Silver Triflate and Palladium Acetate Co-catalyzed Reaction of *N'*-(2-Alkynylbenzylidene)hydrazide with *N*-Allyl Ynamide

Ping Huang,[†] Zhiyuan Chen,*[,†] Qin Yang,[‡] and Yiyuan Peng*[,†,‡]

[†] *Key Laboratory of Functional Small Organic Molecules, Ministry of Education and College of Chemistry & Chemical Engineering, Jiangxi Normal University, Nanchang, Jiangxi 330022, China*

[‡] *Jiangxi's Key Laboratory o f Green Chemistry and College of Life Science, Jiangxi Normal University, 99 Ziyang Road, Nanchang, Jiangxi 330022, China. Fax: 86 791 8812 0396; Tel: 86 791 8812 0396;*

E-mail: yiyuanpeng@yahoo.com; zchenjx@yahoo.cn

Supporting Information

1. General experimental methods (S2)

2. General experimental procedure and characterization data (S2-S15)

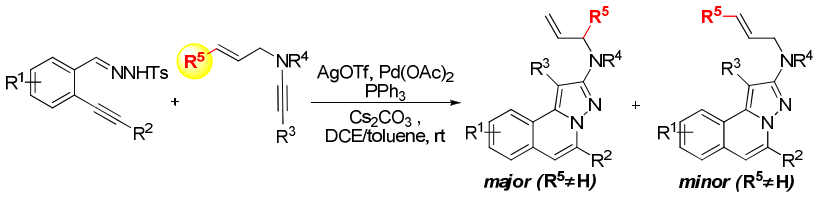
3. ^{1}H and ^{13}C NMR spectra of compound **3** and **4** (S16-S73)

4. X-ray ORTEP illustration of compound **3a**, **4a'** and **4c** (S74-S76)

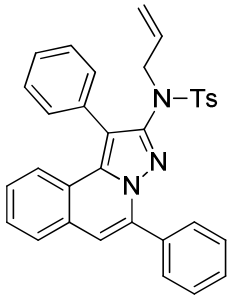
General experimental methods:

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 Silver Triflate and Palladium Acetate Co-catalyzed tandem reaction of N'-(2-alkynylbenzylidene)hydrazide with N-Allyl Ynamides

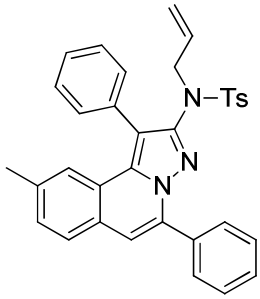


A mixture of *N'*-(2-alkynylbenzylidene)hydrazide **1** (0.20 mmol) and AgOTf (10 mol %) in anhydrous DCE (0.5 mL) was heated at 70 □for 3 hours. The mixture was then cooled to room temperature. Then ynamide with $Pd(OAc)_2$ (10 mol %), PPh_3 (20 mol %) and Cs_2CO_3 (1.2 equiv) was added followed by toluene (2.0 mL).The mixture was stirred at room temperature overnight. After completion of the reaction as indicated by TLC, the reaction was quenched with aqueous NH_4Cl (10 mL, 1.0 M), extracted with EtOAc (2×10 mL), dried by anhydrous Na_2SO_4. Purification of the crude residue using silica gel flash column chromatography (eluent: hexane/EtOAc, 8:1) gave the desired product as a white solid.



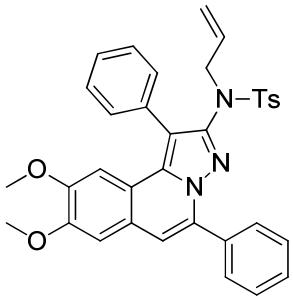
***N*-Allyl-*N*-(1,5-diphenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3a**.

Yield: 90%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3H), 3.91 (d, *J* = 6.4 Hz, 2H), 4.79-4.83 (m, 2H), 5.35-5.39 (m, 1H), 7.09 (s, 1H), 7.15 (d, *J* = 7.8 Hz, 2H), 7.26 (t, *J* = 8.2 Hz, 1H), 7.45-7.56 (m, 7H), 7.65-7.70 (m, 3H), 7.79-7.83 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 54.1, 113.3, 114.9, 118.4, 123.3, 124.4, 127.1, 127.3, 127.9, 128.5, 128.7, 129.0, 129.1, 129.4, 129.6, 131.2, 132.1, 132.5, 133.5, 135.8, 136.8, 137.8, 143.0, 147.1; HRMS calcd. for $C_{33}H_{27}N_3O_2S^+$[M+H] $^+$: 530.1902, found 530.1913.



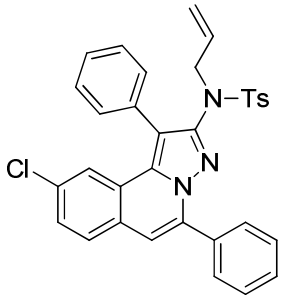
***N*-Allyl-4-methyl-*N*-(9-methyl-1,5-diphenylpyrazolo[5,1-*a*]isoquinolin-2-yl)benzenesulfonamide 3b.**

Yield: 66%; ^{1}H NMR (400 MHz, $CDCl_3$): 2.24 (s, 3H), 2.42 (s, 3H), 3.91 (d, *J* = 6.0 Hz, 2H), 4.79-4.83 (m, 2H), 5.36-5.40 (m, 1H), 7.05 (s, 1H), 7.14 (d, *J* = 7.8 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.4-7.58 (m, 8H), 7.66 (d, *J* = 6.8 Hz, 2H), 7.78 (d, *J* = 7.3 Hz, 2H), 7.83 (d, *J* = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 21.8, 54.1, 113.2, 114.7, 118.4, 123.1, 124.4, 127.1, 127.2, 127.8, 128.5, 128.7, 128.8, 129.0, 129.4, 129.6, 131.2, 132.1, 132.5, 133.7, 135.7, 136.8, 136.9, 137.0, 142.9, 146.9; HRMS calcd. for $C_{34}H_{29}N_3O_2S^+$[M+H] $^+$: 544.2059, found 544.2040.



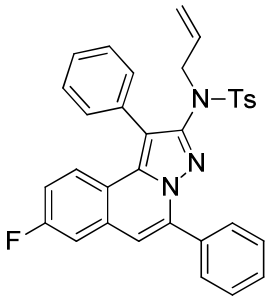
***N*-Allyl-*N*-(8,9-dimethoxy-1,5-diphenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methyl benzenesulfonamide 3c.**

Yield: 63%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3H), 3.49 (s, 3H), 3.94-3.96 (m, 5H), 4.81-4.86 (m, 2H), 5.38-5.48 (m, 1H), 7.02 (s, 1H), 7.06 (s, 1H), 7.16 (d, J = 8.3 Hz, 3H), 7.25-7.55 (m, 6H), 7.66 (d, J = 6.8 Hz, 2H), 7.78-7.84 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 54.2, 55.4, 55.9, 104.4, 107.4, 112.7, 113.2, 118.4, 118.7, 124.2, 127.7, 127.8, 128.5, 128.6, 128.7, 129.0, 129.5, 131.7, 132.4, 132.6, 133.7, 135.7, 136.3, 136.8, 142.9, 146.7, 149.1, 149.7; HRMS calcd. for $C_{35}H_{31}N_3O_4S^+$[M+H] $^+$: 590.2114, found 590.2125.



***N*-Allyl-*N*-(9-chloro-1,5-diphenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzen esulfonamide 3d.**

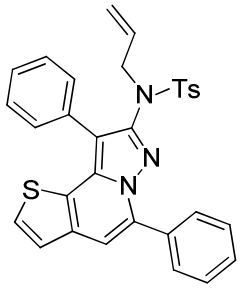
Yield: 80%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3H), 3.92 (d, J = 6.3 Hz, 2H), 4.82 (d, J = 12.1 Hz, 2H), 5.34-5.43 (m, 1H), 7.05 (s, 1H), 7.15 (d, J = 7.6 Hz, 2H), 7.39 (d, J = 8.4 Hz, 1H), 7.43-7.48 (m, 2H), 7.49-7.53 (m, 2H), 7.55-7.60 (m, 3H), 7.62-7.66 (m, 2H), 7.74 (s, 1H), 7.77-7.82 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 54.0, 112.5, 115.4, 118.5, 122.7, 125.3, 127.8, 127.9, 128.2, 128.4, 128.5, 128.6, 128.9, 129.1, 129.2, 129.6, 130.9, 131.3, 132.4, 132.8, 133.2, 134.8, 136.7, 138.1, 143.0, 147.3; HRMS calcd. for $C_{33}H_{26}ClN_3O_2S^+$[M+H]$^+$: 564.1513, found 564.1490.



***N*-Allyl-*N*-(8-fluoro-1,5-diphenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzen esulfonamide 3e.**

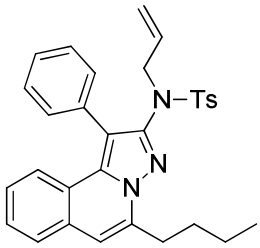
Yield: 88%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.42 (s, 3H), 3.91 (d, J = 6.0 Hz, 2H), 4.80-4.83 (m, 2H), 5.35-5.39 (m, 1H), 6.97 (t, J = 8.5 Hz, 2H), 7.14 (d, J = 7.8 Hz, 2H), 7.31 (d, J = 8.2 Hz, 2H), 7.42-7.56 (m, 6H), 7.64 (d, J = 6.4 Hz, 2H), 7.76-7.83 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 54.0, 111.9, 112.1 ($^{2}J_{CF}$ = 21.0 Hz), 112.4, 114.5, 115.5, 115.7 ($^{2}J_{CF}$ = 22.9 Hz), 118.5, 120.9, 125.5, 125.6 ($^{3}J_{CF}$ = 8.6 Hz), 127.9, 128.0 ($^{3}J_{CF}$ = 7.6 Hz), 128.5, 128.8, 129.0, 129.2, 129.6, 131.1, 131.8, 132.4,

133.1, 135.6, 136.7, 138.8, 143.0, 147.4, 160.5, 163.0 (d, $^{1}J_{CF}$ = 247.0 Hz); HRMS calcd. for $C_{33}H_{26}FN_3O_2S^+$[M+H] $^+$: 548.1808, found 548.1794.



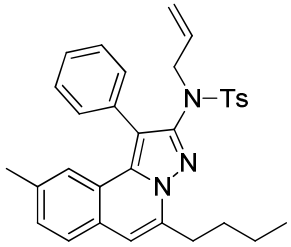
N-Allyl-N-(5,9-diphenylpyrazolo[1,5-a]thieno[2,3-c]pyridin-8-yl)-4-methylbenzenesulfonamide 3f.

Yield: 85%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.42 (s, 3H), 3.97 (d, *J* = 6.0 Hz, 2H), 4.78-4.83 (m, 2H), 5.37-5.41 (m, 1H), 7.14 (d, *J* = 7.3 Hz, 2H), 7.21 (s, 1H), 7.27 (d, *J* = 6.8 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.42-7.55 (m, 6H), 7.72-7.78 (m, 4H), 7.85 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 54.0, 109.1, 118.5, 123.7, 126.5, 126.8, 127.8, 127.9, 128.5, 128.9, 129.0, 129.5, 130.6, 132.3, 133.6, 135.2, 135.5, 136.8, 137.1, 143.0, 146.9; HRMS calcd. for $C_{31}H_{25}N_3O_2S_2^+$[M+H] $^+$: 536.1466, found 536.1452.



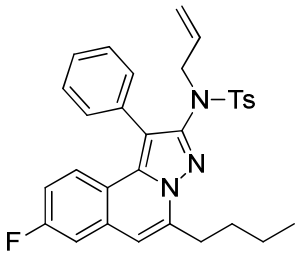
N-Allyl-N-(5-butyl-1-phenylpyrazolo[5,1-a]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3g.

Yield: 51%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.99 (t, *J* = 7.1 Hz, 3H), 1.44-1.50 (m, 2H), 1.75-1.81 (m, 2H), 2.45 (s, 3H), 2.99-3.03 (m, 2H), 4.00 (d, *J* = 6.2 Hz, 2H), 4.84-4.89 (m, 2H), 5.43-5.53 (m, 1H), 6.86 (s, 1H), 7.20 (d, *J* = 7.3 Hz, 1H), 7.29 (d, *J* = 7.5 Hz, 2H), 7.40-7.54 (m, 4H), 7.62 (d, *J* = 7.1 Hz, 3H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.8, 21.6, 22.5, 29.0, 30.6, 54.2, 110.4, 114.7, 118.5, 123.2, 123.9, 126.3, 126.5, 127.6, 127.7, 128.6, 129.1, 129.4, 131.2, 132.3, 132.5, 135.3, 136.9, 139.0, 143.2, 146.8; HRMS calcd. for $C_{31}H_{31}N_3O_2S^+$[M+H] $^+$: 510.2215, found 510.2202.



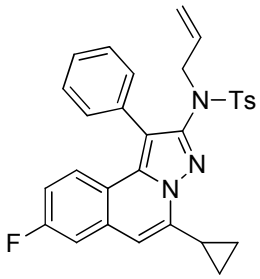
***N*-Allyl-*N*-(5-butyl-9-methyl-1-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3h.**

Yield: 40%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.98 (t, J = 7.3 Hz, 3H), 1.43-1.49 (m, 2H), 1.74-1.79 (m, 2H), 2.23 (s, 3H), 2.45 (s, 3H), 2.97-3.01 (m, 2H), 4.00 (d, J = 6.2 Hz, 2H), 4.83-4.89 (m, 2H), 5.43-5.53 (m, 1H), 6.81 (s, 1H), 7.26-7.29 (m, 4H), 7.48-7.51 (m, 4H), 7.61 (d, J = 7.2 Hz, 2H), 7.86 (d, J = 7.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.9, 21.5, 21.7, 22.5, 29.0, 30.6, 54.2, 110.3, 114.6, 118.4, 123.0, 123.9, 126.4, 127.1, 127.7, 128.5, 128.7, 129.0, 129.2, 131.2, 132.3, 132.6, 135.2, 136.1, 136.9, 138.1, 143.1, 146.6; HRMS calcd. for $C_{32}H_{33}N_3O_2S^+$[M+H] $^+$: 524.2372, found 524.2349.



***N*-Allyl-*N*-(5-butyl-8-fluoro-1-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3i.**

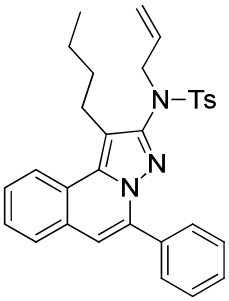
Yield: 64%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.98 (t, J = 7.3 Hz, 3H), 1.44-1.49 (m, 2H), 1.74-1.80 (m, 2H), 2.45 (s, 3H), 3.00 (t, J = 7.3 Hz, 2H), 3.99 (t, J = 6.4 Hz, 2H), 4.84-4.87 (m, 2H), 5.44-5.51 (m, 1H), 6.80 (s, 1H), 6.94 (t, J = 8.0 Hz, 1H), 7.28 (t, J = 9.5 Hz, 3H), 7.47-7.54 (m, 3H), 7.60 (d, J = 7.4 Hz, 2H), 7.71 (t, J = 8.0 Hz, 1H), 7.84 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.8, 21.5, 22.5, 28.9, 30.6, 54.1, 109.7, 111.2, 111.4 (d, $^{2}J_{CF}$ = 21.9 Hz), 114.4, 114.8, 115.0 (d, $^{2}J_{CF}$ = 22.9 Hz), 118.5, 120.5, 125.4, 125.5 (d, $^{3}J_{CF}$ = 8.6 Hz), 127.9, 128.6, 128.7, 129.1, 131.1, 131.3, 131.4 (d, $^{3}J_{CF}$ = 8.6 Hz), 132.0, 132.5, 135.0, 136.8, 140.2, 143.2, 147.1, 160.4, 162.9 (d, $^{1}J_{CF}$ = 246.0 Hz); HRMS calcd. for $C_{31}H_{30}FN_3O_2S^+$[M+H] $^+$: 528.2121, found 528.2115.



***N*-Allyl-*N*-(5-cyclopropyl-8-fluoro-1-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3j.**

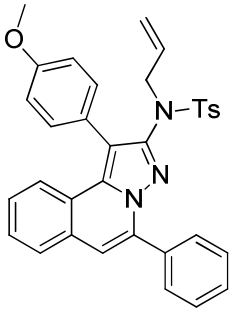
Yield: 46%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.93-0.94 (m, 2H), 1.11-1.13 (m, 2H), 2.45 (s, 3H), 2.48-2.52 (m, 1H), 4.00 (d, J = 6.0 Hz, 2H), 4.85-4.92 (m, 2H), 5.45-5.51 (m, 1H), 6.61 (s, 1H), 6.94 (t, J = 8.2 Hz, 1H), 7.22-7.28 (m, 3H), 7.48-7.55 (m, 3H), 7.60 (d, J = 7.4 Hz, 2H), 7.70 (t, J = 7.2 Hz, 1H), 7.88 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 7.2, 11.3, 21.6, 54.1, 106.7, 111.2, 111.4 (d, $^{2}J_{CF}$ =

21.9 Hz), 114.6, 114.8, 115.0, 118.6, 120.3, 125.4, 125.5 (d, $^{3}J_{CF}$=8.6 Hz), 127.9, 128.7, 128.8 (d, $^{3}J_{CF}$ = 7.6 Hz), 129.1, 129.4, 130.6, 131.2, 131.4 (d, $^{2}J_{CF}$ = 18.1 Hz), 132.0, 132.5, 135.0, 136.8, 141.6, 143.2, 147.3, 160.4, 162.9 (d, $^{1}J_{CF}$ = 247.0 Hz) ; HRMS calcd. for $C_{30}H_{26}FN_3O_2S^+$[M+H] $^+$: 512.1808, found 512.1790.



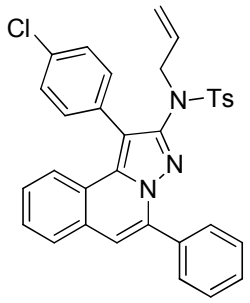
***N*-Allyl-*N*-(1-butyl-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3k.**

Yield: 84%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.07 (t, *J* = 6.9 Hz, 3H), 1.59-1.64 (m, 2H), 1.75-1.79 (m, 2H), 2.45 (s, 3H), 3.14-3.18 (m, 2H), 4.15 (d, *J* = 6.3 Hz, 2H), 4.95-5.01 (m, 2H), 5.73-5.83 (m, 1H), 7.02 (s, 1H), 7.21 (d, *J* = 7.6 Hz, 2H), 7.41 (t, *J* = 7.3 Hz, 2H), 7.43 (d, *J* = 7.0 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.65 (d, *J* = 7.3 Hz, 2H), 7.70-7.75 (m, 3H), 8.23 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.0, 21.6, 23.1, 23.8, 31.4, 54.8, 112.9, 114.9, 118.8, 123.1, 124.9, 127.3, 127.7, 128.5, 128.8, 128.8, 129.0, 129.2, 129.4, 132.8, 133.5, 135.6, 135.7, 137.9, 143.0, 147.6; HRMS calcd. for $C_{31}H_{31}N_3O_2S^+$[M+H] $^+$: 510.2215, found 510.2205.



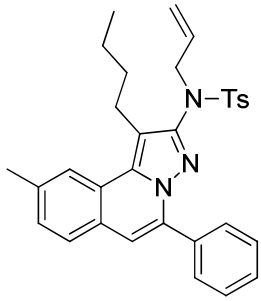
***N*-allyl-*N*-(1-(4-methoxyphenyl)-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3l.**

Yield: 85%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3H), 3.78-3.95 (m, 5H), 4.81-4.86 (m, 2H), 5.37-5.47 (m, 1H), 7.08-7.11 (m, 3H), 7.16 (d, *J* = 7.8 Hz, 2H), 7.28-7.34 (m, 2H), 7.43-7.50 (m, 4H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.79-7.86 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8, 54.2, 55.4, 61.0, 113.4, 114.3, 114.7, 118.6, 123.2, 124.1, 124.5, 124.9, 126.8, 127.2, 128.0, 128.1, 128.7, 129.1, 129.2, 129.8, 132.5, 132.8, 133.7, 136.1, 136.9, 137.8, 143.1, 144.9, 147.4, 159.4; HRMS calcd. for$C_{34}H_{29}N_3O_3S^+$[M+H]$^+$: 560.2008, found 560.1991.



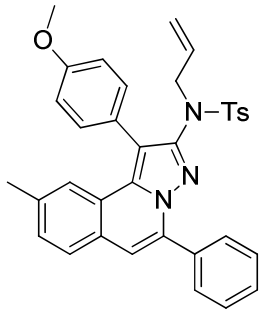
***N*-Allyl-*N*-(1-(4-chlorophenyl)-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methyl benzenesulfonamide 3m.**

Yield: 88%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.45 (s, 3H), 3.94 (d, *J* = 6.0 Hz, 2H), 4.82-4.85 (m, 2H), 5.36-5.40 (m, 1H), 7.11 (s, 1H), 7.17 (d, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.45-7.54 (m, 6H), 7.62 (d, *J* = 7.9 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.76-7.83 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8, 54. 5, 113.7, 114.0, 118.9, 123.2, 124.3, 127.5,128.1, 128.3, 128.7, 129.1, 129.2, 129.3, 129.8, 130.8, 132.5, 132.8, 133.5, 134.0, 136.0, 136.6, 138.0, 143.3, 147.3; HRMS calcd. for $C_{33}H_{26}ClN_3O_2S^+$[M+H]$^+$: 564.1513, found 564.1536.



***N*-Allyl-*N*-(1-butyl-9-methyl-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylb enzenesulfonamide 3n.**

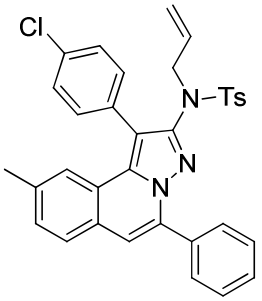
Yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.08 (t, *J* = 6.9 Hz, 3H), 1.58-1.62 (m, 2H), 1.76-1.78 (m, 2H), 2.44 (s, 3H), 2.55 (s, 3H), 3.12-3.16 (m, 2H), 4.13 (d, *J* = 6.0 Hz, 2H), 4.93-4.99 (m, 2H), 5.72-5.77 (m, 1H), 6.97 (s, 1H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.34-7.43 (m, 4H), 7.58-7.64 (m, 3H), 7.73 (d, *J* = 7.3 Hz, 2H), 8.01 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.9, 21.6, 22.0, 23.1, 23.9, 54.8, 112.9, 114.8, 118.7, 123.1, 125.0, 127.0, 127.2, 127.6, 128.5, 128.7, 128.8, 129.0, 129.4, 132.8, 133.6, 135.5, 135.8, 137.1, 137.3, 143.0, 147.4; HRMS calcd. for $C_{32}H_{33}N_3O_2S^+$[M+H] $^+$: 524.2372, found 524.2338.



***N*-Allyl-*N*-(1-(4-methoxyphenyl)-9-methyl-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-**

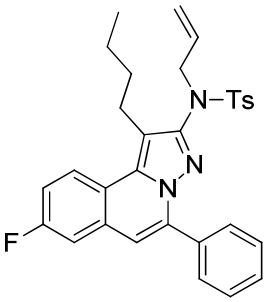
yl)-4-methylbenzenesulfonamide 3o.

Yield: 68%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.28 (s, 3H), 2.43 (s, 3H), 3.94 (d, *J* = 0.7 Hz, 5H), 4.81-4.85 (m, 2H), 5.36-5.46 (m, 1H), 7.05 (s, 1H), 7.10 (d, *J* = 7.4 Hz, 2H), 7.16 (d, *J* = 7.3 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 1H), 7.42-7.49 (m, 3H), 7.57-7.59 (m, 3H), 7.64 (s, 1H), 7.79 (d, *J* = 7.0 Hz, 2H), 7.86 (d, *J* = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 21.8, 54.0, 55.3, 113.2, 114.0, 114.3, 118.3, 123.0, 124.2, 124.5, 127.1, 127.8, 128.5, 128.8, 129.0, 129.4, 129.6, 132.3, 132.6, 133.7, 135.7, 136.9, 137.0, 142.9, 147.0, 159.2; HRMS calcd. for$C_{35}H_{31}N_3O_3S^+$[M+H]$^+$: 574.2164, found 574.2143.



***N*-Allyl-*N*-(1-(4-chlorophenyl)-9-methyl-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl) -4-methylbenzenesulfonamide 3p.**

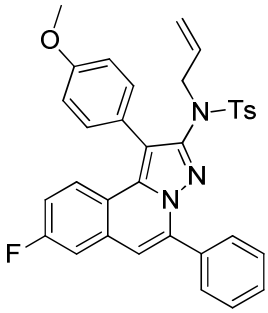
Yield: 71%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.32 (s, 3H), 2.43 (s, 3H), 3.91-3.93 (d, *J* = 5.9 Hz, 2H), 4.79-4.83 (m, 2H), 5.36-5.40 (m, 1H), 7.06 (s, 1H), 7.15-7.16 (d, *J* = 7.8 Hz, 2H), 7.28-7.30 (d, *J* = 7.8 Hz, 1H), 7.41-7.48 (m, 3H), 7.51-7.53 (d, *J* = 7.8 Hz, 2H), 7.57-7.63 (m, 4H), 7.74-7.76 (d, *J* = 7.8 Hz, 2H), 7.80-7.82 (d, *J* = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 21.8, 54.3, 113.4, 113.6, 118.6, 122.8, 124.1, 127.2, 127.8, 128.5, 128.8, 128.9, 129.1, 129.6, 129.7, 130.7, 132.4, 132.6, 133.5, 133.8, 135.6, 136.5, 137.0, 137.2, 143.1, 146.9; HRMS calcd. for$C_{34}H_{28}ClN_3O_2S^+$[M+H]$^+$: 578.1669, found 578.1676.



***N*-Allyl-*N*-(1-butyl-8-fluoro-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbe nzenesulfonamide 3q.**

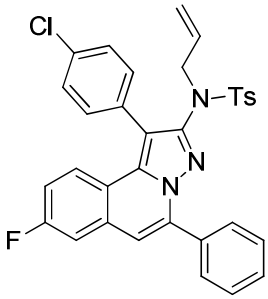
Yield: 85%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.06 (t, *J* = 7.1 Hz, 3H), 1.57-1.63 (m, 2H), 1.74-1.76 (m, 2H), 2.45 (s, 3H), 3.10-3.14 (m, 2H), 4.14 (d, *J* = 6.3 Hz, 2H), 4.95-5.01 (m, 2H), 5.71-5.82 (m, 1H), 6.95 (s, 1H), 7.21 (d, *J* = 7.6 Hz, 2H), 7.32-7.38 (m, 4H), 7.44 (d, *J* = 7.1 Hz, 1H), 7.64 (d, *J* = 7.3 Hz, 2H), 7.73 (d, *J* = 7.7 Hz, 2H), 8.19 (t, *J* = 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.9, 21.6, 23.1, 23.7, 31.3, 54.8, 112.0, 112.2 (d, $^2J_{CF}$ = 21.0 Hz), 114.5, 115.7, 116.0 (d, $^2J_{CF}$ = 22.9 Hz), 118.8, 121.6, 125.3, 125.4 (d, $^3J_{CF}$ = 8.6 Hz), 127.7, 128.5, 129.1, 129.4, 131.0,

131.1 (d, $^{3}J_{CF}$ = 9.5 Hz), 132.7, 133.1, 135.4, 135.6, 138.9, 143.1, 148.0, 160.2, 162.6 (d, $^{1}J_{CF}$ = 246.9 Hz); HRMS calcd. for $C_{31}H_{30}FN_3O_2S^+$[M+H] $^+$: 528.2121, found 528.2101.



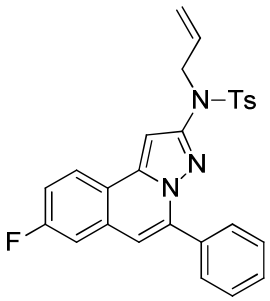
***N*-Allyl-*N*-(8-fluoro-1-(4-methoxyphenyl)-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3r.**

Yield: 87%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3H), 3.84-3.93 (m, 5H), 4.81-4.84 (m, 2H), 5.36-5.40 (m, 1H), 7.01 (s, 2H), 7.09 (d, *J* = 7.3 Hz, 2H), 7.15 (d, *J* = 7.3 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.43-7.55 (m, 5H), 7.77-7.83 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 54.0, 55.3, 111.9, 112.1 (d, $^{2}J_{CF}$ = 21.0 Hz), 112.3, 114.3, 115.5, 115.8 (d, $^{2}J_{CF}$ = 22.9 Hz), 118.4, 121.1, 123.8, 125.5, 125.6 (d, $^{3}J_{CF}$ = 8.6 Hz), 127.9, 128.5, 129.1, 129.2, 129.6, 131.3, 132.2, 132.5, 133.2, 135.7, 136.8, 138.9, 143.0, 147.6, 159.4, 160.5, 163.0 (d, $^{3}J_{CF}$ = 247.0 Hz); HRMS calcd. for$C_{34}H_{28}FN_3O_3S^+$[M+H]$^+$: 578.1914, found 578.1916.



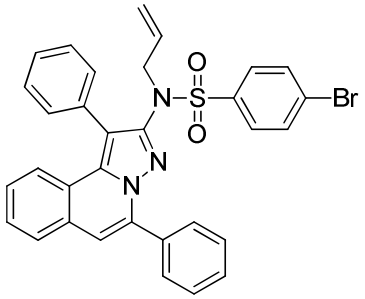
***N*-Allyl-*N*-(1-(4-chlorophenyl)-8-fluoro-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3s.**

Yield: 92%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3H), 3.92 (d, *J* = 6.4 Hz, 2H), 4.80-4.84 (m, 2H), 5.36-5.40 (m, 1H), 7.00-7.03 (m, 2H), 7.16 (d, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.41-7.53 (m, 5H), 7.59 (d, *J* = 7.8 Hz, 2H), 7.73-7.80 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 54.2, 112.0, 112.2 (d, $^{2}J_{CF}$ = 21.0 Hz), 112.6, 113.4, 115.7, 115.9 (d, $^{2}J_{CF}$ = 22.9 Hz), 118.7, 120.7, 125.3, 125.4 (d, $^{3}J_{CF}$ = 8.6 Hz), 127.9, 128.5, 129.0, 129.1, 129.3, 129.6, 130.4, 131.3, 132.3, 132.5 (d, $^{2}J_{CF}$ = 24.8 Hz), 132.9, 134.0, 135.6, 136.3, 138.9, 147.4, 160.6, 163.0 (d, $^{1}J_{CF}$ = 247.9 Hz); HRMS calcd. for $C_{33}H_{25}ClFN_3O_2S^+$[M+H]$^+$: 582.1418, found 582.1438.



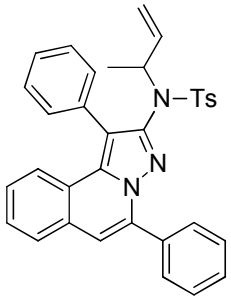
***N*-Allyl-*N*-(8-fluoro-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 3t.**

Yield: 61%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (s, 3H), 4.44 (d, J = 5.0 Hz, 2H), 5.13 (d, J = 10.1 Hz, 1H), 5.25 (d, J = 17.4 Hz, 1H), 5.87-5.91 (m, 1H), 6.92 (s, 1H), 7.17-7.21 (m, 4H), 7.44 (d, J = 6.0 Hz, 4H), 7.68 (d, J = 7.3 Hz, 2H), 7.77 (d, J = 7.4 Hz, 2H), 8.06-8.08 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.5, 51.6, 92.2, 111.0, 111.7, 111.9 (d, $^{2}J_{CF}$ = 21.9 Hz), 115.9, 116.2 (d, $^{2}J_{CF}$ = 23.8 Hz), 118.1, 120.0, 125.9, 126.0 (d, $^{3}J_{CF}$ = 9.5 Hz), 127.0, 127.4, 128.0, 129.3, 129.4 (d, $^{3}J_{CF}$ = 8.6 Hz), 130.8, 133.0, 133.2, 136.0, 138.8 (d, $^{1}J_{CF}$ = 276.5 Hz), 139.8, 143.6, 149.5; HRMS calcd. for $C_{27}H_{22}FN_3O_2S^{+}$[M+H] $^{+}$: 472.1495, found 472.1485.



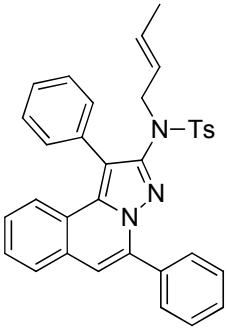
***N*-Allyl-4-bromo-*N*-(1,5-diphenylpyrazolo[5,1-*a*]isoquinolin-2-yl)benzenesulfonamide 3u.**

Yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.94 (d, J = 5.7 Hz, 2H), 4.83-4.88 (m, 2H), 5.36-5.44 (m, 1H), 7.11 (s, 1H), 7.25-7.30 (m, 1H), 7.39-7.51 (m, 6H), 7.55-7.58 (m, 3H), 7.65-7.71 (m, 3H), 7.74-7.76 (m, 2H), 7.80 (d, J = 8.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 54.2, 113.4, 114.5, 118.8, 123.2, 124.3, 127.2, 127.3, 128.0, 128.8, 129.2, 129.4, 129.6, 130.1, 131.1, 131.6, 131.8, 132.1, 133.3, 135.8, 137.8, 138.9, 146.8; HRMS calcd. for $C_{32}H_{24}BrN_3O_2S^{+}$[M+H]$^{+}$: 594.0851, found 594.0866.

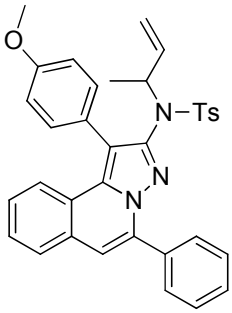


***N*-(but-3-en-2-yl)-*N*-(1,5-diphenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 4a.**

Yield: 55%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.83 (d, *J* = 6.7 Hz, 3H), 2.39 (s, 3H), 4.41-4.44 (m, 1H), 4.70 (t, *J* = 13.3 Hz, 2H), 5.39-5.47 (m, 1H), 7.05 (d, *J* = 7.9 Hz, 2H), 7.12 (s, 1H), 7.25 (m, 1H), 7.43-7.54 (m, 7H), 7.68-7.75 (m, 3H), 7.83-7.86 (m, 5H);^{13}C NMR (100 MHz, $CDCl_3$): δ 18.2, 21.7, 57.6, 113.5, 115.2, 116.6, 123.3, 124.5, 127.2, 127.4, 127.9, 128.6, 129.2, 129.5, 129.8, 131.0, 131.7, 132.5, 133.6, 135.7, 137.9, 138.4, 142.9, 144.7; HRMS calcd. for $C_{34}H_{29}N_3O_2S^+$[M+H] $^+$: 544.2059, found 544.1966.

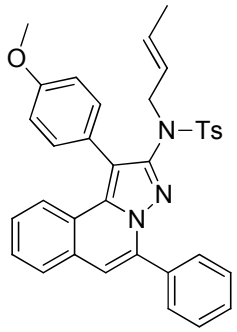


Yield: 27%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.39 (d, *J* = 5.9 Hz, 3H), 2.43 (s, 3H), 3.84 (d, *J* = 6.5 Hz, 2H), 4.91-4.98 (m, 1H), 5.15-5.23 (m, 1H), 7.10 (s, 1H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.25-7.30 (m, 2H), 7.45-7.51 (m, 5H), 7.53-7.57 (m, 2H), 7.64 (d, *J* = 7.0 Hz, 2H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.82 (t, *J* = 8.4 Hz, 4H); ^{13}C NMR (10 MHz, $CDCl_3$): δ 17.7, 21.7, 53.8, 113.4, 115.3, 123.4, 124.5, 125.4, 127.2, 127.9, 128.6, 129.1, 129.7, 131.3, 132.3, 133.6, 135.8, 137.0, 137.9, 142.9, 147.3; HRMS calcd. for $C_{34}H_{29}N_3O_2S^+$[M+H] $^+$: 544.2059, found 544.1978.



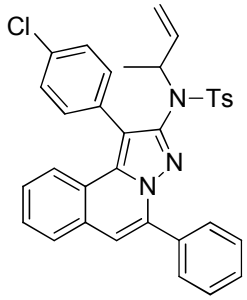
***N*-(but-2-en-1-yl)-*N*-(1-(4-methoxyphenyl)-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 4b.**

Yield: 53%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.84 (d, *J* = 6.4 Hz, 3H), 2.40 (s, 3H), 3.93 (s, 3H), 4.40-4.45 (m, 1H), 4.72 (t, *J* = 8.6 Hz, 2H), 5.42-5.50 (m, 1H), 7.05-7.12 (m, 5H), 7.30-7.33 (m, 2H), 7.47 (d, *J* = 6.4 Hz, 4H), 7.71 (d, *J* = 6.8 Hz), 7.83-7.85 (m, 5H);^{13}C NMR (100 MHz, $CDCl_3$): δ 13.1, 18.2, 21.6, 55.3, 57.5, 64.2, 113.3, 114.0, 115.1, 116.3, 121.7, 123.3, 124.6, 127.3, 127.9, 128.6, 129.2, 129.5, 129.9, 130.0, 131.3, 132.8, 133.6, 135.7, 137.8, 138.4, 142.8, 144.7, 159.3; HRMS calcd. for $C_{35}H_{31}N_3O_2S^+$[M+H] $^+$: 574.2164, found 574.2113.



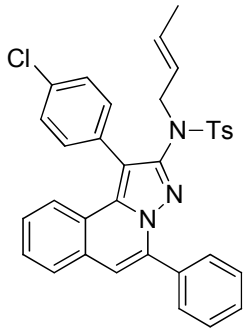
(*E*)-*N*-(but-2-en-1-yl)-N-(1-(4-methoxyphenyl)-5-phenylpyrazolo[5,1-*a*]isoquinoli n-2-yl)-4-methylbenzenesulfonamide 4b'.

