Supporting Information

SYNTHESIS AND CHARACTERIZATION OF PHENYL(1,3,6,8-TETRAAZATRICYCLO[4.3.1.1^{3,8}]UNDECAN-4-YL) METHANONE AND ITS DERIVATIVES

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Contents of Supporting Information

Contents:	**Pages:**
Experimental section	
Identification datas of compounds **7** and **6a-j**	2-4
^{13}C NMR and ^{1}H NMR spectra of compounds **7** and **6a-j**	5-26
Check cif	27-29

Experimental section

General. All reagents and solvents were purchased from J&K Chemical Co. and used without further purification. Melting points were determined on a SGW X-4 micro melting point instrument. ^{1}H and ^{13}C NMR spectra were recorded on Varian 400 or Bruker 500 MHz spectrometer. IR spectra were obtained on a Perkin Elmer FT-IR system. HRMS spectra were obtained by a LTQ Orbitrap Discovery spectrometer from Thermo.

General procedure for the synthesis of compounds 6a-k

1 mmol 2-bromo-1-arylethanone and 3 mmol hexamine (0.42 g) were mixed in 2 mL DMF. The mixture was stirred at 70 ℃ for 1 h. After cooling to room temperature, the mixture was washed twice with CH_2Cl_2, and the combined organic extracts were dried, filtered and concentrated under reduced pressure to give aryl(1,3,6,8-tetraazatricyclo[4.3.1.13,8]undecan-4-yl)methanone.

Procedure for the synthesis of compound 7

1 mmol 2-bromo-1-arylethanone and 3 mmol hexamine (0.42 g) were mixed in 2 mL DMF. The mixture was stirred at 20 ℃ for 1 h. White solid doposited from the mixture. The obtained solid was filtered off and washed 2 times by acetone to give compound 7.

1-phenacyl-3, 5, 7-triaza-1-azoniaadamantane bromide (**7**)

White solid. Mp: 147-149 ℃. NMR (400 MHz, DMSO-*d*6): δ 8.00 (d, *J* = 7.6 Hz, 2H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 2H), 5.43 (t, *J* = 8.4 Hz, 1H), 4.83 (s, 2H), 4.70 (m, 5H), 4.51 (t, *J* = 14 Hz, 2H), 4.23 (d, *J* = 13.2 Hz, 1H), 4.11 (d, *J* = 12.4 Hz, 1H), 3.75 (dd, *J* = 14.8 Hz, *J* = 9.2 Hz, 1H), 3.32 (dd, *J* = 14.4 Hz, *J* = 8 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-*d*6): δ 197.0, 135.5, 133.6, 128.8, 128.7, 72.7, 72.0, 70.5, 68.4, 68.3, 66.0, 57.3.

phenyl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (**6a**)

Yellow solid. Mp: 131-132 ℃. NMR (500 MHz, acetone): δ 8.03 (dt, *J* = 7 Hz, *J* = 1.5 Hz, 2H), 7.58 (tt, *J* = 6 Hz, *J* = 1.5 Hz, 1H), 7.48 (tt, *J* = 6 Hz, *J* = 1 Hz, 2H), 5.00 (t, *J* = 6.5 Hz, 1H), 4.70 (dd, *J* = 11 Hz, *J* = 2 Hz, 1H), 4.61 (dq, *J* = 11.5 Hz, *J* = 1 Hz, 1H), 4.56 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.33 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.27 (s, 2H), 4.13 (d, *J* = 11 Hz, 1H), 4.00 (d, *J* = 11.5 Hz, 1H), 3.82 (d, *J* = 11.5 Hz, 1H), 3.74 (d, *J* = 11.5 Hz, 1H), 3.62 (ddd, *J* = 12.5 Hz, *J* = 6 Hz, *J* = 1 Hz, 1H), 3.47 (dd, *J* = 12.5 Hz, *J* = 7 Hz, 1H). ^{13}C NMR (125 MHz, acetone): δ 198.7, 137.7, 133.6, 129.7, 129.2, 76.5, 75.9, 73.5, 72.1, 70.3, 68.2, 58.3. IR (KBr, cm^{-1}): 2908, 1675, 1446, 1257, 1146, 1009, 907, 810, 734, 690. HRMS (ESI-Orbitrap) *m/z*: $[M + H]^+$ Calcd for $C_{14}H_{18}N_4O+H^+$ 259.15534; Found 259.15521.

p-tolyl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (**6b**)

Yellow oil. NMR (500 MHz, acetone): δ 7.92 (d, *J* = 7 Hz, 2H), 7.29 (d, *J* = 6.5 Hz, 2H), 4.96 (t, *J* = 6.5 Hz, 1H), 4.69 (dd, *J* = 11 Hz, *J* = 2 Hz, 1H), 4.60 (dq, *J* = 11.5 Hz, *J* = 1 Hz, 1H), 4.55 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.32 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.27 (s, 2H), 4.12 (d, *J* = 11 Hz, 1H), 4.00 (d, *J* = 11.5 Hz, 1H), 3.84 (d, *J* = 12 Hz, 1H), 3.73 (d, *J* = 11 Hz, 1H), 3.60 (dd, *J* = 12 Hz, *J* = 6 Hz, 1H), 3.46 (dd, *J* = 12.5 Hz, *J* = 7.5 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (125 MHz, acetone): δ 198.3, 144.3, 135.2, 129.9, 129.8, 76.4, 75.9, 73.6, 72.1, 70.1, 68.2, 58.4, 21.5. IR (KBr, cm^{-1}): 2908, 1669, 1607, 1457, 1382, 1235, 1150, 1041, 1006, 974, 904, 820, 795, 768, 676, 643, 597, 490. HRMS (ESI-Orbitrap) *m/z*: $[M + H]^+$ Calcd for $C_{15}H_{20}N_4O+H^+$ 273.17099; Found 273.17096.

(3-methoxyphenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (**6c**)

Yellow oil. NMR (500 MHz, acetone): δ 7.61 (dt, *J* = 6.5 Hz, *J* = 1 Hz, 1H), 7.53 (dd, *J* = 2 Hz, *J* = 1.5 Hz, 1H), 7.40 (t, *J* = 6.5 Hz, 1H), 7.15 (ddd, *J* = 6.5 Hz, *J* = 2 Hz, *J* = 0.5 Hz, 1H), 4.98 (t, *J* =

6.5 Hz, 1H), 4.69 (dd, *J* = 11.5 Hz, *J* = 1.5 Hz, 1H), 4.60 (dq, *J* = 11.5 Hz, *J* = 1 Hz, 1H), 4.56 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.34 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.27 (s, 2H), 4.13 (d, *J* = 11.5 Hz, 1H), 4.00 (d, *J* = 11.5 Hz, 1H), 3.85 (m, 4H), 3.73 (d, *J* = 11.5 Hz, 1H), 3.59 (ddd, *J* = 12 Hz, *J* = 6 Hz, *J* = 0.5 Hz, 1H), 3.48 (dd, *J* = 12 Hz, *J* = 7 Hz, 1H). ^{13}C NMR (125 MHz, acetone): δ 198.5, 160.7, 139.2, 130.3, 122.1, 119.4, 114.5, 76.4, 75.9, 73.5, 72.0, 70.4, 68.2, 58.4, 55.7. IR (KBr, cm^{-1}): 2906, 1617, 1453, 1387, 1258, 1150, 1046, 1008, 961, 777, 619, 480. HRMS (ESI-Orbitrap) *m/z*: [M + H]$^+$ Calcd for $C_{15}H_{20}N_4O_2$+H$^+$ 289.16590; Found 289.16595.

(4-methoxyphenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (**6d**)

Yellow needles. Mp: 152-153 ℃. NMR (500 MHz, acetone): δ 8.02 (dt, *J* = 8 Hz, *J* = 2 Hz, 2H), 6.99 (dt, *J* = 8 Hz, *J* = 2 Hz, 2H), 4.93 (t, *J* = 6.5 Hz, 1H), 4.69 (dd, *J* = 11 Hz, *J* = 1.5 Hz, 1H), 4.60 (dq, *J* = 11.5 Hz, *J* = 1 Hz, 1H), 4.55 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.31 (dd, *J* = 12 Hz, *J* = 2 Hz, 1H), 4.26 (s, 2H), 4.12 (d, *J* = 11.5 Hz, 1H), 3.99 (d, *J* = 11 Hz, 1H), 3.88 (s, 3H), 3.84 (d, *J* = 11.5 Hz, 1H), 3.73 (d, *J* = 11 Hz, 1H), 3.62 (dd, *J* = 12.5 Hz, *J* = 6 Hz, 1H), 3.44 (dd, *J* = 12.5 Hz, *J* = 7.5 Hz, 1H). ^{13}C NMR (125 MHz, acetone): δ 197.1, 164.3, 132.1, 130.4, 114.4, 76.4, 75.8, 73.6, 72.2, 70.0, 68.2, 58.4, 55.9. IR (KBr, cm^{-1}): 2903, 1669, 1598, 1508, 1457, 1315, 1259, 1234, 1172, 1147, 1023, 1007, 973, 906, 837, 795, 676, 644, 506. HRMS (ESI-Orbitrap) *m/z*: [M + H]$^+$ Calcd for $C_{15}H_{20}N_4O_2$+H$^+$ 289.16590; Found 289.16586.

[1,1'-biphenyl]-4-yl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (**6e**)

Yellow solid. Mp: 168 ℃. NMR (500 MHz, acetone): δ 8.12 (dt, *J* = 7.5 Hz, *J* = 1.5 Hz, 2H), 7.77 (dt, *J* = 7 Hz, *J* = 1.5 Hz, 2H), 7.73 (dt, *J* = 7 Hz, *J* = 1 Hz, 2H), 7.50 (t, *J* = 6.5 Hz, 2H), 7.42 (td, *J* = 6.5 Hz, *J* = 1 Hz, 1H), 5.03 (t, *J* = 6.5 Hz, 1H), 4.72 (dd, *J* = 11 Hz, *J* = 2 Hz, 1H), 4.62 (dq, *J* = 11.5 Hz, *J* = 1 Hz, 1H), 4.57 (dd, *J* = 11 Hz, *J* = 1.5 Hz, 1H), 4.35 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.28 (s, 2H), 4.17 (d, *J* = 11 Hz, 1H), 4.02 (d, *J* = 11.5 Hz, 1H), 3.84 (d, *J* = 12 Hz, 1H), 3.76 (d, *J* = 11 Hz, 1H), 3.67 (dd, *J* = 12.5 Hz, *J* = 5.5 Hz, 1H), 3.49 (dd, *J* = 12 Hz, *J* = 7 Hz, 1H). ^{13}C NMR (125 MHz, acetone): δ 198.3, 146.0, 140.7, 136.5, 130.5, 129.9, 129.1, 128.0, 127.7, 76.5, 75.9, 73.6, 72.2, 70.3, 68.3, 58.2. IR (KBr, cm^{-1}): 2904, 1673, 1601, 1446, 1382, 1258, 1240, 1146, 1007, 975, 904, 767, 751, 698, 661, 494. HRMS (ESI-Orbitrap) *m/z*: [M + H]$^+$ Calcd for $C_{20}H_{22}N_4O$+H$^+$ 335.18664; Found 335.18671.

(3-fluorophenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (**6f**)

Yellow solid. Mp: 134-135 ℃. NMR (500 MHz, acetone): δ 7.86 (d, *J* = 6.5 Hz, 1H), 7.73 (dq, *J* = 8 Hz, *J* = 1 Hz, 1H), 7.54 (td, *J* = 7 Hz, *J* = 5 Hz, 1H), 7.37 (td, *J* = 7.5 Hz, *J* = 2.5 Hz, 1H), 4.99 (t, *J* = 6.5 Hz, 1H), 4.71 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.61 (d, *J* = 11.5 Hz, 1H), 4.56 (dd, *J* = 11 Hz, *J* = 1.5 Hz, 1H), 4.34 (dd, *J* = 11.5 Hz, *J* = 1.5 Hz, 1H), 4.27 (s, 2H), 4.15 (d, *J* = 11 Hz, 1H), 4.00 (d, *J* = 11.5 Hz, 1H), 3.77 (d, *J* = 11.5 Hz, 1H), 3.73 (d, *J* = 11.5 Hz, 1H), 3.64 (dd, *J* = 12.5 Hz, *J* = 6 Hz, 1H), 3.48 (dd, *J* = 12.5 Hz, *J* = 7.5 Hz, 1H). ^{13}C NMR (125 MHz, acetone): δ 197.7, 197.7, 164.3, 162.7, 140.1, 140.0, 131.3, 131.2, 125.8, 125.8, 120.4, 120.3, 116.2, 116.1, 76.3, 75.9, 73.5, 72.1, 70.6, 68.3, 58.0. IR (KBr, cm^{-1}): 2908, 1677, 1586, 1480, 1438, 1385, 1300, 1247, 1168, 1149, 1039, 960, 845, 764, 677, 629, 556, 475. HRMS (ESI-Orbitrap) *m/z*: [M + H]$^+$ Calcd for $C_{14}H_{17}FN_4O$+H$^+$ 277.14592; Found 277.14590.

