Supporting Information for:

Copper-Catalyzed Intermolecular Cyclization of Nitriles and 2-Aminobenzylamine for 3,4-Dihydroquinazolines and Quinazolines Synthesis via Cascade Coupling and Aerobic Oxidation

Cheng Li, Shujuan An, Yuelu Zhu, Jin Zhang, Yifan Kang, Ping Liu,* Yaoyu Wang, Jianli Li*

Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, Department of Chemistry & Materials Science, Northwest University, Xi'an 710069, P. R. China

E-mail: lijianli@nwu.edu.cn; liuping@nwu.edu.cn

CONTENTS

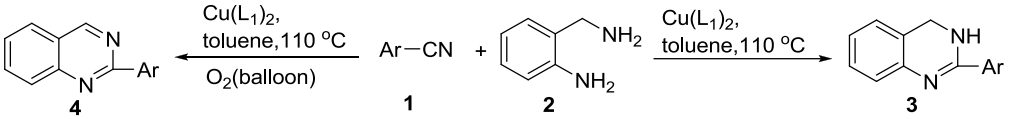
1. General information

^{1}H and ^{13}C NMR spectra were recorded on Varian instrument (400 MHz) and (100 MHz). The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad. Chemical shifts (δ) are reported in ppm using TMS as internal standard and spin-spin coupling constants (*J*) are given in Hz. IR spectra were recorded on a FT-IR spectrometer. Preparative TLC was performed on TLC plates, analytical thin layer chromatography was performed on 10-25um silica gel GF254, visualization was carried out with UV light. Flash column chromatography was performed with SiO_2 (Silica Gel 60 (200-300 mesh)). Melting points were determined using a standard melting point instrument and are uncorrected. The high resolution mass spectra (HRMS) were measured by ESI. Unless otherwise stated, all reagents and solvents were purchased from commercial suppliers and used without further purification.

2. Preparation of copper cinnamate

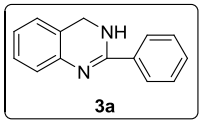
Cinnamic acid (10 mmol) was slowly added into the solution of NaOH (8 mmol NaOH in 10 mL of water) whilst stirring. To the solution, an aqueous solution of $CuCl_2$ (4 mmol $CuCl_2$•$2H_2O$ in 14 mL of water) was added, and the mixture was stirred for 5 min to give a blue precipitate, which was collected by filtration, washed with water, and dried in vacuo to provide copper cinnamate (1.48 g, 94% yield).

3. Procedure for synthesis of dihydroquinazolines and quinazolines



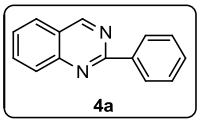
Nitrile (1 mmol), 2-aminobenzylamine (1.25 mmol), $Cu(L_1)_2$ (L_1=cinnamate, 0.1 mmol) and toluene (2 mL) were charged in a 10 mL round bottom flask. Then, the reaction mixture was stirred at 110 ℃ under air and oxygen atmosphere. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was cooled to room temperature, diluted with ethyl acetate (10 mL) and the catalyst was removed by filtration. The solvent was evaporated in vacuo, and the residue was purified by silica gel chromatography to afford the corresponding 3,4-dihydroquinazolines and quinazolines with ethyl acetate/ petroleum ether as eluent**.**

4. Characterization data of products



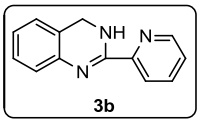
3a

2-phenyl-3,4-dihydroquinazoline (3a): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.57); white solid; mp 142-143 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.5 Hz, 2H), 7.43-7.36 (m, 3H), 7.17 (t, *J* = 7.3 Hz, 1H), 7.07-7.00 (m, 2H), 6.91 (d, *J* = 7.2 Hz, 1H), 4.72 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.04, 141.21, 135.24, 130.57, 128.56, 128.07, 126.49, 125.52, 124.49, 121.57, 120.15, 44.67; IR (KBr): 3213, 3030, 2832, 1585, 1540, 1520, 1475, 1453, 1332, 758, 709, 694, 557, 489 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{14}H_{13}N_2$: 209.1079 ; found: 209.1083.



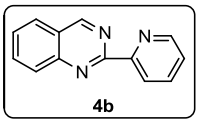
4a

2-phenylquinazoline (4a): eluent (petroleum ether/ethyl acetate =1:3, Rf = 0.46); white solid; mp 102-103 °C (lit.[1] 97-99 °C); ^{1}H NMR (400 MHz, DMSO) δ 9.71 (s, 1H), 8.59 (dd, 7.2, 3.2 Hz, 1H), 8.57 (d, *J* = 1.9 Hz, 1H), 8.17 (d, *J* = 8.2 Hz, 1H), 8.08-8.01 (m, 2H), 7.76-7.72 (m, 1H), 7.58 (d, *J* = 1.8 Hz, 1H), 7.57 (d, *J* = 1.8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 161.30, 159.72, 149.81, 137.41, 134.81, 130.80, 128.72, 128.07, 127.87, 127.79, 127.73, 123.32; IR (KBr): 3063, 2920, 1614, 1586, 1566, 1551, 1483, 1380, 1341, 779, 705, 636 cm^{-1};



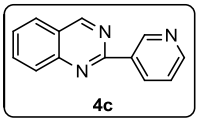
3b

2-(pyridin-2-yl)-3,4-dihydroquinazoline (3b): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.33); yellow solid, mp 79-80 °C; ^{1}H NMR (400 MHz, DMSO) δ 8.55 (s, 1H), 7.79 (t, *J* = 7.2 Hz, 1H), 7.36 (d, *J* = 4.7 Hz, 1H), 7.18 (s, 2H), 7.02-6.97 (m, 3H), 4.83 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.85, 159.71, 154.96, 150.57, 150.07, 136.90, 134.26, 129.00, 128.00, 127.02, 124.69, 123.97, 123.90, 45.75; IR (KBr): 3375, 3053, 2851, 1655, 1562, 1520, 1480, 1434, 1343, 766, 727, 573 cm^{-1}; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{13}H_{12}N_3$: 210.1031; found: 210.1034.



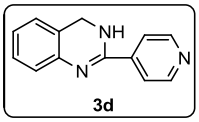
4b

2-(pyridin-2-yl)quinazoline (4b): eluent (petroleum ether/ethyl acetate =1:3, Rf = 0.29); yellow solid, mp 90-92 °C; ^{1}H NMR (400 MHz, DMSO) δ 9.58 (s, 1H), 8.91 (s, 1H), 8.71 (d, *J* = 7.6 Hz, 1H), 8.25 (d, *J* = 8.3 Hz, 1H), 7.98-7.90 (m, 3H), 7.69 (t, *J* = 7.1 Hz, 1H), 7.45-7.42 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.94, 155.08，150.33, 147.80, 136.97, 136.81, 134.33, 129.12, 128.07, 127.97, 127.11, 125.77, 125.14, 124.46, 121.32; IR (KBr): 3055, 1617, 1586, 1551, 1487, 1442, 1397, 1380, 783, 737, 703, 638 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{13}H_{10}N_3$: 208.0875; found: 208.0877.



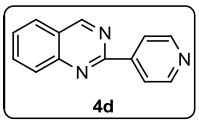
4c

2-(pyridin-3-yl)quinazoline (4c): eluent (petroleum ether/ethyl acetate =1:3, Rf = 0.24); yellow solid; mp 97-99 °C (lit.[2] 94-96 °C); ^{1}H NMR (400 MHz, DMSO) δ 9.76 (s, 1H), 9.69 (s, 1H), 8.85-8.83 (m, 1H), 8.76 (d, *J* = 4.0 Hz, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 8.09 (q, *J* = 8.5 Hz, 2H), 7.79 (t, *J* = 7.1 Hz, 1H), 7.62 (dd, *J* = 7.7, 4.9 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 166.75, 163.38, 156.53, 154.84, 154.41, 140.52, 140.26, 138.05, 133.36, 133.09, 133.05, 129.04, 128.69; IR (KBr): 3038, 2922, 1619, 1582, 1565, 1551, 1424, 1401, 1021, 977, 823, 768, 716, 638, 621, 474 cm^{-1}.



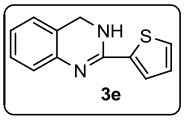
3d

2-(pyridin-4-yl)-3,4-dihydroquinazoline (3d): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.29); yellow solid; mp 83-85 °C; ^{1}H NMR (400 MHz, DMSO) δ 8.68 (s, 2H), 7.86 (s, 2H), 7.13 (s, 1H), 6.99 (d, *J* = 3.7 Hz, 3H), 4.68 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 166.91, 157.43, 155.70, 155.10, 146.80, 140.40, 132.95, 130.86, 129.58, 125.86, 49.04; IR (KBr): 3414, 3286, 3093, 2853, 1666, 1607, 1576, 1561, 1491, 1542, 1336, 1282, 1204, 861, 840, 761 cm^{-1}. HRMS (ESI): m/z [(M+H)$^{+}$] calcd for $C_{13}H_{12}N_3$: 210.1031 ; found: 210.1033.



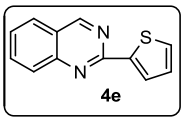
4d

2-(pyridin-4-yl)quinazoline (4d): eluent (petroleum ether/ethyl acetate =1:3, Rf = 0.25); white solid; mp 134-138 °C; ^{1}H NMR (400 MHz, DMSO) δ 9.78 (s, 1H), 8.83 (d, *J* = 4.4 Hz, 2H), 8.42 (d, *J* = 4.0 Hz, 2H), 8.24 (d, *J* = 8.0 Hz, 1H), 8.15-8.09 (m, 2H), 7.84 (t, *J* = 7.1 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 166.84, 163.06, 155.66, 154.77, 149.68, 140.35, 133.85, 133.24, 133.08, 129.02, 127.00; IR (KBr): 3023, 1616, 1598, 1581, 1543, 1488, 1450, 1410, 1401, 1381, 795, 760, 739, 704, 668, 634 cm^{-1}; HRMS (ESI): m /z [(M+H)$^{+}$] calcd for $C_{13}H_{10}N_3$: 208.0875; found: 208.0876.



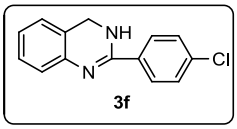
3e

2-(thiophen-2-yl)-3,4-dihydroquinazoline (3e): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.35); yellow solid; mp 152-153 °C; ^{1}H NMR (400 MHz, DMSO) δ 7.81 (s, 1H), 7.72 (s, 1H), 7.66 (d, *J* = 4.5 Hz, 1H), 7.15-7.12 (m, 2H), 6.98 (d, *J* = 7.1 Hz, 1H), 6.95-6.92 (m, 1H), 4.59 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 155.98, 148.79, 145.36, 134.76, 132.85, 132.71, 131.56, 130.77, 128.99, 128.64, 126.70, 46.99; IR (KBr): 3419, 3193, 3066, 1583, 1558, 1504, 1479, 1453, 1424, 1315, 1273, 854, 768, 722 cm^{-1}; HRMS (ESI): m/z [(M+H)$^{+}$] calcd for $C_{12}H_{11}N_2S$: 215.0643; found: 215.0648.



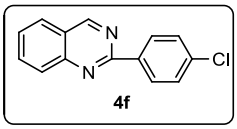
4e

2-(thiophen-2-yl)quinazoline (4e): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.50); yellow solid; mp 136-137 °C (lit.[3] 132-134 °C); ^{1}H NMR (400 MHz, DMSO) δ 9.62 (s, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 8.10 (dd, *J* = 3.7, 1.3 Hz, 1H), 8.02-7.99 (m, 2H), 7.82 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.73-7.69 (m, 1H), 7.27 (dd, *J* = 5.0, 3.7 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 161.43, 149.66, 143.28, 135.07, 131.02, 129.24, 128.66, 128.01, 127.43, 127.32, 123.08; IR (KBr): 2923, 2852, 1617, 1584, 1567, 1554, 1530, 1485, 1452, 1424, 1397, 1379, 1379, 1045, 765, 711 cm^{-1}; HRMS (ESI): m /z [(M + H)$^{+}$] calcd for $C_{12}H_9N_2S$: 213.0486; found: 213.0492.



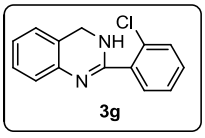
3f

2-(4-chlorophenyl)-3,4-dihydroquinazoline (3f): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.48); white solid; mp 171-172 °C; ^{1}H NMR (400 MHz, DMSO) δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.15-7.11 (m, 1H), 6.95-6.98 (m, 3H), 4.64 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 158.04, 140.09, 138.69, 134.94, 133.55, 133.30, 132.75, 130.63, 128.92, 125.54, 49.04; IR (KBr): 3426, 3195, 3036, 2824, 1587, 1550, 1532, 1489, 1478, 1445, 1342, 1091, 834, 763, 721 cm^{-1}; HRMS (ESI): m/z [(M+H)$^{+}$] calcd for $C_{14}H_{12}ClN_2$: 243.0689; found: 243.0691.



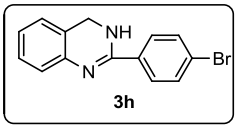
4f

2-(4-chlorophenyl)quinazoline (4f): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.31); white solid; mp 139-140 °C (lit.[4] 133-135 °C); ^{1}H NMR (400 MHz, DMSO) δ 9.72 (s, 1H), 8.57 (d, *J* = 8.4 Hz, 2H), 8.19 (d, *J* = 8.0 Hz, 1H), 8.06 (d, *J* = 3.6 Hz, 2H), 7.78-7.75 (m, 1H), 7.64 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 161.46, 158.73, 149.72, 136.26, 135.69, 134.98, 129.79, 128.84, 127.97, 127.85, 123.35; IR (KBr): 1619, 1585, 1562, 1549, 1405, 1489, 1449, 1405, 1380, 1340, 1083, 1008, 850, 799, 764, 728, 690, 453 cm^{-1};



3g

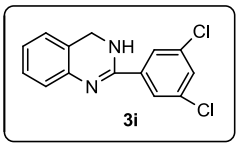
2-(2-chlorophenyl)-3,4-dihydroquinazoline (3g): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.43); ^{1}H NMR (400 MHz, DMSO) δ 6.99 (d, *J* = 7.4 Hz, 2H), 6.93 (t, *J* = 8.0 Hz, 1H), 6.85 (d, *J* = 7.0 Hz, 1H), 6.63 (d, *J* = 11.1 Hz, 2H), 6.52 (dd, *J* = 13.2, 7.4 Hz, 2H), 5.20 (s, 1H), 4.75 (s, 1H); ^{13}C NMR (100 MHz, DMSO) δ 153.15, 147.25, 135.53, 133.42, 133.33, 132.91, 128.73, 125.90, 121.39, 121.11, 120.03, 119.57, 57.27; IR (KBr): 3376, 3207, 3043, 2923, 2851, 1606, 1494, 1459, 1280, 1115, 1087, 1266, 750 cm^{-1}; HRMS (ESI): m/z [(M+H)$^{+}$] calcd for $C_{14}H_{12}ClN_2$: 243.0689 ; found: 243.0693.



3h

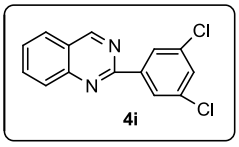
2-(4-bromophenyl)-3,4-dihydroquinazoline (3h): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.45); yellow solid; mp 170-172 °C; ^{1}H NMR (400 MHz, DMSO) δ 6.98 (d, *J* = 7.3 Hz, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.84 (d, *J* = 7.1 Hz, 1H), 6.60-6.62 (d, *J* = 7.2 Hz, 1H), 6.53-6.48 (m, 2H), 5.20 (s, 1H),

4,73 (s, 1H). ^{13}C NMR (100 MHz, DMSO) δ 153.10, 147.20, 135.48, 133.37, 133.28, 132.86, 128.69, 125.86, 121.35, 121.07, 120.00, 119.53, 57.22; IR (KBr): 3423, 3368, 3034, 2929, 2860, 1607, 1495, 1383, 1323, 1115, 1065, 758, 746 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{14}H_{12}BrN_2$: 287.0184 ; found: 287.0188.



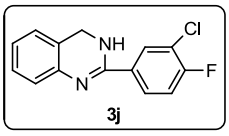
3i

2-(3,5-dichlorophenyl)-3,4-dihydroquinazoline (3i): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.59); yellow solid; mp 162-163 °C; ^{1}H NMR (400 MHz, DMSO) δ 7.98 (s, 2H), 7.75-7.73 (m, 1H), 7.12-7.16 (m, 1H), 7.00 (d, *J* = 8.4 Hz, 3H), 4.66 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 156.43, 143.12, 139.16, 134.62, 132.80, 131.44, 130.65, 130.38, 129.30, 125.46, 120.89, 48.67; IR (KBr): 3428, 3013, 2832, 1590, 1572, 1550, 1481, 1455, 1414, 1390, 1339, 866, 802, 765 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{14}H_{11}Cl_2N_2$: 277. 0299; found: 277.0292.



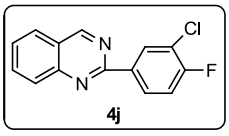
4i

2-(3,5-dichlorophenyl)quinazoline (4i): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.38); white solid; mp 170-171 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 (s, 1H), 8.53 (d, *J* = 1.7 Hz, 2H), 8.09 (d, *J* = 8.8 Hz, 1H), 7.95 (t, *J* = 7.3 Hz, 2H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.48 (d, *J* = 1.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.53, 158.36, 150.45, 140.86, 135.24, 134.41, 130.18, 128.62, 127.91, 127.09, 126.84, 123.80; IR (KBr): 3421, 3091, 1621, 1584, 1549, 1494, 1398, 1384, 1336, 1282, 1246, 860, 799, 761, 721, 666 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{14}H_9Cl_2N_2$: 275. 0143; found: 275.0143.



3j

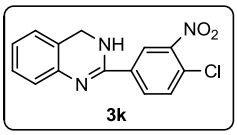
2-(3-chloro-4-fluorophenyl)-3,4-dihydroquinazoline (3j): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.47); yellow solid; mp 130-132 °C; ^{1}H NMR (400 MHz, DMSO) δ 7.75 (s, 1H), 7.47 (d, *J* = 8.6 Hz, 1H), 6.97 (d, *J* = 6.1 Hz, 2H), 6.63 (dd, *J* = 15.9, 8.2 Hz, 2H), 6.49 (t, *J* = 7.3 Hz, 1H), 5.13 (s, 1H), 4.31 (s, 1H); ^{13}C NMR (100 MHz, DMSO) δ 161.45 (d, J_{CF}= 291 Hz), 142.03, 139.86, 129.19, 128.00, 127.27, 124.42 (d, J_{CF}= 28 Hz), 121.47, 120.32, 115.44 (d, J_{CF}= 5 Hz), 113.84 (d, J_{CF}= 26 Hz), 111.18, 105.94, 40.22; IR (KBr): 3404, 3361, 3218, 3069, 1629, 1620, 1600, 1520, 1495, 1458, 1336, 775 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{14}H_{11}ClFN_2$:261. 0595; found: 261.0590.



4j

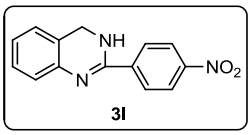
2-(3-chloro-4-fluorophenyl)quinazoline (4j): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.30); white solid; mp 195-196 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.46 (s, 1H), 8.73 (dd, *J* = 7.3, 2.0 Hz, 1H), 8.55-8.52 (m, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.94 (t, *J* = 7.8 Hz, 2H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.30 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.94, 159.68 (d, J_{CF}= 167 Hz), 158.43, 150.53, 135.14,

134.33, 130.93, 128.48, 128.39, 127.56, 127.10, 123.54, 121.44, 116.57 (d, J_{CF}= 22 Hz); IR (KBr): 3033, 1618, 1582, 1566, 1502, 1487, 1452, 1408, 1341, 1287, 1257, 1069, 895, 783, 757, 723 cm^{-1}; HRMS (ESI): m/z [$(M+H)^+$] calcd for $C_{14}H_9ClFN_2$:259.0438; found: 261.0443.



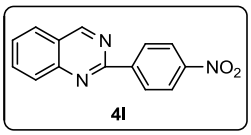
3k

2-(4-chloro-3-nitrophenyl)quinazoline (3k): eluent (petroleum ether/ethyl acetate =2:1, Rf = 0.37); yellow solid; mp 206-208 °C; ^{1}H NMR (400 MHz, DMSO) δ 8.99 (s, 1H), 8.50 (s, 1H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.05-6.96 (m, 2H), 6.68 (d, *J* = 7.8 Hz, 1H), 6.51 (t, *J* = 7.2 Hz, 1H), 5.21 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 152.06, 151.43, 142.59, 136.94, 136.15, 133.33, 133.22, 124.69, 123.39, 121.35, 121.27, 120.38, 101.64, 48.38. IR (KBr): 3444, 3370, 3234, 3034, 2922, 2869, 1826, 1622, 1581, 1556, 1521, 1406, 1361, 1269, 919, 819, 786 cm^{-1}; HRMS (ESI): m/z [$(M+H)^+$] calcd for $C_{14}H_{11}ClN_3O_2$: 288.0540; found: 288.0546.



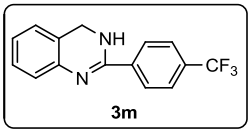
3l

2-(4-nitrophenyl)-3,4-dihydroquinazoline (3l): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.45); yellow solid; mp 128-130 °C; ^{1}H NMR (400 MHz, DMSO) δ 8.32 (d, *J* = 8.7 Hz, 2H), 8.19 (d, *J* = 8.7 Hz, 2H), 7.18-7.13 (m, 1H), 7.00-7.03 (m, 3H), 4.70 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 153.53, 147.20, 145.85, 138.60, 133.05, 132.92, 130.78, 129.58, 128.53, 121.32, 118.59, 69.30; IR (KBr): 3375, 2851, 1645, 1588, 1567, 1516, 1492, 1347, 1108, 857, 752, 702 cm^{-1}; HRMS (ESI): m/z [$(M+H)^+$] calcd for $C_{14}H_{12}N_3O_2$: 254.0930; found: 254.0937.



4l

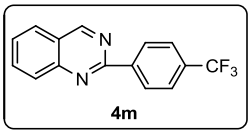
2-(4-nitrophenyl)quinazoline (4l): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.42); white solid; mp 227-228 °C (lit.[5] 218-219); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.54 (s, 1H), 8.84 (d, *J* = 9.0 Hz, 2H), 8.40 (d, *J* = 9.0 Hz, 2H), 8.15-8.17 (m, 1H), 8.01 (dd, *J* = 11.7, 4.7 Hz, 2H), 7.75-7.71 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.25, 158.31, 150.12, 148.69, 143.35, 134.15, 128.91, 128.38, 127.86, 126.75, 123.40, 123.29; IR (KBr): 3068, 1618, 1555, 1517, 1486, 1410, 1347, 861, 847, 802, 766, 748, 710 cm^{-1};



3m

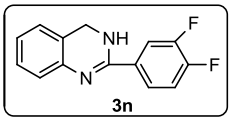
2-(4-(trifluoromethyl)phenyl)-3,4-dihydroquinazoline (3m): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.54); white solid; mp 189-190 °C; ^{1}H NMR (400 MHz, DMSO) δ 8.15 (d, *J* = 7.9 Hz, 2H), 7.84 (d, *J* = 8.2 Hz, 2H), 7.17-7.13 (m, 1H), 7.00-7.02 (m, 3H), 4.69 (s, 2H). ^{13}C NMR (100 MHz, DMSO) δ 158.57, 143.82, 135.36 (dd, J_{CF}= 63, 31 Hz), 133.32, 132.86, 132.56, 130.74, 130.62, 130.27 (d, J_{CF}= 4 Hz), 129.44 (d, J_{CF}= 12 Hz), 127.91, 123.72 (d, J_{CF}= 294 Hz), 47.35; IR (KBr): 3230, 3072, 1598, 1566, 1487, 1457, 1406, 1327, 1175, 1123, 1068, 1019, 941, 765, 697 cm^{-1}. HRMS (ESI): m/z

[(M+H)$^+$] calcd for $C_{15}H_{12}F_3N_2$: 277.0953; found: 277.0956.



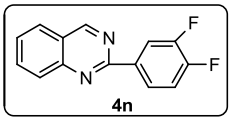
4m

2-(4-(trifluoromethyl)phenyl)quinazoline (4m): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.39); white solid; mp 146-147 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 9.78 (s, 1H), 8.76 (d, *J* = 8.1 Hz, 2H), 8.23 (d, *J* = 8.0 Hz, 1H), 8.10 (q, *J* = 8.4 Hz, 2H), 7.95 (d, *J* = 8.1 Hz, 2H), 7.81 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 161.57, 158.30, 149.67, 141.16, 135.09, 131.03, 130.71, 130.39, 128.69, 128.35, 127.94 (d, J_{CF}= 9 Hz), 125.65 (dd, J_{CF}= 7, 4 Hz), 124.55 (d, J_{CF}= 200 Hz); IR (KBr): 1620, 1584, 1566, 1553, 1489, 1453, 1414, 1325, 1162, 1069, 1069, 858, 803, 765, 704, 646 cm^{-1}. HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{15}H_{10}F_3N_2$: 275.0796; found: 275.0798.



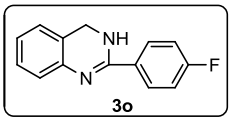
3n

2-(3,4-difluorophenyl)-3,4-dihydroquinazoline (3n): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.48); white solid; mp 144 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 8.00-7.95 (m, 1H), 7.81 (s, 1H), 7.59-7.52 (m, 1H), 7.16-7.12 (m, 1H), 6.99-6.97 (m, 3H), 4.64 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 152.67, 151.96, 149.13 (d, J_{CF}= 243 Hz), 149.00 (d, J_{CF}= 244 Hz), 132.31, 127.76, 125.51, 124.32, 124.05, 123.69 (dd, J_{CF}= 6, 3 Hz), 121.35, 121.29, 117.29 (d, J_{CF}= 17 Hz), 115.79 (d, J_{CF}= 19 Hz), 41.93; IR (KBr): 3200, 3025, 2829, 1618, 1582, 1550, 1531, 1511, 1476, 1334, 1274, 889, 836, 776, 762, 597, 478 cm^{-1}; HRMS (ESI): m/z [(M+H)]$^+$ calcd for $C_{14}H_{11}F_2N_2$: 245.0890; found: 245.0886.



4n

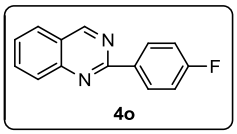
2-(3,4-difluorophenyl)quinazoline (4n): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.31); white solid; mp 141-142 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 (s, 1H), 8.48 (dd, *J* = 11.0, 8.7 Hz, 1H), 8.41 (d, *J* = 4.0 Hz, 1H), 8.08 (d, *J* = 8.3 Hz, 1H), 7.94 (t, *J* = 8.2 Hz, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.34-7.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.46, 158.88, 152.54 (dd, J_{CF}=166, 13Hz), 150.05 (dd, J_{CF}= 161, 13 Hz), 150.49, 135.11 (dd, J_{CF}= 6, 4 Hz), 134.28, 128.47, 127.52, 127.07, 124.79 (dd, J_{CF}= 7, 4 Hz), 123.51, 117.36 (dd, J_{CF}= 33, 19 Hz); IR (KBr): 3064, 1615, 1583, 1567, 1553, 1519, 1490, 1457, 1406, 1273, 1224, 979, 926, 798, 774, 759, 722 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{14}H_9F_2N_2$: 243.0734; found: 243.0733.



3o

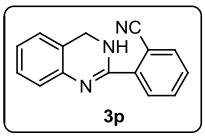
2-(4-fluorophenyl)-3,4-dihydroquinazoline (3o): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.47); white solid; mp 161-162 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 8.02-7.99 (m, 2H), 7.30 (t, *J* = 8.9 Hz, 2H), 7.13-7.11 (m, 1H), 6.98 (dd, *J* = 7.0, 4.2 Hz, 3H), 4.64 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 163.35 (d, J_{CF}= 247 Hz), 149.00, 143.89, 131.28 (d, J_{CF}= 3 Hz), 129.49 (d, J_{CF}= 9 Hz), 127.62, 125.47, 124.51, 123.90, 120.64, 115.00 (d, J_{CF}= 21 Hz), 42.06; IR (KBr): 3211, 3056, 2823, 1589,

1575, 1546, 1499, 1480, 1454, 1345, 1323, 1020, 841, 774, 726 cm^{-1}; HRMS (ESI): m/z [$(M+H)^+$] calcd for $C_{14}H_{12}FN_2$: 227.0985 ; found: 227.0979.



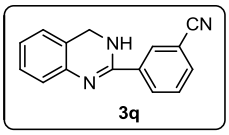
4o

2-(4-fluorophenyl)quinazoline (4o): eluent (petroleum ether/ethyl acetate =1:1, Rf = 0.28); white solid; mp 134-135 ºC (lit.[5] 129-130 ºC); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.63-8.61 (m, 2H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.3 Hz, 1H), 7.23-7.18 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.56 (d, J_{CF}= 249.0 Hz), 160.40, 159.99, 150.59, 134.10, 130.56(d, J_{CF}= 9.0 Hz), 130.09, 128.43, 127.11 (d, J_{CF}= 13.0 Hz), 126.64, 123.37, 115.45 (d, J_{CF}= 22.0 Hz).



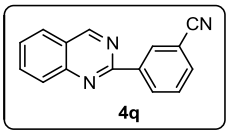
3p

2-(3,4-dihydroquinazolin-2-yl)benzonitrile (3p): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.39); yellow solid; mp 212-213 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 5.6, 3.6 Hz 1H), 7.83 (dd, *J* = 5.4, 3.4 Hz, 1H), 7.76 (dd, *J* = 8.2, 4.8 Hz, 2H), 7.67-7.65 (m, 1H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.32 (t, *J* = 6.5 Hz, 1H), 7.21 (d, *J* = 6.4 Hz, 1H), 5.06 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.88, 140.98, 133.54, 133.32, 133.08, 131.63, 131.49, 128.62, 127.35, 126.82, 126.77, 122.38, 121.15, 120.89, 41.59; IR (KBr): 3423, 3222, 2891, 2232, 1660, 1624, 1596, 1571, 1486, 1428, 1169, 1135, 1108, 890, 858, 765, 688, 525 cm^{-1}; HRMS (ESI): m/z [$(M+H)^+$] calcd for $C_{15}H_{12}N_3$: 234.1031; found: 234.1032.



3q

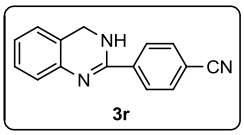
3-(3,4-dihydroquinazolin-2-yl)benzonitrile (3q): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.31); yellow solid; mp 72-73 ºC; ^{1}H NMR (400 MHz, DMSO) δ 8.34 (s, 1H), 8.28 (d, *J* = 7.9 Hz, 1H), 7.97 (d, *J* = 7.5 Hz, 1H), 7.69 (t, *J* = 7.8 Hz, 1H), 7.15 (dd, *J* = 7.3, 3.8 Hz, 1H), 7.00 (d, *J* = 3.7 Hz, 3H), 4.68 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 157.28, 146.83, 140.95, 138.87, 136.49, 135.27, 134.72, 132.88, 130.75, 129.27, 125.52, 123.69, 116.50, 48.95; IR (KBr): 3321, 3069, 2920, 2851, 2231, 1691, 1592, 1560, 1544, 1488, 1455, 1335, 1272, 814, 758, 708, 572 cm^{-1}; HRMS (ESI): m/z [$(M+H)^+$] calcd for $C_{15}H_{12}N_3$: 234.1031; found: 234.1035.



4q

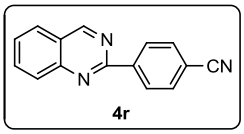
3-(quinazolin-2-yl)benzonitrile (4q): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.43); yellow solid; mp 197-198 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.52 (s, 1H), 9.00 (t, *J* = 1.4 Hz, 1H), 8.92-8.89 (m, 1H), 8.15-8.13 (m, 1H), 8.02-7.97 (m, 2H), 7.81 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.73-7.66 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.27, 158.31, 150.11, 138.71, 134.11, 133.19, 132.13, 131.88, 128.97, 128.24, 127.57, 126.76, 123.43, 118.35, 112.41; IR (KBr): 3069, 2923, 2224, 1620, 1583, 1566, 1553, 1489, 1448, 1391, 1381, 791, 756, 719, 677, 637 cm^{-1}; HRMS (ESI): m/z [$(M+H)^+$] calcd for $C_{15}H_{10}N_3$:

232.0875; found: 232.0918.



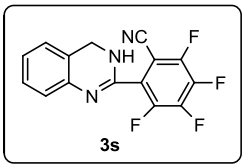
3r

4-(3,4-dihydroquinazolin-2-yl)benzonitrile (3r): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.40); yellow solid; mp 174-175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.3 Hz, 2H), 7.67 (d, *J* = 8.3 Hz, 2H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.07 (t, *J* = 6.8 Hz, 2H), 6.95 (d, *J* = 7.4 Hz, 1H), 4.78 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.04, 139.46, 132.31, 128.27, 127.13, 125.62, 125.26, 119.93, 118.29, 113.83, 44.63; IR (KBr): 3211, 3056, 2822, 2224, 1589, 1546, 1499, 1481, 1455, 1346, 1323, 1241, 1200, 841, 774, 727 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{15}H_{12}N_3$: 234.1031; found: 234.1034.



4r

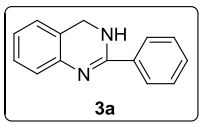
3-(quinazolin-2-yl)benzonitrile (4r): eluent (petroleum ether/ethyl acetate =10:1, Rf = 0.45); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.50 (s, 1H), 8.75 (d, *J* = 8.1 Hz, 2H), 8.11 (d, *J* = 8.3 Hz, 1H), 7.97 (t, *J* = 8.1 Hz, 2H), 7.82 (d, *J* = 8.1 Hz, 2H), 7.69 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.59, 158.98, 150.49, 142.01, 134.45, 132.30, 128.90, 128.70, 128.08, 127.11, 123.76, 118.81, 113.68; IR (KBr): 2922, 2851, 2225, 1617, 1585, 1548, 1450, 1403, 1379, 1055, 860, 802, 802, 772, 737, 564 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{15}H_{10}N_3$: 232.0875; found: 232.0875.

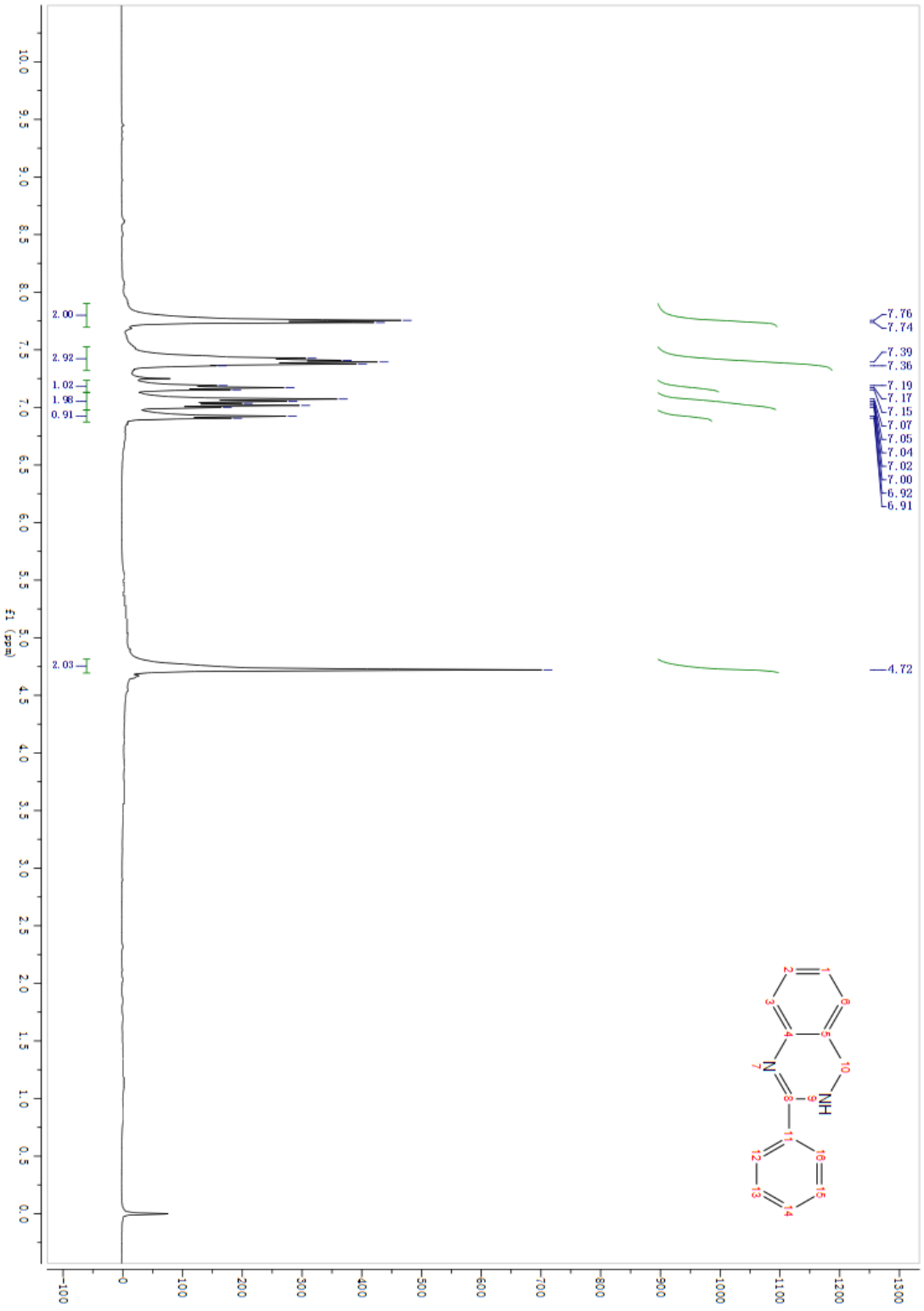


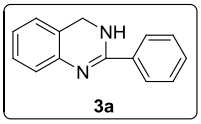
3s

2-(3,4-dihydroquinazolin-2-yl)-3,4,5,6-tetrafluorobenzonitrile (3s): eluent (petroleum ether/ethyl acetate =2:1, Rf = 0.39); white solid; mp 142-144 °C; ^{1}H NMR (400 MHz, DMSO) δ 7.77 (s, 1H), 6.96 (t, *J* = 7.5 Hz, 1H), 6.64 (d, *J* = 8.0 Hz, 1H), 6.51 (t, *J* = 7.3 Hz, 1H), 5.07 (s, 1H), 4.44 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 157.00, 154.95 (dd, J_{CF}=252, 14 Hz), 154.13 (dd, J_{CF}=252, 10 Hz), 150.85, 146.09 (dd, J_{CF}=249, 10 Hz), 145.94 (dd, J_{CF}=248, 10 Hz), 133.00, 132.19, 126.56, 121.05, 120.01, 116.28 (d, J_{CF}= 55 Hz), 103.89 (dd, J_{CF}=16, 4 Hz), 91.28 (dd, J_{CF}=16, 3 Hz), 49.57; IR (KBr): 3425, 3370, 3314, 2242, 1619, 1585, 1542, 1504, 1458, 1442, 1425, 1320, 1275, 1107, 952, 762 cm^{-1}; HRMS (ESI): m/z [(M+H)$^+$] calcd for $C_{15}H_8F_4N_3$: 306.0654; found: 306.0659.

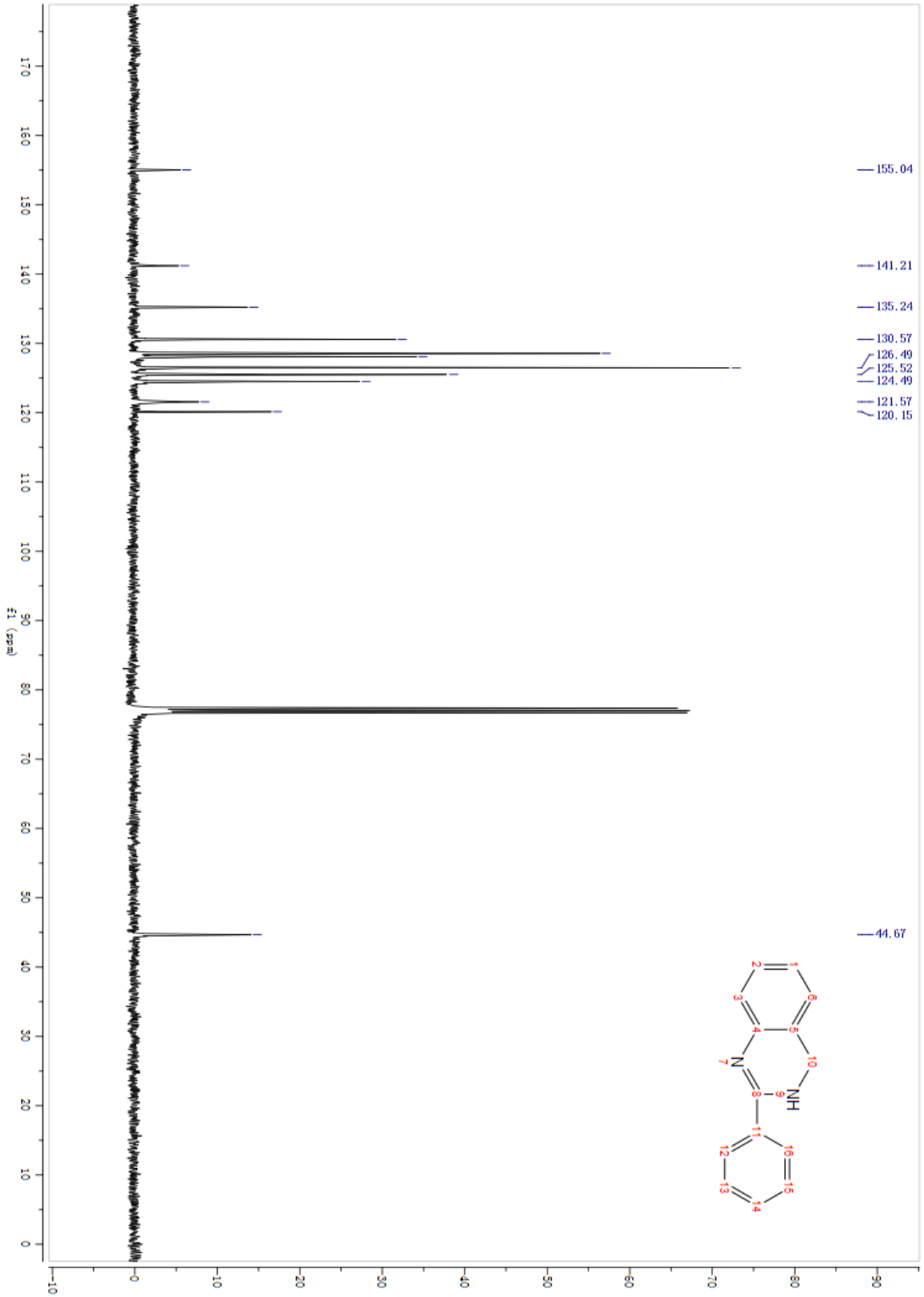
5. Copies of ^{1}H and ^{13}C NMR, IR spectra

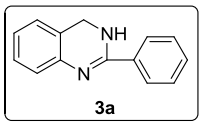




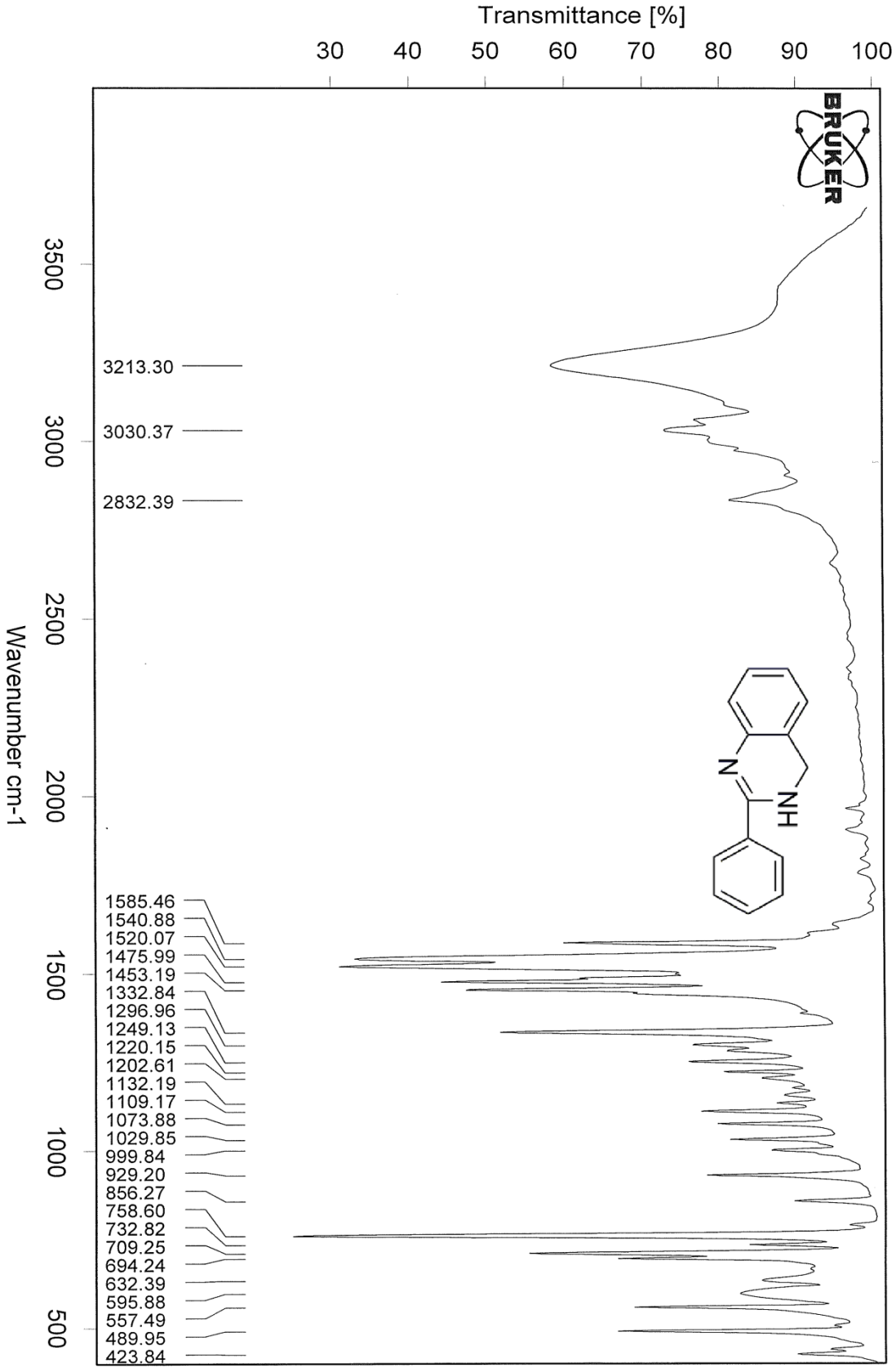

NH
N

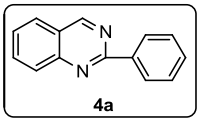
3a


155.04
141.21
135.24
130.57
126.49
125.52
124.49
121.57
120.15
44.67
f1 (ppm)

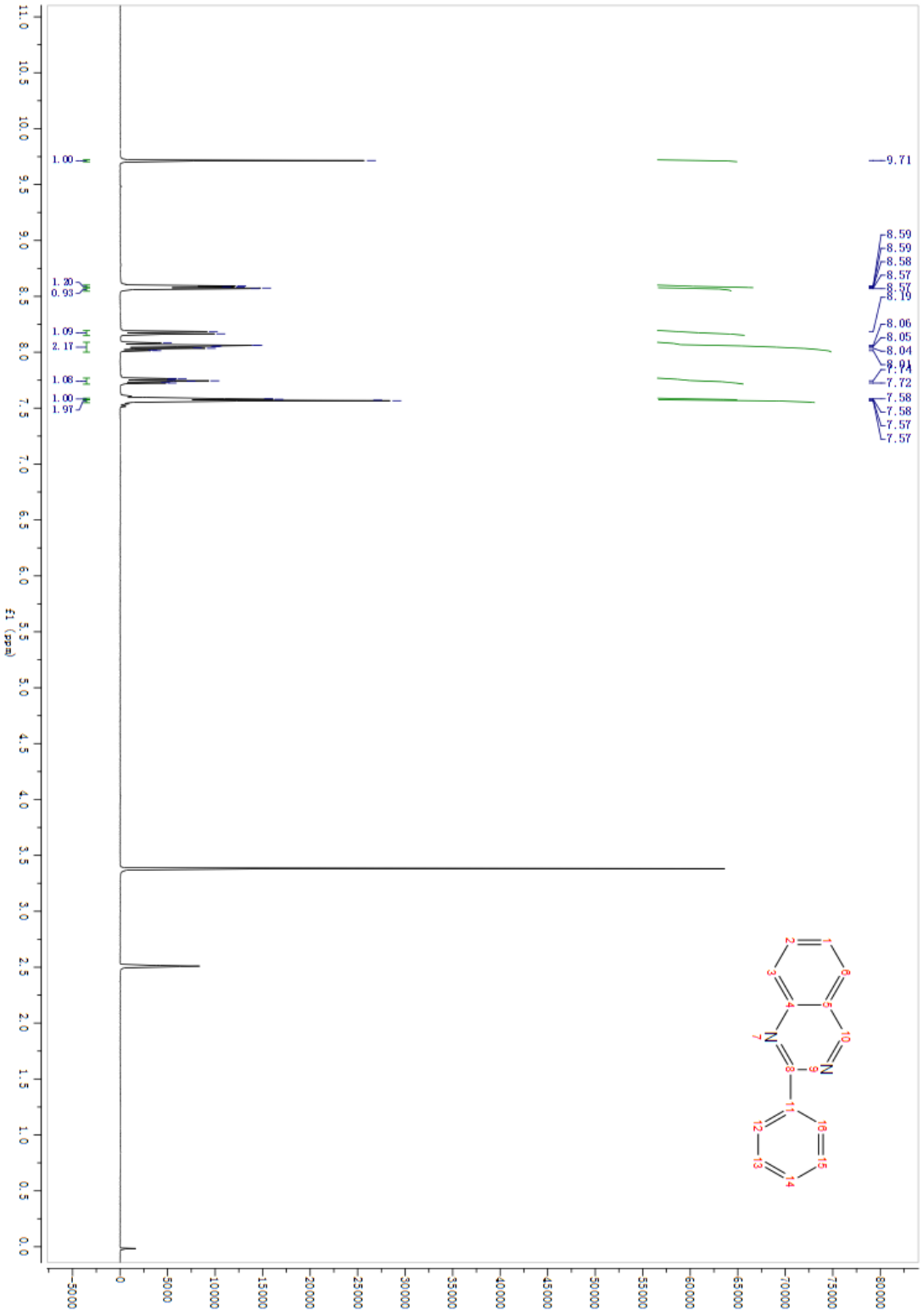

NH
N

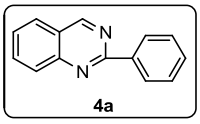
3a

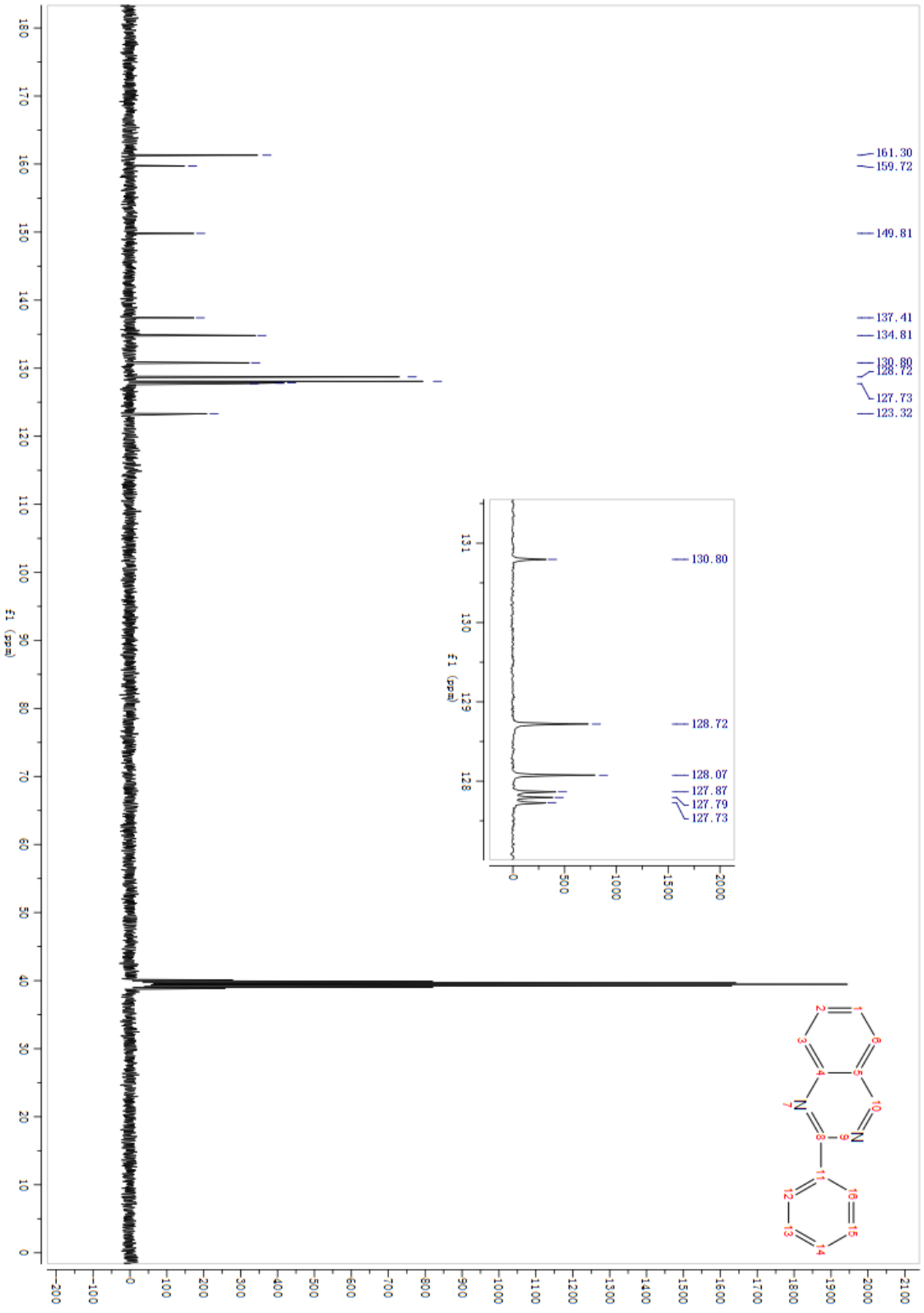

Transmittance [%]
30
40
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3213.30
3030.37
2832.39
1585.46
1540.88
1520.07
1475.99
1453.19
1332.84
1296.96
1249.13
1220.15
1202.61
1132.19
1109.17
1073.88
1029.85
999.84
929.20
856.27
758.60
732.82
709.25
694.24
632.39
595.88
557.49
489.95
423.84
N
HN