Yield: 32%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.40 (d, *J* = 5.9 Hz, 3H), 2.44 (s, 3H), 3.85 (d, *J* = 6.4 Hz, 2H), 3.94 (s, 3H), 4.94-5.04 (m, 1H), 5.15-5.24 (m, 1H), 7.09 (d, *J* = 6.4 Hz, 3H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.25-7.31 (m, 2H), 7.45-7.50 (m, 4H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.79-7.84 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 17.6, 21.7, 53.7, 55.3, 113.3, 114.1, 115.0, 123.3, 124.3, 124.6, 125.4, 127.2, 127.9, 128.6, 129.1,129.5, 129.7, 132.4, 133.7, 135.9, 137.1, 137.9, 142.8, 147.4, 159.3; HRMS calcd. for $C_{35}H_{31}N_3O_2S^+$[M+H] $^+$: 574.2164, found 574.2003.



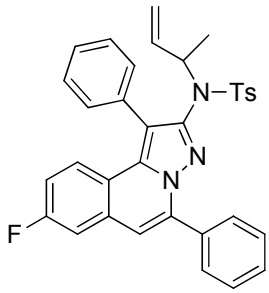
***N*-(but-3-en-2-yl)-*N*-(1-(4-chlorophenyl)-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl) -4-methylbenzenesulfonamide 4c.**

Yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.84 (d, *J* = 5.1 Hz, 3H), 2.40 (s, 3H), 4.41-4.46 (m, 1H), 4.72 (t, *J* = 12.7 Hz, 2H), 5.37-5.48 (m, 1H), 7.07 (d, *J* = 6.8 Hz, 2H), 7.15 (s, 1H), 7.33 (d, *J* = 6.2 Hz, 2H), 7.47-7.53 (m, 6H), 7.67-7.73 (m, 3H), 7.82 (d, *J* = 6.5 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 18.1, 21.6, 57.5, 76.8,,77.1, 77.4, 113.6, 115.3, 123.1, 124.3, 127.3, 127.5, 127.9, 128.2, 128.6, 129.5, 129.6, 129.8, 130.0, 131.0, 132.8, 133.0, 133.1, 133.3, 133.9, 135.7, 137.6, 137.9, 138.2, 143.0, 144.6; HRMS calcd. for $C_{34}H_{28}ClN_3O_2S^+$[M+H] $^+$: 578.1669, found 578.1623.



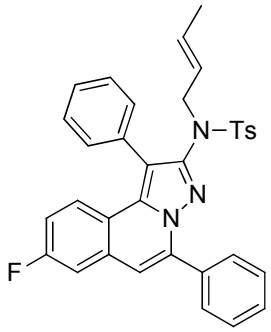
(*E*)-*N*-(but-2-en-1-yl)-*N*-(1-(4-chlorophenyl)-5-phenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 4c'.

Yield: 20%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.40 (d, J = 5.6 Hz, 3H), 2.44 (s, 3H), 3.85 (d, J = 5.9 Hz, 2H), 4.94-5.01 (m, 1H), 5.16-5.24 (m, 1H), 7.12 (s, 1H), 7.16 (d, J = 7.5 Hz, 2H), 7.31-7.34 (m, 1H), 7.43-7.54 (m, 6H), 7.59 (d, J = 6.5 Hz, 2H), 7.72 (d, J = 7.4 Hz, 1H), 7.77-7.81 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 17.7, 21.7, 53.8, 113.4, 115.3, 123.4, 124.5, 125.4, 127.3, 127.9, 128.6, 129.1, 129.7, 131.3, 132.3, 133.6, 135.8, 137.0, 137.9, 142.9, 147.3; HRMS calcd. for $C_{34}H_{28}ClN_3O_2S^+$[M+H] $^+$: 578.1669, found 578.1651.



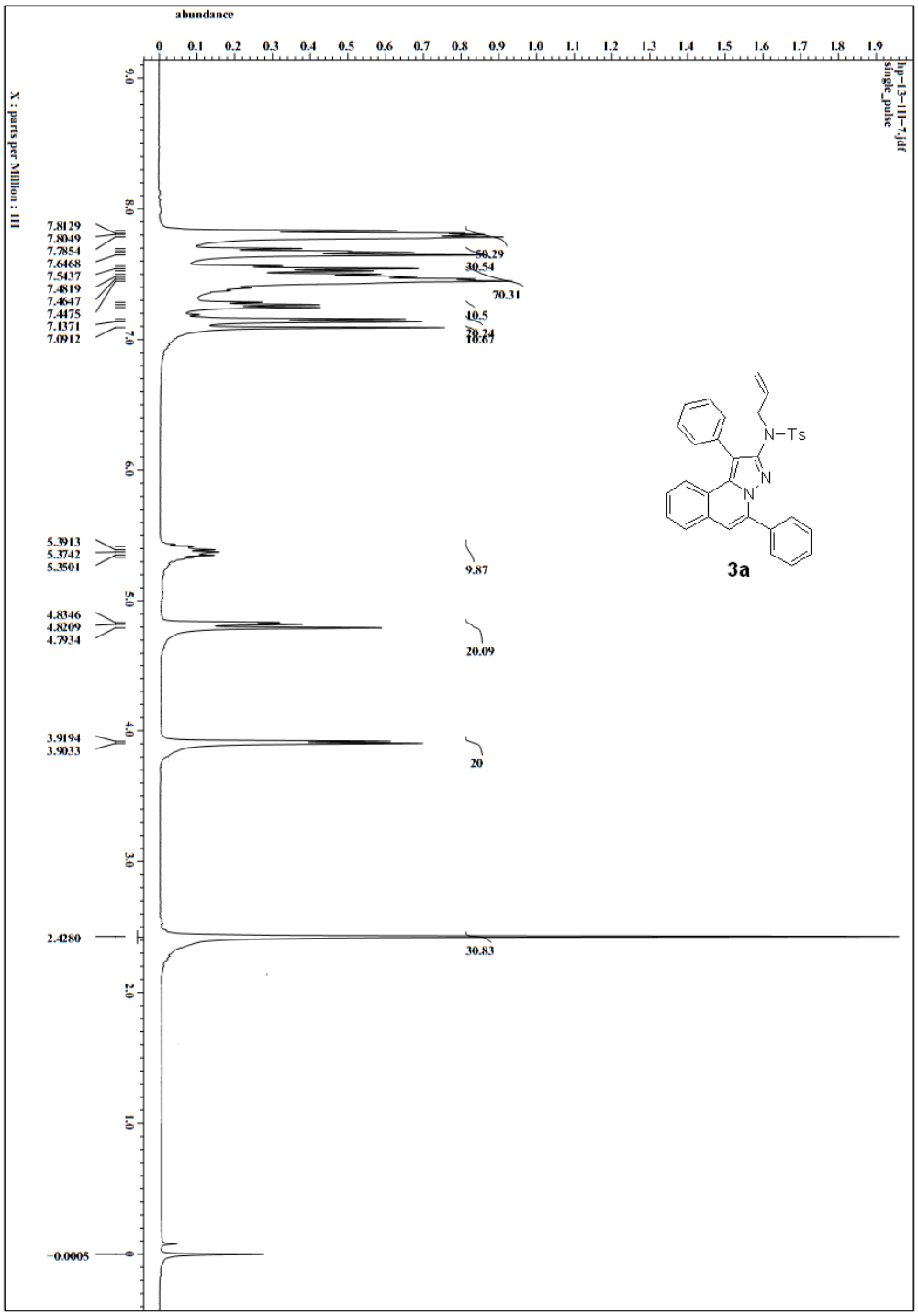
***N*-(but-3-en-2-yl)-*N*-(8-fluoro-1,5-diphenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 4d.**

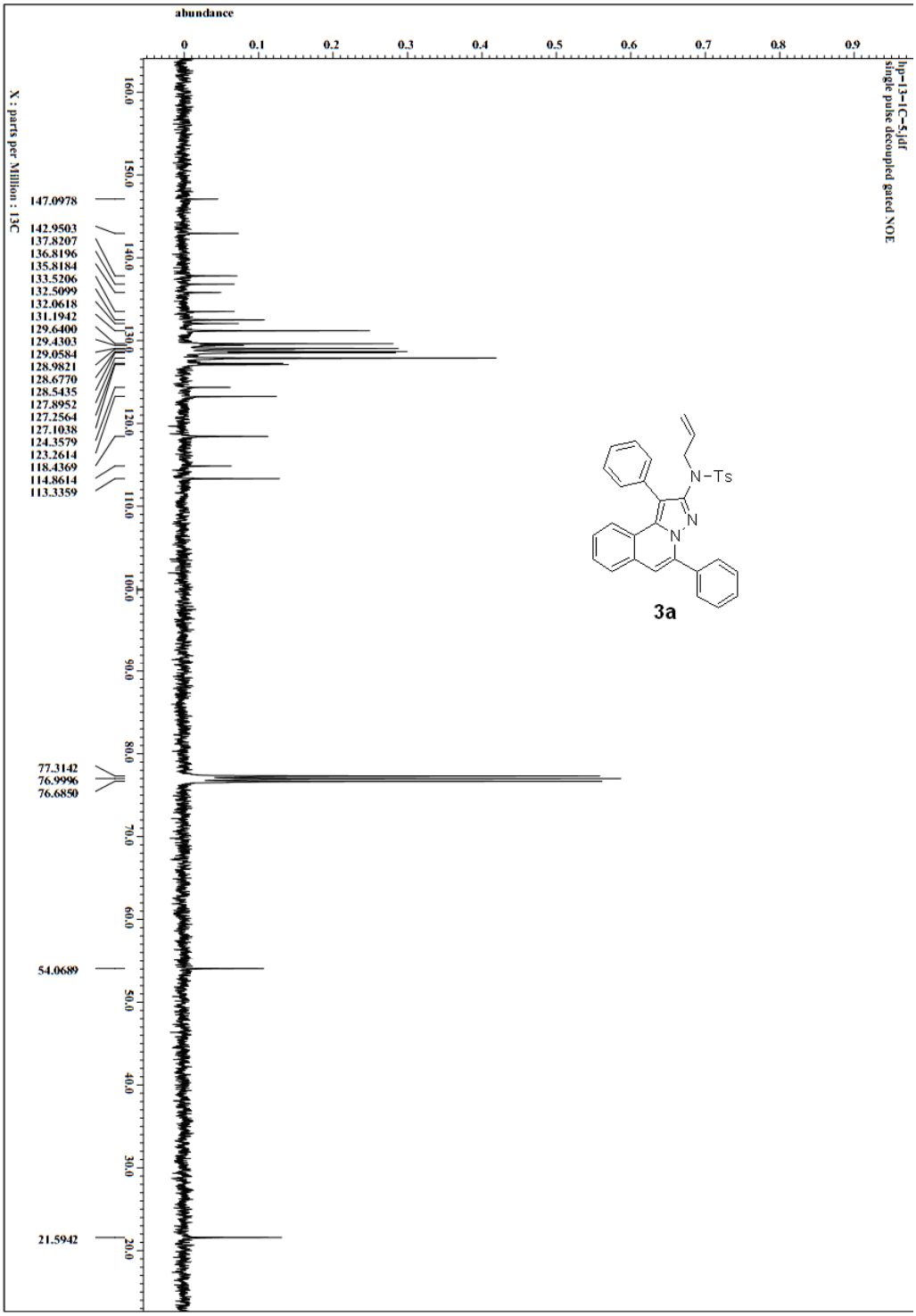
Yield: 59%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.82 (d, J = 6.4 Hz, 3H), 2.40 (s, 3H), 4.41 (m, 1H), 4.71 (t, J = 12.7 Hz, 2H), 5.38-5.46 (m, 1H), 7.06 (d, J = 8.8 Hz, 4H), 7.36 (d, J = 8.2 Hz, 2H), 7.48-7.55 (m, 6H), 7.67 (s, 1H), 7.72 (s, 1H), 7.83 (d, J = 6.4 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 18.1, 21.6, 57.5,112.1, 112.2 (d, $^{2}J_{CF}$ = 23.5 Hz), 112.5, 115.2, 115.6, 115.9 (d, $^{2}J_{CF}$ = 23.0 Hz), 116.3, 121.2, 125.6, 125.7 (d, $^{3}J_{CF}$ = 8.5Hz), 127.9, 128.0 (d, $^{4}J_{CF}$ = 4.7 Hz), 128.8, 128.9 (d, $^{4}J_{CF}$ = 6.7 Hz), 129.3, 129.8, 131.3, 131.4 (d, $^{3}J_{CF}$ = 8.9 Hz), 131.8, 132.2, 133.2, 135.5, 137.7, 138.3, 138.9, 142.9, 144.9, 160.6, 163.1 (d, $^{1}J_{CF}$ = 247.0 Hz); HRMS calcd. for $C_{34}H_{28}FN_3O_2S^+$[M+H] $^+$: 562.1965, found 562.1894.

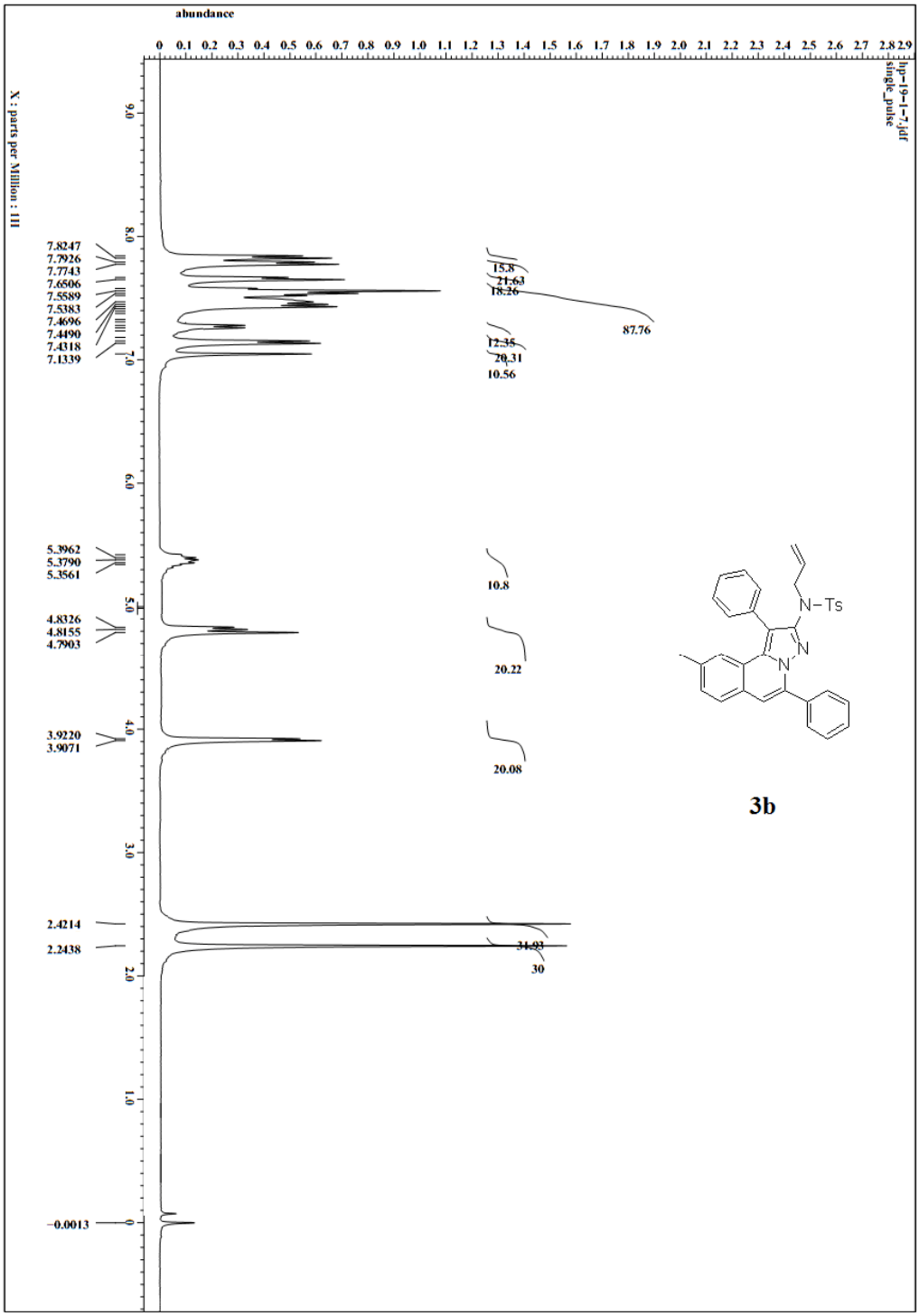


(*E*)-*N*-(but-2-en-1-yl)-*N*-(8-fluoro-1,5-diphenylpyrazolo[5,1-*a*]isoquinolin-2-yl)-4-methylbenzenesulfonamide 4d'.

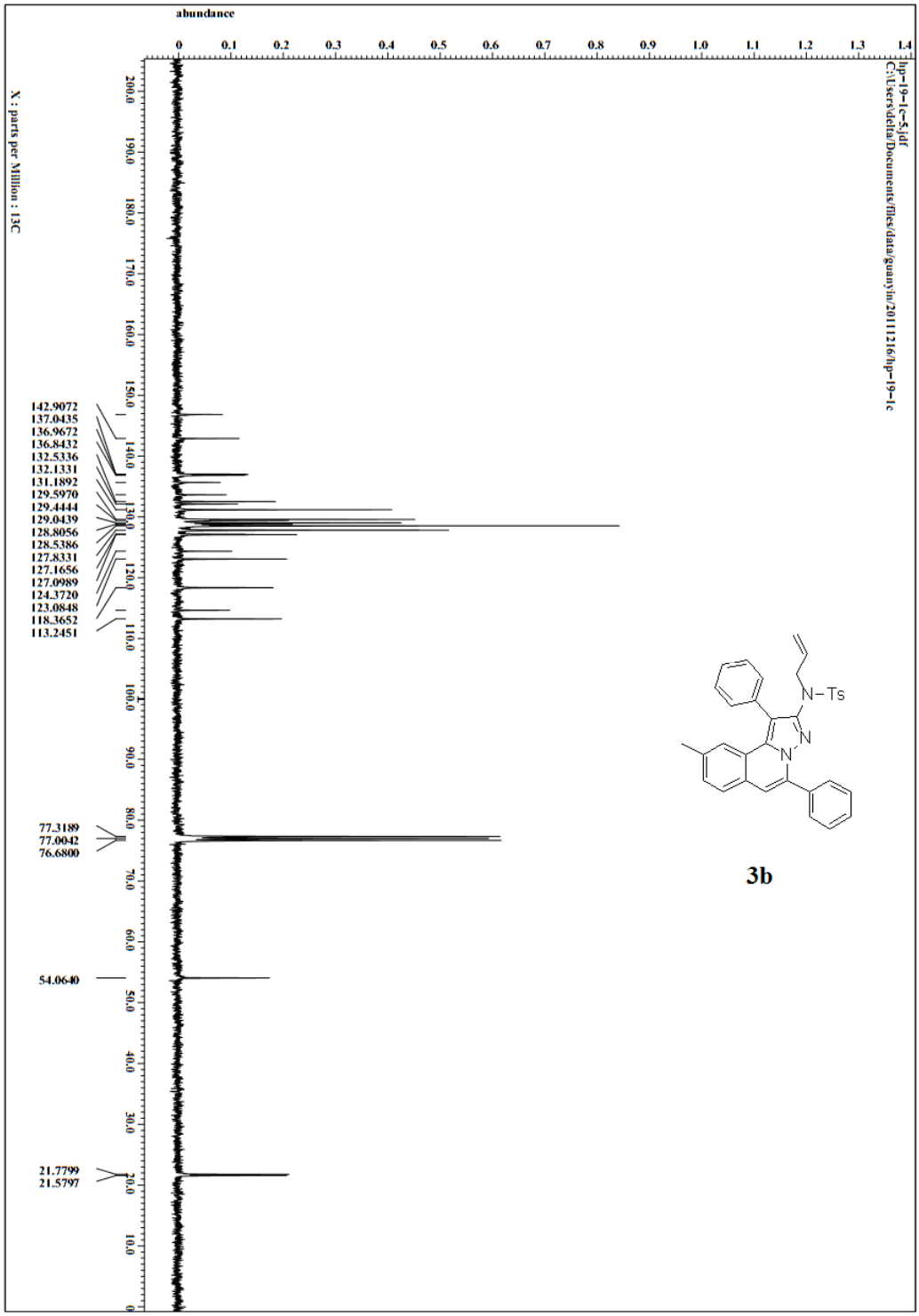
Yield: 29%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.40 (d, J = 5.2 Hz, 3H), 2.44 (s, 3H), 3.84 (d, J = 5.5 Hz, 2H), 4.91-4.97 (m, 1H), 5.15-5.23 (m, 1H), 7.02-7.05 (m, 2H), 7.15 (d, J = 7.6 Hz, 2H), 7.35 (d, J = 8.7 Hz, 1H), 7.46-7.57 (m, 6H), 7.62 (d, J = 6.0 Hz, 2H), 7.80 (t, J = 7.6 Hz, 5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 17.6, 21.7, 53.7, 111.9, 112.2 (d, $^{2}J_{CF}$ = 21.3 Hz), 112.5, 115.0, 115.6, 115.9 (d, $^{2}J_{CF}$ = 23.2 Hz), 121.1, 125.3, 125.7, 125.8 (d, $^{3}J_{CF}$ = 8.5 Hz), 128.0, 128.6, 128.8, 129.1, 129.3 (d, $^{2}J_{CF}$ = 22.2 Hz), 129.7, 129.8, 131.2, 131.3, 131.4 (d, $^{3}J_{CF}$ = 8.9 Hz), 132.0, 133.2, 135.6, 137.0, 139.0, 142.9, 147.6, 163.1 (d, $^{1}J_{CF}$ = 246.8 Hz); HRMS calcd. for $C_{34}H_{28}FN_3O_2S^{+}$[M+H] $^{+}$: 562.1965, found 562.1912.

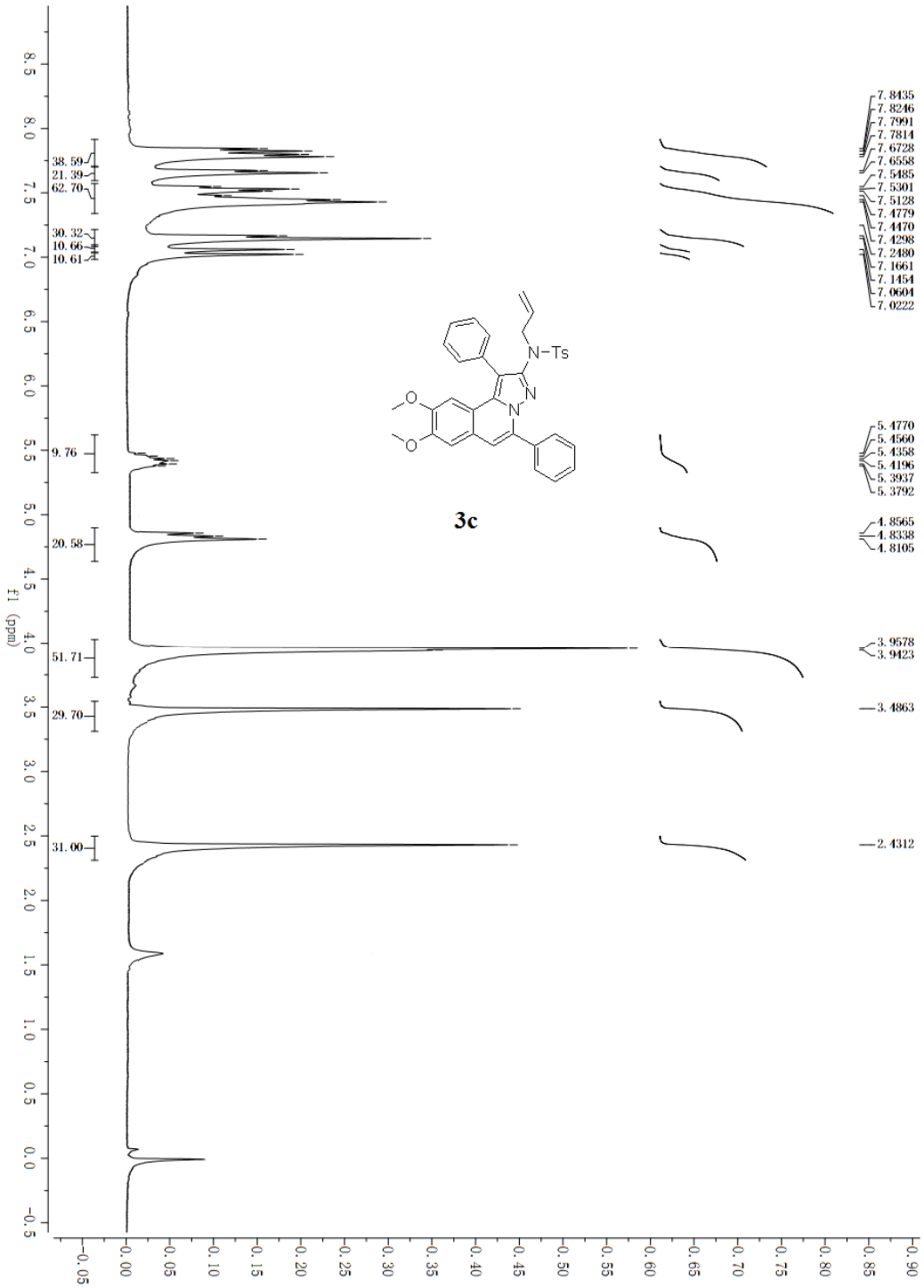

abundance
X : parts per Million : 1H
hrp-13-111-7.jdf
single_pulse
7.8129
7.8049
7.7854
7.6468
7.5437
7.4819
7.4647
7.4475
7.1371
7.0912
5.3913
5.3742
5.3501
4.8346
4.8209
4.7934
3.9194
3.9033
2.4280
-0.0005
50.29
30.54
70.31
10.5
70.24
10.67
9.87
20.09
20
30.83
N-Ts
N
N
3a

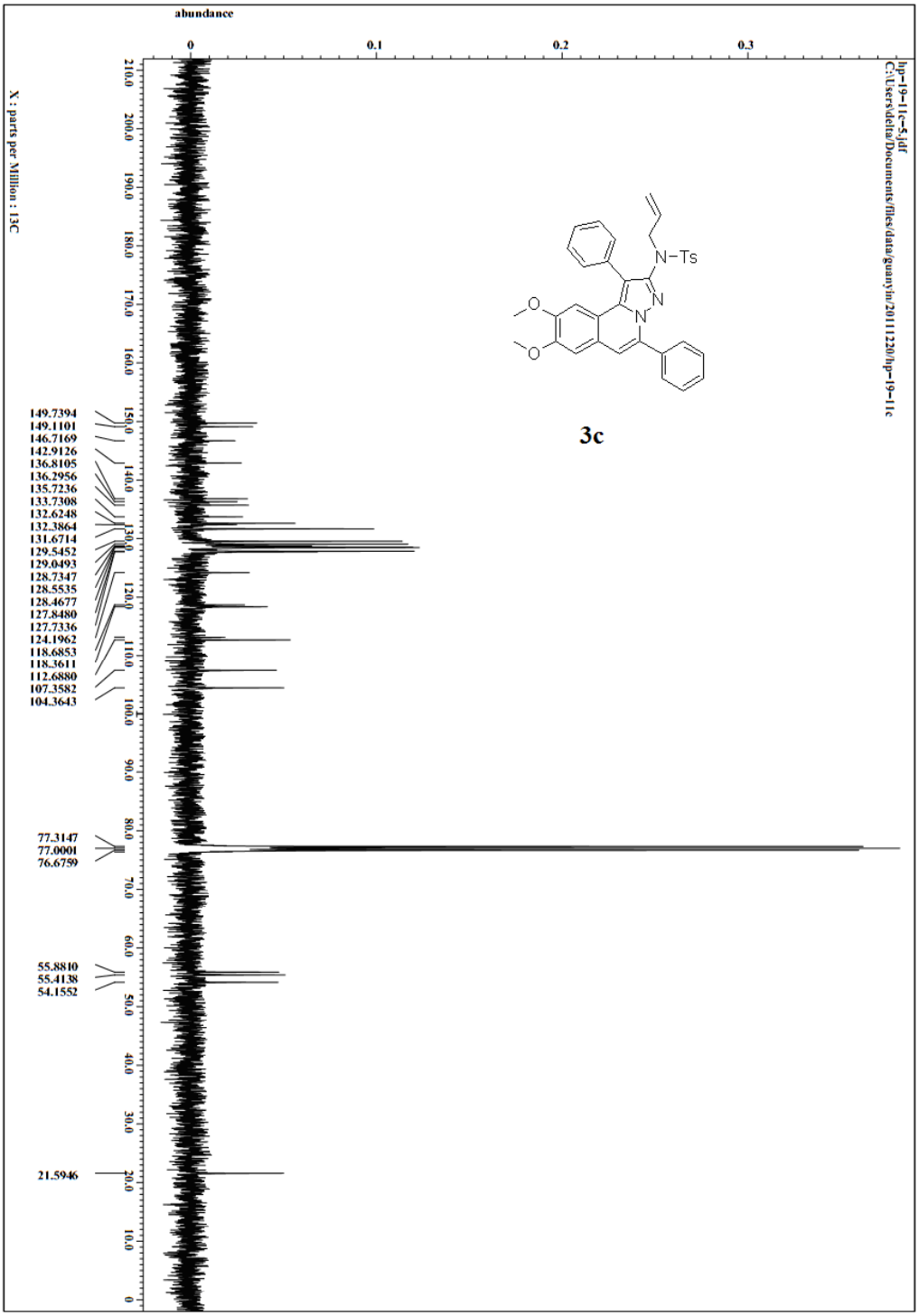

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
hp-13-1C-5.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
147.0978
142.9503
137.8207
136.8196
135.8184
133.5206
132.5099
132.0618
131.1942
129.6400
129.4303
129.0584
128.9821
128.6770
128.5435
127.8952
127.2564
127.1038
124.3579
123.2614
118.4369
114.8614
113.3359
77.3142
76.9996
76.6850
54.0689
21.5942
N-Ts
N
N
3a

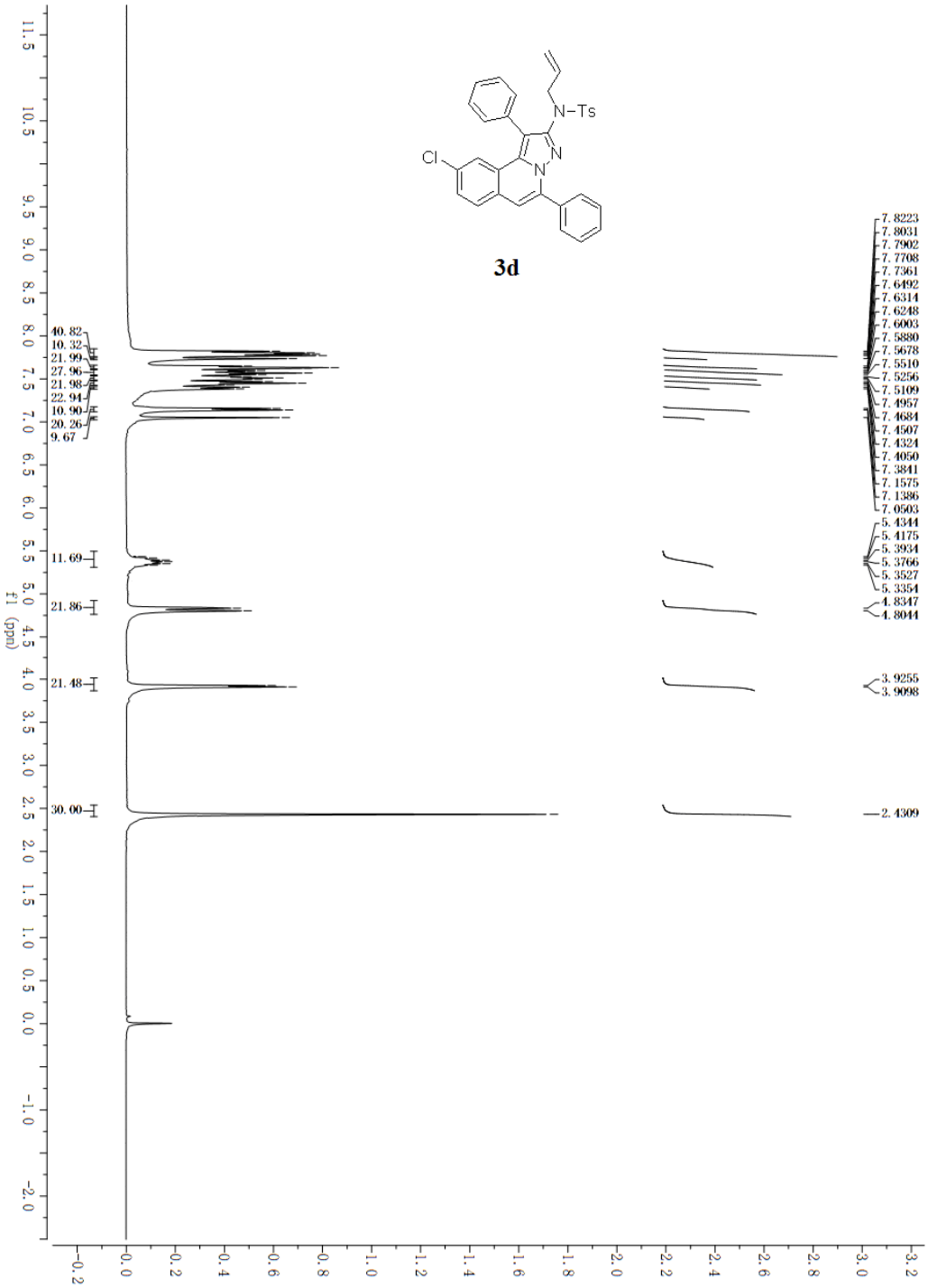

abundance
hp-19-1-7.jdf
single_pulse
X : parts per Million : 111
7.8247
7.7926
7.7743
7.6506
7.5589
7.5383
7.4696
7.4490
7.4318
7.1339
5.3962
5.3790
5.3561
4.8326
4.8155
4.7903
3.9220
3.9071
2.4214
2.2438
-0.0013
15.8
21.63
18.26
87.76
12.35
20.31
10.56
10.8
20.22
20.08
31.93
30
N-Ts
N
N

