Synthesis and Fungicidal Activities of 5-Aryl-1,3,4-oxadiazolyl 2-Thioether Derivatives Containing Strobilurin Motif

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Supporting Information

Table of Contents **Page**

1. Data of intermediates 4a-4o

4-(5-(allylthio)-1,3,4-oxadiazol-2-yl)phenol(4a)

Yield:90.2%. White solid, mp 140.1-141.3 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.34 (s, 1H), 7.88 – 7.71 (m, 2H), 7.03 – 6.88 (m, 2H), 5.99 (ddt, J = 16.9, 9.9, 7.0 Hz, 1H), 5.34 (dt, J = 17.0, 1.4 Hz, 1H), 5.17 (dd, J = 10.0, 1.6 Hz, 1H), 3.94 (d, J = 7.0 Hz, 2H).

4-(5-(prop-2-yn-1-ylthio)-1,3,4-oxadiazol-2-yl)phenol(4b)

Yield:98.3%. Brown solid, mp 163.5-164.0 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.36 (s, 1H), 7.90 – 7.74 (m, 2H), 7.06 – 6.86 (m, 2H), 4.18 (d, J = 2.6 Hz, 2H).

4-(5-((3-methylbut-2-en-1-yl)thio)-1,3,4-oxadiazol-2-yl)phenol(4c)

Yield:93.2%. White solid, mp 126.3-127.4 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.91 – 7.68 (m, 2H), 7.02 – 6.84 (m, 2H), 5.38 (tdt, J = 7.9, 3.0, 1.5 Hz, 1H), 3.93 (d, J = 7.9 Hz, 2H), 1.68 (dd, J = 6.9, 1.4 Hz, 6H).

4-(5-((3-chlorobut-2-en-1-yl)thio)-1,3,4-oxadiazol-2-yl)phenol(4d)

Yield:85.1%. Beige solid, mp 126.8-127.1 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.35 (d, J = 1.6 Hz, 1H), 8.14 – 7.55 (m, 2H), 7.21 – 6.78 (m, 2H), 6.74 – 6.36 (m, 1H), 6.36 – 6.00 (m, 1H), 4.02 (ddd, J = 24.4, 7.6, 1.2 Hz, 2H).

4-(5-(methylthio)-1,3,4-oxadiazol-2-yl)phenol(4e)

Yield:77.6%. White solid, mp 180.2-181.6 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.99 – 7.61 (m, 2H), 7.06 – 6.73 (m, 2H), 2.74 (s, 3H).

4-(5-(benzylthio)-1,3,4-oxadiazol-2-yl)phenol(4f)

Yield:96.3%. White solid, mp 174.3-175.2 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.89 – 7.68 (m, 2H), 7.60 – 7.43 (m, 2H), 7.42 – 7.16 (m, 3H), 7.03 – 6.82 (m, 2H), 4.55 (s, 2H).

4-(5-((4-chlorobenzyl)thio)-1,3,4-oxadiazol-2-yl)phenol(4g)

Yield:62.4%. White solid, mp 200.3-201.2 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.35 (s, 1H), 7.86 – 7.70 (m, 2H), 7.58 – 7.46 (m, 2H), 7.46 – 7.33 (m, 2H), 7.00 – 6.83 (m, 2H), 4.54 (s, 2H).

4-(5-((4-fluorobenzyl)thio)-1,3,4-oxadiazol-2-yl)phenol(4h)

Yield:96.8%. White solid, mp 177.2-177.6 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 – 7.69 (m, 2H), 7.62 –

7.40 (m, 2H), 7.32 – 7.10 (m, 2H), 7.01 – 6.84 (m, 2H), 4.55 (s, 2H).

4-(5-((2-methylbenzyl)thio)-1,3,4-oxadiazol-2-yl)phenol(4i)

Yield:82.4%. White solid, mp 187.6-188.1 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.37 (s, 1H), 7.88 – 7.72 (m, 2H), 7.39 – 7.23 (m, 2H), 7.14 (d, J = 7.8 Hz, 2H), 6.99 – 6.91 (m, 2H), 4.50 (s, 2H), 2.26 (s, 3H).

4-(5-((4-(trifluoromethyl)benzyl)thio)-1,3,4-oxadiazol-2-yl)phenol(4j)

Yield:93.4%. White solid, mp 155.0-156.0 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.36 (s, 1H), 7.83 – 7.58 (m, 6H), 7.05 – 6.85 (m, 2H), 4.63 (s, 2H).

4-(5-((2-methylbenzyl)thio)-1,3,4-oxadiazol-2-yl)phenol(4k)

Yield:82.1%. White solid, mp 174.8-175.2 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.91 – 7.63 (m, 2H), 7.44 – 7.33 (m, 1H), 7.31 – 7.08 (m, 3H), 7.02 – 6.82 (m, 2H), 4.56 (s, 2H), 2.40 (s, 3H).

4-(5-((3-(trifluoromethyl)benzyl)thio)-1,3,4-oxadiazol-2-yl)phenol(4l)

Yield:96.2%. White solid, mp 154.3-154.8℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.37 (s, 1H), 7.87 (d, J = 2.1 Hz, 1H), 7.83 – 7.69 (m, 3H), 7.69 – 7.52 (m, 2H), 7.06 – 6.80 (m, 2H), 4.64 (s, 2H).

4-(5-((2-(trifluoromethyl)benzyl)thio)-1,3,4-oxadiazol-2-yl)phenol(4m)

Yield:99.2%. White solid, mp 156.5-157.2 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 – 7.73 (m, 4H), 7.72 – 7.65 (m, 1H), 7.55 (dd, J = 8.4, 6.9 Hz, 1H), 7.01 – 6.84 (m, 2H), 4.78 – 4.65 (m, 2H).

4-(5-((3-methoxybenzyl)thio)-1,3,4-oxadiazol-2-yl)phenol(4n)

Yield:96.6%. White solid, mp 139.5-139.8 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.93 – 7.65 (m, 2H), 7.31 – 7.21 (m, 1H), 7.09 – 6.99 (m, 2H), 6.99 – 6.89 (m, 2H), 6.89 – 6.81 (m, 1H), 4.52 (s, 2H), 3.72 (s, 3H).

4-(5-((2-methoxybenzyl)thio)-1,3,4-oxadiazol-2-yl)phenol(4o)

Yield:90.3%. White solid, mp 155.7-156.9 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.92 – 7.71 (m, 2H), 7.39 (dd, J = 7.5, 1.8 Hz, 1H), 7.31 (td, J = 7.9, 1.8 Hz, 1H), 7.02 (dd, J = 8.3, 1.1 Hz, 1H), 6.99 – 6.82 (m, 3H), 4.46 (s, 2H), 3.79 (s, 3H).

2. ^{1}H NMR, ^{13}C NMR spectra for 4a-4o:

