Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supporting Information

Visible-Light-Induced Bifunctionalisation of (Homo)Propargylic Amines with CO_2 and Arylsulfinates

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1. General considerations

Chemicals were purchased and used without further purification unless otherwise stated. The ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on Varian VNMR spectrometers (400 and 500 MHz for ^{1}H NMR; 101 and 126 MHz for ^{13}C NMR) with TMS as an internal standard. Mass spectra were recorded on Agilent-6546-QToF spectrometer. TLC was performed on using Merck pre-coated TLC plates (Merck 60 F_{254}) and detected under UV light. Flash column chromatography (FCC) was performed using either silica gel [Davisil, 230-400 mesh (40-63 µm)] or using a Biotage Isolera® UV-VIS Flash Purification System Version 2.3.1 with Sfär Silica HC D (20 µm) prepacked silica cartridges.

Details of Light source:

Manufacturer: Kessil; Model: PR160L; Wavelength: 456 nm, Distance: 5 cm. Manufacturer gives spectral width as ~430-510 nm with radiant flux max at 456 nm of ~0.3 W/nm and 'average intensity of PR160 series' as 399mW/cm^2 (measured from 1 cm distance), max power consumption 50W.

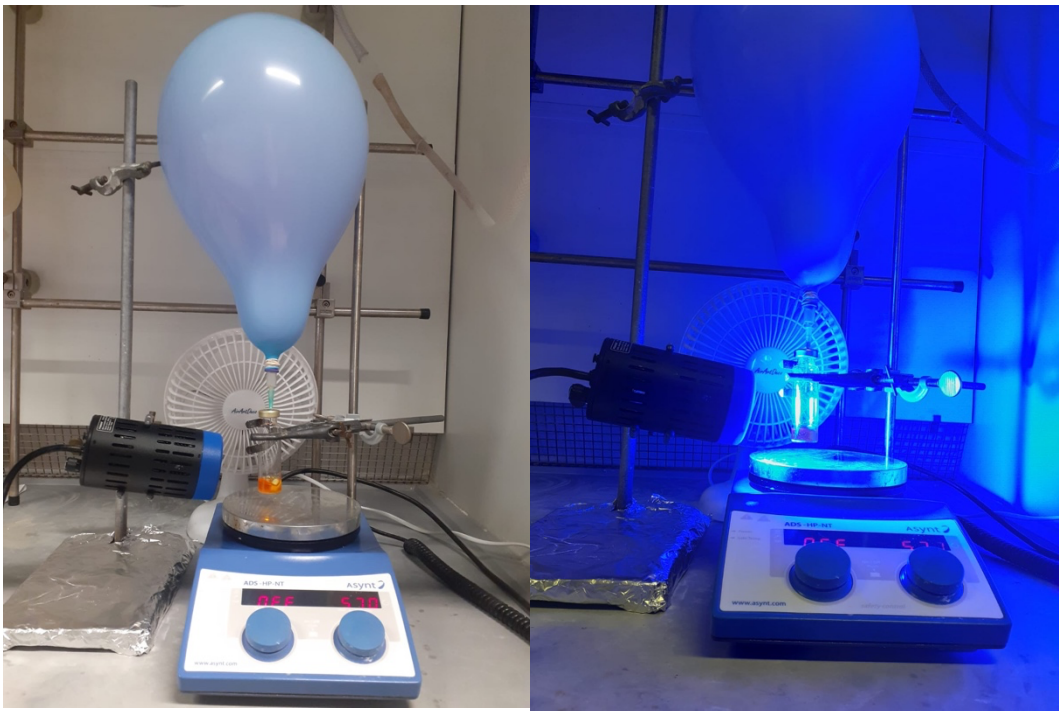


Fig. S1. Reaction setup for photochemical carboxylative sulfonylation reactions.

2. General procedures and spectroscopic data

2.1 General procedure for synthesis of *N*-Benzylpropargylamine (1aa-1au).

Propargylamines were synthesized using the literature procedure. [1,2]

Propargyl bromide (1 equiv.) was added dropwise to the solution of benzylamine (6 equiv.). The reaction was stirred 15 h at room temperature and then 2 M NaOH and Et_2O were added. The layer were separated and the aqueous layer was extracted with Et_2O. The combined organic layers were dried over Na_2SO_4 and then evaporated under reduced pressure. The crude product was purified by flash column chromatography using EtOAc/pentane as an eluent to furnish the corresponding *N*-benzylpropargylamine.

2.2 General procedure for synthesis of *N*-Benzyl homopropargylamines (1ba-1bh).[2,3]

Homopropargylamines were synthesized using the literature procedure. [2,3]

To a solution of homo propargyl alcohol (1 equiv.) and triethylamine (1.5 equiv.) in DCM (7 mL/mmol) was added methanesulfonyl chloride (1.2 equiv.) dropwise at 0 °C. The reaction mixture was allowed to stir at 0 °C for 1 hour and then quenched with 1N aqueous HCl. The aqueous layer extracted with DCM and the organic layers were washed with brine and dried over Na_2SO_4. Crude mesylate was dissolved in DMSO (2 mL/mmol). The benzyl amine (2 equiv.) and sodium iodide (0.1 equiv.) were then added and the reaction mixture was stirred at 50 °C for 16 hours. The solution was then cooled to room temperature and diluted with saturated aqueous $NaHCO_3$ and ethyl acetate. The phases were separated and the aqueous layer extracted with ethyl acetate. The organic layer was dried over Na_2SO_4 and then evaporated under reduced pressure. The crude product was purified by flash column chromatography using EtOAc/pentane as an eluent to furnish the corresponding *N*-benzyl homopropargylamine.

2.3 General procedure A for carboxylative sulfonylation

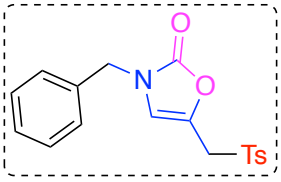
The reaction tube was charged with propargylamine (0.14 mmol), sodium arylsulfinate (0.21 mmol), Cs_2CO_3 (0.28 mmol) and $Ru(bpy)_3Cl_2.6H_2O$ (2 mol%) in DMSO (2 mL). The mixture was stirred under blue LED irradiation for 14 hours. Then, the reaction mixture was quenched with H_2O (20 mL) and aqueous layer was extracted with ethyl acetate (2x10 mL). The combined organic layer was dried over Na_2SO_4 and then evaporated under reduced pressure. The crude product was purified by flash column chromatography using EtOAc/pentane as an eluent to furnish the corresponding final product.

Note: the lights heat the reaction slightly. The reaction temperature was measured to be 27 °C. A control experiment carried out at 27 °C without light gave no reaction.

2.4 Scale-up reaction

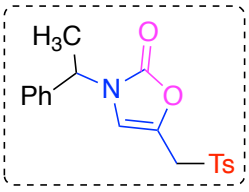
A 50 mL round bottom flask was charged with *N*-benzylprop-2-yn-1-amine (1.40 mmol), Sodium benzenesulfinate (2.10 mmol), Cs_2CO_3 (2.80 mmol) and $Ru(bpy)_3Cl_2.6H_2O$ (2 mol%) in DMSO (15 mL). The mixture was stirred under blue LED irradiation for 24 hours. Then, the reaction mixture was quenched with H_2O (75 mL) and aqueous layer was extracted with ethyl acetate (2x20 mL). The combined organic layer was dried over Na_2SO_4 and then evaporated under reduced pressure. The crude product was purified by flash column chromatography using EtOAc/pentane 2:3 as an eluent to furnish the 3-benzyl-5-(tosylmethyl)oxazol-2(3*H*)-one as a white solid (346 mg, 73%).

3-Benzyl-5-(tosylmethyl)oxazol-2(3*H*)-one (3a)



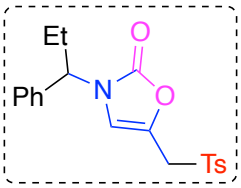
3a (40 mg) was synthesized following general procedure A; white solid; 84% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, *J* = 8.3 Hz, 2H), 7.42-7.32 (m, 3H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.26-7.20 (m, 2H), 6.43 (s, 1H), 4.66 (s, 2H), 4.13-4.08 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.6, 145.5, 134.9, 134.8, 130.0, 129.1, 128.6, 128.6, 128.4, 128.0, 116.1, 54.0, 47.8, 21.7; HRMS: $[M+H]^+$ calculated for $C_{18}H_{18}NO_4S$: 344.0956; found: 344.0951.

3-(1-Phenylethyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3b)



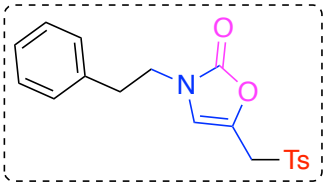
3b (33 mg) was synthesized following general procedure A; white solid; 68% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.64 (d, *J* = 8.3 Hz, 2H), 7.41-7.33 (m, 3H), 7.29-7.26 (m, 4H), 6.46 (s, 1H), 5.26 (q, *J* = 7.1 Hz, 1H), 4.11 (s, 2H), 2.44 (s, 3H), 1.67 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 154.1, 145.5, 139.3, 134.7, 129.9, 129.0, 128.5, 128.5, 128.4, 126.5, 113.9, 54.1, 52.8, 21.7, 19.2; HRMS: $[M+H]^+$ calculated for $C_{19}H_{20}NO_4S$: 358.1113; found: 358.1108.

3-(1-Phenylpropyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3c)



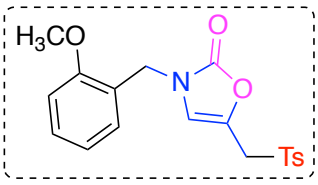
3c (34 mg) was synthesized following general procedure A; white solid; 65% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, *J* = 8.3 Hz, 2H), 7.38-7.31 (m, 3H), 7.27-7.23 (m, 4H), 6.52 (s, 1H), 4.93 (dd, *J* = 9.0, 6.8 Hz, 1H), 4.11 (s, 2H), 2.41 (s, 3H), 2.12-1.97 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.4, 145.5, 138.6, 134.6, 129.9, 129.0, 128.6, 128.5, 128.4, 126.9, 113.8, 59.2, 54.1, 26.4, 21.7, 10.9; HRMS: $[M+H]^+$ calculated for $C_{20}H_{22}NO_4S$: 372.1269; found: 372.1265.

3-Phenethyl-5-(tosylmethyl)oxazol-2(3*H*)-one (3d)



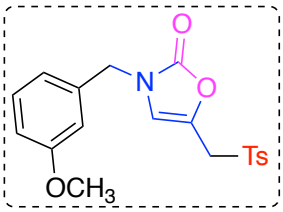
3d (40 mg) was synthesized following general procedure A; white solid; 82% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.66 (d, *J* = 7.9 Hz, 2H), 7.33-7.28 (m, 4H), 7.26-7.24 (m, 1H), 7.17 (d, *J* = 7.4 Hz, 2H), 6.35 (s, 1H), 4.08 (s, 2H), 3.80 (t, *J* = 7.1 Hz, 2H), 2.96 (t, *J* = 7.1 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 154.4, 145.6, 137.1, 135.1, 130.0, 128.9, 128.7, 128.4, 128.0, 127.1, 116.8, 53.9, 45.5, 35.0, 21.7; HRMS: $[M+H]^+$ calculated for $C_{19}H_{20}NO_4S$: 358.1113; found: 358.1110.

3-(2-Methoxybenzyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3e)



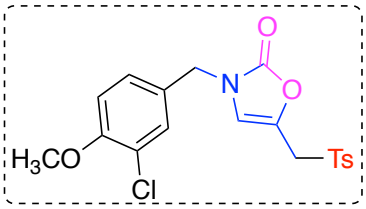
3e (42 mg) was synthesized following general procedure A; white solid; 79% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.32 (td, *J* = 7.9, 1.8 Hz, 1H), 7.23 (app td, *J* = 7.9, 3.3 Hz, 3H), 6.98-6.87 (m, 2H), 6.56 (s, 1H), 4.66 (s, 2H), 4.08 (s, 2H), 3.85 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.3, 154.6, 145.4, 134.9, 130.5, 130.1, 129.9, 128.4, 127.8, 123.2, 120.9, 117.1, 110.7, 55.4, 54.1, 43.2, 21.7; HRMS: $[M+H]^+$ calculated for $C_{19}H_{20}NO_5S$: 374.1062; found: 374.1059.

3-(3-Methoxybenzyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3f)



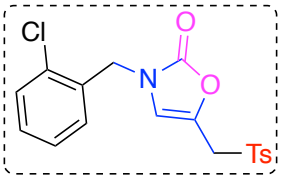
3f (35 mg) was synthesized following general procedure A; white solid; 66% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.3 Hz, 2H), 7.35-7.28 (m, 3H), 6.89 (ddd, *J* = 8.3, 2.6, 0.9 Hz, 1H), 6.81 (ddd, *J* = 7.6, 1.6, 0.9 Hz, 1H), 6.77 (t, *J* = 2.1 Hz, 1H), 6.45 (s, 1H), 4.65 (s, 2H), 4.11 (d, *J* = 0.9 Hz, 2H), 3.81 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 160.2, 154.6, 145.6, 136.4, 134.8, 130.2, 130.0, 128.6, 128.4, 120.1, 116.1, 113.9, 113.7, 55.3, 54.0, 47.8, 21.7; HRMS: $[M+H]^+$ calculated for $C_{19}H_{20}NO_5S$: 374.1062; found: 374.1059.

3-(3-Chloro-4-methoxybenzyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3g)



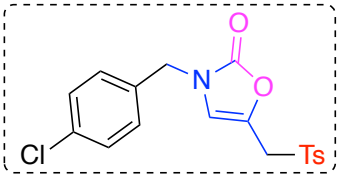
3g (39 mg) was synthesized following general procedure A; white solid; 69% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.32 (app d, *J* = 8.1 Hz, 3H), 7.14 (dd, *J* = 8.4, 2.2 Hz, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 6.46 (s, 1H), 4.59 (s, 2H), 4.12 (s, 2H), 3.91 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.2, 154.4, 145.6, 134.8, 130.0, 129.8, 128.7, 128.4, 128.0, 127.7, 123.1, 115.9, 112.3, 56.2, 53.9, 46.9, 21.7; HRMS: $[M+H]^+$ calculated for $C_{19}H_{19}ClNO_5S$: 408.0672 and 410.0643; found: 408.0668 and 410.0636.

3-(2-Chlorobenzyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3h)



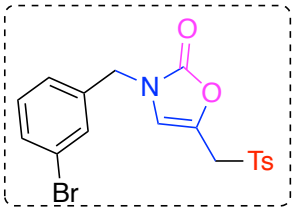
3h (38 mg) was synthesized following general procedure A; white solid; 71% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.3 Hz, 2H), 7.44-7.39 (m, 1H), 7.33-7.26 (m, 5H), 6.54-6.49 (m, 1H), 4.79 (s, 2H), 4.10 (d, *J* = 1.0 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 154.4, 145.6, 134.8, 133.6, 132.5, 130.7, 130.2, 130.0, 128.6, 128.4, 127.5, 116.4, 116.4, 54.0, 45.5, 21.7; HRMS: $[M+H]^+$ calculated for $C_{18}H_{17}ClNO_4S$: 378.0566 and 380.0537; Found: 378.0562 and 380.0530.

3-(4-Chlorobenzyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3i)



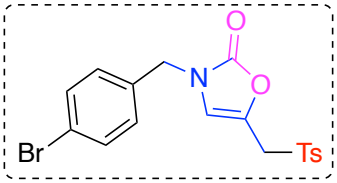
3i (37 mg) was synthesized following general procedure A; white solid; 70% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.66 (d, J = 8.3 Hz, 2H), 7.35 (d, J = 8.4 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 7.18 (d, J = 8.5 Hz, 2H), 6.45 (s, 1H), 4.65 (s, 2H), 4.12 (d, J = 1.0 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 154.5, 145.6, 134.8, 134.6, 133.5, 130.0, 129.4, 129.3, 128.8, 128.4, 115.9, 53.9, 47.2, 21.7; HRMS: $[M+Na]^+$ calculated for $C_{18}H_{16}ClNO_4SNa$: 400.0386 and 402.0356; found: 400.0380 and 402.0350.

3-(3-Bromobenzyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3j)



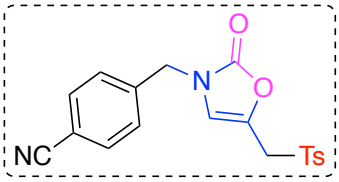
3j (42 mg) was synthesized following general procedure A; white solid; 72% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65 (d, J = 8.3 Hz, 2H), 7.48 (ddd, J = 7.9, 1.9, 1.1 Hz, 1H), 7.37 (s, 1H), 7.33-7.28 (m, 2H), 7.25-7.21 (m, 1H), 7.19-7.14 (m, 1H), 6.46 (t, J = 0.9 Hz, 1H), 4.63 (s, 2H), 4.11 (s, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.5, 145.7, 137.2, 134.8, 131.7, 130.8, 130.7, 130.0, 128.9, 128.4, 126.5, 123.1, 115.9, 53.9, 47.2, 21.7; HRMS: $[M+H]^+$ calculated for $C_{18}H_{17}BrNO_4S$: 422.0061 and 424.0037; found: 422.0058 and 424.0038.

3-(4-Bromobenzyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3k)



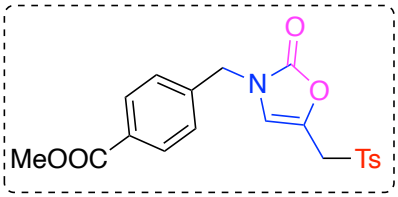
3k (44 mg) was synthesized following general procedure A; white solid; 75% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, J = 8.3 Hz, 2H), 7.49 (d, J = 8.4 Hz, 2H), 7.28 (dt, J = 7.9, 0.7 Hz, 2H), 7.10 (d, J = 8.4 Hz, 2H), 6.43 (s, 1H), 4.61 (s, 2H), 4.10 (d, J = 1.0 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.5, 145.6, 134.8, 134.0, 132.3, 130.0, 129.6, 128.8, 128.4, 122.7, 115.9, 53.9, 47.2, 21.7; $[M+H]^+$ calculated for $C_{18}H_{17}BrNO_4S$: 422.0061 and 424.0037; found: 422.0056 and 424.0036.

4-((2-Oxo-5-(tosylmethyl)oxazol-3(2*H*)-yl)methyl)benzonitrile (3l)



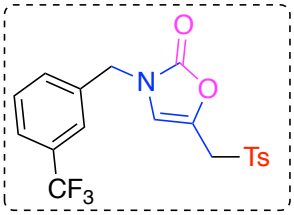
3l (34 mg) was synthesized following general procedure A; white solid; 65% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (app t, *J* = 8.3 Hz, 4H), 7.33 (app dd, *J* = 8.1 Hz, 4H), 6.53 (s, 1H), 4.74 (s, 2H), 4.12 (d, *J* = 1.0 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.5, 145.7, 140.2, 135.0, 132.9, 130.1, 129.1, 128.4, 128.3, 118.1, 116.0, 112.6, 53.8, 47.3, 21.7; HRMS: $[M+H]^+$ calculated for $C_{19}H_{17}N_2O_4S$: 369.0909; found: 369.0903.

Methyl 4-((2-oxo-5-(tosylmethyl)oxazol-3(2*H*)-yl)methyl)benzoate (3m)



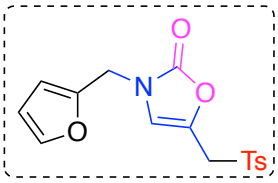
3m (34 mg) was synthesized following general procedure A; white solid; 61% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.3 Hz, 2H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.34-7.25 (m, 4H), 6.45 (s, 1H), 4.72 (s, 2H), 4.11 (d, *J* = 1.0 Hz, 2H), 3.91 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.4, 154.5, 145.6, 139.8, 134.8, 130.4, 130.3, 130.0, 128.9, 128.4, 127.7, 116.0, 53.9, 52.3, 47.5, 21.7; HRMS: $[M+H]^+$ calculated for $C_{20}H_{20}NO_6S$: 402.1011; found: 402.1004.

5-(Tosylmethyl)-3-(3-(trifluoromethyl)benzyl)oxazol-2(3*H*)-one (3n)



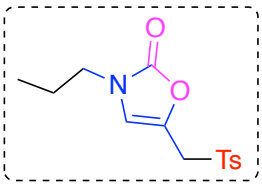
3m (37 mg) was synthesized following general procedure A; white solid; 65% yield (eluent: EtOAc/Pentane = 3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68-7.64 (m, 2H), 7.62 (d, *J* = 7.7 Hz, 1H), 7.54-7.42 (m, 3H), 7.32-7.27 (m, 2H), 6.49 (s, 1H), 4.73 (s, 2H), 4.12 (d, *J* = 1.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.5, 145.7, 136.0, 134.8, 131.6 (app d, *J* = 32.5 Hz), 131.2, 130.0, 129.7, 129.0, 128.4, 125.5 (q, *J* = 3.7 Hz), 124.5 (q, *J* = 3.7 Hz), 123.1 (app d, *J* = 272.9 Hz), 115.9, 53.9, 47.4, 21.7; HRMS: $[M+H]^+$ calculated for $C_{19}H_{17}F_3NO_4S$: 412.0830; found: 412.0826.

3-(Furan-2-ylmethyl)-5-(tosylmethyl)oxazol-2(3*H*)-one (3o)



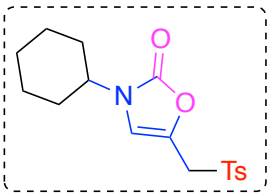
3o (38 mg) was synthesized following general procedure A; white solid; 82% yield (eluent: EtOAc/Pentane = 3:7); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.3 Hz, 2H), 7.40 (dd, *J* = 1.8, 0.9 Hz, 1H), 7.33-7.28 (m, 2H), 6.59 (t, *J* = 1.0 Hz, 1H), 6.36-6.33 (m, 2H), 4.66 (s, 2H), 4.10 (d, *J* = 1.0 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.1, 147.8, 145.6, 143.4, 134.9, 130.0, 128.6, 128.4, 116.1, 110.7, 109.7, 54.0, 40.4, 21.7; HRMS: $[M+H]^+$ calculated for $C_{16}H_{16}NO_5S$: 334.0749; found: 334.0746.

3-Propyl-5-(tosylmethyl)oxazol-2(3*H*)-one (3p)



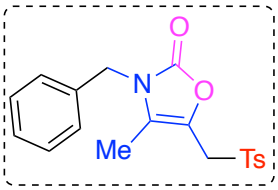
3p (25 mg) was synthesized following general procedure A; white solid; 62% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.39-7.30 (m, 2H), 6.56 (d, *J* = 0.9 Hz, 1H), 4.14 (d, *J* = 1.0 Hz, 2H), 3.47 (t, 7.24 Hz, 2H), 2.43 (s, 3H), 1.68-1.59 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.6, 145.6, 135.0, 130.0, 128.4, 128.2, 116.5, 77.3, 77.0, 76.7, 54.0, 45.7, 22.1, 21.7, 10.9; HRMS: $[M+H]^+$ calculated for $C_{14}H_{18}NO_4S$: 296.0956; found: 296.0953.

3-Cyclohexyl-5-(tosylmethyl)oxazol-2(3*H*)-one (3q)



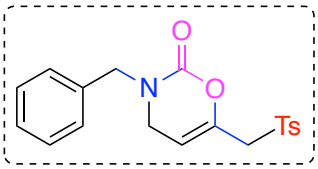
3p (33 mg) was synthesized following general procedure A; white solid; 70% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.73-7.67 (m, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.61 (s, 1H), 4.14 (s, 2H), 3.79 (tt, *J* = 7.8, 4.0 Hz, 1H), 2.45 (s, 3H), 1.94-1.93 (m, 2H), 1.90-1.82 (m, 2H), 1.73-1.70 (m, 1H), 1.37 (qd, *J* = 12.1, 6.2 Hz, 4H), 1.22-1.09 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 154.1, 145.6, 135.0, 130.0, 128.4, 128.3, 113.8, 54.1, 53.4, 32.1, 25.2, 25.0, 21.7; HRMS: $[M+H]^+$ calculated for $C_{17}H_{22}NO_4S$: 336.1269; Found: 336.1267.

3-Benzyl-4-methyl-5-(tosylmethyl)oxazol-2(3*H*)-one (3u)



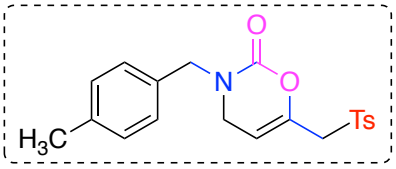
3u (28 mg) was synthesized following general procedure A; white solid; 57% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.38-7.30 (m, 3H), 7.27-7.23 (m, 2H), 7.22-7.17 (m, 2H), 4.70 (s, 2H), 4.11 (s, 2H), 2.40 (s, 3H), 1.77 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.9, 145.4, 135.7, 134.8, 130.0, 129.0, 128.4, 128.2, 127.1, 125.4, 123.8, 53.2, 45.5, 21.7, 8.3; HRMS: $[M+H]^+$ calculated for $C_{19}H_{20}NO_4S$: 358.1113; found: 358.1110.

3-Benzyl-6-(tosylmethyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4a)



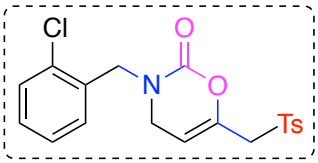
4a (26 mg) was synthesized following general procedure A; white solid; 52% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81-7.72 (m, 2H), 7.37-7.30 (m, 5H), 7.27-7.23 (m, 2H), 5.23 (t, *J* = 3.4 Hz, 1H), 4.49 (s, 2H), 3.84 (s, 2H), 3.73 (d, *J* = 3.4 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.4, 145.4, 140.6, 135.5, 135.1, 129.9, 128.8, 128.4, 128.2, 128.1, 102.6, 59.4, 52.1, 44.7, 21.7; HRMS: $[M+H]^+$ calculated for $C_{24}H_{22}NO_4S$: 358.1113; found: 358.1108.

3-(4-Methylbenzyl)-6-(tosylmethyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4b)



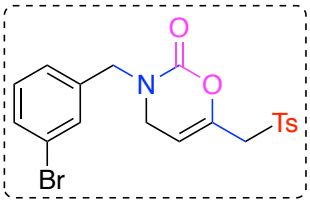
4b (26 mg) was synthesized following general procedure A; white solid; 50% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 7.14 (s, 4H), 5.22 (t, *J* = 3.4 Hz, 1H), 4.45 (s, 2H), 3.83 (s, 2H), 3.71 (d, *J* = 3.4 Hz, 2H), 2.44 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.4, 145.4, 140.5, 137.9, 135.5, 132.0, 129.9, 129.5, 128.4, 128.2, 102.6, 59.4, 51.8, 44.5, 21.7, 21.1; HRMS: $[M+H]^+$ calculated for $C_{20}H_{22}NO_4S$: 372.1269; found: 372.1266.

3-(2-Chlorobenzyl)-6-(tosylmethyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4c)



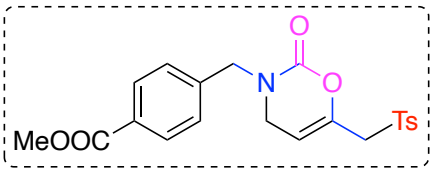
4c (24 mg) was synthesized following general procedure A; white solid; 44% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.1 Hz, 2H), 7.41-7.39 (m, 1H), 7.36-7.32 (m, 3H), 7.28 (dd, *J* = 6.4, 2.7 Hz, 2H), 5.28 (t, *J* = 3.4 Hz, 1H), 4.67 (s, 2H), 3.87 (s, 2H), 3.82 (d, *J* = 3.4 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.4, 145.4, 140.7, 135.5, 133.9, 132.6, 129.9, 129.8, 129.5, 129.4, 128.4, 127.3, 102.7, 59.4, 49.3, 45.2, 21.7; HRMS: $[M+H]^+$ calculated for $C_{19}H_{19}ClNO_4S$: 392.0723 and 394.0694; found: 392.0719 and 394.0689.

3-(3-Bromobenzyl)-6-(tosylmethyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4d)



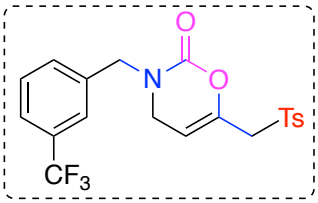
4d (27 mg) was synthesized following general procedure A; white solid; 45% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.45 (dt, *J* = 7.5, 1.8 Hz, 1H), 7.41 (d, *J* = 1.8 Hz, 1H), 7.37-7.33 (m, 2H), 7.24-7.19 (m, 2H), 5.25 (t, *J* = 3.4 Hz, 1H), 4.45 (s, 2H), 3.84 (s, 2H), 3.75 (d, *J* = 3.4 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.3, 145.5, 140.7, 137.5, 135.4, 131.3, 131.0, 130.4, 130.0, 128.4, 126.8, 122.9, 102.5, 59.4, 51.6, 44.9, 21.7; HRMS: $[M+H]^+$ calculated for $C_{19}H_{19}BrNO_4S$: 436.0218 and 438.0194; found: 436.0210 and 438.0191.

Methyl 4-((2-oxo-6-(tosylmethyl)-2*H*-1,3-oxazin-3(4*H*)-yl)methyl)benzoate (4e)



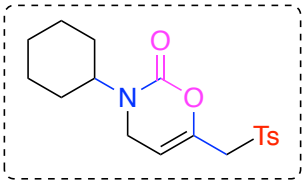
4e (28 mg) was synthesized following general procedure A; white solid; 48% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.02 (s, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.36-7.32 (m, 4H), 5.27 (t, *J* = 3.4 Hz, 1H), 4.56 (s, 2H), 3.92 (s, 3H), 3.86 (s, 2H), 3.77 (d, *J* = 3.4 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.6, 149.4, 145.4, 140.7, 140.2, 135.5, 130.1, 130.0, 129.9, 128.4, 127.9, 102.5, 59.4, 52.2, 51.9, 45.0, 21.7; HRMS: $[M+H]^+$ calculated for $C_{21}H_{22}NO_6S$: 416.1167; found: 416.1161.

6-(Tosylmethyl)-3-(3-(trifluoromethyl)benzyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4f)



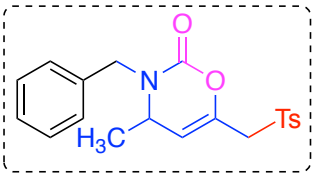
4f (23 mg) was synthesized following general procedure A; white solid; 39% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.61-7.54 (m, 1H), 7.52-7.44 (m, 3H), 7.33 (d, *J* = 8.1 Hz, 2H), 5.26 (t, *J* = 3.4 Hz, 1H), 4.55 (s, 2H), 3.85 (s, 2H), 3.77 (d, *J* = 3.4 Hz, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.4, 145.5, 140.7, 136.2, 135.5, 131.5, 131.2 (app d, *J* = 32.3 Hz), 129.9, 129.4, 128.4, 125.1 (q, *J* = 3.7 Hz), 124.8 (q, *J* = 3.7 Hz), 123.8 (app d, *J* = 272.3 Hz), 102.5, 59.3, 51.8, 45.0, 21.7; HRMS: $[M+H]^+$ calculated for $C_{20}H_{19}F_3NO_4S$: 426.0986; found: 426.0977.

3-Cyclohexyl-6-(tosylmethyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4g)



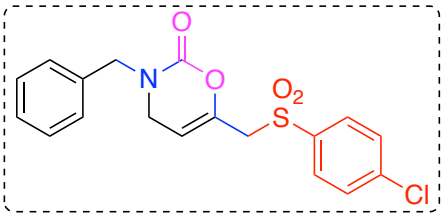
4g (25 mg) was synthesized following general procedure A; white solid; 51% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 5.33-5.25 (m, 1H), 4.04 (ddd, *J* = 11.6, 7.8, 3.7 Hz, 1H), 3.83 (s, 2H), 3.77 (d, *J* = 3.5 Hz, 2H), 2.43 (s, 3H), 1.85-1.75 (m, 2H), 1.69-1.64 (m, 2H), 1.43-1.32 (m, 4H), 1.12-0.99 (m, 1H), 0.86-0.83 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 148.8, 145.3, 140.2, 135.5, 129.9, 128.4, 102.7, 59.3, 55.6, 39.8, 28.9, 25.5, 25.3, 21.7; HRMS: $[M+H]^+$ calculated for $C_{18}H_{24}NO_4S$: 350.1426; found: 350.1421.

3-Benzyl-4-methyl-6-(tosylmethyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4h)



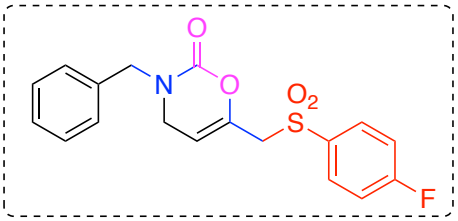
4h (18 mg) was synthesized following general procedure A; brown gummy; 36% yield (eluent: EtOAc/Pentane = 2:3); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.3 Hz, 2H), 7.38-7.30 (m, 5H), 7.24 (d, *J* = 7.6 Hz, 2H), 5.24 (d, *J* = 4.6 Hz, 1H), 5.05 (d, *J* = 15.2 Hz, 1H), 4.08 (d, *J* = 15.3 Hz, 1H), 3.87 (s, 2H), 3.83 (dd, *J* = 6.5, 5.0 Hz, 1H), 2.45 (s, 3H), 1.23 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.9, 145.4, 139.8, 135.7, 135.2, 129.9, 128.8, 128.5, 128.0, 127.9, 108.9, 77.3, 77.0, 76.7, 59.3, 49.9, 49.1, 21.7, 20.6; HRMS: $[M+H]^+$ calculated for $C_{20}H_{22}NO_4S$: 372.1269; found: 372.1266.