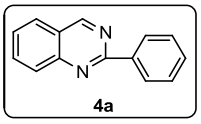

N
N

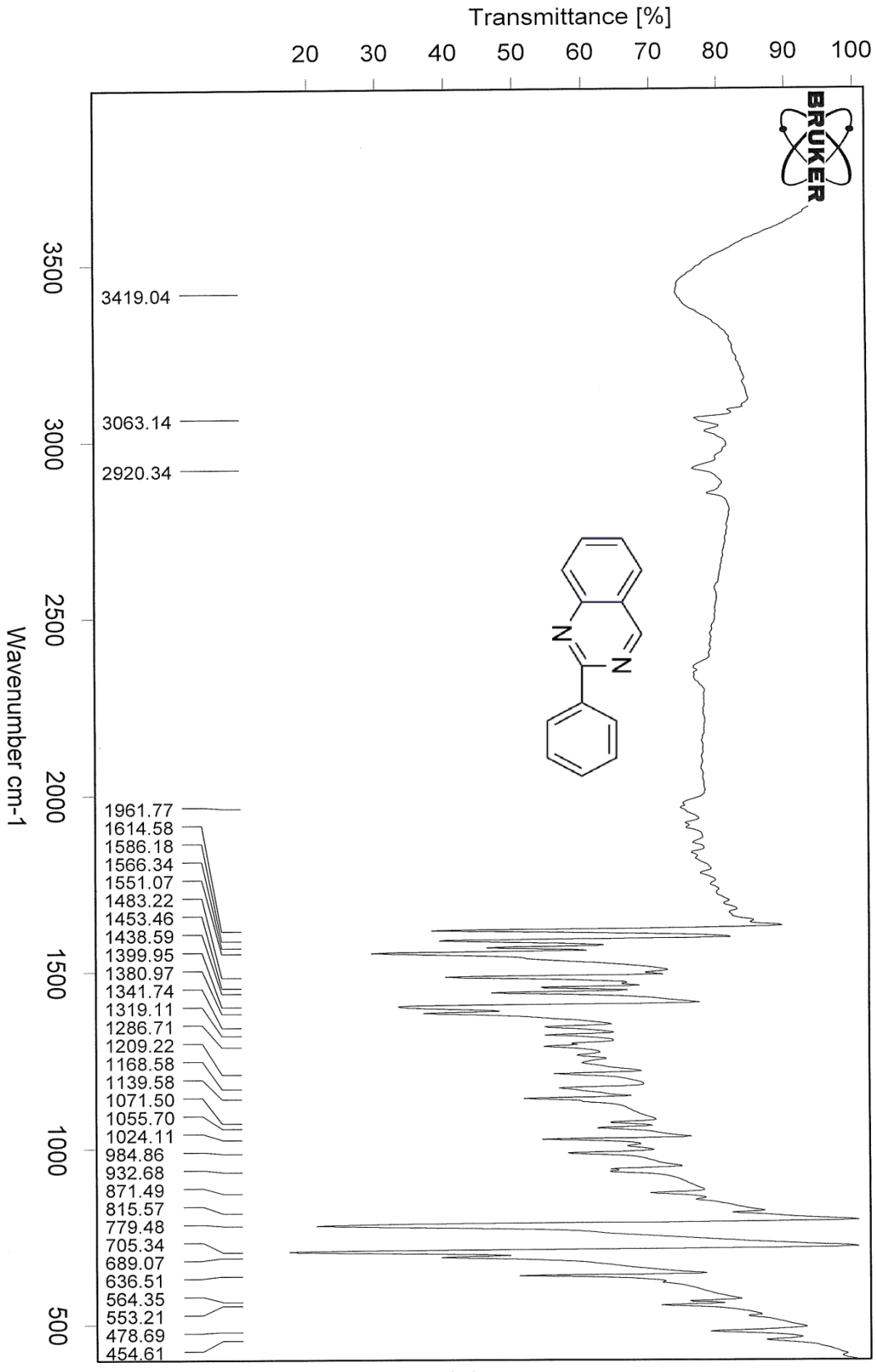
4a

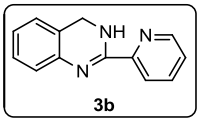

1.00
1.20
0.93
1.09
2.17
1.08
1.00
1.97
9.71
8.59
8.59
8.58
8.57
8.57
8.19
8.06
8.05
8.04
7.74
7.72
7.58
7.58
7.57
7.57
f1 (ppm)


4a

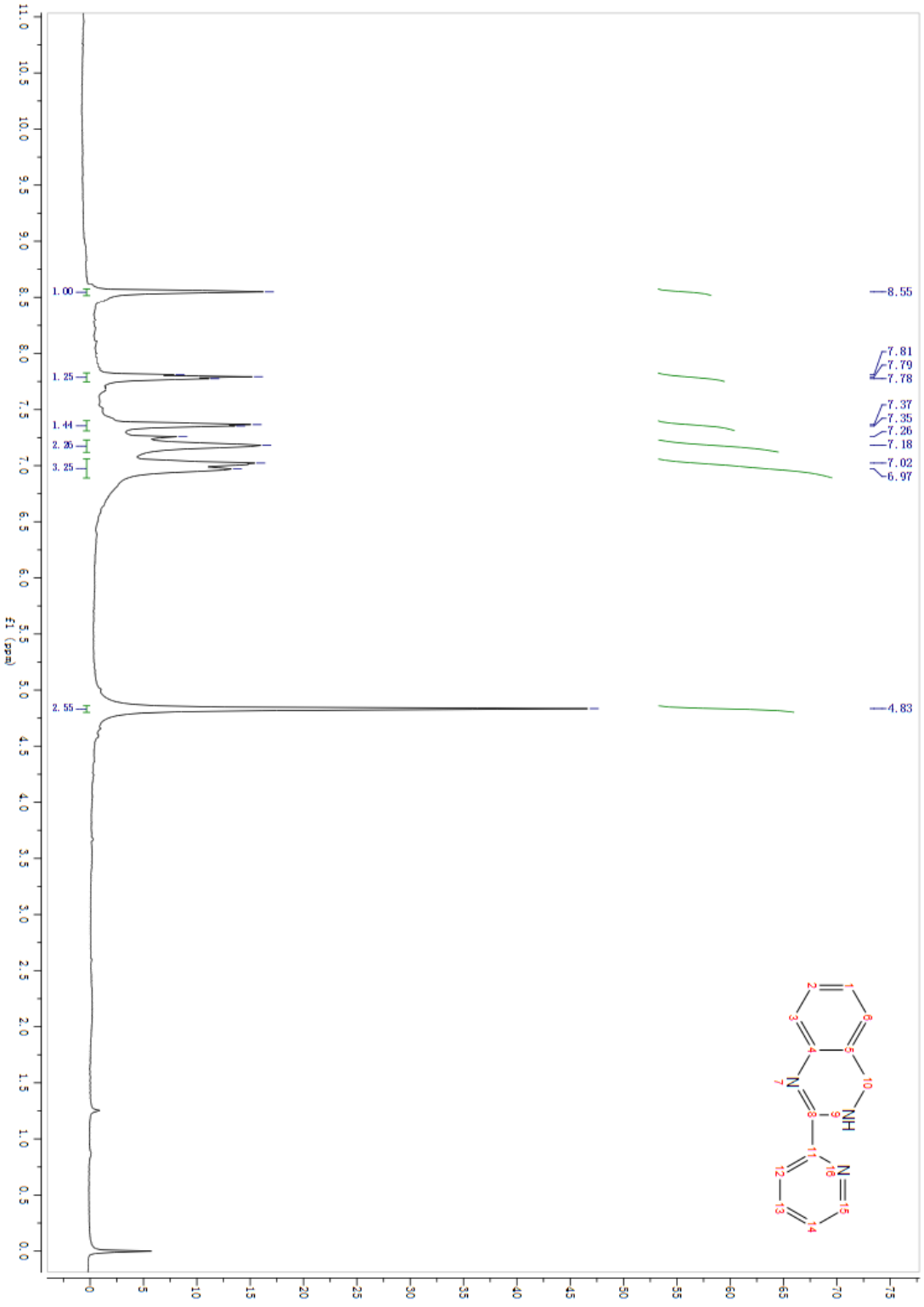

161.30
159.72
149.81
137.41
134.81
130.80
128.72
127.73
123.32
130.80
128.72
128.07
127.87
127.79
127.73
f1 (ppm)

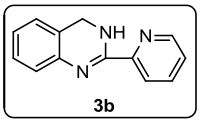

4a


Transmittance [%]
20
30
40
50
60
70
80
90
100
BRUKER
3419.04
3063.14
2920.34
1961.77
1614.58
1586.18
1566.34
1551.07
1483.22
1453.46
1438.59
1399.95
1380.97
1341.74
1319.11
1286.71
1209.22
1168.58
1139.58
1071.50
1055.70
1024.11
984.86
932.68
871.49
815.57
779.48
705.34
689.07
636.51
564.35
553.21
478.69
454.61
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500

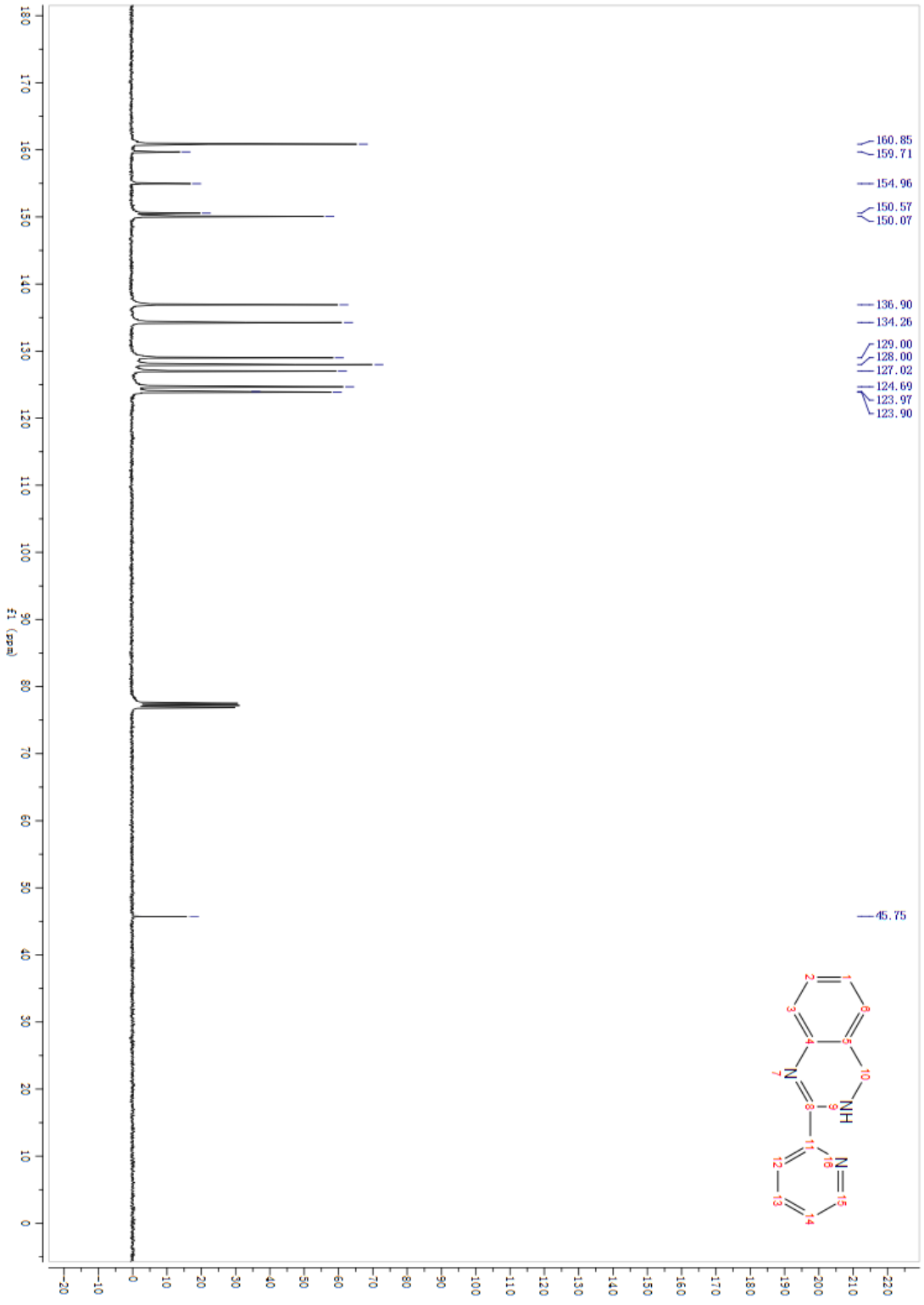

NH
N
N

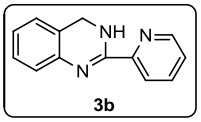
3b


1.00
1.25
1.44
2.26
3.25
2.55
8.55
7.81
7.79
7.78
7.37
7.35
7.26
7.18
7.02
6.97
4.83
f1 (ppm)

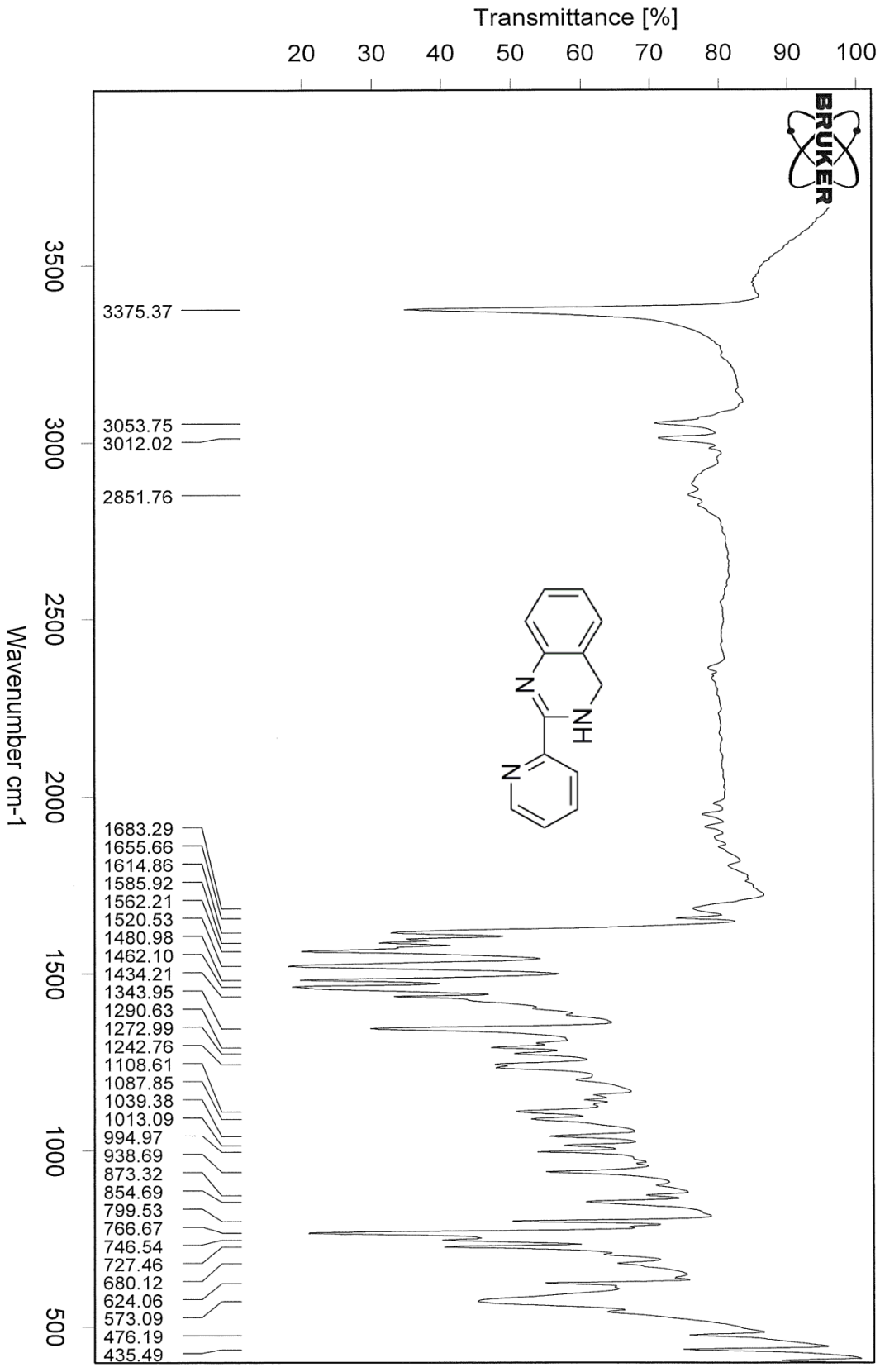

NH
N
N

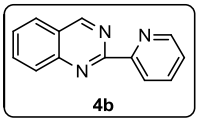
3b


160.85
159.71
154.96
150.57
150.07
136.90
134.26
129.00
128.00
127.02
124.69
123.97
123.90
45.75
f1 (ppm)
NH
N
N

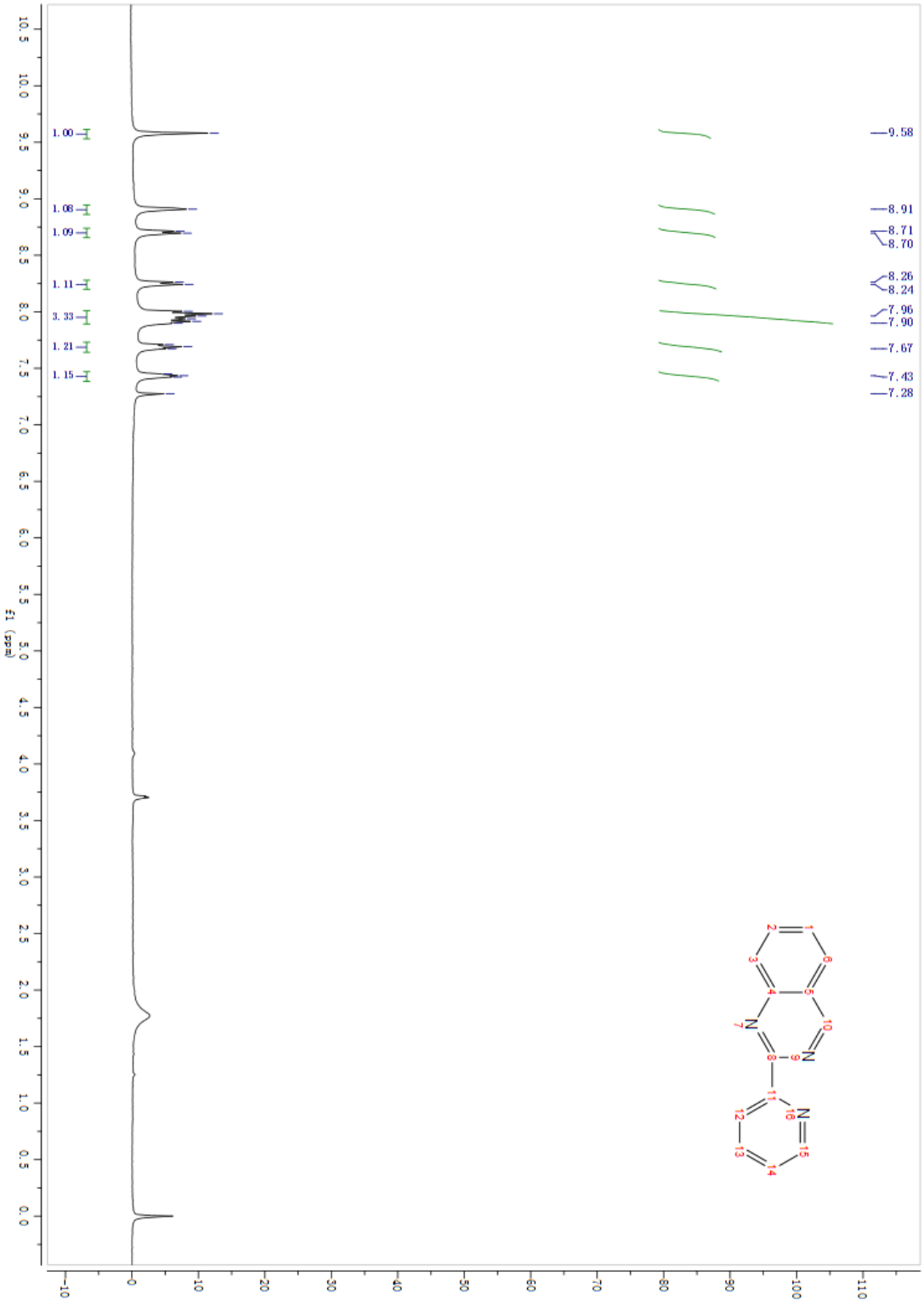

NH
N
N

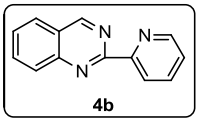
3b

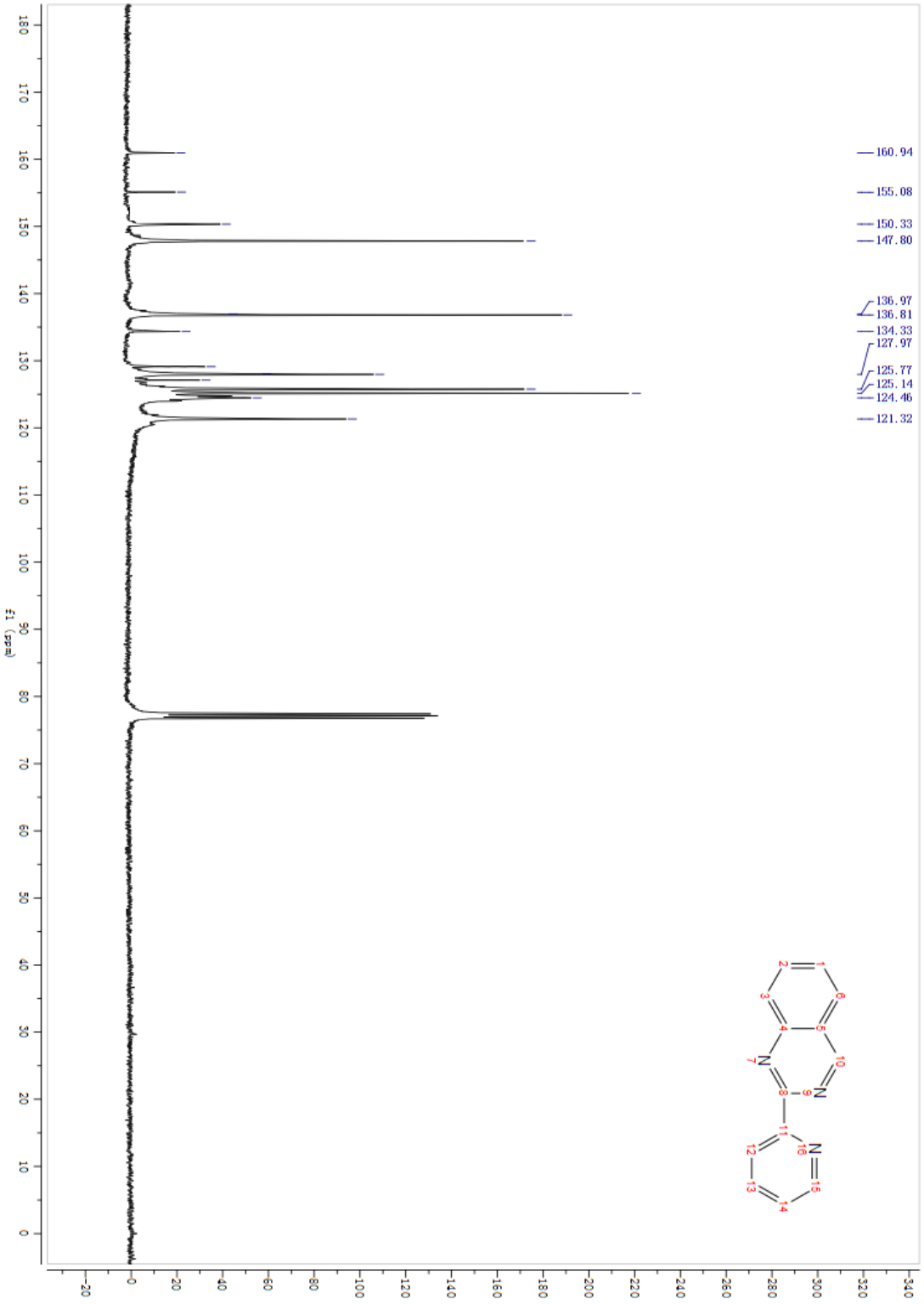

Transmittance [%]
20
30
40
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3375.37
3053.75
3012.02
2851.76
1683.29
1655.66
1614.86
1585.92
1562.21
1520.53
1480.98
1462.10
1434.21
1343.95
1290.63
1272.99
1242.76
1108.61
1087.85
1039.38
1013.09
994.97
938.69
873.32
854.69
799.53
766.67
746.54
727.46
680.12
624.06
573.09
476.19
435.49
N
NH
N

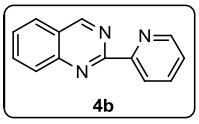

N
N
N

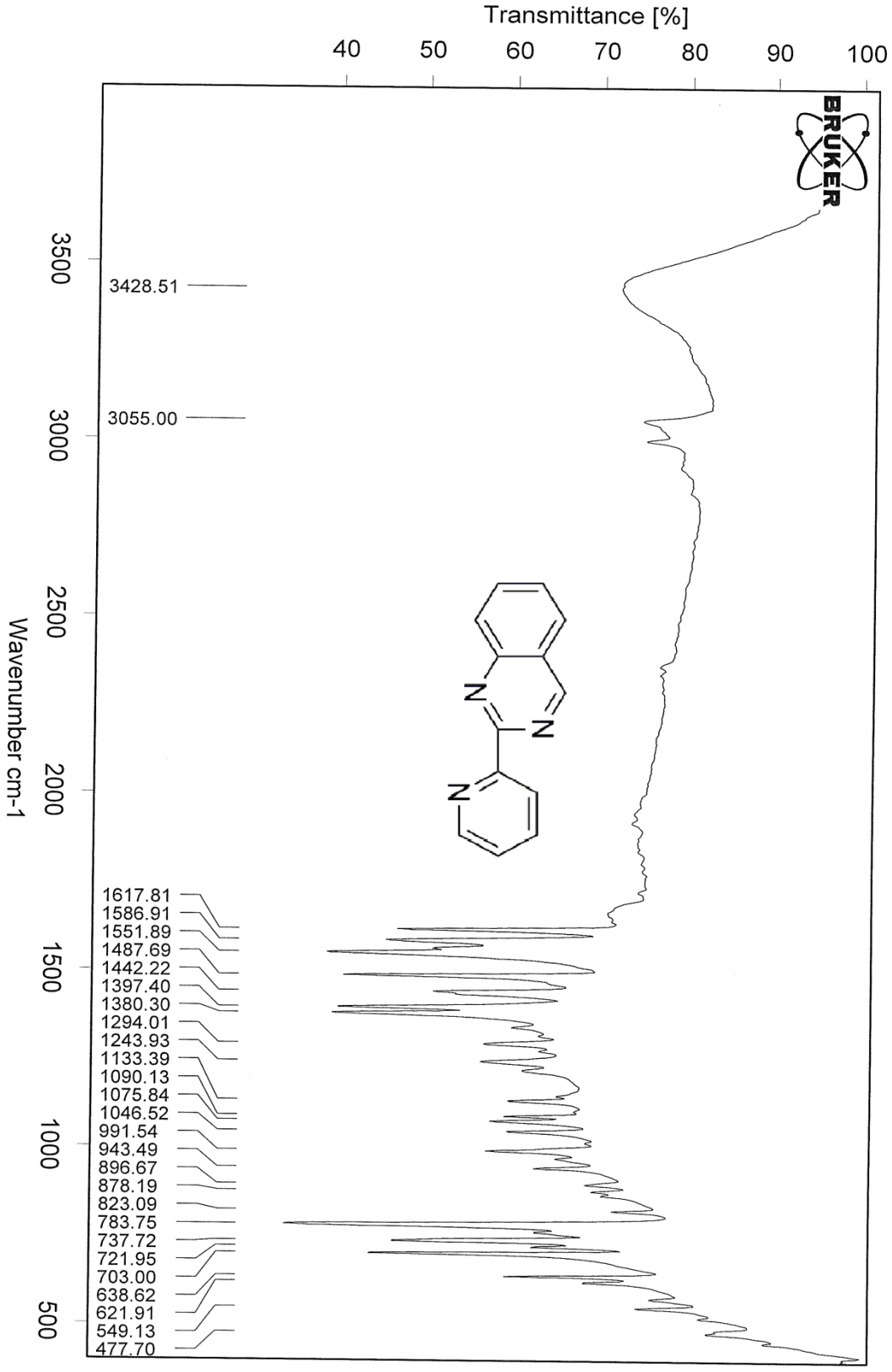
4b

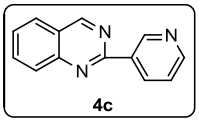

1.00
1.08
1.09
1.11
3.33
1.21
1.15
9.58
8.91
8.71
8.70
8.26
8.24
7.96
7.90
7.67
7.43
7.28
f1 (ppm)

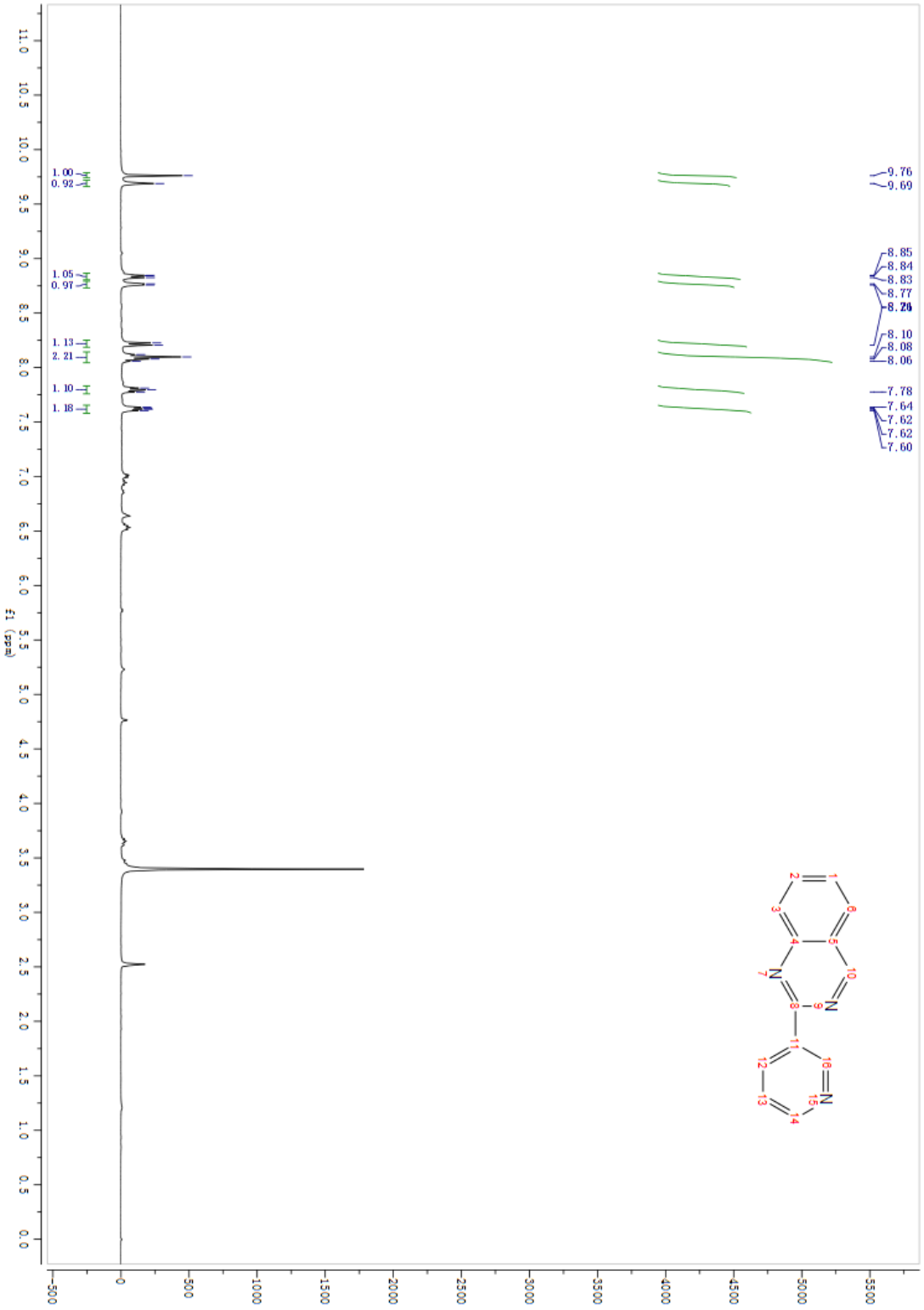

4b

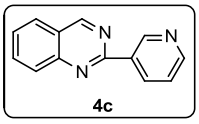

160.94
155.08
150.33
147.80
136.97
136.81
134.33
127.97
125.77
125.14
124.46
121.32
f1 (ppm)

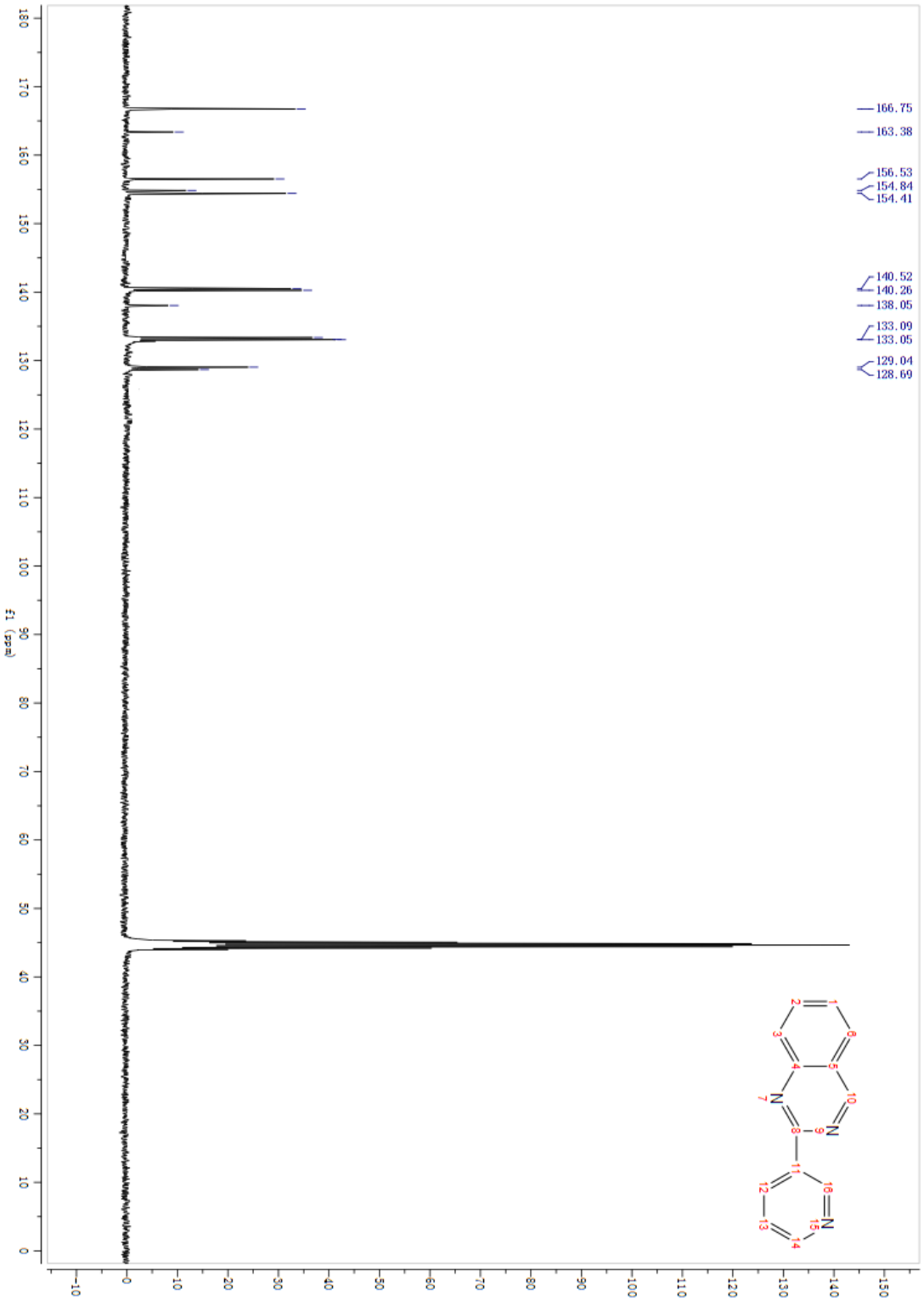

4b

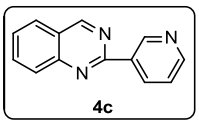

Transmittance [%]
40
50
60
70
80
90
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3428.51
3055.00
1617.81
1586.91
1551.89
1487.69
1442.22
1397.40
1380.30
1294.01
1243.93
1133.39
1090.13
1075.84
1046.52
991.54
943.49
896.67
878.19
823.09
783.75
737.72
721.95
703.00
638.62
621.91
549.13
477.70
N
N
N

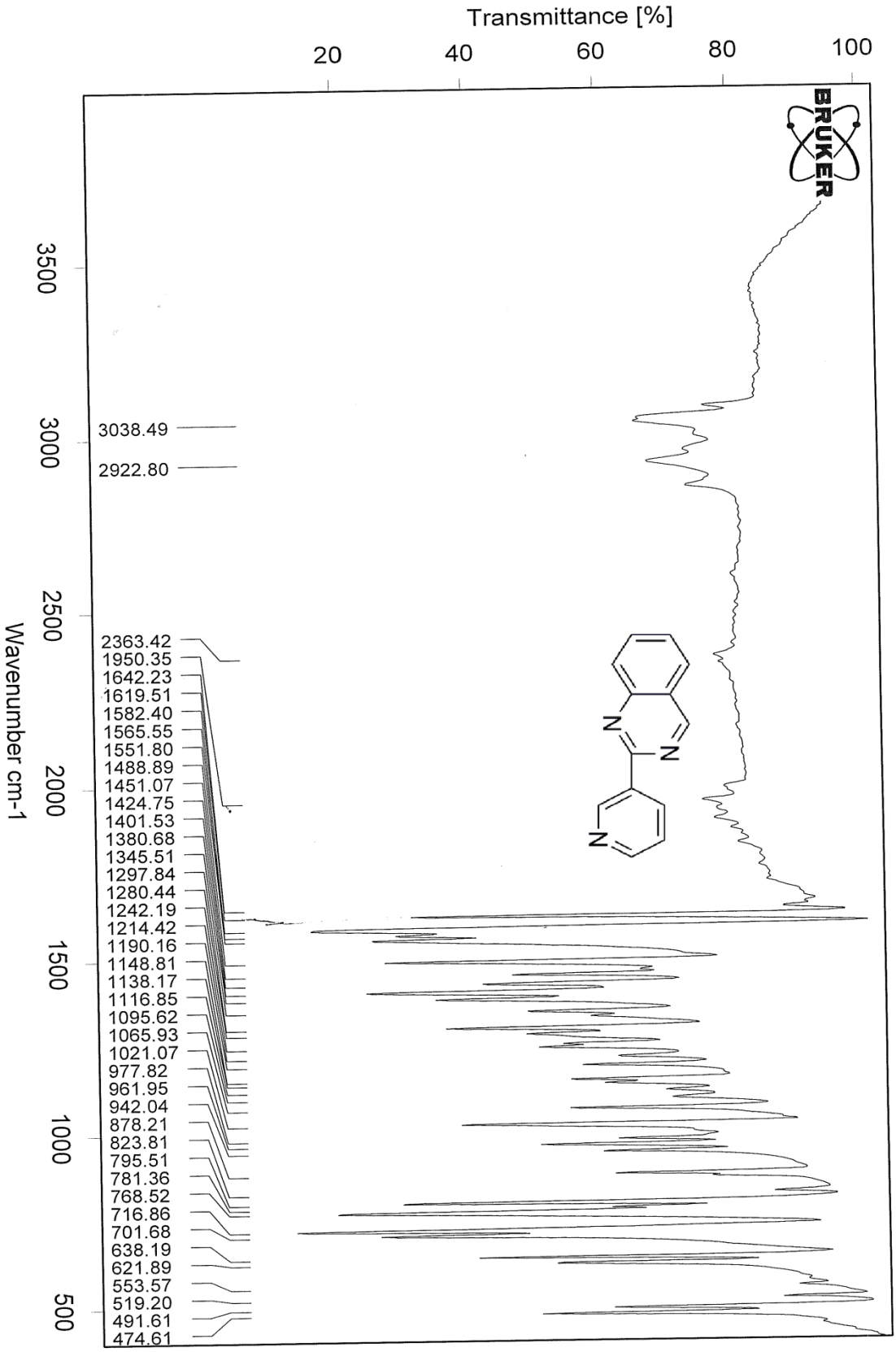

4c

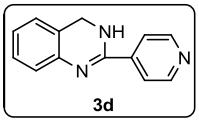

1.00
0.92
1.05
0.97
1.13
2.21
1.10
1.18
9.76
9.69
8.85
8.84
8.83
8.77
8.10
8.08
8.06
7.78
7.64
7.62
7.62
7.60
f1 (ppm)


4c

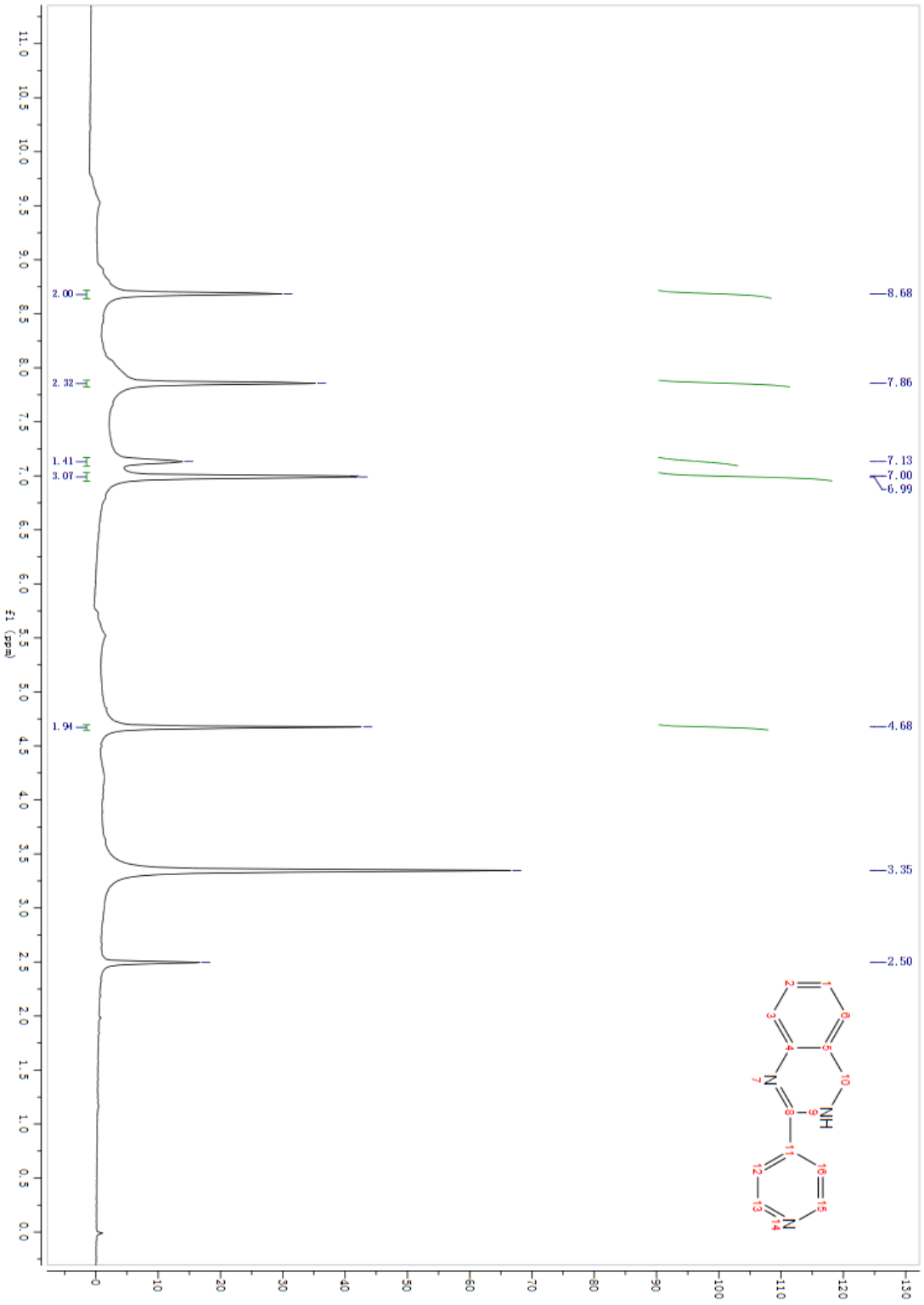

166.75
163.38
156.53
154.84
154.41
140.52
140.26
138.05
133.09
133.05
129.04
128.69
f1 (ppm)

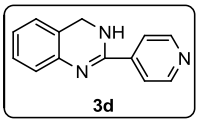

4c


Transmittance [%]
20
40
60
80
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3038.49
2922.80
2363.42
1950.35
1642.23
1619.51
1582.40
1565.55
1551.80
1488.89
1451.07
1424.75
1401.53
1380.68
1345.51
1297.84
1280.44
1242.19
1214.42
1190.16
1148.81
1138.17
1116.85
1095.62
1065.93
1021.07
977.82
961.95
942.04
878.21
823.81
795.51
781.36
768.52
716.86
701.68
638.19
621.89
553.57
519.20
491.61
474.61
N
N
N

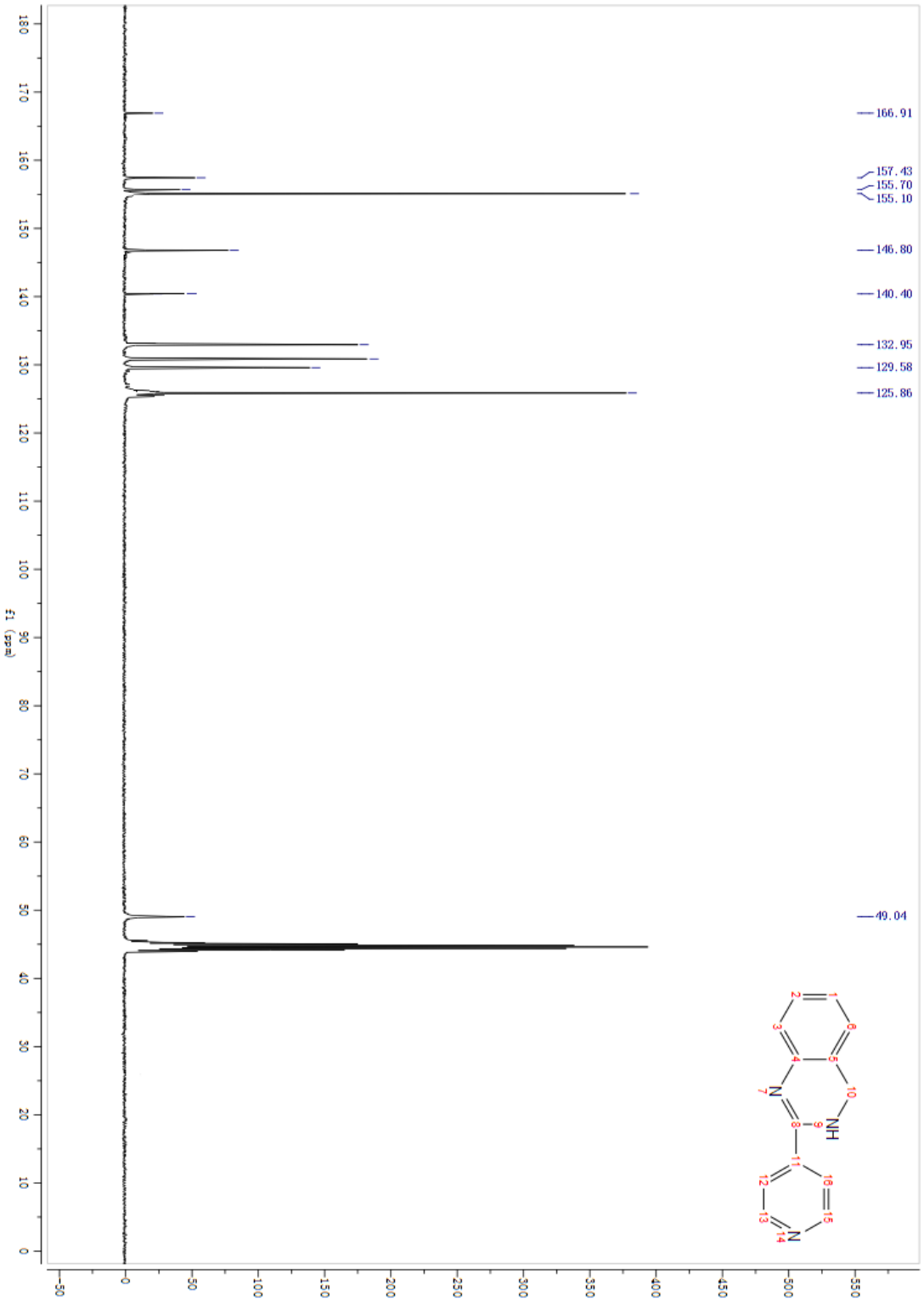


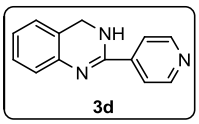
3d

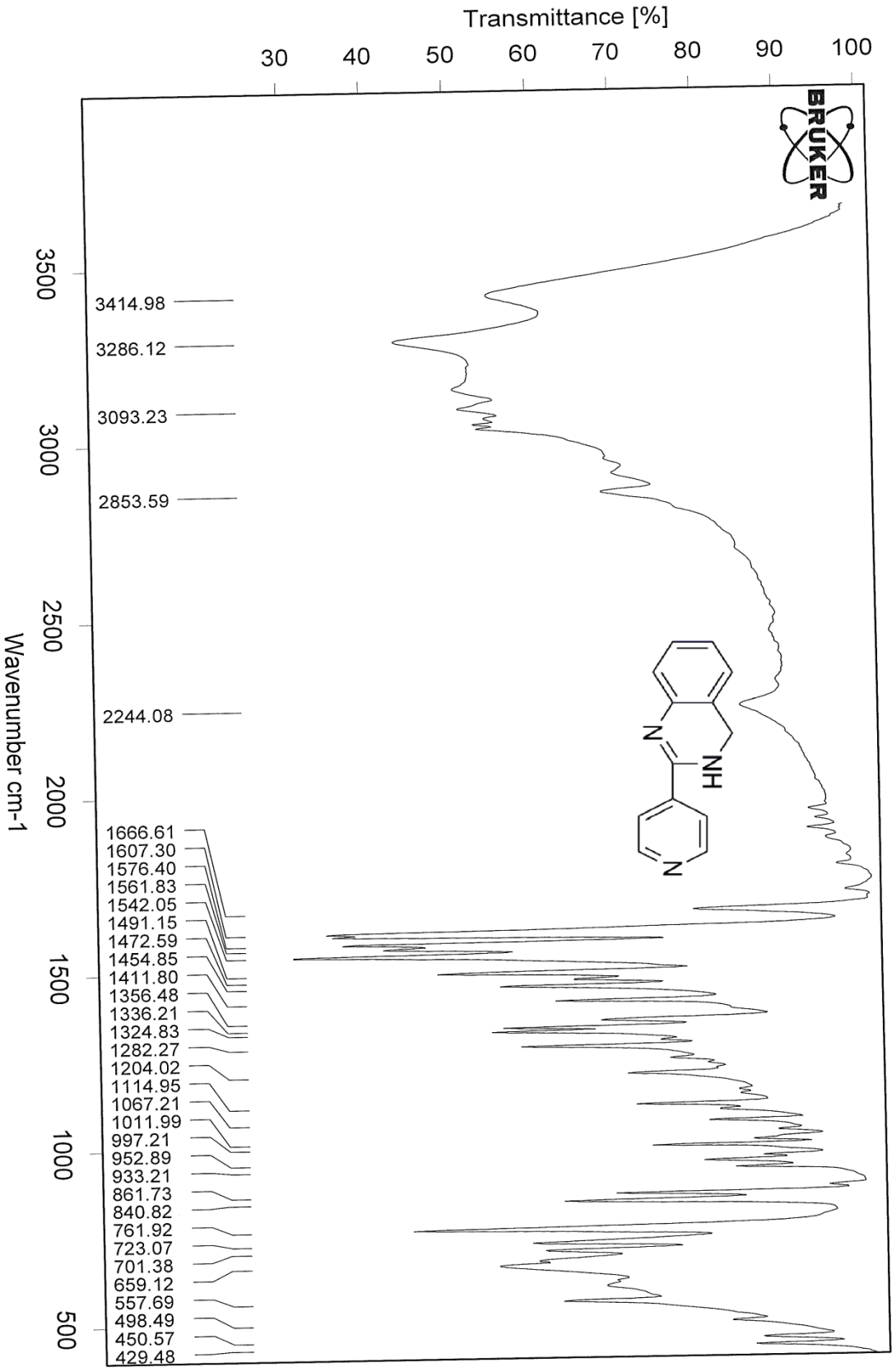


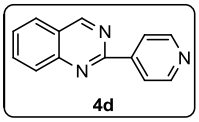

NH
N
N

3d

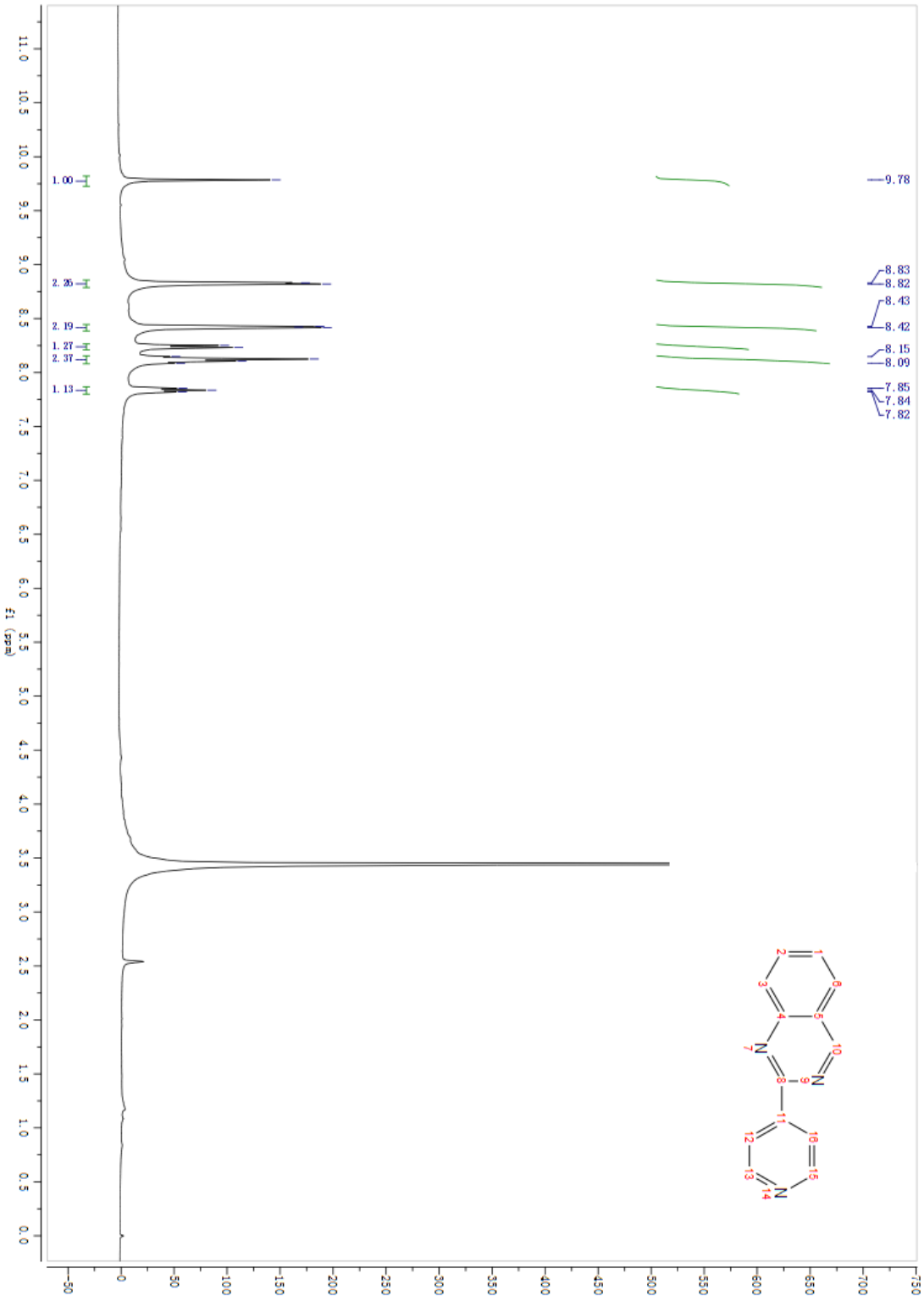

166.91
157.43
155.70
155.10
146.80
140.40
132.95
129.58
125.86
49.04
f1 (ppm)

