

Electronic Supplementary Information

Ruthenium (II)-Catalyzed Switchable C3-Alkylation *verses* Alkenylation with Acrylates of 2-Pyridylbenzofurans *via* C–H Activation[†]

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General information: Reactions were carried out in anhydrous solvents under an atmosphere of argon in oven-dried glassware. ¹H NMR spectra were recorded on JEOL AL-400 (400 MHz), Bruker AC 200 MHz, Bruker DRX 400 MHz and Bruker DRX 500 MHz spectrometers, and TMS was used as an internal standard of spectrometers. The chemical shifts were reported in parts per million (δ) relative to internal standard TMS (0 ppm) and for CDCl₃ (7.27 ppm). The peak patterns are indicated as follows: s, singlet; d, doublet; dd, doublet of doublet; t, triplet; dt, doublet of triplet, td, triplet of doublet, m, multiplet; q, quartet. The coupling constants, *J* are reported in Hertz (Hz). ¹³C NMR spectra were obtained by JEOL AL-400 (100 MHz), (125 MHz), (100 MHz) and (50 MHz) spectrometers and referenced to the internal solvent signals (central peak is 77.0 ppm in CDCl₃). CDCl₃ was used as a NMR solvent. Mass spectroscopy was carried out on PI QStar Pulsar (Hybrid Quadrupole-TOF LC/MS/MS) and High-resolution mass spectra (HRMS) were recorded on a Thermo Scientific Q-Exactive, Accela 1250 pump. Column chromatography was performed over silica gel 100-200 mesh. All reagents were weighed and handled in air and backfilled under argon at room temperature. Unless otherwise noted, all reactions were performed under an argon atmosphere. All reagents were purchased from Aldrich and Alfa Easer and used without further purification. Compounds **1a–1c** are prepared according the procedures reported.^{1,2}

References:

- 1) Y. Komagalla, K. Srinivas and C. V. Ramana, *Tetrahedron Lett.*, 2013, **54**, 1824-1827.
- 2) N. Ortega, S. Urban, B. Beiring and F. Glorius, *Angew. Chem. Int. Ed.*, 2012, **51**, 1710-1713.

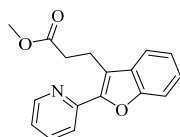
General procedure for preparation of 2-(benzofuran-2-yl)pyridine derivatives (**1a-1c**):

To a solution of alkyne (1.0 mmol), iodobenzene (1.5 mmol) in Et₃N (5.0 mL) and DMF (2.5 mL), PPh₃ (0.1 mmol) was added followed by Pd(PPh₃)₂Cl₂ (0.05 mmol), and the reaction mixture was flushed with argon for 5 min. CuI (0.05 mmol) was added and flushed with argon for 10 min and stirred at rt for 6 h. The reaction mixture was partitioned between ethyl acetate and water. Then the organic layer was separated and the aqueous layer was extracted with ethyl acetate. The combined organic layer was washed with brine, dried (Na₂SO₄) and concentrated. The crude residue was purified by column chromatography.

General procedure A: Linear alkylation using Ru(PPh₃)₃Cl₂:

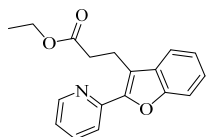
2-(Benzofuran-2-yl)pyridine (0.1 mmol) was placed in a screw cap pressure tube and dissolved in anhydrous toluene (2 mL), which was then evacuated and back filled with argon. To the reaction vessel alkene (acrylate) (0.3 mmol), RuCl₂(PPh₃)₃ (0.005 mmol) and AgOAc (0.03 mmol) were added. The solution was then stirred at 140 °C (bath temperature) for 24 h. The reaction mixture was cooled to room temperature. The solvent were evaporated and the crude products were purified by column chromatography (pet ether/AcOEt) to give analytically pure.

Methyl 3-(2-(pyridin-2-yl)benzofuran-3-yl)propanoate (3aa): Isolated by column chromatography (pet.ether/AcOEt = 8:2, R_f = 0.6). The title compound was



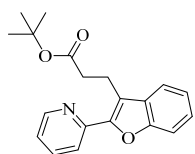
determined as colourless gum (75%). ¹H NMR (200 MHz, CDCl₃): δ 2.83 (t, *J* = 8.1 Hz, 2H), 3.58 (t, *J* = 8.2 Hz, 2H), 3.65 (s, 3H), 7.17–7.24 (m, 1H), 7.28–7.39 (m, 2H), 7.52 (dd, *J* = 1.4, 7.1 Hz, 1H), 7.65–7.69 (m, 1H), 7.78 (dt, *J* = 1.8, 7.9 Hz, 1H), 7.95 (dd, *J* = 0.9, 7.9 Hz, 1H), 8.69 (d, *J* = 4.8 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 19.7 (t), 33.9 (t), 51.5 (q), 111.2 (d), 118.7 (s), 120.1 (d), 120.6 (d), 122.0 (d), 122.7 (d), 125.3 (d), 130.0 (s), 136.4 (d), 149.4 (s), 149.6 (d), 150.8 (s), 153.9 (s), 173.9 (s) ppm; HRMS(ESI) calcd for C₁₇H₁₆O₃N (M⁺+H): 282.1125; found: 282.1125.

Ethyl 3-(2-(pyridin-2-yl)benzofuran-3-yl)propanoate (3ab): Isolated by column chromatography (pet.ether/AcOEt = 8:2, R_f = 0.6). The title compound was



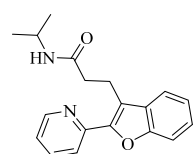
determined as colourless gum (78%). ¹H NMR (400 MHz, CDCl₃): δ 1.20 (t, *J* = 7.3 Hz, 3H), 2.81 (t, *J* = 8.0 Hz, 2H), 3.58 (t, *J* = 8.0 Hz, 2H), 3.65 (q, *J* = 7.3 Hz, 2H), 7.21 (dd, *J* = 4.8, 7.5 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 7.3 Hz, 1H), 7.78 (dt, *J* = 1.8, 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 8.69 (d, *J* = 4.8 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 14.2 (q), 19.8 (t), 34.1 (t), 60.3 (t), 111.2 (d), 118.8 (s), 120.2 (d), 120.6 (d), 122.0 (d), 122.7 (d), 125.3 (d), 130.1 (s), 136.4 (d), 149.3 (s), 149.6 (d), 150.9 (s), 153.9 (s), 173.5 (s) ppm; HRMS(ESI) calcd for C₁₈H₁₈O₃N (M⁺+H): 296.1281; found: 296.1281.

Tert-butyl 3-(2-(pyridin-2-yl)benzofuran-3-yl)propanoate (3ac): Isolated by column chromatography (pet.ether/AcOEt = 8:2, R_f = 0.7). The title compound was determined as colourless gum (80%). ¹H NMR (500 MHz, CDCl₃): δ 1.41 (s, 9H), 2.81 (t, *J* = 7.9 Hz, 2H), 3.58 (t, *J* = 7.9 Hz, 2H), 7.21 (dd, *J* = 4.6, 7.6 Hz, 1H), 7.26–7.30 (m, 1H), 7.34 (dt, *J* = 1.2, 8.2 Hz,



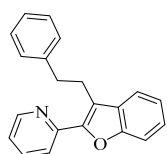
1H), 7.51 (d, $J = 8.2$ Hz, 1H), 7.69 (d, $J = 7.6$ Hz, 1H), 7.77 (dt, $J = 1.8, 7.9$ Hz, 1H), 7.93 (d, $J = 7.9$ Hz, 1H), 8.70 (d, $J = 4.9$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 19.8 (t), 28.1 (q, 3C), 35.3 (t), 80.1 (s), 111.2 (d), 119.0 (s), 120.3 (d), 120.6 (d), 121.9 (d), 122.6 (d), 125.2 (d), 130.1 (s), 136.3 (d), 149.3 (s), 149.6 (d), 150.9 (s), 153.9 (s), 172.8 (s) ppm; HRMS(ESI) calcd for $\text{C}_{20}\text{H}_{22}\text{O}_3\text{N}$ (M^+H): 324.1594; found: 324.1589.

N-isopropyl-3-(2-(pyridin-2-yl)benzofuran-3-yl)propanamide (3ad): Isolated by column



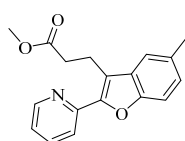
chromatography (pet.ether/AcOEt = 5:5, $R_f = 0.3$). The title compound was determined as white colour solid (53%). Mp: 149-150 °C; ^1H NMR (400 MHz, CDCl_3): δ 0.97 (d, $J = 6.6$ Hz, 6H), 2.81 (t, $J = 7.1$ Hz, 2H), 3.56 (t, $J = 7.1$ Hz, 2H), 3.97–4.06 (m, 1H), 6.82 (d, $J = 6.9$ Hz, 1H), 7.30 (d, $J = 7.6$ Hz, 1H), 7.32–7.39 (m, 2H), 7.52 (d, $J = 8.1$ Hz, 1H), 7.70 (d, $J = 7.8$ Hz, 1H), 7.91 (t, $J = 7.6$ Hz, 1H), 8.04 (d, $J = 8.1$ Hz, 1H), 8.73 (d, $J = 3.9$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 20.2 (t), 22.5 (q, 2C), 36.3 (t), 41.2 (d), 111.3 (d, 2C), 120.2 (s), 120.7 (d, 2C), 121.6 (d), 122.6 (d), 123.1 (d), 125.9 (d), 129.6 (s, 2C), 154.2 (s, 2C), 171.6 (s) ppm; HRMS(ESI) calcd for $\text{C}_{19}\text{H}_{21}\text{O}_2\text{N}_2$ (M^+H): 309.1598; found: 309.1600.

2-(3-Phenethylbenzofuran-2-yl)pyridine (3ae): Isolated by column chromatography



(pet.ether/AcOEt = 8:2, $R_f = 0.7$). The title compound was determined as colourless gum (83%). ^1H NMR (500 MHz, CDCl_3): δ 3.06 (t, $J = 8.2$ Hz, 2H), 3.57 (t, $J = 8.2$ Hz, 2H), 7.18–7.26 (m, 3H), 7.29–7.36 (m, 5H), 7.53 (d, $J = 8.2$ Hz, 1H), 7.57 (d, $J = 7.6$ Hz, 1H), 7.77 (d, $J = 7.6$ Hz, 1H), 7.89 (d, $J = 7.6$ Hz, 1H), 8.74 (d, $J = 3.7$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 26.4 (t), 35.9 (t), 111.3 (d), 120.0 (d, 2C), 120.6 (d), 121.9 (d), 122.6 (d), 125.1 (d), 125.8 (d), 128.3 (d, 2C), 128.6 (d, 2C), 130.3 (s, 2C), 136.3 (d), 142.4 (s), 149.2 (s), 149.6 (d), 151.1 (s), 154.0 (s) ppm; HRMS(ESI) calcd for $\text{C}_{21}\text{H}_{18}\text{ON}$ (M^+H): 300.1383; found: 300.1380.

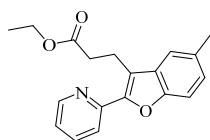
Methyl 3-(5-methyl-2-(pyridin-2-yl)benzofuran-3-yl)propanoate (3ba): Isolated by column



chromatography (pet.ether/AcOEt = 8:2, $R_f = 0.6$). The title compound was determined as pale yellow colour gum (67%). ^1H NMR (400 MHz, CDCl_3): δ 2.48 (s, 3H), 2.81 (t, $J = 8.1$ Hz, 2H), 3.55 (t, $J = 8.1$ Hz, 2H), 3.66 (s, 3H), 7.16 (d, $J = 8.4$ Hz, 1H), 7.22 (dd, $J = 5.1, 7.0$ Hz, 1H), 7.40 (d, $J = 8.4$ Hz, 1H), 7.43 (s, 1H), 7.79 (t,

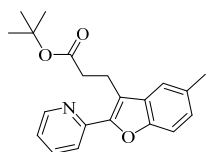
$J = 7.7$ Hz, 1H), 7.93 (d, $J = 8.1$ Hz, 1H), 8.71 (d, $J = 3.7$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 19.8 (t), 21.4 (q), 33.8 (t), 51.6 (q), 110.8 (d), 118.8 (s), 119.8 (d), 120.7 (d), 122.0 (d), 126.8 (d), 130.0 (s), 132.2 (s), 136.7 (d), 149.1 (s), 149.3 (d), 150.6 (s), 152.4 (s), 173.9 (s) ppm; HRMS(ESI) calcd for $\text{C}_{18}\text{H}_{18}\text{O}_3\text{N}$ (M^+H): 296.1281; found: 296.1282.

Ethyl 3-(5-methyl-2-(pyridin-2-yl)benzofuran-3-yl)propanoate (3bb): Isolated by column



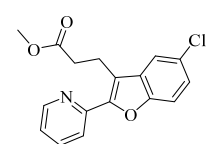
chromatography (pet.ether/AcOEt = 8:2, $R_f = 0.6$). The title compound was determined as pale yellow colour gum (64%). ^1H NMR (400 MHz, CDCl_3): δ 1.21 (t, $J = 7.1$ Hz, 3H), 2.48 (s, 3H), 2.80 (t, $J = 7.6$ Hz, 2H), 3.55 (t, $J = 7.6$ Hz, 2H), 4.11 (q, $J = 7.1$ Hz, 2H), 7.18 (d, $J = 8.3$ Hz, 1H), 7.27 (s, 1H), 7.42 (d, $J = 8.8$ Hz, 1H), 7.44 (s, 1H), 7.85 (t, $J = 7.6$ Hz, 1H), 7.98 (d, $J = 8.1$ Hz, 1H), 8.74 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 14.2 (q), 19.8 (t), 21.4 (q), 34.0 (t), 60.4 (t), 110.9 (d, 2C), 119.9 (s), 119.9 (d, 2C), 121.0 (d), 122.2 (d), 127.1 (d), 132.3 (s, 2C), 152.6 (s, 3C), 173.4 (s) ppm; HRMS(ESI) calcd for $\text{C}_{19}\text{H}_{20}\text{O}_3\text{N}$ (M^+H): 310.1438; found: 310.1439.

Tert-butyl 3-(5-methyl-2-(pyridin-2-yl)benzofuran-3-yl)propanoate (3bc): Isolated by



column chromatography (pet.ether/AcOEt = 8:2, $R_f = 0.7$). The title compound was determined as pale yellow colour gum (65%). ^1H NMR (500 MHz, CDCl_3): δ 1.42 (s, 9H), 2.48 (s, 3H), 2.70 (t, $J = 7.9$ Hz, 2H), 3.51 (t, $J = 7.9$ Hz, 2H), 7.15 (d, $J = 7.9$ Hz, 1H), 7.20 (dd, $J = 5.5, 6.7$ Hz, 1H), 7.39 (d, $J = 8.2$ Hz, 1H), 7.44 (s, 1H), 7.78 (t, $J = 7.6$ Hz, 1H), 7.91 (d, $J = 7.9$ Hz, 1H), 8.70 (d, $J = 4.0$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 19.9 (t), 21.4 (q), 28.1 (q, 3C), 35.3 (t), 80.2 (s), 110.7 (d), 118.9 (s), 120.0 (d), 120.7 (d), 121.9 (d), 126.6 (d), 130.1 (s), 132.1 (s), 136.5 (d), 149.2 (s), 149.4 (d), 150.8 (s), 152.4 (s), 172.8 (s) ppm; HRMS(ESI) calcd for $\text{C}_{21}\text{H}_{24}\text{O}_3\text{N}$ (M^+H): 338.1751; found: 338.1753.

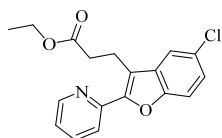
Methyl 3-(5-chloro-2-(pyridin-2-yl)benzofuran-3-yl)propanoate (3ca): Isolated by column



chromatography (pet.ether/AcOEt = 8:2, $R_f = 0.6$). The title compound was determined as white colour solid (86%). Mp: 87-88 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.81 (t, $J = 7.8$ Hz, 2H), 3.53 (t, $J = 8.0$ Hz, 2H), 3.66 (s, 3H), 7.23 (ddd, $J = 1.0, 5.0, 7.5$ Hz, 1H), 7.29 (dd, $J = 2.3, 8.5$ Hz, 1H), 7.43 (d, $J = 8.5$ Hz, 1H), 7.63 (d, $J = 2.0$ Hz, 1H), 7.79 (dt, $J = 1.8, 8.0$ Hz, 1H), 7.92 (d, $J = 8.0$ Hz, 1H), 8.69 (d, $J = 4.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 19.7 (t), 33.7 (t), 51.6 (q), 112.3 (d), 118.3 (s), 119.7 (d), 120.7

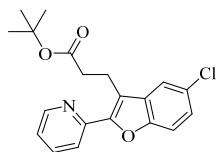
(d), 122.4 (d), 125.4 (d), 128.4 (s), 131.5 (s), 136.5 (d), 149.7 (d), 150.4 (s), 150.7 (s), 152.2 (s), 173.7 (s) ppm; HRMS(ESI) calcd for C₁₇H₁₅O₃NCl (M⁺+H): 316.0735; found: 316.0736.

Ethyl 3-(5-chloro-2-(pyridin-2-yl)benzofuran-3-yl)propanoate (3cb): Isolated by column



chromatography (pet.ether/AcOEt = 8:2, R_f = 0.6). The title compound was determined as white colour solid (81%). Mp: 84-85 °C; ¹H NMR (400 MHz, CDCl₃): δ 1.22 (t, J = 7.3 Hz, 3H), 2.79 (t, J = 7.3 Hz, 2H), 3.53 (t, J = 7.3 Hz, 2H), 4.11 (t, J = 7.3 Hz, 2H), 7.23 (ddd, J = 0.9, 5.0, 7.3 Hz, 1H), 7.29 (dd, J = 1.8, 8.7 Hz, 1H), 7.43 (d, J = 8.7 Hz, 1H), 7.63 (d, J = 2.3 Hz, 1H), 7.79 (dt, J = 1.8, 8.2 Hz, 1H), 7.92 (d, J = 7.8 Hz, 1H), 8.69 (d, J = 4.1 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 14.1 (q), 19.6 (t), 34.0 (t), 60.4 (t), 112.2 (d), 118.4 (s), 119.8 (d), 120.7 (d), 122.4 (d), 125.4 (d), 128.4 (s), 131.5 (s), 136.5 (d), 149.7 (d), 150.4 (s), 150.7 (s), 152.2 (s), 173.2 (s) ppm; HRMS(ESI) calcd for C₁₈H₁₇O₃NCl (M⁺+H): 330.0891; found: 330.0892.

Tert-butyl 3-(5-chloro-2-(pyridin-2-yl)benzofuran-3-yl)propanoate (3cc): Isolated by column

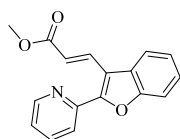


chromatography (pet.ether/AcOEt = 8:2, R_f = 0.7). The title compound was determined as white colour solid (83%). Mp: 90-91 °C; ¹H NMR (400 MHz, CDCl₃): δ 1.41 (s, 9H), 2.69 (t, J = 8.0 Hz, 2H), 3.49 (t, J = 7.8 Hz, 2H), 7.23 (dd, J = 5.0, 6.5 Hz, 1H), 7.29 (dd, J = 2.0, 8.5 Hz, 1H), 7.42 (d, J = 8.5 Hz, 1H), 7.64 (d, J = 1.8 Hz, 1H), 7.78 (dt, J = 1.8, 8.0 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 8.70 (d, J = 4.3 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 19.8 (t), 28.1 (q, 3C), 33.7 (t), 80.3 (s), 112.2 (d), 118.6 (s), 119.9 (d), 120.8 (d), 122.3 (d), 125.4 (d), 128.3 (s), 131.5 (s), 136.4 (d), 149.7 (d), 150.4 (s), 150.7 (s), 152.3 (s), 172.6 (s) ppm; HRMS(ESI) calcd for C₂₀H₂₁O₃NCl (M⁺+H): 358.1204; found: 358.1207.

General procedure B: Linear alkenylation using Ru(PPh₃)₃Cl₂ :

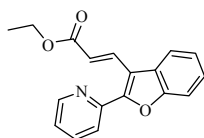
2-(benzofuran-2-yl)pyridine (0.1 mmol) was placed in a screw cap pressure tube and dissolved in anhydrous toluene (2 mL), which was then evacuated and back filled with argon. To the reaction vessel alkene (acrylate) (0.3 mmol), K₂CO₃ (0.3 mmol), RuCl₂(PPh₃)₃ (0.005 mmol) and AgOAc (0.03 mmol) were added. The solution was then stirred at 140 °C (bath temperature) for 24 h. The reaction mixture was cooled to room temperature. The solvent were evaporated and the crude products were purified by column chromatography (pet ether/AcOEt) to give analytically pure.

Methyl (*E*)-3-(2-(pyridin-2-yl)benzofuran-3-yl)acrylate (4aa): The title compound was



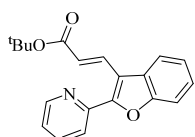
isolated by column chromatography (pet.ether/AcOEt = 8:2, R_f = 0.4) and determined as pale yellow colour solid (77%). Mp: 116-117 °C; ^1H NMR (500 MHz, CDCl_3): δ 3.86 (s, 3H), 6.74 (d, J = 16.5 Hz, 1H), 7.29 (dd, J = 0.9, 4.6 Hz, 1H), 7.35 (dt, J = 0.9, 7.9 Hz, 1H), 7.41 (dt, J = 1.5, 8.2 Hz, 1H), 7.57 (d, J = 7.9 Hz, 1H), 7.82 (dt, J = 1.8, 7.9 Hz, 1H), 7.94 (d, J = 7.6 Hz, 1H), 7.99 (d, J = 7.9 Hz, 1H), 8.79 (dddd, J = 0.9, 1.5, 2.4, 4.6 Hz, 1H), 9.02 (d, J = 16.5 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 51.7 (q), 111.7 (d), 115.5 (s), 119.7 (d), 121.7 (d), 122.1 (d), 123.2 (d), 124.0 (d), 126.0 (d), 126.9 (s), 136.6 (d), 137.6 (d), 149.9 (d), 149.9 (s), 153.5 (s), 154.4 (s), 167.8 (s) ppm; HRMS(ESI) calcd for $\text{C}_{17}\text{H}_{14}\text{O}_3\text{N}$ (M^+H): 280.0968; found: 280.0968.

Ethyl (*E*)-3-(2-(pyridin-2-yl)benzofuran-3-yl)acrylate (4ab): Isolated by column



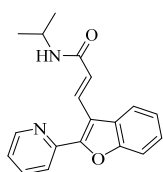
chromatography (pet.ether/AcOEt = 8:2, R_f = 0.4). The title compound was determined as yellow colour solid (72%). Mp: 124-125 °C; ^1H NMR (500 MHz, CDCl_3): δ 1.38 (t, J = 7.3 Hz, 3H), 4.32 (q, J = 7.3 Hz, 2H), 6.74 (d, J = 16.5 Hz, 1H), 7.29 (dddd, J = 0.9, 4.9, 7.6, 12.5 Hz, 1H), 7.35 (dt, J = 0.9, 7.9 Hz, 1H), 7.41 (dt, J = 1.2, 8.2 Hz, 1H), 7.57 (d, J = 7.9 Hz, 1H), 7.82 (dt, J = 1.8, 7.9 Hz, 1H), 7.95 (d, J = 7.6 Hz, 1H), 7.99 (d, J = 8.2 Hz, 1H), 8.79 (ddd, J = 0.9, 1.5, 4.6 Hz, 1H), 9.02 (d, J = 16.5 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 14.4 (q), 60.4 (t), 111.7 (d), 115.6 (s), 120.1 (d), 121.8 (d), 122.1 (d), 123.1 (d), 123.9 (d), 126.0 (d), 126.9 (s), 136.6 (d), 137.3 (d), 149.8 (s), 149.9 (d), 153.4 (s), 154.4 (s), 167.4 (s) ppm; HRMS(ESI) calcd for $\text{C}_{18}\text{H}_{16}\text{O}_3\text{N}$ (M^+H): 294.1125; found: 294.1125.

Tert-butyl (*E*)-3-(2-(pyridin-2-yl)benzofuran-3-yl)acrylate (4ac): Isolated by column



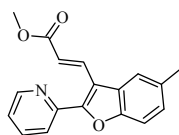
chromatography (pet.ether/AcOEt = 8:2, R_f = 0.6). The title compound was determined as white colour solid (70%). Mp: 131-133 °C; ^1H NMR (400 MHz, CDCl_3): δ 1.59 (s, 9H), 6.59 (d, J = 16.6 Hz, 1H), 7.29 (dd, J = 5.3, 7.3 Hz, 1H), 7.36 (t, J = 7.3 Hz, 1H), 7.41 (t, J = 7.5 Hz, 1H), 7.57 (d, J = 8.0 Hz, 1H), 7.82 (dt, J = 1.5, 8.0 Hz, 1H), 7.97 (d, J = 8.5 Hz, 1H), 7.99 (d, J = 8.3 Hz, 1H), 8.79 (d, J = 4.3 Hz, 1H), 8.97 (d, J = 16.6 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 28.3 (q, 3C), 80.3 (s), 111.7 (d), 115.7 (s), 121.8 (d), 121.9 (d), 122.1 (d), 123.1 (d), 123.8 (d), 125.9 (d), 126.9 (s), 136.3 (d), 136.6 (d), 149.9 (d), 149.9 (s), 153.2 (s), 154.4 (s), 166.7 (s) ppm; HRMS(ESI) calcd for $\text{C}_{20}\text{H}_{20}\text{O}_3\text{N}$ (M^+H): 322.1438; found: 322.1431.

(E)-N-isopropyl-3-(2-(pyridin-2-yl)benzofuran-3-yl)acrylamide (4ad): Isolated by column



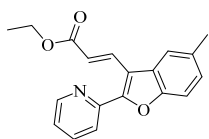
chromatography (pet.ether/AcOEt = 5:5, R_f = 0.2). The title compound was determined as white colour solid (51%). Mp: 196-198 °C; ^1H NMR (500 MHz, CDCl_3): δ 1.27 (d, J = 6.6 Hz, 6H), 4.25–4.32 (m, 1H), 5.57 (d, J = 6.4 Hz, 1H), 6.68 (d, J = 16.2 Hz, 1H), 7.28–7.30 (m, 1H), 7.33–7.37 (m, 1H), 7.41 (t, J = 7.9 Hz, 1H), 7.59 (d, J = 7.9 Hz, 1H), 7.82 (d, J = 7.9 Hz, 1H), 7.92 (d, J = 7.6 Hz, 1H), 7.98 (d, J = 7.9 Hz, 1H), 7.89 (d, J = 4.6 Hz, 1H), 8.80 (d, J = 16.2 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 22.9 (q, 2C), 41.6 (d), 111.8 (d), 115.7 (s), 121.5 (d), 122.1 (d), 123.0 (d), 123.4 (d), 123.7 (d), 125.8 (d), 127.1 (s), 132.9 (d), 136.6 (d), 149.9 (s), 150.0 (d), 152.9 (s), 154.4 (s), 165.5 (s) ppm; HRMS(ESI) calcd for $\text{C}_{19}\text{H}_{19}\text{O}_2\text{N}_2$ ($\text{M}^+\text{+H}$): 307.1441; found: 307.1436.

Methyl (E)-3-(5-methyl-2-(pyridin-2-yl)benzofuran-3-yl)acrylate (4ba): Isolated by column



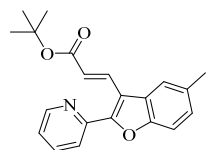
chromatography (pet.ether/AcOEt = 8:2, R_f = 0.5). The title compound was determined as white colour solid (65%). Mp: 110-111 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.51 (s, 3H), 3.87 (s, 3H), 6.74 (d, J = 16.6 Hz, 1H), 7.23 (d, J = 8.5 Hz, 1H), 7.28–7.31 (m, 1H), 7.46 (d, J = 8.5 Hz, 1H), 7.73 (s, 1H), 7.83 (dt, J = 1.8, 8.0 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 8.00 (d, J = 4.5 Hz, 1H), 9.01 (d, J = 16.6 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 21.5 (q), 51.7 (q), 111.2 (d), 115.4 (s), 119.5 (d), 121.6 (d), 122.1 (d), 123.1 (d), 126.9 (s), 127.3 (d), 133.6 (s), 136.7 (d), 137.7 (d), 149.8 (d), 149.9 (s), 152.9 (s), 153.6 (s), 167.9 (s) ppm; HRMS(ESI) calcd for $\text{C}_{18}\text{H}_{16}\text{O}_3\text{N}$ ($\text{M}^+\text{+H}$): 294.1125; found: 294.1122.

Ethyl (E)-3-(5-methyl-2-(pyridin-2-yl)benzofuran-3-yl)acrylate (4bb): Isolated by column



chromatography (pet.ether/AcOEt = 8:2, R_f = 0.5). The title compound was determined as yellow colour gum (65%). ^1H NMR (500 MHz, CDCl_3): δ 1.40 (t, J = 7.3 Hz, 3H), 2.52 (s, 3H), 4.32 (q, J = 7.3 Hz, 2H), 6.74 (d, J = 16.2 Hz, 1H), 7.23 (d, J = 5.8 Hz, 1H), 7.30 (t, J = 5.8 Hz, 1H), 7.46 (d, J = 8.2 Hz, 1H), 7.74 (s, 1H), 7.84 (t, J = 7.6 Hz, 1H), 7.99 (d, J = 7.6 Hz, 1H), 8.80 (bs, 1H), 9.00 (d, J = 16.2 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 14.4 (q), 21.5 (q), 60.5 (t), 111.2 (d), 115.5 (s), 119.9 (d), 121.6 (d), 122.1 (d), 123.1 (d), 126.9 (s), 127.3 (d), 133.6 (s), 136.8 (d), 137.4 (d), 149.7 (d), 149.8 (s), 152.9 (s), 165.4 (s), 167.5 (s) ppm; HRMS(ESI) calcd for $\text{C}_{19}\text{H}_{18}\text{O}_3\text{N}$ ($\text{M}^+\text{+H}$): 308.1281; found: 308.1283.

Tert-butyl (E)-3-(5-methyl-2-(pyridin-2-yl)benzofuran-3-yl)acrylate (4bc): Isolated by

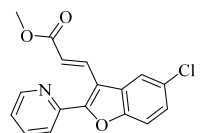


column chromatography (pet.ether/AcOEt = 8:2, R_f = 0.5). The title compound

was determined as yellow colour gum (66%). ^1H NMR (500 MHz, CDCl_3): δ

1.59 (s, 9H), 2.52 (s, 3H), 6.66 (d, J = 16.2 Hz, 1H), 7.22 (d, J = 7.9 Hz, 1H), 7.28–7.29 (m, 1H), 7.45 (d, J = 8.2 Hz, 1H), 7.74 (s, 1H), 7.82 (dt, J = 1.5, 7.9 Hz, 1H), 7.97 (d, J = 7.9 Hz, 1H), 8.79 (d, J = 4.3 Hz, 1H), 8.94 (d, J = 16.2 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 21.5 (q), 28.3 (q, 3C), 80.3 (s), 111.2 (d), 115.5 (s), 121.7 (d, 2C), 122.1 (d), 123.0 (d), 127.0 (s), 127.2 (d), 133.5 (s), 136.4 (d), 136.6 (d), 149.8 (d), 150.0 (s), 152.9 (s), 153.3 (s), 166.8 (s) ppm; HRMS(ESI) calcd for $\text{C}_{21}\text{H}_{22}\text{O}_3\text{N}$ ($\text{M}^+\text{+H}$): 336.1594; found: 336.1594.

Methyl (E)-3-(5-chloro-2-(pyridin-2-yl)benzofuran-3-yl)acrylate (4ca): Isolated by column

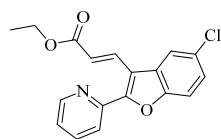


chromatography (pet.ether/AcOEt = 8:2, R_f = 0.4). The title compound was

determined as white colour solid (81%). Mp: 122-123 °C; ^1H NMR (400 MHz,

CDCl_3): δ 3.87 (s, 3H), 6.74 (d, J = 16.5 Hz, 1H), 7.32 (ddd, J = 0.9, 4.6, 7.3 Hz, 1H), 7.37 (dd, J = 2.3, 8.7 Hz, 1H), 7.49 (d, J = 8.7 Hz, 1H), 7.84 (dt, J = 1.8, 8.2 Hz, 1H), 7.89 (d, J = 1.8 Hz, 1H), 7.98 (d, J = 7.8 Hz, 1H), 8.80 (d, J = 4.6 Hz, 1H), 8.96 (d, J = 16.5 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 51.8 (q), 112.7 (d), 115.0 (s), 119.9 (d), 121.3 (d), 122.2 (d), 123.5 (d), 126.2 (d), 128.1 (s), 129.7 (s), 136.7 (d), 136.9 (d), 149.4 (s), 150.0 (d), 152.7 (s), 154.5 (s), 167.6 (s) ppm; HRMS(ESI) calcd for $\text{C}_{17}\text{H}_{13}\text{O}_3\text{NCl}$ ($\text{M}^+\text{+H}$): 314.0578; found: 314.0580.

