

Chemoselective Synthesis of Novel Coumarin-based Cyclopenta[*c*]pyrans *via* Base-mediated Reaction of α,β -Unsaturated Coumarins and β -Ketodinitriles

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This version of the Electronic Supplementary Information replaces a previous copy in which the crystallographic details for compound **3d** was incorrect.

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Experimental section

General

Keywords: 4-chloro-3-vinyl coumarins, 2-(2-oxo-2-phenylethyl)malononitriles β -ketodinitriles, α,β -unsaturated coumarins, coumarin-based cyclopenta[*c*]pyrans.

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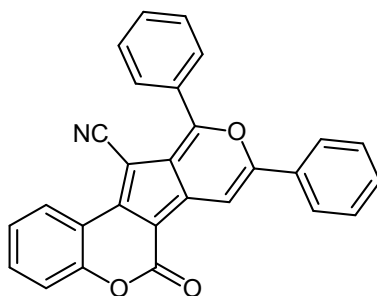
Melting points were measured on an Electrothermal 9100 apparatus. IR spectra were recorded as KBr pellets on a Nicolet FTIR 100 spectrophotometer. ¹H NMR (500 MHz, 300 MHz) and ¹³C NMR (75 MHz) spectra were obtained using Bruker DRX-500 Avance and Bruker DRX-300 Avance spectrometers. All NMR spectra were recorded at r.t. in DMSO-*d*₆ and CDCl₃. Chemical shifts are reported in parts per million (δ) downfield from an internal TMS reference. Coupling constants (*J* values) are reported in hertz (Hz), and standard abbreviations were used to indicate spin multiplicities. Elemental analyses for C, H, and N were performed using a Heraeus CHN-O-Rapid analyzer. Mass spectra were recorded on a Finnigan-MATT 8430 mass spectrometer operating at an ionization potential of 70 eV. All chemicals and solvents were purchased from Merck or Aldrich and were used without further purification. Starting materials were synthesized according to the procedures reported in the literature. Single crystals of compounds **3d** were formed in CH₂Cl₂.

General procedure for the preparation of 3a-3g.

To a magnetically stirred solution of phenacyl bromide (1 mmol, 199 mg), and malononitrile (1 mmol, 66 mg), was added Et₃N (1 mmol, 101 mg) in absolute EtOH (5 ml). After 2 h, α,β -unsaturated coumarin **2** (1 mmol, 310 mg), and Et₃N (2 mmol) were added to the reaction mixture. The reaction was carried out at 80 °C, and it was monitored by TLC. After 12 h a brilliant orange product was isolated by filtration, and purified by washing with EtOH (96%).

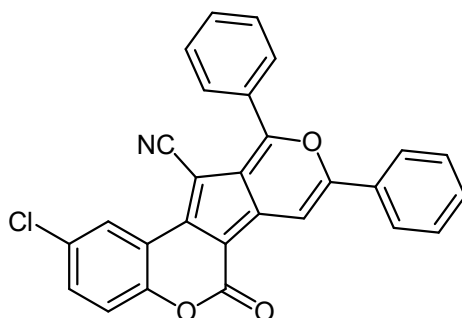
Characteristic data for compounds 3a-3g.

6-Oxo-8,10-diphenyl-6H-pyrano[3',4':4,5]cyclopenta[1,2-*c*]chromene-11-carbonitrile (3a).



Orange powder, dec point = 310-312 °C, 0.32 g, yield: 79%. IR (KBr): 2201 (C≡N), 1720 (C=O), 1643, 1601, and 1542 (Ar), 1225, 1177, 1114, and 999 (C-O) cm⁻¹. Anal. calcd. for C₂₈H₁₅NO₃ (413.42): C, 81.35; H, 3.66, N, 3.39%. Found: C, 81.34; H, 3.62, N, 3.36%. ¹H NMR (500 MHz, DMSO-*d*₆): δ = 7.46 (1H, t, ³J_{HH} = 8.5 Hz, CH² of coumarin), 7.47 (1H, d, ³J_{HH} = 8.3 Hz, CH⁴ of coumarin), 7.63-7.66 (4H, m, 4CH of Ph), 7.77 (2H, t, ³J_{HH} = 7.2 Hz, 2CH_{para} of Ph), 7.83 (1H, t, ³J_{HH} = 7.7 Hz, CH² of coumarin), 8.15 (2H, t, ³J_{HH} = 7.2 Hz, 2CH_{ortho} of Ph), 8.17 (2H, t, ³J_{HH} = 7.2 Hz, 2CH_{ortho} of Ph), 8.55 (1H, d, ³J_{HH} = 7.8 Hz, CH¹ of coumarin), 8.62 (1H, s, CH⁷). MS (EI, 70 eV): *m/z* (%) = 414 (M⁺, 100), 384 (12), 356 (24), 327 (24), 251 (22), 206 (18), 105 (13), 77 (16).

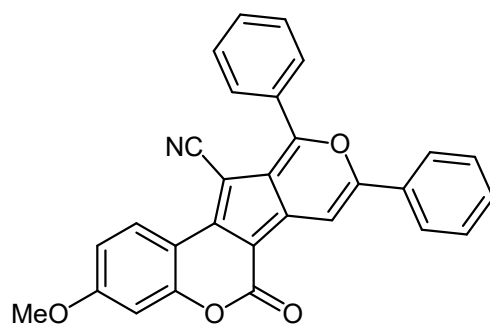
2-Chloro-6-oxo-8,10-diphenyl-6H-pyrano[3',4':4,5]cyclopenta[1,2-c]chromene-11-carbonitrile (3b).



Orange powder, dec point = 318-320 °C, 0.37 g, yield: 84%. IR (KBr): 2202 (C≡N), 1730 (C=O), 1615, 1555, 1541, and 1468 (Ar), 1228, 1176, and 1005 (C-O) cm⁻¹. Anal. calcd. for

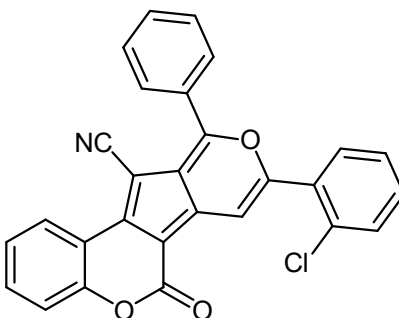
C₂₈H₁₄ClNO₃ (447.87): C, 75.09; H, 3.15, N, 3.13%. Found C, 75.07; H, 3.12, N, 3.12%. ¹H NMR (300 MHz, CDCl₃), δ = 7.35 (1H, d, ³J_{HH} = 8.8 Hz, CH² of coumarin), 7.49 (1H, dd, ³J_{HH} = 8.8 Hz, ²J_{HH} = 2.5 Hz, CH⁴ of coumarin), 7.56-7.60 (3H, m, 3CH of Ph), 7.73-7.76 (3H, m, 3CH of Ph), 8.07 (2H, t, ³J_{HH} = 6.2 Hz, 2CH_{ortho} of Ph), 8.09 (2H, t, ³J_{HH} = 6.2 Hz, 2CH_{ortho} of Ph), 8.66 (1H, d, ³J_{HH} = 2.6 Hz, CH¹ of coumarin), 8.74 (1H, s, CH⁷). MS (EI, 70 eV): *m/z* (%) = 447 (M⁺, 100), 427 (3), 390 (6), 327 (13), 251 (9), 105 (11), 77 (14).

3-Methoxy-6-oxo-8,10-diphenyl-6*H*-pyrano[3',4':4,5]cyclopenta[1,2-*c*]chromene-11-carbonitrile (3c).



Orange powder, dec point = 343-345 °C, 0.34 g, yield: 77%. IR (KBr): 2198 (C≡N), 1727 (C=O), 1614, 1556, 1460, and 1421 (Ar), 1205, 1166, 1117, and 1035 (C-O) cm⁻¹. Anal. calcd. for C₂₉H₁₇NO₄ (443.45): C, 78.55; H, 3.86, N, 3.16%. Found: C, 78.54; H, 3.85, N, 3.14%. ¹H NMR (500 MHz, CDCl₃): δ = 3.92 (3H, s, OCH₃), 6.92 (1H, d, ³J_{HH} = 2.5 Hz, CH⁴ of coumarin), 6.95 (1H, dd, ³J_{HH} = 8.5 Hz, ²J_{HH} = 2.5 Hz, CH² of coumarin), 7.55-7.60 (3H, m, 3CH of Ph), 7.72-7.75 (3H, m, 3CH of Ph), 8.07 (4H, d, ³J_{HH} = 8.7 Hz 4CH_{ortho} of Ph), 8.66 (1H, d, ³J_{HH} = 8.5 Hz, CH¹ of coumarin), 8.74 (1H, s, CH⁷). MS (EI, 70 eV): *m/z* (%) = 443 (M⁺, 100), 400 (20), 372 (10), 314 (18), 221 (23), 105 (38), 77 (24).

8-(2-Chlorophenyl)-6-oxo-10-phenyl-6H-pyrano[3',4':4,5]cyclopenta[1,2-c]chromene-11-carbonitrile (3d).



Orange powder, dec point = 255-257 °C, 0.38 g, yield: 86%. IR (KBr): 2204 (C≡N), 1706 (C=O),

1605, 1548, and 1468 (Ar), 1176, 1115, 1045, and 1029 (C-O) cm⁻¹. Anal. calcd. for

C₂₈H₁₄ClNO₃ (447.87): C, 75.09; H, 3.15, N, 3.13%. Found: C, 75.06; H, 3.12, N, 3.12%. ¹H

NMR (500 MHz, DMSO-*d*₆): δ = 7.42 (1H, t, ³J_{HH} = 7.4 Hz, CH² of coumarin), 7.47 (1H, d, ³J_{HH}

= 8.0 Hz, CH⁴ of coumarin), 7.59-7.66 (3H, m, 3CH of Ar), 7.70-7.74 (3H, m, 3CH of Ph), 7.78

(1H, t, ³J_{HH} = 7.4 Hz, CH³ of coumarin), 7.98 (1H, d, ³J_{HH} = 7.0 Hz, CH of Ar), 8.11 (2H, d, ³J_{HH}

= 7.2 Hz, 2CH of Ar), 8.50 (1H, d, ³J_{HH} = 7.8 Hz, CH¹ of coumarin), 8.51 (1H, s, CH⁷). ¹³C NMR

(75 MHz, CDCl₃): δ = 80.76, 111.48, 117.00, 117.70, 117.94, 123.74, 124.72, 125.59, 127.49,

128.86, 129.77, 130.77, 131.01, 131.09, 131.10, 131.47, 131.97, 132.20, 133.07, 139.31, 148.03,

153.31, 155.44, 158.49, 162.77. MS (EI, 70 eV): *m/z* (%) = 447 (M⁺, 7), 308 (13), 251 (11), 139

(100), 105 (46), 77 (34), . Crystal data for 3d C₂₈H₁₄ClNO₃ (CCDC 1970237): MW = 575.55,

monoclinic, P 1 21/n 1, a = 7.4936(15) Å, b = 24.222(5) Å, c = 13.519(3) Å, α = 90, β =

101.90(3), γ = 90, V = 2401.1(9) Å³, Z = 4, D_c = 1.474 mg/m³, F(000) = 1088, crystal

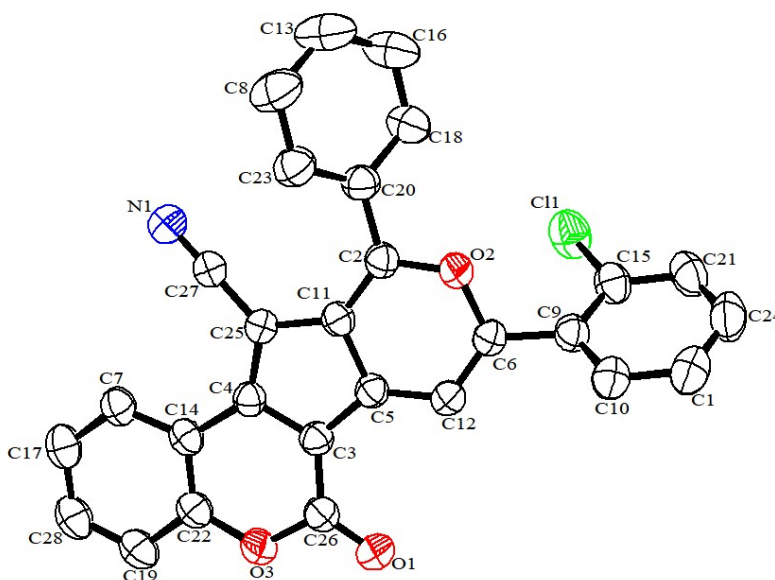
dimension 0.50 × 0.30 × 0.20 mm, radiation, Mo Kα (λ = 0.71073 Å), 2.280 × 2 × 24.499,

intensity data were collected at 293(2) K with a Bruker APEX area-detector diffractometer, and

employing ω/2θ scanning technique, in the range of -8 ≤ h ≤ 8, 0 ≤ k ≤ 28, 0 ≤ l ≤ 15; the

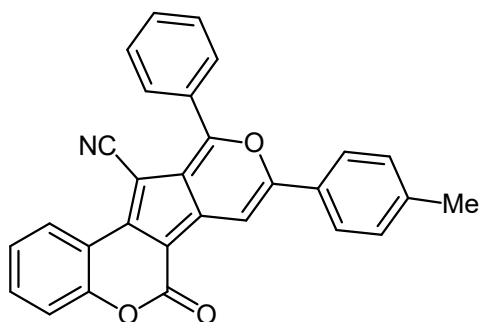
structure was solved by a direct method, all non-hydrogen atoms were positioned and anisotropic

thermal parameters refined from 3827 observed reflections with $R(\text{int}) = 0.0286$ by a full-matrix least-squares technique converged to $R1 = 0.0695$, and $wR2 = 0.1724$ [$I > 2\sigma(I)$].



ORTEP diagram of **3d** (CCDC 1970237).

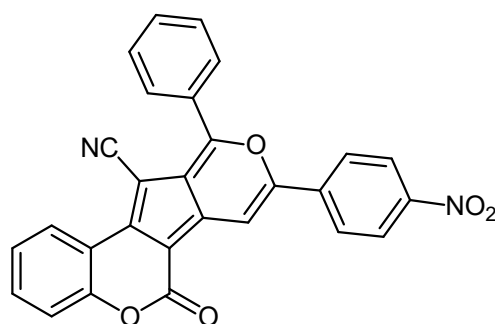
6-Oxo-8-phenyl-10-(*p*-tolyl)-6*H*-pyrano[3',4':4,5]cyclopenta[1,2-*c*]chromene-11-carbonitrile (3e**).**



Orange powder, dec point = 342-345 °C, 0.32 g, yield: 75%. IR (KBr): 2198 (C≡N), 1730 (C=O), 1605, 1560, 1543, and 1511 (Ar), 1176, 1112, 1052, and 1036 (C-O) cm^{-1} . Anal. calcd. for $\text{C}_{29}\text{H}_{17}\text{NO}_3$ (427.45): C, 81.49; H, 4.01, N, 3.28%. Found: C, 81.44; H, 4.02, N, 3.26%. ^1H NMR (300 MHz, $\text{DMSO-}d_6$): $\delta = 2.41$ (3H, s, CH_3), 7.44 (2H, d, $^3J_{\text{HH}} = 8.0$ Hz, 2CH of Ar), 7.45 (1H,

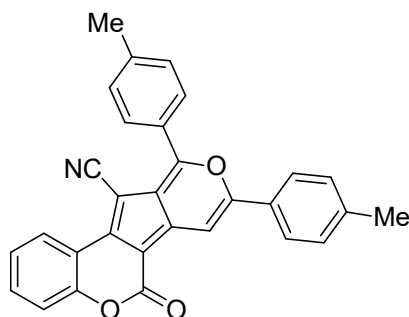
t, $^3J_{\text{HH}} = 7.8$ Hz, CH² of coumarin), 7.49 (1H, d, $^3J_{\text{HH}} = 7.8$ Hz, CH⁴ of coumarin), 7.67 (1H, t, $^3J_{\text{HH}} = 7.4$ Hz, CH³ of coumarin), 7.74 (1H, t, $^3J_{\text{HH}} = 8.5$ Hz, CH_{para} of Ph), 7.77 (2H, t, $^3J_{\text{HH}} = 8.5$ Hz, 2CH_{meta} of Ph), 8.05 (2H, d, $^3J_{\text{HH}} = 8.0$ Hz, 2CH of Ar), 8.15 (2H, d, $^3J_{\text{HH}} = 8.4$ Hz, 2CH_{ortho} of Ph), 8.58 (1H, d, $^3J_{\text{HH}} = 7.7$ Hz, CH¹ of coumarin), 8.62 (1H, s, CH⁷). MS (EI, 70 eV): *m/z* (%) = 427 (M⁺, 100), 370 (6), 354 (8), 340 (10), 327 (14), 264 (12), 105 (55), 77 (21).

8-(4-Nitrophenyl)-6-oxo-10-phenyl-6H-pyrano[3',4':4,5]cyclopenta[1,2-c]chromene-11-carbonitrile (3f).



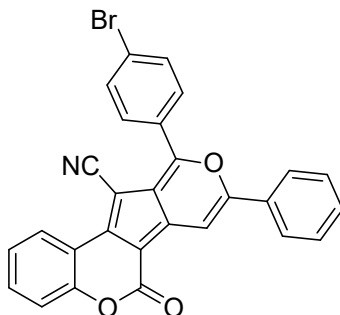
Orange powder, dec point = 367-369 °C, 0.41 g, yield: 91%. IR (KBr): 2204 (C≡N), 1720 (C=O), 1594, 1542, 1521, and 1424 (Ar), 1175, 1111, 1051, and 1000 (C-O) cm⁻¹. Anal. calcd. for C₂₈H₁₄N₂O₅ (458.09): C, 73.36; H, 3.08, N, 6.11%. Found: C, 73.34; H, 3.10, N, 6.13%. ¹H NMR (500 MHz, DMSO-*d*₆): δ = 7.43 (1H, t, $^3J_{\text{HH}} = 8.4$ Hz, CH² of coumarin), 7.46 (1H, d, $^3J_{\text{HH}} = 8.6$ Hz, CH⁴ of coumarin), 7.63 (1H, t, $^3J_{\text{HH}} = 8.0$ Hz, CH³ of coumarin), 7.76 (2H, t, $^3J_{\text{HH}} = 7.6$ Hz, 2CH_{meta} of Ph), 7.82 (1H, t, $^3J_{\text{HH}} = 7.4$ Hz, CH_{para} of Ph), 8.17 (2H, d, $^3J_{\text{HH}} = 7.6$ Hz, 2CH_{ortho} of Ph), 8.38 (2H, d, $^3J_{\text{HH}} = 8.6$ Hz, 2CH of Ar), 8.41 (2H, d, $^3J_{\text{HH}} = 8.6$ Hz, 2CH of Ar), 8.55 (1H, d, $^3J_{\text{HH}} = 7.9$ Hz, CH¹ of coumarin), 8.80 (1H, s, CH⁷). MS (EI, 70 eV): *m/z* (%) = 458 (M⁺, 100), 412 (23), 354 (30), 327 (62), 251 (28), 105 (71), 77 (46).

6-Oxo-8,10-di-*p*-tolyl-6H-pyrano[3',4':4,5]cyclopenta[1,2-c]chromene-11-carbonitrile (3g).



