Electronic Supplementary Material (ESI) for Green Chemistry.

Waste-Minimized Synthesis of C2 Functionalized Quinolines Exploiting Iron-Catalysed C–H activation

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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 100.6 MHz). Chemical shifts are reported in ppm and coupling constants in Hertz. Flash chromatography was carried out on a Büchi Reveleris® X2-UV system. Iron(II) sulfate heptahydrate (CAS 7782-63-0) has been purchased by Sigma Aldrich and has been used without further purification. Yields refer to isolated compounds, estimated to be >95% pure as determined by ^{1}H NMR spectroscopy. Melting points were measured on a Büchi 510 apparatus.

2. General Procedures

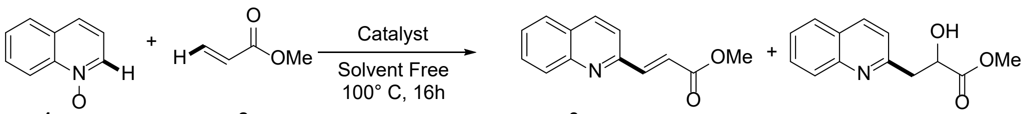
2.1 General procedure for synthesis of quinoline *N*-oxide. In a 100 mL round bottom flask equipped with a magnetic stirrer quinoline (5mmol) was placed in 50 mL DCM. The solution was cooled to 0°C and m-CPBA (1.3 eq, 6.5 mmol, 1.121 g) was added portion wise. The reaction was heated at 28°C and kept under stirring. After 24h the reaction crude was washed with aqueous KOH [1M] (3x30 mL). The organic phase was dried over sodium sulphate and concentrated under reduced pressure. Silica plug purification (DCM) afforded the desired quinolines in yields range 60-70%

2.2 General procedure used in the optimization of quinoline *N*-Oxides alkenylation. Catalyst (1 mol%) and quinoline *N*-Oxide (**1a**) (1mmol) were added in a 2mL screw-capped vial equipped with a magnetic stirrer. The solvent was added in the indicated amount followed by acrylate (**2**) or styrene (**5**) (in the quantity indicated in tables). The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for the time indicated. After this time, the crude mixture was diluted with methanol (2 mL) and filtered over a celite plug to eventually remove the catalyst. The solvent has been removed under reduced pressure. Small samples of the mixture has been diluted with ethyl acetate or chloroform and analyzed by GLC using pure compounds as reference standard. The crude mixture has been purified by column chromatography (ETP/EtOAc).

2.3 General procedure for $FeSO_4$ catalyzed quinoline *N*-Oxides alkenylation. $FeSO_4$ (2.78 mg, 1 mol%) and quinoline *N*-Oxide (**1a**) (145 mg, 1mmol) were added in a 2mL screw-capped vial equipped with a magnetic stirrer. Toluene (50 uL) followed by acrylate (**2**) or styrene (**5**) (2 eq) were added. The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for 16h. After this time, the crude mixture was diluted with methanol (2 mL) and filtered over a celite plug. The solvent has been removed under reduced pressure crude mixture has been purified by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80 for **3a** or EtOAc/Petroleum Ether 1/99 → 10/90 for **6a**).

3. Optimization of reaction condition

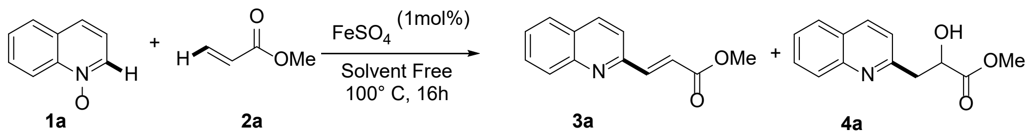
3.1 Screening of Transition Metal Catalysts



Entry	Catalyst	Moles %	T (°C)	GC Conversion %	Selectivity 3a:4a
1	Catalyst free	1	100 °C	30%	[8:92]
2	$Pd(OAc)_2$	1	100 °C	52%	[50:50]
3	Pd/C	1	100 °C	48%	[30:70]
4	$CuSO_4$	1	100 °C	82%	[5:95]
5	$CuSO_4$	1	100 °C	95%	[10:90][b]
6	Cu powder		100 °C	80%	[52:48]
7	$NiCl_2$	1	100 °C	61%	[41:59]
8	$NaIO_4$	1	100 °C	86%	[40:60]
9	$CoSO_4$	1	100 °C	91%	[50:50]
10	$BrMn(CO)_5$	1	100 °C	95%	[23:77]
11	$FeCl_3$	1	100 °C	93%	[50:50]
12	$FeSO_4$	1	100 °C	83%	[95:5]
13	$FeSO_4$	0.5	100 °C	68%	[70:30]
14	$FeSO_4$	0.1	100 °C	47%	[70:30]
15	$C_{32}H_{16}FeN_8$	1	100 °C	64%	[85:15]

[a] Reaction conditions: **1a** (1mmol), **2a** (2mmol) at 100° C for 16h. [b] 4A molecular sieves has been added to the reaction mixture.

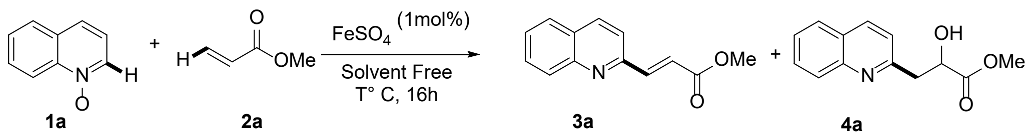
3.2 Screening of stoichiometry between 1a and 2a



Entry	Equivalents of 2a	GC Conversion %	Selectivity 3a:4a
1	5	84%	[80:20]
2	10	45%	[78:22]
3	20	23%	[50:50]
4	1	30%	[40:60]

[a] Reaction conditions: **1a** (1mmol), **2a** (as table) at 100° C for 16h

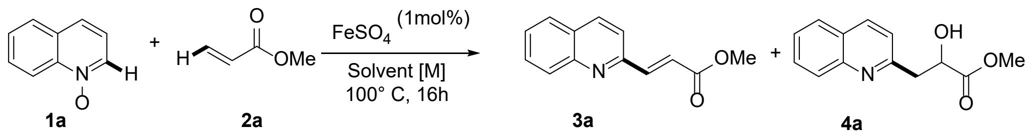
3.3 Screening of temperature in the reaction between 1a and 2a



Entry	T (°C)	GC Conversion %	Selectivity 3a:4a
1	110 °C	87%	[98:2]
2	80 °C	74%	[95:5]
3	60 °C	43%	[100:0]
4	50 °C	40%	[100:0]
5	25 °C	12%	[100:0]

[a] Reaction conditions: **1a** (1mmol), **2a** (2mmol) at temperature indicated in table. for 16h

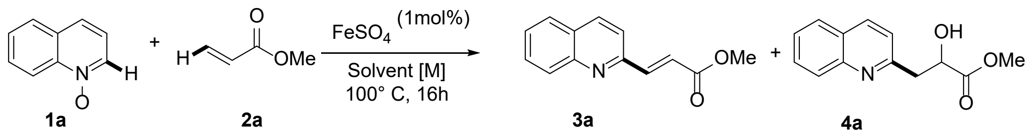
3.4 Screening of solvents and molarity of reaction mixture in the iron-catalyzed reaction between 1a and 2a



Entry	Solvent (0.3 M)	GC Conversion %	Selectivity 3a:4a
1	Water	81%	[0:100]
2	1,4-Dioxane	61%	[5:95]
3	THF	58%	[0:100]

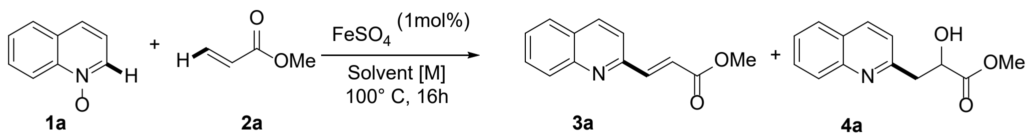
4	2-MeTHF	44%	[0:100]
5	DMF	47%	[0:100]
6	Ethanol abs.	47%	[2:98]
7	Acetonitrile	40%	[13:87]
8	NMP	54%	[0:100]
9	GVL	53%	[2:98]
10	n-BuOH	36%	[5:95]

[a] Reaction conditions: **1a** (1mmol), **2a** (2 mmol) at 100° C for 16h



Entry	Solvent (2 M)	GC Conversion %	Selectivity 3a:4a
1	Water + SDS	30 %	[15:75]
2	Heptane	0 %	-
3	Hexane	14 %	[15:75]
4	Cyclohexane	35 %	[12:88]
5	1,4-dioxane	63 %	[25:75]
6	Methanol	32 %	[8:92]
7	Ethanol abs.	58 %	[20:80]
8	Isopropanol	28 %	[15:85]
9	THF	56 %	[40:60]
10	2-methyl THF	33 %	[70:30]
11	Toluene	66 %	[40:60]
12	DMF	50 %	[20:80]
13	GVL	52 %	[2:98]
14	Acetonitrile	48 %	[20:80]

[a] Reaction conditions: **1a** (1mmol), **2a** (2 mmol) at 100° C for 16h

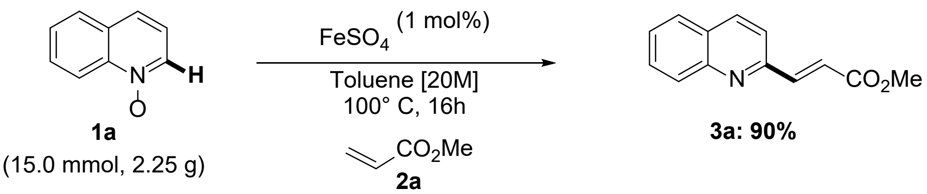


Catalyst	Solvent (20 M)	GC Conversion %	Selectivity 3a:4a

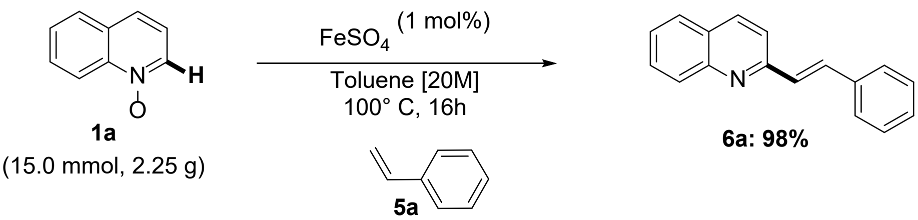
1	Water + SDS	55 %	[32:68]
2	Heptane	98 %	[64:36]
3	Hexane	99 %	[65:35]
4	Cyclohexane	99 %	[70:30]
5	1,4-dioxane	68 %	[45:55]
6	Methanol	85 %	[78:22]
7	Ethanol abs.	50 %	[35:65]
8	Isopropanol	99 %	[67:33]
9	THF	50 %	[50:50]
10	2-methyl THF	99 %	[74:26]
11	Toluene	98 %	[100:0]
12	DMF	90 %	[52:48]
13	GVL	98 %	[31:69]
14	Acetonitrile	66 %	[35:65]

[a] Reaction conditions: **1a** (1mmol), **2a** (2 mmol) at 100° C for 16h

4. Gram Scale Reaction Procedures



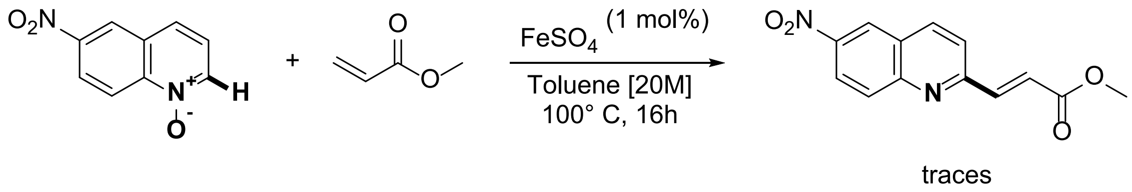
$FeSO_4$ (41 mg, 1 mol%) and quinoline *N*-Oxide (**1a**) (2.2 g, 15 mmol) were added in a 4mL screw-capped vial tube equipped with a magnetic stirrer. Toluene (0.75 mL) followed by methyl acrylate (**2a**) (2.7 mL, 30 mmol) were added. The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for 16h. After this time, the crude mixture was poured into methanol (5 mL) and filtered over a celite plug. The solvent has been removed under reduced pressure and the crude mixture has been purified by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80). yielding **3a** in 90% (2.8 g)