3-Benzyl-6-(((4-chlorophenyl)sulfonyl)methyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4i)



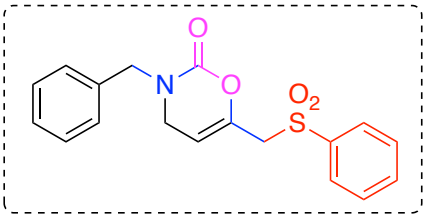
4i (18 mg) was synthesized following general procedure A; white solid; 42% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, *J* = 8.7 Hz, 2H), 7.51 (d, *J* = 8.8 Hz, 2H), 7.39-7.31 (m, 3H), 7.25 (d, *J* = 6.3 Hz, 2H), 5.24 (t, *J* = 3.4 Hz, 1H), 4.49 (s, 2H), 3.86 (s, 2H), 3.74 (d, *J* = 3.4 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.2, 141.2, 140.3, 136.9, 135.0, 129.9, 129.6, 128.9, 128.2, 128.2, 103.0, 59.5, 52.2, 44.7; HRMS: $[M+H]^+$ calculated for $C_{18}H_{17}ClNO_4S$: 378.0566 and 380.0537; found: 378.0563 and 380.0532.

3-Benzyl-6-(((4-fluorophenyl)sulfonyl)methyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4j)



4j (15 mg) was synthesized following general procedure A; white solid; 38% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99-7.87 (m, 2H), 7.41-7.31 (m, 3H), 7.28-7.26 (m, 2H), 7.25-7.19 (m, 2H), 5.26 (t, *J* = 3.4 Hz, 1H), 4.51 (s, 2H), 3.88 (s, 2H), 3.76 (d, *J* = 3.5 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 166.2 (d, *J* = 257.6 Hz), 149.2, 140.4, 135.0, 134.4, 131.2 (d, *J* = 9.9 Hz), 128.9, 128.3, 116.8, 116.6, 102.9, 59.6, 52.2, 44.7; HRMS: $[M+H]^+$ calculated for $C_{18}H_{17}FNO_4S$: 362.0862; found: 362.0858.

3-Benzyl-6-((phenylsulfonyl)methyl)-3,4-dihydro-2*H*-1,3-oxazin-2-one (4k):

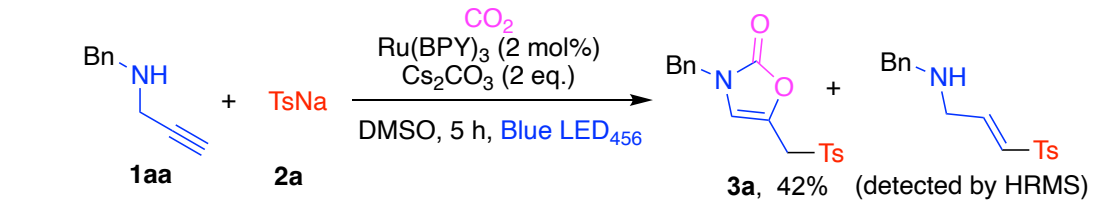


4j (18 mg) was synthesized following general procedure A; white solid; 49% yield (eluent: EtOAc/Pentane = 1:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.95 – 7.88 (m, 2H), 7.72 – 7.65 (m, 1H), 7.60 – 7.53 (m, 2H), 7.38-7.33 (m, 3H), 7.28 – 7.24 (m, 2H), 5.26 (t, *J* = 3.4 Hz, 1H), 4.50 (s, 2H), 3.88 (s, 2H), 3.75 (d, *J* = 3.5 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 149.3, 140.4, 138.4, 135.1, 134.3, 129.3, 128.8, 128.4, 128.2, 128.2, 102.8, 59.4, 52.1, 44.7; HRMS: $[M+H]^+$ calculated for $C_{18}H_{18}NO_4S$: 344.0956; Found: 344.0953.

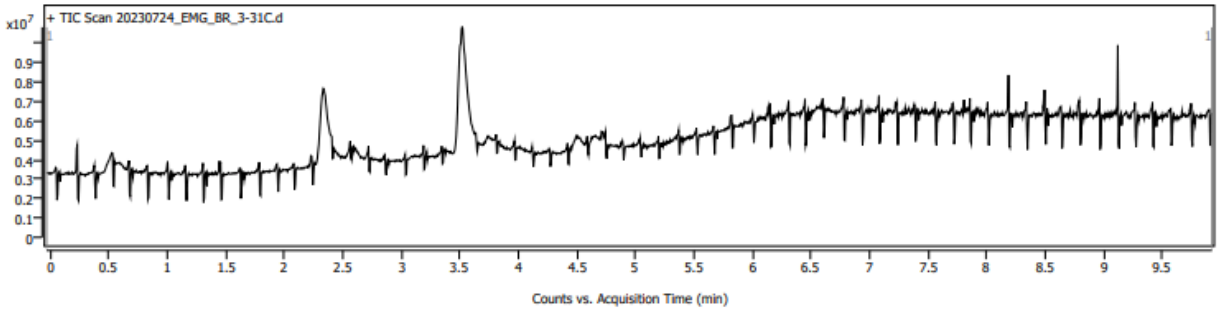
3. Intermediate trapping experiment

3.a HRMS analysis of reaction mixture

General Procedure **A** was followed except except the reaction was quenched after 5 hours. After completion of the reaction, the reaction mixture was directly analysed by HRMS.



Sample Chromatograms



Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
1		C17 H19 N O2 S	2.343	301.1135		FBF	97.48				FBF
2		C18 H17 N O4 S	3.521	343.0876		FBF	98.57				FBF

Compound Details

Cpd. 1: C17 H19 N O2 S

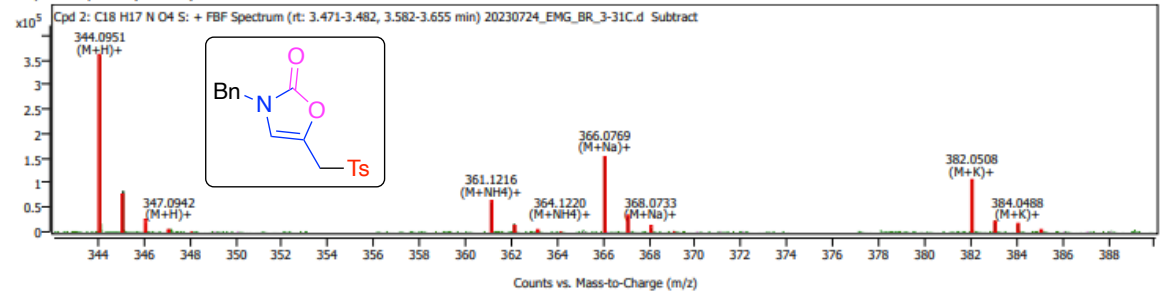
Name	Formula	RT	RI	Mass	Score	Algorithm	Lib/DB
	C17 H19 N O2 S	2.343		301.1135	97.48	FBF	

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Score (MFG)	Score (RT)
M+ (M+H)+ (M+Na)+ (M+K)+	301.1147 302.1209 324.1027 340.0768					

Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (DB)	Score (MFG)
	C17 H19 N O2 S	M+ (M+H)+ (M+Na)+ (M+K)+	2.343		301.1135		FBF	97.48		

Compound Spectra (overlaid)



Compound Spectra (overlaid)

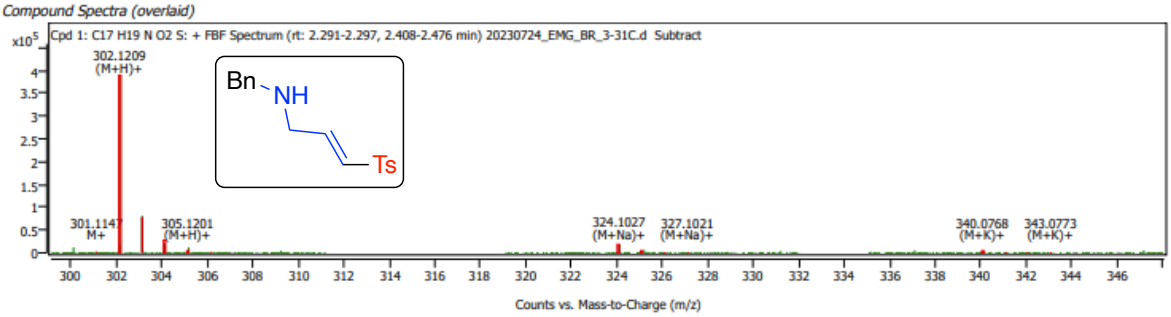


Fig. S2. HRMS spectra.

5. X-ray crystallographic studies

a) X-ray crystallographic studies of compound 3a (CCDC 2287477)

A single crystals of compound **3a** for X-ray diffraction analysis were grown using $CHCl_3$ solvent under slow evaporation method.

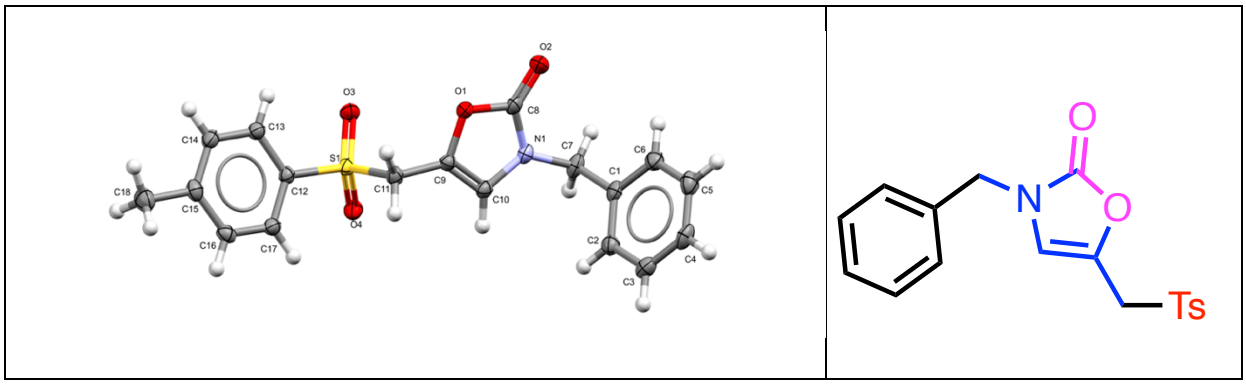


Fig. S3. Asymmetric unit, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Experimental:

Data were obtained at a temperature of 92(6) K in a SuperNova, Dual, Cu at home/near four-circle diffractometer with a microfocus sealed X-ray tube, using a mirror as a monochromator and an Atlas detector and with Cu Kα radiation (λ = 1.54184 Å).

All data were integrated with CrysAlisPro and a gaussian absorption correction using SCALE3 ABSPACK was applied. All structures was solved by dual methods using SHELXT and refined by full-matrix least-squares methods against F^2 by SHELXL using OLEX2 as an interface.

Table 1. Crystal data and structure refinement for **3a**

CCDC	2287477
Empirical formula	C18H17NO4S
Formula weight	343.38
Temperature [K]	104.4(5)
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	12.30520(10)
b [Å]	7.33200(10)
c [Å]	18.7530(2)
α [°]	90
β [°]	102.2920(10)
γ [°]	90
Volume [Å3]	1653.14(3)
Z	4

ρcalc [gcm−3]	1.380
μ [mm−1]	1.933
F(000)	720
Crystal size [mm3]	0.18×0.12×0.05
Crystal colour	translucent intense colourless
Crystal shape	block
Radiation	Cu Kα (λ=1.54184 Å)
2θ range [°]	7.35 to 145.37 (0.81 Å)
Index ranges	−15 ≤ h ≤ 15 −9 ≤ k ≤ 8 −23 ≤ l ≤ 19
Reflections collected	22109
Independent reflections	3235 Rint = 0.0364 Rsigma = 0.0185
Completeness to θ = 67.684°	99.9 %
Data / Restraints / Parameters	3235/0/218
Goodness-of-fit on F2	1.040
Final R indexes [I≥2σ(I)]	R1 = 0.0322 wR2 = 0.0832
Final R indexes [all data]	R1 = 0.0377 wR2 = 0.0877
Largest peak/hole [eÅ−3]	0.45/-0.48

b) X-ray crystallographic studies of compound 4a (CCDC 2287478)

A single crystals of compound **3a** for X-ray diffraction analysis were grown using $CHCl_3$ solvent under slow evaporation method.

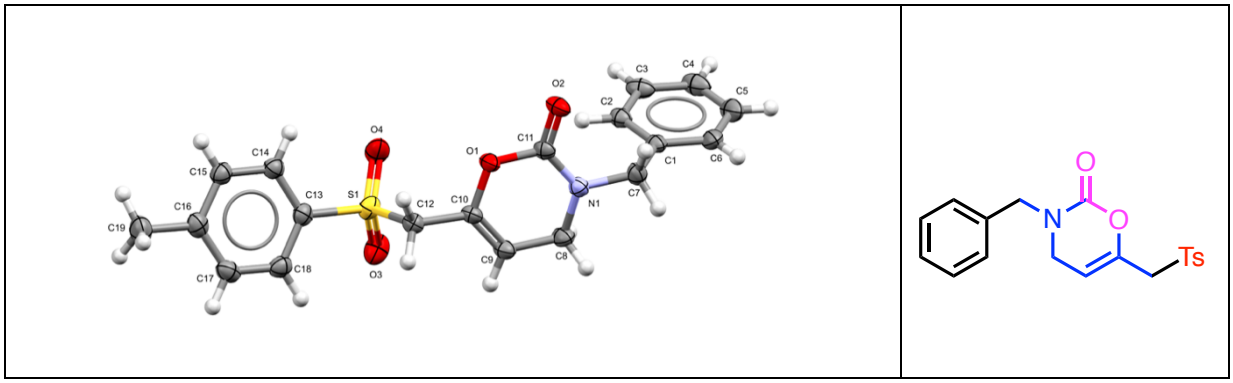


Fig. S4. Asymmetric unit, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table 2. Crystal data and structure refinement for **4a**

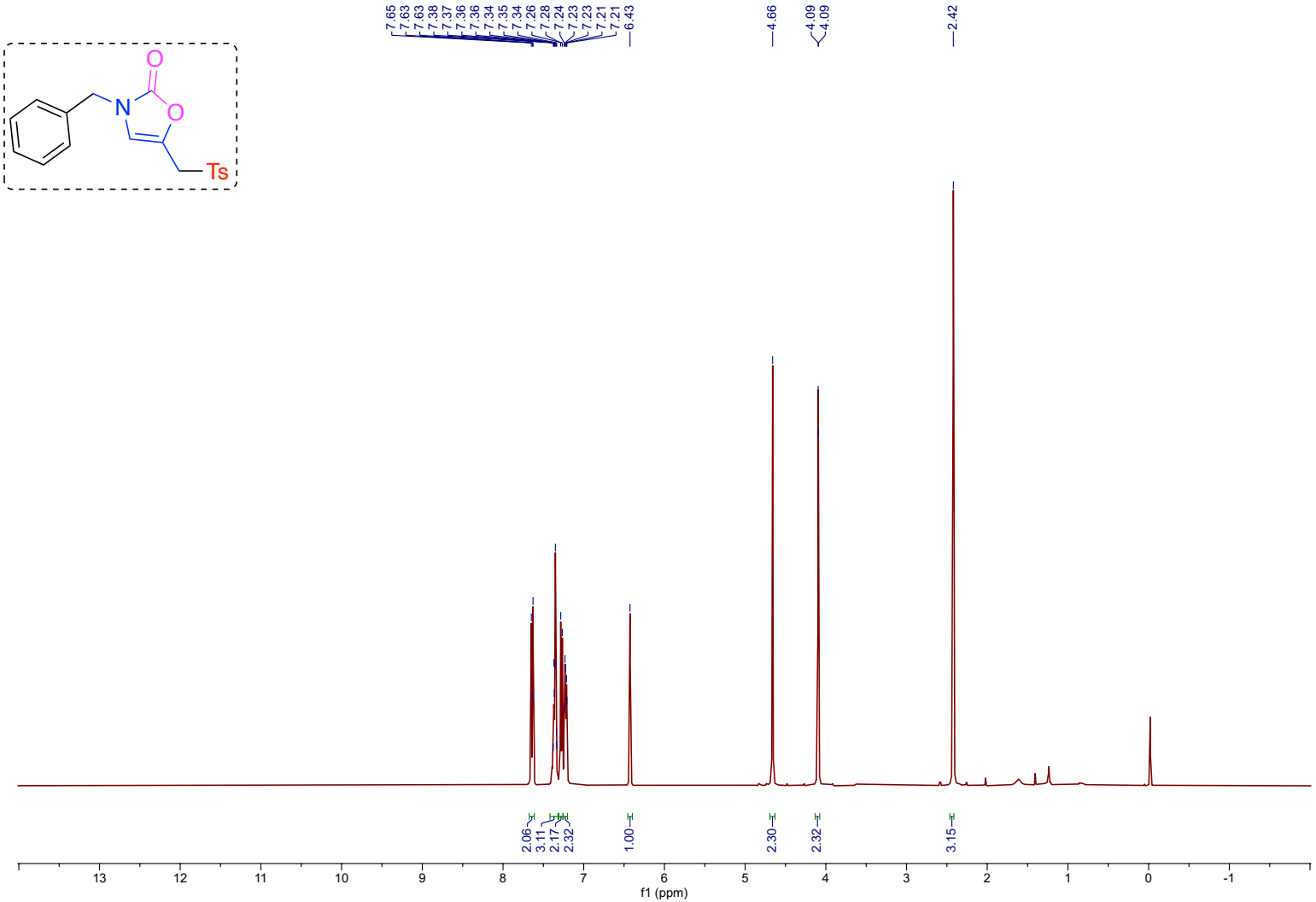
CCDC	2287478
Empirical formula	C19H19NO4S
Formula weight	357.41
Temperature [K]	104.60(14)
Crystal system	orthorhombic
Space group (number)	$P2_12_12_1$ (19)
a [Å]	7.37430(10)
b [Å]	15.0097(2)
c [Å]	15.6382(2)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å3]	1730.93(4)
Z	4
ρcalc [gcm−3]	1.372
μ [mm−1]	1.867
F(000)	752
Crystal size [mm3]	0.34×0.22×0.15
Crystal colour	metallic dark yellow
Crystal shape	block
Radiation	Cu Kα (λ=1.54184 Å)
2θ range [°]	8.16 to 145.27 (0.81 Å)
Index ranges	−8 ≤ h ≤ 6 −18 ≤ k ≤ 18 −18 ≤ l ≤ 19
Reflections collected	16147
Independent reflections	3386 Rint = 0.0314 Rsigma = 0.0213
Completeness to θ = 67.684°	100.0 %

Data / Restraints / Parameters	3386/0/227
Goodness-of-fit on F2	1.064
Final R indexes [I≥2σ(I)]	R1 = 0.0270 wR2 = 0.0682
Final R indexes [all data]	R1 = 0.0293 wR2 = 0.0703
Largest peak/hole [eÅ−3]	0.22/-0.26
Flack X parameter	-0.004(7)

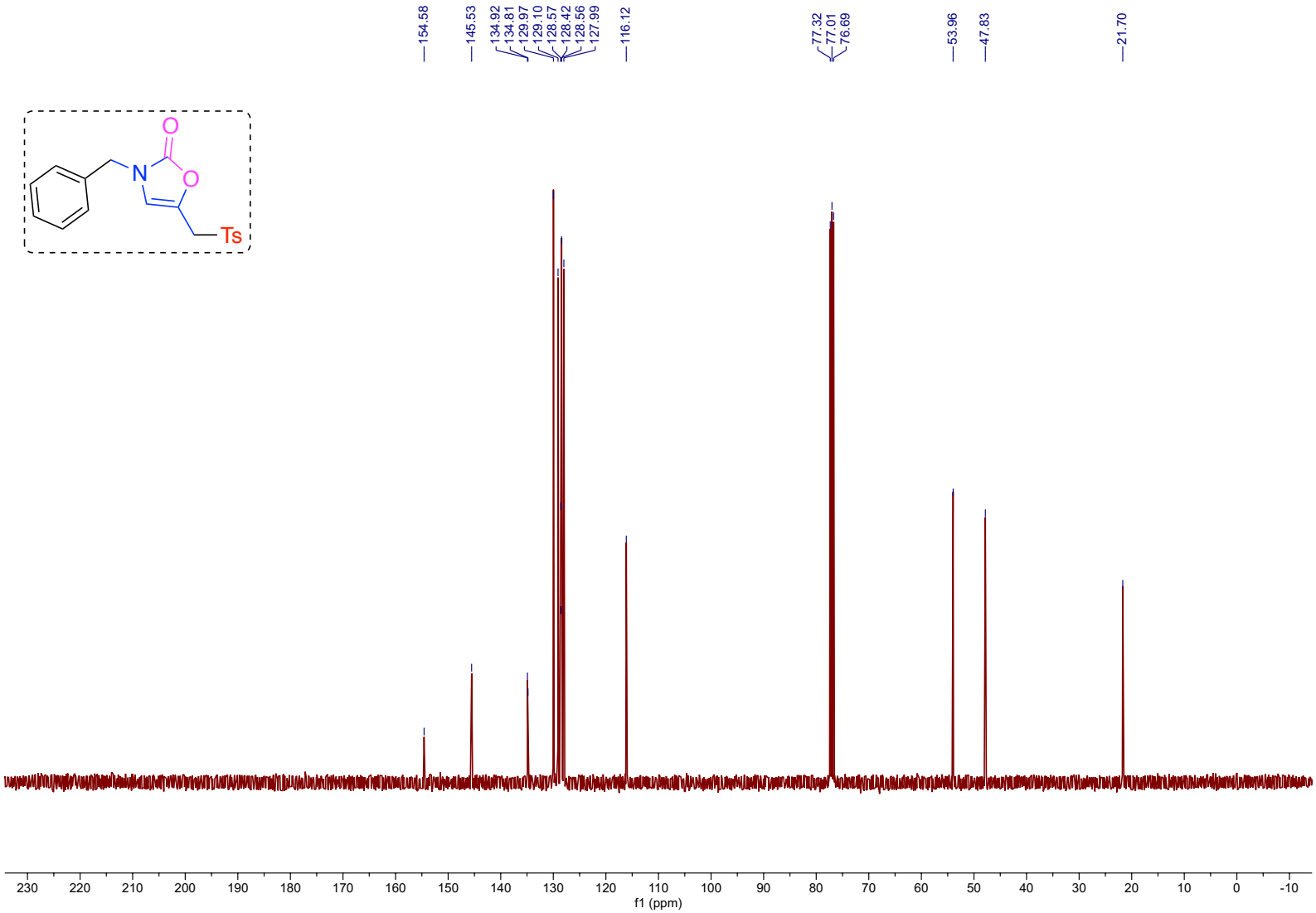
5. References:

1. Q.-W. Song and L.-N. He, *Adv. Synth. Catal.*, 2016, **358**, 1251–1258.
2. W. Hess and J. W. Burton, *Chem.-Eur., J.* 2010, **16**, 12303– 12306.
3. P. Quinodoz, A. Quelhas, K. Wright, B. Drouillat, J. Marrot and F. Couty, *Eur. J. Org. Chem.,* 2017, **2017**, 2621– 2626.

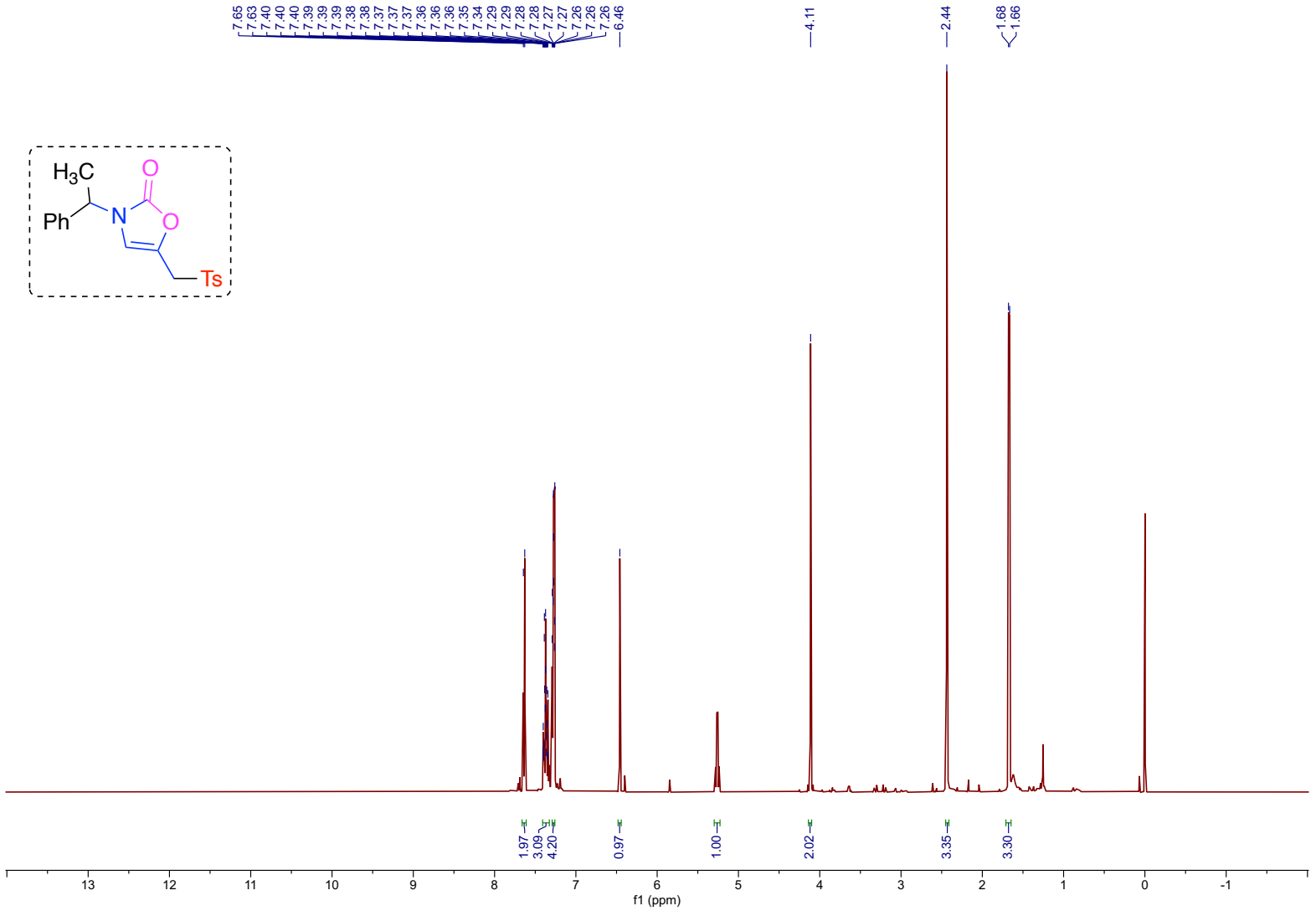
6. Copies of 1H and 13C NMR spectra:



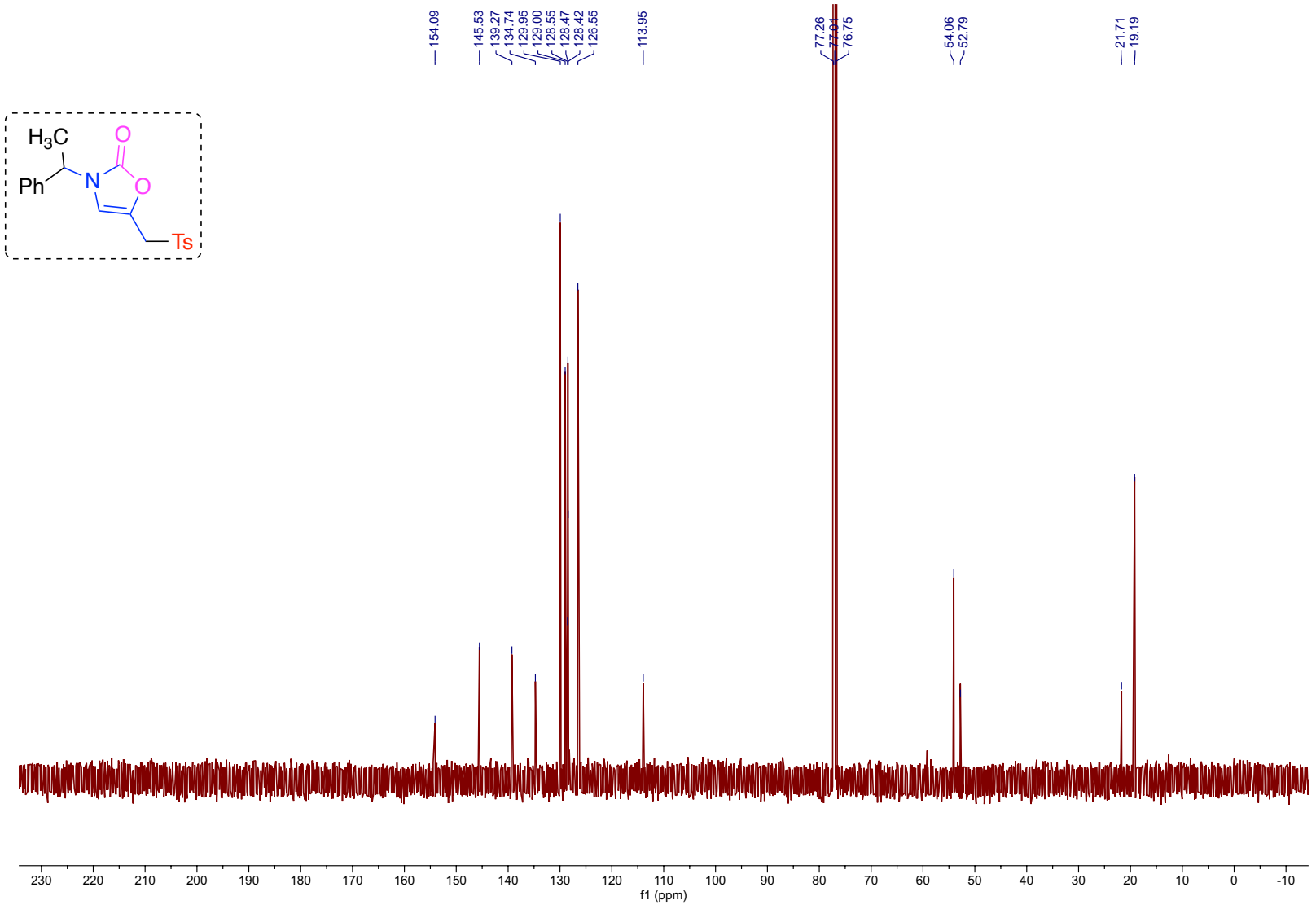
^{1}H (400 MHz) spectrum of compound 3a in $CDCl_3$



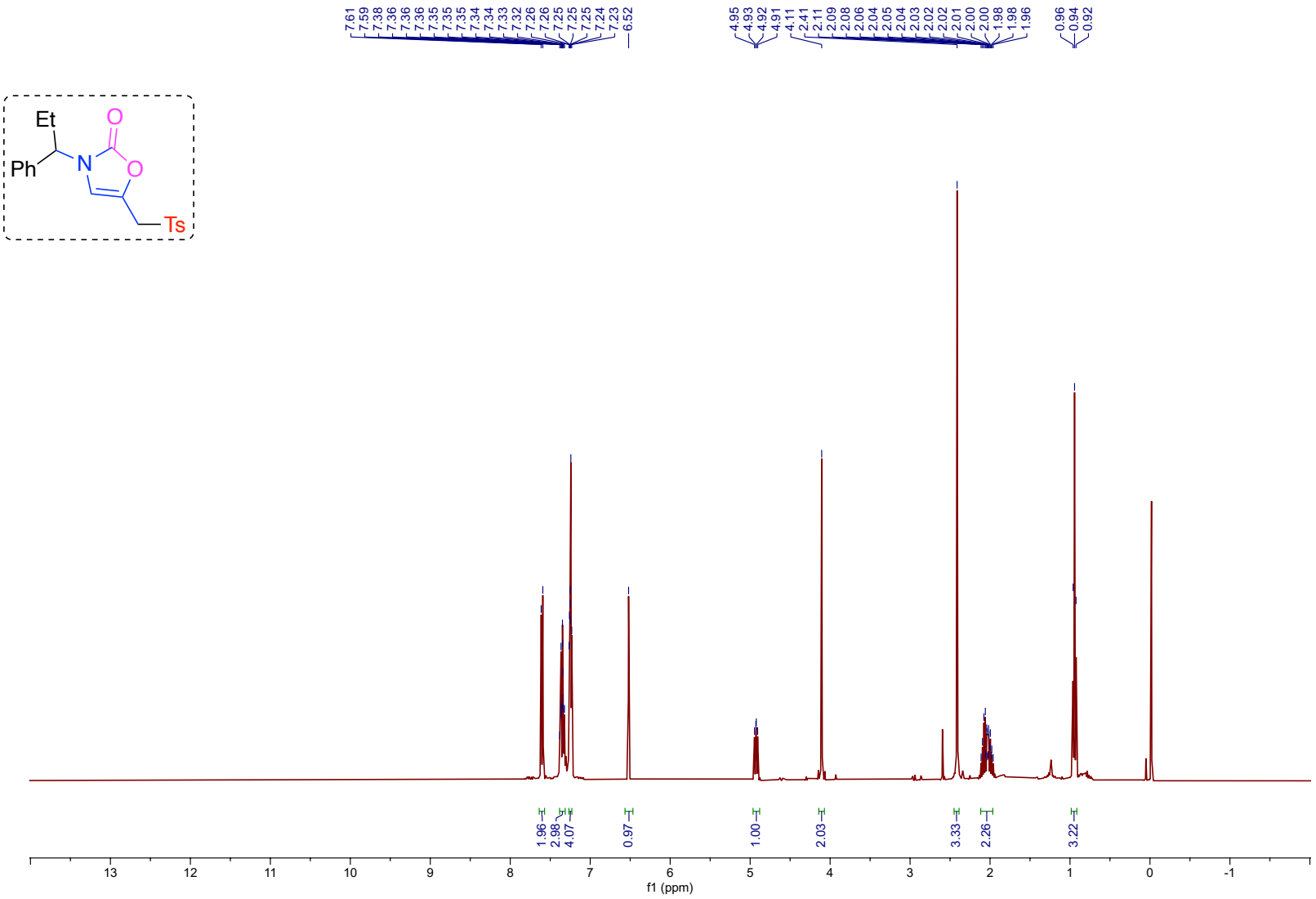
^{13}C (101 MHz) spectrum of compound 3a in $CDCl_3$