Orange powder, dec point = 348-350 °C, 0.31 g, yield: 72%. IR (KBr): 2198 (C≡N), 1730 (C=O), 1604, 1563, 1484, and 1422 (Ar), 1175, 1112, 1051, and 998 (C-O) cm⁻¹. Anal. calcd. for C₃₀H₁₉NO₃ (441.14): C, 81.62; H, 4.34, N, 3.17%. Found: C, 81.63; H, 4.36, N, 3.15%. ¹H NMR (500 MHz, DMSO-*d*₆): δ = 2.47 (3H, s, CH₃), 2.55 (3H, s, CH₃), 7.37 (2H, d, ³J_{HH} = 7.7 Hz, 2CH of Ar), 7.38 (1H, t, ³J_{HH} = 7.2 Hz, CH² of coumarin), 7.43 (1H, d, ³J_{HH} = 8.2 Hz, CH⁴ of coumarin), 7.53 (2H, d, ³J_{HH} = 7.7 Hz, 2CH of Ar), 7.56 (1H, t, ³J_{HH} = 7.7 Hz, CH³ of coumarin), 7.96 (2H, d, ³J_{HH} = 7.8 Hz, 2CH of Ar), 7.99 (2H, d, ³J_{HH} = 7.9 Hz, 2CH of Ar), 8.72 (1H, s, CH⁷), 8.77 (1H, d, ³J_{HH} = 7.9 Hz, CH¹ of coumarin). MS (EI, 70 eV): *m/z* (%) = 441 (M⁺, 100), 354 (16), 264 (19), 220 (29), 119 (25), 91 (57).

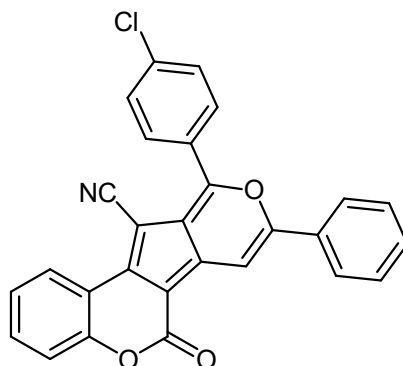
10-(4-Bromophenyl)-6-oxo-8-phenyl-6H-pyrano[3',4':4,5]cyclopenta[1,2-c]chromene-11-carbonitrile (3h).



Orange powder, dec point = 357-359 °C, 0.40 g, yield: 83%. IR (KBr): 2204 (C≡N), 1729 (C=O), 1602, 1563, 1541, and 1425 (Ar), 1175, 1113, 1051, and 1005 (C-O) cm⁻¹. Anal. calcd. for

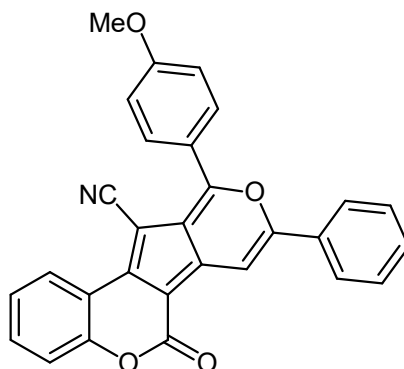
C₂₈H₁₄BrNO₃ (491.02): C, 68.31; H, 2.87, N, 2.85%. Found: C, 68.33; H, 2.85, N, 2.86%. ¹H NMR (500 MHz, DMSO-*d*₆): δ = 7.48 (1H, t, ³J_{HH} = 8.2 Hz, CH² of coumarin), 7.49 (1H, d, ³J_{HH} = 8.4 Hz, CH⁴ of coumarin), 7.63 (2H, d, ³J_{HH} = 7.0 Hz, 2CH of Ar), 7.64 (1H, t, ³J_{HH} = 8.2 Hz, CH_{para} of Ph), 7.67 (1H, t, 7.2 Hz, CH³ of coumarin), 7.98 (2H, d, ³J_{HH} = 8.2 Hz, 2CH_{meta} of Ph), 8.11 (2H, d, ³J_{HH} = 8.2 Hz, 2CH_{ortho} of Ph), 8.16 (2H, d, ³J_{HH} = 7.0 Hz, 2CH of Ar), 8.56 (1H, d, ³J_{HH} = 7.0 Hz, CH¹ of coumarin), 8.66 (1H, s, CH⁷). MS (EI, 70 eV): *m/z* (%) = 493 (M⁺+1, 100), 491 (M⁺, 98), 327 (26), 251 (30), 105 (27), 77 (41).

10-(4-Chlorophenyl)-6-oxo-8-phenyl-6H-pyrano[3',4':4,5]cyclopenta[1,2-*c*]chromene-11-carbonitrile (3i).



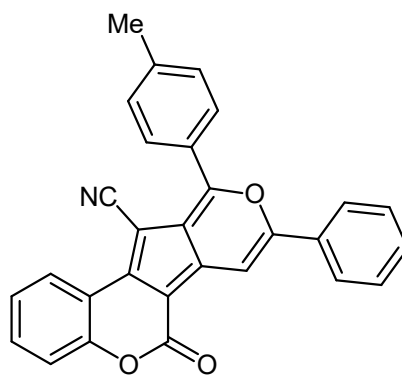
Orange powder, dec point = 370-373 °C, 0.36 g, yield: 81%. IR (KBr): 2200 (C≡N), 1729 (C=O), 1602, 1563, 1468, and 1423 (Ar), 1225, 1175, 1112, and 1051 (C-O) cm⁻¹. Anal. calcd. for C₂₈H₁₄ClNO₃ (447.87): C, 75.09; H, 3.15, N, 3.13%. Found: C, 75.06; H, 3.13, N, 3.12%. ¹H NMR (500 MHz, CDCl₃): δ = 7.42 (1H, t, ³J_{HH} = 7.3 Hz, CH² of coumarin), 7.46 (1H, d, ³J_{HH} = 8.2 Hz, CH⁴ of coumarin), 7.50-7.64 (4H, m, 2CH_{meta} of Ph, CH_{para} of Ph, and CH³ of coumarin), 7.74 (2H, d, ³J_{HH} = 8.5 Hz, 2CH of Ar), 8.06 (2H, d, ³J_{HH} = 8.5 Hz, 2CH of Ar), 8.09 (2H, d, ³J_{HH} = 8.0 Hz, 2CH_{meta} of Ph), 8.78 (1H, d, ³J_{HH} = 7.9 Hz, CH¹ of coumarin), 8.81 (1H, s, CH⁷). MS (EI, 70 eV): *m/z* (%) = 447 (M⁺, 2), 327 (10), 308 (9), 251 (18), 138 (100), 105 (31), 77 (28).

8-(4-Methoxyphenyl)-6-oxo-10-phenyl-6H-pyrano[3',4':4,5]cyclopenta[1,2-*c*]chromene-11-carbonitrile (3j).

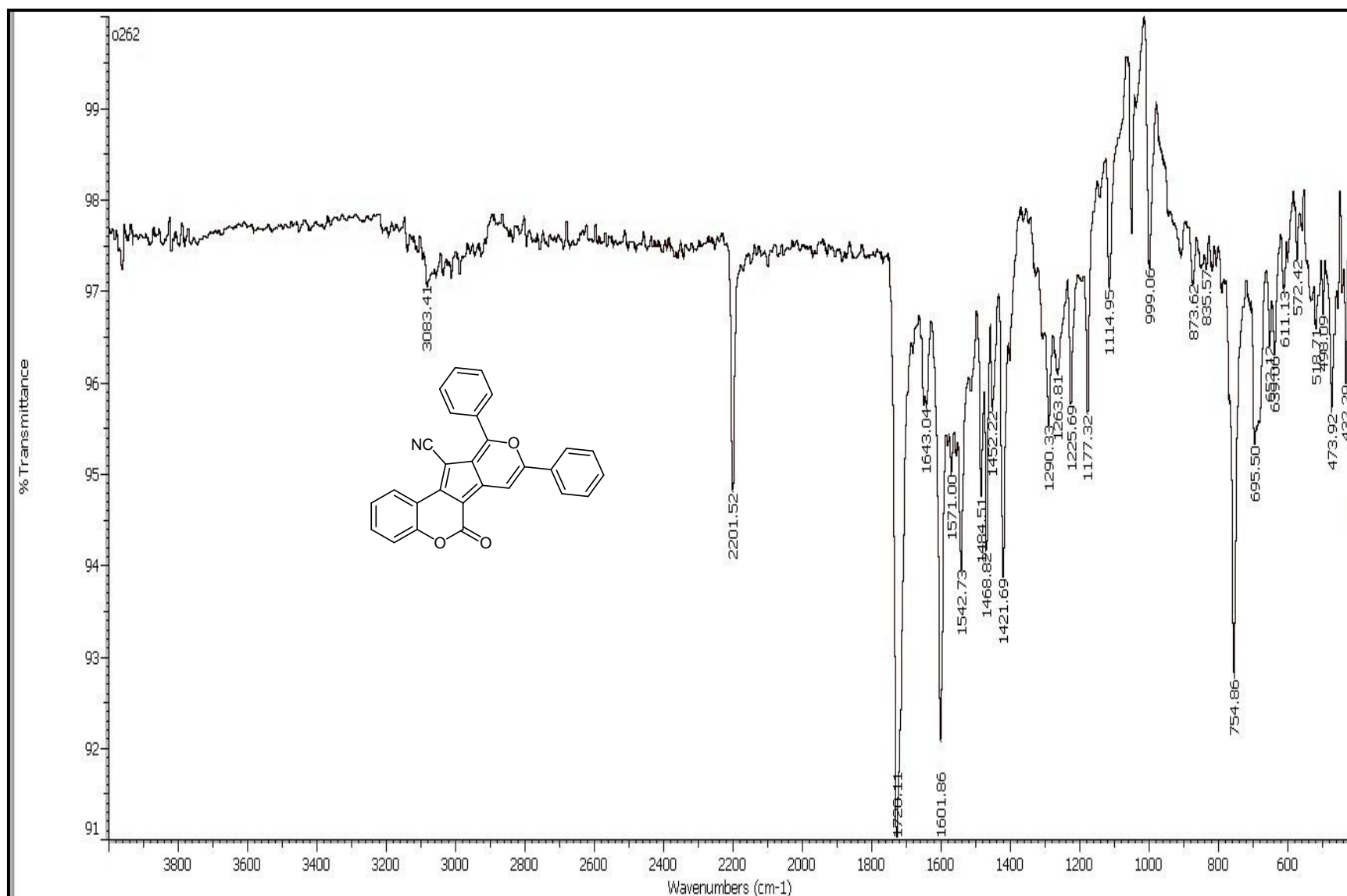


Orange powder, dec point = 318-320 °C, 0.35 g, yield: 80%. IR (KBr): 2198 (C≡N), 1735 (C=O), 1603, 1559, 1547, and 1470 (Ar), 1000 (C-O) cm⁻¹. Anal. calcd. for C₂₉H₁₇NO₄ (443.45): C, 78.55; H, 3.86, N, 3.16%. Found: C, 78.54; H, 3.84, N, 3.15%. ¹H NMR (500 MHz, DMSO-*d*₆): δ = 3.95 (3H, s, OCH₃), 7.28 (2H, d, ³J_{HH} = 8.7 Hz, 2CH of Ar), 7.40 (1H, t, ³J_{HH} = 7.1 Hz, CH⁴ of coumarin), 7.41 (1H, d, ³J_{HH} = 7.1 Hz, CH² of coumarin), 7.50-7.60 (3H, m, 3CH of Ph), 7.60 (1H, t, ³J_{HH} = 6.8 Hz, CH³ of coumarin), 8.07 (2H, d, ³J_{HH} = 7.3 Hz, 2CH_{ortho} of Ph), 8.11 (2H, d, ³J_{HH} = 8.6 Hz, 2CH of Ar), 8.48 (1H, s, CH⁷), 8.51 (1H, d, ³J_{HH} = 7.0 Hz, CH¹ of coumarin). MS (EI, 70 eV: *m/z* (%) = 443 (M⁺, 100), 428 (2), 372 (7), 344 (7), 314 (9), 221 (16), 105 (20), 77 (13).

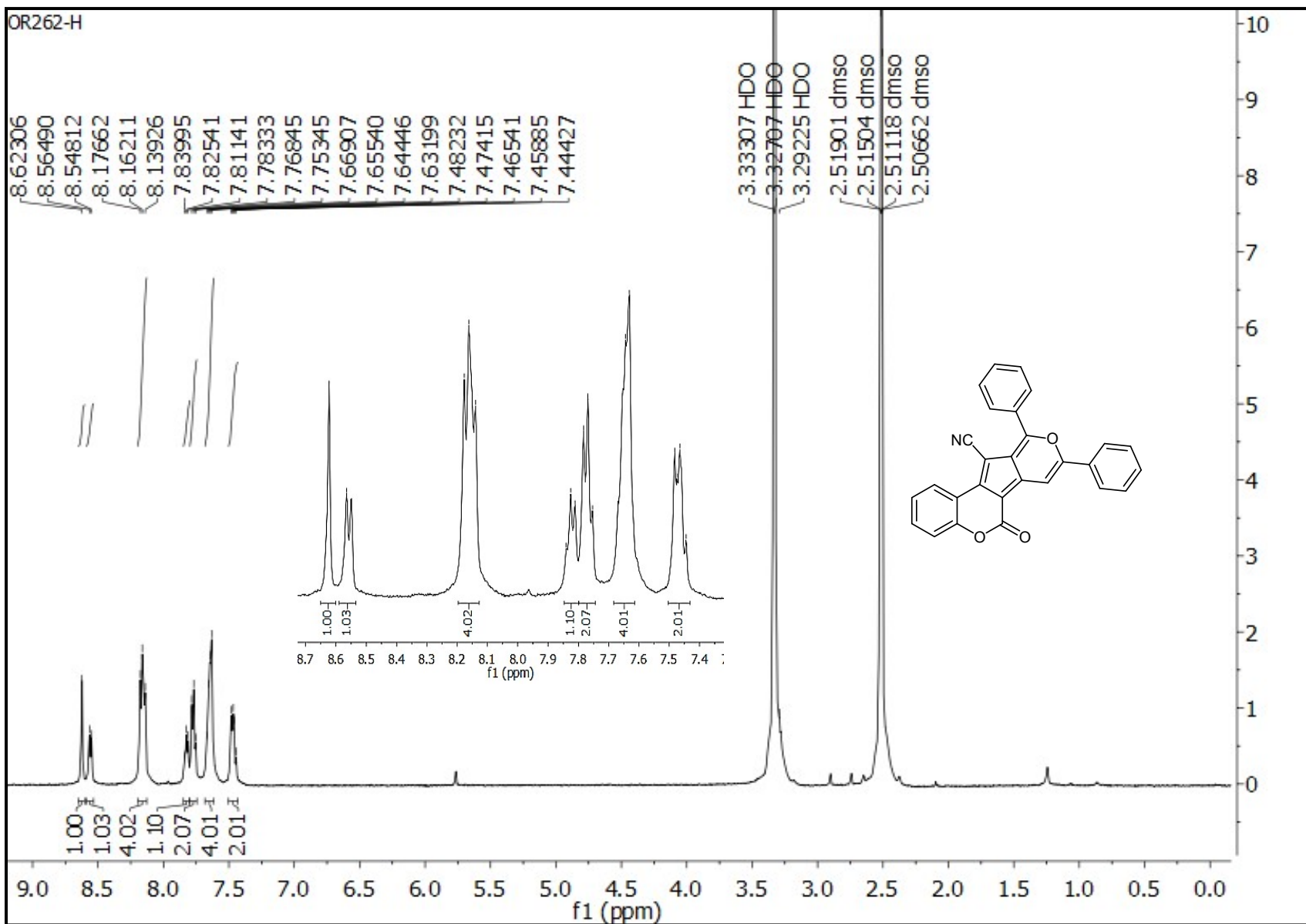
6-Oxo-8-phenyl-10-(*p*-tolyl)-6H-pyrano[3',4':4,5]cyclopenta[1,2-*c*]chromene-11-carbonitrile (3k).



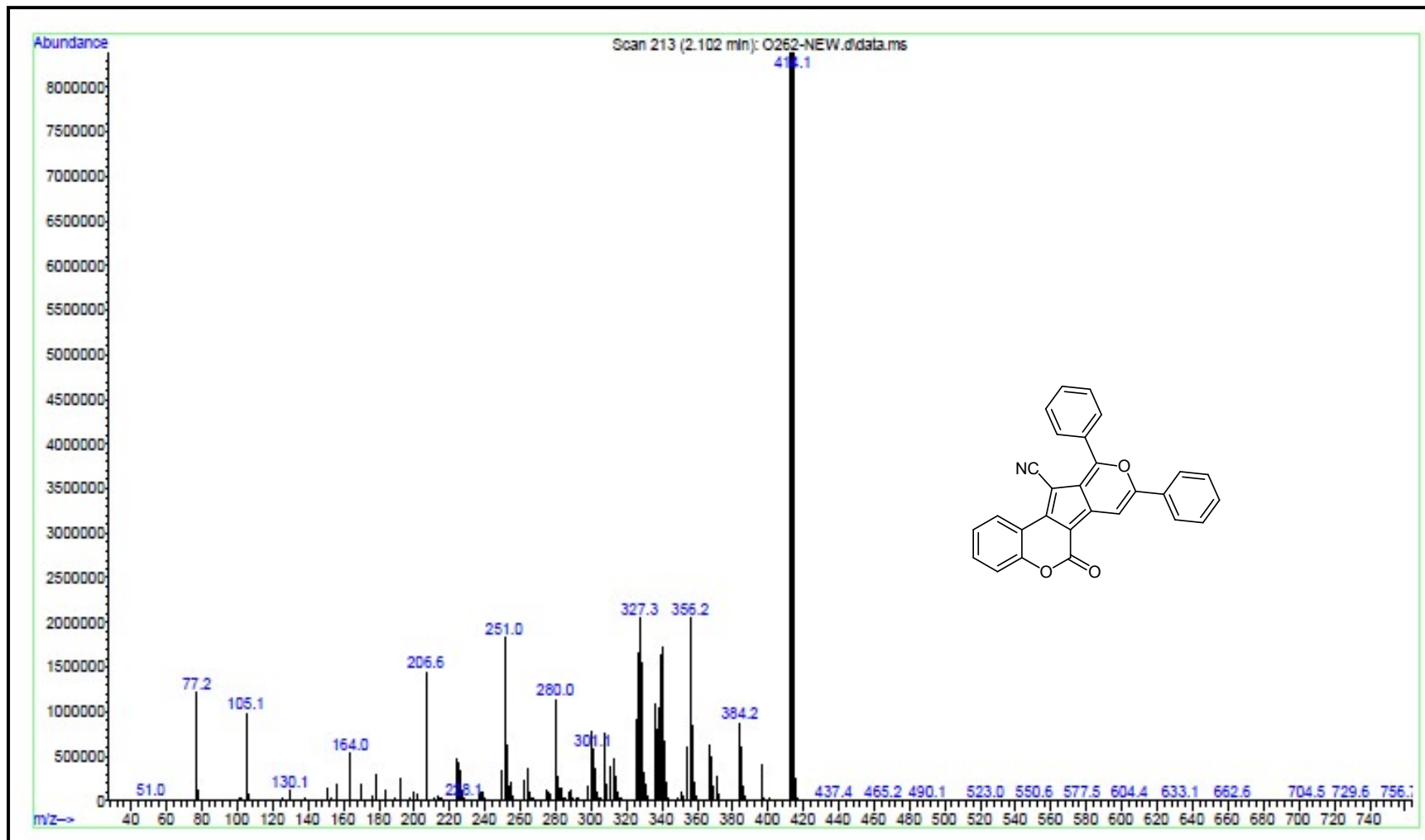
Orange powder, dec point = 301-305 °C, 0.33 g, yield: 78%. IR (KBr): 2181 (C≡N), 1680 (C=O), 1652, 1616, 1598, and 1486 (Ar), 1218, 1201, 1169, and 1105 (C-O) cm⁻¹. Anal. calcd. for C₂₉H₁₇NO₃ (427.12): C, 81.49; H, 4.01, N, 3.28%. Found: C, 81.51; H, 4.02, N, 3.28%. ¹H NMR (500 MHz, DMSO-*d*₆): δ = 2.56 (3H, s, CH₃), 7.38 (1H, t, ³J_{HH} = 7.6 Hz, CH² of coumarin), 7.43 (1H, d, ³J_{HH} = 8.3 Hz, CH² of coumarin), 7.52-7.60 (6H, m, 6CH of Ar), 8.00 (2H, d, ³J_{HH} = 7.7 Hz, 2CH_{ortho} of Ph), 8.07 (2H, d, ³J_{HH} = 7.5 Hz, 2CH of Ar), 8.77 (1H, s, CH⁷), 8.78 (1H, d, ³J_{HH} = 7.9 Hz, CH¹ of coumarin). MS (EI, 70 eV: *m/z* (%) = 427 (M⁺, 100), 370 (4), 340 (5), 327 (4), 213 (9).