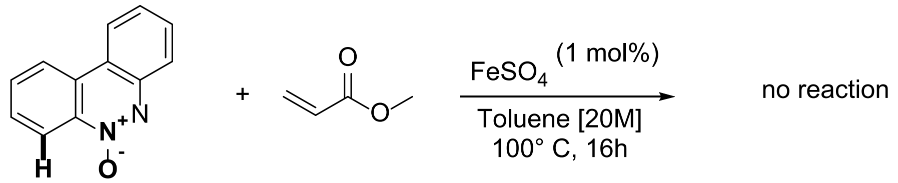


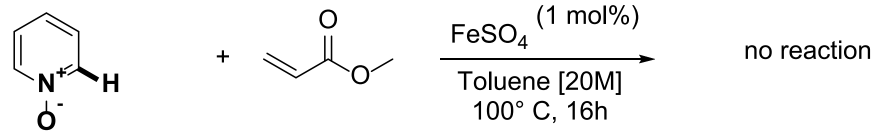
$FeSO_4$ (41 mg, 1 mol%) and quinoline *N*-Oxide (**1a**) (2.2 g, 15 mmol) were added in a 4mL screw-capped vial tube equipped with a magnetic stirrer. Toluene (50 uL) followed by styrene (**5a**) (3.4 mL, 30mmol) were added. The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for 16h. After this time, the crude mixture was poured into methanol (5 mL) and filtered over a celite plug. The solvent has been removed under reduced pressure crude mixture has been purified by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielding **6a** in 98% (3.4 g)

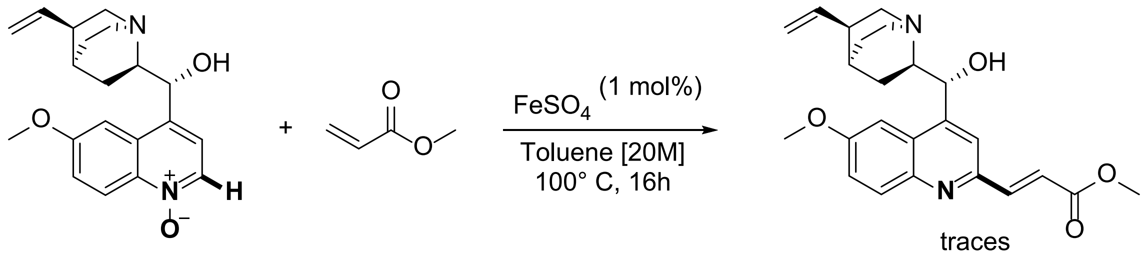
4.1 Unsuccessful reaction with N-oxide and alkene substrates

***N*-oxide Substrates**

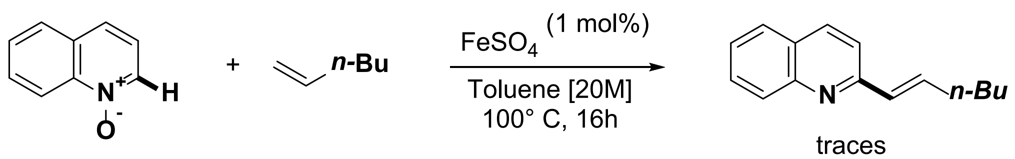


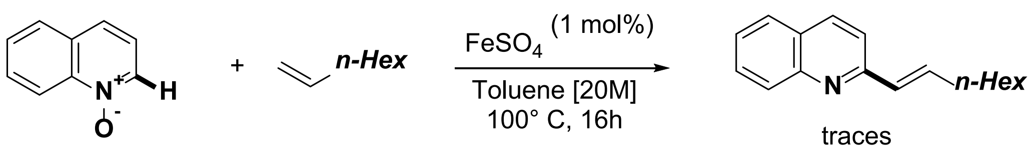






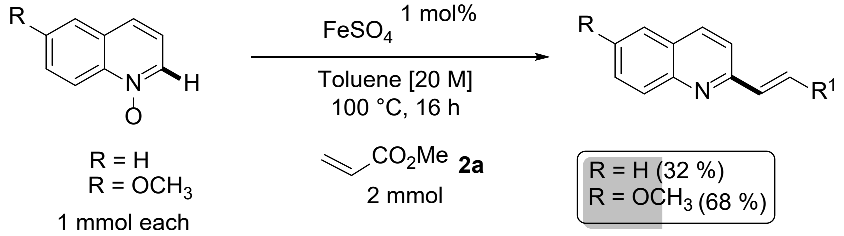
Alkene Substrates





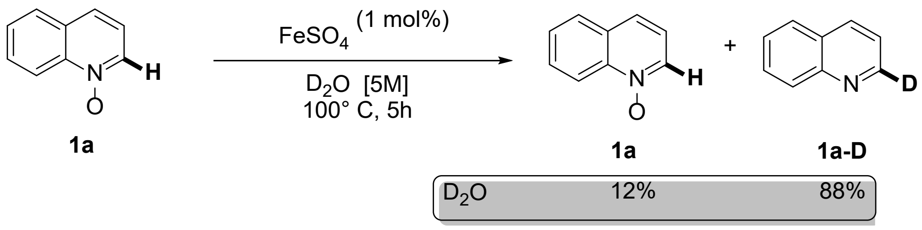
5. Mechanistic Investigation

5.1 Procedure for Competition Experiments

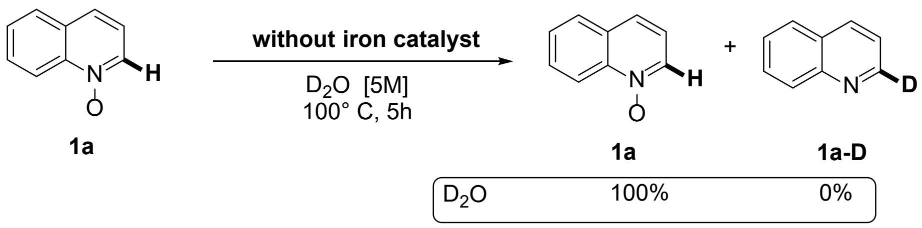


$FeSO_4$ (2.78 mg, 1 mol%), quinoline *N*-Oxide (**1a**) (145 mg, 1mmol) and 6-methoxyquinoline *N*-oxide (175 mg, 1mmol) were added in a 2mL screw-capped vial equipped with a magnetic stirrer. Toluene (50 uL) followed by methyl acrylate (**2a**) (2 mmol, 172 mg, 180 µL) were added. The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for 16h. After this time, the crude mixture was diluted with methanol (2 mL) and filtered over a celite plug. The solvent has been removed under reduced pressure and dissolved in ethyl acetate (2mL) and analyzed by GLC using pure compounds as reference standard.

5.2 Procedure for H/D scrambling

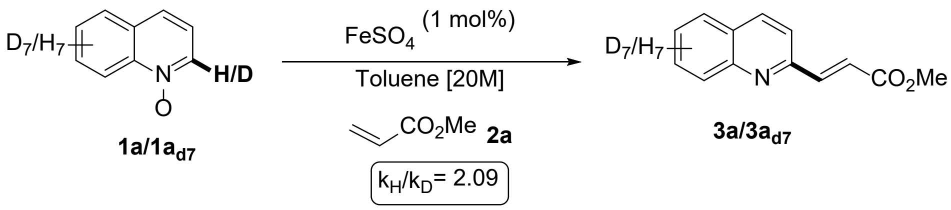


$FeSO_4$ (2.78 mg, 1 mol%), quinoline *N*-Oxide (**1a**) (145 mg, 1mmol) were added in a 2mL screw-capped vial equipped with a magnetic stirrer. D_2O (200 uL) was added. The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for 5h. After this time, the crude mixture was evaporated and analyzed by ^{1}H-NMR to estimate the ratio between product **1a and 1a-D**



quinoline *N*-Oxide (**1a**) (145 mg, 1mmol) were added in a 2mL screw-capped vial equipped with a magnetic stirrer. D_2O (200 uL) was added. The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for 5h. After this time, the crude mixture was evaporated and analyzed by ^{1}H-NMR to estimate the ratio between product **1a and 1a-D**

5.3 Procedure for Intermolecular KIE determination in independent reaction

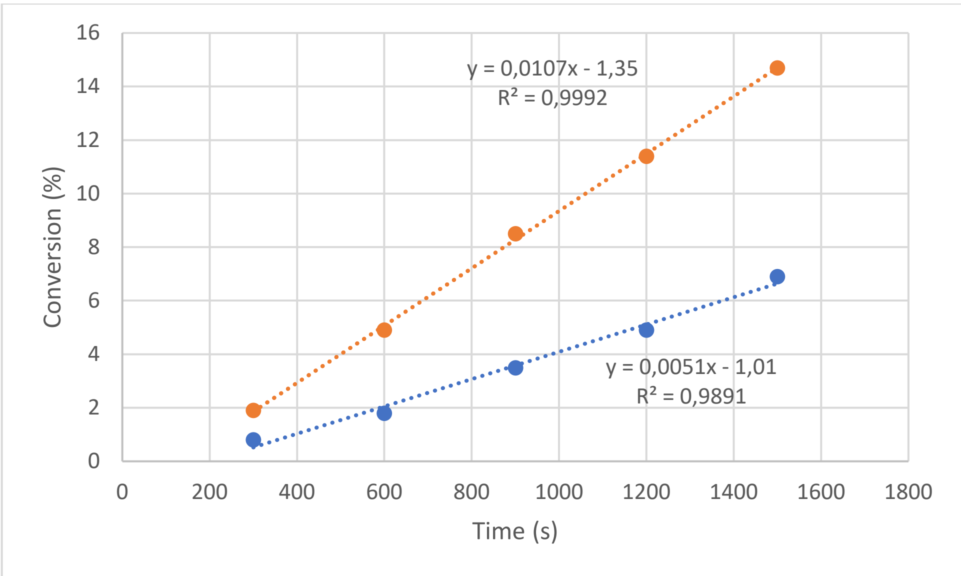


Two separate experiment were carried out:

Experiment 1: $FeSO_4$ (2.78 mg, 1 mol%), quinoline *N*-Oxide (**1a**) (145 mg, 1mmol) were added in a 2mL screw-capped vial equipped with a magnetic stirrer. Toluene (50 uL) followed by methyl acrylate (**2a**) (2 mmol, 172 mg, 180 μL) were added. The resulting mixture was sealed with a Teflon lined cap and left stirred at 100°C. Samples were taken each 300 s and analyzed by GLC analysis using samples of pure compound as references.

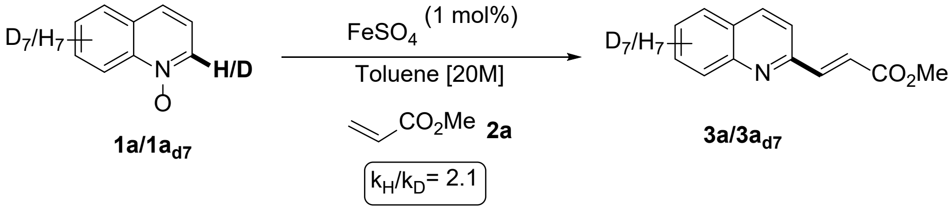
Experiment 2: $FeSO_4$ (2.78 mg, 1 mol%), quinoline *N*-Oxide-d7 (**1a$_{d7}$**) (152 mg, 1mmol) were added in a 2mL screw-capped vial equipped with a magnetic stirrer. Toluene (50 uL) followed by methyl acrylate (**2a**) (2 mmol, 172 mg, 180 μL) were added. The resulting mixture was sealed with a Teflon lined cap and left stirred at 100°C. Samples were taken each 300 s and analyzed by GLC analysis using samples of pure compound as references.

