Electronic Supplementary Information

Aerobic waste-minimized Pd-catalyzed C–H alkenylation in GVL using a tube-in-tube heterogeneous flow reactor

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CONTENTS

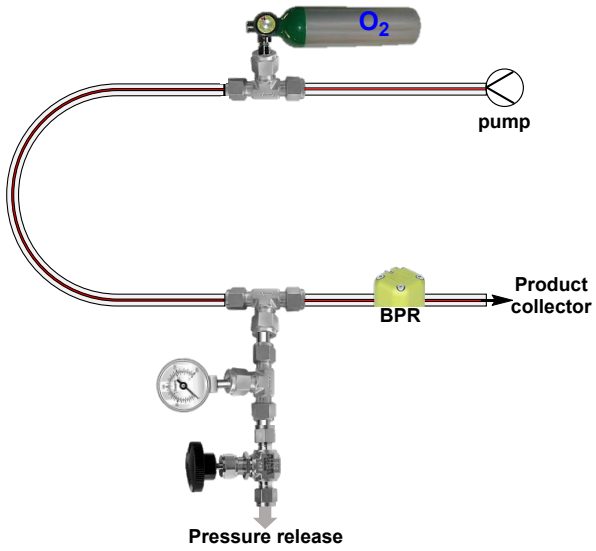
1. General Remarks

All chemicals were used without any further purification unless otherwise noted. GLC analyses were performed by using Agilent 6850 Series GC System equipped with a capillary column DB-5MS (30 m, 0.32 mm), a FID detector and helium as gas carrier. GC-EIMS analyses were carried out by using a Hewlett-Packard HP 6890N Network GC system/5975 Mass Selective Detector equipped with an electron impact ionizer at 70 eV. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker DRX-ADVANCE 400 MHz (^{1}H at 400 MHz and ^{13}C at 101 MHz and ^{19}F at 376 MHz). Chemical shifts are reported in ppm and coupling constants in Hertz. Flash chromatography was carried out on a Büchi Reveleris® X2-UV system. Melting points were collected using Büchi 510 analyser. Elemental Analysis (EA) were conducted on Elementar UNICUBE® elemental analyzer. Palladium content was measured by using an Agilent MP-AES 4210 instrument. Flow systems were implemented using PTFE tubes and PTFE or stainless-steel connectors purchased from Swagelok. The variable back-pressure regulator used was provided by Zaiput Inc. HPLC pumps Shimadzu Prominence LC20-AD were used for the flow procedures.

Characterization data and copies of the ^{1}H and ^{13}C NMR and ^{19}FNMR are reported below.

2. General Assembly of the reactor

The gas-liquid-solid reactor assembly was implemented with a variable (1, 2, 2.5 m) section of Teflon AF2400 tubing (with variable internal diameters 0.79, 1.59, 3.18 mm) placed within PTFE tubing (6 mm o.d.). These tubings were coiled and each end fastened to the proper Swagelok fitting. The liquid inlet section was connected to a stainless-steel T-piece in which the oxygen was supplied. The outlet section was mounted with a T-piece stainless steel connector in which a pressure gauge and a pressure release valve were connected (Figure S1). The heterogeneous catalyst (Pd/C, 10% w/w) was packed inside the Teflon AF2400 tube by placing in the tube outlet a piece of silica wool, then the catalyst was sucked into the inner tube by a vacuum pump. The amount of catalyst used in all experiments was 60 mg.



3. General Procedures

3.1 General flow procedure for the oxidative C–H alkenylation

The flow streams driven by the HPLC pump containing a 0.2 M GVL solution of the starting acetanilides or *N*-methoxybenzamide (**1a-f**, **4a-c**, 1 eq), the olefin (**2a-f**, 1.5 eq), *p*-TsOH (1eq), and *p*-benzoquinone (10 mol%) was directed through the tube-in-tube reactor packed with Pd/C (10% w/w, 60 mg, 0.056 mmol of Pd) placed in a thermostated box at 85 °C, with a flow rate of 15 μL min^{-1} and at a pressure of 5 Bar of O_2. A back-pressure regulator (5.2 bar) was placed immediately after the gas-liquid-solid reactor. The reaction mixture was continuously pumped with a residence time inside the reactor of 140 min. The reaction mixture at the outlet of the reactor was collected into a flask and the solvent was removed *via* distillation under vacuum and the crude mixture was purified by column chromatography or crystallization.

3.2 General procedure for leaching determination

At the outlet of the reactor, samples of the reaction mixture were taken and digested into 2 mL of aqua regia for 1h. The digested material was diluted with milli-Q water to a final volume of 10 mL and the amount of palladium leached in solution was measured with a microwave plasma-atomic emission spectrometer (MP-AES 4210).

4. E-factor calculations

Ref (18a): M. D. K. Boele, G. P. F. van Strijdonck, A. H. M. de Vries, P. C. J. Kamer, J. G. de Vries and P. W. N. M. van Leeuwen, *J. Am. Chem. Soc.*, 2002, **124**, 1586–1587

$[(0.447_{[4\text{-Me-acetanlide}]} + 0.381_{[\text{butyl acrylate}]} + 4.725_{[\text{acetic acid}]} + 2.167_{[\text{toluene}]} + 0.013_{[\text{Pd(OAc)2}]} + 0.324_{[\text{benzoquinone}]} + 0.286_{[\text{TsOH}]} + 21.390_{[\text{Et2O}]}) - 0.702_{[\text{product}]}]/ 0.702_{[\text{product}]} = \mathbf{41.3}$

Ref (18b): T. Nishikata, B. H. Lipshutz, *Org. Lett*., 2010, **12**, 1972–1975

$[(0.041_{[3\text{-OMe-acetanlide}]} + 0.064_{[\text{butyl acrylate}]} + 1.000_{[\text{water}]} + 0.030_{[\text{surfactant}]} + 0.011_{[\text{Pd-cat}]} + 0.027_{[\text{benzoquinone}]} + 0.085_{[\text{AgNO3}]}) - 0.061_{[\text{product}]}]/ 0.061_{[\text{product}]} = \mathbf{19.3}$

Ref (18c): F. W. Patureau and F. Glorius, *J. Am. Chem. Soc.,* 2010, **132**, 9982–9983

$[(0.149_{[4\text{-Me-acetanlide}]} + 0.190_{[\text{butyl acrylate}]} + 4.025_{[\text{t-amyl-alchol}]} + 0.003_{[\text{Rh-cat}]} + 0.381_{[\text{CuOAc2}]} + 0.006_{[\text{AgSbF6}]}) - 0.269_{[\text{product}]}]/ 0.269_{[\text{product}]} = \mathbf{16.6}$

Ref (18c): F. W. Patureau and F. Glorius, *J. Am. Chem. Soc.,* 2010, **132**, 9982–9983 (*under air*)

$[(0.149_{[4\text{-Me-acetanlide}]} + 0.190_{[\text{butyl acrylate}]} + 4.025_{[\text{t-amyl-alchol}]} + 0.003_{[\text{Rh-cat}]} + 0.018_{[\text{CuOAc2}]} + 0.006_{[\text{AgSbF6}]}) - 0.267_{[\text{product}]}]/ 0.267_{[\text{product}]} = \mathbf{15.4}$

Ref (18d): L. L. Chng, J. Zhang, J. Yang, M. Amoura and J. Y. Ying, *Adv. Synth. Catal.,* 2011, **353**, 2988–2998 (heterogeneous catalyst has been recovered and is not accounted in the calculation)

$[(0.027_{[\text{acetanlide}]} + 0.050_{[\text{butyl acrylate}]} + 0.390_{[\text{toluene}]} + 3.975_{[\text{DCM}]} + 1.965_{[\text{hexane}]}) - 0.039_{[\text{product}]}]/ 0.039_{[\text{product}]} = \mathbf{160.3}$

Ref (18e): Y. Takahama, Y. Shibata and K. Tanaka, *Chem. Eur. J.,* 2015, **21**, 9053–9056

$[(0.108_{[\text{acetanlide}]} + 0.034_{[\text{methyl acrylate}]} + 1.568_{[\text{acetone}]} + 0.008_{[\text{Rh-cat}]} + 0.013_{[\text{AgSbF6}]} + 0.016_{[\text{CuOAc2}]}) - 0.072_{[\text{product}]}]/ 0.072_{[\text{product}]} = \mathbf{23.3}$

Ref (18f): G. N. Hermann, P. Becker and C. Bolm, *Angew. Chem., Int. Ed.*, 2015, **54**, 7414–7417

$[(0.081_{[\text{acetanlide}]} + 0.083_{[\text{butyl acrylate}]} + 0.009_{[\text{Rh-cat}]} + 0.012_{[\text{AgBF4}]} + 0.027_{[\text{Cu(OAc)2}]} + 79.5_{[\text{DCM}]} + 54.12_{[\text{EtOAc}]}) - 0.111_{[\text{product}]}]/ 0.111_{[\text{product}]} = \mathbf{1201.2}$

Ref (18g): C. J. Mulligan, J. S. Parker, K. K. M. Hii, *React. Chem. Eng.*, 2020, **5**, 1104-1111

$[(0.178_{[4\text{-Me-acetanlide}]} + 0.127_{[\text{butyl acrylate}]} + 12.6_{[\text{acetic acid}]} + 0.011_{[\text{Pd(OAc)2}]} + 0.108_{[\text{benzoquinone}]} + 0.095_{[\text{TsOH}]}) - 0.250_{[\text{product}]}]/ 0.250_{[\text{product}]} = \mathbf{51.4}$

Ref (18h): R. Zhu, S. Lu, Q. Wang, J. Bai, Y. Wang, Q. Yu, J. Huang, *Tetrahedron* 2018, **74**, 3879–3887.

$[(0.027_{[\text{acetanlide}]} + 0.076_{[\text{butyl acrylate}]} + 1.102_{[\text{TFA}]} + 1.256_{[\text{DCE}]} + 0.004_{[\text{Pd(OAc)2}]} + 0.142_{[\text{selectfluor}]} + 0.095_{[\text{TsOH}]} + 27.06_{[\text{EtOAc}]}) - 0.042_{[\text{product}]}]/ 0.042_{[\text{product}]} = \mathbf{707.6}$

Ref (15c): F. Ferlin, S. Santoro, L. Ackermann and L. Vaccaro, *Green Chem*., 2017, **19**, 2510–2514 (*Batch*) (heterogeneous base and catalyst have been recovered and not accounted in the calculation)

$[(0.067_{[\text{acetanlide}]} + 0.069_{[\text{butyl acrylate}]} + 1.054_{[\text{GVL}]} + 0.108_{[\text{benzoquinone}]} + 2.000_{[\text{NaHCO3}]} + 1.804_{[\text{EtOAc}]}) - 0.124_{[\text{product}]}]/ 0.124_{[\text{product}]} = \mathbf{40.1}$

Ref (15c): F. Ferlin, S. Santoro, L. Ackermann and L. Vaccaro, *Green Chem*., 2017, **19**, 2510–2514 (*Flow*) (heterogeneous catalyst has been recovered and not accounted in the calculation)

$[(58.121_{[\text{acetanlide}]} + 60.151_{[\text{butyl acrylate}]} + 906.95_{[\text{GVL}]} + 92.961_{[\text{benzoquinone}]} + 81.794_{[\text{TsOH}]} + 1500_{[\text{NaHCO3}]} + 665_{[\text{EtOAc}]}) - 108.996_{[\text{product}]}]/ 108.996_{[\text{product}]} = \mathbf{29.8}$

***This work*:**

$[(0.337_{[\text{acetanlide}]} + 0.476_{[\text{butyl acrylate}]} + 12.655_{[\text{GVL}]} + 0.027_{[\text{benzoquinone}]} + 0.475_{[\text{TsOH}]}) - (0.489_{[\text{product}]} + 12.02_{\text{GVL recovered}})]/ 0.489_{[\text{product}]} = \mathbf{3.0}$

5. RME and MRP calculation

RME = [(Mass of Product/(Total imput mass – Mass of recovered materials)]*100

Ref 18a = [(0.702/(29.735 – 0)]*100 = **2.4**

Ref 18b = [(0.061/(1.258 – 0)]*100 = **4.9**

Ref 18c = [(0.269/(4.756 – 0)]*100 = **5.7**

Ref 18c (*under air*)= [(0.267/(4.399 – 0)]*100 = **6.1**

Ref 18d = [(0.039/(6.408 – 0.001)]*100 = **0.6** (heterogeneous catalyst recovered)

Ref 18e = [(0.072/(1.784 – 0)]*100 = **4.1**

Ref 18f = [(0.111/(133.833 – 0)]*100 = **0.1**

Ref 18g = [(0.250/(13.120 – 0)]*100 = **1.9**

Ref 18h = [(0.042/(29.763 – 0)]*100 = **0.1**

Ref 15c = [(0.124/(5.104 – 0.163)]*100 = **2.5** (heterogeneous catalyst and base recovered)

Ref 15c = [(108.996/(3364.983 – 2.00)]*100 = **3.2** (heterogeneous catalyst recovered)

This work = [(0.489/(13.972 – 12.082)]*100 = **25.8** (solvent and heterogeneous catalyst recovered)

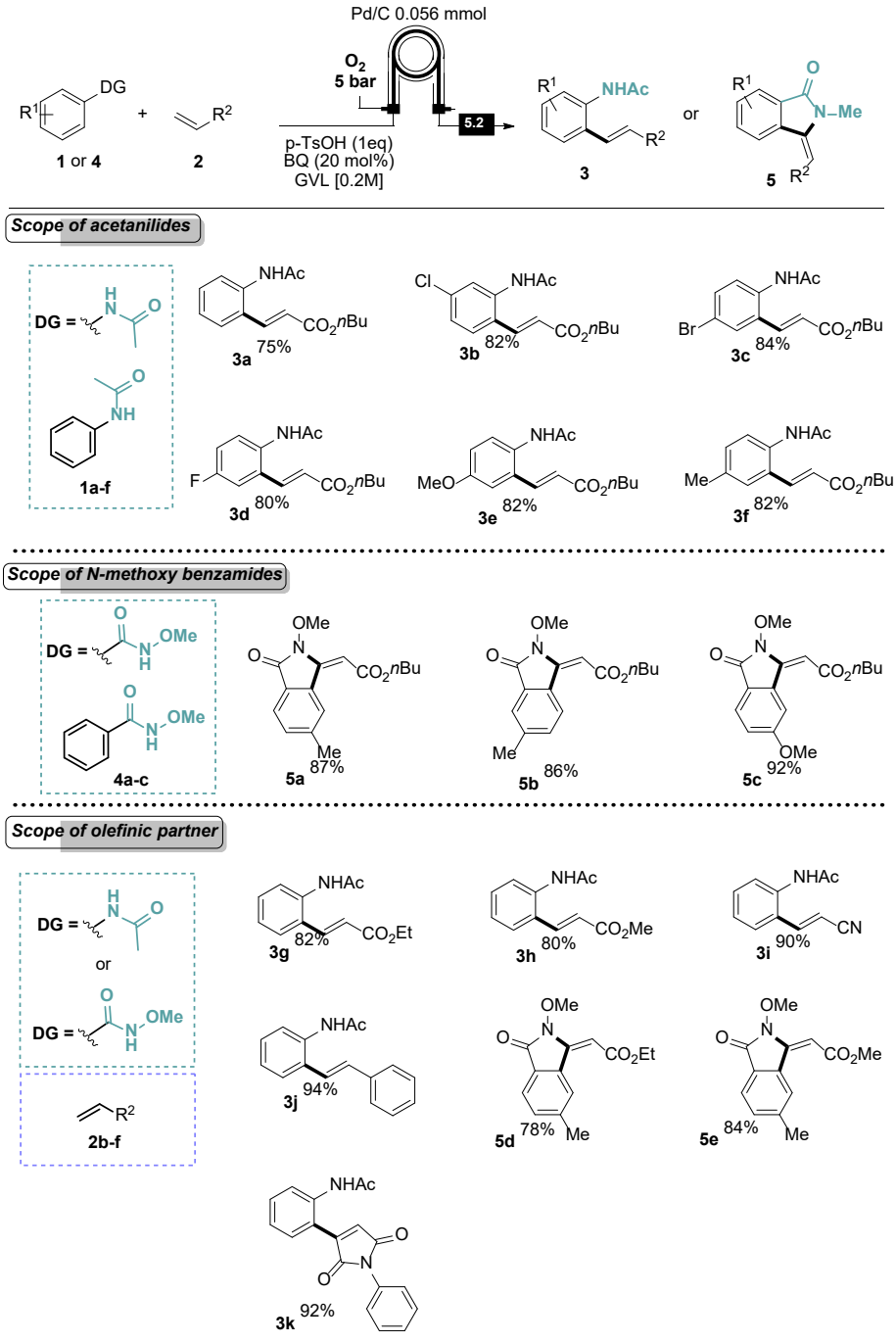
MRP = [(RME/100)*(Stoichiometric factor)]/[(AE/100)*(Yield/100)]

Stoichiometric factor (SF) = (Actual mass of reagent)/(Stoichiometric mass of reagent)

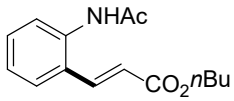
AE is 99.6 % for all the protocols analyzed

Ref 18a: SF= 1	**MRP**= [(2.4/100)*(1)]/[(0.996)*(85/100)] = **0.028**
Ref 18b: SF= 1.43	**MRP**= [(4.9/100)*(1.43)]/[(0.996)*(85/100)] = **0.083**
Ref 18c: SF= 1.23	**MRP**= [(5.7/100)*(1.23)]/[(0.996)*(98/100)] = **0.071**
Ref 18c (*under air*): SF= 1.23	**MRP**= [(6.1/100)*(1.23)]/[(0.996)*(97/100)] = **0.077**
Ref 18d: SF= 1.48	**MRP**= [(0.6/100)*(1.48)]/[(0.996)*(76/100)] = **0.012**
Ref 18e: SF= 1.61	**MRP**= [(4.1/100)*(1.68)]/[(0.996)*(82/100)] = **0.084**
Ref 18f: SF= 1.05	**MRP**= [(0.1/100)*(1.05)]/[(0.996)*(71/100)] = **0.001**
Ref 18g: SF= 1.11	**MRP**= [(1.9/100)*(1.11)]/[(0.996)*(91/100)] = **0.023**
Ref 18h: SF= 1.97	**MRP**= [(0.1/100)*(1.97)]/[(0.996)*(80/100)] = **0.002**
Ref 15c: SF= 1.05	**MRP**= [(2.5/100)*(1.05)]/[(0.996)*(95/100)] = **0.027**
Ref 15c: SF= 1.05	**MRP**= [(3.2/100)*(1.05)]/[(0.996)*(97/100)] = **0.035**
This work: SF= 1.24	**MRP**= [(25.8/100)*(1.24)]/[(0.996)*(75/100)] = **0.428**

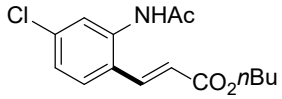
6. Substrates scope using 20 mol% of *p*-benzoquinone in Flow



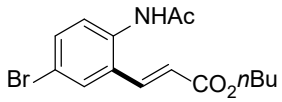
7. Characterization data of products



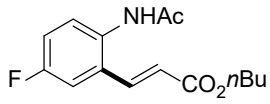
butyl (E)-3-(2-acetamidophenyl)acrylate (3a): The general flow procedure was followed using *N*-phenylacetamide (**1a**) (337.9 mg, 2.5 mmol) and butyl acrylate (**2a**) (537 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 4/1) yielded **3a** (489.9 mg, 75%) as white solid. **M.p.** 82-85 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 15.8 Hz, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.55 – 7.53 (m, 2H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 6.38 (d, *J* = 15.7 Hz, 1H), 4.18 (t, *J* = 6.7 Hz, 2H), 2.21 (s, 3H), 1.70 – 1.63 (m, 2H), 1.46 – 1.37 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.1, 167.0, 139.5, 136.0, 130.9, 127.9, 127.2, 126.0, 125.5, 120.6, 64.8, 30.8, 24.2, 19.3, 13.9. **GC-EIMS (m/z, %):** 261 (M^+, 80), 219 (25), 146 (100), 128 (43), 126 (25). **Elemental Analysis**: Calc: C, 68.94; H, 7.33; N, 5.36. Found: C, 68.93; H, 7.34; N, 5.37.



