Ring-Opening Reactions of Aziridines with Carboxylic Acids Catalyzed by DBU

Yanqin Guo [a], Yepeng Xie[a], Qin Yang [a,b], Songsong Xu[a], Zhihong Deng[b], Xuechun Mao[b], Yiyuan Peng*[a,b]

[a]*Key Laboratory of Functional Small Organic Molecules, Ministry of Education and Key Laboratory of Green Chemistry, Jiangxi Province, Nanchang, Jiangxi 330022, China*

[b] *College of Chemistry & Chemical Engineering, Jiangxi Normal University, Nanchang, Jiangxi 330022, China*

Fax: 86 791 8812 0388; Tel: 86 791 8812 0388;

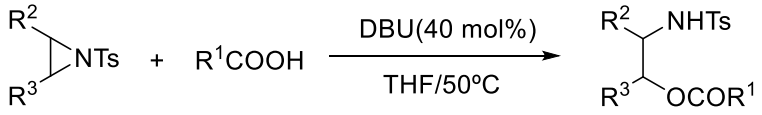
E-mail: yiyuanpeng@yahoo.com; yypeng@jxnu.edu.cn

Supporting Information

General Materials and Methods:

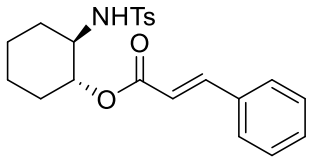
All reactions were performed in reaction tubes under nitrogen atmosphere. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63 μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr (house vacuum) at 25–35 °C. Commercial reagents and solvents were used as received. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale.

General procedure for synthesis of 3:



1 **2** **3**

A mixture of aziridines **1** (0.20 mmol), carboxylic acids **2** (0.24 mmol), and DBU (0.08 mmol, 40 mol%) in THF (2.0 ml) were added subsequently. The mixture was stirred at 50°C for 24-36 hours. After completion of the reaction as indicated by TLC, evaporation of the solvent followed by purification on silica gel provided the corresponding product **3**.



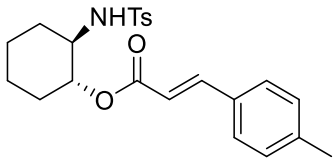
2-((4-Methylphenyl)sulfonamido)cyclohexyl cinnamate (3aa)

Yield: 74.2 mg (93%); white solid; mp 93–94 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.71 (d, *J* = 8.0 Hz, 2H), 7.49–7.39 (m, 6H), 7.12 (d, *J* = 7.6 Hz, 2H), 5.99 (d, *J* = 16.0 Hz, 1H), 5.41 (d, *J* = 7.6 Hz, 1H), 4.71 (td, *J* = 10.4, 4.8 Hz, 1H), 3.33–3.25 (m, 1H), 2.17–2.11 (m, 4H), 2.01–1.98 (m, 1H), 1.71–1.69 (m, 2H), 1.40–1.26 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.1, 144.9, 142.7, 138.4, 134.1, 130.4, 129.5, 128.9, 128.0, 126.8, 117.4, 74.1, 57.3, 34.1, 31.2, 24.2, 23.7, 21.1.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{25}NO_4SNa$: 422.1402; found: 422.1423. IR(KBr) (cm^{-1}) v 3430, 3309, 3061, 2944, 2863, 1723, 1636, 1598, 1448, 1366, 1329, 1163, 1025.



2-((4-Methylphenyl)sulfonamido)cyclohexyl (*E*)-3-(*p*-tolyl)acrylate (3ab)

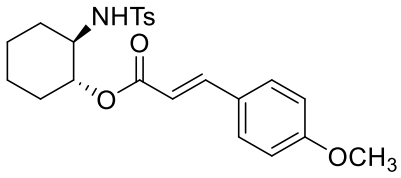
Yield: 75.2 mg (91%); white solid; mp 134–136 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 15.6 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 8.4 Hz, 2H), 5.93 (d, *J* = 15.6 Hz, 1H), 5.27–5.24 (m, 1H), 4.69 (td, *J* = 10.4, 4.4 Hz, 1H), 3.31–3.23(m, 1H), 2.38 (s, 3H), 2.20–2.16 (m, 1H), 2.13 (s, 3H), 2.00–1.96 (m, 1H), 1.71–1.68 (m, 2H), 1.42–1.25 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.3, 145.0, 142.8, 140.9, 138.5, 131.5, 129.6, 129.5, 128.1, 126.9, 116.5, 74.0, 57.4, 34.1, 31.3, 24.3, 23.8, 21.5, 21.2.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{23}H_{27}NO_4SNa$: 436.1558; found: 436.1543.

IR(KBr) (cm^{-1}) v 3451, 3299, 3031, 2949, 2920, 2856, 1684, 1631, 1605, 1511, 1426, 1358, 1334, 1182, 1020.



2-((4-Methylphenyl)sulfonamido)cyclohexyl-(*E*)-3-(4-methoxyphenyl)acrylate (3ac)

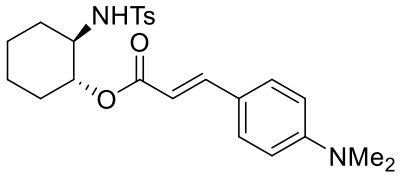
Yield: 84.9 mg (99%); white solid; mp 133–134 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.69 (d, *J* = 8.4 Hz, 2H), 7.44–7.38 (m, 3H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 5.85 (d, *J* = 15.6 Hz, 1H), 5.28–5.22 (m, 1H), 4.69 (td, *J* = 10.4, 4.4 Hz, 1H), 3.85 (s, 3H), 3.30–3.22 (m, 1H), 2.20–2.14 (m, 4H), 1.99–1.96 (m,1H), 1.72–1.69 (m, 2H), 1.43–1.27 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.4, 161.6, 144.6, 142.7, 138.7, 129.8, 129.5, 127.1, 126.9, 115.2, 114.4, 74.0, 57.3, 55.4, 34.0, 31.3, 24.3, 23.8, 21.2.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{23}H_{27}NO_5SNa$: 452.1508, found: 452.1478.

IR(KBr) (cm^{-1}) v 3442, 3293, 2929, 2856, 1703, 1514, 1457, 1325, 1170, 1159, 1028.



2-((4-Methylphenyl)sulfonamido)cyclohexyl (*E*)-3-(4-(dimethylamino)phenyl)acrylate (3ad)

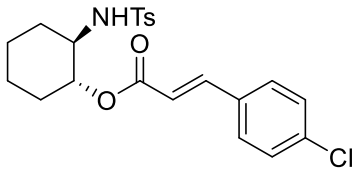
Yield: 87.5 mg (99%); brown solid; mp 146–148 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.69 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 16.0 Hz, 1H), 7.32 (d, *J* = 8.8 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.66 (d, *J* = 8.8 Hz, 2H), 5.74 (d, *J* = 15.6 Hz, 1H), 5.36–5.30 (m, 1H), 4.68 (td, *J* = 10.0, 4.4 Hz, 1H), 3.26–3.18 (m, 1H), 3.05 (s, 6H), 2.23–2.20 (m, 1H), 2.16 (s, 3H), 1.97–1.94 (m, 1H), 1.75–1.60 (m, 2H), 1.40–1.26 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 168.3, 151.9, 145.7, 142.8, 138.2, 129.9, 129.5, 126.9, 121.9, 111.7, 112.6, 73.6, 57.6, 40.2, 34.3, 31.4, 24.3, 23.9, 21.4.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{24}H_{30}N_2O_4SNa$: 465.1824; found: 465.1836 .

IR(KBr) (cm^{-1}) v 3431, 3322, 3046, 2926, 2859, 2810, 1698, 1627, 1601, 1527, 1446, 1364, 1326, 1159, 1036.



2-((4-Methylphenyl)sulfonamido)cyclohexyl (*E*)-3-(4-chlorophenyl)acrylate (3ae)

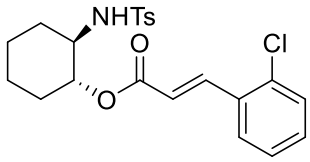
Yield: 81.4 mg (94%); white solid; mp 124–125 ℃.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.71 (d, *J* = 8.0 Hz, 2H), 7.46–7.28 (m, 5H), 7.13 (d, *J* = 7.6 Hz, 2H), 6.00 (d, *J* = 16.0 Hz, 1H), 5.37 (d, *J* = 8.0 Hz, 1H), 4.71 (td, *J* = 10.0, 4.4 Hz, 1H), 3.34–3.26 (m, 1H), 2.16 (s, 3H), 2.12–2.09 (m, 1H), 2.01–1.99 (m, 1H), 1.72–1.67 (m, 2H), 1.38–1.27 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.8, 143.4, 142.7, 138.7, 136.3, 132.8, 129.5, 129.3, 129.2, 126.9, 118.3, 74.4, 57.1, 33.8, 31.2, 24.3, 23.7, 21.3.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{24}NO_4SClNa$: 456.1012; found: 456.0994.

IR(KBr) (cm^{-1}) v 3427, 3278, 3065, 2940, 2862, 1688, 1636, 1592, 1491, 1325, 1160, 1092, 1024, 1011.



2-((4-Methylphenyl)sulfonamido)cyclohexyl (*E*)-3-(2-chlorophenyl)acrylate (3af)

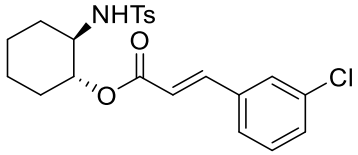
Yield: 85.7 mg (99%); white solid; mp 146–148 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82 (d, *J* = 16.0 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.51 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.44 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.36–7.27 (m, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 5.97 (d, *J* = 16.0 Hz, 1H), 4.99–4.96 (m, 1H), 4.71 (td, *J* = 10.4, 4.4 Hz, 1H), 3.34–3.26 (m, 1H), 2.22–2.19 (m, 1H), 2.07 (s, 3H), 2.00–1.97 (m, 1H), 1.74–1.66 (m, 2H), 1.47–1.27 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.5, 142.7, 140.5, 138.7, 135.0, 132.6, 131.1, 130.3, 129.5, 127.6, 127.1, 126.9, 120.2, 74.3, 57.4, 34.1, 31.2, 24.2, 23.8, 21.0.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{24}NO_4SClNa$: 456.1012; found: 456.1031.

IR(KBr) (cm^{-1}) v 3450, 3271, 3067, 2943, 2864, 1706, 1630, 1590, 1450, 1325, 1188, 1086, 1027.



2-((4-Methylphenyl)sulfonamido)cyclohexyl (*E*)-3-(3-chlorophenyl)acrylate (3ag)

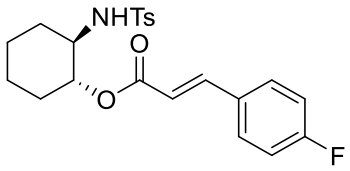
Yield: 82.3 mg (95%); pale yellow solid; mp 55–56 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.71 (d, *J* = 7.6 Hz, 2H), 7.42–7.33 (m, 5H), 7.15 (d, *J* = 7.6 Hz, 2H), 6.00 (d, *J* = 16.0 Hz, 1H), 5.36 (d, *J* = 7.6 Hz, 1H), 4.73–4.68 (m, 1H), 3.33–3.23 (m, 1H), 2.17–2.12 (m,4H), 2.01–1.99 (m, 1H), 1.71–1.67 (m, 2H), 1.40–1.28 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.6, 143.2, 142.8, 138.6, 136.1, 134.9, 130.2, 130.2, 129.5, 127.6, 126.9, 126.4, 119.2, 74.4, 57.1, 33.9, 31.2, 24.3, 23.7, 21.3.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{24}NO_4SClNa$: 456.1012; found: 456.1027.

IR(KBr) (cm^{-1}) v 3500, 3274, 3064, 2940, 2861, 1707, 1639, 1597, 1565, 1452, 1325, 1160, 1093, 1030.



2-((4-Methylphenyl)sulfonamido)cyclohexyl (*E*)-3-(4-fluorophenyl)acrylate (3ah)

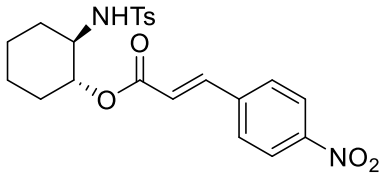
Yield: 70.9 mg (85%); pale yellow solid; mp 82–84 °C.

^1H NMR (400 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 8.4 Hz, 2H), 7.46–7.42 (m, 3H), 7.15–7.07 (m, 4H), 5.94 (d, *J* = 16.0 Hz, 1H), 5.12 (d, *J* = 7.2 Hz, 1H), 4.70 (td, *J* = 10.0, 4.0 Hz, 1H), 3.33–3.25 (m, 1H), 2.15–2.13 (m, 4H), 2.00–1.97 (m, 1H), 1.73–1.70 (m, 2H), 1.44–1.28 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.9, 165.2 (d, $^1J_{C-F}$ = 250 Hz), 143.6, 142.6, 138.8, 130.6, 130.0 (d, $^3J_{C-F}$ = 10 Hz), 129.5, 126.9, 117.6, 116.1(d, $^2J_{C-F}$ = 20 Hz), 74.3, 57.1, 33.8, 31.2, 24.3, 23.7, 21.2.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{24}NO_4SFNa$: 440.1308; found: 440.1331.

IR(KBr) (cm^{-1}) v 3450, 3324, 3070, 2948, 2862, 1687, 1635, 1600, 1509, 1415, 1331, 1239, 1179, 1093, 1019, 1002.



2-((4-Methylphenyl)sulfonamido)cyclohexyl (*E*)-3-(4-nitrophenyl)acrylate (3ai)

Yield: 70.2 mg (79%); pale yellow solid; mp 160–161 °C.

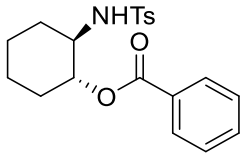
^1H NMR (400 MHz, $CDCl_3$): δ = 8.25 (d, *J* = 7.6 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.63–7.56 (m, 3H), 7.18 (d, *J* = 7.6 Hz, 2H), 6.22 (d, *J* = 16.0 Hz, 1H), 5.16–5.14 (m,

1H), 4.77–4.68 (m, 1H), 3.37–3.28 (m, 1H), 2.21 (s, 3H), 2.04–2.02 (m, 2H), 1.76–1.67 (m, 2H), 1.44–1.29 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 148.5, 142.8, 141.9, 140.5, 138.7, 129.5, 128.7, 126.9, 124.1, 122.0, 74.8, 57.0, 33.5, 31.2, 24.3, 23.7, 21.3.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{24}N_2O_6SNa$: 467.1253; found: 467.1268.

IR(KBr) (cm^{-1}) v 3441, 3284, 2939, 2862, 1712, 1640, 1599, 1520, 1344, 1061, 1091, 1032.



2-((4-Methylphenyl)sulfonamido)cyclohexyl benzoate (3aj)[1]

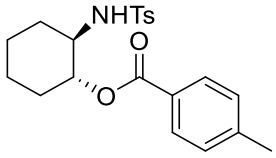
Yield: 62.7 mg (84%); white solid; mp 170–172 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.77 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.54 (t, *J* = 6.8 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 5.20 (d, *J* = 7.2 Hz, 1H), 4.82 (td, *J* = 10.4, 4.4 Hz, 1H), 3.36–3.28 (m, 1H), 2.18 (s, 4H), 2.04–2.01 (m, 1H), 1.73–1.70 (m, 2H), 1.51–1.30 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.8, 142.7, 138.1, 133.0, 129.7, 129.4, 128.1, 126.6, 74.6, 57.2, 34.0, 31.2, 24.2, 23.8, 21.4.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{20}H_{23}NO_4SNa$: 396.1245; found: 396.1259.

IR(KBr) (cm^{-1}) v 3440, 3329, 2927, 2862, 1707, 1599, 1450, 1323, 1158, 1015.



2-((4-Methylphenyl)sulfonamido)cyclohexyl 4-methylbenzoate (3ak)[2]

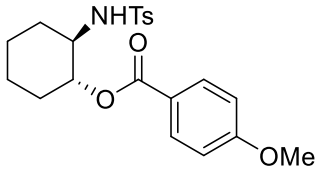
Yield: 76.6 mg (99%); white solid; mp 147–149 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.64 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 5.13 (d, *J* = 6.4 Hz, 1H), 4.80 (td, *J* = 10.4, 4.4 Hz, 1H), 3.33–3.25 (m, 1H), 2.42 (s, 3H), 2.23–2.18 (m, 4H), 2.02–1.99 (m, 1H), 1.76–1.69 (m, 2H), 1.51–1.30 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.9, 143.7, 142.6, 138.0, 129.8, 129.4, 128.8, 126.9, 126.5, 74.4, 57.4, 34.2, 31.3, 24.2, 23.8, 21.7, 21.4.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{21}H_{25}NO_4SNa$: 410.1402; found: 410.1413.

IR(KBr) (cm^{-1}) v 3410, 3323, 3052, 3035, 2930, 2919, 2855, 1708, 1613, 1443, 1324, 1272, 1157, 1087, 1027, 1020.



2-((4-Methylphenyl)sulfonamido)cyclohexyl 4-methoxybenzoate (3al)[1]

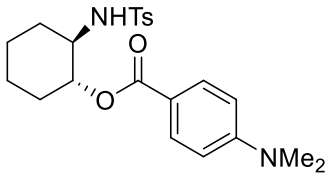
Yield: 74.2 mg (92%); white solid; mp 132–134 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.71 (d, *J* = 8.8 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 5.29 (d, *J* = 6.8 Hz, 1H), 4.78 (td, *J* = 10.4, 4.4 Hz, 1H), 3.87 (s, 3H), 3.33–3.25 (m, 1H), 2.20–2.17 (m, 4H), 2.03–1.99 (m, 1H), 1.74–1.68 (m,2H), 1.49–1.26 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.6, 163.4, 142.6, 138.1, 131.8, 129.4, 126.6, 122.1, 113.3, 74.3, 57.3, 55.5, 34.0, 31.3, 24.2, 23.8, 21.4.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{21}H_{25}NO_5SNa$: 426.1351; found: 426.1355.

IR(KBr) (cm^{-1}) v 3399, 3331, 3083, 2932, 2863, 1706, 1607, 1441, 1326, 1261, 1158, 1080, 1033, 1016.



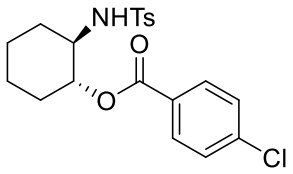
2-((4-Methylphenyl)sulfonamido)cyclohexyl 4-(dimethylamino)benzoate (3am)

Yield: 78.2 mg (94%); pale yellow solid; mp 148–150 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.61–7.57 (m,4H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.56 (d, *J* = 9.2 Hz, 2H), 5.33 (d, *J* = 6.4 Hz, 1H), 4.75 (td, *J* = 10.4, 4.4 Hz, 1H), 3.26–3.18 (m, 1H), 3.05 (s, 6H), 2.26–2.19 (m, 4H), 2.00–1.96 (m, 1H), 1.77–1.63 (m, 2H), 1.46–1.28 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.5, 153.4, 142.4, 137.8, 131.5, 129.4, 126.6, 116.3, 110.4, 73.7, 57.7, 40.1, 34.3, 31.4, 24.2, 23.9, 21.4.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{28}N_2O_4SNa$: 439.1667; found: 439.1647. IR(KBr) (cm^{-1}) v 3422, 3303, 3066, 2935, 2863, 1679, 1609, 1534, 1443, 1374, 1330, 1284, 1181, 1088, 1026.



2-((4-Methylphenyl)sulfonamido)cyclohexyl 4-chlorobenzoate (3an)[1]

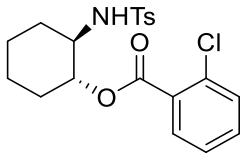
Yield: 74.9 mg (92%); white solid; mp 145–146 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 8.0 Hz, 2H), 5.18–5.15 (m, 1H), 4.81 (td, *J* = 10.4, 4.0 Hz, 1H), 3.38–3.30 (m, 1H), 2.22 (s, 3H), 2.15–2.12 (m, 1H), 2.04–2.01 (m, 1H), 1.75–1.68 (m, 2H), 1.50–1.29 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.8, 142.8, 139.4, 138.2, 131.1, 129.4, 128.4, 128.2, 126.5, 74.9, 57.2, 34.0, 31.3, 24.3, 23.8, 21.4.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{20}H_{22}NO_4SClNa$: 430.0856; found: 430.0864.

IR(KBr) (cm^{-1}) v 3435, 3271, 2940, 1712, 1595, 1467, 1400, 1327,1280, 1154, 1093, 1014.



2-((4-Methylphenyl)sulfonamido)cyclohexyl 2-chlorobenzoate (3ao)[1]

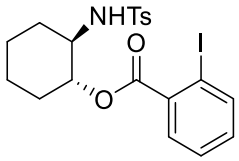
Yield: 75.7 mg (93%); white solid; mp 138–140 °C.

^1H NMR (400 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 3.6 Hz, 2H), 7.28–7.23 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 5.28 (d, *J* = 7.6 Hz, 1H), 4.85 (td, *J* = 10.0, 4.4 Hz, 1H), 3.39–3.31 (m, 1H), 2.23 (s, 3H), 2.10–2.03 (m, 2H), 1.74–1.64 (m, 2H), 1.52–1.29 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.3, 142.8, 138.2, 134.0, 132.7, 131.9, 131.0 , 129.4, 129.3, 126.6, 126.5, 75.3, 56.8, 33.4, 31.0, 24.2, 23.7, 21.5.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{20}H_{22}NO_4SClNa$: 430.0856; found: 430.0833.

IR(KBr) (cm^{-1}) v 3442, 3261, 2942, 2862, 1733, 1590, 1472, 1440, 1324,1254, 1158, 1117, 1084, 1052, 1013.



2-((4-Methylphenyl)sulfonamido)cyclohexyl 2-iodobenzoate (3ap)

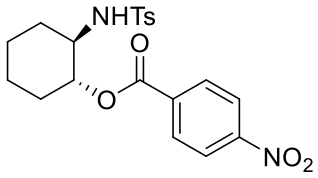
Yield: 88.8 mg (89%); white solid; mp 165–167 °C.

^1H NMR (400 MHz, $CDCl_3$): δ = 7.97 (d, *J* = 8.0 Hz, 1H), 7.67–7.64 (m, 3H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.14 (td, *J* = 7.6, 1.2 Hz, 1H), 7.00 (d, *J* = 8.0 Hz, 2H), 5.13–5.11 (m, 1H), 4.84 (td, *J* = 10.0, 4.4 Hz, 1H), 3.40–3.32 (m, 1H), 2.23 (s, 3H), 2.12–2.09 (m, 2H), 1.76–1.66 (m, 2H), 1.54–1.27 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.0, 142.8, 141.3, 138.2, 133.8, 132.8, 131.5, 129.5, 127.8, 126.6, 94.7, 75.6, 56.8, 33.6, 31.2, 24.3, 23.7, 21.6.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{20}H_{22}NO_4SINa$: 522.0212; found: 522.0177.

IR(KBr) (cm^{-1}) v 3435, 3264, 2938, 2861, 1728, 1582, 1452, 1323,1254, 1160, 1086, 1045, 1016.



2-((4-Methylphenyl)sulfonamido)cyclohexyl 4-nitrobenzoate (3aq)[2]

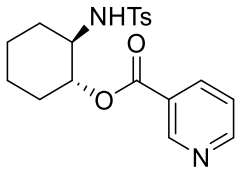
Yield: 64.4 mg (77%); white solid; mp 151–153 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.20 (d, *J* = 8.4 Hz, 2H), 8.01 (d, *J* = 8.8 Hz, 2H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 7.6 Hz, 2H), 5.17–5.06 (m, 1H), 4.85 (td, *J* = 10.0, 4.4 Hz, 1H), 3.46–3.37 (m, 1H), 2.24 (s, 3H), 2.10–2.00 (m, 2H), 1.77–1.68 (m, 2H), 1.54–1.29 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.6, 150.4, 143.0, 138.4, 135.3, 130.9, 129.5, 126.6, 123.2, 75.9, 56.7, 33.3, 31.1, 24.3, 23.7, 21.4.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{20}H_{22}N_2O_6SNa$: 441.1096; found: 441.1116.

IR(KBr) (cm^{-1}) v 3429, 3305, 2952, 2860, 1724, 1608, 1600, 1527, 1436, 1328, 1272, 1163, 1088, 1011.



2-((4-Methylphenyl)sulfonamido)cyclohexyl nicotinate (3ar)

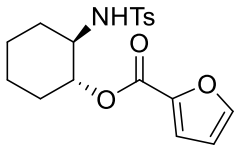
Yield: 65.8 mg (88%); white solid; mp 151–153 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.94 (s, 1H), 8.75 (d, *J* = 3.6 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.35–7.30 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 2H), 5.57–5.54 (m, 1H), 4.87 (td, *J* = 10.4, 4.4 Hz, 1H), 3.42–3.34 (m, 1H), 2.22 (s, 3H), 2.10–2.03 (m, 2H), 1.77–1.69 (m, 2H), 1.50–1.29 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.1, 153.1, 150.7, 142.9, 138.4, 137.3, 129.4, 126.5, 125.7, 123.2, 75.3, 56.8, 33.6, 31.1, 24.3, 23.7, 21.5.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{19}H_{22}N_2O_4SNa$: 397.1198; found: 397.1222.

IR(KBr) (cm^{-1}) v 3431, 3095, 2942, 2868, 1730, 1595, 1474, 1430, 1315,1276, 1157, 1093, 1027, 1014.



2-((4-Methylphenyl)sulfonamido)cyclohexyl furan-2-carboxylate (3as)[1]

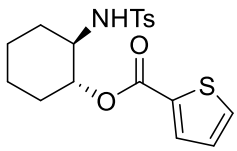
Yield: 66.1 mg (91%); white solid; mp 124–127 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.65 (d, *J* = 8.0 Hz, 2H), 7.53 (s, 1H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 3.2 Hz, 1H), 6.46 (t, *J* = 1.6 Hz, 1H), 5.26–5.24 (m, 1H), 4.78 (td, *J* = 10.8, 4.4 Hz, 1H), 3.35–3.27 (m, 1H), 2.29 (s, 3H), 2.15–2.12 (m, 1H), 2.03–1.99 (m, 1H), 1.72–1.67 (m, 2H), 1.50–1.26 (m, 4H).

^{13}C NMR (100MHz, $CDCl_3$): δ = 158.8, 146.4, 144.1, 142.7, 138.1, 129.3, 126.7, 118.4, 111.8, 74.7, 57.1, 33.9, 31.2, 24.2, 23.7, 21.5.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{18}H_{21}NO_5SNa$: 386.1038; found: 386.1012.

IR(KBr) (cm^{-1}) v 3424, 3318, 2936, 2859, 1716, 1472, 1398, 1321,1296, 1235, 1158, 1085, 1012.



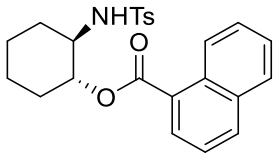
2-((4-Methylphenyl)sulfonamido)cyclohexyl thiophene-2-carboxylate (3at)

Yield: 70.5 mg (93%); white solid; mp 179–181 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.62 (d, *J* = 8.0 Hz, 2H), 7.54–7.52 (m, 2H), 7.05–7.02 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 2H), 5.25 (d, *J* = 7.2 Hz, 1H), 4.77 (td, *J* = 10.0, 4.8 Hz, 1H), 3.34–3.25 (m, 1H), 2.24 (s, 3H), 2.19–2.15(m, 1H), 2.03–1.99 (m, 1H), 1.75–1.67 (m, 2H), 1.52–1.29 (m, 4H).

^{13}C NMR (100MHz, $CDCl_3$): δ = 162.5, 142.7, 138.0, 133.8, 133.5, 132.7, 129.4, 127.6, 126.6, 74.9, 57.1, 33.9, 31.2, 24.1, 23.7, 21.5.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{18}H_{21}NO_4S_2Na$: 402.0810; found: 402.0790. IR(KBr) (cm^{-1}) v 3434, 3272, 3096, 3059, 2924, 2854, 1685, 1597, 1523, 1455, 1416, 1364, 1287, 1267, 1163, 1107, 1094, 1039, 1006.



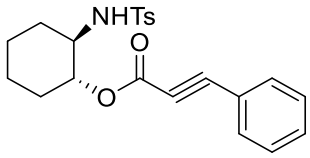
2-((4-Methylphenyl)sulfonamido)cyclohexyl 1-naphthoate (3au)[1]

Yield: 82.1 mg (97%); white solid; mp 125–126 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.85 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 6.8 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.59–7.50 (m, 4H), 7.37 (t, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 8.0 Hz, 2H), 5.46–5.44 (m, 1H), 4.93 (td, *J* = 10.4, 4.8 Hz, 1H), 3.44–3.36 (m, 1H), 2.12–2.09 (m, 2H), 1.97 (s, 3H), 1.73–1.64 (m, 2H), 1.55–1.29 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.4, 142.5, 138.2, 133.7, 133.5, 131.5, 130.7, 129.2, 128.5, 127.8, 126.5, 126.3, 126.2, 125.9, 124.4, 74.6, 57.2, 33.9, 31.3, 24.3, 23.8, 21.2.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{24}H_{25}NO_4SNa$: 446.1402; found: 446.1413. IR(KBr) (cm^{-1}) v 3405, 3275, 2939, 2859, 1713, 1595, 1510, 1430, 1330, 1083, 1022.



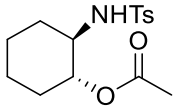
2-((4-Methylphenyl)sulfonamido)cyclohexyl 3-phenylpropiolate (3av)

Yield: 31.8 mg (40%); white solid; mp 149–150 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.77 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 7.2 Hz, 2H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 4.92–4.88 (m, 1H), 4.73 (td, *J* = 10.0, 4.4 Hz, 1H), 3.33–3.25 (m, 1H), 2.20–2.17 (m,4H), 2.02–1.99 (m, 1H), 1.73–1.68 (m, 2H), 1.46–1.27 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 153.9, 143.0, 138.3, 133.0, 130.8, 129.6, 128.6, 127.0, 119.6, 87.0, 80.5, 75.8, 56.6, 33.6, 30.8, 24.0, 23.6, 21.2.

HRMS (ESI): *m/z* $[M+K]^+$ calcd for $C_{22}H_{23}NO_4SK$: 436.0985, found: 436.1009. IR(KBr) (cm^{-1}) v 3386, 3251, 3064, 2939, 2859, 2224, 1706, 1596, 1468, 1360, 1325, 1161, 1023.



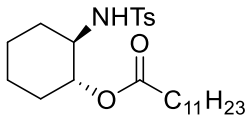
2-((4-Methylphenyl)sulfonamido)cyclohexyl acetate (3aw)[1]

Yield: 37.9 mg (61%); white solid; mp 123–125 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.75 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.08 (d, *J* = 7.6 Hz, 1H), 4.56 (td, *J* = 10.0, 4.4 Hz, 1H), 3.22–3.15 (m, 1H), 2.42 (s, 3H), 2.05–1.90 (m, 2H), 1.78 (s, 3H), 1.70–1.63 (m, 2H), 1.37–1.24 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 171.5, 143.1, 138.6, 129.6, 126.9, 74.1, 56.9, 33.4, 31.1, 24.2, 23.7, 21.5, 21.0.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{15}H_{21}NO_4SNa$: 334.1089; found: 334.1055. IR(KBr) (cm^{-1}) v 3406, 3245, 2942, 2865, 1715, 1597, 1494, 1454, 1373, 1336, 1259, 1160, 1090, 1039.



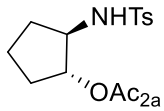
2-((4-Methylphenyl)sulfonamido)cyclohexyl dodecanoate (3ax)

Yield: 67.7 mg (75%); white solid; mp 38–39 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.75 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 7.2 Hz, 2H), 5.22 (d, *J* = 7.6 Hz, 1H), 4.60–4.55 (m, 1H), 3.26–3.17 (m, 1H), 2.41 (s, 3H), 2.04–1.91 (m, 5H), 1.69–1.61 (m, 2H), 1.49–1.46 (m, 3H), 1.40–1.26 (m, 21H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 174.1, 142.8, 138.9, 129.5, 126.9, 73.8, 56.8, 34.2, 33.2, 31.9, 31.0, 29.6, 29.5, 29.3, 29.3, 29.1, 24.7, 24.2, 23.6, 22.6, 21.4, 14.1.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{25}H_{41}NO_4SNa$: 474.2654; found: 474.2650. IR(KBr) (cm^{-1}) v 3305, 2923, 2853, 1731, 1455, 1383, 1326, 1304, 1206, 1161, 1090, 1020.



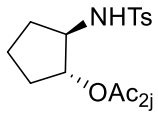
2-((4-Methylphenyl)sulfonamido)cyclopentyl cinnamate (3ba)[4]

Yield: 67.0 mg (87%); white solid; mp 125–126 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.77 (d, *J* = 8.0 Hz, 2H), 7.55–7.39 (m, 6H), 7.21 (d, *J* = 7.6 Hz, 2H), 6.21 (d, *J* = 16.0 Hz, 1H), 5.71–5.70 (m, 1H), 5.03–4.98 (m, 1H), 3.62–3.56 (m,1H), 2.24 (s, 3H), 2.10–2.03 (m, 2H), 1.74–1.52 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.9, 145.1, 143.2, 137.5, 134.2, 130.5, 129.6, 129.0, 128.1, 127.2, 117.6, 79.6, 59.9, 31.3, 29.5, 21.4, 20.8.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{21}H_{23}NO_4SNa$: 408.1245; found: 408.1248. IR(KBr) (cm^{-1}) v 3270, 3059, 2866, 1702, 1630, 1576, 1493, 1449, 1326, 1152, 1088, 1074, 1018, 991.



2-((4-Methylphenyl)sulfonamido)cyclopentyl benzoate (3bj)

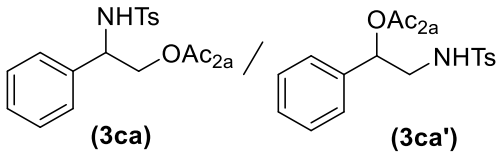
Yield: 61.0 mg (85%); white solid; mp 147–148 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 5.32–5.28 (m, 1H), 5.11–5.06 (m, 1H), 3.63–3.57 (m, 1H), 2.23–2.08 (m, 5H), 1.74–1.59 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ =166.6, 143.2, 137.0, 133.2, 129.6, 129.6, 129.6, 128.3, 127.1, 80.0, 60.1, 31.6, 29.5, 21.4, 20.8.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{19}H_{21}NO_4SNa$: 382.1089; found: 382.1074.

IR(KBr) (cm^{-1}) v 3321, 2961, 2927, 2870, 1712, 1599, 1450, 1358, 1322, 1274, 1151, 1113, 1091, 1070, 1029.



(3ca) **(3ca')**

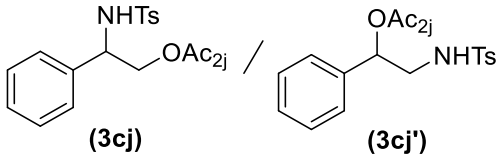
2-((4-Methylphenyl)sulfonamido)-2-phenylethyl cinnamate (3ca)/2-((4-methylphenyl)sulfonamido)-1-phenylethyl cinnamate (3ca')

Yield: 74.9 mg (89%, 80/20); white solid; mp 106–108 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.73 (d, *J* = 8.0 Hz, 0.4H), 7.64–7.21 (m, 13H), 7.06 (d, *J* = 7.6 Hz, 1.6H), 6.36 (d, *J* = 16.0 Hz, 0.2H), 6.21 (d, *J* = 16.0 Hz, 0.8H), 6.09–6.08 (m, 0.8H), 5.88–5.85 (m, 0.2H), 5.55–5.52 (m, 0.2H), 4.74–4.69 (m, 0.8H), 4.36–4.24 (m, 1.6H), 3.43–3.38 (m, 0.4H), 2.33 (s, 0.6H), 2.20 (s, 2.4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.6, 165.9, 145.7, 145.6, 143.4, 143.1, 137.8, 137.5, 137.3, 134.2, 130.5, 129.7, 129.4, 128.9, 128.7, 128.6, 128.2, 128.0, 127.1, 126.9, 126.4, 117.5, 117.2, 74.3, 66.6, 57.2, 47.9, 21.4, 21.3.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{24}H_{23}NO_4SNa$: 444.1245; found: 444.1256. IR(KBr) (cm^{-1}) v 3446, 3258, 3063, 3030, 2922, 1719, 1698, 1638, 1495, 1450, 1331, 1283, 1205, 1161, 1091, 1021.



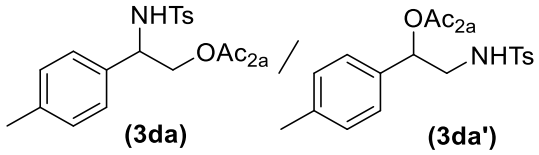
2-((4-Methylphenyl)sulfonamido)-2-phenylethyl benzoate (3cj)/2-((4-methylphenyl)sulfonamido)-1-phenylethyl benzoate (3cj')

Yield: 52.9 mg (67%, 70/30); white solid; mp 160–162 °C.

^1H NMR (400 MHz, $CDCl_3$): δ = 8.00 (d, *J* = 7.2 Hz, 0.6H), 7.87 (d, *J* = 7.2 Hz, 1.4H), 7.70 (d, *J* = 8.4 Hz, 0.6H), 7.59–7.22 (m, 10H), 7.02 (d, *J* = 8.0 Hz, 1.4H), 5.97–5.94 (m, 0.3H), 5.47–5.44 (m, 0.7H), 4.91–4.86 (m, 0.3H), 4.77–4.73 (m, 0.7H), 4.49–4.35 (m, 1.4H), 3.54–3.47 (m, 0.6H), 2.38 (s, 0.9H), 2.27 (s, 2.1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 165.6, 143.6, 143.2, 137.3, 137.2, 133.4, 133.4, 129.8, 129.8, 129.7, 129.5, 129.2, 128.9, 128.7, 128.5, 128.4, 128.2, 127.0, 127.0, 126.9, 126.4, 74.6, 67.0, 57.2, 47.9, 21.6, 21.5.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{21}NO_4SNa$: 418.1089; found: 418.1070. IR(KBr) (cm^{-1}) v 3437, 3343, 3062, 2924, 1709, 1600, 1495, 1434, 1322, 1278, 1157, 1128, 1090, 1026.



2-((4-Methylphenyl)sulfonamido)-2-(p-tolyl)ethyl cinnamate(3da)/2-((4-methylphenyl)sulfonamido)-1-(p-tolyl)ethyl cinnamate (3da')[4]

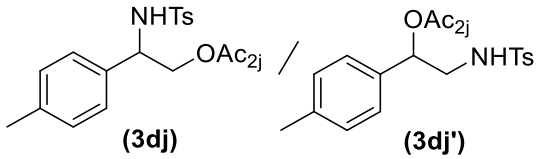
Yield: 78.3 mg (90%,70/30); white solid; mp 128–130 ℃.

^{1}H NMR (400 MHz, $CDCl_3$): δ =7.73 (d, *J* = 8.0 Hz, 0.6H), 7.63–7.08 (m, 12H), 7.02 (d, *J* = 8.0 Hz, 1.4H), 6.34 (d, *J* = 16.0 Hz, 0.3H), 6.21 (d, *J* = 16.0 Hz, 0.7H), 5.88–5.80 (m, 1H), 5.39–5.31 (m, 0.3H), 4.68–4.64 (m, 0.7H), 4.36–4.23(m, 1.4H), 3.46–3.33 (m, 0.6H), 2.34 (s, 0.9H), 2.30 (s, 0.9H), 2.27 (s, 2.1H), 2.22 (s, 2.1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.8, 166.1, 145.7, 145.6, 143.5, 143.1, 138.5, 137.8, 137.6, 137.0, 134.4, 134.2, 134.2, 134.1, 130.6, 130.5, 129.8, 129.4, 129.3, 128.9, 128.9, 128.2, 127.1, 127.1, 126.9, 126.4, 117.4, 117.1, 74.3, 66.7, 56.9, 47.9, 21.5, 21.4, 21.2, 21.1.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{25}H_{25}NO_4SNa$: 458.1402; found: 458.1411.

IR(KBr) (cm^{-1}) v 3312, 3061, 3027, 2955, 2922, 1698, 1634, 1598, 1578, 1516, 1496, 1450, 1384, 1330, 1285, 1156, 1118, 1089, 1017, 982.



(3dj) **(3dj')**

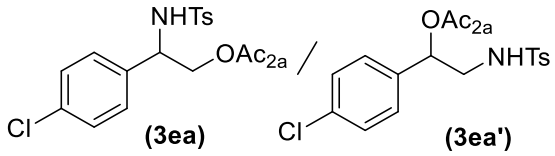
2-((4-Methylphenyl)sulfonamido)-2-(p-tolyl)ethyl benzoate(3dj)/2-((4-methylphenyl)sulfonamido)-1-(p-tolyl)ethyl benzoate (3dj')[4]

Yield: 66.3 mg (81%, 70/30); pale yellow solid; mp 151–154 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.97 (d, *J* = 7.2Hz, 0.6H), 7.88–7.85 (m, 1.4H), 7.70 (d, *J* = 8.0 Hz, 0.6H), 7.59–6.98 (m, 10.4H), 5.95–5.91 (m, 0.3H), 5.87 (d, *J* = 6.8 Hz, 0.7H), 5.31 (t, *J* = 6.8 Hz, 0.3H), 4.73–4.68 (m, 0.7H), 4.45–4.33 (m, 1.4H), 3.53–3.38 (m, 0.6H), 2.35 (s, 0.9H), 2.29 (s, 0.9H), 2.27 (s, 2.1H), 2.25 (s, 2.1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 165.7, 143.4, 143.1, 138.5, 137.8, 137.4, 137.1, 134.4, 134.2, 133.2, 129.8, 129.5, 129.4, 129.3, 128.4, 128.3, 127.0, 126.8, 126.4, 74.7, 67.1, 56.9, 47.9, 21.5, 21.4, 21.2, 21.1.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{23}H_{23}NO_4SNa$: 432.1245; found: 432.1264. IR(KBr) (cm^{-1}) v 3332, 3030, 2956, 2921, 1712, 1599, 1515, 1494, 1449, 1384, 1321, 1270, 1152, 1122, 1090, 1019, 996.



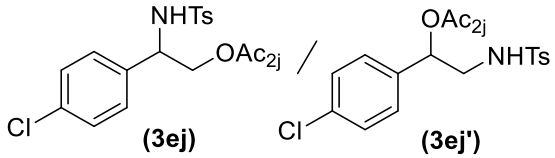
2-(4-Chlorophenyl)-2-((4-methylphenyl)sulfonamido)ethyl cinnamate(3ea)/1-(4-chlorophenyl)-2-((4-methylphenyl)sulfonamido)ethyl cinnamate (3ea')[4]

Yield: 65.5 mg (72%, 80/20); white solid; mp 160–163 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 8.0Hz, 0.4H), 7.66–7.14 (m, 12H), 7.11 (d, *J* = 8.0Hz, 1.6H), 6.36 (d, *J* = 16.0 Hz, 0.2H), 6.22 (d, *J* = 16.0 Hz, 0.8H), 5.95–5.88 (m, 0.8H), 5.82 (t, *J* = 6.0 Hz, 0.2H), 5.38–5.31 (m, 0.2H), 4.70–4.64 (m, 0.8H), 4.34–4.21 (m, 1.6H), 3.43–3.34 (m, 0.4H), 2.37 (s, 0.6H), 2.25 (s, 2.4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.6, 145.9, 143.4, 137.4, 135.9, 134.1, 134.0, 130.6, 129.8, 129.5, 128.9, 128.8, 128.4, 128.2, 127.8, 127.1, 127.0, 116.8, 66.3, 56.6, 21.3.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{24}H_{22}NO_4SClNa$: 478.0856; found: 478.0861. IR(KBr) (cm^{-1}) v 3442, 3271, 2924, 1717, 1707, 1636, 1599, 1494, 1450, 1319, 1170, 1156, 1091, 1014, 980.



2-(4-Chlorophenyl)-2-((4-methylphenyl)sulfonamido)ethyl benzoate(3ej)/1-(4-chlorophenyl)-2-((4-methylphenyl)sulfonamido)ethyl benzoate (3ej')[4]

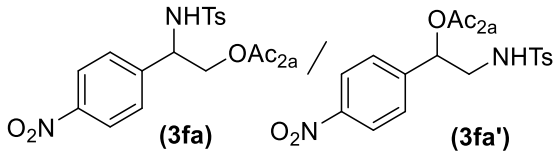
Yield: 71.2 mg (83%, 84/16); white solid; mp 155–156 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.98 (d, *J* = 7.2 Hz, 0.32H), 7.86 (d, *J* = 7.2 Hz, 1.68H), 7.68 (d, *J* = 8.4 Hz, 0.32H), 7.59–7.18(m, 9H), 7.02 (d, *J* = 7.2 Hz, 1.68H), 5.95–5.92(m, 0.16H), 5.72 (d, *J* = 6.8 Hz, 0.84H), 5.10 (t, *J* = 6.4 Hz, 0.16H),

4.74–4.69 (m, 0.84H), 4.44–4.32 (m, 1.68H), 3.49–3.44 (m, 0.32H), 2.39 (s, 0.48H), 2.28 (s, 2.52H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 143.5, 137.0, 135.8, 135.6, 134.0, 133.5, 133.4, 129.8, 129.8, 129.7, 129.5, 129.1, 129.0, 128.8, 128.5, 128.4, 128.3, 127.8, 126.9, 74.1, 66.7, 56.6, 47.7, 21.6, 21.5.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{20}NO_4SClNa$: 452.0699; found: 452.0672. IR(KBr) (cm^{-1}) v 3429, 3272, 2955, 2923, 1721, 1697, 1599, 1491, 1441, 1385, 1330, 1269, 1156, 1123, 1092, 1071, 1027, 1015, 989.



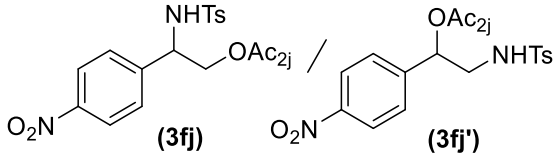
2-((4-Methylphenyl)sulfonamido)-2-(4-nitrophenyl)ethyl cinnamate(3fa)/2-((4-methylphenyl)sulfonamido)-1-(4-nitrophenyl)ethyl cinnamate (3fa')

Yield: 25.2 mg (27%, 55/45); pale yellow solid; mp 139–142 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.16–8.09(m, 2.0H), 7.70–7.24 (m, 10.9H), 7.13 (d, *J* = 8.0 Hz, 1.1H), 6.41 (d, *J* = 16.0 Hz, 0.45H), 6.21 (d, *J* = 16.0 Hz, 0.55H), 6.15–6.02 (m, 0.55H), 5.94 (t, *J* = 5.6 Hz, 0.45H), 5.47–5.34 (m, 0.45H), 4.80–4.77 (m, 0.55H), 4.37–4.22(m, 1.1H), 3.63–3.44 (m, 0.9H), 2.37 (s, 1.35H)，2.24 (s, 1.65H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.6, 165.6, 147.8, 147.6, 146.7, 146.4, 144.7, 144.4, 143.9, 136.9, 136.8, 133.8, 130.9, 129.9, 129.7, 129.0, 129.0, 128.3, 128.3, 128.0, 127.3, 127.0, 127.0, 123.9, 123.8, 116.5, 116.3, 73.5, 65.9, 56.8, 47.5, 21.5, 21.4.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{24}H_{22}N_2O_6SNa$: 489.1096; found: 489.1107. IR(KBr) (cm^{-1}) v 3447, 3273, 2923, 2853, 1709, 1636, 1600, 1520, 1450, 1347, 1332, 1204, 1164, 1090, 1018, 982.



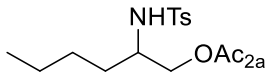
2-((4-Methylphenyl)sulfonamido)-2-(4-nitrophenyl)ethyl benzoate(3fj)/2-((4-methylphenyl)sulfonamido)-1-(4-nitrophenyl)ethyl benzoate (3fj')

Yield: 20.2 mg (23%, 67/33); pale yellow solid; mp 139–142 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.16–8.10 (m, 2.0H), 8.01 (d, *J* = 7.6 Hz, 0.66H), 7.84 (d, *J* = 7.6 Hz, 1.34H), 7.68–7.38 (m, 7.0H), 7.21 (d, *J* = 8.0 Hz, 0.66H), 7.03 (d, *J* = 8.0 Hz, 1.34H), 6.11–6.05 (m, 1H), 5.45–5.30 (m, 0.33H), 4.85–4.82 (m, 0. 67H), 4.47–4.37 (m, 1.34H), 3.52–3.44 (m, 0.66H), 2.38 (s, 0.99H), 2.27 (s, 2.01H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 165.3, 147.9, 147.6, 144.7, 144.3, 143.9, 143.8, 136.7, 133.8, 133.6, 129.8, 129.8, 129.7, 129.6, 128.9, 128.8, 128.6, 128.5, 128.0, 127.3, 126.9, 124.0, 123.9, 73.9, 66.4, 56.8, 47.5, 21.5, 21.5.

HRMS (ESI): *m/z*$[M+Na]^+$ calcd for $C_{22}H_{20}N_2O_6SNa$: 463.0940; found: 463.0941. IR(KBr) (cm^{-1}) v 3436, 3276, 3066, 2924, 2853, 1714, 1600, 1520, 1451, 1439, 1348, 1271, 1158, 1090, 1027.



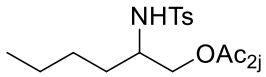
2-((4-Methylphenyl)sulfonamido)hexyl cinnamate (3ga)

Yield: 56.9 mg (71%); white solid; mp 105–106 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.78 (d, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 16.0 Hz, 1H), 7.48–7.46 (m, 2H), 7.38–7.37 (m, 3H), 7.23 (d, *J* = 8.0 Hz, 2H), 6.23 (d, *J* = 16.0 Hz, 1H), 5.43 (d, *J* = 8.4 Hz, 1H), 4.15–4.00 (m, 2H), 3.58–3.50 (m, 1H), 2.29 (s, 3H), 1.54–1.47 (m, 2H), 1.26–1.20 (m, 4H), 0.81 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ =166.7, 145.3, 143.2, 138.4, 134.3, 130.4, 129.6, 128.9, 128.1, 127.0, 117.4, 65.8, 53.2, 32.2, 27.5, 22.3, 21.3, 13.7.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{22}H_{27}NO_4SNa$: 424.1558; found: 424.1580. IR(KBr) (cm^{-1}) v 3320, 2956, 2853, 1704, 1634, 1579, 1499, 1453, 1430, 1389, 1317, 1286, 1187, 1159, 1142, 1093, 1008, 983.



2-((4-Methylphenyl)sulfonamido)hexyl benzoate (3gj)

Yield: 49.5 mg (66%); white solid; mp 104–106 °C.

^1H NMR (400 MHz, $CDCl_3$): δ = 7.91 (d, *J* = 7.6 Hz, 2H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 5.19 (d, *J* = 8.0, 1H), 4.27–4.11 (m, 2H), 3.64–3.56 (m, 1H), 2.32 (s, 3H), 1.60–1.51 (m, 2H), 1.30–1.20 (m, 4H), 0.80 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 143.3, 137.9, 133.2, 129.7, 129.6, 129.5, 128.4, 126.9, 66.2, 53.1, 32.3, 27.6, 22.3, 21.5, 13.9.

HRMS (ESI): *m/z* $[M+Na]^+$ calcd for $C_{20}H_{25}NO_4SNa$: 398.1402; found: 398.1412.

IR(KBr) (cm^{-1}) v 3406, 3299, 2933, 2858, 1709, 1601, 1495, 1452, 1428, 1395, 1325, 1280, 1164, 1114, 1092, 1044, 1028, 971.

Reference:

1. Liu, Y. K.; Li, R.; Yue, L.; Li, B. J.; Chen, Y. C.; Wu, Y.; Ding, L. S. *Org. Lett.* **2006**, *8*, 152.

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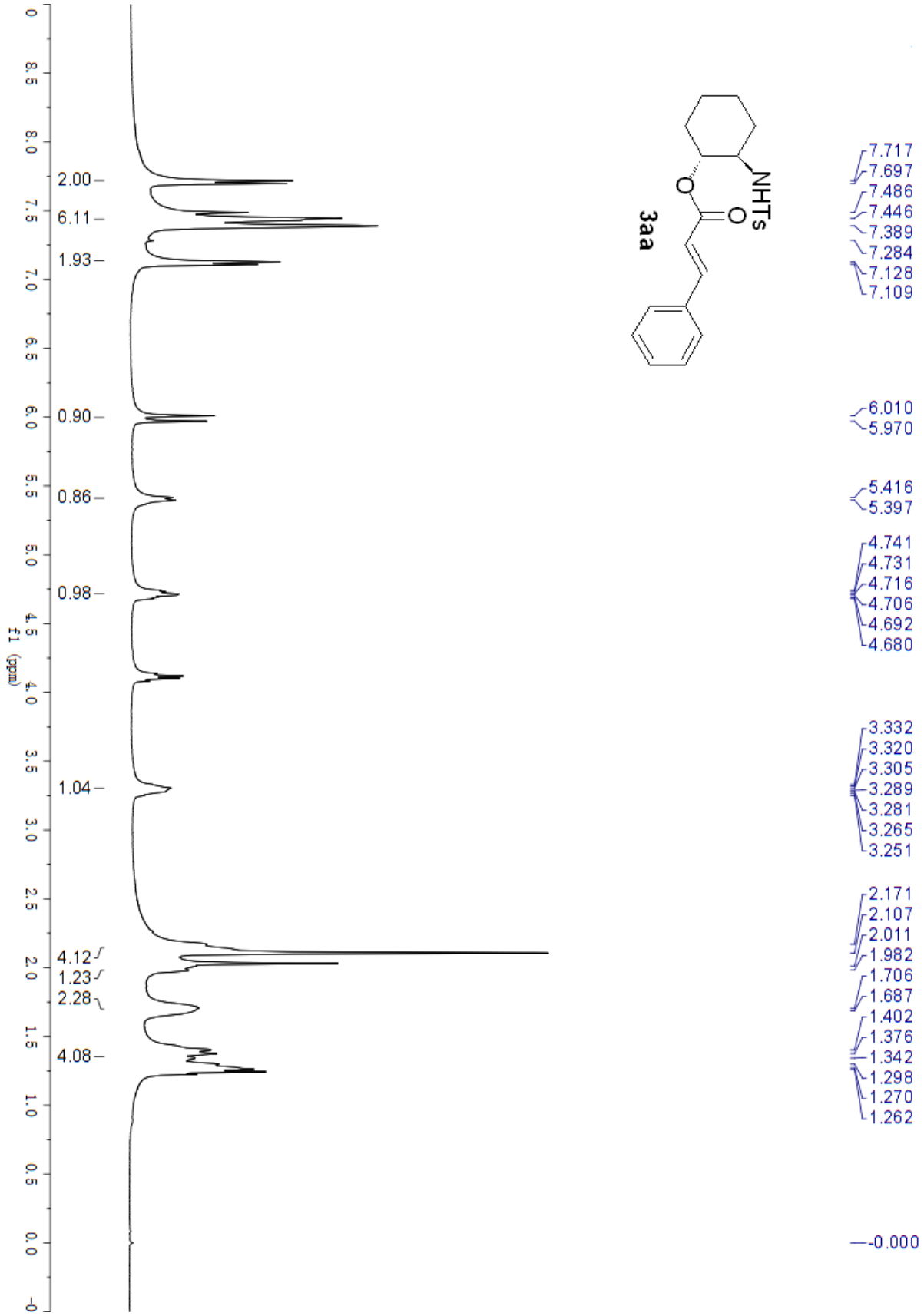
3. Zhang, F.; Chamg, H.; Wei, W. *J. Heterocyclic Chem*., **2015**, *52*, 284.