Ethyl (E)-3-(5-chloro-2-(pyridin-2-yl)benzofuran-3-yl)acrylate (4cb): Isolated by column

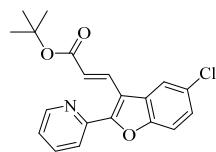


chromatography (pet.ether/AcOEt = 8:2, R_f = 0.4). The title compound was

determined as white colour solid (78%). Mp: 117-118 °C; ^1H NMR (400

MHz, CDCl_3): δ 1.39 (t, J = 7.1 Hz, 3H), 4.33 (q, J = 7.1 Hz, 2H), 6.64 (d, J = 16.4 Hz, 1H), 7.23 (dd, J = 4.9, 6.9 Hz, 1H), 7.36 (dd, J = 2.0, 8.6 Hz, 1H), 7.48 (d, J = 8.6 Hz, 1H), 7.8 (dd, J = 1.5, 7.8 Hz, 1H), 7.89 (d, J = 1.7 Hz, 1H), 7.96 (d, J = 8.1 Hz, 1H), 8.79 (d, J = 4.7 Hz, 1H), 8.96 (d, J = 16.4 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 14.7 (q), 60.8 (t), 113.0 (d), 115.4 (s), 120.7 (d), 121.7 (d), 122.5 (d), 123.8 (d), 126.5 (d), 128.5 (s), 129.9 (s), 137.0 (d, 2C), 149.7 (s), 150.3 (d), 153.0 (s), 154.7 (s), 167.5 (s) ppm; HRMS(ESI) calcd for $\text{C}_{18}\text{H}_{15}\text{O}_3\text{NCl}$ ($\text{M}^+\text{+H}$): 328.0735; found: 328.0737.

Tert-butyl (E)-3-(5-chloro-2-(pyridin-2-yl)benzofuran-3-yl)acrylate (4cc): Isolated by



column chromatography (pet.ether/AcOEt = 8:2, R_f = 0.6). The title compound

was determined as white colour solid (80%). Mp: 136-137 °C; ^1H NMR (400

MHz, CDCl_3): δ 1.59 (s, 9H), 6.59 (d, J = 16.3 Hz, 1H), 7.31 (dd, J = 4.8, 7.5

Hz, 1H), 7.38 (dd, J = 2.0, 8.8 Hz, 1H), 7.50 (d, J = 8.5 Hz, 1H), 7.83 (dt, J = 1.8, 8.0 Hz, 1H),

7.93 (d, J = 2.0 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 8.79 (td, J = 0.8, 4.8 Hz, 1H), 8.90 (d, J = 16.6

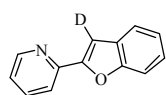
Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 28.3 (q, 3C), 80.6 (s), 112.7 (d), 115.2 (s), 121.5 (d),

122.2 (d), 122.3 (d), 123.4 (d), 126.1 (d), 128.3 (s), 129.6 (s), 135.6 (d), 136.7 (d), 149.5 (s),

150.0 (d), 152.8 (s), 154.3 (s), 166.5 (s) ppm; HRMS(ESI) calcd for $\text{C}_{20}\text{H}_{19}\text{O}_3\text{NCl}$ ($\text{M}^+\text{+H}$):

356.1048; found: 356.1043.

2-(Benzofuran-2-yl-3-D)pyridine (5): Isolated by column chromatography (pet.ether/AcOEt =



9:1, R_f = 0.4). The title compound was determined as white colour solid (83%).

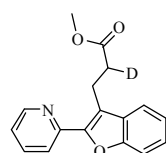
Mp: 82-83 °C; ^1H NMR (200 MHz, CDCl_3): δ 7.27–7.44 (m, 2H and 1H extra due

to CDCl_3), 7.50 (s, 0.30H (30%)), 7.63 (d, J = 8.1 Hz, 1H), 7.72 (d, J = 7.5 Hz, 1H), 7.84 (dt, J =

1.0, 7.5 Hz, 1H), 7.96 (d, J = 7.8 Hz, 1H), 8.74 (d, J = 3.9 Hz, 1H); HRMS(ESI) calcd for

$\text{C}_{13}\text{H}_9^2\text{HON}$ ($\text{M}^+\text{+H}$): 197.0820; found: 197.0816.

Methyl 3-(2-(pyridin-2-yl)benzofuran-3-yl)propanoate-2-D (6): Isolated by column



chromatography (pet.ether/AcOEt = 9:1, R_f = 0.4). The title compound was

determined as white colour sticky solid (76%). ^1H NMR (200 MHz, CDCl_3): δ

2.83 (t, J = 8.2 Hz, 1.91H (9%)), 3.58 (t, J = 8.2 Hz, 2H), 3.65 (s, 3H), 7.21 (dd, J

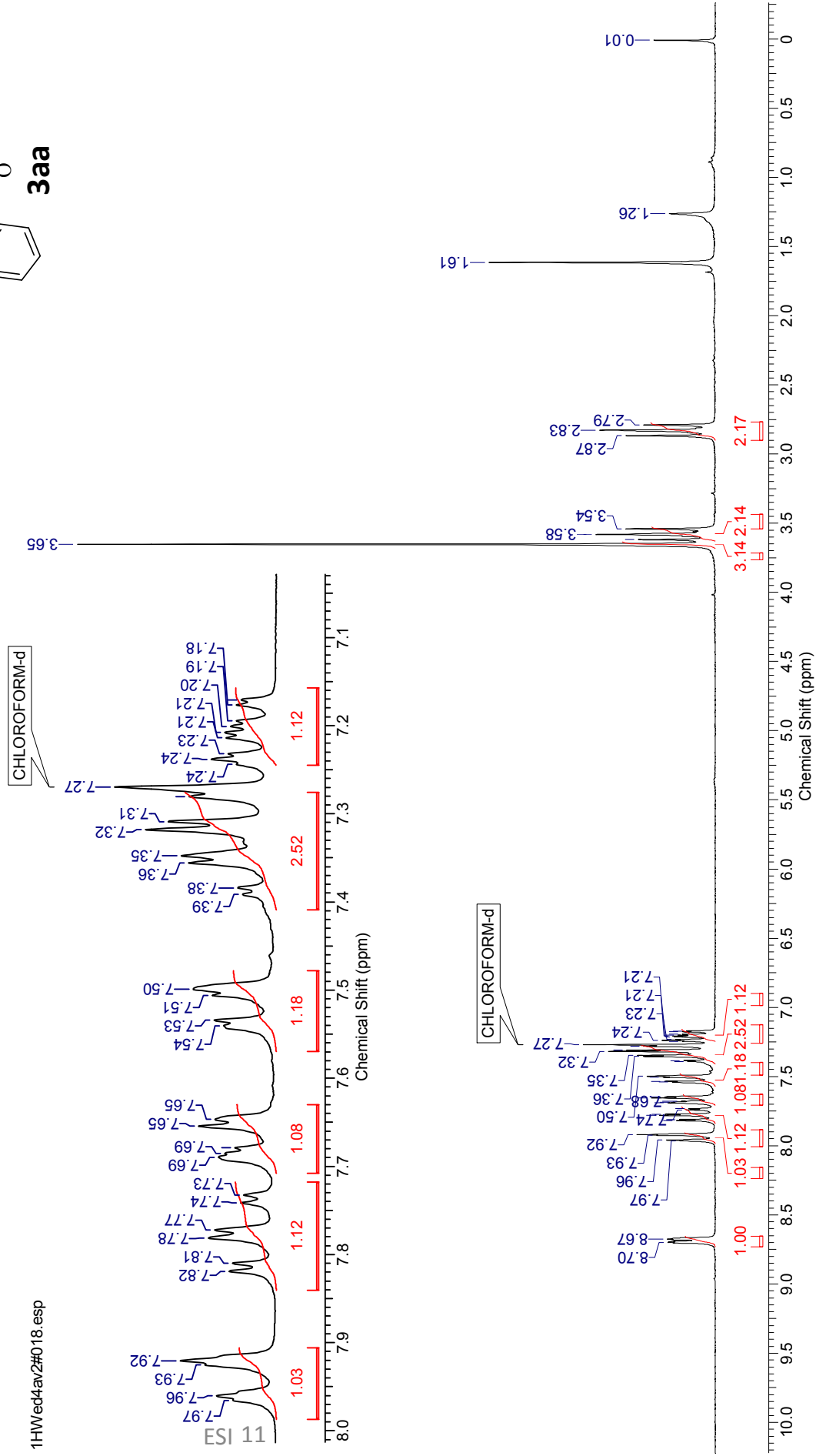
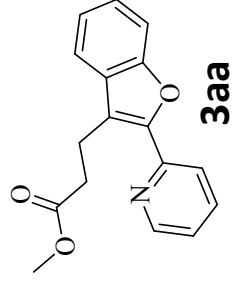
= 1.1, 4.8 Hz, 1H), 7.28–7.39 (m, 2H), 7.49–7.54 (m, 1H), 7.64–7.69 (m, 1H),

7.78 (dt, J = 1.8, 7.9 Hz, 1H), 7.95 (td, J = 1.0, 8.1 Hz, 1H), 8.69 (ddd, J = 0.9, 1.8, 4.8 Hz, 1H);

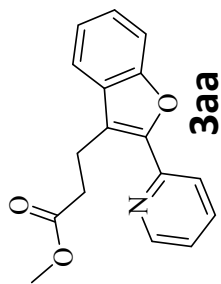
HRMS(ESI) calcd for $\text{C}_{17}\text{H}_{14}^2\text{HO}_3\text{N}$ ($\text{M}^+\text{+H}$): 282.1109; found: 282.1121.

200 MHz, CDCl₃

1HWed4av2#018.esp



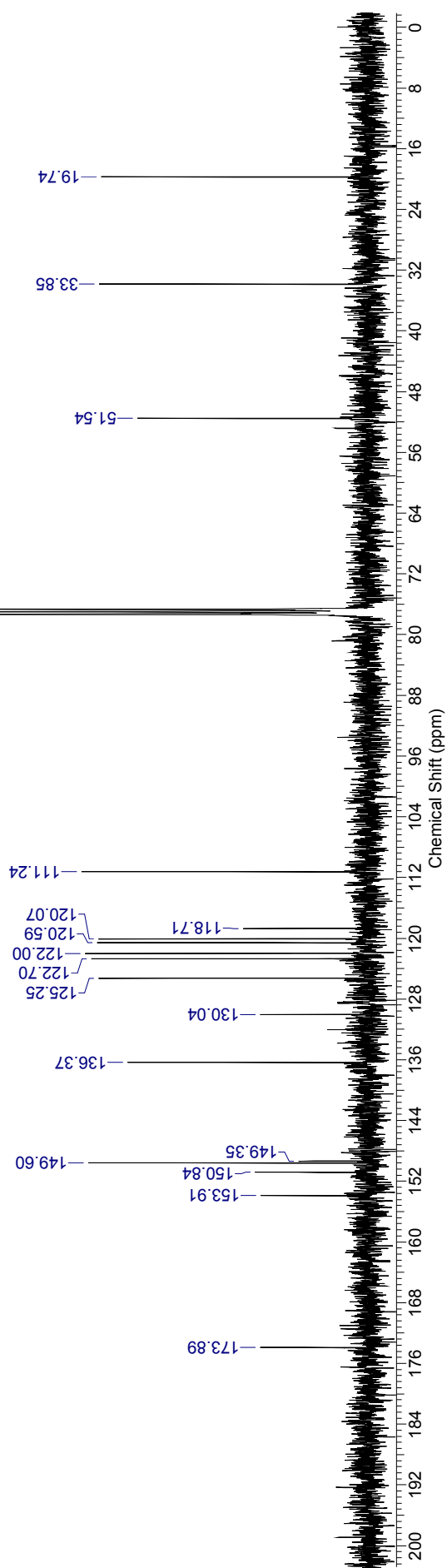
400 MHz, CDCl₃



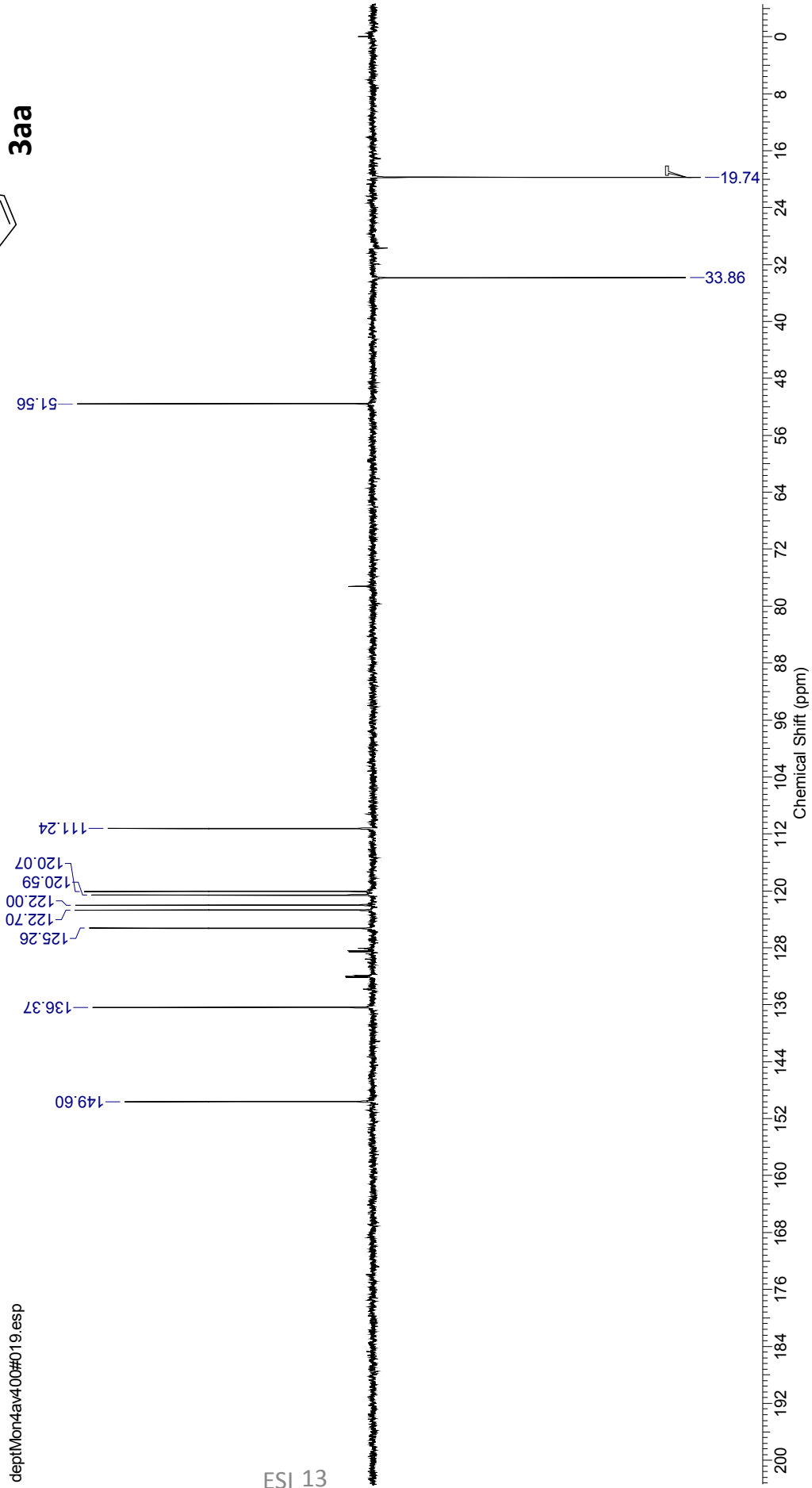
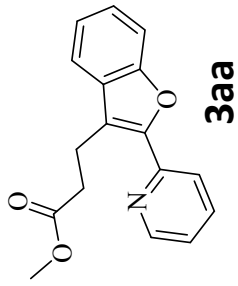
13CMon4av400#019.esp

CHLOROFORM-d

ESI 12



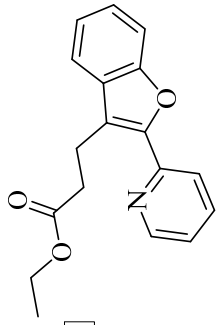
400 MHz, CDCl₃



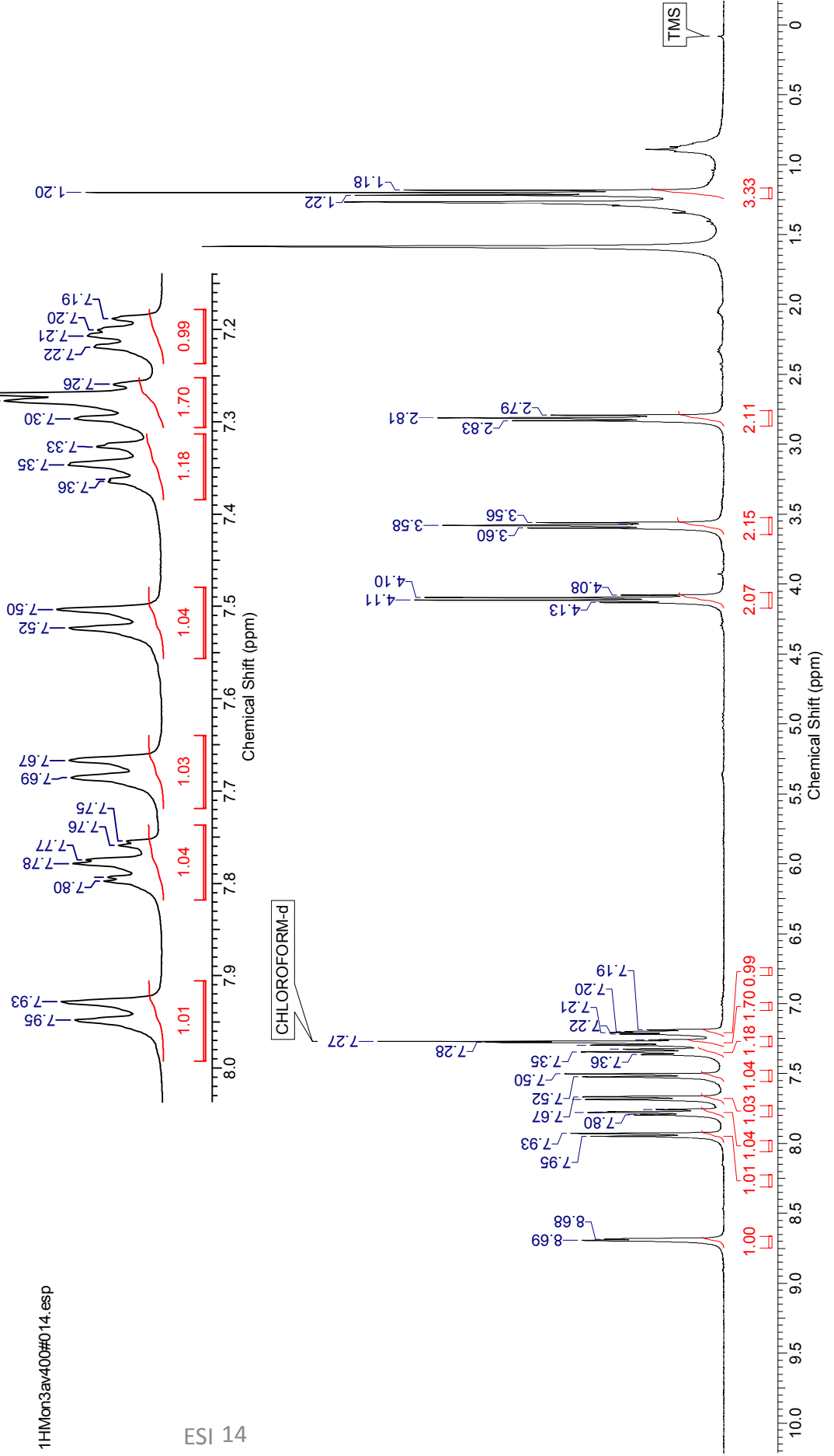
deptMon4av400#019.esp

ESI 13

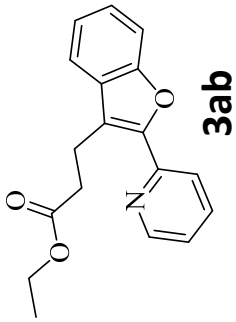
400 MHz, CDCl₃



3ab



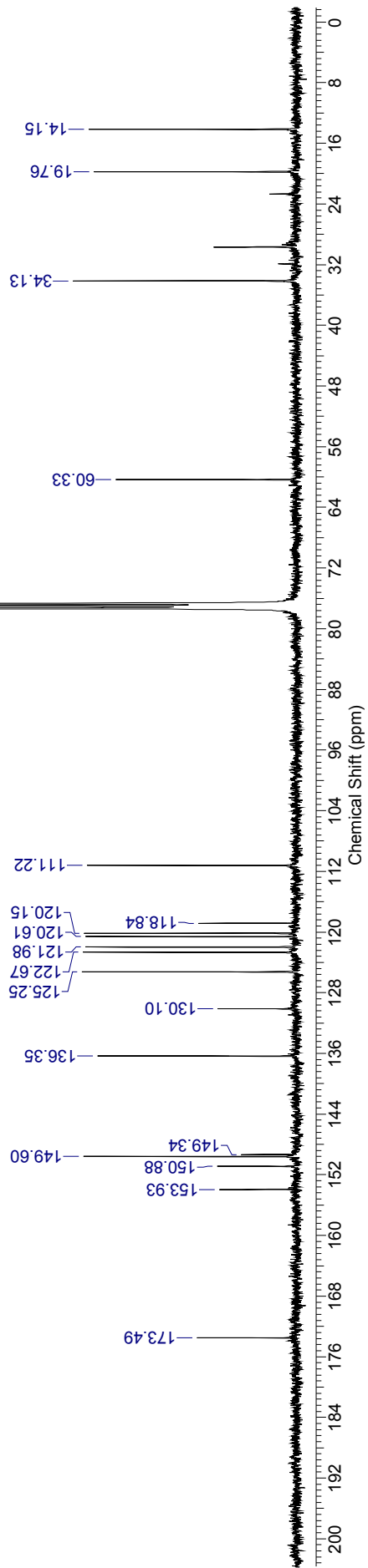
400 MHz, CDCl₃



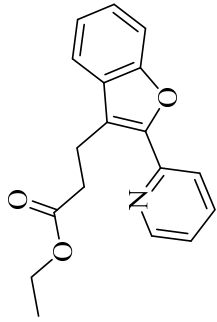
13CMon3av400#014.esp

CHLOROFORM-d

ESI 15



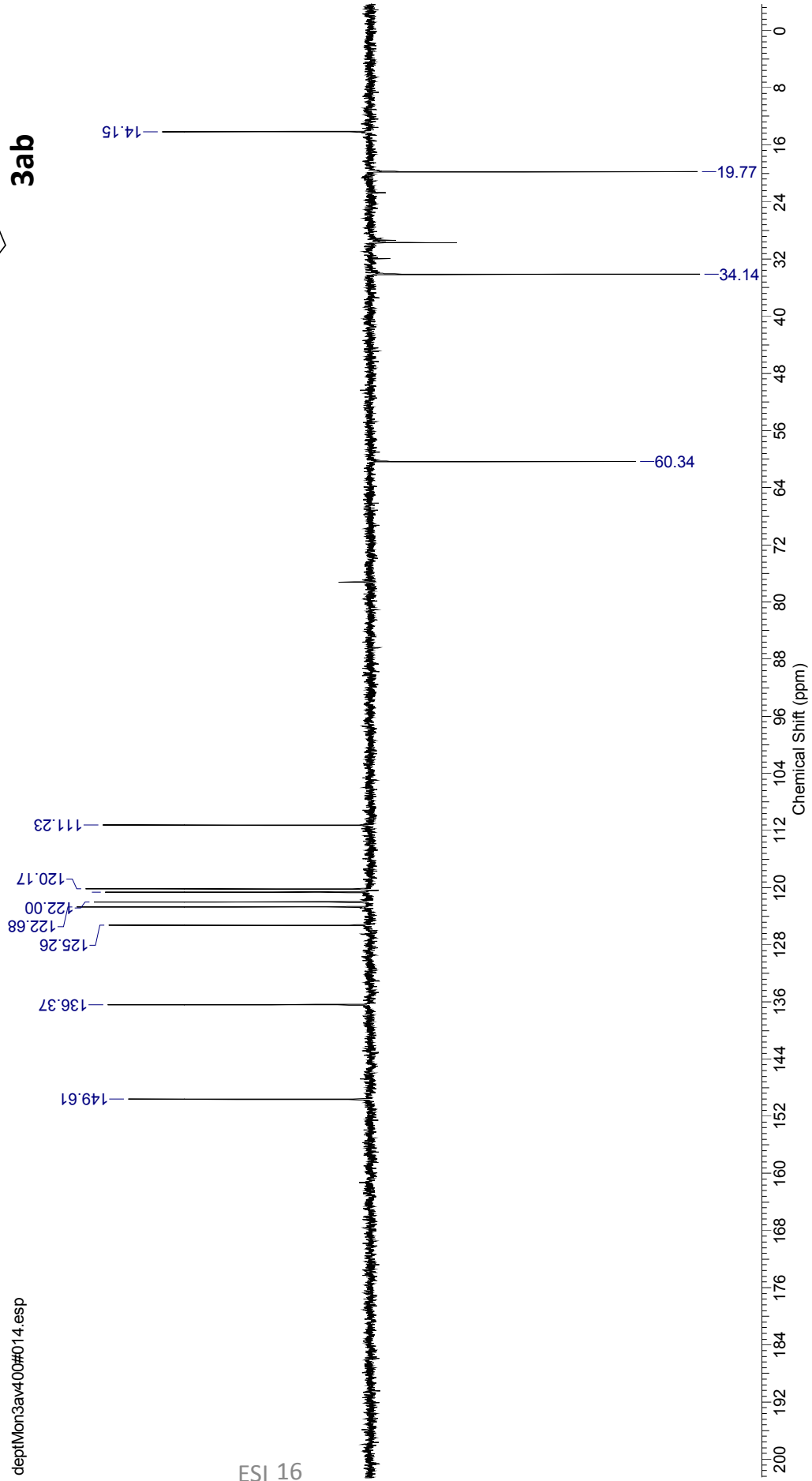
400 MHz, CDCl₃



3ab

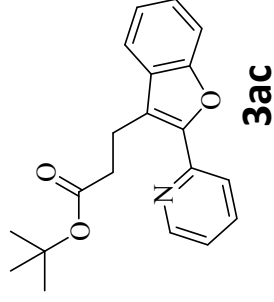
deptMon3av400#014.esp

ESI 16

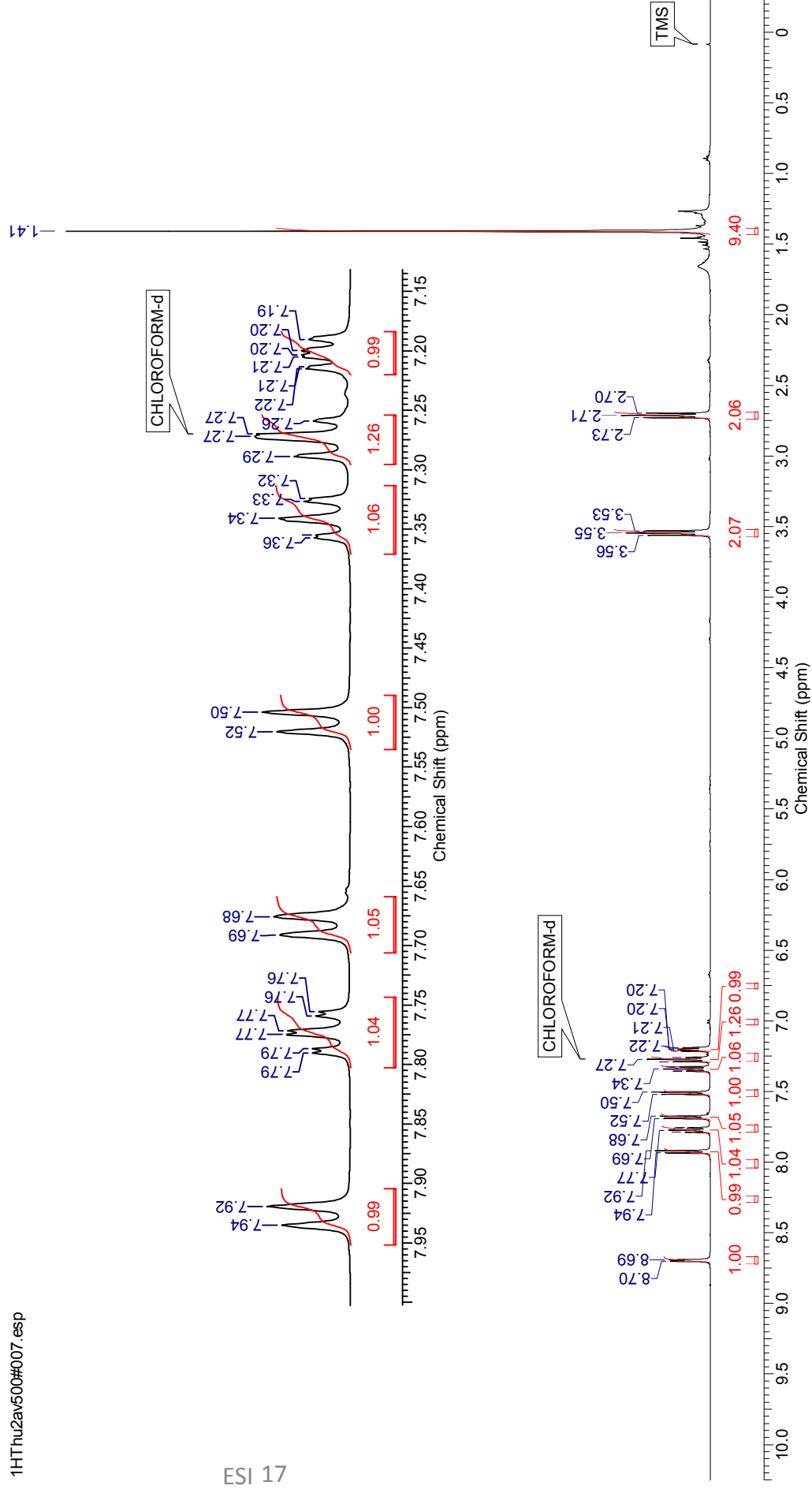


1HThu2av500#007.esp

500 MHz, CDCl₃

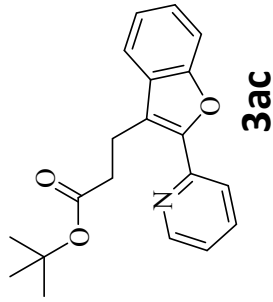


1HThu2av500#007.esp

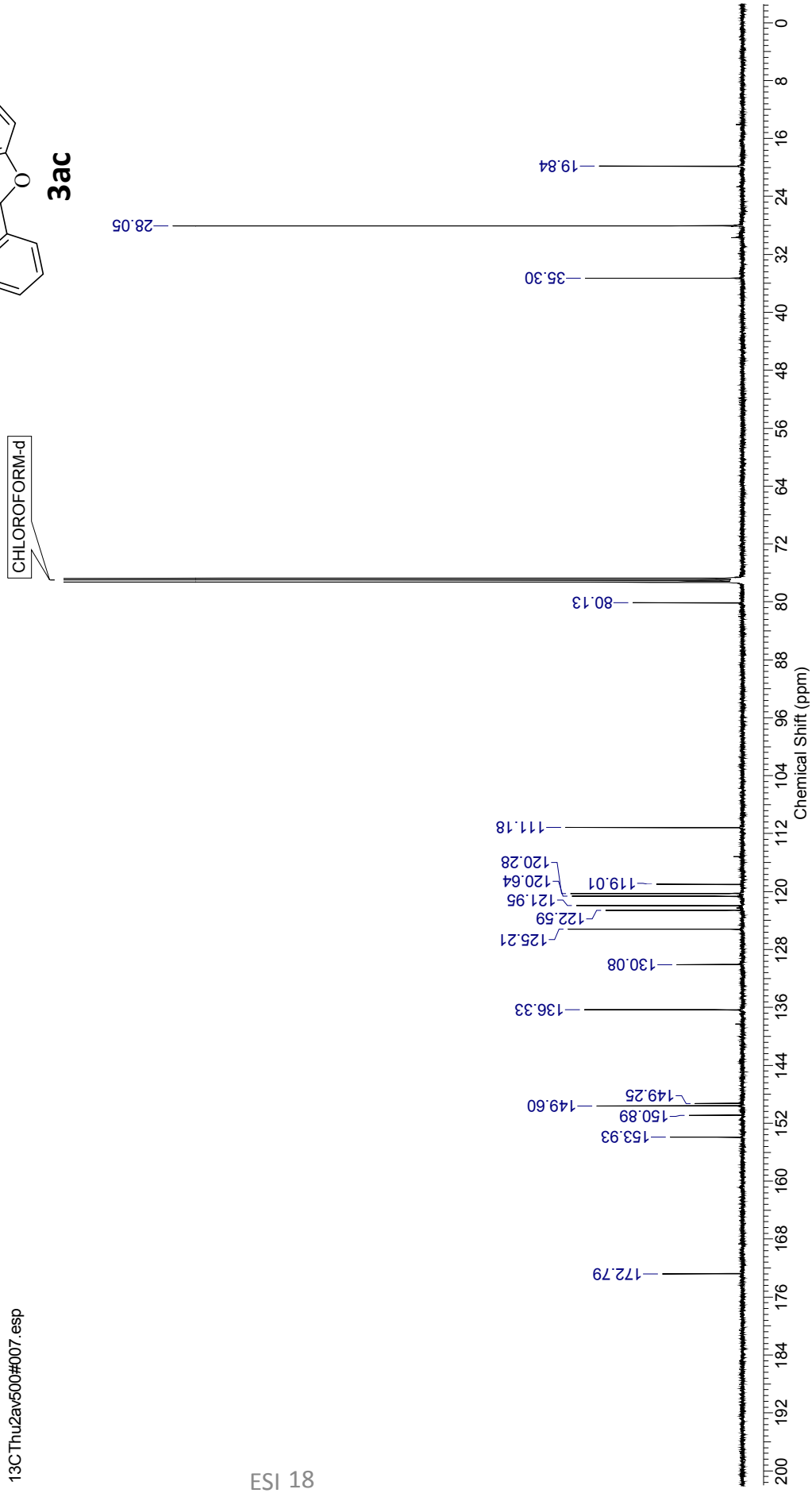


ESI 17

500 MHz, CDCl₃

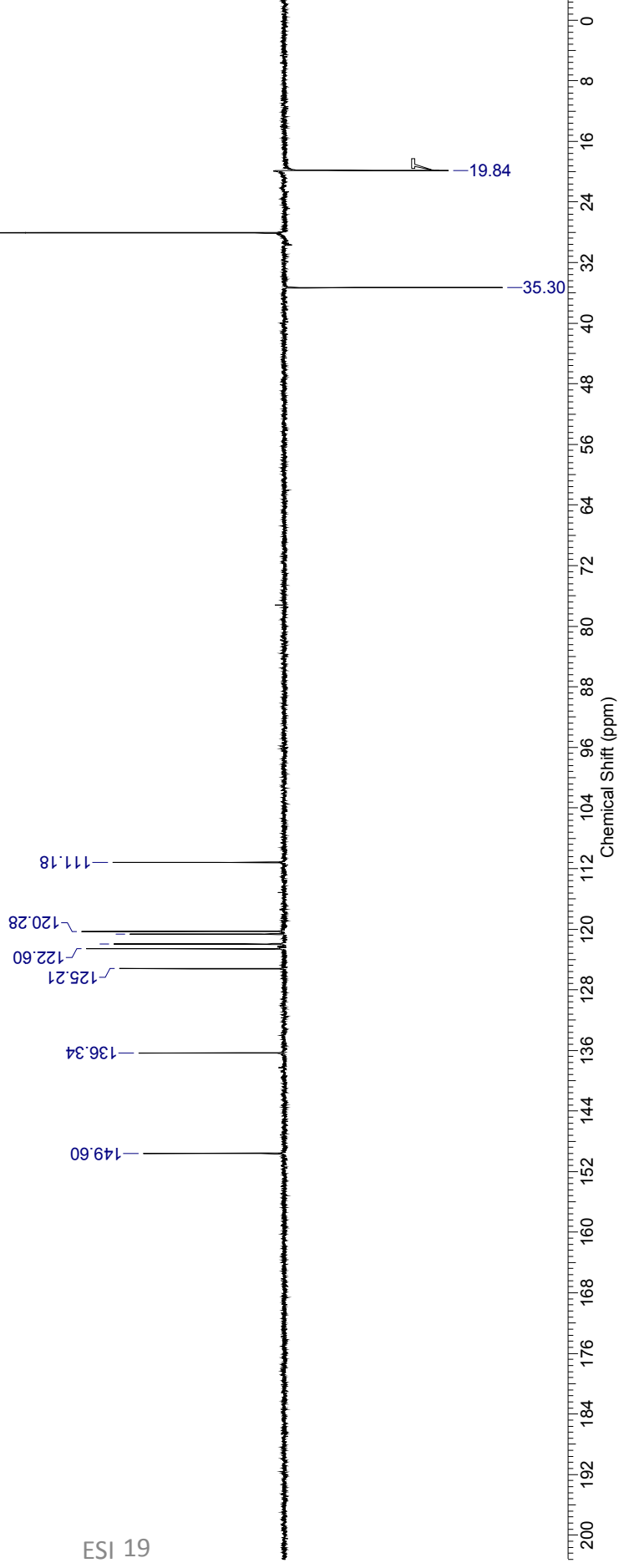
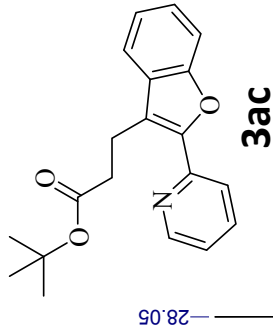