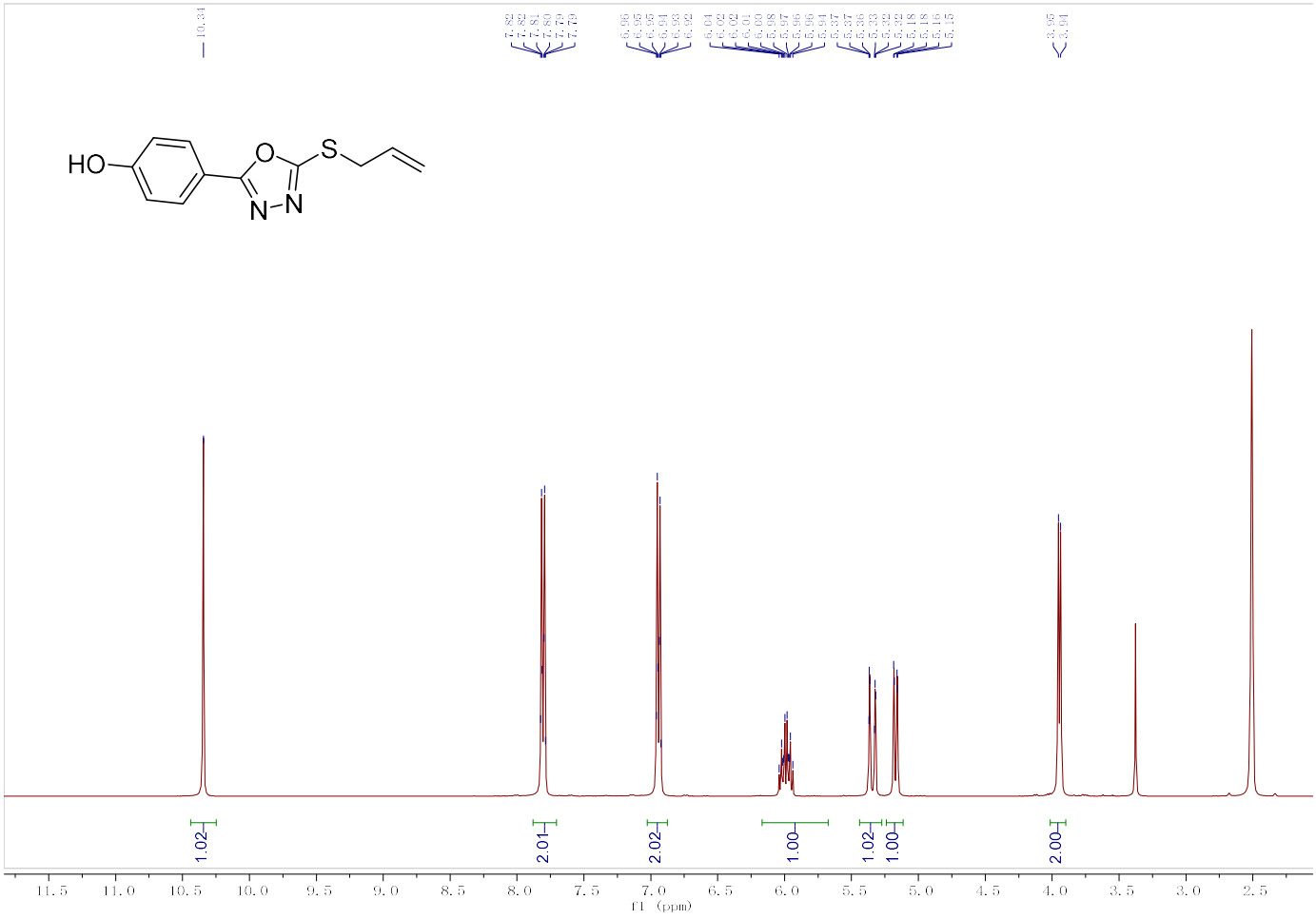

Fig. S01 ^{1}H NMR of compound **4a**

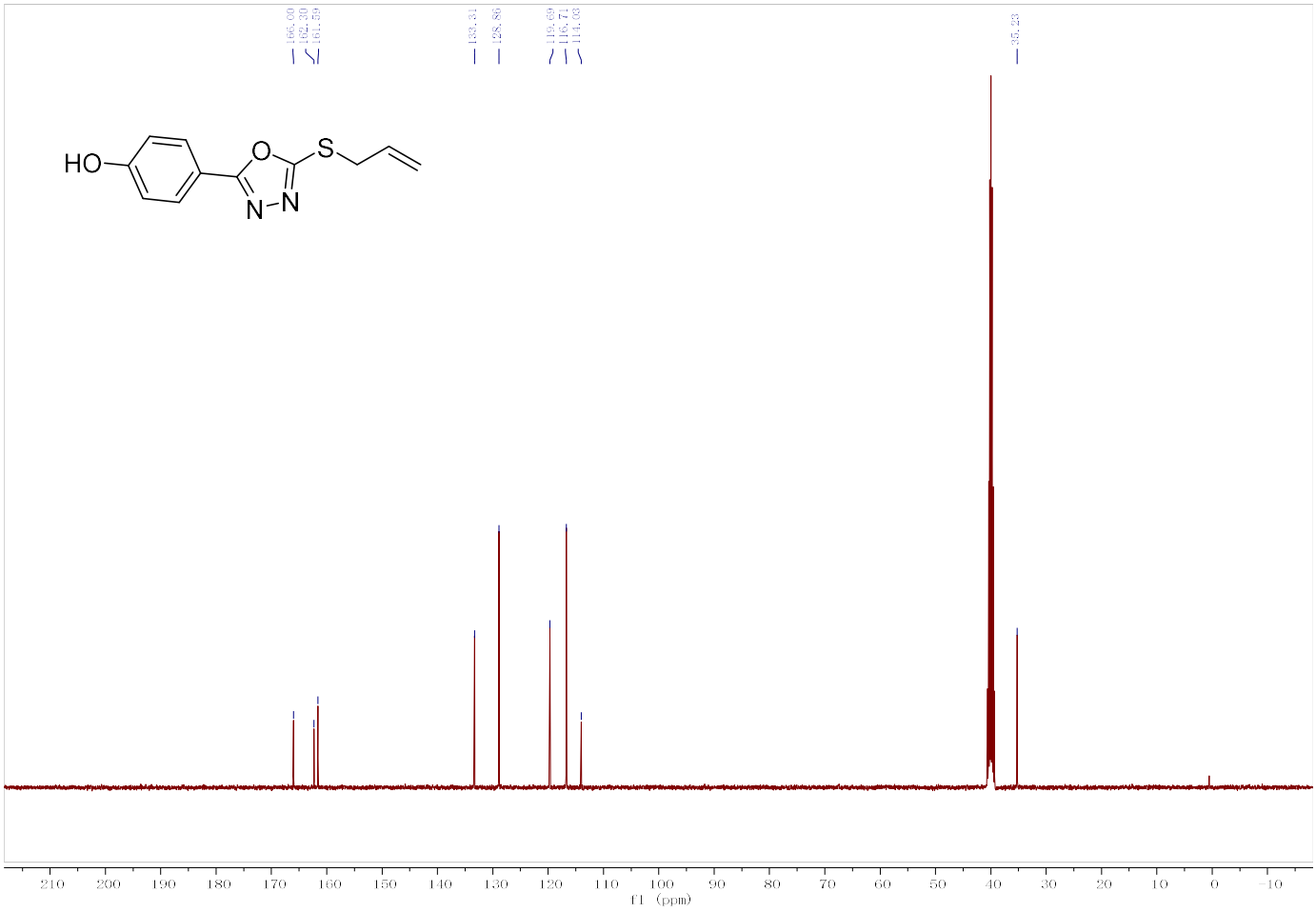

Fig. S02 ^{13}C NMR of compound **4a**

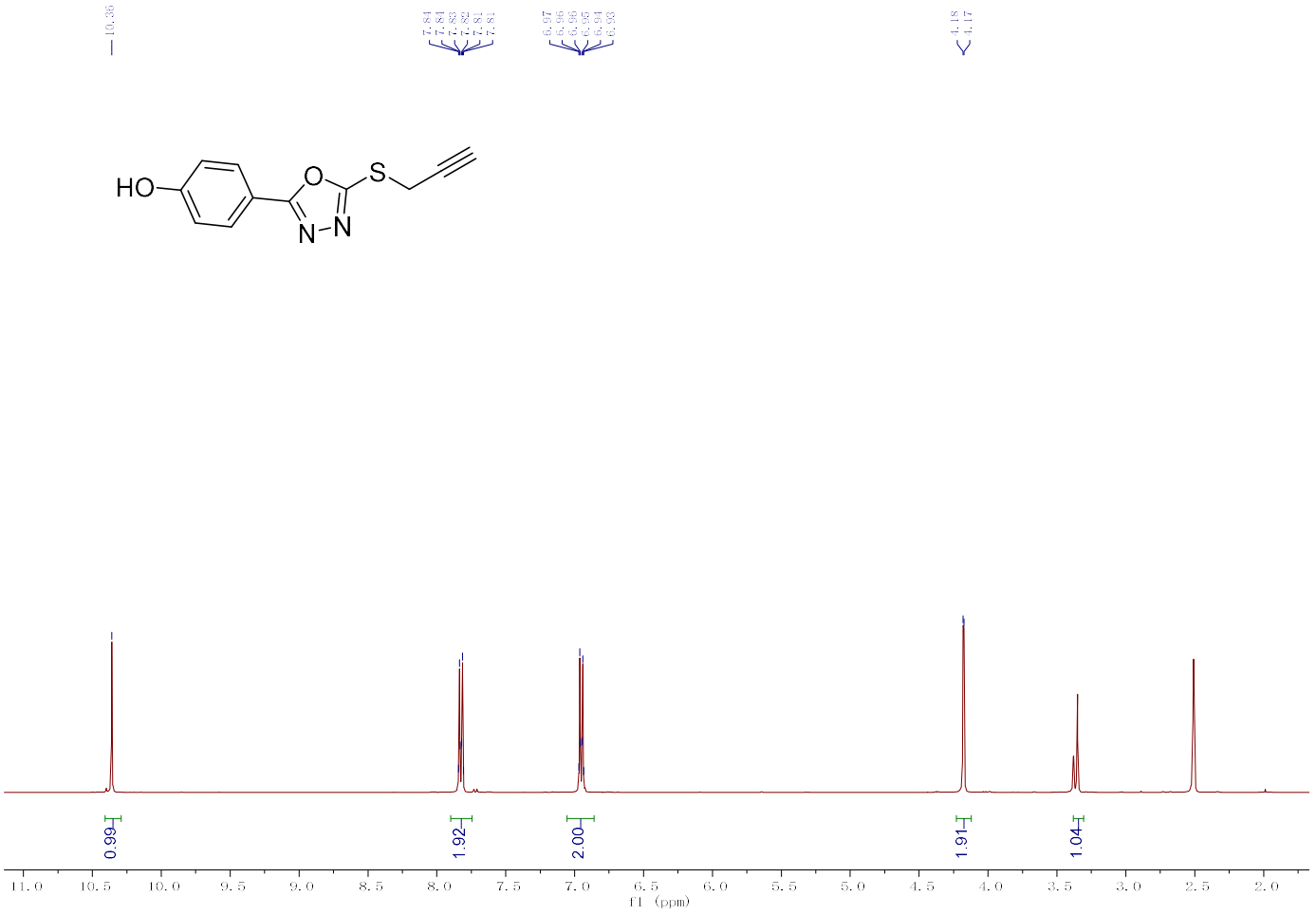

Fig. S03 ^{1}H NMR of compound **4b**

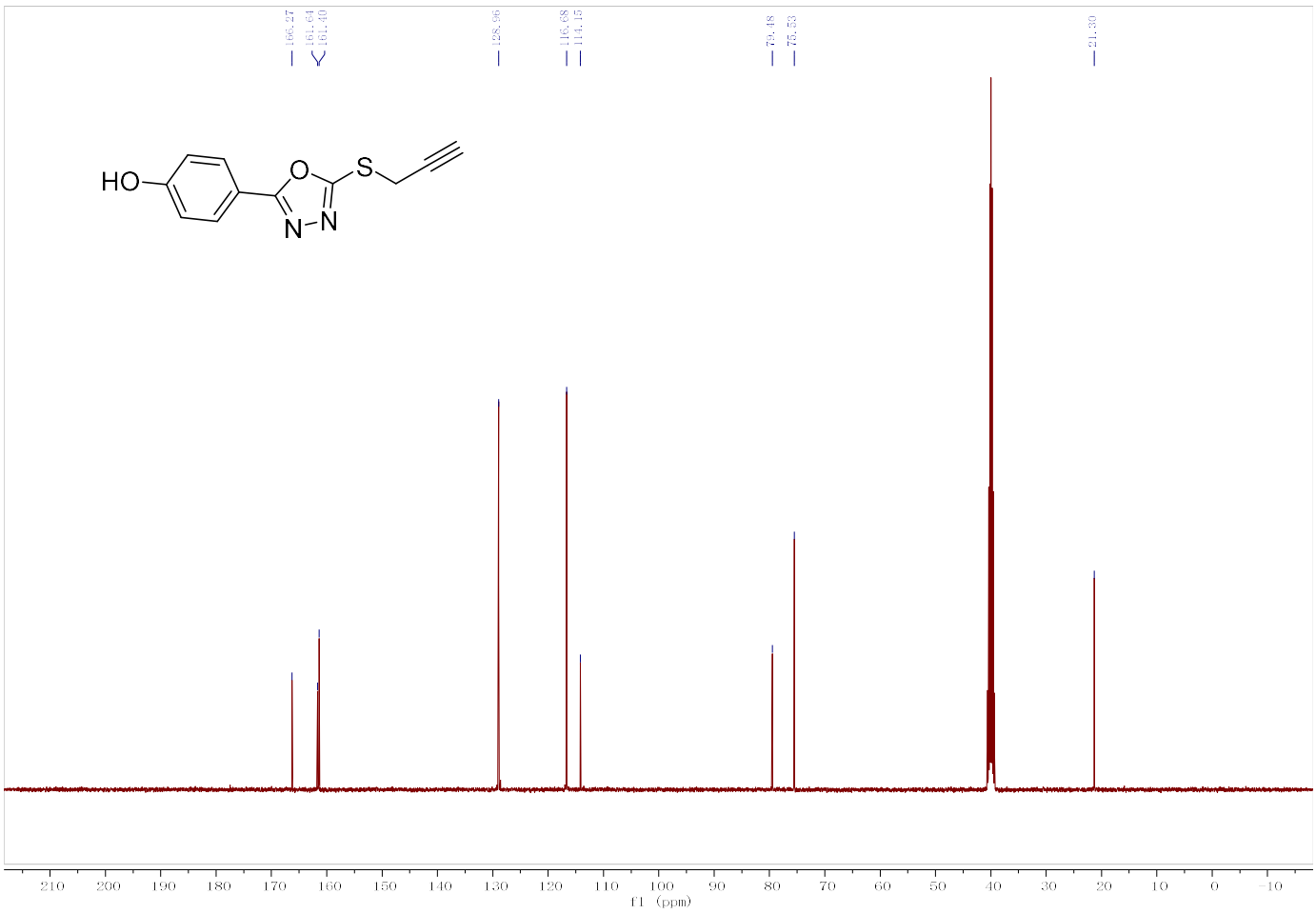

Fig. S04 ^{13}C NMR of compound **4b**

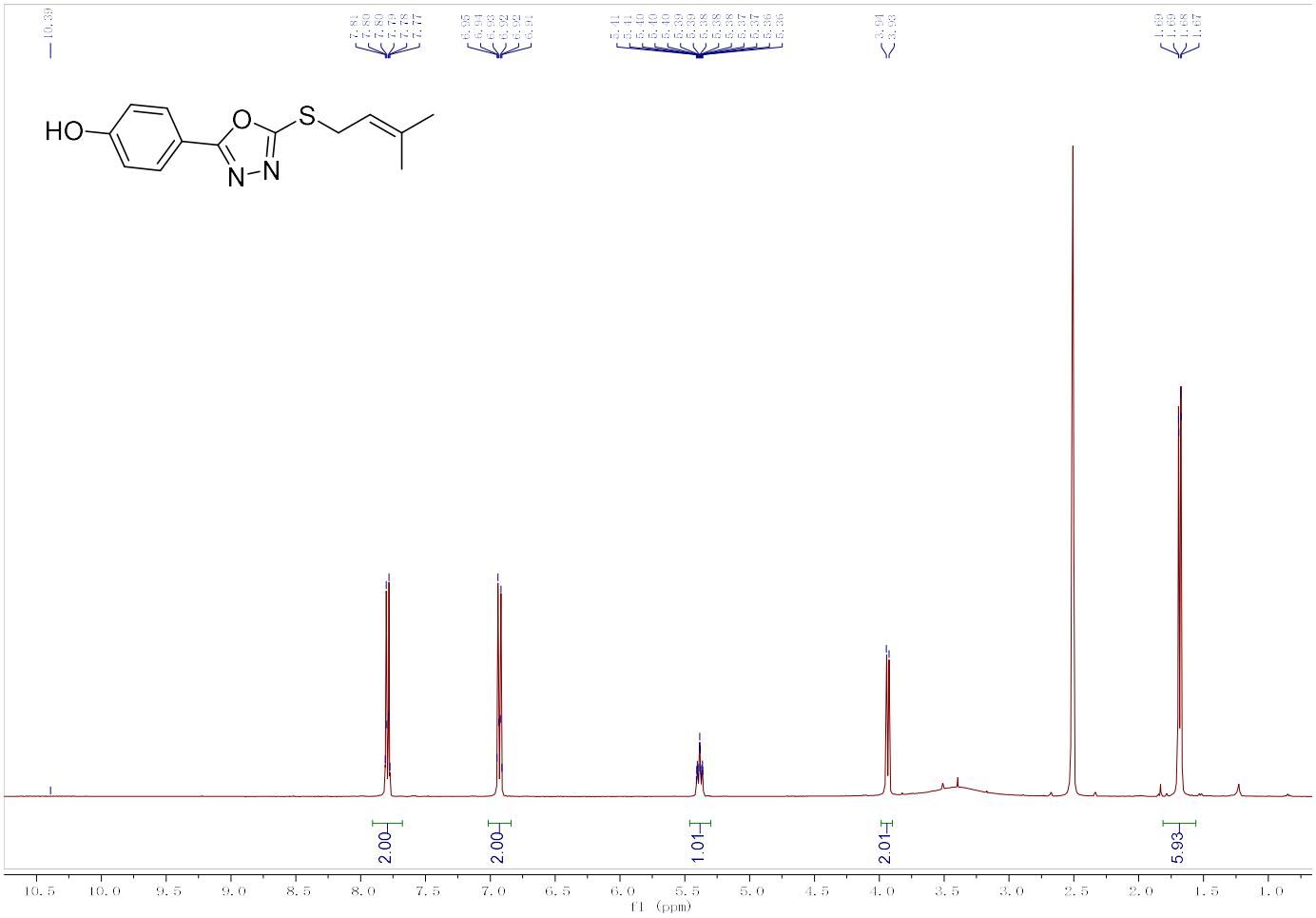

Fig. S05 ^{1}H NMR of compound **4c**

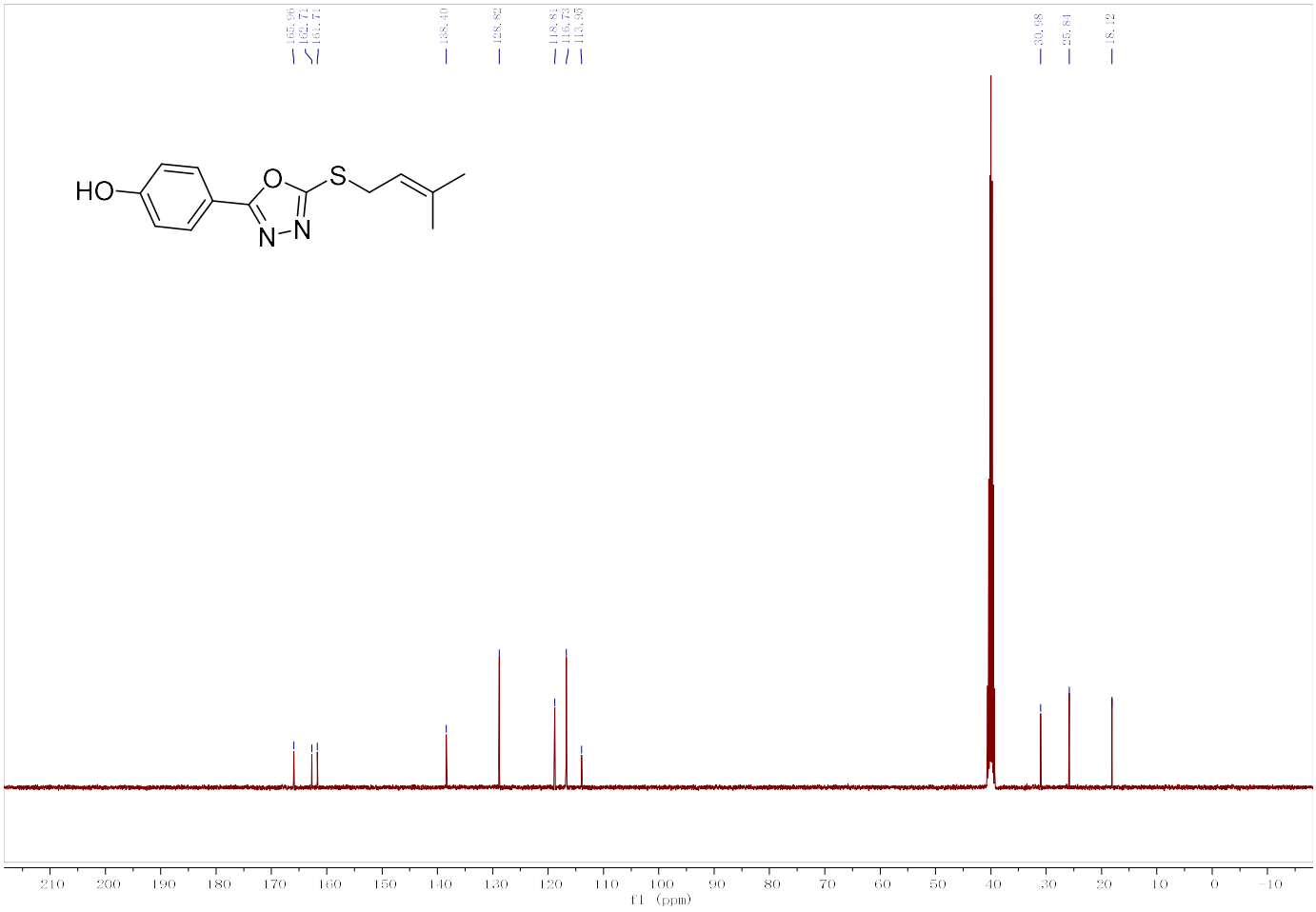

Fig. S06 ^{13}C NMR of compound **4c**

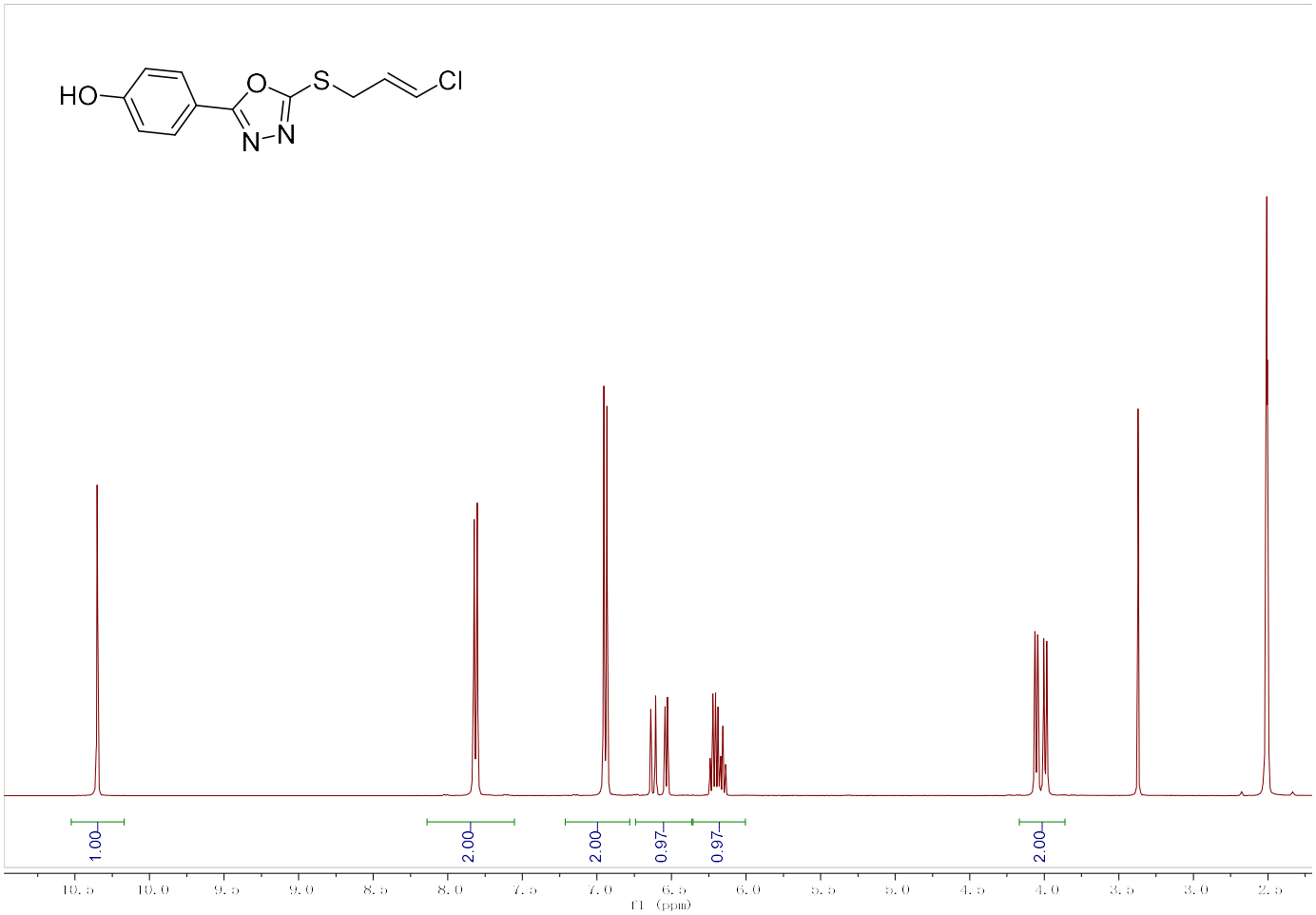

Fig. S07 ^{1}H NMR of compound **4d**

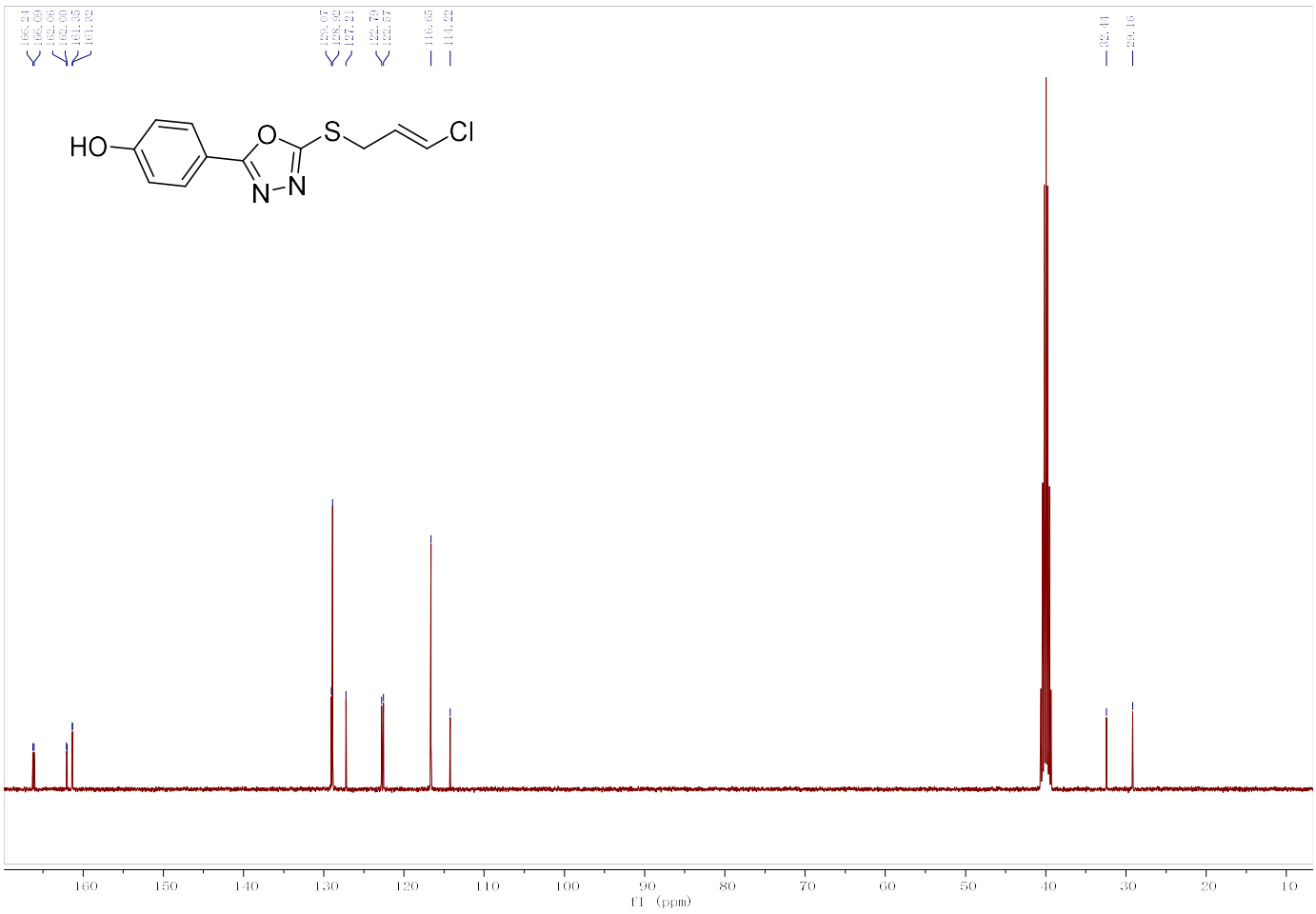