	300 s	600 s	900 s	1200 s	1500 s
Exp. 1 (Conversion to **3a**)	1.9	4.9	8.5	11.4	14.7
Exp. 2 (Conversion to **3a$_{d7}$**)	0.8	1.8	3.5	4.9	6.9

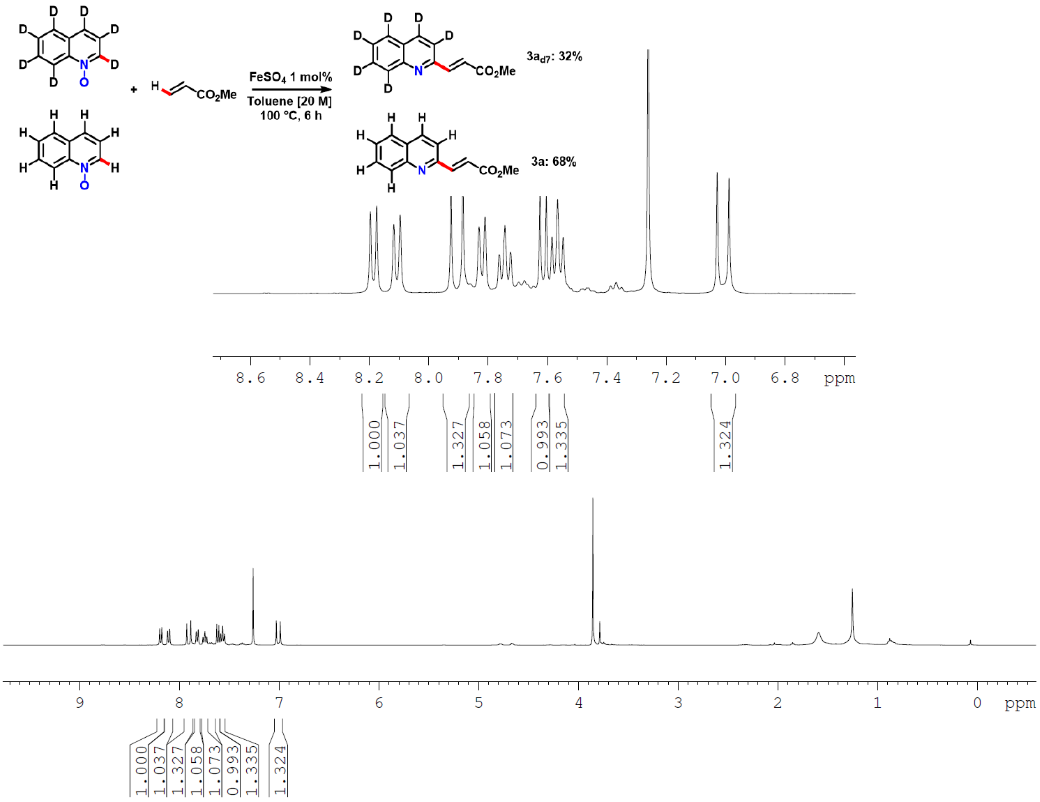


K_H= 1.07 x 10^{-2} K_D= 5.1 x 10^{-3} KIE : 2.09

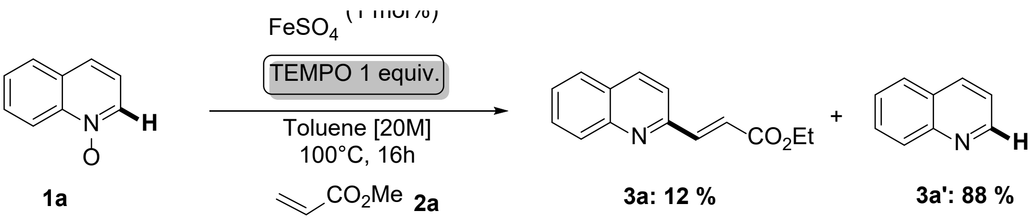
5.4 Procedure for Intermolecular KIE determination in one-pot



$FeSO_4$ (2.78 mg, 1 mol%), quinoline *N*-Oxide (**1a**) (145 mg, 1mmol) and quinoline *N*-Oxide-d7 (**1a$_{d7}$**) (152 mg, 1mmol) were added in a 2mL screw-capped vial equipped with a magnetic stirrer. Toluene (50 uL) followed by methyl acrylate (**2a**) (2 mmol, 172 mg, 180 µL) were added. The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for 8h. After this time, the crude mixture was filtered over a silica plug eluting with EtOAc/Petroleum Ether 1/99. The solvent was evaporated under reduced pressure and the crude was analyzed by ^{1}H-NMR to estimate the ratio between **3a** and **3a$_{d7}$**.



5.5 Procedure for Radical scavenging experiment



$FeSO_4$ (2.78 mg, 1 mol%), quinoline *N*-Oxide (**1a**) (145 mg, 1mmol) and TMEPO (156 mg, 1mmol) were added in a 2mL screw-capped vial equipped with a magnetic stirrer. Toluene (50 uL) followed by methyl acrylate (**2a**) (2 mmol, 172 mg, 180 µL) were added. The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for 16h. After this time, the crude mixture was diluted with methanol (2 mL) and filtered over a celite plug. The solvent has been removed under reduced pressure and dissolved in ethyl acetate (2mL) and analyzed by GLC using pure compounds as reference standard.

6. Mechanistic Investigation Based on DFT Calculations

6.1 Computational methods

All calculations were carried out using density functional theory with the B3LYP functional,[1] as implemented in the Gaussian09 program package.[2] For geometry optimizations, the def2-SVP basis set was used for all elements.[3] The stationary points were confirmed as minima (no imaginary frequencies) or transition states (only one imaginary frequency) by analytical frequency calculations at the same theory level as the geometry optimizations. The vibrational analyses were conducted with the GoodVibes program[4] at 373 K using the quasi-rigid-rotor-harmonic-oscillator approximation proposed by Grimme.[5] Based on the optimized geometries, single-point calculations were carried out with the def2-TZVP basis set for all elements.[3] Energies were also corrected for dispersion effects using the DFT-D3 method of Grimme with Becke and Johnson damping.[6] The reported energies are the gas-phase Gibbs free energies, calculated with the bigger basis set and including all the mentioned corrections.

For all stationary points different spin states were evaluated, and in all cases the quintet state was found to be significantly more stable than the alternatives. Since the reaction is performed in solvent-free conditions or in the presence of minimal amounts of an apolar solvent, only neutral species have been considered in this investigation.

6.2 DFT Results

To gain more insight into the mechanism of the alkenylation of quinoline-*N*-oxide, we performed DFT calculations on different mechanistic possibilities. We chose as a model the reaction between unsubstituted quinoline-*N*-oxide **1a** and methyl acrylate **2a**. First we will illustrate the most favorable mechanism according to the calculated free energies (Figure S1). The process starts from the quinoline-*N*-oxide-coordinated iron complex **A**, that we take as a reference point for the energy. A slightly endergonic dissociation of a water molecule (from **A** to **B**) precedes the first key step, a ligand-promoted deprotonation of C2 mediated by sulfate (**TS1$_{C2}$**, see Figure S2 for the optimized geometry), associated with a reasonable free energy barrier of 20.4 kcal/mol. In the resulting intermediate **C** the deprotonated substrate coordinates iron with both oxygen and C2. Next, a slightly exergonic proton transfer from a water ligand to the oxygen of the substrate leads to intermediate **D**, which can further evolve to intermediate **E** through a shift of the hydroxy group from nitrogen to iron (the transition states for these two steps could not be located). The reaction can then proceed through an insertion of the methyl acrylate double bond on the C2−Fe bond (**TS2$_{C2}$**, see Figure S2 for the optimized geometry). This step is associated with a free energy barrier of 27.5 kcal/mol, still reasonable considering the reaction temperature, and leads exergonically to intermediate **F**, in which iron is coordinated to the α-position (relative to the carbonyl group). This can rearrange with a gain of ca. 10 kcal/mol to intermediate **G**, in which the functionalized substrate coordinates iron through the enolate oxygen (the transition state for this rearrangement could not be located). Finally, one of the hydroxy ligand can abstract a benzylic hydrogen through **TS3$_{C2}$** (see Figure S2 for the optimized geometry), to give intermediate **H**, in which the final product is coordinated to the iron complex through its carbonyl oxygen. This step is associated to a barrier of 17.3 kcal/mol and is exergonic by 25.1 kcal/mol. Overall, this mechanism has reasonable energy barriers.

We also considered the possibility of the reaction occurring through an initial [3+2] cycloaddition, followed by a N–O cleavage step and a dehydration.[7] However the transition state for the initial cycloaddition occurring with [$FeSO_4(H_2O)_3$] acting as a Lewis acid catalyst by coordination on the carbonyl (**TS$_{[3+2]}$**) is 39.3 kcal/mol higher in energy than complex **A** (see grey profile in Figure S1). The uncatalyzed [3+2] cycloaddition has expectedly an even higher energy relative to complex **A** (45.9 kcal/mol, see **TS$_{[3+2]U}$** in Figure S1). These findings essentially rule out the possibility for this reaction to occur through an initial [3+2] cycloaddition.

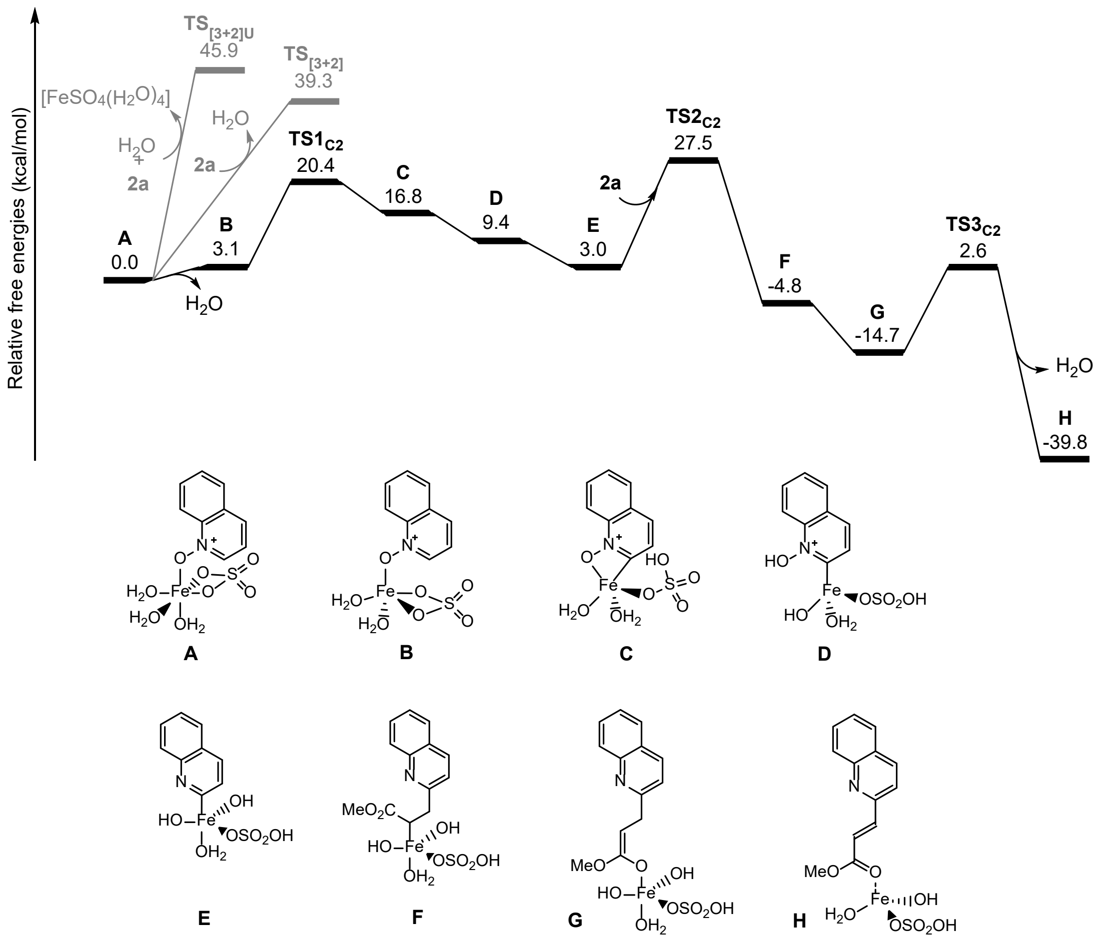


Figure S1. Calculated free energy profile and structures of the intermediates for the reaction between **1a** and **2a** occurring on C2.

Next, in order to investigate whether this mechanism is able to account for the observed C2 selectivity, we located the key transition states also for the functionalization on the C8 position, the only other position apart from C2 that could potentially benefit from a directing effect of the *N*-oxide group. The C−H activation step for the reaction occurring on C8 through **TS1**$_{C8}$ (see Figure S2 for the optimized geometry) is associated with a barrier of 26.2 kcal/mol, 5.8 kcal/mol higher than the corresponding transition state for the C2−H activation (**TS1**$_{C2}$ in Figure S2). Importantly, also the transition states for the insertion step show the same trend, with the transition state for the insertion occurring on C8 being 4.2 kcal/mol higher in energy than the corresponding transition state for the reaction occurring on C2 (see **TS2**$_{C2}$ and **TS2**$_{C8}$ in Figure S2). This demonstrates that the proposed mechanism is able to account for the experimentally observed regioselectivity. Concerning the origins of the selectivity, a simple analysis of the transition states for the C–H activation step reveal that **TS1**$_{C2}$ is a later transition state compared to **TS1**$_{C8}$. Less pronounced differences are observed between **TS2**$_{C2}$ and **TS2**$_{C8}$. The considerable differences between **TS1**$_{C2}$ and **TS1**$_{C8}$ can possibly depend on the substantial difference in acidity between C2–H and C8–H (ca. 11.5 kcal/mol in the gas phase, corresponding to a difference of ca. 8 units of pKa). However, a more detailed investigation is needed to address the origins of the observed selectivity and to verify whether this preliminary mechanistic proposal holds also for other substrates. Further mechanistic investigations are ongoing in our laboratories and the results will be published in due course.

