Mn-Catalyzed oxo-alkylation of 1,2,4-triazine-3,5(2*H*, 4*H*)-diones with cyclic alkanols via oxidative cross-dehydrogenative-coupling

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Supporting Information

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I. General methods and materials

^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded on a Bruker AC-P 400 spectrometer (400 MHz for ^{1}H, 100 MHz for $^{13}C\{^{1}H\}$) in $CDCl_3$ (with TMS as internal standard). Chemical shifts (δ) were measured in ppm relative to TMS δ = 0 for ^{1}H, or to chloroform δ = 77.0 for $^{13}C\{^{1}H\}$ as internal standard. Coupling constants, *J*, are reported in hertz. High-resolution mass spectra (HRMS) were recorded on a quadrupole time-of-flight mass spectrometer (Q-TOF-MS) using electrospray ionization (ESI) as an ionization method. Melting points were obtained on the Shanghai Inesa WRS-3 melting point apparatus. Unless otherwise noted, the starting materials were purchased from J&K Chemical or Energy Chemicals and used without further purification. Some reactions were tried on the microreactor (Chemtrix BV, Kilo Flow, Labtrix Start, or Protrix) to obtain the product in a better yield during the preparation of the substrates. Solvents were dried and purified according to the procedure from "The Purification of Laboratory Chemicals book". The crude products were purified by flash column chromatography on silica gel and the reported yields are the actual isolated yields of pure products. Thin-layer chromatography (TLC) was performed using 60 mesh silica gel plates visualized with short-wavelength UV light (254 nm). IR spectra were recorded on an FT-IR spectrometer (Bruker Alpha), and only major peaks were reported in cm^{-1}.

II. General procedure

1. General procedure for the cross-dehydrocoupling of 1,2,4-triazine-3,5(2*H*,4*H*)-dione derivatives with cyclopropanol.

1,2,4-triazine-3,5(2*H*, 4*H*)-diones derivative (**1a**-**1s**) (0.3 mmol), manganese acetylacetonate (0.045 mmol), iodobenzene diacetate (0.45 mmol), and magnets were added to a Schlenk capped tube. Subsequently, a solution of ethyl acetate (1.5 mL) of the cyclopropanol derivative (**2a**-**2h**) (0.75 mmol) was added and the reaction was carried out at room temperature until the substrate was depleted (monitored by TLC for about 10 hours). Afterwards, the solvent was removed under reduced pressure. The residue was separated and purified by silica gel column chromatography to give the corresponding alkylated product (**3a**-**3aa**).

2. General procedure for the cross-dehydrocoupling of 1,2,4-triazine-3,5(2*H*,4*H*)-dione derivatives with cyclopropanol.(Mechanism control experiments A)

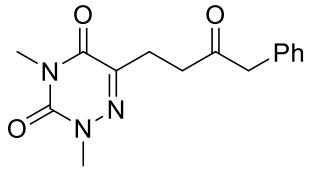
N2, N4-dimethyl-1,2,4-triazine-3,5(2*H*, 4*H*)-dione (**1a**) (0.3 mmol), manganese acetylacetonate (0.045 mmol), iodobenzene diacetate (0.45 mmol), TEMPO (0.6 mmol), and magnets were added to the Schlenk capped tube, followed by 1-phenylmethylcyclopropanol (**3a**) (0.75 mmol) to a solution of ethyl acetate (1.5 mL) and reacted for 10 h at room temperature. The solvent was removed under reduced pressure and the residue was isolated and purified by silica gel column chromatography in 19% yield for 3a and 77% recovery for **1a**.

3. General procedure for the cross-dehydrocoupling of 1,2,4-triazine-3,5(2*H*,4*H*)-dione derivatives with cyclopropanol.(Mechanism control experiments B)

N2, N4-dimethyl-1,2,4-triazine-3,5(2*H*, 4*H*)-dione (**1a**) (0.3 mmol), manganese acetylacetonate (0.045 mmol), iodobenzene diacetate (0.45 mmol), 1,1-diphenylethene (0.6 mmol), and magnets were added to the Schlenk capped tube, followed by the addition of 1-phenylmethylcyclopropanol (**2a**) (0.75

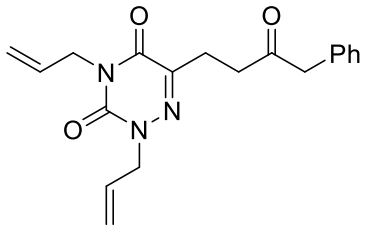
mmol) to a solution of ethyl acetate (1.5 mL) and reacted for 10 h at room temperature. The solvent was removed under reduced pressure and the residue was isolated and purified by silica gel column chromatography in 47% yield for 3a and 45% recovery for **1a**.

III. Characterization of the products



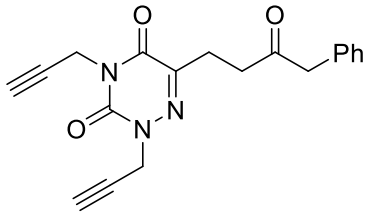
2,4-dimethyl-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3a)

Colorless oil (72.4 mg, 84%), (petroleum ether/EtOAc = 3:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35−7.27 (m, 3H), 7.23-7.21 (m, 2H), 3.74 (s, 2H), 3.47 (s, 3H), 3.31 (s, 3H), 2.86 (dd, J = 4 Hz, J = 4 Hz, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.3, 156.2, 149.0, 142.9, 133.9, 129.3, 128.6, 127.0, 50.1, 39.2, 37.0, 27.0, 24.0. HRMS (ESI): m/z calcd for $C_{15}H_{17}N_3NaO_3^+$ $[M+Na]^+$ 310.1162. Found 310.1159. IR (KBr, cm^{-1}): 2980, 2850, 1712, 1663, 1448, 1321, 1063, 760, 738.



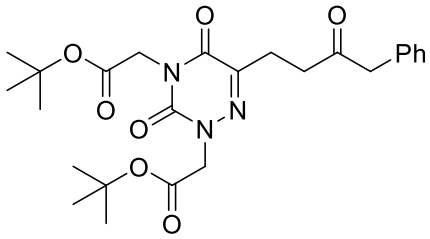
2,4-diallyl-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3b)

Colorless oil (84.6 mg, 83%), (petroleum ether/EtOAc = 2:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.28 (m, 3H), 7.21 (d, J = 8 Hz, 2H), 5.90-5.79 (m, 2H), 5.31-5.19 (m, 4H), 4.50 (d, J = 8 Hz, 2H), 4.43 (d, J = 4 Hz, 2H), 3.73 (s, 2H), 2.88 (d, J = 4 Hz, 2H), 2.84 (d, J = 8 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.2, 155.5, 148.3, 143.7, 134.0, 131.5, 130.3, 129.4, 128.7, 127.0, 119.2, 118.8, 53.7, 50.1, 42.8, 36.9, 24.1. HRMS (ESI): m/z calcd for $C_{19}H_{21}N_3NaO_3^+$ $[M+Na]^+$ 362.1475. Found 362.1473. IR (KBr, cm^{-1}): 3086, 3027, 2947, 1710, 1663, 1453, 1420, 1354, 1272, 934, 768, 743, 696.



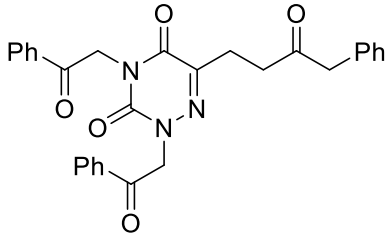
6-(3-oxo-4-phenylbutyl)-2,4-di(prop-2-yn-1-yl)-1,2,4-triazine-3,5(2H,4H)-dione (3c)

Colorless oil (52.6 mg, 52%), (petroleum ether/EtOAc = 3:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.32 (m, 2H), 7.26-7.22 (m, 3H), 4.65 (s, 2H), 4.58 (s, 2H), 3.76 (s, 2H), 2.92 (d, J = 8 Hz, 2H), 2.88 (d, J = 4 Hz, 2H), 2.34 (s, 1H), 2.31 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.1, 154.8, 147.5, 144.4, 134.0, 129.4, 128.7, 127.1, 76.8, 76.4, 73.4, 71.7, 50.1, 41.1, 36.8, 30.0, 24.1; HRMS (ESI): m/z calcd for $C_{19}H_{17}N_3NaO_3^+$ $[M+Na]^+$ 358.1162. Found 358.1163. IR (KBr, cm^{-1}): 3274, 3307, 2985, 1713, 1663, 1615, 1452, 1411, 1319, 1153, 1084, 938, 759, 662, 689.



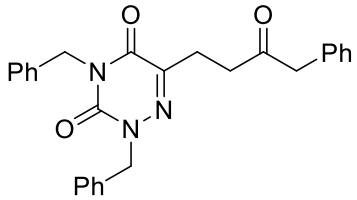
di-tert-butyl 2,2'-(3,5-dioxo-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-2,4(3*H*,5*H*)-diyl)diacetate (3d)

White solid (111.5 mg, 76%), (petroleum ether/EtOAc = 3:1 as the eluet): m. p. = 103-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.31 (m, 3H), 7.21 (d, J = 8 Hz, 2H), 4.53 (s, 2H), 4.41 (s, 2H), 3.71 (s, 2H), 2.89 (d, J = 8 Hz, 2H), 2.83 (d, J = 8 Hz, 2H), 1.47 (s, 9H), 1.46 (s, 9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 205.9, 166.3, 165.5, 155.4, 148.5, 144.0, 134.0, 129.4, 128.7, 127.0, 82.9, 82.8, 53.2, 50.1, 42.1, 37.1, 28.0, 27.9, 24.1; HRMS (ESI): m/z calcd for $C_{25}H_{33}N_3NaO_7^+$ $[M+Na]^+$ 510.2211. Found 510.2210. IR (KBr, cm^{-1}): 2984, 2916, 2848, 1747, 1719, 1672, 1453, 1366, 1260, 1232, 1151, 804, 771, 749, 702.



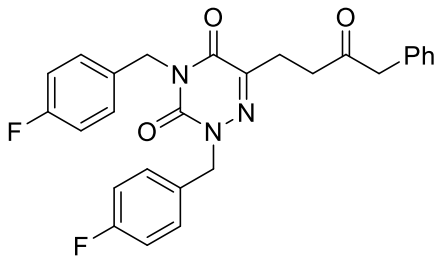
2,4-bis(2-oxo-2-phenylethyl)-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3e)

Colorless oil (121.5 mg, 79%), (petroleum ether/EtOAc = 2:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, J = 8 Hz, J = 12 Hz, 4H), 7.66-7.59 (m, 2H), 7.54-7.47 (m, 4H), 7.26-7.19 (m, 5H), 5.36 (s, 2H), 5.22 (s, 2H), 3.69 (s, 2H), 2.92 (d, J = 8 Hz, 2H), 2.85 (d, J = 8 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.0, 191.4, 190.2, 155.6, 148.9, 144.3, 134.4, 134.3, 134.1, 134.0, 129.4, 128.9, 128.8, 128.7, 128.6, 128.1, 128.0, 126.9, 57.2, 50.0, 46.5, 37.1, 24.1. HRMS (ESI): m/z calcd for $C_{29}H_{25}N_3NaO_5^+$ $[M+Na]^+$ 518.1686. Found 518.1689. IR (KBr, cm^{-1}): 2917, 2847, 1718, 1701, 1660, 1451, 1356, 1225, 912, 742, 686.



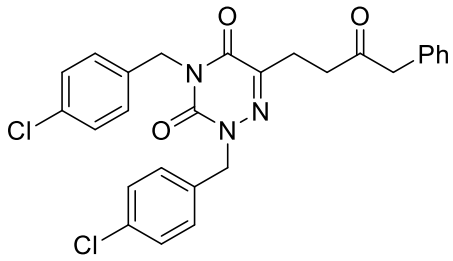
2,4-dibenzyl-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3f)

Colorless oil (103.2 mg, 78%), (petroleum ether/EtOAc = 3:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 8 Hz, 2H), 7.30-7.23 (m, 11H), 7.16 (d, J = 8 Hz, 2H), 5.03 (s, 2H), 4.94 (s, 2H), 3.67 (s, 2H), 2.86 (d, J = 4 Hz, 2H), 2.80 (d, J = 4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.1, 155.7, 148.8, 143.7, 135.6, 135.4, 133.9, 130.3, 129.3, 128.6, 128.6, 128.4, 128.1, 127.9, 127.0, 55.0, 50.0, 44.1, 36.9, 24.0. HRMS (ESI): m/z calcd for $C_{27}H_{25}N_3NaO_3^+$ $[M+Na]^+$ 462.1788. Found 462.1785. IR (KBr, cm^{-1}): 3017, 2987, 2907, 2836, 2359, 2321, 1702, 1649, 1592, 1483, 1439, 1342, 1225, 1069, 1018, 754, 733, 689.



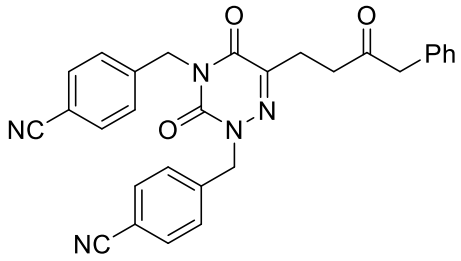
2,4-bis(4-fluorobenzyl)-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3g)

Colorless oil (71.1 mg, 50%), (petroleum ether/EtOAc = 3:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.42 (m, 2H), 7.31-7.23 (m, 5H), 7.18 (d, J = 4 Hz, 2H), 6.98 (dd, J = 8 Hz, J = 16 Hz, 4H), 4.98 (s, 2H), 4.88 (s, 2H), 3.69 (s, 2H), 2.86 (d, J = 4 Hz, 2H), 2.82 (d, J = 4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.0, 162.5 (d, J = 246 Hz), 162.4 (d, J = 245 Hz), 155.6, 148.7, 143.9, 133.9, 131.4 (d, J = 8 Hz), 131.3, 130.4 (d, J = 8 Hz), 129.4, 129.3 (d, J = 10 Hz), 128.7, 127.1, 115.5 (d, J = 18 Hz), 115.3 (d, J = 18 Hz), 54.4, 50.0, 43.4, 36.9, 24.0. HRMS (ESI): m/z calcd for $C_{27}H_{23}F_2N_3NaO_3^+$ $[M+Na]^+$ 498.1600. Found 498.1604. IR (KBr, cm^{-1}): 2939, 2902, 1709, 1658, 1603, 1507, 1448, 1337, 1218, 1158, 1094, 768, 731, 689, 585.



2,4-bis(4-chlorobenzyl)-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3h)

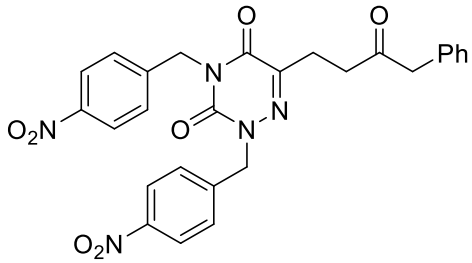
White solid (100.9 mg, 66%), (petroleum ether/EtOAc = 3:1 as the eluet): m. p. = 110-112 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, J = 8 Hz, 2H), 7.29-7.25 (m, 7H), 7.19-7.16 (m, 4H), 4.98 (s, 2H), 4.88 (s, 2H), 3.68 (s, 2H), 2.86 (d, J = 8 Hz, 2H), 2.82 (d, J = 8 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.0, 155.6, 148.7, 144.0, 134.1, 134.0, 133.9, 133.9, 133.8, 130.9, 129.9, 129.4, 128.8, 128.7, 128.7, 127.1, 54.4, 50.0, 43.5, 36.9, 24.0. HRMS (ESI): m/z calcd for $C_{27}H_{23}Cl_2N_3NaO_3^+$ $[M+Na]^+$ 530.1009. Found 530.1011. IR (KBr, cm^{-1}): 2949, 2902, 1710, 1654, 1419, 1445, 1355, 1089, 1009, 804, 740, 698, 552.



4,4'-((3,5-dioxo-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-2,4(3*H*,5*H*)-diyl)bis(methylene))dibenzonitrile (3i)

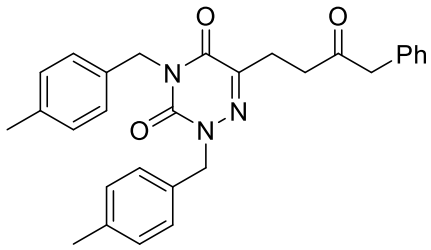
White solid (75.9 mg, 52%), (petroleum ether/EtOAc = 2:1 as the eluet): m. p. = 138-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.58 (m, 3H), 7.52 (d, J = 8 Hz, 2H), 7.32-7.26 (m, 6H), 7.17 (d, J = 8 Hz, 4H), 5.05 (s, 2H), 4.93 (s, 2H), 3.69 (s, 2H), 2.87 (s, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 205.9, 155.5, 148.6, 144.4, 140.4, 140.2, 133.8, 132.4, 132.3, 129.9, 129.3, 128.9, 128.7, 127.1, 118.4, 118.3,

112.1, 112.0, 54.7, 49.9, 43.7, 36.8, 23.9; HRMS (ESI): m/z calcd for $C_{29}H_{23}N_5NaO_3^+$ $[M+Na]^+$ 512.1693. Found 512.1696. IR (KBr, cm^{-1}): 3034, 2999, 2228, 1708, 1651, 1601, 1450, 1406, 1353, 1218, 1143, 764, 723, 694, 579.



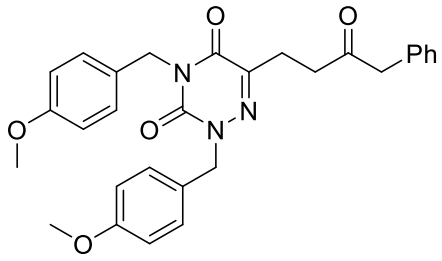
2,4-bis(4-nitrobenzyl)-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3j)

White solid (95.6 mg, 60%), (petroleum ether/EtOAc = 2:1 as the eluet): m. p. = 113-116 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.11 (m, 4H), 7.58 (d, J = 8 Hz, 2H), 7.38 (d, J = 8 Hz, 2H), 7.26-7.17 (m, 5H), 5.10 (s, 2H), 4.98 (s, 2H), 3.70 (s, 2H), 2.89 (s, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 205.9, 155.5, 148.6, 147.7, 147.6, 144.6, 142.3, 142.2, 133.8, 130.1, 129.3, 129.1, 128.7, 127.1, 123.8, 123.7, 54.4, 49.9, 43.4, 36.8, 24.0; HRMS (ESI): m/z calcd for $C_{27}H_{23}N_5NaO_7^+$ $[M+Na]^+$ 552.1490. Found 552.1488. IR (KBr, cm^{-1}): 2951, 2921, 1707, 1660, 1603, 1519, 1453, 1345, 1104, 940, 853, 799, 736, 695.



2,4-bis(4-methylbenzyl)-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3k)

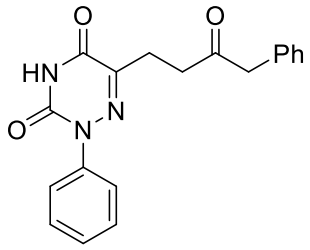
White solid (126.9 mg, 90%), (petroleum ether/EtOAc = 3:1 as the eluet): m. p. = 84-87 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8 Hz, 2H), 7.30-7.23 (m, 3H), 7.19-7.17 (m, 4H), 7.16-7.09 (m, 4H), 4.99 (s, 2H), 4.91 (s, 2H), 3.67 (s, 2H), 2.85 (d, J = 8 Hz, 2H), 2.79 (d, J = 8 Hz, 2H), 2.32 (s, 3H), 2.30 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.1, 155.8, 148.8, 143.6, 137.9, 137.8, 134.0, 132.7, 132.6, 129.4, 129.3, 129.2, 129.1, 128.7, 128.5, 127.0, 54.8, 50.1, 43.8, 36.9, 24.1, 21.1; HRMS (ESI): m/z calcd for $C_{29}H_{29}N_3NaO_3^+$ $[M+Na]^+$ 490.2101. Found 490.2102. IR (KBr, cm^{-1}): 3032, 2911, 1716, 1697, 1660, 1510, 1453, 1352, 1314, 1072, 766, 729, 696, 585.



2,4-bis(4-methoxybenzyl)-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3l)

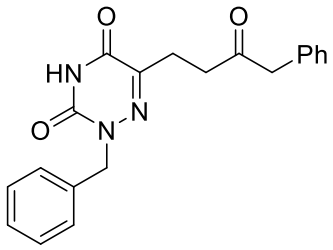
Colorless oil (115.6 mg, 77%), (petroleum ether/EtOAc = 3:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 8 Hz, 2H), 7.29-7.21 (m, 5H), 7.17 (d, J = 8 Hz, 2H), 6.84-6.80 (m, 4H), 4.96 (s, 2H), 4.88 (s, 2H), 3.77 (s, 3H), 3.76 (s, 3H), 3.69 (s, 2H), 2.85 (d, J = 8 Hz, 2H), 2.80 (d, J = 8 Hz, 2H);

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 206.1, 159.4, 159.2, 155.7, 148.7, 143.6, 133.9, 130.9, 130.0, 129.3, 128.6, 127.8, 127.7, 127.0, 113.9, 113.7, 55.1, 55.1, 54.5, 50.0, 43.5, 36.9, 24.0; HRMS (ESI): m/z calcd for $C_{29}H_{29}N_3NaO_5^+$ $[M+Na]^+$ 522.1999. Found 522.1987. IR (KBr, cm^{-1}): 2933, 2831, 1716, 1697, 1646, 1610, 1510, 1448, 1353, 1247, 1177, 1037, 767, 733, 693, 644, 587.



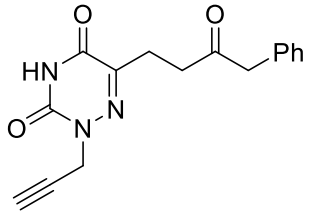
6-(3-oxo-4-phenylbutyl)-2-phenyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3m)

White solid (59.2 mg, 59%), (petroleum ether/EtOAc = 2:1 as the eluet): m. p. = 170-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.95 (s, 1H), 7.52-7.46 (m, 3H), 7.33-7.29 (m, 3H), 7.25-7.19 (m, 4H), 3.73 (s, 2H), 2.90 (d, J = 4 Hz, 2H), 2.85 (d, J = 8 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 206.5, 155.8, 149.7, 145.2, 134.0, 132.2, 129.5, 129.4, 128.8, 128.7, 127.8, 127.1, 50.2, 36.7, 24.2. HRMS (ESI): m/z calcd for $C_{19}H_{17}N_3NaO_3^+$ $[M+Na]^+$ 358.1162. Found 358.1161. IR (KBr, cm^{-1}): 3194, 3079, 2945, 1710, 1665, 1613, 1493, 1432, 1319, 1237, 1185, 1105, 750, 696.



2-benzyl-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3n)

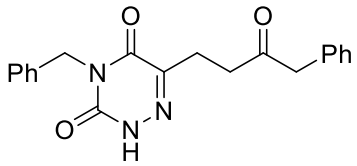
White solid (78.8 mg, 75%), (petroleum ether/EtOAc = 2:1 as the eluet): m. p. = 126-128 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (s, 1H), 7.45 (d, J = 8 Hz, 2H), 7.32-7.29 (m, 6H), 7.19 (d, J = 8 Hz, 2H), 5.03 (s, 2H), 3.72 (s, 2H), 2.86 (d, J = 4 Hz, 2H), 2.80 (d, J = 4 Hz, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 206.5, 155.8, 149.9, 144.8, 135.2, 134.0, 129.4, 129.3, 128.7, 128.6, 128.1, 127.0, 50.1, 43.5, 36.9, 24.2; HRMS (ESI): m/z calcd for $C_{20}H_{19}N_3NaO_3^+$ $[M+Na]^+$ 372.1319. Found 372.1317. IR (KBr, cm^{-1}): 3116, 3000, 2810, 1742, 1708, 1653, 1495, 1458, 1363, 1239, 1154, 1084, 1032, 839, 4744, 696.



6-(3-oxo-4-phenylbutyl)-2-(prop-2-yn-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3o)

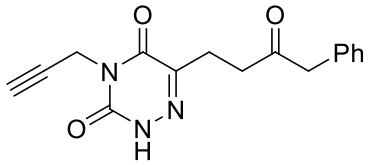
White solid (35.4 mg, 40%), (petroleum ether/EtOAc = 2:1 as the eluet): m. p. = 96-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 7.38-7.35 (m, 3H), 7.24 (d, J = 4 Hz, 2H), 4.67 (s, 2H), 3.77 (s, 2H), 2.92 (d, J = 8 Hz, 2H), 2.88 (d, J = 4 Hz, 2H), 2.26 (s, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 206.4, 155.0, 149.0, 144.7, 134.0, 129.4, 128.7, 127.1, 76.4, 71.8, 50.2, 36.8, 29.3, 24.1; HRMS (ESI): m/z calcd for $C_{16}H_{15}N_3NaO_3^+$ $[M+Na]^+$ 320.1006. Found 320.1007. IR (KBr, cm^{-1}): 3263, 3102, 2911,

1719, 1662, 1606, 1451, 1347, 1213, 1166, 1086, 1037, 749, 716, 697.



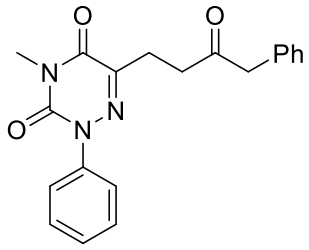
4-benzyl-6-(3-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3p)

White solid (73.7 mg, 70%), (petroleum ether/EtOAc = 2:1 as the eluet): m. p. = 91-94 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.83 (s, 1H), 7.31-7.25 (m, 8H), 7.16 (d, J = 4 Hz, 2H), 4.94 (s, 2H), 3.67 (s, 2H), 2.84 (d, J = 4 Hz, 2H), 2.80 (d, J = 4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.1, 156.2, 148.5, 145.0, 135.4, 133.9, 129.4, 128.7, 128.6, 128.5, 128.1, 127.0, 54.0, 50.1, 36.9, 23.6; HRMS (ESI): m/z calcd for $C_{20}H_{19}N_3NaO_3^+$ $[M+Na]^+$ 372.1319. Found 372.1320. IR (KBr, cm^{-1}): 2990, 2818, 1714, 1677, 1587, 1460, 1354, 1296, 1068, 889, 733, 691.



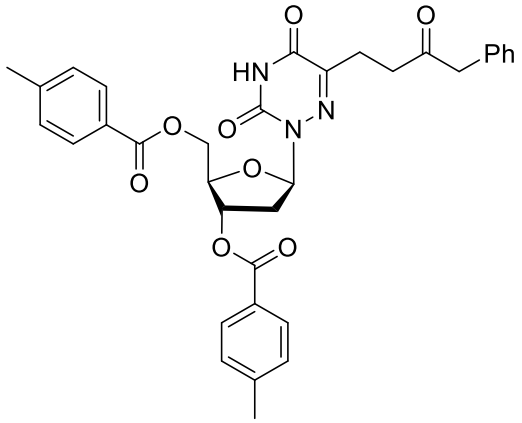
6-(3-oxo-4-phenylbutyl)-4-(prop-2-yn-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3q)

Colorless oil (44.6 mg, 50%), (petroleum ether/EtOAc = 2:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.75 (s, 1H), 7.35-7.32 (m, 2H), 7.28-7.22 (m, 3H), 4.56 (s, 2H), 3.76 (s, 2H), 2.90-2.85 (m, 4H), 2.33 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.2, 156.1, 147.9, 145.6, 134.0, 129.4, 128.7, 127.1, 76.8, 73.4, 50.1, 40.1, 36.8, 23.6; HRMS (ESI): m/z calcd for $C_{16}H_{15}N_3NaO_3^+$ $[M+Na]^+$ 320.1006. Found 320.1008. IR (KBr, cm^{-1}): 3274, 2990, 2893, 1714, 1670, 1617, 1410, 1321, 1150, 1080, 936, 756, 689.



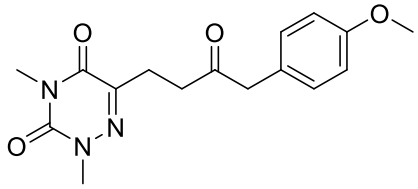
4-methyl-6-(3-oxo-4-phenylbutyl)-2-phenyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3r)

Colorless oil (53.5 mg, 51%), (petroleum ether/EtOAc = 3:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.43 (m, 3H), 7.36-7.23 (m, 5H), 7.18 (d, J = 8 Hz, 2H), 3.75 (s, 2H), 3.50 (s, 3H), 2.92-2.88 (m, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.4, 155.9, 148.7, 144.0, 134.0, 133.0, 129.4, 129.4, 129.2, 128.7, 127.7, 127.1, 50.1, 39.3, 37.0, 24.2; HRMS (ESI): m/z calcd for $C_{20}H_{19}N_3NaO_3^+$ $[M+Na]^+$ 372.1319. Found 372.1320. IR (KBr, cm^{-1}): 2955, 1714, 1665, 1609, 1495, 1439, 1349, 1305, 1220, 1152, 1025, 738, 714, 699, 632.



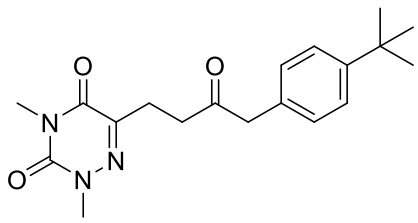
(2R,3S,5R)-5-(3,5-dioxo-6-(3-oxo-4-phenylbutyl)-4,5-dihydro-1,2,4-triazin-2(3*H*)-yl)-2-(((4-methyl benzoyl)oxy)methyl)tetrahydrofuran-3-yl 4-methylbenzoate (3s)

White solid (157.6 mg, 86%), (petroleum ether/EtOAc = 3:1 as the eluet): m. p. = 111-114 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 7.96-7.89 (m, 4H), 7.27-7.17 (m, 9H), 6.63-6.60 (m, 1H), 5.62 (s, 1H), 4.50-4.48 (m, 2H), 4.44-4.41 (m, 1H), 3.76 (s, 2H), 3.00-2.87 (m, 2H), 2.82-2.71 (m, 4H), 2.43 (s, 3H), 2.38 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.1, 166.2, 165.9, 155.5, 148.5, 146.3, 144.3, 144.0, 134.0, 129.8, 129.7, 129.4, 129.2, 129.1, 128.7, 127.0, 126.8, 126.5, 85.6, 81.8, 74.7, 64.1, 49.7, 37.2, 34.6, 23.7, 21.7, 21.6; HRMS (ESI): m/z calcd for $C_{34}H_{33}N_3NaO_8^+$ $[M+Na]^+$ 634.2160. Found 634.2164. IR (KBr, cm^{-1}): 3073, 2818, 1725, 1706, 1689, 1611, 1454, 1259, 1177, 1099, 842, 749, 681, 565.



6-(4-(4-methoxyphenyl)-3-oxobutyl)-2,4-dimethyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3t)

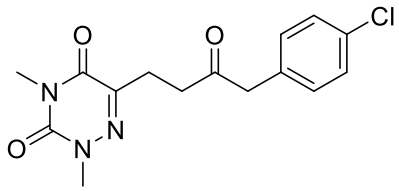
Colorless oil (75.3 mg, 79%), (petroleum ether/EtOAc = 2:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (d, J = 8 Hz, 2H), 6.86 (d, J = 4 Hz, 2H), 3.79 (s, 3H), 3.67 (s, 2H), 3.50 (s, 3H), 3.31 (s, 3H), 2.86-2.82 (m, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.7, 158.6, 156.2, 149.1, 143.1, 130.4, 125.9, 114.1, 55.2, 49.2, 39.2, 36.9, 27.0, 24.2; HRMS (ESI): m/z calcd for $C_{16}H_{19}N_3NaO_4^+$ $[M+Na]^+$ 340.1268. Found 340.1270. IR (KBr, cm^{-1}): 3031, 2956, 2911, 2836, 1704, 1657, 1613, 1509, 1464, 1321, 1246, 1091, 1032, 804, 740,, 1246, 1091, 1032, 804, 740,630.



6-(4-(4-(tert-butyl)phenyl)-3-oxobutyl)-2,4-dimethyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3u)

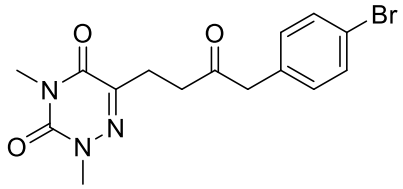
Colorless oil (92.6 mg, 90%), (petroleum ether/EtOAc = 3:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, J = 4 Hz, 2H), 7.16 (d, J = 4 Hz, 2H), 3.70 (s, 2H), 3.45 (s, 3H), 3.31 (s, 3H), 2.86 (s, 4H), 1.30 (s, 9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.5, 156.2, 149.9, 149.1, 143.0, 130.9, 129.0, 125.6, 49.5, 39.2, 37.0, 34.4, 31.2, 27.0, 24.0; HRMS (ESI): m/z calcd for $C_{19}H_{25}N_3NaO_3^+$ $[M+Na]^+$ 366.1788.

Found 366.1785. IR (KBr, cm^{-1}): 2956, 2909, 2873, 1712, 1660, 1602, 1467, 1354, 1413, 1314, 1265, 1053, 971, 827, 756, 740, 620.



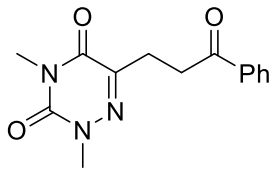
6-(4-(4-chlorophenyl)-3-oxobutyl)-2,4-dimethyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3v)

Colorless oil (76.6 mg, 79%), (petroleum ether/EtOAc = 2:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, J = 8 Hz, 2H), 7.15 (d, J = 8 Hz, 2H), 3.72 (s, 2H), 3.50 (s, 3H), 3.32 (s, 3H), 2.88-2.84 (m, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 205.6, 156.2, 149.1, 142.9, 133.0, 132.3, 130.7, 128.8, 49.1, 39.2, 37.3, 27.0, 24.1; HRMS (ESI): m/z calcd for $C_{15}H_{16}ClN_3NaO_3^+$ $[M+Na]^+$ 344.0772. Found 344.0775. IR (KBr, cm^{-1}): 2949, 2912, 1714, 1661, 1491, 1406, 1361, 1319, 1214, 1093, 1058, 1016, 797, 740, 628, 576.



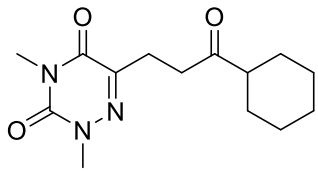
6-(4-(4-bromophenyl)-3-oxobutyl)-2,4-dimethyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3w)

White solid (91.0 mg, 83%), (petroleum ether/EtOAc = 2:1 as the eluet): m. p. = 98-101 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 8 Hz, 2H), 7.09 (d, J = 8 Hz, 2H), 3.70 (s, 2H), 3.50 (s, 3H), 3.32 (s, 3H), 2.88-2.84 (m, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 205.6, 156.2, 149.1, 142.9, 132.8, 131.7, 131.1, 121.1, 49.2, 39.2, 37.3, 27.1, 24.1; HRMS (ESI): m/z calcd for $C_{15}H_{16}BrN_3NaO_3^+$ $[M+Na]^+$ 388.0267. Found 388.0269. IR (KBr, cm^{-1}): 2952, 2900, 1715, 1658, 1463, 1317, 1060, 1006, 800, 750, 654.