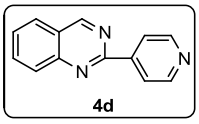

NH
N
N
3d

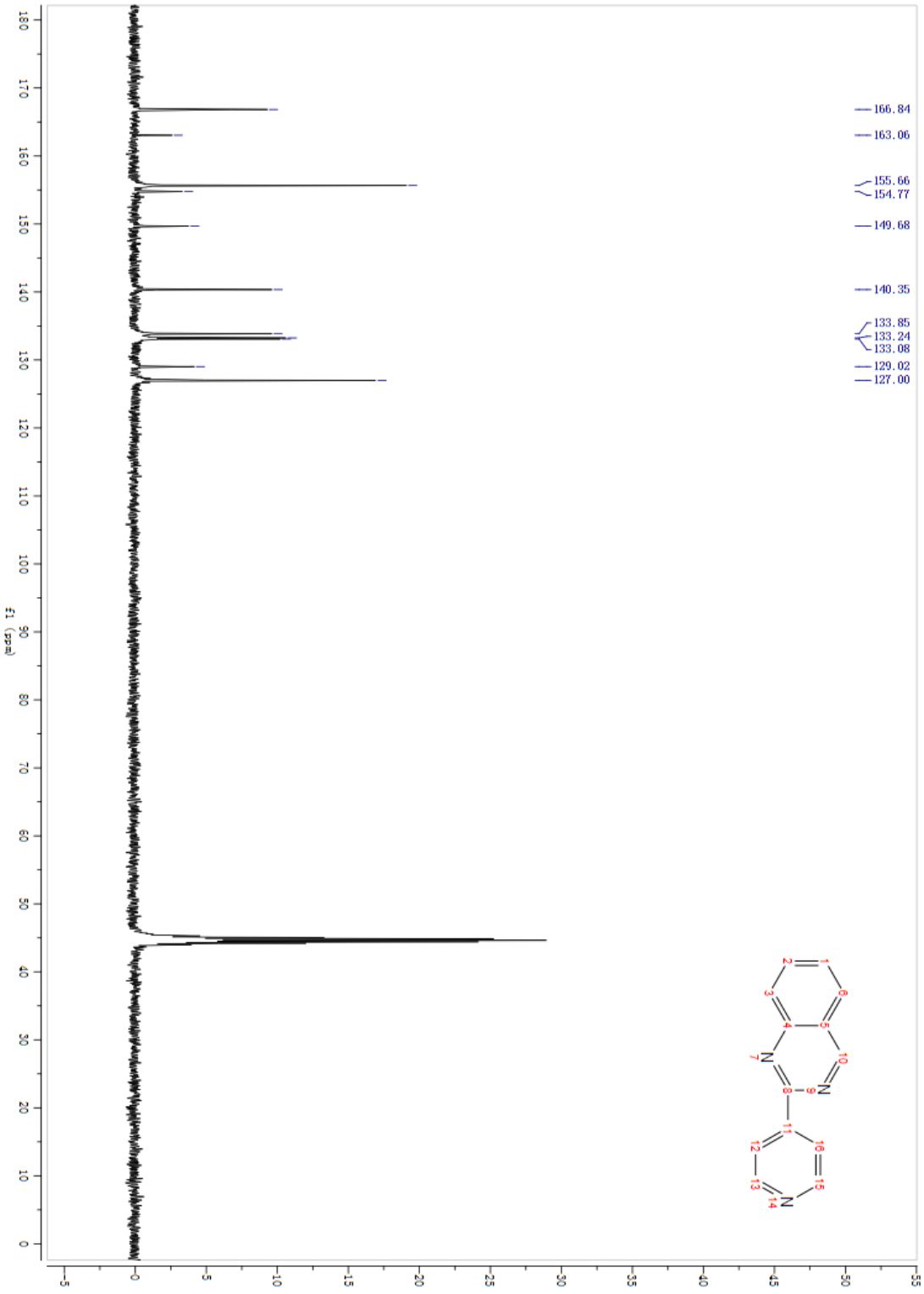

Transmittance [%]
30
40
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3414.98
3286.12
3093.23
2853.59
2244.08
1666.61
1607.30
1576.40
1561.83
1542.05
1491.15
1472.59
1454.85
1411.80
1356.48
1336.21
1324.83
1282.27
1204.02
1114.95
1067.21
1011.99
997.21
952.89
933.21
861.73
840.82
761.92
723.07
701.38
659.12
557.69
498.49
450.57
429.48
N
NH
N

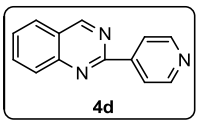

N
N
N

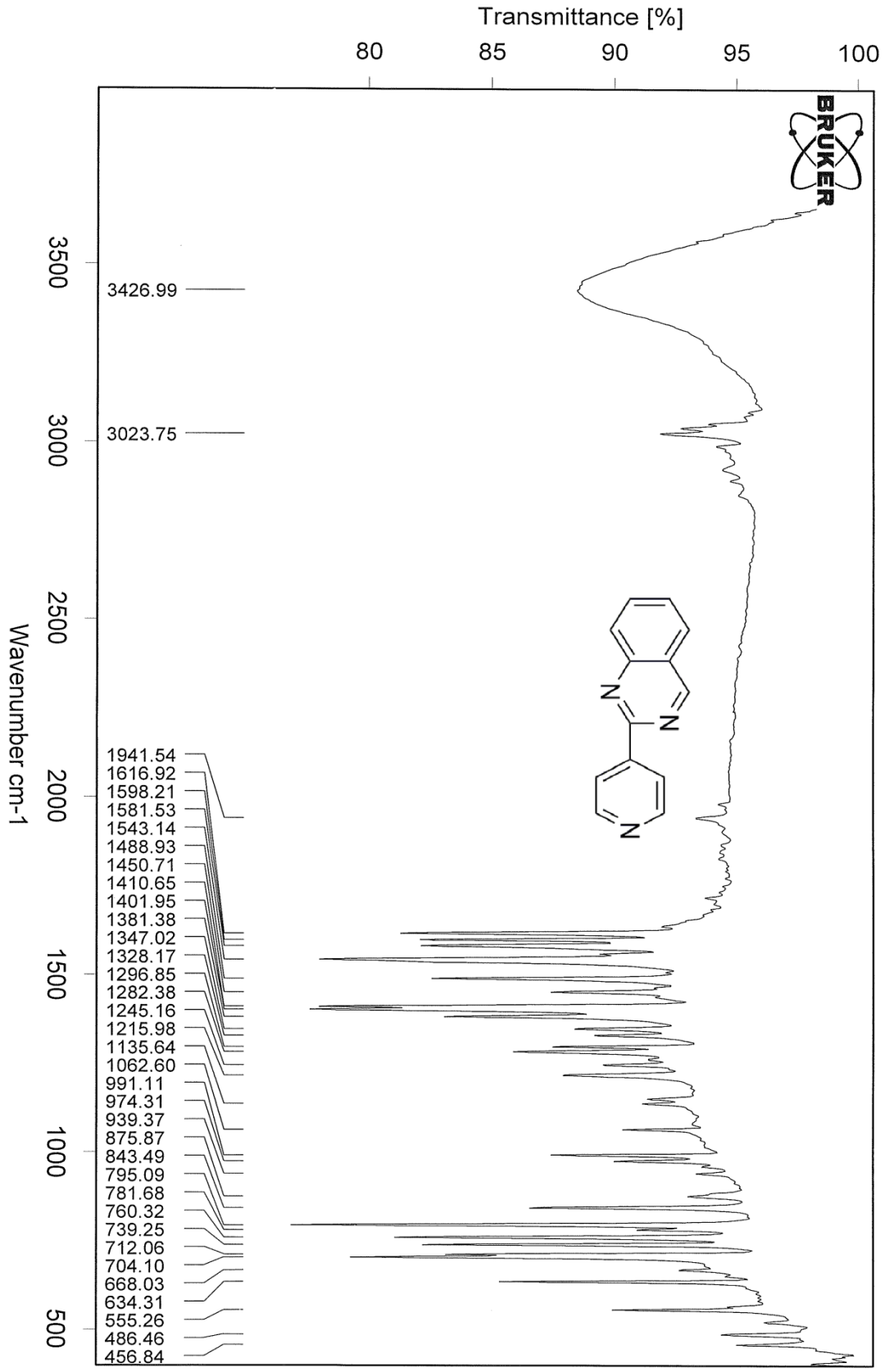
4d

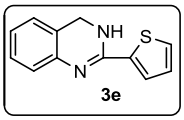

1.00
2.26
2.19
1.27
2.37
1.13
9.78
8.83
8.82
8.43
8.42
8.15
8.09
7.85
7.84
7.82
f1 (ppm)


4d

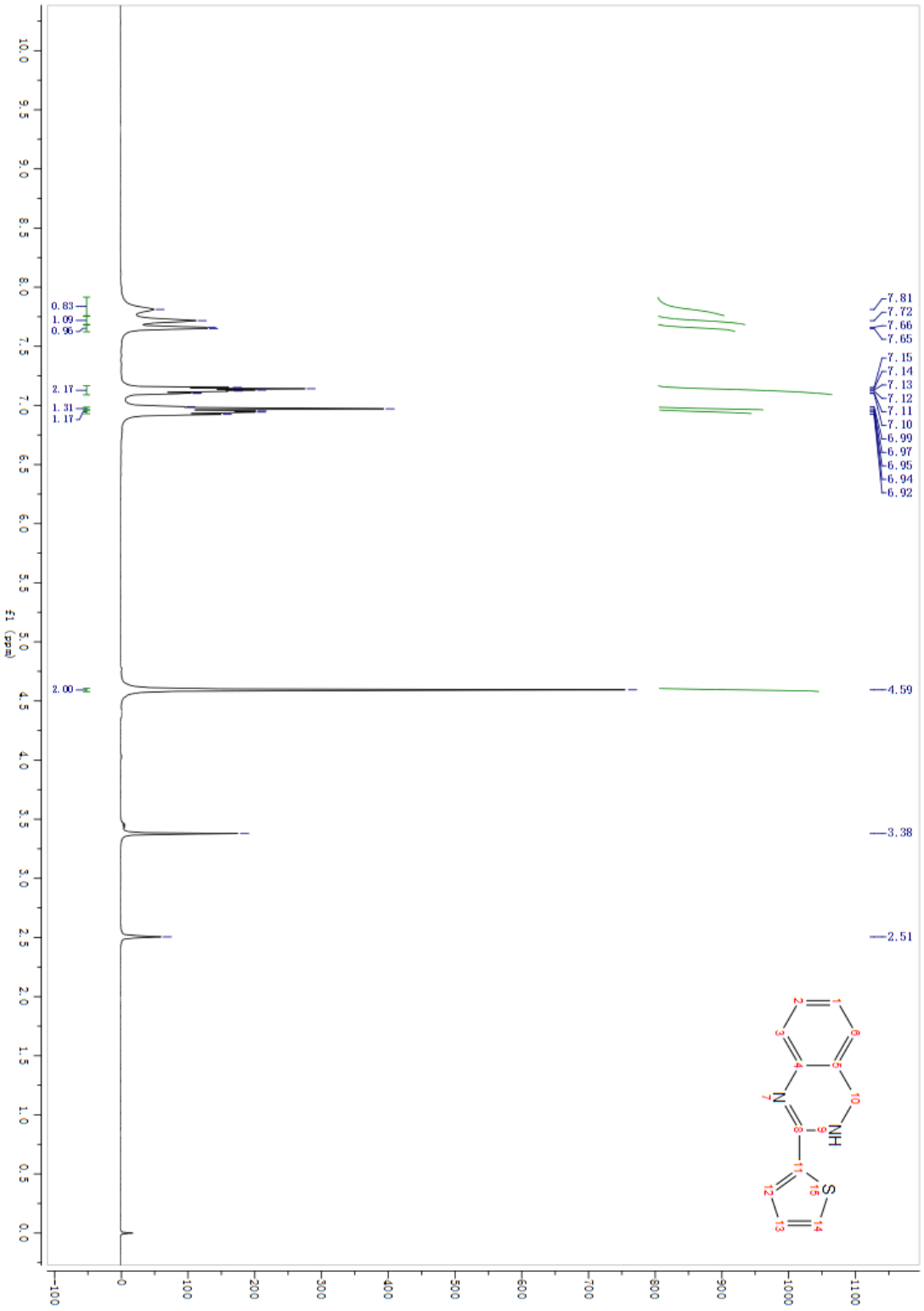

166.84
163.06
155.66
154.77
149.68
140.35
133.85
133.24
133.08
129.02
127.00
f1 (ppm)

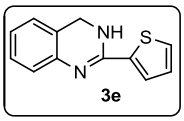

4d

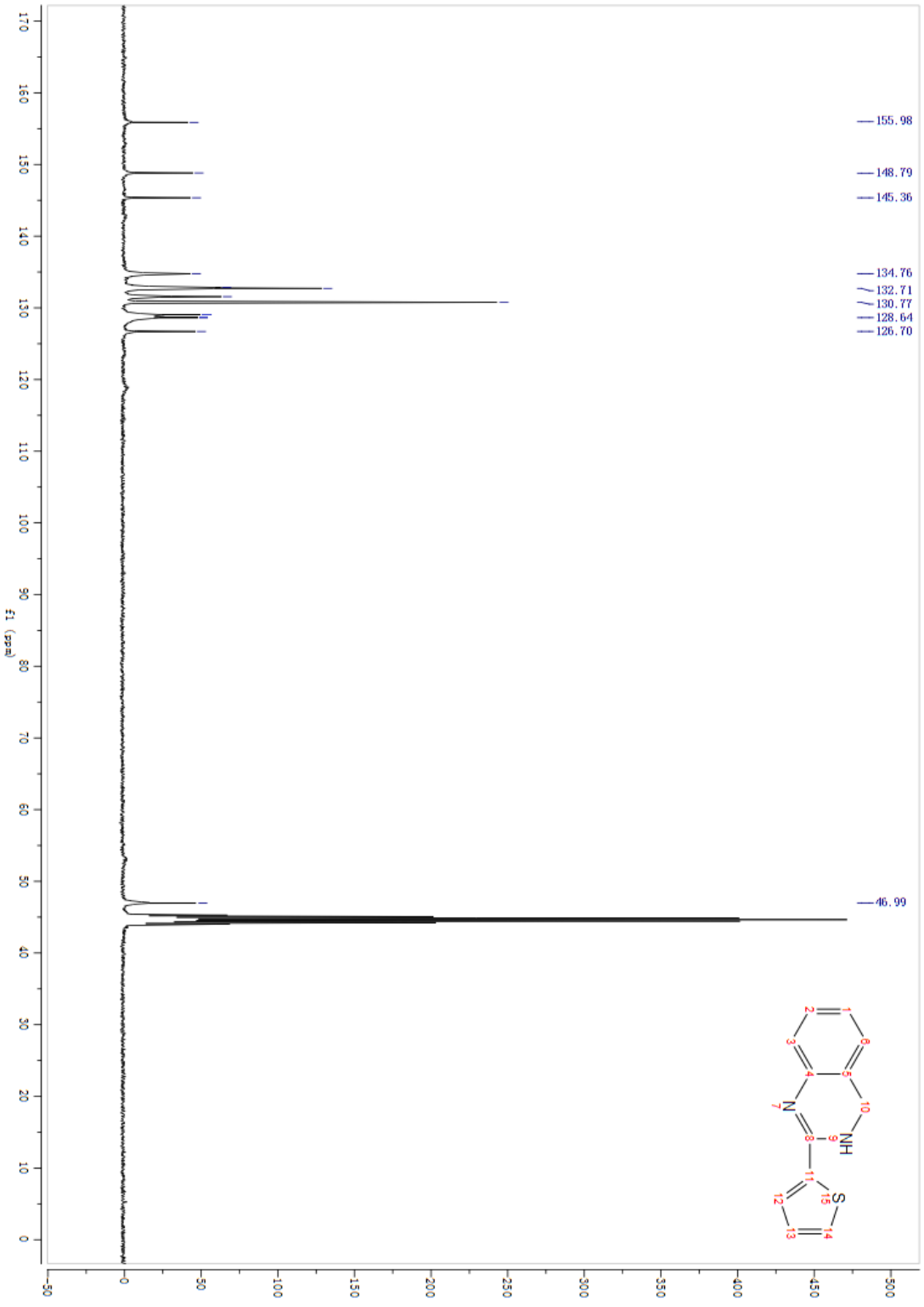

Transmittance [%]
80
85
90
95
100
BRUKER
3426.99
3023.75
1941.54
1616.92
1598.21
1581.53
1543.14
1488.93
1450.71
1410.65
1401.95
1381.38
1347.02
1328.17
1296.85
1282.38
1245.16
1215.98
1135.64
1062.60
991.11
974.31
939.37
875.87
843.49
795.09
781.68
760.32
739.25
712.06
704.10
668.03
634.31
555.26
486.46
456.84
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
N
N
N

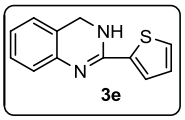

NH
S
N

3e

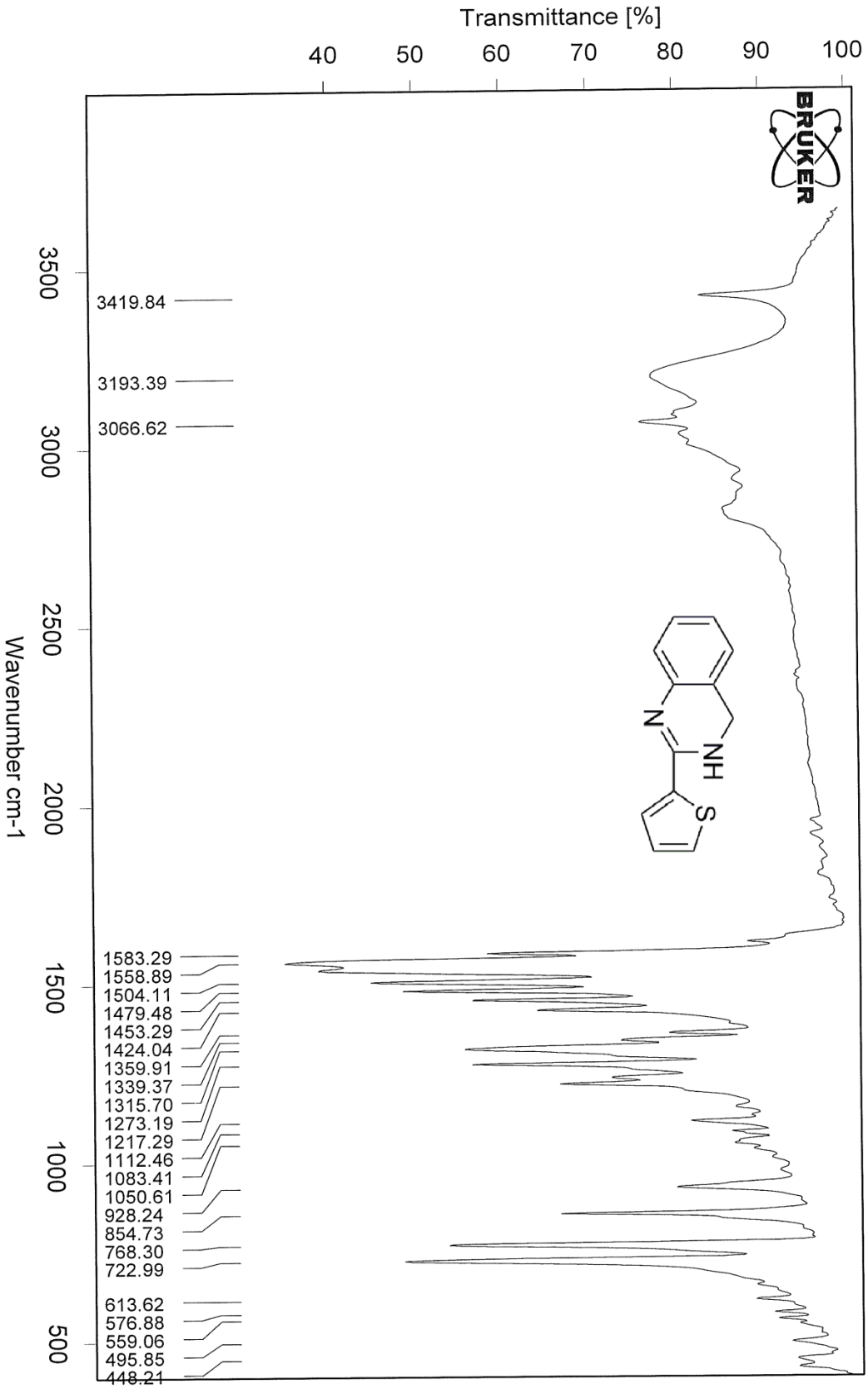

7.81
7.72
7.66
7.65
7.15
7.14
7.13
7.12
7.11
7.10
6.99
6.97
6.95
6.94
6.92
4.59
3.38
2.51
0.83
1.09
0.96
2.17
1.31
1.17
2.00
f1 (ppm)

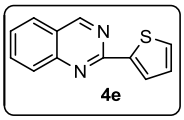

NH
S
N
3e

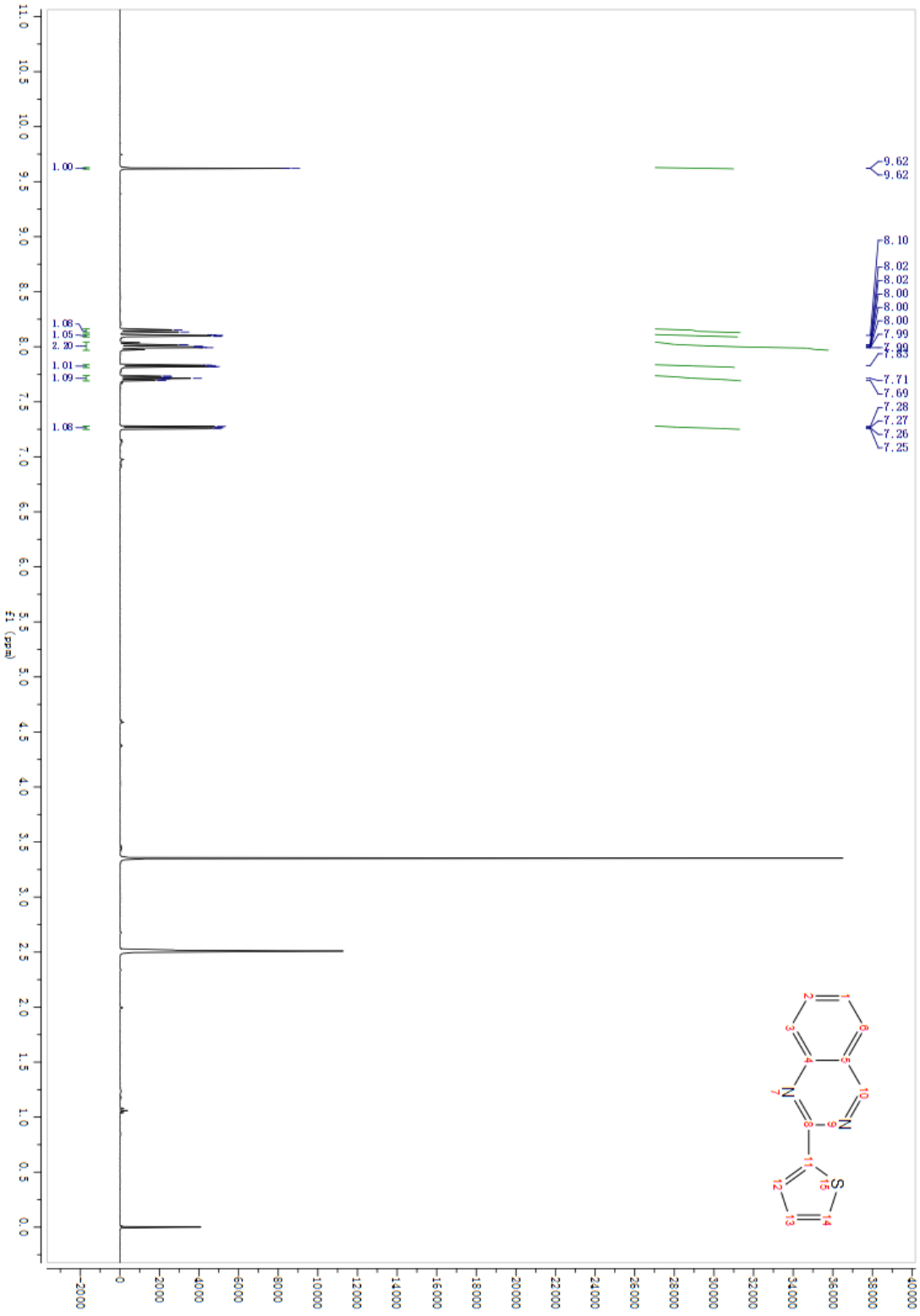

155.98
148.79
145.36
134.76
132.71
130.77
128.64
126.70
46.99
f1 (ppm)


NH
S
N

3e


Transmittance [%]
40
50
60
70
80
90
100
BRUKER
3419.84
3193.39
3066.62
1583.29
1558.89
1504.11
1479.48
1453.29
1424.04
1359.91
1339.37
1315.70
1273.19
1217.29
1112.46
1083.41
1050.61
928.24
854.73
768.30
722.99
613.62
576.88
559.06
495.85
448.21
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
N
NH
S


N
S
N
4e


9.62
9.62
8.10
8.02
8.02
8.00
8.00
8.00
7.99
7.71
7.69
7.28
7.27
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7.25
1.00
1.08
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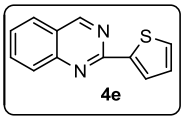
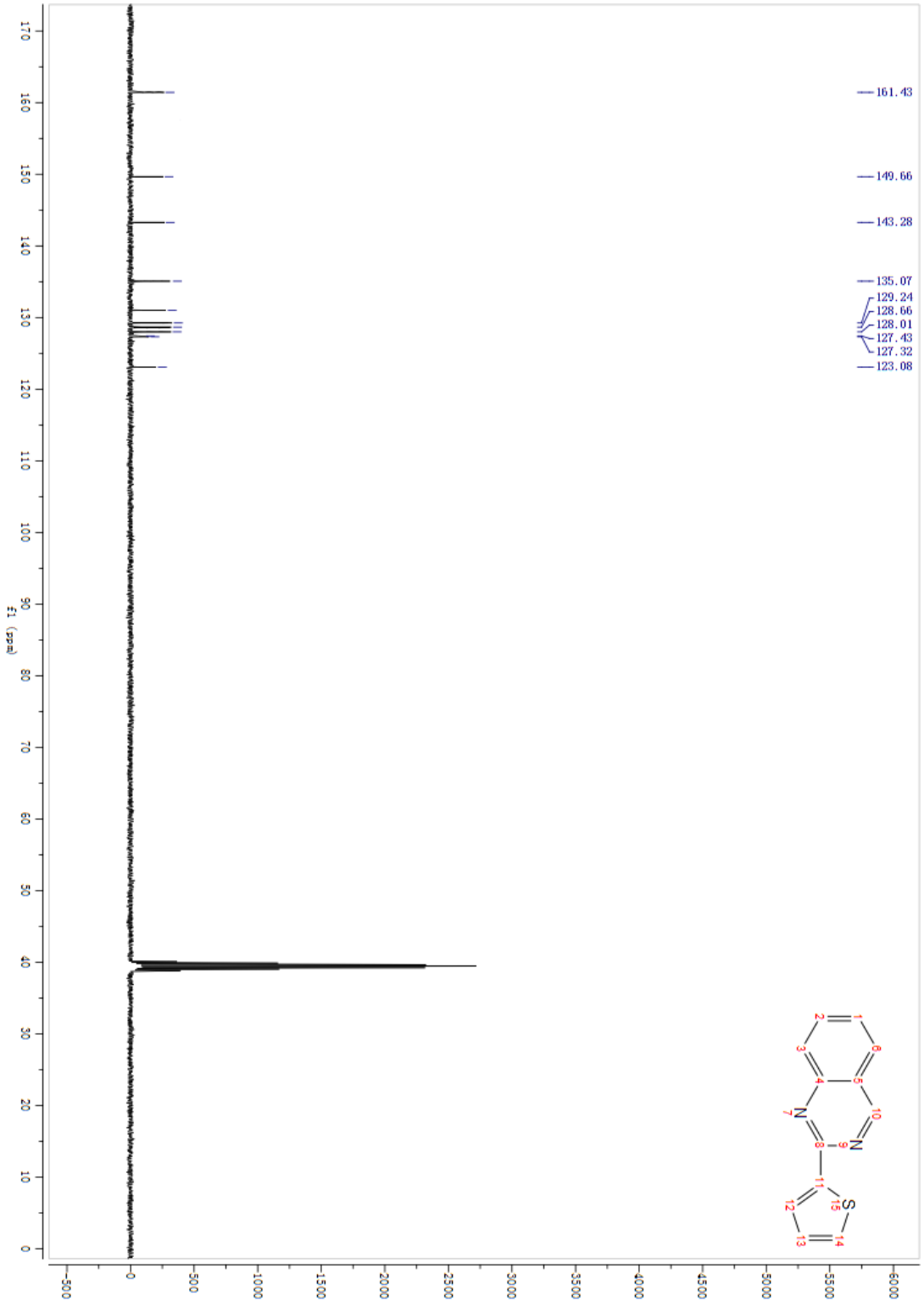
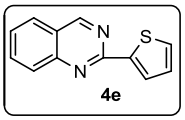
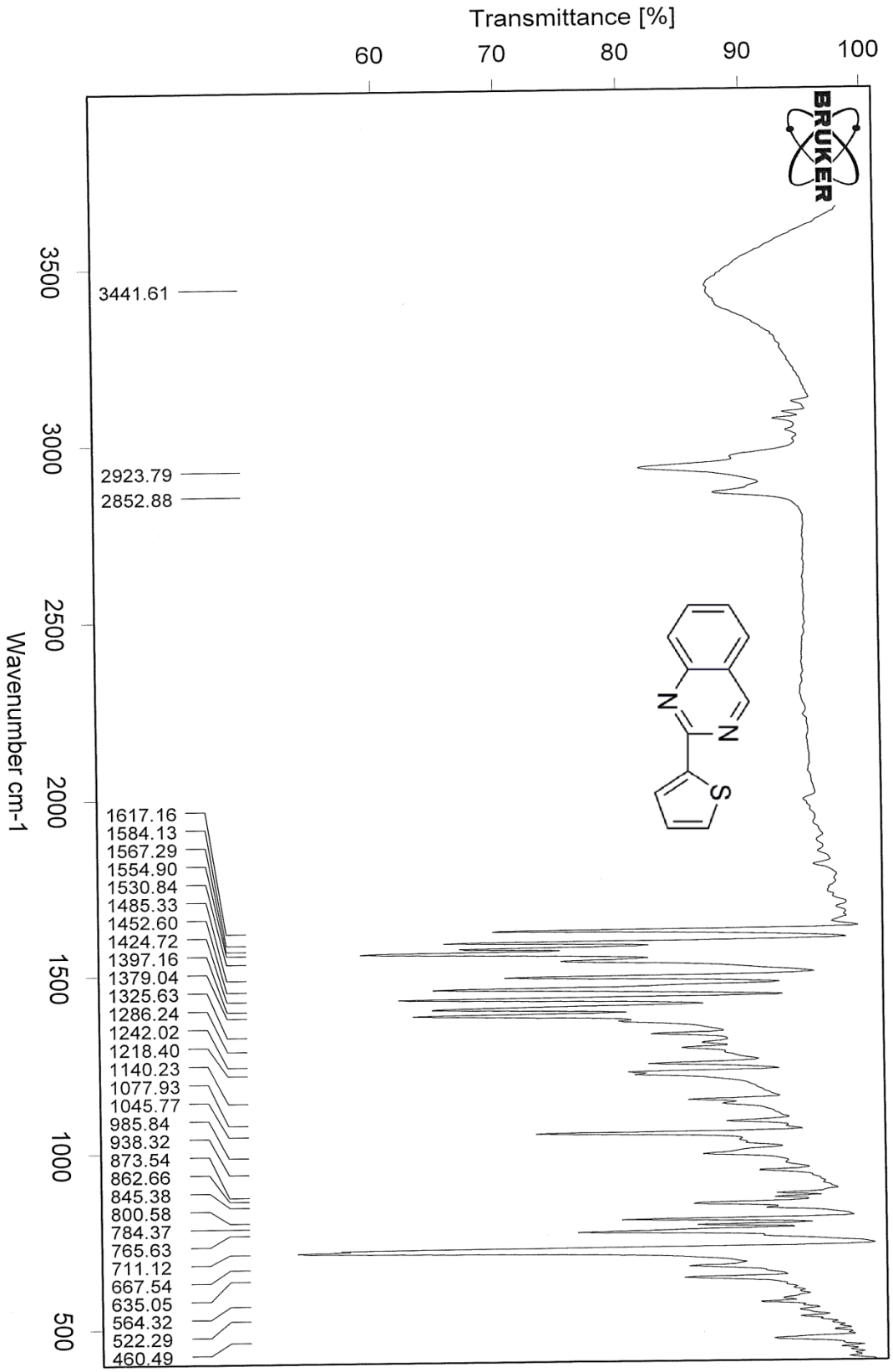
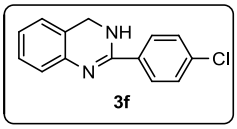
1.09
1.08
f1 (ppm)


N
S
N
4e

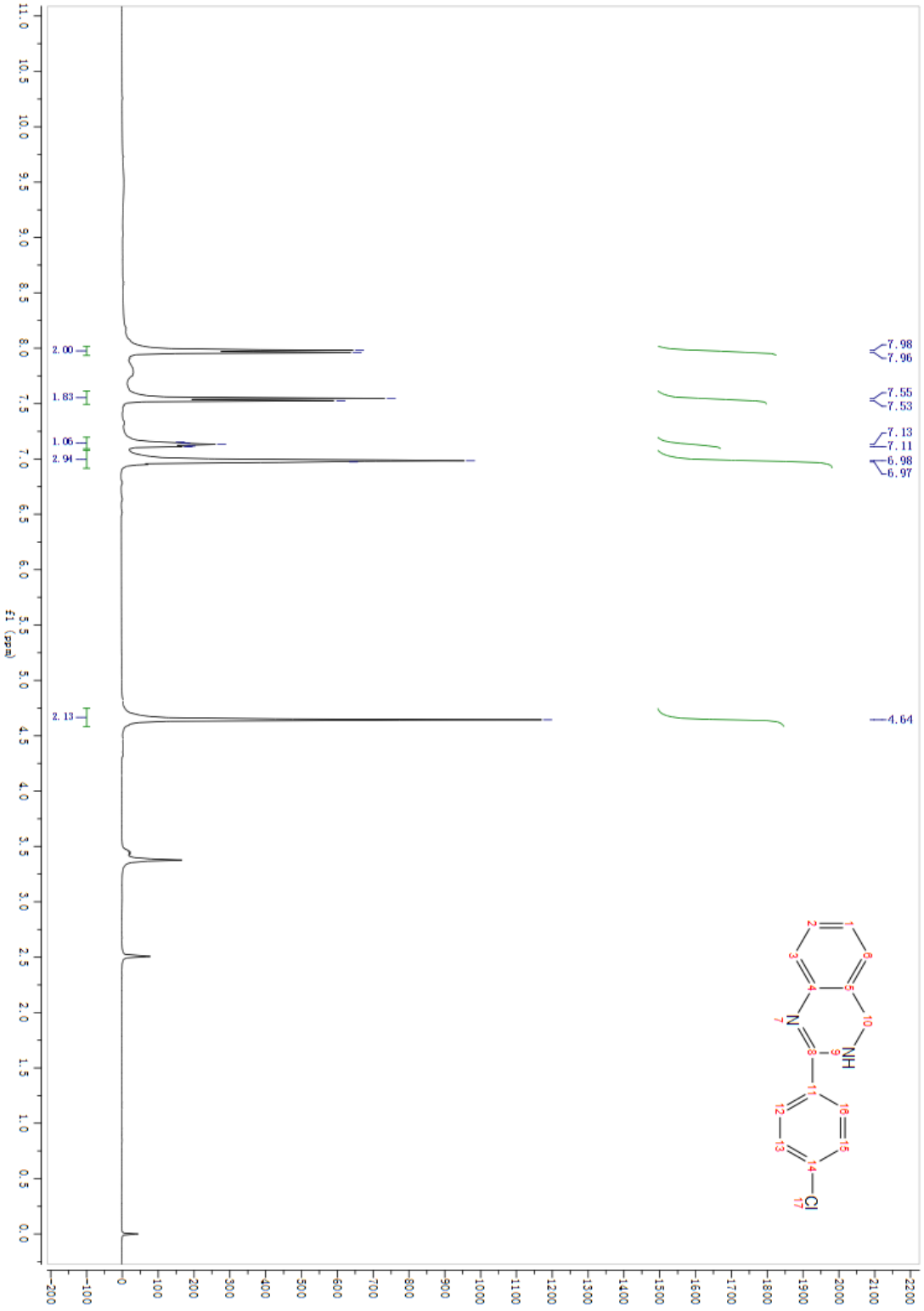

161.43
149.66
143.28
135.07
129.24
128.66
128.01
127.43
127.32
123.08
f1 (ppm)

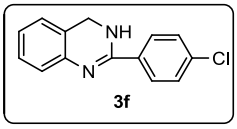

N
S
N
4e


Transmittance [%]
60
70
80
90
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3441.61
2923.79
2852.88
1617.16
1584.13
1567.29
1554.90
1530.84
1485.33
1452.60
1424.72
1397.16
1379.04
1325.63
1286.24
1242.02
1218.40
1140.23
1077.93
1045.77
985.84
938.32
873.54
862.66
845.38
800.58
784.37
765.63
711.12
667.54
635.05
564.32
522.29
460.49
N
N
S

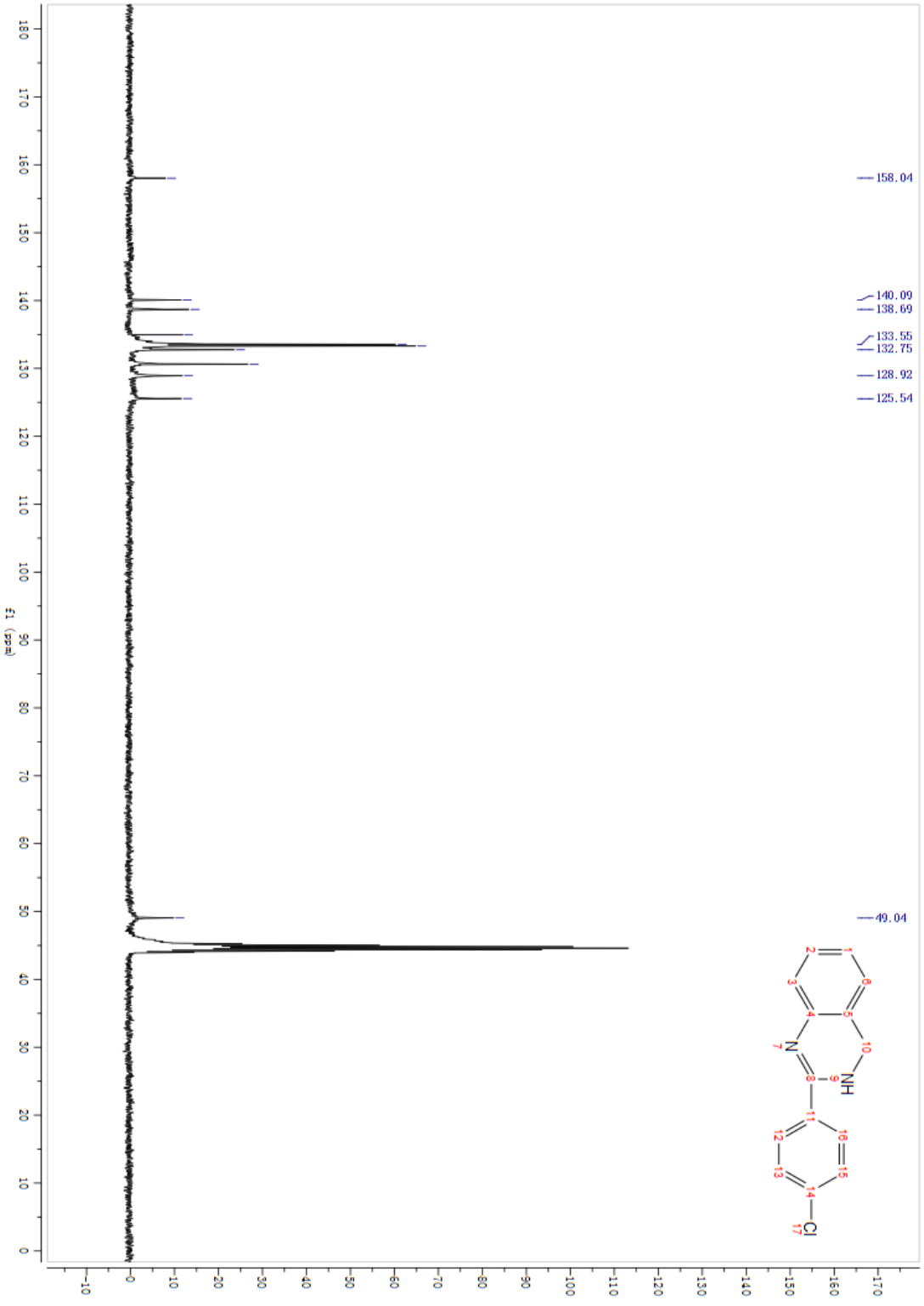

NH
N
Cl

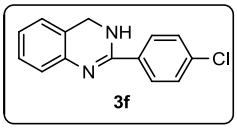
3f


2.00
1.83
1.06
2.94
2.13
7.98
7.96
7.55
7.53
7.13
7.11
6.98
6.97
4.64
f1 (ppm)

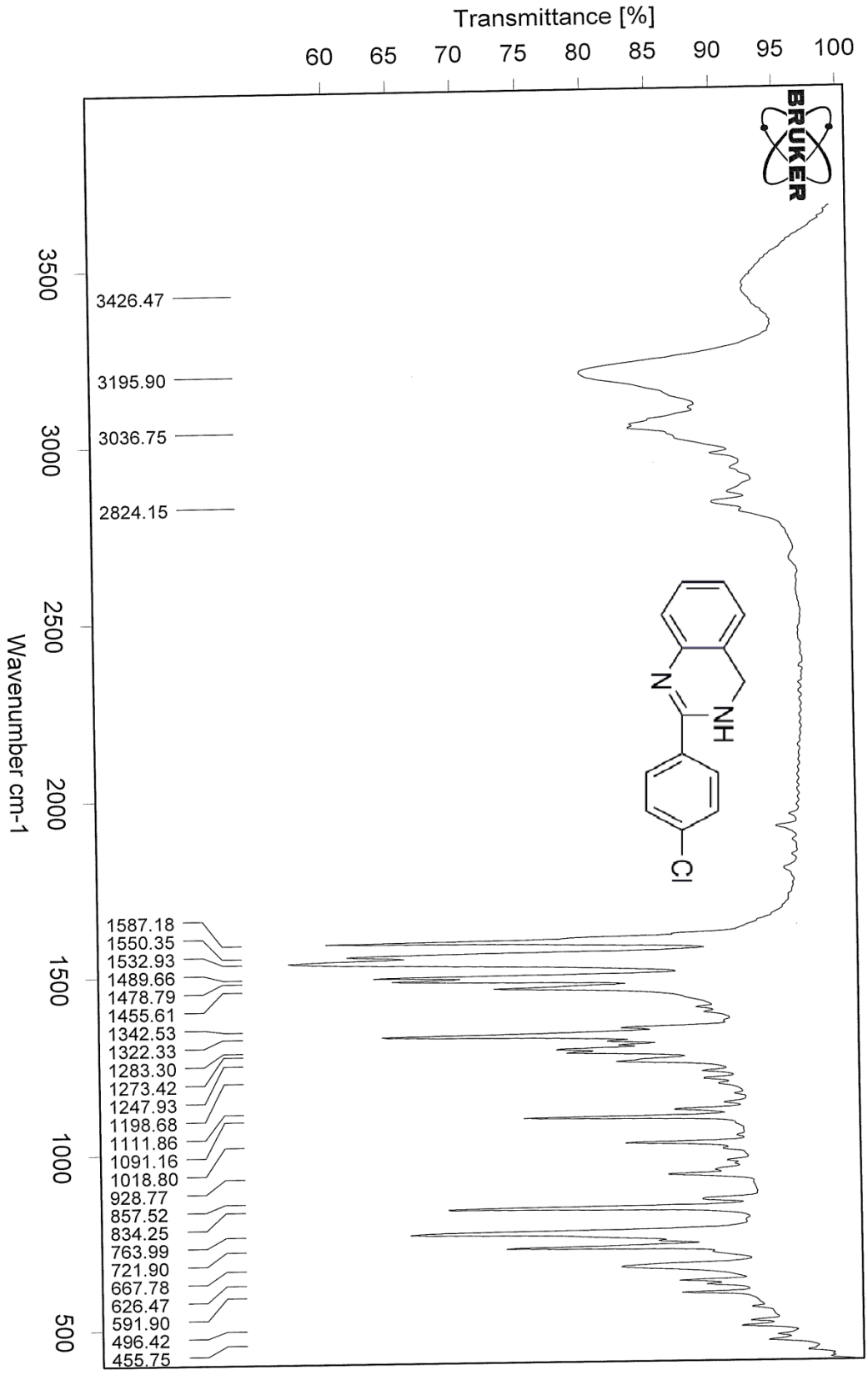


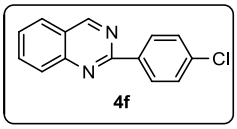
3f



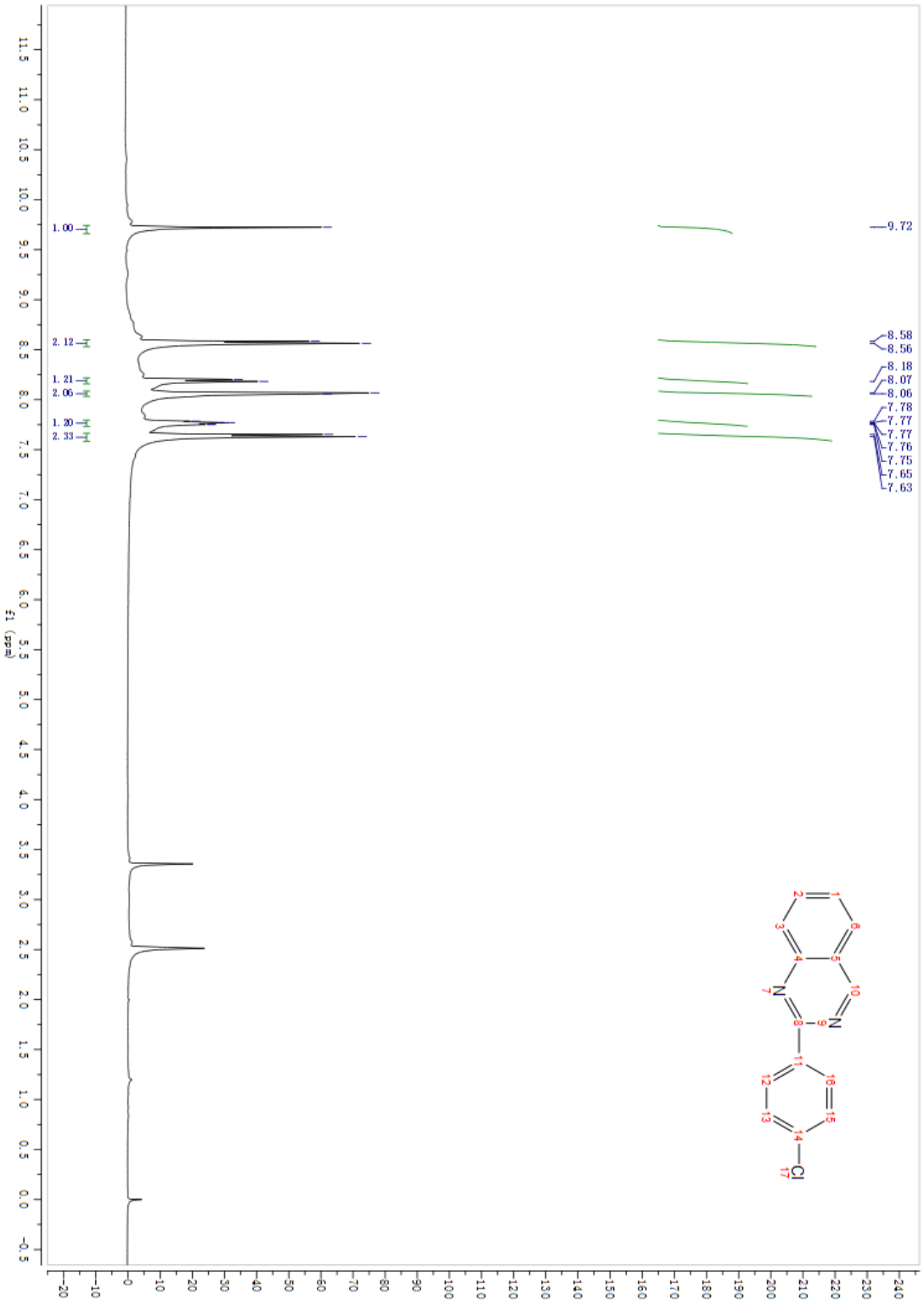

NH
N
Cl

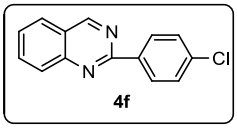
3f


Transmittance [%]
60
65
70
75
80
85
90
95
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3426.47
3195.90
3036.75
2824.15
1587.18
1550.35
1532.93
1489.66
1478.79
1455.61
1342.53
1322.33
1283.30
1273.42
1247.93
1198.68
1111.86
1091.16
1018.80
928.77
857.52
834.25
763.99
721.90
667.78
626.47
591.90
496.42
455.75
N
NH
Cl