13C.Thu2av500#007.esp



500 MHz, CDCl₃

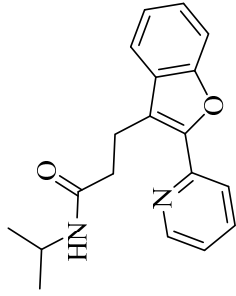
deptThu2av500#007.esp



ESI 19

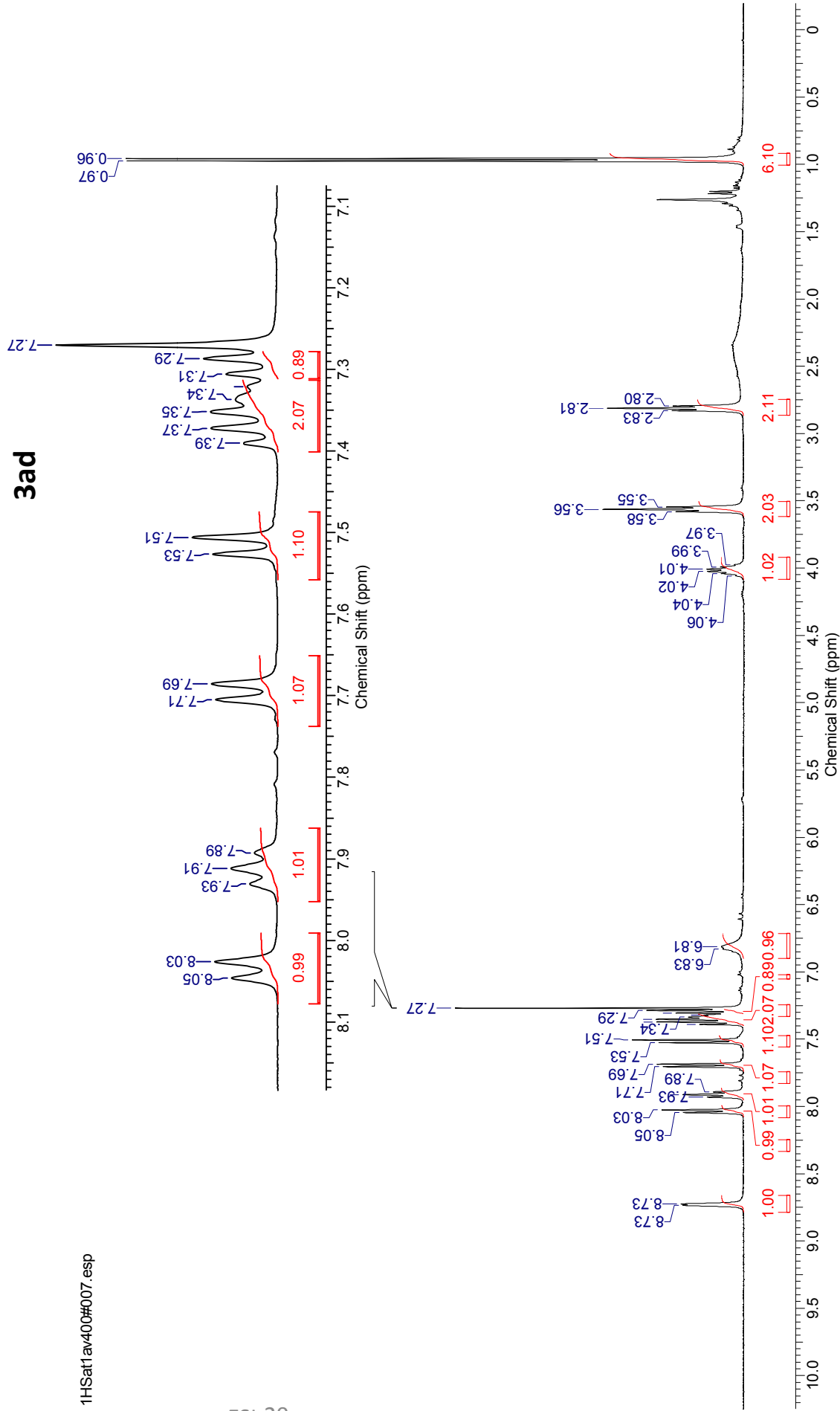
1HSat1av400#007.esp

400 MHz, CDCl₃



3ad

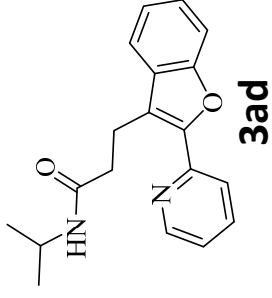
CHLOROFORM-d



1HSat1av400#007.esp

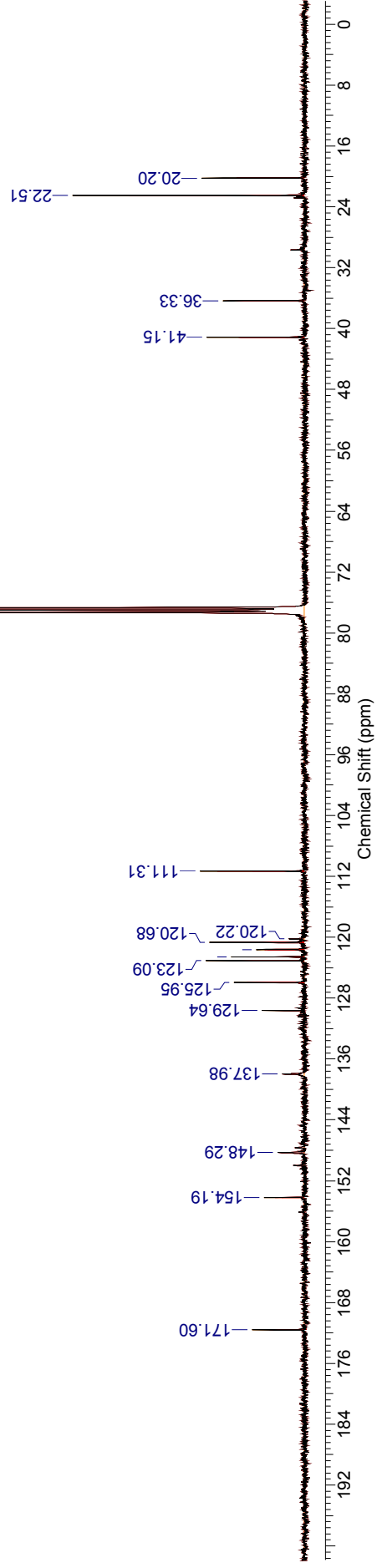
ESI 20

400 MHz, CDCl₃

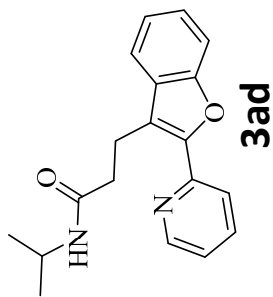


13CSatt1av400#007.esp

CHLOROFORM-d

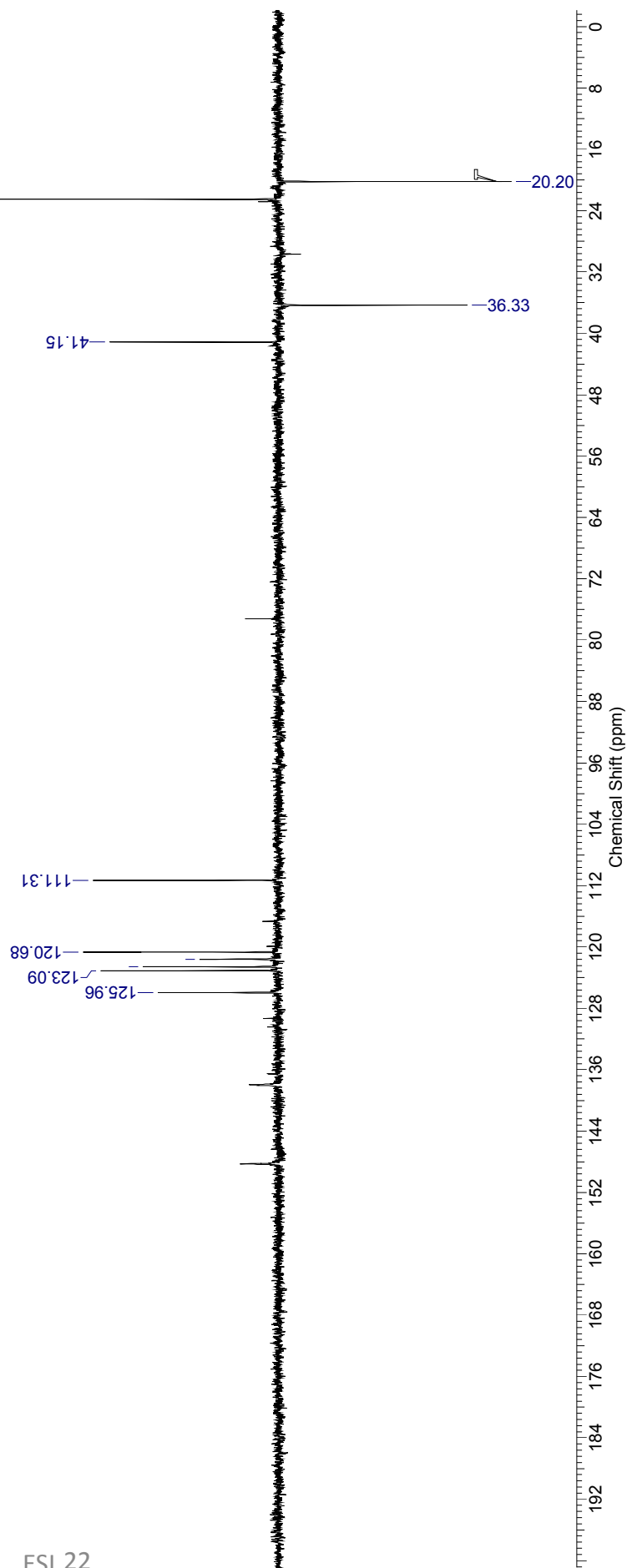


400 MHz, CDCl₃

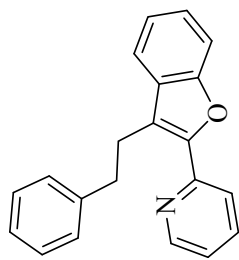


deptSat1av400#007.esp

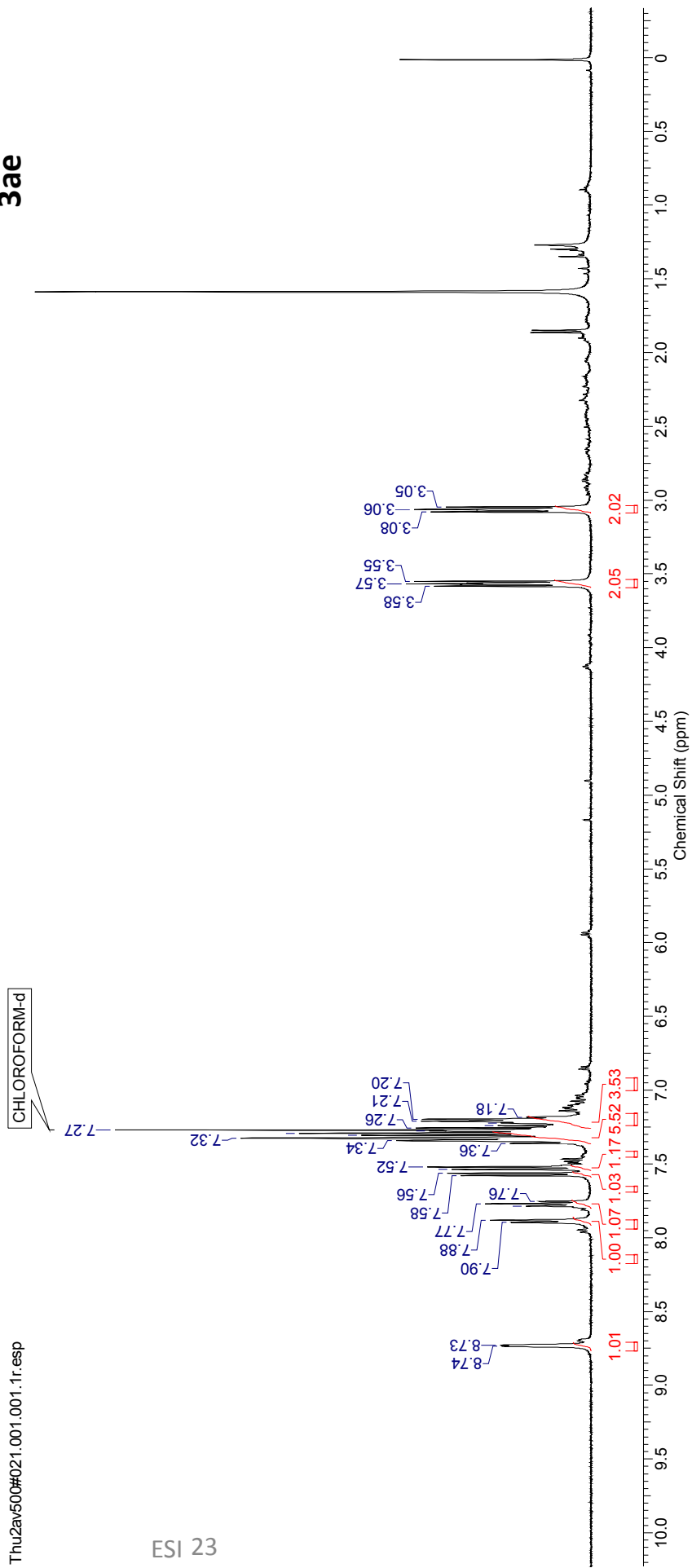
ESI 22



500 MHz, CDCl₃



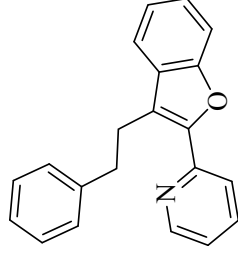
3ae



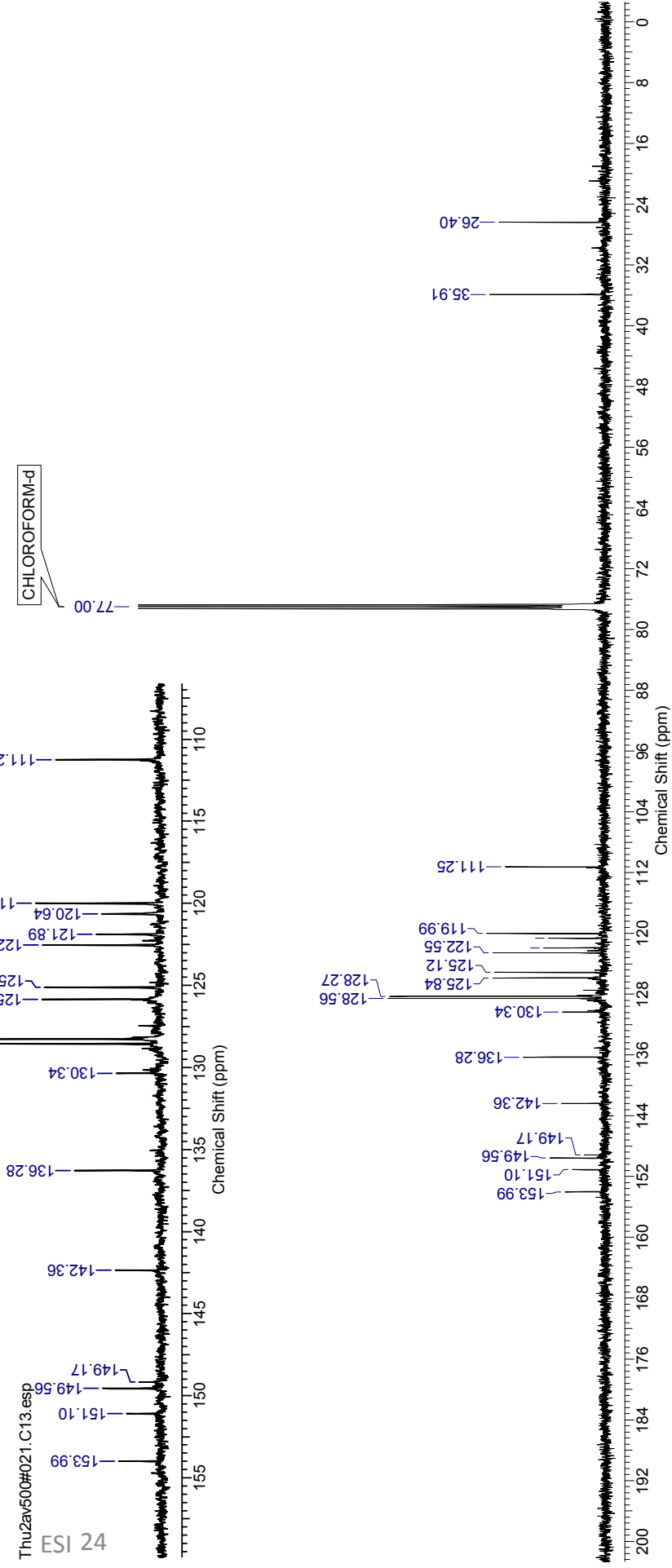
ESI 23

500 MHz, CDCl₃

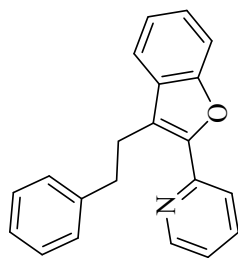
Thu2av500#021.C13.esp



3ae



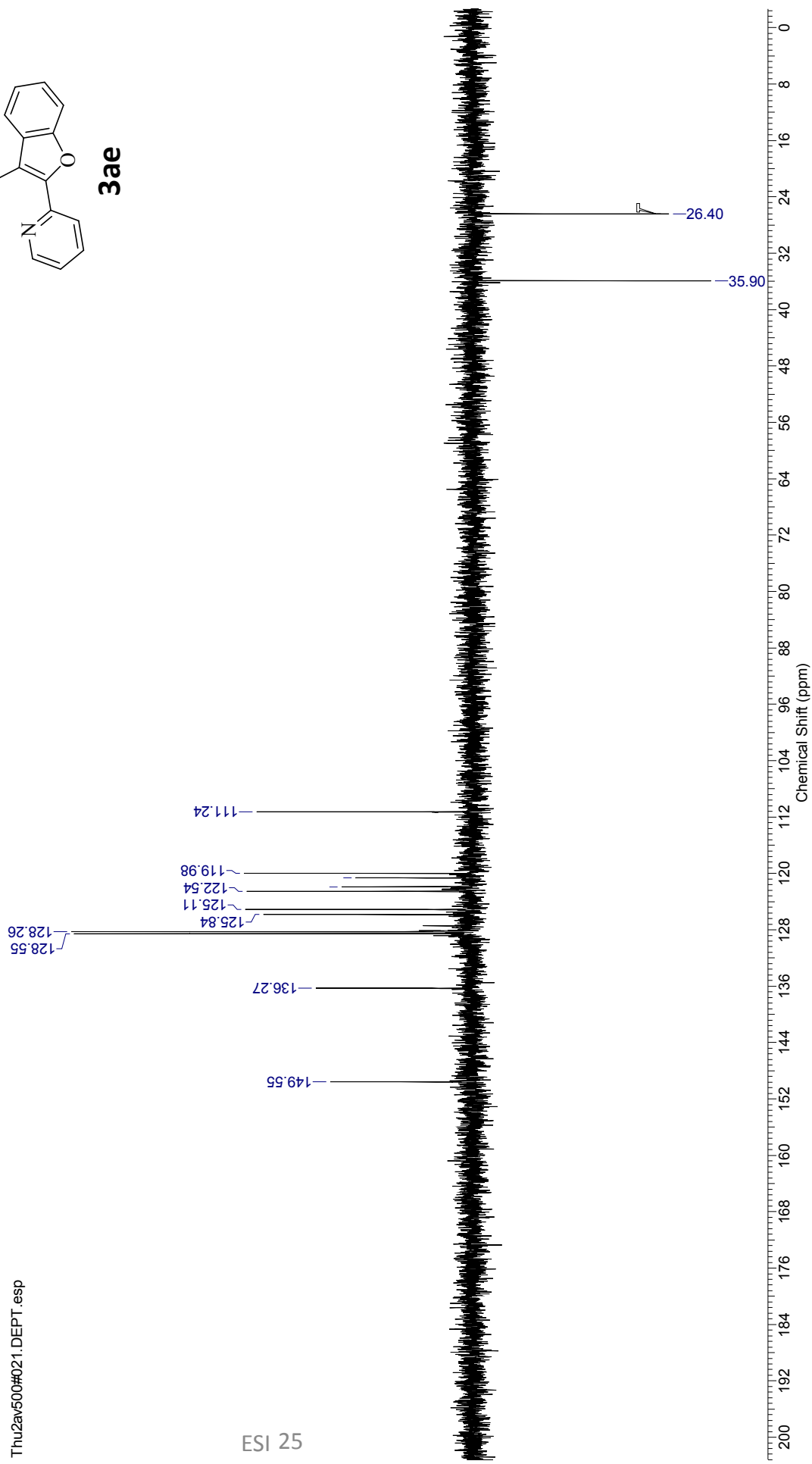
500 MHz, CDCl₃



3ae

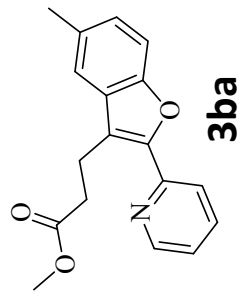
Thu2av500#021.DEPT.esp

ESI 25



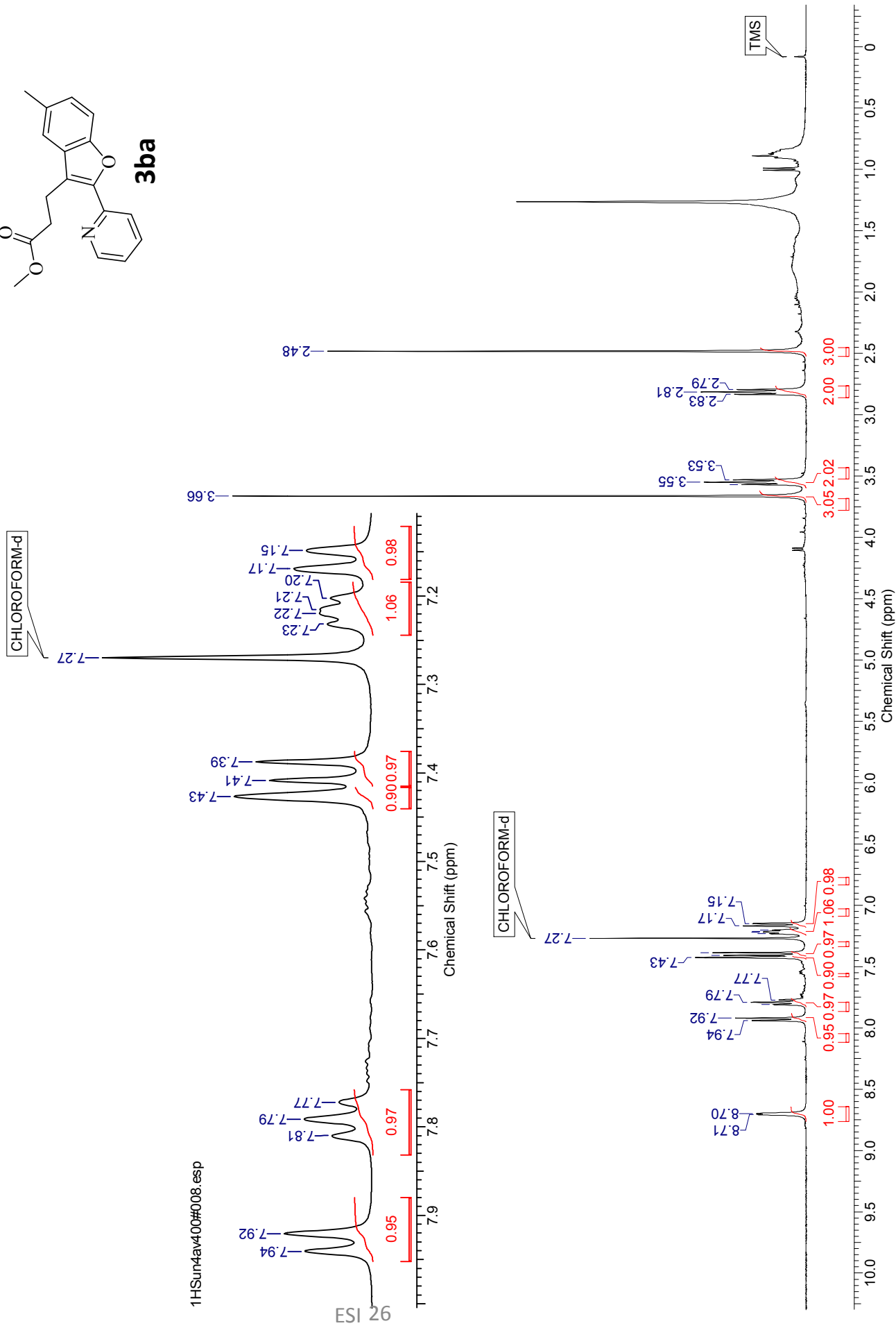
1HSun4av400#008.esp

400 MHz, CDCl₃

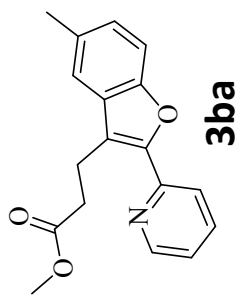


3ba

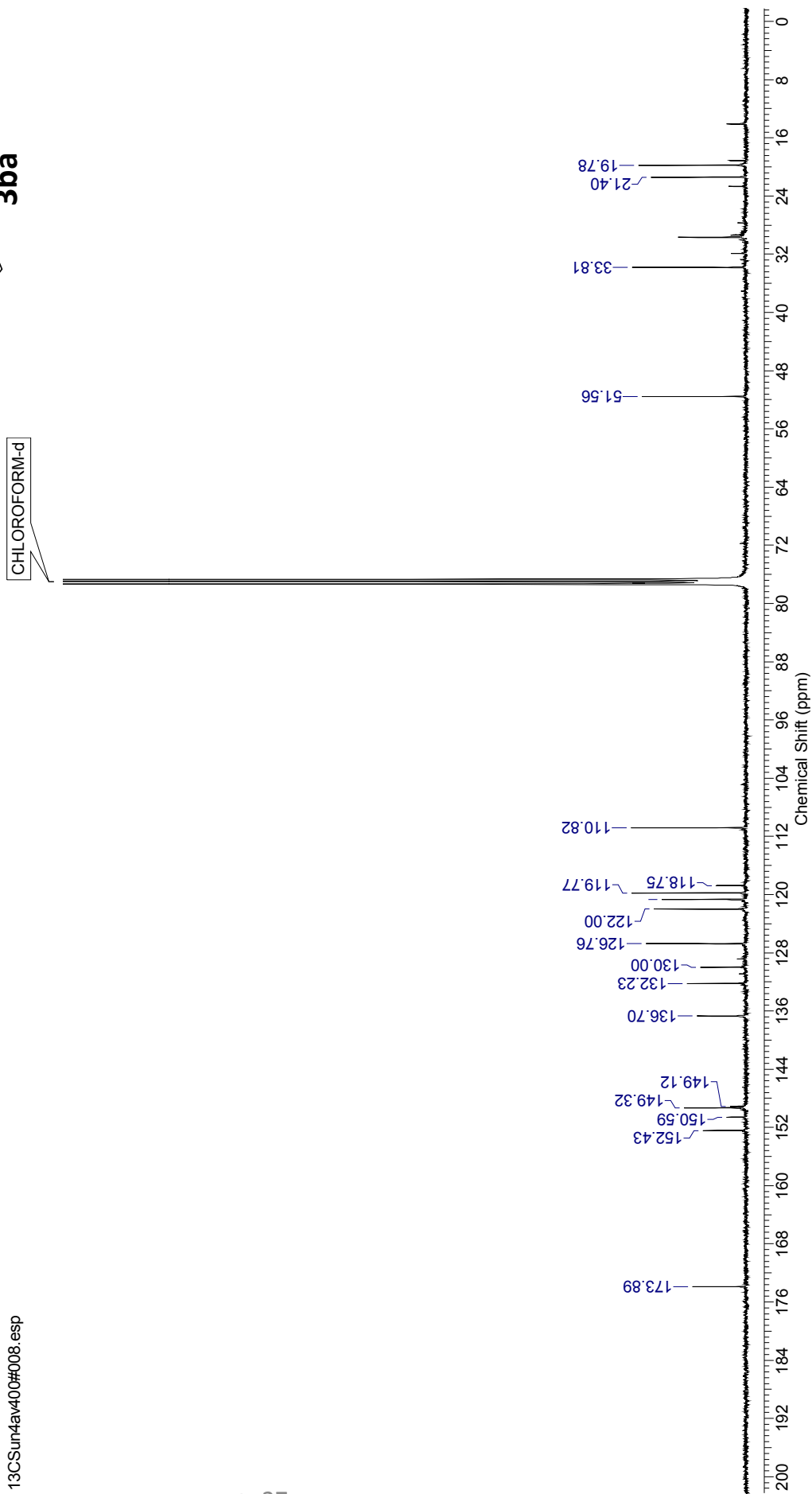
1HSun4av400#008.esp



400 MHz, CDCl₃

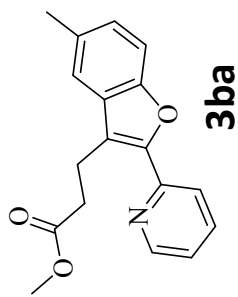


13CSun4av400#008.esp



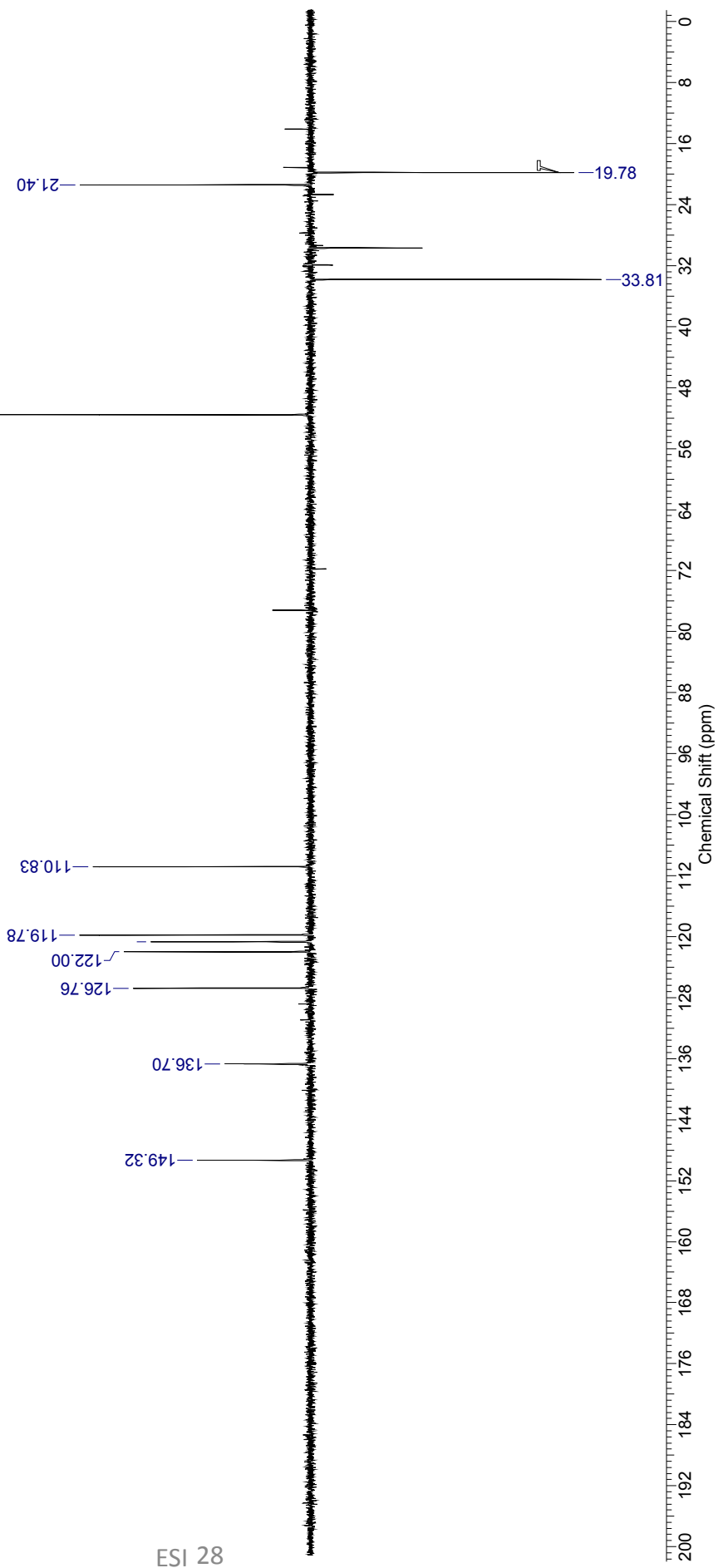
ESI 27

400 MHz, CDCl₃

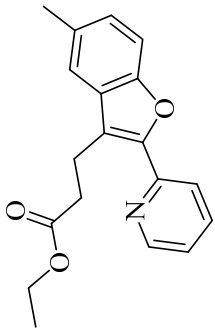


DEPTSun4av400#008.esp

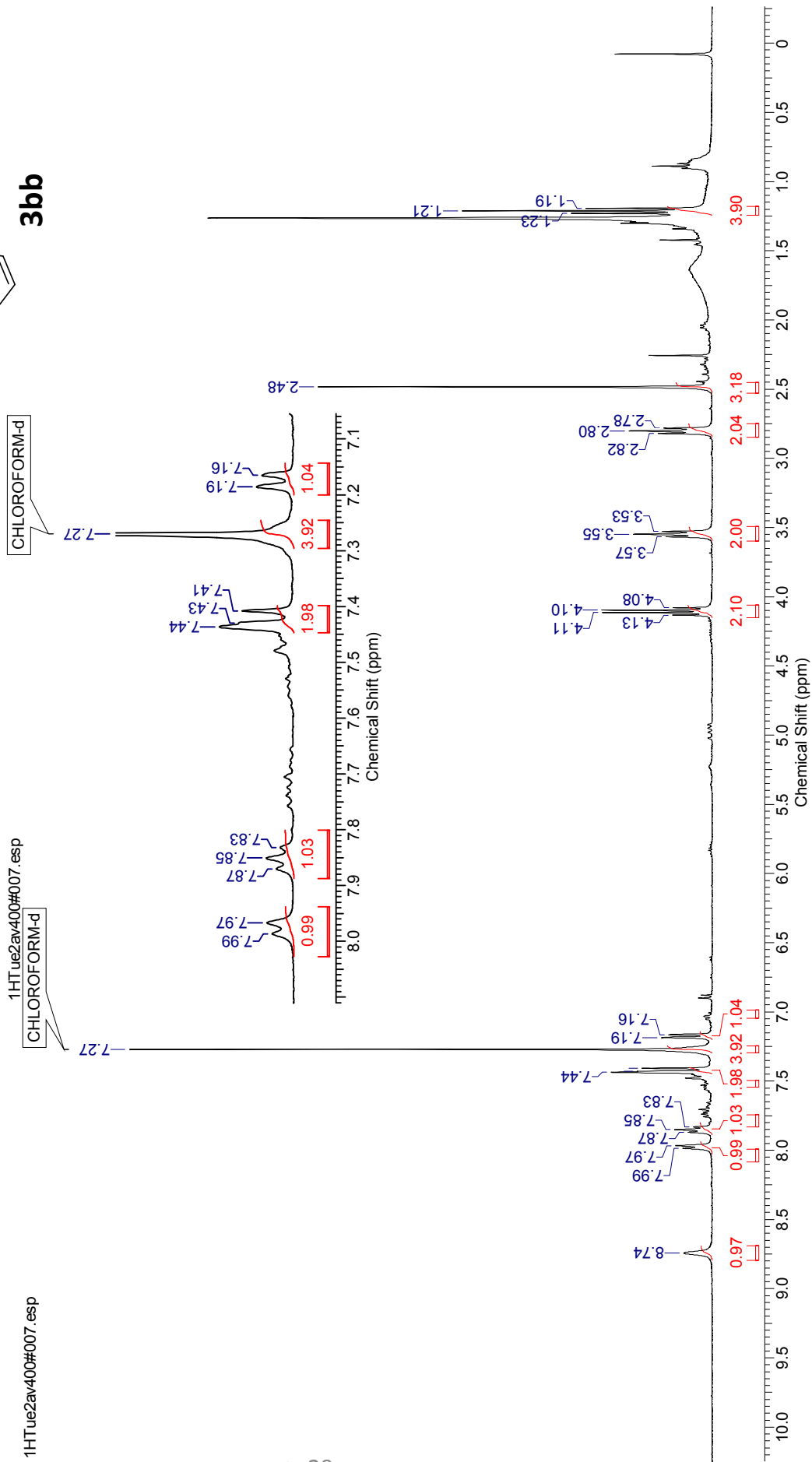
ESI 28



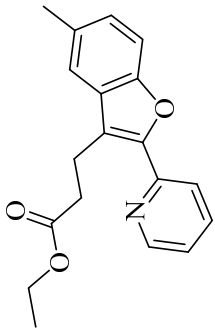
400 MHz, CDCl₃



3bb



400 MHz, CDCl₃

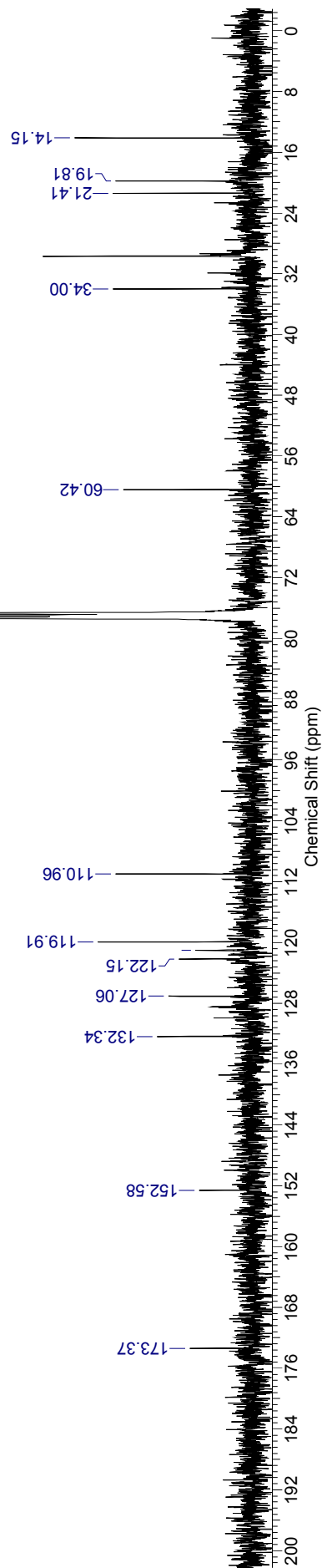


3bb