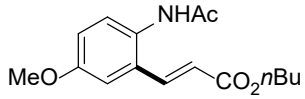
butyl (E)-3-(2-acetamido-4-chlorophenyl)acrylate (3b): The general flow procedure was followed using *N*-(3-chlorophenyl)acetamide (**1b**) (424.0 mg, 2.5 mmol) and butyl acrylate (**2a**) (537 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 4/1 → 3/1) yielded **3b** (598.9 mg, 81%) as off-white solid. **M.p.** 152-154 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.72 – 7.66 (m, 3H), 7.48 – 7.46 (m, 1H), 7.39 (s, 1H), 6.38 (d, *J* = 15.8 Hz, 1H), 4.20 (t, *J* = 6.7 Hz, 2H), 2.21 (s, 3H), 1.71 – 1.64 (m, 2H), 1.47 – 1.36 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.0, 166.7, 137.9, 134.9, 133.6, 129.9, 129.3, 126.7, 122.1, 119.1, 65.0, 30.8, 24.3, 19.3, 13.9. **GC-EIMS (m/z, %):** 295 (M^+, 45), 253 (30), 182 (45), 180 (100), 162 (50), 154 (25). **Elemental Analysis:** Calc: C, 60.92; H, 6.13; N, 4.74. Found: C, 60.91; H, 6.15; N, 4.73.



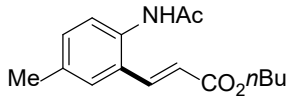
butyl (E)-3-(2-acetamido-5-bromophenyl)acrylate (3c): The general flow procedure was followed using *N*-(4-bromophenyl)acetamide (**1c**) (535.1 mg, 2.5 mmol) and butyl acrylate (**2a**) (537 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 4/1 → 3/1) yielded **3c** (714.4 mg, 84%) as off-white solid. **M.p.** 121-123 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 – 7.77 (m, 2H), 7.70 (d, *J* = 15.8 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.11 (d, *J* = 8.2 Hz, 1H), 6.32 (d, *J* = 15.7 Hz, 1H), 4.16 (t, *J* = 6.7 Hz, 2H), 2.20 (s, 3H), 1.68 – 1.61 (m, 2H), 1.44 – 1.35 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.2, 166.9, 138.4, 137.0, 136.5, 128.0, 126.0, 125.8, 125.1, 120.8, 64.9, 30.8, 24.2, 19.3, 13.8. **GC-EIMS (m/z, %):** 341 (M^++1, 25), 339 (M^+-1, 25), 299 (28), 297 (28), 224 (100), 198 (35). **Elemental Analysis**: Calc: C, 52.96; H, 5.33; N, 4.12. Found: C, 52.95; H, 5.34; N, 4.14.



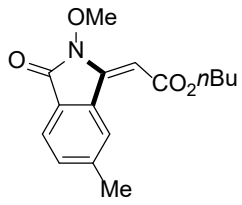
butyl (E)-3-(2-acetamido-5-fluorophenyl)acrylate (3d): The general flow procedure was followed using *N*-(4-fluorophenyl)acetamide (**1d**) (382.9 mg, 2.5 mmol) and butyl acrylate (**2a**) (537 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 4/1) yielded **3d** (558.6 mg, 80%) as white solid. **M.p.** 137-139 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 15.9 Hz, 1H), 7.62 (dd, *J* = 8.9, 5.2 Hz, 1H), 7.38 (s, 1H), 7.24 (dd, *J* = 9.2, 3.0 Hz, 1H), 7.07 (td, *J* = 8.3, 2.9 Hz, 1H), 6.37 (d, *J* = 15.9 Hz, 1H), 4.20 (t, *J* = 6.7 Hz, 2H), 2.21 (s, 3H), 1.71 – 1.64 (m, 2H), 1.47 – 1.37 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.2, 166.7, 160.5 ($^1J_{C\text{-}F}$ = 246), 138.3, 132.0, 130.2 ($^3J_{C\text{-}F}$ = 8), 127.9 ($^3J_{C\text{-}F}$ = 8), 121.8, 117.8 ($^2J_{C\text{-}F}$ = 23), 113.3 ($^2J_{C\text{-}F}$ = 23), 65.0, 30.8, 24.1, 19.3, 13.9. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -115.41 (q, *J* = 7.8 Hz). **GC-EIMS (m/z, %):** 279 (M^+, 28), 237 (50), 164 (100), 136 (44), 135 (25). **Elemental Analysis:** Calc: C, 64.50; H, 6.50; N, 5.01. Found: C, 64.48; H, 6.51; N, 5.02.



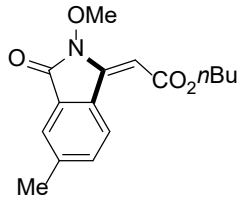
butyl (E)-3-(2-acetamido-5-methoxyphenyl)acrylate (3e): The general flow procedure was followed using *N*-(4-methoxyphenyl)acetamide (**1e**) (412.9 mg, 2.5 mmol) and butyl acrylate (**2a**) (537 µL, 3.75 mmol). Purification by crystallization (hexane/acetone: 9/1) yielded **3e** (582.7 mg, 80%) as off-white solid. **M.p.** 128-130 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 15.9 Hz, 1H), 7.49 (d, *J* = 8.8 Hz, 1H), 7.07 (d, *J* = 2.9 Hz, 2H), 6.96 – 6.93 (m, 2H), 6.38 (d, *J* = 15.9 Hz, 1H), 4.21 (t, *J* = 6.7 Hz, 2H), 3.82 (s, 3H), 2.21 (s, 3H), 1.72 – 1.65 (m, 2H), 1.48 – 1.39 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.2, 166.9, 157.9, 139.4, 130.1, 129.0, 127.9, 120.9, 117.0, 111.4, 64.8, 55.7, 30.9, 24.1, 19.3, 13.9. **GC-EIMS (m/z, %):** 291 (M^+, 45), 249 (20), 176 (100), 175 (52). **Elemental Analysis**: Calc: C, 65.96; H, 7.27; N, 4.81. Found: C, 65.96; H, 7.29; N, 4.82.



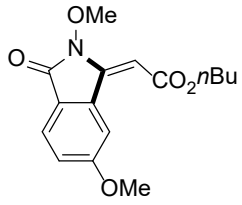
butyl (E)-3-(2-acetamido-5-methylphenyl)acrylate (3f): The general flow procedure was followed using *N*-(p-tolyl)acetamide (**1f**) (372.9 mg, 2.5 mmol) and butyl acrylate (**2a**) (537 µL, 3.75 mmol). Purification by crystallization (hexane/acetone: 9/1) yielded **3f** (564.4 mg, 82%) as white solid. **M.p.** 127-129 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 15.9 Hz, 1H), 7.55 (d, *J* = 8.2 Hz, 1H), 7.36 (s, 1H), 7.29 (s, 1H), 7.18 (d, *J* = 8.2 Hz, 1H), 6.38 (d, *J* = 15.9 Hz, 1H), 4.19 (t, *J* = 6.6 Hz, 2H), 2.33 (s, 3H), 2.21 (s, 3H), 1.69 – 1.64 (m, 2H), 1.45 – 1.40 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.1, 167.1, 139.5, 135.9, 133.5, 131.7, 128.0, 127.5, 125.7, 120.4, 64.7, 30.8, 24.2, 21.0, 19.3, 13.9. **GC-EIMS (m/z, %):** 275 (M^+, 45), 233 (15), 161 (18), 160 (100), 142 (25). **Elemental Analysis:** Calc: C, 69.79; H, 7.69; N, 5.09. Found: C, 69.80; H, 7.70; N, 5.07.



butyl (E)-2-(2-methoxy-6-methyl-3-oxoisoindolin-1-ylidene)acetate (5a): The general flow procedure was followed using *N*-methoxy-4-methylbenzamide (**4a**) (412.9 mg, 2.5 mmol) and butyl acrylate (**2a**) (537 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 6/1→ 4/1) yielded **5a** (622.1 mg, 86%) as white solid. **M.p.** 62-64 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.81 (s, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.39 (d, *J* = 7.7 Hz, 1H), 5.95 (s, 1H), 4.22 (t, *J* = 6.7 Hz, 2H), 4.01 (s, 3H), 2.50 (s, 3H), 1.72 – 1.67 (m, 2H), 1.48 – 1.42 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.2, 161.9, 144.7, 144.1, 132.3, 130.5, 128.8, 124.9, 123.3, 97.5, 64.7, 64.4, 30.9, 22.5, 19.3, 13.9. **GC-EIMS (m/z, %):** 289 (M^+, 20), 259 (77), 258 (20), 202 (100), 158 (25). **Elemental Analysis**: Calc: C, 66.42; H, 6.62; N, 4.84. Found: C, 66.40; H, 6.63; N, 4.85.

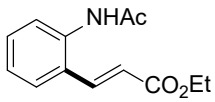


butyl (E)-2-(2-methoxy-5-methyl-3-oxoisoindolin-1-ylidene)acetate (5b): The general flow procedure was followed using *N*-methoxy-3-methylbenzamide (**4b**) (412.9 mg, 2.5 mmol) and butyl acrylate (**2a**) (537 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 6/1→ 4/1) yielded **5b** (607.6 mg, 84%) as white solid. **M.p.** 79-81 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 8.0 Hz, 1H), 7.63 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 5.93 (s, 1H), 4.21 (t, *J* = 6.7 Hz, 2H), 4.02 (s, 3H), 2.46 (s, 3H), 1.73 – 1.66 (m, 2H), 1.47 – 1.41 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.2, 162.0, 144.1, 142.5, 134.3, 128.2, 127.7, 123.8, 97.1, 64.6, 64.5, 30.9, 21.8, 19.3, 13.9. **GC-EIMS (m/z, %):** 289 (M^+, 15), 260 (35), 259 (45), 202 (100), 147 (80). **Elemental Analysis**: Calc: C, 66.42; H, 6.62; N, 4.84. Found: Calc: C, 66.43; H, 6.63; N, 4.82.

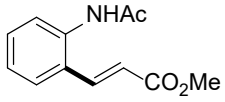


butyl (E)-2-(2,6-dimethoxy-3-oxoisoindolin-1-ylidene)acetate (5c): The general flow procedure was followed using *N*,4-dimethoxybenzamide (**4c**) (452.9 mg, 2.5 mmol) and butyl acrylate (**2a**) (537 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 6/1→ 4/1) yielded **5c** (687.0 mg, 90%) as white solid. **M.p.** 88-90 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.06 (d, *J* = 8.3 Hz, 1H), 5.93 (s, 1H), 4.20 (t, *J* = 6.7 Hz, 2H), 4.00 (s, 3H), 3.91 (s, 3H), 1.69 (p, *J* = 7.0 Hz, 2H), 1.43 (q, *J* = 7.5 Hz, 2H), 0.95 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.1, 164.4, 161.9, 144.1, 132.5,

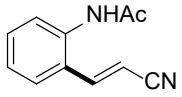
124.9, 119.6, 118.1, 113.1, 97.5, 64.6, 64.4, 55.9, 30.8, 19.3, 13.8. **GC-EIMS (m/z, %):** 305 (M^+, 35), 274 (55), 233 (22), 193 (100), 191 (58), 163 (24). **Elemental Analysis**: Calc: C, 62.94; H, 6.27; N, 4.59. Found: C, 62.93; H, 6.26; N, 4.60.



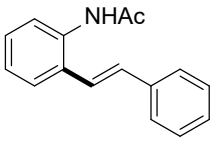
ethyl (E)-3-(2-acetamidophenyl)acrylate (3g): The general flow procedure was followed using *N*-phenylacetamide (**1a**) (337.9 mg, 2.5 mmol) and ethyl acrylate (**2b**) (408 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 4/1→ 2/1) yielded **3g** (478.1 mg, 82%) as white solid. **M.p.** 140-143 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 15.8, 2.9 Hz, 1H), 7.74 – 7.55 (m, 2H), 7.55 – 7.49 (m, 1H), 7.37 – 7.32 (m, 1H), 7.19 – 7.14 (m, 1H), 6.36 (dd, *J* = 15.8, 6.6 Hz, 1H), 4.26 – 4.21 (m, 2H), 2.19 (d, *J* = 7.2 Hz, 3H), 1.31 (td, *J* = 7.1, 4.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.2, 166.9, 139.6, 136.1, 130.8, 127.9, 127.2, 126.0, 125.6, 120.4, 60.8, 24.2, 14.4. **GC-EIMS (m/z, %):** 233 (M^+, 45), 191 (25), 146 (100), 145 (48), 128 (52), 118 (36). **Elemental Analysis**: Calc: C, 66.94; H, 6.48; N, 6.00. Found: C, 66.92; H, 6.49; N, 6.01.



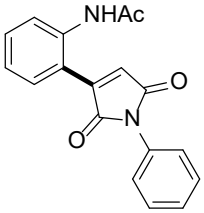
methyl (E)-3-(2-acetamidophenyl)acrylate (3h): The general flow procedure was followed using *N*-phenylacetamide (**1a**) (337.9 mg, 2.5 mmol) and methyl acrylate (**2c**) (338 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 4/1→ 2/1) yielded **3h** (438.4 mg, 80%) as off-white solid. **M.p.** 136-138 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 15.8 Hz, 1H), 7.67 – 7.63 (m, 2H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.36 (d, *J* = 15.7 Hz, 1H), 3.78 (s, 3H), 2.20 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.2, 167.3, 139.8, 136.1, 130.9, 127.9, 127.2, 126.1, 125.6, 120.1, 51.9, 24.2. **GC-EIMS (m/z, %):**219 (M^+, 25), 177 (32), 176 (46), 146 (100), 118 (55). **Elemental Analysis**: Calc: C, 65.74; H, 5.98; N, 6.39. Found: C, 65.73; H, 5.97; N, 6.40.



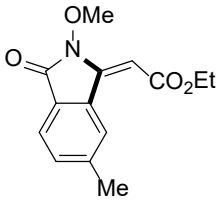
(E)-N-(2-(2-cyanovinyl)phenyl)acetamide (3i): The general flow procedure was followed using *N*-phenylacetamide (**1a**) (337.9 mg, 2.5 mmol) and acrylonitrile (**2d**) (246 µL, 3.75 mmol). Purification by crystallization (hexane/acetone: 9/1) yielded **3i** (418.9 mg, 90%) as pale brown solid. **M.p.** 171-174 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 – 7.57 (m, 3H), 7.48 – 7.42 (m, 2H), 7.40 – 7.21 (m, 1H), 5.82 (d, *J* = 16.5 Hz, 1H), 2.22 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.3, 146.4, 135.6, 131.8, 127.7, 126.4, 126.1, 126.1, 118.3, 97.8, 23.9. **GC-EIMS (m/z, %)**: 186 (M^+, 28), 171 (25), 144 (100), 117 (70). **Elemental Analysis**: Calc: C, 70.95; H, 5.41; N, 15.04. Found: C, 70.93; H, 5.42; N, 15.03.



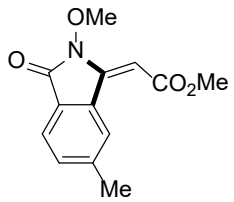
(E)-N-(2-styrylphenyl)acetamide (3j): The general flow procedure was followed using *N*-phenylacetamide (**1a**) (337.9 mg, 2.5 mmol) and styrene (**2e**) (430 µL, 3.75 mmol). Purification by crystallization (hexane/acetone: 9/1) yielded **3j** (551.7 mg, 93%) as white solid. **M.p.** 141-143 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 – 7.76 (m, 1H), 7.54 – 7.50 (m, 3H), 7.40 – 7.36 (m, 2H), 7.32 – 7.28 (m, 2H), 7.20 – 7.11 (m, 2H), 6.99 (d, *J* = 16.1 Hz, 1H), 2.20 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.7, 137.1, 134.8, 132.6, 132.5, 130.5, 128.9, 128.5, 128.3, 127.0, 126.8, 125.8, 124.5, 124.4, 123.6, 24.4. **GC-EIMS (m/z, %)**: 237 (M^+, 34), 222 (18), 195 (20), 194 (100), 165 (32). **Elemental Analysis**: Calc: C, 80.98; H, 6.37; N, 5.90. Found: C, 80.97; H, 6.38; N, 5.91.