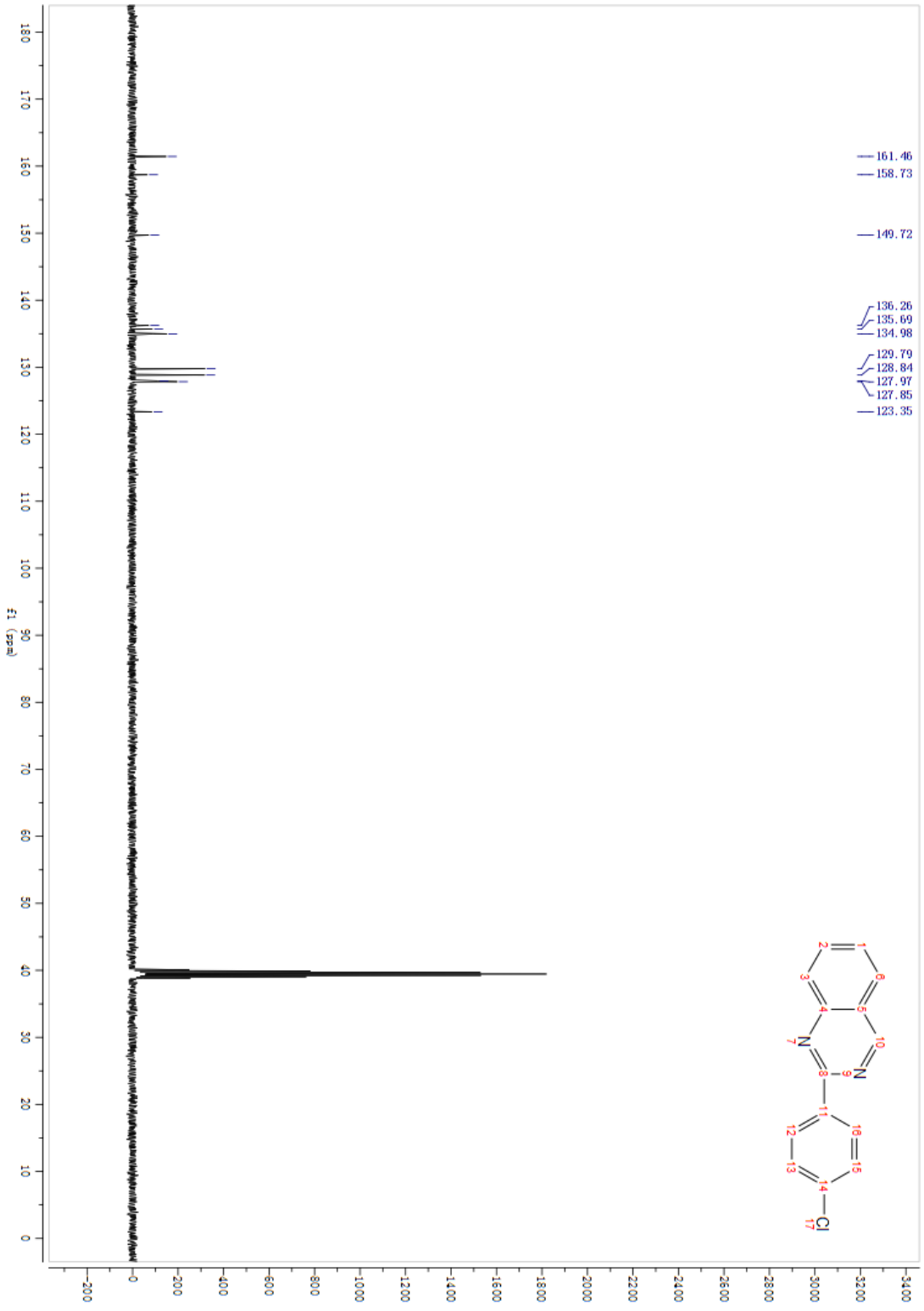

N
N
Cl

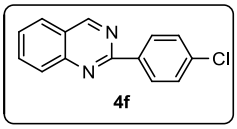
4f


1.00
2.12
1.21
2.06
1.20
2.33
9.72
8.58
8.56
8.18
8.07
8.06
7.78
7.77
7.77
7.76
7.75
7.65
7.63
f1 (ppm)

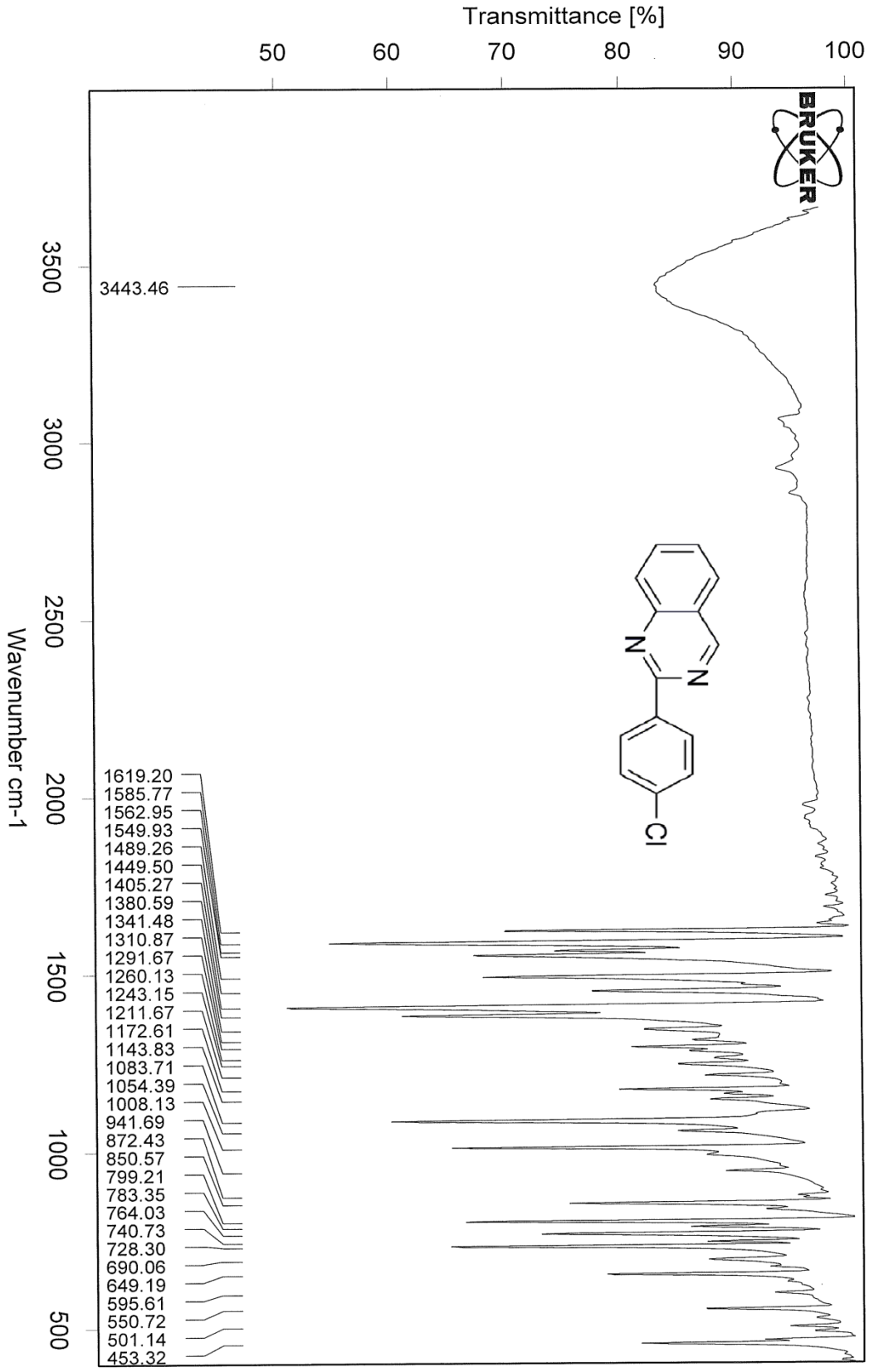

N
N
Cl

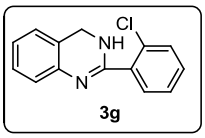
4f


161.46
158.73
149.72
136.26
135.69
134.98
129.79
128.84
127.97
127.85
123.35
f1 (ppm)
Cl

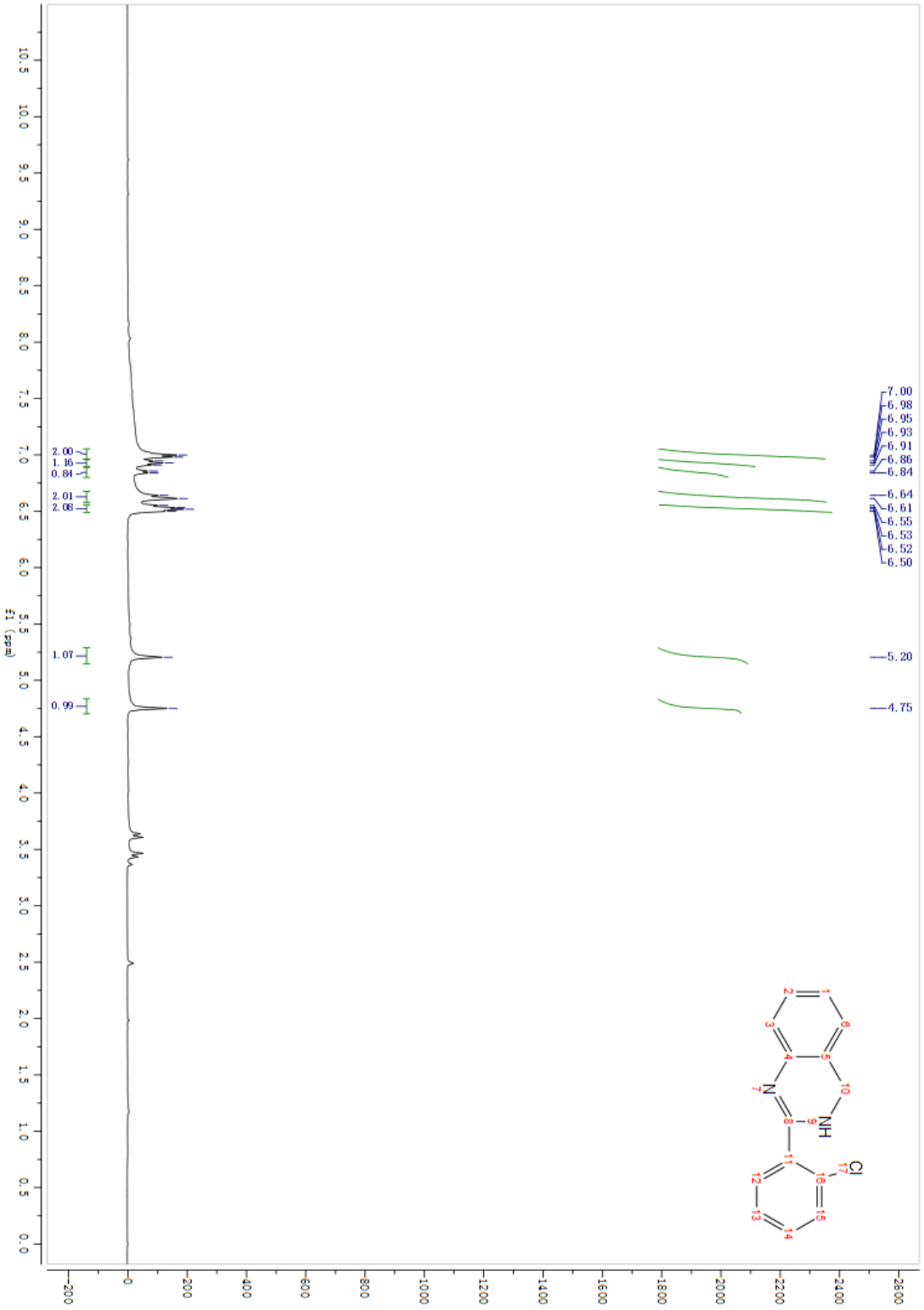

N
N
Cl

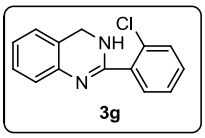
4f


Transmittance [%]
50
60
70
80
90
100
BRUKER
3443.46
1619.20
1585.77
1562.95
1549.93
1489.26
1449.50
1405.27
1380.59
1341.48
1310.87
1291.67
1260.13
1243.15
1211.67
1172.61
1143.83
1083.71
1054.39
1008.13
941.69
872.43
850.57
799.21
783.35
764.03
740.73
728.30
690.06
649.19
595.61
550.72
501.14
453.32
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
N
N
Cl

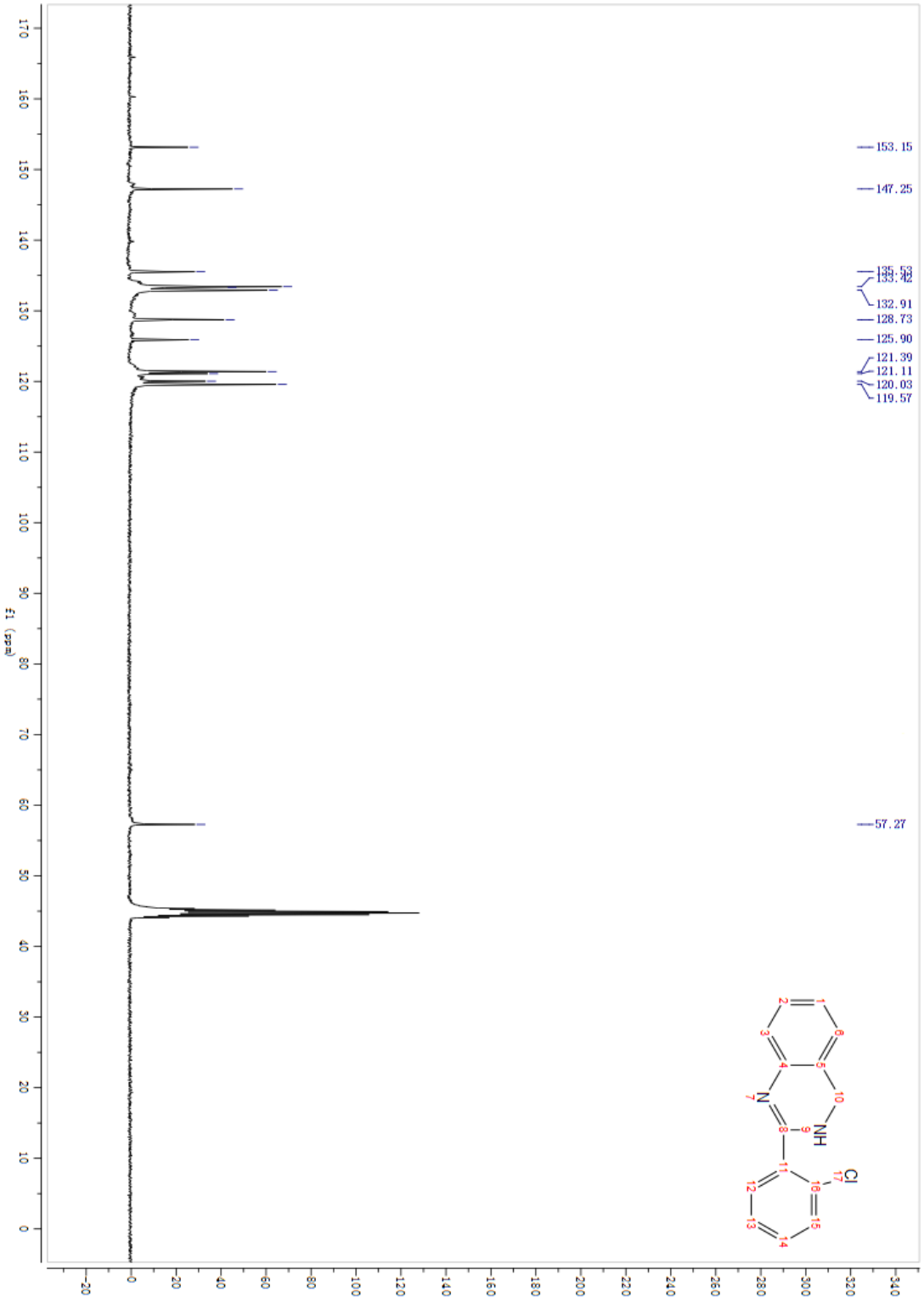

Cl
NH
N

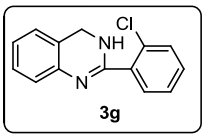
3g


7.00
6.98
6.95
6.93
6.91
6.86
6.84
6.64
6.61
6.55
6.53
6.52
6.50
5.20
4.75
2.00
1.16
0.84
2.01
2.08
1.07
0.99
f1 (ppm)
NH
N
Cl

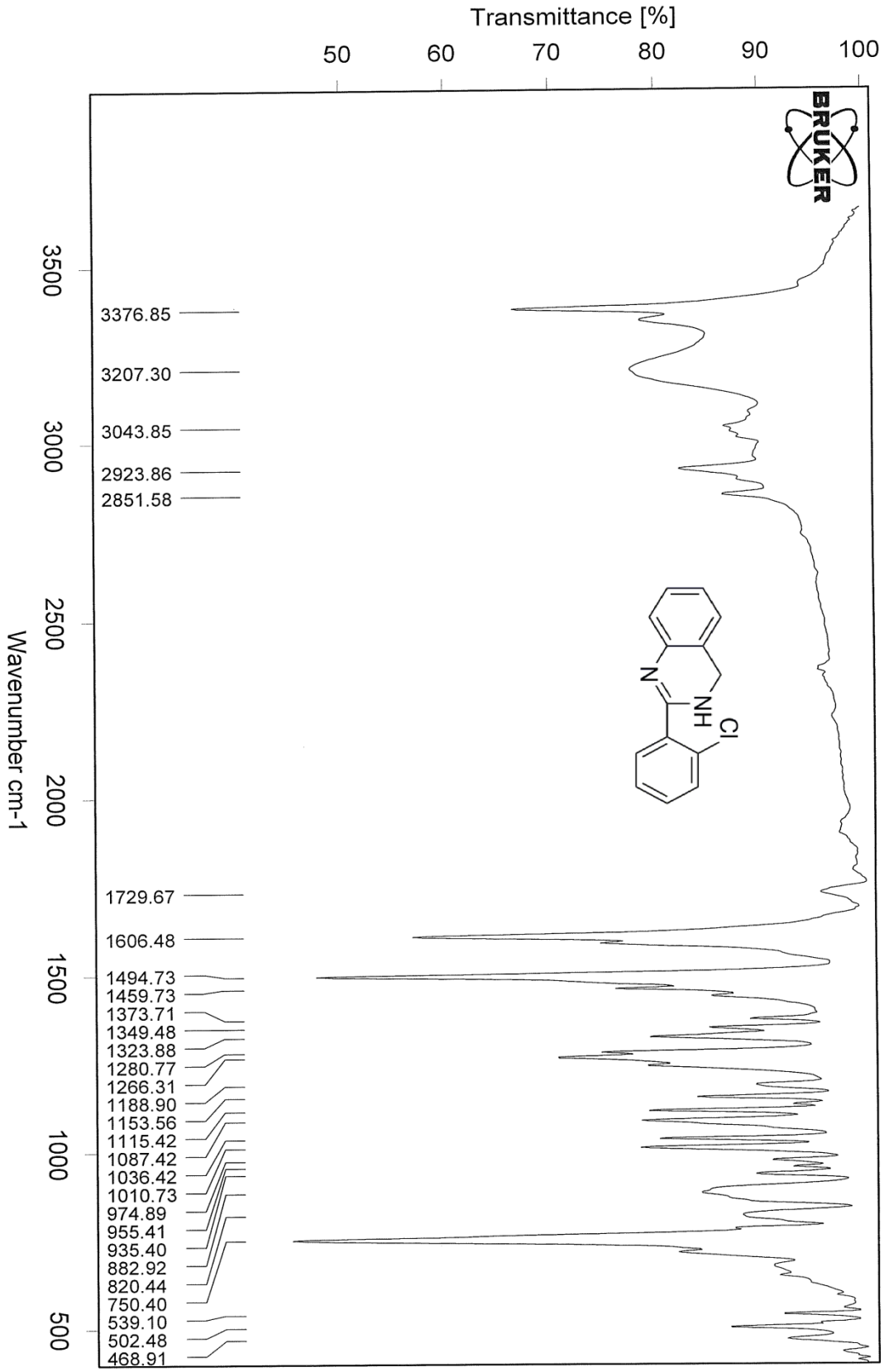

Cl
NH
N

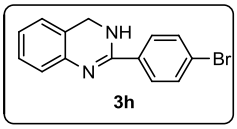
3g


153.15
147.25
135.53
133.42
132.91
128.73
125.90
121.39
121.11
120.03
119.57
57.27
f1 (ppm)
NH
N
Cl

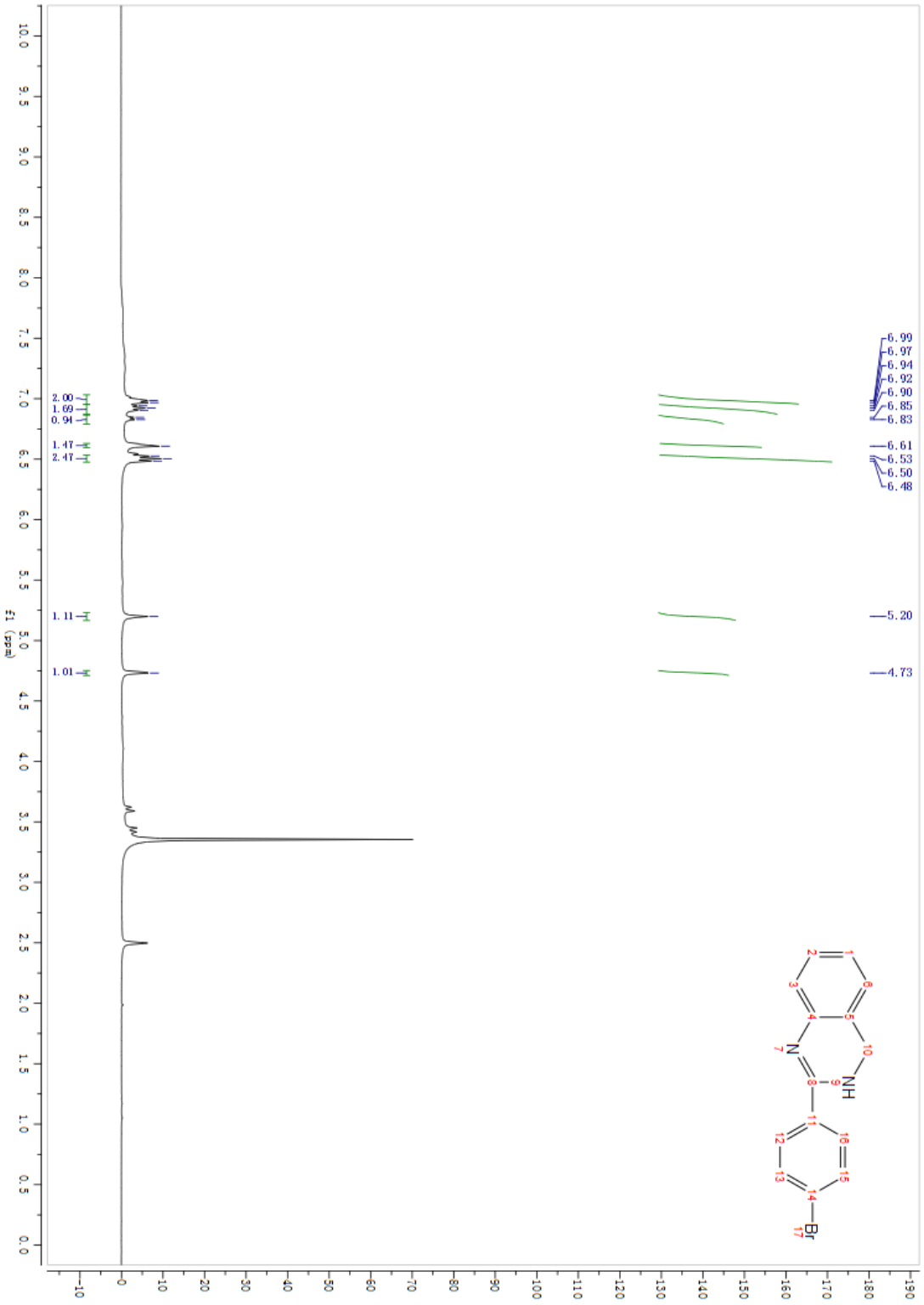

Cl
NH
N

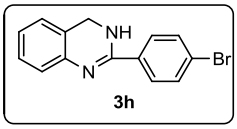
3g


Transmittance [%]
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3376.85
3207.30
3043.85
2923.86
2851.58
1729.67
1606.48
1494.73
1459.73
1373.71
1349.48
1323.88
1280.77
1266.31
1188.90
1153.56
1115.42
1087.42
1036.42
1010.73
974.89
955.41
935.40
882.92
820.44
750.40
539.10
502.48
468.91
N
NH
Cl

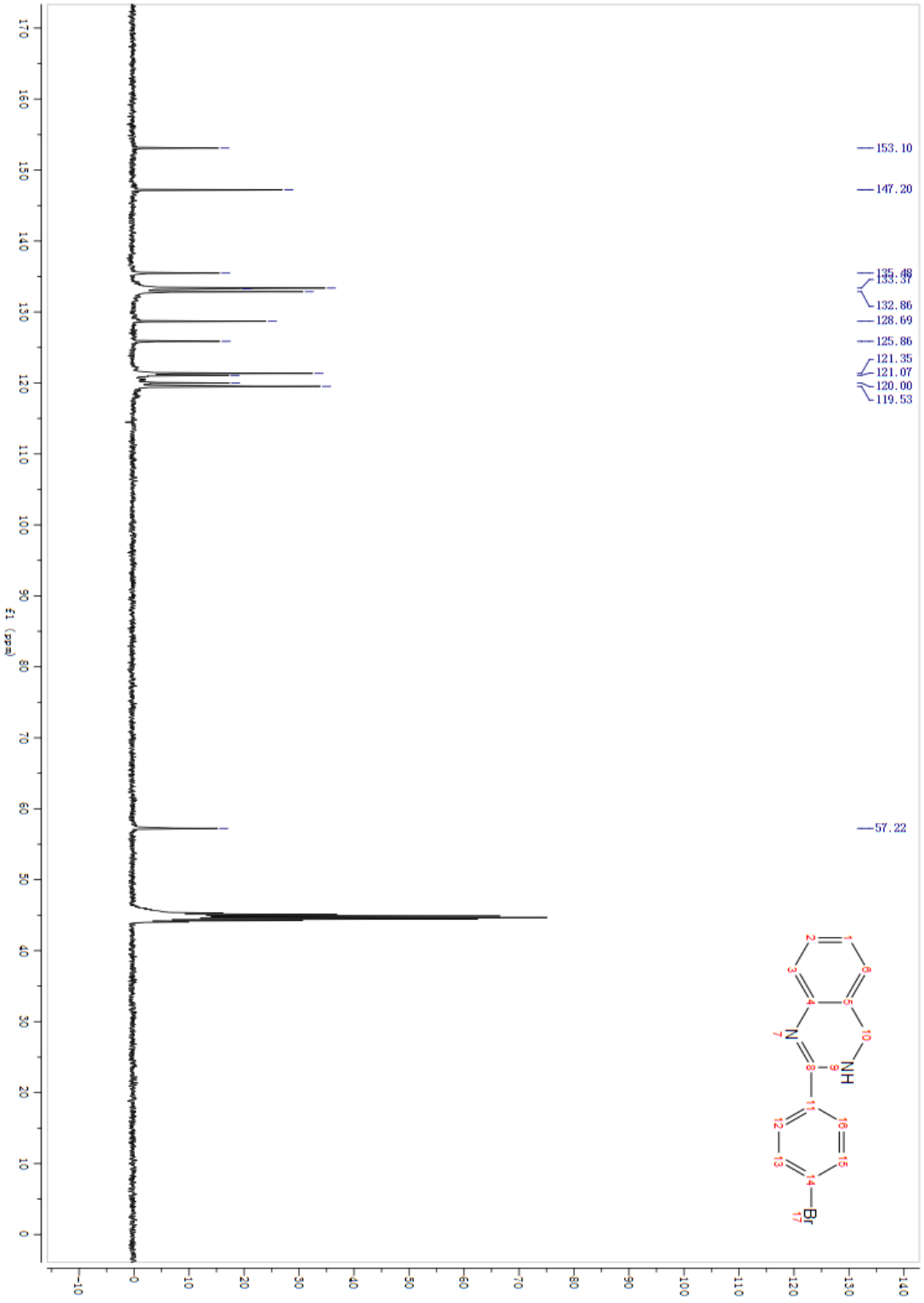

NH
N
Br

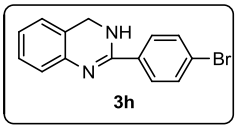
3h


6.99
6.97
6.94
6.92
6.90
6.85
6.83
6.61
6.53
6.50
6.48
5.20
4.73
2.00
1.69
0.94
1.47
2.47
1.11
1.01
f1 (ppm)
NH
N
Br

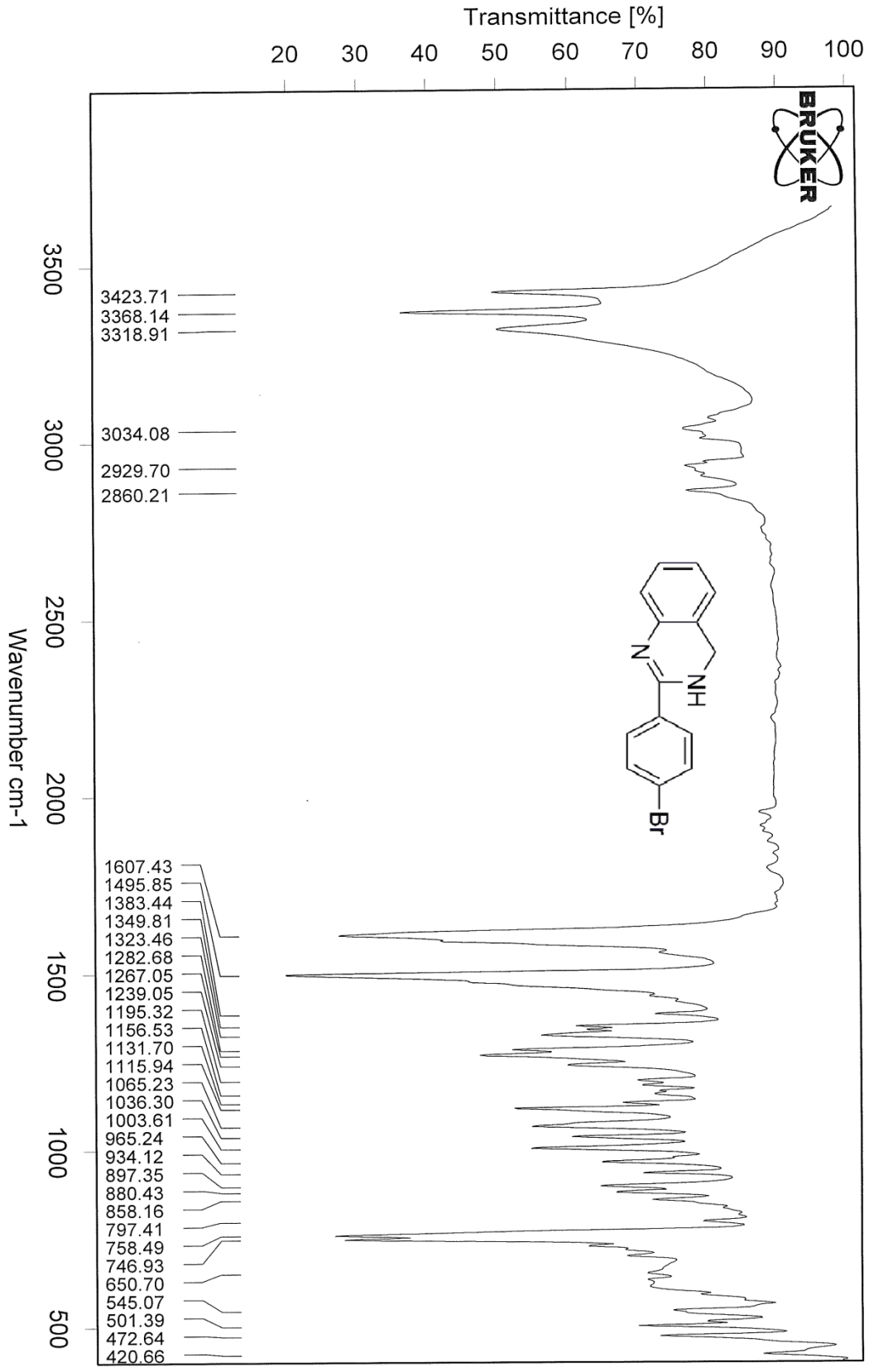

NH
N
Br

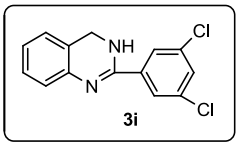
3h


153.10
147.20
135.48
133.37
132.86
128.69
125.86
121.35
121.07
120.00
119.53
57.22
f1 (ppm)
NH
Br

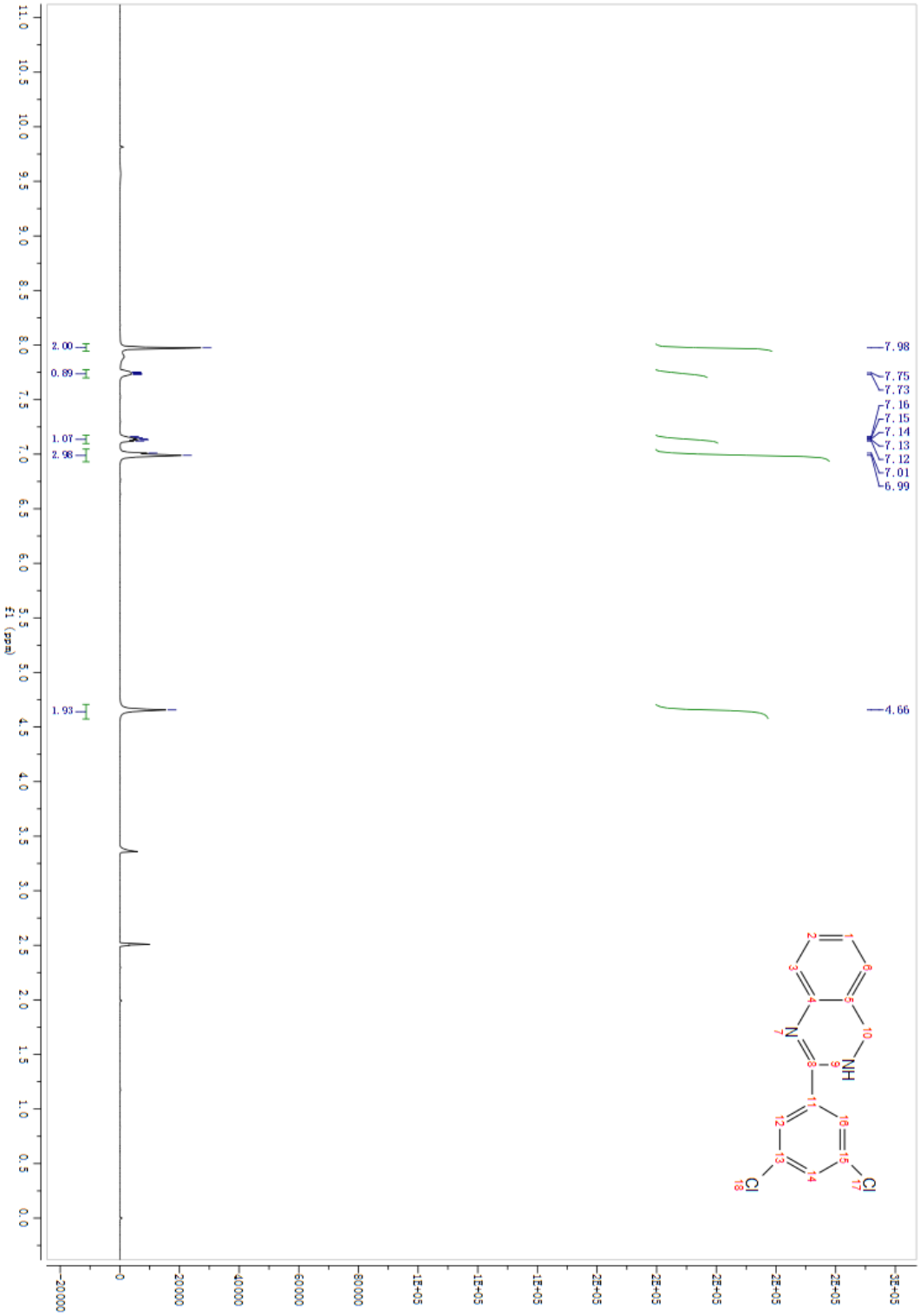

NH
N
Br

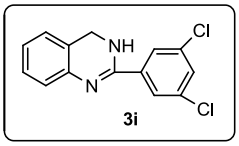
3h


Transmittance [%]
20
30
40
50
60
70
80
90
100
BRUKER
3423.71
3368.14
3318.91
3034.08
2929.70
2860.21
1607.43
1495.85
1383.44
1349.81
1323.46
1282.68
1267.05
1239.05
1195.32
1156.53
1131.70
1115.94
1065.23
1036.30
1003.61
965.24
934.12
897.35
880.43
858.16
797.41
758.49
746.93
650.70
545.07
501.39
472.64
420.66
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
N
NH
Br

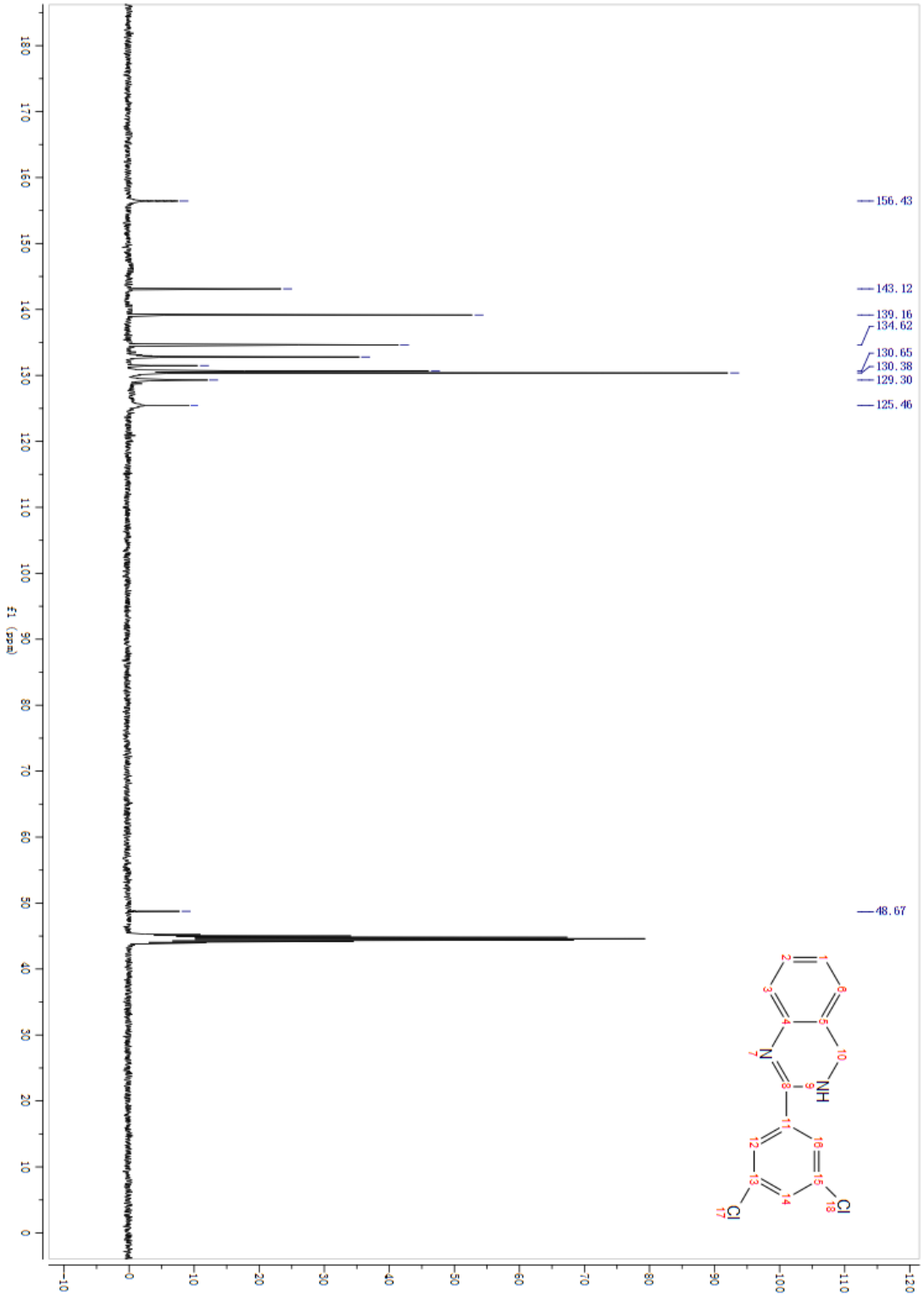

NH
N
Cl
Cl

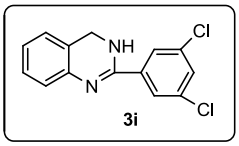
3i


2.00
0.89
1.07
2.98
1.93
7.98
7.75
7.73
7.16
7.15
7.14
7.13
7.12
7.01
6.99
4.66
f1 (ppm)

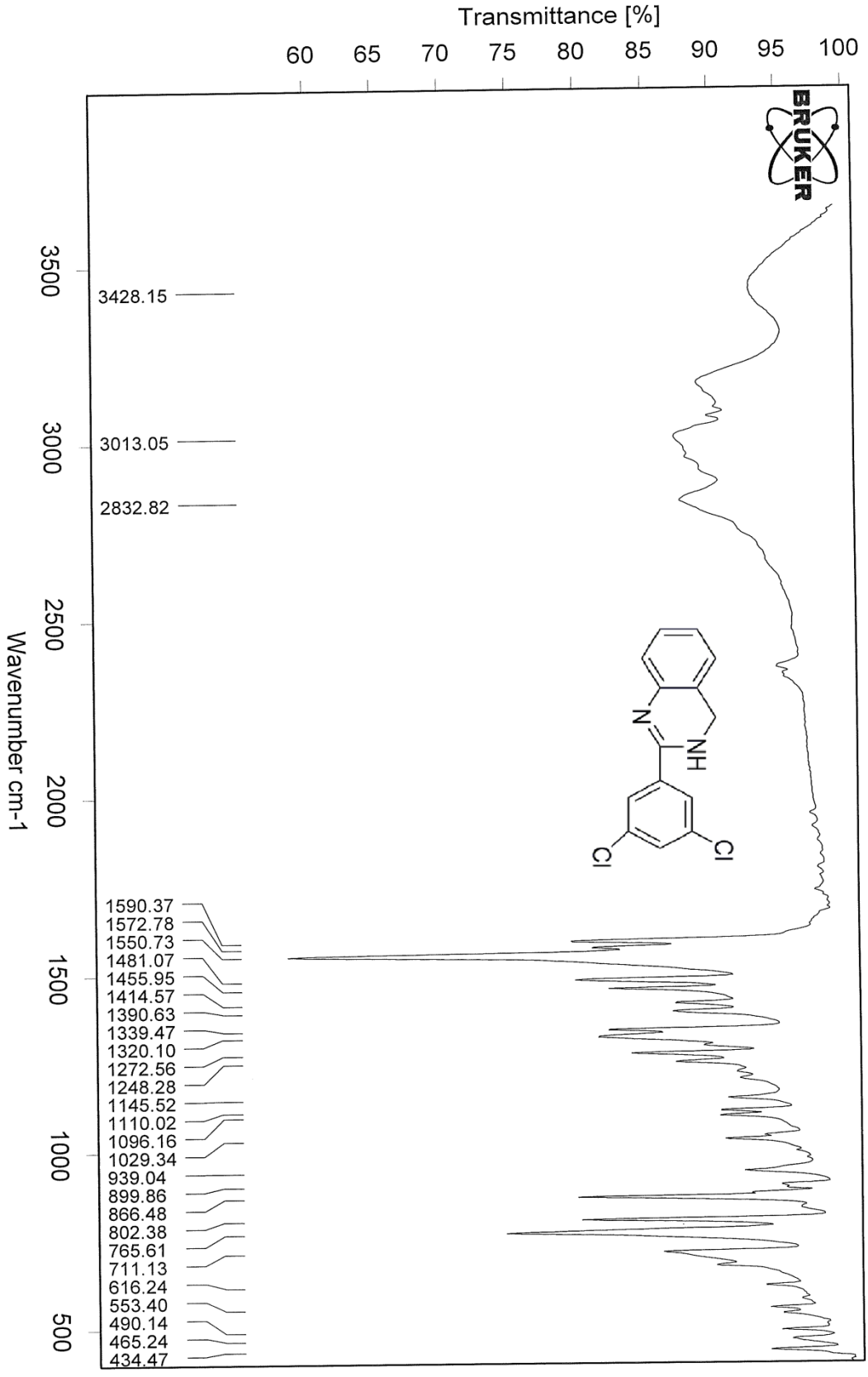

NH
N
Cl
Cl

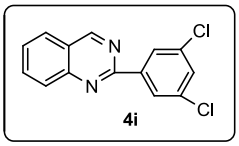
3i


156.43
143.12
139.16
134.62
130.65
130.38
129.30
125.46
48.67
f1 (ppm)

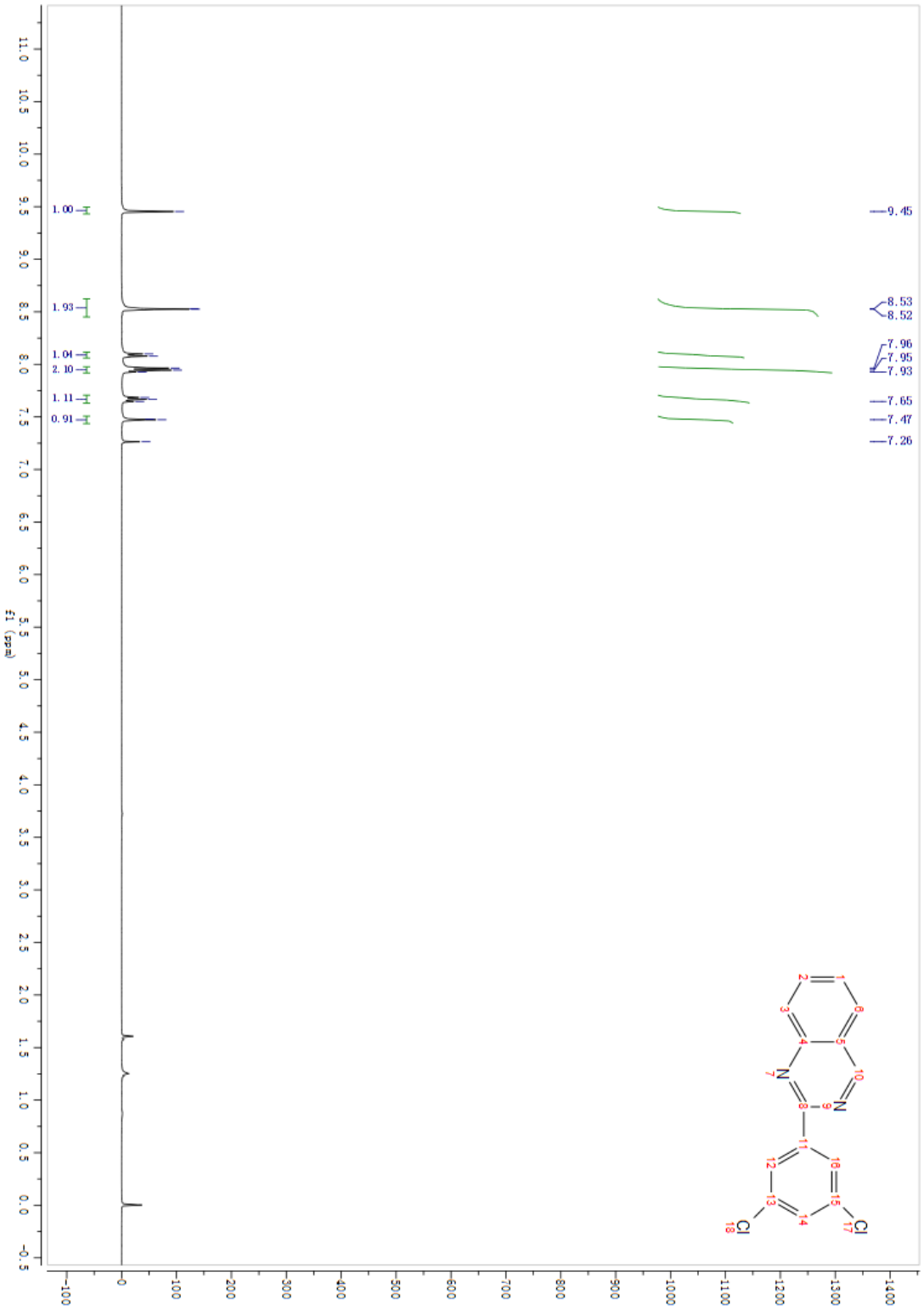

NH
N
Cl
Cl

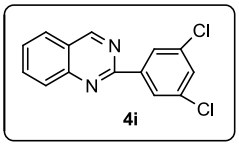
3i


Transmittance [%]
60
65
70
75
80
85
90
95
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3428.15
3013.05
2832.82
1590.37
1572.78
1550.73
1481.07
1455.95
1414.57
1390.63
1339.47
1320.10
1272.56
1248.28
1145.52
1110.02
1096.16
1029.34
939.04
899.86
866.48
802.38
765.61
711.13
616.24
553.40
490.14
465.24
434.47
N
NH
Cl
Cl

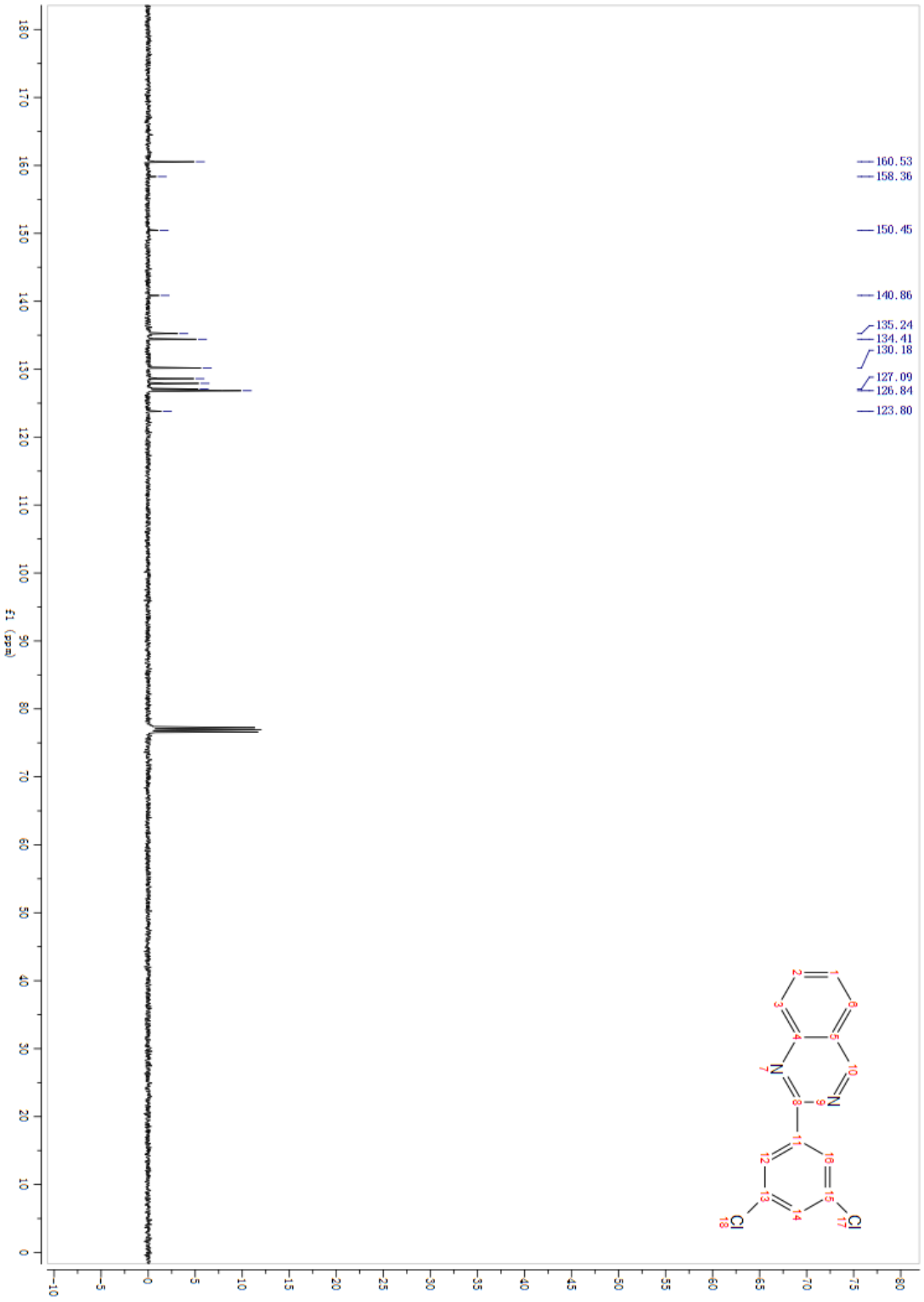

N
N
Cl
Cl

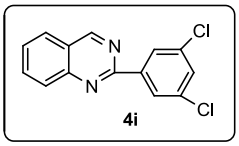
4i


1.00
1.93
1.04
2.10
1.11
0.91
9.45
8.53
8.52
7.96
7.95
7.93
7.65
7.47
7.26
f1 (ppm)

