Supporting information

for

Synthetic and mechanistic study on the conjugate isothiocyanation of enones with trimethylsilyl isothiocyanate

Table of Contents

1. General methods and starting materials 2
2. Synthesis and characterization data of enones 2
2.1 General procedures: synthesis of chalcones via Claisen-Schmidt condensation and enones via Aldol reaction 2
2.2 Characterization data of enones 4
3. Optimization of the reaction conditions 10
4. Synthesis and characterization data of isothiocyanation products 12
4.1 General procedure 12
4.2 Spectral identification of isothiocyanate vs thiocyanate isomers 12
4.3 Characterization data of isothiocyanation products and derivatives 16
5. Additional control experiments 27
6. Computational details 28
7. Additional Figures/Schemes 29
8. Complete energy data 36
9. XYZ coordinates for all computed structures 39
10. Spectral data 51
10.1 ^{1}H NMR for enone substrates 51
10.2 ^{1}H, ^{13}C, and ^{19}F NMR for isothiocyanation products and derivatives 67
11. References 108

1. General methods and starting materials

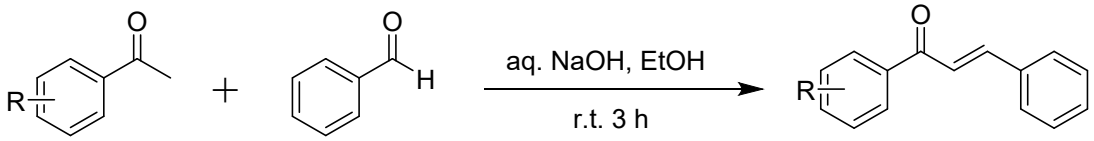
All solvents were used as commercially supplied. All reagents were purchased from commercial sources such as Sigma-Aldrich, TCI, VWR and used as obtained. Thin-layer chromatography was performed using 200 μm aluminum-backed plates purchased from Silicycle, which were visualized under UV light. Flash chromatography was carried out using silica gel from Silicycle (siliaflash P60, 40-63 μm).

^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz) spectra were recorded on a 500 MHz Bruker ultrashield spectrometer. ^{19}F NMR (283 MHz) spectra were recorded on a 300 MHz Bruker ultrashield spectrometer. Chemical shifts are given in parts per million (ppm, δ), referenced to the tetramethylsilane internal standard in all NMR solvents, calibrated at 0.0 ppm. ^{1}H and ^{13}C (where applicable) NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), pentet (p), sextet (sext) or heptet (hept). Mass spectrums were recorded on a high-resolution Orbitrap Q Exactive mass spectrometer (Thermo Scientific, San Jose, CA). FTIR spectra were collected by Shimadzu IRAffinity-1 Fourier transform infrared spectrophotometer.

2. Synthesis and characterization data of enones

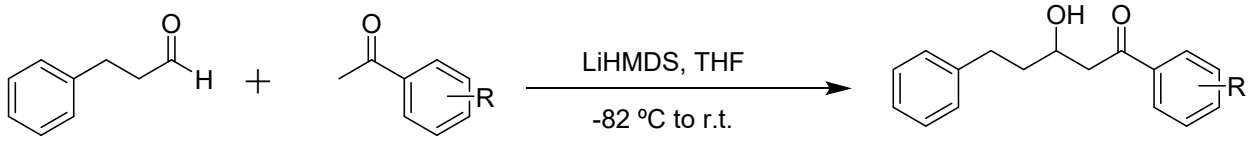
2.1 General procedures: synthesis of chalcones via Claisen-Schmidt condensation and enones via Aldol reaction

Procedure A: Following a modified literature procedure (Claisen-Schmidt condensation):[1]



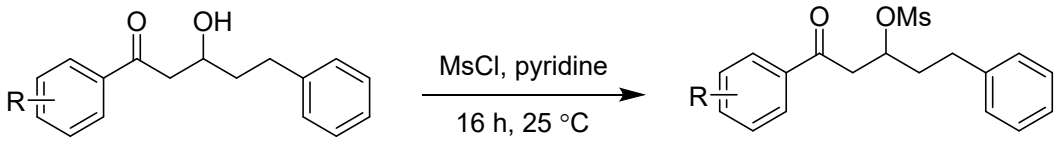
In a round-bottom flask, benzaldehyde (0.52 mL, 5 mmol) and acetophenone (0.73 mL, 6 mmol, 1.2 equiv.) were dissolved in ethanol (95%). Then, a solution of sodium hydroxide (2 mL, 3 M) was added at room temperature and the mixture stirred for 3 hours. After the reaction was finished, ice cold water was added, then the solid was filtered and washed with cold water.

Procedure B: Following a modified literature procedure (Aldol reaction):[2]

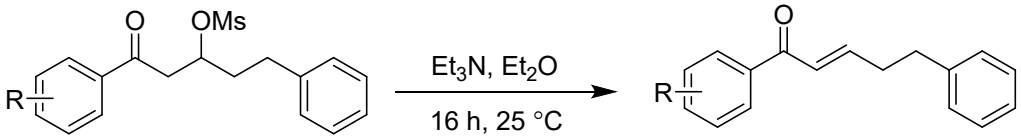


To a flame-dried round-bottom flask, Lithium bis(trimethylsilyl)amide solution in toluene (6 mL, 6 mmol, 1.2 equiv.) was added to anhydrous tetrahydrofuran (20 mL) under argon atmosphere and the solution was cooled to -82 °C using a liquid nitrogen/ethyl acetate bath and stirred for 30 minutes. Then, acetophenone (0.58 mL, 5 mmol, 1.0 equiv.) was added at -82 °C and the solution

was stirred for another 30 minutes. Then, the 3-phenylpropionaldehyde (1.4 mL, 10 mmol, 2.0 equiv.) was added dropwise and the mixture was stirred at -82 °C for 2 hours. After the reaction was finished, it was quenched with a mixture of H_2O:AcOH (1:1, 1 mL) and allowed to warm to room temperature. Water was added (5 mL) and the aqueous phase was extracted twice with diethyl ether (2 x 20 mL). The combined organic phases were washed with $NaHCO_3$ (sat), then brine, and the organic solution was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude mixture obtained was used without further purification.

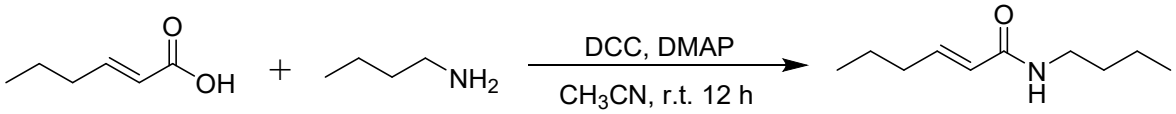


The aldol was dissolved in pyridine (1.1 M) and cooled to 0 °C. Methanesulfonyl chloride (5 mmol) was added dropwise at 0 °C and the reaction was stirred 16 hours at room temperature. Then, a mixture of water and diethyl ether (1:1) was added. The two phases were separated, and the organic phase was washed twice with a saturated aqueous solution of $CuSO_4$, then with brine. The organic phase was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The mesylated aldol was used without further purification.



The mesylated aldol was dissolved in diethyl ether (1.4 M). Then, trimethylamine (5 mmol) was added dropwise, and the reaction was stirred for 16 hours at room temperature. Then, a mixture of water and diethyl ether were added (1:1). The two phases were separated, and the organic phase was washed with HCl (1M), $NaHCO_3$ (sat) and brine. The organic phase was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by flash chromatography (hexane/ethyl acetate) to afford the desired product.

Procedure C: Following a modified literature procedure:[3, 4]

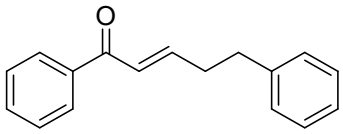


In a round-bottom flask, to a stirred solution of trans-2-hexenoic acid (5 mmol, 1.0 eq) in anhydrous acetonitrile (50 mL), n-butylamine (6 mmol, 1.2 eq) and dicyclohexylcarbodiimide (6 mmol, 1.2 eq) were added at 0 °C and stirred for 10 min, then 4-Dimethylaminopyridine (0.5 mmol, 0.1 eq) was added and the mixture was stirred at room temperature for 12 hours. After completion of the reaction, the mixture was concentrated under reduced pressure, then extracted with dichloromethane (2 x 20 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered,

and concentrated under reduced pressure. The crude compound was purified by flash chromatography (hexane/ethyl acetate) to afford the desired product.

2.2 Characterization data of enones

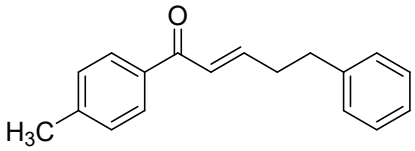
(*E*)-1,5-diphenylpent-2-en-1-one (**1a**)



Following procedure B, acetophenone (0.58 mL, 5 mmol), 3-phenylpropionaldehyde (1.4 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1a** as a yellowish oil (0.53 g, 2.25 mmol, 45% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 25:1). All characterization data were consistent with those reported.[2]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.92 (dt, *J* = 8.3, 1.1 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.49 (dd, *J* = 8.4, 7.0 Hz, 2H), 7.37 – 7.31 (m, 3H), 7.24 (s, 2H), 7.12 (dt, *J* = 15.6, 6.8 Hz, 1H), 6.94 – 6.83 (m, 1H), 2.89 (t, *J* = 7.7 Hz, 2H), 2.72 – 2.66 (m, 2H).

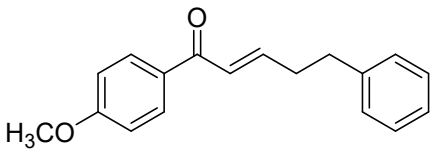
(*E*)-5-phenyl-1-(p-tolyl)pent-2-en-1-one (**1b**)



Following procedure B, 4'-Methylacetophenone (0.68 mL, 5 mmol), 3-phenylpropionaldehyde (1.4 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1b** as a colorless oil (0.65 g, 2.6 mmol, 52% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 20:1). All characterization data were consistent with those reported.[5]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.82 – 7.76 (m, 2H), 7.31 – 7.27 (m, 2H), 7.24 – 7.18 (m, 5H), 7.05 (dt, *J* = 15.4, 6.9 Hz, 1H), 6.85 (dt, *J* = 15.4, 1.5 Hz, 1H), 2.82 (t, *J* = 7.7 Hz, 2H), 2.61 (dtd, *J* = 8.7, 7.0, 1.5 Hz, 2H), 2.38 (s, 3H).

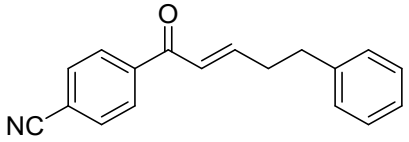
(*E*)-1-(4-methoxyphenyl)-5-phenylpent-2-en-1-one (**1c**)



Following procedure B, 4'-methoxyacetophenone (0.67 mL, 5 mmol), 3-phenylpropionaldehyde (1.4 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1c** as a light-yellow oil (0.64 g, 2.4 mmol, 48% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 15:1). All characterization data were consistent with those reported.[6]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.98 – 7.83 (m, 2H), 7.32 – 7.26 (m, 2H), 7.20 (m, *J* = 7.1, 3.7, 2.2 Hz, 3H), 7.05 (dt, *J* = 15.3, 6.8 Hz, 1H), 6.93 – 6.90 (m, 2H), 6.87 (dt, *J* = 15.3, 1.5 Hz, 1H), 3.83 (s, 3H), 2.82 (t, *J* = 7.7 Hz, 2H), 2.61 (dtd, *J* = 8.8, 7.0, 1.5 Hz, 2H).

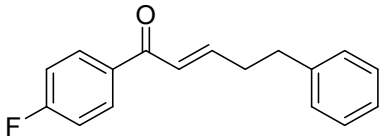
(*E*)-4-(5-phenylpent-2-enoyl)benzonitrile (**1d**)



Following procedure B, 4-acetylbenzonitrile (0.73 g, 5 mmol), 3-phenylpropionaldehyde (1.4 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1d** as a white solid (0.73 g, 2.4 mmol, 48% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 15:1). All characterization data were consistent with those reported.[6]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.93 – 7.89 (m, 2H), 7.76 – 7.72 (m, 2H), 7.33 – 7.29 (m, 2H), 7.25 – 7.18 (m, 3H), 7.10 (dt, *J* = 15.4, 6.9 Hz, 1H), 6.79 (dt, *J* = 15.5, 1.5 Hz, 1H), 2.86 (t, *J* = 7.6 Hz, 2H), 2.67 (dtd, *J* = 8.8, 7.0, 1.5 Hz, 2H).

(*E*)-1-(4-fluorophenyl)-5-phenylpent-2-en-1-one (**1e**)

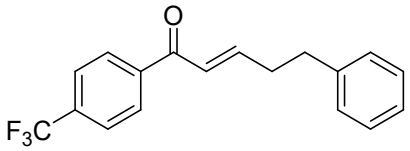


Following procedure B, 4'-fluoroacetophenone (0.61 mL, 5 mmol), 3-phenylpropionaldehyde (1.4 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1e** as a colorless oil (0.64 g, 2.5 mmol, 50% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 20:1). All characterization data were consistent with those reported.[6]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.89 (m, 2H), 7.29 (m, 2H), 7.20 (m, 3H), 7.10 (m, 3H), 6.84 (dq, 1H), 2.83 (t, 2H), 2.63 (m, 2H).

^{19}F NMR (283 MHz, Chloroform-d) δ -109.55.

(*E*)-5-phenyl-1-(4-(trifluoromethyl)phenyl)pent-2-en-1-one (**1f**)

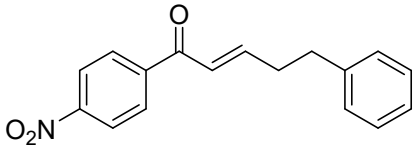


Following procedure B, 4'-(Trifluoromethyl)acetophenone (0.96 g, 5 mmol), 3-phenylpropionaldehyde (1.4 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1f** as a yellow solid (0.63 g, 2.4 mmol, 48% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 20:1). All characterization data were consistent with those reported.[6]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.96 – 7.91 (m, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.34 – 7.29 (m, 2H), 7.25 – 7.19 (m, 3H), 7.10 (dt, *J* = 15.5, 6.9 Hz, 1H), 6.81 (dt, *J* = 15.5, 1.5 Hz, 1H), 2.86 (t, *J* = 7.6 Hz, 2H), 2.67 (dtd, *J* = 8.8, 7.0, 1.5 Hz, 2H).

^{19}F NMR (283 MHz, Chloroform-d) δ -64.61.

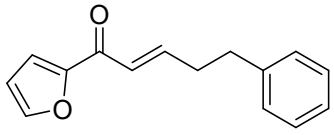
(*E*)-1-(4-nitrophenyl)-5-phenylpent-2-en-1-one (**1g**)



Following procedure B, 4'-nitroacetophenone (0.83 g, 5 mmol), 3-phenylpropionaldehyde (1.4 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1g** as a yellowish solid (0.36 g, 1.28 mmol, 26% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 10:1). All characterization data were consistent with those reported.[7]

^{1}H NMR (500 MHz, Chloroform-d) δ 8.32 – 8.27 (m, 2H), 8.00 – 7.95 (m, 2H), 7.34 – 7.30 (m, 2H), 7.22 (dd, *J* = 9.5, 7.8 Hz, 3H), 7.11 (dt, *J* = 15.4, 6.9 Hz, 1H), 6.81 (dt, *J* = 15.5, 1.5 Hz, 1H), 2.87 (t, *J* = 7.6 Hz, 2H), 2.73 – 2.65 (m, 2H).

(*E*)-1-(furan-2-yl)-5-phenylpent-2-en-1-one (**1h**)

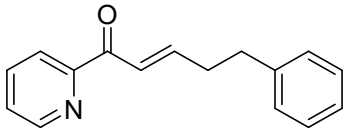


Following procedure B, 2-acetylfuran (0.50 mL, 5 mmol), 3-phenylpropionaldehyde (1.4 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1h** as a yellowish oil (0.51 g, 2.25 mmol, 45% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 25:1). All characterization data were consistent with those reported.[8]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.59 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.21 – 7.15 (m, 5H), 6.80 (dt, *J* = 15.4, 1.5 Hz, 1H), 6.53 (dd, *J* = 3.6, 1.7 Hz, 1H), 2.86 – 2.80 (m, 2H), 2.62 (dtd, *J* = 8.9, 7.0, 1.6 Hz, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 178.09, 153.33, 147.81, 146.47, 140.83, 128.50, 126.20, 125.43, 120.44, 117.60, 112.39, 34.47, 29.71.

(*E*)-5-phenyl-1-(pyridin-2-yl)pent-2-en-1-one (**1i**)

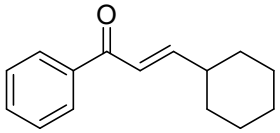


Following procedure B, 2-acetylpyridine (0.56 mL, 5 mmol), 3-phenylpropionaldehyde (1.4 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1i** as a yellowish oil (0.56 g, 2.35 mmol, 47% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 20:1). All characterization data were consistent with those reported.[8]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.93 – 7.89 (m, 2H), 7.77 – 7.73 (m, 2H), 7.34 – 7.29 (m, 2H), 7.25 – 7.18 (m, 3H), 7.09 (dt, *J* = 15.5, 6.9 Hz, 1H), 6.78 (dt, *J* = 15.5, 1.5 Hz, 1H), 2.86 (t, *J* = 7.6 Hz, 2H), 2.72 – 2.62 (m, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 189.34, 155.99, 150.71, 150.04, 142.73, 140.44, 129.45, 128.60, 128.41, 126.37, 126.32, 123.74, 34.54, 34.33.

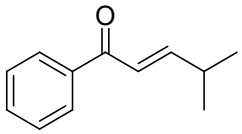
(*E*)-3-cyclohexyl-1-phenylprop-2-en-1-one (**1j**)



Following procedure B, acetophenone (0.58 mL, 5 mmol), cyclohexane carbaldehyde (1.3 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1j** as a light-yellow solid (0.40 g, 2.0 mmol, 40% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 25:1). All characterization data were consistent with those reported.[9]

^{1}H NMR (500 MHz, Chloroform-d) δ 8.00 – 7.87 (m, 2H), 7.59 – 7.50 (m, 1H), 7.44 (ddt, *J* = 9.5, 7.6, 2.0 Hz, 2H), 7.00 (ddd, *J* = 15.7, 6.8, 1.9 Hz, 1H), 6.82 (dd, *J* = 15.5, 1.5 Hz, 1H), 2.24 (m, 1H), 1.81 (dqt, *J* = 12.7, 5.0, 2.7 Hz, 4H), 1.37 – 1.18 (m, 6H).

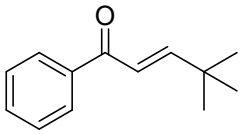
(*E*)-4-methyl-1-phenylpent-2-en-1-one (**1k**)



Following procedure B, acetophenone (0.58 mL, 5 mmol), isobutyraldehyde (0.92 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1k** as a light-yellow oil (0.48 g, 2.75 mmol, 55% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 30:1). All characterization data were consistent with those reported.[10]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.97 – 7.88 (m, 2H), 7.60 – 7.51 (m, 1H), 7.50 – 7.44 (m, 2H), 7.04 (dd, *J* = 15.5, 6.7 Hz, 1H), 6.83 (dd, *J* = 15.5, 1.4 Hz, 1H), 2.57 (m, *J* = 13.5, 6.7, 1.4 Hz, 1H), 1.13 (d, *J* = 6.8 Hz, 6H).

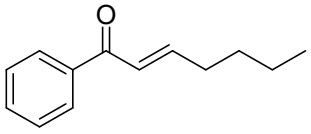
(*E*)-4,4-dimethyl-1-phenylpent-2-en-1-one (**1l**)



Following procedure B, acetophenone (0.58 mL, 5 mmol), pivalaldehyde (1.10 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1l** as a colorless oil (0.50 g, 2.65 mmol, 53% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 35:1). All characterization data were consistent with those reported.[2]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.95 – 7.90 (m, 2H), 7.56 – 7.51 (m, 1H), 7.45 (t, *J* = 8.1, 6.6 Hz, 2H), 7.07 (d, *J* = 15.7 Hz, 1H), 6.79 (d, *J* = 15.7 Hz, 1H), 1.14 (s, 9H).

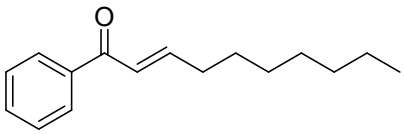
(*E*)-1-phenylhept-2-en-1-one (**1m**)



Following procedure B, acetophenone (0.58 mL, 5 mmol), pentanal (1.08 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1m** as a light-yellow oil (0.42 g, 2.25 mmol, 45% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 25:1). All characterization data were consistent with those reported.[11]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.94 – 7.91 (m, 2H), 7.58 – 7.53 (m, 1H), 7.48 – 7.44 (m, 2H), 7.07 (dt, *J* = 15.3, 6.9 Hz, 1H), 6.88 (dt, *J* = 15.4, 1.5 Hz, 1H), 2.32 (qd, *J* = 7.0, 1.5 Hz, 2H), 1.55 – 1.48 (m, 2H), 1.44 – 1.34 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H).

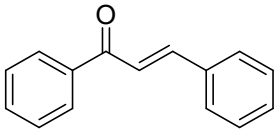
(*E*)-1-phenyloct-2-en-1-one (**1n**)



Following procedure B, acetophenone (0.58 mL, 5 mmol), octanal (1.6 mL, 10 mmol), methanesulfonyl chloride (0.39 mL, 5 mmol) and trimethylamine (0.45 mL, 5 mmol) gave **1n** as a yellowish oil (0.40 g, 2.0 mmol, 40% overall yield). Purification was performed by flash column chromatography (hexane/ethyl acetate 25:1). All characterization data were consistent with those reported.[2]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.97 – 7.93 (m, 2H), 7.59 – 7.56 (m, 1H), 7.51 – 7.47 (m, 2H), 7.10 (dt, *J* = 15.3, 6.9 Hz, 1H), 6.90 (dt, *J* = 15.4, 1.5 Hz, 1H), 2.35 (q, *J* = 7.0 Hz, 2H), 1.58 –1.27 (m, 10H), 0.96 (t, *J* = 7.3 Hz, 3H).

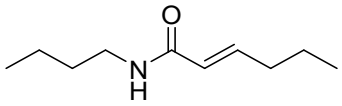
(*E*)-chalcone (**1q**)



Following procedure A, benzaldehyde (0.52 mL, 5 mmol) and acetophenone (0.73 mL, 6 mmol, 1.2 equiv.) gave **1q** as a yellow solid (1.79 g, 4.30 mmol, 86% overall yield). All characterization data were consistent with those reported.[12]

^{1}H NMR (500 MHz, Chloroform-d) δ 8.02 (s, 2H), 7.80 (s, 1H), 7.65 (s, 2H), 7.59 (s, 1H), 7.51 (s, 3H), 7.42 (s, 3H).

(*E*)-N-butylhex-2-enamide (**1r**)



Following procedure C, trans-2-hexenoic acid (0.57 g, 5 mmol), n-butylamine (0.44 g, 6 mmol), dicyclohexylcarbodiimide (1.24 g, 6 mmol) and 4-Dimethylaminopyridine (0.06 g, 0.5 mmol) gave **1r** as a white solid (0.38 g, 2.25 mmol, 45% yield). All characterization data were consistent with those reported.[13]

^{1}H NMR (500 MHz, Chloroform-d) δ 6.82 (dt, J = 15.0, 7.0 Hz, 1H), 5.75 (dt, J = 15.3, 1.7 Hz, 1H), 5.48 (s, 1H), 3.32 (td, J = 7.2, 5.9 Hz, 2H), 2.15 (m, 2H), 1.53 – 1.45 (m, 4H), 1.39 – 1.35 (m, 2H), 0.93 (t, J = 7.4 Hz, 6H).

3. Optimization of the reaction conditions

Initial procedure

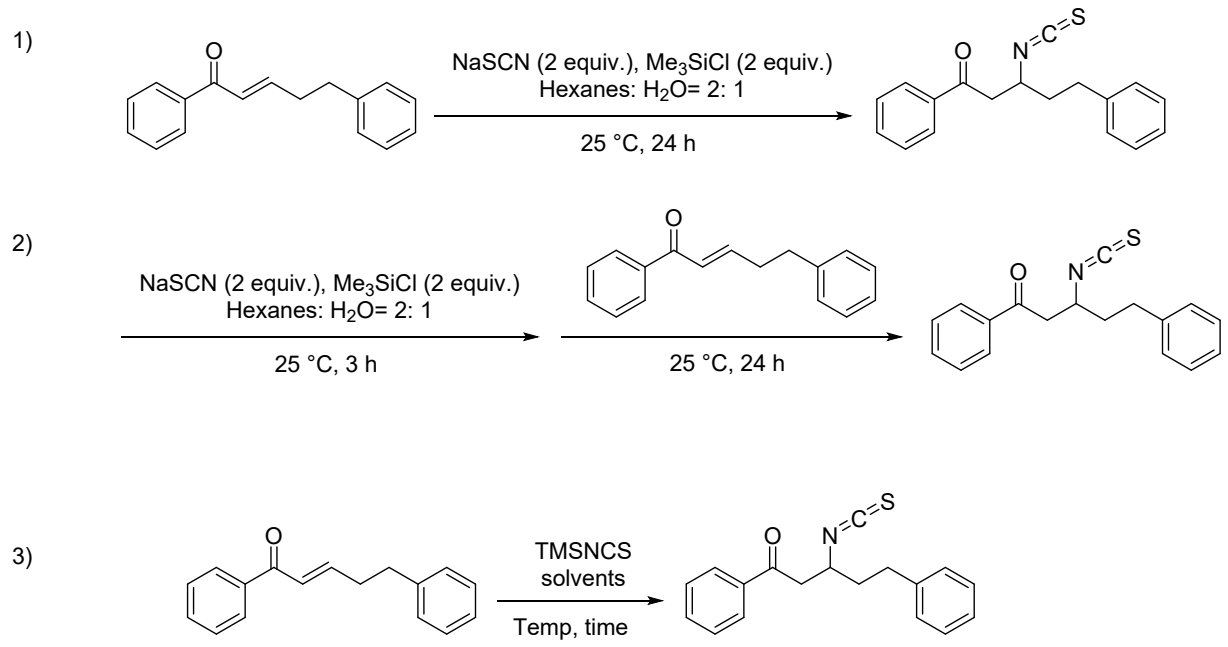


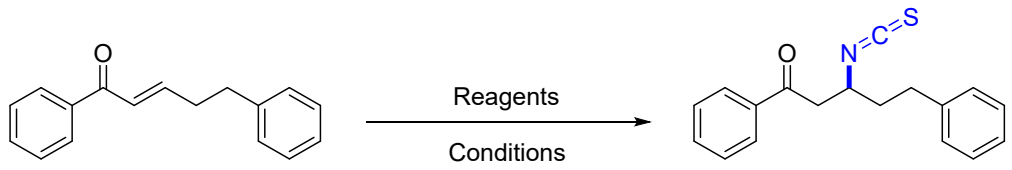
Figure S1 Initial procedures

Procedure 1: to a round-bottom flask, sodium thiocyanate (2.0 equiv.) and trimethylsilyl chloride (2.0 equiv.) were dissolved in a mixture of hexanes and water, then (*E*)-1,5-diphenylpent-2-en-1-one (**1a**) was added. The resulting mixture was stirred at 25 °C for 24 hours.

Procedure 2: to a round-bottom flask, sodium thiocyanate (2.0 equiv.) in water, trimethylsilyl chloride (2.0 equiv.) in hexanes, mixed these two solutions and stirred for 3 hours at 25 °C, (*E*)-1,5-diphenylpent-2-en-1-one (**1a**) was added and stirred at 25°C for 24 hours.

Procedure 3: to a round-bottom flask, (trimethylsilyl)isothiocyanate and (*E*)-1,5-diphenylpent-2-en-1-one (**1a**) were dissolved into solvents, then stirred to give 1,5-diphenyl-3-thiocyanatopentan-1-one (**2a**).

Optimization Table S1



Entry	Reagents	Solvents	Temperature (°C)	Time (h)	Yield [a] (%)
1	NaSCN (5 equiv.)	Hexanes: H_2O (2:1)	25	24[b]	0
2	TMSCl &NaSCN	Hexanes: H_2O (2:1)	25	24[b]	90
3	TMSCl &NaSCN	Hexanes: H_2O (2:1)	25	27[c]	96
4	TMSCl &NaSCN	Hexanes: EtOH (2:1)	25	27[c]	99
5	TMSNCS (5 equiv.)	Hexanes: EtOH (2:1)	25	27[d]	95
6	TMSNCS (5 equiv.)	Hexanes: EtOH (2:1)	25	6[d]	98
7	TMSNCS (5 equiv.)	Hexanes: EtOH (2:1)	25	3[d]	93
8	TMSNCS (5 equiv.)	Hexanes: EtOH (2:1)	25	1.5[d]	100
9	TMSNCS (5 equiv.)	Hexanes	25	1.5	48
10	TMSNCS (5 equiv.)	Hexanes: EtOH (2:1)	0	1.5	100
11	TMSNCS (5 equiv.)	CH_2Cl_2: EtOH (2:1)	0	1.5	100
12	TMSNCS (5 equiv.)	THF: EtOH (2:1)	0	1.5	57
13	TMSNCS (5 equiv.)	Octanol	0	6	0
14	TMSNCS (5 equiv.)	EtOH	0	6	100
15	TMSNCS (5 equiv.)	EtOH	0	3	100
16	TMSNCS (5 equiv.)	EtOH	0	1.5	100
17	TMSNCS (2 equiv.)	EtOH	0	0.5	100 (90)[e]
18	TMSNCS (1.1 equiv.)	EtOH	0	0.5	80
19	TMSNCS (1.1 equiv.)	EtOH	0	6	95

[a] Reactions were run on 0.15 mmol scale. Yield was estimated by ^{1}H NMR of the crude mixture with dibenzyl ether as internal standard. [b] Reaction condition: Procedure 1; [c] Reaction condition: Procedure 2; [d] Reaction condition: Procedure 3. [e] isolated yield.

4. Synthesis and characterization data of isothiocyanation products

4.1 General procedure

In a round-bottom flask, (trimethylsilyl)isothiocyanate (0.3 mmol, 2.0 equiv.) and an enone (0.15 mmol, 1.0 equiv.) were dissolved into 95% ethanol (1.5 mL) or 95% ethanol/dichloromethane (1.5 mL, 2/1), and the mixture was then stirred 30 mins to 6 hours at 0 ℃. Then, the solvents were evaporated under reduced pressure and the resulting crude mixture was purified by flash column chromatography (hexanes/ethyl acetate) to afford the desired products.

4.2 Spectral identification of isothiocyanate vs thiocyanate isomers

There is great selectivity for the isothiocyanato group in products. The combined NMR and FTIR can show the difference between isothiocyanate and thiocyanate.[14-16] From NMR, we can identify the ratio between isothiocyanato- and thiocyanato- product. Figure S2 shows the NMR difference between ethyl isothiocyanate and ethyl thiocyanate, where the chemical shift of the-CH_2 group is 3.00 ppm for ethyl thiocyanate and 3.58 ppm for ethyl isothiocyanate, in line with the increased electronegativity of nitrogen. For the reaction starting with but-3-en-2-one, the crude ratio between 4-isothiocyanatobutan-2-one (**2p**) and 4-thiocyanatobutan-2-one is almost 1:1 which is shown in Figure S3, and we can obtain the pure **2p** of 55% yield. For the reaction started with 3-cyclohexyl-1-phenylprop-2-en-1-one (**1j**), the crude ratio between 3-cyclohexyl-3-isothiocyanato-1-phenylpropan-1-one (**2j**) and 3-cyclohexyl-3-thiocyanato-1-phenylpropan-1-one is about 86:14 which is shown in Figure S4, while after column only **2j** is detected (Figure S5). Purification usually reduces the amount of thiocyanato- product in our system. There is a high selectivity for isothiocyanates from the results of the other substrates.

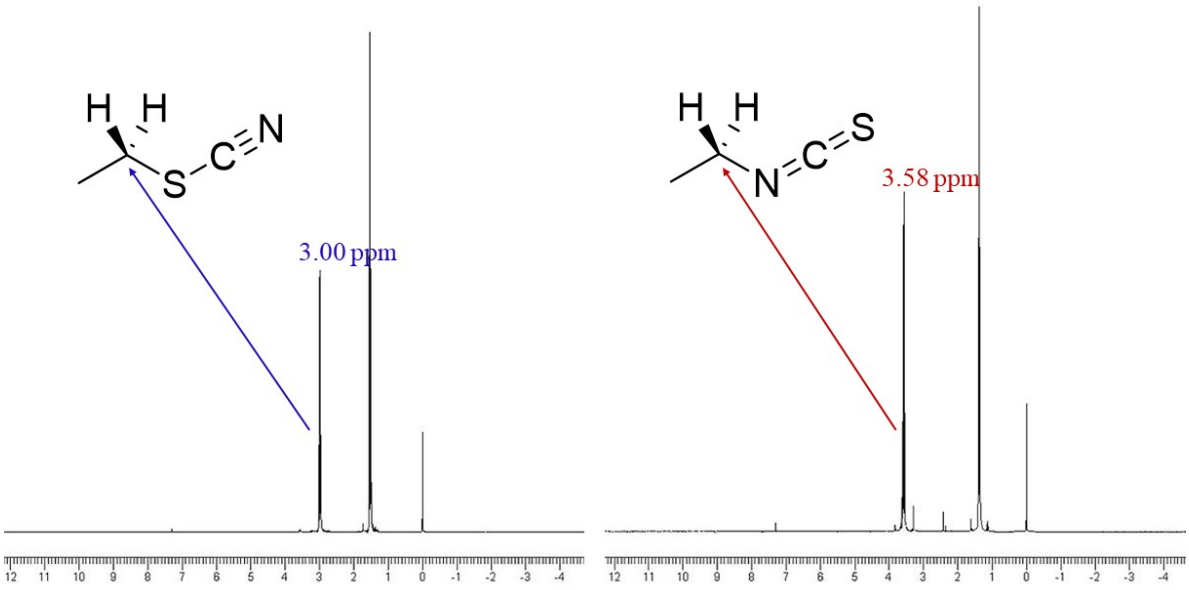


Figure S2 NMR of ethyl isothiocyanate and ethyl thiocyanate[17, 18]

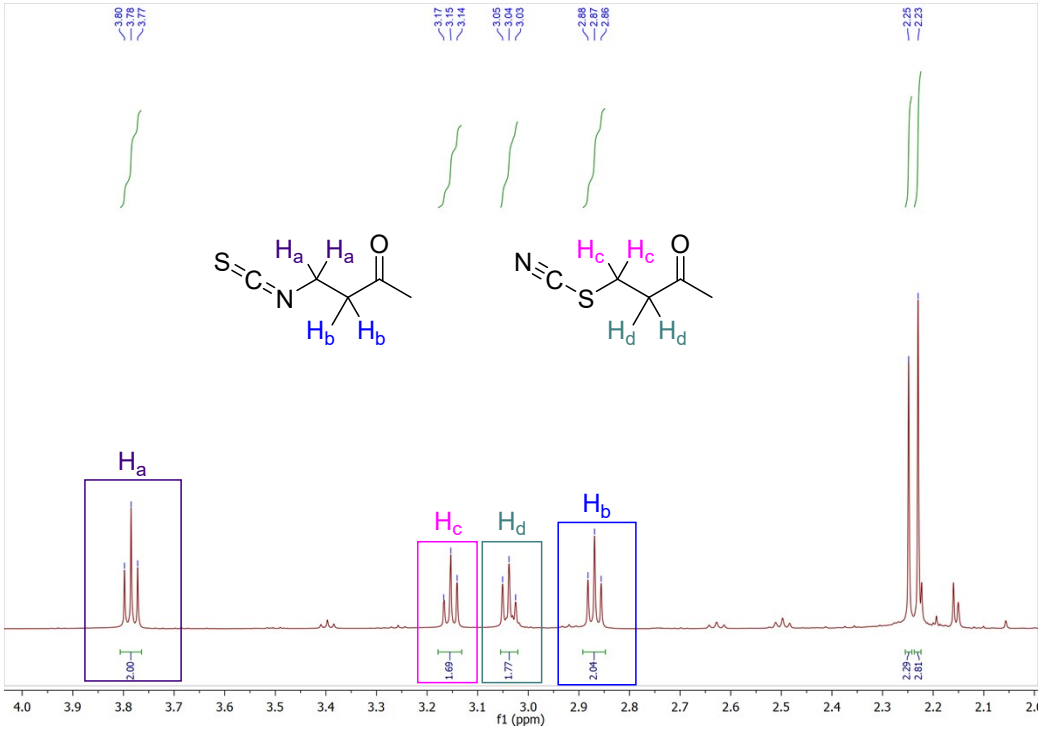


Figure S3 Crude NMR of 4-isothiocyanatobutan-2-one (**2p**) and 4-thiocyanatobutan-2-one (**2p'**)

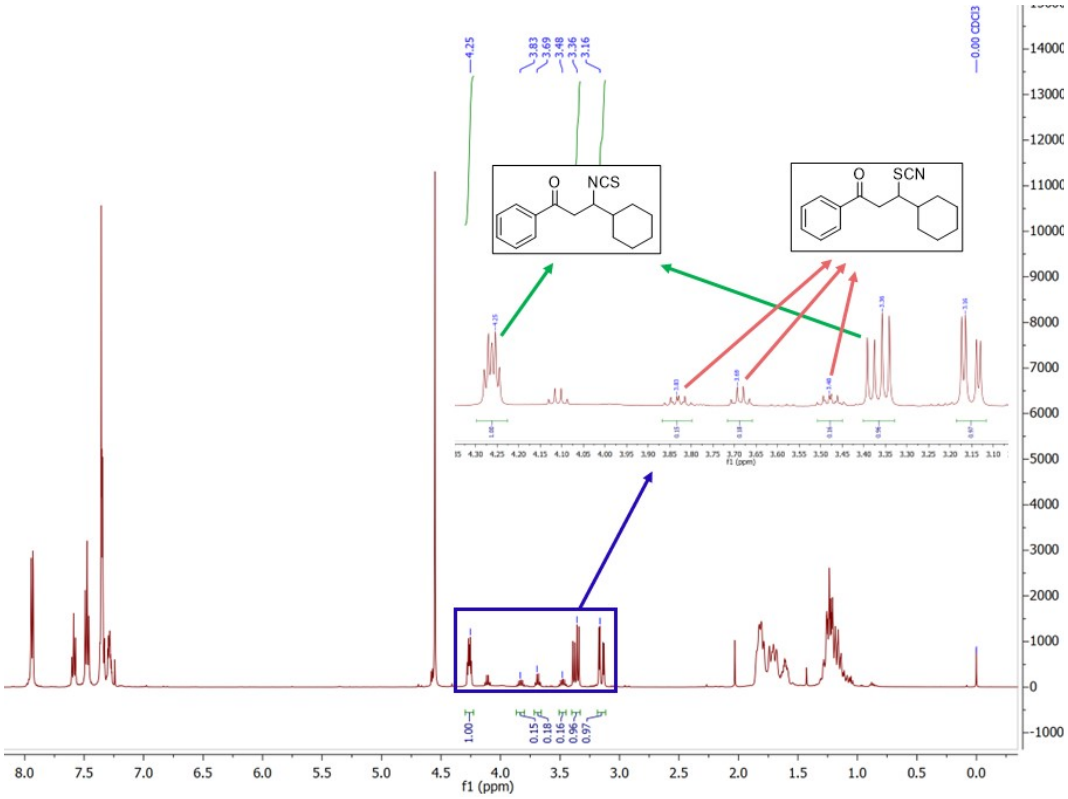


Figure S4 Crude NMR of 3-cyclohexyl-3-isothiocyanato-1-phenylpropan-1-one (**2j**) and 3-cyclohexyl-3-thiocyanato-1-phenylpropan-1-one (**2j'**)

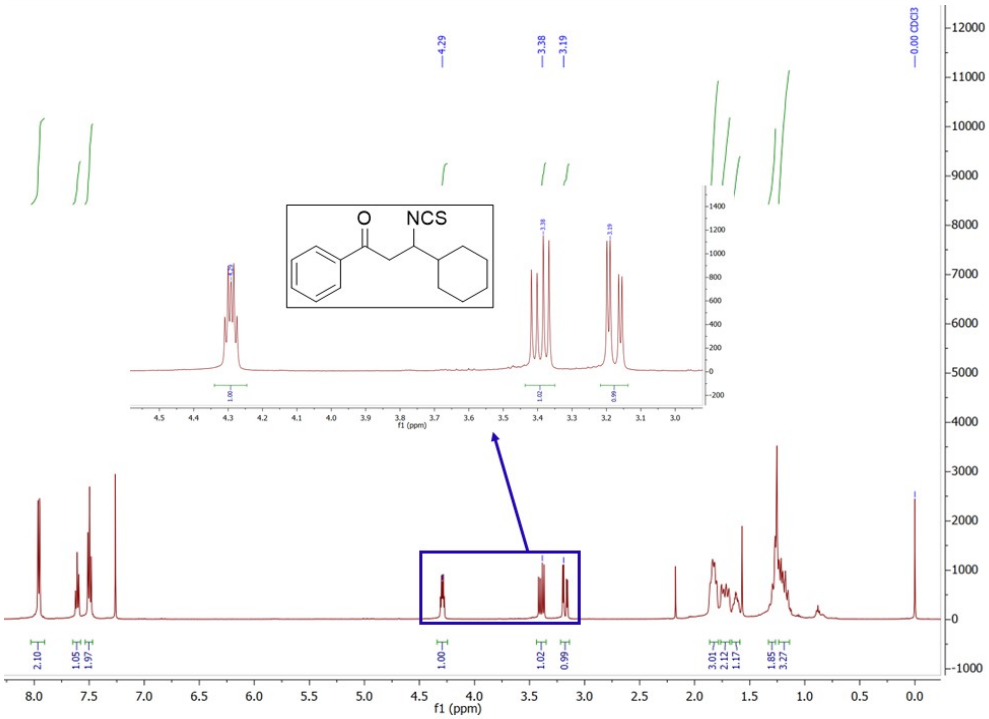


Figure S5 NMR after column of 3-cyclohexyl-3-isothiocyanato-1-phenylpropan-1-one (**2j**)

FTIR showed that the peak at 2098 cm^{-1} is broad for **2a** (Figure S6) which matches the lower wavenumber and broad signal of isothiocyanates, compared with the IR spectrums of ethyl isothiocyanate and ethyl thiocyanate and the wavenumber from the literature (Figure S7).[19, 20]

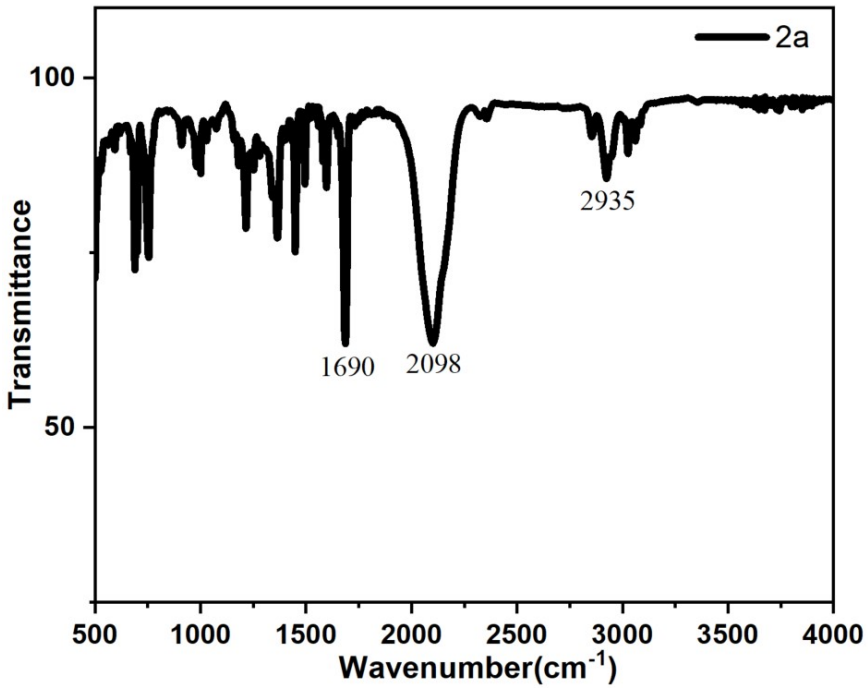


Figure S6 FTIR of **2a**

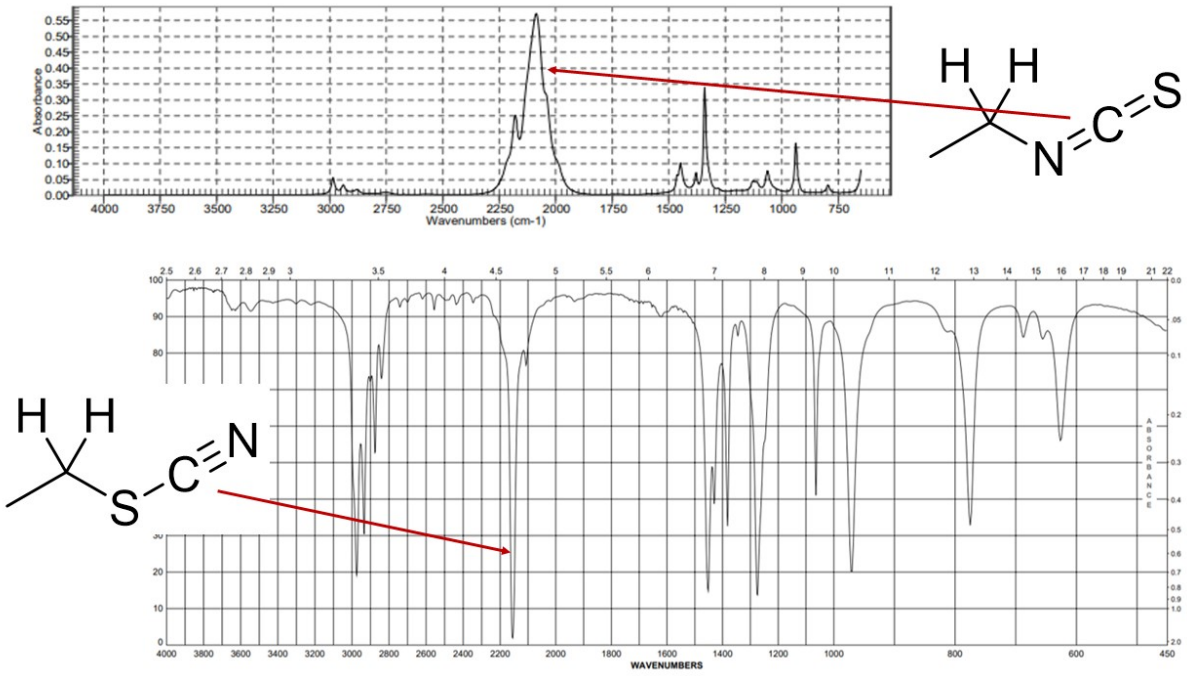
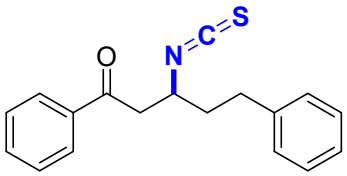


Figure S7 IR of ethyl isothiocyanate and ethyl thiocyanate (*Spectral Data were obtained from Sigma-Aldrich)*

4.3 Characterization data of isothiocyanation products and derivatives

3-isothiocyanato-1,5-diphenylpentan-1-one (2a)



Molecular formula: $C_{18}H_{17}NOS$ MW = 295.40 g/mol

Following the general procedure, enone **1a** (0.15 mmol, 35.5 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2a**. Purification by flash column chromatography (hexane/ethyl acetate 20/1) gave the title compound (40.0 mg, 90%) as a yellow solid.