4. Yadav, J. S. *Tetrahedron Lett.* **2002**, *43*, 2099.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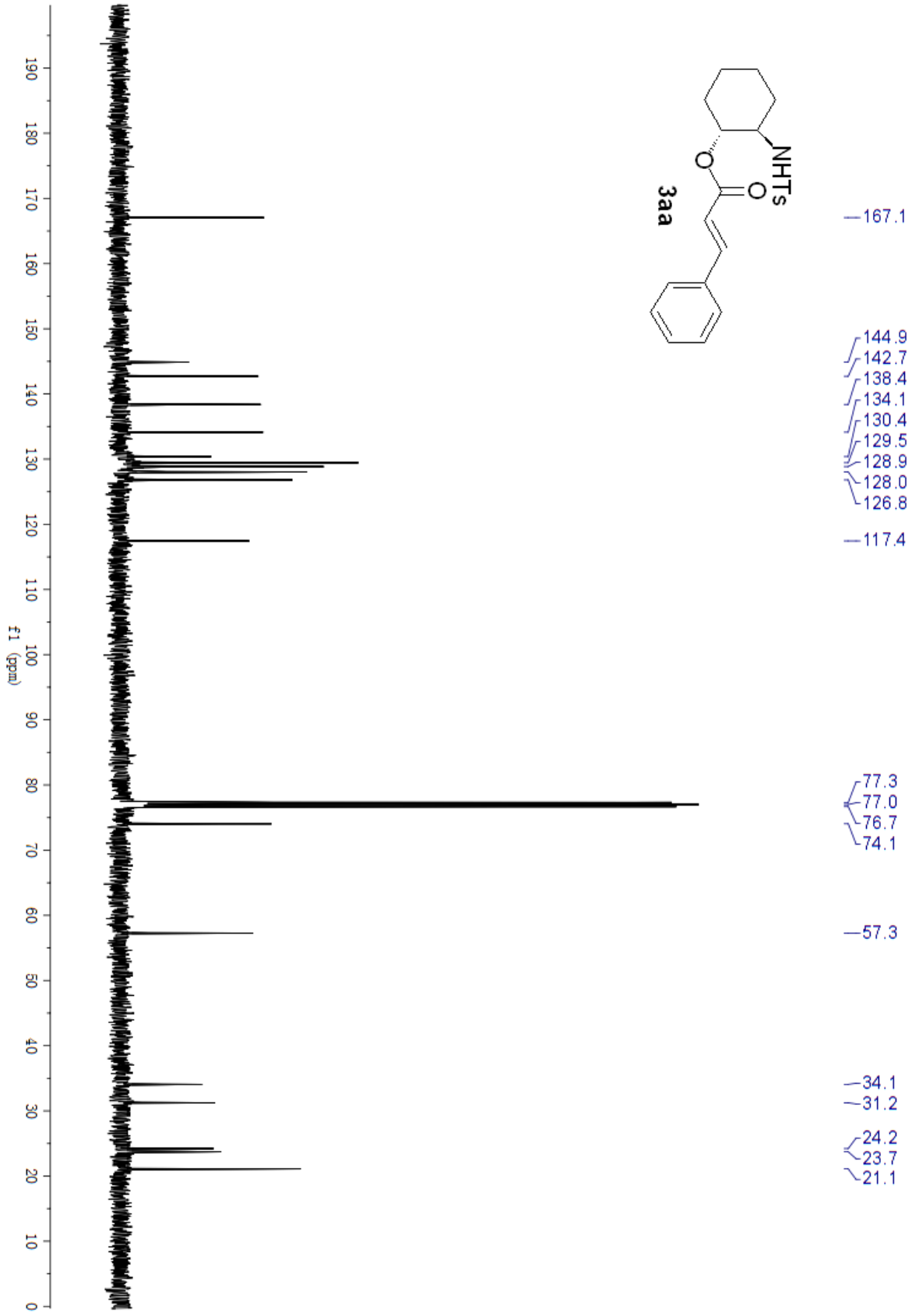
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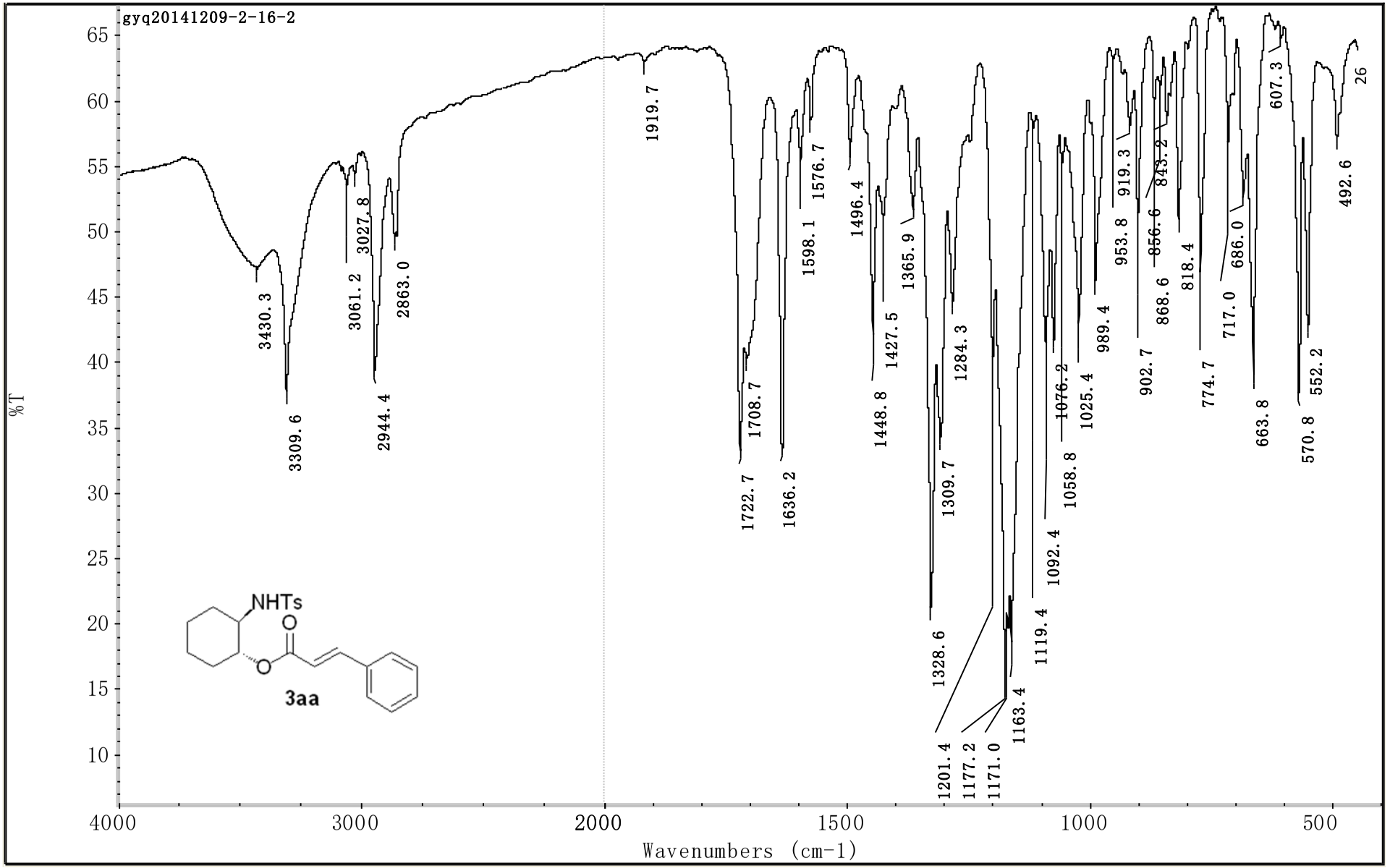
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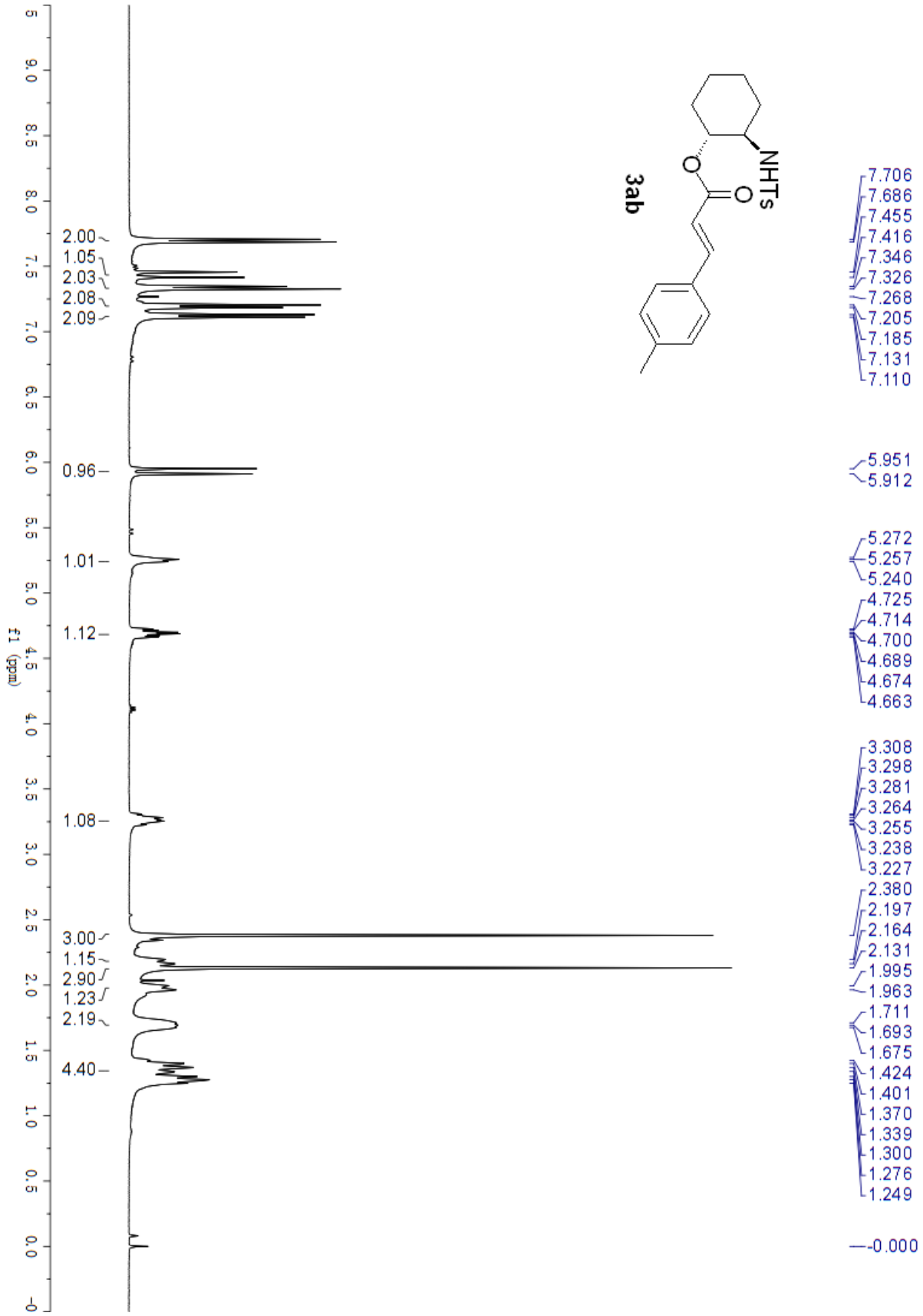
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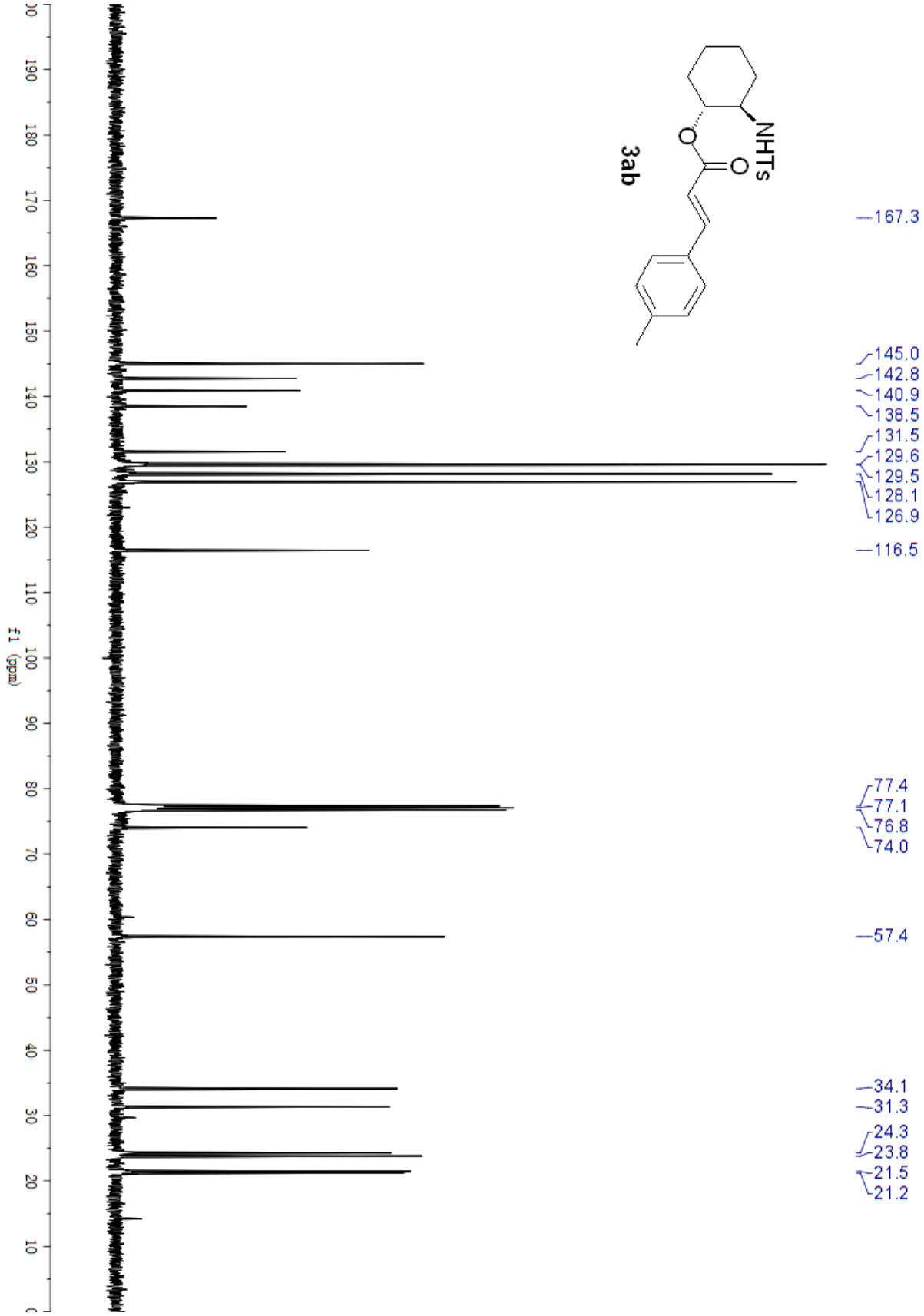
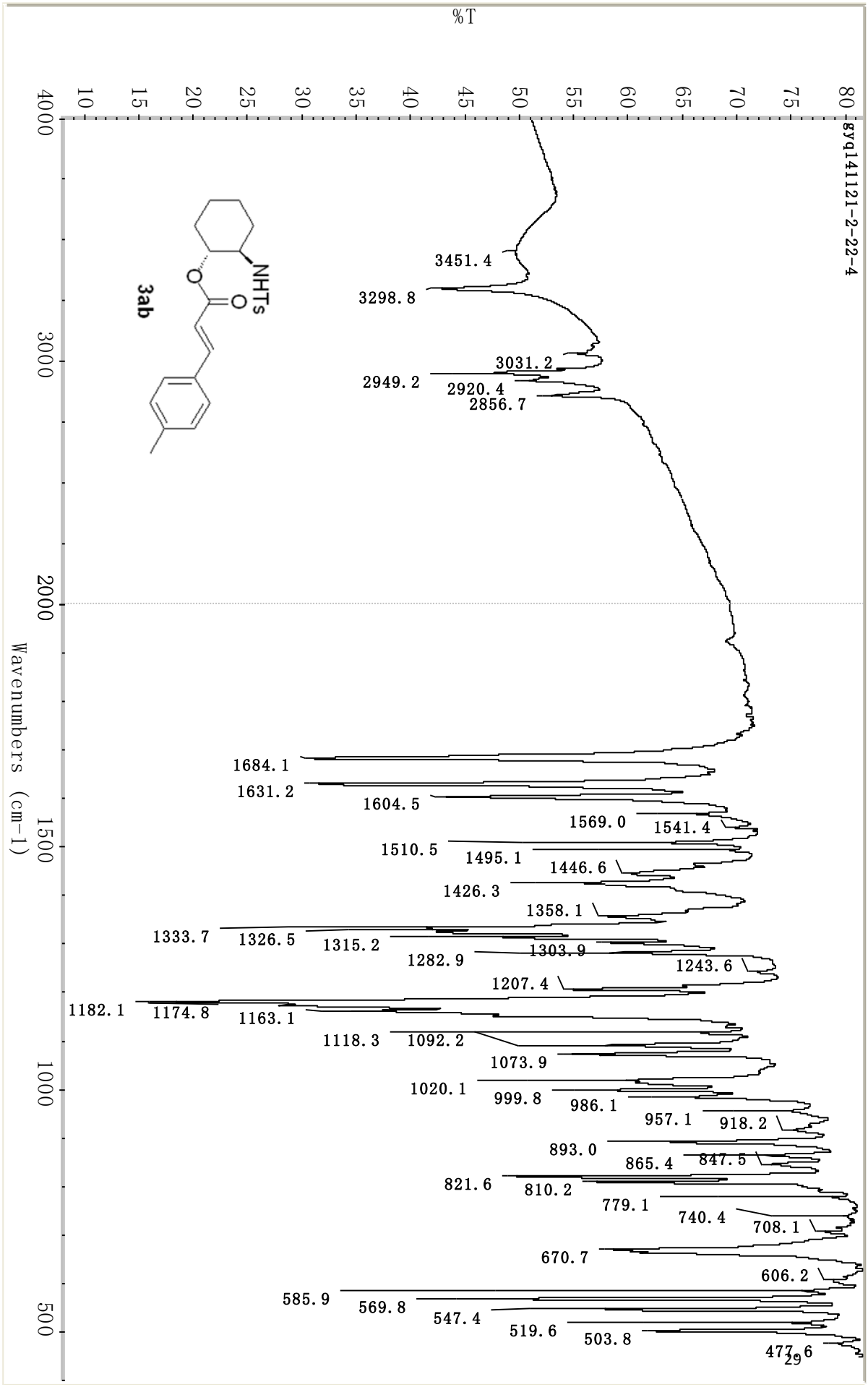
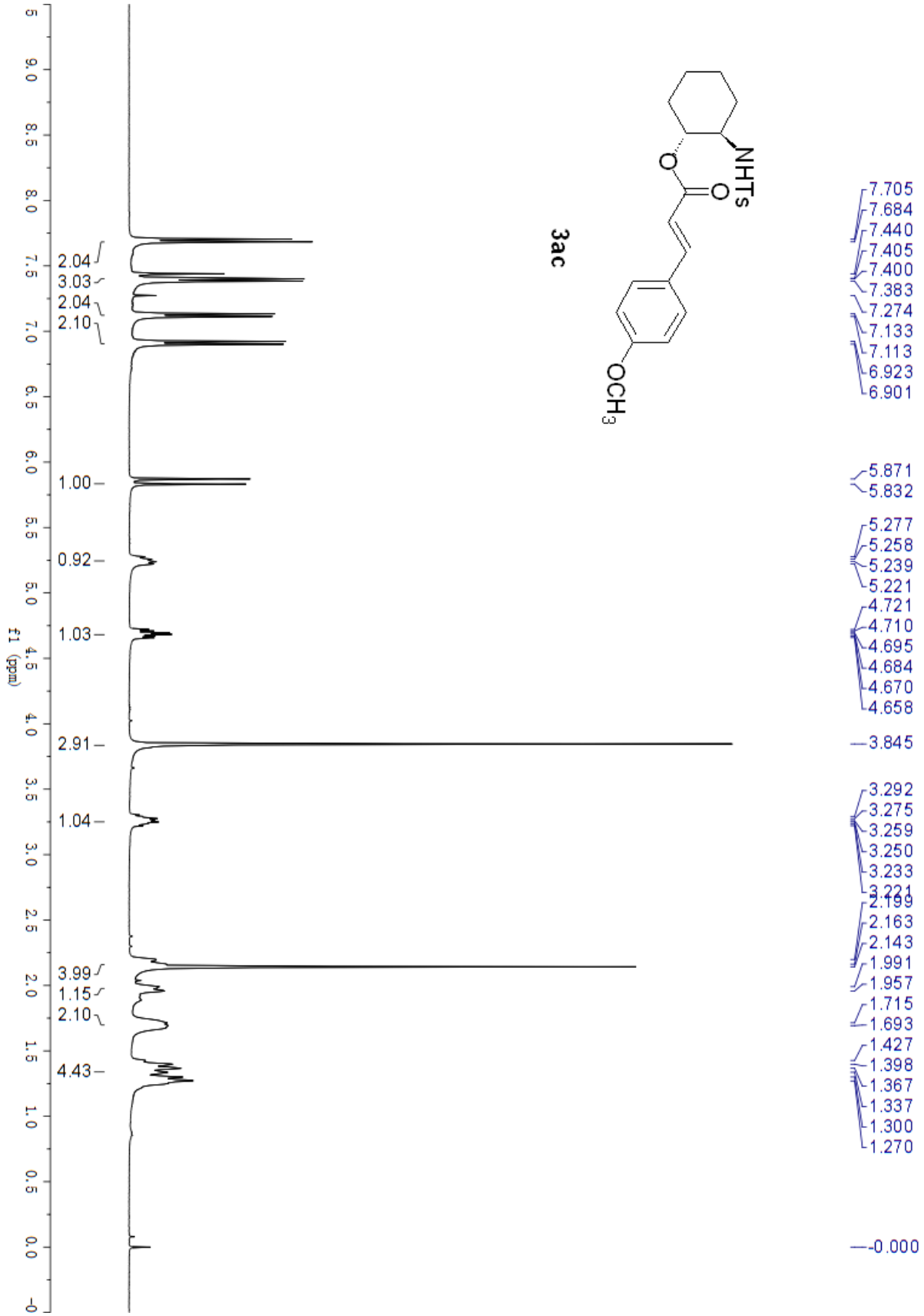
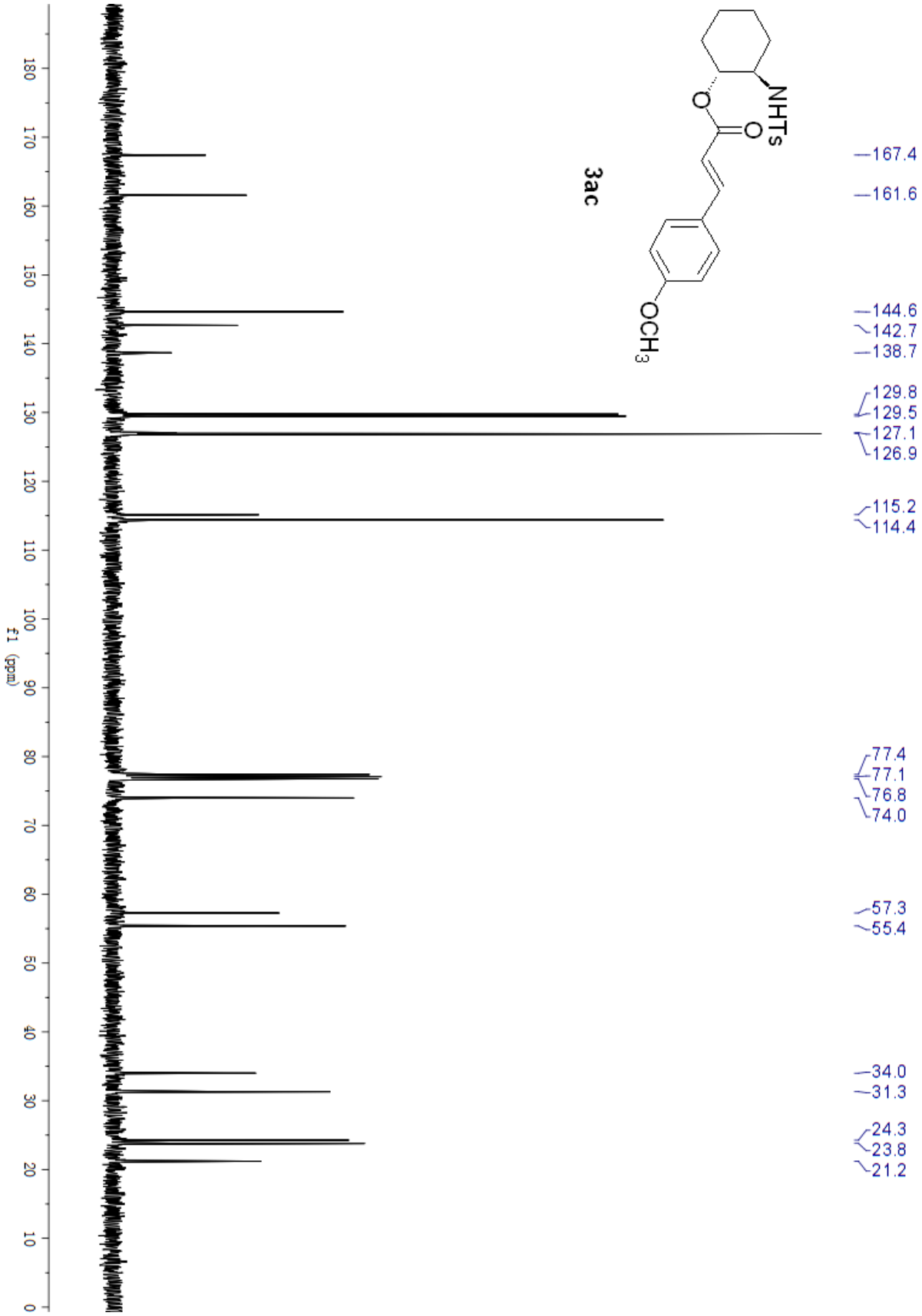
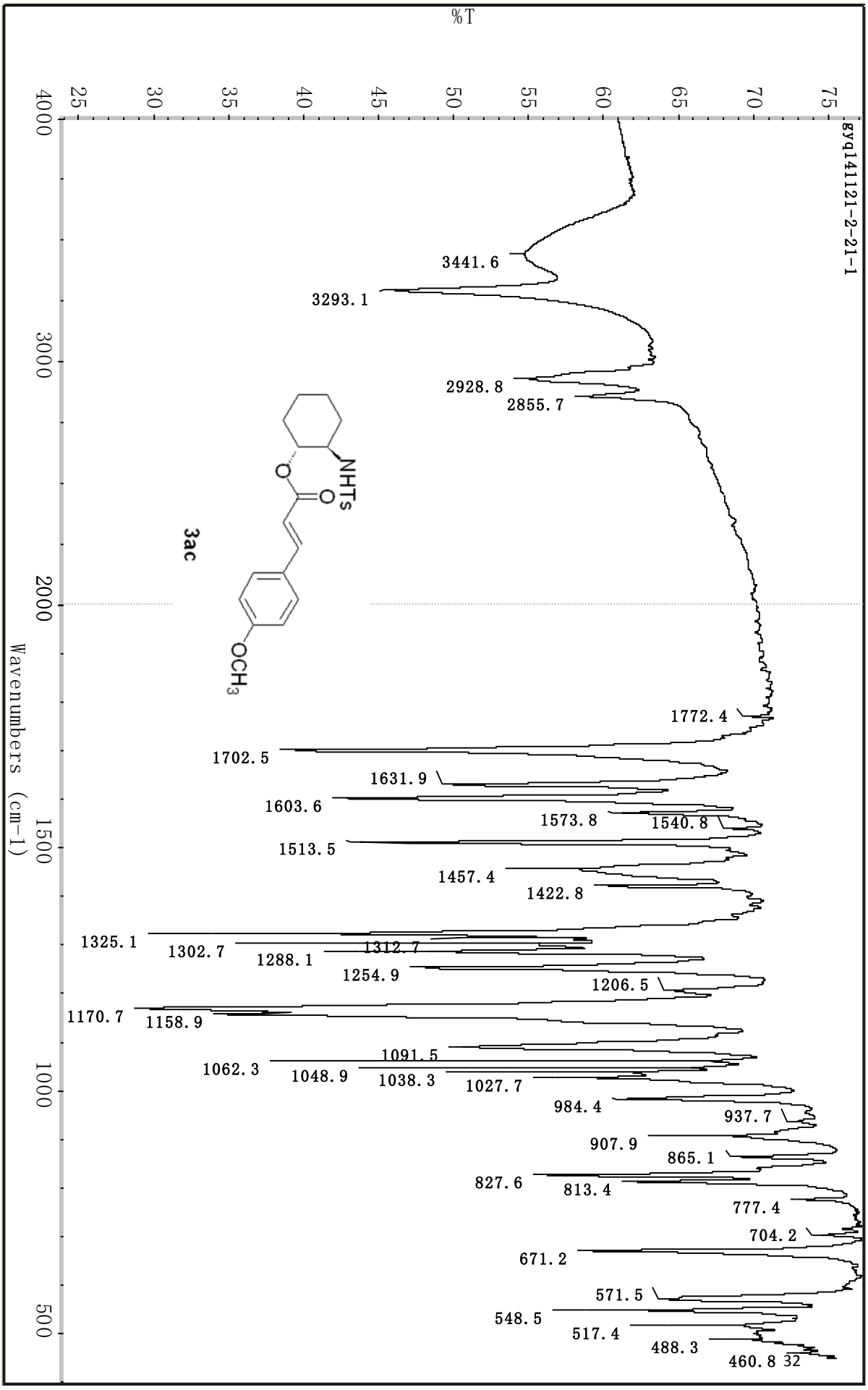
1.693
1.675
1.424
1.401
1.370
1.339
1.300
1.276
1.249
-0.000

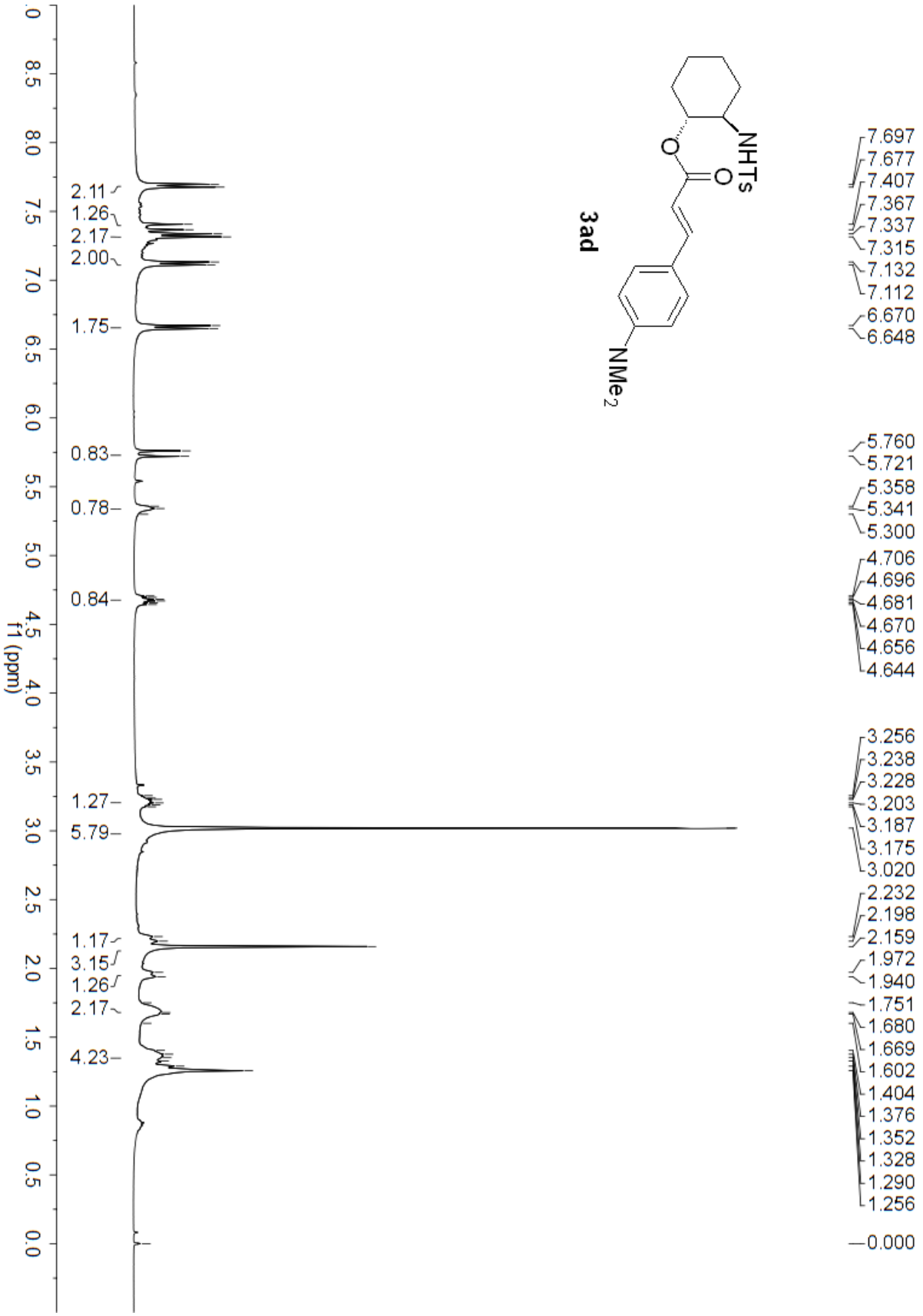

3ab
NHTs
O
O
167.3
145.0
142.8
140.9
138.5
131.5
129.6
129.5
128.1
126.9
116.5
77.4
77.1
76.8
74.0
57.4
34.1
31.3
24.3
23.8
21.5
21.2
f1 (ppm)

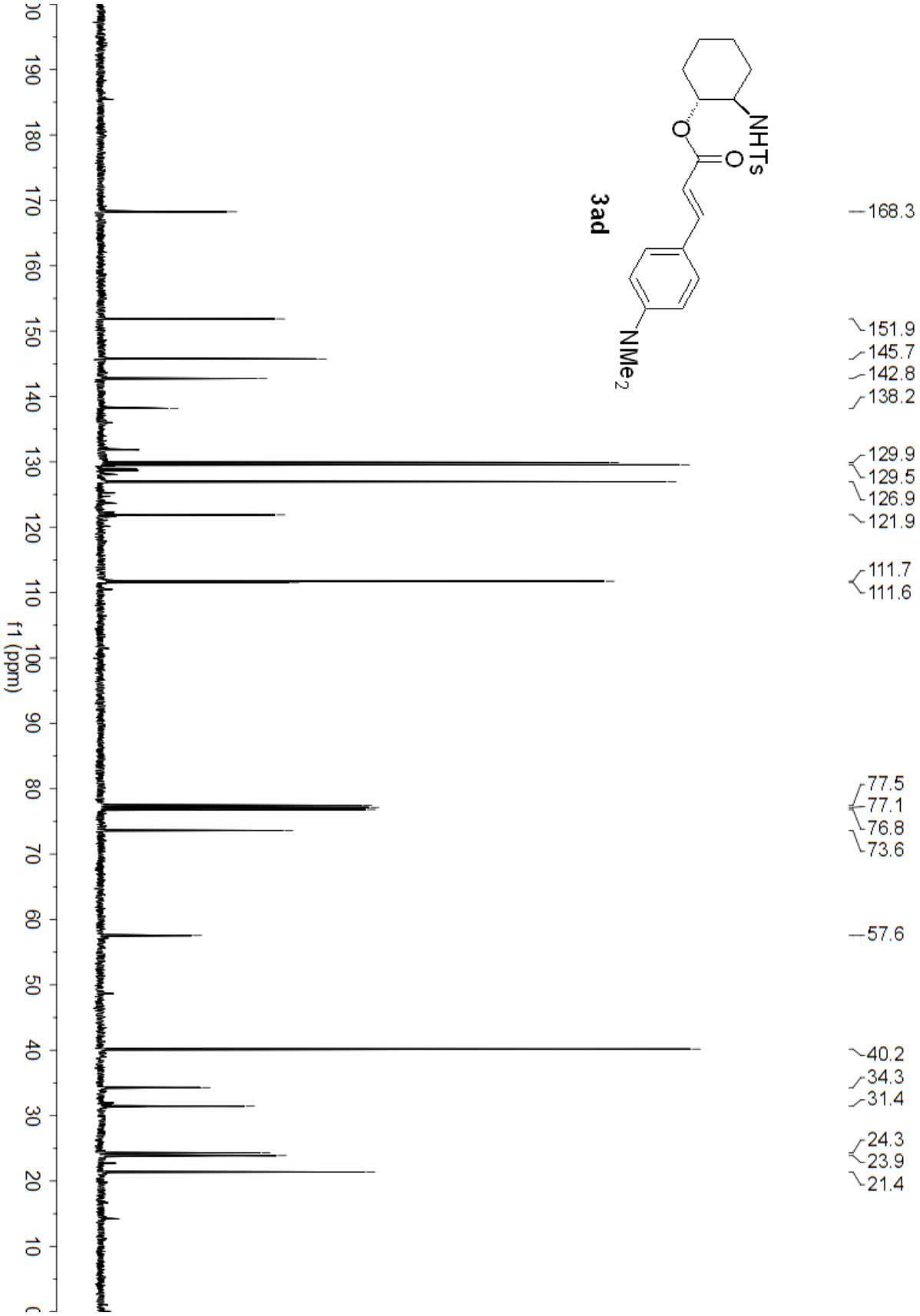

%T
Wavenumbers (cm-1)
gyq141121-2-22-4
3ab
NHTs
O
O
3451.4
3298.8
3031.2
2949.2
2920.4
2856.7
1684.1
1631.2
1604.5
1569.0
1541.4
1510.5
1495.1
1446.6
1426.3
1358.1
1333.7
1326.5
1315.2
1303.9
1282.9
1243.6
1207.4
1182.1
1174.8
1163.1
1118.3
1092.2
1073.9
1020.1
999.8
986.1
957.1
918.2
893.0
865.4
847.5
821.6
810.2
779.1
740.4
708.1
670.7
606.2
585.9
569.8
547.4
519.6
503.8
477.6

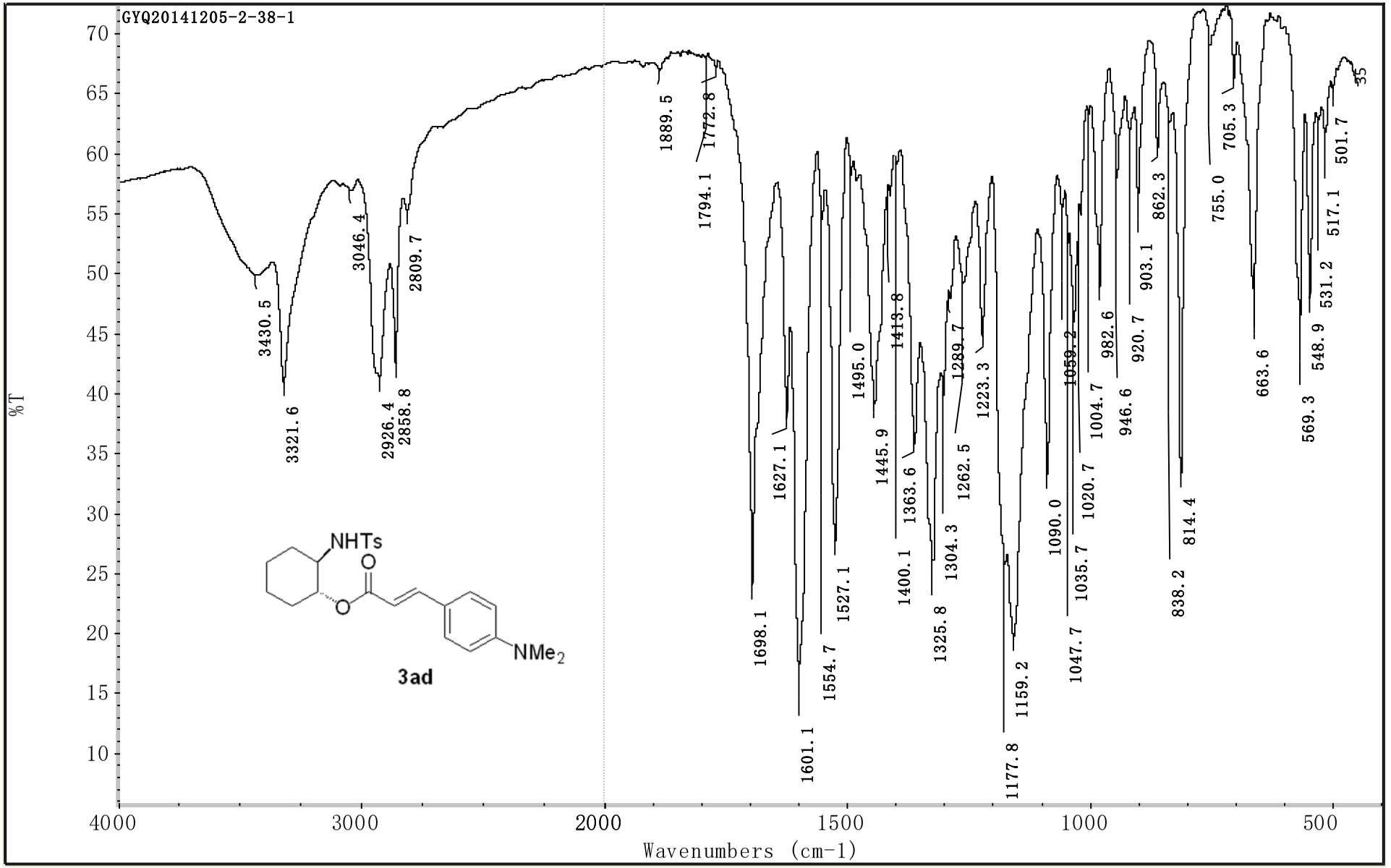

3ac
NHTs
O
O
OCH3
f1 (ppm)
2.04
3.03
2.04
2.10
1.00
0.92
1.03
2.91
1.04
3.99
1.15
2.10
4.43
7.705
7.684
7.440
7.405
7.400
7.383
7.274
7.133
7.113
6.923
6.901
5.871
5.832
5.277
5.258
5.239
5.221
4.721
4.710
4.695
4.684
4.670
4.658
3.845
3.292
3.275
3.259
3.250
3.233
2.199
2.163
2.143
1.991
1.957
1.715
1.693
1.427
1.398
1.367
1.337
1.300
1.270
0.000

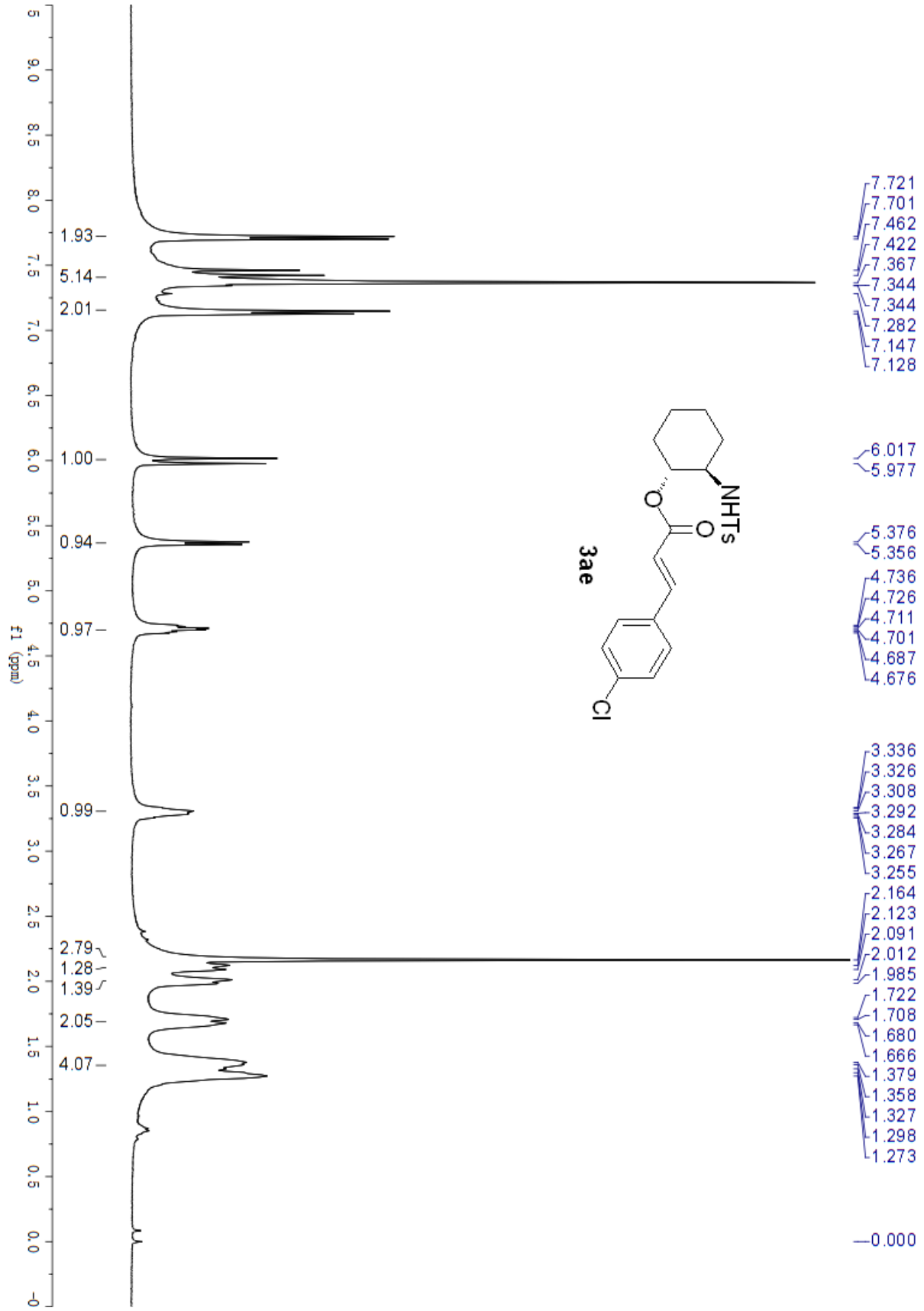

3ac
NHTs
O
O
OCH3
167.4
161.6
144.6
142.7
138.7
129.8
129.5
127.1
126.9
115.2
114.4
77.4
77.1
76.8
74.0
57.3
55.4
34.0
31.3
24.3
23.8
21.2
f1 (ppm)

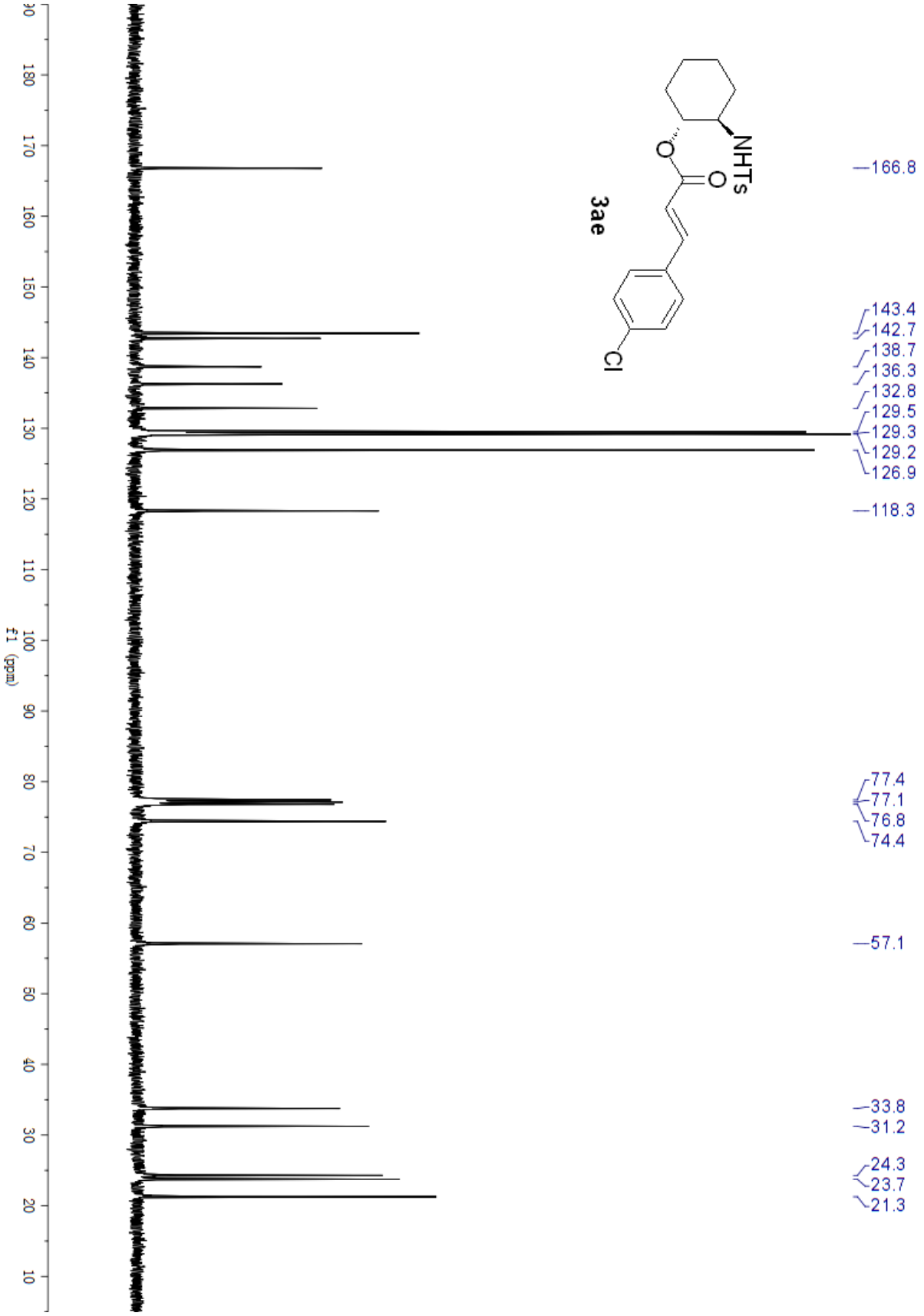

%T
25
30
35
40
45
50
55
60
65
70
75
gyq141121-2-21-1
3441.6
3293.1
2928.8
2855.7
3ac
NHTs
O
O
OCH3
1772.4
1702.5
1631.9
1603.6
1573.8
1540.8
1513.5
1457.4
1422.8
1325.1
1302.7
1312.7
1288.1
1254.9
1206.5
1170.7
1158.9
1091.5
1062.3
1048.9
1038.3
1027.7
984.4
937.7
907.9
865.1
827.6
813.4
777.4
704.2
671.2
571.5
548.5
517.4
488.3
460.8
4000
3000
2000
1500
1000
500
Wavenumbers (cm-1)

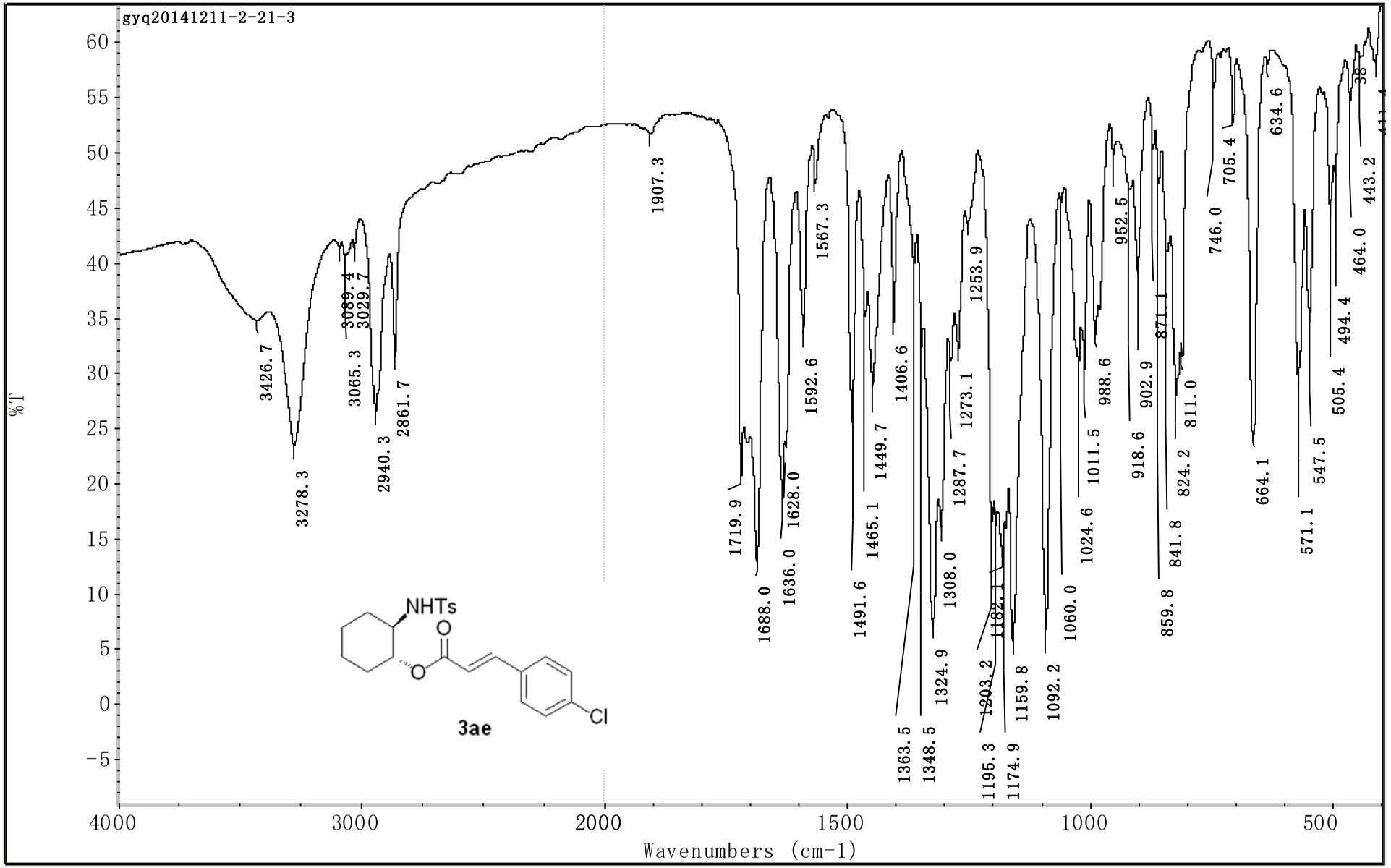

3ad
NHTs
O
O
NMe2
7.697
7.677
7.407
7.367
7.337
7.315
7.132
7.112
6.670
6.648
5.760
5.721
5.358
5.341
5.300
4.706
4.696
4.681
4.670
4.656
4.644
3.256
3.238
3.228
3.203
3.187
3.175
3.020
2.232
2.198
2.159
1.972
1.940
1.751
1.680
1.669
1.602
1.404
1.376
1.352
1.328
1.290
1.256
0.000
2.11
1.26
2.17
2.00
1.75
0.83
0.78
0.84
1.27
5.79
1.17
3.15
1.26
2.17
4.23
f1 (ppm)

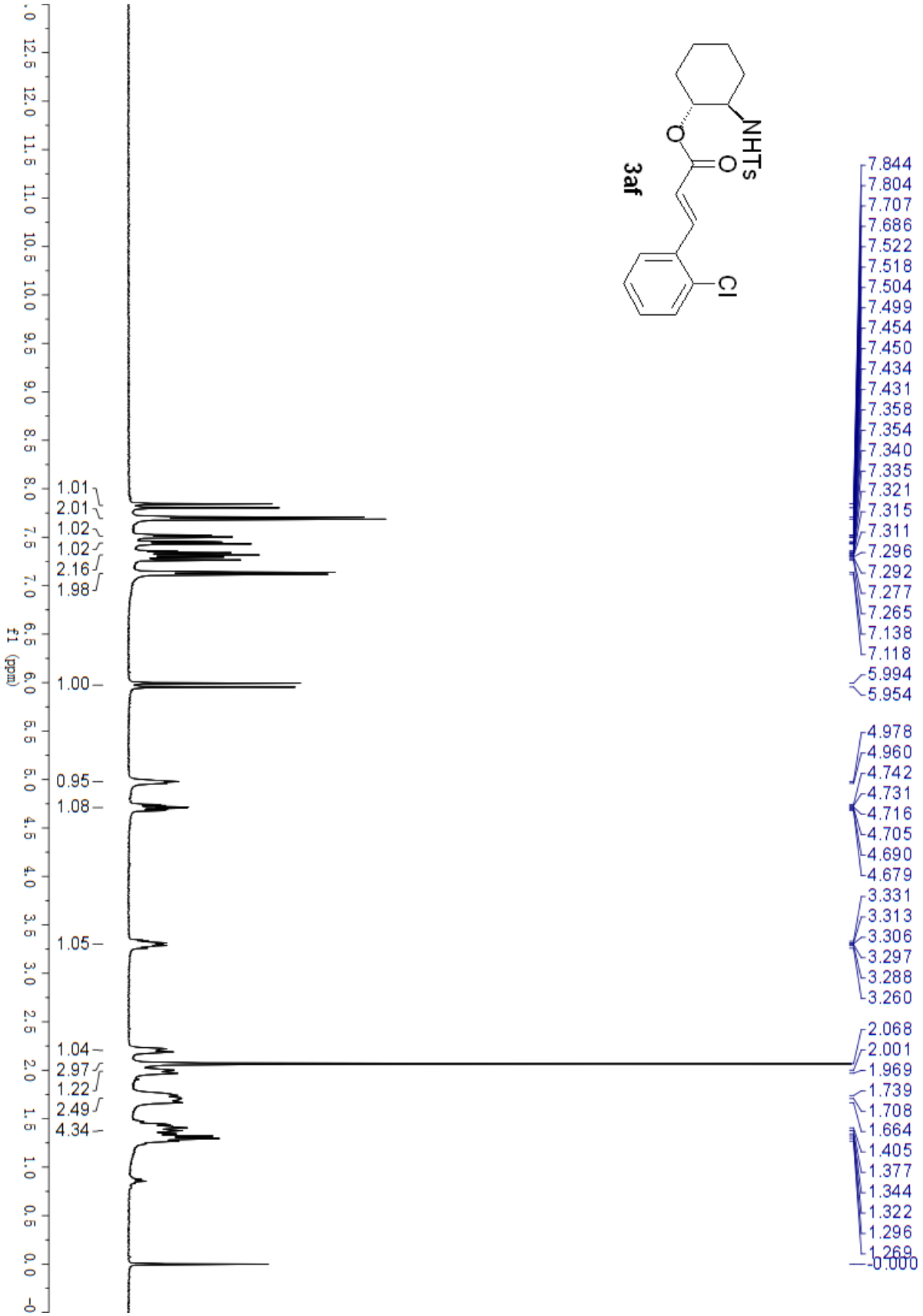

3ad
NHTs
O
O
NMe2
168.3
151.9
145.7
142.8
138.2
129.9
129.5
126.9
121.9
111.7
111.6
77.5
77.1
76.8
73.6
57.6
40.2
34.3
31.4
24.3
23.9
21.4
f1 (ppm)

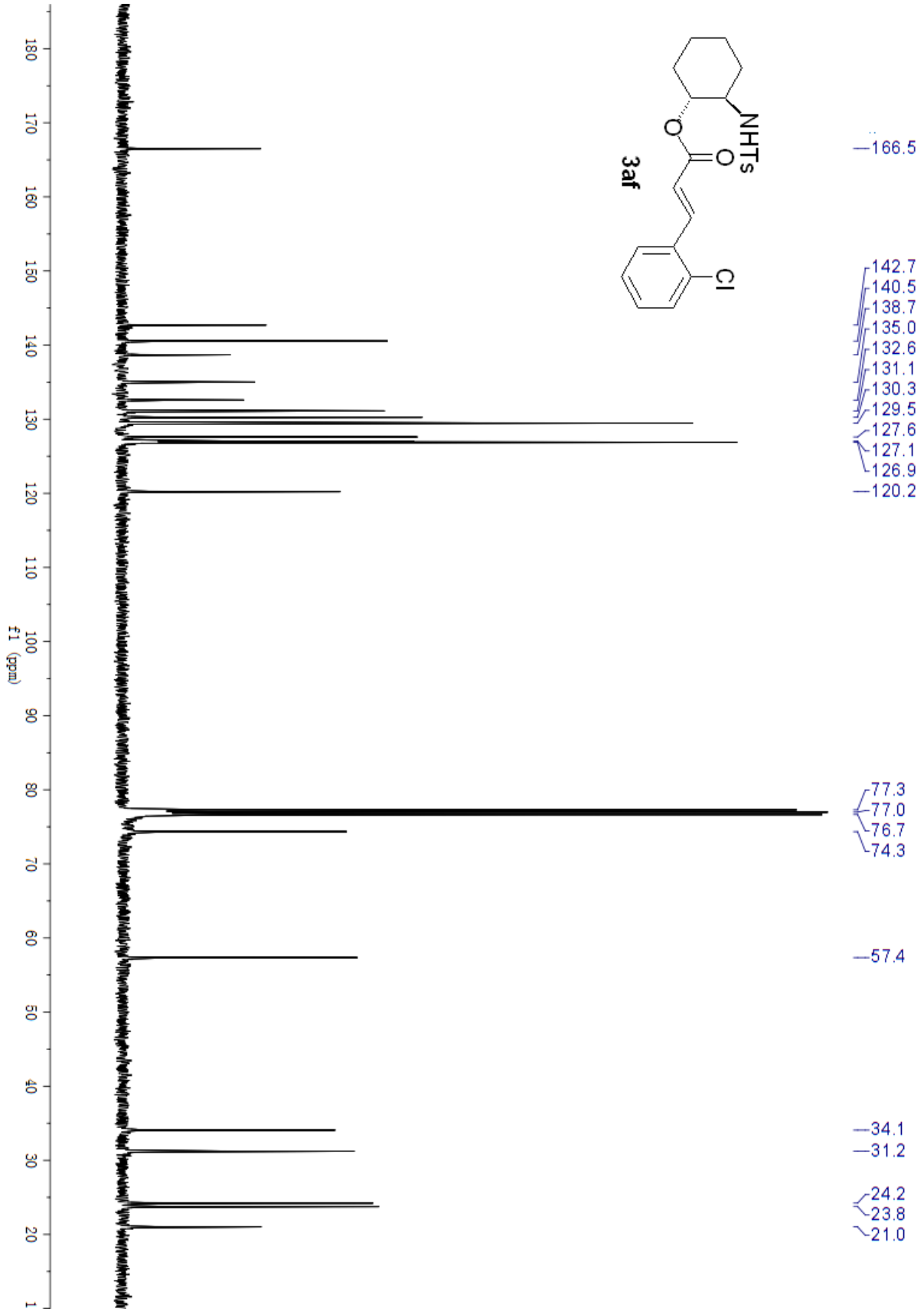

GYQ20141205-2-38-1
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
70
65
60
55
50
45
40
35
30
25
20
15
10
3430.5
3321.6
3046.4
2926.4
2858.8
2809.7
1889.5
1794.1
1772.8
1698.1
1627.1
1601.1
1554.7
1527.1
1495.0
1445.9
1418.8
1400.1
1363.6
1325.8
1304.3
1289.7
1262.5
1223.3
1177.8
1159.2
1090.0
1059.2
1047.7
1035.7
1020.7
1004.7
982.6
946.6
920.7
903.1
862.3
838.2
814.4
755.0
705.3
663.6
569.3
548.9
531.2
517.1
501.7
NHTs
O
O
NMe2
3ad

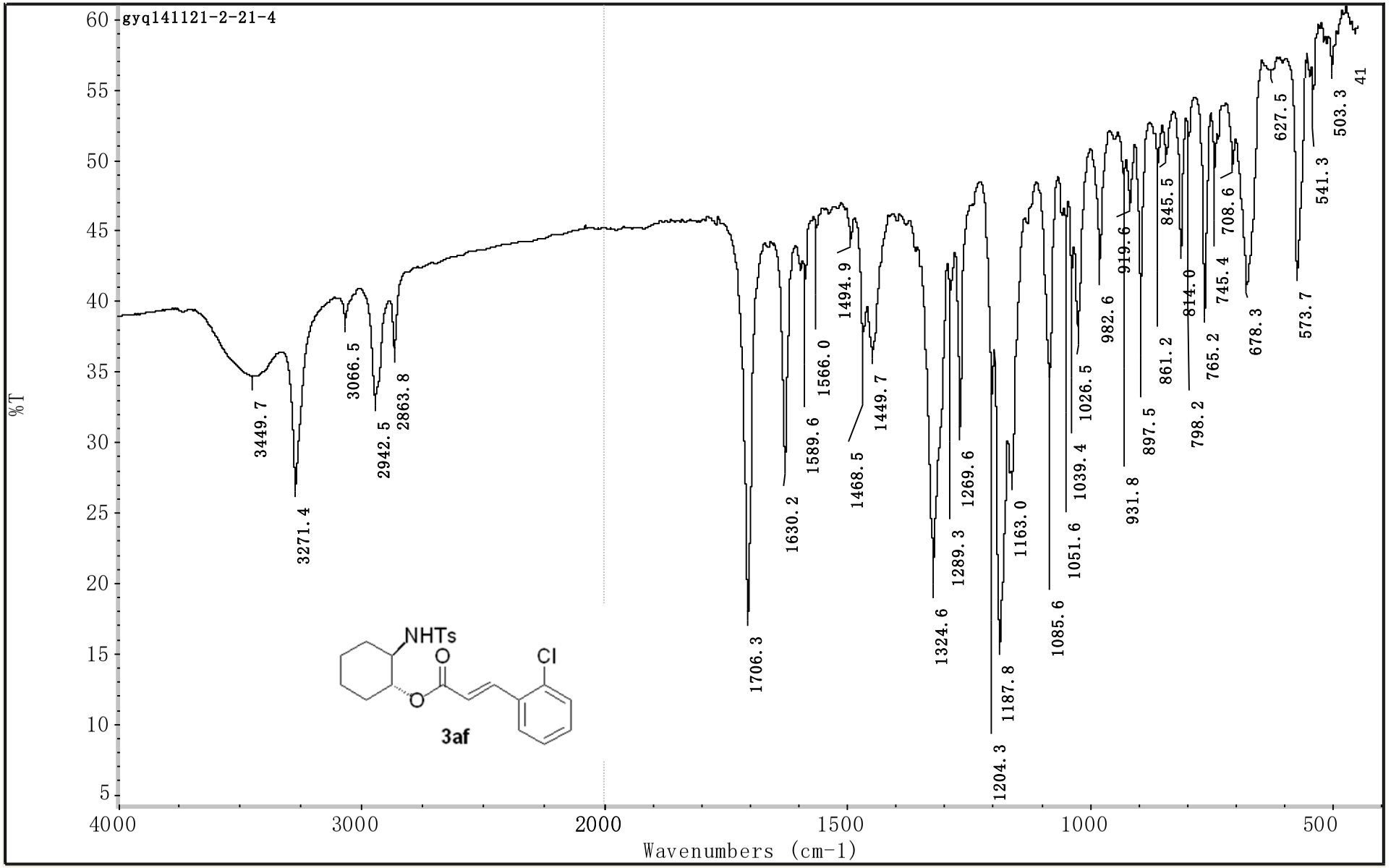

7.721
7.701
7.462
7.422
7.367
7.344
7.344
7.282
7.147
7.128
6.017
5.977
5.376
5.356
4.736
4.726
4.711
4.701
4.687
4.676
3.336
3.326
3.308
3.292
3.284
3.267
3.255
2.164
2.123
2.091
2.012
1.985
1.722
1.708
1.680
1.666
1.379
1.358
1.327
1.298
1.273
0.000
1.93
5.14
2.01
1.00
0.94
0.97
0.99
2.79
1.28
1.39
2.05
4.07
f1 (ppm)
NHTs
O
O
Cl
3ae

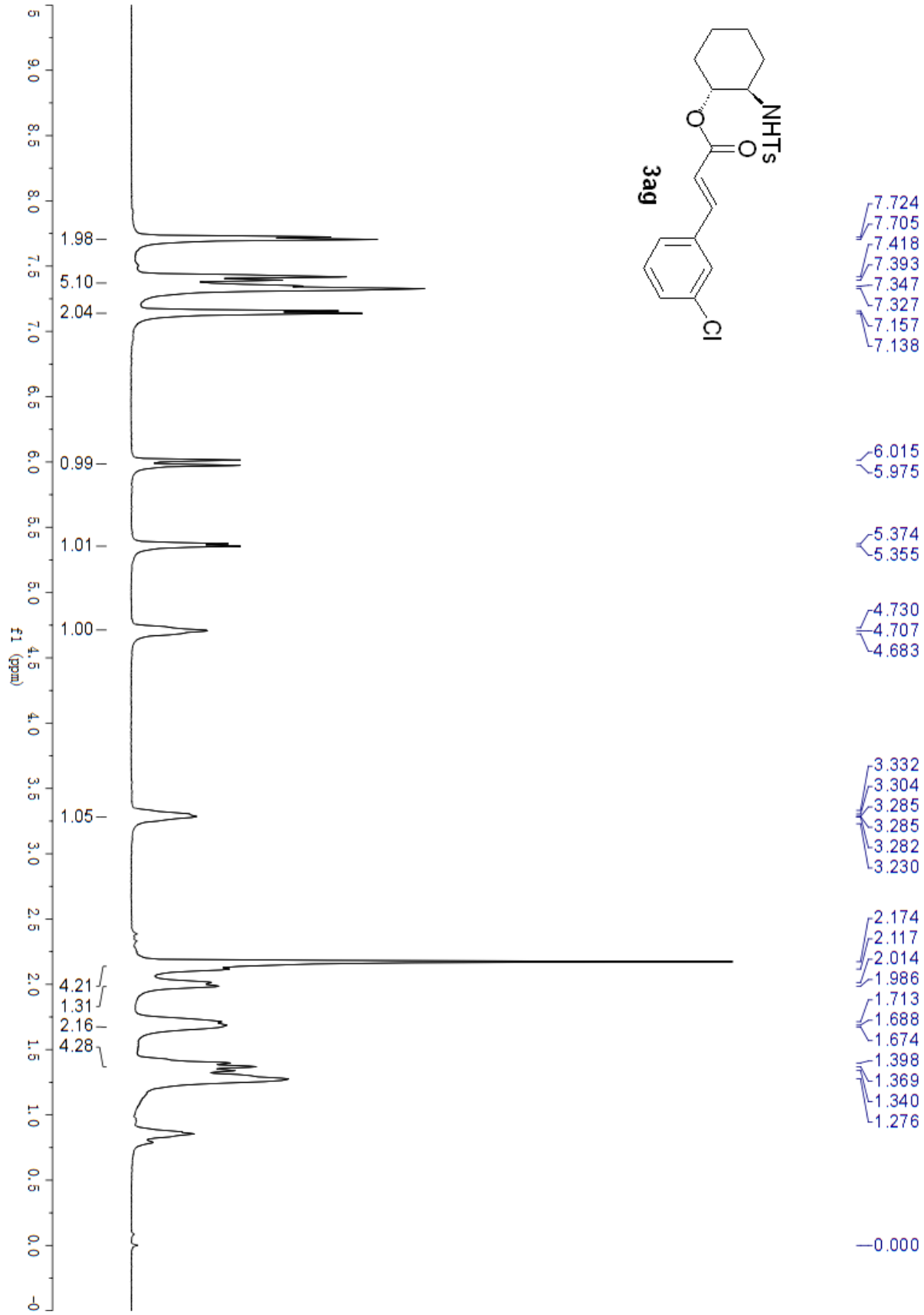

3ae
NHTs
O
O
Cl
166.8
143.4
142.7
138.7
136.3
132.8
129.5
129.3
129.2
126.9
118.3
77.4
77.1
76.8
74.4
57.1
33.8
31.2
24.3
23.7
21.3
f1 (ppm)