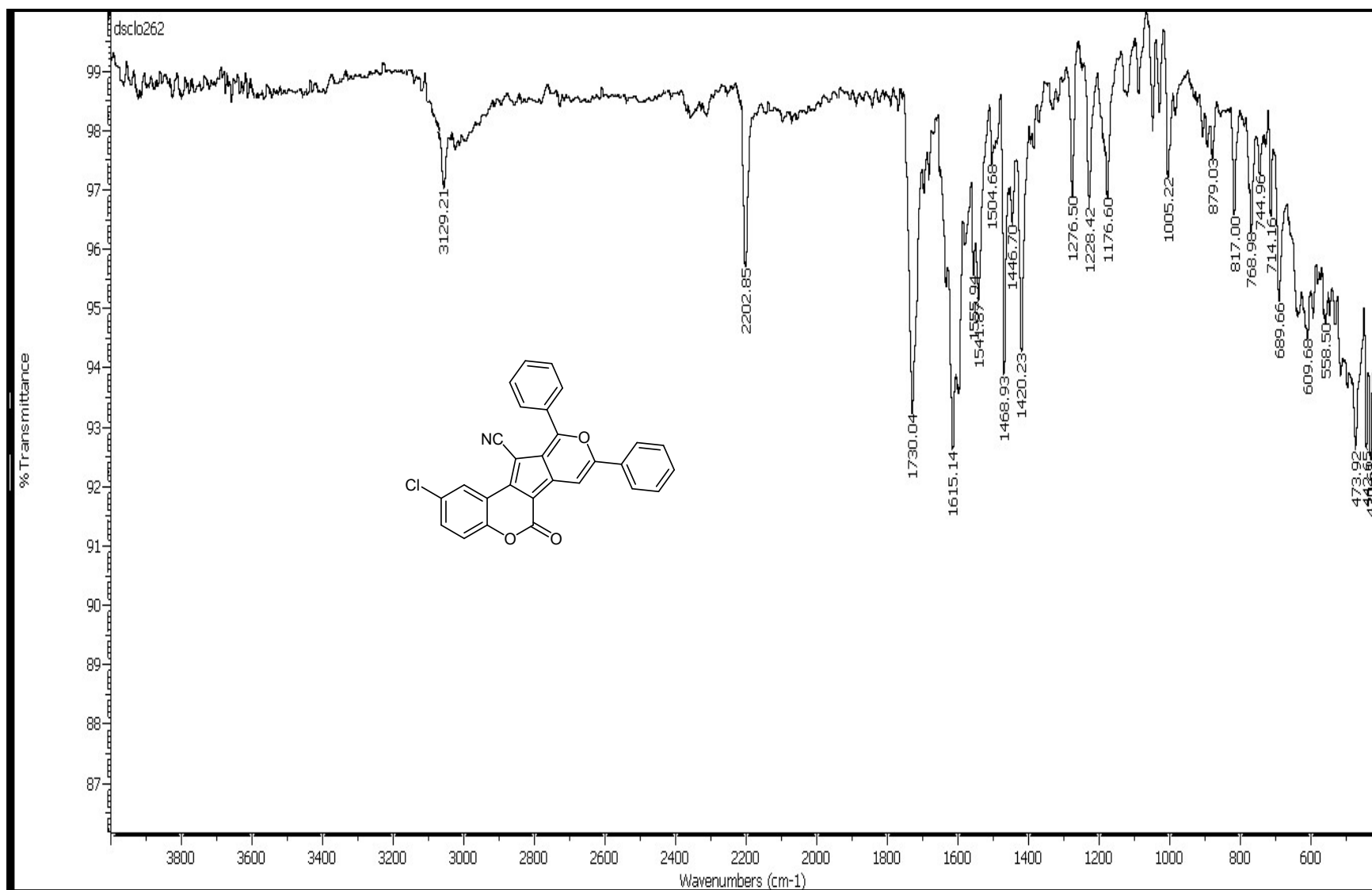
IR spectrum of 3a



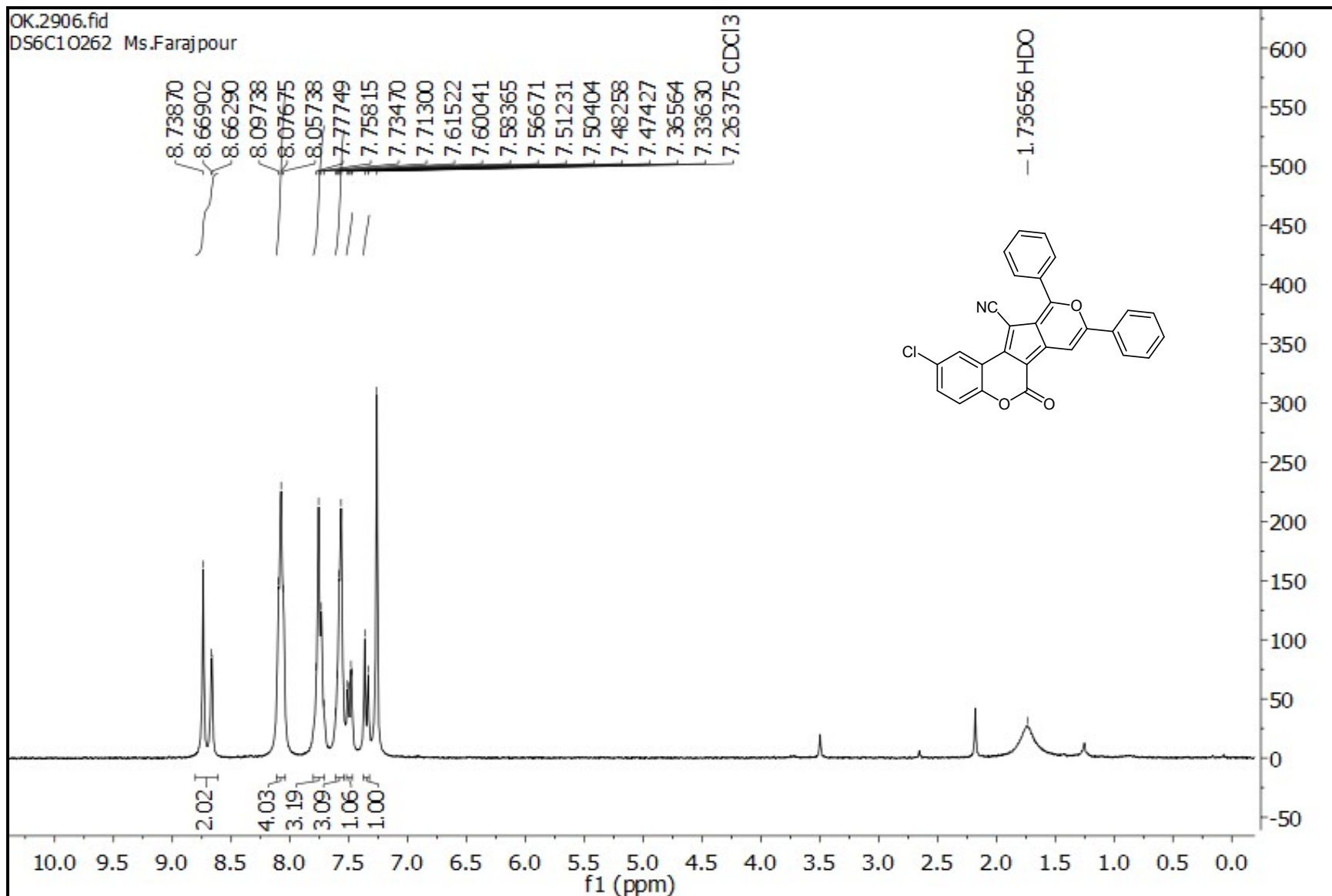
¹H NMR (DMSO-*d*₆, 500 MHz) of **3a**



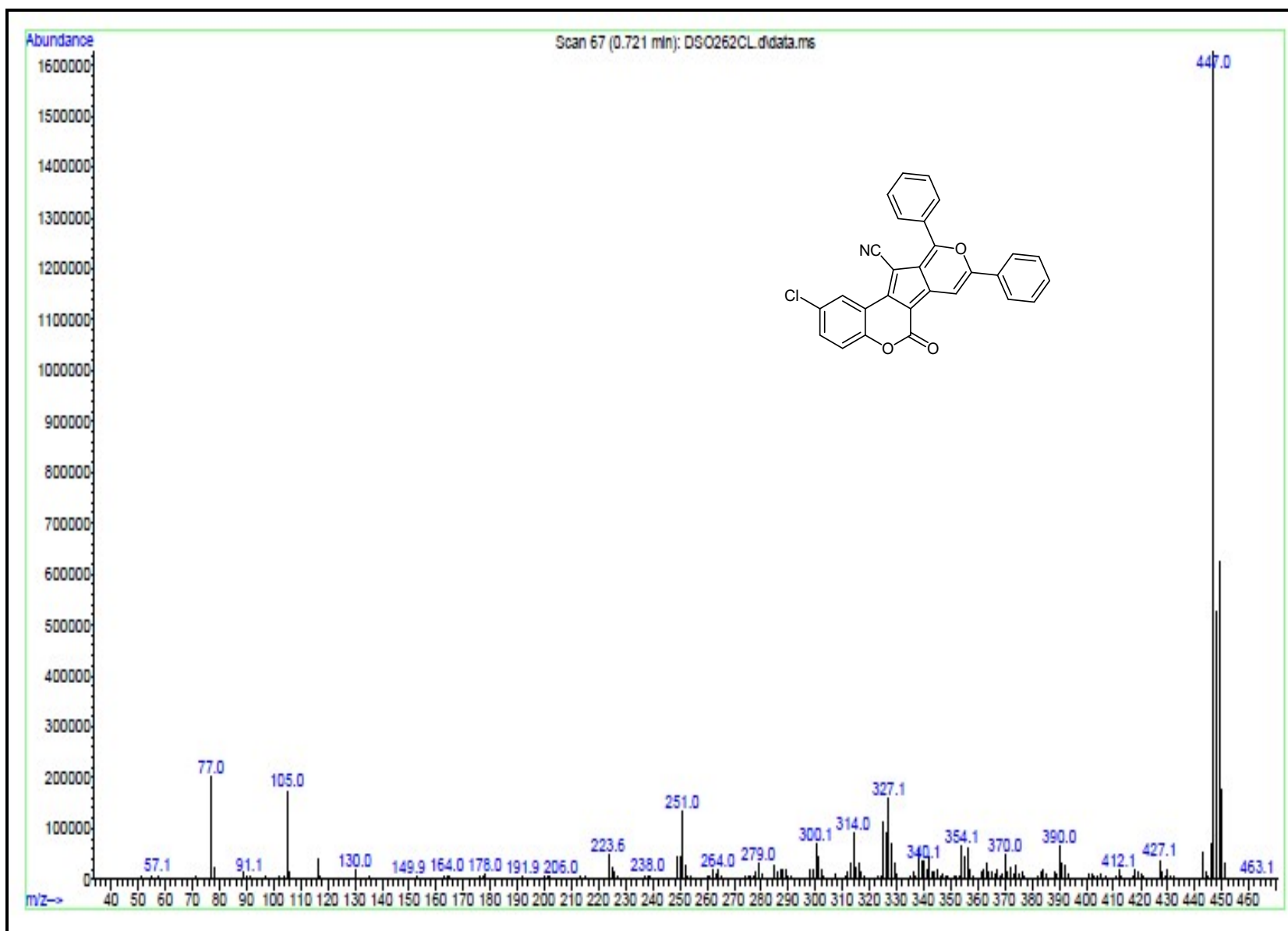
Mass spectrum of **3a**



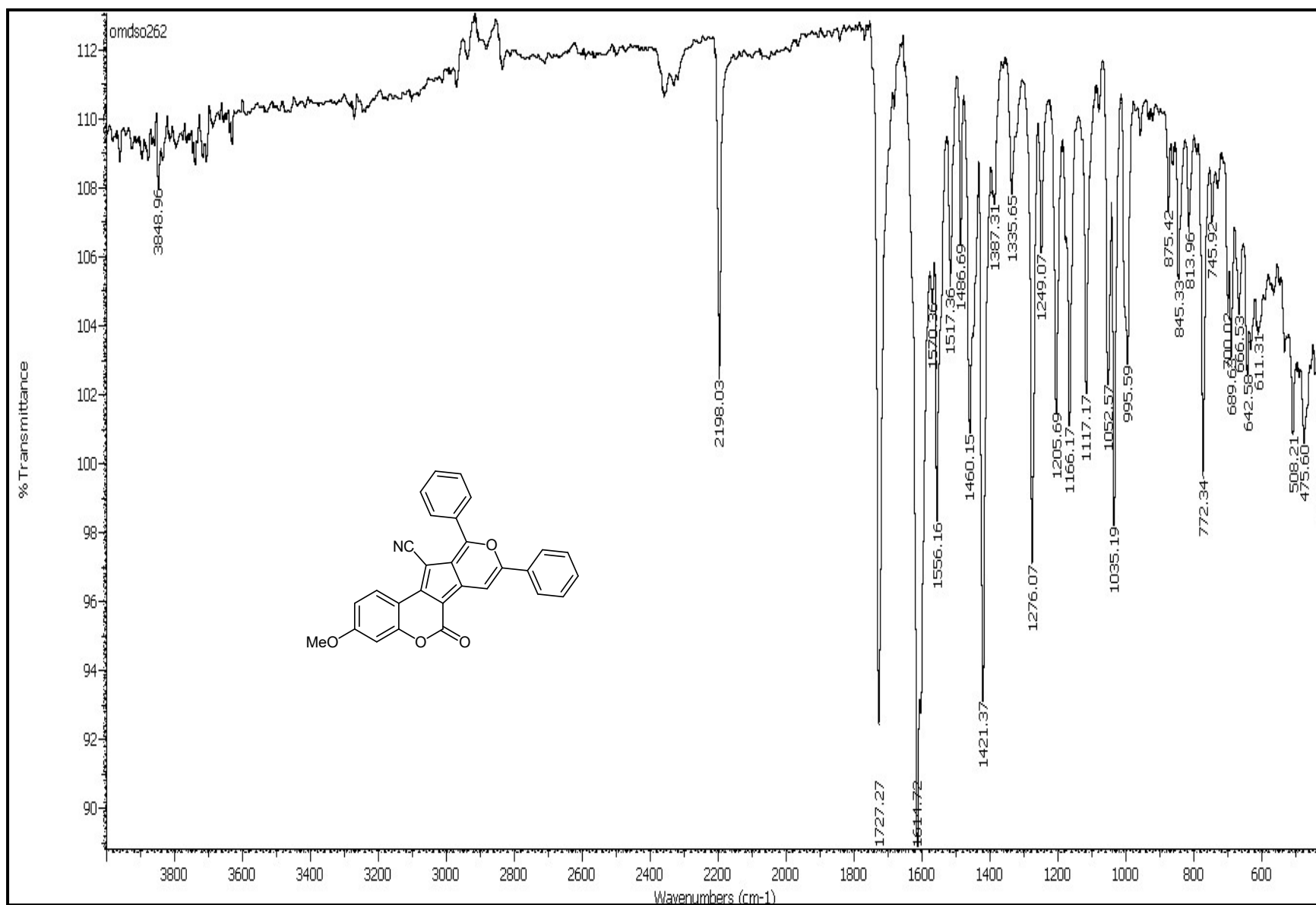
IR spectrum of 3b



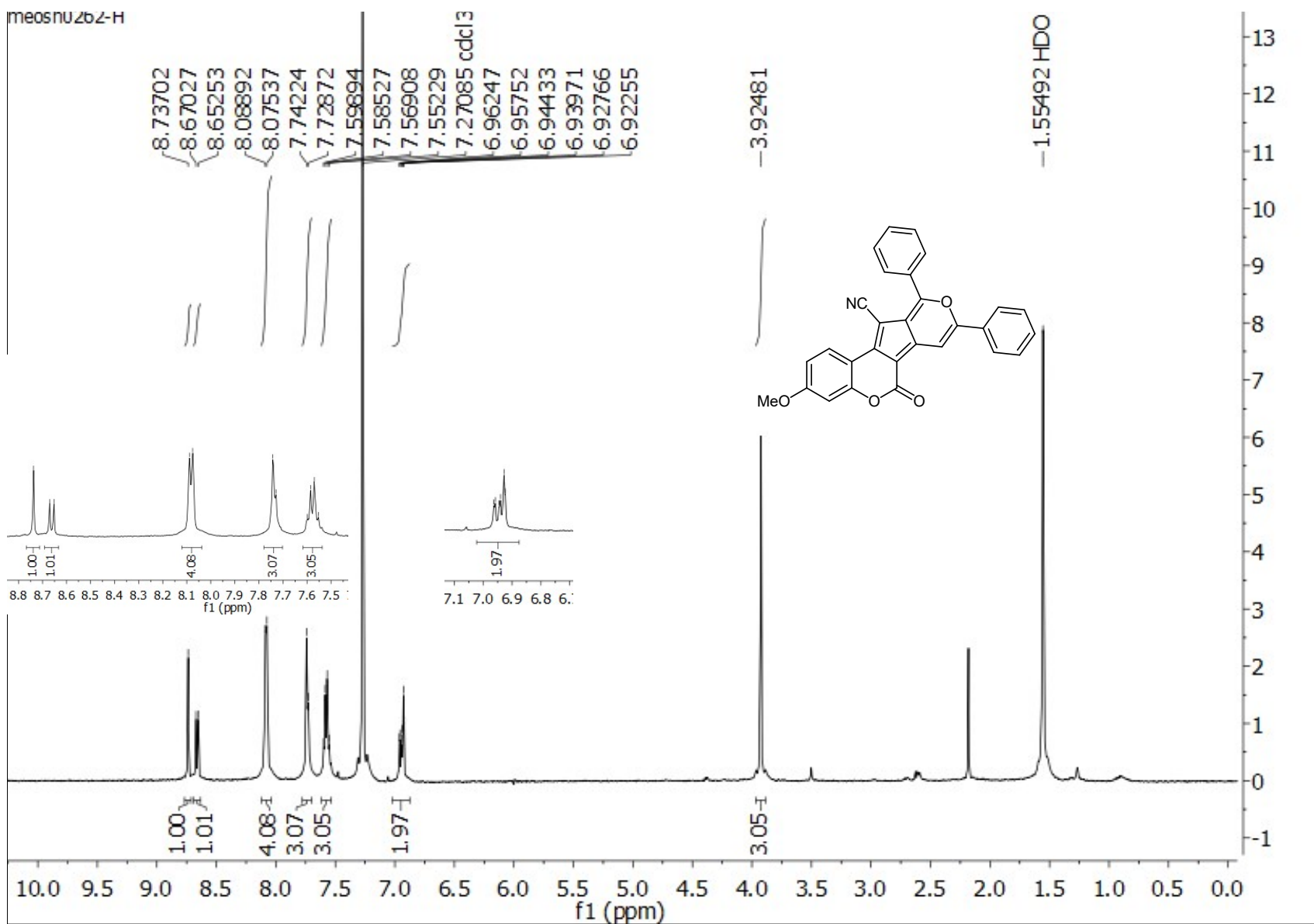
¹H NMR (CDCl₃, 300 MHz) of **3b**



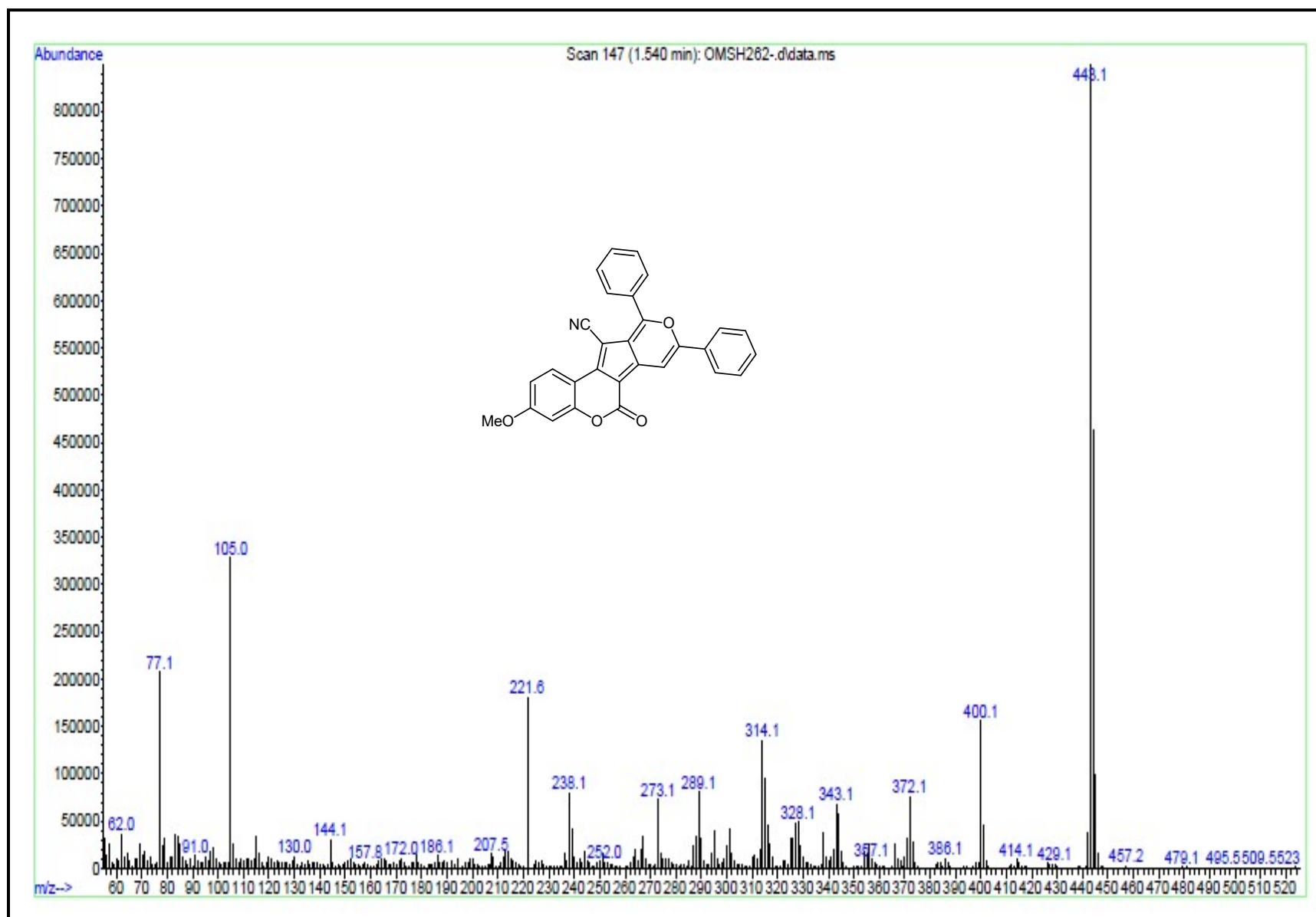