(4-chlorophenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (**6g**)

Yellow oil. NMR (500 MHz, acetone): δ 8.04 (d, *J* = 7 Hz, 2H), 7.52 (d, *J* = 7 Hz, 2H), 4.97 (t, *J* = 6 Hz, 1H), 4.70 (d, *J* = 11.5 Hz, 1H), 4.61 (d, *J* = 11 Hz, 1H), 4.56 (d, *J* = 11 Hz, 1H), 4.32 (d, *J* = 11.5 Hz, 1H), 4.27 (s, 2H), 4.14 (d, *J* = 11 Hz, 1H), 3.99 (d, *J* = 11.5 Hz, 1H), 3.73 (t, *J* = 10 Hz, 2H), 3.65 (dd, *J* = 12.5 Hz, *J* = 5.5 Hz, 1H), 3.46 (dd, *J* = 12.5 Hz, *J* = 7.5 Hz, 1H). ^{13}C NMR (125 MHz, acetone): δ 197.7, 139.2, 136.3, 131.6, 129.4, 76.3, 75.8, 73.4, 72.2, 70.4, 68.3, 57.9. IR (KBr, cm^{-1}): 2920, 1681, 1617, 1589, 1452, 1400, 1255, 1152, 1092, 1010, 961, 909, 875, 842, 783, 635, 476. HRMS (ESI-Orbitrap) *m/z*: [M + H]$^+$ Calcd for $C_{14}H_{17}ClN_4O$+H$^+$ 293.116367; Found 293.11636.

1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl(4-(trifluoromethyl)phenyl)methanone (**6h**)

Yellow solid. Mp: 94 ℃. NMR (500 MHz, acetone): δ 8.21 (d, *J* = 7 Hz, 2H), 7.83 (d, *J* = 6.5 Hz, 2H), 5.04 (t, *J* = 6.5 Hz, 1H), 4.71 (dd, *J* = 11 Hz, *J* = 2 Hz, 1H), 4.62 (dq, *J* = 11.5 Hz, *J* = 1 Hz, 1H), 4.57 (dd, *J* = 11 Hz, *J* = 2 Hz, 1H), 4.32 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.27 (s, 2H), 4.16 (d, *J* = 11.5 Hz, 1H), 4.00 (d, *J* = 11.5 Hz, 1H), 3.73 (m, 3H), 3.48 (dd, *J* = 12.5 Hz, *J* = 7 Hz, 1H). ^{13}C NMR (125 MHz, acetone): δ 198.3, 141.1, 134.1, 133.9, 130.5, 126.2, 76.4, 75.9, 73.4, 72.2, 70.8, 68.3, 57.7. IR (KBr, cm^{-1}): 2912, 1687, 1458, 1411, 1327, 1260, 1132, 1068, 1040, 1012, 978, 960, 900, 858, 788, 636, 480. HRMS (ESI-Orbitrap) *m/z*: [M + H]$^+$ Calcd for $C_{15}H_{17}F_3N_4O+H^+$ 327.14272; Found 327.14273.

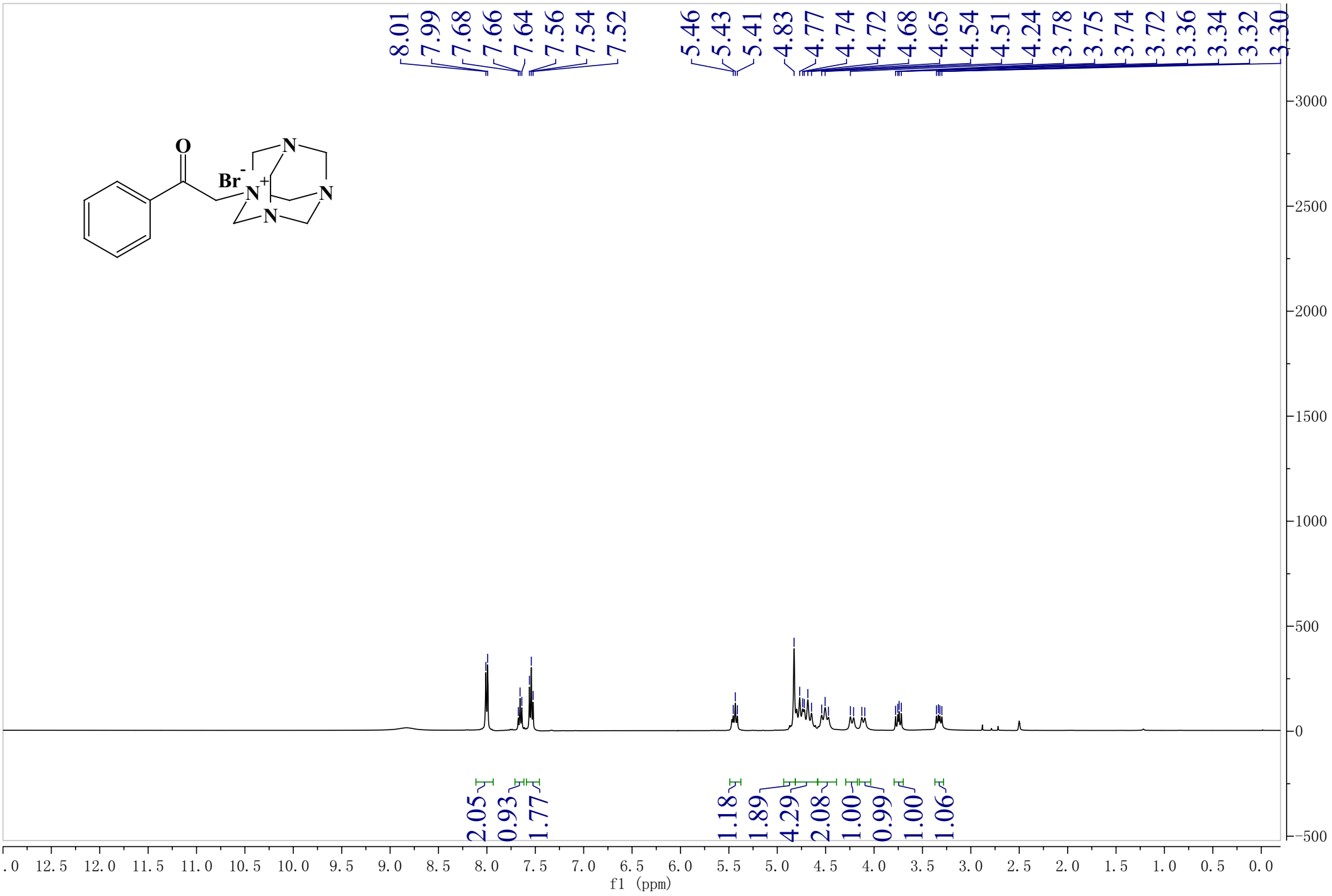
thiophen-2-yl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (**6i**)

Yellow solid. Mp: 135-136 ℃. NMR (500 MHz, acetone): δ 7.95 (dd, *J* = 3.5 Hz, *J* = 1 Hz, 1H), 7.82 (dd, *J* = 4 Hz, *J* = 1 Hz, 1H), 7.17 (dd, *J* = 4.5 Hz, *J* = 3.5 Hz, 1H), 4.75 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.66 (t, *J* = 6.5 Hz, 1H), 4.61 (dq, *J* = 11 Hz, *J* = 1 Hz, 1H), 4.56 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.41 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.29 (s, 2H), 4.08 (d, *J* = 11 Hz, 1H), 3.98 (d, *J* = 11 Hz, 1H), 3.79 (d, *J* = 12 Hz, 1H), 3.73 (d, *J* = 11.5 Hz, 1H), 3.65 (ddd, *J* = 12 Hz, *J* = 5.5 Hz, *J* = 0.5 Hz, 1H), 3.49 (dd, *J* = 12.5 Hz, *J* = 7.5 Hz, 1H). ^{13}C NMR (125 MHz, acetone): δ 192.4, 143.0, 135.1, 134.3, 128.5, 76.2, 76.0, 73.3, 72.8, 72.0, 69.0, 58.3. IR (KBr, cm^{-1}): 2859, 1639, 1408, 1248, 1012, 746, 626, 485. HRMS (ESI-Orbitrap) *m/z*: [M + H]$^+$ Calcd for $C_{12}H_{16}N_4OS+H^+$ 265.11176; Found 265.11179.

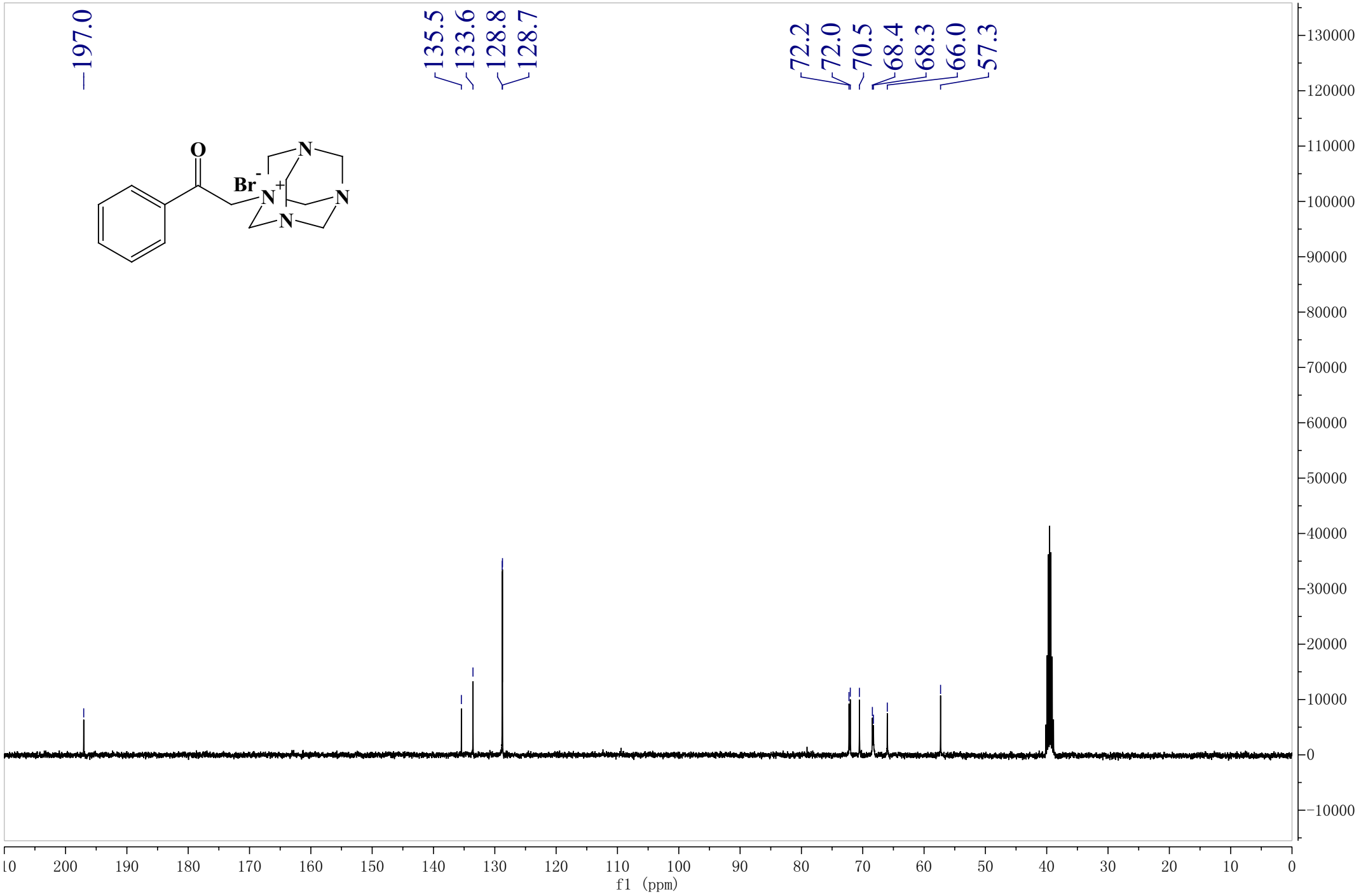
naphthalen-2-yl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (**6j**)