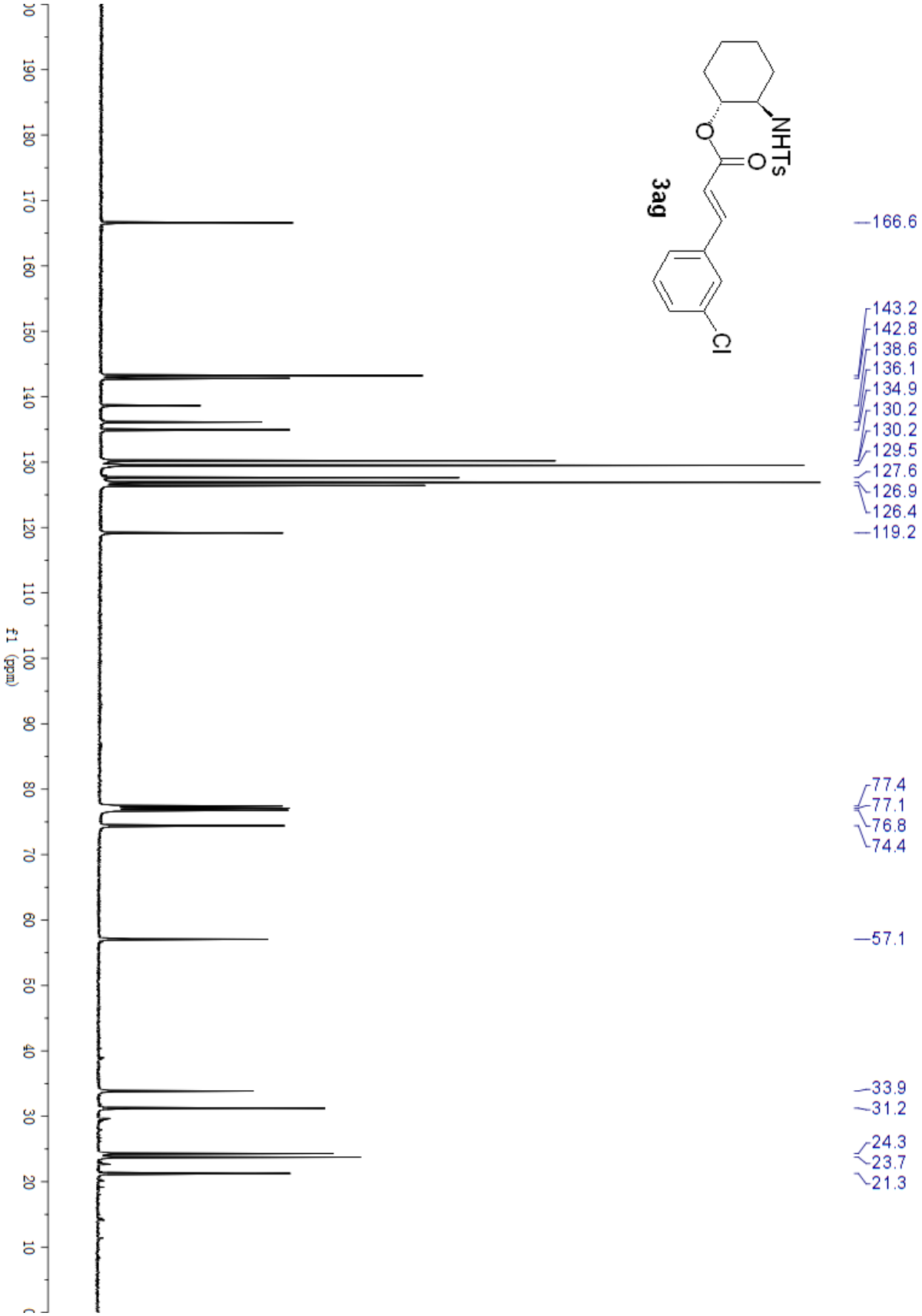

gyq20141211-2-21-3
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3426.7
3278.3
3089.4
3065.3
3029.7
2940.3
2861.7
1907.3
1719.9
1688.0
1636.0
1628.0
1592.6
1567.3
1491.6
1465.1
1449.7
1406.6
1363.5
1348.5
1324.9
1308.0
1287.7
1273.1
1253.9
1203.2
1195.3
1182.1
1174.9
1159.8
1092.2
1060.0
1024.6
1011.5
988.6
952.5
918.6
902.9
871.1
859.8
841.8
824.2
811.0
746.0
705.4
664.1
634.6
571.1
547.5
505.4
494.4
464.0
443.2
NHTs
O
O
Cl
3ae

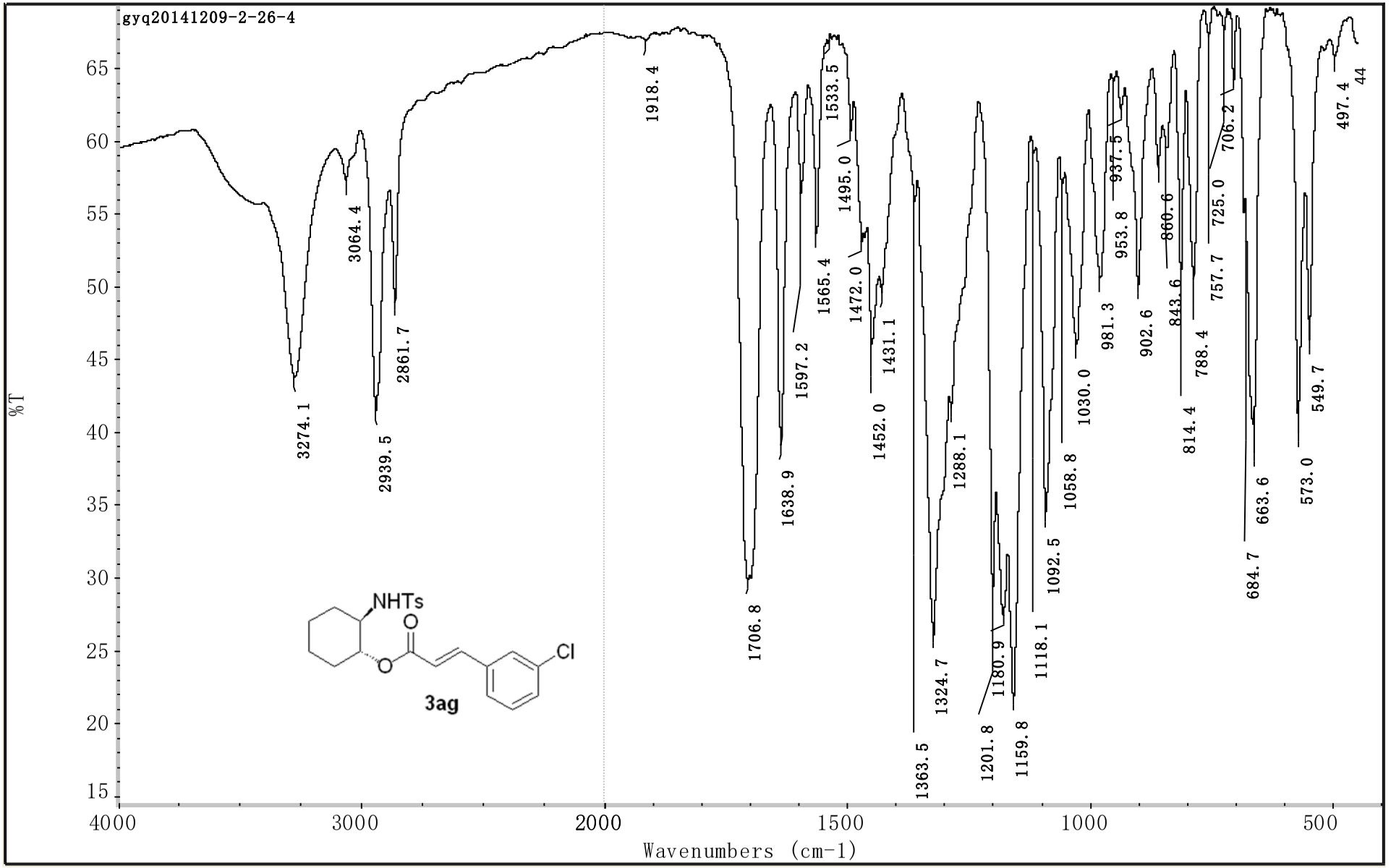

3af
NHTs
O
O
Cl
f1 (ppm)
1.01
2.01
1.02
1.02
2.16
1.98
1.00
0.95
1.08
1.05
1.04
2.97
1.22
2.49
4.34
7.844
7.804
7.707
7.686
7.522
7.518
7.504
7.499
7.454
7.450
7.434
7.431
7.358
7.354
7.340
7.335
7.321
7.315
7.311
7.296
7.292
7.277
7.265
7.138
7.118
5.994
5.954
4.978
4.960
4.742
4.731
4.716
4.705
4.690
4.679
3.331
3.313
3.306
3.297
3.288
3.260
2.068
2.001
1.969
1.739
1.708
1.664
1.405
1.377
1.344
1.322
1.296
1.269
0.000

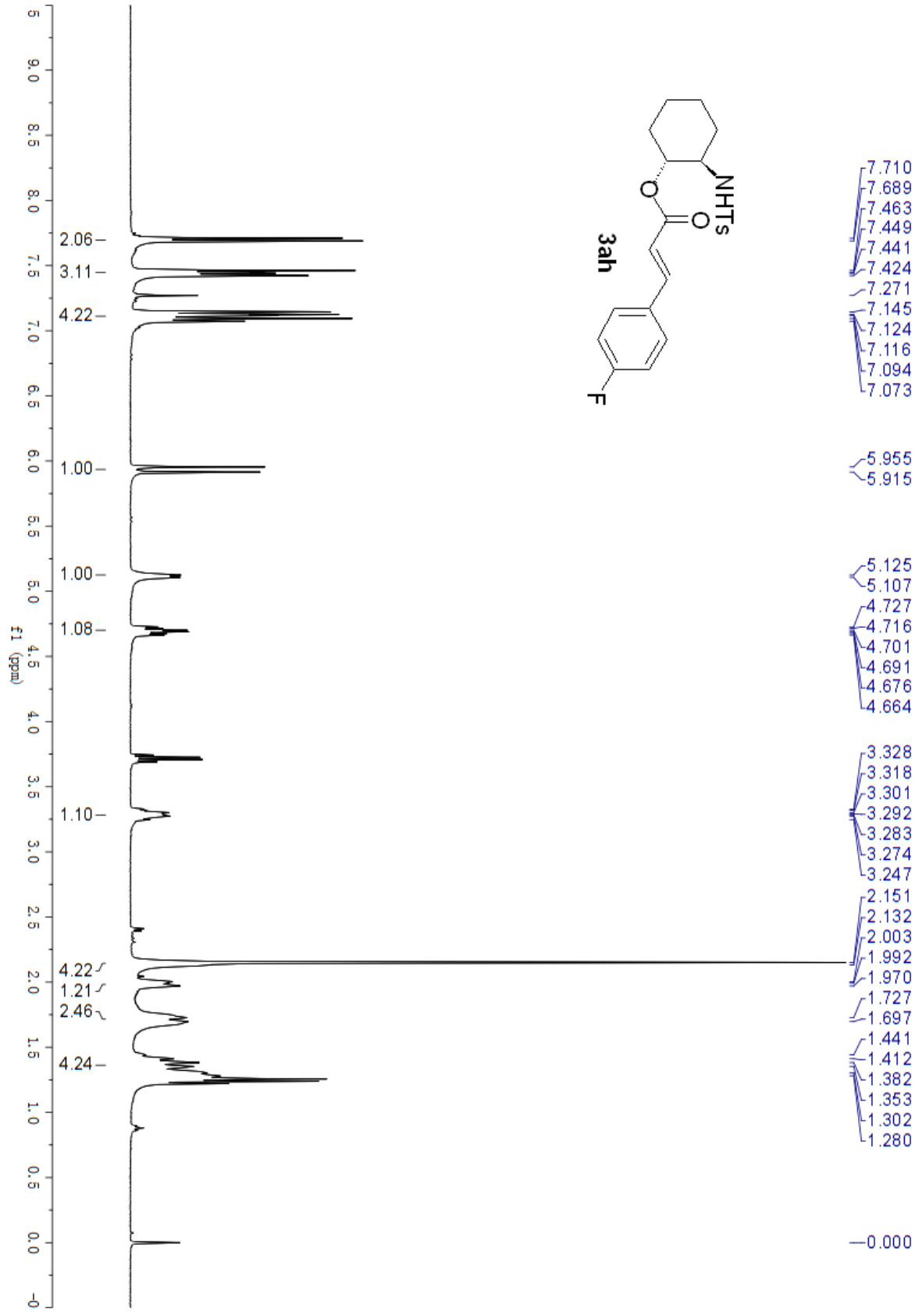

3af
NHTs
O
O
Cl
166.5
142.7
140.5
138.7
135.0
132.6
131.1
130.3
129.5
127.6
127.1
126.9
120.2
77.3
77.0
76.7
74.3
57.4
34.1
31.2
24.2
23.8
21.0
f1 (ppm)

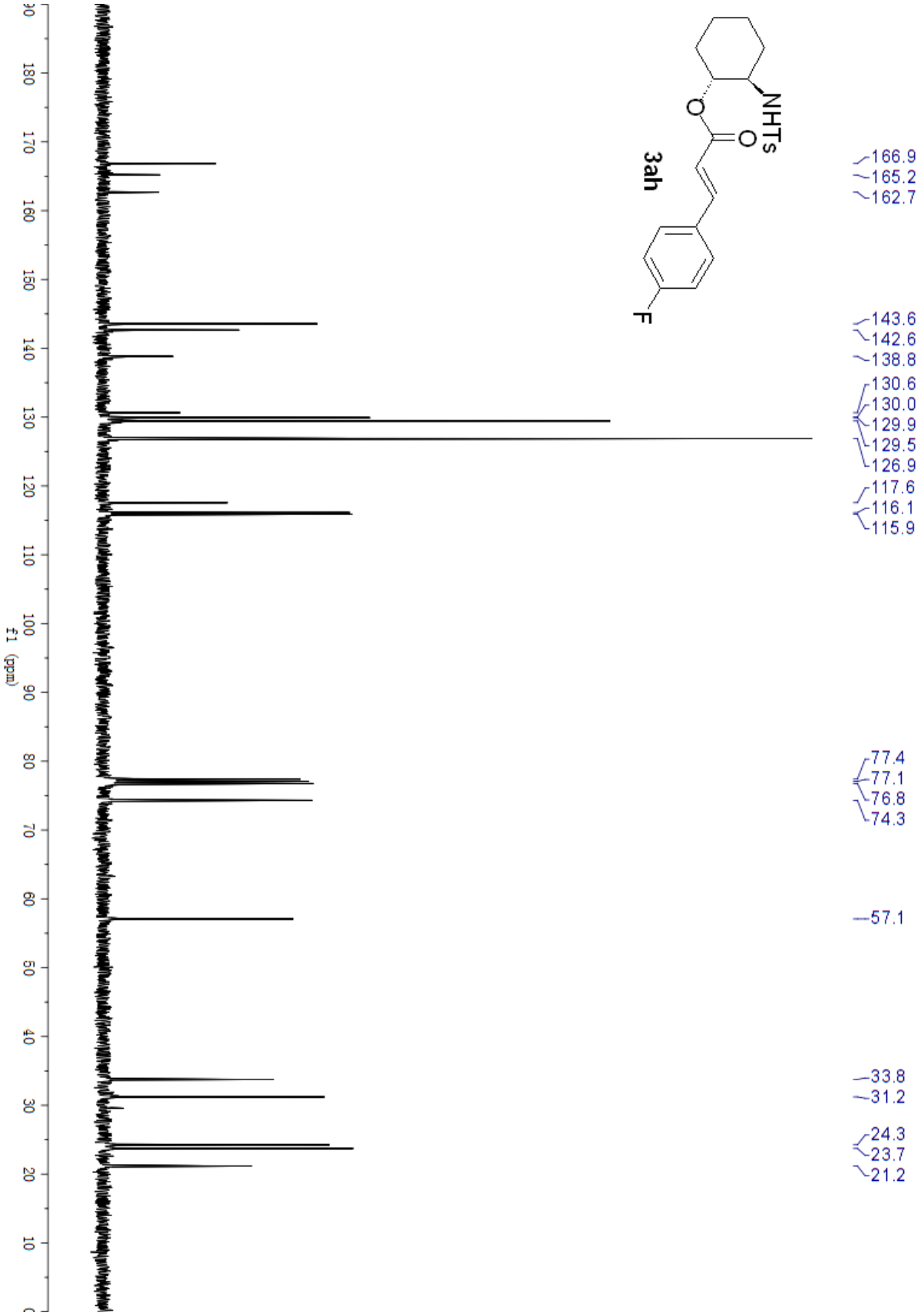

gyq141121-2-21-4
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
60
55
50
45
40
35
30
25
20
15
10
5
3449.7
3271.4
3066.5
2942.5
2863.8
1706.3
1630.2
1589.6
1566.0
1494.9
1468.5
1449.7
1324.6
1289.3
1269.6
1204.3
1187.8
1163.0
1085.6
1051.6
1039.4
1026.5
982.6
931.8
919.6
897.5
861.2
845.5
814.0
798.2
765.2
745.4
708.6
678.3
627.5
573.7
541.3
503.3
41
NHTs
O
Cl
O
3af

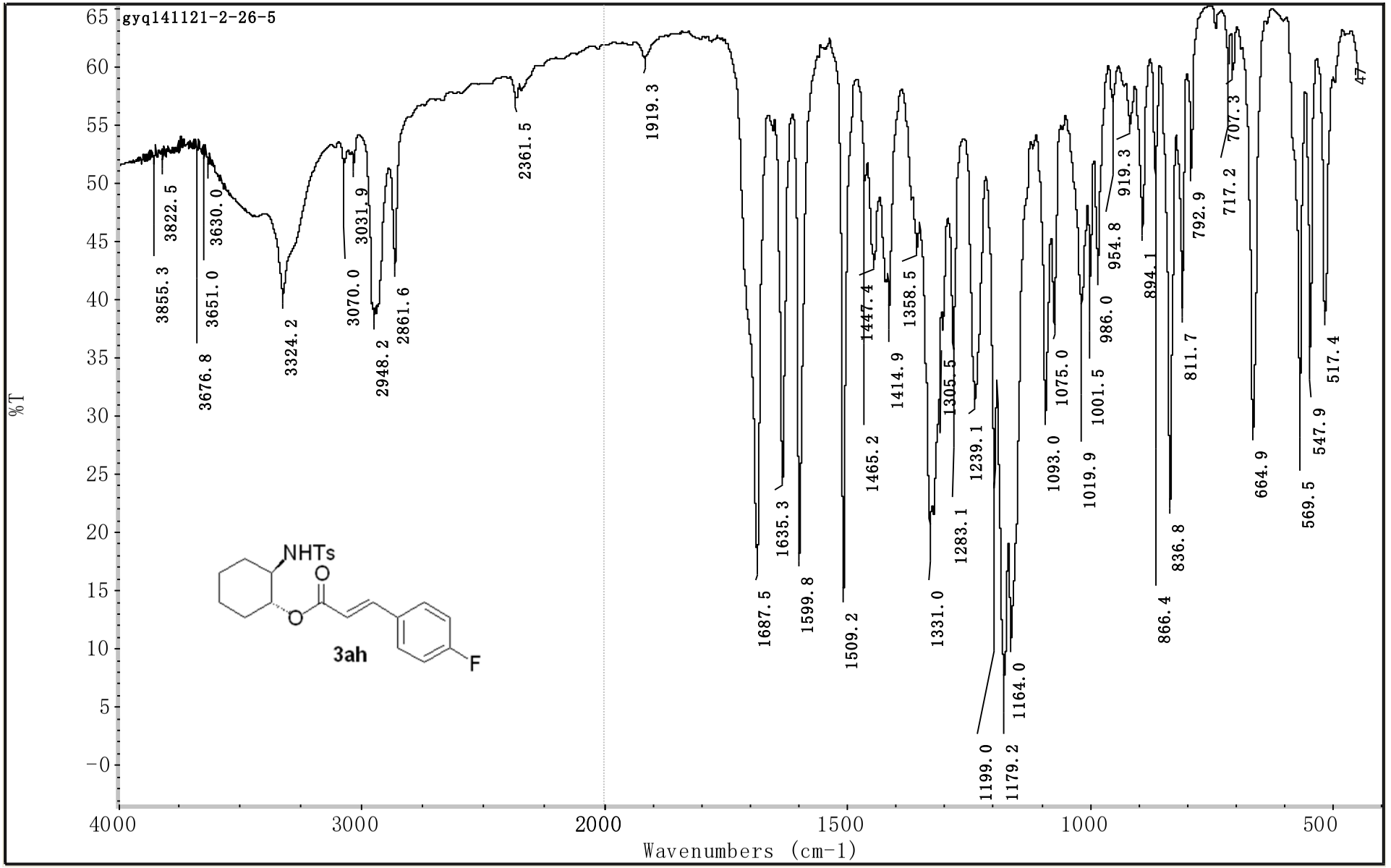

3ag
NHTs
O
O
Cl
f1 (ppm)
1.98
5.10
2.04
0.99
1.01
1.00
1.05
4.21
1.31
2.16
4.28
7.724
7.705
7.418
7.393
7.347
7.327
7.157
7.138
6.015
5.975
5.374
5.355
4.730
4.707
4.683
3.332
3.304
3.285
3.285
3.282
3.230
2.174
2.117
2.014
1.986
1.713
1.688
1.674
1.398
1.369
1.340
1.276
0.000

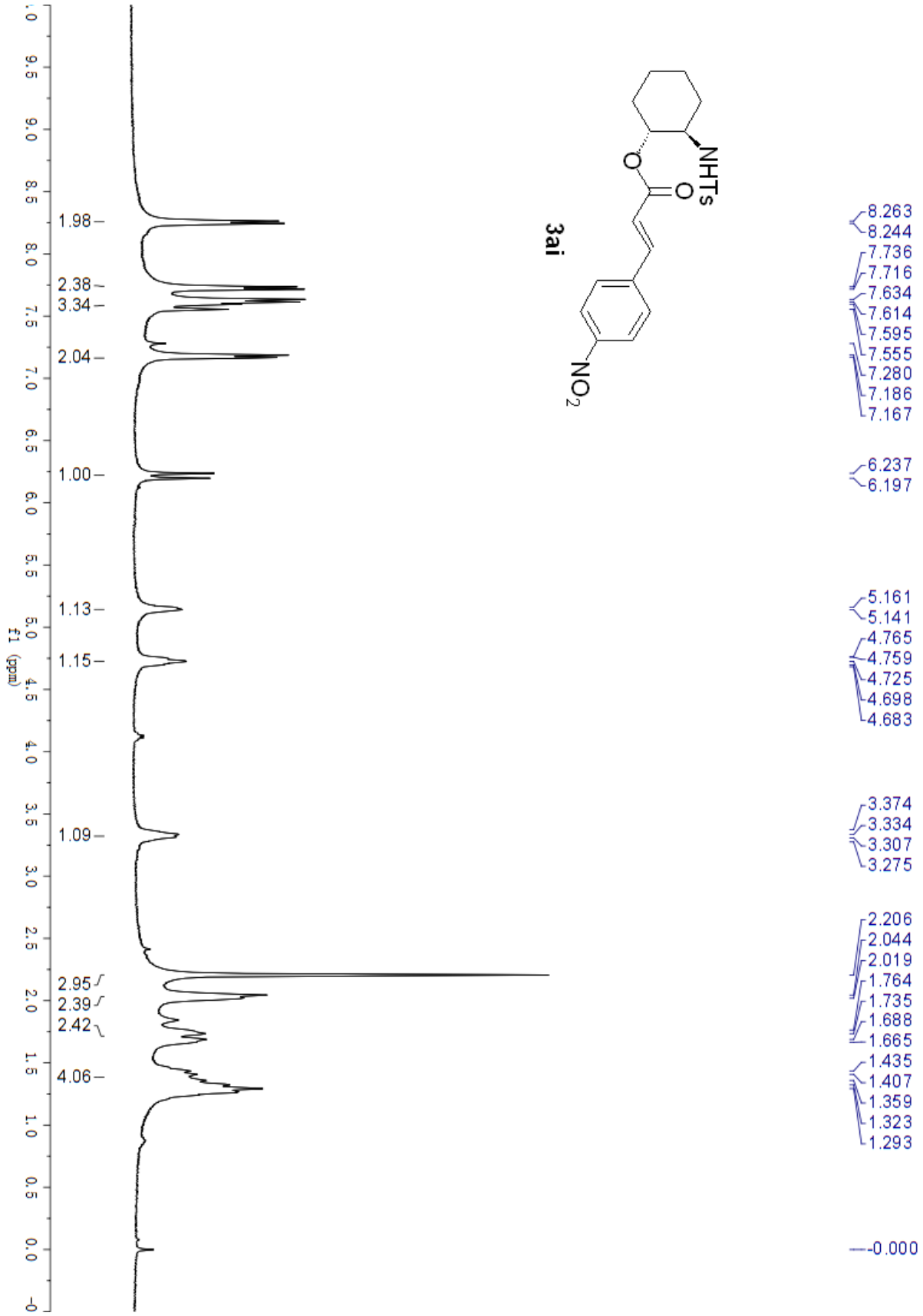

3ag
NHTs
O
O
Cl
166.6
143.2
142.8
138.6
136.1
134.9
130.2
130.2
129.5
127.6
126.9
126.4
119.2
77.4
77.1
76.8
74.4
57.1
33.9
31.2
24.3
23.7
21.3
f1 (ppm)

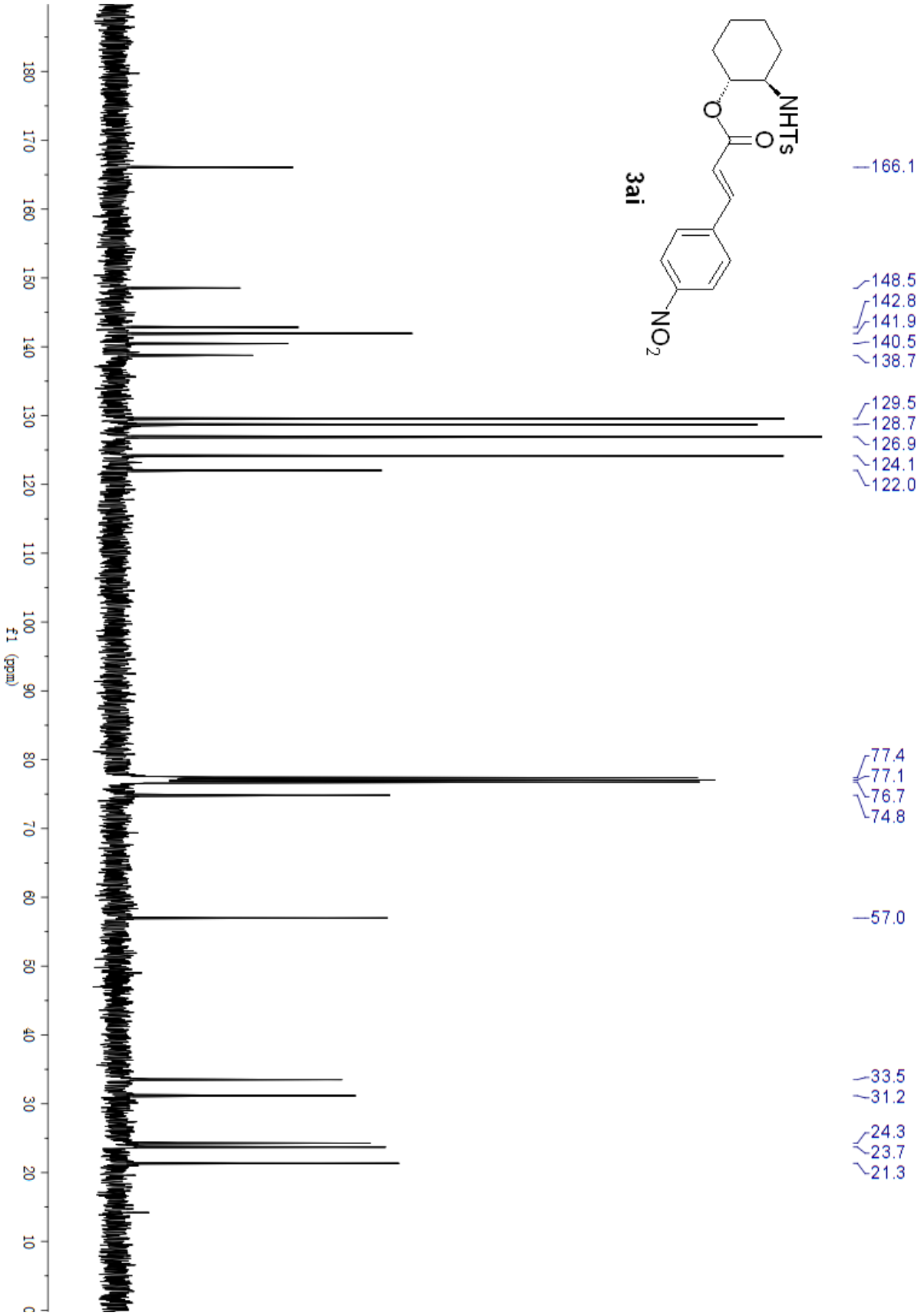

gyq20141209-2-26-4
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
65
60
55
50
45
40
35
30
25
20
15
3274.1
3064.4
2939.5
2861.7
1918.4
1706.8
1638.9
1597.2
1565.4
1533.5
1495.0
1472.0
1452.0
1431.1
1363.5
1324.7
1288.1
1201.8
1180.9
1159.8
1118.1
1092.5
1058.8
1030.0
981.3
953.8
937.5
902.6
860.6
843.6
814.4
788.4
757.7
725.0
706.2
684.7
663.6
573.0
549.7
497.4
44
NHTs
O
O
Cl
3ag

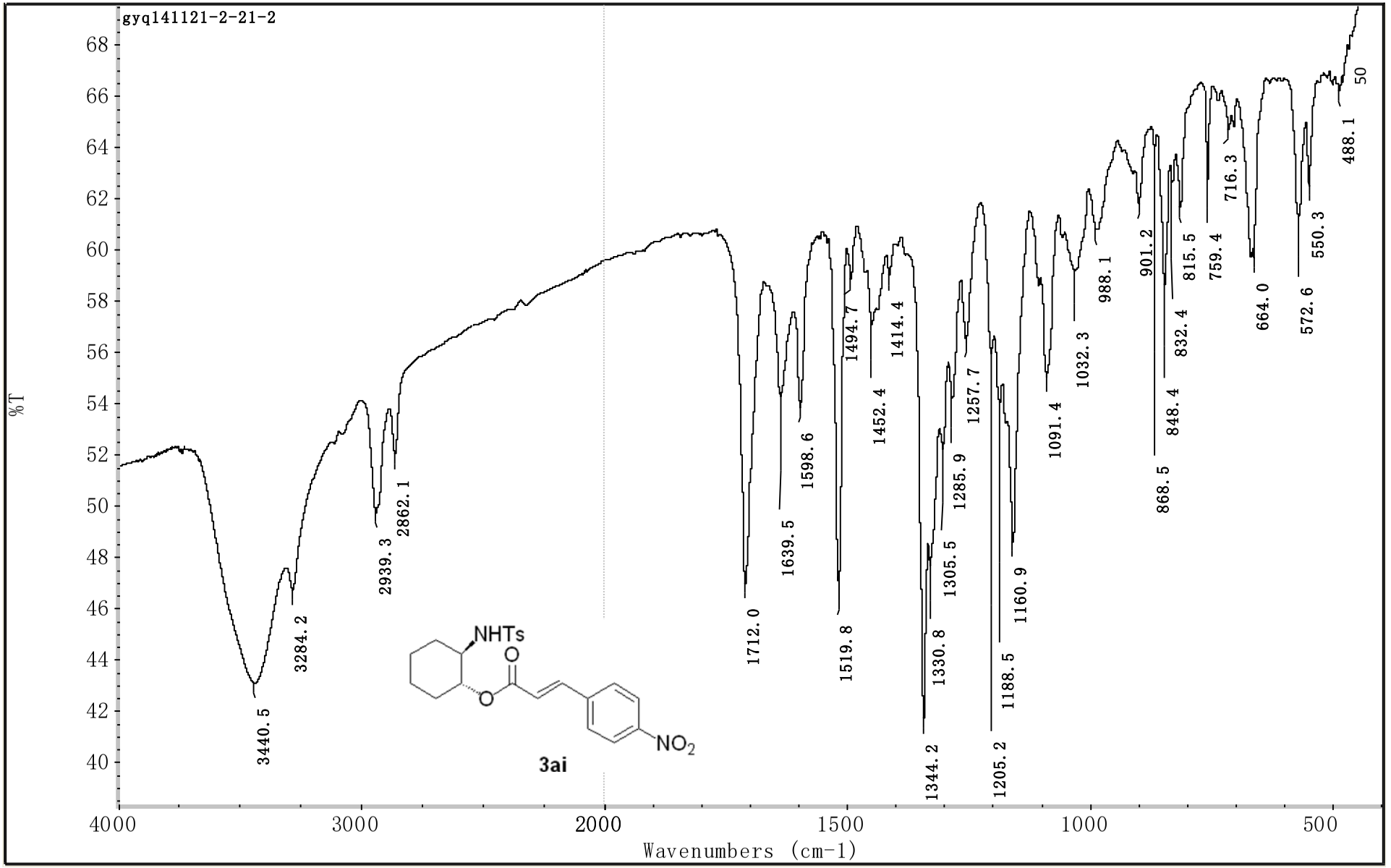

3ah
NHTs
O
O
F
7.710
7.689
7.463
7.449
7.441
7.424
7.271
7.145
7.124
7.116
7.094
7.073
5.955
5.915
5.125
5.107
4.727
4.716
4.701
4.691
4.676
4.664
3.328
3.318
3.301
3.292
3.283
3.274
3.247
2.151
2.132
2.003
1.992
1.970
1.727
1.697
1.441
1.412
1.382
1.353
1.302
1.280
0.000
2.06
3.11
4.22
1.00
1.00
1.08
1.10
4.22
1.21
2.46
4.24
f1 (ppm)

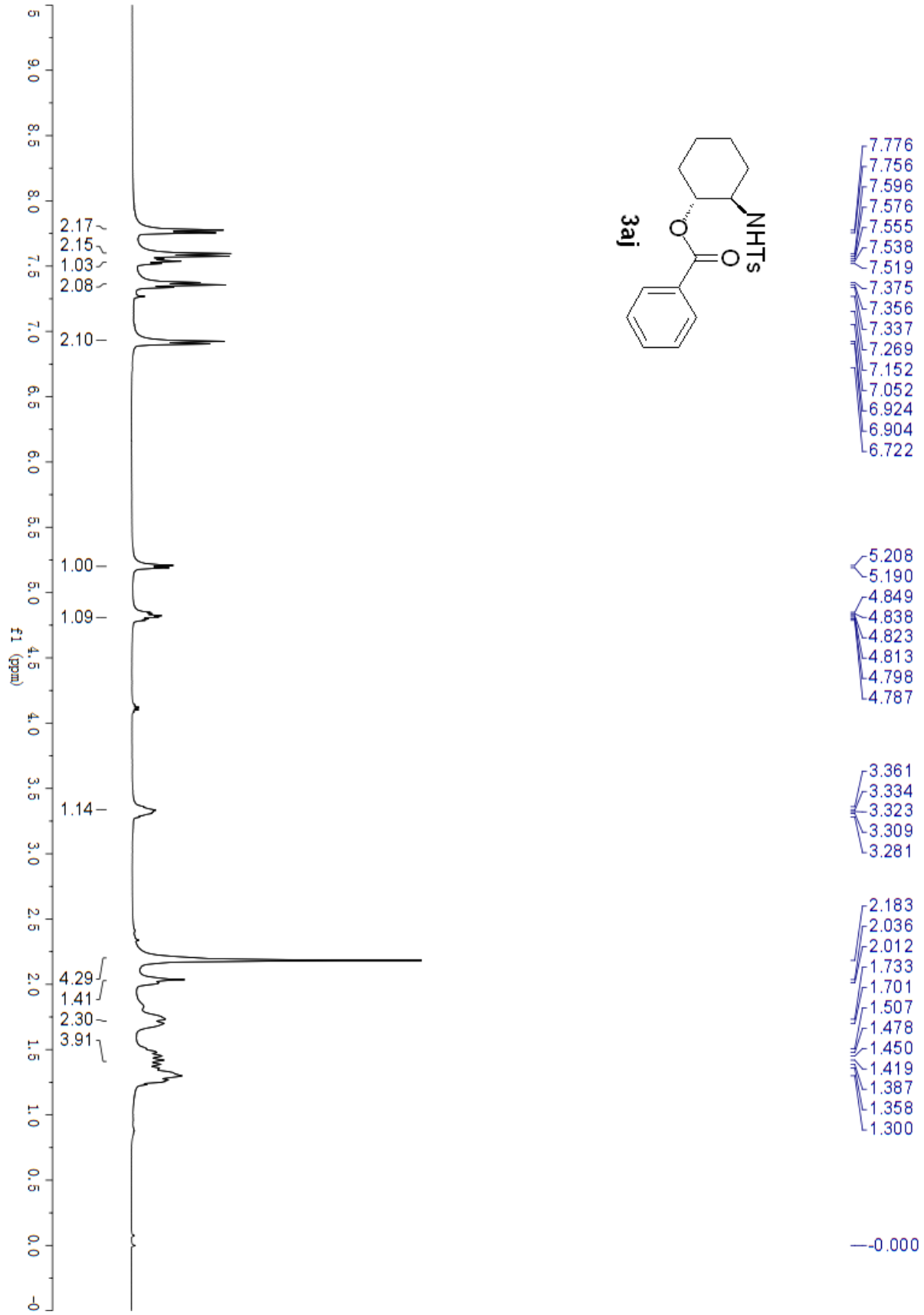

3ah
NHTs
O
O
F
166.9
165.2
162.7
143.6
142.6
138.8
130.6
130.0
129.9
129.5
126.9
117.6
116.1
115.9
77.4
77.1
76.8
74.3
57.1
33.8
31.2
24.3
23.7
21.2
f1 (ppm)

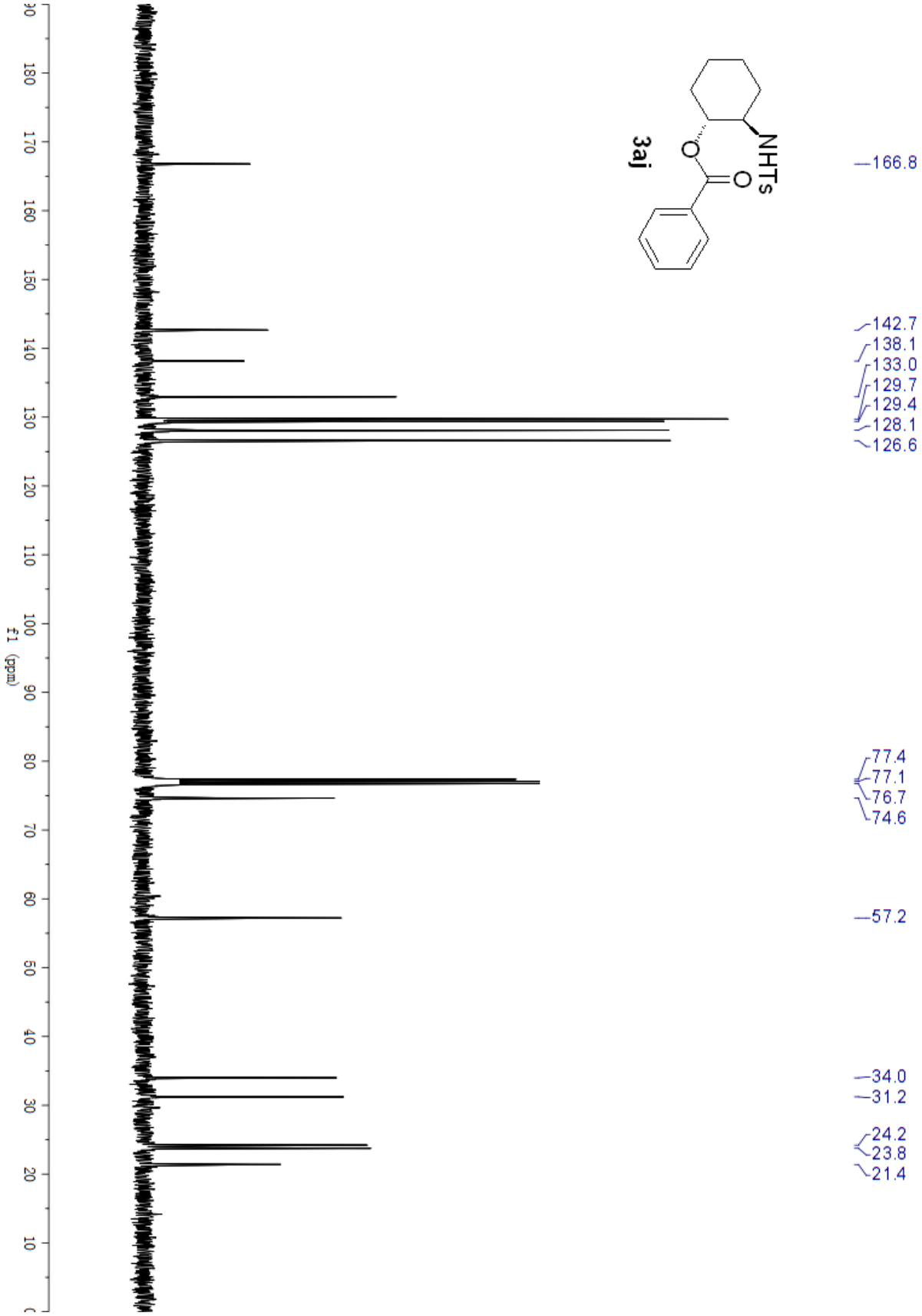

gyq141121-2-26-5
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
65
60
55
50
45
40
35
30
25
20
15
10
5
-0
3855.3
3822.5
3676.8
3651.0
3630.0
3324.2
3070.0
3031.9
2948.2
2861.6
2361.5
1919.3
1687.5
1635.3
1599.8
1509.2
1465.2
1447.4
1414.9
1358.5
1331.0
1305.5
1283.1
1239.1
1199.0
1179.2
1164.0
1093.0
1075.0
1019.9
1001.5
986.0
954.8
919.3
894.1
866.4
836.8
811.7
792.9
717.2
707.3
664.9
569.5
547.9
517.4
NHTs
O
O
3ah
F

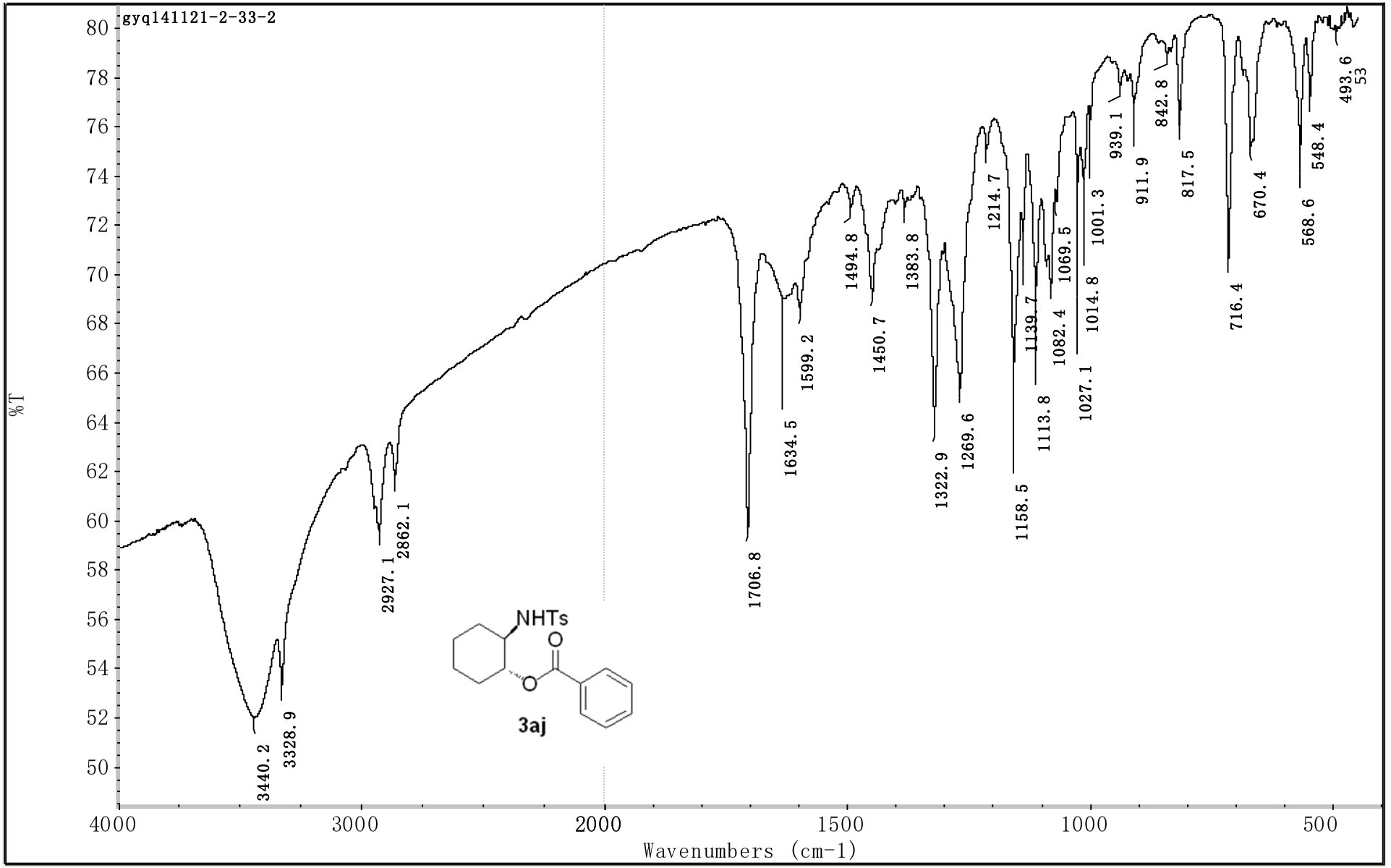

3ai
NHTs
O
O
O
NO2
f1 (ppm)
1.98
2.38
3.34
2.04
1.00
1.13
1.15
1.09
2.95
2.39
2.42
4.06
8.263
8.244
7.736
7.716
7.634
7.614
7.595
7.555
7.280
7.186
7.167
6.237
6.197
5.161
5.141
4.765
4.759
4.725
4.698
4.683
3.374
3.334
3.307
3.275
2.206
2.044
2.019
1.764
1.735
1.688
1.665
1.435
1.407
1.359
1.323
1.293
0.000

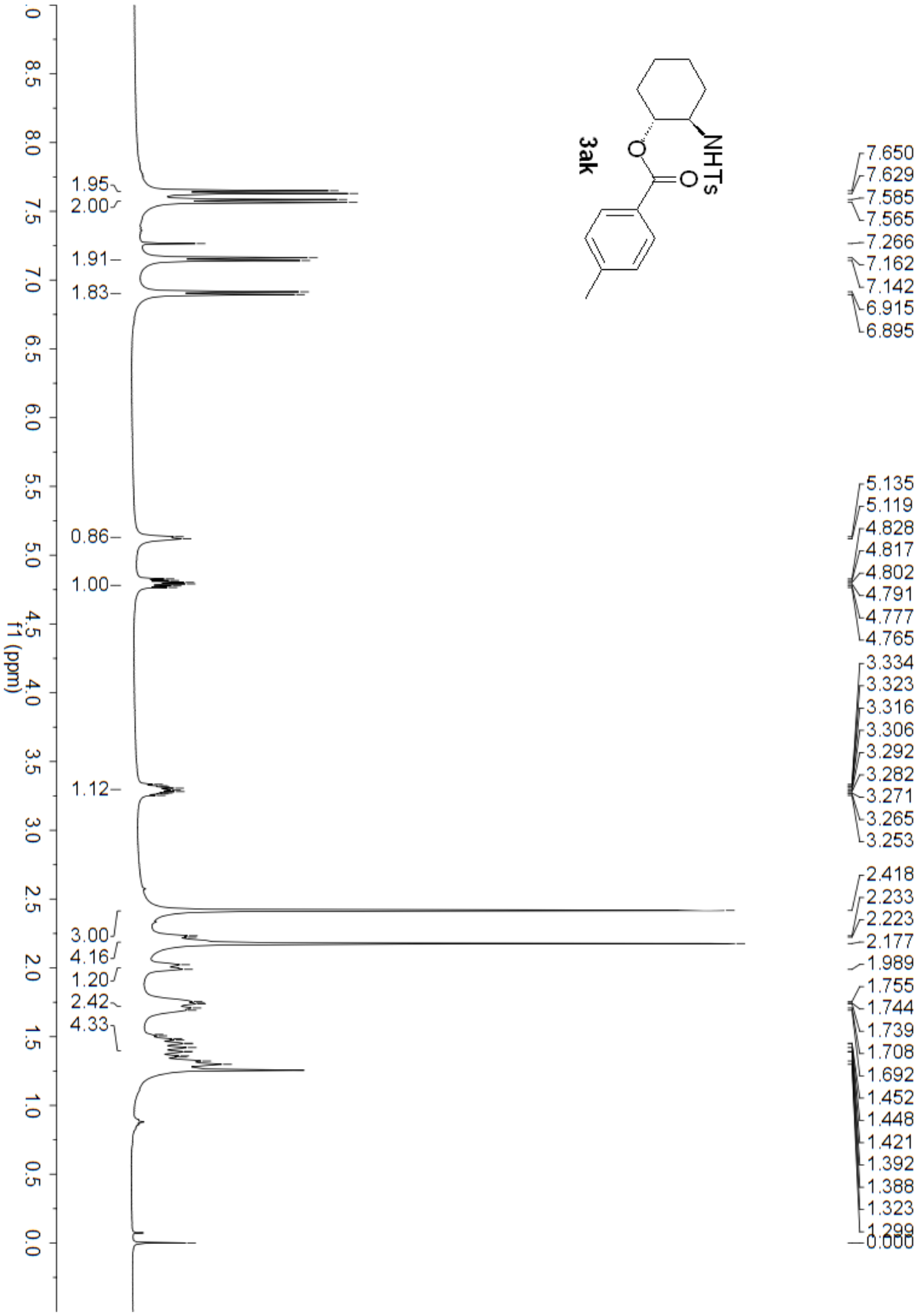

3ai
NHTs
O
O
NO2
166.1
148.5
142.8
141.9
140.5
138.7
129.5
128.7
126.9
124.1
122.0
77.4
77.1
76.7
74.8
57.0
33.5
31.2
24.3
23.7
21.3
f1 (ppm)

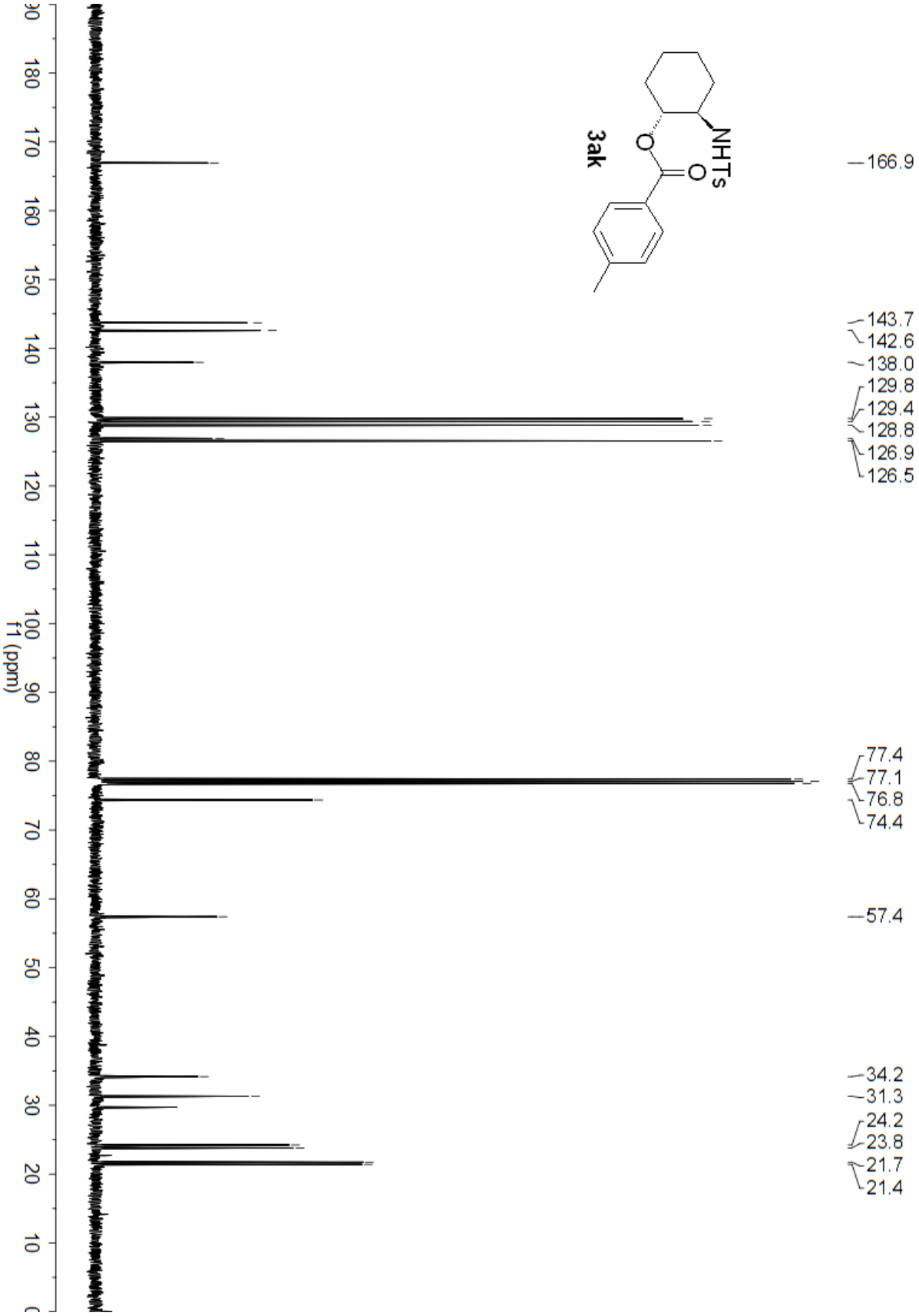

gyq141121-2-21-2
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3440.5
3284.2
2939.3
2862.1
1712.0
1639.5
1598.6
1519.8
1494.7
1452.4
1414.4
1344.2
1330.8
1305.5
1285.9
1257.7
1205.2
1188.5
1160.9
1091.4
1032.3
988.1
901.2
868.5
848.4
832.4
815.5
759.4
716.3
664.0
572.6
550.3
488.1
NHTs
O
O
NO2
3ai

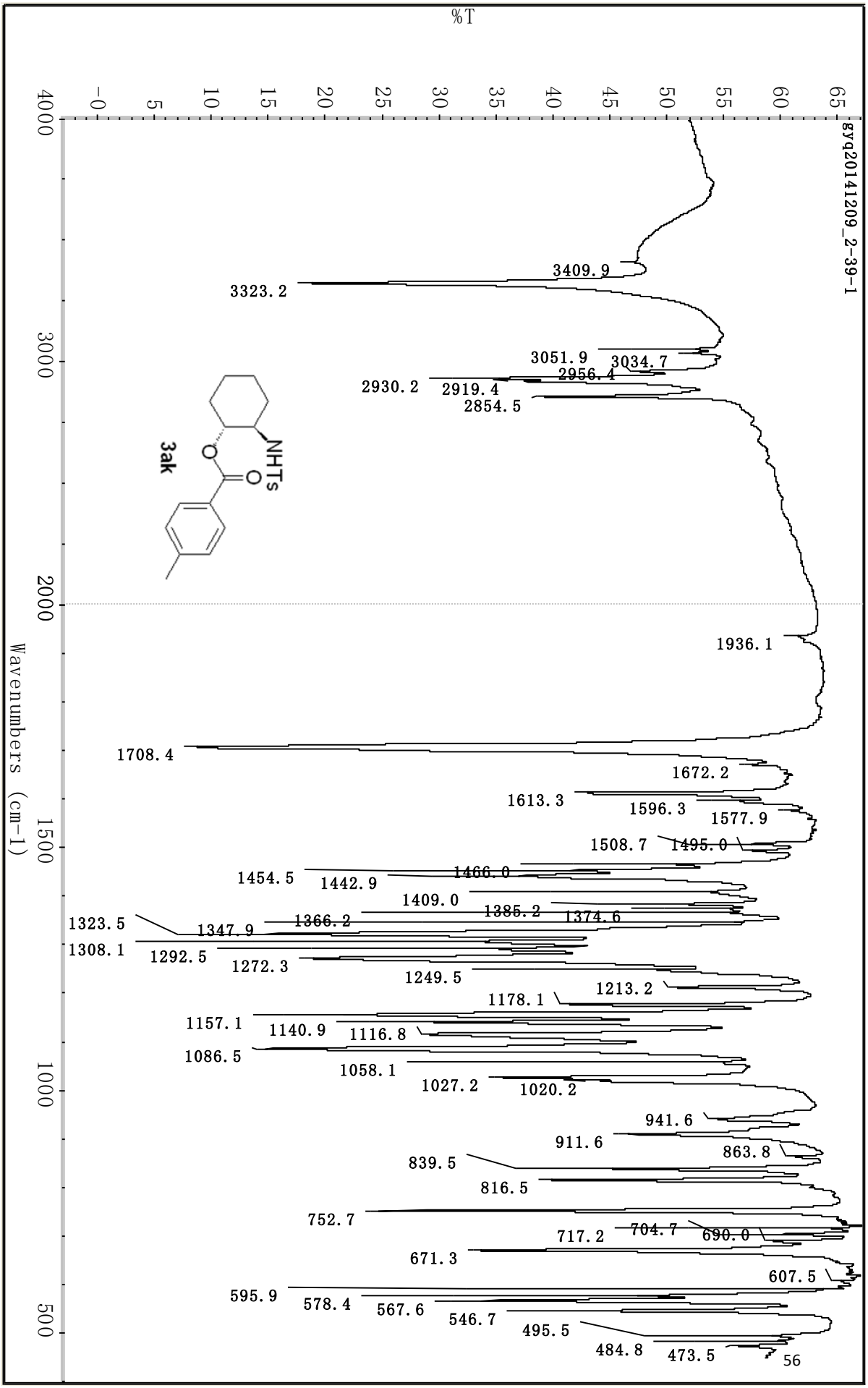

3aj
NHTs
O
O
7.776
7.756
7.596
7.576
7.555
7.538
7.519
7.375
7.356
7.337
7.269
7.152
7.052
6.924
6.904
6.722
5.208
5.190
4.849
4.838
4.823
4.813
4.798
4.787
3.361
3.334
3.323
3.309
3.281
2.183
2.036
2.012
1.733
1.701
1.507
1.478
1.450
1.419
1.387
1.358
1.300
0.000
2.17
2.15
1.03
2.08
2.10
1.00
1.09
1.14
4.29
1.41
2.30
3.91
f1 (ppm)

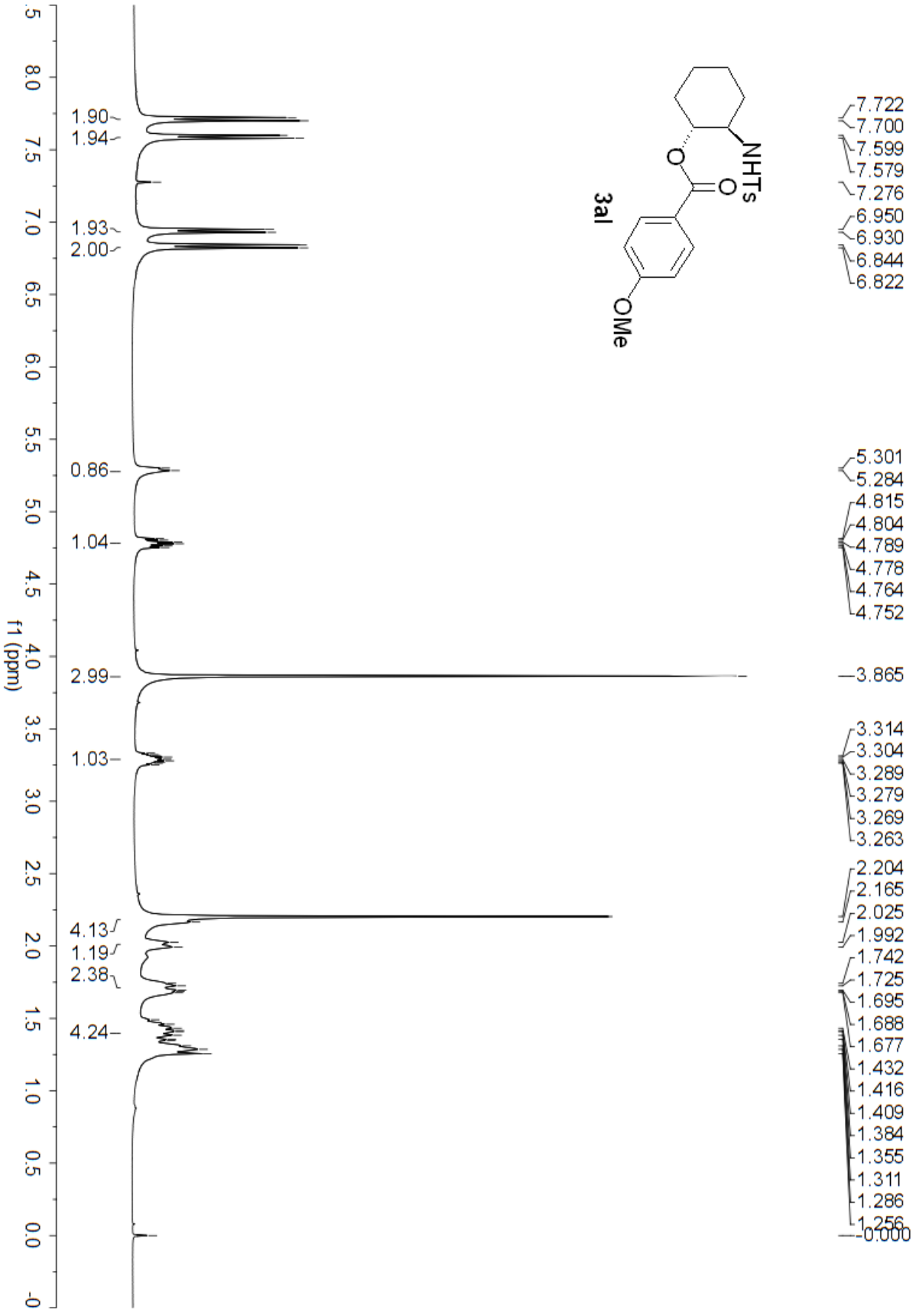

3aj
NHTs
O
O
166.8
142.7
138.1
133.0
129.7
129.4
128.1
126.6
77.4
77.1
76.7
74.6
57.2
34.0
31.2
24.2
23.8
21.4
f1 (ppm)