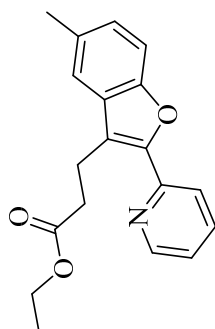
13CTue2av400#007r.esp

CHLOROFORM-d

ESI 30



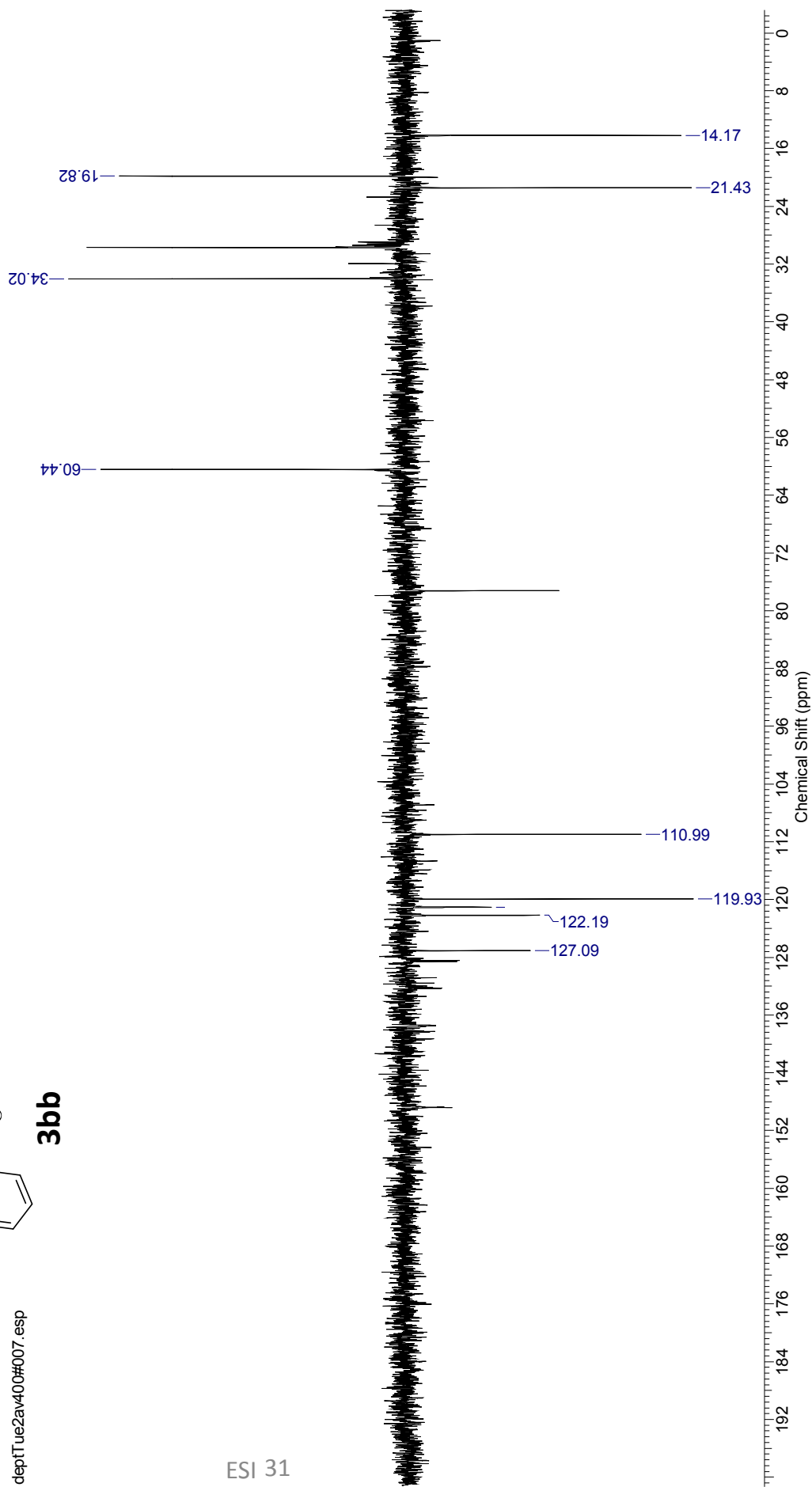
400 MHz, CDCl₃



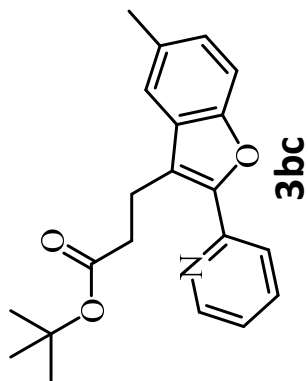
3bb

deptTue2av400#007.esp

ESI 31

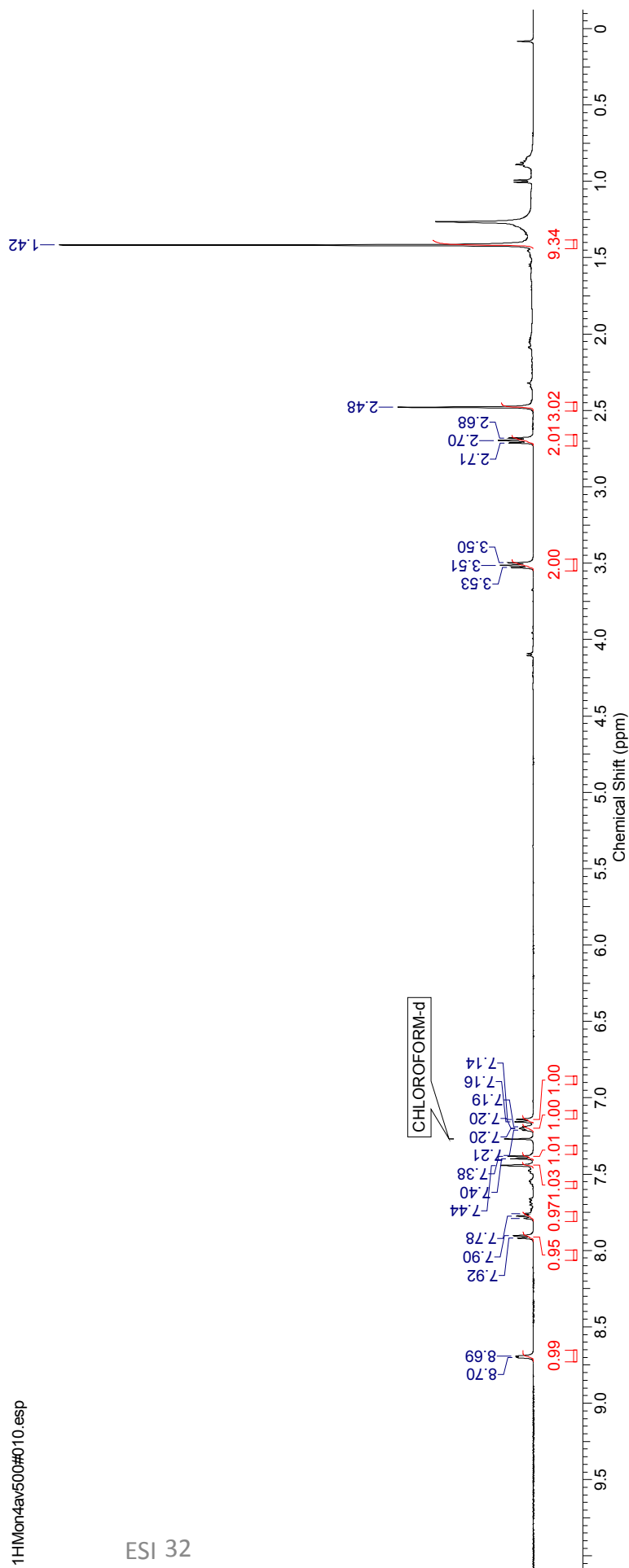


500 MHz, CDCl₃

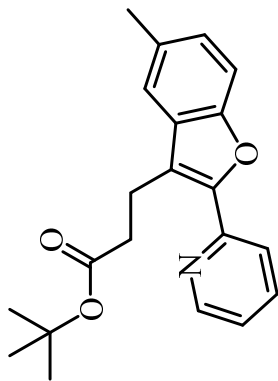


1HMon4av500#010.esp

ESI 32



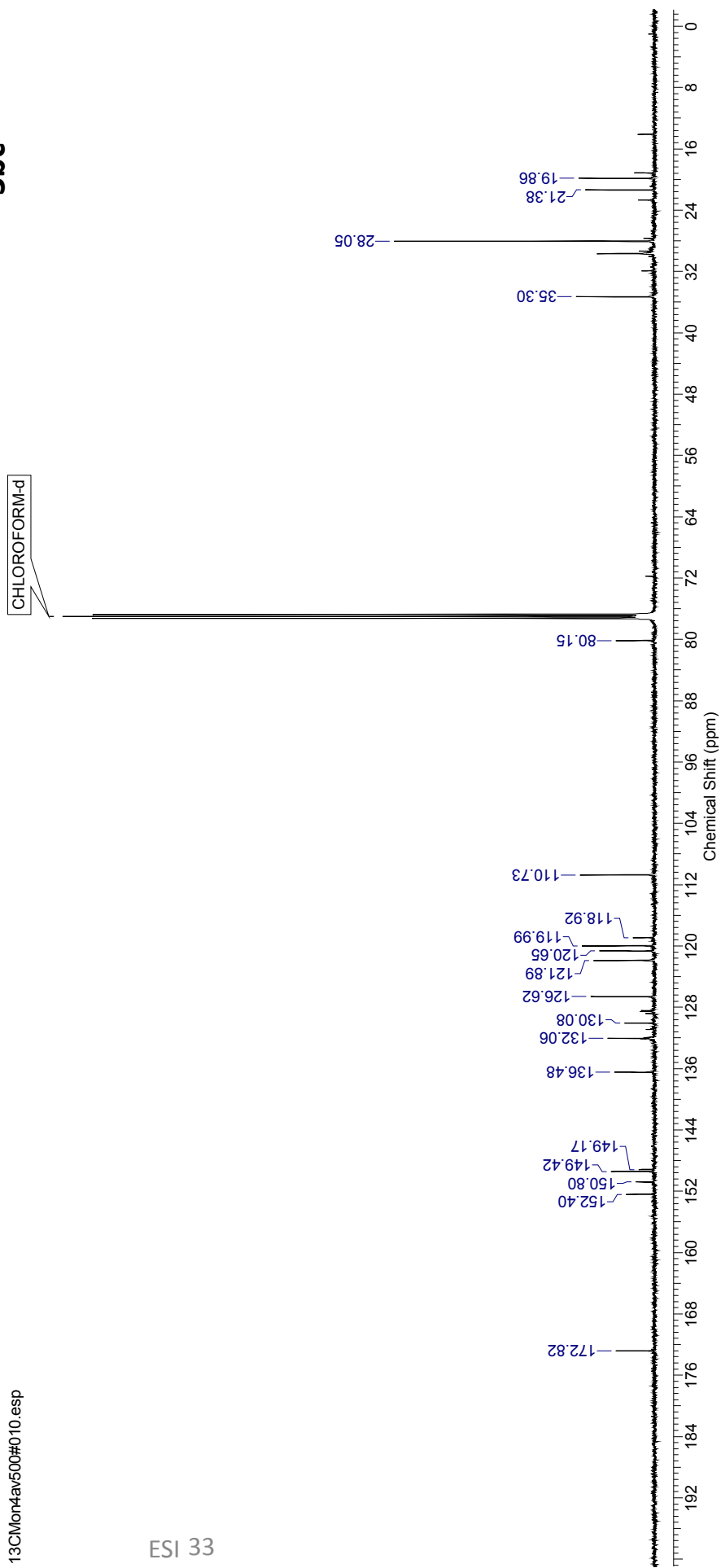
500 MHz, CDCl₃



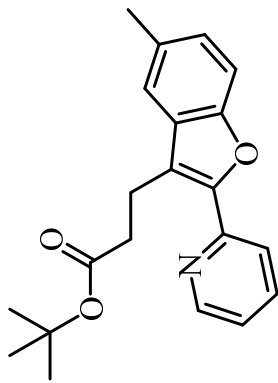
3bc

13CMon4av500#010.esp

ESI 33



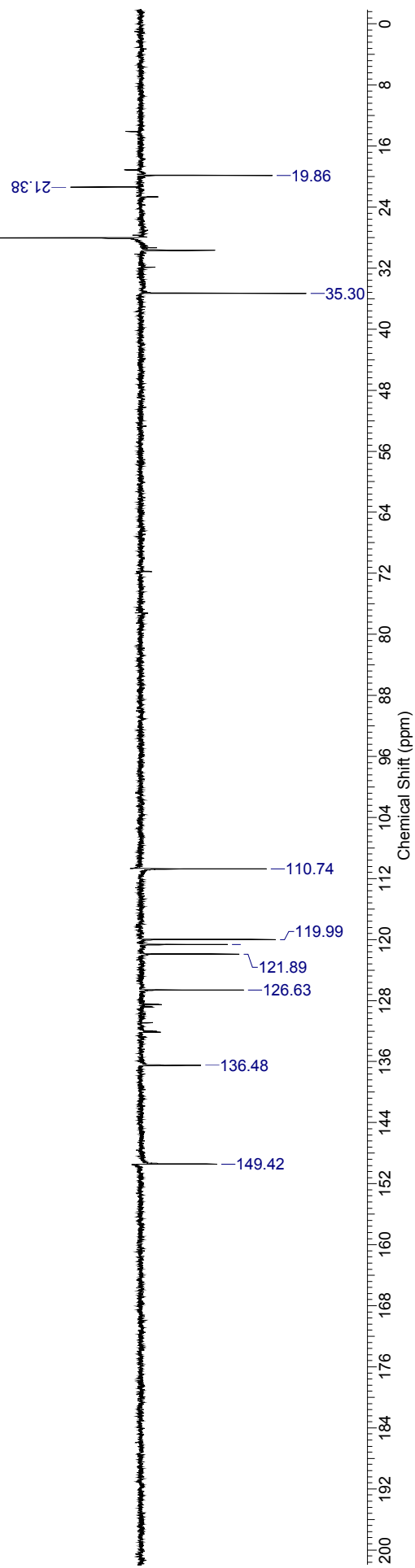
500 MHz, CDCl₃



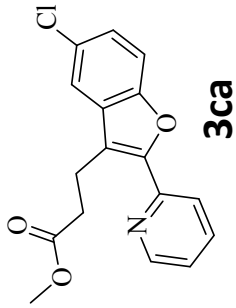
3bc

deptMon4av500#010_1r.esp

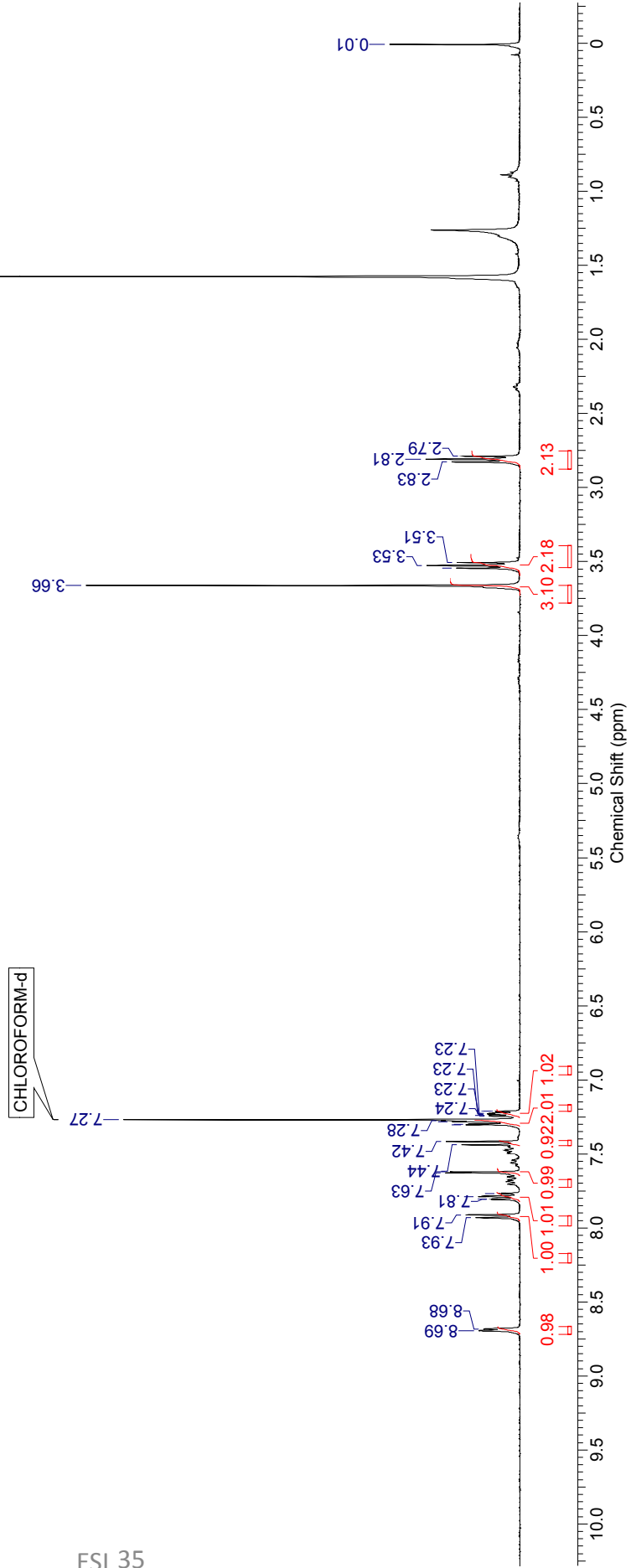
ESI 34



400 MHz, CDCl₃

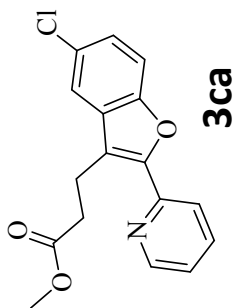


1HWed5av400#009.1r.esp



ESI 35

400 MHz, CDCl₃

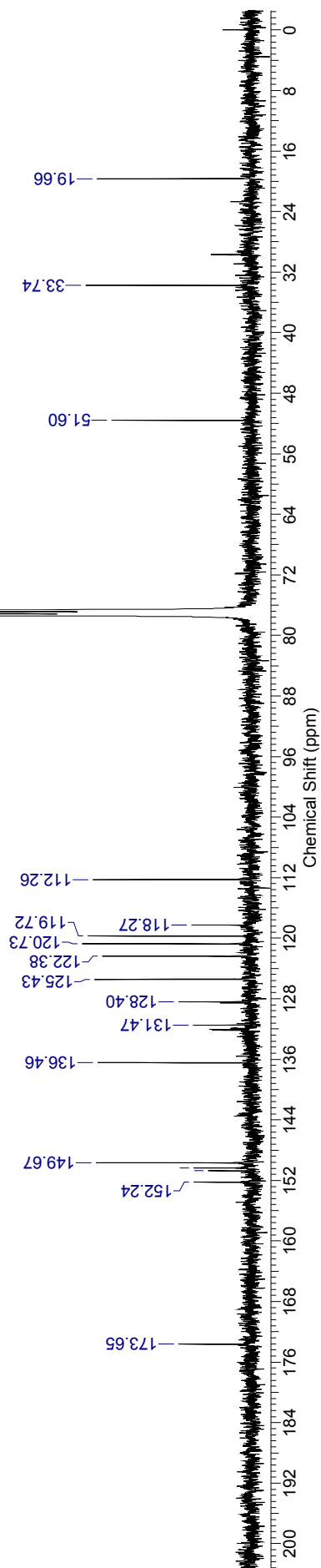


3ca

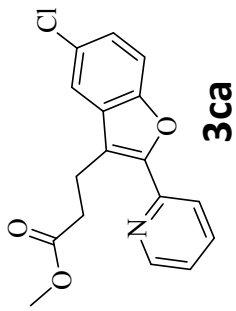
Wed5av400#009.1r.esp

CHLOROFORM-d

ESI 36

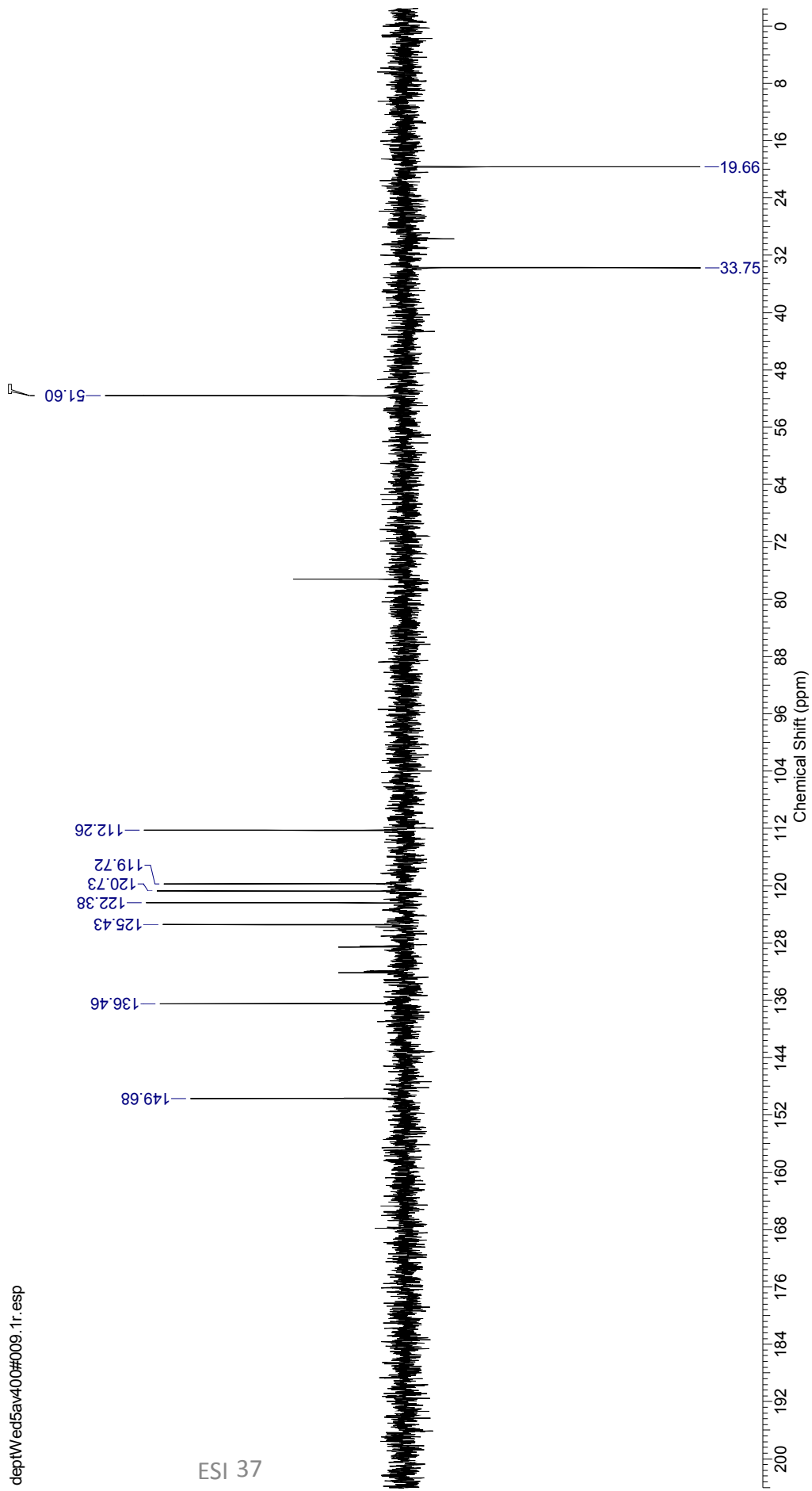


400 MHz, CDCl₃

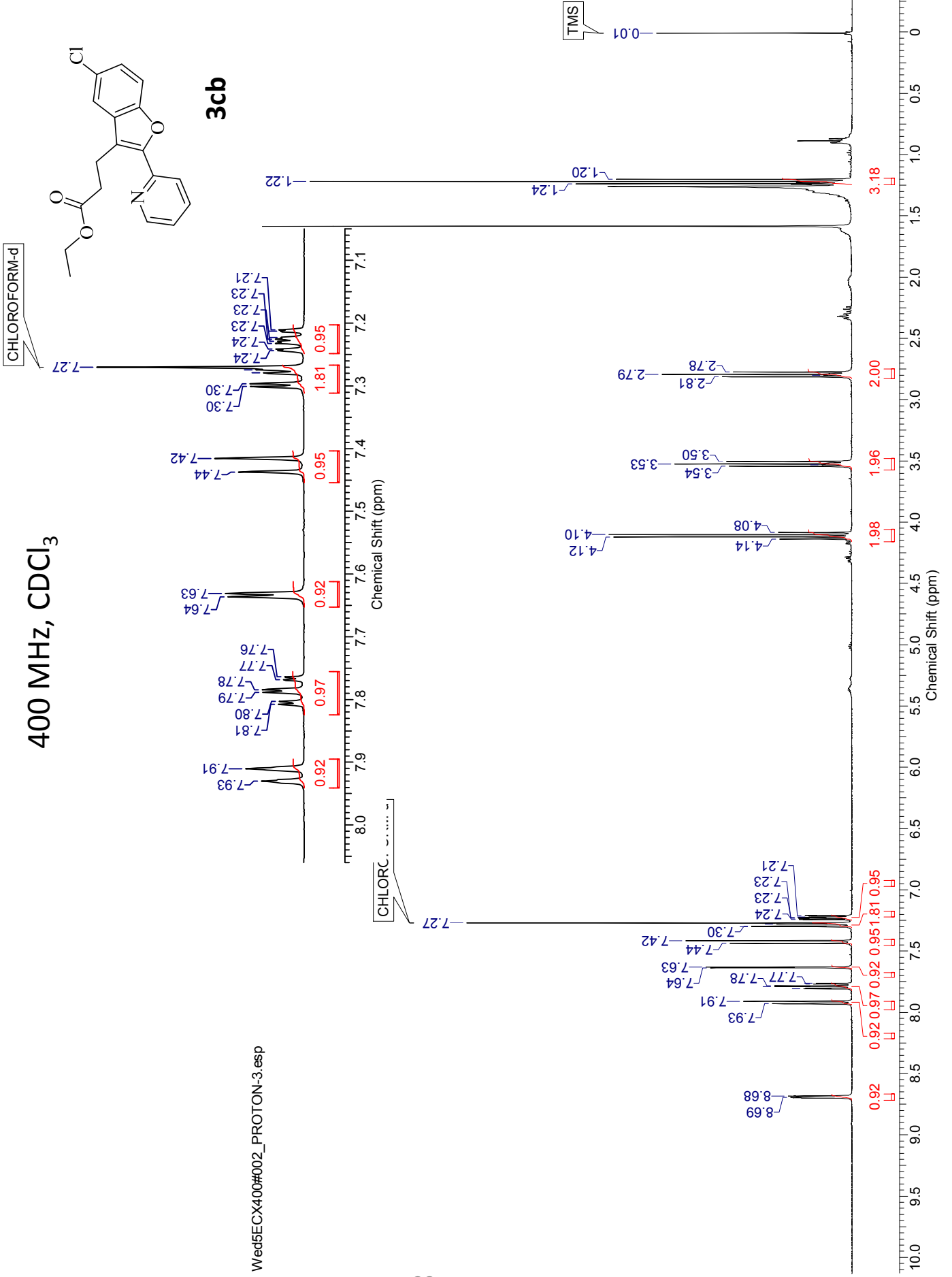


dep1W\ed5av40#009_1r.esp

ESI 37

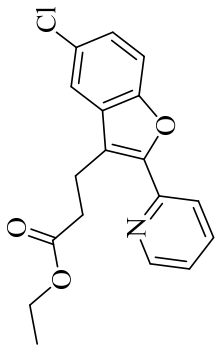


400 MHz, CDCl₃



Wed5ECX400#002_PROTON-3.esp

400 MHz, CDCl₃

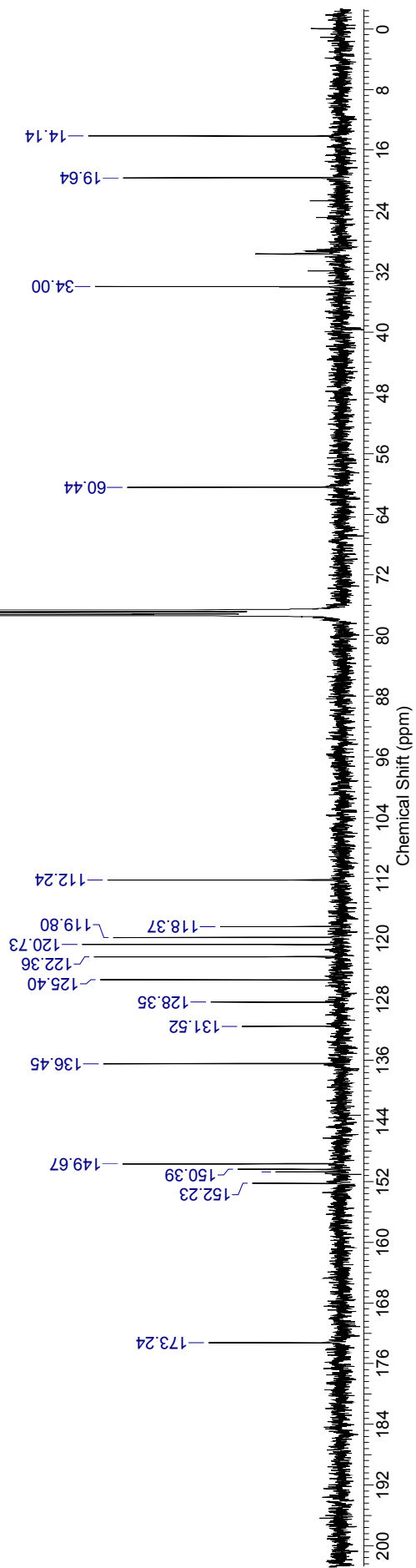


3cb

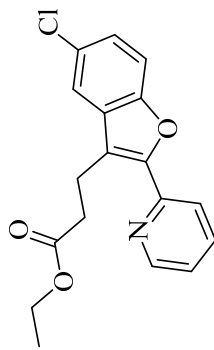
Wed5ECX400#002_CARBO-3.esp

CHLOROFORM-d

ESI 39



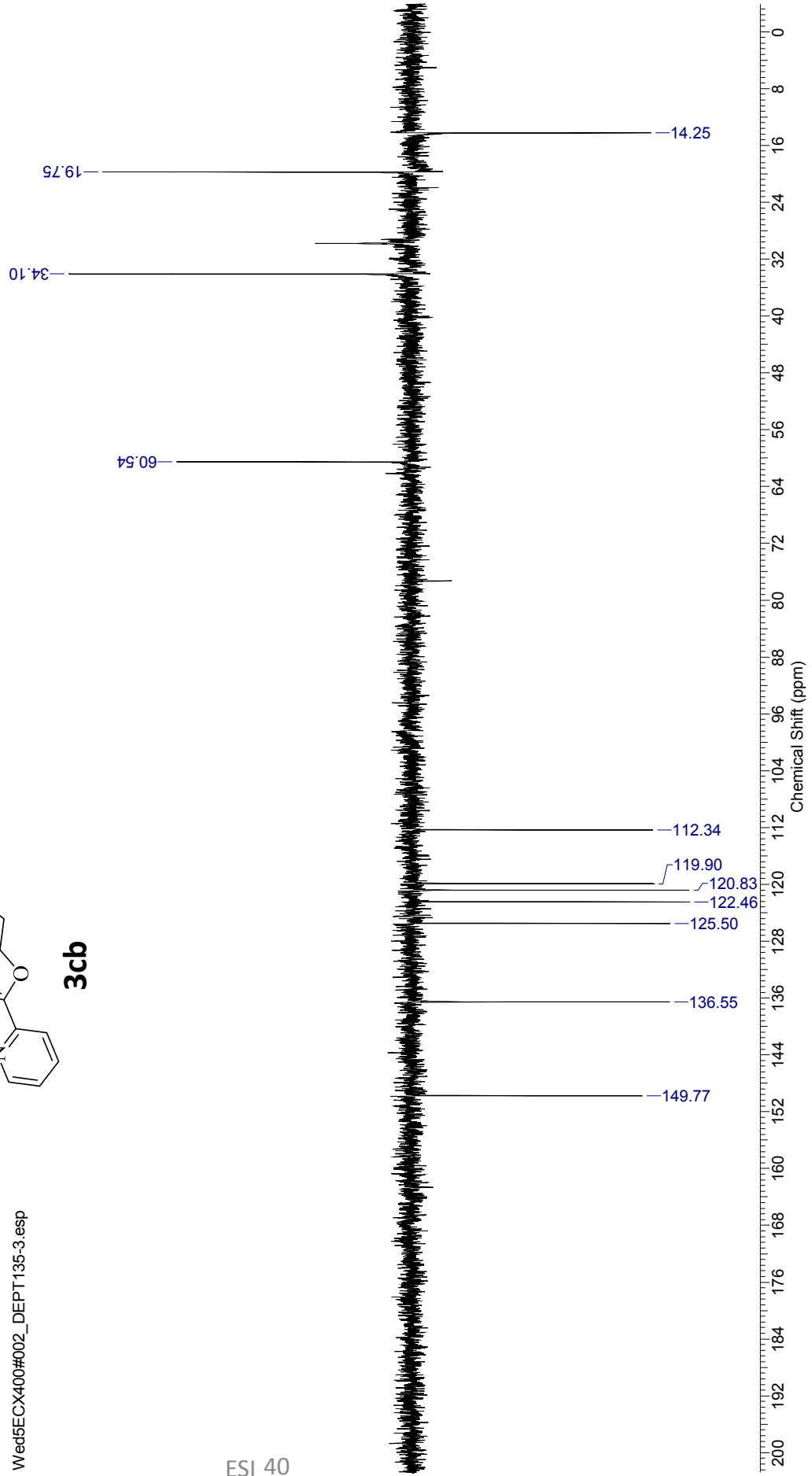
400 MHz, CDCl₃



3cb

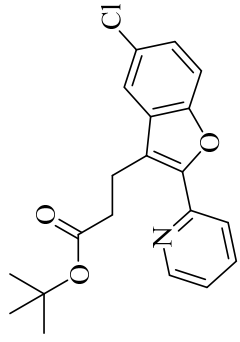
Wed5ECX400#002_DEPT135-3.esp

ESI 40



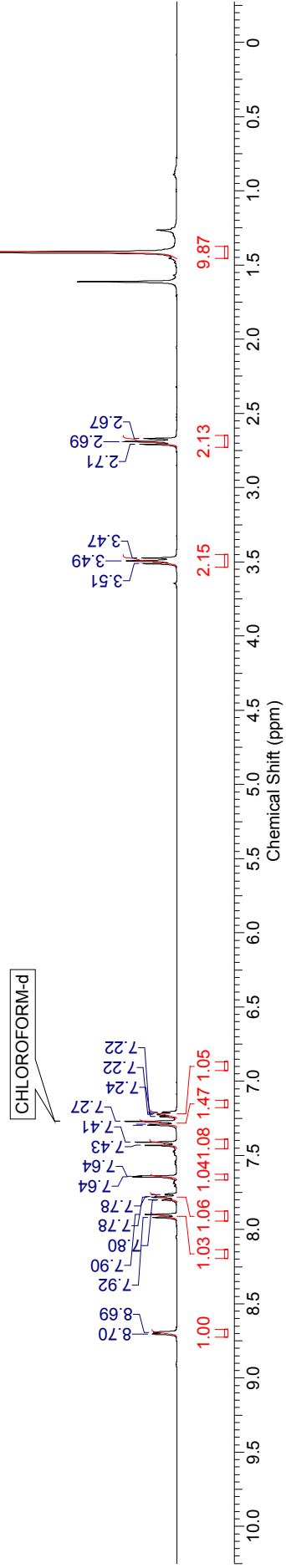
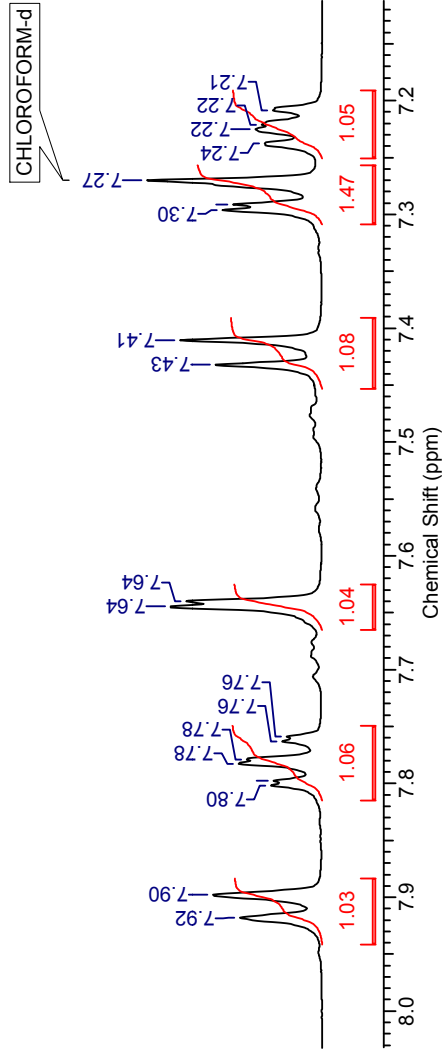
400 MHz, CDCl₃