Mass spectrum of **3b**



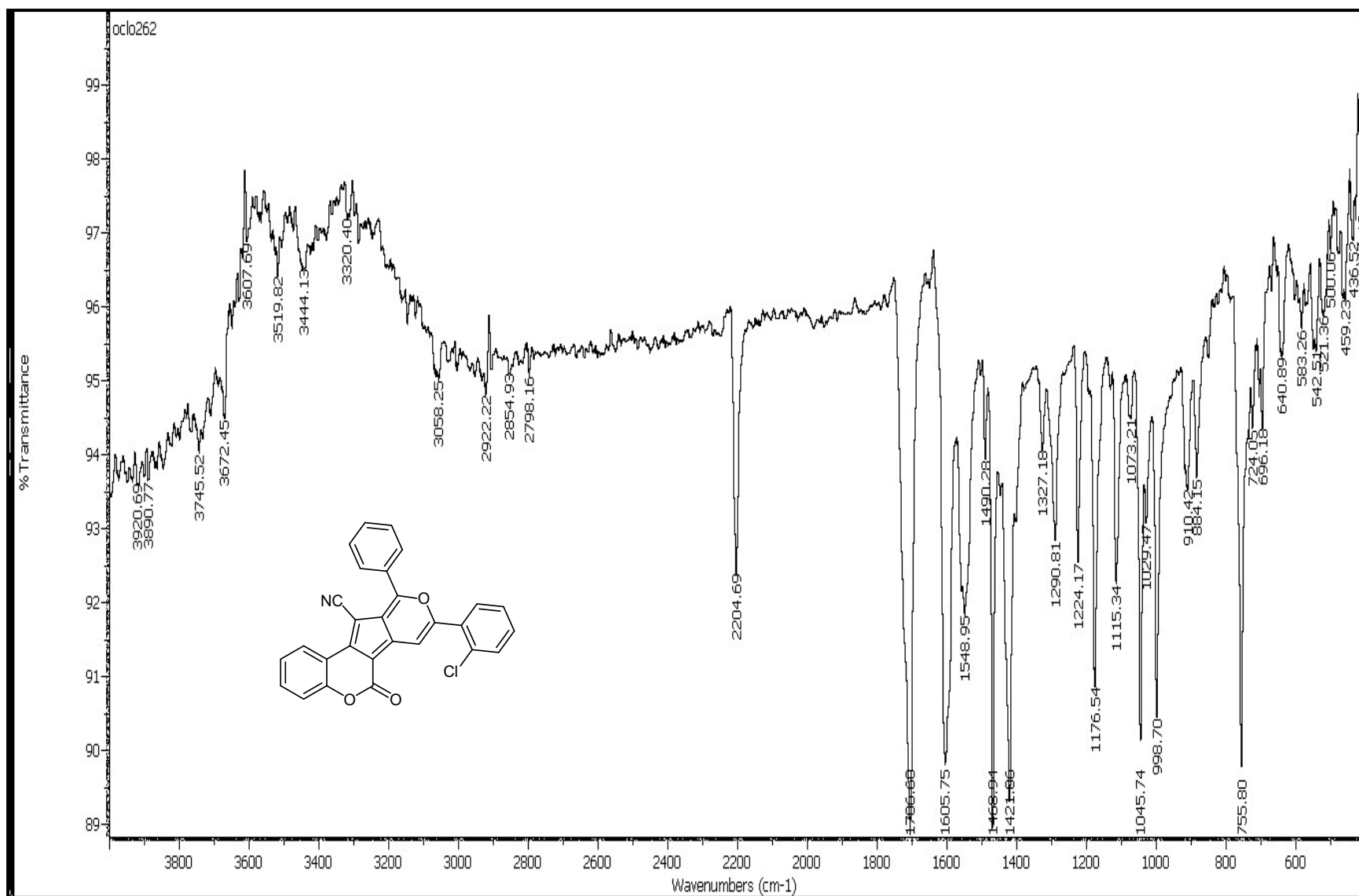
IR spectrum of 3c



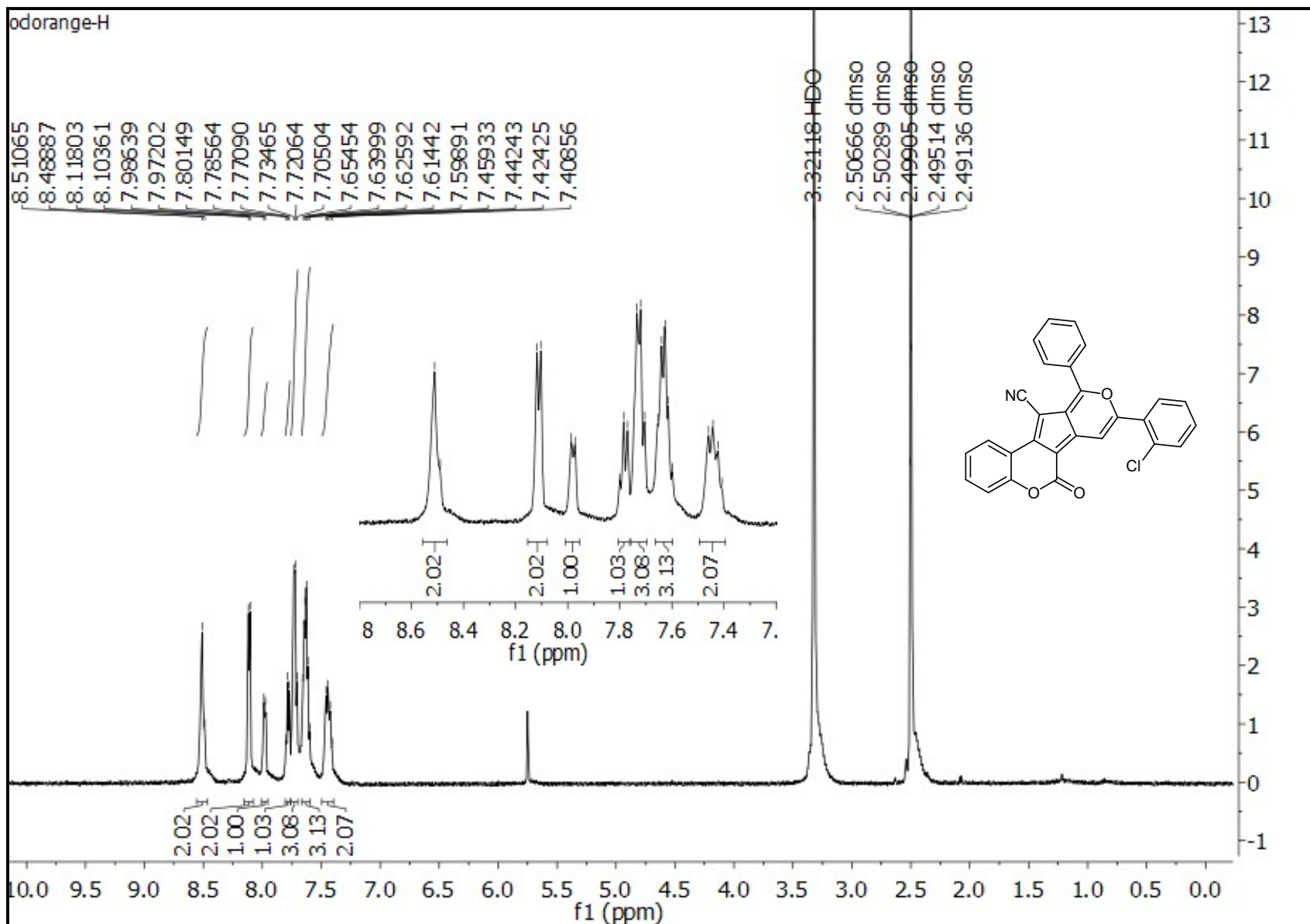
¹H NMR (CDCl₃, 500 MHz) of **3c**



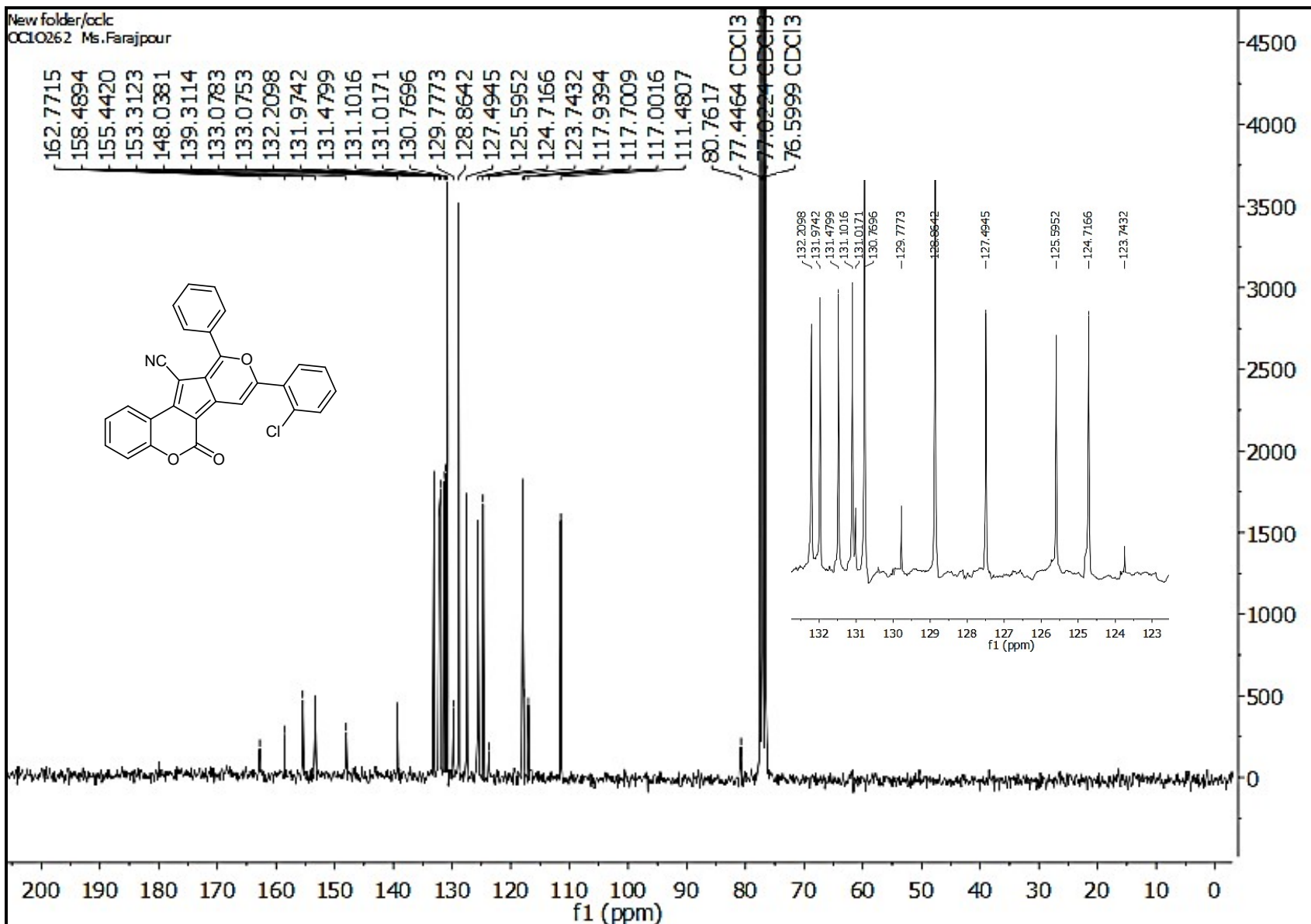
Mass spectrum of 3c



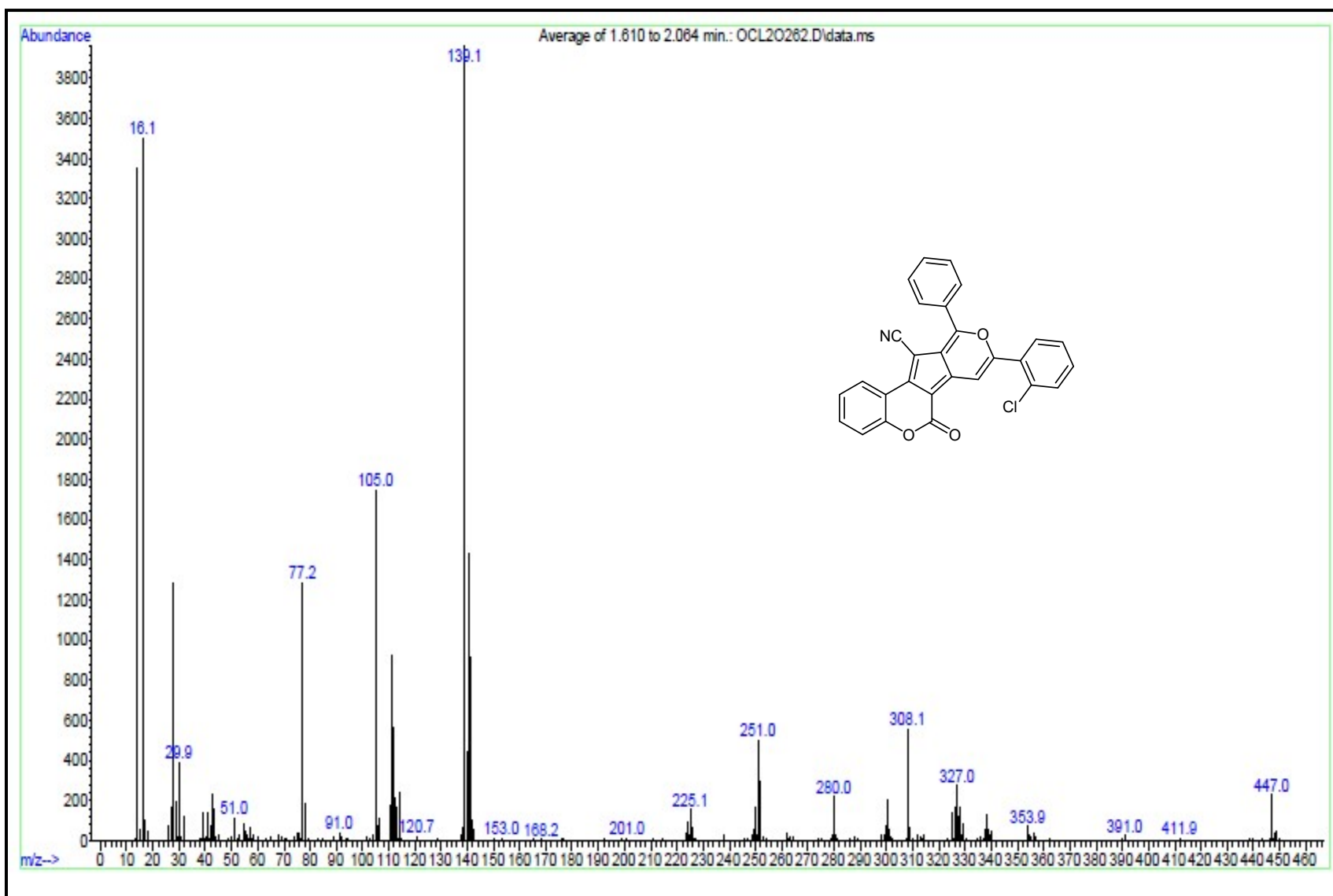
IR spectrum of 3d



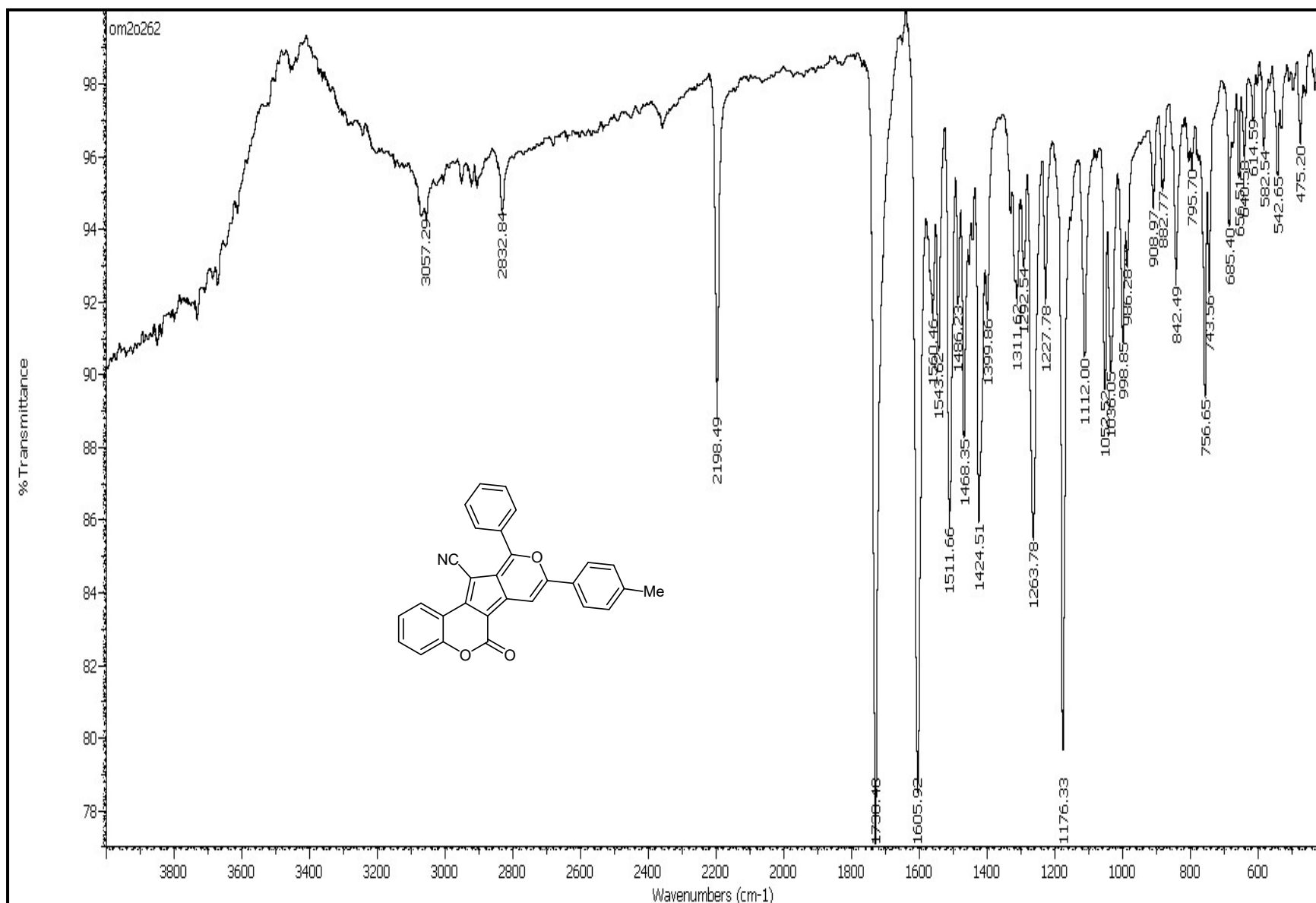
¹H NMR (DMSO-*d*₆, 500 MHz) of **3d**