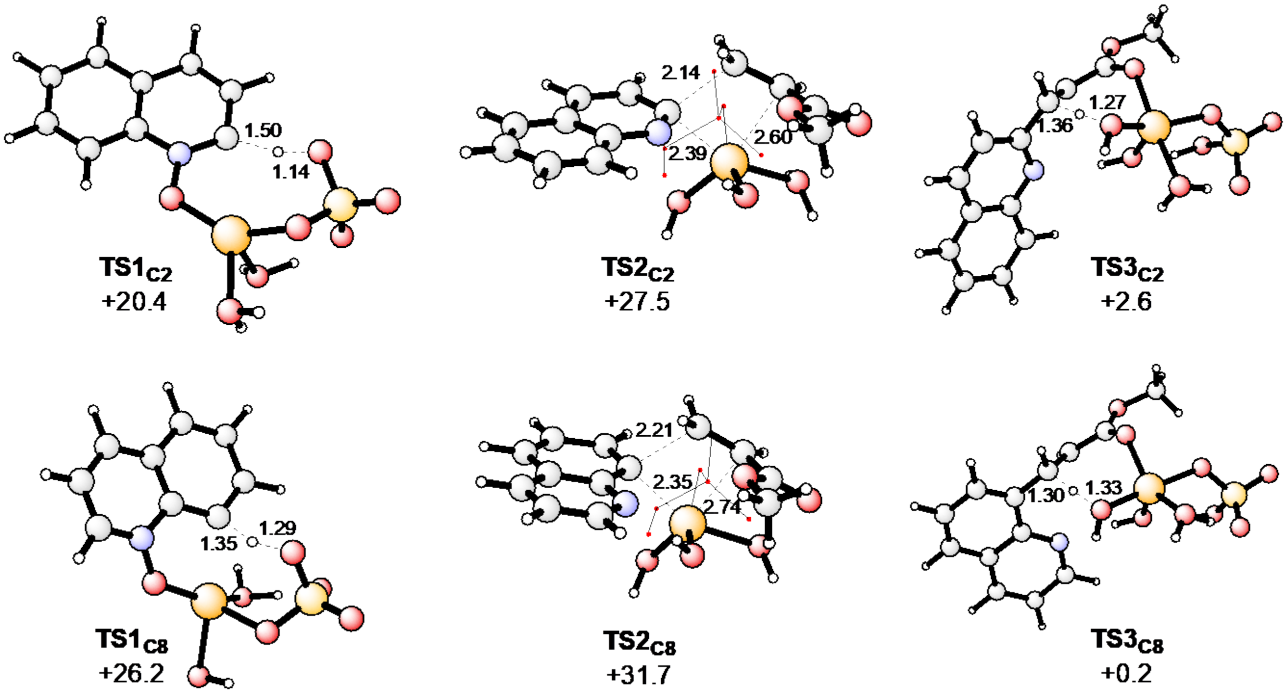


Figure S2. Optimized structures of key transition states for the reaction occurring on C2 or on C3 position of quinoline-N-oxide. Free energies relative to complex **A** are given in kcal/mol. Distances are in Å.

6.3 Energies and energy corrections of the stationary points (in atomic units)

Stationary point	B3LYP/def2-SVP	B3LYP/def2-TZVP	Thermal correction to Gibbs free energy	D3 correction
A	-2668.2692070	-2669.8112788	0.1681480	-0.07896771
B	-2591.8754531	-2593.3279686	0.1451290	-0.06889794
TS1$_{C2}$	-2591.8408937	-2593.2943611	0.1401490	-0.07005821
C	-2591.8489228	-2593.3024835	0.1425380	-0.07007006
D	-2591.8580975	-2593.3147153	0.1409430	-0.06804080
E	-2591.8647211	-2593.3220252	0.1429470	-0.07284258
TS2$_{C2}$	-2898.0838742	-2899.8884663	0.2255110	-0.10539071
F	-2898.1486672	-2899.9505934	0.2314770	-0.10063292
G	-2898.1669967	-2899.9677807	0.2302650	-0.09811029
TS3$_{C2}$	-2898.1373814	-2899.9346886	0.2258040	-0.09918900
H	-2821.8229646	-2823.5318572	0.2065880	-0.08496347
TS1$_{C8}$	-2591.8317445	-2593.2804608	0.1407330	-0.07530376
TS2$_{C8}$	-2898.0754541	-2899.8792136	0.2260090	-0.10843848
H_2O	-76.3583153	-76.4628741	-0.0019230	-0.00057395
2a	-306.2420201	-306.5965207	0.0550060	-0.01393392
[$FeSO_4(H_2O)_4$]	-2267.8610108	-2268.9814264	0.0618200	-0.03485307
TS$_{[3+2]}$	-2974.4822865	-2976.3665412	0.2570640	-0.10543373
TS$_{[3+2]U}$	-782.9642303	-783.8337392	0.1832780	-0.06480201

7. E-factor calculations for literature protocols and for the reported procedure

Reference	Procedure	E-factor calculation[a]
J. Am. Chem. Soc. 2009, **131**, 13888–13889	5 mmol olefins in 1 mL NMP was added into the flask charged with 1 mmol N-oxide, 5 mol% $Pd(OAc)_2$ (11.2 mg). The mixture was stirred at 110 °C for 20 hours, then cooled down to room temperature, diluted with 10 mL ether and washed with 10 mL H_2O. The aqueous layer was extracted twice with ether (5 mL) and the combined organic phase was dried over Na_2SO_4. After evaporation of the solvents the residue was purified by silica gel chromatography or thin layer chromatography (TLC) (elute: hexane-EtOAc). (E)-Ethyl-3-(2-quinolyl)acrylate (86 %)	E-factor = [500.6 mg (Ethyl acrylate) + 145.2 mg (Quinoline *N*-oxide) + 1030 mg (NMP) + 11.2 mg (Palladium acetate) + 14260 mg (diethyl ether) + 10000 mg (Water)] – 195.5 mg (product) / 195.5 mg (product) = **131.7**
Tetrahedron Letters 2016, **57,** 3920–3923	2.5 mmol olefins in 1 mL DMSO was added into the flask charged with 0.5 mmol *N*-oxide, 10 mol% $PdCl_2$ (8.8 mg). The mixture was stirred at 100 °C for 20 hours, then cooled down to room temperature, diluted with 10 mL ethyl acetate and washed with 10 mL H_2O. The aqueous layer was extracted twice with ethyl acetate (5 mL) and the combined organic phase was dried over Na_2SO_4. After evaporation of the solvents the residue was purified by flash column chromatography (silica gel, hexane/EtOAc) to afford the desired products (E)-2-Styrylquinoline (56 %).	E-factor = [260.37 mg (styrene) + 72.6 mg (Quinoline *N*-oxide) + 1100 mg (DMSO) + 8.8 mg (Palladium chloride) + 18040 mg (ethyl acetate) + 10000 mg (Water)] – 64.7 mg (product) / 64.7 mg (product) = **458.6**
Org. Biomol. Chem., 2016, **14**, 5820–5825	An oven-dried re-sealable tube, fitted with a magnetic stirrer, was charged with N-oxide substrate (0.143 mmol). The tube was fitted with a rubber septum and purged with nitrogen. A solution of styrene (450 mol%) and TsOH (5 mol%) in the appropriate solvent (50:1 v/v mixture with H_2O, 1.5 M concentration with respect to substrate) was added via syringe and the tube was sealed with a Young's tap. The reaction vessel was placed into a pre-heated heating block at 120-140 °C and stirred for 24 hours. The reaction mixture was cooled to room temperature and concentrated in vacuo. Purification of the residue by FCC (10% EtOAc/hexane to 30% EtOAc/hexane) afforded pure (E)-2-Styrylquinoline (96 %).	E-factor = [67 mg (styrene) + 20 mg (Quinoline *N*-oxide) + 110 mg (DMSO) + 2 mg (water) + 1.3 mg (TsOH)] – 31.7 mg (product) / 31.7 mg (product) = **5.3**
Org. Lett. 2016, **18**, 1796−1799	Quinoline N-oxide (0.1 mmol) was weighed into a 15 mL dried screw-capped tube, which was followed by the addition of DMSO (0.5 mL), styrene (1.0	E-factor = [104,15 mg (styrene) + 14.5 mg (Quinoline *N*-oxide) + 550 mg (DMSO) + 18 mg (AcOH)] –

	mmol) and AcOH (0.3 mmol). The tube was sealed and stirred at 120 °C for 40 hours. The reaction mixture was cooled to room temperature and then subjected to silica gel column chromatography (EtOAc/petroleum ether) to obtain the desired (E)-2-Styrylquinoline (75 %).	17.34 mg (product) / 17.34 mg (product) = **37.6**
This work	$FeSO_4$ (41 mg, 1 mol%) and quinoline *N*-Oxide (**1a**) (2.2 g, 15 mmol) were added in a 4mL screw-capped vial tube equipped with a magnetic stirrer. Toluene (50 uL) followed by styrene (**5a**) (3.4 mL, 30mmol) were added. The resulting mixture was sealed with a Teflon lined cap and stirred at 100°C for 16h. After this time, the crude mixture was poured into methanol (5 mL) and filtered over a celite plug. The solvent has been removed under reduced pressure crude mixture has been purified by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielding **6a** in 98% (3.4 g)	E-factor = [3.1 g (styrene) + 2.2 g (Quinoline *N*-oxide) + 0.64 g (toluene) + 0.04 g (Iron sulfate) + 3,9 g (methanol)] – 3.4 g (product) / 3.4 g (product) = **0.92**

[a] Solvents and solid materials used for chromatography were not included in the calculation

8. Methods, source and references for safety/hazard analysis

List of abbreviations:

AE = atom economy

ARDP = abiotic resource depletion potential

CGP = corrosiveness potential as a gas

CLP = corrosiveness potential as a liquid/solid

ECHA = European Chemicals Agency

FP = flammability potential

FLP = flash point (closed cup)

LC50 (inhalation) = lethal concentration to kill 50% of

population via inhalation route

LD50 (dermal) = lethal dose to kill 50% of population via dermal route

MCM = multicompartment model

MRP = material recovery parameter

MW = molecular weight

MSDS = material safety data sheets

NOISH = National Institute for Occupational Safety and Health (U.S.)

OEL = occupational exposure limit

OELP = occupational exposure limit potential

OSHA = Occupational Safety and Health Administration (U.S.)

PMI = process mass intensity

RPP = risk phrase potential

RME = reaction mass efficiency

RTECS = Registry of Toxic Effects of Chemical Substances

SHI = Safety/Hazard Index

SHZI = Safety/Hazard Impact

SF = stoichiometric factor

TWA = time weighted average

VMR = vector magnitude ratio

The safety/hazard analysis have been conducted in accordance with the methods, calculations and equation reported by J. Andraos in *Org. Process Res. Dev.* 2013, **17**, 175−192.

Definitions and equation for multicompartment method (MCM) and for Abiotic resource depletion potential (ARDP) have been used in accordance with the data reported by J. Andraos in *Org. Process Res. Dev*. 2012, **16**, 1482−1506.

Log Kow reference: CRC Handbook of Chemistry and Physics, 91st ed., CRC Press: Boca Raton, 2009, Chapter 16, pp. 43-47

ARDP and Metal abundance references: Guinée, J.B., ed., Handbook on Life Cycle Assessment, Kluwer Academic Publishers: Dordrecht, 2002, Part 2b, p. 167

LD50 and LC50 and OEL, Flash point and risk phrases references and sources: MSDS files for each compound, Registry of Toxic Effects of Chemical Substances (RTECS) and NIOSH POCKET GUIDE TO CHEMICAL HAZARDS, National Institute for Occupational Safety and Health, September 2007, Publication No. 2005-149 (http://www.cdc.gov/niosh).

