Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

A concise synthesis of 4-imino-3,4-dihydroquinazolin-2-ylphosphonates via a palladium-catalyzed reaction of carbodiimide, isocyanide, and phosphite

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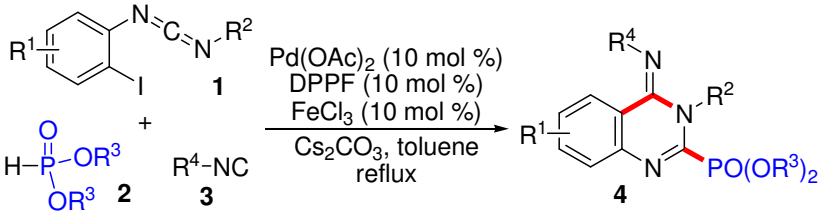
Supporting Information

1. General experimental methods (S2).
2. General experimental procedure and characterization data (S2-S8).
3. ^{1}H and ^{13}C NMR spectra of compounds **4** (S9-S36).

General Materials and Methods:

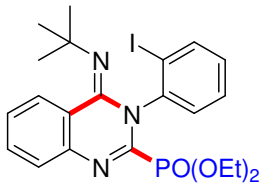
Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using 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 at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument. The carbodiimides **1** were synthesized according to literature method (1) F. Zeng, H. Alper, *Org. Lett*. 2010, **12,** 3642. 2) F. Zeng and H. Alper, *Org. Lett.* 2010, **12**, 1188.)

General procedure of the synthesis of 4-imino-3,4-dihydroquinazolin-2-ylphosphonates via a palladium-catalyzed reaction of carbodiimide, isocyanide, and phosphite

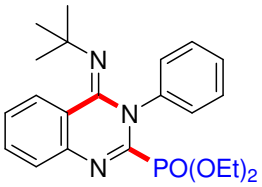


$Pd(OAc)_2$ (10 mol %), DPPF (10 mol %), and $FeCl_3$ (10 mol %) were added to a solution of carbodiimides **1** (0.2 mmol) in toluene (2.0 mL) under N_2 atmosphere at room temperature. Then phosphite **2** (1.5 equiv) was added. After the mixture was stirred at room temperature for 1 hour, isocyanide **3** (2.0 euqiv) and Cs_2CO_3 (2.0 equiv) was added. Then the mixture was stirred at reflux. After completion of reaction

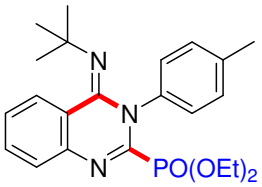
as indicated by TLC (8-12 hrs), the solvent was evaporated and the residue was purified on silica gel to provide the desired product **4**.



Diethyl (*E*)-4-(*tert*-butylimino)-3,4-dihydro-3-(2-iodophenyl)quinazolin-2-yl-2-phosphonate (**4a**)**:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.14 (t, *J* = 7.2 Hz, 3H), 1.23 (s, 9H), 1.36 (t, *J* = 7.2 Hz, 3H), 3.66-3.71 (m, 1H), 3.72-3.93 (m, 1H), 4.22-4.28 (m, 2H), 7.01-7.06 (m, 1H), 7.41-7.61 (m, 5H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.98 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.1, 16.3, 31.0, 53.0, 63.0, 64.6, 102.6, 122.3, 125.8, 127.9, 128.8, 128.9, 129.6, 131.6, 132.9, 138.5, 142.6, 146.5, 151.8; HRMS Calcd for $C_{22}H_{28}IN_3O_3P^+$ (ESI, $M+H^+$): 540.0907; found: 540.0920.

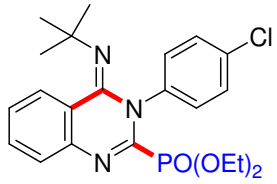


Diethyl (*E*)-4-(*tert*-butylimino)-3,4-dihydro-3-phenylquinazolin-2-yl-2-phosphonate (**4b**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.14 (t, *J* = 7.2 Hz, 3H), 1.23 (s, 9H), 1.36 (t, *J* = 7.2 Hz, 3H), 3.66-3.70 (m, 1H), 3.87-3.91 (m, 1H), 4.24-4.28 (m, 2H), 6.90-6.94 (m, 1H), 7.05-7.28 (m, 7H), 7.61 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.1, 16.3, 31.0, 53.0, 62.9, 64.6, 121.1, 122.9, 123.1, 123.7, 124.2, 127.5, 128.6, 130.8 141.9, 145.6, 148.1, 153.6; HRMS Calcd for $C_{22}H_{29}N_3O_3P^+$ (ESI, $M+H^+$): 414.1941; found: 414.1940.

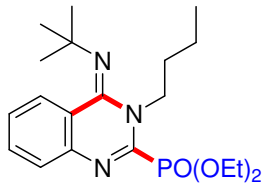


Diethyl (*E*)-4-(*tert*-butylimino)-3,4-dihydro-3-*p*-tolylquinazolin-2-yl-2-phosphonate (**4c**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.12 (t, *J* = 7.2 Hz, 3H), 1.22 (s, 9H), 1.35 (t, *J* =

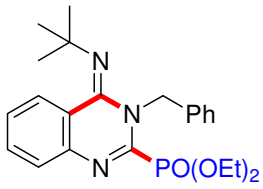
7.2 Hz, 3H), 2.40 (s, 3H), 3.64-3.70 (m, 1H), 3.85-3.93 (m, 1H), 4.23-4.26 (m, 2H), 7.00-7.03 (m, 1H), 7.24-7.41 (m, 3H), 7.60 (d, J = 8.0 Hz, 2H), 7.84 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.3, 16.5, 20.2, 31.2, 53.1, 63.2, 63.9, 122.5, 126.2, 128.9, 129.3, 129.8, 131.8, 133.2, 138.7, 142.8, 146.9, 149.5, 152.0; HRMS Calcd for $C_{23}H_{31}N_3O_3P^+$ (ESI, M+H$^+$): 428.2098; found: 428.2135.



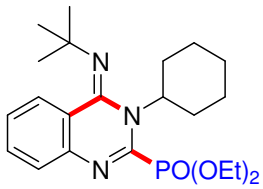
Diethyl (*E*)-4-(*tert*-butylimino)-3-(4-chlorophenyl)-3,4-dihydroquinazolin-2-yl-2-phosphonate (**4d**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.12 (t, J = 7.2 Hz, 3H), 1.21 (s, 9H), 1.34 (t, J = 7.2 Hz, 3H), 3.64-3.70 (m, 1H), 3.85-3.89 (m, 1H), 4.23-4.26 (m, 2H), 7.00-7.04 (m, 1H), 7.22-7.41 (m, 3H), 7.50-7.54 (m, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.97 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.1, 16.3, 31.0, 53.0, 62.9, 64.6, 122.3, 126.1, 128.1, 128.8, 129.1, 129.7, 131.2, 132.9, 138.5, 146.5, 149.2, 151.8; HRMS Calcd for $C_{22}H_{28}ClN_3O_3P^+$ (ESI, M+H$^+$): 448.1551; found: 448.1553.



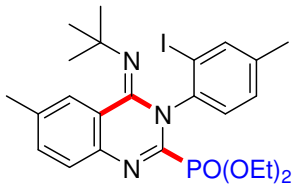
Diethyl (*E*)-4-(*tert*-butylimino)-3-butyl-3,4-dihydroquinazolin-2-yl-2-phosphonate (**4e**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.94 (t, J = 7.2 Hz, 3H), 1.25-1.38 (m, 8H), 1.41 (s, 9H), 1.55-1.62 (m, 2H), 4.29-4.36 (m, 6H), 7.25-7.27 (m, 1H), 7.46-7.48 (m, 2H), 7.93 (d, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 16.3, 16.3, 20.3, 30.1, 31.7, 46.5, 53.3, 64.0, 64.1, 121.2, 125.2, 127.8, 129.3, 131.1, 146.8, 149.8, 152.4, ; HRMS Calcd for $C_{20}H_{33}N_3O_3P^+$ (ESI, M+H$^+$): 394.2254; found: 394.2265.



Diethyl (*E*)-4-(*tert*-butylimino)-3-benzyl-3,4-dihydroquinazolin-2-yl-2-phosphonate (**4f**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.26-1.37 (m, 15H), 4.22-4.24 (m, 4H), 5.53 (s, 2H), 7.15-7.27 (m, 6H), 7.49-7.53 (m , 2H), 7.84 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.0, 31.3, 49.6, 53.2, 64.1, 121.4, 125.4, 126.2, 127.1, 127.7, 127.8, 129.2, 131.2, 138.3, 150.2, 152.7; HRMS Calcd for $C_{23}H_{31}N_3O_3P^+$ (ESI, M+H$^+$): 428.2098; found: 428.2098.

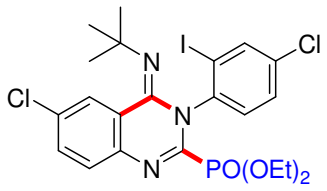


Diethyl (*E*)-4-(*tert*-butylimino)-3-cyclohexyl-3,4-dihydroquinazolin-2-yl-2-phosphonate (**4g**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.38-1.41 (m, 17H), 1.78-1.86 (m, 6H), 2.72-2.78 (m, 2H), 4.29-4.33 (m, 5H), 7.18-7.20 (m, 1H), 7.40-7.41 (m , 2H), 7.72 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.3, 16.4, 25.9, 26.8, 30.7, 31.7, 31.9, 54.3, 63.3, 64.0, 64.1, 122.1, 124.7, 126.6, 128.4, 130.8, 146.7, 150.4, 152.9; HRMS Calcd for $C_{22}H_{34}N_3NaO_3P^+$ (ESI, M+Na$^+$): 442.2230; found: 442.2248.

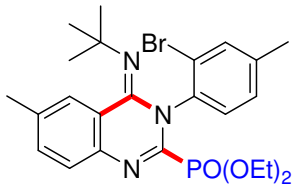


Diethyl (*E*)-4-(*tert*-butylimino)-3,4-dihydro-3-(2-iodo-4-methylphenyl)-6-methylquinazolin-2-yl-2-phosphonate (**4h**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.14 (t, *J* = 7.2 Hz, 3H), 1.23 (s, 9H), 1.36 (t, *J* = 7.2 Hz, 3H), 2.41 (s, 3H), 2.45 (s, 3H), 3.66-3.70 (m, 1H), 3.87-3.91 (m, 1H), 4.24-4.28 (m, 2H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.33-7.35 (m, 2H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.87 (s, 1H), 7.93 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.1, 16.3, 20.6, 20.6, 31.0, 52.9, 63.0, 64.6, 122.3, 126.0, 128.1, 128.7, 128.8, 129.1,

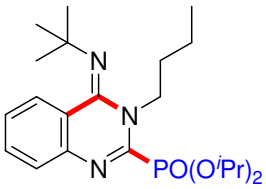
129.7, 131.7, 133.0, 138.6, 140.4, 142.6, 146.5; HRMS Calcd for $C_{24}H_{32}IN_3O_3P^+$ (ESI, M+H$^+$):568.1220; found: 568.1220.



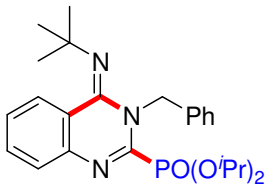
Diethyl (*E*)-4-(*tert*-butylimino)-6-chloro-3-(4-chloro-2-iodophenyl)-3,4-dihydroquinazolin-2-yl-2-phosphonate (**4i**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.16 (t, *J* = 7.2 Hz, 3H), 1.23 (s, 9H), 1.36 (t, *J* = 7.2 Hz, 3H), 3.78-3.82 (m, 1H), 3.92-3.98 (m, 1H), 4.22-4.26 (m, 2H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.48-7.52 (m, 2H), 7.83 (s, 1H), 7.93 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.0, 16.2, 30.9, 53.2, 63.2, 63.7, 102.5, 122.9, 128.2, 129.2, 130.0, 131.6, 131.9, 133.4, 133.9, 137.8, 139.1, 140.9, 144.8, 151.7; HRMS Calcd for $C_{22}H_{26}Cl_2IN_3O_3P^+$ (ESI, M+H$^+$): 608.0128; found: 608.0122.



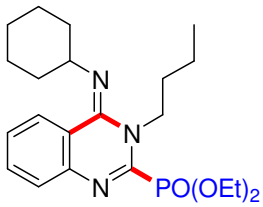
Diethyl (*E*)-4-(*tert*-butylimino)-3-(2-bromo-4-methylphenyl)-3,4-dihydro-6-methylquinazolin-2-yl-2-phosphonate (**4j**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.14 (t, *J* = 7.2 Hz, 3H), 1.23 (s, 9H), 1.36 (t, *J* = 7.2 Hz, 3H), 2.40 (s, 3H), 2.44 (s, 3H), 3.76-3.79 (m, 1H), 3.87-3.91 (m, 1H), 4.31-4.38 (m, 2H), 7.09 (d, *J* = 7.6 Hz, 1H), 7.27-7.33 (m, 2H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.86 (s, 1H), 7.95 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.3, 16.5, 20.6, 21.3, 31.2, 53.5, 63.4, 65.0, 102.8, 123.3, 128.5, 129.5, 130.3, 131.9, 132.2, 133.7, 134.2, 138.2, 141.3, 152.1; HRMS Calcd for $C_{24}H_{32}BrN_3O_3P^+$ (ESI, M+H$^+$):520.1359; found: 520.1359.



Dipropyl (*E*)-4-(*tert*-butylimino)-3-butyl-3,4-dihydroquinazolin-2-yl-2-phosphonate (**4k**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.94 (t, *J* = 7.6 Hz, 3H), 1.38-1.49 (m, 23H), 1.68-1.73 (m, 2H), 4.27 (t, *J* = 7.2 Hz, 2H), 4.87-4.91 (m, 2H), 7.23-7.26 (m, 1H), 7.43-7.47 (m, 2H), 7.91 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 20.3, 23.7, 23.7, 24.2, 24.2, 29.6, 31.8, 46.5, 53.3, 121.2, 125.0, 127.6, 129.3, 131.1, 146.9, 150.4, 152.9; HRMS Calcd for $C_{22}H_{37}N_3O_3P^+$ (ESI, M+H$^+$): 422.2567; found: 422.2565.

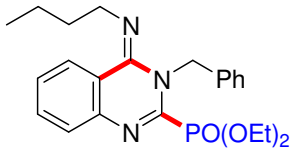


Dipropyl (*E*)-4-(*tert*-butylimino)-3-benzyl-3,4-dihydroquinazolin-2-yl-2-phosphonate (**4l**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.25 (s, 9H), 1.34 (s, 6H), 1.35 (s, 6H), 4.83-4.91 (m, 2H), 5.52 (s, 2H), 7.13-7.26 (m, 6H), 7.46-7.49 (m, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.4, 24.0, 31.2, 49.8, 53.2, 73.2, 73.3, 121.4, 125.2, 126.1, 127.2, 127.6, 129.2, 131.1, 138.5, 139.5, 146.5, 153.3; HRMS Calcd for $C_{25}H_{35}N_3O_3P^+$ (ESI, M+H$^+$): 456.2411; found: 456.2413.

