Tandem Addition-Cyclization Reactions of 2-Alkynylbenzenamines with Isocyanates Catalyzed by $PdCl_2$

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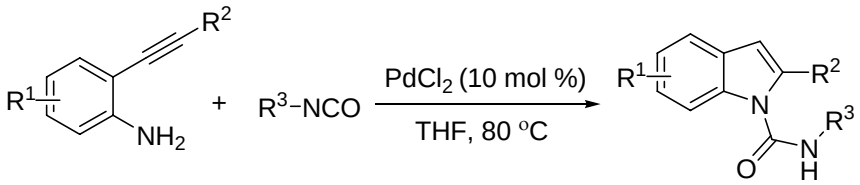
Supporting Information

Experimental Section

All reactions were performed in test 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.

*General procedure for reaction of 2-alkynylbenzenamine **1** with isocyanate **2** catalyzed by palladium chloride:* A solution of 2-alkynylbenzenamine **1** (0.50 mmol) and isocyanate **2** (0.75 mmol, 1.5 equiv) in THF (2.0 mL) was stirred at 80 °C for 3 h. Then $PdCl_2$ (10 mol %) was added to the mixture. After completion of reaction as indicated by TLC, the solvent was evaporated and the residue was quenched with water (10 mL), extracted with EtOAc (2 × 10 mL), dried by anhydrate Na_2SO_4. Evaporation of the solvent followed by purification on silica gel provided the corresponding product **3**.



1 **2** **3**

*N,2-Diphenyl-1H-indole-1-carboxamide **3a***

Yield: 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.69 (s, 1H), 6.72 (br, 1H), 7.04 - 7.08 (m, 3H), 7.20 - 7.27 (m, 3H), 7.33 (dt, *J* = 1.5, 7.82 Hz, 1H), 7.42 - 7.47 (m, 3H), 7.54 - 7.56 (m, 2H), 7.59 (d, *J* = 7.8 Hz, 1H), 8.20 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 109.1, 114.3, 119.6, 120.6, 122.7,124.4, 124.6, 128.6, 128.8, 128.9, 129.1, 132.0, 136.7, 137.6, 137.9, 149.4; MS (ESI) *m/z* 313 (M^++H); HRMS calcd for $C_{21}H_{16}N_2O$ (M^++H): 313.1341; Found: 313.1372.

*2-(4-Methoxyphenyl)-N-phenyl-1H-indole-1-carboxamide **3b**:* Yield: 53%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.85 (s, 3H), 6.64 (s, 1H), 6.82 (br, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 7.06 - 7.13 (m, 3H), 7.23 - 7.27 (m, 3H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.50 (d, *J* = 8.8 Hz, 2H), 7.58 (d, *J* = 7.8 Hz, 1H), 8.23 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 108.6, 114.5, 114.6, 119.7, 120.4,

122.7, 124.2, 124.3, 124.6, 128.7, 129.0, 130.3, 136.8, 137.4, 137.8, 149.5, 160.2; MS (ESI) *m/z* 343 (M^++H); HRMS calcd for $C_{22}H_{18}N_2O_2$ (M^++H): 343.1447; Found: 343.1470.

N,2-Diphenyl-5-(trifluoromethyl)-1H-indole-1-carboxamide ***3c***: Yield: 46%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.75 (br, 1H), 6.77 (s, 1H), 7.04 - 7.12 (m, 3H), 7.23 - 7.27 (m, 2H), 7.49 - 7.51 (m, 3H), 7.56 - 7.59 (m, 3H), 7.89 (s, 1H), 8.30 (d, J = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 108.9, 114.9, 118.1 (q, $^3J_{CF}$ = 3.8 Hz), 119.7, 121.1 (q, $^3J_{CF}$ = 3.8 Hz), 124.8 (q, $^1J_{CF}$ = 270.8 Hz), 124.9, 125.0 (q, $^2J_{CF}$ = 31.5 Hz), 128.2, 129.0, 129.1, 129.3, 129.5, 131.3, 136.4, 139.3, 148.9; MS (ESI) *m/z* 381 (M^++H); HRMS calcd for $C_{22}H_{15}F_3N_2O$ (M^++H): 381.1215; Found: 381.1251.

5-Methyl-N,2-diphenyl-1H-indole-1-carboxamide ***3d:*** Yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.45 (s, 3H), 6.62 (s, 1H), 6.70 (br, 1H), 7.04 - 7.06 (m, 3H), 7.15 (d, J = 8.3 Hz, 1H), 7.22 (t, J = 7.8 Hz, 2H), 7.37 (s, 1H), 7.42 - 7.48 (m, 3H), 7.54 - 7.56 (m, 2H), 8.10 (d, J = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 109.1, 114.2, 119.6, 120.4, 124.5, 126.0, 128.9, 129.0, 129.1, 132.1, 132.2, 136.2, 136.8, 137.6, 149.5; MS (ESI) *m/z* 327 (M^++H); HRMS calcd for $C_{22}H_{18}N_2O$ (M^++H): 327.1497; Found: 327.1527.

2-Cyclopropyl-N-phenyl-1H-indole-1-carboxamide ***3e*****:** Yield: 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.71 - 1.75 (m, 2H), 1.87 - 1.91 (m, 2H), 2.90 - 3.00 (m, 1H), 7.03 (s, 1H), 7.89 - 7.93 (m, 2H), 7.96 - 8.00 (m, 1H), 8.13 (t, J = 8.3 Hz, 2H), 8.20 (d, J = 8.3 Hz, 1H), 8.32 (d, J = 8.3 Hz, 2H), 8.83 (d, J = 8.3 Hz, 1H), 9.05 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 8.2, 10.3, 105.4, 114.1, 119.6, 120.1, 122.3, 123.6, 124.5, 128.4, 129.2, 137.0, 137.3, 140.0, 149.8; MS (ESI) *m/z* 277 (M^++H); HRMS calcd for $C_{18}H_{16}N_2O$ (M^++H): 277.1341; Found: 277.1358.

N-(4-Fluorophenyl)-2-phenyl-1H-indole-1-carboxamide **3f**: Yield: 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.69 (br, 1H), 6.70 (s, 1H), 6.91 (t, J = 8.7 Hz, 2H), 6.98 - 7.02 (m, 2H), 7.24 - 7.28 (m, 1H), 7.34 (dt, J = 1.5, 8.3 Hz, 1H), 7.44 - 7.49 (m, 3H), 7.54 - 7.57 (m, 2H), 7.59 (d, J = 7.8 Hz, 1H), 8.19 (d, J = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 109.3, 114.4, 115.6 (d, $^2J_{CF}$ = 22.9 Hz), 120.6, 121.4 (d, $^3J_{CF}$ = 7.6 Hz), 122.8, 124.6, 128.6, 128.9, 129.0, 129.1, 132.0, 132.7 (d, $^4J_{CF}$ = 2.8 Hz), 137.5, 137.9, 149.5, 159.6 (d, $^1J_{CF}$ = 243.1 Hz); MS (ESI) *m/z* 331 (M^++H); HRMS calcd for $C_{21}H_{15}FN_2O$ (M^++H): 331.1247; Found: 331.1271.

N-(4-Fluorophenyl)-2-(4-methoxyphenyl)-1H-indole-1-carboxamide **3g**: Yield: 65%; ^{1}H NMR(400 MHz,$CDCl_3$) δ 3.86 (s, 3H), 6.64 (s, 1H), 6.81 (br, 1H), 6.94 (t, J = 8.3 Hz, 2H), 7.00 (d, J = 8.8 Hz, 2H), 7.05 - 7.09 (m, 2H), 7.25 (dt, J = 1.5, 8.3 Hz, 1H), 7.33 (dt, J = 1.5, 8.3

Hz, 1H), 7.49 (d, *J* = 8.8 Hz, 2H), 7.58 (d, *J* = 7.8 Hz, 1H), 8.21 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 108.7, 114.4, 114.6, 115.6 (d, $^2J_{CF}$ = 22.9 Hz), 120.4, 121.5 (d, $^3J_{CF}$ = 8.6 Hz), 122.7, 124.1, 124.3, 128.7, 130.3, 132.8, 137.3, 137.8, 149.7, 159.6 (d, $^1J_{CF}$ = 242.1 Hz), 160.2; MS (ESI) *m/z* 383 (M^++Na); HRMS calcd for $C_{22}H_{17}FN_2O_2$ (M^++Na): 383.1172; Found: 383.1200.

N-(4-Fluorophenyl)-2-phenyl-5-(trifluoromethyl)-1H-indole-1-carboxamide **3h**: Yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.70(br,1H), 6.77(s,1H), 6.91-7.00(m,4H), 7.50-7.52(m,3H), 7.56-7.58(m,3H), 7.89(s,1H), 8.28(d,J=8.8Hz,1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 109.0, 114.8, 115.8 (d, $^2J_{CF}$ = 22.9 Hz), 118.1 (q, $^3J_{CF}$ = 3.8 Hz), 121.1 (q, $^3J_{CF}$ = 3.1 Hz), 121.6 (d, $^3J_{CF}$ = 7.6 Hz), 124.7 (q, $^1J_{CF}$ = 270.2 Hz), 125.2 (q, $^2J_{CF}$ = 32.1 Hz), 128.1, 129.1, 129.4, 129.6, 131.3, 132.3, 139.1, 139.2, 149.0, 159.8 (d, $^1J_{CF}$ = 243.4 Hz); MS (ESI) *m/z* 399 (M^++H); HRMS calcd for $C_{22}H_{14}F_4N_2O$ (M^++H): 399.1121; Found: 399.1150.

N-(4-Fluorophenyl)-5-methyl-2-phenyl-1H-indole-1-carboxamide **3i**: Yield: 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.45 (s, 3H), 6.62 (s, 1H), 6.68 (br, 1H), 6.90 (t, *J* = 8.8 Hz, 2H), 6.98 - 7.01 (m, 2H), 7.15 (d, *J* = 8.3 Hz, 1H), 7.37 (s, 1H), 7.42 - 7.48 (m, 3H), 7.52 - 7.55 (m, 2H), 8.07 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 109.3, 114.2, 115.7 (d, $^2J_{CF}$ = 21.9 Hz), 120.5, 121.6 (d, $^3J_{CF}$ = 7.6 Hz), 126.2, 129.0, 129.2, 132.3, 132.4, 132.9 (d, $^4J_{CF}$ = 2.8 Hz), 136.3, 137.6, 149.8, 159.7 (d, $^1J_{CF}$ = 243.1 Hz); MS (ESI) *m/z* 345 (M^++H); HRMS calcd for $C_{22}H_{17}FN_2O$ (M^++H): 345.1403; Found: 345.1432.

2-Cyclopropyl-N-(4-fluorophenyl)-1H-indole-1-carboxamide **3j**: Yield: 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.97 - 1.01 (m, 2H), 1.12 - 1.17 (m, 2H), 2.15 - 2.24 (m, 1H), 6.30 (s, 1H), 7.08 (t, *J* = 7.3 Hz, 2H), 7.18 (dt, *J* = 1.3, 7.8 Hz, 1H), 7.25 (dt, *J* = 1.5, 8.6 Hz, 1H), 7.47 (d, *J* = 7.3 Hz, 1H), 7.52 - 7.55 (m, 2H), 8.08 (d, *J* = 8.3 Hz, 1H), 8.33 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 8.2, 10.4, 105.7, 114.4, 115.9 (d, $^2J_{CF}$ = 21.9 Hz), 120.1, 121.4 (d, $^3J_{CF}$ = 8.6 Hz), 122.4, 123.7, 128.4, 133.3 (d, $^4J_{CF}$ = 2.8 Hz), 137.0, 139.9, 150.0, 159.5 (d, $^1J_{CF}$ = 242.1 Hz); MS (ESI) *m/z* 317 (M^++Na); HRMS calcd for $C_{18}H_{15}FN_2O$ (M^++Na): 317.1066; Found: 317.1092.

N-(4-Methoxyphenyl)-2-phenyl-1H-indole-1-carboxamide **3k**: Yield: 86%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.73 (s, 1H), 6.61 (br, 1H), 6.69 (s, 1H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 8.3 Hz, 2H), 7.24 (t, *J* = 7.3 Hz, 1H), 7.32 (dt, *J* = 1.5, 8.3 Hz, 1H), 7.42 - 7.47 (m, 3H), 7.54 - 7.60 (m, 3H), 8.18 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 108.8, 114.1, 114.2, 120.6,

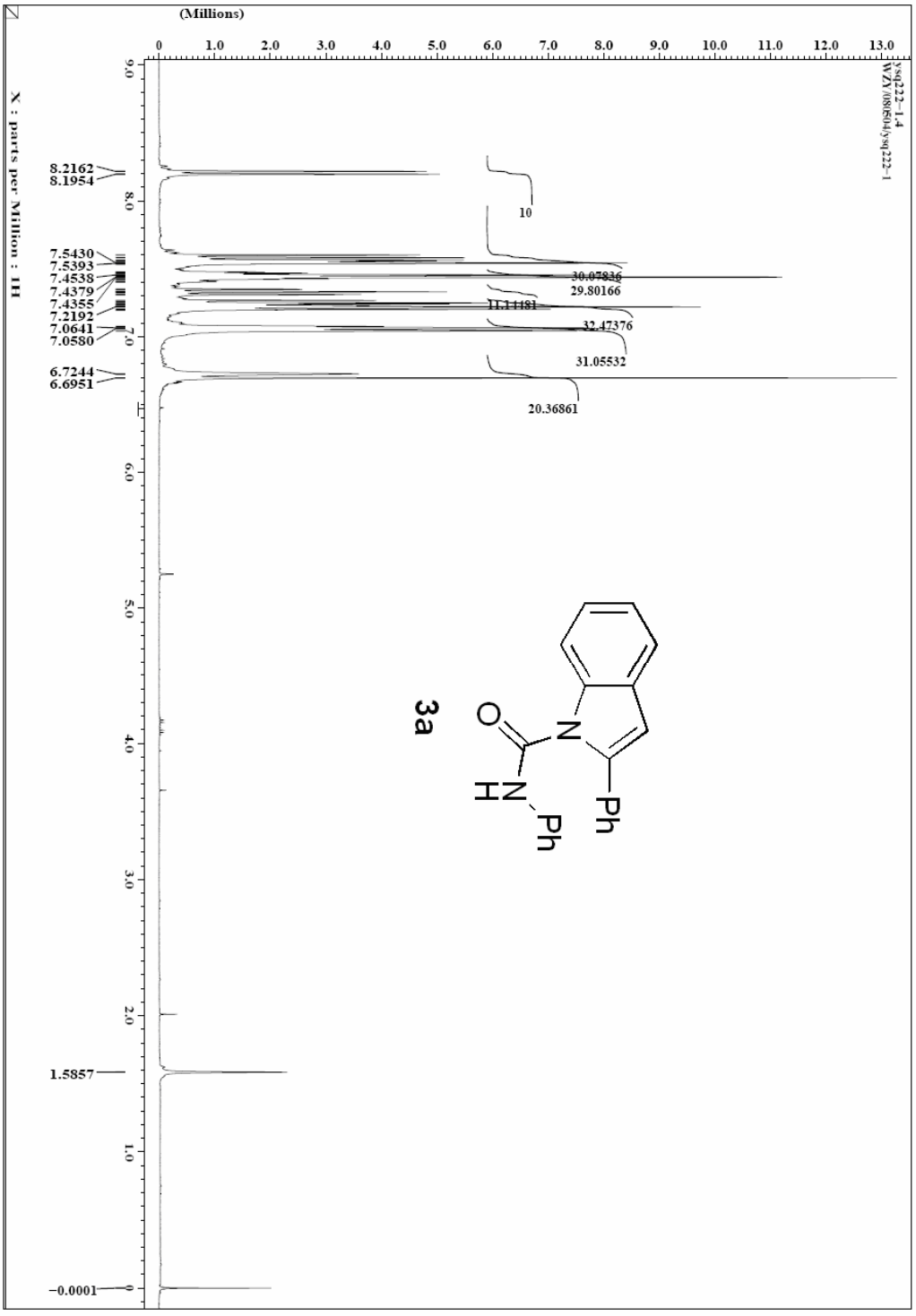
121.7, 122.6, 124.4, 128.6, 128.8, 129.0, 129.7, 132.0, 137.6, 137.9, 149.6, 156.7; MS (ESI) *m/z* 343 (M^++H); HRMS calcd for $C_{22}H_{18}N_2O_2$ (M^++H): 343.1477; Found: 343.1487.

N,2-Bis(4-methoxyphenyl)-1H-indole-1-carboxamide **3l**: Yield: 73%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.75 (s, 3H), 3.85 (s, 3H), 6.62 (s, 1H), 6.70 (br, 1H), 6.78 (d, *J* = 8.8 Hz, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 7.03 (d, *J* = 8.3 Hz, 2H), 7.24 (d, *J* = 7.3 Hz, 1H), 7.31 (dt, *J* = 1.0, 8.3 Hz, 1H), 7.49 (d, *J* = 8.3 Hz, 2H), 7.57 (d, *J* = 7.8 Hz, 1H), 8.20 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 108.3, 114.1, 114.4, 114.5, 120.3, 121.7, 122.6, 124.1, 124.2, 128.7, 129.8, 130.2, 137.5, 137.8, 149.8, 156.7, 160.1; MS (ESI) *m/z* 373 (M^++H); HRMS calcd for $C_{23}H_{20}N_2O_3$ (M^++H): 373.1552; Found: 373.1579.