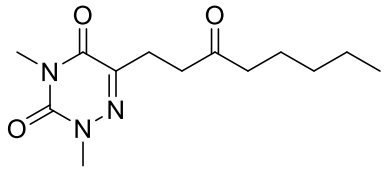
2,4-dimethyl-6-(3-oxo-3-phenylpropyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3x)

White solid (48.2 mg, 59%), (petroleum ether/EtOAc = 3:1 as the eluet): m. p. = 110-113 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8 Hz, 2H), 7.60-7.56 (m, 1H), 7.50-7.46 (m, 2H), 3.52 (s, 3H), 3.39-3.36 (m, 5H), 3.09 (t, J = 8 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 198.3, 156.4, 149.2, 143.4, 136.8, 133.1, 128.6, 128.0, 39.3, 34.0, 27.1, 24.7; HRMS (ESI): m/z calcd for $C_{14}H_{15}N_3NaO_3^+$ $[M+Na]^+$ 296.1006. Found 296.1009. IR (KBr, cm^{-1}): 2957, 2897, 1713, 1691, 1654, 1590, 1452, 1371, 1319, 1264, 1181, 1061, 984, 740, 713, 694.



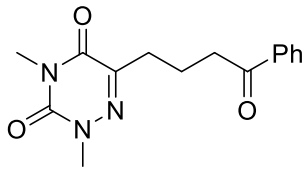
6-(3-cyclohexyl-3-oxopropyl)-2,4-dimethyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3y)

Colorless oil (72.0 mg, 86%), (petroleum ether/EtOAc = 3:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.56 (s, 3H), 3.34 (s, 3H), 2.88 (d, J = 8 Hz, 2H), 2.83 (d, J = 8 Hz, 2H), 2.42-2.37 (m, 1H), 1.88-1.85 (m, 2H), 1.80-1.78 (m, 2H), 1.68 (d, J = 8 Hz, 1H), 1.41-1.19 (m, 5H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 211.9, 156.3, 149.1, 143.4, 50.7, 39.2, 35.7, 28.5, 27.0, 25.8, 25.6, 24.0; HRMS (ESI): m/z calcd for $C_{14}H_{21}N_3NaO_3^+$ $[M+Na]^+$ 302.1475. Found 302.1476. IR (KBr, cm^{-1}): 2928, 250, 1712, 1663, 1448, 1321, 1063, 760, 738.



2,4-dimethyl-6-(3-oxooctyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3z)

Colorless oil (69.8 mg, 87%), (petroleum ether/EtOAc = 3:1 as the eluet): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.57 (s, 3H), 3.34 (s, 3H), 2.90 (t, J = 8 Hz, 2H), 2.79 (t, J = 8 Hz, 2H), 2.46 (t, J = 8 Hz, 2H), 1.64-1.56 (m, 2H), 1.35-1.26 (m, 4H), 0.90 (t, J = 8 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 209.2, 156.3, 149.2, 143.3, 42.8, 39.3, 37.7, 31.4, 27.1, 24.2, 23.5, 22.4, 13.8; HRMS (ESI): m/z calcd for $C_{13}H_{21}N_3NaO_3^+$ $[M+Na]^+$ 290.1475. Found 290.1473. IR (KBr, cm^{-1}): 2956, 2925, 2866, 1712, 1665, 1457, 1325, 1126, 1062, 839, 744.

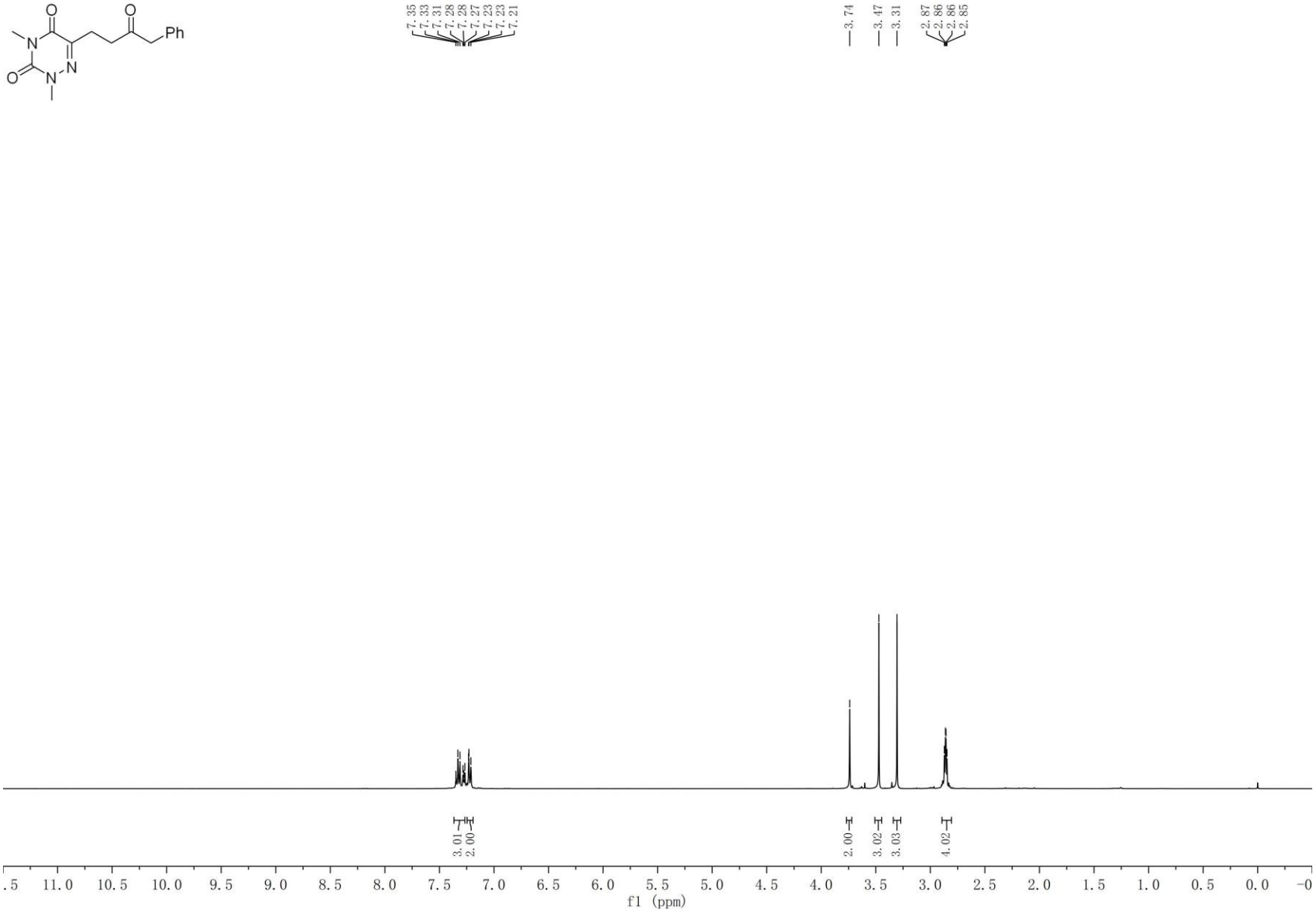


2,4-dimethyl-6-(4-oxo-4-phenylbutyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3aa)

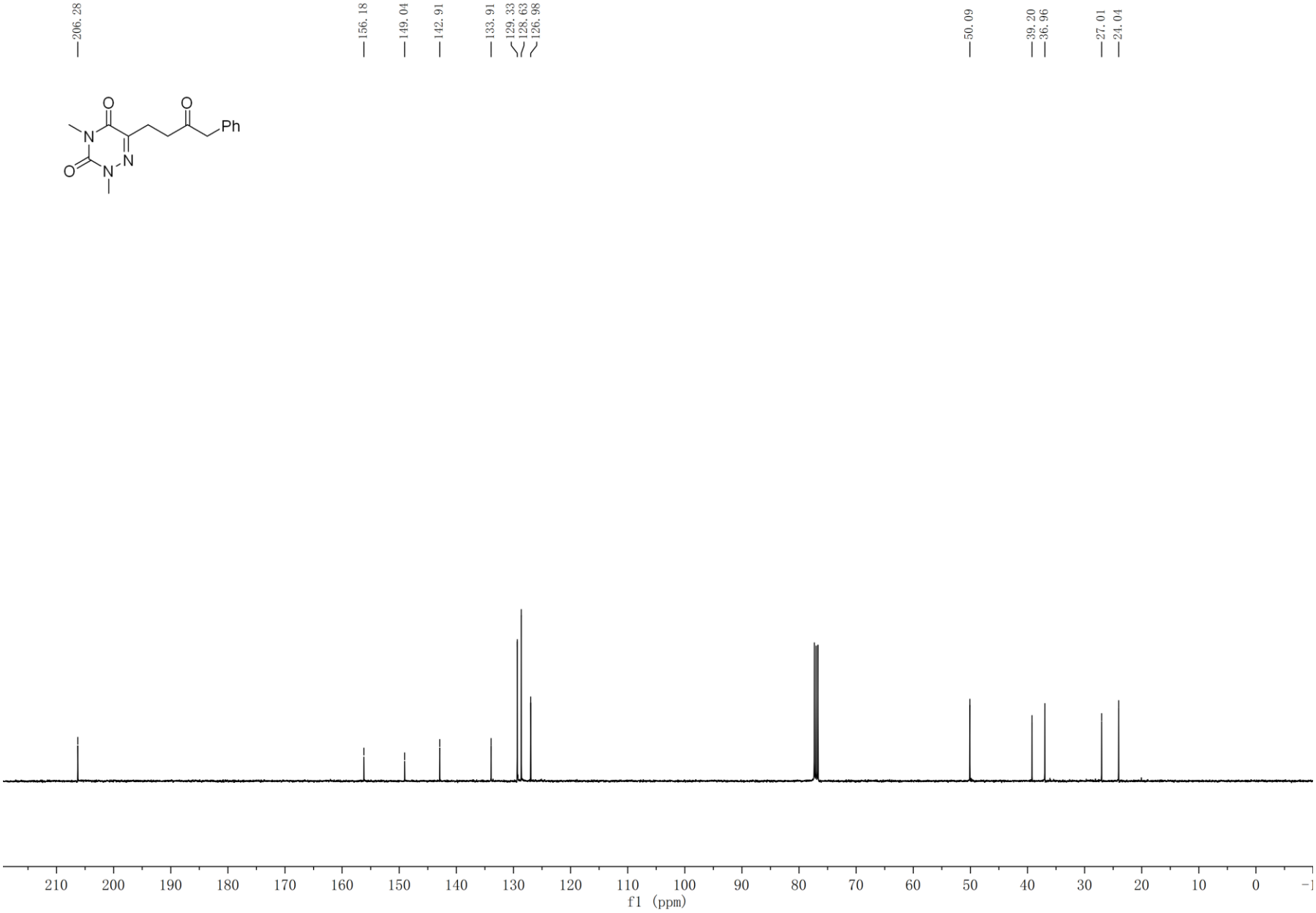
White solid (56.9 mg, 66%), (petroleum ether/EtOAc = 3:1 as the eluet): m. p. = 136-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 8 Hz, 2H), 7.58-7.55 (m, 1H), 7.48-7.45 (m, 2H), 3.56 (s, 3H), 3.35 (s, 3H), 3.07 (t, J = 8 Hz, 2H), 2.72 (t, J = 8 Hz, 2H), 2.16-2.08 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 199.5, 156.4, 149.2, 144.2, 136.8, 133.0, 128.6, 127.9, 39.3, 37.6, 29.7, 27.1, 20.6; HRMS (ESI): m/z calcd for $C_{15}H_{17}N_3NaO_3^+$ $[M+Na]^+$ 310.1162. Found 310.1163. IR (KBr, cm^{-1}): 2957, 2897, 1691, 1654, 1590, 1452, 1371, 1319, 1264, 1181, 1061, 984, 740, 713, 694.

IV. NMR Charts

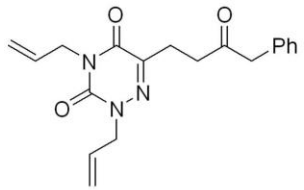
3a-^{1}H NMR (400 MHz, $CDCl_3$)

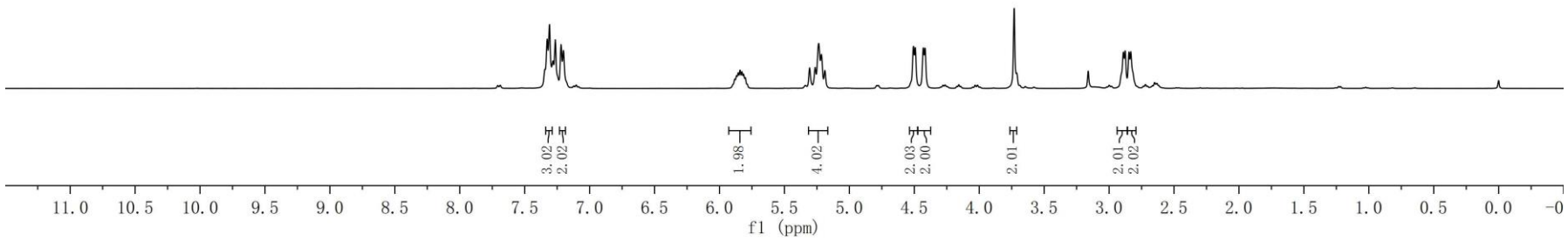


3a-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

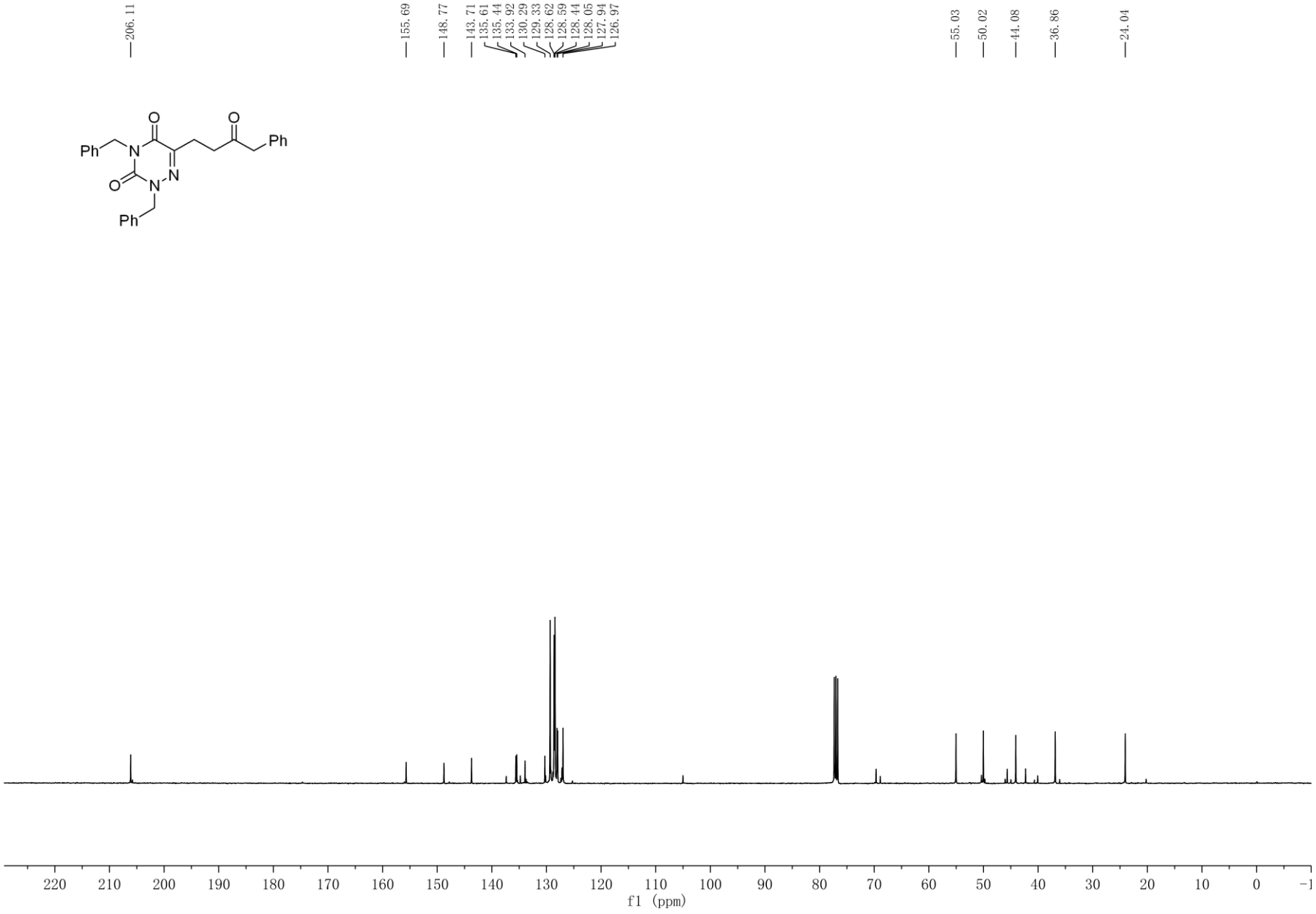


3b-^{1}H NMR (400 MHz, $CDCl_3$)

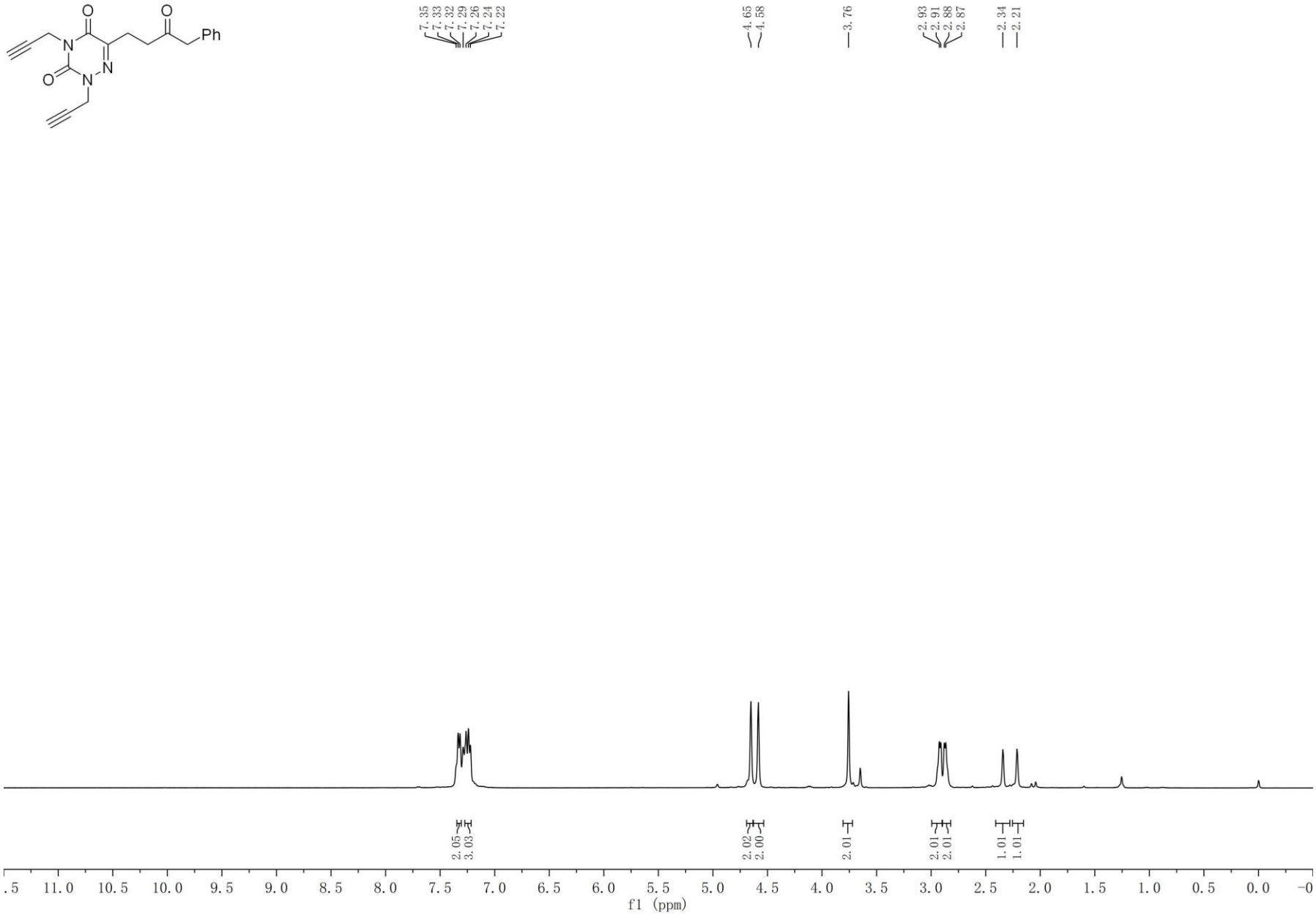




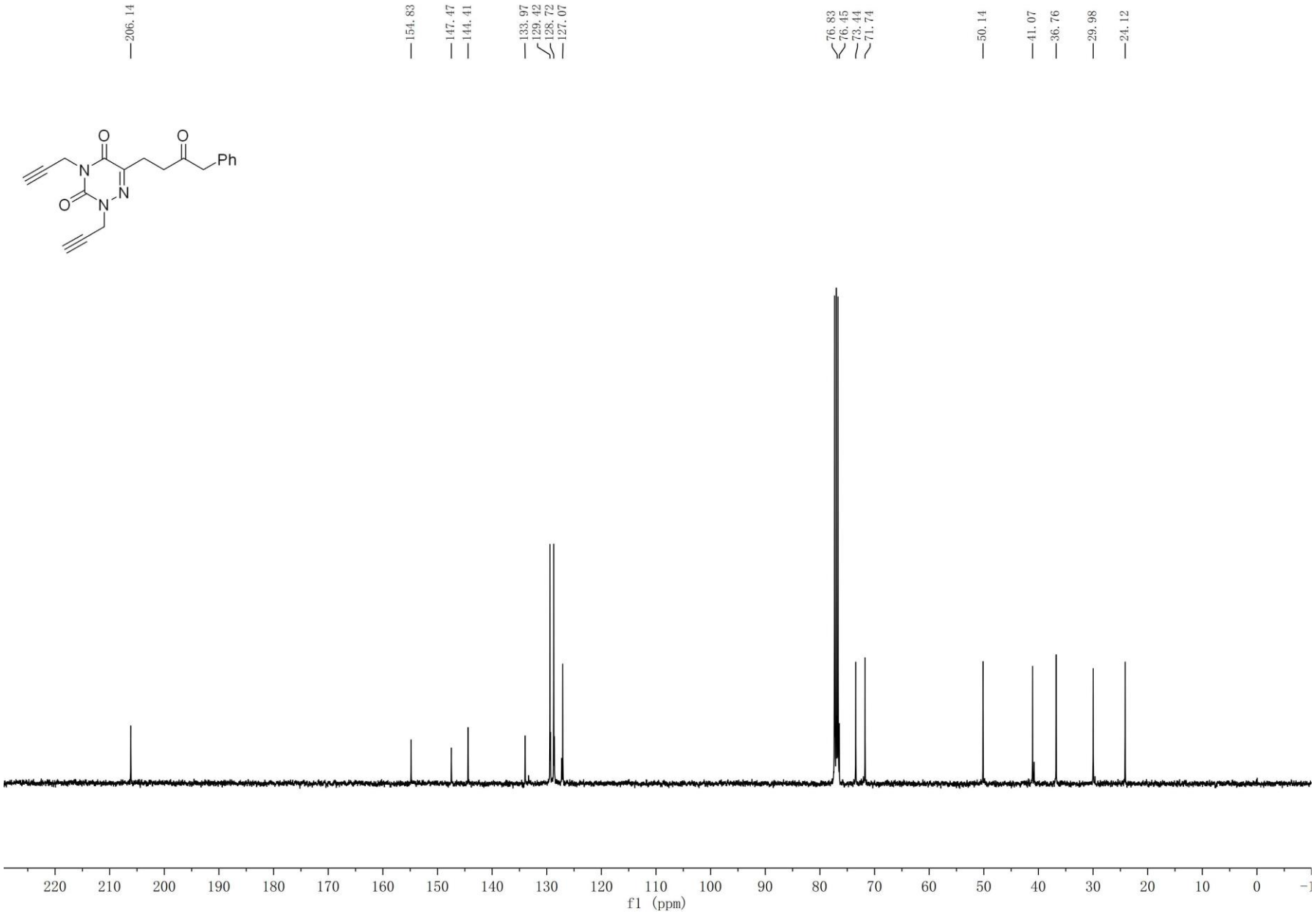
3b-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



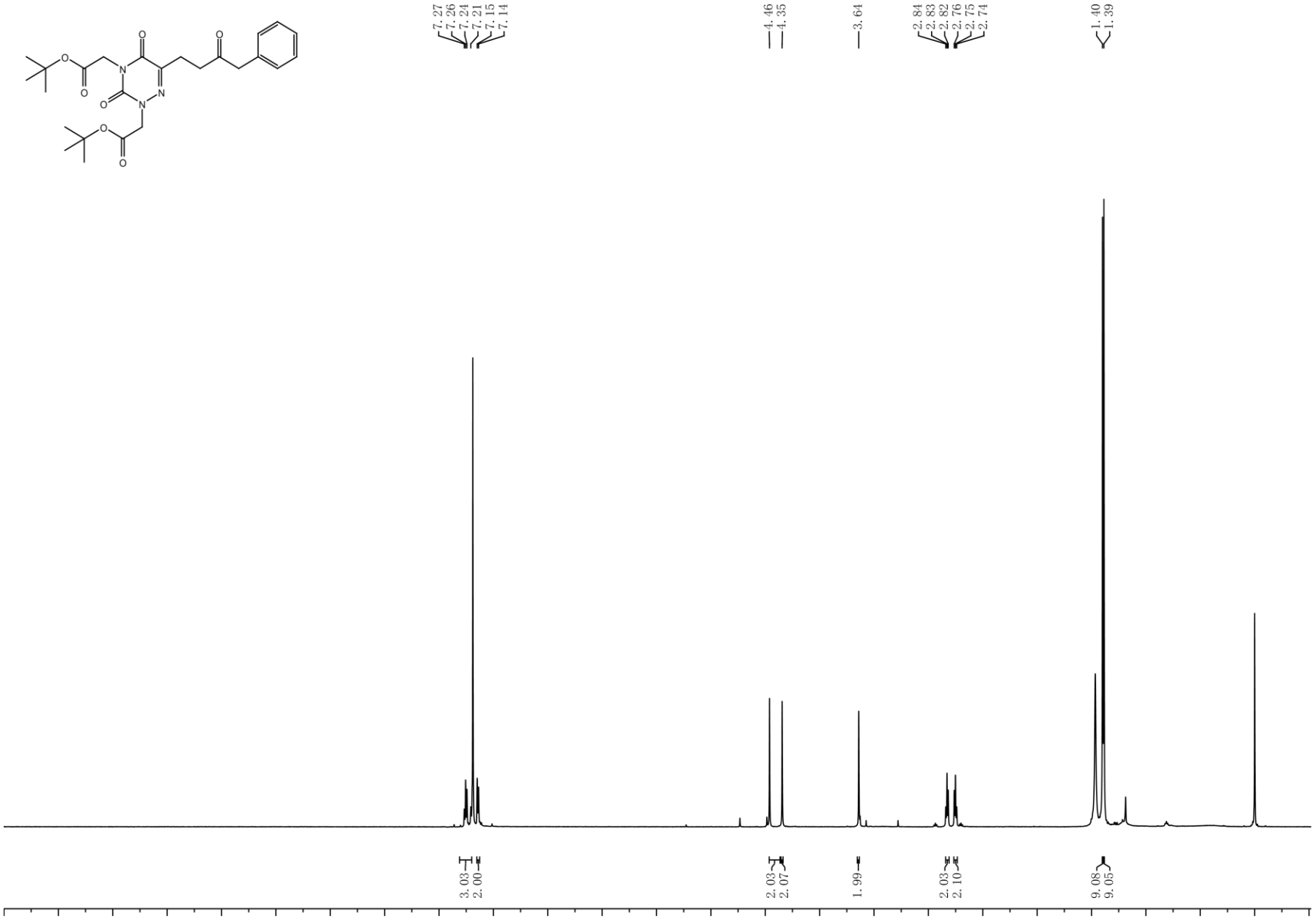
3c-^{1}H NMR (400 MHz, $CDCl_3$)



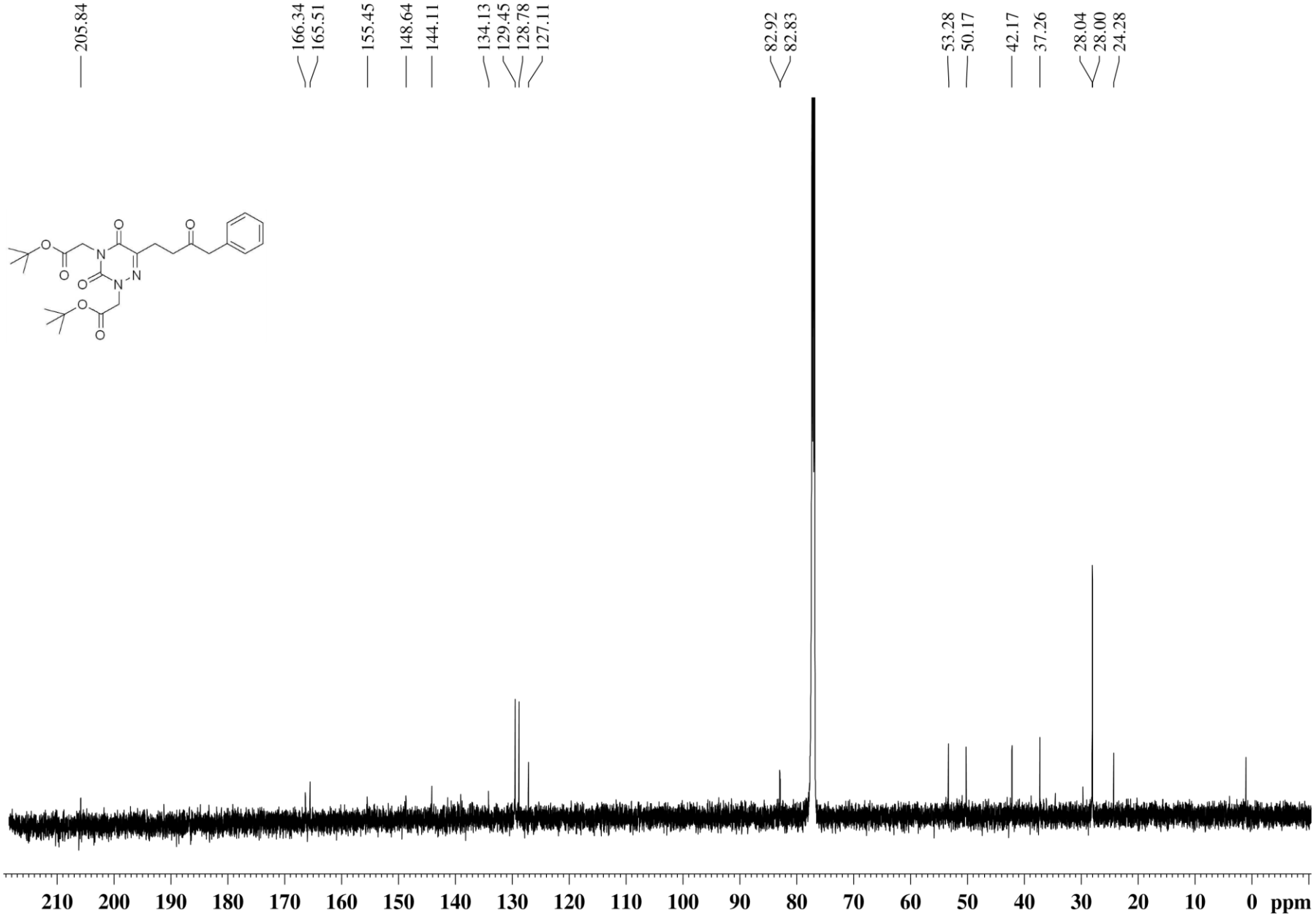
3c-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



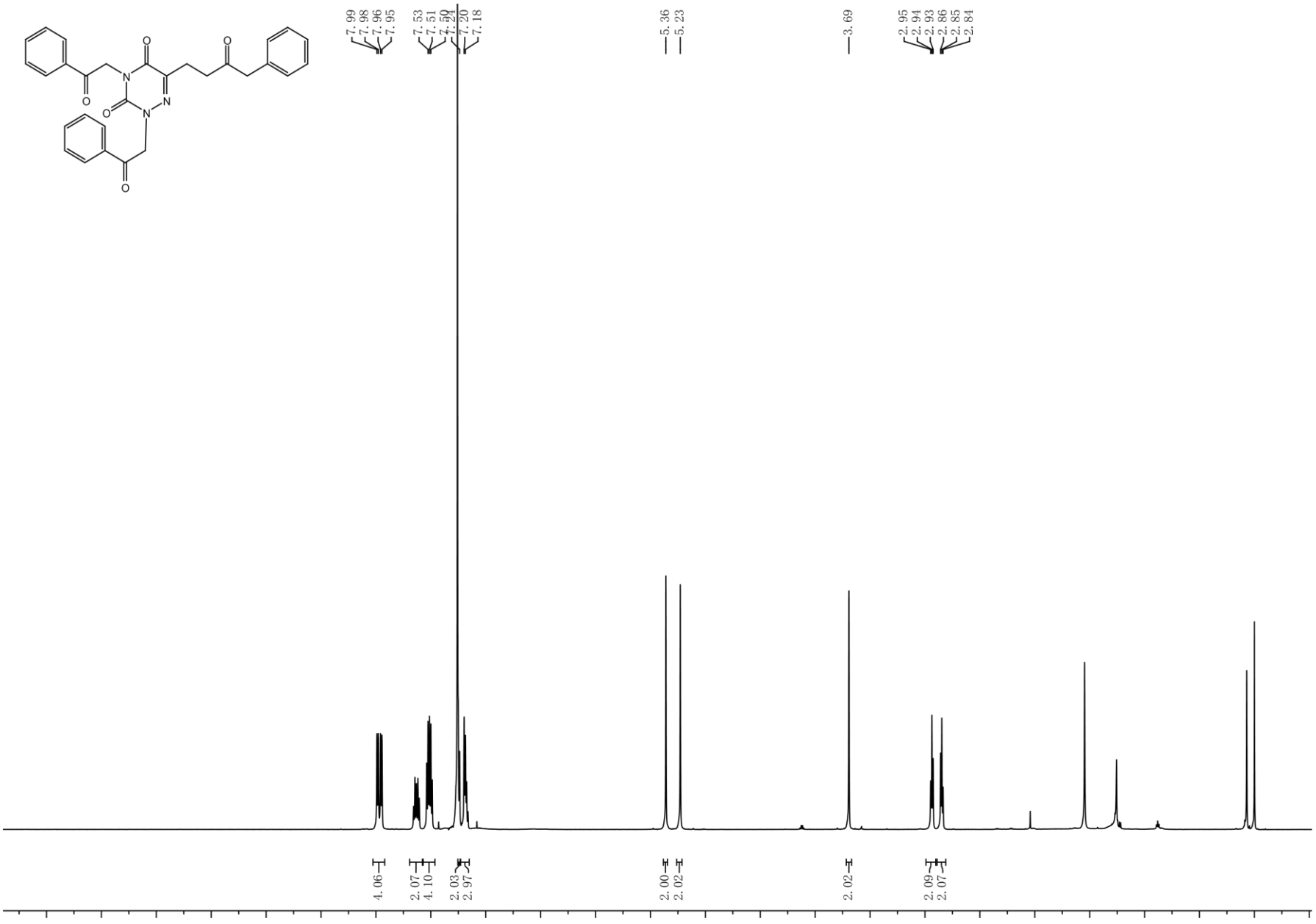
3d-^{1}H NMR (400 MHz, $CDCl_3$)