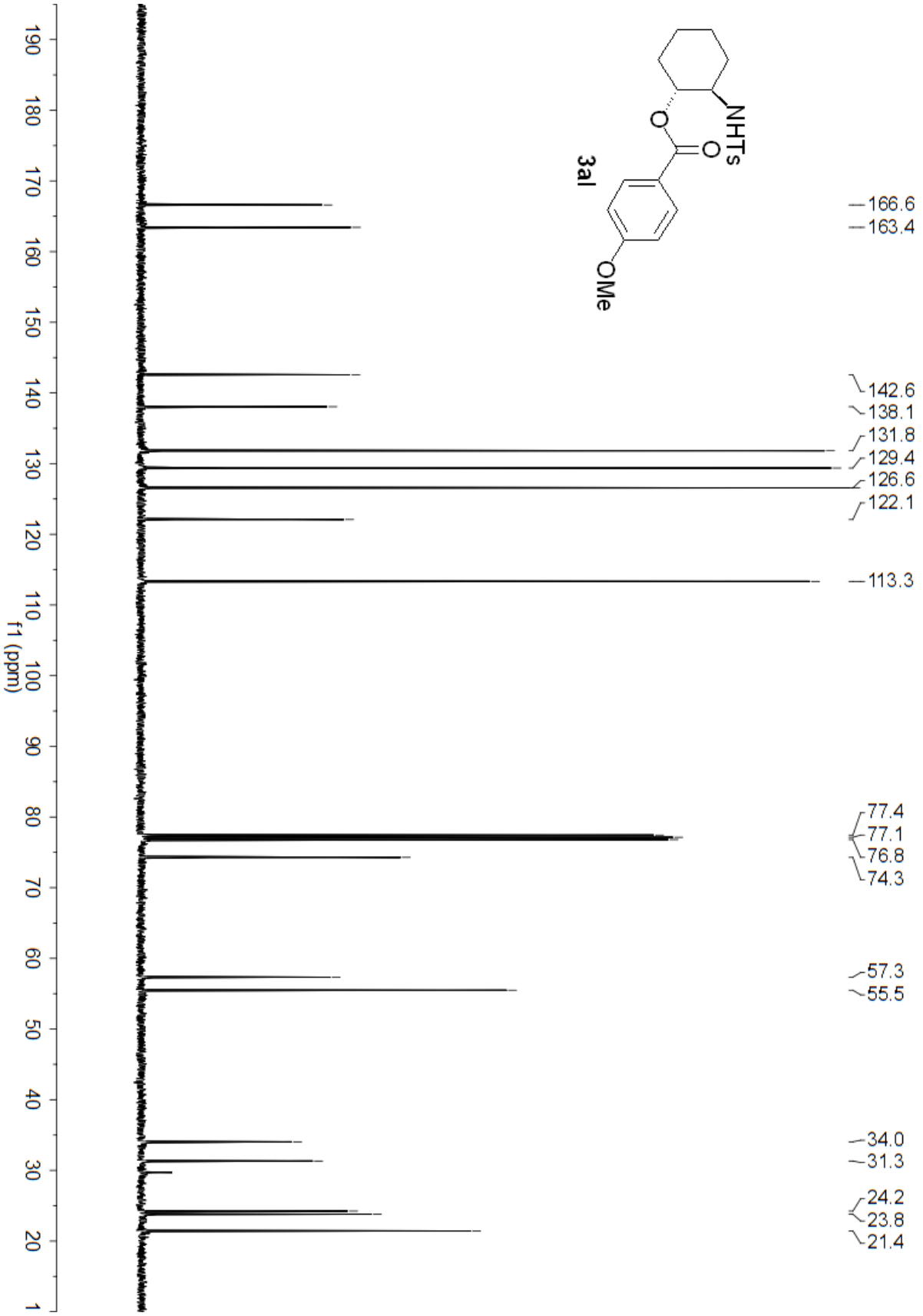

gyq141121-2-33-2
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
80
78
76
74
72
70
68
66
64
62
60
58
56
54
52
50
3440.2
3328.9
2927.1
2862.1
1706.8
1634.5
1599.2
1494.8
1450.7
1383.8
1322.9
1269.6
1214.7
1158.5
1139.7
1113.8
1082.4
1069.5
1027.1
1014.8
1001.3
939.1
911.9
842.8
817.5
716.4
670.4
568.6
548.4
493.6
53
NHTs
O
O
3aj

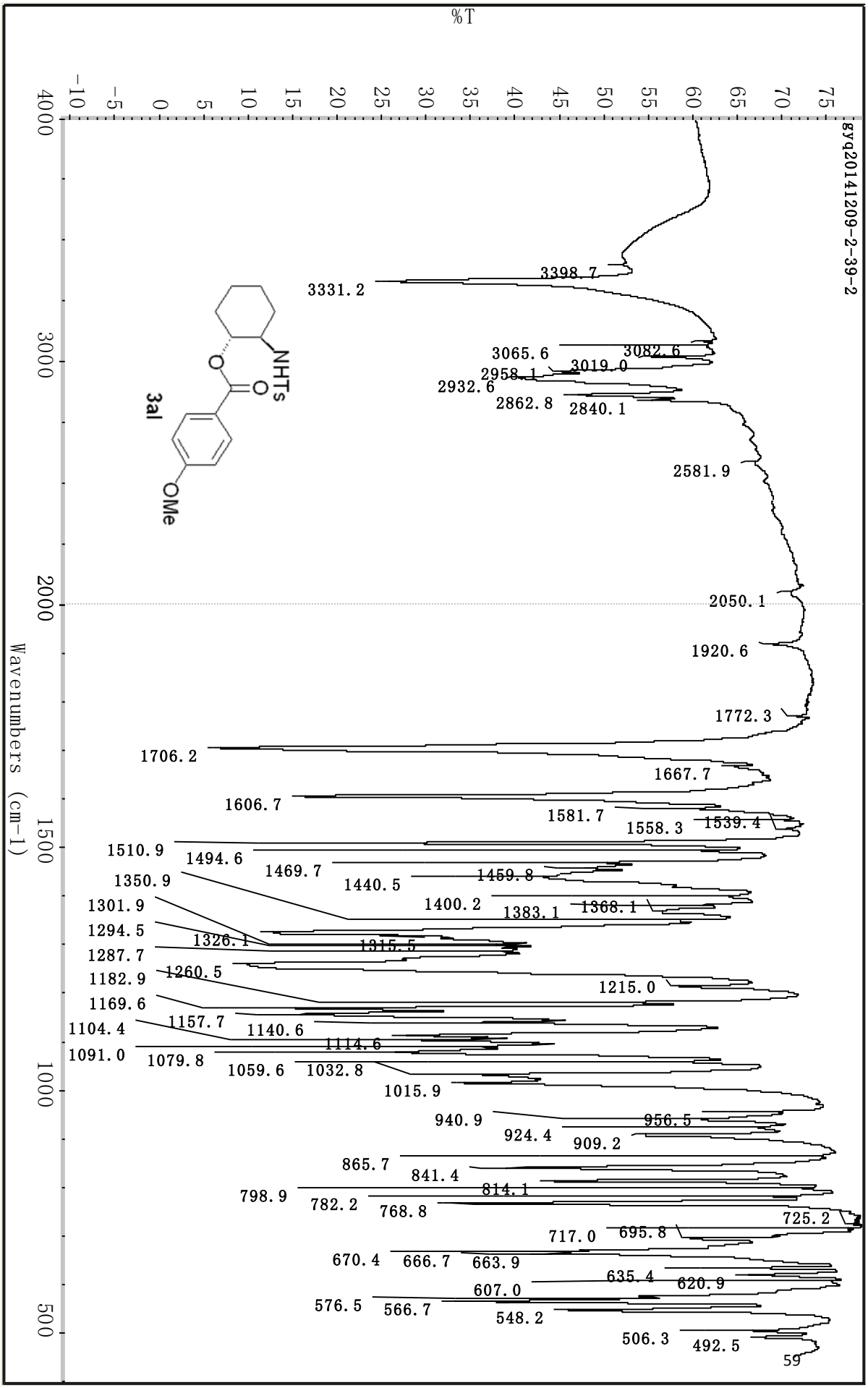

3ak
NHTs
O
O
7.650
7.629
7.585
7.565
7.266
7.162
7.142
6.915
6.895
5.135
5.119
4.828
4.817
4.802
4.791
4.777
4.765
3.334
3.323
3.316
3.306
3.292
3.282
3.271
3.265
3.253
2.418
2.233
2.223
2.177
1.989
1.755
1.744
1.739
1.708
1.692
1.452
1.448
1.421
1.392
1.388
1.323
1.299
0.000
1.95
2.00
1.91
1.83
0.86
1.00
1.12
3.00
4.16
1.20
2.42
4.33
f1 (ppm)

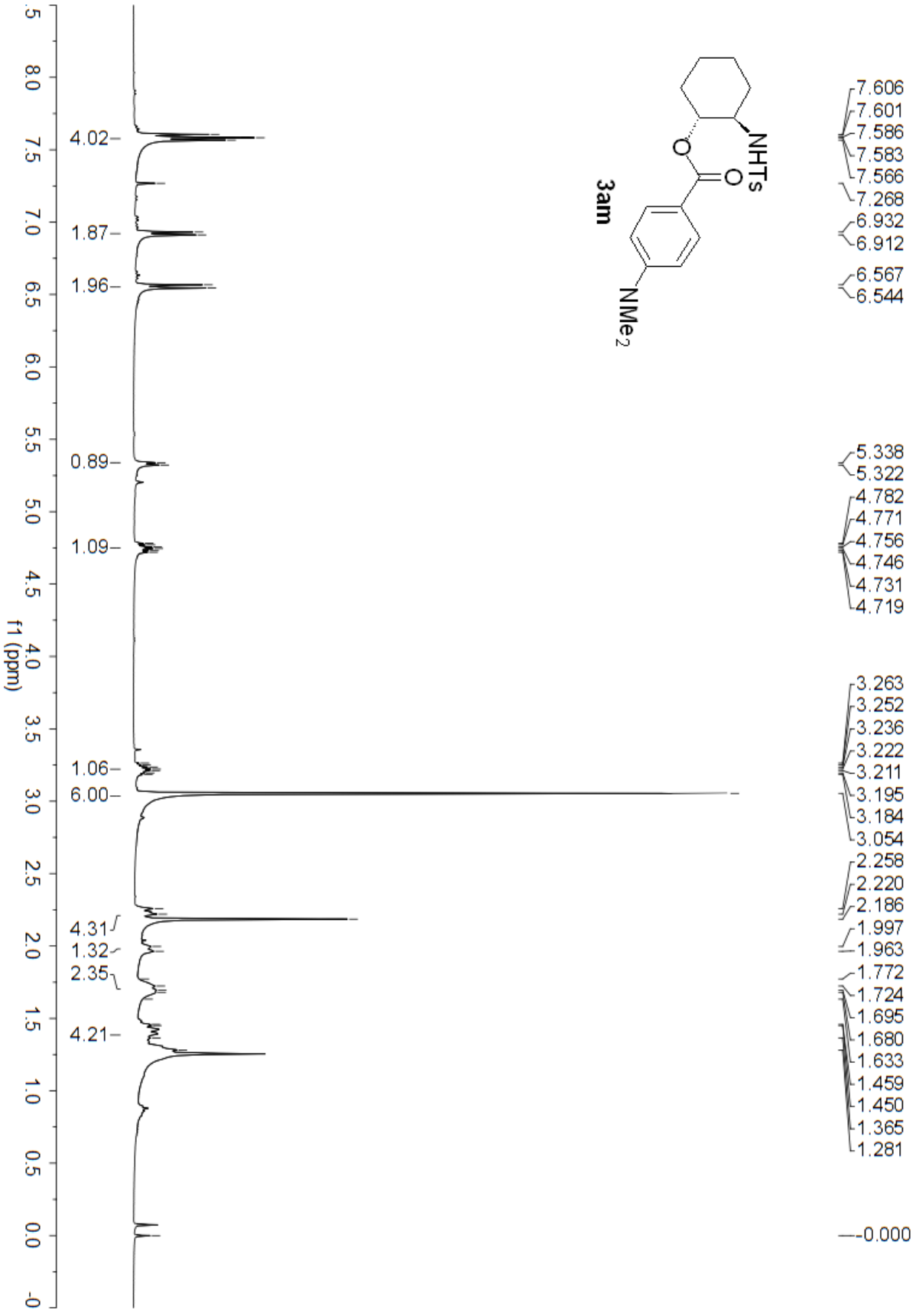

3ak
NHTs
O
O
166.9
143.7
142.6
138.0
129.8
129.4
128.8
126.9
126.5
77.4
77.1
76.8
74.4
57.4
34.2
31.3
24.2
23.8
21.7
21.4
f1 (ppm)

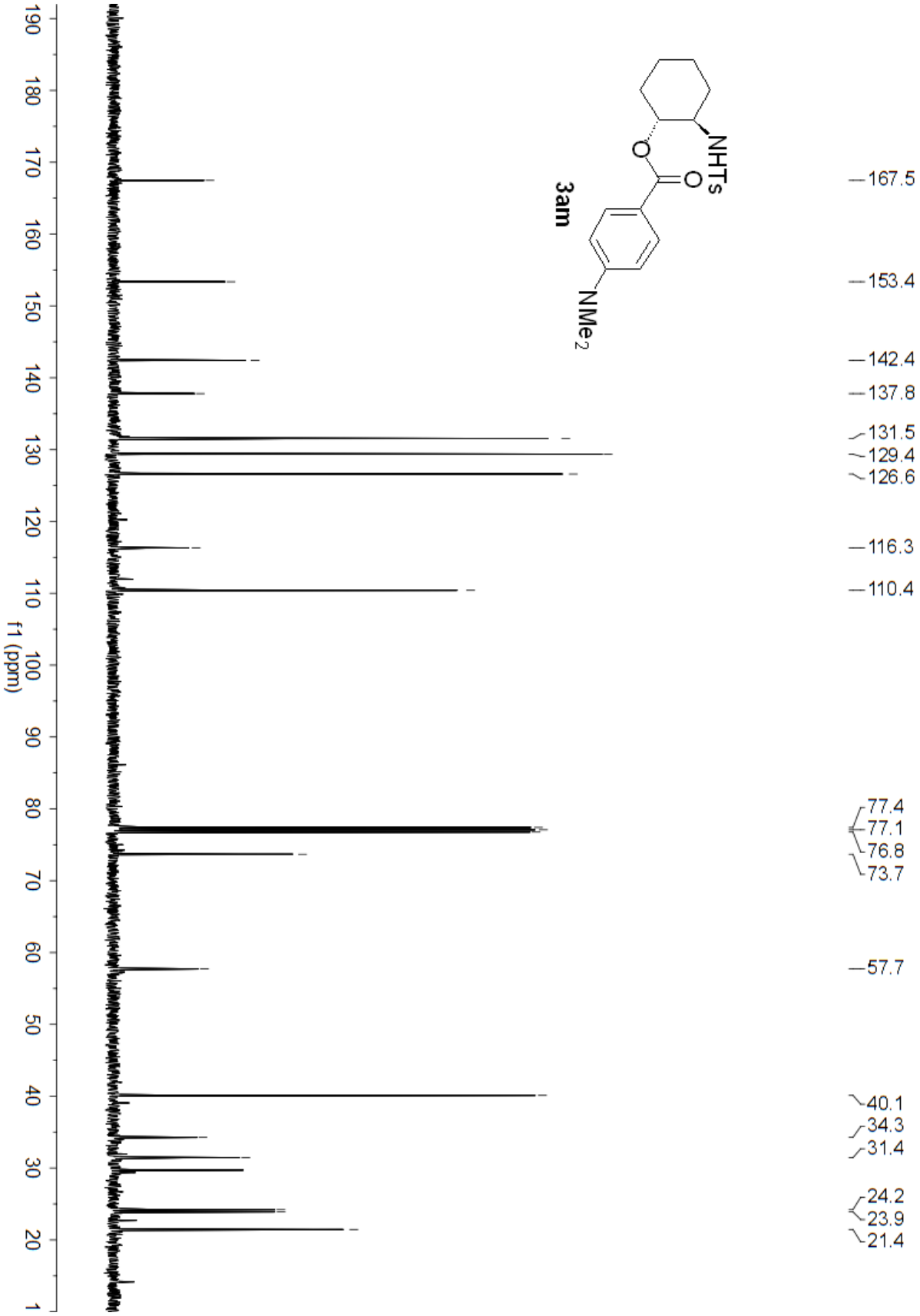

%T
gyq20141209_2-39-1
3409.9
3323.2
3051.9
3034.7
2956.4
2930.2
2919.4
2854.5
1936.1
1708.4
1672.2
1613.3
1596.3
1577.9
1508.7
1495.0
1466.0
1454.5
1442.9
1409.0
1385.2
1374.6
1366.2
1347.9
1323.5
1308.1
1292.5
1272.3
1249.5
1213.2
1178.1
1157.1
1140.9
1116.8
1086.5
1058.1
1027.2
1020.2
941.6
911.6
863.8
839.5
816.5
752.7
717.2
704.7
690.0
671.3
607.5
595.9
578.4
567.6
546.7
495.5
484.8
473.5
3ak
NHTs
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
0
5
10
15
20
25
30
35
40
45
50
55
60
65

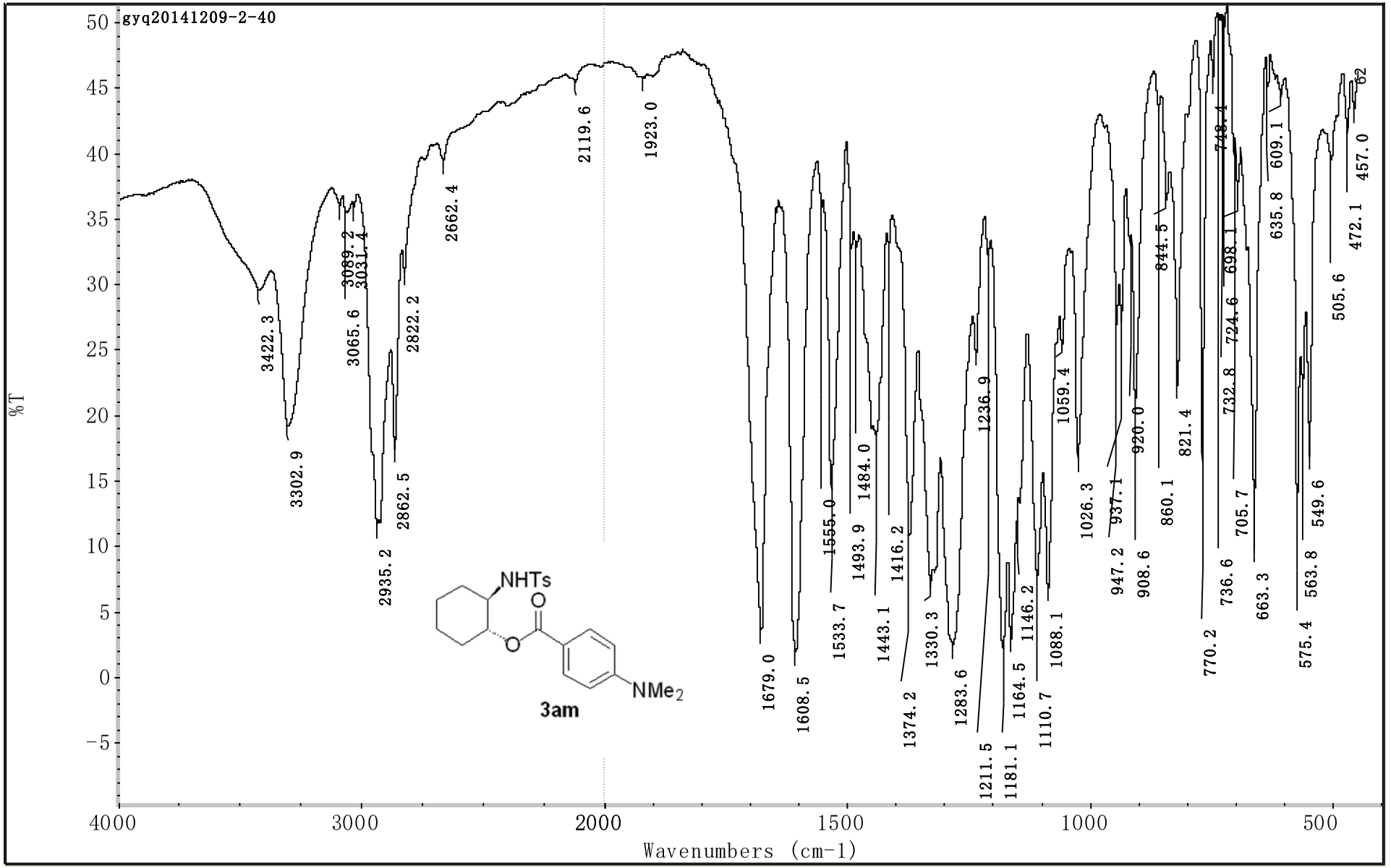

3al
NHTs
OMe
f1 (ppm)
1.90
1.94
1.93
2.00
0.86
1.04
2.99
1.03
4.13
1.19
2.38
4.24
7.722
7.700
7.599
7.579
7.276
6.950
6.930
6.844
6.822
5.301
5.284
4.815
4.804
4.789
4.778
4.764
4.752
3.865
3.314
3.304
3.289
3.279
3.269
3.263
2.204
2.165
2.025
1.992
1.742
1.725
1.695
1.688
1.677
1.432
1.416
1.409
1.384
1.355
1.311
1.286
1.256
0.000

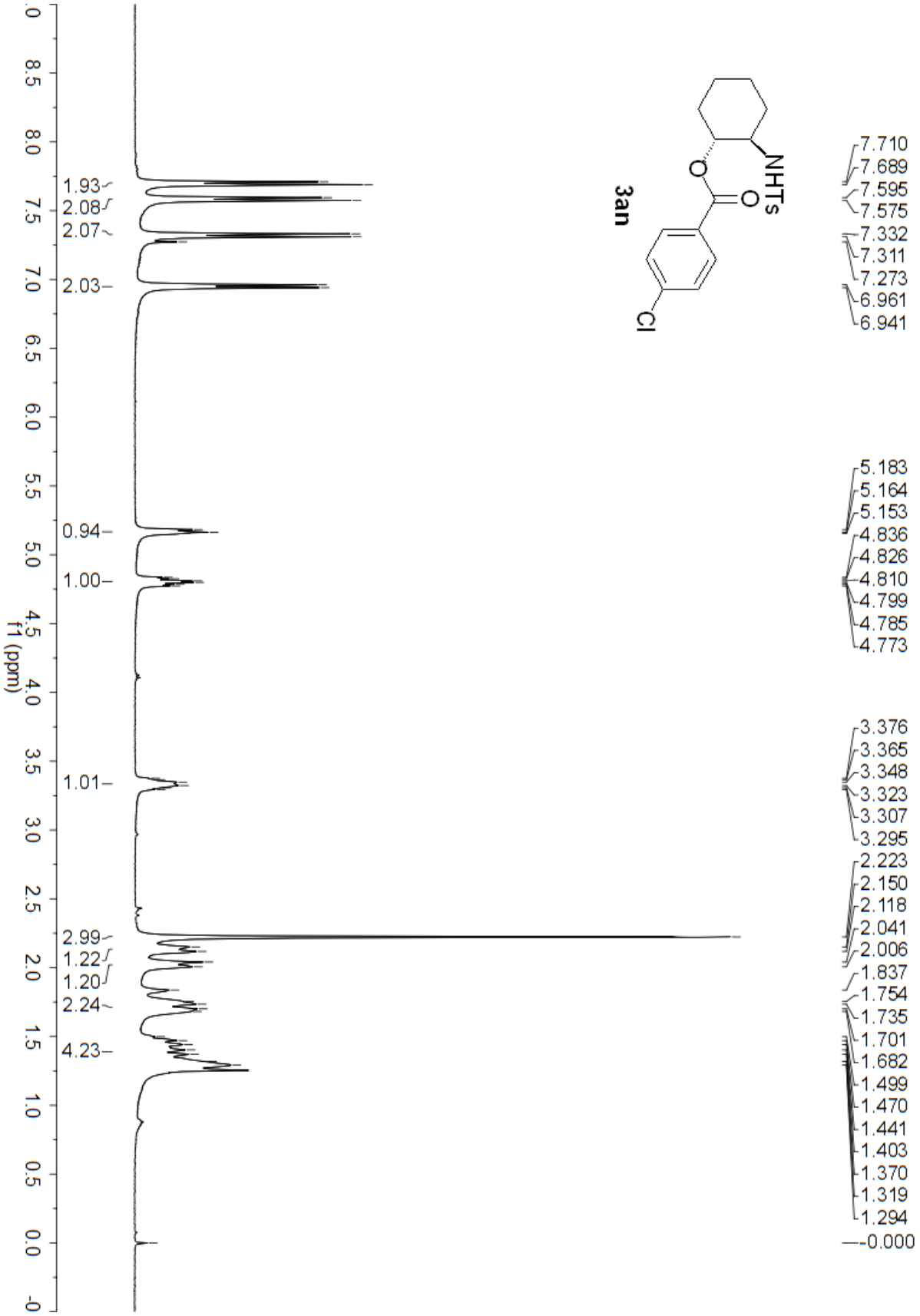

3al
NHTs
O
O
OMe
166.6
163.4
142.6
138.1
131.8
129.4
126.6
122.1
113.3
77.4
77.1
76.8
74.3
57.3
55.5
34.0
31.3
24.2
23.8
21.4
f1 (ppm)

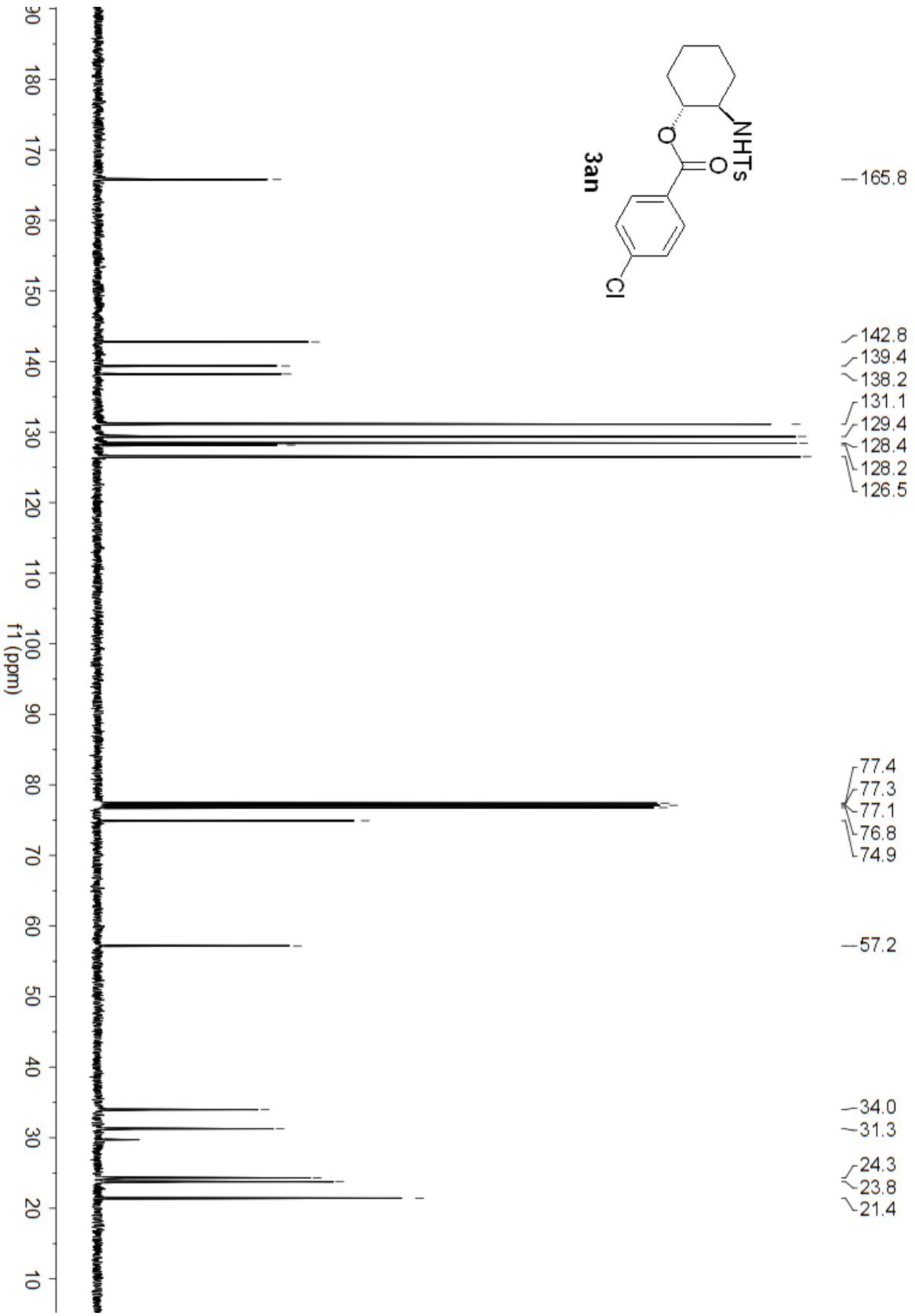

%T
Wavenumbers (cm-1)
gyq20141209-2-39-2
3398.7
3331.2
3065.6
3082.6
3019.0
2958.1
2932.6
2862.8
2840.1
2581.9
2050.1
1920.6
1772.3
1706.2
1667.7
1606.7
1581.7
1558.3
1539.4
1510.9
1494.6
1469.7
1459.8
1440.5
1400.2
1383.1
1368.1
1350.9
1326.1
1315.5
1301.9
1294.5
1287.7
1260.5
1215.0
1182.9
1169.6
1157.7
1140.6
1114.6
1104.4
1091.0
1079.8
1059.6
1032.8
1015.9
956.5
940.9
924.4
909.2
865.7
841.4
814.1
798.9
782.2
768.8
725.2
717.0
695.8
670.4
666.7
663.9
635.4
620.9
607.0
576.5
566.7
548.2
506.3
492.5
3al
NHTs
OMe

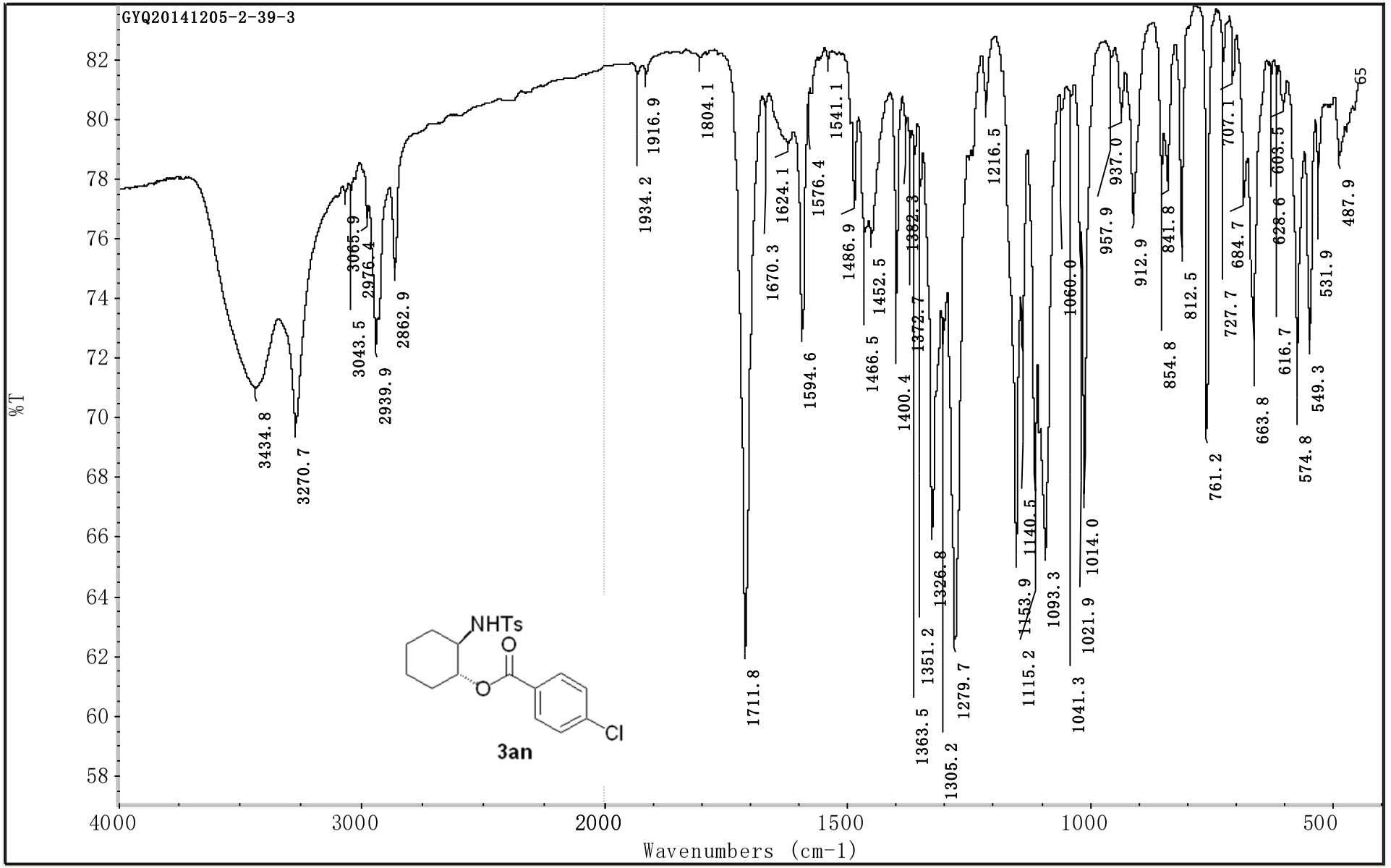

3am
NHTs
O
O
NMe2
7.606
7.601
7.586
7.583
7.566
7.268
6.932
6.912
6.567
6.544
5.338
5.322
4.782
4.771
4.756
4.746
4.731
4.719
3.263
3.252
3.236
3.222
3.211
3.195
3.184
3.054
2.258
2.220
2.186
1.997
1.963
1.772
1.724
1.695
1.680
1.633
1.459
1.450
1.365
1.281
0.000
4.02
1.87
1.96
0.89
1.09
1.06
6.00
4.31
1.32
2.35
4.21
f1 (ppm)

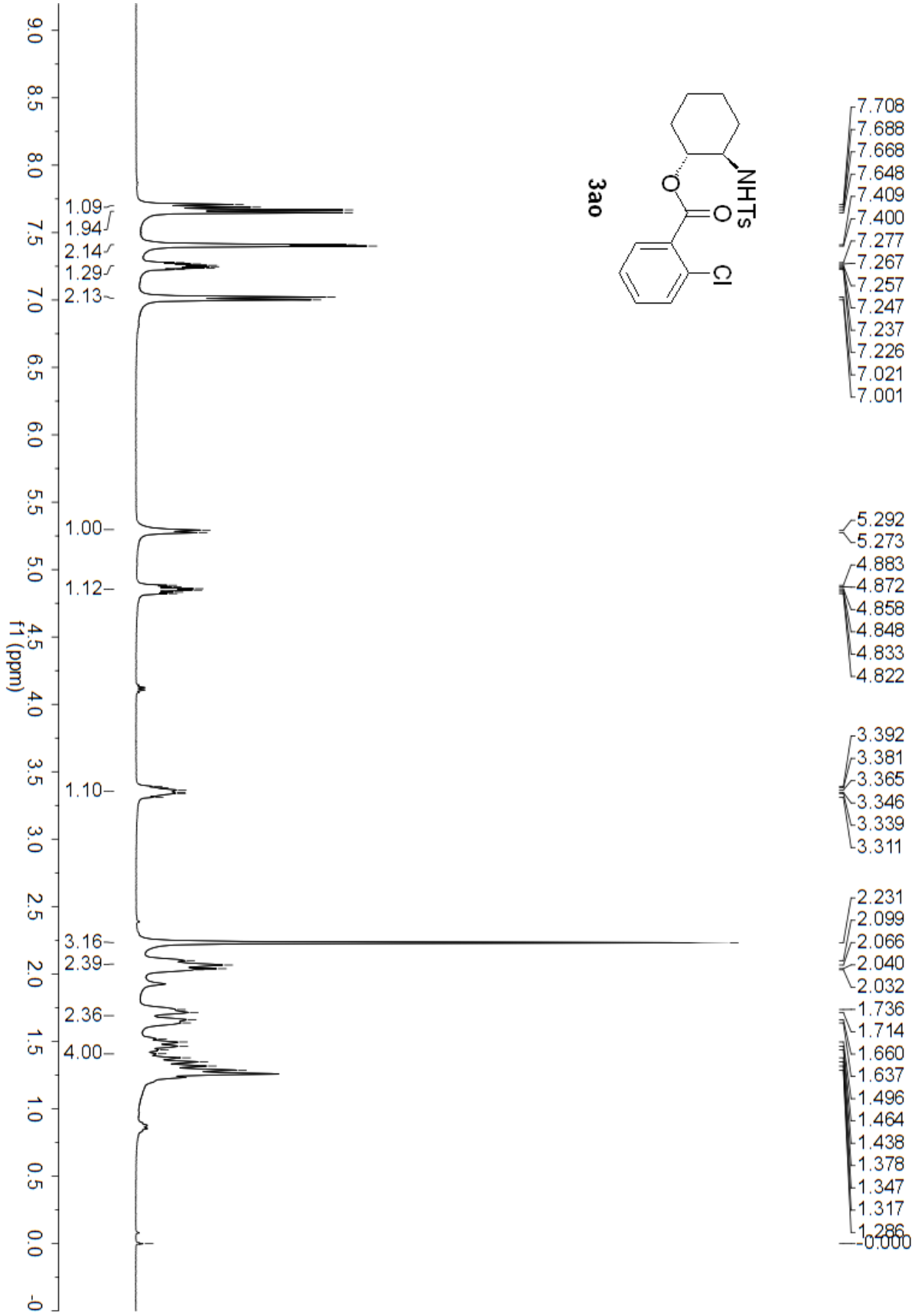

3am
NHTs
O
O
NMe2
167.5
153.4
142.4
137.8
131.5
129.4
126.6
116.3
110.4
77.4
77.1
76.8
73.7
57.7
40.1
34.3
31.4
24.2
23.9
21.4
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
1

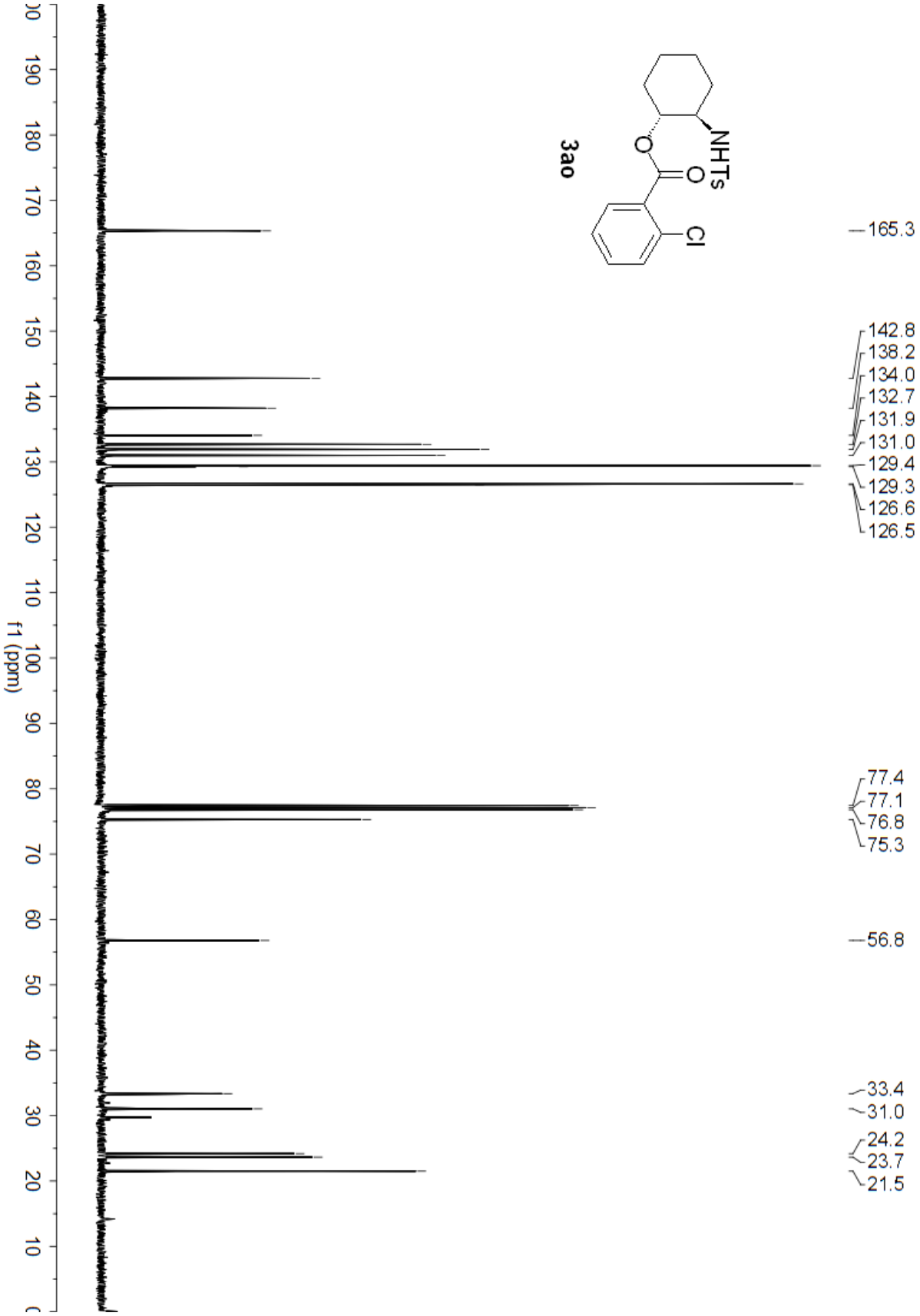

gyq20141209-2-40
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
50
45
40
35
30
25
20
15
10
5
0
-5
3422.3
3302.9
3089.2
3065.6
3031.4
2935.2
2862.5
2822.2
2662.4
2119.6
1923.0
1679.0
1608.5
1555.0
1533.7
1493.9
1484.0
1443.1
1416.2
1374.2
1330.3
1283.6
1236.9
1211.5
1181.1
1164.5
1146.2
1110.7
1088.1
1059.4
1026.3
947.2
937.1
920.0
908.6
860.1
844.5
821.4
770.2
748.4
736.6
732.8
724.6
705.7
698.1
663.3
635.8
609.1
575.4
563.8
549.6
505.6
472.1
457.0
NHTs
O
O
NMe2
3am

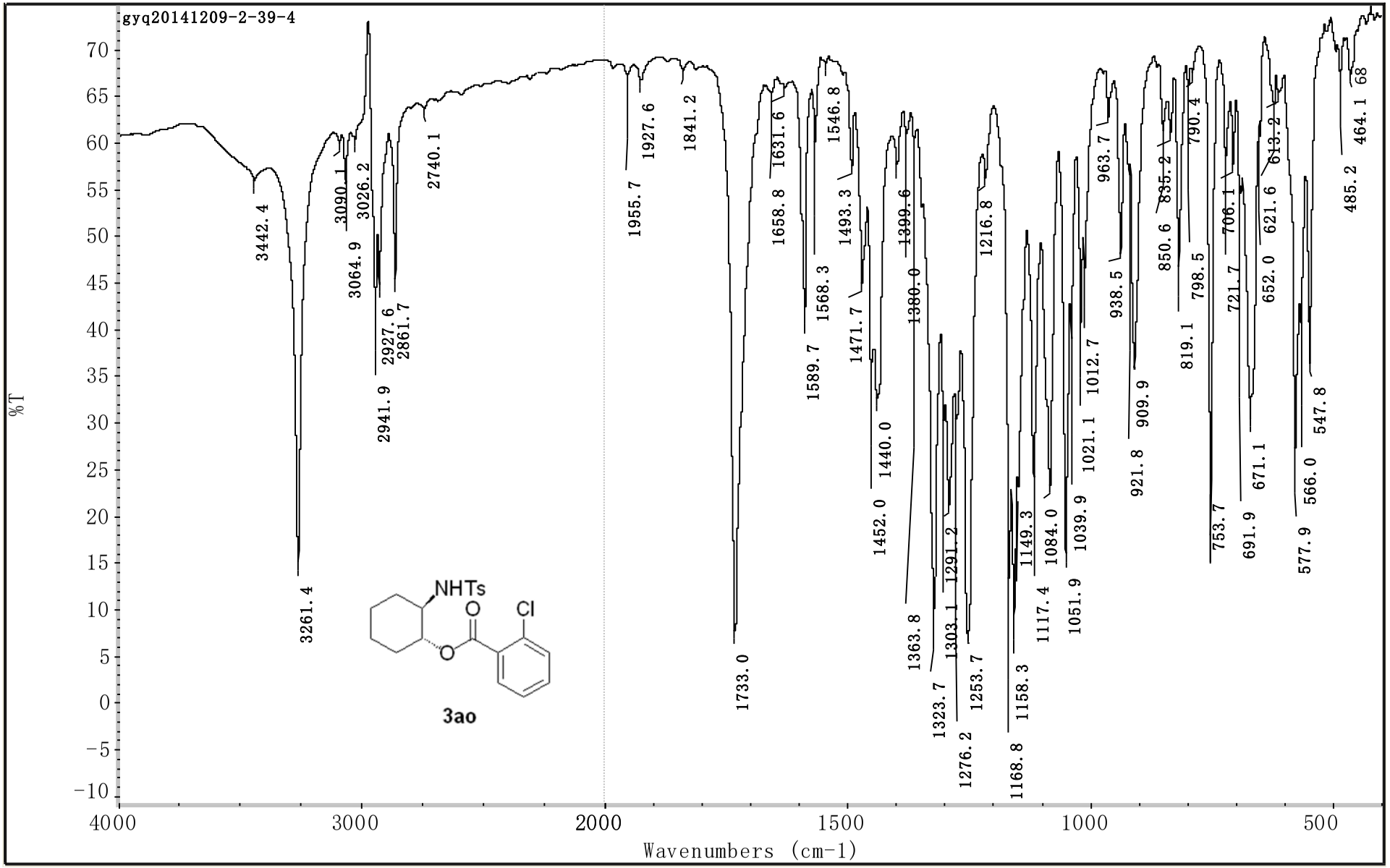

3an
NHTs
O
O
Cl
f1 (ppm)
1.93
2.08
2.07
2.03
0.94
1.00
1.01
2.99
1.22
1.20
2.24
4.23
7.710
7.689
7.595
7.575
7.332
7.311
7.273
6.961
6.941
5.183
5.164
5.153
4.836
4.826
4.810
4.799
4.785
4.773
3.376
3.365
3.348
3.323
3.307
3.295
2.223
2.150
2.118
2.041
2.006
1.837
1.754
1.735
1.701
1.682
1.499
1.470
1.441
1.403
1.370
1.319
1.294
-0.000

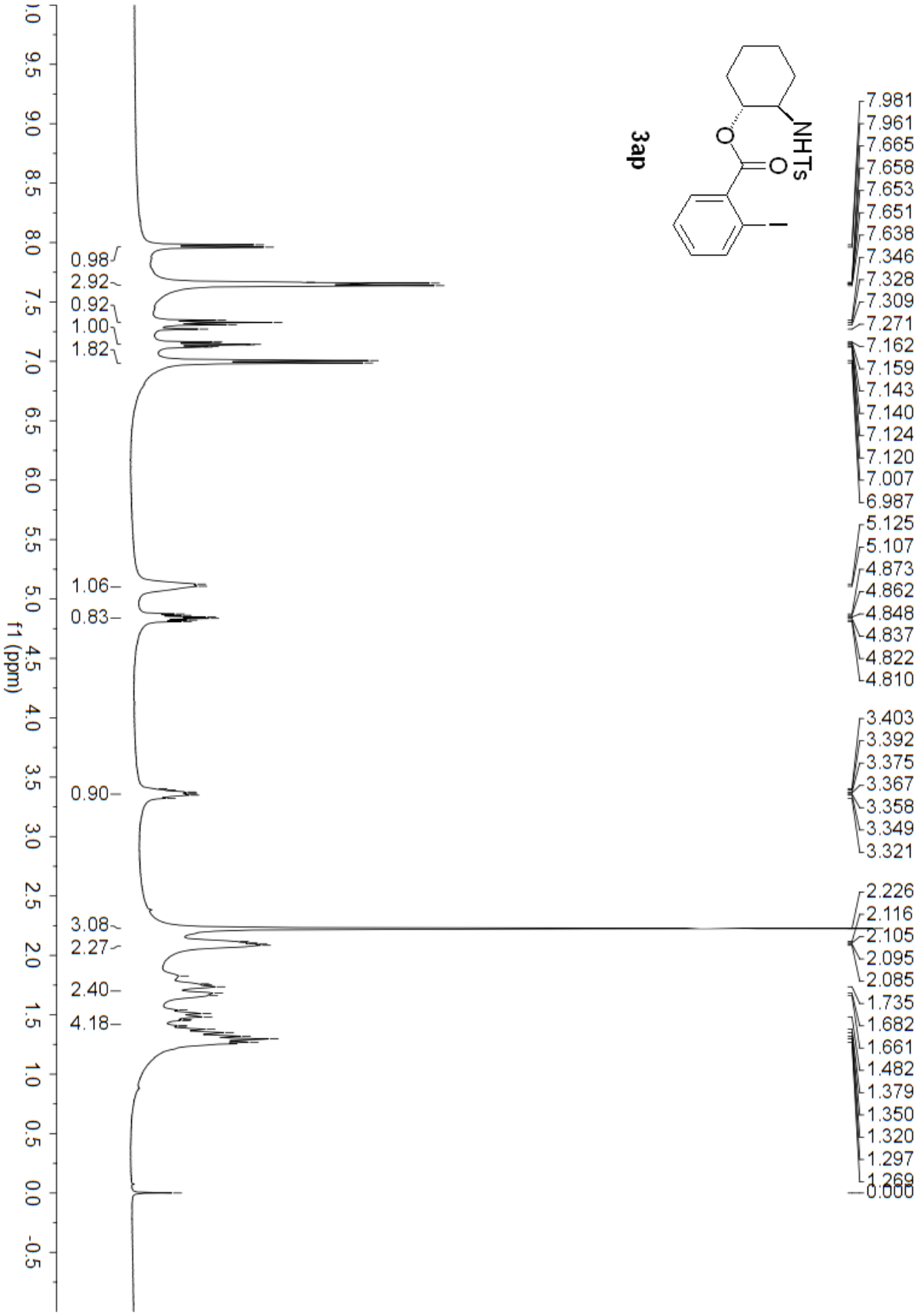

3an
NHTs
O
O
Cl
165.8
142.8
139.4
138.2
131.1
129.4
128.4
128.2
126.5
77.4
77.3
77.1
76.8
74.9
57.2
34.0
31.3
24.3
23.8
21.4
f1 (ppm)

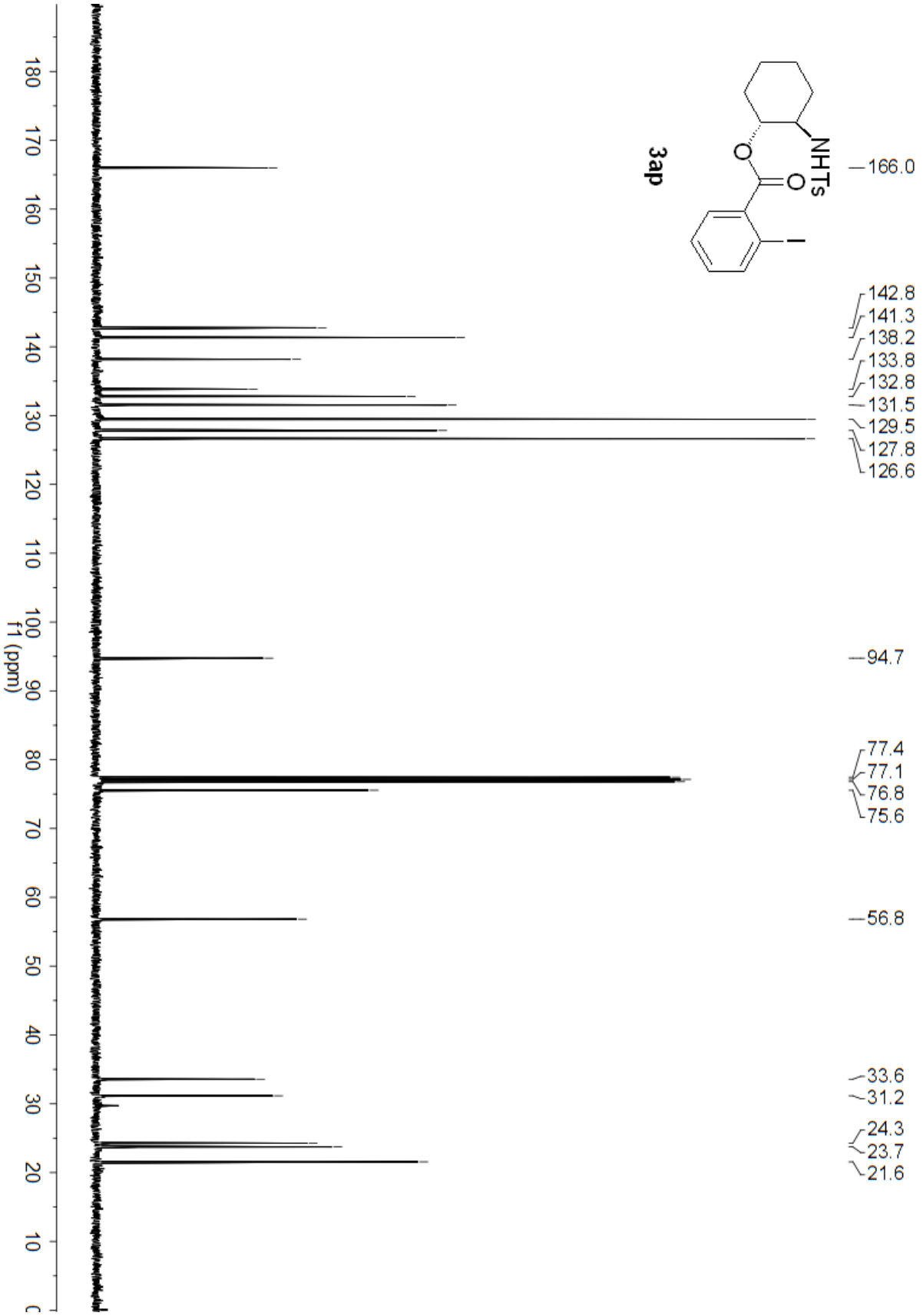

GYQ20141205-2-39-3
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
82
80
78
76
74
72
70
68
66
64
62
60
58
3434.8
3270.7
3065.9
3043.5
2976.4
2939.9
2862.9
1934.2
1916.9
1804.1
1711.8
1670.3
1624.1
1594.6
1576.4
1541.1
1486.9
1466.5
1452.5
1400.4
1382.3
1372.7
1363.5
1351.2
1326.8
1305.2
1279.7
1216.5
1153.9
1140.5
1115.2
1093.3
1060.0
1041.3
1021.9
1014.0
957.9
937.0
912.9
854.8
841.8
812.5
761.2
727.7
707.1
684.7
663.8
628.6
616.7
603.5
574.8
549.3
531.9
487.9
NHTs
O
O
Cl
3an

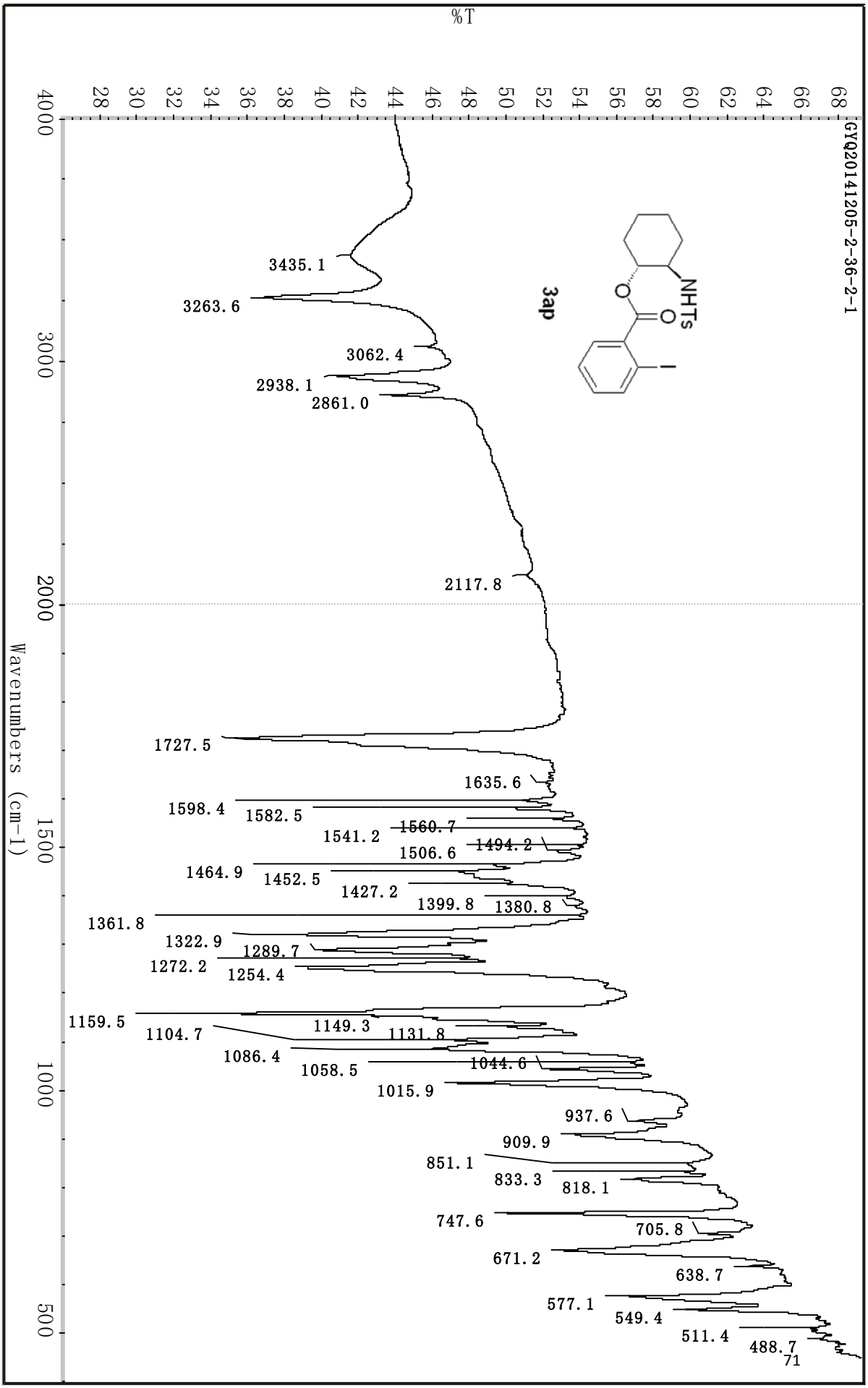

3ao
NHTs
O
O
Cl
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
1.09
1.94
2.14
1.29
2.13
1.00
1.12
1.10
3.16
2.39
2.36
4.00
7.708
7.688
7.668
7.648
7.409
7.400
7.277
7.267
7.257
7.247
7.237
7.226
7.021
7.001
5.292
5.273
4.883
4.872
4.858
4.848
4.833
4.822
3.392
3.381
3.365
3.346
3.339
3.311
2.231
2.099
2.066
2.040
2.032
1.736
1.714
1.660
1.637
1.496
1.464
1.438
1.378
1.347
1.317
1.286
0.000