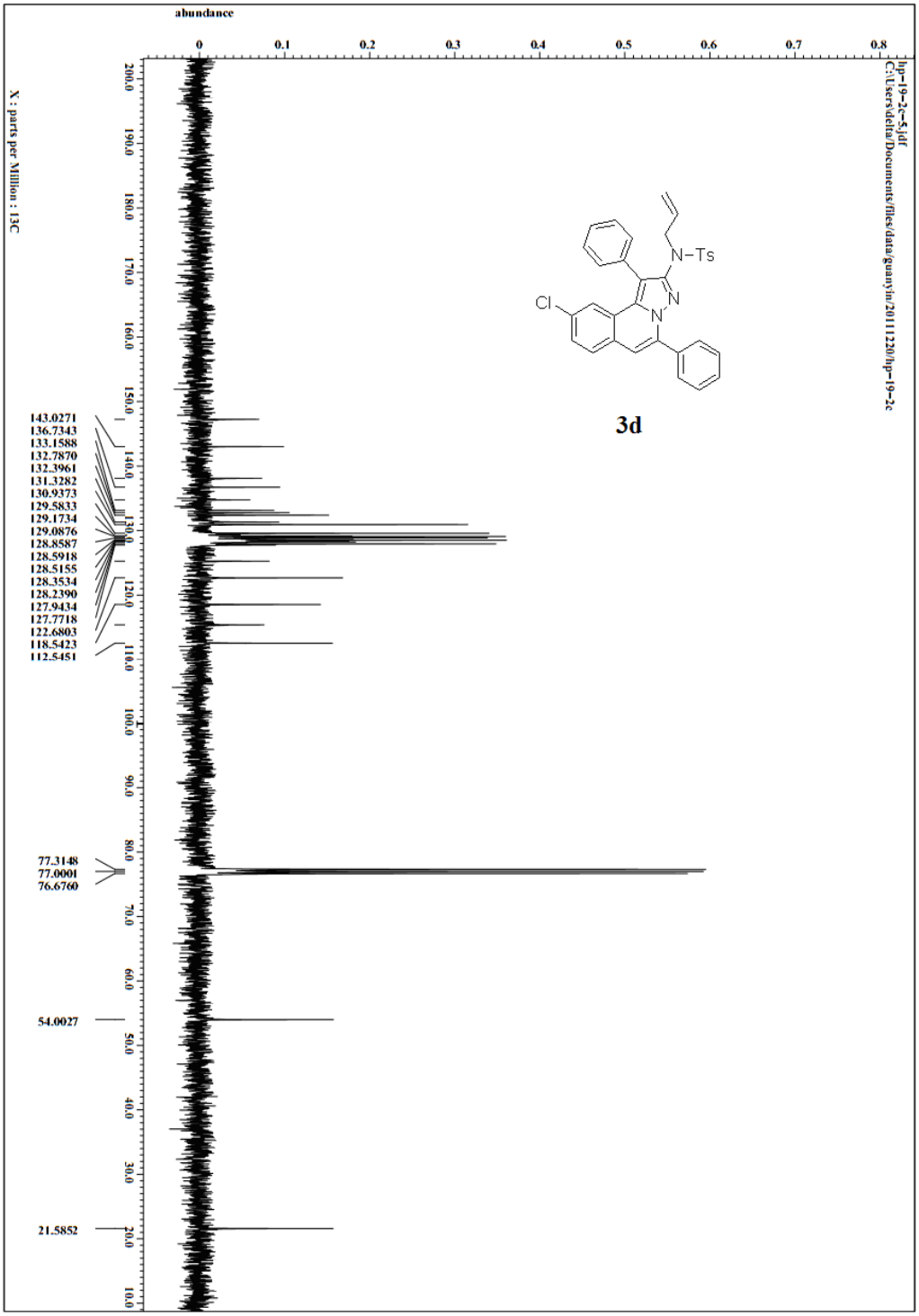
3b

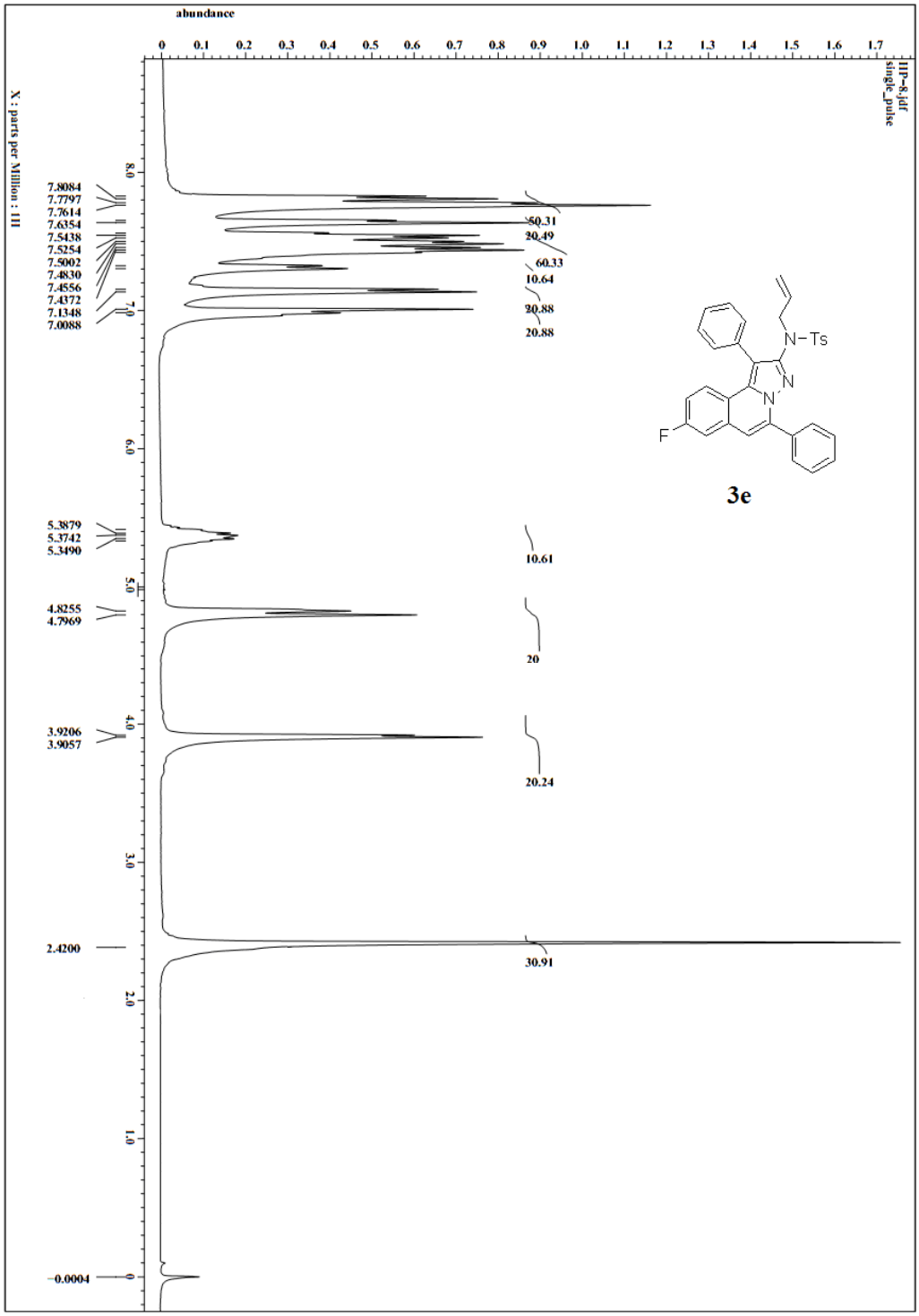

hp-19-1c-5.jdf
C:\Users\delfa\Documents\files\data\guanyin\20111216\hp-19-1c
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4
X : parts per Million : 13C
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
142.9072
137.0435
136.9672
136.8432
132.5336
132.1331
131.1892
129.5970
129.4444
129.0439
128.8056
128.5386
127.8331
127.1656
127.0989
124.3720
123.0848
118.3652
113.2451
77.3189
77.0042
76.6800
54.0640
21.7799
21.5797
N-Ts
N
N
3b

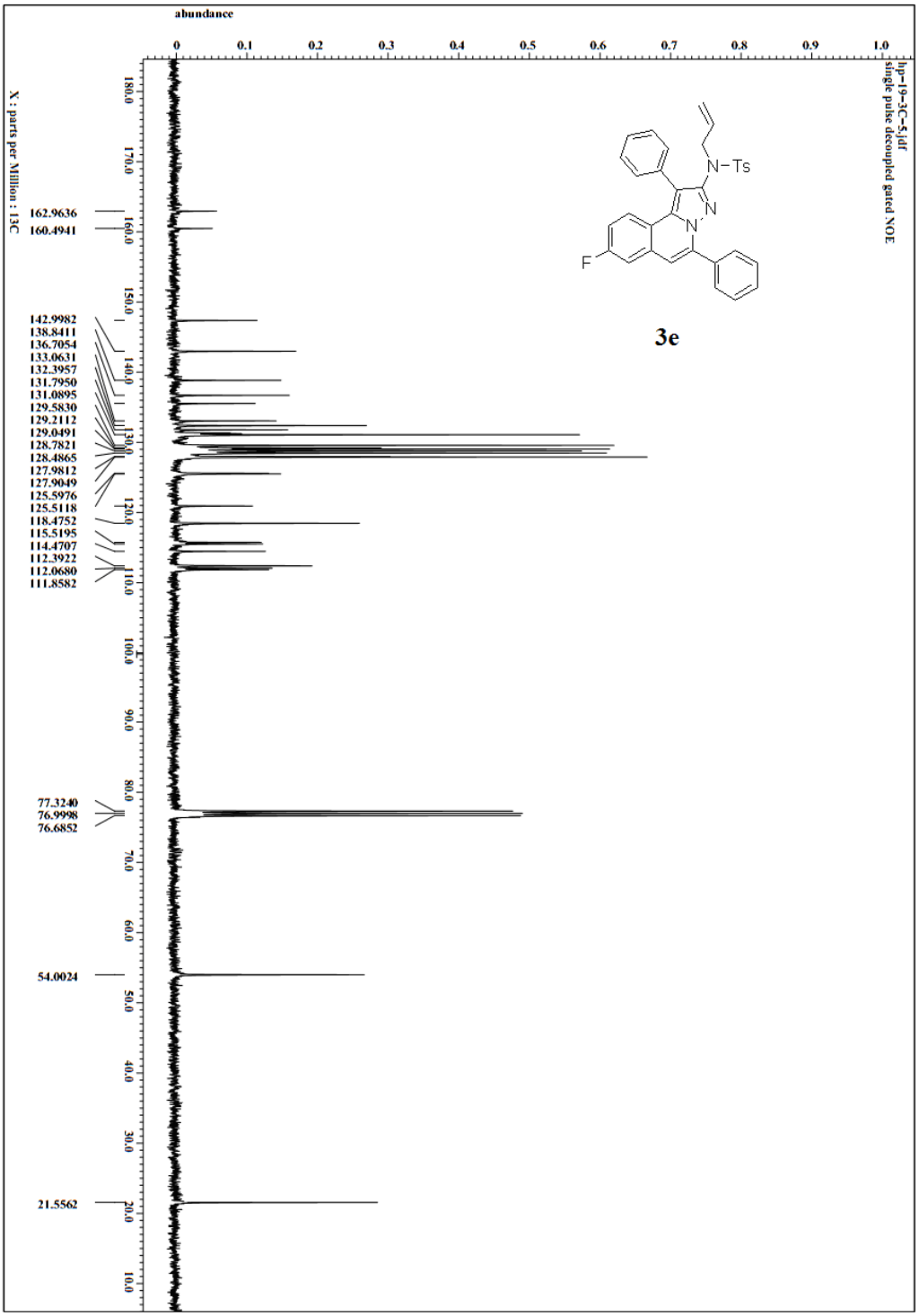

7.8435
7.8246
7.7991
7.7814
7.6728
7.6558
7.5485
7.5301
7.5128
7.4779
7.4470
7.4298
7.2480
7.1661
7.1454
7.0604
7.0222
5.4770
5.4560
5.4358
5.4196
5.3937
5.3792
4.8565
4.8338
4.8105
3.9578
3.9423
3.4863
2.4312
38.59
21.39
62.70
30.32
10.66
10.61
9.76
20.58
51.71
29.70
31.00
N-Ts
N
N
O
O
3c
f1 (ppm)

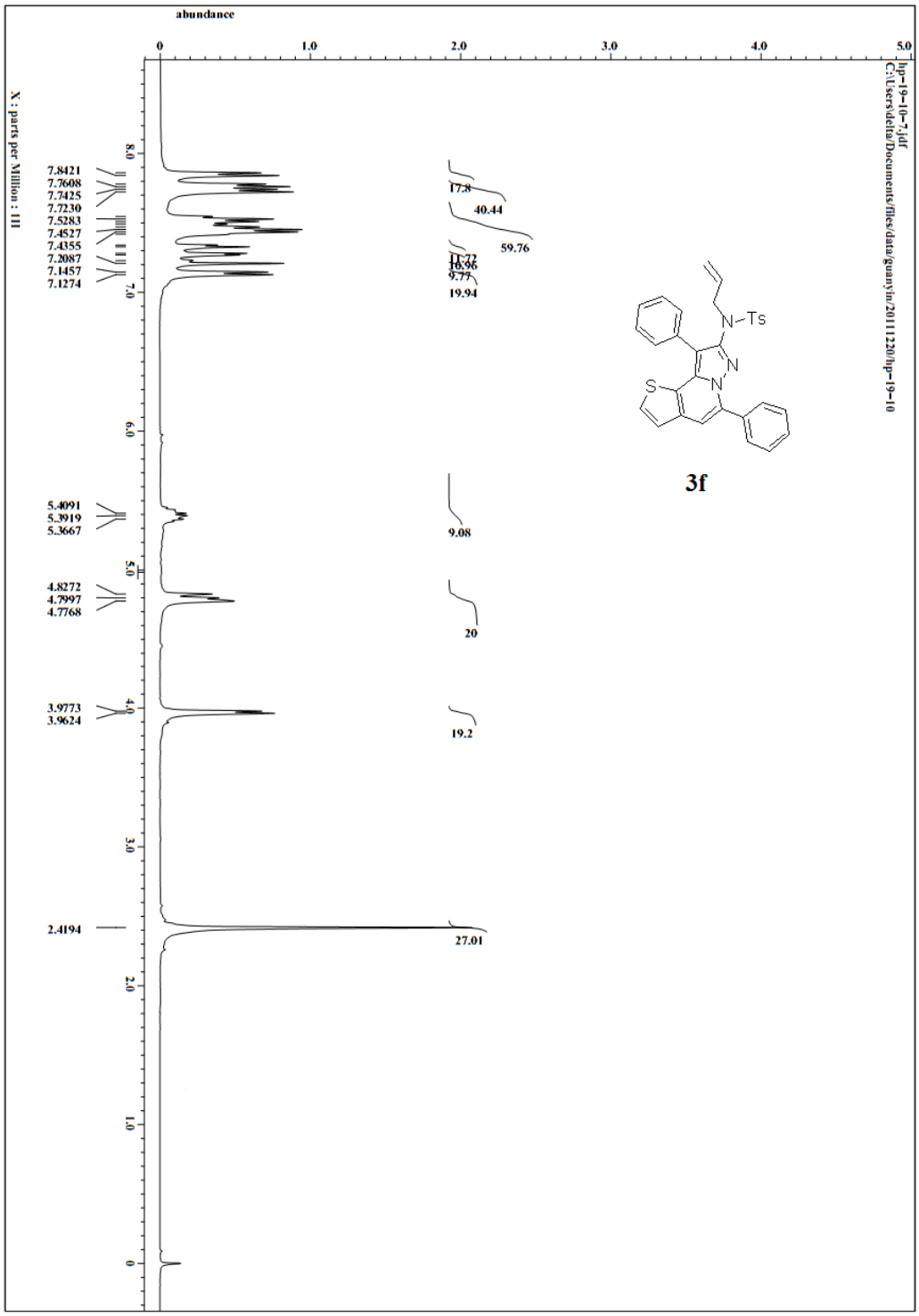

hp-19-11c-5.jdf
C:\Users\delta/Documents/files/data/guanyin/20111220/hp-19-11c
abundance
0
0.1
0.2
0.3
X : parts per Million : 13C
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
149.7394
149.1101
146.7169
142.9126
136.8105
136.2956
135.7236
133.7308
132.6248
132.3864
131.6714
129.5452
129.0493
128.7347
128.5535
128.4677
127.8480
127.7336
124.1962
118.6853
118.3611
112.6880
107.3582
104.3643
77.3147
77.0001
76.6759
55.8810
55.4138
54.1552
21.5946
N-Ts
N
N
O
O
3c

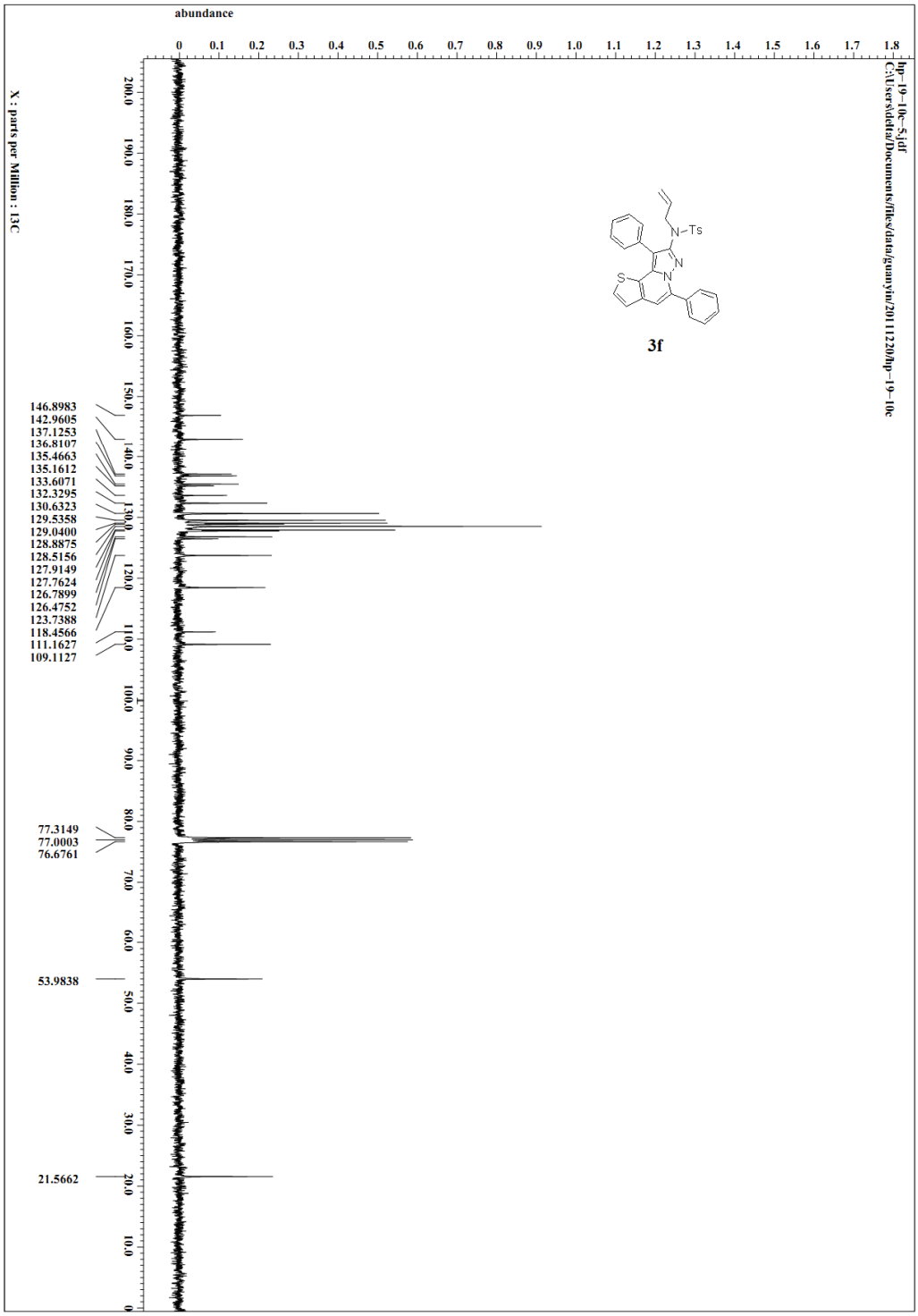

N-Ts
Cl
N
N
3d
40.82
10.32
21.99
27.96
21.98
22.94
10.90
20.26
9.67
11.69
21.86
21.48
30.00
7.8223
7.8031
7.7902
7.7708
7.7361
7.6492
7.6314
7.6248
7.6003
7.5880
7.5678
7.5510
7.5256
7.5109
7.4957
7.4684
7.4507
7.4324
7.4050
7.3841
7.1575
7.1386
7.0503
5.4344
5.4175
5.3934
5.3766
5.3527
5.3354
4.8347
4.8044
3.9255
3.9098
2.4309
f1 (ppm)

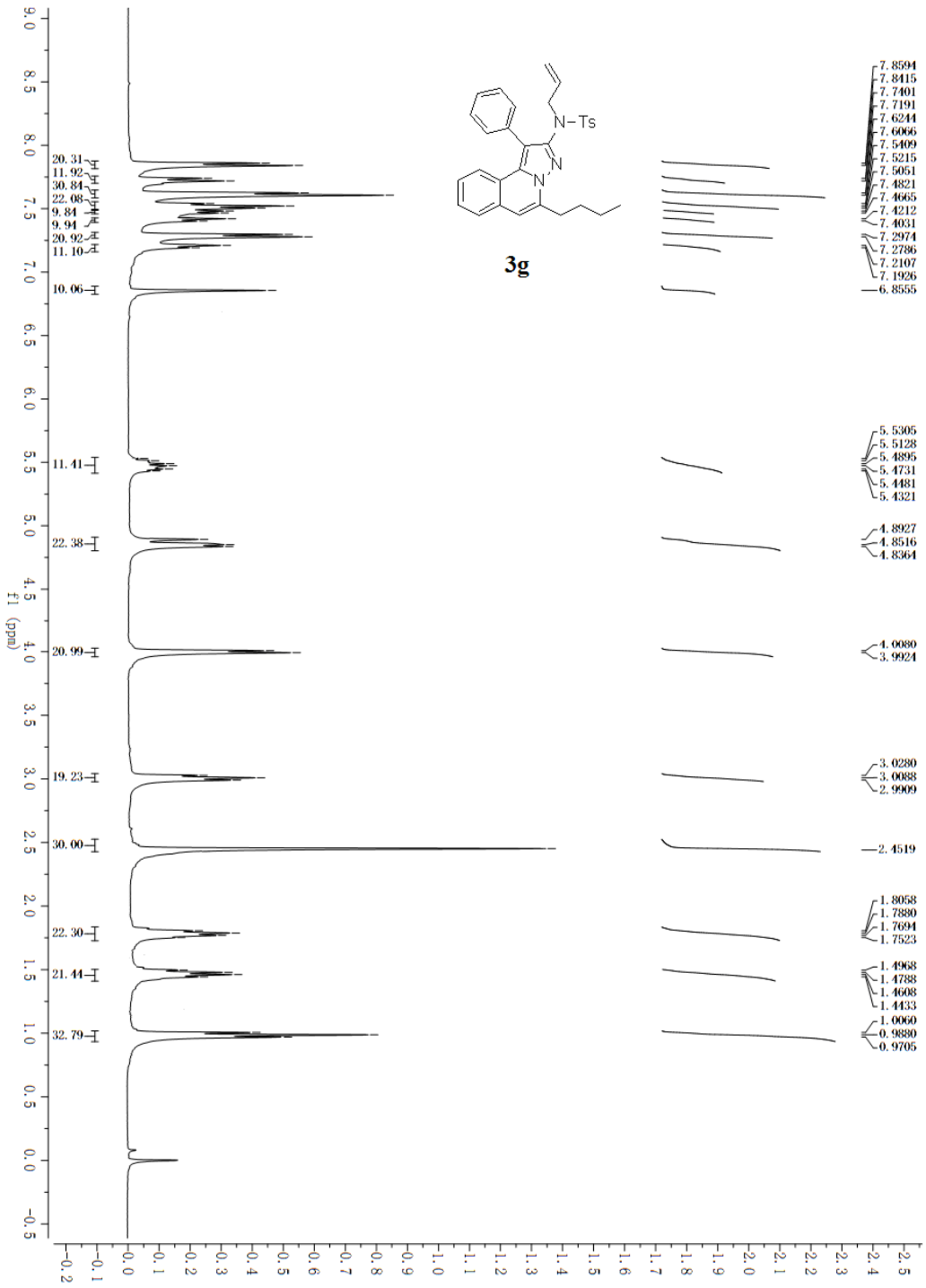

hp-19-2c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-19-2c
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
N-Ts
Cl
N
N
3d
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
143.0271
136.7343
133.1588
132.7870
132.3961
131.3282
130.9373
129.5833
129.1734
129.0876
128.8587
128.5918
128.5155
128.3534
128.2390
127.9434
127.7718
122.6803
118.5423
112.5451
77.3148
77.0001
76.6760
54.0027
21.5852

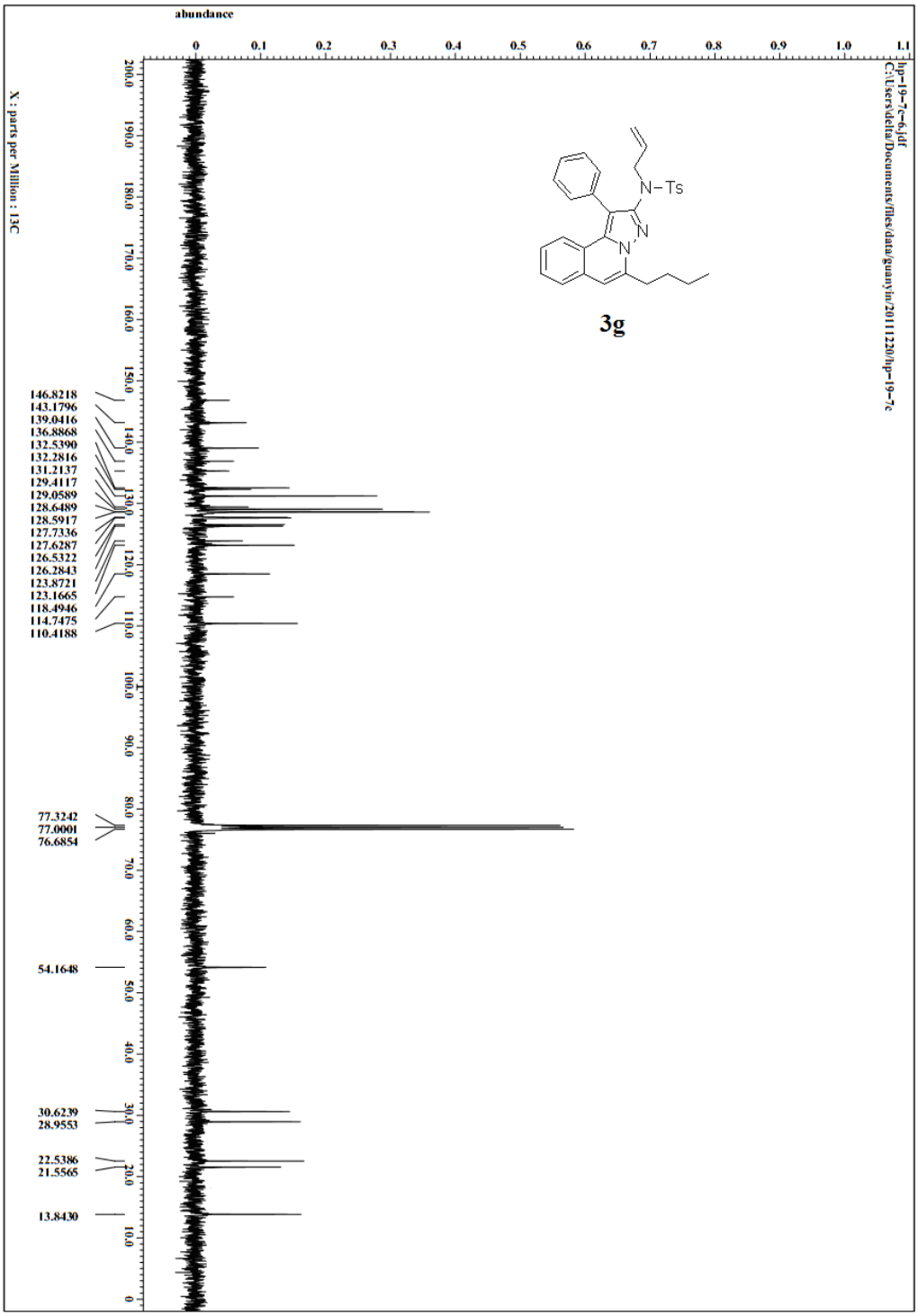

abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7
HP-8.jdf
single_pulse
X : parts per Million : 1H
8.0
7.8084
7.7797
7.7614
7.6354
7.5438
7.5254
7.5002
7.4830
7.4556
7.4372
7.1348
7.0088
7.0
6.0
5.3879
5.3742
5.3490
5.0
4.8255
4.7969
4.0
3.9206
3.9057
3.0
2.4200
2.0
1.0
-0.0004
0
50.31
20.49
60.33
10.64
20.88
20.88
10.61
20
20.24
30.91
N-Ts
N
N
F
3e

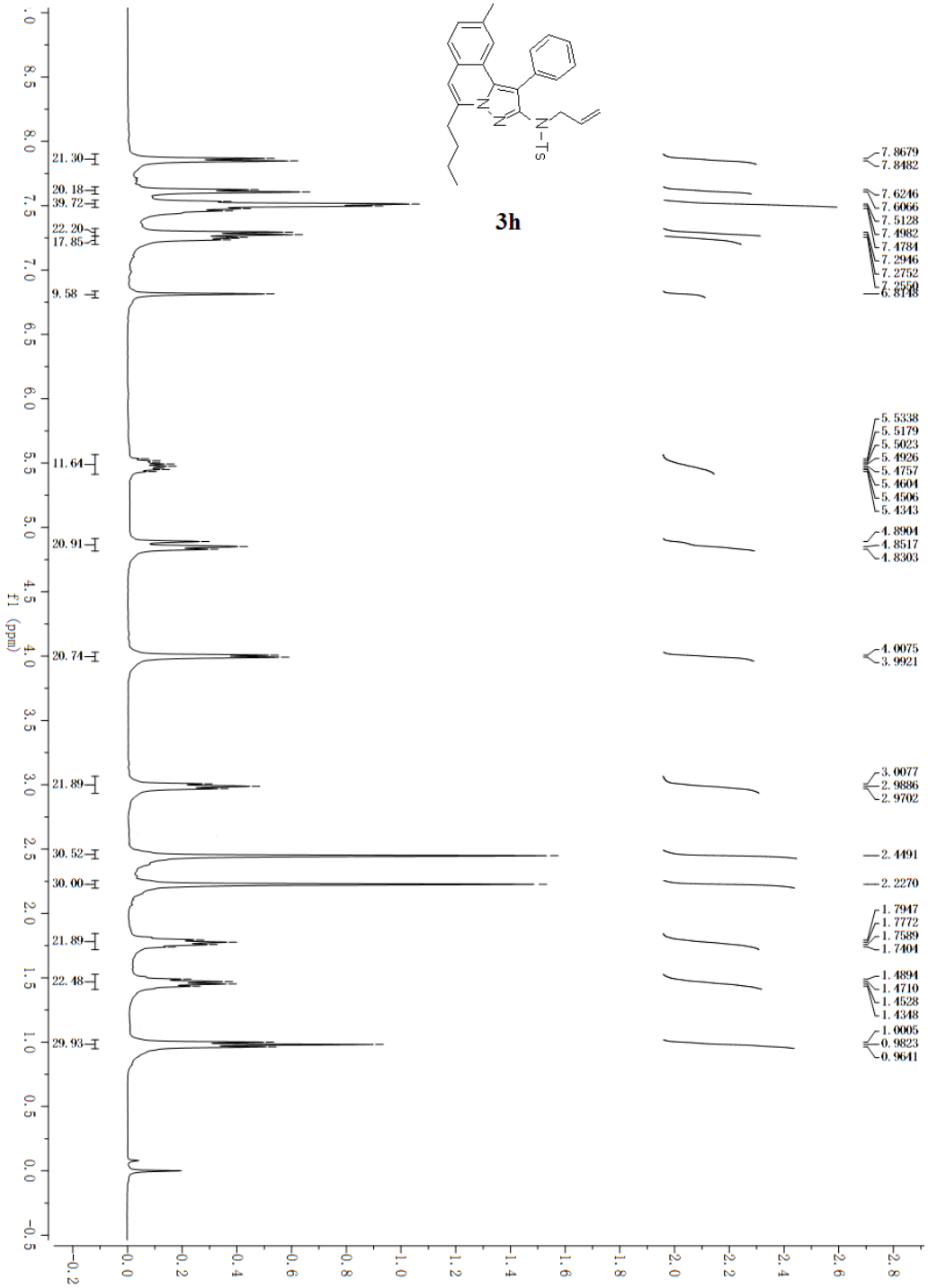

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
hp-19-3C-5.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C
N-Ts
N
N
F
3e
162.9636
160.4941
142.9982
138.8411
136.7054
133.0631
132.3957
131.7950
131.0895
129.5830
129.2112
129.0491
128.7821
128.4865
127.9812
127.9049
125.5976
125.5118
118.4752
115.5195
114.4707
112.3922
112.0680
111.8582
77.3240
76.9998
76.6852
54.0024
21.5562
190.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0

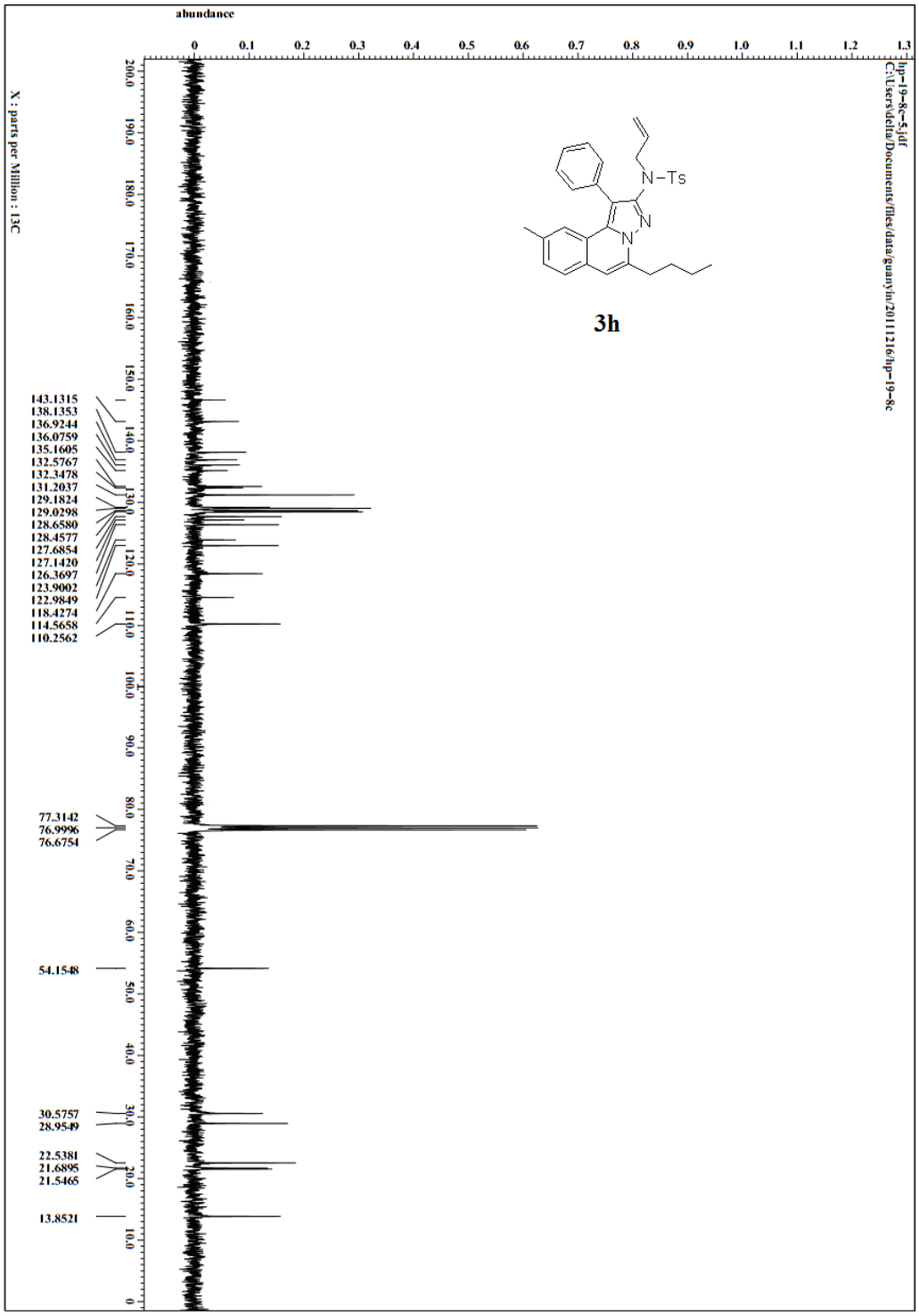

abundance
0
1.0
2.0
3.0
4.0
5.0
hp-19-10-7.jdf
C:\Users\delta/Documents/files/data/guanyin/20111220/hp-19-10
X : parts per Million : 111
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8421
7.7608
7.7425
7.7230
7.5283
7.4527
7.4355
7.2087
7.1457
7.1274
5.4091
5.3919
5.3667
4.8272
4.7997
4.7768
3.9773
3.9624
2.4194
17.8
40.44
59.76
11.72
10.96
9.77
19.94
9.08
20
19.2
27.01
N-Ts
N
N
S
3f

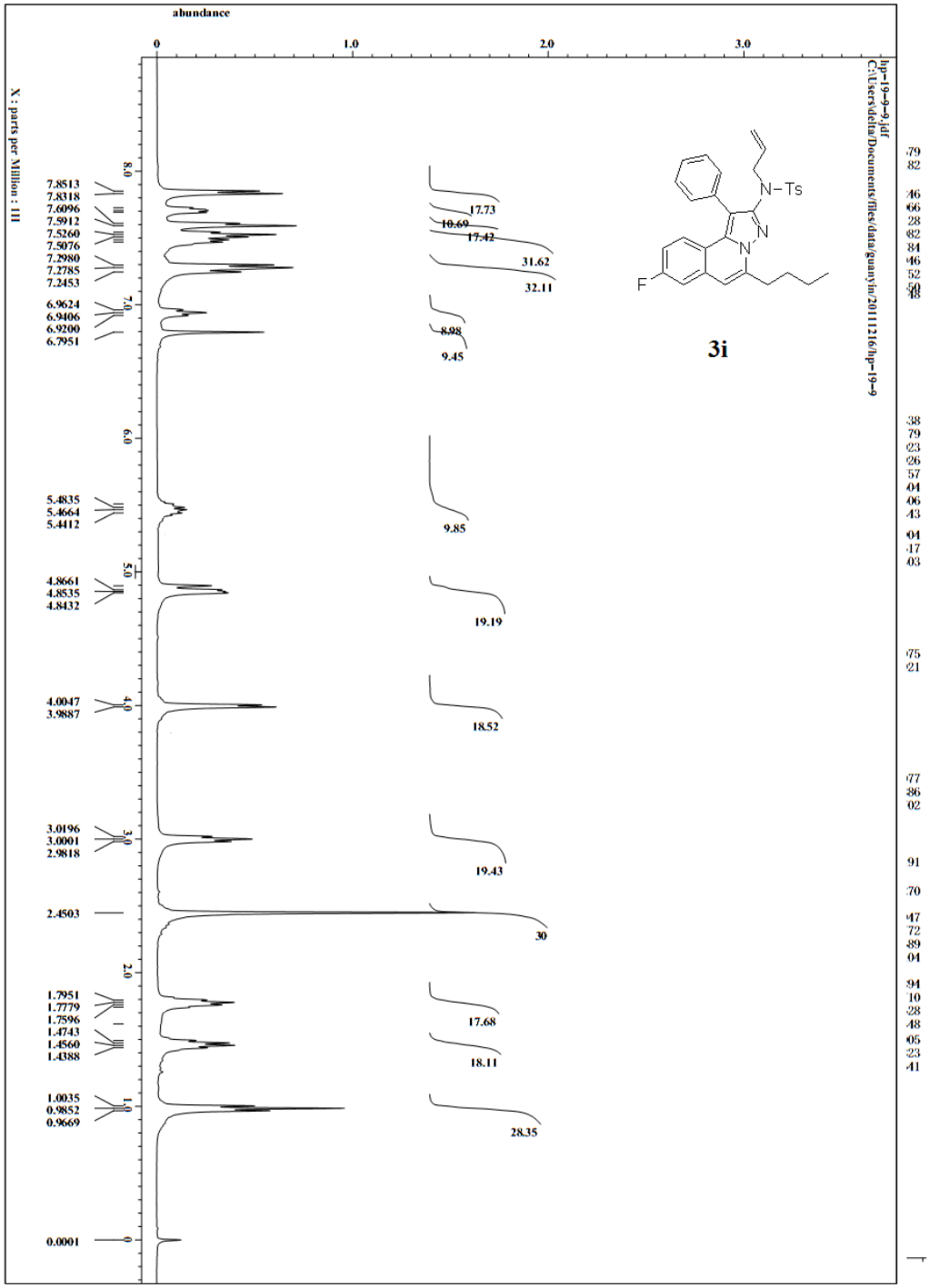

hp-19-10c-5.jdf
C:\Users\deltu\Documents\files\data\guanyin\20111220\hp-19-10c
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8
N-Ts
N
N
S
3f
X : parts per Million : 13C
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
146.8983
142.9605
137.1253
136.8107
135.4663
135.1612
133.6071
132.3295
130.6323
129.5358
129.0400
128.8875
128.5156
127.9149
127.7624
126.7899
126.4752
123.7388
118.4566
111.1627
109.1127
77.3149
77.0003
76.6761
53.9838
21.5662