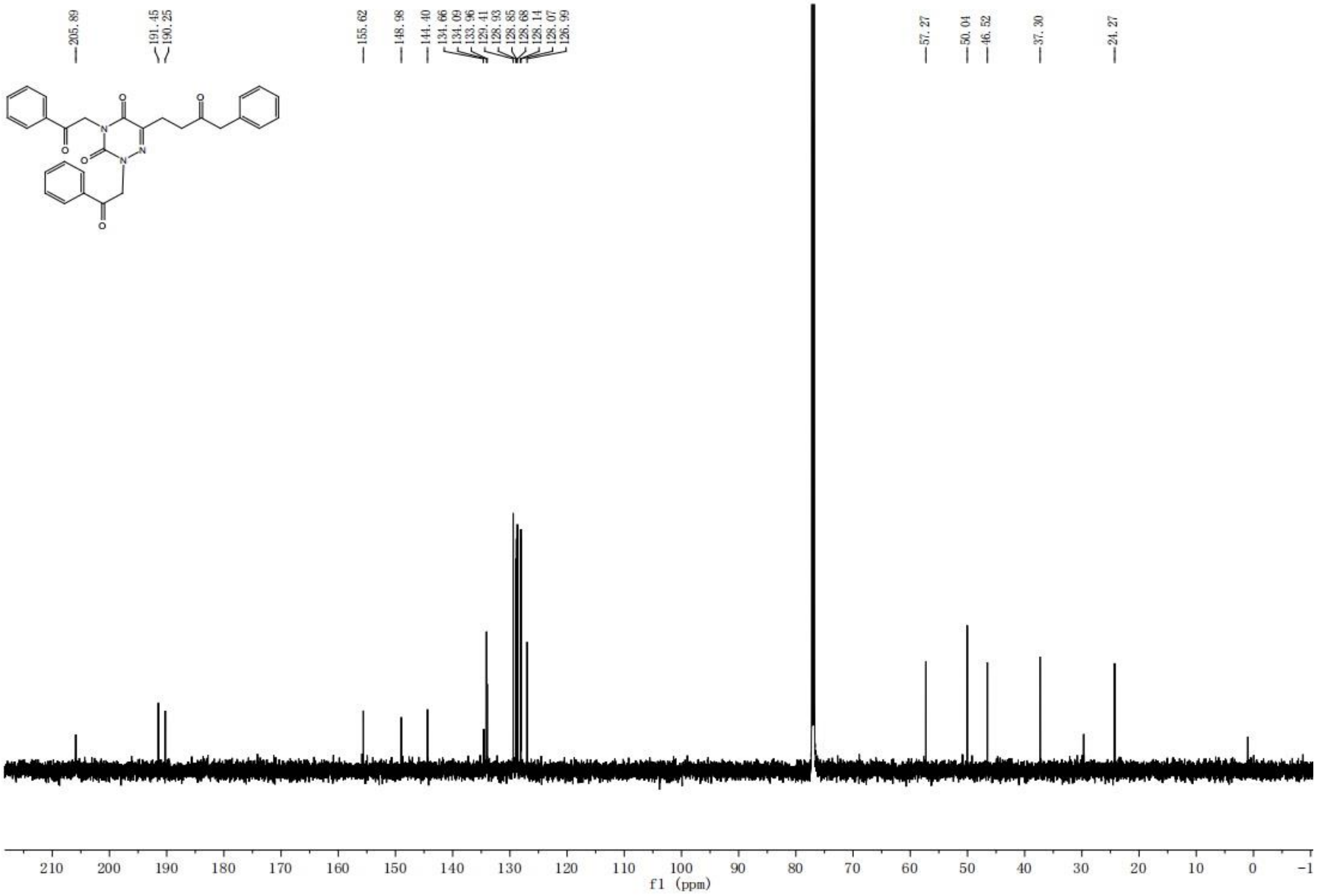
3d-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



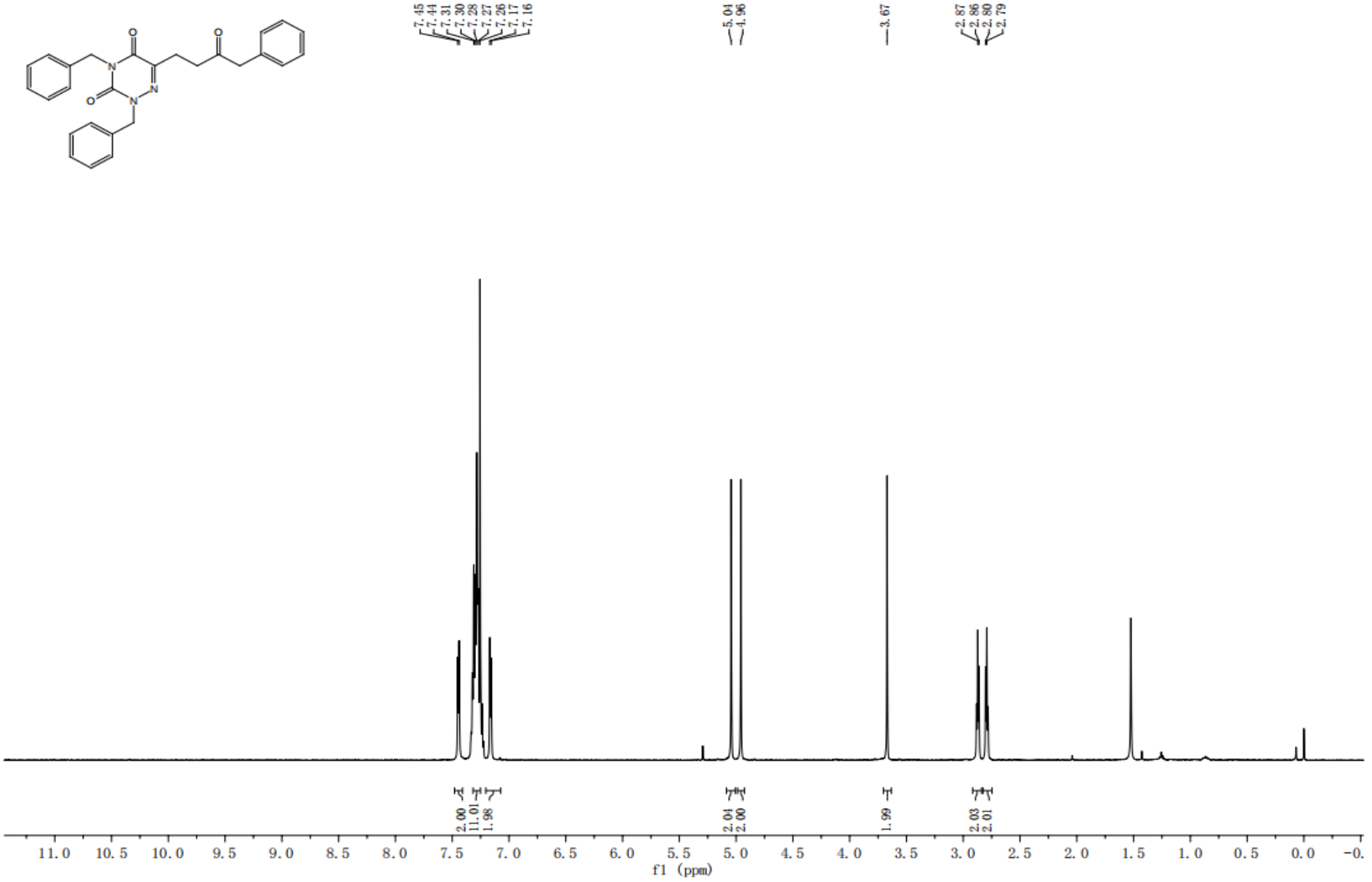
3e-^{1}H NMR (400 MHz, $CDCl_3$)



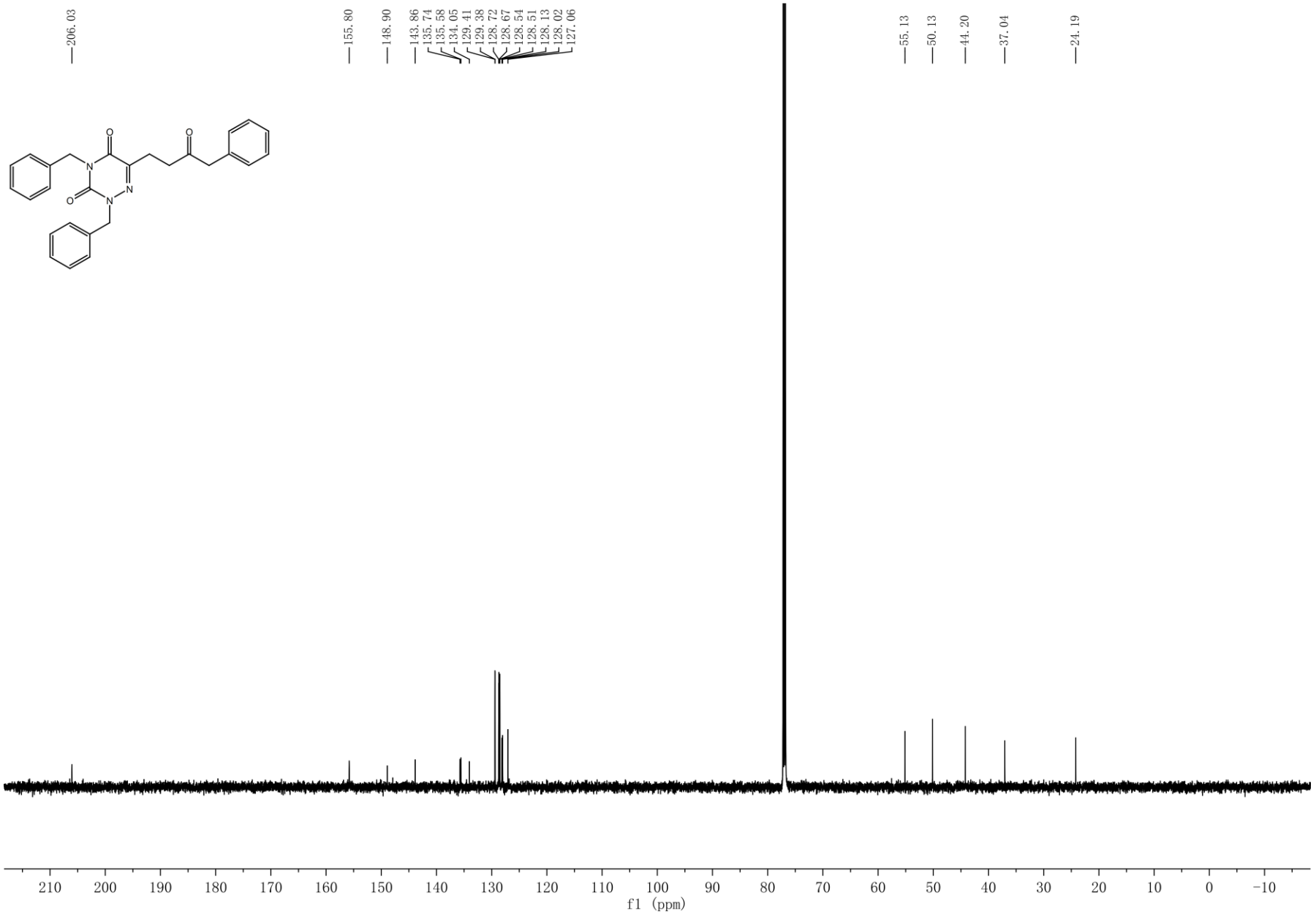
3e-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



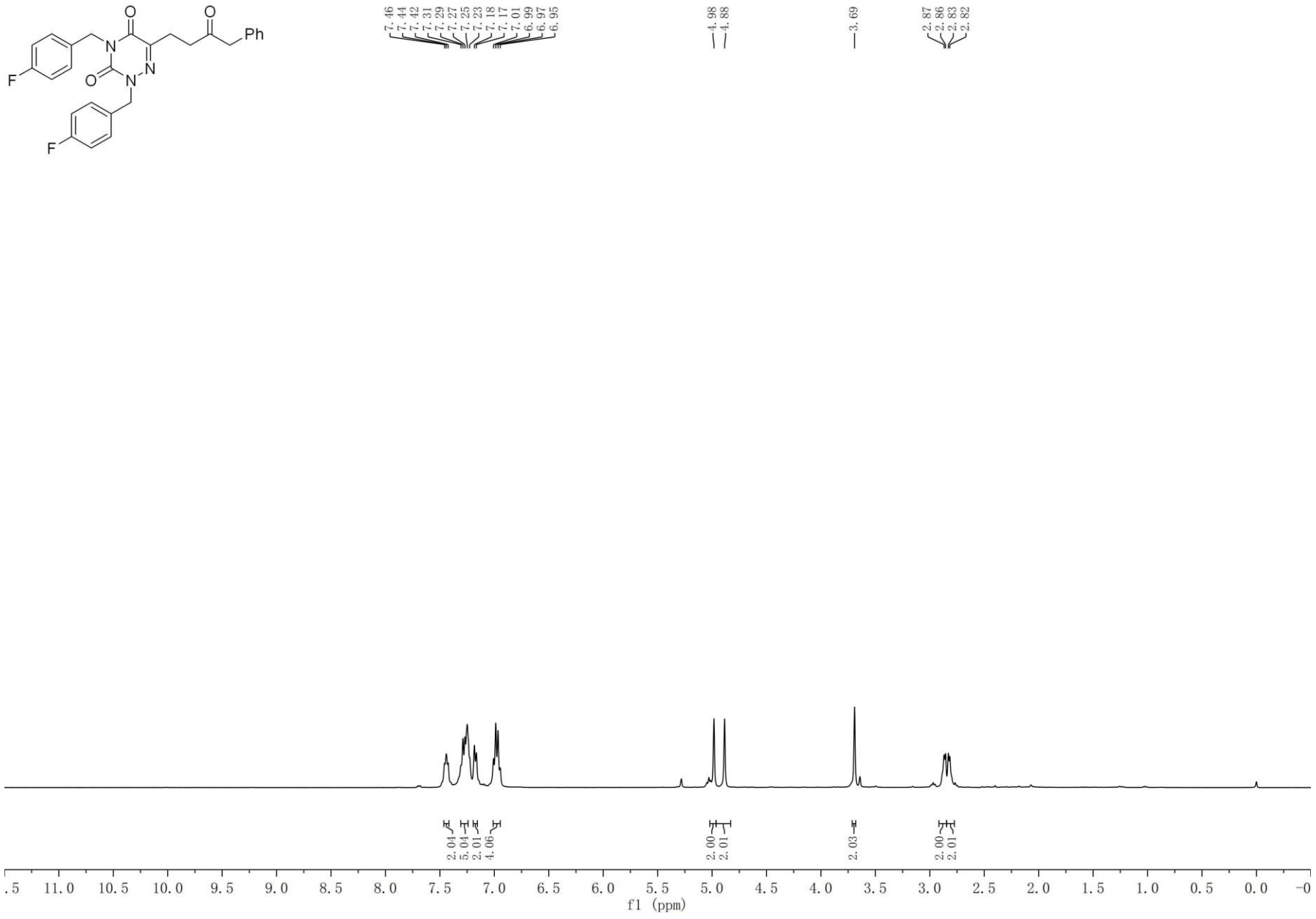
3f-^{1}H NMR (400 MHz, $CDCl_3$)



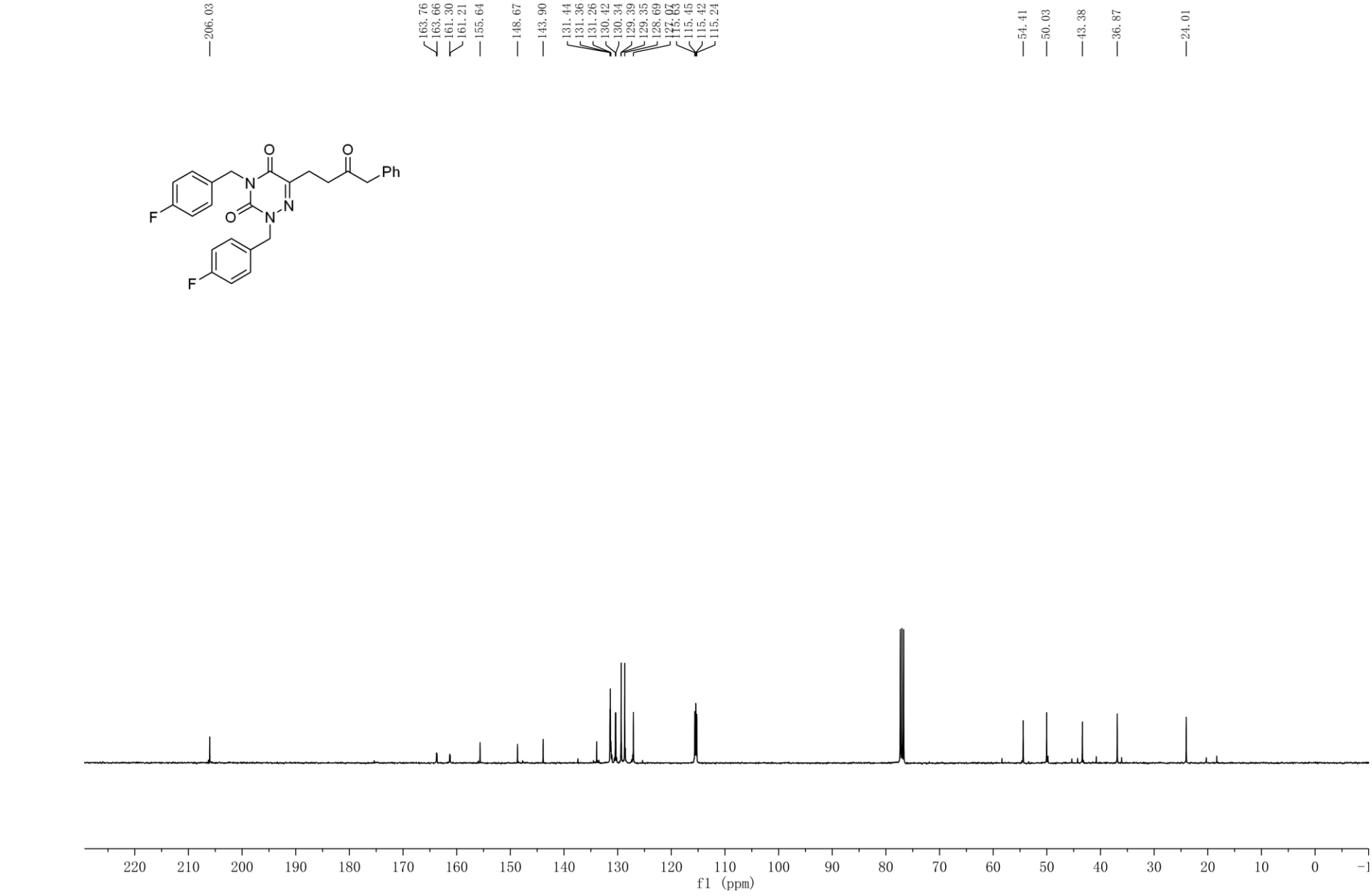
3f-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



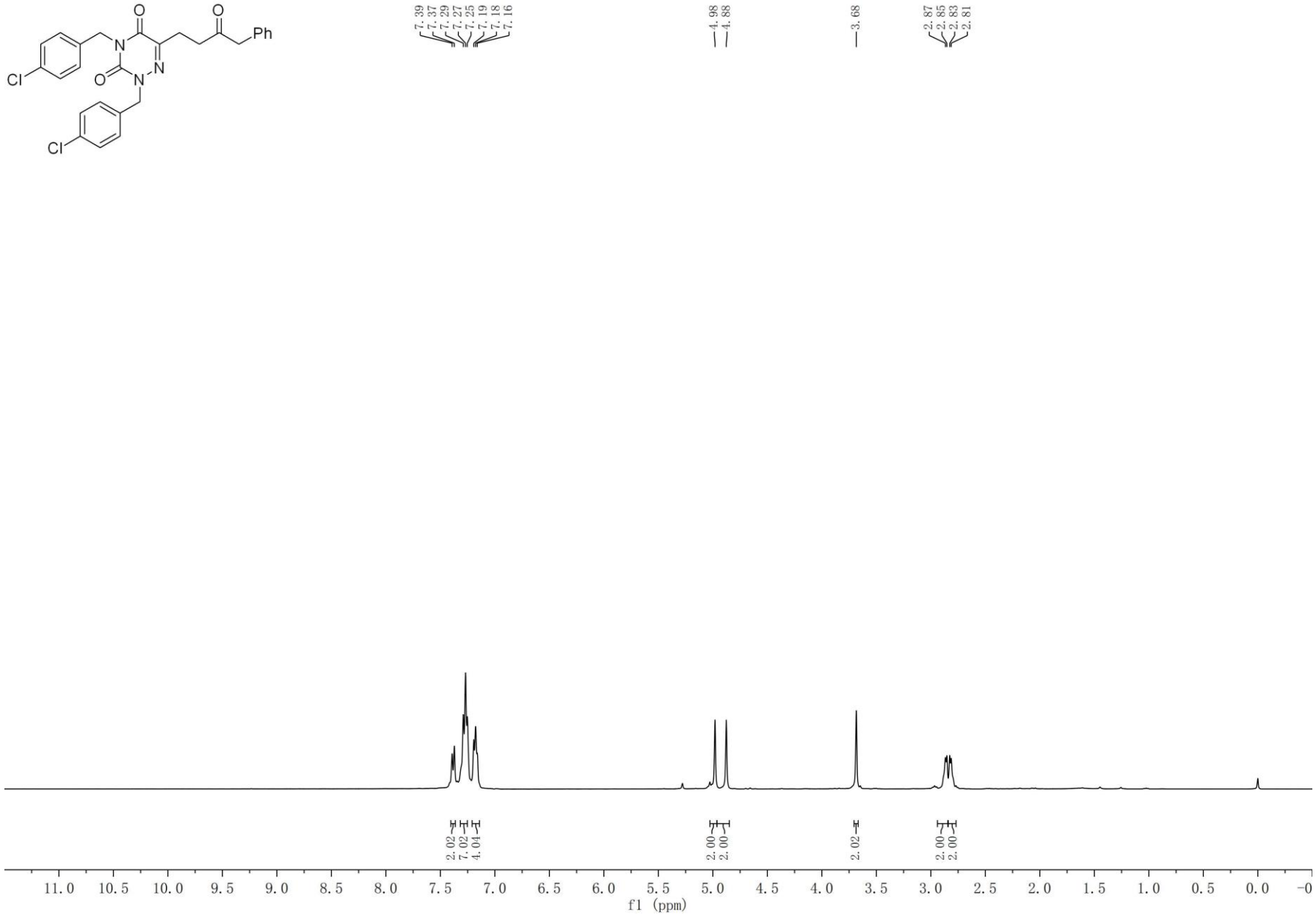
3g-^{1}H NMR (400 MHz, $CDCl_3$)



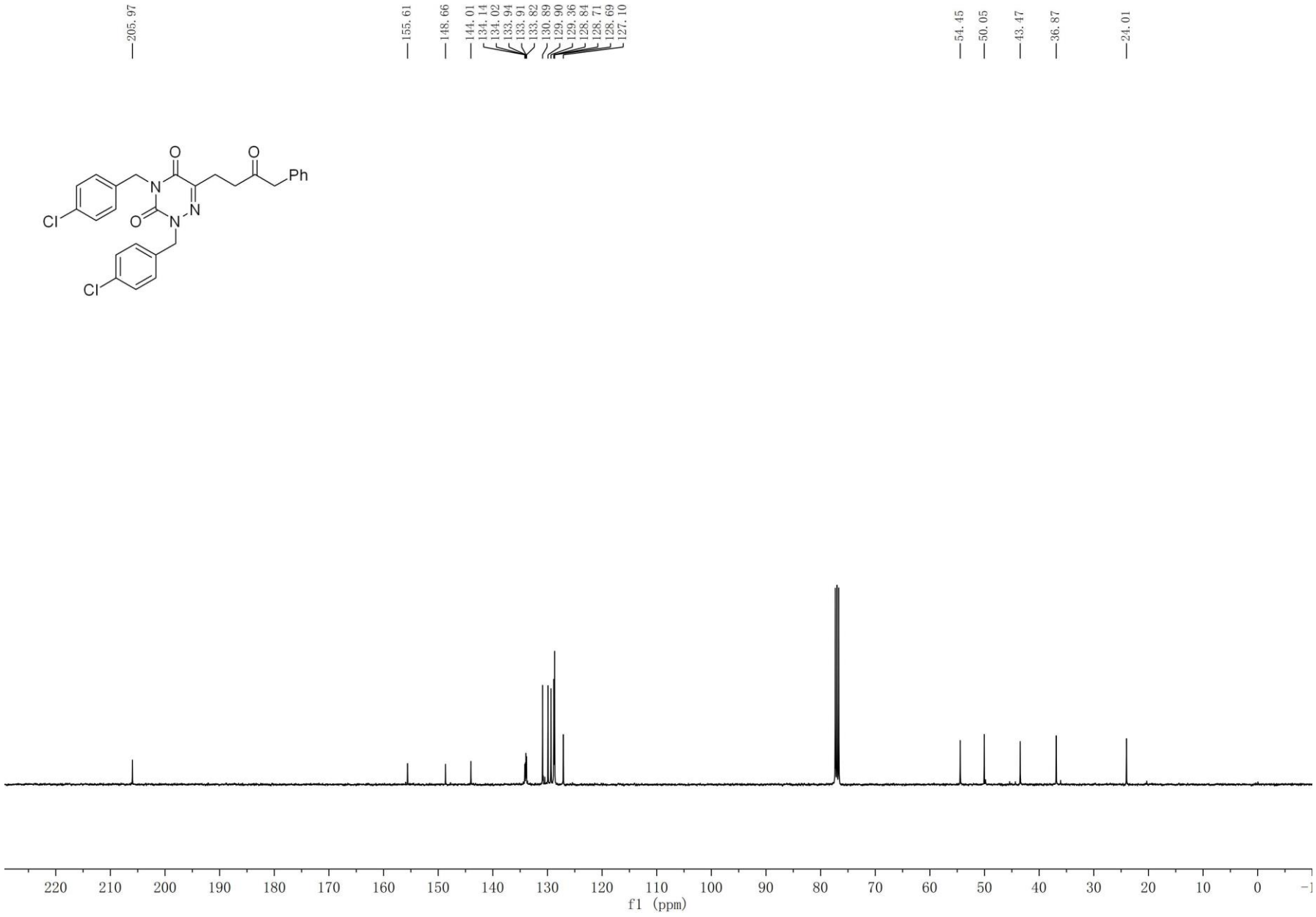
3g-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



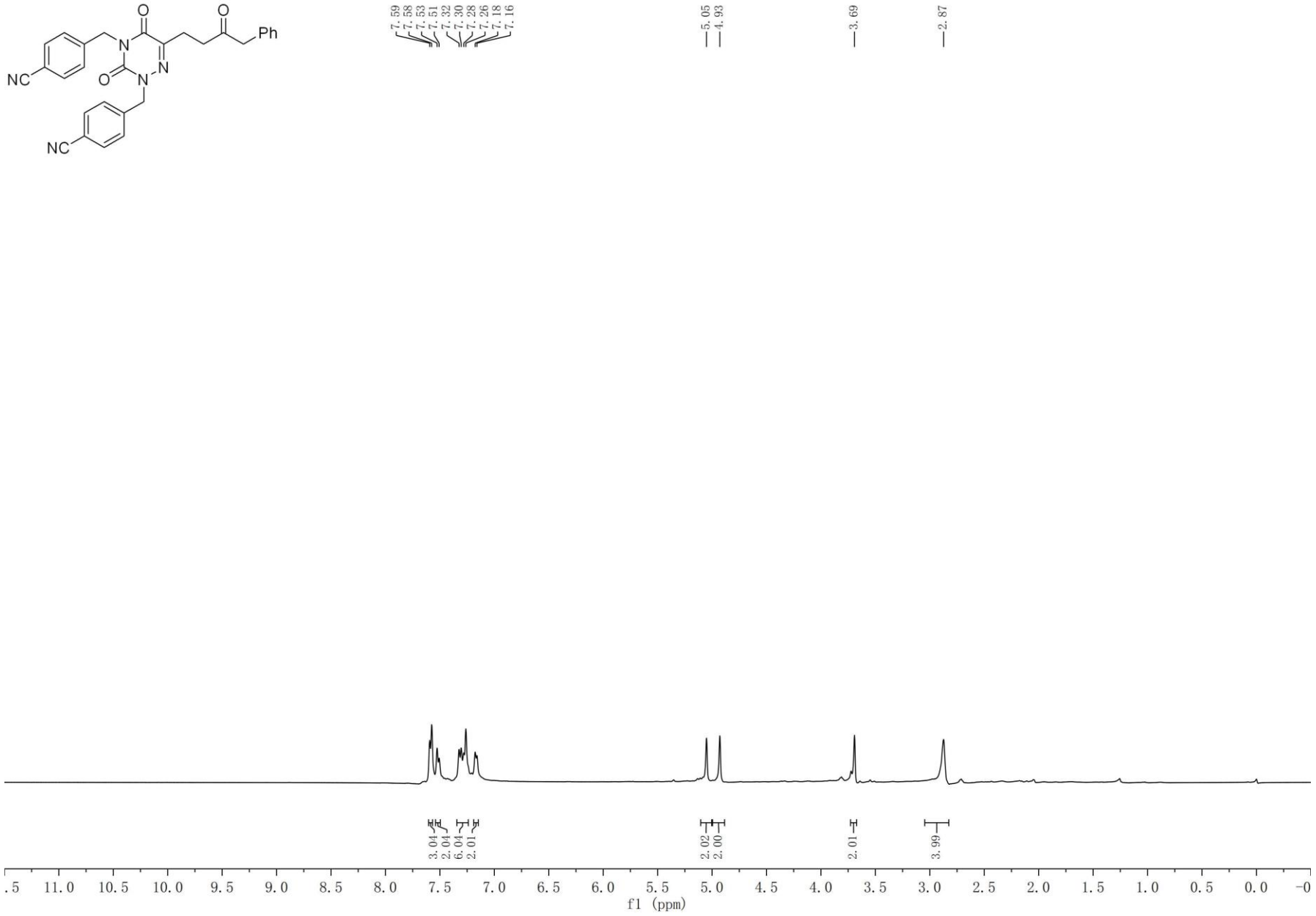
3h-^{1}H NMR (400 MHz, $CDCl_3$)



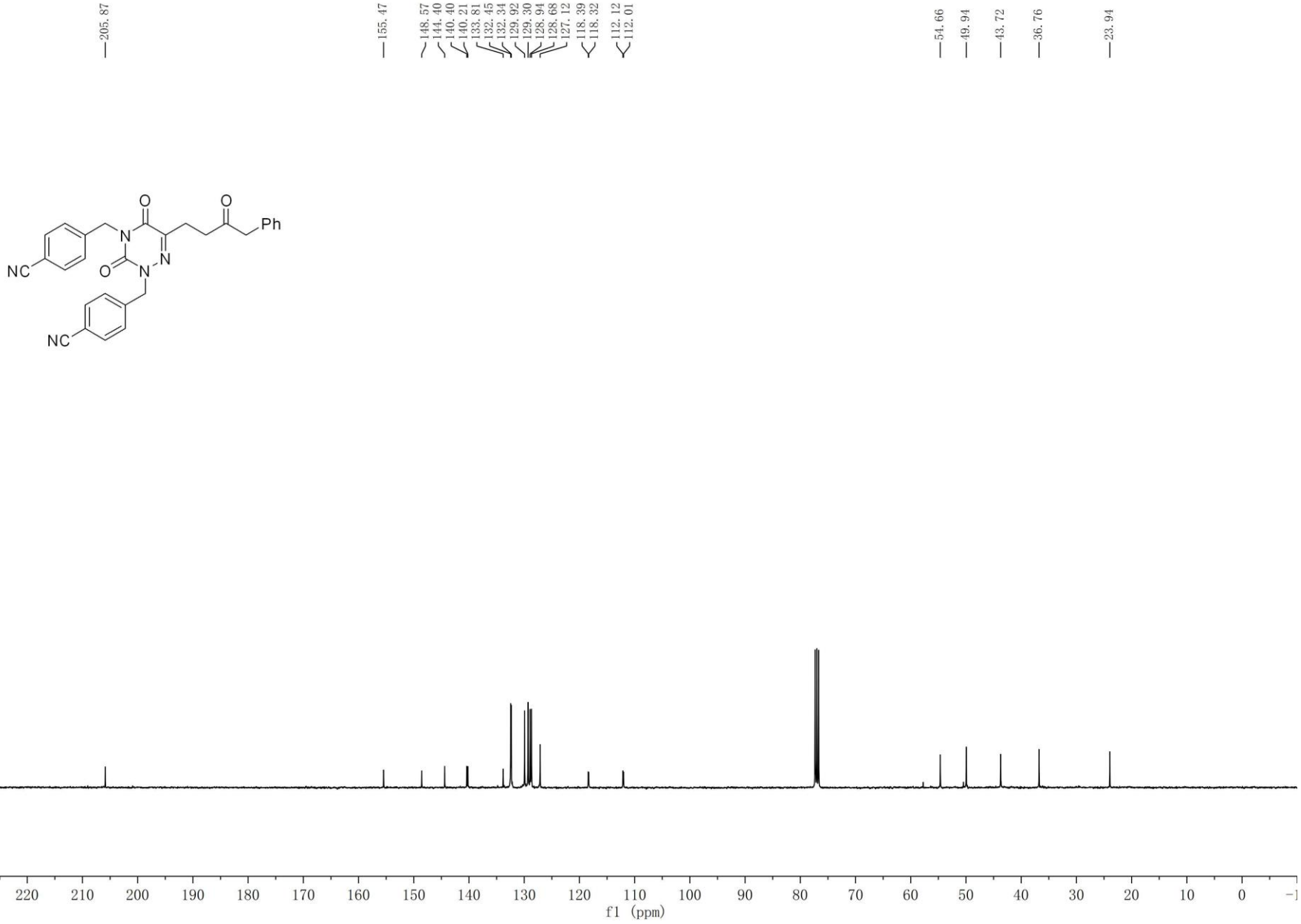
3h-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