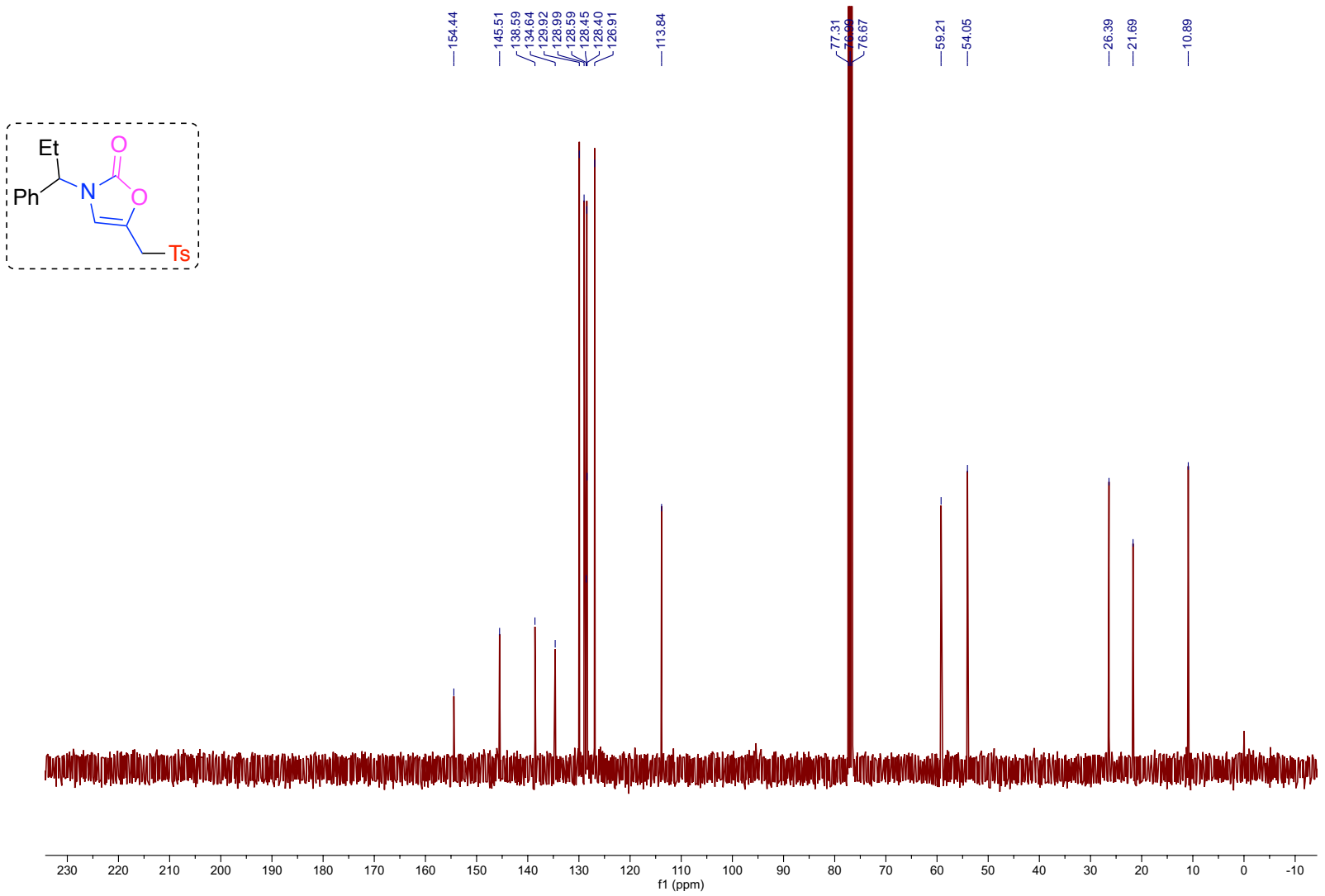
^{1}H (500 MHz) spectrum of compound 3b in $CDCl_3$



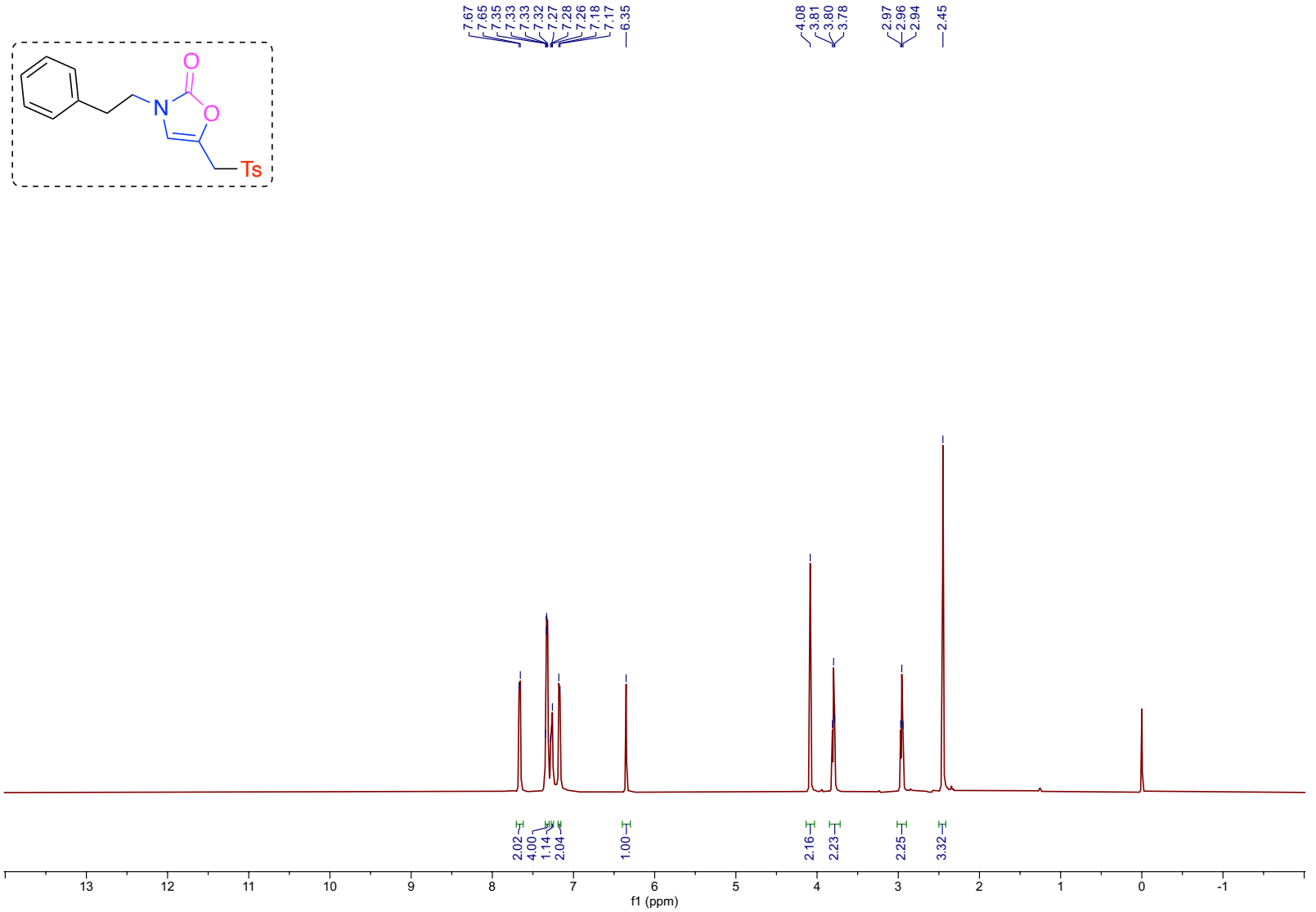
^{13}C (126 MHz) spectrum of compound 3b in $CDCl_3$



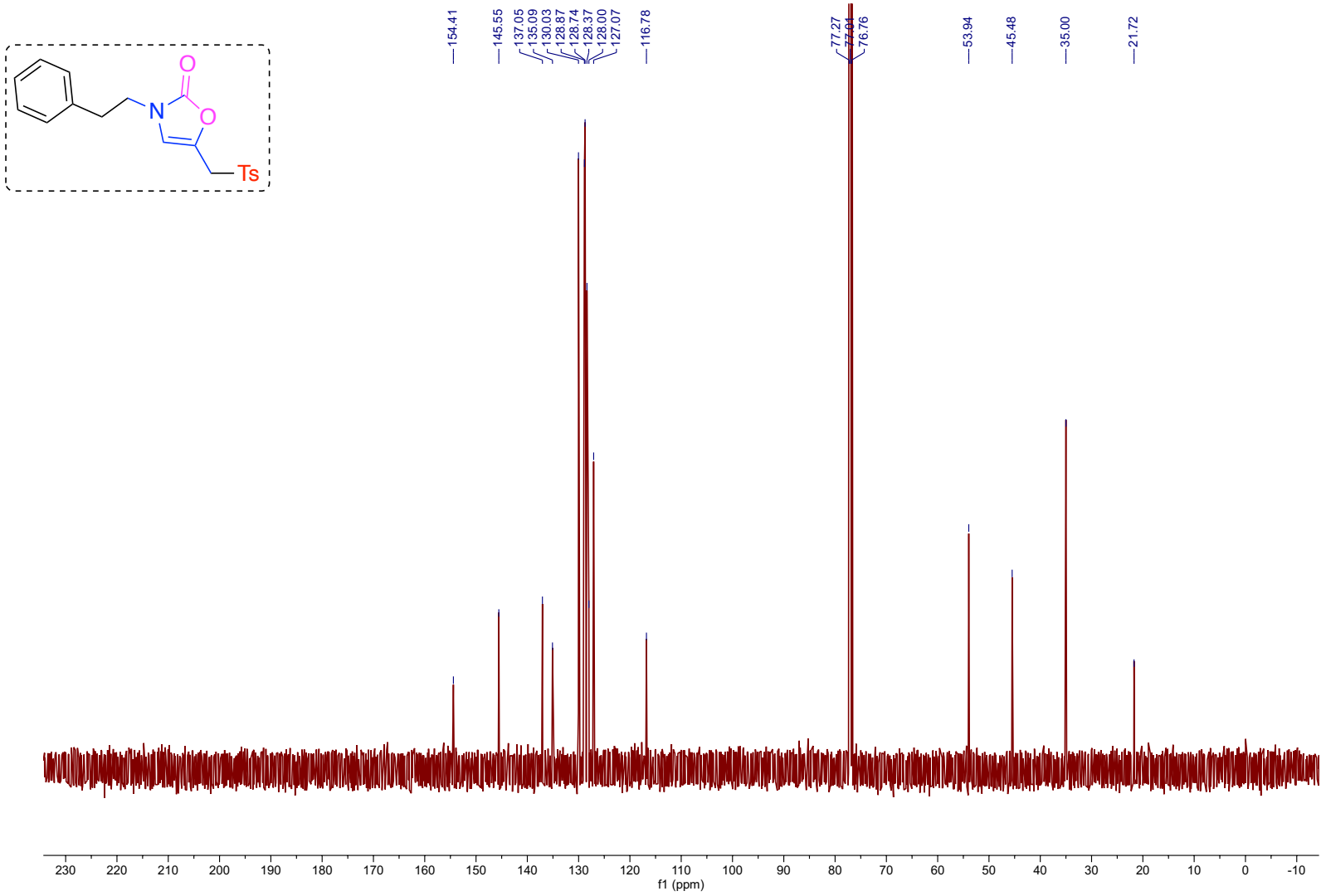
^{1}H (400 MHz) spectrum of compound 3c in $CDCl_3$



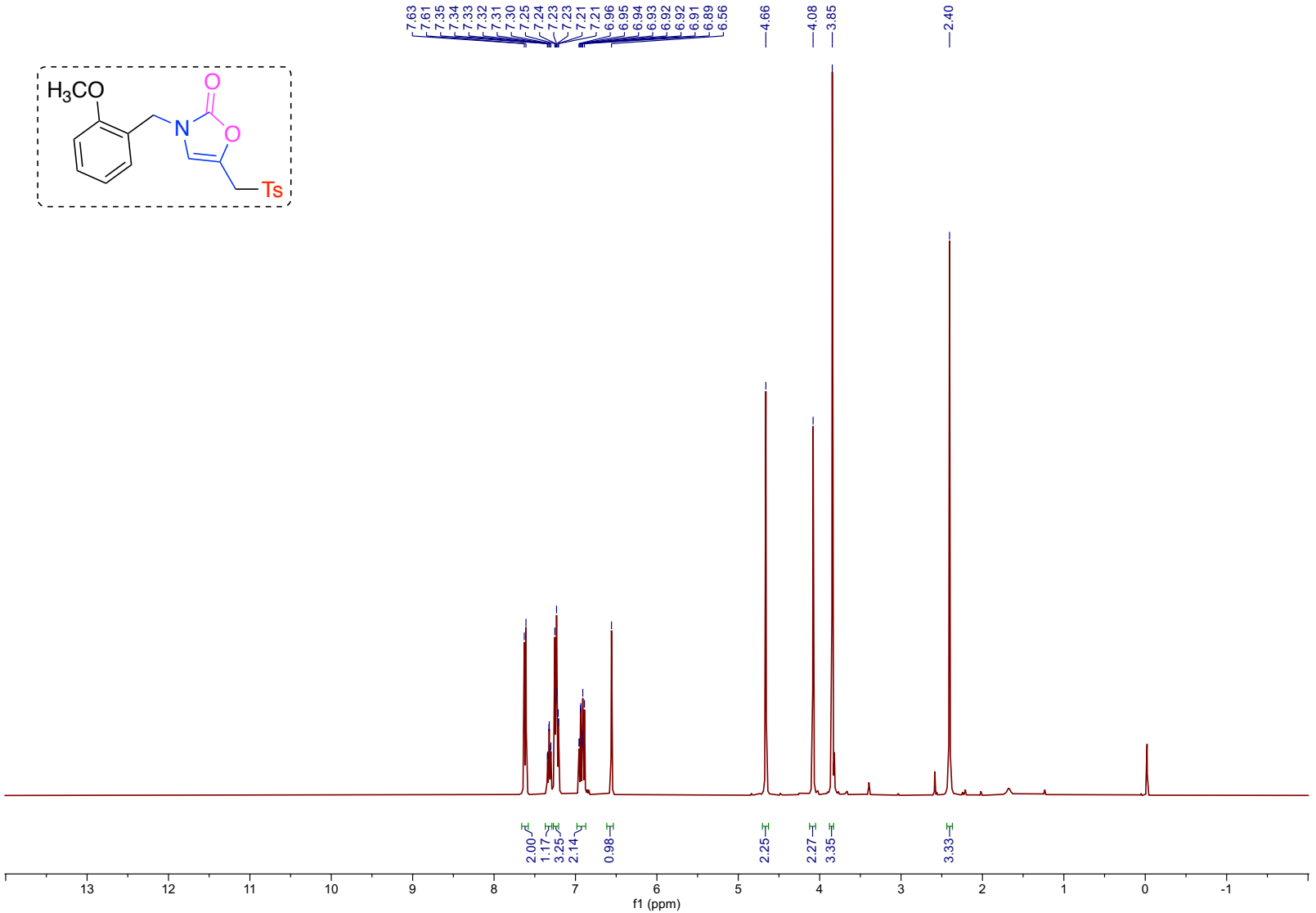
^{13}C (101 MHz) spectrum of compound 3c in $CDCl_3$



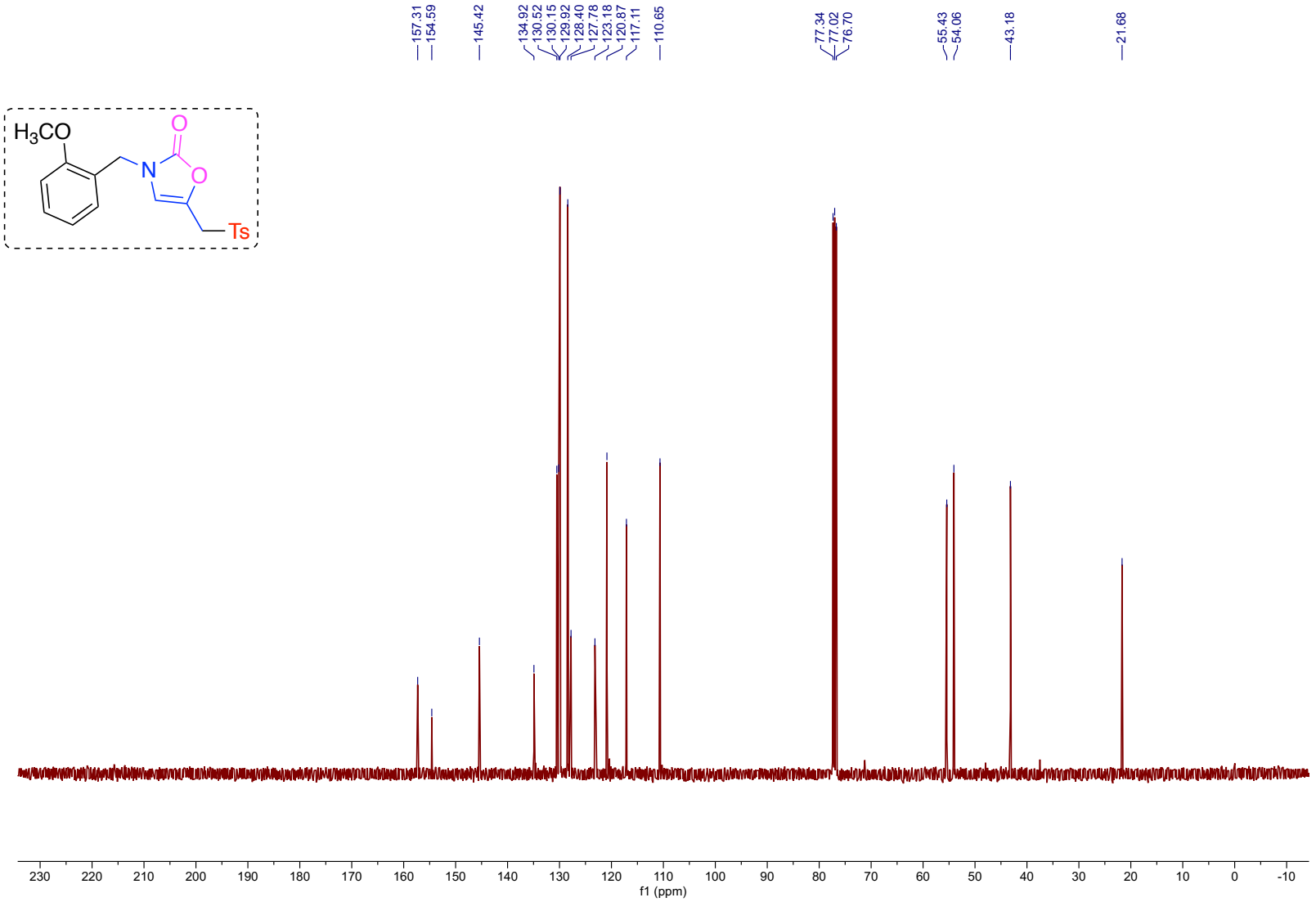
^{1}H (500 MHz) spectrum of compound 3d in $CDCl_3$



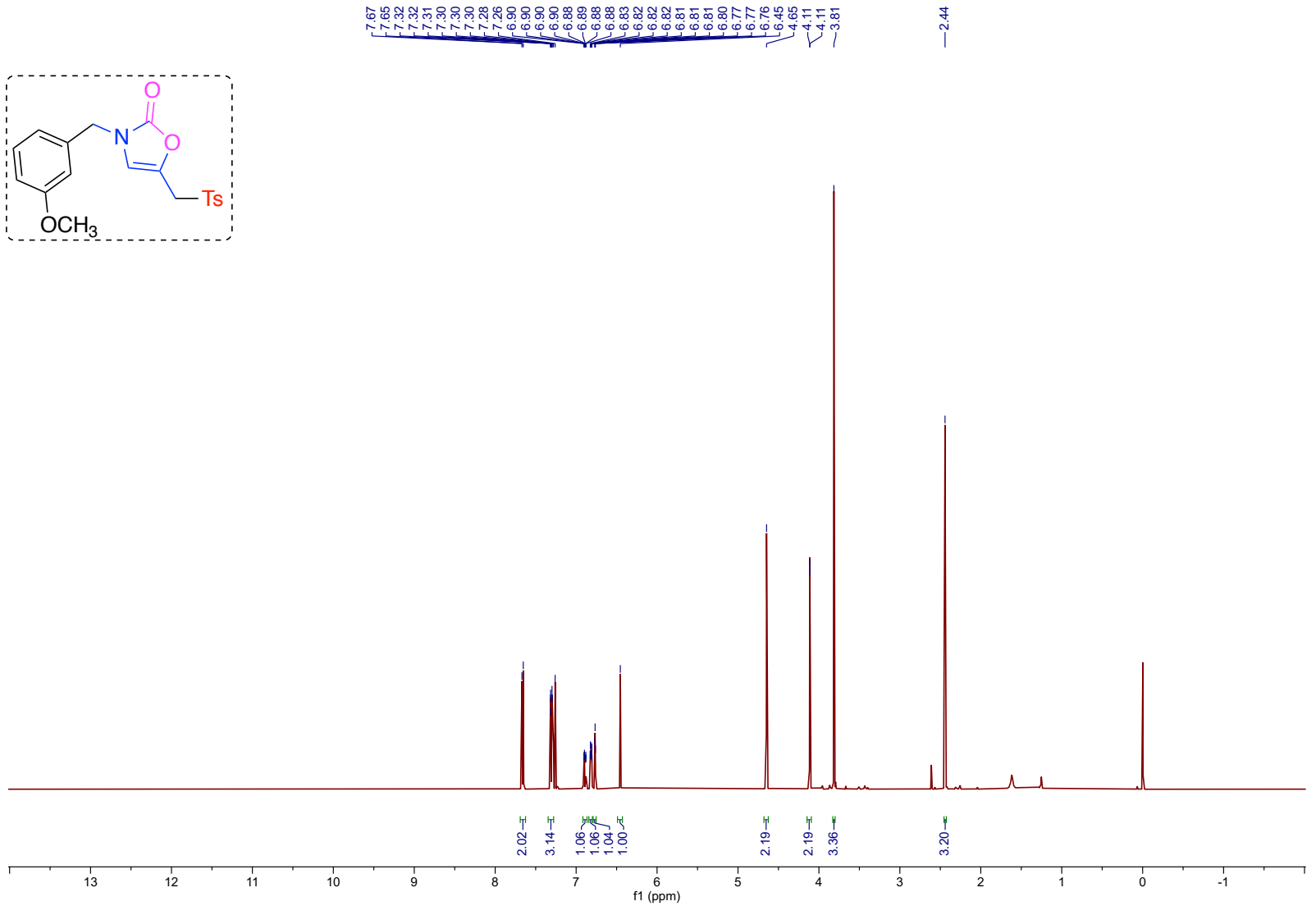
^{13}C (126 MHz) spectrum of compound 3d in $CDCl_3$



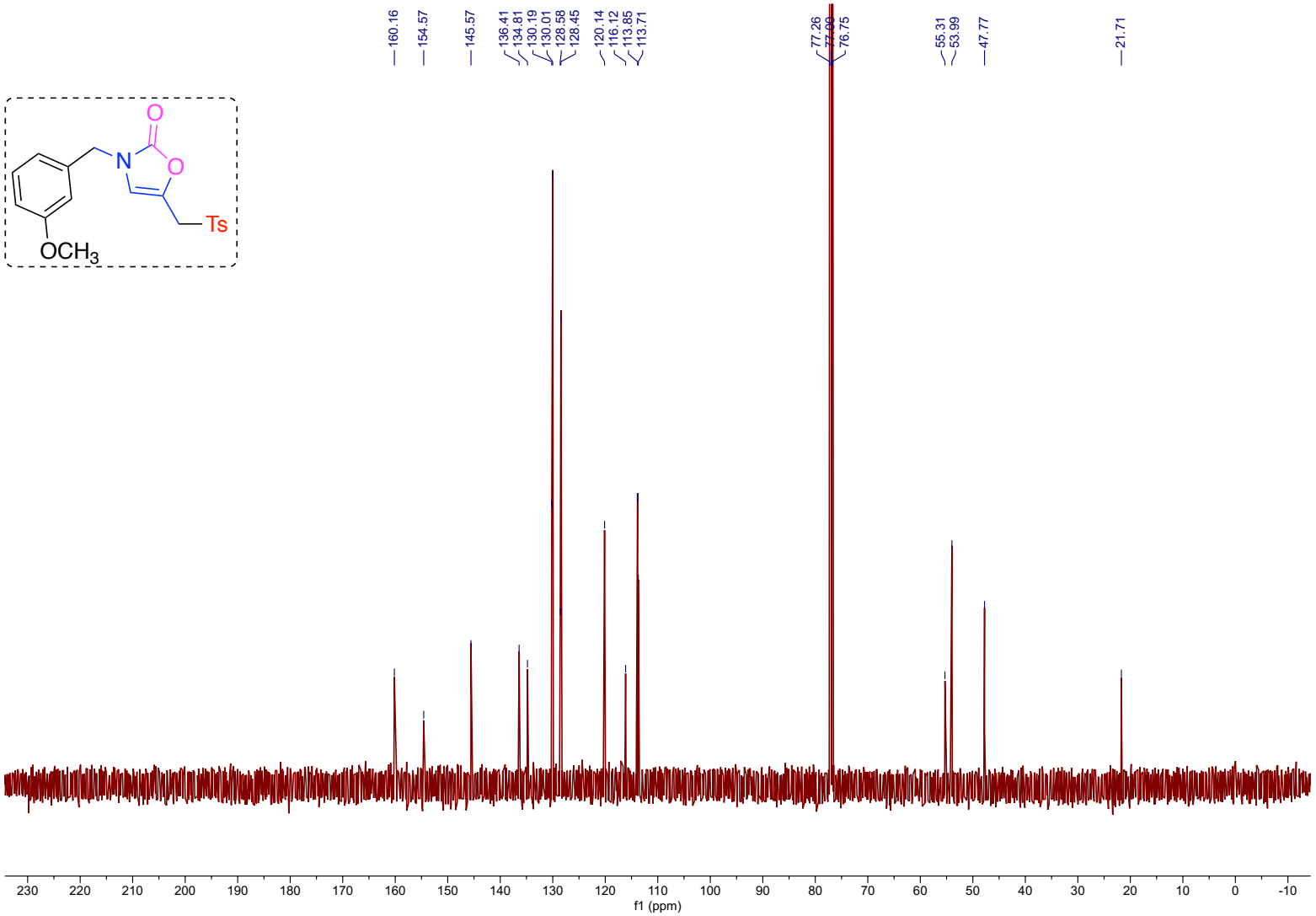
^{1}H (400 MHz) spectrum of compound 3e in $CDCl_3$



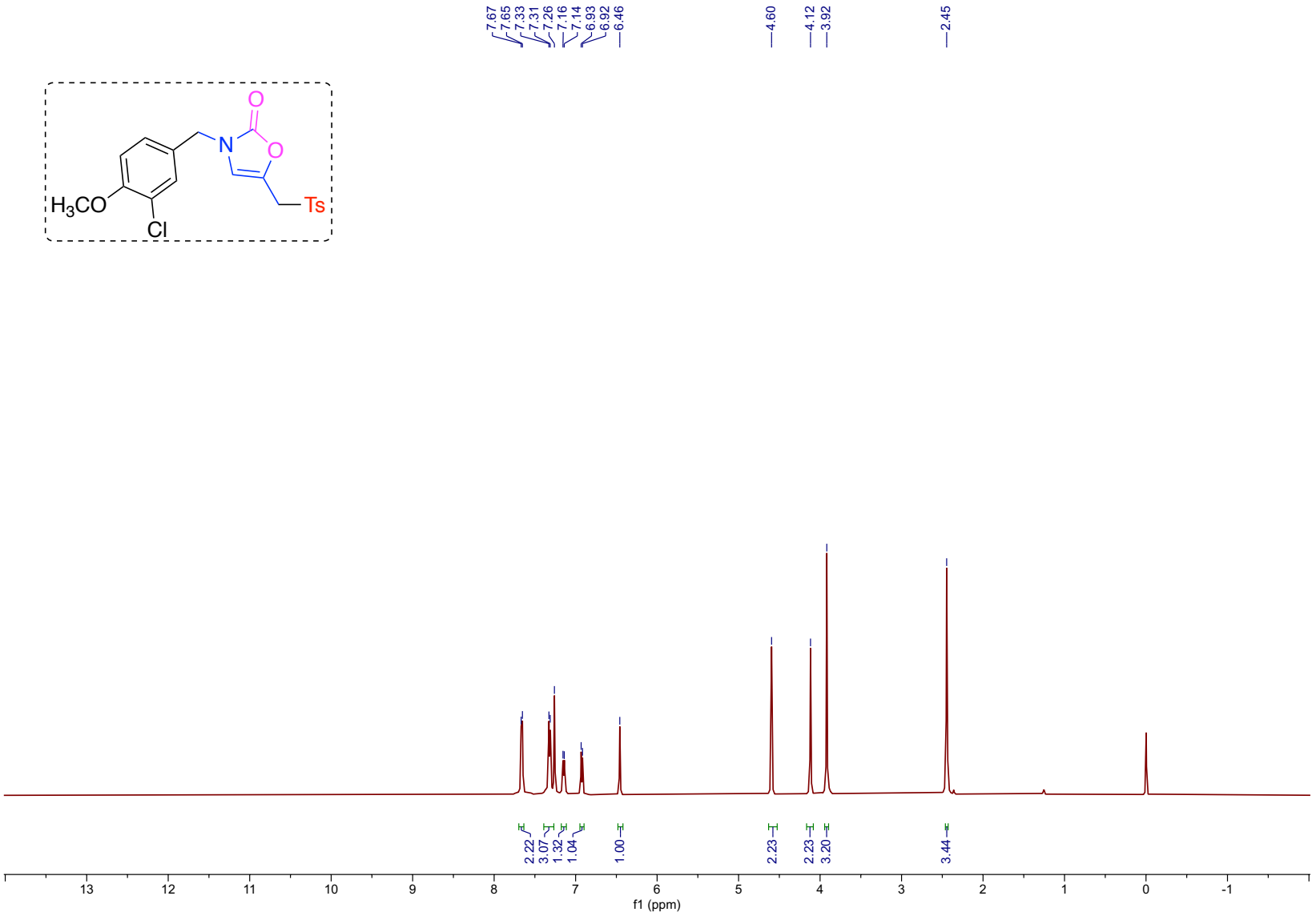
^{13}C (101 MHz) spectrum of compound 3e in $CDCl_3$



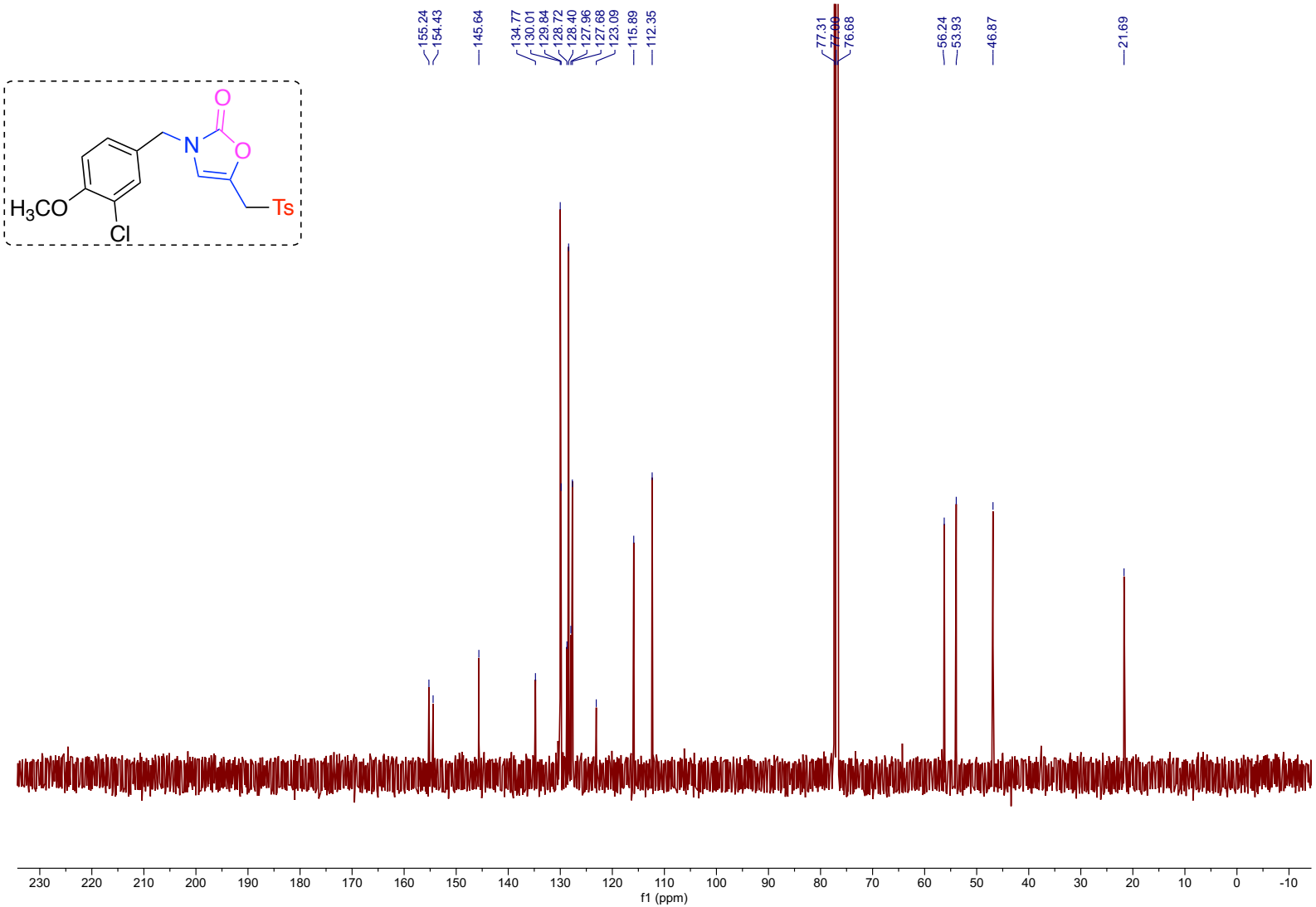
^{1}H (500 MHz) spectrum of compound 3f in $CDCl_3$