Yellow solid. Mp: 101 ℃. NMR (500 MHz, acetone): δ 8.67 (s, 1H), 8.06 (dq, *J* = 7 Hz, *J* = 1 Hz, 2H), 7.97 (d, *J* = 7.5 Hz, 2H), 7.65 (td, *J* = 6 Hz, *J* = 1.5 Hz, 1H), 7.60 (td, *J* = 6 Hz, *J* = 1 Hz, 1H), 5.17 (t, *J* = 7 Hz, 1H), 4.74 (dd, *J* = 11 Hz, *J* = 2 Hz, 1H), 4.64 (dq, *J* = 11 Hz, *J* = 1 Hz, 1H), 4.58 (dd, *J* = 11 Hz, *J* = 1.5 Hz, 1H), 4.35 (dd, *J* = 11.5 Hz, *J* = 2 Hz, 1H), 4.29 (s, 2H), 4.21 (d, *J* = 11.5 Hz, 1H), 4.04 (d, *J* = 11.5 Hz, 1H), 3.89 (d, *J* = 11.5 Hz, 1H), 3.77 (d, *J* = 11.5 Hz, 1H), 3.67 (ddd, *J* = 12.5 Hz, *J* = 6 Hz, *J* = 1 Hz, 1H), 3.56 (dd, *J* = 12.5 Hz, *J* = 7.5 Hz, 1H). ^{13}C NMR (125 MHz, acetone): δ 198.7, 136.4, 135.1, 133.6, 131.3, 130.5, 129.3, 128.9, 128.6, 127.6, 125.6, 76.5, 75.9, 73.6, 72.2, 70.4, 68.3, 58.4. IR (KBr, cm^{-1}): 2904, 1619, 1386, 1257, 1150, 1009, 620, 486. HRMS (ESI-Orbitrap) *m/z*: [M + H]$^+$ Calcd for $C_{18}H_{20}N_4O+H^+$ 309.17099; Found 309.17102.

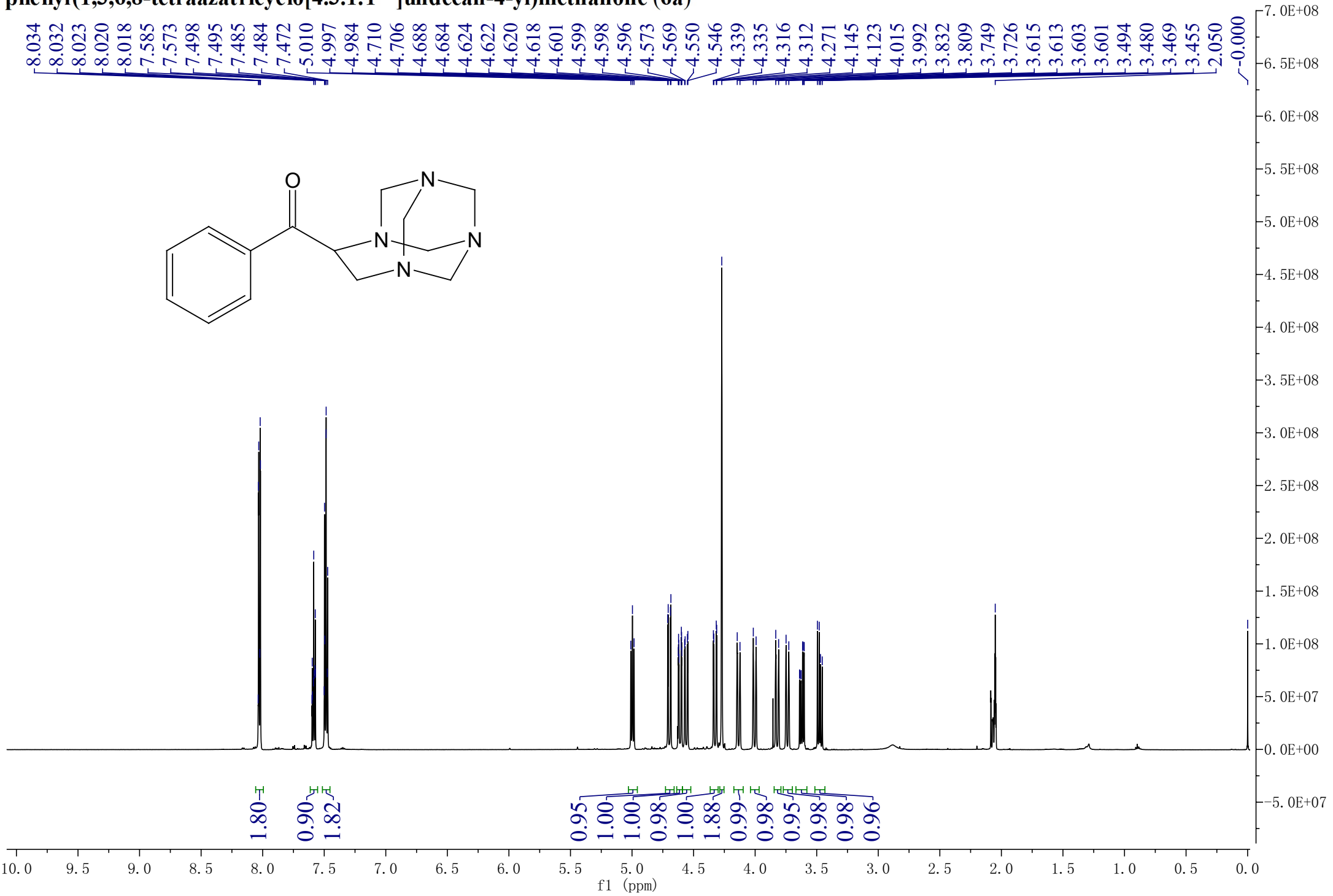
1-phenacyl-3,5,7-triaza-1-azoniaadamantane bromide (7)



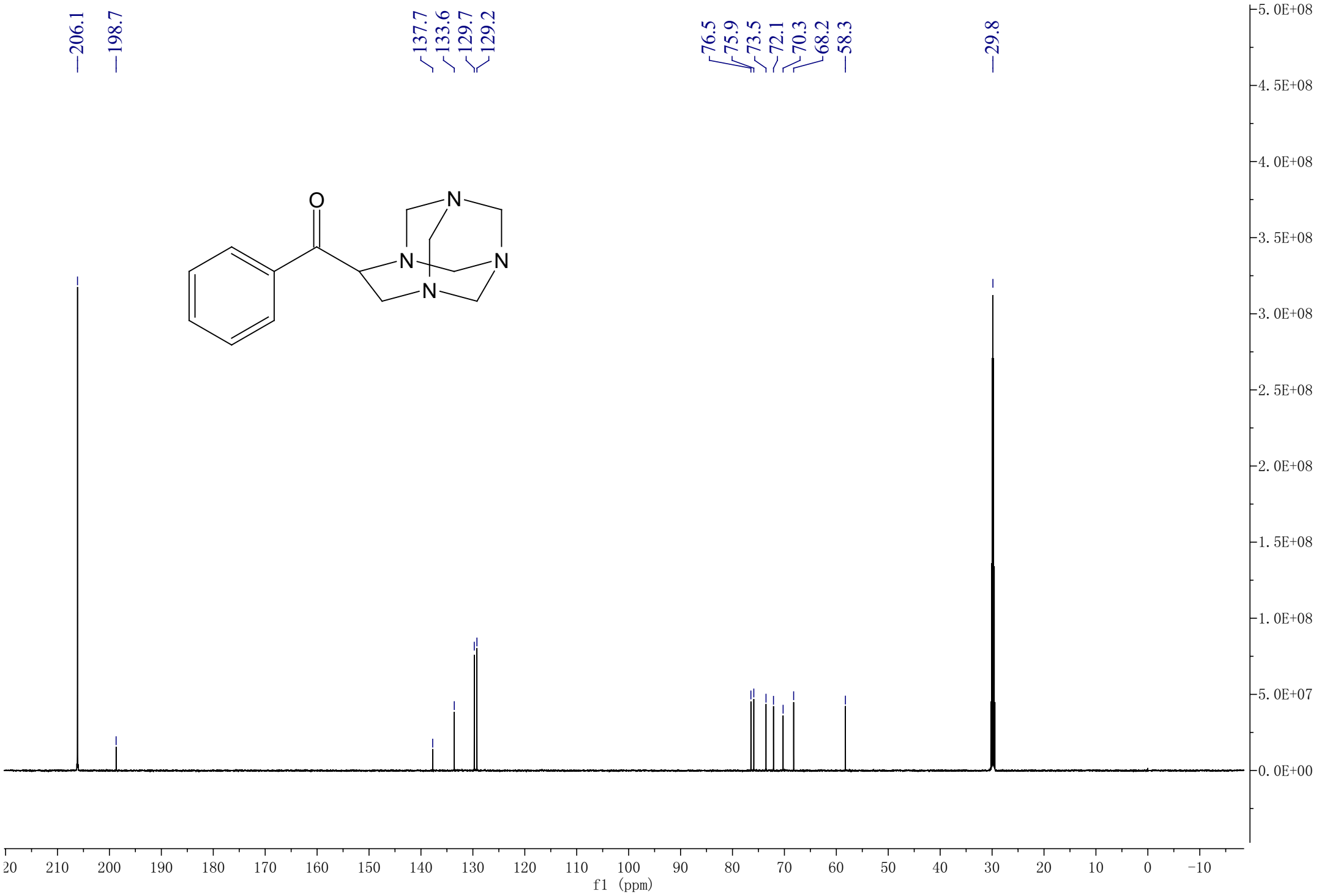
1-phenacyl-3,5,7-triaza-1-azoniaadamantane bromide (7)



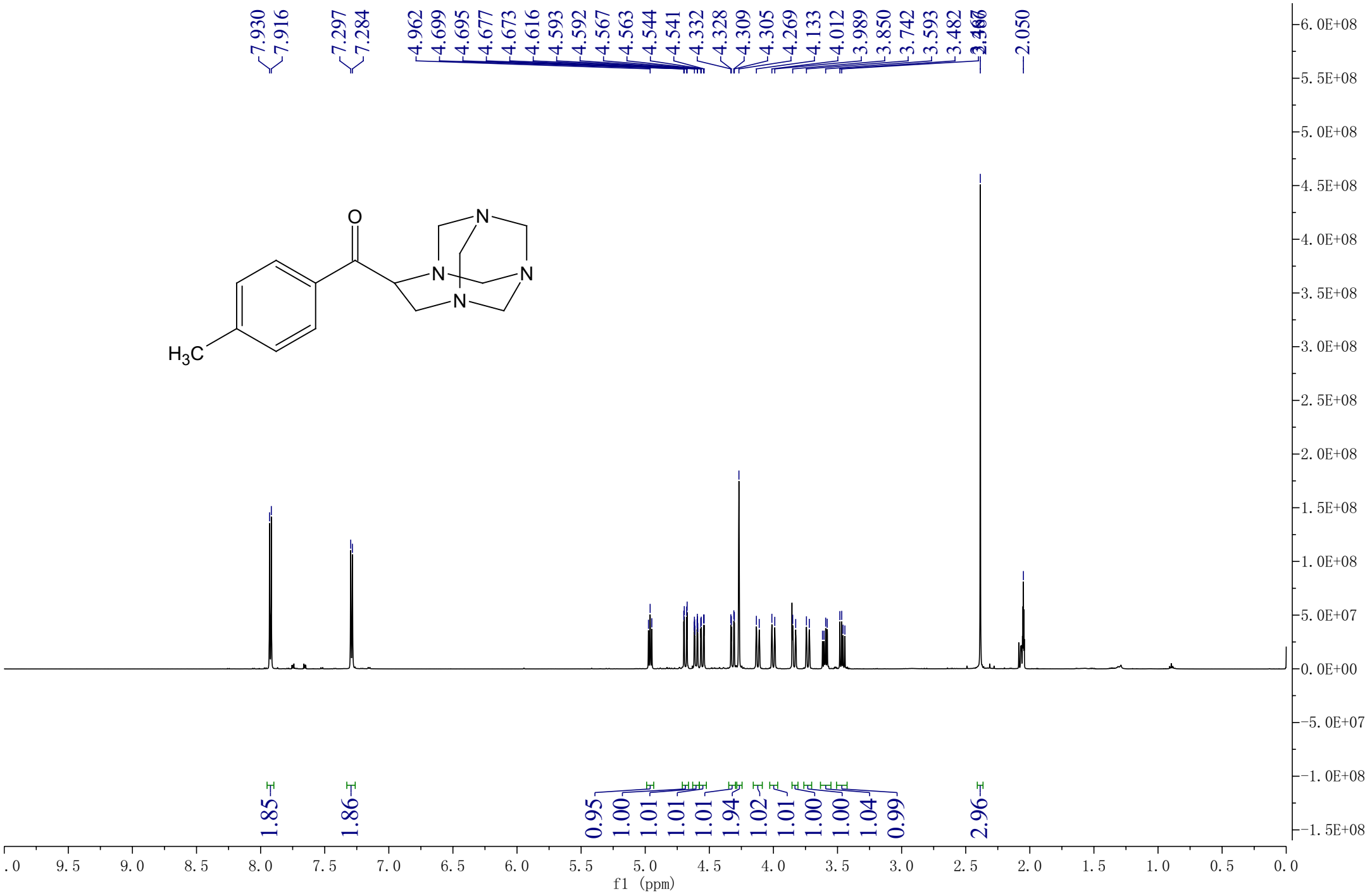
phenyl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6a)