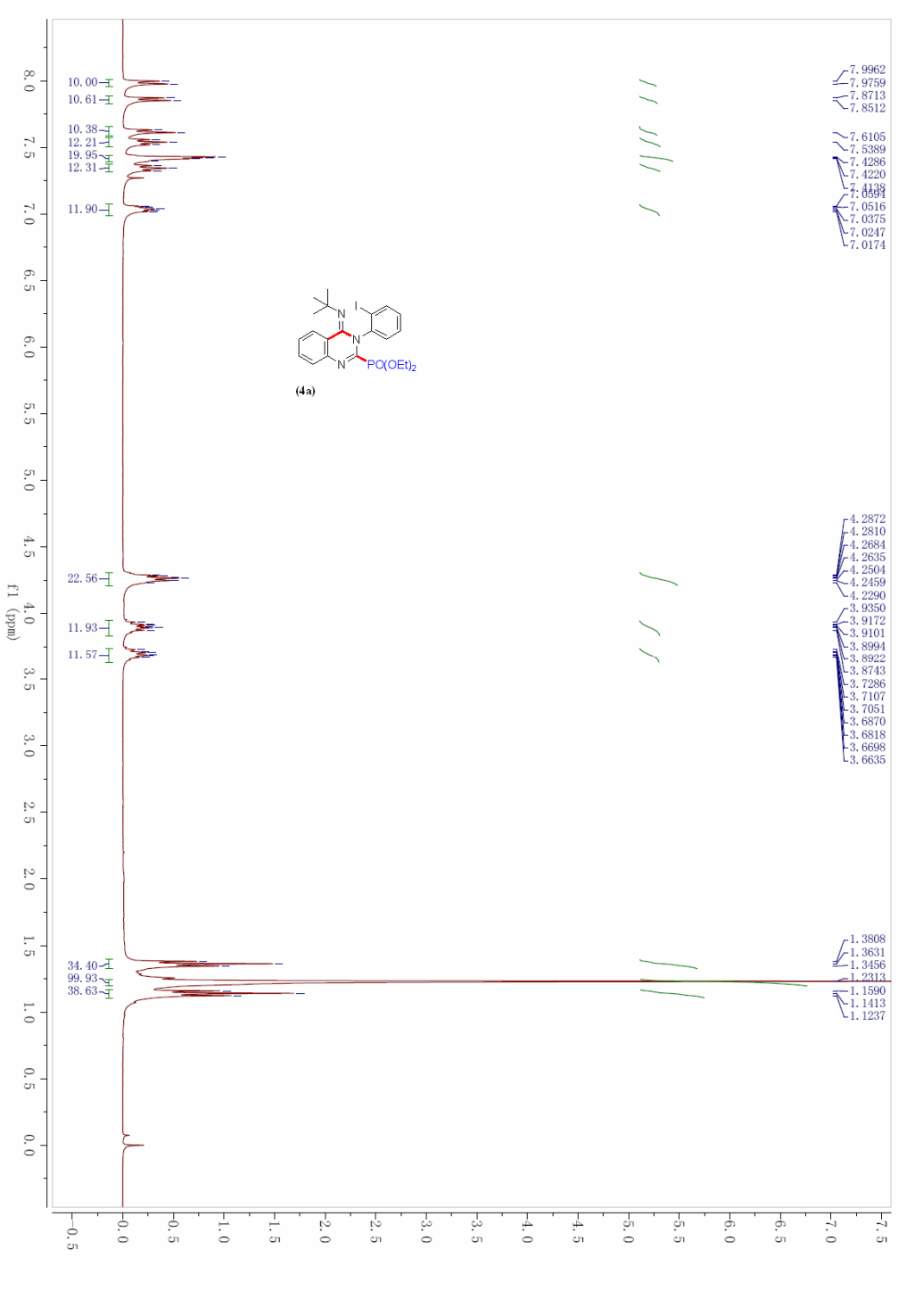


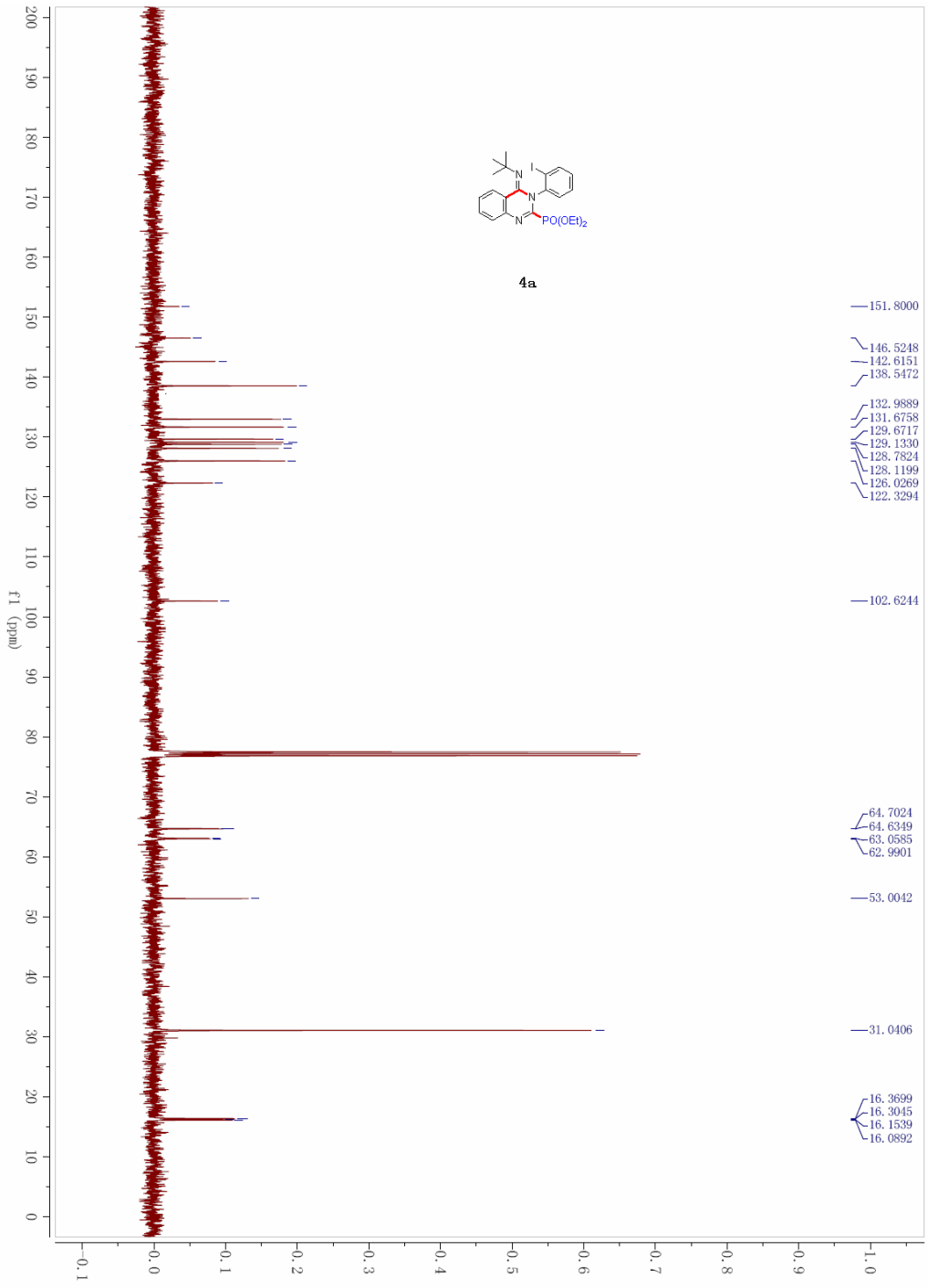
Diethyl (*E*)-3-butyl-4-(cyclohexylimino)-3,4-dihydroquinazolin-2-yl-2-phosphonate (**4m**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.94 (t, *J* = 6.4 Hz, 3H), 1.25-1.45 (m, 15H), 1.81-1.83 (m, 5H), 4.03-4.05 (m, 1H), 4.30-4.33 (m, 6H), 7.26-7.26 (m, 1H), 7.48-7.51 (m, 2H), 7.78 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.9, 16.3, 16.4, 20.3, 24.4, 26.1, 29.9, 35.0, 46.5, 56.3, 64.1, 64.1, 120.8, 126.1, 127.3, 128.3,

131.3, 146.2, 149.3, 151.9; HRMS Calcd for $C_{22}H_{35}N_3O_3P^+$ (ESI, $M+H^+$):420.2411 ; found: 420.2414.



Diethyl (*E*)-3-benzyl-4-(butylimino)-3,4-dihydroquinazolin-2-yl-2-phosphonate (**4n**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.82 (t, *J* = 7.6 Hz, 3H), 1.20-1.28 (m, 8H), 1.47-1.54 (m, 2H), 3.68-3.71 (m, 2H), 4.20-4.27 (m, 4H), 5.63 (s, 2H), 7.14-7.31 (m, 6H), 7.50-7.54 (m, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.8, 15.9, 16.0, 20.2, 35.1, 49.3, 50.4, 64.0, 64.1, 121.6, 126.0,126.3, 126.9, 127.7, 128.3, 131.4, 138.0, 143.5, 135.9; HRMS Calcd for $C_{23}H_{31}N_3O_3P^+$ (ESI, $M+H^+$): 428.2098 ; found: 428.2111.