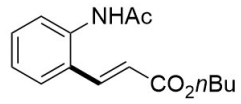
***N*-(2-(2,5-dioxo-1-phenyl-2,5-dihydro-1H-pyrrol-3-yl)phenyl)acetamide (3k):** The general flow procedure was followed using *N*-phenylacetamide (**1a**) (337.9 mg, 2.5 mmol) and *N*-phenylmaleimide (**2f**) (649.4 mg, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 6/1→ 4/1) yielded **3k** (704.5 mg, 92%) as pale-yellow solid. **M.p.** 165-167 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.91 (s, 1H), 7.87 (d, *J* = 8.2 Hz, 1H), 7.53 – 7.47 (m, 4H), 7.44 – 7.37 (m, 3H), 7.29 – 7.25 (m, 1H), 6.80 (s, 1H), 2.12 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.9, 169.0, 168.5, 146.2, 135.6, 132.3, 131.2, 131.1, 129.4, 128.7, 128.4, 126.3, 126.2, 126.0, 122.5, 24.5. **GC-EIMS (m/z, %)**: 306 (M^+, 100), 264 (74), 246 (33), 235 (21), 219 (25), 172 (68). **Elemental Analysis:** Calc: C, 70.58; H, 4.61; N, 9.15. Found: C, 70.56; H, 4.62; N, 9.16.



ethyl (E)-2-(2-methoxy-6-methyl-3-oxoisoindolin-1-ylidene)acetate (5d): The general flow procedure was followed using *N*-methoxy-4-methylbenzamide (**4a**) (412.9 mg, 2.5 mmol) and ethyl acrylate (**2b**) (408 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 6/1→ 4/1) yielded **5d** (509.4 mg, 78%) as colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 7.67 (d, *J* = 7.7 Hz, 1H), 7.35 (d, *J* = 7.7 Hz, 1H), 5.91 (s, 1H), 4.25 (q, *J* = 7.1 Hz, 2H), 3.99 (s, 3H), 2.47 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.0, 161.8, 144.6, 144.0, 132.3, 130.4, 128.7, 124.8, 123.2, 97.4, 64.3, 60.6, 22.4, 14.4. **GC-EIMS (m/z, %):** 261 (M^+,28), 231 (25), 217 (100), 216 (58), 176 (25), 175 (17). **Elemental Analysis**: Calc: C, 64.36; H, 5.79; N, 5.36. Found: C, 64.35; H, 5.78; N, 5.37.



ethyl (E)-2-(2-methoxy-6-methyl-3-oxoisoindolin-1-ylidene)acetate (5e): The general flow procedure was followed using *N*-methoxy-4-methylbenzamide (**4a**) (412.9 mg, 2.5 mmol) and methyl acrylate (**2c**) (338 µL, 3.75 mmol). Purification by column chromatography (petroleum ether/EtOAc: 6/1→ 4/1) yielded **5e** (506.8 mg, 82%) as colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 7.7 Hz, 1H), 5.92 (s, 1H), 3.99 (s, 3H), 3.80 (s, 3H), 2.47 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.4, 161.8, 144.7, 144.3, 132.3, 130.4, 128.7, 124.8, 123.2, 96.8, 64.3, 51.8, 22.4. **GC-EIMS (m/z, %):** 247 (M^+, 15), 231 (44), 217 (100), 216 (18), 147(20). **Elemental Analysis**: Calc: C, 63.15; H, 5.30; N, 5.67. Found: C, 63.17; H, 5.29; N, 5.66.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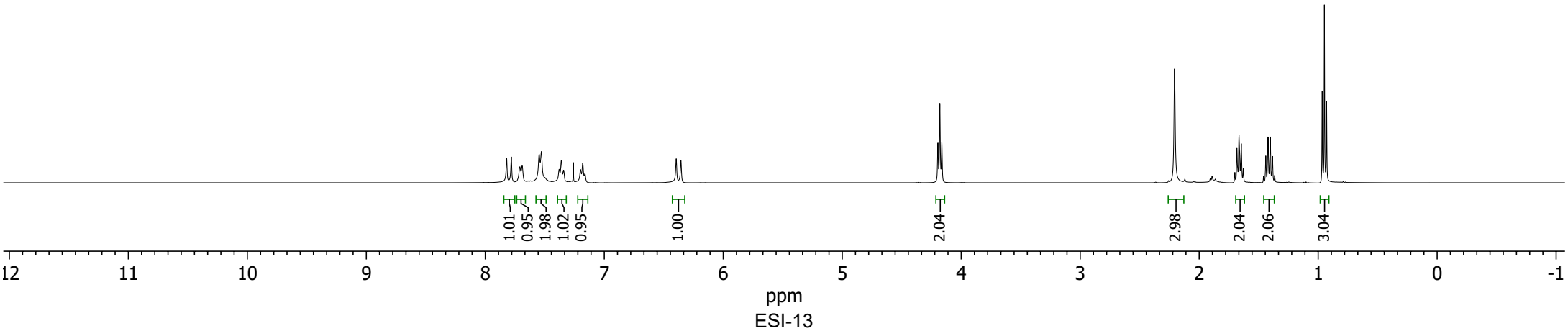
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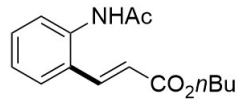
ESI-13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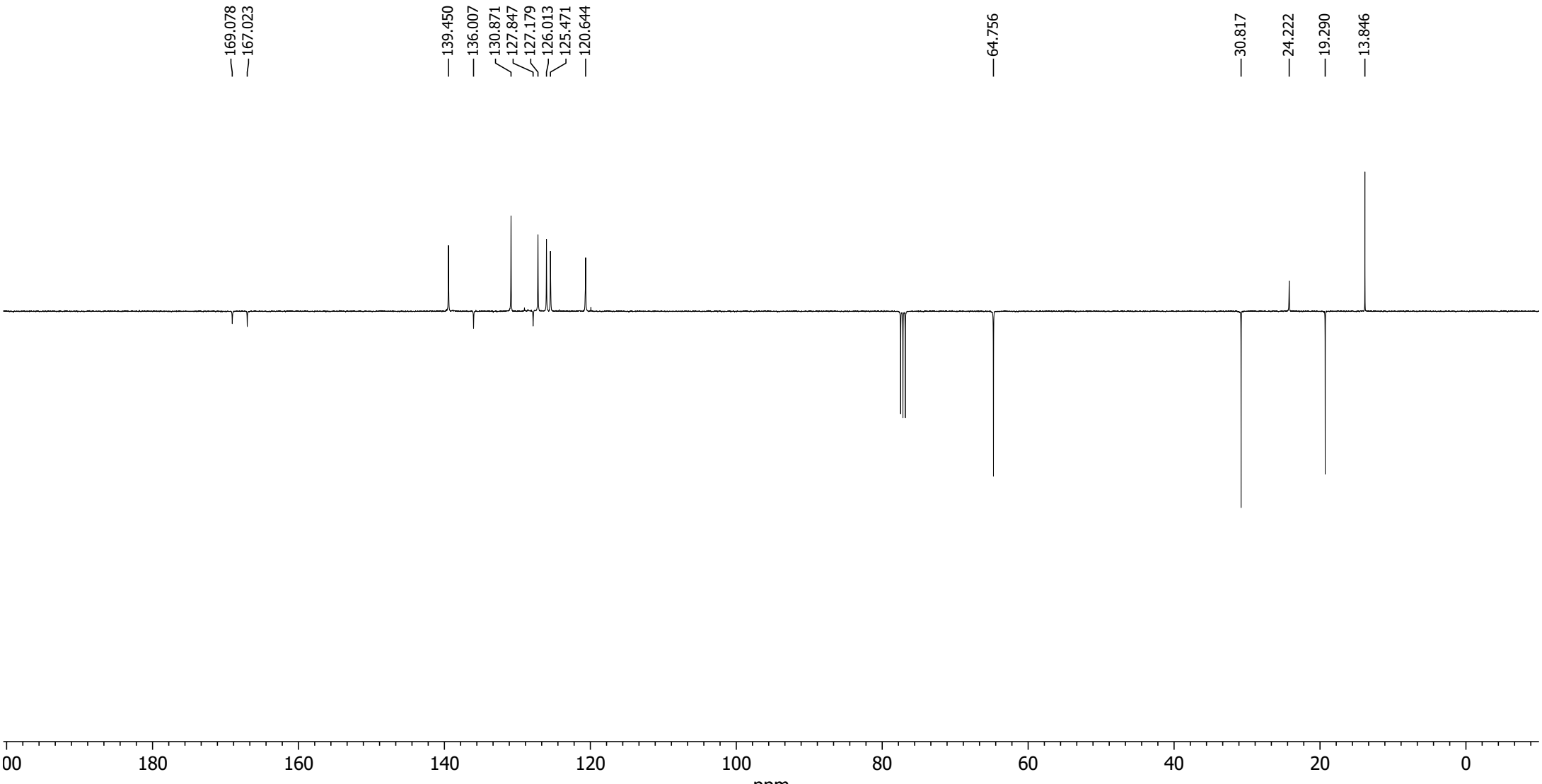
3a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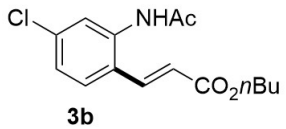
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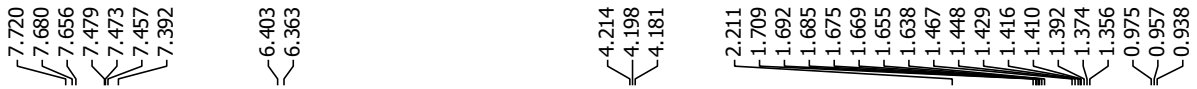
3b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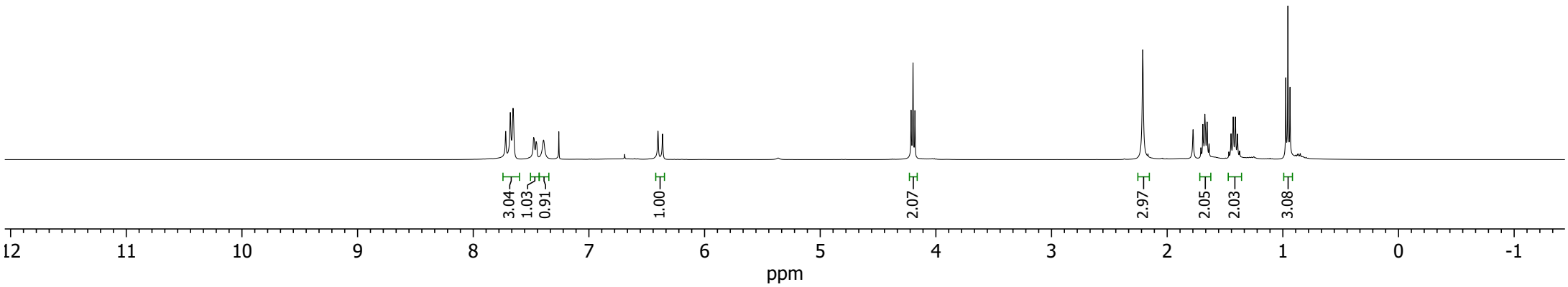
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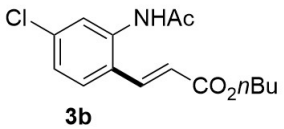
ESI-15



3b

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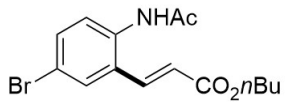
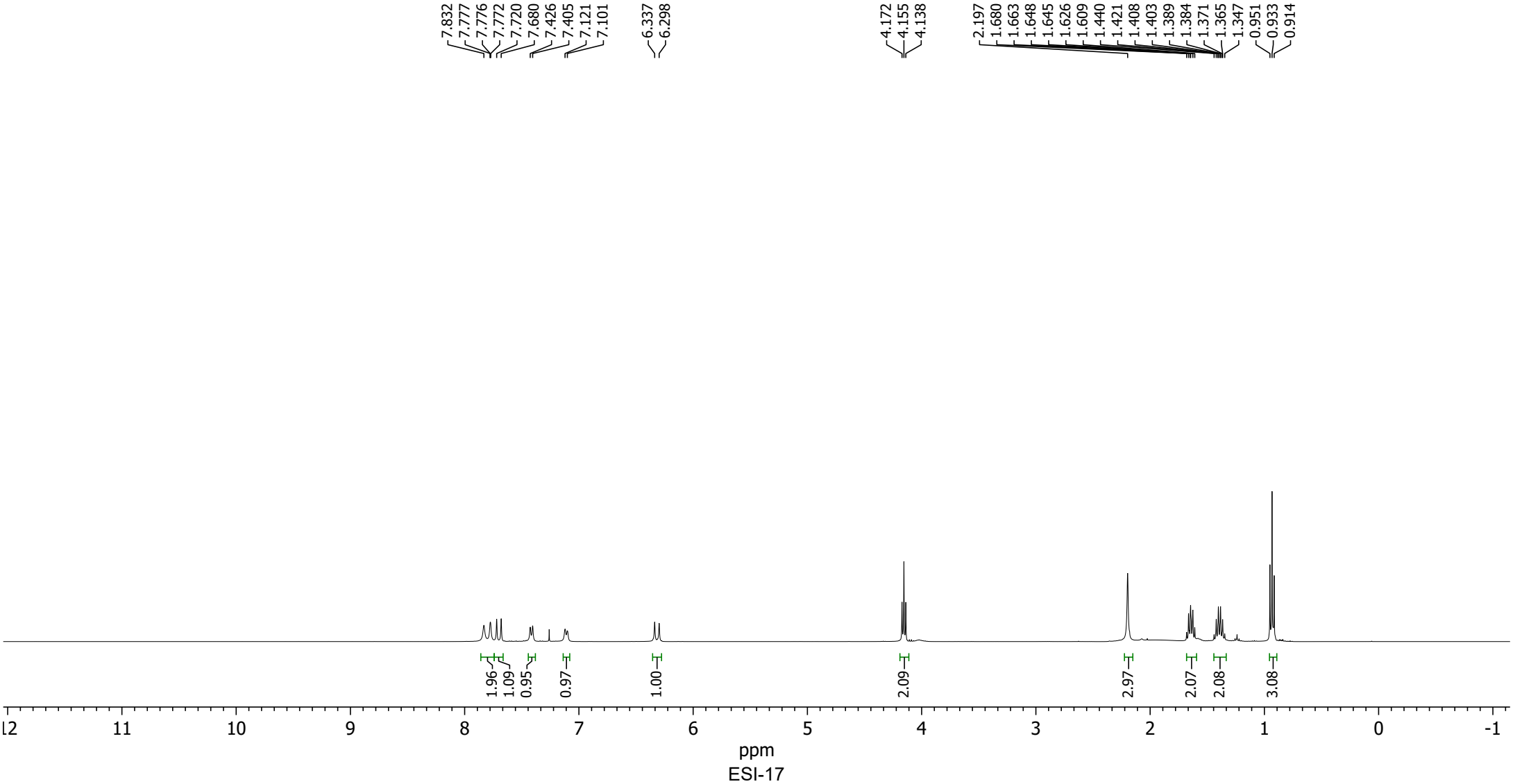
ppm

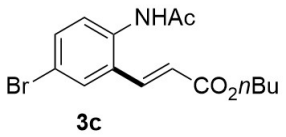
ESI-16


NHAc
Br
CO2nBu

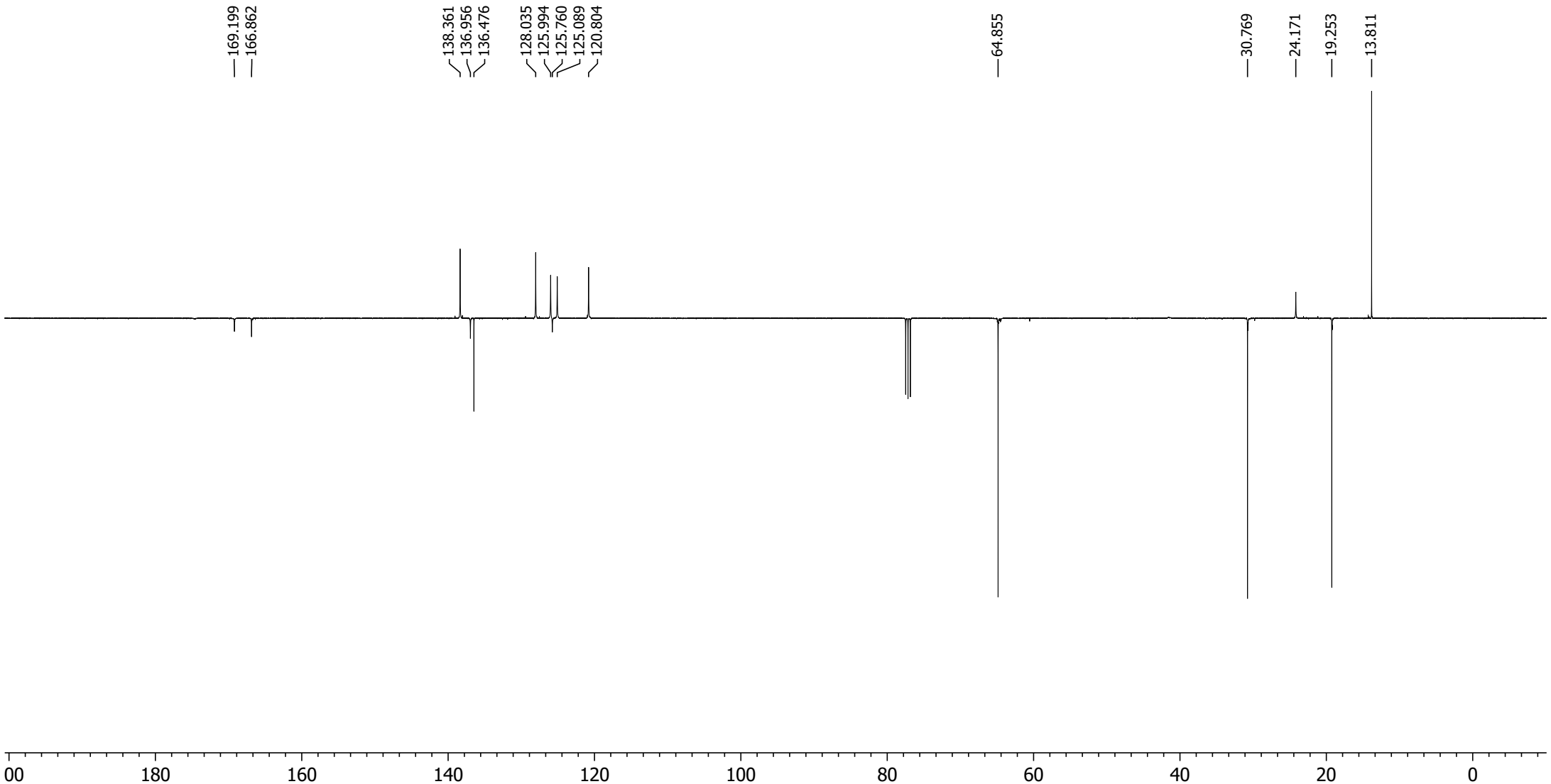
3c


7.832
7.777
7.776
7.772
7.720
7.680
7.426
7.405
7.121
7.101
6.337
6.298
4.172
4.155
4.138
2.197
1.680
1.663
1.648
1.645
1.626
1.609
1.440
1.421
1.408
1.403
1.389
1.384
1.371
1.365
1.347
0.951
0.933
0.914
1.96
1.09
0.95
0.97
1.00
2.09
2.97
2.07
2.08
3.08
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