1HThu4av400#005.esp

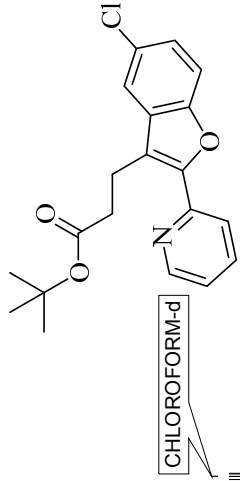


3cc

1HThu4av400#005.esp



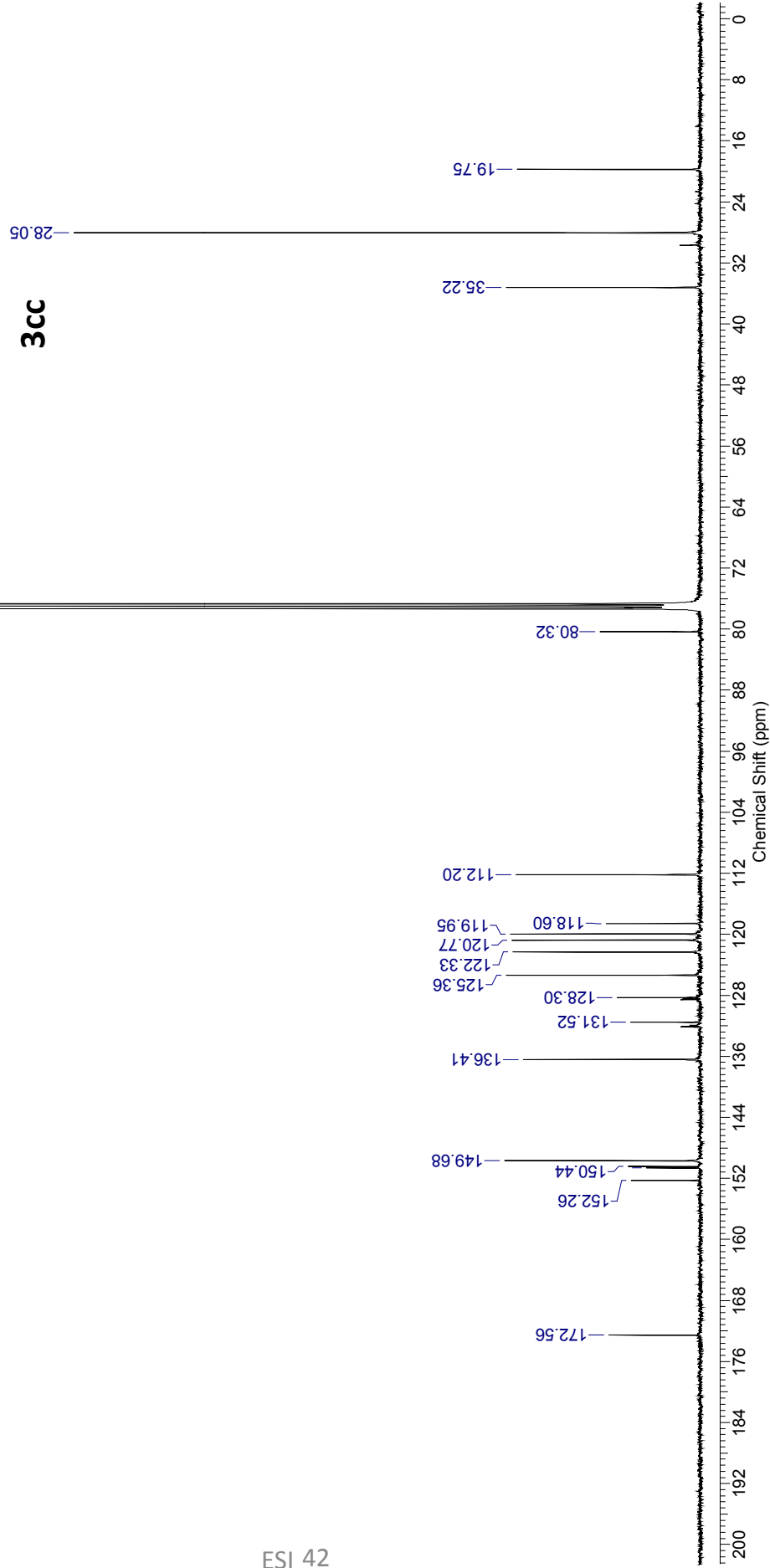
400 MHz, CDCl₃



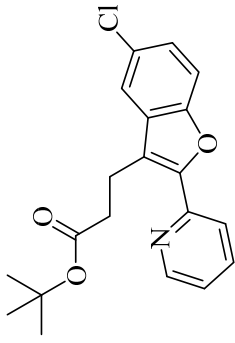
3cc

13CThu4v400#005.esp

ESI 42



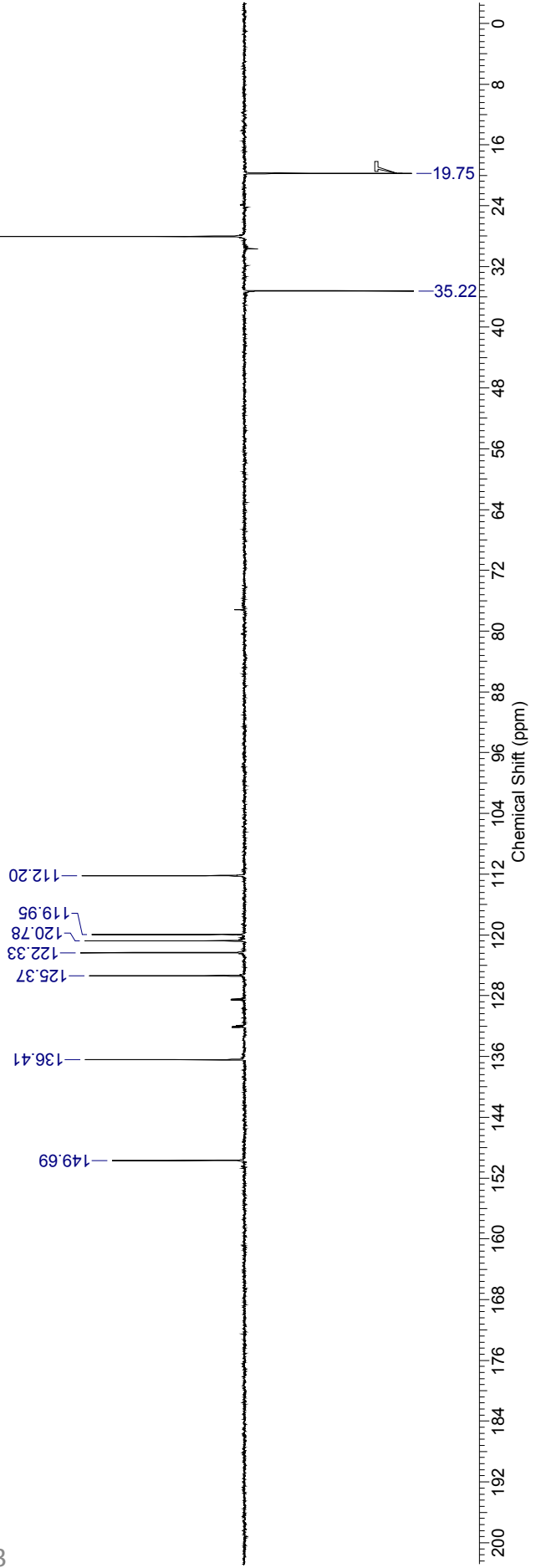
400 MHz, CDCl₃



3cc

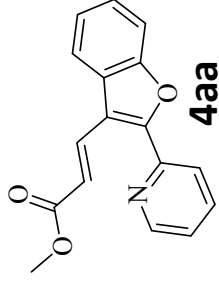
deptThu4v400#005.esp

ESI 43

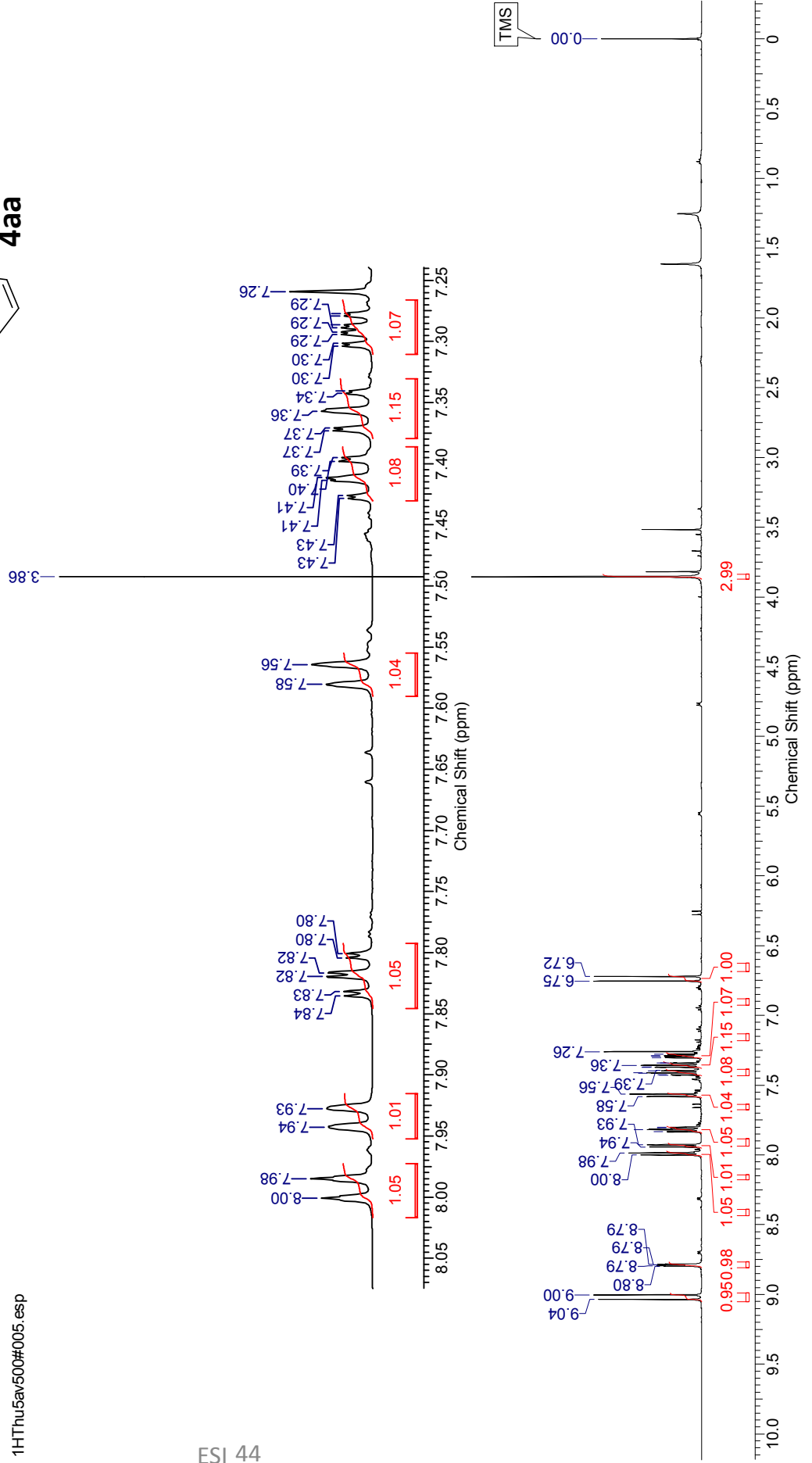


500 MHz, CDCl₃

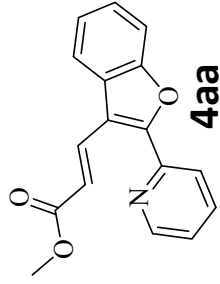
1HThu5av500#005.esp



1HThu5av500#005.esp

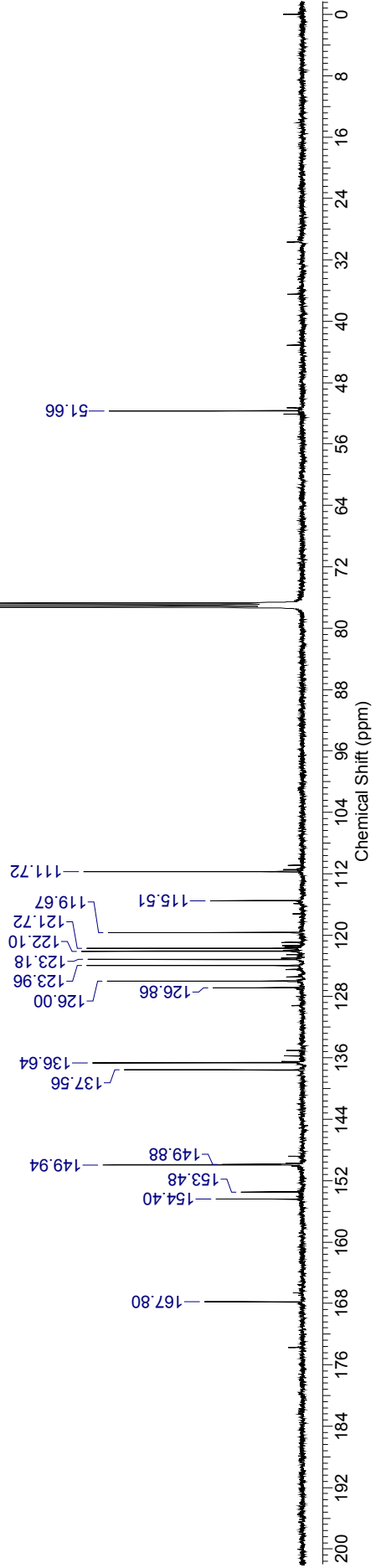


500 MHz, CDCl₃



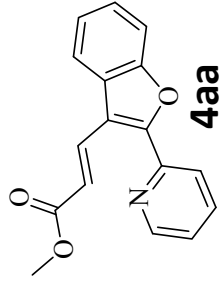
13CThu5av500#005.esp

CHLOROFORM-d



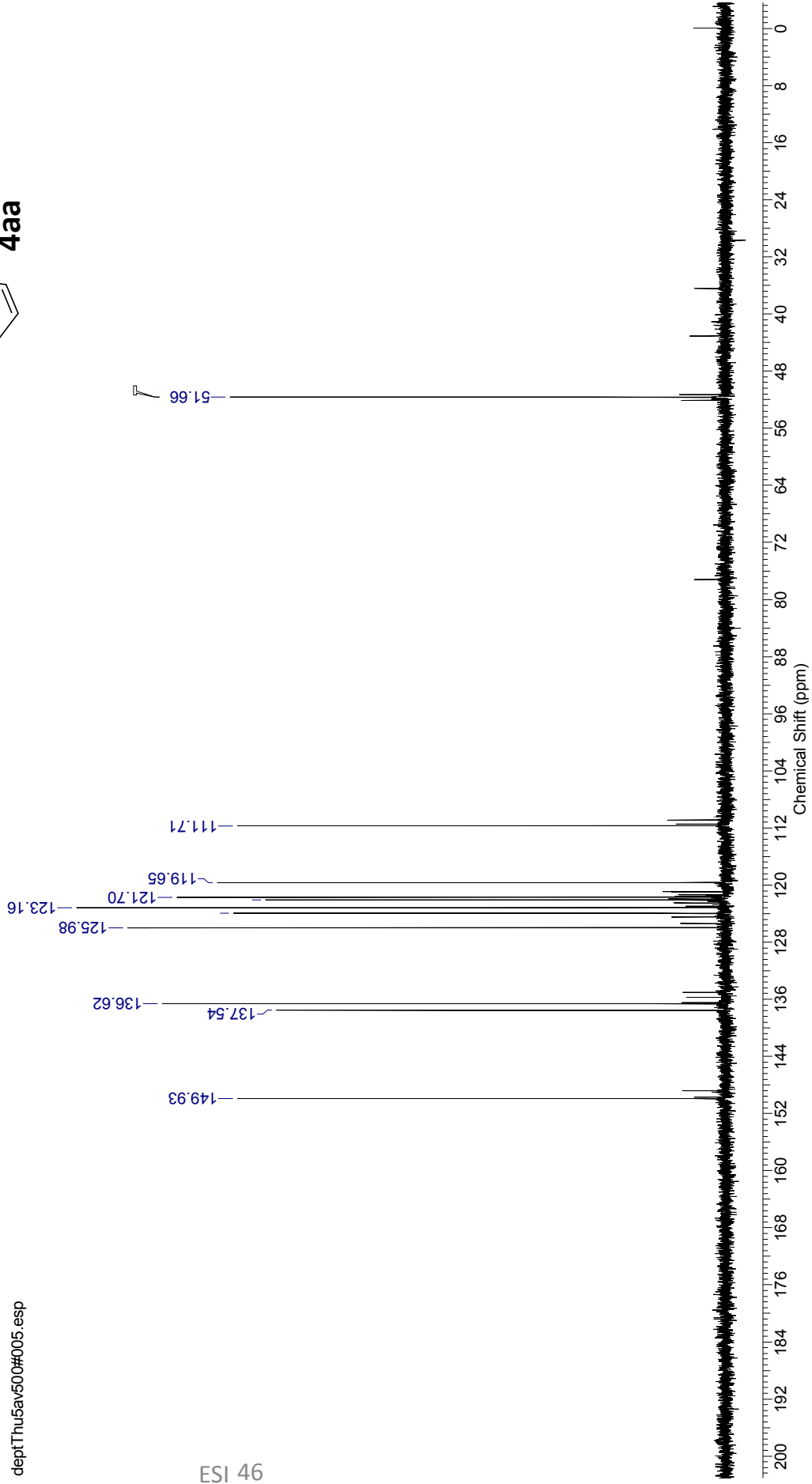
ESI 45

500 MHz, CDCl₃

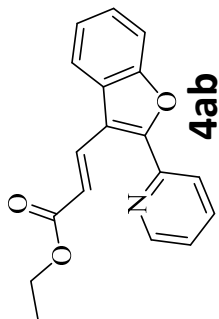


deptThu5av500#005.esp

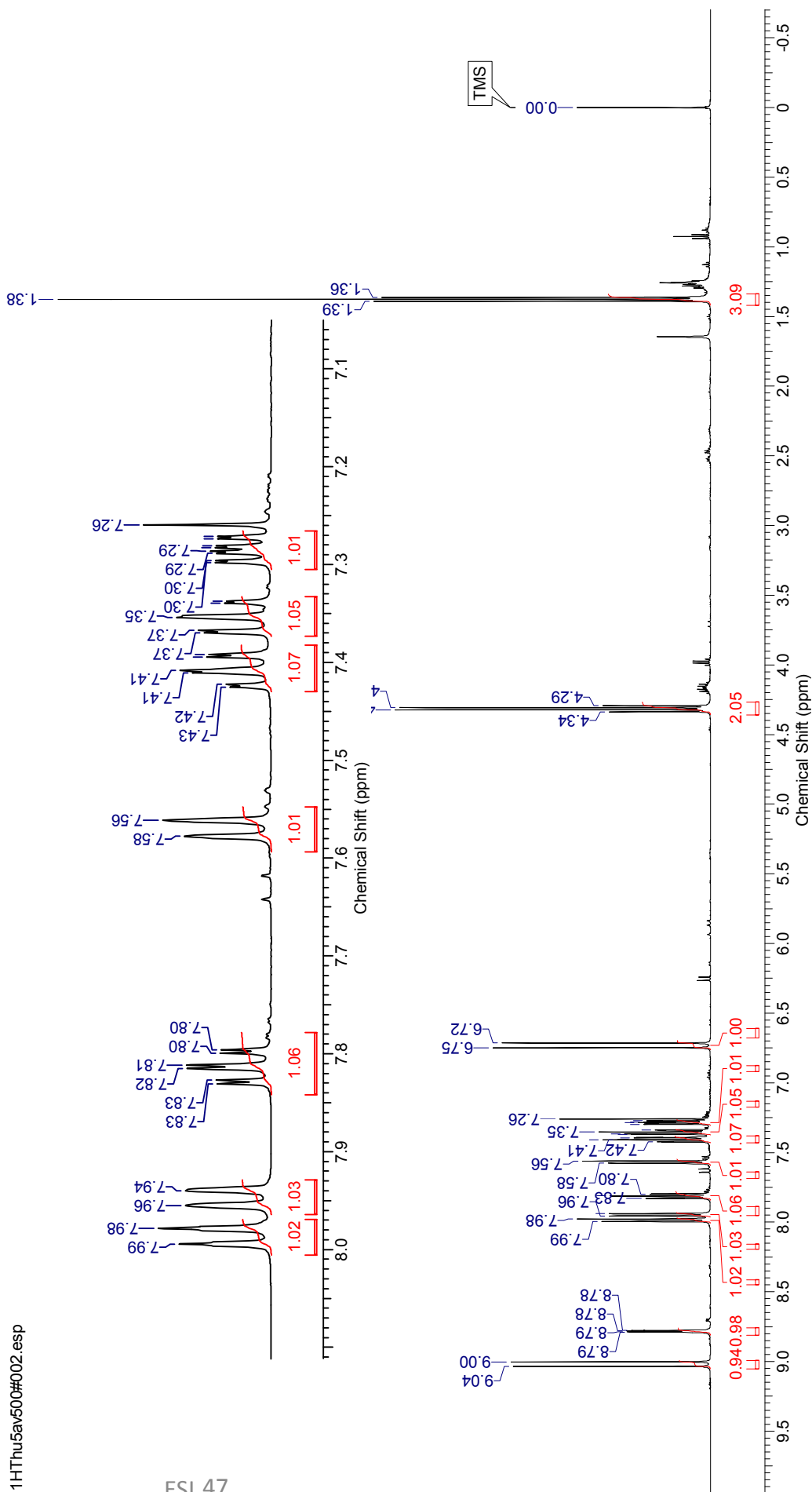
ESI 46



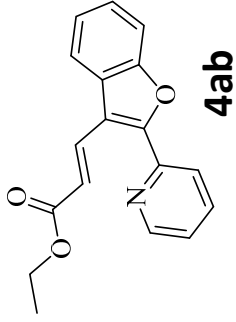
500 MHz, CDCl₃



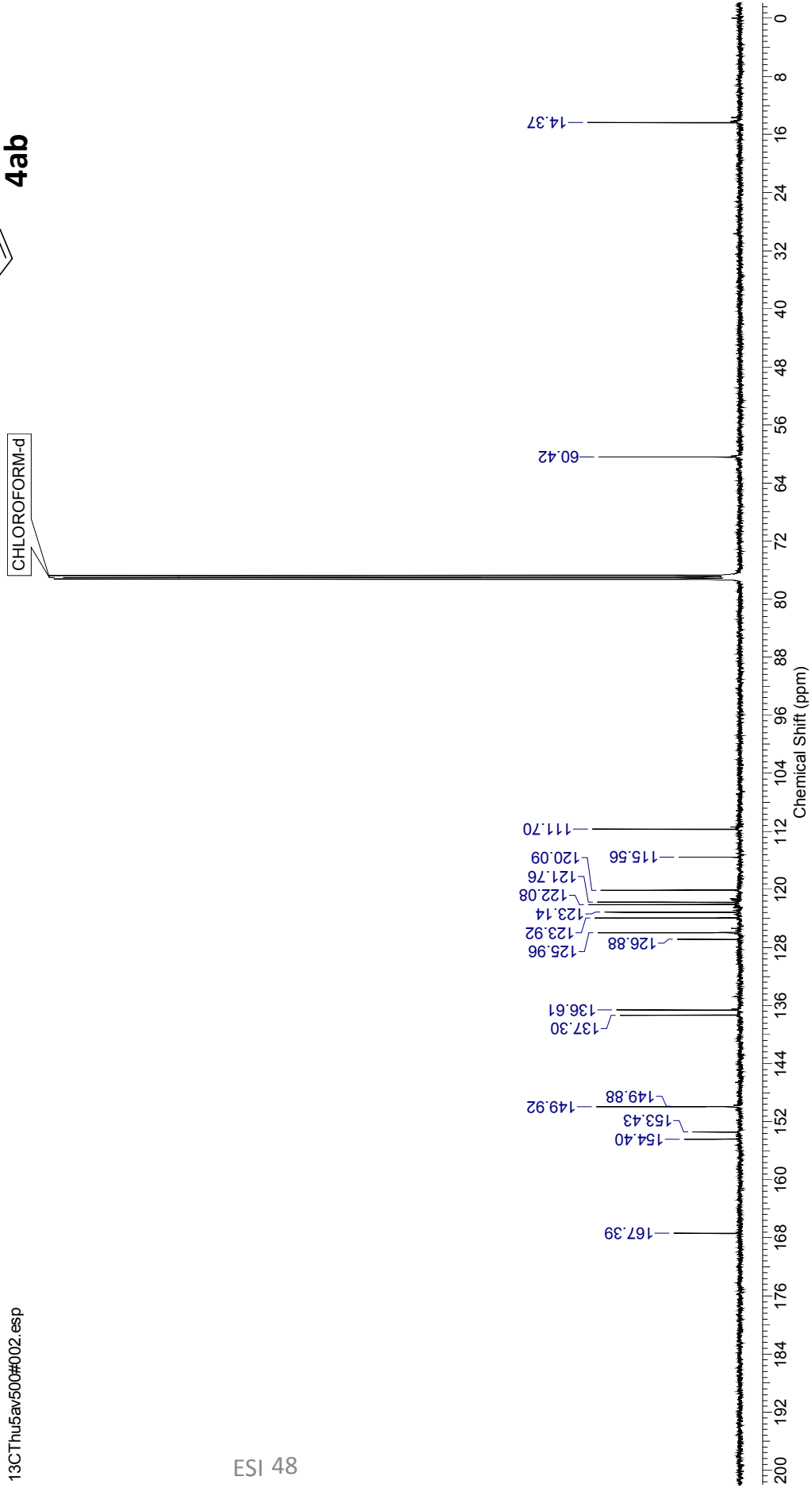
1HThu5av500#002.esp



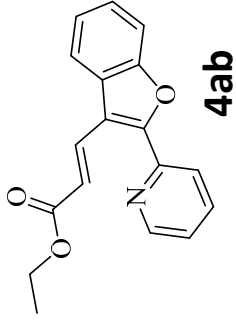
500 MHz, CDCl₃



13CThu5av500#002.esp

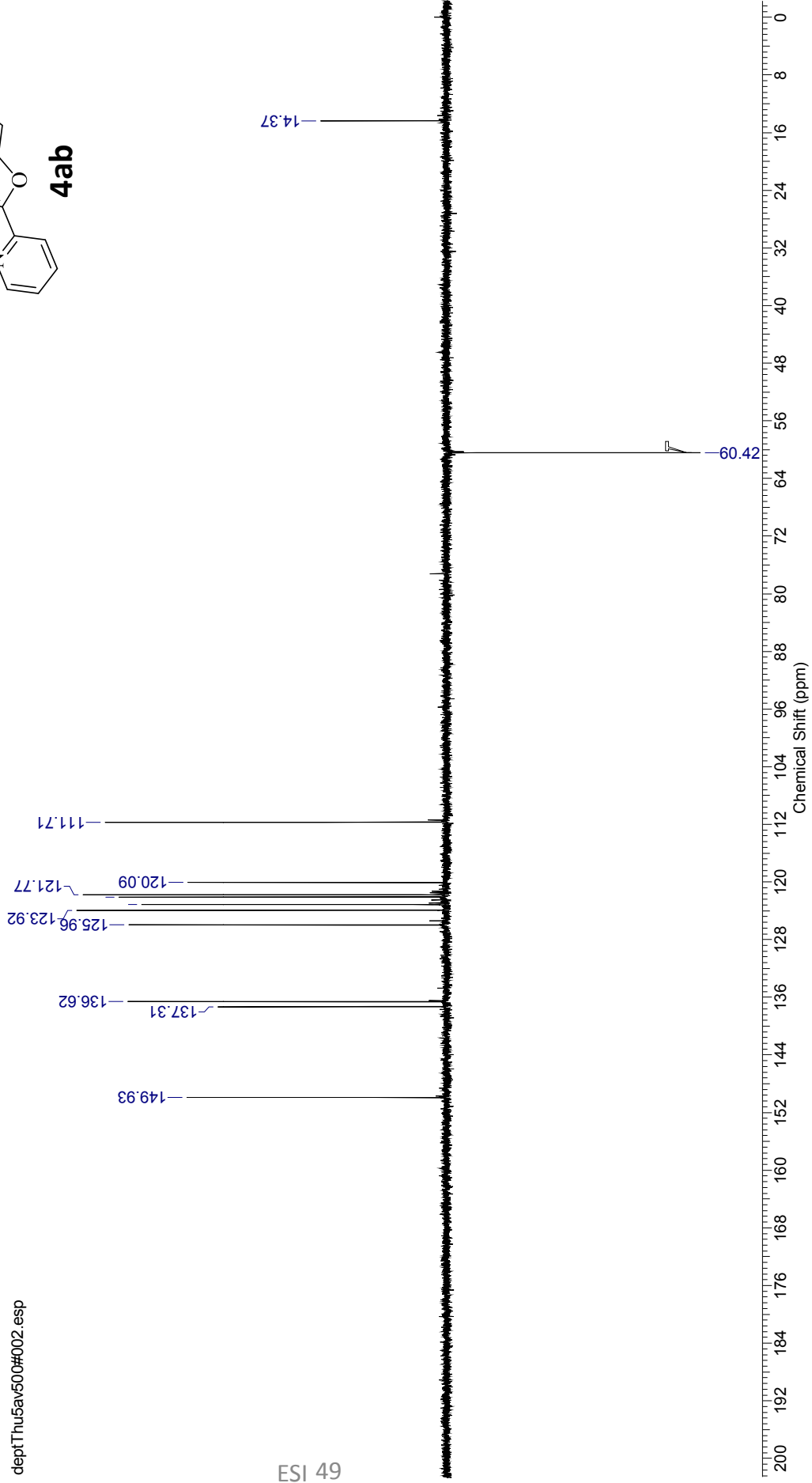


500 MHz, CDCl₃

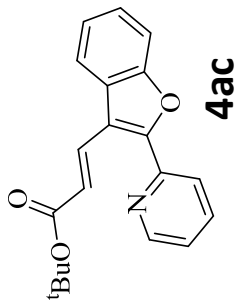


deptThu5av500#002.esp

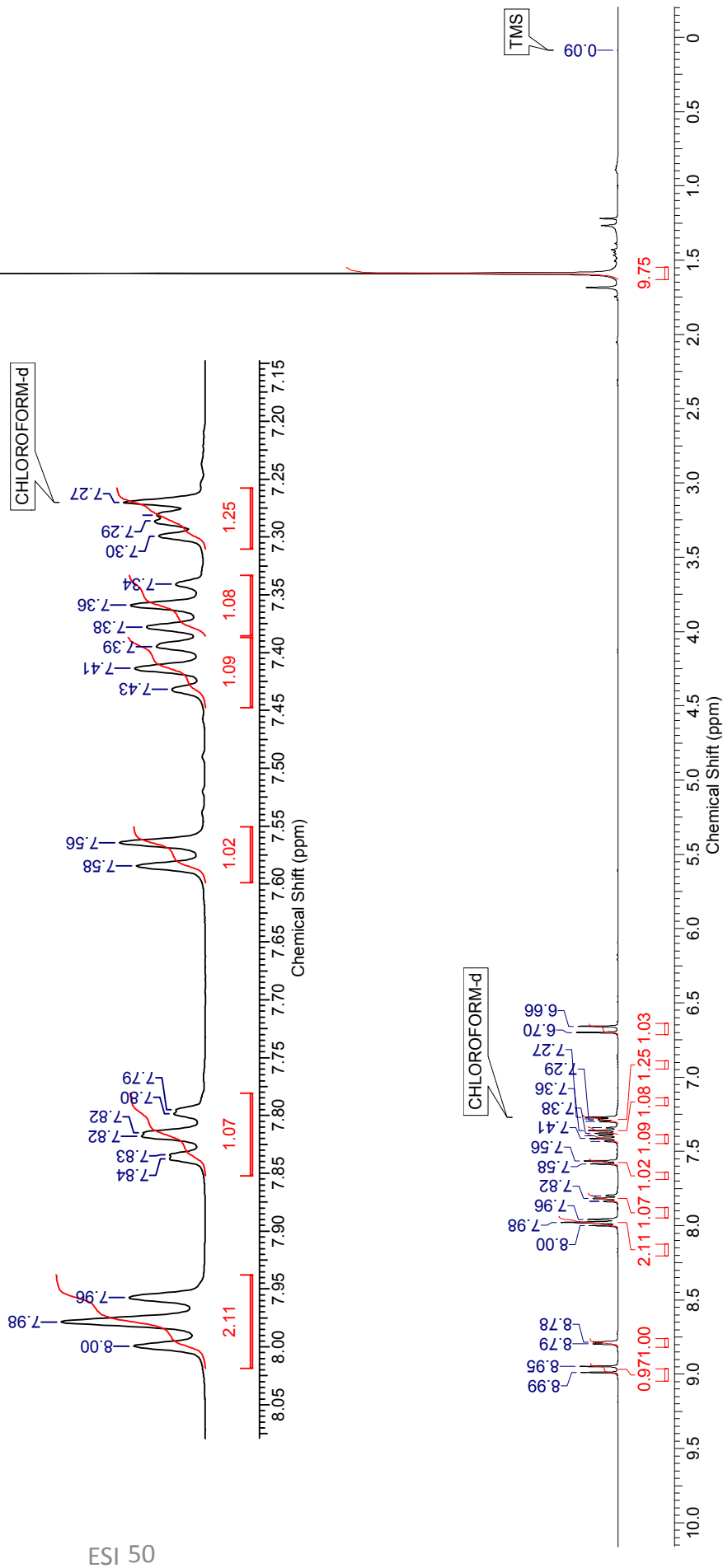
64 ISI



400 MHz, CDCl₃

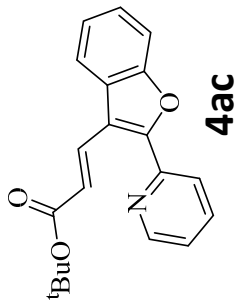


1HFrI5av400#006.esp

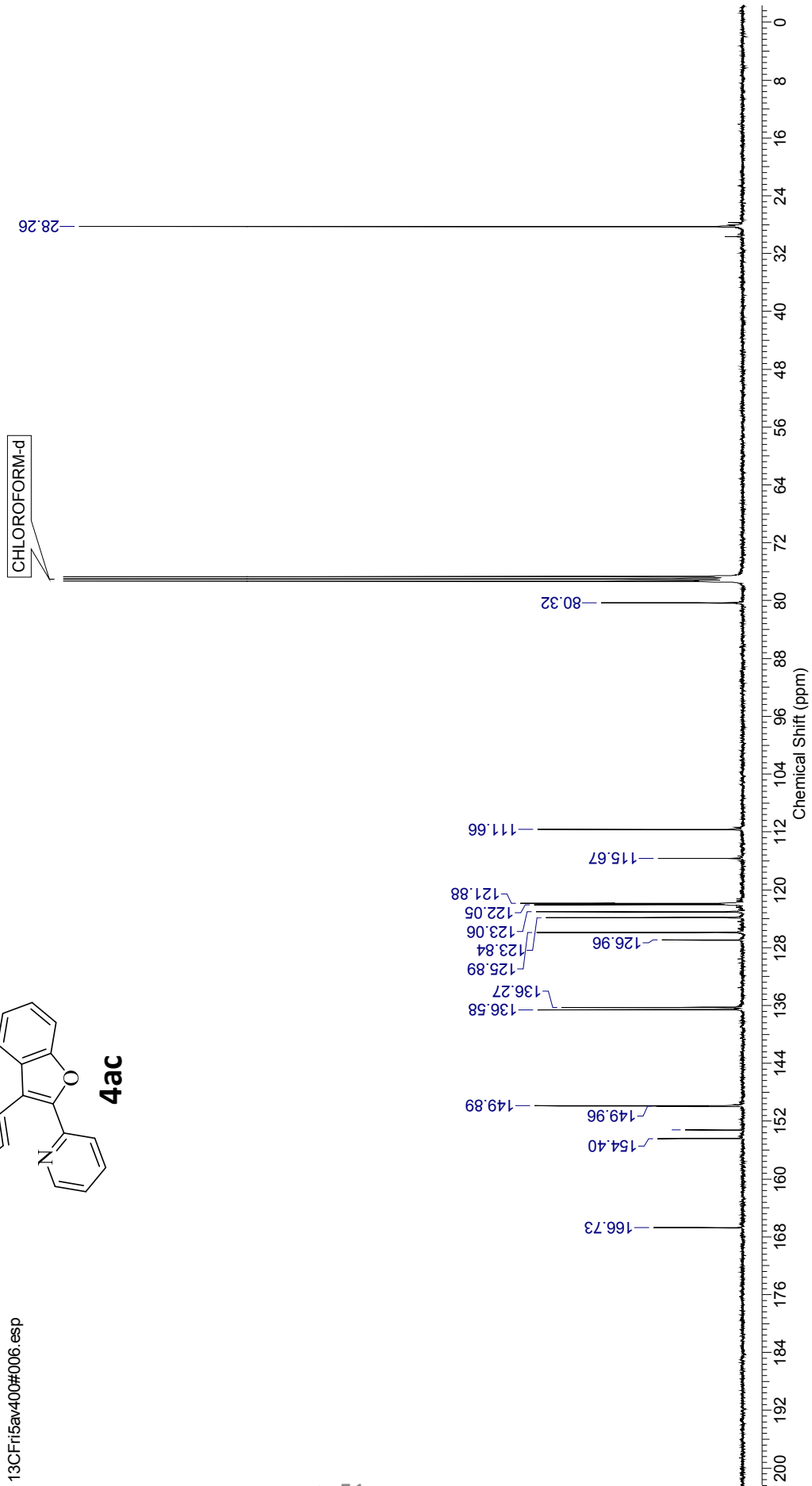


ESI 50

400 MHz, CDCl₃

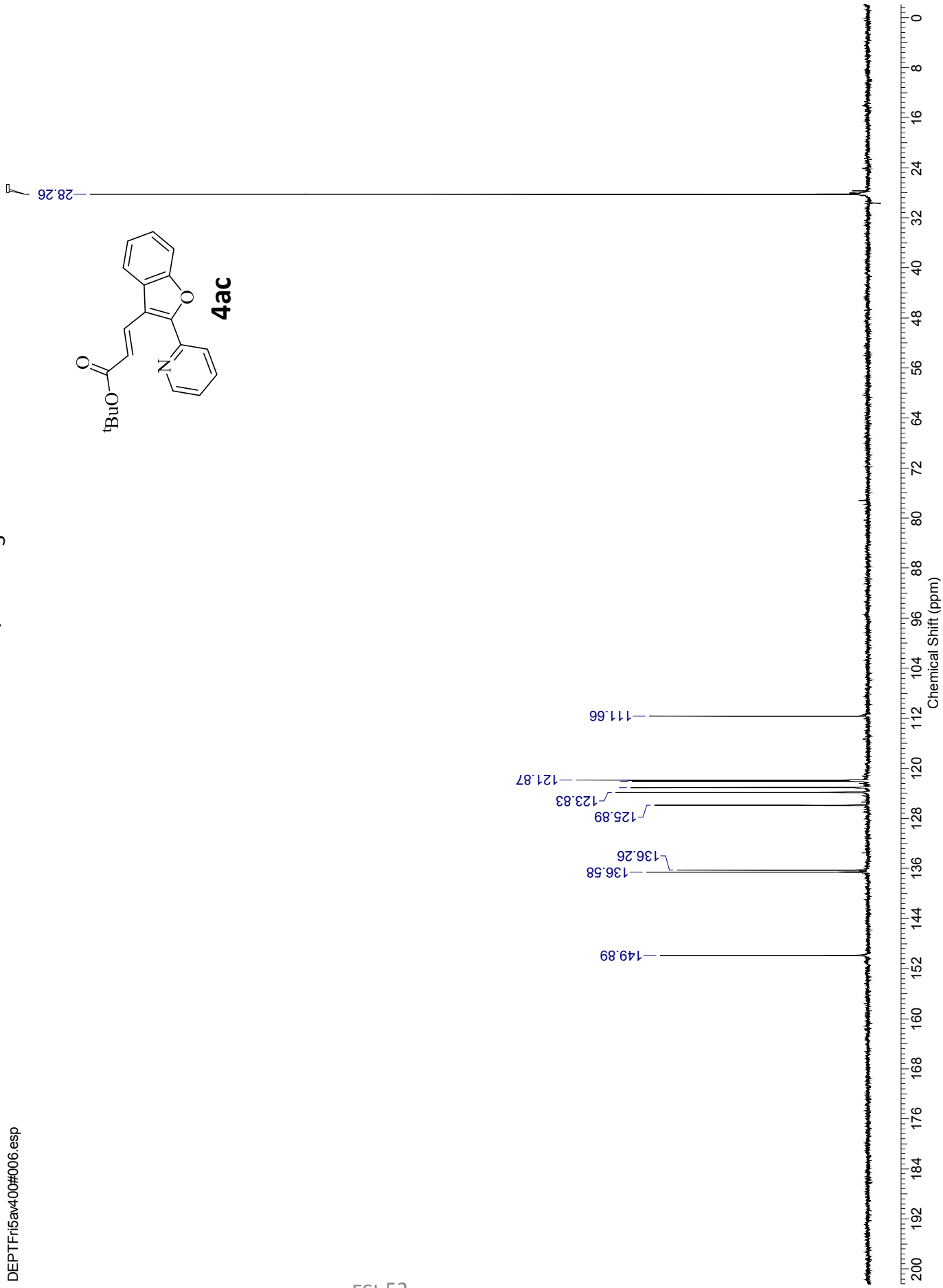
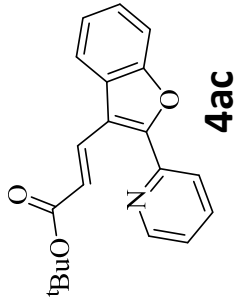