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16.3045
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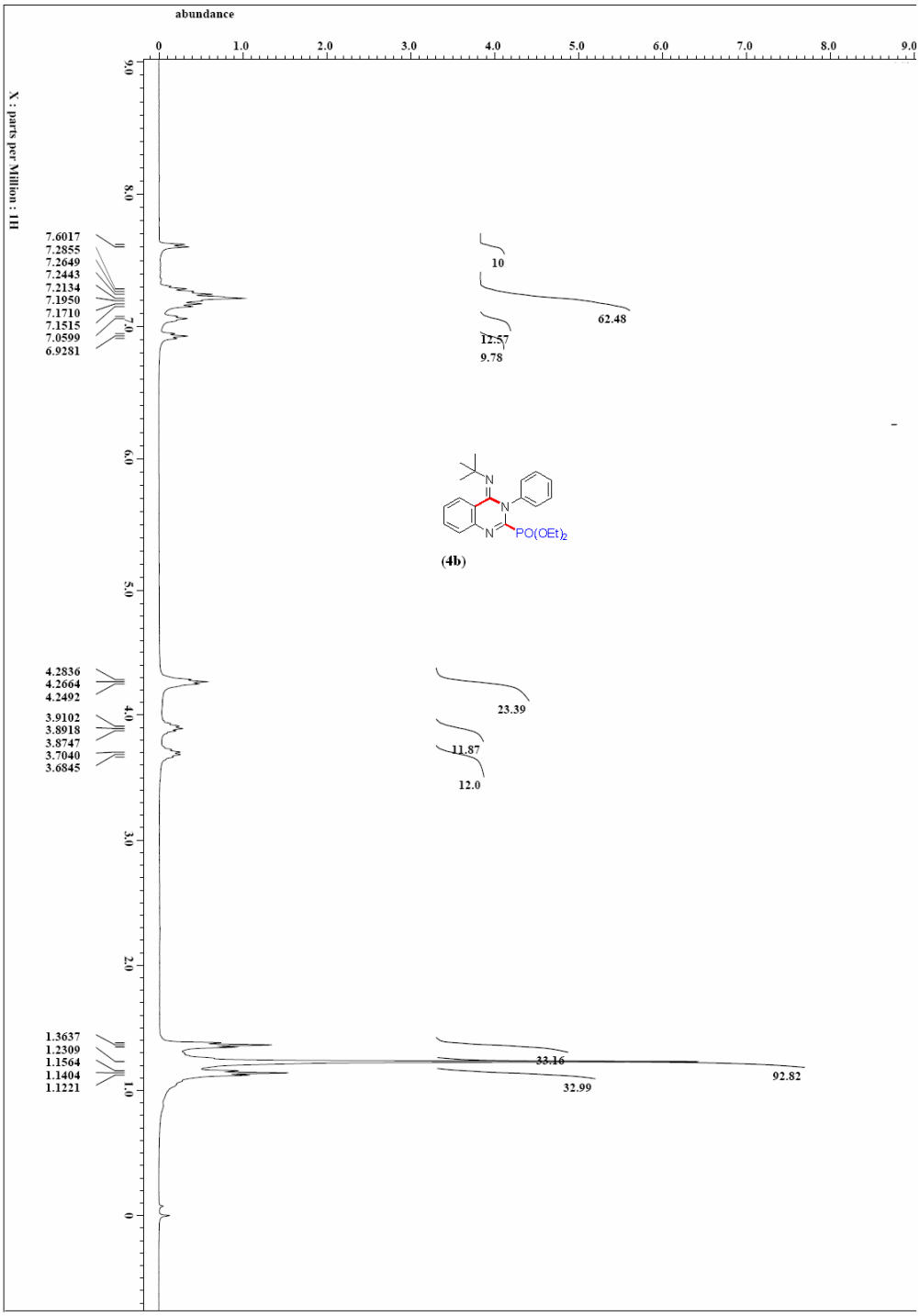
16.0892
f1 (ppm)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7.1950
7.1710
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6.9281
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4.2664
4.2492
3.9102
3.8918
3.8747
3.7040
3.6845
1.3637
1.2309
1.1564
1.1404
1.1221
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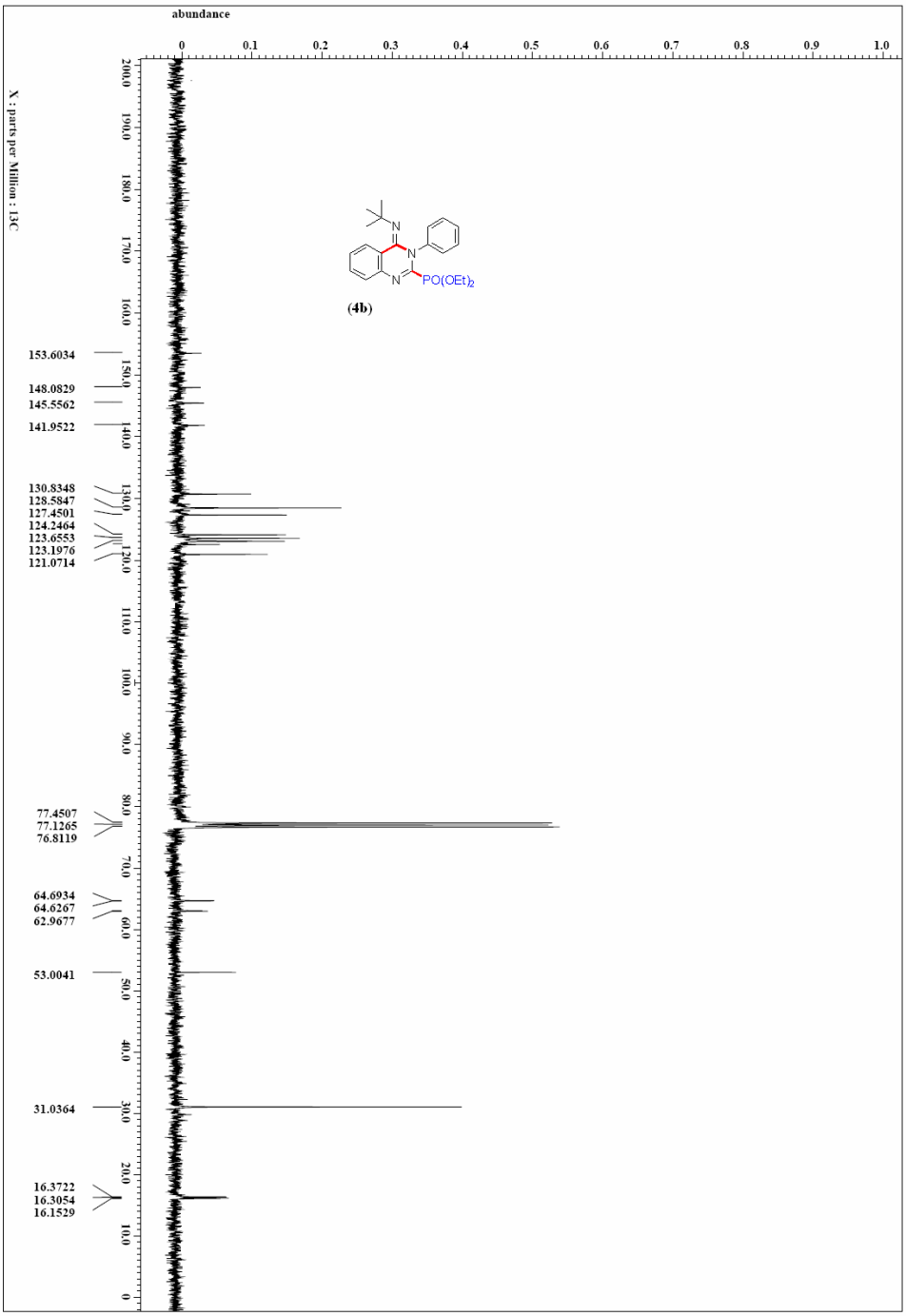
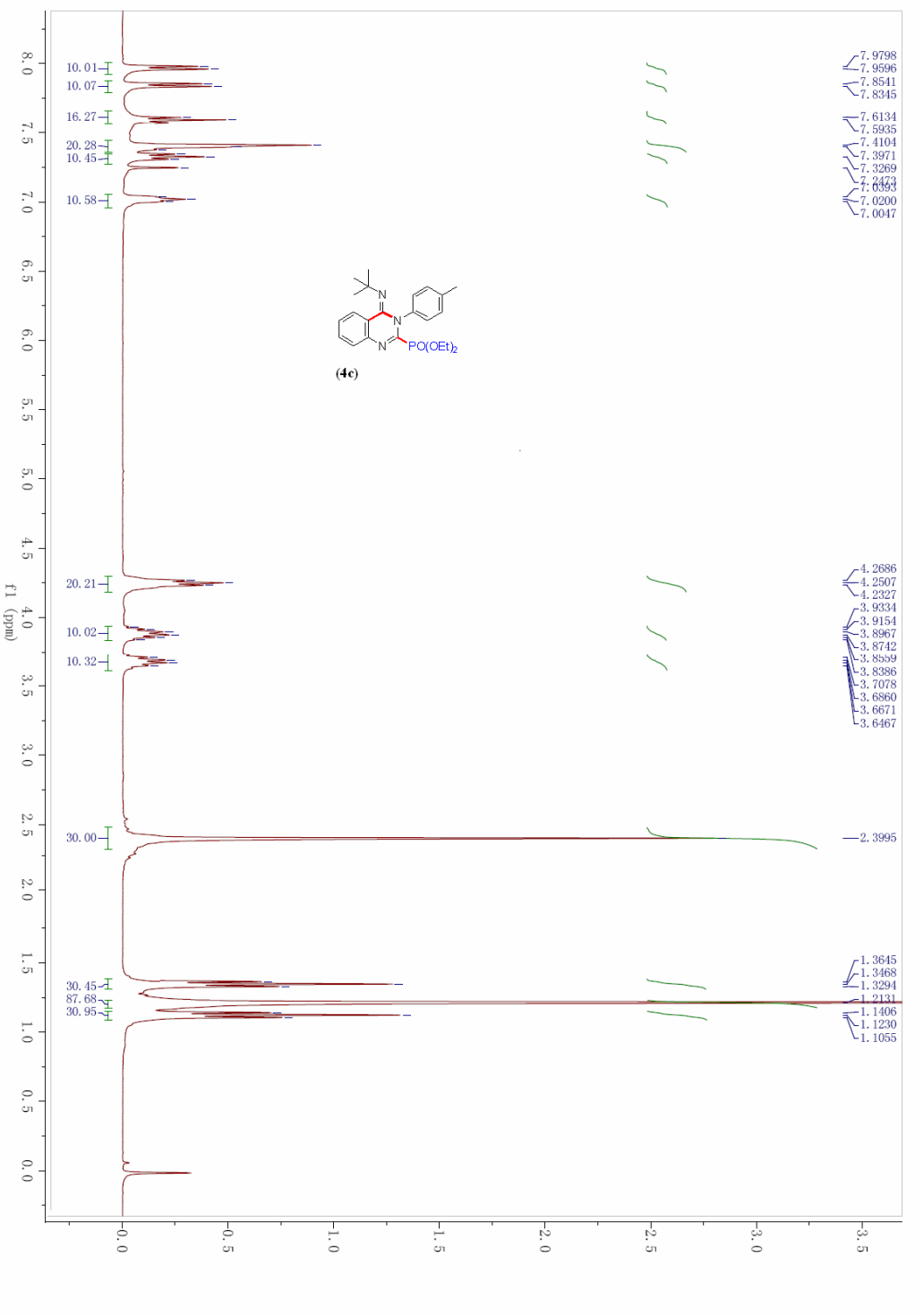
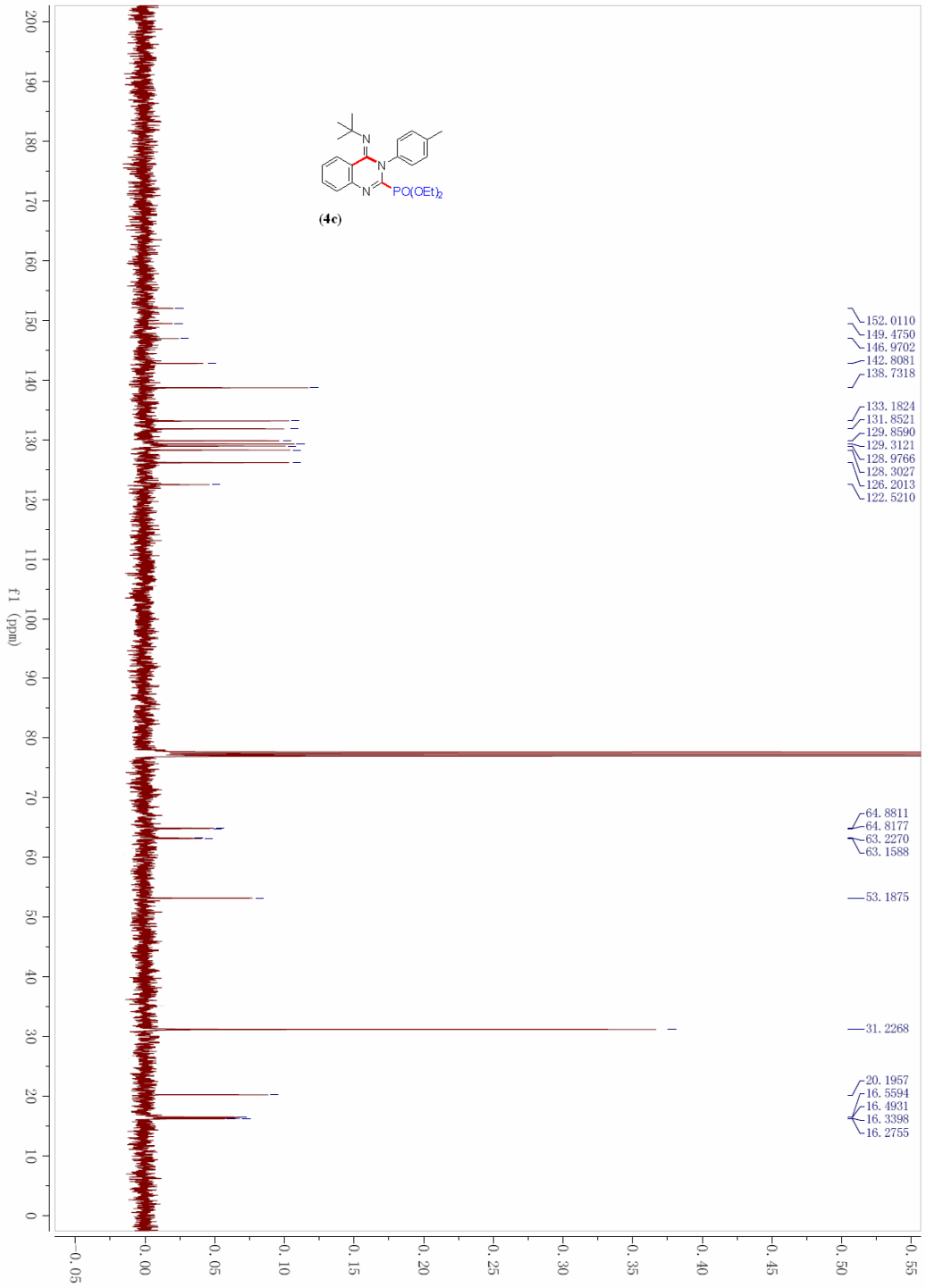
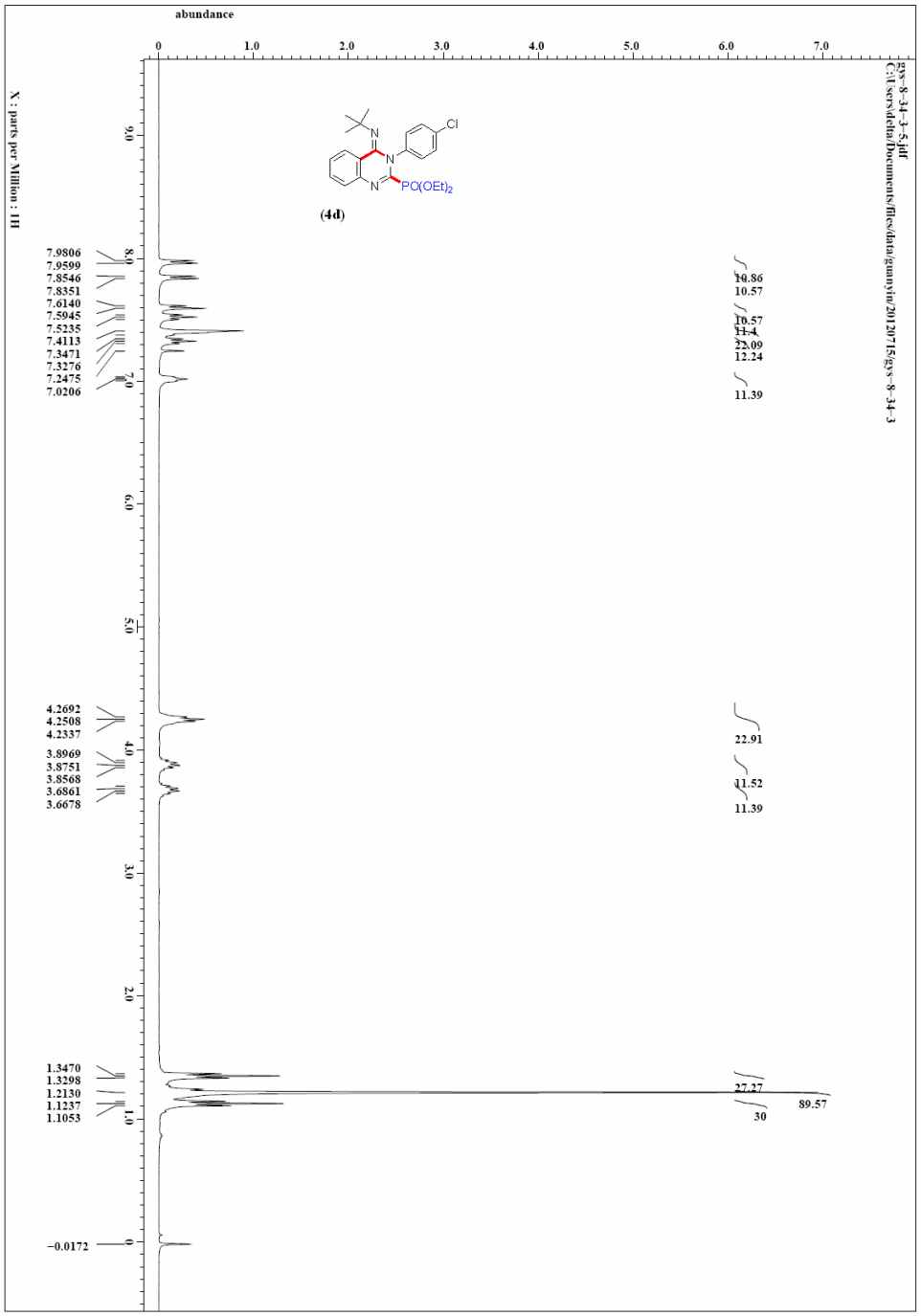
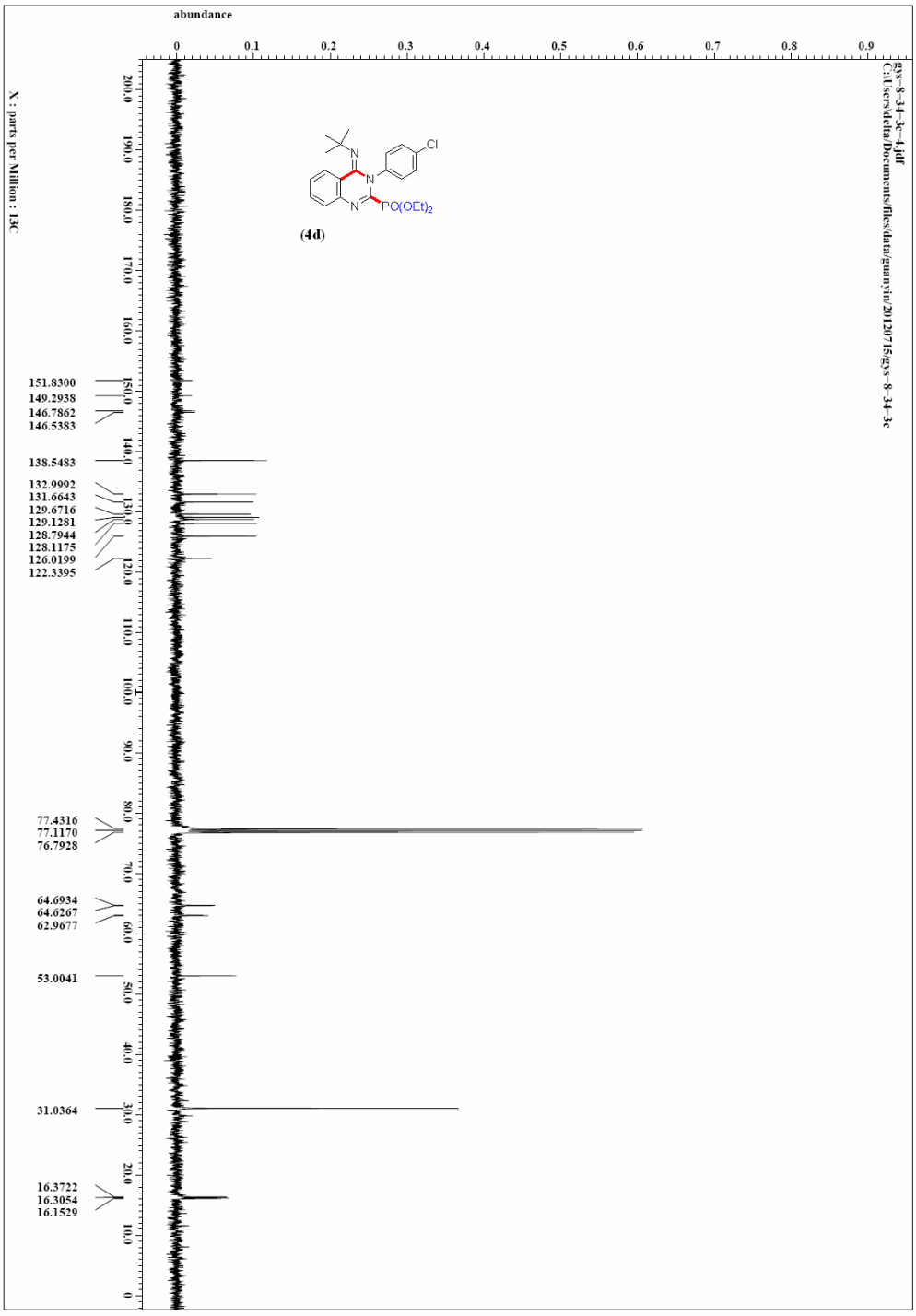
92.82