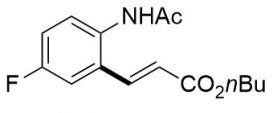
ESI-17


NHAc
Br
CO2nBu

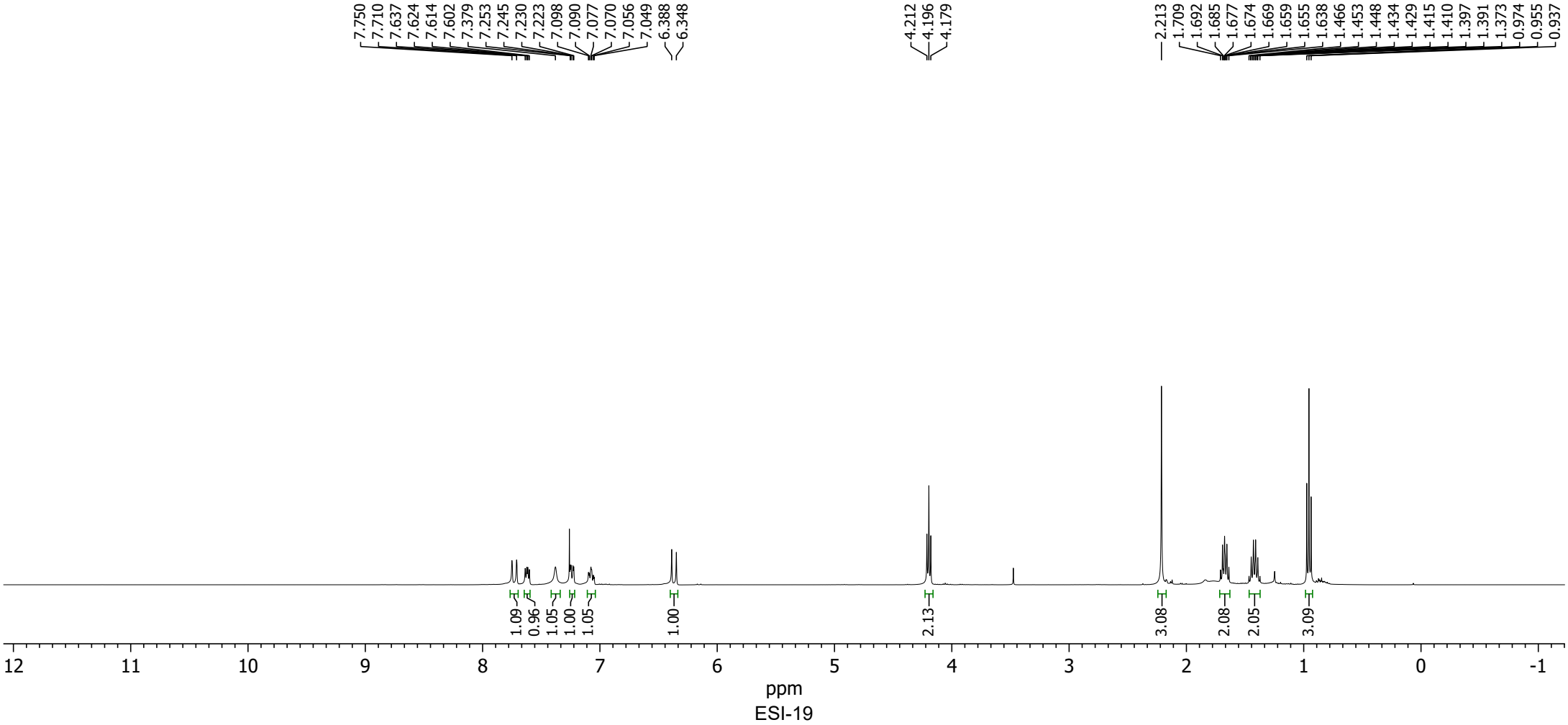
3c


169.199
166.862
138.361
136.956
136.476
128.035
125.994
125.760
125.089
120.804
64.855
30.769
24.171
19.253
13.811
00
180
160
140
120
100
80
60
40
20
0
ppm

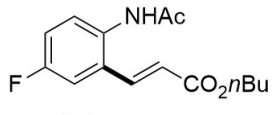
ESI-18


NHAc
F
CO_2nBu

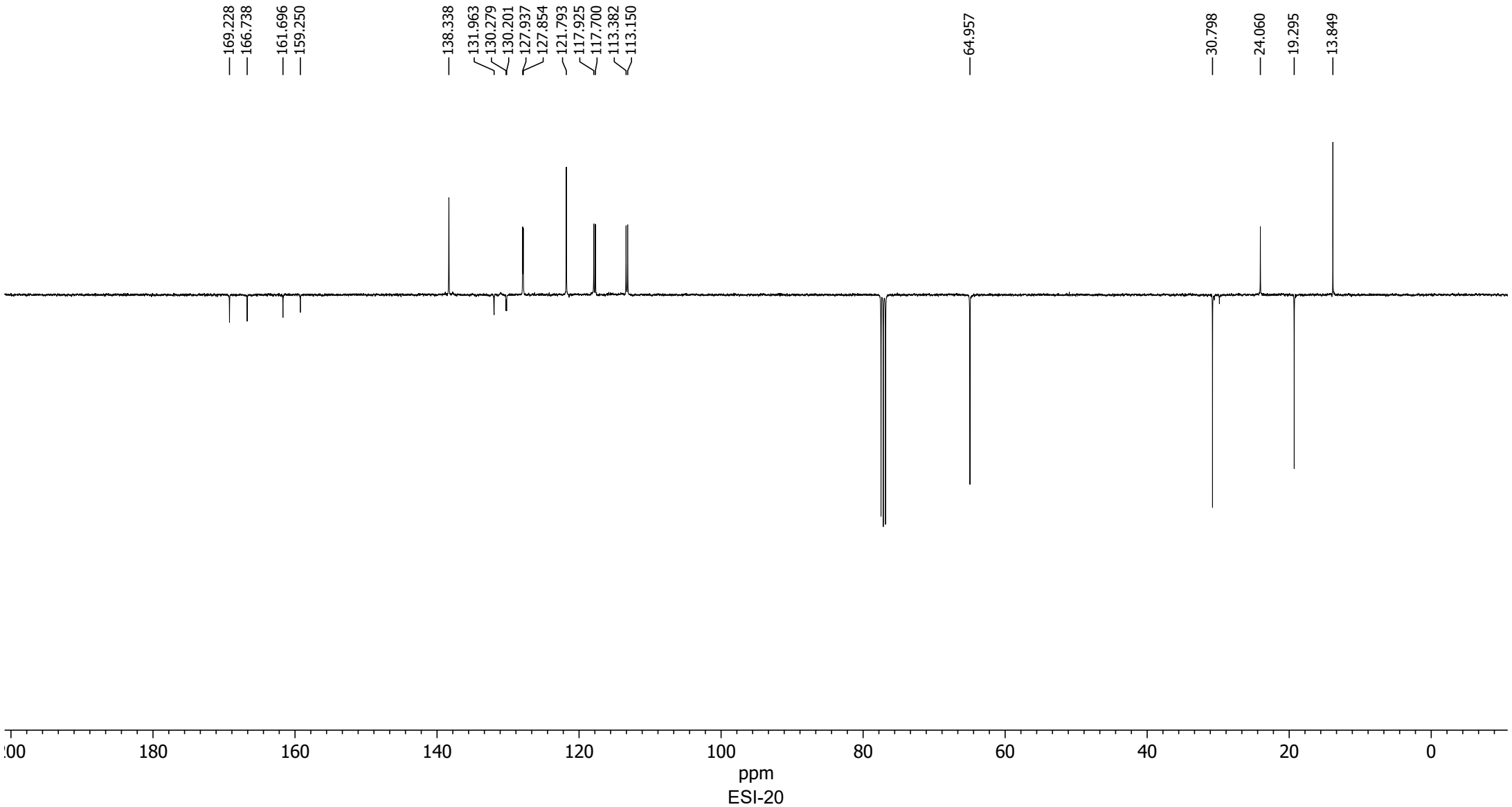
3d


7.750
7.710
7.637
7.624
7.614
7.602
7.379
7.253
7.245
7.230
7.223
7.098
7.090
7.077
7.070
7.056
7.049
6.388
6.348
4.212
4.196
4.179
2.213
1.709
1.692
1.685
1.677
1.674
1.669
1.659
1.655
1.638
1.466
1.453
1.448
1.434
1.429
1.415
1.410
1.397
1.391
1.373
0.974
0.955
0.937
1.09
0.96
1.05
1.00
1.05
1.00
2.13
3.08
2.08
2.05
3.09
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

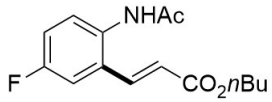
ESI-19


NHAc
F
CO2nBu

3d

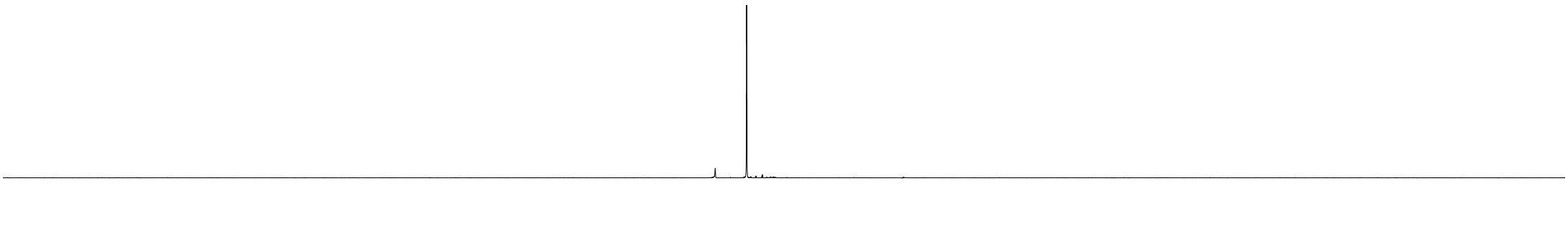

169.228
166.738
161.696
159.250
138.338
131.963
130.279
130.201
127.937
127.854
121.793
117.925
117.700
113.382
113.150
64.957
30.798
24.060
19.295
13.849
200
180
160
140
120
100
80
60
40
20
0
ppm

ESI-20

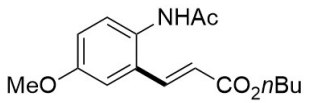


3d

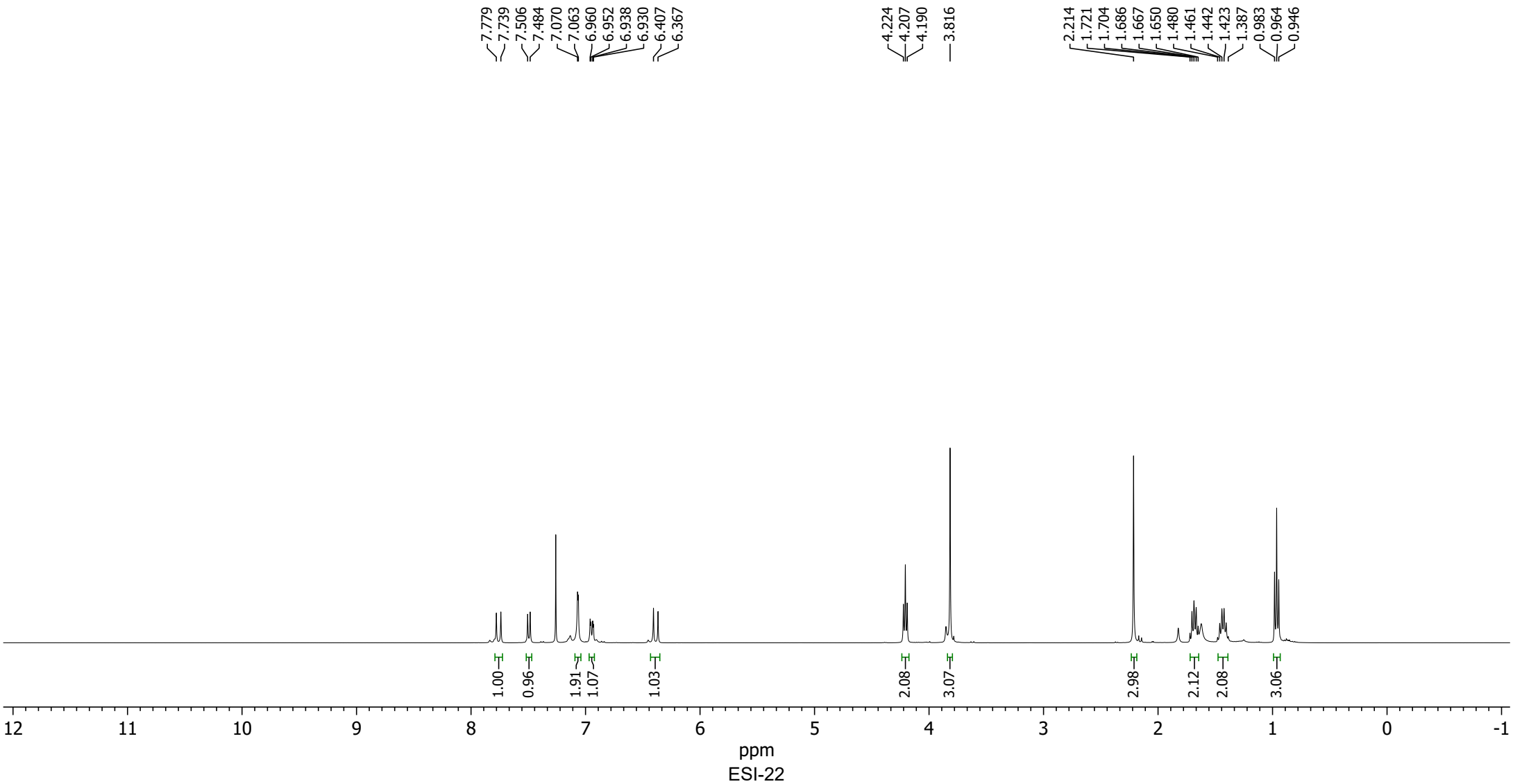
-115.378
-115.399
-115.417
-115.437



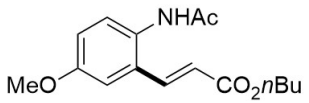
ESI-21


NHAc
MeO
CO2nBu

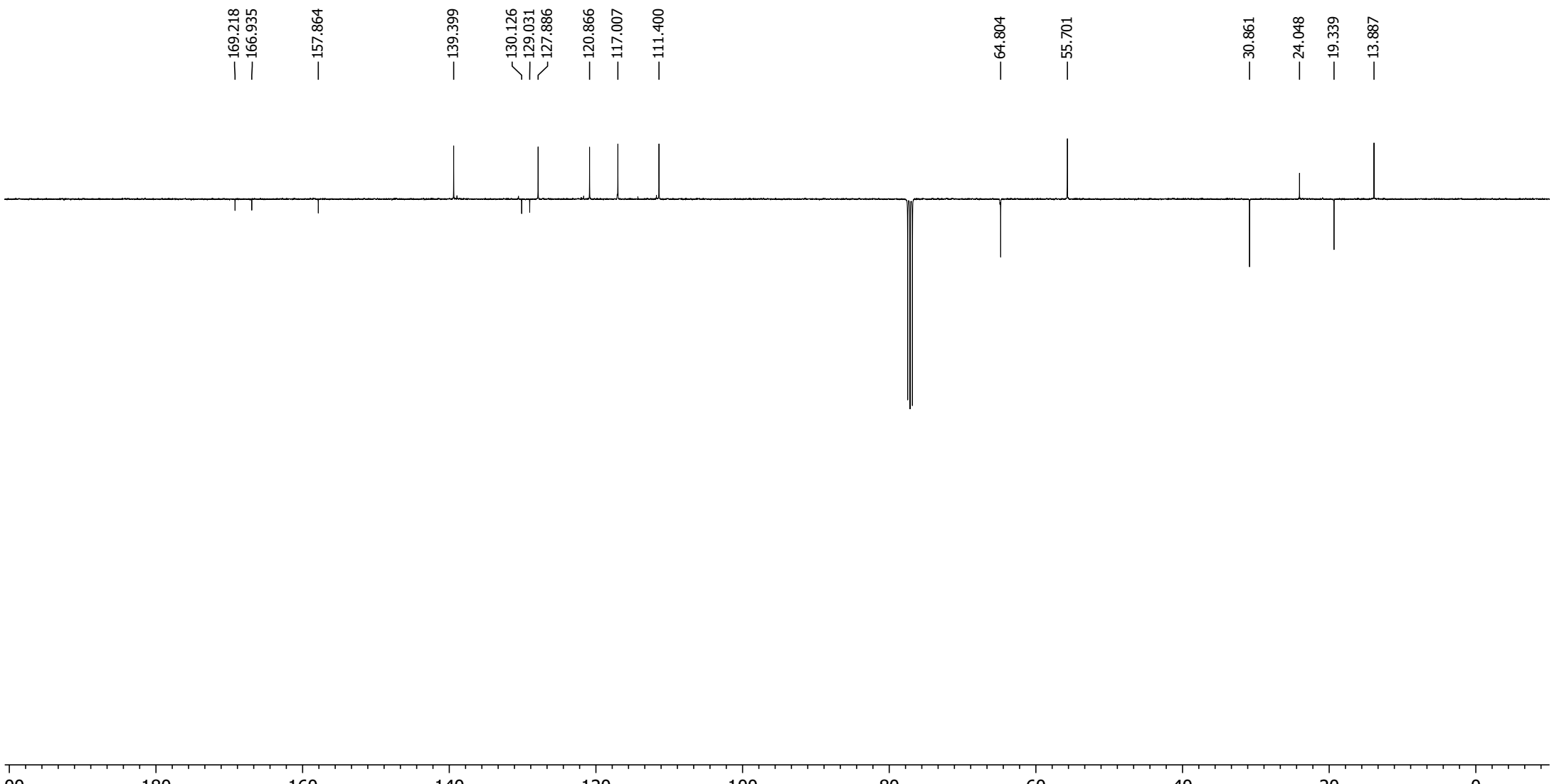
3e


7.779
7.739
7.506
7.484
7.070
7.063
6.960
6.952
6.938
6.930
6.407
6.367
4.224
4.207
4.190
3.816
2.214
1.721
1.704
1.686
1.667
1.650
1.480
1.461
1.442
1.423
1.387
0.983
0.964
0.946
1.00
0.96
1.91
1.07
1.03
2.08
3.07
2.98
2.12
2.08
3.06
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