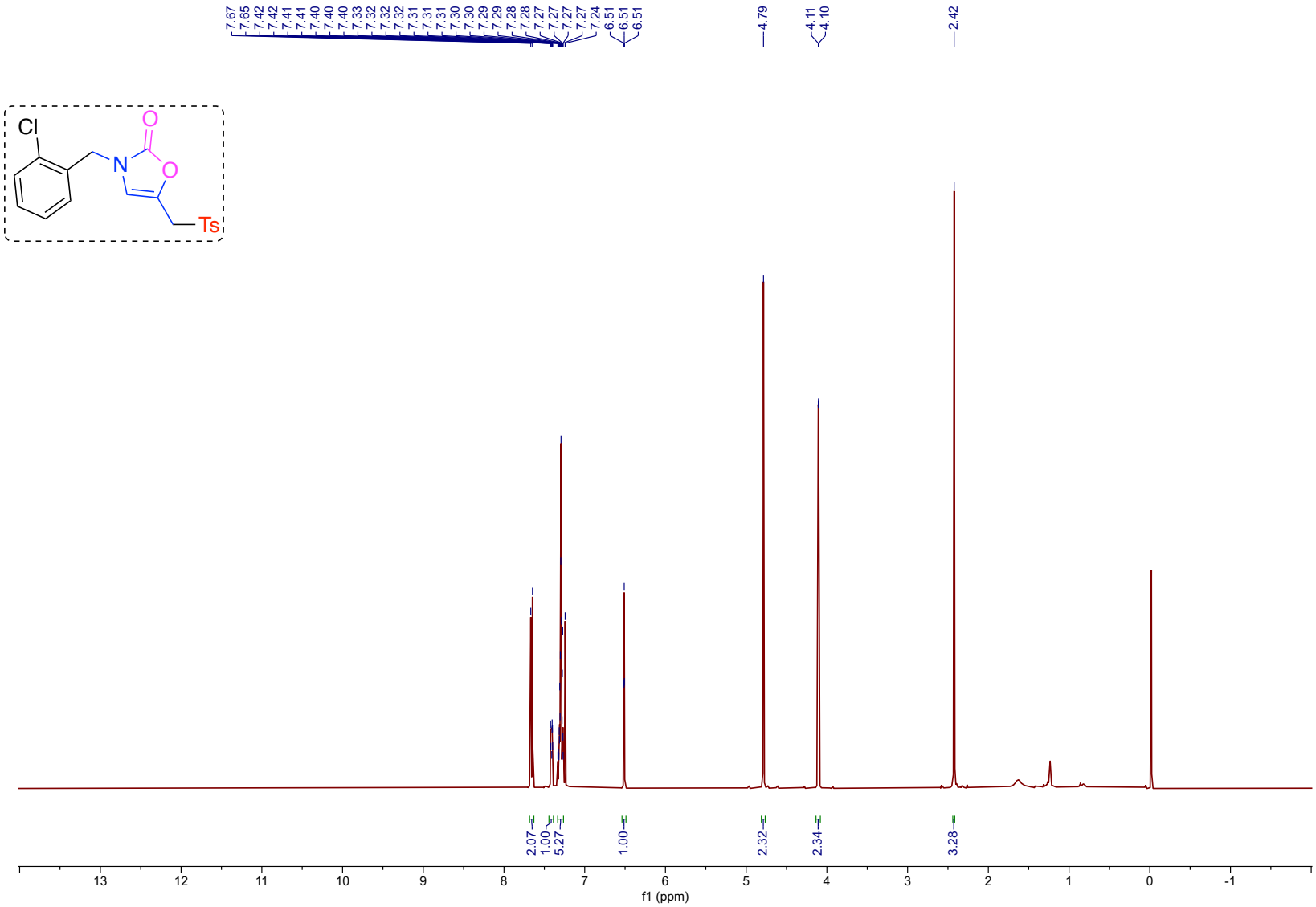
^{13}C (126 MHz) spectrum of compound 3f in $CDCl_3$



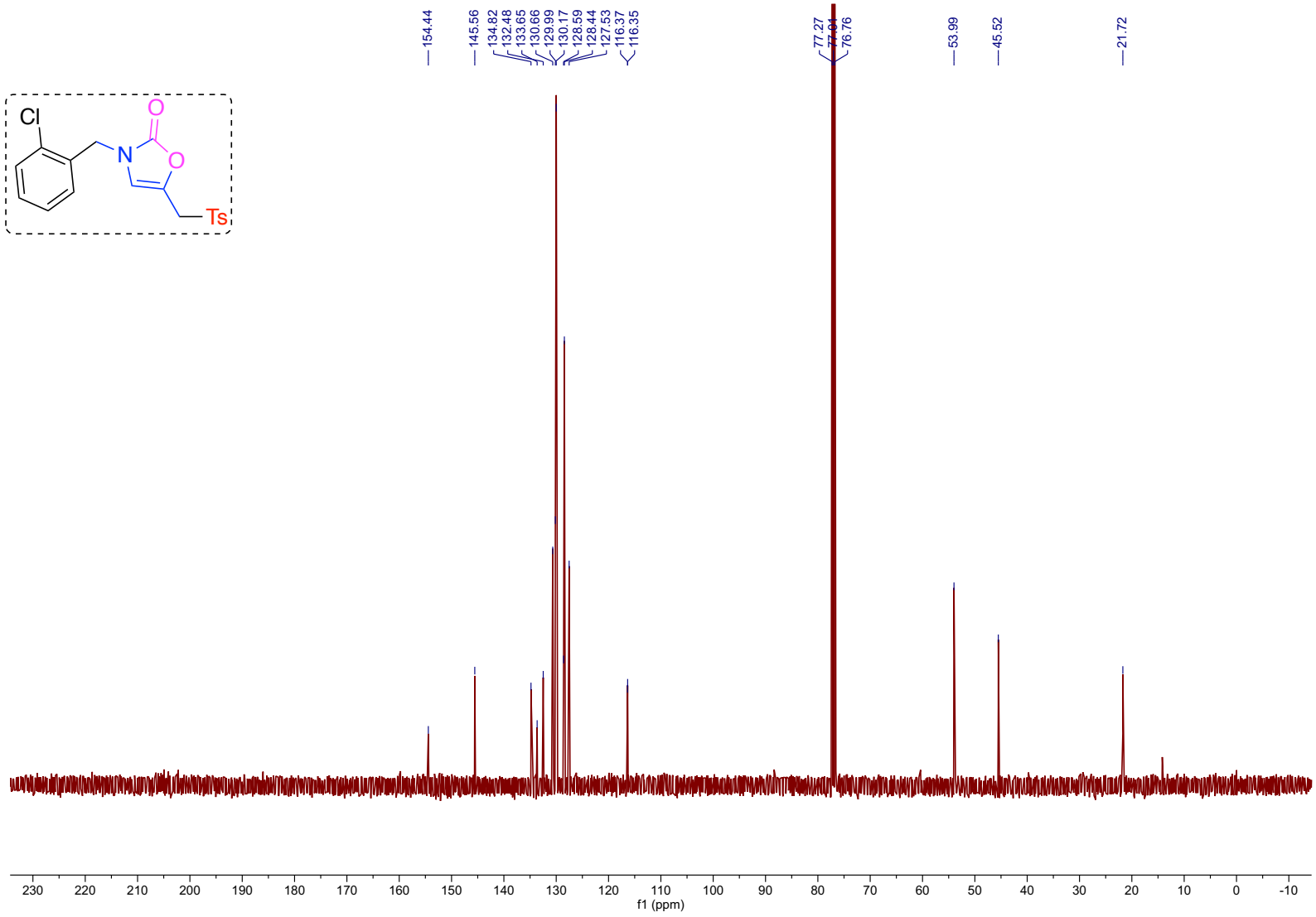
^{1}H (500 MHz) spectrum of compound 3g in $CDCl_3$



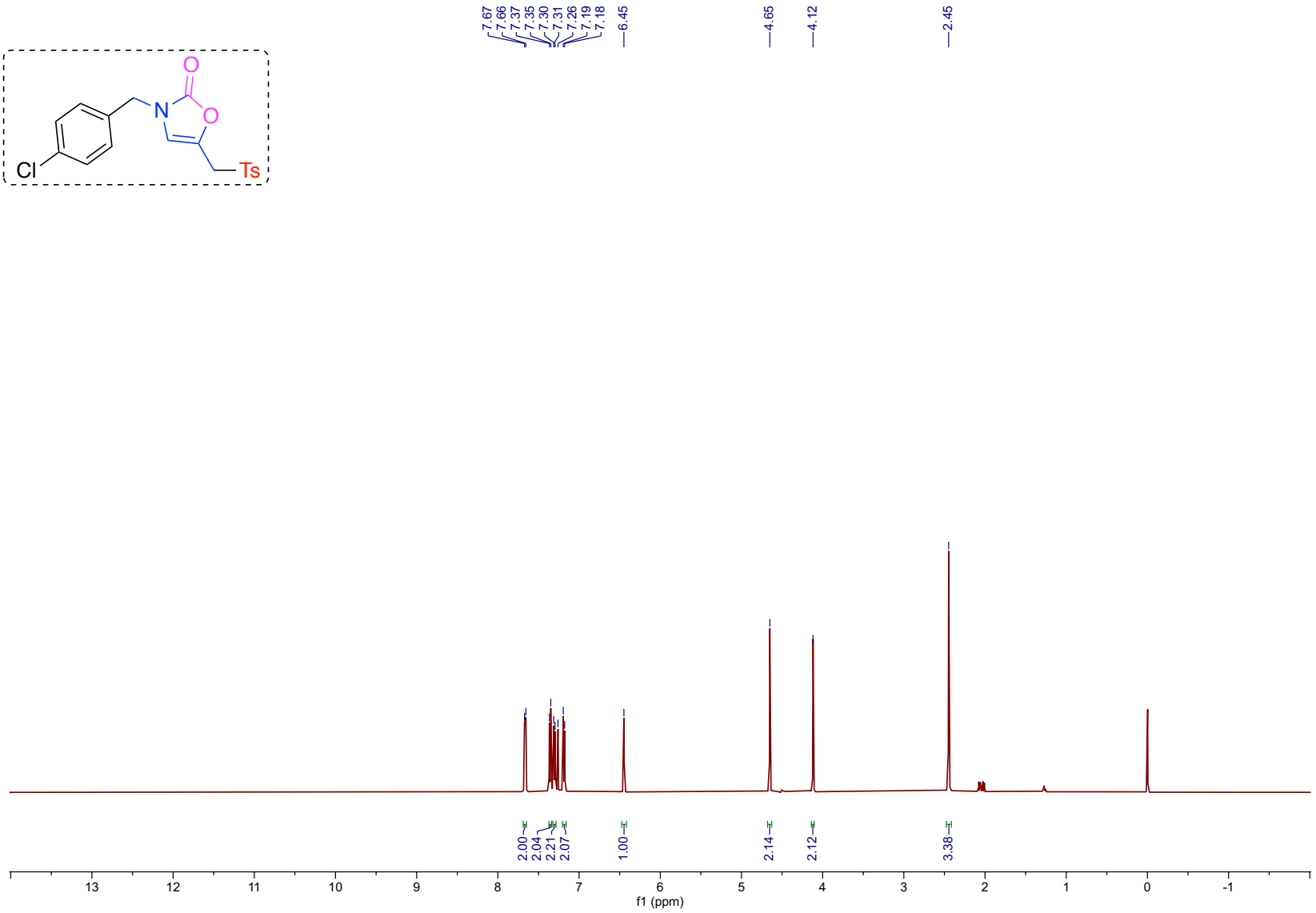
^{13}C (101 MHz) spectrum of compound 3g in $CDCl_3$



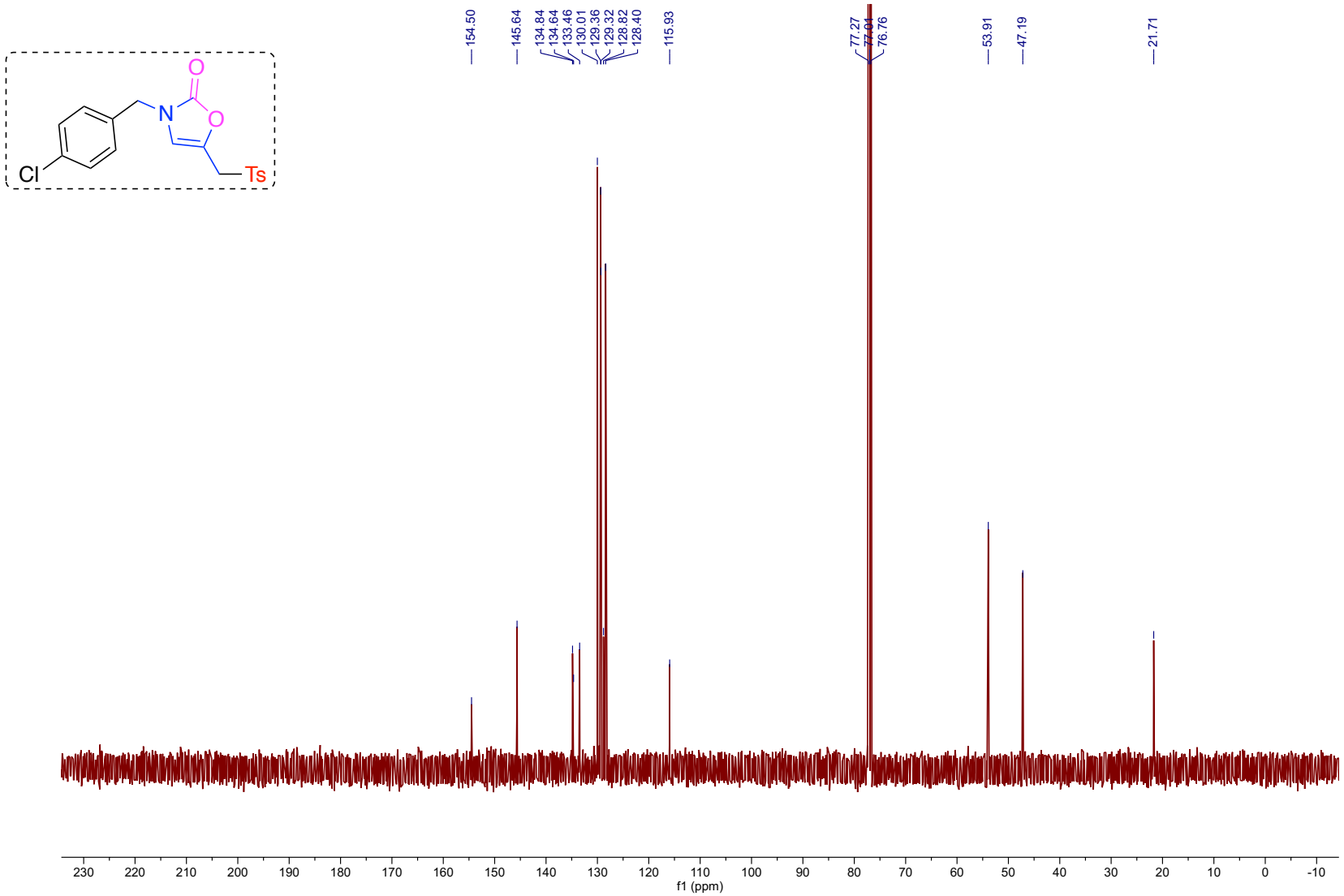
^{1}H (400 MHz) spectrum of compound 3h in $CDCl_3$



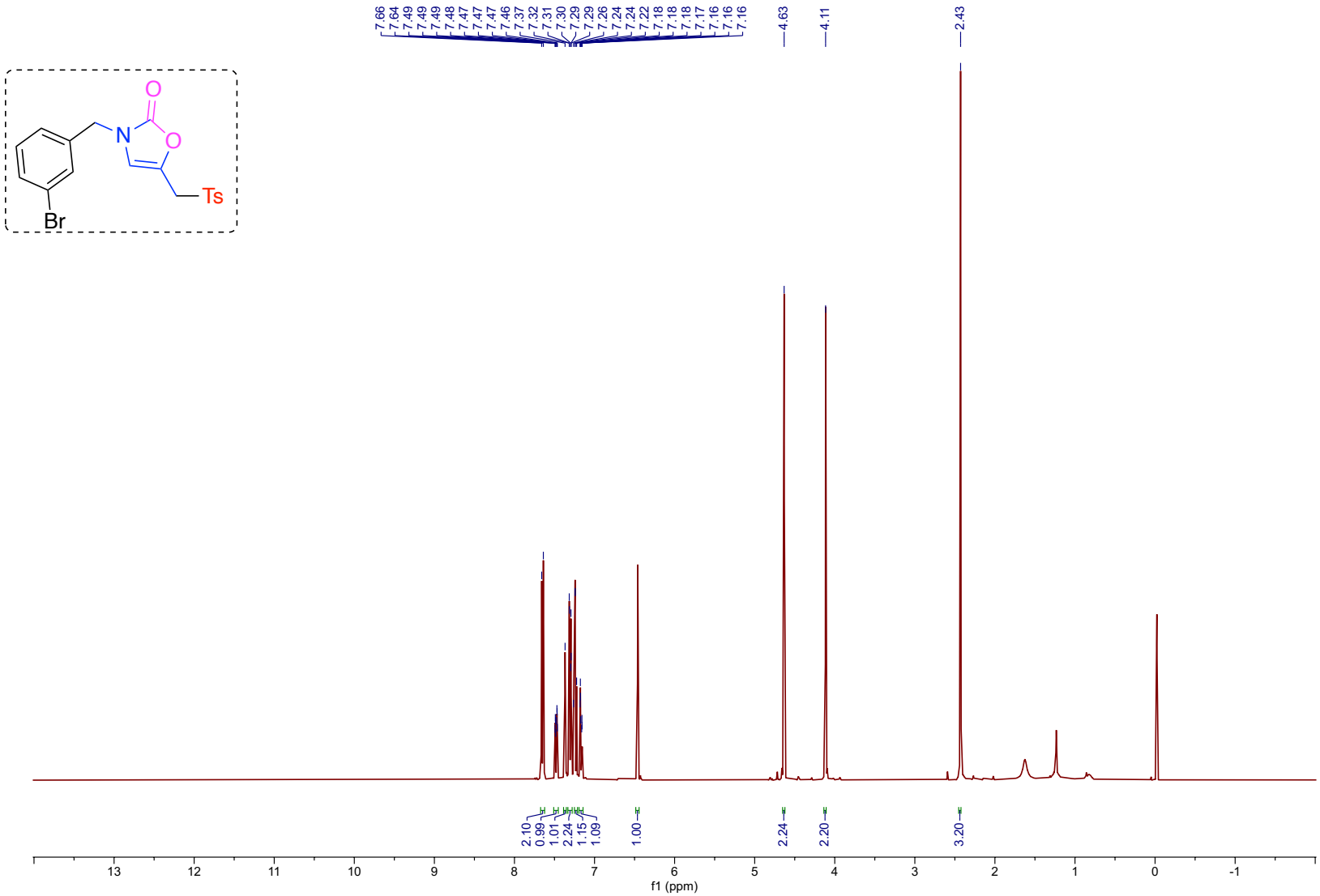
^{13}C (126 MHz) spectrum of compound 3h in $CDCl_3$



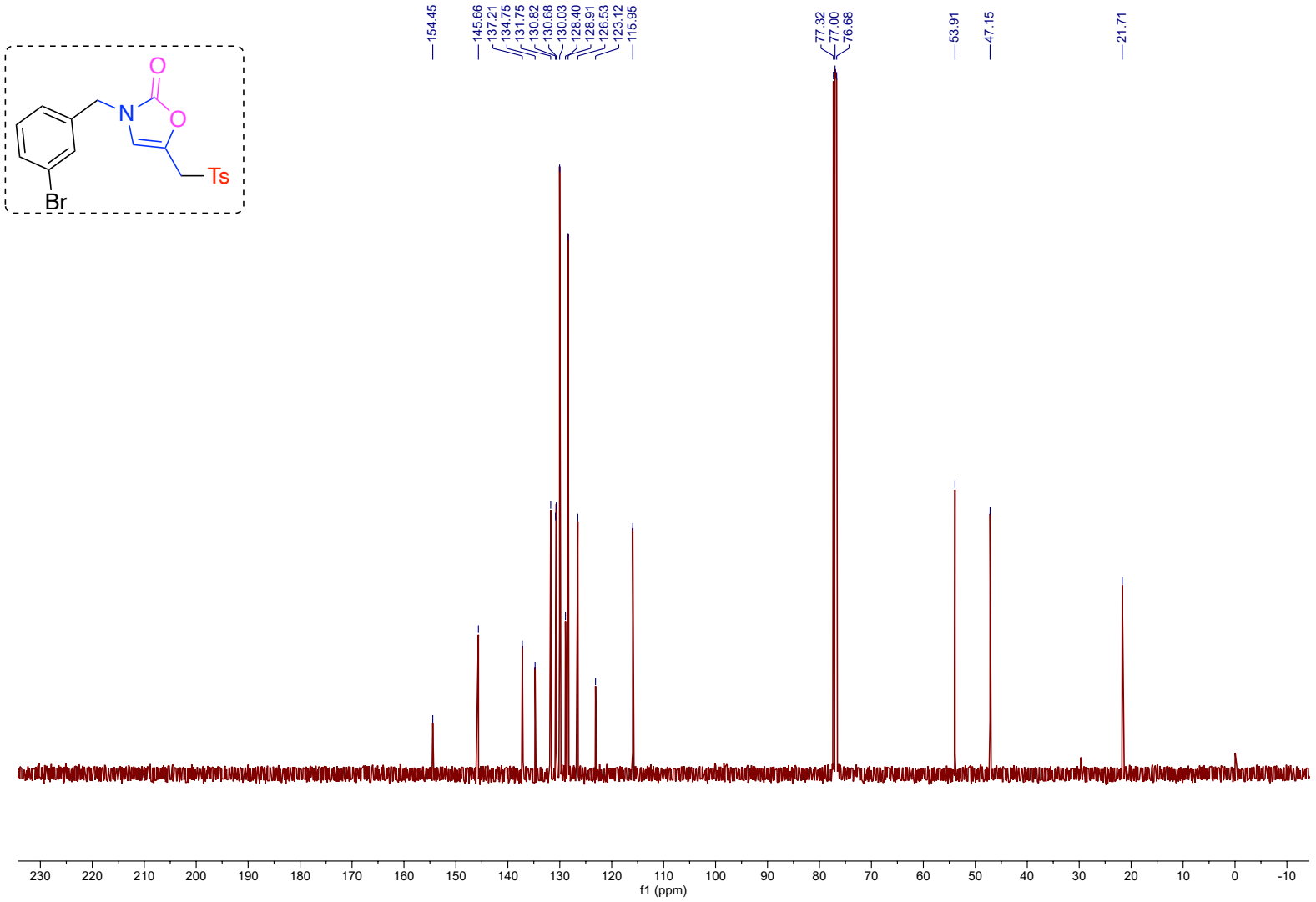
^{1}H (500 MHz) spectrum of compound 3i in $CDCl_3$



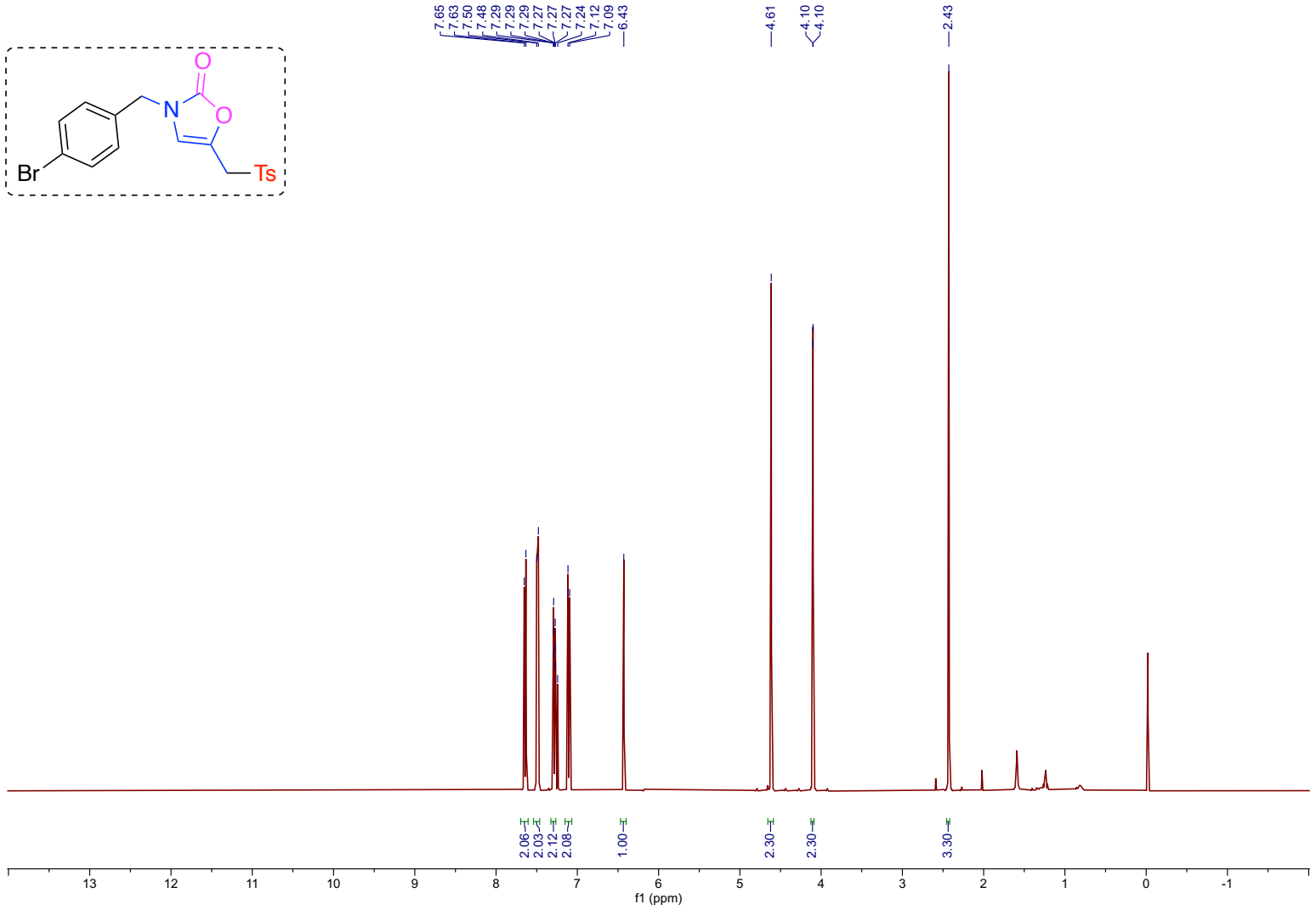
^{13}C (126 MHz) spectrum of compound 3i in $CDCl_3$



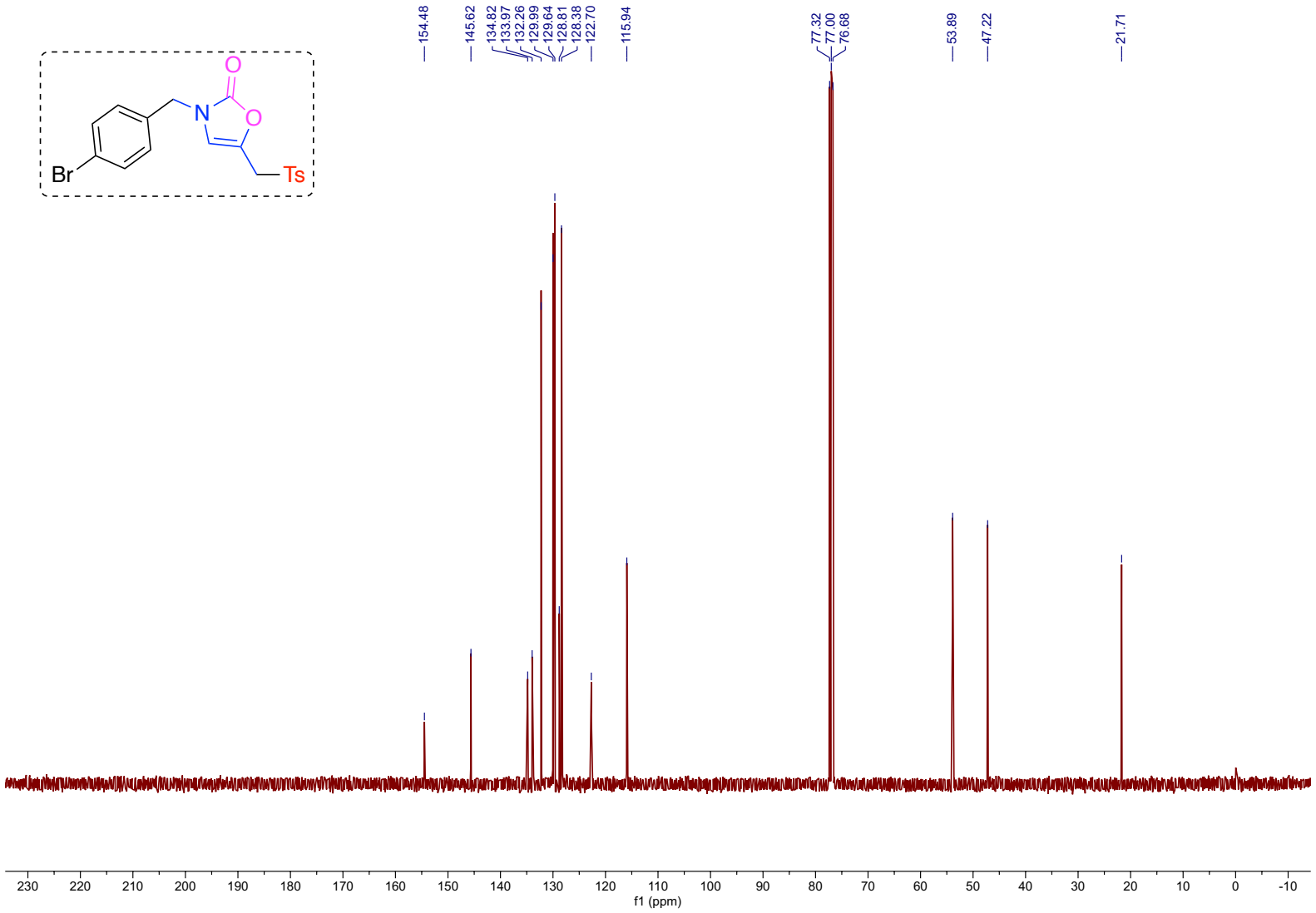
^{1}H (400 MHz) spectrum of compound 3j in $CDCl_3$



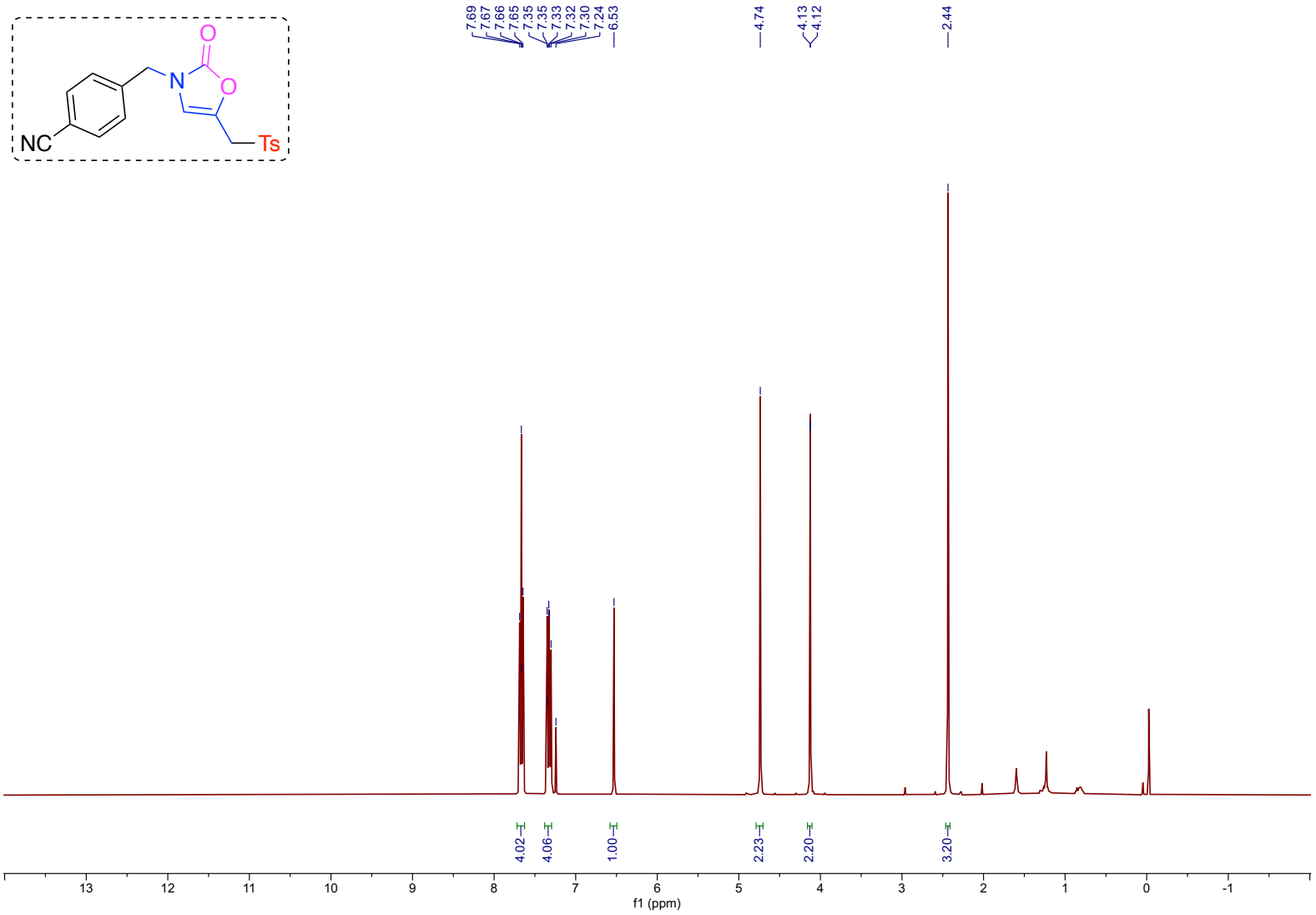
^{13}C (101 MHz) spectrum of compound 3j in $CDCl_3$