$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 75 MHz) of **3d**

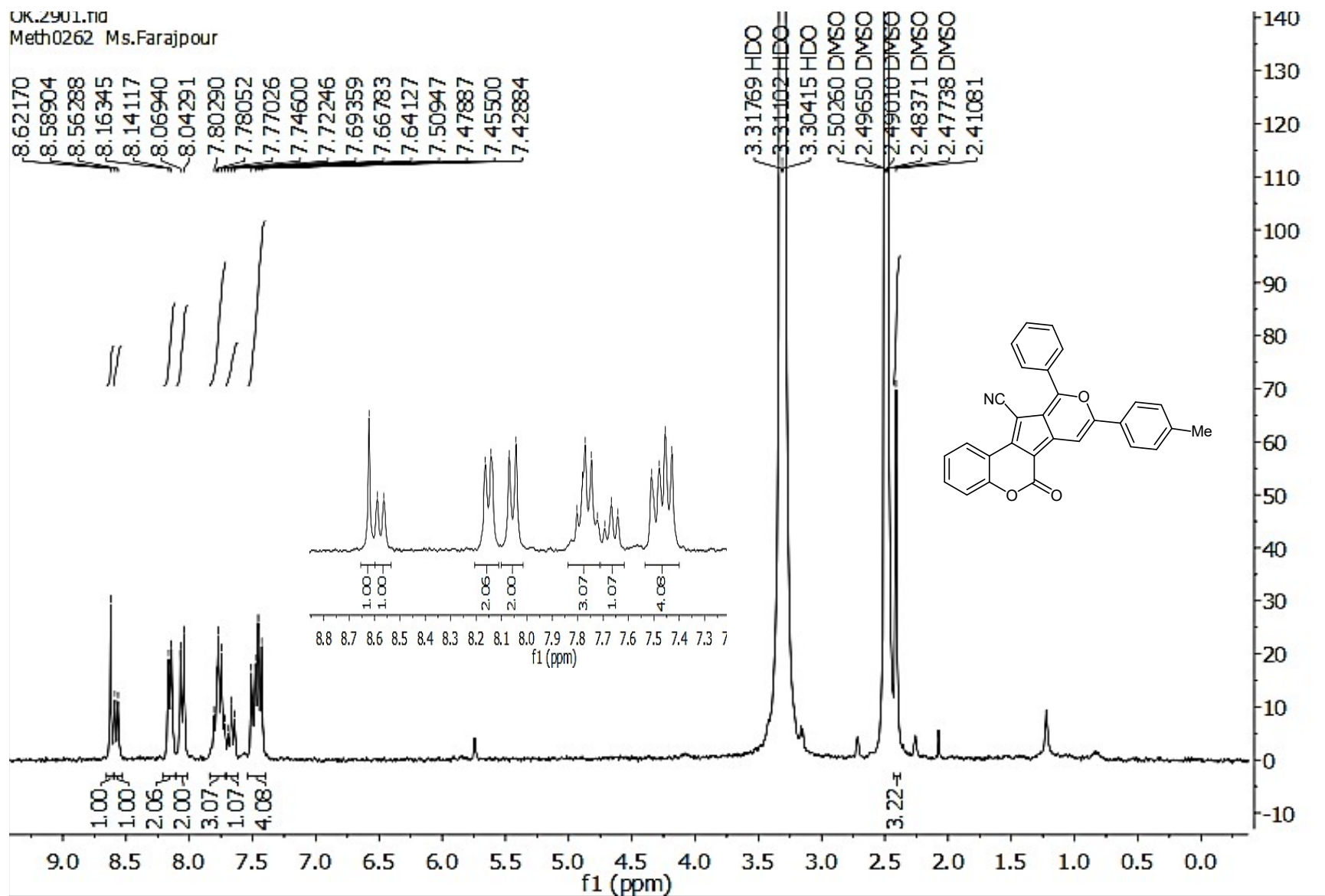


Mass spectrum of **3d**

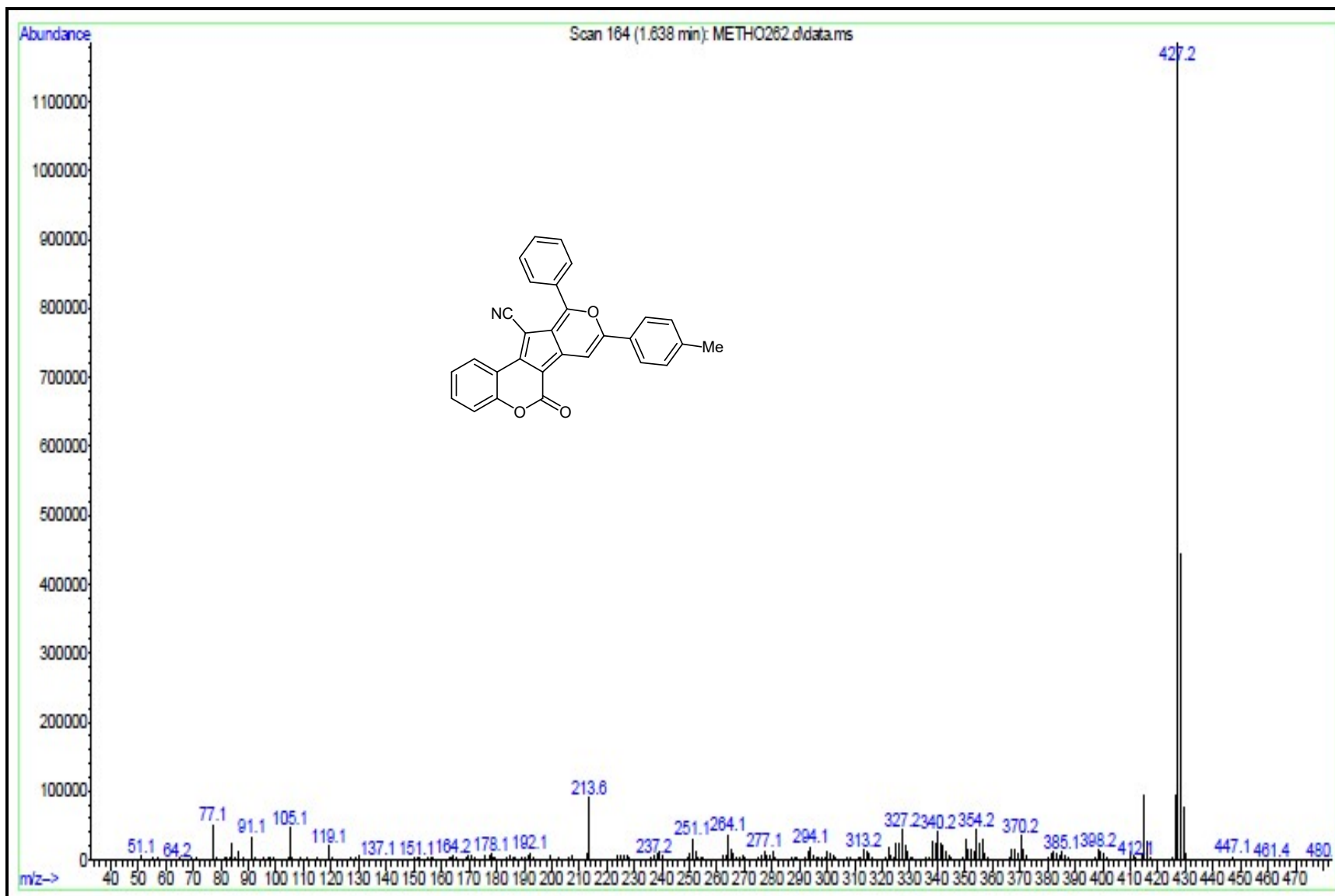


IR spectrum of **3e**

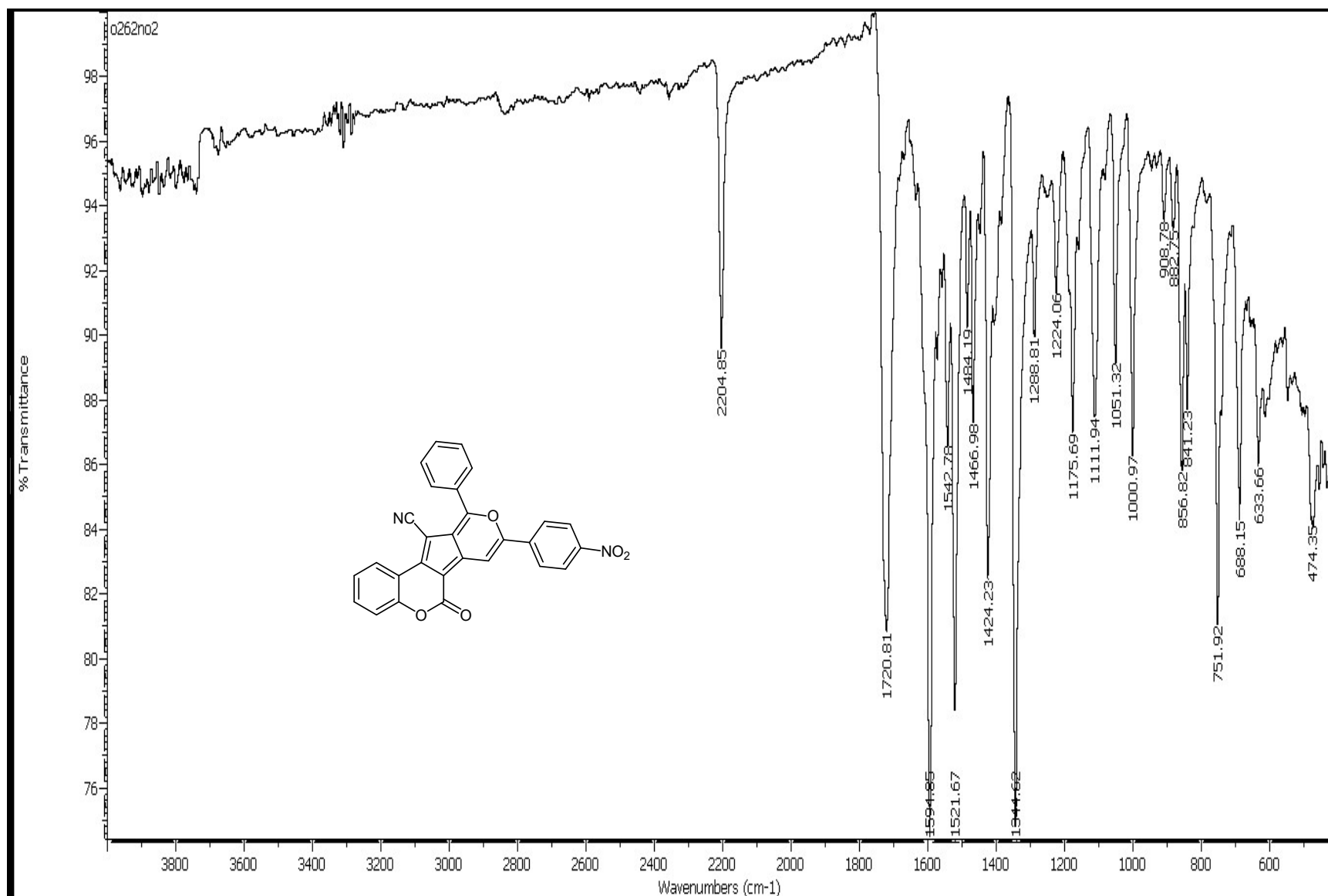
OK_2901.tia
Meth0262 Ms.Farajpour



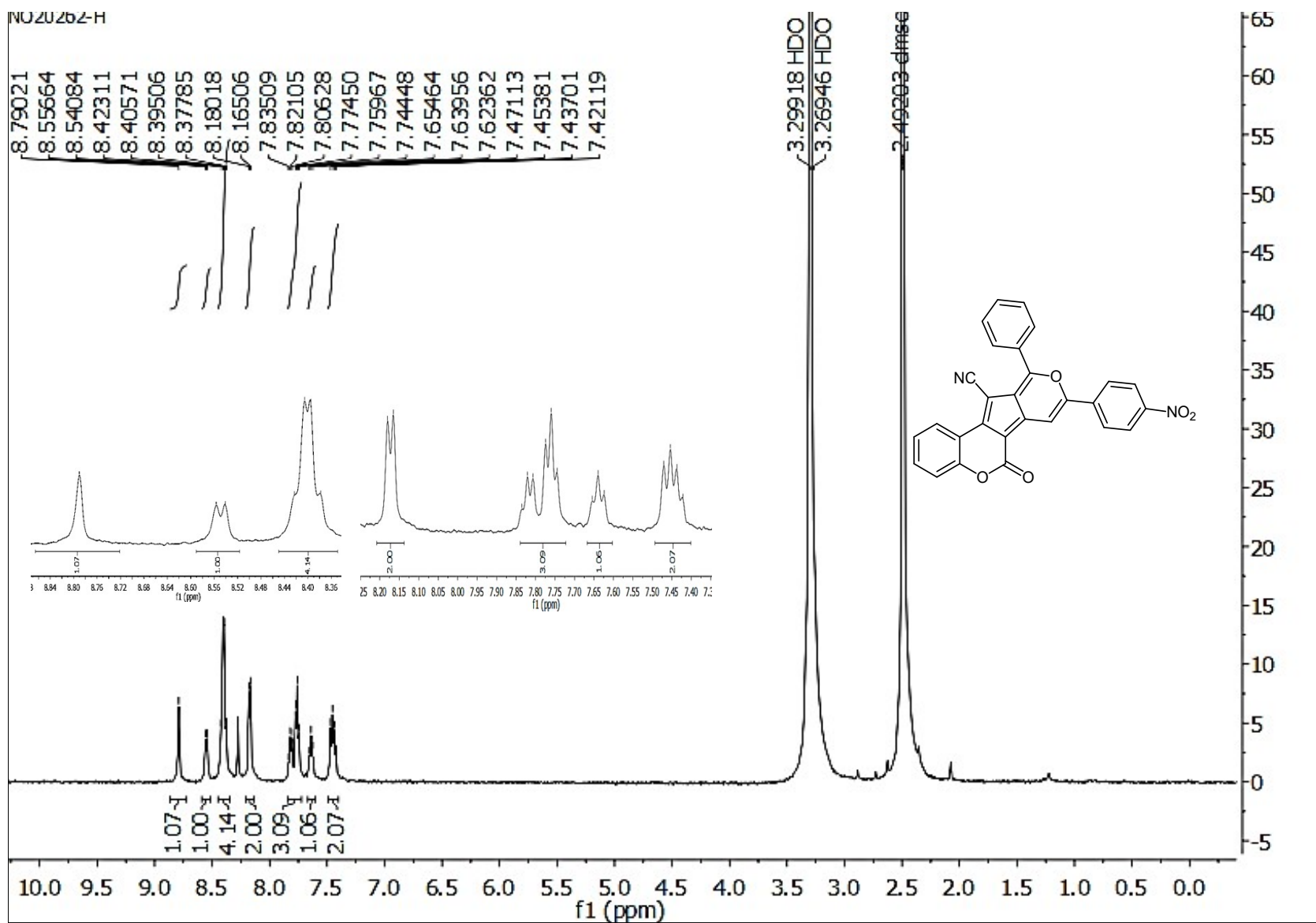
¹H NMR (DMSO-*d*₆, 300 MHz) of 3e



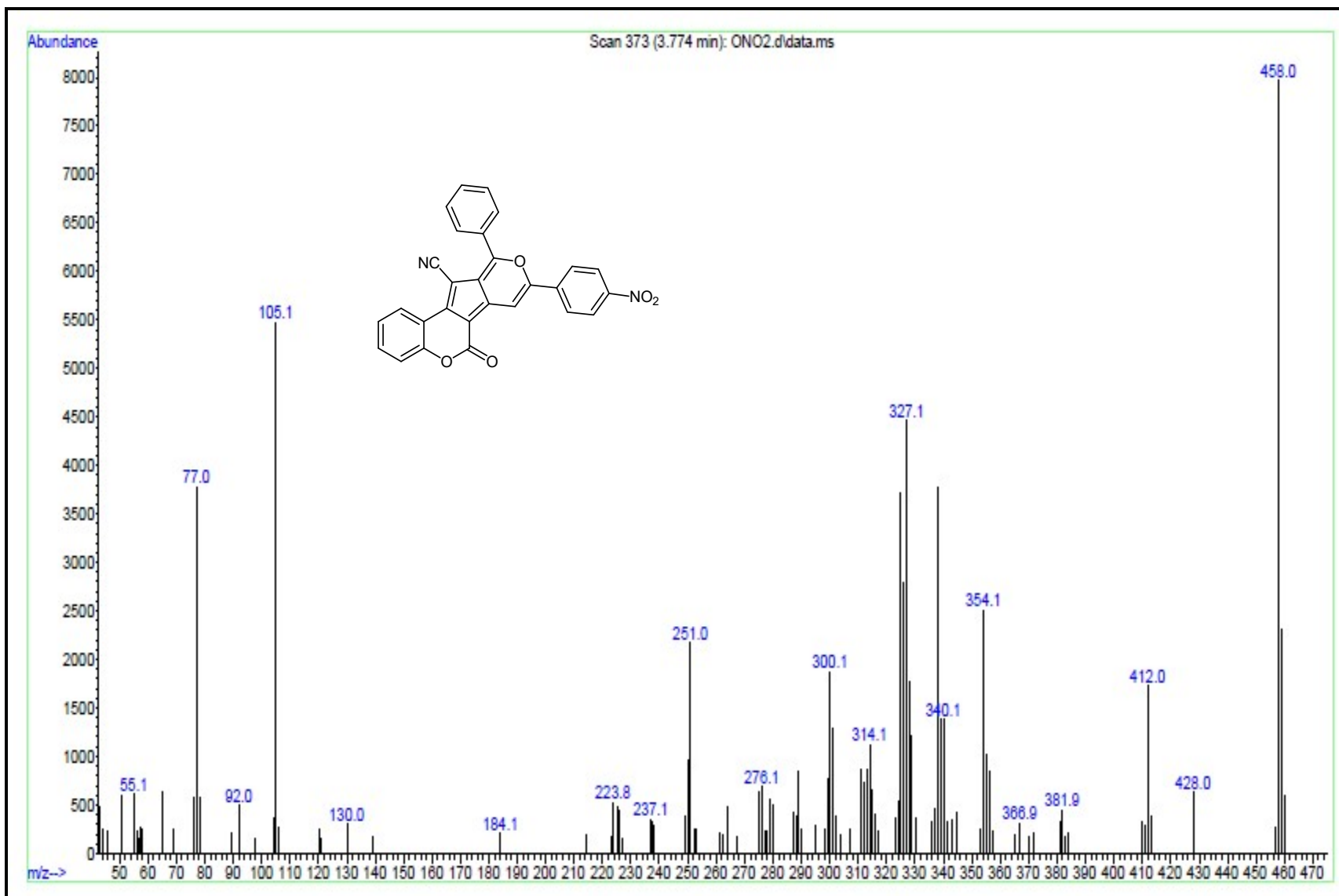