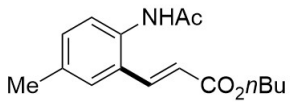
ESI-22


NHAc
MeO
CO2nBu

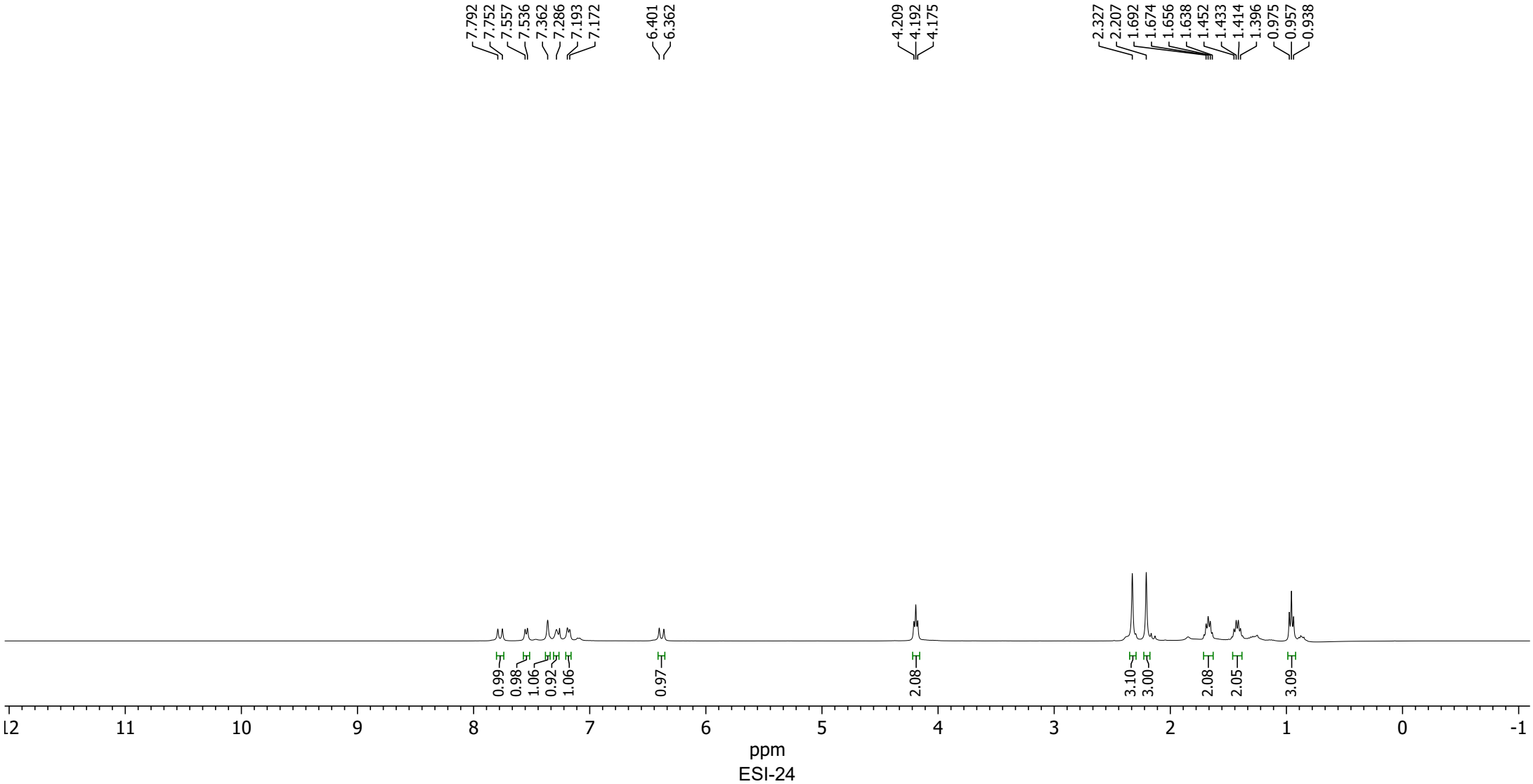
3e


169.218
166.935
157.864
139.399
130.126
129.031
127.886
120.866
117.007
111.400
64.804
55.701
30.861
24.048
19.339
13.887
00
180
160
140
120
100
80
60
40
20
0
ppm

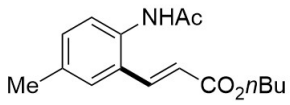
ESI-23


NHAc
Me
CO2nBu

3f


7.792
7.752
7.557
7.536
7.362
7.286
7.193
7.172
6.401
6.362
4.209
4.192
4.175
2.327
2.207
1.692
1.674
1.656
1.638
1.452
1.433
1.414
1.396
0.975
0.957
0.938
0.99
0.98
1.06
0.92
1.06
0.97
2.08
3.10
3.00
2.08
2.05
3.09
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

ESI-24



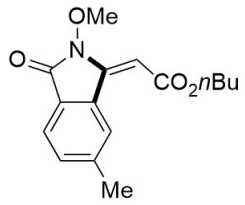
3f

169.071
167.088
139.497
135.926
133.458
131.735
127.962
127.494
125.694
120.399
64.717
30.835
24.178
21.069
19.307
13.855

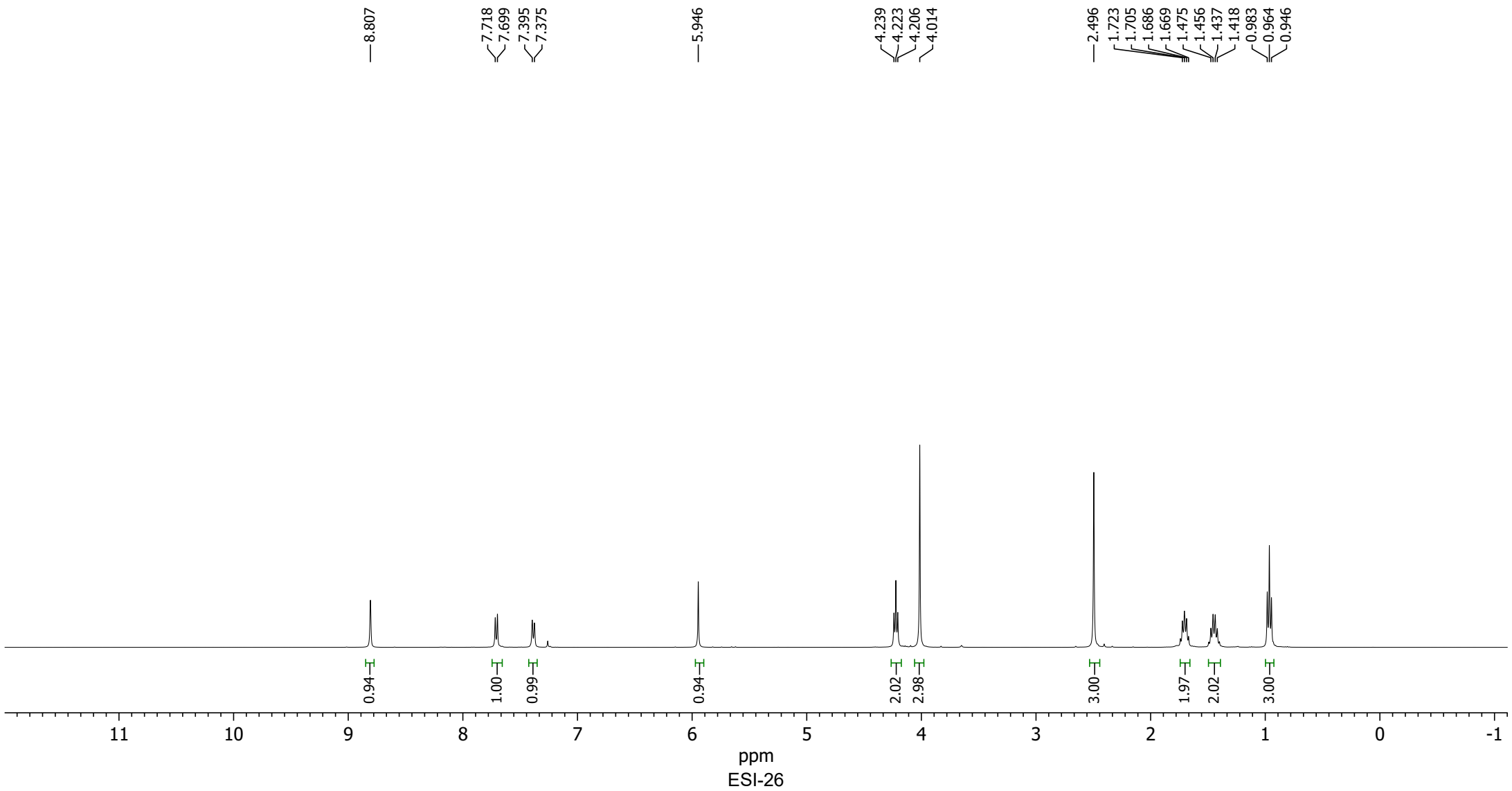
00 180 160 140 120 100 80 60 40 20 0

ppm

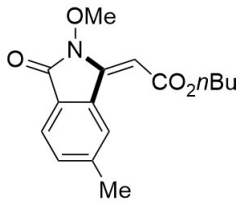
ESI-25


OMe
N
O
CO2nBu
Me

5a

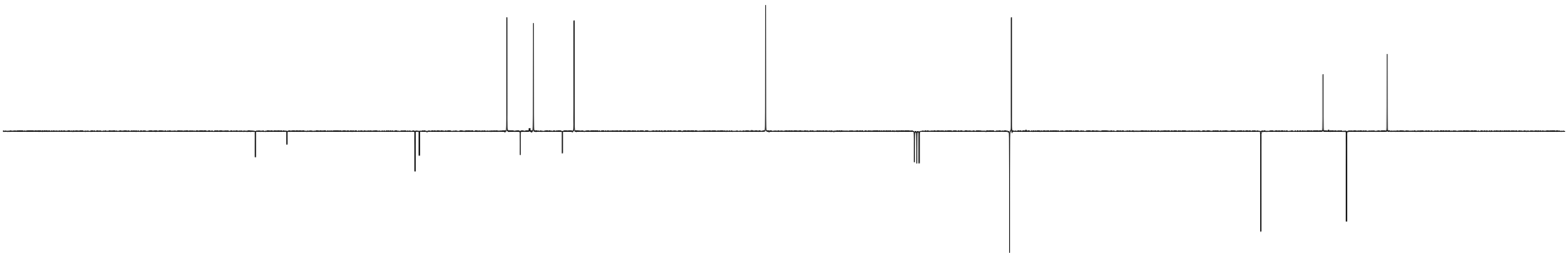

8.807
7.718
7.699
7.395
7.375
5.946
4.239
4.223
4.206
4.014
2.496
1.723
1.705
1.686
1.669
1.475
1.456
1.437
1.418
0.983
0.964
0.946
0.94
1.00
0.99
0.94
2.02
2.98
3.00
1.97
2.02
3.00
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

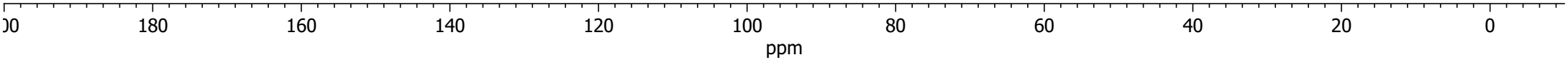
ESI-26



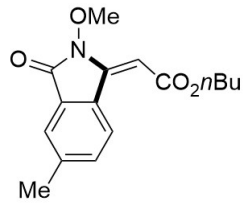
5a

166.173
161.940
144.688
144.113
132.332
130.528
128.766
124.871
123.285
97.500
64.673
64.416
30.857
22.481
19.319
13.853





ESI-27



5b

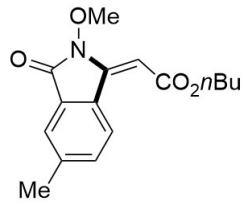
8.856
8.836
7.630
7.467
7.447
5.929
4.232
4.215
4.198
4.016
2.459
1.732
1.715
1.708
1.697
1.678
1.661
1.469
1.450
1.431
1.413
0.979
0.961
0.942

1.00
1.01
1.02
0.99
2.08
3.04
3.12
2.02
2.02
3.10

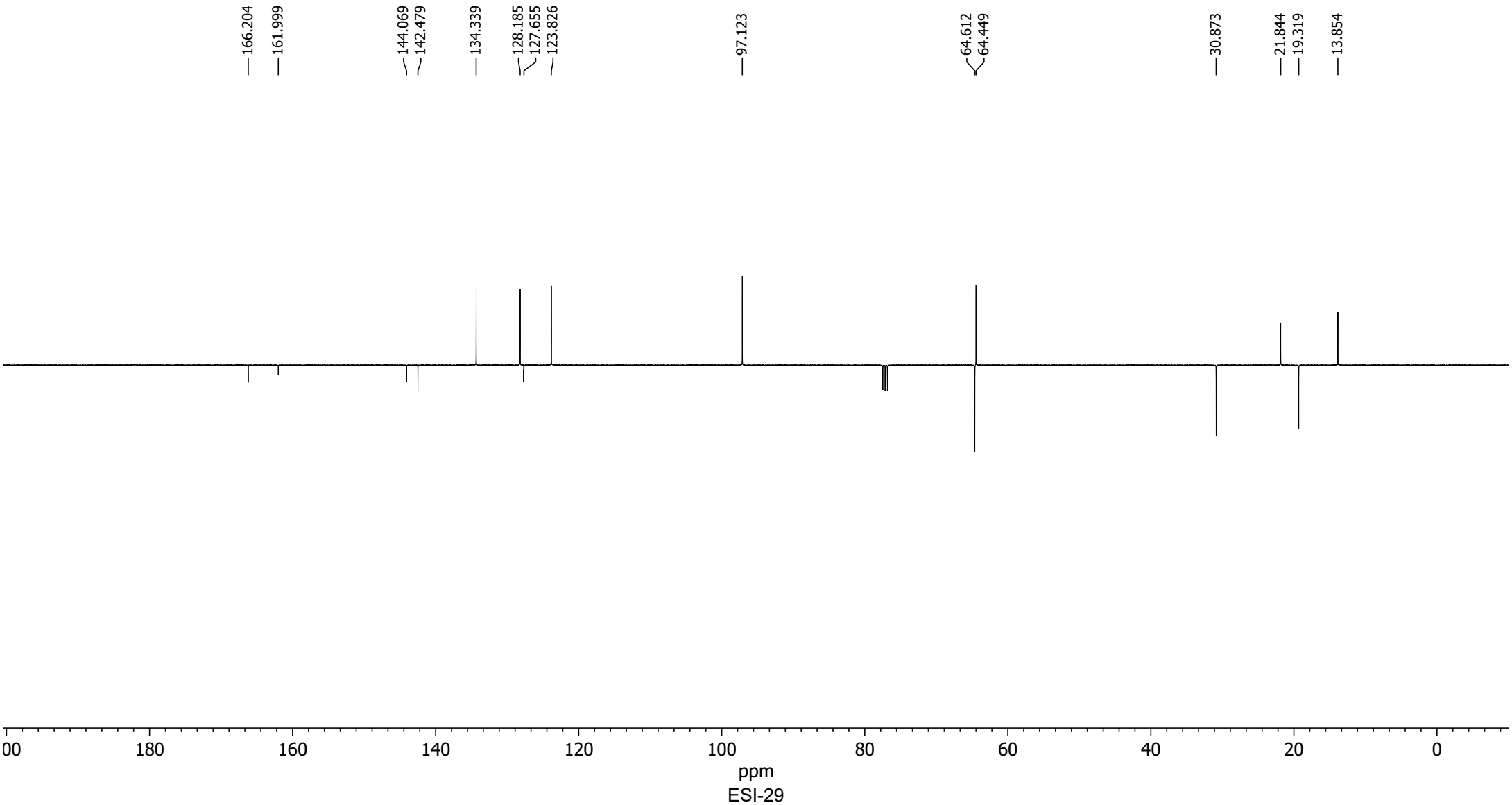
.2 11 10 9 8 7 6 5 4 3 2 1 0 -1

ppm

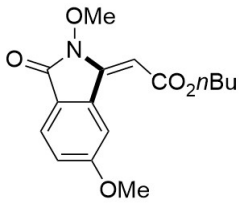
ESI-28


OMe
N
O
CO2nBu
Me

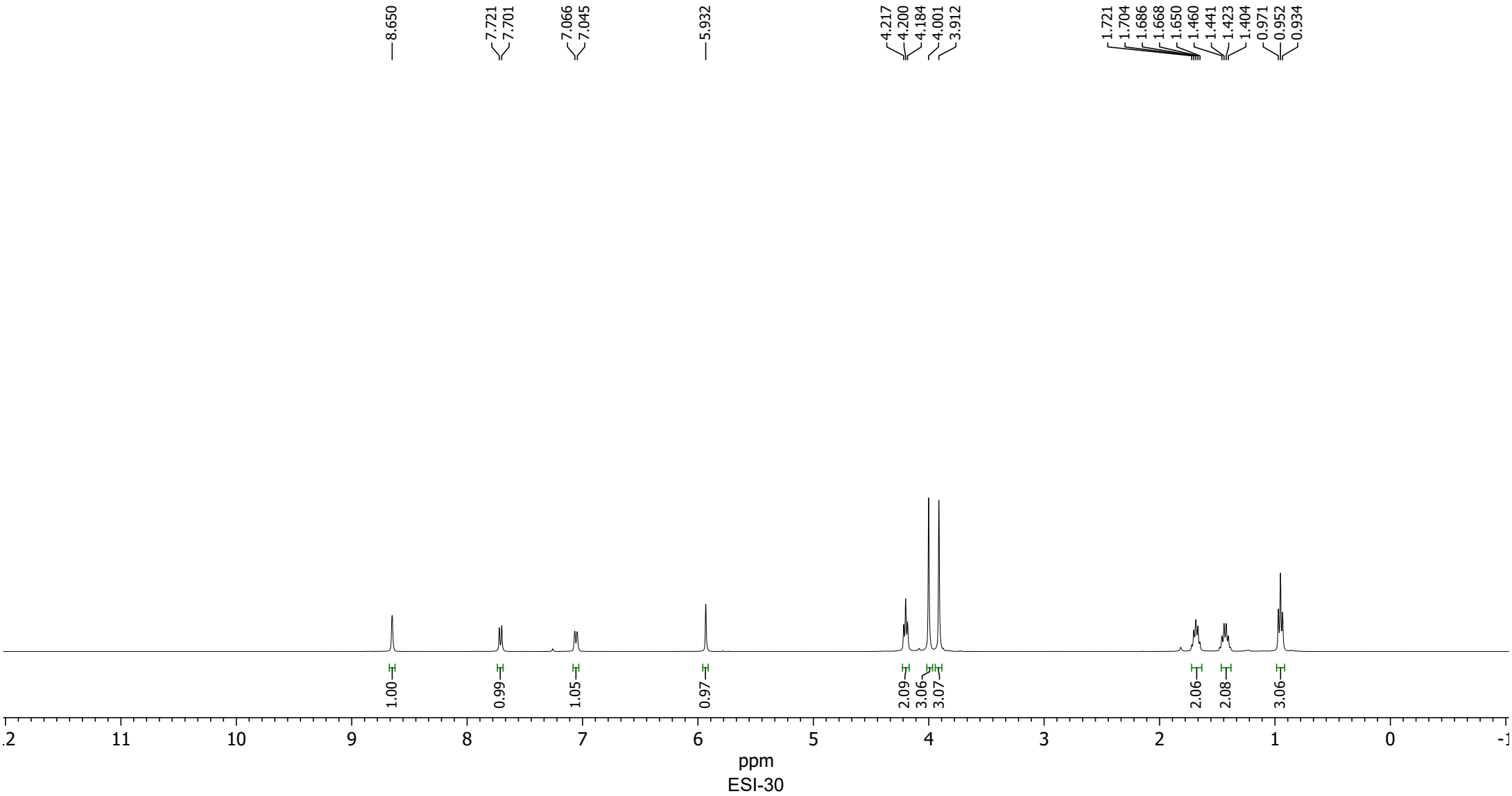
5b


166.204
161.999
144.069
142.479
134.339
128.185
127.655
123.826
97.123
64.612
64.449
30.873
21.844
19.319
13.854
00
180
160
140
120
100
80
60
40
20
0
ppm