13CFri5av400#006.esp



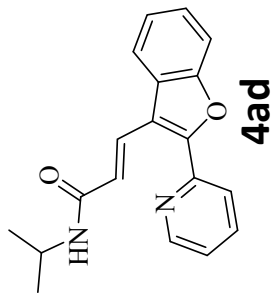
400 MHz, CDCl₃

DEPTF15av400#006.esp



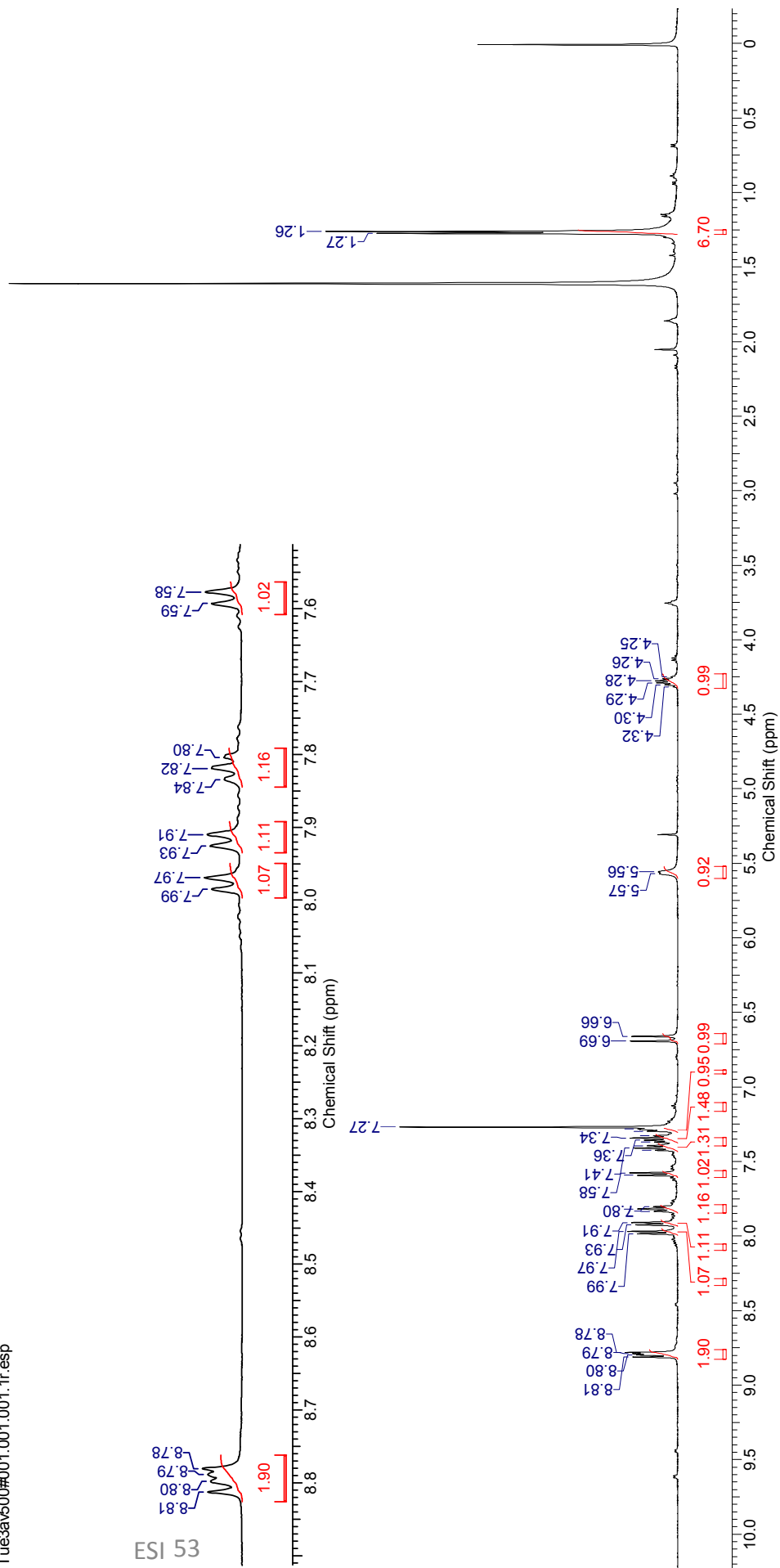
500 MHz, CDCl₃

Tue3av500#001.001.001.1r.esp

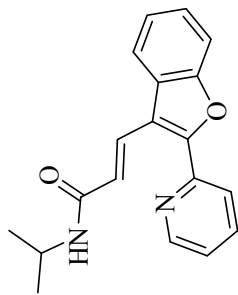


Tue3av500#001.001.001.1r.esp

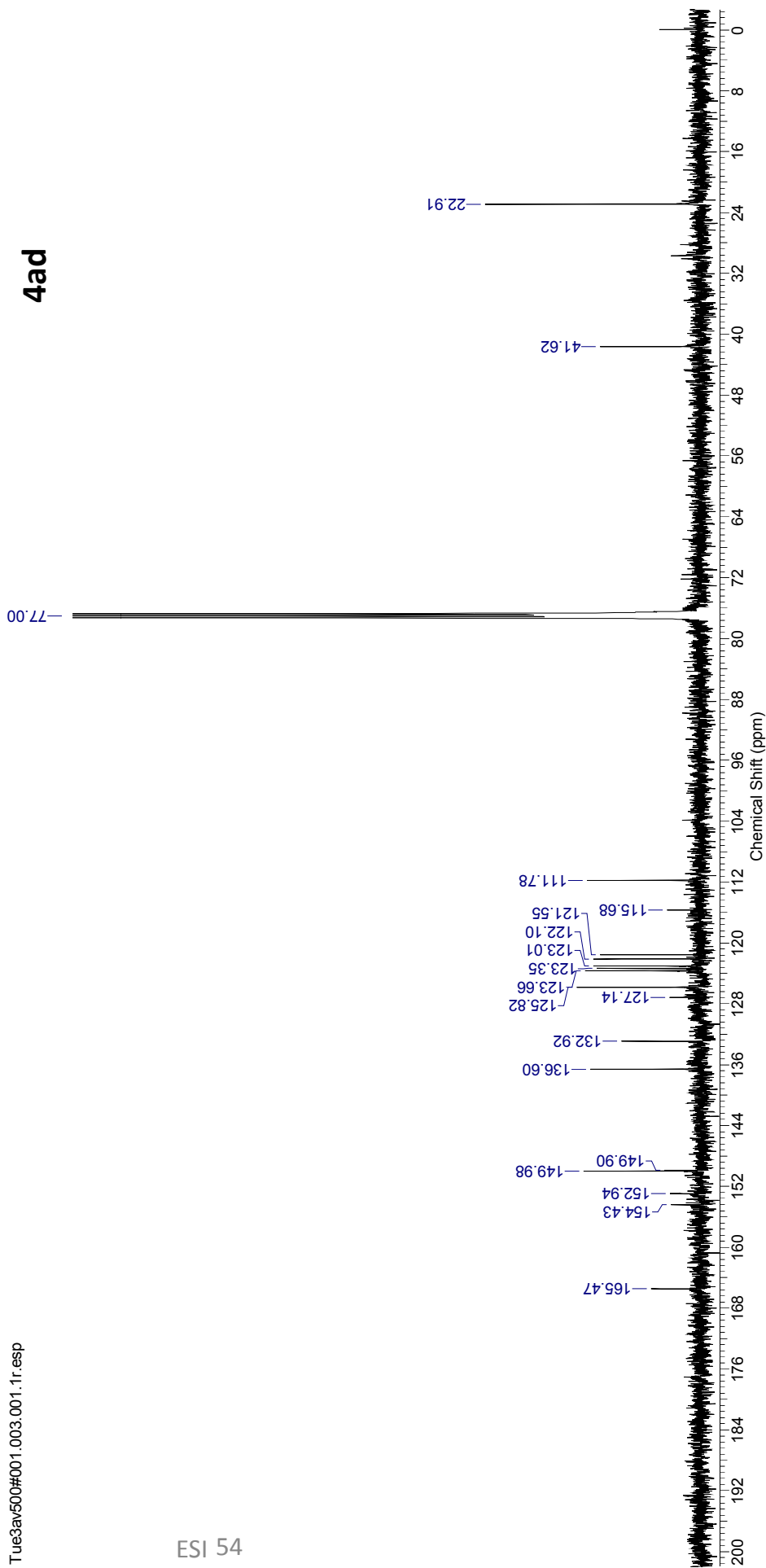
ESI 53



500 MHz, CDCl₃

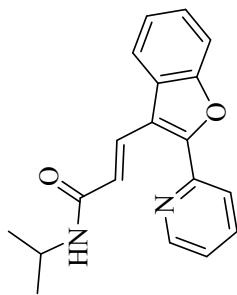


Tue3av500#001.003.001.1r.esp



ESI 54

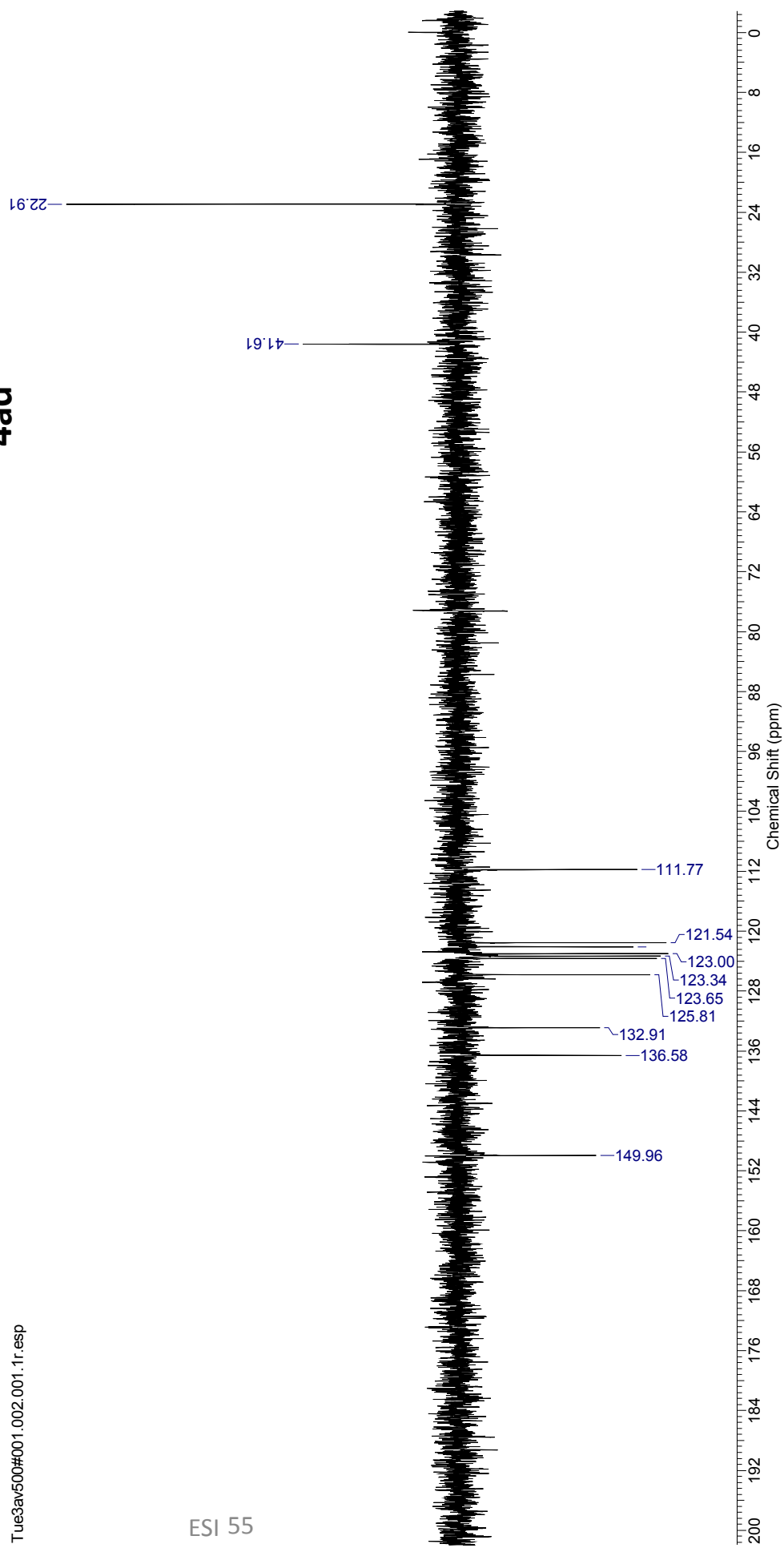
500 MHz, CDCl₃



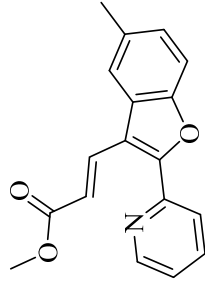
4ad

Tue3av500#001.002.001.1r.esp

ESI 55

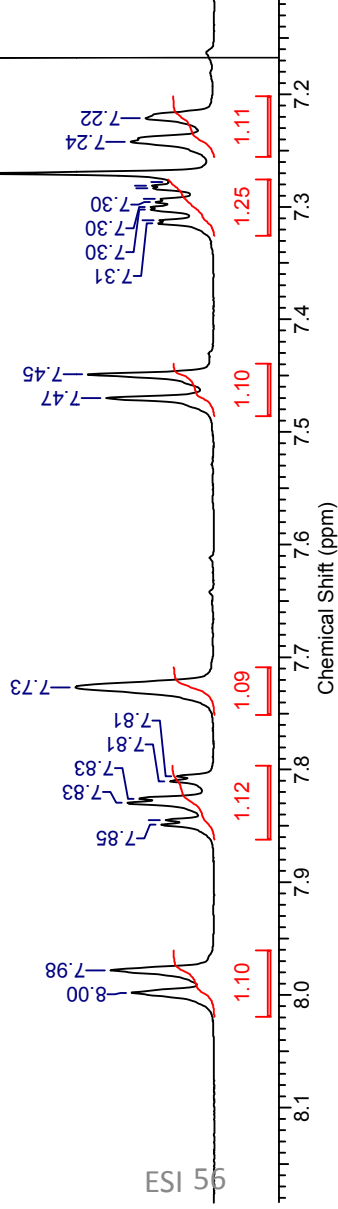


400 MHz, CDCl₃



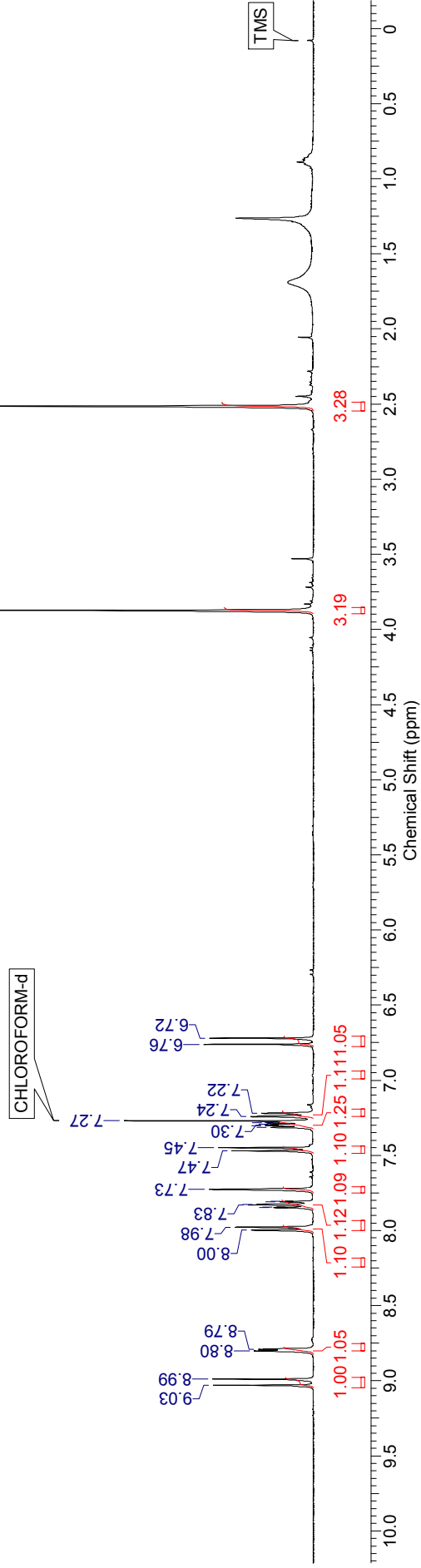
4ba

CHLOROFORM-d

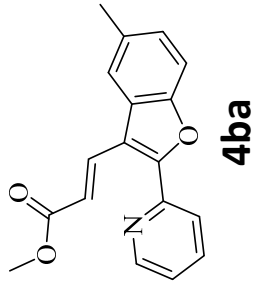


ESI 56

CHLOROFORM-d



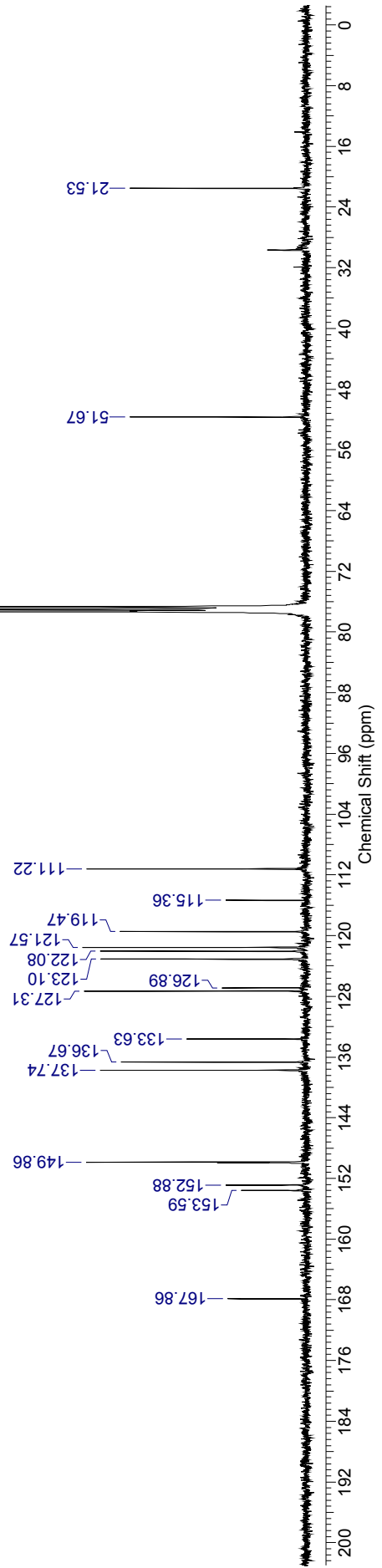
400 MHz, CDCl₃



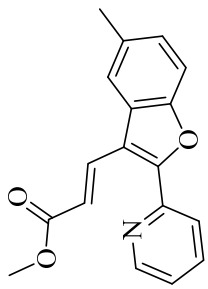
13CSun1av400#002.esp

CHLOROFORM-d

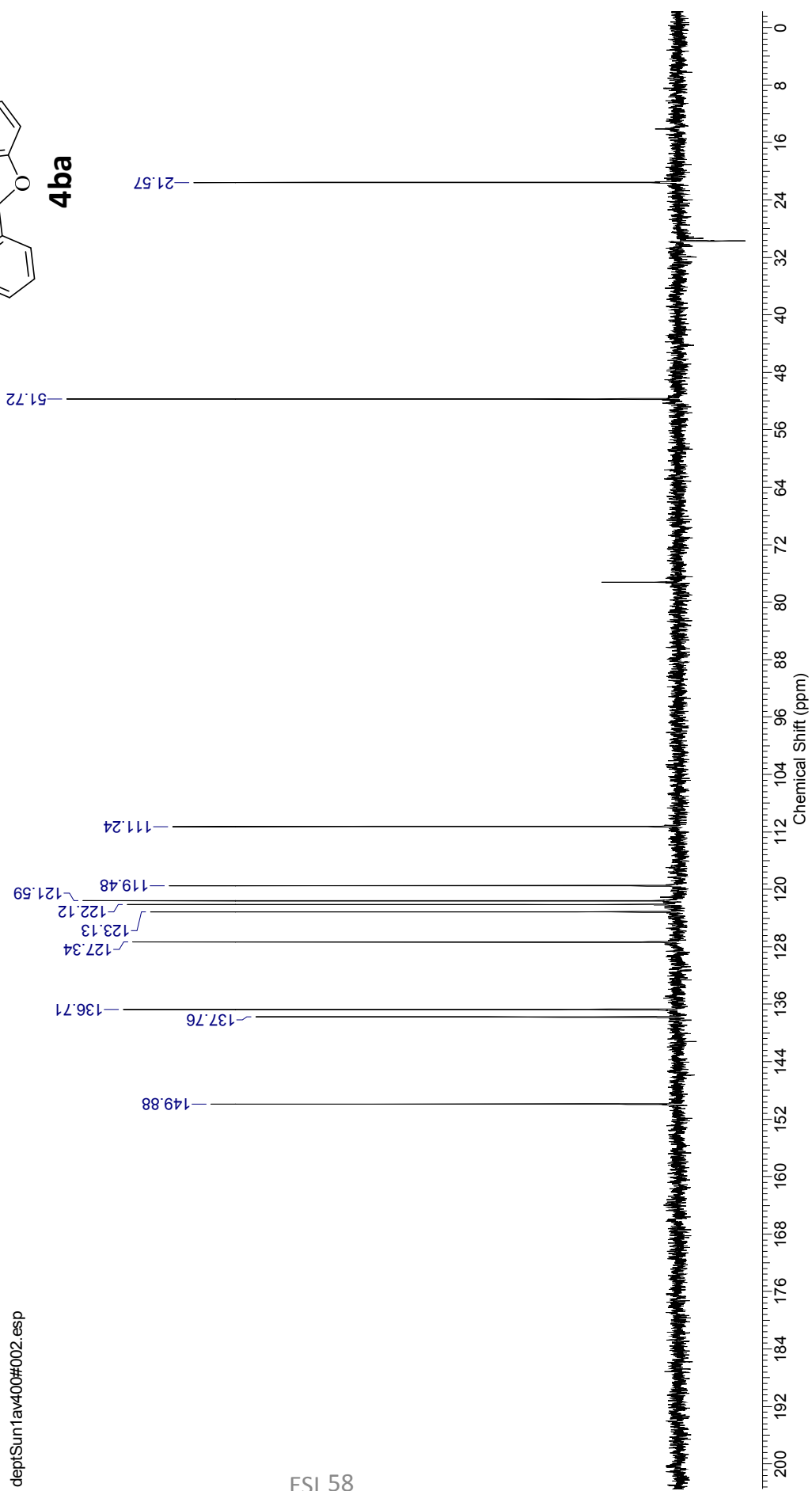
ESI 57



400 MHz, CDCl₃



4ba

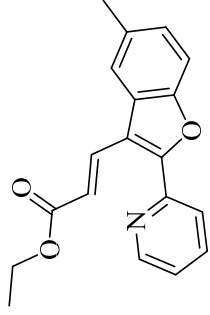


deptSun1av400#002.esp

1HThu1av500#017.esp