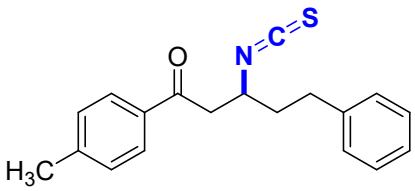
^{1}H NMR (500 MHz, Chloroform-d) δ 7.93 – 7.90 (m, 2H), 7.62 – 7.57 (m, 1H), 7.50 – 7.45 (m, 2H), 7.33 – 7.28 (m, 2H), 7.24 – 7.19 (m, 3H), 4.37 (m, 1H), 3.41 (dd, *J* = 17.3, 7.1 Hz, 1H), 3.16 (dd, *J* = 17.3, 5.8 Hz, 1H), 2.92 (m, 1H), 2.78 (m, 1H), 2.09 – 1.96 (m, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 195.88, 140.12, 136.19, 133.79, 132.37, 128.84, 128.69, 128.49, 128.10, 126.42, 53.40, 43.97, 37.36, 32.32.

IR (cm^{-1}) 2935, 2098 (broad), 1690.

HRMS (ESI+) calculated for $C_{18}H_{18}NOS$ $[M+H]^+$ 296.1104, found 296.1107.

3-isothiocyanato-5-phenyl-1-(p-tolyl)pentan-1-one (2b)



Molecular formula: $C_{19}H_{19}NOS$ MW = 309.43 g/mol

Following the general procedure, enone **1b** (0.15 mmol, 37.5 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2b**. Purification by flash column chromatography (hexane/ethyl acetate 20/1) gave the title compound (42.6 mg, 92%) as a light-yellow oil.

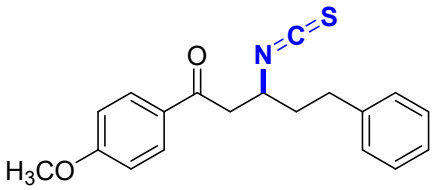
^{1}H NMR (500 MHz, Chloroform-d) δ 7.81 – 7.76 (m, 2H), 7.27 (dd, *J* = 8.3, 6.9 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.19 (d, *J* = 7.4 Hz, 3H), 4.31 (m, 1H), 3.32 (dd, *J* = 17.3, 7.1 Hz, 1H), 3.08 (dd, *J* = 17.3, 5.8 Hz, 1H), 2.87 (ddd, *J* = 14.2, 9.0, 5.2 Hz, 1H), 2.73 (ddd, *J* = 13.6, 9.0, 7.3 Hz, 1H), 2.38 (s, 3H), 2.03 – 1.92 (m, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 195.25, 144.70, 140.16, 133.81, 132.37, 129.49, 128.65, 128.46, 128.21, 126.37, 53.53, 43.84, 37.38, 32.32, 21.70.

IR (cm^{-1}) 2930, 2918 (broad), 2093, 1698, 1453.

HRMS (ESI+) calculated for $C_{19}H_{20}NOS$ $[M+H]^+$ 310.1260, found 310.1262.

3-isothiocyanato-1-(4-methoxyphenyl)-5-phenylpentan-1-one (2c)



Molecular formula: $C_{19}H_{19}NO_2S$ MW = 325.43 g/mol

Following the general procedure, enone **1c** (0.15 mmol, 40.0 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2c**. Purification by flash column chromatography (hexane/ethyl acetate 20/1) gave the title compound (42.4 mg, 87%) as a yellowish oil.

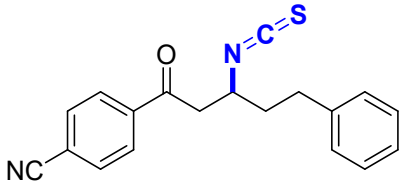
^{1}H NMR (500 MHz, Chloroform-d) δ 7.91 – 7.87 (d, *J* = 9.0 Hz, 2H), 7.33 – 7.27 (m, 2H), 7.23 – 7.19 (m, 3H), 6.95 – 6.92 (m, 2H), 4.35 (m, 1H), 3.87 (s, 3H), 3.36 (dd, *J* = 17.0, 7.0 Hz, 1H), 3.11 (dd, *J* = 17.0, 5.9 Hz, 1H), 2.91 (m, 1H), 2.77 (m, 1H), 2.09 – 1.95 (m, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 194.11, 164.01, 140.19, 132.27, 130.44, 129.37, 128.65, 128.47, 126.37, 113.98, 55.56, 53.66, 43.59, 37.40, 32.34.

IR (cm^{-1}) 2920, 2100 (broad), 1702, 1456, 1257.

HRMS (ESI+) calculated for $C_{19}H_{20}NO_2S$ $[M+H]^+$ 326.1209, found 326.1212.

4-(3-isothiocyanato-5-phenylpentanoyl)benzonitrile (2d)



Molecular formula: $C_{19}H_{16}N_2OS$ MW = 320.41 g/mol

Following the general procedure, enone **1d** (0.15 mmol, 39.2 mg) and TMSNCS (0.3 mmol, 42 µL) in ethanol/dichloromethane gave the product **2d**. Purification by flash column chromatography (hexane/ethyl acetate 20/1) gave the title compound (42.2 mg, 88%) as a light-yellow oil.

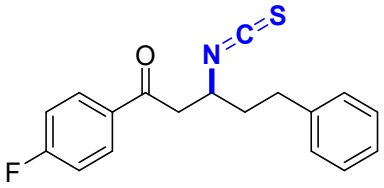
^{1}H NMR (500 MHz, Chloroform-d) δ 7.61 (dd, *J* = 1.7, 0.8 Hz, 1H), 7.33 – 7.28 (m, 2H), 7.25 – 7.19 (m, 4H), 6.57 (dd, *J* = 3.6, 1.7 Hz, 1H), 4.31 (m, 1H), 3.29 (dd, *J* = 16.5, 7.6 Hz, 1H), 3.02 (dd, *J* = 16.5, 5.7 Hz, 1H), 2.90 (dt, *J* = 14.2, 7.2 Hz, 1H), 2.76 (dt, *J* = 13.9, 8.2 Hz, 1H), 2.06 – 1.96 (m, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 184.75, 152.27, 147.00, 140.04, 132.55, 128.68, 128.47, 126.42, 117.99, 117.63, 112.71, 53.30, 43.77, 37.41, 32.24.

IR (cm^{-1}) 2960, 2260 (w), 2100 (broad), 1744.

HRMS (ESI+) calculated for $C_{19}H_{17}N_2OS$ $[M+H]^+$ 321.1056, found 321.1064.

1-(4-fluorophenyl)-3-isothiocyanato-5-phenylpentan-1-one (2e)



Molecular formula: $C_{18}H_{16}FNOS$ MW = 313.39 g/mol

Following the general procedure, enone **1e** (0.15 mmol, 38.0 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2e**. Purification by flash column chromatography (hexane/ethyl acetate 20/1) gave the title compound (43.2 mg, 92%) as a yellowish oil.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.96 – 7.89 (m, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.22 – 7.18 (m, 3H), 7.16 – 7.08 (m, 2H), 4.39 – 4.28 (m, 1H), 3.36 (dd, *J* = 17.3, 7.2 Hz, 1H), 3.10 (dd, *J* = 17.3, 5.8 Hz, 1H), 2.89 (m, 1H), 2.76 (m, 1H), 2.01 (m, 2H).

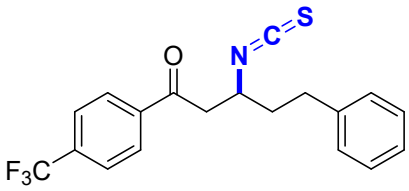
^{13}C NMR (126 MHz, Chloroform-d) δ 194.12, 166.10 (*J* = 256.30 Hz), 140.11, 132.68, 132.66, 132.51, 130.84 (*J* = 9.85 Hz), 128.59 (*J* = 27.15 Hz), 126.46, 116.02 (*J* = 22.01 Hz), 53.38, 43.86, 37.32, 32.30.

^{19}F NMR (283 MHz, Chloroform-d) δ -105.36.

IR (cm^{-1}) 2930, 2097 (broad), 1702, 1683.

HRMS (ESI+) calculated for $C_{18}H_{17}FNOS$ $[M+H]^+$ 314.1009, found 314.1010.

3-isothiocyanato-5-phenyl-1-(4-(trifluoromethyl)phenyl)pentan-1-one (2f)



Molecular formula: $C_{19}H_{16}F_3NOS$ MW = 363.40 g/mol

Following the general procedure, enone **1f** (0.15 mmol, 45.6 mg) and TMSNCS (0.3 mmol, 42 µL) in ethanol/dichloromethane gave the product **2f**. Purification by flash column chromatography (hexane/ethyl acetate 20/1) gave the title compound (49 mg, 90%) as a yellow solid.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.94 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.65 – 7.60 (m, 1H), 7.50 (t, *J* = 7.8 Hz, 2H), 7.37 – 7.31 (m, 2H), 7.24 (d, *J* = 1.9 Hz, 2H), 4.45 – 4.34 (m, 1H), 3.44 (dd, *J* = 17.3, 7.3 Hz, 1H), 3.19 (dd, *J* = 17.3, 5.8 Hz, 1H), 2.99 – 2.92 (m, 1H), 2.81 (m, 1H), 2.13 – 2.00 (m, 2H).

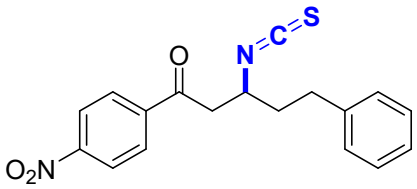
^{13}C NMR (126 MHz, Chloroform-d) δ 195.66, 140.13, 136.24, 133.75, 132.54, 128.83, 128.68, 128.48, 128.09, 126.41, 53.44, 43.96, 37.36, 32.32.

^{19}F NMR (283 MHz, Chloroform-d) δ -63.17.

IR (cm^{-1}) 2970, 2103 (broad), 1737, 1420.

HRMS (ESI+) calculated for $C_{19}H_{17}F_3NOS$ $[M+H]^+$ 364.0977, found 364.0975.

3-isothiocyanato-1-(4-nitrophenyl)-5-phenylpentan-1-one (2g)



Molecular formula: $C_{18}H_{16}N_2O_3S$ MW = 340.40 g/mol

Following the general procedure, enone **1g** (0.15 mmol, 42.17 mg) and TMSNCS (0.3 mmol, 42 μL) in ethanol/dichloromethane gave the product **2g**. Purification by flash column chromatography (hexane/ethyl acetate 20/1) gave the title compound (47.9 mg, 94%) as a yellow solid.

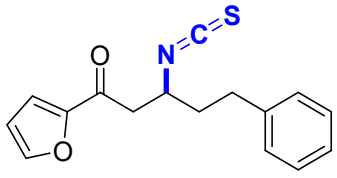
^{1}H NMR (500 MHz, Chloroform-d) δ 8.35 – 8.32 (m, 2H), 8.09 – 8.06 (m, 2H), 7.34 – 7.30 (m, 2H), 7.25 – 7.21 (m, 3H), 4.40 – 4.34 (m, 1H), 3.46 (dd, *J* = 17.5, 7.5 Hz, 1H), 3.18 (dd, *J* = 17.5, 5.3 Hz, 1H), 2.94 (dt, *J* = 14.0, 7.0 Hz, 1H), 2.80 (dt, *J* = 14.0, 8.2 Hz, 1H), 2.09 – 2.03 (m, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 194.33, 150.79, 140.42, 139.88, 133.39, 129.17, 128.76, 128.48, 126.54, 124.08, 53.08, 44.48, 37.27, 32.22.

IR (cm^{-1}) 2931, 2103 (broad), 1690, 1540.

HRMS (ESI+) calculated for $C_{18}H_{17}N_2O_3S$ $[M+H]^+$ 341.0954, found 341.0960.

1-(furan-2-yl)-3-isothiocyanato-5-phenylpentan-1-one (2h)



Molecular formula: $C_{16}H_{15}NO_2S$ MW = 285.36 g/mol

Following the general procedure, enone **1h** (0.15 mmol, 34.0 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2h**. Purification by flash column chromatography (hexane/ethyl acetate 20/1) gave the title compound (38.5 mg, 90%) as a yellowish solid.

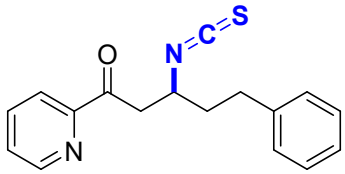
^{1}H NMR (500 MHz, Chloroform-d) δ 7.61 (dd, *J* = 1.7, 0.8 Hz, 1H), 7.33 – 7.28 (m, 2H), 7.24 (dd, *J* = 3.6, 0.8 Hz, 1H), 7.23 – 7.20 (m, 3H), 6.57 (dd, *J* = 3.6, 1.7 Hz, 1H), 4.35 – 4.26 (m, 1H), 3.29 (dd, *J* = 16.5, 7.6 Hz, 1H), 3.02 (dd, *J* = 16.5, 5.7 Hz, 1H), 2.90 (dt, *J* = 14.2, 7.2 Hz, 1H), 2.77 (dt, *J* = 14.0, 8.2 Hz, 1H), 2.02 (dt, *J* = 8.2, 6.9 Hz, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 184.77, 152.25, 147.00, 140.03, 132.56, 128.68, 128.47, 126.41, 118.00, 112.71, 53.30, 43.77, 37.41, 32.23.

IR (cm^{-1}) 2930, 2093 (broad), 1675, 1330, 750.

HRMS (ESI+) calculated for $C_{16}H_{16}NO_2S$ $[M+H]^+$ 286.0896, found 286.0893.

3-isothiocyanato-5-phenyl-1-(pyridin-2-yl)pentan-1-one (2i)



Molecular formula: $C_{17}H_{16}N_2OS$ MW = 296.39 g/mol

Following the general procedure, enone **1i** (0.15 mmol, 35.6 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2i**. Purification by flash column chromatography (hexane/ethyl acetate 15/1) gave the title compound (40 mg, 90%) as a yellow solid.

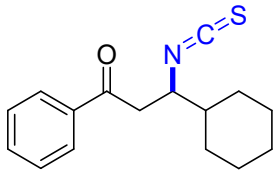
^{1}H NMR (500 MHz, Chloroform-d) δ 8.35 – 8.32 (m, 2H), 8.09 – 8.06 (m, 2H), 7.34 – 7.30 (m, 2H), 7.23 (ddt, *J* = 8.4, 3.8, 1.8 Hz, 3H), 4.37 (tt, *J* = 7.4, 5.4 Hz, 1H), 3.46 (dd, *J* = 17.5, 7.5 Hz, 1H), 3.18 (dd, *J* = 17.5, 5.3 Hz, 1H), 2.94 (dt, *J* = 14.0, 7.0 Hz, 1H), 2.80 (dt, *J* = 14.0, 8.2 Hz, 1H), 2.09 – 2.03 (m, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 194.33, 150.67, 140.42, 139.87, 133.40, 129.17, 128.76, 128.48, 126.53, 126.28, 124.08, 53.08, 44.48, 37.27, 32.22.

IR (cm^{-1}) 2930, 2100 (broad), 1691, 1350.

HRMS (ESI+) calculated for $C_{17}H_{16}N_2OS$ $[M+2H]^{2+}$ 149.0564, found 149.0575.

3-cyclohexyl-3-isothiocyanato-1-phenylpropan-1-one (2j)



Molecular formula: $C_{16}H_{19}NOS$ MW = 273.39 g/mol

Following the general procedure, enone **1j** (0.15 mmol, 32.2 mg) and TMSNCS (0.3 mmol, 42 µL) in ethanol/dichloromethane gave the product **2j**. Purification by flash column chromatography (hexane/ethyl acetate 15/1) gave the title compound (36 mg, 88%) as a yellowish oil.

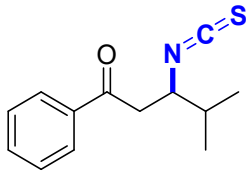
^{1}H NMR (500 MHz, Chloroform-d) δ 8.00 – 7.92 (m, 2H), 7.61 (td, *J* = 7.2, 1.3 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 2H), 4.29 (dt, *J* = 8.7, 4.6 Hz, 1H), 3.39 (dd, *J* = 17.2, 8.2 Hz, 1H), 3.18 (dd, *J* = 17.2, 4.7 Hz, 1H), 1.86 – 1.80 (m, 3H), 1.78 – 1.67 (m, 2H), 1.66 – 1.59 (m, 1H), 1.33 – 1.14 (m, 5H).

^{13}C NMR (126 MHz, Chloroform-d) δ 196.08, 136.33, 133.72, 131.03, 128.83, 128.14, 58.75, 42.42, 30.25, 27.81, 25.98, 25.77.

IR (cm^{-1}) 2935, 2103 (broad), 1685.

HRMS (ESI+) calculated for $C_{16}H_{20}NOS$ $[M+H]^+$ 274.1260, found 274.1265.

3-isothiocyanato-4-methyl-1-phenylpentan-1-one (2k)



Molecular formula: $C_{13}H_{15}NOS$ MW = 233.33 g/mol

Following the general procedure, enone **1k** (0.15 mmol, 26.2 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2k**. Purification by flash column chromatography (hexane/ethyl acetate 30/1) gave the title compound (33 mg, 95%) as a yellowish oil.

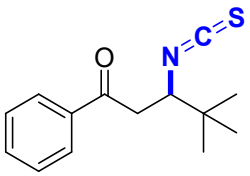
^{1}H NMR (500 MHz, Chloroform-d) δ 7.99 – 7.92 (m, 2H), 7.64 – 7.58 (m, 1H), 7.53 – 7.43 (m, 2H), 4.32 (dt, *J* = 8.6, 4.4 Hz, 1H), 3.39 (dd, *J* = 17.2, 8.3 Hz, 1H), 3.13 (dd, *J* = 17.2, 4.6 Hz, 1H), 1.99 (hept, *J* = 6.7, 4.3 Hz, 1H), 1.09 (d, *J* = 6.8 Hz, 3H), 1.05 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-d) δ 196.01, 136.31, 133.75, 131.34, 128.84, 128.14, 59.37, 41.52, 33.03, 19.91, 17.10.

IR (cm^{-1}) 2920, 2093 , 1685, 1450.

HRMS (ESI+) calculated for $C_{13}H_{16}NOS$ $[M+H]^+$ 234.0947, found 234.0950.

3-isothiocyanato-4,4-dimethyl-1-phenylpentan-1-one (2l)



Molecular formula: $C_{14}H_{17}NOS$ MW = 247.36 g/mol

Following the general procedure, enone **1l** (0.15 mmol, 28.4 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2l**. Purification by flash column chromatography (hexane/ethyl acetate 35/1) gave the title compound (35.5 mg, 96%) as a pale oil.

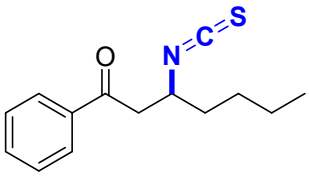
^{1}H NMR (500 MHz, Chloroform-d) δ 7.98 – 7.94 (m, 2H), 7.60 (tt, *J* = 7.0, 1.3 Hz, 1H), 7.53 – 7.47 (m, 2H), 4.19 (dd, *J* = 9.9, 2.6 Hz, 1H), 3.35 (dd, *J* = 17.0, 9.9 Hz, 1H), 3.10 (dd, *J* = 17.0, 2.6 Hz, 1H), 1.06 (s, 9H).

^{13}C NMR (126 MHz, Chloroform-d) δ 196.28, 136.44, 133.70, 128.82, 128.17, 63.06, 39.50, 35.66, 26.29.

IR (cm^{-1}) 2970, 2097 (broad), 1689, 1450.

HRMS (ESI+) calculated for $C_{14}H_{18}NOS$ $[M+H]^+$ 248.1104, found 248.1105.

3-isothiocyanato-1-phenylheptan-1-one (2m)



Molecular formula: $C_{14}H_{17}NOS$ MW = 247.36 g/mol

Following the general procedure, enone **1m** (0.15 mmol, 30.3 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2m**. Purification by flash column chromatography (hexane/ethyl acetate 20/1) gave the title compound (36.9 mg, 90%) as a yellowish oil.

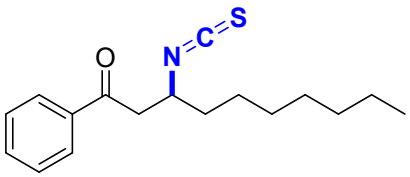
^{1}H NMR (500 MHz, Chloroform-d) δ 8.00 – 7.93 (m, 2H), 7.67 – 7.61 (m, 1H), 7.56 – 7.47 (m, 2H), 4.40 (tt, *J* = 7.1, 5.7 Hz, 1H), 3.43 (dd, *J* = 17.2, 7.1 Hz, 1H), 3.19 (dd, *J* = 17.2, 5.7 Hz, 1H), 1.77 – 1.69 (m, 2H), 1.32 (h, *J* = 2.9, 2.2 Hz, 4H), 0.93 – 0.91 (m, 3H).

^{13}C NMR (126 MHz, Chloroform-d) δ 195.90, 136.25, 133.75, 131.38, 128.84, 128.11, 53.97, 43.98, 35.55, 28.14, 22.14, 13.94.

IR (cm^{-1}) 2970, 2097 (broad), 1747, 1448, 1375.

HRMS (ESI+) calculated for $C_{14}H_{18}NOS$ $[M+H]^+$ 248.1104, found 248.1103.

3-isothiocyanato-1-phenyldecan-1-one (2n)



Molecular formula: $C_{17}H_{23}NOS$ MW = 289.44 g/mol

Following the general procedure, enone **1n** (0.15 mmol, 34.5 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2n**. Purification by flash column chromatography (hexane/ethyl acetate 25/1) gave the title compound (40.4 mg, 93%) as a yellowish oil.

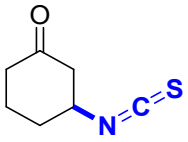
^{1}H NMR (500 MHz, Chloroform-d) δ 7.98 – 7.92 (m, 2H), 7.63 – 7.57 (m, 1H), 7.52 – 7.43 (m, 2H), 4.38 (s, 1H), 3.40 (dd, *J* = 17.2, 7.1 Hz, 1H), 3.16 (dd, *J* = 17.2, 5.7 Hz, 1H), 1.75 – 1.67 (m, 2H), 1.34 – 1.27 (m, 10H), 0.89 (t, *J* = 2.7 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-d) δ 195.91, 136.27, 133.75, 131.44, 128.84, 128.12, 54.00, 43.98, 36.86, 31.74, 29.11, 28.96, 26.04, 22.64, 14.11.

IR (cm^{-1}) 2930, 2135 (broad), 1680, 1450.

HRMS (ESI+) calculated for $C_{17}H_{24}NOS$ $[M+H]^+$ 290.1573, found 290.1574.

3-isothiocyanatocyclohexan-1-one (2o)



Molecular formula: C_7H_9NOS MW = 155.22 g/mol

Following the general procedure, cyclohex-2-en-1-one (0.15 mmol, 14.5 mg) and TMSNCS (0.3 mmol, 42 µL) gave the product **2o**. Purification by flash column chromatography (hexane/ethyl acetate 10/1) gave the title compound (22.8 mg, 98%) as a yellowish solid.

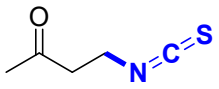
^{1}H NMR (500 MHz, Chloroform-d) δ 4.20 (m, 1H), 2.71 (m, 1H), 2.60 (m, 1H), 2.41 – 2.36 (m, 2H), 2.19 – 1.99 (m, 3H), 1.87 – 1.78 (m, 1H).

^{13}C NMR (126 MHz, Chloroform-d) δ 206.31, 133.48, 55.45, 47.60, 40.63, 31.55, 21.37.

IR (cm^{-1}) 2084 (broad), 1725,1465.

HRMS (ESI+) calculated for $C_7H_{10}NOS$ $[M+H]^+$ 156.0478, found 156.0480.

4-isothiocyanatobutan-2-one (2p)



Molecular formula: C_5H_7NOS MW = 129.18 g/mol

Following the general procedure, but-3-en-2-one (0.3 mmol, 21.0 mg) and TMSNCS (0.6 mmol, 84 µL) gave the product **2p**. Purification by flash column chromatography (hexane/ethyl acetate 5/1) gave the title compound (21.2 mg, 55%) as a yellowish solid.

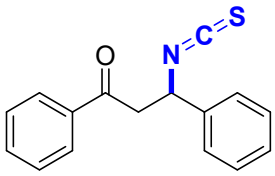
^{1}H NMR (500 MHz, Chloroform-d) δ 3.77 (t, *J* = 6.6 Hz, 2H), 2.85 (t, *J* = 6.6 Hz, 2H), 2.22 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-d) δ 204.27, 131.60, 42.83, 39.51, 30.13.

IR (cm^{-1}) 2927, 2123, 1722, 1440.

HRMS (ESI+) calculated for C_5H_8NOS $[M+H]^+$ 130.0321 found 130.0322.

3-isothiocyanato-1,3-diphenylpropan-1-one (2q)

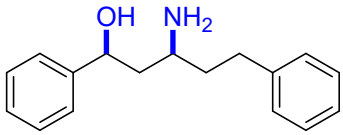


Molecular formula: $C_{16}H_{13}NOS$ MW = 267.35 g/mol

Following the general procedure, chalcone (0.3 mmol, 62.5 mg) and TMSNCS (1.5 mmol, 210 µL) gave the product **2q**. Purification by flash column chromatography (hexane/ethyl acetate 10/1) gave the title compound (yield is in range of 6.4-20.0 mg, 8-25%) as a yellowish solid. All characterization data were consistent with those reported.[21]

^{1}H NMR (500 MHz, Chloroform-d) δ 7.95 – 7.91 (m, 2H), 7.59 (m, 1H), 7.49 – 7.44 (m, 2H), 7.40 (d, J = 4.4 Hz, 4H), 7.36 – 7.33 (m, 1H), 5.54 (dd, J = 8.4, 4.8 Hz, 1H), 3.71 (dd, J = 17.4, 8.4 Hz, 1H), 3.40 (dd, J = 17.4, 4.8 Hz, 1H).

3-amino-1,5-diphenylpentan-1-ol (P1)



Molecular formula: $C_{17}H_{21}NO$ MW = 255.36 g/mol

To a round-bottom flask, **2a** (0.3 mmol, 88.62 mg) was dissolved into methanol (10 mL) and the solution cooled to 0 °C. $NaBH_4$ (0.9 mmol, 13.62 mg) was added and the mixture refluxed at 70 °C for 12 h. Ammounia solution (1 mL) was added dropwise. Then, the mixture was extracted with dichloromethane, the organic phase was washed with brine and dried over $NaSO_4$. The dichloromethane was removed by rotary evaporator.[22]

Purification of the crude mixture by flash column chromatography (hexane/ethyl acetate 10/1) afforded compound 3-amino-1,5-diphenylpentan-1-ol **P1** (68.9 mg, 90%, syn: anti= 5:4) as a white solid.

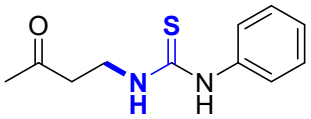
^{1}H NMR (500 MHz, Chloroform-d) δ 8.24 (s, 1H), 7.37 (d, *J* = 3.5 Hz, 4H), 7.32 – 7.27 (m, 3H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.18 – 7.14 (m, 2H), 5.25 (dd, *J* = 11.8, 2.4 Hz, 1H), 3.66 (ddd, *J* = 11.7, 6.8, 3.7 Hz, 1H), 2.70 (dtd, *J* = 18.5, 6.4, 1.8 Hz, 2H), 2.34 – 2.26 (m, 1H), 2.13 – 2.00 (m, 2H), 1.94 – 1.83 (m, 2H).

^{13}C NMR (126 MHz, Chloroform-d) δ 139.61, 137.56, 129.04, 128.87, 128.78, 128.21, 126.69, 126.17, 80.63, 52.17, 36.88, 34.42, 31.18.

IR (cm^{-1}) 3854, 3183, 2323, 1150.

HRMS (ESI+) calculated for $C_{17}H_{22}NO$ $[M+H]^+$ requires 256.1696 found 256.1699.

1-(3-oxobutyl)-3-phenylthiourea (P2)



Molecular formula: $C_{11}H_{14}N_2OS$ MW = 222.31 g/mol

To a round-bottom flask, **2p** (0.3 mmol, 38.75 mg) and aniline (0.45 mmol, 41 µL) were dissolved into methanol (10 mL), then refluxed for 8h. The solvents were evaporated under reduced pressure and the resulting materials were purified by flash column chromatography (hexanes/ethyl acetate 5/1) to afford the 1-(3-oxobutyl)-3-phenylthiourea **P2** (53.4 mg, 80%) as a white solid.[23]

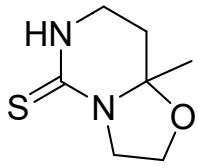
^{1}H NMR (500 MHz, Chloroform-d) δ 7.68 (s, 1H), 7.44 (tt, *J* = 8.4, 1.9 Hz, 2H), 7.34 – 7.29 (m, 1H), 7.15 (d, *J* = 7.8 Hz, 2H), 6.77 (s, 1H), 3.87 (q, *J* = 5.7 Hz, 2H), 2.89 (t, *J* = 5.5 Hz, 2H), 2.16 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-d) δ 208.87, 180.09, 135.98, 130.21, 127.26, 124.83, 42.32, 39.91, 30.12.

IR (cm^{-1}) 3280, 2330, 1700, 1540.

HRMS (ESI+) calculated for $C_{11}H_{15}N_2OS$ $[M+H]^+$ 223.0900 found 223.0902.

hexahydro-8a-methyl-6H-oxazolo[3,2-c]pyrimidine-5-thione (P3)



Molecular formula: $C_7H_{12}N_2OS$ MW = 172.25 g/mol

To a round-bottom flask, **2p** (0.2 mmol, 25.80 mg) and ethanolamine (0.25 mmol, 15 μL) were dissolved into methanol (5 mL), then refluxed under argon for 12 h. The methanol was removed by rotary evaporator. Water was added, and the mixture was extracted with dichloromethane (2× 20 mL), the organic phase was washed with brine and dried over $NaSO_4$. The dichloromethane was removed by rotary evaporator. The residue was purified by flash column chromatography by using benzene and ethyl acetate mixture (5/1) as eluent to afford hexahydro-8a-methyl-6H-oxazolo[3,2-c]pyrimidine-5-thione **P3**(18.3 mg, 53%) as a solid.[24]

^{1}H NMR (500 MHz, Chloroform-d) δ 6.44 (s, 1H), 4.25 (ddd, *J* = 10.9, 8.3, 7.4 Hz, 1H), 4.11 (dqt, *J* = 12.6, 8.8, 4.9 Hz, 2H), 3.83 (ddd, *J* = 11.0, 7.1, 4.7 Hz, 1H), 3.42 (m, 1H), 3.28 (td, *J* = 13.3, 4.6 Hz, 1H), 2.19 (ddt, *J* = 12.7, 4.6, 1.6 Hz, 1H), 1.83 (m, 1H), 1.40 (d, *J* = 0.9 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-d) δ 175.18, 90.16, 62.79, 48.54, 38.44, 31.61, 22.56.

IR (cm^{-1}) 1653, 1457, 906, 722.

HRMS (ESI+) calculated for $C_7H_{13}N_2OS$. $[M+H]^+$ requires 173.0743 found 173.0741.

5. Additional control experiments

The reaction between TMSNCS and ethanol (95%) can proceed to isothiocyanic acid and CH_3CH_2OTMS, as detected by ^1H NMR (Figure S8).[25] There is no reaction between TMSNCS and hexanes.

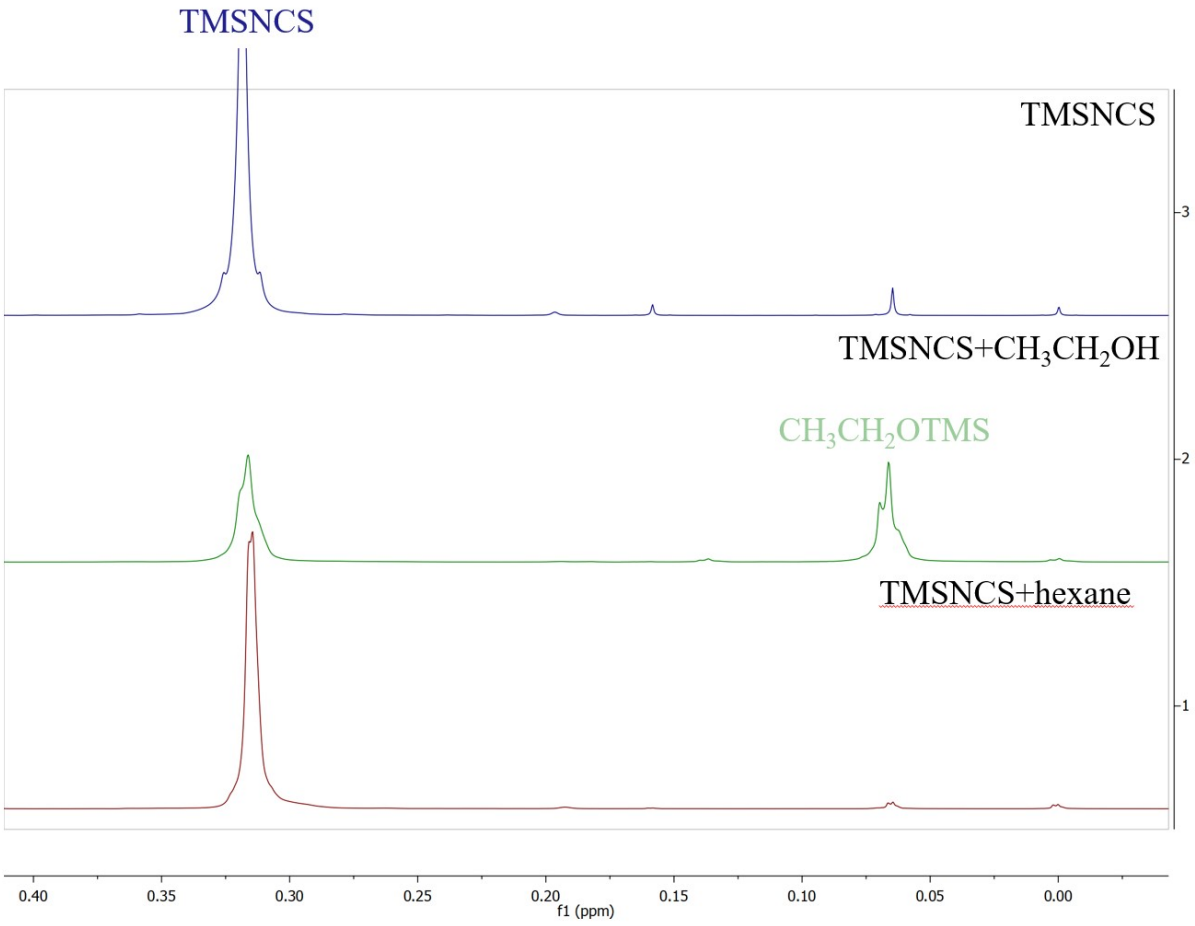


Figure S8 NMR comparison between TMSNCS in ethanol and TMSNCS in hexane[a]

[a] Reaction condition: TMSNCS (0.3 mmol, 42 μL) and ethanol (0.3 mmol, 18.4 μL); TMSNCS (0.3 mmol, 42 μL) and hexane (0.3 mmol, 39.1 μL) for 12 h at 25 ℃

6. Computational details

Density functional theory (DFT) calculations were performed using Gaussian 16.[26] Geometry optimizations were done with the M06-2X functional,[27] using the 6-31+G(d,p) basis set, and SMD implicit solvation[28] to model the effects of ethanol solution (the experimental solvent). Vibrational analysis on the stationary points allowed for the confirmation of minima structures (zero imaginary frequencies) and transition structures (TS, exactly one imaginary frequency). Zero-point energy, enthalpy and free energy corrections were obtained with a state of 1 atm pressure and 298.15 K temperature using Goodvibes version 3.2,[29] applying Grimme's quasiharmonic oscillator approximation with a frequency cut-off value of 100 cm^{-1}.[30] To obtain accurate energies, single-point energy refinements were then performed at the M06−2X/def2tzvpp level of theory (this basis set affords more relevant energy values in our system, Table S2), using the SMD ethanol solvation model. The free energy values reported were then obtained by adding the free energy corrections obtained from the frequency analysis to the single-point electronic energies. Visualizations of the computed structures were prepared using CYLview.[31]

Benchmark of single point refinement methods:

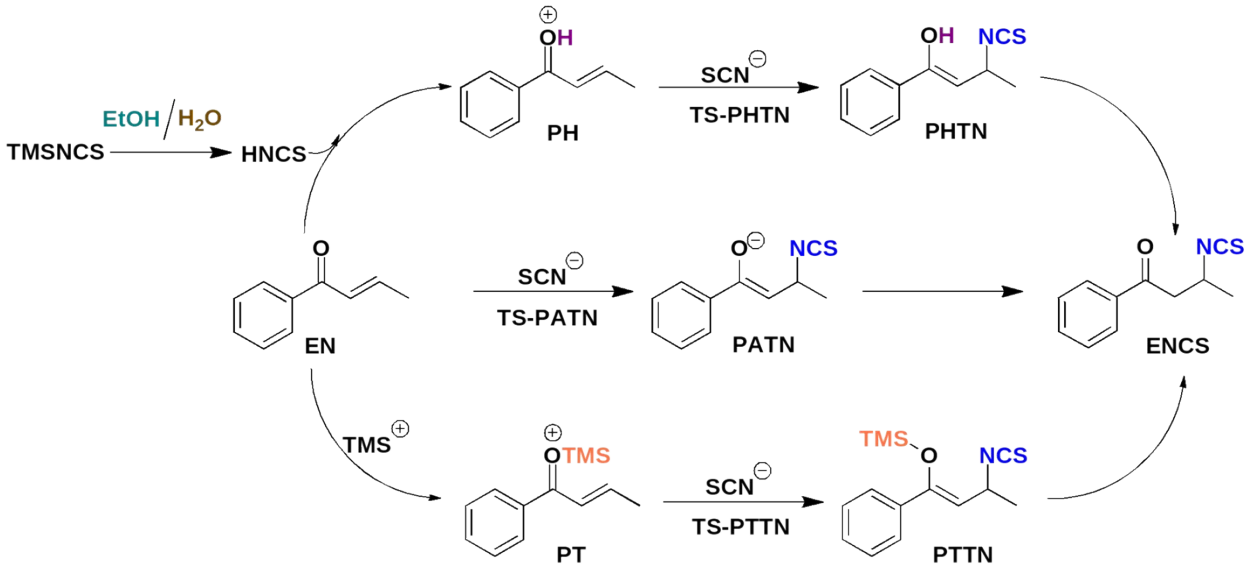


Table S2. Intermediates single-point energy refinement methods screening

Entry	SPE method[a]	PHTN[b]	PHTN[c]	PATN	PTTN
1	M062X/def2tzvpp	9.2	8.5	24.2	10.2
2	M062X/aug-cc-pVTZ	10.0	9.6	24.8	10.5
3	ωB97X-D/aug-cc-pVTZ	13.2	12.9	26.5	12.5

4	B3LYP-D3(BJ)/aug-cc-pVTZ	15.8	15.8	27.8	15.1

[a] Single-point energy refinement method with the SMD solvation model. [b] Protonic pathway with EtOH involved. [c] Protonic pathway with H_2O involved

Table S3. TS single-point energy refinement methods screening

Entry	SPE method[a]	TS-PHTN[b]	TS-PHTN[c]	TS-PATN	TS-PTTN
1	M062X/def2tzvpp	26.0	25.4	29.3	29.3
2	M062X/aug-cc-pVTZ	26.2	25.7	29.6	28.7
3	wB97X-D/aug-cc-pVTZ	30.0	29.2	31.5	31.0
4	B3LYP-D3(BJ)/aug-cc-pVTZ	26.3	26.3	29.4	27.0

[a] Single-point energy refinement method with the SMD solvation model. [b] Protonic pathway with EtOH involved. [c] Protonic pathway with H_2O involved

7. Additional Figures/Schemes

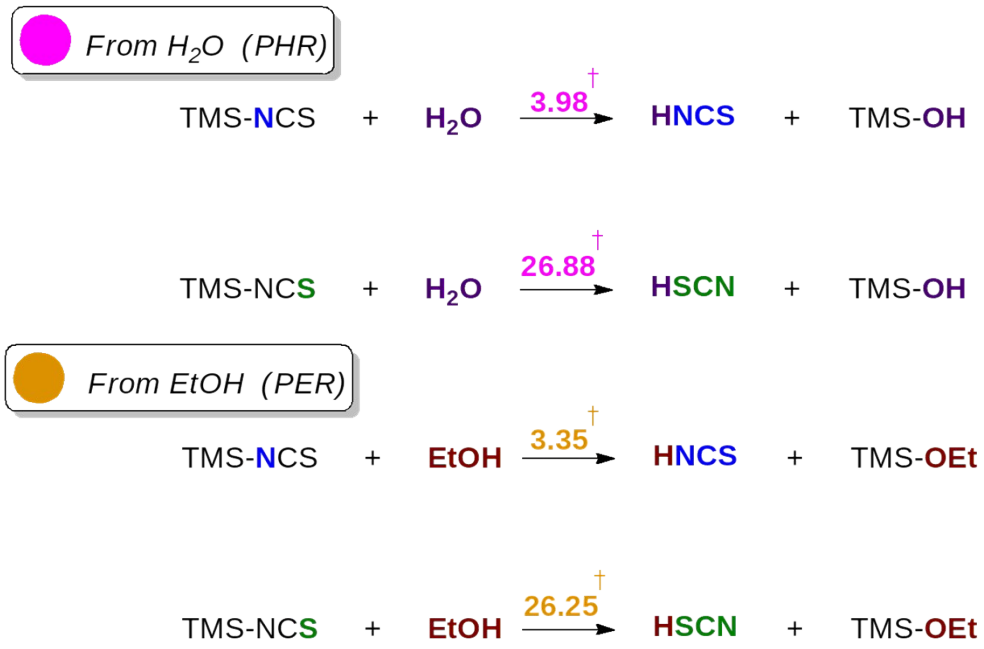
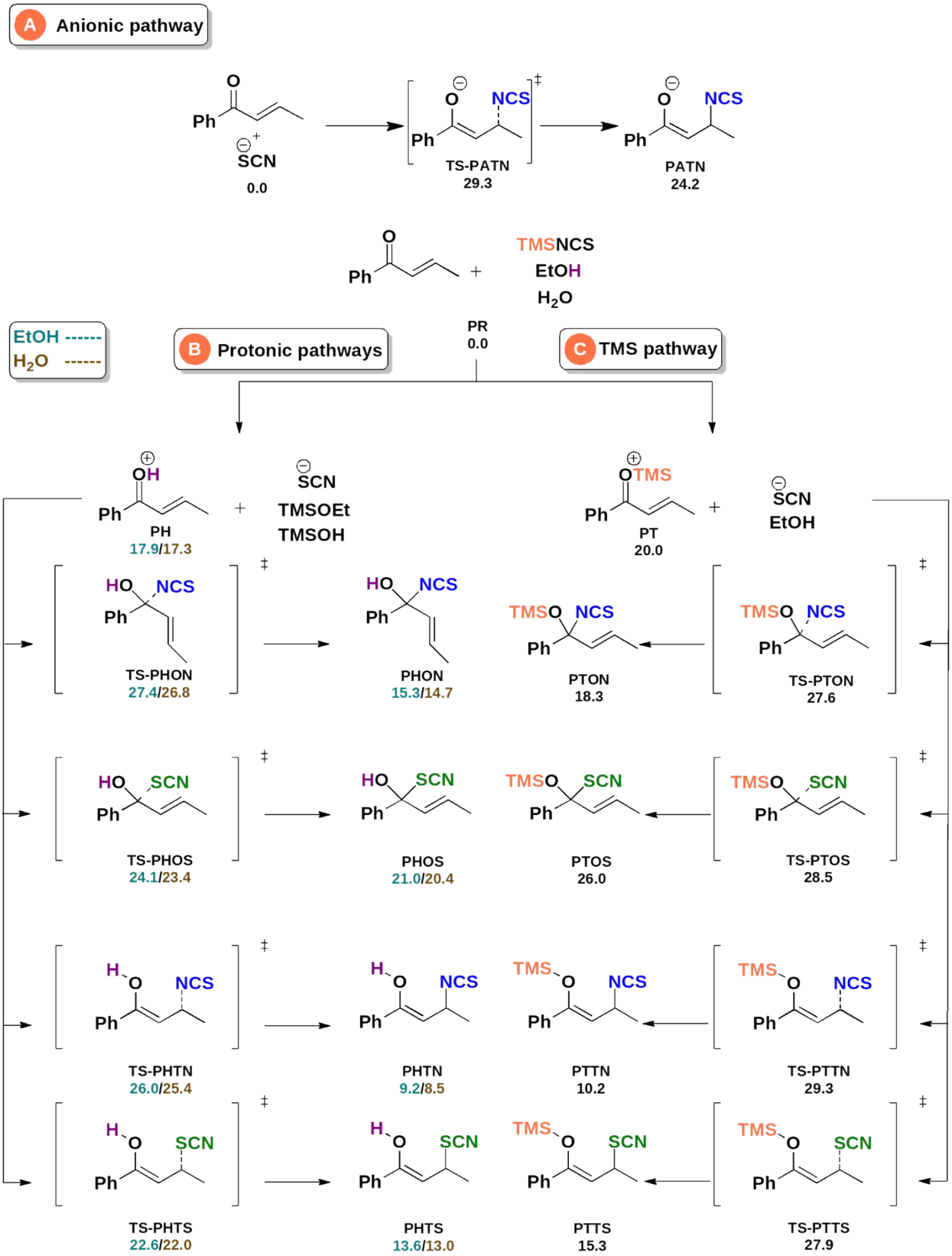


Figure S9. The first step of the reactions protonated pathways H_2O and EtOH

For the case of the plausible protonated pathways of EtOH and H_2O, the first step involves the protic solvent forming isothiocyanic acid, HNCS or thiocyanic acid HSCN (Figure S9). Because of this, the difference in free energies were calculated between both species: for HSCN, it is approximately 23 kcal/mol energetically lower in free energy. Guda et al.[32] reported similar

experimental observations and showed that the formation of HNCS is more favorable, as reported by our DFT studies.

Figure S10 shows the most plausible reaction mechanisms: in the top is shown the anionic pathway; in light blue the EtOH-involved pathway; in brown is shown the H_2O-involved pathway; and in black is the TMS-involved pathway. The reactants, enone, EtOH, TMSNCS and H_2O, are the reference states.