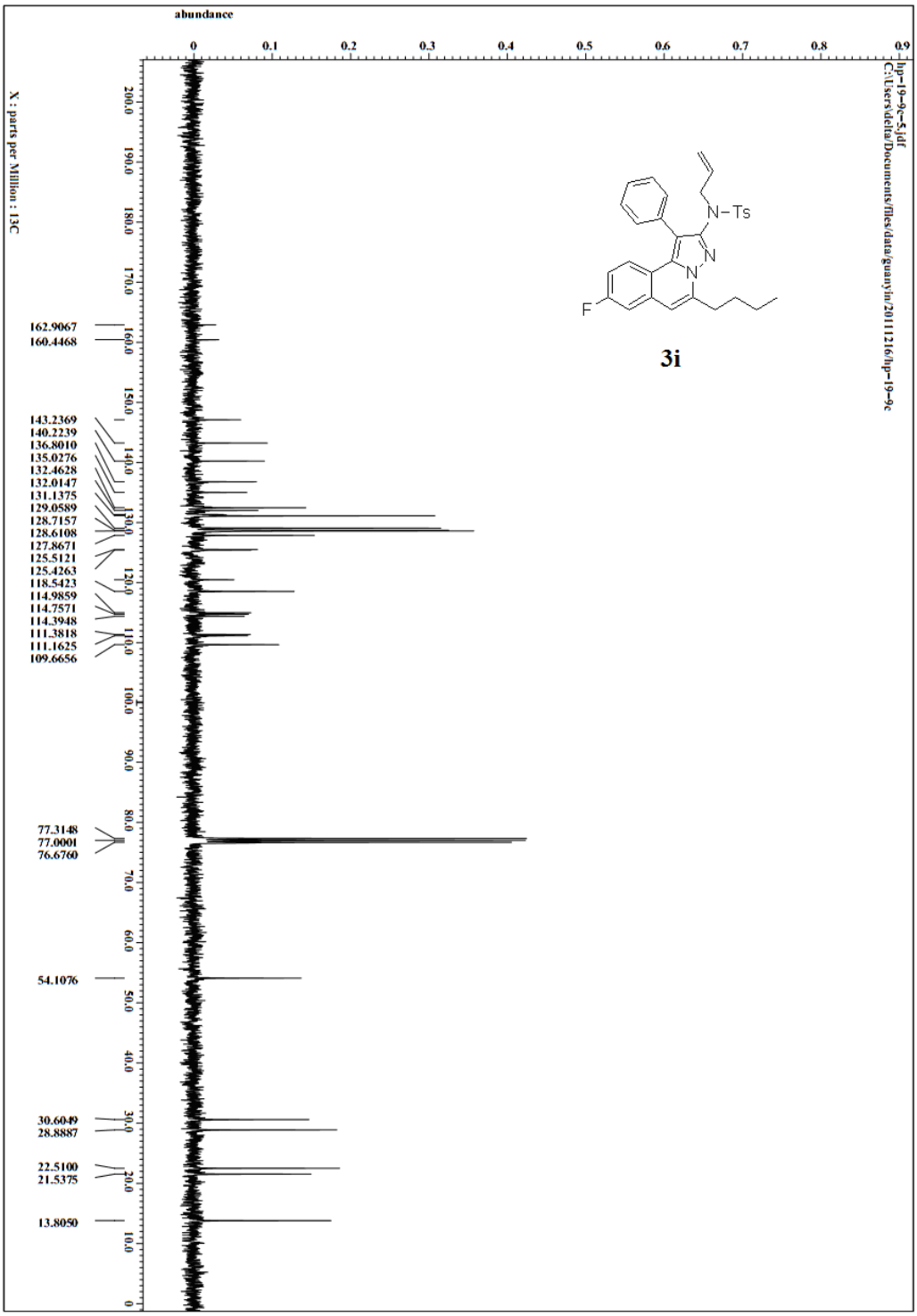

N-Ts
N
N
3g
f1 (ppm)
20.31
11.92
30.84
22.08
9.84
9.94
20.92
11.10
10.06
11.41
22.38
20.99
19.23
30.00
22.30
21.44
32.79
7.8594
7.8415
7.7401
7.7191
7.6244
7.6066
7.5409
7.5215
7.5051
7.4821
7.4665
7.4212
7.4031
7.2974
7.2786
7.2107
7.1926
6.8555
5.5305
5.5128
5.4895
5.4731
5.4481
5.4321
4.8927
4.8516
4.8364
4.0080
3.9924
3.0280
3.0088
2.9909
2.4519
1.8058
1.7880
1.7694
1.7523
1.4968
1.4788
1.4608
1.4433
1.0060
0.9880
0.9705


abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1
hp-19-7c-6.jdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-19-7c
X : parts per Million : 13C
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
146.8218
143.1796
139.0416
136.8868
132.5390
132.2816
131.2137
129.4117
129.0589
128.6489
128.5917
127.7336
127.6287
126.5322
126.2843
123.8721
123.1665
118.4946
114.7475
110.4188
77.3242
77.0001
76.6854
54.1648
30.6239
28.9553
22.5386
21.5565
13.8430
N-Ts
N
N
3g

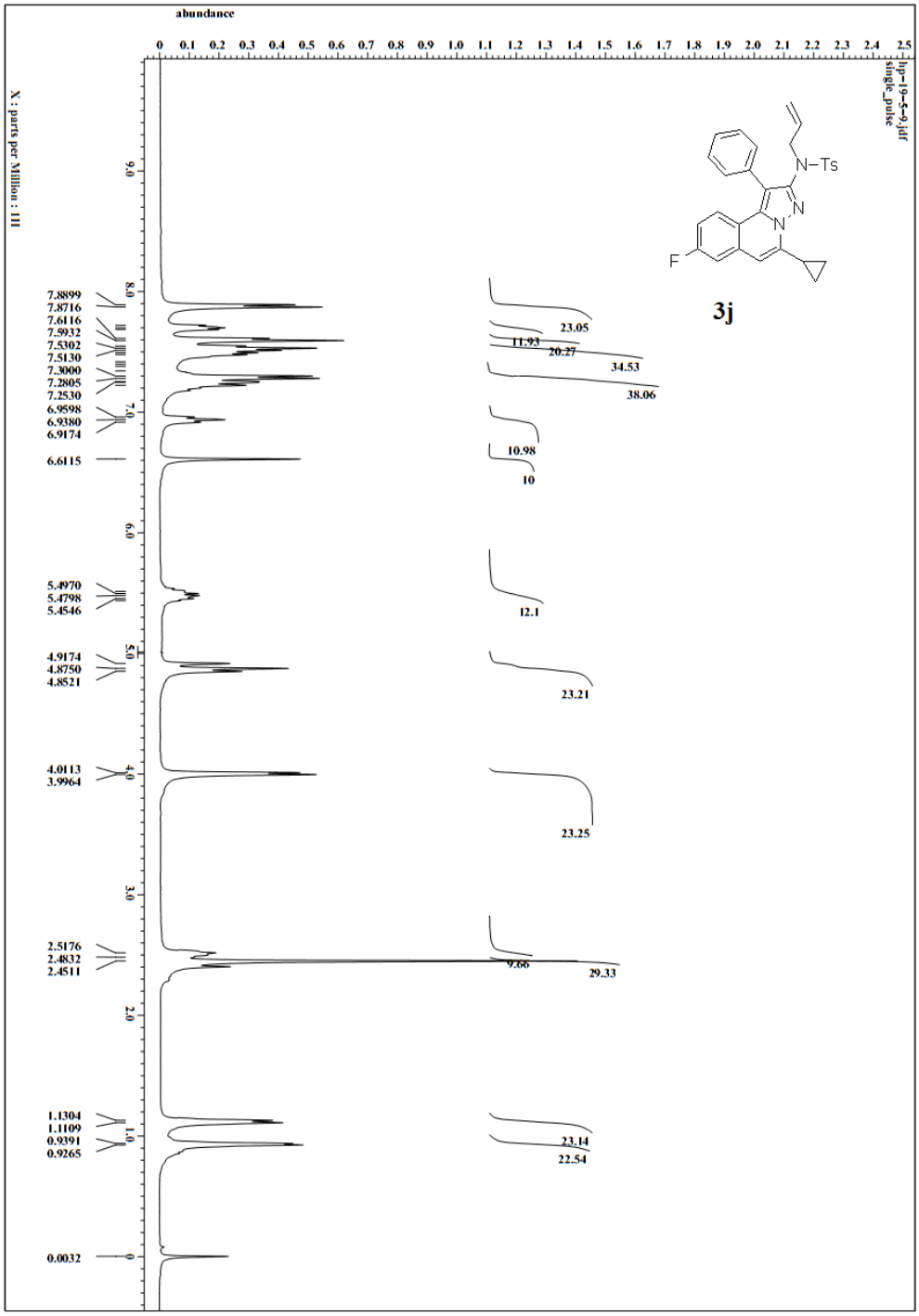

3h
N-Ts
21.30
20.18
39.72
22.20
17.85
9.58
11.64
20.91
20.74
21.89
30.52
30.00
21.89
22.48
29.93
7.8679
7.8482
7.6246
7.6066
7.5128
7.4982
7.4784
7.2946
7.2752
7.2550
6.8148
5.5338
5.5179
5.5023
5.4926
5.4757
5.4604
5.4506
5.4343
4.8904
4.8517
4.8303
4.0075
3.9921
3.0077
2.9886
2.9702
2.4491
2.2270
1.7947
1.7772
1.7589
1.7404
1.4894
1.4710
1.4528
1.4348
1.0005
0.9823
0.9641
f1 (ppm)

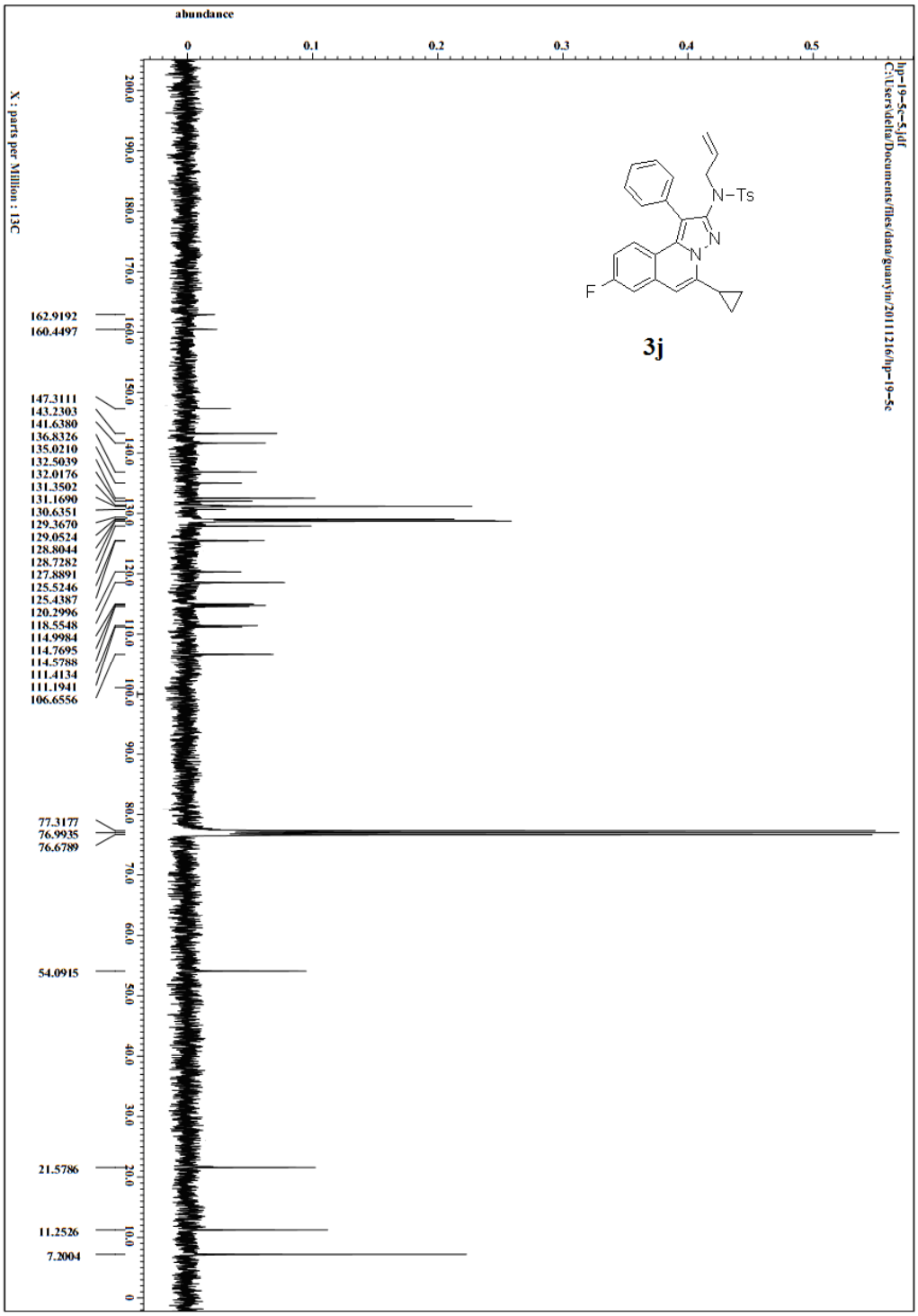

hp-19-8c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111216\hp-19-8c
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
N-Ts
N
N
3h
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
143.1315
138.1353
136.9244
136.0759
135.1605
132.5767
132.3478
131.2037
129.1824
129.0298
128.6580
128.4577
127.6854
127.1420
126.3697
123.9002
122.9849
118.4274
114.5658
110.2562
77.3142
76.9996
76.6754
54.1548
30.5757
28.9549
22.5381
21.6895
21.5465
13.8521

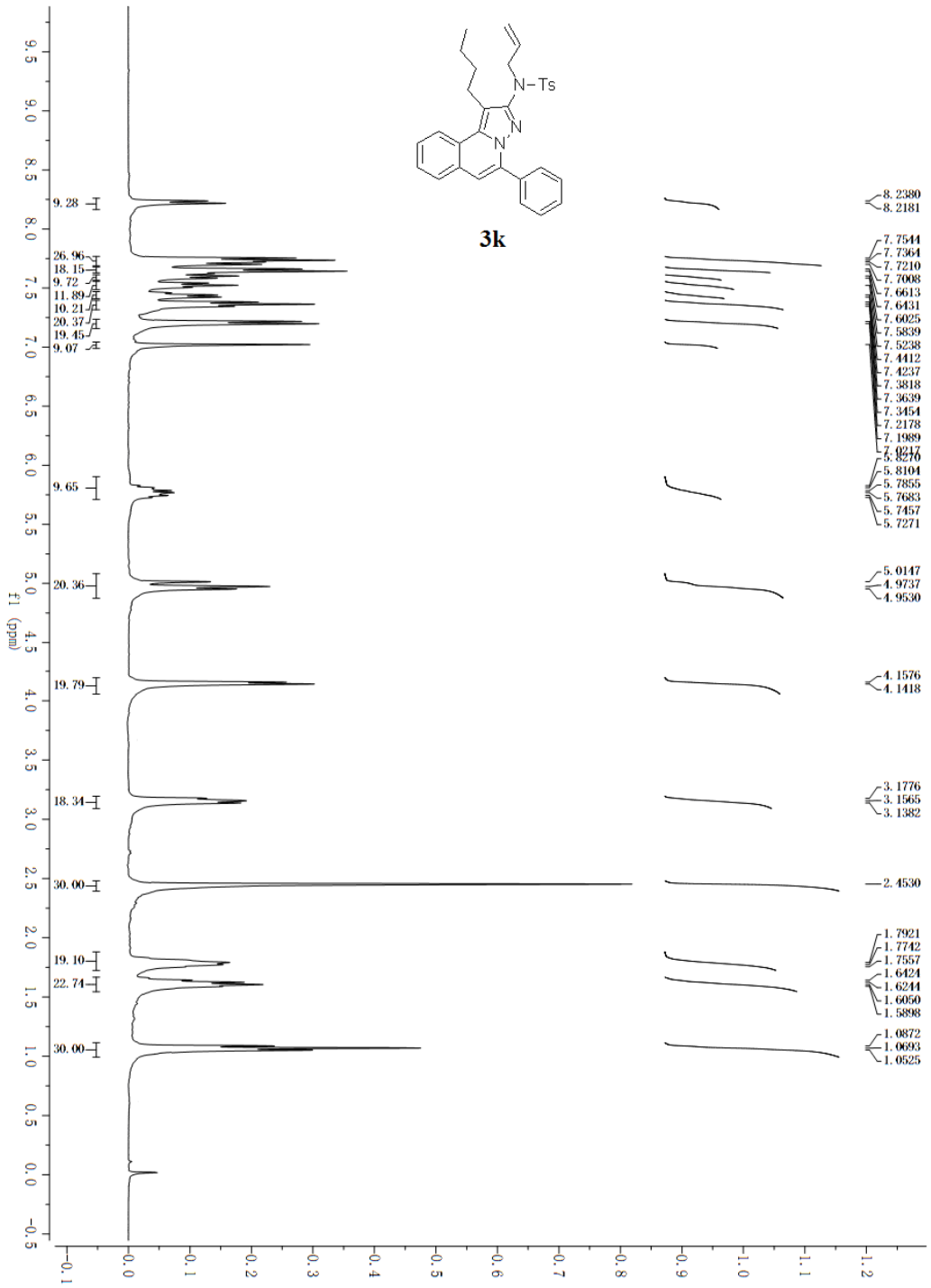

abundance
0
1.0
2.0
3.0
hp-19-9-9.jdf
C:\Users\dcha\Documents\files\data\guanyin\20111216\hp-19-9
N-Ts
N
N
F
3i
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8513
7.8318
7.6096
7.5912
7.5260
7.5076
7.2980
7.2785
7.2453
6.9624
6.9406
6.9200
6.7951
5.4835
5.4664
5.4412
4.8661
4.8535
4.8432
4.0047
3.9887
3.0196
3.0001
2.9818
2.4503
1.7951
1.7779
1.7596
1.4743
1.4560
1.4388
1.0035
0.9852
0.9669
0.0001
17.73
10.69
17.42
31.62
32.11
8.98
9.45
9.85
19.19
18.52
19.43
30
17.68
18.11
28.35

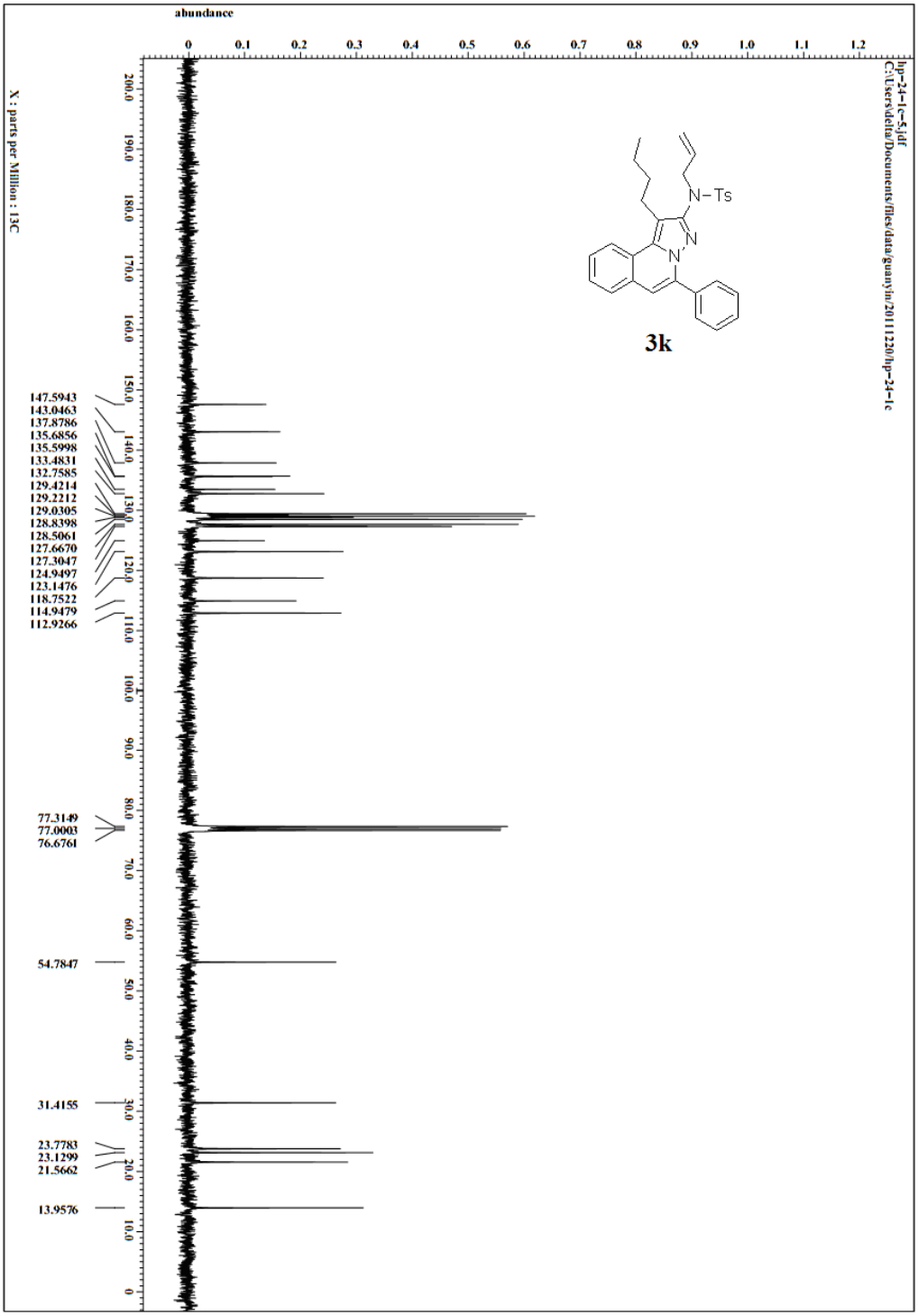

hp-19-9c-5.dif
C:\Users\delta\Documents\files\data\guanyin\20111216\hp-19-9c
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.9067
160.4468
143.2369
140.2239
136.8010
135.0276
132.4628
132.0147
131.1375
129.0589
128.7157
128.6108
127.8671
125.5121
125.4263
118.5423
114.9859
114.7571
114.3948
111.3818
111.1625
109.6656
77.3148
77.0001
76.6760
54.1076
30.6049
28.8887
22.5100
21.5375
13.8050
N-Ts
N
N
F

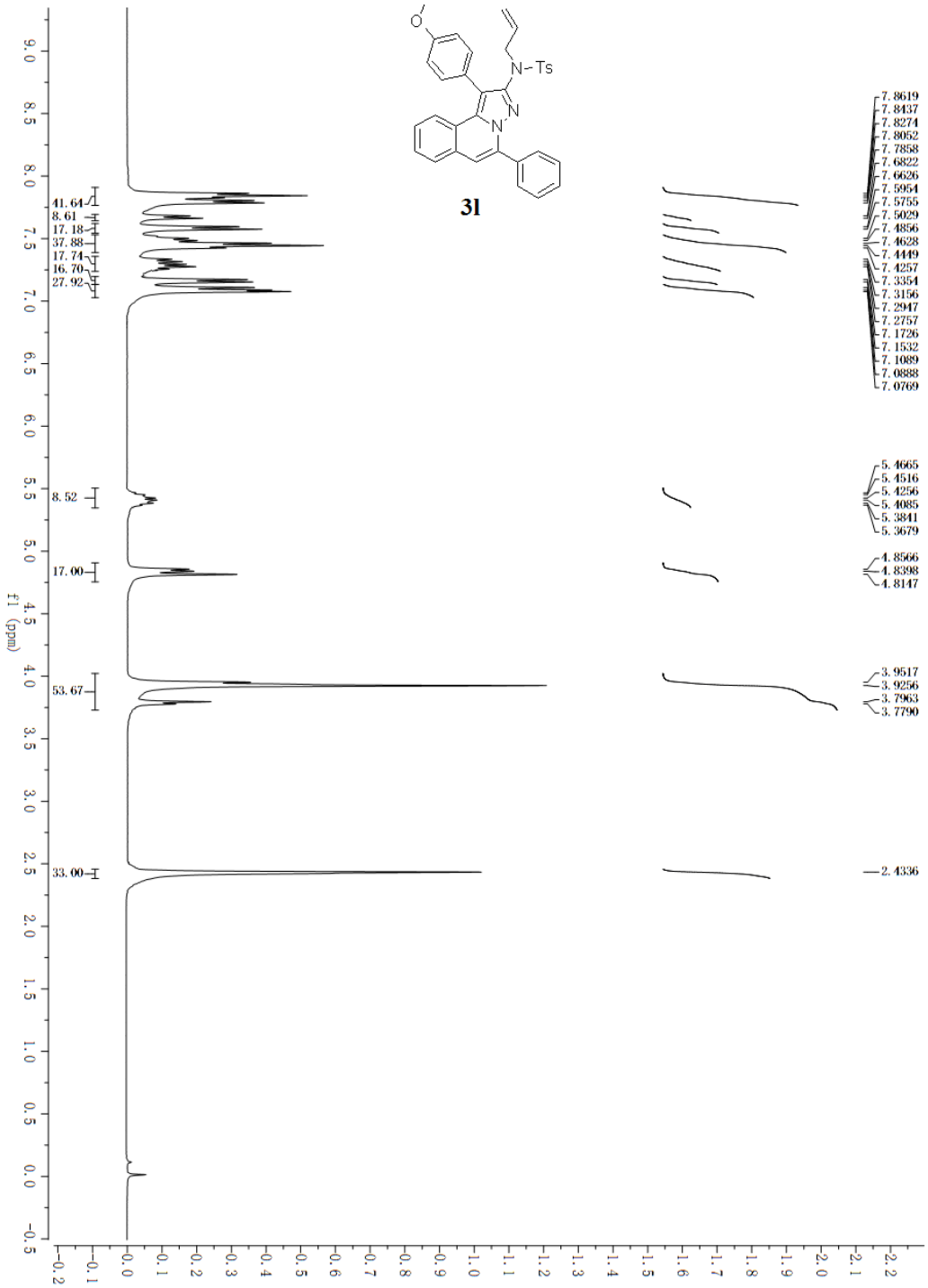
3i

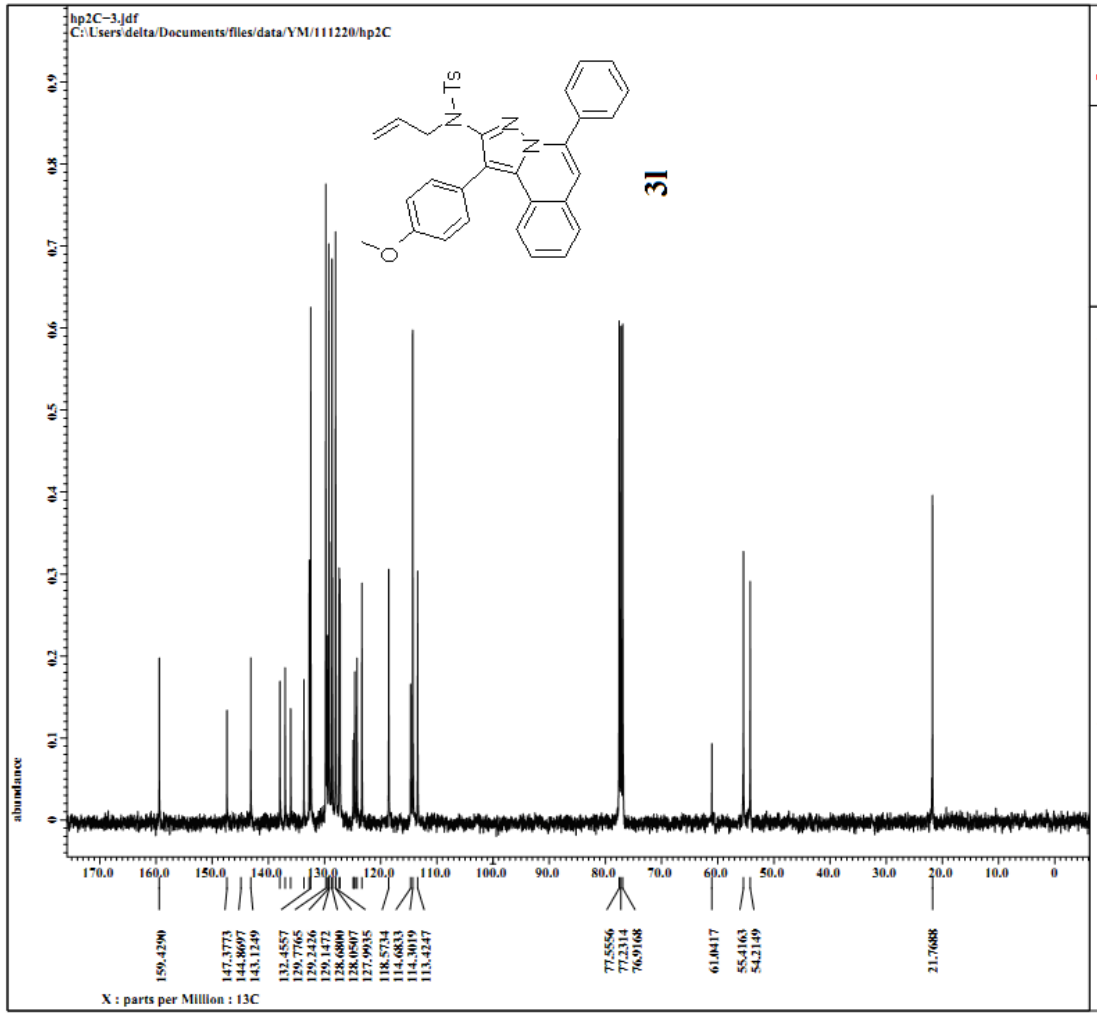

abundance
X : parts per Million : 1H
hp-19-5-9.jdf
single_pulse
N-Ts
N
N
F
3j
7.8899
7.8716
7.6116
7.5932
7.5302
7.5130
7.3000
7.2805
7.2530
6.9598
6.9380
6.9174
6.6115
5.4970
5.4798
5.4546
4.9174
4.8750
4.8521
4.0113
3.9964
2.5176
2.4832
2.4511
1.1304
1.1109
0.9391
0.9265
0.0032
23.05
11.93
20.27
34.53
38.06
10.98
10
12.1
23.21
23.25
9.66
29.33
23.14
22.54


hp-19-5c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111216\hp-19-5c
abundance
0
0.1
0.2
0.3
0.4
0.5
N-Ts
N
N
F
3j
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.9192
160.4497
147.3111
143.2303
141.6380
136.8326
135.0210
132.5039
132.0176
131.3502
131.1690
130.6351
129.3670
129.0524
128.8044
128.7282
127.8891
125.5246
125.4387
120.2996
118.5548
114.9984
114.7695
114.5788
111.4134
111.1941
106.6556
77.3177
76.9935
76.6789
54.0915
21.5786
11.2526
7.2004


N-Ts
N
N
3k
f1 (ppm)
9.28
26.96
18.15
9.72
11.89
10.21
20.37
19.45
9.07
9.65
20.36
19.79
18.34
30.00
19.10
22.74
30.00
8.2380
8.2181
7.7544
7.7364
7.7210
7.7008
7.6613
7.6431
7.6025
7.5839
7.5238
7.4412
7.4237
7.3818
7.3639
7.3454
7.2178
7.1989
7.0217
5.8270
5.8104
5.7855
5.7683
5.7457
5.7271
5.0147
4.9737
4.9530
4.1576
4.1418
3.1776
3.1565
3.1382
2.4530
1.7921
1.7742
1.7557
1.6424
1.6244
1.6050
1.5898
1.0872
1.0693
1.0525


abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2
hp-24-1c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-24-1c
X : parts per Million : 13C
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
147.5943
143.0463
137.8786
135.6856
135.5998
133.4831
132.7585
129.4214
129.2212
129.0305
128.8398
128.5061
127.6670
127.3047
124.9497
123.1476
118.7522
114.9479
112.9266
77.3149
77.0003
76.6761
54.7847
31.4155
23.7783
23.1299
21.5662
13.9576
N-Ts
N
N
3k

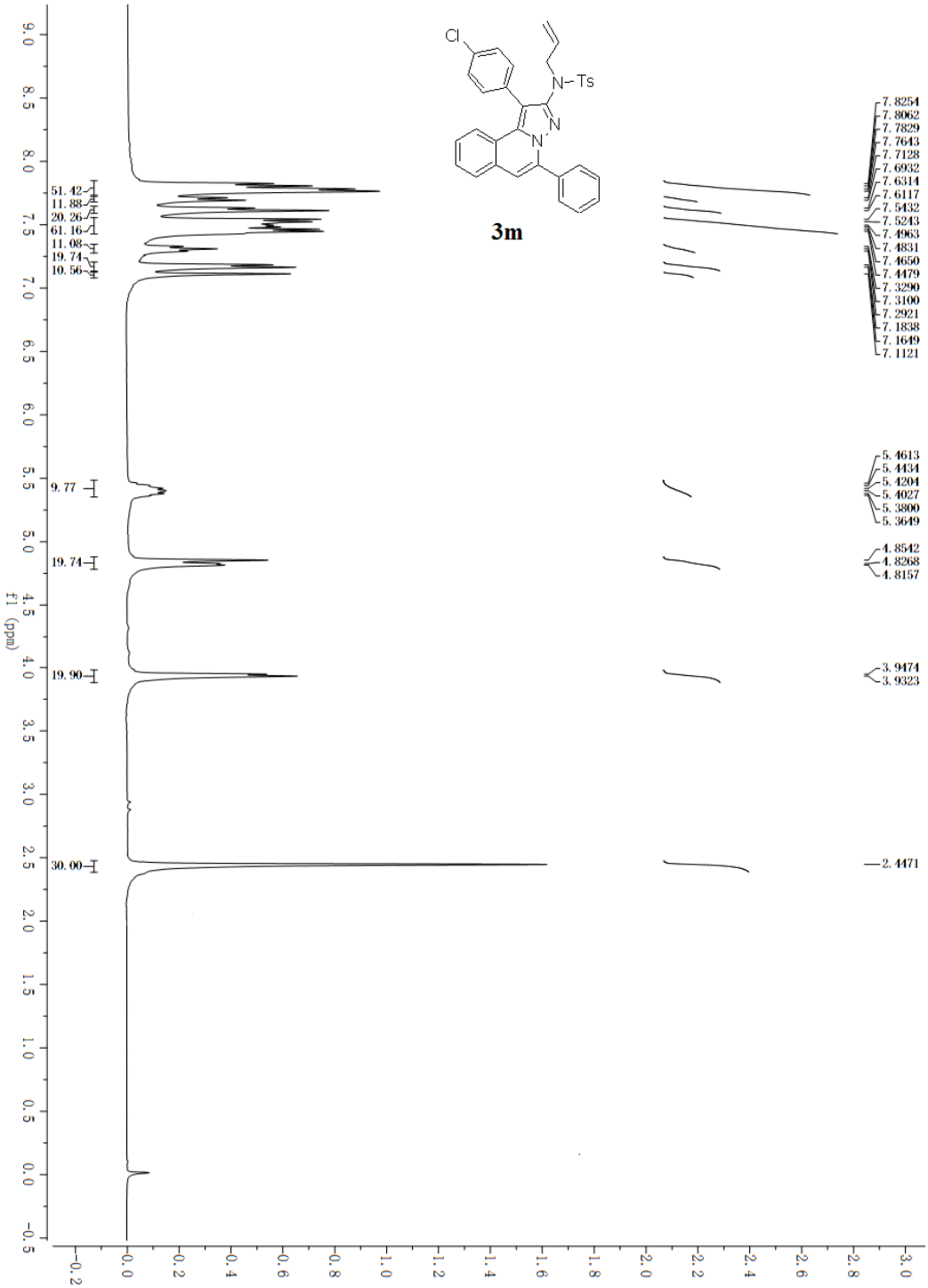

3l
N-Ts
41.64
8.61
17.18
37.88
17.74
16.70
27.92
8.52
17.00
53.67
33.00
7.8619
7.8437
7.8274
7.8052
7.7858
7.6822
7.6626
7.5954
7.5755
7.5029
7.4856
7.4628
7.4449
7.4257
7.3354
7.3156
7.2947
7.2757
7.1726
7.1532
7.1089
7.0888
7.0769
5.4665
5.4516
5.4256
5.4085
5.3841
5.3679
4.8566
4.8398
4.8147
3.9517
3.9256
3.7963
3.7790
2.4336
f1 (ppm)