N-(4-Methoxyphenyl)-2-phenyl-5-(trifluoromethyl)-1H-indole-1-carboxamide **3m**: Yield: 43%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 6.62 (br, 1H), 6.76 - 6.79 (m, 3H), 6.98 (d, *J* = 7.3 Hz, 2H), 7.49 - 7.51 (m, 3H), 7.55 - 7.58 (m, 3H), 7.89 (s, 1H), 7.28 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.5, 108.8, 114.3, 114.8, 118.2 (q, $^3J_{CF}$ = 4.7 Hz), 121.1 (q, $^3J_{CF}$ = 2.9 Hz), 121.9, 124.9 (q, $^1J_{CF}$ = 269.8 Hz), 125.1 (q, $^2J_{CF}$ = 31.5 Hz), 128.2, 129.1, 129.5, 129.7, 131.5, 139.3, 139.4, 149.3, 157.1; MS (ESI) *m/z* 433 (M^++Na); HRMS calcd for $C_{23}H_{17}F_3N_2O_2$ (M^++Na): 433.1140; Found: 433.1173.

N-(4-Methoxyphenyl)-5-methyl-2-phenyl-1H-indole-1-carboxamide **3n**: Yield: 83%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.44 (s, 3H), 3.73 (s, 3H), 6.60 (br, 1H), 6.61 (s, 1H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 7.14 (d, *J* = 8.1 Hz, 1H), 7.36 (s, 1H), 7.41 - 7.46 (m, 3H), 7.51 - 7.55 (m, 2H), 8.06 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 55.4, 108.8, 114.0, 114.1, 120.3, 121.6, 125.9, 128.7, 128.8, 129.0, 129.8, 132.0, 132.2, 136.2, 137.6, 149.7, 156.6; MS (ESI) *m/z* 357 (M^++H); HRMS calcd for $C_{23}H_{20}N_2O_2$ (M^++H): 357.1603; Found: 357.1629.