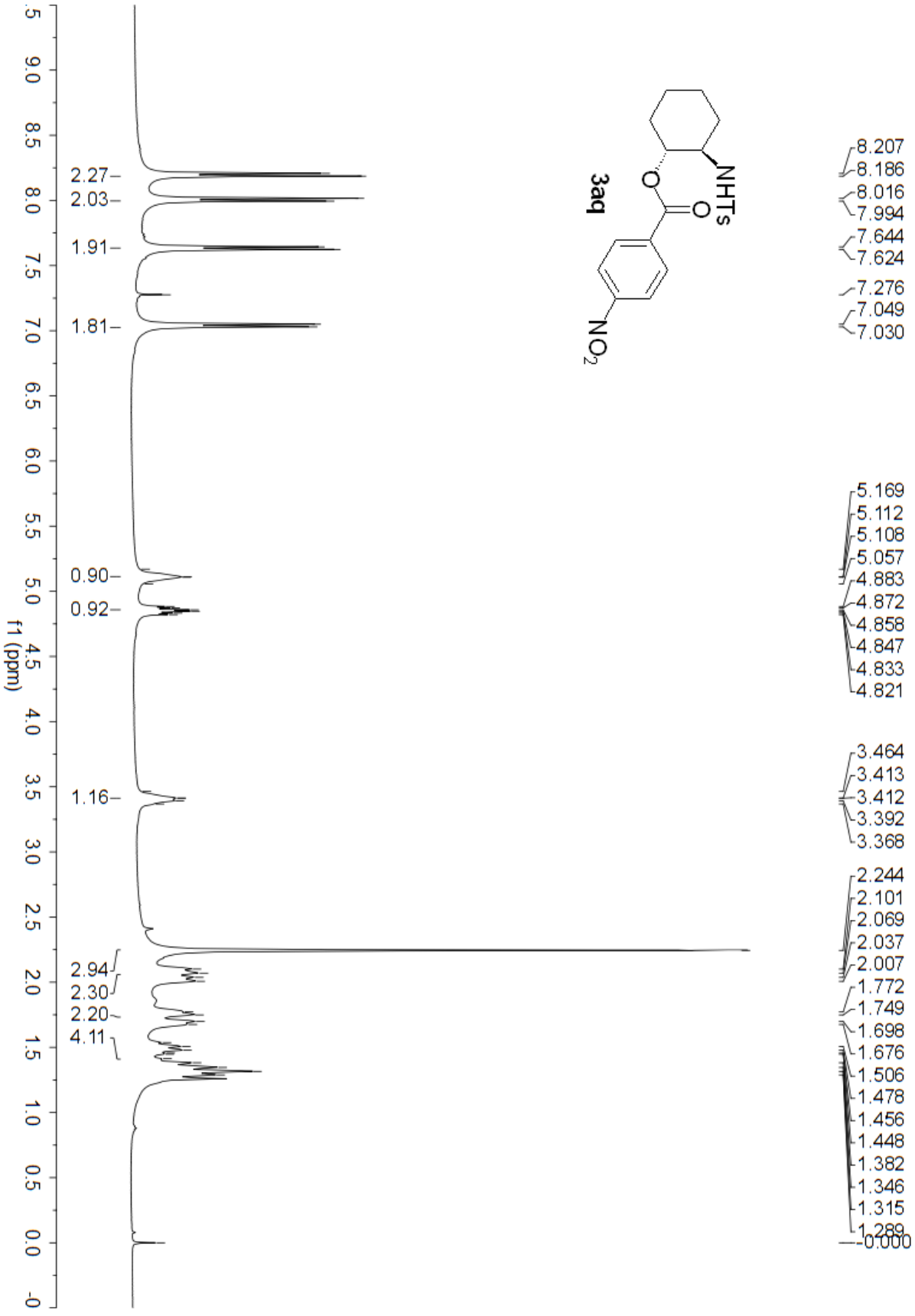

3ao
NHTs
O
O
Cl
165.3
142.8
138.2
134.0
132.7
131.9
131.0
129.4
129.3
126.6
126.5
77.4
77.1
76.8
75.3
56.8
33.4
31.0
24.2
23.7
21.5
f1 (ppm)

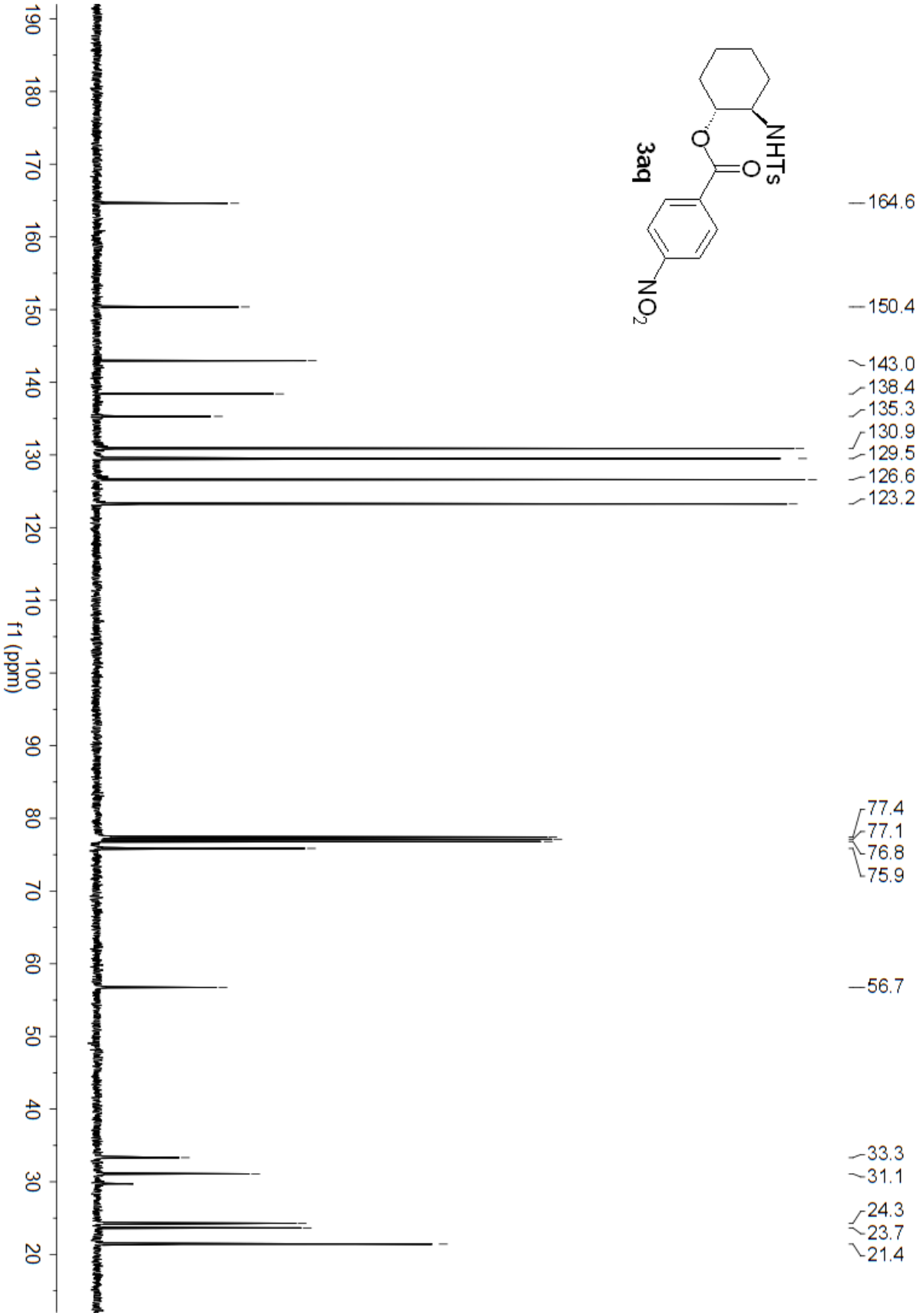

gyq20141209-2-39-4
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3442.4
3261.4
3090.1
3064.9
3026.2
2941.9
2927.6
2861.7
2740.1
1955.7
1927.6
1841.2
1733.0
1658.8
1631.6
1589.7
1568.3
1546.8
1493.3
1471.7
1452.0
1440.0
1399.6
1380.0
1363.8
1323.7
1303.1
1291.2
1276.2
1253.7
1216.8
1168.8
1158.3
1149.3
1117.4
1084.0
1051.9
1039.9
1021.1
1012.7
963.7
938.5
921.8
909.9
850.6
835.2
819.1
798.5
790.4
753.7
721.7
706.1
691.9
671.1
652.0
621.6
613.2
577.9
566.0
547.8
485.2
464.1
NHTs
O
Cl
O
3ao

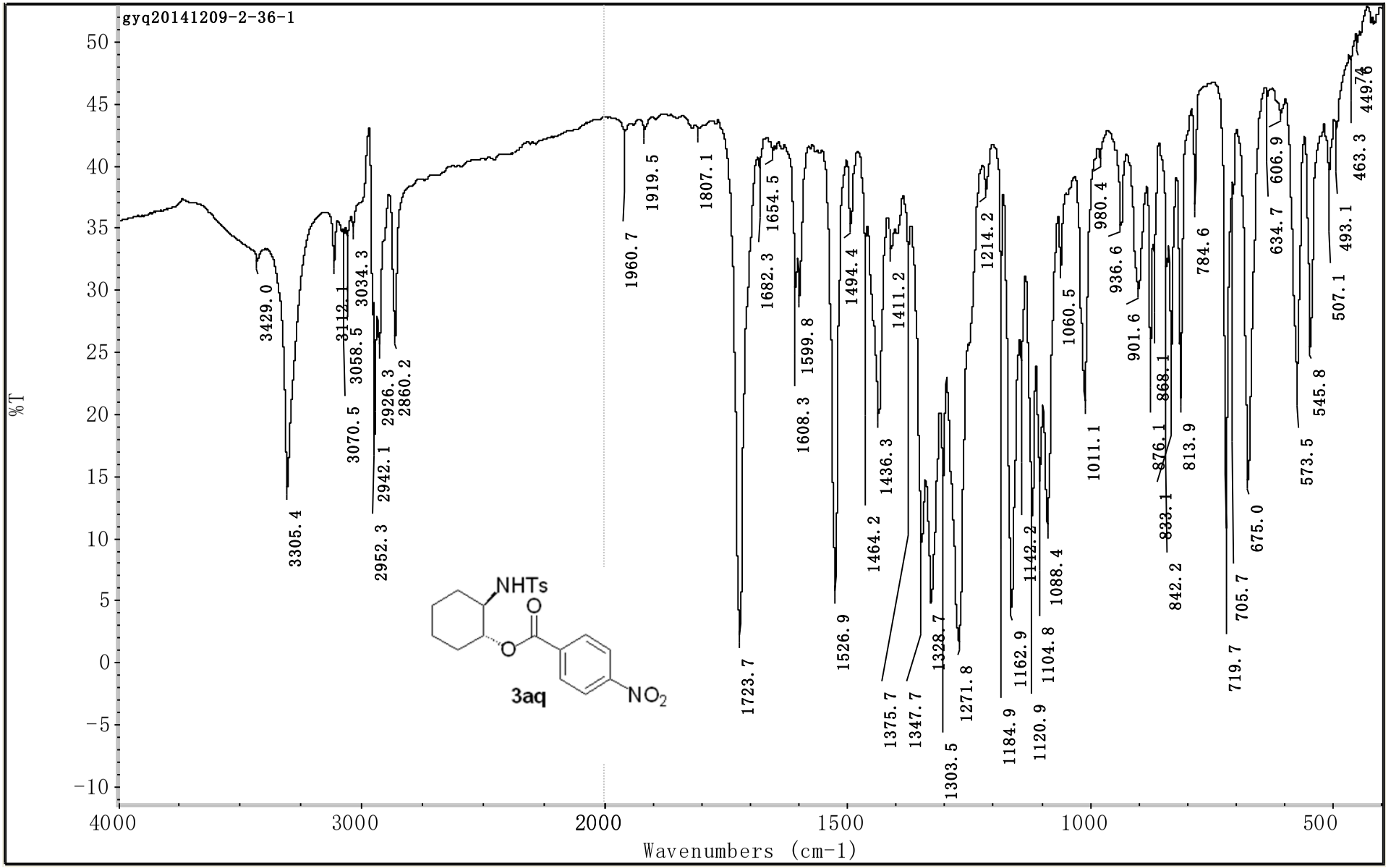

3ap
NHTs
O
O
I
7.981
7.961
7.665
7.658
7.653
7.651
7.638
7.346
7.328
7.309
7.271
7.162
7.159
7.143
7.140
7.124
7.120
7.007
6.987
5.125
5.107
4.873
4.862
4.848
4.837
4.822
4.810
3.403
3.392
3.375
3.367
3.358
3.349
3.321
2.226
2.116
2.105
2.095
2.085
1.735
1.682
1.661
1.482
1.379
1.350
1.320
1.297
1.269
0.000
0.98
2.92
0.92
1.00
1.82
1.06
0.83
0.90
3.08
2.27
2.40
4.18
f1 (ppm)

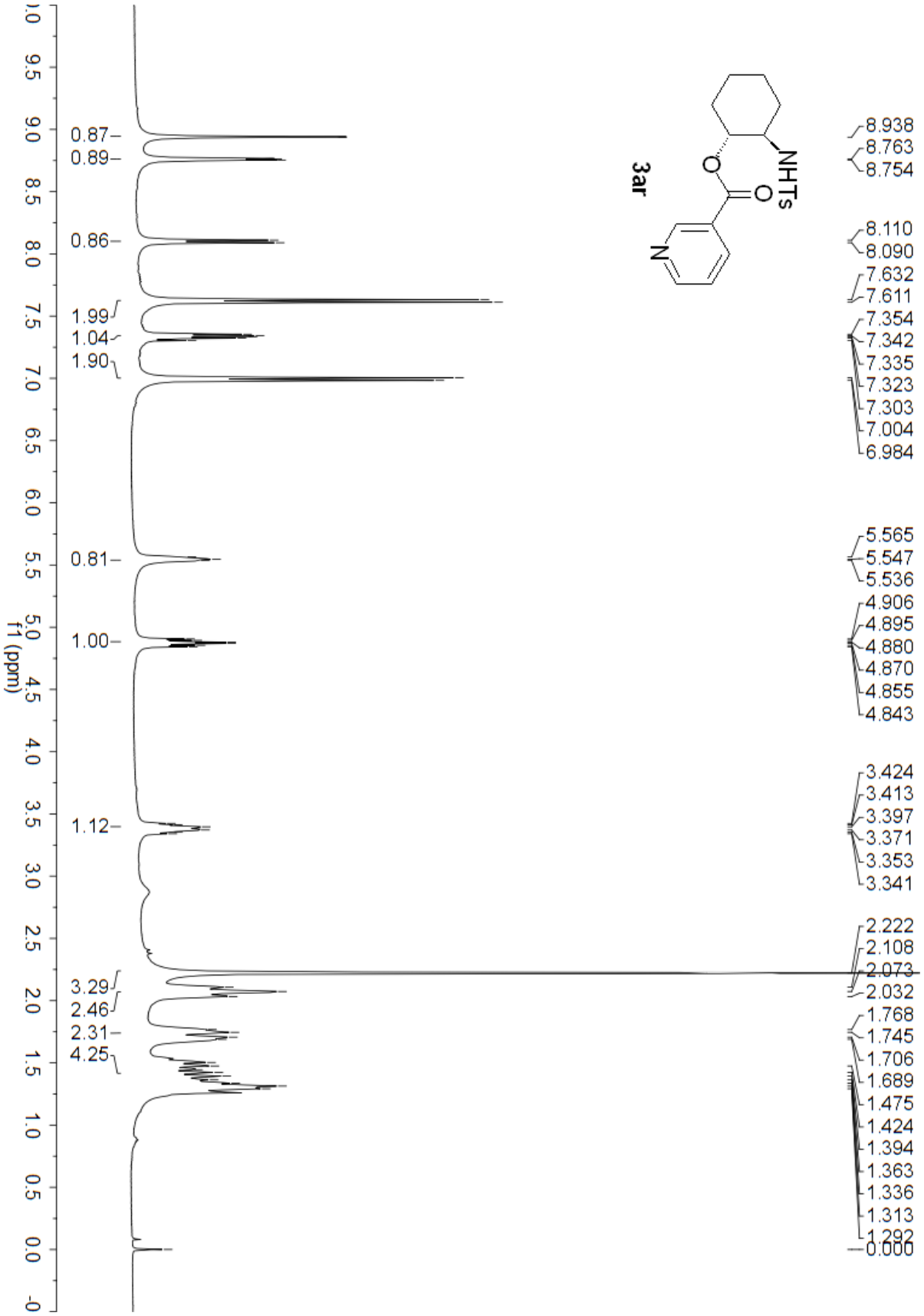

3ap
NHTs
O
O
I
166.0
142.8
141.3
138.2
133.8
132.8
131.5
129.5
127.8
126.6
94.7
77.4
77.1
76.8
75.6
56.8
33.6
31.2
24.3
23.7
21.6
f1 (ppm)

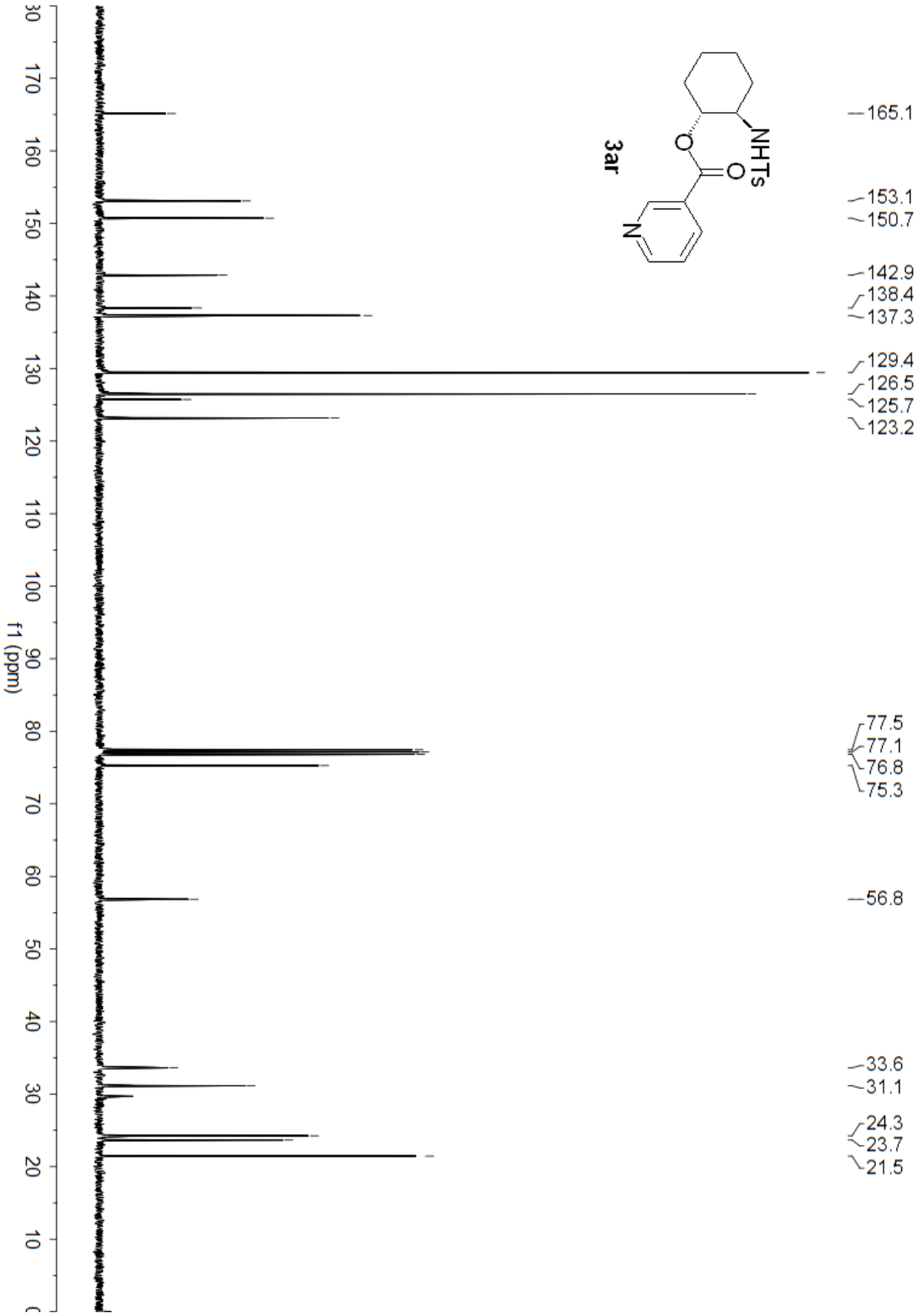

%T
Wavenumbers (cm-1)
GYQ20141205-2-36-2-1
3ap
NHTs
O
O
I
3435.1
3263.6
3062.4
2938.1
2861.0
2117.8
1727.5
1635.6
1598.4
1582.5
1541.2
1560.7
1494.2
1506.6
1464.9
1452.5
1427.2
1399.8
1380.8
1361.8
1322.9
1289.7
1272.2
1254.4
1159.5
1104.7
1149.3
1131.8
1086.4
1058.5
1044.6
1015.9
937.6
909.9
851.1
833.3
818.1
747.6
705.8
671.2
638.7
577.1
549.4
511.4
488.7

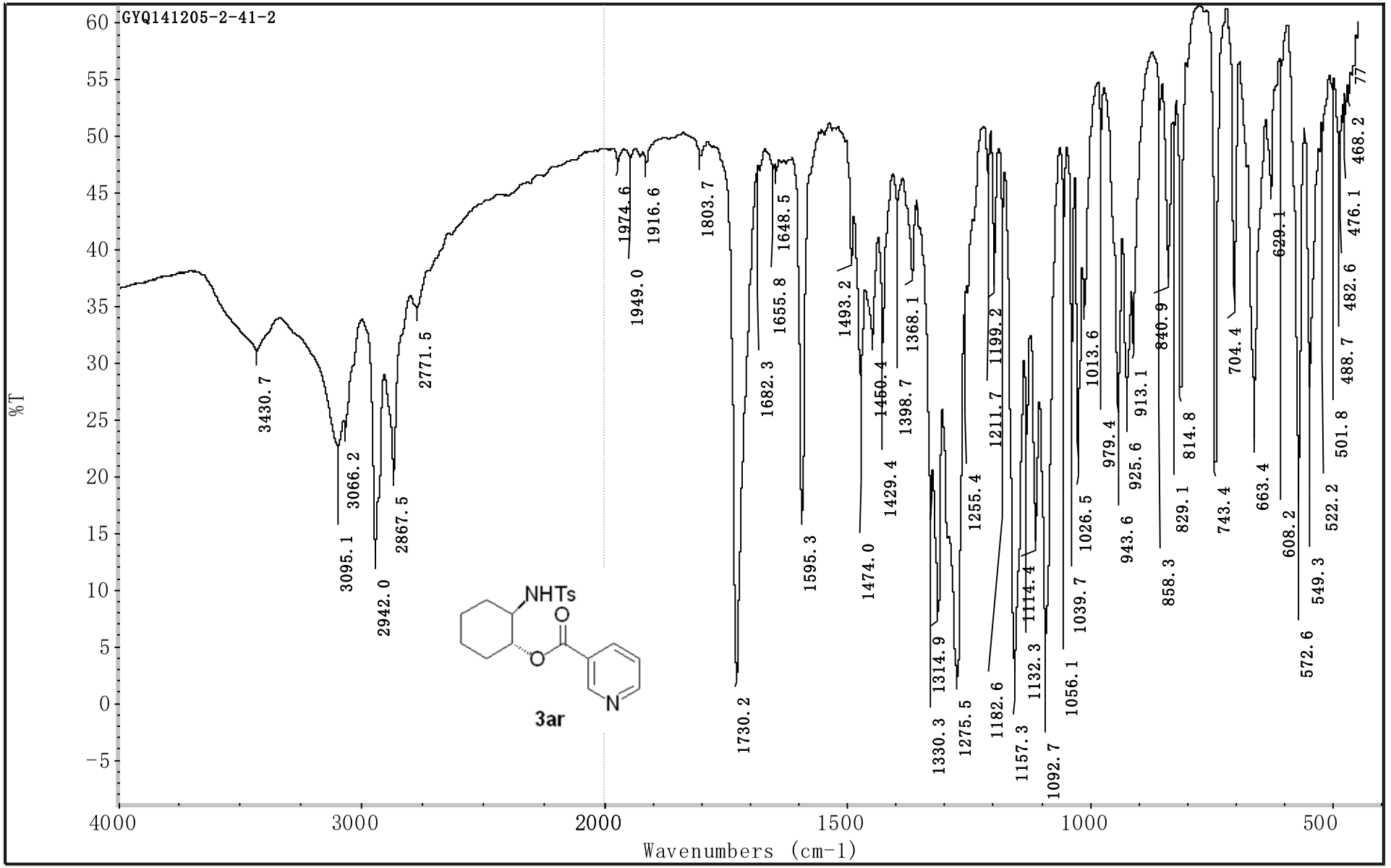

3aq
NHTs
O
O
NO2
8.207
8.186
8.016
7.994
7.644
7.624
7.276
7.049
7.030
5.169
5.112
5.108
5.057
4.883
4.872
4.858
4.847
4.833
4.821
3.464
3.413
3.412
3.392
3.368
2.244
2.101
2.069
2.037
2.007
1.772
1.749
1.698
1.676
1.506
1.478
1.456
1.448
1.382
1.346
1.315
1.289
0.000
2.27
2.03
1.91
1.81
0.90
0.92
1.16
2.94
2.30
2.20
4.11
f1 (ppm)

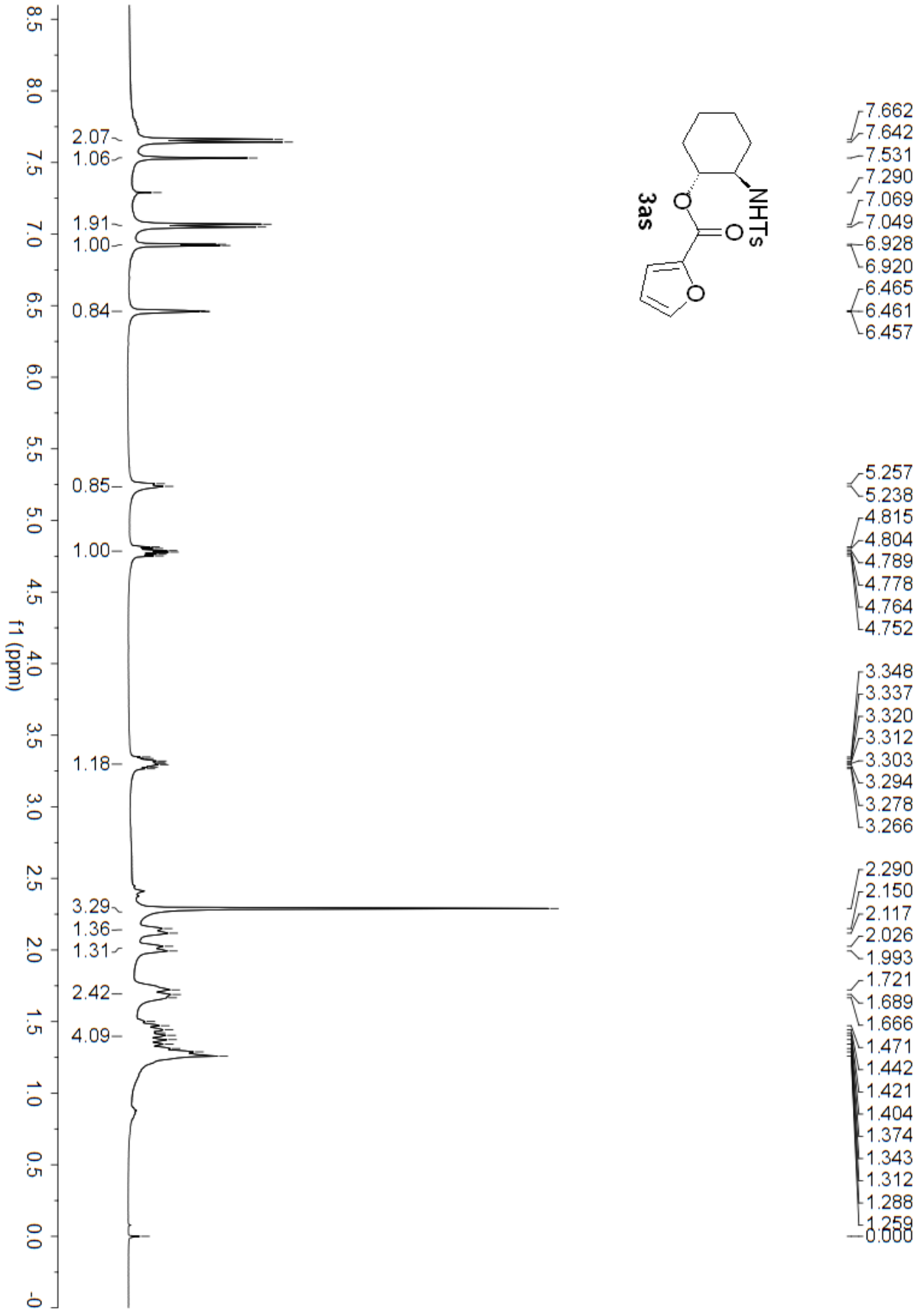

3aq
NHTs
O
O
NO2
164.6
150.4
143.0
138.4
135.3
130.9
129.5
126.6
123.2
77.4
77.1
76.8
75.9
56.7
33.3
31.1
24.3
23.7
21.4
f1 (ppm)

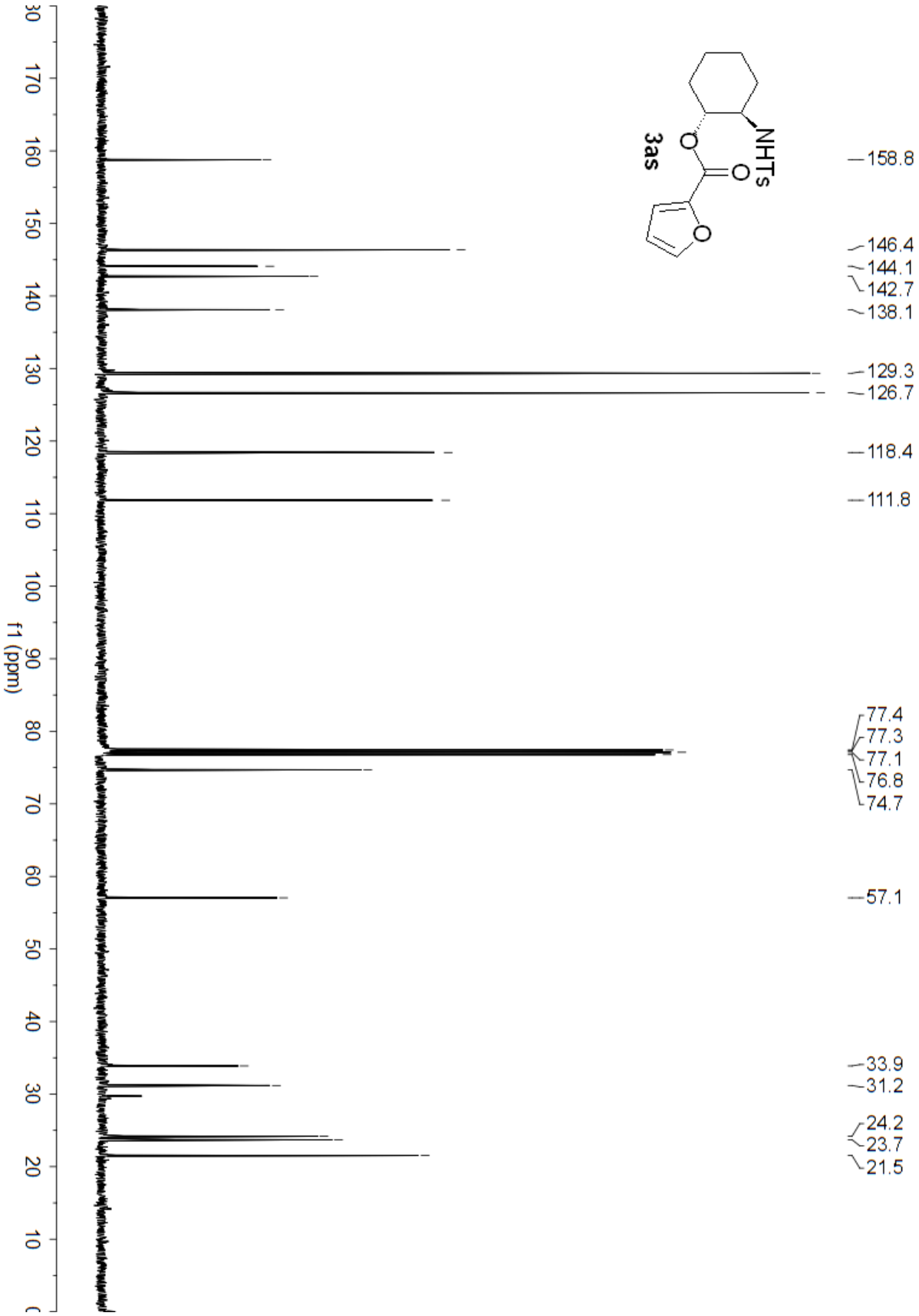

gyq20141209-2-36-1
%T
Wavenumbers (cm-1)
3429.0
3305.4
3112.1
3070.5
3058.5
3034.3
2952.3
2942.1
2926.3
2860.2
1960.7
1919.5
1807.1
1723.7
1682.3
1654.5
1608.3
1599.8
1526.9
1494.4
1464.2
1436.3
1411.2
1375.7
1347.7
1328.7
1303.5
1271.8
1214.2
1184.9
1162.9
1142.2
1120.9
1104.8
1088.4
1060.5
1011.1
980.4
936.6
901.6
876.1
868.1
842.2
833.1
813.9
784.6
719.7
705.7
675.0
634.7
606.9
573.5
545.8
507.1
493.1
463.3
449.6
NHTs
O
O
3aq
NO2

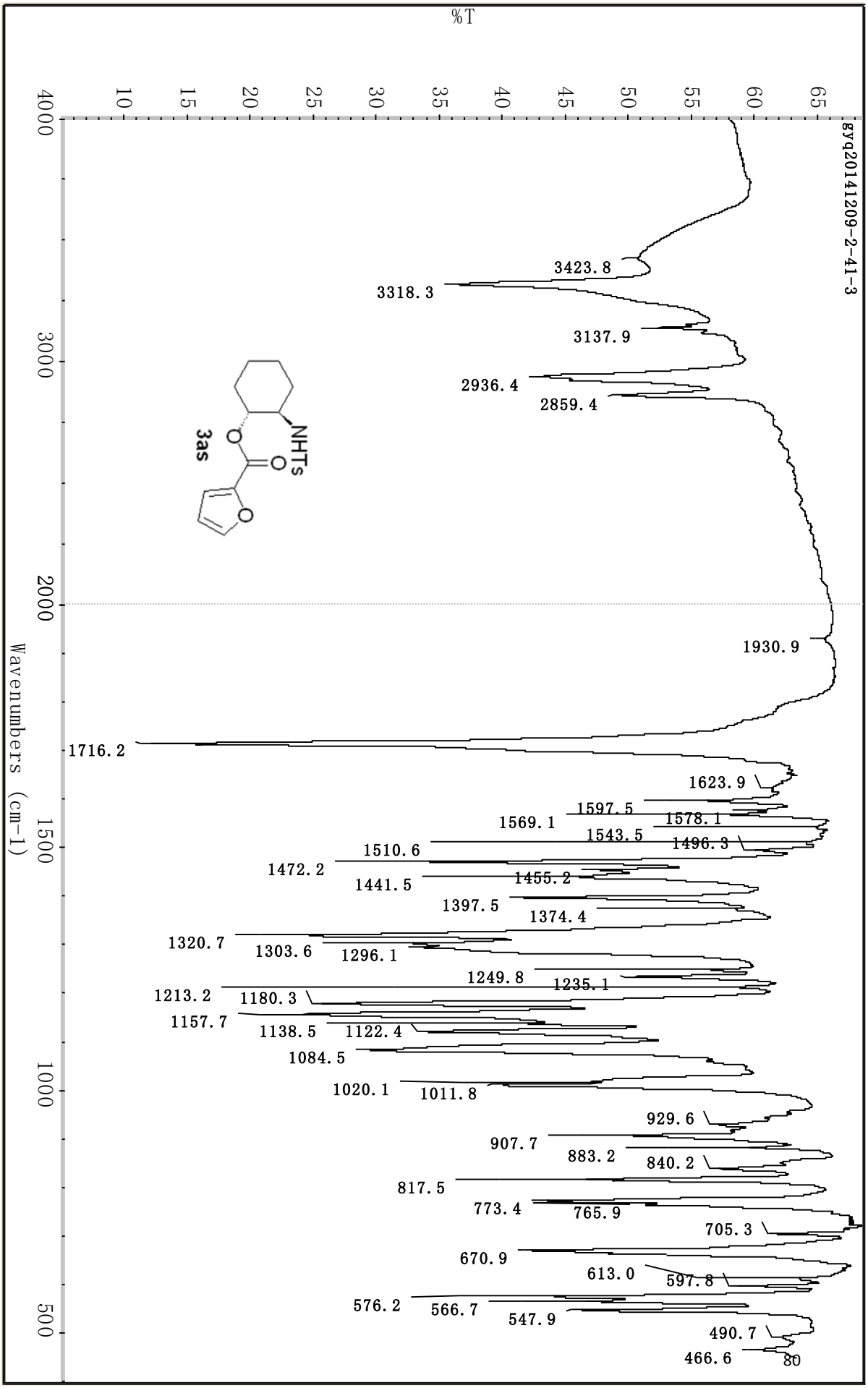

3ar
NHTs
O
O
N
8.938
8.763
8.754
8.110
8.090
7.632
7.611
7.354
7.342
7.335
7.323
7.303
7.004
6.984
5.565
5.547
5.536
4.906
4.895
4.880
4.870
4.855
4.843
3.424
3.413
3.397
3.371
3.353
3.341
2.222
2.108
2.073
2.032
1.768
1.745
1.706
1.689
1.475
1.424
1.394
1.363
1.336
1.313
1.292
0.000
0.87
0.89
0.86
1.99
1.04
1.90
0.81
1.00
1.12
3.29
2.46
2.31
4.25
f1 (ppm)

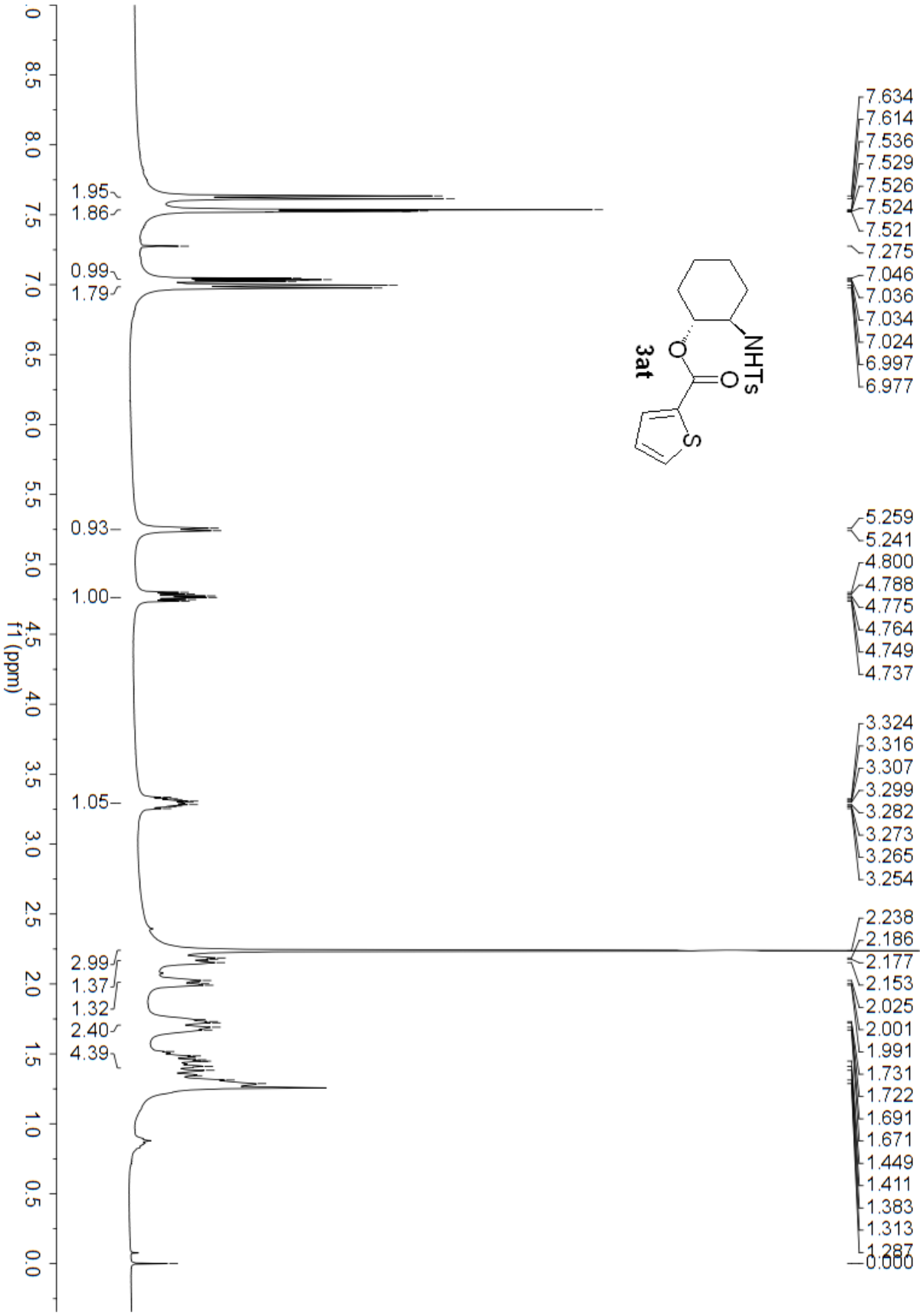

3ar
NHTs
O
O
N
165.1
153.1
150.7
142.9
138.4
137.3
129.4
126.5
125.7
123.2
77.5
77.1
76.8
75.3
56.8
33.6
31.1
24.3
23.7
21.5
f1 (ppm)

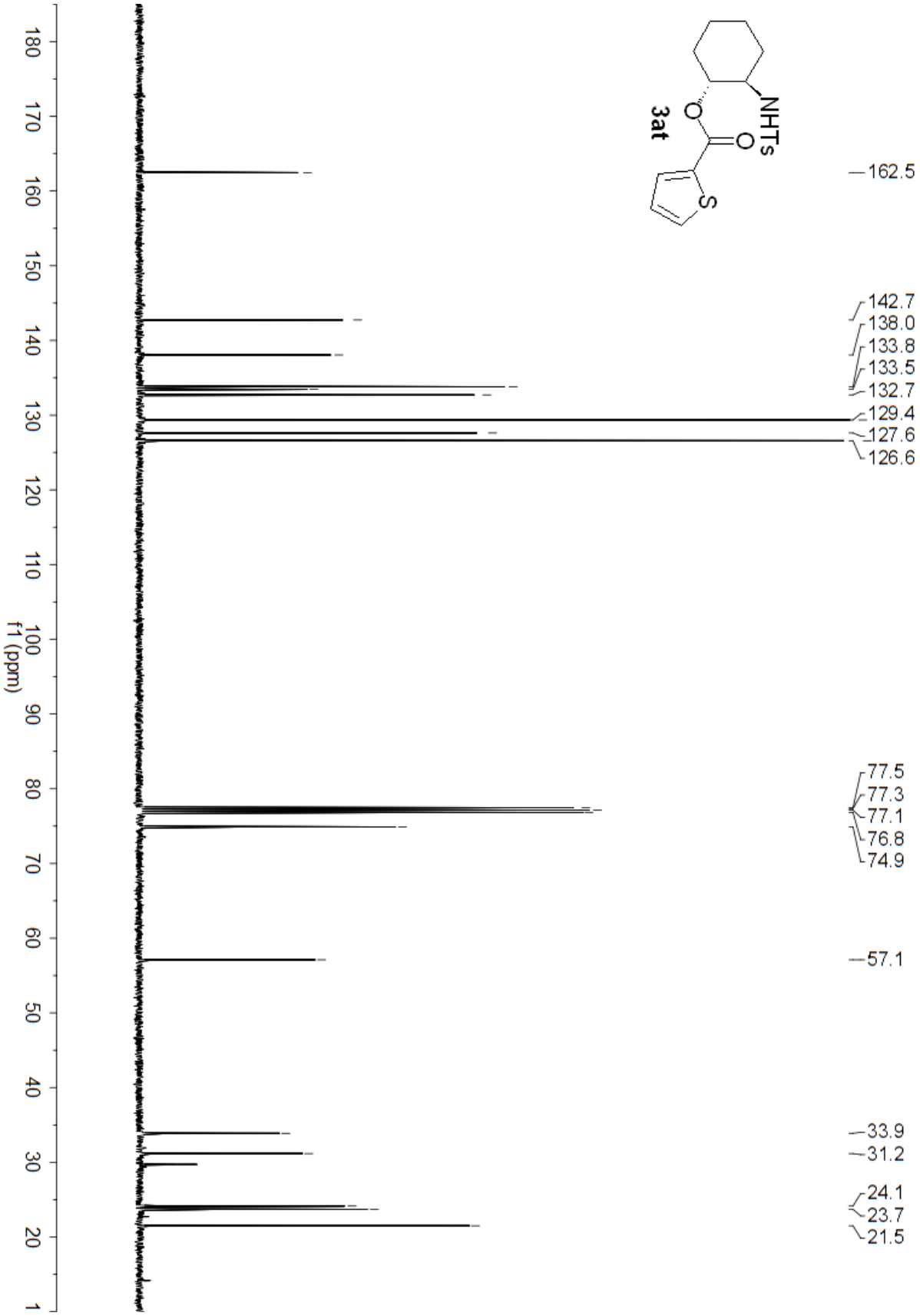

GYQ141205-2-41-2
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3430.7
3095.1
3066.2
2942.0
2867.5
2771.5
1974.6
1949.0
1916.6
1803.7
1730.2
1682.3
1655.8
1648.5
1595.3
1493.2
1474.0
1460.4
1429.4
1398.7
1368.1
1330.3
1314.9
1275.5
1255.4
1211.7
1199.2
1182.6
1157.3
1132.3
1114.4
1092.7
1056.1
1039.7
1026.5
1013.6
979.4
943.6
925.6
913.1
858.3
840.9
829.1
814.8
743.4
704.4
663.4
629.1
608.2
572.6
549.3
522.2
501.8
488.7
482.6
476.1
468.2
77
NHTs
O
O
N
3ar

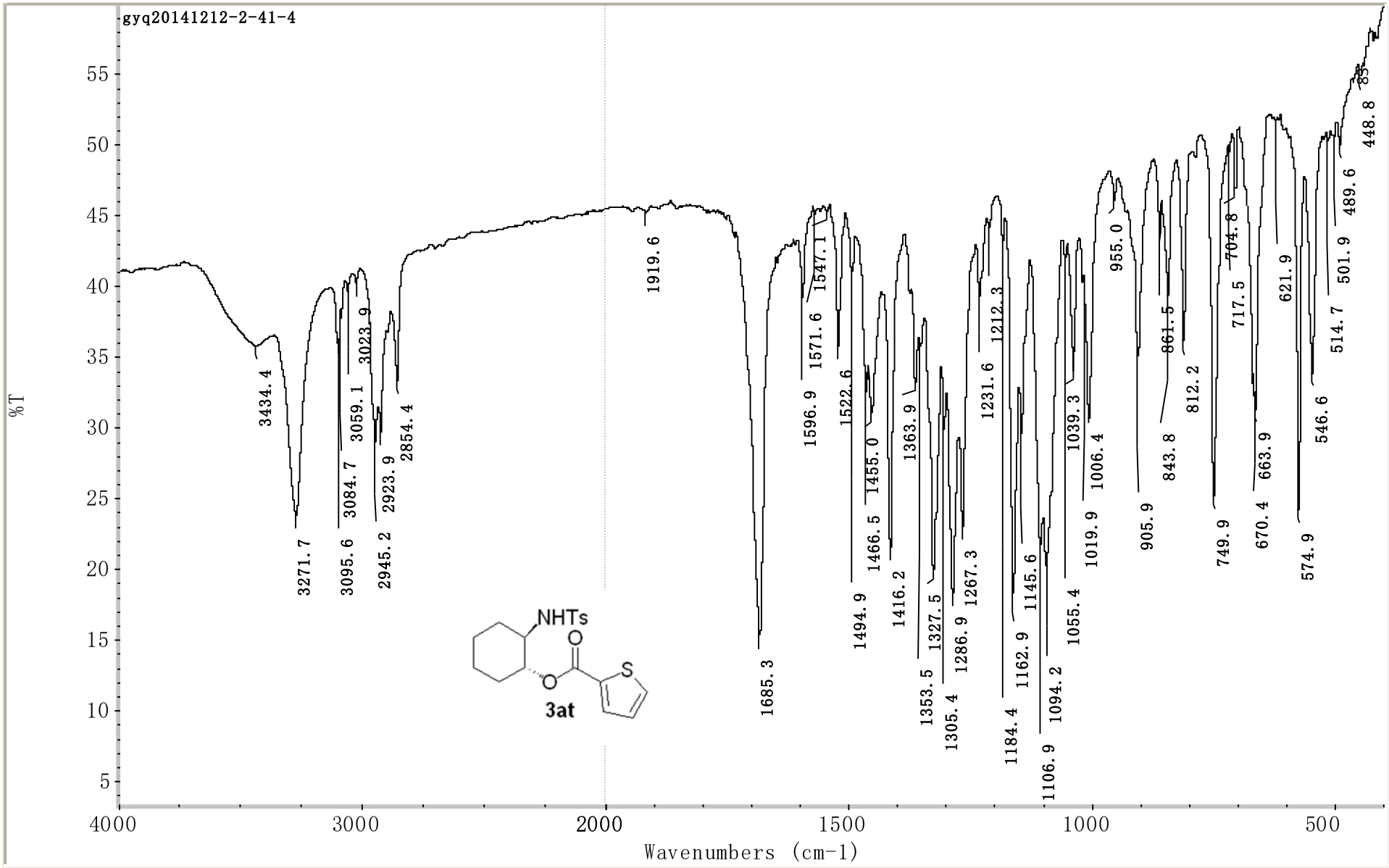

3as
NHTs
O
O
O
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
2.07
1.06
1.91
1.00
0.84
0.85
1.00
1.18
3.29
1.36
1.31
2.42
4.09
7.662
7.642
7.531
7.290
7.069
7.049
6.928
6.920
6.465
6.461
6.457
5.257
5.238
4.815
4.804
4.789
4.778
4.764
4.752
3.348
3.337
3.320
3.312
3.303
3.294
3.278
3.266
2.290
2.150
2.117
2.026
1.993
1.721
1.689
1.666
1.471
1.442
1.421
1.404
1.374
1.343
1.312
1.288
1.259
0.000

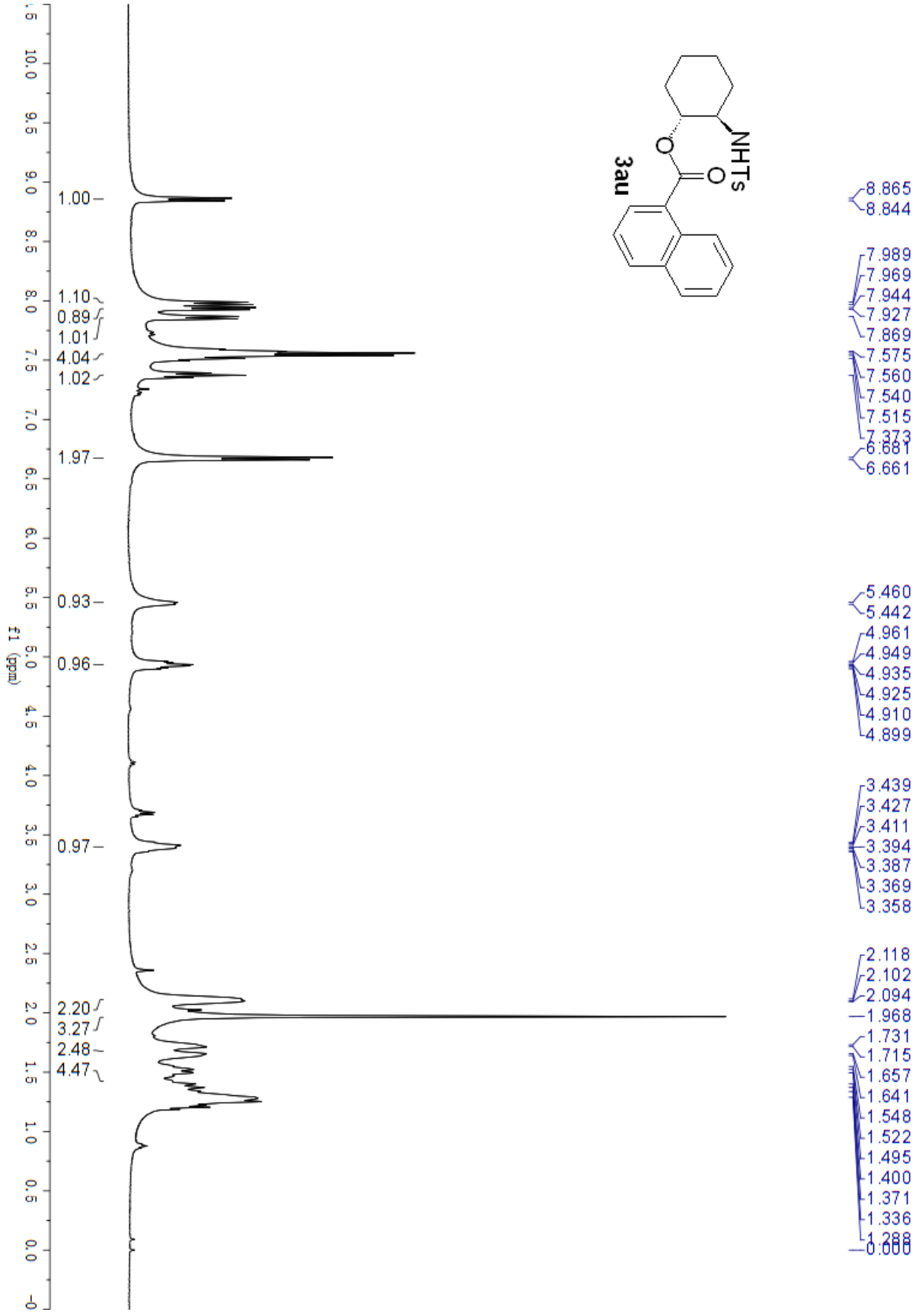

3as
NHTs
O
O
O
158.8
146.4
144.1
142.7
138.1
129.3
126.7
118.4
111.8
77.4
77.3
77.1
76.8
74.7
57.1
33.9
31.2
24.2
23.7
21.5
f1 (ppm)

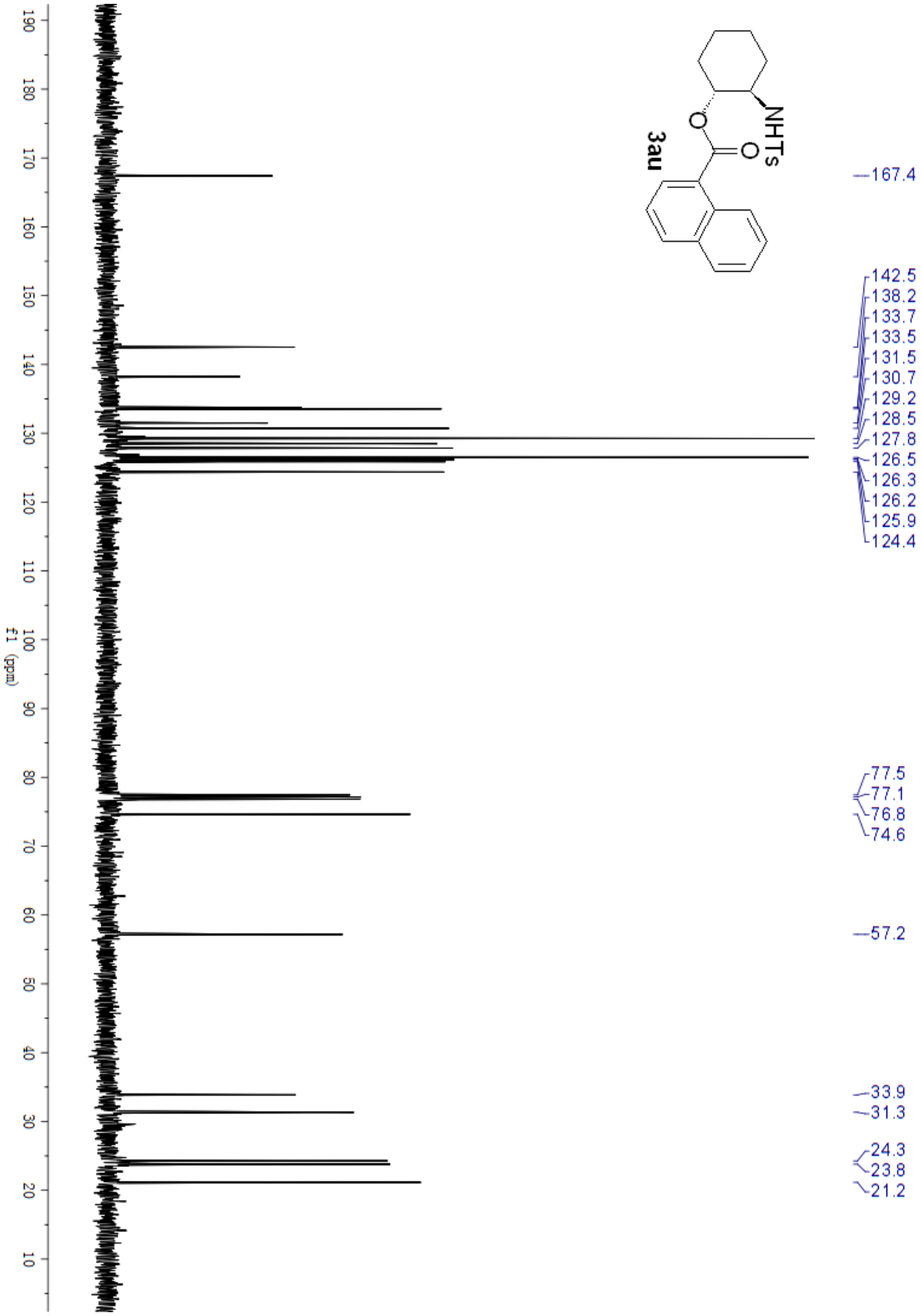

%T
Wavenumbers (cm-1)
gyq20141209-2-41-3
3as
NHTs
3423.8
3318.3
3137.9
2936.4
2859.4
1930.9
1716.2
1623.9
1597.5
1578.1
1569.1
1543.5
1496.3
1510.6
1472.2
1455.2
1441.5
1397.5
1374.4
1320.7
1303.6
1296.1
1249.8
1235.1
1213.2
1180.3
1157.7
1138.5
1122.4
1084.5
1020.1
1011.8
929.6
907.7
883.2
840.2
817.5
773.4
765.9
705.3
670.9
613.0
597.8
576.2
566.7
547.9
490.7
466.6

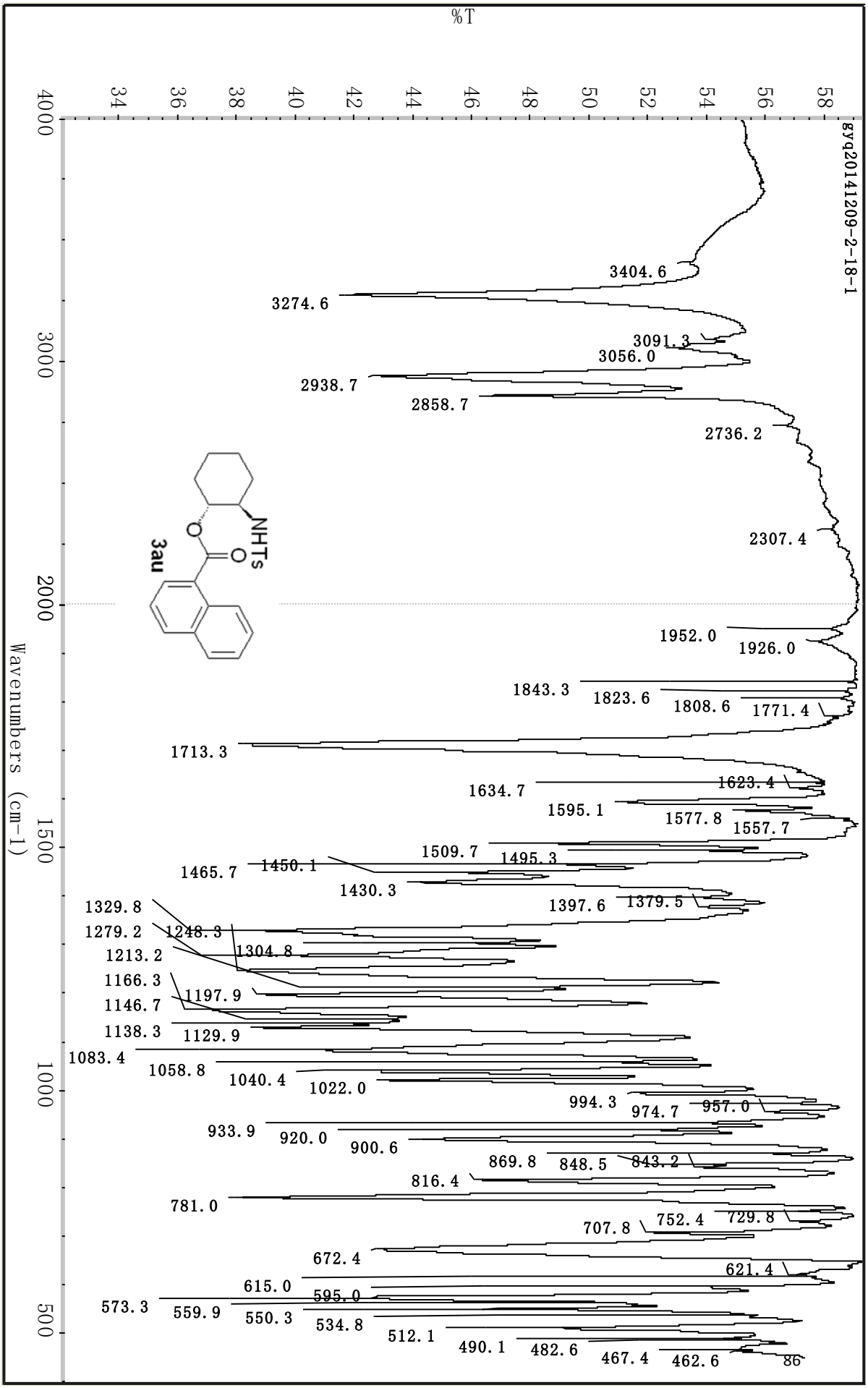

3at
NHTs
O
O
S
f1 (ppm)
1.95
1.86
0.99
1.79
0.93
1.00
1.05
2.99
1.37
1.32
2.40
4.39
7.634
7.614
7.536
7.529
7.526
7.524
7.521
7.275
7.046
7.036
7.034
7.024
6.997
6.977
5.259
5.241
4.800
4.788
4.775
4.764
4.749
4.737
3.324
3.316
3.307
3.299
3.282
3.273
3.265
3.254
2.238
2.186
2.177
2.153
2.025
2.001
1.991
1.731
1.722
1.691
1.671
1.449
1.411
1.383
1.313
1.287
0.000