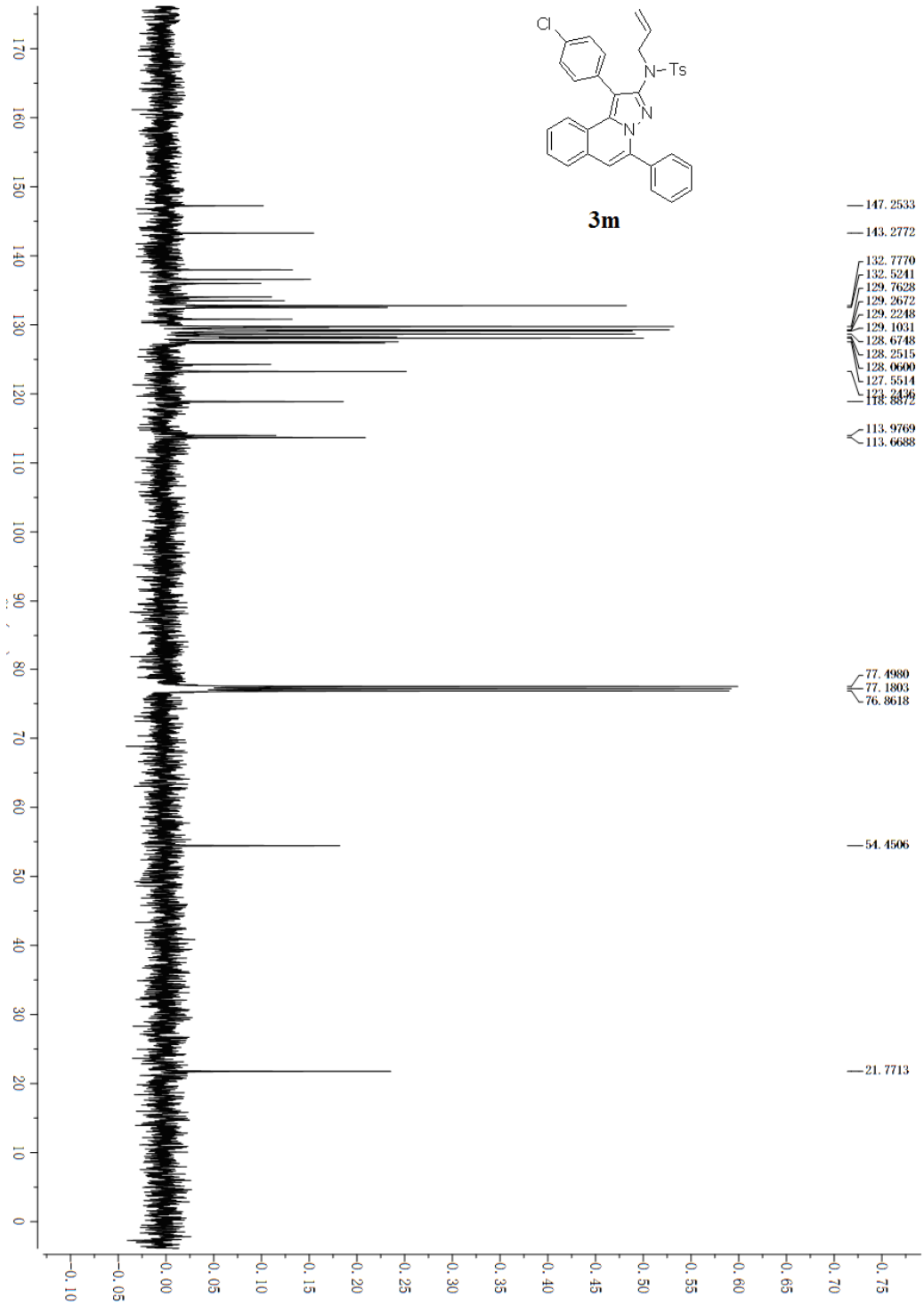


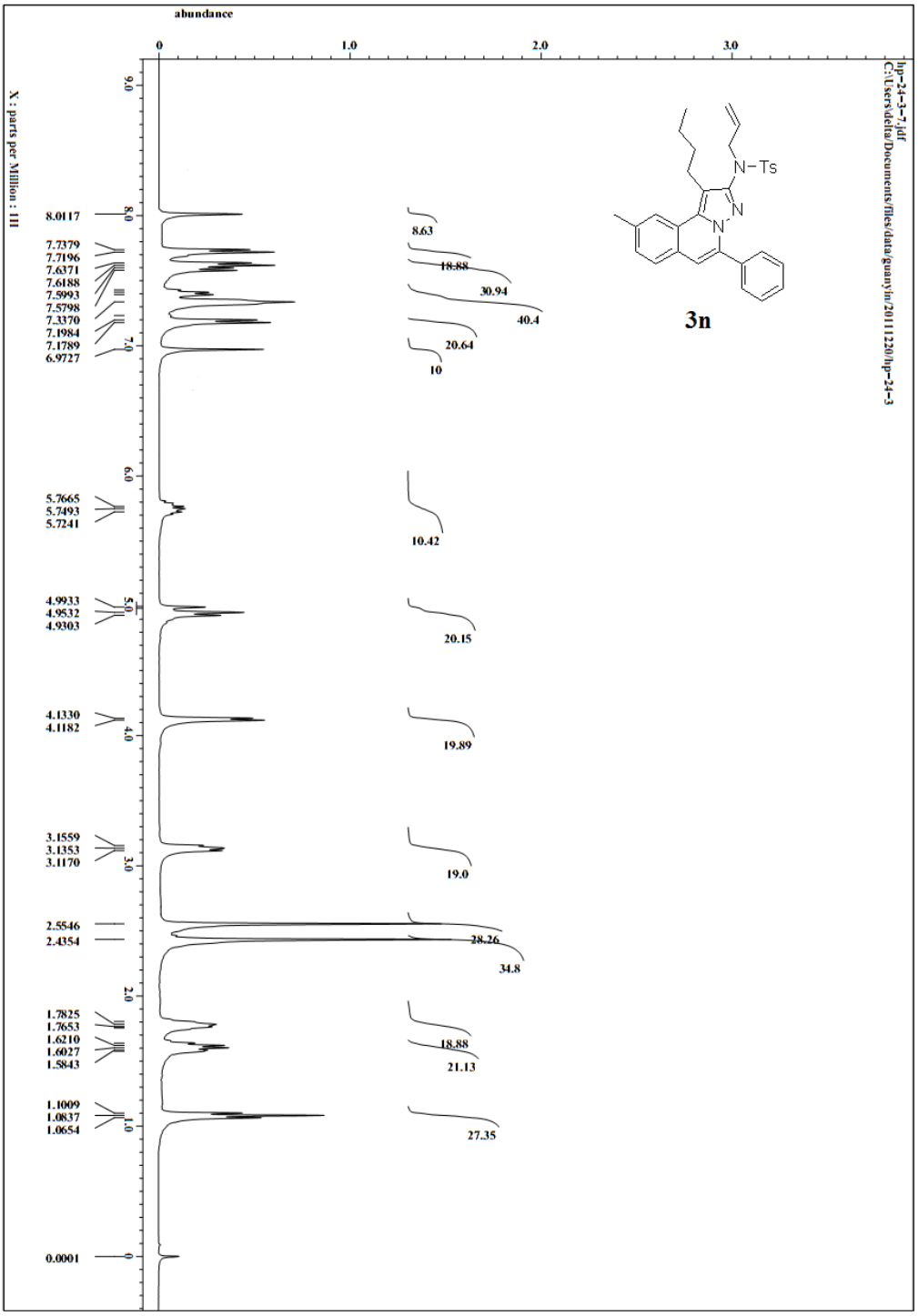
JEOL

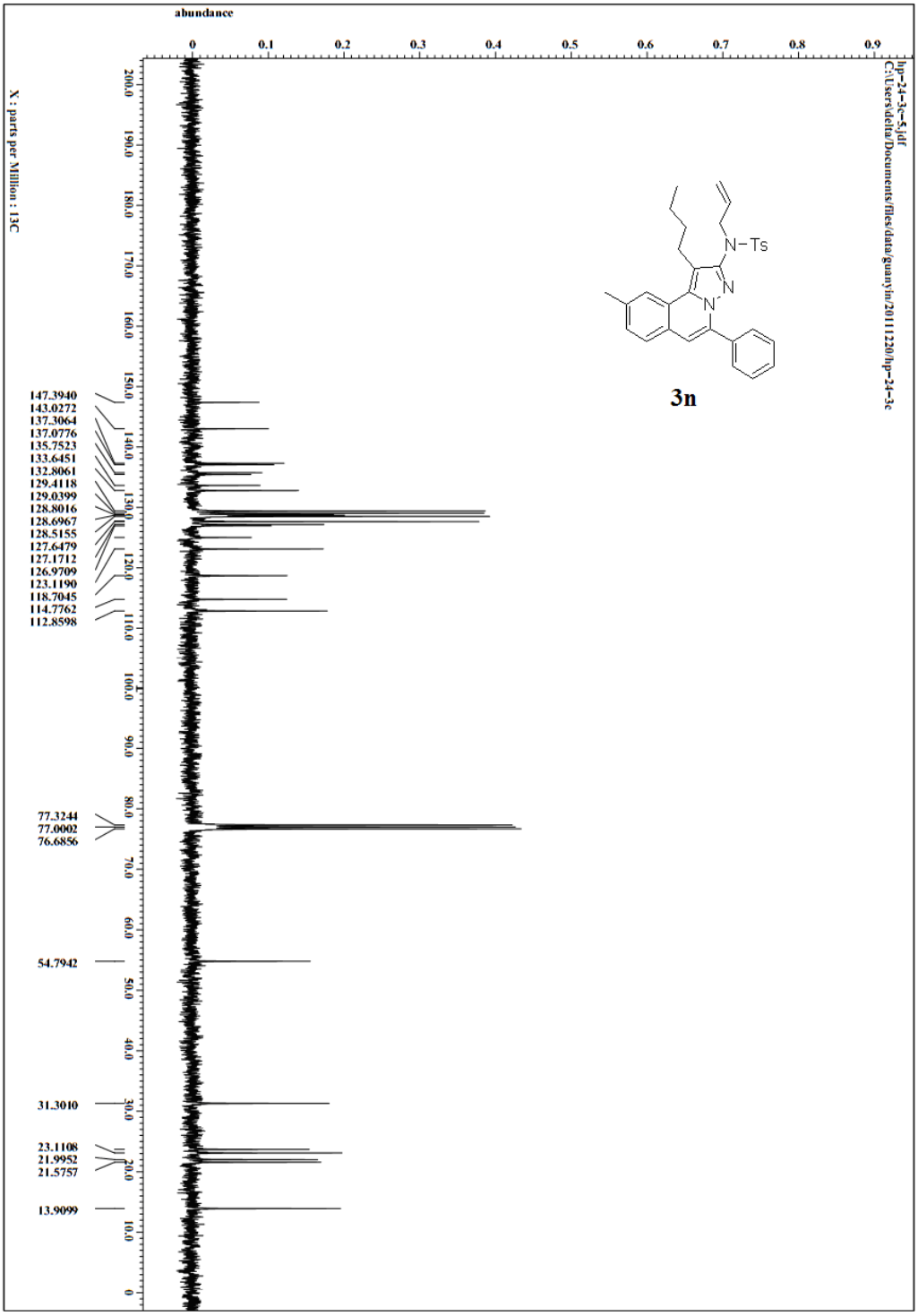
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: hp2C-1.jdf
```

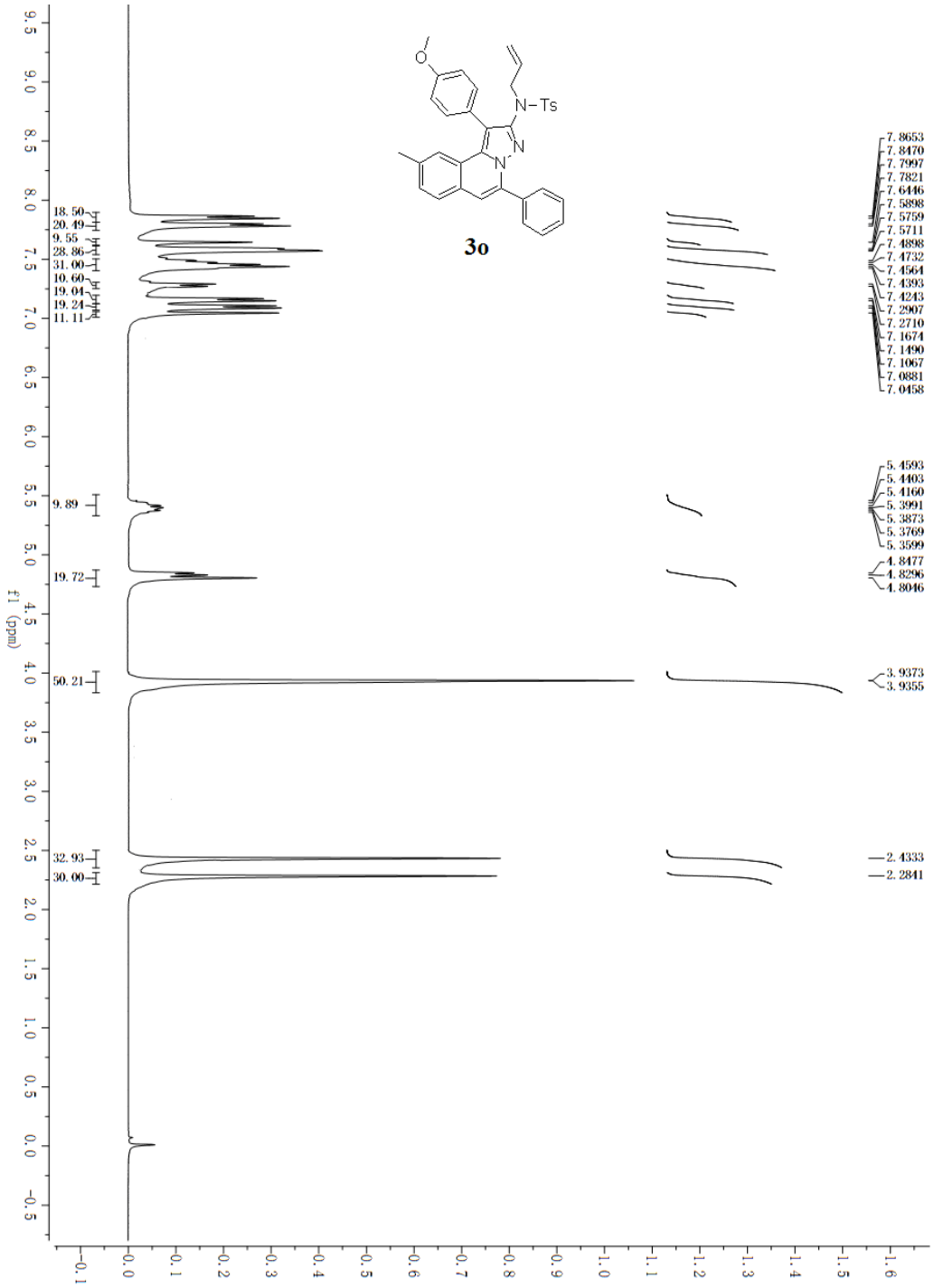
```
Filename          = hp2C-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = C:\Users\delta/Docume
Solvent           = CHLOROFORM-D
Creation_time     = 20-DEC-2011 09:08:32
Revision_time     = 20-DEC-2011 09:20:21
Current_time      = 20-DEC-2011 09:21:19

Comment           = C:\Users\delta/Docume
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 173
Total_scans       = 173