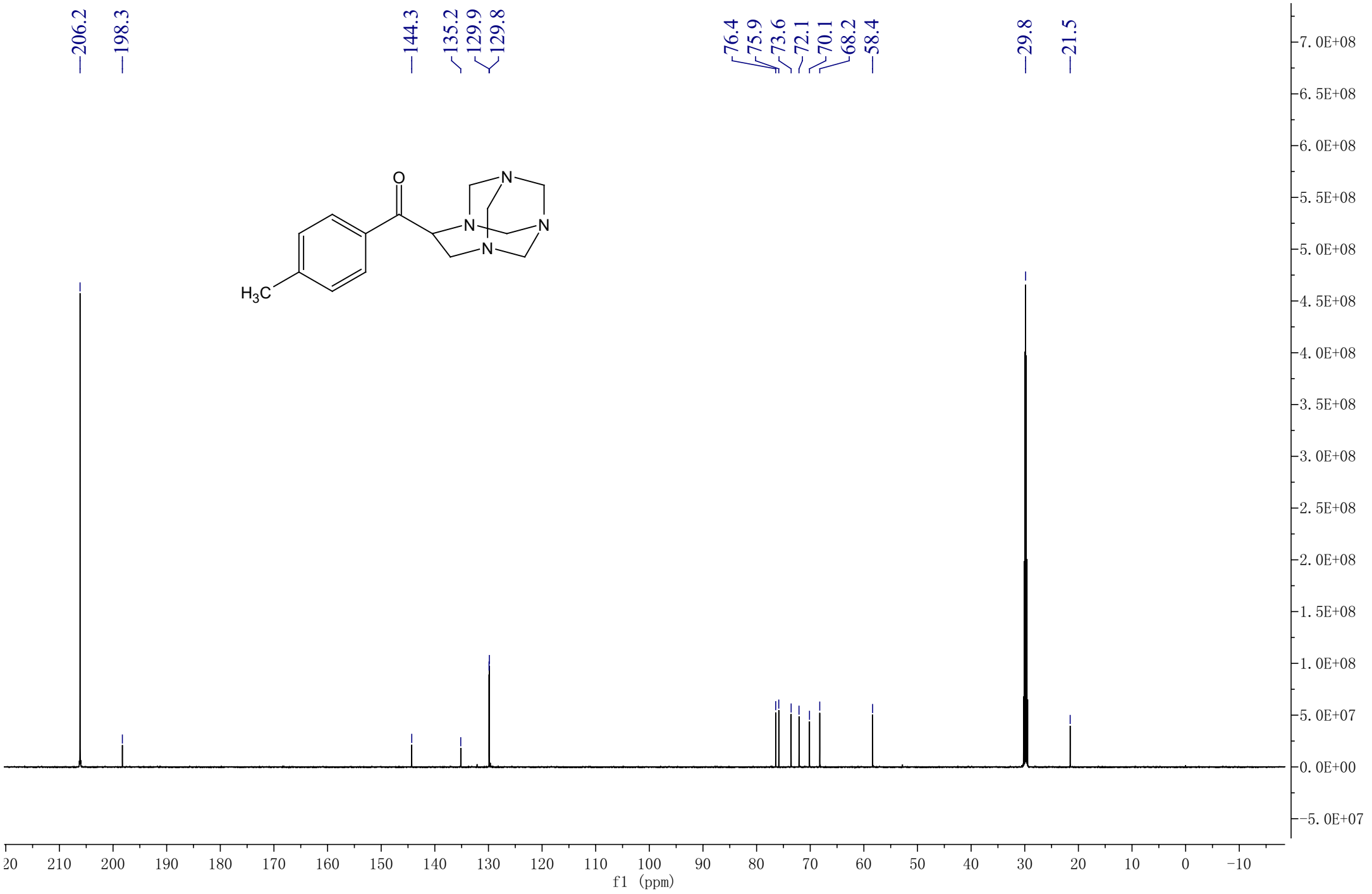
phenyl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6a)



p-tolyl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6b)



p-tolyl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6b)



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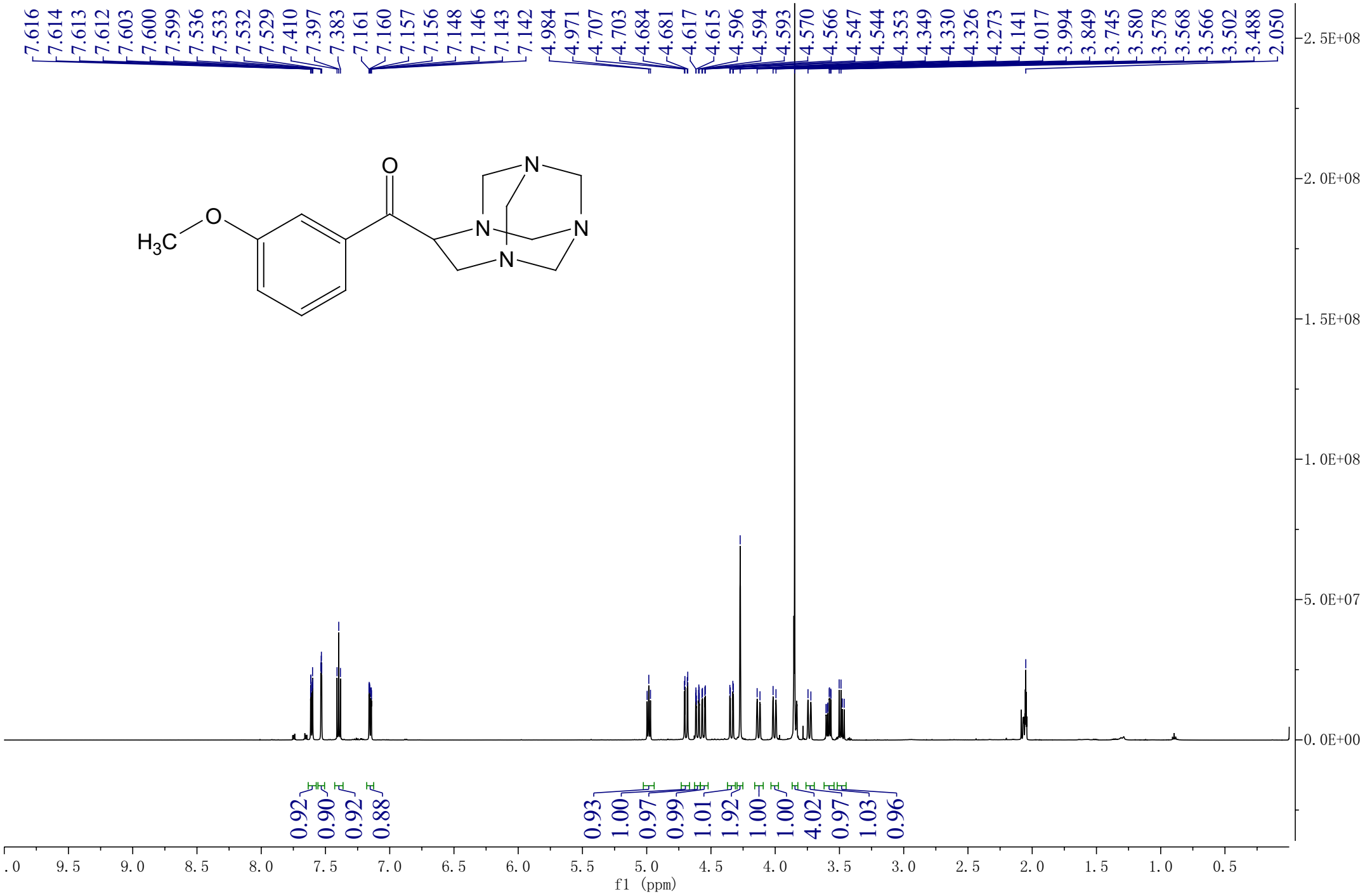
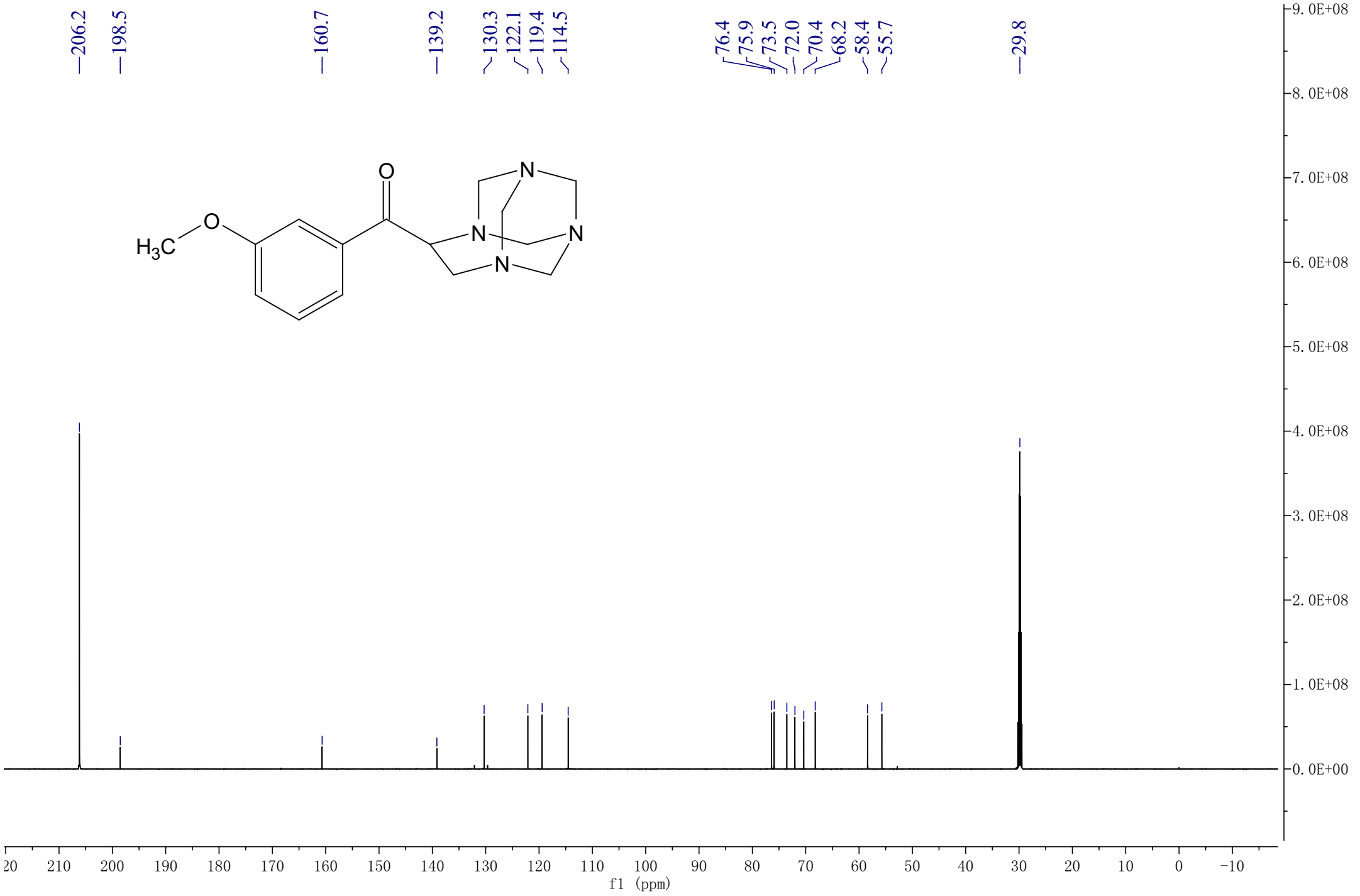
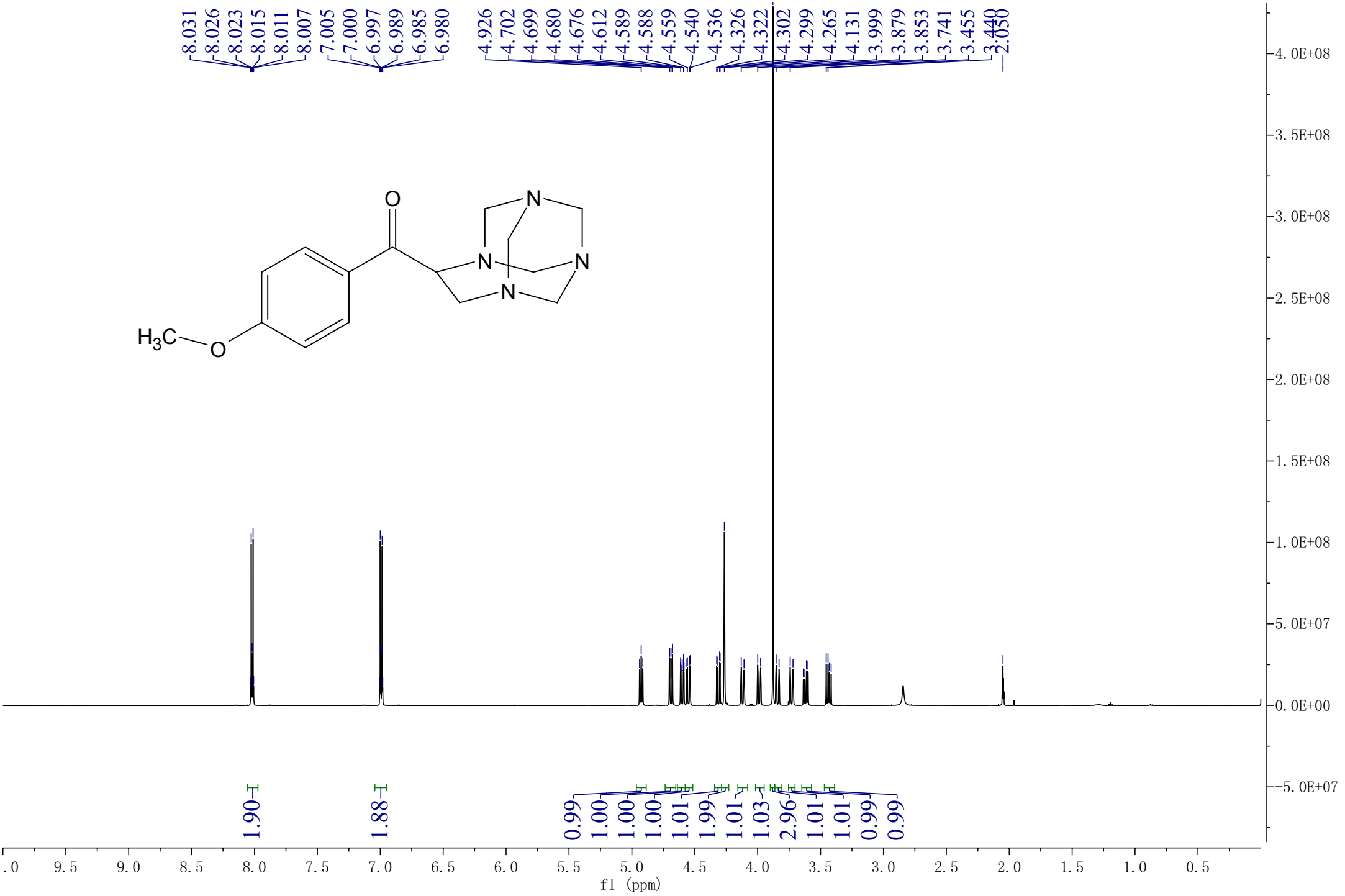