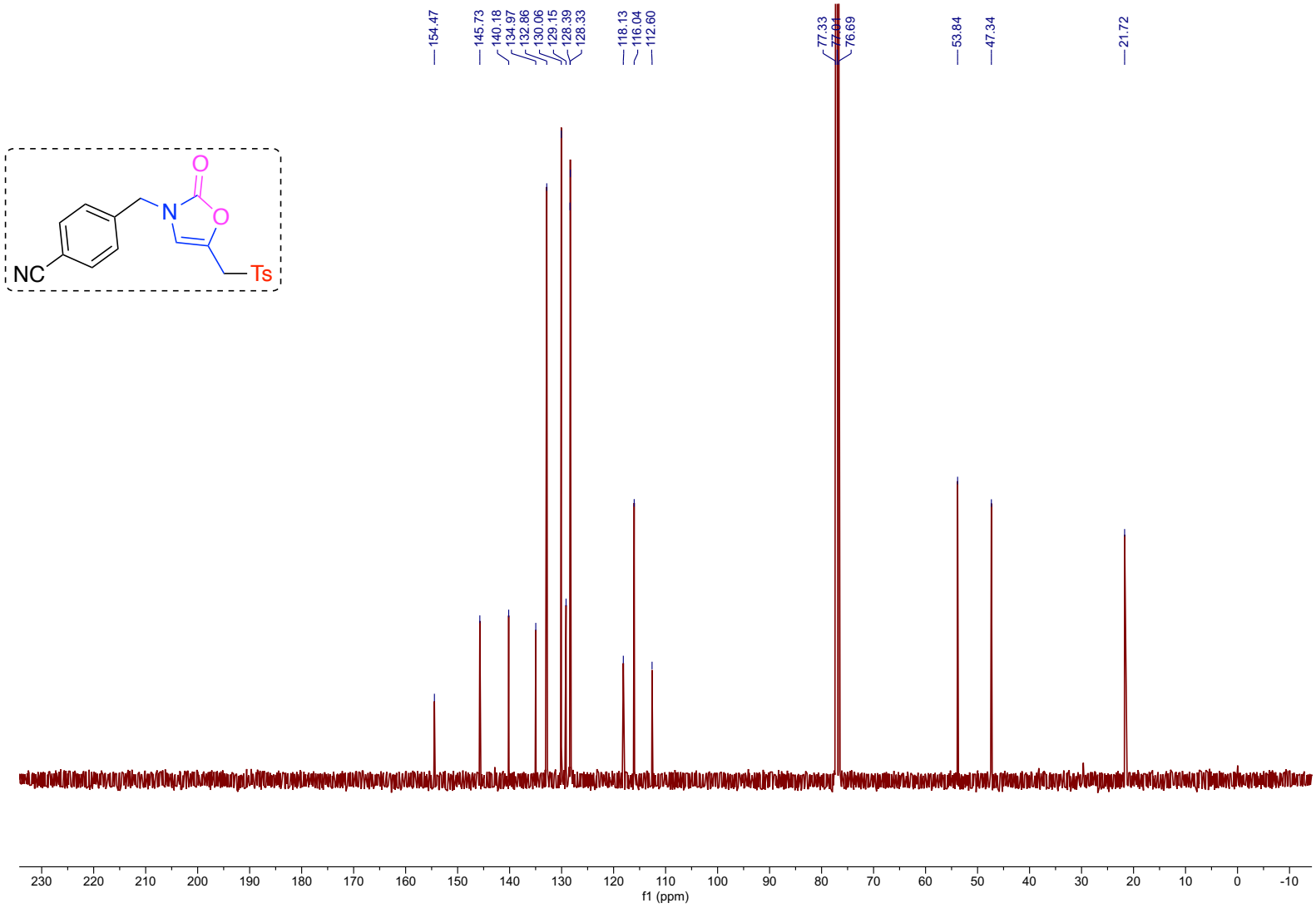
^{1}H (400 MHz) spectrum of compound 3k in $CDCl_3$



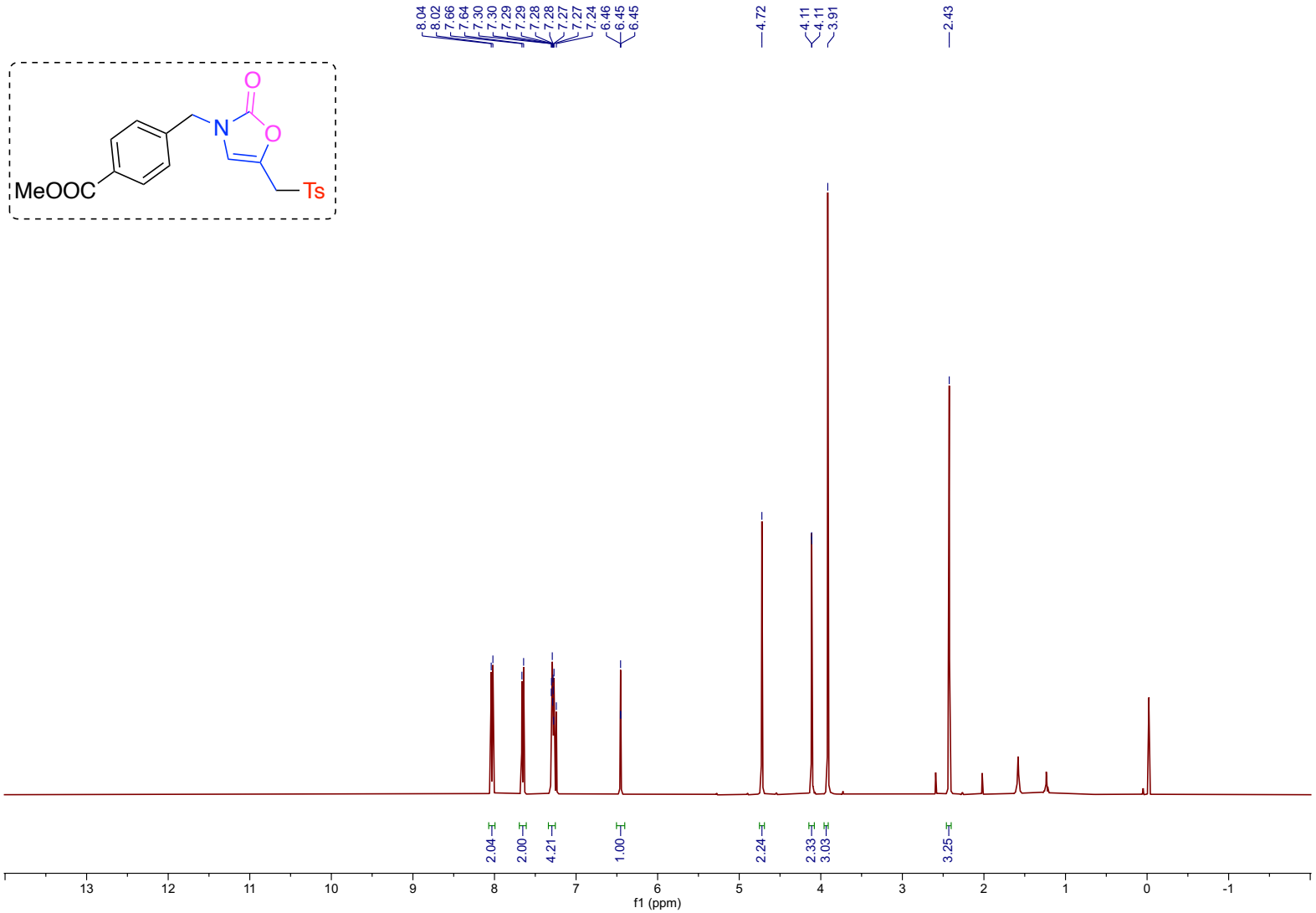
^{13}C (101 MHz) spectrum of compound 3k in $CDCl_3$



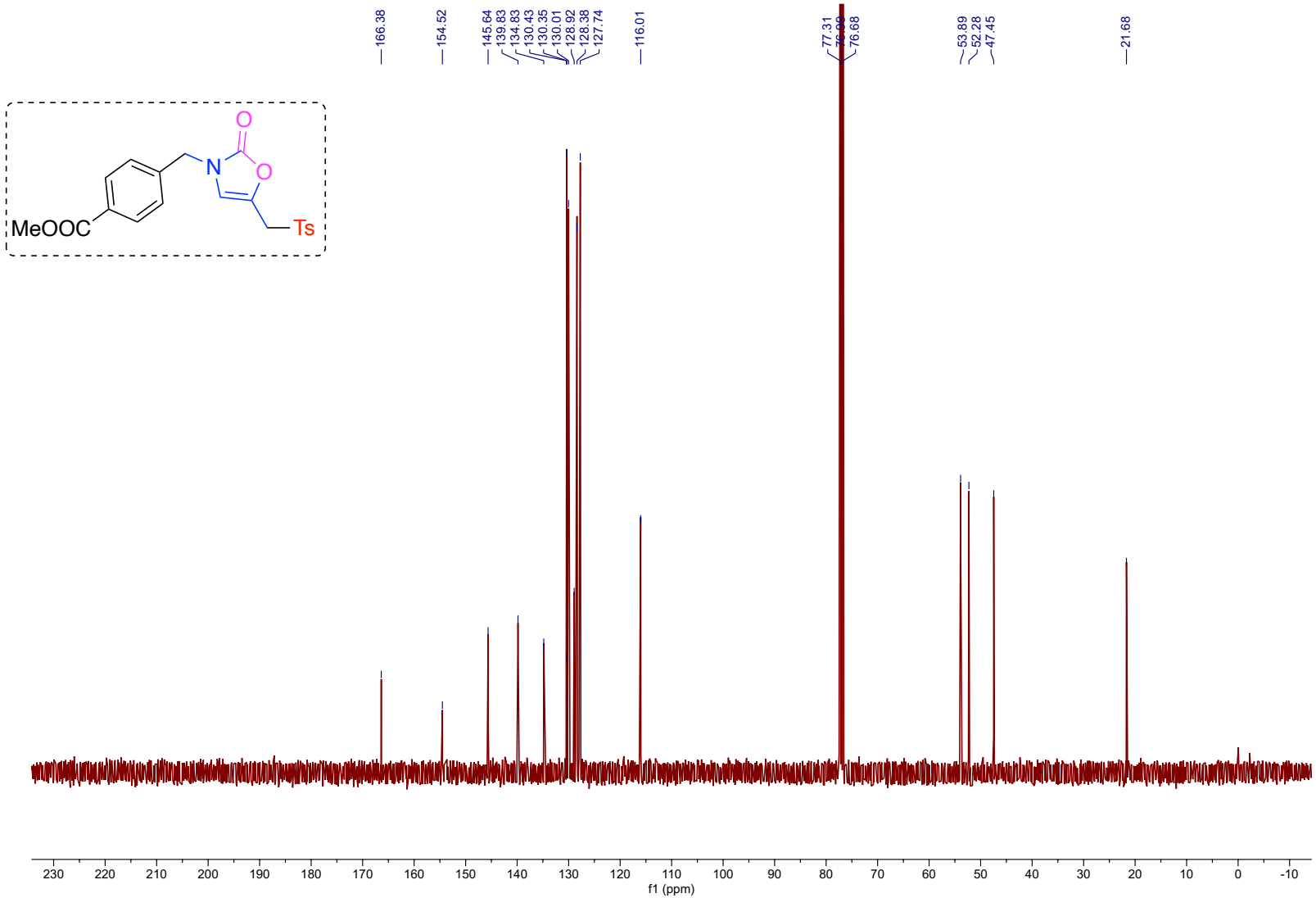
^{1}H (400 MHz) spectrum of compound 3l in $CDCl_3$



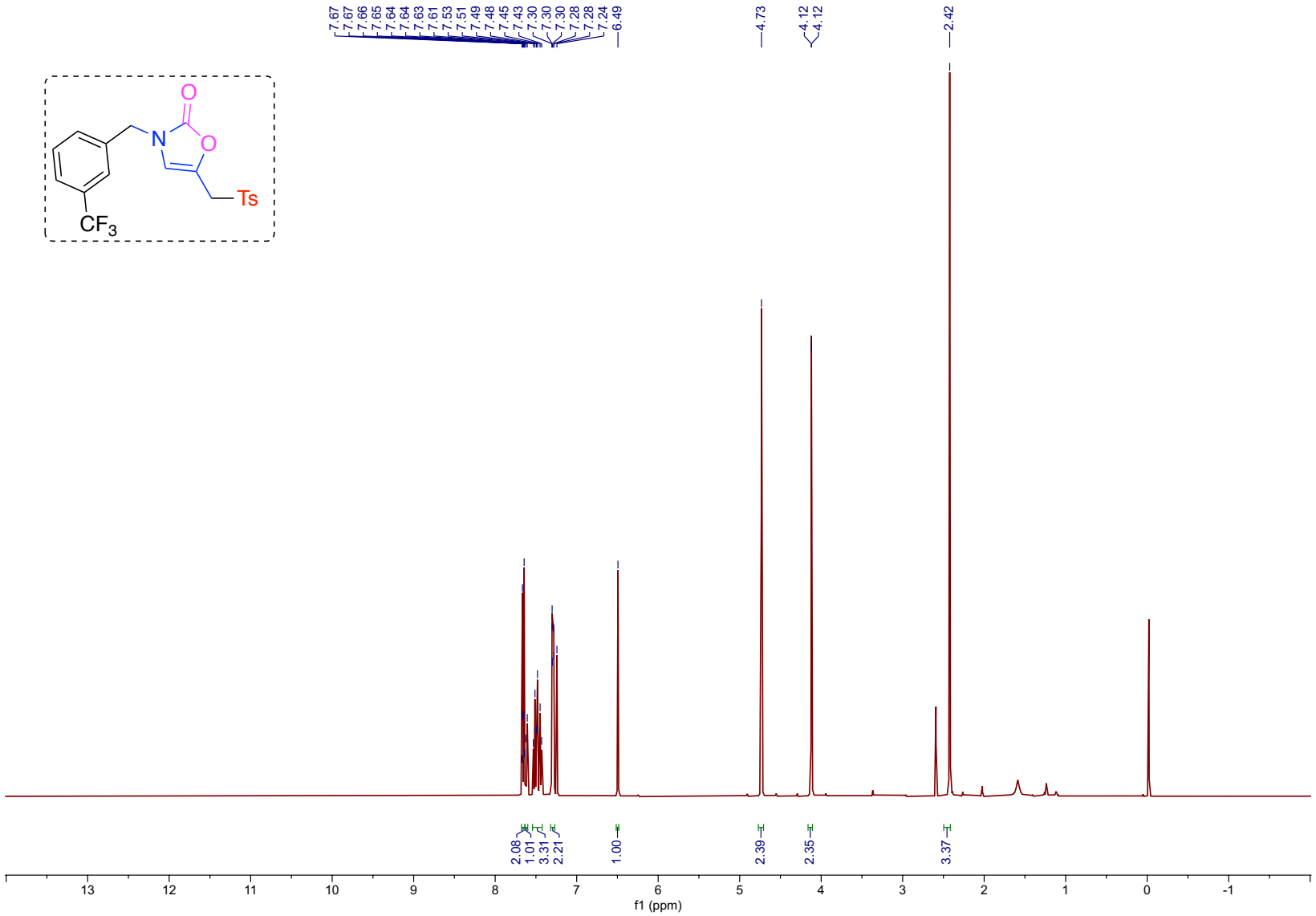
^{13}C (101 MHz) spectrum of compound 3l in $CDCl_3$



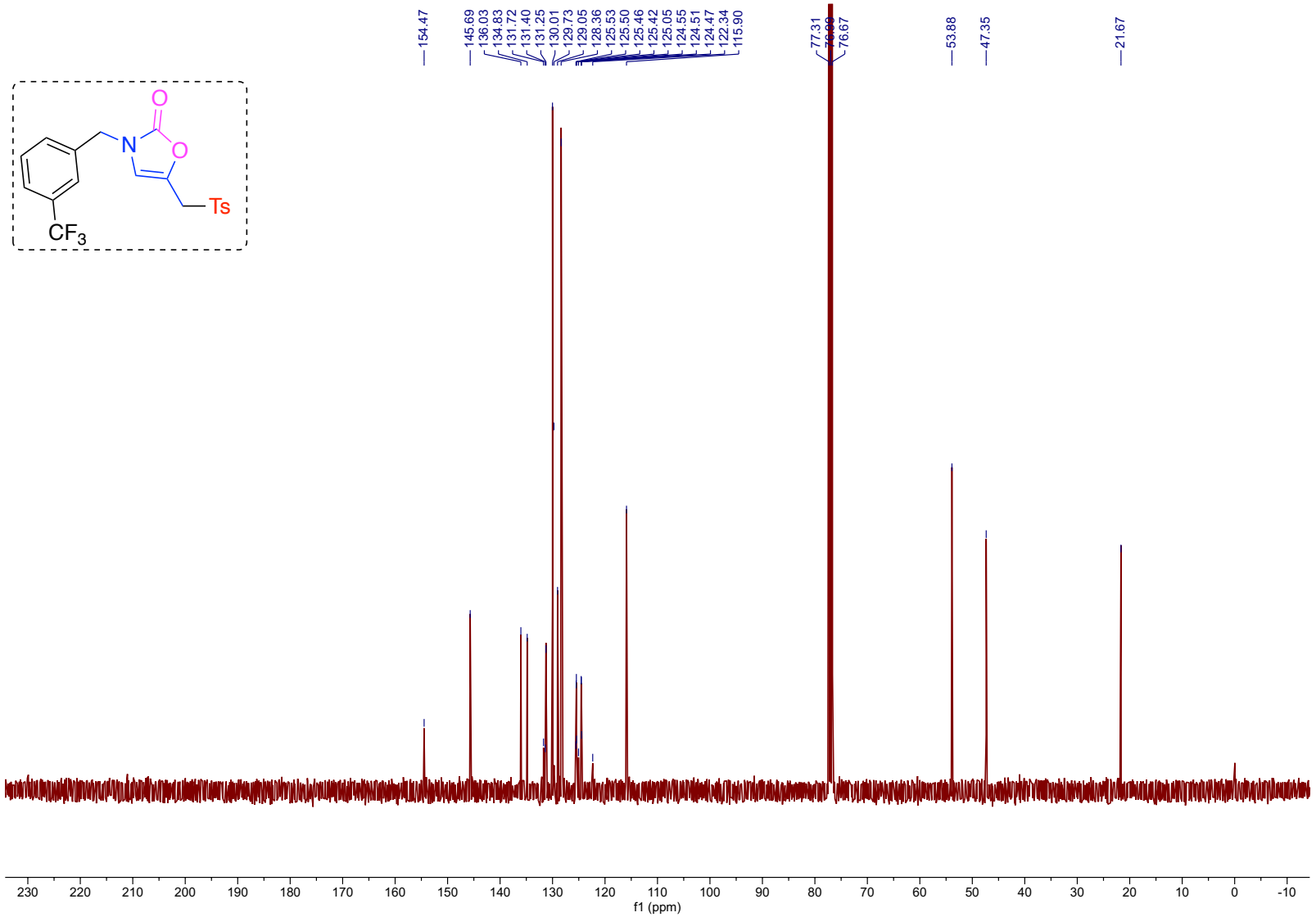
^{1}H (400 MHz) spectrum of compound 3m in $CDCl_3$



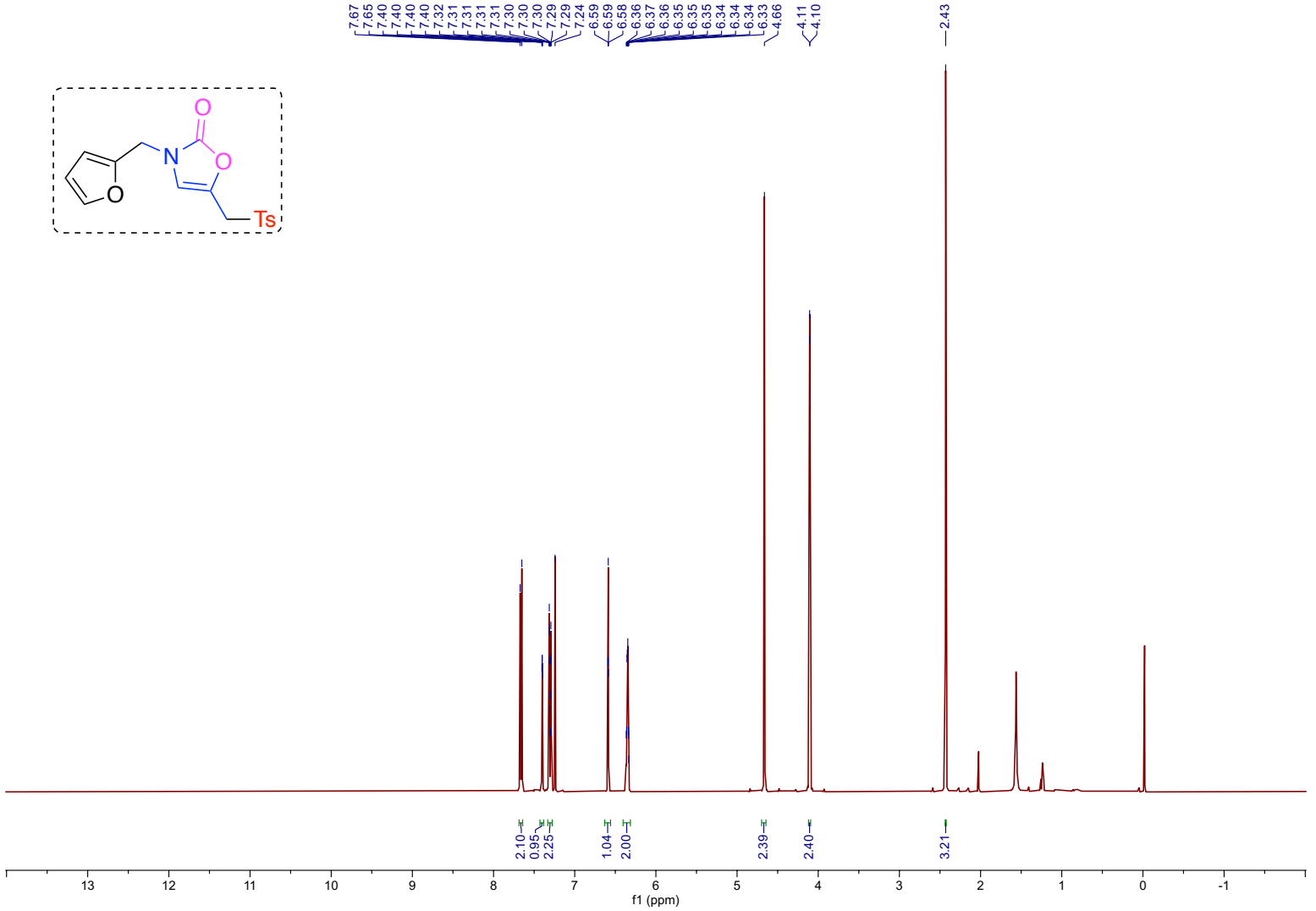
^{13}C (101 MHz) spectrum of compound 3m in $CDCl_3$



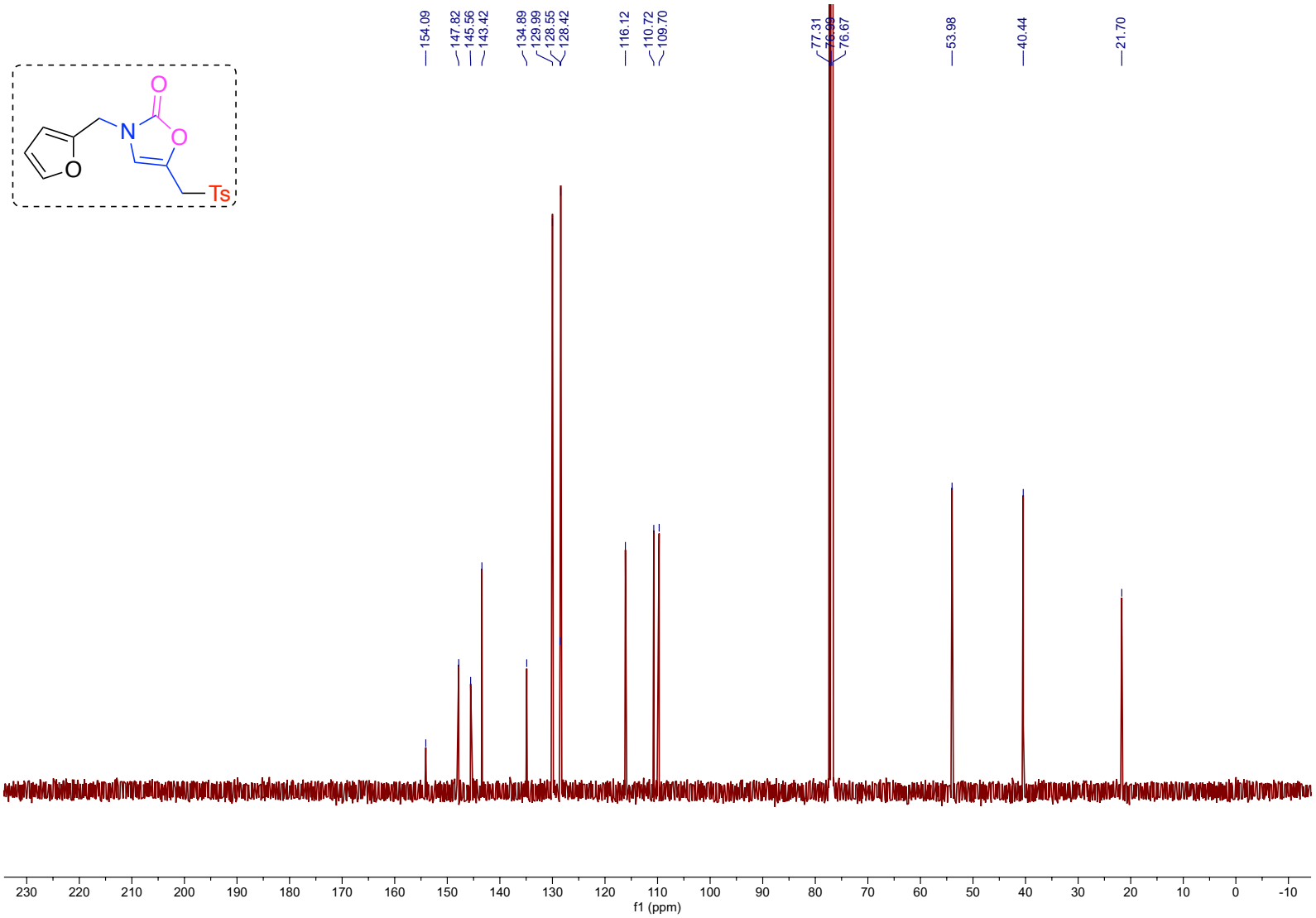
^{1}H (400 MHz) spectrum of compound 3n in $CDCl_3$



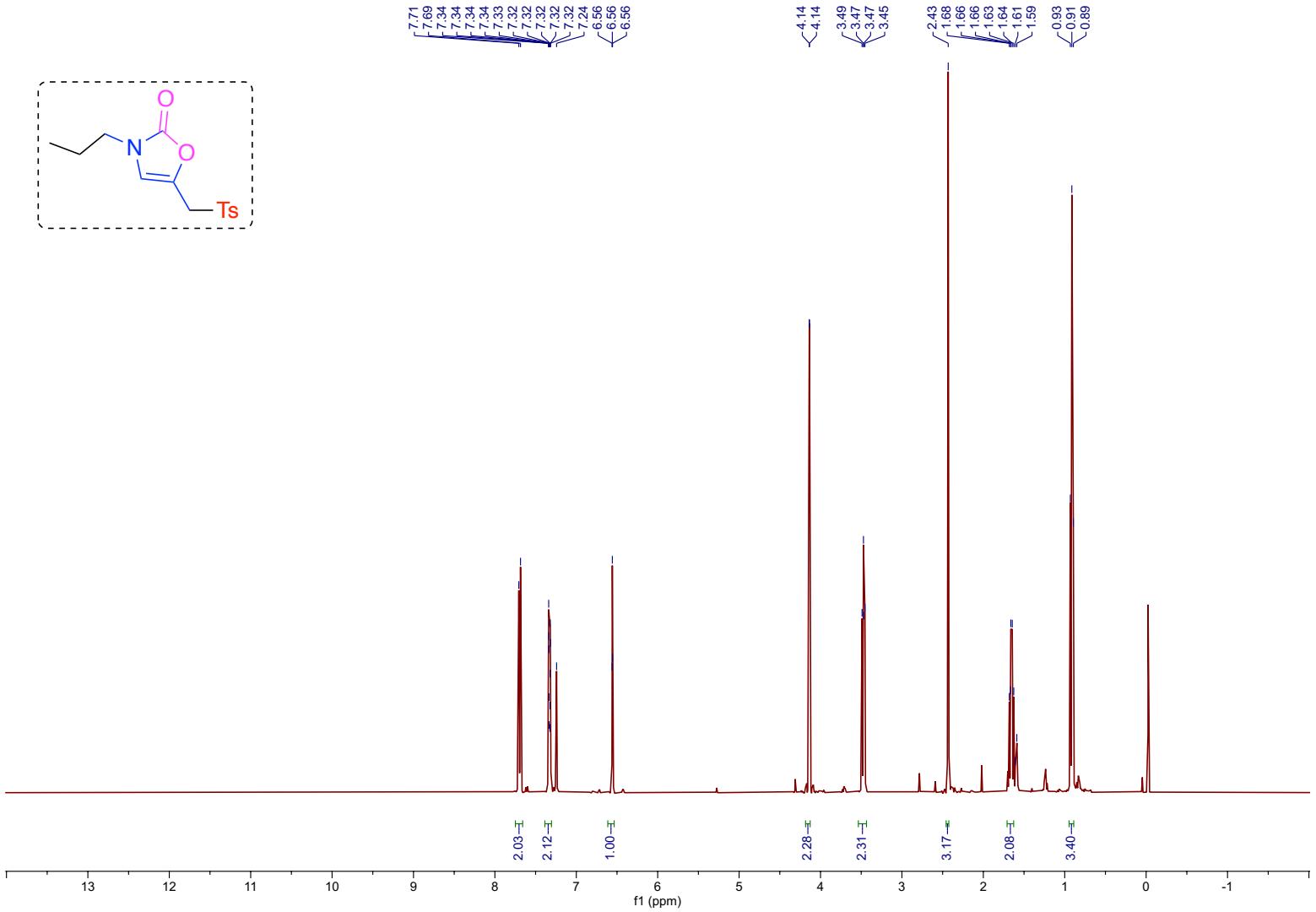
^{13}C (101 MHz) spectrum of compound 3n in $CDCl_3$



