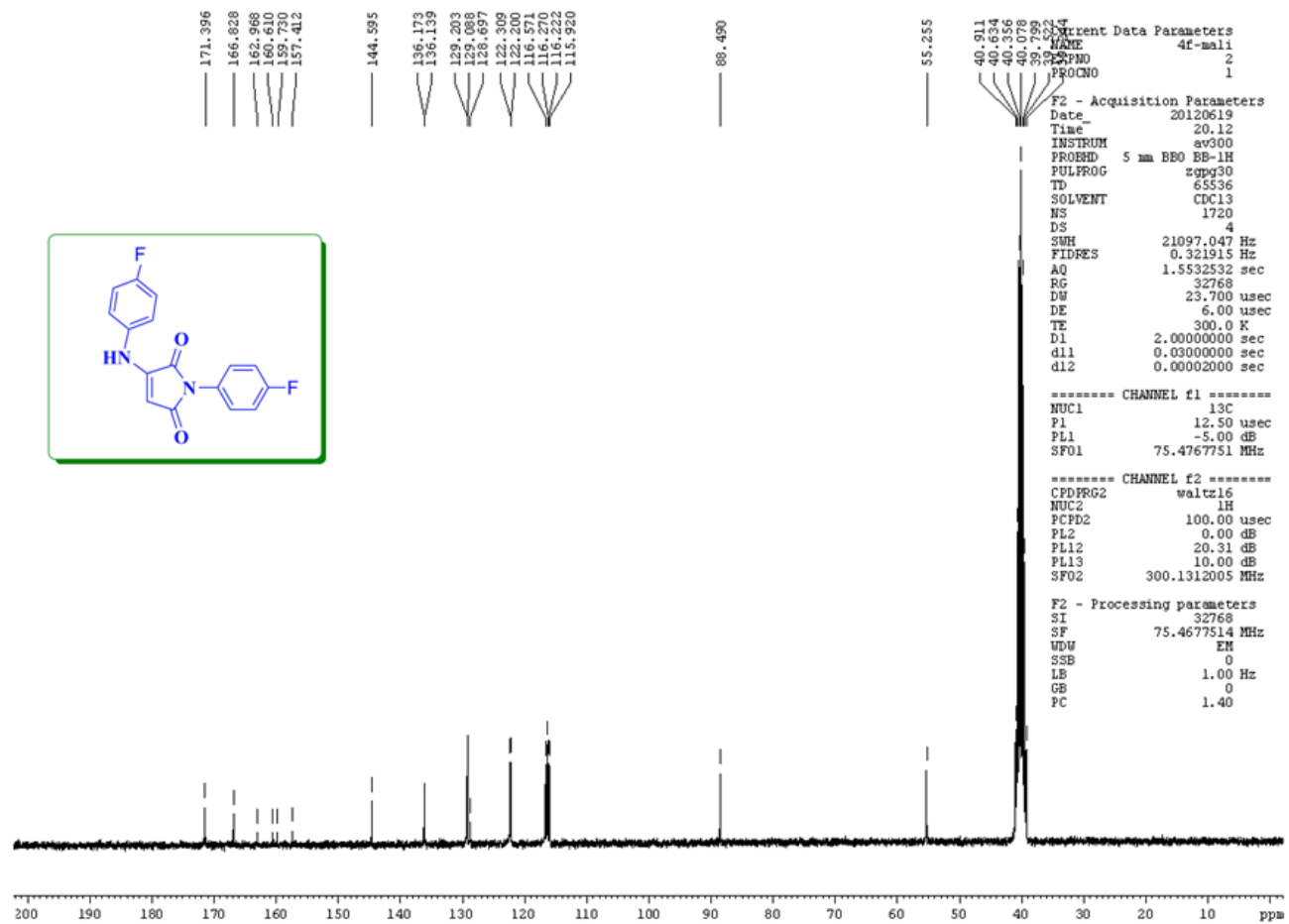


FIG 14: ^{13}C NMR spectrum of **3e**

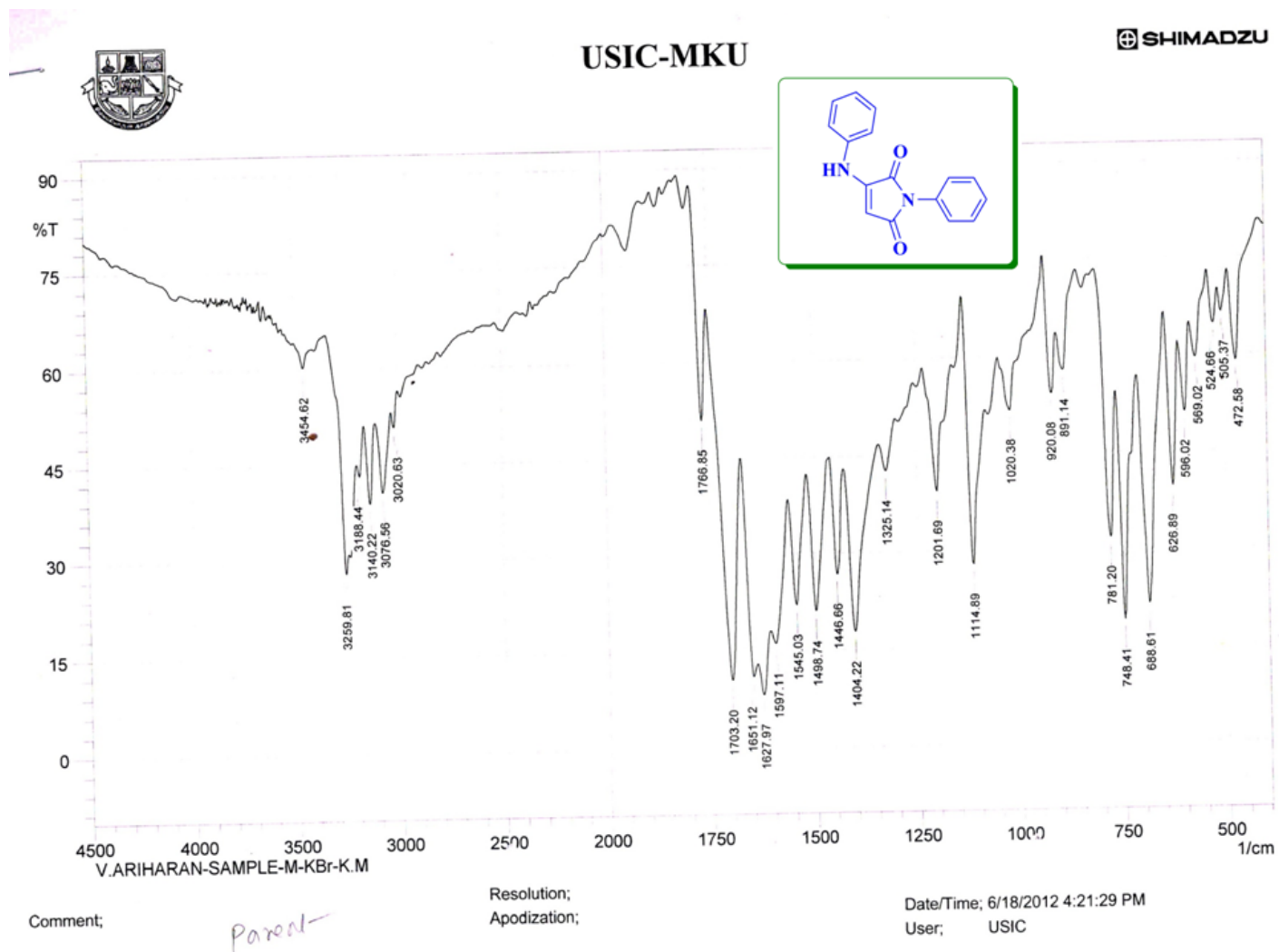


FIG 18: IR spectrum of **3a**

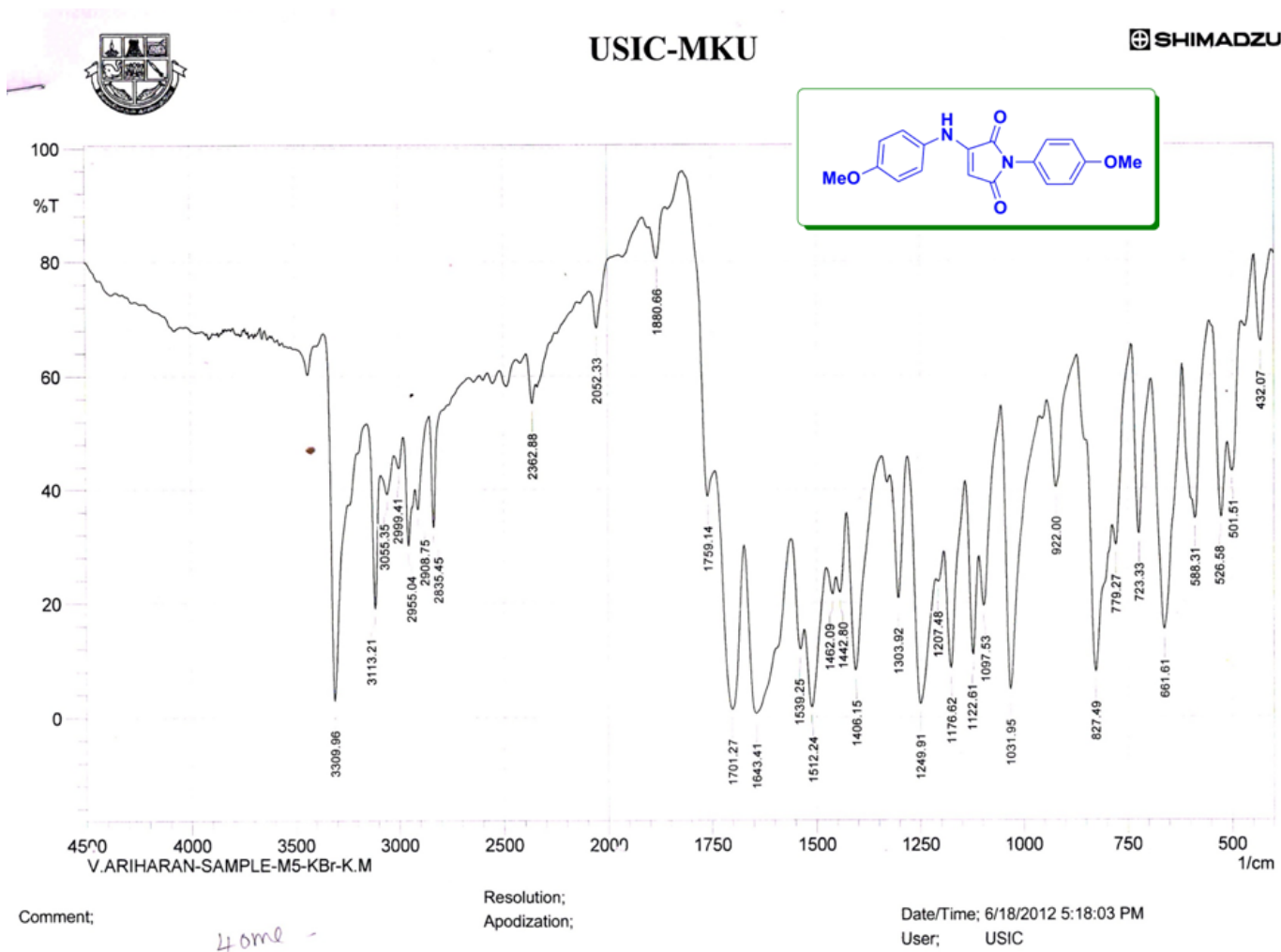


FIG 19: IR spectrum of **3b**