A Anionic pathway
Ph
O
SCN
0.0
NCS
TS-PATN
29.3
PATN
24.2
TMSNCS
EtOH
H2O
PR
0.0
EtOH ------
H2O ------
B Protonic pathways
C TMS pathway
OH
PH
17.9/17.3
SCN
TMSOEt
TMSOH
OTMS
PT
20.0
EtOH
HO
TS-PHON
27.4/26.8
PHON
15.3/14.7
TMSO
PTON
18.3
TS-PTON
27.6
TS-PHOS
24.1/23.4
PHOS
21.0/20.4
PTOS
26.0
TS-PTOS
28.5
H
TMS
TS-PHTN
26.0/25.4
PHTN
9.2/8.5
PTTN
10.2
TS-PTTN
29.3
TS-PHTS
22.6/22.0
PHTS
13.6/13.0
PTTS
15.3
TS-PTTS
27.9

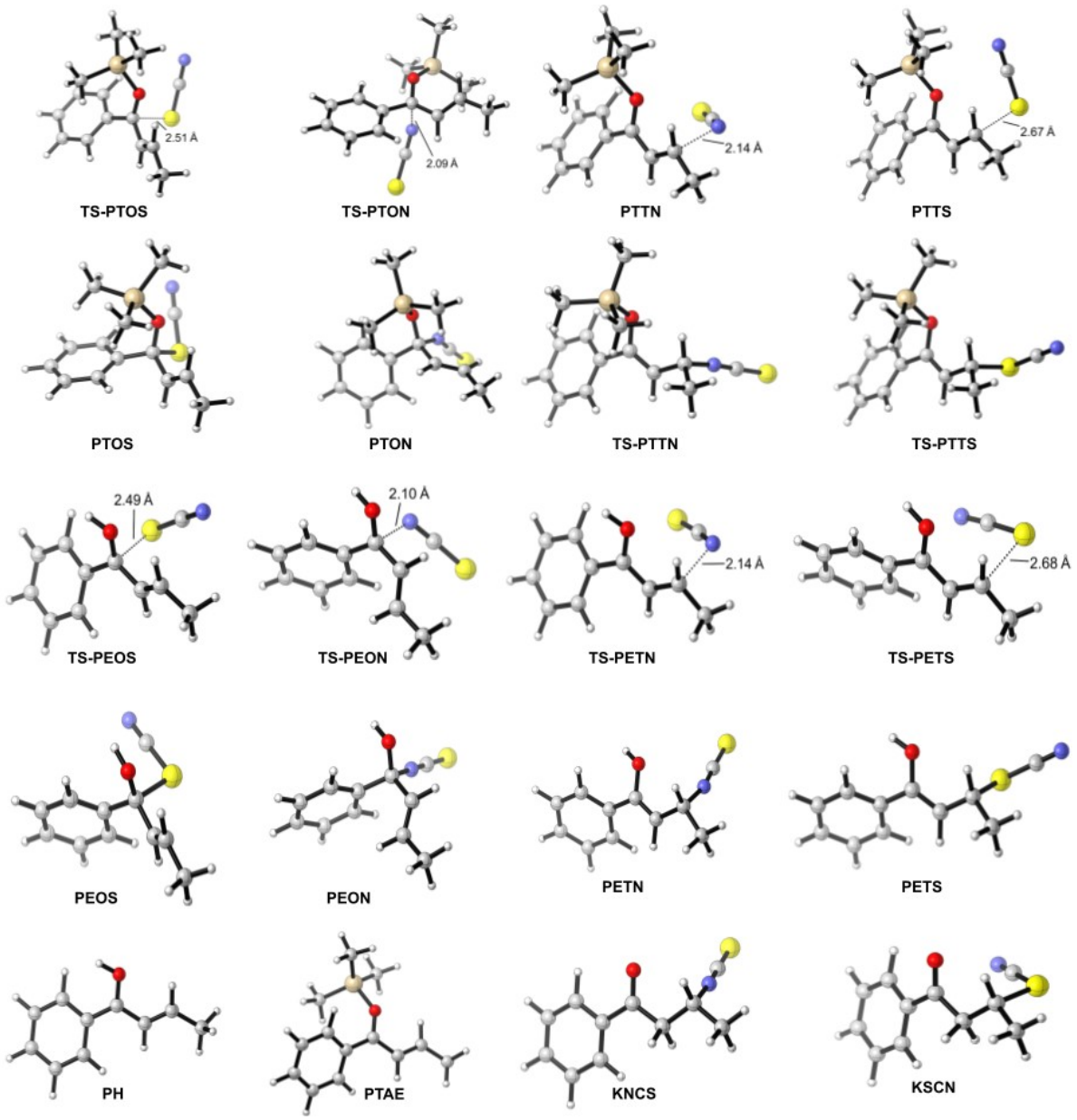


Figure S10. Plausible reaction mechanisms

Figure S11 depicts the reaction mechanism for the protonated pathway that shows more favorable activation and reaction energies than the TMS-involved pathway. Also, the reaction can happen with anhydrous ethanol like the EtOH-involved pathway. However, the reaction can occur at a lower energy cost with the presence of water in the reaction media, shown by the H_2O-involved pathway.

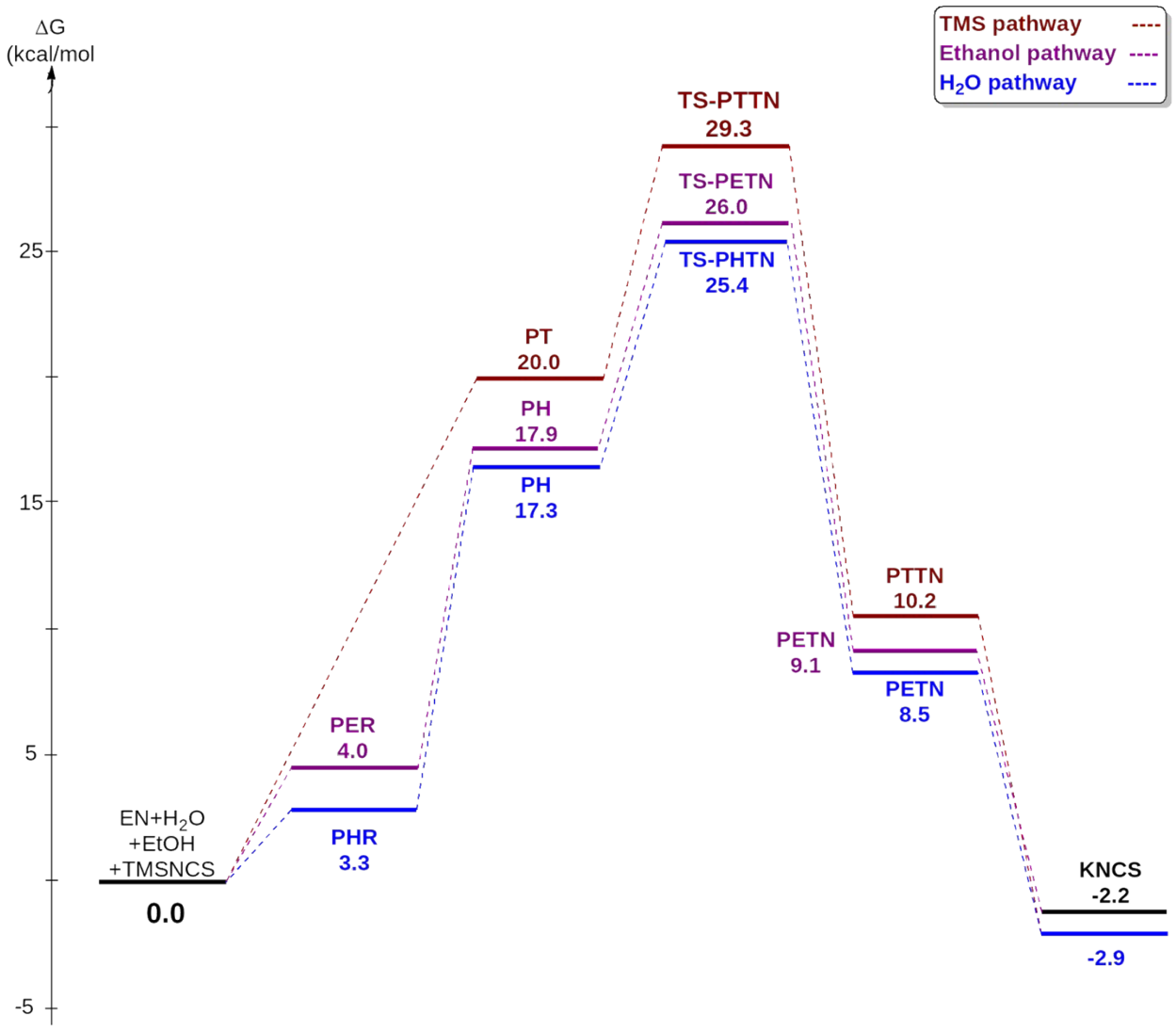


Figure S11. PES pathways of the plausible mechanisms

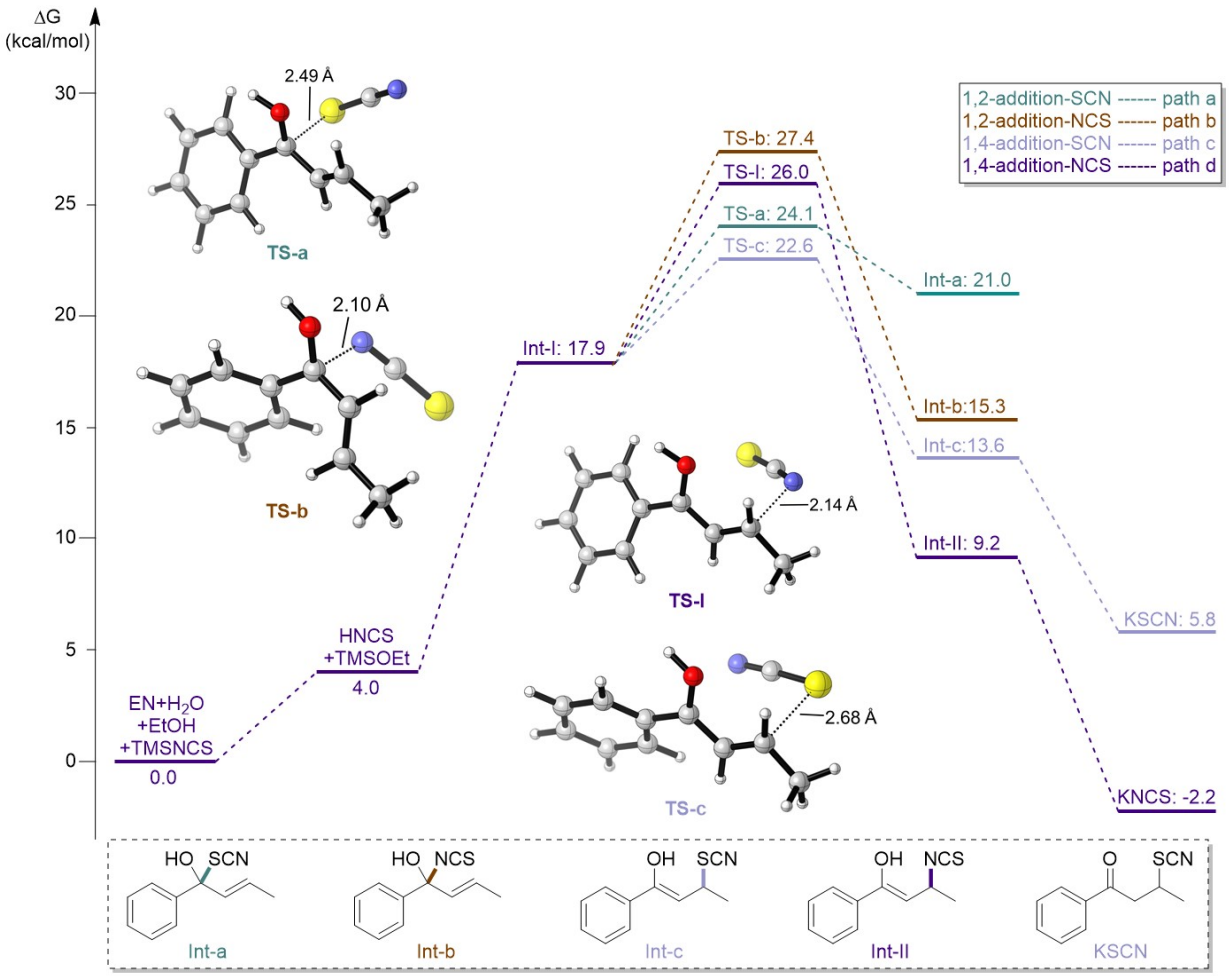


Figure S12. PES pathways of the ethanol pathway

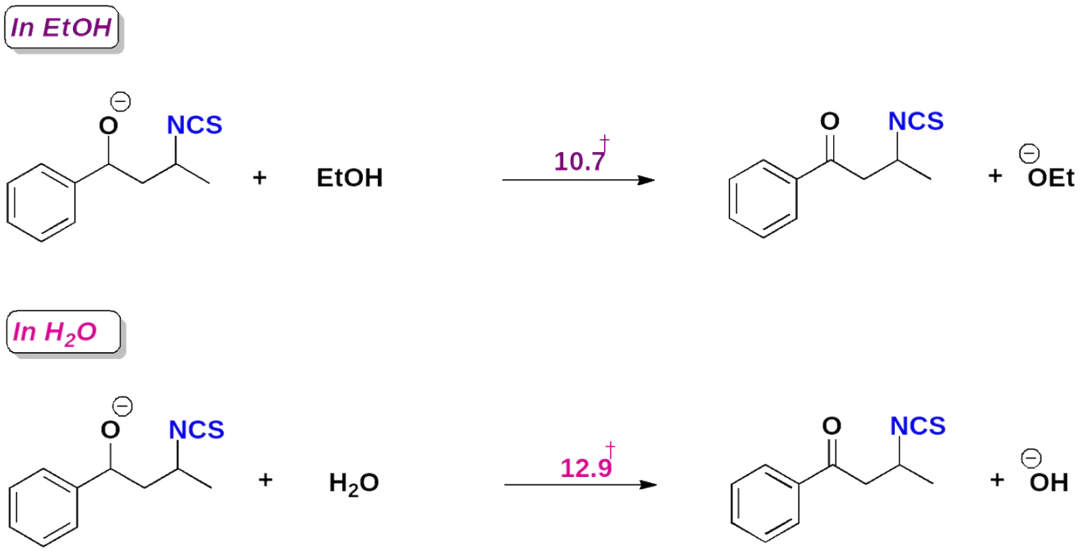


Figure S13. PES pathways of the ethanol pathway

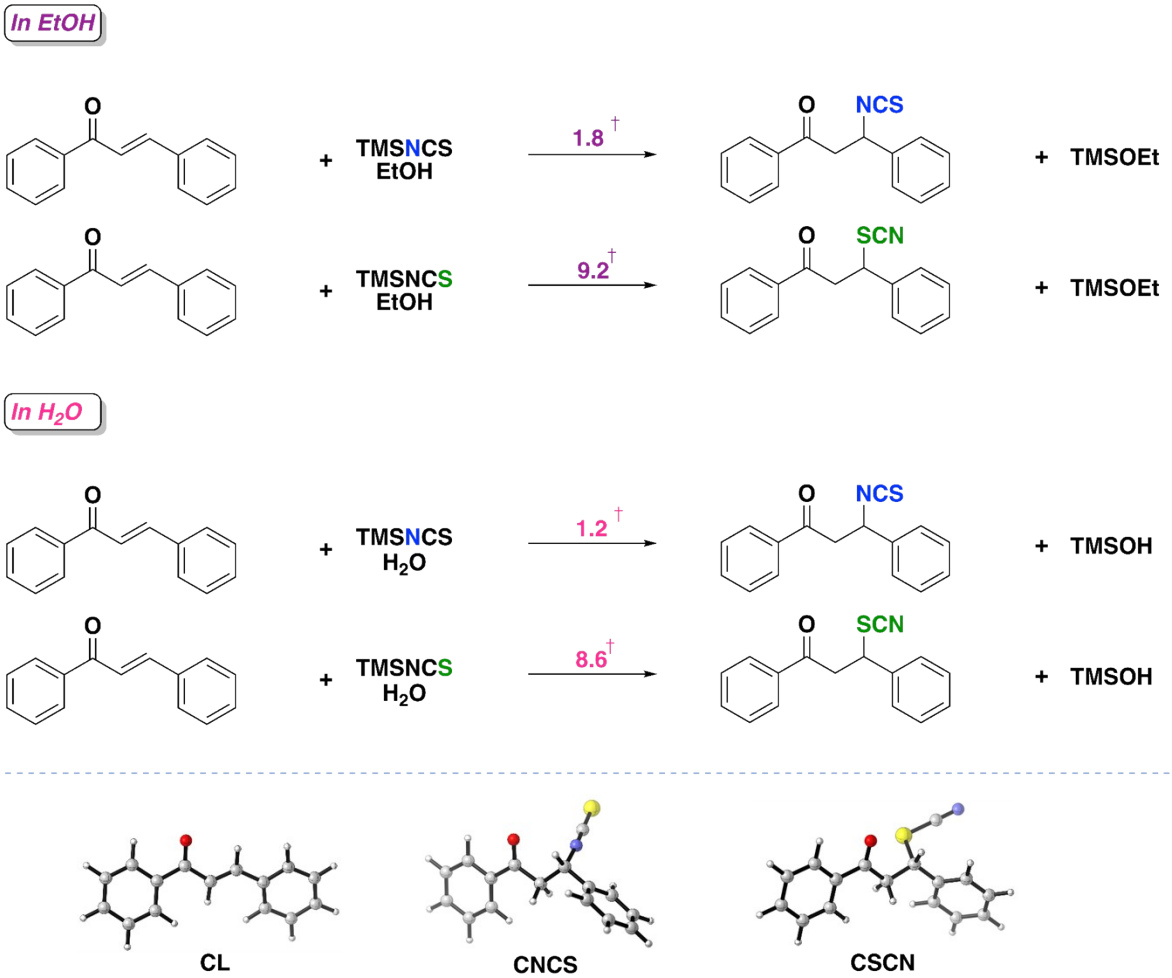


Figure S14. Free energies for chalcone substrate

8. Complete energy data

Energy (E), enthalpy (H) and quasi-harmonic-corrected free energy (qh-G(T)) are obtained from the M06−2X/6−31+G(d,p)/SMD(EtOH) optimizations and frequency calculations. Single-point refinements (SPE) are obtained at the M06−2X/def2tzvpp/SMD(EtOH) level of theory.

Table S4. Absolute energy (in Hartrees) of all computed structures

Structure	E	H	qh-G(T)	SPE
		Base system		
EtOH	-154.982973	-154.89987	-154.930527	-155.039706
EtO	-154.475204	-154.405884	-154.435663	-154.527196
H_2O	-76.409008	-76.384653	-76.406744	-76.441022
HNCS	-491.568024	-491.545712	-491.574353	-491.637086
HSCN	-491.549788	-491.52868	-491.558093	-491.598621
OH	-75.903301	-75.891456	-75.911013	-75.927883
SCN	-491.121805	-491.109371	-491.135902	-491.195226
TMS-NCS	-900.195263	-900.064751	-900.112522	-900.335425
TMS cation	-408.965707	-408.850592	-408.891033	-409.036509
TMSCl	-869.39592	-869.276832	-869.319205	-869.502479
TMSOEt	-563.598478	-563.409384	-563.458898	-563.729765
TMSOH	-485.023038	-484.892326	-484.935576	-485.13015
EN	-462.126989	-461.948865	-461.995663	-462.279853
KNCS	-953.733063	-953.527192	-953.582489	-953.952428
KSCN	-953.717462	-953.512704	-953.567802	-953.938666
		Activated enones		
PT (Int-IV)	-871.165967	-870.869556	-870.93336	-871.392704

PH (Int-I)	-462.549882	-462.359069	-462.405867	-462.704425
		TMS pathway		
TSs				
TS-PTTN (TS-III)	-1362.299651	-1361.990534	-1362.061414	-1362.592699
TS-PTTS	-1362.301097	-1361.992023	-1362.063481	-1362.594305
TS-PTON	-1362.302112	-1361.993112	-1362.064396	-1362.594921
TS-PTOS	-1362.299984	-1361.991176	-1362.062608	-1362.593112
Intermediates				
PTTN (Int-V)	-1362.331611	-1362.01988	-1362.09138	-1362.625244
PTTS	-1362.320746	-1362.010067	-1362.081379	-1362.616217
PTON	-1362.318603	-1362.007987	-1362.078967	-1362.611661
PTOS	-1362.304313	-1361.994581	-1362.065334	-1362.598752
		Protonated pathway		
TSs				
TS-PHTN (TS-I)	-953.684354	-953.481304	-953.536191	-953.904945
TS-PHTS	-953.690857	-953.487249	-953.541773	-953.911387
TS-PHON	-953.682589	-953.479375	-953.534118	-953.903073
TS-PHOS	-953.687704	-953.484321	-953.538941	-953.908712
Intermediates				
PHTN (Int-II)	-953.713545	-953.507655	-953.563012	-953.934245
PHTS	-953.703422	-953.498587	-953.553981	-953.925996
PHON	-953.703691	-953.500027	-953.554008	-953.923546
PHOS	-953.691735	-953.487683	-953.543068	-953.913476
		Anionic Pathway		

PATN (Int-III)	-953.238021	-953.045493	-953.100644	-953.456646
TS-PATN (TS-II)	-953.229263	-953.038621	-953.092691	-953.447725
		Chalcone		
CL	-653.806323	-653.573029	-653.627328	-654.019061
CNCS	-1145.405568	-1145.144981	-1145.2079	-1145.684575
CSCN	-1145.391435	-1145.13152	-1145.194298	-1145.672339

9. XYZ coordinates for all computed structures

Output files for all Gaussian 16 optimized geometries have been archived and can be accessed on Zenodo (DOI: 10.5281/zenodo.8432613).

TMS cation

C	-1.53105	-0.99839	-0.00112
H	-2.16557	-0.68669	-0.84012
H	-1.32732	-2.06873	-0.06712
H	-2.09198	-0.78553	0.91888
C	1.63219	-0.82416	-0.00412
C	-0.10020	1.82326	0.00488
H	2.44571	-0.12196	-0.19912
H	1.78595	-1.28308	0.98288
H	1.64223	-1.63565	-0.74012
H	0.59717	2.23623	0.74088
H	0.22283	2.18642	-0.98112
H	-1.11375	2.17930	0.20288
Si	-0.00007	-0.00176	-0.00112

KSCN

C	-0.09404	-0.20786	0.78706
C	3.31305	-1.89968	0.08506
H	3.06009	-2.75670	0.71606
H	3.21807	-2.19669	-0.96294
C	2.36199	-0.75773	0.42206
H	2.43798	-0.49173	1.47706
C	1.65687	1.69023	-0.68094
H	4.35504	-1.63263	0.28506
O	0.23893	0.47016	1.74806
C	-1.51103	-0.21993	0.31706
C	-2.38209	0.76603	0.79906
C	-1.98199	-1.18295	-0.58294
C	-3.70909	0.78896	0.38406
H	-2.00512	1.51405	1.49006
C	-3.31599	-1.16502	-0.98694
H	-1.32095	-1.95592	-0.96394
C	-4.17804	-0.17906	-0.50694
H	-4.37813	1.56093	0.75306
H	-3.68095	-1.91904	-1.67794
H	-5.21504	-0.16212	-0.82894
C	0.92001	-1.07281	0.06106
H	0.76001	-1.03481	-1.02194
H	0.71606	-2.10982	0.36606
N	0.73383	2.37618	-0.84494
S	3.03292	0.71430	-0.51794

SCN

S	0.00000	0.00000	1.02934
C	0.00000	0.00000	-0.63365
N	0.00000	0.00000	-1.80966

TMSOEt

C	-1.14319	-1.34795	-1.23421
H	-0.86421	-1.04372	-2.24925
H	-0.58023	-2.25380	-0.98113
H	-2.20721	-1.61385	-1.24402
C	-1.15403	-0.59244	1.73822
C	-1.85498	1.54239	-0.38194
H	-0.91896	0.17717	2.48167
H	-2.21104	-0.85975	1.85340
H	-0.56108	-1.48422	1.96835
H	-2.92399	1.31719	-0.30062
H	-1.62691	2.35414	0.31765
H	-1.66000	1.90262	-1.39780
Si	-0.83206	0.02710	-0.00082
O	0.76997	0.54341	-0.12923
C	1.83591	-0.39899	-0.02328
H	1.80284	-1.08926	-0.87749
H	1.72391	-0.99292	0.89483
C	3.15696	0.34286	-0.00296
H	3.98792	-0.36641	0.06774
H	3.27996	0.93078	-0.91809
H	3.20403	1.02012	0.85521

H_2O

O	0.00000	0.00000	0.11780

H	0.00000	0.76600	-0.47120
H	-0.00000	-0.76600	-0.47120

EtOH

C	-0.00000	0.55308	0.00000
H	0.02718	1.19707	0.88800
H	0.02718	1.19707	-0.88800
C	1.17674	-0.39725	0.00000
H	1.15656	-1.03524	-0.88900
H	2.11589	0.16449	0.00000
H	1.15656	-1.03524	0.88900
O	-1.19822	-0.22459	0.00000
H	-1.95805	0.37362	0.00000

TMS-NCS

C	1.69489	0.00030	0.00091
S	3.29689	-0.00013	-0.00001
N	0.51389	0.00031	0.00091
Si	-1.26311	-0.00008	-0.00000
C	-1.77212	-0.72816	1.63720
H	-1.39611	-0.12601	2.47046
H	-2.86612	-0.76142	1.70701
H	-1.39313	-1.74958	1.74831
C	-1.77012	-1.05428	-1.45006
H	-1.39213	-2.07593	-1.34433
H	-2.86313	-1.10097	-1.51238
H	-1.39212	-0.63924	-2.38922
C	-1.77110	1.78269	-0.18848
H	-1.39409	2.38949	0.64049
H	-1.39210	2.20170	-1.12614
H	-2.86410	1.85962	-0.19788

TMSCl

C	0.88543	-1.06662	-1.43672
H	1.97945	-1.10789	-1.48799
H	0.50933	-2.08846	-1.32480
H	0.51379	-0.66276	-2.38367
C	0.88238	-0.71164	1.64219
C	0.88019	1.77949	-0.20414
H	1.97636	-0.73671	1.70619
H	0.50513	-0.10451	2.47264
H	0.51027	-1.73365	1.76412
H	0.50094	2.39677	0.61646
H	1.97419	1.85049	-0.20765
H	0.50855	2.19330	-1.14793
Si	0.36100	0.00112	-0.00006
Cl	-1.76000	-0.00174	-0.00085

HNCS

C	-0.00000	0.50536	0.00000
S	0.03566	-1.08726	0.00000
N	-0.12501	1.68132	0.00000
H	0.30455	2.59472	0.00000

EN

C	2.35301	-1.55700	-0.16808
C	1.01900	-1.15303	-0.19208
C	0.69097	0.19796	-0.02008
C	1.71395	1.13498	0.17992
C	3.04296	0.72801	0.21892
C	3.36399	-0.62098	0.04292
H	2.60103	-2.60400	-0.31408
H	0.24401	-1.89205	-0.36808
H	1.45393	2.18098	0.31192
H	3.82894	1.45803	0.38492
H	4.40199	-0.93896	0.06992
C	-0.72204	0.68593	-0.07108
O	-0.94707	1.87493	-0.29608
C	-1.82002	-0.27809	0.16792
C	-3.09703	0.05988	-0.06308
H	-1.57500	-1.26708	0.54392
H	-3.30605	1.05888	-0.44708
C	-4.26601	-0.83614	0.16192
H	-4.96502	-0.37215	0.86692
H	-4.81700	-0.98115	-0.77408
H	-3.96299	-1.81113	0.55092

HSCN

C	0.67285	-0.00833	0.00014
N	1.81876	0.04148	-0.00007

S	-0.94499	-0.07914	-0.00002
H	-1.64849	1.02583	-0.00000

KNCS

C	0.39583	0.29288	0.66400
C	-2.53126	2.72977	-0.11100
H	-2.01929	3.63479	0.22500
H	-2.51226	2.69677	-1.20400
C	-1.82621	1.51079	0.47300
H	-1.85021	1.55179	1.56600
C	-2.96413	-0.72425	-0.21600
H	-3.57026	2.76973	0.22600
O	-0.11014	-0.37014	1.55800
N	-2.53317	0.31777	0.09600
S	-3.58808	-2.14727	-0.64500
C	1.79784	0.02893	0.21800
C	2.50188	-1.02805	0.81000
C	2.41881	0.80995	-0.76400
C	3.80989	-1.30000	0.42600
H	2.01290	-1.63106	1.56900
C	3.73182	0.53800	-1.14500
H	1.89078	1.63393	-1.23400
C	4.42686	-0.51597	-0.55200
H	4.35092	-2.12098	0.88600
H	4.20980	1.14802	-1.90500
H	5.44887	-0.72694	-0.85200
C	-0.38021	1.40885	-0.00500
H	-0.35420	1.27585	-1.09300
H	0.12876	2.35587	0.21200

TMSOH

C	-0.90220	-1.53428	-0.55492
H	-0.39171	-2.44411	-0.21968
H	-1.92741	-1.55649	-0.16741
H	-0.95766	-1.56143	-1.64891
C	-0.89907	1.53472	-0.55720
C	1.78136	-0.00227	-0.55720
H	-0.38791	2.44388	-0.22391
H	-0.95551	1.56056	-1.65225
H	-1.92426	1.55951	-0.17074
H	1.83191	-0.00346	-1.65117
H	2.31250	0.88492	-0.19488
H	2.31085	-0.88908	-0.19298
Si	0.00507	0.00000	0.02090
O	0.10822	0.00177	1.70695
H	-0.72803	0.00259	2.18953

TS-PATN (TS-II)

Imaginary frequency: -430.0791 cm^{-1}

C	-0.14610	-0.48893	0.74109
C	2.79684	-2.61401	-0.39191
H	2.36682	-3.58500	-0.12291
H	2.71485	-2.49201	-1.47591
C	2.03187	-1.53599	0.32909
H	2.20187	-1.50399	1.40409
C	2.77794	1.01699	-0.24591
C	0.70088	-1.26295	-0.07491
H	0.38587	-1.54594	-1.07391
H	3.85284	-2.61304	-0.11191
O	0.21092	0.03306	1.83809
N	3.10191	-0.09502	0.00909
S	2.29998	2.52000	-0.62591
C	-1.56209	-0.24389	0.28209
C	-2.21806	0.91913	0.70209
C	-2.24912	-1.14787	-0.53891
C	-3.52505	1.18416	0.30009
H	-1.68704	1.62011	1.34109
C	-3.56211	-0.88984	-0.93291
H	-1.76614	-2.06789	-0.85591
C	-4.20208	0.27918	-0.51891
H	-4.01703	2.09718	0.62509
H	-4.08613	-1.60482	-1.56091
H	-5.22407	0.48021	-0.82891

PATN (Int-III)

C	0.48306	0.37301	0.62794
C	-2.23498	2.69996	-0.60106
H	-1.59200	3.56797	-0.43206
H	-2.23698	2.46996	-1.67107
C	-1.68796	1.51897	0.19393
H	-1.71196	1.74897	1.26594
C	-3.22892	-0.59406	-0.05207

C	-0.30795	1.11499	-0.21707
H	0.03704	1.42600	-1.19707
H	-3.25299	2.94994	-0.29107
O	0.13007	-0.02400	1.80594
N	-2.62494	0.40096	0.04994
S	-4.09190	-1.95807	-0.20106
C	1.88007	0.01203	0.17694
C	2.88907	-0.13295	1.13793
C	2.20707	-0.20196	-1.16907
C	4.19307	-0.45593	0.76494
H	2.64406	0.01705	2.18493
C	3.50807	-0.53494	-1.54506
H	1.43507	-0.12798	-1.93006
C	4.50908	-0.65892	-0.57907
H	4.96408	-0.55291	1.52493
H	3.73808	-0.70693	-2.59206
H	5.52208	-0.91890	-0.87206

TS-PTTN (TS-III)

Imaginary frequency: -325.0110 cm^{-1}

C	-0.17798	-0.36198	-0.51209
C	-3.45095	-1.02612	-2.28509
H	-3.12796	-0.89910	-3.32709
H	-3.53191	-2.09712	-2.08409
C	-2.42098	-0.38807	-1.42109
H	-2.44602	0.69293	-1.32609
C	-2.85196	-0.82209	1.27591
C	-1.19795	-1.02602	-1.17109
H	-1.05991	-2.07002	-1.43309
H	-4.42397	-0.54916	-2.16909
O	-0.40303	0.84001	-0.02209
Si	0.56091	2.28505	-0.00109
C	-0.66914	3.56800	-0.55709
H	-0.21518	4.56602	-0.54109
H	-1.01313	3.36699	-1.57809
H	-1.54214	3.58096	0.10491
C	1.96692	2.09211	-1.21209
H	2.40388	3.08113	-1.39909
H	2.75995	1.43714	-0.83809
H	1.61194	1.70009	-2.17209
C	1.11190	2.58207	1.75491
H	1.31986	3.64908	1.89491
H	0.32291	2.29904	2.45991
H	2.01992	2.02511	2.00591
N	-3.53998	-0.41312	0.39991
S	-1.82093	-1.40905	2.38691
C	1.16105	-0.95593	-0.32109
C	1.84104	-0.75890	0.88791
C	1.76308	-1.68890	-1.35109
C	3.11506	-1.28784	1.06291
H	1.35602	-0.21792	1.69591
C	3.04510	-2.20485	-1.17609
H	1.24108	-1.82692	-2.29409
C	3.72109	-2.00482	0.02791
H	3.63505	-1.14582	2.00491
H	3.51812	-2.75783	-1.98109
H	4.72011	-2.40878	0.16191

TS-PTON

Imaginary frequency: -285.8242 cm^{-1}

C	1.08706	3.32137	-0.95992
H	2.14807	3.28365	-0.70592
H	0.97210	3.16933	-2.03892
H	0.69579	4.32126	-0.73892
C	0.83758	1.42530	0.65508
H	1.89157	1.45958	0.91808
C	0.30634	2.28615	-0.22392
H	-0.76765	2.26286	-0.40792
C	0.25788	0.31514	2.86908
H	-0.19287	-0.60898	3.23008
H	1.32487	0.34343	3.09208
H	-0.22635	1.16901	3.36308
C	0.01283	0.48107	1.40808
N	1.05532	-1.30664	0.84608
C	2.00332	-1.29839	0.13808
S	3.29831	-1.26103	-0.85692
O	-1.18308	0.18675	1.00708
Si	-1.85990	-0.50044	-0.44992
C	-2.09041	-2.29950	-0.03592
H	-2.68028	-2.78566	-0.82092
H	-1.12727	-2.81324	0.04008
H	-2.62438	-2.41664	0.91308
C	-3.47415	0.41213	-0.59692
H	-4.04504	0.02397	-1.44892

H	-4.08311	0.28396	0.30408
H	-3.31344	1.48317	-0.75792
C	-0.76697	-0.25414	-1.93892
H	-1.13578	-0.92824	-2.72192
H	-0.81224	0.76585	-2.33092
H	0.27810	-0.51285	-1.74592

PTON

C	0.65660	3.58802	-0.10102
H	-0.15742	3.85495	0.57698
H	1.55855	4.13310	0.19998
H	0.39957	3.93200	-1.10902
C	0.19380	1.23598	0.60098
H	-0.61423	1.58191	1.24698
C	0.90673	2.11104	-0.10702
H	1.71576	1.75711	-0.74502
C	0.44098	-0.81900	2.02198
H	0.53407	-1.90699	1.98698
H	1.29994	-0.39092	2.54598
H	-0.47405	-0.55207	2.55798
C	0.35993	-0.26900	0.59898
N	1.58396	-0.62790	-0.08902
C	2.74497	-0.76580	-0.23302
S	4.30699	-0.97667	-0.51302
O	-0.67402	-0.91509	-0.10502
Si	-2.29906	-0.45523	-0.28602
C	-3.02693	-1.91129	-1.19802
H	-4.09795	-1.75838	-1.37102
H	-2.54292	-2.04525	-2.17202
H	-2.90385	-2.83728	-0.62502
C	-3.10608	-0.23630	1.38898
H	-4.17409	-0.02939	1.24898
H	-3.01600	-1.14329	1.99598
H	-2.67915	0.60174	1.95198
C	-2.46119	1.10676	-1.30902
H	-1.77719	1.08881	-2.16502
H	-3.48420	1.17567	-1.69802
H	-2.26027	2.01177	-0.72802

PTTS

C	-0.36199	-0.45102	-0.07204
C	2.74602	-0.96595	1.84796
H	2.20701	-0.46896	2.66196
H	2.73705	-2.04394	2.03296
C	2.05202	-0.63096	0.53896
H	2.08599	0.43904	0.32796
S	2.92704	-1.43894	-0.92204
C	4.47702	-0.77690	-0.72404
N	5.54301	-0.32987	-0.60304
C	0.65303	-1.14700	0.46796
H	0.46505	-2.14200	0.86196
H	3.78002	-0.61092	1.85996
O	-0.14002	0.75898	-0.66304
Si	-0.51706	2.24097	0.11196
C	0.35291	3.50800	-0.94004
H	0.18989	4.51499	-0.54304
H	1.43192	3.32102	-0.96404
H	-0.02209	3.48499	-1.96904
C	0.15495	2.15799	1.85496
H	-0.10708	3.07598	2.39396
H	-0.27703	1.31598	2.40896
H	1.24595	2.06102	1.86996
C	-2.36606	2.51393	0.14296
H	-2.57209	3.50292	0.57096
H	-2.79506	2.48692	-0.86304
H	-2.88004	1.76891	0.75996
C	-1.76298	-0.94106	-0.11604
C	-2.58298	-0.59208	-1.19704
C	-2.28496	-1.74407	0.90696
C	-3.89597	-1.05111	-1.26204
H	-2.18400	0.03693	-1.98804
C	-3.59994	-2.20010	0.84096
H	-1.66795	-1.99405	1.76596
C	-4.40795	-1.85612	-0.24304
H	-4.51998	-0.78013	-2.10804
H	-3.99693	-2.81411	1.64396
H	-5.43394	-2.20915	-0.29104

PT (Int-IV)

C	0.19721	0.84703	-0.27205
C	2.66578	3.75755	-0.16505
H	1.92293	4.55769	-0.17805
H	3.29179	3.84742	0.73095

H	3.34280	3.86842	-1.02105
C	0.71547	2.18693	-0.23705
H	0.00863	3.00907	-0.24405
C	2.04951	2.41267	-0.20005
H	2.72435	1.55654	-0.19105
Si	1.27570	-1.75518	0.17095
O	1.02002	-0.12113	-0.45305
C	-0.03837	-2.13092	1.43195
H	-0.98843	-2.43674	0.98595
H	0.32447	-2.95600	2.05595
H	-0.21821	-1.27389	2.09095
C	1.27249	-2.84318	-1.33305
H	1.61929	-3.84325	-1.05105
H	0.27847	-2.94399	-1.77705
H	1.95856	-2.45232	-2.09205
C	2.95873	-1.57751	0.93695
H	2.94488	-0.84051	1.74695
H	3.28155	-2.53657	1.35695
H	3.69880	-1.26665	0.19195
C	-1.23484	0.58631	-0.15905
C	-1.79506	-0.51658	-0.82405
C	-2.05068	1.44347	0.59895
C	-3.15911	-0.75732	-0.73305
H	-1.17118	-1.15570	-1.44305
C	-3.40973	1.17673	0.70995
H	-1.61851	2.28738	1.12695
C	-3.96394	0.08284	0.04095
H	-3.59727	-1.59623	-1.26305
H	-4.03860	1.82186	1.31395
H	-5.02898	-0.11295	0.11895

PTTN (Int-V)

C	-0.27082	-0.27803	0.04193
C	2.39209	0.87917	2.20893
H	1.53605	1.32710	2.71993
H	2.69316	-0.02381	2.74993
C	1.99012	0.52614	0.77693
H	1.70805	1.43112	0.23093
C	4.06220	-0.56271	-0.37807
C	0.86719	-0.47095	0.72693
H	1.01026	-1.39894	1.27393
H	3.22104	1.59123	2.21093
O	-0.44691	0.82895	-0.74307
Si	-1.40201	2.16388	-0.26107
C	-1.16510	3.38490	-1.64607
H	-1.72617	4.30485	-1.44707
H	-0.10812	3.64998	-1.76007
H	-1.52007	2.97187	-2.59707
C	-0.73206	2.78493	1.37093
H	-1.32912	3.63789	1.71393
H	-0.78800	2.00993	2.14293
H	0.30892	3.11701	1.28393
C	-3.19197	1.65974	-0.07107
H	-3.78204	2.54170	0.20693
H	-3.60194	1.26071	-1.00507
H	-3.32491	0.90673	0.71393
N	3.13816	-0.01978	0.09193
S	5.33725	-1.29061	-1.04607
C	-1.38675	-1.25912	0.01993
C	-2.16274	-1.39718	-1.13807
C	-1.68569	-2.04614	1.13993
C	-3.20767	-2.31626	-1.18107
H	-1.94078	-0.78216	-2.00607
C	-2.73362	-2.96322	1.09593
H	-1.11170	-1.92410	2.05393
C	-3.49661	-3.10228	-0.06407
H	-3.79766	-2.41830	-2.08707
H	-2.96157	-3.56124	1.97293
H	-4.31656	-3.81334	-0.09607

TS-PTOS

Imaginary frequency: -129.9882 cm^{-1}

C	-2.98245	-3.04727	-1.51635
H	-2.48223	-3.98821	-1.27356
H	-3.97843	-3.04558	-1.05928
H	-3.13454	-2.99010	-2.59933
C	-1.03963	-1.94906	-0.38126
H	-0.58340	-2.90901	-0.15547
C	-2.20568	-1.86719	-1.03917
H	-2.62292	-0.88125	-1.24495
C	-0.30186	-0.75498	0.03193
C	-1.08194	0.38532	2.75020
S	-0.60661	-1.18752	2.48286
N	-1.41518	1.49722	2.89943

O	-0.92212	0.38990	-0.06781
Si	-0.57451	1.86815	-0.93755
C	0.45550	1.39066	-2.41671
H	0.05167	0.49767	-2.90685
H	0.43128	2.21080	-3.14455
H	1.50256	1.20484	-2.15381
C	-2.29665	2.40086	-1.39834
H	-2.91562	2.52255	-0.50227
H	-2.26790	3.36196	-1.92415
H	-2.77753	1.66788	-2.05445
C	0.24529	3.12012	0.17164
H	0.02804	4.12014	-0.22115
H	-0.15664	3.06483	1.18966
H	1.33131	3.00135	0.21055
C	1.18313	-0.74364	-0.00316
C	1.86528	-1.64233	-0.82838
C	1.89496	0.23838	0.69998
C	3.25125	-1.54400	-0.96445
H	1.32041	-2.39534	-1.38949
C	3.27393	0.32871	0.56491
H	1.36585	0.91113	1.37114
C	3.95407	-0.56098	-0.27331
H	3.77536	-2.23475	-1.61762
H	3.82180	1.08673	1.11702
H	5.03205	-0.48672	-0.38036

PTOS

C	3.35971	-2.46530	-1.42209
H	2.90087	-3.00202	-2.25615
H	4.31267	-2.04099	-1.75837
H	3.59578	-3.18286	-0.62807
C	1.25248	-1.11644	-1.38574
H	0.84764	-1.68118	-2.22565
C	2.46449	-1.38654	-0.90014
H	2.83932	-0.79383	-0.06638
C	0.36225	-0.02857	-0.84384
C	0.09982	2.67332	-1.40287
S	0.44313	1.27743	-2.29211
N	-0.11240	3.64564	-0.80227
O	0.88605	0.61861	0.25162
Si	0.67097	0.34187	1.92617
C	1.19324	-1.39759	2.37188
H	2.26128	-1.55842	2.18985
H	1.00518	-1.56070	3.43978
H	0.62941	-2.15479	1.81603
C	1.82569	1.61213	2.65422
H	1.52554	2.62346	2.36058
H	1.81662	1.55820	3.74854
H	2.85374	1.44742	2.31421
C	-1.09113	0.65756	2.46529
H	-1.10723	0.72464	3.55993
H	-1.47126	1.60329	2.06500
H	-1.77197	-0.14722	2.16770
C	-1.08069	-0.48668	-0.63741
C	-1.31548	-1.82491	-0.30799
C	-2.15884	0.40606	-0.65345
C	-2.60243	-2.26237	0.01134
H	-0.49236	-2.53369	-0.29199
C	-3.44279	-0.03144	-0.34111
H	-2.01201	1.45274	-0.89825
C	-3.66859	-1.36762	-0.00371
H	-2.76527	-3.30499	0.26712
H	-4.26791	0.67433	-0.36010
H	-4.67155	-1.70645	0.24010

TS-PTTS

Imaginary frequency: -189.4777 cm^{-1}

C	-0.33298	-0.69907	0.20995
C	2.51609	-2.80597	1.54495
H	2.26709	-2.86198	2.61495
H	2.24012	-3.75998	1.08795
C	1.73805	-1.67500	0.97495
H	2.13302	-0.67098	1.10495
S	3.01705	-1.44996	-1.36205
C	3.27699	0.18505	-1.16905
N	3.46396	1.33206	-1.01605
C	0.40106	-1.80804	0.63095
H	-0.07091	-2.78506	0.62695
H	3.59109	-2.64394	1.46095
O	0.29399	0.42896	-0.00205
Si	0.02893	2.06695	0.52895
C	0.15790	3.09795	-1.01105
H	0.18786	4.16095	-0.74605
H	1.07991	2.85698	-1.55205

H	-0.69410	2.93892	-1.67905
C	1.41992	2.36699	1.72995
H	1.36289	3.38799	2.12295
H	1.36095	1.67499	2.57795
H	2.38893	2.23802	1.23795
C	-1.62407	2.17789	1.38595
H	-1.66310	3.13489	1.92095
H	-2.47107	2.14187	0.69595
H	-1.74405	1.38089	2.12895
C	-1.76697	-0.77611	-0.10505
C	-2.29400	0.03787	-1.11805
C	-2.60595	-1.66314	0.58695
C	-3.64600	-0.03617	-1.43705
H	-1.63902	0.70489	-1.67205
C	-3.96094	-1.71818	0.27695
H	-2.20392	-2.28213	1.38395
C	-4.47997	-0.90820	-0.73605
H	-4.04802	0.58381	-2.23205
H	-4.61292	-2.39020	0.82595
H	-5.53697	-0.95924	-0.97905

PHTN (Int-II)

C	0.35902	0.33489	0.52303
C	-2.37199	2.83404	-0.24344
H	-1.77600	3.68997	0.08477
H	-2.32496	2.77130	-1.33446
C	-1.80699	1.56790	0.38627
H	-1.88601	1.63265	1.47729
C	-3.00195	-0.66298	-0.17827
C	-0.37398	1.31901	-0.01776
H	0.06703	1.97319	-0.76260
H	-3.40899	2.98896	0.06257
O	-0.20199	-0.42434	1.50884
N	-2.62597	0.43098	0.01299
S	-3.57593	-2.13991	-0.46862
H	0.31002	-1.23237	1.65966
C	1.76403	0.04199	0.14999
C	2.67902	-0.38023	1.12391
C	2.19406	0.19030	-1.17497
C	4.00503	-0.63713	0.77887
H	2.36600	-0.48547	2.15988
C	3.52007	-0.06460	-1.51600
H	1.48407	0.48847	-1.94091
C	4.42905	-0.47982	-0.54108
H	4.70702	-0.95530	1.54281
H	3.84109	0.04764	-2.54697
H	5.46106	-0.68275	-0.80911

TS-PHTS

Imaginary frequency: -149.3720 cm^{-1}

C	-0.11994	-0.57512	0.50295
C	3.06799	-2.01027	-0.96505
H	2.88093	-3.09226	-0.90805
H	2.91300	-1.69426	-1.99905
C	2.11502	-1.34522	-0.03605
H	2.35002	-1.36823	1.02295
S	3.31713	1.04972	0.08295
C	1.83517	1.79079	0.06095
N	0.75119	2.23784	0.03595
C	0.82103	-1.03816	-0.41705
H	0.52103	-1.13715	-1.45505
H	4.10499	-1.84132	-0.67305
O	0.25206	-0.46813	1.76295
H	-0.41792	-0.03410	2.31695
C	-1.51493	-0.28205	0.14095
C	-2.53794	-0.50100	1.07595
C	-1.82991	0.19797	-1.13905
C	-3.86193	-0.24793	0.72895
H	-2.31296	-0.90501	2.05895
C	-3.15389	0.46003	-1.47305
H	-1.03990	0.40093	-1.85505
C	-4.17091	0.23508	-0.54205
H	-4.65094	-0.43290	1.45095
H	-3.39188	0.84704	-2.45805
H	-5.20390	0.43713	-0.80905