Fig. S08 ^{13}C NMR of compound **4d**

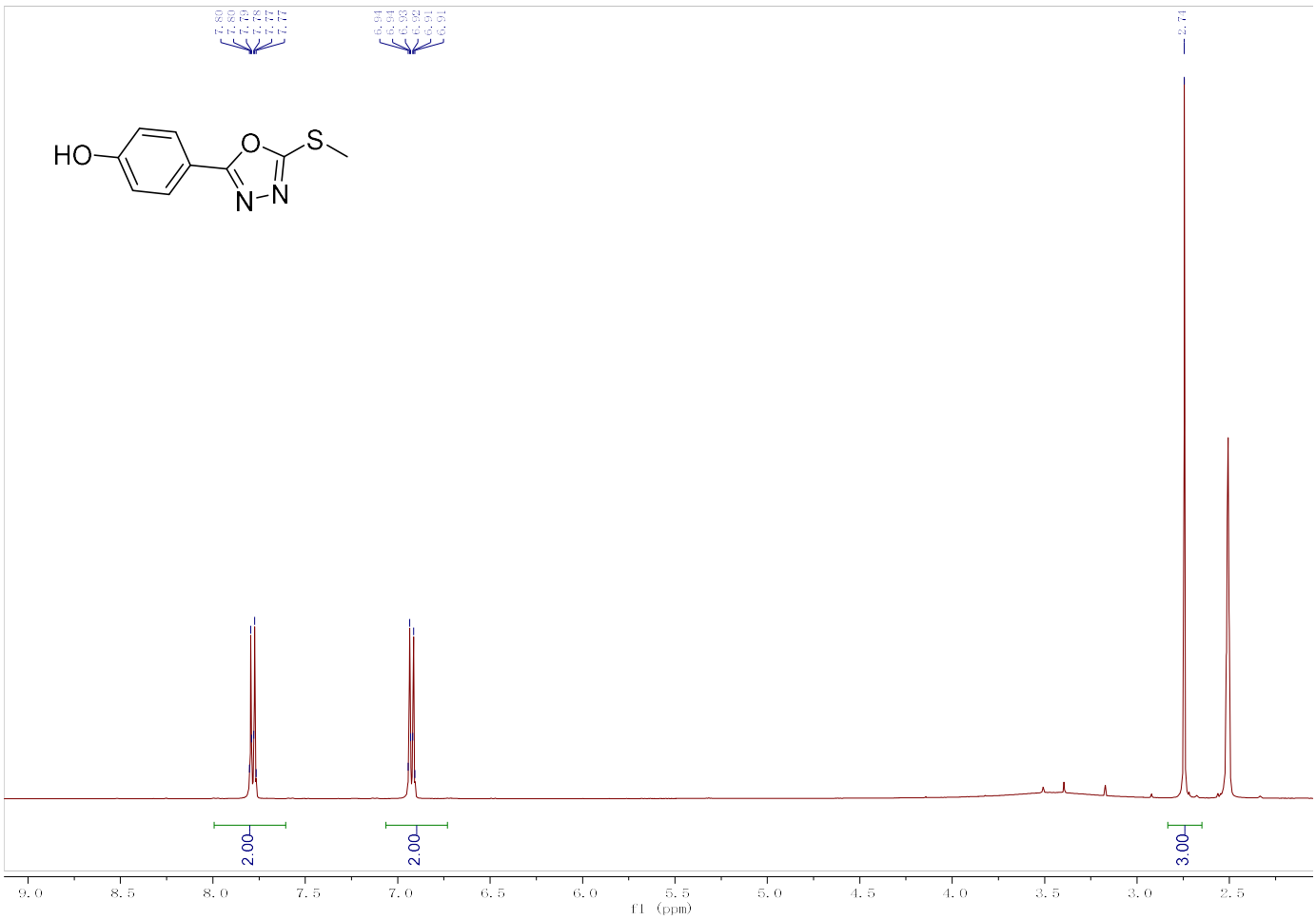

Fig. S09 ^{1}H NMR of compound **4e**

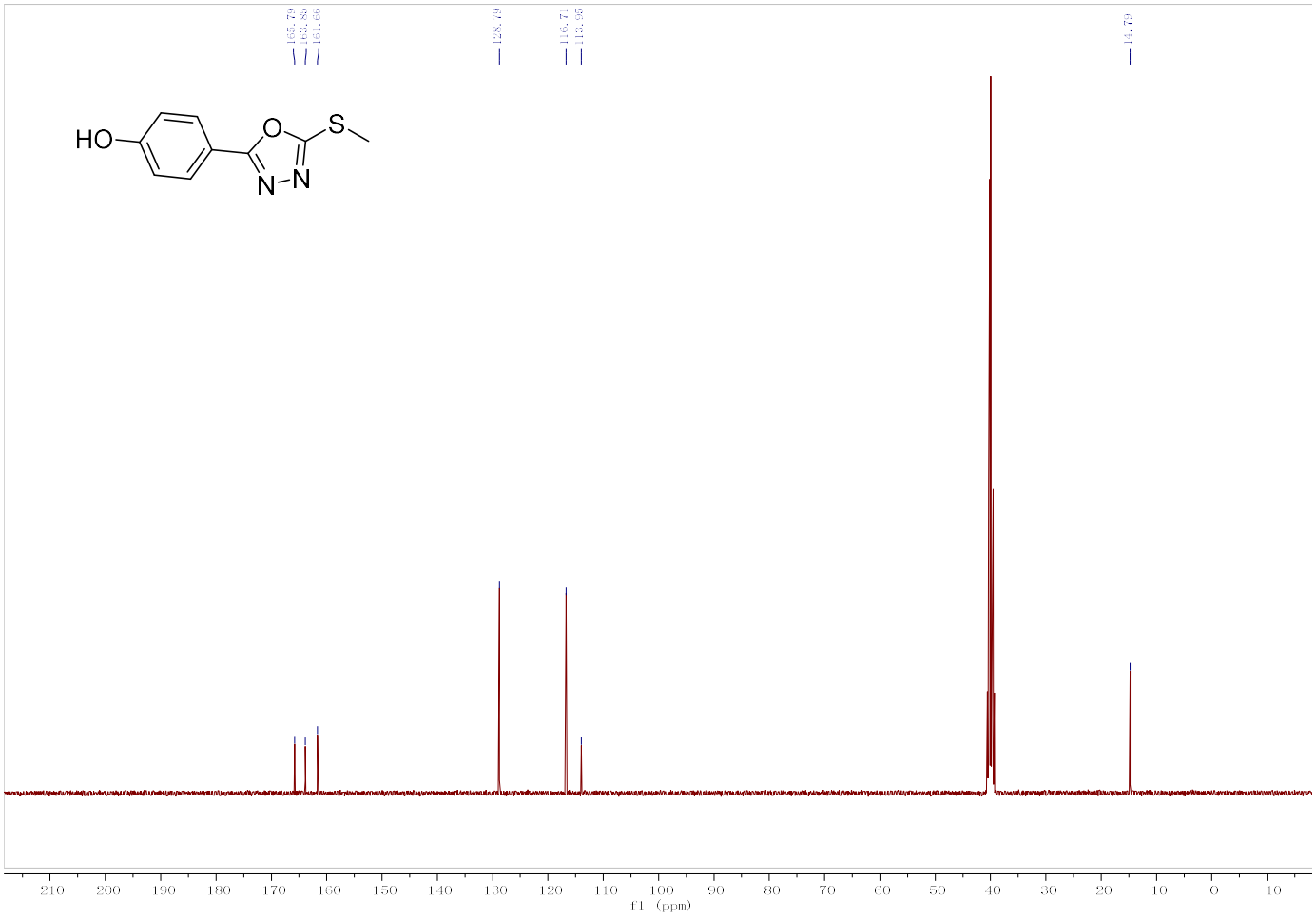

Fig. S10 ^{13}C NMR of compound **4e**

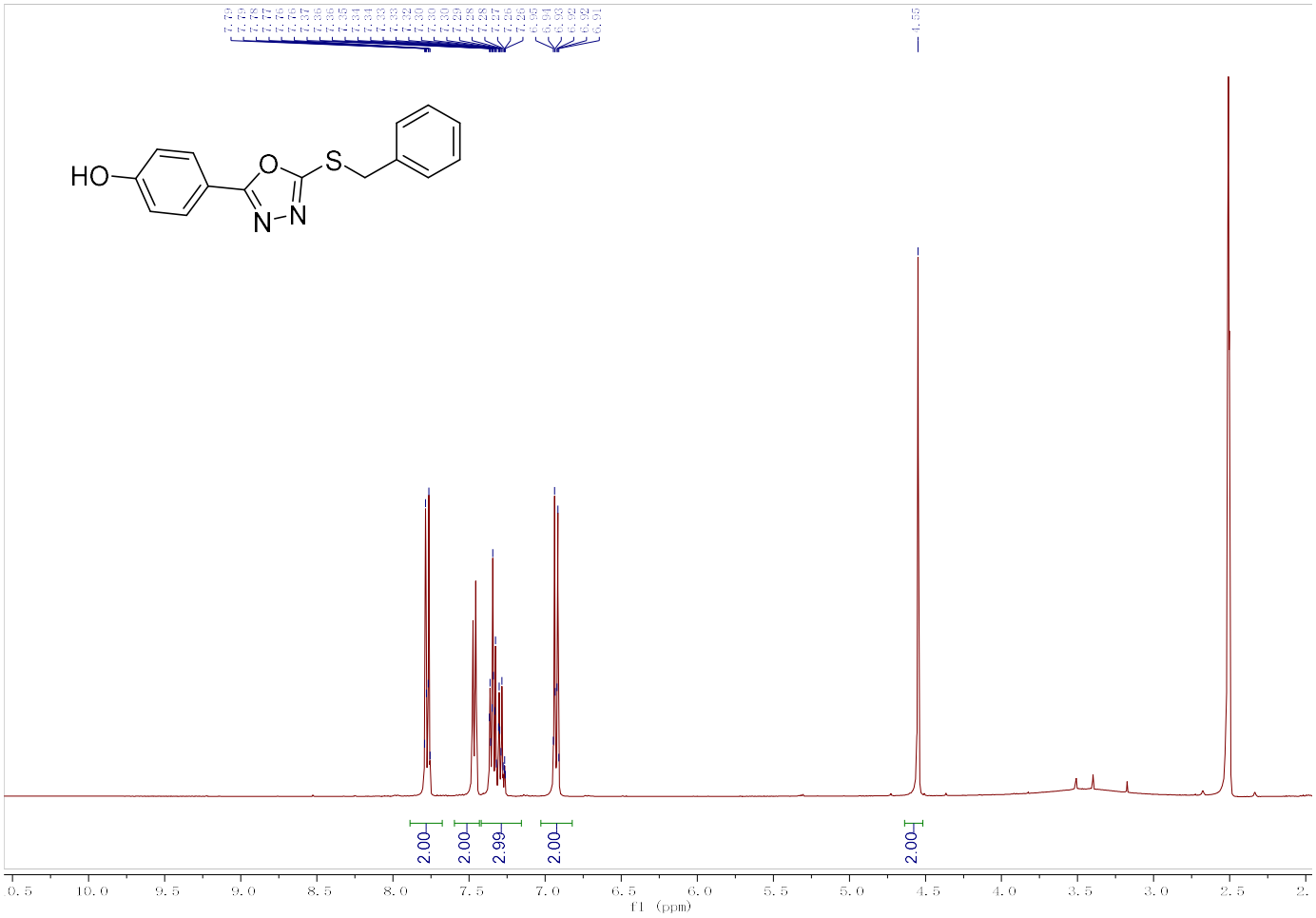

Fig. S11 ^{1}H NMR of compound **4f**

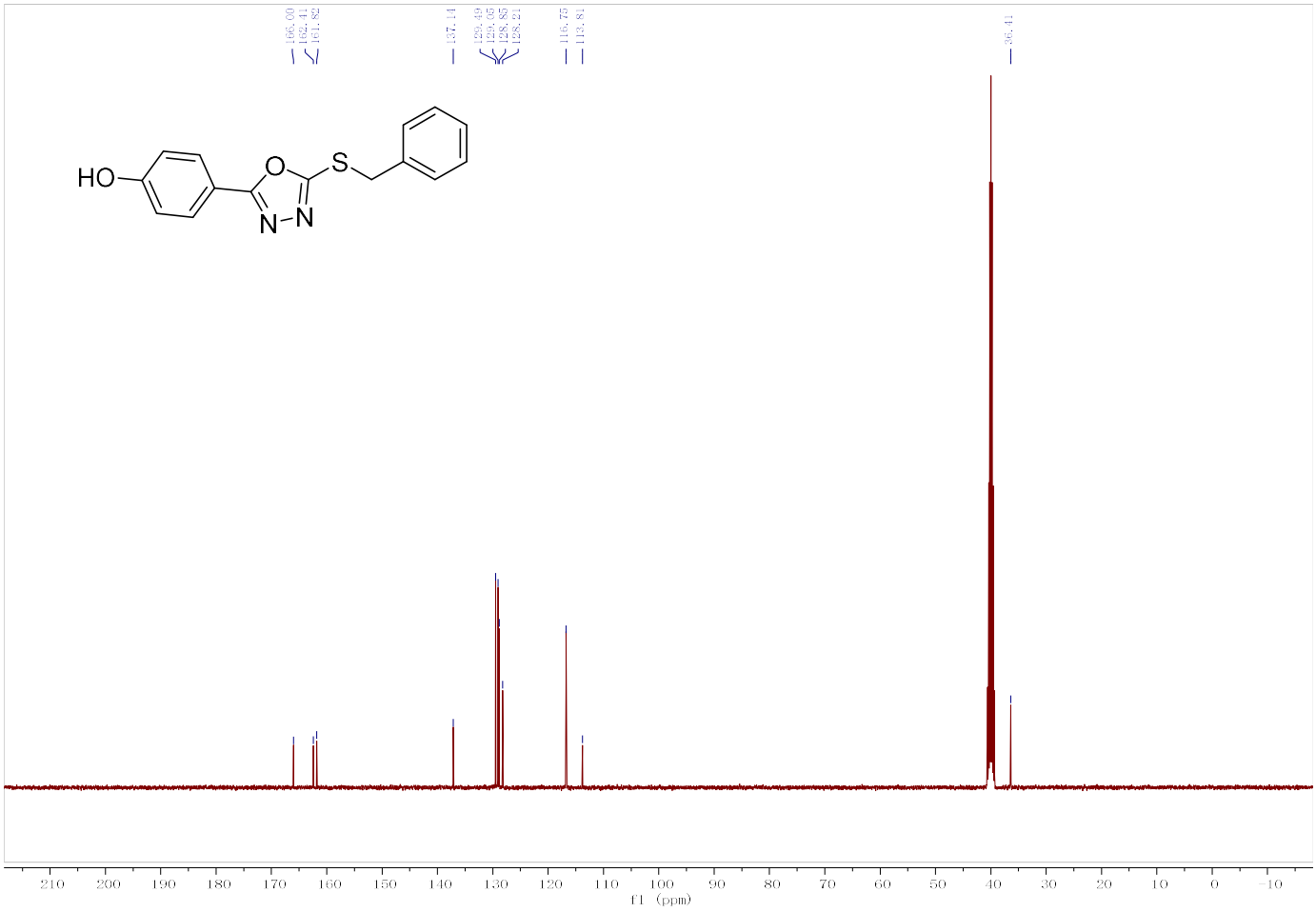

Fig. S12 ^{13}C NMR of compound **4f**

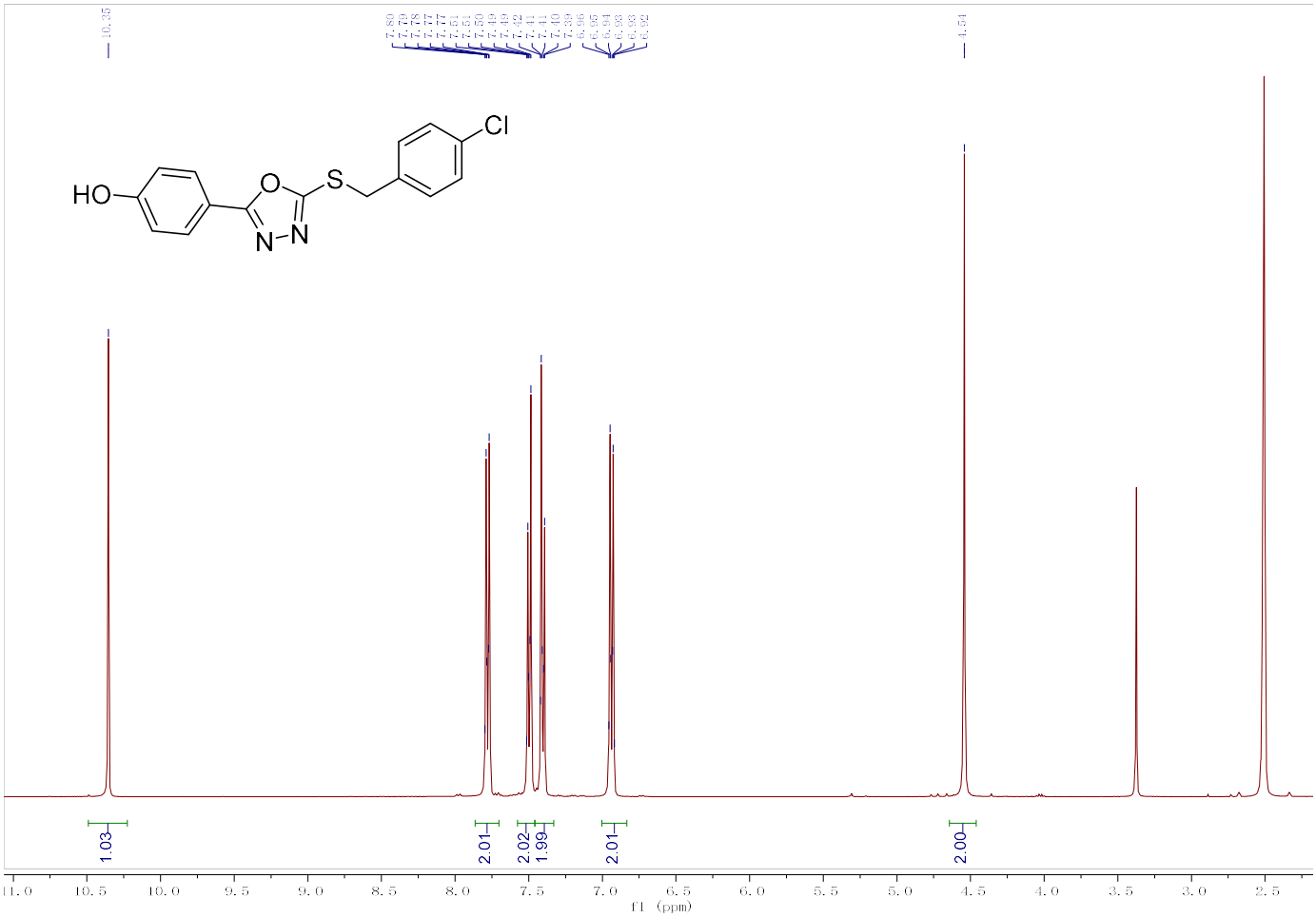

Fig. S13 ^{1}H NMR of compound **4g**

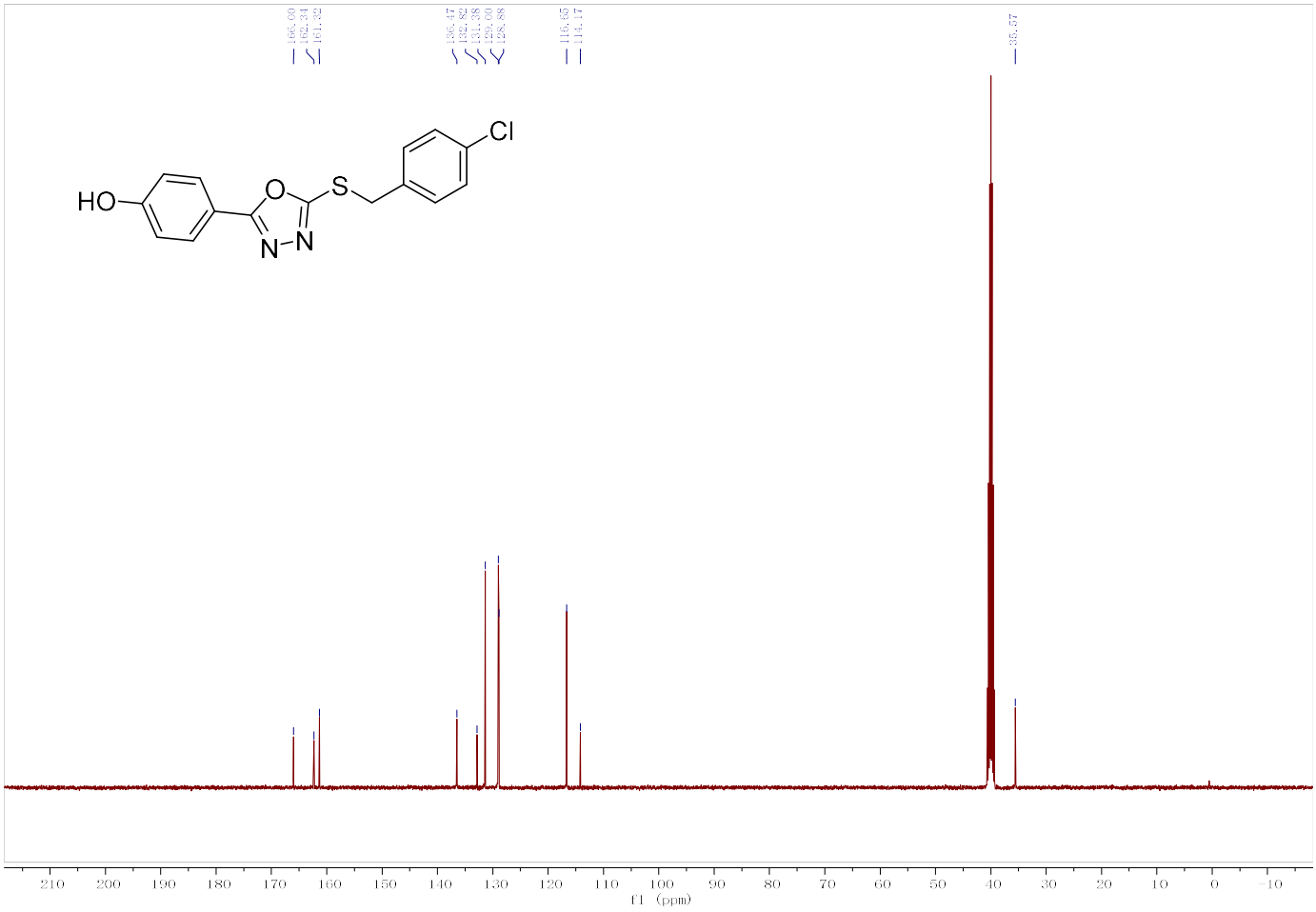

Fig. S14 ^{13}C NMR of compound **4g**

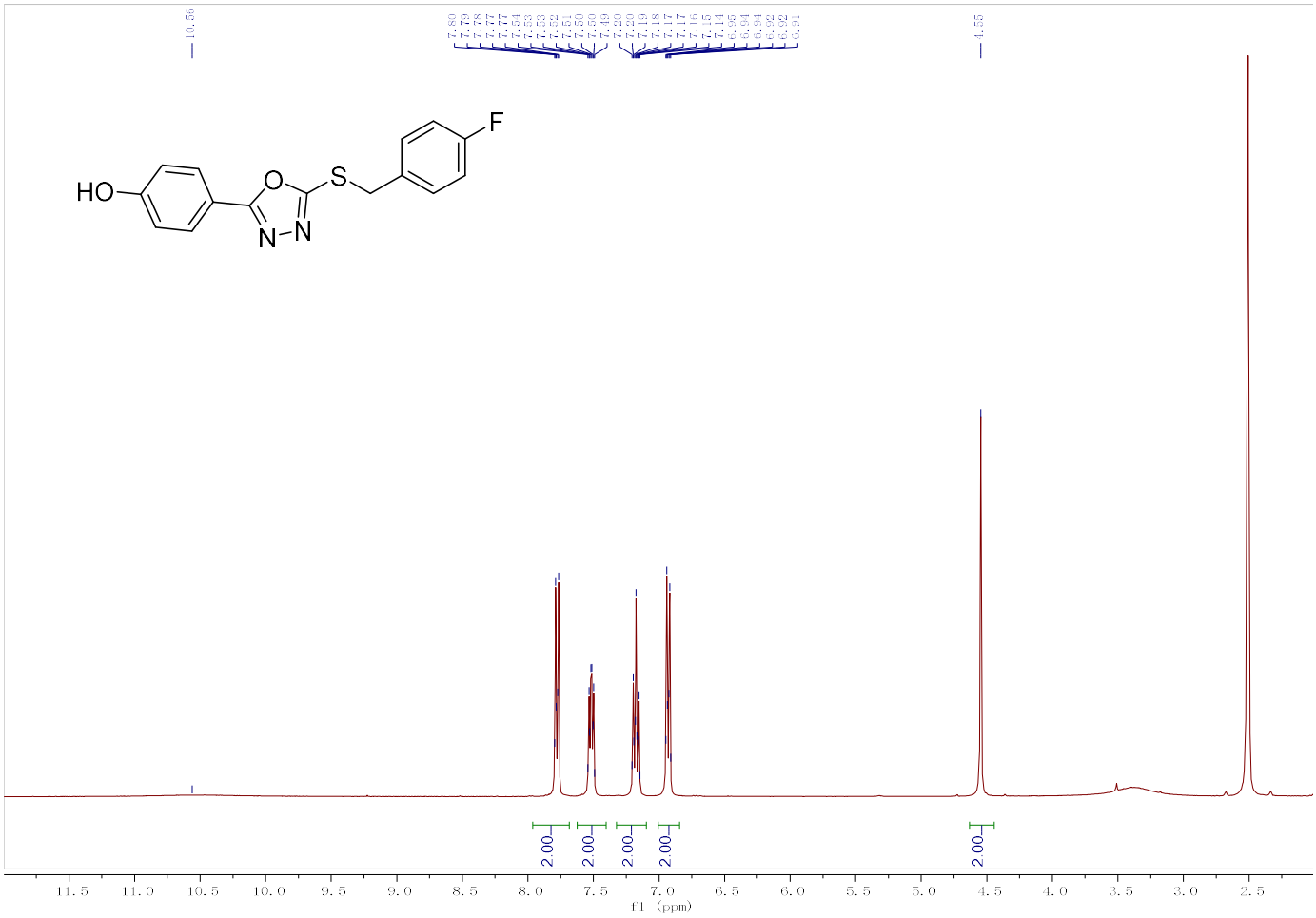

Fig. S15 ^{1}H NMR of compound **4h**

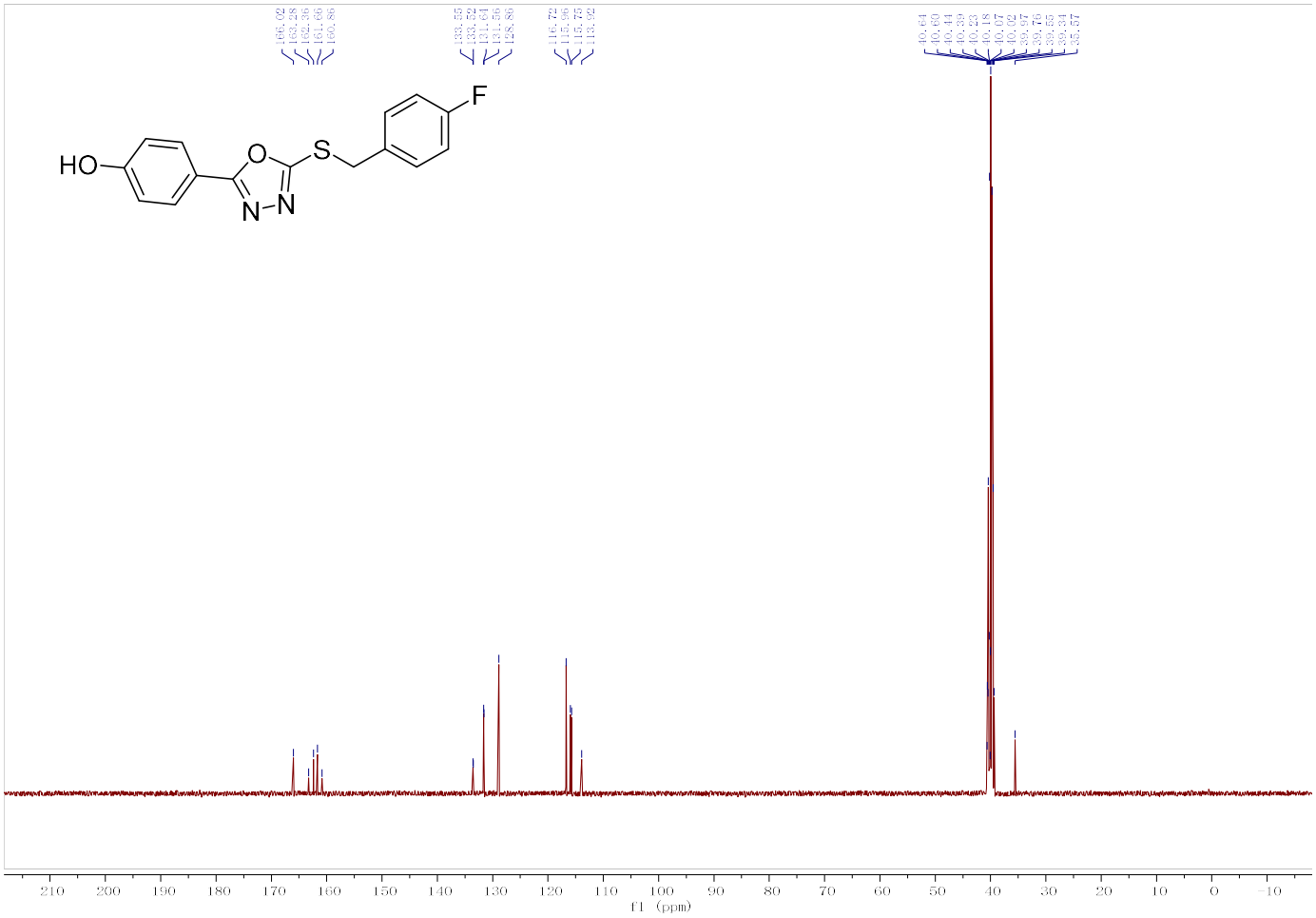