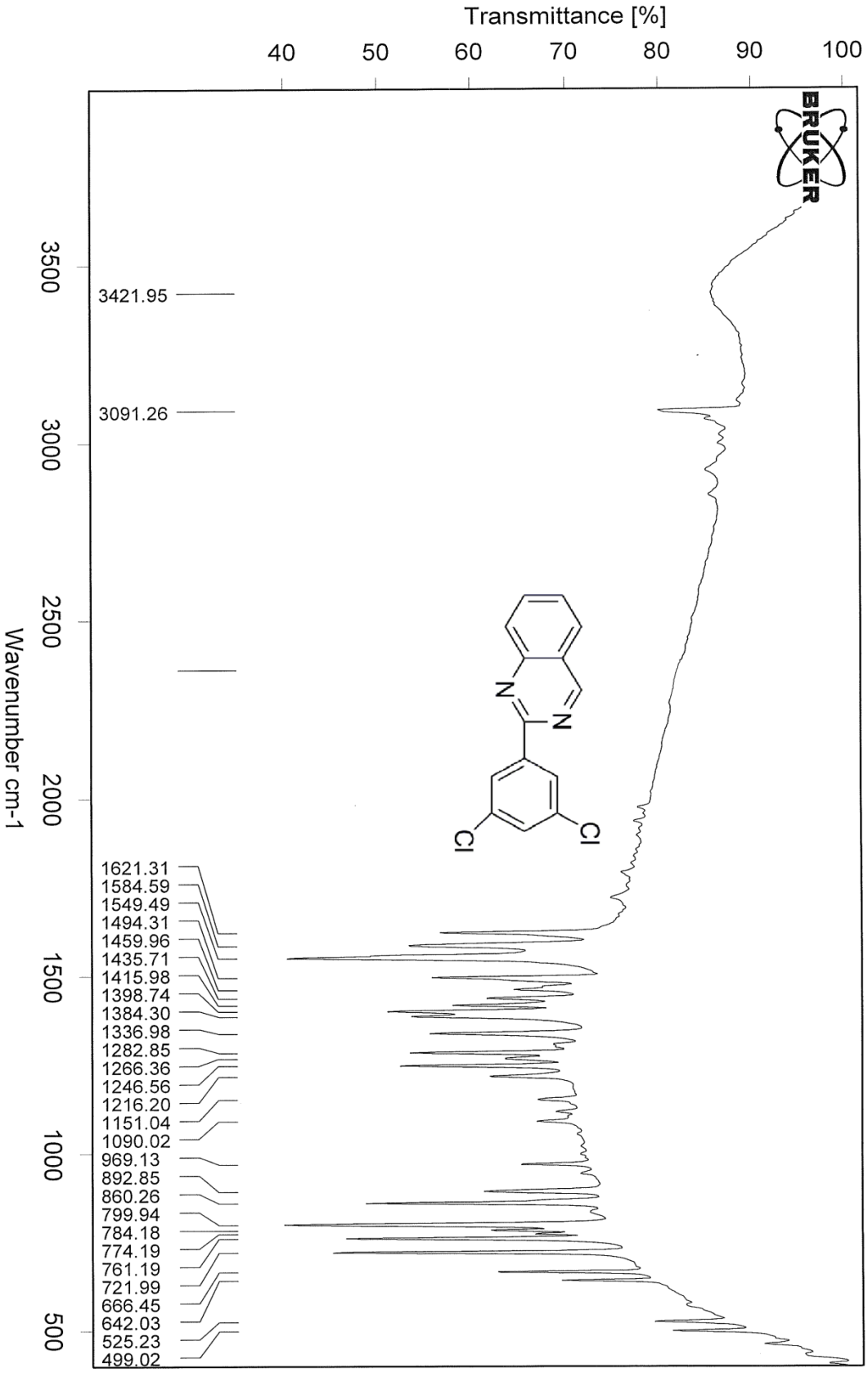

Cl
N
N
Cl

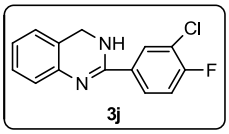
4i


160.53
158.36
150.45
140.86
135.24
134.41
130.18
127.09
126.84
123.80
f1 (ppm)

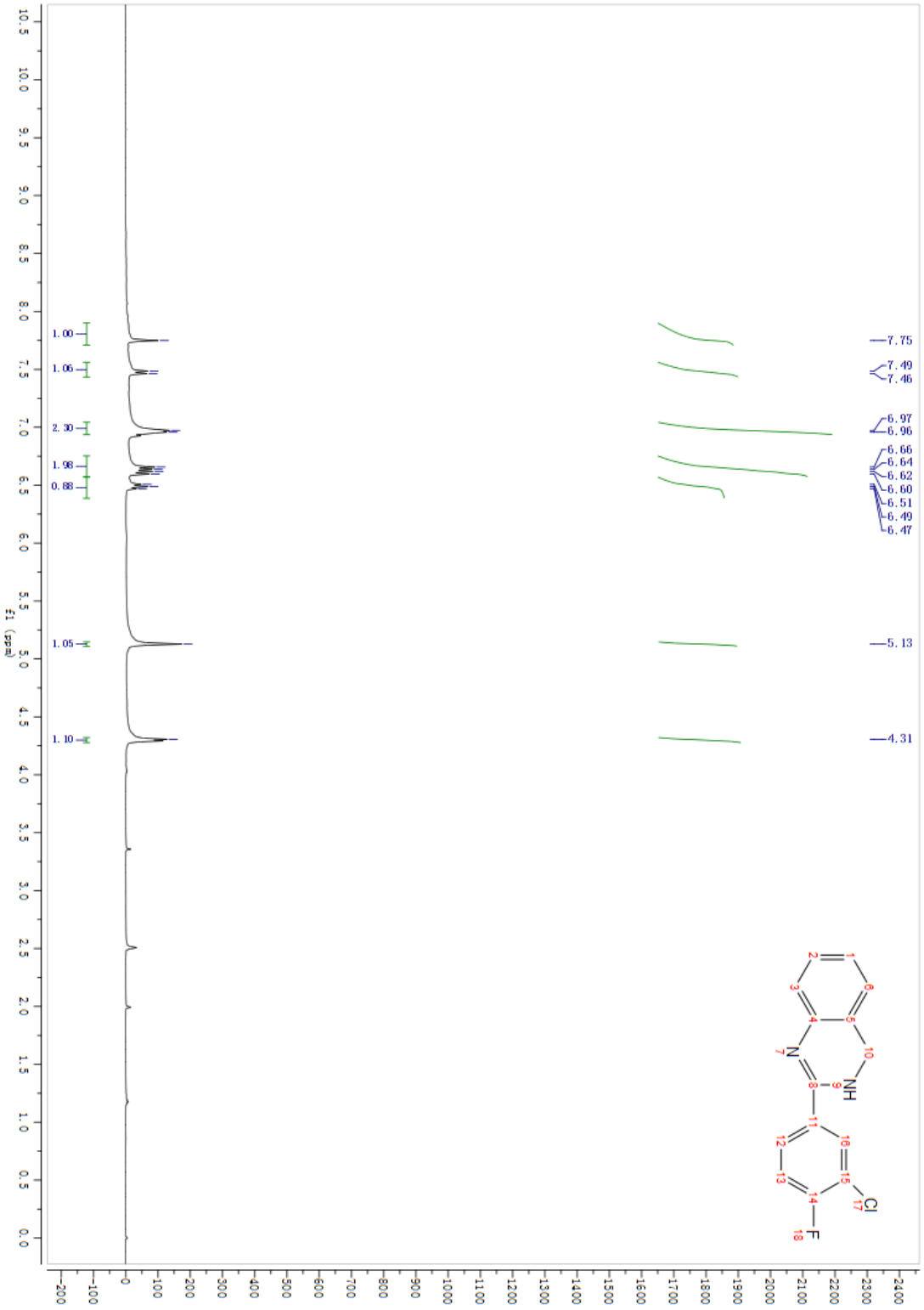

Cl
N
N
Cl

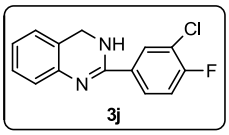
4i


Transmittance [%]
40
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3421.95
3091.26
1621.31
1584.59
1549.49
1494.31
1459.96
1435.71
1415.98
1398.74
1384.30
1336.98
1282.85
1266.36
1246.56
1216.20
1151.04
1090.02
969.13
892.85
860.26
799.94
784.18
774.19
761.19
721.99
666.45
642.03
525.23
499.02
N
N
Cl
Cl

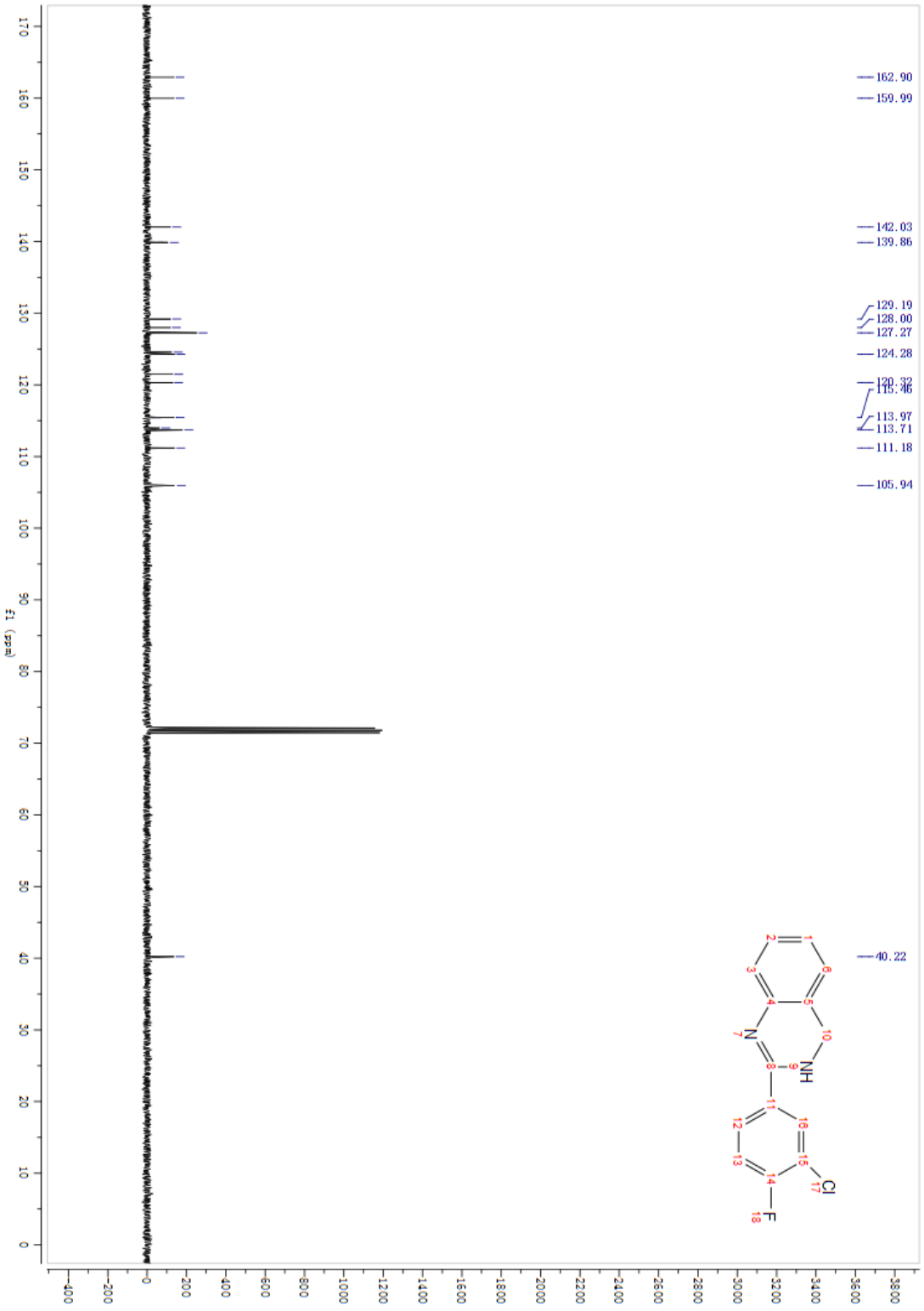

NH
N
Cl
F

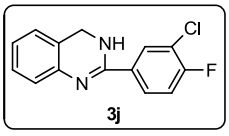
3j


1.00
1.06
2.30
1.98
0.88
1.05
1.10
7.75
7.49
7.46
6.97
6.96
6.66
6.64
6.62
6.60
6.51
6.49
6.47
5.13
4.31
f1 (ppm)

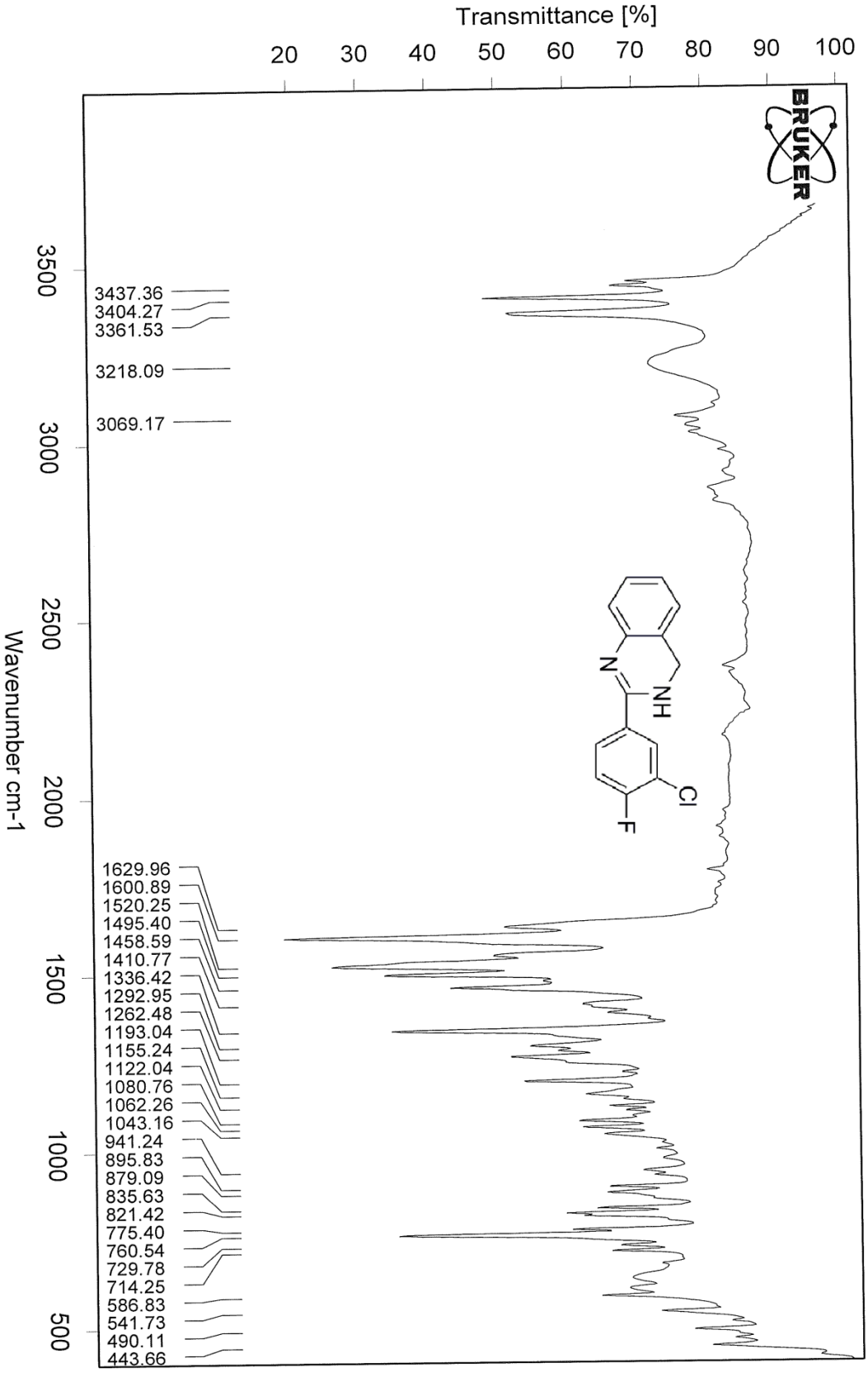

NH
N
Cl
F

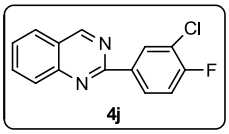
3j


162.90
159.99
142.03
139.86
129.19
128.00
127.27
124.28
120.32
115.46
113.97
113.71
111.18
105.94
40.22
f1 (ppm)
NH
N
Cl
F

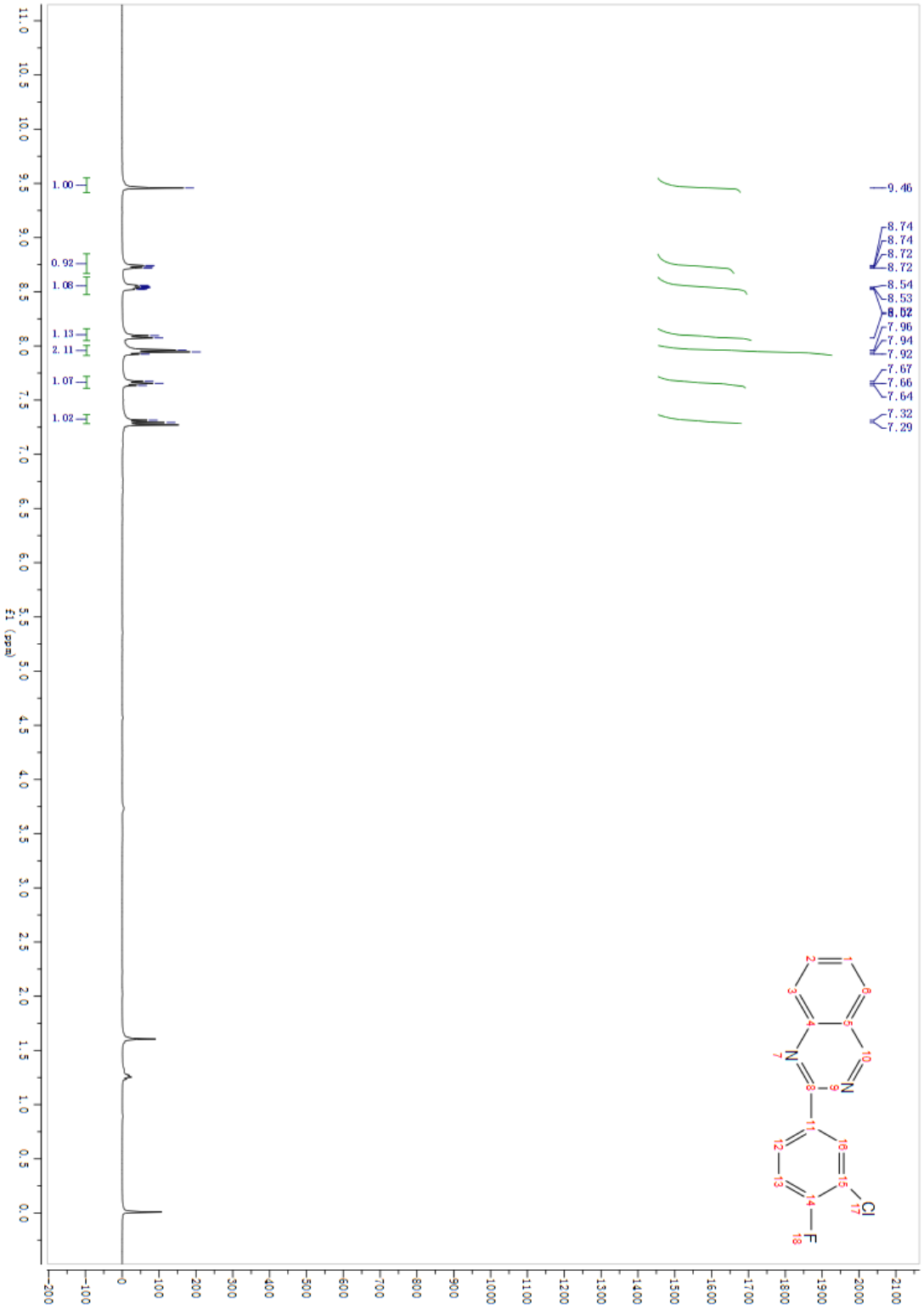

NH
Cl
N
F

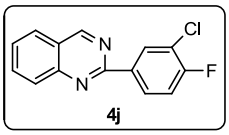
3j


Transmittance [%]
20
30
40
50
60
70
80
90
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3437.36
3404.27
3361.53
3218.09
3069.17
1629.96
1600.89
1520.25
1495.40
1458.59
1410.77
1336.42
1292.95
1262.48
1193.04
1155.24
1122.04
1080.76
1062.26
1043.16
941.24
895.83
879.09
835.63
821.42
775.40
760.54
729.78
714.25
586.83
541.73
490.11
443.66
N
NH
Cl
F

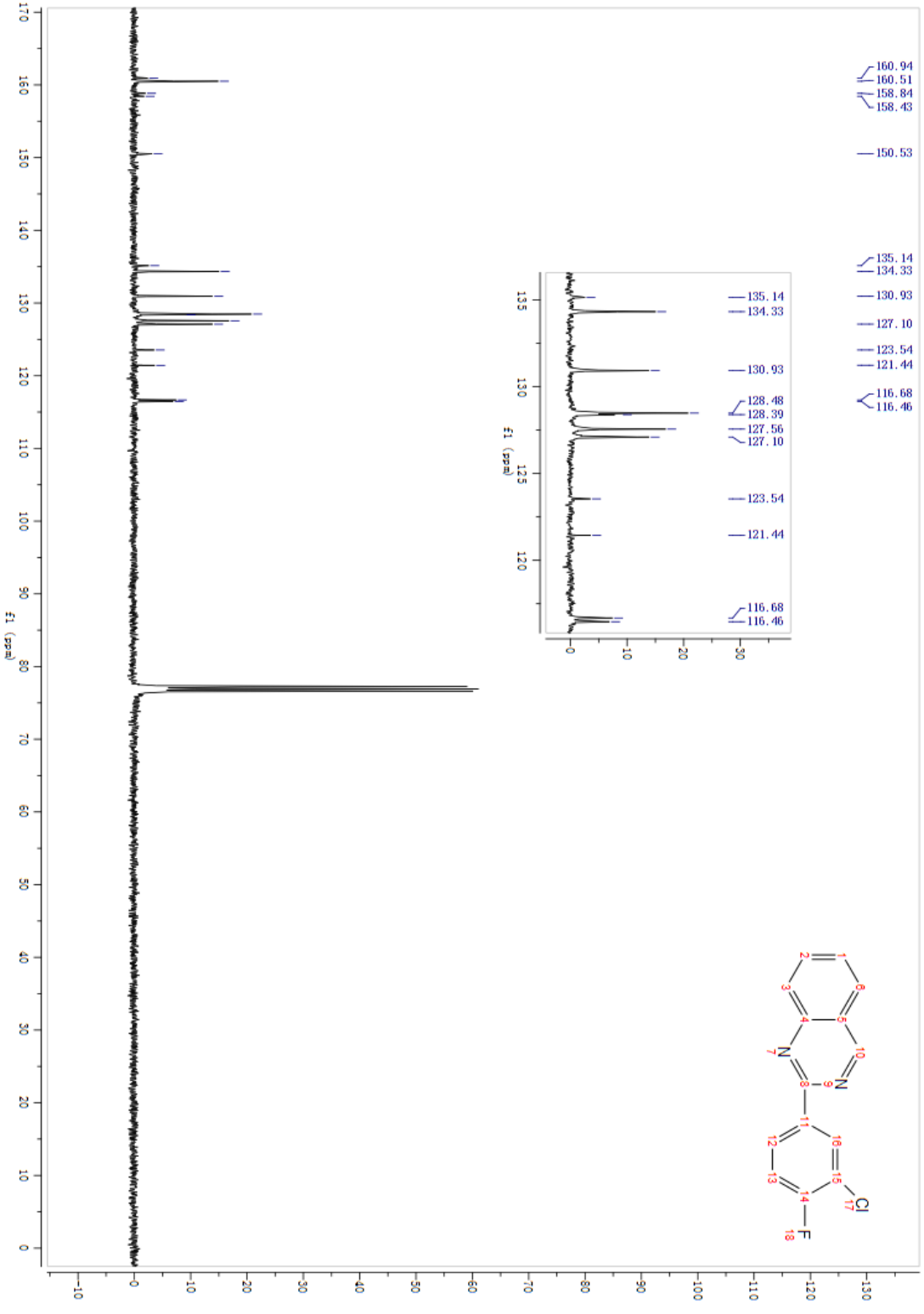

Cl
N
N
F

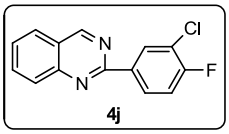
4j


9.46
8.74
8.74
8.72
8.72
8.54
8.53
7.96
7.94
7.92
7.67
7.66
7.64
7.32
7.29
1.00
0.92
1.08
1.13
2.11
1.07
1.02
f1 (ppm)

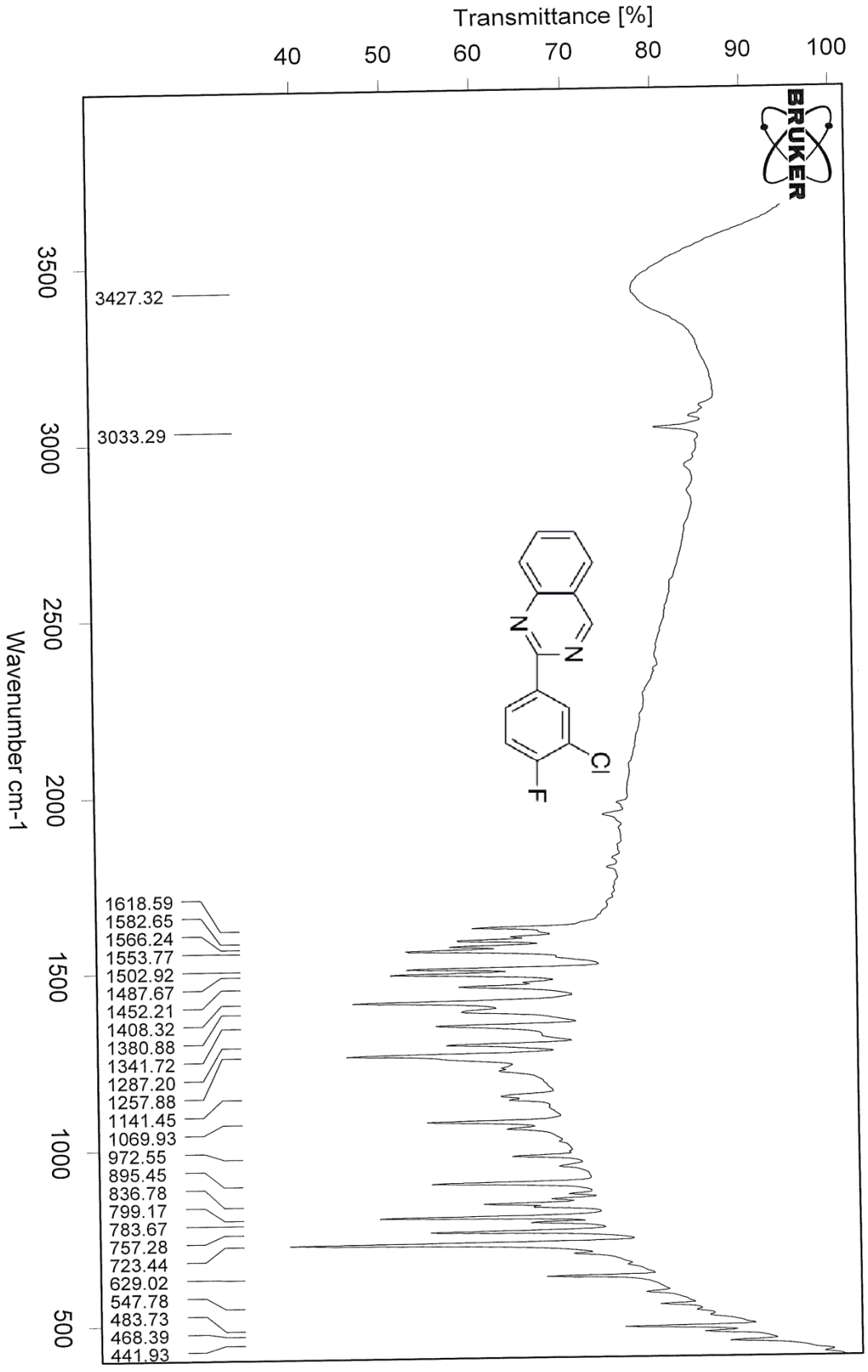

Cl
N
N
F

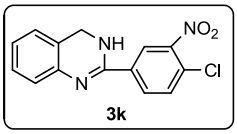
4j


160.94
160.51
158.84
158.43
150.53
135.14
134.33
130.93
127.10
123.54
121.44
116.68
116.46
128.48
128.39
127.56
f1 (ppm)

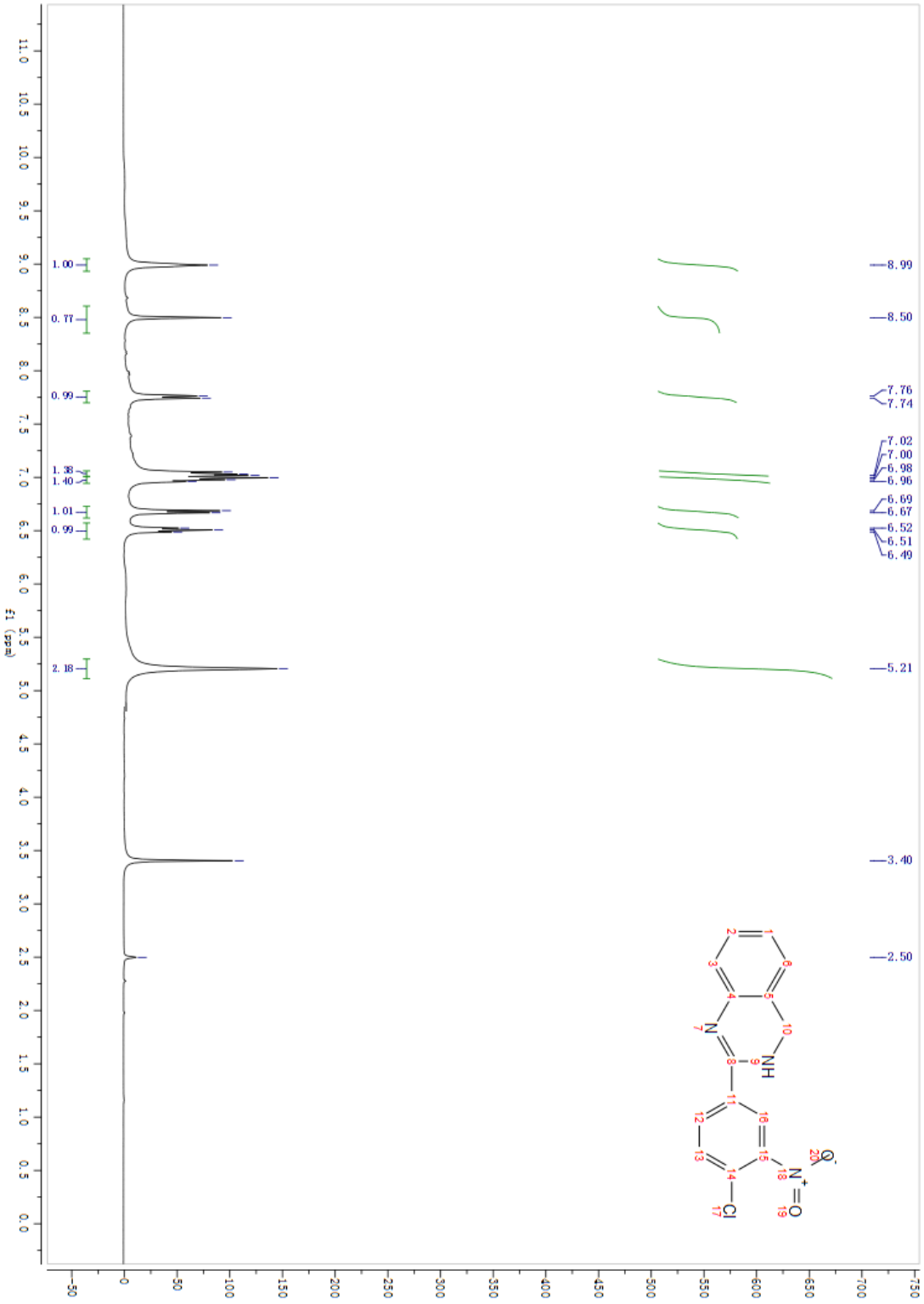

Cl
N
N
F

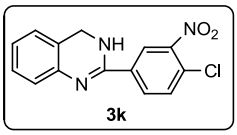
4j


Transmittance [%]
40
50
60
70
80
90
100
BRUKER
3427.32
3033.29
1618.59
1582.65
1566.24
1553.77
1502.92
1487.67
1452.21
1408.32
1380.88
1341.72
1287.20
1257.88
1141.45
1069.93
972.55
895.45
836.78
799.17
783.67
757.28
723.44
629.02
547.78
483.73
468.39
441.93
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
N
N
Cl
F

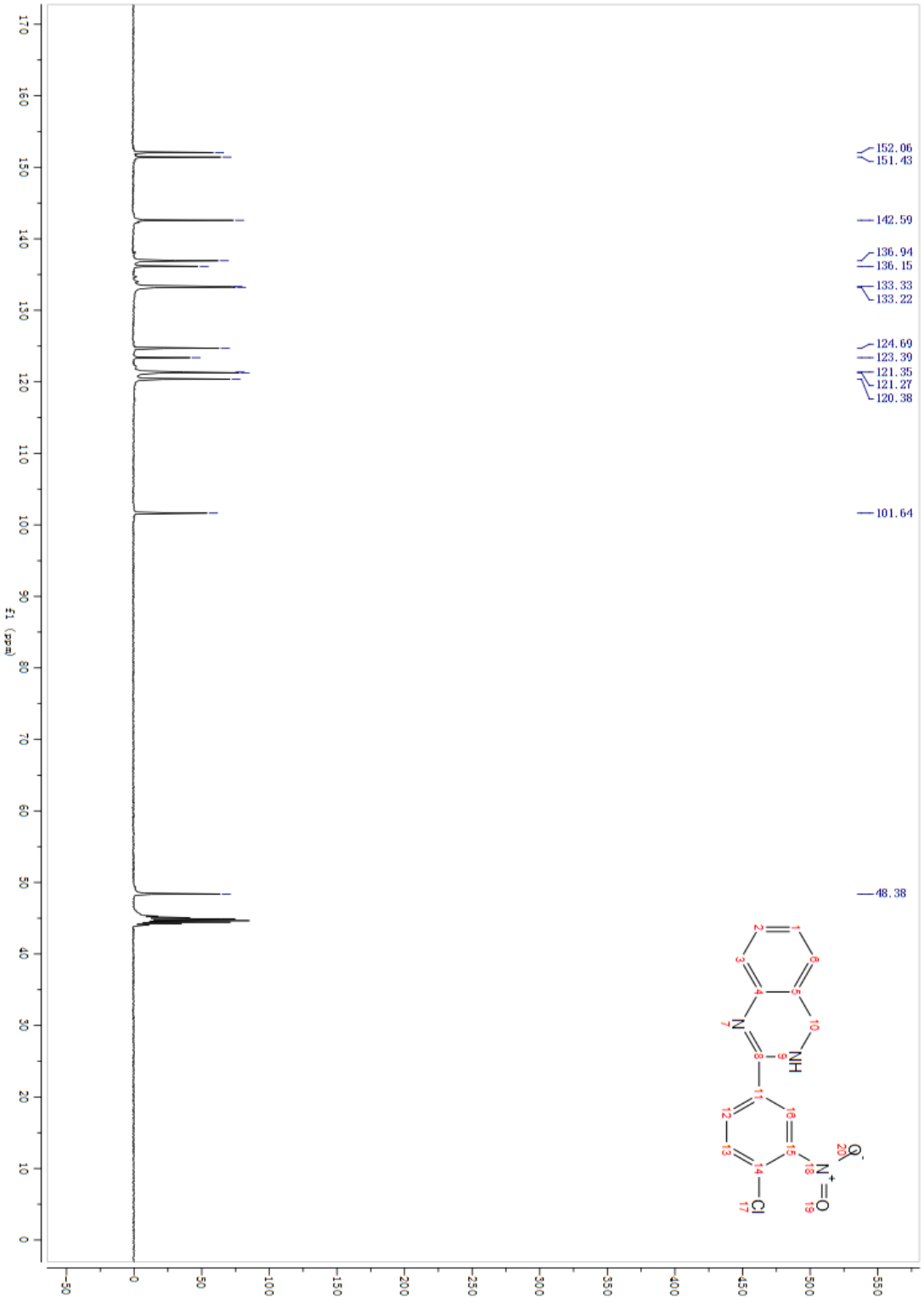

NH
N
NO2
Cl

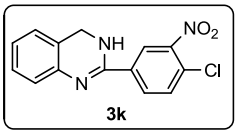
3k


1.00
0.77
0.99
1.38
1.40
1.01
0.99
2.18
8.99
8.50
7.76
7.74
7.02
7.00
6.98
6.96
6.69
6.67
6.52
6.51
6.49
5.21
3.40
2.50
f1 (ppm)

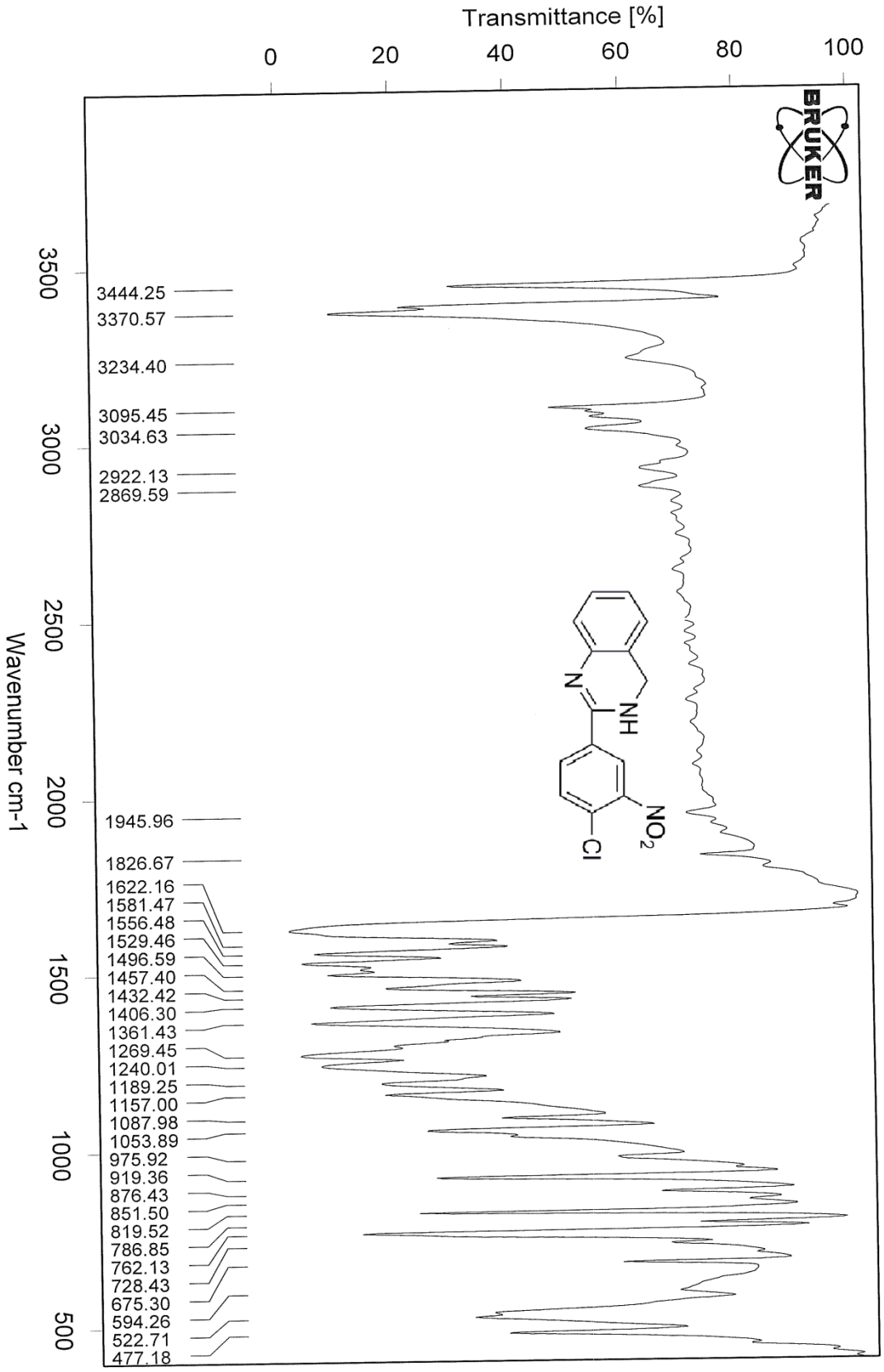

NH
N
NO2
Cl

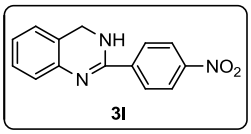
3k


152.06
151.43
142.59
136.94
136.15
133.33
133.22
124.69
123.39
121.35
121.27
120.38
101.64
48.38
f1 (ppm)

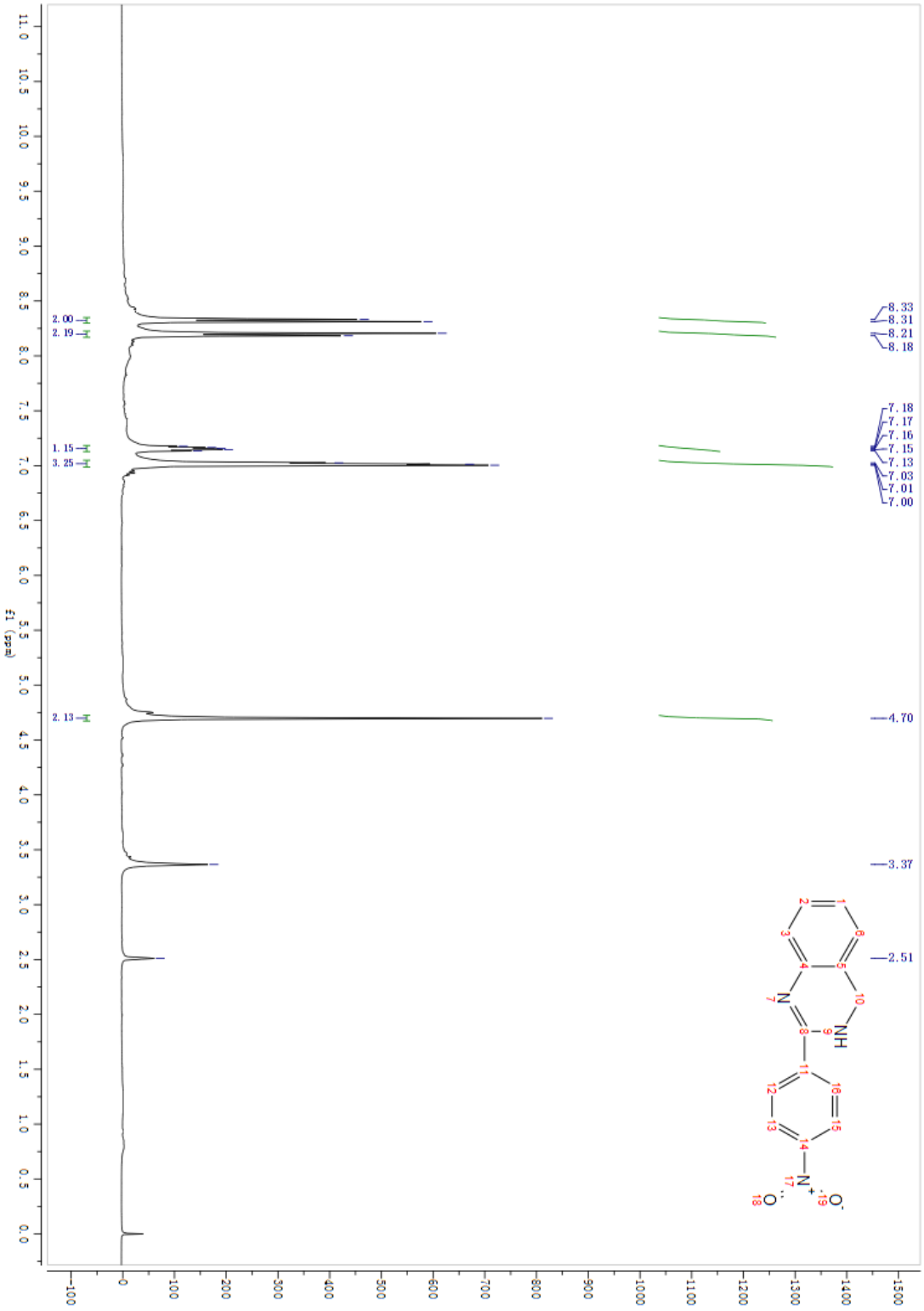

NH
NO2
N
Cl

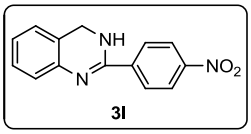
3k


Transmittance [%]
0
20
40
60
80
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3444.25
3370.57
3234.40
3095.45
3034.63
2922.13
2869.59
1945.96
1826.67
1622.16
1581.47
1556.48
1529.46
1496.59
1457.40
1432.42
1406.30
1361.43
1269.45
1240.01
1189.25
1157.00
1087.98
1053.89
975.92
919.36
876.43
851.50
819.52
786.85
762.13
728.43
675.30
594.26
522.71
477.18
N
NH
NO2
Cl

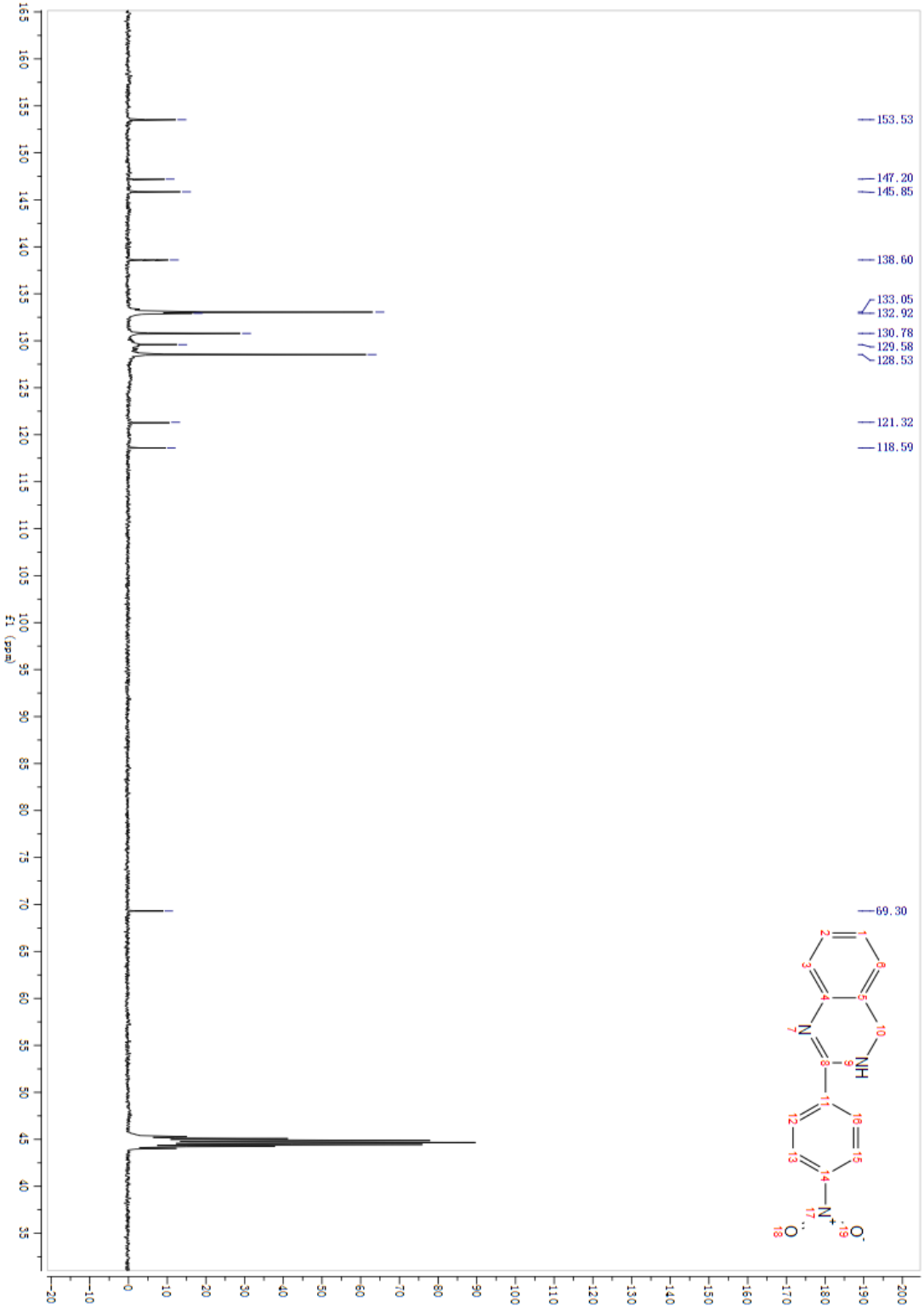

NH
N
NO2

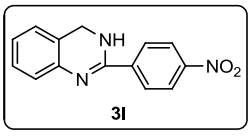
3l


2.00
2.19
1.15
3.25
2.13
8.33
8.31
8.21
8.18
7.18
7.17
7.16
7.15
7.13
7.03
7.01
7.00
4.70
3.37
2.51
f1 (ppm)

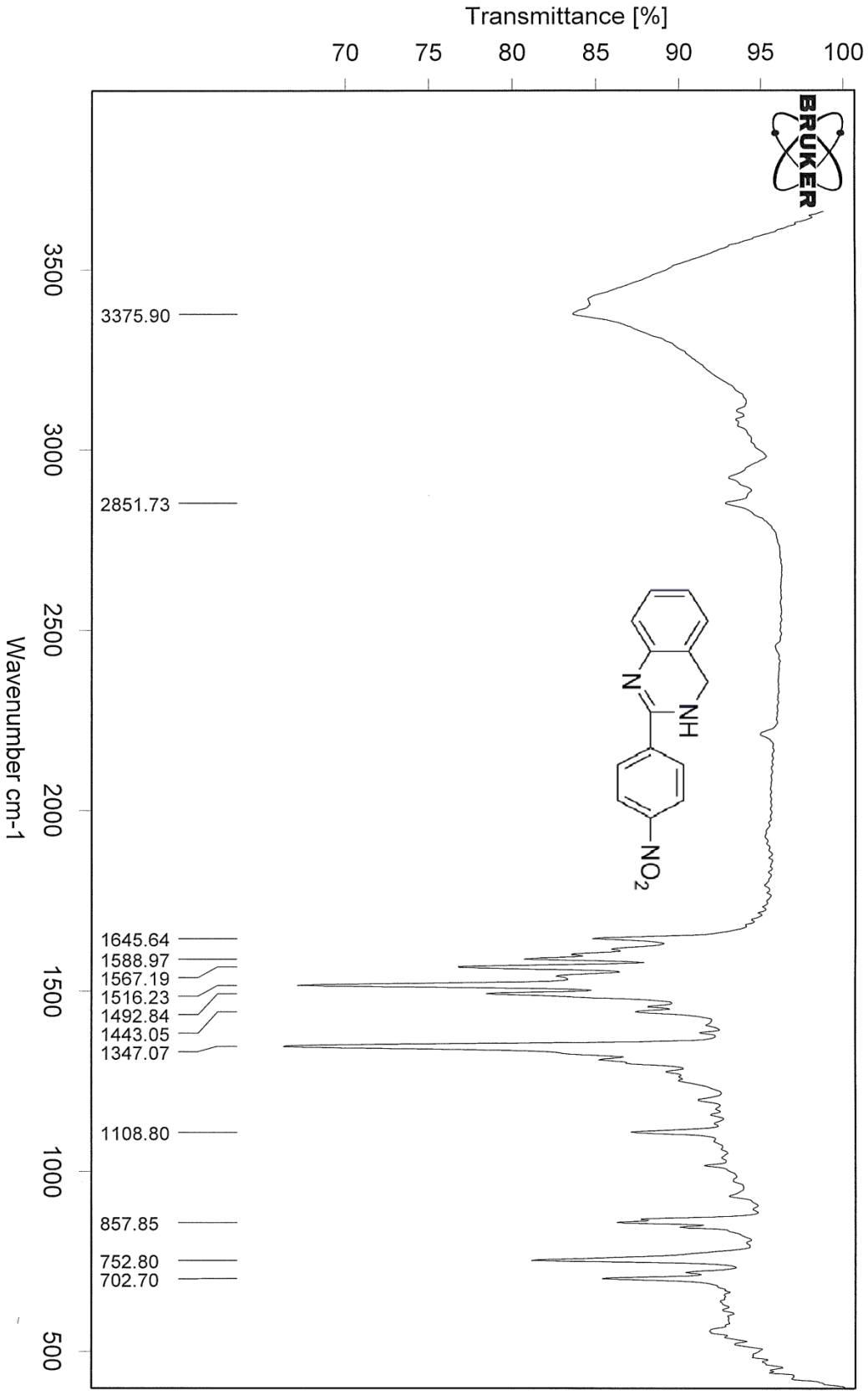

NH
N
NO2

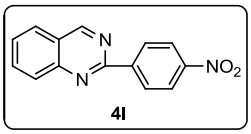
3l


153.53
147.20
145.85
138.60
133.05
132.92
130.78
129.58
128.53
121.32
118.59
69.30
f1 (ppm)