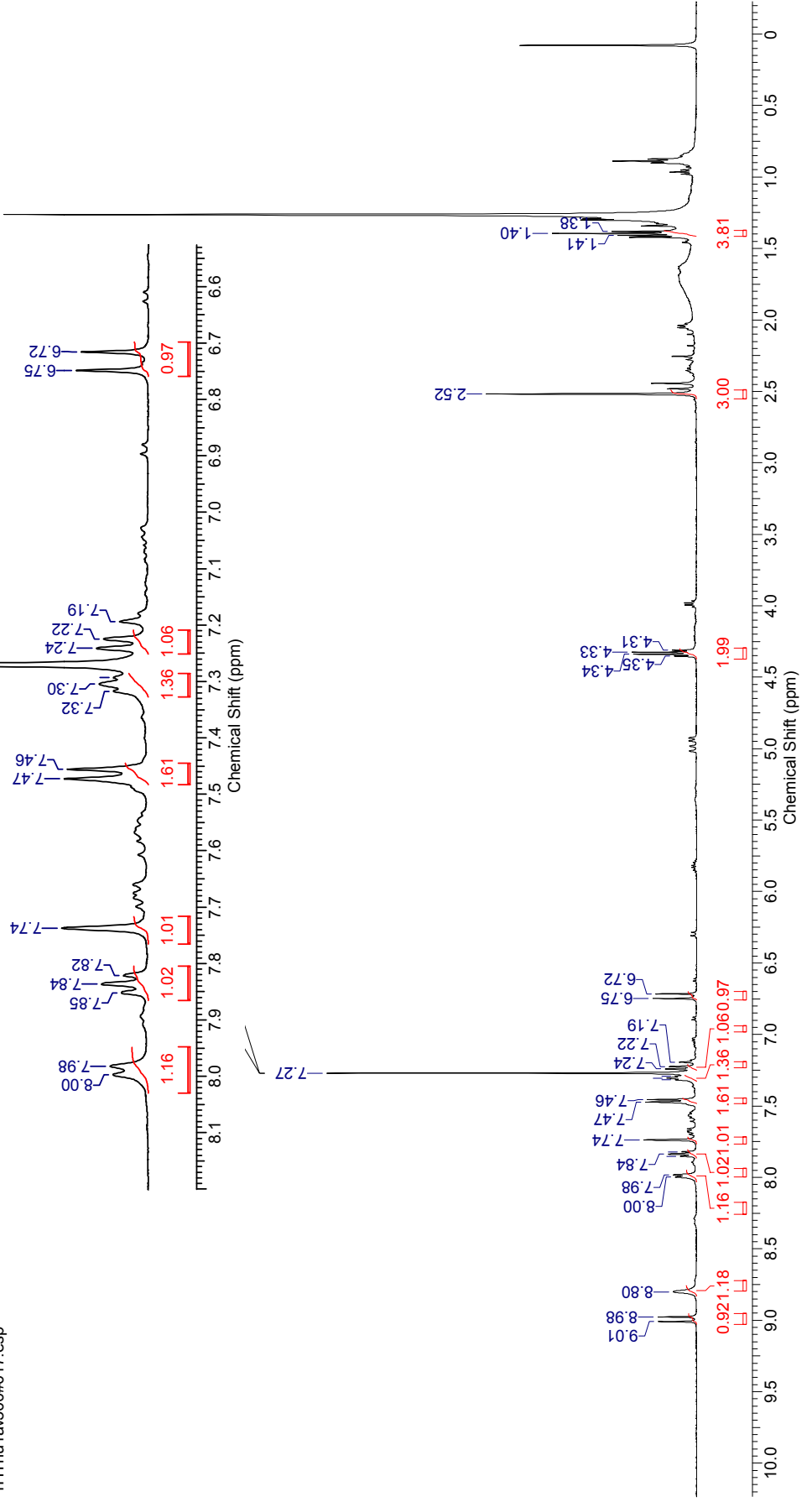
500 MHz, CDCl₃

CHLOROFORM-d



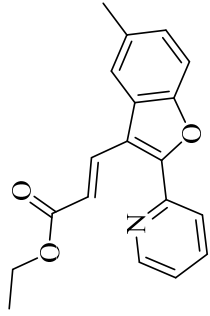
4bb

1HThu1av500#017.esp



ESI 59

500 MHz, CDCl₃

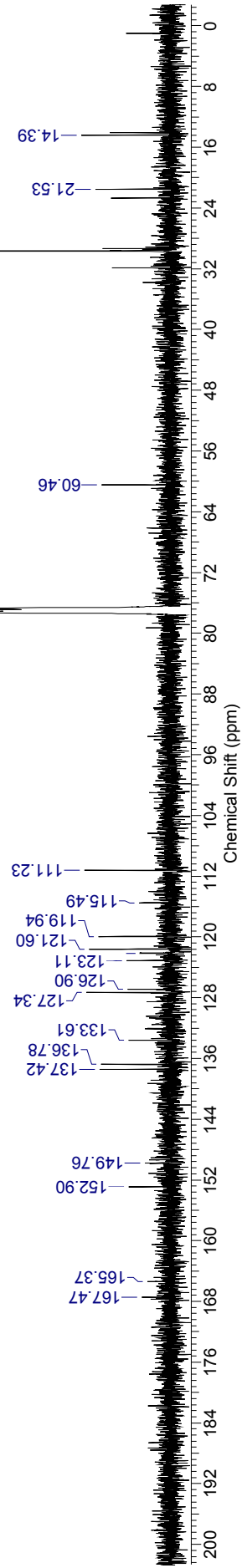


4bb

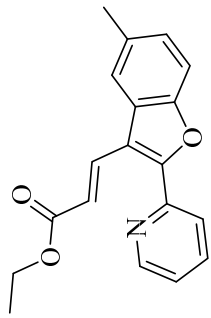
13CThu1av500#017.esp

CHLOROFORM-d

ESI 60

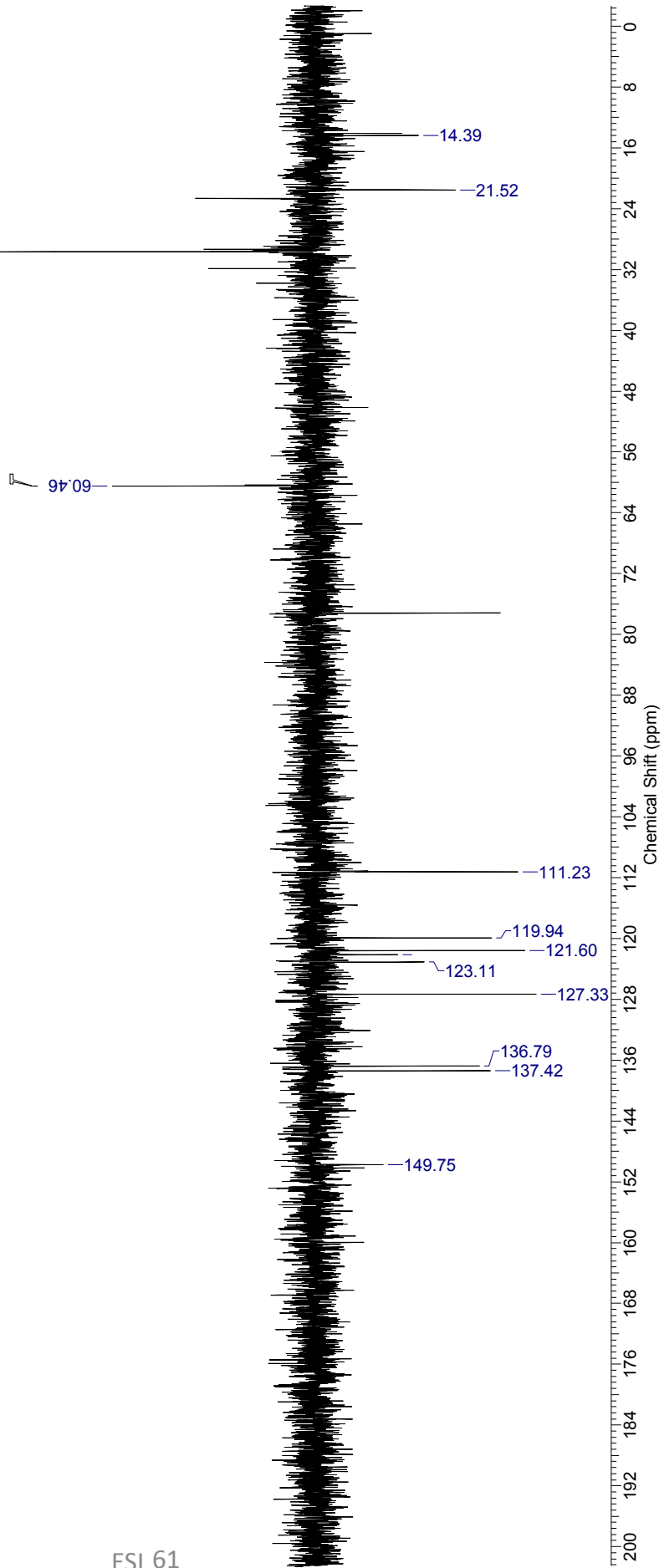


500 MHz, CDCl₃



deptThu1av500#017.esp

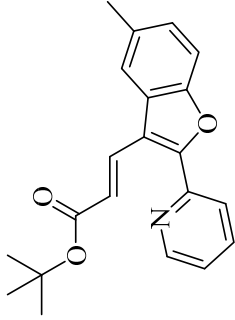
4bb



ESI 61

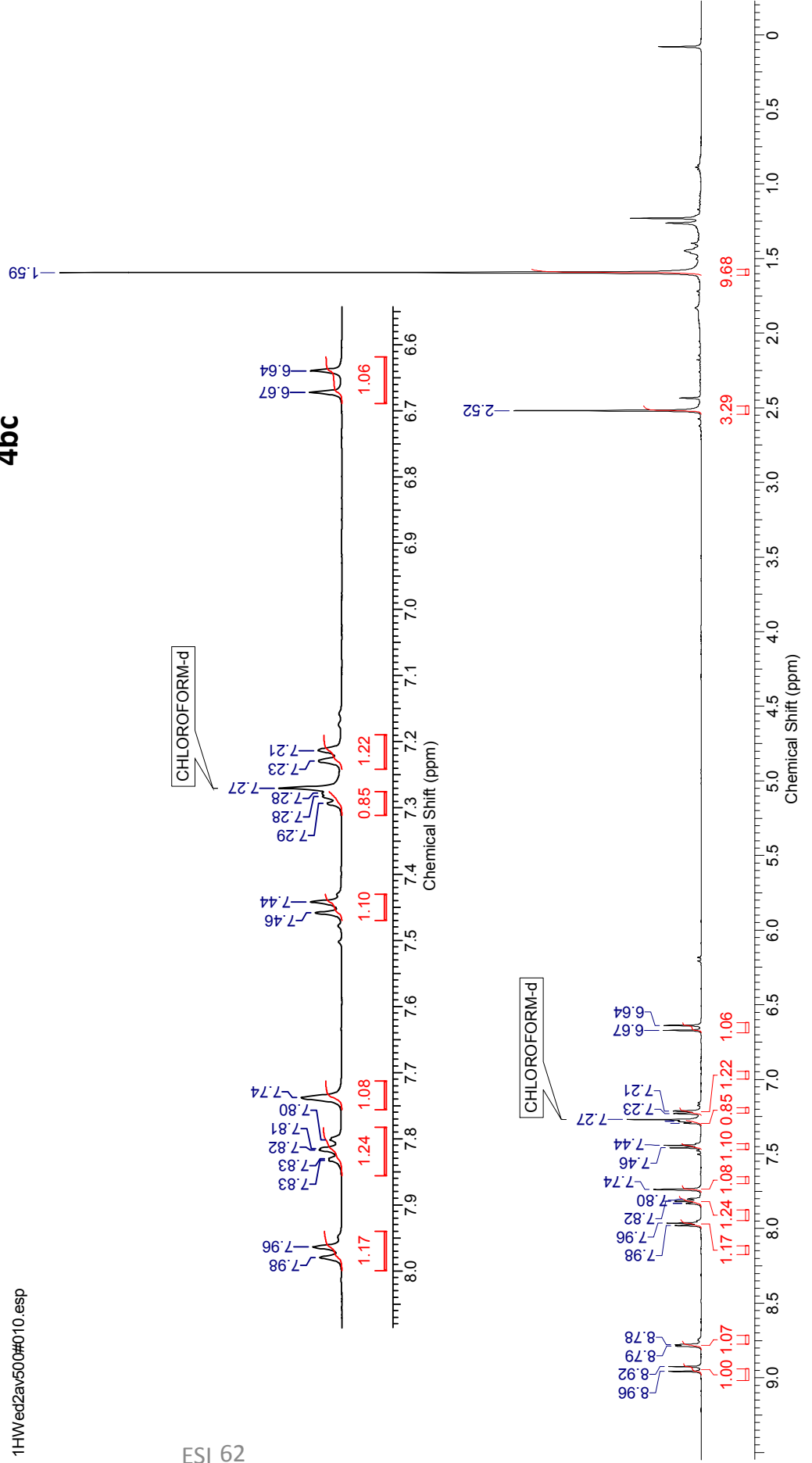
500 MHz, CDCl₃

1HWed2av500#010.esp



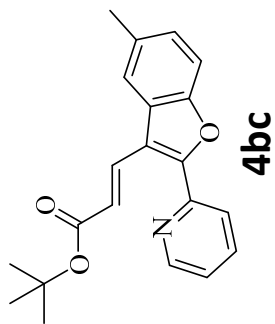
4bc

1HWed2av500#010.esp

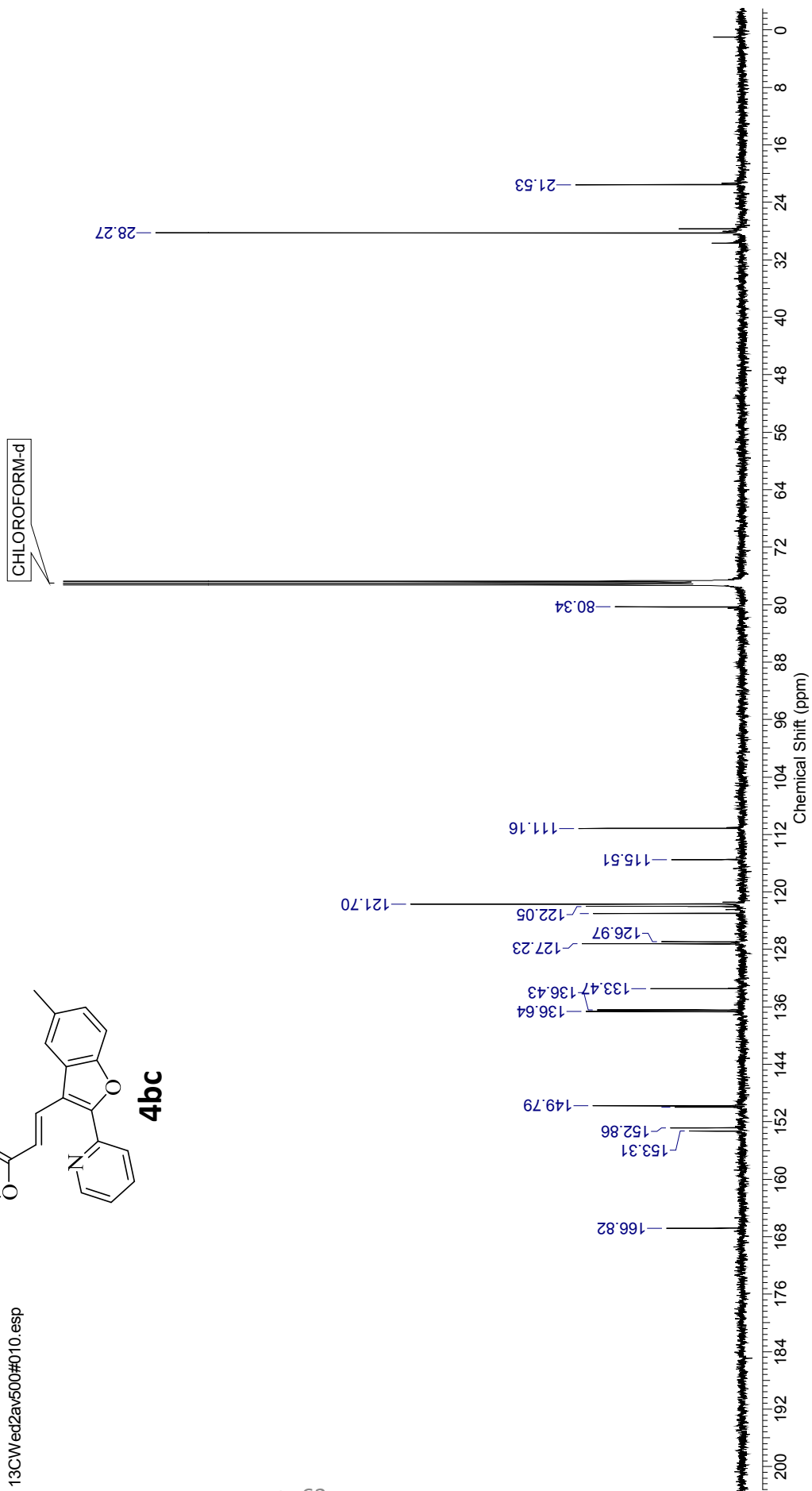


ESI 62

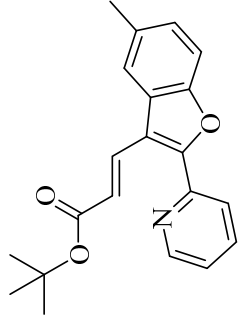
500 MHz, CDCl₃



13CWed2av500#010.esp



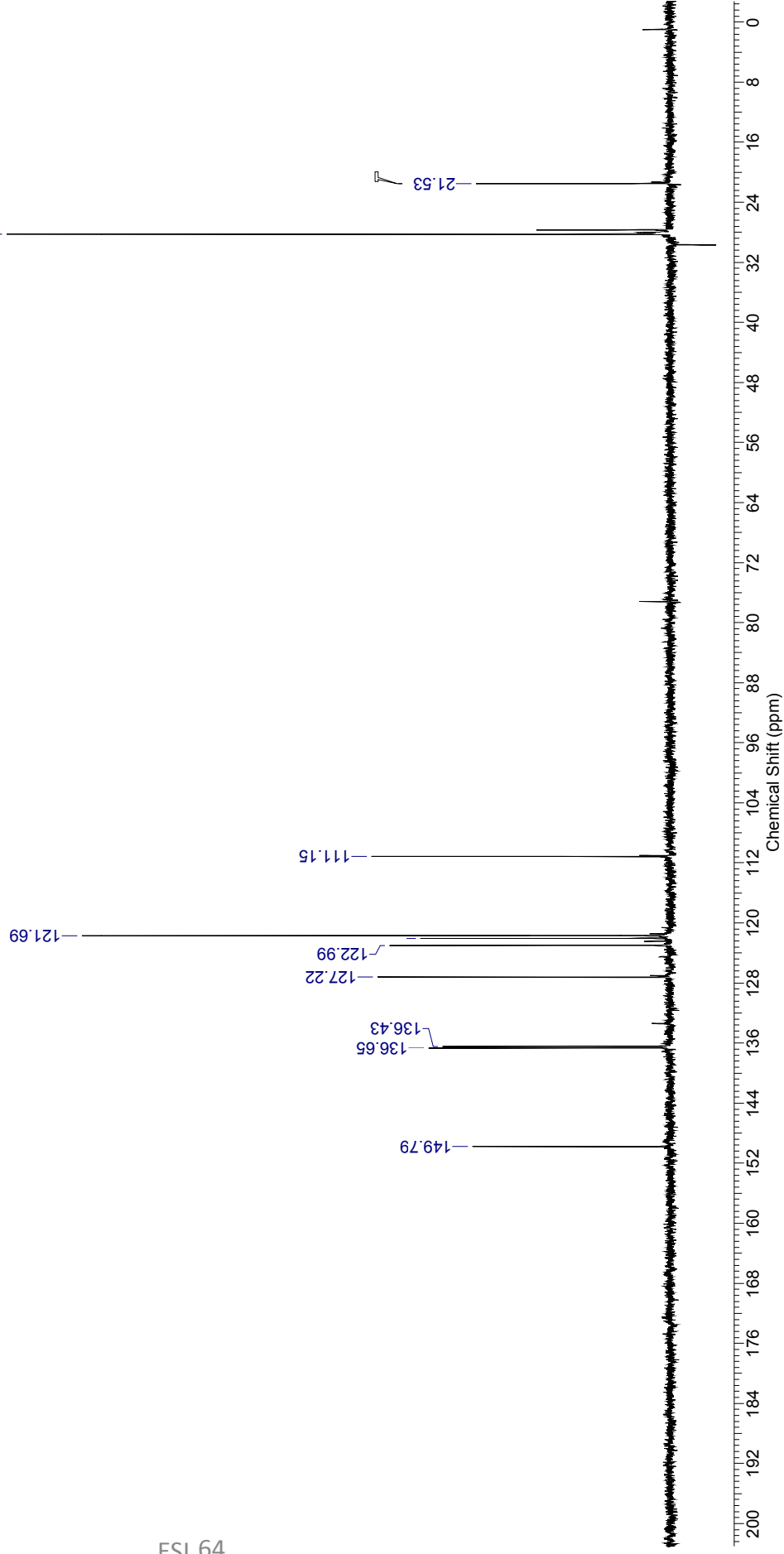
500 MHz, CDCl₃



4bc

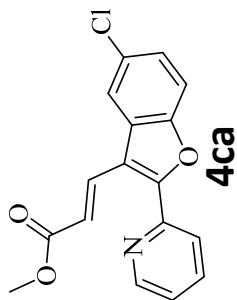
deptWed2av500#010.esp

ESI 64

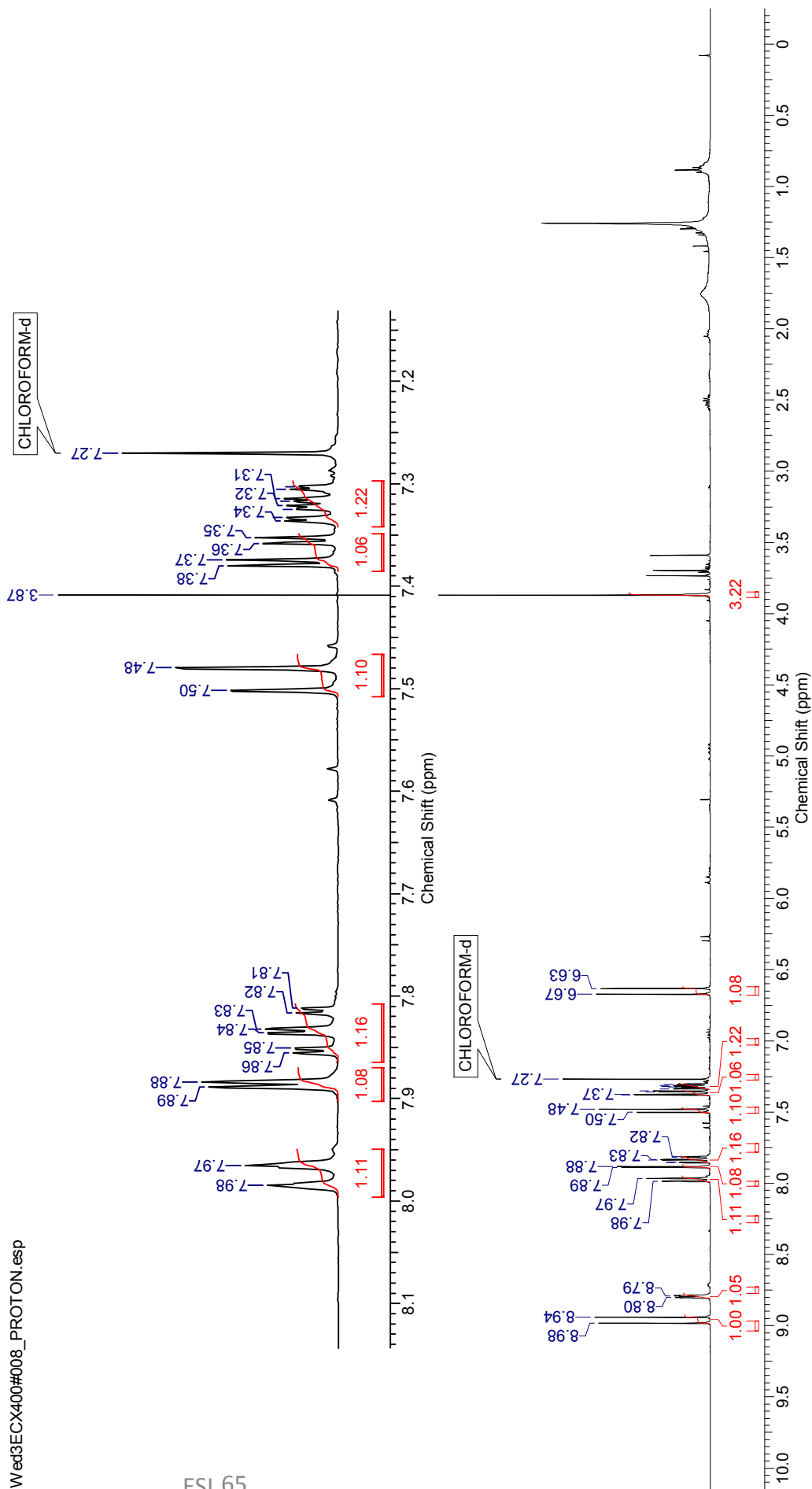


400 MHz, CDCl₃

Wed3ECX400#008_PROTON.esp

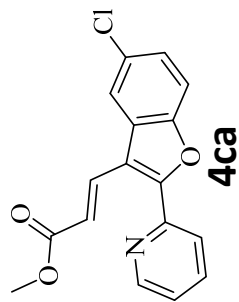


Wed3ECX400#008_PROTON.esp



ESI 65

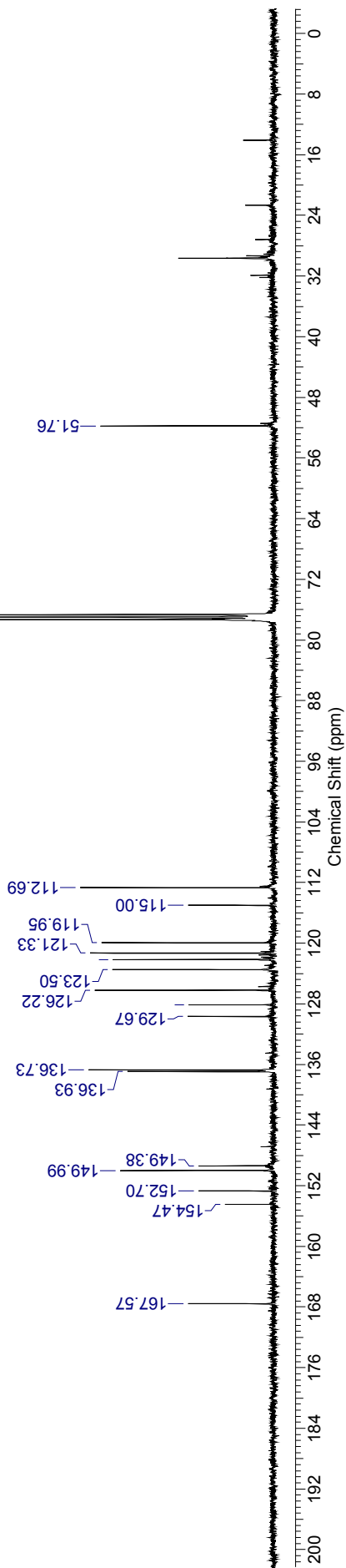