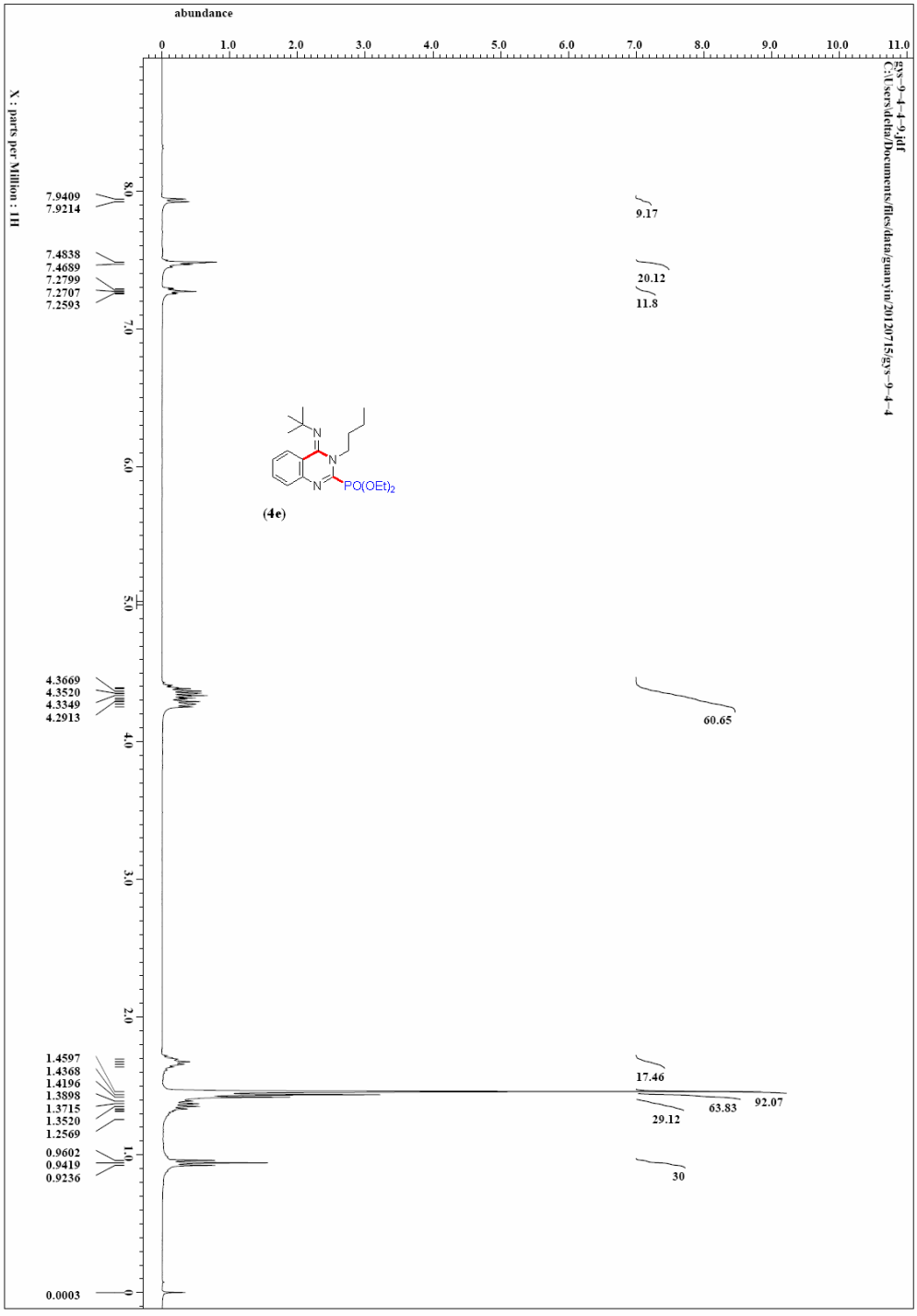


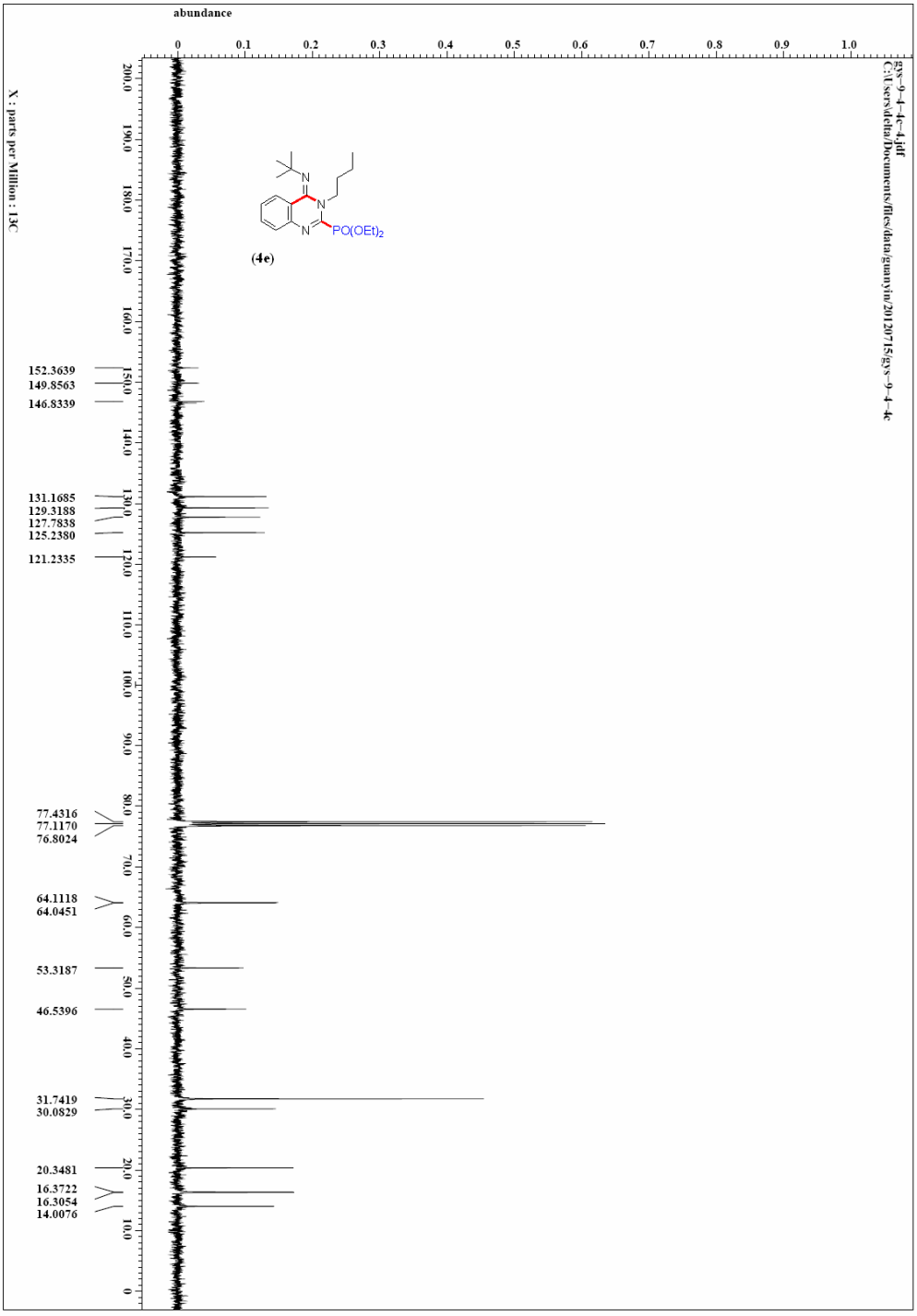


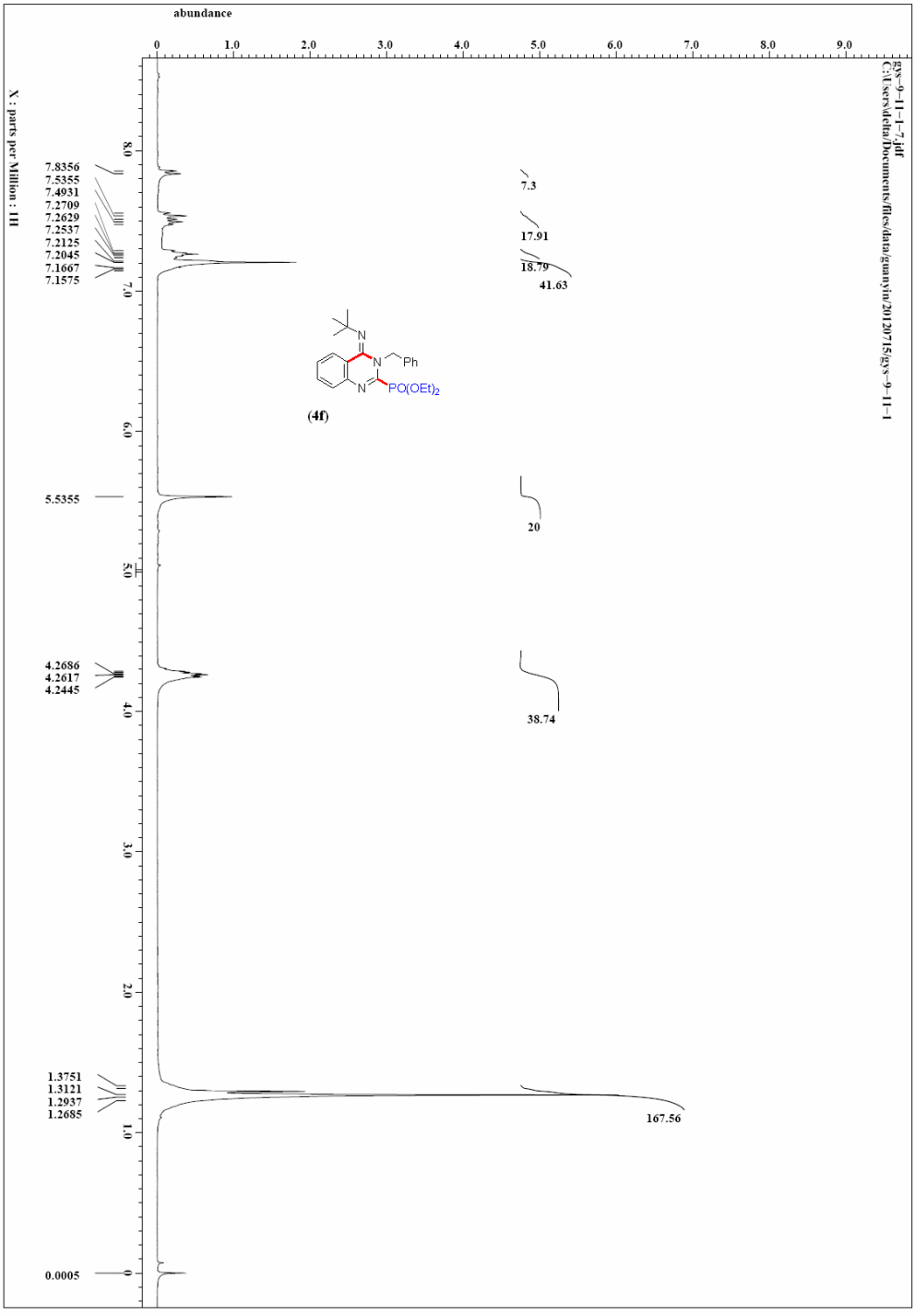


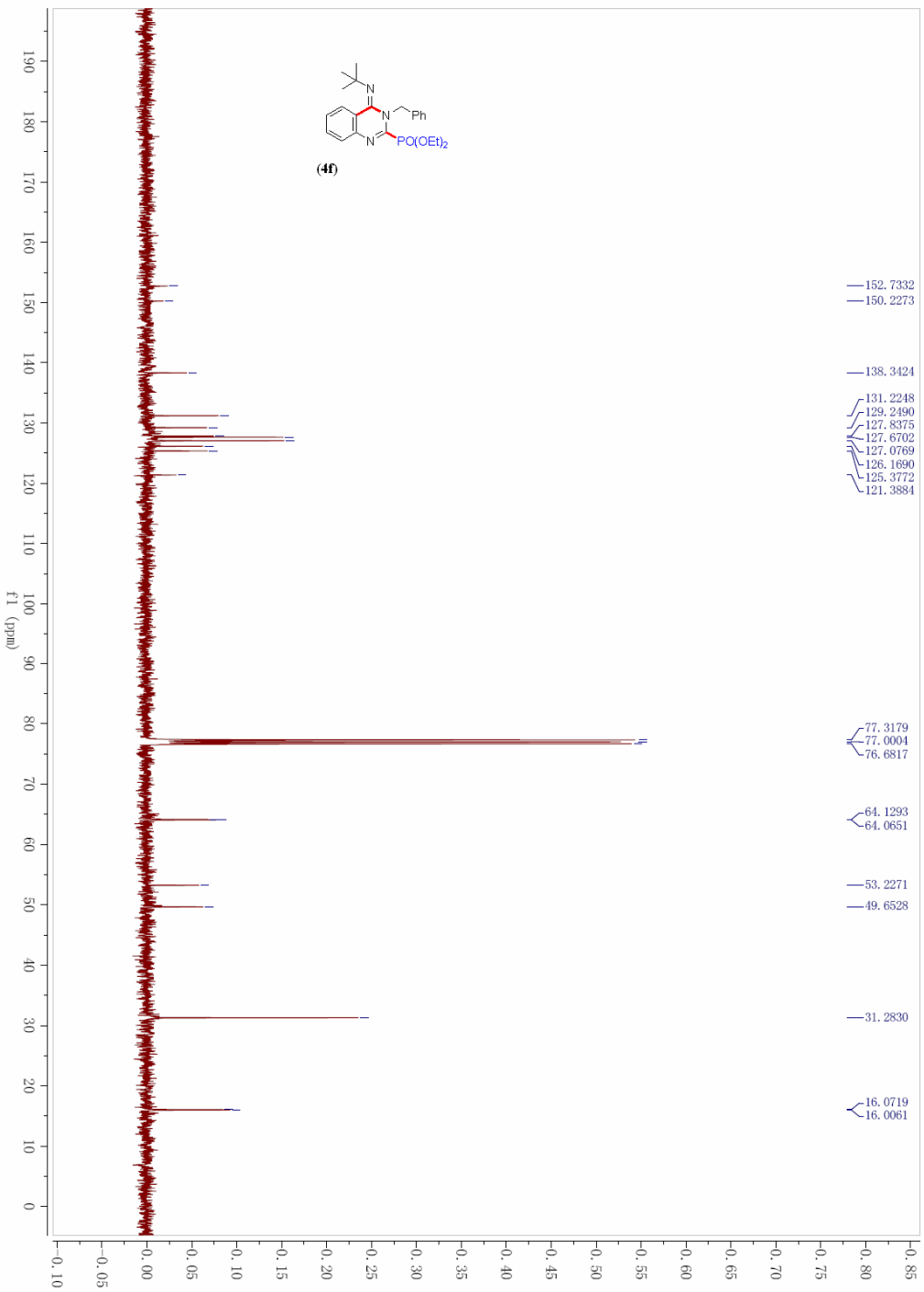


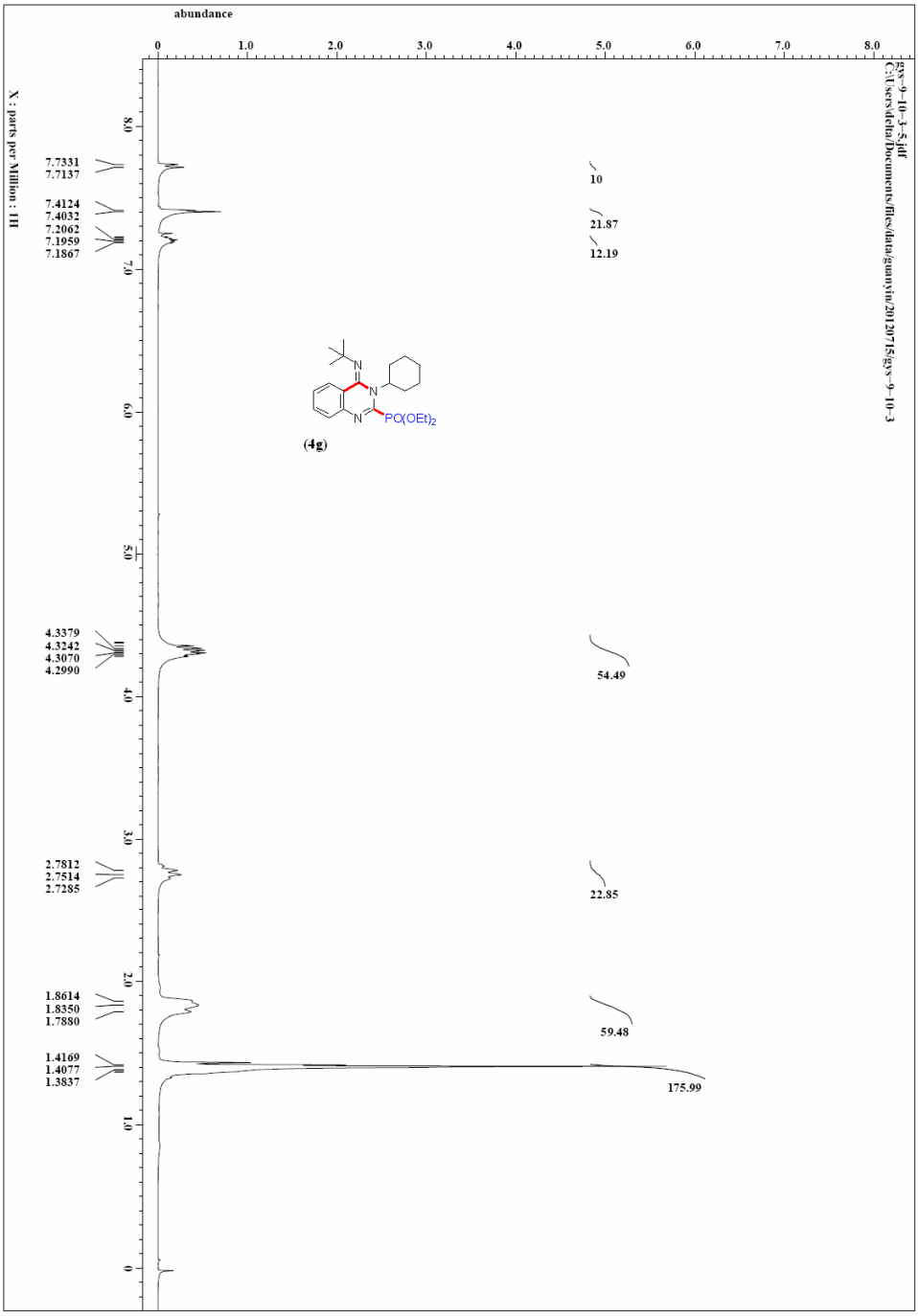

abundance
X : parts per Million : 13C
gsy-8-34-3c-4.jdf
C:\Users\dcfta\Documents\files\data\gsunyin\20120715\gsy-8-34-3c
(4d)
151.8300
149.2938
146.7862
146.5383
138.5483
132.9992
131.6643
129.6716
129.1281
128.7944
128.1175
126.0199
122.3395
77.4316
77.1170
76.7928
64.6934
64.6267
62.9677
53.0041
31.0364
16.3722
16.3054
16.1529

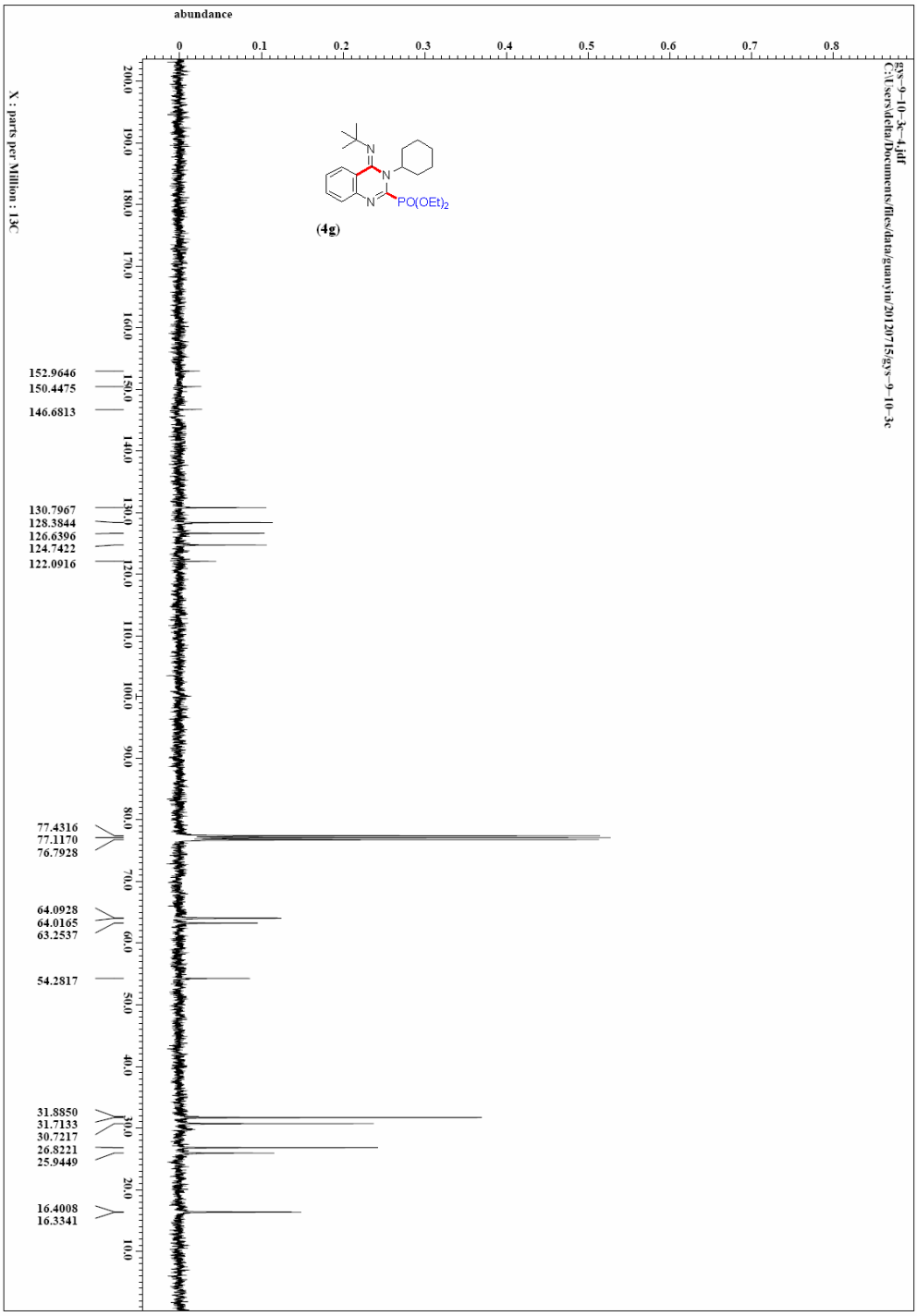

abundance
X : parts per Million : 1H
gys-9-4-4-9.jdf