Mass spectrum of 3e



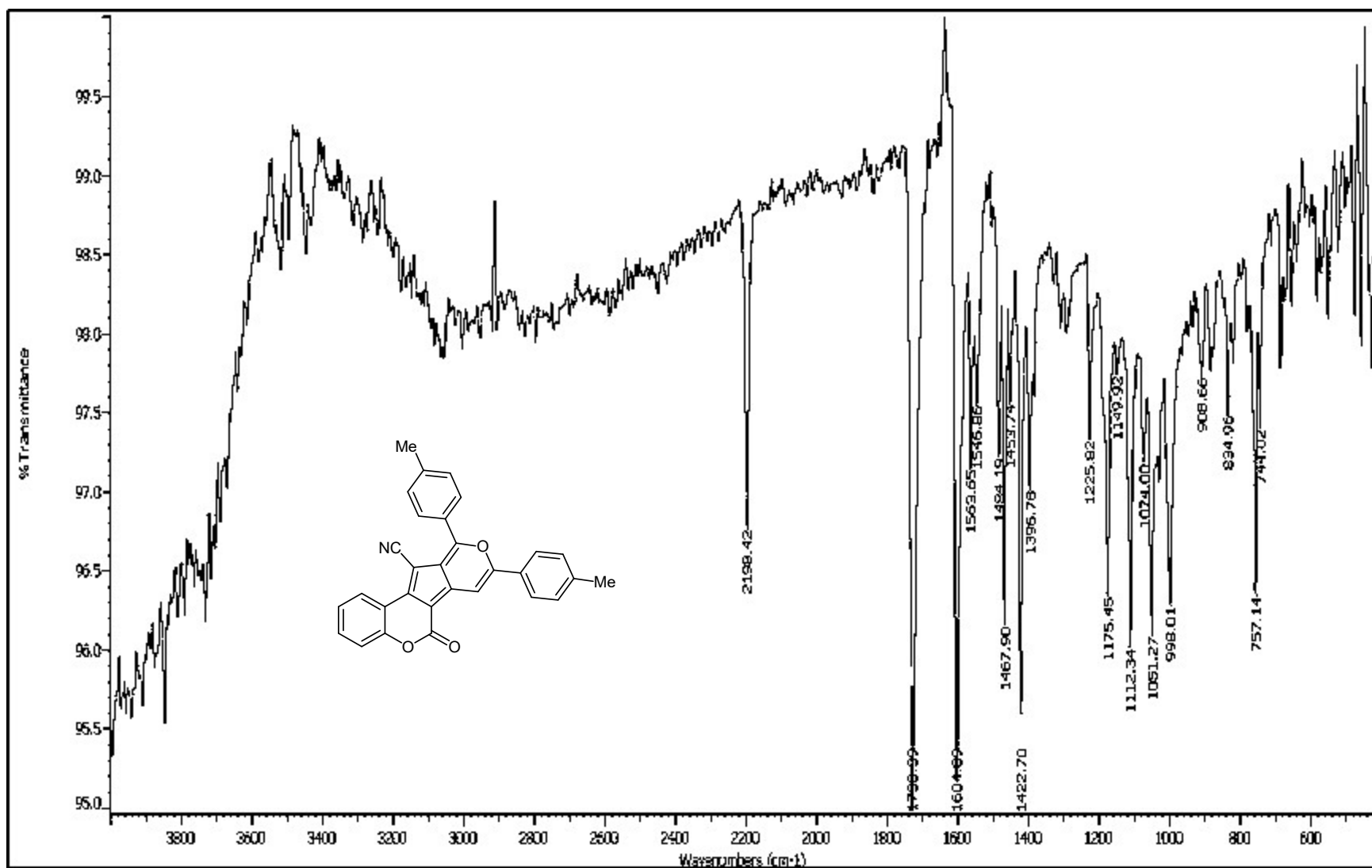
IR spectrum of **3f**



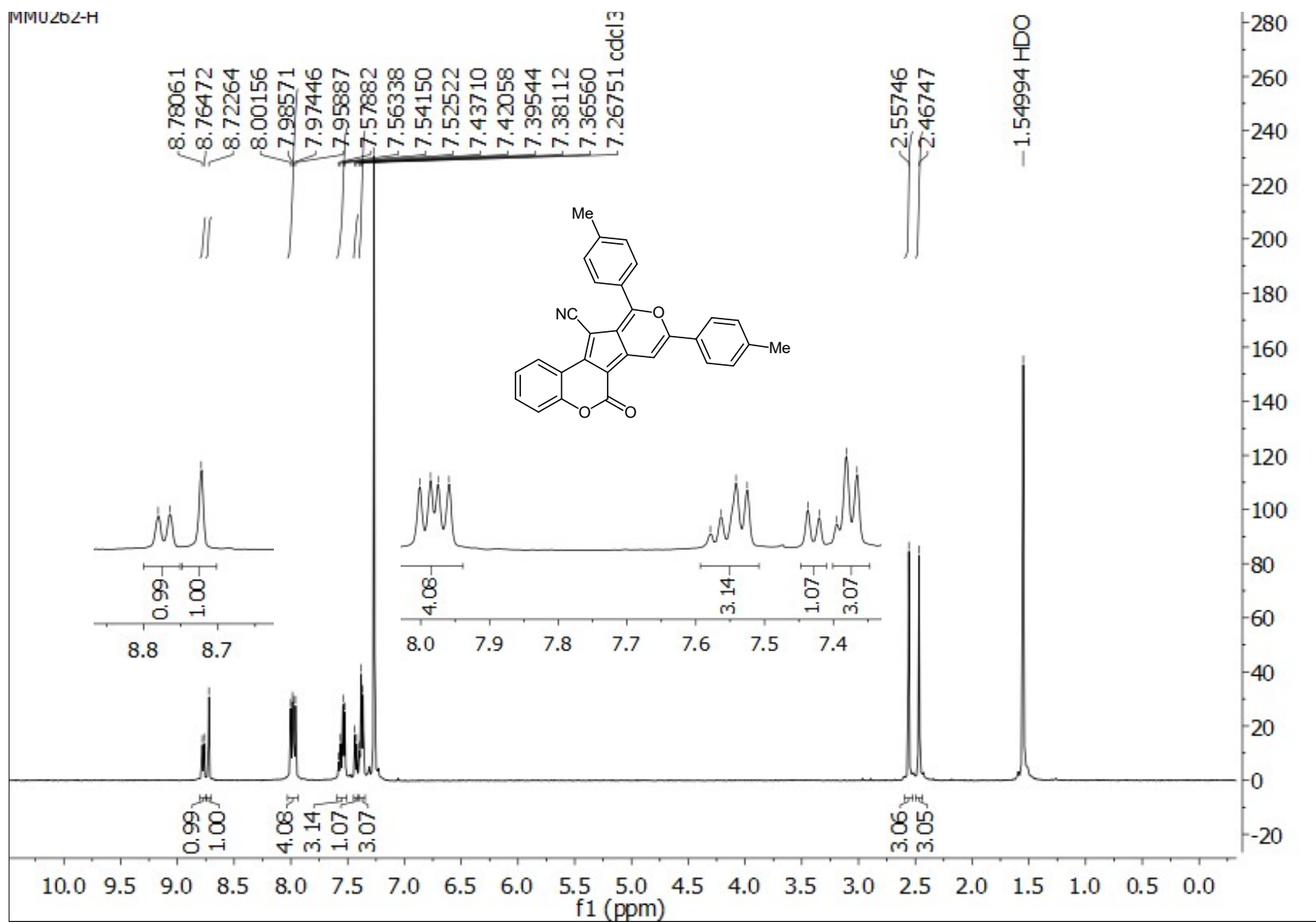
¹H NMR (DMSO-*d*₆, 300 MHz) of 3f



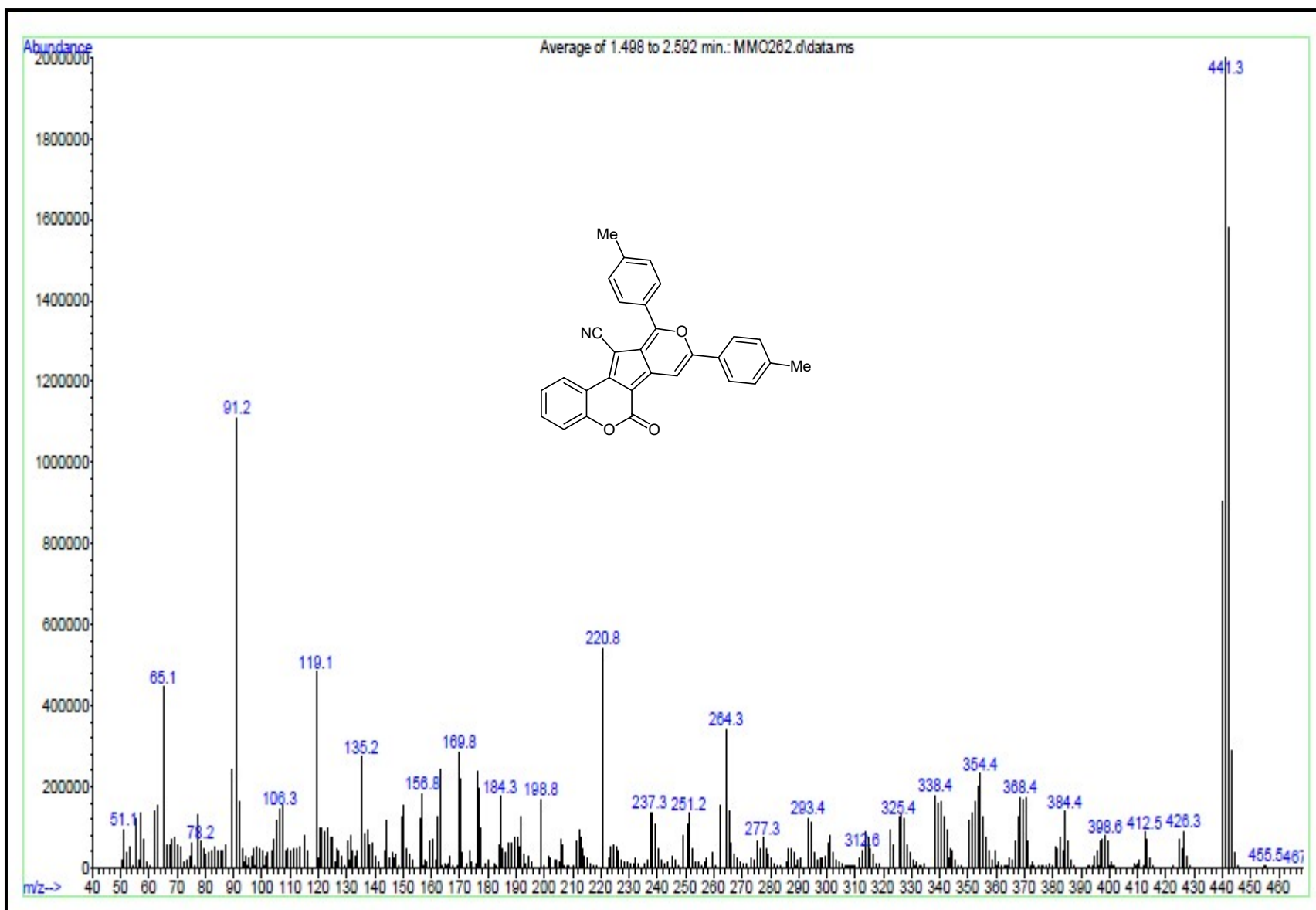
Mass spectrum of **3f**



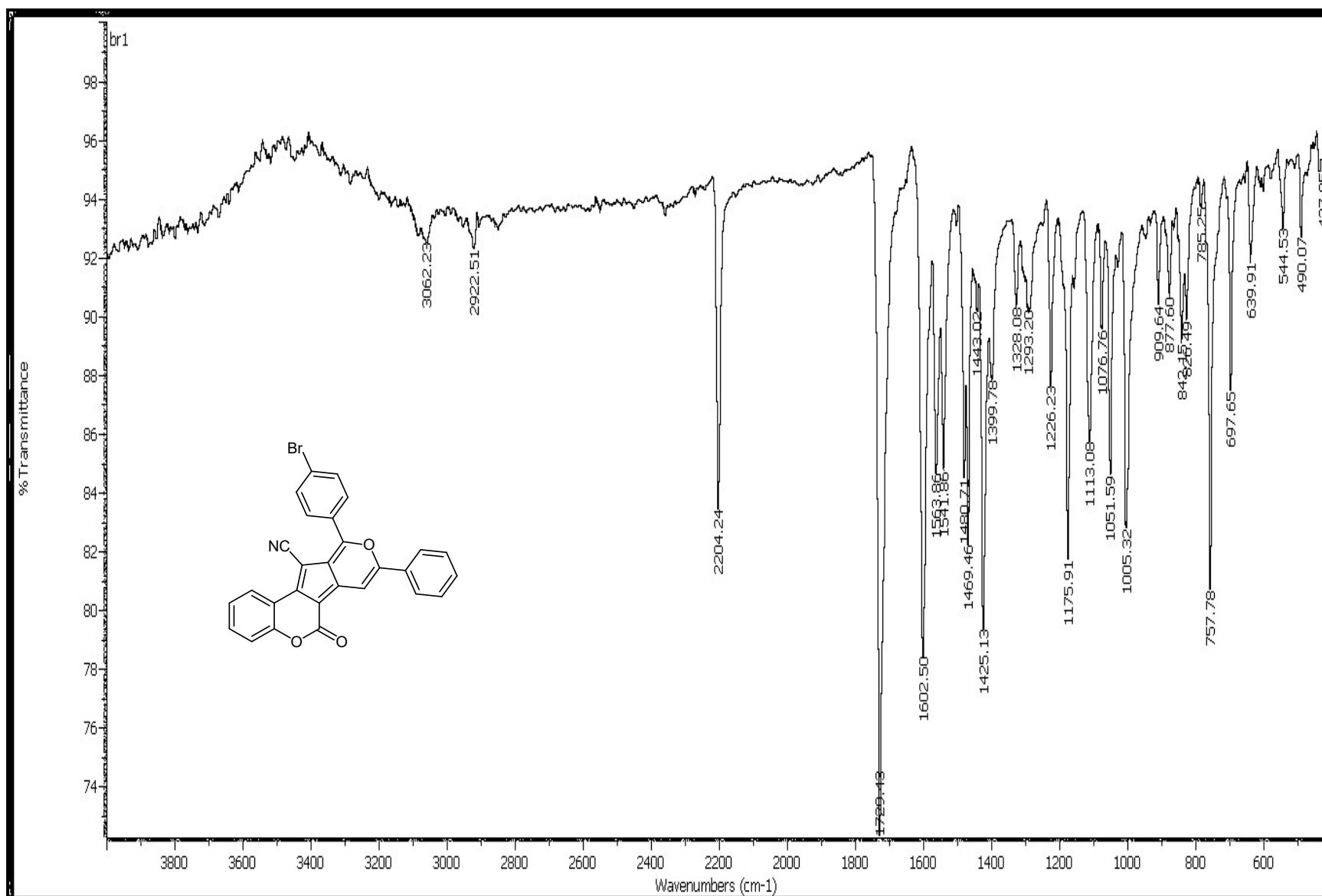
IR spectrum of 3g



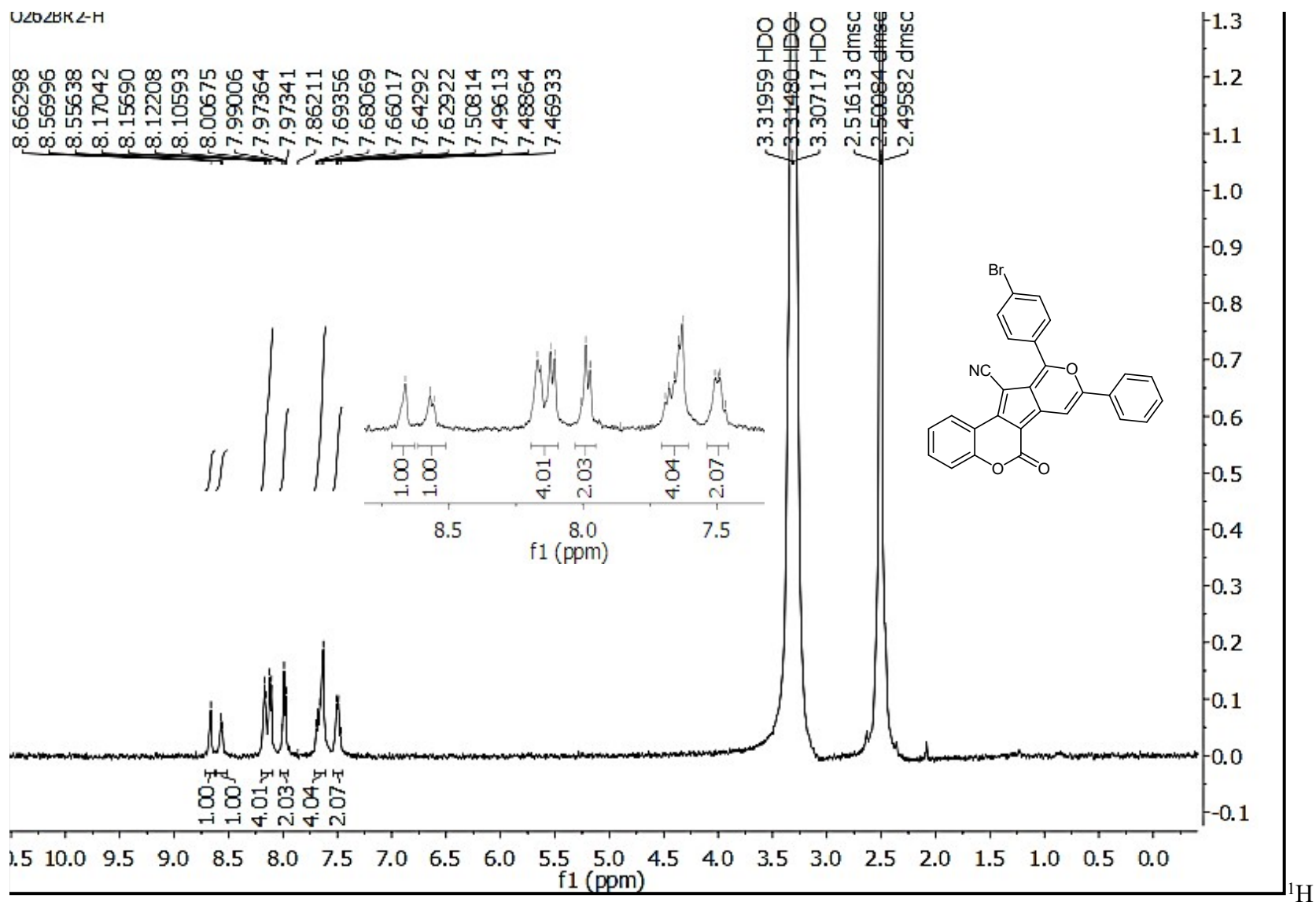
¹H NMR (CDCl₃, 500 MHz) of **3g**