2-Cyclopropyl-N-(4-methoxyphenyl)-1H-indole-1-carboxamide **3o**: Yield: 88%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.94 - 0.98 (m, 2H), 1.10 - 1.05 (m, 2H), 2.16 - 2.24 (m, 1H), 3.80 (s, 3H), 6.27 (s, 1H), 6.91 (d, *J* = 9.3 Hz, 2H), 7.16 (t, *J* = 7.3 Hz, 1H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.46 (t, *J* = 8.8 Hz, 3H), 8.07 (d, J = 8.3, 1H), 8.17 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 8.2, 10.3, 55.5, 105.2, 114.0, 114.4, 120.0, 121.6, 122.2, 123.5, 128.4, 130.3, 137.0, 140.1, 150.1, 156.7; MS (ESI) *m/z* 307 (M^++H); HRMS calcd for $C_{19}H_{18}N_2O_2$ (M^++H): 307.1447; Found: 307.1473.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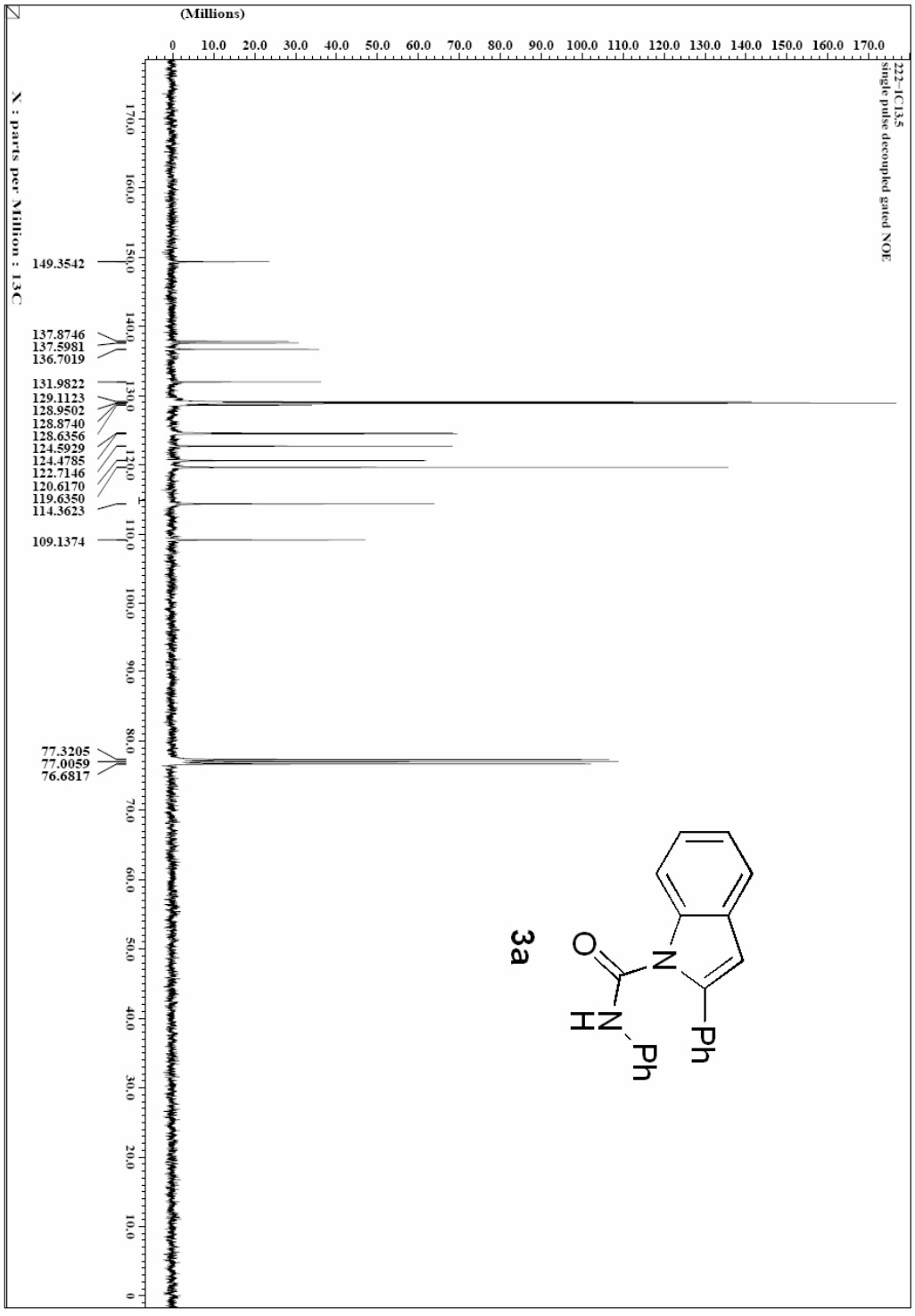
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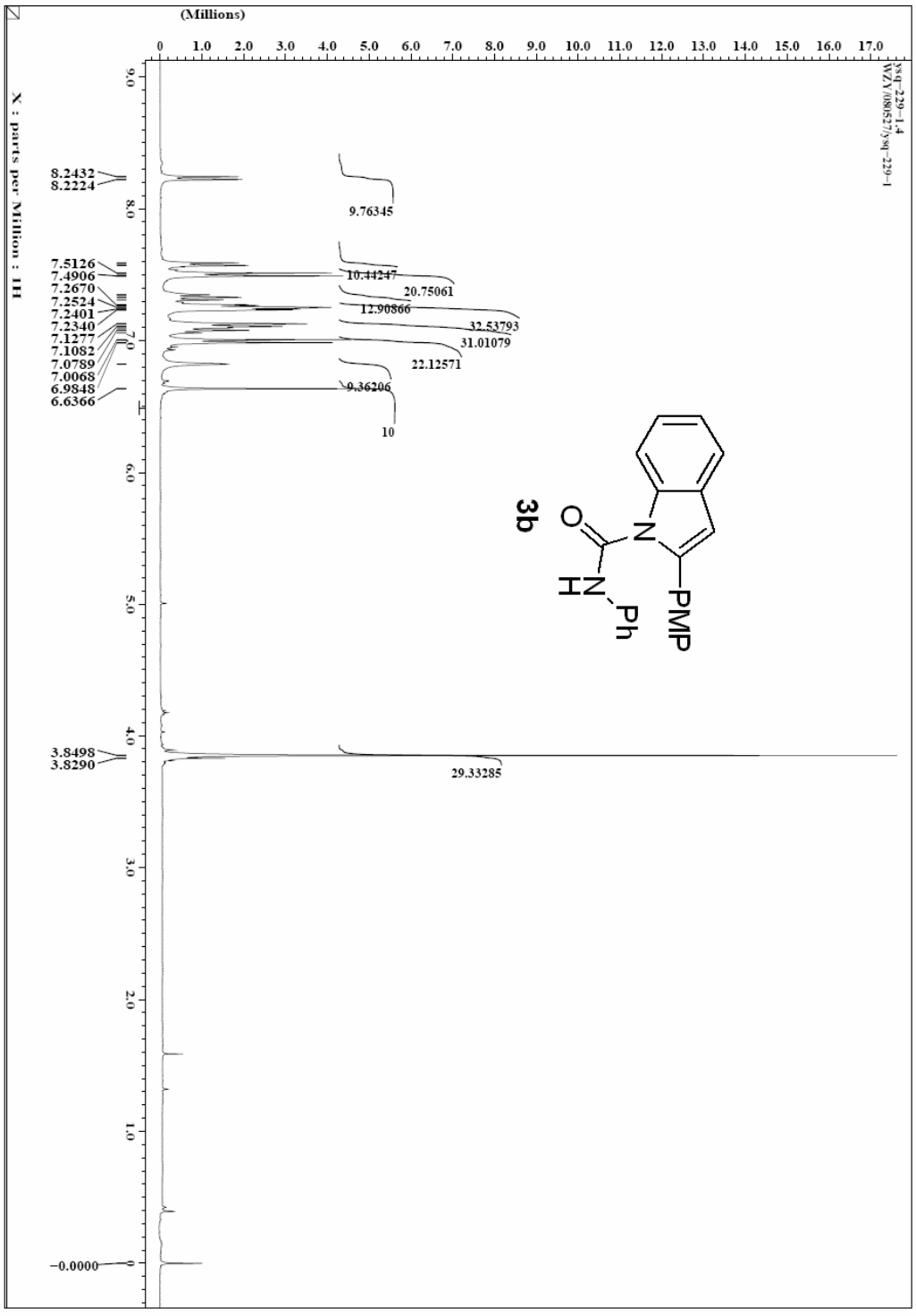
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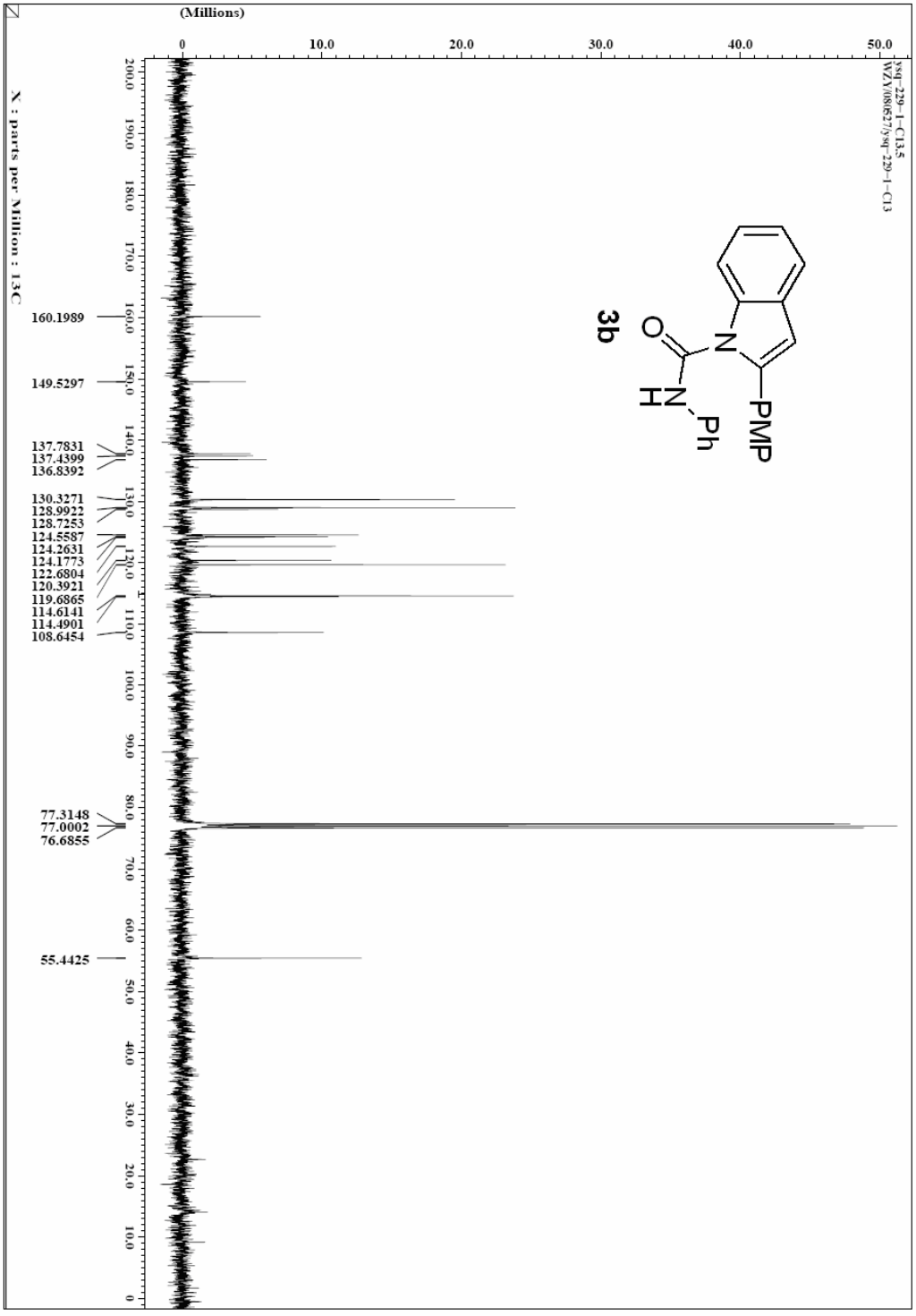
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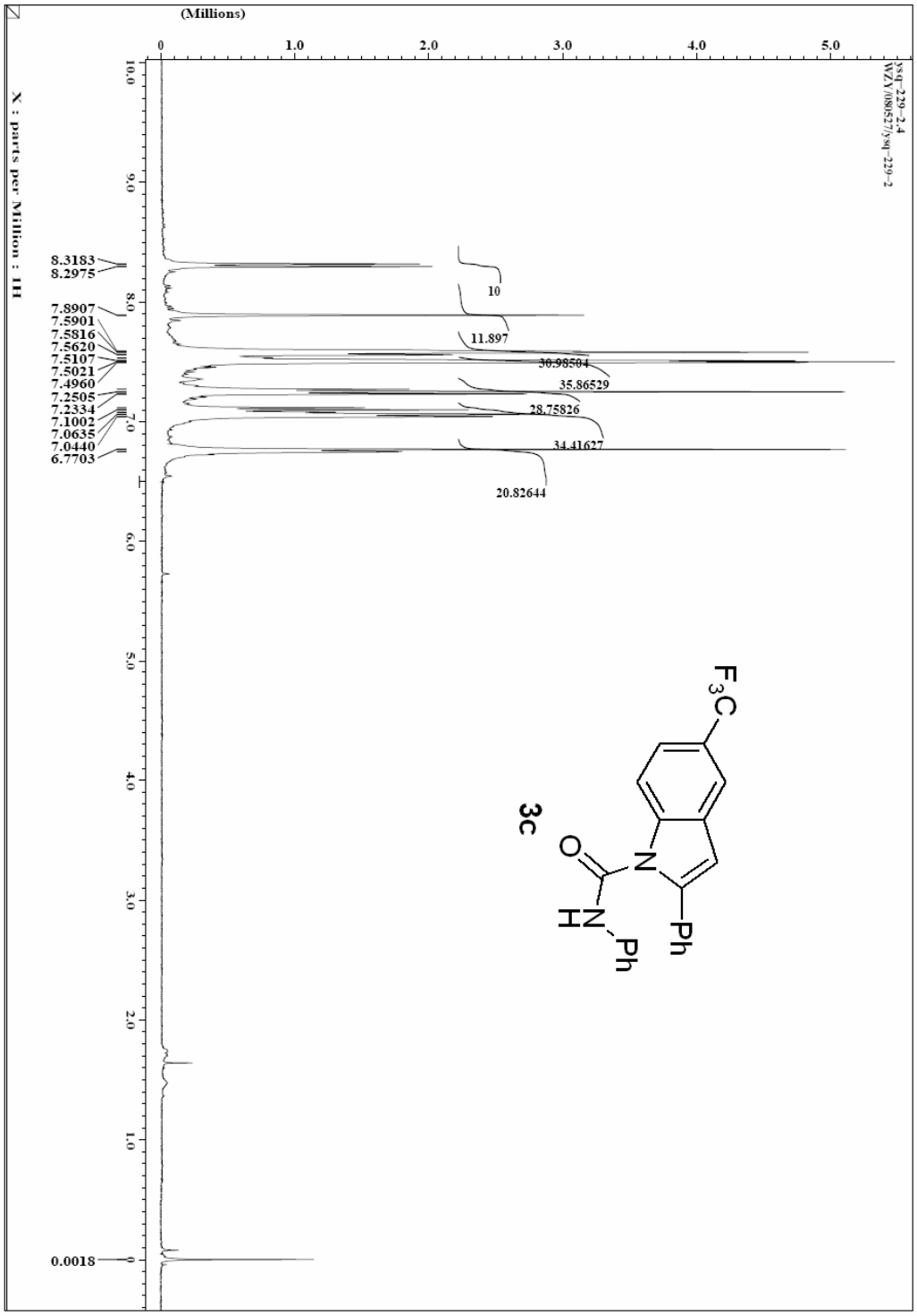
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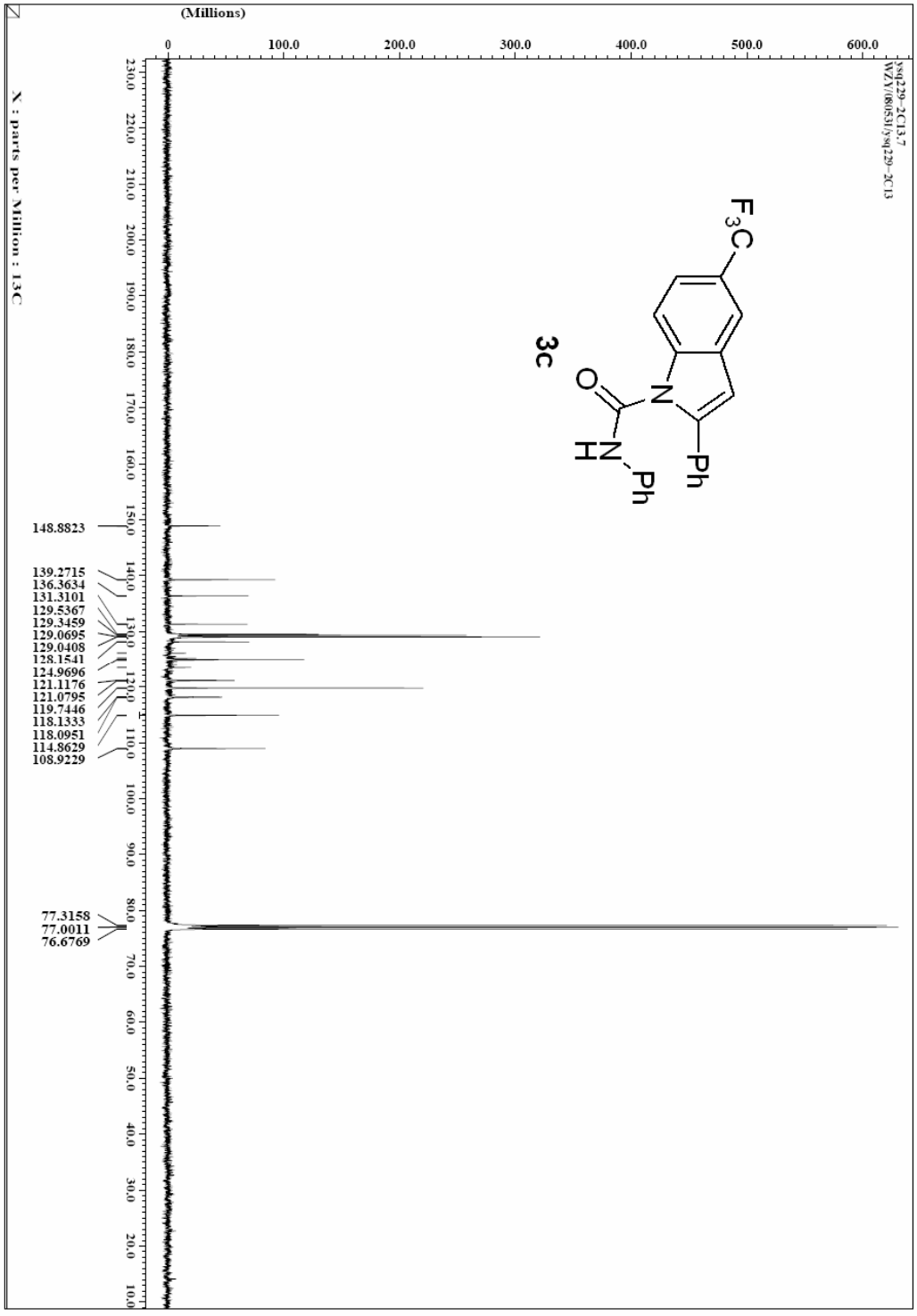
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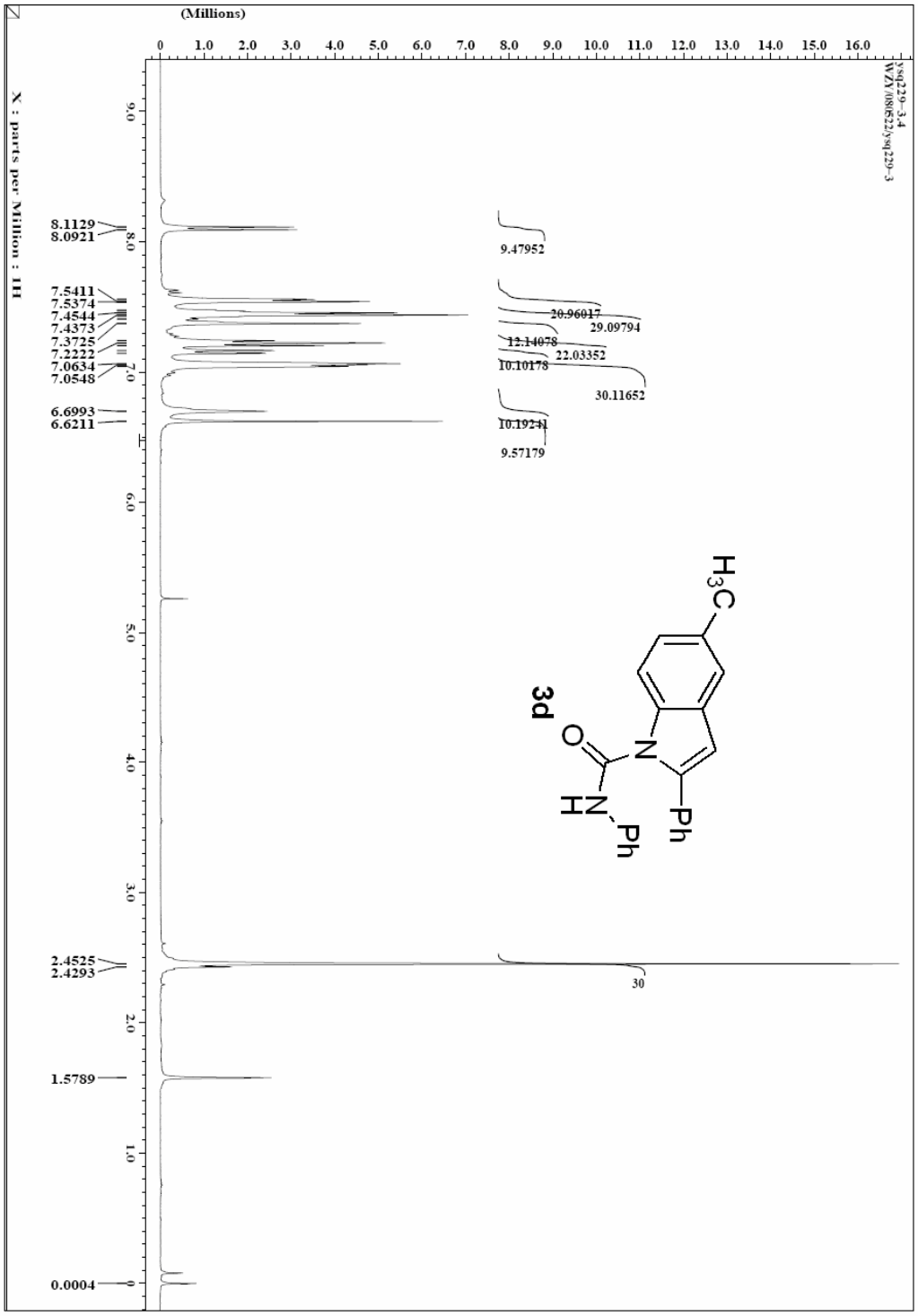
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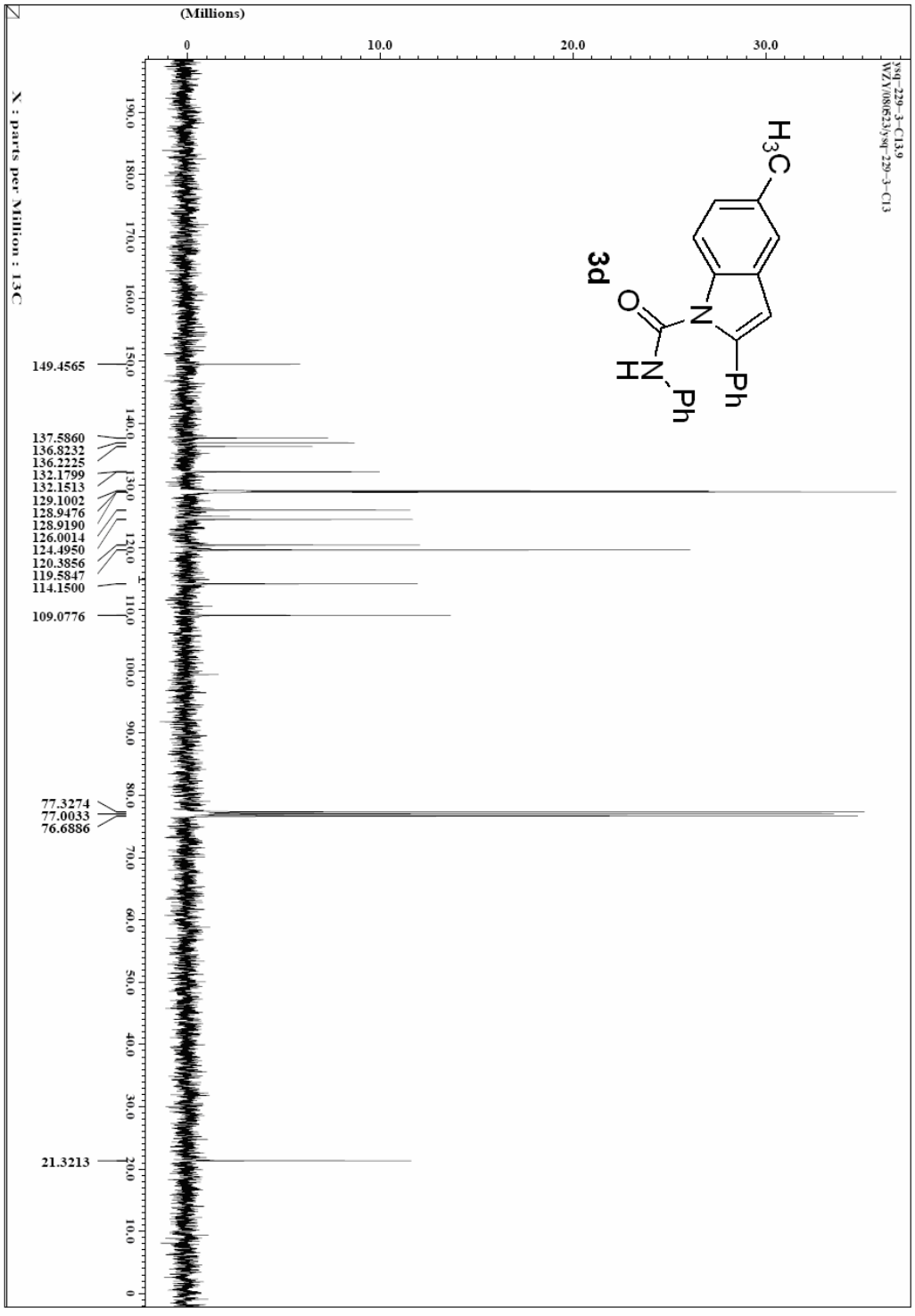
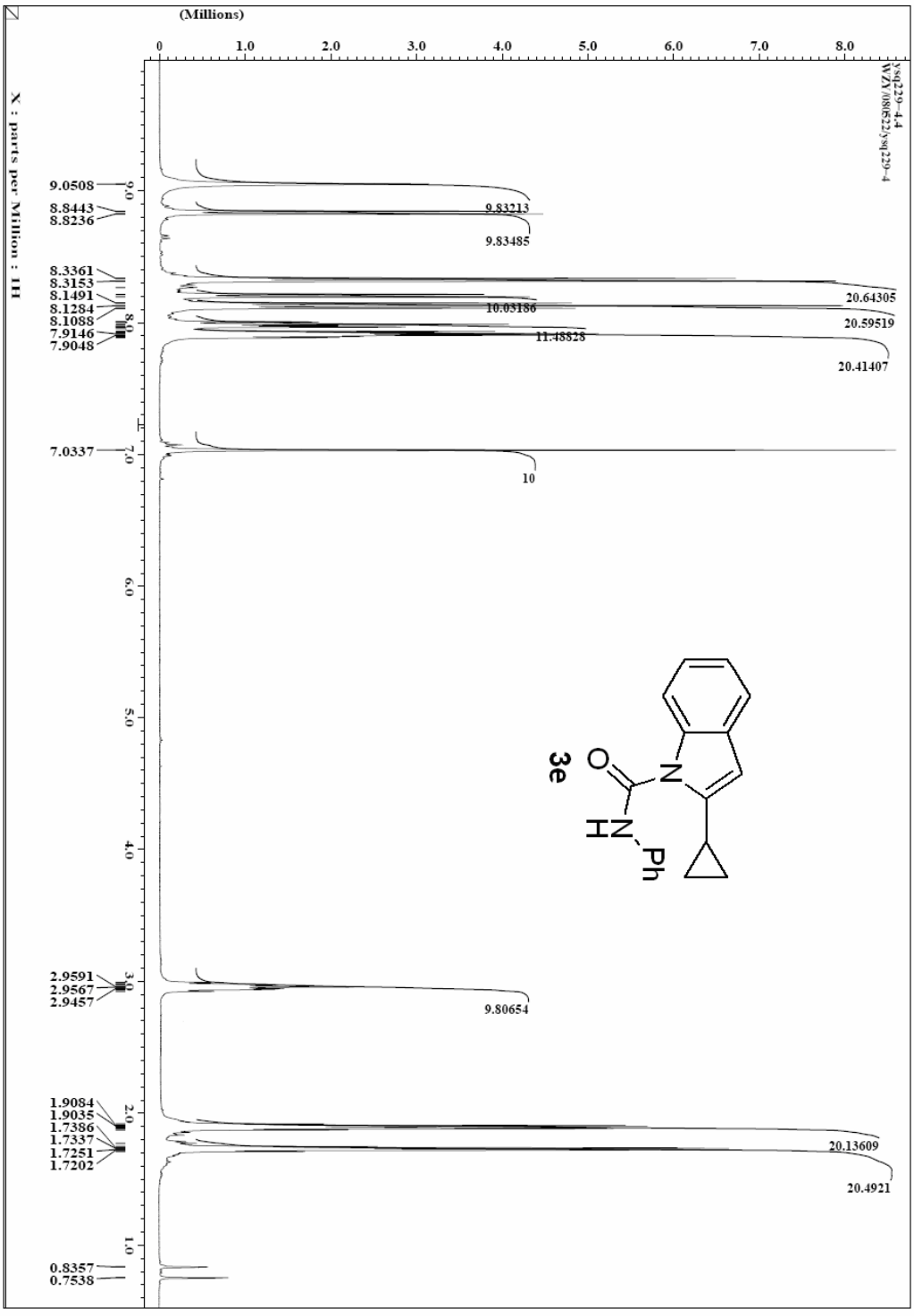
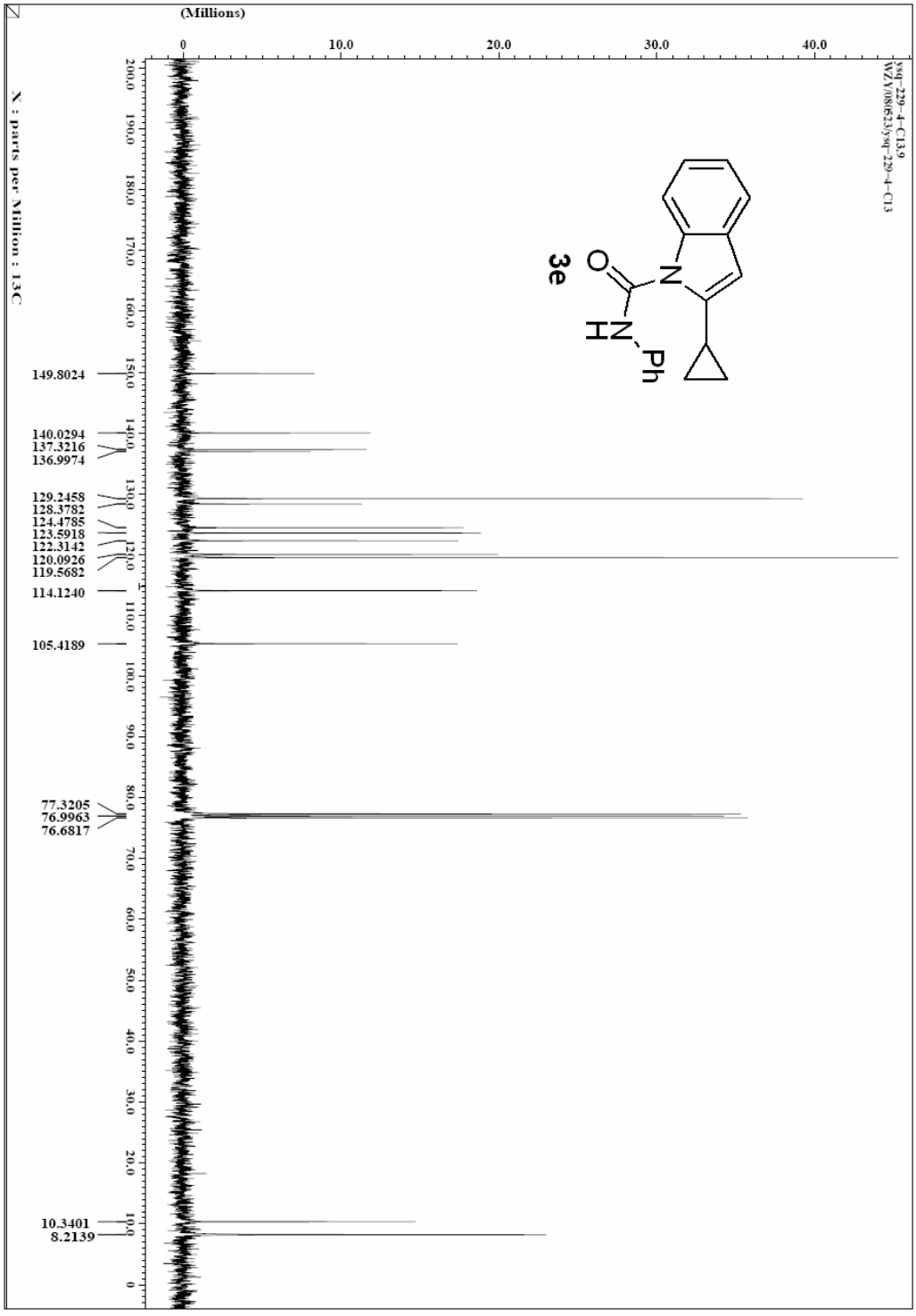
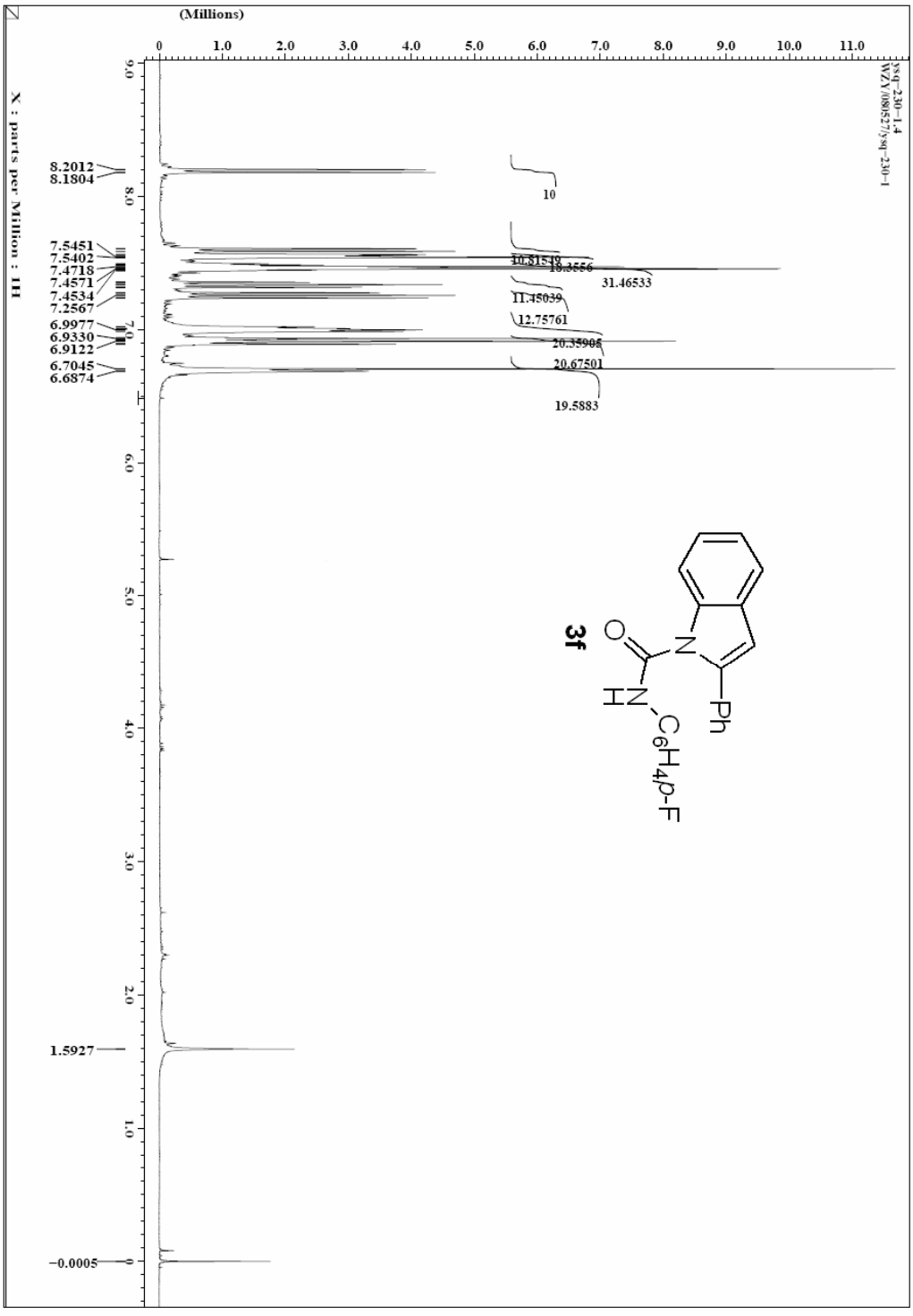
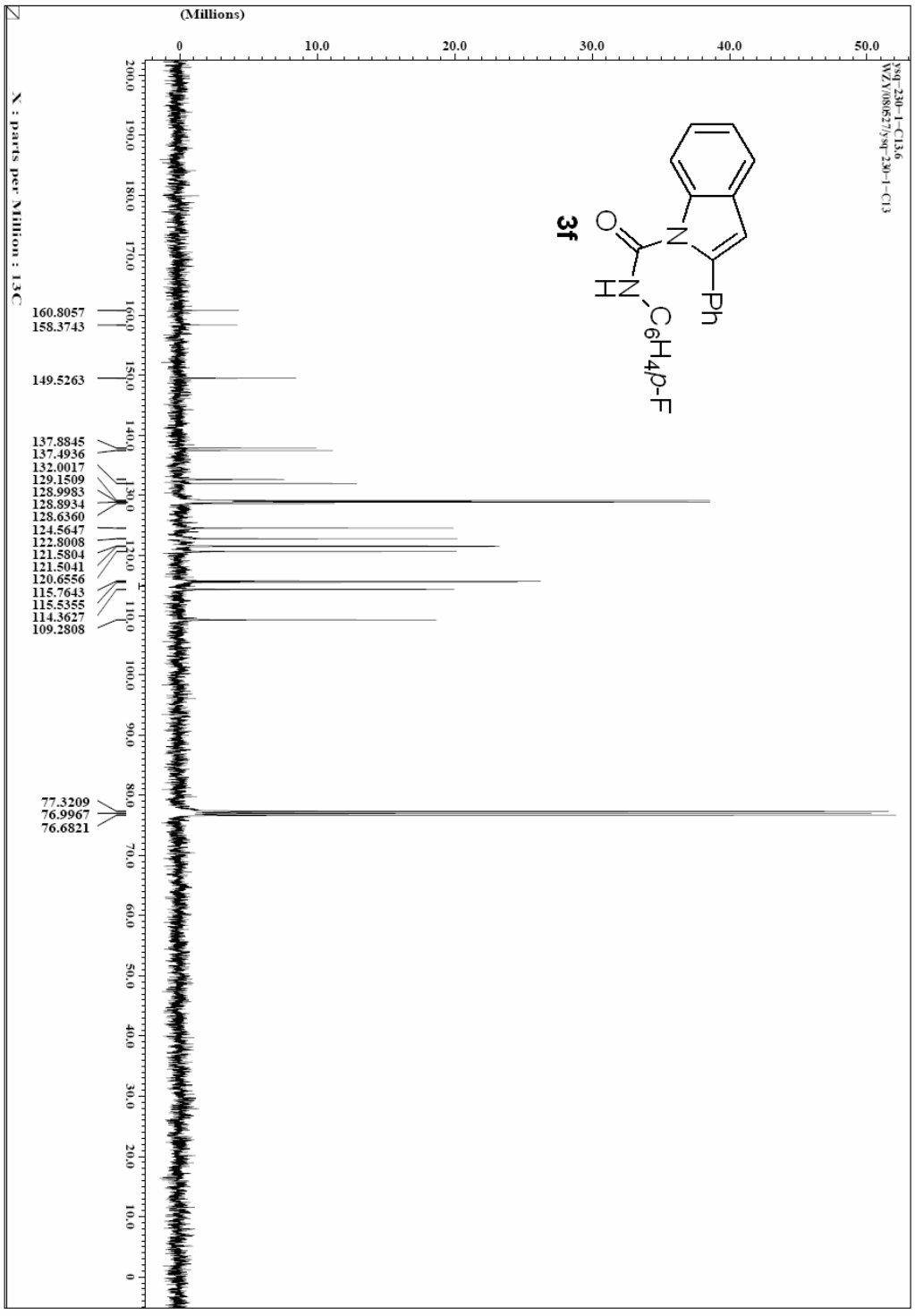
Ph
Ph