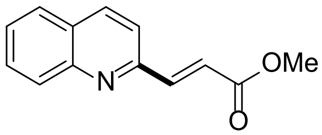
QEissen factors: Eissen, M. Bewertung der Umweltverträglichkeit organisch-chemischer Synthesen. PhD thesis 2001, Universität Oldenburg, and *Org. Process Res. Dev.* 2013, **17**, 175−192.

Safety Index Analysis

Substance		LD50 mg/k	LC50 g m3	Risk Phrases	QEissen	FLP (C)	FLP(K)	FP	OEL (mg/m	OEL (mmo	CGP	CLP	OELP	RPP	Ω	Metal Abbundance %	logARDP	ADP
Ethyl acryl	140-88-5	1120	9,13	R 11-20/21/22-36/37/38-43	18	9	282,15	0,826334	100	0,99	0,056955	0,567857	4,111111	2,121628	7,683885			
methyl acr	96-33-3	277	3,58	R 11-20/21/22-36/37/38-43	18	-2,7	270,45	0,862082	35	0,4	0,145251	2,296029	10,175	2,121628	15,59999			
styrene	100-42-5	2650	11,78	R 10-20-36/38-48/20	3,37	31	304,15	0,766563	215	2,06	0,044143	0,24	1,975728	1,424154	4,450588			
solvents																		
DMSO	67-68-5	28300	5330	R 10-24/25-36/37/38	3,75	87	360,15	0,647369	160	2,04	9,76E-05	0,022473	1,995098	1,846601	4,511639			
AcOH	64-19-7	3310	39,3	R 10	1	40	313,15	0,744531	25	0,4	0,013232	0,192145	10,175	1,614857	12,73976			
toluene	108-88-3	636	49	R 11-20	3	4	277,15	0,841241	375	4,07	0,010612	1	1	1,807477	4,659331			
EtOAc	141-78-6	5620	200	R 11-36	3	-4	269,15	0,866246	1400	15,89	0,0026	0,113167	0,256136	1,807477	3,045626			
diethyl eth	60-29-7	1211	0,52	R 12-19	9	-40	233,15	1	1200	16,19	1	0,525186	0,25139	2,000098	4,776673			
NMP	872-50-4	4150	5,1	R 61-36/37/38	7,5	91	364,15	0,640258	40	0,4	0,101961	0,153253	10,175	1,968131	13,0386			
methanol	67-56-1	2769	128,2	R 11-23/24/25	5	9,7	282,85	0,824288	260	8,11	0,004056	0,229686	0,50185	1,897041	3,456921			
additives																		
TsOH	6192-52-5	2570		R 34-36/37/38	3	180	453,15	0,51451	10			0,247471		1,807477	2,569458			
Catalyst																		
iron sulfat	7782-63-0	1520		R 22-36/38	0,75				10	0,17		0,418421	23,94118	1,564417	25,92401	5,6	-7,07	3,58E-04
palladium	7647-10-1.	479		R 22-41-43-50/53	4				0,5	0,004		1,327766	1017,5	1,857917	1020,686	0,015	-0,49	0,32
palladium	3375-31-3	2100		R 41	2				0,5	0,004		0,302857	1017,5	1,736387	1019,539	0,015	-0,49	0,32

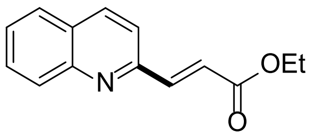
	fractional weighting factors			SHZI input	SHI imput	f waste			$SHZI_{waste}$	SHI_{waste}	f_{excess}	$SHZI_{excess}$	SHI_{excess}
	$f_{ethyl\ acrylate}$	f_{NMP}				$f_{ethyl\ acrylate}$	f_{NMP}	$f_{diethylether}$			$f_{ethyl\ acrylate}$		
J. Am. Chem. Soc. 2009, 131, 13888–13889	0,298759	0,614705		0,497552	0,502448	0,027285	0,065647	0,972715	0,389709	0,610291	0,733945	0,733945	0,266055
	$f_{styrene}$	f_{DMSO}				$f_{styrene}$	f_{DMSO}	$f_{ethylacetate}$			$f_{styrene}$		
Tetrahedron Letters 2016, 57, 3920–3923	0,181823	0,768156		0,476987	0,523013	0,011198	0,055815	0,969475	0,400535	0,599465	0,744179	0,744179	0,255821
	$f_{styrene}$	f_{DMSO}	f_{TsOH}			$f_{styrene}$	f_{DMSO}				$f_{styrene}$		
Org. Biomol. Chem., 2016, **14**, 5820–5825	0,34277	0,55814	0,006572	0,451189	0,548811	0,327649	0,669915		0,499948	0,500052	0,728997	0,728997	0,271003
	$f_{styrene}$	f_{DMSO}	f_{AcOH}			$f_{styrene}$	f_{DMSO}				$f_{styrene}$		
Org. Lett. 2016, 18, 1796–1799	0,147727	0,78125	0,025568	0,466646	0,533354	0,145552	0,855365		0,502876	0,497124	0,74872	0,74872	0,25128
	$f_{styrene}$	$f_{toluene}$				$f_{styrene}$	$f_{toluene}$	$f_{methanol}$			$f_{styrene}$		
This work	0,521886	0,107744		0,31007	0,68993	0,253731	0,106136	0,646766	0,307125	0,692875	0,410188	0,410188	0,589812

9. Characterization Data



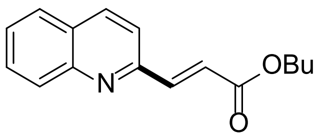
Methyl (*E*)-3-(quinolin-2-yl)acrylate (3a)[8]

General procedure has been followed using quinoline *N*-oxide (**1a**) (1 mmol, 145 mg) and methyl acrylate (172 mg, 180 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80) yielded **3a** (183 mg, 86%) as white solid. M. p. 75-77. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.19 (d, *J* = 8.5 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 7.91 (d, *J* = 15.9 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.77 – 7.72 (m, 1H), 7.63 – 7.55 (m, 2H), 7.01 (d, *J* = 15.9 Hz, 1H), 3.85 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 167.2, 153.3, 148.4, 144.5, 136.9, 130.2, 130.0, 128.2, 127.7, 127.5, 123.4, 120.5, 52.08. **GC-EIMS (m/z, %):** 213 (100), 199 (75), 185 (45), 143 (60), 129 (45).



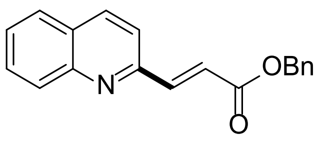
Ethyl (*E*)-3-(quinolin-2-yl)acrylate (3b)[9]

General procedure has been followed using quinoline *N*-oxide (**1a**) (1 mmol, 145 mg) and ethyl acrylate (2 mmol, 200 mg, 218 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 15/85) yielded **3b** (186 mg, 82%) as white solid. M. p. 80-81. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.18 (d, *J* = 8.5 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 16.0 Hz, 1H), 7.82 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.76 – 7.72 (m, 1H), 7.62 (d, *J* = 8.5 Hz, 1H), 7.58 – 7.54 (m, 1H), 6.99 (d, *J* = 16.0 Hz, 1H), 4.31 (q, *J* = 7.2 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.7, 153.4, 148.4, 144.2, 136.9, 130.2, 130.0, 128.2, 127.7, 127.5, 123.9, 120.4, 60.9, 14.4. **GC-EIMS (m/z, %):** 227 (100), 199 (40), 155 (65), 143 (70), 129 (55).



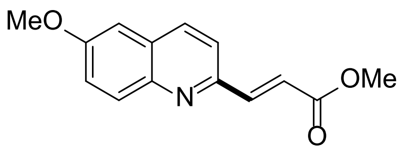
Butyl (*E*)-3-(quinolin-2-yl)acrylate (3c)[9]

General procedure has been followed using quinoline *N*-oxide (**1a**) (1 mmol, 145 mg) and buthyl acrylate (256 mg, 287 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80) yielded **3c** (224 mg, 88 %) as white solid. M. p. 75-77. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.17 (d, *J* = 8.5 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.89 (d, *J* = 15.9 Hz, 1H), 7.81 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.75 – 7.71 (m, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.57 – 7.53 (m, 1H), 6.98 (d, *J* = 16.0 Hz, 1H), 4.25 (t, *J* = 6.6 Hz, 2H), 1.75 – 1.67 (m, 2H), 1.50 – 1.41 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.7, 153.3, 148.3, 144.0, 136.8, 130.1, 129.8, 128.1, 127.6, 127.3, 123.8, 120.3, 64.7, 30.7, 19.2, 13.8. **GC-EIMS (m/z, %):** 255 (100), 226 (75), 183 (45), 143 (65), 129 (45).



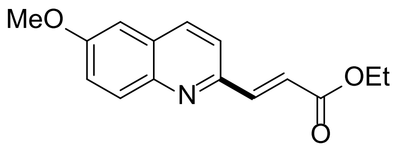
Benzyl (*E*)-3-(quinolin-2-yl)acrylate (3d)[10]

General procedure has been followed using quinoline *N*-oxide (**1a**) (1 mmol, 145 mg) and benzyl acrylate (324 mg, 306 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80) yielded **3d** (231 mg, 80 %) as pale-yellow solid. M. p. 80-82. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.17 (d, *J* = 8.5 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 15.9 Hz, 1H), 7.81 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.76 – 7.71 (m, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.46 – 7.35 (m, 6H), 7.05 (d, *J* = 15.9 Hz, 1H), 5.30 (s, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.4, 153.1, 148.3, 144.6, 136.8, 135.9, 131.1, 130.1, 129.9, 128.6, 128.3, 128.1, 127.6, 127.4, 123.4, 120.3, 66.6. **GC-EIMS (m/z, %):** 289 (10), 244 (100), 182 (50), 155 (45), 128(40).



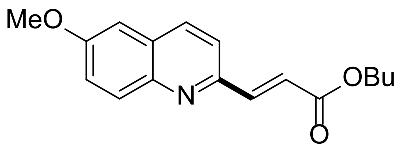
Methyl (*E*)-3-(6-methoxyquinolin-2-yl)acrylate (3e)

General procedure has been followed using 6-methoxyquinoline *N*-oxide (1 mmol, 175 mg) and methyl acrylate (172 mg, 180 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80) yielded **3e** (199 mg, 82%) as white solid. M. p. 80-81. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.06 (d, *J* = 8.6 Hz, 1H), 8.01 (d, *J* = 8.8 Hz, 1H), 7.87 (d, *J* = 15.9 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 1H), 7.41 – 7.38 (m, 1H), 7.06 (d, *J* = 2.9 Hz, 1H), 6.94 (d, *J* = 15.9 Hz, 1H), 3.94 (s, 3H), 3.84 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 167.3, 158.7, 150.9, 144.5, 144.6, 135.5, 131.4, 129.5, 123.3, 122.3, 120.9, 105.1, 55.8, 52.0. **GC-EIMS (m/z, %):** 243 (100), 212 (60), 185 (75), 169 (30), 141(25).



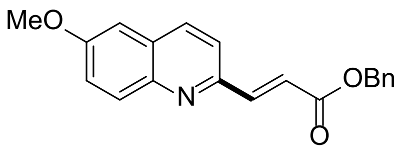
Ethyl (*E*)-3-(6-methoxyquinolin-2-yl)acrylate (3f)

General procedure has been followed using 6-methoxyquinoline *N*-oxide (1 mmol, 175 mg) and ethyl acrylate (2 mmol, 200 mg, 218 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80) yielded **3f** (218 mg, 85%) as white solid. M. p. 78-80. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.06 (d, *J* = 8.5 Hz, 1H), 7.99 (d, *J* = 9.2 Hz, 1H), 7.87 (d, *J* = 15.9 Hz, 1H), 7.58 (d, *J* = 8.5 Hz, 1H), 7.39 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.07 (d, *J* = 2.8 Hz, 1H), 6.92 (d, *J* = 15.9 Hz, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 3.95 (s, 3H), 1.36 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.88, 158.66, 151.02, 144.58, 144.39, 135.44, 131.47, 129.43, 123.16, 122.69, 120.79, 105.09, 60.84, 55.76, 14.45. **GC-EIMS (m/z, %):** 257 (95), 212 (10), 185 (100), 141 (30), 115 (10).