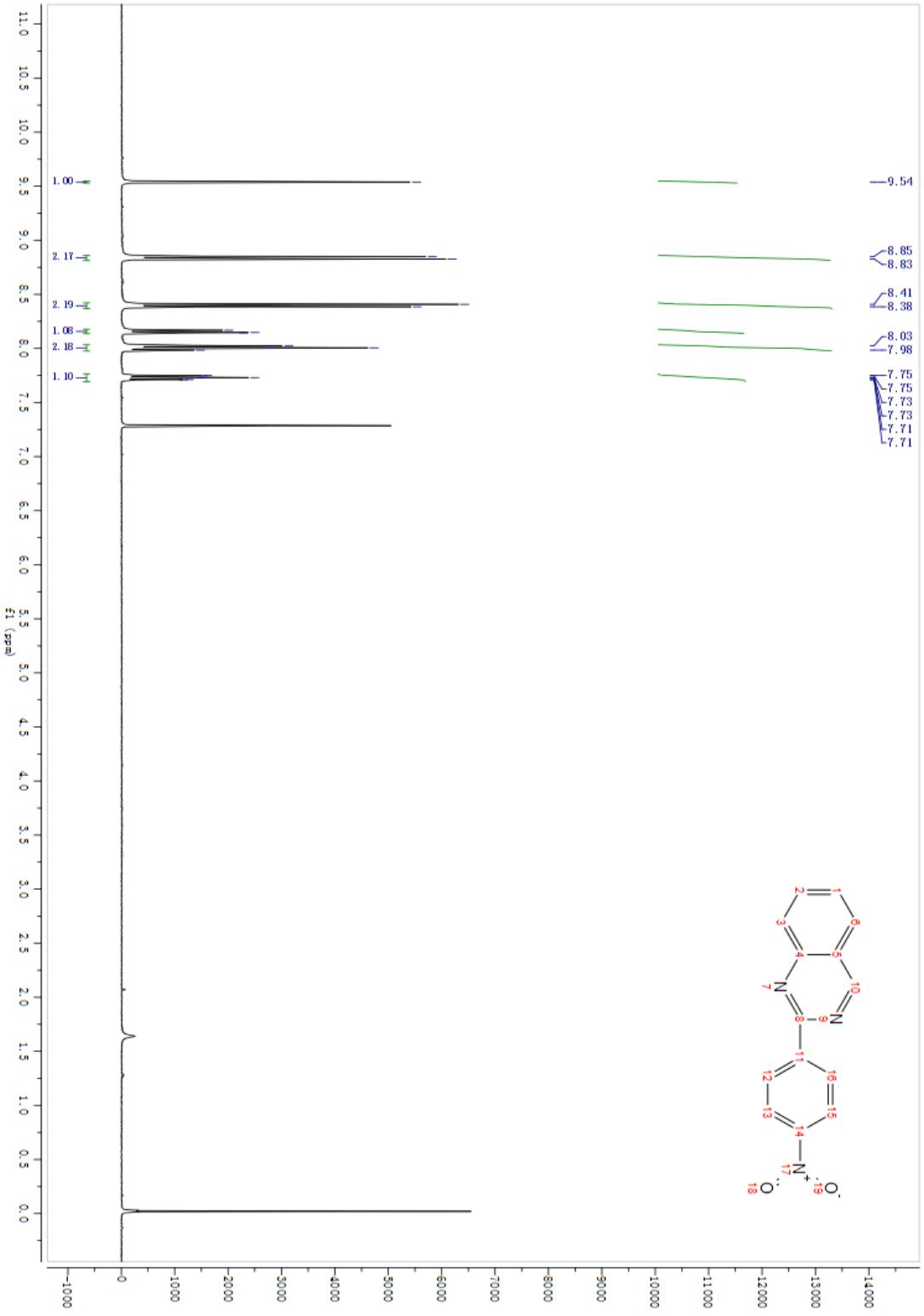

NH
N
NO2

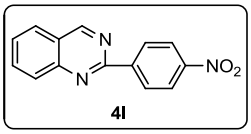
3l


Transmittance [%]
70
75
80
85
90
95
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3375.90
2851.73
1645.64
1588.97
1567.19
1516.23
1492.84
1443.05
1347.07
1108.80
857.85
752.80
702.70
N
NH
NO2

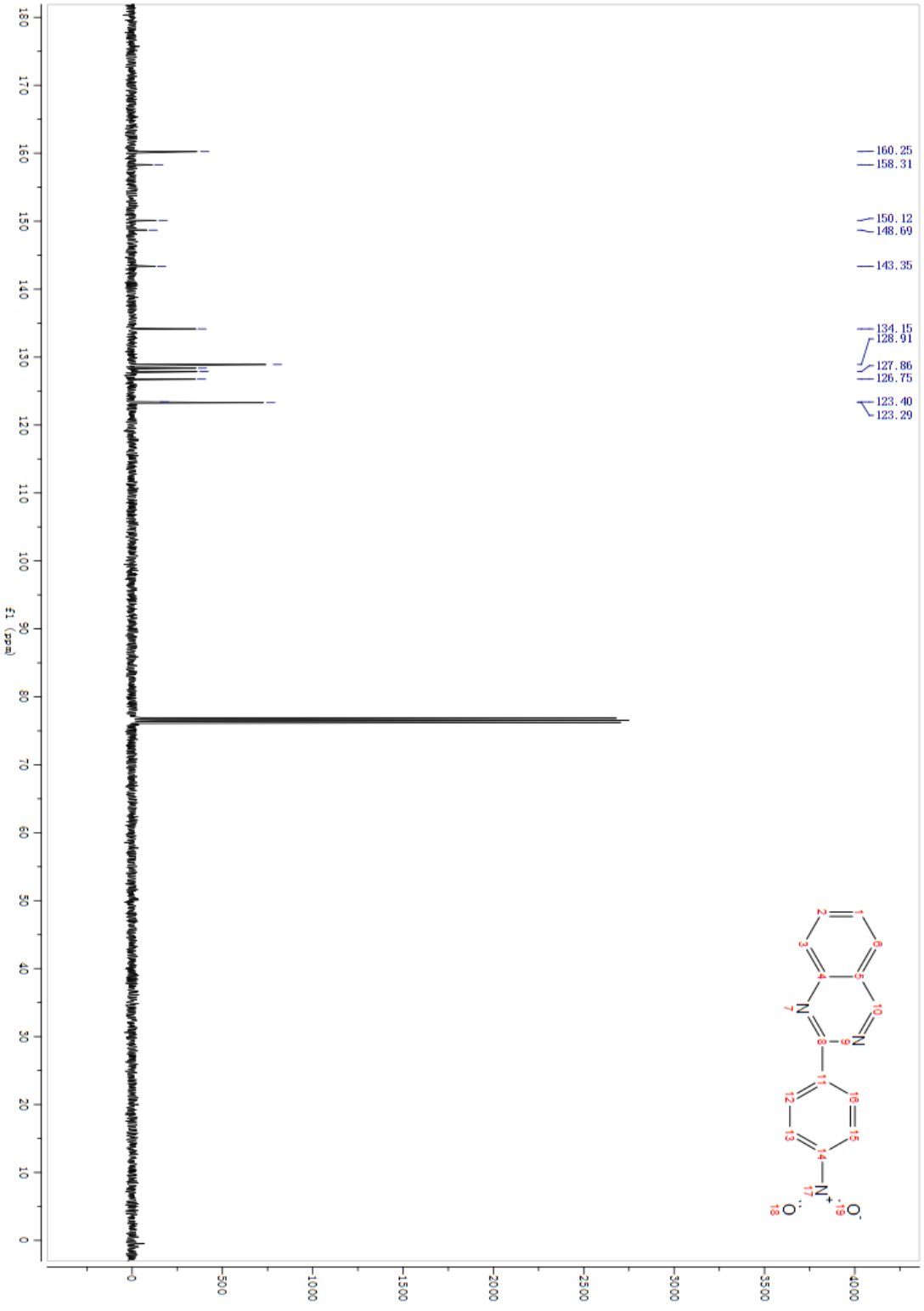

N
N
NO2

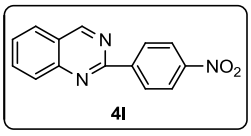
4l


1.00
2.17
2.19
1.08
2.18
1.10
9.54
8.85
8.83
8.41
8.38
8.03
7.98
7.75
7.75
7.73
7.73
7.71
7.71
f1 (ppm)

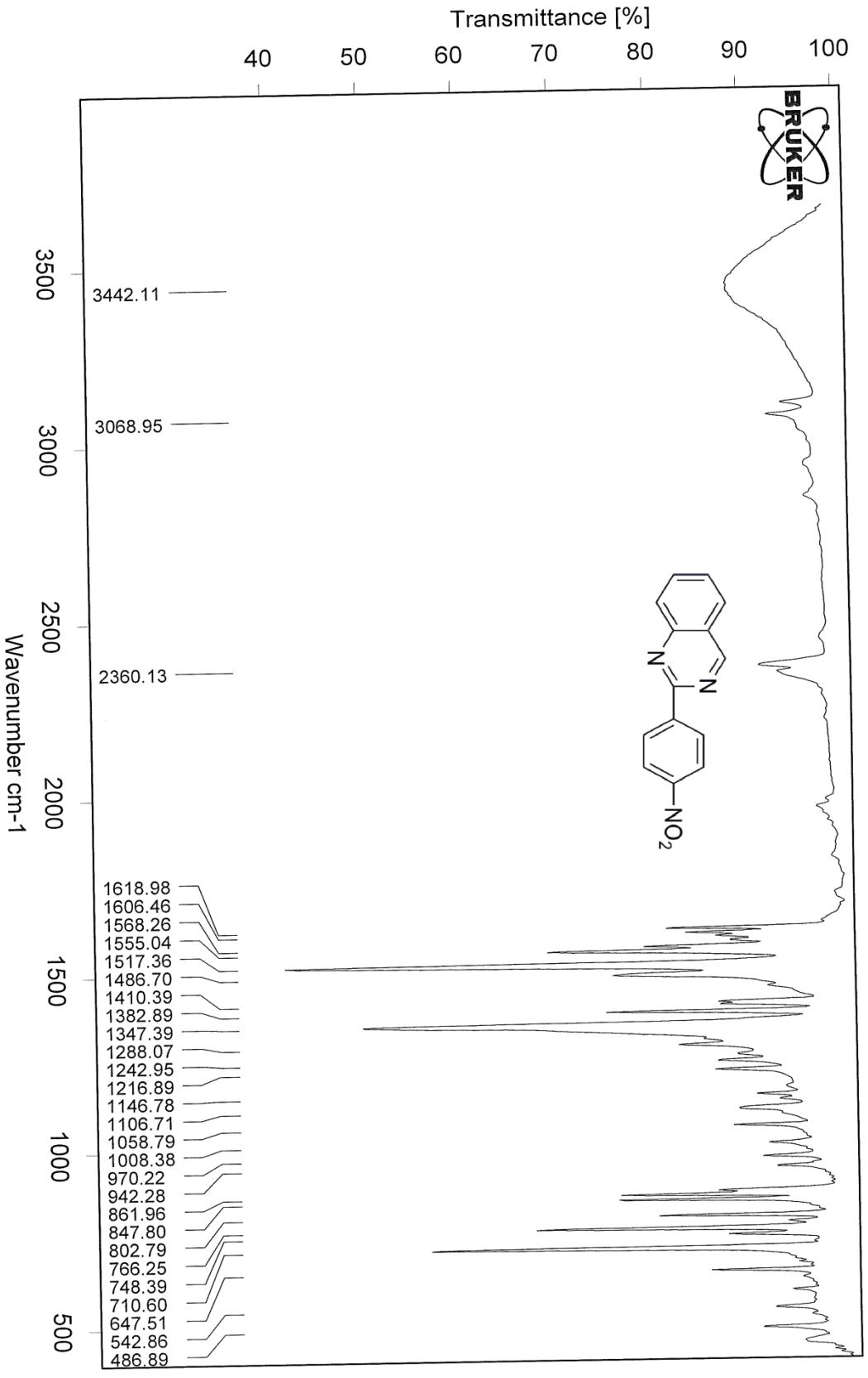

N
N
NO2

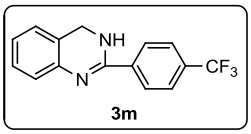
4l


160.25
158.31
150.12
148.69
143.35
134.15
128.91
127.86
126.75
123.40
123.29
f1 (ppm)

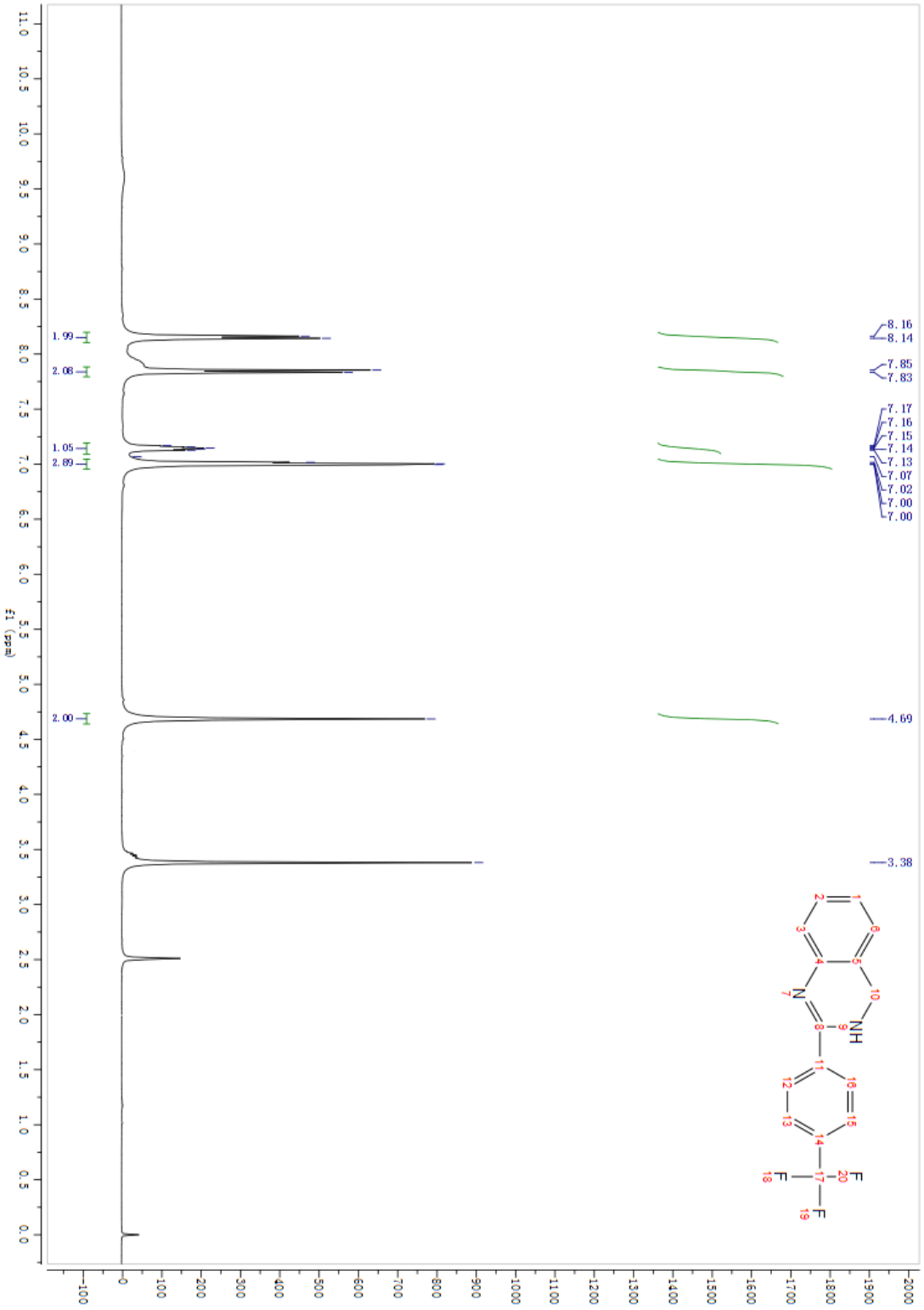

N
N
NO2

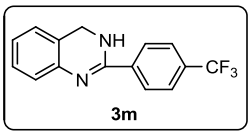
4l


Transmittance [%]
40
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3442.11
3068.95
2360.13
1618.98
1606.46
1568.26
1555.04
1517.36
1486.70
1410.39
1382.89
1347.39
1288.07
1242.95
1216.89
1146.78
1106.71
1058.79
1008.38
970.22
942.28
861.96
847.80
802.79
766.25
748.39
710.60
647.51
542.86
486.89
N
N
NO2

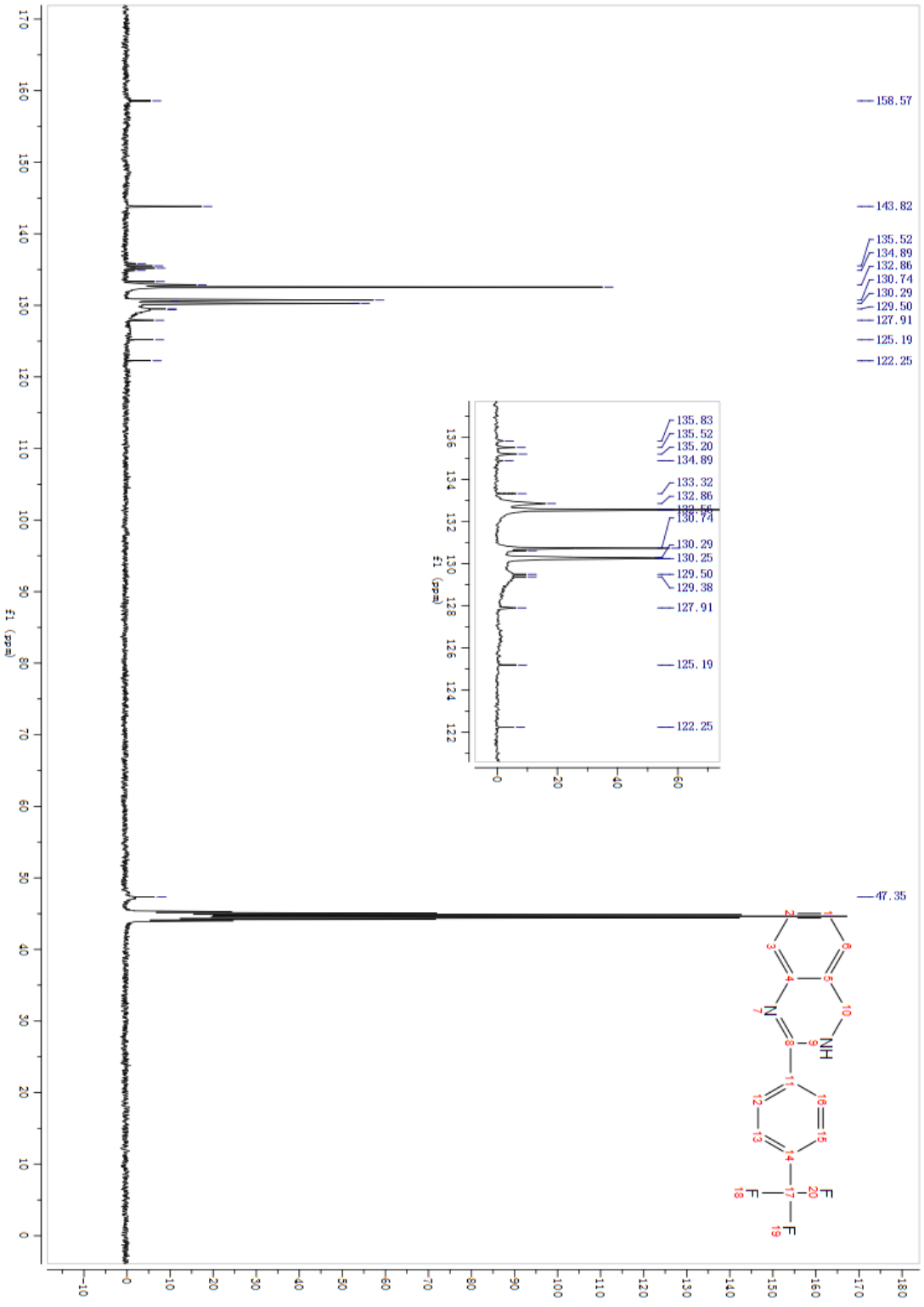

NH
N
CF3

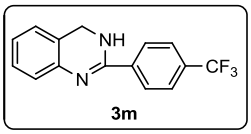
3m


8.16
8.14
7.85
7.83
7.17
7.16
7.15
7.14
7.13
7.07
7.02
7.00
7.00
4.69
3.38
1.99
2.08
1.05
2.89
2.00
f1 (ppm)

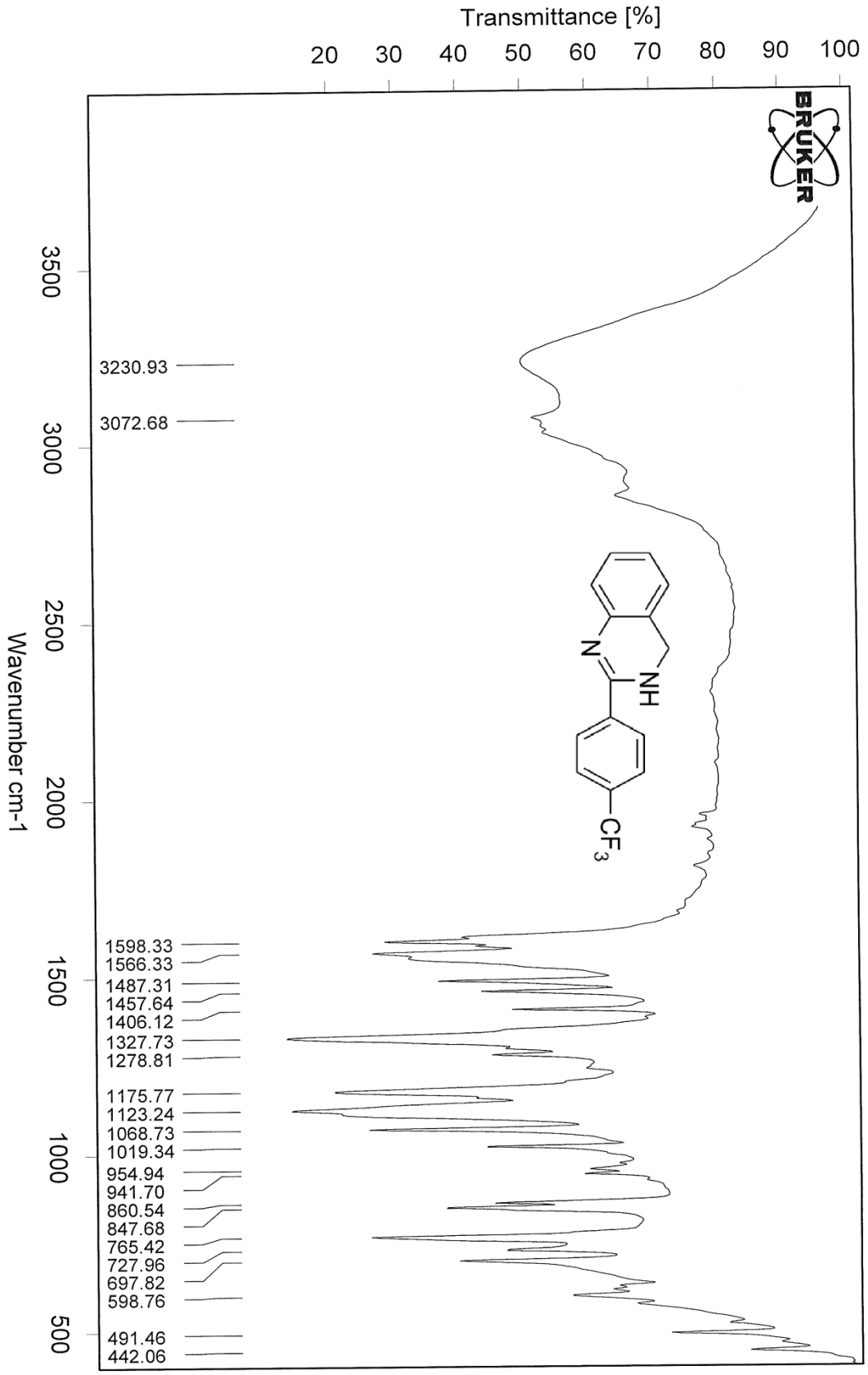

NH
N
CF3

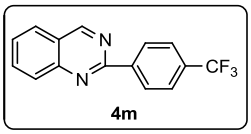
3m


158.57
143.82
135.52
134.89
132.86
130.74
130.29
129.50
127.91
125.19
122.25
47.35
135.83
135.52
135.20
134.89
133.32
132.86
130.74
130.29
130.25
129.50
129.38
127.91
125.19
122.25
f1 (ppm)

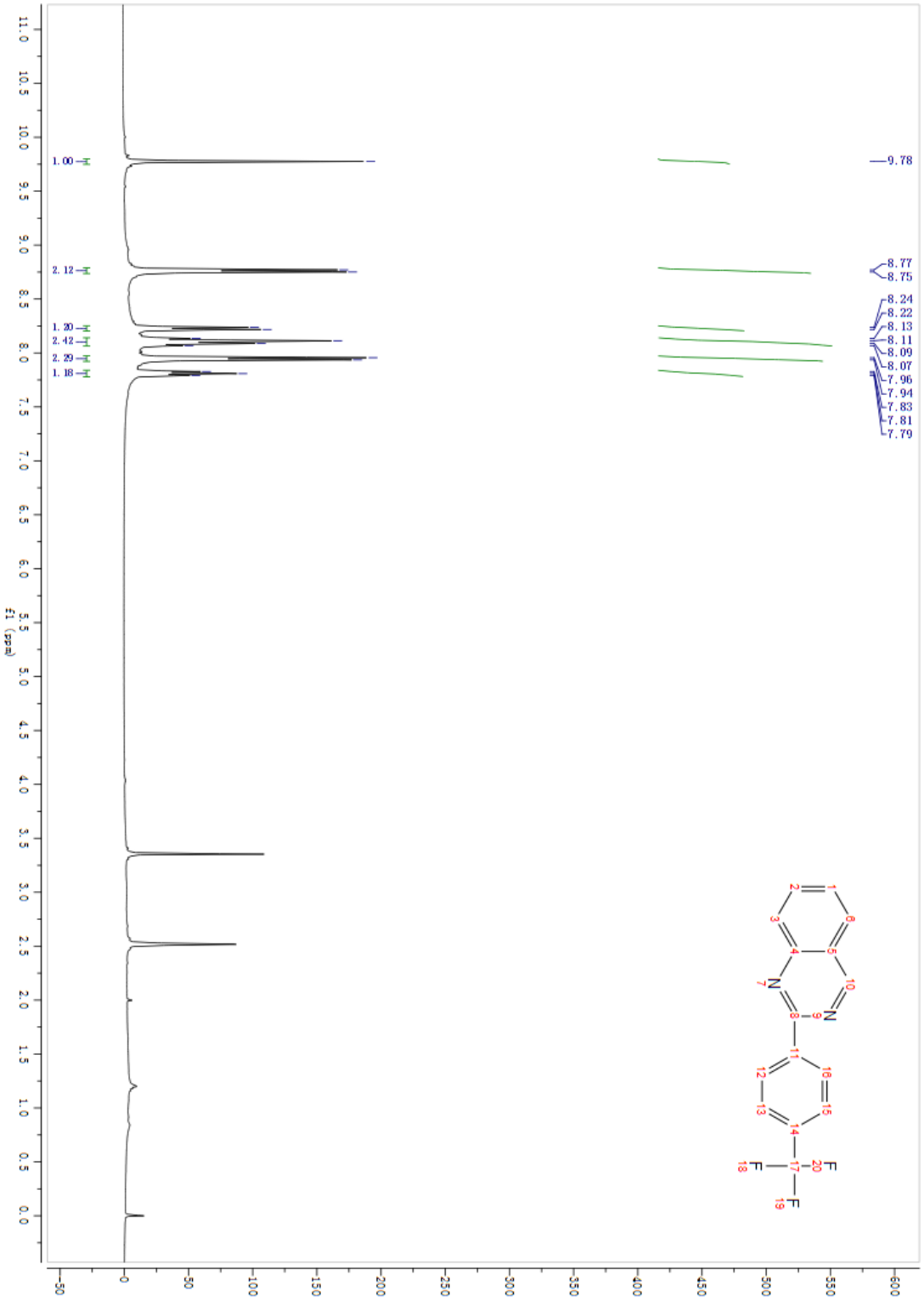

NH
N
CF3

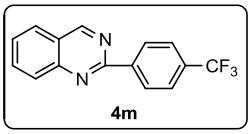
3m


Transmittance [%]
20
30
40
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3230.93
3072.68
1598.33
1566.33
1487.31
1457.64
1406.12
1327.73
1278.81
1175.77
1123.24
1068.73
1019.34
954.94
941.70
860.54
847.68
765.42
727.96
697.82
598.76
491.46
442.06
N
NH
CF3

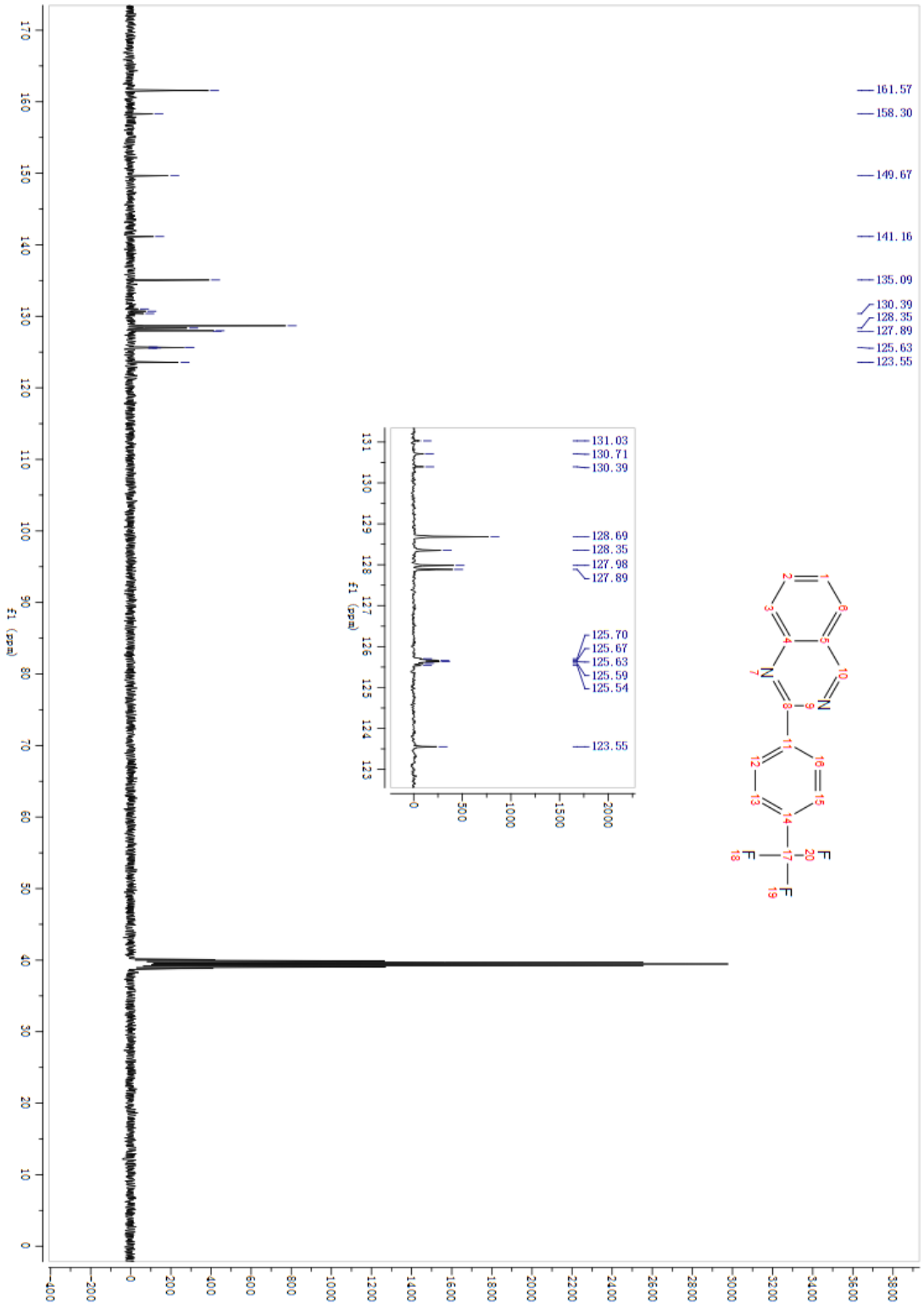

N
N
CF3

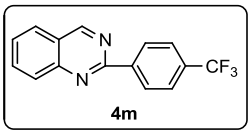
4m


1.00
2.12
1.20
2.42
2.29
1.18
9.78
8.77
8.75
8.24
8.22
8.13
8.11
8.09
8.07
7.96
7.94
7.83
7.81
7.79
f1 (ppm)

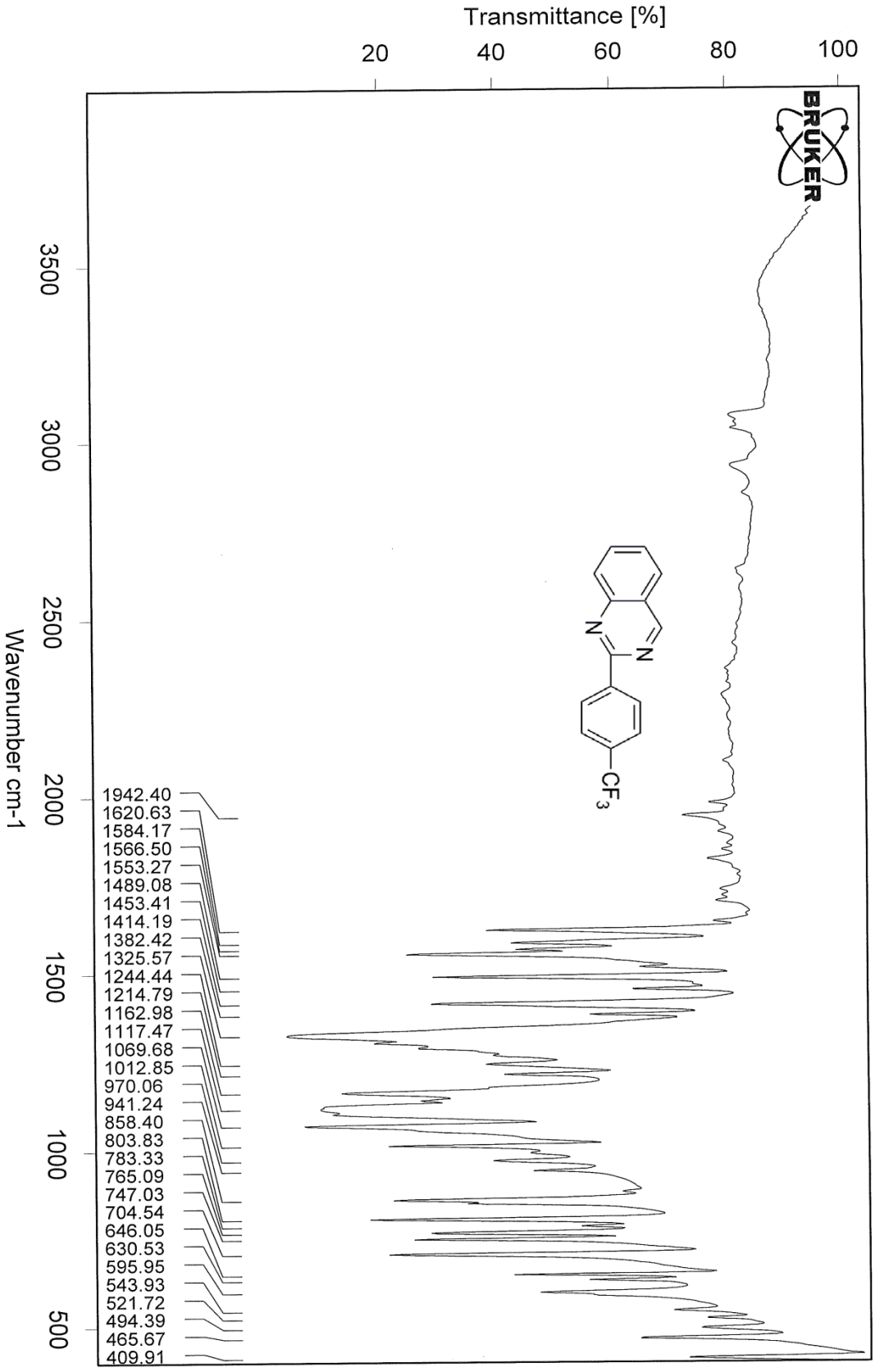

N
N
CF3

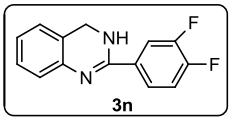
4m


161.57
158.30
149.67
141.16
135.09
130.39
128.35
127.89
125.63
123.55
131.03
130.71
130.39
128.69
128.35
127.98
127.89
125.70
125.67
125.63
125.59
125.54
123.55
f1 (ppm)

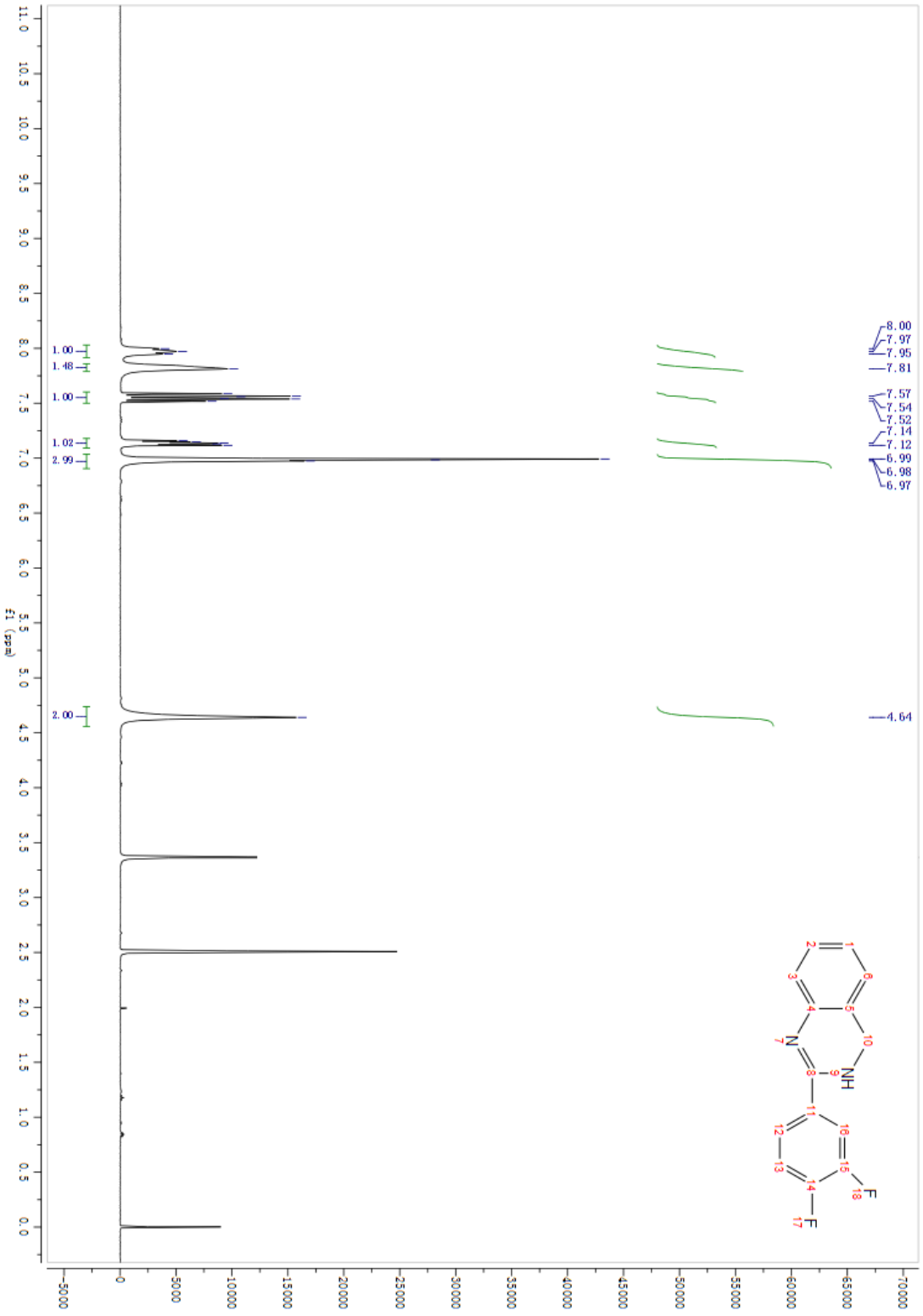

N
N
CF3

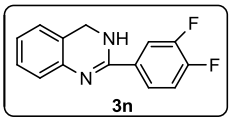
4m


Transmittance [%]
20
40
60
80
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
N
N
CF3
1942.40
1620.63
1584.17
1566.50
1553.27
1489.08
1453.41
1414.19
1382.42
1325.57
1244.44
1214.79
1162.98
1117.47
1069.68
1012.85
970.06
941.24
858.40
803.83
783.33
765.09
747.03
704.54
646.05
630.53
595.95
543.93
521.72
494.39
465.67
409.91

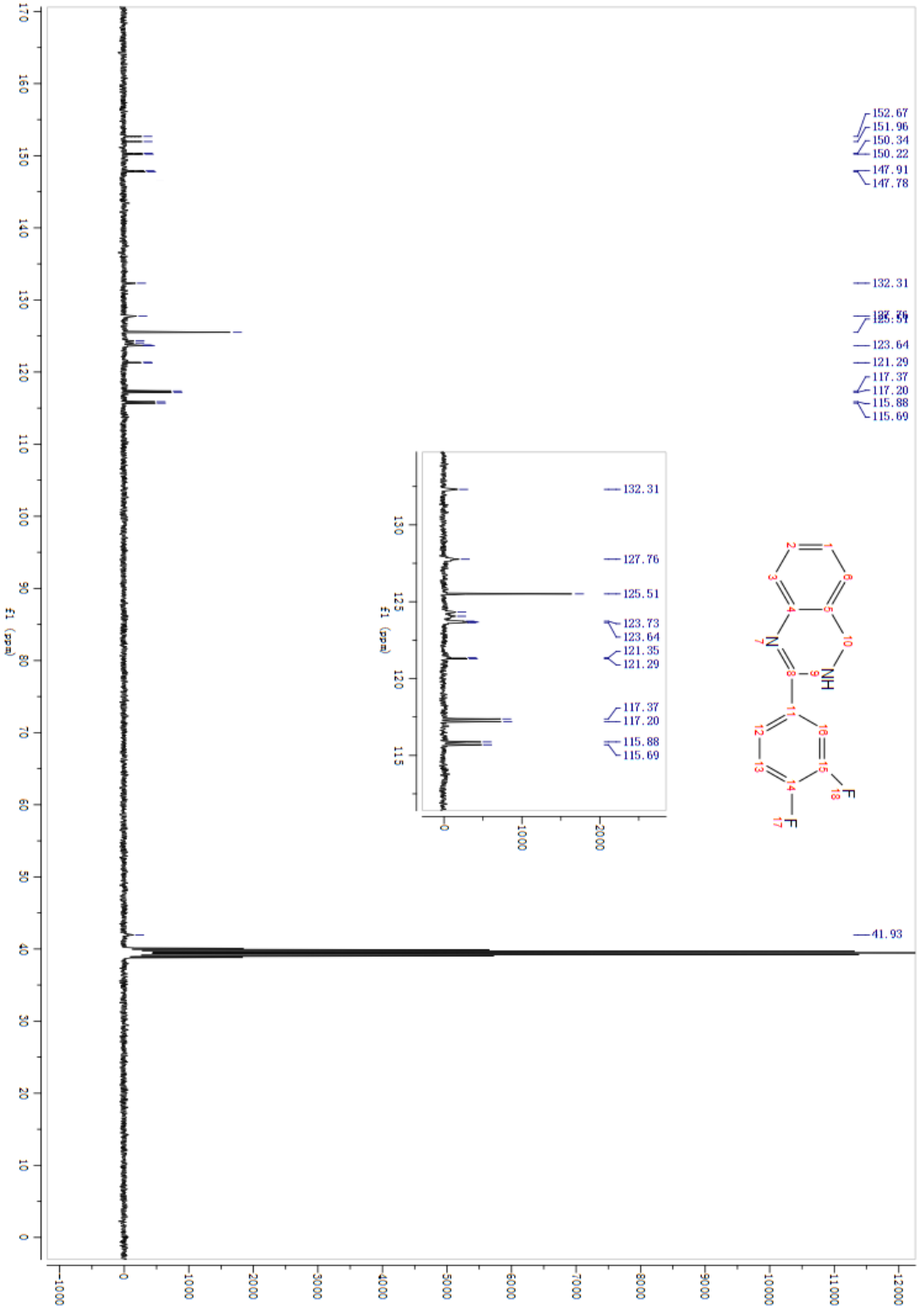

NH
N
F
F

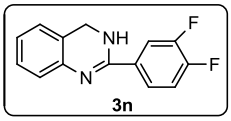
3n

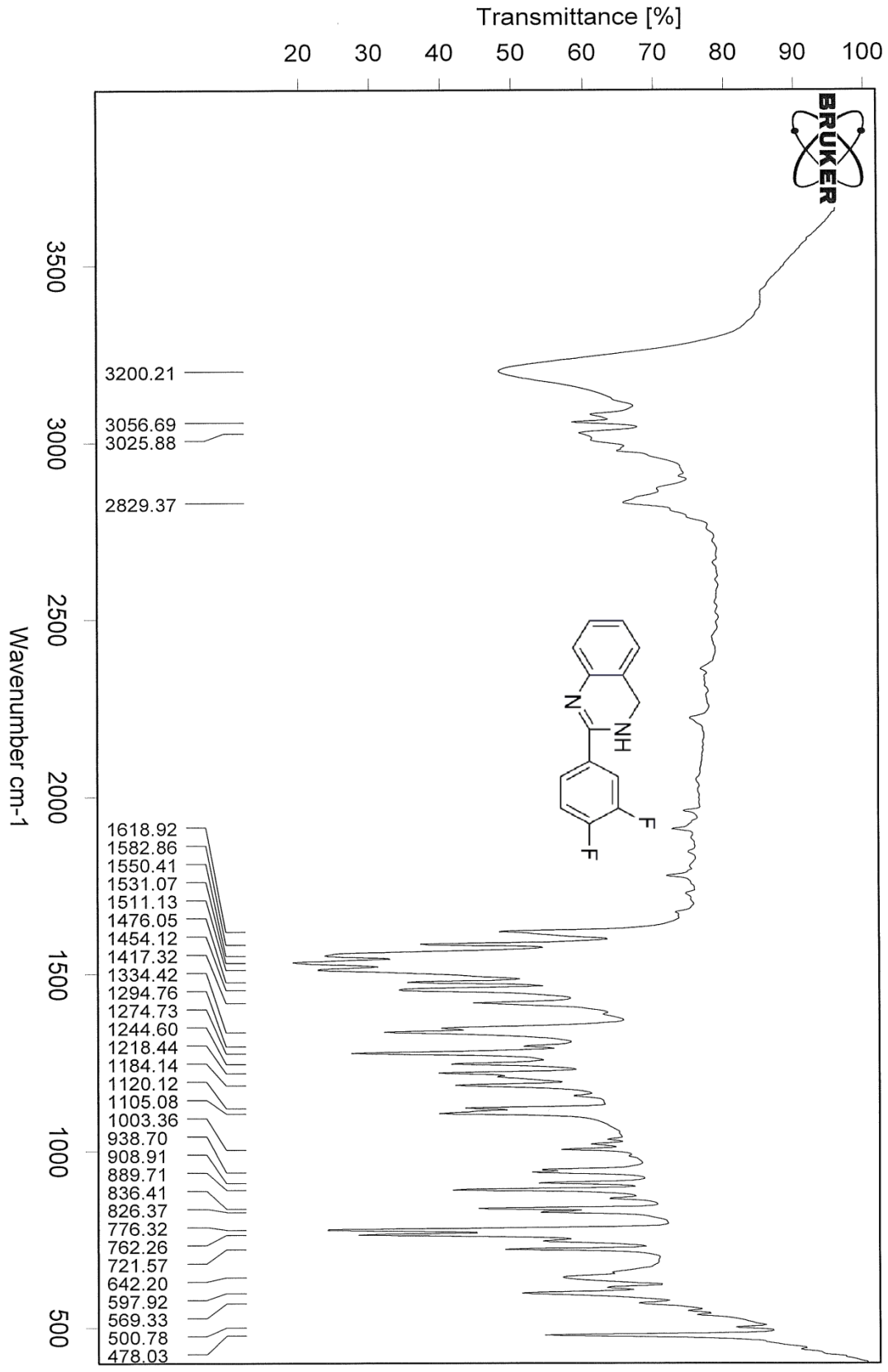

8.00
7.97
7.95
7.81
7.57
7.54
7.52
7.14
7.12
6.99
6.98
6.97
4.64
1.00
1.48
1.00
1.02
2.99
2.00
f1 (ppm)

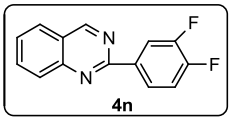

NH
N
F
F

3n

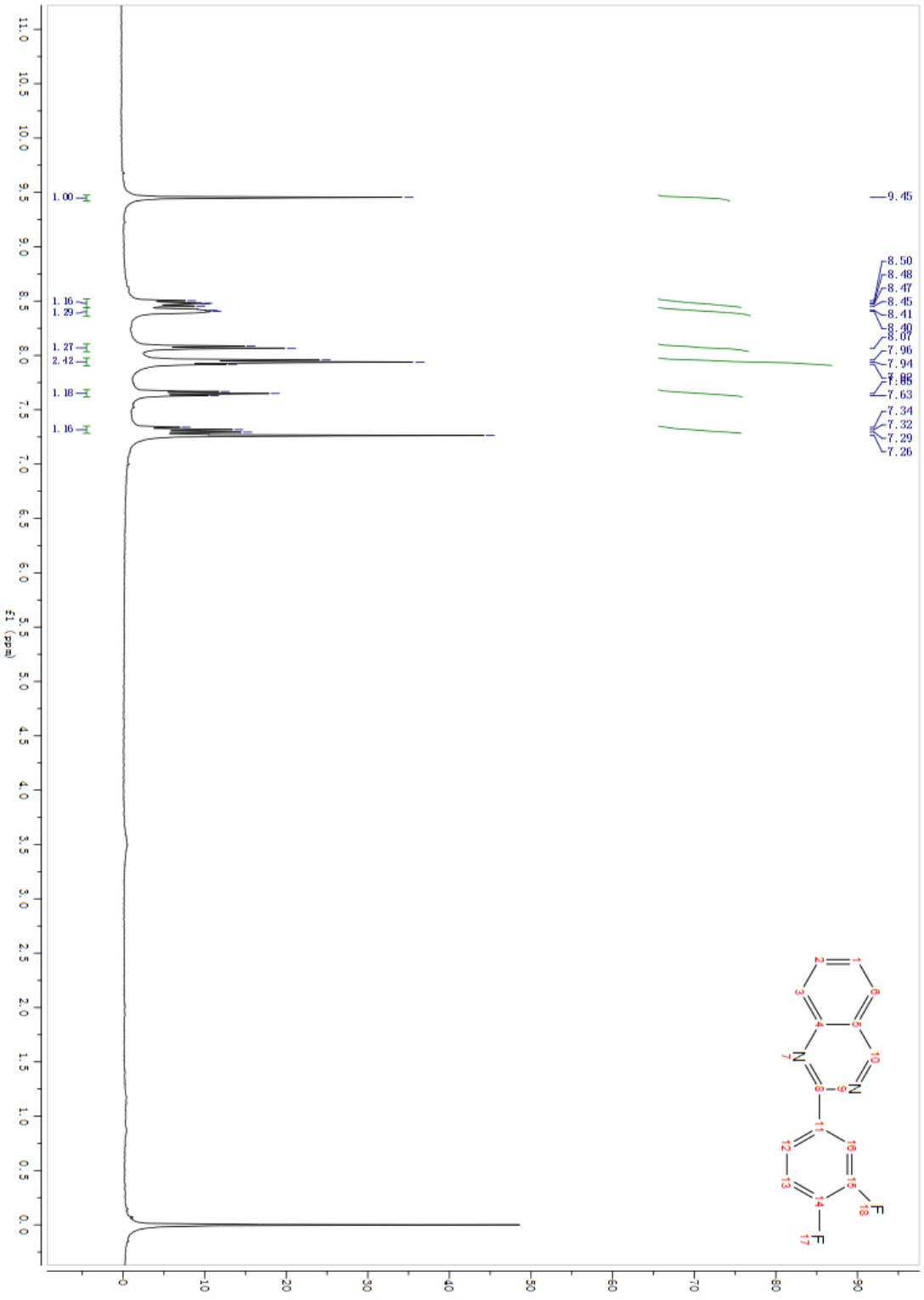

152.67
151.96
150.34
150.22
147.91
147.78
132.31
123.64
121.29
117.37
117.20
115.88
115.69
41.93
f1 (ppm)
132.31
127.76
125.51
123.73
123.64
121.35
121.29
117.37
117.20
115.88
115.69
NH
F
F

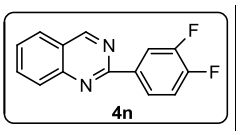

NH
F
F
N
3n


Transmittance [%]
20
30
40
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3200.21
3056.69
3025.88
2829.37
1618.92
1582.86
1550.41
1531.07
1511.13
1476.05
1454.12
1417.32
1334.42
1294.76
1274.73
1244.60
1218.44
1184.14
1120.12
1105.08
1003.36
938.70
908.91
889.71
836.41
826.37
776.32
762.26
721.57
642.20
597.92
569.33
500.78
478.03
N
NH
F
F