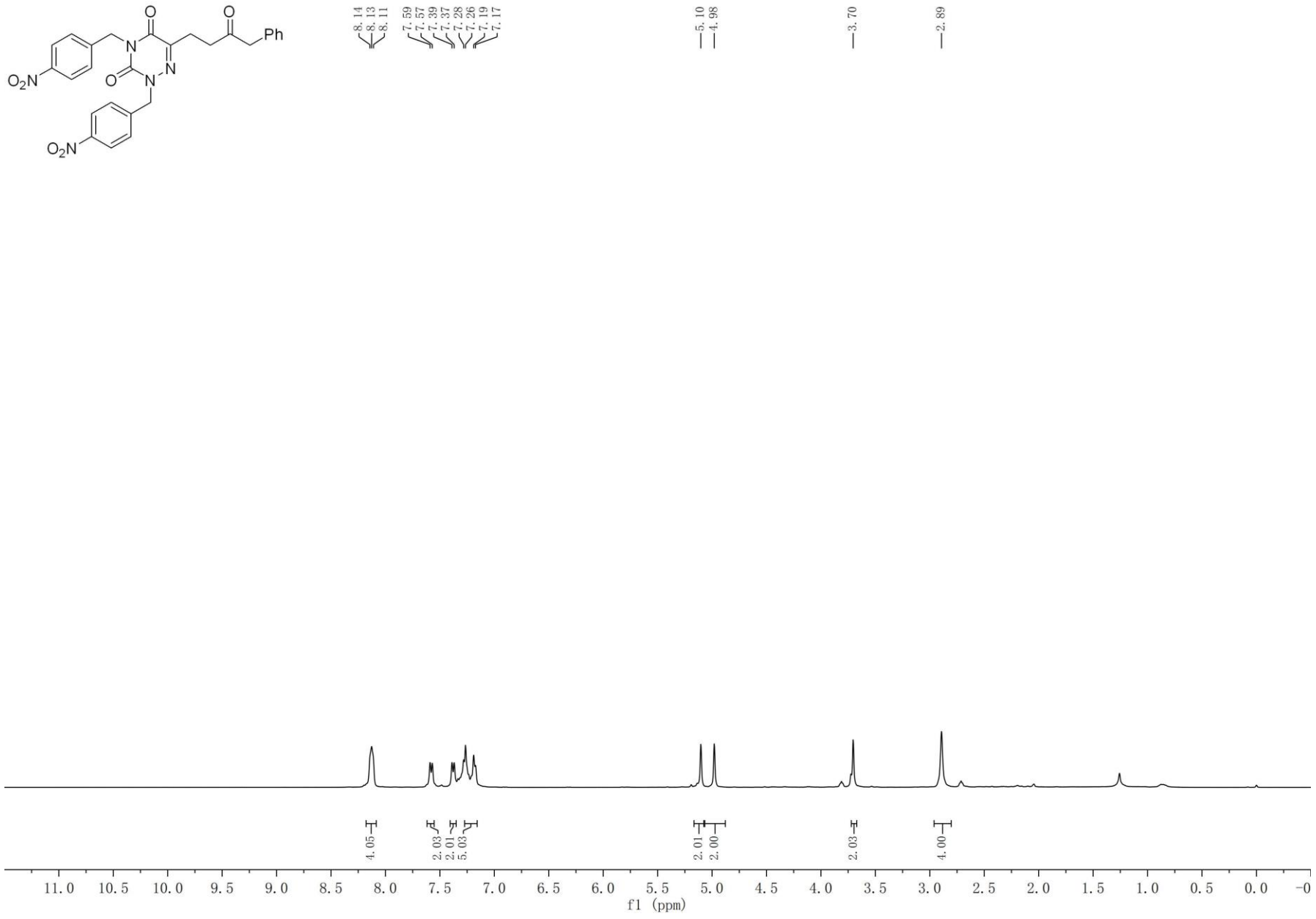
3i-^{1}H NMR (400 MHz, $CDCl_3$)



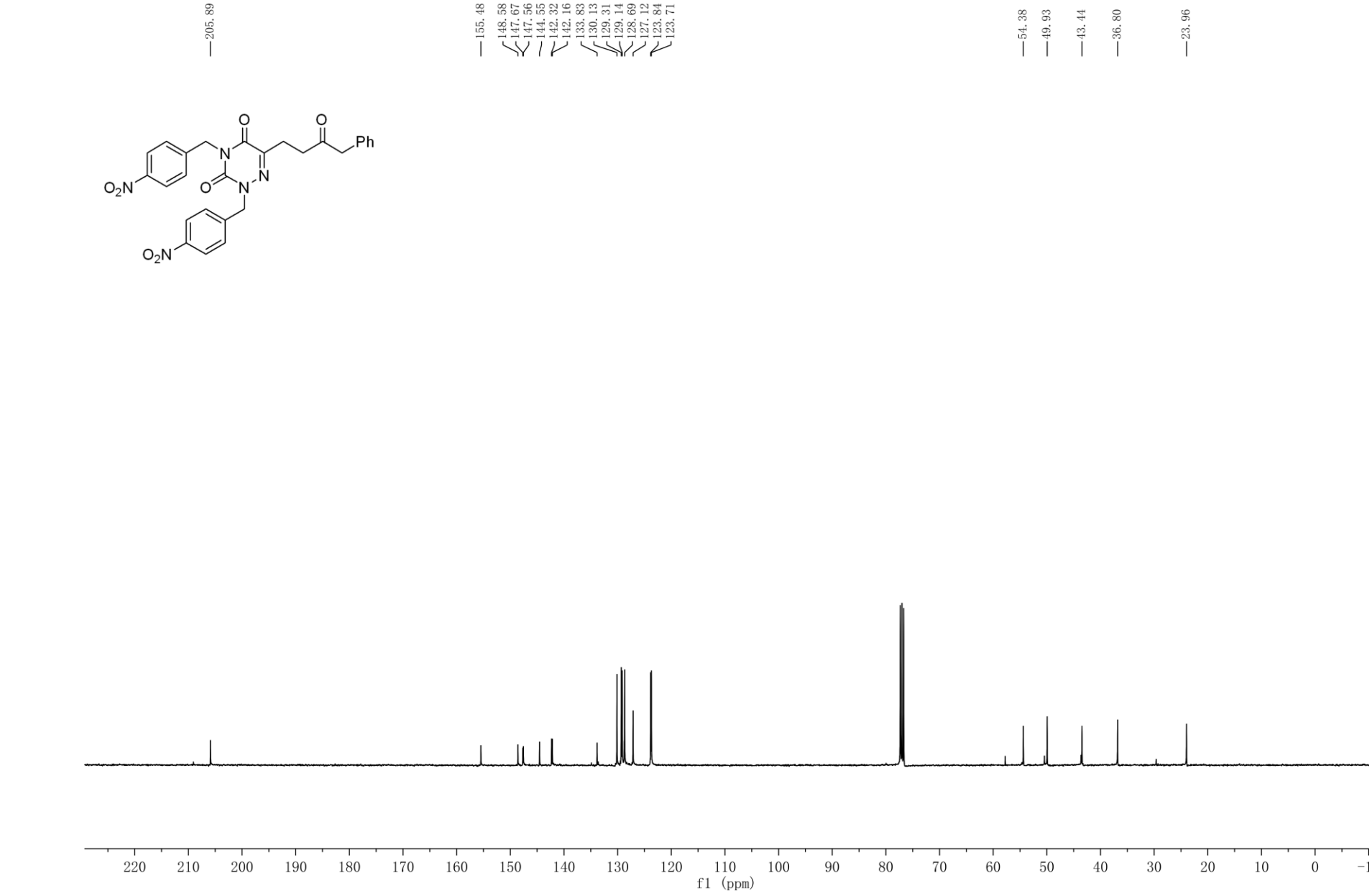
3i-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



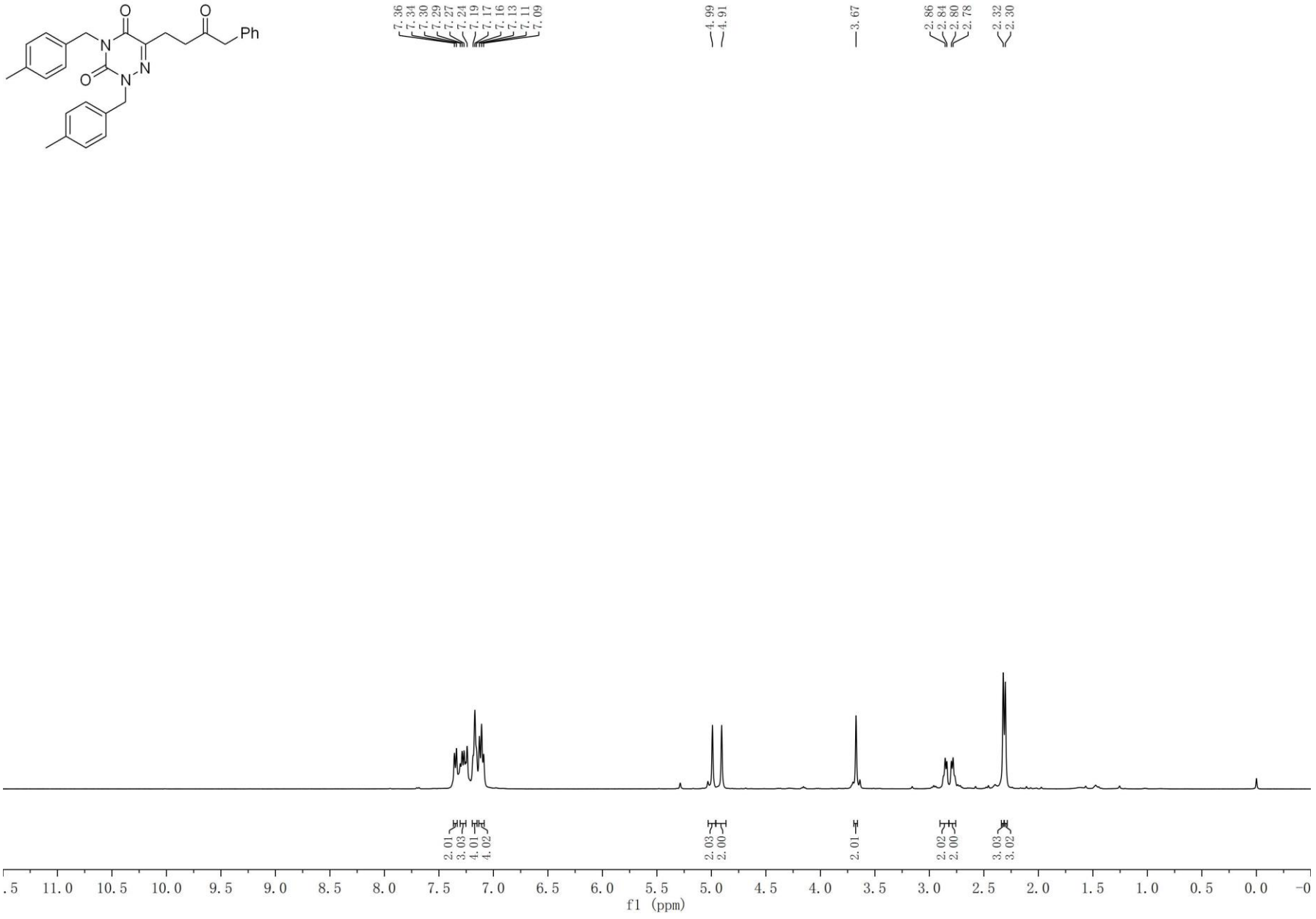
3j-^{1}H NMR (400 MHz, $CDCl_3$)



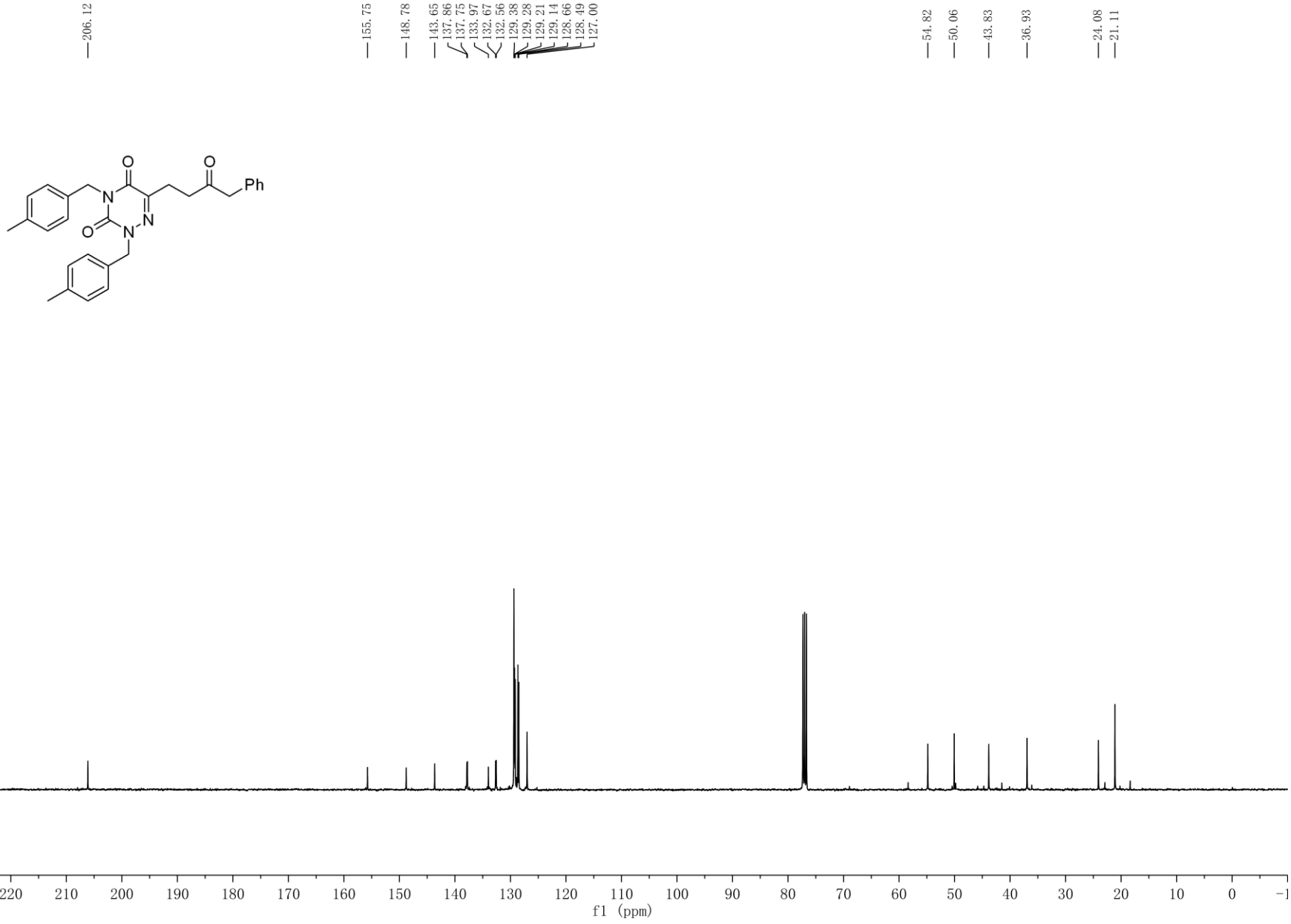
3j-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



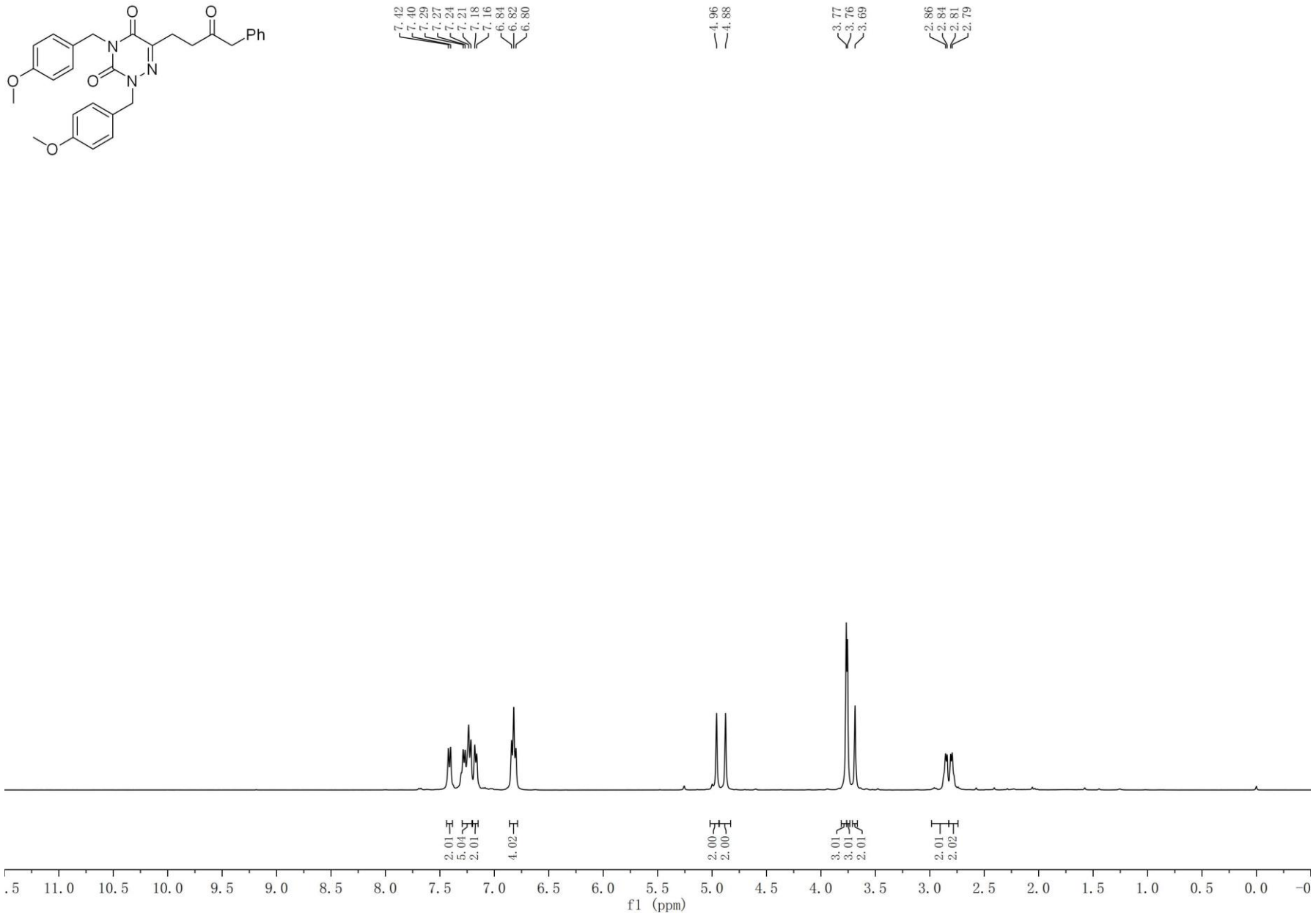
3k-^{1}H NMR (400 MHz, $CDCl_3$)



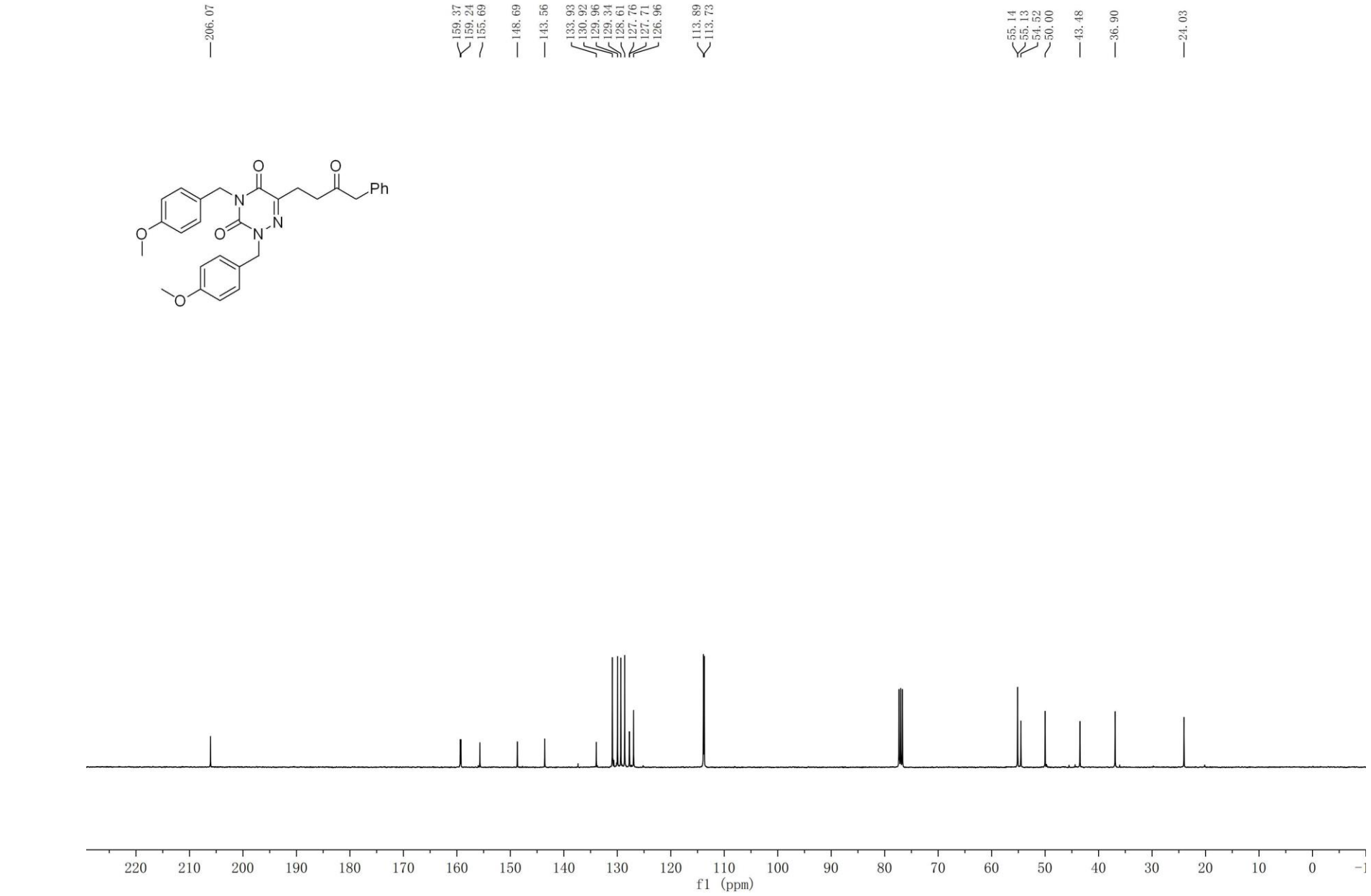
3k-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



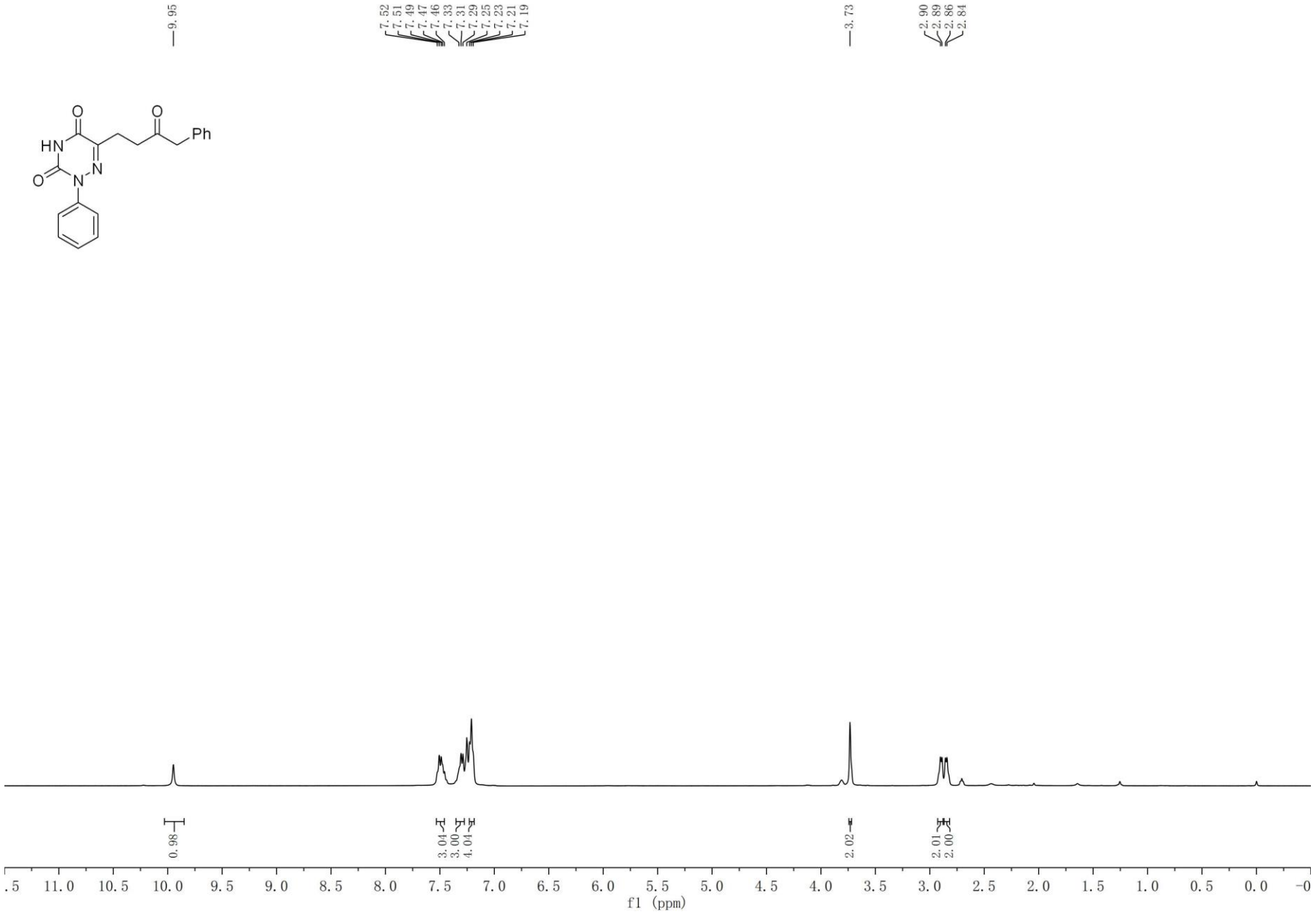
3l-^{1}H NMR (400 MHz, $CDCl_3$)



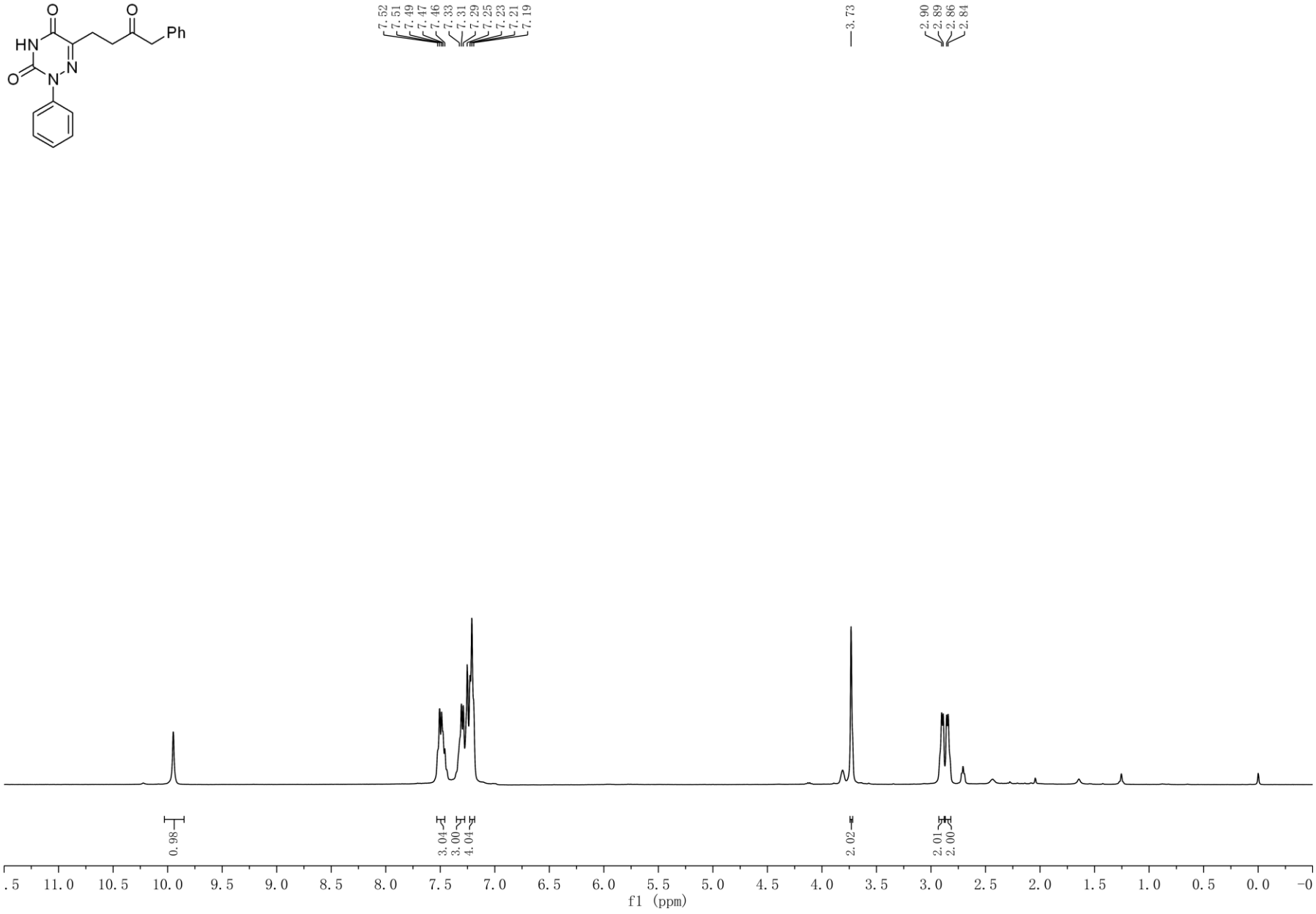
3l-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



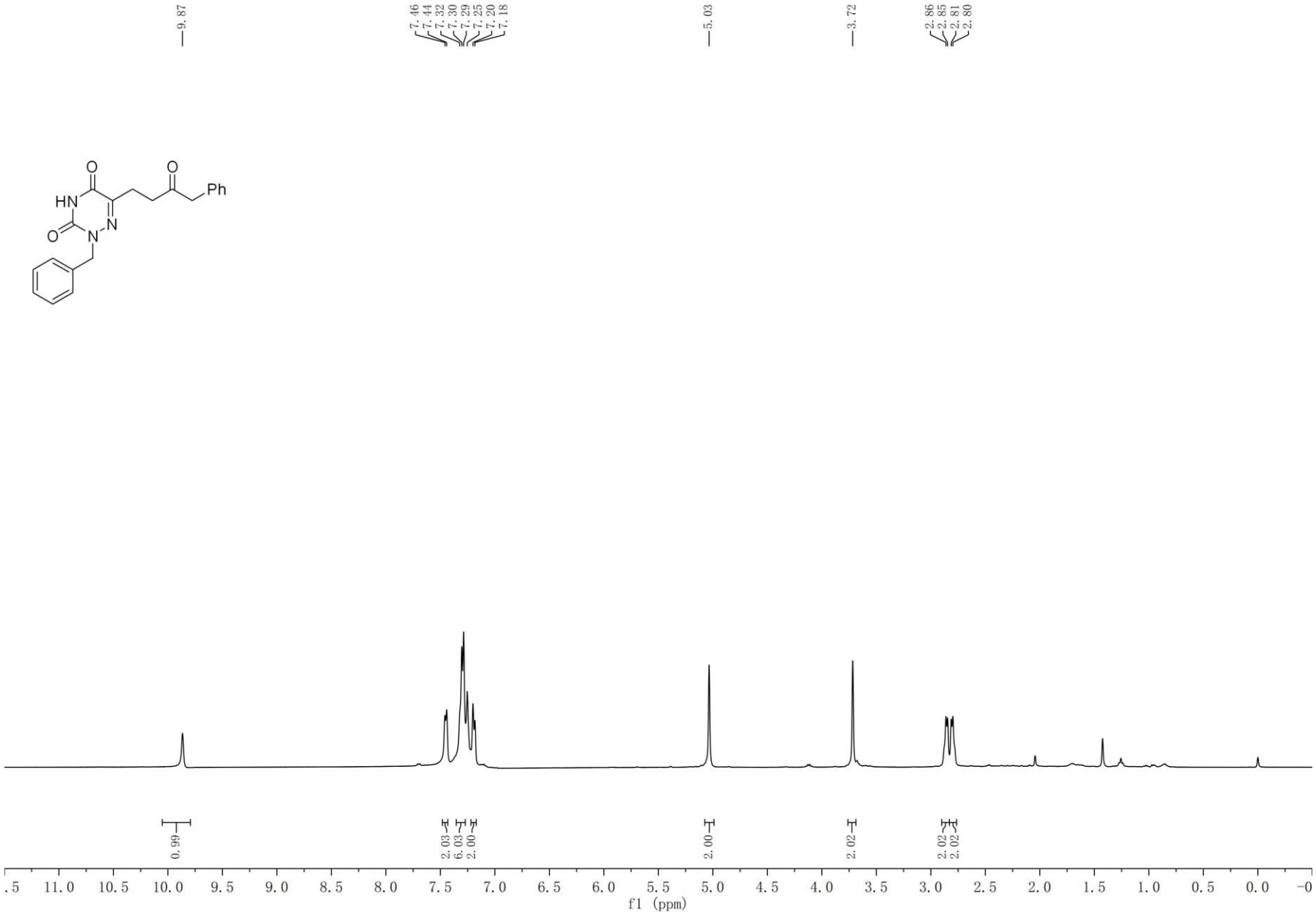
3m-^{1}H NMR (400 MHz, $CDCl_3$)