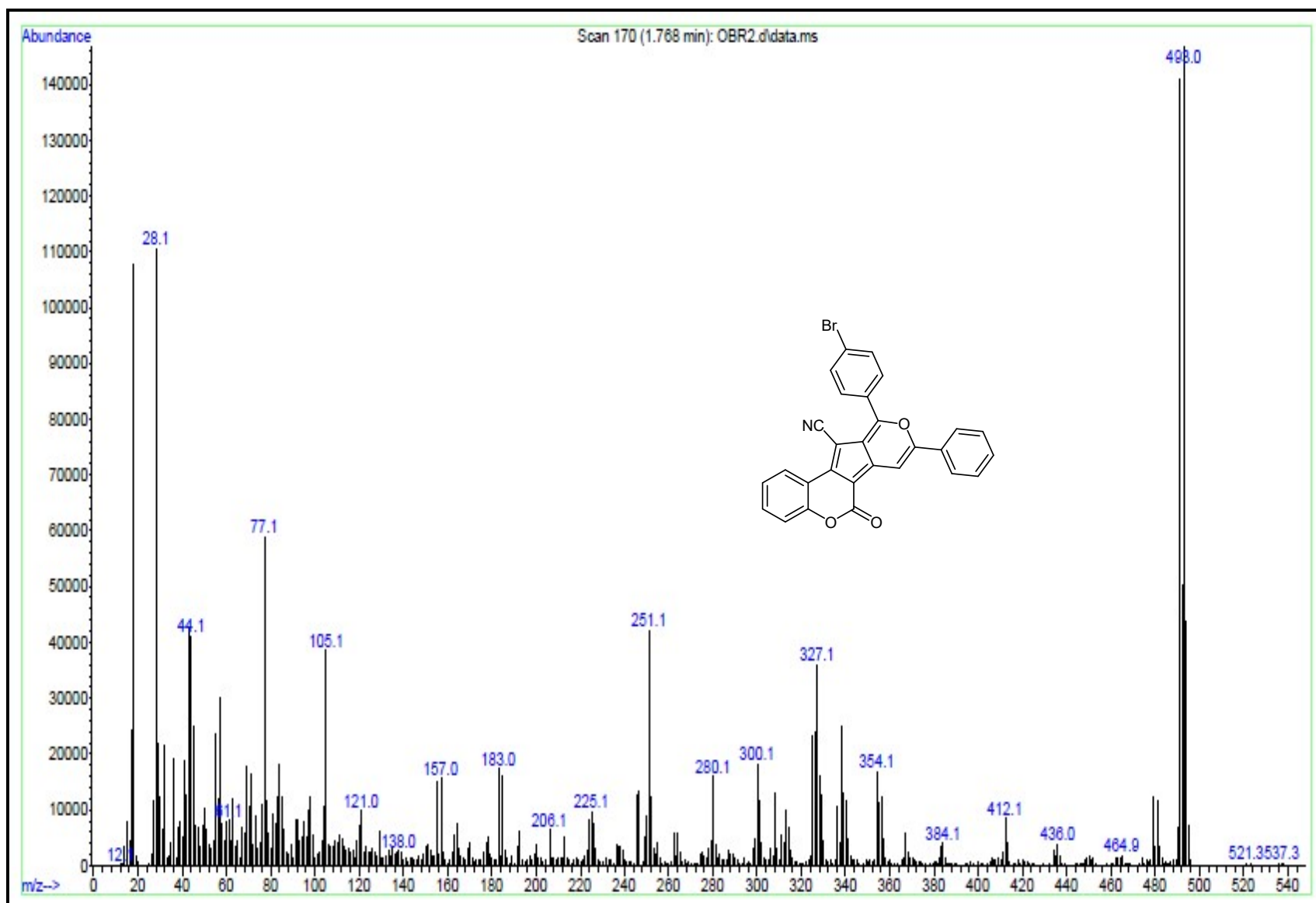
Mass spectrum of **3g**



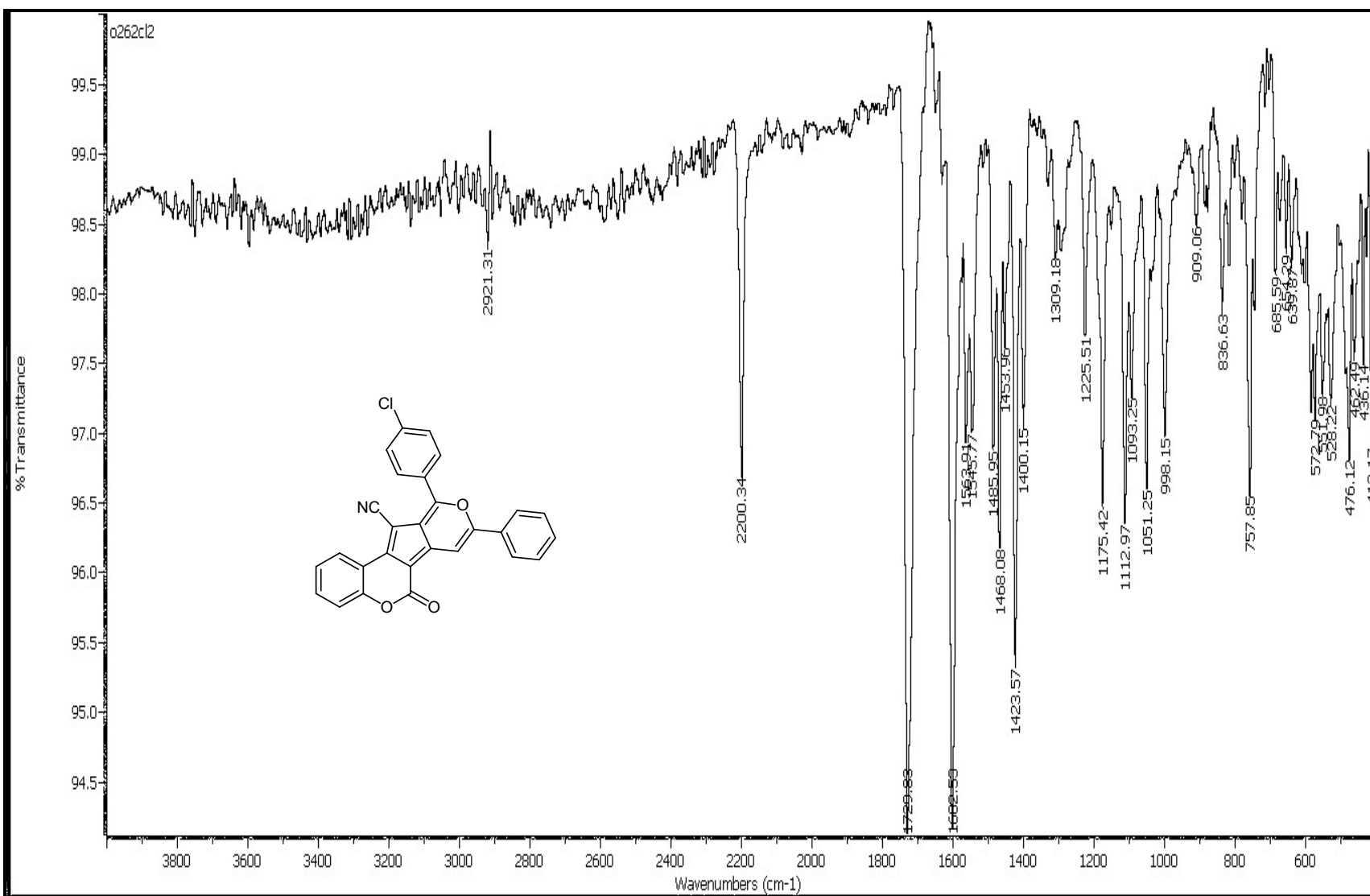
IR spectrum of 3h



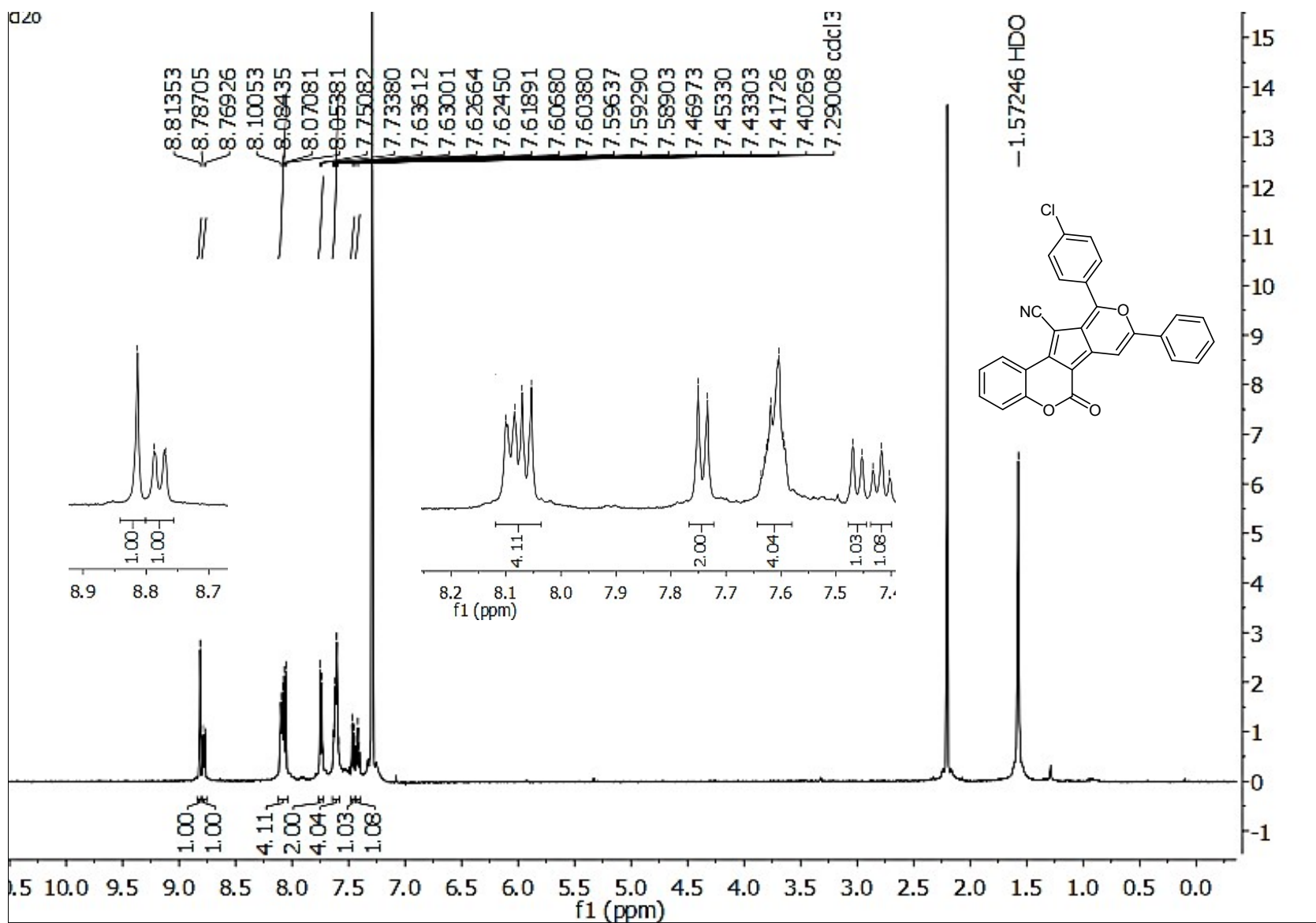
NMR (DMSO- d_6 , 500 MHz) of **3h**



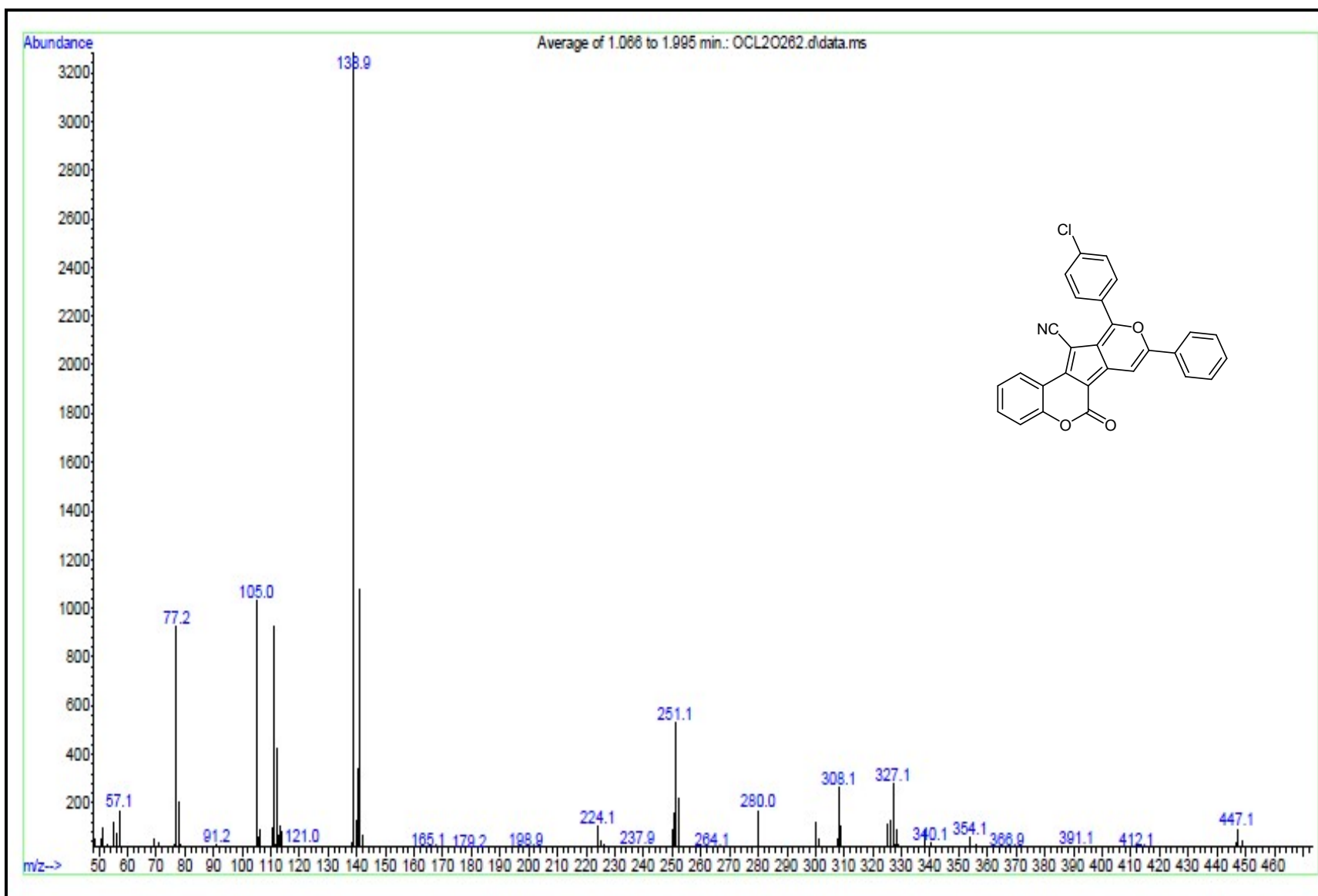
Mass spectrum of **3h**



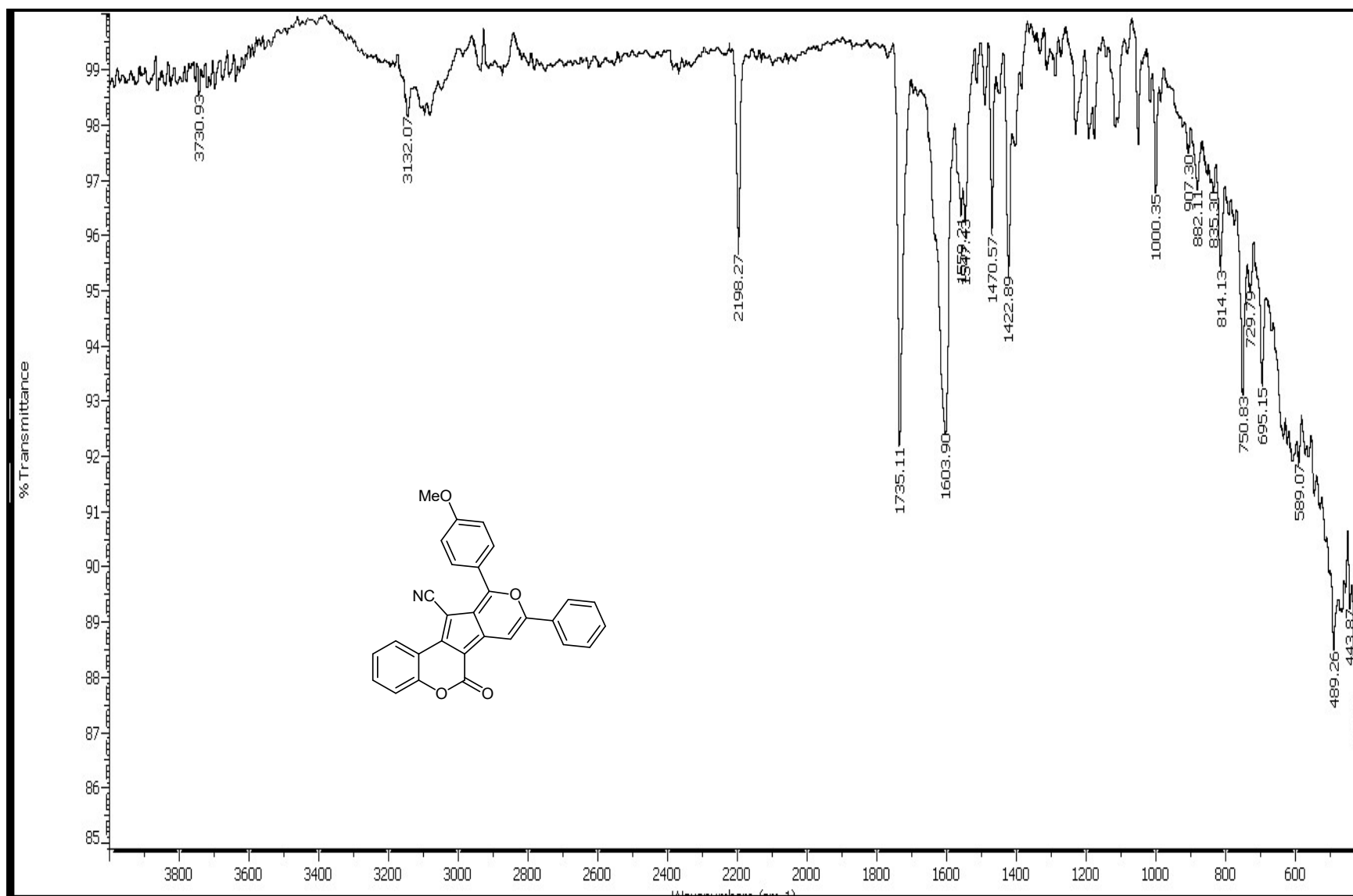
IR spectrum of **3i**



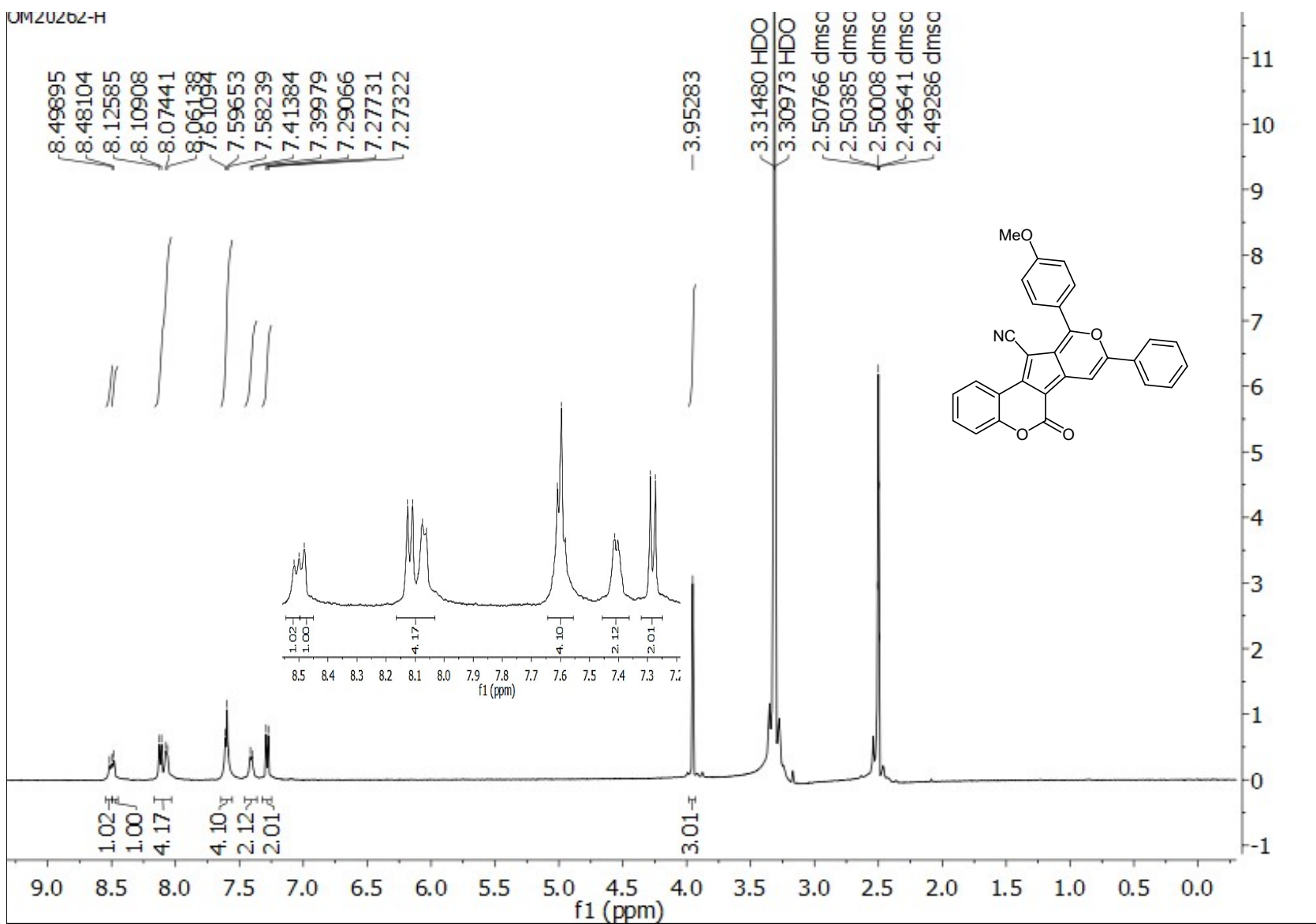