Fig. S16 ^{13}C NMR of compound **4h**

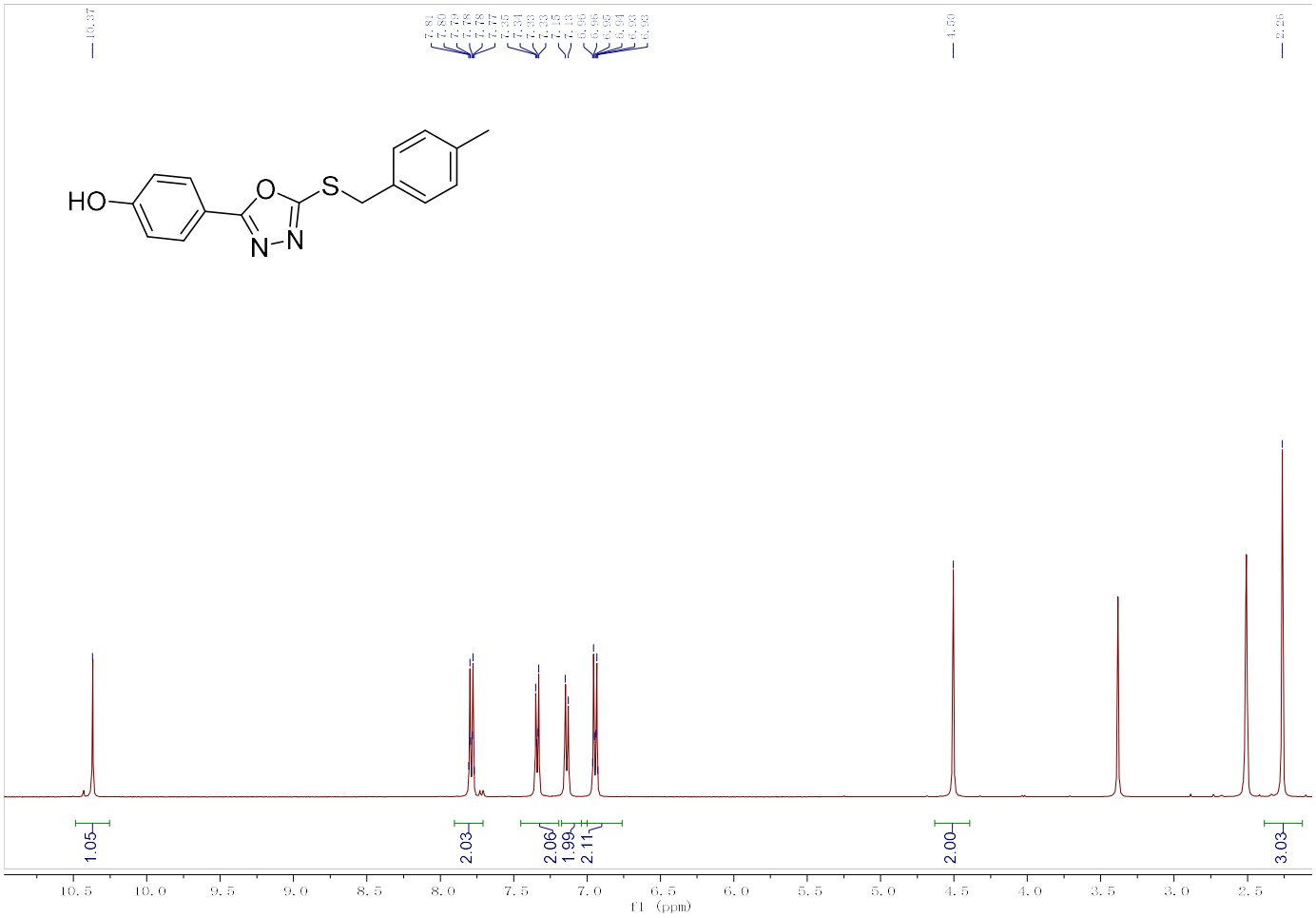

Fig. S17 ^{1}H NMR of compound **4i**

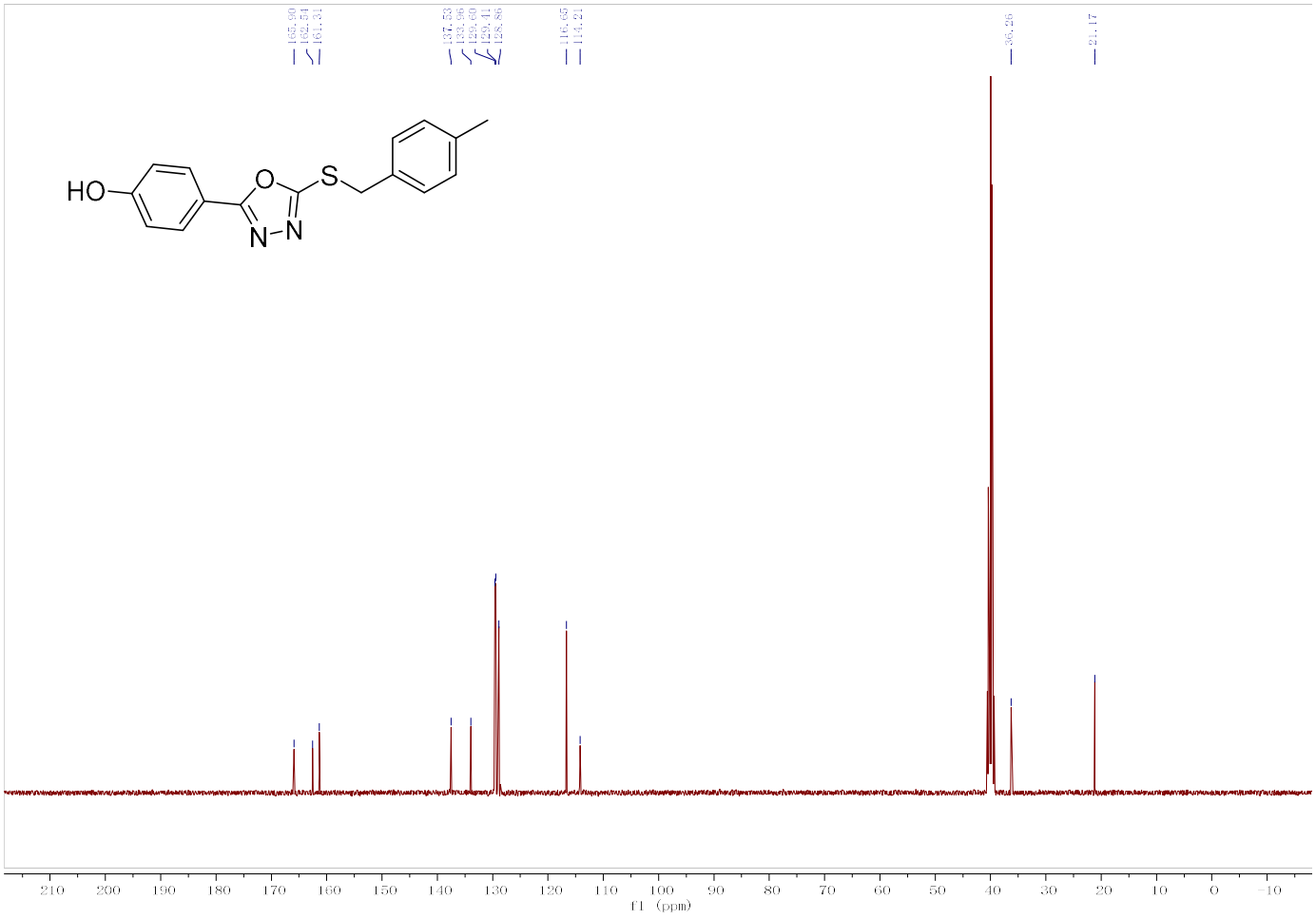

Fig. S18 ^{13}C NMR of compound **4i**

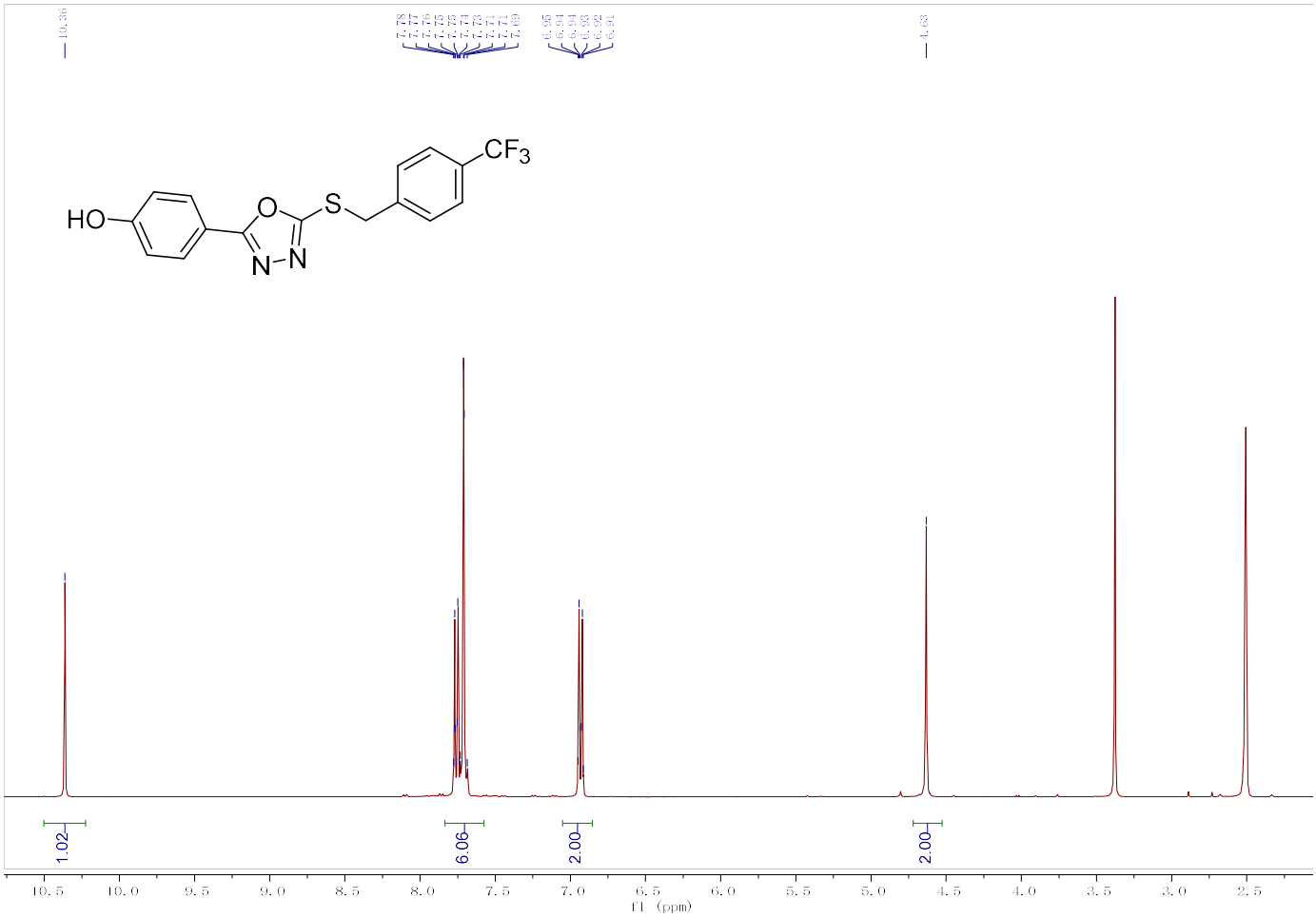

Fig. S19 ^{1}H NMR of compound **4j**

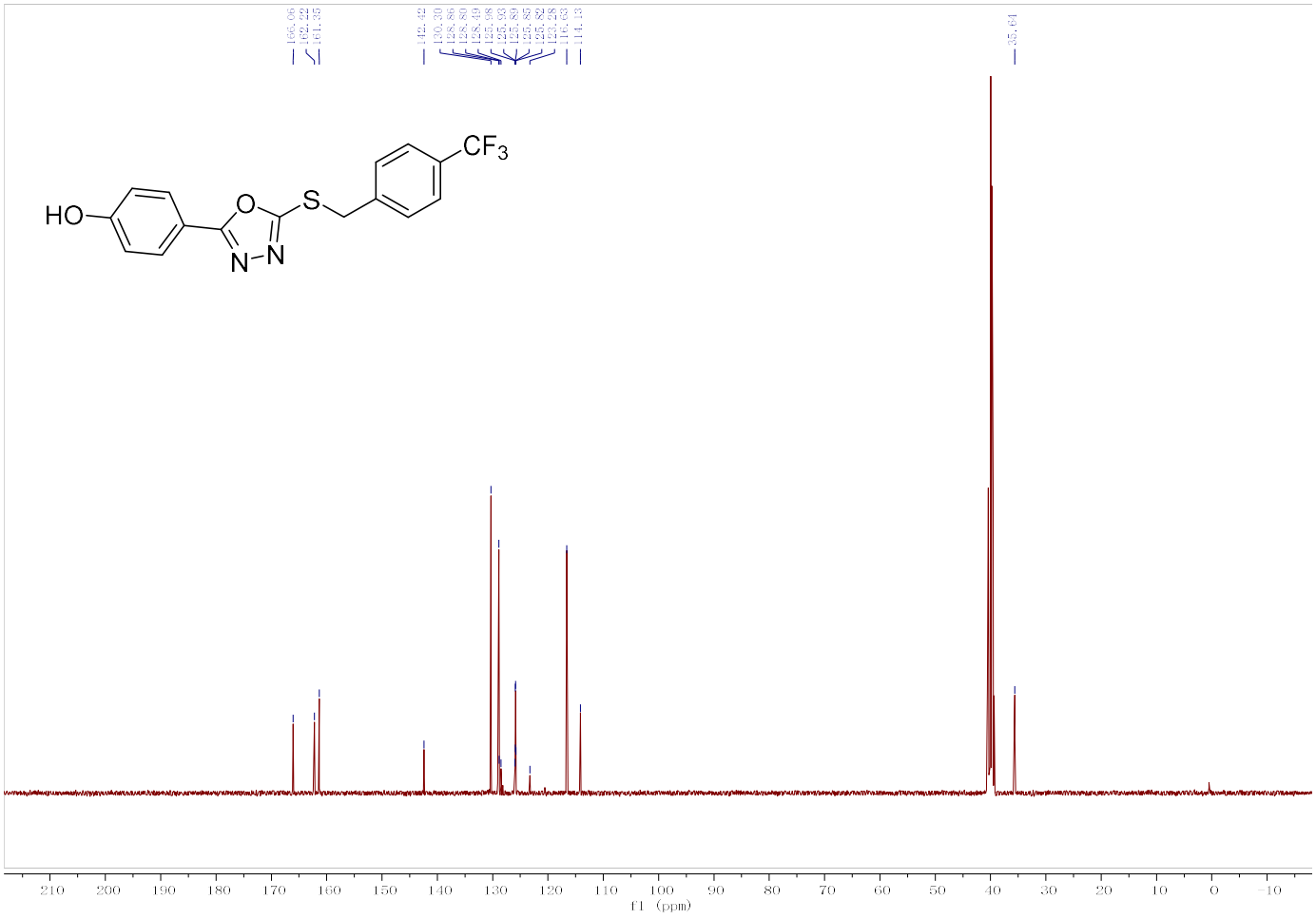

Fig. S20 ^{13}C NMR of compound **4j**

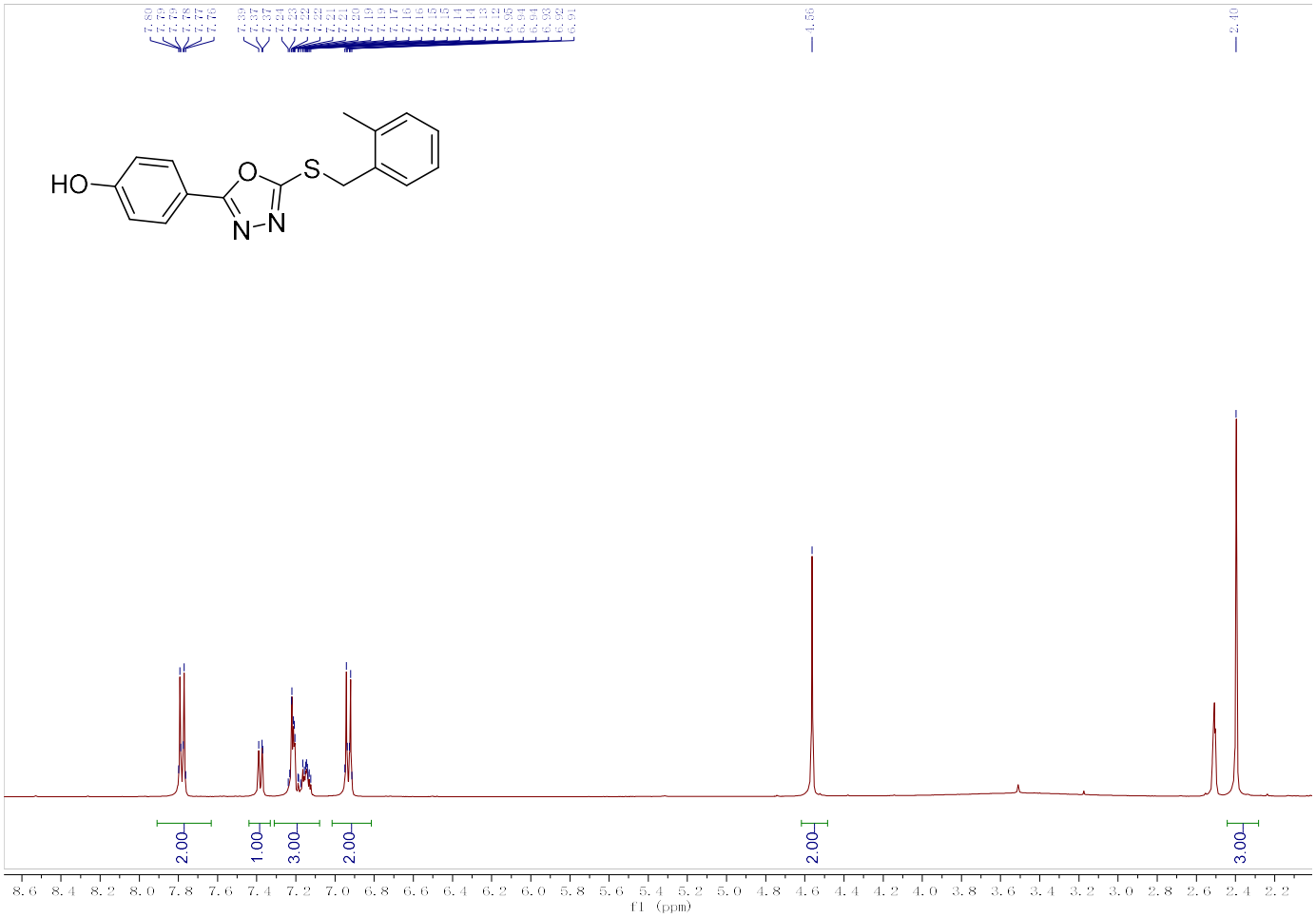

Fig. S21 ^{1}H NMR of compound **4k**

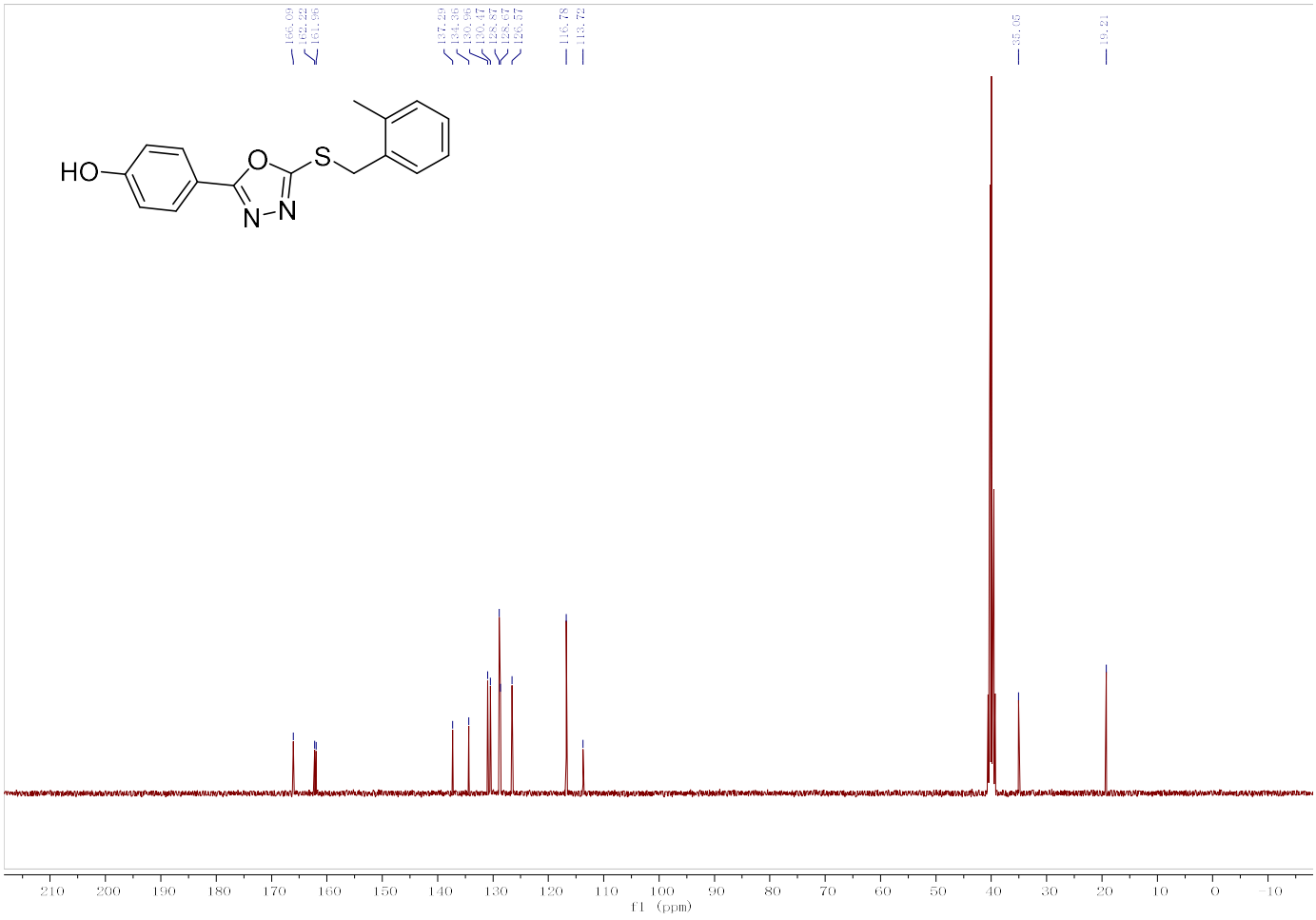

Fig. S22 ^{13}C NMR of compound **4k**

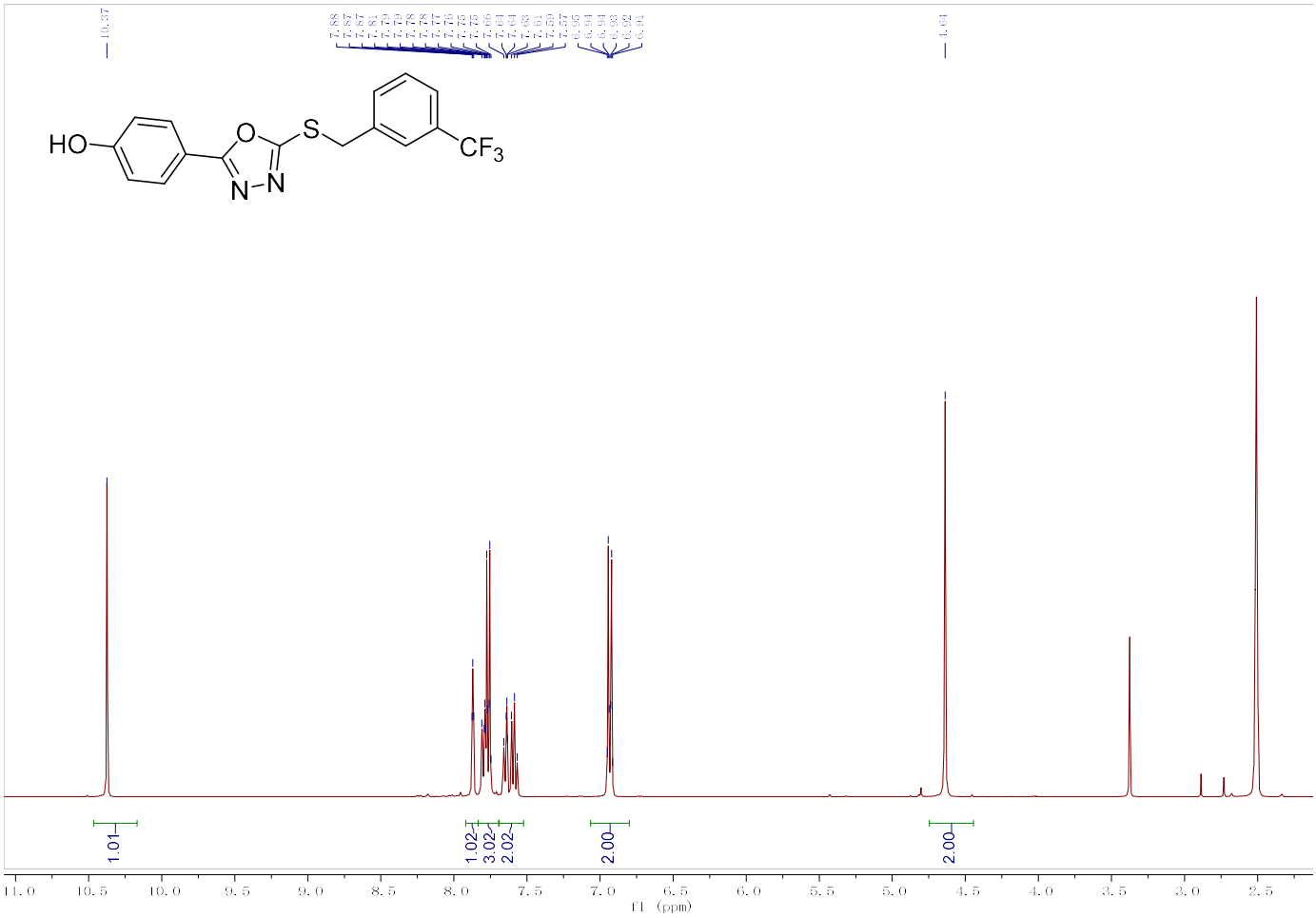

Fig. S23 ^{1}H NMR of compound **4l**