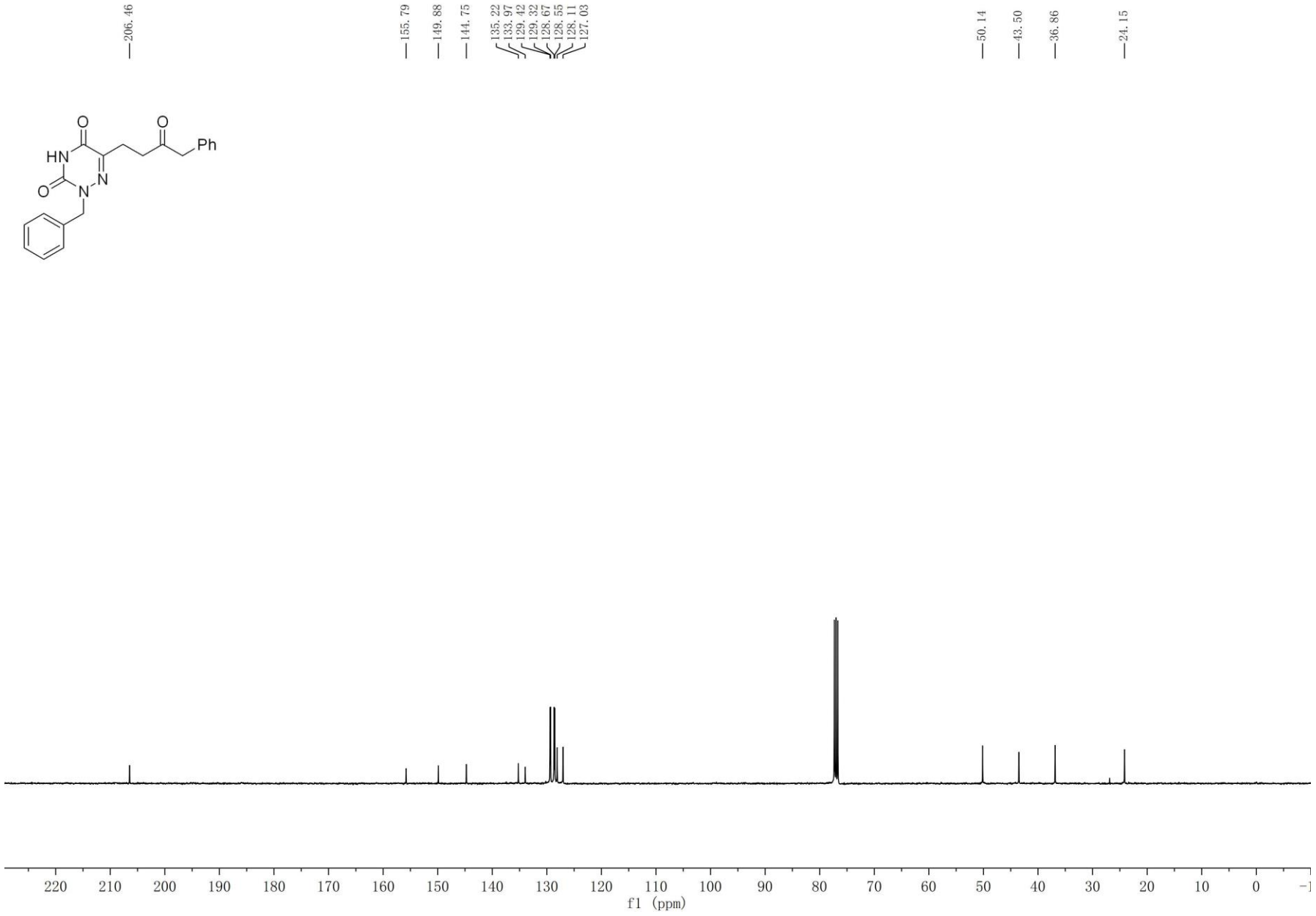
3m-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



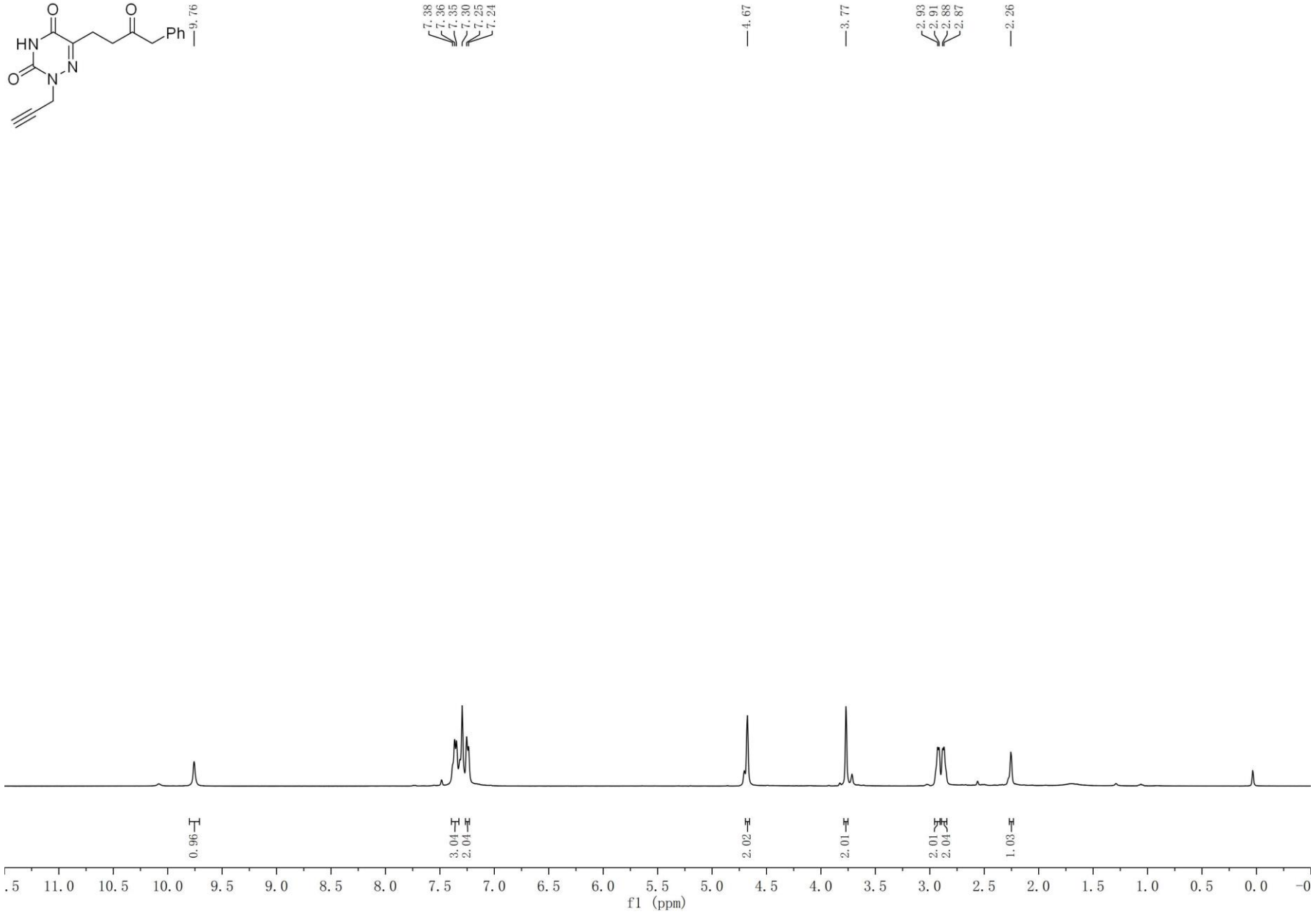
3n-^{1}H NMR (400 MHz, $CDCl_3$)



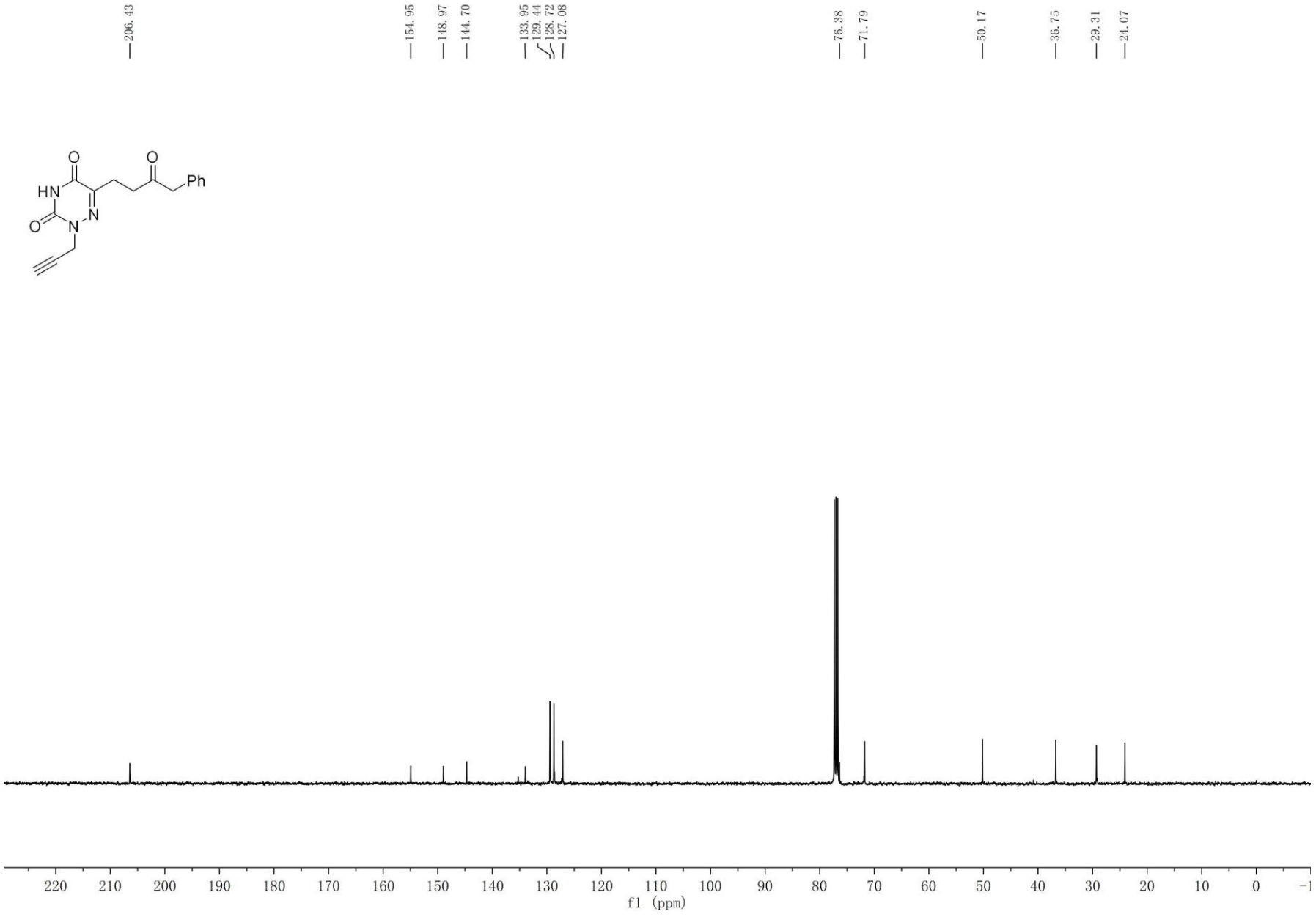
3n-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



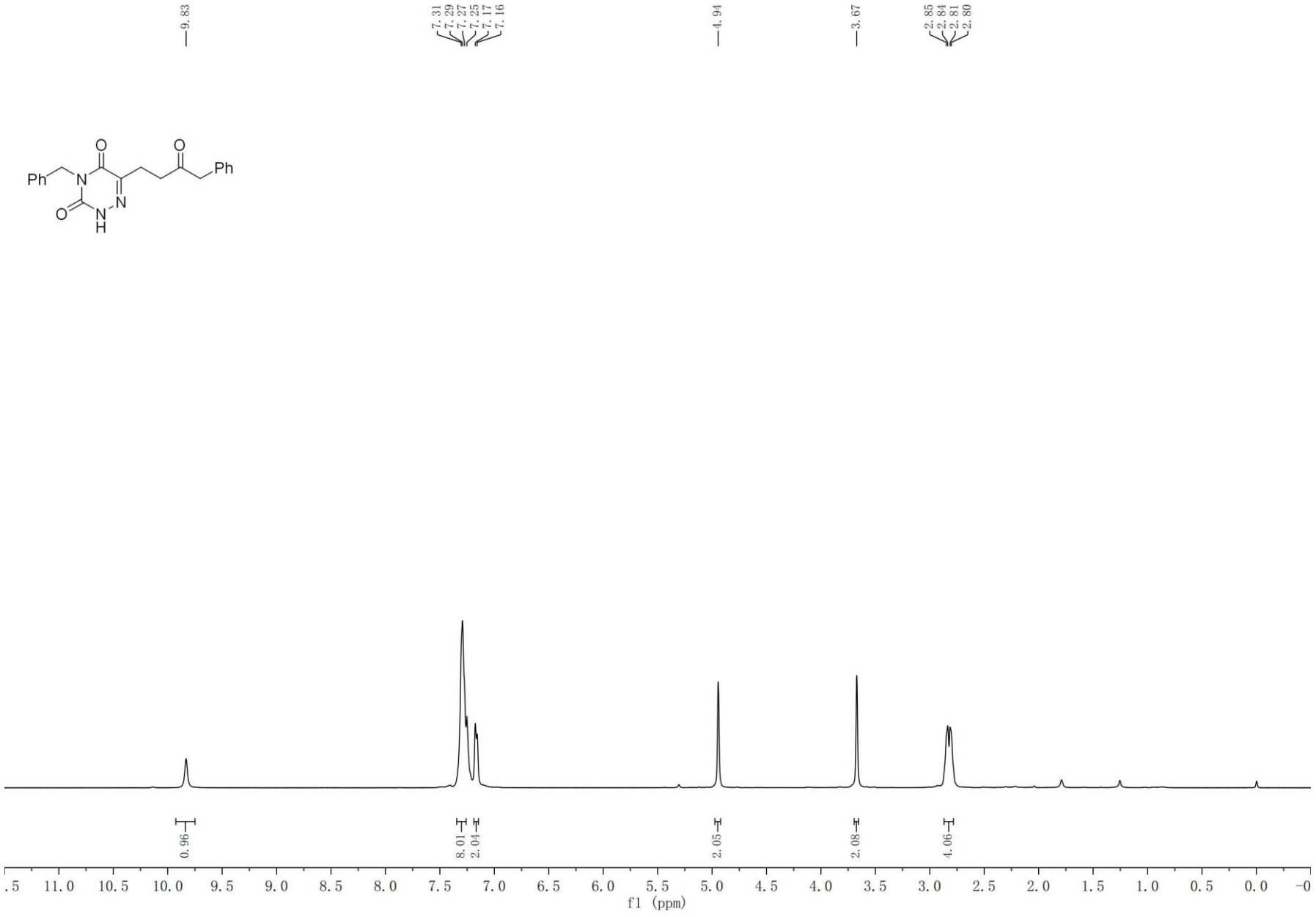
3o-^{1}H NMR (400 MHz, $CDCl_3$)



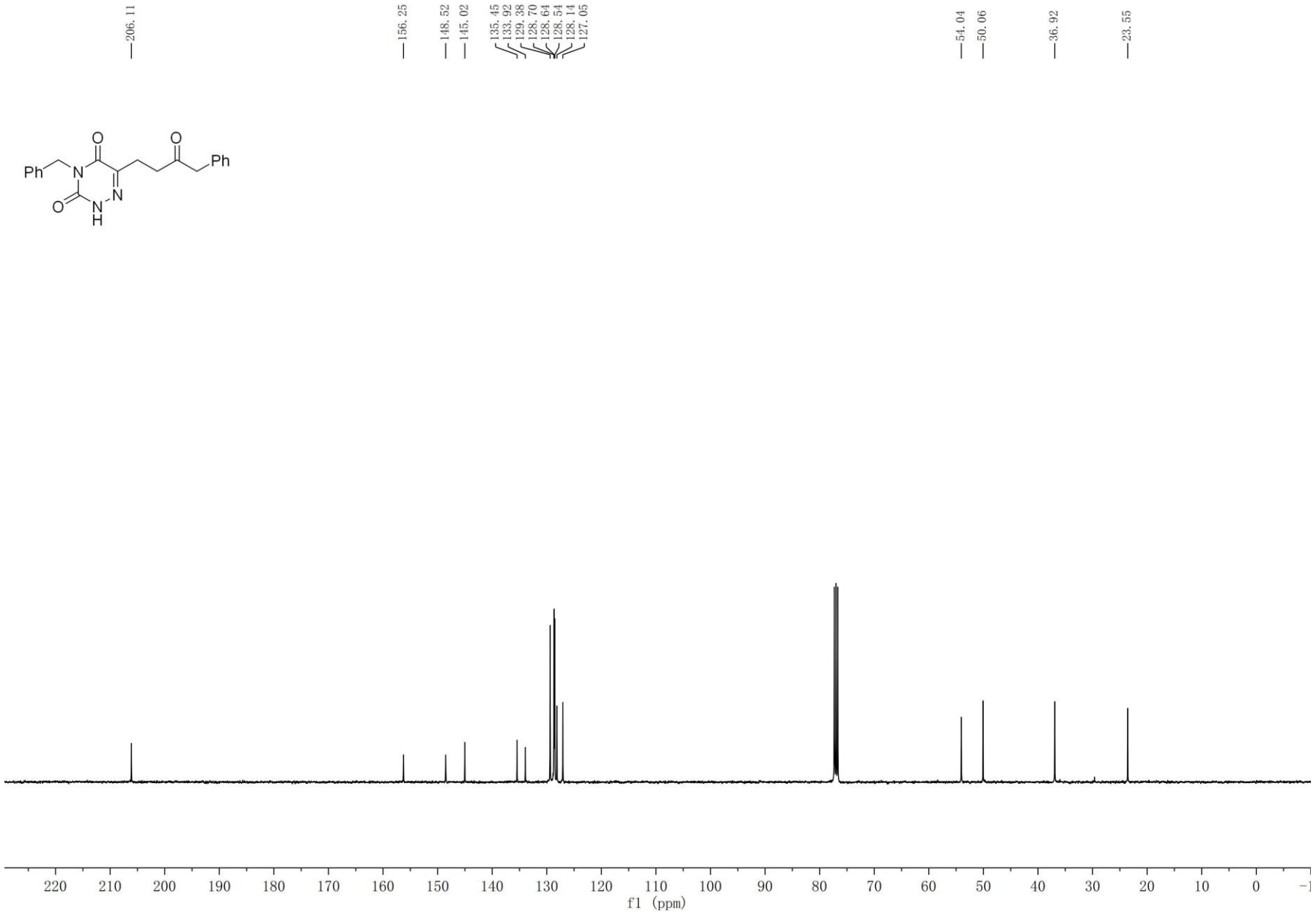
3o-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



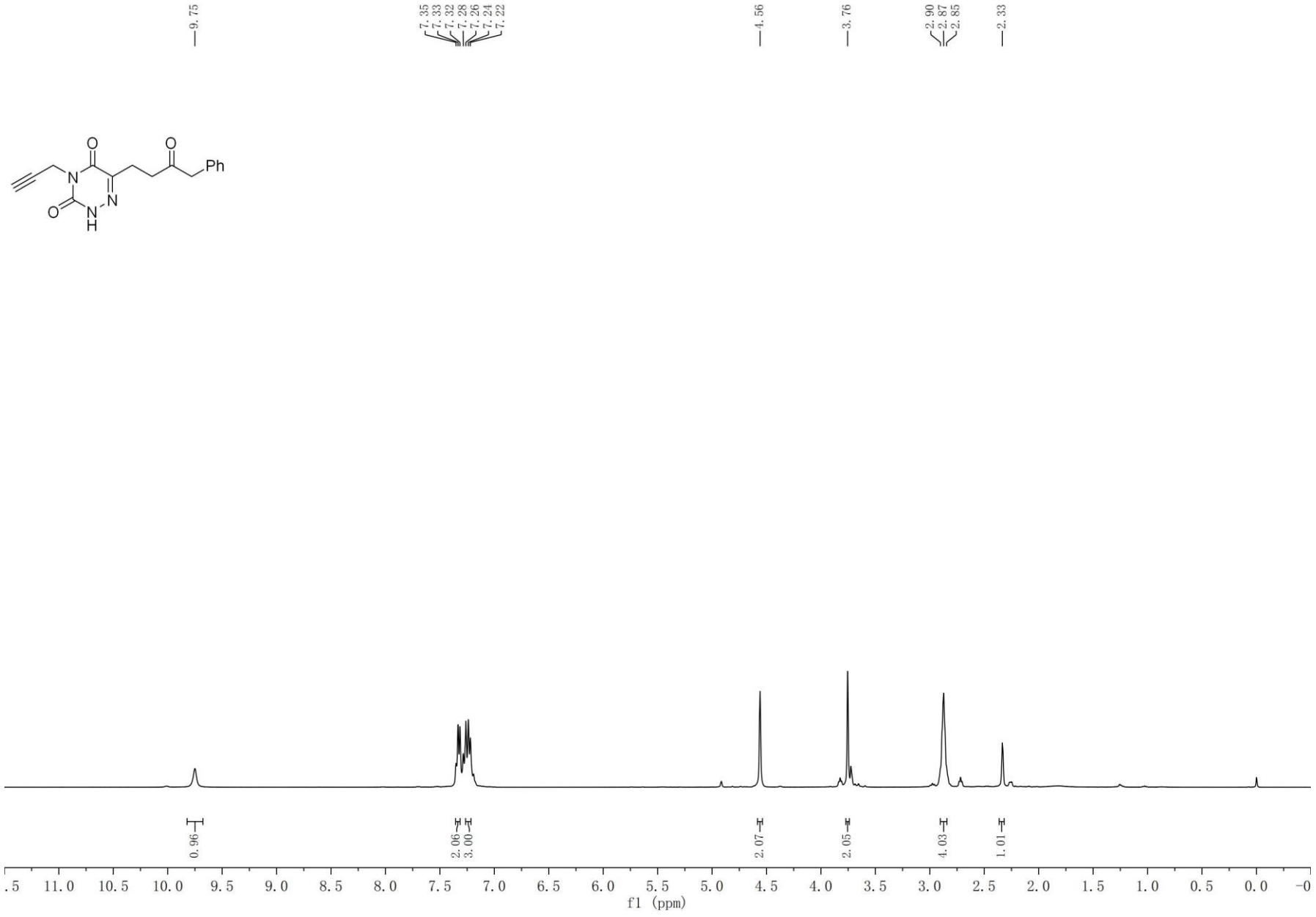
3p-^{1}H NMR (400 MHz, $CDCl_3$)



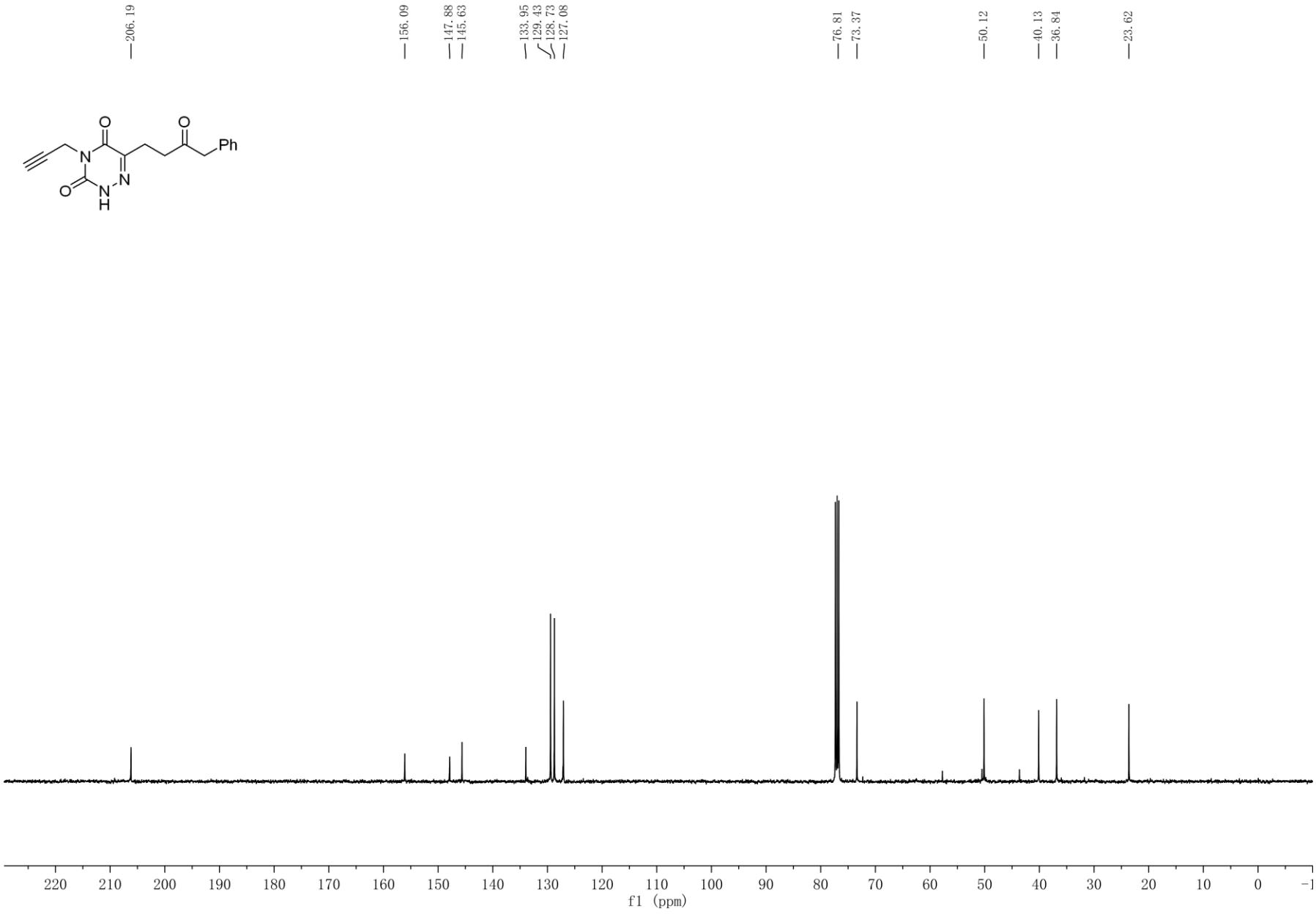
3p-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



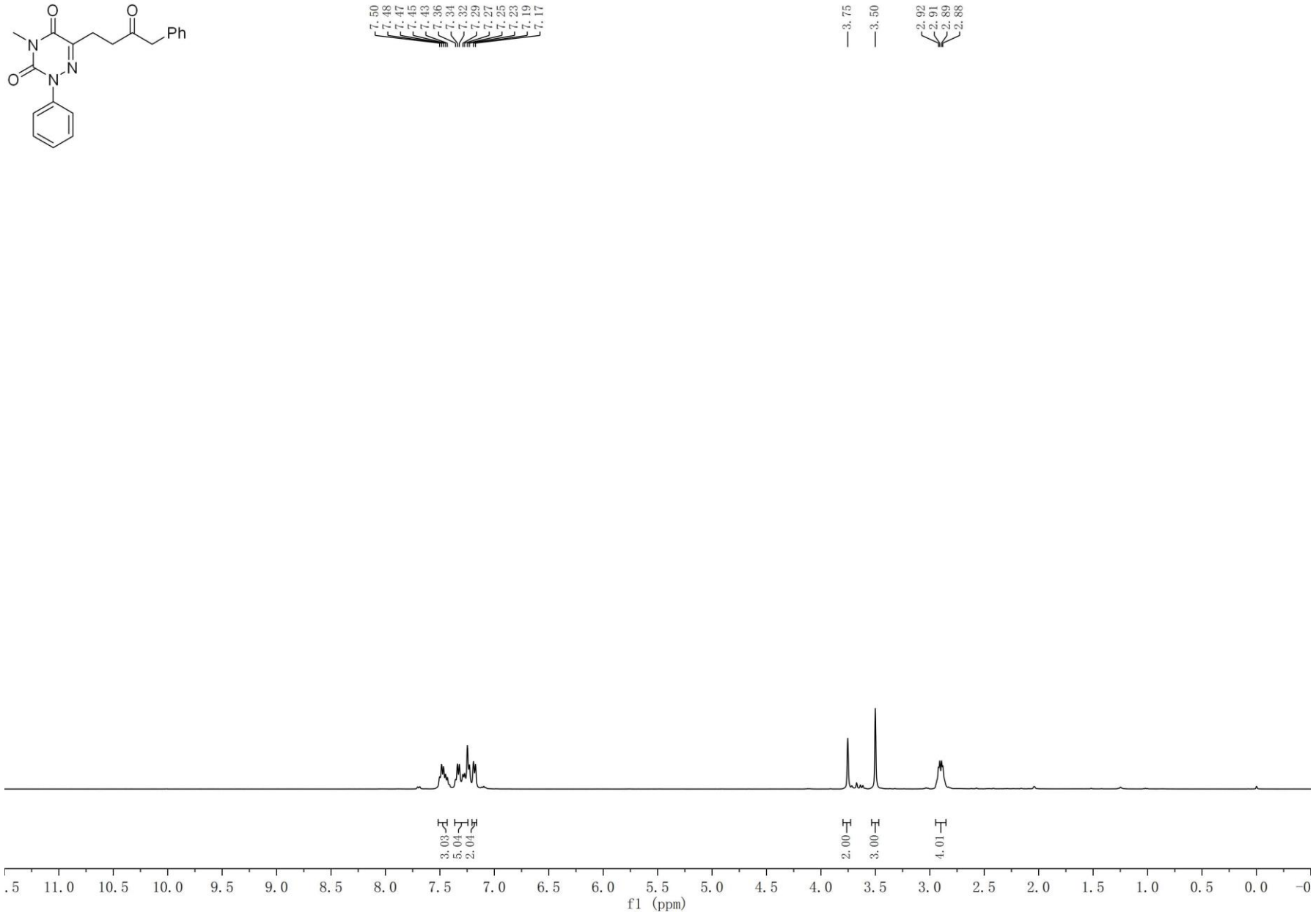
3q-^{1}H NMR (400 MHz, $CDCl_3$)



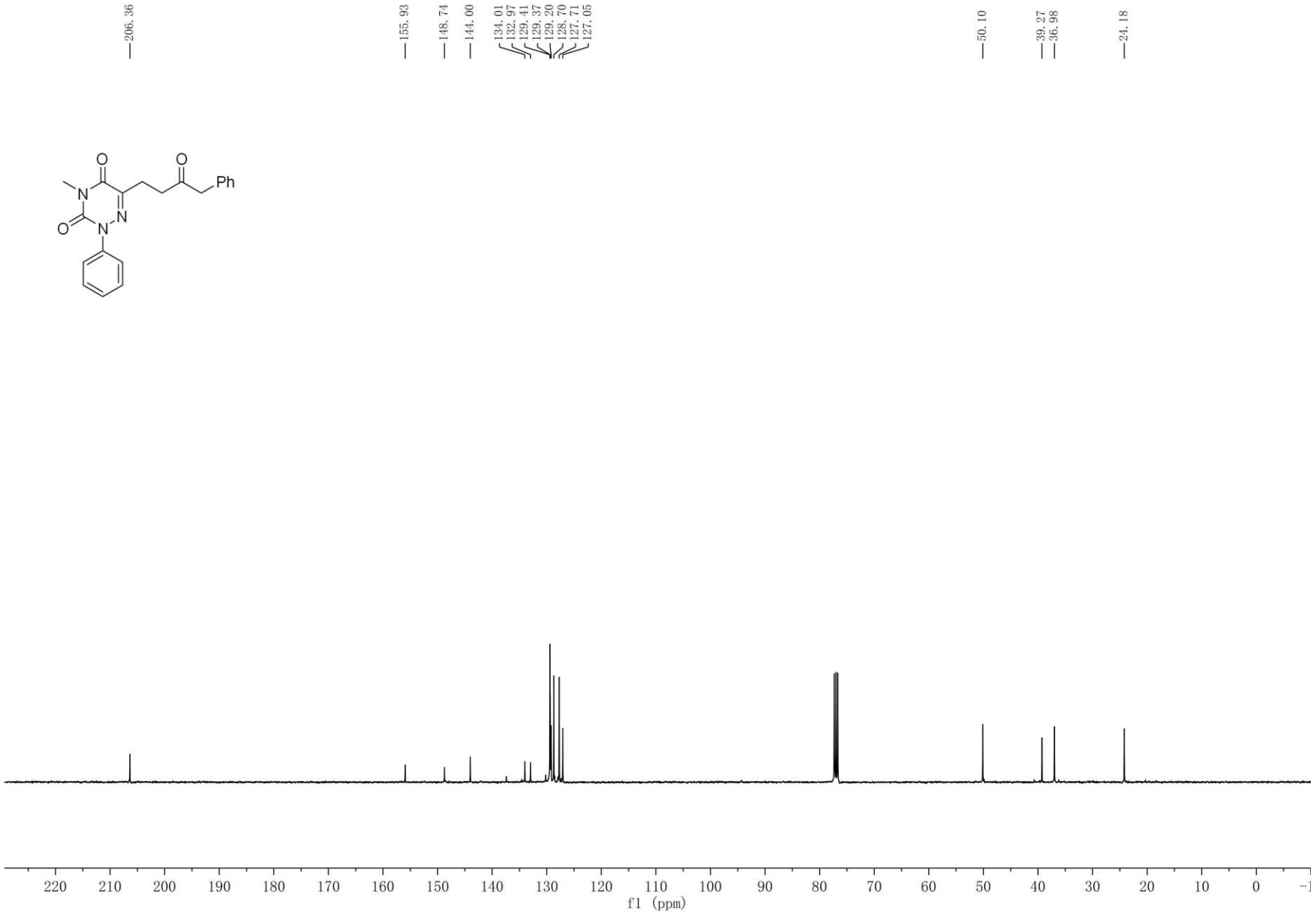
3q-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



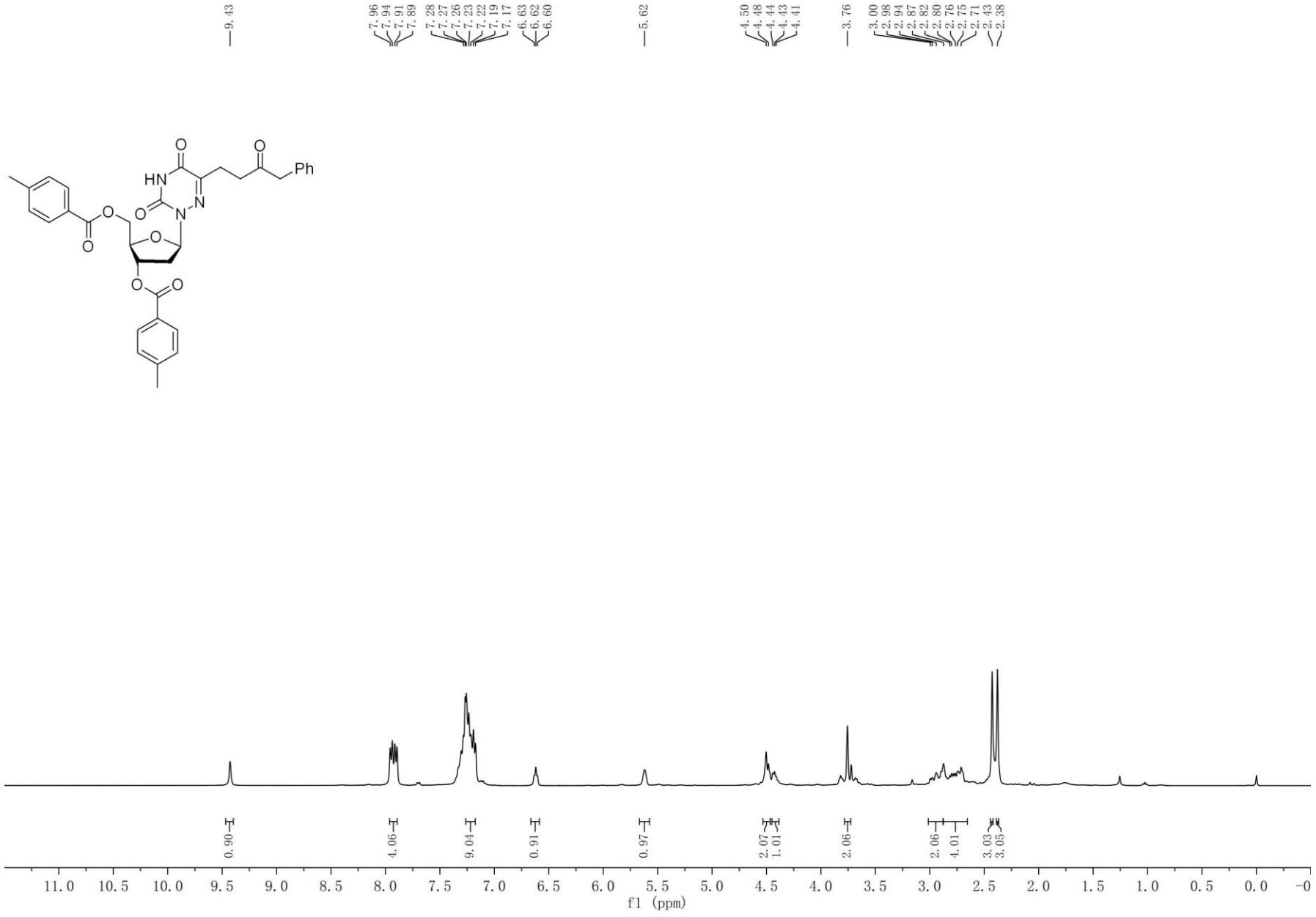
3r-^{1}H NMR (400 MHz, $CDCl_3$)