¹H NMR (CDCl₃, 500 MHz) of **3i**



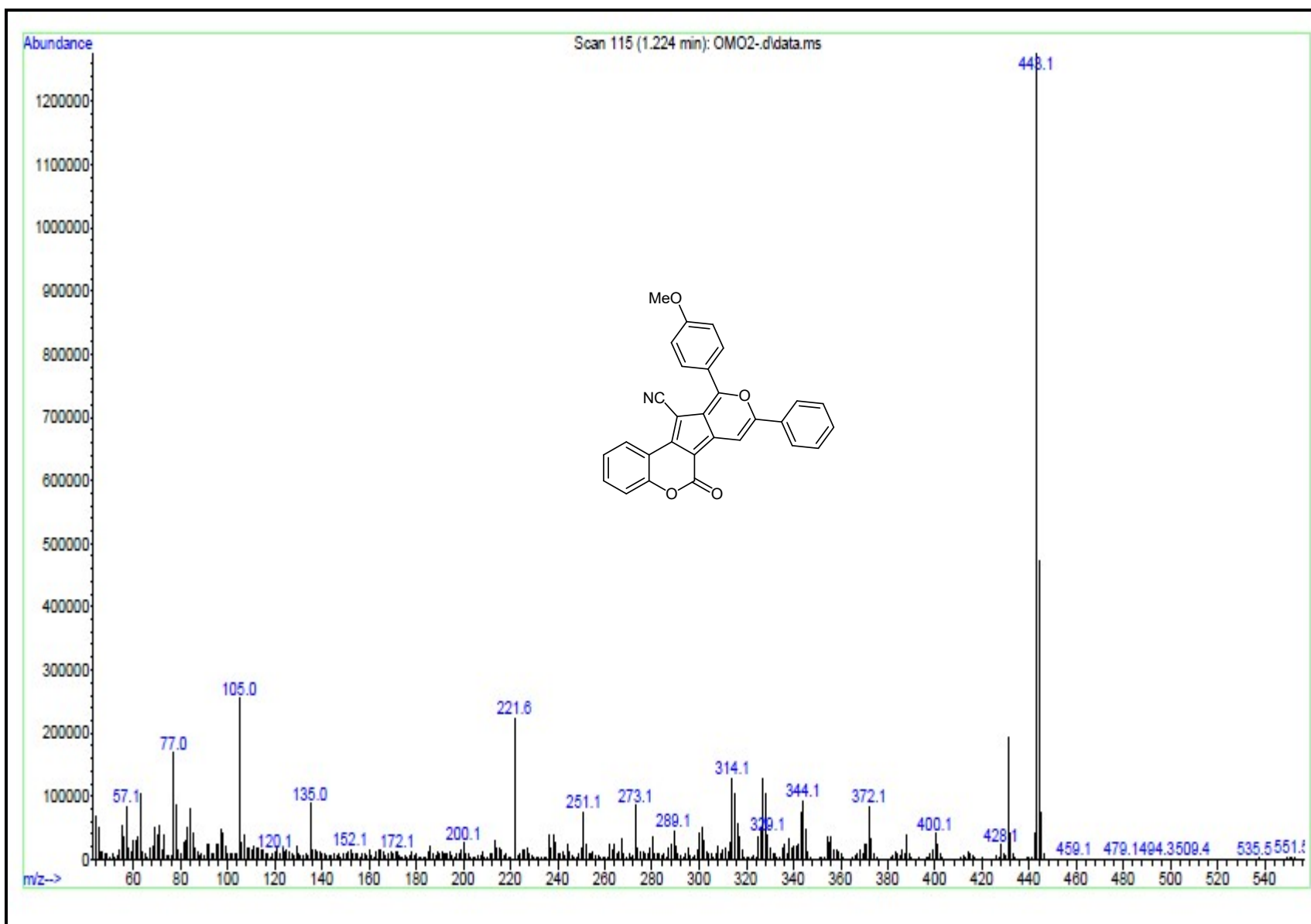
Mass spectrum of **3i**



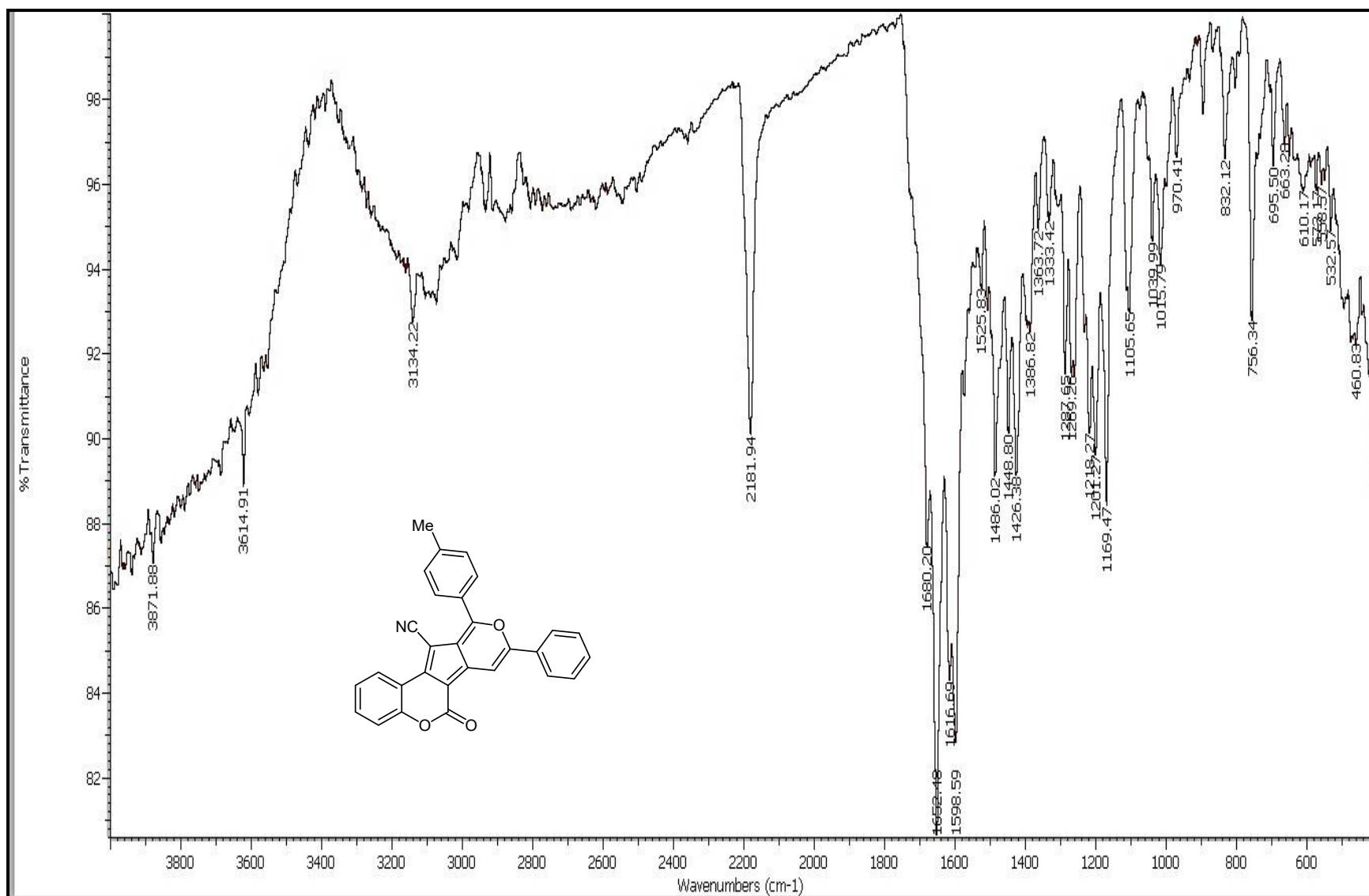
IR spectrum of **3j**



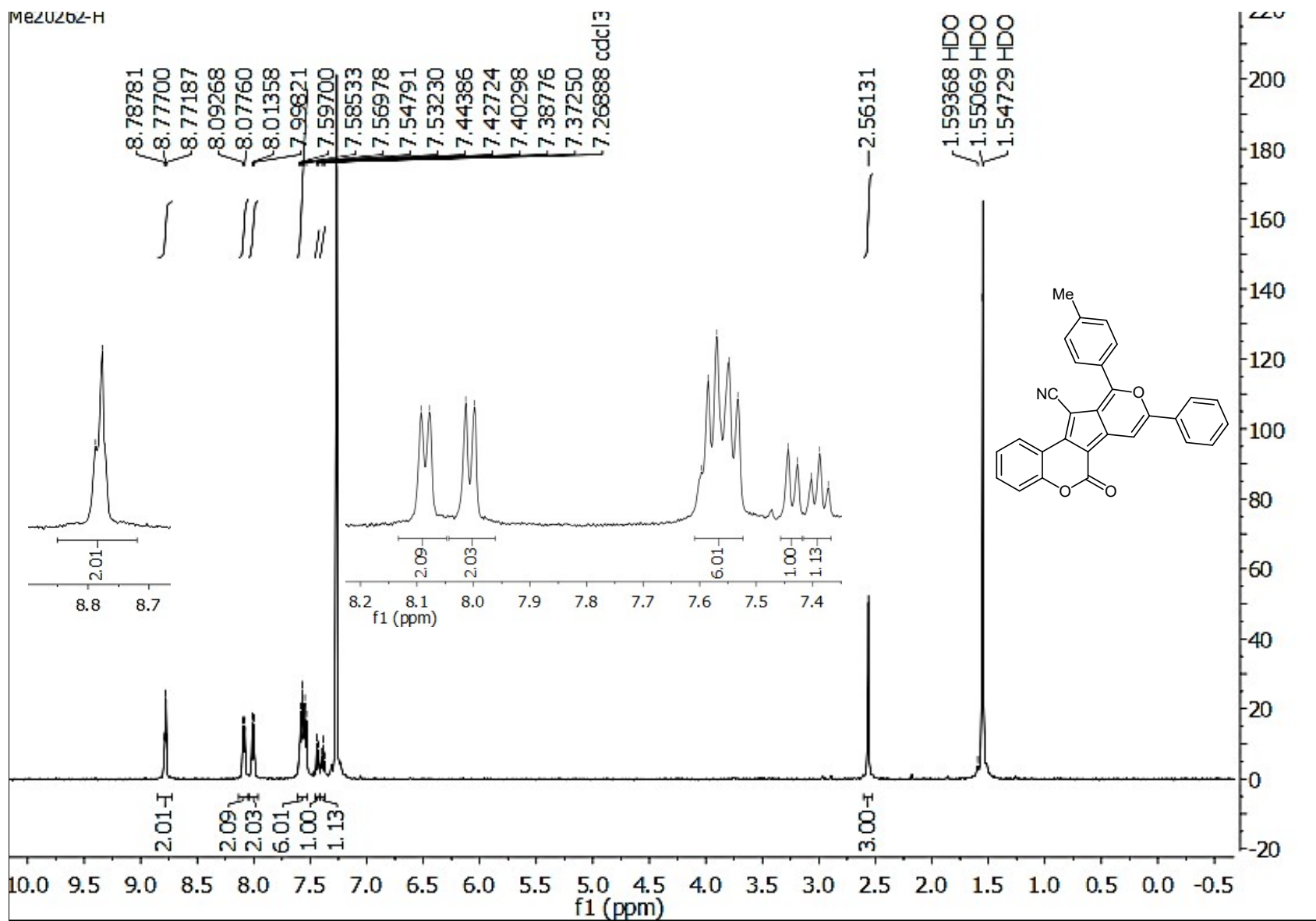
^1H NMR (DMSO- d_6 , 500 MHz) of **3j**



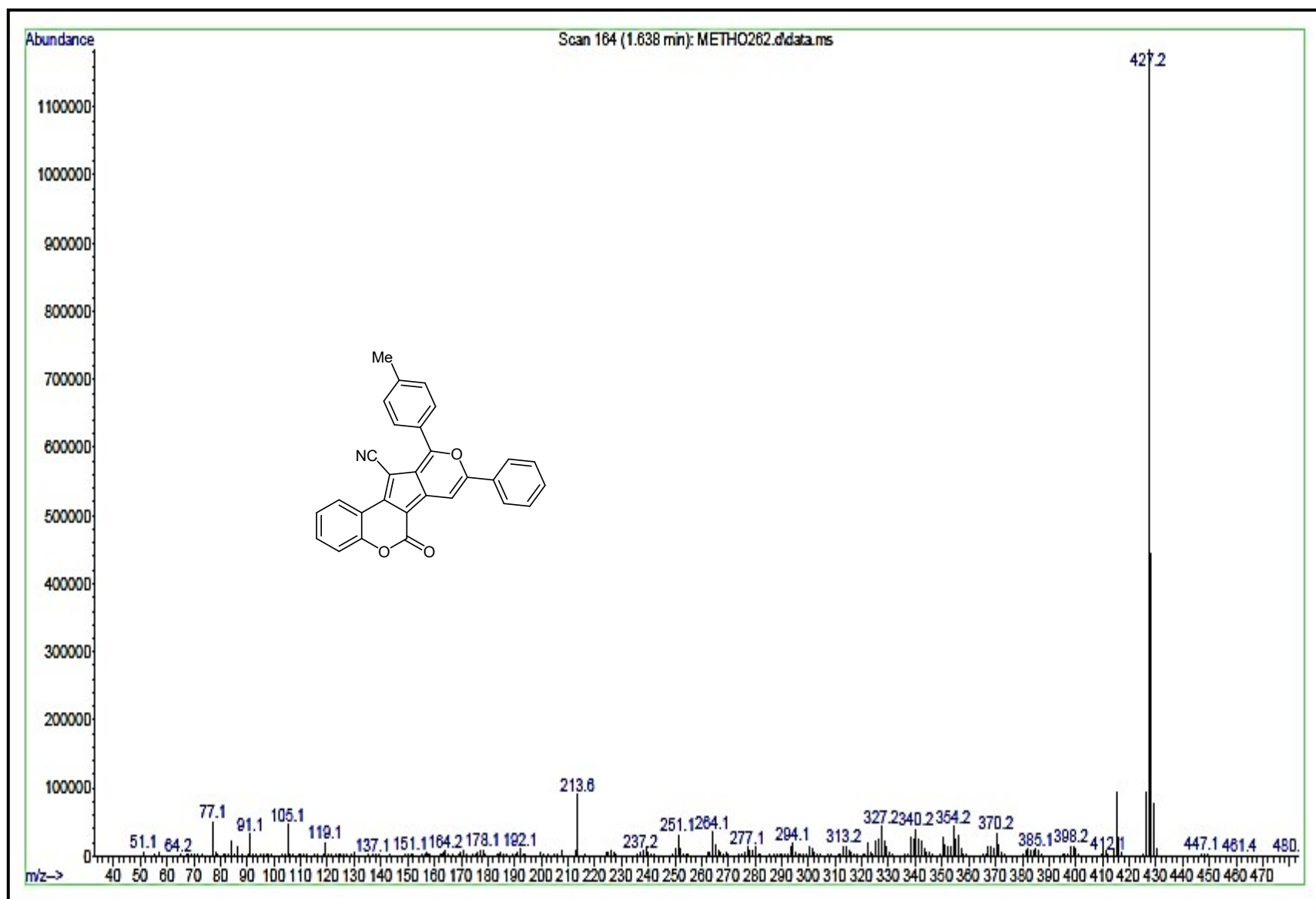
Mass spectrum of **3j**



IR spectrum of 3k



¹H NMR (CDCl₃, 500 MHz) of **3k**



Mass spectrum of **3k**