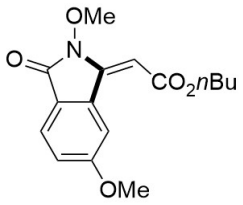
ESI-29


OMe
N
O
CO2nBu
OMe

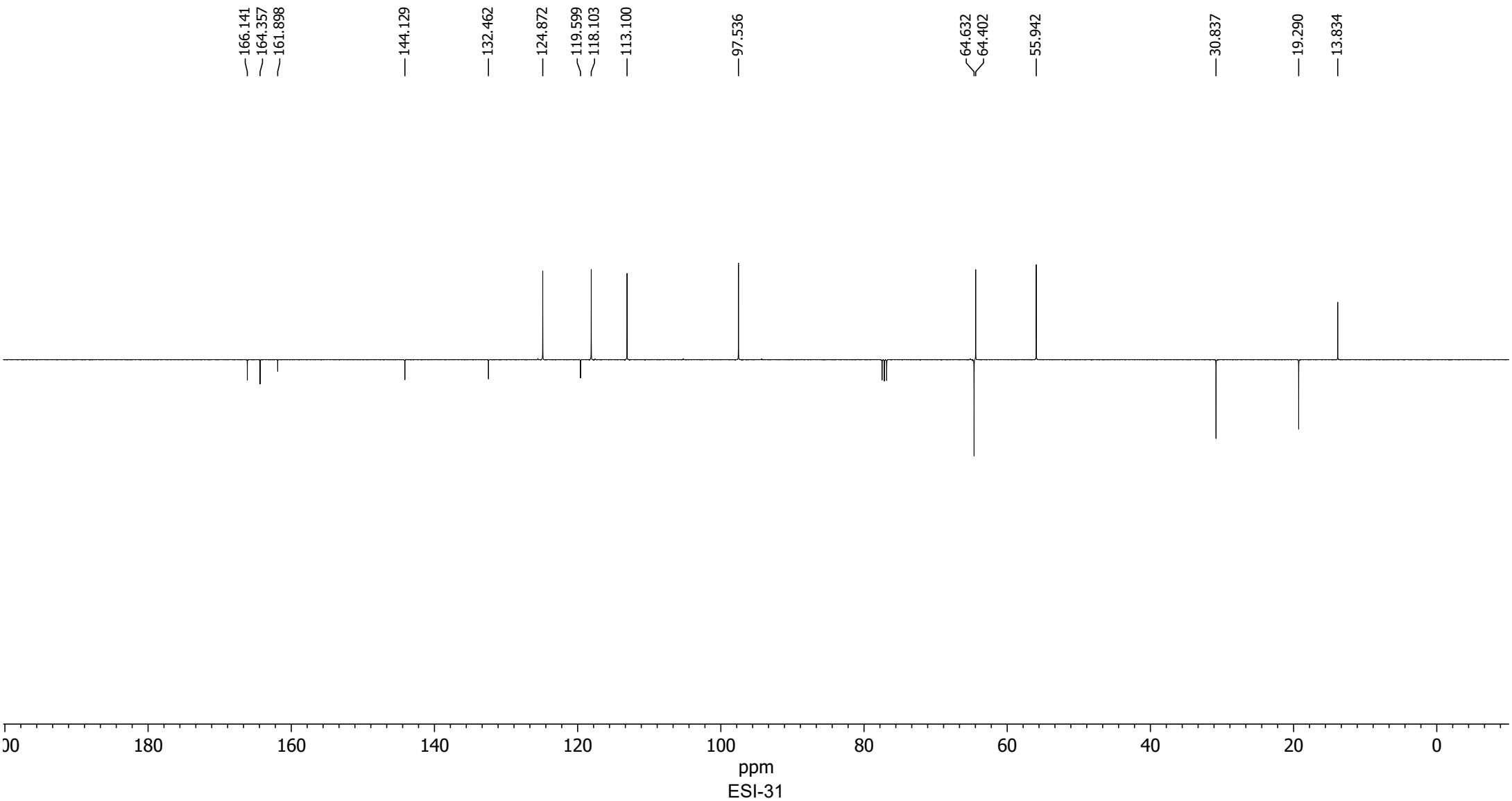
5c


8.650
7.721
7.701
7.066
7.045
5.932
4.217
4.200
4.184
4.001
3.912
1.721
1.704
1.686
1.668
1.650
1.460
1.441
1.423
1.404
0.971
0.952
0.934
1.00
0.99
1.05
0.97
2.09
3.06
3.07
2.06
2.08
3.06
ppm

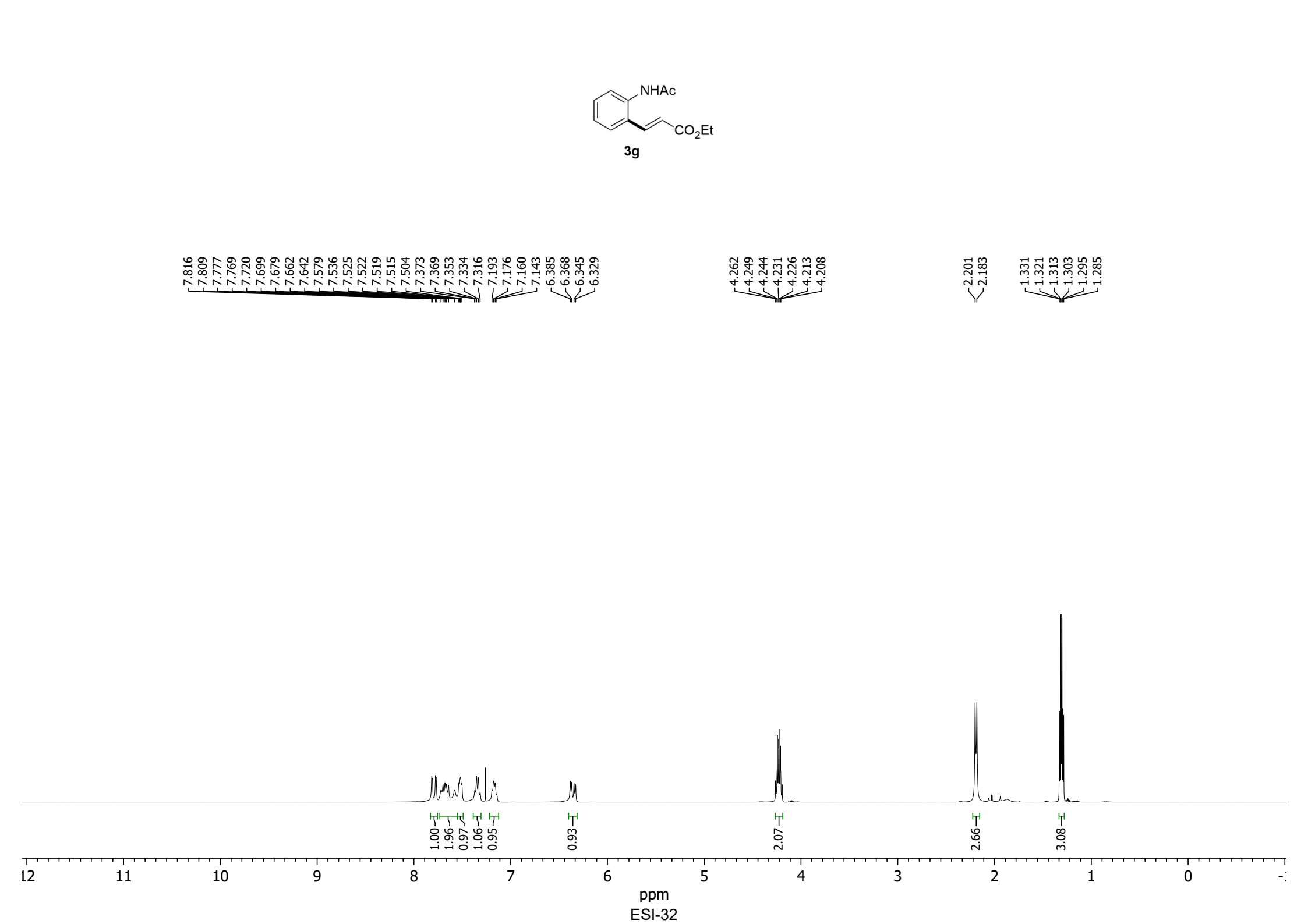
ESI-30

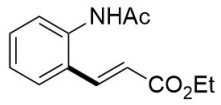

OMe
N
O
CO2nBu
OMe

5c

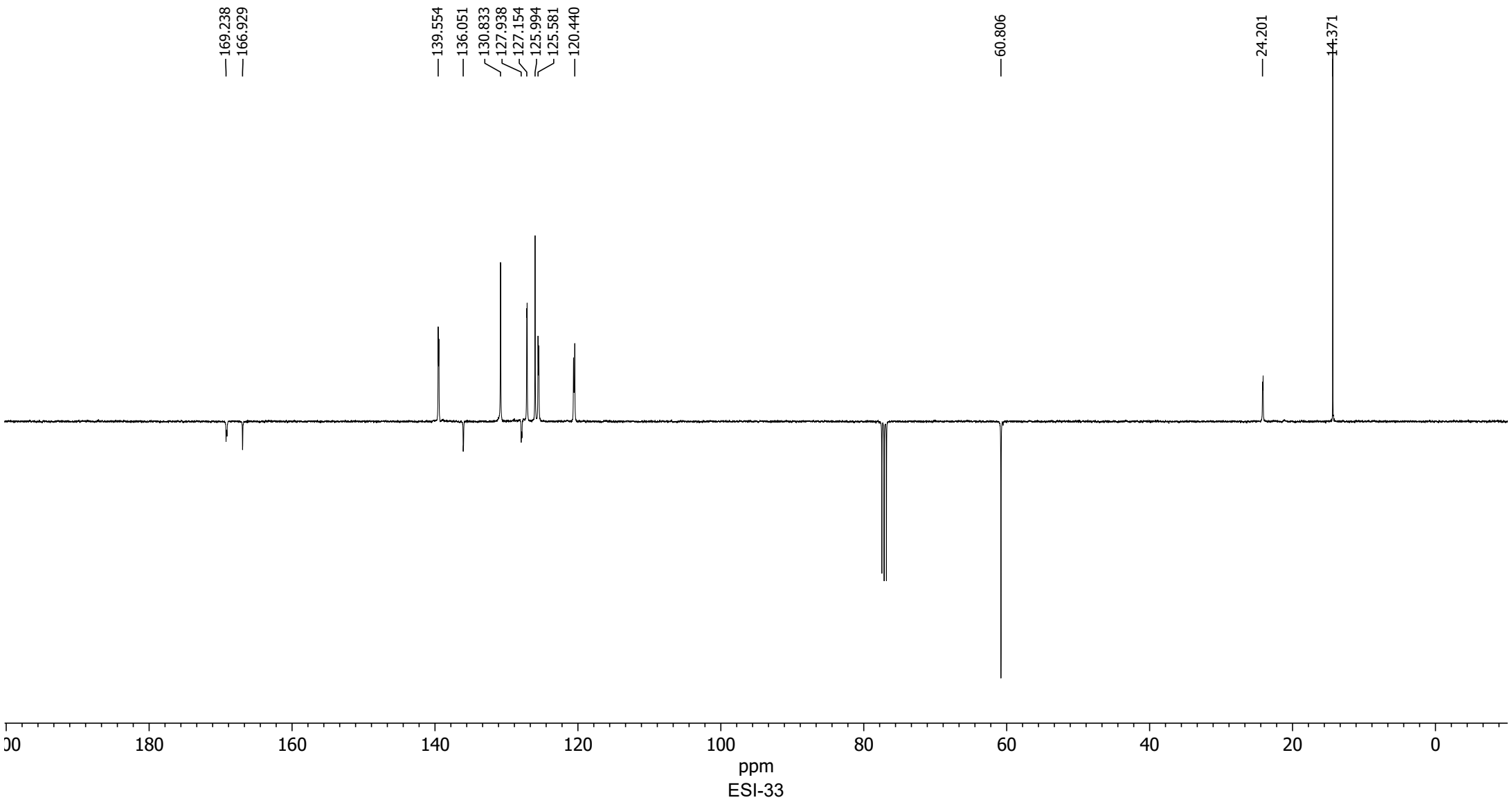

166.141
164.357
161.898
144.129
132.462
124.872
119.599
118.103
113.100
97.536
64.632
64.402
55.942
30.837
19.290
13.834
00
180
160
140
120
100
80
60
40
20
0
ppm

ESI-31

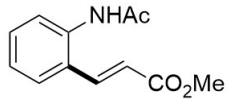

NHAc
CO2Et
3g
7.816
7.809
7.777
7.769
7.720
7.699
7.679
7.662
7.642
7.579
7.536
7.525
7.522
7.519
7.515
7.504
7.373
7.369
7.353
7.334
7.316
7.193
7.176
7.160
7.143
6.385
6.368
6.345
6.329
4.262
4.249
4.244
4.231
4.226
4.213
4.208
2.201
2.183
1.331
1.321
1.313
1.303
1.295
1.285
1.00
1.96
0.97
1.06
0.95
0.93
2.07
2.66
3.08
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
ESI-32


NHAc
CO2Et

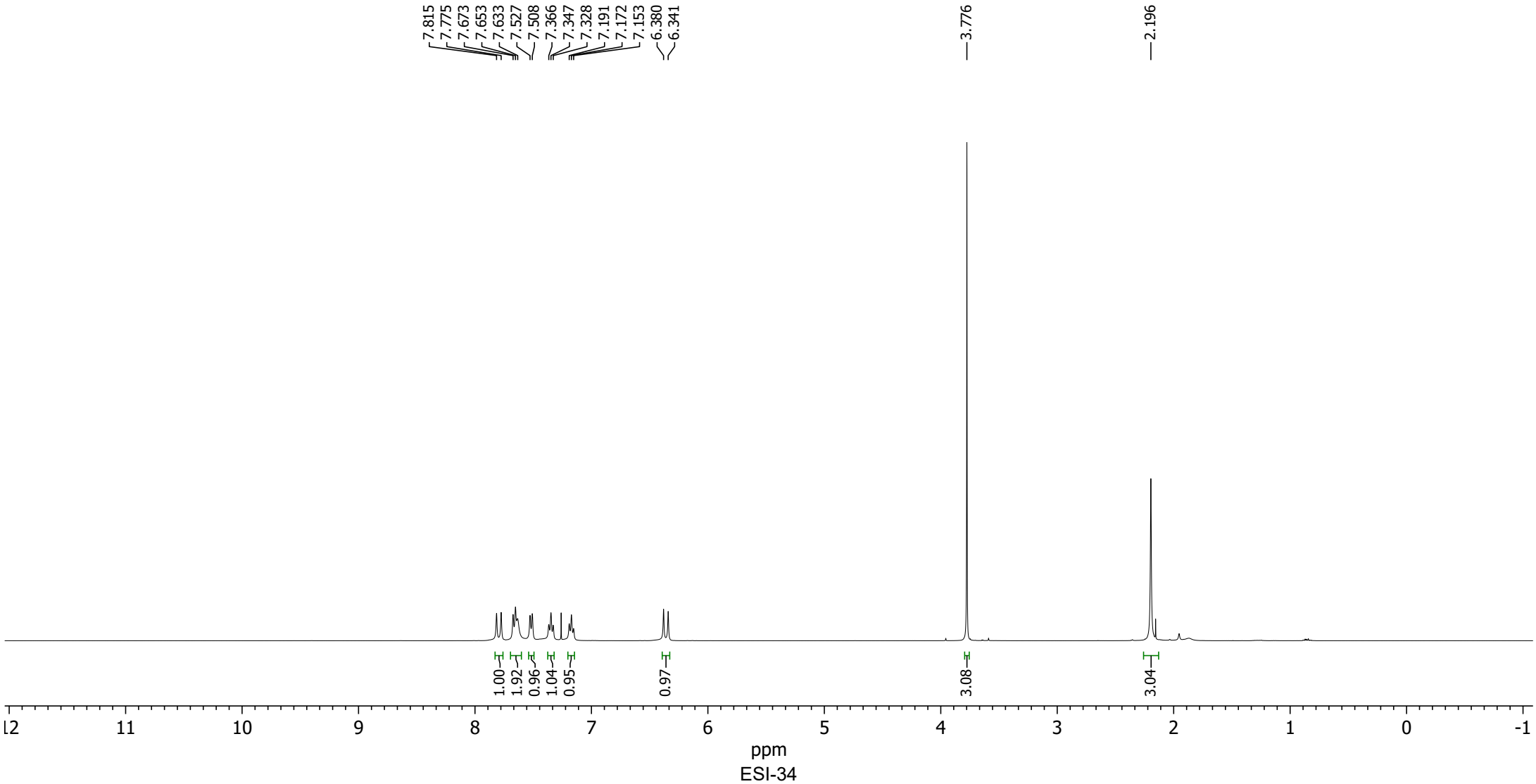
3g


169.238
166.929
139.554
136.051
130.833
127.938
127.154
125.994
125.581
120.440
60.806
24.201
14.371
180
160
140
120
100
80
60
40
20
0
ppm

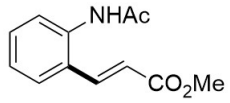
ESI-33


NHAc
CO2Me

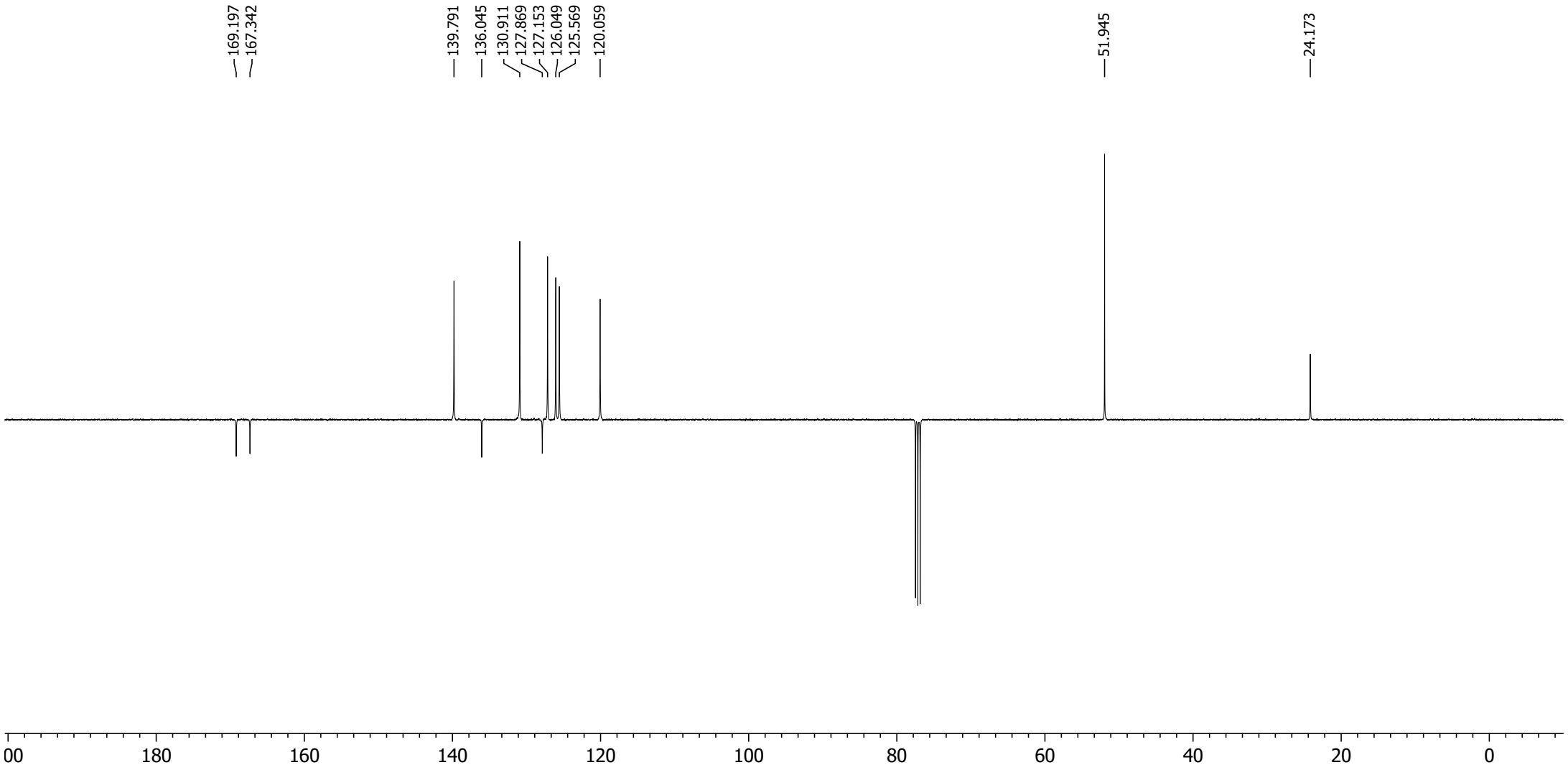
3h

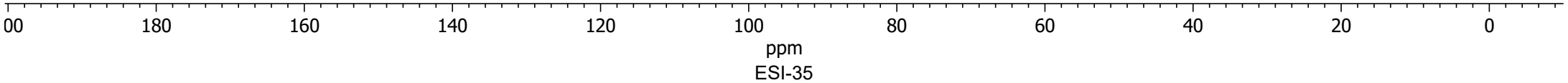

7.815
7.775
7.673
7.653
7.633
7.527
7.508
7.366
7.347
7.328
7.191
7.172
7.153
6.380
6.341
3.776
2.196
1.00
1.92
0.96
1.04
0.95
0.97
3.08
3.04
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