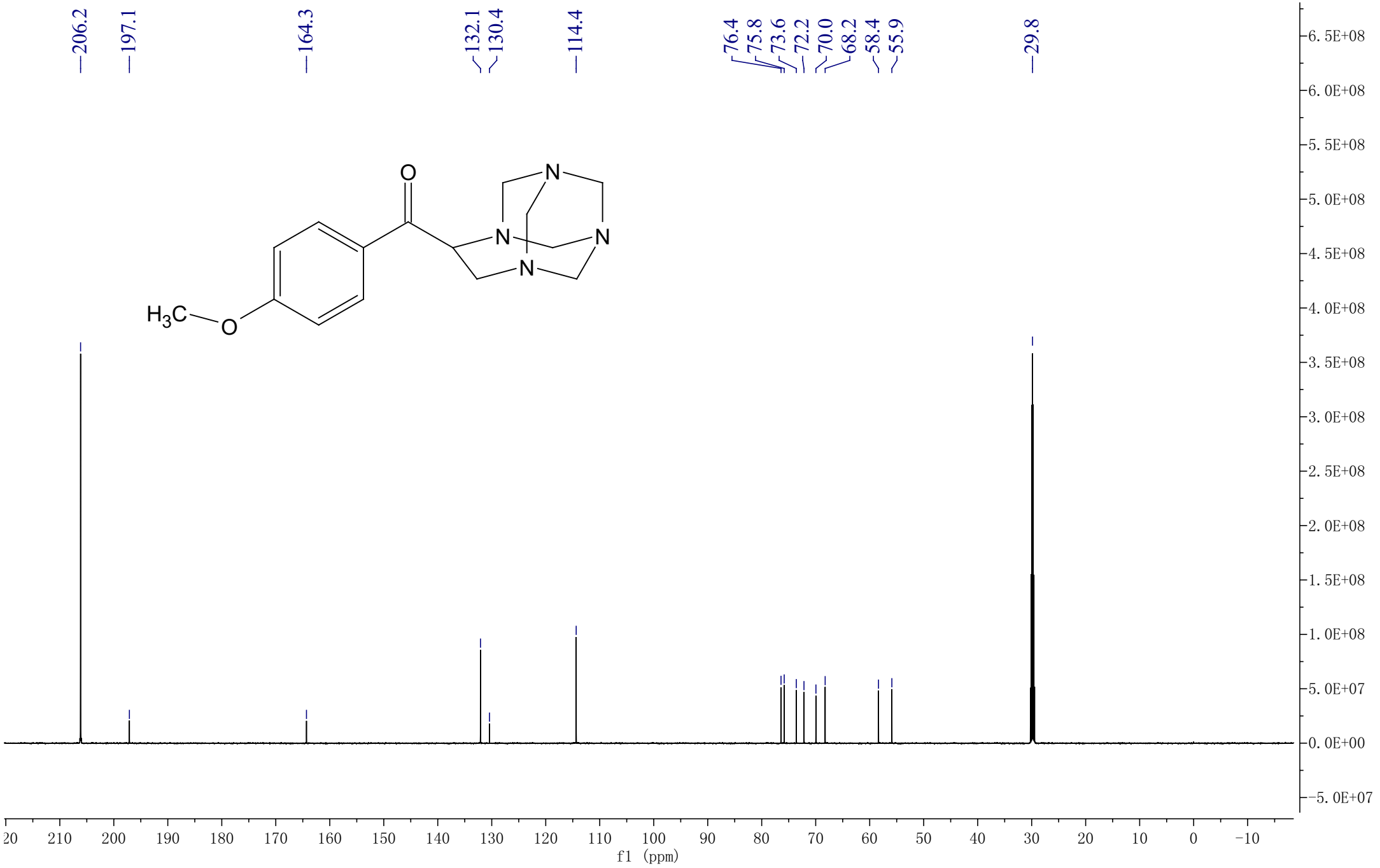
(3-methoxyphenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6c)



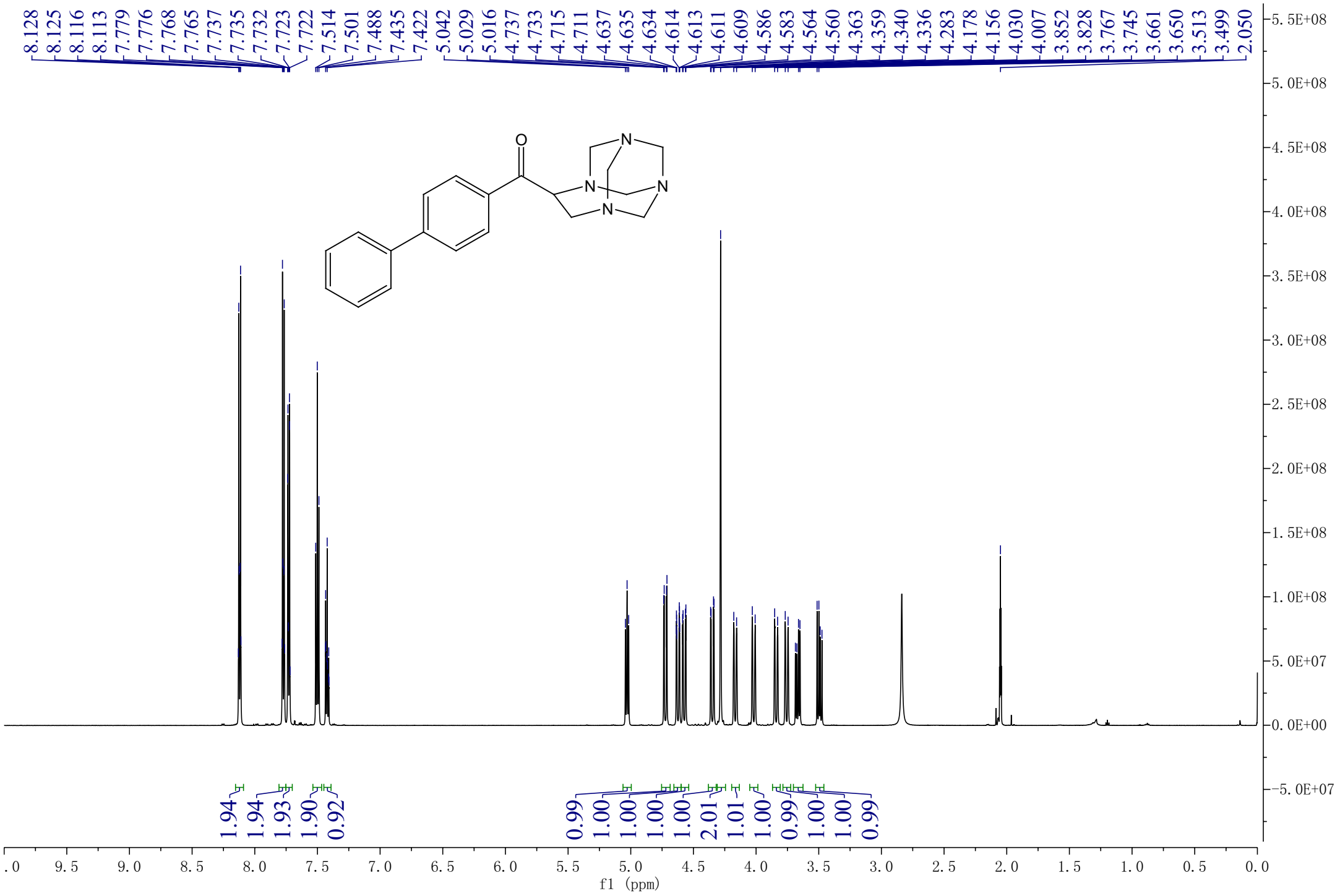
(4-methoxyphenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6d)