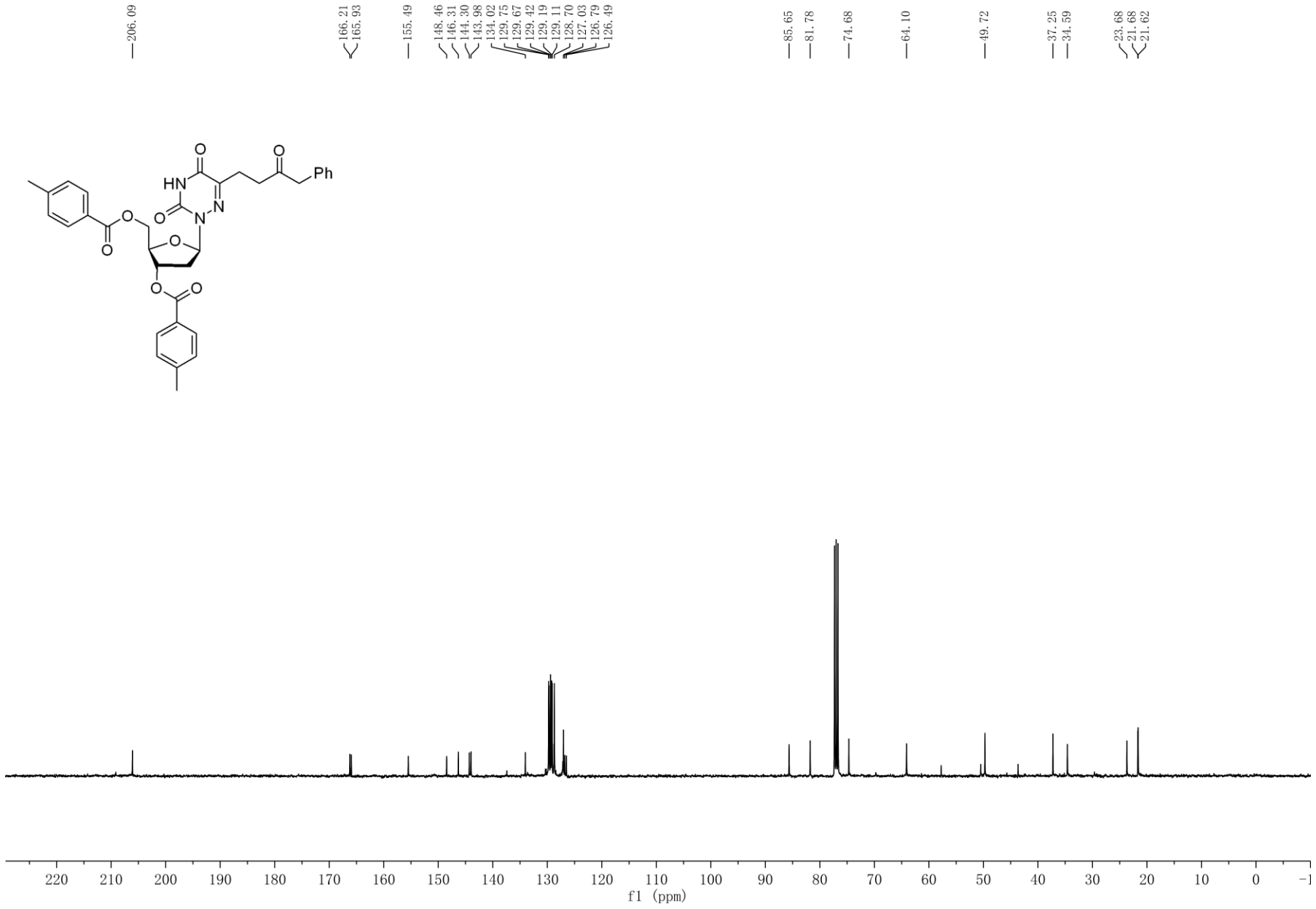
3r-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



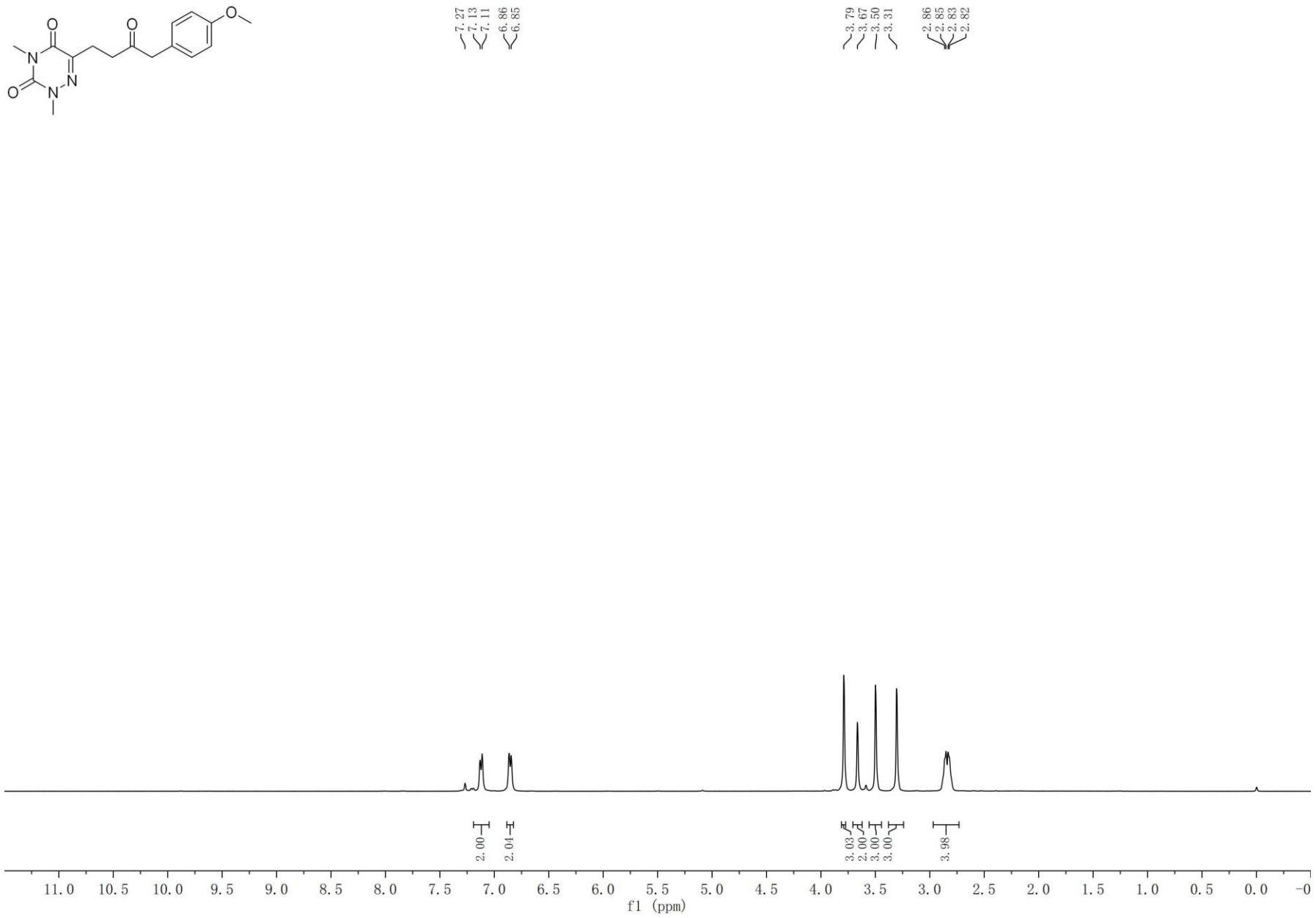
3s-^{1}H NMR (400 MHz, $CDCl_3$)



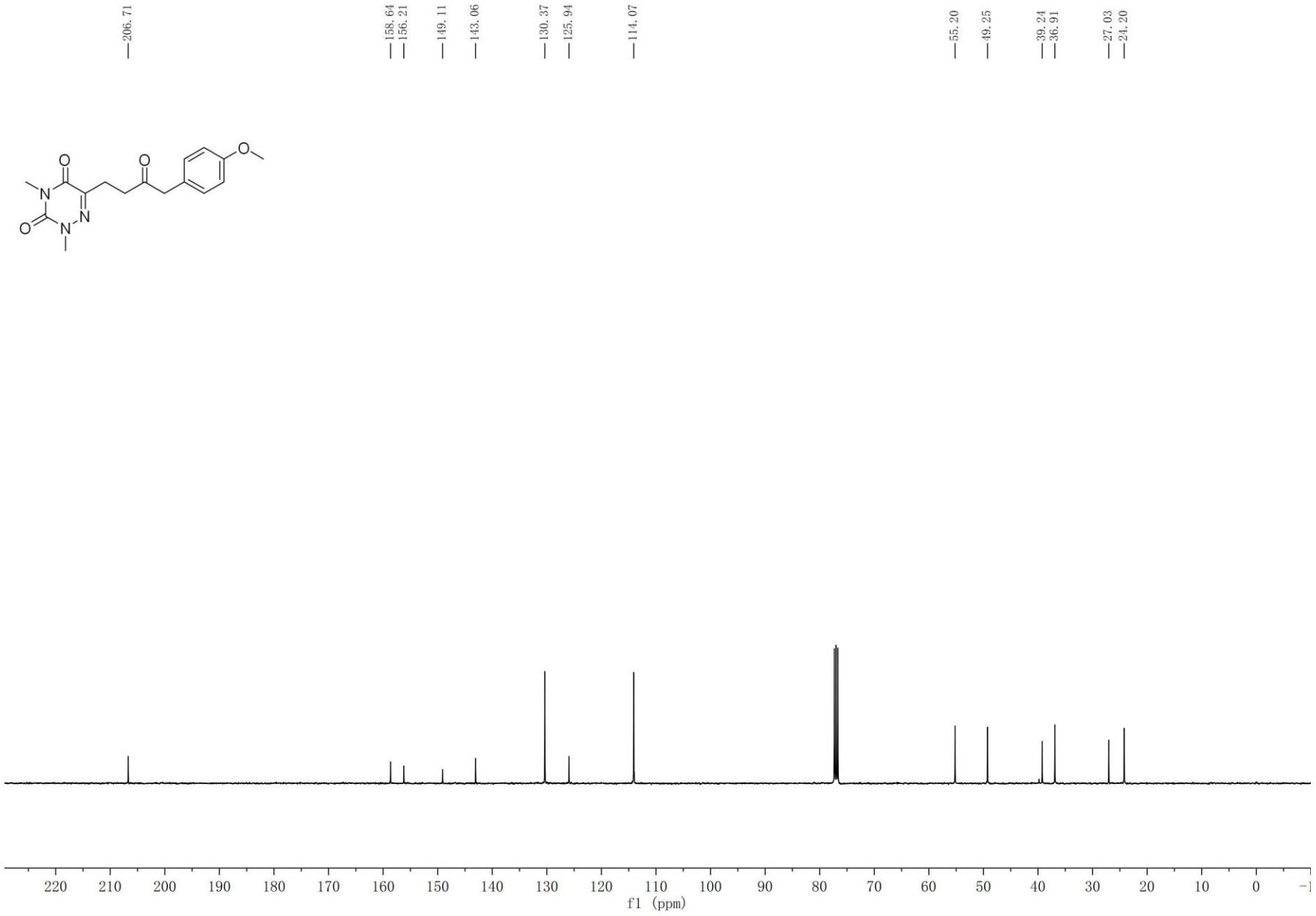
3s-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



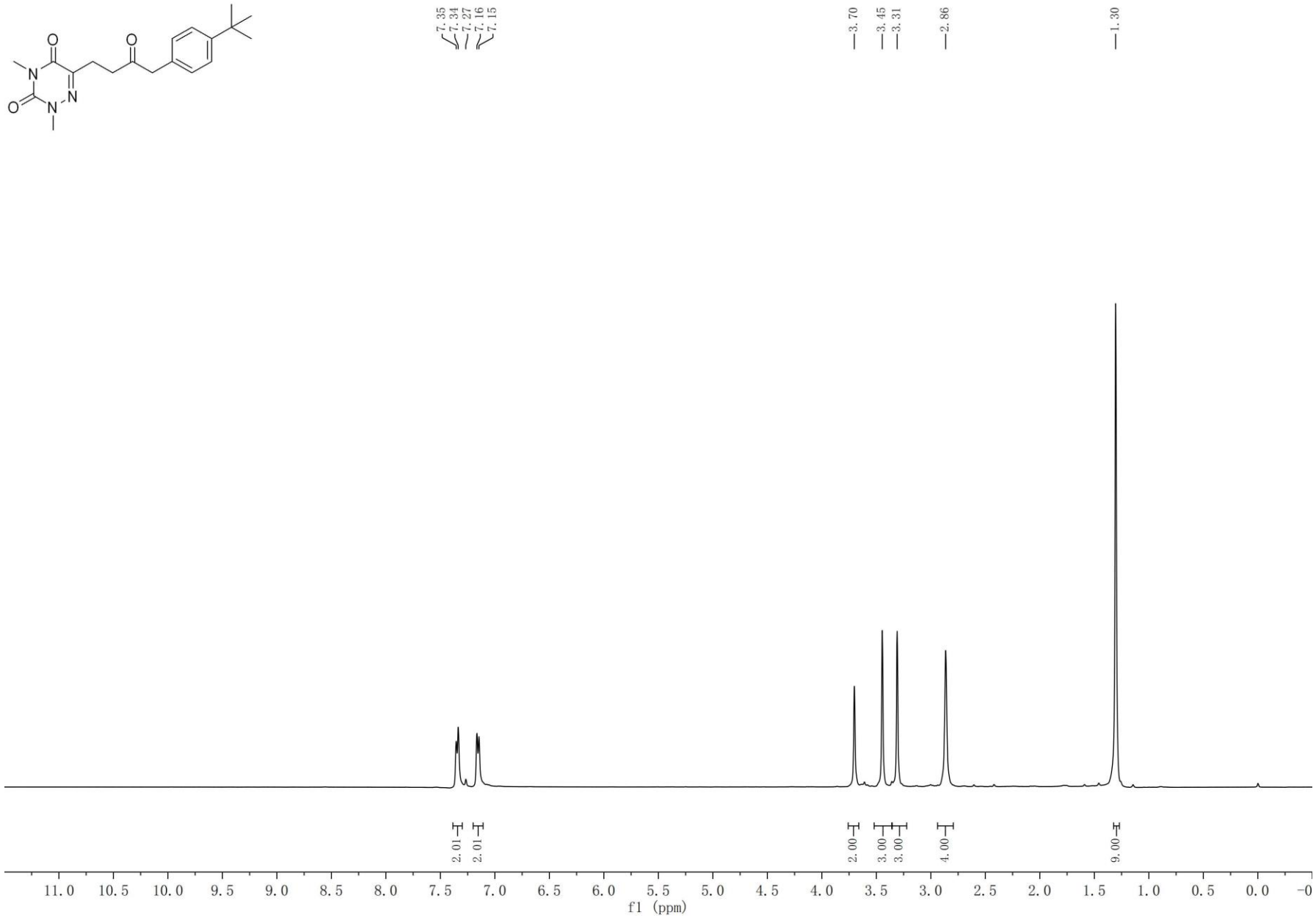
3t-^{1}H NMR (400 MHz, $CDCl_3$)



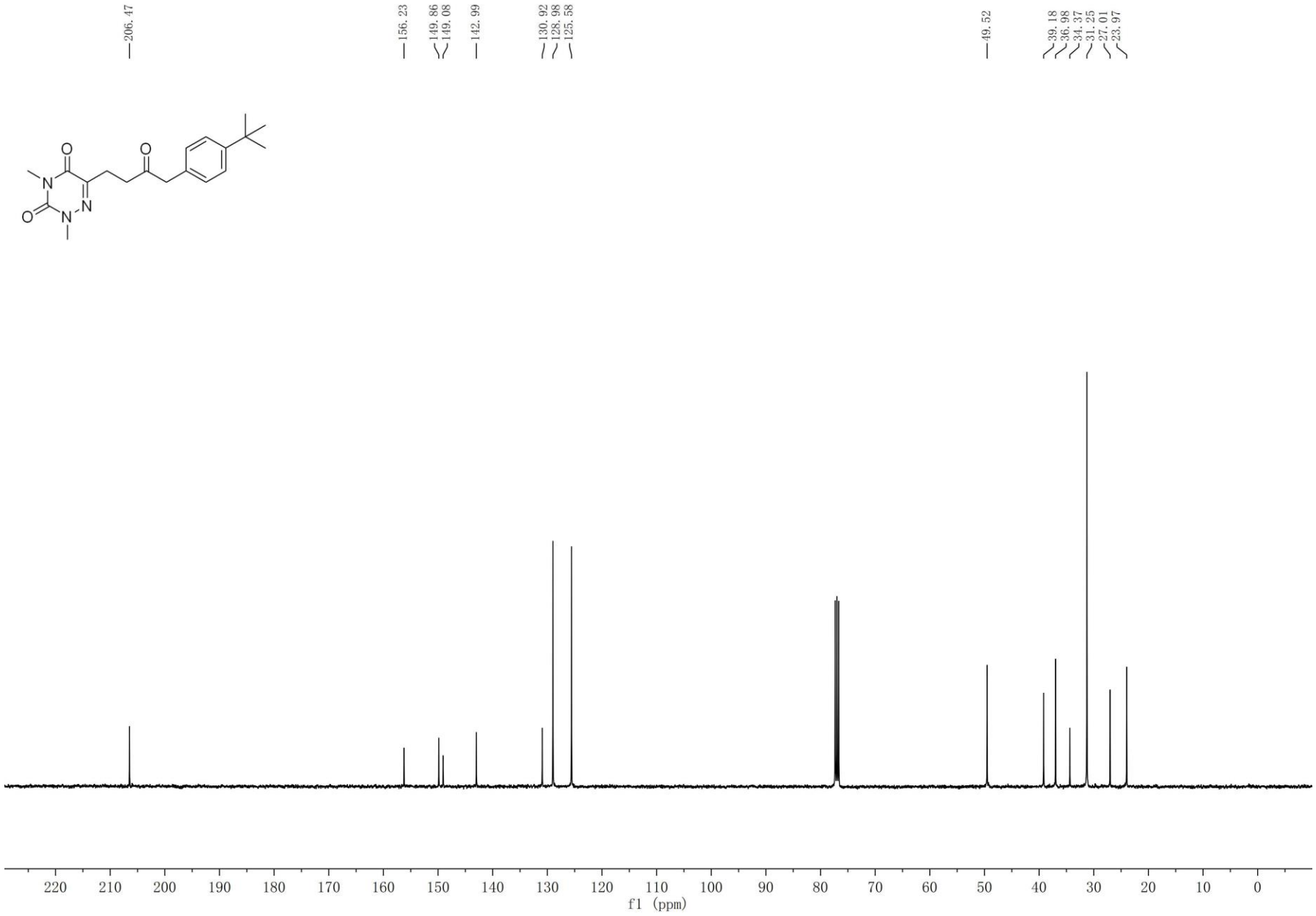
3t-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



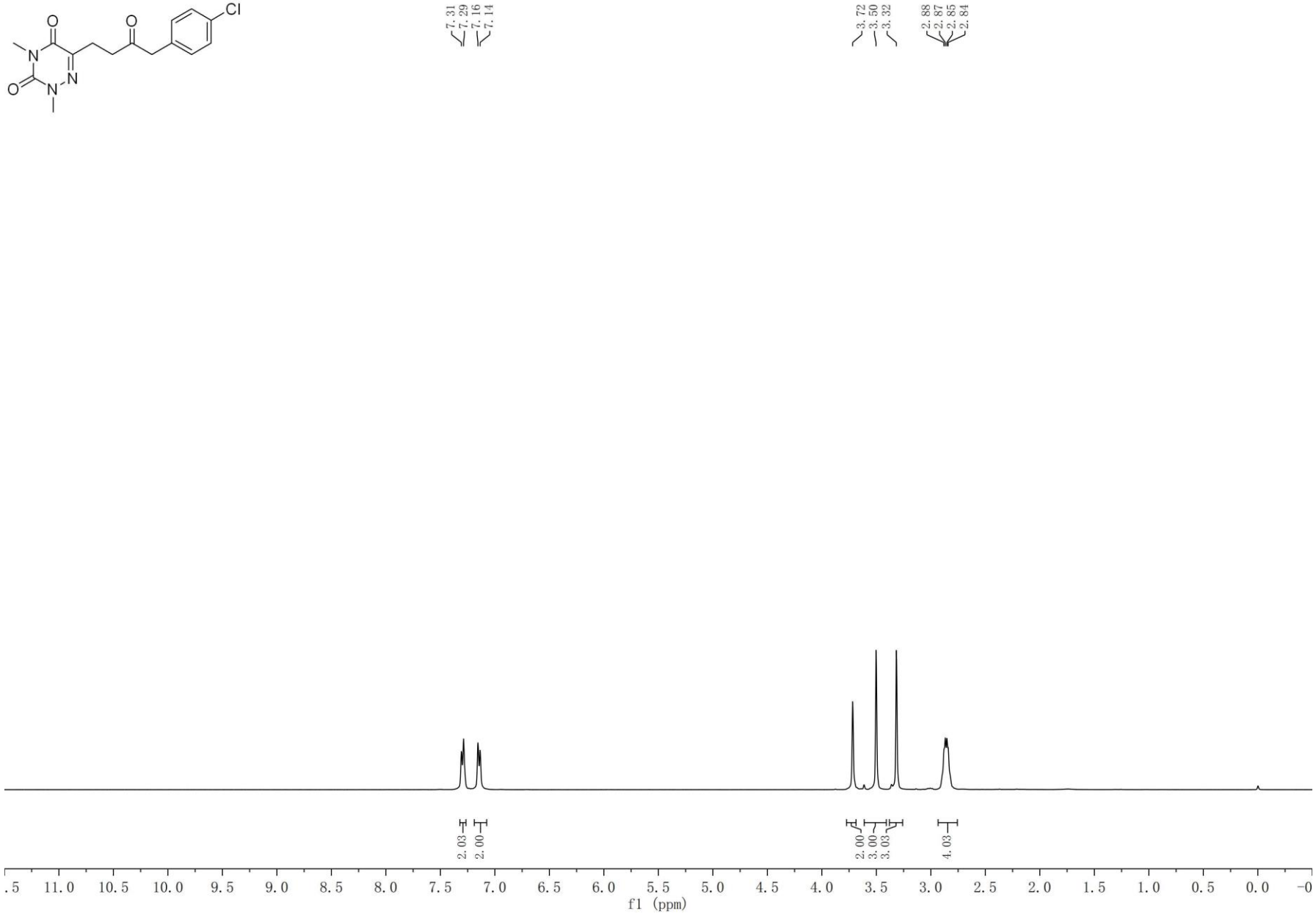
3u-^{1}H NMR (400 MHz, $CDCl_3$)



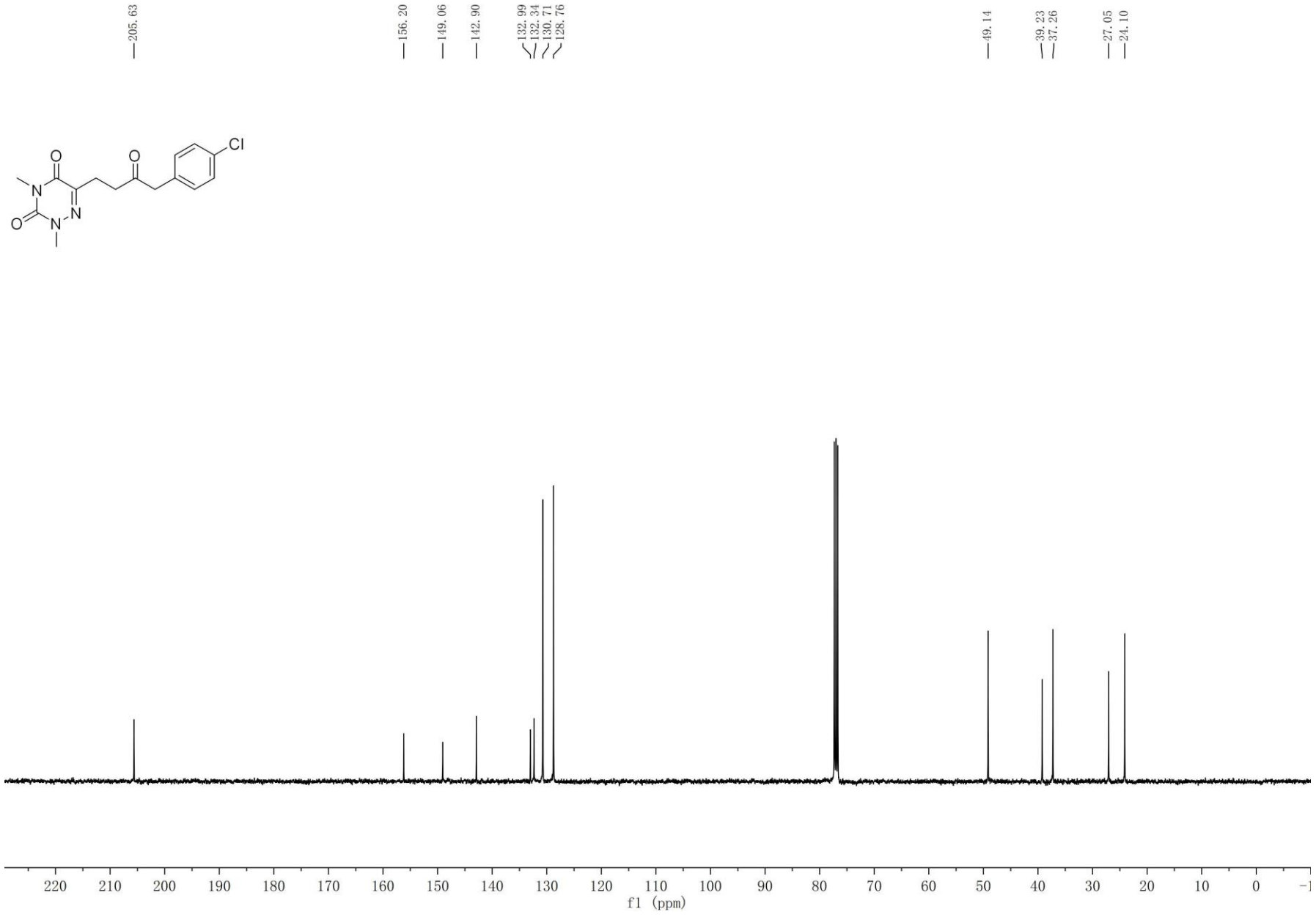
3u-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



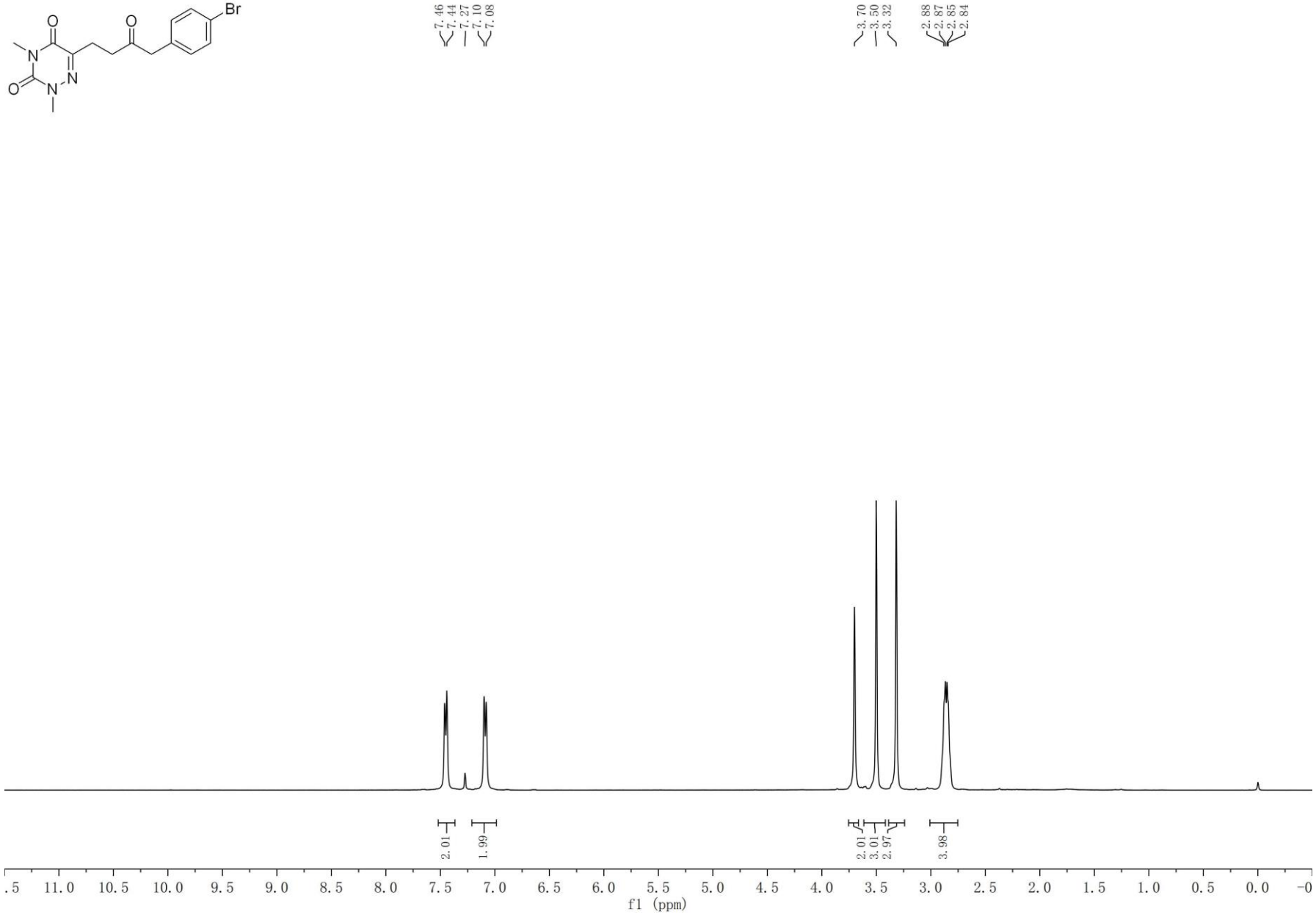
3v-^{1}H NMR (400 MHz, $CDCl_3$)



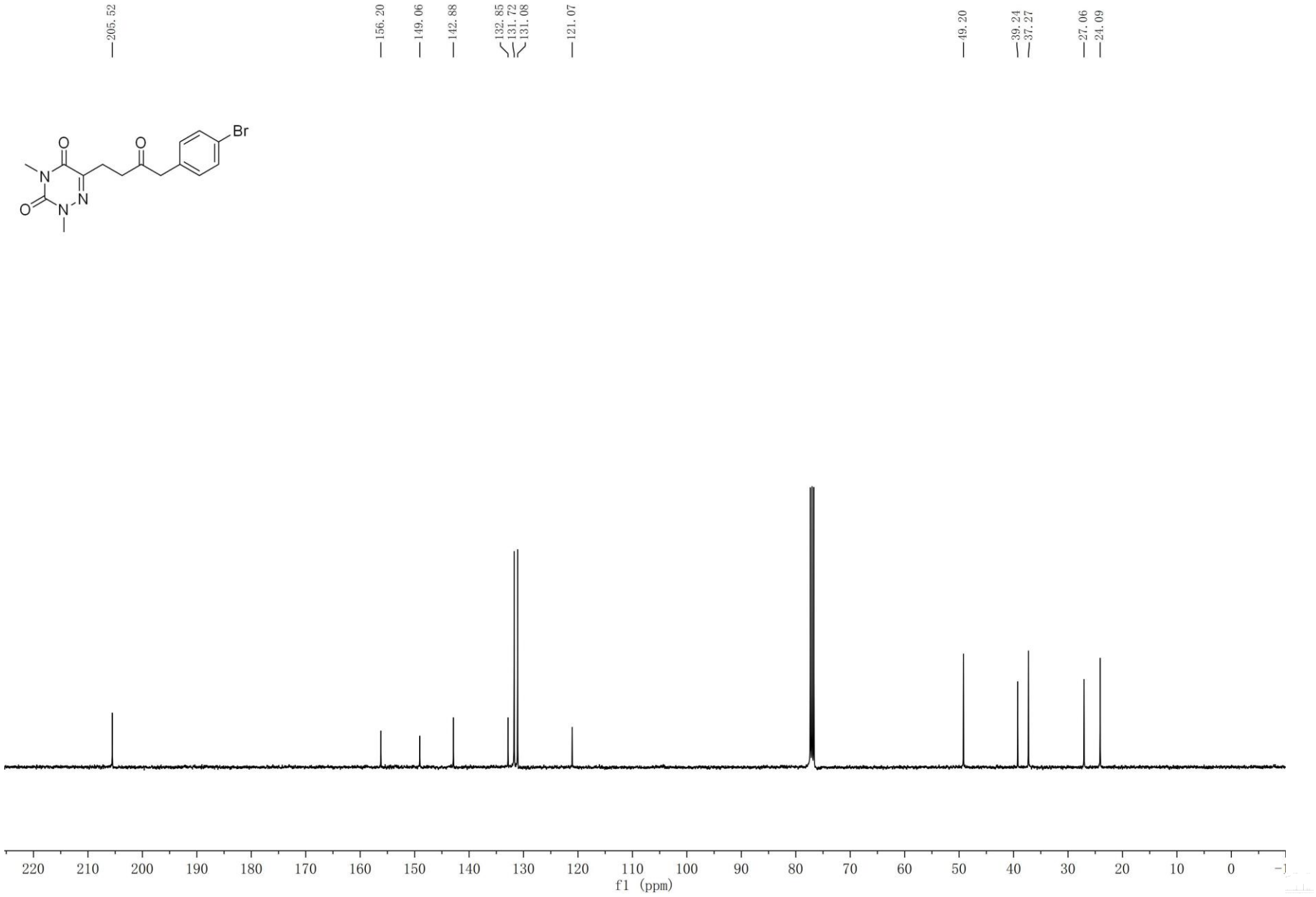
3v-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