ESI-34

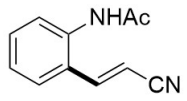

NHAc
CO2Me

3h


169.197
167.342
139.791
136.045
130.911
127.869
127.153
126.049
125.569
120.059
51.945
24.173

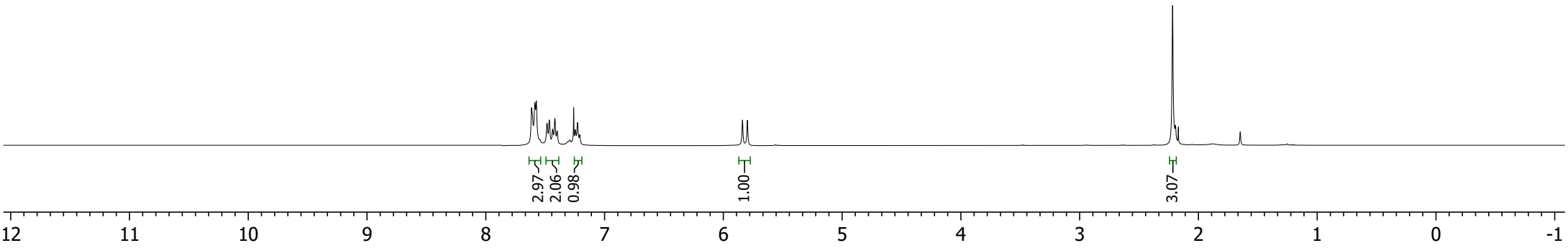

00
180
160
140
120
100
80
60
40
20
0
ppm

ESI-35

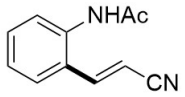

NHAc
CN

3i

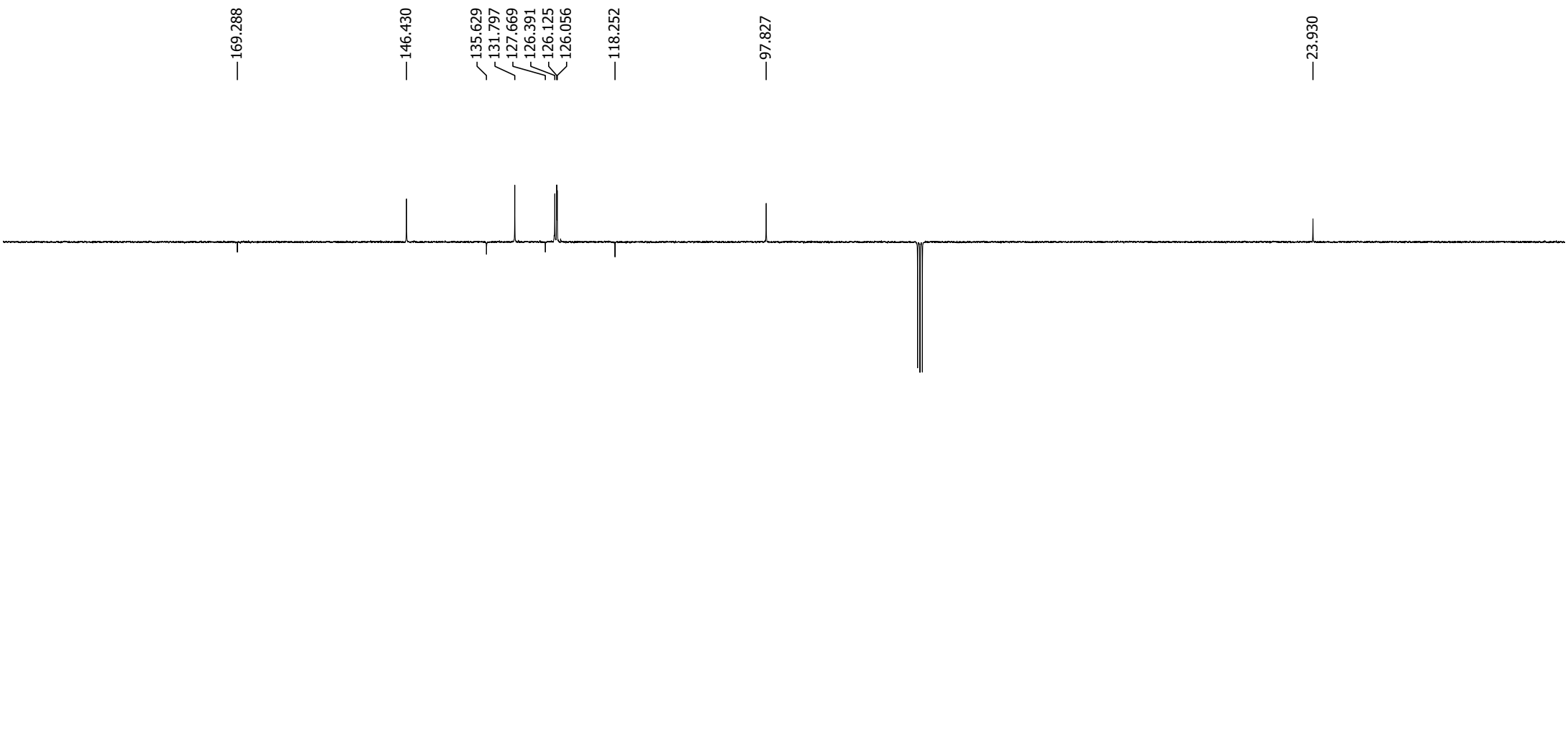

7.615
7.607
7.587
7.574
7.484
7.465
7.437
7.418
7.399
7.247
7.228
7.209
5.839
5.798
2.218


2.97
2.06
0.98
1.00
3.07
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

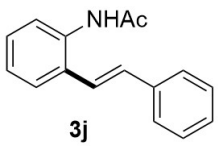
ESI-36


NHAc
CN

3i


169.288
146.430
135.629
131.797
127.669
126.391
126.125
126.056
118.252
97.827
23.930
200
180
160
140
120
100
80
60
40
20
0
ppm

ESI-37



3j

7.799
7.779
7.760
7.538
7.515
7.495
7.397
7.379
7.360
7.319
7.301
7.282
7.199
7.180
7.157
7.116
7.010
6.969

2.204

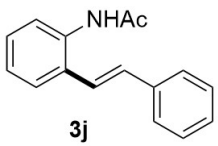
0.98
3.03
2.07
2.08
2.09
1.00

2.97

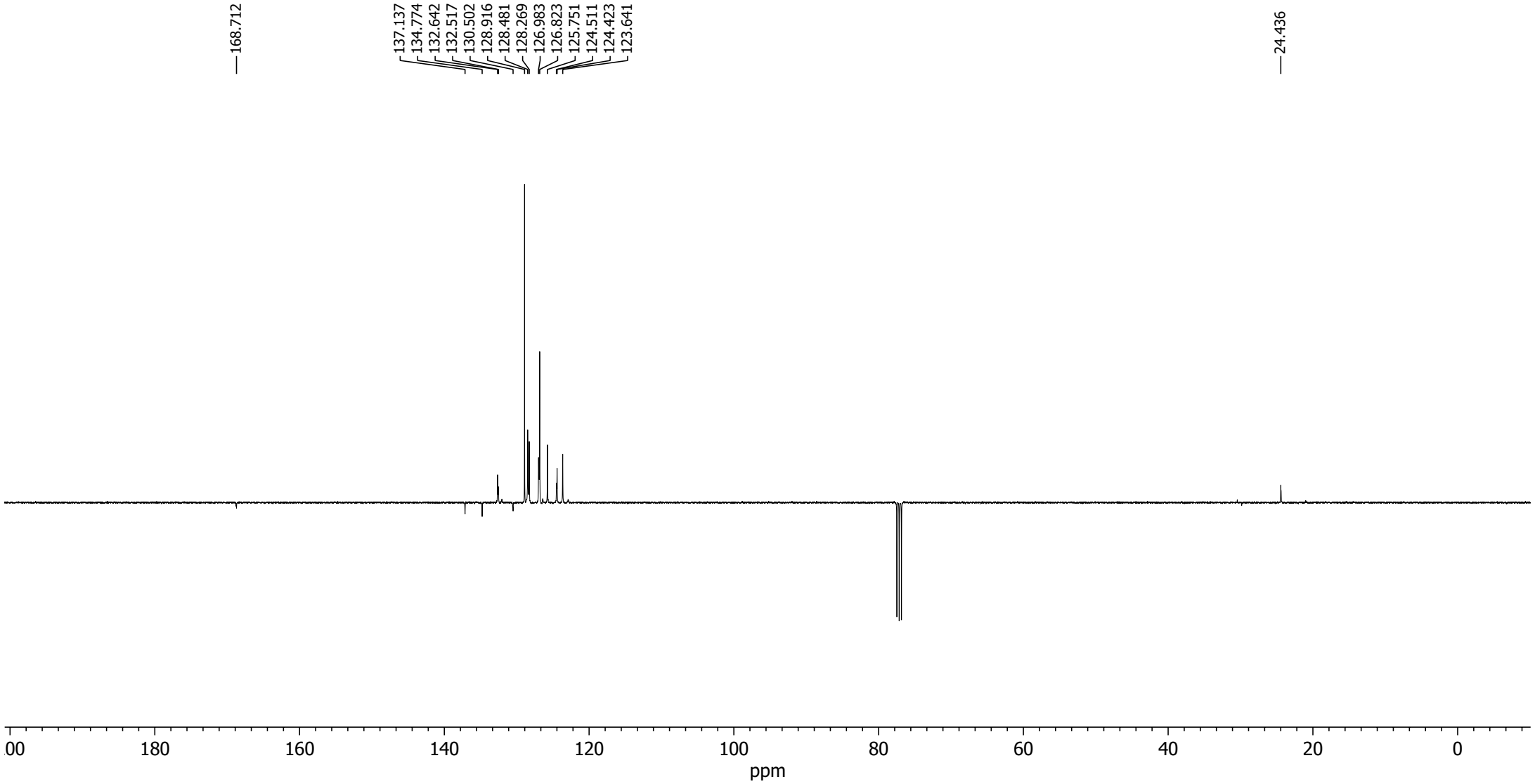
12 11 10 9 8 7 6 5 4 3 2 1 0 -1

ppm

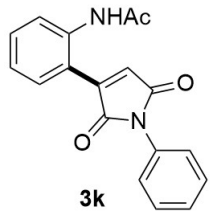
ESI-38


NHAc

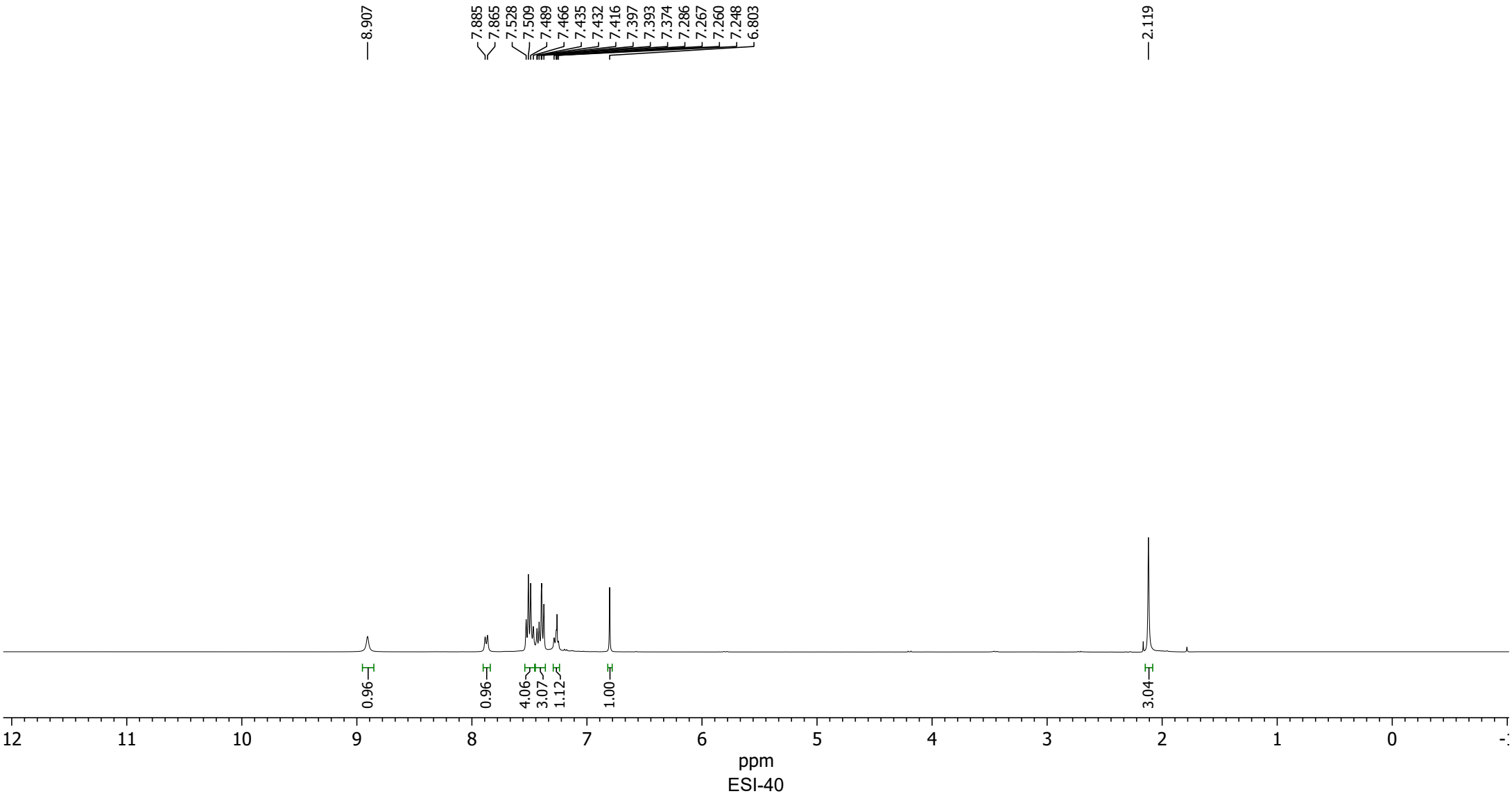
3j


168.712
137.137
134.774
132.642
132.517
130.502
128.916
128.481
128.269
126.983
126.823
125.751
124.511
124.423
123.641
24.436
00
180
160
140
120
100
80
60
40
20
0
ppm

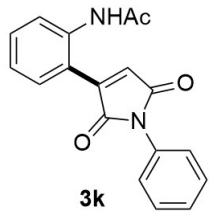
ESI-39


NHAc
O
O
N

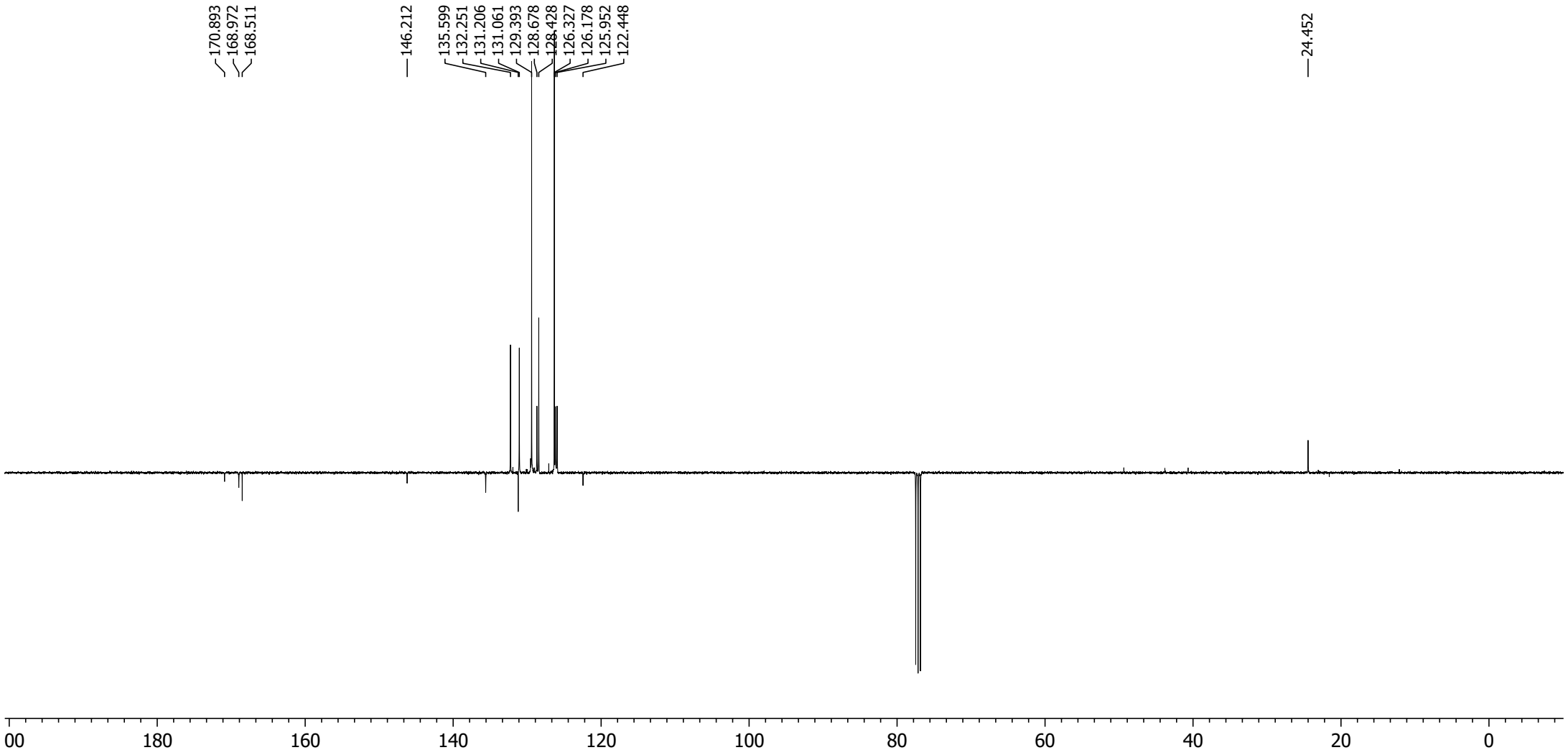
3k


8.907
7.885
7.865
7.528
7.509
7.489
7.466
7.435
7.432
7.416
7.397
7.393
7.374
7.286
7.267
7.260
7.248
6.803
2.119
0.96
0.96
4.06
3.07
1.12
1.00
3.04
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