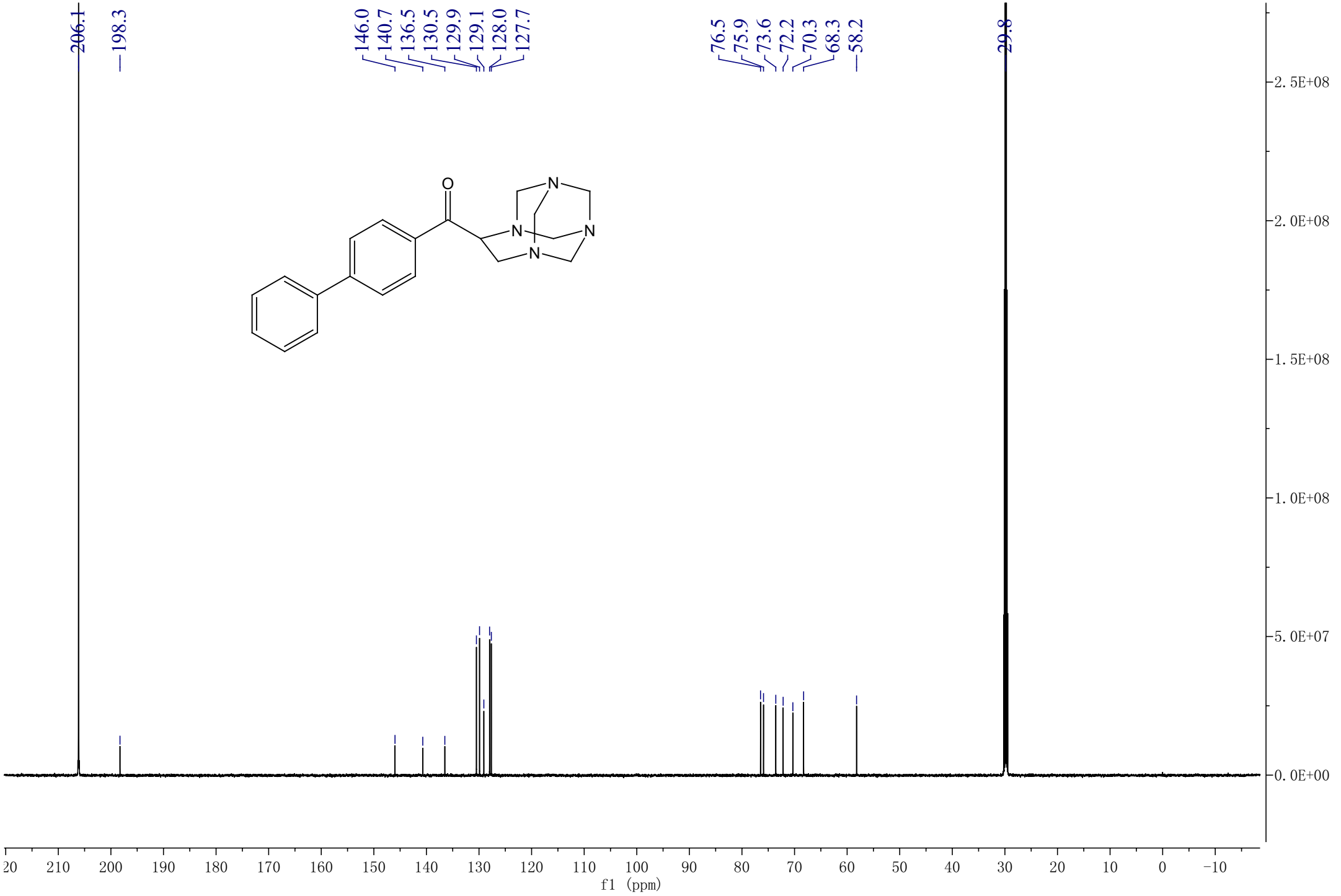
(4-methoxyphenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6d)



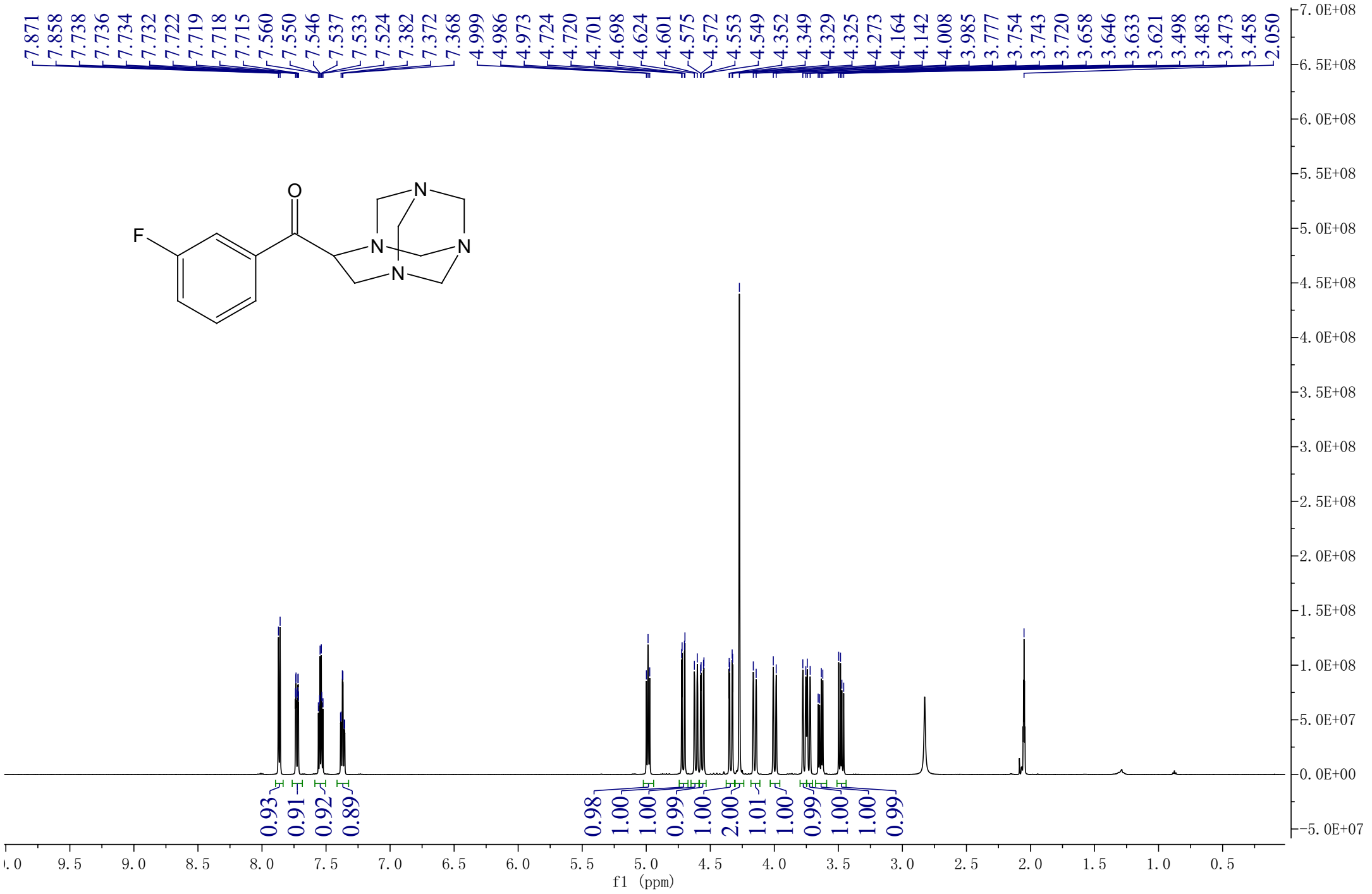
[1,1'-biphenyl]-4-yl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6e)



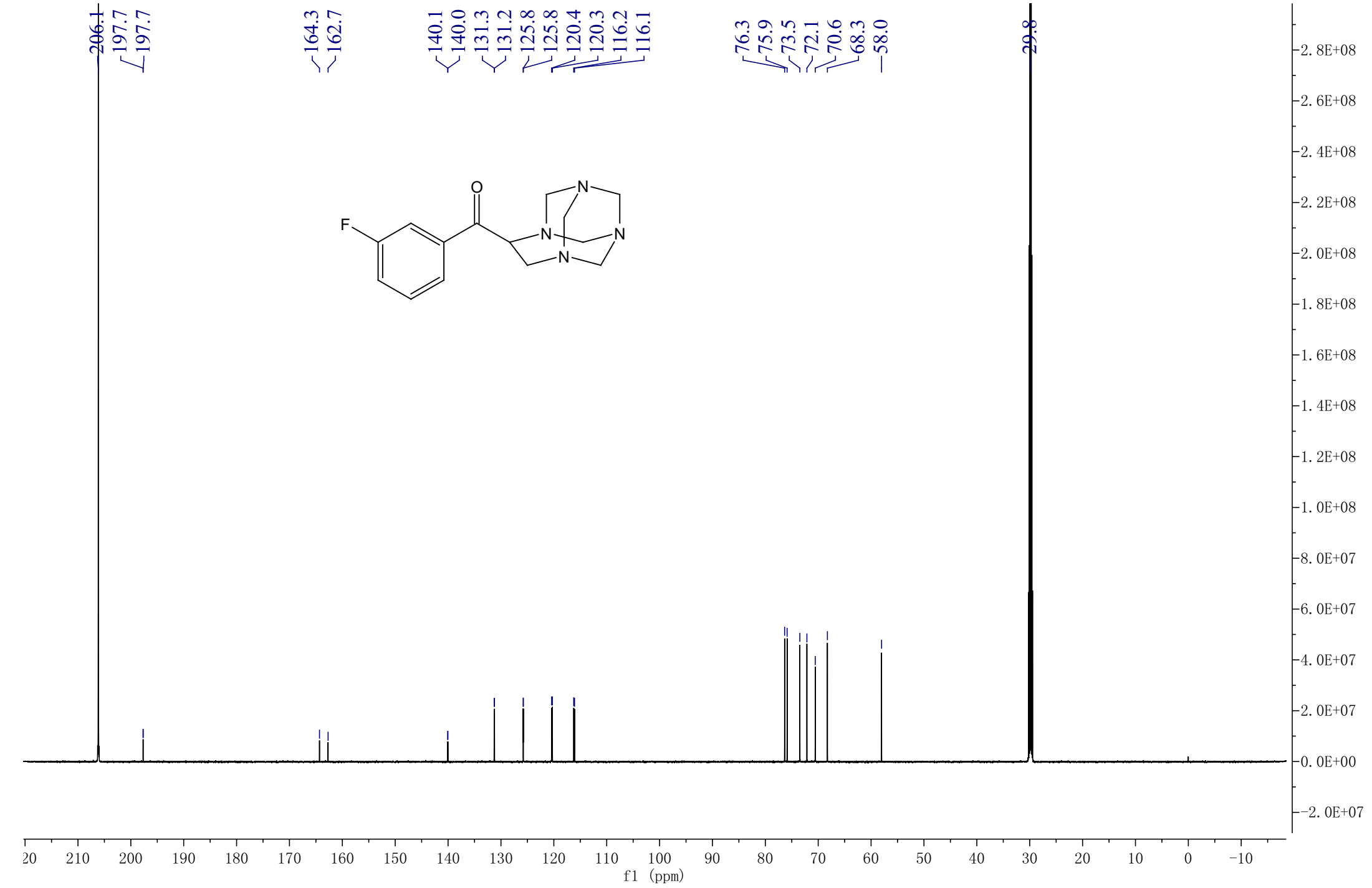
[1,1'-biphenyl]-4-yl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6e)