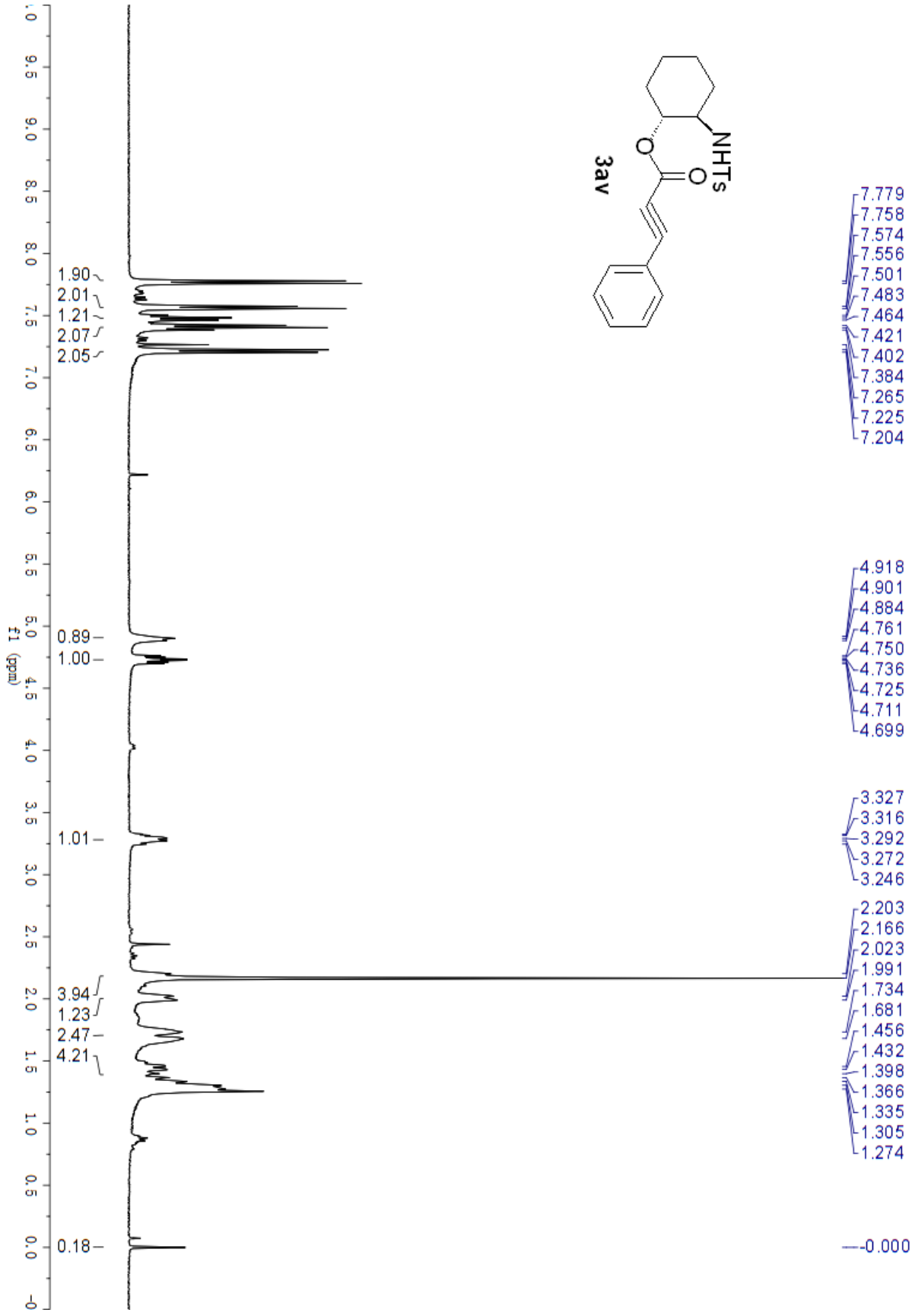

3at
NHTs
O
O
S
162.5
142.7
138.0
133.8
133.5
132.7
129.4
127.6
126.6
77.5
77.3
77.1
76.8
74.9
57.1
33.9
31.2
24.1
23.7
21.5
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
1

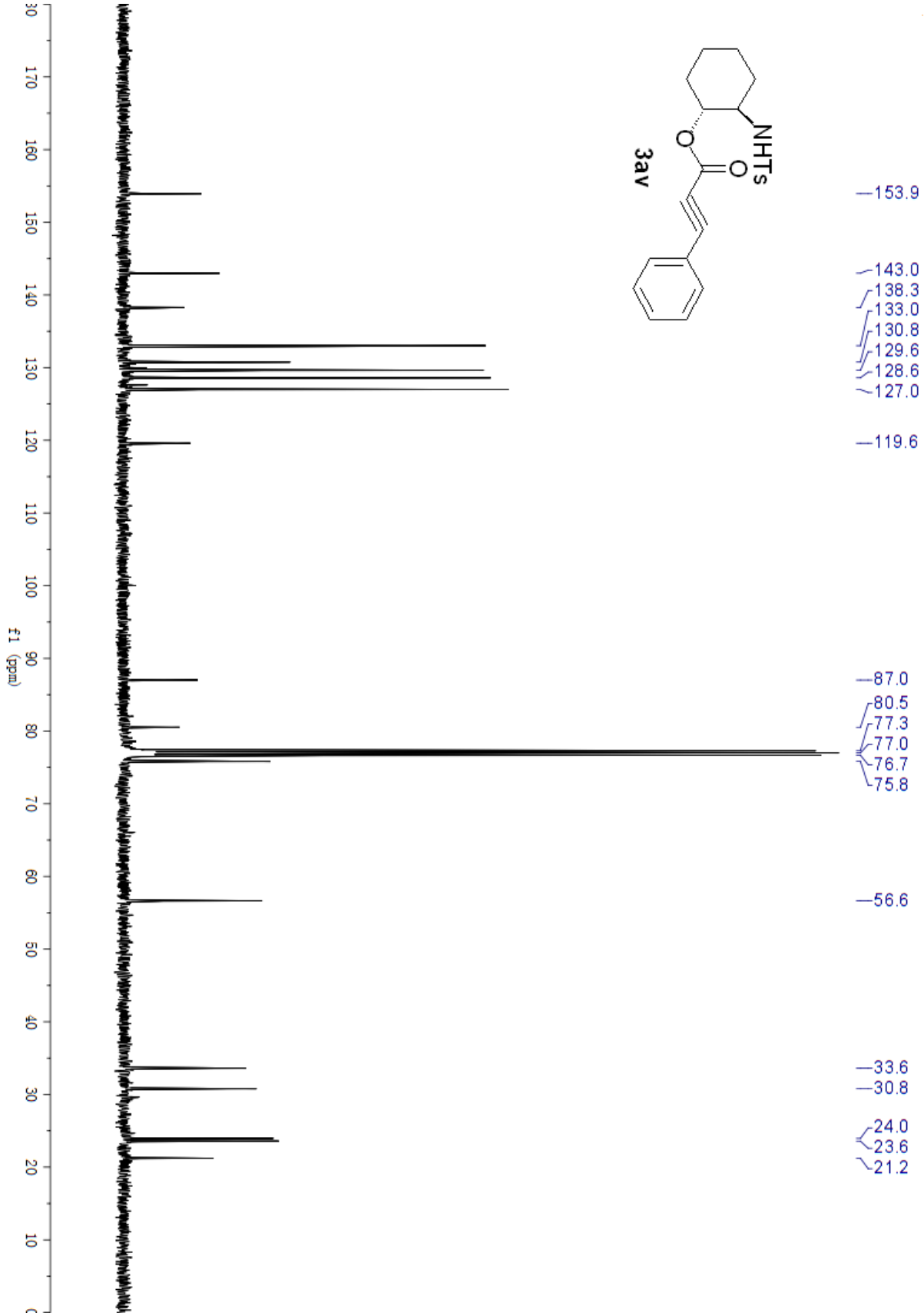

gyq20141212-2-41-4
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
55
50
45
40
35
30
25
20
15
10
5
3434.4
3271.7
3095.6
3084.7
3059.1
3023.9
2945.2
2923.9
2854.4
1919.6
1685.3
1596.9
1571.6
1547.1
1522.6
1494.9
1466.5
1455.0
1416.2
1363.9
1353.5
1327.5
1305.4
1286.9
1267.3
1231.6
1212.3
1184.4
1162.9
1145.6
1106.9
1094.2
1055.4
1039.3
1019.9
1006.4
955.0
905.9
861.5
843.8
812.2
749.9
717.5
704.8
670.4
663.9
621.9
574.9
546.6
514.7
501.9
489.6
448.8
NHTs
O
O
S
3at

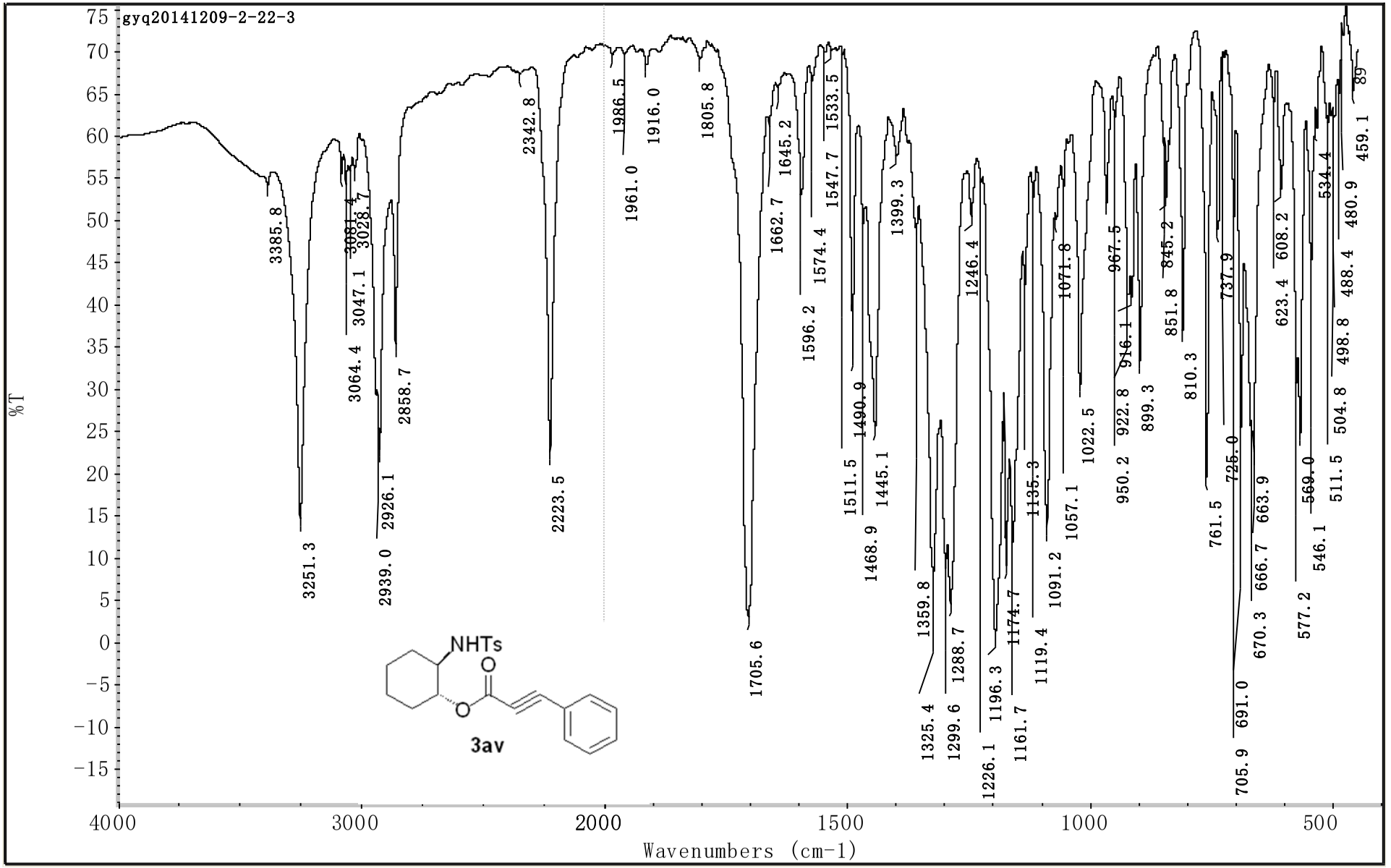

3au
NHTs
O
O
f1 (ppm)
1.00
1.10
0.89
1.01
4.04
1.02
1.97
0.93
0.96
0.97
2.20
3.27
2.48
4.47
8.865
8.844
7.989
7.969
7.944
7.927
7.869
7.575
7.560
7.540
7.515
7.373
6.681
6.661
5.460
5.442
4.961
4.949
4.935
4.925
4.910
4.899
3.439
3.427
3.411
3.394
3.387
3.369
3.358
2.118
2.102
2.094
1.968
1.731
1.715
1.657
1.641
1.548
1.522
1.495
1.400
1.371
1.336
0.000

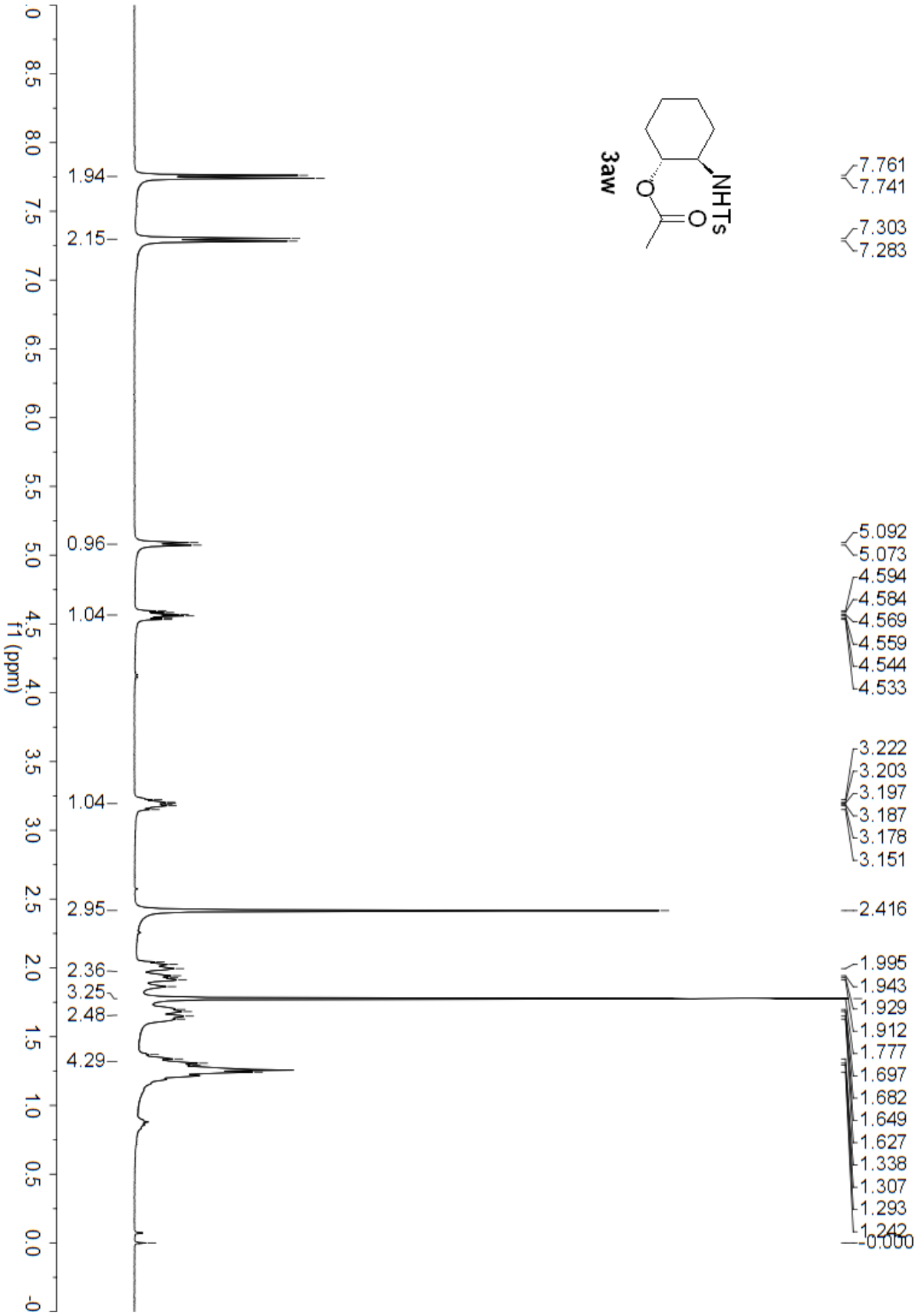

3au
NHTs
O
O
167.4
142.5
138.2
133.7
133.5
131.5
130.7
129.2
128.5
127.8
126.5
126.3
126.2
125.9
124.4
77.5
77.1
76.8
74.6
57.2
33.9
31.3
24.3
23.8
21.2
f1 (ppm)

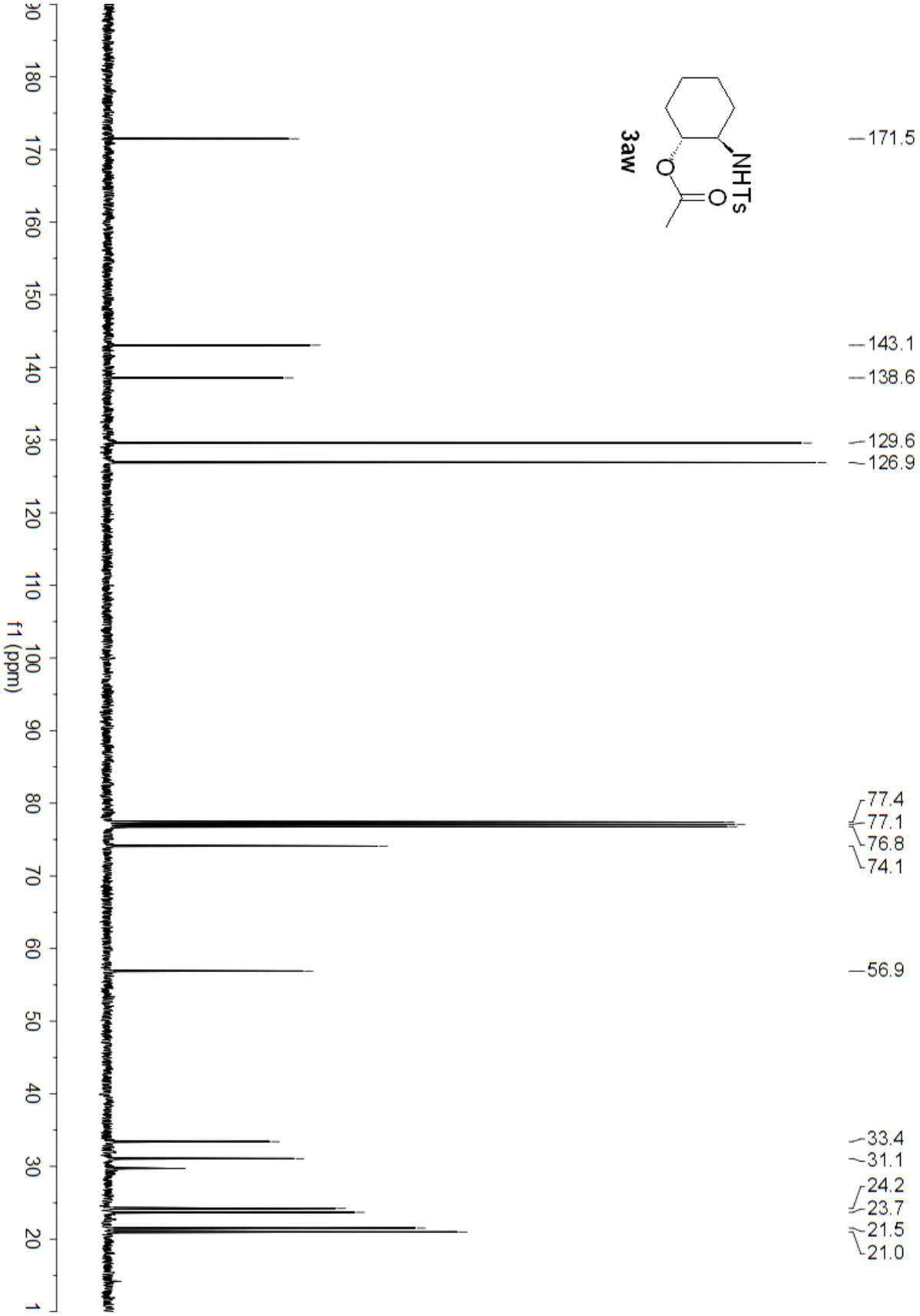

%T
34
36
38
40
42
44
46
48
50
52
54
56
58
gyq20141209-2-18-1
3404.6
3274.6
3091.3
3056.0
2938.7
2858.7
2736.2
2307.4
1952.0
1926.0
1843.3
1823.6
1808.6
1771.4
1713.3
1634.7
1623.4
1595.1
1577.8
1557.7
1509.7
1495.3
1465.7
1450.1
1430.3
1397.6
1379.5
1329.8
1279.2
1248.3
1213.2
1304.8
1166.3
1197.9
1146.7
1138.3
1129.9
1083.4
1058.8
1040.4
1022.0
994.3
974.7
957.0
933.9
920.0
900.6
869.8
848.5
843.2
816.4
781.0
752.4
729.8
707.8
672.4
621.4
615.0
595.0
573.3
559.9
550.3
534.8
512.1
490.1
482.6
467.4
462.6
86
NHTs
O
O
3au
4000
3000
2000
1500
1000
500
Wavenumbers (cm-1)

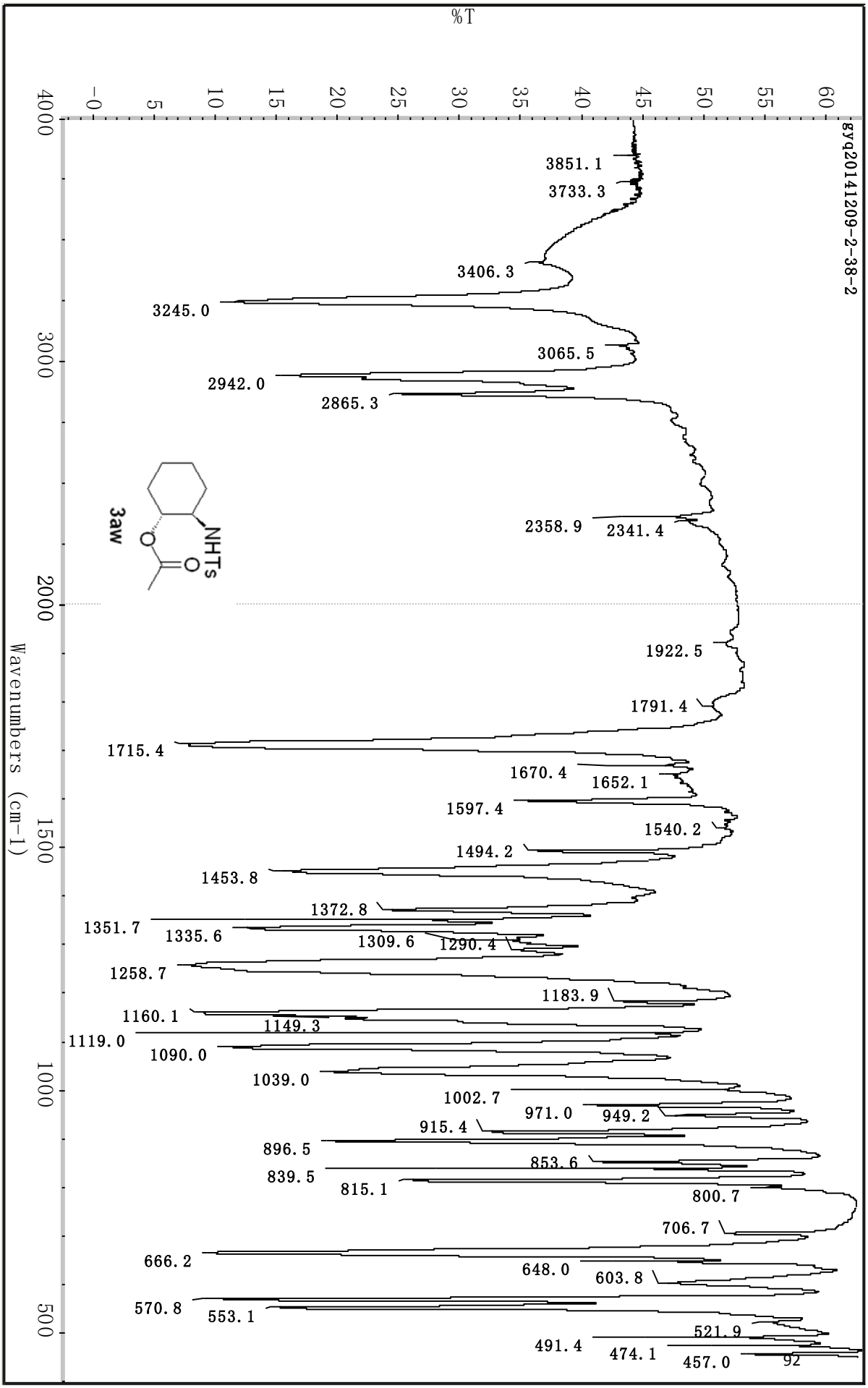

3av
NHTs
O
O
7.779
7.758
7.574
7.556
7.501
7.483
7.464
7.421
7.402
7.384
7.265
7.225
7.204
4.918
4.901
4.884
4.761
4.750
4.736
4.725
4.711
4.699
3.327
3.316
3.292
3.272
3.246
2.203
2.166
2.023
1.991
1.734
1.681
1.456
1.432
1.398
1.366
1.335
1.305
1.274
0.000
1.90
2.01
1.21
2.07
2.05
0.89
1.00
1.01
3.94
1.23
2.47
4.21
0.18
f1 (ppm)

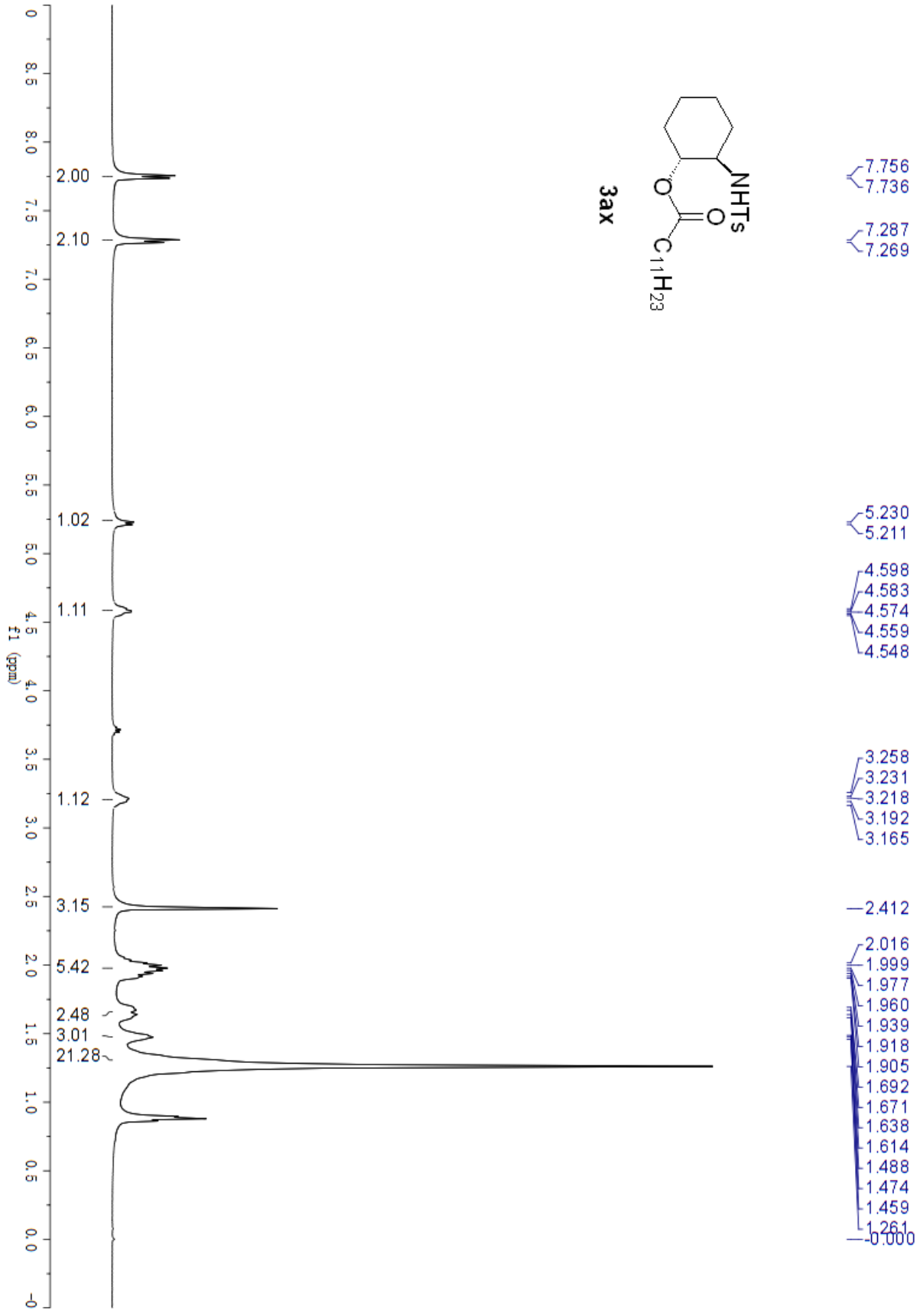

3av
NHTs
O
O
153.9
143.0
138.3
133.0
130.8
129.6
128.6
127.0
119.6
87.0
80.5
77.3
77.0
76.7
75.8
56.6
33.6
30.8
24.0
23.6
21.2
f1 (ppm)

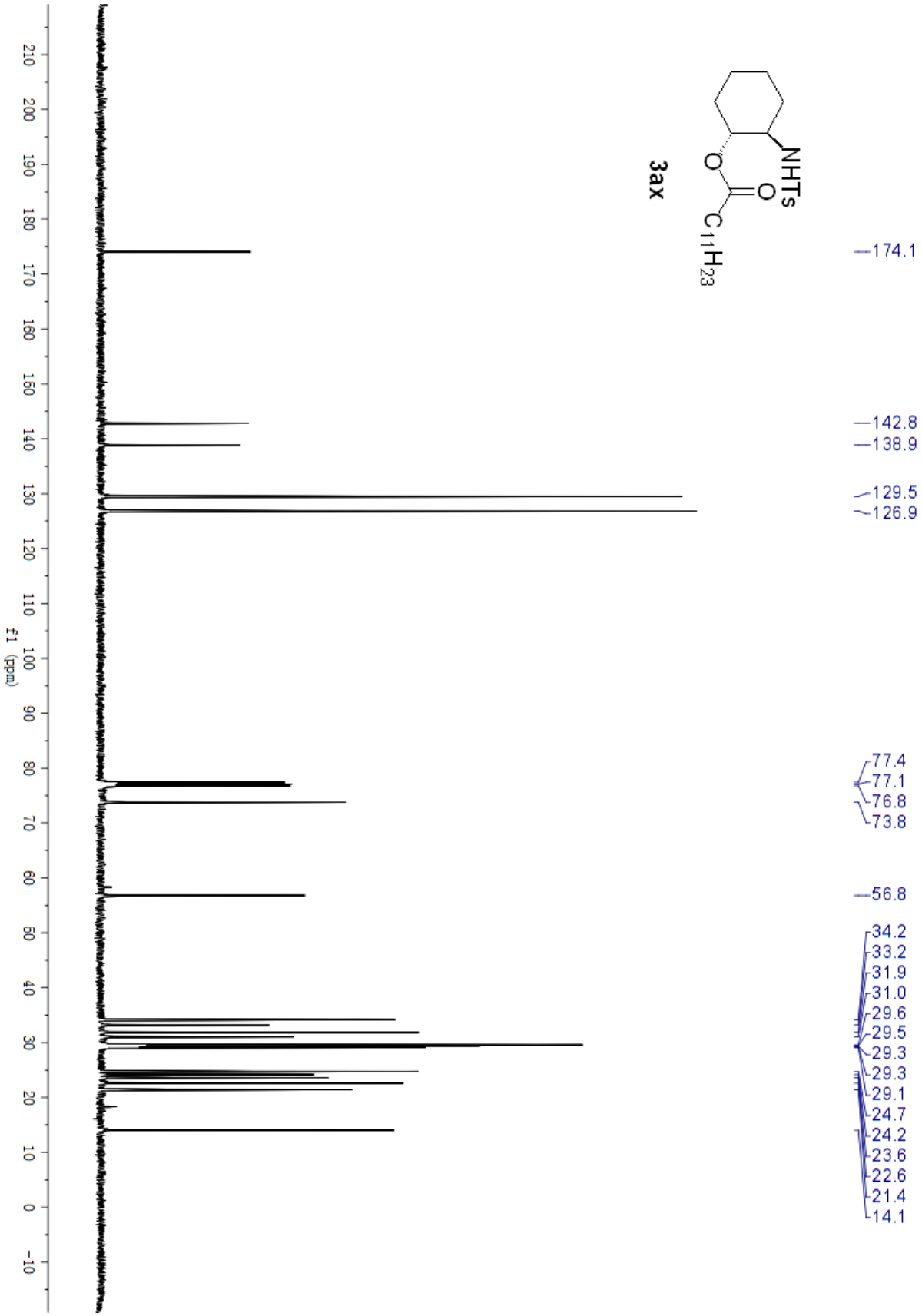

gyq20141209-2-22-3
%T
Wavenumbers (cm-1)
3385.8
3251.3
3081.4
3064.4
3047.1
3028.7
2939.0
2926.1
2858.7
2342.8
2223.5
1986.5
1961.0
1916.0
1805.8
1705.6
1662.7
1645.2
1596.2
1574.4
1547.7
1533.5
1511.5
1490.9
1468.9
1445.1
1399.3
1359.8
1325.4
1299.6
1288.7
1246.4
1226.1
1196.3
1174.7
1161.7
1135.3
1119.4
1091.2
1071.8
1057.1
1022.5
967.5
950.2
922.8
916.1
899.3
851.8
845.2
810.3
761.5
737.9
726.0
705.9
691.0
670.3
666.7
663.9
623.4
608.2
577.2
569.0
546.1
534.4
511.5
504.8
498.8
488.4
480.9
459.1
NHTs
O
O
3av

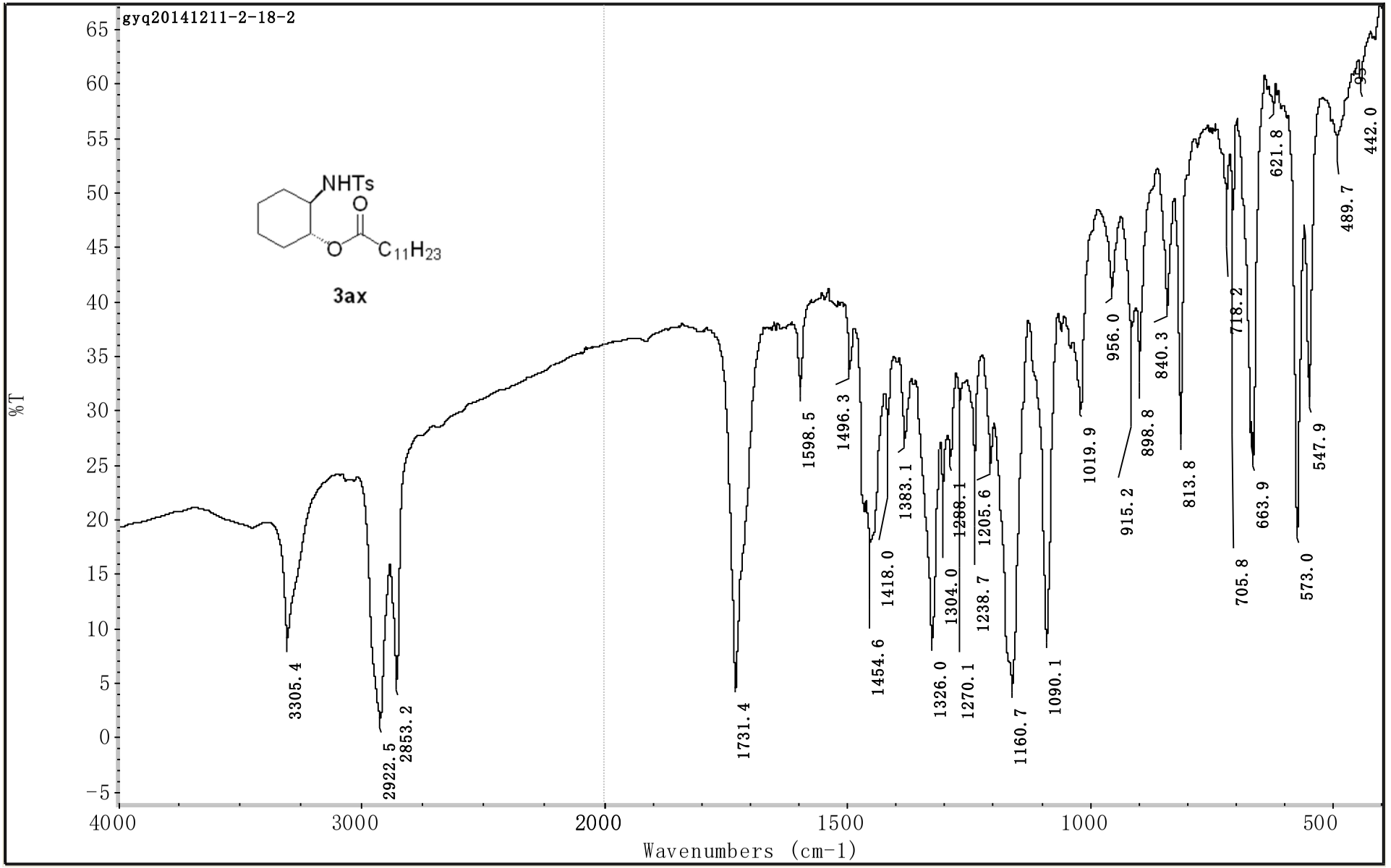

3aw
NHTs
O
O
f1 (ppm)
1.94
2.15
0.96
1.04
1.04
2.95
2.36
3.25
2.48
4.29
7.761
7.741
7.303
7.283
5.092
5.073
4.594
4.584
4.569
4.559
4.544
4.533
3.222
3.203
3.197
3.187
3.178
3.151
2.416
1.995
1.943
1.929
1.912
1.777
1.697
1.682
1.649
1.627
1.338
1.307
1.293
1.242
0.000

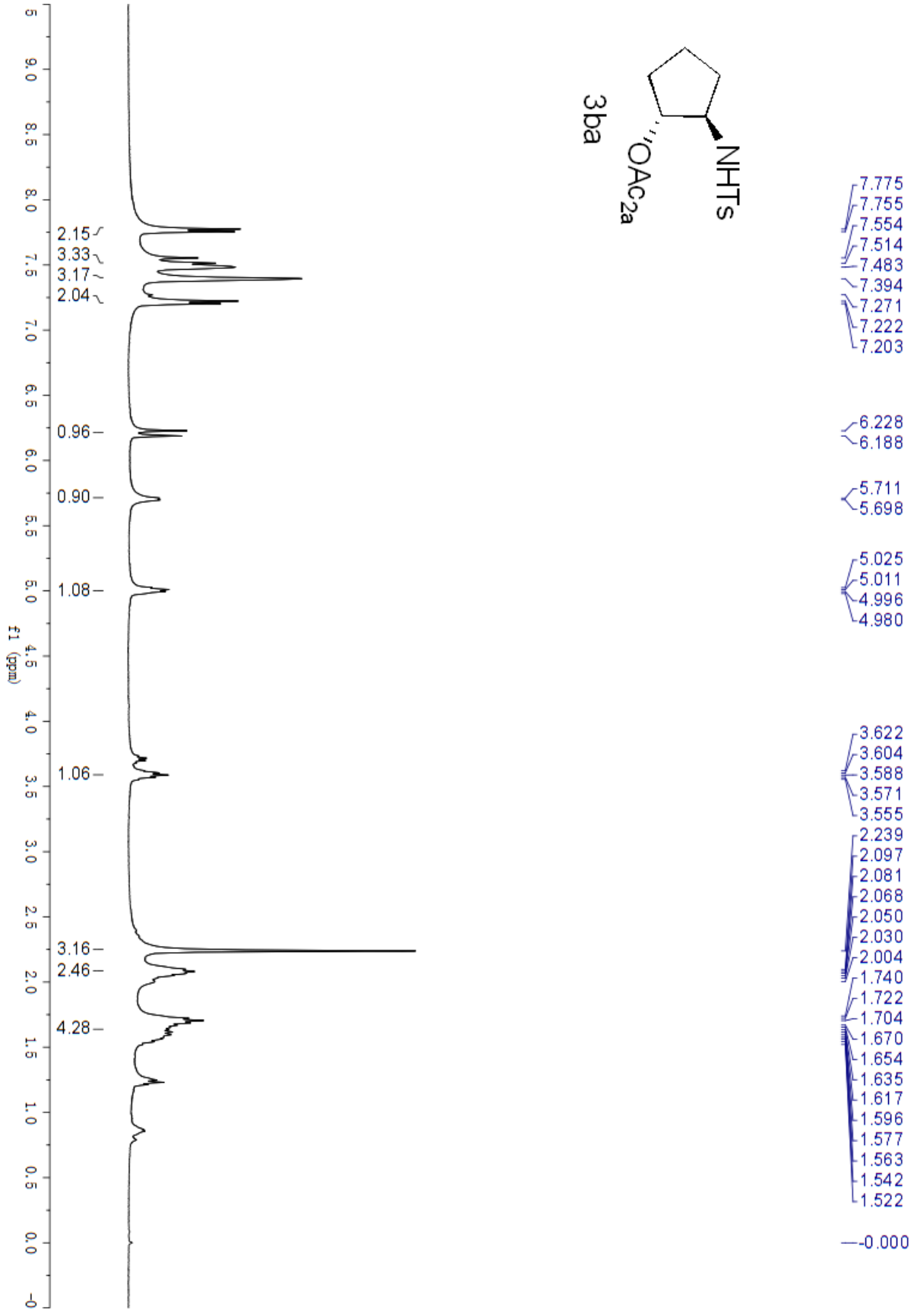

3aw
NHTs
O
O
171.5
143.1
138.6
129.6
126.9
77.4
77.1
76.8
74.1
56.9
33.4
31.1
24.2
23.7
21.5
21.0
f1 (ppm)

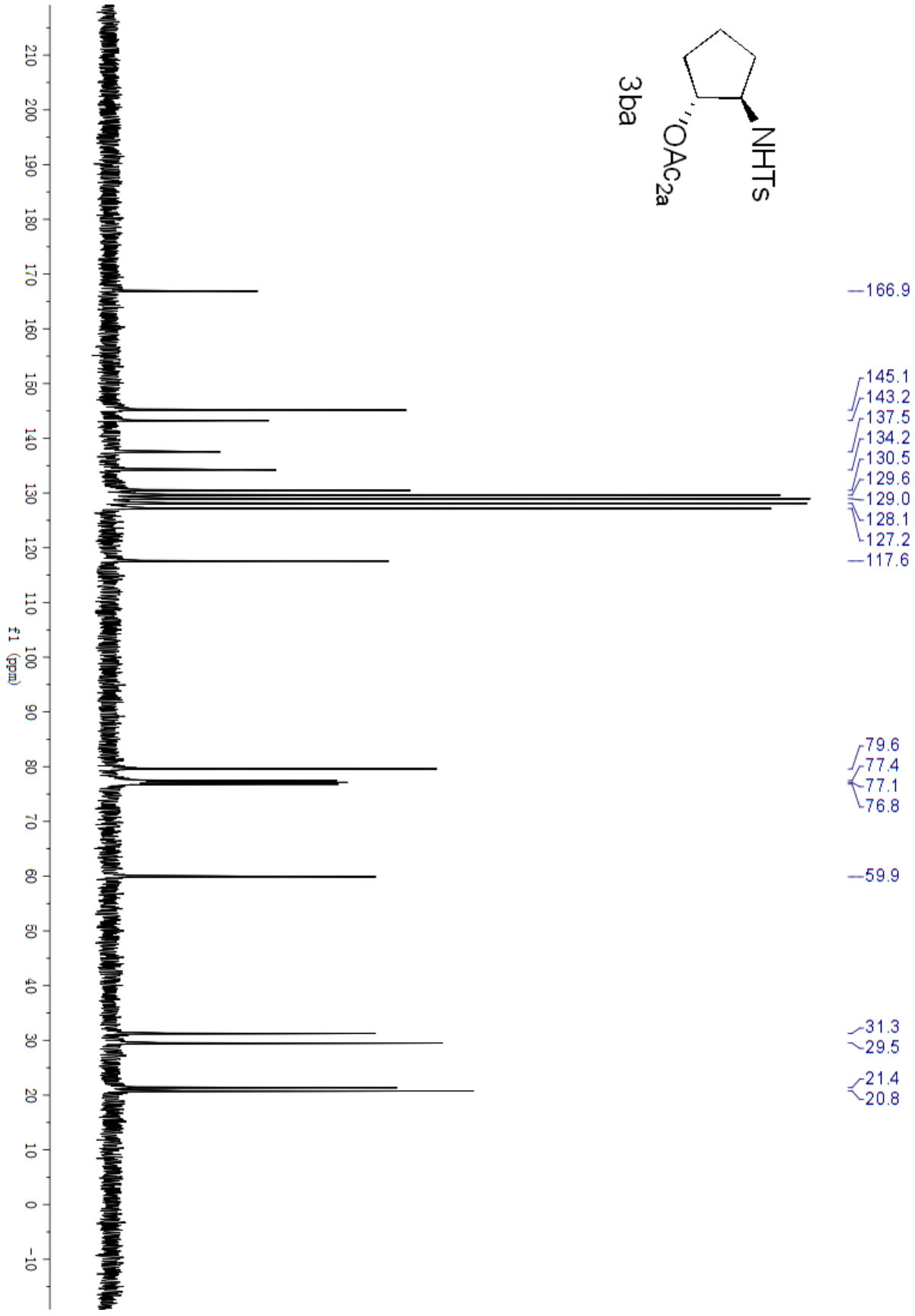

%T
Wavenumbers (cm-1)
gyq20141209-2-38-2
3aw
NHTs
O
O
3851.1
3733.3
3406.3
3245.0
3065.5
2942.0
2865.3
2358.9
2341.4
1922.5
1791.4
1715.4
1670.4
1652.1
1597.4
1540.2
1494.2
1453.8
1372.8
1351.7
1335.6
1309.6
1290.4
1258.7
1183.9
1160.1
1149.3
1119.0
1090.0
1039.0
1002.7
971.0
949.2
915.4
896.5
853.6
839.5
815.1
800.7
706.7
666.2
648.0
603.8
570.8
553.1
521.9
491.4
474.1
457.0
92

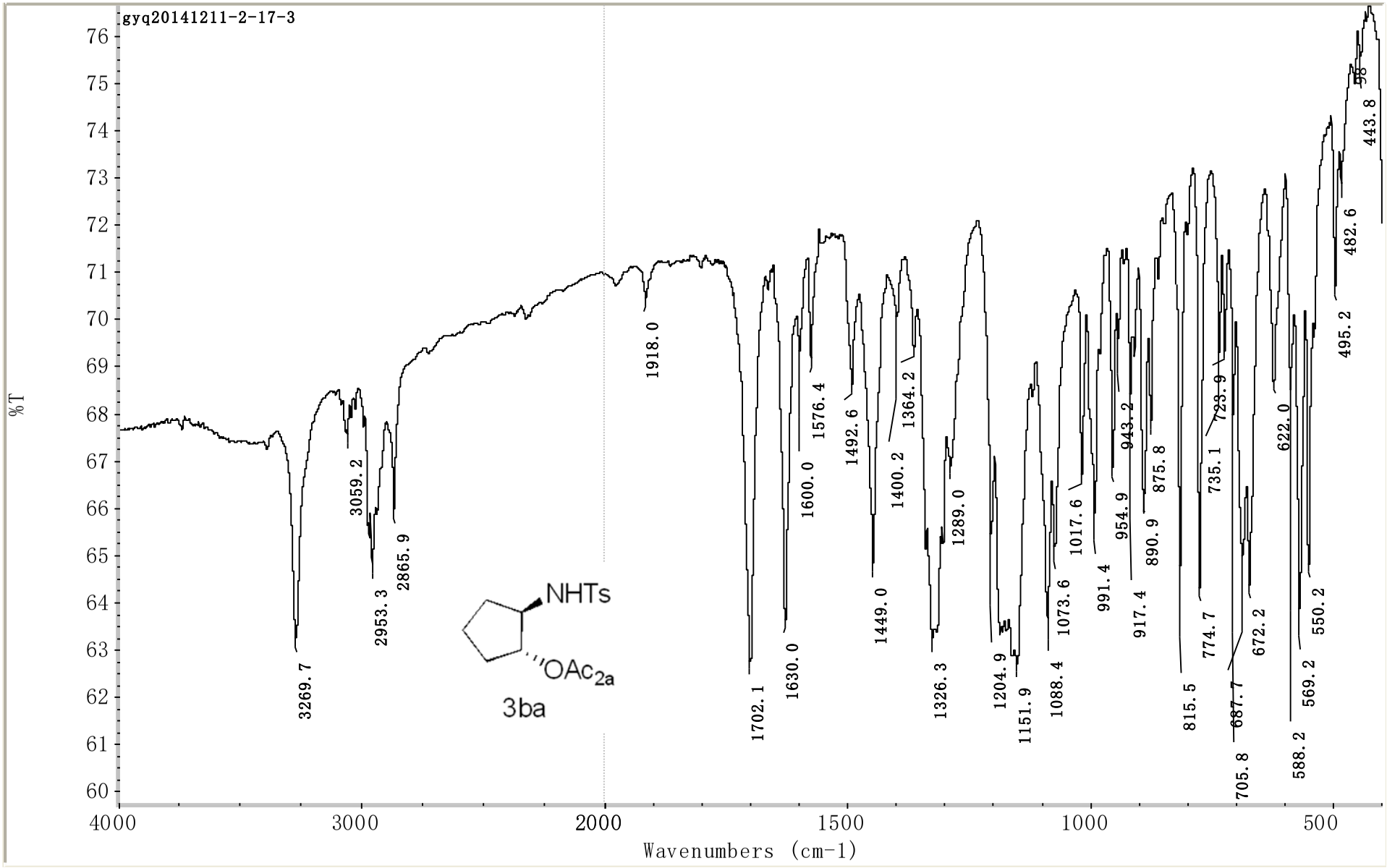

3ax
NHTs
O
O
$C_{11}H_{23}$
f1 (ppm)
2.00
2.10
1.02
1.11
1.12
3.15
5.42
2.48
3.01
21.28
7.756
7.736
7.287
7.269
5.230
5.211
4.598
4.583
4.574
4.559
4.548
3.258
3.231
3.218
3.192
3.165
2.412
2.016
1.999
1.977
1.960
1.939
1.918
1.905
1.692
1.671
1.638
1.614
1.488
1.474
1.459
1.261
0.000

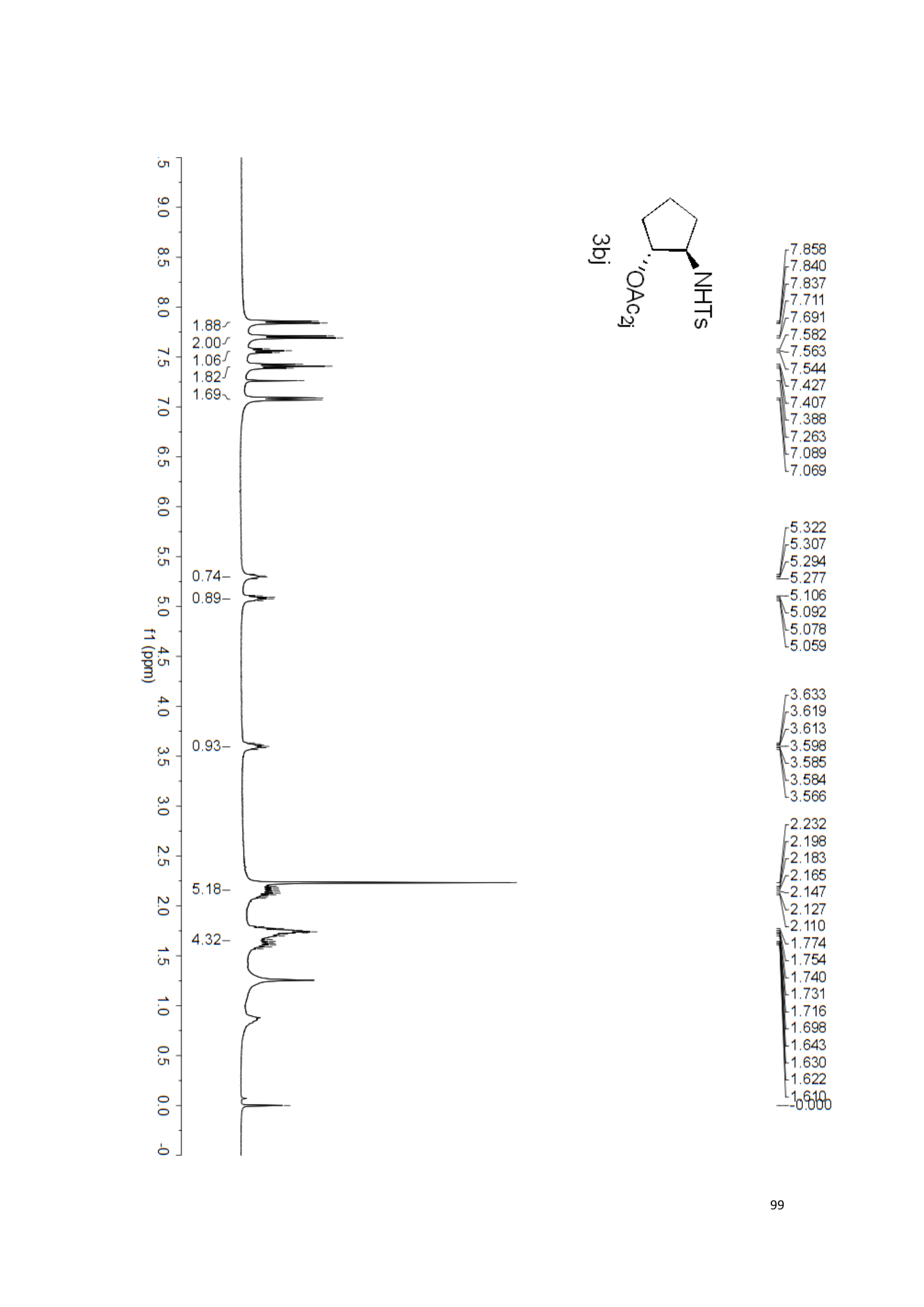

3ax
NHTs
O
O
C11H23
174.1
142.8
138.9
129.5
126.9
77.4
77.1
76.8
73.8
56.8
34.2
33.2
31.9
31.0
29.6
29.5
29.3
29.3
29.1
24.7
24.2
23.6
22.6
21.4
14.1
f1 (ppm)

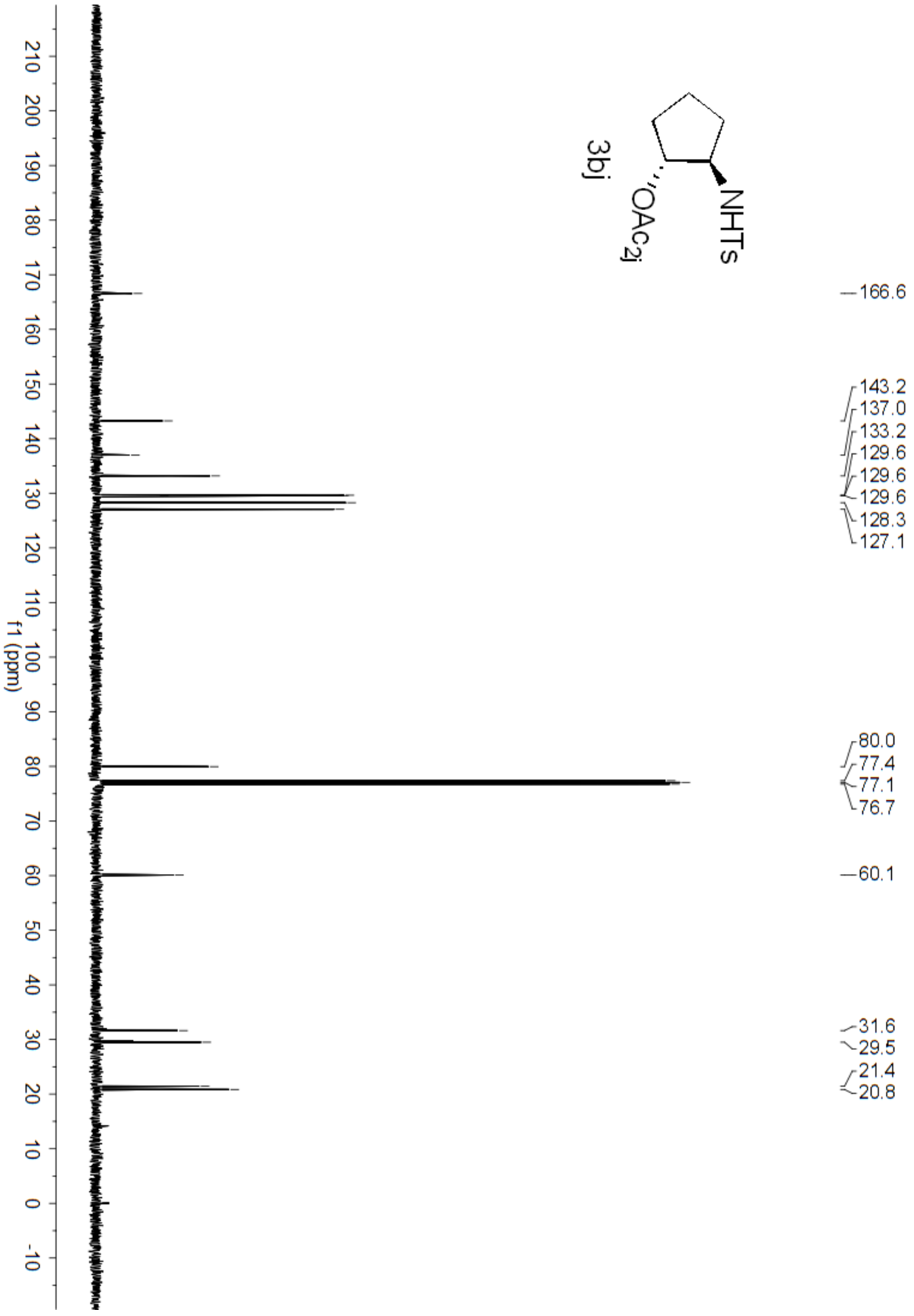

gyq20141211-2-18-2
NHTs
O
O
$C_{11}H_{23}$
3ax
%T
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
4000
3000
2000
1500
1000
500
Wavenumbers (cm-1)
3305.4
2922.5
2853.2
1731.4
1598.5
1496.3
1454.6
1418.0
1383.1
1326.0
1304.0
1288.1
1270.1
1238.7
1205.6
1160.7
1090.1
1019.9
956.0
915.2
898.8
840.3
813.8
718.2
705.8
663.9
621.8
573.0
547.9
489.7
442.0

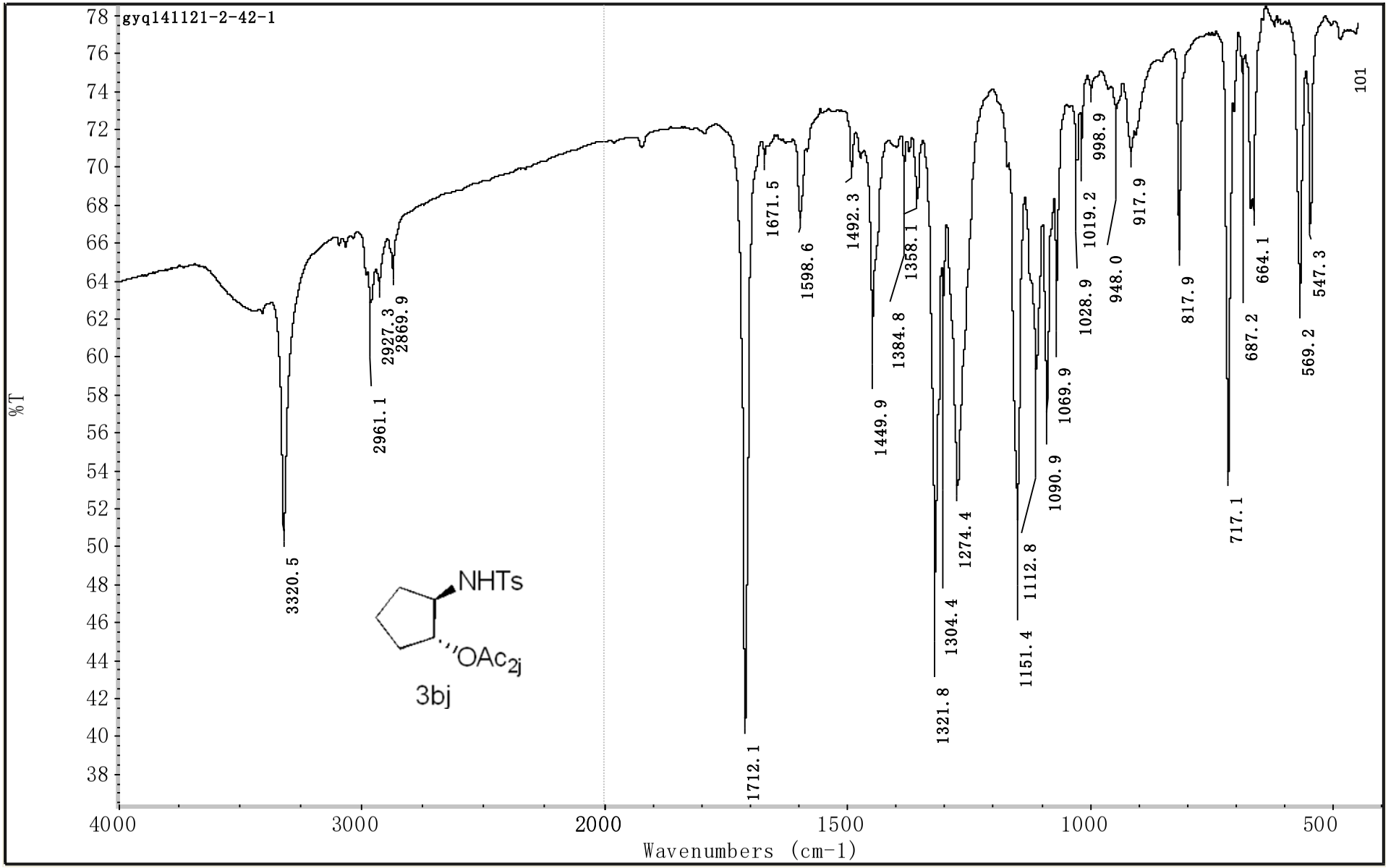

3ba
NHTs
OAc
2a
7.775
7.755
7.554
7.514
7.483
7.394
7.271
7.222
7.203
6.228
6.188
5.711
5.698
5.025
5.011
4.996
4.980
3.622
3.604
3.588
3.571
3.555
2.239
2.097
2.081
2.068
2.050
2.030
2.004
1.740
1.722
1.704
1.670
1.654
1.635
1.617
1.596
1.577
1.563
1.542
1.522
-0.000
2.15
3.33
3.17
2.04
0.96
0.90
1.08
1.06
3.16
2.46
4.28
f1 (ppm)