X_90_width        = 9.15[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 7[dB]
X_pulse           = 3.05[us]
Irr_atn_dec       = 25.20784[dB]
Irr_atn_noe       = 25.20784[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 19.8[dC]
```

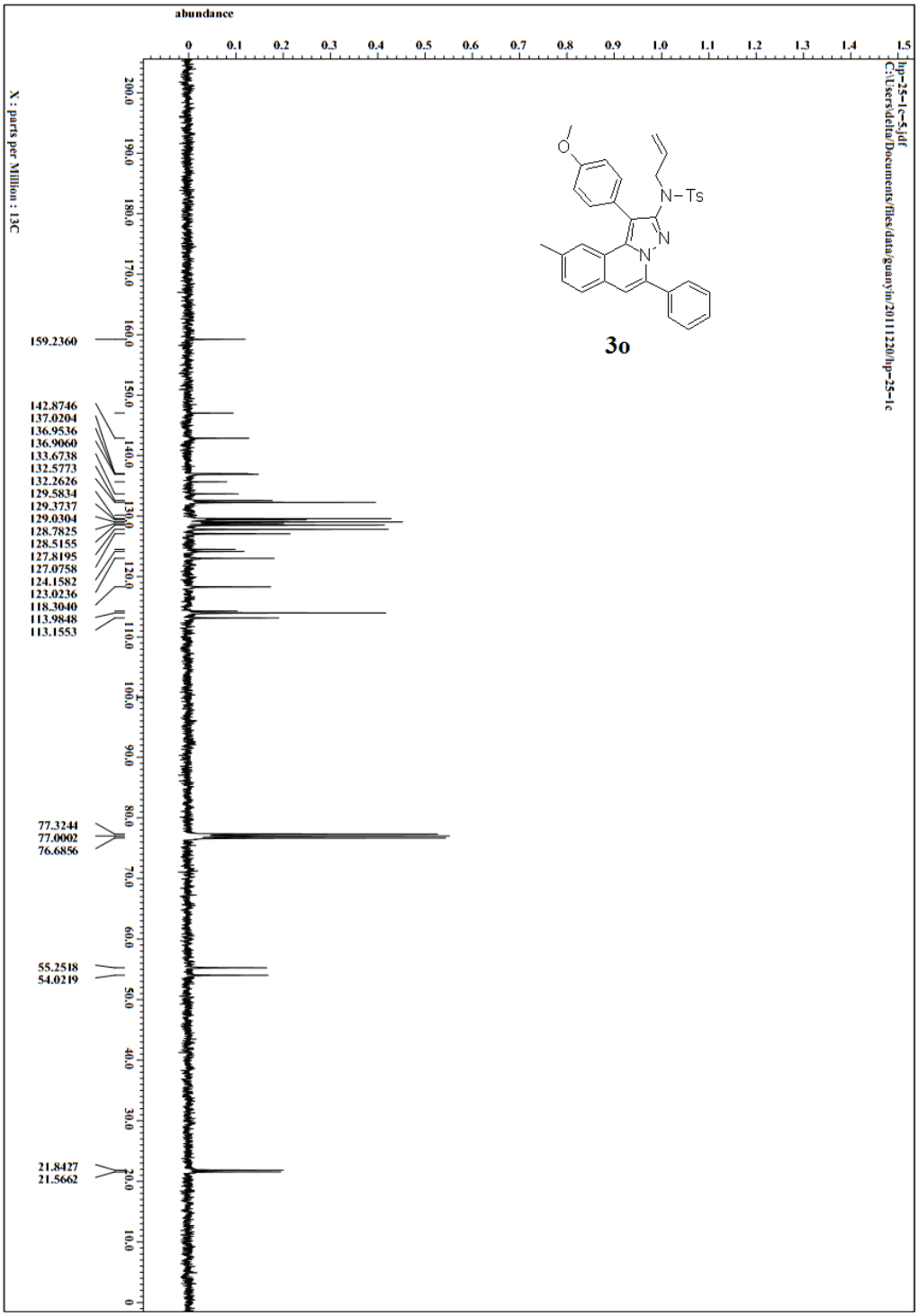

Cl
N-Ts
N
N
3m
7.8254
7.8062
7.7829
7.7643
7.7128
7.6932
7.6314
7.6117
7.5432
7.5243
7.4963
7.4831
7.4650
7.4479
7.3290
7.3100
7.2921
7.1838
7.1649
7.1121
5.4613
5.4434
5.4204
5.4027
5.3800
5.3649
4.8542
4.8268
4.8157
3.9474
3.9323
2.4471
51.42
11.88
20.26
61.16
11.08
19.74
10.56
9.77
19.74
19.90
30.00
f1 (ppm)

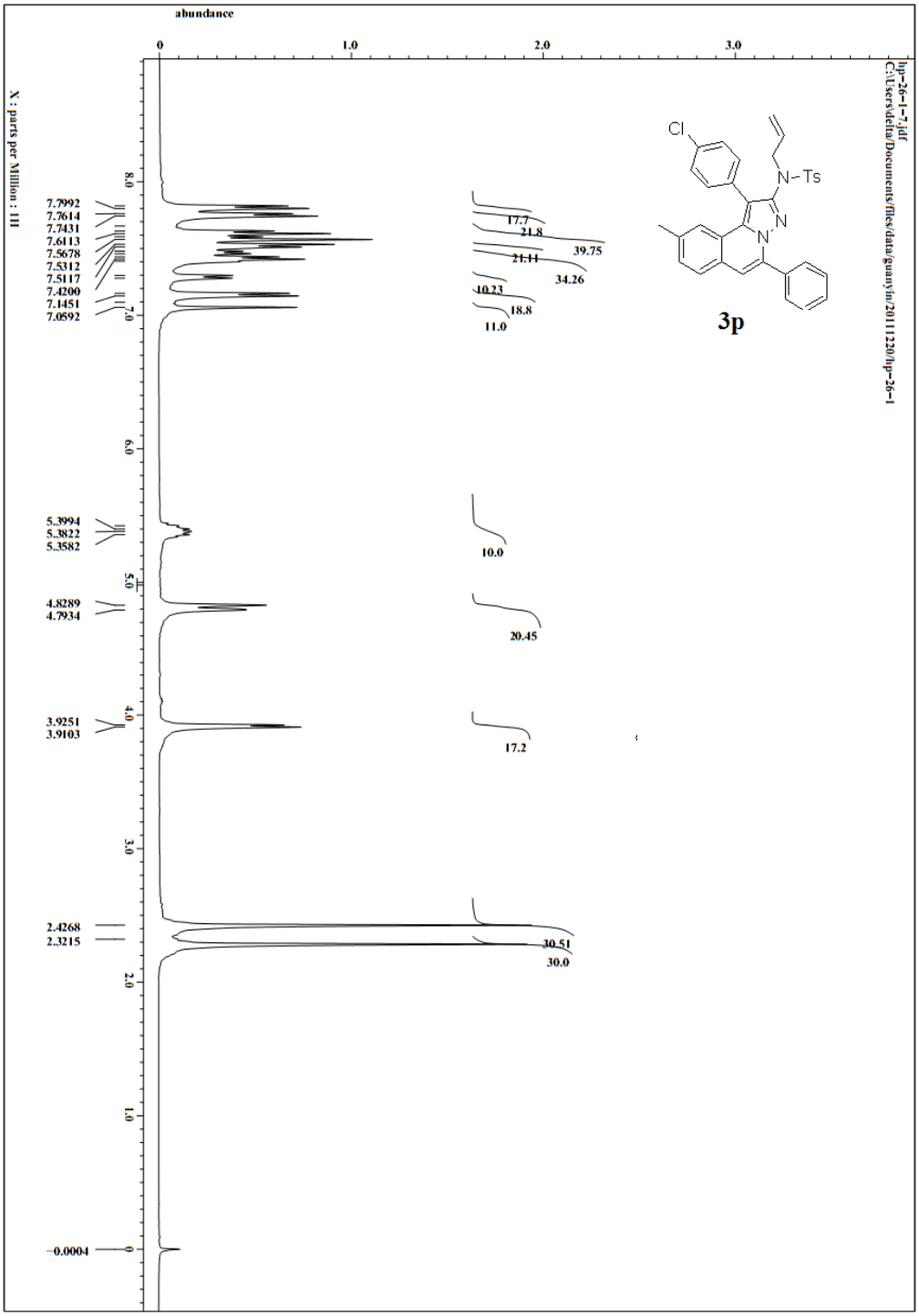

Cl
N-Ts
N
N
3m
147.2533
143.2772
132.7770
132.5241
129.7628
129.2672
129.2248
129.1031
128.6748
128.2515
128.0600
127.5514
123.2436
118.8872
113.9769
113.6688
77.4980
77.1803
76.8618
54.4506
21.7713

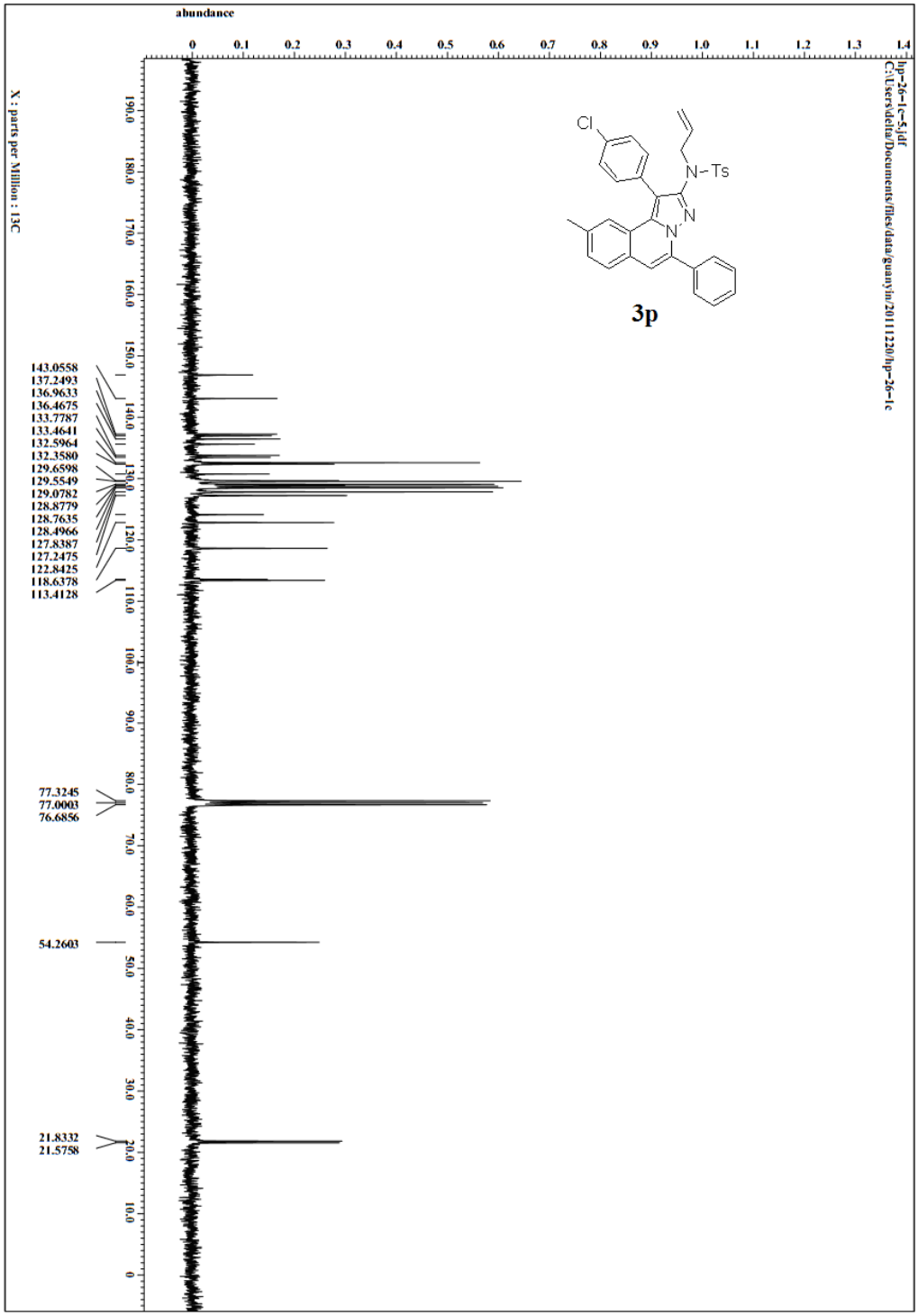

hp-24-3-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-24-3
3n
N-Ts
N
N
abundance
0
1.0
2.0
3.0
X : parts per Million : 111
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.0117
7.7379
7.7196
7.6371
7.6188
7.5993
7.5798
7.3370
7.1984
7.1789
6.9727
5.7665
5.7493
5.7241
4.9933
4.9532
4.9303
4.1330
4.1182
3.1559
3.1353
3.1170
2.5546
2.4354
1.7825
1.7653
1.6210
1.6027
1.5843
1.1009
1.0837
1.0654
0.0001
8.63
18.88
30.94
40.4
20.64
10
10.42
20.15
19.89
19.0
28.26
34.8
18.88
21.13
27.35

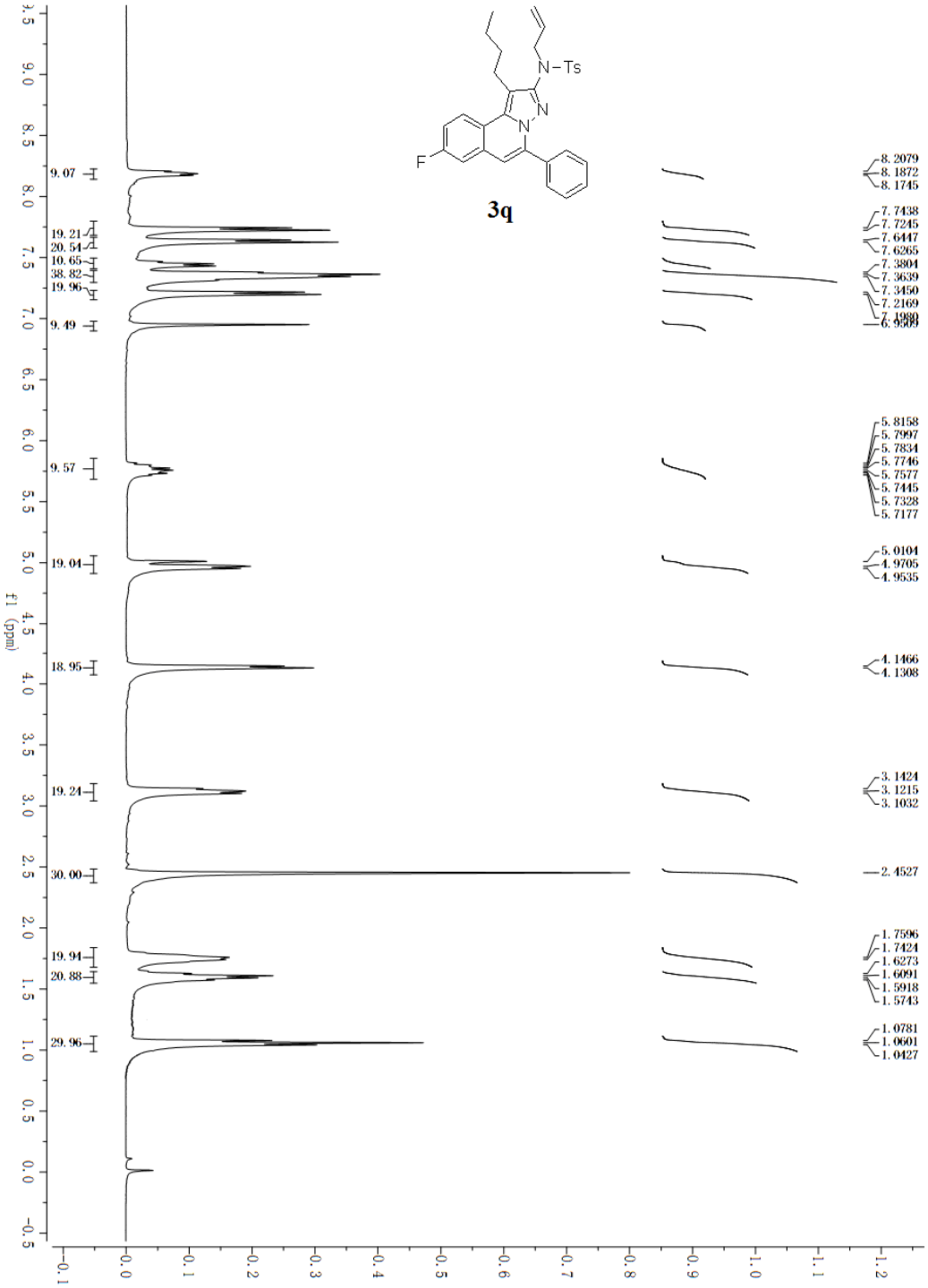

hp-24-3c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-24-3c
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
N-Ts
N
N
3n
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
147.3940
143.0272
137.3064
137.0776
135.7523
133.6451
132.8061
129.4118
129.0399
128.8016
128.6967
128.5155
127.6479
127.1712
126.9709
123.1190
118.7045
114.7762
112.8598
77.3244
77.0002
76.6856
54.7942
31.3010
23.1108
21.9952
21.5757
13.9099

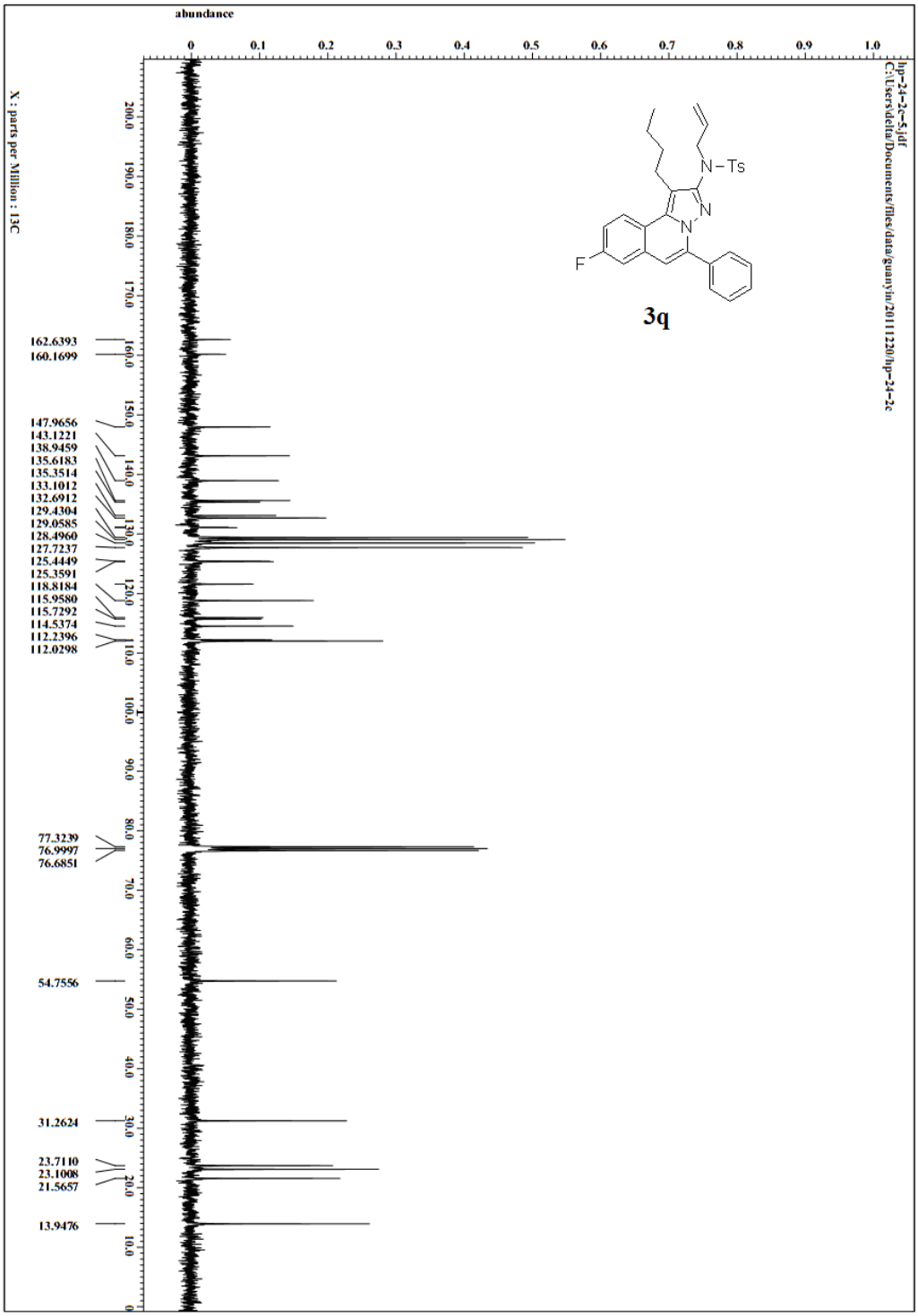

3o
N-Ts
O
N
N
18.50
20.49
9.55
28.86
31.00
10.60
19.04
19.24
11.11
9.89
19.72
50.21
32.93
30.00
7.8653
7.8470
7.7997
7.7821
7.6446
7.5898
7.5759
7.5711
7.4898
7.4732
7.4564
7.4393
7.4243
7.2907
7.2710
7.1674
7.1490
7.1067
7.0881
7.0458
5.4593
5.4403
5.4160
5.3991
5.3873
5.3769
5.3599
4.8477
4.8296
4.8046
3.9373
3.9355
2.4333
2.2841
f1 (ppm)

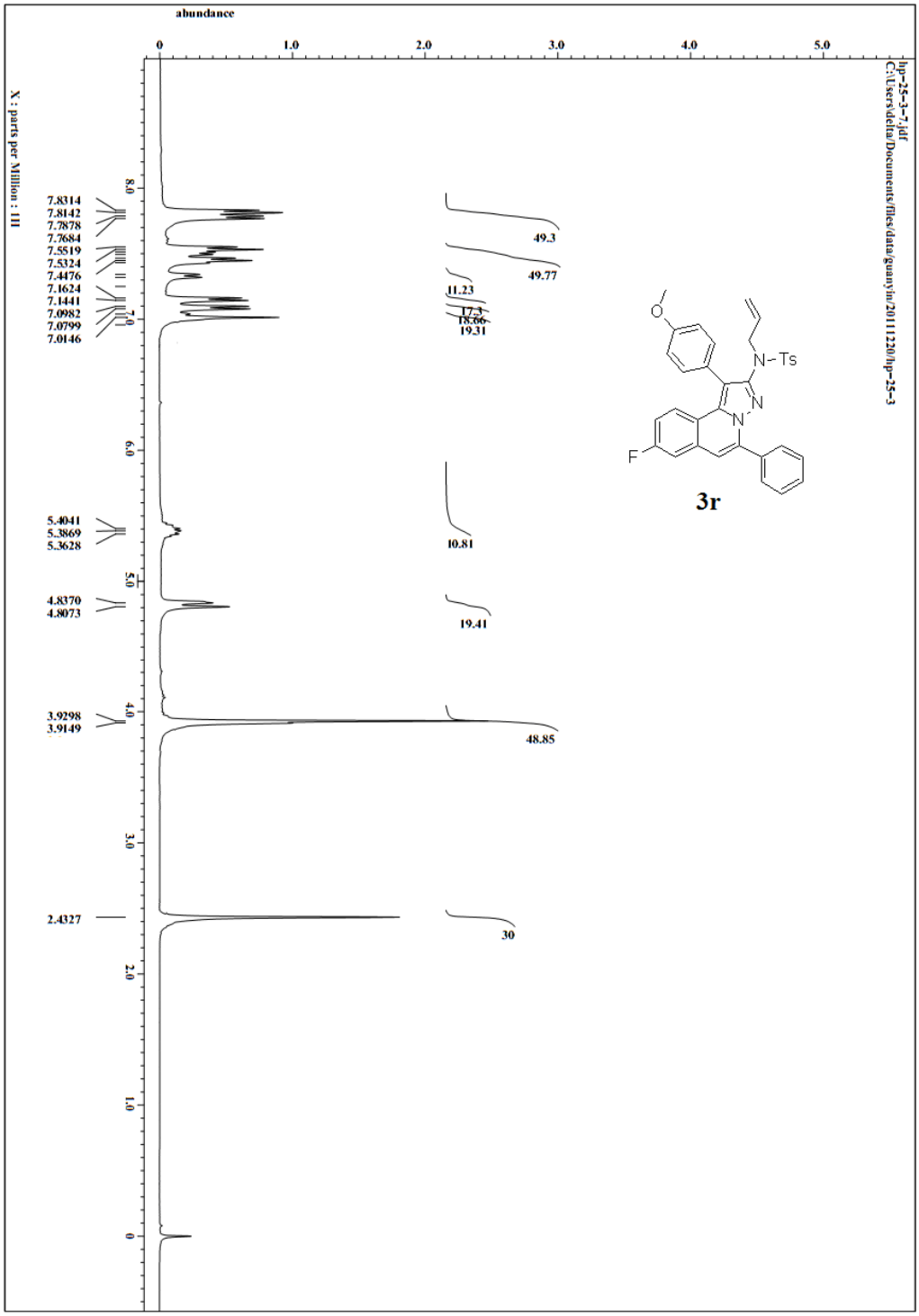

hp-25-1c-5.dif
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-25-1c
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5
X : parts per Million : 13C
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
159.2360
142.8746
137.0204
136.9536
136.9060
133.6738
132.5773
132.2626
129.5834
129.3737
129.0304
128.7825
128.5155
127.8195
127.0758
124.1582
123.0236
118.3040
113.9848
113.1553
77.3244
77.0002
76.6856
55.2518
54.0219
21.8427
21.5662
O
N-Ts
N
N
3o

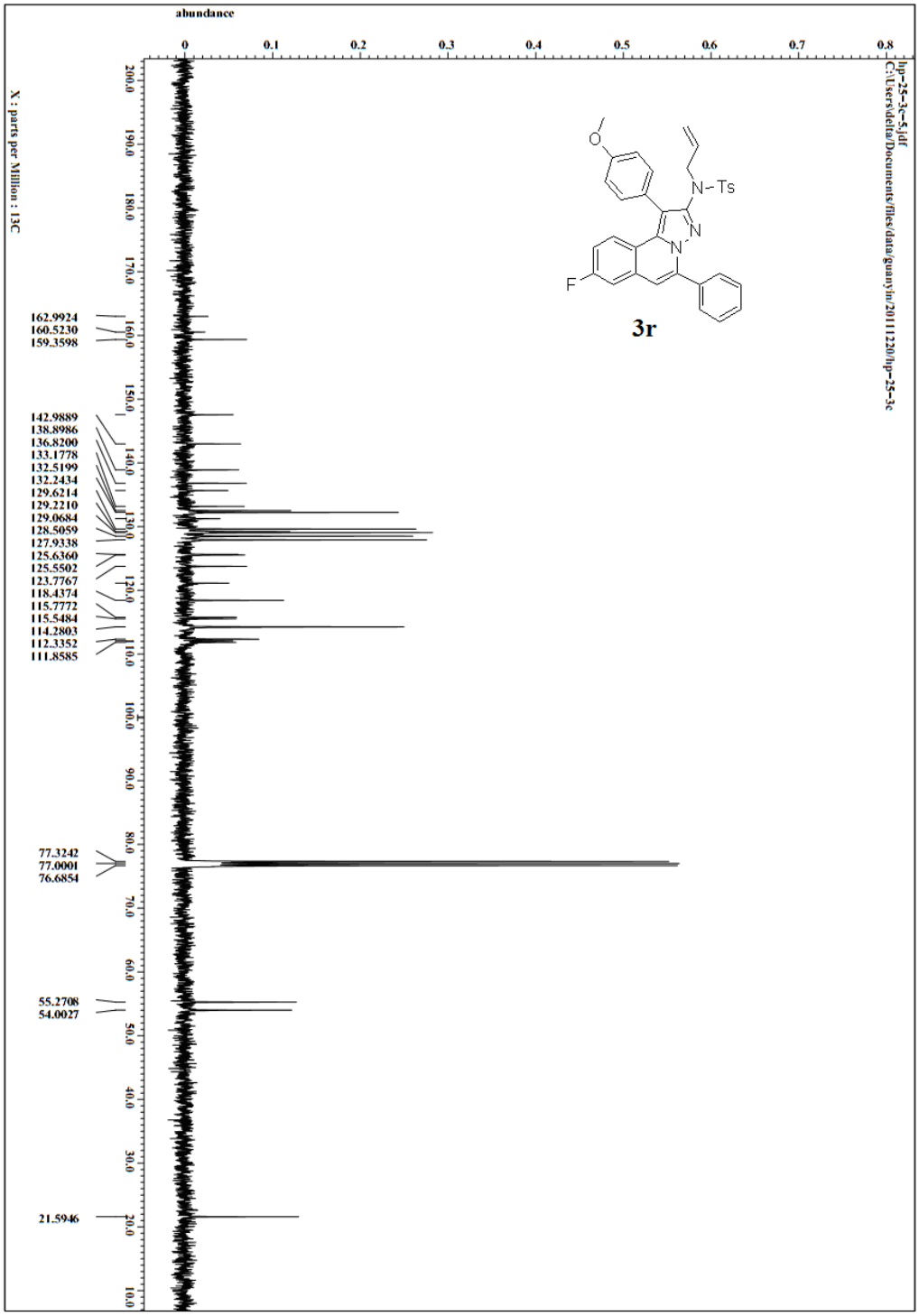

hp-26-1-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-26-1
3p
Cl
N-Ts
N
N
abundance
X : parts per Million : 1H
7.7992
7.7614
7.7431
7.6113
7.5678
7.5312
7.5117
7.4200
7.1451
7.0592
5.3994
5.3822
5.3582
4.8289
4.7934
3.9251
3.9103
2.4268
2.3215
-0.0004
17.7
21.8
39.75
21.11
34.26
10.23
18.8
11.0
10.0
20.45
17.2
30.51
30.0

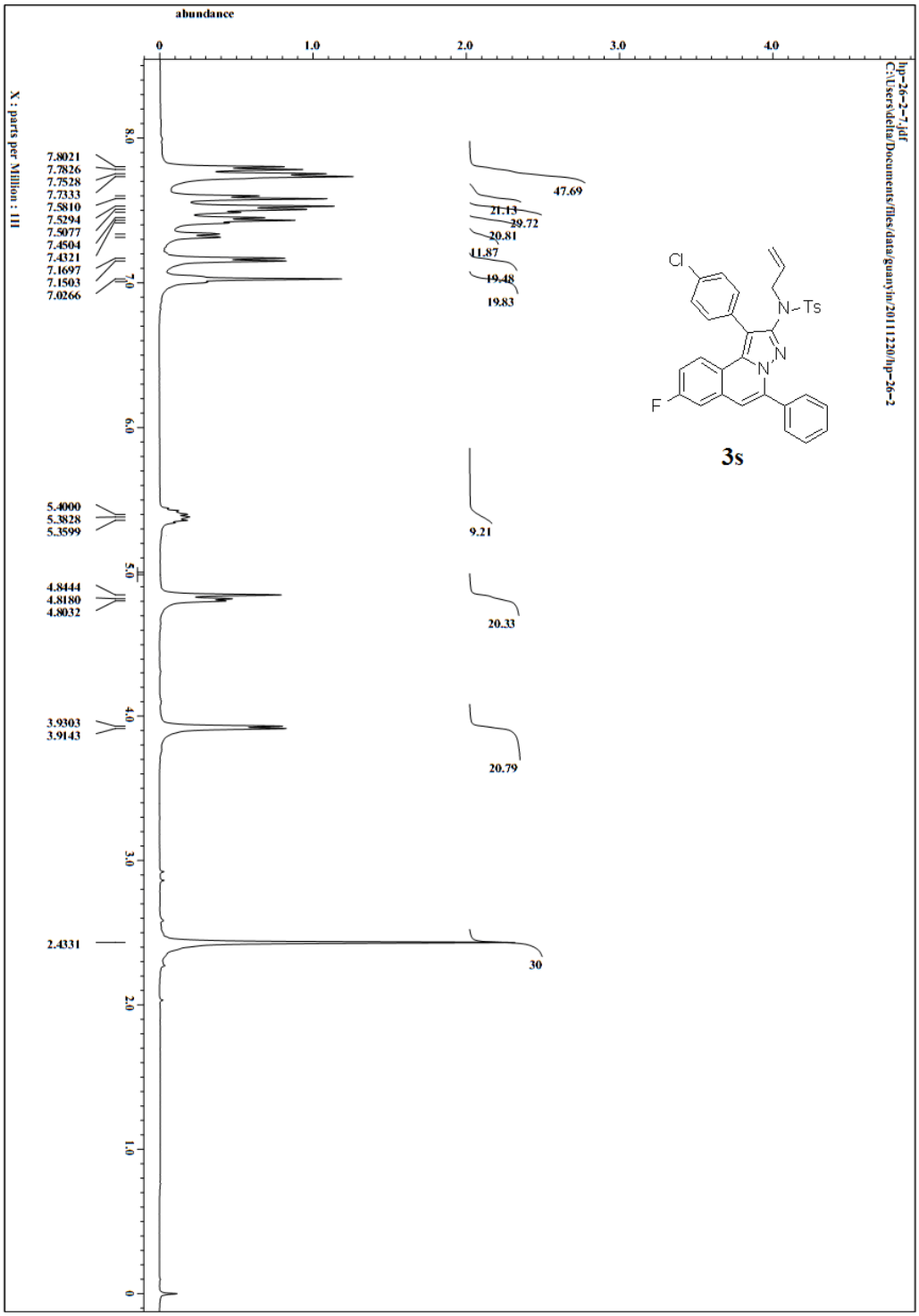

abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4
hp-26-1c-5.dff
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-26-1c
X : parts per Million : 13C
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
143.0558
137.2493
136.9633
136.4675
133.7787
133.4641
132.5964
132.3580
129.6598
129.5549
129.0782
128.8779
128.7635
128.4966
127.8387
127.2475
122.8425
118.6378
113.4128
77.3245
77.0003
76.6856
54.2603
21.8332
21.5758
Cl
N-Ts
N
N
3p

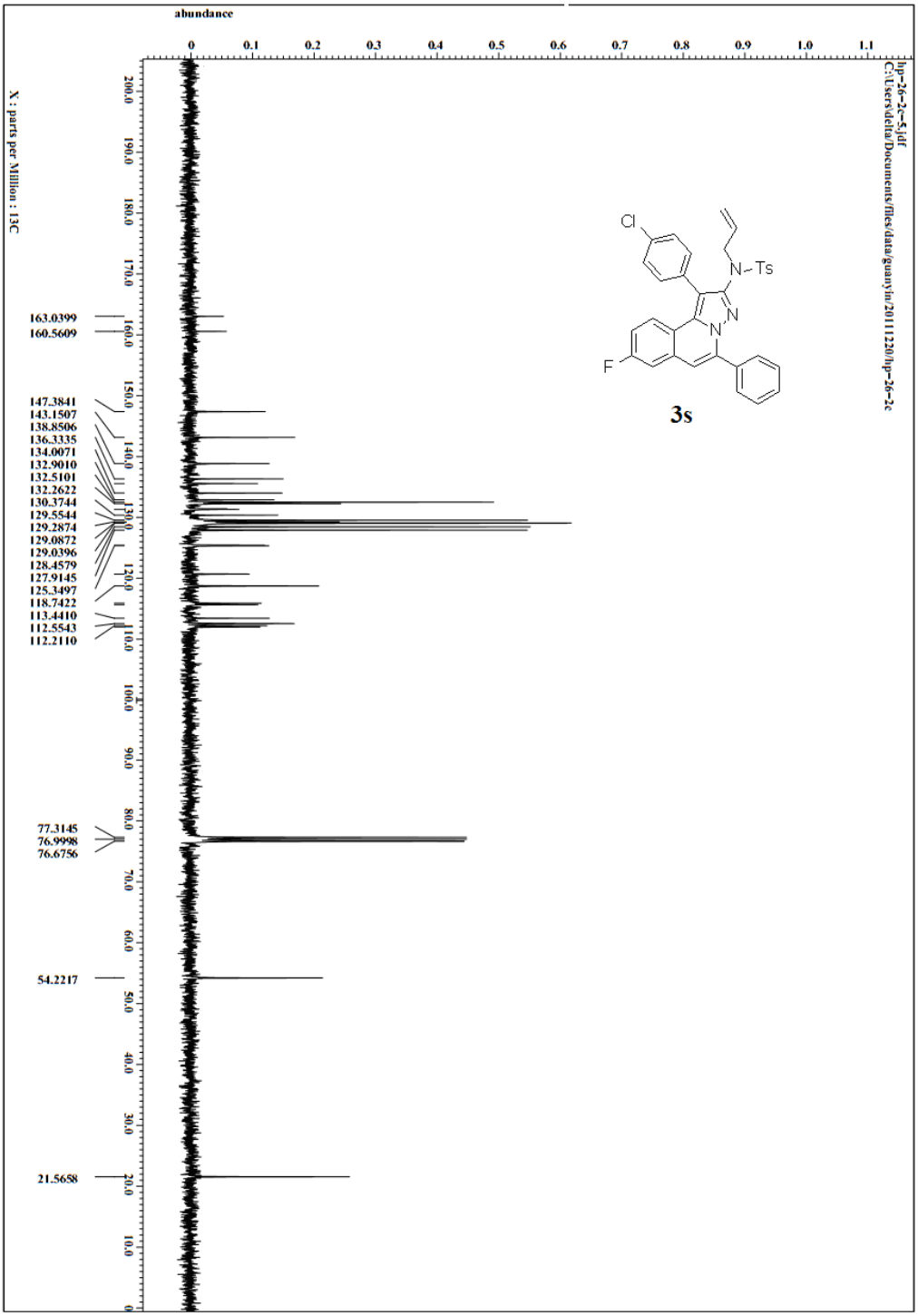

N-Ts
N
N
F
3q
f1 (ppm)
9.07
19.21
20.54
10.65
38.82
19.96
9.49
9.57
19.04
18.95
19.24
30.00
19.94
20.88
29.96
8.2079
8.1872
8.1745
7.7438
7.7245
7.6447
7.6265
7.3804
7.3639
7.3450
7.2169
7.1989
6.9609
5.8158
5.7997
5.7834
5.7746
5.7577
5.7445
5.7328
5.7177
5.0104
4.9705
4.9535
4.1466
4.1308
3.1424
3.1215
3.1032
2.4527
1.7596
1.7424
1.6273
1.6091
1.5918
1.5743
1.0781
1.0601
1.0427

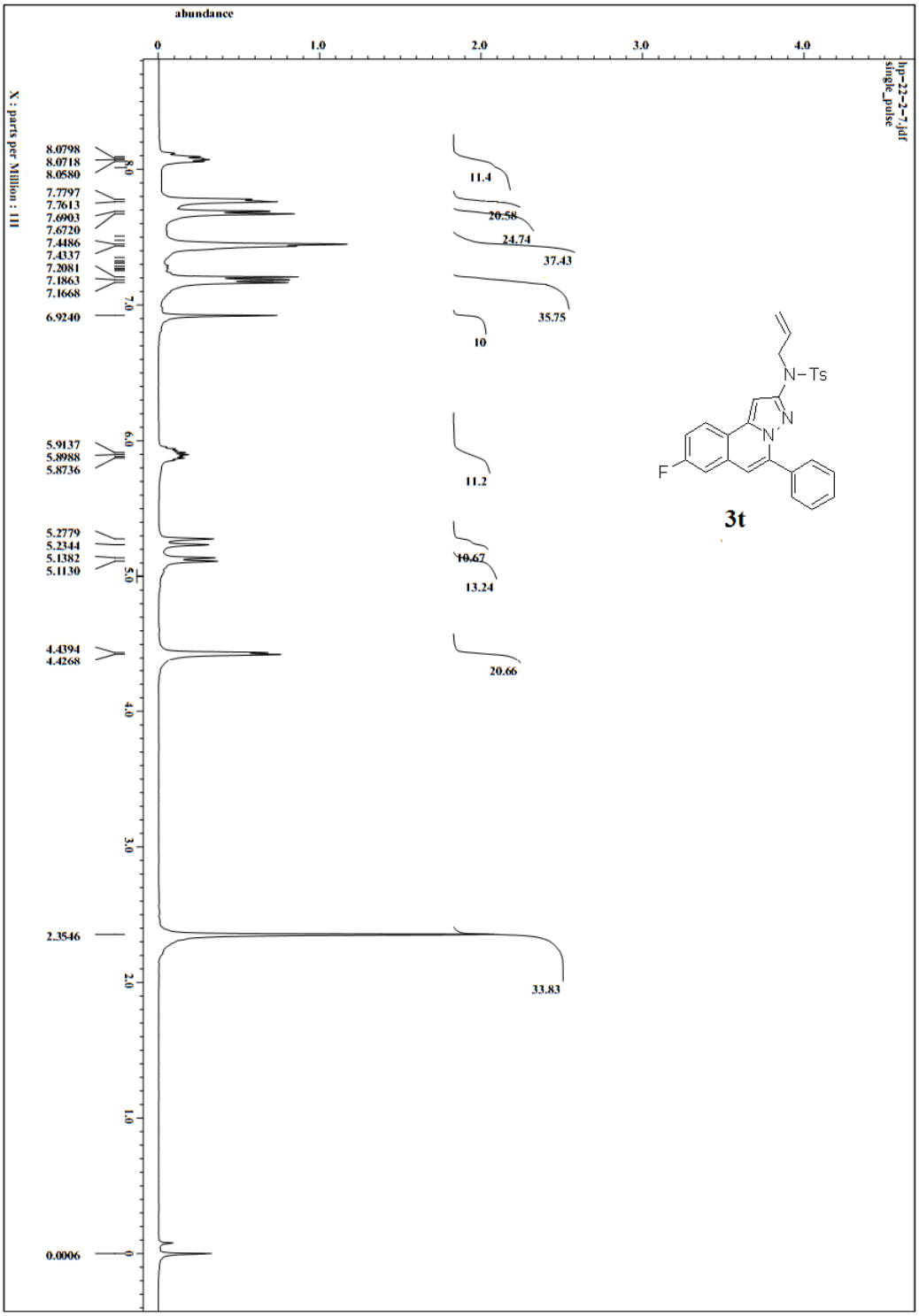

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
hp-24-2c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-24-2c
N-Ts
N
N
F
3q
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.6393
160.1699
147.9656
143.1221
138.9459
135.6183
135.3514
133.1012
132.6912
129.4304
129.0585
128.4960
127.7237
125.4449
125.3591
118.8184
115.9580
115.7292
114.5374
112.2396
112.0298
77.3239
76.9997
76.6851
54.7556
31.2624
23.7110
23.1008
21.5657
13.9476

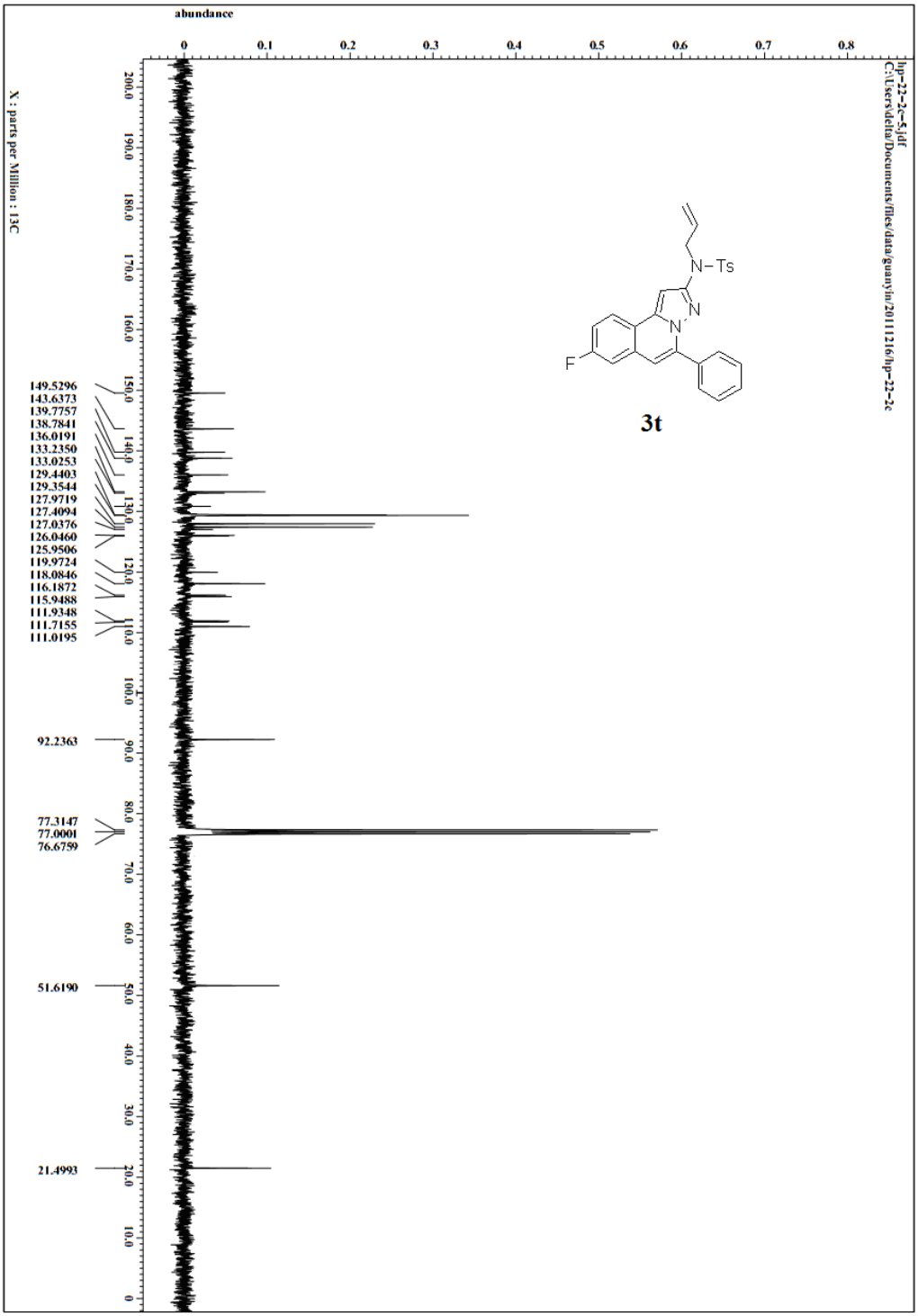

hp-25-3-7.jdf