400 MHz, CDCl₃



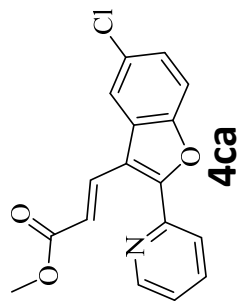
Wed3ECX400#008_CARBON.esp

CHLOROFORM-d

ESI 66

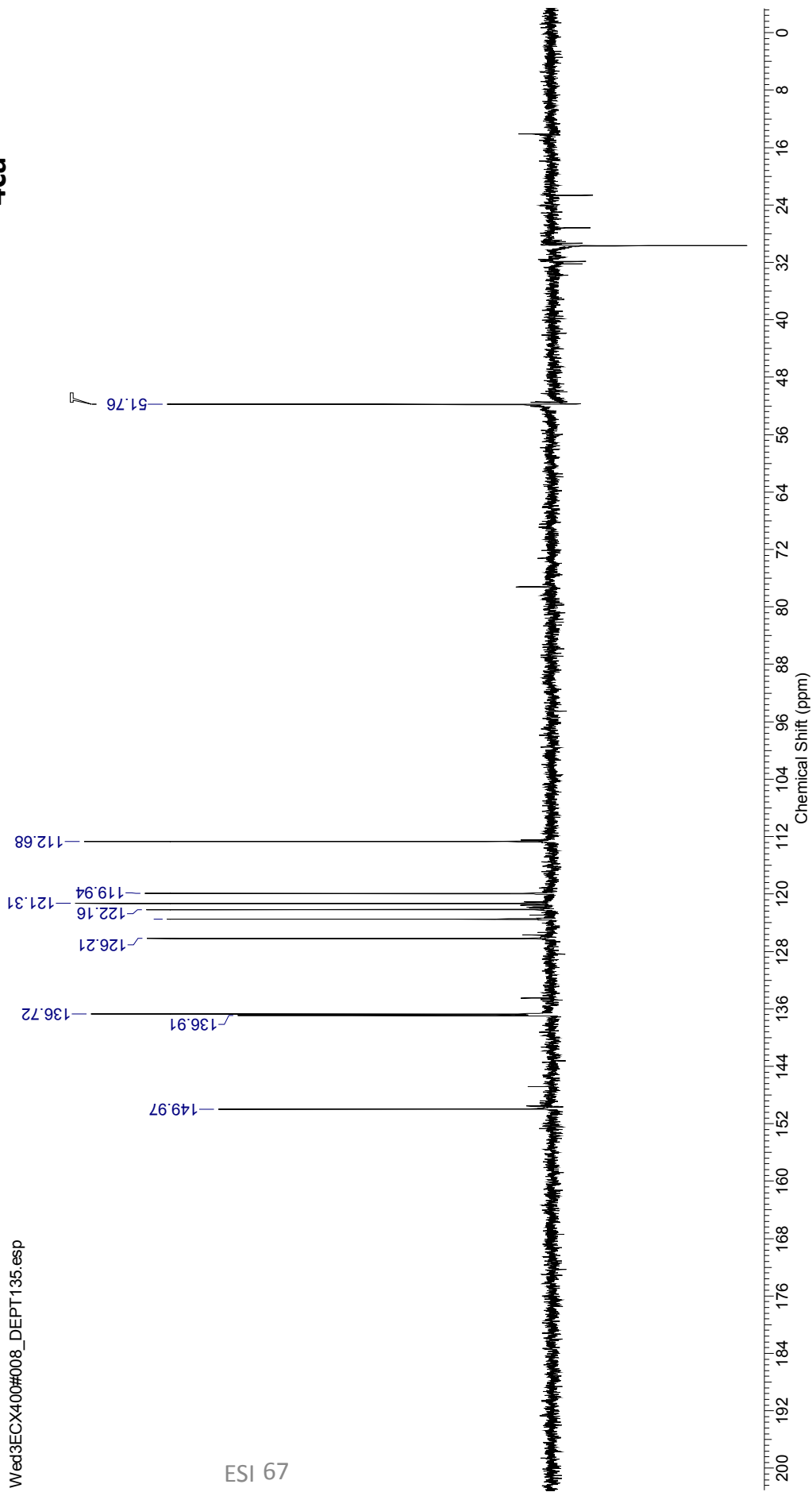


400 MHz, CDCl₃

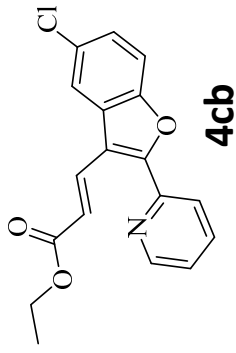


Wed3ECX400#008_DEPT135.esp

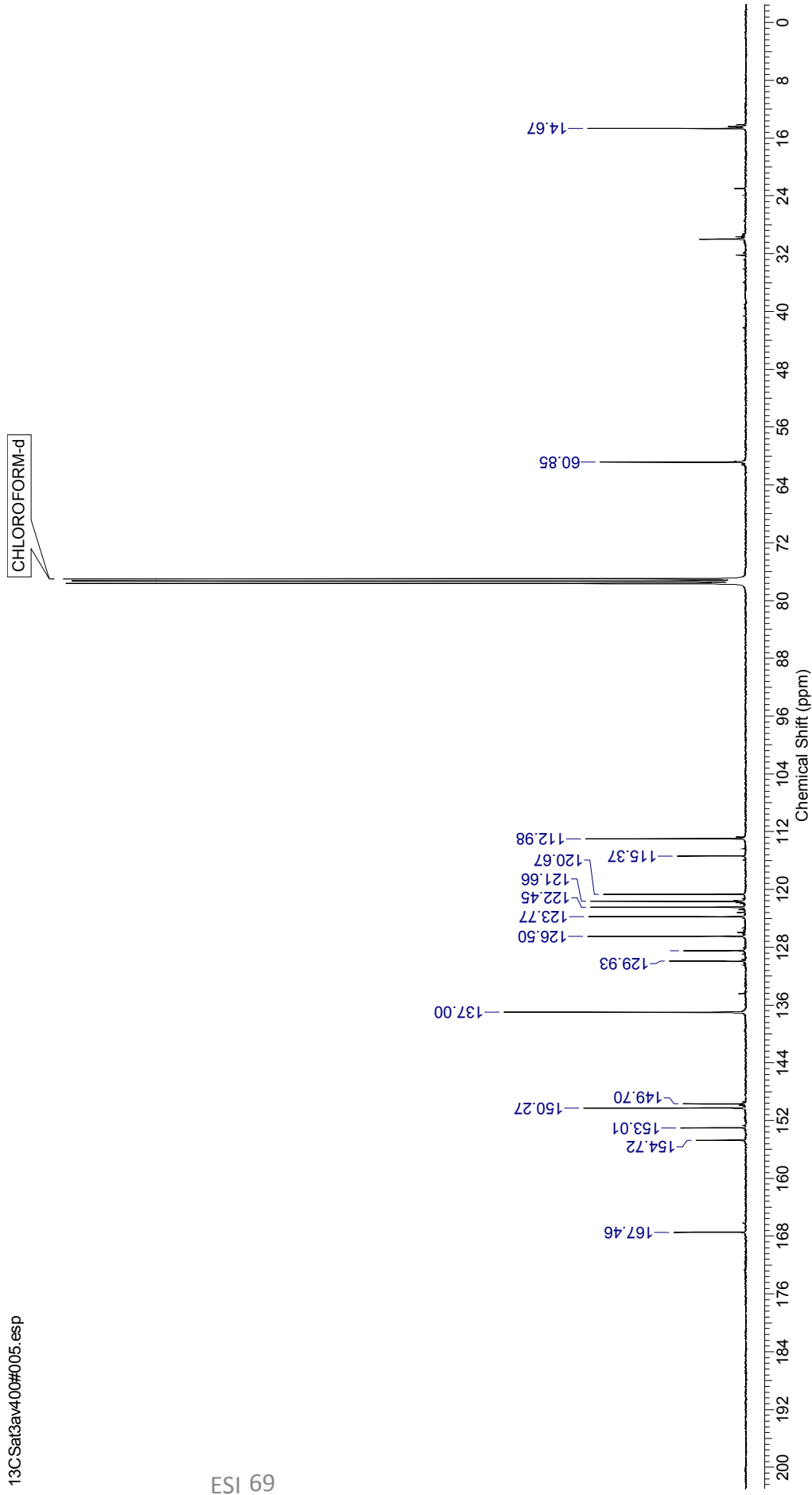
ESI 67



400 MHz, CDCl₃

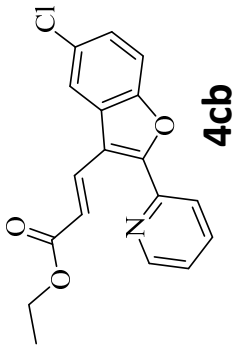


13CSat3av400#005.esp

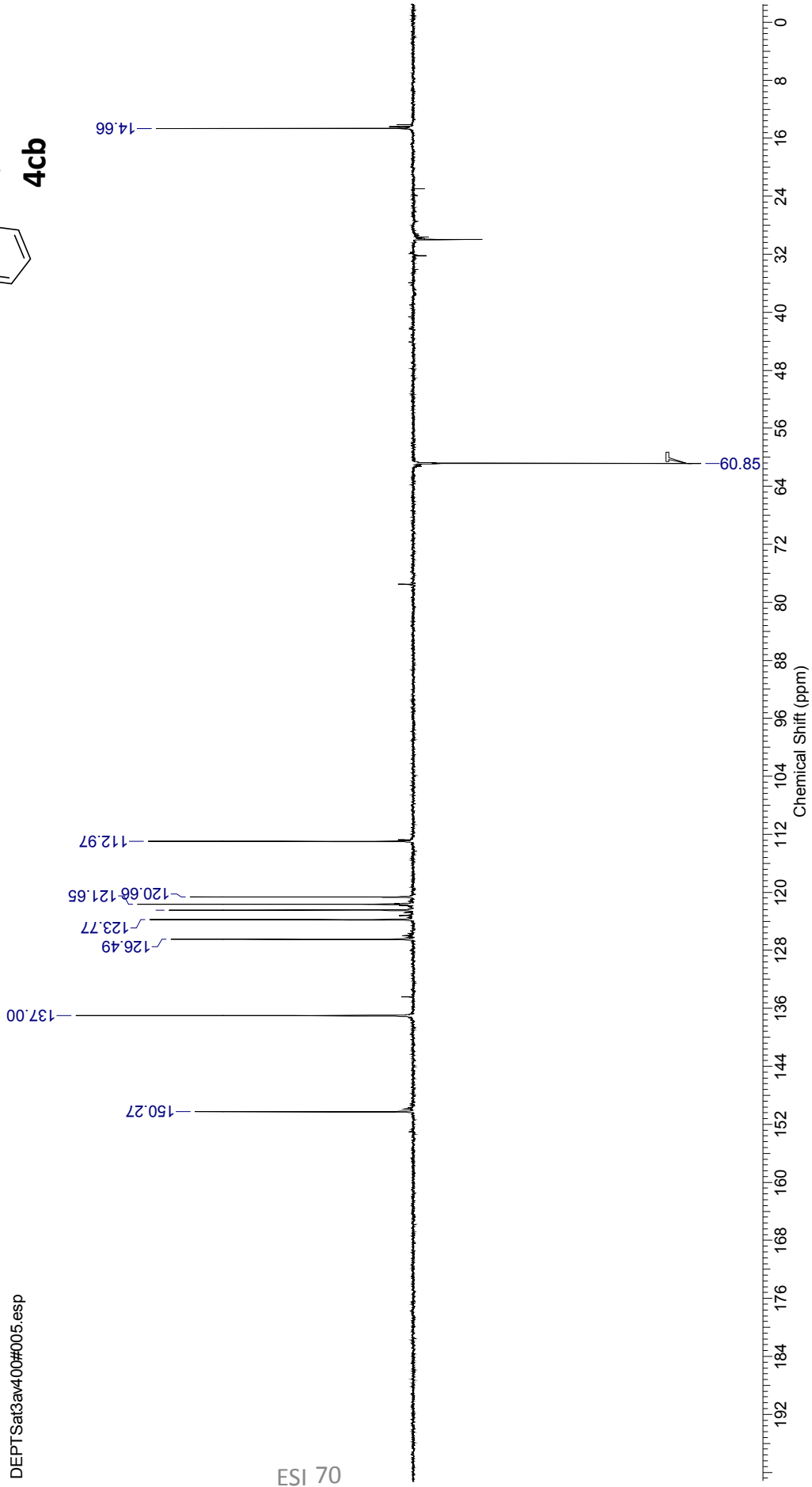


69 ISI

400 MHz, CDCl₃



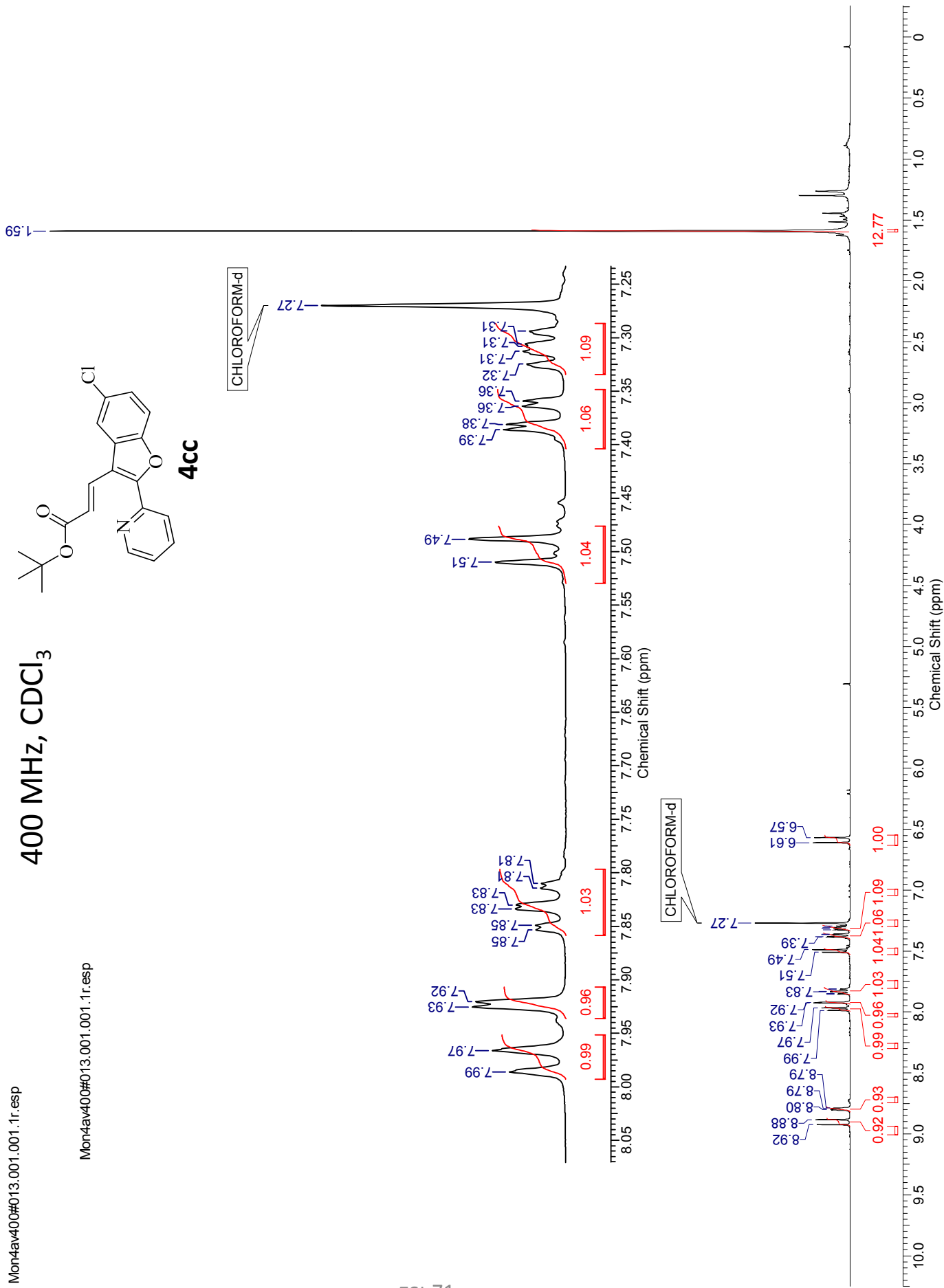
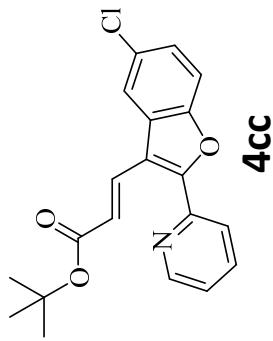
DEPTSat3av400#005.esp



ESI 70

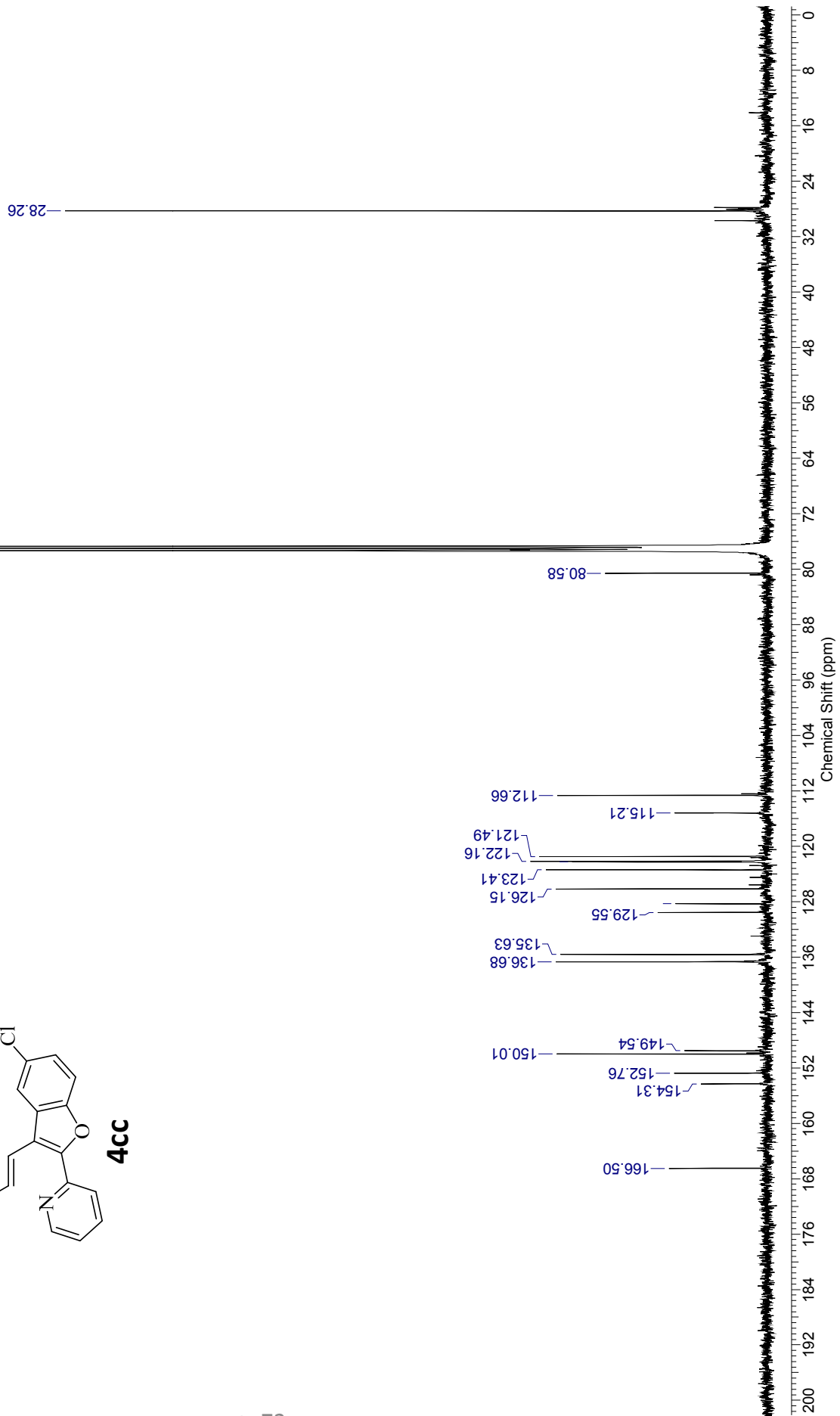
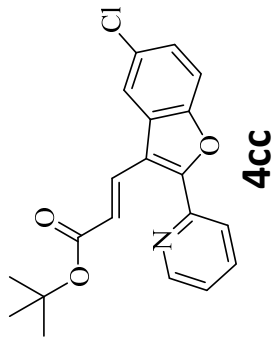
400 MHz, CDCl₃

Mon4av400#013.001.001.1r.esp

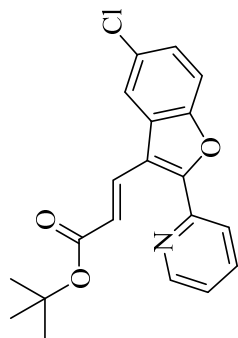


400 MHz, CDCl₃

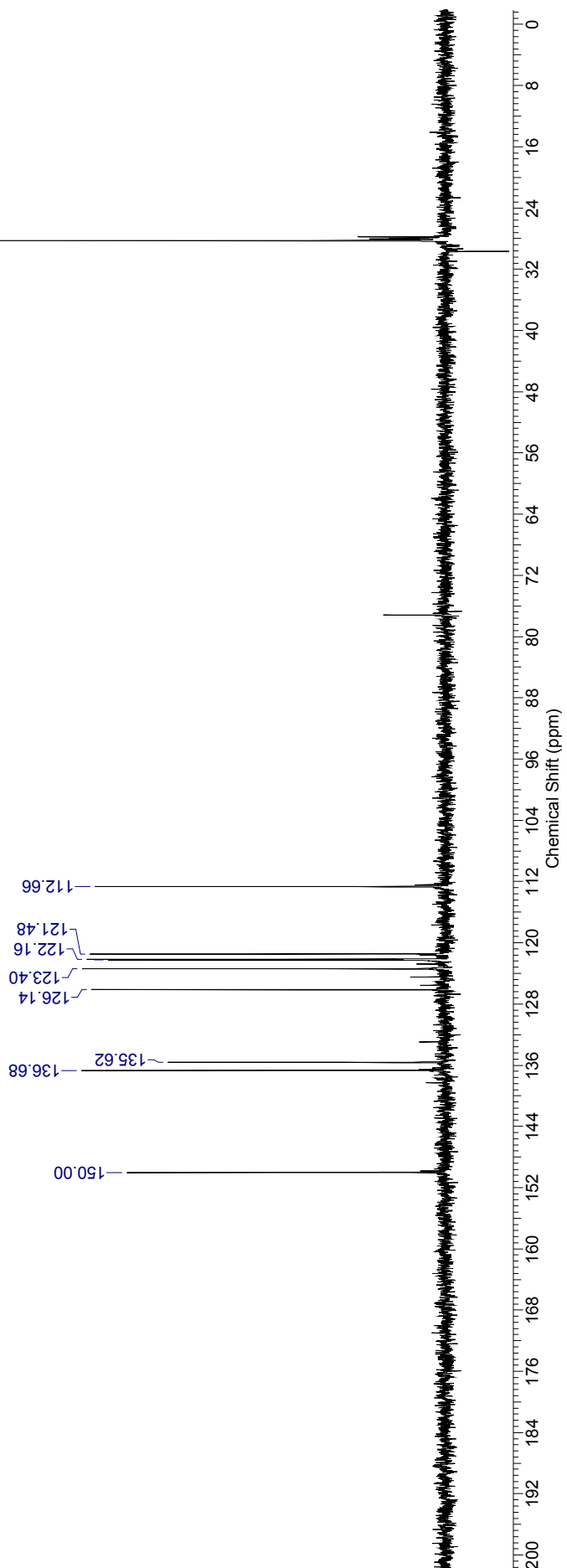
CHLOROFORM-d



400 MHz, CDCl₃

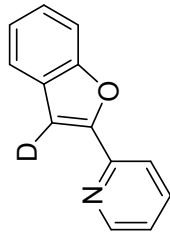


4cc



200 MHz, CDCl₃

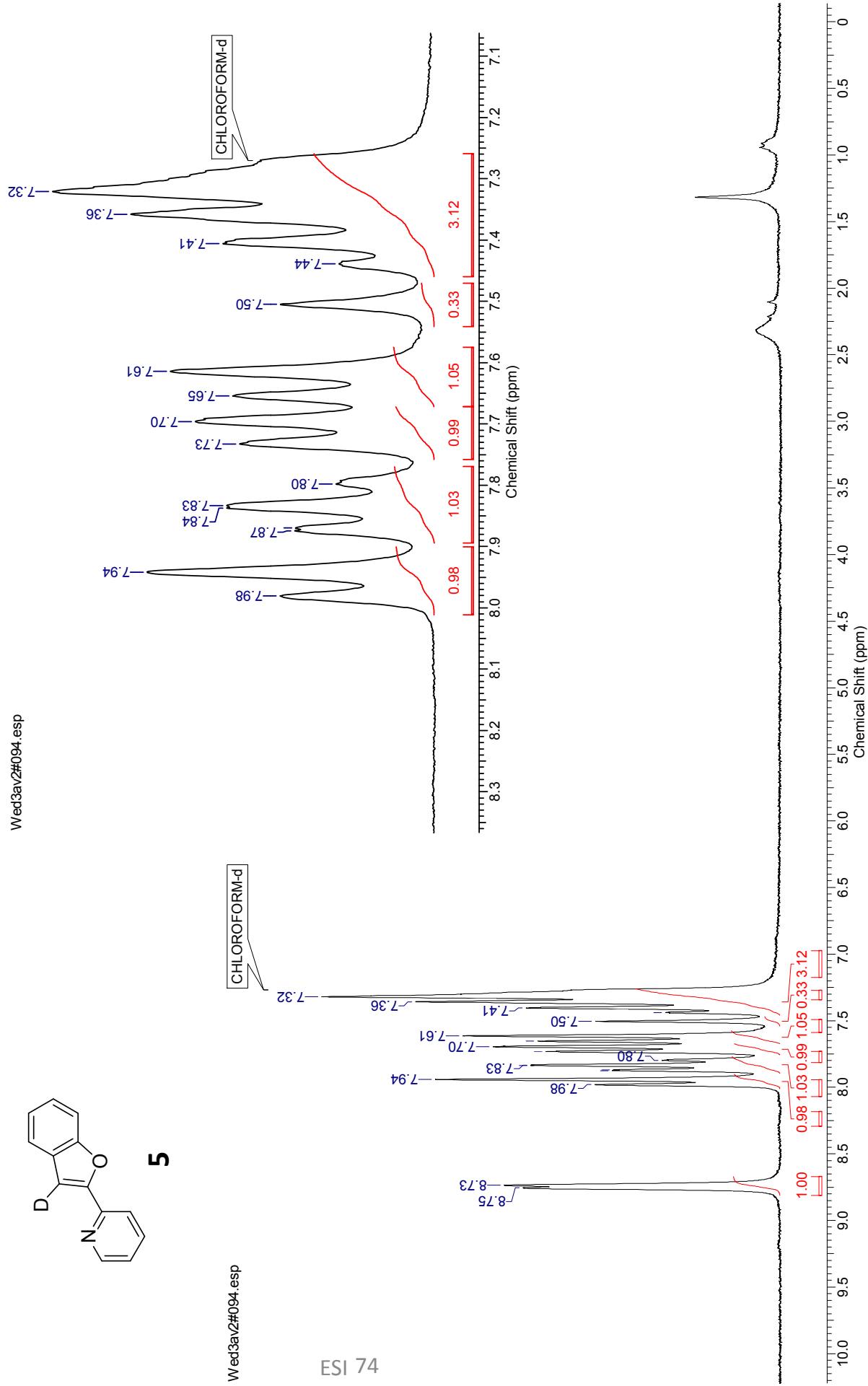
Wed3av2#094.esp



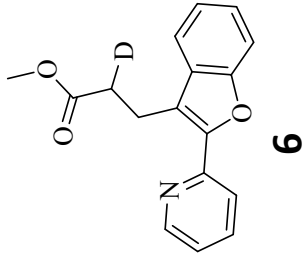
5

Wed3av2#094.esp

ESI 74



200 MHz, CDCl₃



Thu4av2#066.001.001.1r.esp

ESI 75