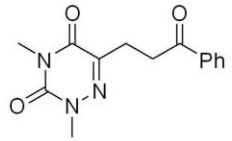
3w-^{1}H NMR (400 MHz, $CDCl_3$)

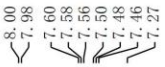


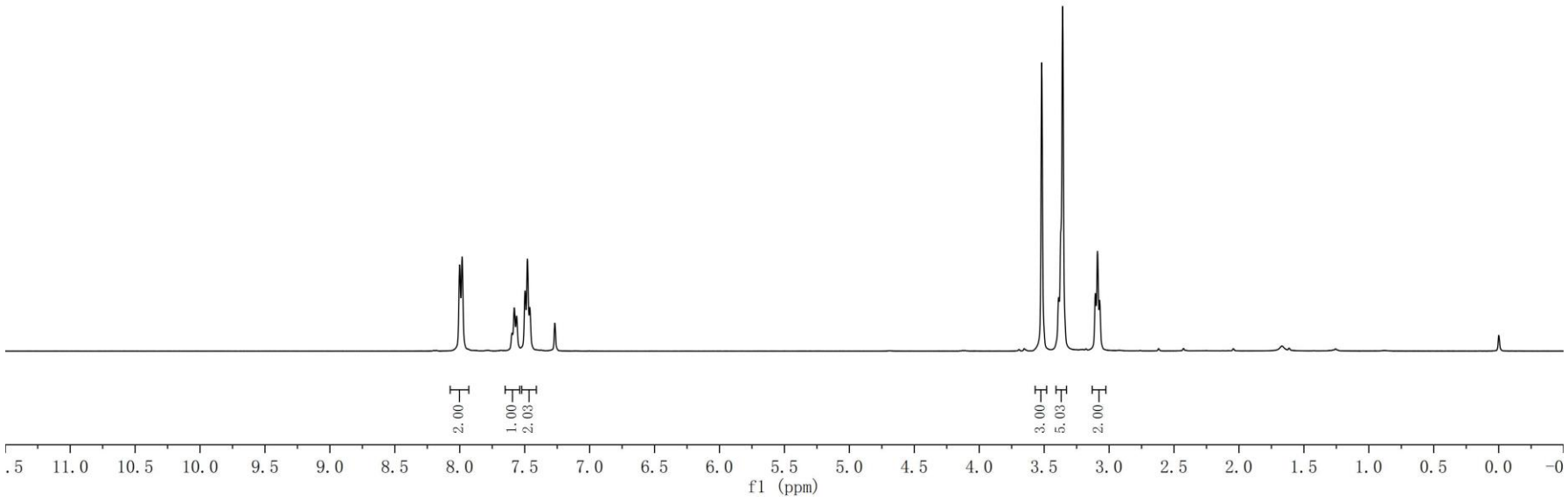
3w-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



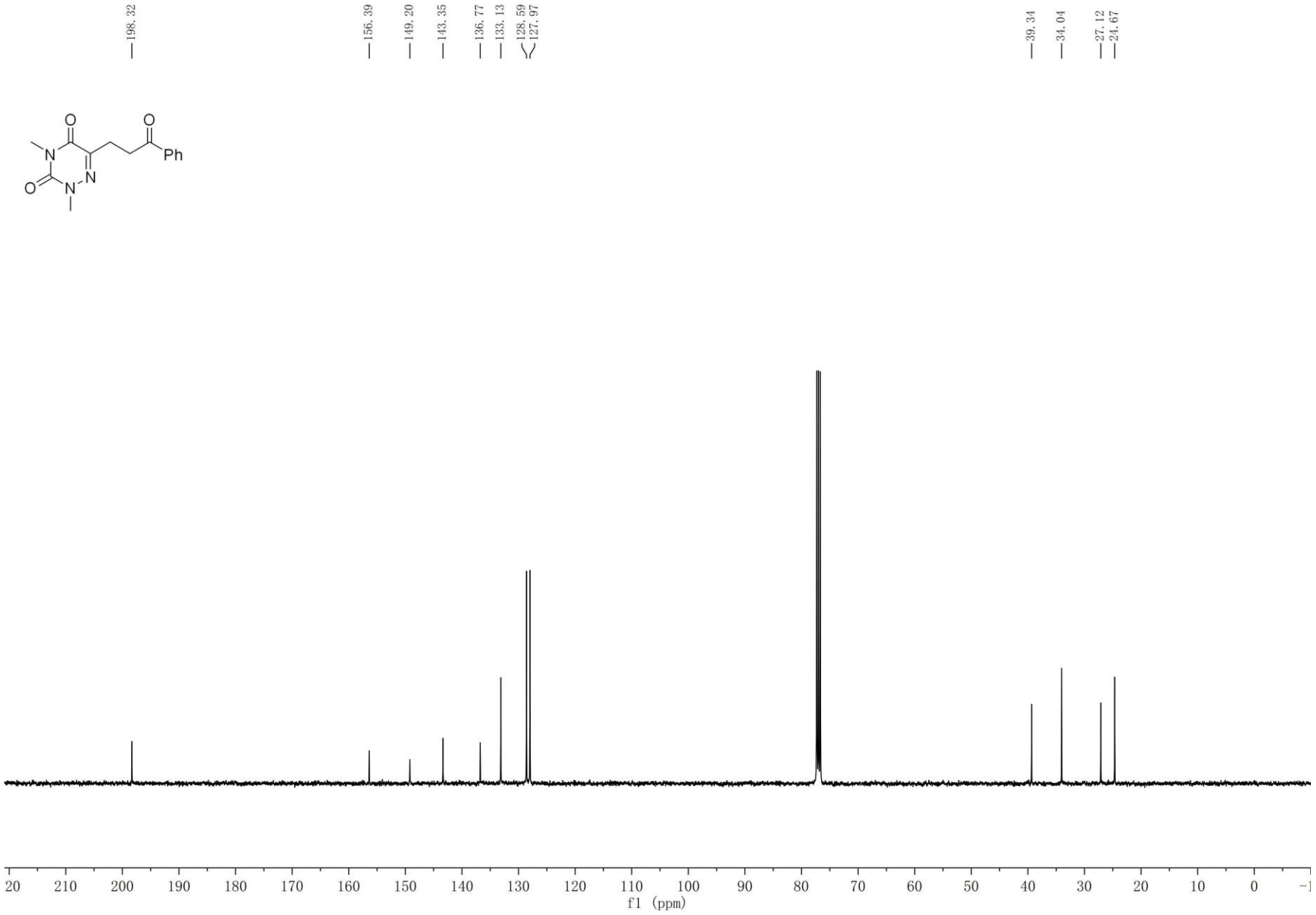
3x-^{1}H NMR (400 MHz, $CDCl_3$)



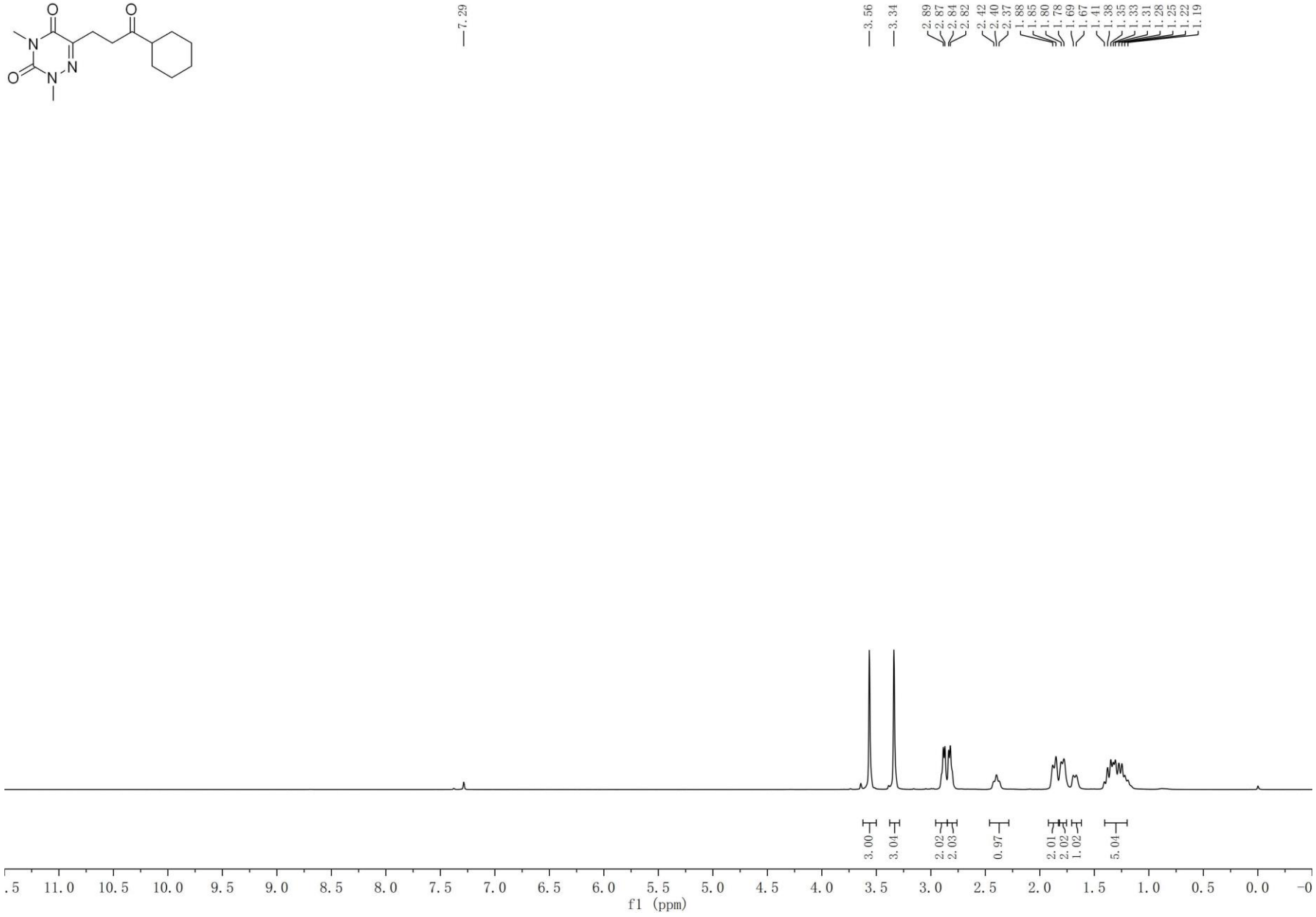




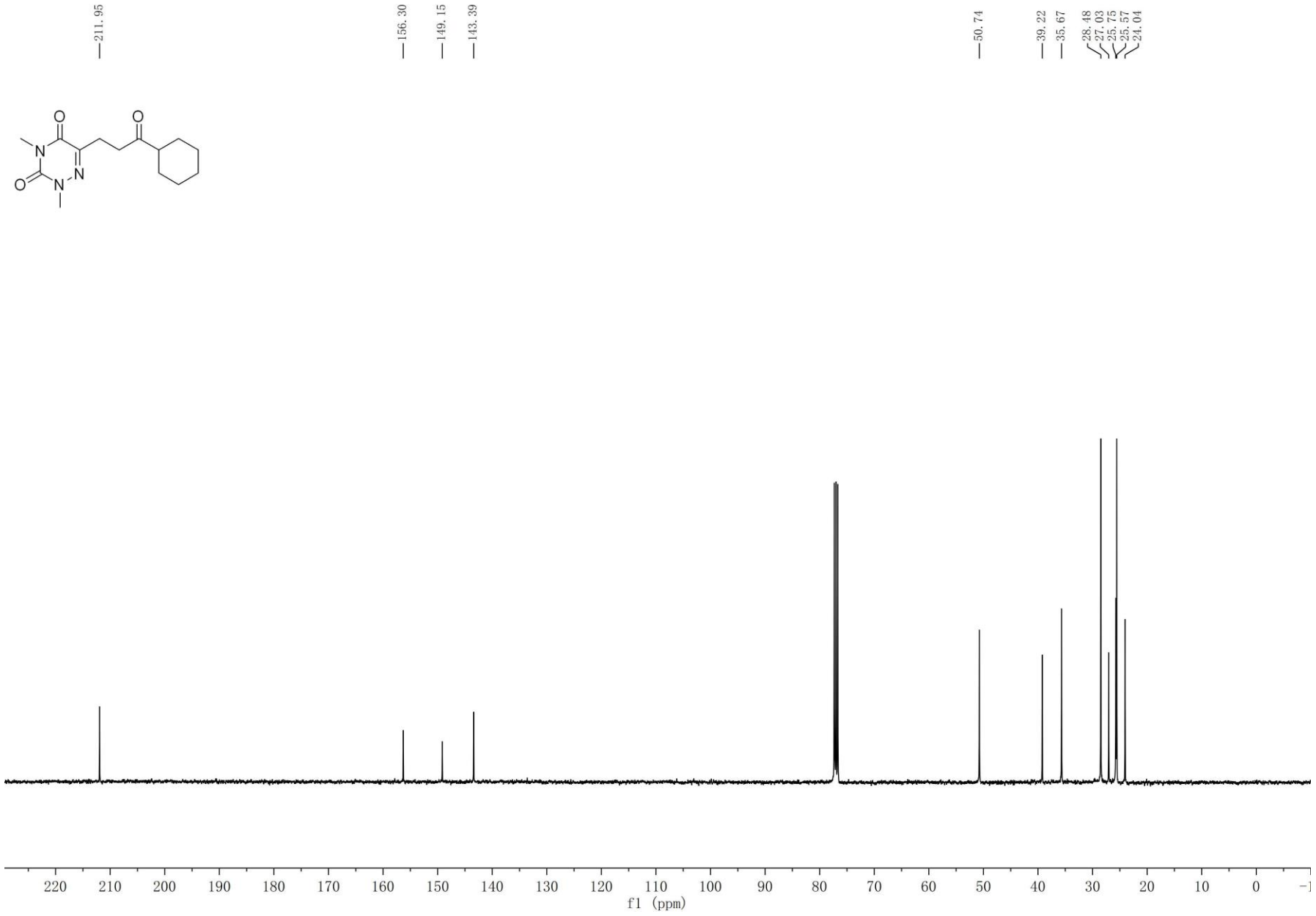
3x-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



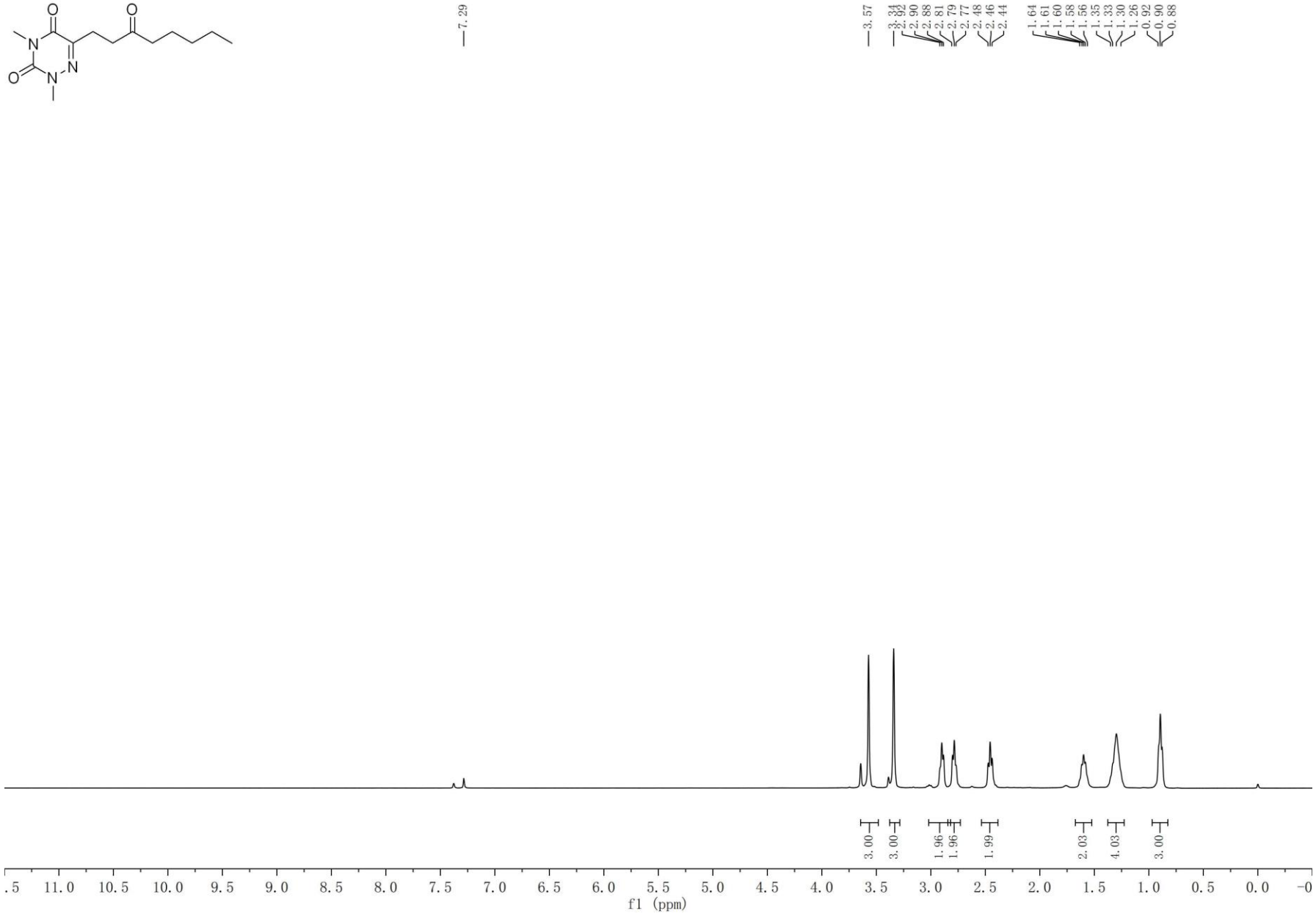
3y-^{1}H NMR (400 MHz, $CDCl_3$)



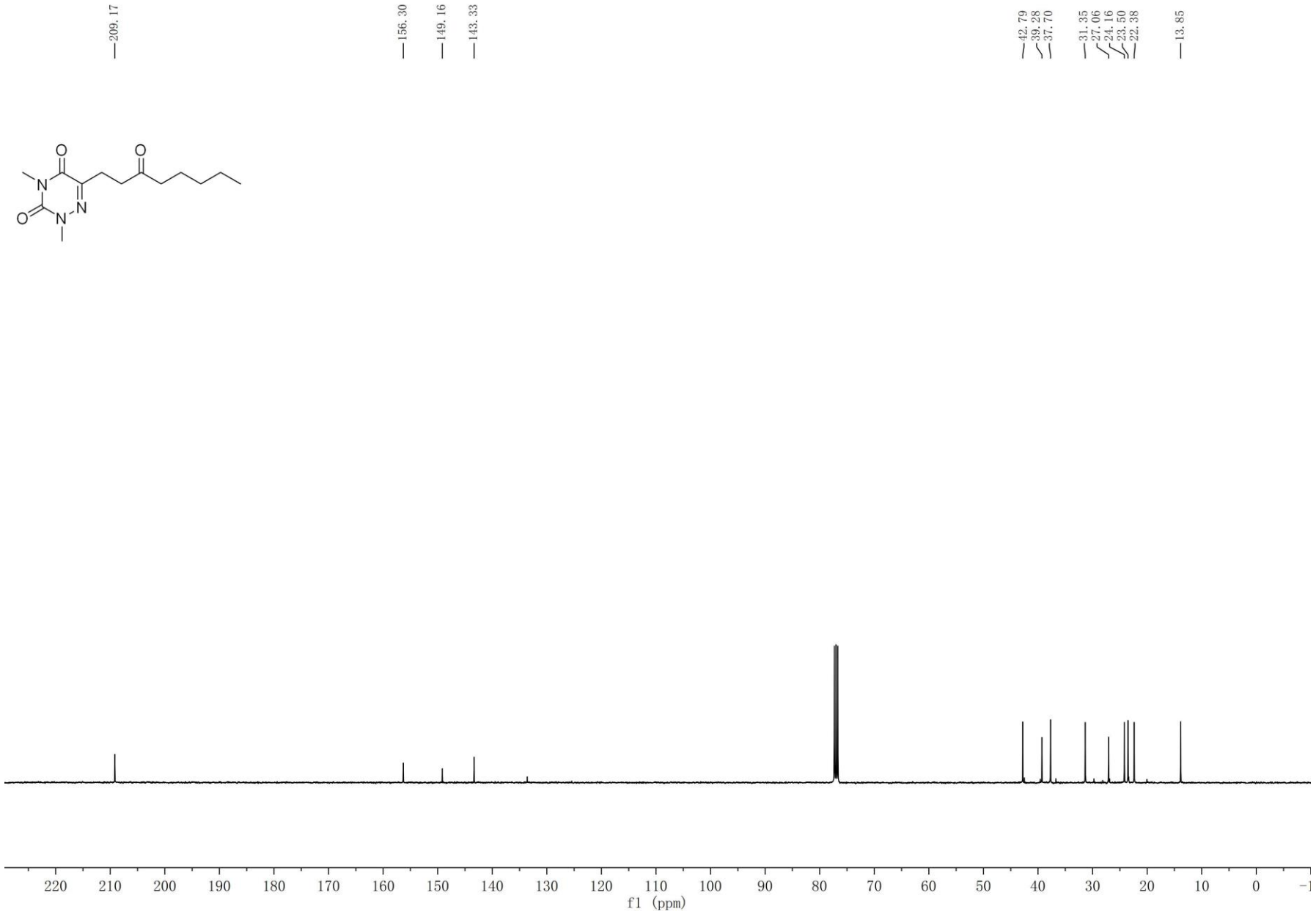
3y-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



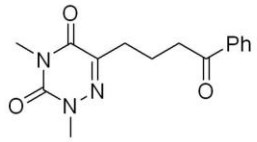
3z-^{1}H NMR (400 MHz, $CDCl_3$)

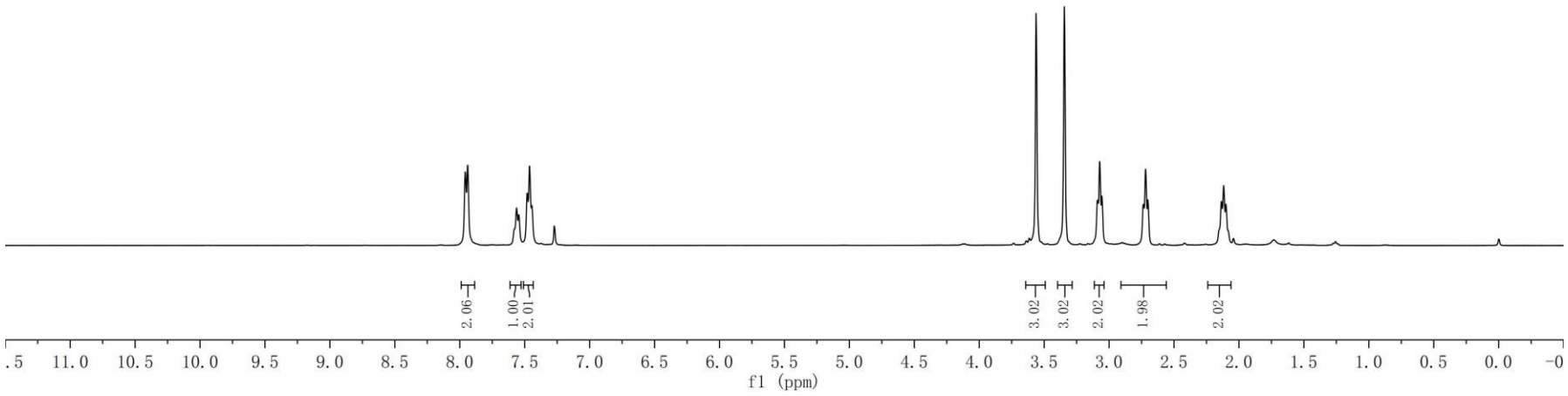


3z-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

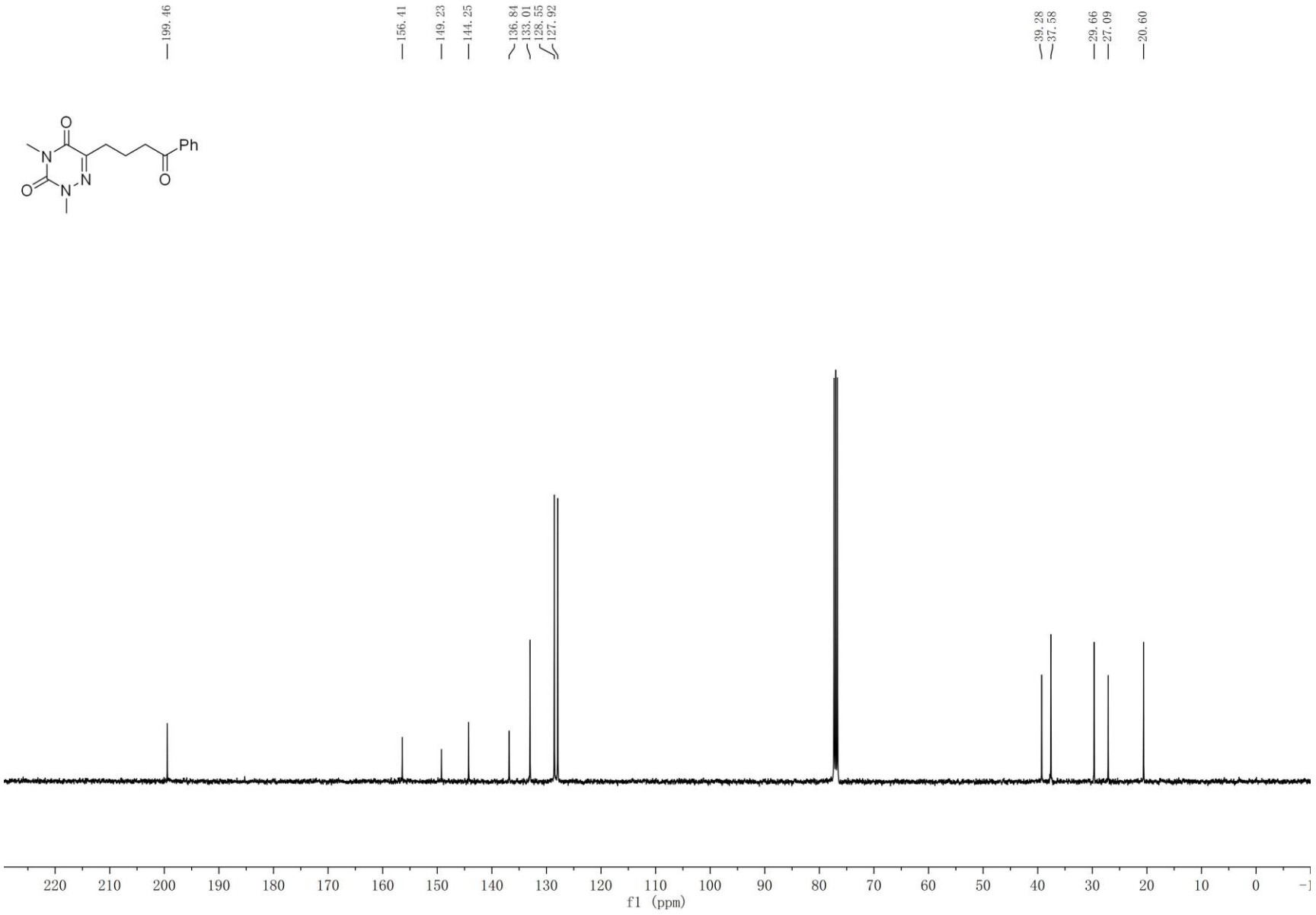


3aa-^{1}H NMR (400 MHz, $CDCl_3$)



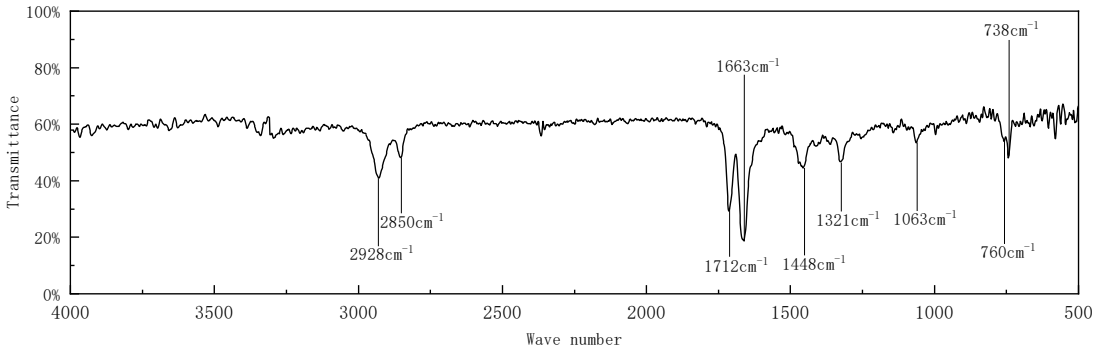


3aa-$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

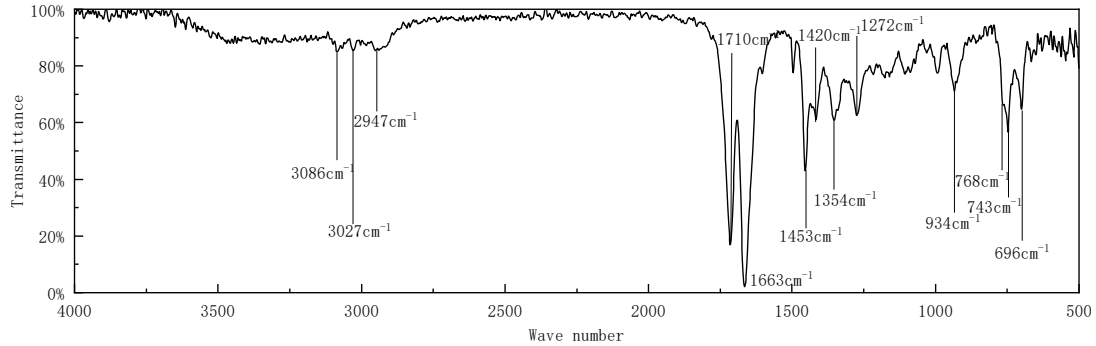


V. IR Spectrum

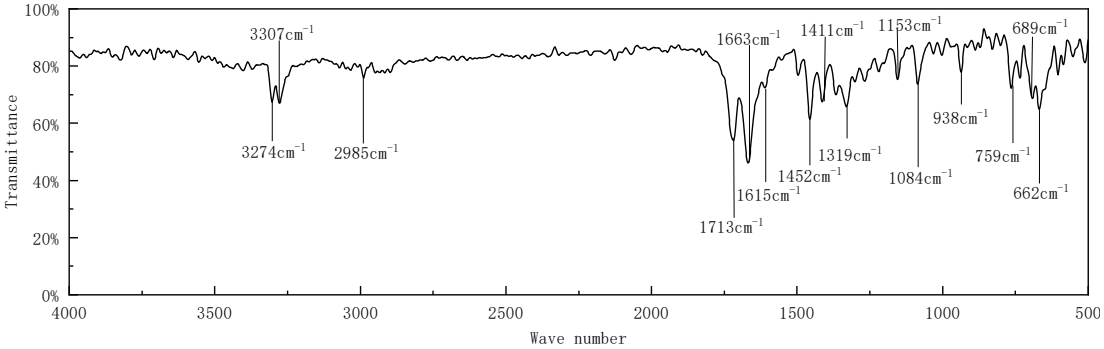
3a



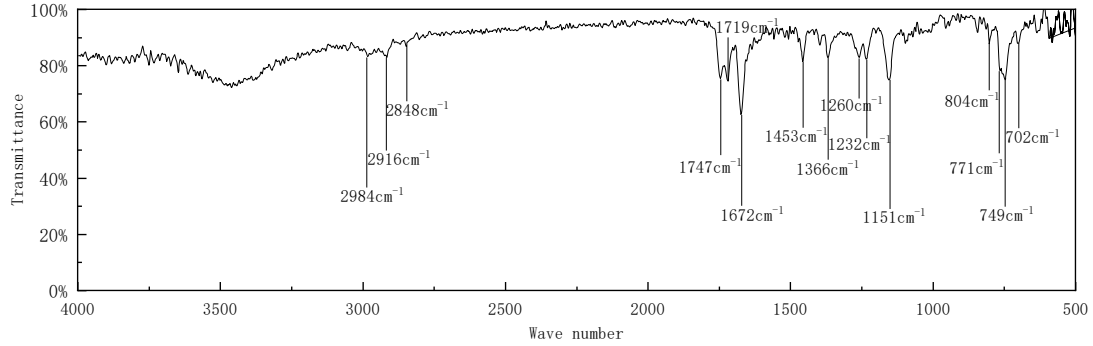
3b



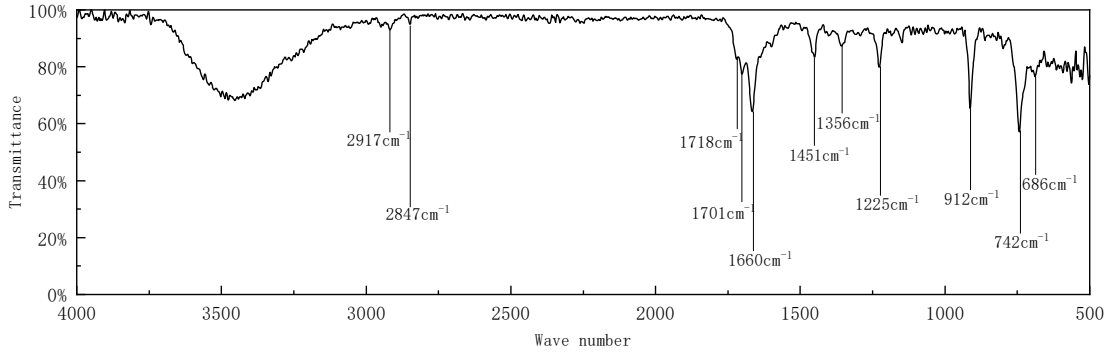
3c



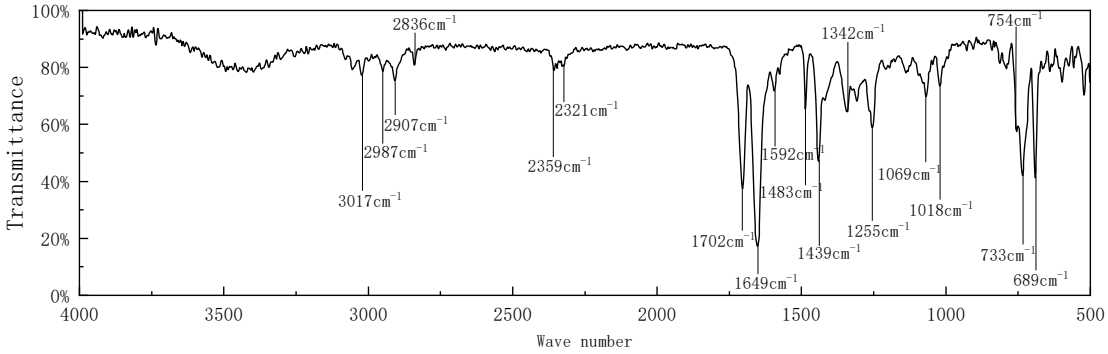
3d



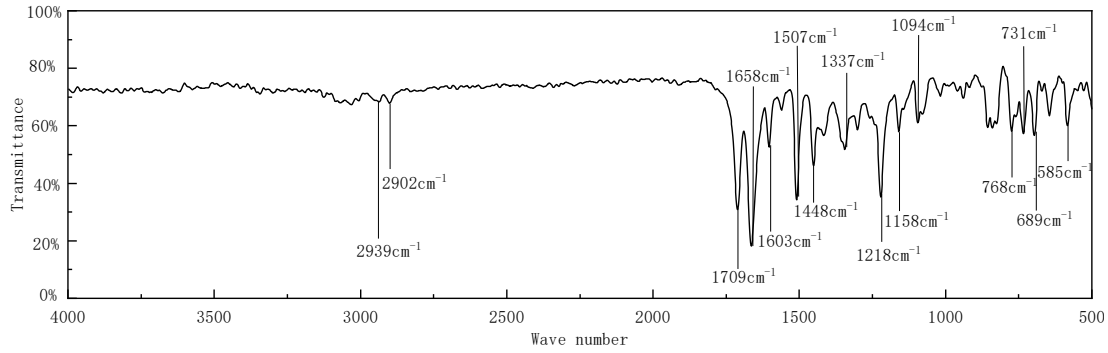
3e


Transmittance
Wave number
2917cm-1
2847cm-1
1718cm-1
1701cm-1
1660cm-1
1451cm-1
1356cm-1
1225cm-1
912cm-1
742cm-1
686cm-1