TS-PHON

Imaginary frequency: -315.3124 cm^{-1}

C	-2.03985	2.45211	-1.74783
H	-2.83990	2.75777	-1.07073
H	-1.61079	3.34035	-2.22532
H	-2.46380	1.83754	-2.55019
C	-0.97905	1.45900	0.28273

H	-1.78409	1.83069	0.91386
C	-0.97193	1.69070	-1.03915
H	-0.14189	1.33601	-1.64727
C	0.07588	0.74960	0.99344
C	-1.89315	-1.30223	0.76719
O	0.24179	1.18594	2.22369
H	0.92974	0.69167	2.70448
C	1.22892	0.11994	0.30220
C	2.52290	0.48570	0.69051
C	1.04599	-0.77549	-0.76029
C	3.62594	-0.04497	0.02232
H	2.67885	1.20528	1.48990
C	2.14903	-1.30317	-1.41948
H	0.04301	-1.07331	-1.05153
C	3.44101	-0.93941	-1.02818
H	4.62692	0.24685	0.32455
H	2.00208	-2.00373	-2.23486
H	4.30004	-1.35615	-1.54533
N	-0.98220	-0.99662	1.46343
S	-3.12708	-1.67968	-0.22012

TS-PHTN (TS-I)

Imaginary frequency: -320.3873 cm^{-1}

C	-0.00097	-0.51088	0.64909
C	3.16614	-2.24090	-0.47758
H	2.88822	-3.28888	-0.29835
H	3.07812	-2.04613	-1.54862
C	2.23009	-1.39380	0.30825
H	2.42210	-1.29356	1.37223
C	2.55090	1.29511	-0.25333
C	0.92307	-1.16698	-0.14178
H	0.64208	-1.44122	-1.15272
H	4.19814	-2.10376	-0.15562
O	0.41301	-0.02060	1.80998
N	3.30296	0.45024	0.10385
S	1.42682	2.35892	-0.75154
H	-0.32100	0.28946	2.36592
C	-1.41398	-0.33306	0.26907
C	-2.12506	0.79898	0.69484
C	-2.05392	-1.30327	-0.51472
C	-3.45907	0.95881	0.33282
H	-1.63210	1.57614	1.27366
C	-3.38994	-1.14044	-0.86674
H	-1.51486	-2.19230	-0.82553
C	-4.09301	-0.01140	-0.44597
H	-4.00013	1.84384	0.65063
H	-3.88489	-1.90060	-1.46357
H	-5.13503	0.11447	-0.72398

PHON

Imaginary frequency: -10.2852 cm^{-1}

C	0.75427	3.72098	-1.21713
H	-0.00669	4.35304	-0.75113
H	1.73930	4.16691	-1.04213
H	0.59427	3.71999	-2.30113
C	-0.15587	1.90605	0.23587
H	-0.90282	2.57910	0.65687
C	0.71216	2.32298	-0.68513
H	1.44211	1.62393	-1.09213
C	-0.23597	0.49706	0.78987
C	-2.54305	-0.49978	0.04287
O	-0.24696	0.62806	2.18887
H	-0.25303	-0.25194	2.59987
C	0.88396	-0.42203	0.30687
C	2.10696	-0.39012	0.98387
C	0.73590	-1.23302	-0.81913
C	3.17090	-1.17320	0.53987
H	2.22601	0.25087	1.85187
C	1.80384	-2.01410	-1.26113
H	-0.20710	-1.25695	-1.35813
C	3.02084	-1.98819	-0.58313
H	4.11691	-1.14627	1.07287
H	1.67979	-2.64509	-2.13713
H	3.84980	-2.59825	-0.92813
N	-1.51101	-0.05385	0.37687
S	-3.95309	-1.11267	-0.42013

PH (Int-I)

C	-0.70587	0.57396	-0.07494
C	-4.22897	-0.85880	0.19706
H	-3.93204	-1.84382	0.55806
H	-4.90494	-0.38575	0.92006
H	-4.80298	-0.95876	-0.73194

C	-1.78194	-0.33897	0.15906
H	-1.54100	-1.33698	0.50506
C	-3.07091	0.03012	-0.03694
H	-3.28484	1.03614	-0.39594
O	-1.03179	1.80698	-0.31194
H	-0.28175	2.37693	-0.56094
C	0.69210	0.17186	-0.02594
C	1.70017	1.12380	0.22106
C	1.03701	-1.17716	-0.22894
C	3.02814	0.72670	0.26806
H	1.45624	2.16381	0.41906
C	2.37098	-1.56025	-0.19694
H	0.27296	-1.91611	-0.44294
C	3.36405	-0.61332	0.05606
H	3.80119	1.45765	0.47706
H	2.63691	-2.59827	-0.36894
H	4.40603	-0.91839	0.09106

TS-PHOS

Imaginary frequency: -140.1976 cm^{-1}

C	-3.27598	2.37803	-0.23194
H	-2.93898	2.70602	-1.21694
H	-4.23100	1.84905	-0.33893
H	-3.47296	3.25503	0.39406
C	-1.11702	1.11797	-0.13594
H	-0.84901	1.44897	-1.13494
C	-2.28201	1.48600	0.42706
H	-2.52602	1.12301	1.42406
C	-0.19504	0.20995	0.52207
C	-2.35909	-1.66500	-0.40593
S	-0.76509	-1.76904	-0.87894
N	-3.46309	-1.52597	-0.04494
O	-0.58605	-0.21904	1.70707
H	0.11994	-0.67706	2.19507
C	1.25696	0.20891	0.21207
C	2.07593	-0.84111	0.65507
C	1.82299	1.28790	-0.47493
C	3.44293	-0.80714	0.41407
H	1.64491	-1.70410	1.16006
C	3.19699	1.31686	-0.71193
H	1.20701	2.11591	-0.80693
C	4.00696	0.27284	-0.27093
H	4.06891	-1.62716	0.75106
H	3.63101	2.16085	-1.23794
H	5.07596	0.29681	-0.45993

PHTS

C	-0.52501	0.54097	0.07611
C	2.55299	-0.39801	1.95511
H	2.08799	0.04499	2.84211
H	2.44700	-1.48601	2.01411
C	1.85299	0.14799	0.72311
H	1.98098	1.22899	0.63711
S	2.61899	-0.55501	-0.85389
C	4.22299	-0.04100	-0.65089
N	5.32499	0.30701	-0.52289
C	0.41399	-0.23603	0.64411
H	0.11800	-1.18603	1.07911
H	3.61499	-0.14200	1.96411
O	-0.16802	1.76297	-0.40889
H	-0.86702	2.13397	-0.96689
C	-1.95801	0.16796	-0.01089
C	-2.95002	1.14595	0.14411
C	-2.33500	-1.16104	-0.24289
C	-4.29702	0.79594	0.07811
H	-2.67402	2.17795	0.34311
C	-3.68300	-1.50705	-0.30789
H	-1.57200	-1.92004	-0.39189
C	-4.66700	-0.53006	-0.14789
H	-5.05702	1.55994	0.20811
H	-3.96399	-2.53806	-0.49489
H	-5.71700	-0.80007	-0.20189

PHOS

C	4.06513	-1.68103	-0.37219
H	3.80113	-1.98803	-1.38719
H	4.98814	-1.09203	-0.41119
H	4.28513	-2.57503	0.22081
C	1.80914	-0.60902	-0.33119
H	1.60314	-0.95202	-1.34319
C	2.97014	-0.88703	0.26581
H	3.14314	-0.53003	1.27981
C	0.70414	0.17798	0.31781

C	-0.66285	2.53098	-0.09519
S	0.78914	1.86298	-0.65519
N	-1.65985	2.98499	0.29381
O	1.00714	0.42398	1.63881
H	0.28014	0.88998	2.08281
C	-0.66586	-0.45102	0.10381
C	-1.39286	-0.91802	1.20081
C	-1.18786	-0.61401	-1.18519
C	-2.63387	-1.53101	1.01081
H	-0.99686	-0.82402	2.20681
C	-2.42186	-1.22801	-1.37119
H	-0.63486	-0.25302	-2.04919
C	-3.15187	-1.68601	-0.27119
H	-3.18987	-1.88701	1.87281
H	-2.81587	-1.34501	-2.37619
H	-4.11687	-2.16101	-0.41719

EtO anion

C	-0.00000	0.53600	0.00000
H	0.22700	1.17900	0.88100
H	0.22700	1.17900	-0.88100
C	1.02900	-0.60000	0.00000
H	0.89500	-1.23200	-0.88600
H	2.06100	-0.22200	0.00000
H	0.89500	-1.23200	0.88600
O	-1.31000	0.08900	0.00000

OH anion

O	0.00000	0.00000	0.10700
H	0.00000	0.00000	-0.85800

CL

C	3.78800	1.75600	0.42200
C	2.55600	1.10500	0.39800
C	2.47900	-0.23900	0.01000
C	3.64800	-0.92000	-0.35600
C	4.87400	-0.26300	-0.34700
C	4.94600	1.07600	0.04400
H	3.84300	2.79400	0.73600
H	1.66500	1.64400	0.70600
H	3.58300	-1.96100	-0.65500
H	5.77500	-0.79200	-0.64400
H	5.90300	1.58800	0.05500
C	1.18600	-0.99000	0.00100
O	1.19400	-2.21900	0.05300
C	-0.07600	-0.22500	-0.09000
C	-1.25600	-0.84600	0.08500
H	-0.01700	0.83600	-0.30700
H	-1.23800	-1.91200	0.31000
C	-2.58900	-0.24000	0.01400
C	-3.70300	-1.05100	0.28200
C	-2.79900	1.11200	-0.30900
C	-4.99400	-0.52900	0.23400
H	-3.54800	-2.09800	0.53000
C	-4.08700	1.63200	-0.35700
H	-1.95500	1.76000	-0.52600
C	-5.18800	0.81400	-0.08500
H	-5.84500	-1.16900	0.44500
H	-4.23700	2.67800	-0.60900
H	-6.19300	1.22500	-0.12400

CNCS

C	3.99700	-1.87700	1.25300
C	2.76100	-1.44600	0.77600
C	2.69700	-0.43300	-0.18800
C	3.88000	0.14500	-0.66600
C	5.11300	-0.28400	-0.18500
C	5.17200	-1.29700	0.77500
H	4.04300	-2.66500	1.99900
H	1.85500	-1.90700	1.15700
H	3.82300	0.93100	-1.41300
H	6.02700	0.16800	-0.55700
H	6.13400	-1.63400	1.14900
C	1.39400	0.05100	-0.73700
O	1.36100	0.89800	-1.61800
C	-2.39600	-0.63200	-0.32900
C	-2.87300	-1.67900	-1.12000
C	-3.03800	-0.32500	0.87300
C	-3.98500	-2.41600	-0.71200
H	-2.37400	-1.91500	-2.05700
C	-4.15200	-1.06000	1.27800
H	-2.67300	0.49200	1.49100
C	-4.62700	-2.10700	0.48700
H	-4.35200	-3.22600	-1.33600
H	-4.65000	-0.81200	2.21100

H	-5.49600	-2.67600	0.80200
C	-1.14600	0.10800	-0.77100
H	-1.08700	0.09800	-1.86400
N	-1.19800	1.48000	-0.36800
C	-1.07100	2.56500	0.05500
S	-0.93600	4.06600	0.61700
C	0.11300	-0.54500	-0.18900
H	0.09600	-1.61400	-0.43300
H	0.09800	-0.46500	0.90400

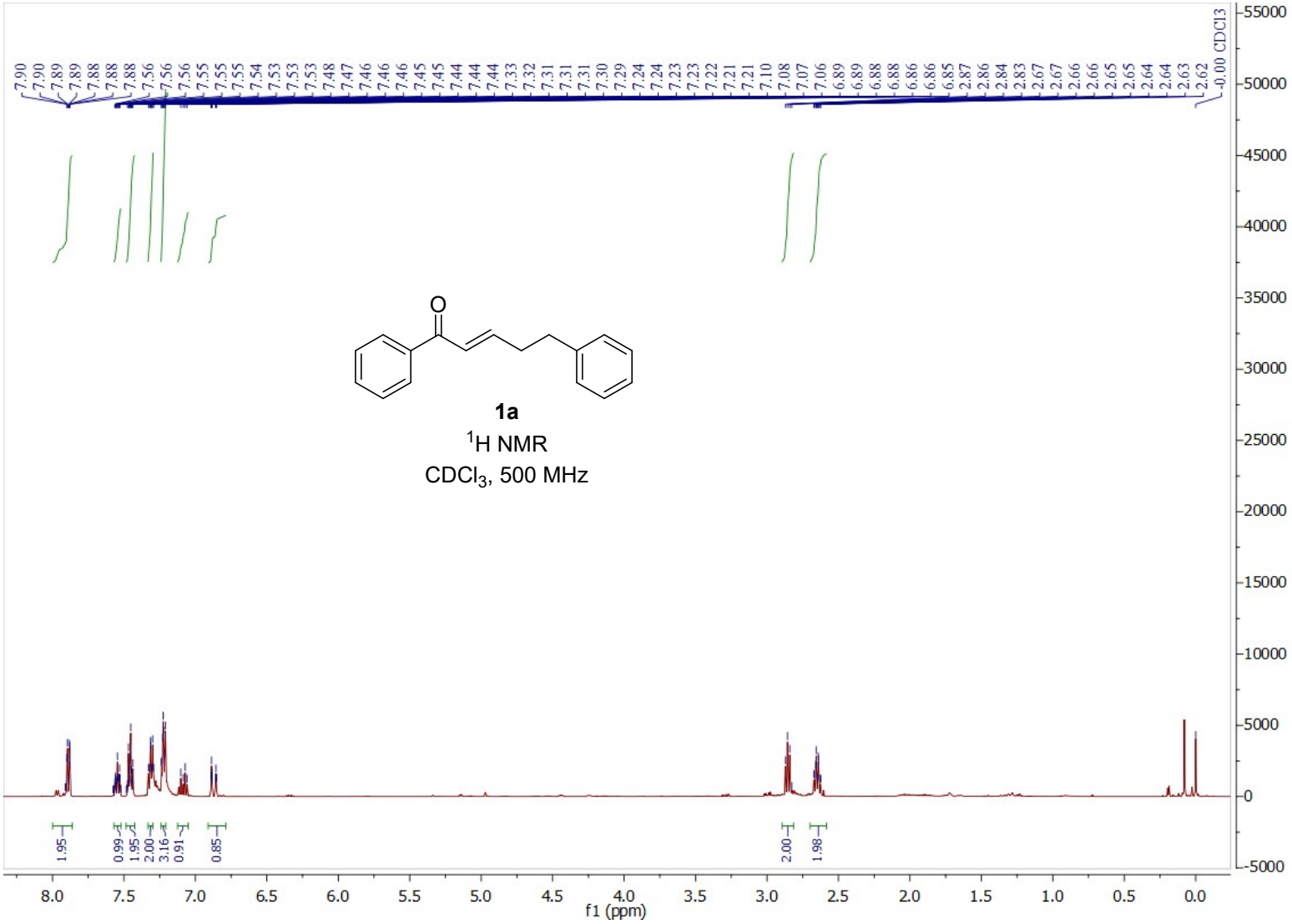
N	3.65000	2.80000	-0.27300
C	-0.38700	-0.28000	0.04300
H	-0.40300	-1.19900	0.64400
H	-0.50100	-0.60100	-0.99900

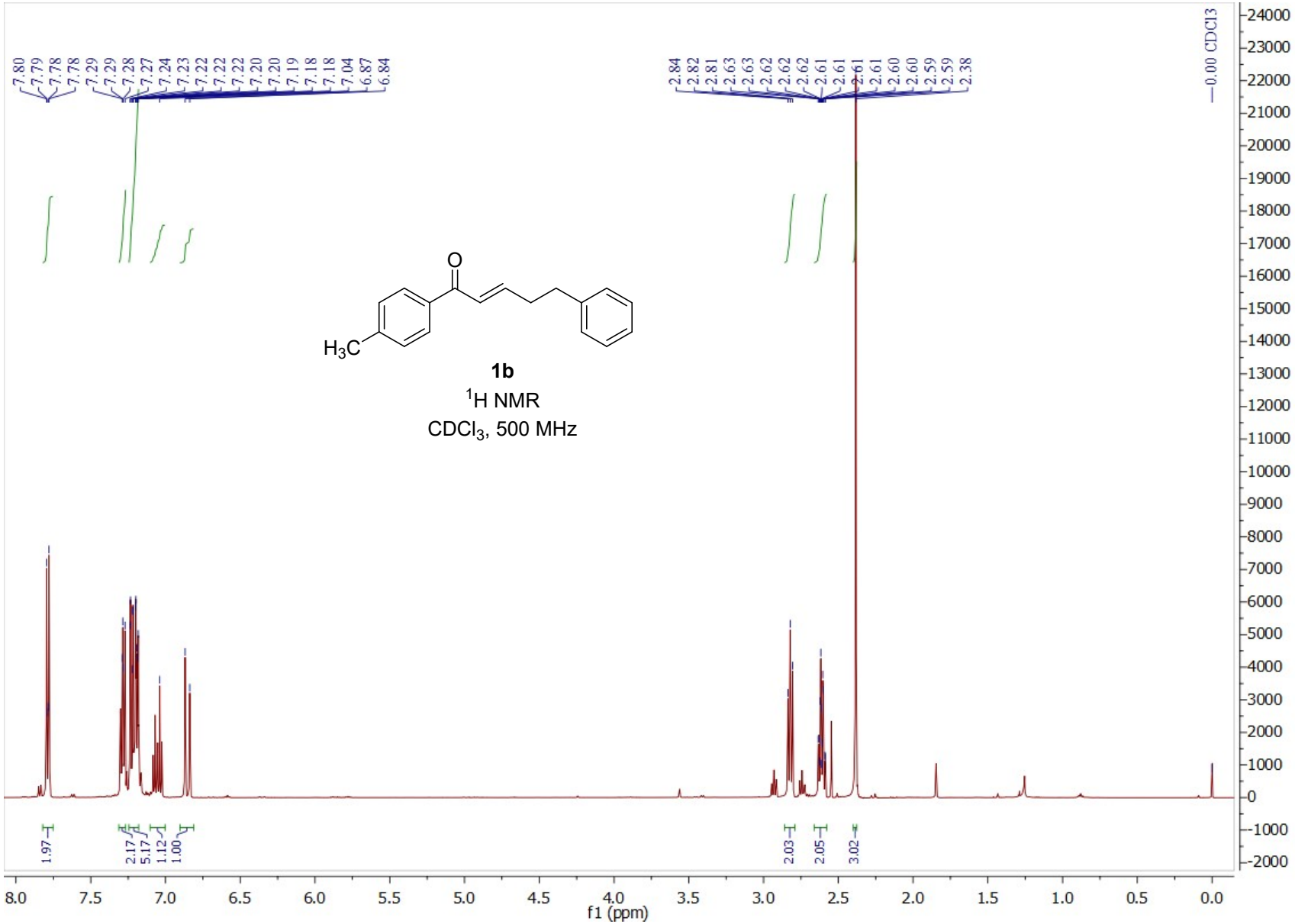
CSCN

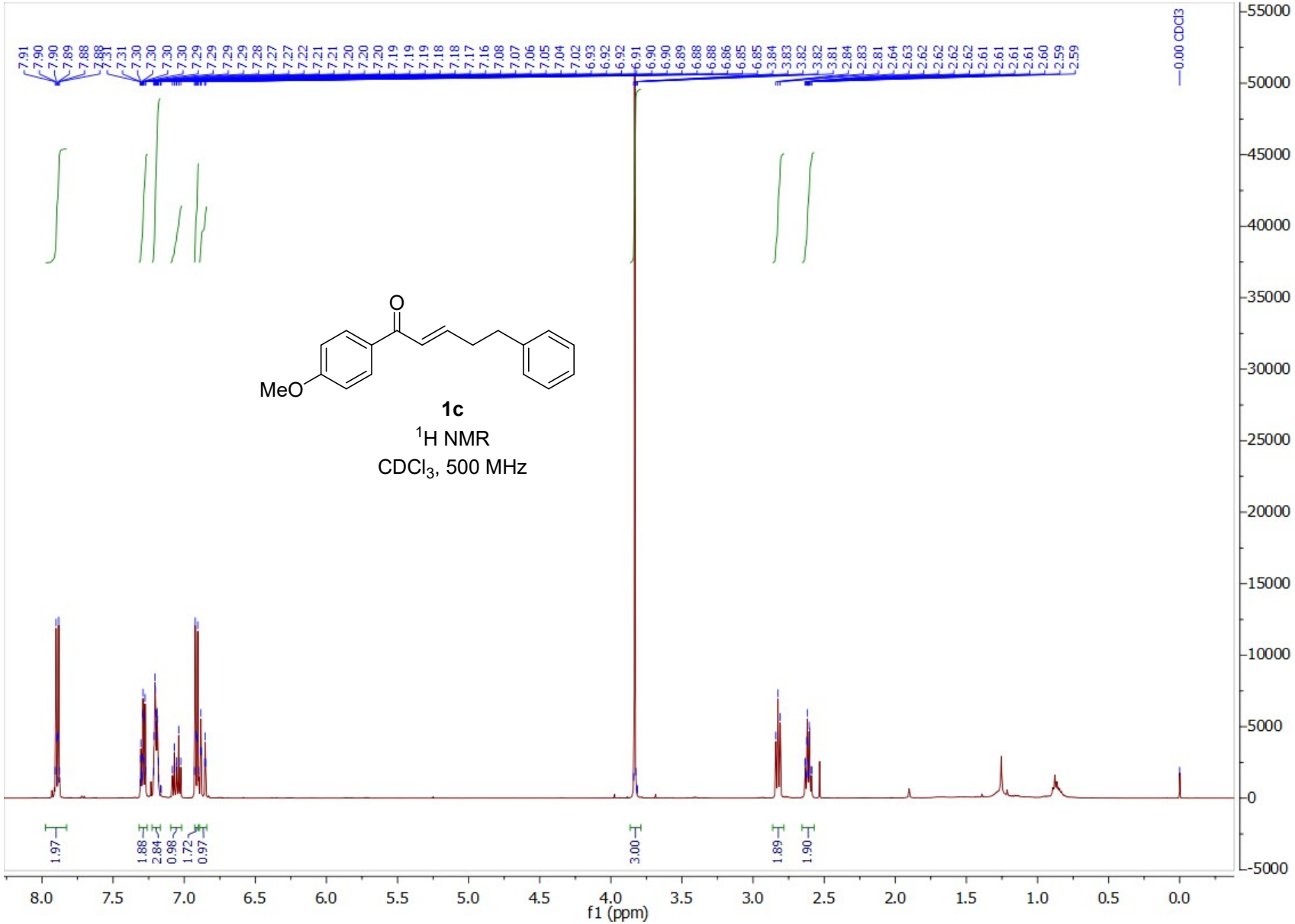
C	-4.44200	-1.75600	-0.53700
C	-3.14900	-1.27900	-0.32800
C	-2.95200	0.00200	0.20300
C	-4.06100	0.79900	0.51900
C	-5.34900	0.32300	0.30500
C	-5.54100	-0.95700	-0.22300
H	-4.58900	-2.75100	-0.94500
H	-2.30500	-1.91500	-0.57600
H	-3.90100	1.79100	0.93000
H	-6.20500	0.94500	0.54800
H	-6.54700	-1.33000	-0.38900
C	-1.58600	0.55200	0.45600
O	-1.43700	1.63700	0.99800
C	2.13600	-0.51900	0.23600
C	3.10100	-0.44400	1.24400
C	2.29800	-1.44900	-0.79900
C	4.20800	-1.29400	1.22800
H	2.98200	0.28100	2.04600
C	3.40300	-2.29600	-0.81500
H	1.56500	-1.50900	-1.60000
C	4.36000	-2.22200	0.20000
H	4.95000	-1.22700	2.01900
H	3.51800	-3.01500	-1.62100
H	5.22100	-2.88400	0.18500
C	0.95200	0.41100	0.28600
H	0.92500	0.93800	1.24200
C	2.61300	2.36700	-0.56600
S	1.10100	1.75200	-1.01800

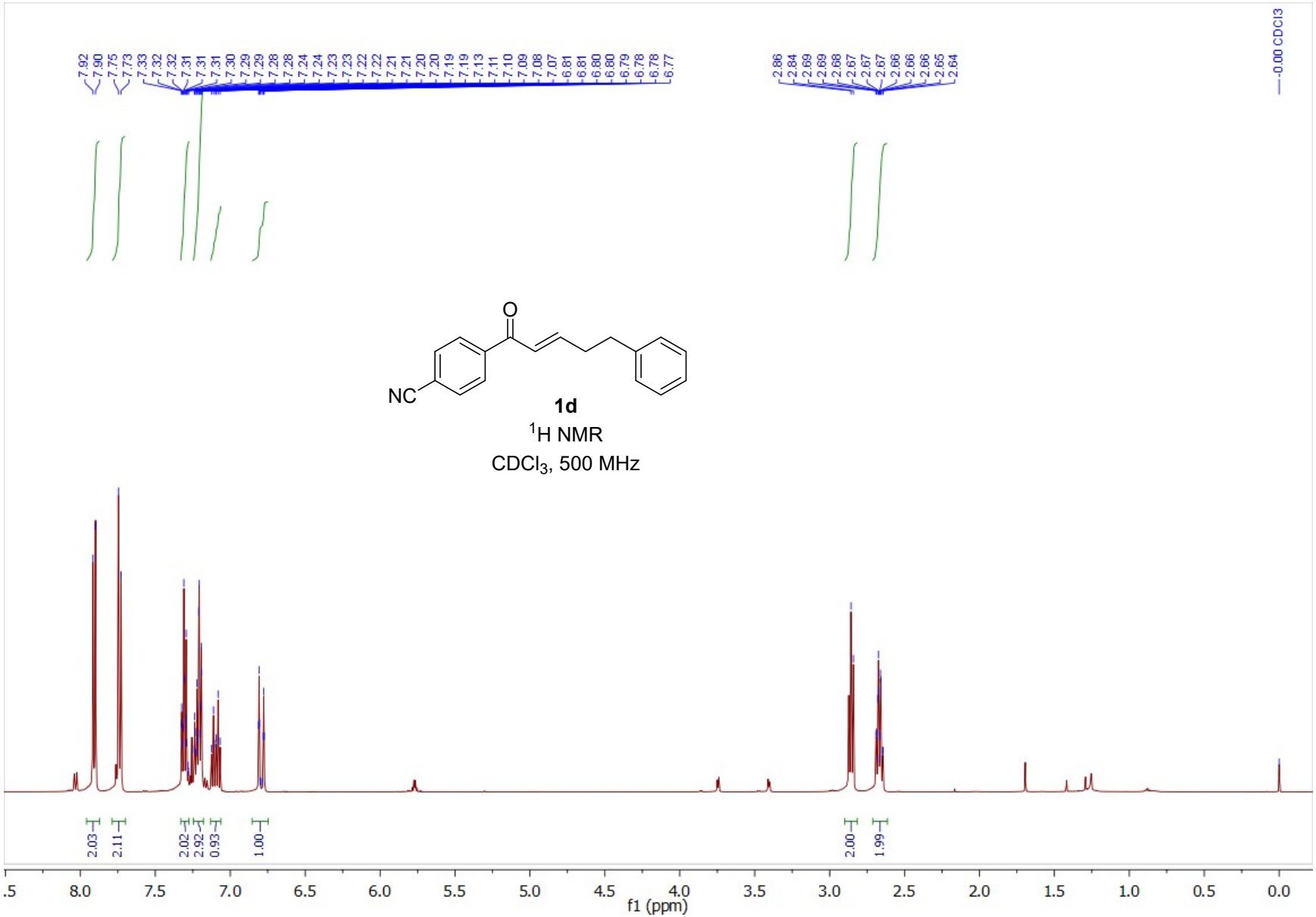
10. Spectral data

10.1 *^{1}H NMR for enone substrates*




7.80
7.79
7.78
7.78
7.29
7.29
7.28
7.27
7.24
7.23
7.22
7.22
7.22
7.20
7.20
7.19
7.18
7.18
7.04
6.87
6.84
2.84
2.82
2.81
2.63
2.63
2.62
2.62
2.62
2.61
2.61
2.61
2.61
2.60
2.60
2.59
2.59
2.38
0.00 CDCl3
O
H3C
1b
1H NMR
CDCl3, 500 MHz
1.97
2.17
5.17
1.12
1.00
2.03
2.05
3.02
f1 (ppm)

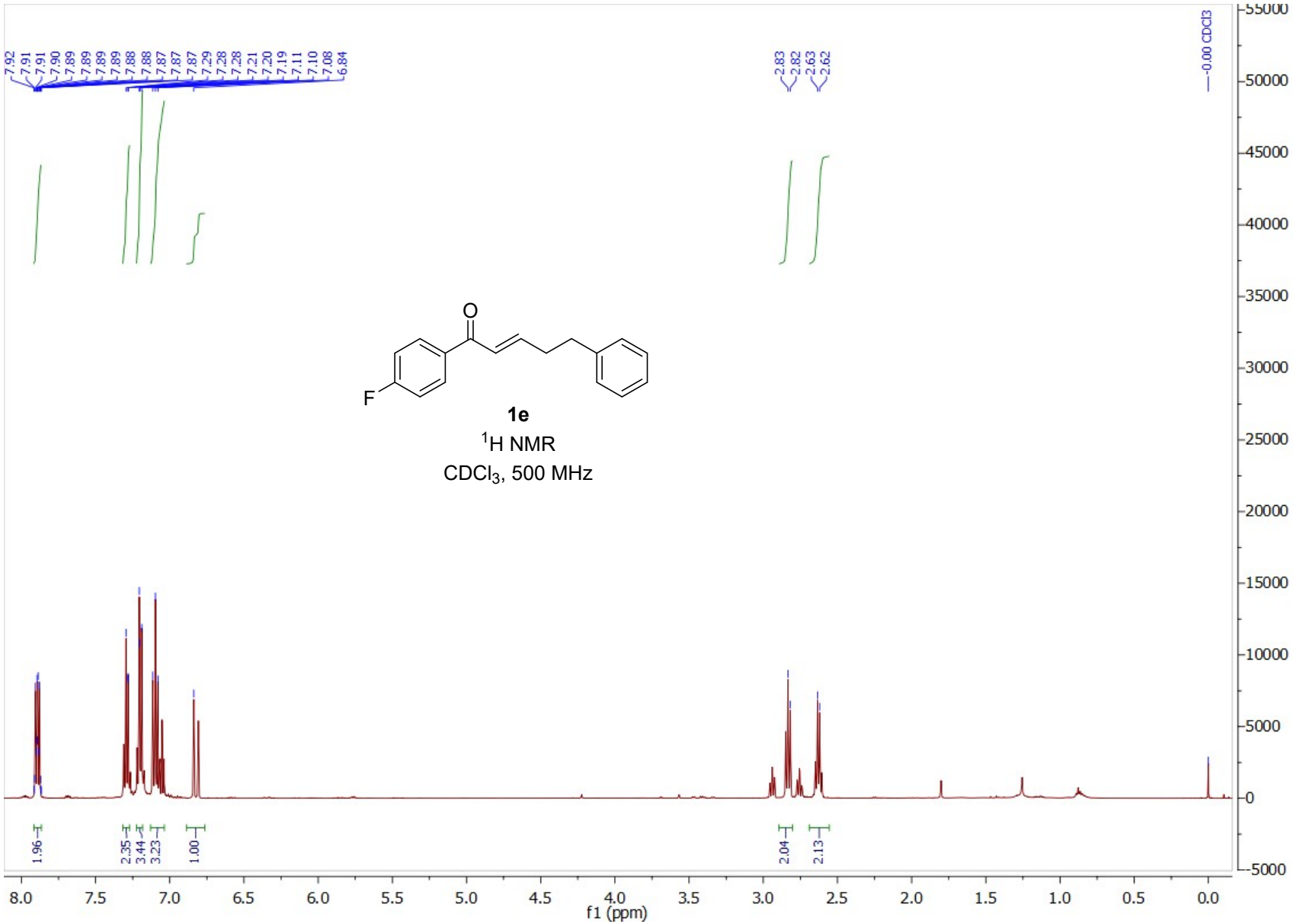

MeO
O
1c
1H NMR
CDCl3, 500 MHz
f1 (ppm)



1d

^{1}H NMR

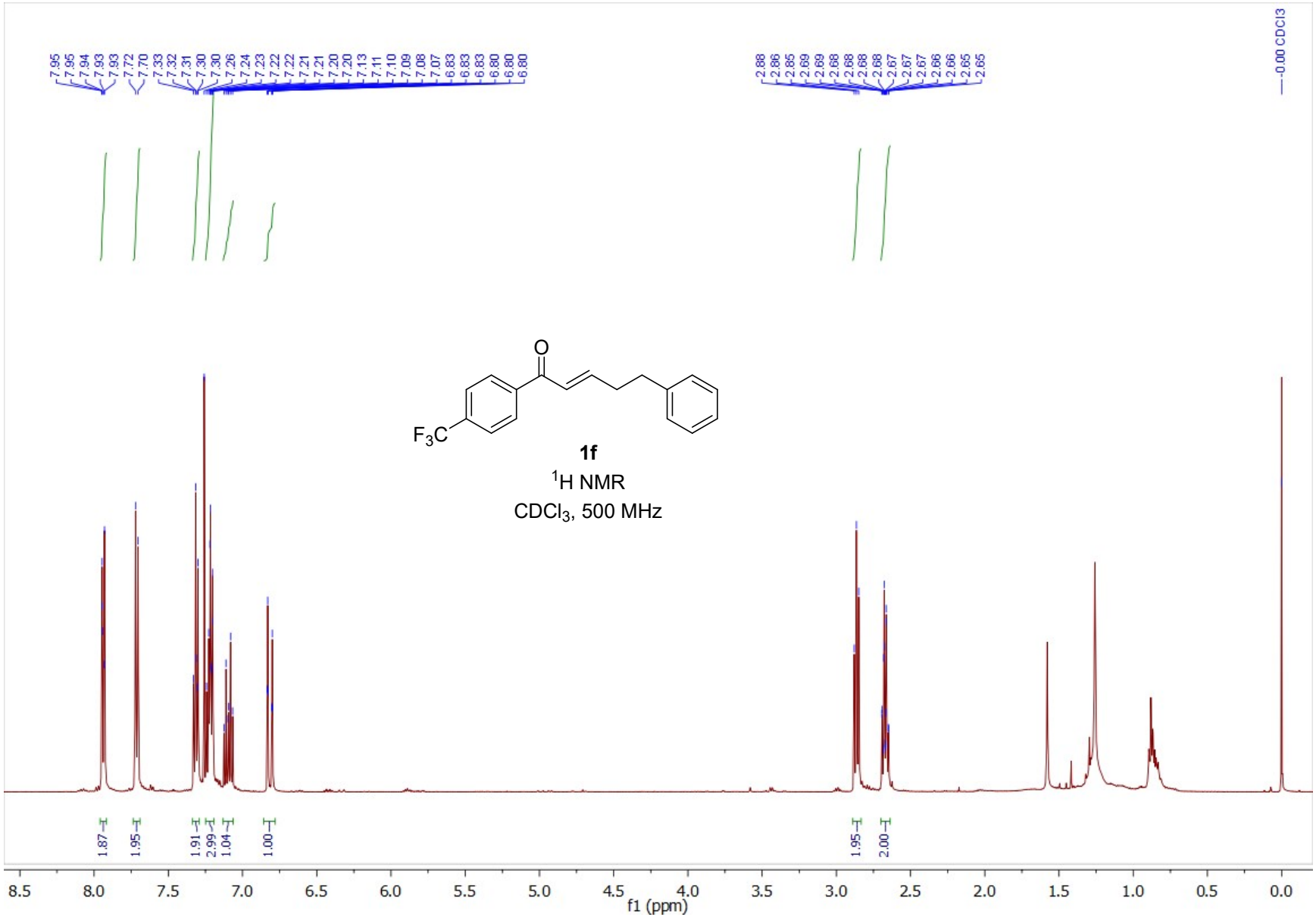
$CDCl_3$, 500 MHz

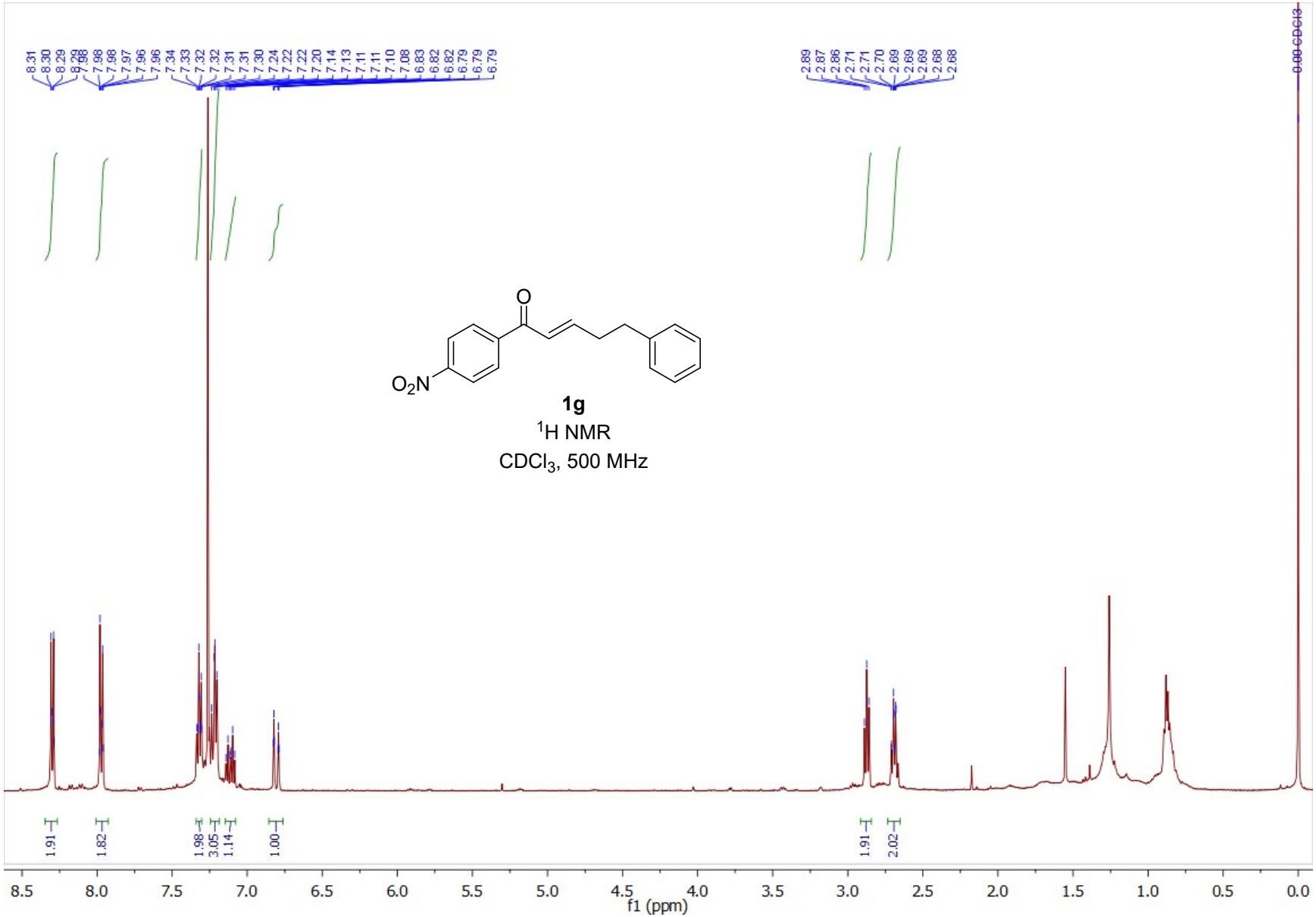


1e

^{1}H NMR

$CDCl_3$, 500 MHz

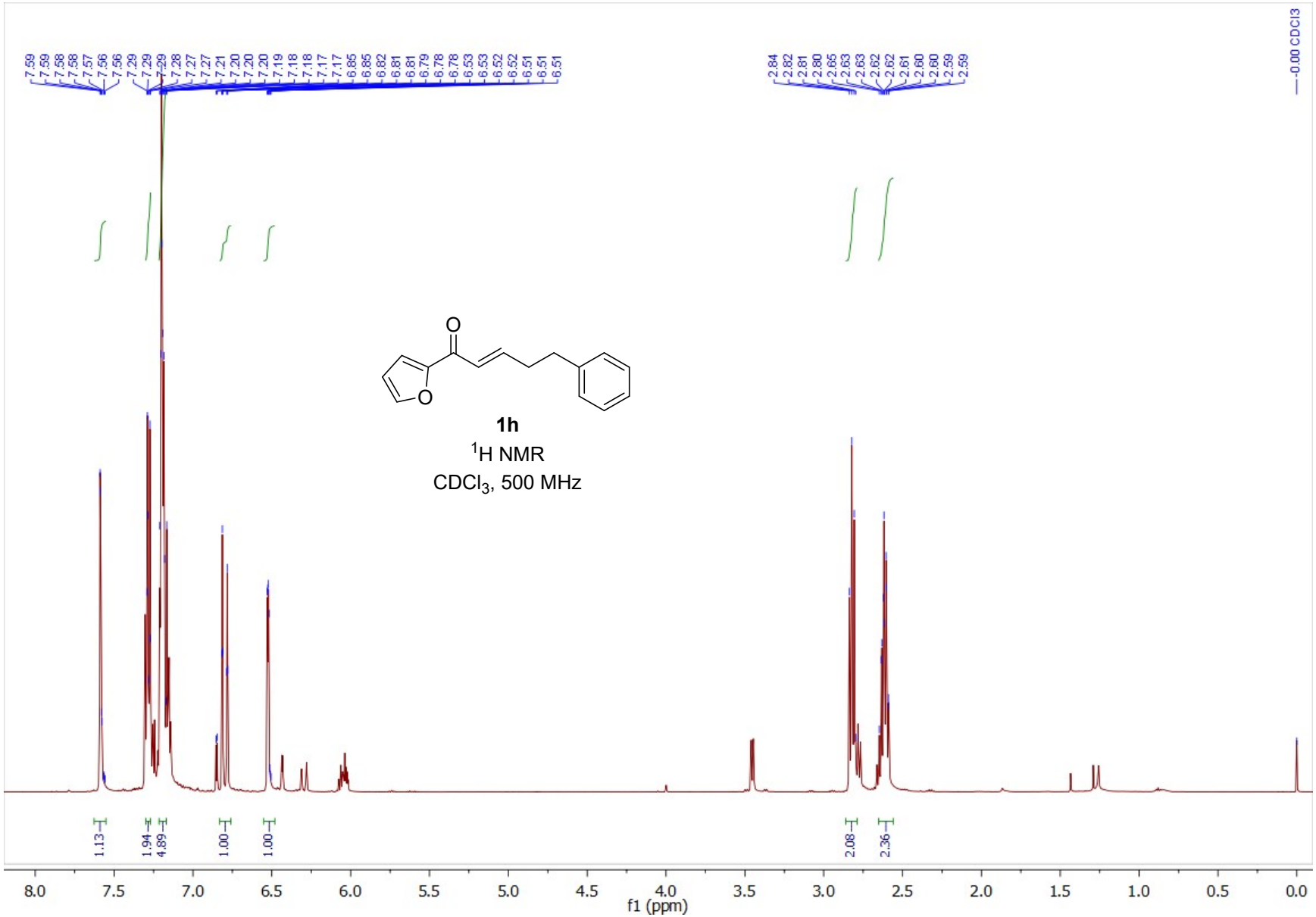

7.95
7.95
7.94
7.93
7.93
7.72
7.70
7.33
7.32
7.31
7.30
7.30
7.26
7.24
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.13
7.11
7.10
7.09
7.08
7.07
6.83
6.83
6.80
6.80
6.80
2.88
2.86
2.85
2.69
2.69
2.68
2.68
2.68
2.68
2.67
2.67
2.67
2.66
2.66
2.65
2.65
0.00 CDCl3
O
F3C
1f
1H NMR
CDCl3, 500 MHz
1.87
1.95
1.91
2.99
1.04
1.00
1.95
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