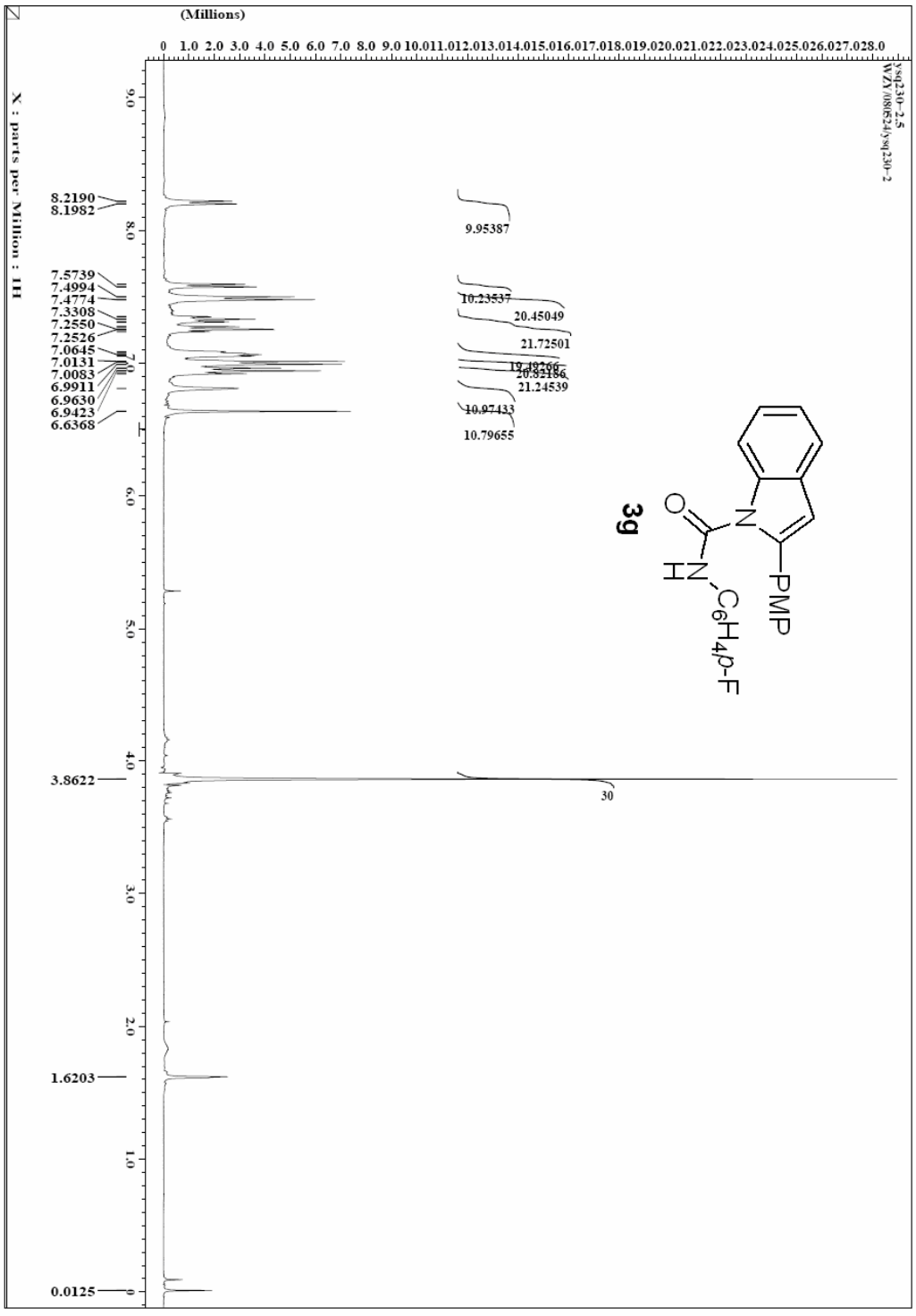

(Millions)
0
10.0
20.0
30.0
N : parts per Million : 13C
149.4565
137.5860
136.8232
136.2225
132.1799
132.1513
129.1002
128.9476
128.9190
126.0014
124.4950
120.3856
119.5847
114.1500
109.0776
77.3274
77.0033
76.6886
21.3213
3d
H3C
O
N
H
N
Ph
Ph

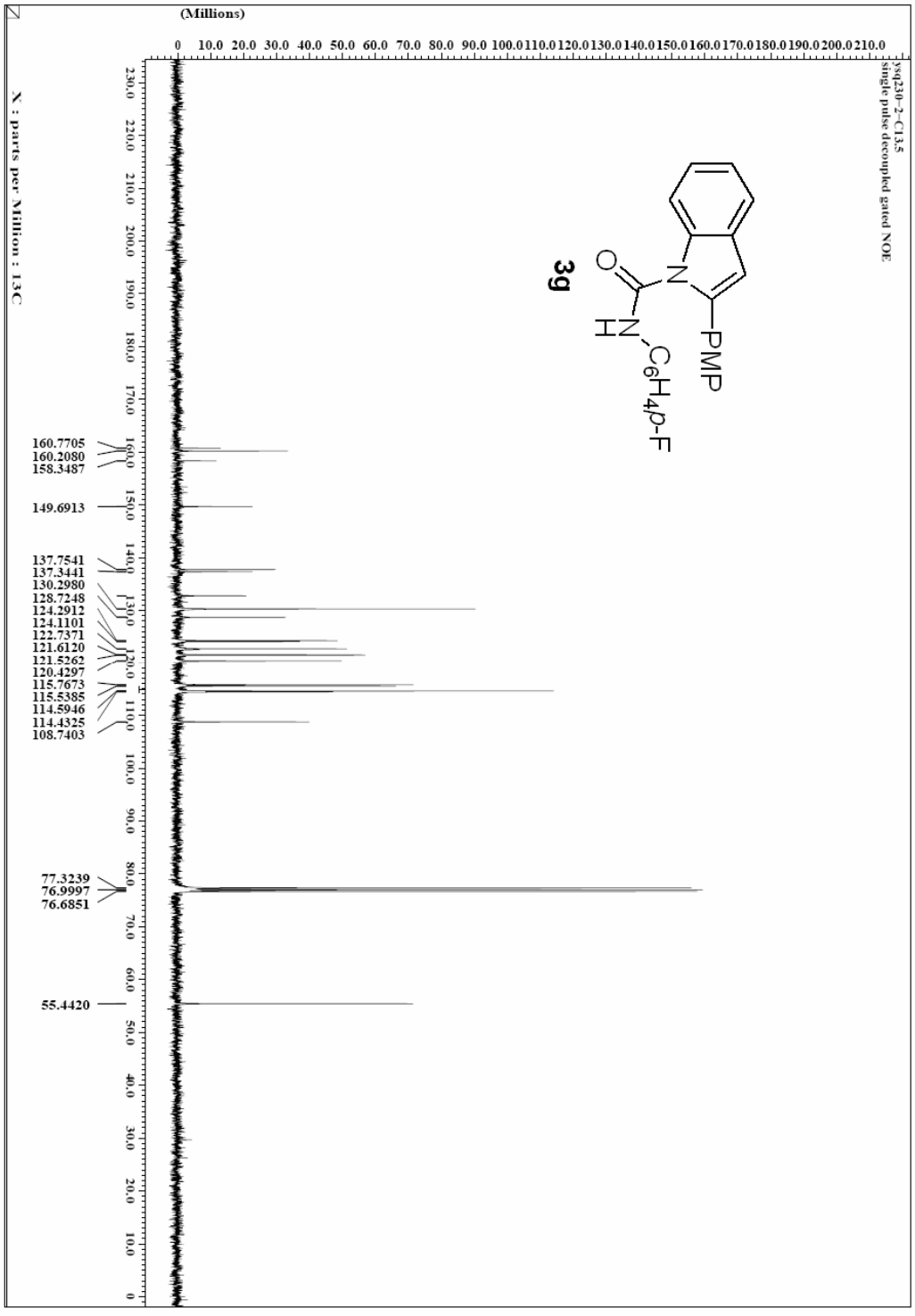

(Millions)
X : parts per Million : 1H
9.0508
8.8443
8.8236
8.3361
8.3153
8.1491
8.1284
8.1088
7.9146
7.9048
7.0337
2.9591
2.9567
2.9457
1.9084
1.9035
1.7386
1.7337
1.7251
1.7202
0.8357
0.7538
9.83213
9.83485
10.03186
11.48828
20.64305
20.59519
20.41407
10
9.80654
20.13609
20.4921
3e