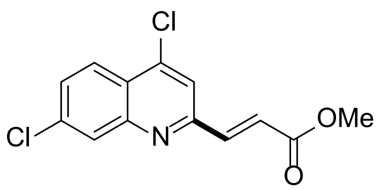
Butyl (*E*)-3-(6-methoxyquinolin-2-yl)acrylate (3g)

General procedure has been followed using 6-methoxyquinoline *N*-oxide (1 mmol, 175 mg) and buthyl acrylate (256 mg, 287 μL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 15/85) yielded **3g** (222 mg, 78%) as white solid. M. p. 74-75. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.03 – 7.96 (m, 2H), 7.84 (d, *J* = 15.9 Hz, 1H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.36 (dd, *J* = 9.3, 2.8 Hz, 1H), 7.03 (d, *J* = 2.8 Hz, 1H), 6.91 (d, *J* = 15.9 Hz, 1H), 4.23 (t, *J* = 6.6 Hz, 2H), 3.92 (s, 3H), 1.73 – 1.66 (m, 2H), 1.47 – 1.42 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.92, 158.59, 150.95, 144.50, 144.27, 135.38, 131.38, 129.36, 123.10, 122.64, 120.73, 105.03, 64.70, 55.68, 30.85, 19.31, 13.85. **GC-EIMS (m/z, %):** 285 (60), 242 (5), 212 (10), 185 (100), 141 (25).



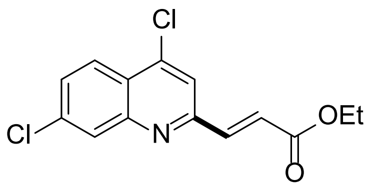
Benzyl (*E*)-3-(6-methoxyquinolin-2-yl)acrylate (3h)

General procedure has been followed using 6-methoxyquinoline *N*-oxide (1 mmol, 175 mg) and benzyl acrylate (324 mg, 306 μL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80) yielded **3h** (223 mg, 70 %) as pale-yellow solid. M. p. 85-87. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.02 (d, *J* = 8.5 Hz, 1H), 7.97 (d, *J* = 9.3 Hz, 1H), 7.90 (d, *J* = 15.9 Hz, 1H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.45 – 7.34 (m, 6H), 7.04 (d, *J* = 2.8 Hz, 1H), 6.98 (d, *J* = 15.9 Hz, 1H), 5.29 (s, 2H), 3.92 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.6, 158.6, 150.8, 144.9, 144.5, 136.1, 135.4, 131.4, 129.4, 128.7, 128.4, 123.2, 122.2, 120.8, 105.0, 66.6, 55.7. **GC-EIMS (m/z, %):** 319 (65), 274 (60), 212 (50), 185 (100), 169 (25).



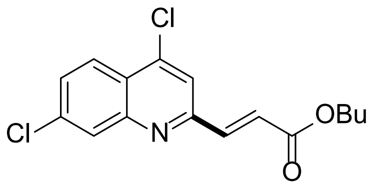
Methyl (*E*)-3-(4,7-dichloroquinolin-2-yl)acrylate (3i)

General procedure has been followed using 4,7-dichloroquinoline *N*-oxide (1 mmol, 214 mg) and methyl acrylate (172 mg, 180 μL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 15/85) yielded **3i** (245 mg, 87%) as pale-yellow solid. M. p. 127-129. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.16 – 8.11 (m, 2H), 7.78 (d, *J* = 15.9 Hz, 1H), 7.65 (s, 1H), 7.60 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.02 (d, *J* = 15.8 Hz, 1H), 3.86 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.7, 154.3, 149.5, 143.4, 142.8, 137.3, 129.4, 129.2, 125.6, 124.9, 124.8, 120.9, 52.2. **GC-EIMS (m/z, %):** 281 (60), 266 (20), 250 (95), 223 (100), 196 (40), 186 (25), 161 (45).



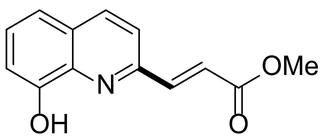
Ethyl (*E*)-3-(4,7-dichloroquinolin-2-yl)acrylate (3j)

General procedure has been followed using 4,7-dichloroquinoline *N*-oxide (1 mmol, 214 mg) and ethyl acrylate (2 mmol, 200 mg, 218 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 15/85) yielded **3j** (251 mg, 85%) as white solid. M. p. 115-116. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.15 – 8.10 (m, 2H), 7.77 (d, *J* = 15.9 Hz, 1H), 7.65 (s, 1H), 7.59 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.00 (d, *J* = 15.9 Hz, 1H), 4.31 (q, *J* = 7.2 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.3, 154.4, 149.5, 143.4, 142.5, 137.3, 129.3, 129.2, 125.6, 125.5, 124.8, 120.8, 61.1, 14.4. **GC-EIMS (m/z, %):** 295 (50), 266 (20), 250 (100), 223 (100), 196 (40), 161 (45), 125 (20).



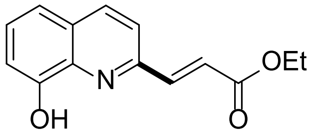
Butyl (*E*)-3-(4,7-dichloroquinolin-2-yl)acrylate (3k)

General procedure has been followed using 4,7-dichloroquinoline *N*-oxide (1 mmol, 214 mg) and buthyl acrylate (256 mg, 287 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80) yielded **3k** (265 mg, 82%) as white solid. M. p. 110-113. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.15 – 8.11 (m, 2H), 7.76 (d, *J* = 15.9 Hz, 1H), 7.66 (s, 1H), 7.59 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.00 (d, *J* = 15.9 Hz, 1H), 4.26 (t, *J* = 6.6 Hz, 2H), 1.75 – 1.68 (m, 2H), 1.51 – 1.41 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.3, 154.4, 149.4, 143.4, 142.4, 137.3, 129.4, 129.2, 125.6, 124.8, 120.8, 65.1, 30.8, 19.3, 13.9. **GC-EIMS (m/z, %):** 326 (28), 324 (100), 322 (32), 288 (65), 268 (40), 254 (25), 252 (35).



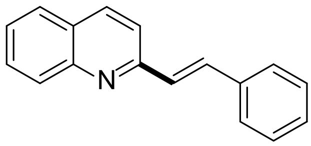
Methyl (*E*)-3-(8-hydroxyquinolin-2-yl)acrylate (3l)

General procedure has been followed using 8-hydroxyquinoline *N*-oxide (1 mmol, 161 mg) and methyl acrylate (172 mg, 180 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 15/85) yielded **3l** (201 mg, 88%) as white solid. M. p. 72-74. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.17 (d, *J* = 8.5 Hz, 1H), 7.86 (d, *J* = 15.9 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.47 (t, *J* = 7.9 Hz, 1H), 7.33 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.19 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.00 (d, *J* = 15.9 Hz, 1H), 3.87 (s, 3H). **^{13}C** NMR (101 MHz, $CDCl_3$) **δ** 166.9, 150.7, 143.4, 138.1, 137.0, 128.8, 128.4, 123.1, 121.3, 117.7, 110.6, 52.0. **GC-EIMS (m/z, %):** 229 (100), 228 (15), 212 (25), 198 (15), 189 (35), 144 (50), 129 (15).



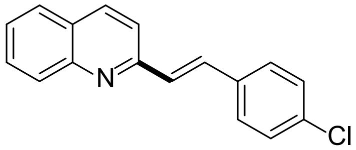
Ethyl (*E*)-3-(8-hydroxyquinolin-2-yl)acrylate (3m).

General procedure has been followed using 8-hydroxyquinoline *N*-oxide (1 mmol, 161 mg) and Ethyl acrylate (2 mmol, 200 mg, 218 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 15/85) yielded **3m** (201 mg, 88%) as white solid. M. p. 78-79. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.17 (d, *J* = 8.5 Hz, 2H), 7.85 (d, *J* = 15.9 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.47 (t, *J* = 7.9 Hz, 1H), 7.33 (d, *J* = 8.3, 1H), 7.19 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.99 (d, *J* = 15.9 Hz, 1H), 4.32 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 4H). **^{13}C** NMR (101 MHz, $CDCl_3$) **δ** 166.6, 152.5, 150.9, 143.2, 138.2, 137.1, 128.9, 128.5, 123.8, 121.4, 117.9, 110.7, 61.1, 14.4. **GC-EIMS (m/z, %):** 243 (100), 227 (20), 226 (15), 214 (45), 189 (50), 144 (45), 129 (20).



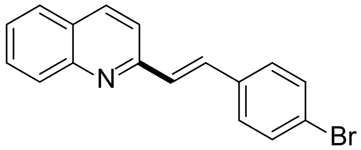
(*E*)-2-styrylquinoline (6a)[8]

General procedure has been followed using quinoline *N*-oxide (**1a**) (1 mmol, 145 mg) and styrene (208 mg, 230 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6a** (203 mg, 88 %) as pale-orange solid. M. p. 98-99. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.16 (d, *J* = 8.6 Hz, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 7.81 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.76 – 7.67 (m, 5H), 7.55 – 7.51 (m, 1H), 7.46 – 7.41 (m, 3H), 7.38 – 7.34 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 156.0, 148.3, 136.5, 136.4, 134.5, 129.8, 129.2, 129.0, 128.8, 128.7, 127.5, 127.4, 127.3, 126.2, 119.3. **GC-EIMS (m/z, %):** 231 (100), 169 (40), 155 (20), 143 (40), 129 (45).



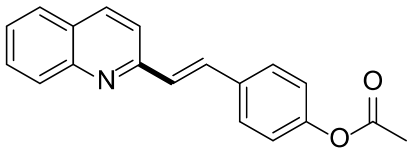
(*E*)-2-(4-chlorostyryl)quinoline (6b)[11]

General procedure has been followed using quinoline *N*-oxide (**1a**) (1 mmol, 145 mg) and 4-chlorostyrene (277 mg, 240 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6b** (229 mg, 86%) as pale-orange solid. M. p. 143-144. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.13 (d, *J* = 8.6 Hz, 1H), 8.09 – 8.07 (m, 1H), 7.79 – 7.77 (m, 1H), 7.73 – 7.69 (m, 1H), 7.66 – 7.62 (m, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.52 – 7.48 (m, 1H), 7.38 – 7.34 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 155.7, 148.4, 136.6, 135.2, 134.4, 133.1, 130.0, 129.7, 129.4, 129.2, 128.5, 127.7, 127.5, 126.4, 119.5. **GC-EIMS (m/z, %):** 267 (75), 265 (100), 231 (60), 229 (55), 143 (80), 129 (30).



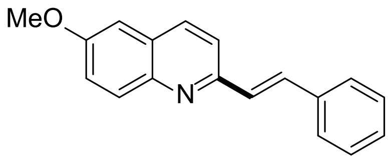
(*E*)-2-(4-bromostyryl)quinoline (6c)

General procedure has been followed using quinoline *N*-oxide (**1a**) (1 mmol, 145 mg) and 4-bromostyrene (366 mg, 261 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6c** (232 mg, 75%) as pale-brown solid. M. p. 138-140. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.13 (d, *J* = 8.6 Hz, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.78 (d, *J* = 6.7 Hz, 1H), 7.73 – 7.69 (m, 1H), 7.65 – 7.61 (m, 2H), 7.54 – 7.48 (m, 5H), 7.38 (d, *J* = 16.3 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 155.7, 148.4, 136.6, 135.6, 133.2, 132.1, 130.0, 129.8, 129.4, 128.8, 127.7, 127.6, 126.5, 122.7, 119.5. **GC-EIMS (m/z, %):** 310 (100), 228 (50), 202 (15), 178 (25), 128 (20), 101 (15).



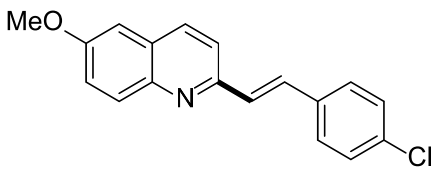
(*E*)-4-(2-(quinolin-2-yl)vinyl)phenyl acetate (6d)

General procedure has been followed using quinoline *N*-oxide (**1a**) (1 mmol, 145 mg) and 4-acetoxystyrene (324 mg, 306 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6d** (223 mg, 77%) as white solid. M. p. 127-128. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.13 (d, *J* = 8.6 Hz, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.79 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.73 – 7.62 (m, 5H), 7.52 – 7.48 (m, 1H), 7.36 (d, *J* = 16.3 Hz, 1H), 7.13 (d, *J* = 8.6 Hz, 1H), 2.32 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 169.5, 155.9, 151.0, 148.3, 136.6, 134.4, 133.6, 130.0, 129.2, 128.4, 127.7, 127.5, 126.4, 122.1, 119.4, 115.8, 21.3. **GC-EIMS (m/z, %):** 289 (30), 246 (100), 217 (25), 191 (15), 128 (25).