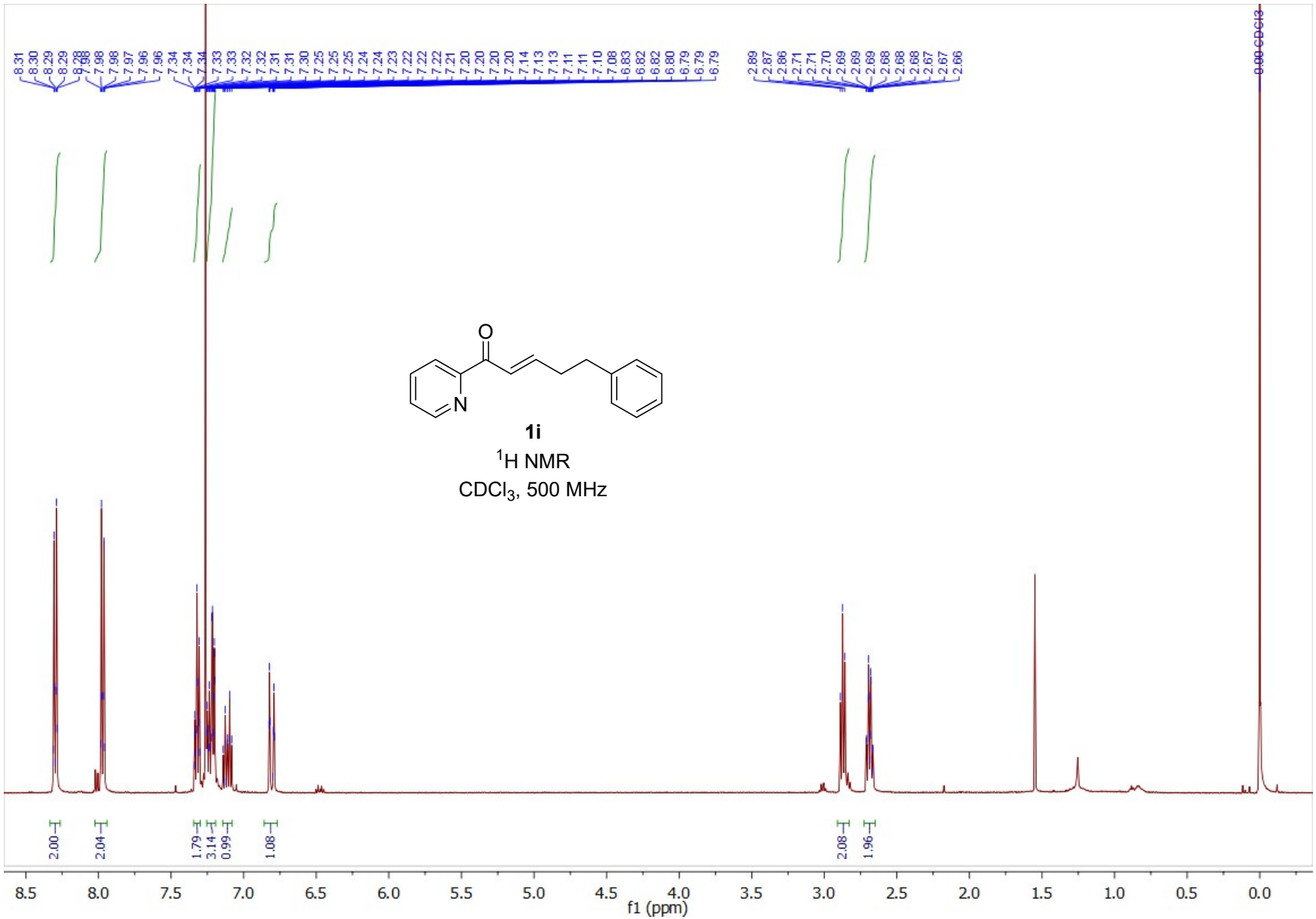


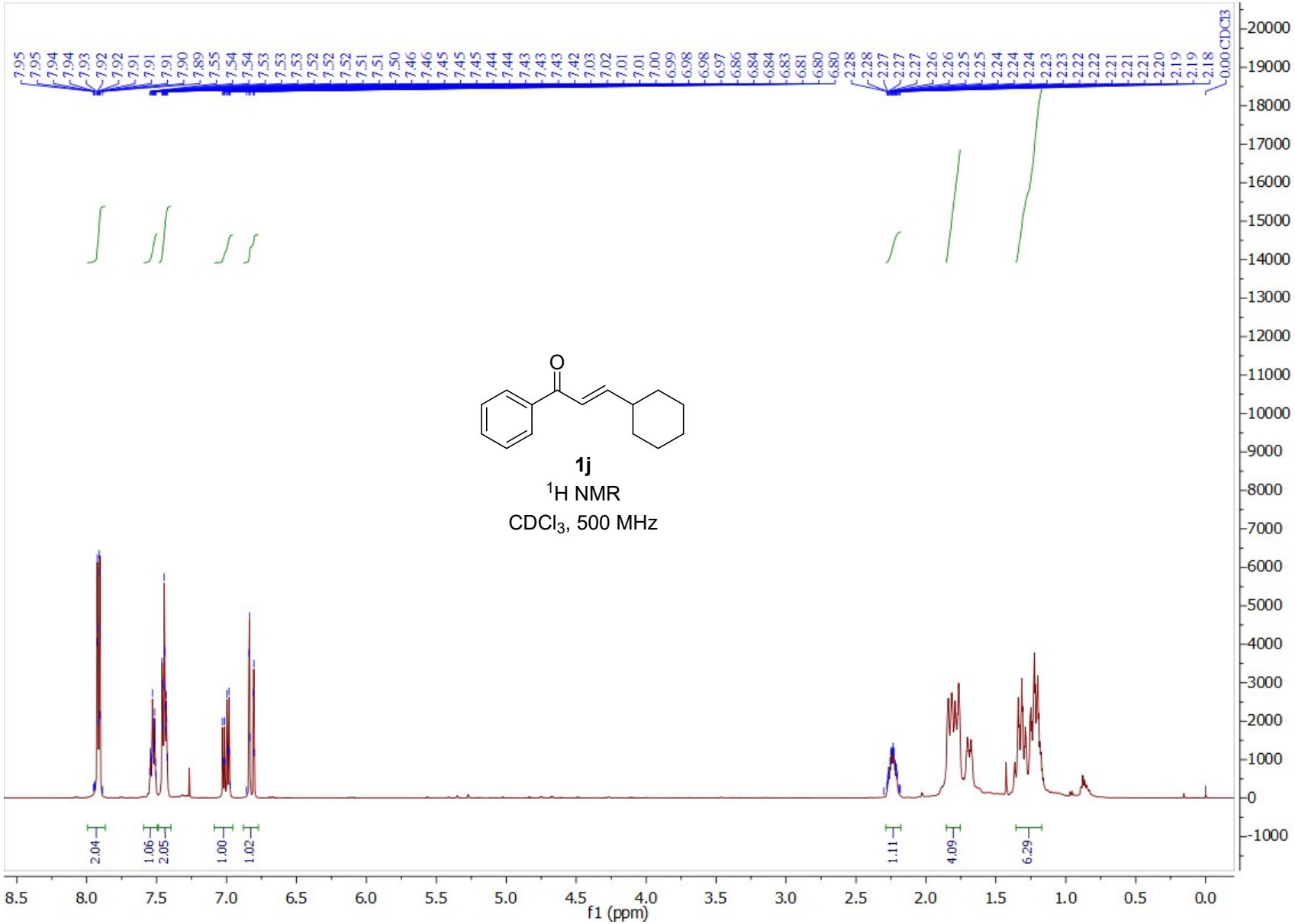
1g

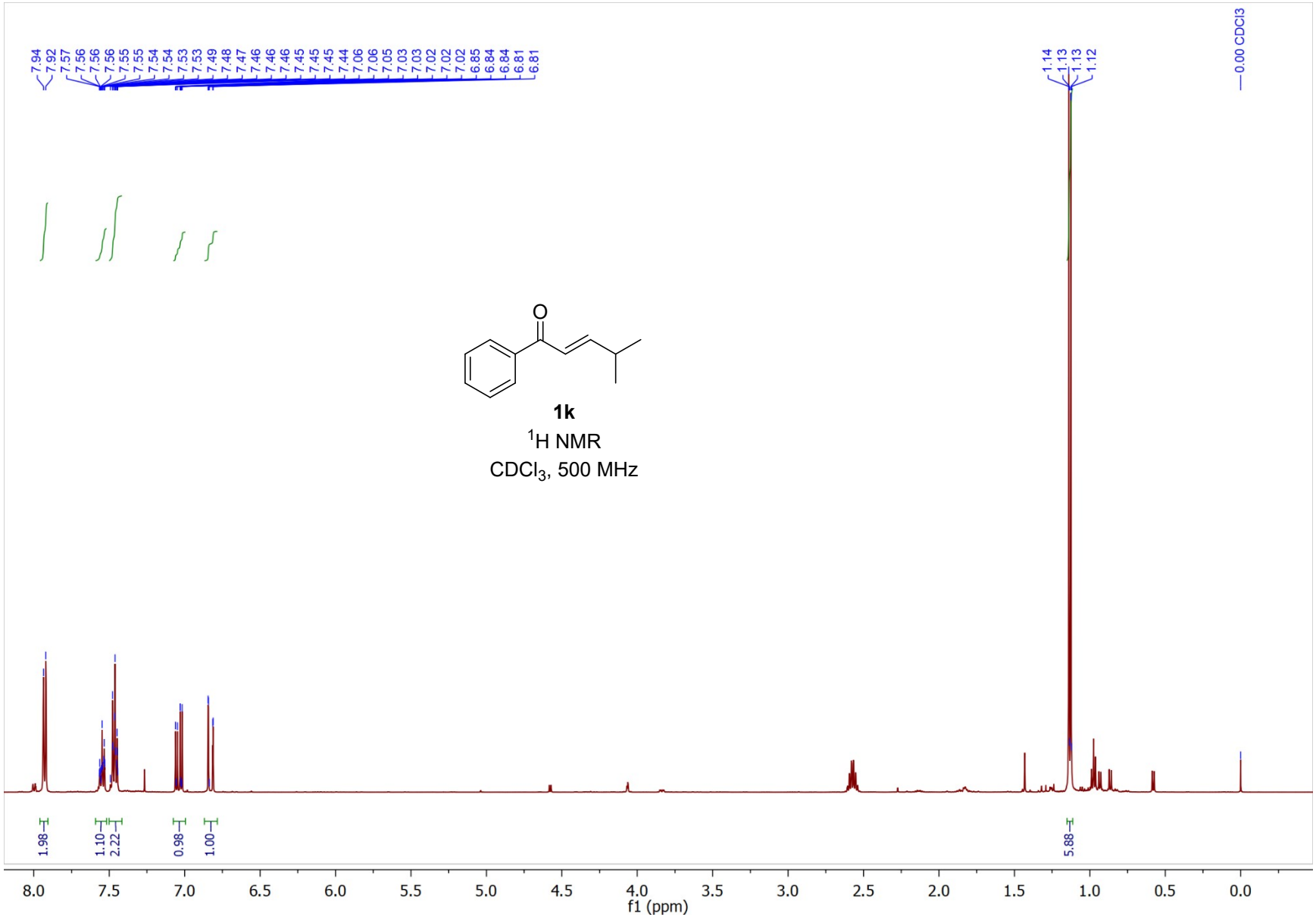
^{1}H NMR

$CDCl_3$, 500 MHz


7.59
7.59
7.58
7.58
7.57
7.56
7.56
7.29
7.29
7.29
7.28
7.27
7.27
7.21
7.20
7.20
7.20
7.19
7.18
7.18
7.17
7.17
6.85
6.85
6.82
6.81
6.81
6.79
6.78
6.78
6.53
6.53
6.52
6.52
6.51
6.51
6.51
2.84
2.82
2.81
2.80
2.65
2.63
2.63
2.62
2.62
2.61
2.60
2.60
2.59
2.59
-0.00 CDCl3
O
O
1h
1H NMR
CDCl3, 500 MHz
1.13
1.94
4.89
1.00
1.00
2.08
2.36
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
N
1i
1H NMR
CDCl3, 500 MHz
f1 (ppm)

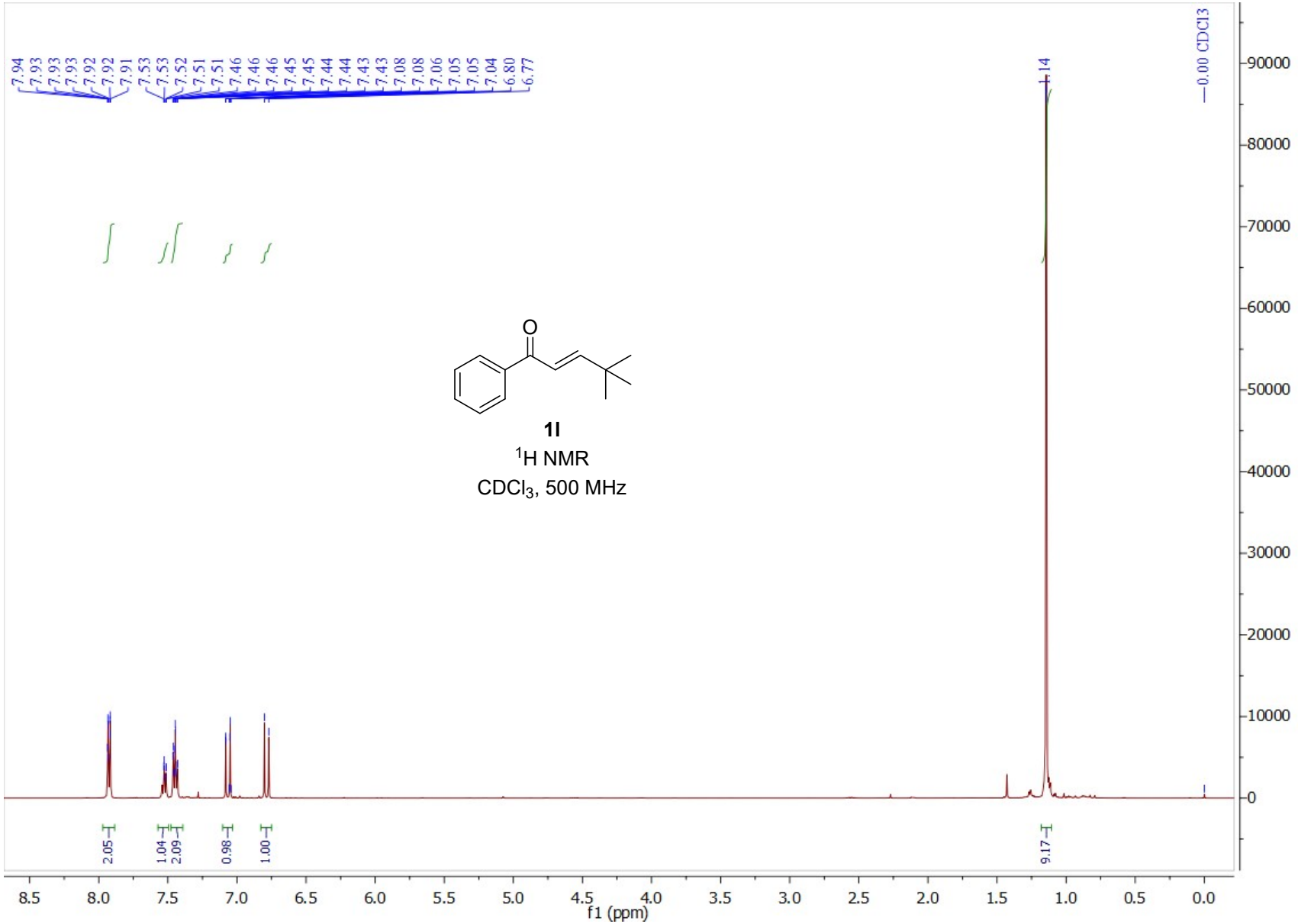

O
1j
1H NMR
CDCl3, 500 MHz
f1 (ppm)



1k

^{1}H NMR

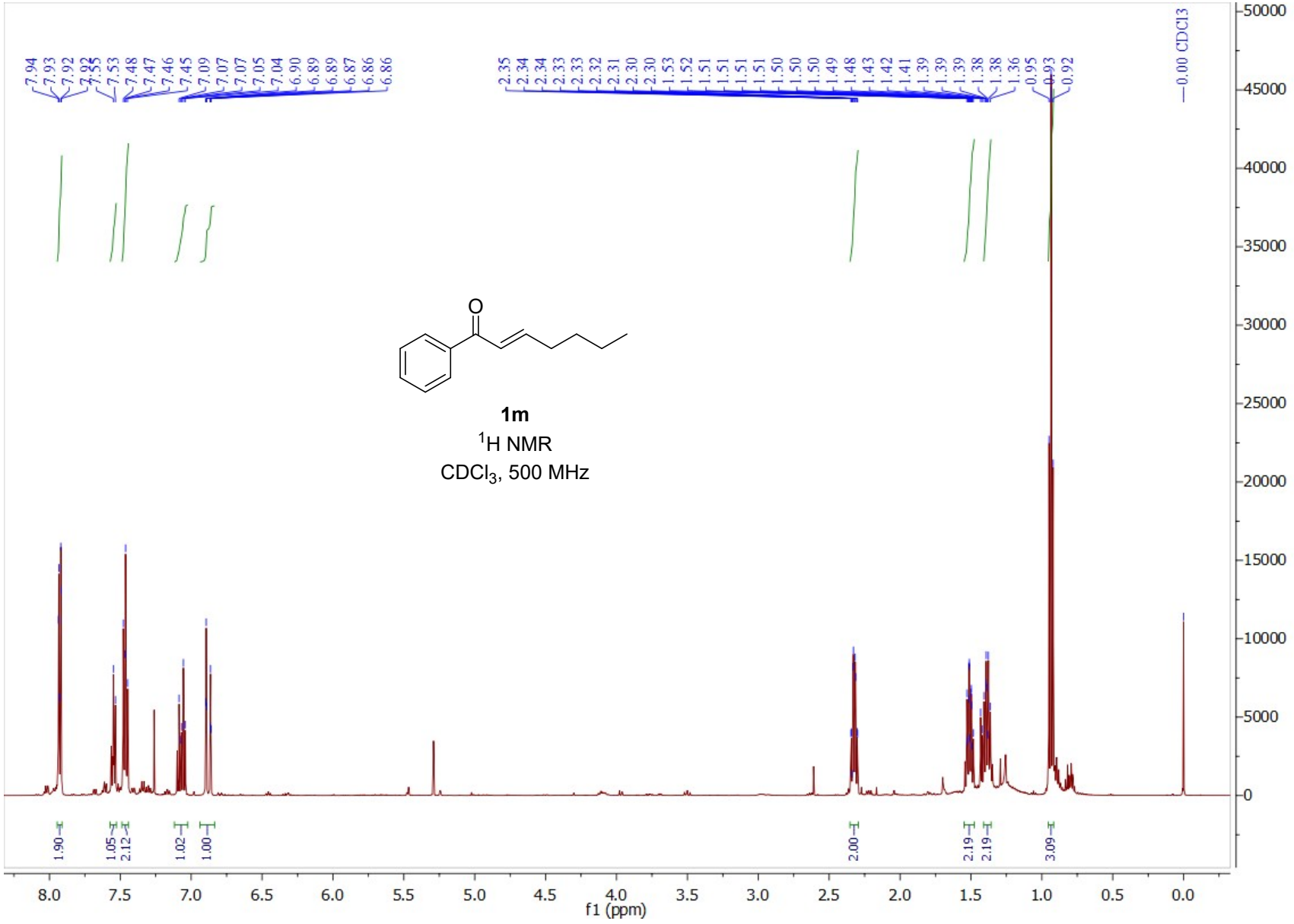
$CDCl_3$, 500 MHz



1l

^{1}H NMR

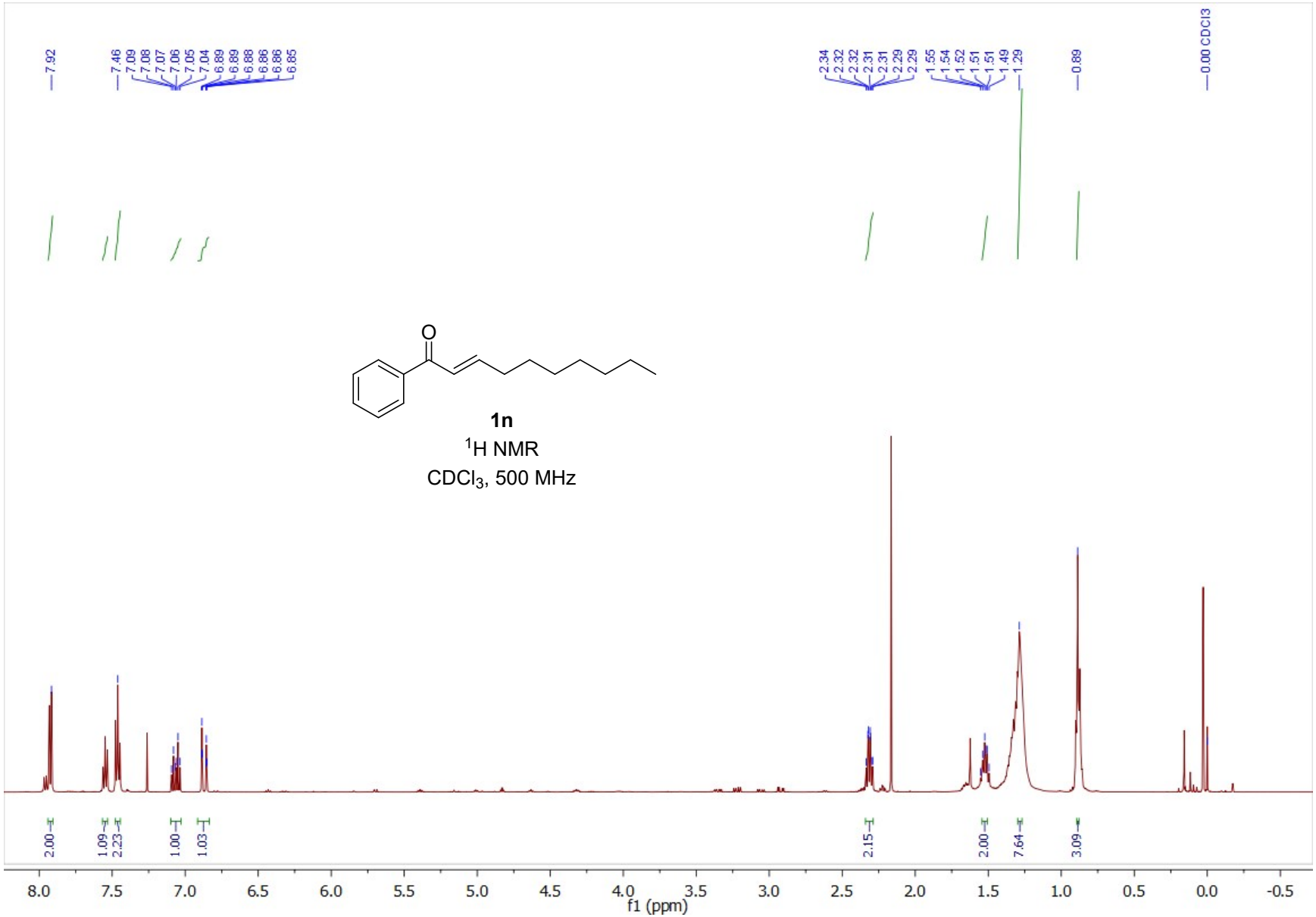
$CDCl_3$, 500 MHz

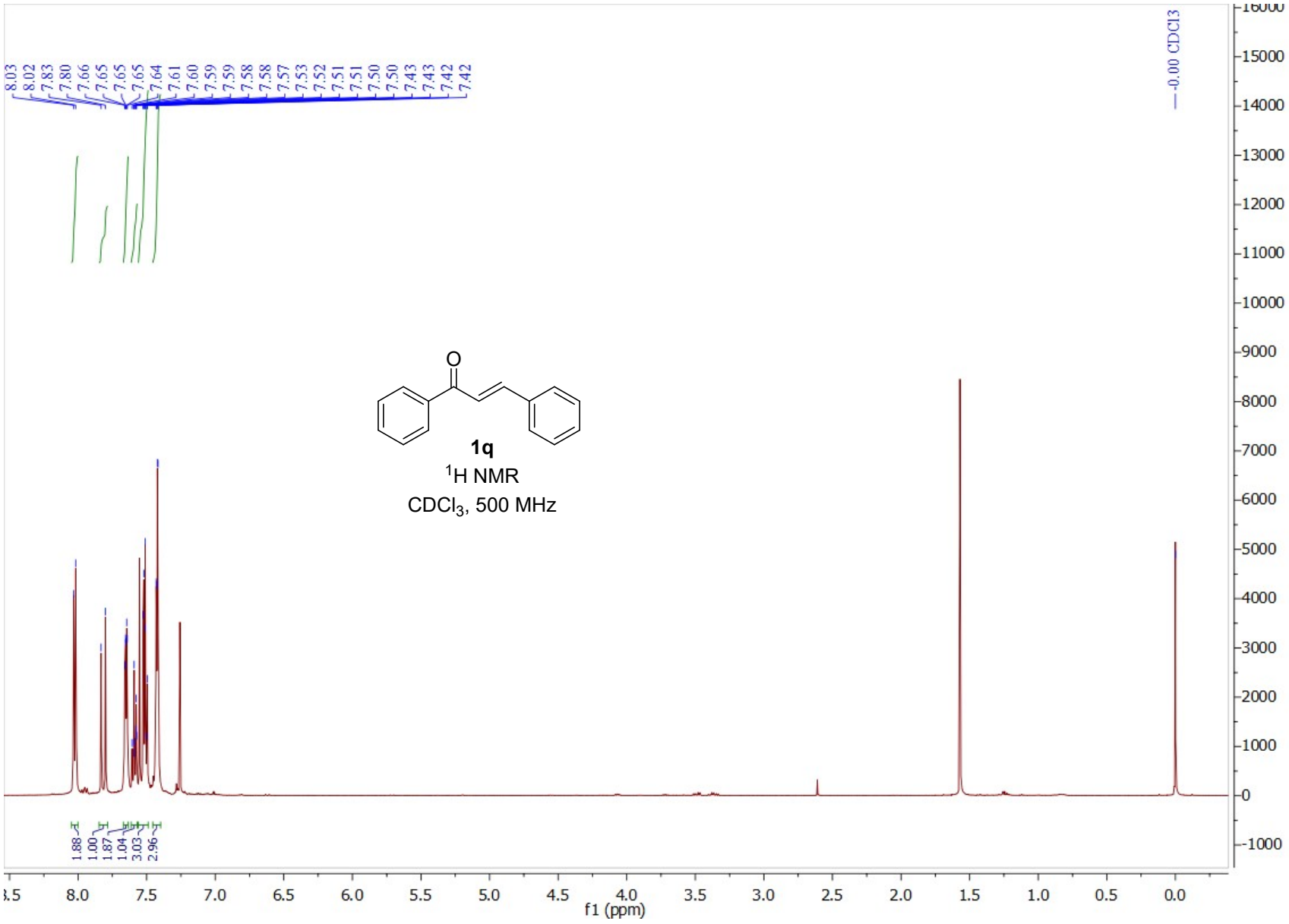


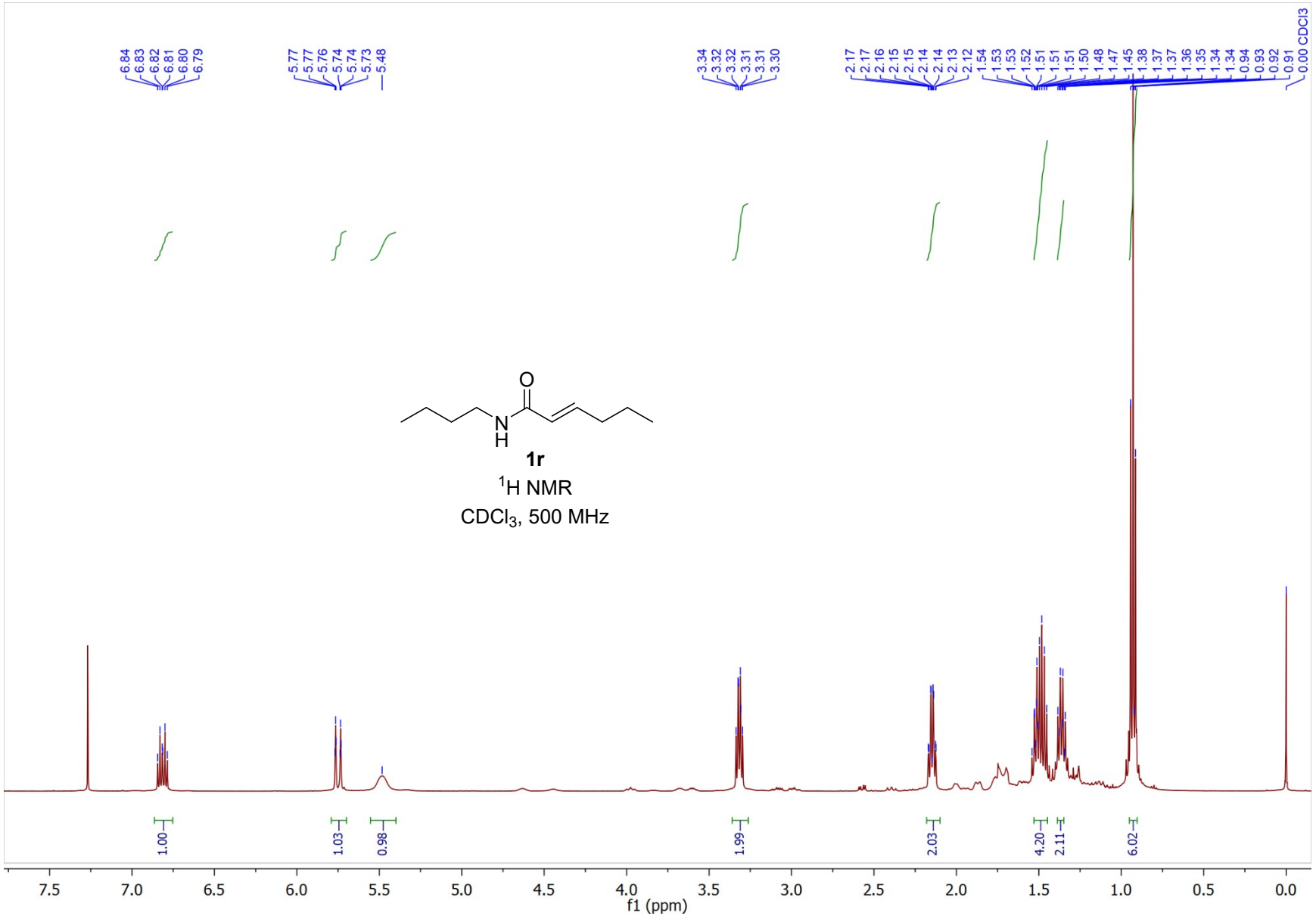
1m

^{1}H NMR

$CDCl_3$, 500 MHz


7.92
7.46
7.09
7.08
7.07
7.06
7.05
7.04
6.89
6.89
6.88
6.86
6.86
6.85
2.34
2.32
2.32
2.31
2.31
2.29
2.29
1.55
1.54
1.52
1.51
1.51
1.49
1.29
0.89
0.00 CDCl3
O
1n
1H NMR
CDCl3, 500 MHz
2.00
1.09
2.23
1.00
1.03
2.15
2.00
7.64
3.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


8.03
8.02
7.83
7.80
7.66
7.65
7.65
7.65
7.64
7.61
7.60
7.59
7.59
7.58
7.58
7.57
7.53
7.52
7.51
7.51
7.50
7.50
7.43
7.43
7.42
7.42
-0.00 CDCl3
O
1q
1H NMR
CDCl3, 500 MHz
1.88
1.00
1.87
1.04
3.03
2.96
f1 (ppm)

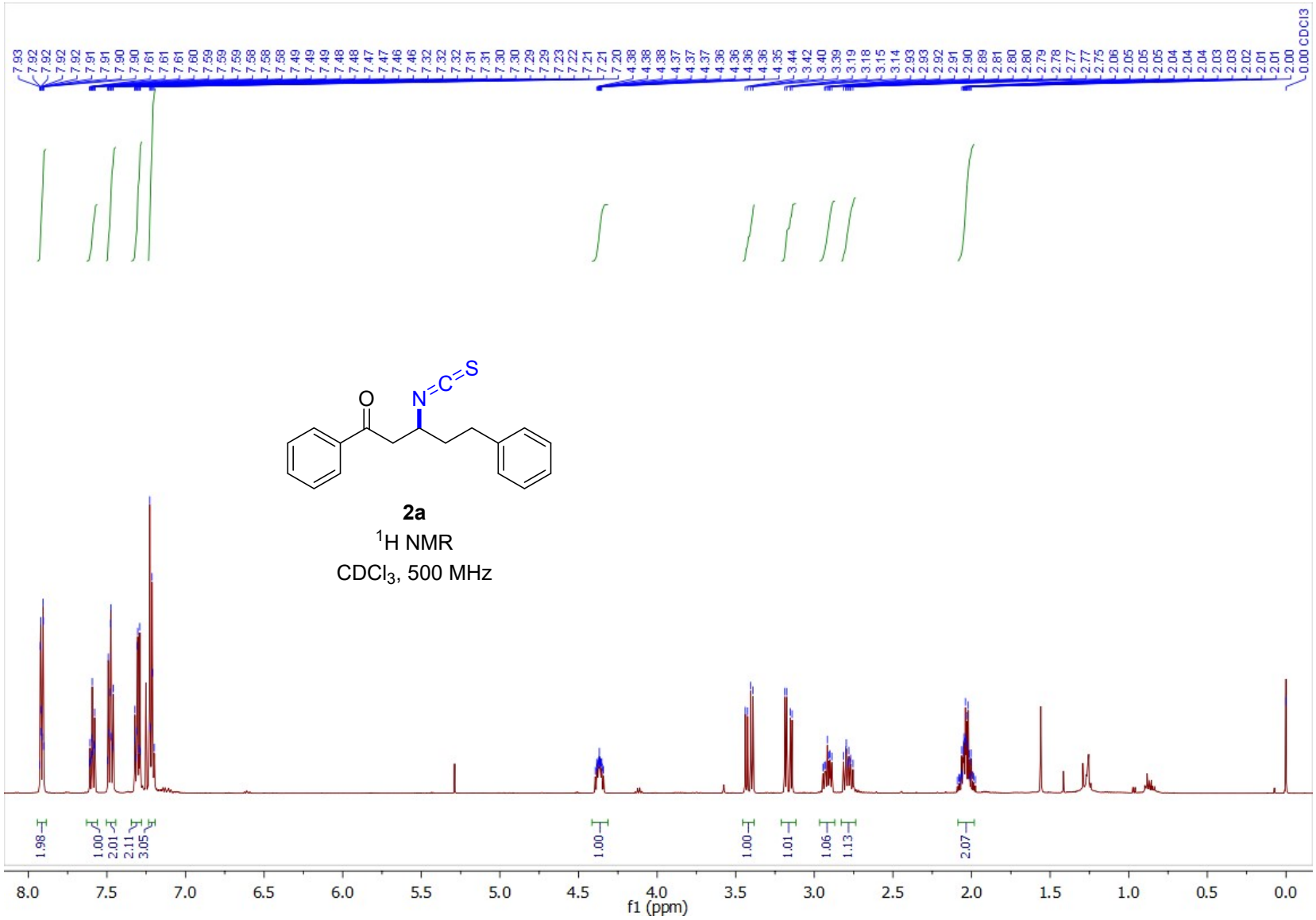


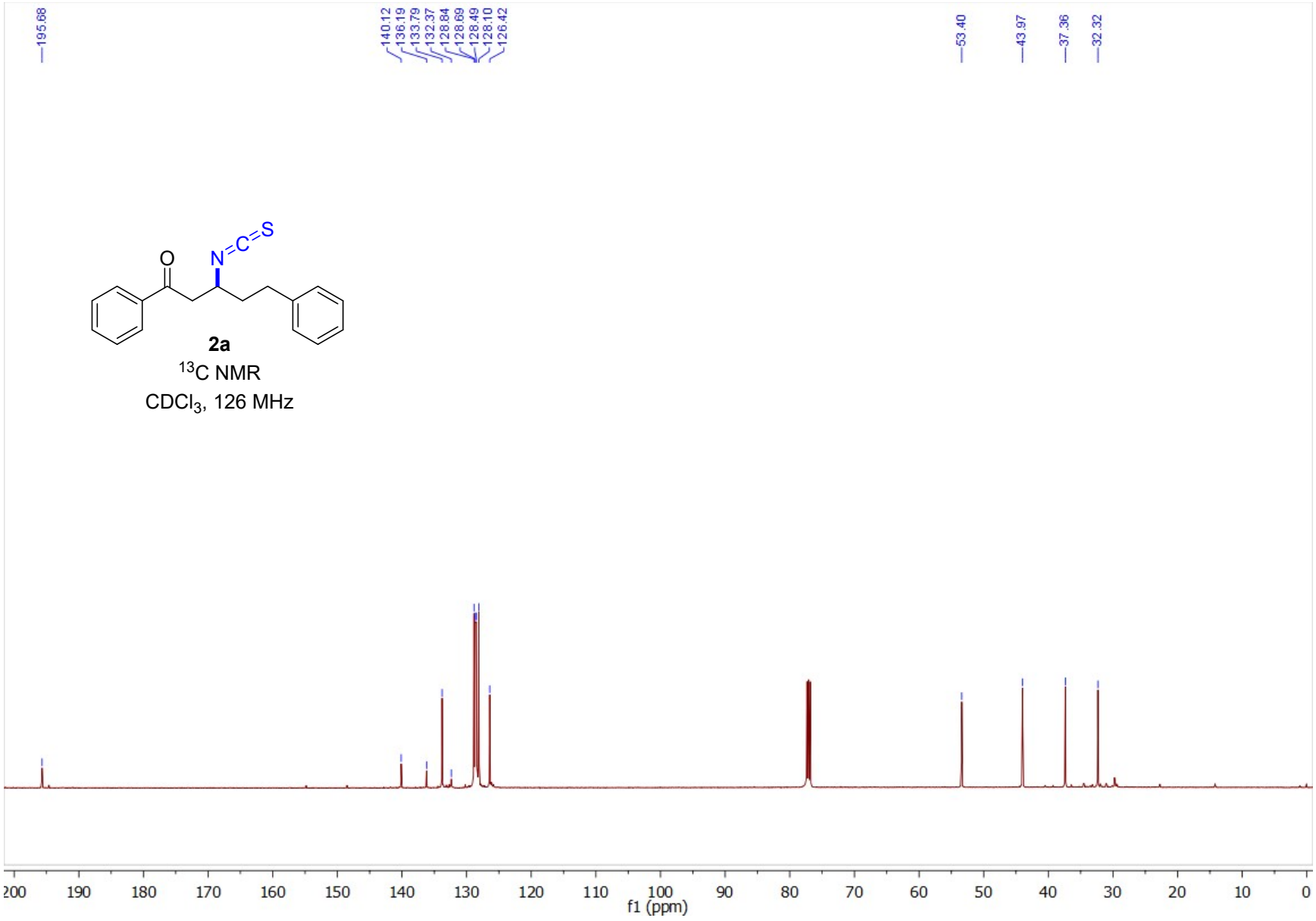
1r

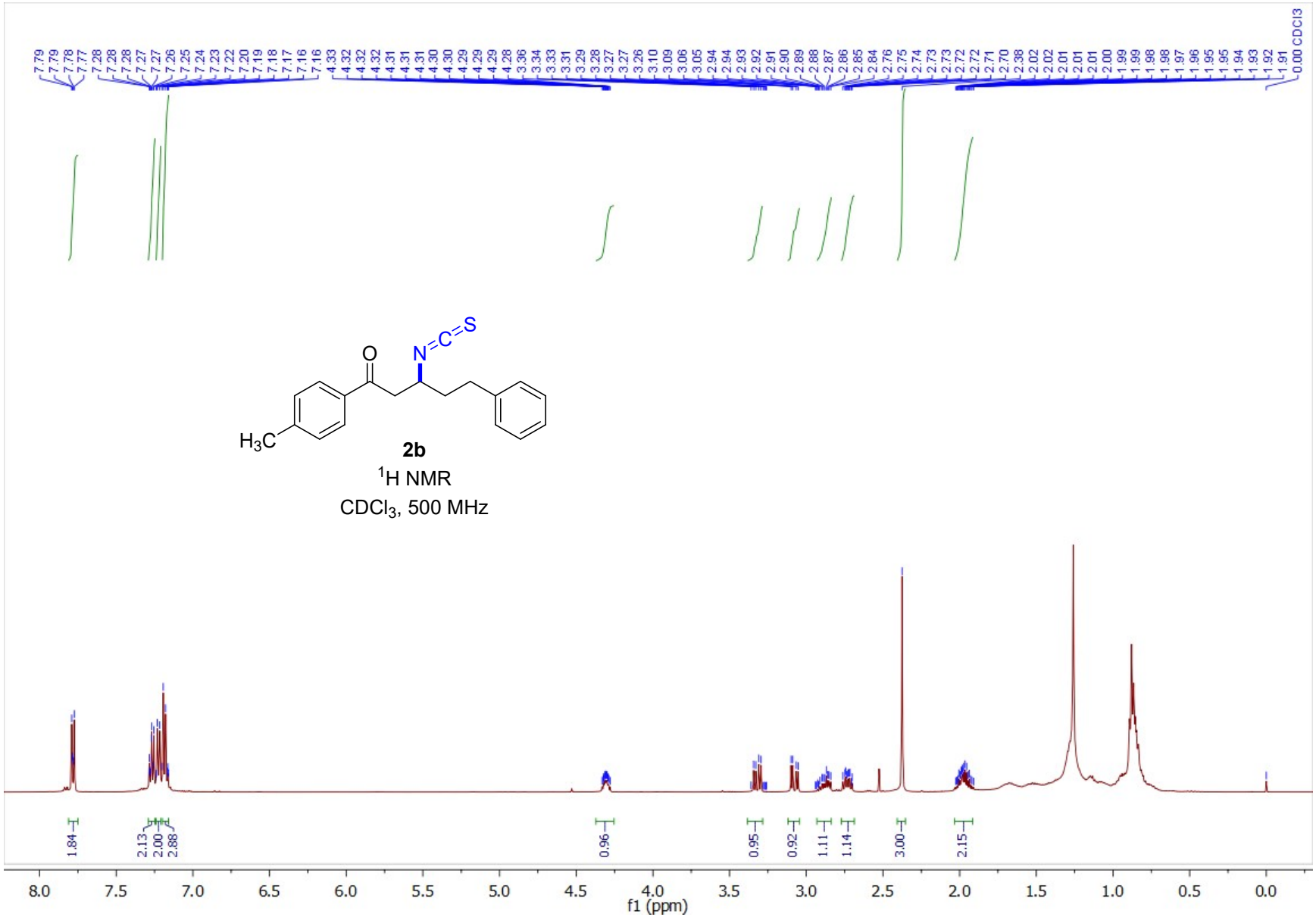
^{1}H NMR

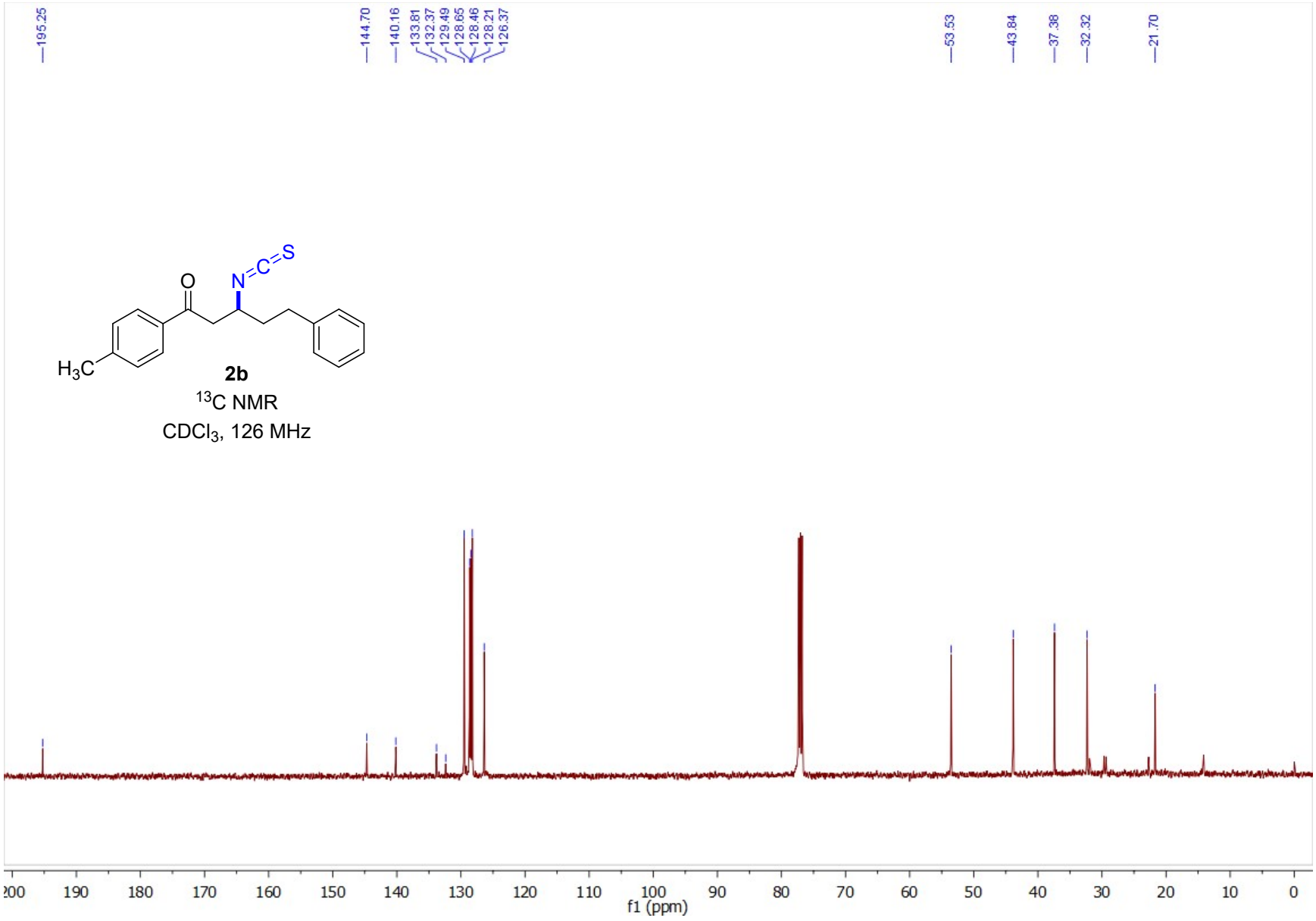
$CDCl_3$, 500 MHz

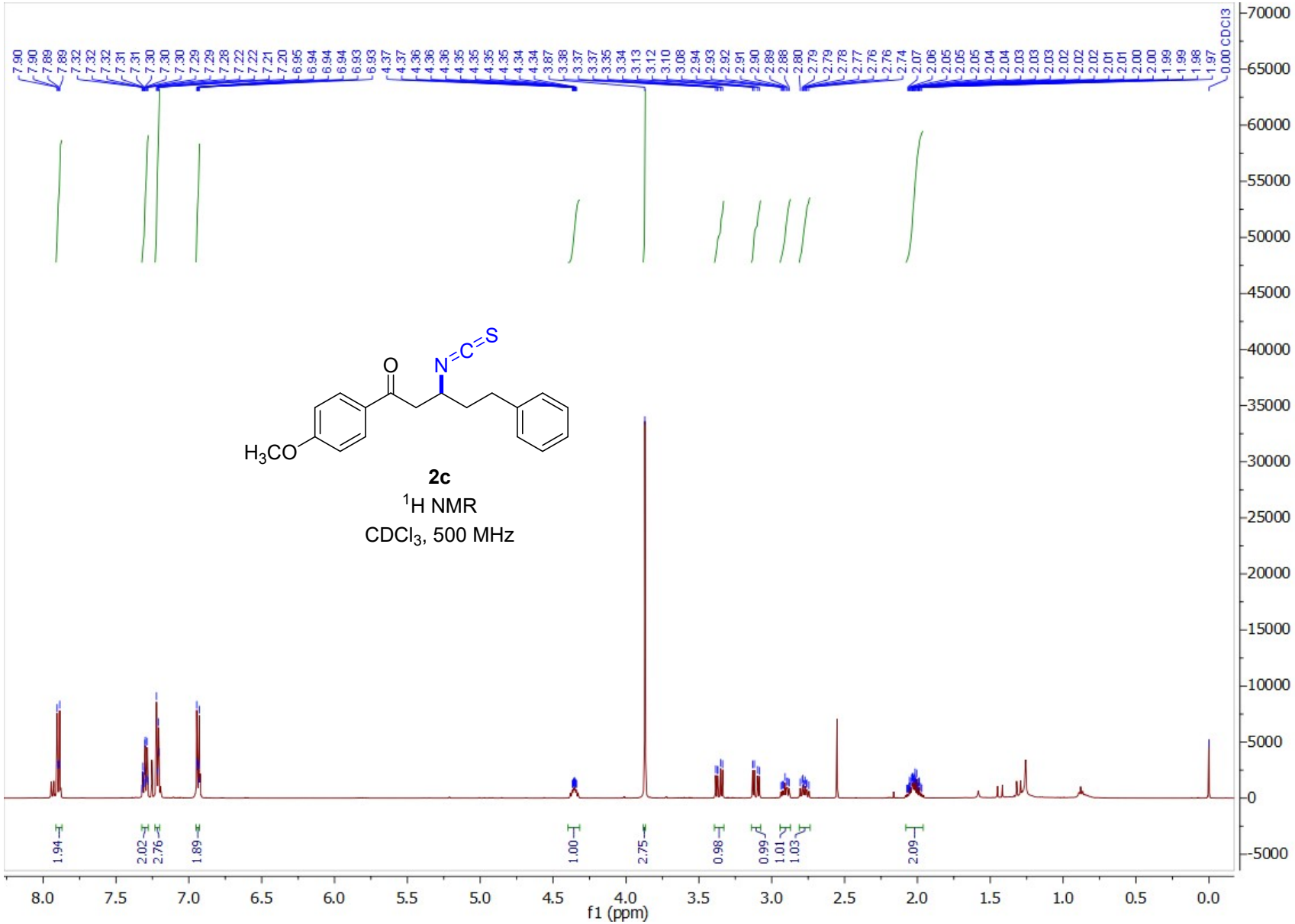
10.2 ^{1}H, ^{13}C, and ^{19}F NMR for isothiocyanation products and derivatives