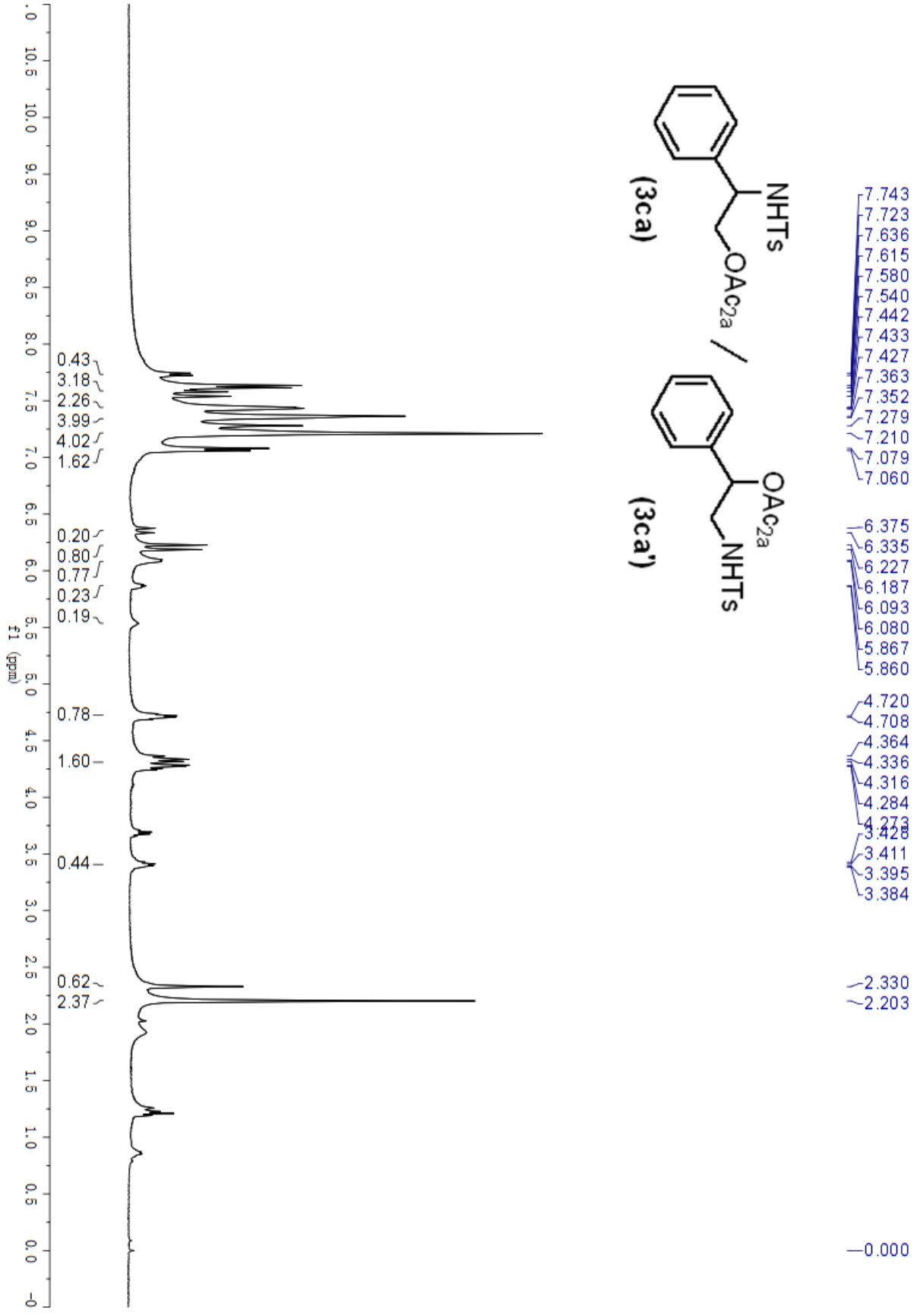

3ba
NHTs
OAc
2a
166.9
145.1
143.2
137.5
134.2
130.5
129.6
129.0
128.1
127.2
117.6
79.6
77.4
77.1
76.8
59.9
31.3
29.5
21.4
20.8
f1 (ppm)

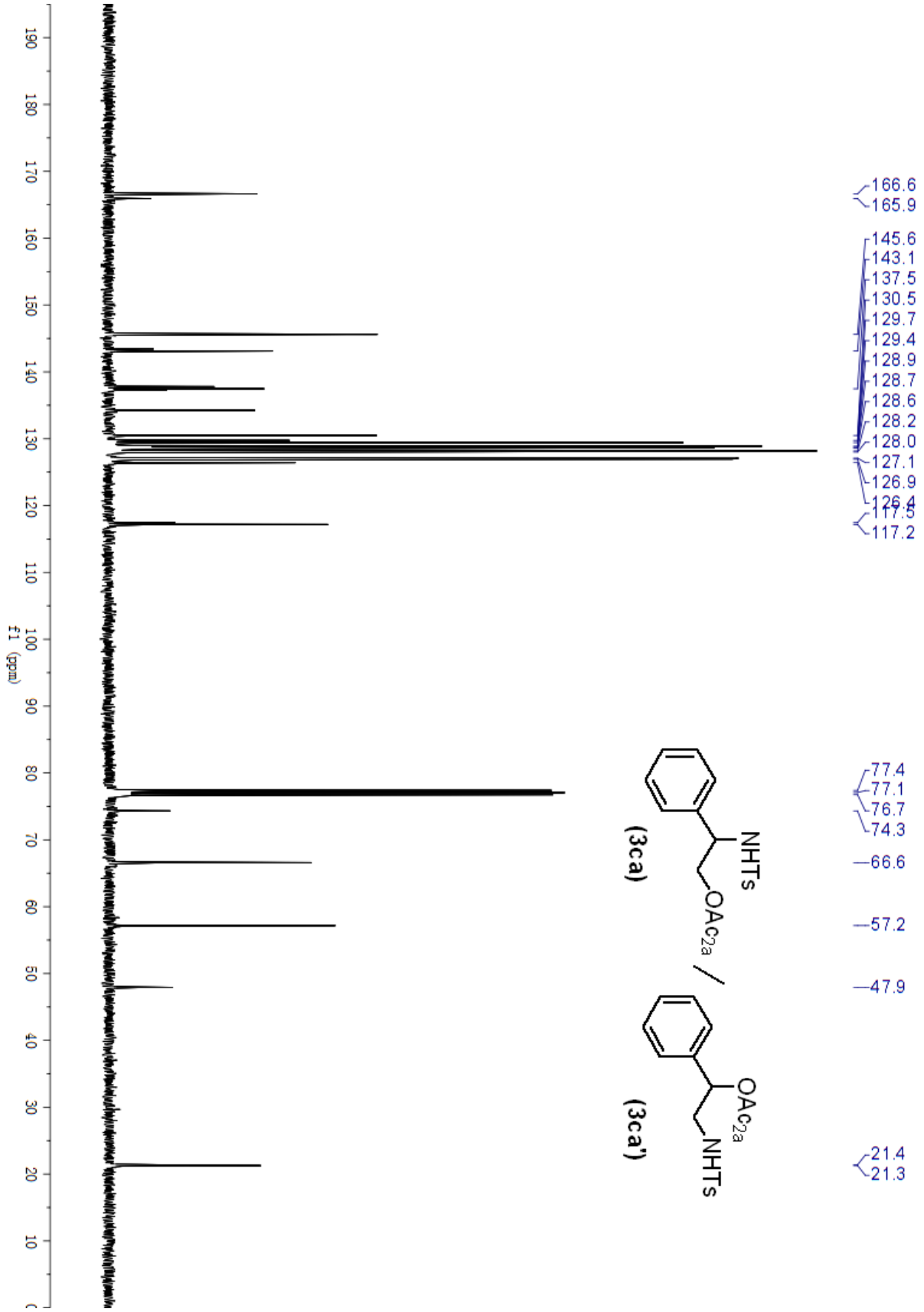

gyq20141211-2-17-3
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3269.7
3059.2
2953.3
2865.9
1918.0
1702.1
1630.0
1600.0
1576.4
1492.6
1449.0
1400.2
1364.2
1326.3
1289.0
1204.9
1151.9
1088.4
1073.6
1017.6
991.4
954.9
943.2
917.4
890.9
875.8
815.5
774.7
735.1
723.9
705.8
687.7
672.2
622.0
588.2
569.2
550.2
495.2
482.6
443.8
NHTs
OAc
2a
3ba

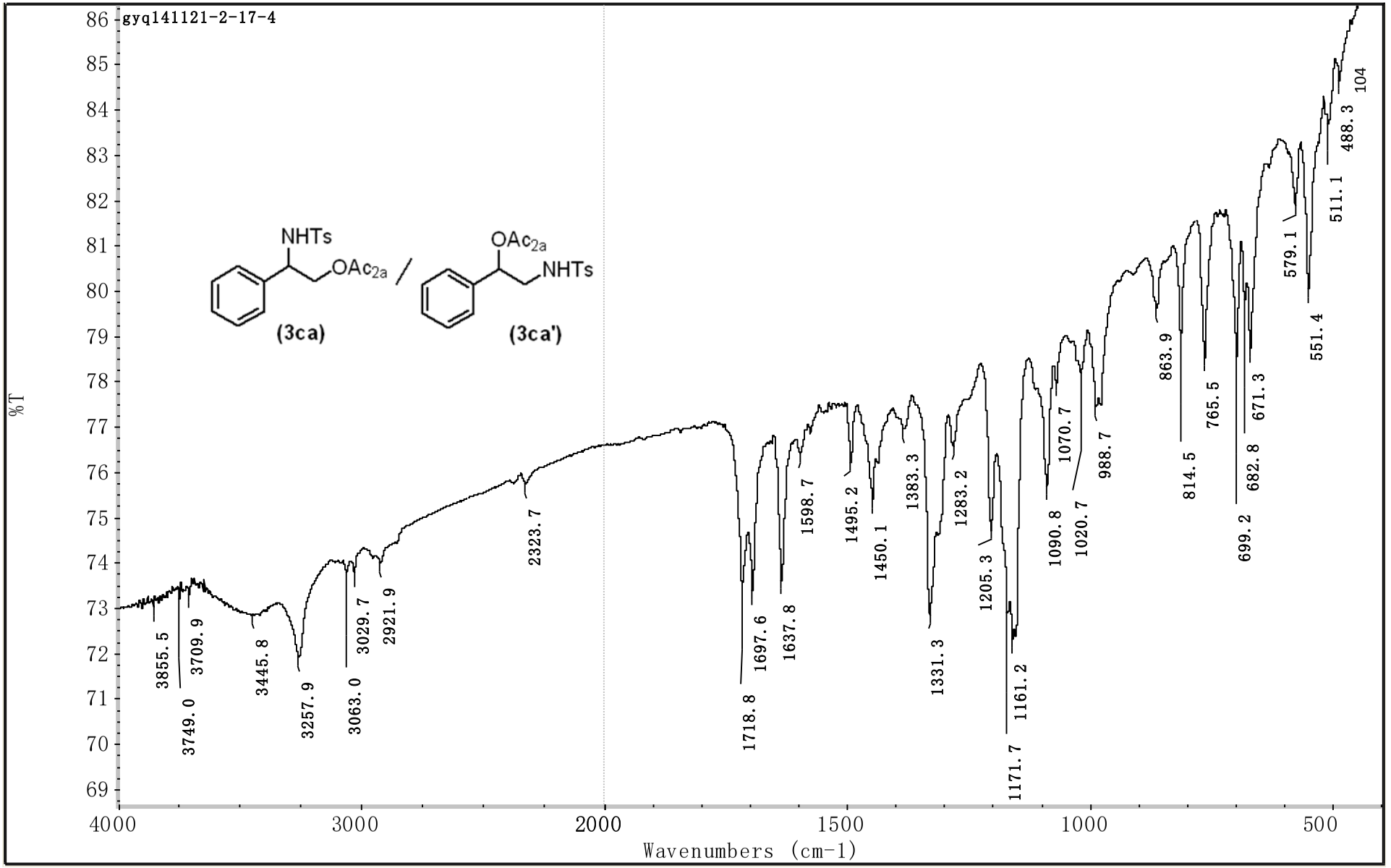

NHTs
OAc
3bj
7.858
7.840
7.837
7.711
7.691
7.582
7.563
7.544
7.427
7.407
7.388
7.263
7.089
7.069
5.322
5.307
5.294
5.277
5.106
5.092
5.078
5.059
3.633
3.619
3.613
3.598
3.585
3.584
3.566
2.232
2.198
2.183
2.165
2.147
2.127
2.110
1.774
1.754
1.740
1.731
1.716
1.698
1.643
1.630
1.622
1.610
0.000
1.88
2.00
1.06
1.82
1.69
0.74
0.89
0.93
5.18
4.32
f1 (ppm)

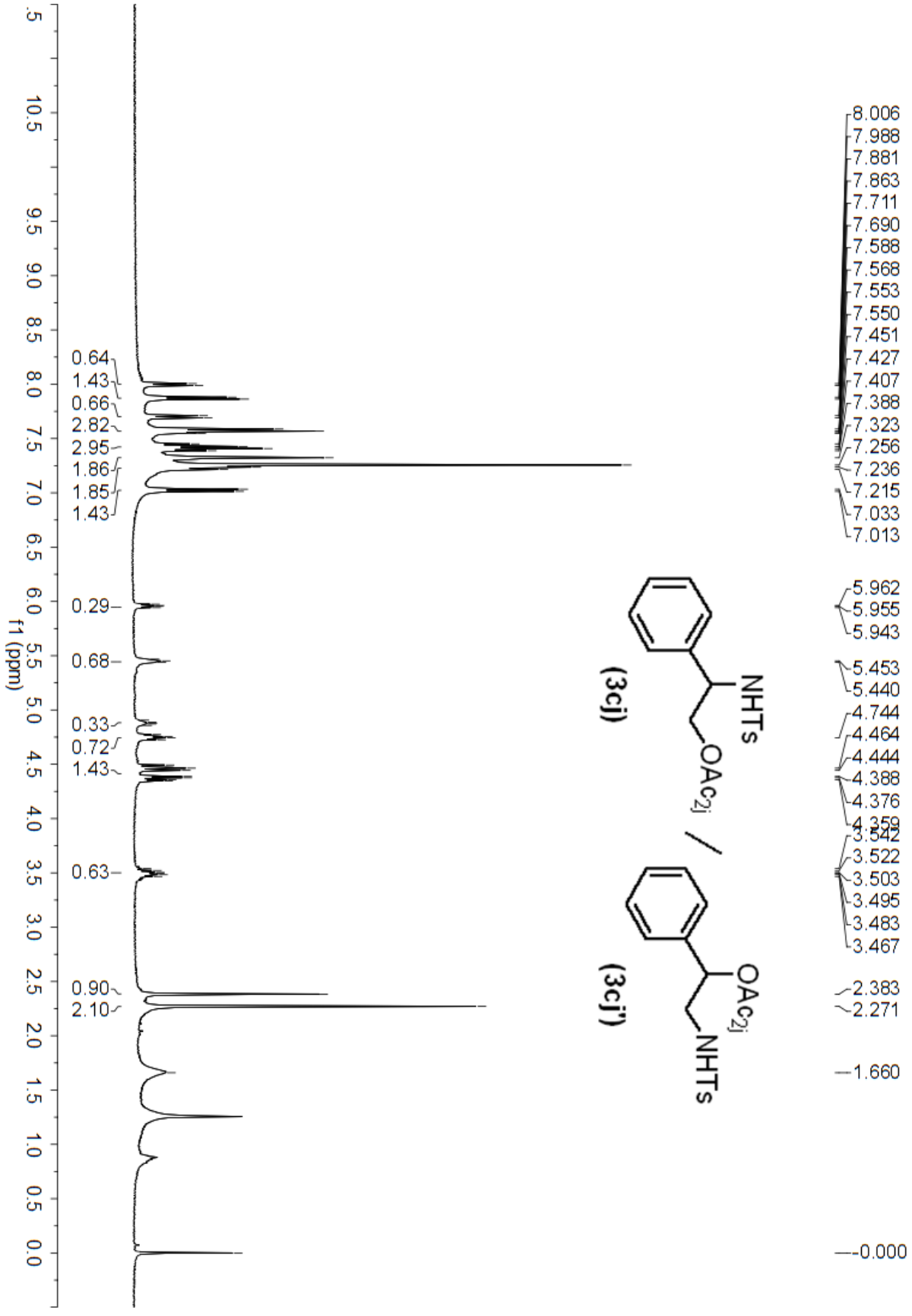

3bj
NHTs
OAc
2j
166.6
143.2
137.0
133.2
129.6
129.6
129.6
128.3
127.1
80.0
77.4
77.1
76.7
60.1
31.6
29.5
21.4
20.8
f1 (ppm)

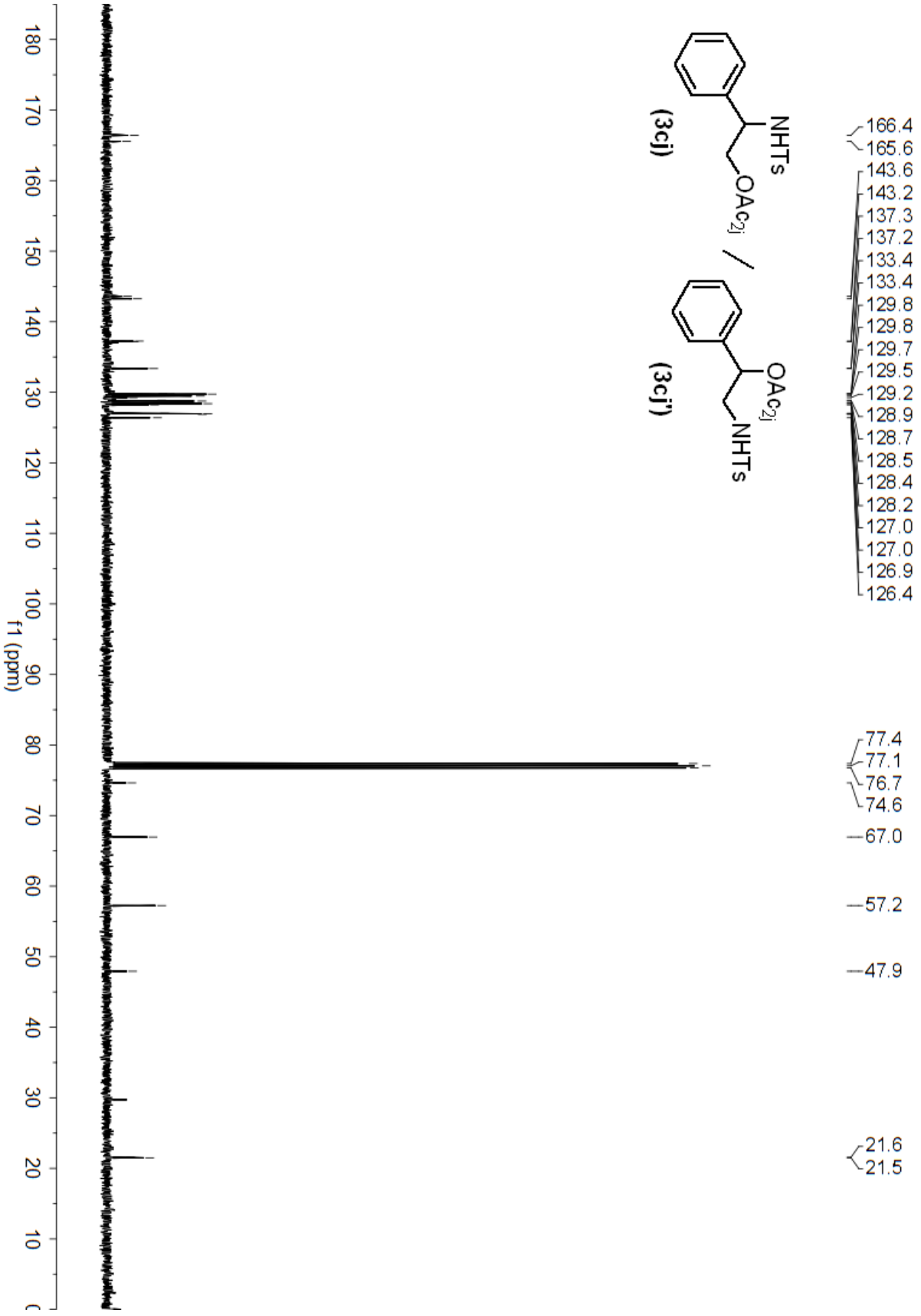

gyq141121-2-42-1
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3320.5
2961.1
2927.3
2869.9
1712.1
1671.5
1598.6
1492.3
1449.9
1384.8
1358.1
1321.8
1304.4
1274.4
1151.4
1112.8
1090.9
1069.9
1028.9
1019.2
998.9
948.0
917.9
817.9
717.1
687.2
664.1
569.2
547.3
NHTs
OAc2j
3bj

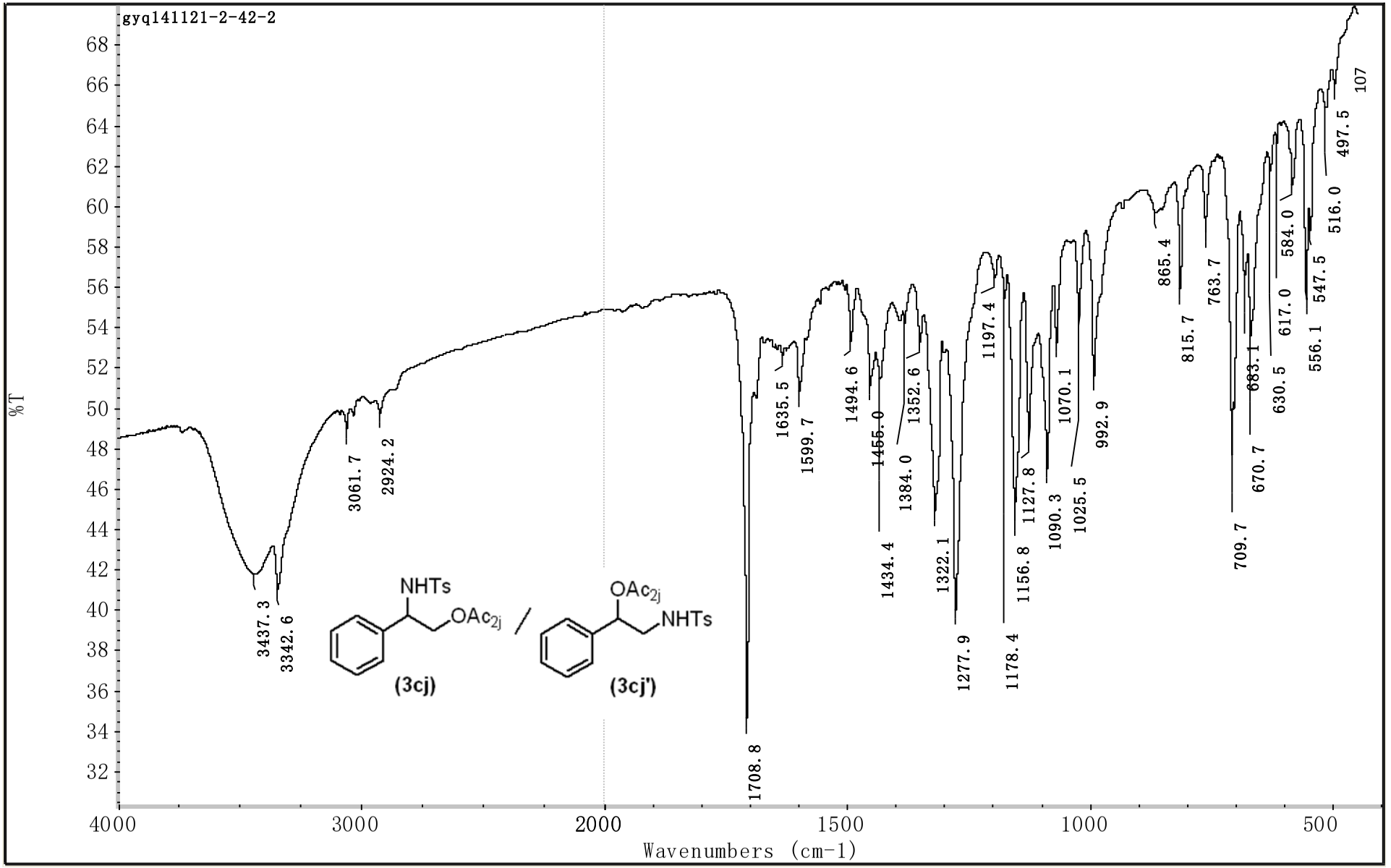

NHTs
OAc2a
(3ca)
OAc2a
NHTs
(3ca')
7.743
7.723
7.636
7.615
7.580
7.540
7.442
7.433
7.427
7.363
7.352
7.279
7.210
7.079
7.060
6.375
6.335
6.227
6.187
6.093
6.080
5.867
5.860
4.720
4.708
4.364
4.336
4.316
4.284
4.273
3.428
3.411
3.395
3.384
2.330
2.203
0.000
0.43
3.18
2.26
3.99
4.02
1.62
0.20
0.80
0.77
0.23
0.19
0.78
1.60
0.44
0.62
2.37
f1 (ppm)

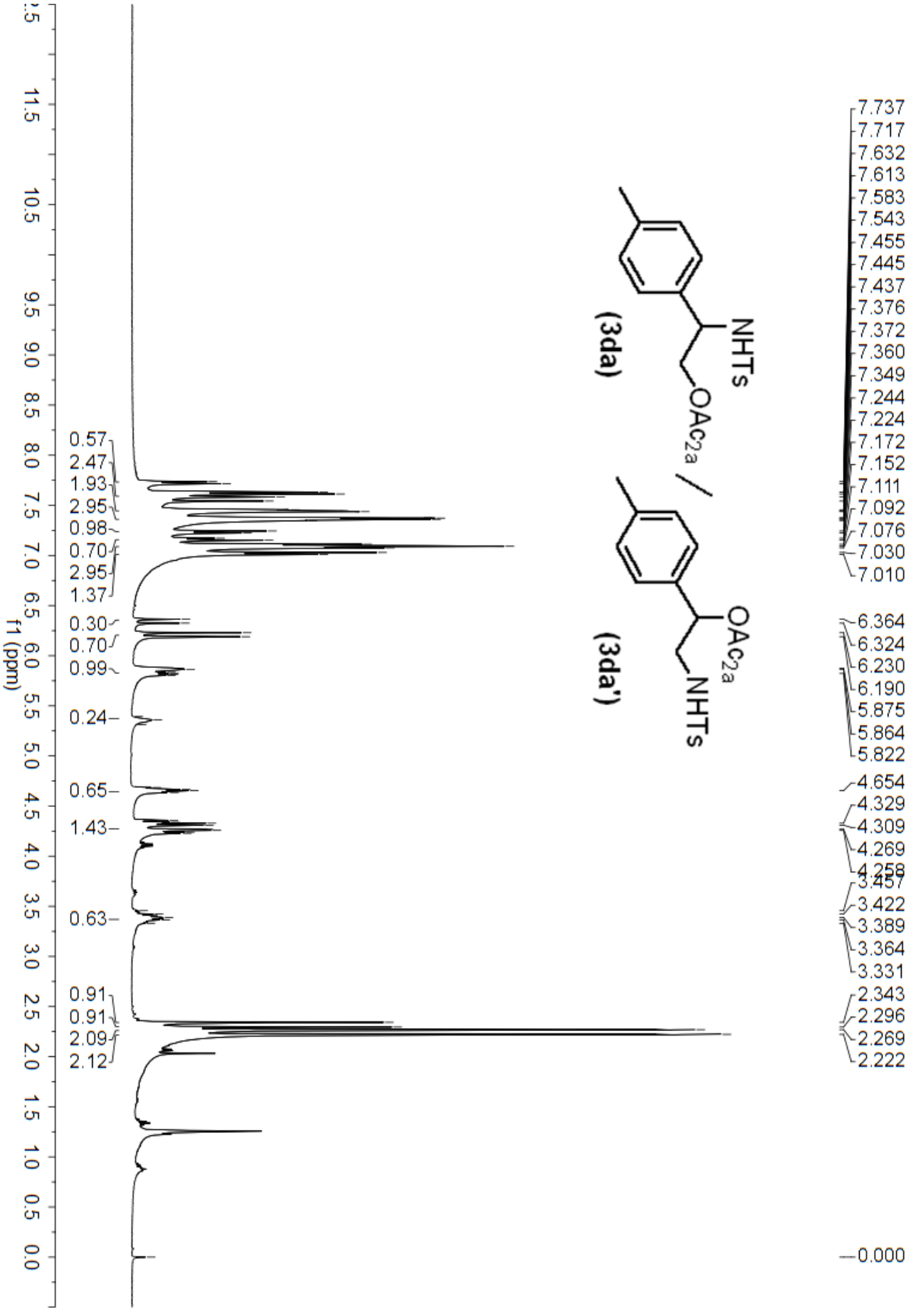

166.6
165.9
145.6
143.1
137.5
130.5
129.7
129.4
128.9
128.7
128.6
128.2
128.0
127.1
126.9
126.4
117.5
117.2
77.4
77.1
76.7
74.3
66.6
57.2
47.9
21.4
21.3
NHTs
OAc2a
(3ca)
OAc2a
NHTs
(3ca')
f1 (ppm)

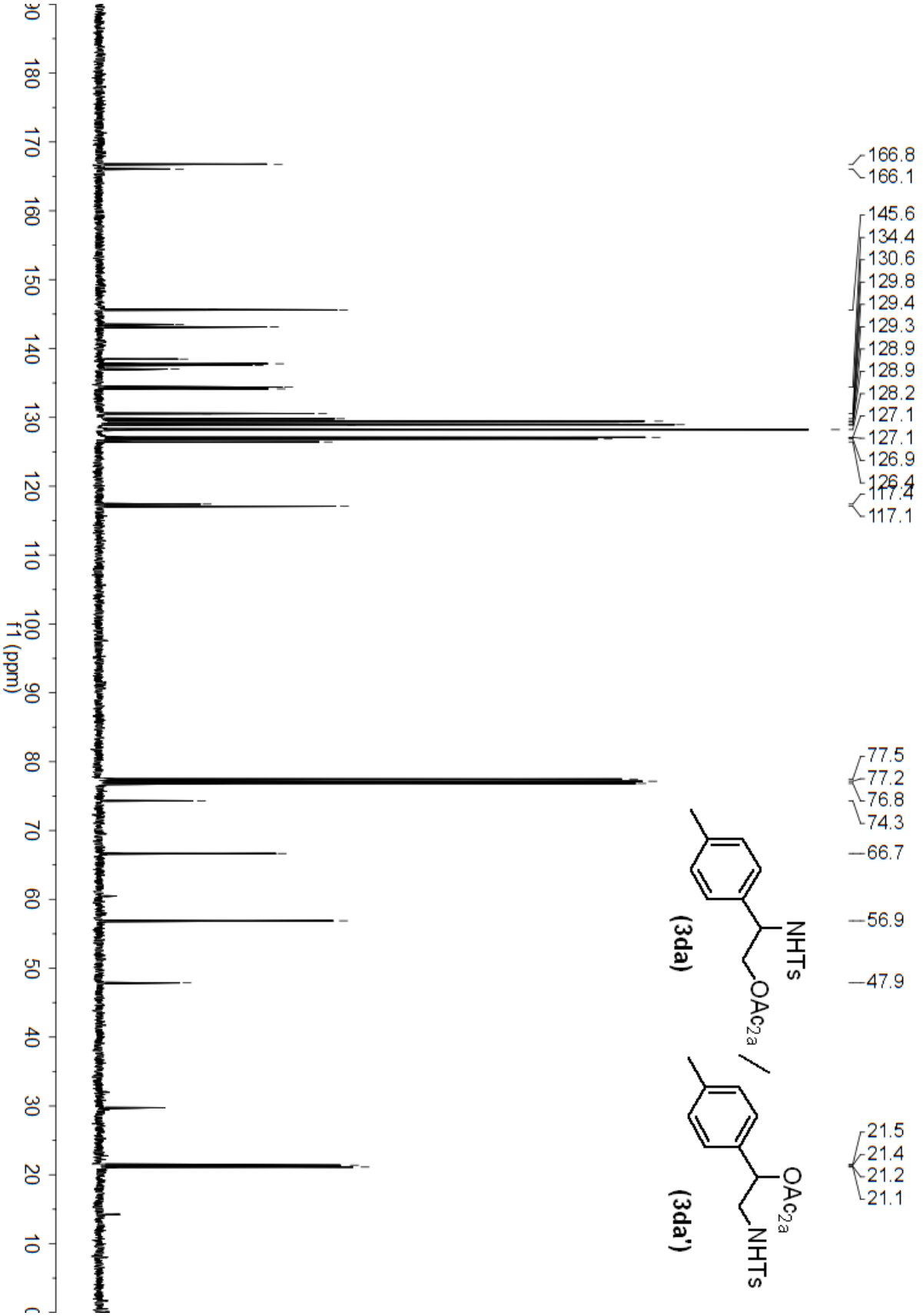

gyq141121-2-17-4
NHTs
OAc2a
(3ca)
OAc2a
NHTs
(3ca')
%T
Wavenumbers (cm-1)
3855.5
3749.0
3709.9
3445.8
3257.9
3063.0
3029.7
2921.9
2323.7
1718.8
1697.6
1637.8
1598.7
1495.2
1450.1
1383.3
1331.3
1283.2
1205.3
1171.7
1161.2
1090.8
1070.7
1020.7
988.7
863.9
814.5
765.5
699.2
682.8
671.3
579.1
551.4
511.1
488.3

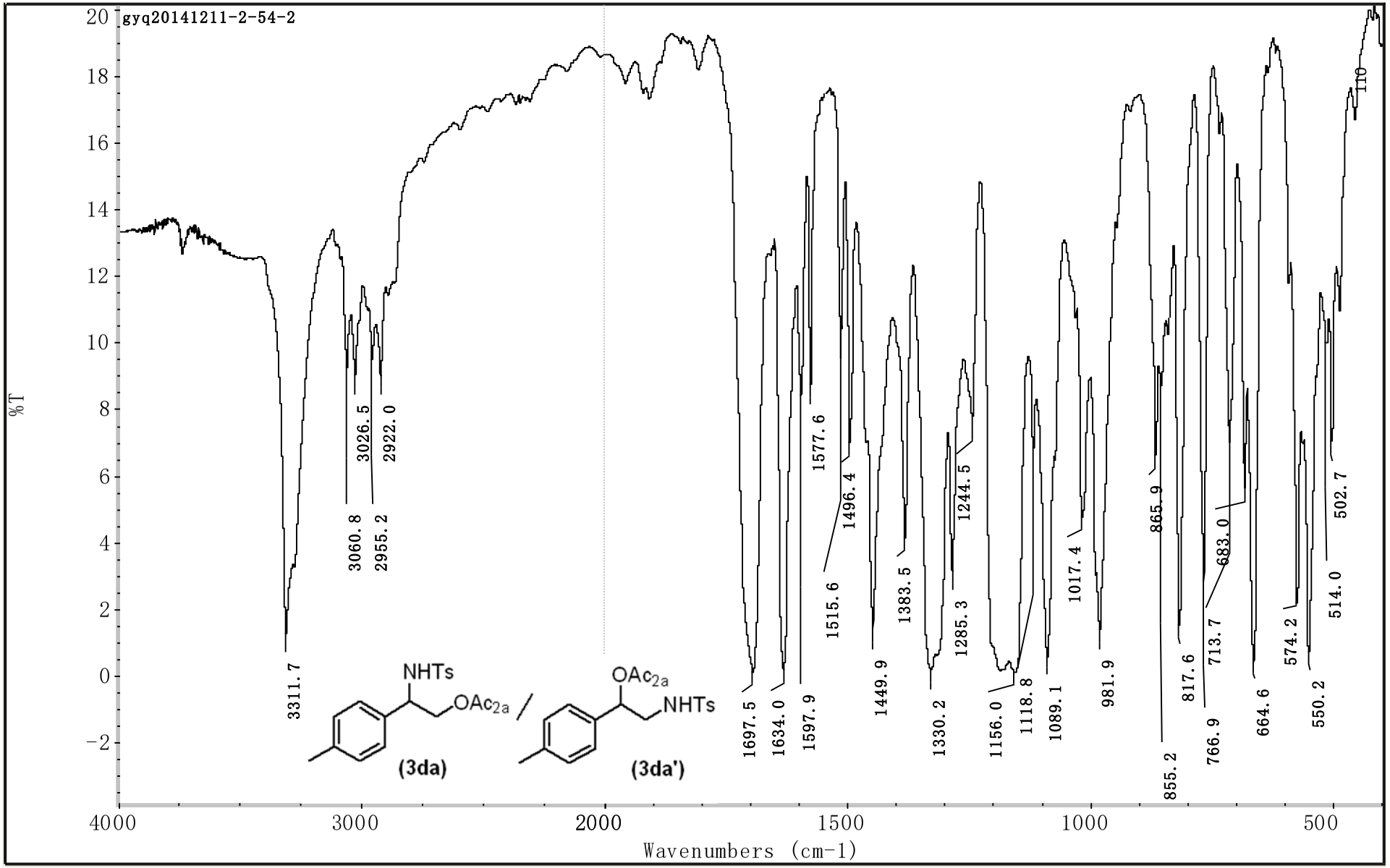

f1 (ppm)
0.64
1.43
0.66
2.82
2.95
1.86
1.85
1.43
0.29
0.68
0.33
0.72
1.43
0.63
0.90
2.10
8.006
7.988
7.881
7.863
7.711
7.690
7.588
7.568
7.553
7.550
7.451
7.427
7.407
7.388
7.323
7.256
7.236
7.215
7.033
7.013
5.962
5.955
5.943
5.453
5.440
4.744
4.464
4.444
4.388
4.376
4.359
3.542
3.522
3.503
3.495
3.483
3.467
2.383
2.271
1.660
0.000
NHTs
OAc2j
(3cj)
OAc2j
NHTs
(3cj')


NHTs
OAc2j
(3cj)
OAc2j
NHTs
(3cj')
166.4
165.6
143.6
143.2
137.3
137.2
133.4
133.4
129.8
129.8
129.7
129.5
129.2
128.9
128.7
128.5
128.4
128.2
127.0
127.0
126.9
126.4
77.4
77.1
76.7
74.6
67.0
57.2
47.9
21.6
21.5
f1 (ppm)

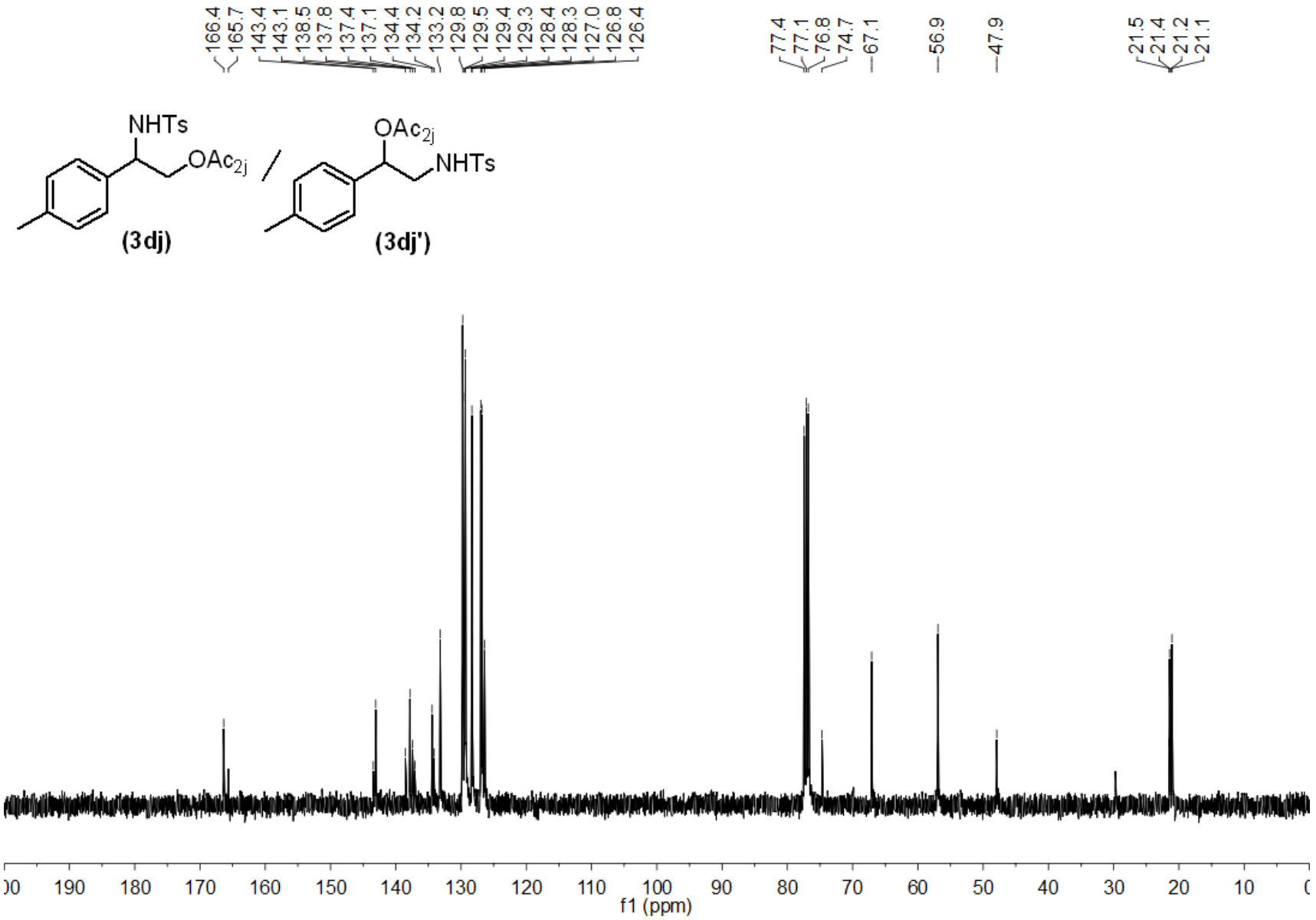

gyq141121-2-42-2
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3437.3
3342.6
3061.7
2924.2
1708.8
1635.5
1599.7
1494.6
1456.0
1434.4
1384.0
1352.6
1322.1
1277.9
1197.4
1178.4
1156.8
1127.8
1090.3
1070.1
1025.5
992.9
865.4
815.7
763.7
709.7
683.1
670.7
630.5
617.0
584.0
556.1
547.5
516.0
497.5
NHTs
OAc2j
(3cj)
OAc2j
NHTs
(3cj')

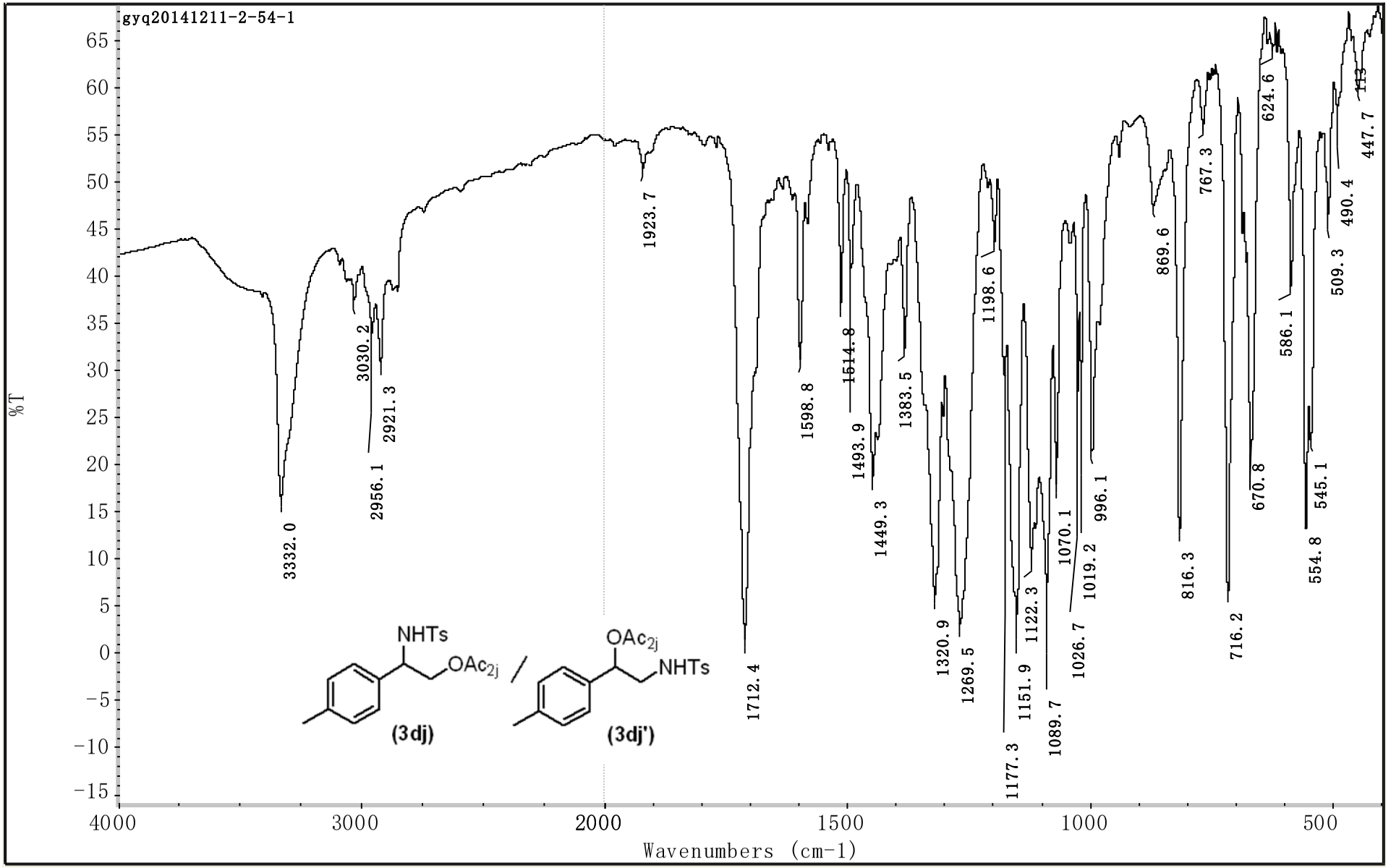

NHTs
OAc2a
(3da)
OAc2a
NHTs
(3da')
f1 (ppm)
0.57
2.47
1.93
2.95
0.98
0.70
2.95
1.37
0.30
0.70
0.99
0.24
0.65
1.43
0.63
0.91
0.91
2.09
2.12
7.737
7.717
7.632
7.613
7.583
7.543
7.455
7.445
7.437
7.376
7.372
7.360
7.349
7.244
7.224
7.172
7.152
7.111
7.092
7.076
7.030
7.010
6.364
6.324
6.230
6.190
5.875
5.864
5.822
4.654
4.329
4.309
4.269
4.258
3.457
3.422
3.389
3.364
3.331
2.343
2.296
2.269
2.222
0.000

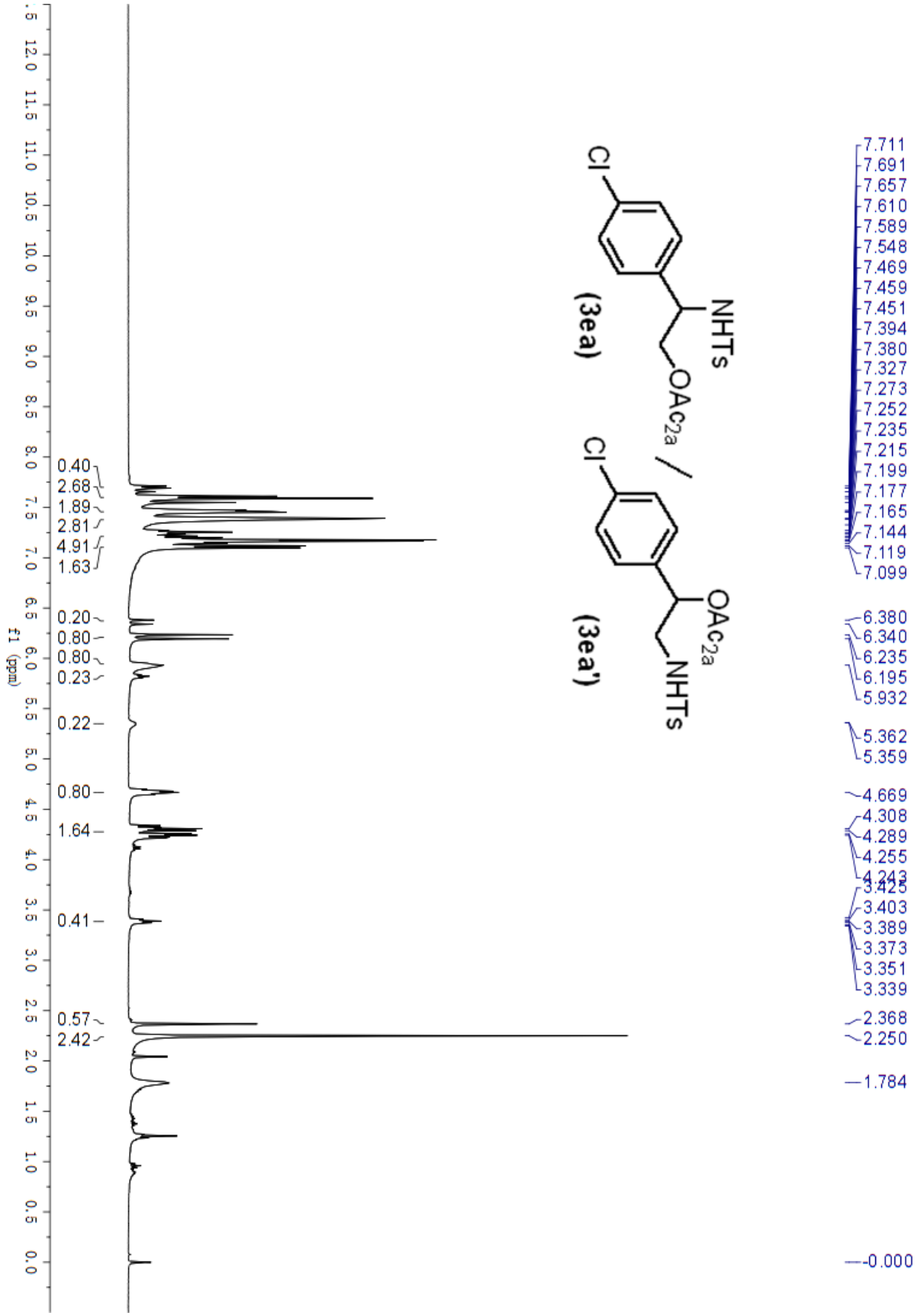

166.8
166.1
145.6
134.4
130.6
129.8
129.4
129.3
128.9
128.9
128.2
127.1
127.1
126.9
126.4
117.4
117.1
77.5
77.2
76.8
74.3
66.7
56.9
47.9
21.5
21.4
21.2
21.1
NHTs
OAc2a
(3da)
OAc2a
NHTs
(3da')
f1 (ppm)

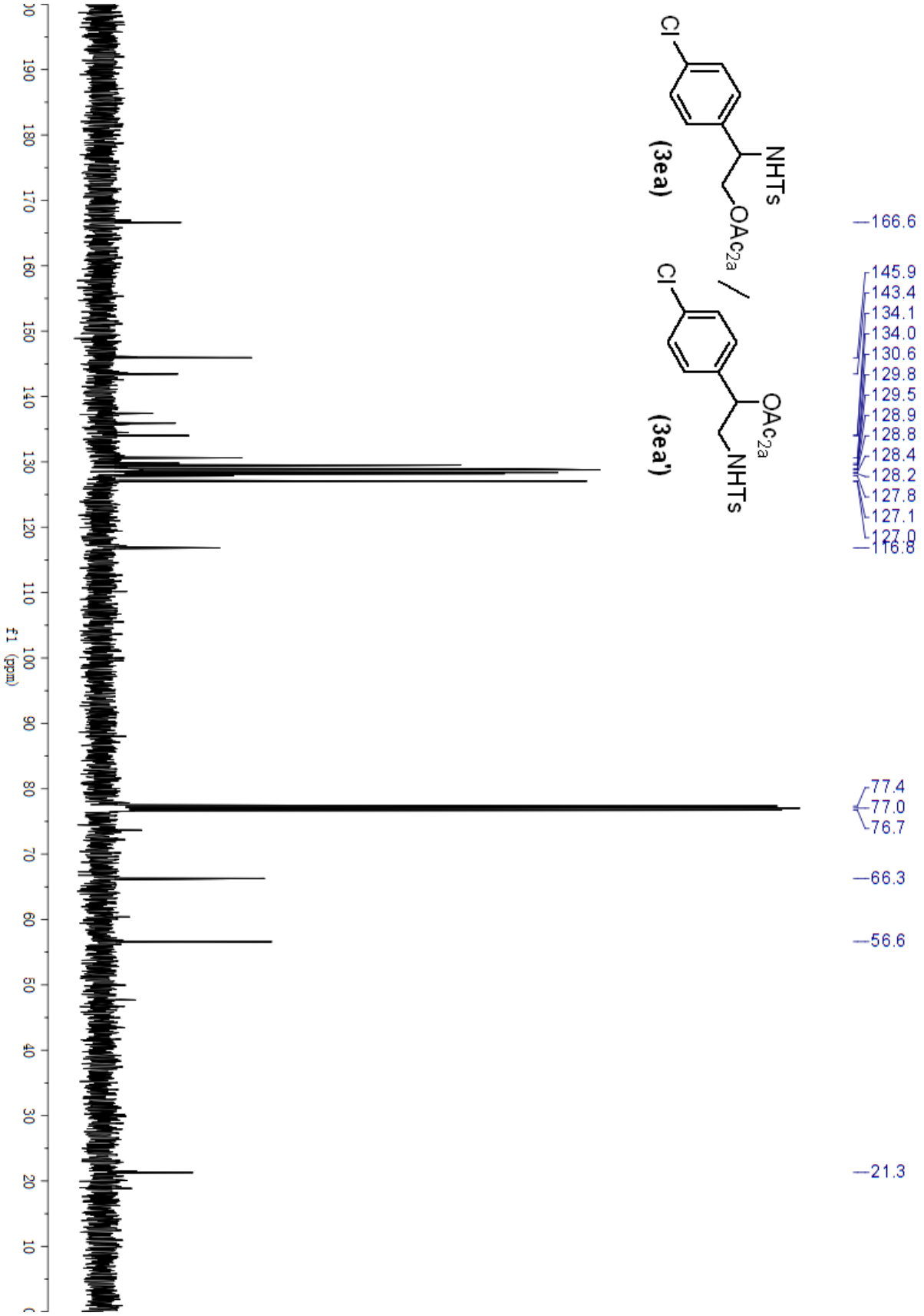

gyq20141211-2-54-2
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3311.7
3060.8
3026.5
2955.2
2922.0
1697.5
1634.0
1597.9
1577.6
1515.6
1496.4
1449.9
1383.5
1330.2
1285.3
1244.5
1156.0
1118.8
1089.1
1017.4
981.9
865.9
855.2
817.6
766.9
713.7
683.0
664.6
574.2
550.2
514.0
502.7
NHTs
OAc2a
(3da)
OAc2a
NHTs
(3da')

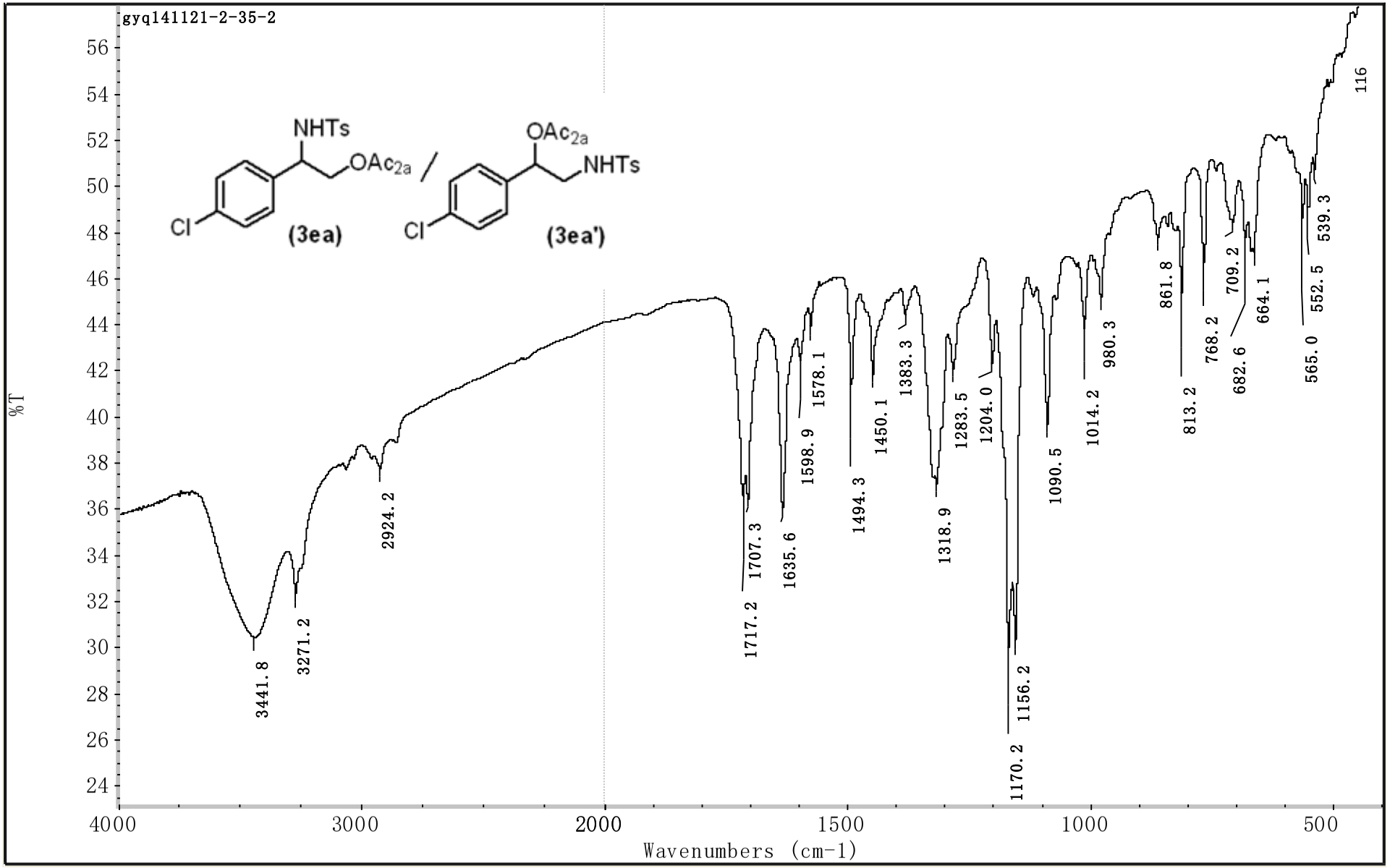
7.980
7.962
7.875
7.857
7.854
7.705
7.685
7.590
7.570
7.548
7.529
7.511
7.396
7.385
7.365
7.346
7.247
7.204
7.190
7.184
7.171
7.134
7.113
7.091
7.038
7.018
6.997
6.977
5.934
5.925
5.914
5.874
5.857
4.421
4.401
4.369
4.357
3.529
3.461
3.407
3.379
2.352
2.291
2.273
2.249
0.000
NHTs
OAc2j
(3dj)
OAc2j
NHTs
(3dj')
0.61
1.43
0.62
2.57
2.04
1.26
2.03
2.97
0.30
0.70
0.27
0.67
1.42
0.62
0.88
0.89
2.13
2.10
f1 (ppm)

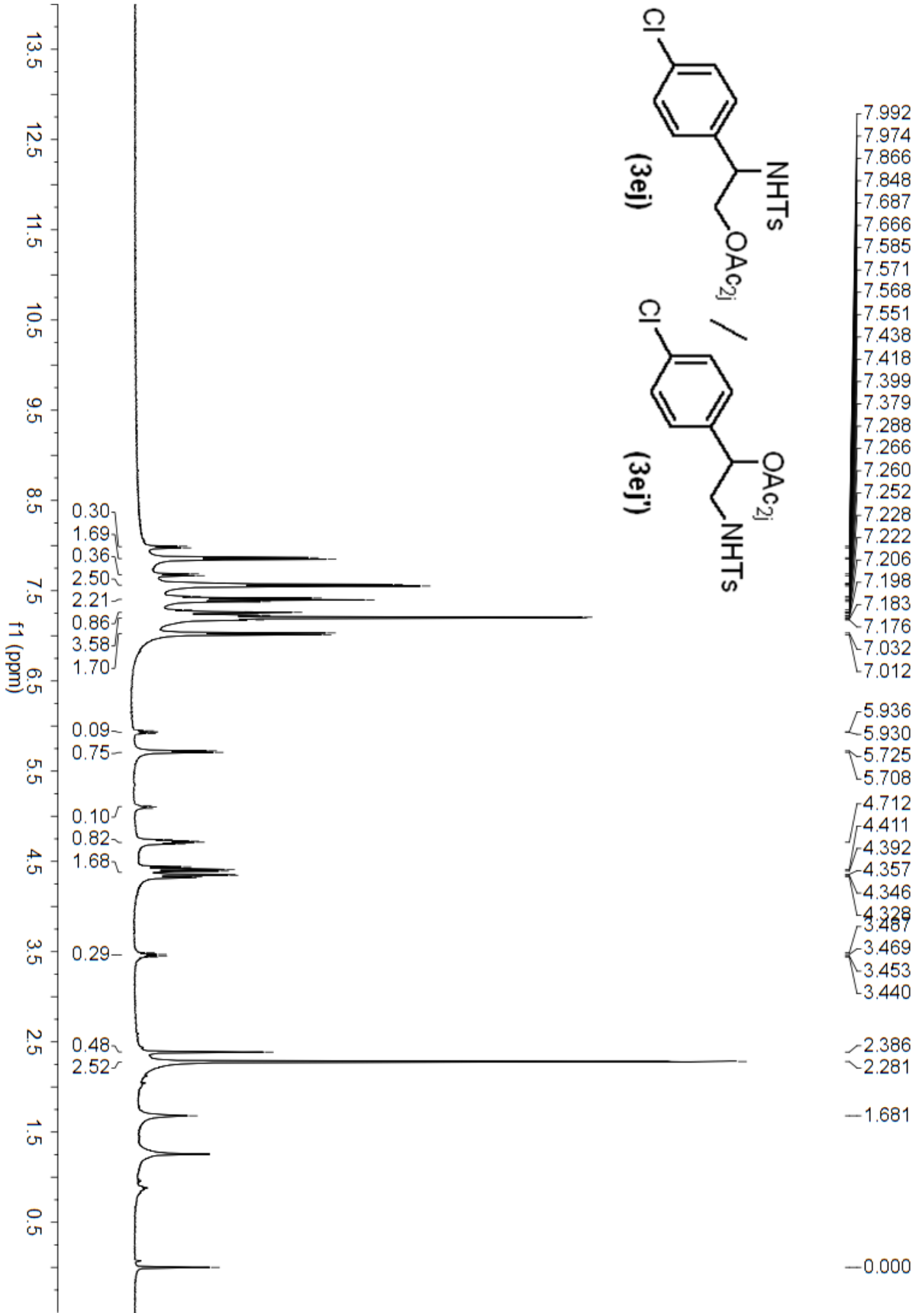

166.4
165.7
143.4
143.1
138.5
137.8
137.4
137.1
134.4
134.2
133.2
129.8
129.5
129.4
129.3
128.4
128.3
127.0
126.8
126.4
77.4
77.1
76.8
74.7
67.1
56.9
47.9
21.5
21.4
21.2
21.1
NHTs
OAc2j
(3dj)
OAc2j
NHTs
(3dj')
f1 (ppm)