C:\Users\dela\Documents\files\data\guanyin\20111220\hp-25-3
abundance
X : parts per Million : 111
7.8314
7.8142
7.7878
7.7684
7.5519
7.5324
7.4476
7.1624
7.1441
7.0982
7.0799
7.0146
5.4041
5.3869
5.3628
4.8370
4.8073
3.9298
3.9149
2.4327
49.3
49.77
11.23
17.3
18.66
19.31
10.81
19.41
48.85
30
N-Ts
3r

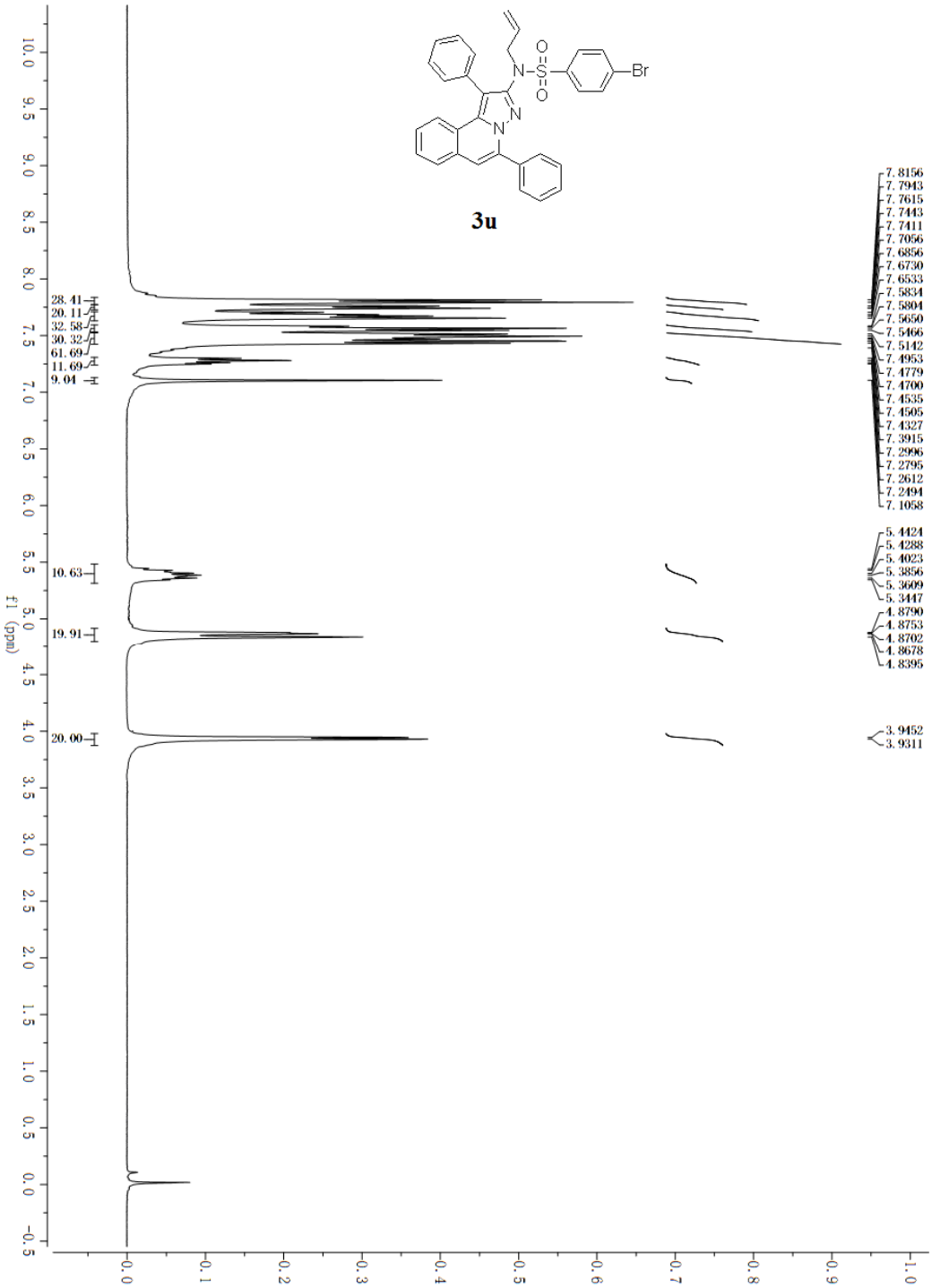

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
hp-25-3c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-25-3c
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
162.9924
160.5230
159.3598
142.9889
138.8986
136.8200
133.1778
132.5199
132.2434
129.6214
129.2210
129.0684
128.5059
127.9338
125.6360
125.5502
123.7767
118.4374
115.7772
115.5484
114.2803
112.3352
111.8585
77.3242
77.0001
76.6854
55.2708
54.0027
21.5946
O
N-Ts
N
N
F
3r

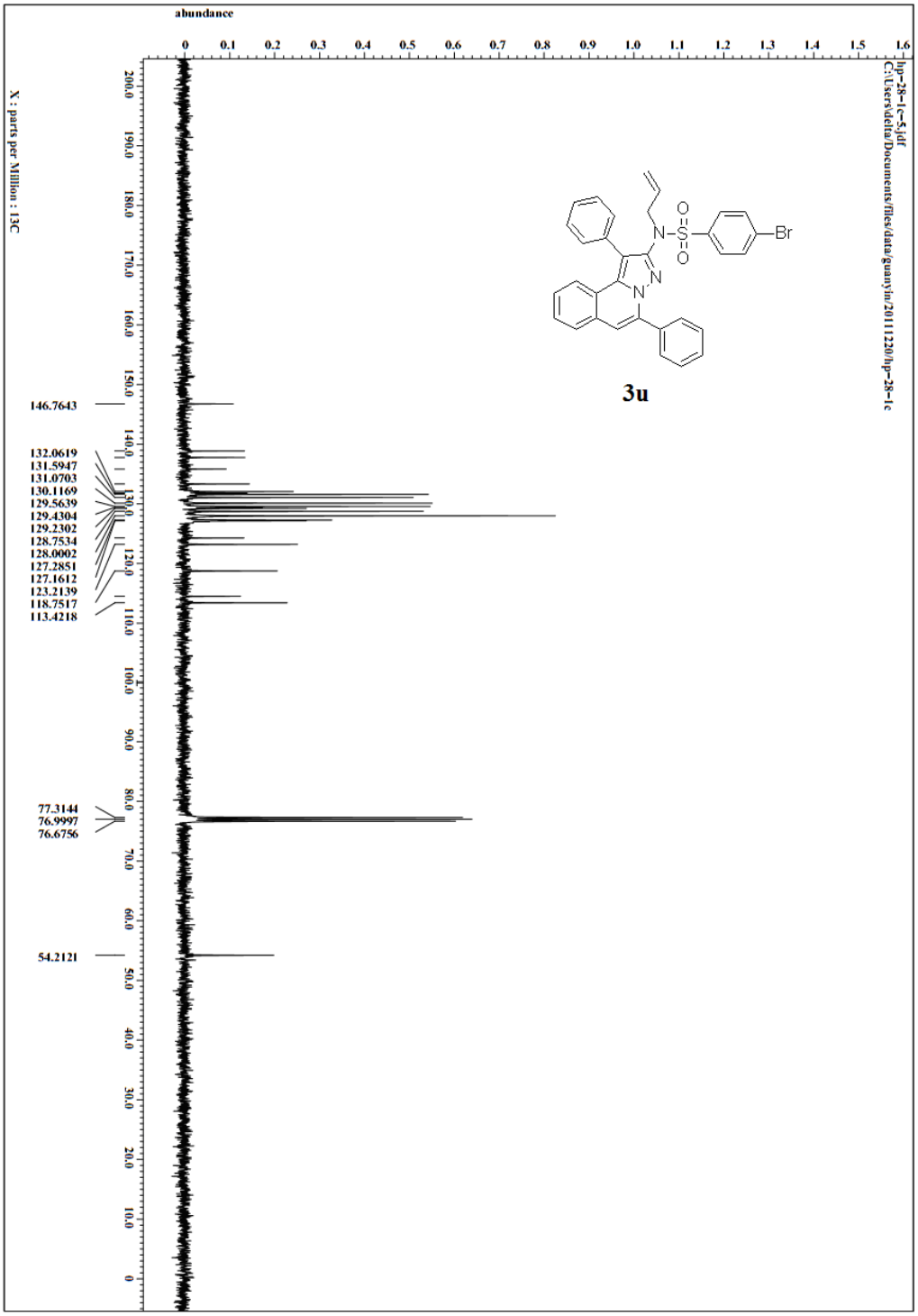

abundance
0
1.0
2.0
3.0
4.0
hp-26-2-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-26-2
X : parts per Million : 1H
7.8021
7.7826
7.7528
7.7333
7.5810
7.5294
7.5077
7.4504
7.4321
7.1697
7.1503
7.0266
5.4000
5.3828
5.3599
4.8444
4.8180
4.8032
3.9303
3.9143
2.4331
47.69
21.13
29.72
20.81
11.87
19.48
19.83
9.21
20.33
20.79
30
Cl
N-Ts
N
N
F
3s

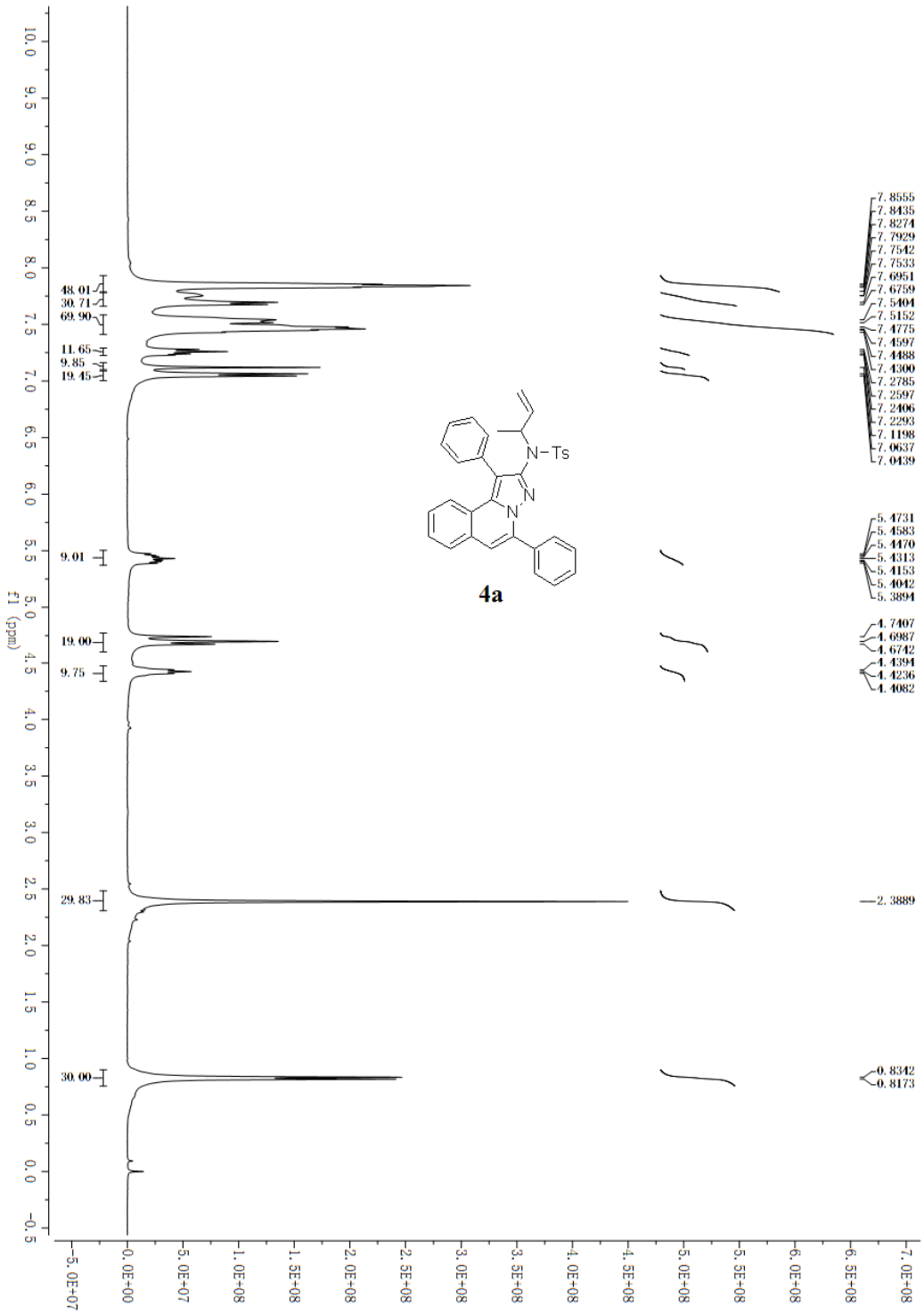

hp-26-2c-5.idf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-26-2c
abundance
X : parts per Million : 13C
163.0399
160.5609
147.3841
143.1507
138.8506
136.3335
134.0071
132.9010
132.5101
132.2622
130.3744
129.5544
129.2874
129.0872
129.0396
128.4579
127.9145
125.3497
118.7422
113.4410
112.5543
112.2110
77.3145
76.9998
76.6756
54.2217
21.5658
Cl
N-Ts
N
N
F
3s

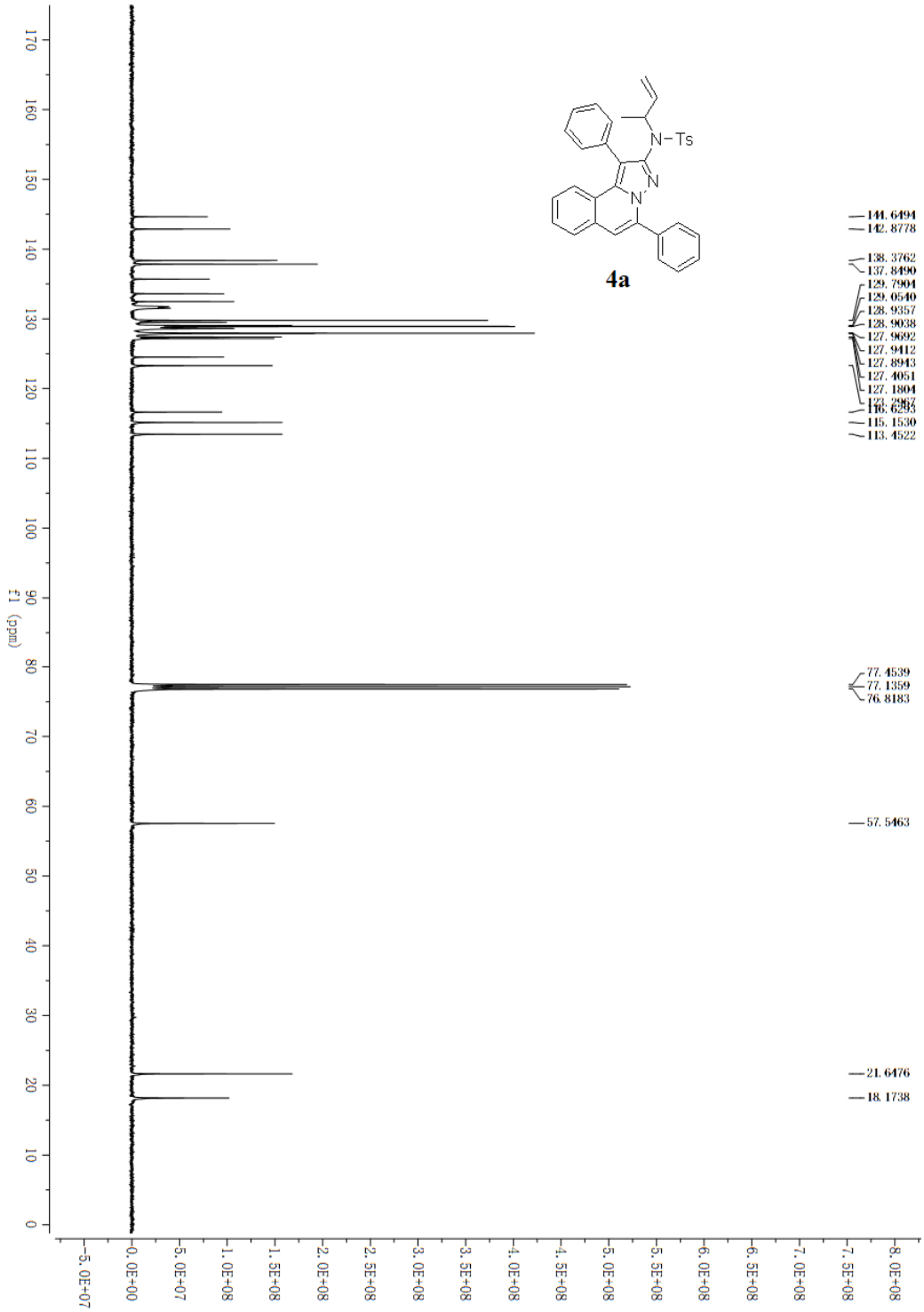

abundance
hp-22-2-7.jdf
single_pulse
X : parts per Million : 111
8.0798
8.0718
8.0580
7.7797
7.7613
7.6903
7.6720
7.4486
7.4337
7.2081
7.1863
7.1668
6.9240
5.9137
5.8988
5.8736
5.2779
5.2344
5.1382
5.1130
4.4394
4.4268
2.3546
0.0006
11.4
20.58
24.74
37.43
35.75
10
11.2
10.67
13.24
20.66
33.83
N-Ts
N
N
F
3t

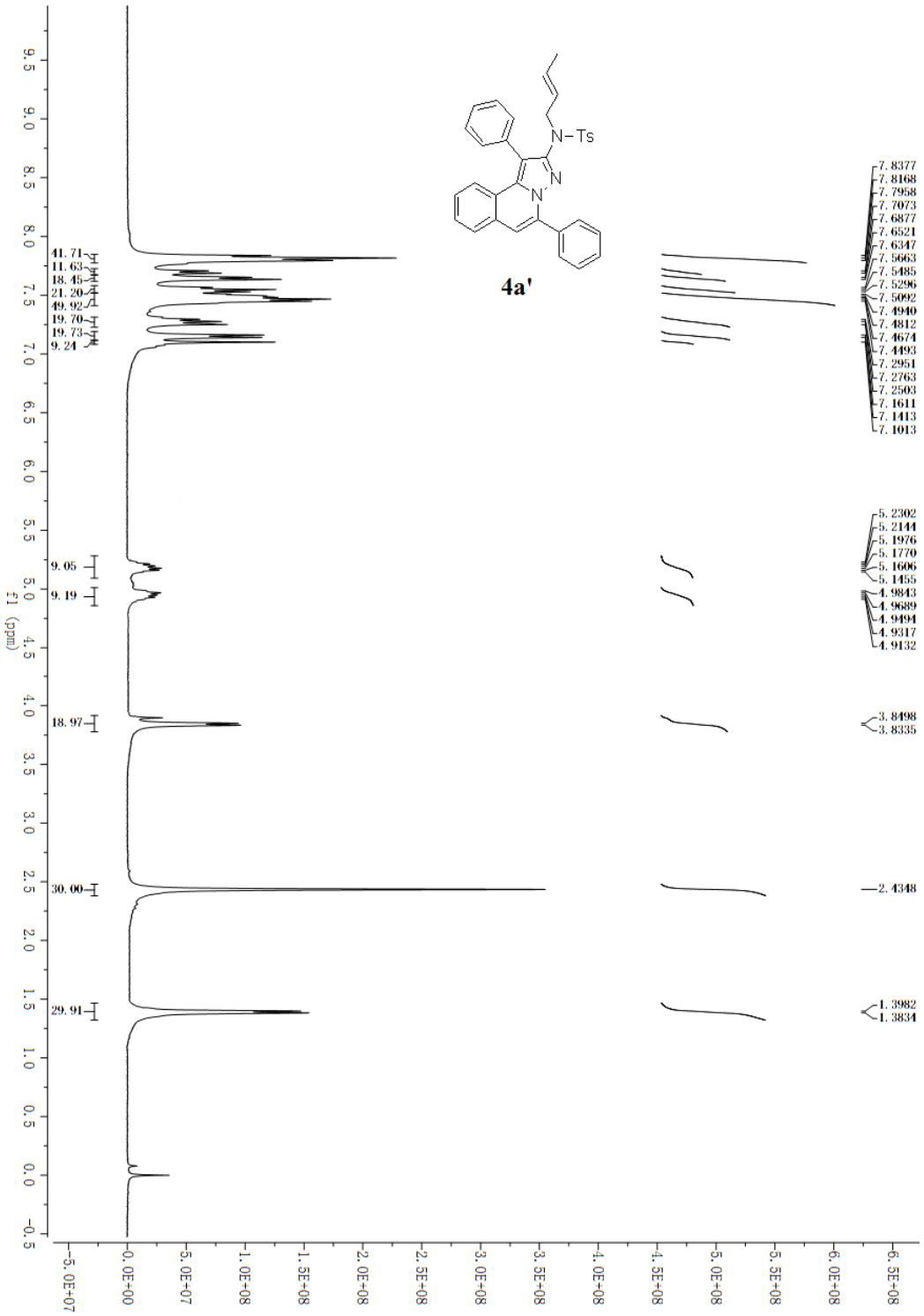

hp-22-2c-5.jdf
C:\Users\delta\Documents\files\data\guanyin\20111216\hp-22-2c
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
N-Ts
N
N
F
3t
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
149.5296
143.6373
139.7757
138.7841
136.0191
133.2350
133.0253
129.4403
129.3544
127.9719
127.4094
127.0376
126.0460
125.9506
119.9724
118.0846
116.1872
115.9488
111.9348
111.7155
111.0195
92.2363
77.3147
77.0001
76.6759
51.6190
21.4993

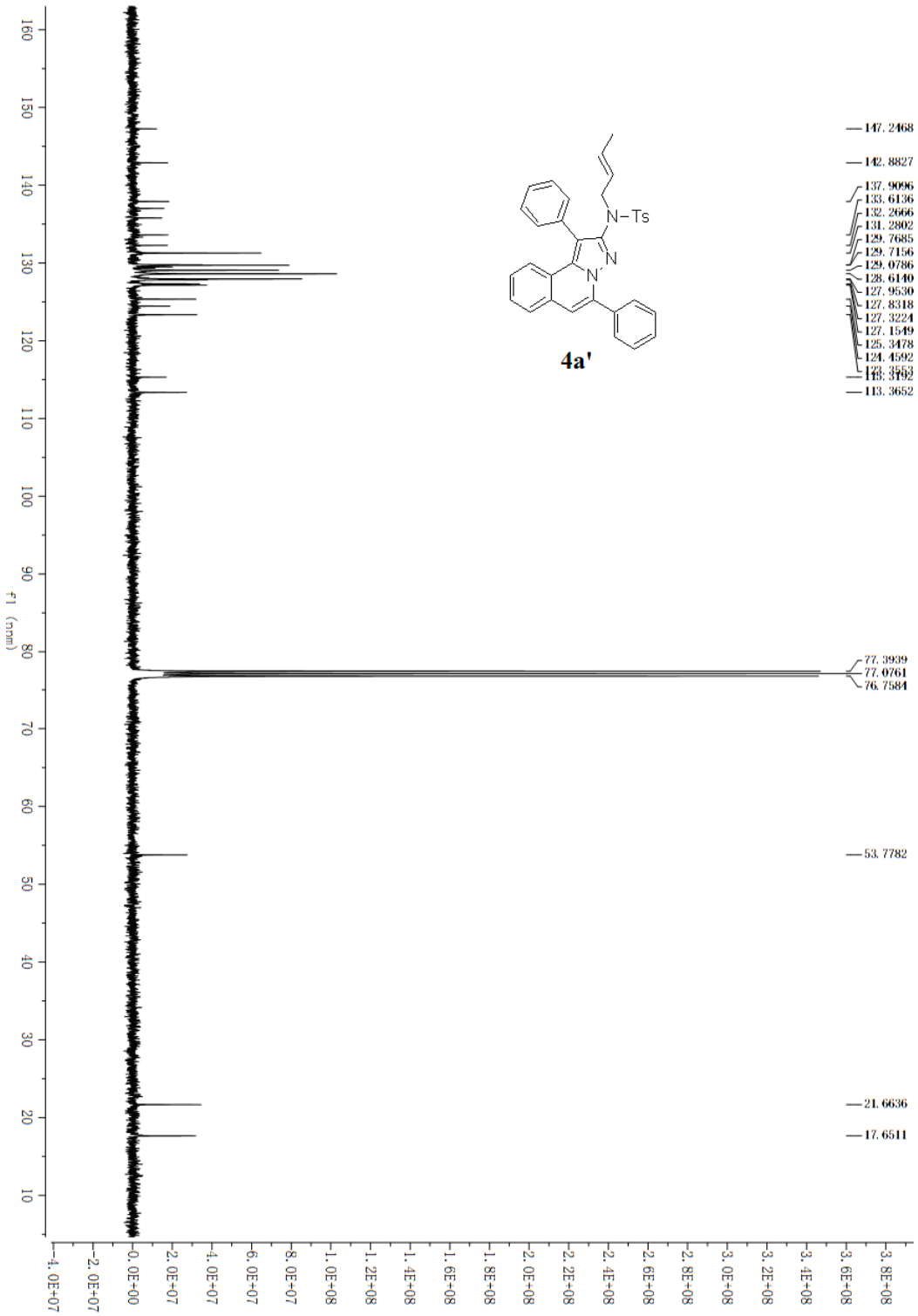

3u
Br
N
S
O
O
N
N
28.41
20.11
32.58
30.32
61.69
11.69
9.04
10.63
19.91
20.00
7.8156
7.7943
7.7615
7.7443
7.7411
7.7056
7.6856
7.6730
7.6533
7.5834
7.5804
7.5650
7.5466
7.5142
7.4953
7.4779
7.4700
7.4535
7.4505
7.4327
7.3915
7.2996
7.2795
7.2612
7.2494
7.1058
5.4424
5.4288
5.4023
5.3856
5.3609
5.3447
4.8790
4.8753
4.8702
4.8678
4.8395
3.9452
3.9311
f1 (ppm)

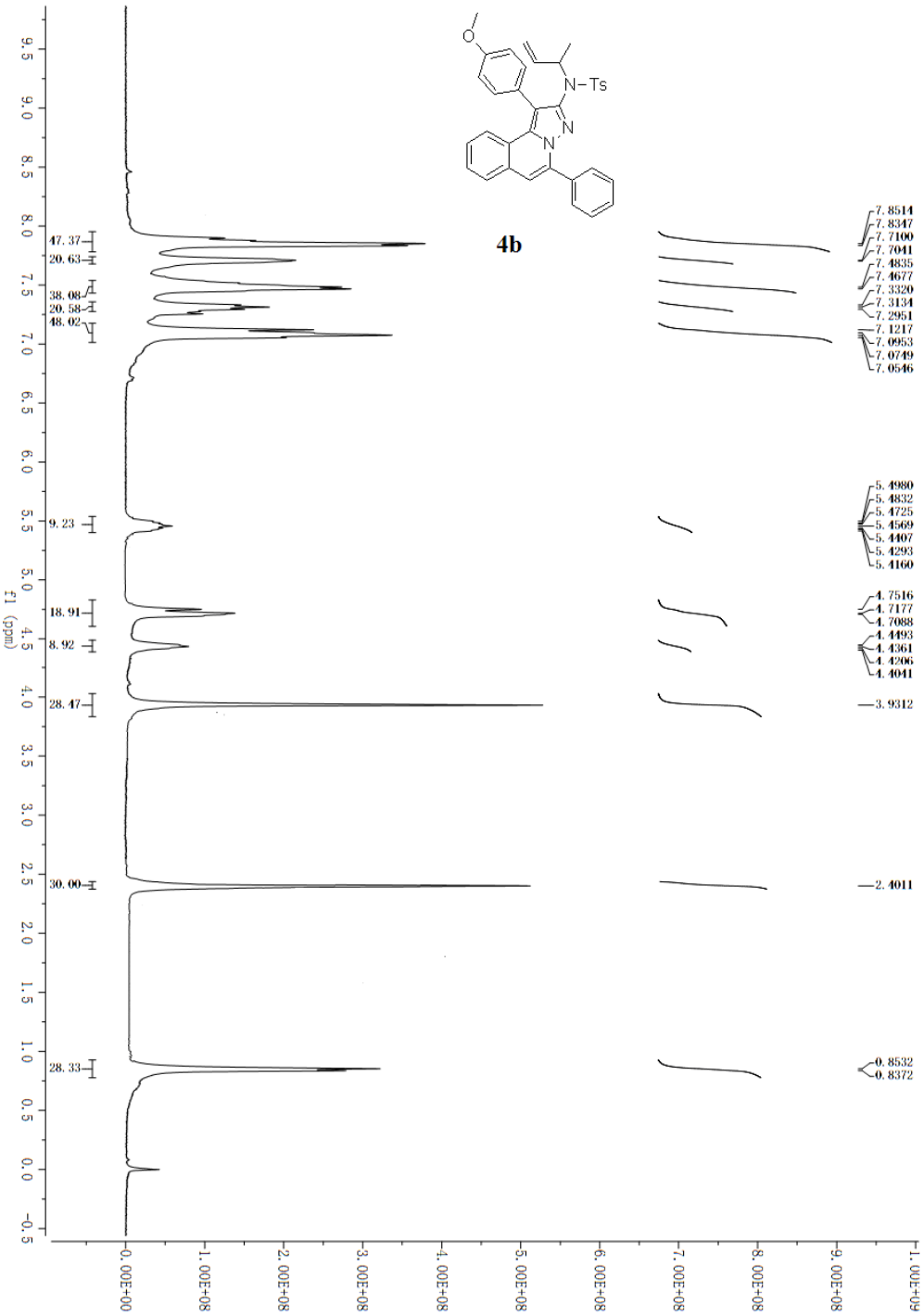

abundance
hp-28-1c-5.fdf
C:\Users\delta\Documents\files\data\guanyin\20111220\hp-28-1c
X : parts per Million : 13C
146.7643
132.0619
131.5947
131.0703
130.1169
129.5639
129.4304
129.2302
128.7534
128.0002
127.2851
127.1612
123.2139
118.7517
113.4218
77.3144
76.9997
76.6756
54.2121
Br
3u

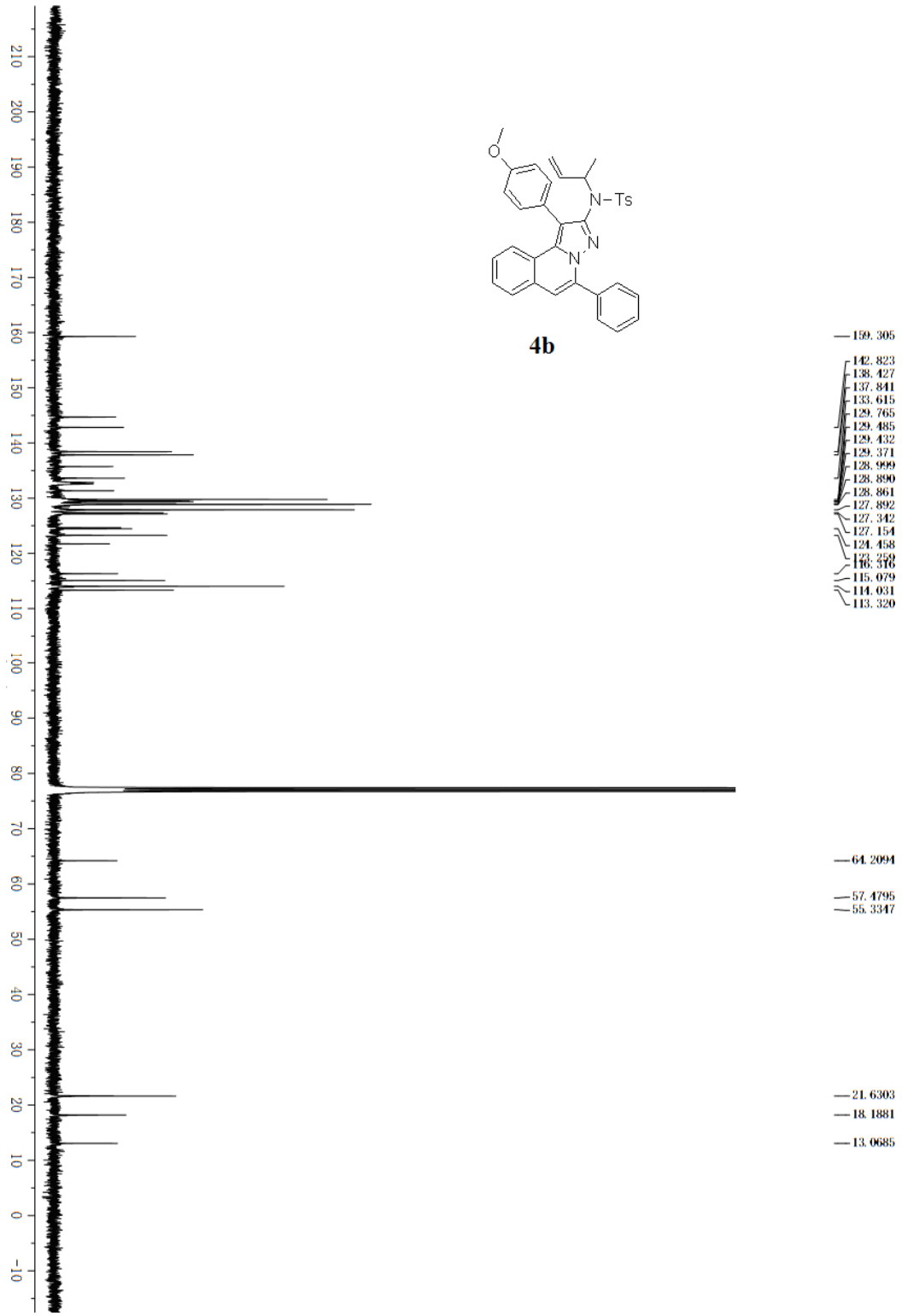

7.8555
7.8435
7.8274
7.7929
7.7542
7.7533
7.6951
7.6759
7.5404
7.5152
7.4775
7.4597
7.4488
7.4300
7.2785
7.2597
7.2406
7.2293
7.1198
7.0637
7.0439
5.4731
5.4583
5.4470
5.4313
5.4153
5.4042
5.3894
4.7407
4.6987
4.6742
4.4394
4.4236
4.4082
2.3889
0.8342
0.8173
48.01
30.71
69.90
11.65
9.85
19.45
9.01
19.00
9.75
29.83
30.00
N-Ts
N
N
4a
f1 (ppm)

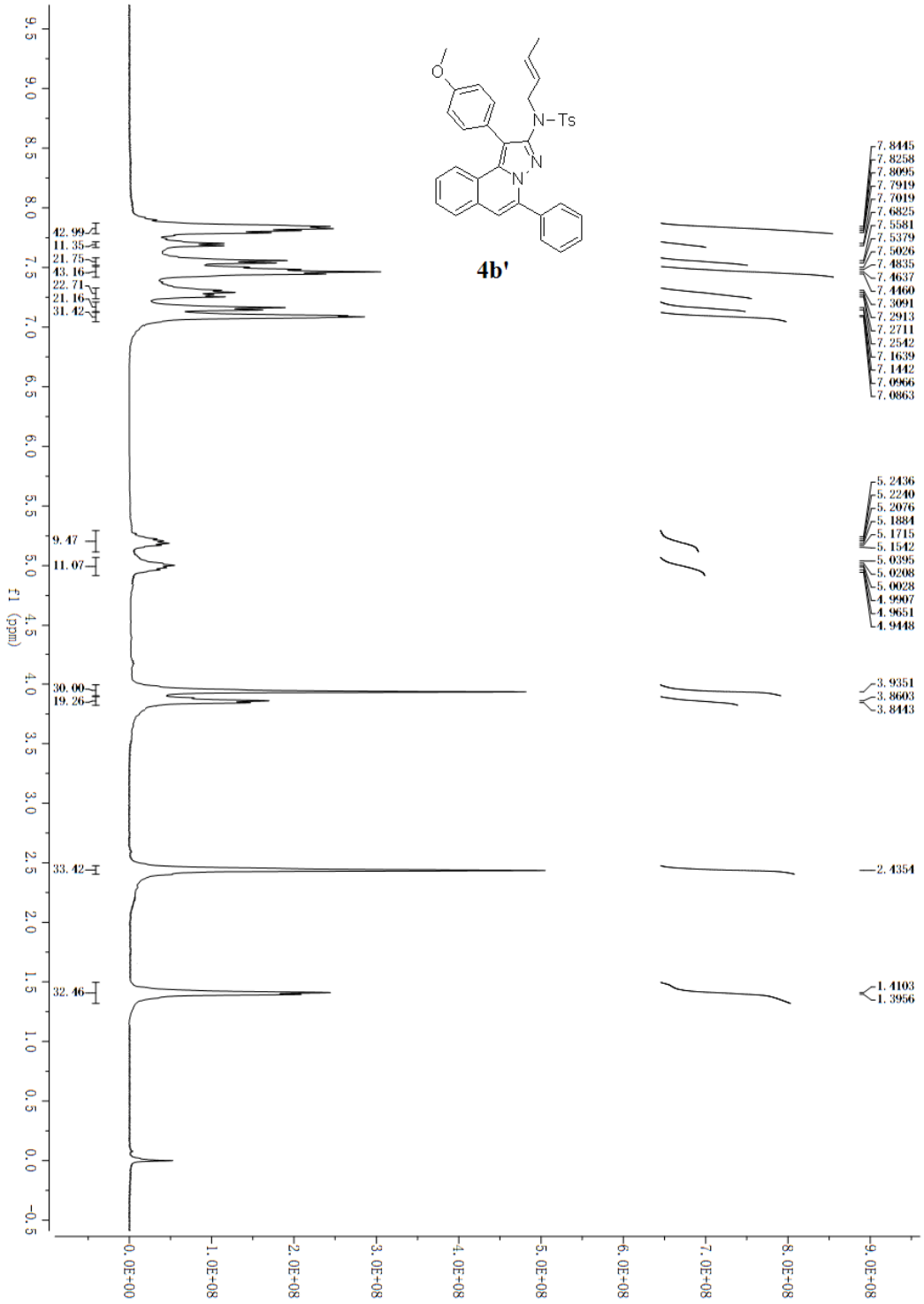

N-Ts
N
N
4a
144.6494
142.8778
138.3762
137.8490
129.7904
129.0540
128.9357
128.9038
127.9692
127.9412
127.8943
127.4051
127.1804
115.1530
113.4522
77.4539
77.1359
76.8183
57.5463
21.6476
18.1738
f1 (ppm)

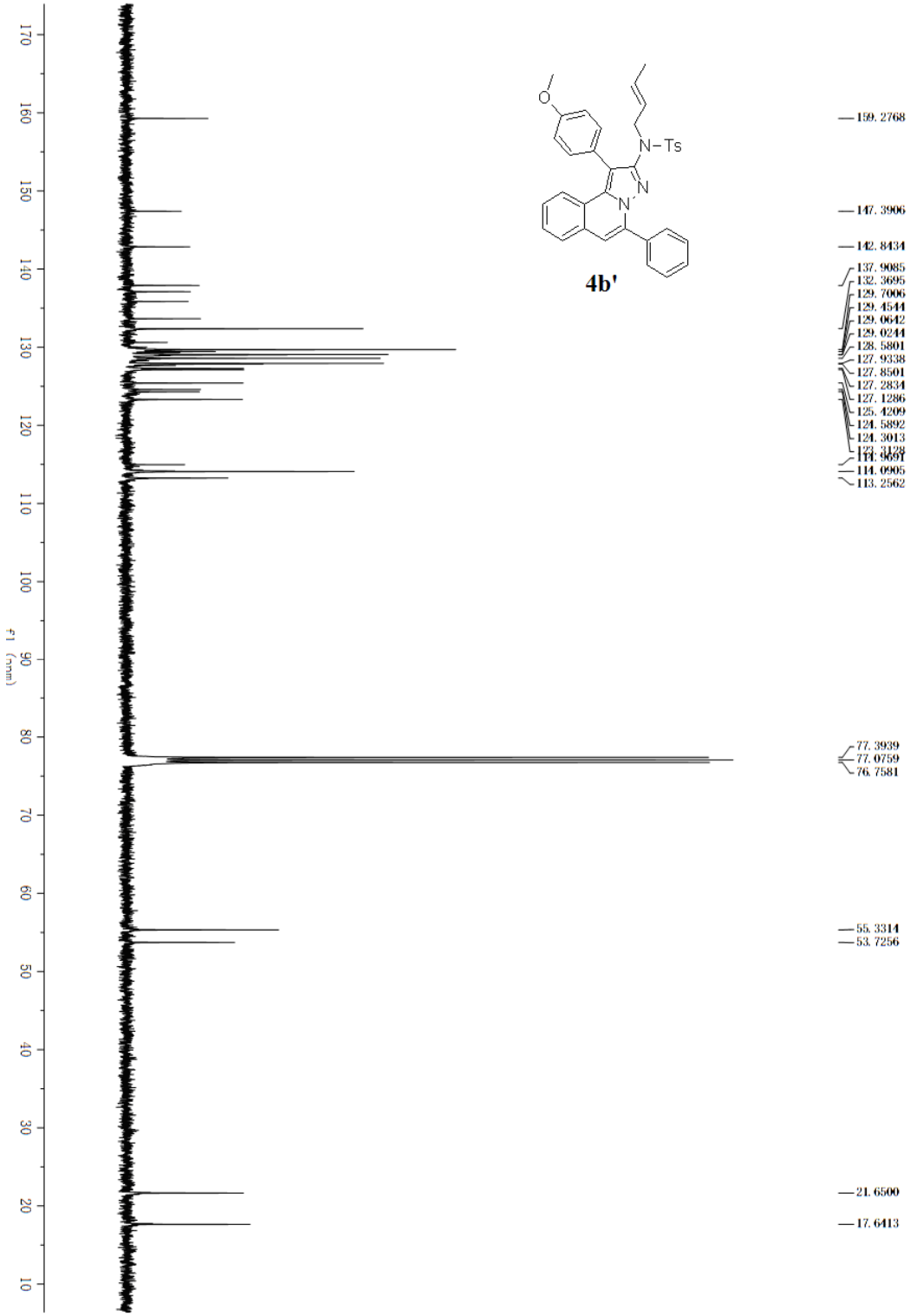

N-Ts
N
N
4a'
7.8377
7.8168
7.7958
7.7073
7.6877
7.6521
7.6347
7.5663
7.5485
7.5296
7.5092
7.4940
7.4812
7.4674
7.4493
7.2951
7.2763
7.2503
7.1611
7.1413
7.1013
5.2302
5.2144
5.1976
5.1770
5.1606
5.1455
4.9843
4.9689
4.9494
4.9317
4.9132
3.8498
3.8335
2.4348
1.3982
1.3834
41.71
11.63
18.45
21.20
49.92
19.70
19.73
9.24
9.05
9.19
18.97
30.00
29.91
f1 (ppm)

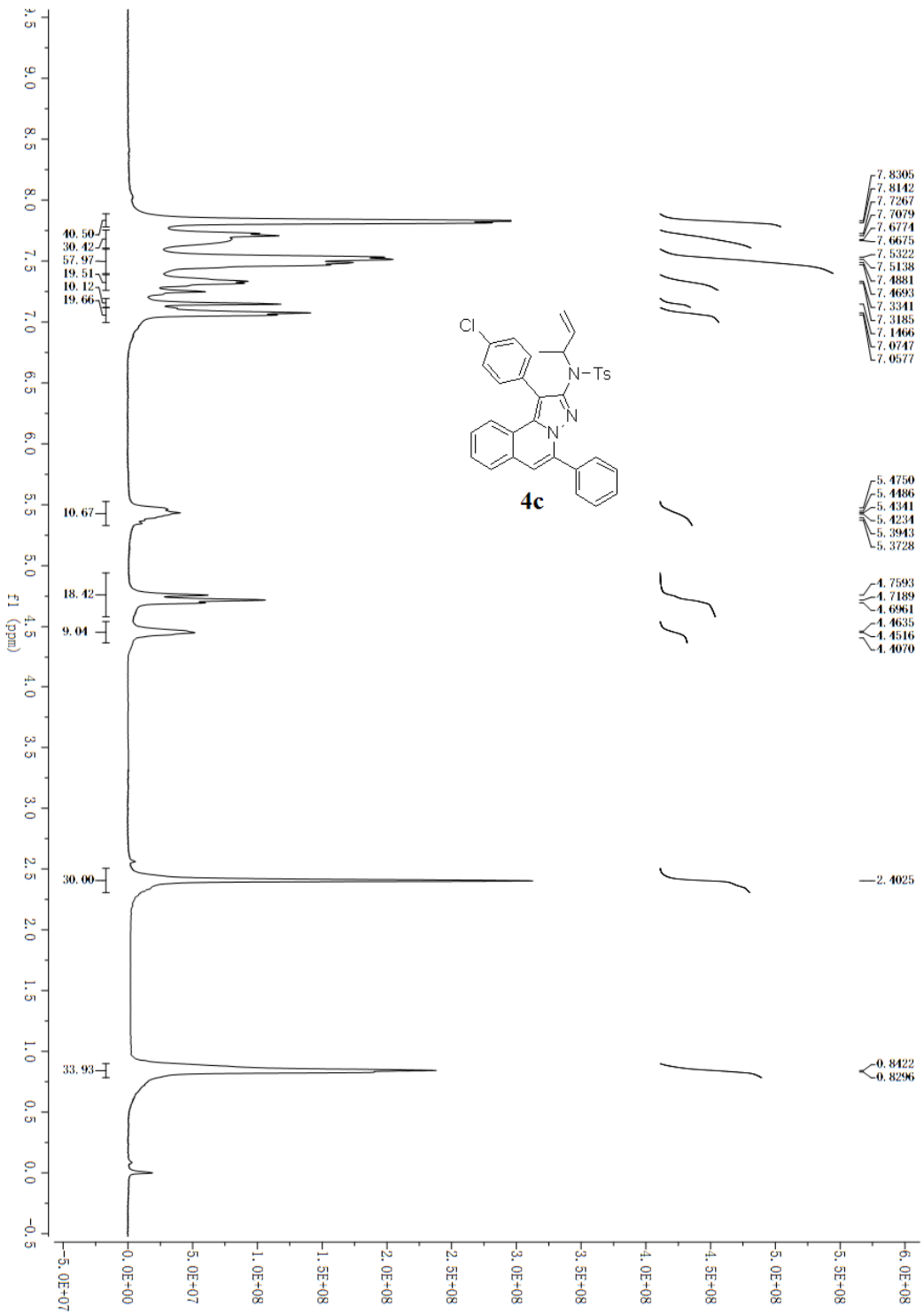

147.2468
142.8827
137.9096
133.6136
132.2666
131.2802
129.7685
129.7156
129.0786
128.6140
127.9530
127.8318
127.3224
127.1549
125.3478
124.4592
123.3553
113.3792
113.3652
77.3939
77.0761
76.7584
53.7782
21.6636
17.6511
N-Ts
N
N
4a'
f1 (ppm)

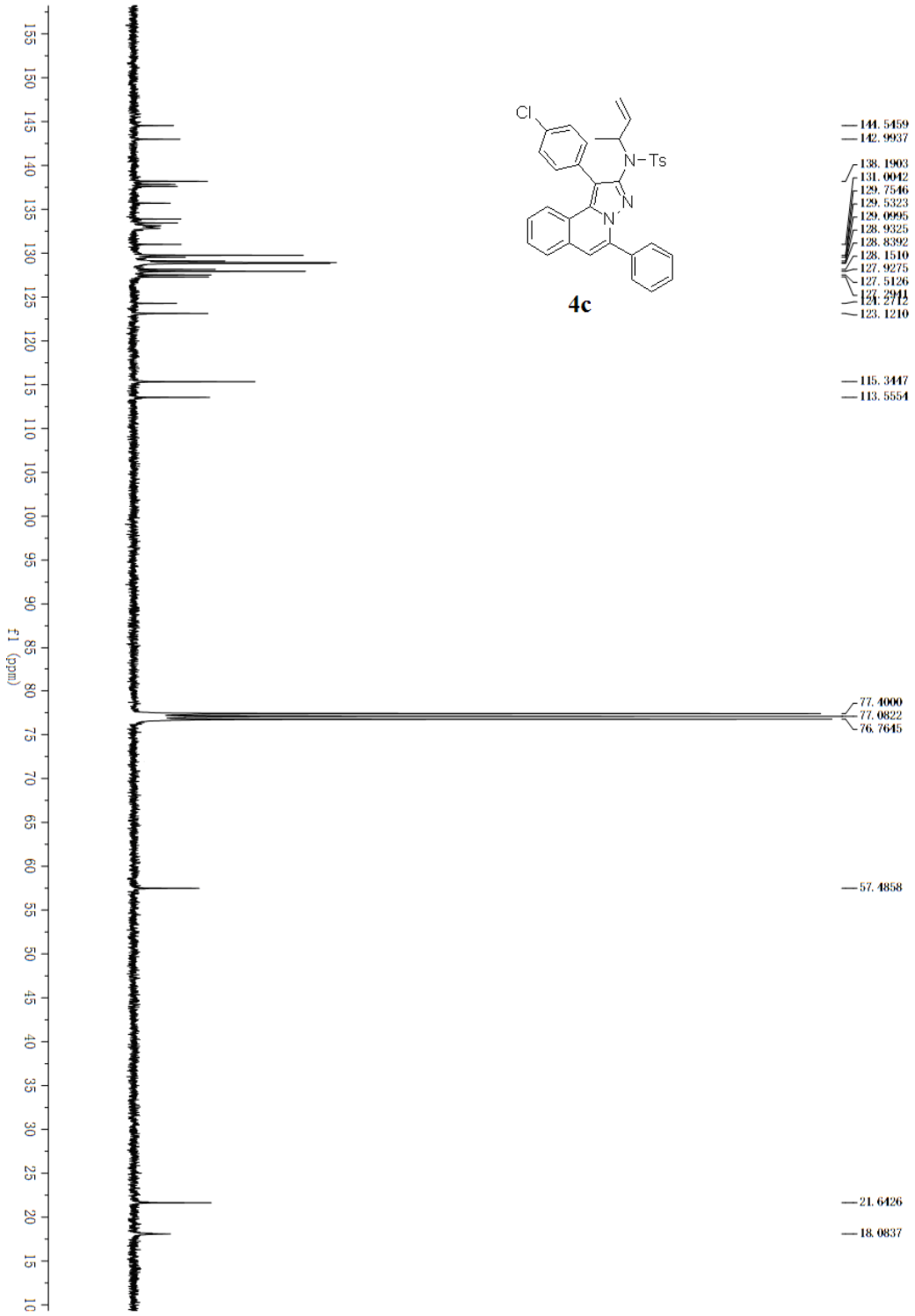

4b
N-Ts
N
N
O
7.8514
7.8347
7.7100
7.7041
7.4835
7.4677
7.3320
7.3134
7.2951
7.1217
7.0953
7.0749