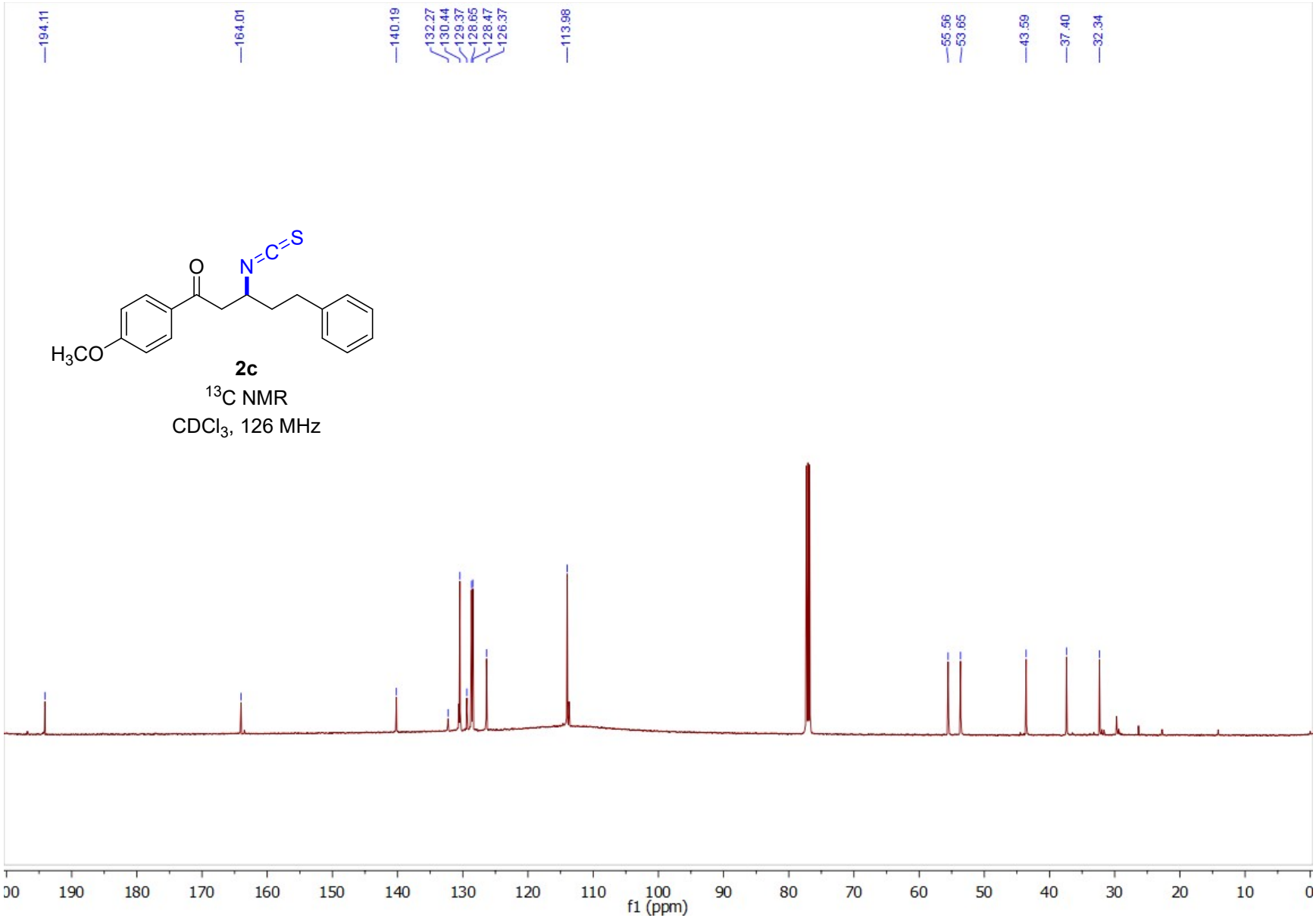


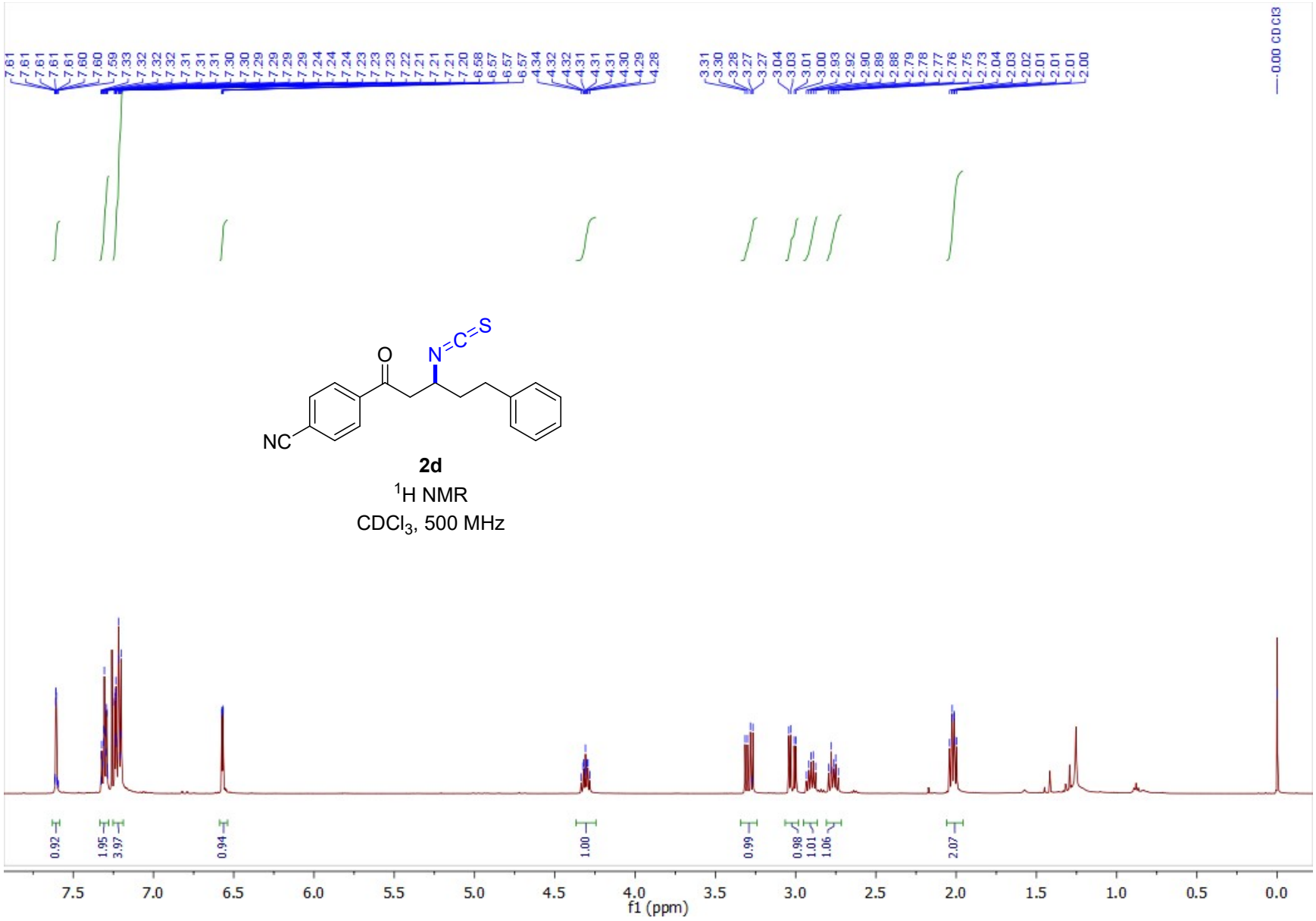

195.68
140.12
136.19
133.79
132.37
128.84
128.69
128.49
128.10
126.42
53.40
43.97
37.36
32.32
O
N=C=S
2a
13C NMR
CDCl3, 126 MHz
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.79 7.79 7.78 7.77 7.28 7.28 7.27 7.27 7.26 7.25 7.24 7.23 7.22 7.20 7.19 7.18 7.17 7.16 7.16 4.33 4.32 4.32 4.31 4.31 4.31 4.30 4.30 4.29 4.29 4.29 4.28 3.36 3.34 3.33 3.31 3.29 3.28 3.27 3.27 3.26 3.10 3.09 3.06 3.05 2.94 2.94 2.93 2.92 2.91 2.90 2.89 2.88 2.87 2.86 2.85 2.84 2.76 2.75 2.74 2.73 2.73 2.72 2.72 2.71 2.70 2.38 2.02 2.02 2.01 2.01 2.01 2.00 1.99 1.99 1.98 1.98 1.97 1.96 1.95 1.95 1.94 1.93 1.92 1.91 0.00 CDCl3
O
N=C=S
H3C
2b
1H NMR
CDCl3, 500 MHz
1.84
2.13
2.00
2.88
0.96
0.95
0.92
1.11
1.14
3.00
2.15
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


195.25
144.70
140.16
133.81
132.37
129.49
128.65
128.46
128.21
126.37
53.53
43.84
37.38
32.32
21.70
O
N=C=S
H3C
2b
13C NMR
CDCl3, 126 MHz
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N=C=S
H3CO
2c
1H NMR
CDCl3, 500 MHz
f1 (ppm)

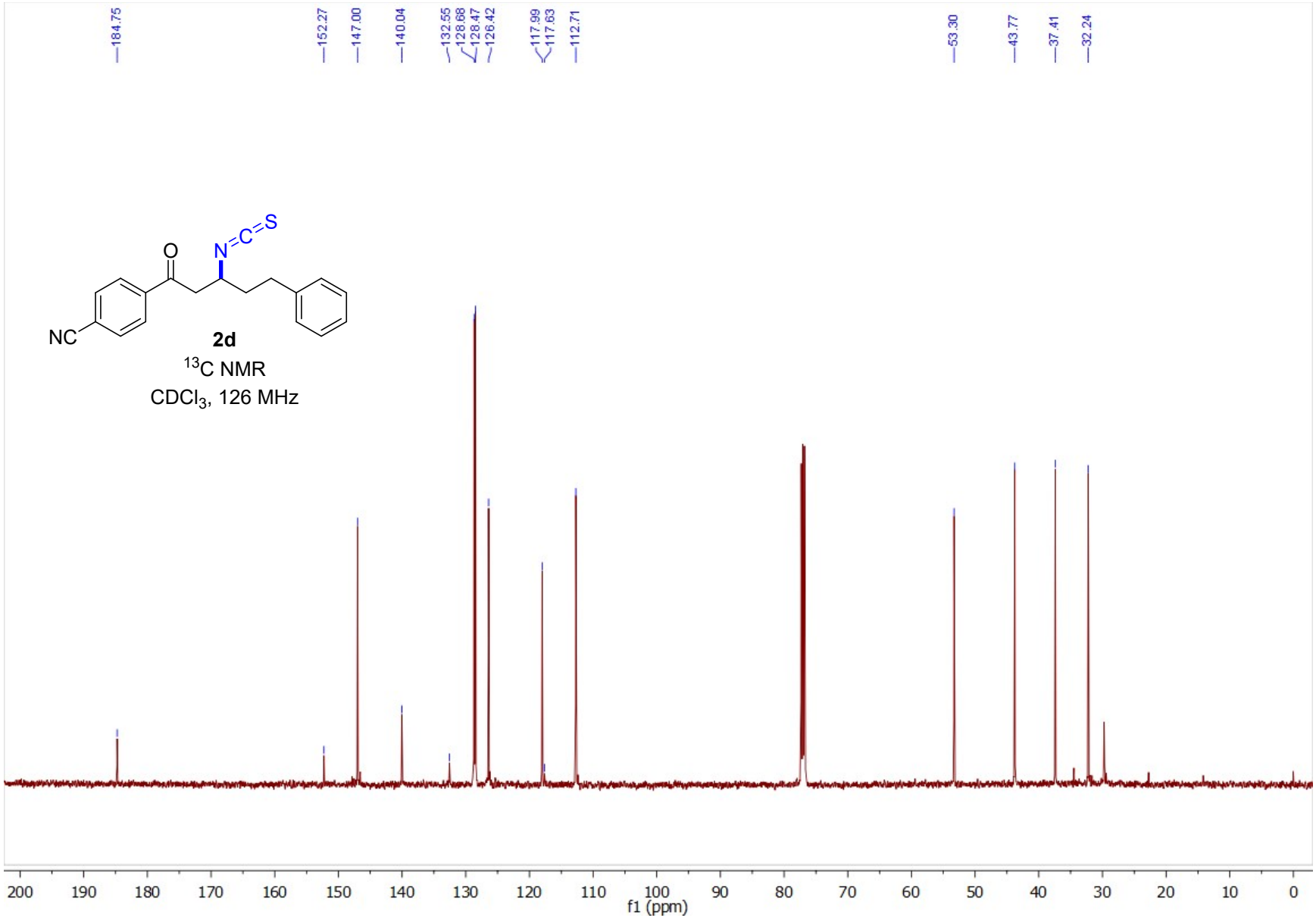

194.11
164.01
140.19
132.27
130.44
129.37
128.65
128.47
126.37
113.98
55.56
53.65
43.59
37.40
32.34
O
N=C=S
H3CO
2c
13C NMR
CDCl3, 126 MHz
f1 (ppm)

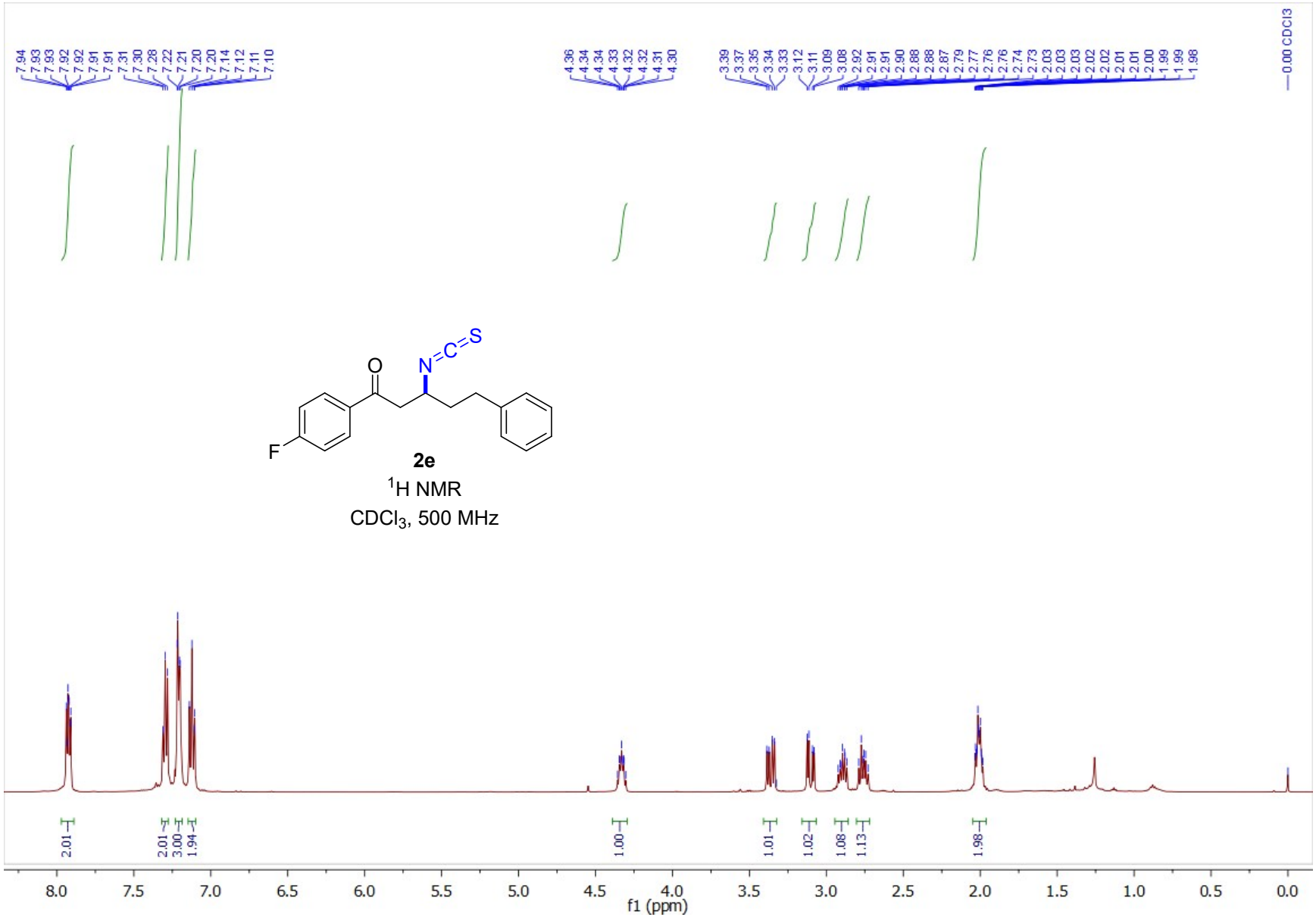


2d

^{1}H NMR

$CDCl_3$, 500 MHz

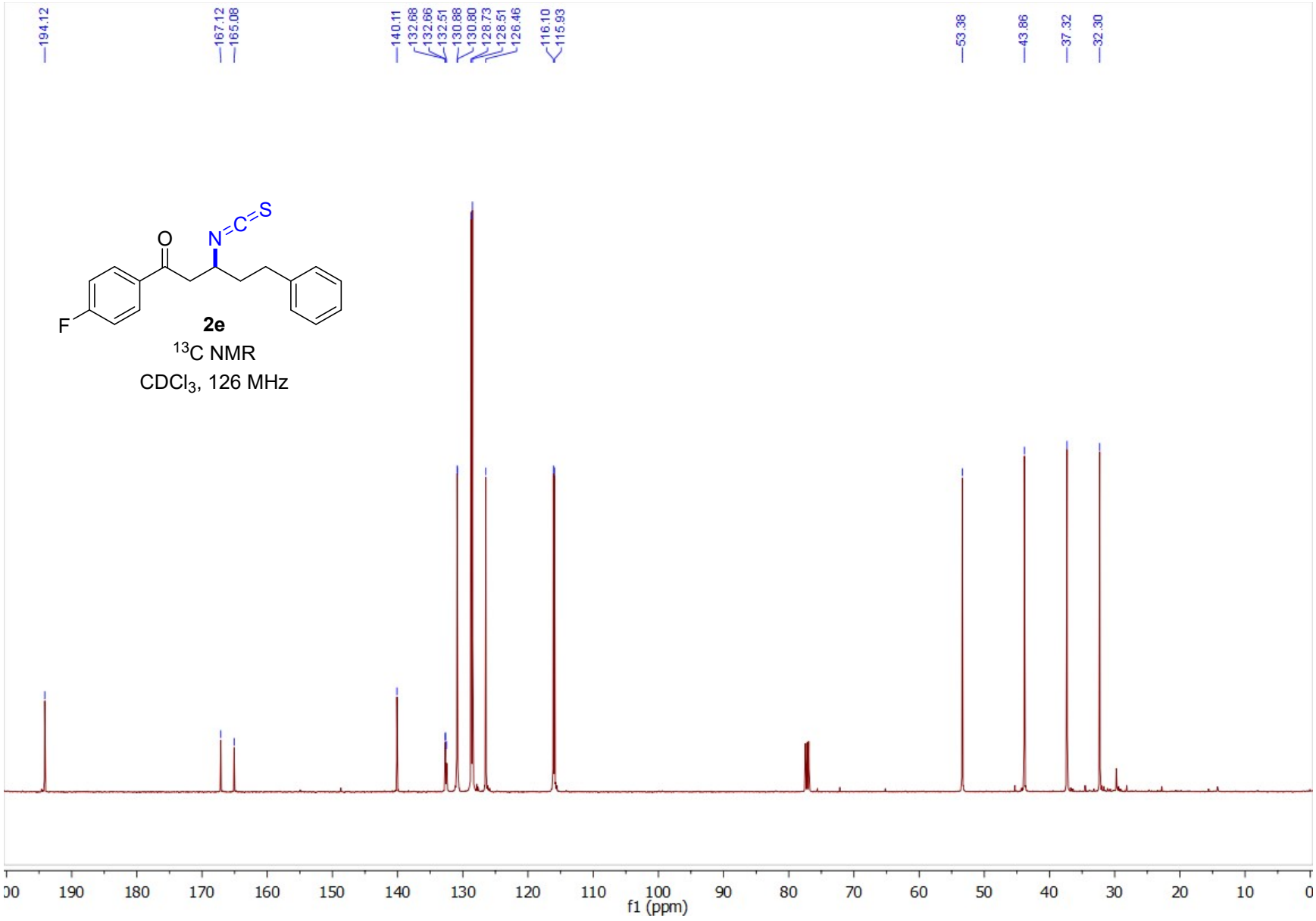

184.75
152.27
147.00
140.04
132.55
128.68
128.47
126.42
117.99
117.63
112.71
53.30
43.77
37.41
32.24
O
N=C=S
NC
2d
13C NMR
CDCl3, 126 MHz
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

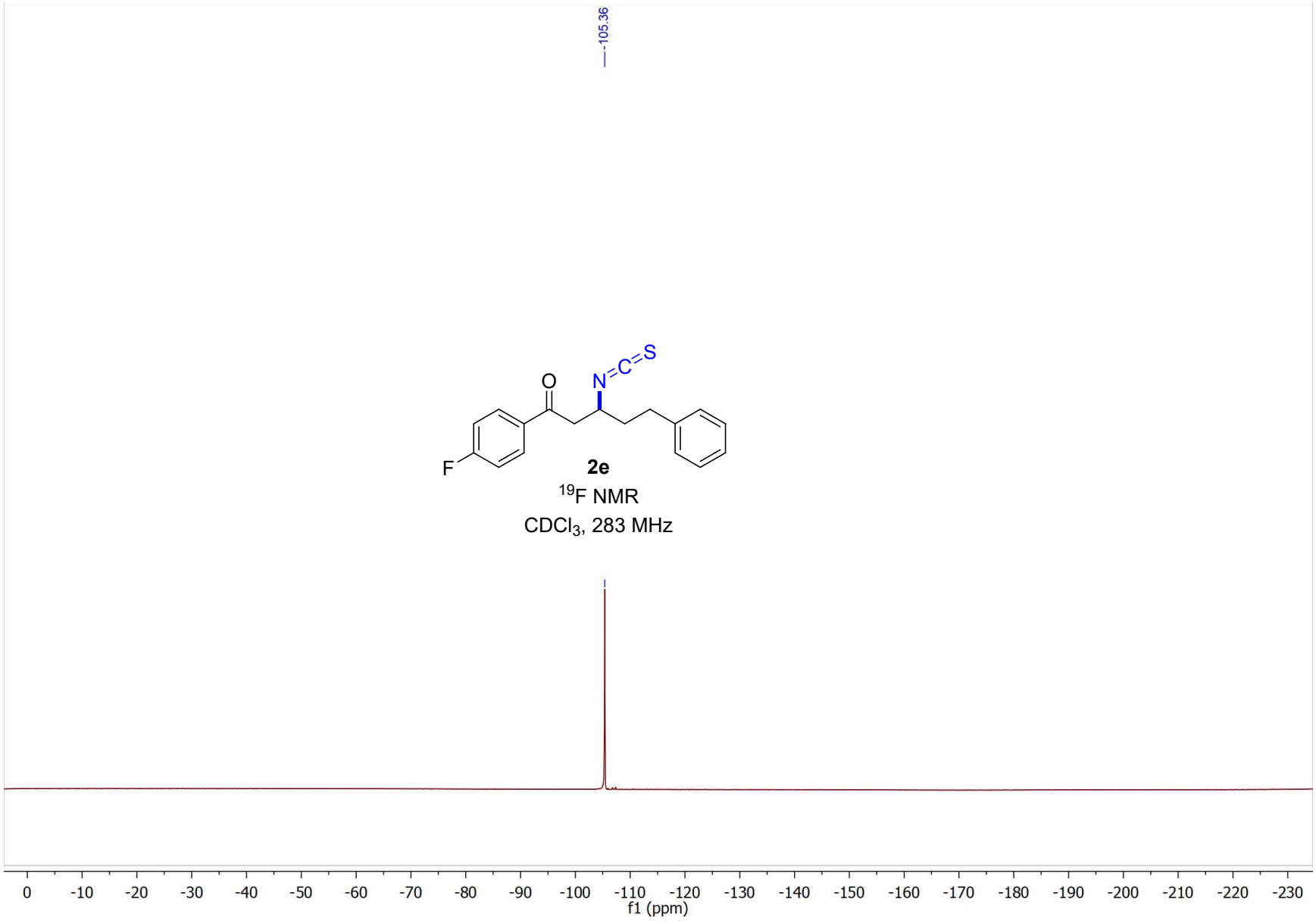


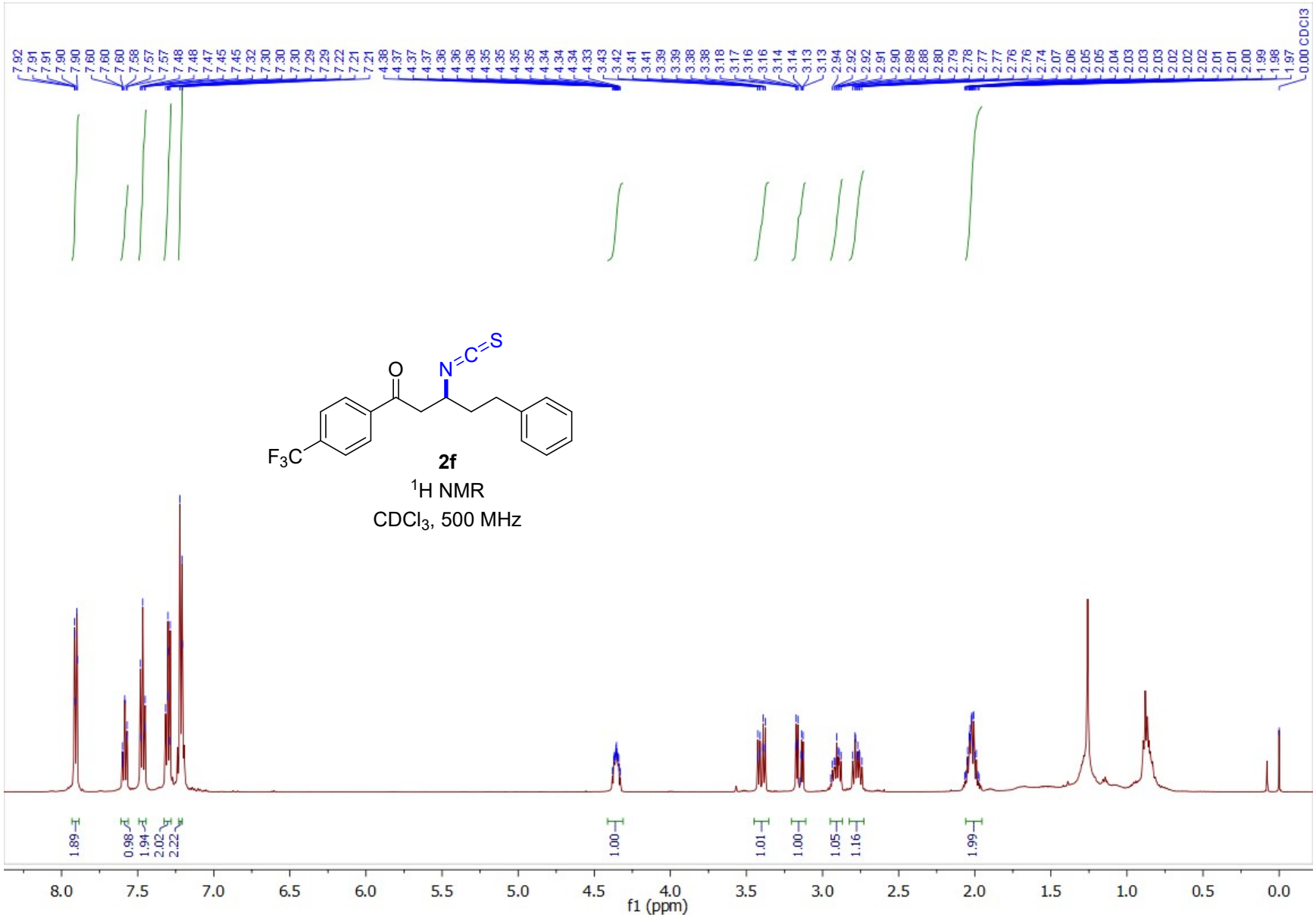
2e

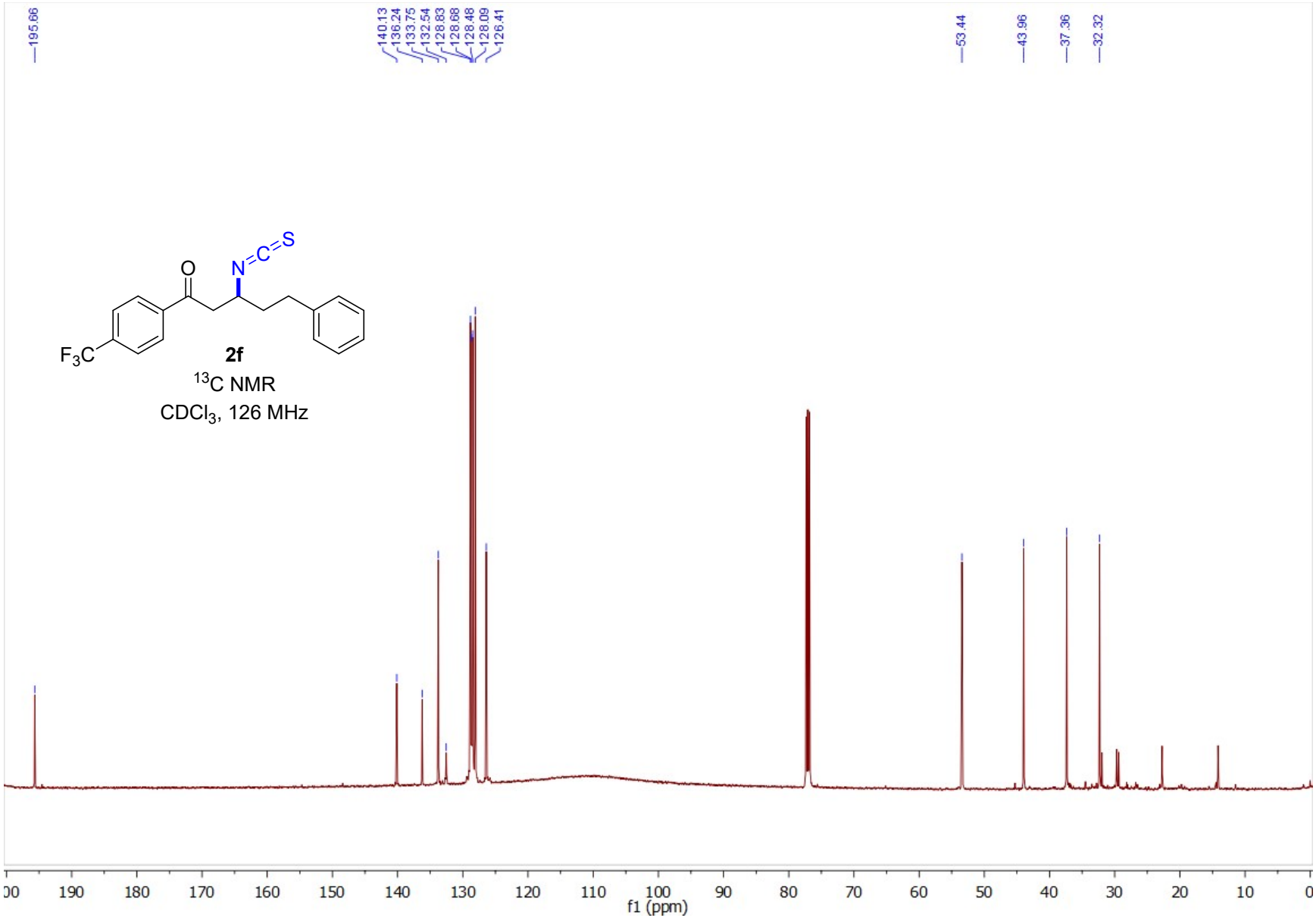
^{1}H NMR

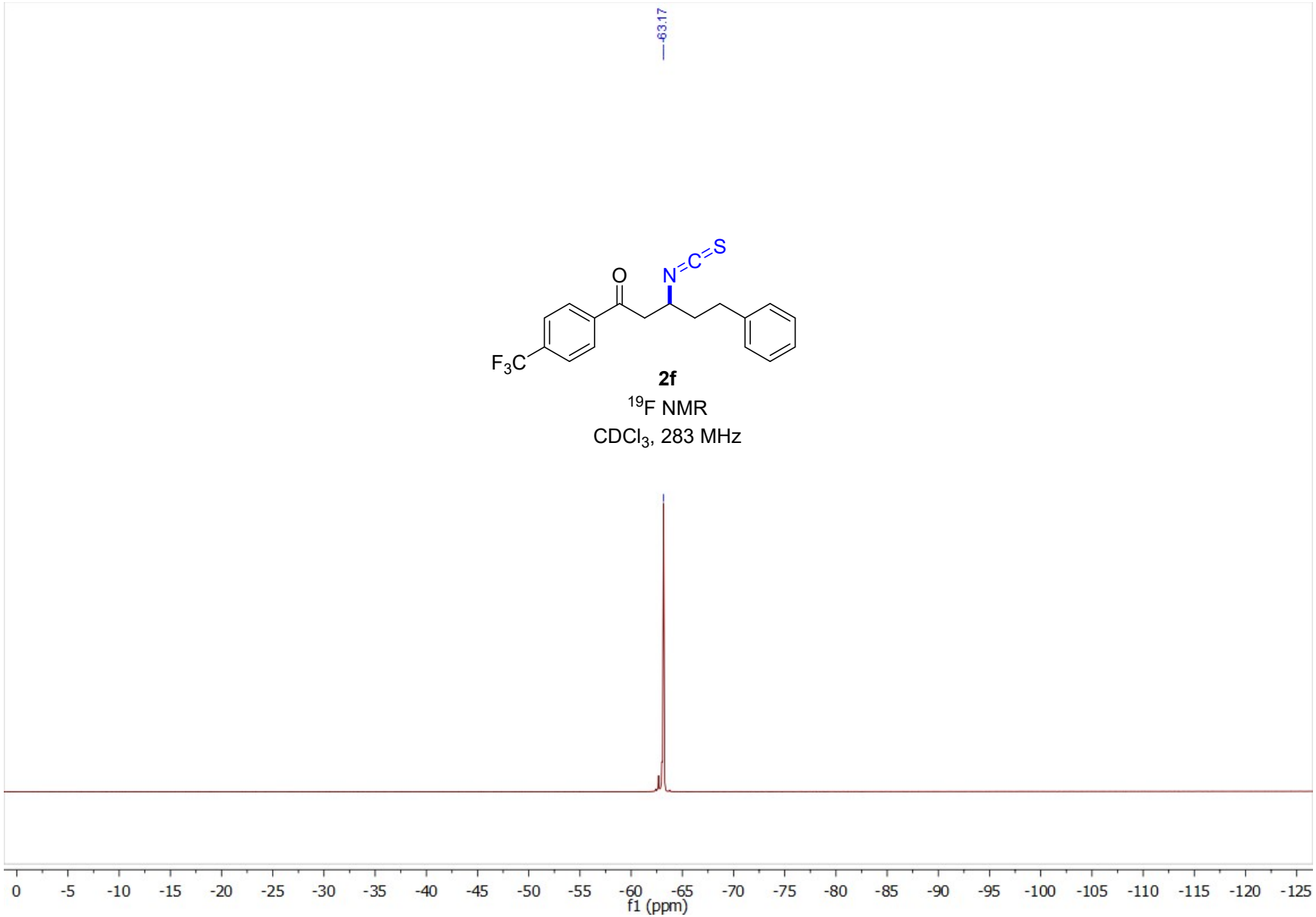
$CDCl_3$, 500 MHz


194.12
167.12
165.08
140.11
132.68
132.66
132.51
130.88
130.80
128.73
128.51
126.46
116.10
115.93
53.38
43.86
37.32
32.30
O
N=C=S
F
2e
13C NMR
CDCl3, 126 MHz
f1 (ppm)


-105.36
O
N=C=S
F
2e
19F NMR
CDCl3, 283 MHz
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230
f1 (ppm)


O
N=C=S
F3C
2f
1H NMR
CDCl3, 500 MHz
f1 (ppm)

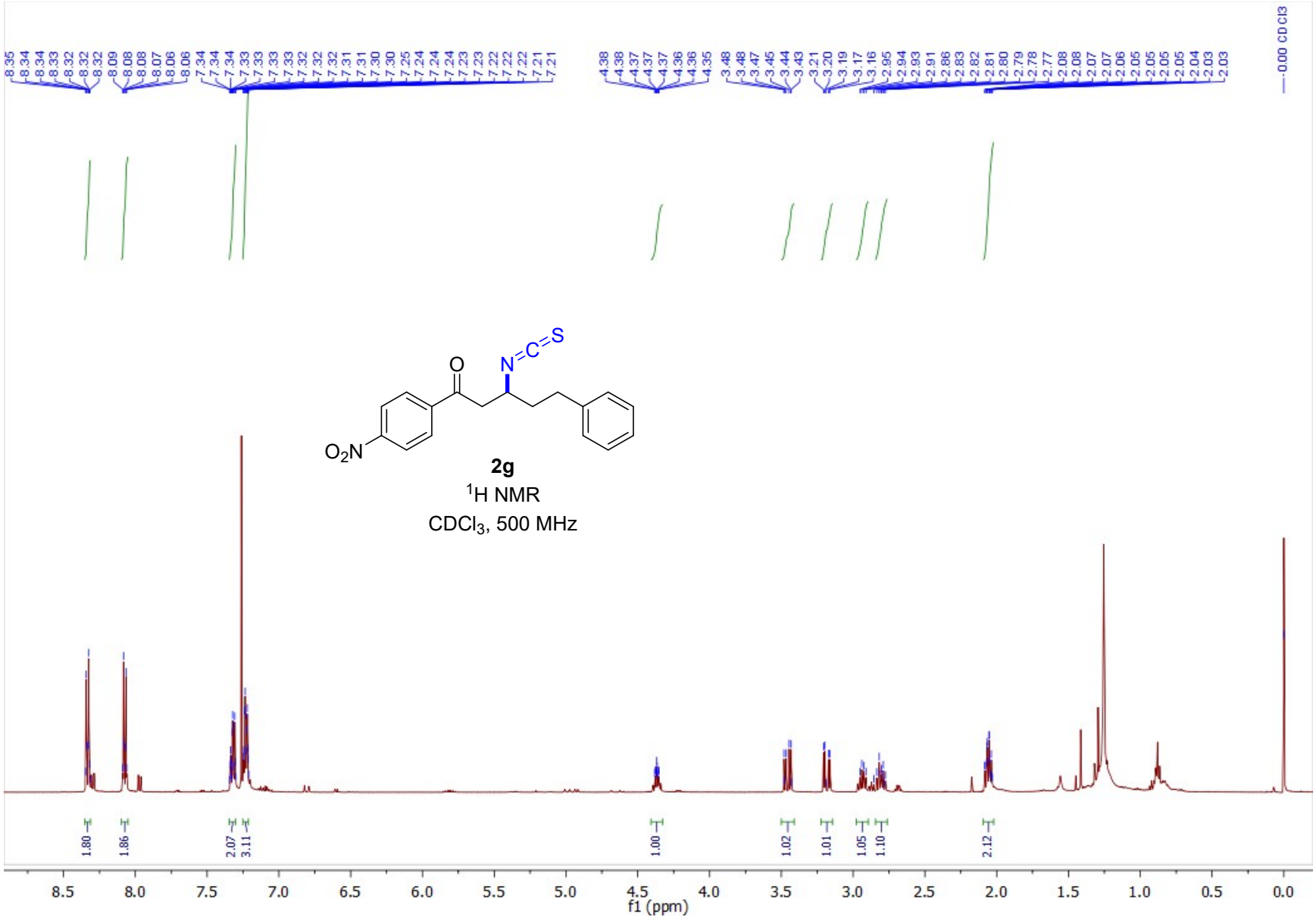

195.66
140.13
136.24
133.75
132.54
128.83
128.68
128.48
128.09
126.41
53.44
43.96
37.36
32.32
O
N=C=S
F3C
2f
13C NMR
CDCl3, 126 MHz
f1 (ppm)

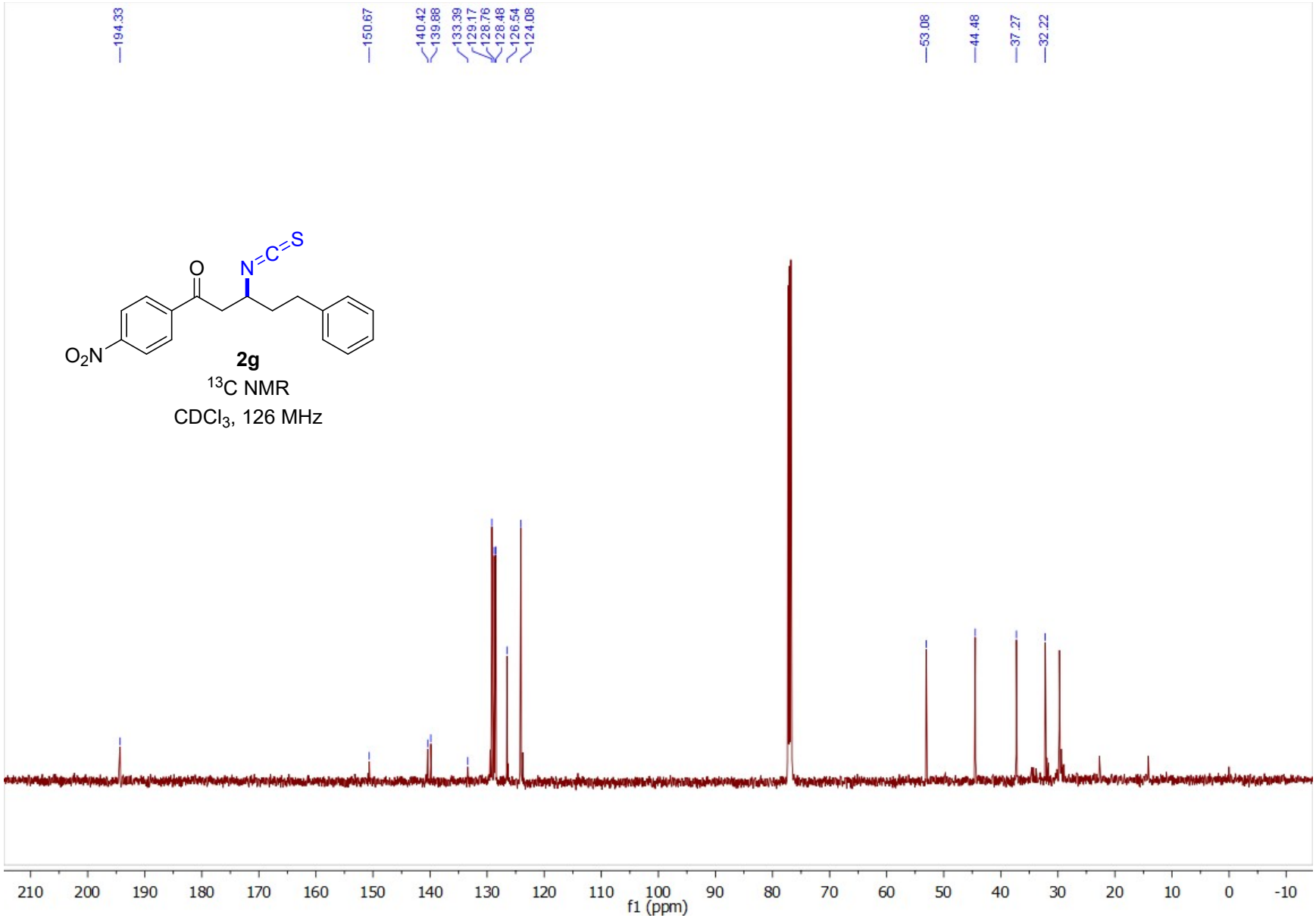


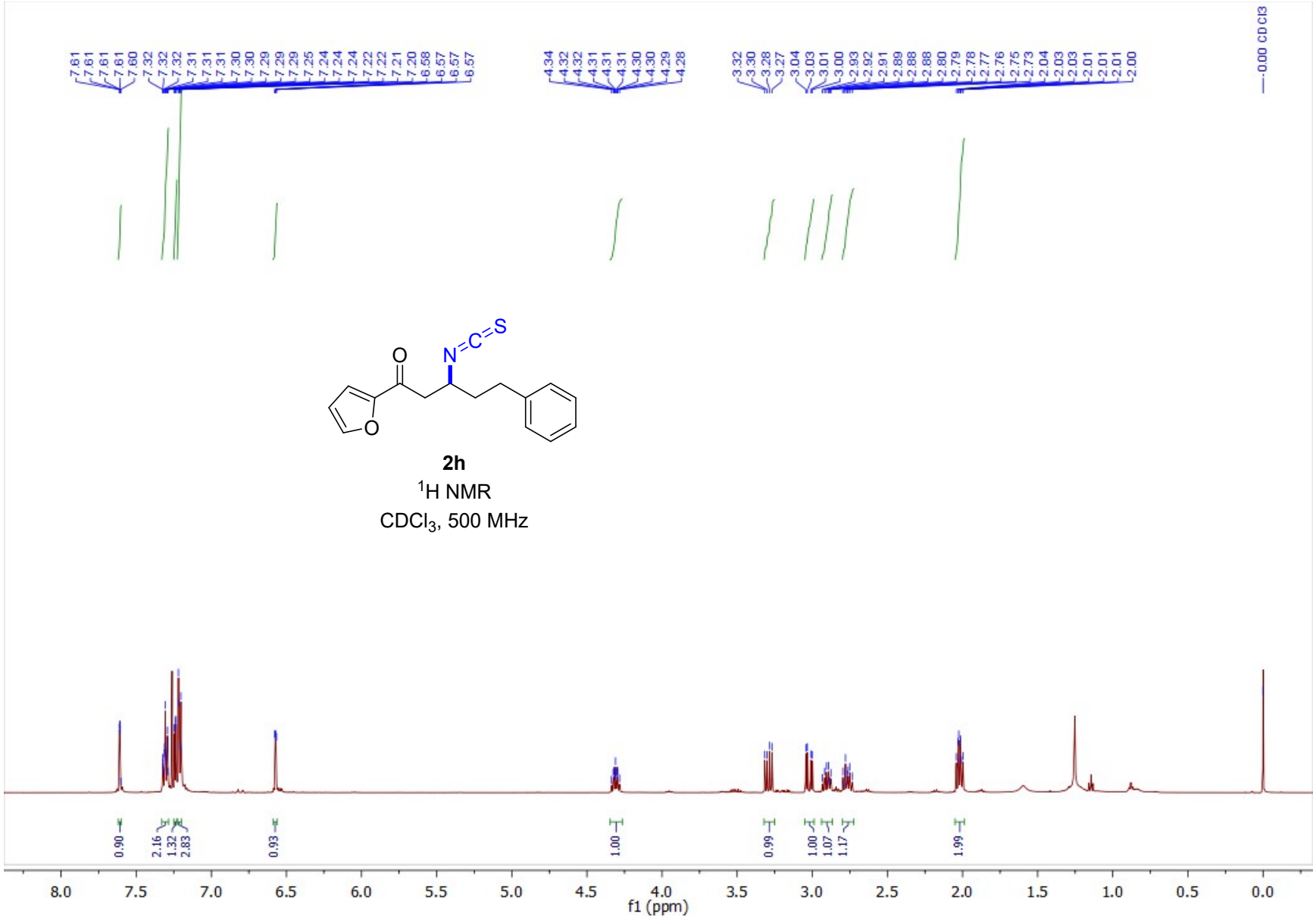
2f

^{19}F NMR

$CDCl_3$, 283 MHz


8.35 8.34 8.34 8.33 8.32 8.32 8.32 8.09 8.08 8.08 8.07 8.06 8.06 7.34 7.34 7.34 7.33 7.33 7.33 7.32 7.32 7.32 7.31 7.31 7.30 7.30 7.25 7.24 7.24 7.24 7.23 7.22 7.22 7.22 7.21 7.21
4.38 4.38 4.37 4.37 4.37 4.36 4.36 4.35 3.48 3.48 3.47 3.45 3.44 3.43 3.21 3.20 3.19 3.17 3.16 2.95 2.94 2.93 2.91 2.86 2.83 2.82 2.81 2.80 2.79 2.78 2.77 2.08 2.08 2.07 2.07 2.06 2.05 2.05 2.05 2.05 2.04 2.03 2.03
0.00 CDCl3
O
N=C=S
O2N
2g
1H NMR
CDCl3, 500 MHz
1.80
1.86
2.07
3.11
1.00
1.02
1.01
1.05
1.10
2.12
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