C:\Users\delta\Documents\files\data\guanyin\20120715\gys-9-4-4
7.9409
7.9214
7.4838
7.4689
7.2799
7.2707
7.2593
4.3669
4.3520
4.3349
4.2913
1.4597
1.4368
1.4196
1.3898
1.3715
1.3520
1.2569
0.9602
0.9419
0.9236
0.0003
9.17
20.12
11.8
60.65
17.46
92.07
63.83
29.12
30
PO(OEt)2
(4e)

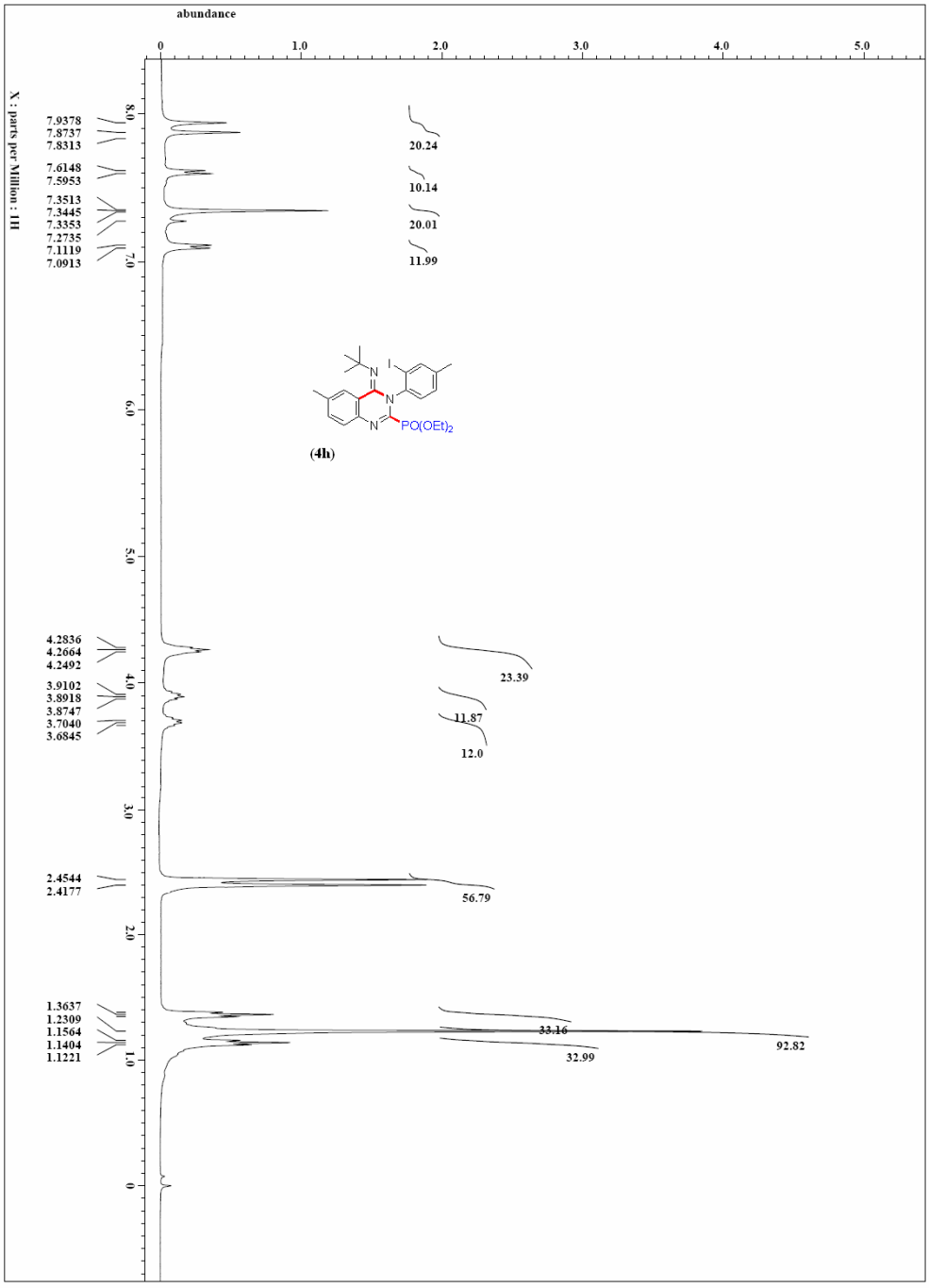


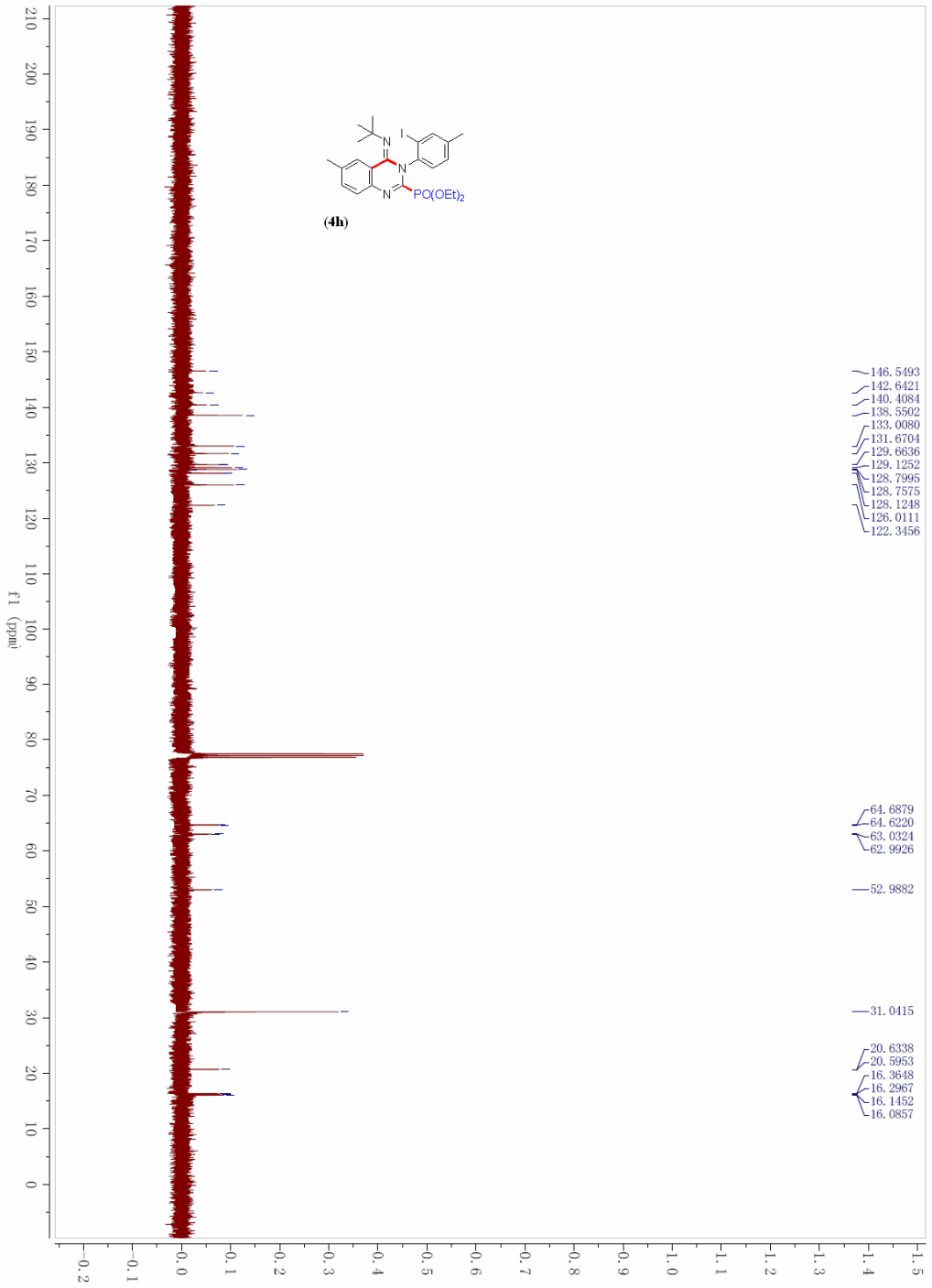

abundance
X : parts per Million : 1H
gys-9-11-1-7.jdf
C:\Users\delta\Documents\files\data\guanyin\20120715\gys-9-11-1
7.8356
7.5355
7.4931
7.2709
7.2629
7.2537
7.2125
7.2045
7.1667
7.1575
5.5355
4.2686
4.2617
4.2445
1.3751
1.3121
1.2937
1.2685
0.0005
7.3
17.91
18.79
41.63
20
38.74
167.56
Ph
PO(OEt)2
(4f)