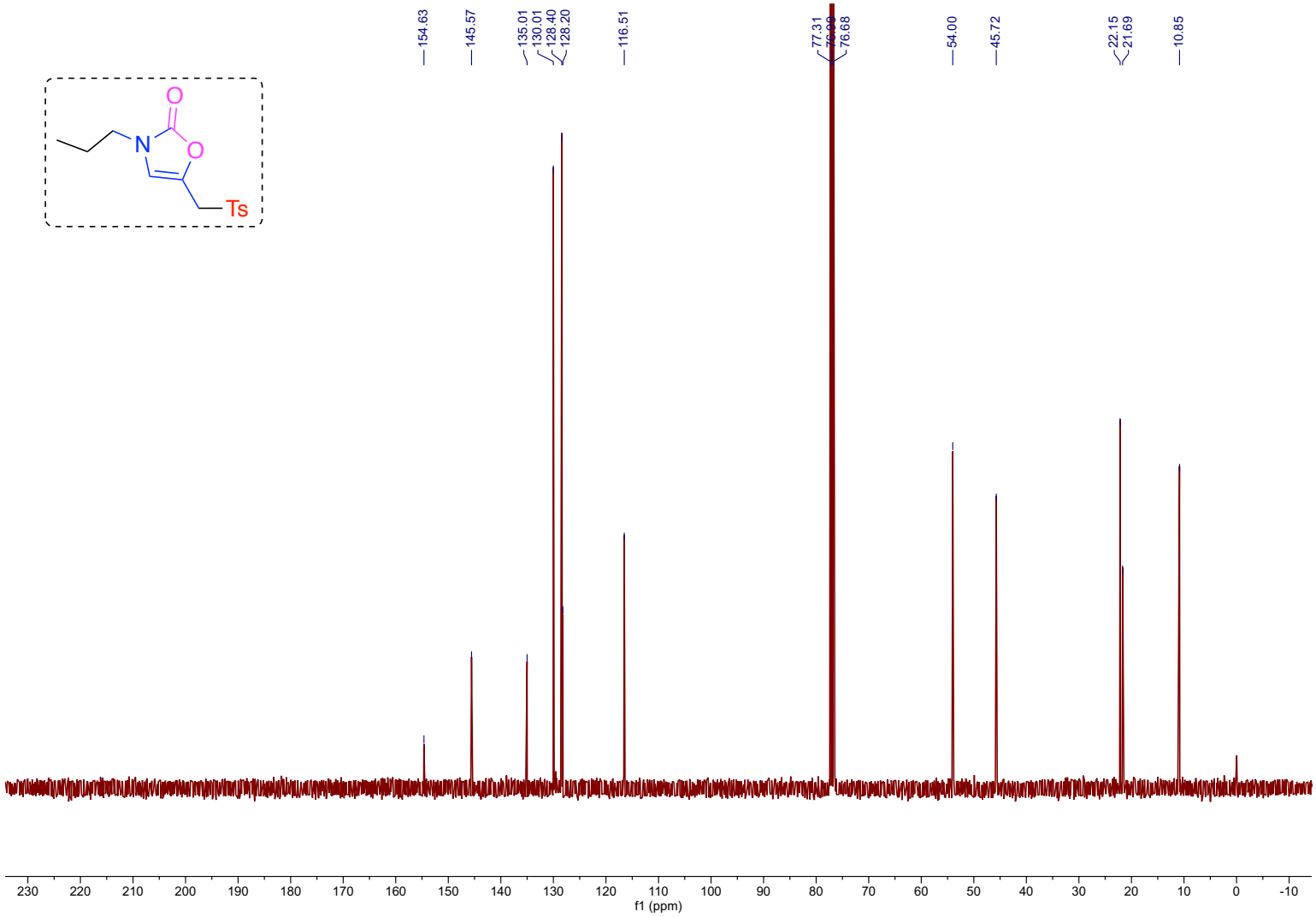
^{1}H (400 MHz) spectrum of compound 3o in $CDCl_3$



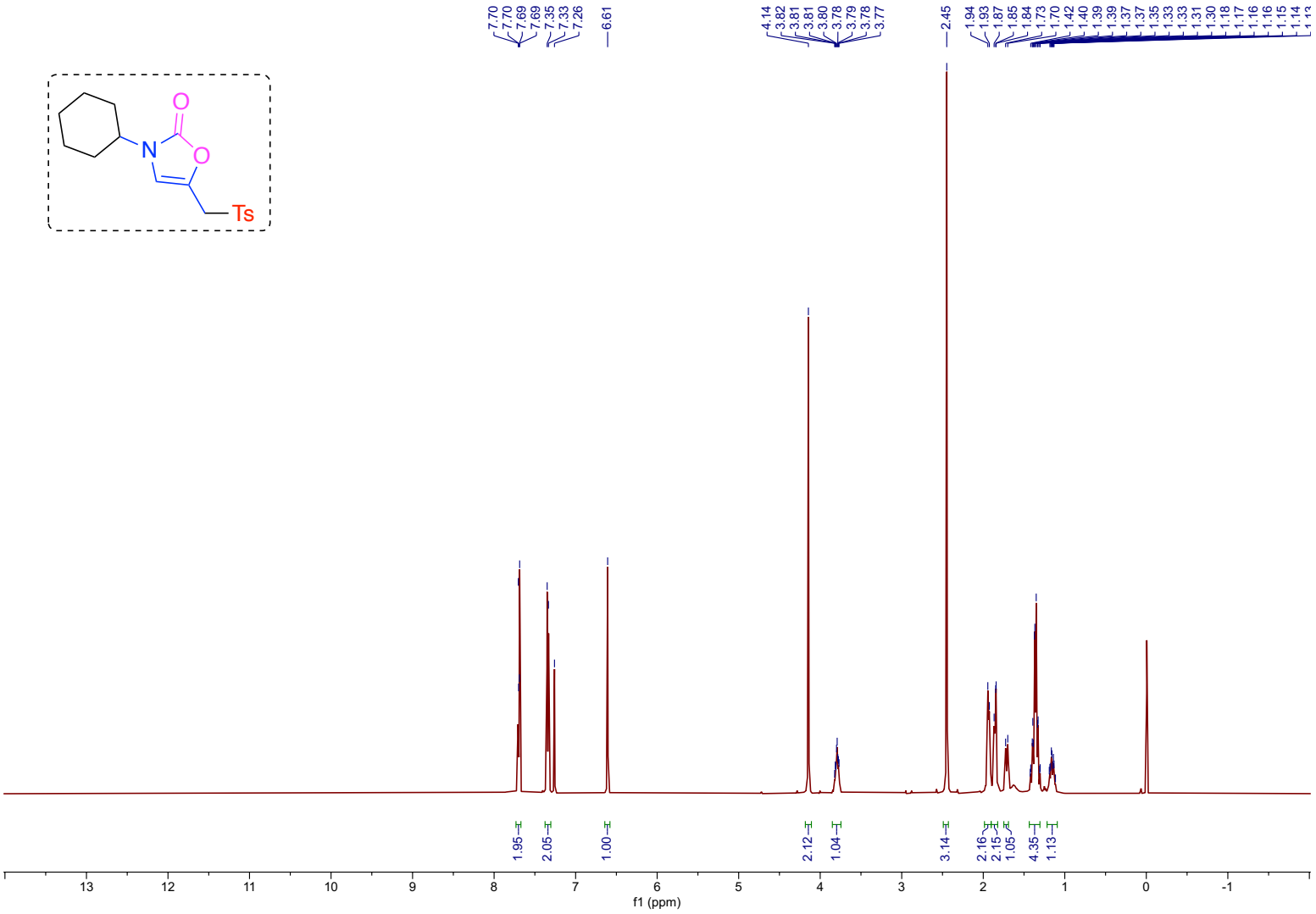
^{13}C (101 MHz) spectrum of compound 3o in $CDCl_3$



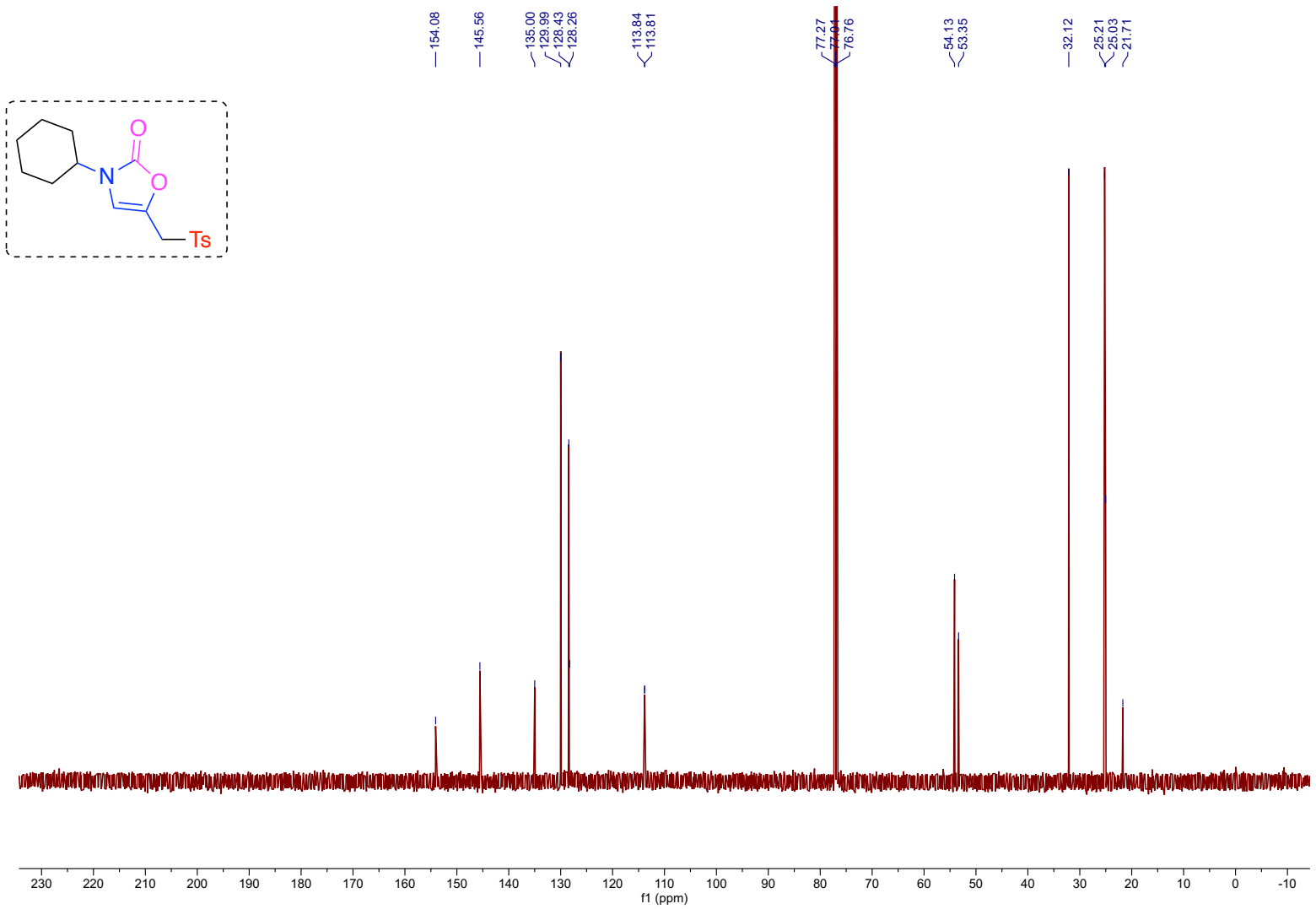
^{1}H (400 MHz) spectrum of compound 3p in $CDCl_3$



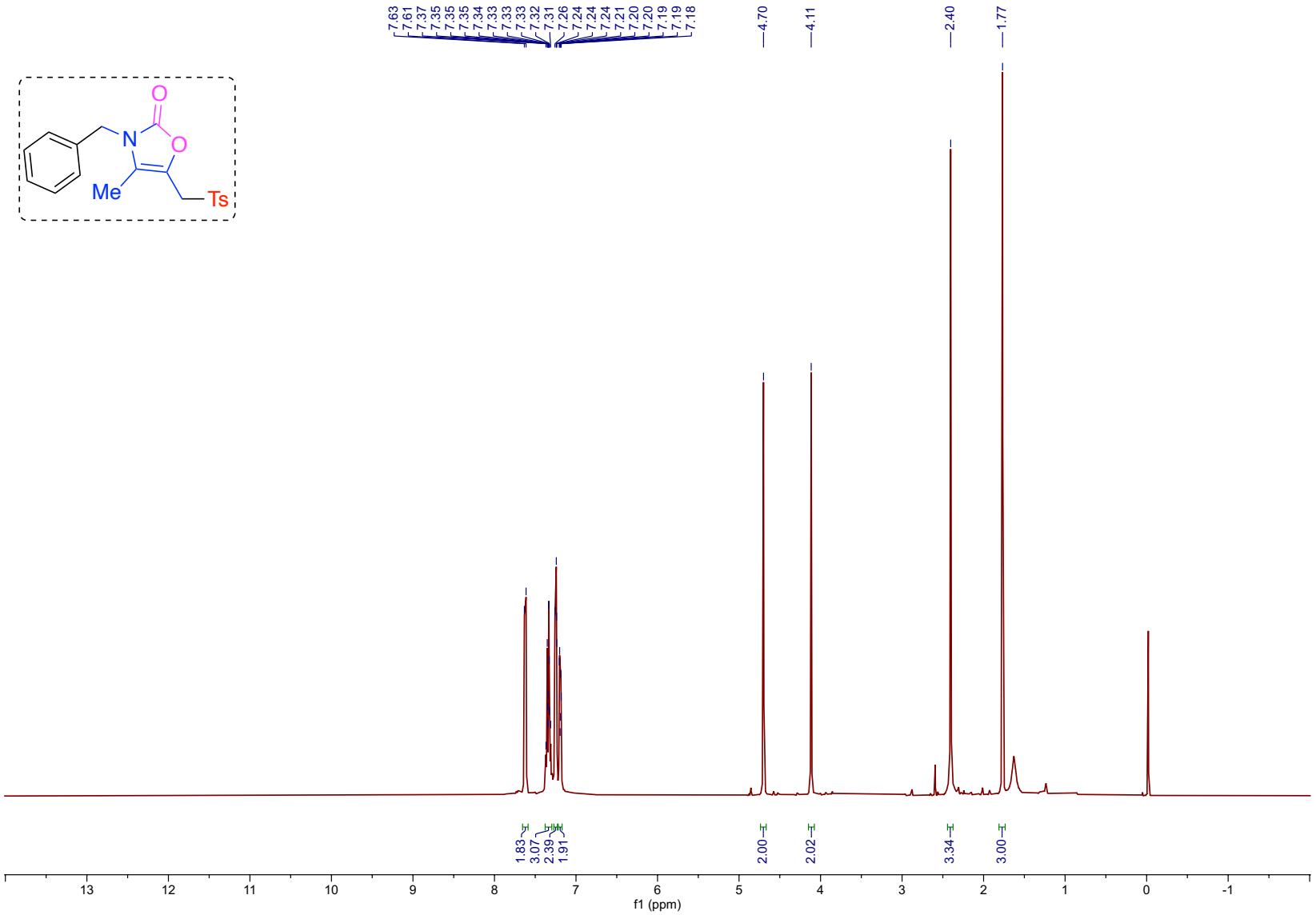
^{13}C (101 MHz) spectrum of compound 3p in $CDCl_3$



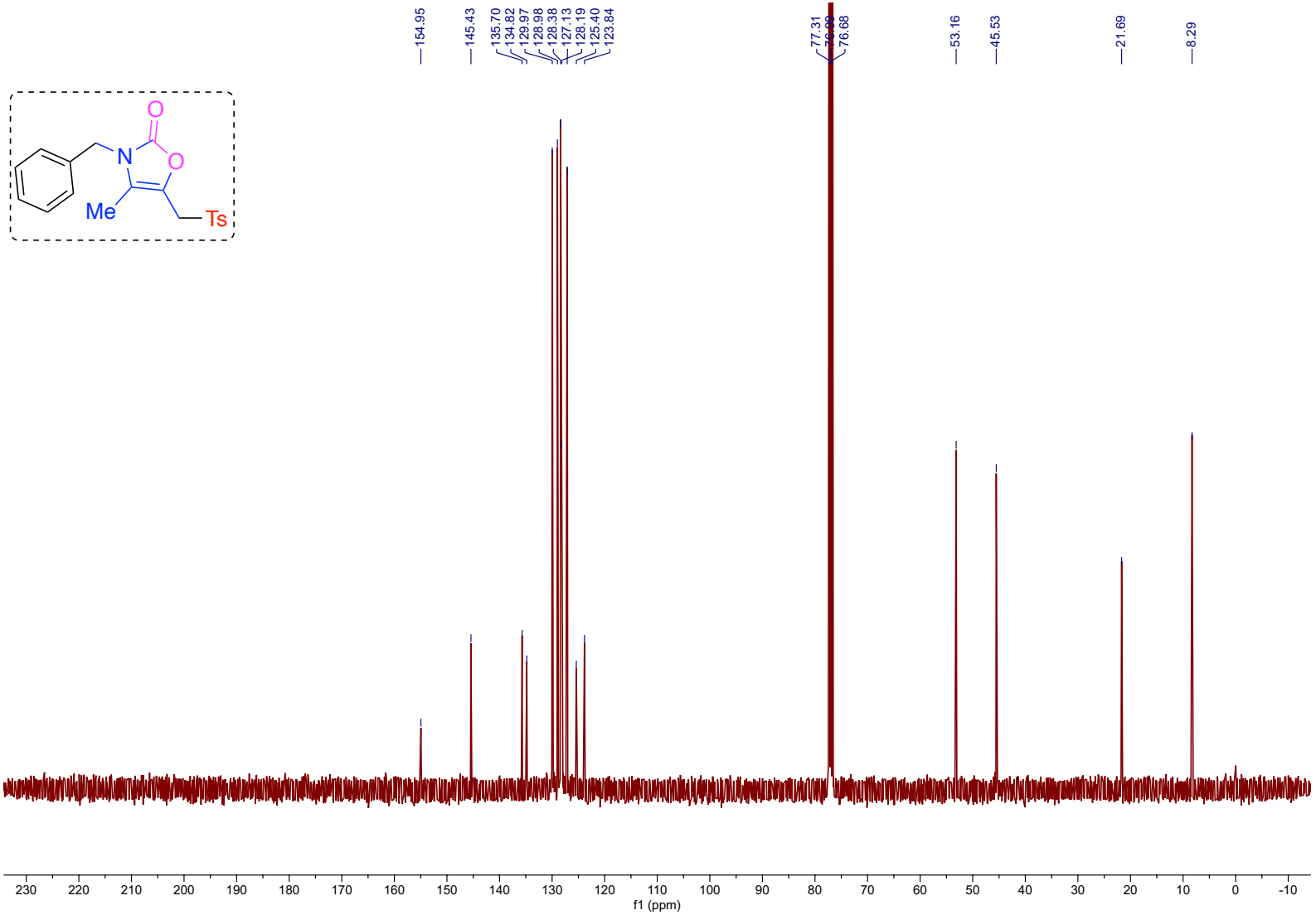
^{1}H (500 MHz) spectrum of compound 3q in $CDCl_3$



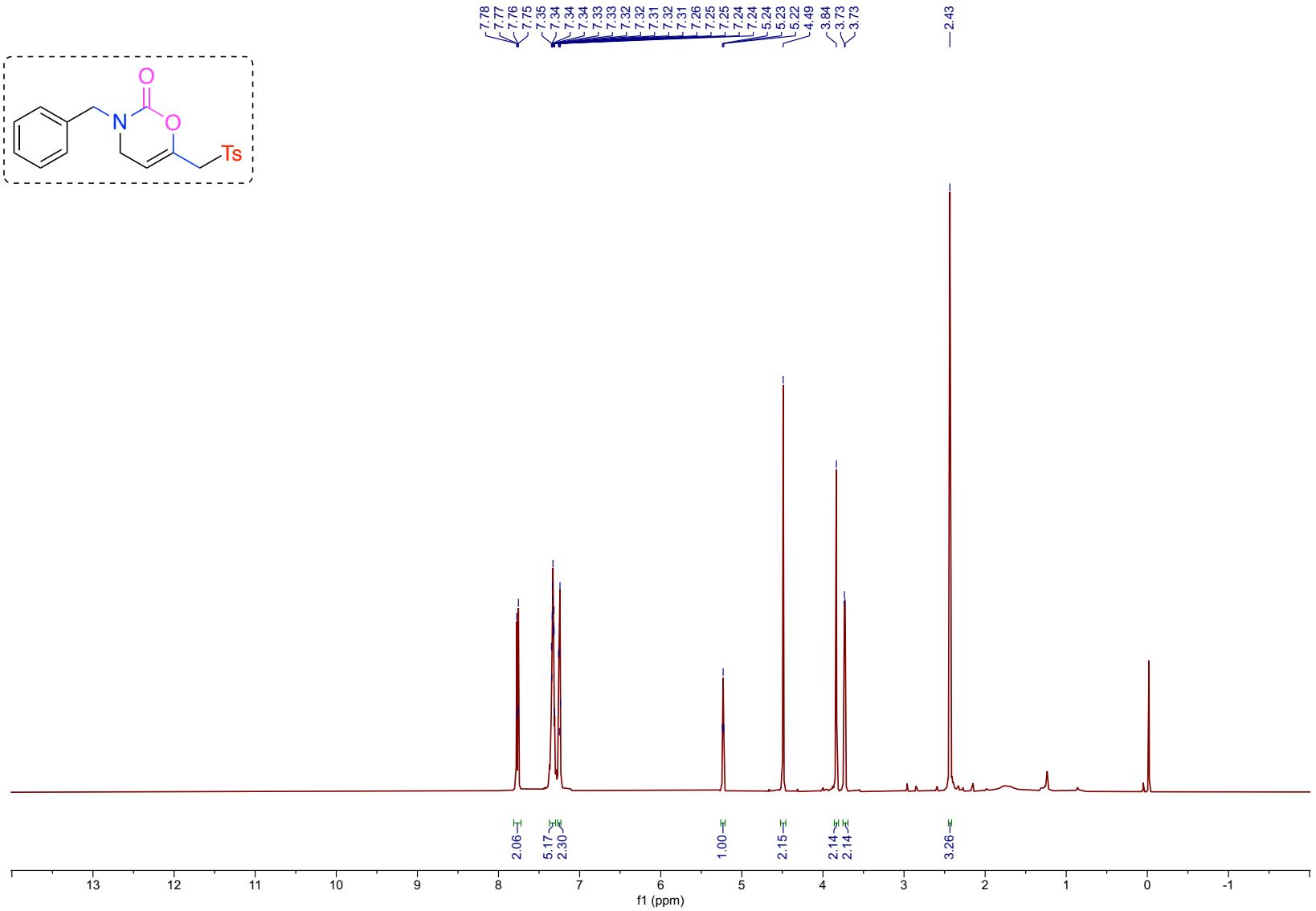
^{13}C (126 MHz) spectrum of compound 3q in $CDCl_3$



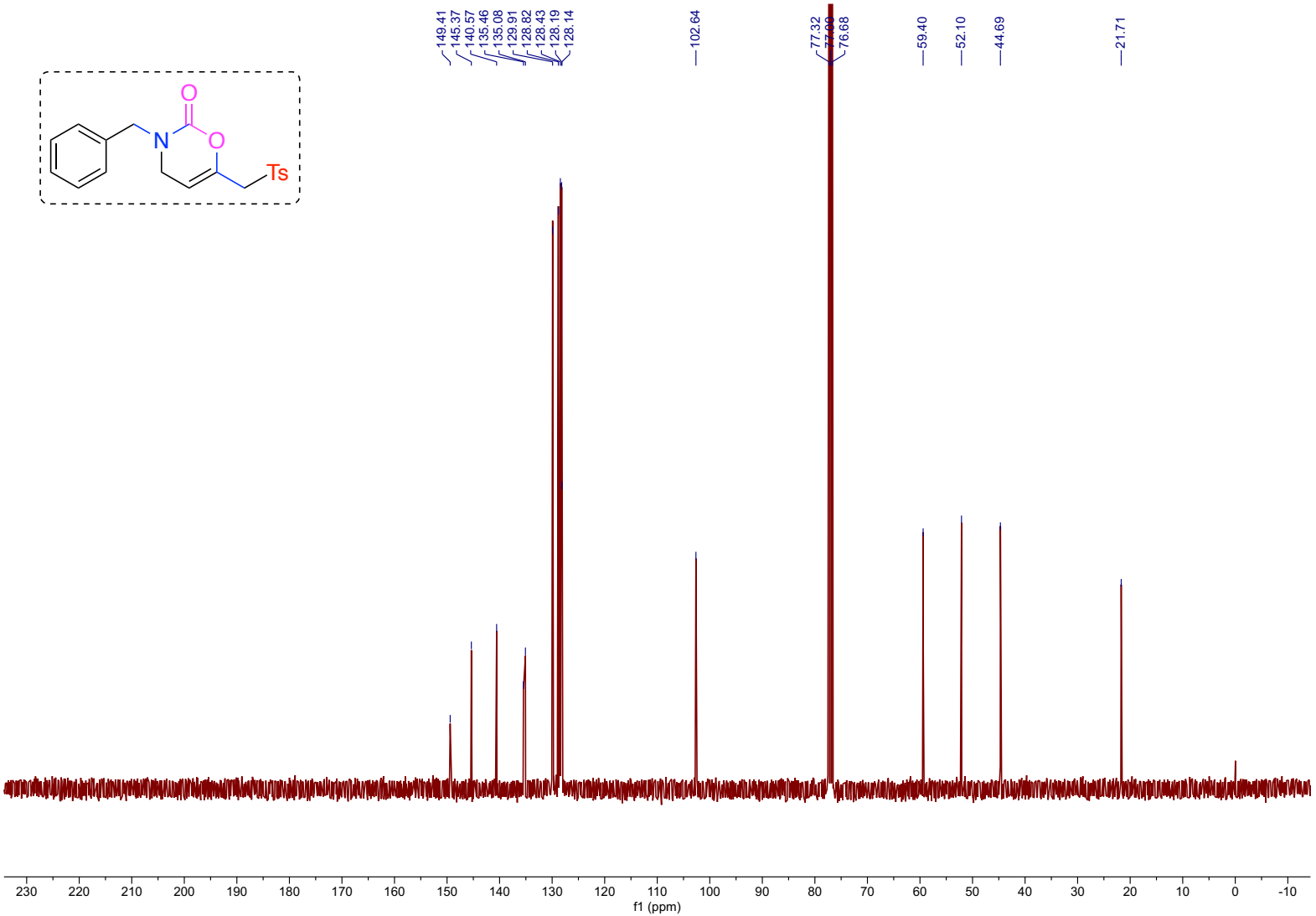
^{1}H (400 MHz) spectrum of compound 3u in $CDCl_3$



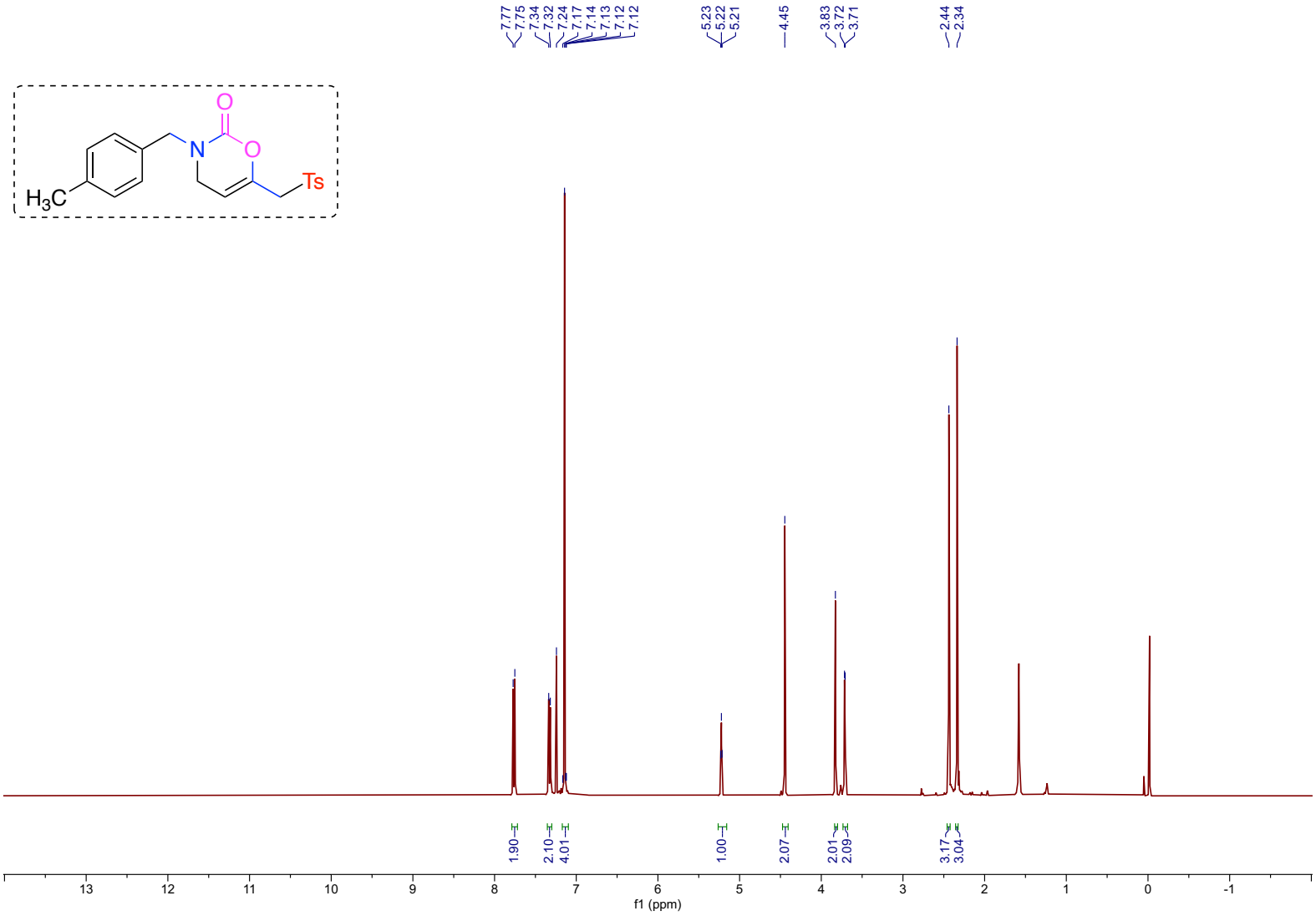
^{13}C (101 MHz) spectra of compound 3u in $CDCl_3$



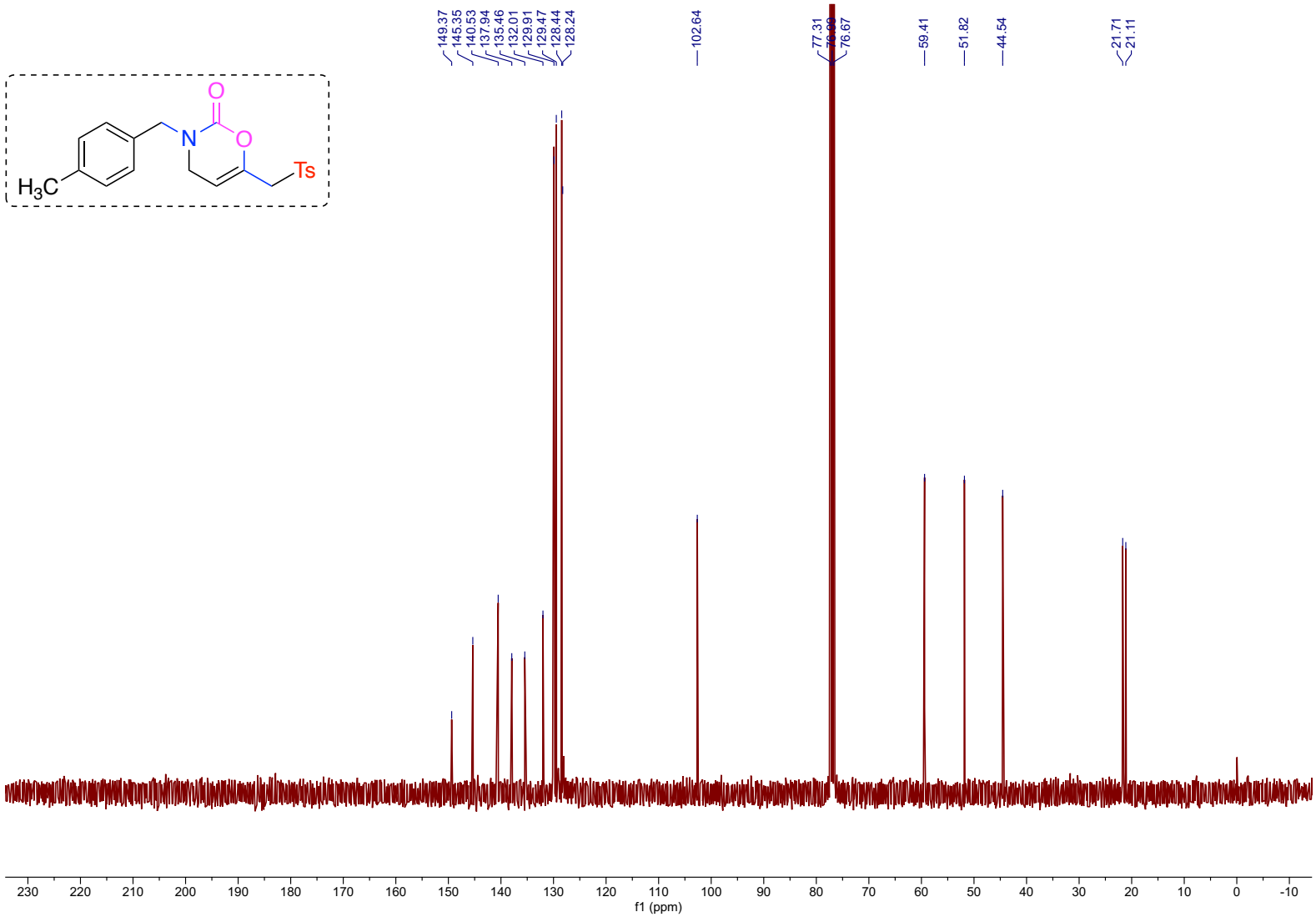
^{1}H (400 MHz) spectrum of compound 4a in $CDCl_3$