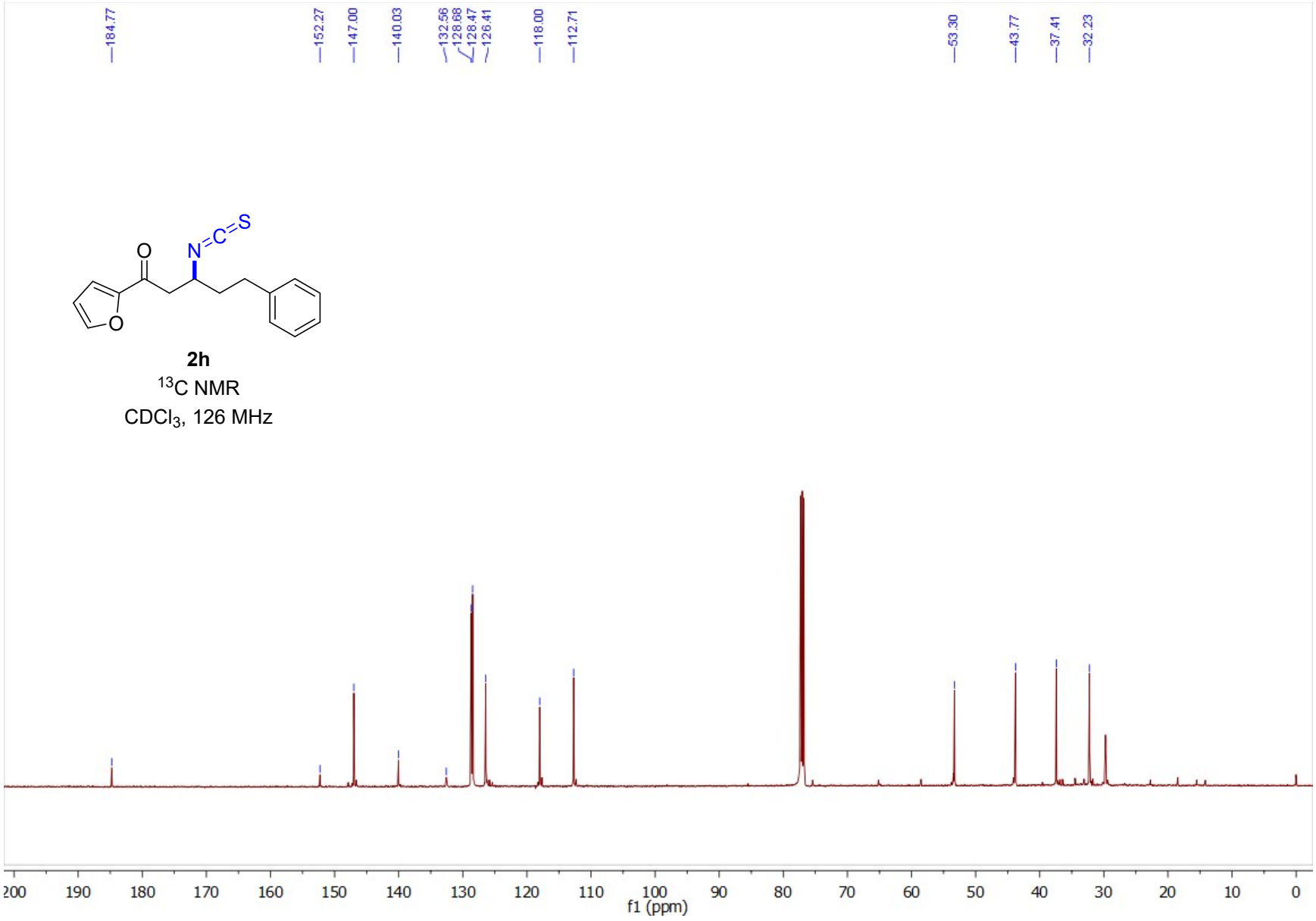

194.33
150.67
140.42
139.88
133.39
129.17
128.76
128.48
126.54
124.08
53.08
44.48
37.27
32.22
O
N=C=S
O2N
2g
13C NMR
CDCl3, 126 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

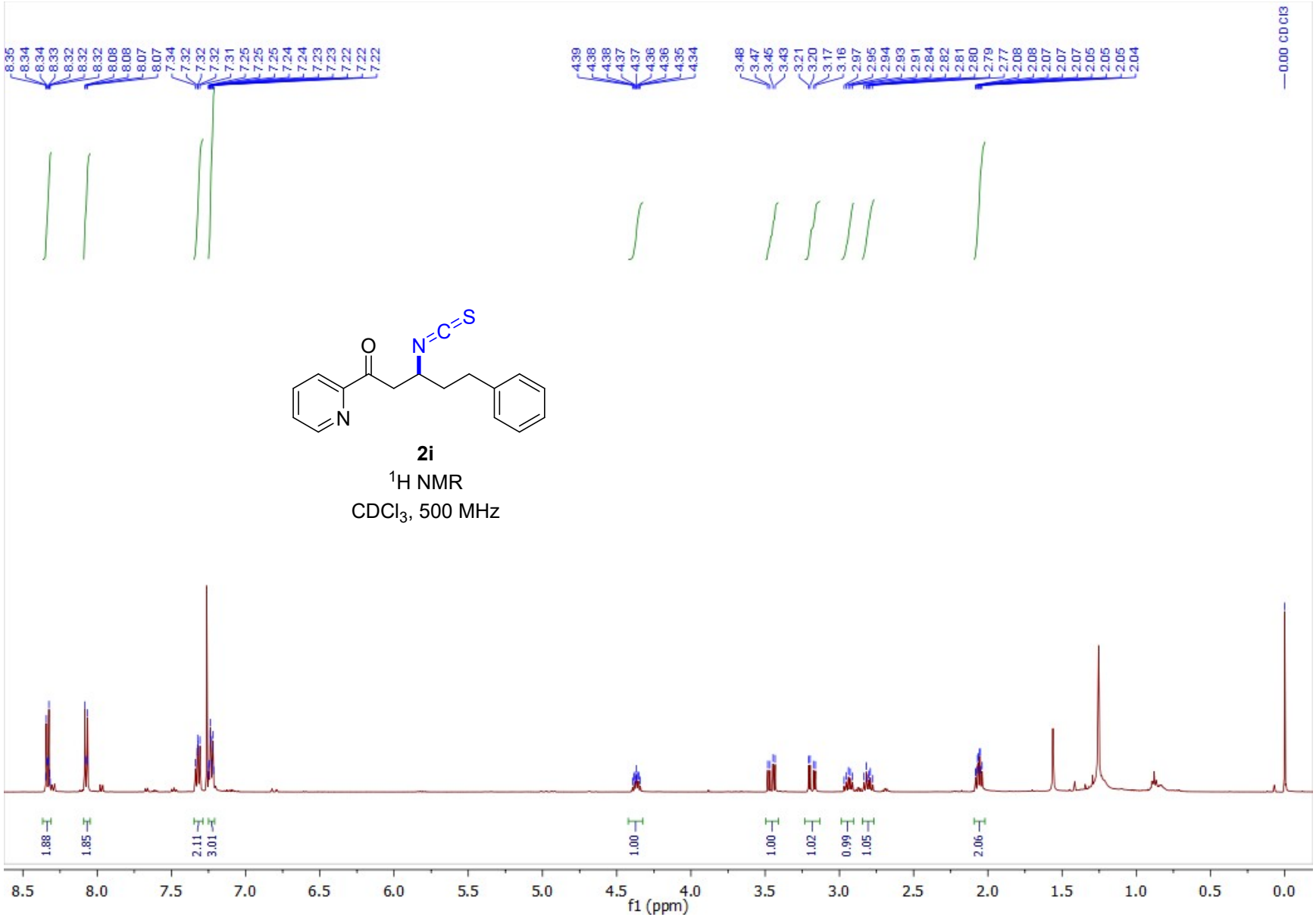


2h

^{1}H NMR

$CDCl_3$, 500 MHz

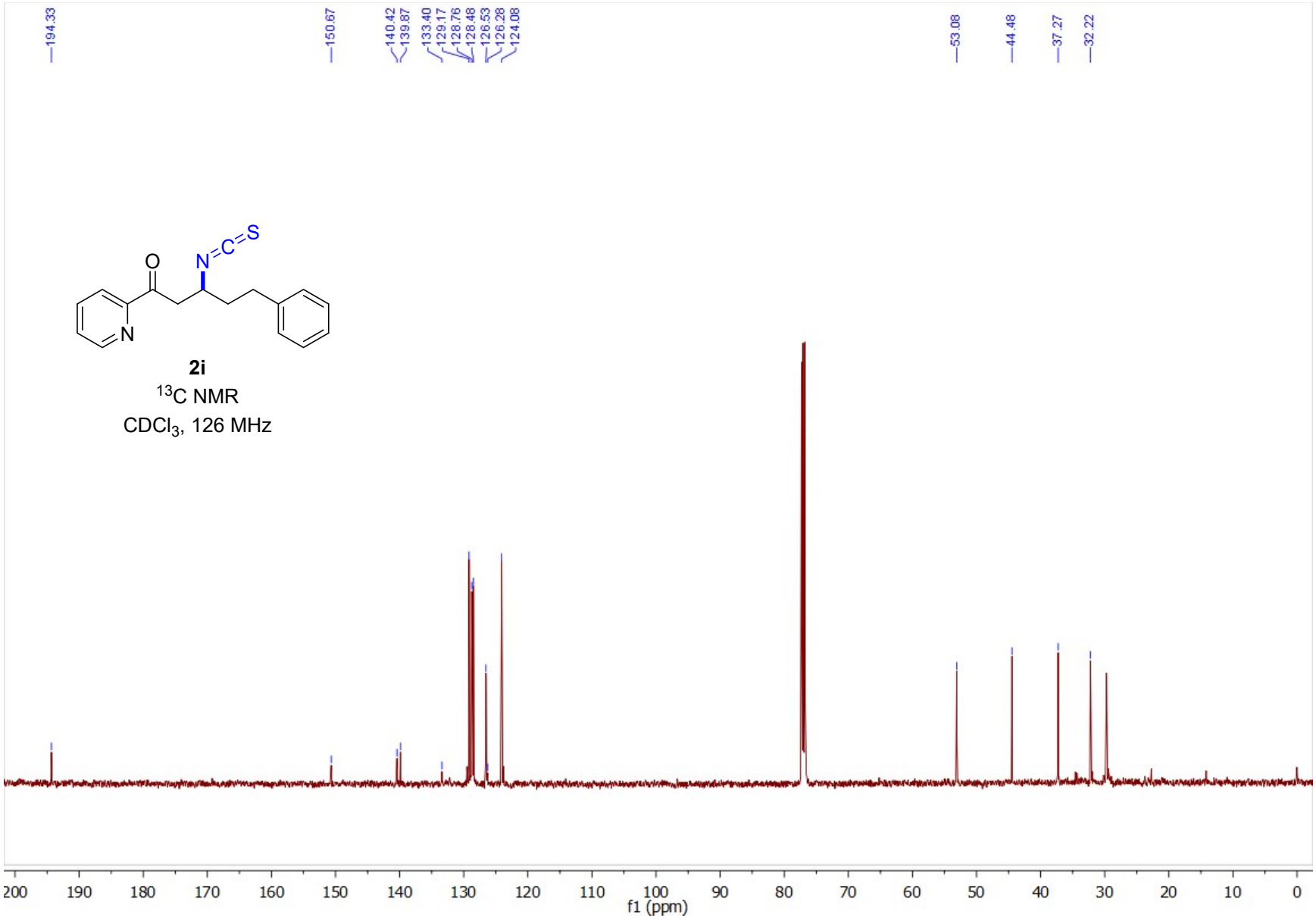

184.77
152.27
147.00
140.03
132.56
128.68
128.47
126.41
118.00
112.71
53.30
43.77
37.41
32.23
O
N=C=S
O
2h
13C NMR
CDCl3, 126 MHz
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

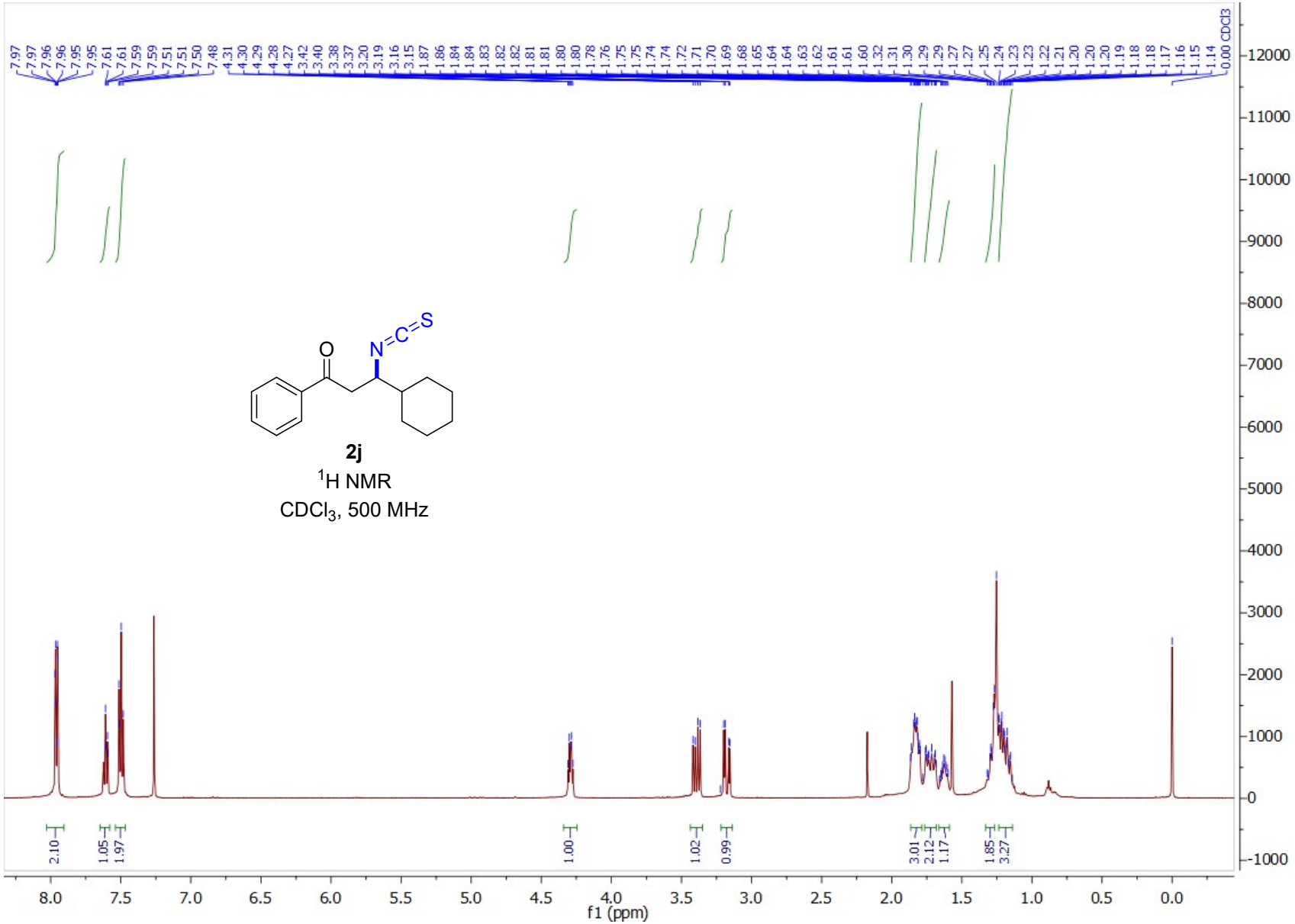


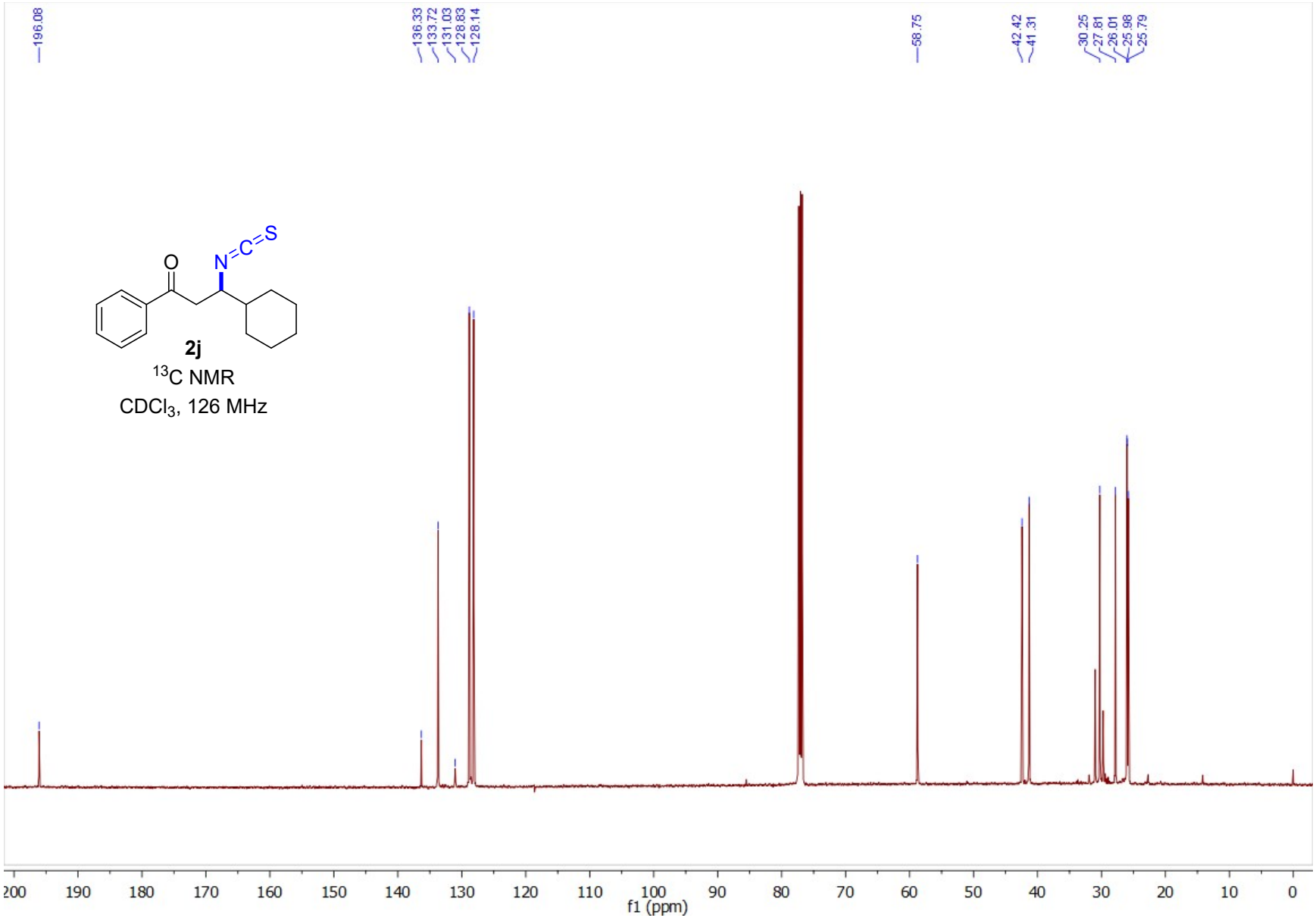
2i

^{1}H NMR

$CDCl_3$, 500 MHz


194.33
150.67
140.42
139.87
133.40
129.17
128.76
128.48
126.53
126.28
124.08
53.08
44.48
37.27
32.22
O
N=C=S
N
2i
13C NMR
CDCl3, 126 MHz
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N=C=S
2j
1H NMR
CDCl3, 500 MHz
f1 (ppm)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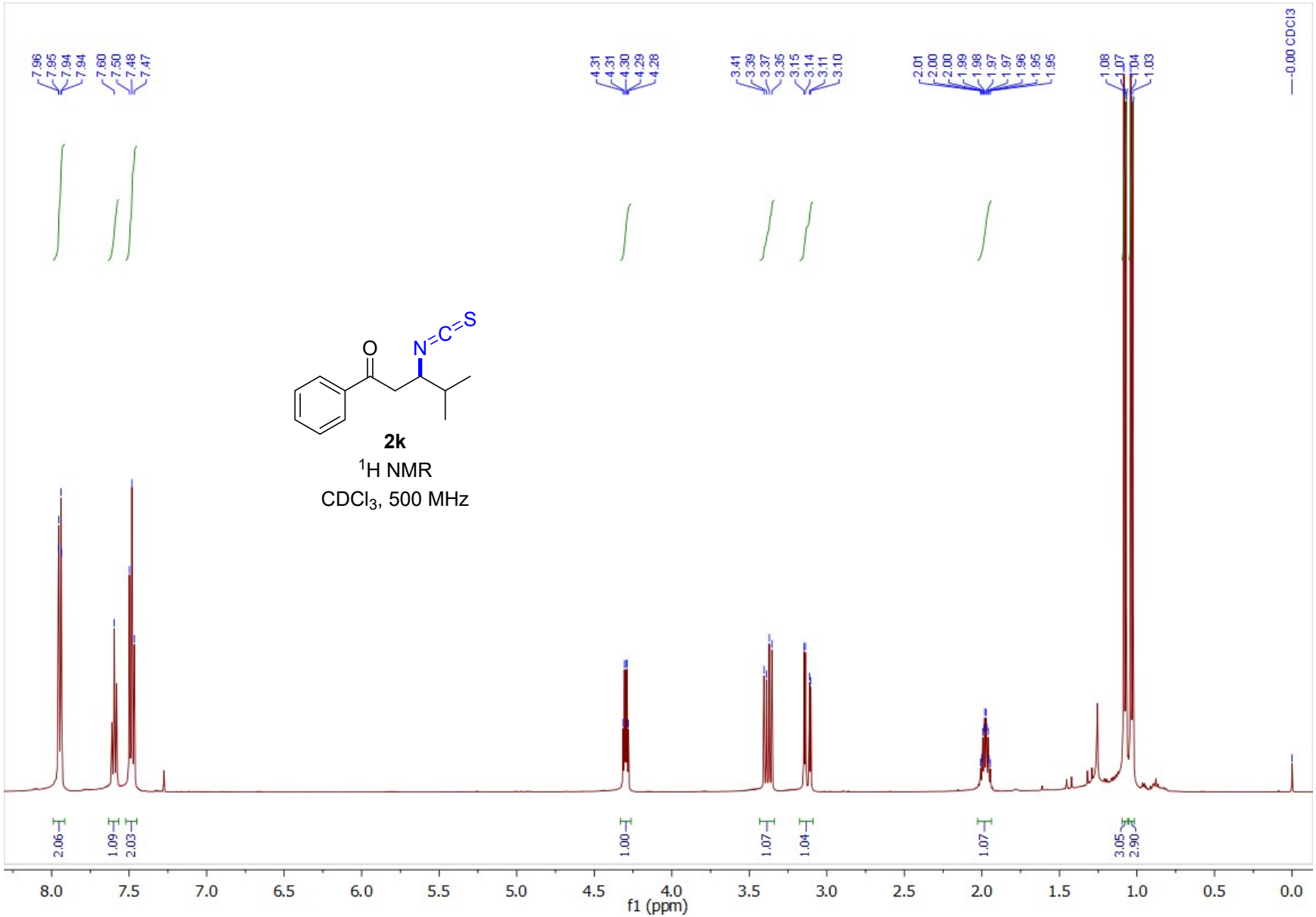
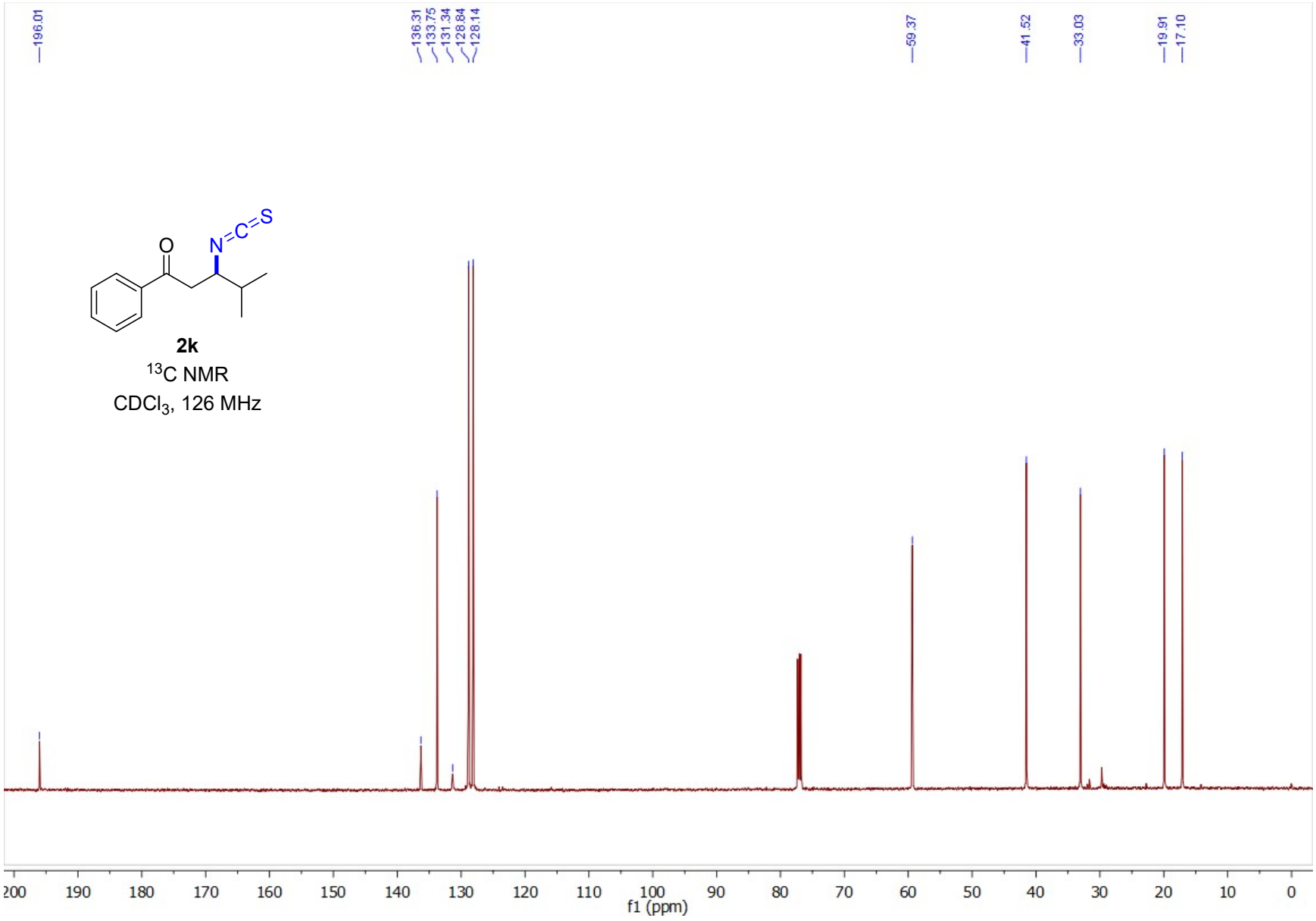
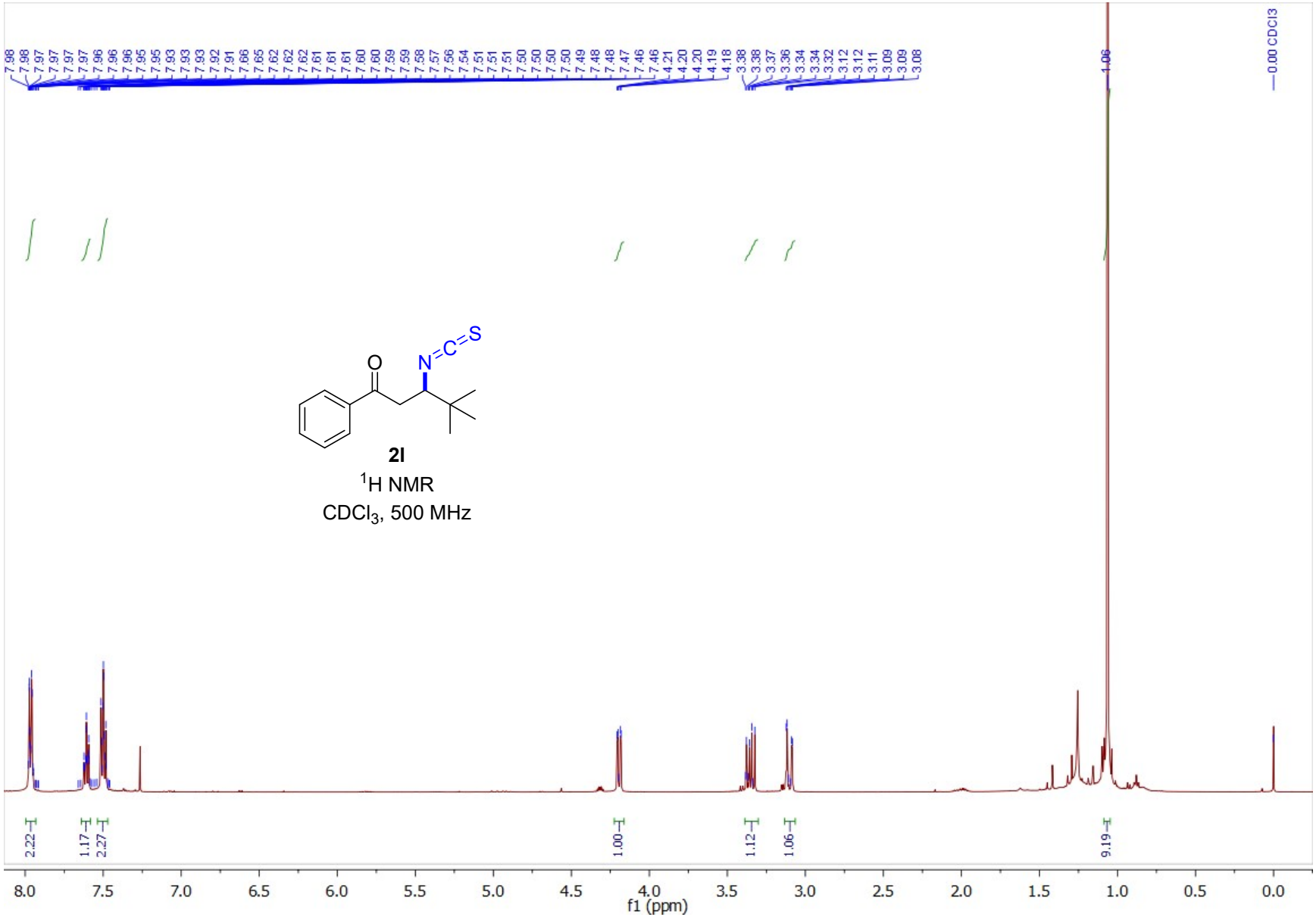
136.33
133.72
131.03
128.83
128.14
58.75
42.42
41.31
30.25
27.81
26.01
25.98
25.79
O
N=C=S
2j
13C NMR
CDCl3, 126 MHz
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.96
7.95
7.94
7.94
7.60
7.50
7.48
7.47
4.31
4.31
4.30
4.29
4.28
3.41
3.39
3.37
3.35
3.15
3.14
3.11
3.10
2.01
2.00
2.00
1.99
1.98
1.97
1.97
1.96
1.95
1.95
1.08
1.07
1.04
1.03
0.00 CDCl3
O
N=C=S
2k
1H NMR
CDCl3, 500 MHz
2.06
1.09
2.03
1.00
1.07
1.04
1.07
3.05
2.90
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

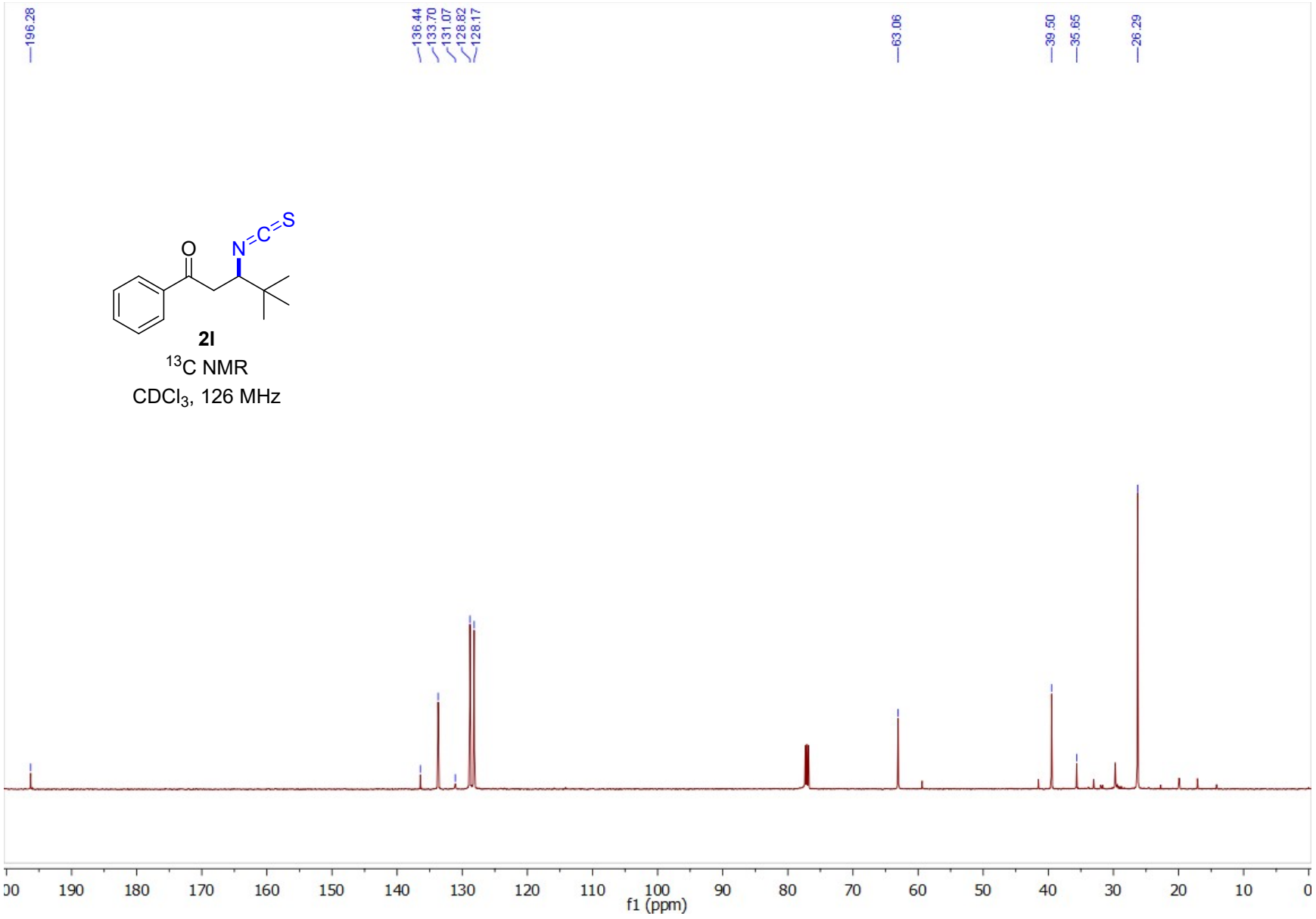

196.01
136.31
133.75
131.34
128.84
128.14
59.37
41.52
33.03
19.91
17.10
O
N=C=S
2k
13C NMR
CDCl3, 126 MHz
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



2l

^{1}H NMR

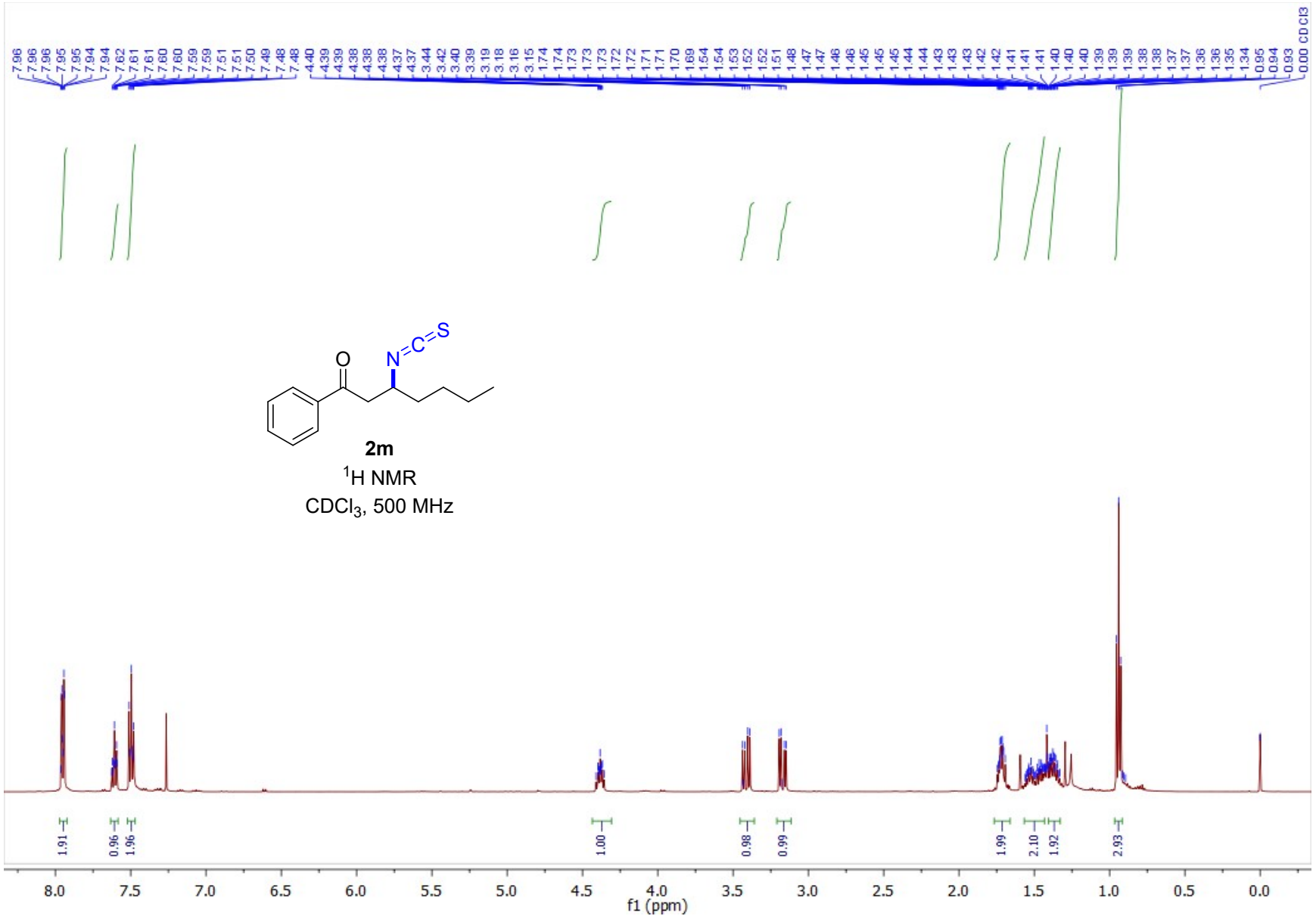
$CDCl_3$, 500 MHz

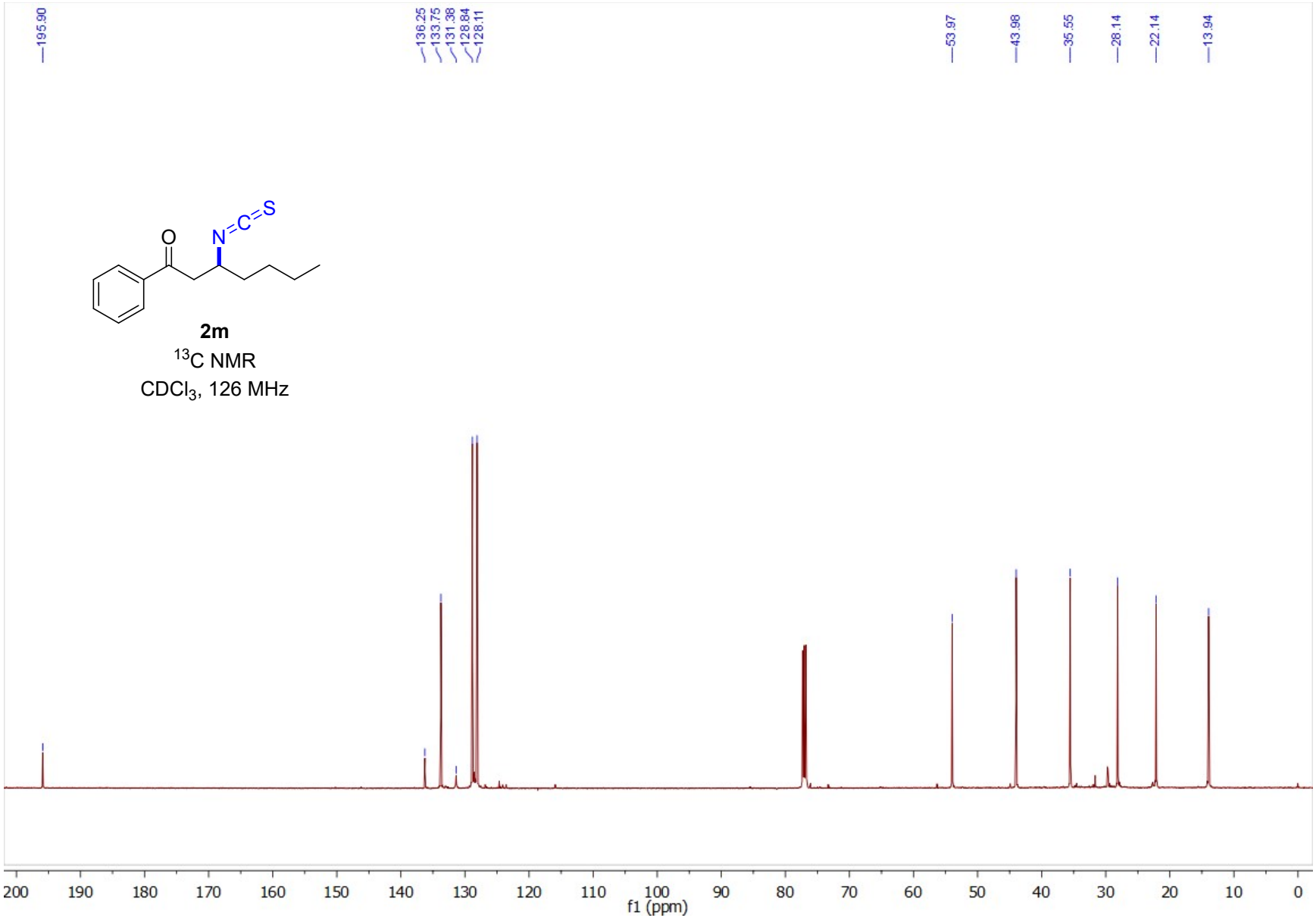


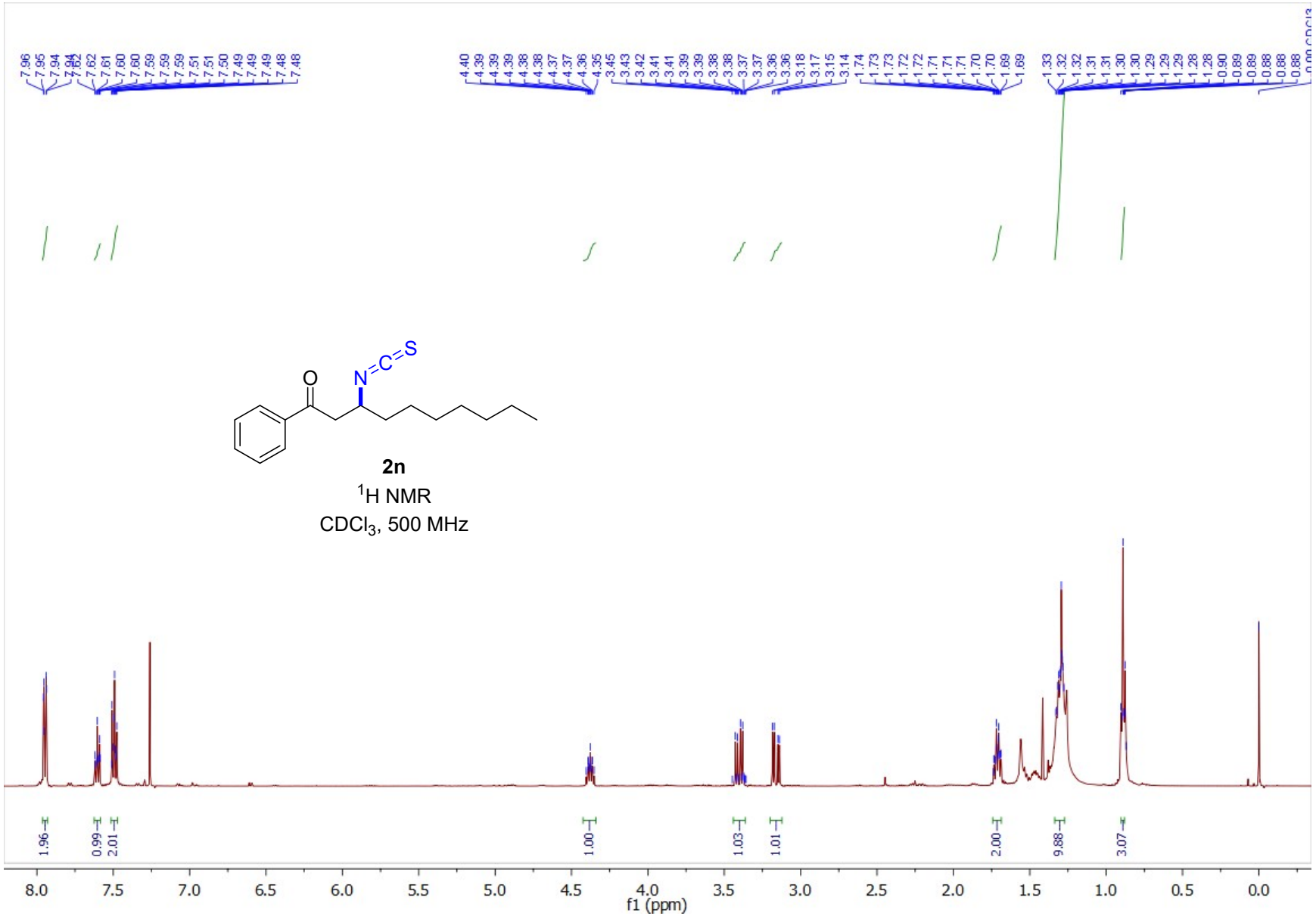
2l

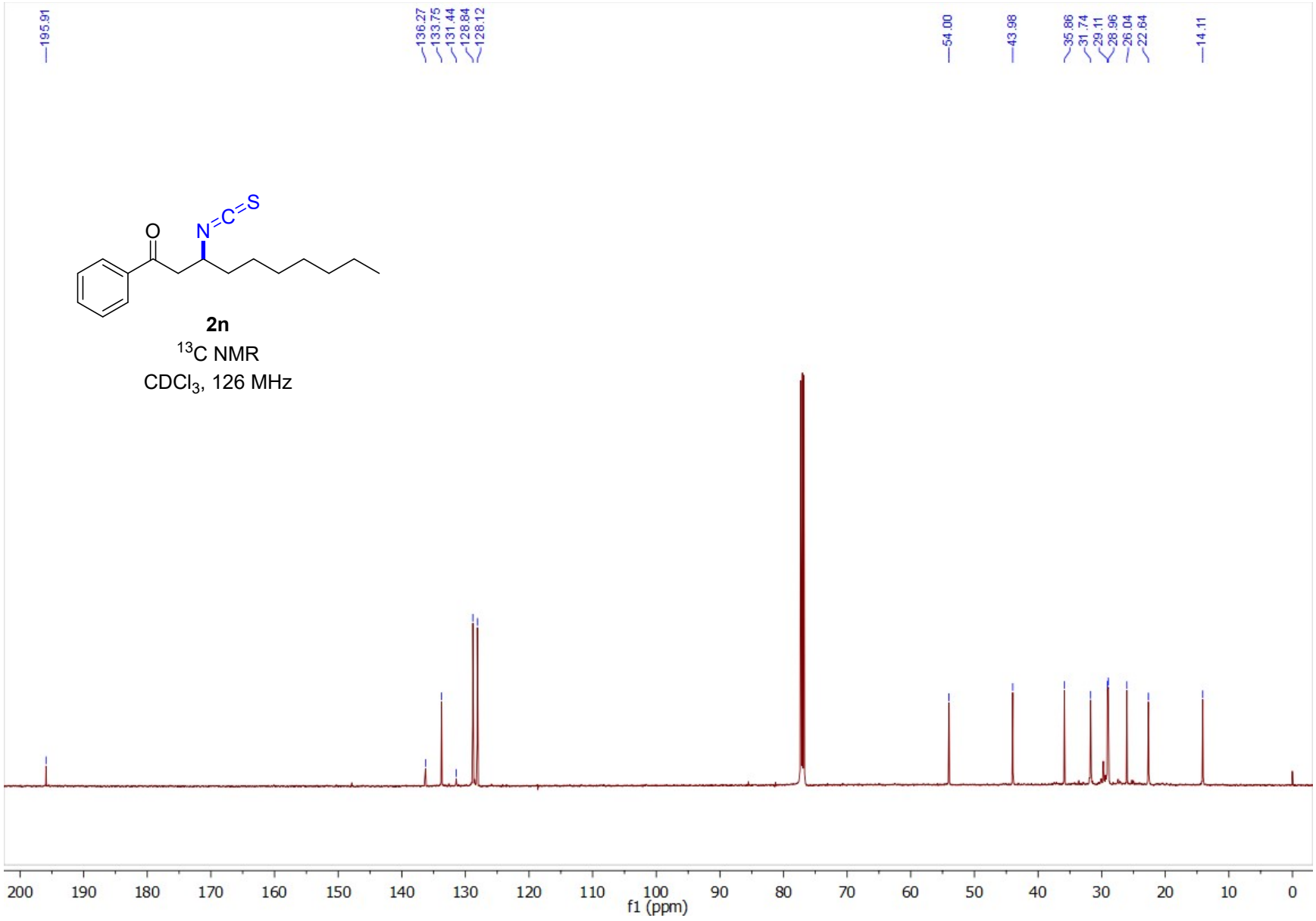
^{13}C NMR

$CDCl_3$, 126 MHz


O
N=C=S
2m
1H NMR
CDCl3, 500 MHz
f1 (ppm)