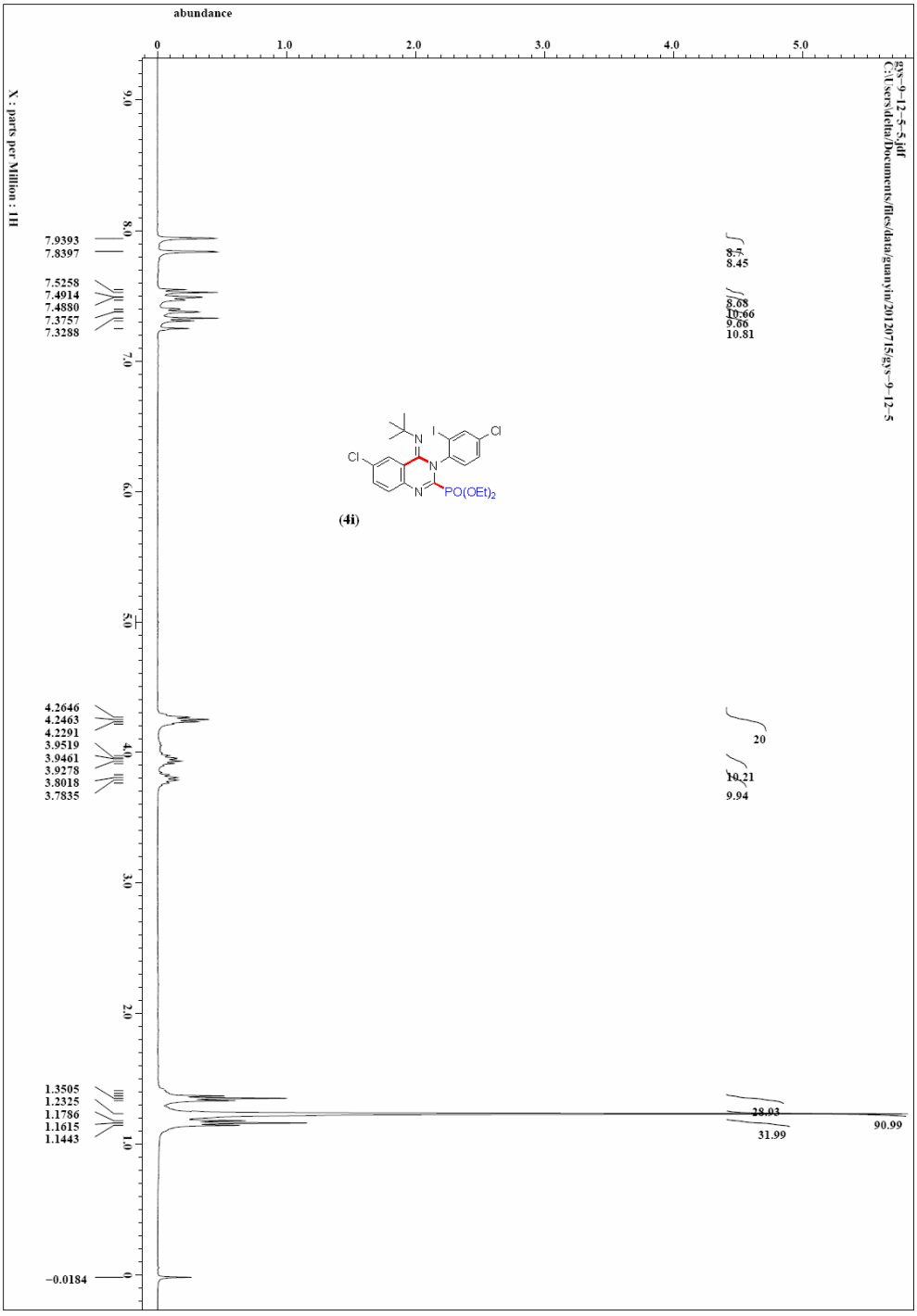

(4f)
152.7332
150.2273
138.3424
131.2248
129.2490
127.8375
127.6702
127.0769
126.1690
125.3772
121.3884
77.3179
77.0004
76.6817
64.1293
64.0651
53.2271
49.6528
31.2830
16.0719
16.0061
f1 (ppm)

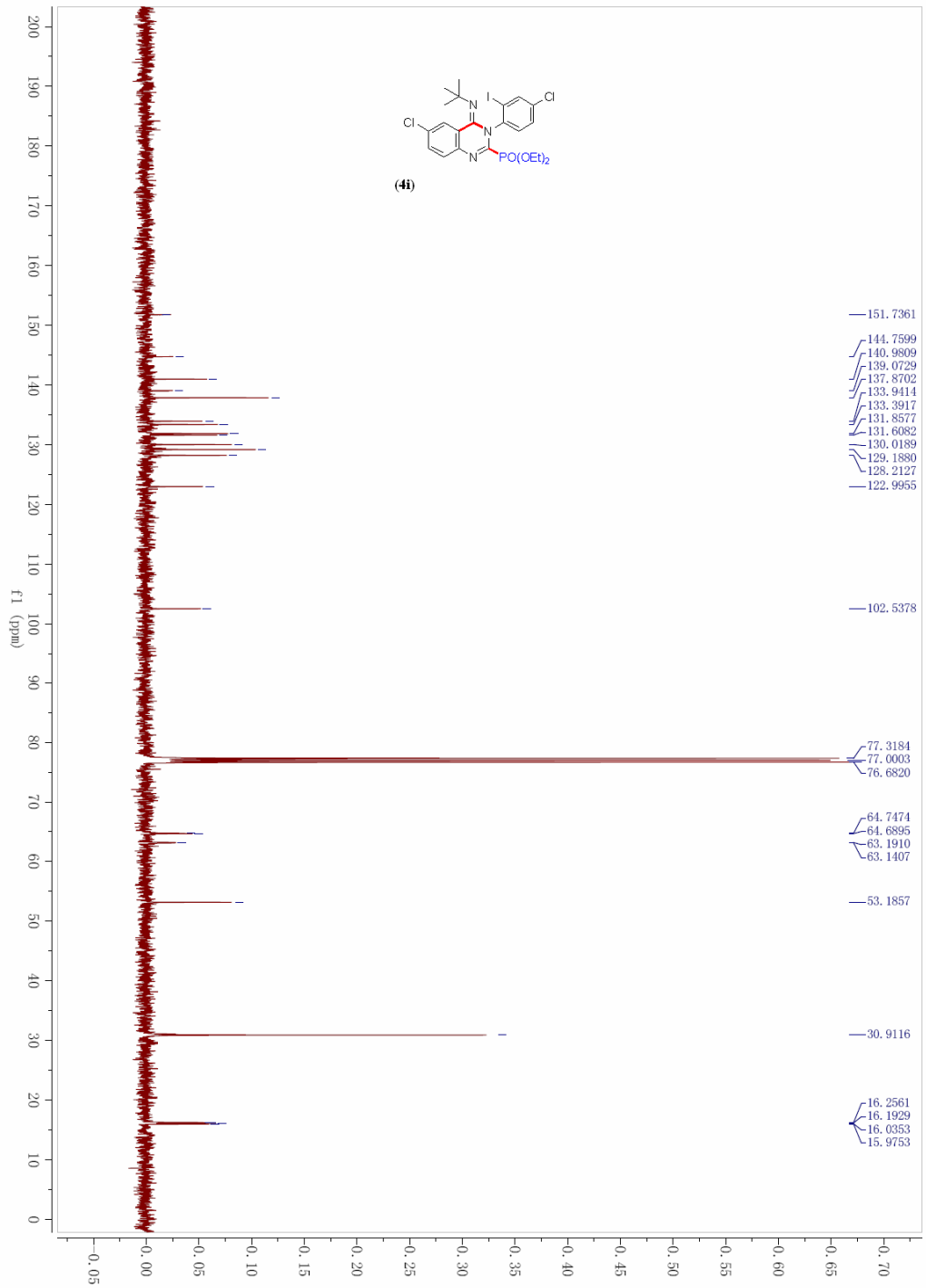


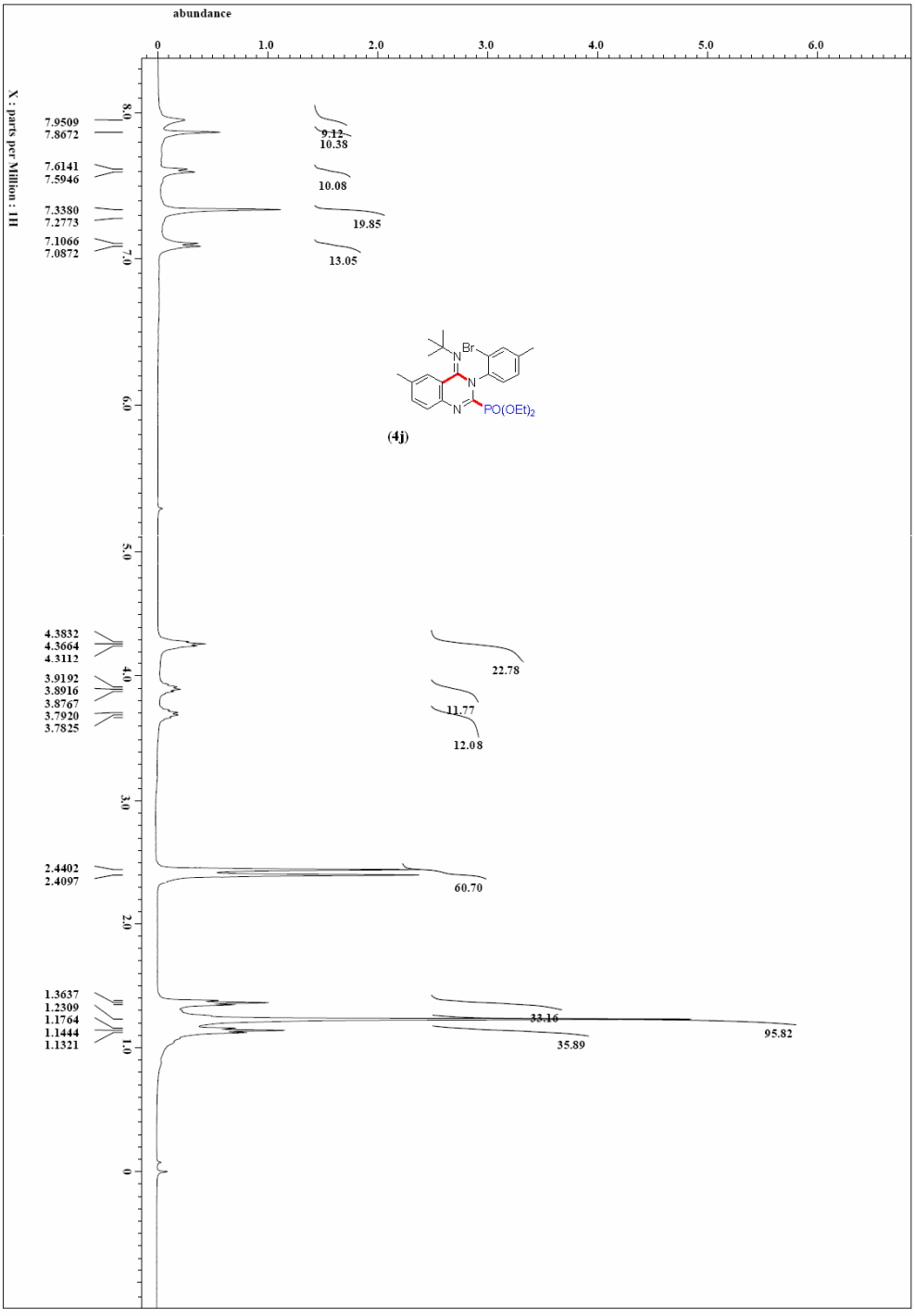

abundance
X : parts per Million : 13C
gys-9-10-3c-4.jdf
C:\Users\delta\Documents\files\data\guanyin\20120715\gys-9-10-3c
PO(OEt)2
(4g)
152.9646
150.4475
146.6813
130.7967
128.3844
126.6396
124.7422
122.0916
77.4316
77.1170
76.7928
64.0928
64.0165
63.2537
54.2817
31.8850
31.7133
30.7217
26.8221
25.9449
16.4008
16.3341