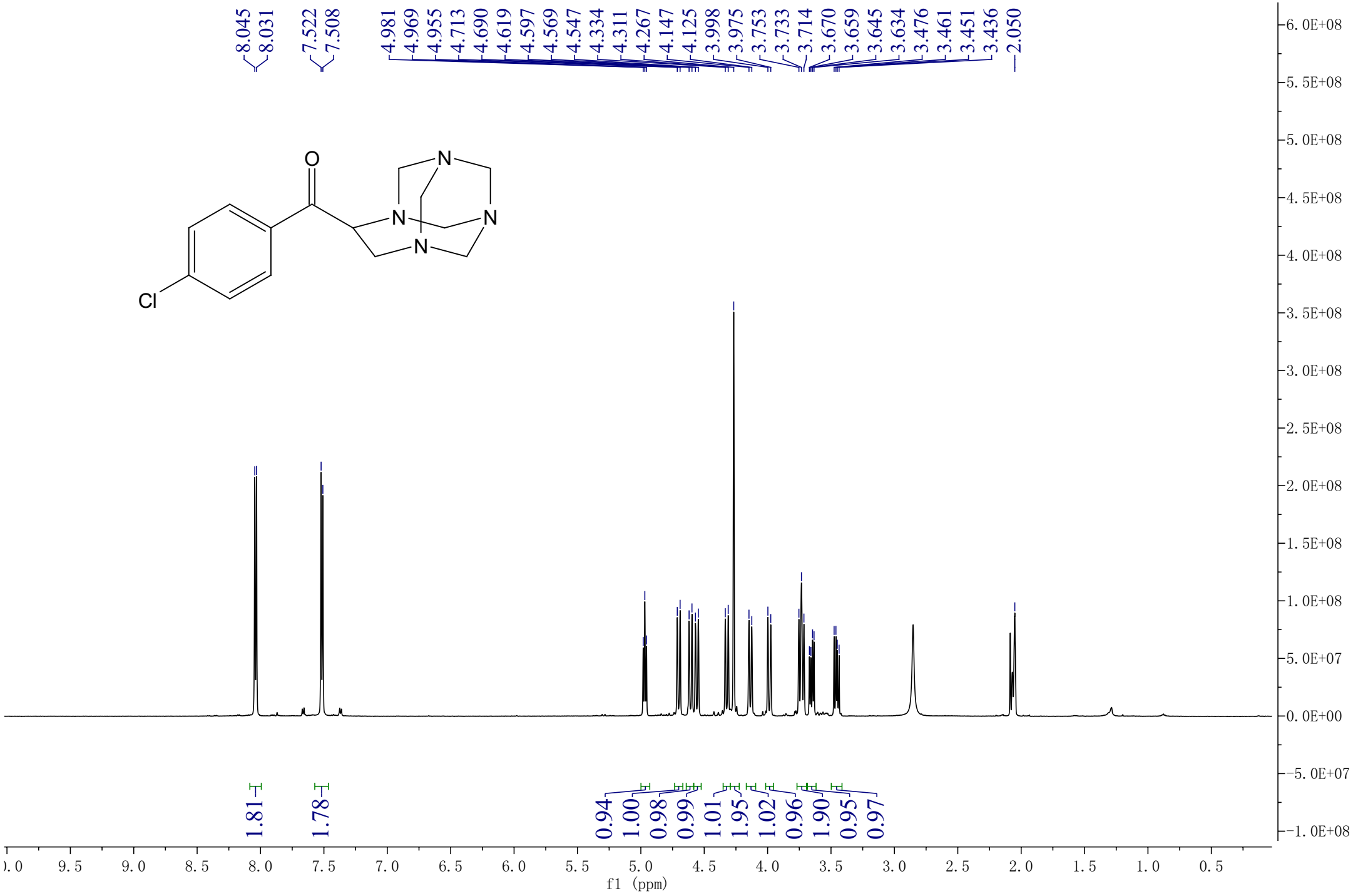
(3-fluorophenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6f)



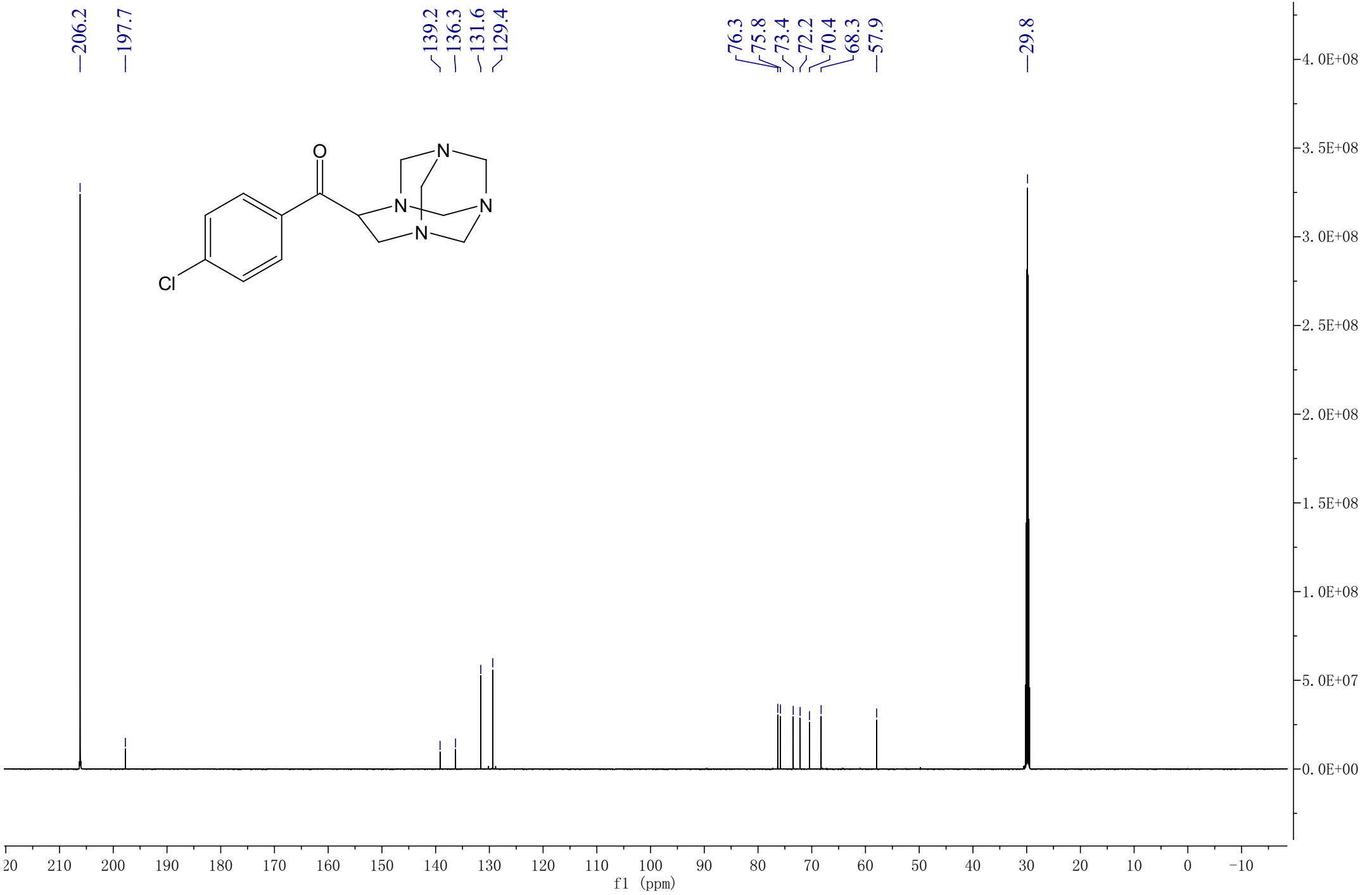
(3-fluorophenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6f)



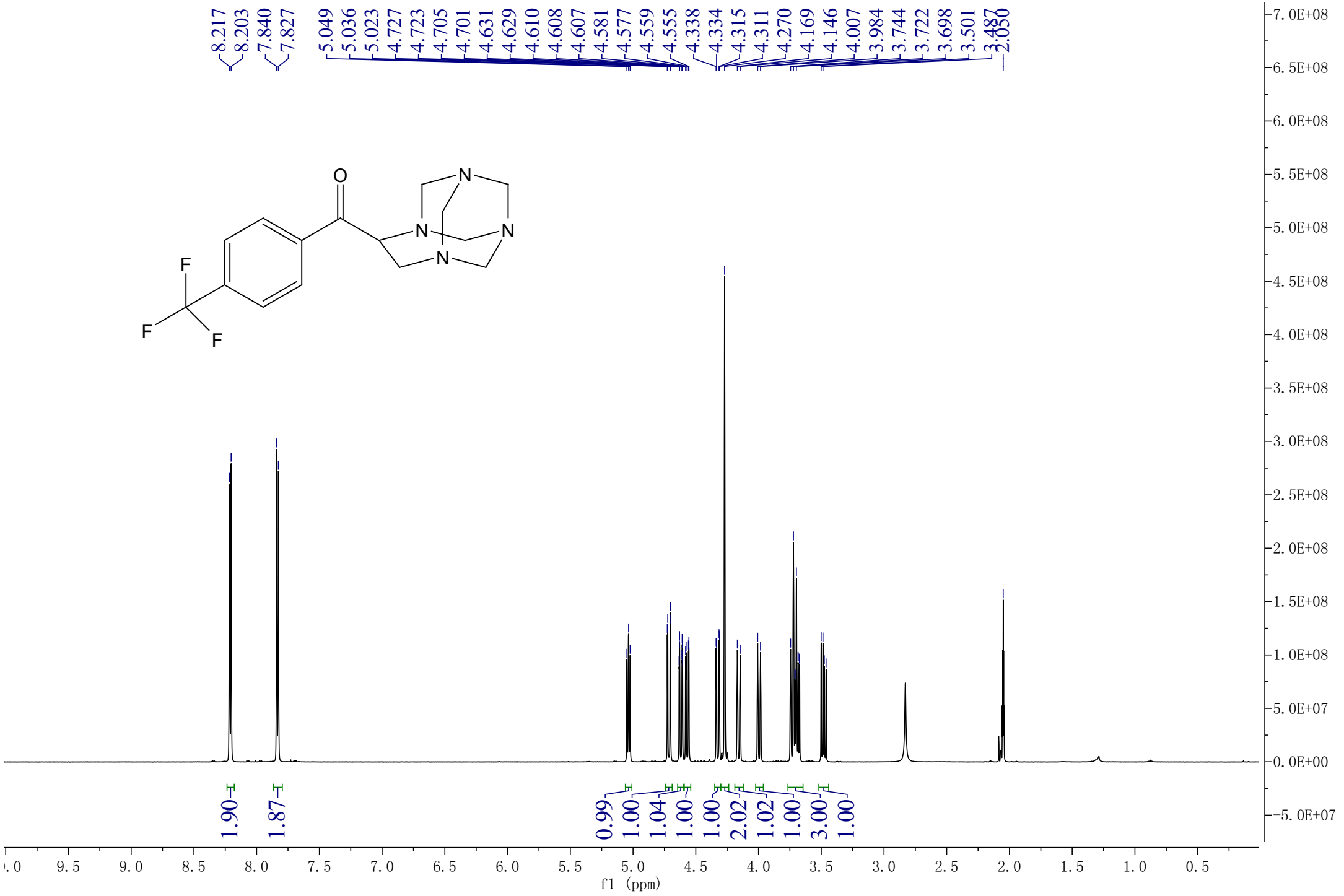
(4-chlorophenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6g)