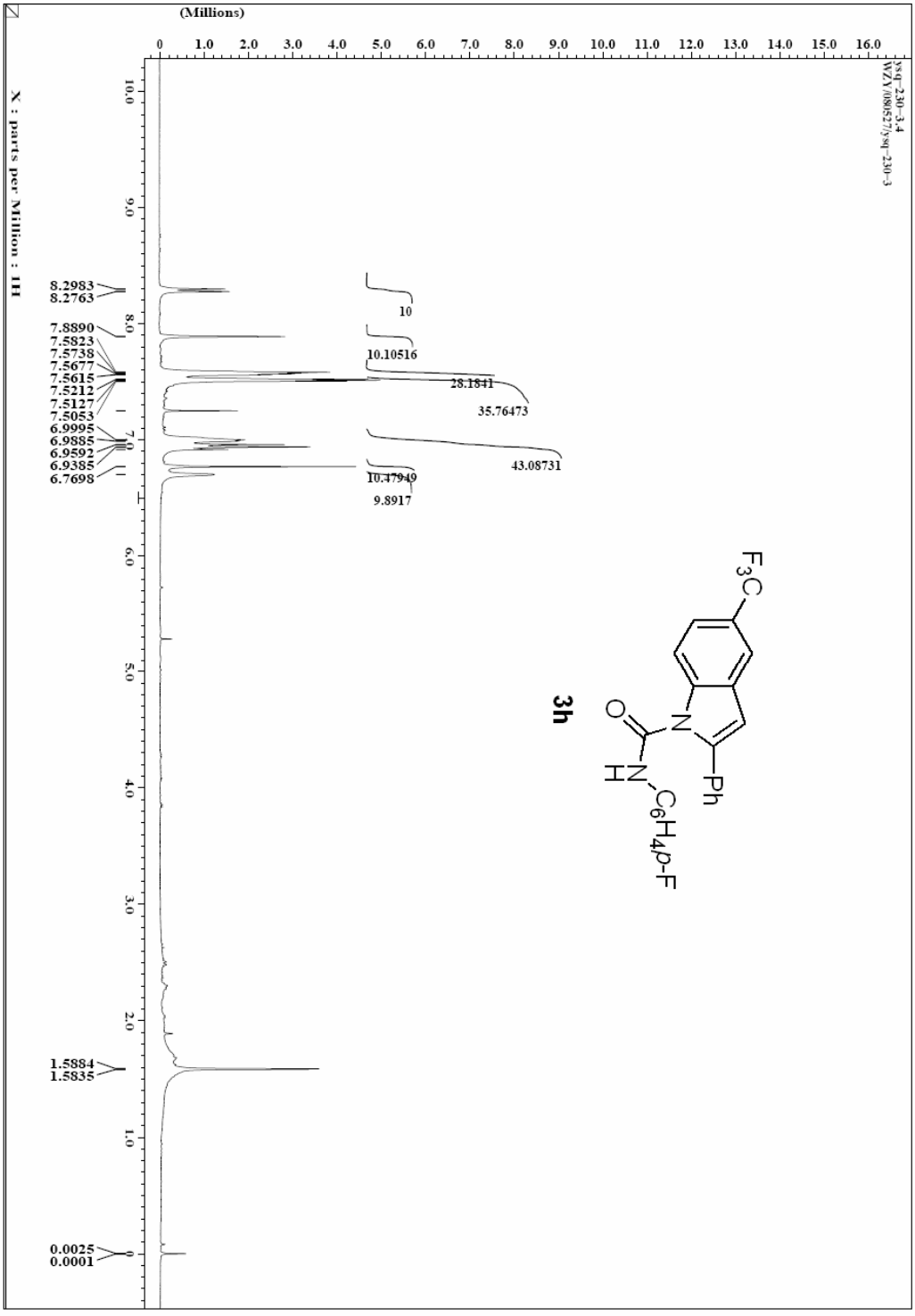

(Millions)
0
10.0
20.0
30.0
40.0
X : parts per Million : 13C
149.8024
140.0294
137.3216
136.9974
129.2458
128.3782
124.4785
123.5918
122.3142
120.0926
119.5682
114.1240
105.4189
77.3205
76.9963
76.6817
10.3401
8.2139
3e
O
N
H
N
Ph

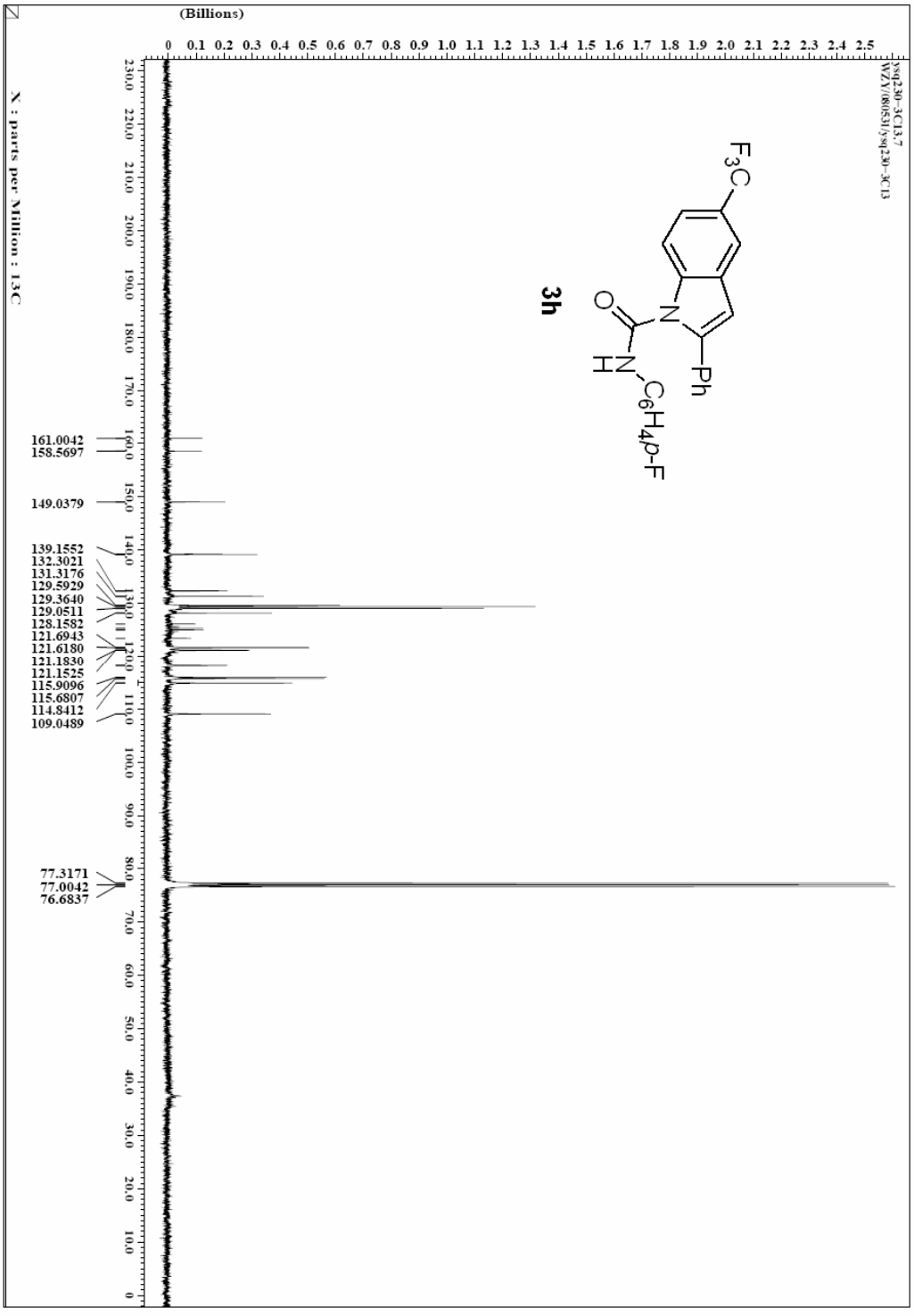

(Millions)
X : parts per Million : 1H
8.2012
8.1804
7.5451
7.5402
7.4718
7.4571
7.4534
7.2567
6.9977
6.9330
6.9122
6.7045
6.6874
1.5927
-0.0005
10
10.81549
18.3556
31.46533
11.45039
12.75761
20.35905
20.67501
19.5883
3f
Ph
C6H4p-F

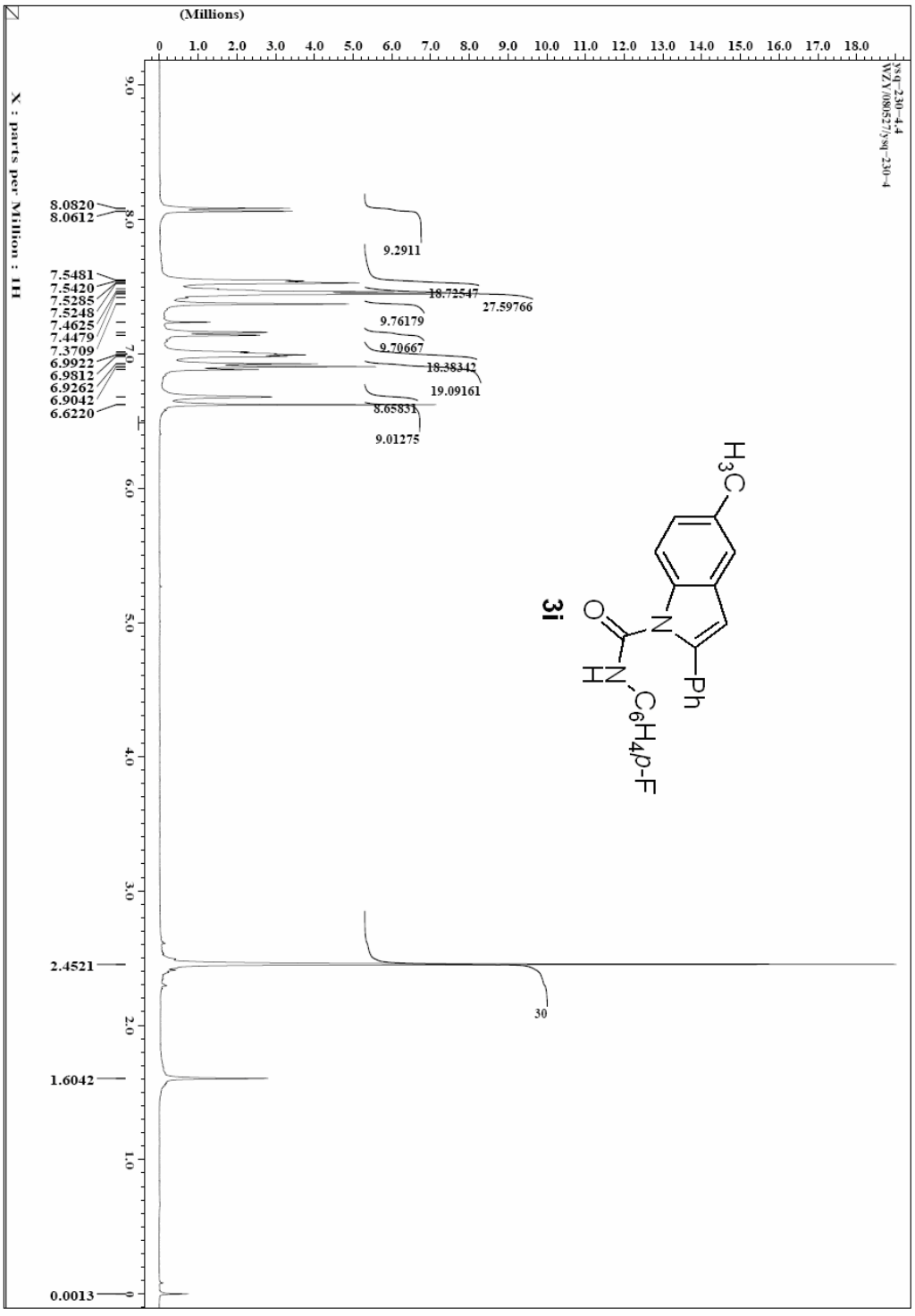

(Millions)
0
10.0
20.0
30.0
40.0
50.0
ssq-230-1-C13.6
WZ\080827\ssq-230-1-C13
X : parts per Million : 13C
160.8057
158.3743
149.5263
137.8845
137.4936
132.0017
129.1509
128.9983
128.8934
128.6360
124.5647
122.8008
121.5804
121.5041
120.6556
115.7643
115.5355
114.3627
109.2808
77.3209
76.9967
76.6821
3f
O
N
H
N
Ph
C6H4p-F

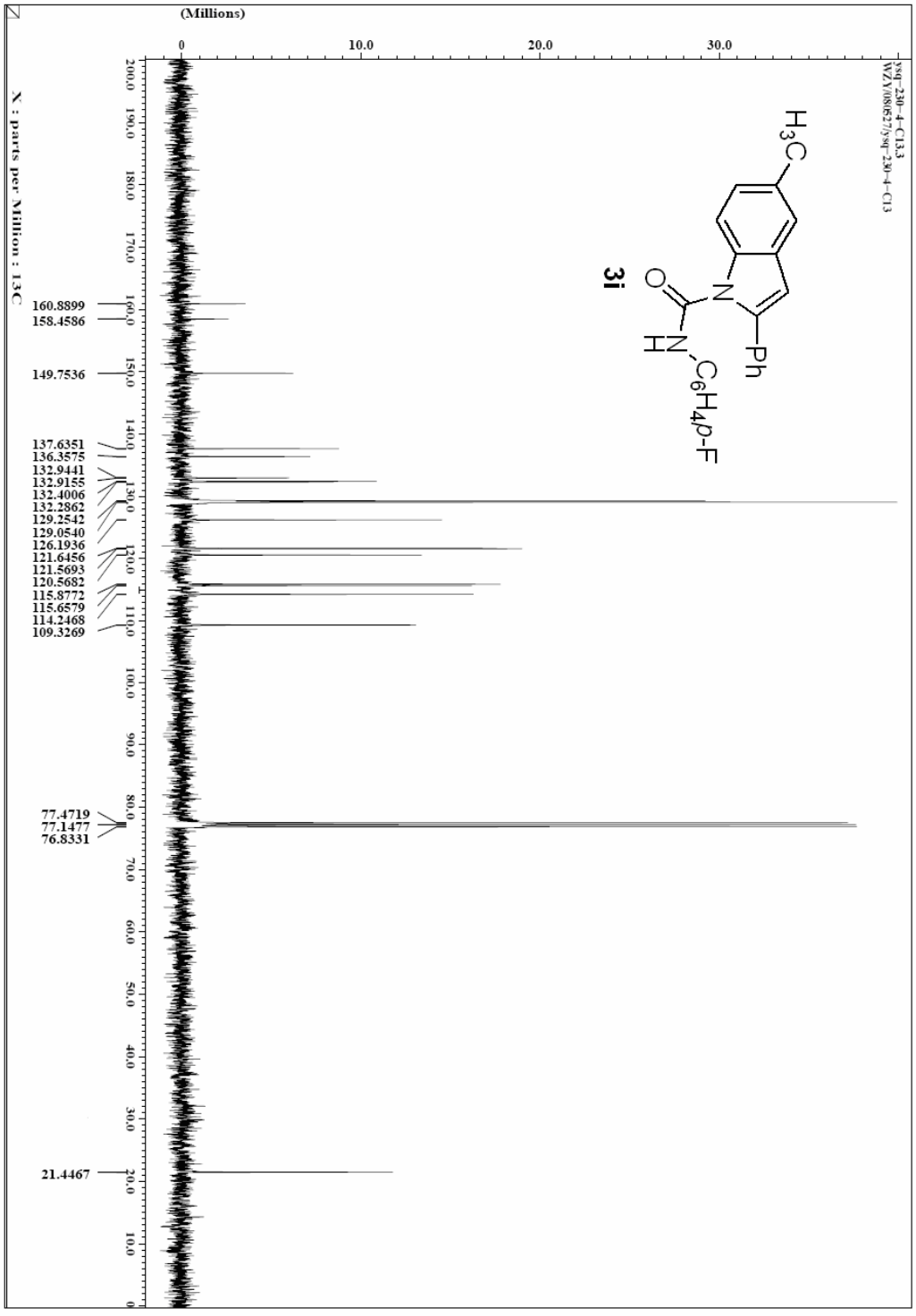

(Millions)
X : parts per Million : 1H
8.2190
8.1982
7.5739
7.4994
7.4774
7.3308
7.2550
7.2526
7.0645
7.0131
7.0083
6.9911
6.9630
6.9423
6.6368
3.8622
1.6203
0.0125
9.95387
10.23537
20.45049
21.72501
21.24539
10.97433
10.79655
30
3g
PMP
C6H4p-F