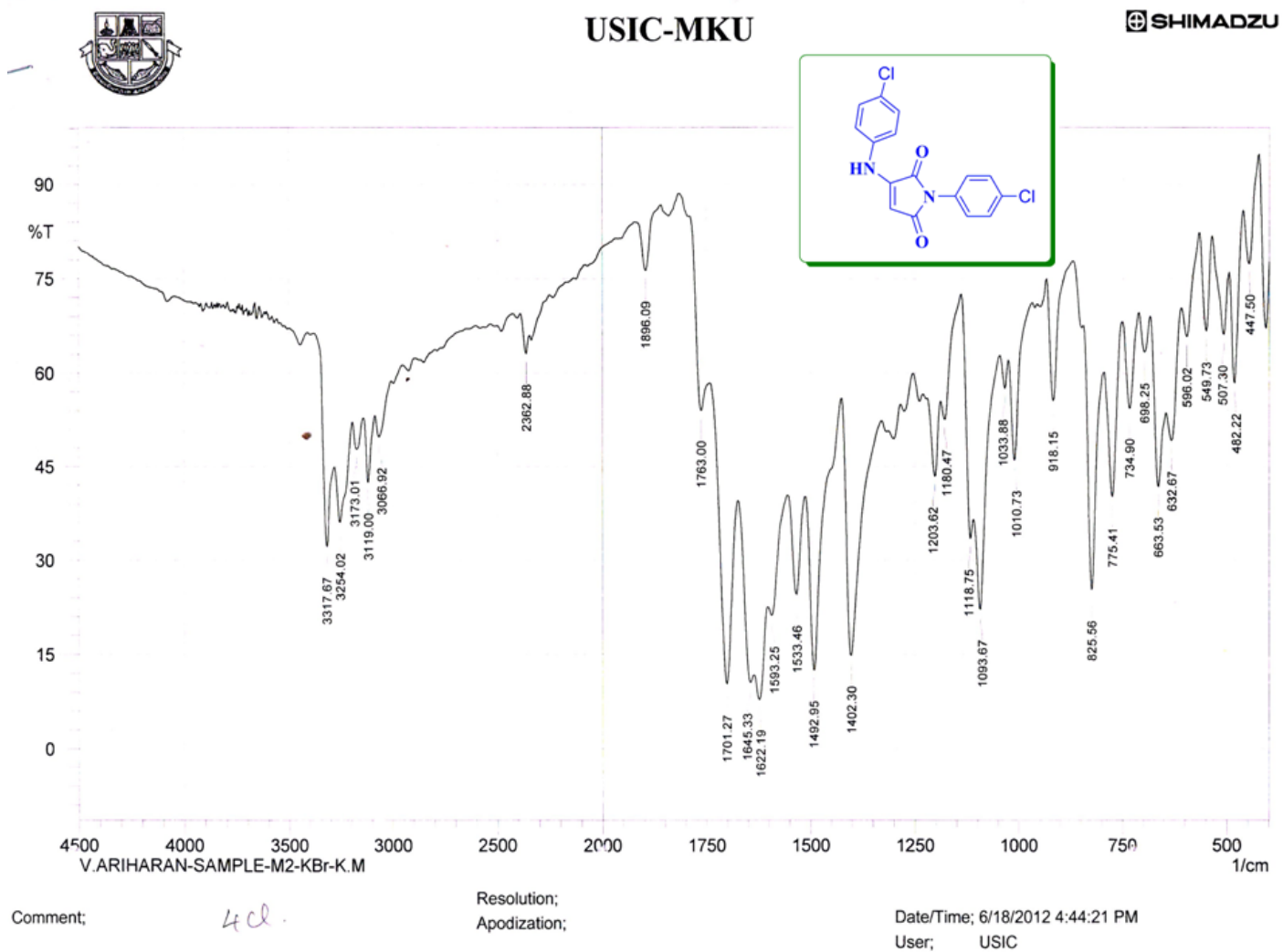


FIG 20: IR spectrum of **3c**

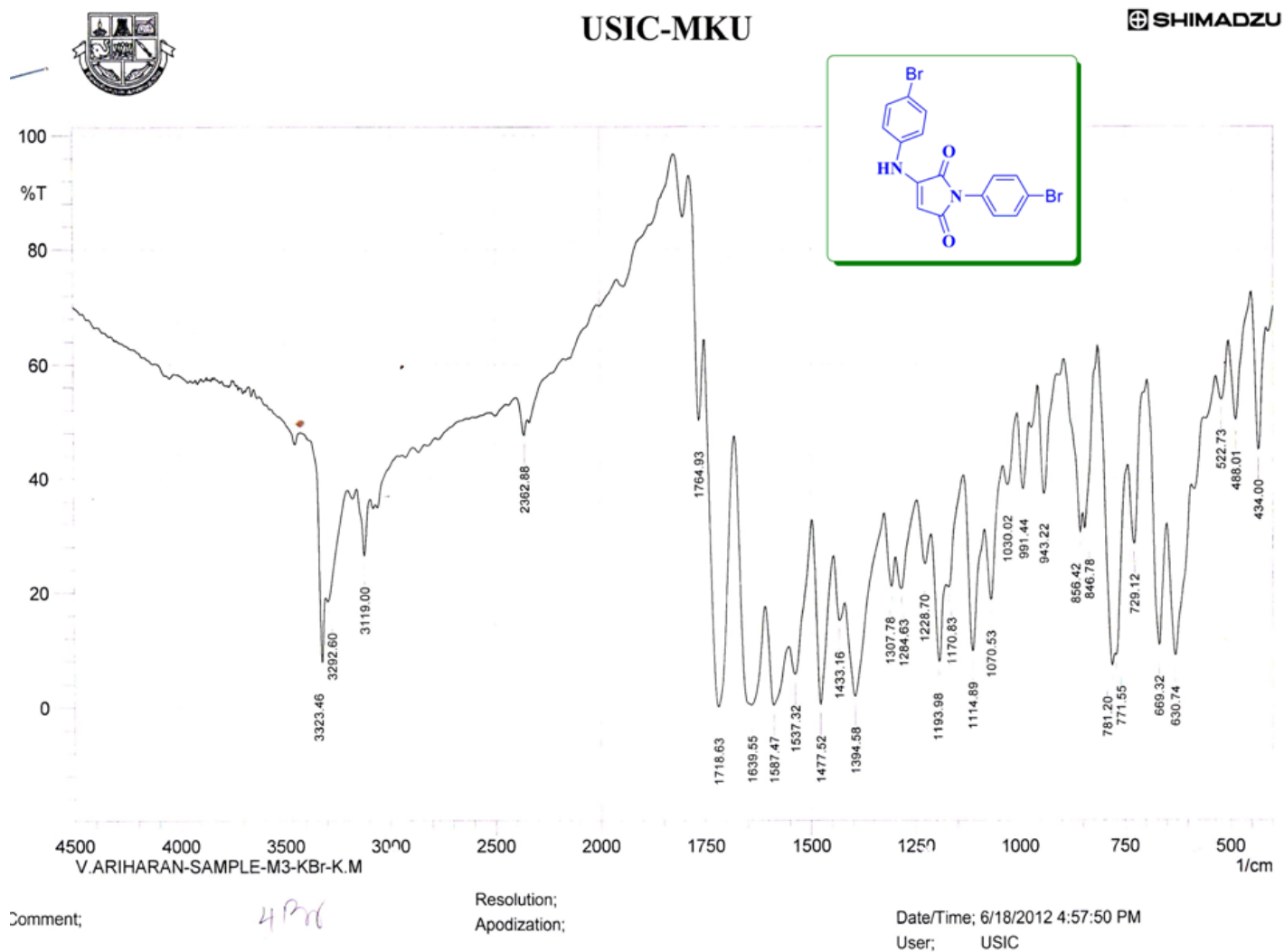


FIG 20: IR spectrum of **3d**

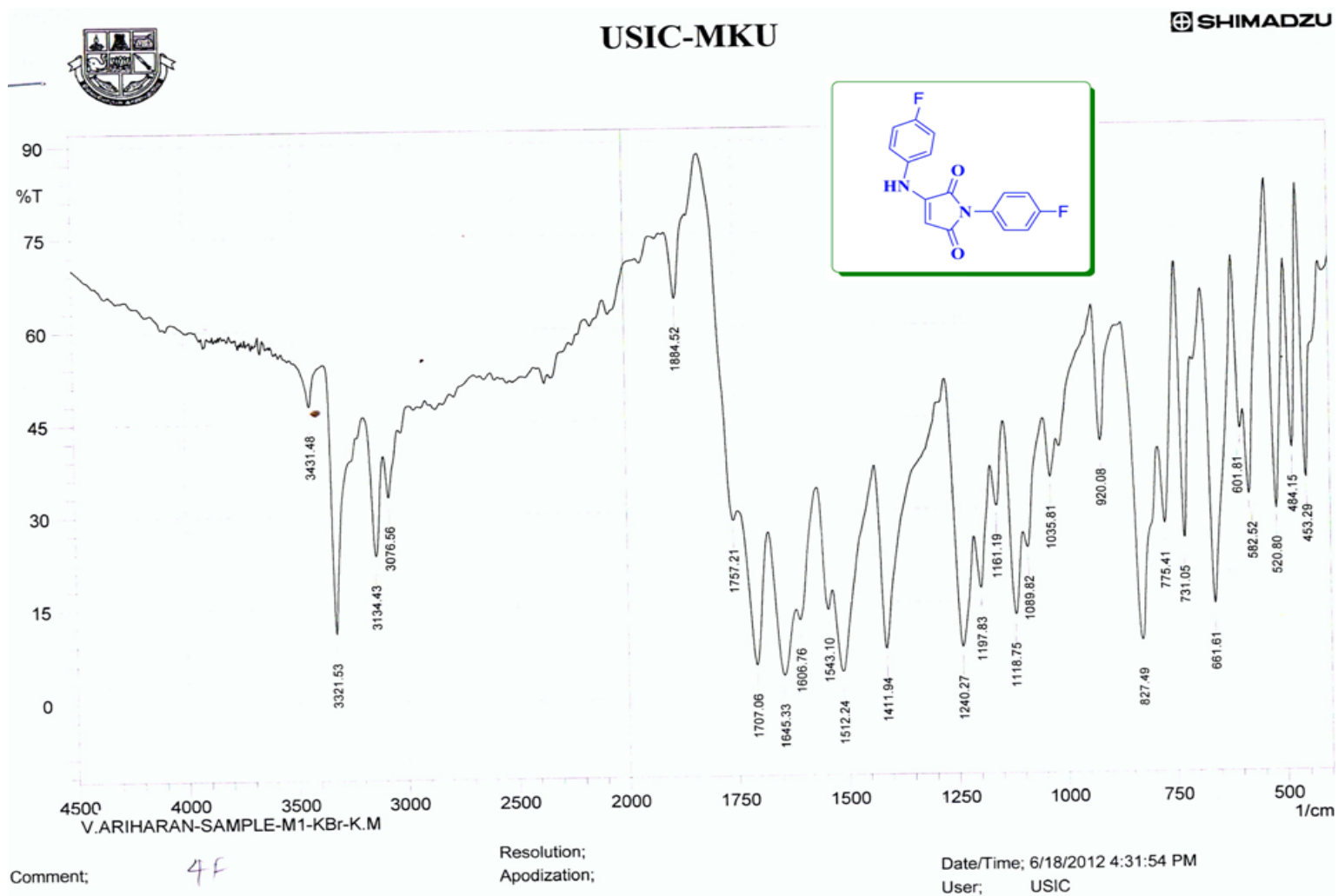


FIG 20: IR spectrum of 3e

Selected Crystallographic Data for 3a

Empirical formula	C ₁₆ H ₁₂ N ₂ O ₂
Formula weight	264.28
Temperature	110(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 7.3183(5) Å alpha = 90°. b = 12.5581(9) Å beta = 90°. c = 27.197(2) Å gamma = 90°.
Volume	2499.5(3) Å ³
Z	8
Density (calculated)	1.405 Mg/m ³
Absorption coefficient	0.768 mm ⁻¹
F(000)	1104
Crystal size	0.17 x 0.08 x 0.03 mm ³
Theta range for data collection	3.25 to 59.99°.
Index ranges	-8<=h<=8, -14<=k<=12, -30<=l<=30
Reflections collected	16898
Independent reflections	3613 [R(int) = 0.0557]
Completeness to theta = 59.99°	98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9773 and 0.8805
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3613 / 0 / 361
Goodness-of-fit on F ²	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0538, wR2 = 0.1386
R indices (all data)	R1 = 0.0663, wR2 = 0.1456
Absolute structure parameter	0.7(5)
Largest diff. peak and hole	0.354 and -0.356 e.Å ⁻³