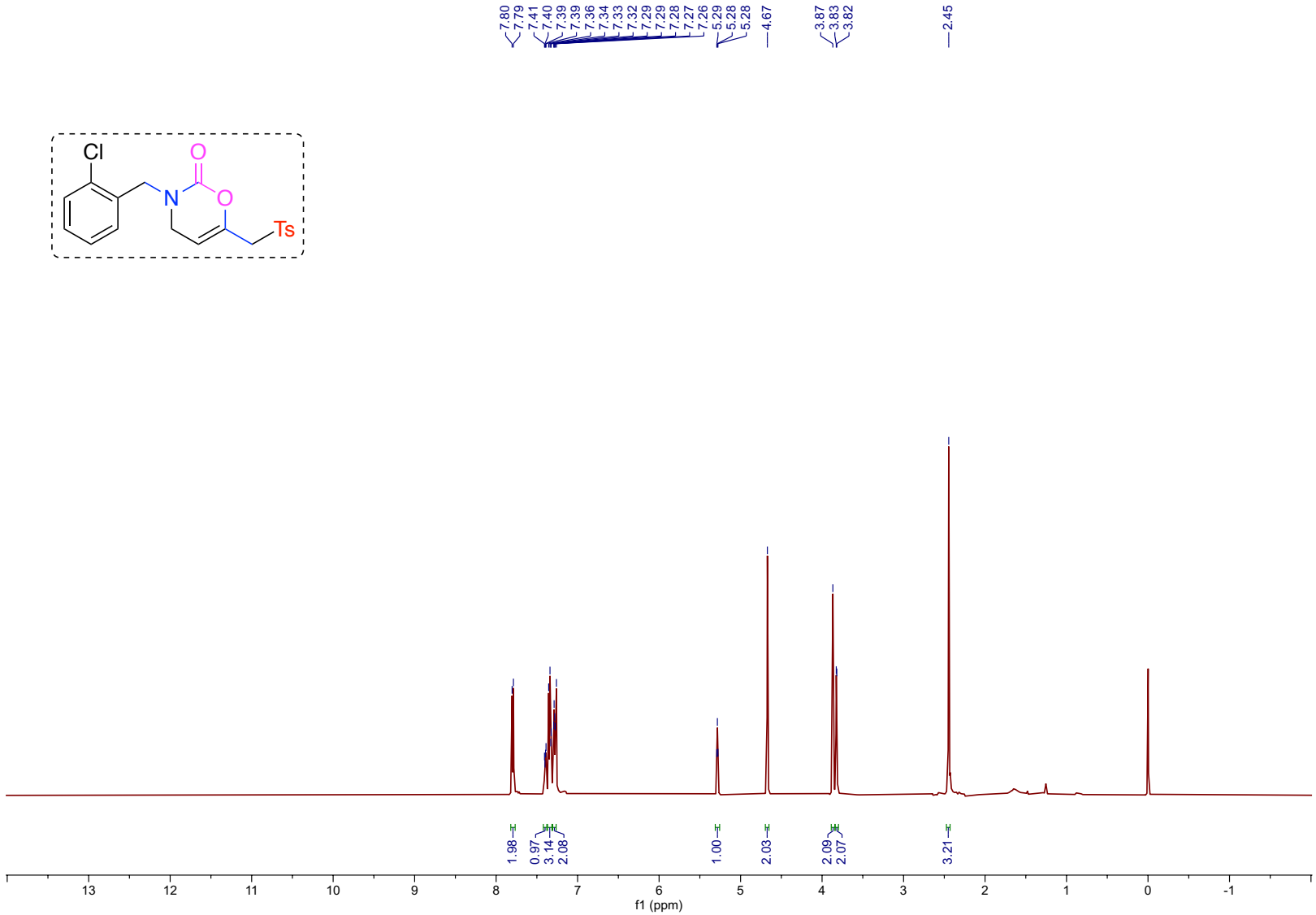
^{13}C (101 MHz) spectrum of compound 4a in $CDCl_3$



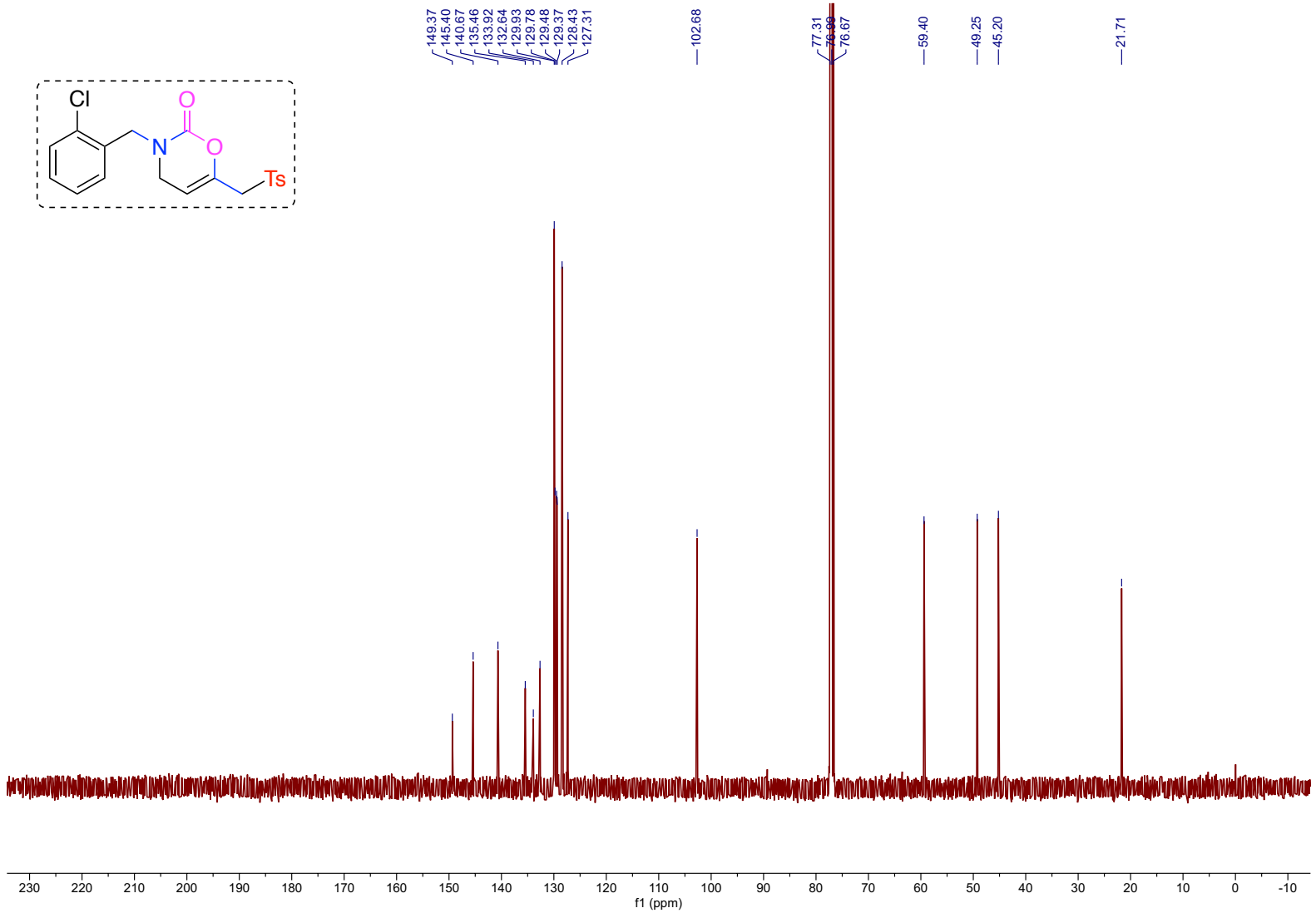
^{1}H (400 MHz) spectrum of compound 4b in $CDCl_3$



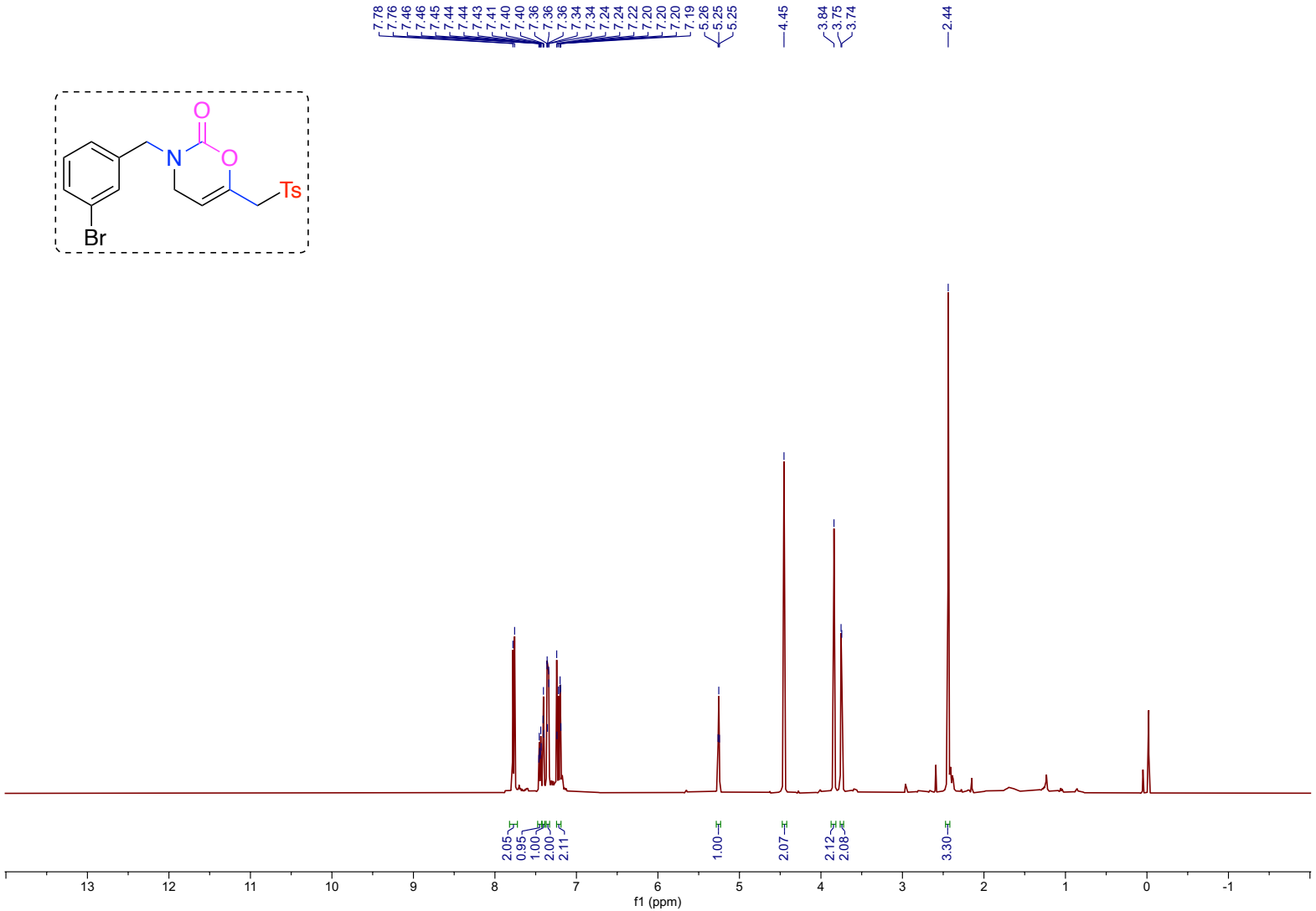
^{13}C (101 MHz) spectrum of compound 4b in $CDCl_3$



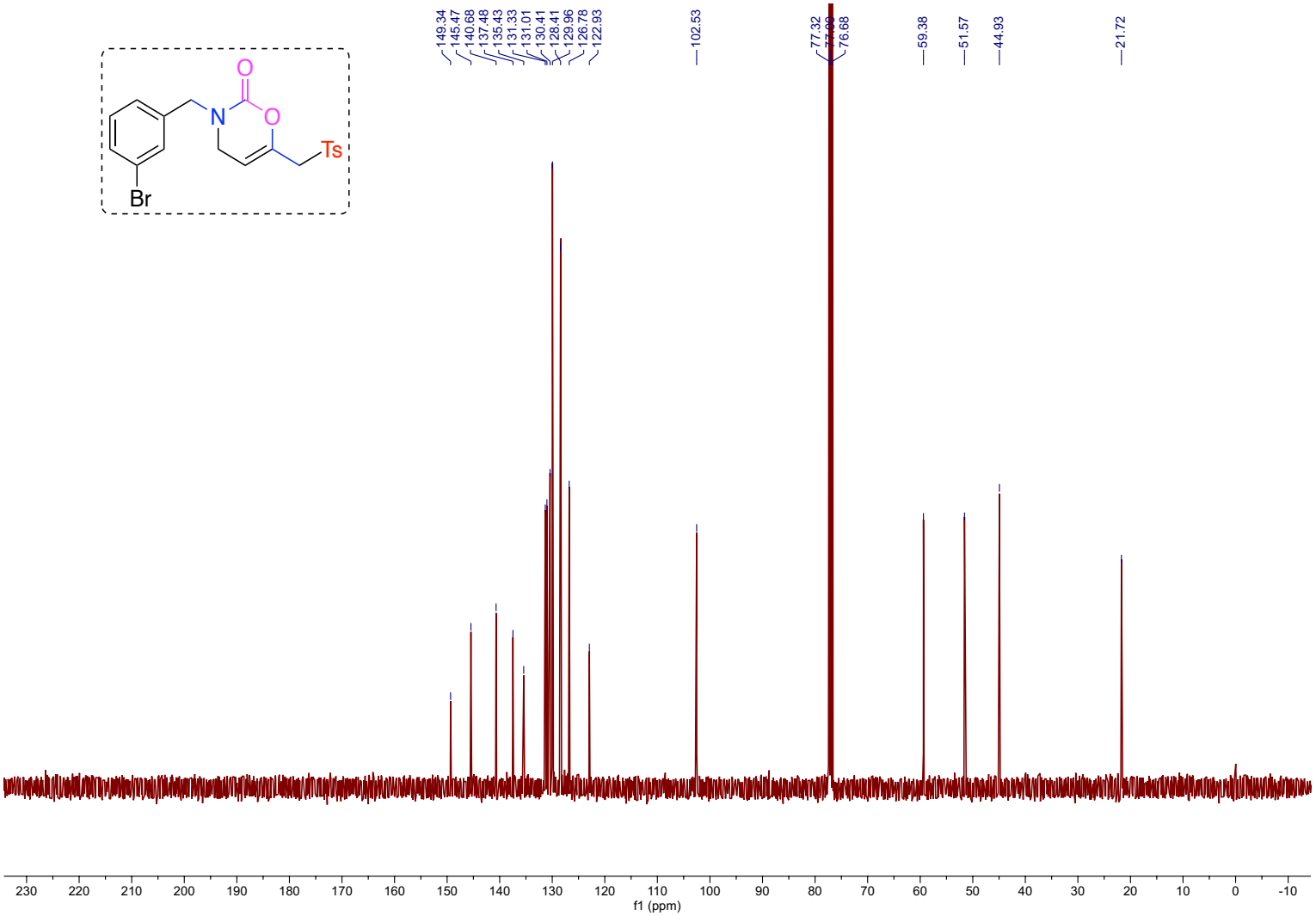
^{1}H (500 MHz) spectrum of compound 4c in $CDCl_3$



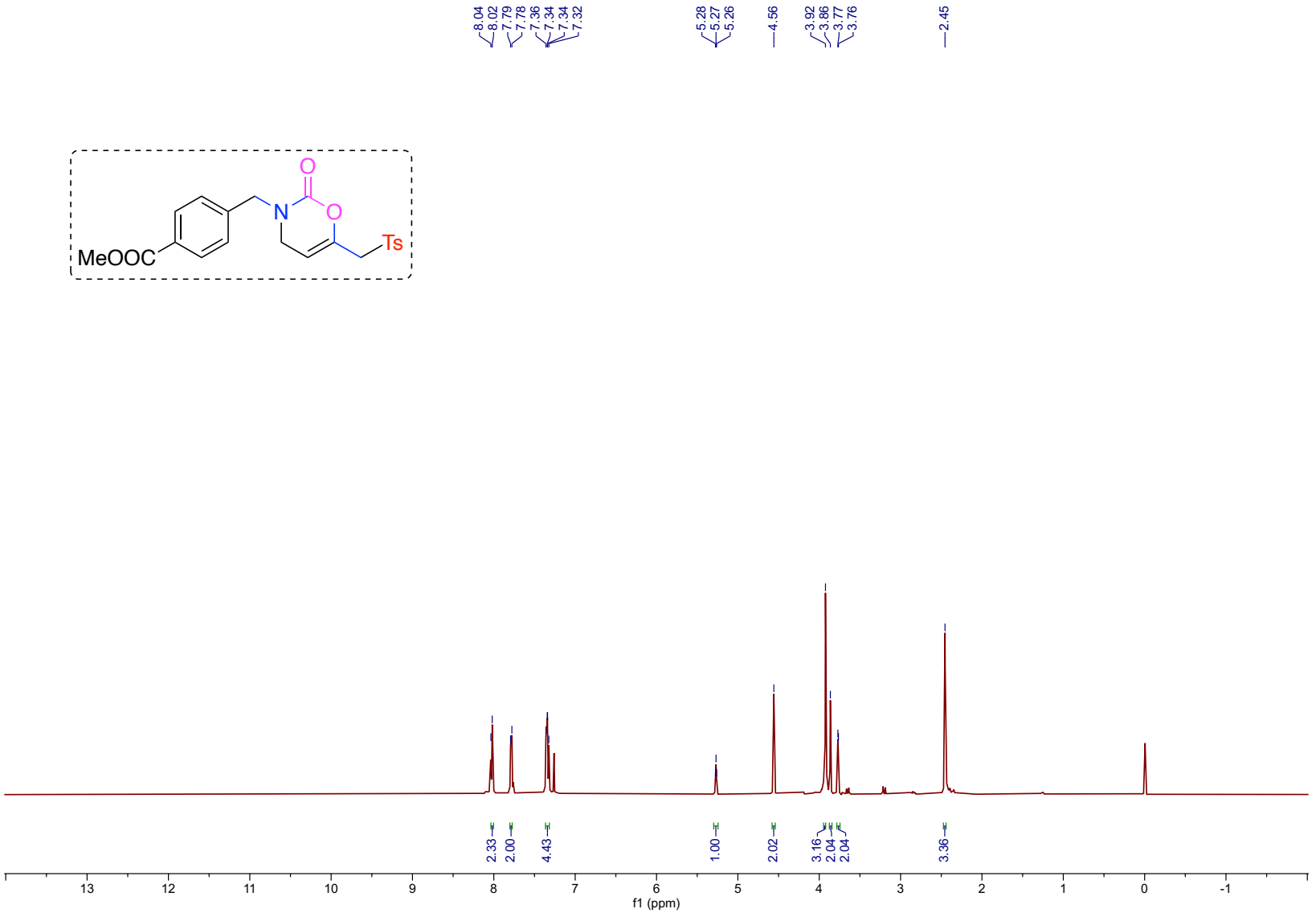
^{13}C (101 MHz) spectrum of compound 4c in $CDCl_3$



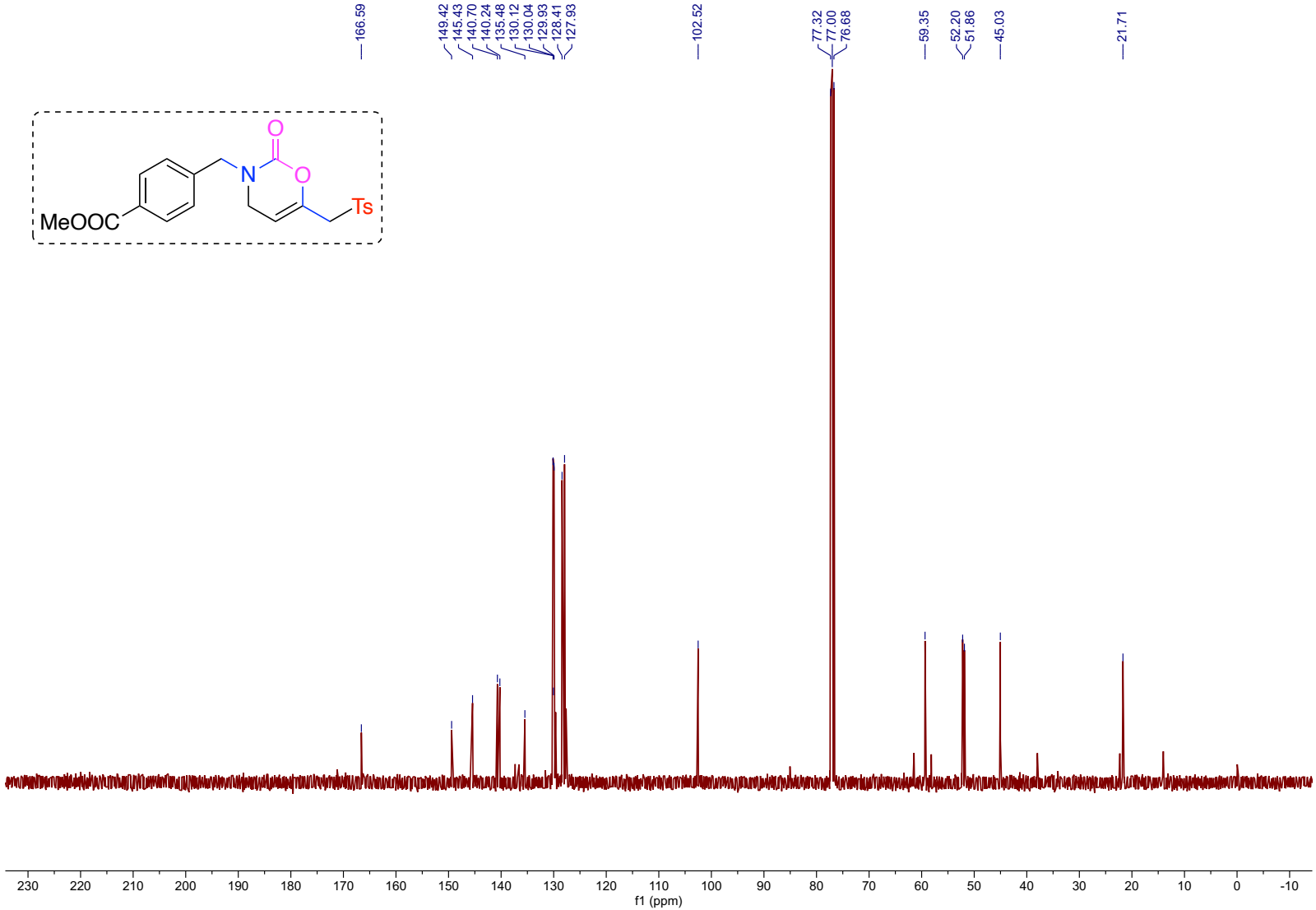
^{1}H (400 MHz) spectrum of compound 4d in $CDCl_3$



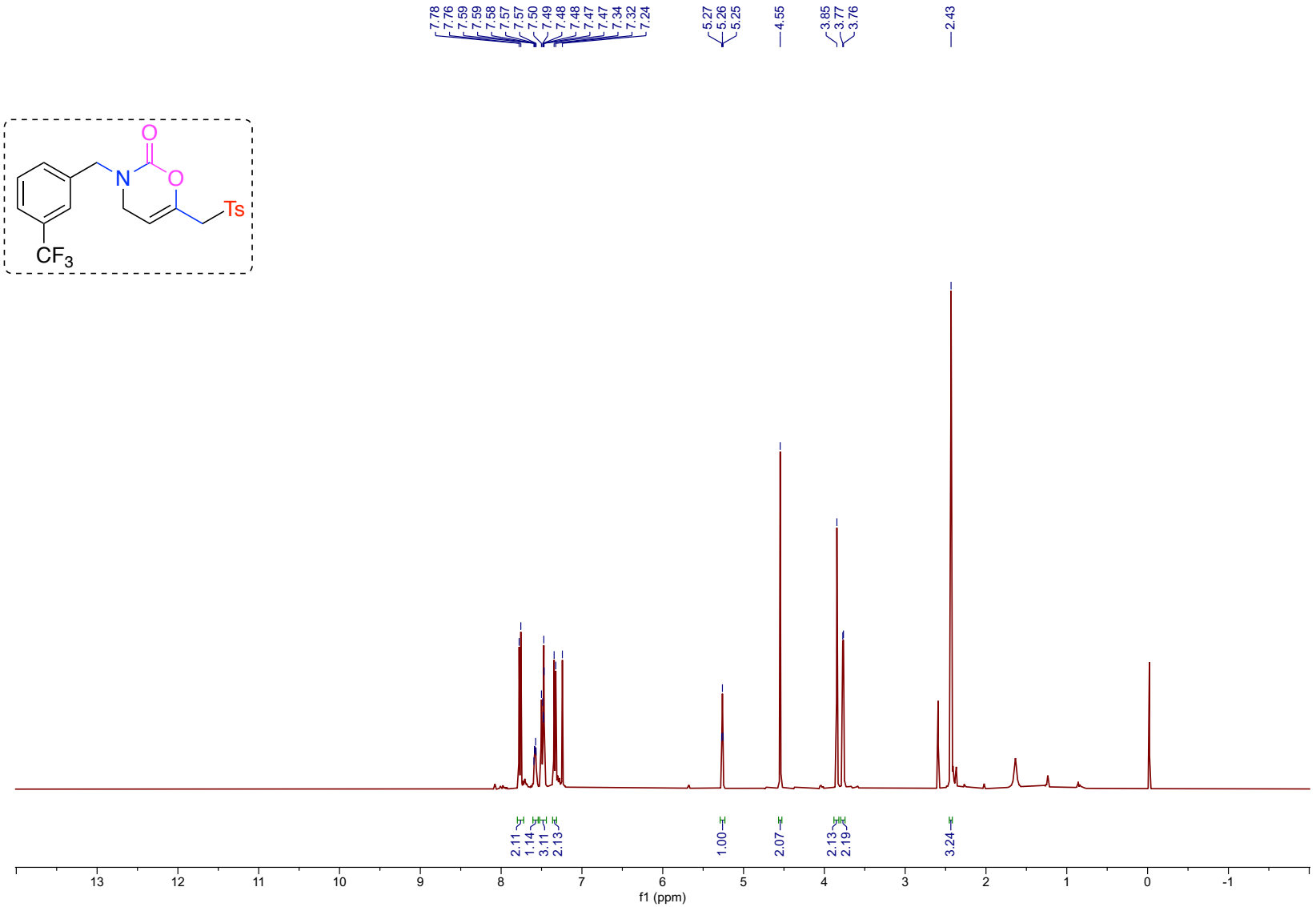
^{13}C (101 MHz) spectrum of compound 4d in $CDCl_3$



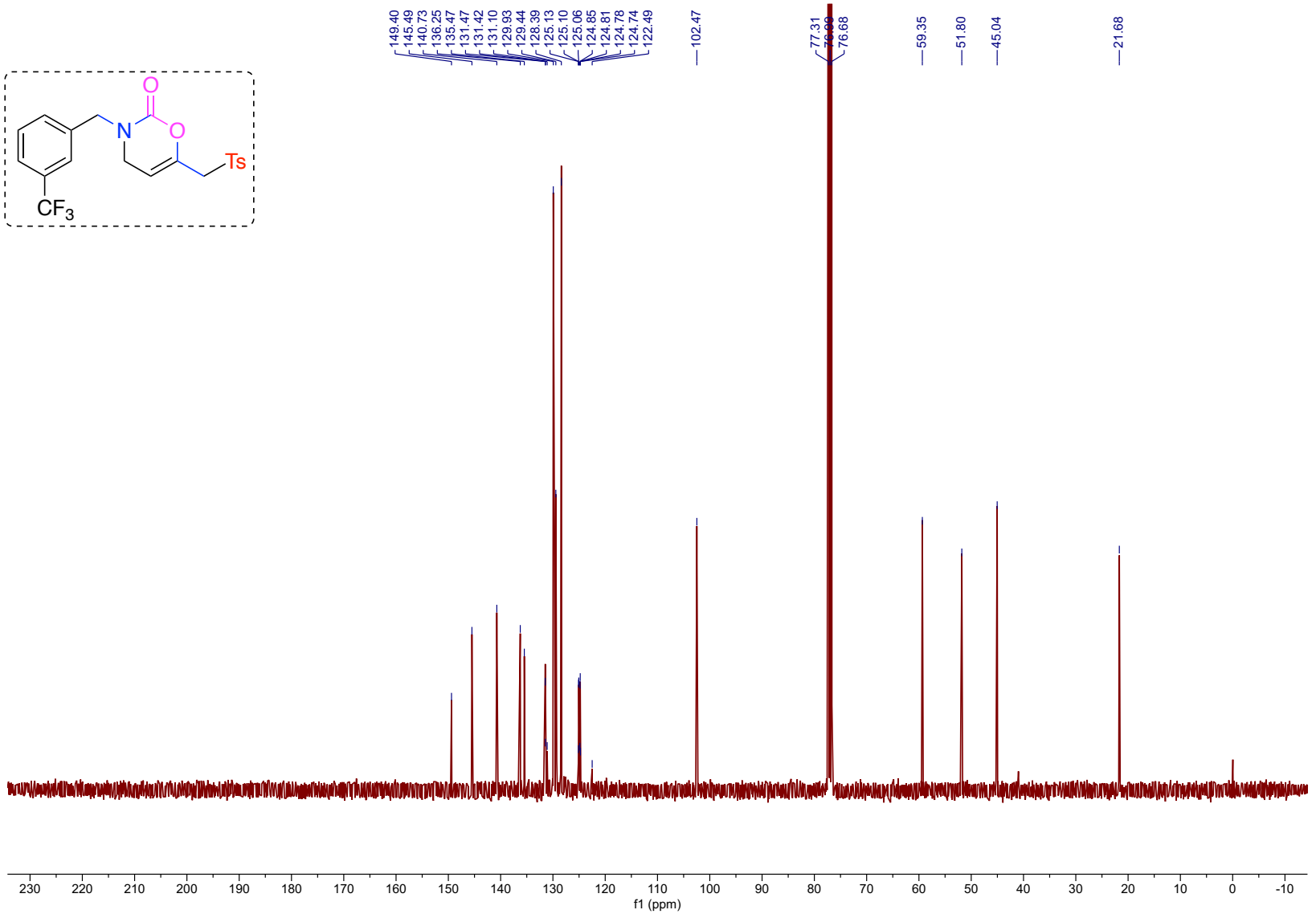
^{1}H (500 MHz) spectrum of compound 4e in $CDCl_3$



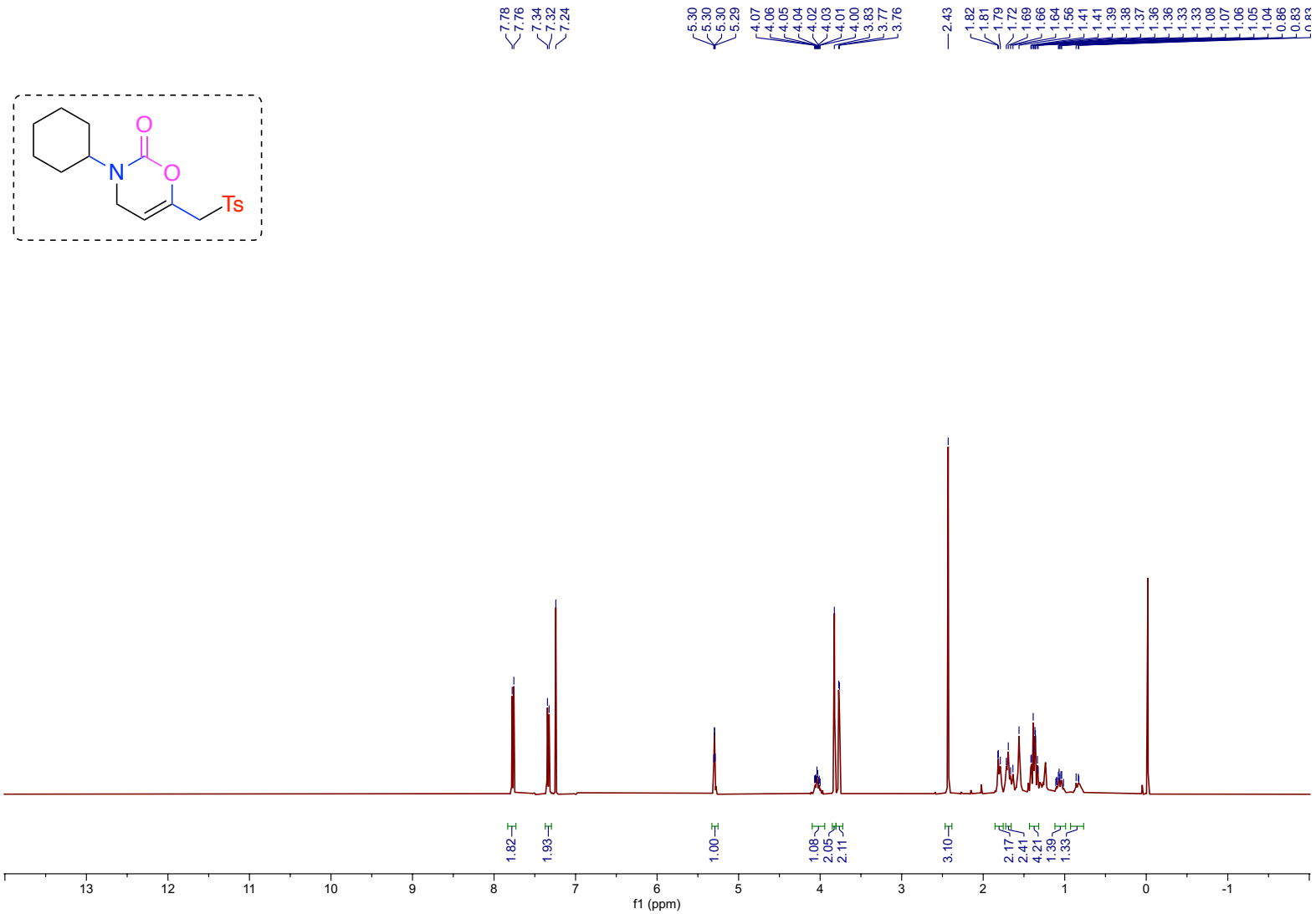
^{13}C (101 MHz) spectrum of compound 4e in $CDCl_3$