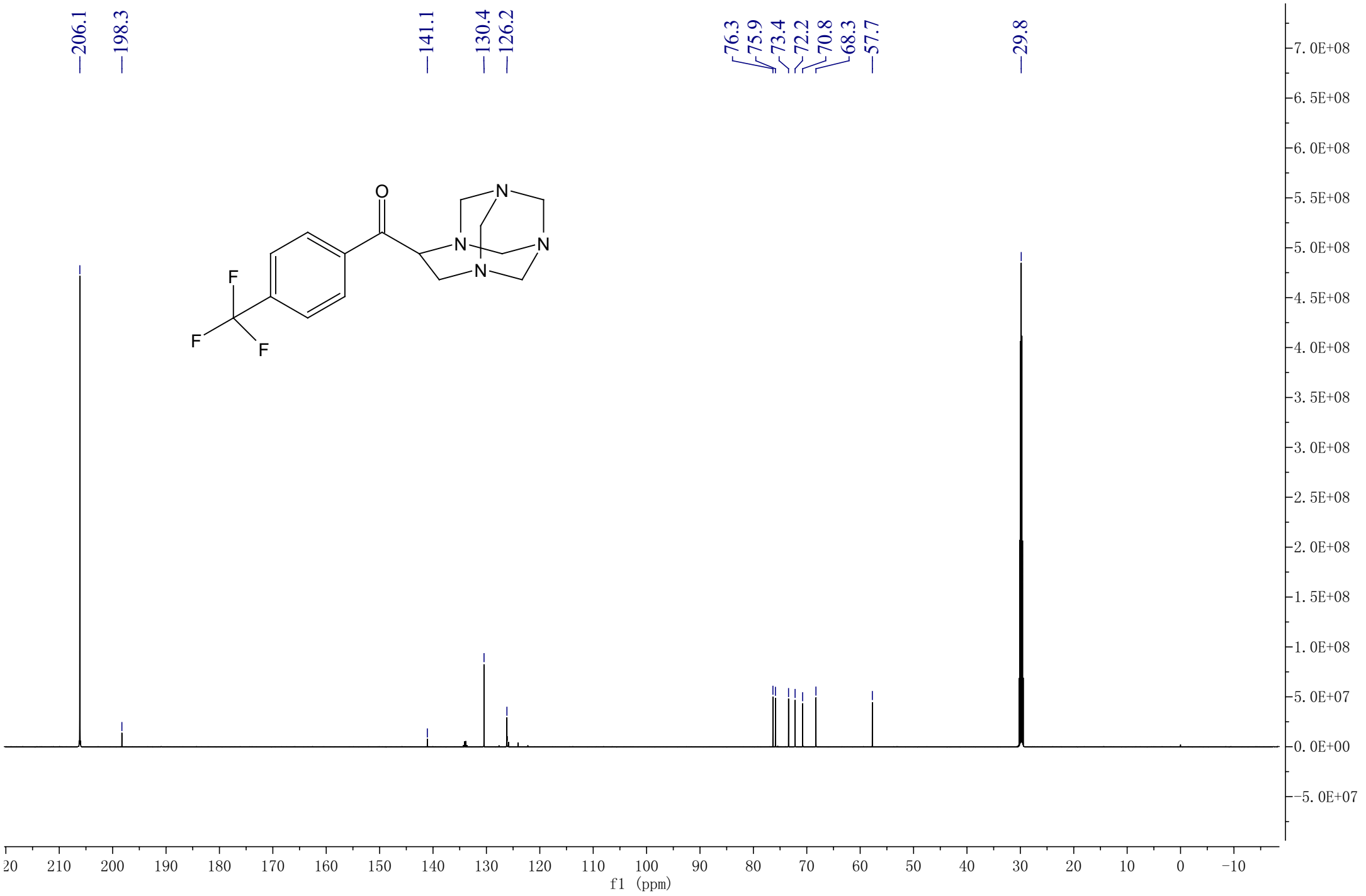
(4-chlorophenyl)(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6g)



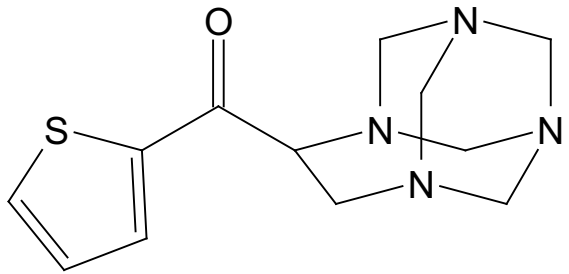
1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl(4-(trifluoromethyl)phenyl)methanone (6h)



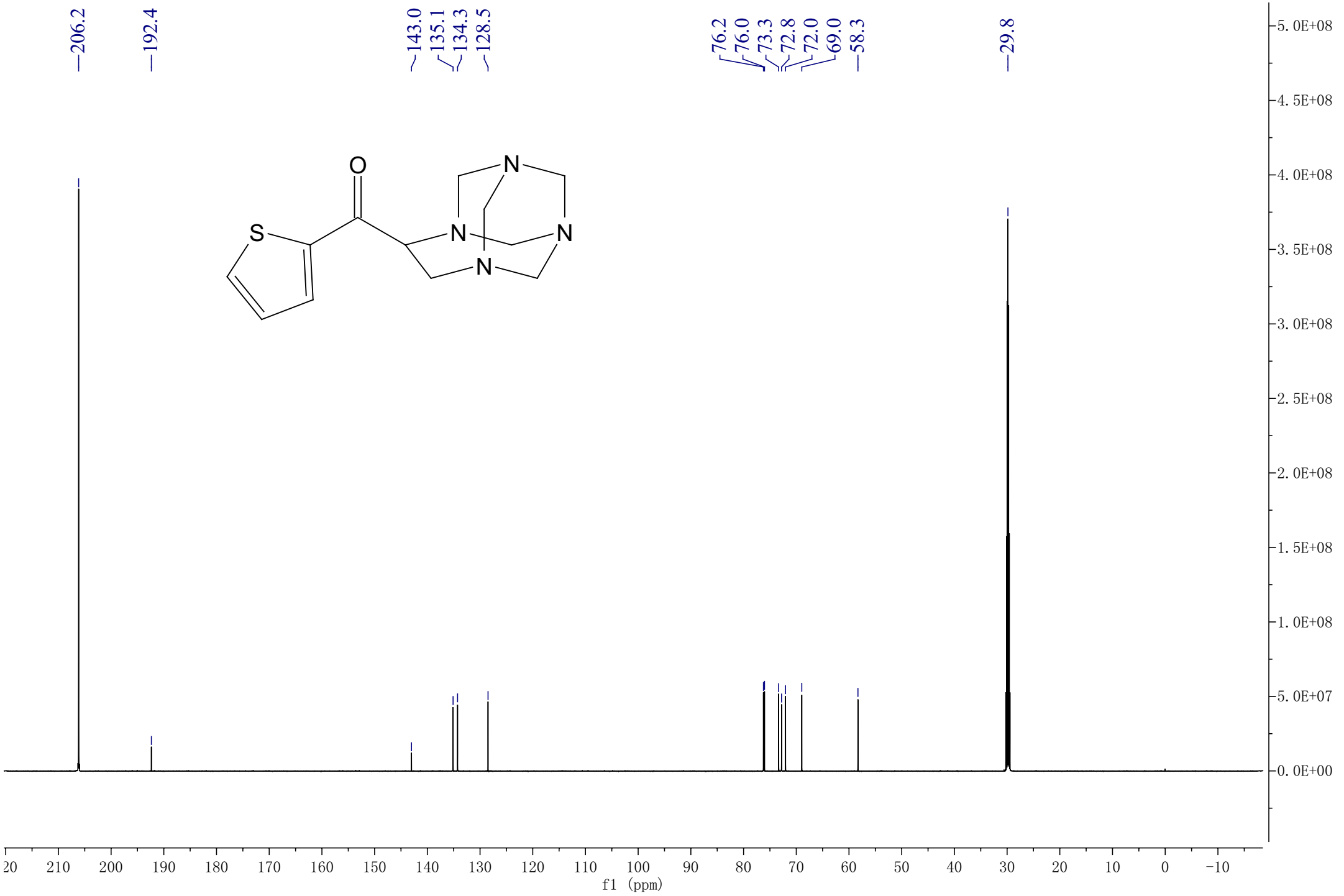
1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl(4-(trifluoromethyl)phenyl)methanone (6h)



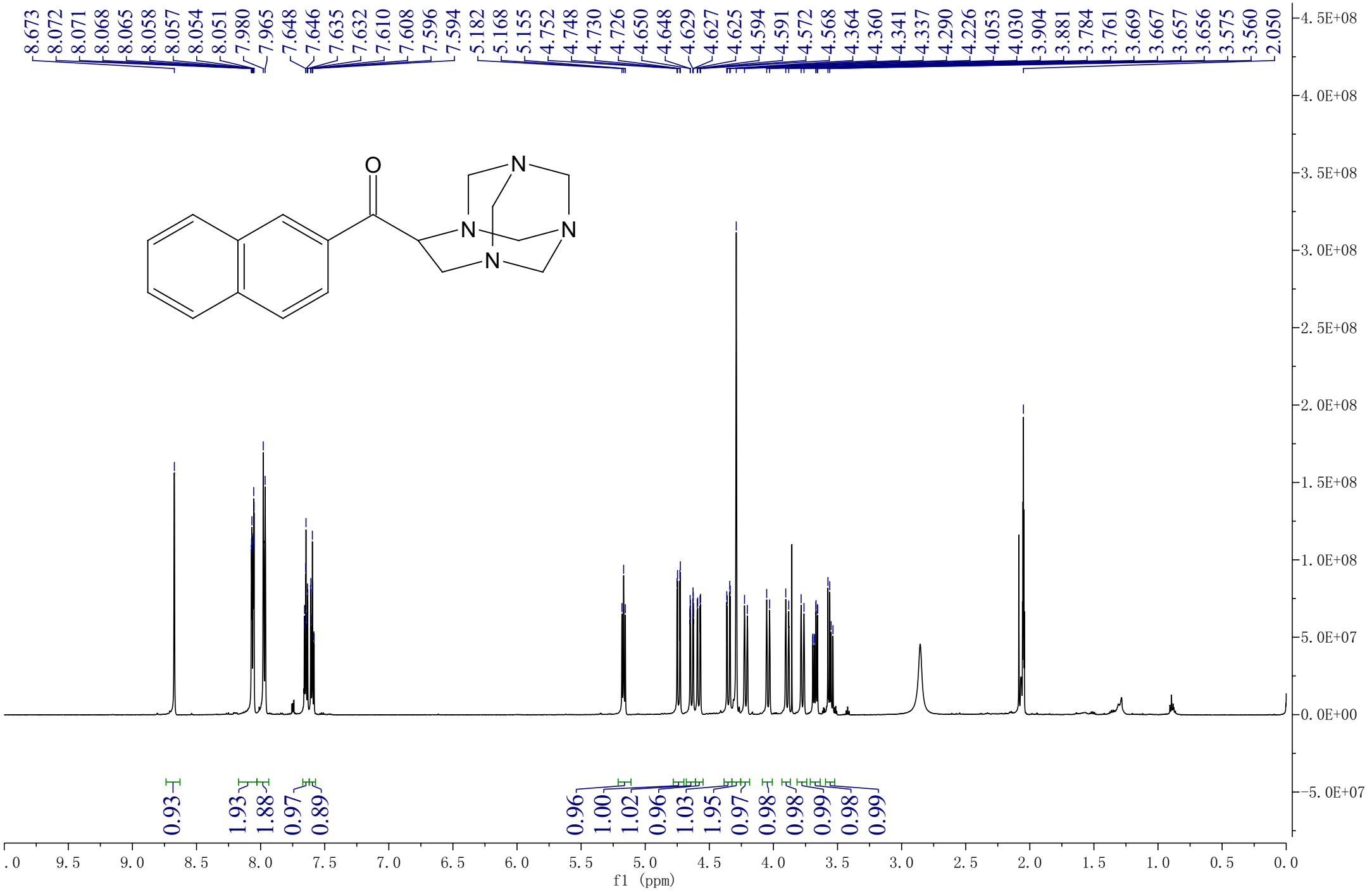
thiophen-2-yl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6i)



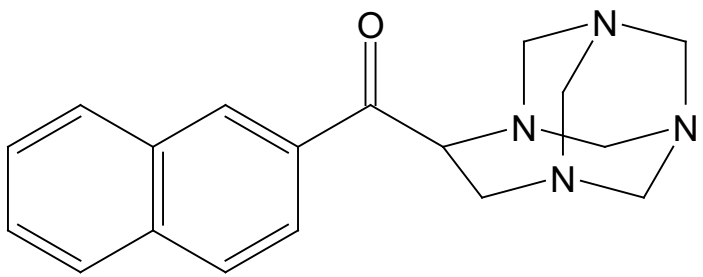
thiophen-2-yl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6i)



naphthalen-2-yl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6j)



naphthalen-2-yl(1,3,6,8-tetraazatricyclo[4.3.1.1^{3,8}]undecan-4-yl)methanone (6j)



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 6d

```
Bond precision:  C-C = 0.0017 A          Wavelength=0.71073

Cell:            a=6.2417(16)     b=18.453(5)        c=12.263(3)
                 alpha=90         beta=99.371(3)     gamma=90
Temperature:     153 K

                Calculated                Reported
Volume          1393.6(6)                 1393.6(6)
Space group     P 21/n                    P2(1)/n
Hall group      -P 2yn                    ?
Moiety formula  C15 H20 N4 O2             ?
Sum formula     C15 H20 N4 O2             C15 H20 N4 O2
Mr              288.35                    288.35
Dx,g cm-3       1.374                     1.374
Z               4                         4
Mu (mm-1)       0.094                     0.094
F000            616.0                     616.0
F000'           616.24
h,k,lmax        8,25,17                   8,25,17
Nref            4058                      4049
Tmin,Tmax       0.956,0.976
Tmin'           0.954

Correction method= Not given

Data completeness= 0.998          Theta(max)= 30.000

R(reflections)= 0.0477( 3618)     wR2(reflections)= 0.1142( 4049)

S = 0.999                 Npar= 191
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT793_ALERT_4_G The Model has Chirality at C8           (Verify)          S
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 18/09/2013; check.def file version of 12/09/2013

Datablock 6d - ellipsoid plot