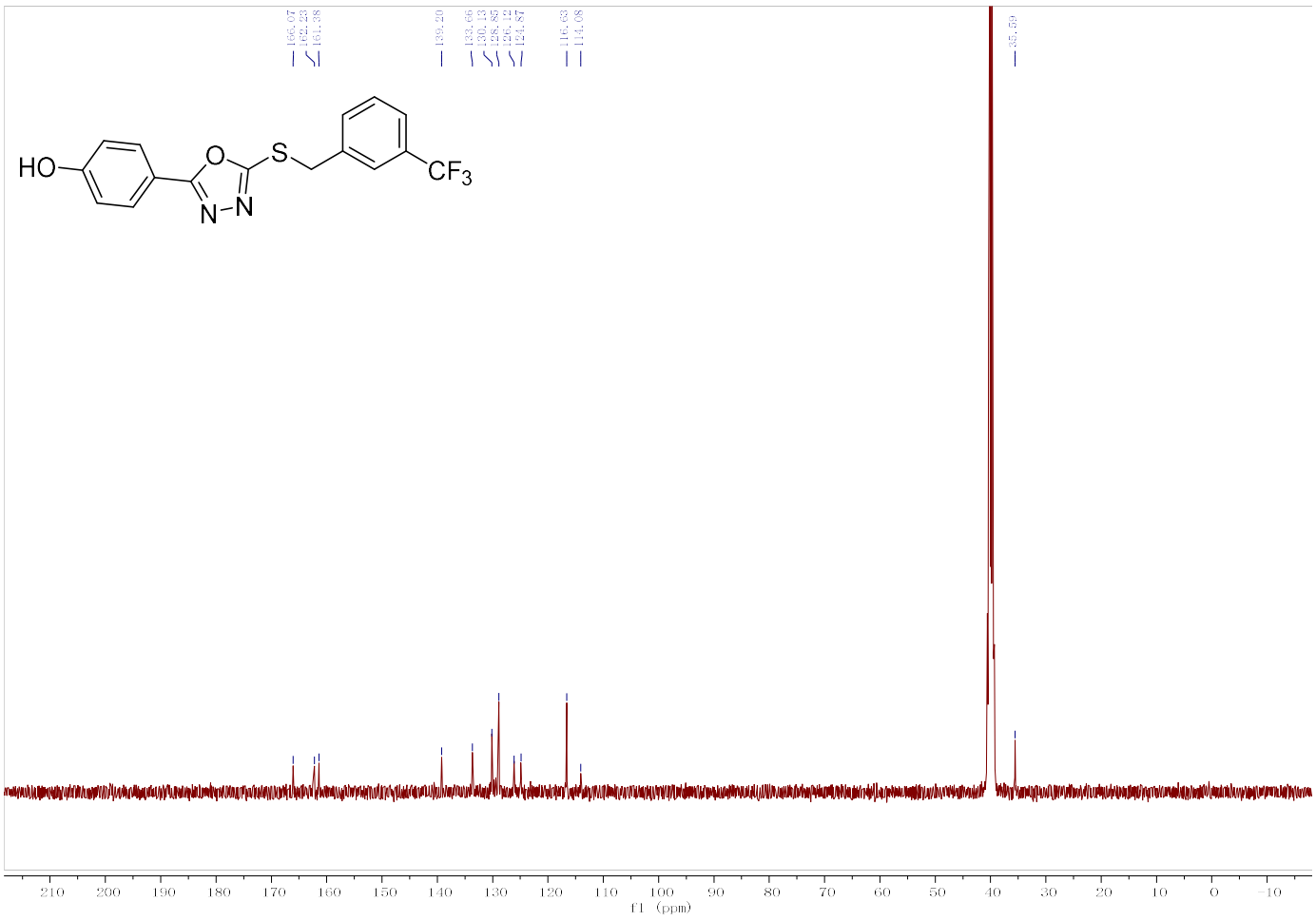

Fig. S24 ^{13}C NMR of compound **4l**

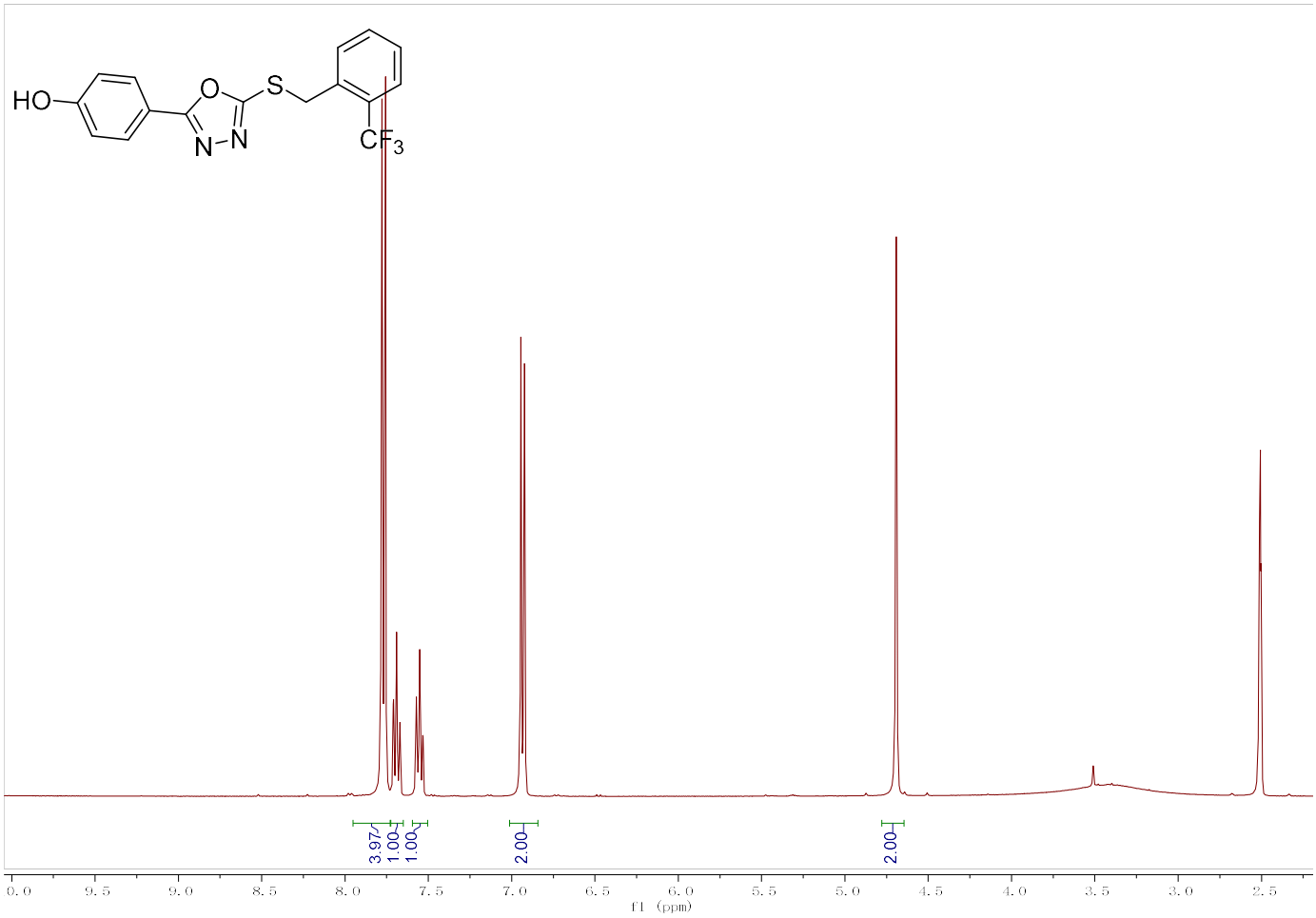

Fig. S25 ^{1}H NMR of compound **4m**

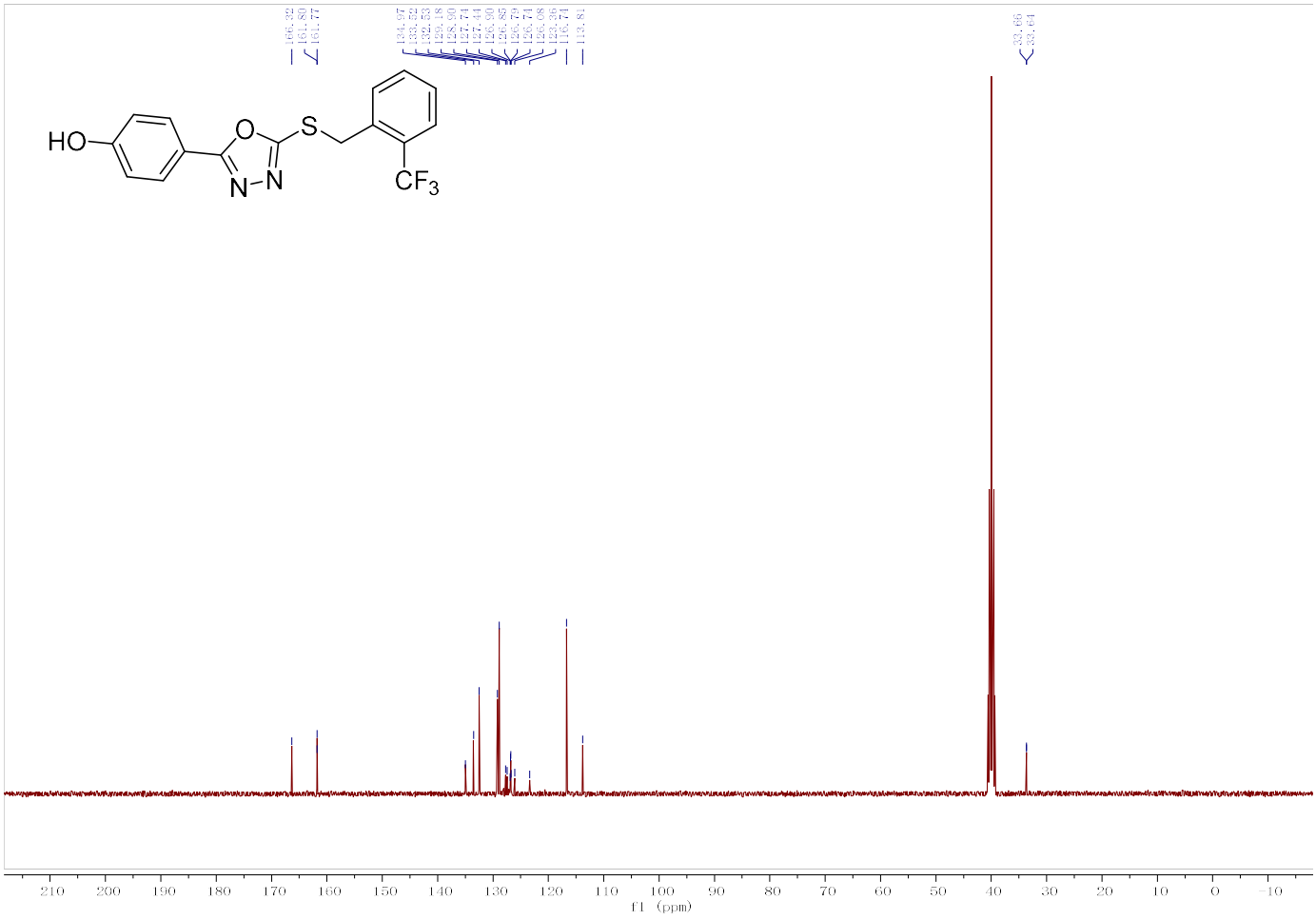

Fig. S26 ^{13}C NMR of compound **4m**

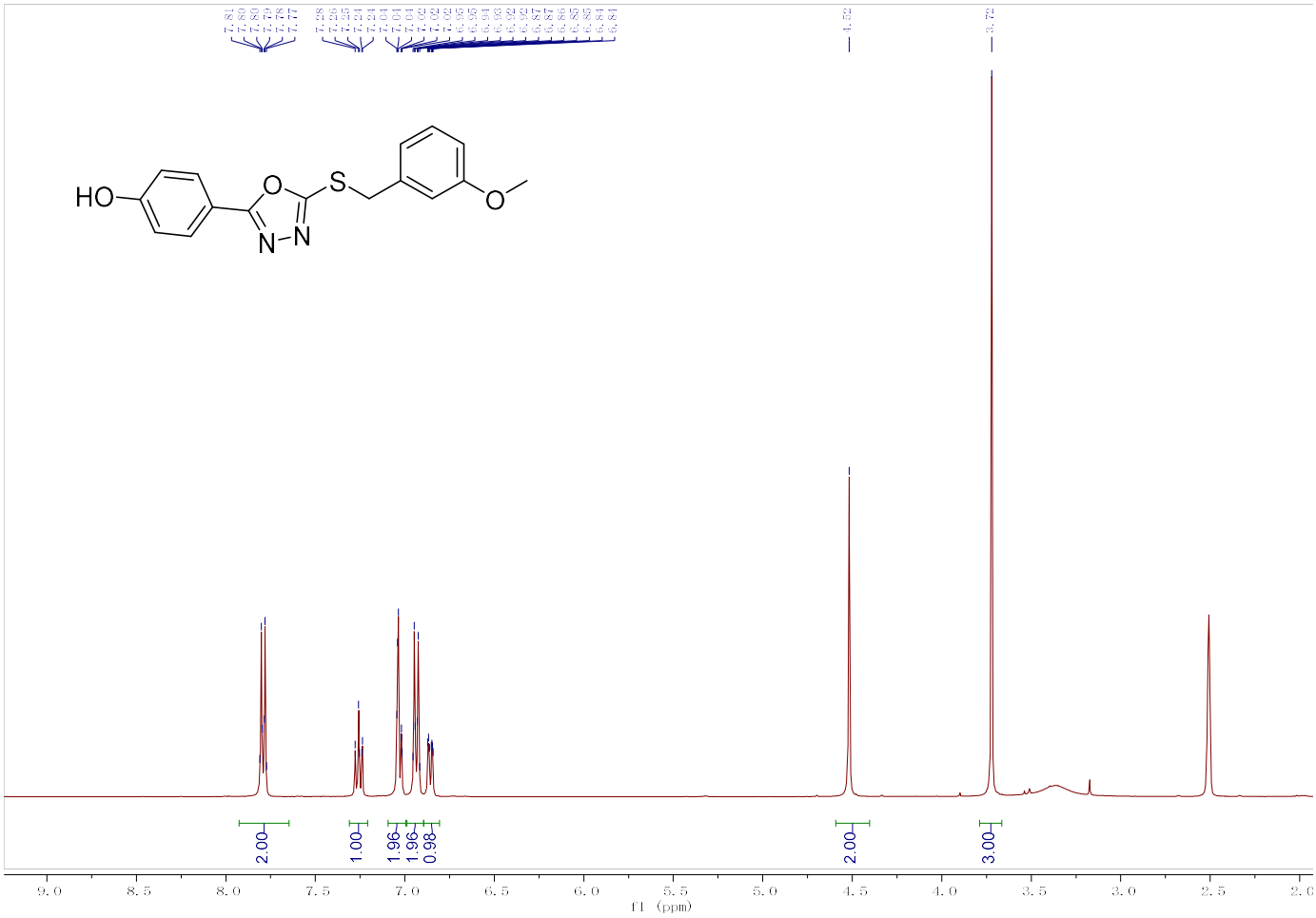

Fig. S27 ^{1}H NMR of compound **4n**

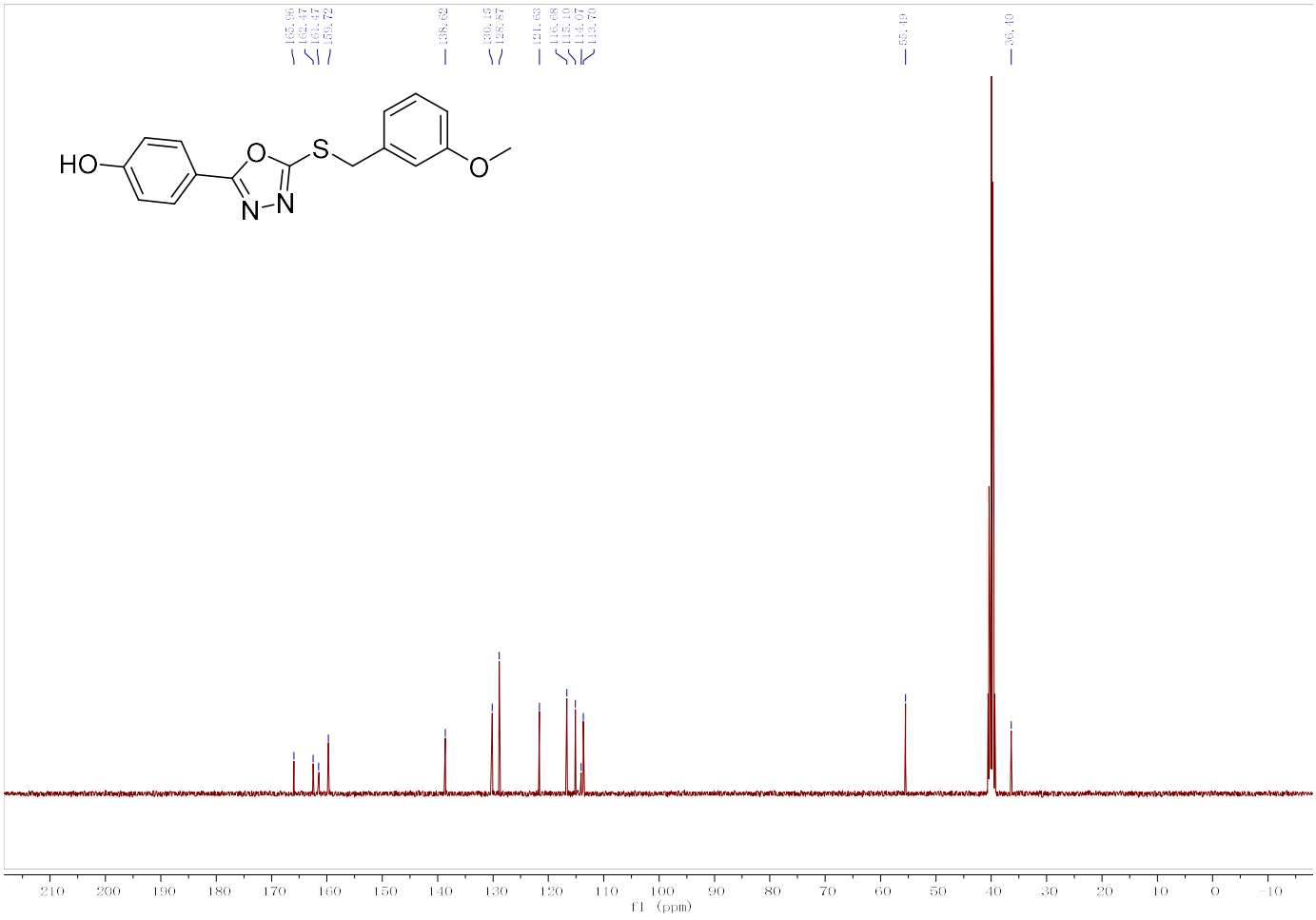

Fig. S28 ^{13}C NMR of compound **4n**

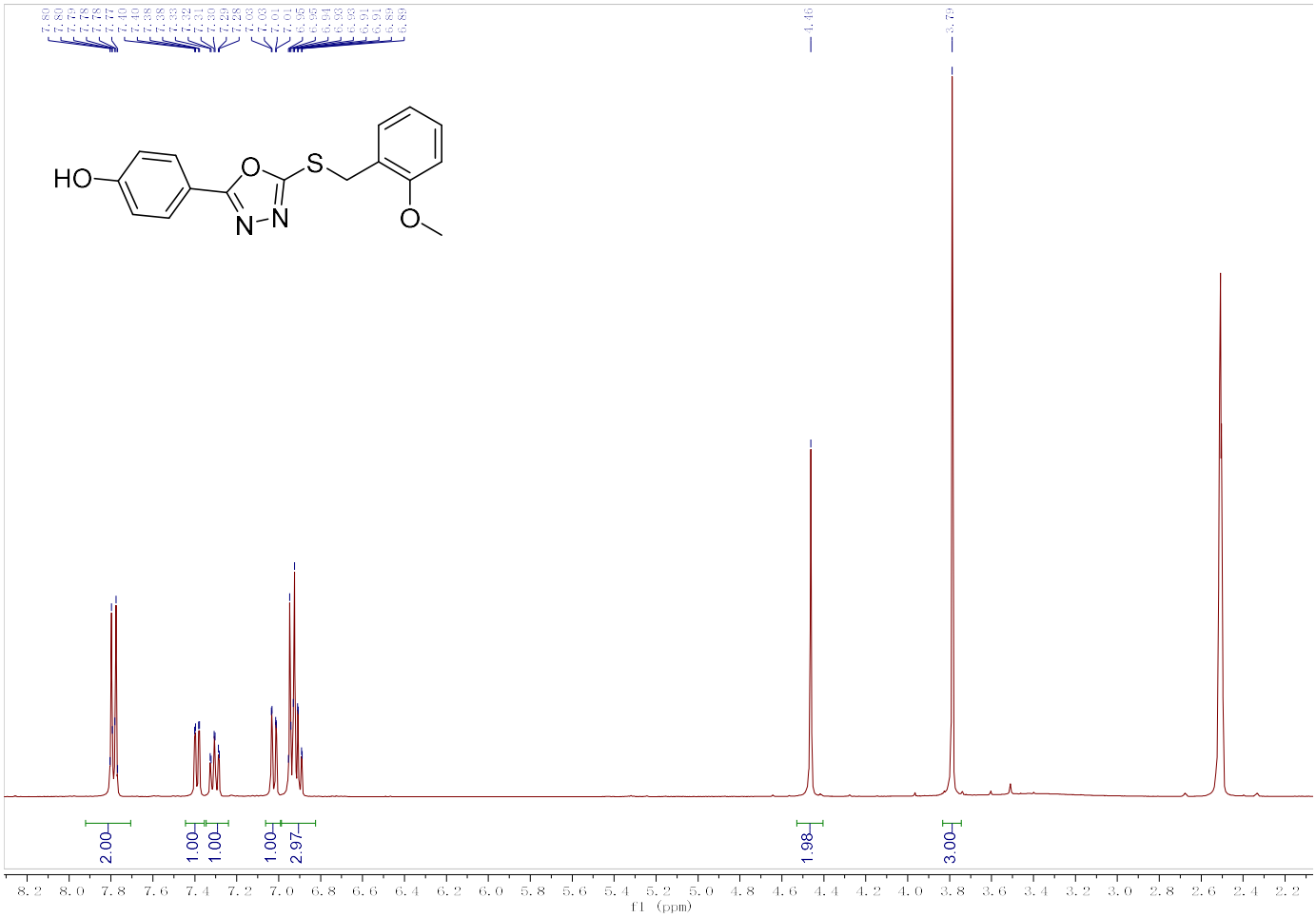

Fig. S29 ^{1}H NMR of compound **4o**

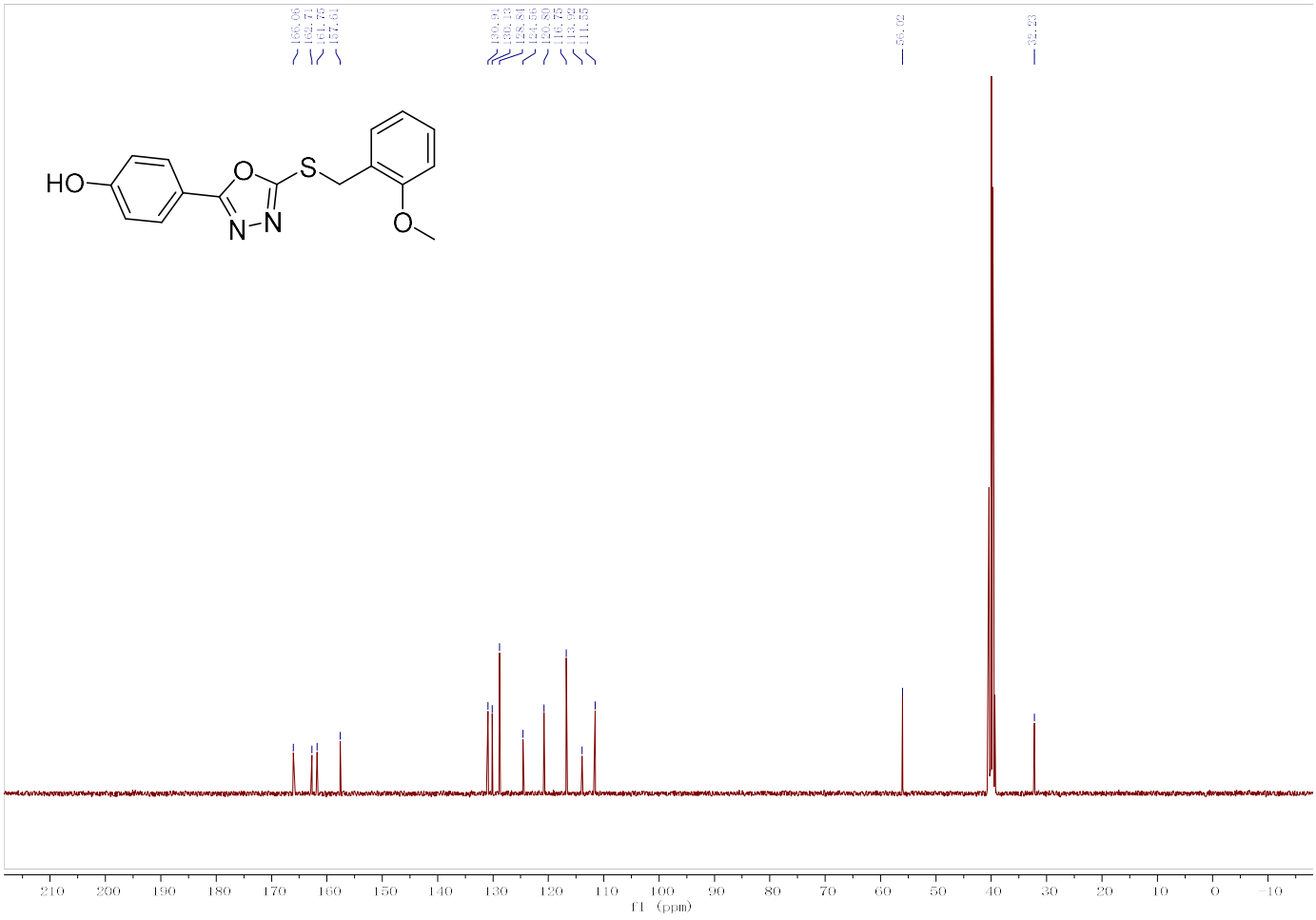

Fig. S30 ^{13}C NMR of compound **4o**

3. ^{1}H NMR, ^{13}C spectra for target compounds:

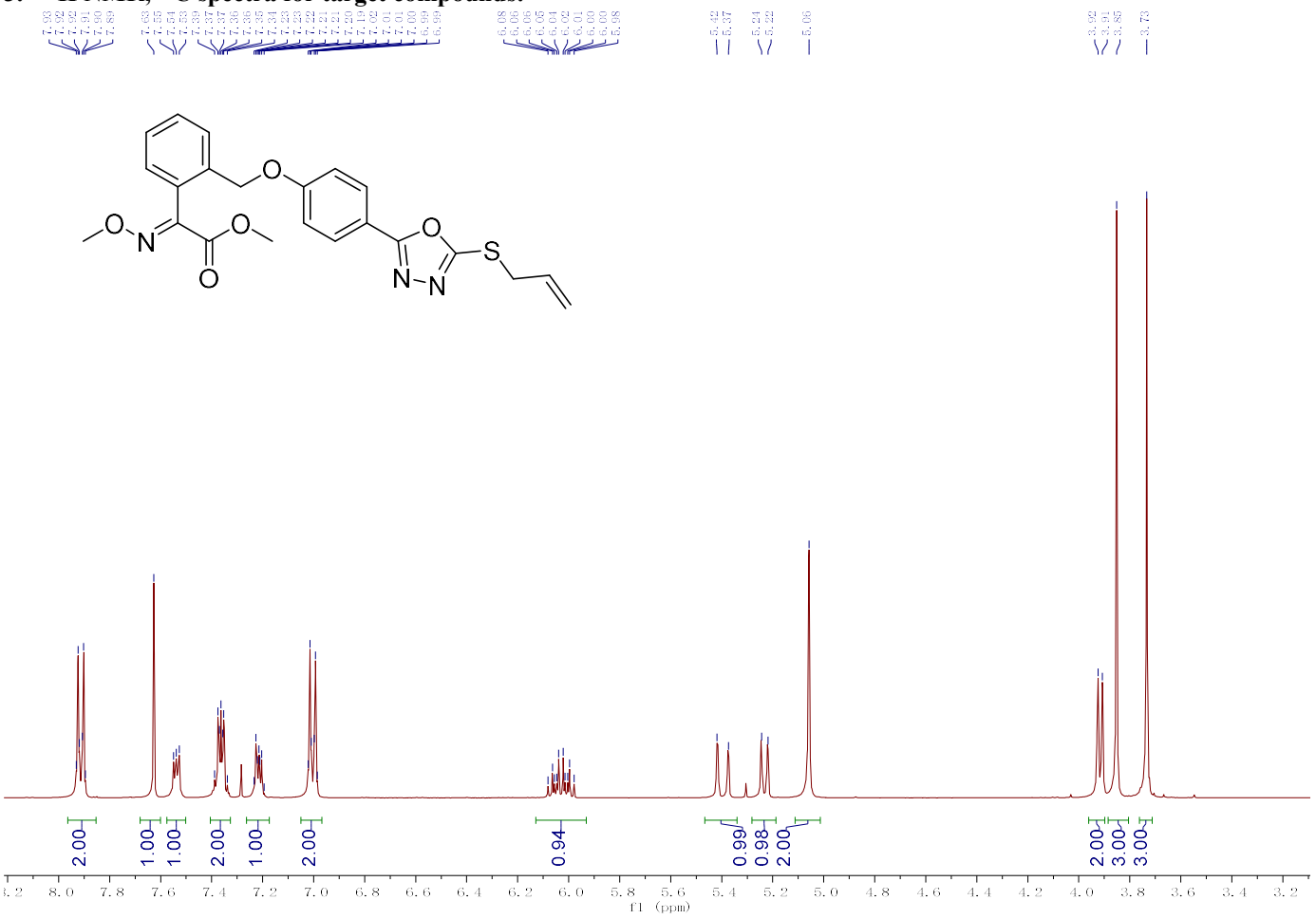

Fig. S31 ^{1}H NMR of compound **6a**

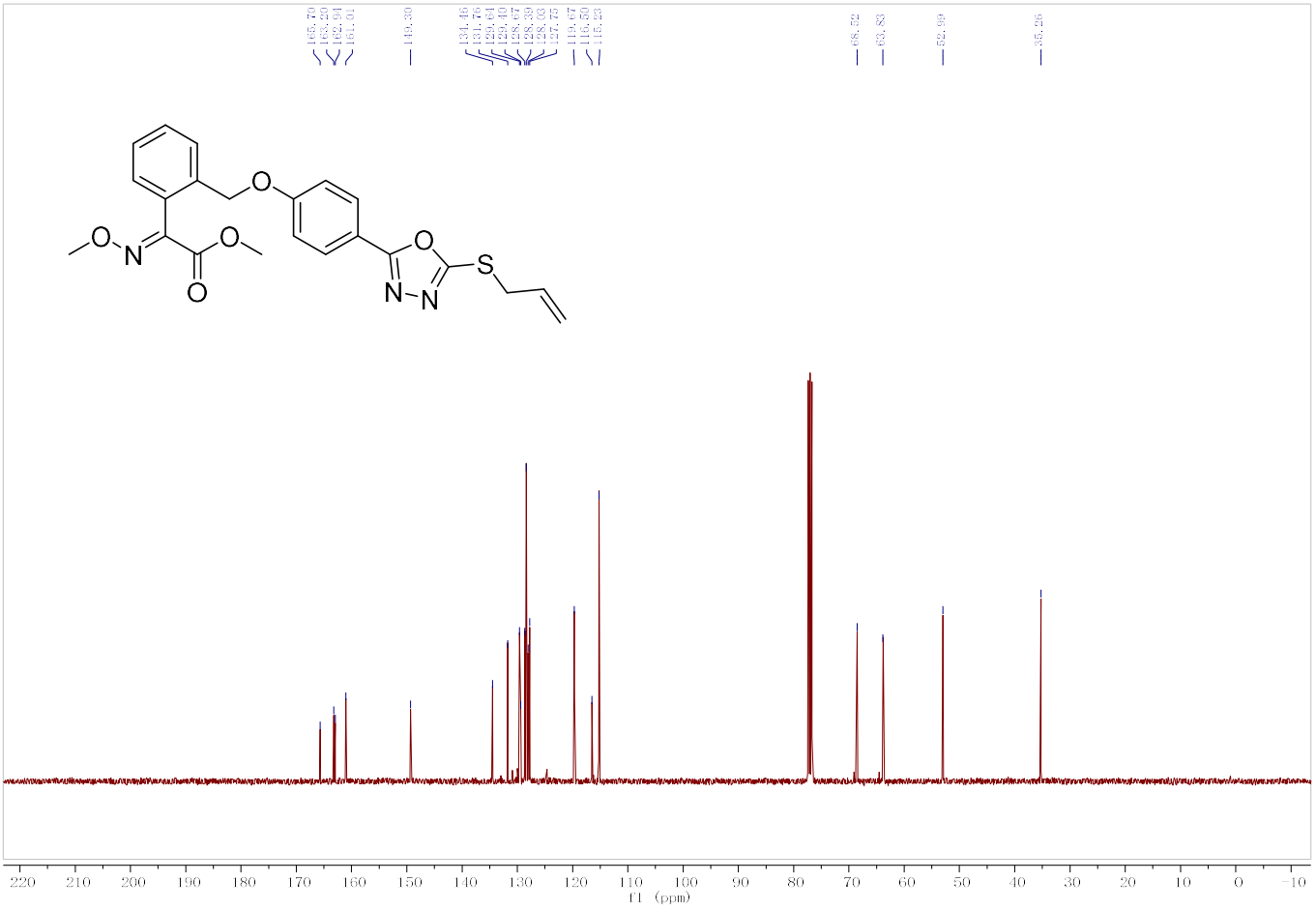

Fig. S32 ^{13}C NMR of compound **6a**

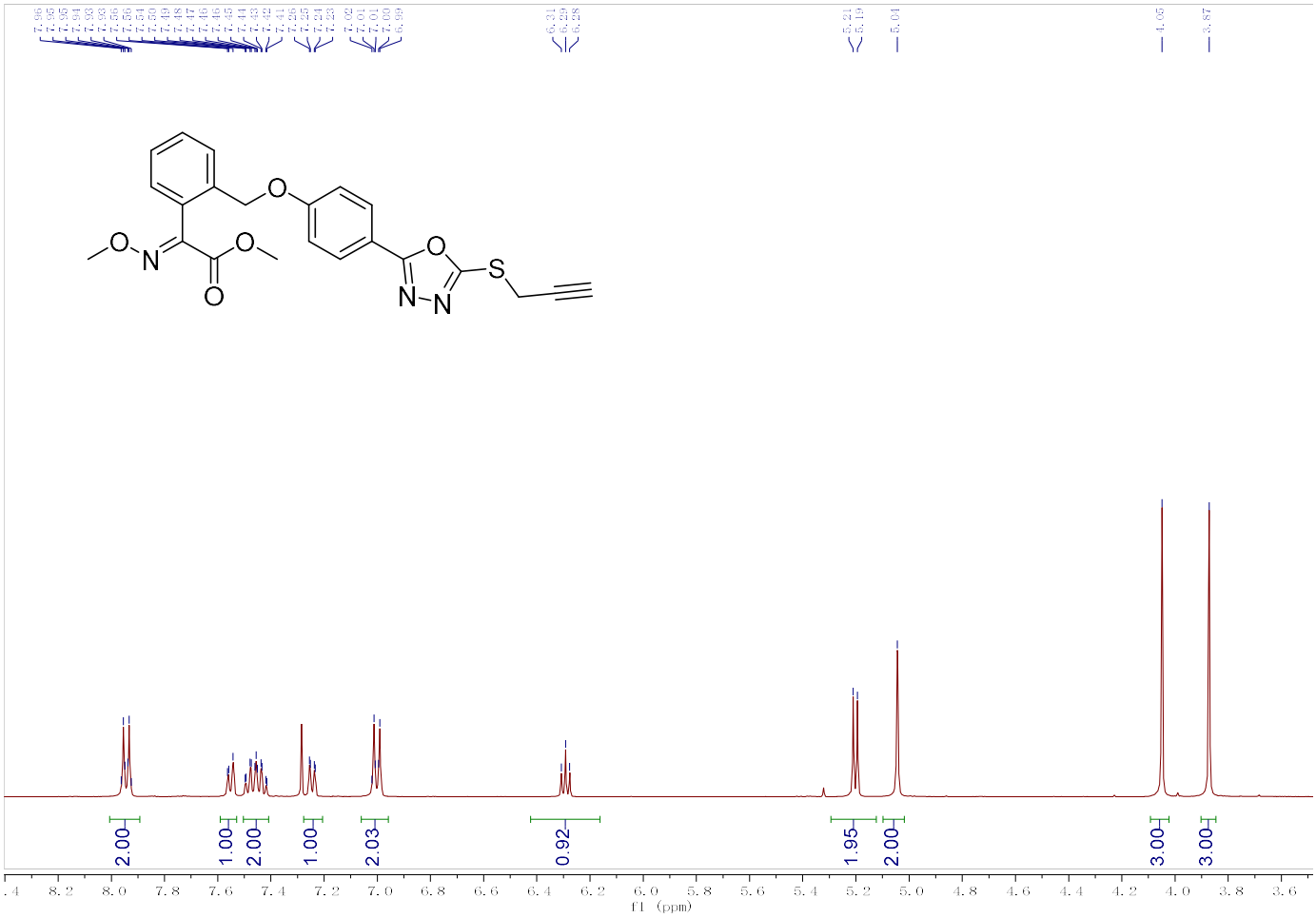

Fig. S33 ^{1}H NMR of compound **6b**

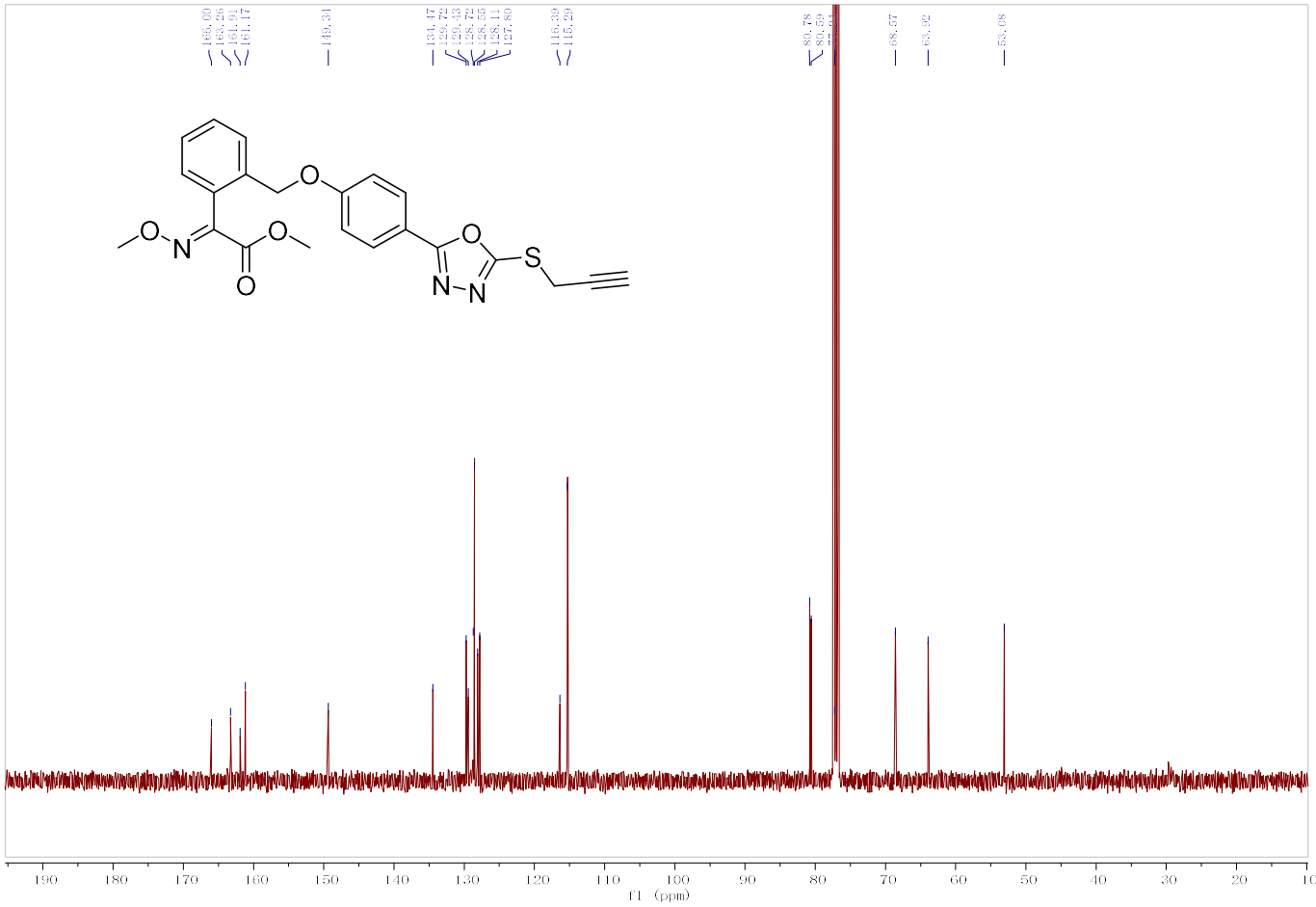

Fig. S34 ^{13}C NMR of compound **6b**

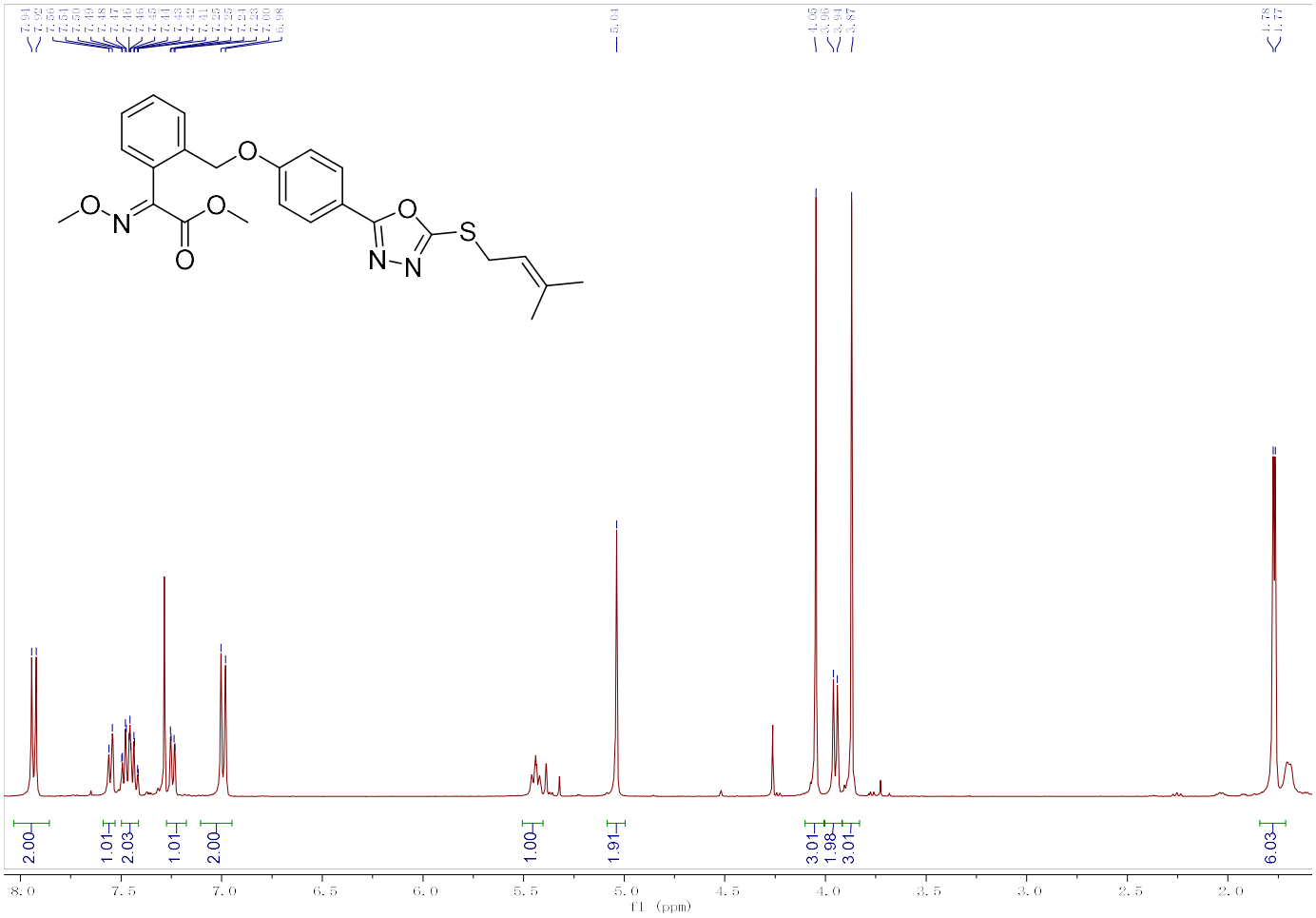

Fig. S35 ^{1}H NMR of compound **6c**

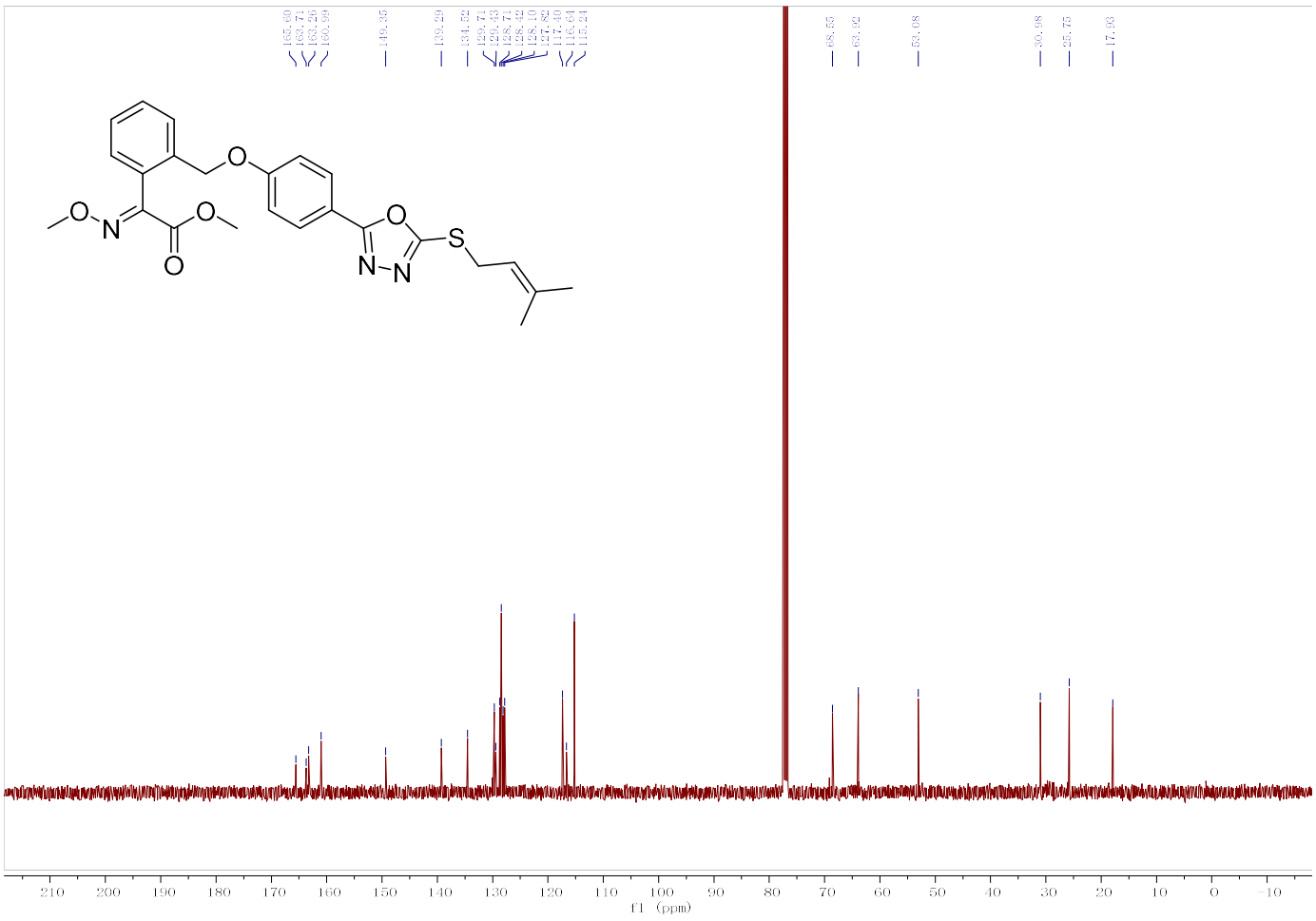

Fig. S36 ^{13}C NMR of compound **6c**

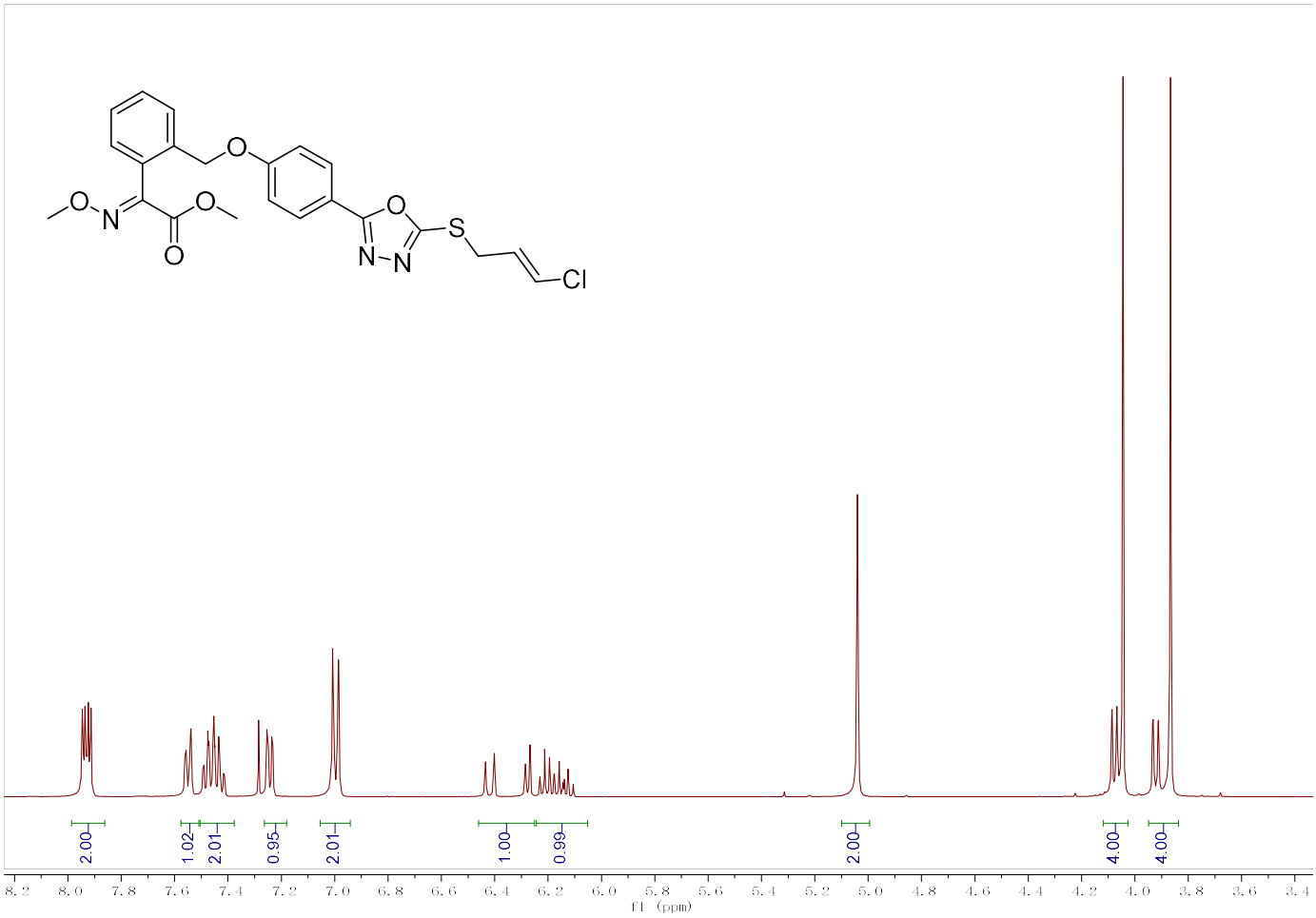

Fig. S37 ^{1}H NMR of compound **6d**

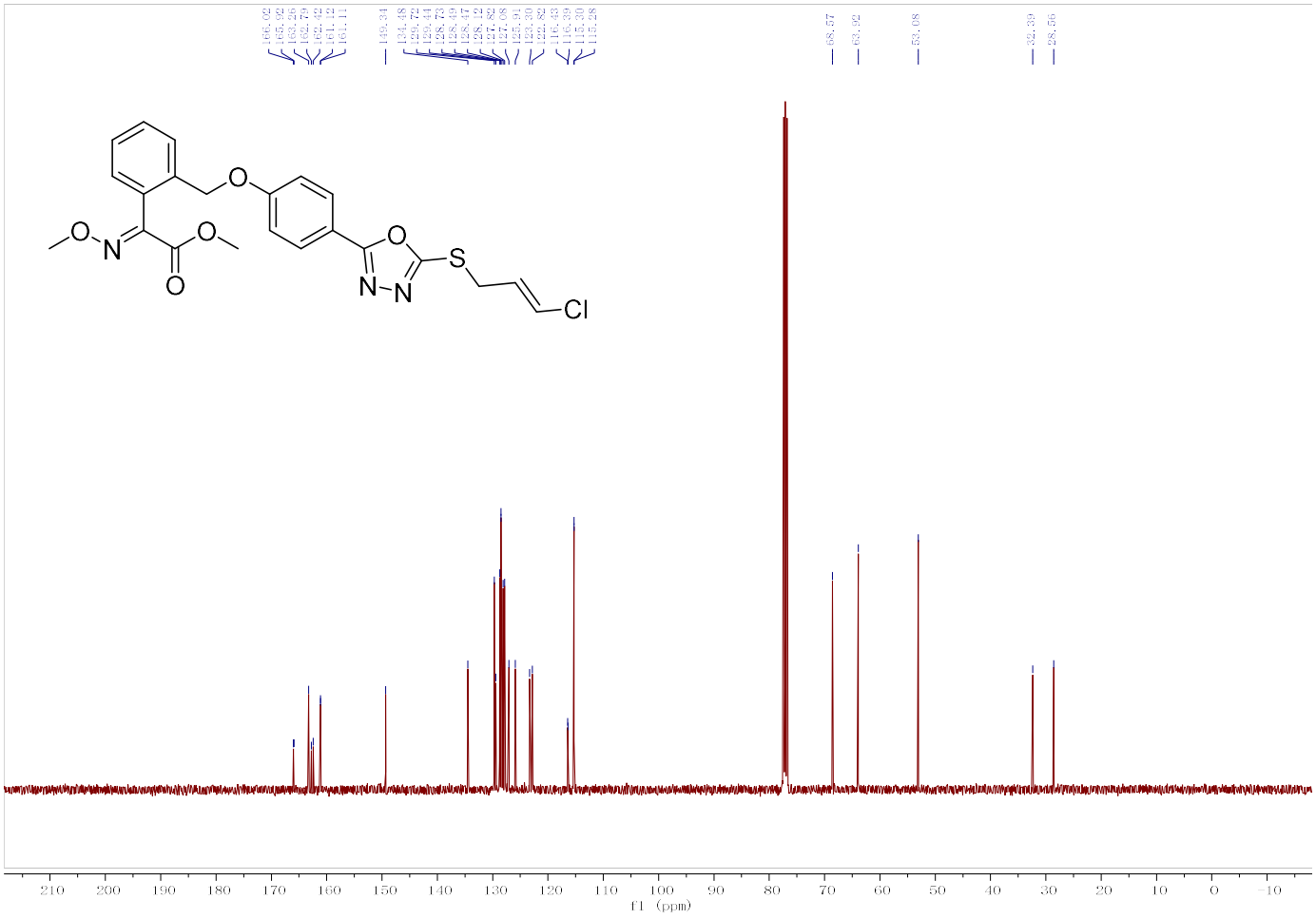

Fig. S38 ^{13}C NMR of compound **6d**

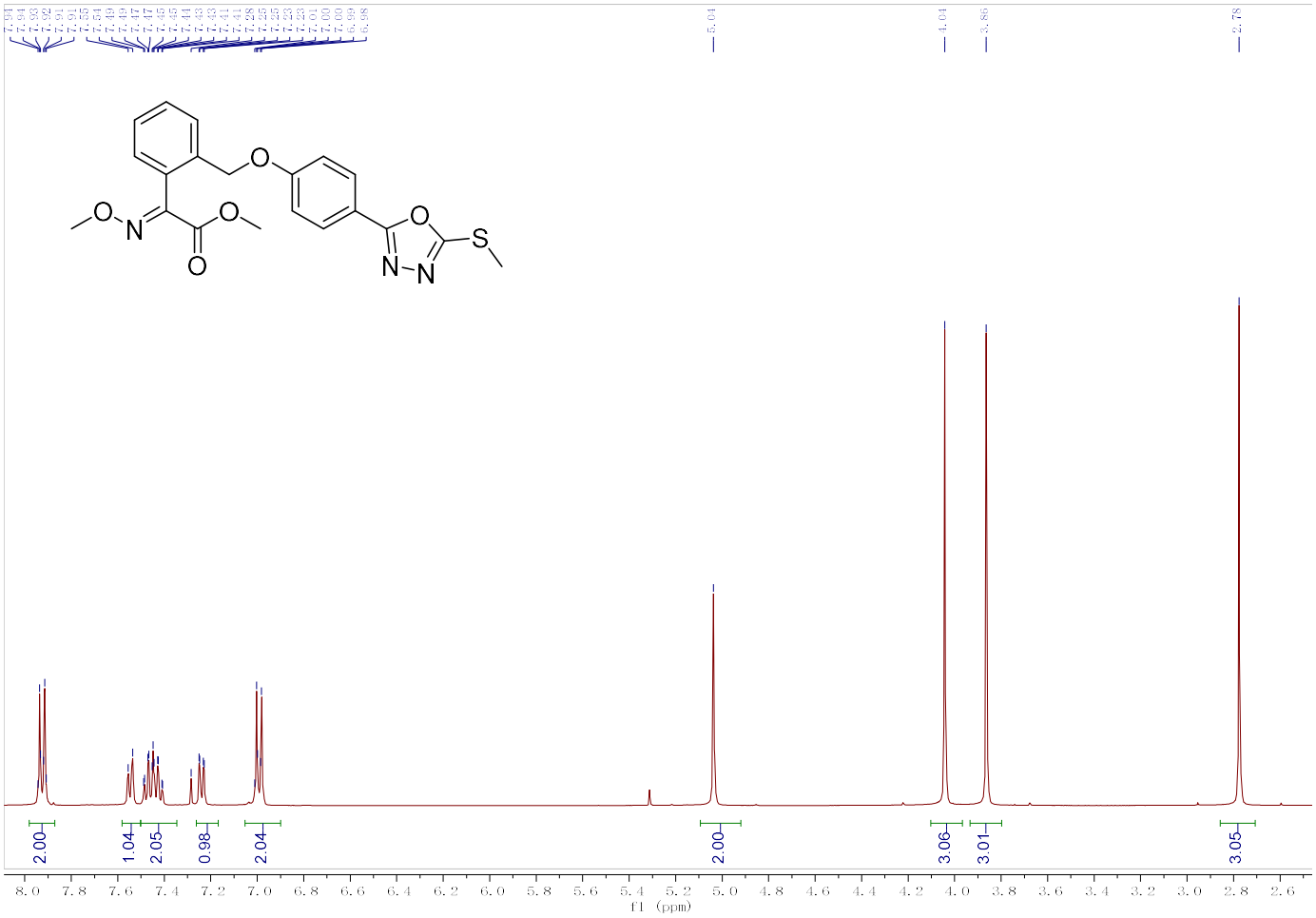

Fig. S39 ^{1}H NMR of compound **6e**

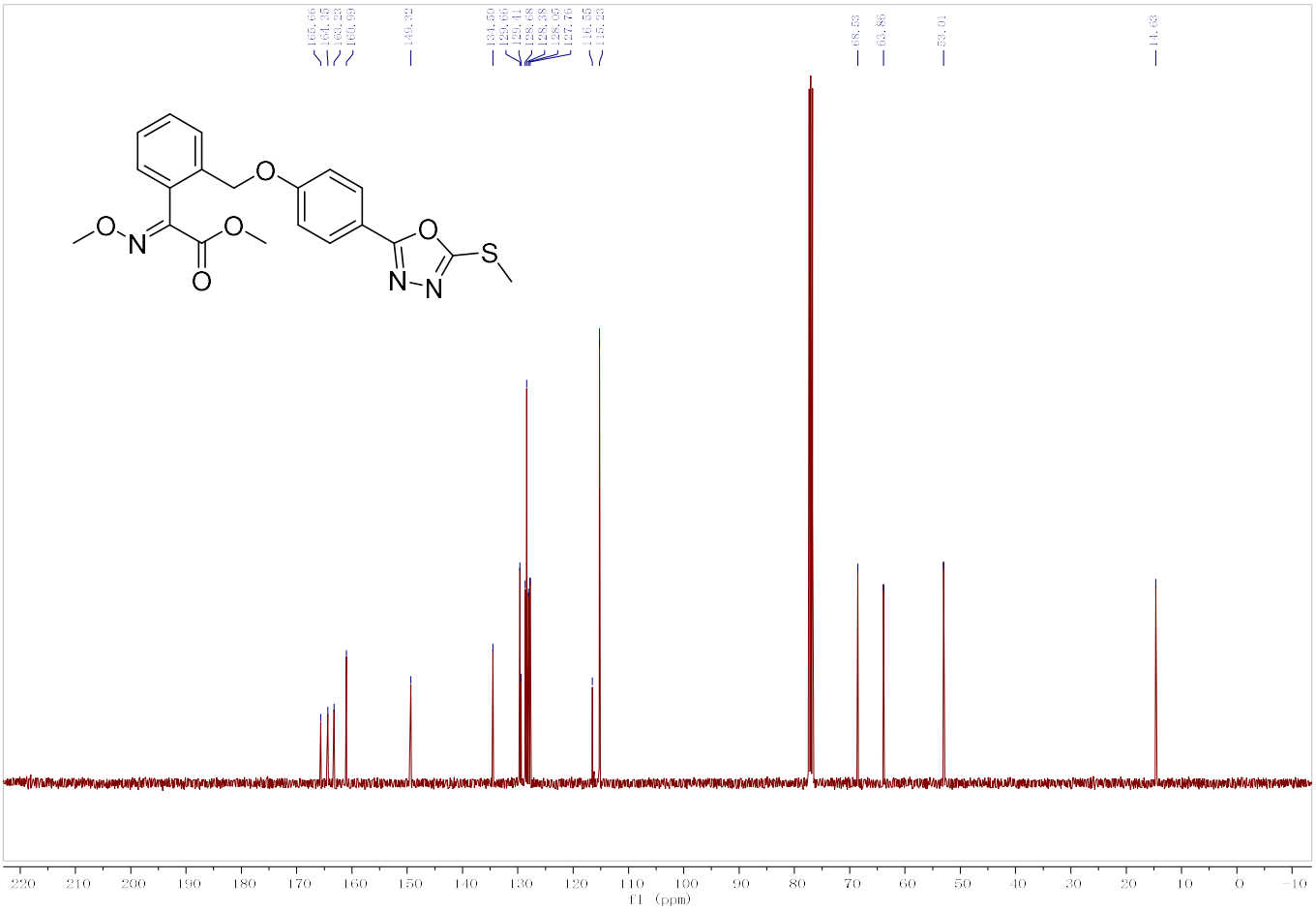

Fig. S40 ^{13}C NMR of compound **6e**