(*E*)-6-methoxy-2-styrylquinoline (6e)

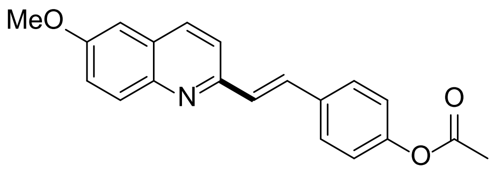
General procedure has been followed using 6-methoxyquinoline *N*-oxide (1 mmol, 175 mg) and styrene (208 mg, 230 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6e** (212 mg, 81%) as pale-yellow solid. M. p. 148-151. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.03 (d, *J* = 8.6 Hz, 1H), 7.98 (d, *J* = 9.2 Hz, 1H), 7.65 – 7.60 (m, 4H), 7.42 – 7.31 (m, 5H), 7.07 (d, *J* = 2.8 Hz, 1H), 3.94 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 157.8, 153.9, 144.4, 136.9, 135.3, 133.4, 130.8, 129.2, 128.9, 128.5, 128.5, 127.3, 122.5, 119.7, 105.4, 55.7. **GC-EIMS (m/z, %):** 261 (100), 247 (35), 231 (40), 173 (25), 159 (60).



(*E*)-2-(4-chlorostyryl)-6-methoxyquinoline (6f)

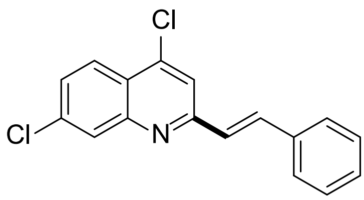
General procedure has been followed using 6-methoxyquinoline *N*-oxide (1 mmol, 175 mg) and 4-chlorostyrene (277 mg, 240 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6f** (237 mg, 80%) as pale-yellow solid. M. p. 158-160. **^{1}H NMR** (400 MHz, $CDCl_3$)

δ 8.03 (d, *J* = 8.6 Hz, 1H), 7.97 (d, *J* = 9.2 Hz, 1H), 7.62 – 7.54 (m, 4H), 7.38 – 7.35 (m, 4H), 7.07 (d, *J* = 2.8 Hz, 1H), 3.94 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 157.9, 153.5, 144.5, 135.4, 135.3, 134.2, 132.0, 130.8, 129.7, 129.1, 128.5, 128.4, 122.6, 119.8, 105.4, 55.7. **GC-EIMS (m/z, %):** 294 (100), 280 (65), 251 (25), 216 (15), 189 (25), 163 (33).



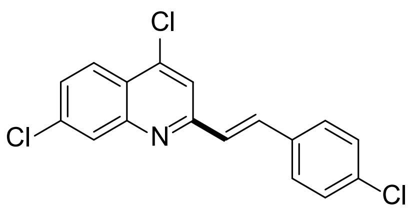
(*E*)-4-(2-(6-methoxyquinolin-2-yl)vinyl)phenyl acetate (6g)

General procedure has been followed using 6-methoxyquinoline *N*-oxide (1 mmol, 175 mg) and 4-acetoxystyrene (324 mg, 306 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6g** (235 mg, 74%) as pale-yellow solid. M. p. 139-141. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.03 (d, *J* = 8.9 Hz, 1H), 7.98 (d, *J* = 9.2 Hz, 1H), 7.64 – 7.57 (m, 3H), 7.40 – 7.30 (m, 2H), 7.11 (d, *J* = 8.8 Hz, 2H), 7.06 (d, *J* = 2.8 Hz, 1H), 3.95 (s, 3H), 2.33 (s, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 169.5, 157.9, 153.6, 150.8, 144.2, 135.4, 134.6, 132.5, 130.5, 129.1, 128.5, 128.2, 122.6, 122.1, 119.7, 105.4, 55.7, 21.3. **GC-EIMS (m/z, %):** 319 (100), 277 (80), 247 (65), 232 (55), 143 (85).



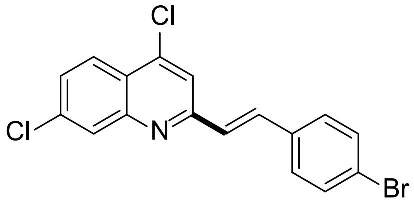
(*E*)-4,7-dichloro-2-styrylquinoline (6h)

General procedure has been followed using 4,7-dichloroquinoline *N*-oxide (1 mmol, 214 mg) and styrene (208 mg, 230 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6h** (273 mg, 91%) as white solid. M. p. 128-129. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.07 – 8.03 (m, 2H), 7.66 (t, *J* = 8.1 Hz, 2H), 7.59 (d, *J* = 7.2 Hz, 2H), 7.48 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.37 (t, *J* = 7.3 Hz, 2H), 7.33 – 7.29 (m, 1H), 7.21 (d, *J* = 2.1 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 157.2, 149.6, 142.8, 136.8, 136.2, 136.1, 129.3, 129.0, 128.6, 128.1, 127.6, 127.6, 125.6, 124.1, 119.8. **GC-EIMS (m/z, %):** 298 (100), 264 (60), 228 (15), 201 (15), 162 (30), 113 (20).



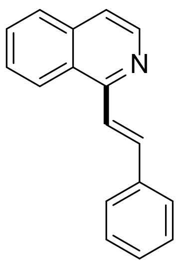
(*E*)-4,7-dichloro-2-(4-chlorostyryl)quinoline (6i)

General procedure has been followed using 4,7-dichloroquinoline *N*-oxide (1 mmol, 214 mg) and 4-chlorostyrene (277 mg, 240 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6i** (287 mg, 86%) as pale-yellow solid. M. p. 150-152. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.16 – 8.11 (m, 2H), 7.73 – 7.69 (m, 2H), 7.60 – 7.56 (m, 3H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 1.7 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 156.7, 149.4, 142.8, 136.8, 134.9, 134.7, 134.5, 129.1, 128.6, 128.5, 128.1, 127.9, 125.4, 124.0, 119.8. **GC-EIMS (m/z, %):** 334 (100), 298 (75), 263 (15), 227 (25), 200 (15), 162 (15), 131 (20).



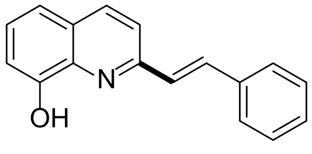
(*E*)-2-(4-bromostyryl)-4,7-dichloroquinoline (6j)

General procedure has been followed using 4,7-dichloroquinoline *N*-oxide (1 mmol, 214 mg) and 4-bromostyrene (366 mg, 261 μL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6j** (333 mg, 88%) as pale-brown solid. M. p. 138-140. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.08 – 8.04 (m, 2H), 7.63 – 7.58 (m, 2H), 7.53 – 7.44 (m, 5H), 7.21 (d, *J* = 16.2 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 156.6, 149.4, 142.8, 136.8, 134.9, 134.7, 132.1, 128.8, 128.4, 128.1, 128.0, 125.4, 123.9, 123.2, 119.7. **GC-EIMS (m/z, %):** 378 (100), 344 (50), 298 (25), 262 (25), 227 (25), 200 (10), 162 (20).



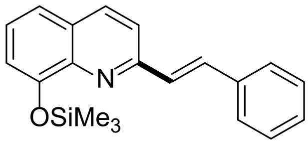
(*E*)-3-styrylisoquinoline (6k)

General procedure has been followed using isoquinoline *N*-oxide (1 mmol, 145 mg) and styrene (208 mg, 230 μL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6k** (171 mg, 74%) as pale-yellow solid. M. p. 115-116. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.57 (d, *J* = 5.6 Hz, 1H), 8.39 – 8.37 (m, 1H), 8.00 (d, *J* = 1.9 Hz, 2H), 7.85 – 7.82 (m, 1H), 7.72 – 7.67 (m, 3H), 7.65 – 7.61 (m, 1H), 7.57 (d, *J* = 5.6 Hz, 1H), 7.44 – 7.41 (m, 2H), 7.37 – 7.33 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 154.6, 142.5, 137.0, 136.8, 135.9, 129.9, 128.8, 128.6, 127.5, 127.3, 127.2, 126.8, 124.5, 122.9, 120.0. **GC-EIMS (m/z, %):** 231 (100), 202 (20), 154 (25), 115 (15), 77 (15).



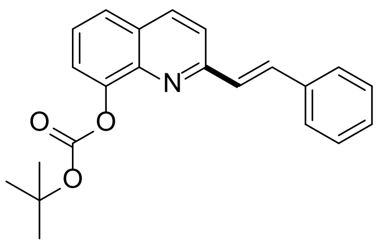
(*E*)-2-styrylquinolin-8-ol (6l)

General procedure has been followed using 8-hydroxyquinoline *N*-oxide (1 mmol, 161 mg) and styrene (208 mg, 230 μL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6l** (218 mg, 88 %) as white solid. M. p. 99-100. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.11 (d, *J* = 8.6 Hz, 1H), 7.72 (d, *J* = 16.3 Hz, 1H), 7.65 – 7.63 (m, 3H), 7.45 – 7.29 (m, 6H), 7.19 – 7.17 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 153.6, 152.1, 138.0, 136.4, 136.4, 134.4, 128.9, 128.8, 128.1, 127.5, 127.3, 127.3, 120.4, 117.7, 110.2. **GC-EIMS (m/z, %):** 247 (100), 217 (25), 189 (35), 114 (15), 89 (16).



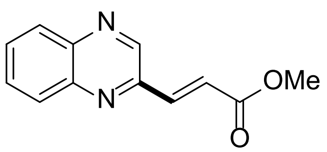
(E)-2-styryl-8-((trimethylsilyl)oxy)quinoline (6m).

General procedure has been followed using 8-((trimethylsilyl)oxy)quinoline *N*-oxide (1 mmol, 233 mg) and styrene (208 mg, 230 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6m** (268 mg, 84%) as pale orange solid. M. p. 98-101. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.12 (d, *J* = 8.5 Hz, 1H), 7.72 (d, *J* = 16.3 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 3H), 7.44 – 7.29 (m, 6H), 7.18 (d, *J* = 7.5 Hz, 1H), 0.08 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 153.8, 152.2, 138.2, 136.6, 136.5, 134.5, 129.0, 128.9, 128.3, 127.6, 127.4, 127.4, 120.5, 117.8, 110.3, 1.2. **GC-EIMS (m/z, %):** 319 (100), 247 (50), 246 (45), 230 (15), 171 (45), 154 (25).



(E)-tert-butyl (2-styrylquinolin-8-yl) carbonate (6n).

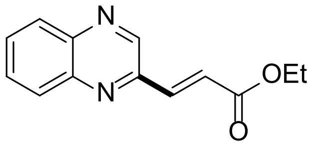
General procedure has been followed using 8-((tert-butoxycarbonyl)oxy)quinoline *N*-oxide (1 mmol, 261 mg) and styrene (208 mg, 230 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **6n** (270 mg, 78%) as white crystals. M. p. 107-109. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.12 (d, *J* = 8.5 Hz, 1H), 7.77 (d, *J* = 16.2 Hz, 1H), 7.67 – 7.59 (m, 4H), 7.52 – 7.33 (m, 6H), 1.65 (s, 9H).. **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 155.8, 152.2, 147.5, 141.3, 136.7, 136.4, 134.8, 129.0, 128.8, 128.7, 127.4, 125.8, 125.6, 121.2, 120.7, 83.5, 27.9. **GC-EIMS (m/z, %):** 347 (100), 290 (25), 247 (75), 271 (35), 246 (55).



Methyl (E)-3-(quinoxalin-2-yl)acrylate (8a)

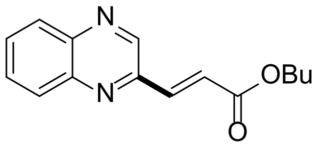
General procedure has been followed using quinoxaline *N*-oxide (1 mmol, 146 mg) and methyl acrylate (172 mg, 180 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 →

15/85) yielded **8a** (171, 80 %) as pale-yellow solid. M. p. 75-76. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.99 (s, 1H), 8.11 – 8.08 (m, 2H), 7.90 (d, *J* = 15.9 Hz, 1H), 7.81 – 7.76 (m, 2H), 7.15 (d, *J* = 15.9 Hz, 1H), 3.86 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.6, 148.0, 144.9, 142.7, 142.6, 140.7, 130.9, 130.9, 130.0, 129.4, 125.1, 52.3. **GC-EIMS (m/z, %):** 214 (100), 199 (90), 183 (80), 155 (65), 129 (50).