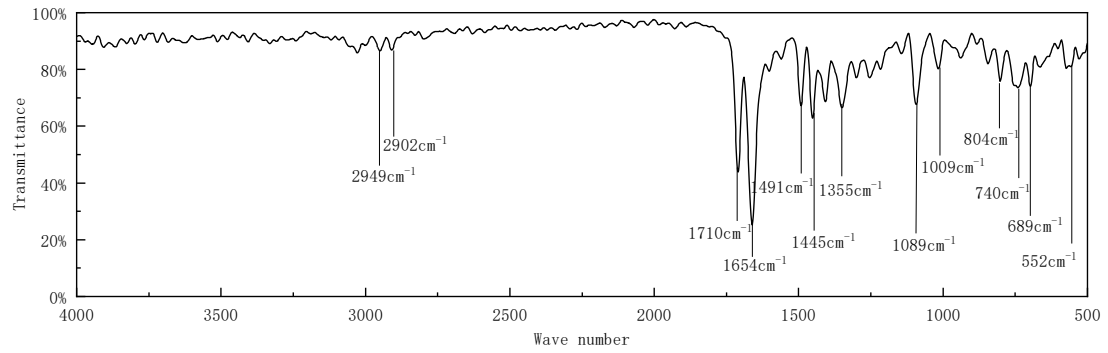
3f


Transmittance
Wave number
3017cm-1
2987cm-1
2907cm-1
2836cm-1
2359cm-1
2321cm-1
1702cm-1
1649cm-1
1592cm-1
1483cm-1
1439cm-1
1342cm-1
1255cm-1
1069cm-1
1018cm-1
754cm-1
733cm-1
689cm-1

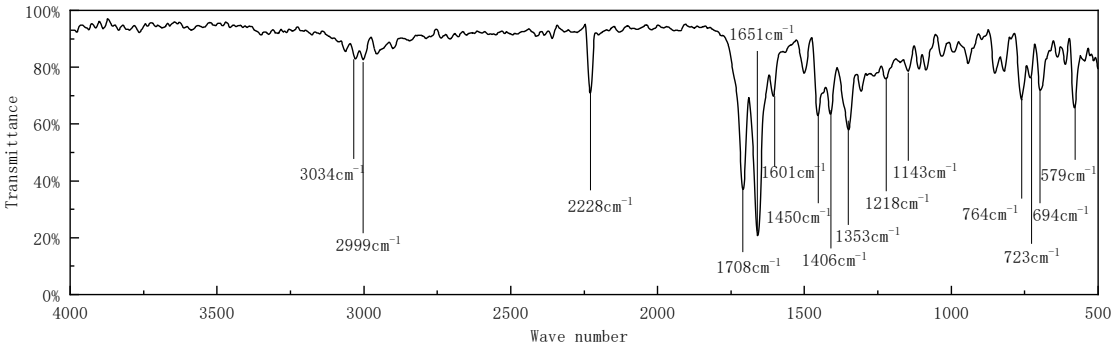
3g


Transmittance
Wave number
2939cm-1
2902cm-1
1709cm-1
1658cm-1
1603cm-1
1507cm-1
1448cm-1
1337cm-1
1218cm-1
1158cm-1
1094cm-1
768cm-1
731cm-1
689cm-1
585cm-1

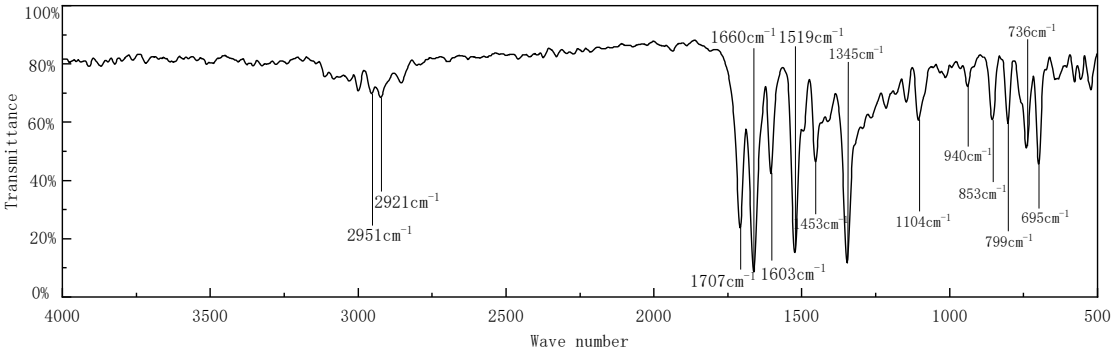
3h


Transmittance
Wave number
2949cm-1
2902cm-1
1710cm-1
1654cm-1
1491cm-1
1445cm-1
1355cm-1
1089cm-1
1009cm-1
804cm-1
740cm-1
689cm-1
552cm-1

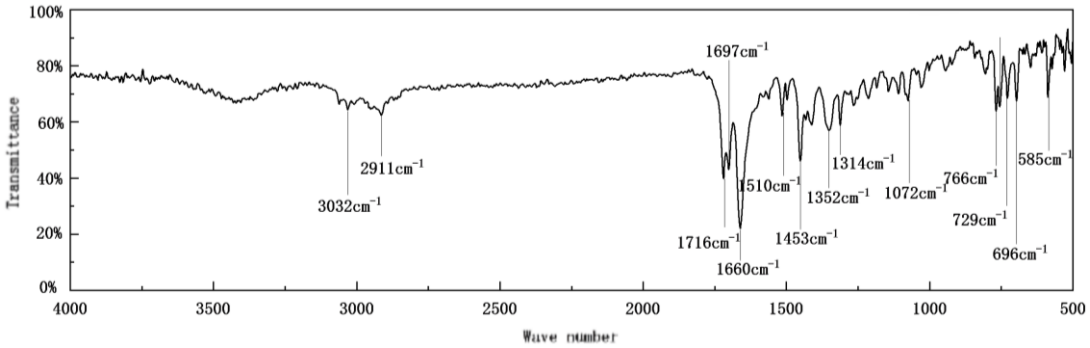
3i


Transmittance
Wave number
3034cm⁻¹
2999cm⁻¹
2228cm⁻¹
1708cm⁻¹
1651cm⁻¹
1601cm⁻¹
1450cm⁻¹
1406cm⁻¹
1353cm⁻¹
1218cm⁻¹
1143cm⁻¹
764cm⁻¹
723cm⁻¹
694cm⁻¹
579cm⁻¹

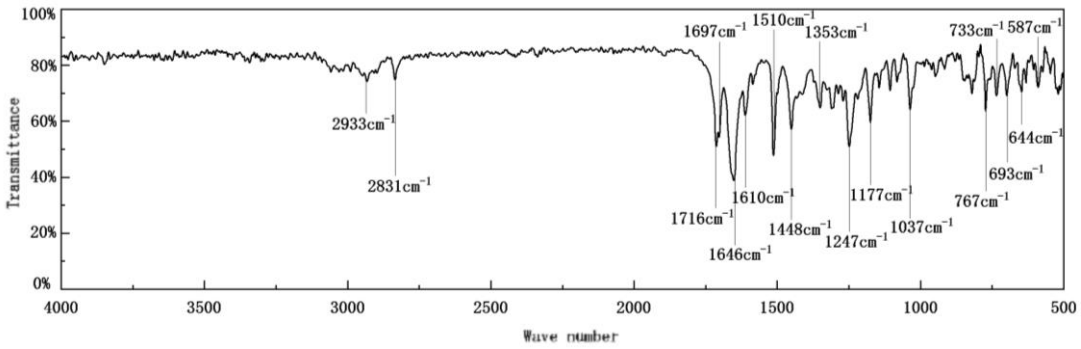
3j


Transmittance
Wave number
2951cm⁻¹
2921cm⁻¹
1707cm⁻¹
1660cm⁻¹
1603cm⁻¹
1519cm⁻¹
1453cm⁻¹
1345cm⁻¹
1104cm⁻¹
940cm⁻¹
853cm⁻¹
799cm⁻¹
736cm⁻¹
695cm⁻¹

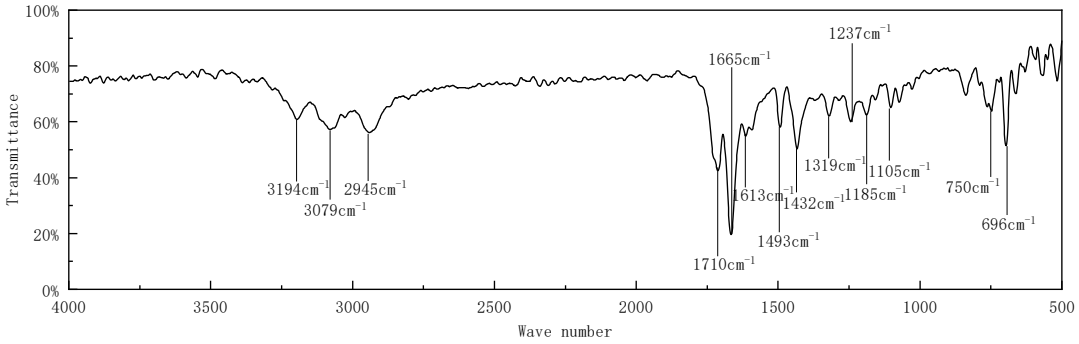
3k


Transmittance
Wave number
3032cm⁻¹
2911cm⁻¹
1716cm⁻¹
1660cm⁻¹
1697cm⁻¹
1510cm⁻¹
1453cm⁻¹
1352cm⁻¹
1314cm⁻¹
1072cm⁻¹
766cm⁻¹
729cm⁻¹
696cm⁻¹
585cm⁻¹

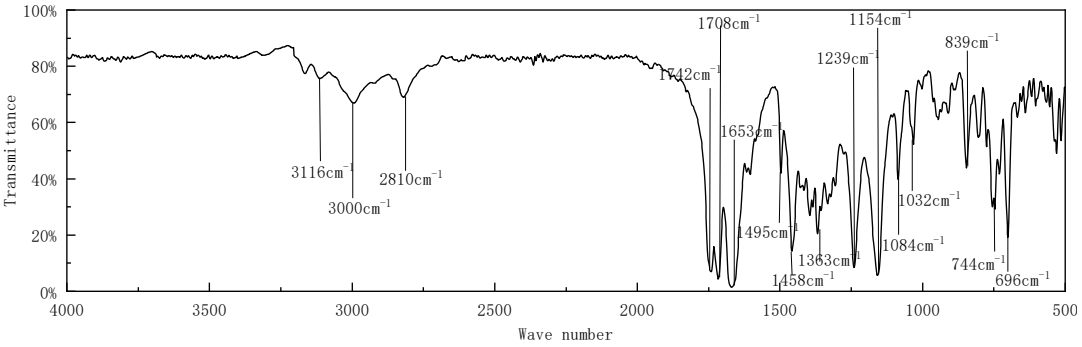
3l


Transmittance
Wave number
2933cm⁻¹
2831cm⁻¹
1716cm⁻¹
1646cm⁻¹
1697cm⁻¹
1510cm⁻¹
1610cm⁻¹
1448cm⁻¹
1353cm⁻¹
1247cm⁻¹
1177cm⁻¹
1037cm⁻¹
767cm⁻¹
733cm⁻¹
693cm⁻¹
644cm⁻¹
587cm⁻¹

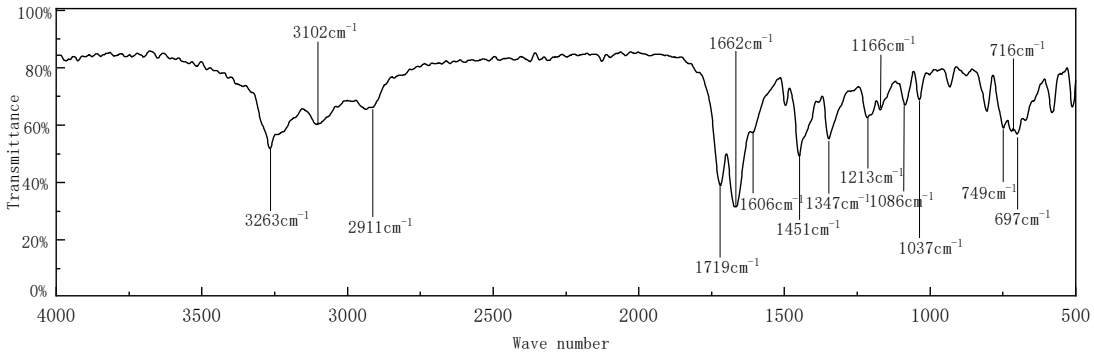
3m


Transmittance
Wave number
3194cm⁻¹
3079cm⁻¹
2945cm⁻¹
1710cm⁻¹
1665cm⁻¹
1613cm⁻¹
1493cm⁻¹
1432cm⁻¹
1319cm⁻¹
1237cm⁻¹
1185cm⁻¹
1105cm⁻¹
750cm⁻¹
696cm⁻¹

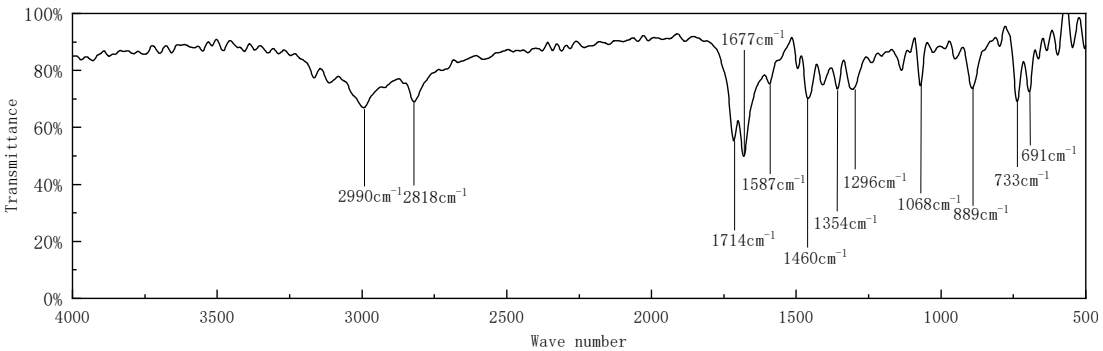
3n


Transmittance
Wave number
3116cm⁻¹
3000cm⁻¹
2810cm⁻¹
1742cm⁻¹
1708cm⁻¹
1653cm⁻¹
1495cm⁻¹
1458cm⁻¹
1363cm⁻¹
1239cm⁻¹
1154cm⁻¹
1084cm⁻¹
1032cm⁻¹
839cm⁻¹
744cm⁻¹
696cm⁻¹

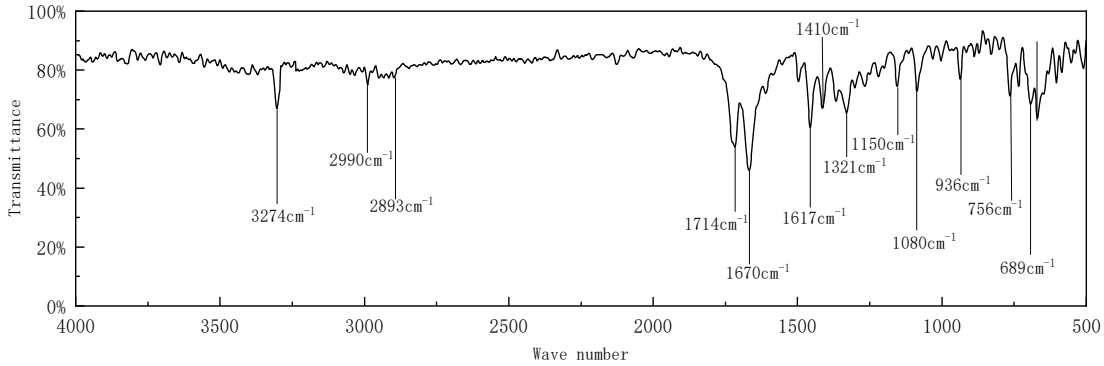
3o


Transmittance
Wave number
3263cm⁻¹
3102cm⁻¹
2911cm⁻¹
1719cm⁻¹
1662cm⁻¹
1606cm⁻¹
1451cm⁻¹
1347cm⁻¹
1213cm⁻¹
1166cm⁻¹
1086cm⁻¹
1037cm⁻¹
749cm⁻¹
716cm⁻¹
697cm⁻¹

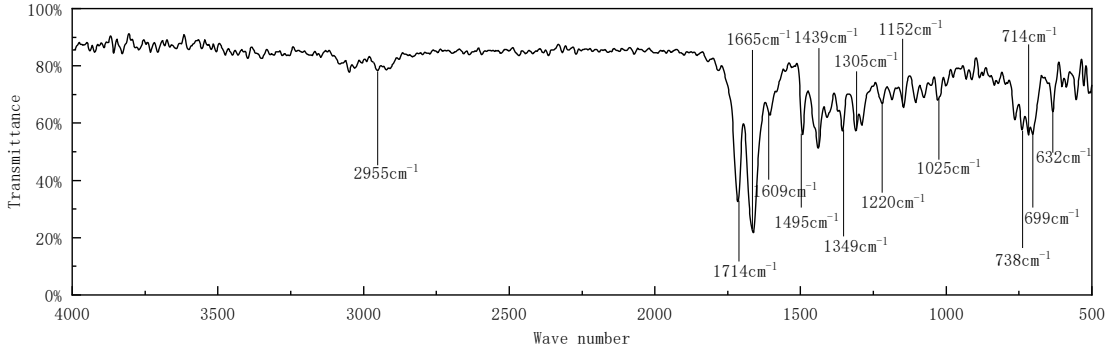
3p


Transmittance
Wave number
2990cm⁻¹
2818cm⁻¹
1714cm⁻¹
1677cm⁻¹
1587cm⁻¹
1460cm⁻¹
1354cm⁻¹
1296cm⁻¹
1068cm⁻¹
889cm⁻¹
733cm⁻¹
691cm⁻¹

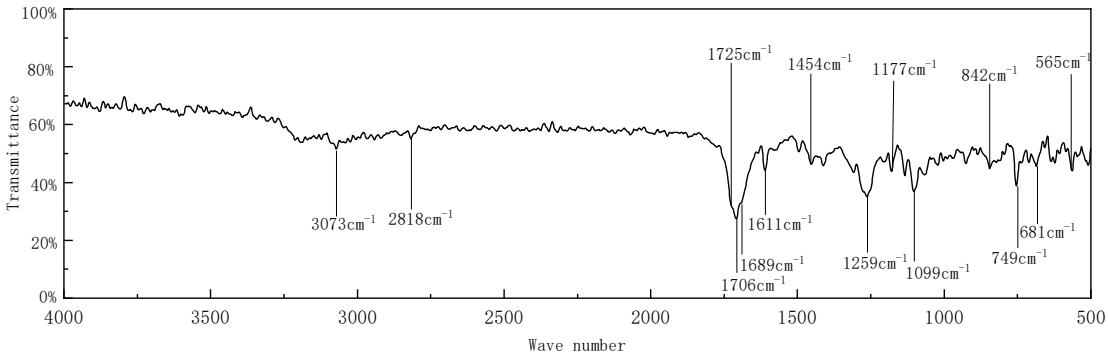
3q


Transmittance
Wave number
3274cm⁻¹
2990cm⁻¹
2893cm⁻¹
1714cm⁻¹
1670cm⁻¹
1617cm⁻¹
1410cm⁻¹
1321cm⁻¹
1150cm⁻¹
1080cm⁻¹
936cm⁻¹
756cm⁻¹
689cm⁻¹

3r


Transmittance
Wave number
2955cm⁻¹
1714cm⁻¹
1665cm⁻¹
1609cm⁻¹
1495cm⁻¹
1439cm⁻¹
1349cm⁻¹
1305cm⁻¹
1220cm⁻¹
1152cm⁻¹
1025cm⁻¹
738cm⁻¹
714cm⁻¹
699cm⁻¹
632cm⁻¹

3s


Transmittance
Wave number
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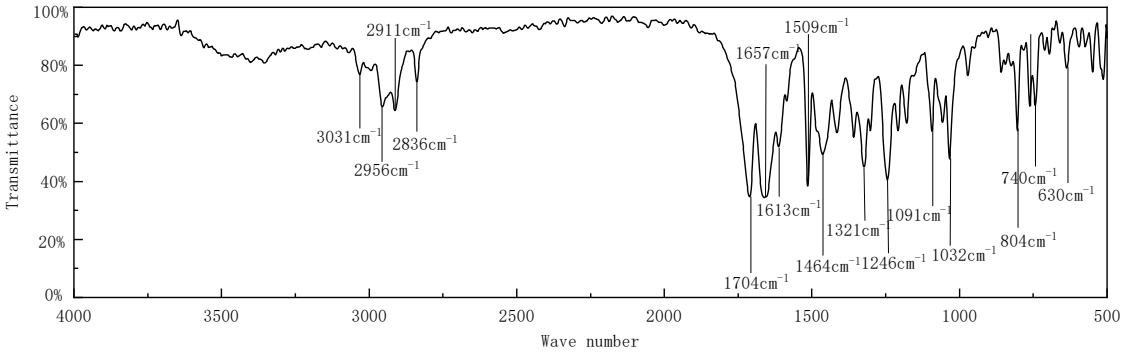
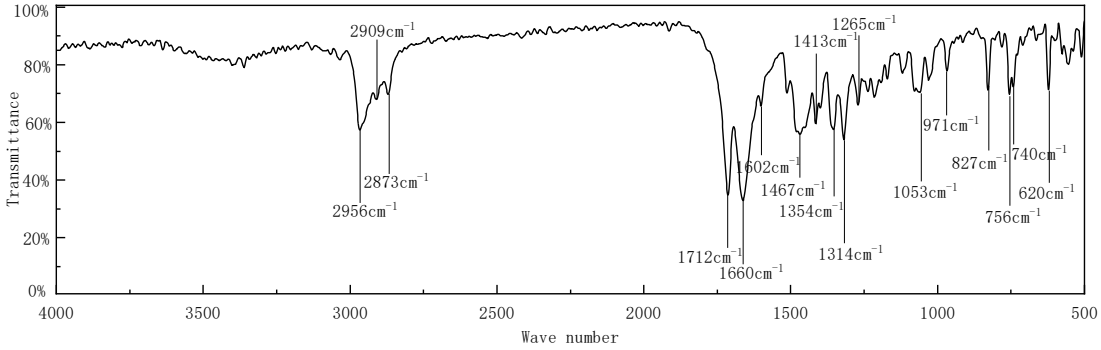
2818cm⁻¹
1706cm⁻¹
1689cm⁻¹
1611cm⁻¹
1725cm⁻¹
1454cm⁻¹
1259cm⁻¹
1099cm⁻¹
1177cm⁻¹
842cm⁻¹
749cm⁻¹
681cm⁻¹
565cm⁻¹

3t


Transmittance
Wave number
3031cm⁻¹
2956cm⁻¹
2836cm⁻¹
2911cm⁻¹
1704cm⁻¹
1657cm⁻¹
1613cm⁻¹
1509cm⁻¹
1464cm⁻¹
1321cm⁻¹
1246cm⁻¹
1091cm⁻¹
1032cm⁻¹
804cm⁻¹
740cm⁻¹
630cm⁻¹

3u


Transmittance
Wave number
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2956cm⁻¹
2873cm⁻¹
1712cm⁻¹
1660cm⁻¹
1602cm⁻¹
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1354cm⁻¹
1314cm⁻¹
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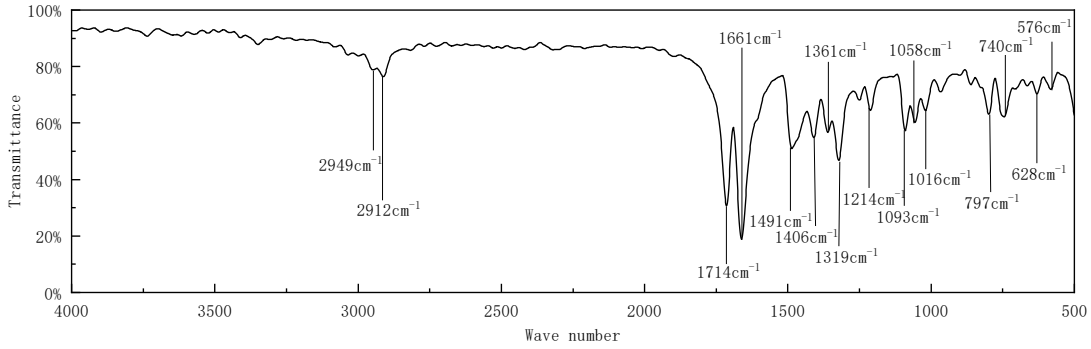
1053cm⁻¹
971cm⁻¹
827cm⁻¹
756cm⁻¹
740cm⁻¹
620cm⁻¹

3v


Transmittance
Wave number
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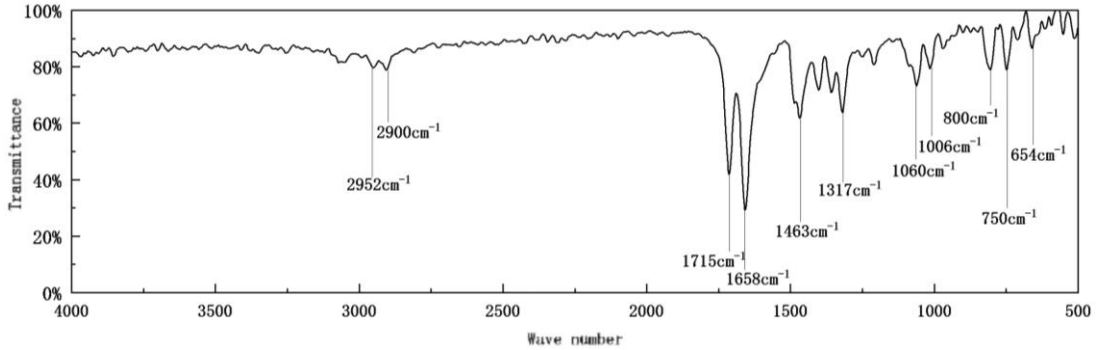
2912cm⁻¹
1714cm⁻¹
1661cm⁻¹
1491cm⁻¹
1406cm⁻¹
1361cm⁻¹
1319cm⁻¹
1214cm⁻¹
1093cm⁻¹
1058cm⁻¹
1016cm⁻¹
797cm⁻¹
740cm⁻¹
628cm⁻¹
576cm⁻¹

3w


Transmittance
Wave number
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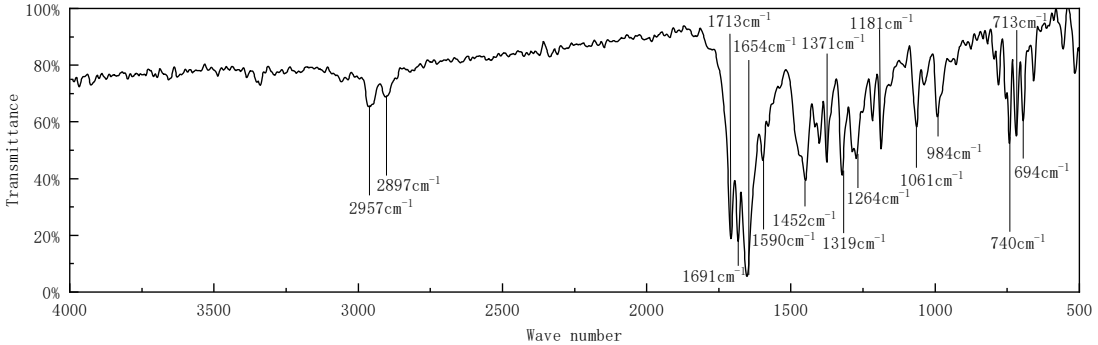
2900cm⁻¹
1715cm⁻¹
1658cm⁻¹
1463cm⁻¹
1317cm⁻¹
1060cm⁻¹
1006cm⁻¹
800cm⁻¹
750cm⁻¹
654cm⁻¹

3x


Transmittance
Wave number
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2897cm⁻¹
1691cm⁻¹
1713cm⁻¹
1654cm⁻¹
1590cm⁻¹
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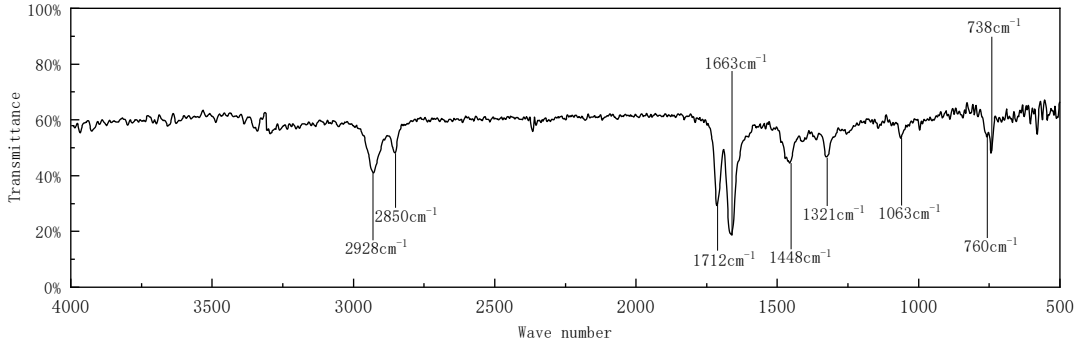
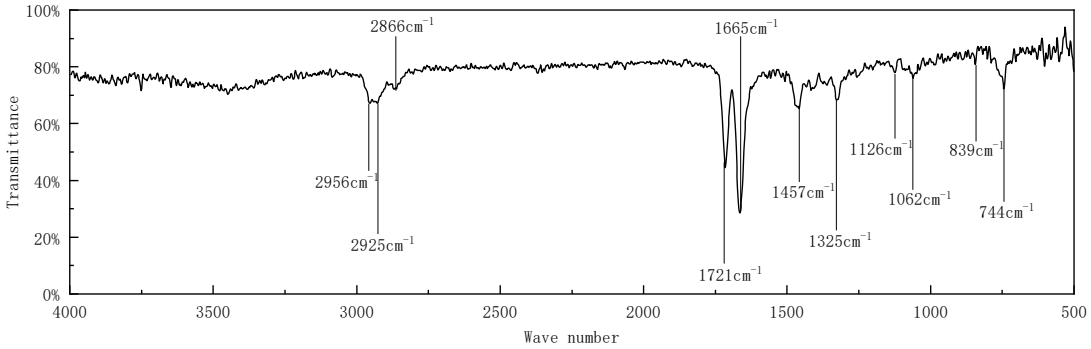
1371cm⁻¹
1319cm⁻¹
1264cm⁻¹
1181cm⁻¹
1061cm⁻¹
984cm⁻¹
740cm⁻¹
713cm⁻¹
694cm⁻¹

3y


Transmittance
Wave number
100%
80%
60%
40%
20%
0%
4000
3500
3000
2500
2000
1500
1000
500
738cm⁻¹
1663cm⁻¹
2850cm⁻¹
2928cm⁻¹
1321cm⁻¹
1063cm⁻¹
1712cm⁻¹
1448cm⁻¹
760cm⁻¹

3z


Transmittance
Wave number
100%
80%
60%
40%
20%
0%
4000
3500
3000
2500
2000
1500
1000
500
2866cm⁻¹
1665cm⁻¹
2956cm⁻¹
1126cm⁻¹
839cm⁻¹
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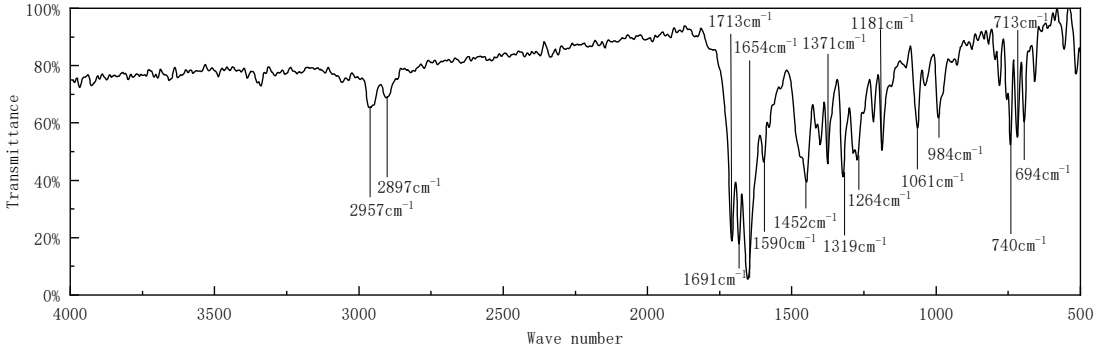
1062cm⁻¹
744cm⁻¹
2925cm⁻¹
1325cm⁻¹
1721cm⁻¹

3aa


Transmittance
Wave number
100%
80%
60%
40%
20%
0%
4000
3500
3000
2500
2000
1500
1000
500
1713cm⁻¹
1654cm⁻¹
1371cm⁻¹
1181cm⁻¹
713cm⁻¹
984cm⁻¹
694cm⁻¹
2897cm⁻¹
1061cm⁻¹
1264cm⁻¹
2957cm⁻¹
1452cm⁻¹
1590cm⁻¹
1319cm⁻¹
740cm⁻¹
1691cm⁻¹