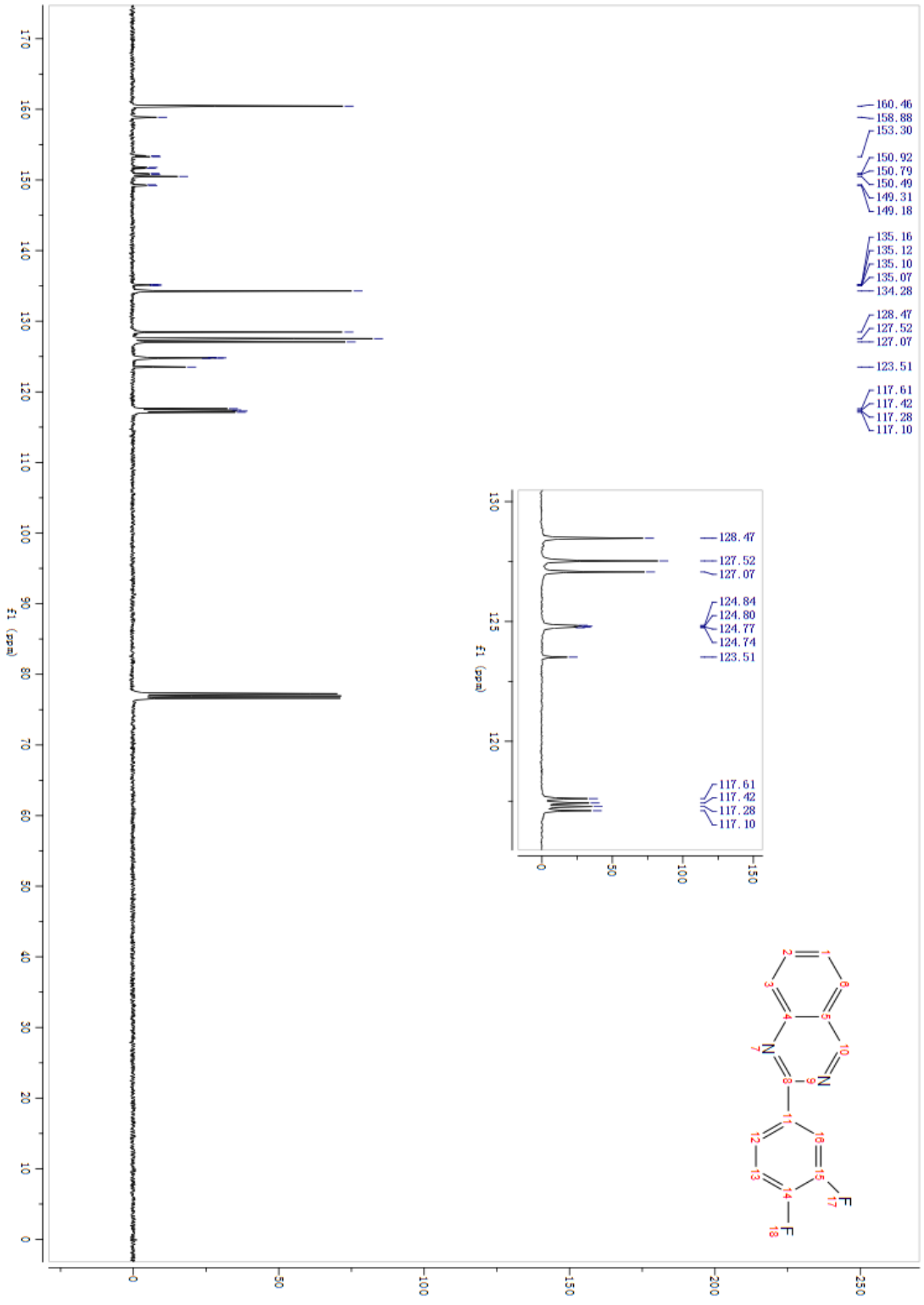

F
N
N
F

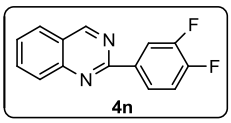
4n


1.00
1.16
1.29
1.27
2.42
1.18
1.16
9.45
8.50
8.48
8.47
8.45
8.41
8.40
8.07
7.96
7.94
7.63
7.34
7.32
7.29
7.26
f1 (ppm)

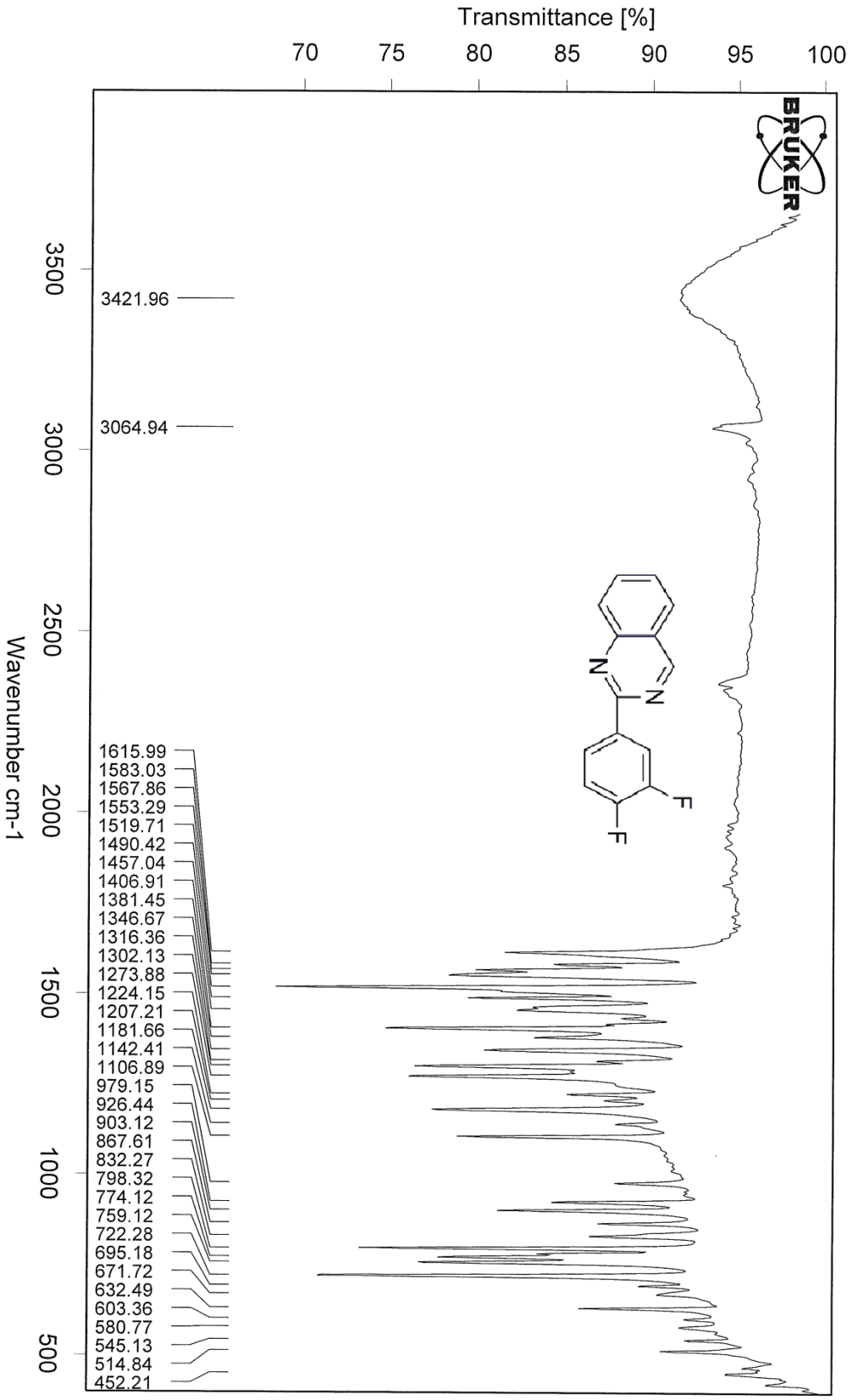

F
N
N
F

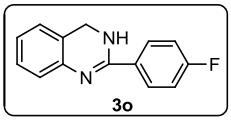
4n


160.46
158.88
153.30
150.92
150.79
150.49
149.31
149.18
135.16
135.12
135.10
135.07
134.28
128.47
127.52
127.07
123.51
117.61
117.42
117.28
117.10
f1 (ppm)

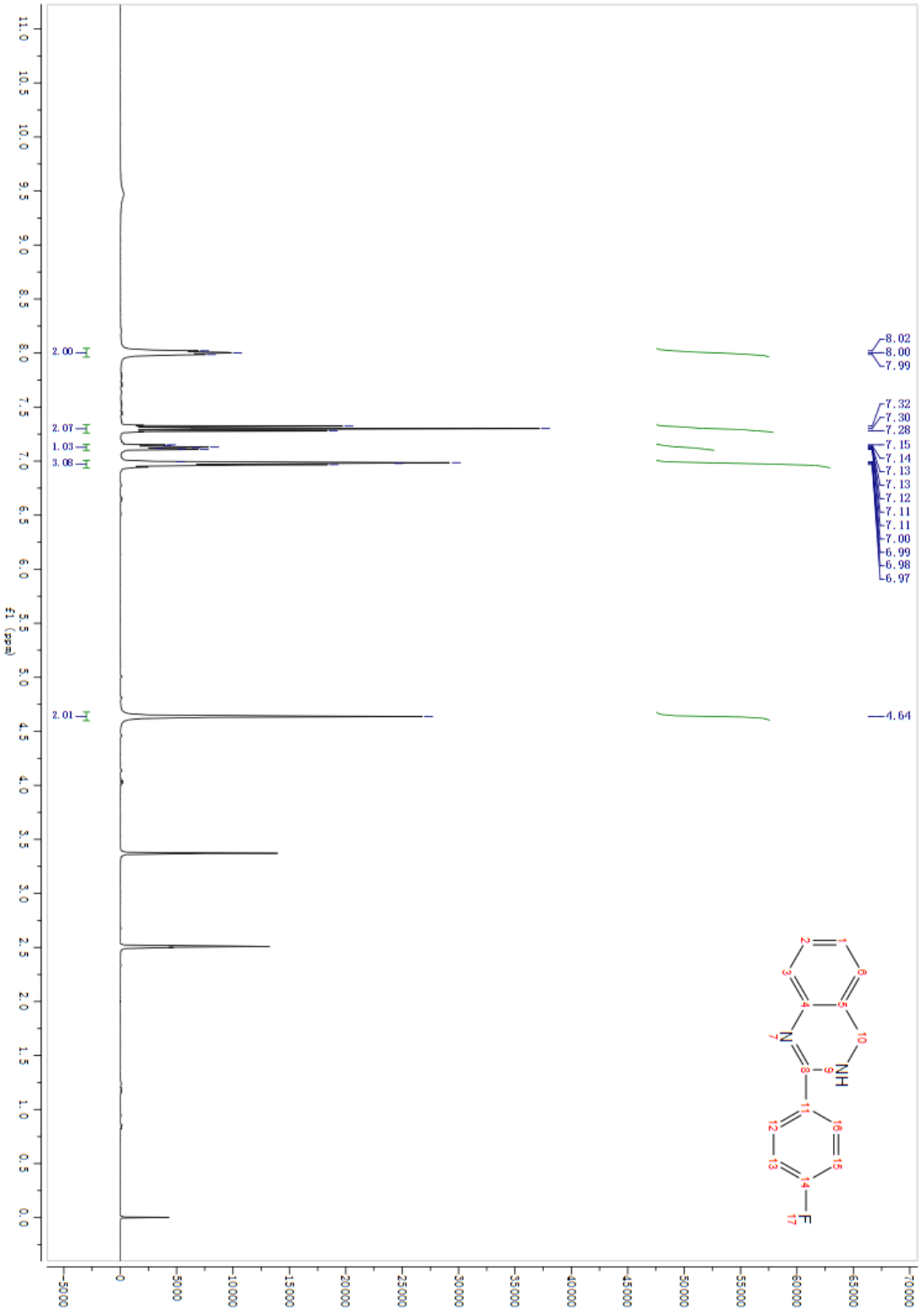

F
N
N
F

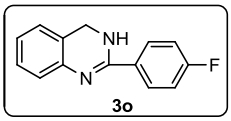
4n


Transmittance [%]
70
75
80
85
90
95
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3421.96
3064.94
1615.99
1583.03
1567.86
1553.29
1519.71
1490.42
1457.04
1406.91
1381.45
1346.67
1316.36
1302.13
1273.88
1224.15
1207.21
1181.66
1142.41
1106.89
979.15
926.44
903.12
867.61
832.27
798.32
774.12
759.12
722.28
695.18
671.72
632.49
603.36
580.77
545.13
514.84
452.21
N
N
F
F

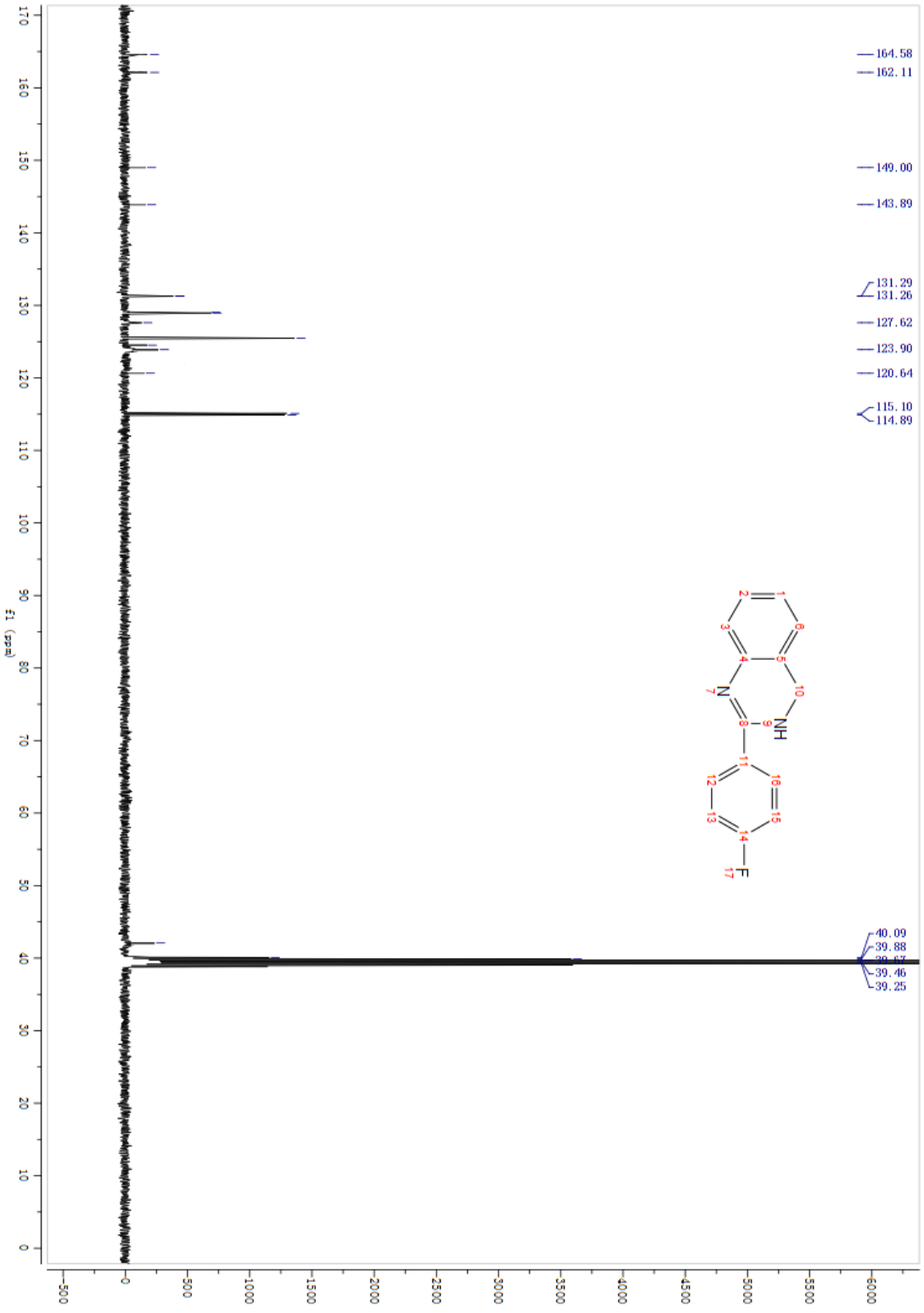

NH
N
F

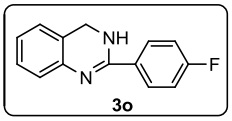
3o


2.00
2.07
1.03
3.08
2.01
8.02
8.00
7.99
7.32
7.30
7.28
7.15
7.14
7.13
7.13
7.12
7.11
7.11
7.00
6.99
6.98
6.97
4.64
f1 (ppm)

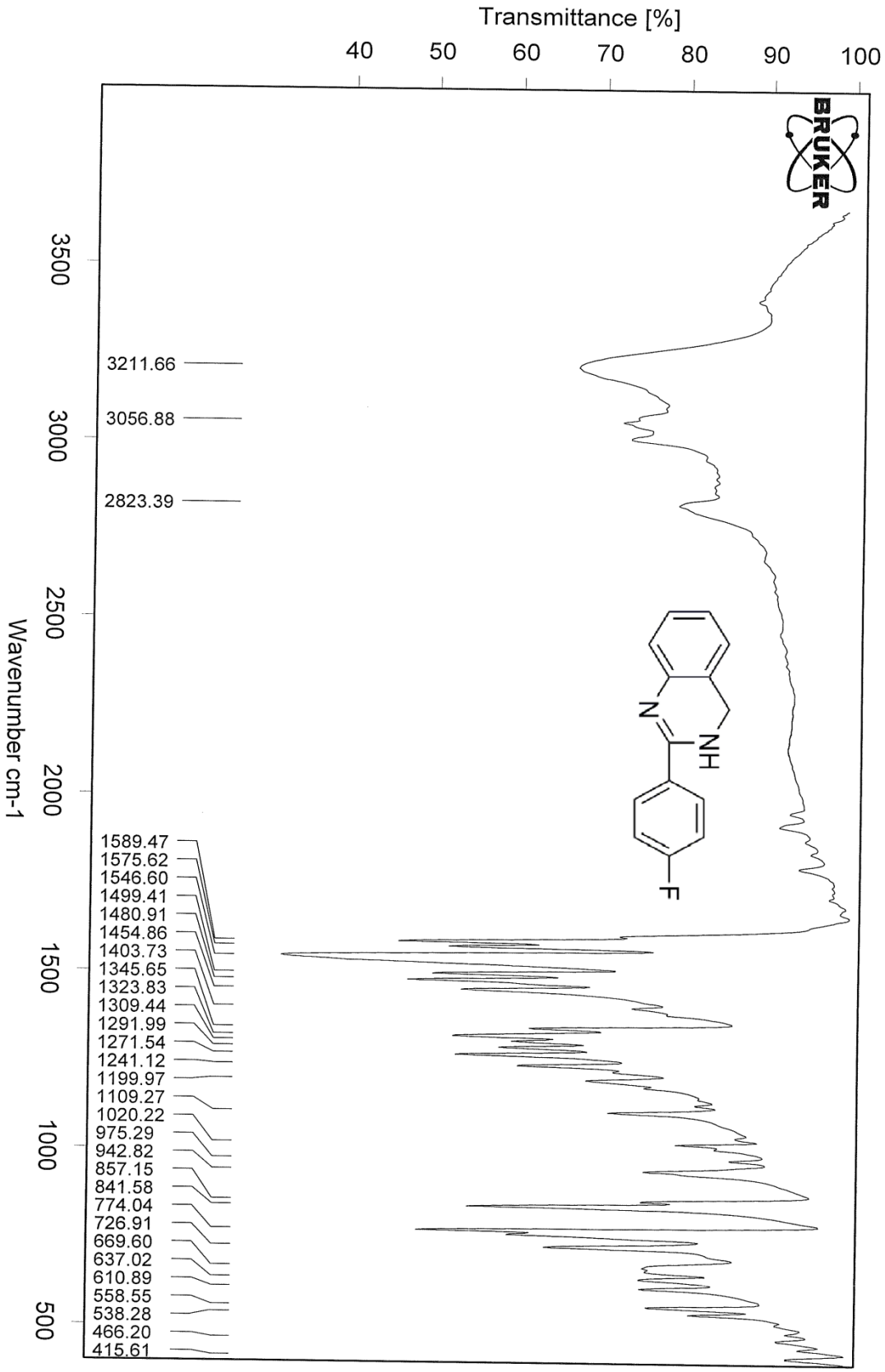

NH
N
F

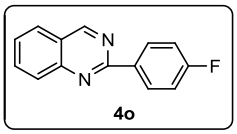
3o


164.58
162.11
149.00
143.89
131.29
131.26
127.62
123.90
120.64
115.10
114.89
40.09
39.88
39.46
39.25
f1 (ppm)

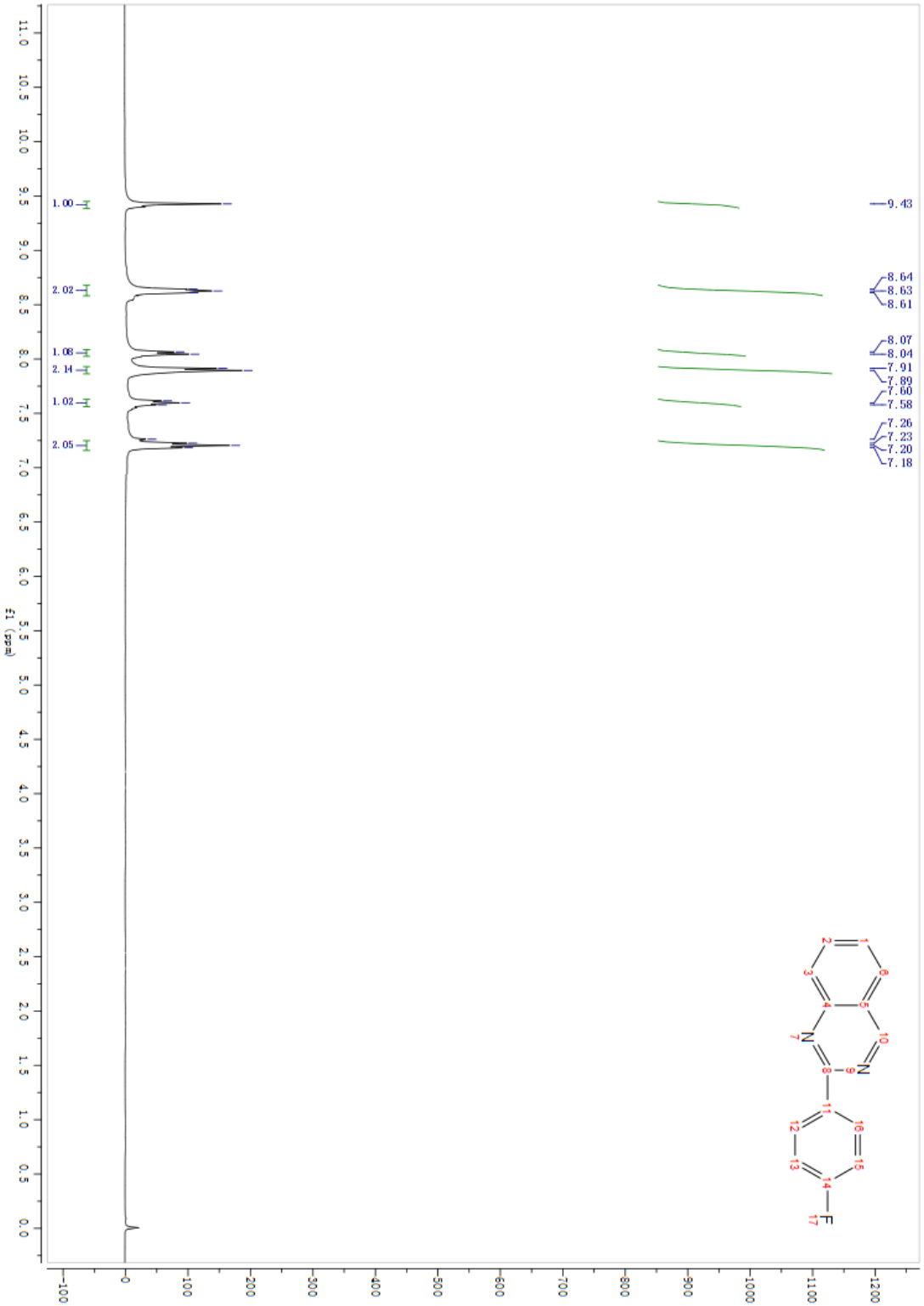

NH
N
F

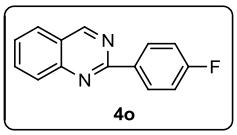
3o


Transmittance [%]
40
50
60
70
80
90
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3211.66
3056.88
2823.39
1589.47
1575.62
1546.60
1499.41
1480.91
1454.86
1403.73
1345.65
1323.83
1309.44
1291.99
1271.54
1241.12
1199.97
1109.27
1020.22
975.29
942.82
857.15
841.58
774.04
726.91
669.60
637.02
610.89
558.55
538.28
466.20
415.61
N
NH
F

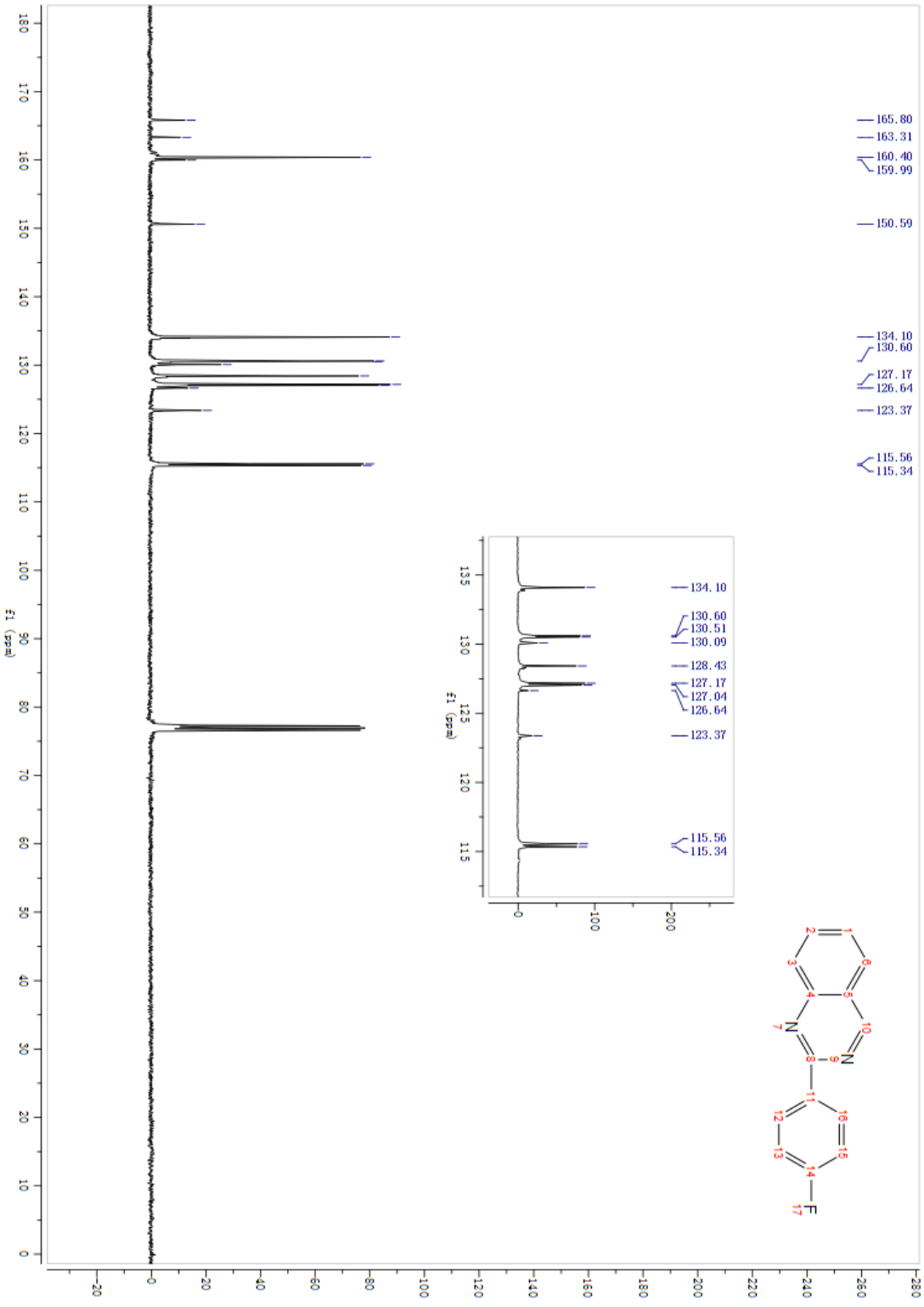

N
N
F

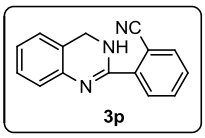
4o

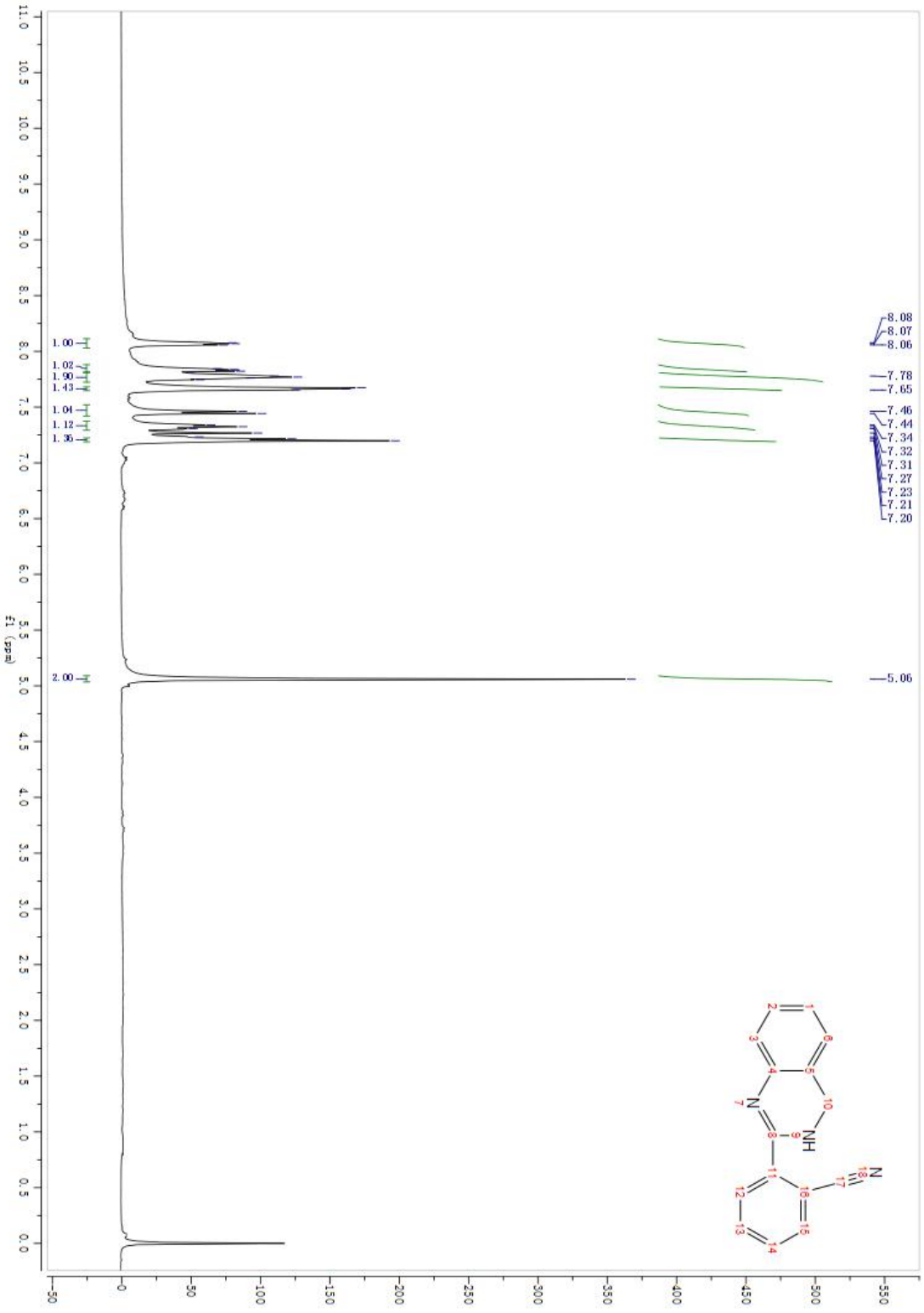

1.00
2.02
1.08
2.14
1.02
2.05
9.43
8.64
8.63
8.61
8.07
8.04
7.91
7.89
7.60
7.58
7.26
7.23
7.20
7.18
f1 (ppm)

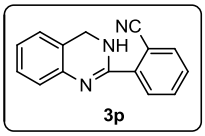

N
N
F

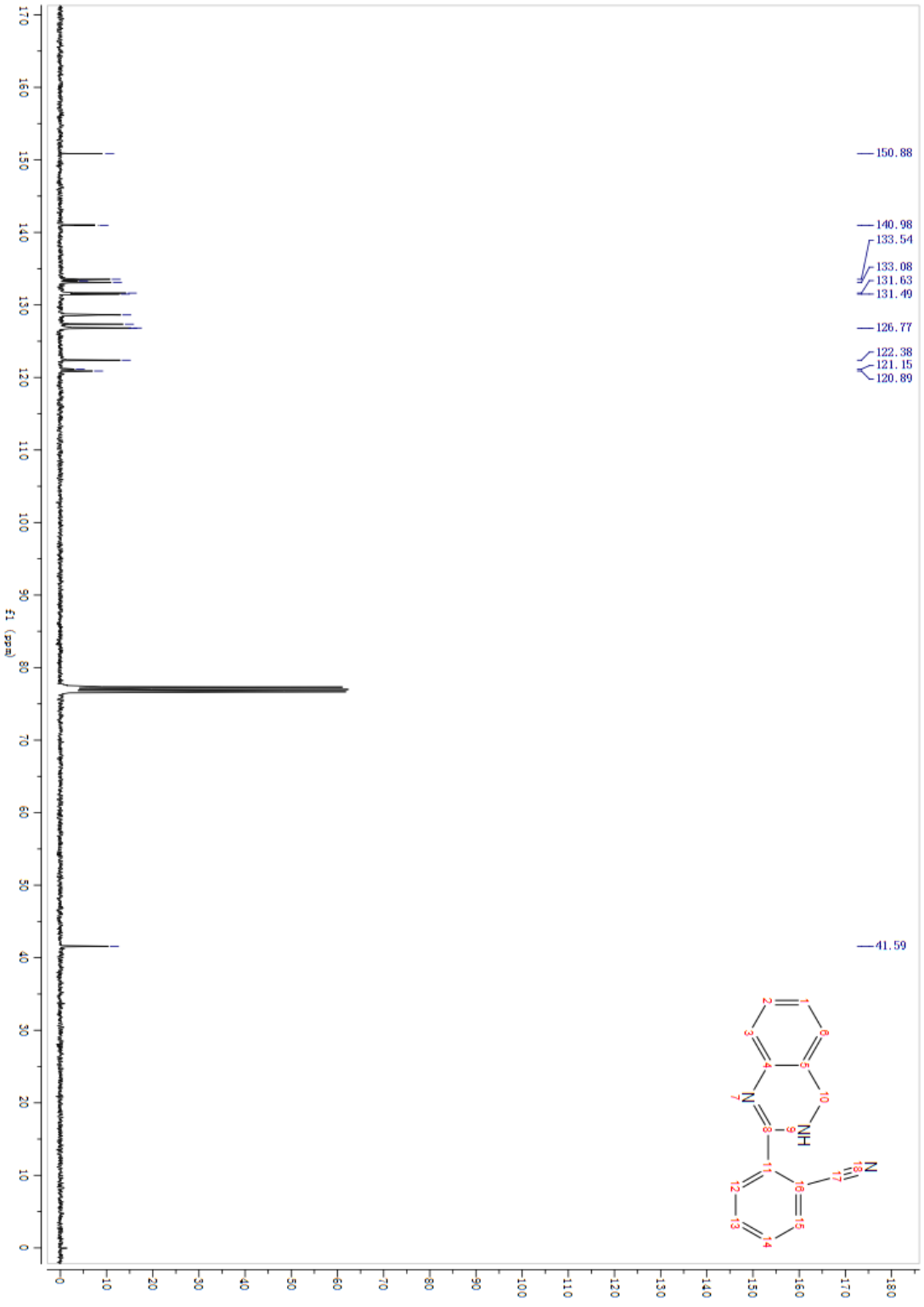
4o

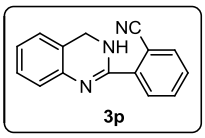

165.80
163.31
160.40
159.99
150.59
134.10
130.60
127.17
126.64
123.37
115.56
115.34
f1 (ppm)
134.10
130.60
130.51
130.09
128.43
127.17
127.04
126.64
123.37
115.56
115.34
f1 (ppm)

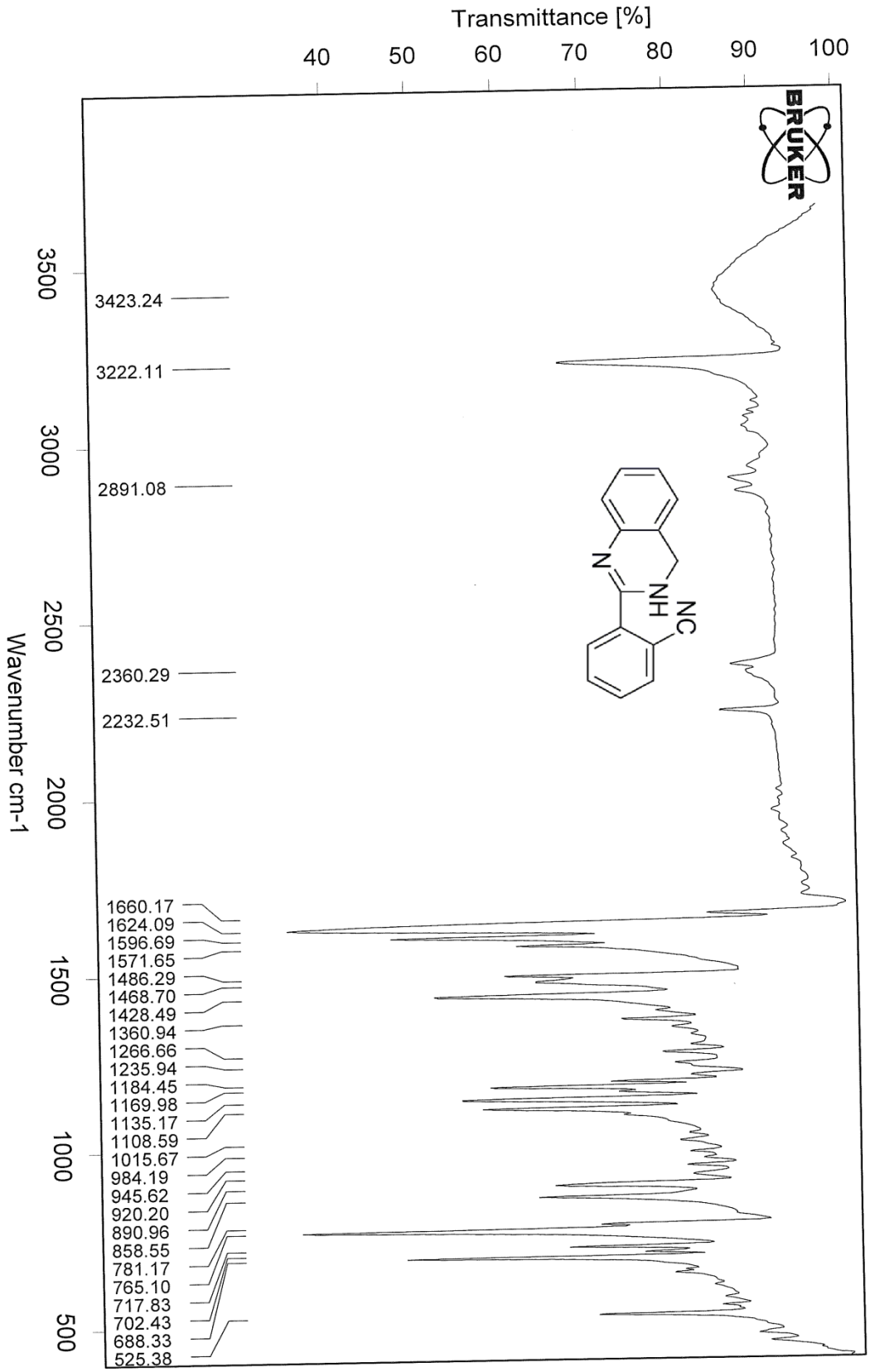

NC
NH
N
3p

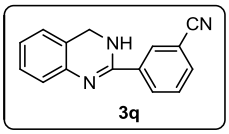

8.08
8.07
8.06
7.78
7.65
7.46
7.44
7.34
7.32
7.31
7.27
7.23
7.21
7.20
5.06
1.00
1.02
1.90
1.43
1.04
1.12
1.36
2.00
f1 (ppm)


NC
NH
N
3p

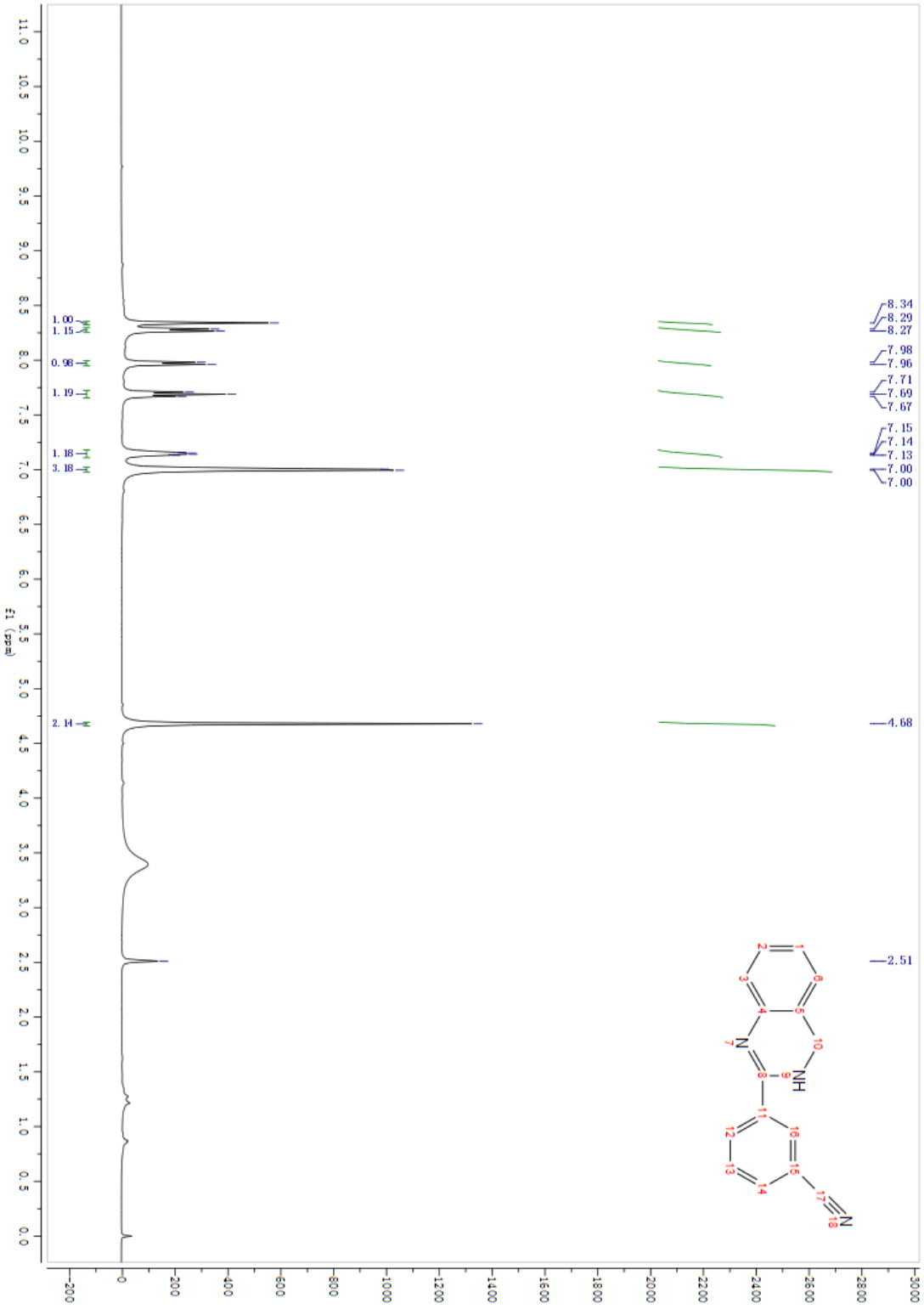

150.88
140.98
133.54
133.08
131.63
131.49
126.77
122.38
121.15
120.89
41.59
f1 (ppm)


NC
NH
N
3p


Transmittance [%]
40
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3423.24
3222.11
2891.08
2360.29
2232.51
1660.17
1624.09
1596.69
1571.65
1486.29
1468.70
1428.49
1360.94
1266.66
1235.94
1184.45
1169.98
1135.17
1108.59
1015.67
984.19
945.62
920.20
890.96
858.55
781.17
765.10
717.83
702.43
688.33
525.38
N
NH
NC


CN
NH
N

3q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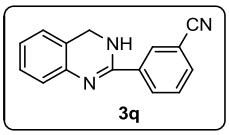
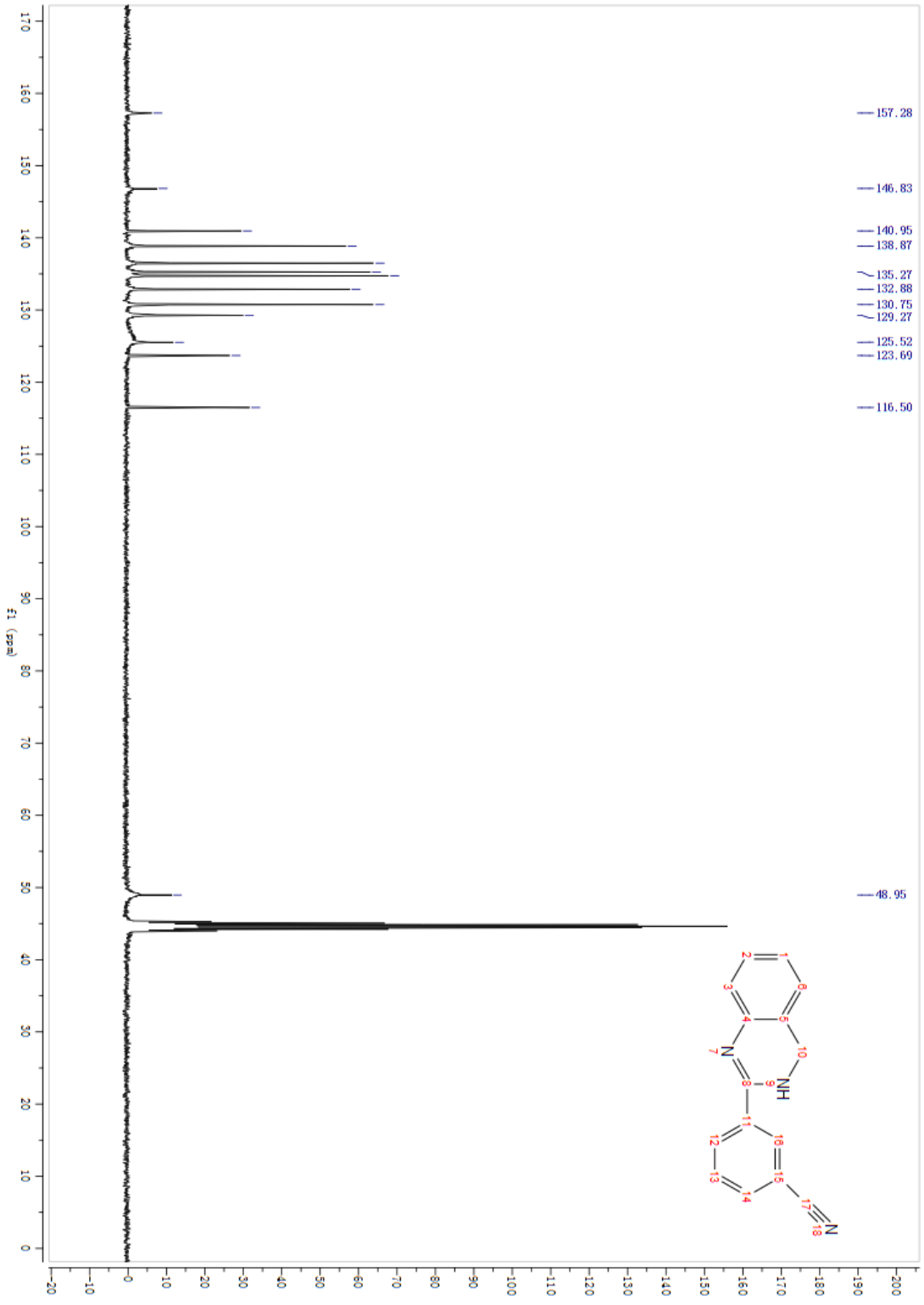
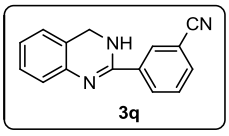
1.15
0.98
1.19
1.18
3.18
2.14
8.34
8.29
8.27
7.98
7.96
7.71
7.69
7.67
7.15
7.14
7.13
7.00
7.00
4.68
2.51
f1 (ppm)

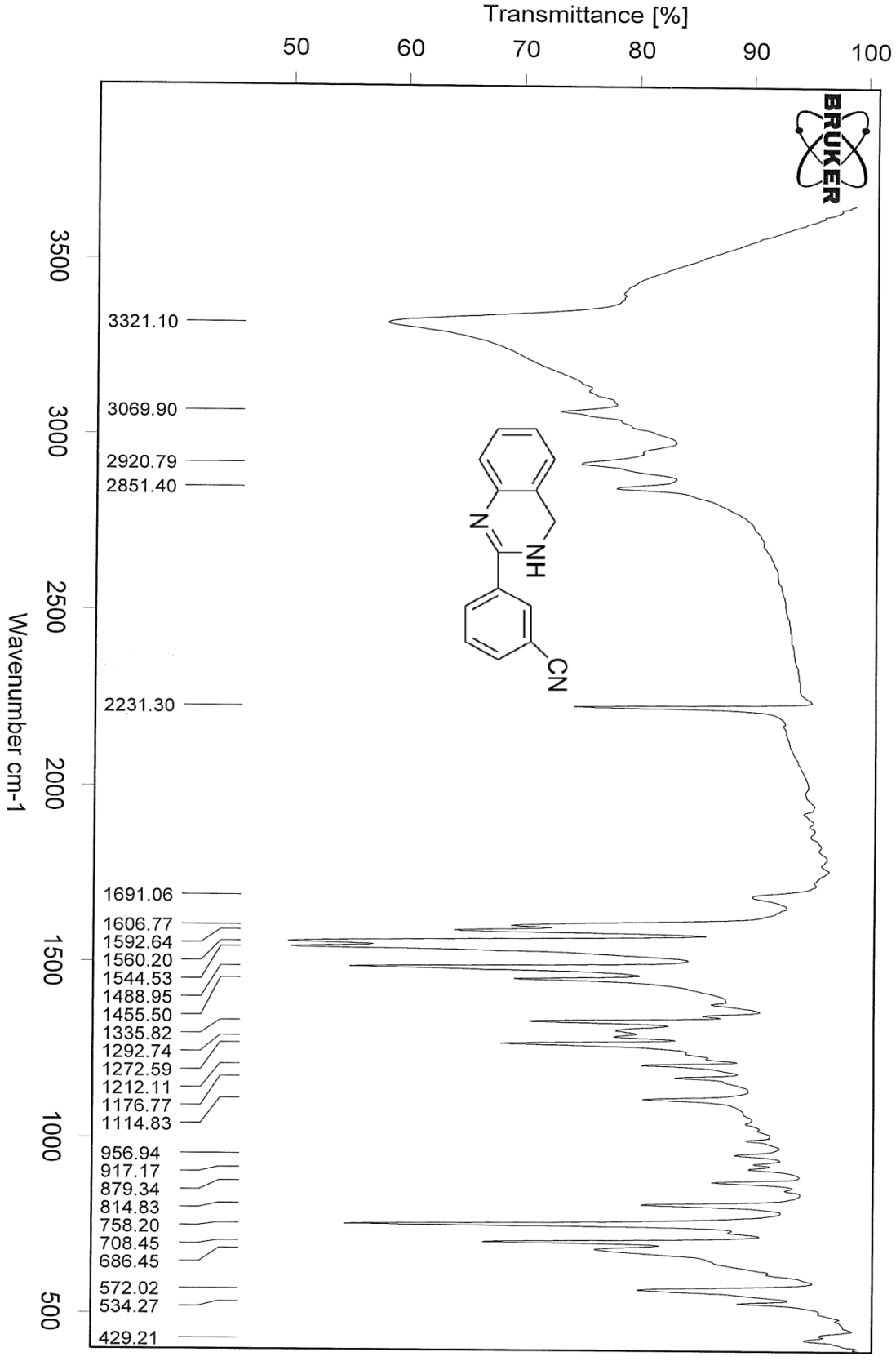

CN
NH
N

3q


157.28
146.83
140.95
138.87
135.27
132.88
130.75
129.27
125.52
123.69
116.50
48.95
f1 (ppm)