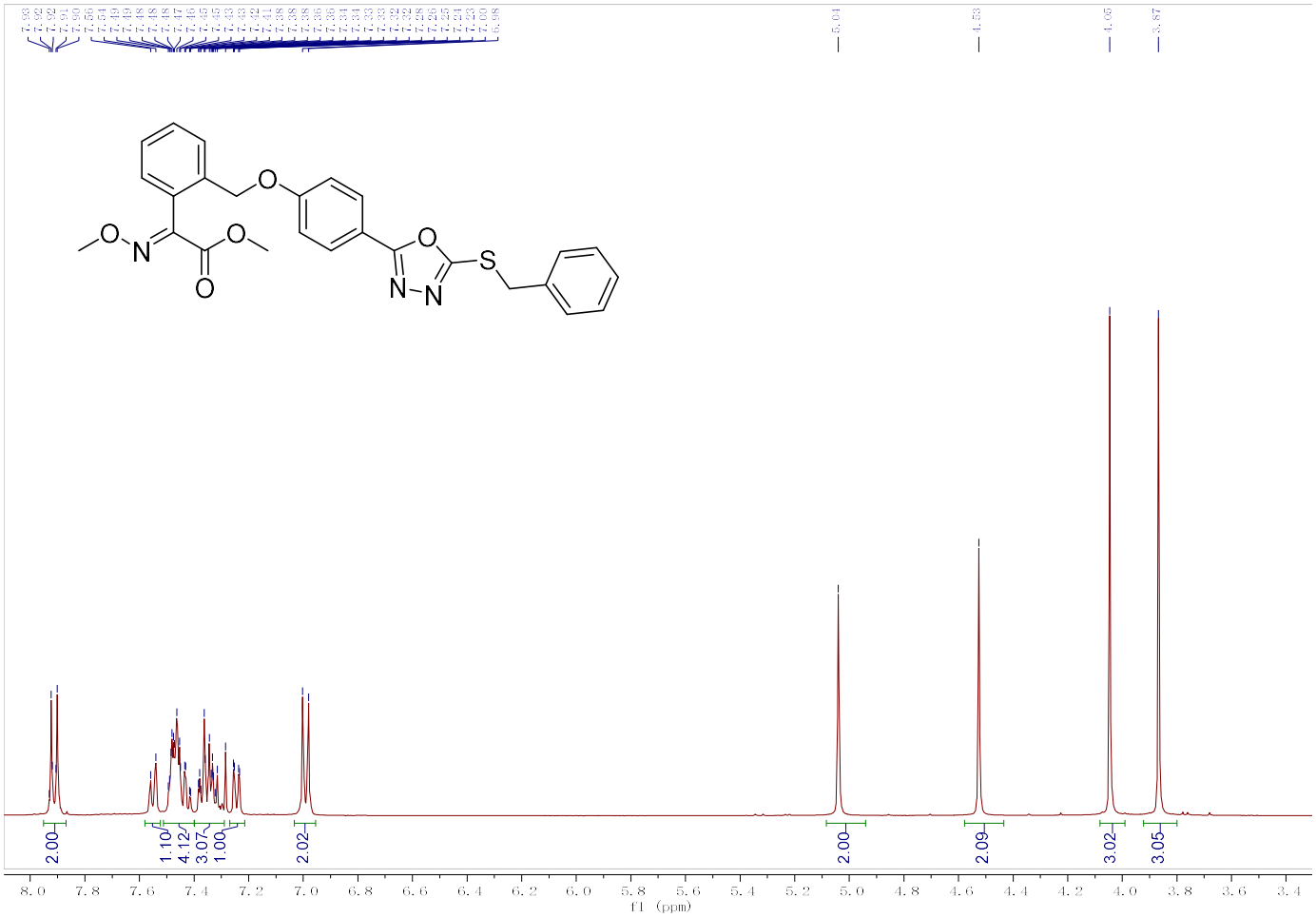

Fig. S41 ^{1}H NMR of compound **6f**

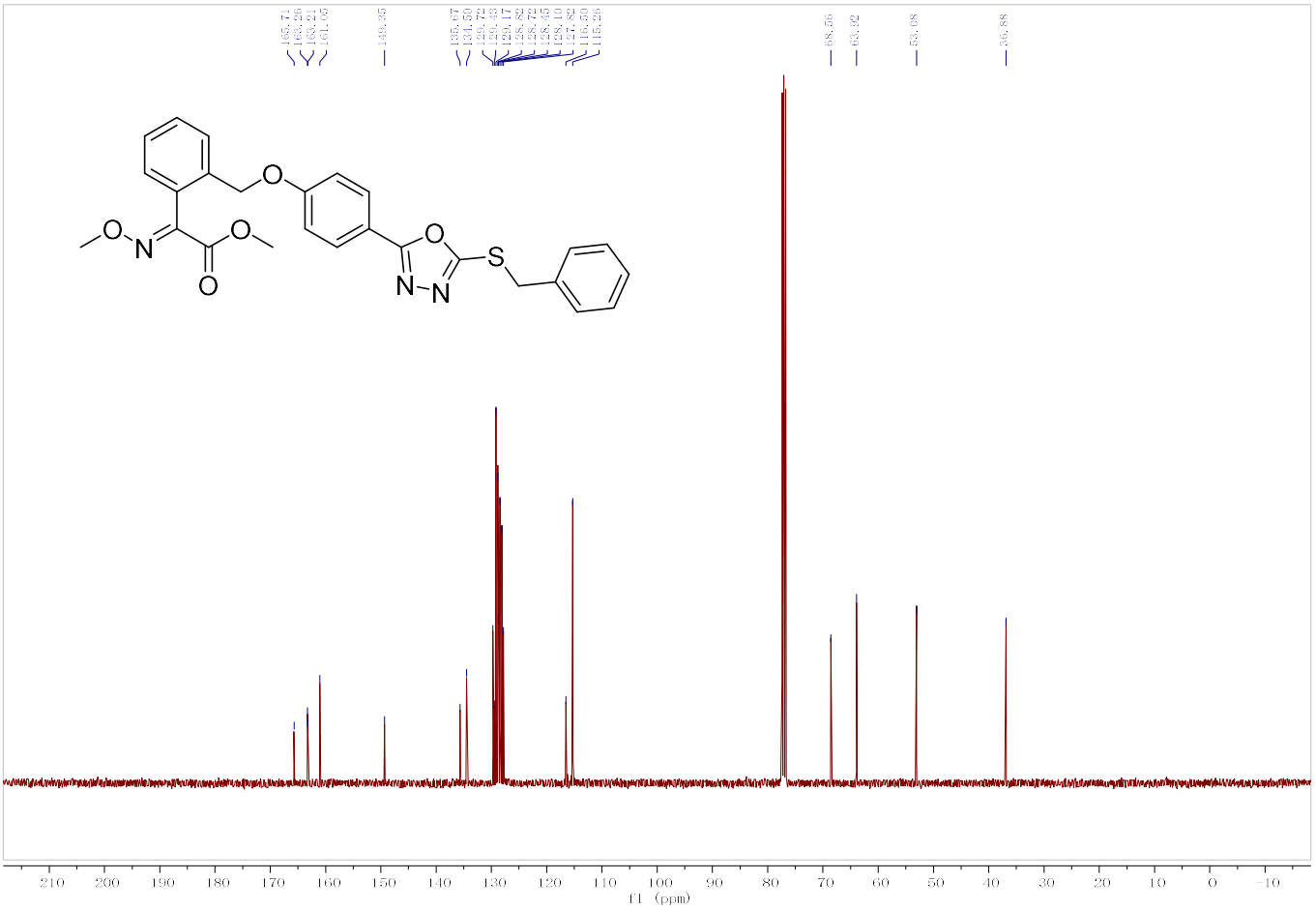

Fig. S42 ^{13}C NMR of compound **6f**

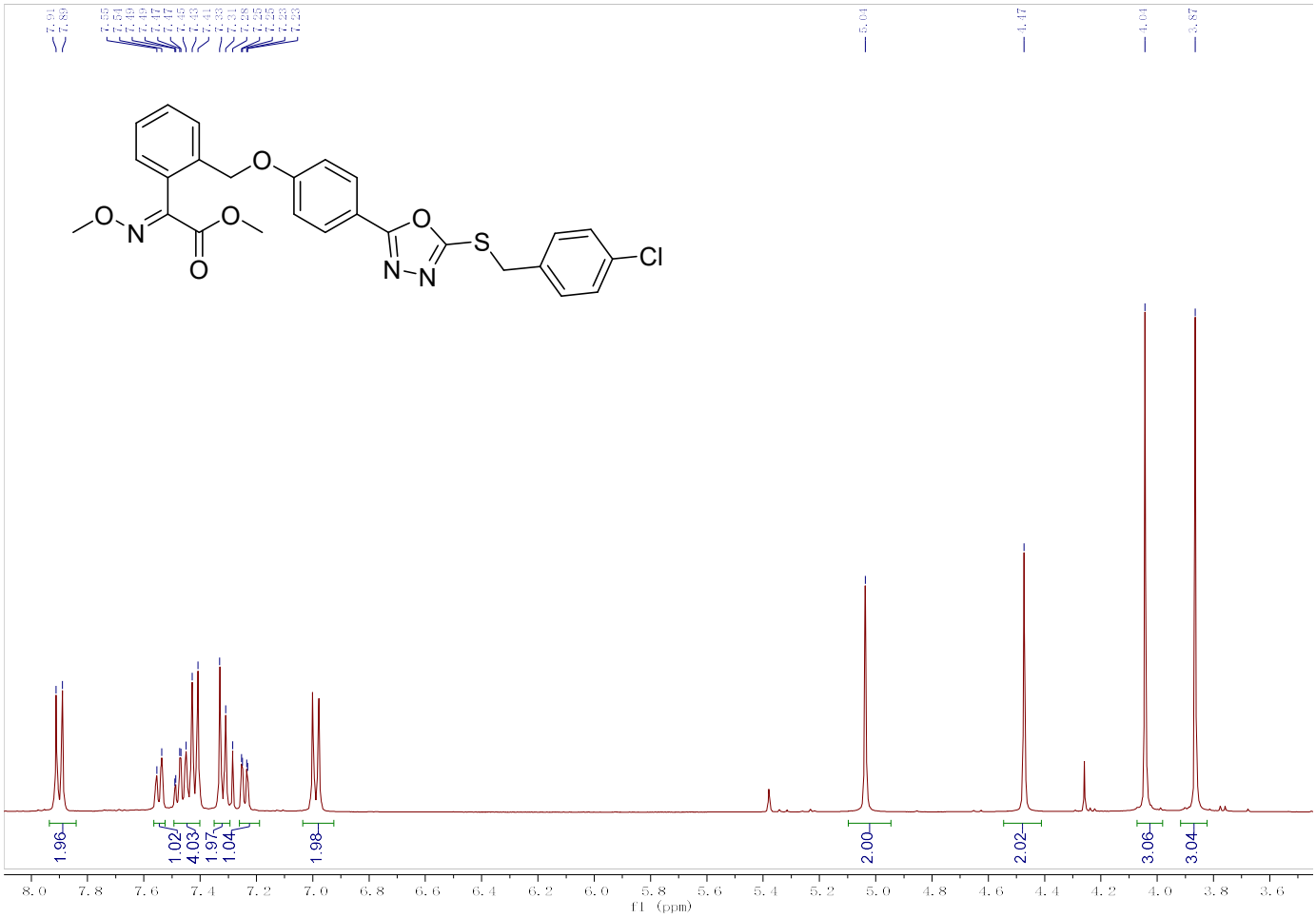

Fig. S43 ^{1}H NMR of compound **6g**

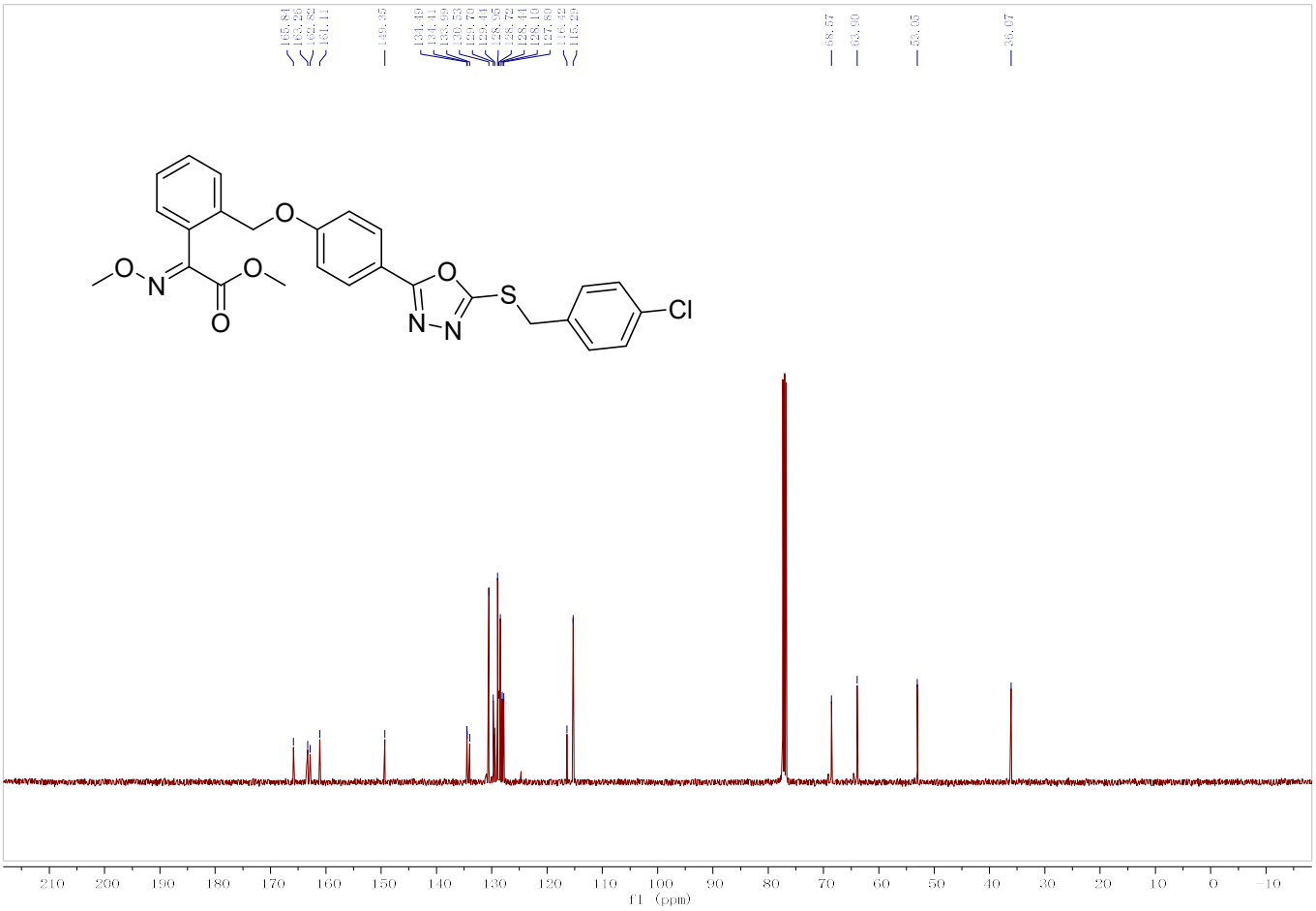

Fig. S44 ^{13}C NMR of compound **6g**

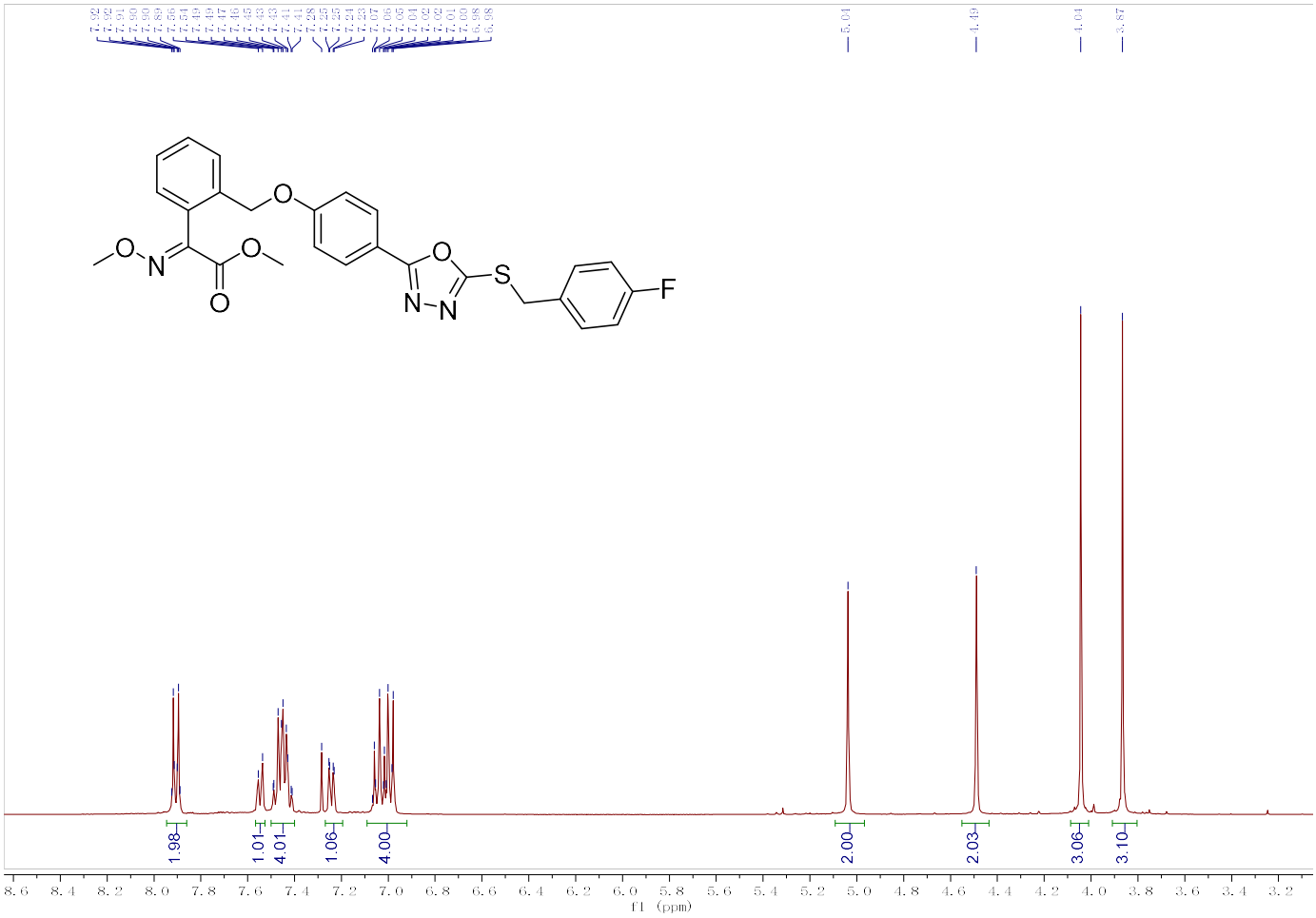

Fig. S45 ^{1}H NMR of compound **6h**

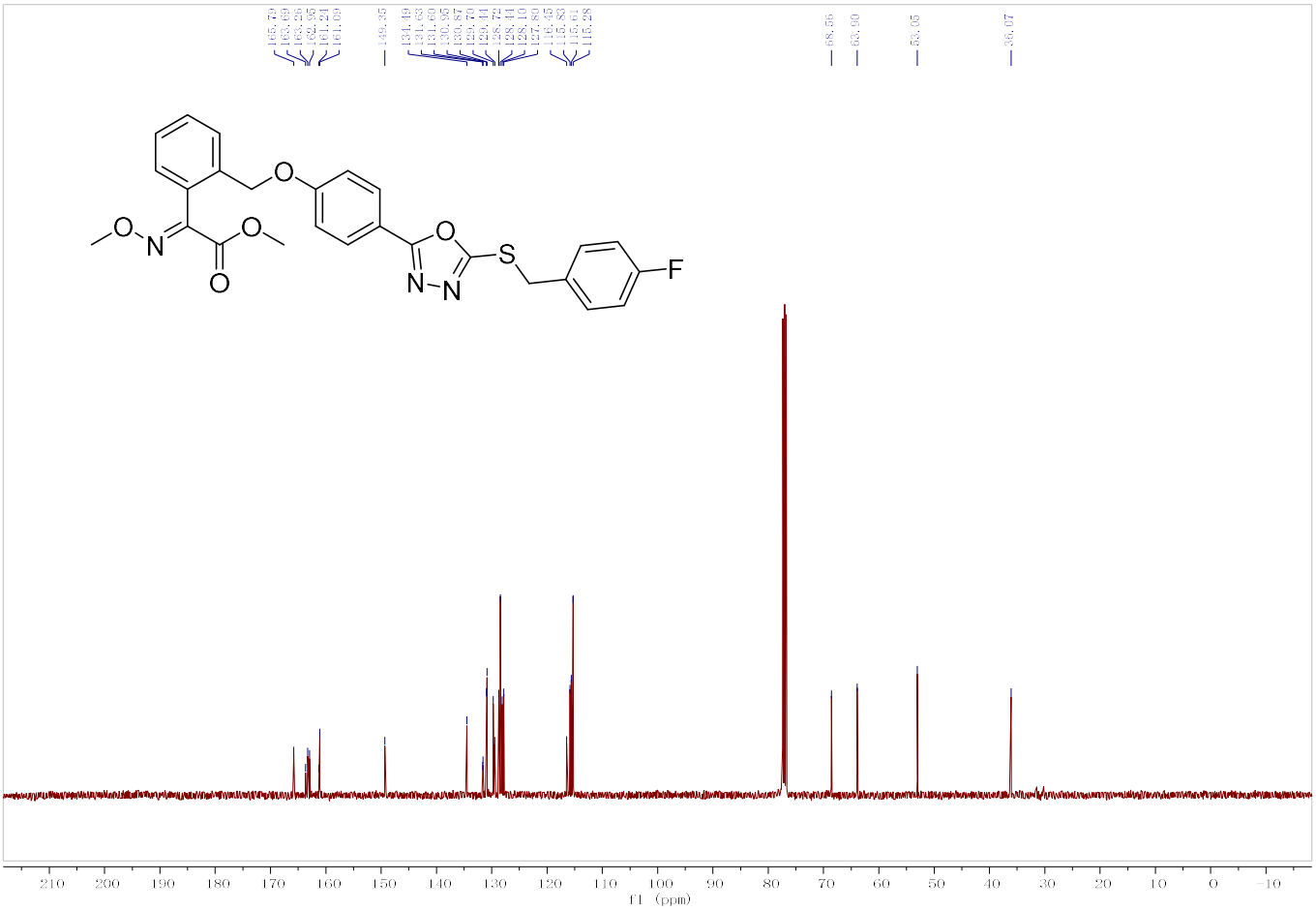

Fig. S46 ^{13}C NMR of compound **6h**

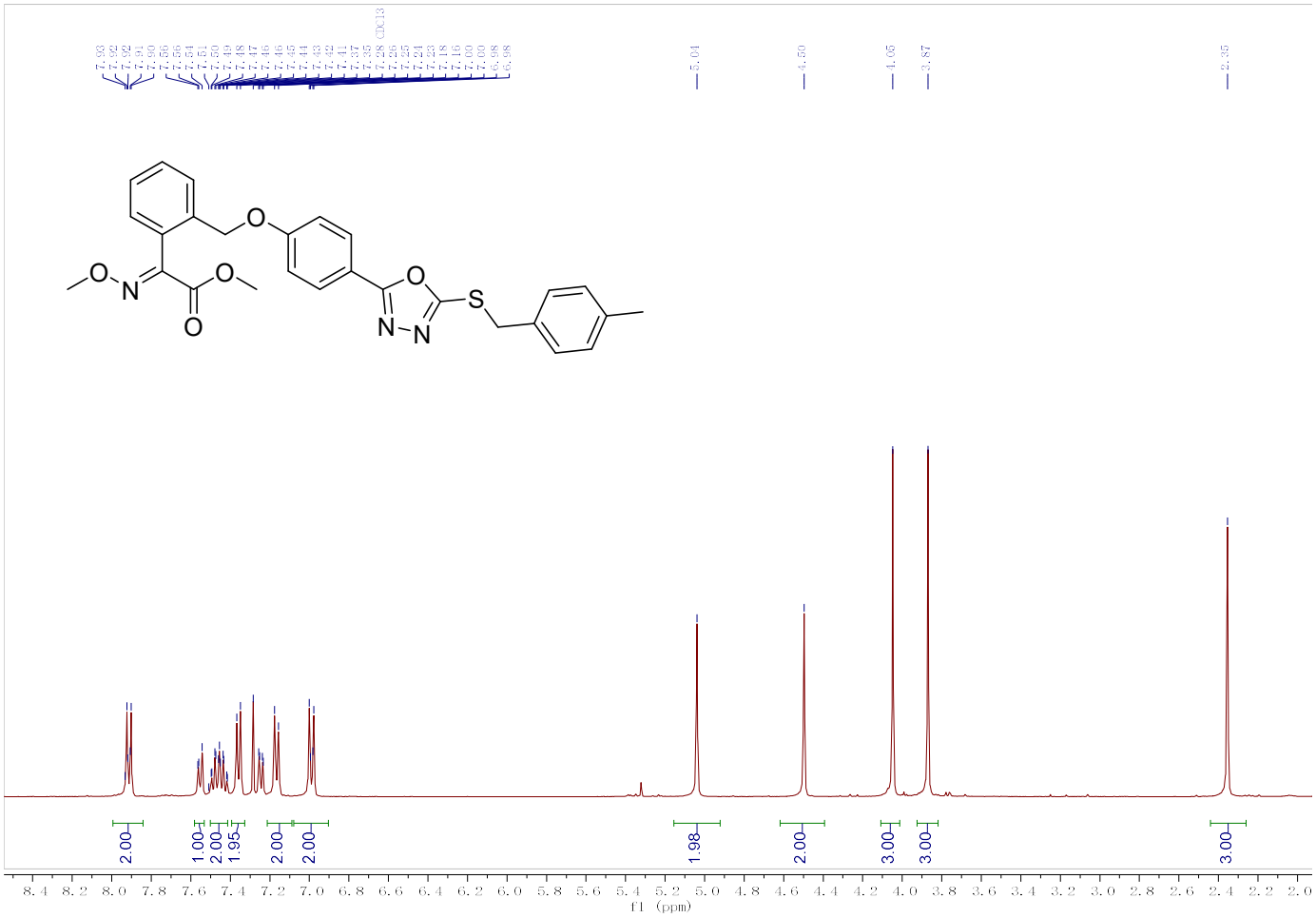

Fig. S47 ^{1}H NMR of compound **6i**

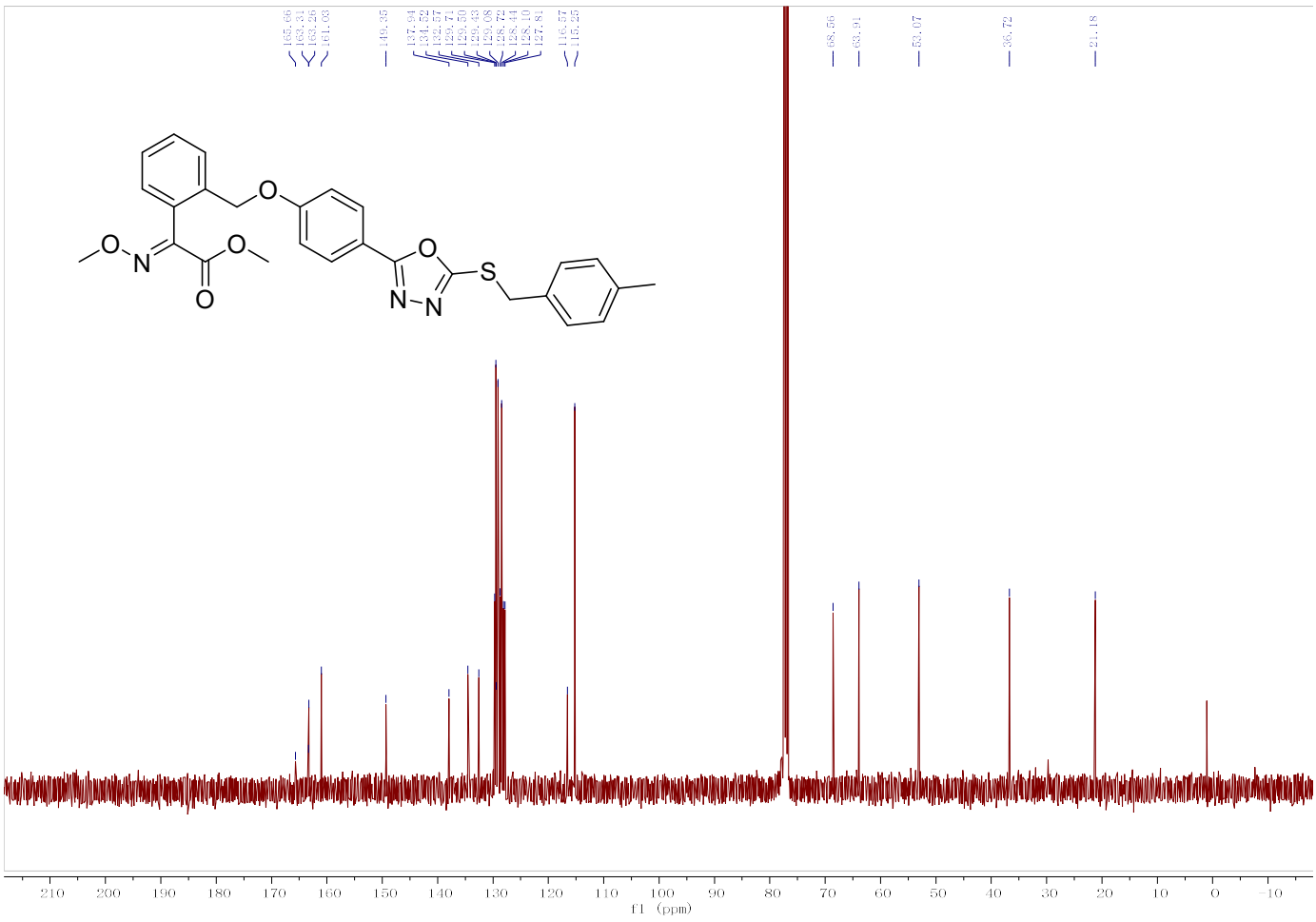

Fig. S48 ^{13}C NMR of compound **6i**

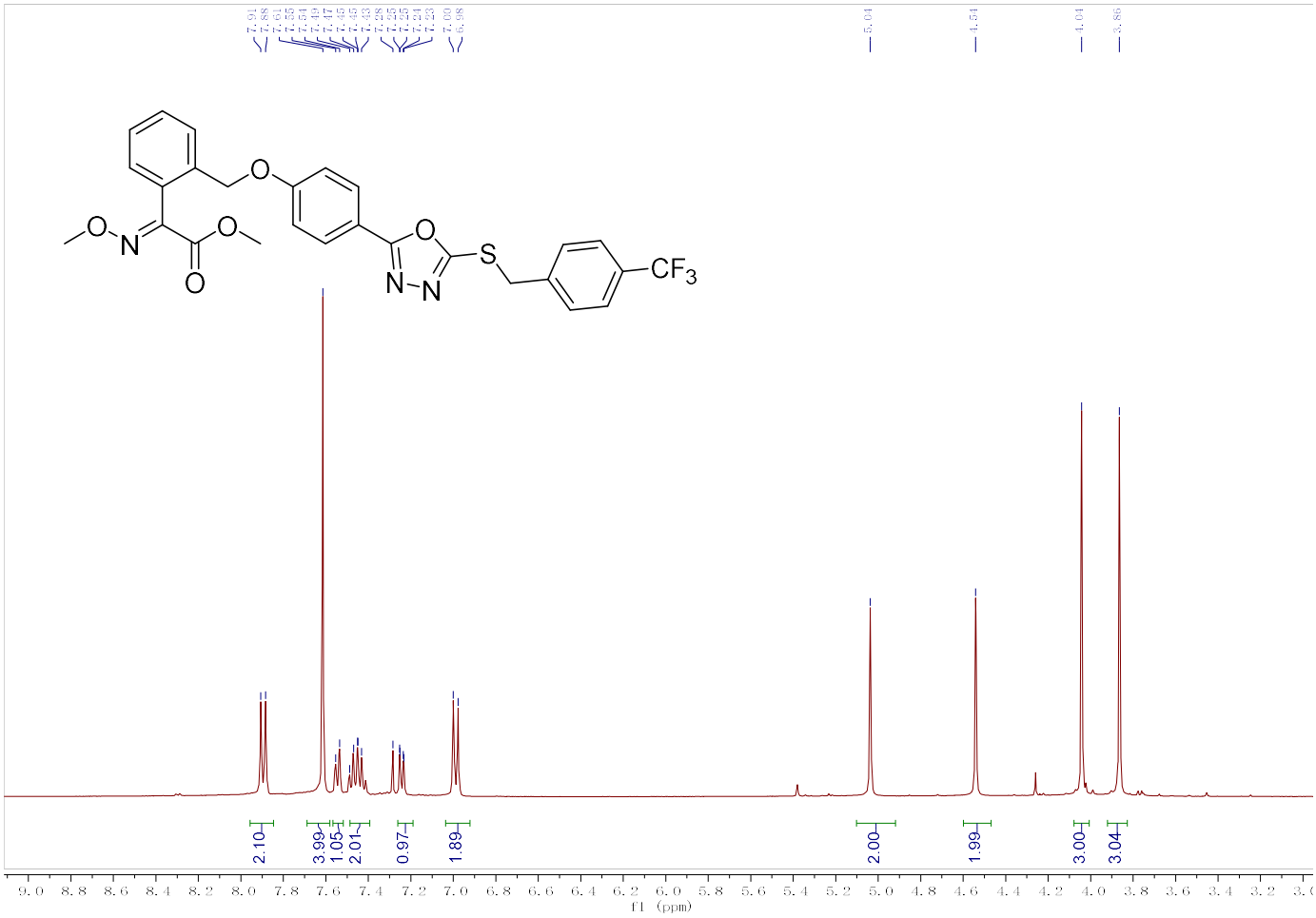

Fig. S49 ^{1}H NMR of compound **6j**

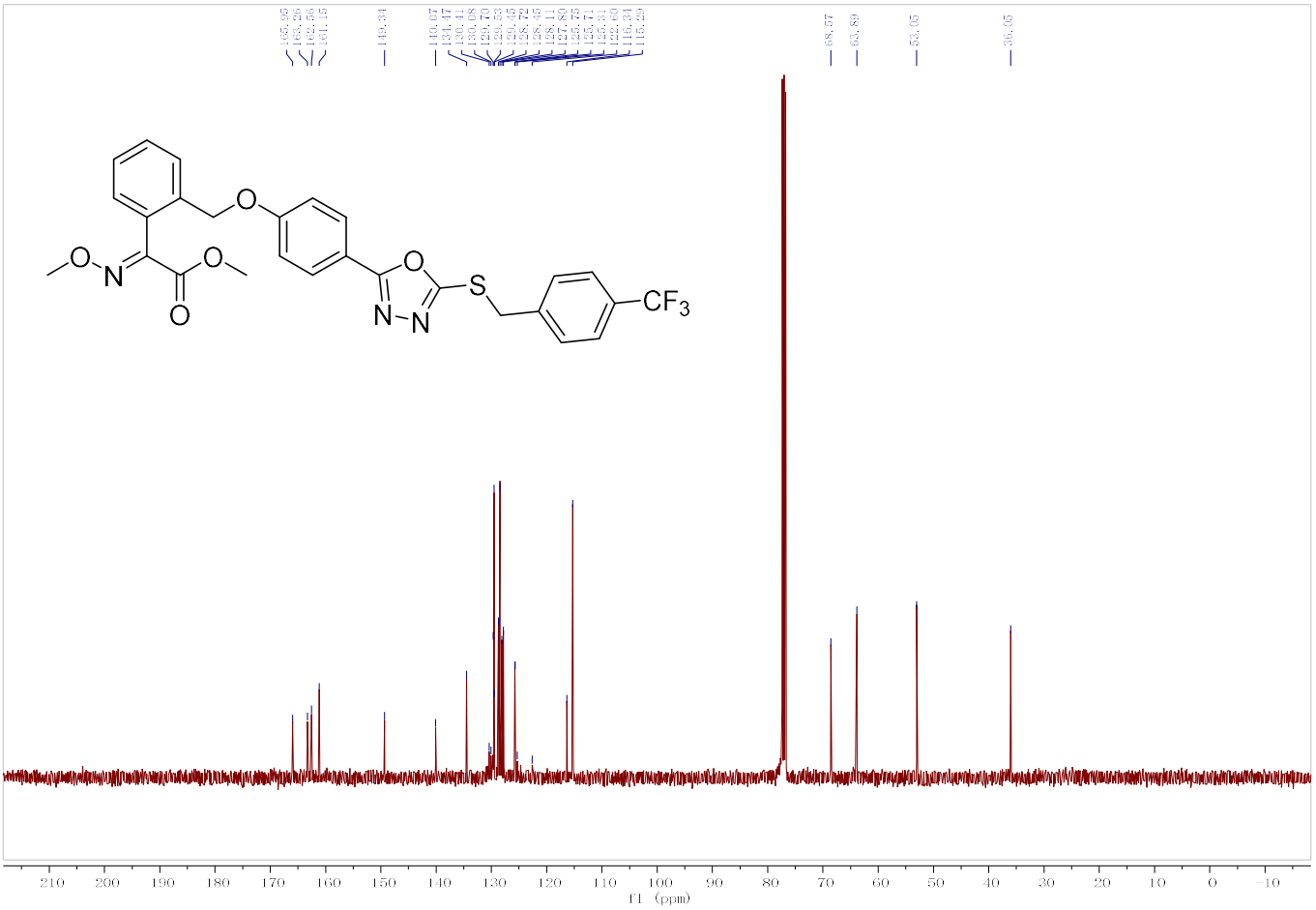

Fig. S50 ^{13}C NMR of compound **6j**