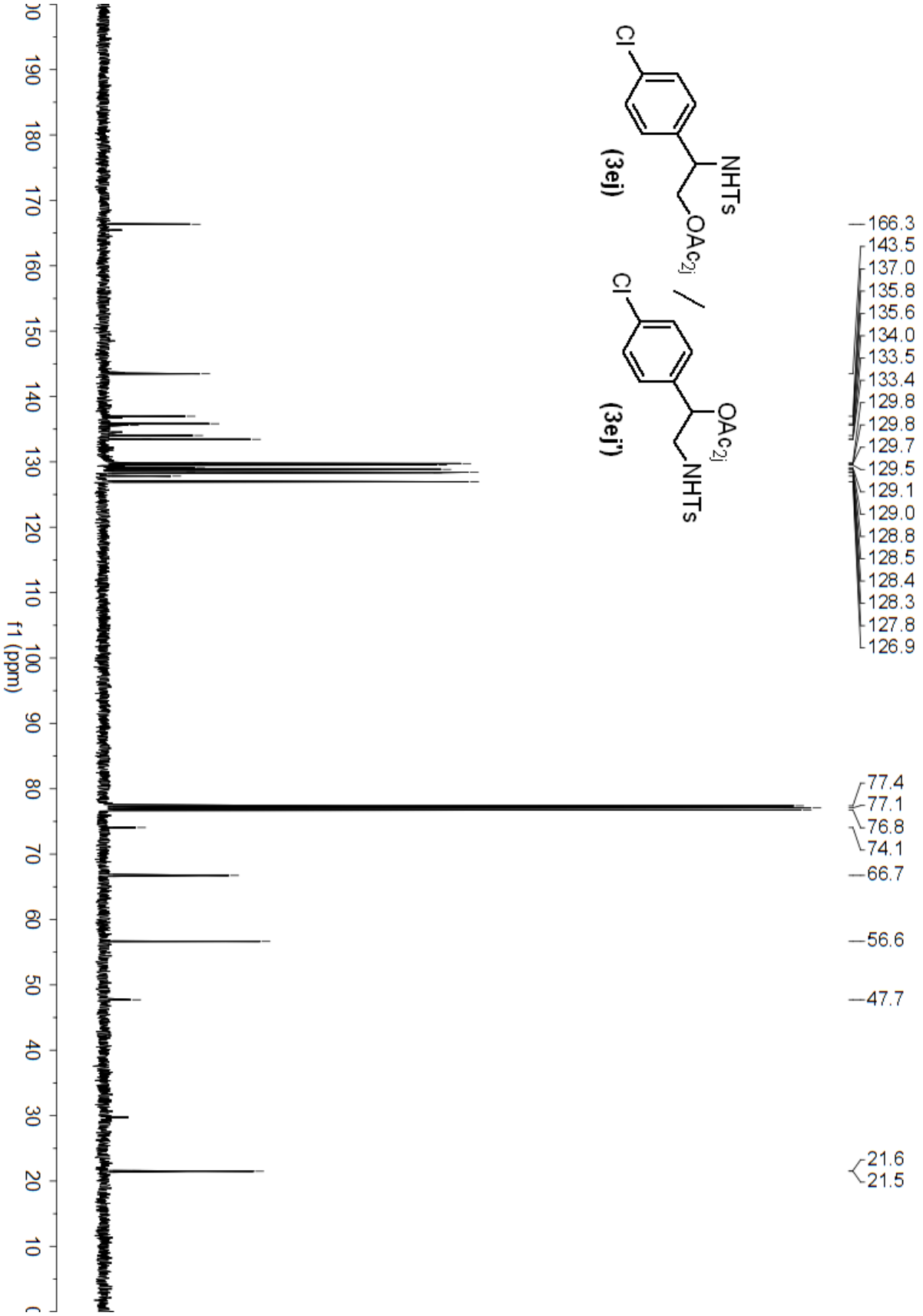

gyq20141211-2-54-1
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
-15
3332.0
3030.2
2956.1
2921.3
1923.7
1712.4
1598.8
1614.8
1493.9
1449.3
1383.5
1320.9
1269.5
1198.6
1177.3
1151.9
1122.3
1089.7
1070.1
1026.7
1019.2
996.1
869.6
816.3
767.3
716.2
670.8
624.6
586.1
554.8
545.1
509.3
490.4
447.7
NHTs
OAc2j
(3dj)
OAc2j
NHTs
(3dj')

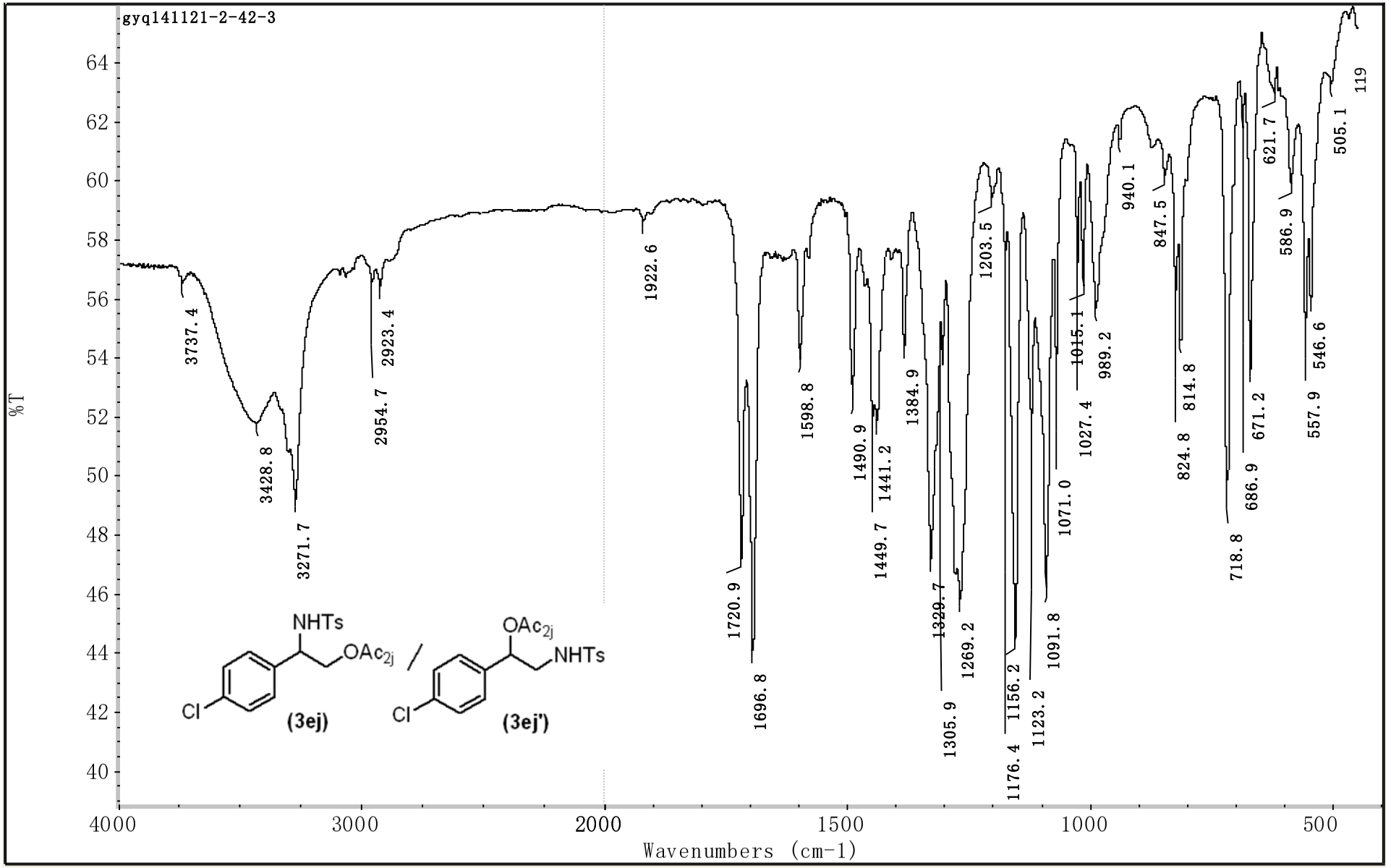

Cl
NHTs
OAc2a
(3ea)
Cl
OAc2a
NHTs
(3ea')
f1 (ppm)
0.40
2.68
1.89
2.81
4.91
1.63
0.20
0.80
0.80
0.23
0.22
0.80
1.64
0.41
0.57
2.42
7.711
7.691
7.657
7.610
7.589
7.548
7.469
7.459
7.451
7.394
7.380
7.327
7.273
7.252
7.235
7.215
7.199
7.177
7.165
7.144
7.119
7.099
6.380
6.340
6.235
6.195
5.932
5.362
5.359
4.669
4.308
4.289
4.255
4.243
3.425
3.403
3.389
3.373
3.351
3.339
2.368
2.250
1.784
0.000

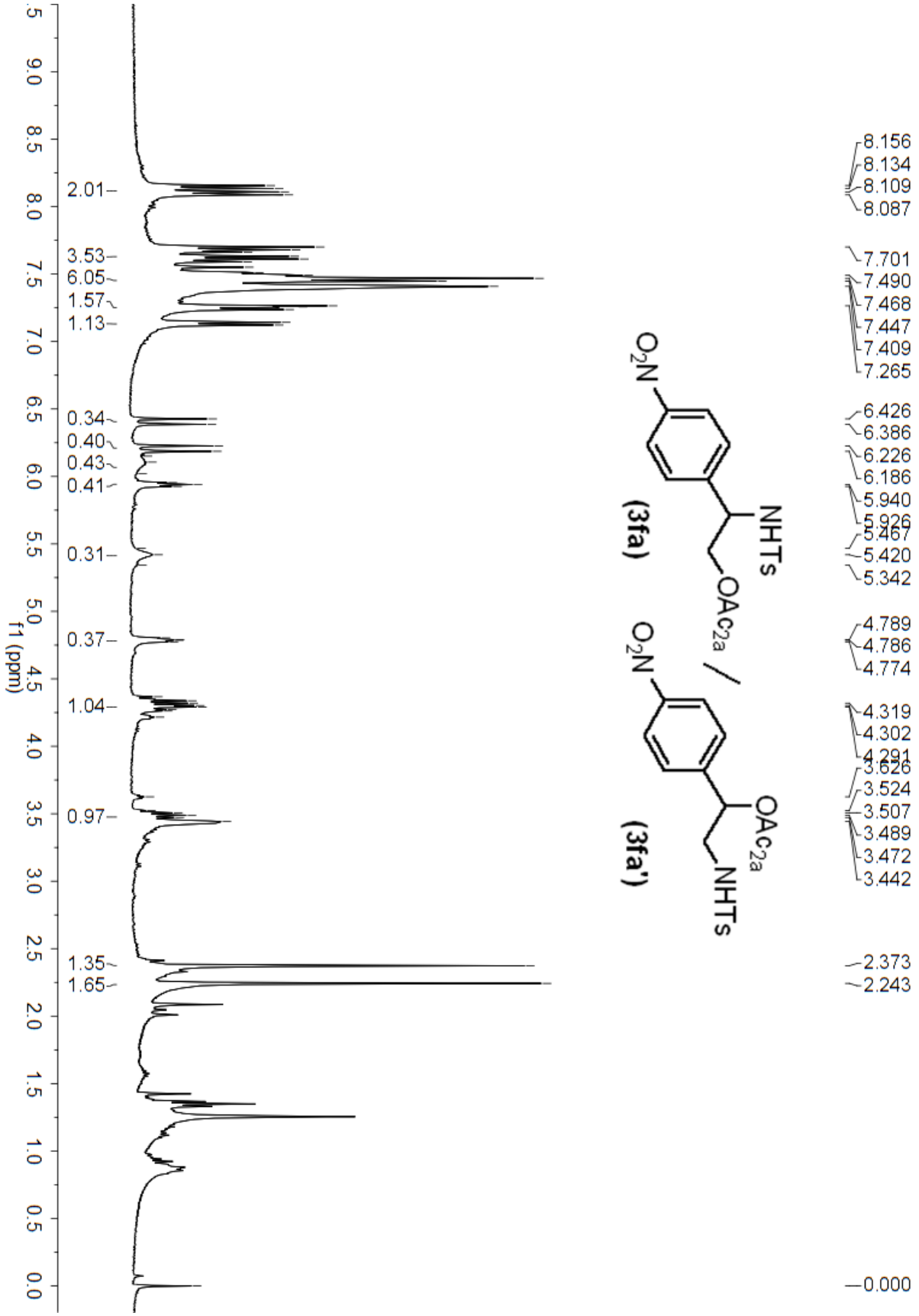

Cl
NHTs
OAc2a
(3ea)
Cl
OAc2a
NHTs
(3ea')
166.6
145.9
143.4
134.1
134.0
130.6
129.8
129.5
128.9
128.8
128.4
128.2
127.8
127.1
127.0
116.8
77.4
77.0
76.7
66.3
56.6
21.3
f1 (ppm)

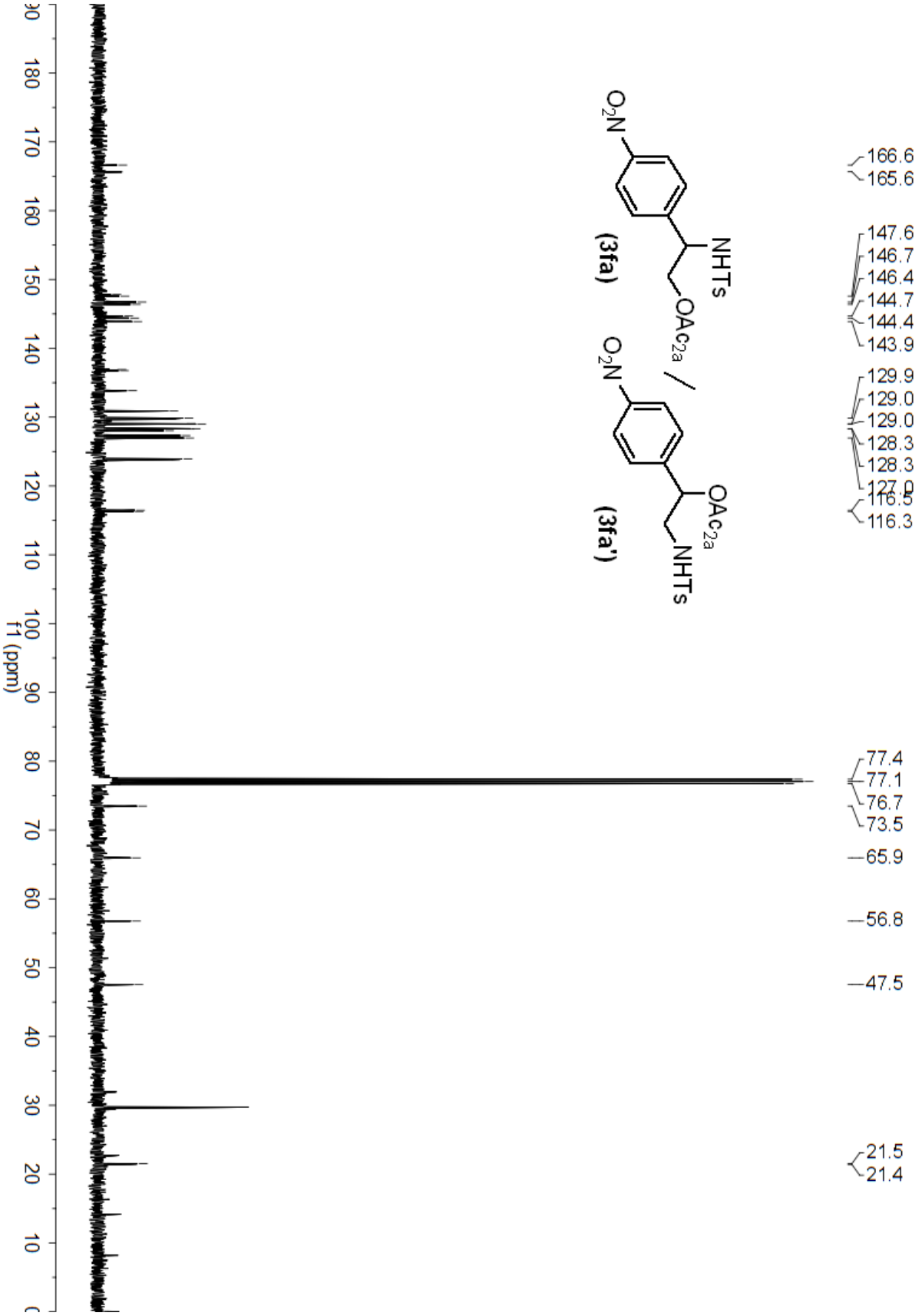

gyq141121-2-35-2
NHTs
OAc2a
Cl
(3ea)
OAc2a
NHTs
Cl
(3ea')
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3441.8
3271.2
2924.2
1717.2
1707.3
1635.6
1598.9
1578.1
1494.3
1450.1
1383.3
1318.9
1283.5
1204.0
1170.2
1156.2
1090.5
1014.2
980.3
861.8
813.2
768.2
709.2
682.6
664.1
565.0
552.5
539.3
116

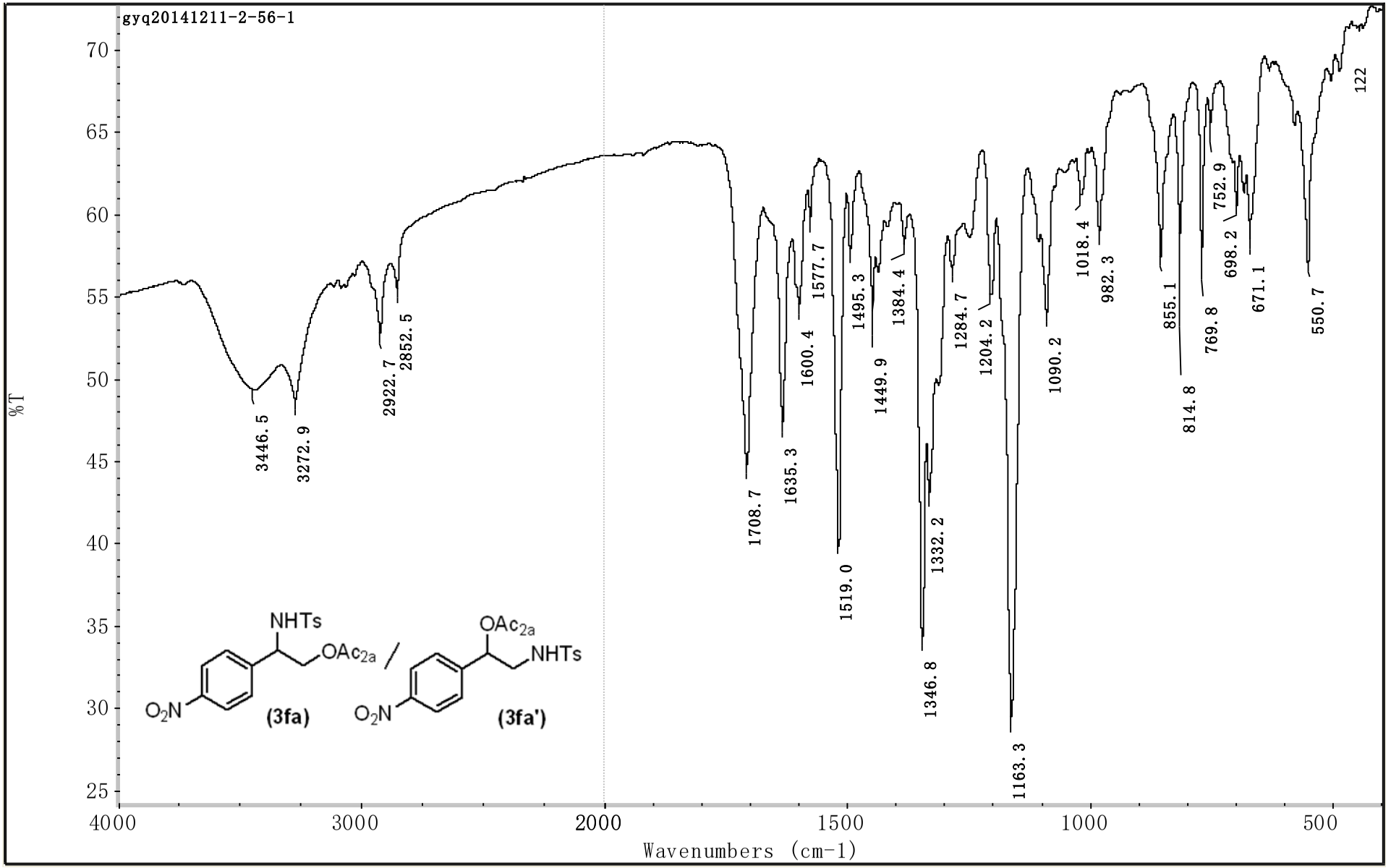

Cl
NHTs
OAc2j
(3ej)
Cl
OAc2j
NHTs
(3ej')
f1 (ppm)
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
0.30
1.69
0.36
2.50
2.21
0.86
3.58
1.70
0.09
0.75
0.10
0.82
1.68
0.29
0.48
2.52
7.992
7.974
7.866
7.848
7.687
7.666
7.585
7.571
7.568
7.551
7.438
7.418
7.399
7.379
7.288
7.266
7.260
7.252
7.228
7.222
7.206
7.198
7.183
7.176
7.032
7.012
5.936
5.930
5.725
5.708
4.712
4.411
4.392
4.357
4.346
4.328
3.487
3.469
3.453
3.440
2.386
2.281
1.681
0.000

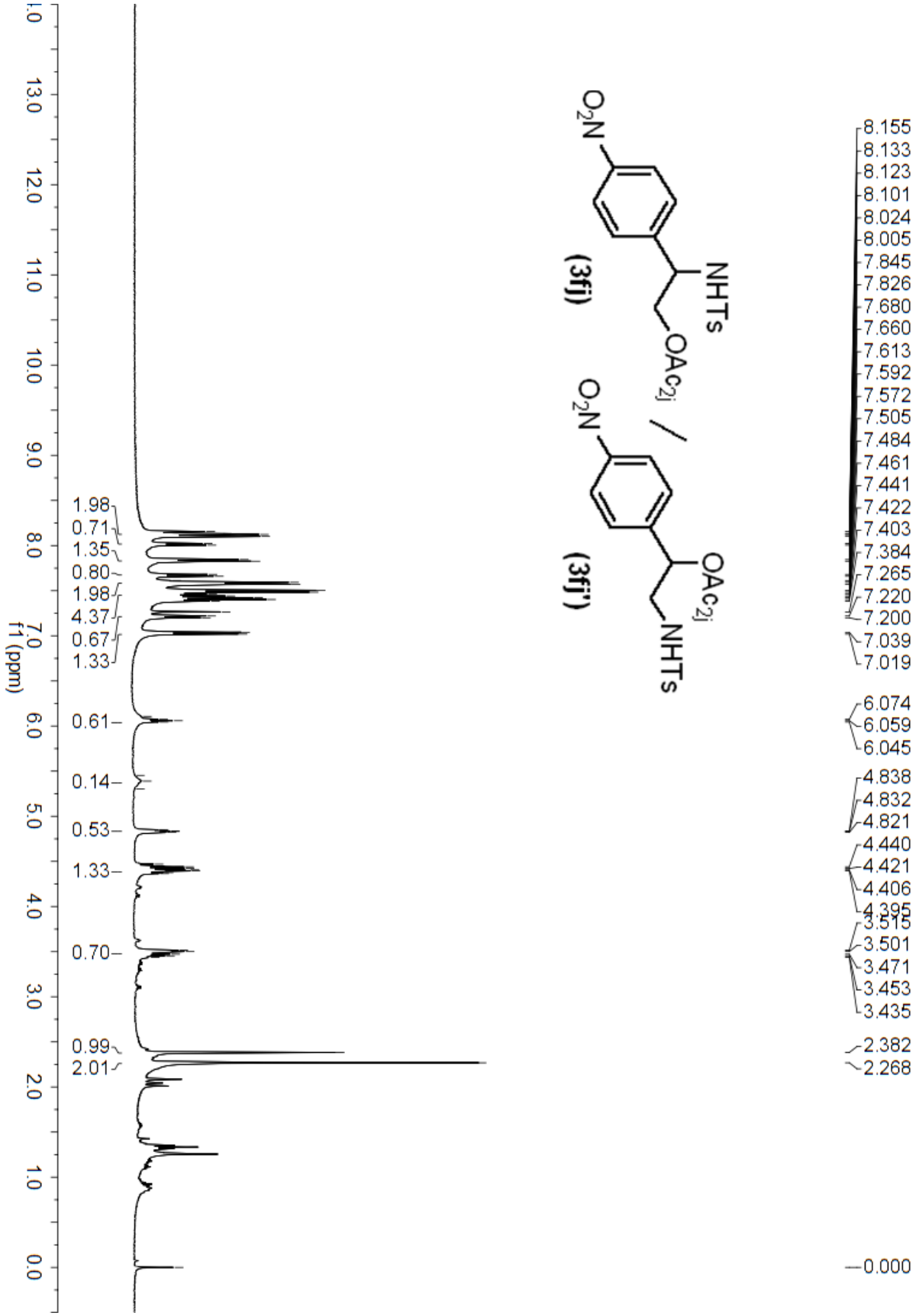

Cl
NHTs
OAc2j
(3ej)
Cl
OAc2j
NHTs
(3ej')
166.3
143.5
137.0
135.8
135.6
134.0
133.5
133.4
129.8
129.8
129.7
129.5
129.1
129.0
128.8
128.5
128.4
128.3
127.8
126.9
77.4
77.1
76.8
74.1
66.7
56.6
47.7
21.6
21.5
f1 (ppm)

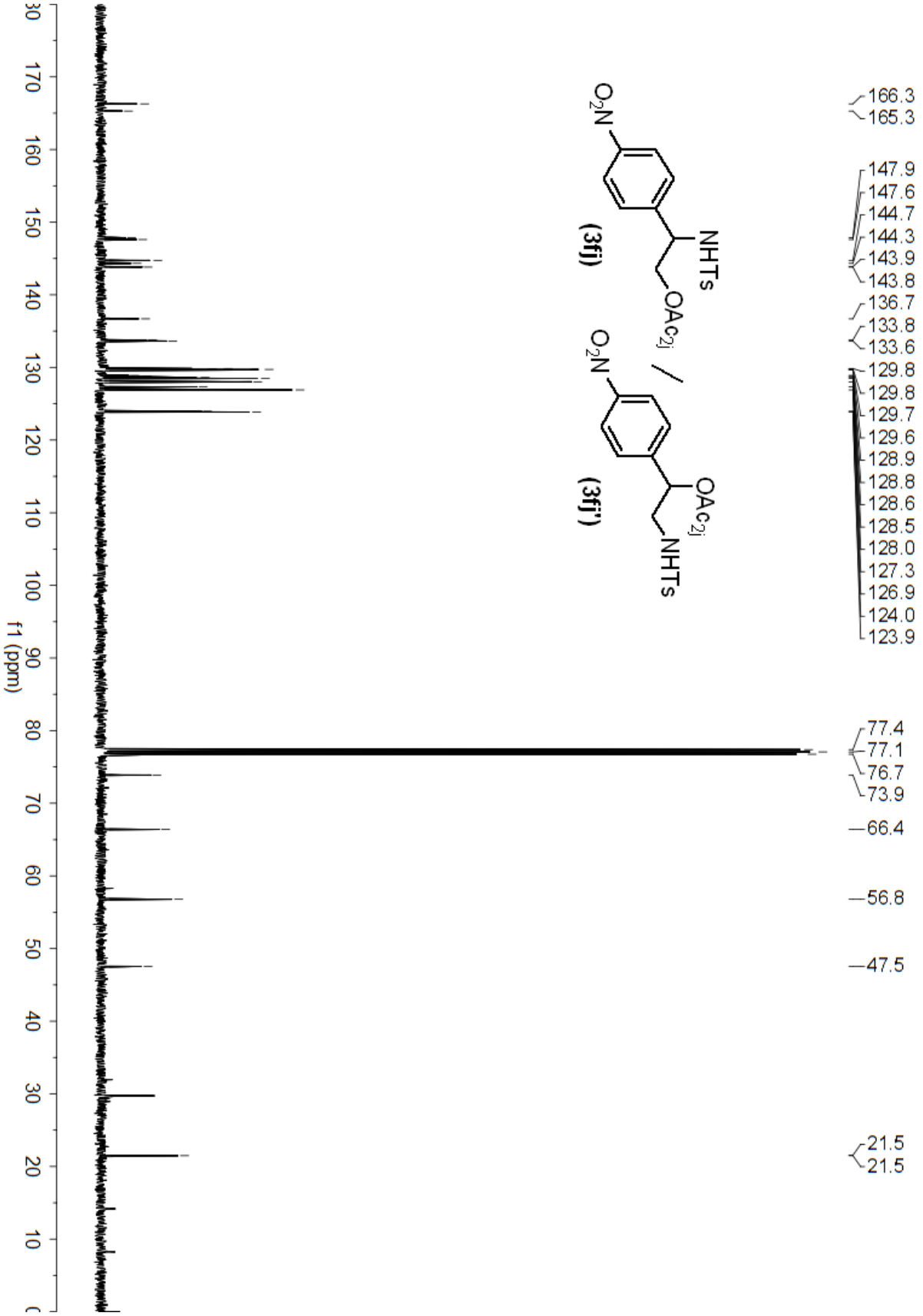

gyq141121-2-42-3
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
64
62
60
58
56
54
52
50
48
46
44
42
40
3737.4
3428.8
3271.7
2954.7
2923.4
1922.6
1720.9
1696.8
1598.8
1490.9
1449.7
1441.2
1384.9
1329.7
1305.9
1269.2
1203.5
1176.4
1156.2
1123.2
1091.8
1071.0
1027.4
1015.1
989.2
940.1
847.5
824.8
814.8
718.8
686.9
671.2
621.7
586.9
557.9
546.6
505.1
119
NHTs
OAc2j
Cl
(3ej)
OAc2j
NHTs
Cl
(3ej')

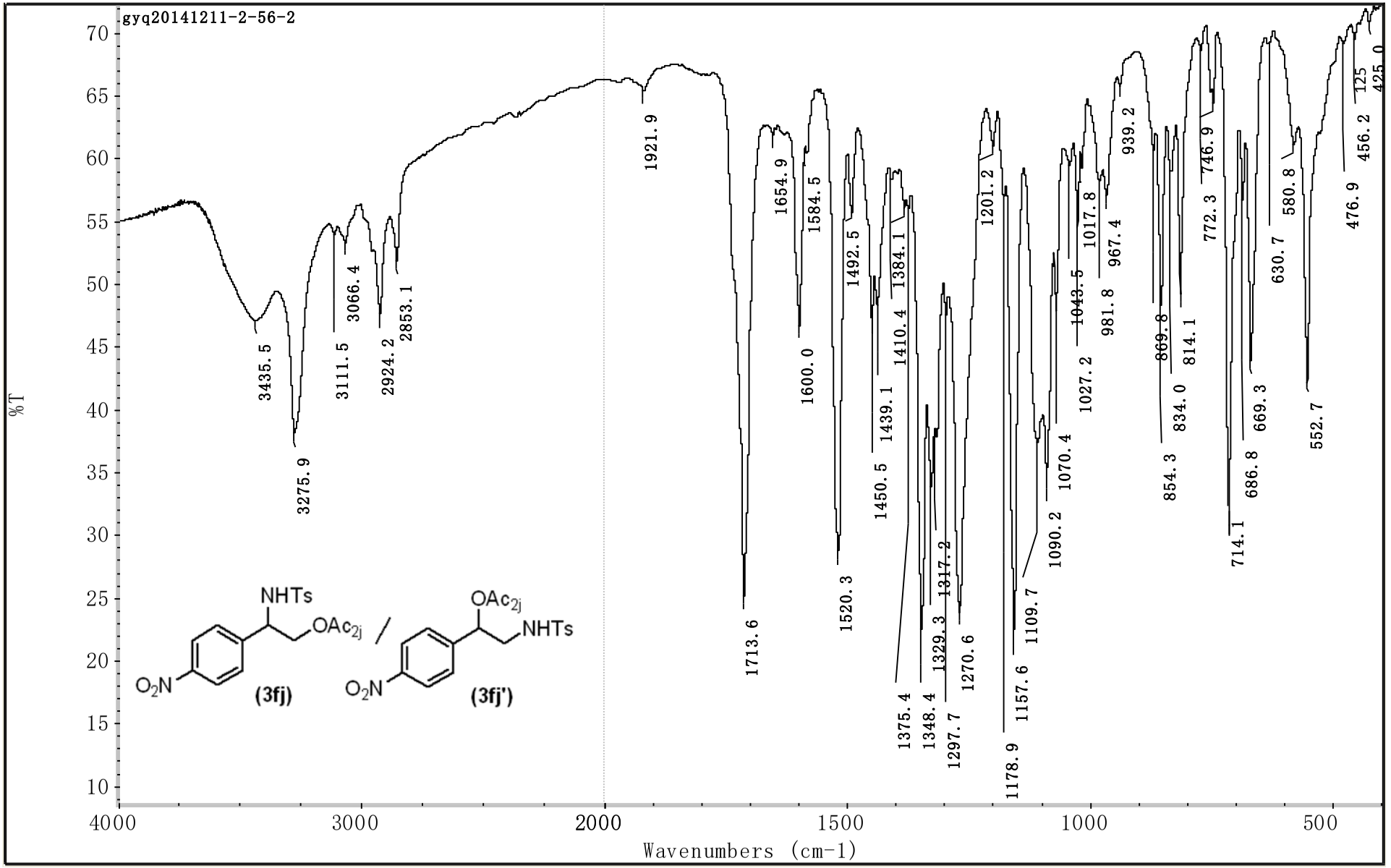

8.156
8.134
8.109
8.087
7.701
7.490
7.468
7.447
7.409
7.265
6.426
6.386
6.226
6.186
5.940
5.926
5.467
5.420
5.342
4.789
4.786
4.774
4.319
4.302
4.291
3.626
3.524
3.507
3.489
3.472
3.442
2.373
2.243
0.000
2.01
3.53
6.05
1.57
1.13
0.34
0.40
0.43
0.41
0.31
0.37
1.04
0.97
1.35
1.65
f1 (ppm)
O2N
NHTs
OAc2a
(3fa)
O2N
OAc2a
NHTs
(3fa')

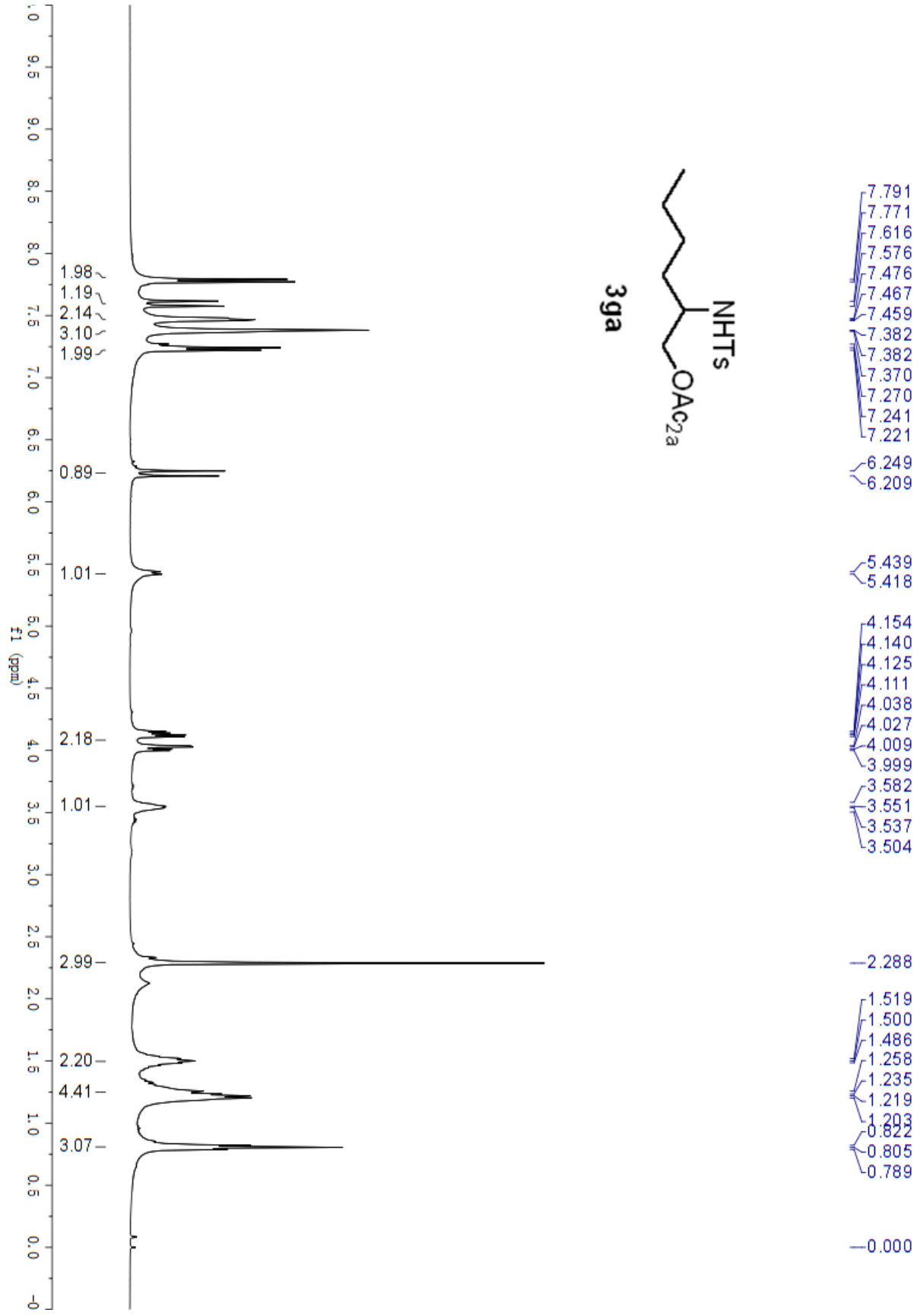

166.6
165.6
147.6
146.7
146.4
144.7
144.4
143.9
129.9
129.0
129.0
128.3
128.3
127.0
116.5
116.3
77.4
77.1
76.7
73.5
65.9
56.8
47.5
21.5
21.4
f1 (ppm)
(3fa)
(3fa')

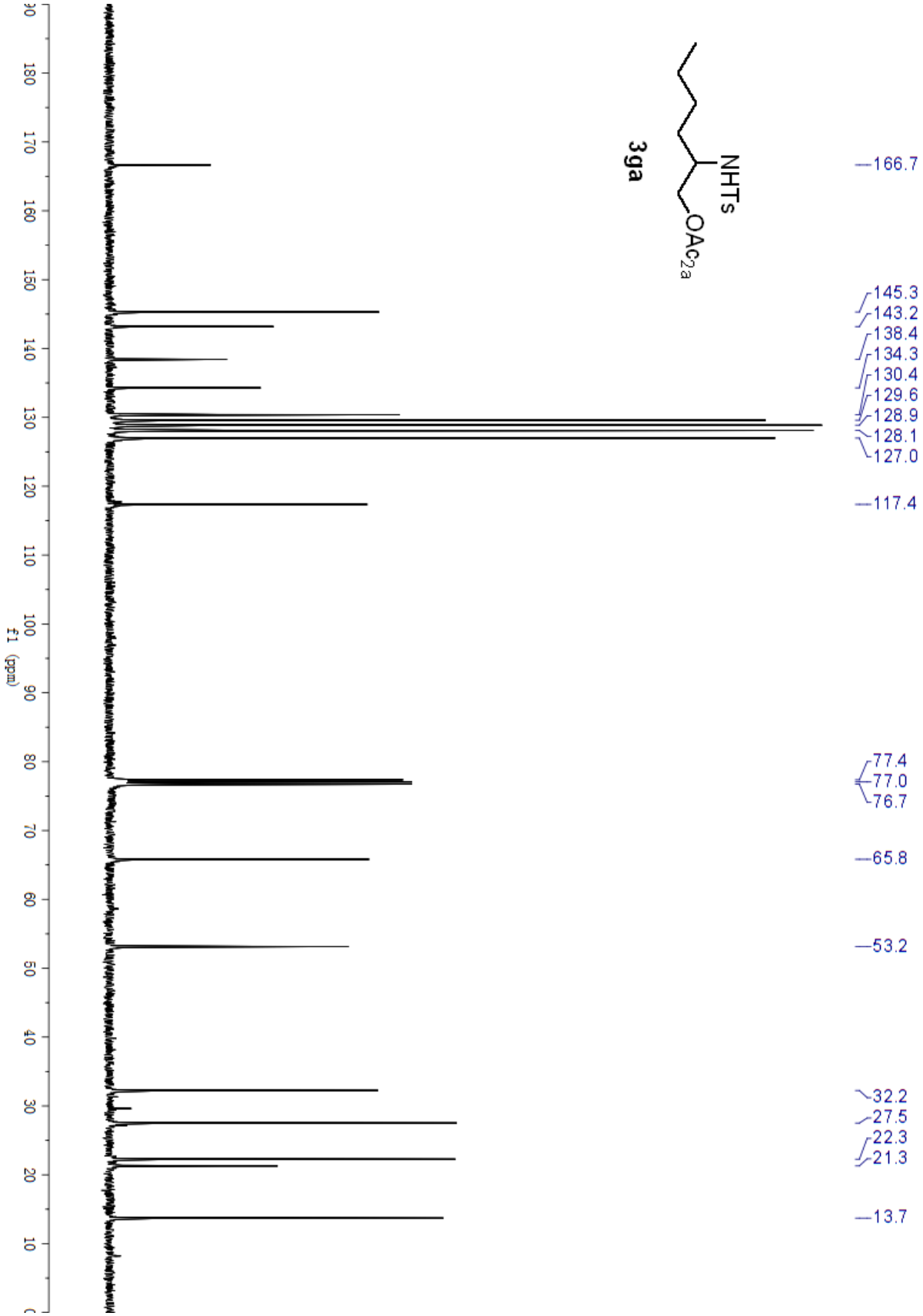

gyq20141211-2-56-1
%T
70
65
60
55
50
45
40
35
30
25
4000
3000
2000
1500
1000
500
Wavenumbers (cm-1)
3446.5
3272.9
2922.7
2852.5
1708.7
1635.3
1600.4
1577.7
1519.0
1495.3
1449.9
1384.4
1346.8
1332.2
1284.7
1204.2
1163.3
1090.2
1018.4
982.3
855.1
814.8
769.8
752.9
698.2
671.1
550.7
122
NHTs
OAc2a
O2N
(3fa)
OAc2a
NHTs
O2N
(3fa')

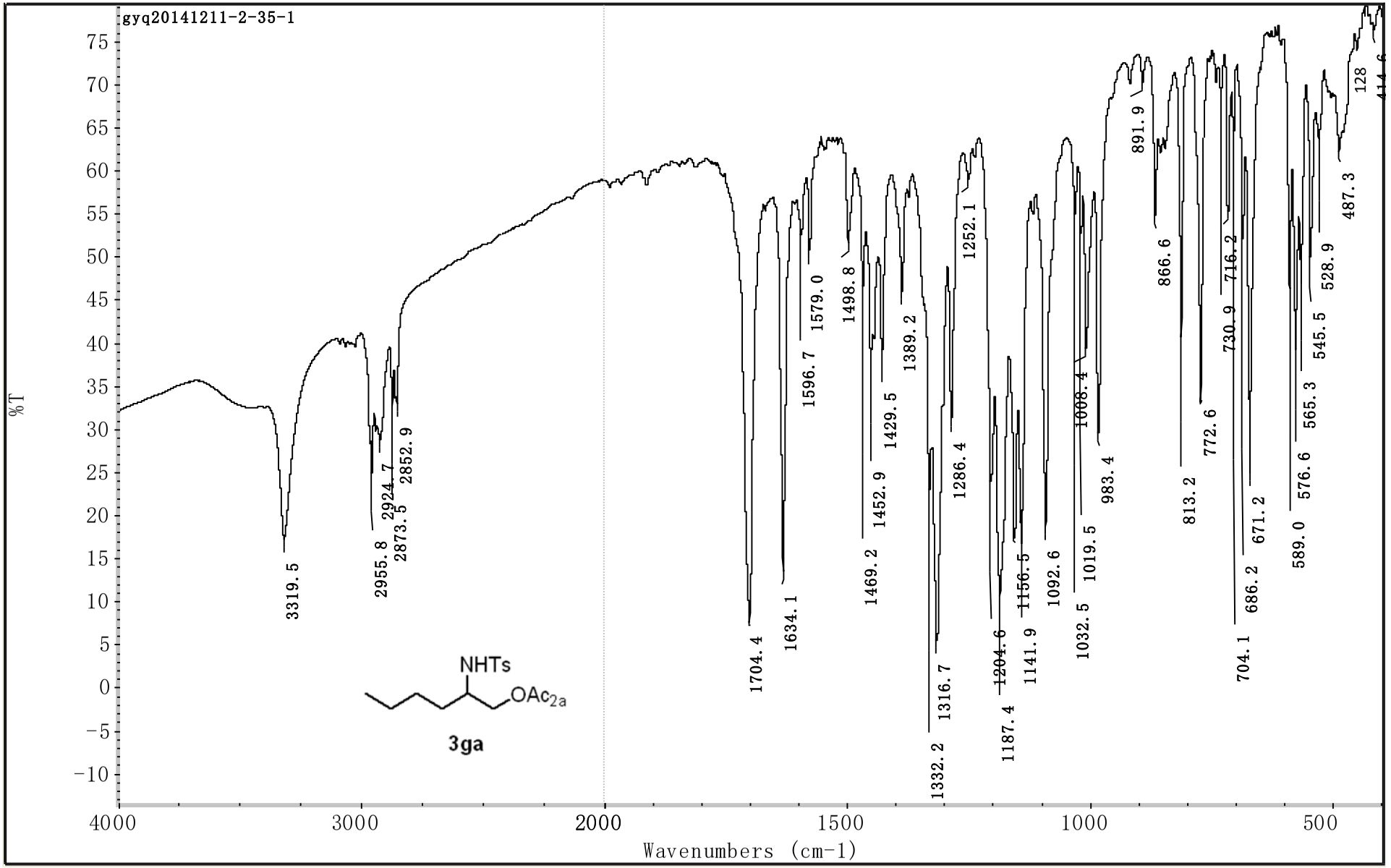

O2N
NHTs
OAc2j
(3fj)
/
O2N
OAc2j
NHTs
(3fj')
8.155
8.133
8.123
8.101
8.024
8.005
7.845
7.826
7.680
7.660
7.613
7.592
7.572
7.505
7.484
7.461
7.441
7.422
7.403
7.384
7.265
7.220
7.200
7.039
7.019
6.074
6.059
6.045
4.838
4.832
4.821
4.440
4.421
4.406
4.395
3.515
3.501
3.471
3.453
3.435
2.382
2.268
0.000
1.98
0.71
1.35
0.80
1.98
4.37
0.67
1.33
0.61
0.14
0.53
1.33
0.70
0.99
2.01
f1 (ppm)

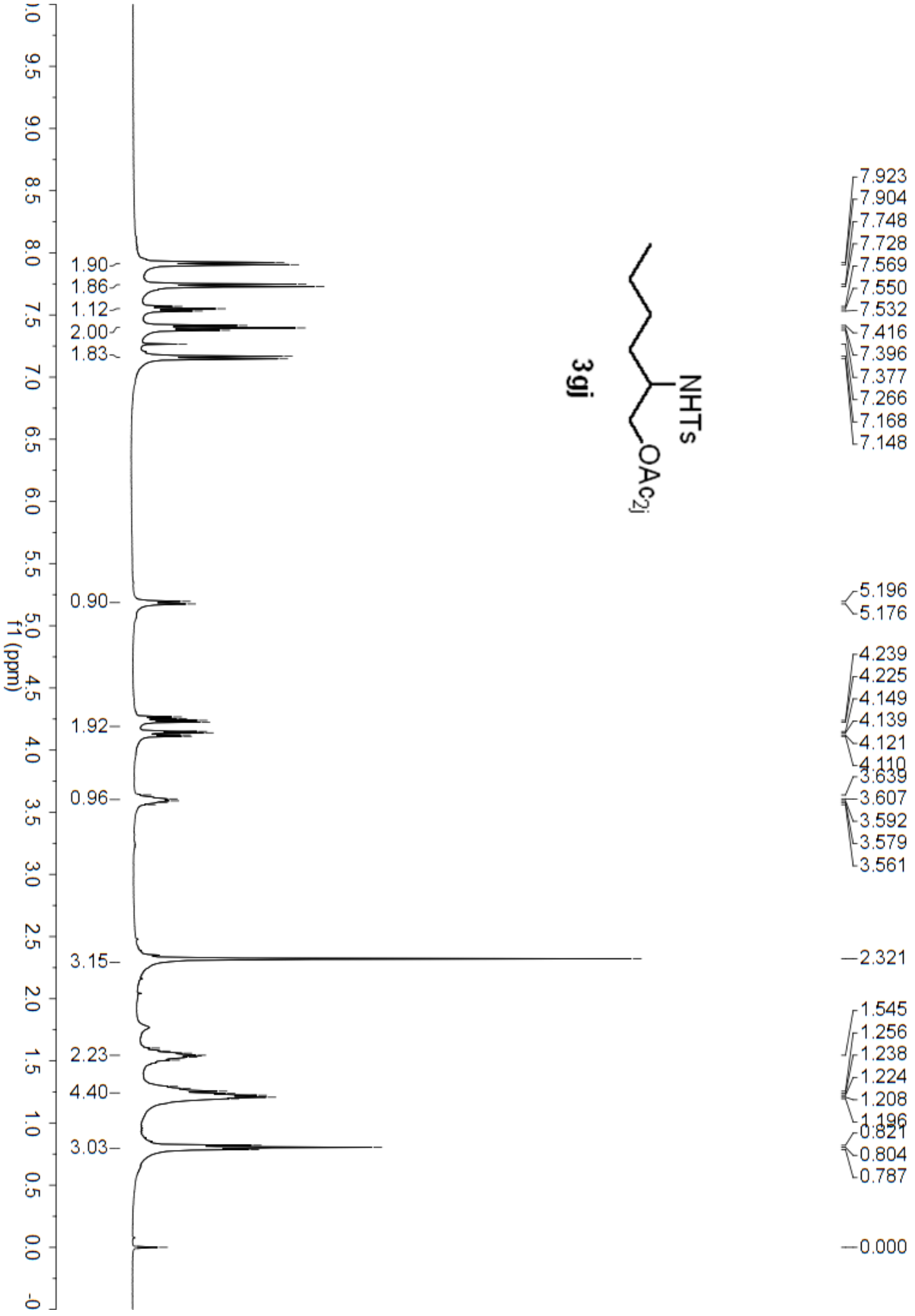

O2N
NHTs
OAc2j
(3fj)
O2N
OAc2j
NHTs
(3fj')
166.3
165.3
147.9
147.6
144.7
144.3
143.9
143.8
136.7
133.8
133.6
129.8
129.8
129.7
129.6
128.9
128.8
128.6
128.5
128.0
127.3
126.9
124.0
123.9
77.4
77.1
76.7
73.9
66.4
56.8
47.5
21.5
21.5
f1 (ppm)

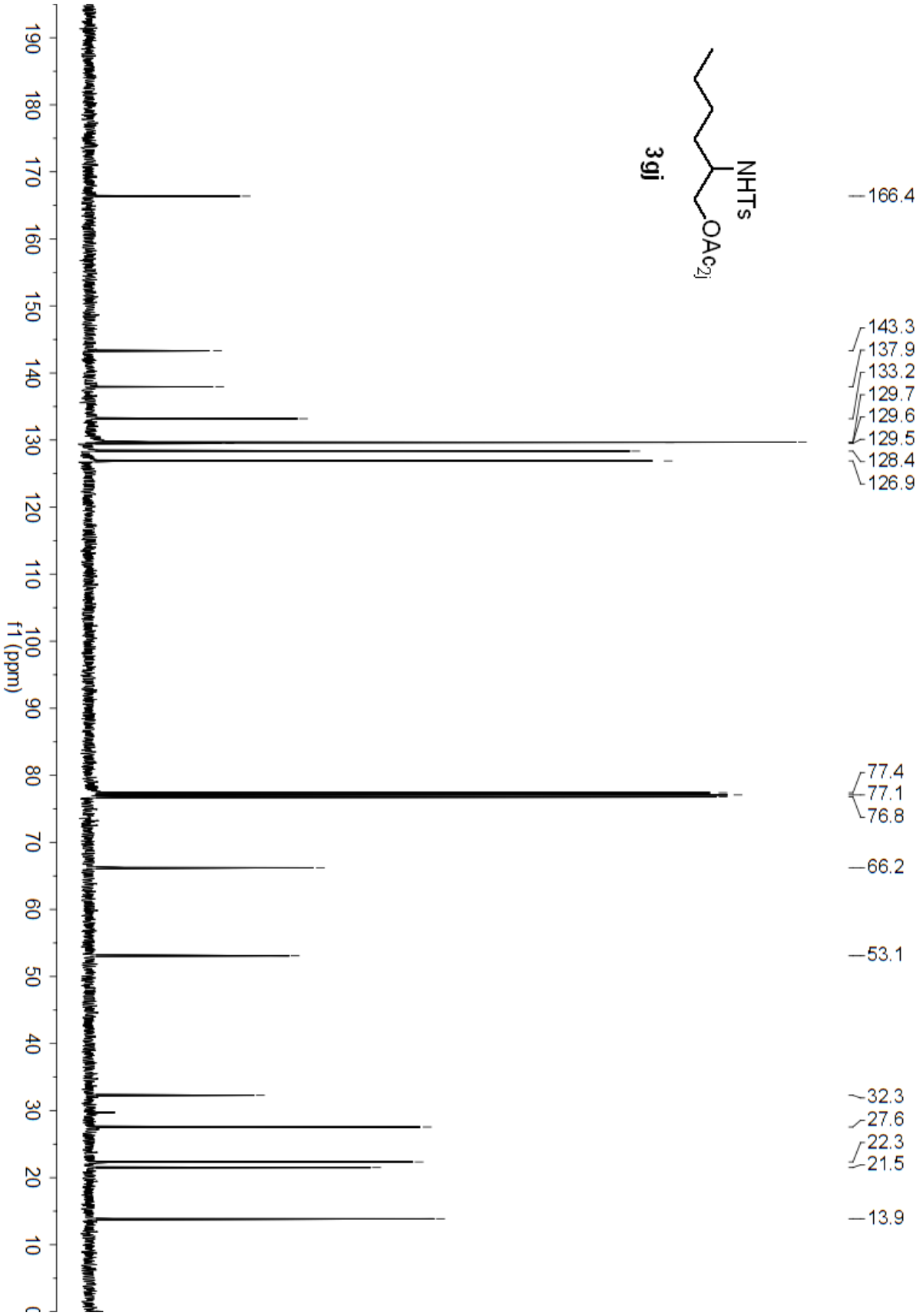

gyq20141211-2-56-2
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
70
65
60
55
50
45
40
35
30
25
20
15
10
3435.5
3275.9
3111.5
3066.4
2924.2
2853.1
1921.9
1713.6
1654.9
1600.0
1584.5
1520.3
1492.5
1450.5
1439.1
1410.4
1384.1
1375.4
1348.4
1329.3
1317.2
1297.7
1270.6
1201.2
1178.9
1157.6
1109.7
1090.2
1070.4
1043.5
1027.2
1017.8
981.8
967.4
939.2
869.8
854.3
834.0
814.1
772.3
746.9
714.1
686.8
669.3
630.7
580.8
552.7
476.9
456.2
125
425.0
NHTs
OAc2j
O2N
(3fj)
OAc2j
NHTs
O2N
(3fj')

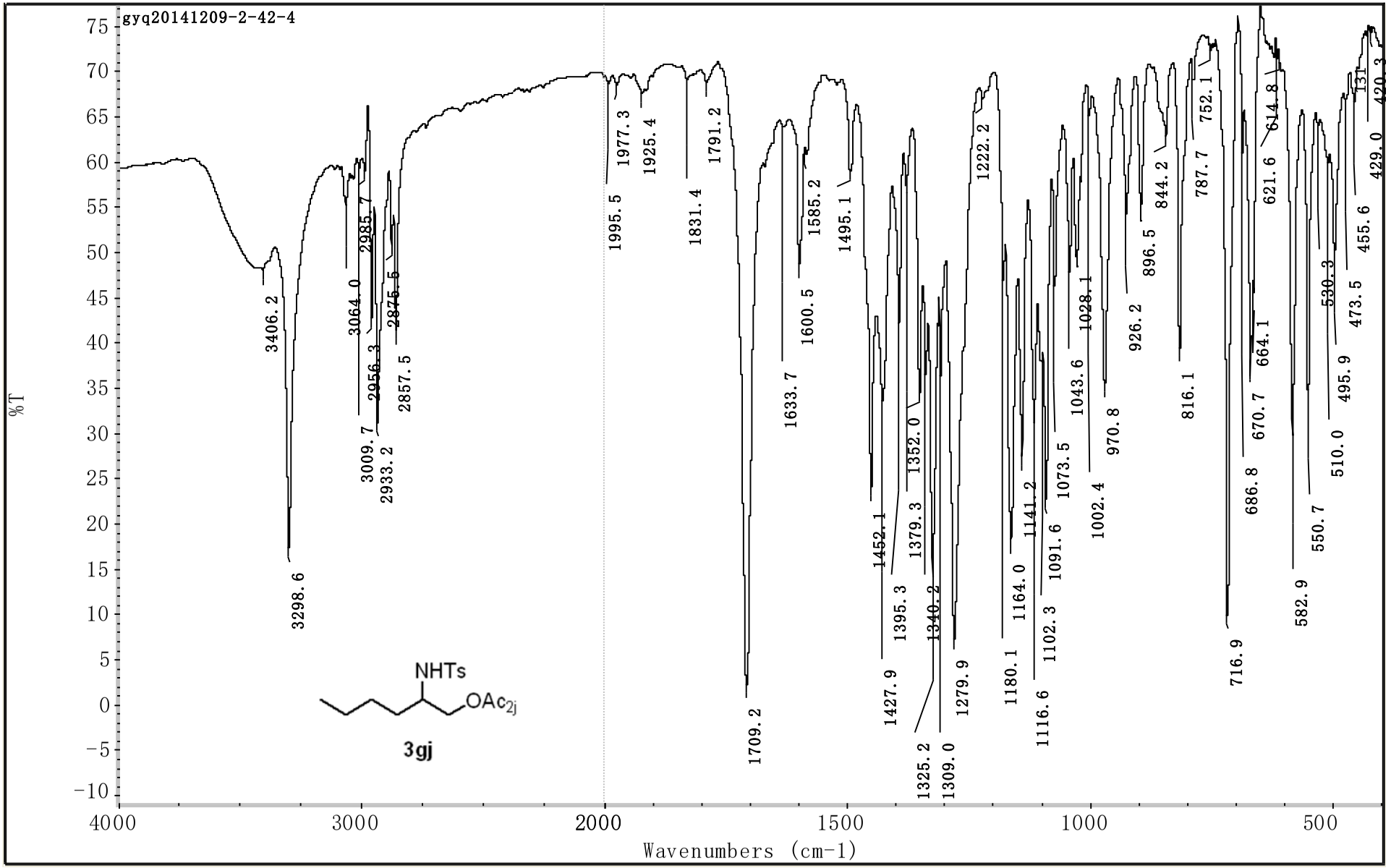

3ga
NHTs
OAc2a
7.791
7.771
7.616
7.576
7.476
7.467
7.459
7.382
7.382
7.370
7.270
7.241
7.221
6.249
6.209
5.439
5.418
4.154
4.140
4.125
4.111
4.038
4.027
4.009
3.999
3.582
3.551
3.537
3.504
2.288
1.519
1.500
1.486
1.258
1.235
1.219
1.203
0.822
0.805
0.789
0.000
1.98
1.19
2.14
3.10
1.99
0.89
1.01
2.18
1.01
2.99
2.20
4.41
3.07
f1 (ppm)


3ga
NHTs
OAc2a
166.7
145.3
143.2
138.4
134.3
130.4
129.6
128.9
128.1
127.0
117.4
77.4
77.0
76.7
65.8
53.2
32.2
27.5
22.3
21.3
13.7
f1 (ppm)


gyq20141211-2-35-1
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3319.5
2955.8
2924.7
2873.5
2852.9
1704.4
1634.1
1596.7
1579.0
1498.8
1469.2
1452.9
1429.5
1389.2
1332.2
1316.7
1286.4
1252.1
1204.6
1187.4
1156.5
1141.9
1092.6
1032.5
1019.5
1008.4
983.4
891.9
866.6
813.2
772.6
730.9
716.2
704.1
686.2
671.2
589.0
576.6
565.3
545.5
528.9
487.3
NHTs
OAc2a
3ga


3gj
NHTs
OAc2j
f1 (ppm)
1.90
1.86
1.12
2.00
1.83
0.90
1.92
0.96
3.15
2.23
4.40
3.03
7.923
7.904
7.748
7.728
7.569
7.550
7.532
7.416
7.396
7.377
7.266
7.168
7.148
5.196
5.176
4.239
4.225
4.149
4.139
4.121
4.110
3.639
3.607
3.592
3.579
3.561
2.321
1.545
1.256
1.238
1.224
1.208
1.196
0.821
0.804
0.787
0.000


3gj
NHTs
OAc
166.4
143.3
137.9
133.2
129.7
129.6
129.5
128.4
126.9
77.4
77.1
76.8
66.2
53.1
32.3
27.6
22.3
21.5
13.9
f1 (ppm)


gyq20141209-2-42-4
%T
Wavenumbers (cm-1)
4000
3000
2000
1500
1000
500
3406.2
3298.6
3064.0
3009.7
2985.7
2956.3
2933.2
2876.6
2857.5
1995.5
1977.3
1925.4
1831.4
1791.2
1709.2
1633.7
1600.5
1585.2
1495.1
1452.1
1427.9
1395.3
1379.3
1352.0
1340.2
1325.2
1309.0
1279.9
1222.2
1180.1
1164.0
1141.2
1116.6
1102.3
1091.6
1073.5
1043.6
1028.1
1002.4
970.8
926.2
896.5
844.2
816.1
787.7
752.1
716.9
686.8
670.7
664.1
621.6
614.8
582.9
550.7
530.3
510.0
495.9
473.5
455.6
429.0
420.3
NHTs
OAc2j
3gj