195.90
136.25
133.75
131.38
128.84
128.11
53.97
43.98
35.55
28.14
22.14
13.94
O
N=C=S
2m
13C NMR
CDCl3, 126 MHz
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

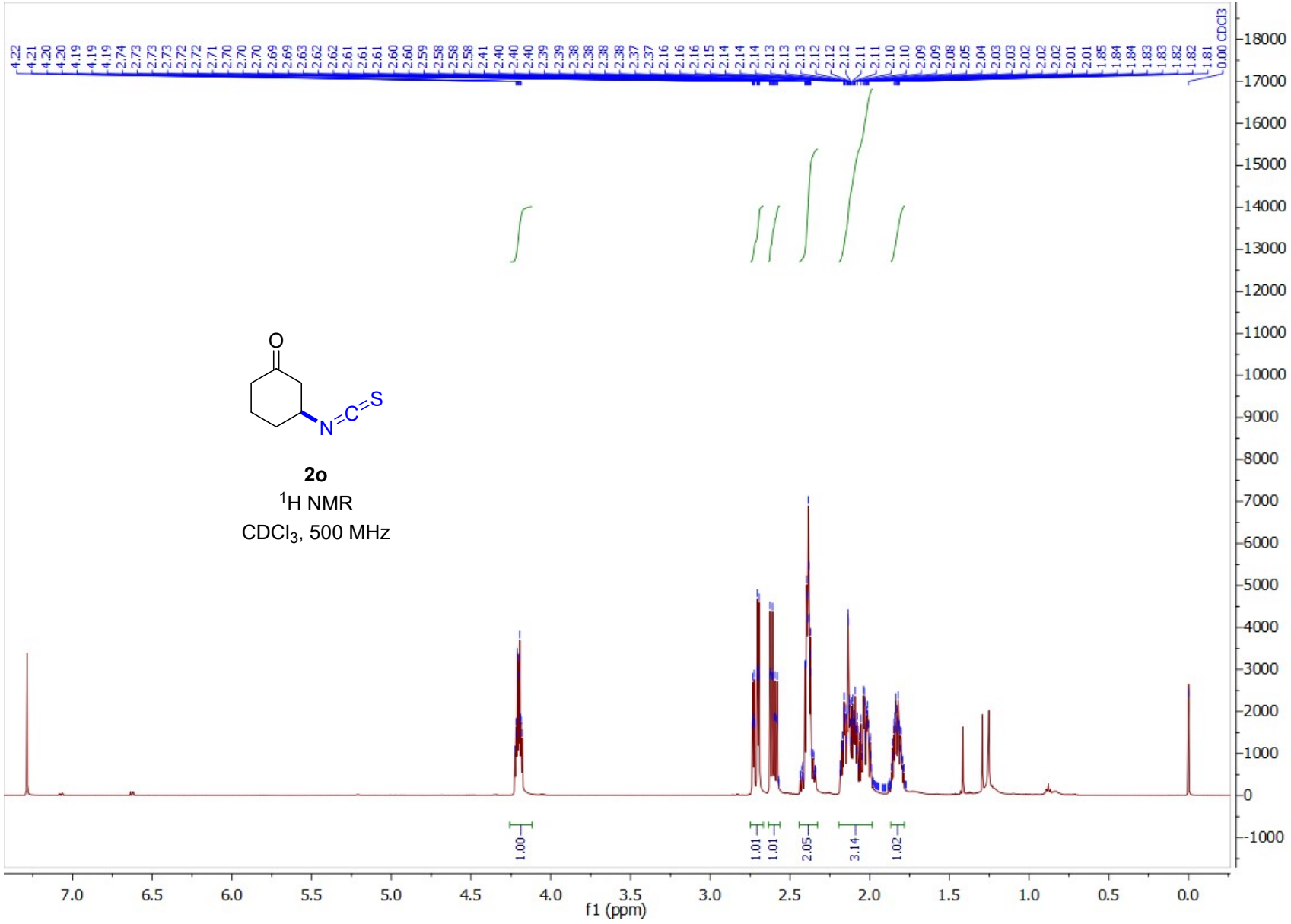

O
N=C=S
2n
1H NMR
CDCl3, 500 MHz
f1 (ppm)

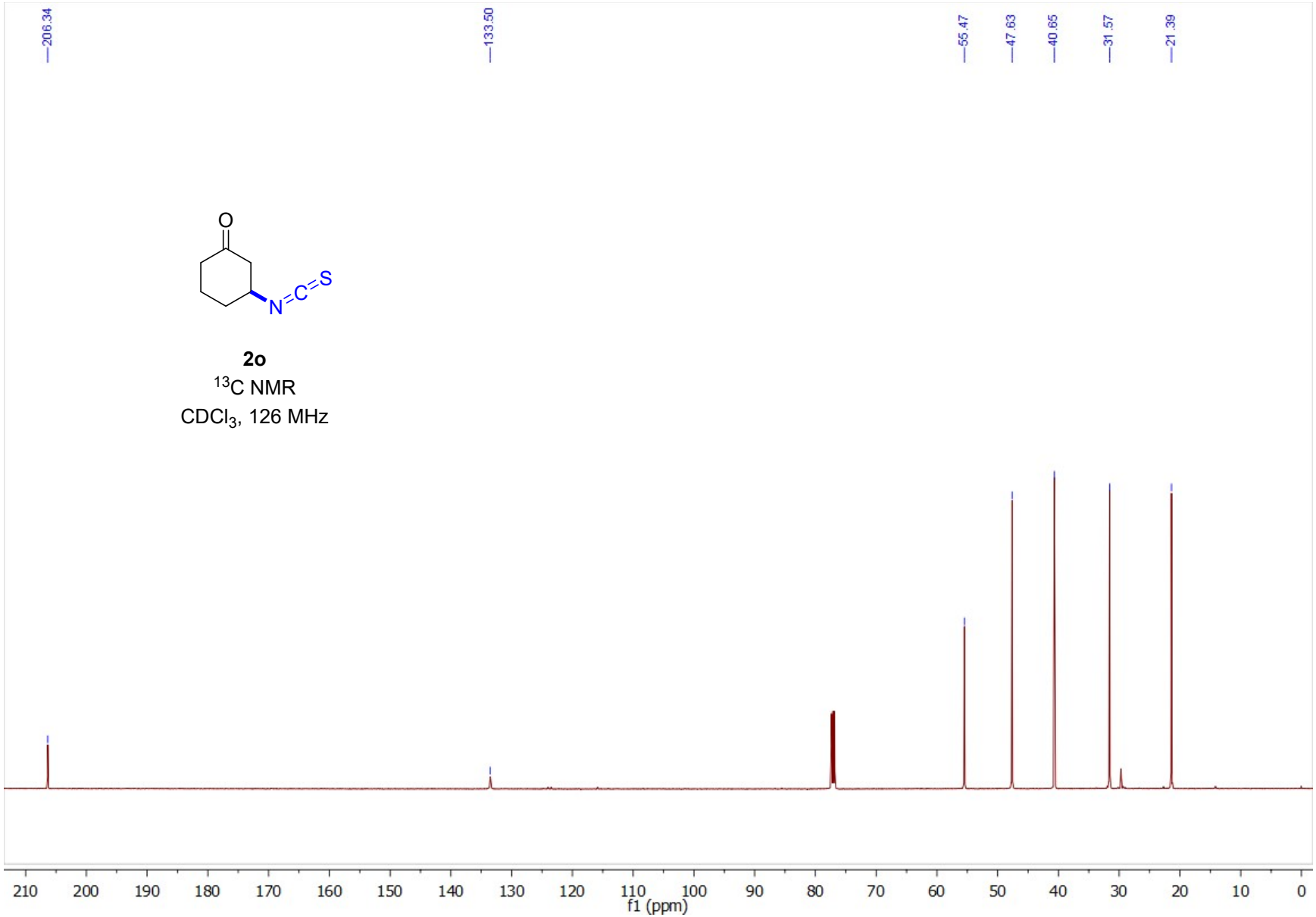


2n

^{13}C NMR

$CDCl_3$, 126 MHz

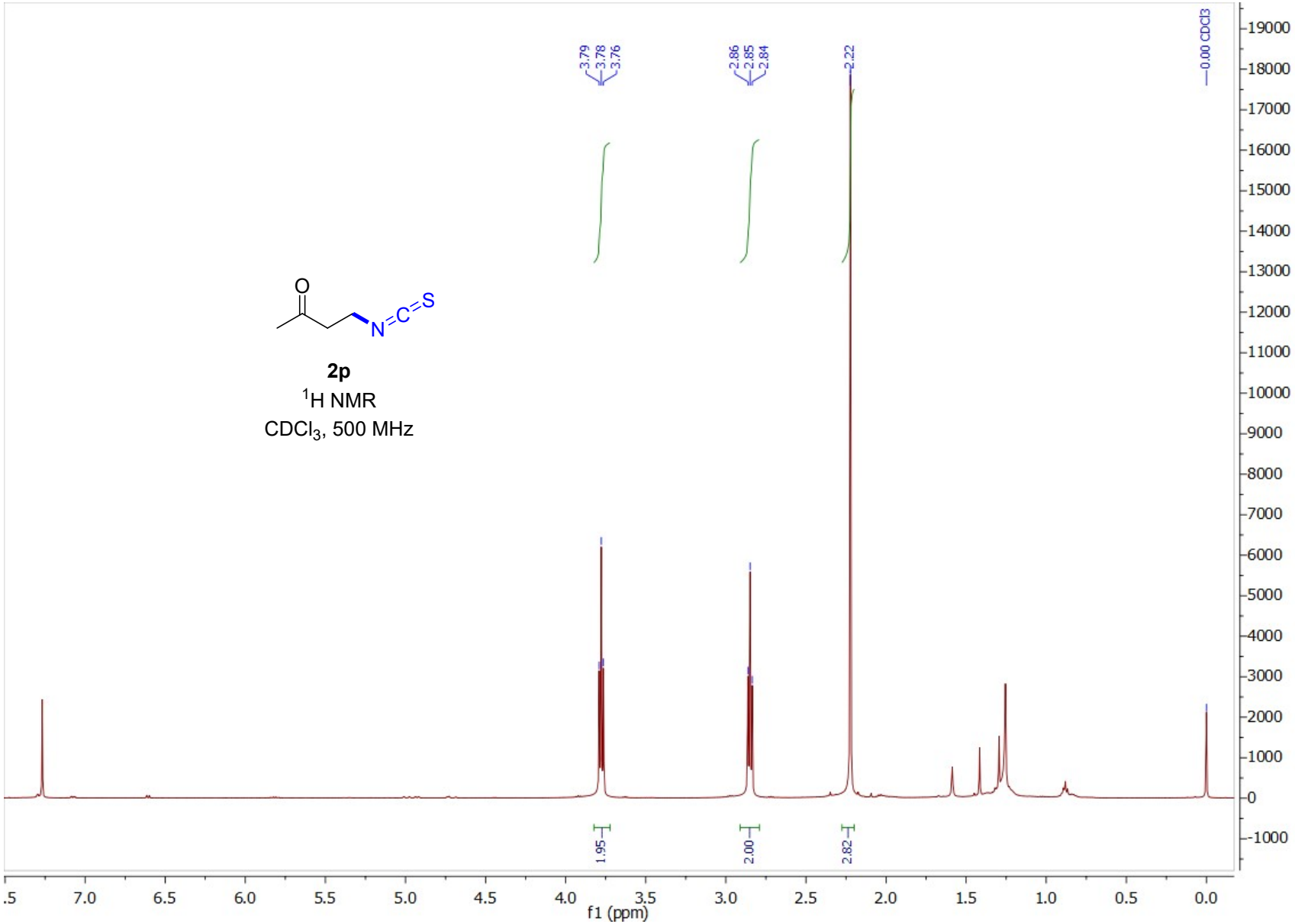

O
N=C=S
2o
1H NMR
CDCl3, 500 MHz
f1 (ppm)



2o

^{13}C NMR

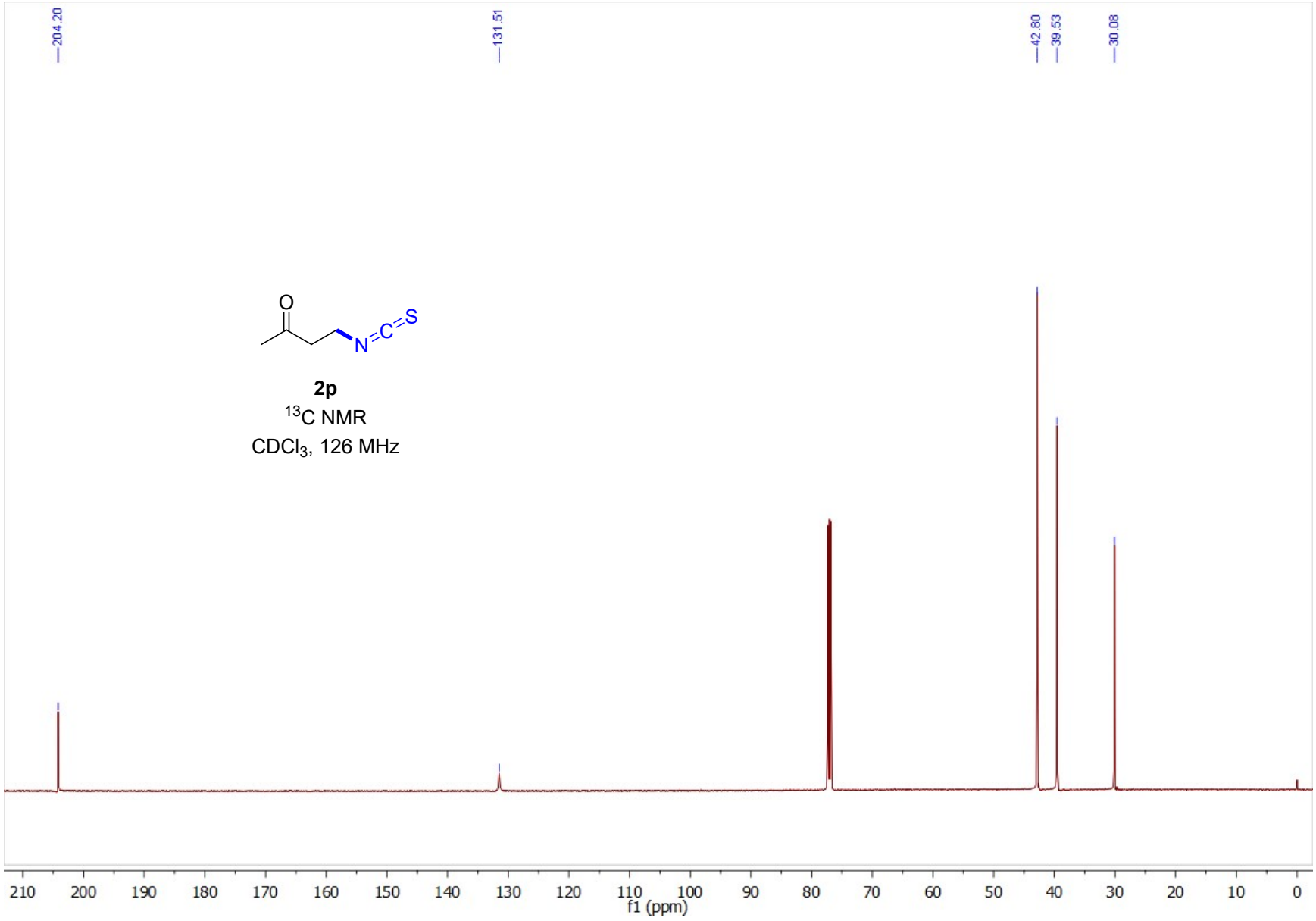
$CDCl_3$, 126 MHz

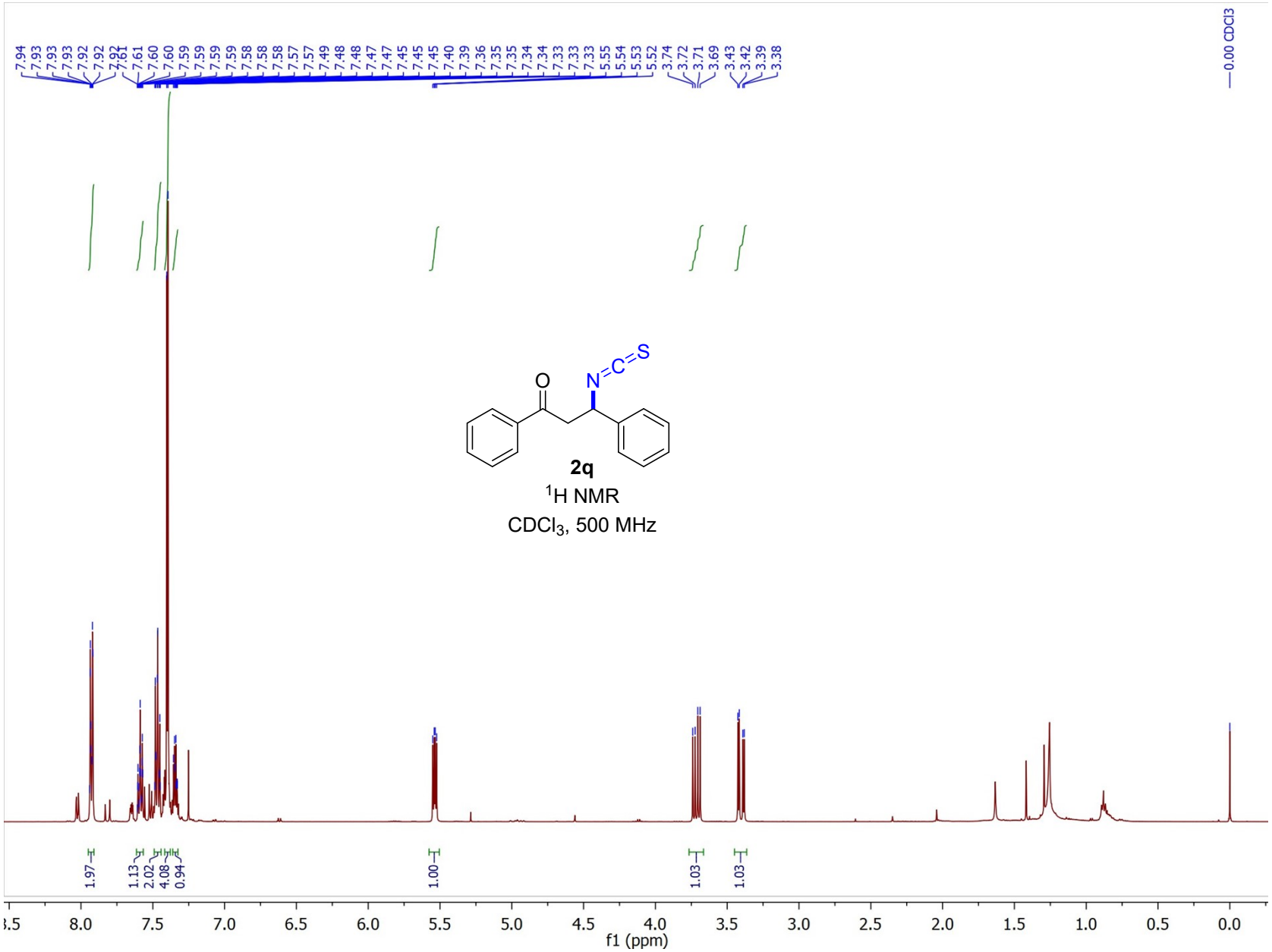


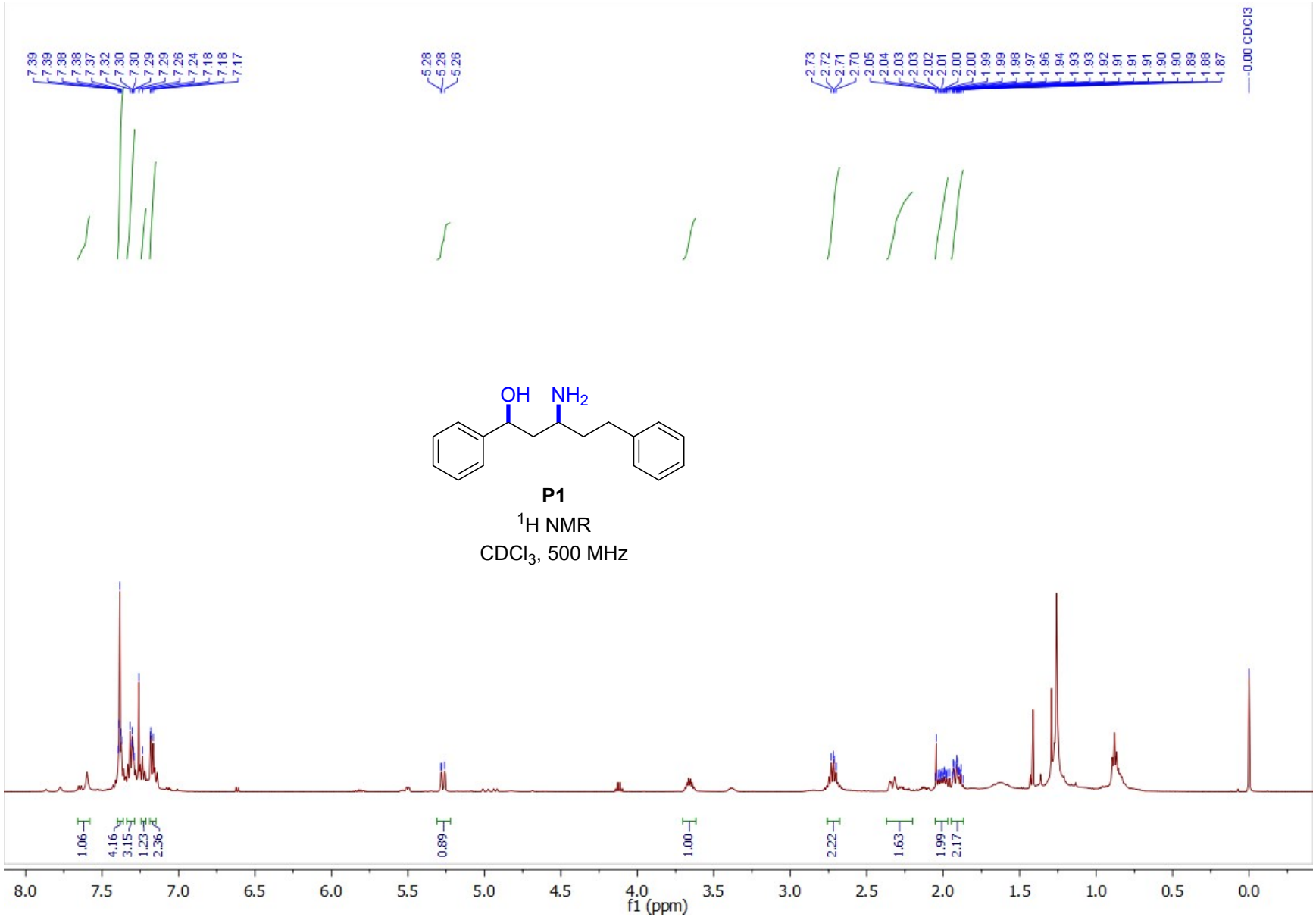
2p

^{1}H NMR

$CDCl_3$, 500 MHz


204.20
131.51
42.80
39.53
30.08
O
N=C=S
2p
13C NMR
CDCl3, 126 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

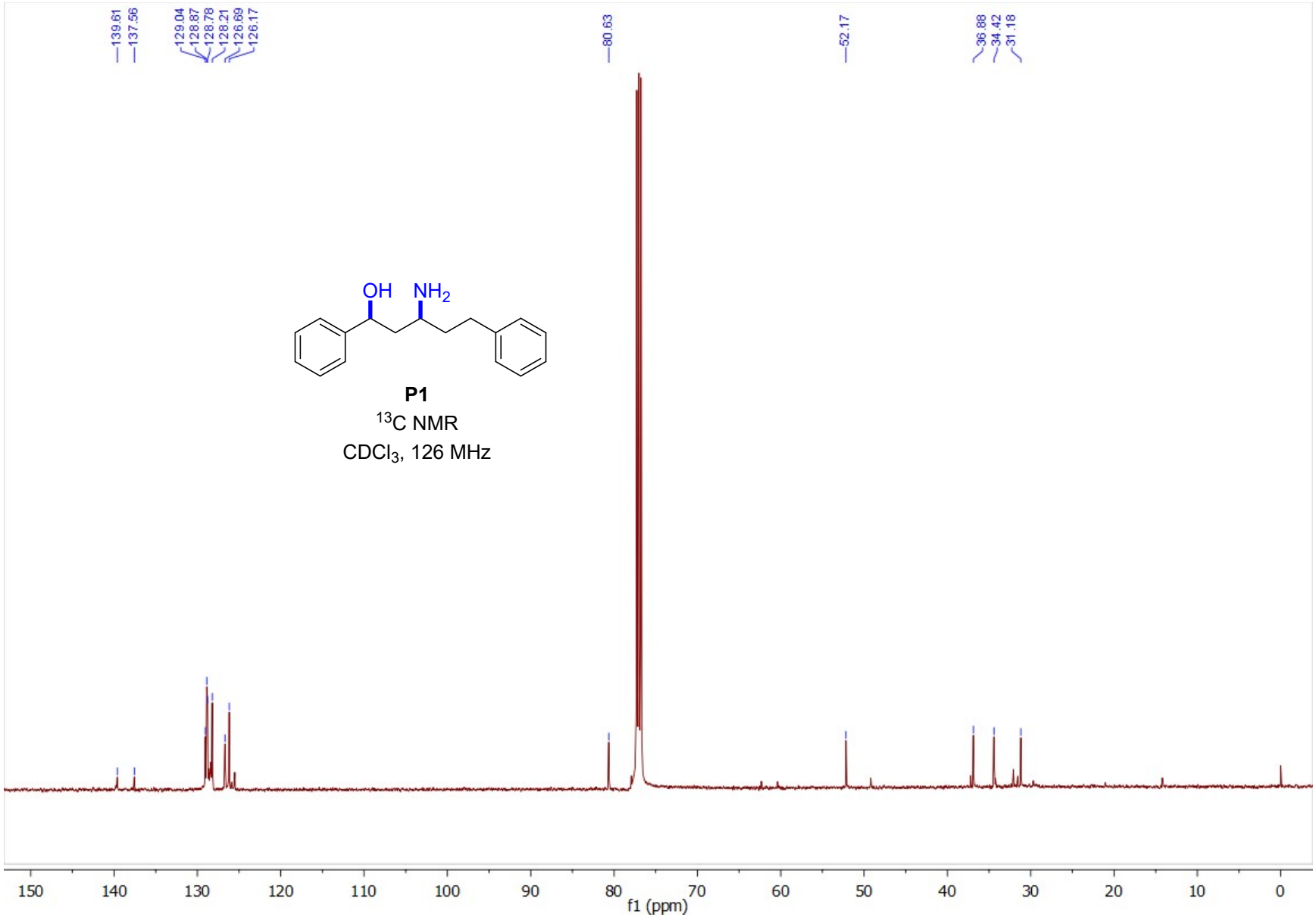

7.94 7.93 7.93 7.93 7.92 7.92 7.92 7.61 7.61 7.60 7.60 7.59 7.59 7.59 7.59 7.58 7.58 7.58 7.57 7.57 7.49 7.48 7.48 7.47 7.47 7.45 7.45 7.45 7.40 7.39 7.36 7.35 7.35 7.34 7.34 7.33 7.33 7.33 5.55 5.54 5.53 5.52 3.74 3.72 3.71 3.69 3.43 3.42 3.39 3.38
0.00 CDCl3
O
N=C=S
2q
1H NMR
CDCl3, 500 MHz
1.97
1.13
2.02
4.08
0.94
1.00
1.03
1.03
f1 (ppm)



P1

^{1}H NMR

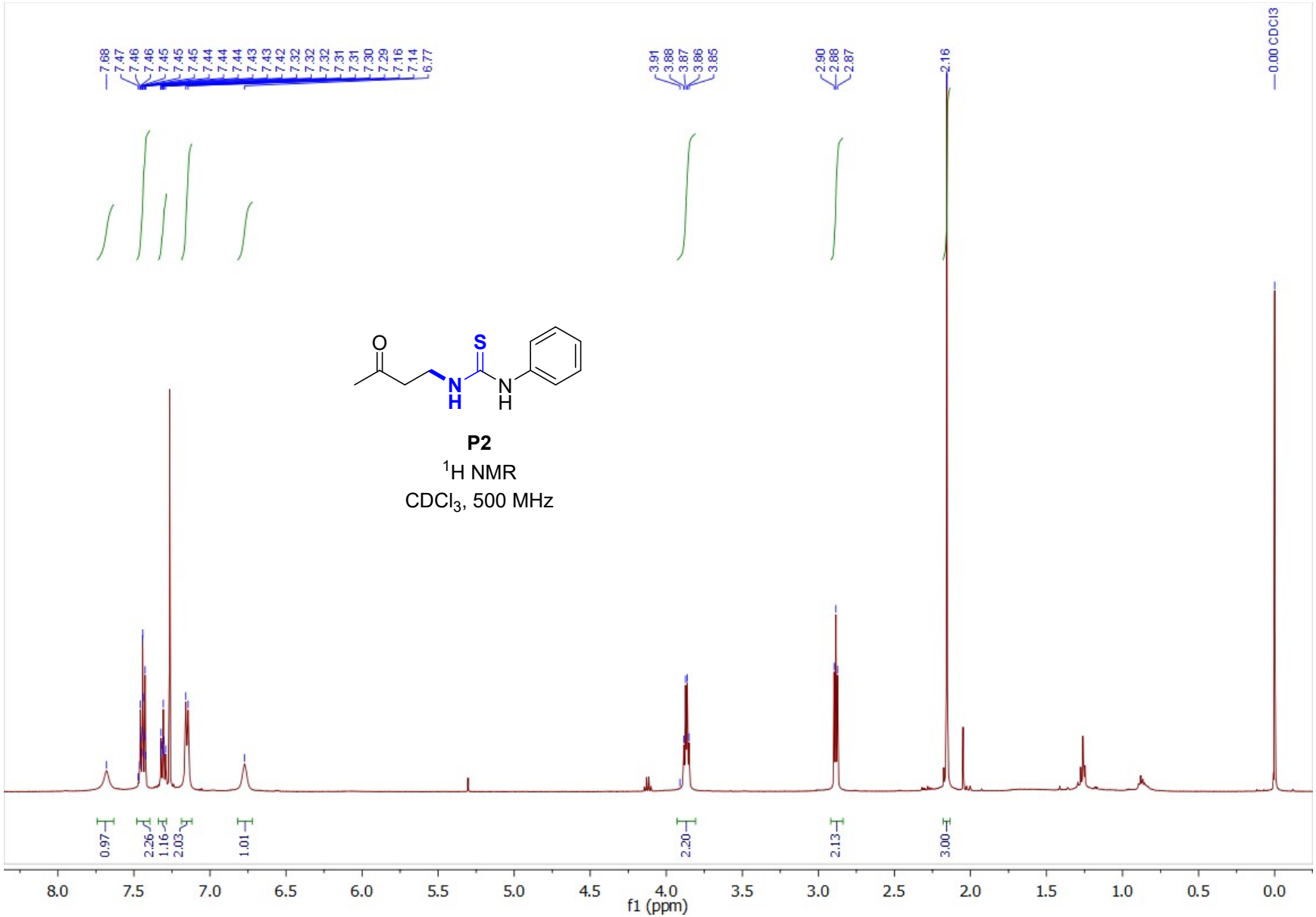
$CDCl_3$, 500 MHz



P1

^{13}C NMR

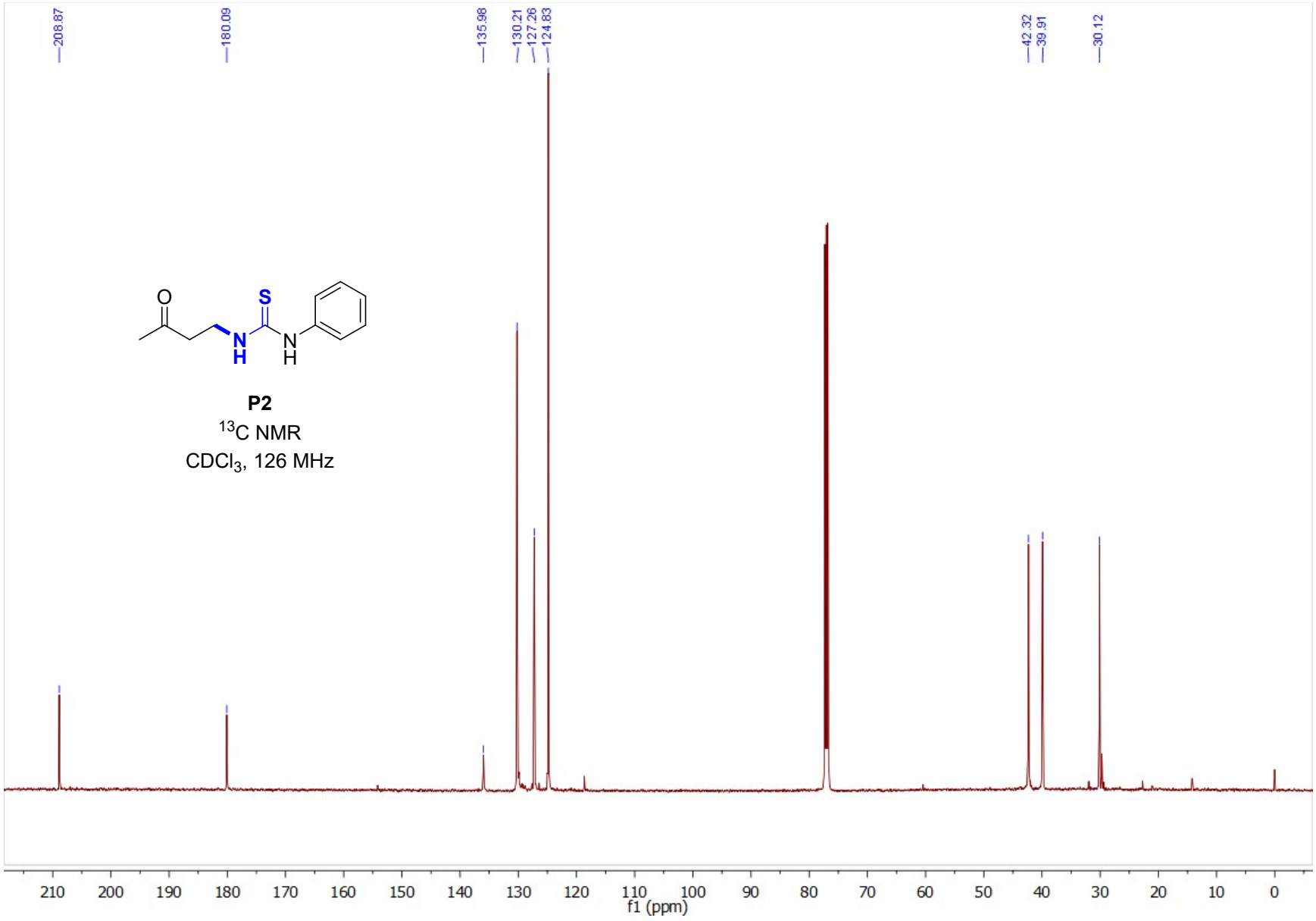
$CDCl_3$, 126 MHz

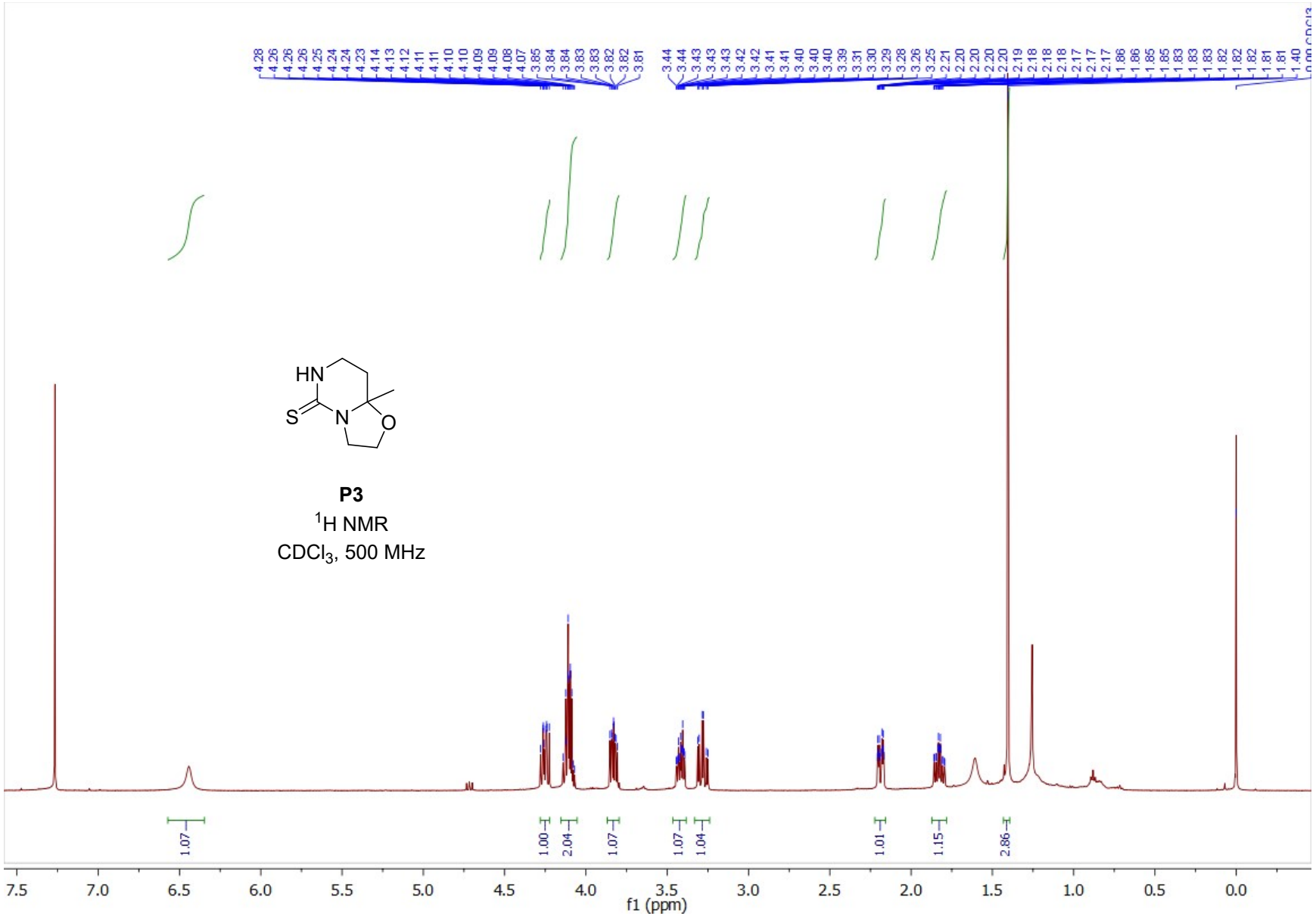


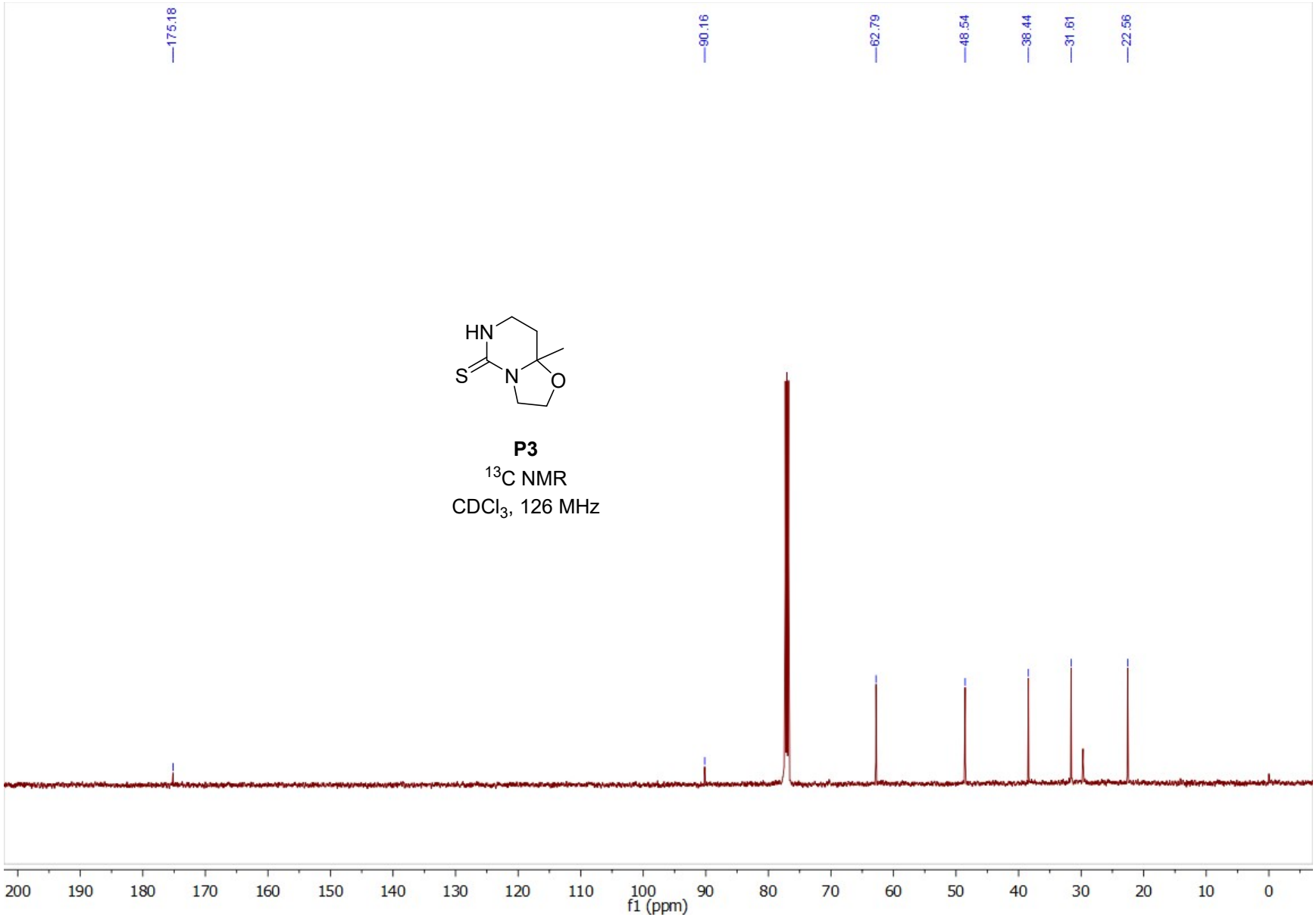
P2

^{1}H NMR

$CDCl_3$, 500 MHz


208.87
180.09
135.98
130.21
127.26
124.83
42.32
39.91
30.12
O
S
N
H
N
H
P2
13C NMR
CDCl3, 126 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


HN
S
N
O
P3
1H NMR
CDCl3, 500 MHz
1.07
1.00
2.04
1.07
1.07
1.04
1.01
1.15
2.86
f1 (ppm)



P3

^{13}C NMR

$CDCl_3$, 126 MHz

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