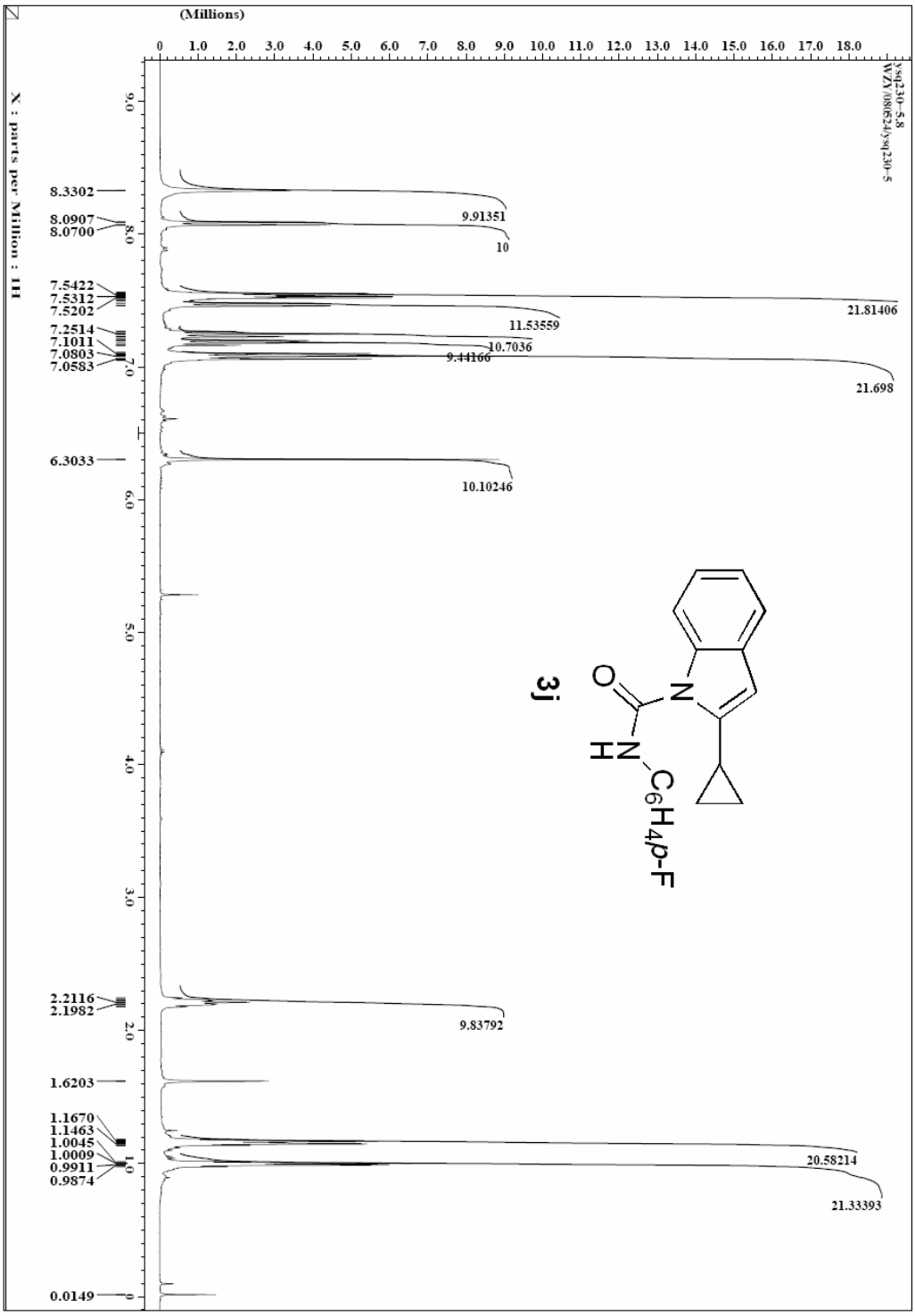

(Millions)
0 10.0 20.0 30.0 40.0 50.0 60.0 70.0 80.0 90.0 100.0 110.0 120.0 130.0 140.0 150.0 160.0 170.0 180.0 190.0 200.0 210.0
ysq230-2-C13.5
single pulse decoupled gated NOE
X : parts per Million : 13C
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
160.7705
160.2080
158.3487
149.6913
137.7541
137.3441
130.2980
128.7248
124.2912
124.1101
122.7371
121.6120
121.5262
120.4297
115.7673
115.5385
114.5946
114.4325
108.7403
77.3239
76.9997
76.6851
55.4420
3g
O
N
H
N
PMP
C6H4p-F

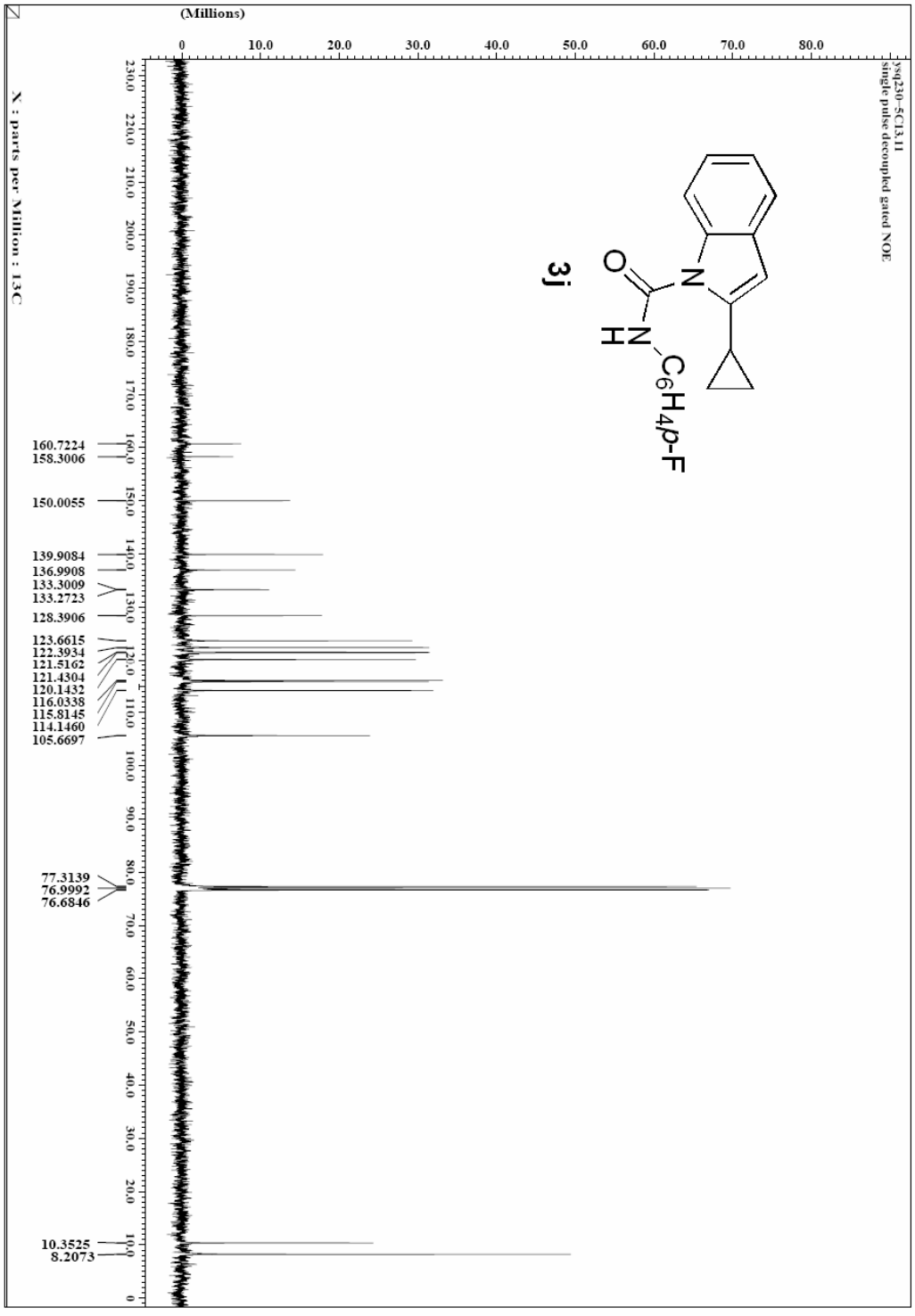

(Millions)
X : parts per Million : 1H
8.2983
8.2763
7.8890
7.5823
7.5738
7.5677
7.5615
7.5212
7.5127
7.5053
6.9995
6.9885
6.9592
6.9385
6.7698
1.5884
1.5835
0.0025
0.0001
10
10.10516
28.1841
35.76473
43.08731
10.47949
9.8917
3h
F3C
O
N
H
Ph
C6H4p-F

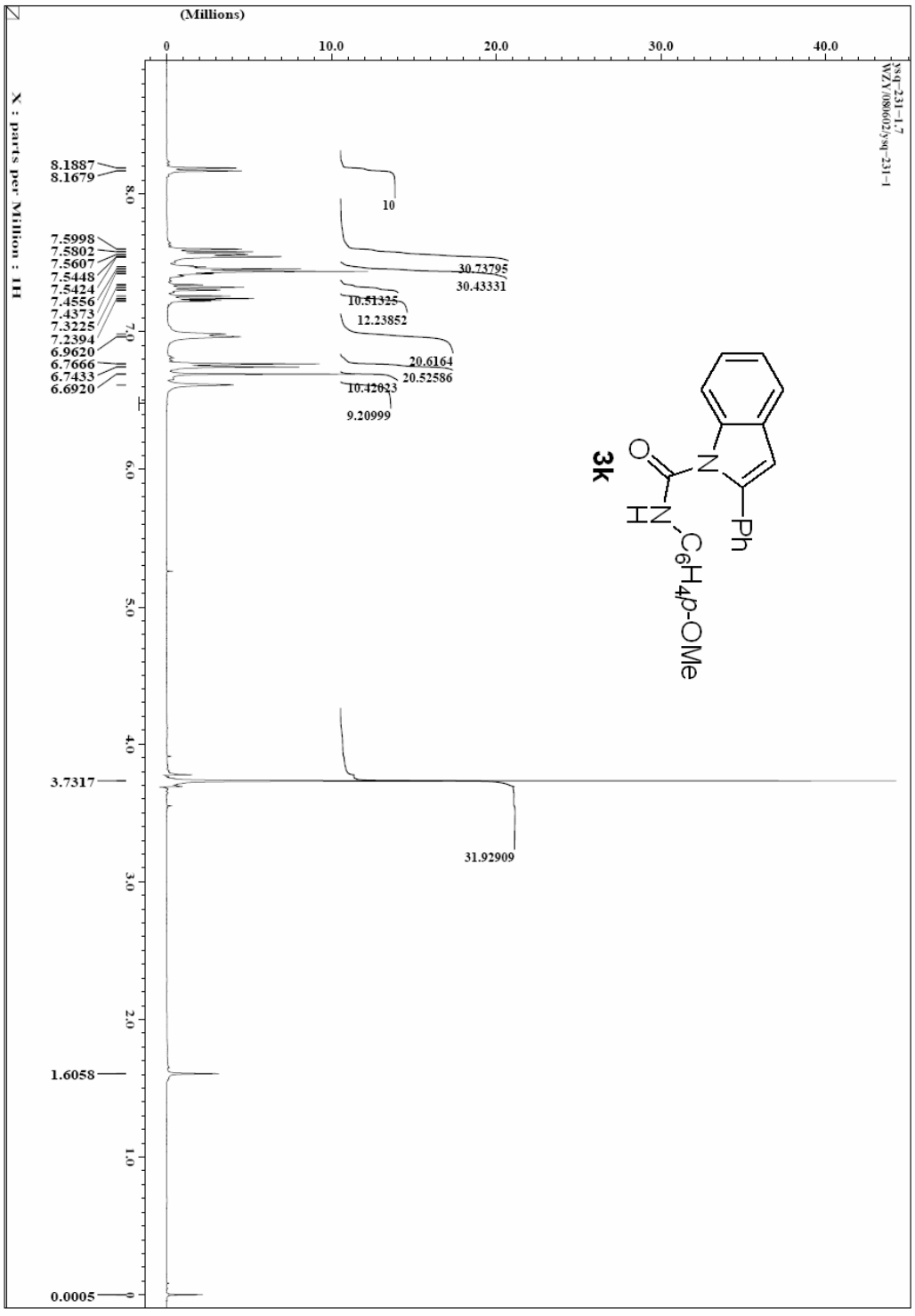

(Billions)
X : parts per Million : 13C
161.0042
158.5697
149.0379
139.1552
132.3021
131.3176
129.5929
129.3640
129.0511
128.1582
121.6943
121.6180
121.1830
121.1525
115.9096
115.6807
114.8412
109.0489
77.3171
77.0042
76.6837
3h

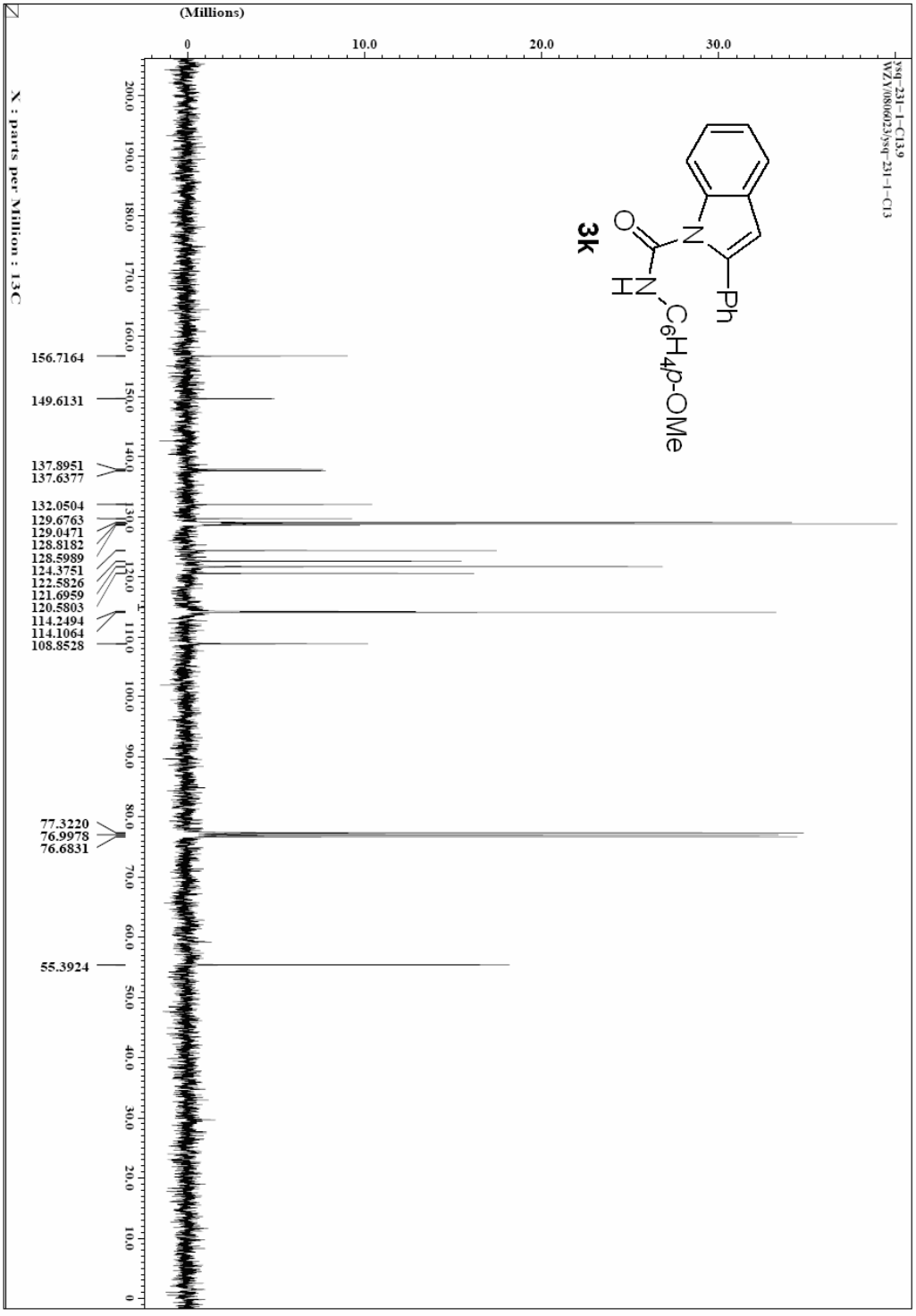

(Millions)
X : parts per Million : 1H
8.0820
8.0612
7.5481
7.5420
7.5285
7.5248
7.4625
7.4479
7.3709
6.9922
6.9812
6.9262
6.9042
6.6220
2.4521
1.6042
0.0013
9.2911
18.72547
27.59766
9.76179
9.70667
18.38342
19.09161
8.65831
9.01275
30
3i
H3C
O
N
H
N
Ph
C6H4p-F