CN
NH
N

3q


Transmittance [%]
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70
80
90
100
BRUKER
Wavenumber cm-1
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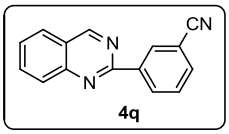
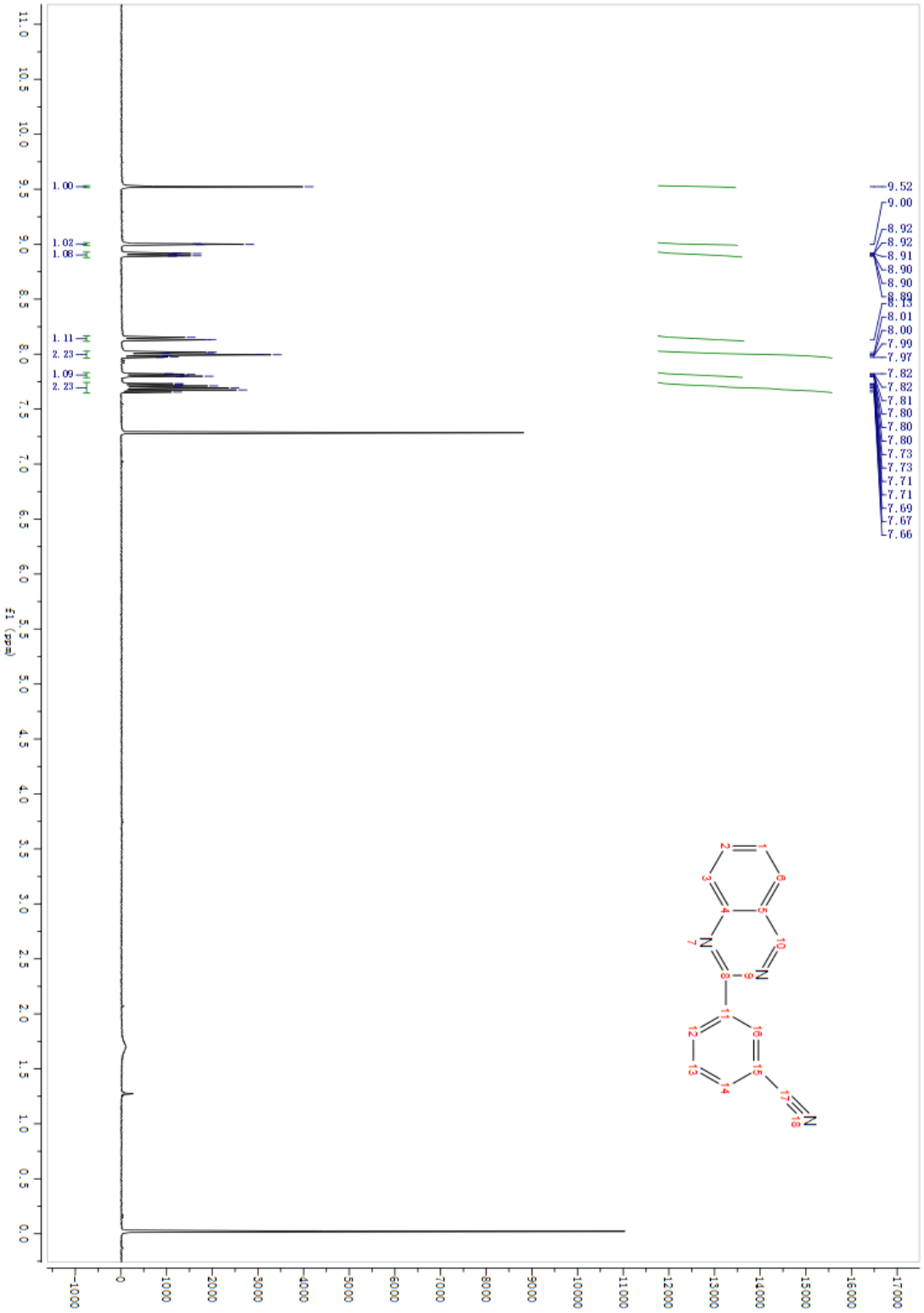
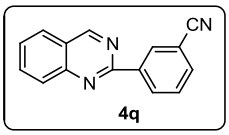
3000
2500
2000
1500
1000
500
3321.10
3069.90
2920.79
2851.40
2231.30
1691.06
1606.77
1592.64
1560.20
1544.53
1488.95
1455.50
1335.82
1292.74
1272.59
1212.11
1176.77
1114.83
956.94
917.17
879.34
814.83
758.20
708.45
686.45
572.02
534.27
429.21
N
NH
CN

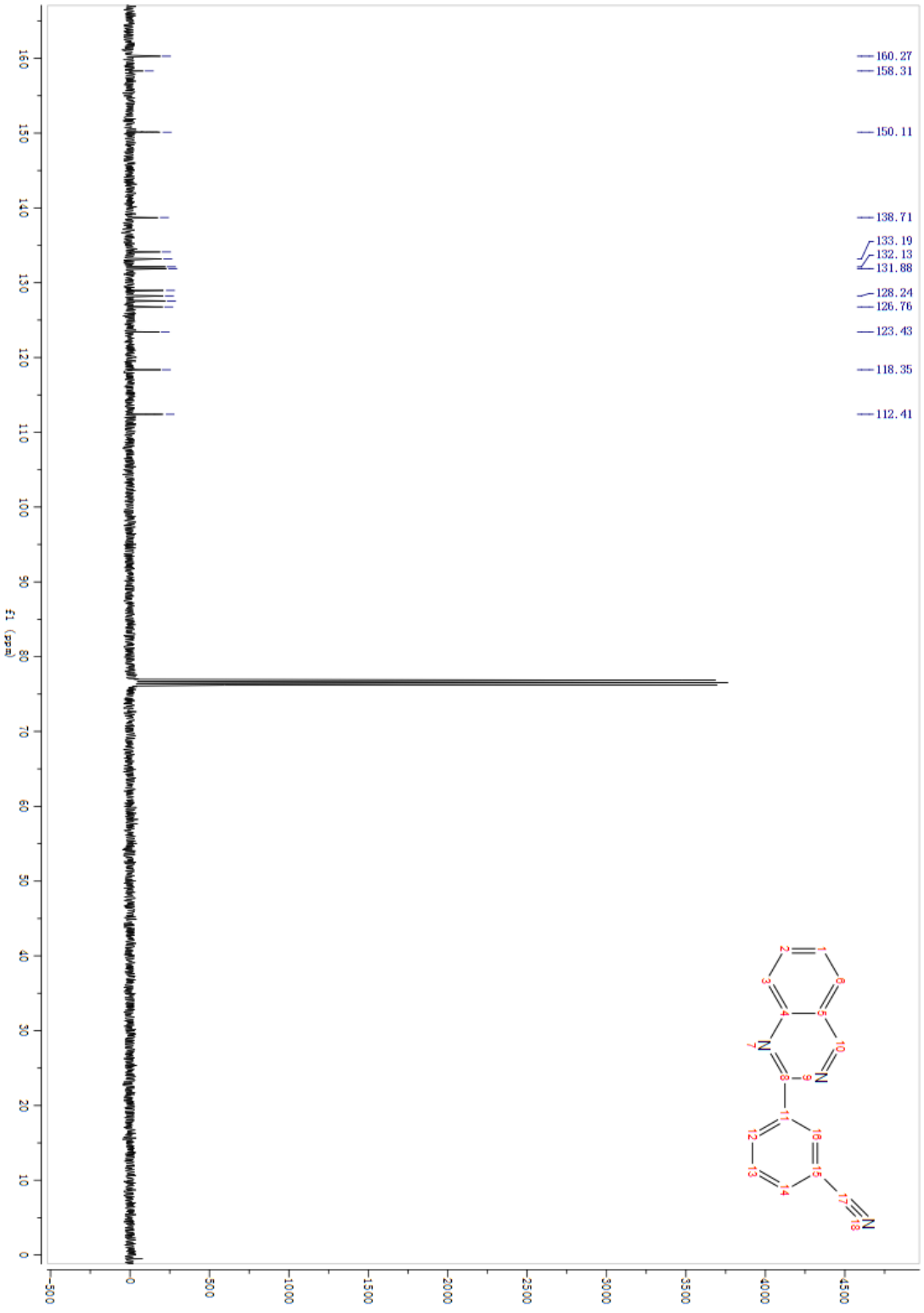

CN
N
N

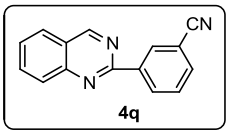
4q


1.00
1.02
1.08
1.11
2.23
1.09
2.23
9.52
9.00
8.92
8.92
8.91
8.90
8.90
8.01
8.00
7.99
7.97
7.82
7.82
7.81
7.80
7.80
7.80
7.73
7.73
7.71
7.71
7.69
7.67
7.66
f1 (ppm)

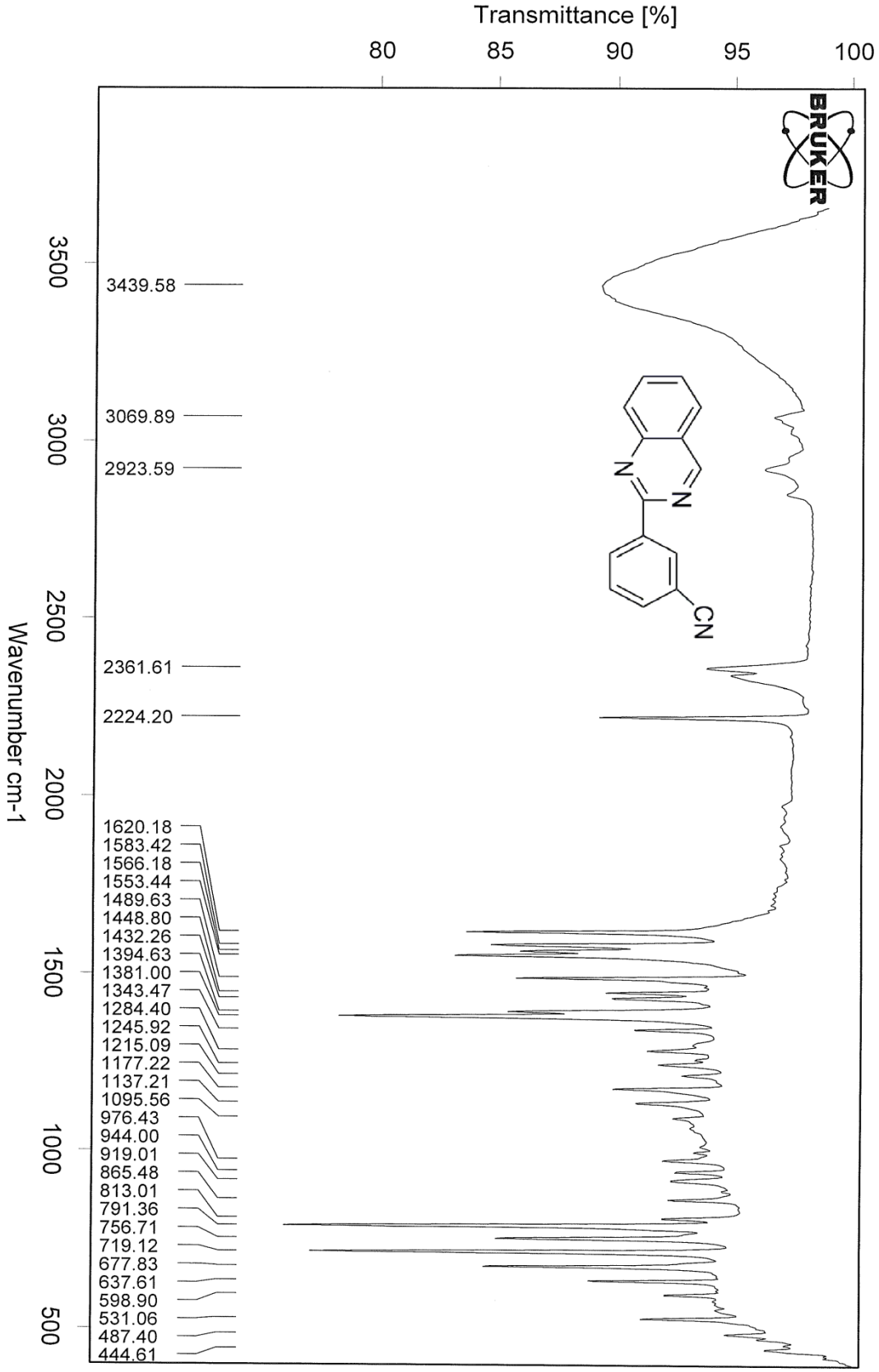

CN
N
N

4q


160.27
158.31
150.11
138.71
133.19
132.13
131.88
128.24
126.76
123.43
118.35
112.41
f1 (ppm)


CN
N
N

4q


Transmittance [%]
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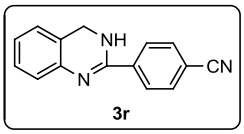
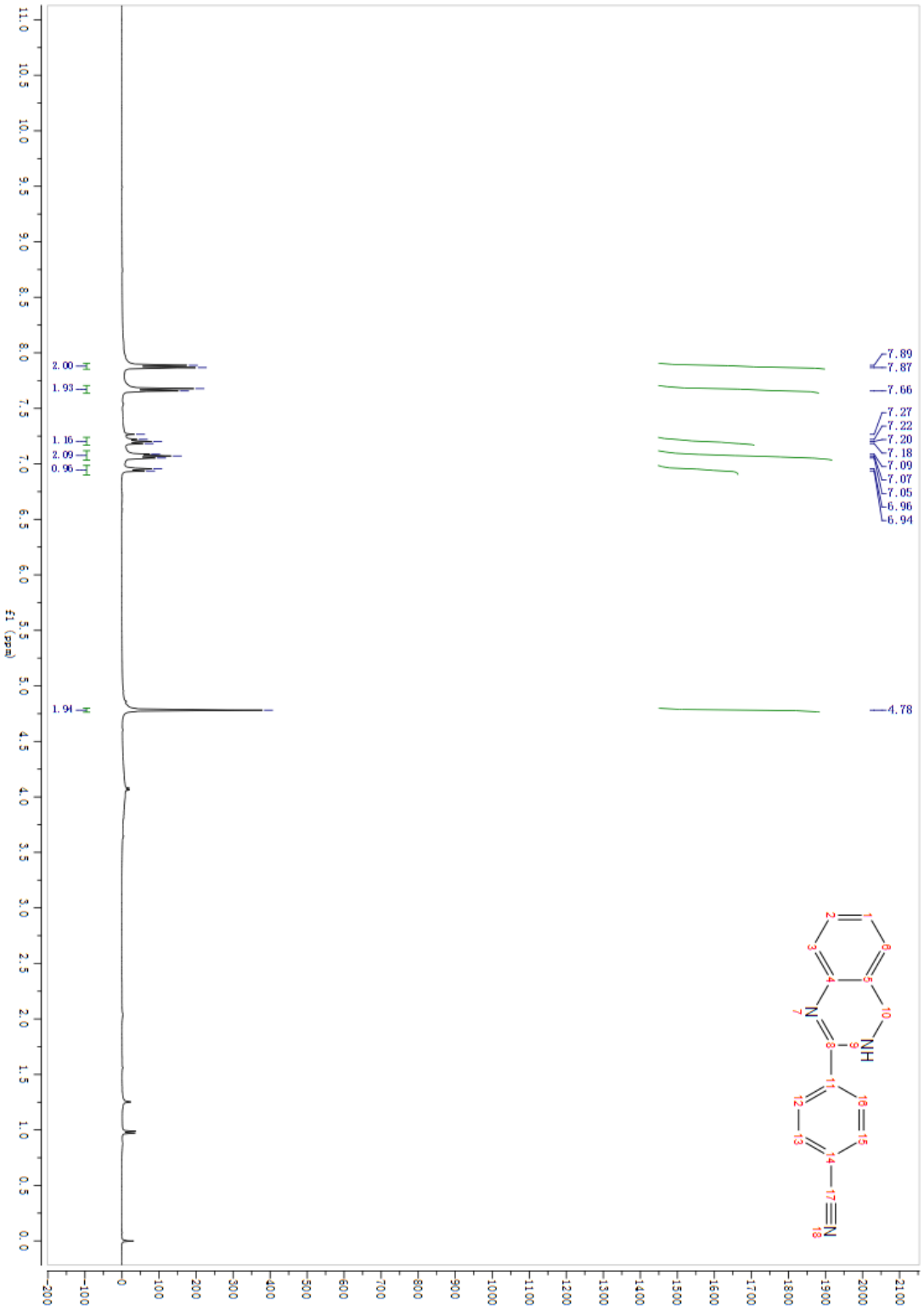
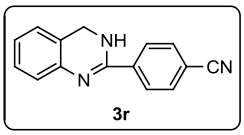
85
90
95
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3439.58
3069.89
2923.59
2361.61
2224.20
1620.18
1583.42
1566.18
1553.44
1489.63
1448.80
1432.26
1394.63
1381.00
1343.47
1284.40
1245.92
1215.09
1177.22
1137.21
1095.56
976.43
944.00
919.01
865.48
813.01
791.36
756.71
719.12
677.83
637.61
598.90
531.06
487.40
444.61
N
N
CN

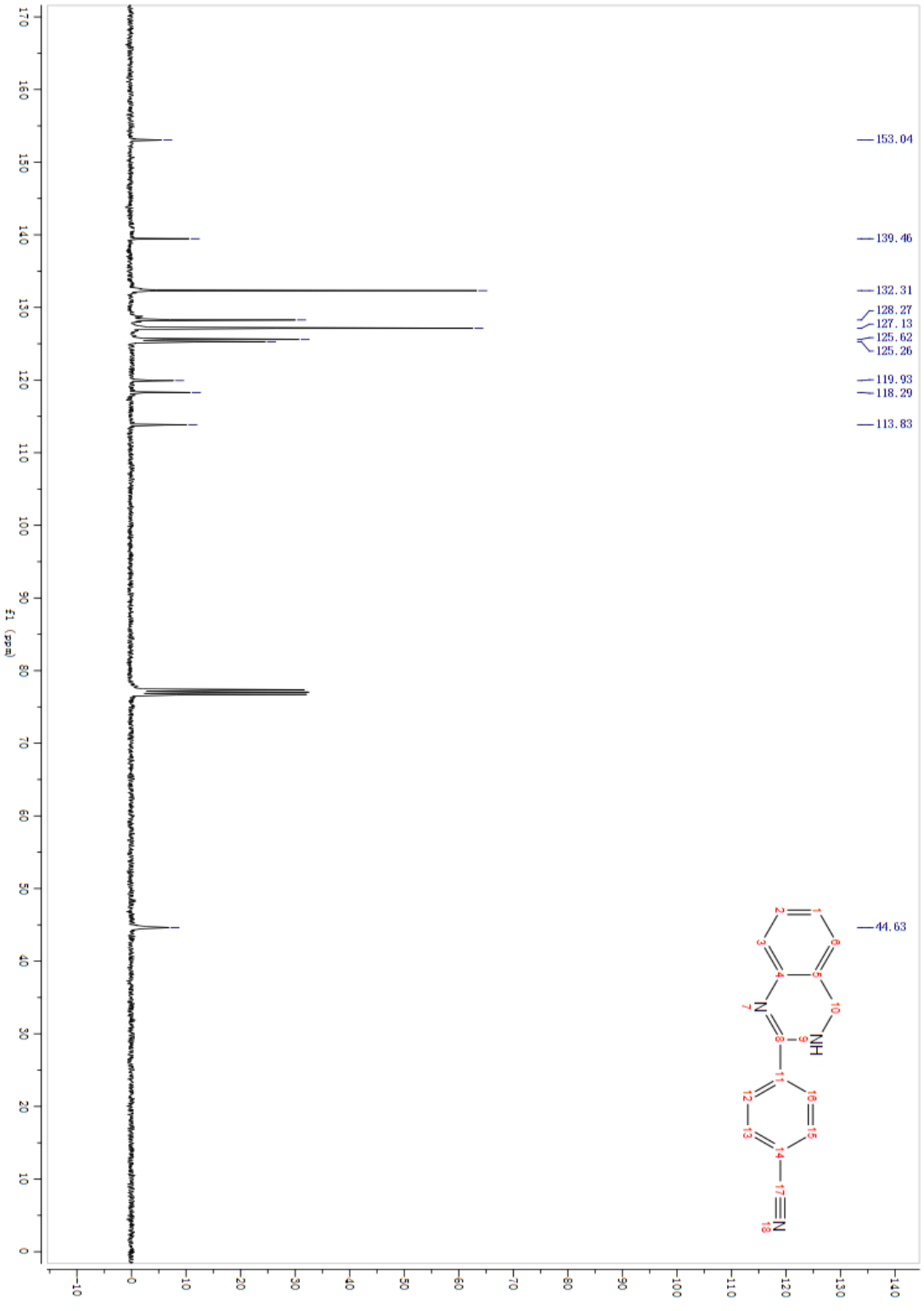

NH
N
CN

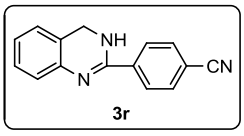
3r


2.00
1.93
1.16
2.09
0.96
1.94
7.89
7.87
7.66
7.27
7.22
7.20
7.18
7.09
7.07
7.05
6.96
6.94
4.78
f1 (ppm)

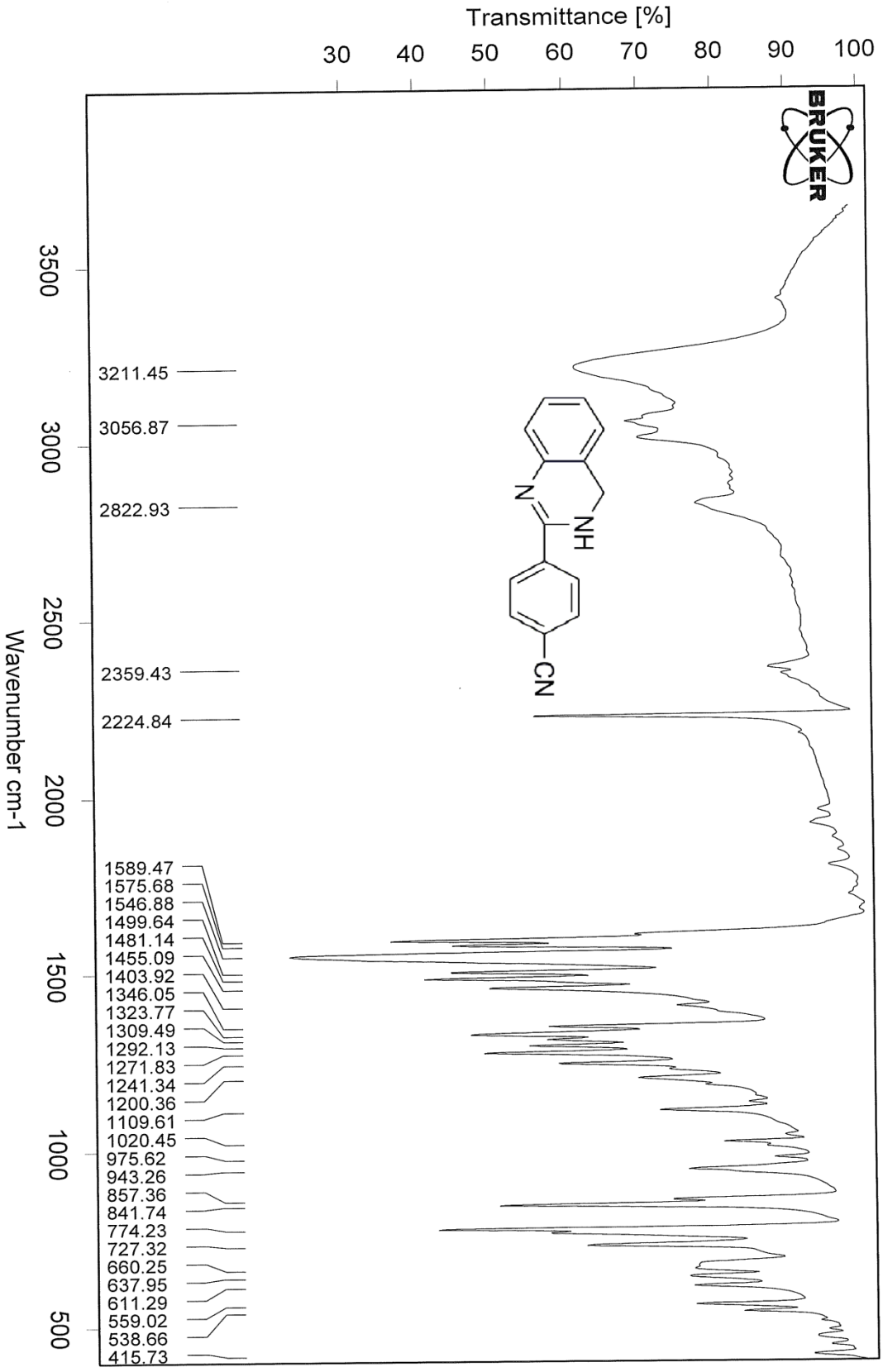

NH
N
CN

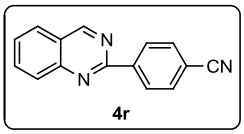
3r


153.04
139.46
132.31
128.27
127.13
125.62
125.26
119.93
118.29
113.83
44.63
f1 (ppm)

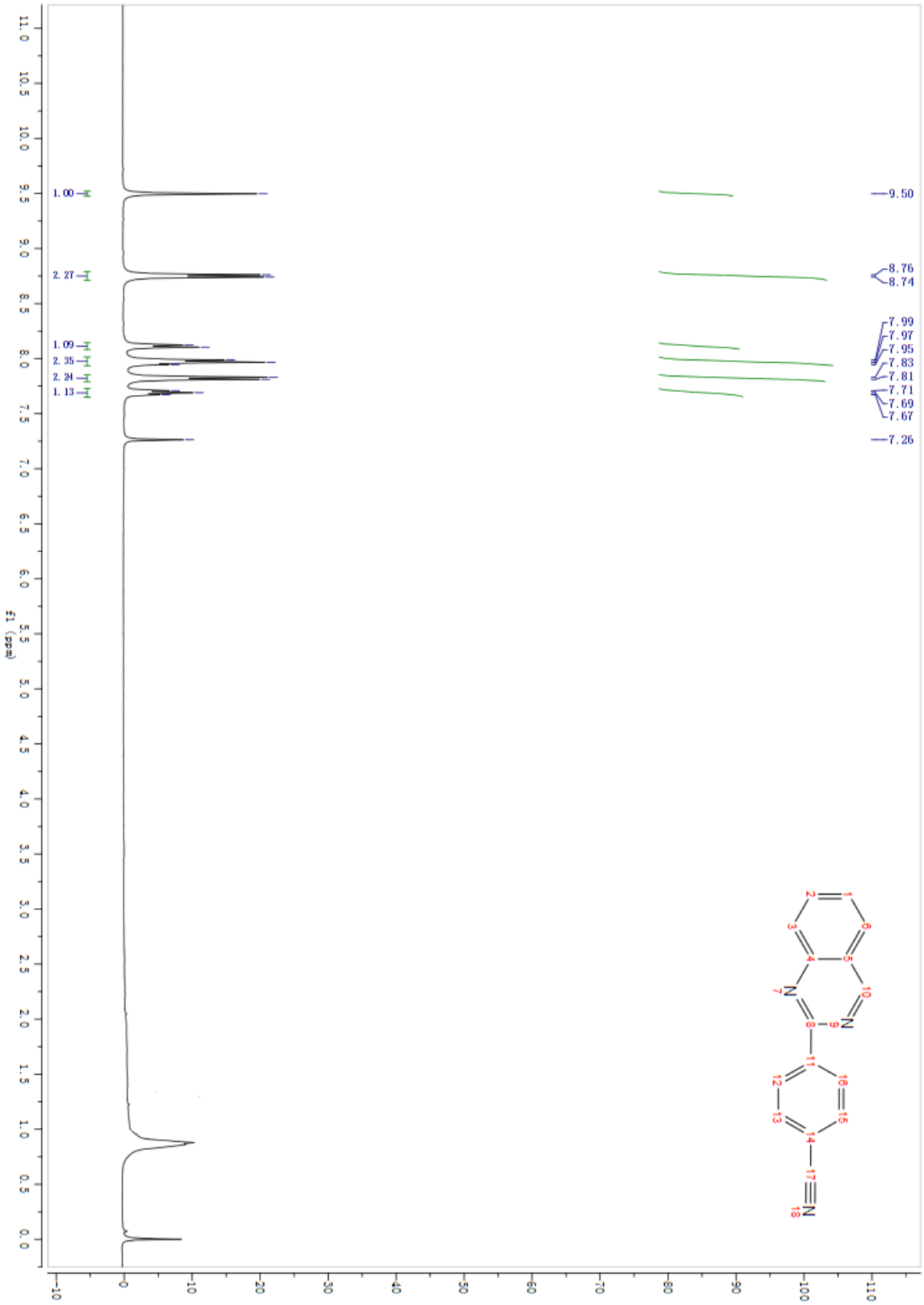

NH
N
CN

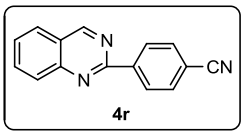
3r


Transmittance [%]
30
40
50
60
70
80
90
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3211.45
3056.87
2822.93
2359.43
2224.84
1589.47
1575.68
1546.88
1499.64
1481.14
1455.09
1403.92
1346.05
1323.77
1309.49
1292.13
1271.83
1241.34
1200.36
1109.61
1020.45
975.62
943.26
857.36
841.74
774.23
727.32
660.25
637.95
611.29
559.02
538.66
415.73
N
NH
CN

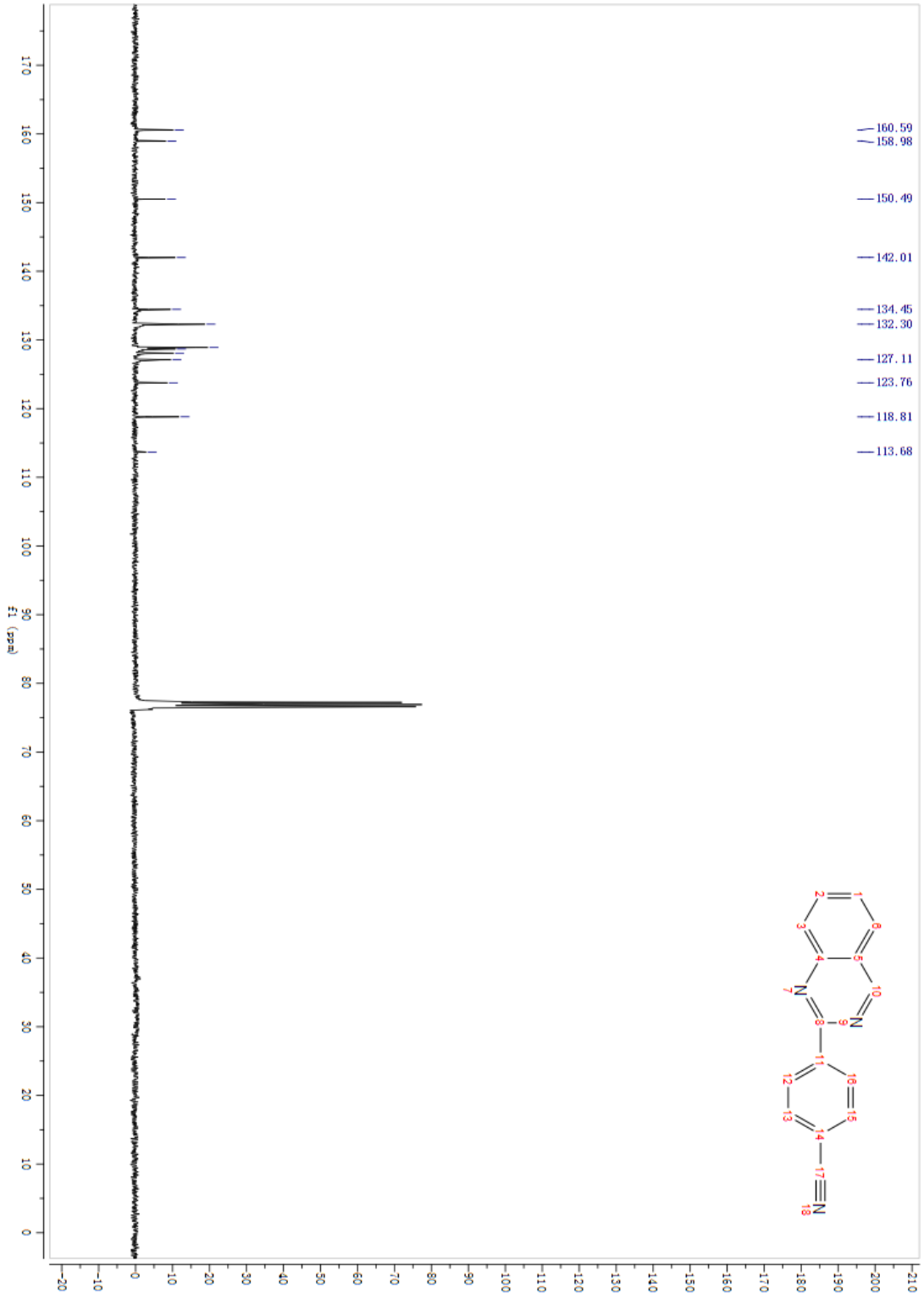

N
N
CN

4r


1.00
2.27
1.09
2.35
2.24
1.13
9.50
8.76
8.74
7.99
7.97
7.95
7.83
7.81
7.71
7.69
7.67
7.26
f1 (ppm)


N
N
CN

4r


160.59
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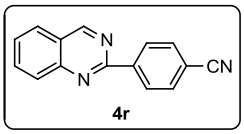
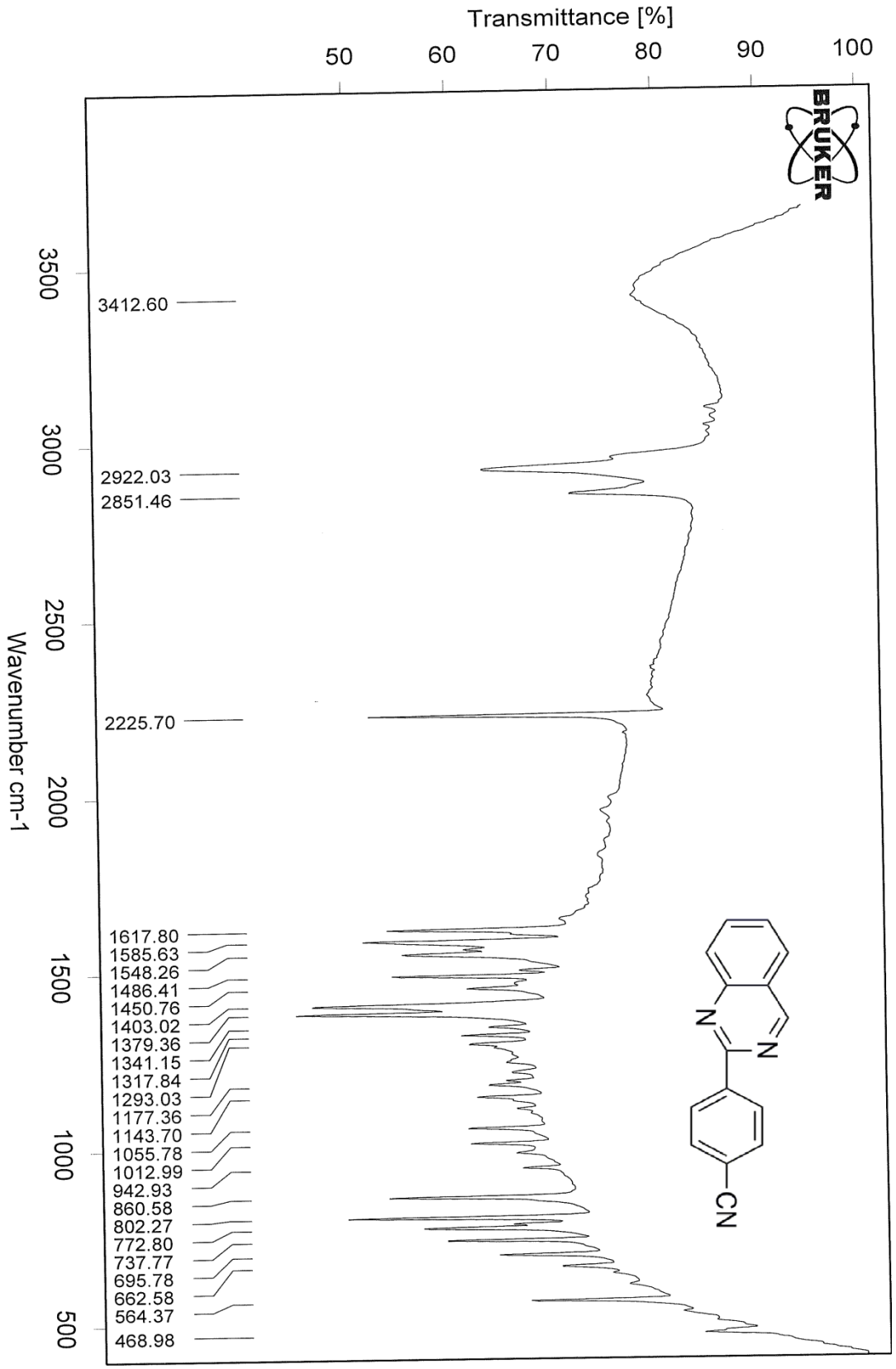
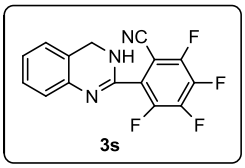
150.49
142.01
134.45
132.30
127.11
123.76
118.81
113.68
f1 (ppm)

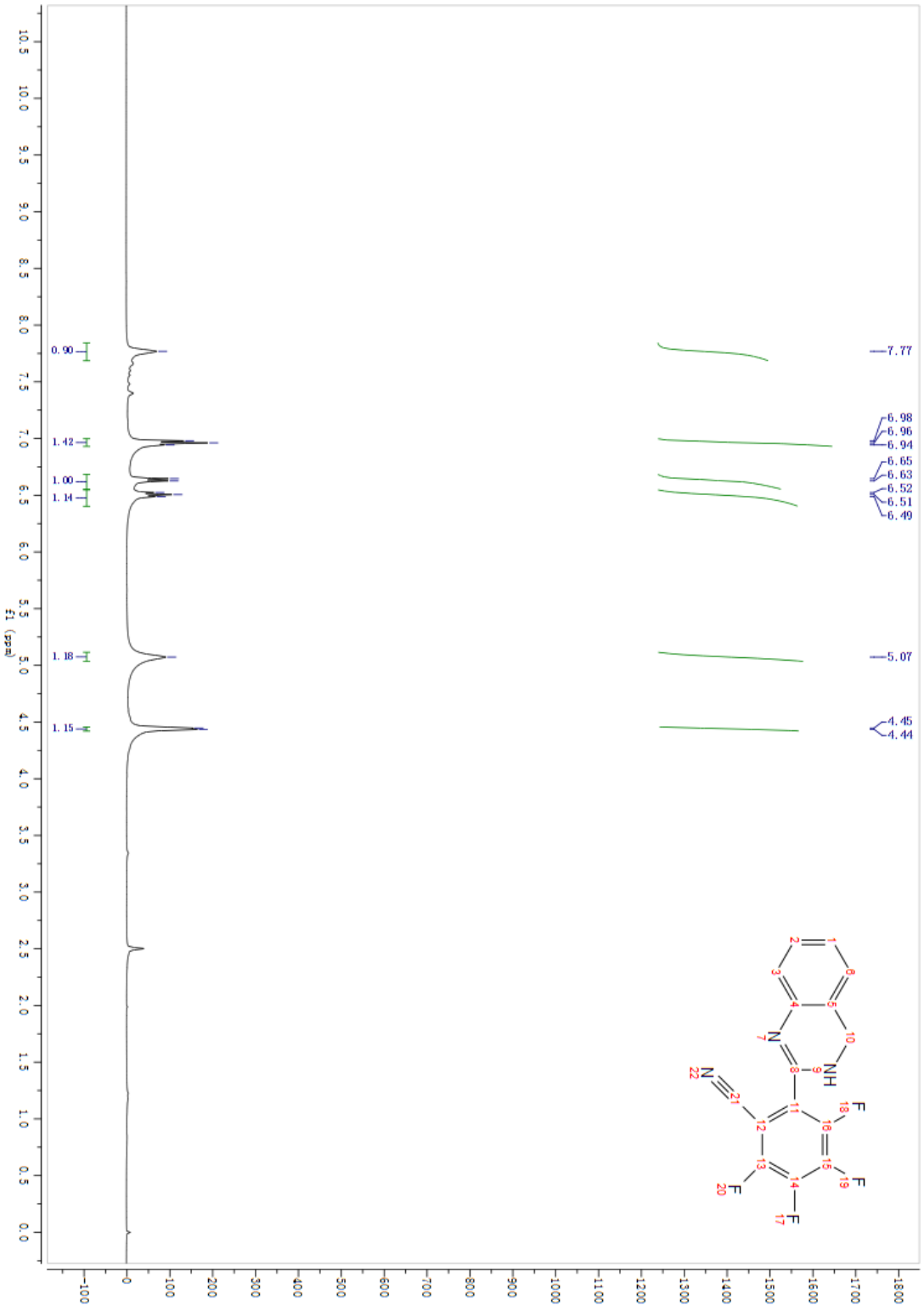

N
N
CN

4r


Transmittance [%]
50
60
70
80
90
100
BRUKER
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3412.60
2922.03
2851.46
2225.70
1617.80
1585.63
1548.26
1486.41
1450.76
1403.02
1379.36
1341.15
1317.84
1293.03
1177.36
1143.70
1055.78
1012.99
942.93
860.58
802.27
772.80
737.77
695.78
662.58
564.37
468.98
N
N
CN


NC
F
NH
F
N
F
F

3s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1.00
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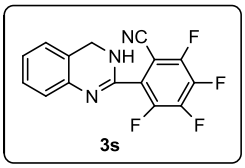
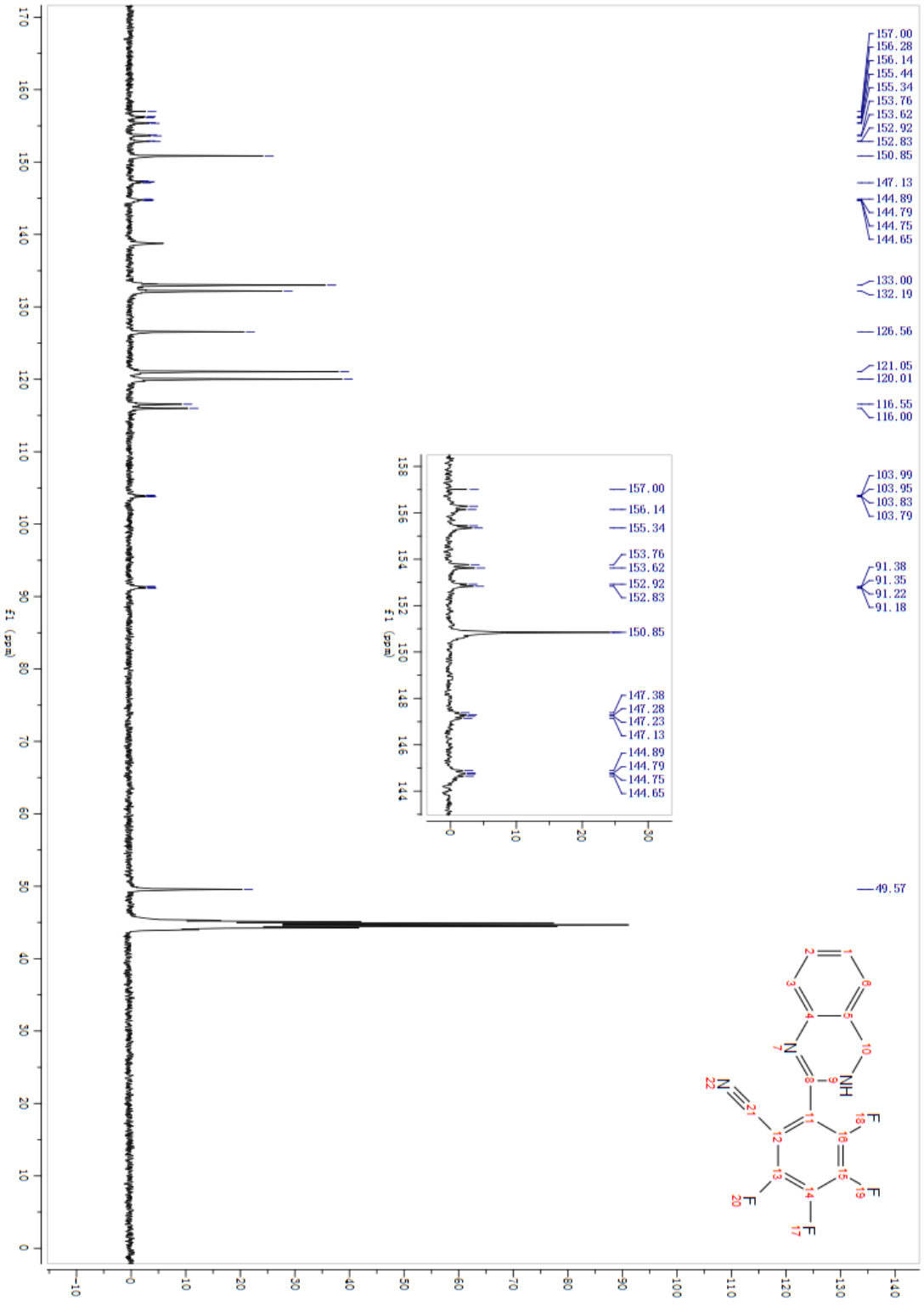
1.18
1.15
7.77
6.98
6.96
6.94
6.65
6.63
6.52
6.51
6.49
5.07
4.45
4.44
f1 (ppm)


NC
F
NH
F
N
F
F
3s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150.85
147.13
144.89
144.79
144.75
144.65
133.00
132.19
126.56
121.05
120.01
116.55
116.00
103.99
103.95
103.83
103.79
91.38
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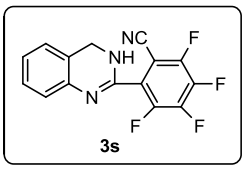
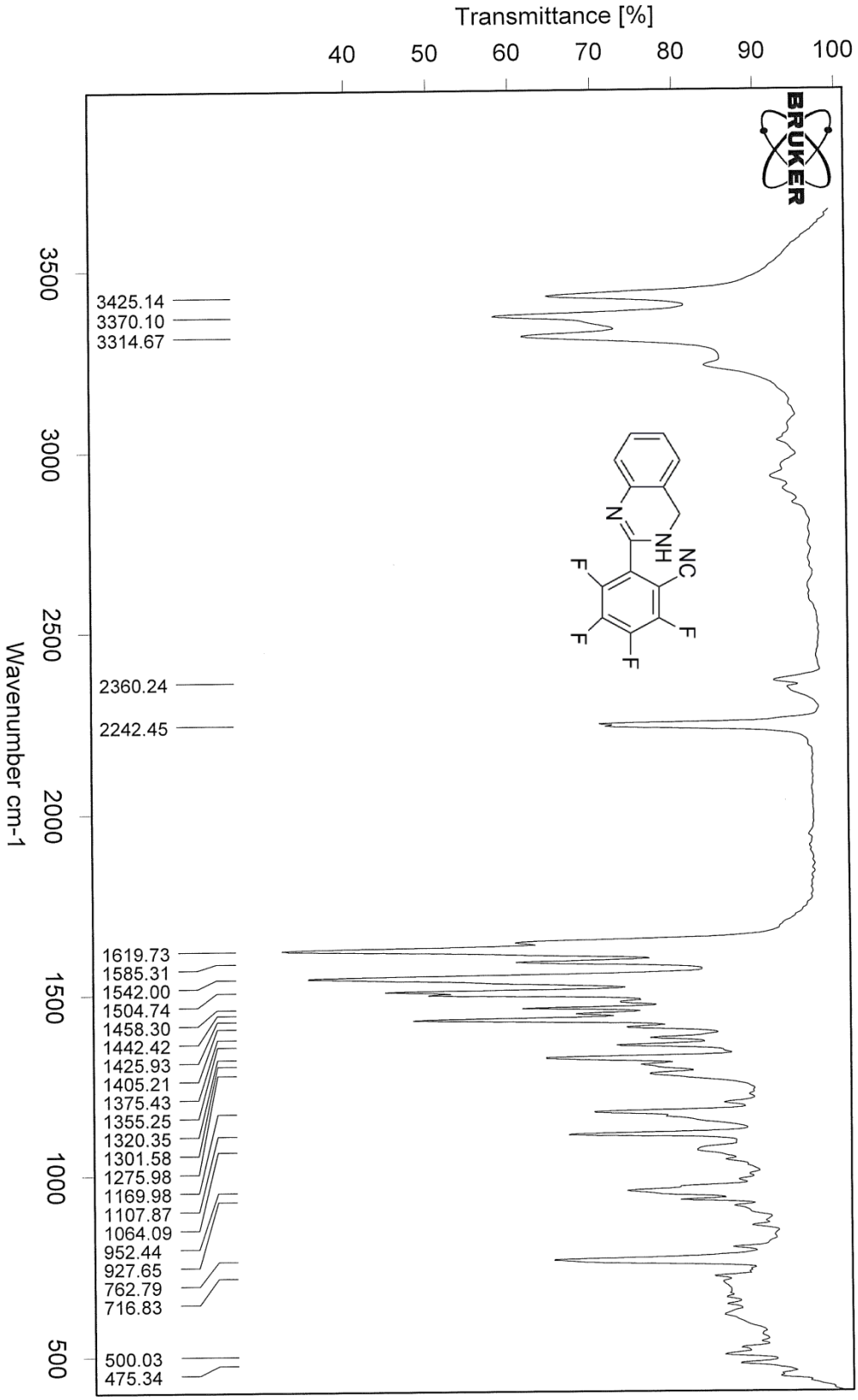
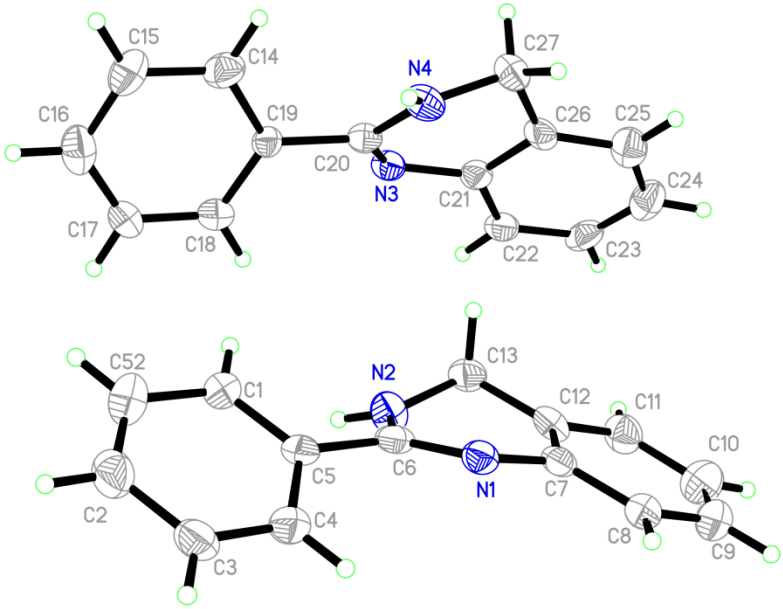
91.18
49.57
f1 (ppm)


NC
F
NH
F
N
F
F
3s

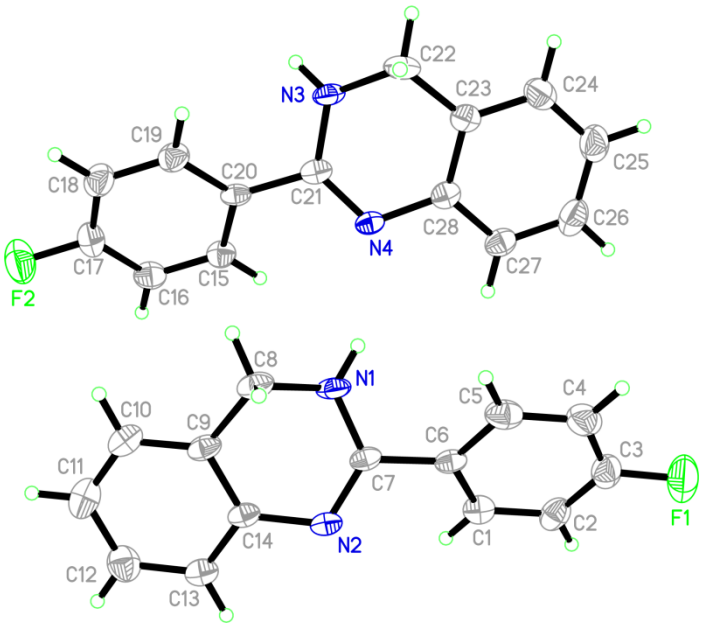

Transmittance [%]
40
50
60
70
80
90
100
BRUKER
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3425.14
3370.10
3314.67
2360.24
2242.45
1619.73
1585.31
1542.00
1504.74
1458.30
1442.42
1425.93
1405.21
1375.43
1355.25
1320.35
1301.58
1275.98
1169.98
1107.87
1064.09
952.44
927.65
762.79
716.83
500.03
475.34
N
NH
NC
F
F
F
F

6. X-Ray structure of 3a and 3o

3a: 2-phenyl-3,4-dihydroquinazoline (CCDC 977533)



3o: 2-(4-fluorophenyl)-3,4-dihydroquinazoline (CCDC 977534)



7. Literature citations for known compounds

1. B. Han, C. Wang, R. F. Han, W. Yu, X. Y. Duan, R. Fang and X. L. Yang. *Chem. Commun.*, 2011, **47**, 7818–7820.
2. H. Yuan, W. J. Yoo, H. Miyamura and S. Kobayashi. *Adv. Synth. Catal.*, 2012, **354**, 2899– 2904.
3. C. Wang, S. Li, H. Liu, Y. Jiang and H. Fu, *J. Org. Chem.*, 2010, **75**, 7936.
4. C. U. Maheswari, G. S. Kumar, M. Venkateshwar, R. A. Kumar, M. L. Kantam, and K. R. Reddy, *Adv. Synth. Catal.*, 2010, **352**, 341 – 346.
5. B. Han, X. L. Yang, C. Wang, Y. W. Bai, T. C. Pan, X. Chen and W. Yu. *J. Org. Chem.*, 2012, **77**, 1136−1142.