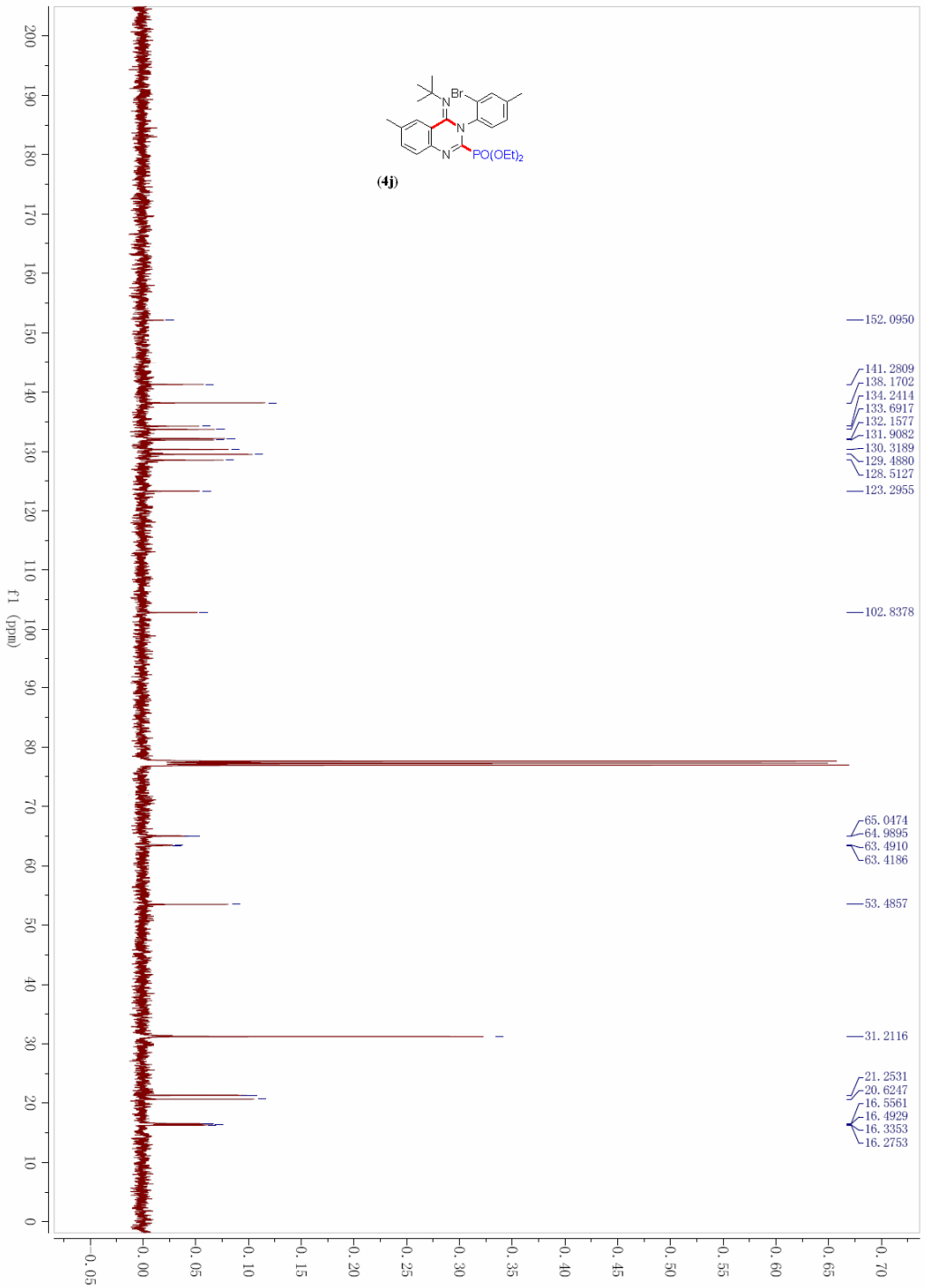


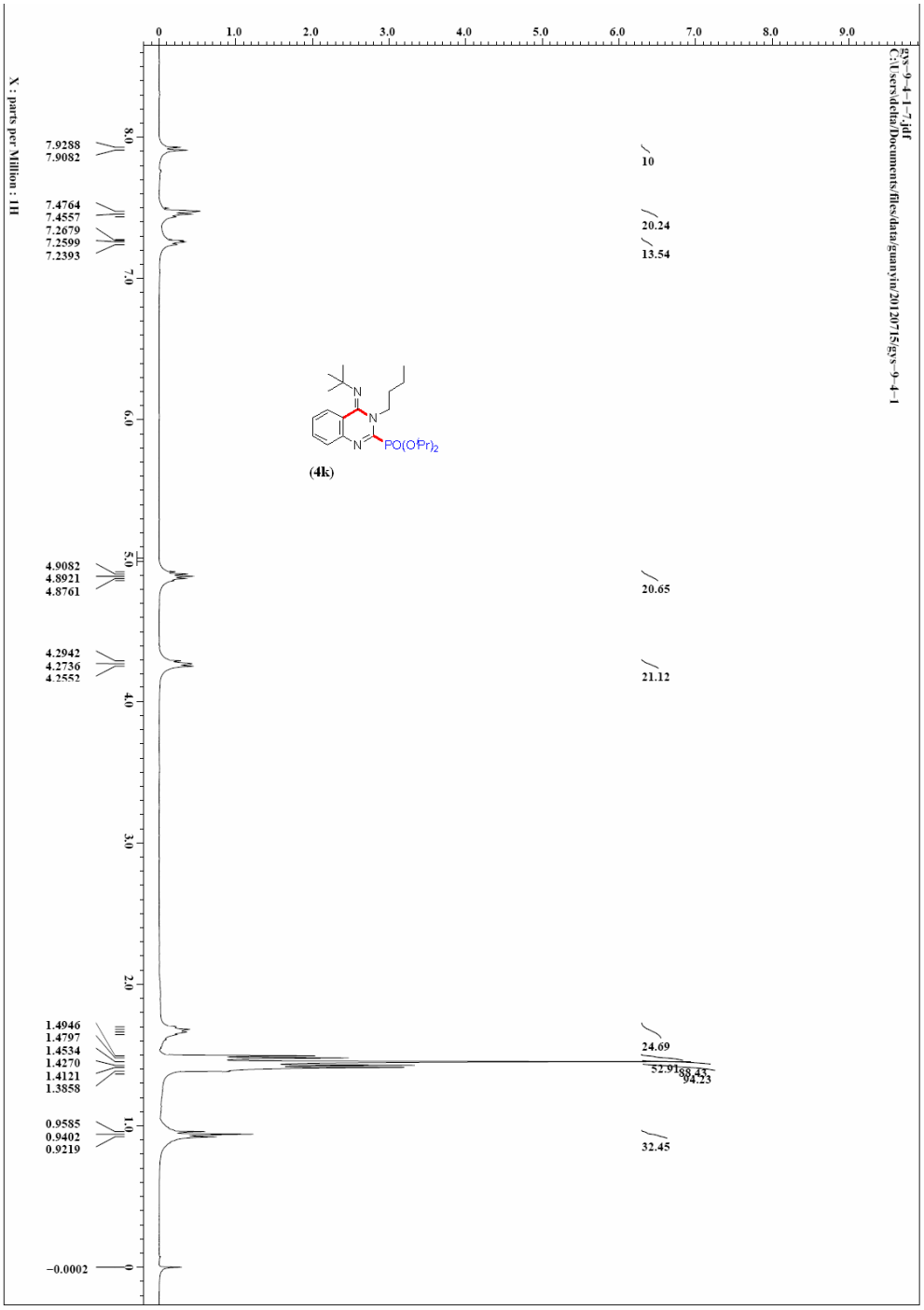


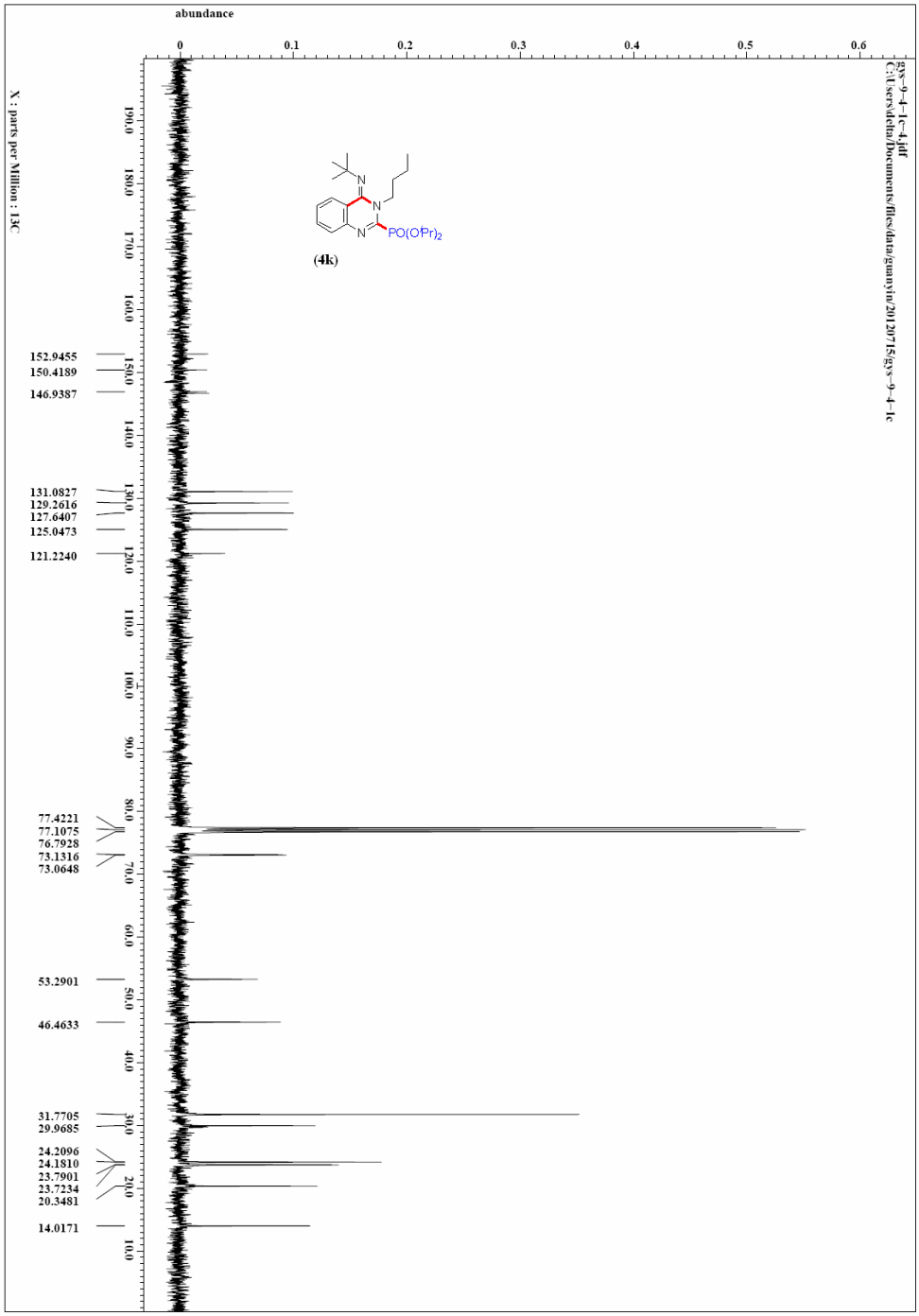

abundance
X : parts per Million : 1H
gsx~9~12~5~5.jdf
C:\Users\delta\Documents\flies\data\guanyin\20120715\gsx~9~12~5
7.9393
7.8397
7.5258
7.4914
7.4880
7.3757
7.3288
4.2646
4.2463
4.2291
3.9519
3.9461
3.9278
3.8018
3.7835
1.3505
1.2325
1.1786
1.1615
1.1443
−0.0184
8.57
8.45
8.08
10.66
9.06
10.81
20
10.21
9.94
28.03
31.99
90.99
PO(OEt)2
(4i)

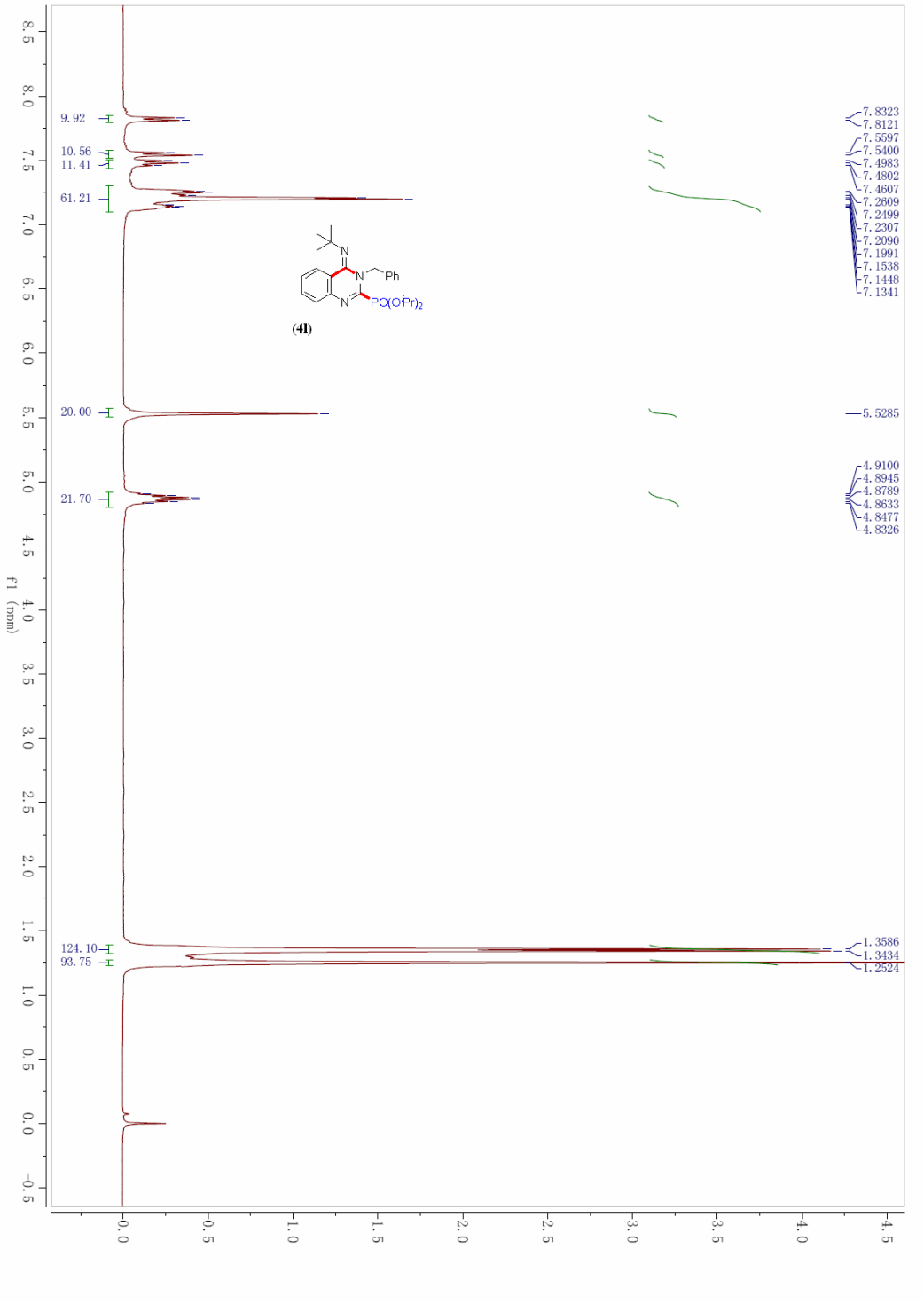

(4i)
151.7361
144.7599
140.9809
139.0729
137.8702
133.9414
133.3917
131.8577
131.6082
130.0189
129.1880
128.2127
122.9955
102.5378
77.3184
77.0003
76.6820
64.7474
64.6895
63.1910
63.1407
53.1857
30.9116
16.2561
16.1929
16.0353
15.9753
f1 (ppm)


abundance
X : parts per Million : 1H
7.9509
7.8672
7.6141
7.5946
7.3380
7.2773
7.1066
7.0872
4.3832
4.3664
4.3112
3.9192
3.8916
3.8767
3.7920
3.7825
2.4402
2.4097
1.3637
1.2309
1.1764
1.1444
1.1321
9.12
10.38
10.08
19.85
13.05
22.78
11.77
12.08
60.70
33.16
95.82
35.89
Br
N
N
N
PO(OEt)2
(4j)