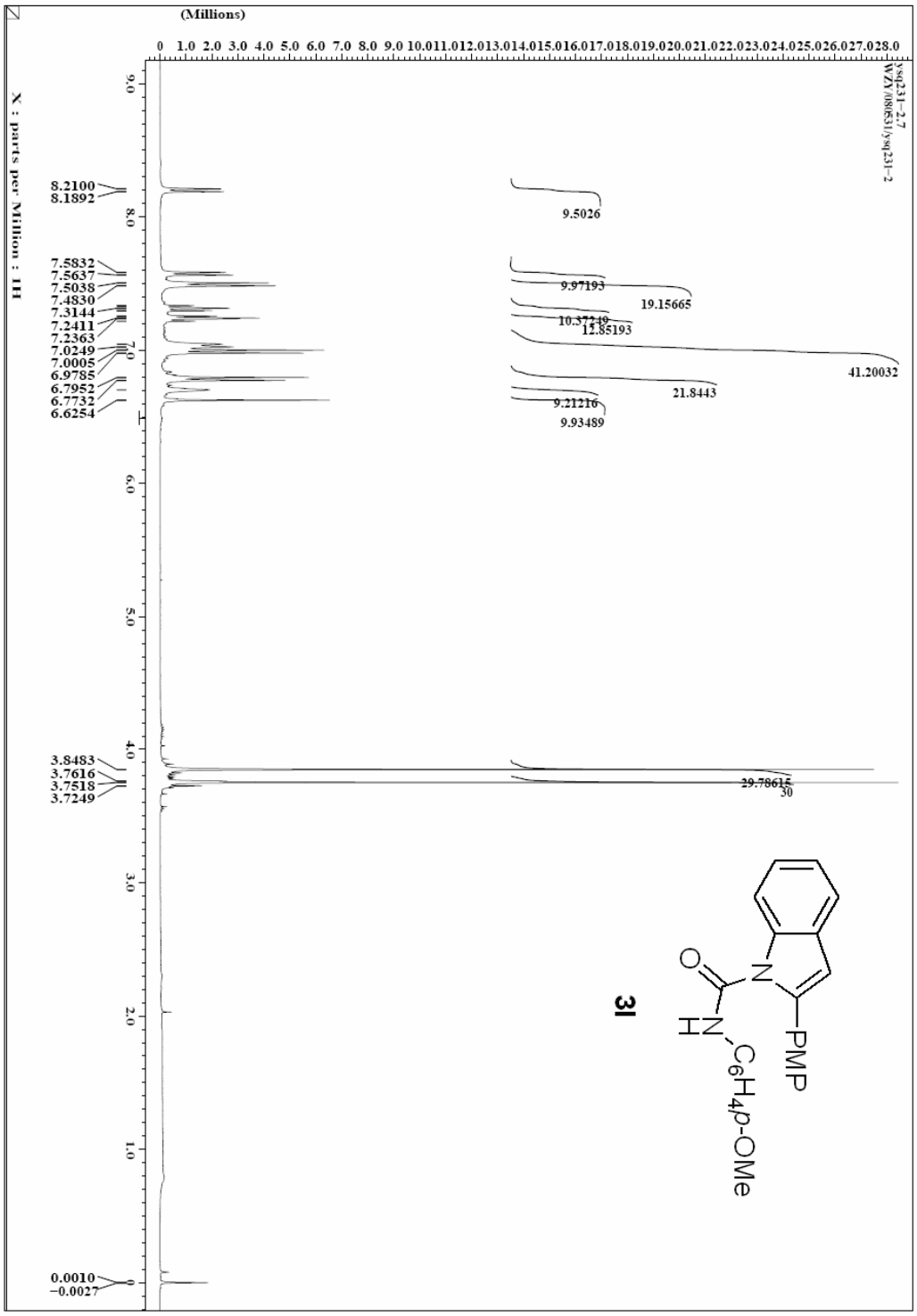

(Millions)
0
10.0
20.0
30.0
ssq-230-4-C13.3
WZ\080827\ssq-230-4-C13
N : parts per Million : 13C
160.8899
158.4586
149.7536
137.6351
136.3575
132.9441
132.9155
132.4006
132.2862
129.2542
129.0540
126.1936
121.6456
121.5693
120.5682
115.8772
115.6579
114.2468
109.3269
77.4719
77.1477
76.8331
21.4467
3i
H3C
Ph
C6H4p-F

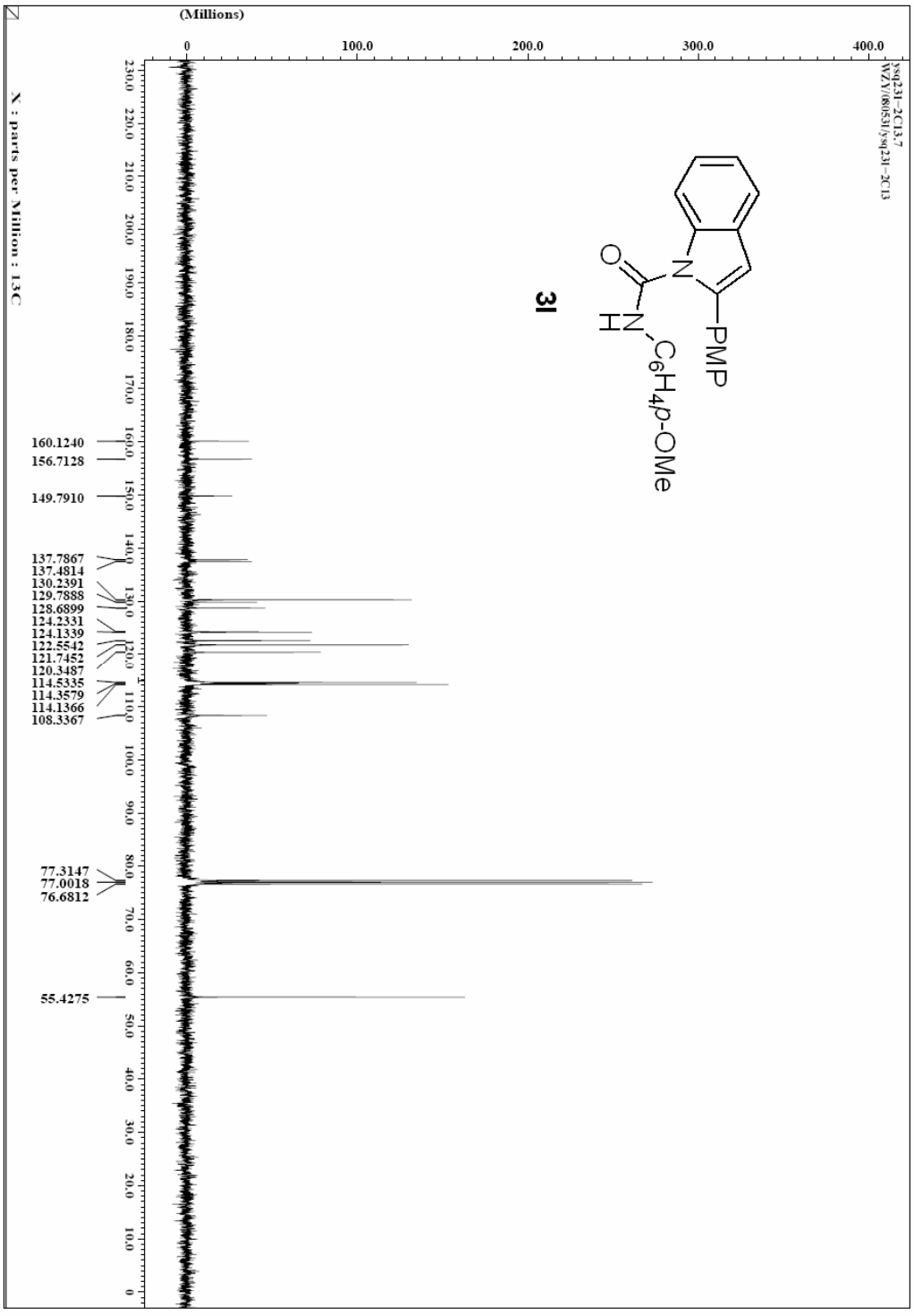

(Millions)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0
X : parts per Million : 1H
8.3302
8.0907
8.0700
7.5422
7.5312
7.5202
7.2514
7.1011
7.0803
7.0583
6.3033
2.2116
2.1982
1.6203
1.1670
1.1463
1.0045
1.0009
0.9911
0.9874
0.0149
9.91351
10
21.81406
11.53559
10.7036
9.44166
21.698
10.10246
9.83792
20.58214
21.33393
3j
C6H4p-F

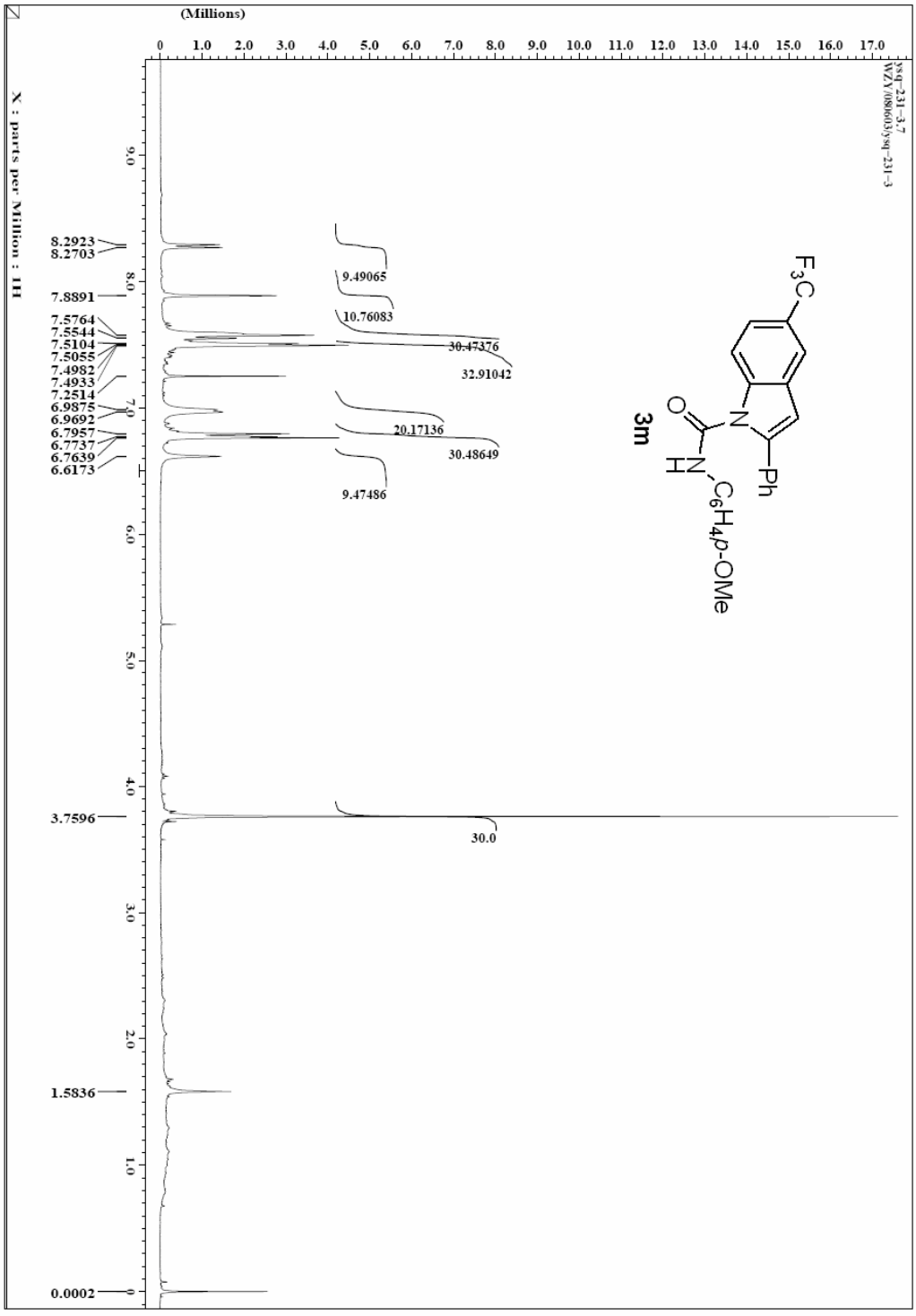

(Millions)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
ysq230-5C13.11
single pulse decoupled gated NOE
X : parts per Million : 13C
160.7224
158.3006
150.0055
139.9084
136.9908
133.3009
133.2723
128.3906
123.6615
122.3934
121.5162
121.4304
120.1432
116.0338
115.8145
114.1460
105.6697
77.3139
76.9992
76.6846
10.3525
8.2073
O
N
H
N
C6H4p-F
3j

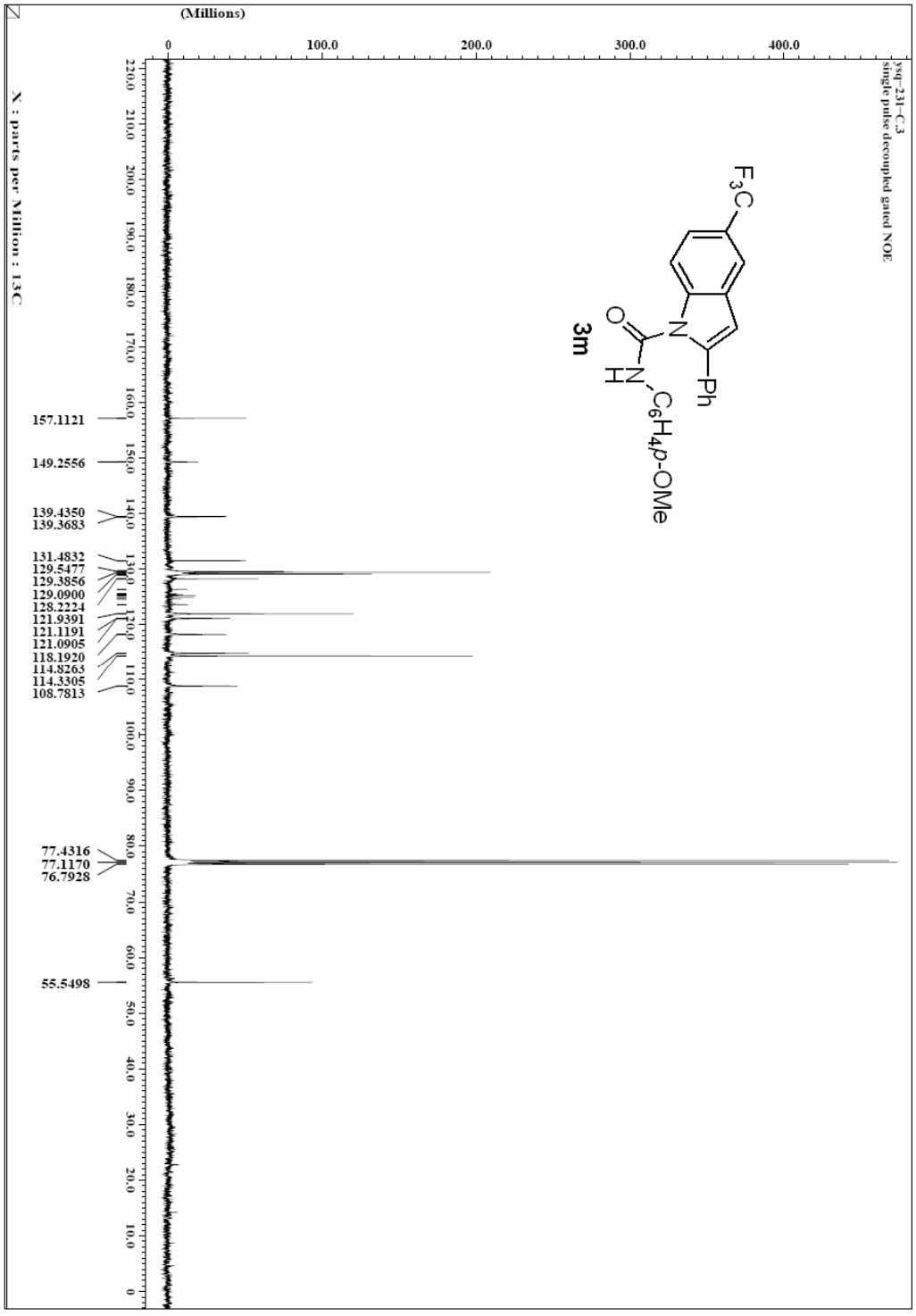

(Millions)
0
10.0
20.0
30.0
40.0
X : parts per Million : 1H
8.1887
8.1679
7.5998
7.5802
7.5607
7.5448
7.5424
7.4556
7.4373
7.3225
7.2394
6.9620
6.7666
6.7433
6.6920
3.7317
1.6058
0.0005
10
30.73795
30.43331
10.51325
12.23852
20.6164
20.52586
10.42623
9.20999
31.92909
3k
Ph
N
O
H
N
C6H4p-OMe