7.0546
5.4980
5.4832
5.4725
5.4569
5.4407
5.4293
5.4160
4.7516
4.7177
4.7088
4.4493
4.4361
4.4206
4.4041
3.9312
2.4011
0.8532
0.8372
47.37
20.63
38.08
20.58
48.02
9.23
18.91
8.92
28.47
30.00
28.33
f1 (ppm)

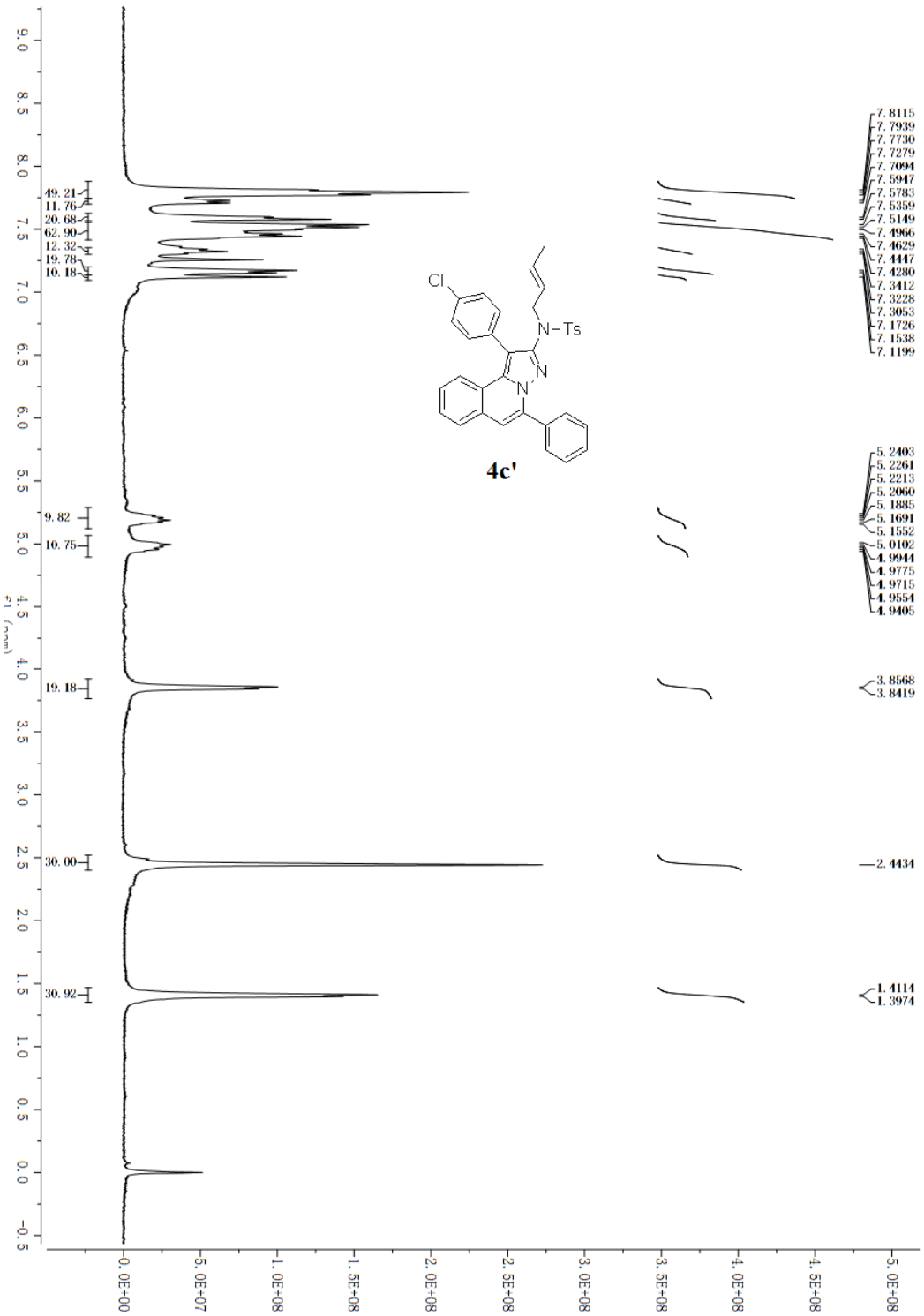

O
N-Ts
N
N
4b
159.305
142.823
138.427
137.841
133.615
129.765
129.485
129.432
129.371
128.999
128.890
128.861
127.892
127.342
127.154
124.458
123.259
116.316
115.079
114.031
113.320
64.2094
57.4795
55.3347
21.6303
18.1881
13.0685

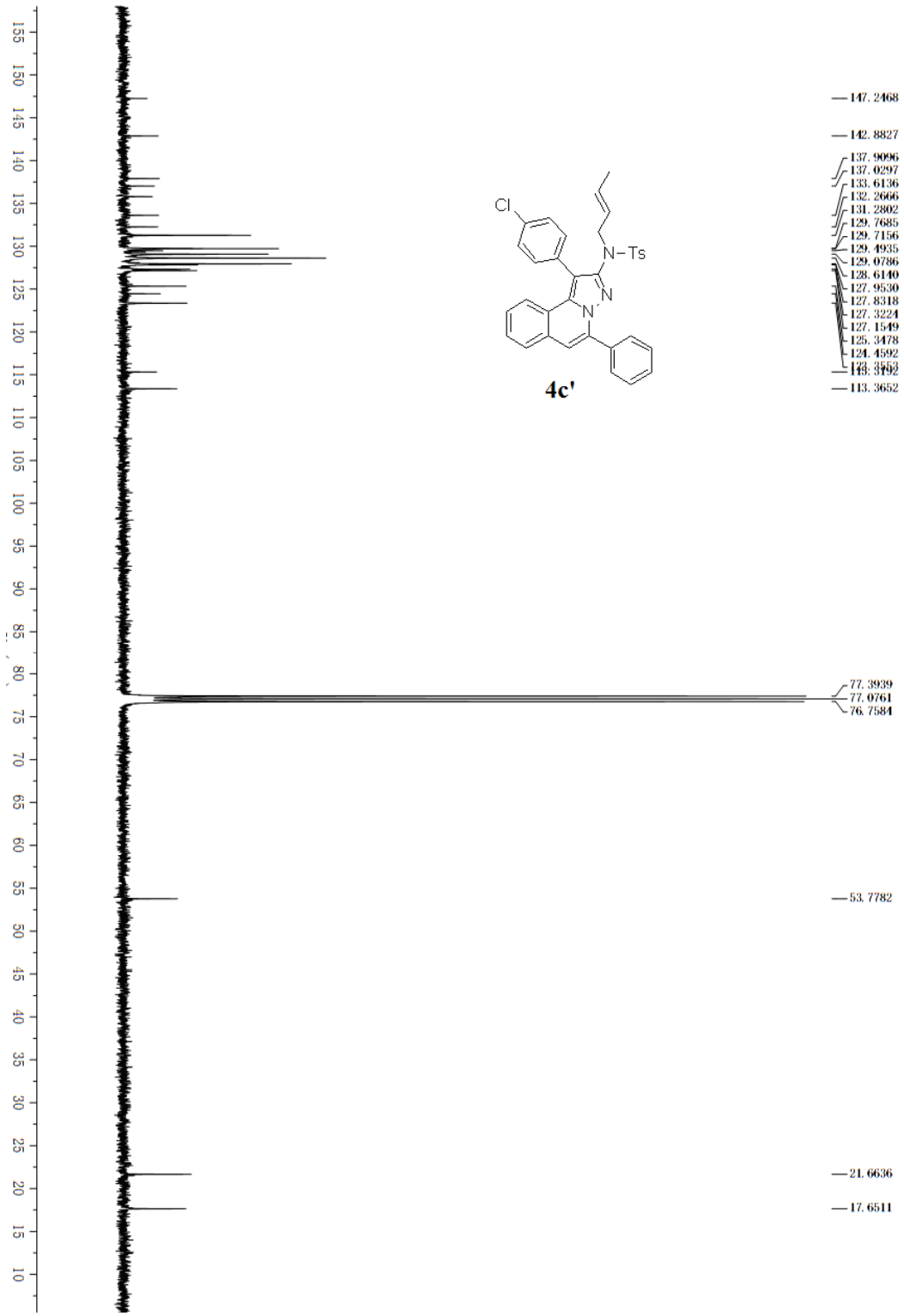

4b'
N-Ts
N
N
O
7.8445
7.8258
7.8095
7.7919
7.7019
7.6825
7.5581
7.5379
7.5026
7.4835
7.4637
7.4460
7.3091
7.2913
7.2711
7.2542
7.1639
7.1442
7.0966
7.0863
5.2436
5.2240
5.2076
5.1884
5.1715
5.1542
5.0395
5.0208
5.0028
4.9907
4.9651
4.9448
3.9351
3.8603
3.8443
2.4354
1.4103
1.3956
42.99
11.35
21.75
43.16
22.71
21.16
31.42
9.47
11.07
30.00
19.26
33.42
32.46
f1 (ppm)

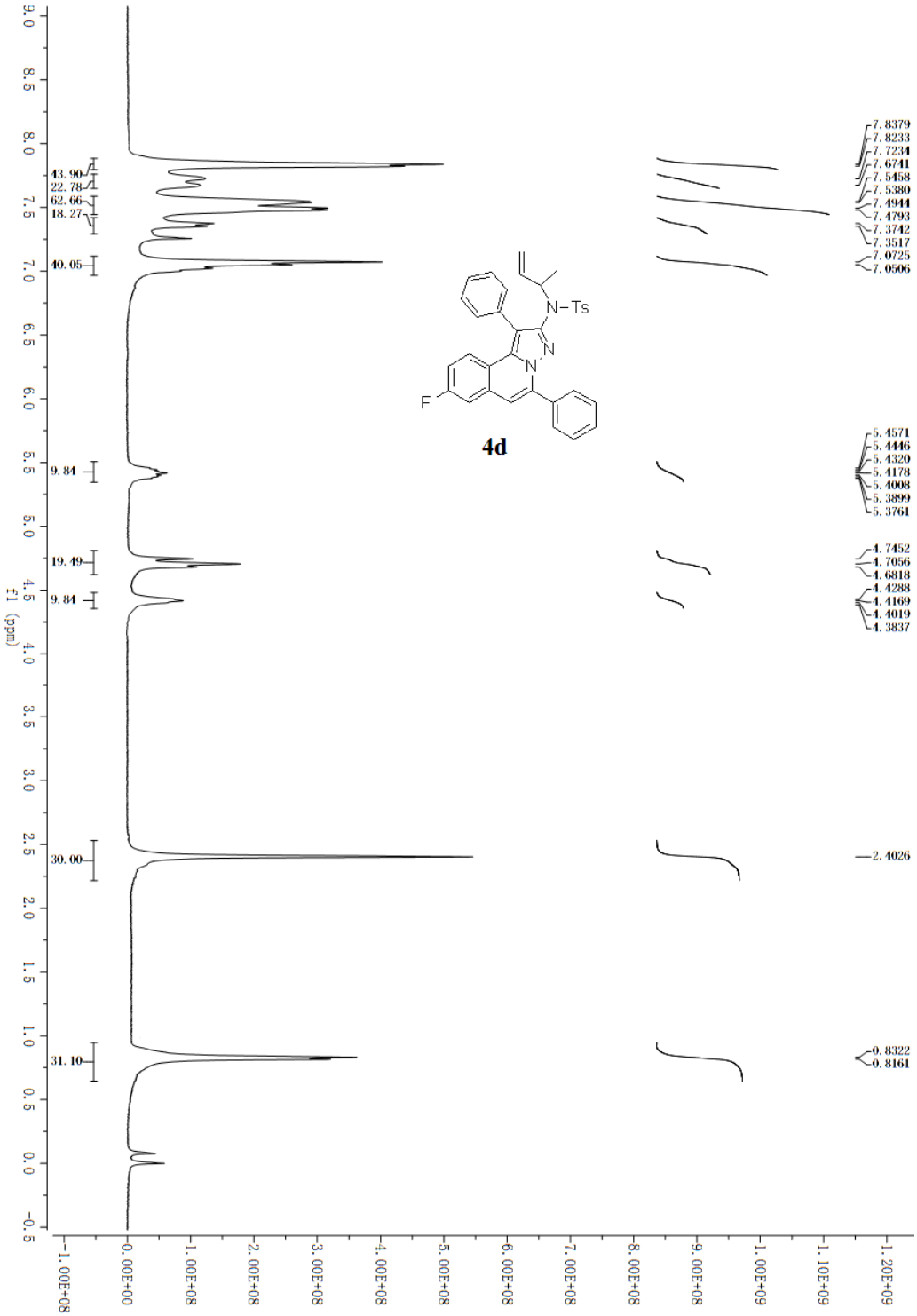

N-Ts
N
N
O
4b'
159.2768
147.3906
142.8434
137.9085
132.3695
129.7006
129.4544
129.0642
129.0244
128.5801
127.9338
127.8501
127.2834
127.1286
125.4209
124.5892
124.3013
123.3128
114.0905
113.2562
77.3939
77.0759
76.7581
55.3314
53.7256
21.6500
17.6413
f1 (ppm)

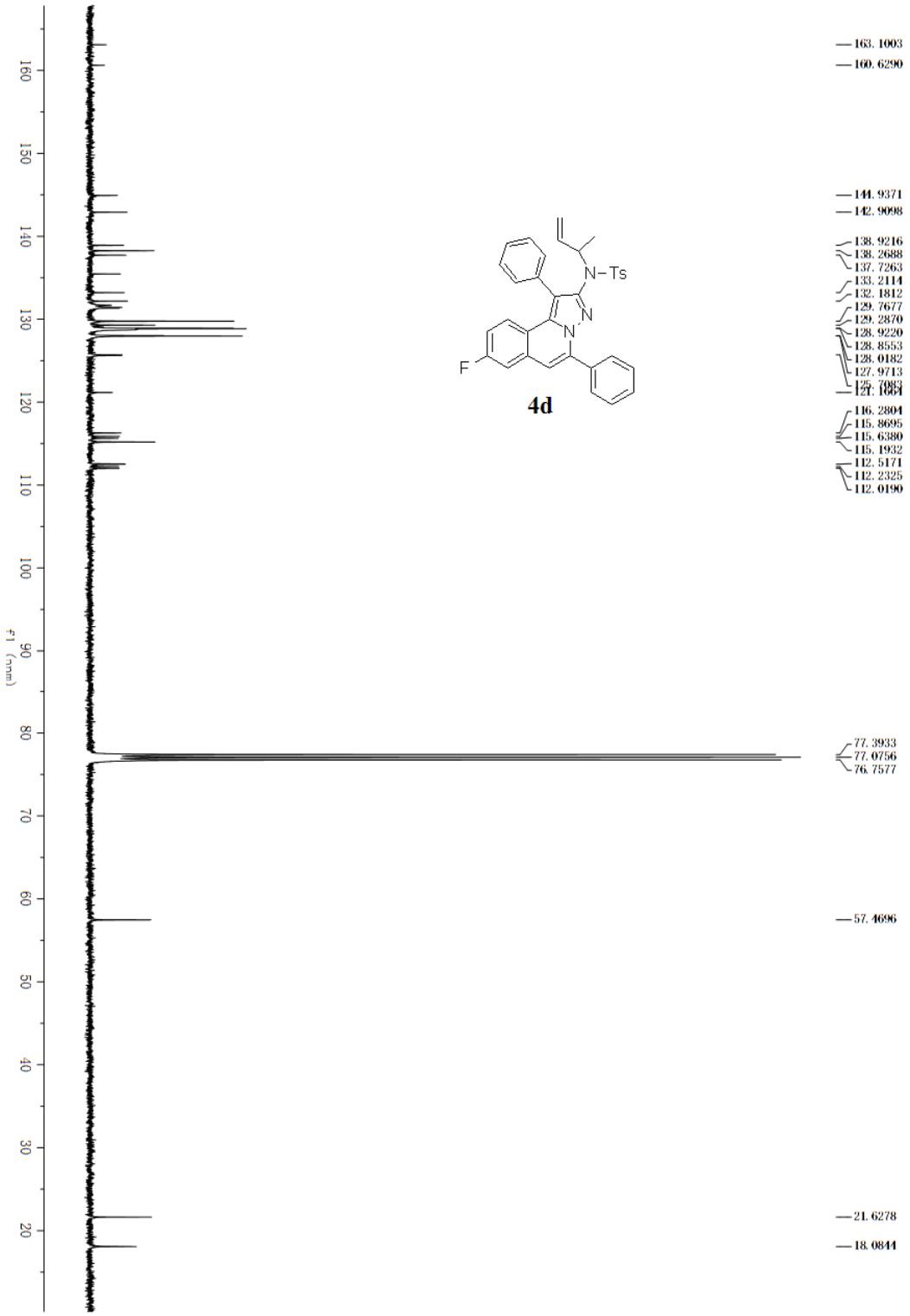

7.8305
7.8142
7.7267
7.7079
7.6774
7.6675
7.5322
7.5138
7.4881
7.4693
7.3341
7.3185
7.1466
7.0747
7.0577
5.4750
5.4486
5.4341
5.4234
5.3943
5.3728
4.7593
4.7189
4.6961
4.4635
4.4516
4.4070
2.4025
0.8422
0.8296
40.50
30.42
57.97
19.51
10.12
19.66
10.67
18.42
9.04
30.00
33.93
Cl
N-Ts
N
N
4c
f1 (ppm)

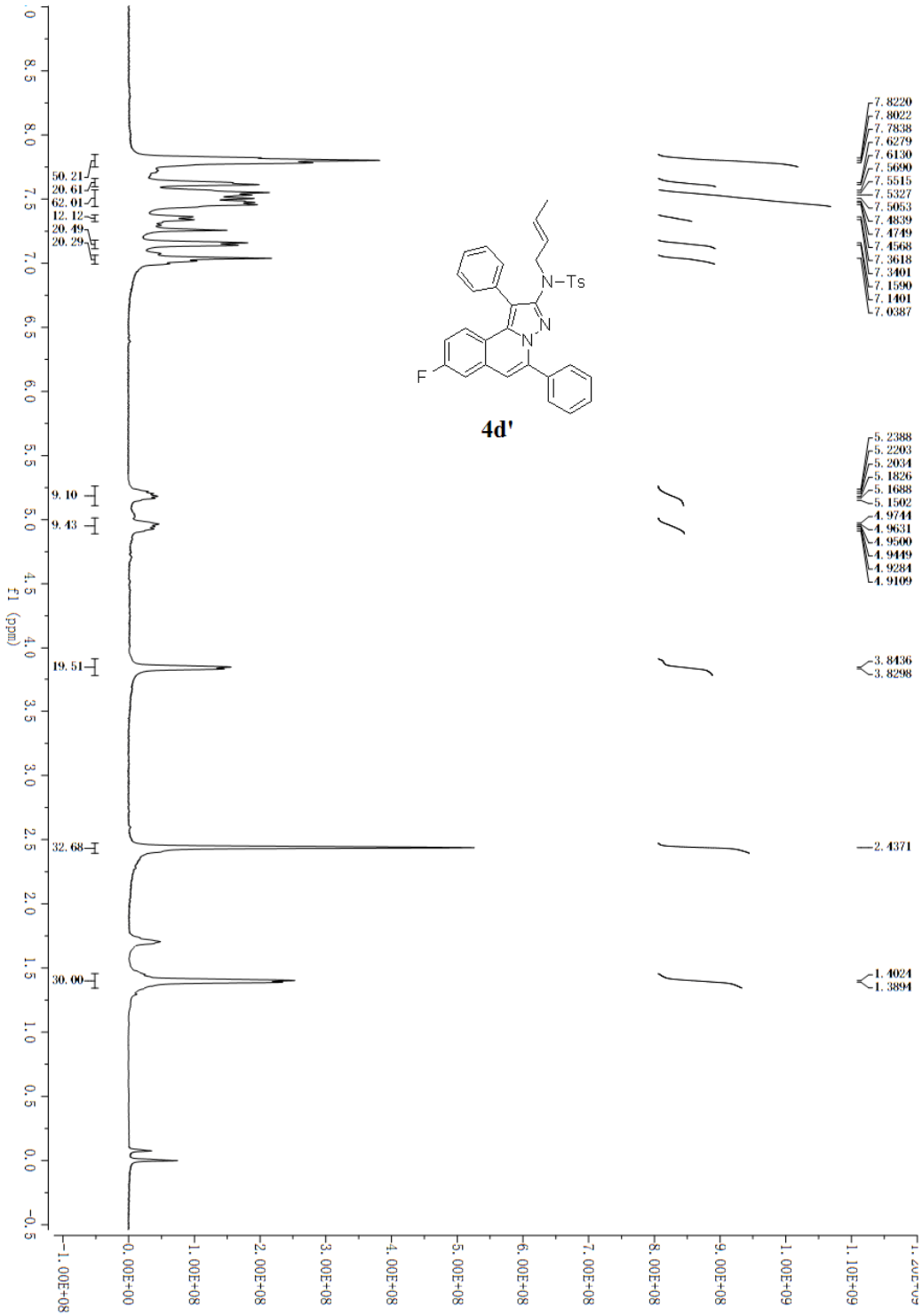

Cl
N-Ts
N
N
4c
144.5459
142.9937
138.1903
131.0042
129.7546
129.5323
129.0995
128.9325
128.8392
128.1510
127.9275
127.5126
127.2941
124.2712
123.1210
115.3447
113.5554
77.4000
77.0822
76.7645
57.4858
21.6426
18.0837
f1 (ppm)

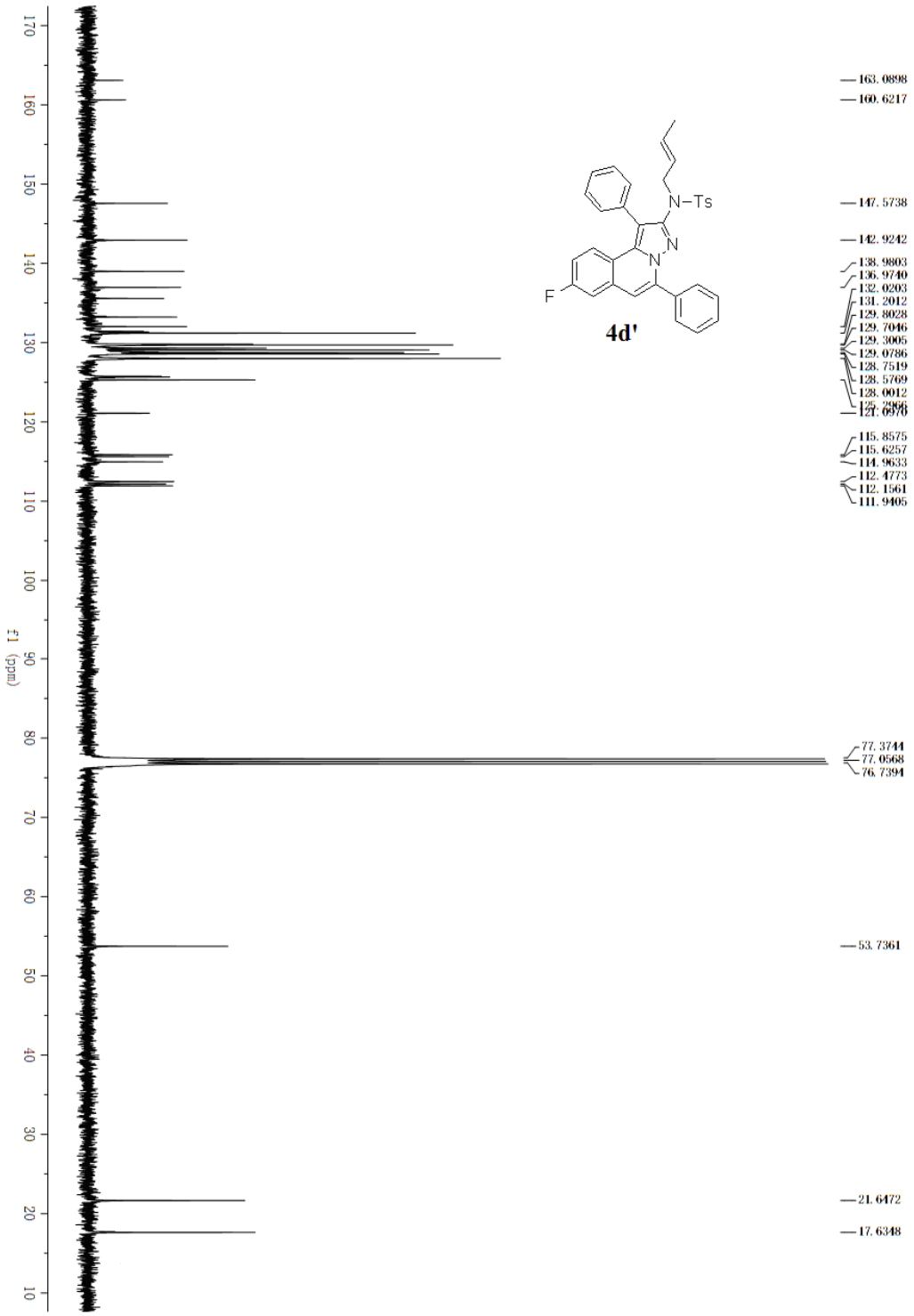

Cl
N-Ts
N
N
4c'
7.8115
7.7939
7.7730
7.7279
7.7094
7.5947
7.5783
7.5359
7.5149
7.4966
7.4629
7.4447
7.4280
7.3412
7.3228
7.3053
7.1726
7.1538
7.1199
5.2403
5.2261
5.2213
5.2060
5.1885
5.1691
5.1552
5.0102
4.9944
4.9775
4.9715
4.9554
4.9405
3.8568
3.8419
2.4434
1.4114
1.3974
49.21
11.76
20.68
62.90
12.32
19.78
10.18
9.82
10.75
19.18
30.00
30.92
f1 (ppm)

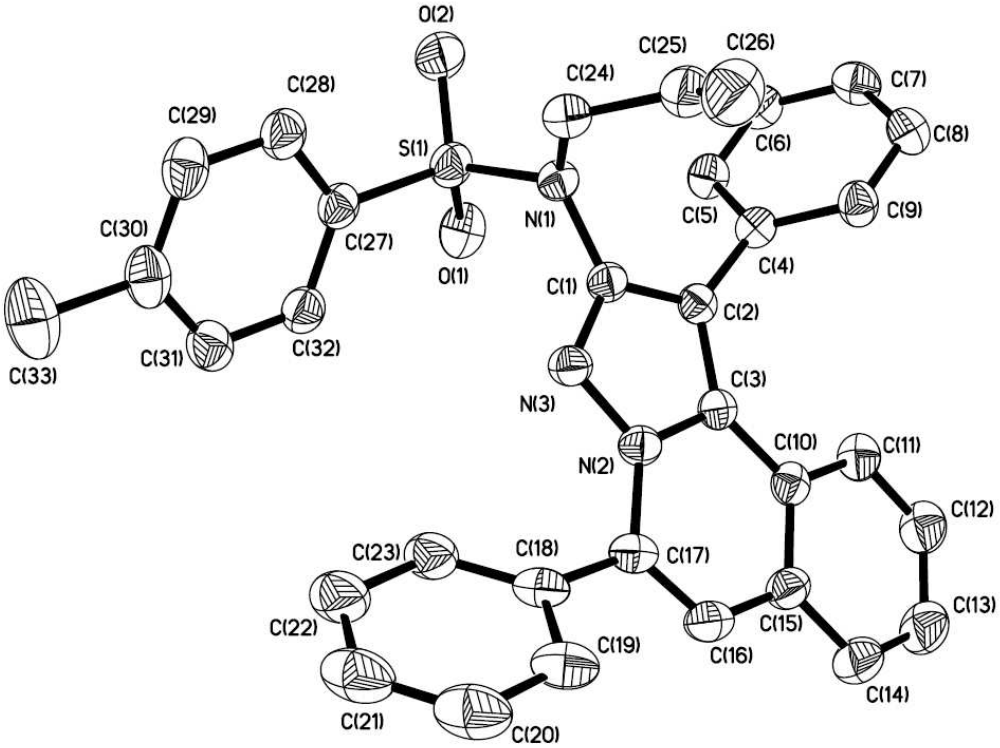

147.2468
142.8827
137.9096
137.0297
133.6136
132.2666
131.2802
129.7685
129.7156
129.4935
129.0786
128.6140
127.9530
127.8318
127.3224
127.1549
125.3478
124.4592
123.3553
113.3652
77.3939
77.0761
76.7584
53.7782
21.6636
17.6511
Cl
N-Ts
N
N
4c'

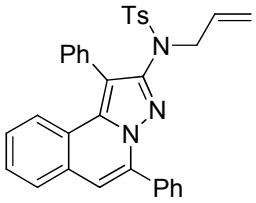

7.8379
7.8233
7.7234
7.6741
7.5458
7.5380
7.4944
7.4793
7.3742
7.3517
7.0725
7.0506
5.4571
5.4446
5.4320
5.4178
5.4008
5.3899
5.3761
4.7452
4.7056
4.6818
4.4288
4.4169
4.4019
4.3837
2.4026
0.8322
0.8161
43.90
22.78
62.66
18.27
40.05
9.84
19.49
9.84
30.00
31.10
N-Ts
N
N
F
4d
f1 (ppm)


163.1003
160.6290
144.9371
142.9098
138.9216
138.2688
137.7263
133.2114
132.1812
129.7677
129.2870
128.9220
128.8553
128.0182
127.9713
125.7083
121.1664
116.2804
115.8695
115.6380
115.1932
112.5171
112.2325
112.0190
77.3933
77.0756
76.7577
57.4696
21.6278
18.0844
N-Ts
N
N
F
4d
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20

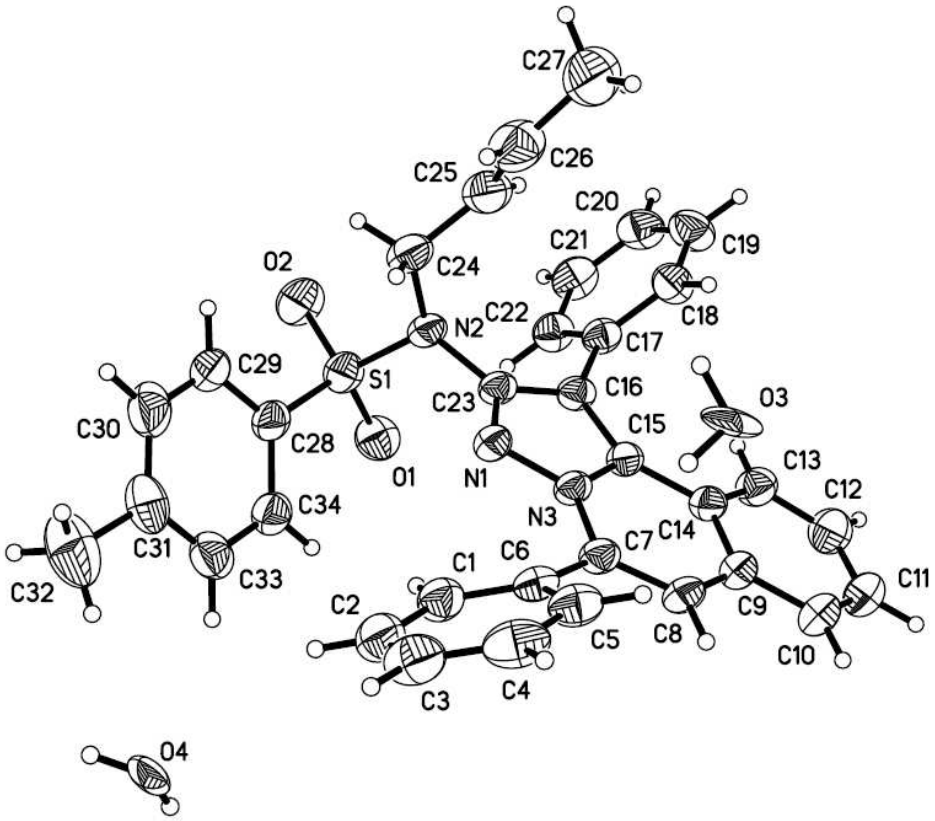

7.8220
7.8022
7.7838
7.6279
7.6130
7.5690
7.5515
7.5327
7.5053
7.4839
7.4749
7.4568
7.3618
7.3401
7.1590
7.1401
7.0387
5.2388
5.2203
5.2034
5.1826
5.1688
5.1502
4.9744
4.9631
4.9500
4.9449
4.9284
4.9109
3.8436
3.8298
2.4371
1.4024
1.3894
50.21
20.61
62.01
12.12
20.49
20.29
9.10
9.43
19.51
32.68
30.00
N-Ts
N
N
F
4d'
f1 (ppm)

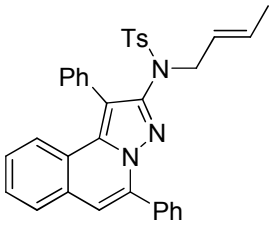

N-Ts
N
N
F
4d'
163.0898
160.6217
147.5738
142.9242
138.9803
136.9740
132.0203
131.2012
129.8028
129.7046
129.3005
129.0786
128.7519
128.5769
128.0012
125.2966
121.0970
115.8575
115.6257
114.9633
112.4773
112.1561
111.9405
77.3744
77.0568
76.7394
53.7361
21.6472
17.6348
f1 (ppm)


O(2)
C(25)
C(26)
C(24)
C(7)
C(28)
C(29)
S(1)
C(6)
C(8)
N(1)
C(5)
C(9)
C(30)
C(27)
O(1)
C(4)
C(1)
C(2)
C(33)
C(31)
C(32)
N(3)
C(3)
N(2)
C(10)
C(11)
C(12)
C(23)
C(18)
C(17)
C(13)
C(22)
C(15)
C(19)
C(16)
C(14)
C(21)
C(20)

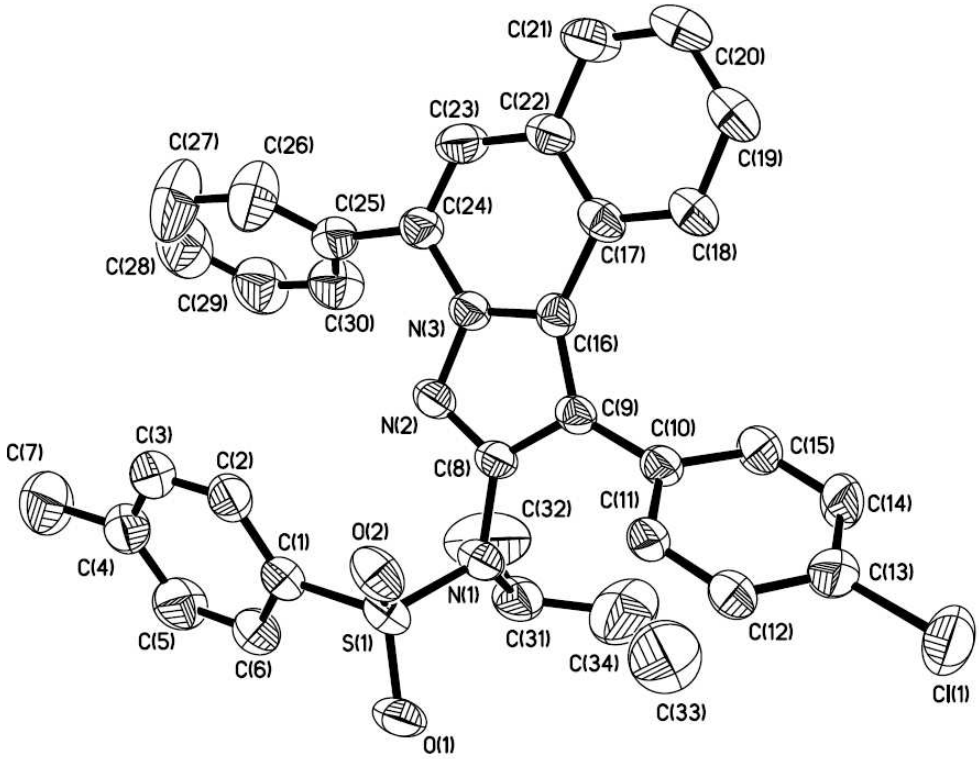

Ts
N
Ph
N
N
Ph

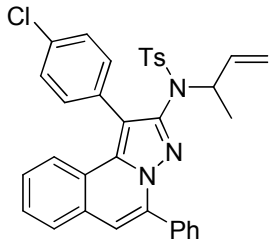
3a


C27
C26
C25
C20
C21
C19
C24
O2
C22
C18
N2
C17
C29
S1
C23
C16
O3
C30
C28
C15
O1
N1
C13
C12
C34
N3
C14
C31
C7
C6
C1
C11
C32
C33
C2
C9
C5
C8
C10
C3
C4
O4


Ts
N
Ph
N
N
Ph

4a'


C(21)
C(20)
C(23)
C(22)
C(19)
C(27)
C(26)
C(25)
C(24)
C(17)
C(18)
C(28)
C(29)
C(30)
N(3)
C(16)
N(2)
C(9)
C(10)
C(15)
C(7)
C(3)
C(2)
C(8)
C(11)
C(14)
C(32)
C(1)
O(2)
C(4)
N(1)
C(13)
C(5)
S(1)
C(31)
C(12)
C(6)
C(34)
Cl(1)
C(33)
O(1)


Cl
Ts
N
N
N
Ph

4c