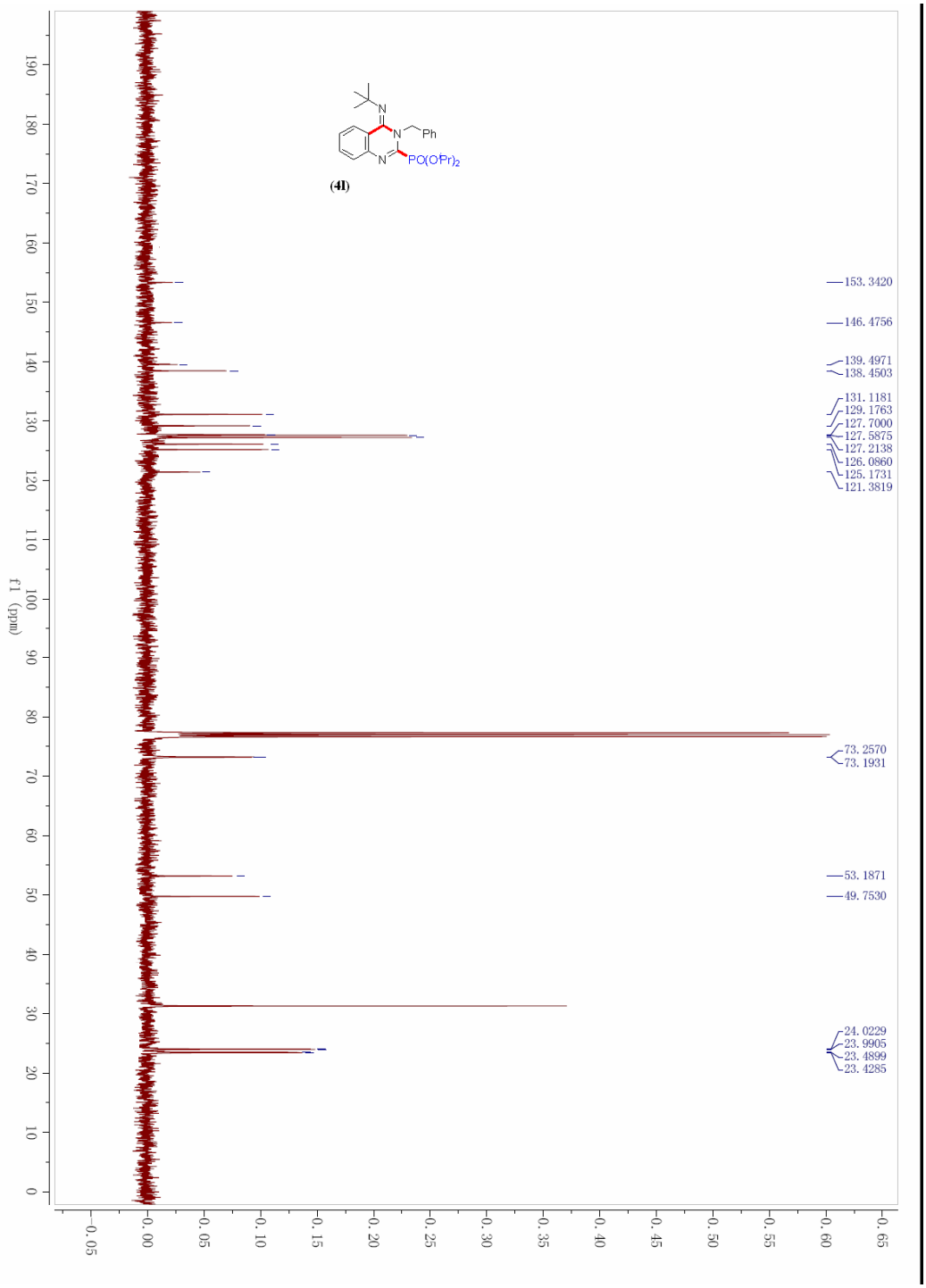


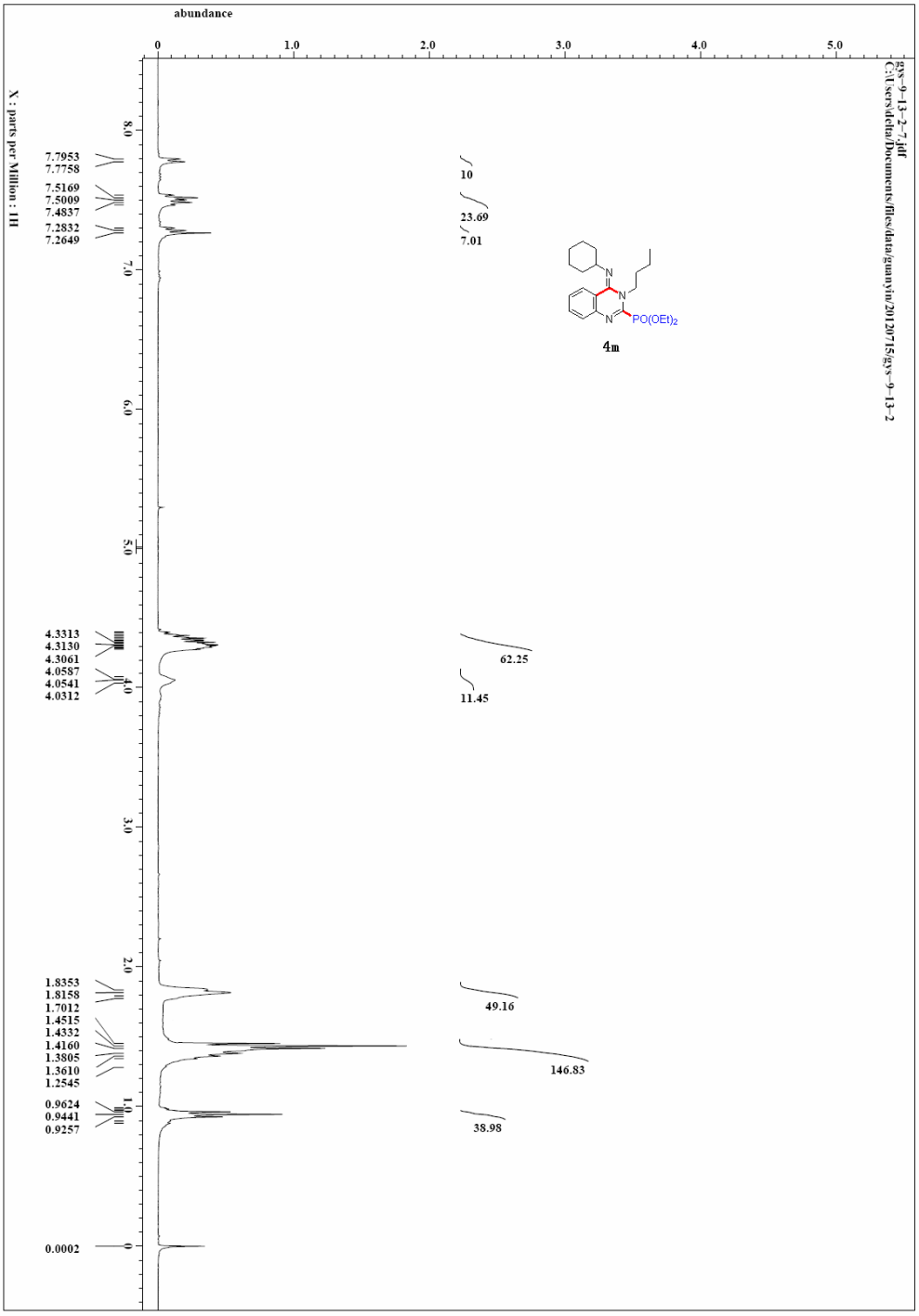

X : parts per Million : 1H
7.9288
7.9082
7.4764
7.4557
7.2679
7.2599
7.2393
4.9082
4.8921
4.8761
4.2942
4.2736
4.2552
1.4946
1.4797
1.4534
1.4270
1.4121
1.3858
0.9585
0.9402
0.9219
−0.0002
10
20.24
13.54
20.65
21.12
24.69
52.91
88.43
94.23
32.45
PO(OPr)2
(4k)
C:\Users\delta\Documents\files\data\guanyin\20120715\gys−9−4−1
gys−9−4−1−7.jdf

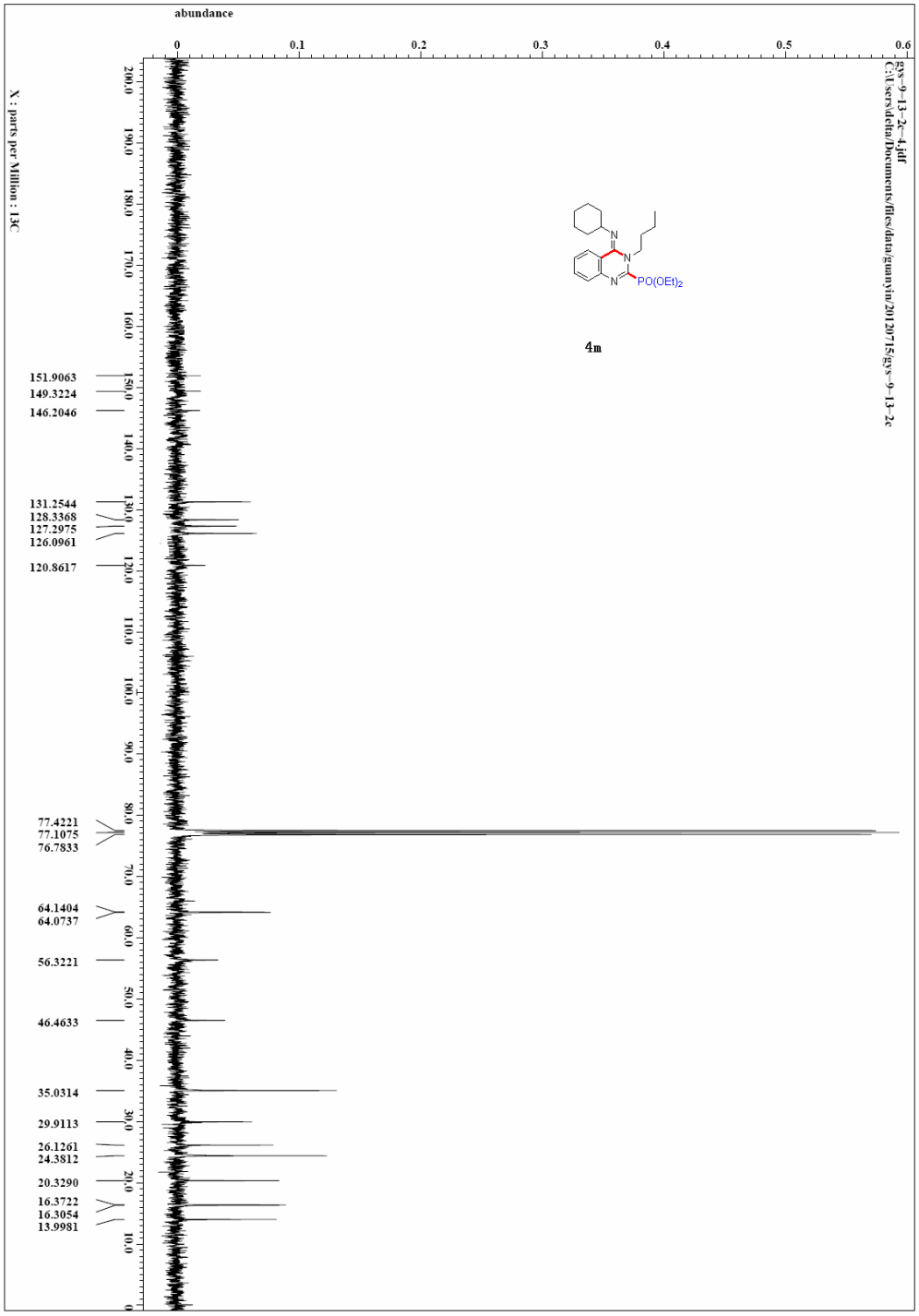

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
gys-9-4-1c-4.jdf
C:\Users\delta\Documents\files\data\guanyin\20120715\gys-9-4-1c
PO(OiPr)2
(4k)
152.9455
150.4189
146.9387
131.0827
129.2616
127.6407
125.0473
121.2240
77.4221
77.1075
76.7928
73.1316
73.0648
53.2901
46.4633
31.7705
29.9685
24.2096
24.1810
23.7901
23.7234
20.3481
14.0171

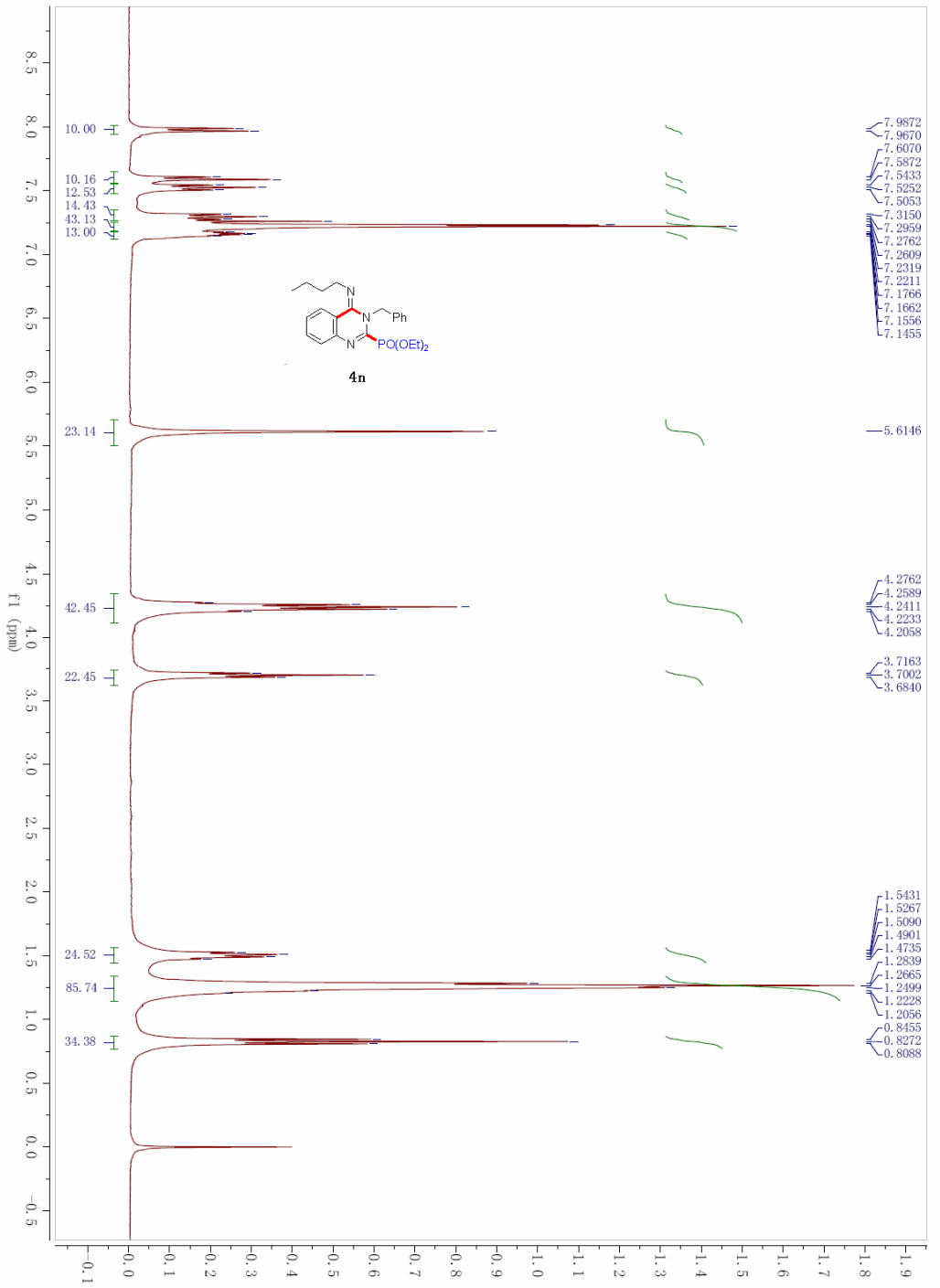

9.92
10.56
11.41
61.21
20.00
21.70
124.10
93.75
7.8323
7.8121
7.5597
7.5400
7.4983
7.4802
7.4607
7.2609
7.2499
7.2307
7.2090
7.1991
7.1538
7.1448
7.1341
5.5285
4.9100
4.8945
4.8789
4.8633
4.8477
4.8326
1.3586
1.3434
1.2524
Ph
PO(OiPr)2
f1 (ppm)

(41)


(4l)
153.3420
146.4756
139.4971
138.4503
131.1181
129.1763
127.7000
127.5875
127.2138
126.0860
125.1731
121.3819
73.2570
73.1931
53.1871
49.7530
24.0229
23.9905
23.4899
23.4285
f1 (ppm)


abundance
0
1.0
2.0
3.0
4.0
5.0
gys-9-13-2-7.jdf
C:\Users\data\Documents\files\data\guanyin\20120715\gys-9-13-2
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.7953
7.7758
7.5169
7.5009
7.4837
7.2832
7.2649
4.3313
4.3130
4.3061
4.0587
4.0541
4.0312
1.8353
1.8158
1.7012
1.4515
1.4332
1.4160
1.3805
1.3610
1.2545
0.9624
0.9441
0.9257
0.0002
10
23.69
7.01
62.25
11.45
49.16
146.83
38.98
N
N
N
PO(OEt)2
4m


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
gys-9-13-2c-4.jdf
C:\1\serv\delta\Documents\files\data\guanxin\20120715\gys-9-13-2c
PO(OEt)2
4m
151.9063
149.3224
146.2046
131.2544
128.3368
127.2975
126.0961
120.8617
77.4221
77.1075
76.7833
64.1404
64.0737
56.3221
46.4633
35.0314
29.9113
26.1261
24.3812
20.3290
16.3722
16.3054
13.9981


10.00
10.16
12.53
14.43
43.13
13.00
23.14
42.45
22.45
24.52
85.74
34.38
7.9872
7.9670
7.6070
7.5872
7.5433
7.5252
7.5053
7.3150
7.2959
7.2762
7.2609
7.2319
7.2211
7.1766
7.1662
7.1556
7.1455
5.6146
4.2762
4.2589
4.2411
4.2233
4.2058
3.7163
3.7002
3.6840
1.5431
1.5267
1.5090
1.4901
1.4735
1.2839
1.2665
1.2499
1.2228
1.2056
0.8455
0.8272
0.8088
Ph
PO(OEt)2
4n
f1 (ppm)