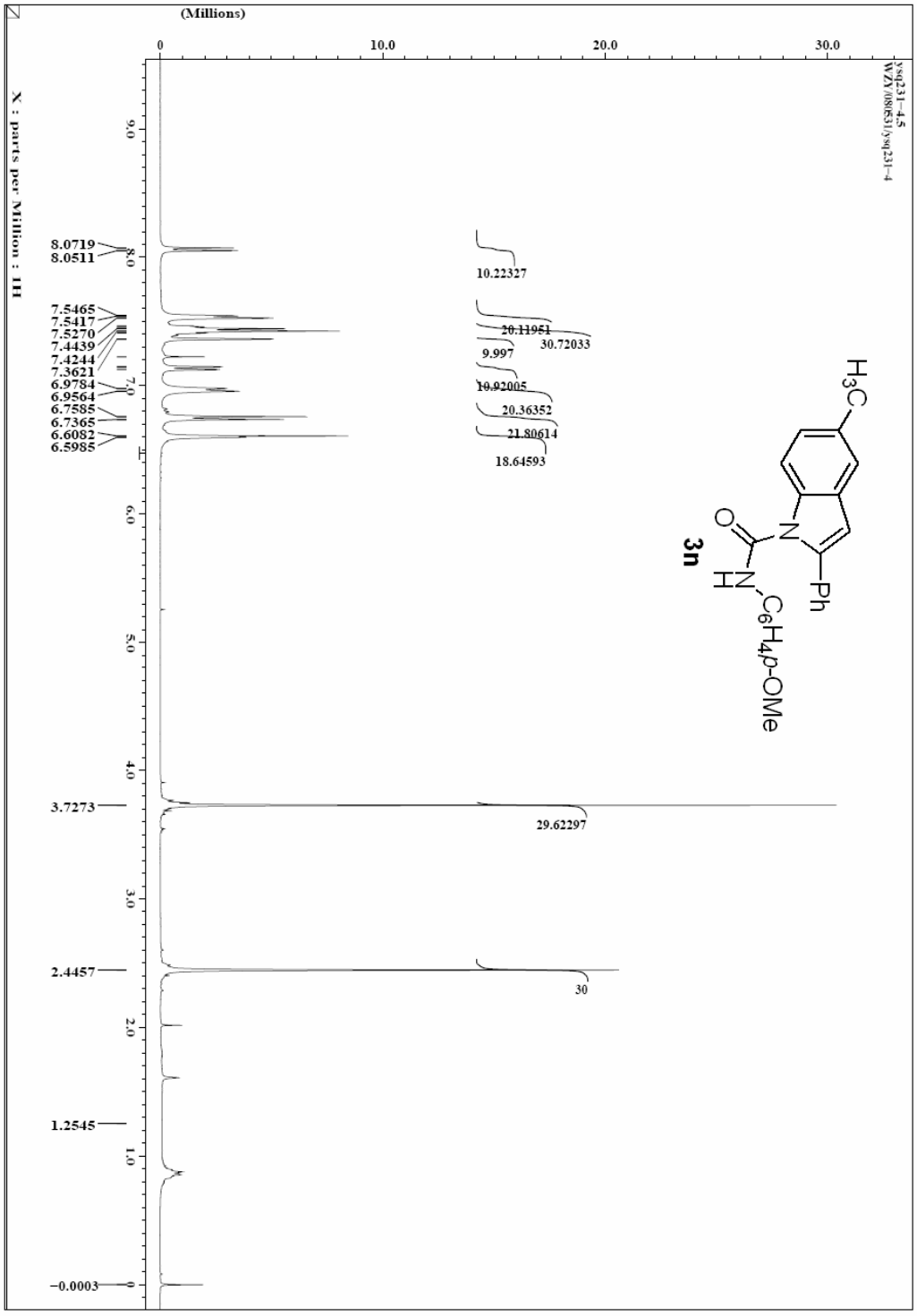

(Millions)
0
10.0
20.0
30.0
ssq-231-1-C13.9
WZY080623/ssq-231-1-C13
X : parts per Million : 13C
156.7164
149.6131
137.8951
137.6377
132.0504
129.6763
129.0471
128.8182
128.5989
124.3751
122.5826
121.6959
120.5803
114.2494
114.1064
108.8528
77.3220
76.9978
76.6831
55.3924
3k
Ph
C6H4p-OMe

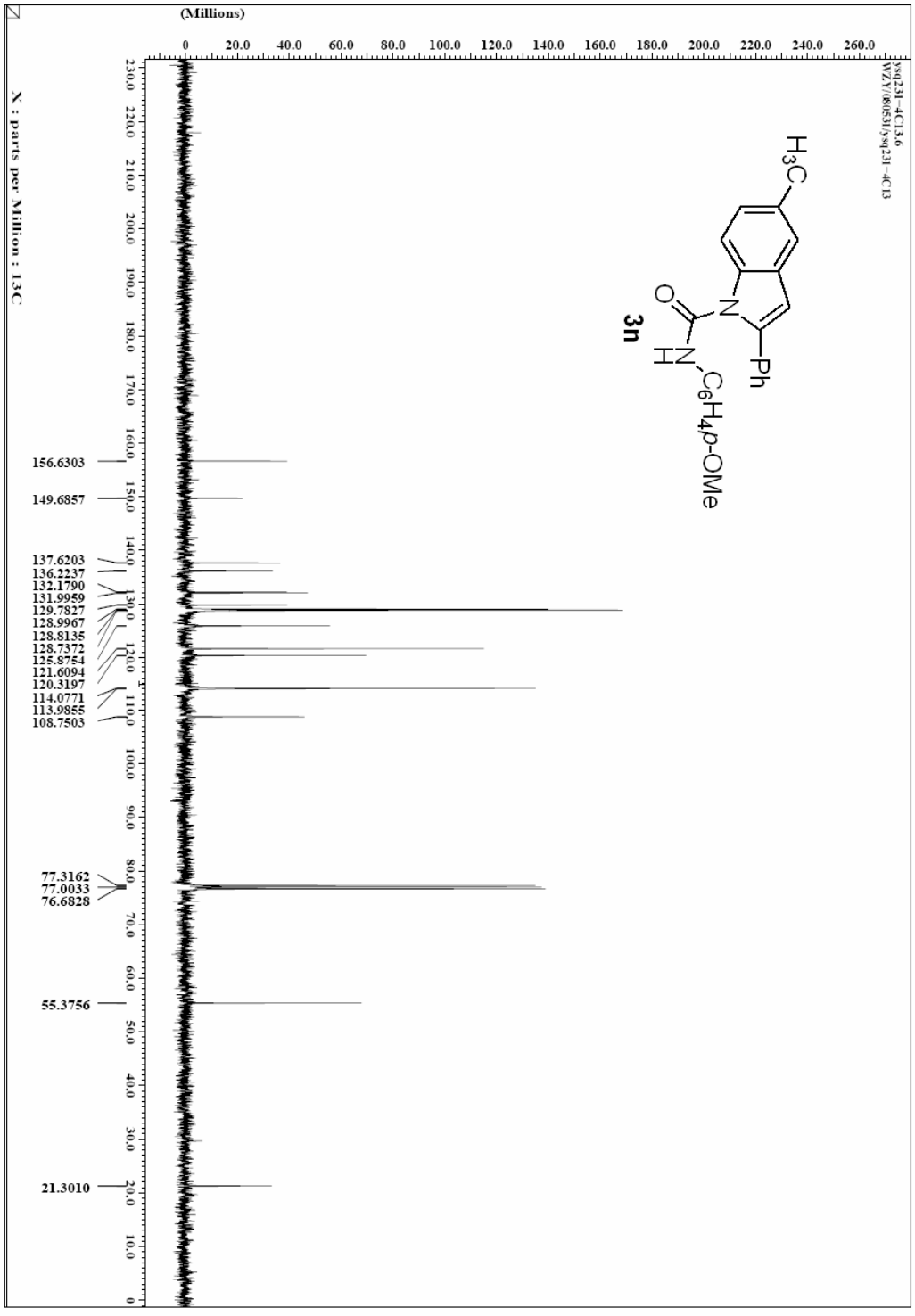

(Millions)
X : parts per Million : 1H
8.2100
8.1892
7.5832
7.5637
7.5038
7.4830
7.3144
7.2411
7.2363
7.0249
7.0005
6.9785
6.7952
6.7732
6.6254
3.8483
3.7616
3.7518
3.7249
0.0010
−0.0027
9.5026
9.97193
19.15665
10.37249
12.85193
41.20032
21.8443
9.21216
9.93489
29.78615
30
3l
PMP
C6H4p-OMe

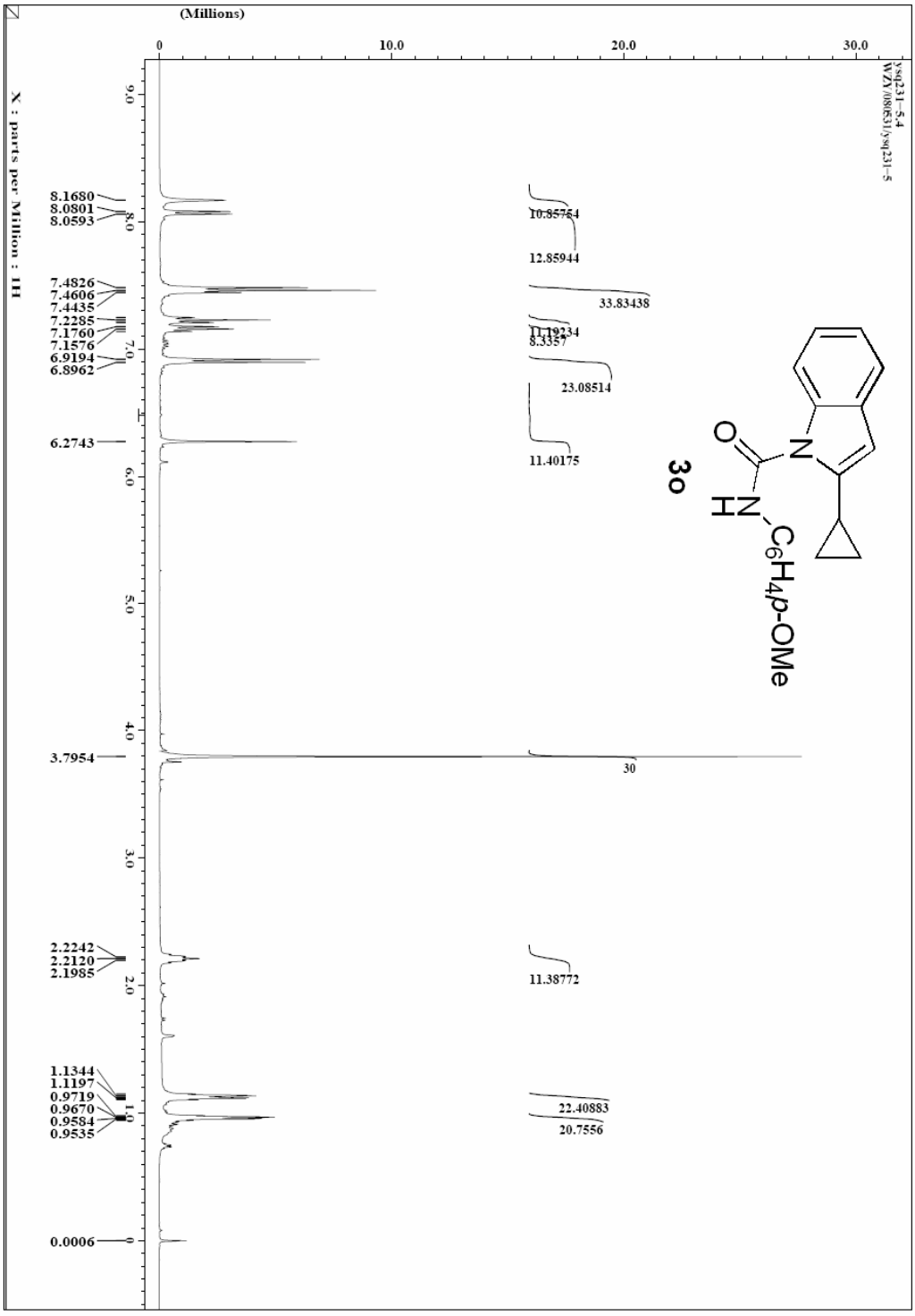

(Millions)
0
100.0
200.0
300.0
400.0
ssq231-2C13.7
WZ\080531\ssq231-2C13
X : parts per Million : 13C
160.1240
156.7128
149.7910
137.7867
137.4814
130.2391
129.7888
128.6899
124.2331
124.1339
122.5542
121.7452
120.3487
114.5335
114.3579
114.1366
108.3367
77.3147
77.0018
76.6812
55.4275
3l
PMP
C6H4p-OMe

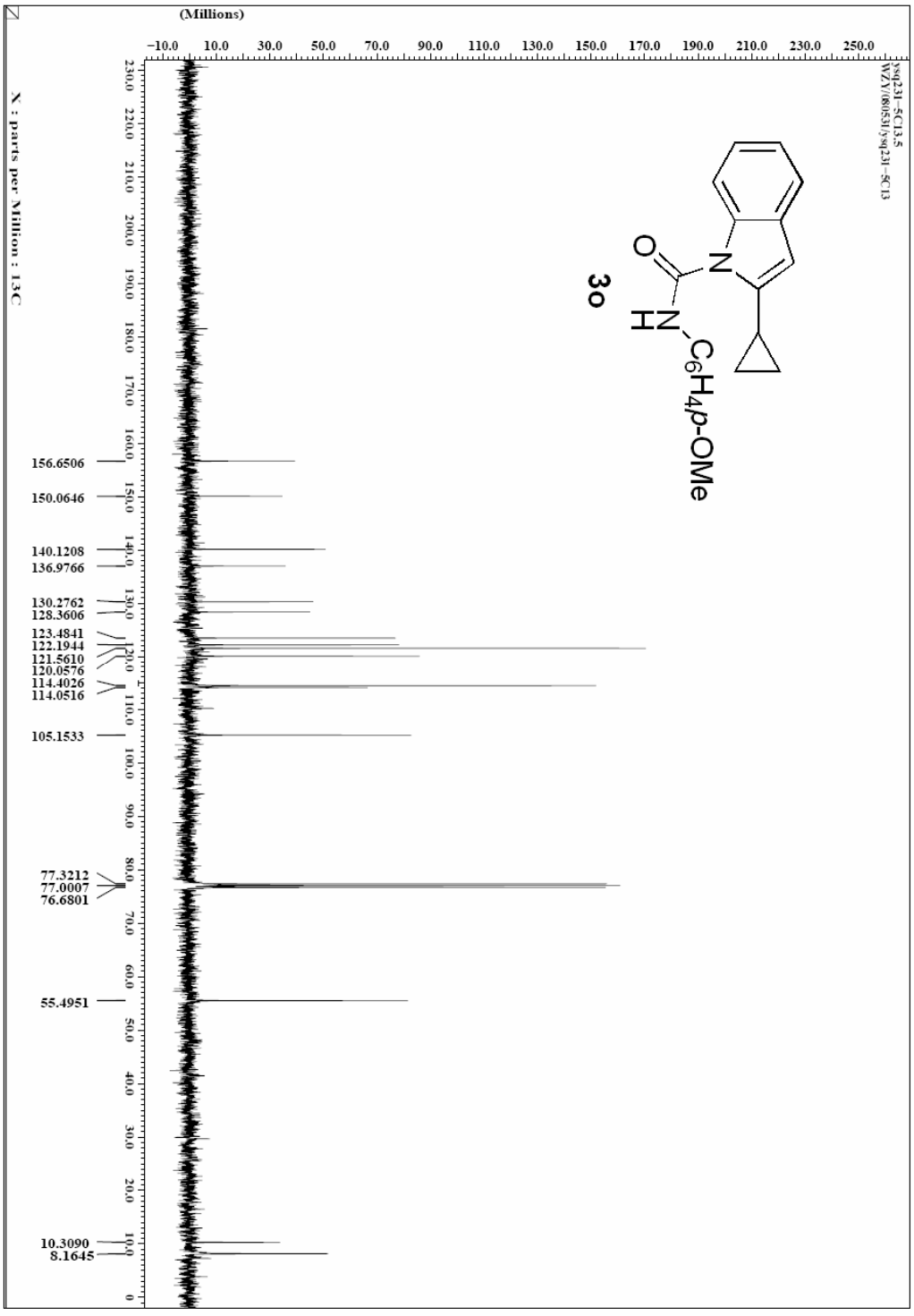

(Millions)
X : parts per Million : 1H
8.2923
8.2703
7.8891
7.5764
7.5544
7.5104
7.5055
7.4982
7.4933
7.2514
6.9875
6.9692
6.7957
6.7737
6.7639
6.6173
3.7596
1.5836
0.0002
9.49065
10.76083
30.47376
32.91042
20.17136
30.48649
9.47486
30.0
F3C
Ph
C6H4p-OMe
3m


(Millions)
0
100.0
200.0
300.0
400.0
X : parts per Million : 13C
157.1121
149.2556
139.4350
139.3683
131.4832
129.5477
129.3856
129.0900
128.2224
121.9391
121.1191
121.0905
118.1920
114.8263
114.3305
108.7813
77.4316
77.1170
76.7928
55.5498
F3C
N
O
N
H
Ph
C6H4p-OMe
3m


(Millions)
0
10.0
20.0
30.0
X : parts per Million : 1H
8.0719
8.0511
7.5465
7.5417
7.5270
7.4439
7.4244
7.3621
6.9784
6.9564
6.7585
6.7365
6.6082
6.5985
3.7273
2.4457
1.2545
−0.0003
10.22327
20.11951
30.72033
9.997
10.92005
20.36352
21.80614
18.64593
29.62297
30
3n
H3C
Ph
C6H4,p-OMe


(Millions)
0 20.0 40.0 60.0 80.0 100.0 120.0 140.0 160.0 180.0 200.0 220.0 240.0 260.0
X : parts per Million : 13C
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
156.6303
149.6857
137.6203
136.2237
132.1790
131.9959
129.7827
128.9967
128.8135
128.7372
125.8754
121.6094
120.3197
114.0771
113.9855
108.7503
77.3162
77.0033
76.6828
55.3756
21.3010
H3C
N
O
N
H
Ph
C6H4p-OMe
3n


(Millions)
0
10.0
20.0
30.0
X : parts per Million : 1H
8.1680
8.0801
8.0593
7.4826
7.4606
7.4435
7.2285
7.1760
7.1576
6.9194
6.8962
6.2743
3.7954
2.2242
2.2120
2.1985
1.1344
1.1197
0.9719
0.9670
0.9584
0.9535
0.0006
10.85754
12.85944
33.83438
11.19234
8.3357
23.08514
11.40175
30
11.38772
22.40883
20.7556
3o
O
N
H
N
C6H4p-OMe


(Millions)
X : parts per Million : 13C
156.6506
150.0646
140.1208
136.9766
130.2762
128.3606
123.4841
122.1944
121.5610
120.0576
114.4026
114.0516
105.1533
77.3212
77.0007
76.6801
55.4951
10.3090
8.1645
3o
C6H4p-OMe