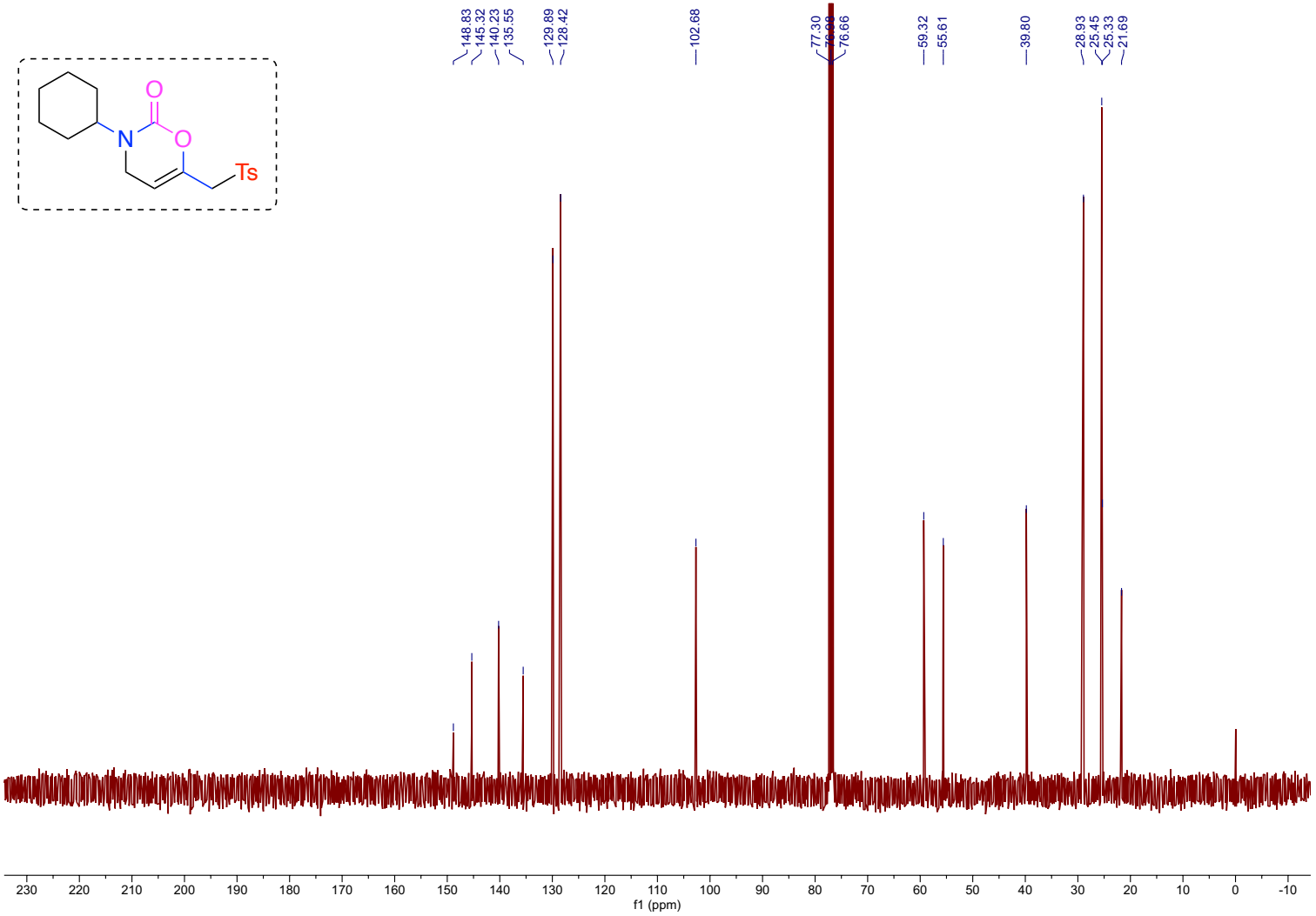
^{1}H (400 MHz) spectrum of compound 4f in $CDCl_3$



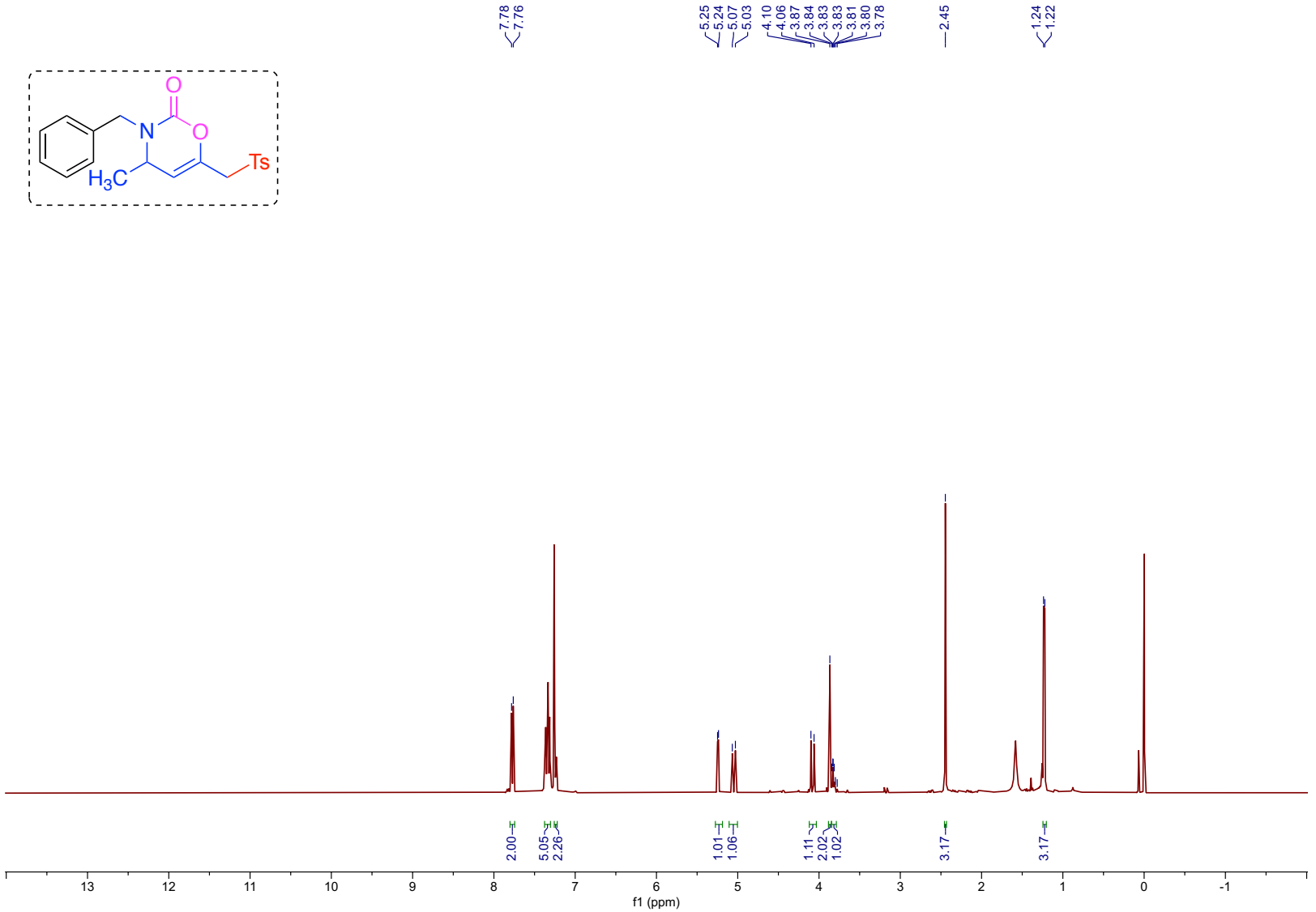
^{13}C (101 MHz) spectrum of compound 4f in $CDCl_3$



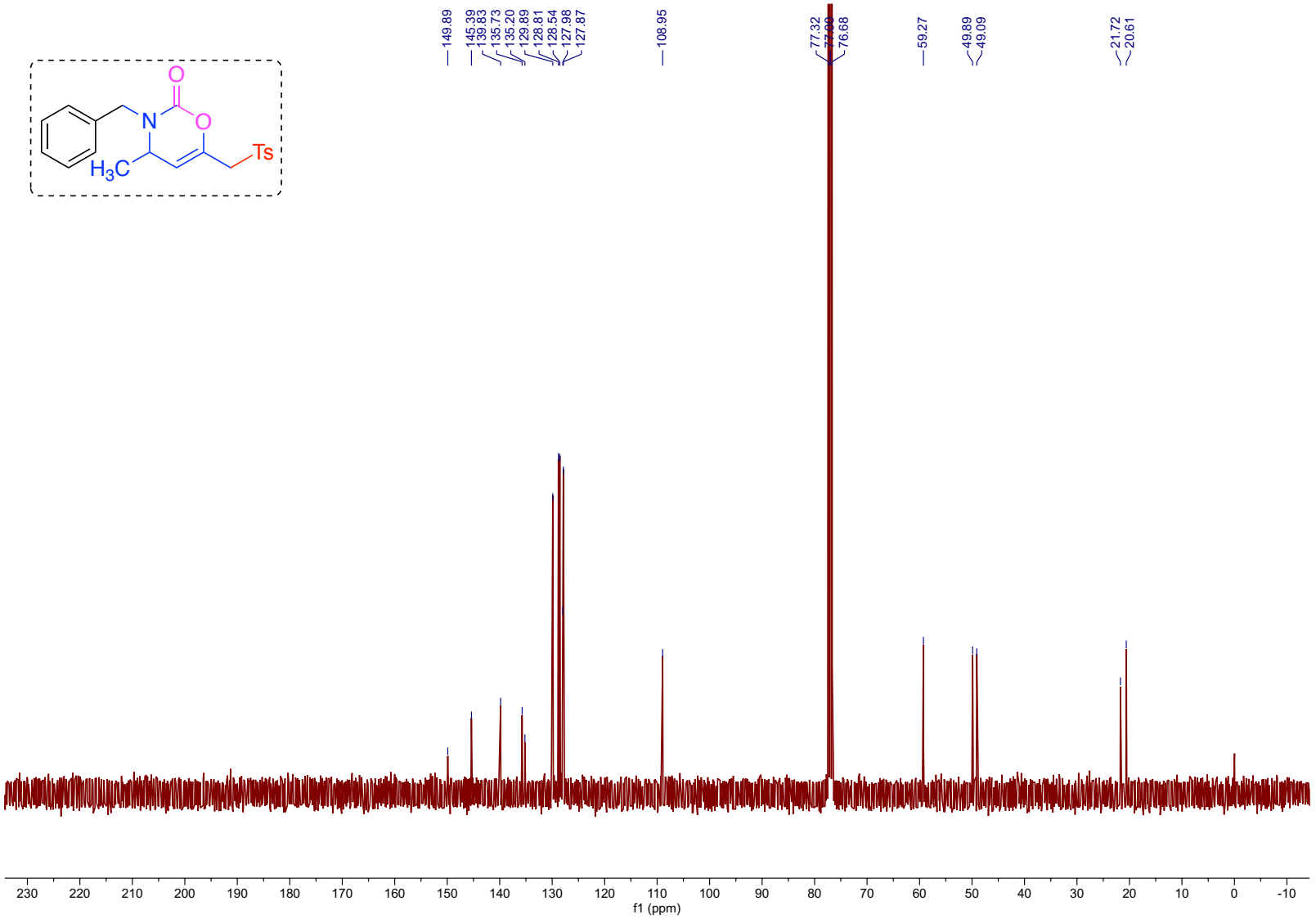
^{1}H (400 MHz) spectrum of compound 4g in $CDCl_3$



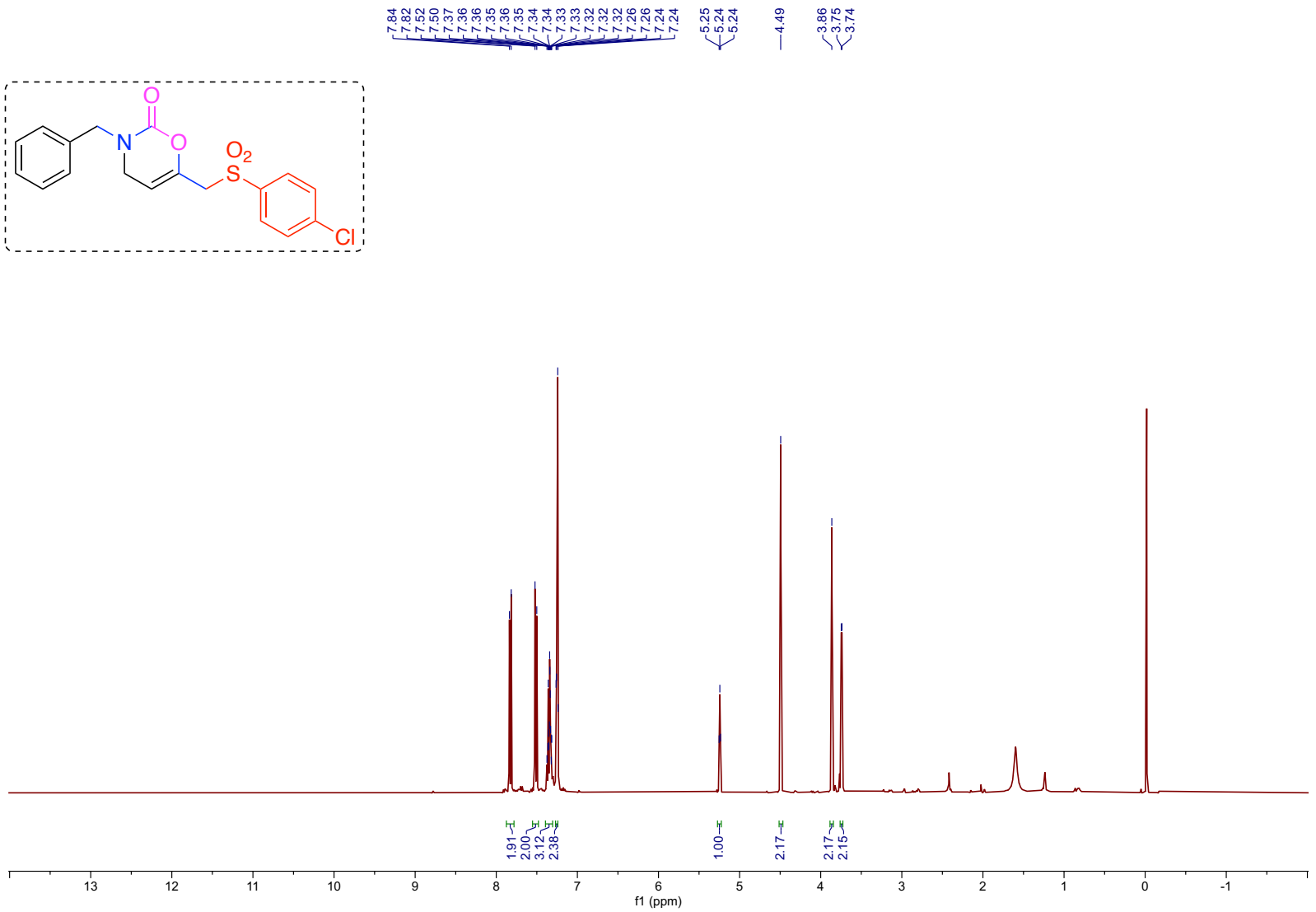
^{13}C (101 MHz) spectrum of compound 4g in $CDCl_3$



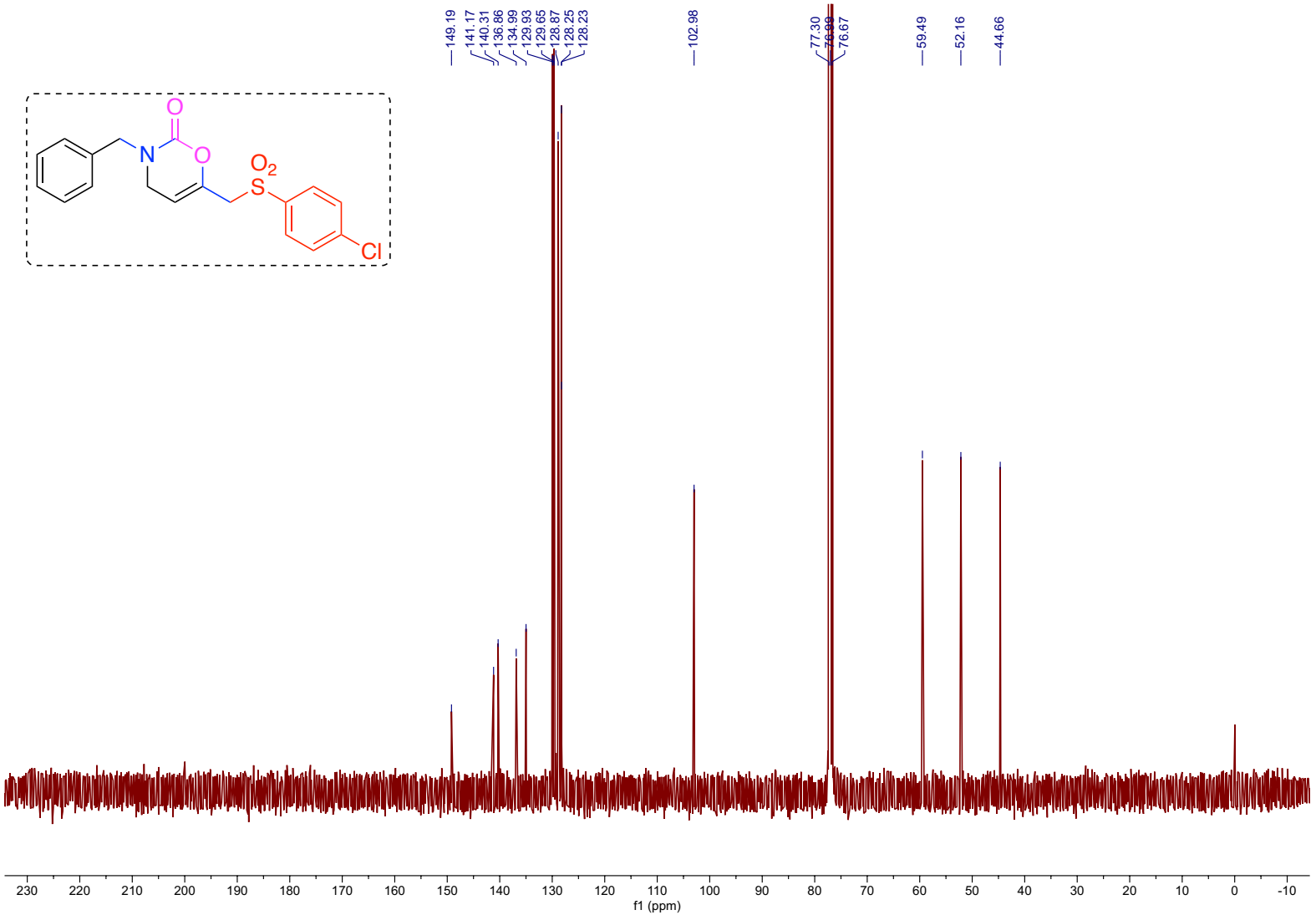
^{1}H (400 MHz) spectrum of compound 4h in $CDCl_3$



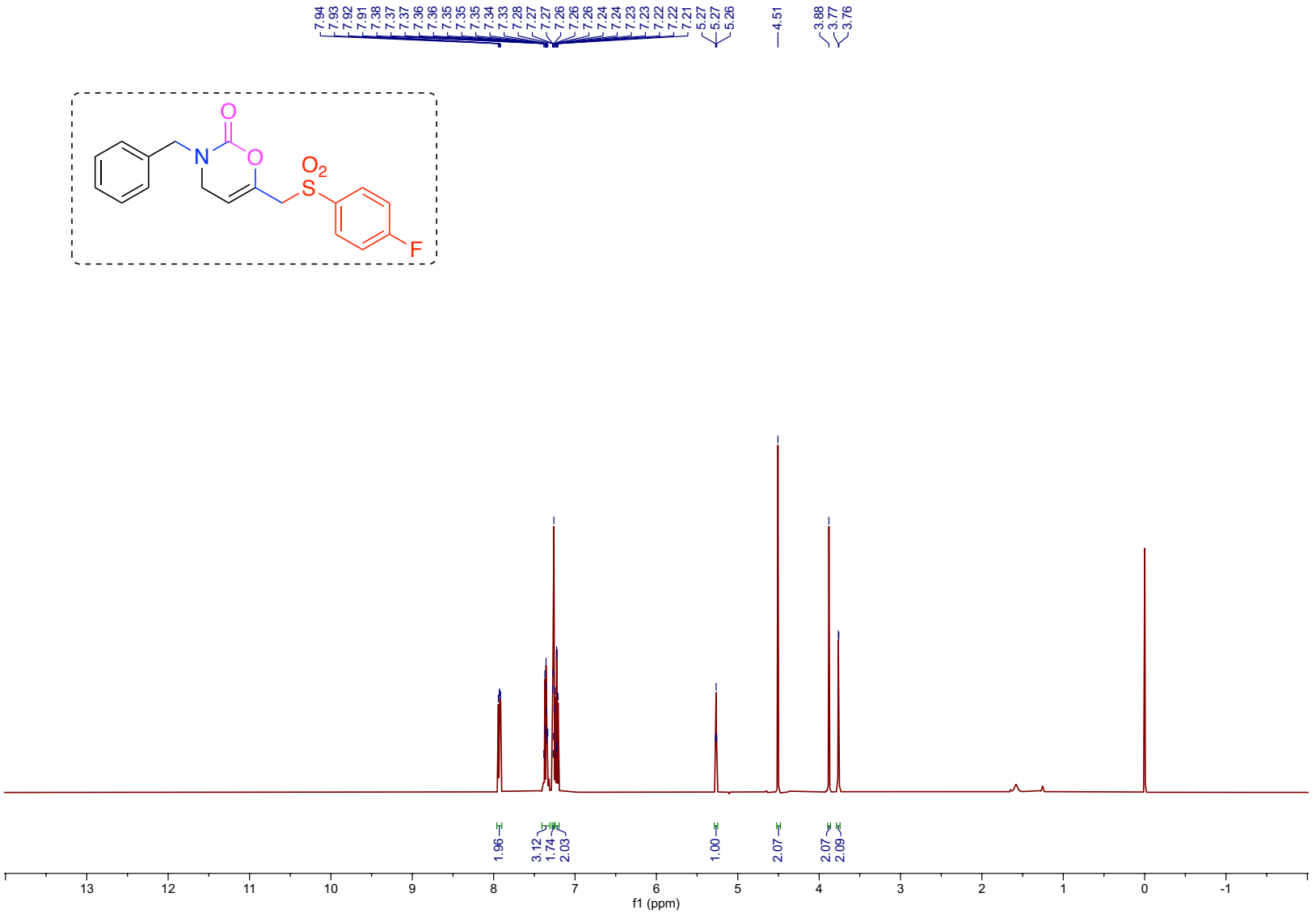
^{13}C (101 MHz) spectrum of compound 4h in $CDCl_3$



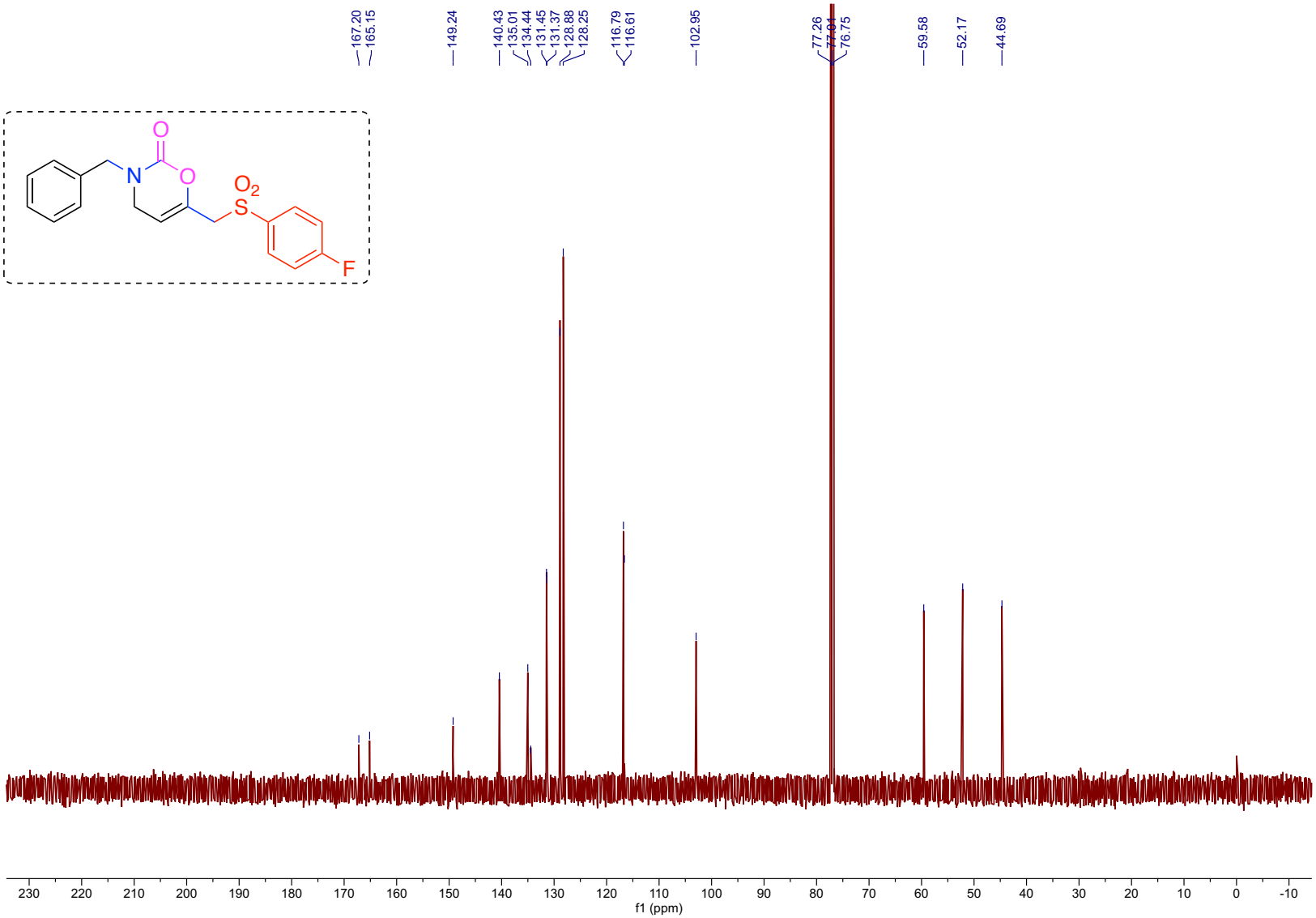
^{1}H (400 MHz) spectrum of compound 4i in $CDCl_3$



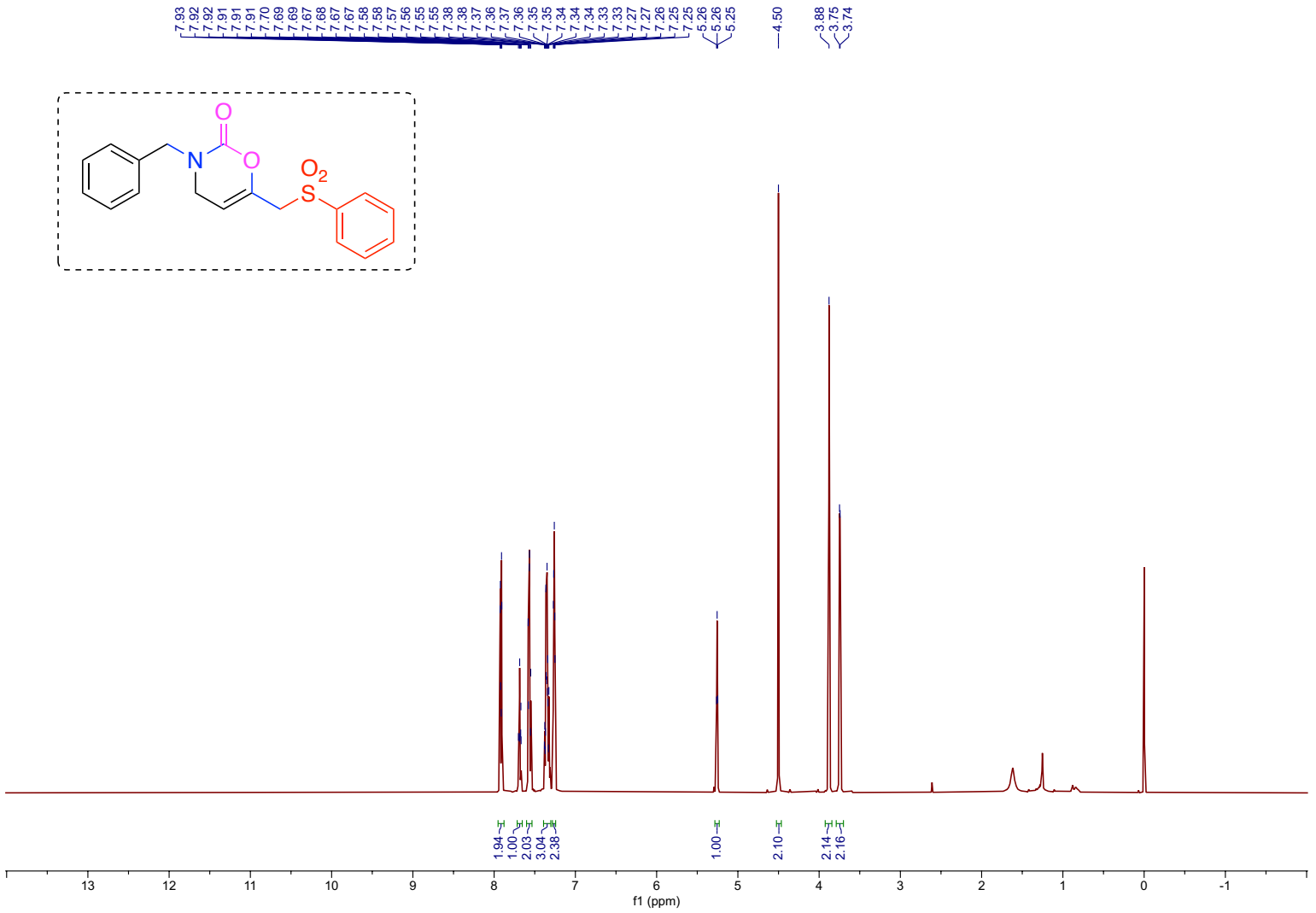
^{13}C (101 MHz) spectrum of compound 4i in $CDCl_3$



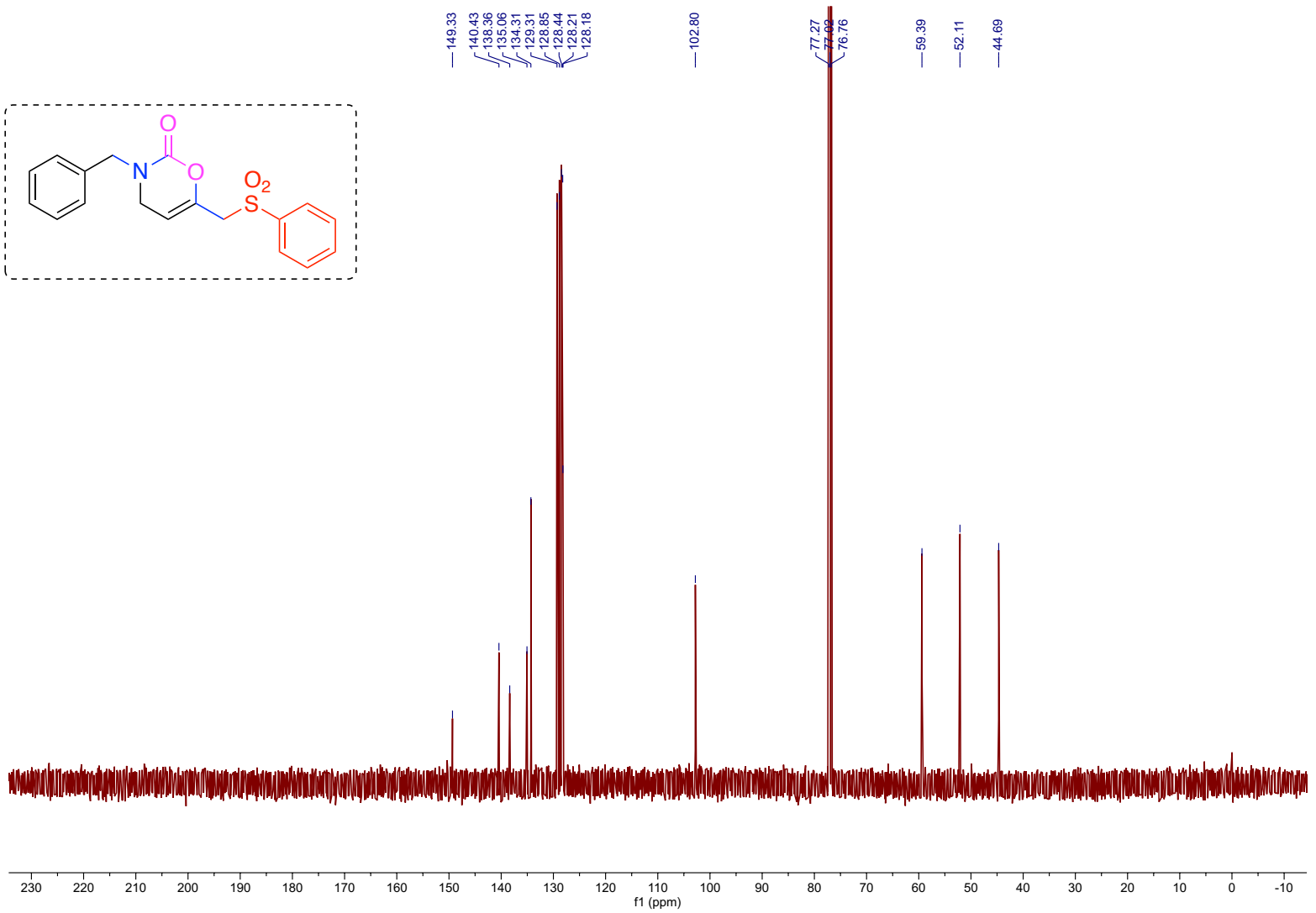
^{1}H (500 MHz) spectrum of compound 4j in $CDCl_3$



^{13}C (126 MHz) spectrum of compound 4j in $CDCl_3$



^{1}H (500 MHz) spectrum of compound 4k in $CDCl_3$



^{13}C (126 MHz) spectrum of compound 4k in $CDCl_3$