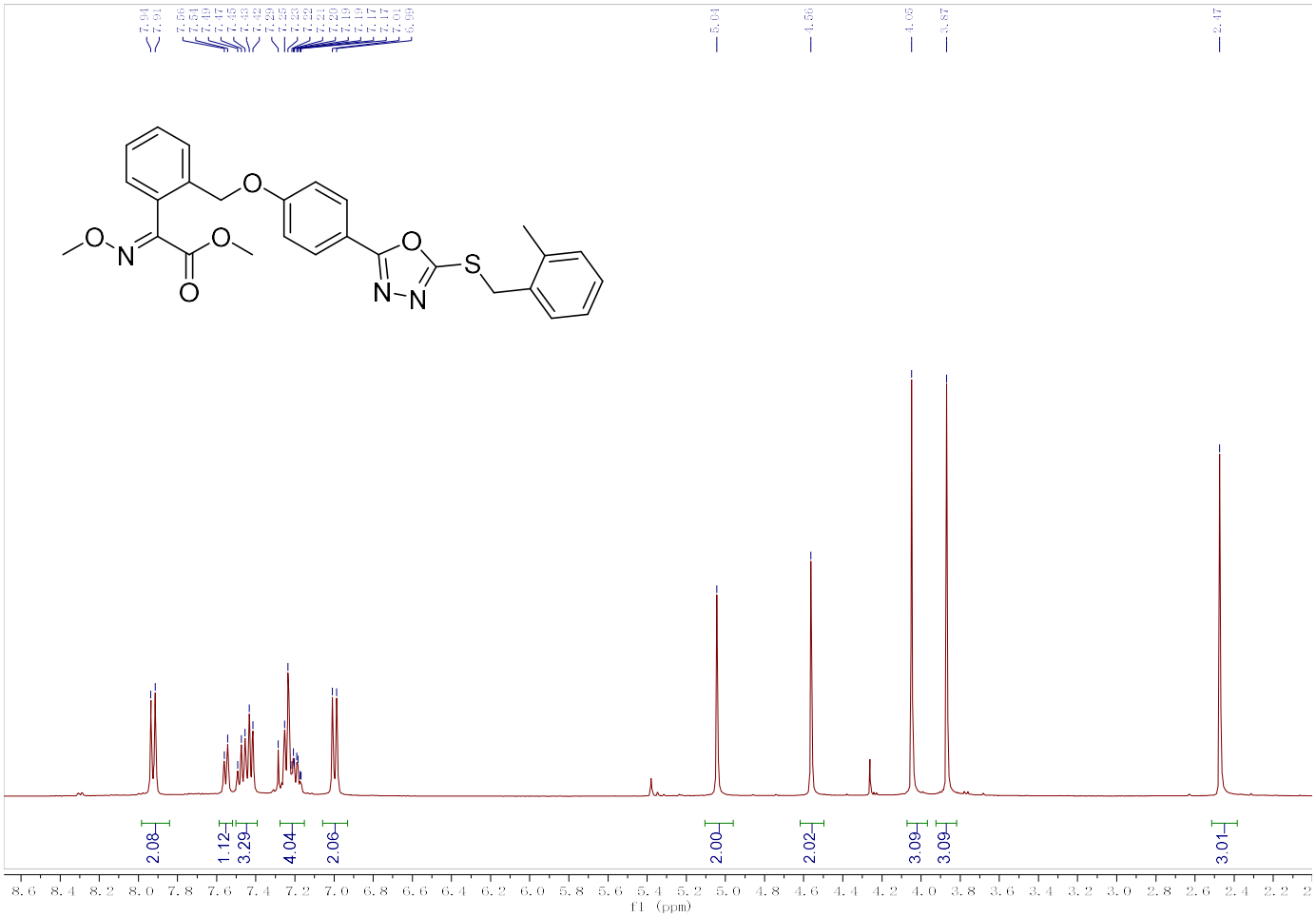

Fig. S51 ^{1}H NMR of compound **6k**

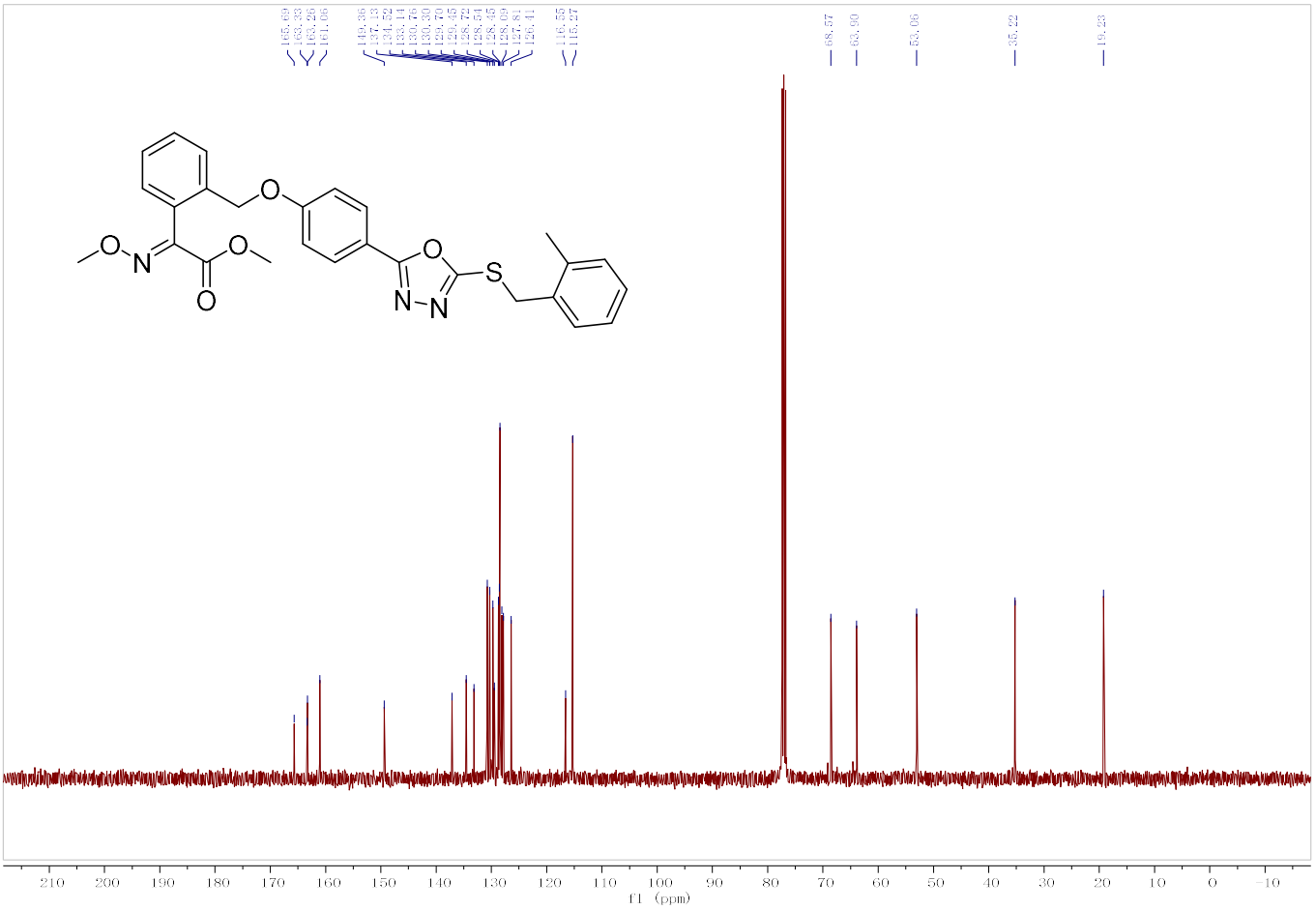

Fig. S52 ^{13}C NMR of compound **6k**

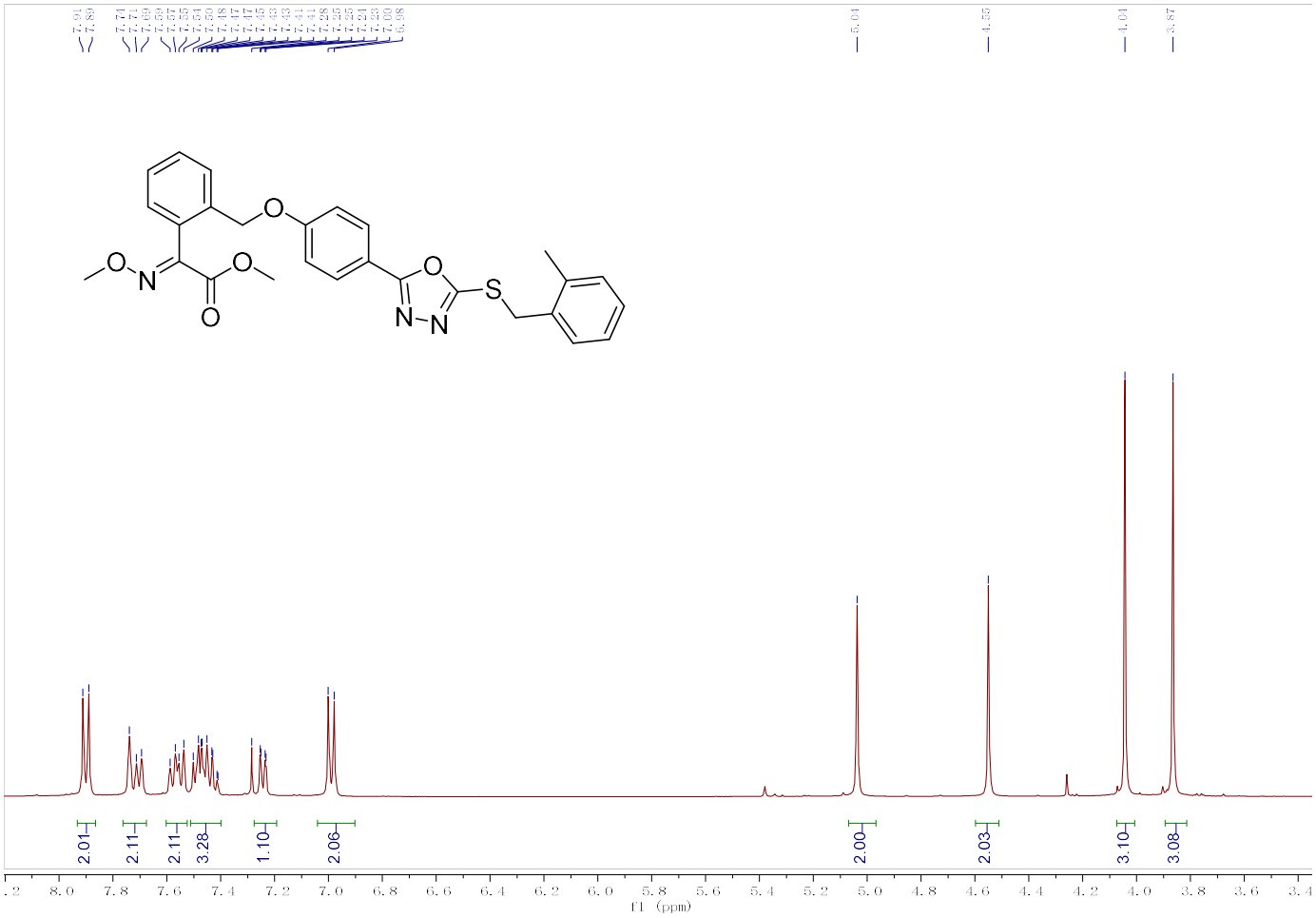

Fig. S53 ^{1}H NMR of compound **6l**

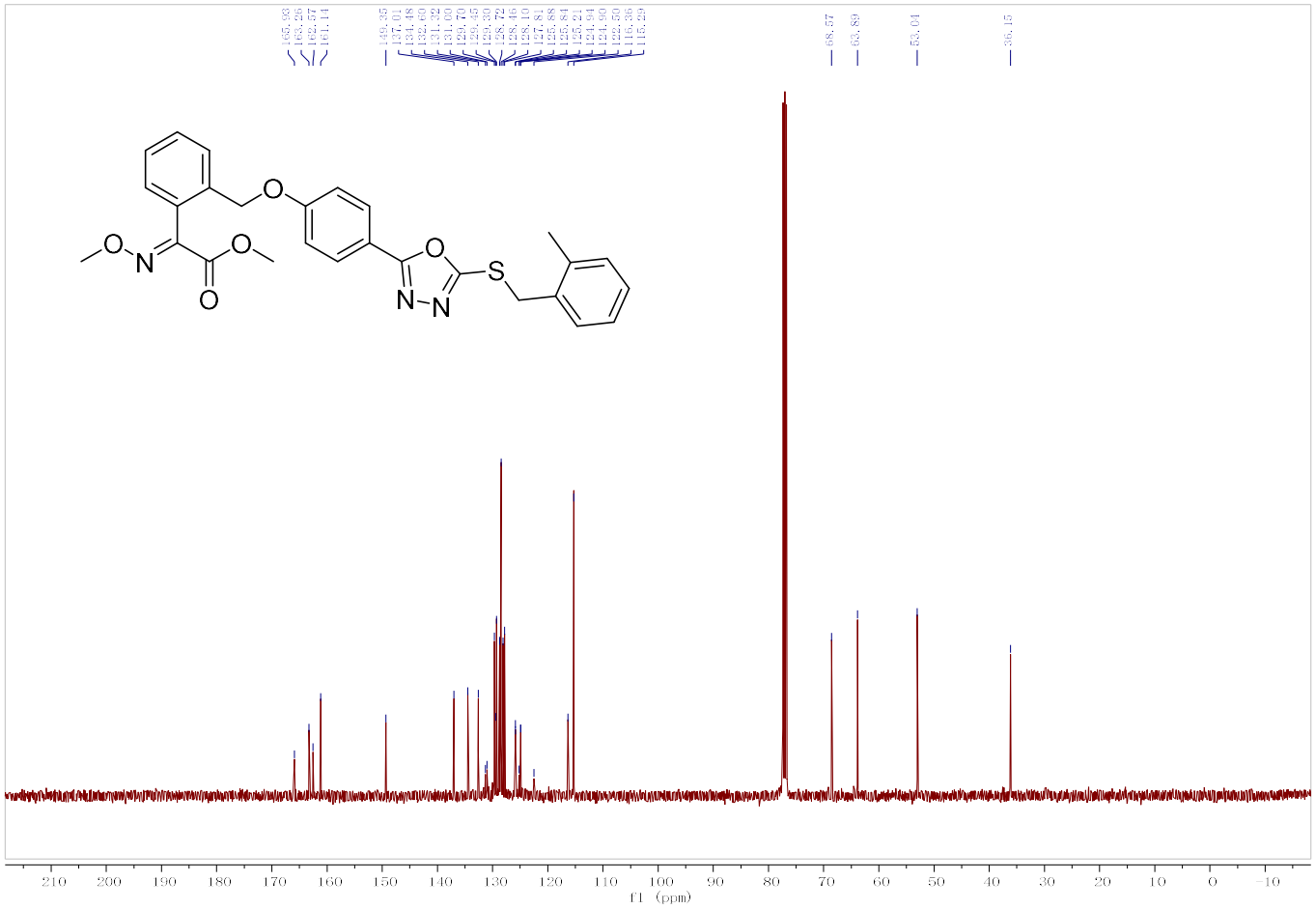

Fig. S54 ^{13}C NMR of compound **6l**

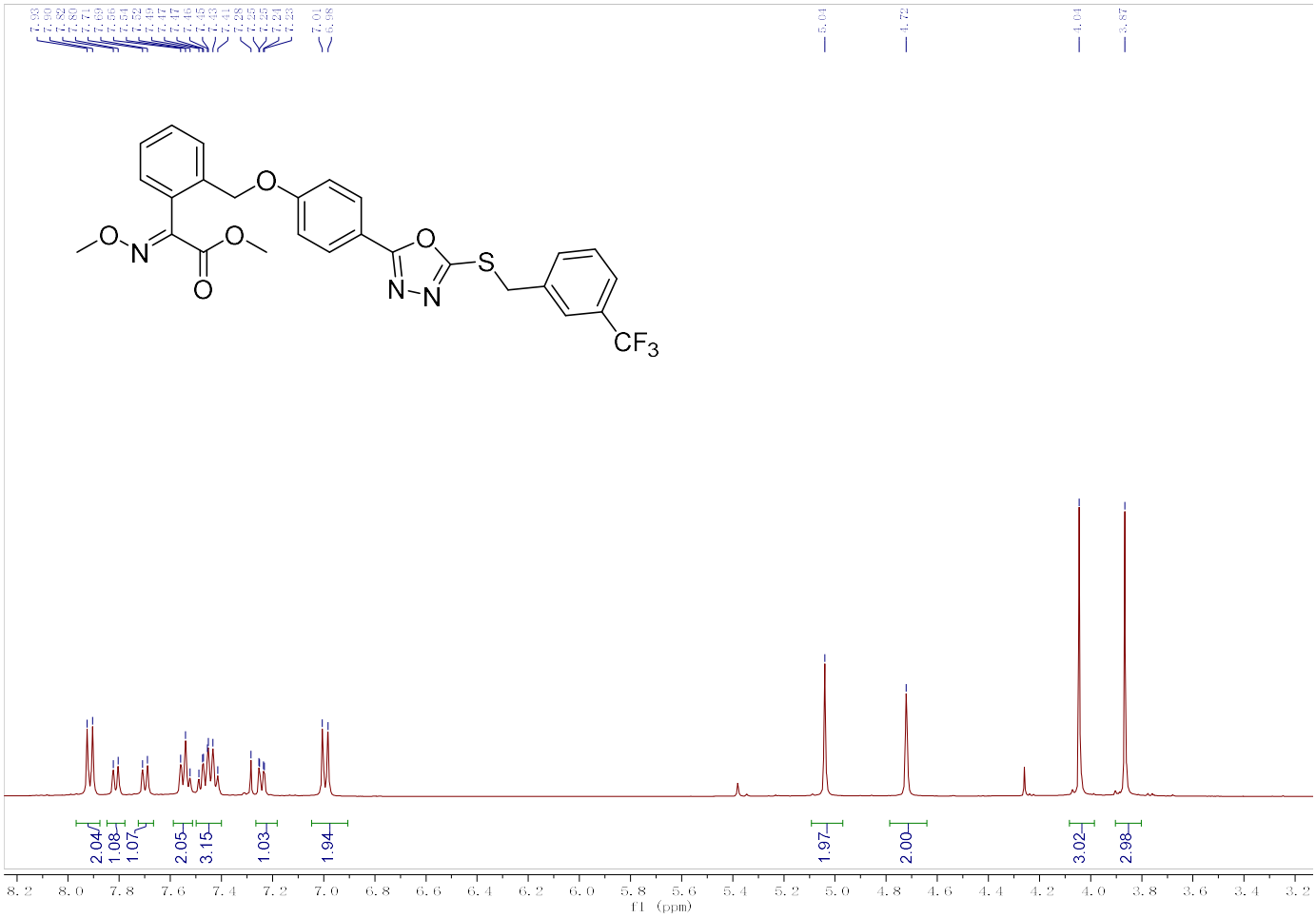

Fig. S55 ^{1}H NMR of compound **6m**

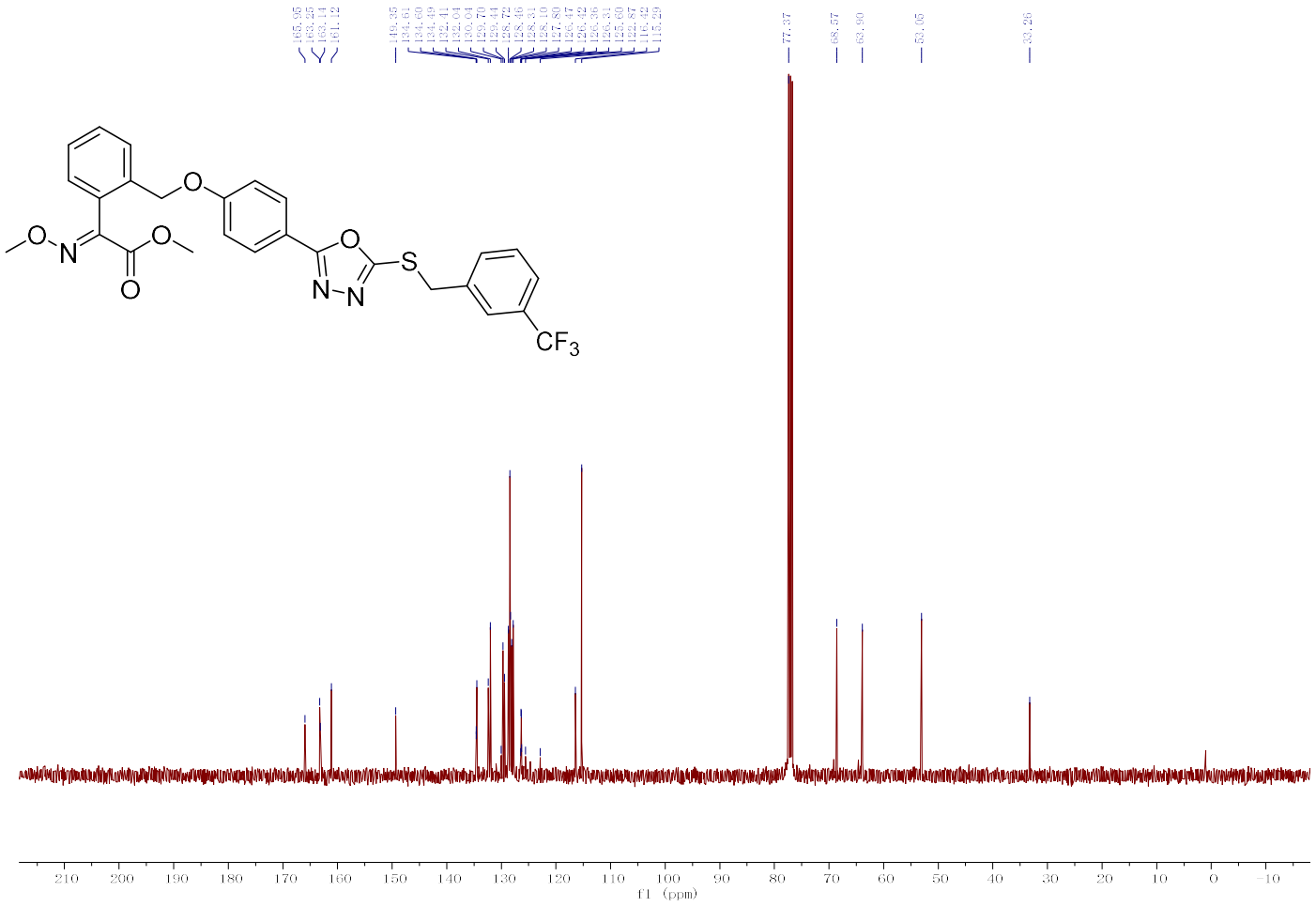

Fig. S56 ^{13}C NMR of compound **6m**

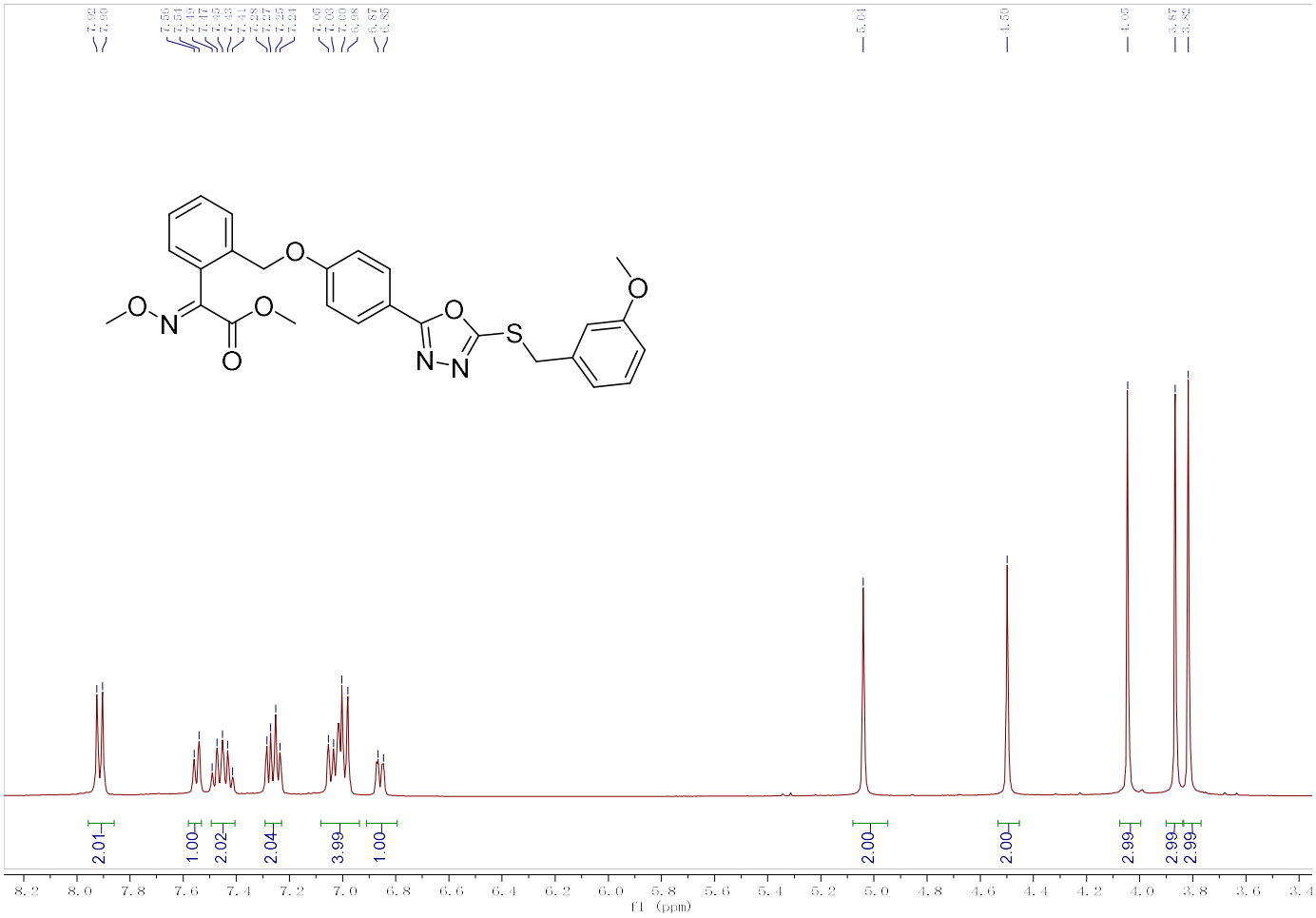

Fig. S57 ^{1}H NMR of compound **6n**

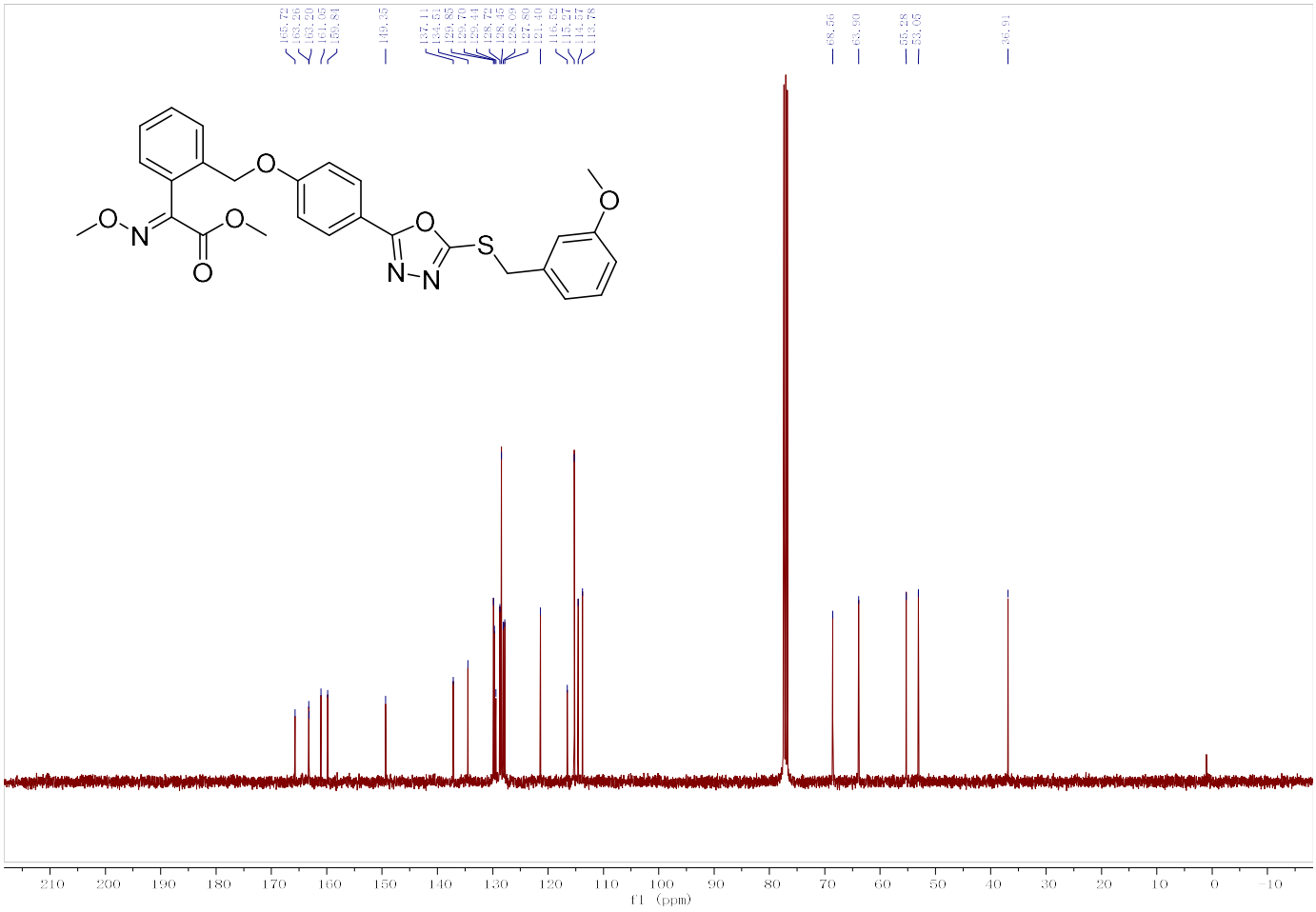

Fig. S58^{13}C NMR of compound **6n**

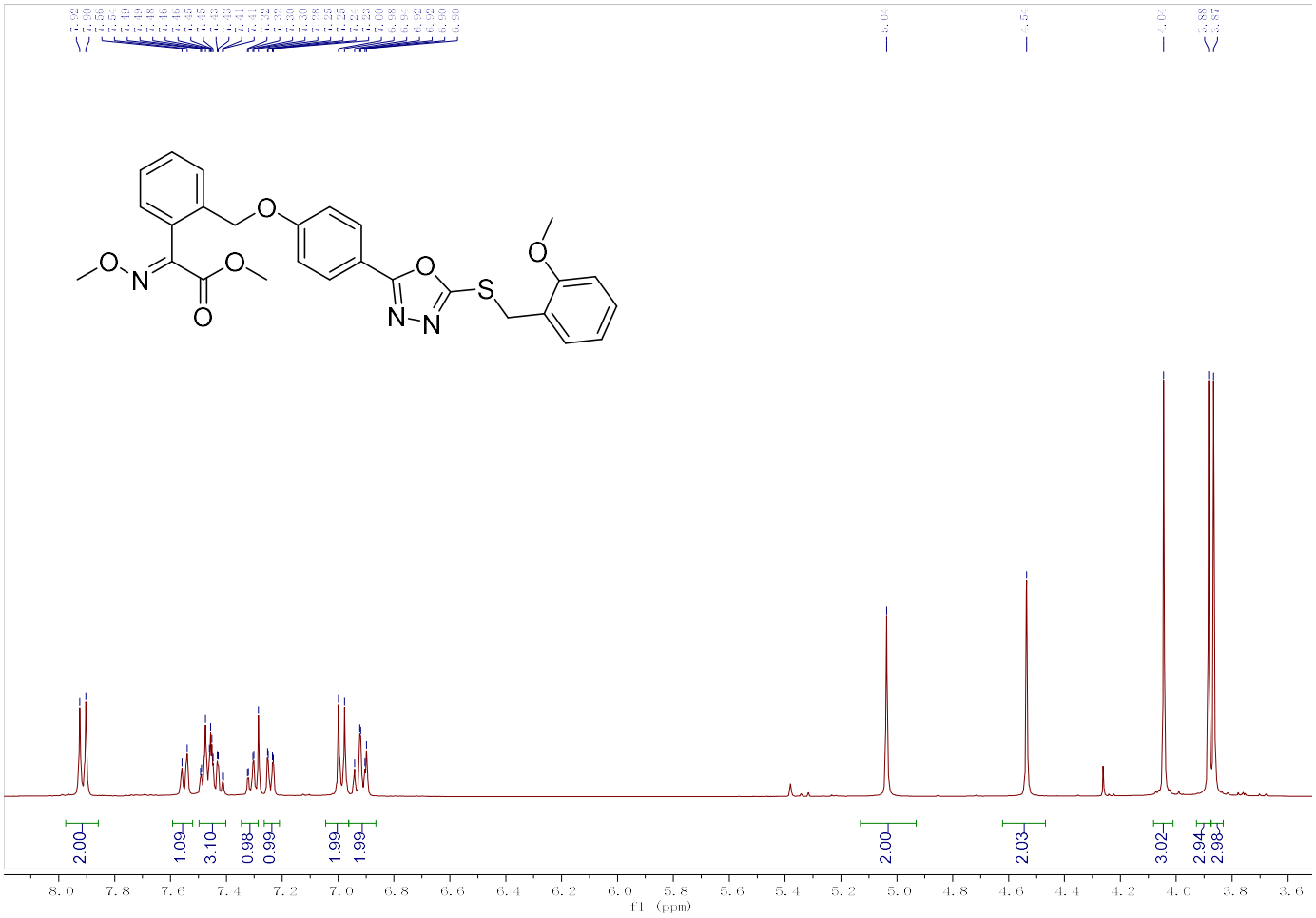

Fig. S59 ^{1}H NMR of compound **6o**

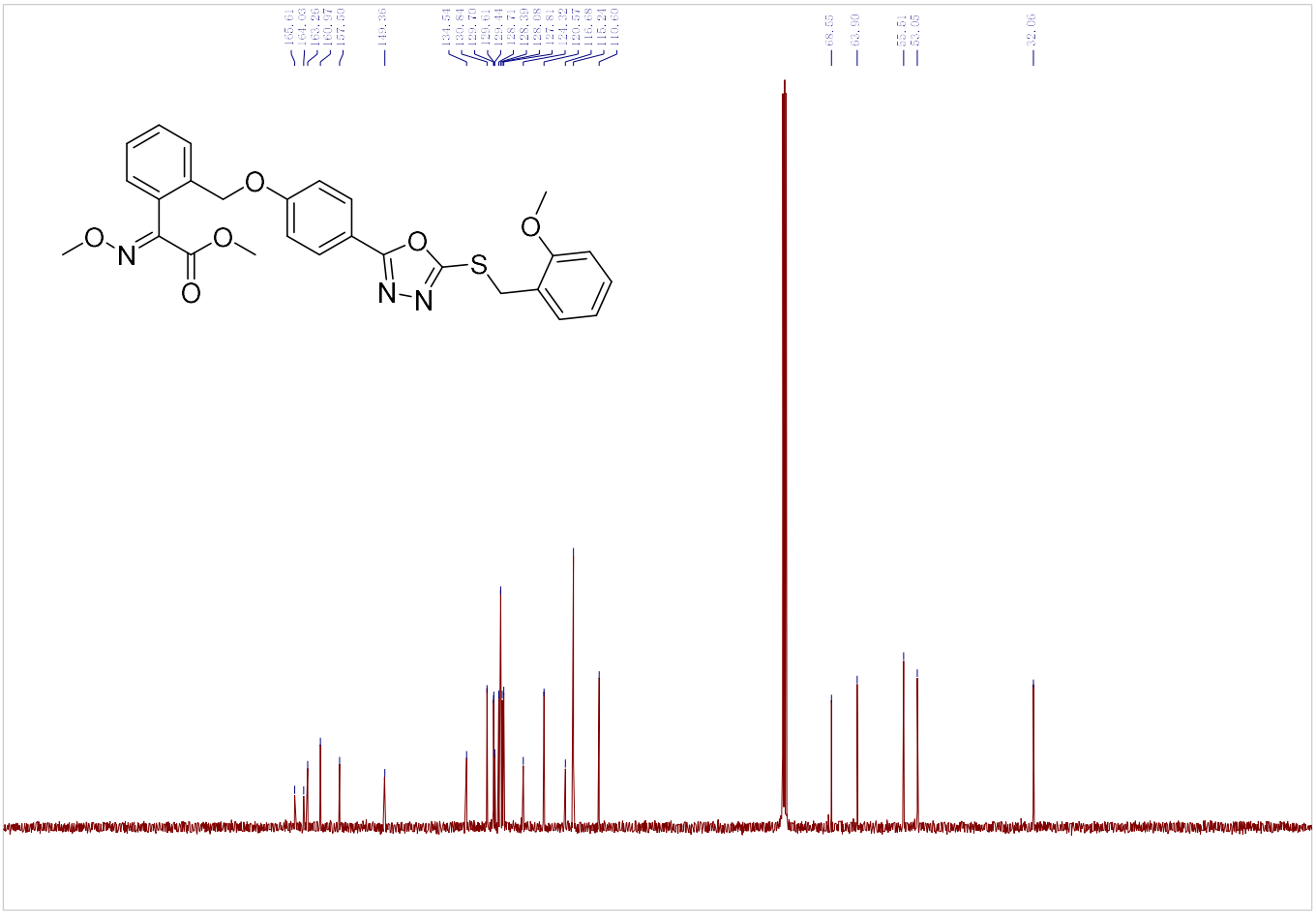

Fig. S60 ^{13}C NMR of compound **6o**