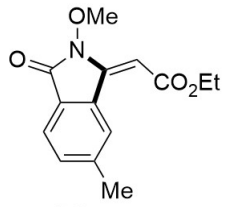
ESI-40


NHAc
O
O
N

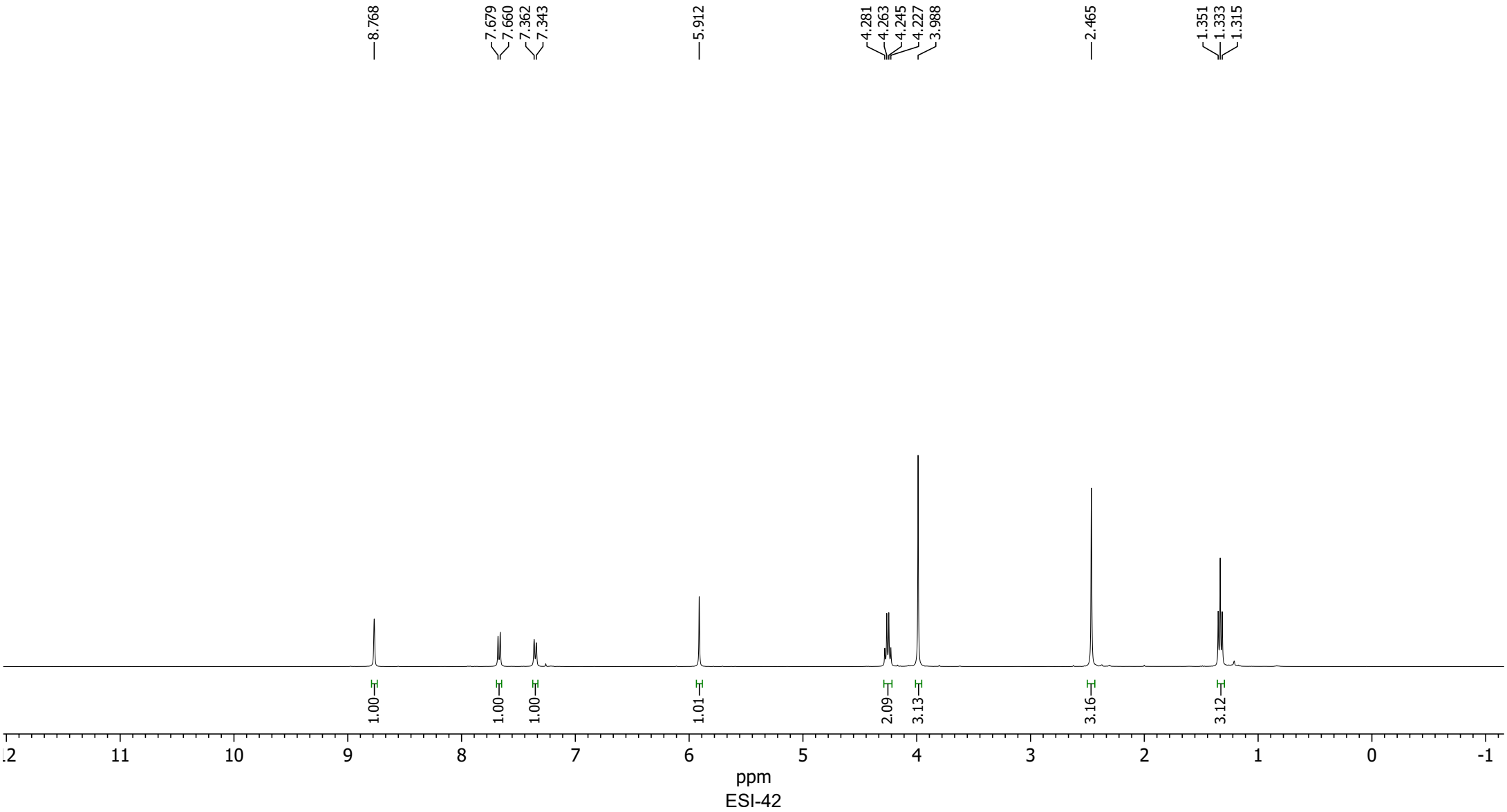
3k


170.893
168.972
168.511
146.212
135.599
132.251
131.206
131.061
129.393
128.678
128.428
126.327
126.178
125.952
122.448
24.452
00
180
160
140
120
100
80
60
40
20
0
ppm

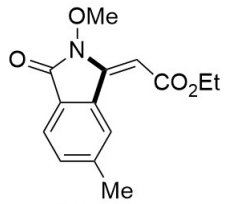
ESI-41


OMe
N
O
CO2Et
Me

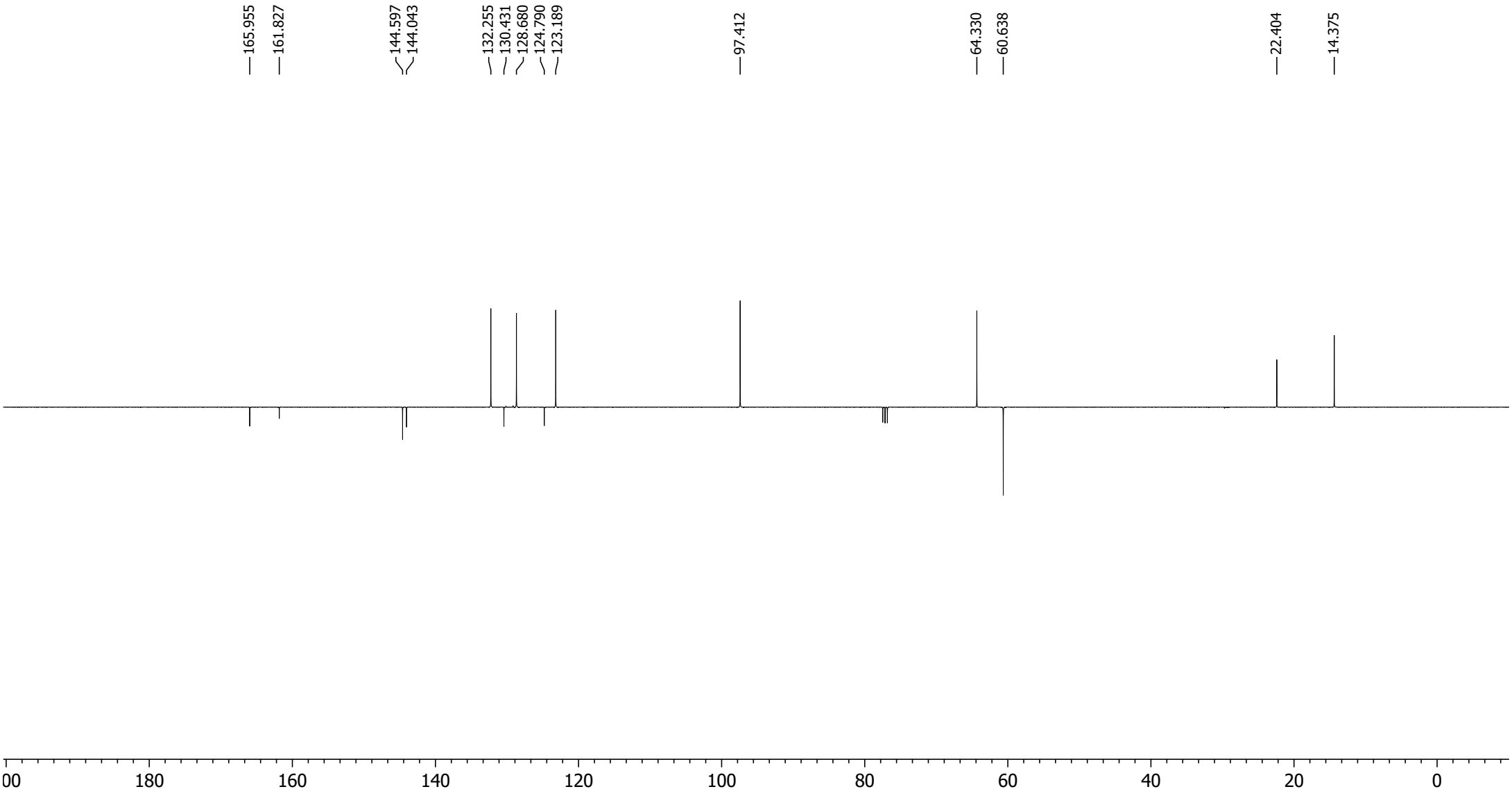
5d


8.768
7.679
7.660
7.362
7.343
5.912
4.281
4.263
4.245
4.227
3.988
2.465
1.351
1.333
1.315
1.00
1.00
1.00
1.01
2.09
3.13
3.16
3.12
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

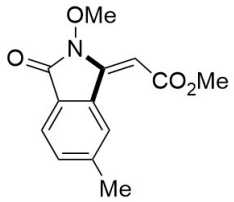
ESI-42


OMe
N
O
CO2Et
Me

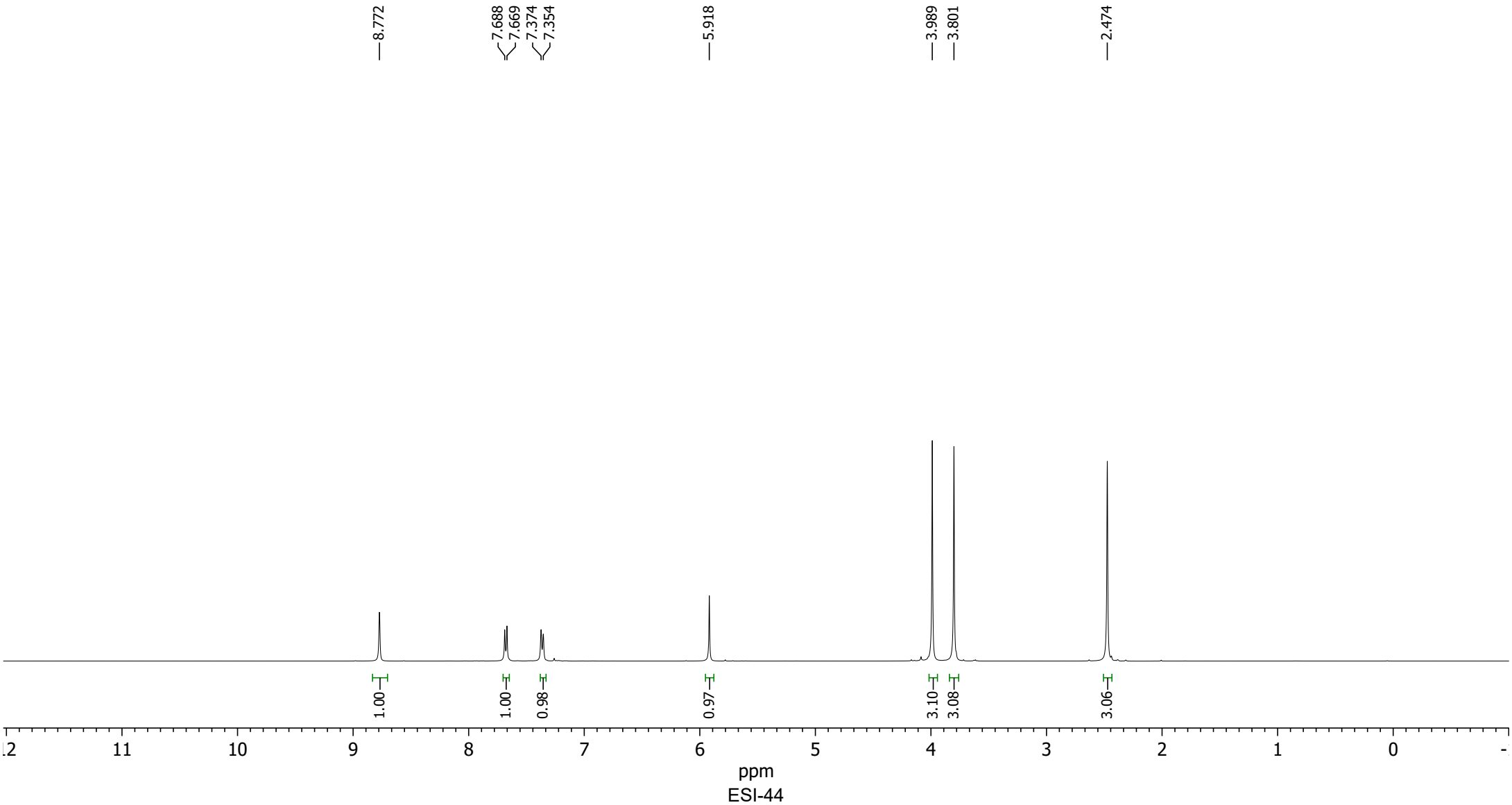
5d


165.955
161.827
144.597
144.043
132.255
130.431
128.680
124.790
123.189
97.412
64.330
60.638
22.404
14.375
00
180
160
140
120
100
80
60
40
20
0
ppm

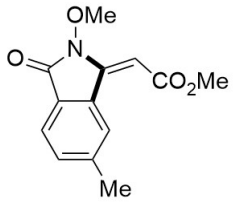
ESI-43


OMe
N
O
CO2Me
Me

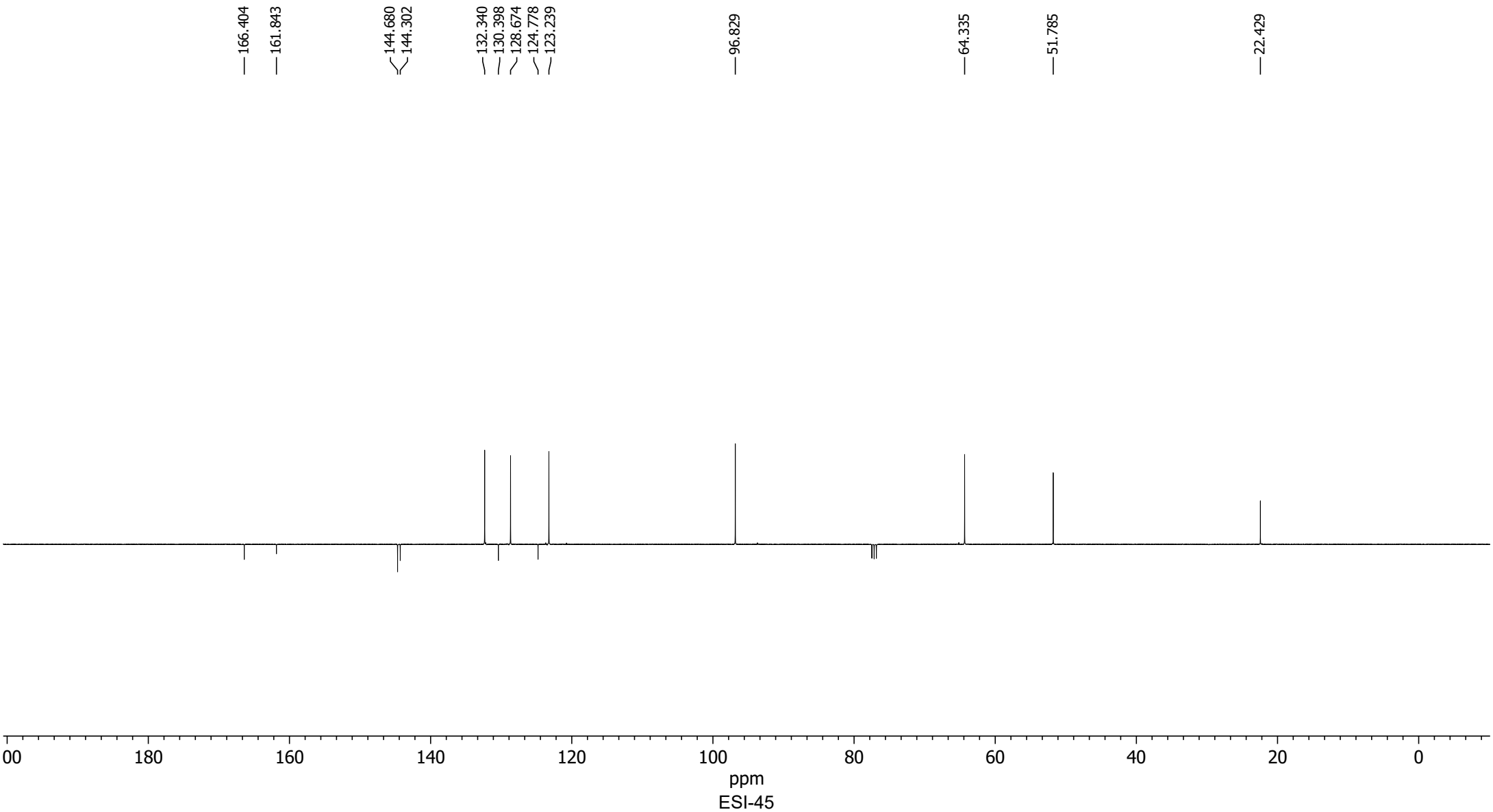
5e


8.772
7.688
7.669
7.374
7.354
5.918
3.989
3.801
2.474
1.00
1.00
0.98
0.97
3.10
3.08
3.06
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

ESI-44


OMe
N
O
CO2Me
Me

5e


166.404
161.843
144.680
144.302
132.340
130.398
128.674
124.778
123.239
96.829
64.335
51.785
22.429
00
180
160
140
120
100
80
60
40
20
0
ppm

ESI-45