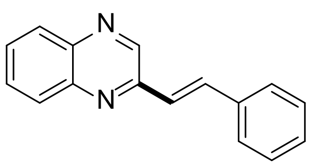
Ethyl (E)-3-(quinoxalin-2-yl)acrylate (8b)

General procedure has been followed using quinoxaline *N*-oxide (1 mmol, 146 mg) and ethyl acrylate (2 mmol, 200 mg, 218 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 15/85) yielded **8b** (172 mg, 75%) as pale-orange solid. M. p. 77-78. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 8.99 (s, 1H), 8.10 – 8.07 (m, 2H), 7.88 (d, *J* = 15.9 Hz, 1H), 7.79 – 7.77 (m, 2H), 7.13 (d, *J* = 16.0 Hz, 1H), 4.31 (q, *J* = 7.1 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.1, 148.2, 144.8, 142.6, 142.5, 140.4, 130.9, 130.8, 129.9, 129.4, 125.7, 61.2, 14.4. **GC-EIMS (m/z, %):** 228 (100), 199 (80), 183 (70), 155 (50), 129 (70).



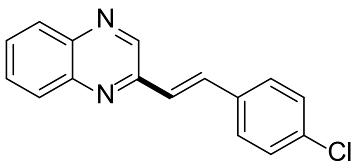
Butyl (E)-3-(quinoxalin-2-yl)acrylate (8c)

General procedure has been followed using quinoxaline *N*-oxide (1 mmol, 146 mg) and buthyl acrylate (256 mg, 287 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 20/80) yielded **8c** (198 mg, 78%) as pale-orange solid. M. p. 72-74. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 9.00 (s, 1H), 8.11 – 8.08 (m, 2H), 7.89 (d, *J* = 15.9 Hz, 1H), 7.81 – 7.76 (m, 2H), 7.14 (d, *J* = 16.0 Hz, 1H), 4.26 (t, *J* = 6.6 Hz, 2H), 1.75 – 1.68 (m, 2H), 1.51 – 1.41 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 166.3, 148.2, 144.8, 142.7, 142.6, 140.4, 130.9, 130.9, 129.9, 129.4, 125.7, 65.1, 30.8, 19.3, 13.9. **GC-EIMS (m/z, %):** 256 (100), 241 (35), 213 (48), 199 (85), 183 (75), 155 (65), 129 (30).



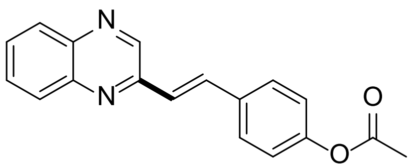
(E)-2-styrylquinoxaline (8d)[11]

General procedure has been followed using quinoxaline *N*-oxide (1 mmol, 146 mg) and styrene (208 mg, 230 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **8d** (208 mg, 90 %) as pale-orange solid. M. p. 105-107. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 9.05 (s, 1H), 8.09 – 8.06 (m, 2H), 7.88 (d, *J* = 16.3 Hz, 1H), 7.79 – 7.70 (m, 2H), 7.69 – 7.66 (m, 2H), 7.45 – 7.41 (m, 3H), 7.39 – 7.35 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 150.8, 144.6, 142.6, 141.7, 136.6, 136.1, 130.5, 129.4, 129.4, 129.3, 129.3, 129.1, 127.6, 125.5. **GC-EIMS (m/z, %):** 232 (100), 203 (25), 176 (15), 128 (25), 102 (40).



(E)-2-(4-chlorostyryl)quinoxaline (8e)[12]

General procedure has been followed using quinoxaline *N*-oxide (1 mmol, 146 mg) and 4-chlorostyrene (277 mg, 240 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **8e** (234 mg, 88%) as pale-orange solid. M. p. 118-120. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 9.02 (s, 1H), 8.09 – 8.05 (m, 2H), 7.83 (d, *J* = 16.3 Hz, 1H), 7.79 – 7.69 (m, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 16.4 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 150.4, 144.6, 142.6, 141.8, 135.1, 134.7, 130.6, 129.6, 129.3, 129.3, 128.7, 125.9. **GC-EIMS (m/z, %):** 265 (100), 231 (35), 203 (15), 176 (15), 128 (20), 102 (35).



(E)-4-(2-(quinoxalin-2-yl)vinyl)phenyl acetate (8f)

General procedure has been followed using quinoxaline *N*-oxide (1 mmol, 146 mg) and 4-acetoxystyrene (324 mg, 306 µL). Isolation by column chromatography (EtOAc/Petroleum Ether 1/99 → 10/90) yielded **8f** (267 mg, 92%) as yellow solid. M. p. 138-140. **^{1}H NMR** (400 MHz, $CDCl_3$) **δ** 9.01 (s, 1H), 8.08 – 8.04 (m, 2H), 7.84 (d, *J* = 16.3 Hz, 1H), 7.77 – 7.65 (m, 4H), 7.32 (d, *J* = 16.3 Hz, 1H), 7.15 (d, *J* = 8.6 Hz, 2H), 2.32 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) **δ** 169.3, 151.3, 150.4, 146.0, 144.5, 142.5, 141.6, 135.3, 133.8, 130.4, 129.4, 129.2, 128.5, 125.5, 122.1, 21.2. **GC-EIMS (m/z, %):** 290 (20), 247 (100), 219 (15), 191 (5), 165 (3).

10. Cartesian Coordinates of Stationary Points

A

Fe	1.36865000	-1.09936900	0.15379800
O	2.19264000	0.59108600	1.02815100
O	1.24952900	0.66454400	-1.16974200
S	2.33986200	1.38781900	-0.33165700
O	2.05909000	2.80827600	-0.14398900
O	3.68870000	1.04963100	-0.89919000
O	3.41570000	-1.51129800	-0.70083500
H	4.09275300	-1.87912700	-0.11703500
O	1.81975500	-1.82081400	2.19431500
H	2.28499800	-0.97967900	2.37473300
O	1.01576000	-1.89366800	-1.84384200
H	1.00893600	-0.95128600	-2.13507400
H	1.93800400	-2.16029800	-2.01479000
H	0.92969300	-1.67627800	2.55896500
H	3.68924800	-0.53750100	-0.86289600
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C	-2.60919800	-0.20336100	0.23576500
C	-3.45438300	0.90907100	-0.05368900
C	-4.76453700	0.63957100	-0.53635300
C	-5.19697800	-0.65774900	-0.71702200
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C	-0.87126200	1.28009500	0.90464500
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H	0.15350300	1.35298400	1.27469300
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B

Fe	1.30678300	0.91794300	0.09870600
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O	4.25964300	-0.46752700	0.45182600
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O	1.99267800	2.66915700	-1.04409800
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H	2.93275600	1.50554900	2.24009200
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H	-1.51161200	-3.47025000	0.26398300
H	0.05257400	-1.49600200	0.41491900
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O	-0.67115700	0.90929200	0.29741700

TS1$_{C2}$

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S	3.05625300	-1.12920900	-0.15367900
O	3.19867100	-0.81808000	1.31162000
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O	2.36939400	3.02492000	-0.23322900
H	3.16477300	2.75541500	-0.72358100
O	1.84891000	1.25302100	1.81137500
H	1.23725100	1.08617400	2.54183400
H	2.45331100	0.41400200	1.75005700
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C	-3.45270900	1.37324300	-0.24256800
C	-2.75860800	0.15011600	-0.10500300
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C

Fe	0.92979700	1.10635600	0.06392200
O	2.08480600	-2.07652600	-0.78195500
O	2.59664700	0.34239100	-0.84839100
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O	2.09386100	2.94770800	-0.22813300
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H	1.42438600	0.78157300	2.72574300
H	2.58486700	0.30953200	1.78551100
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C	-3.33367200	-1.11407300	0.20512000
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D

Fe	1.14450100	1.22281400	-0.03985200
O	2.72848400	-2.24096200	-0.18106600
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S	3.62202700	-0.84875300	-0.24733300
O	3.88090900	-0.55279400	1.17760300
O	4.74970500	-1.12077600	-1.12192600
O	0.37395200	2.90783600	-0.47572600
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C	-5.49469900	0.13372300	-0.16849500
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C	-3.08526200	0.08773400	-0.06330400
C	-3.10422800	-1.32407400	0.11711200
C	-4.36165400	-1.98194400	0.15089800
C	-5.53559300	-1.26855400	0.01148700
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H	-6.49806200	-1.78449600	0.03893900
C	-0.68808100	-1.28747800	0.20220400
C	-0.65443500	0.13178500	0.03920400
H	-1.85515700	-3.08748500	0.37890800
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E

Fe	1.04869800	1.15653400	-0.01137700
O	2.51273800	-1.64993900	1.06131200
O	1.96749900	-0.28786600	-0.94097600
S	3.14712900	-1.11039400	-0.32981200
O	4.23175400	-0.15897400	0.01023400
O	3.46603500	-2.27569500	-1.11908700
O	0.25760800	2.42946300	-0.96068200
H	-0.71371800	2.47262400	-0.89955000
O	2.93062800	2.10112800	0.34088000
H	2.98022800	2.21966200	1.30291300
H	3.60423500	1.38355000	0.15266500
C	-5.54999200	0.56852300	-0.16890200
C	-4.30467500	1.16571500	-0.19512900
C	-3.14168600	0.36750600	-0.07630000
C	-3.25743100	-1.05337400	0.06953000
C	-4.55418900	-1.63229900	0.09177000
C	-5.67597500	-0.83562500	-0.02473800
H	-6.44907300	1.18251900	-0.26093200
H	-4.18663200	2.24515200	-0.30618100
C	-2.05635400	-1.81072200	0.18541300
H	-4.64967000	-2.71558600	0.20114300
H	-6.67031600	-1.28773300	-0.00738000
C	-0.82259600	-1.19557300	0.16405600
C	-0.84904200	0.21764500	0.00876900
H	-2.11735100	-2.89742600	0.29543200
H	0.11048000	-1.74870600	0.25725500
H	2.10606900	-0.86778800	1.53558200
N	-1.89511700	0.93764900	-0.10332000
O	1.19432700	0.58450300	1.77814800
H	0.41827900	0.45485400	2.33963000

$TS2_{C2}$

Fe	0.96815300	0.21675100	0.74400700
O	3.58232800	-2.55060300	-1.52262700
O	1.97849000	-0.83856800	-0.67751800
S	3.03757300	-1.92602900	-0.33653300
O	2.18115200	-3.04022500	0.43584800
O	4.00025400	-1.32747800	0.63200900
O	2.86749700	0.88291500	1.27283900
H	3.48314500	0.08968600	1.13130100
O	0.76145400	-1.34868900	1.76755200
H	0.26050700	-1.32936800	2.59308100
H	1.60384800	-2.55293000	1.10807100
H	3.01237700	1.26332600	2.14955100
C	-5.51599600	-0.36632800	0.67299300
C	-4.32846800	0.32913400	0.56532300
C	-3.18598100	-0.30568100	0.01537300
C	-3.26962200	-1.66782600	-0.42745800
C	-4.50815400	-2.35096800	-0.30252400
C	-5.60712500	-1.71243100	0.23708900
H	-6.39636600	0.12215000	1.09756500
H	-4.23715600	1.36608900	0.89367200
C	-2.09457200	-2.26309100	-0.96954000
H	-4.57699900	-3.38885000	-0.63832500
H	-6.55622500	-2.24533500	0.33077300
C	-0.92320000	-1.54542600	-1.06755900
C	-0.97076400	-0.20750800	-0.58789300
H	-2.12607500	-3.30437500	-1.30337000
H	0.00473900	-1.97361800	-1.44383200
N	-2.00465000	0.37250200	-0.10015800
O	0.04545800	1.55894300	1.55907800
H	-0.85586200	1.74095600	1.24910100
C	0.17038700	1.10853100	-1.83770000
H	-0.78430700	1.55289700	-2.12064400
H	0.54782500	0.26821400	-2.42189400
C	1.10771400	1.92380400	-1.21319400
H	2.16008000	1.63640500	-1.16938100
C	0.81431800	3.27170800	-0.67088200
O	1.66671000	4.03236600	-0.27805400
O	-0.50085800	3.56897000	-0.70041400
C	-0.86306100	4.84277300	-0.16781100
H	-0.34132200	5.65296100	-0.69891500
H	-1.94794000	4.93418800	-0.30272100
H	-0.60359000	4.89983200	0.90041500

F

Fe	1.03811000	-0.11483500	0.84733800
O	3.57811200	-2.43216100	-1.89271300
O	2.30707500	-0.76935600	-0.54136800
S	2.60658700	-2.26909000	-0.83372800
O	1.20619600	-2.82361200	-1.37600400

O	2.89471300	-2.93540600	0.46893200
O	2.18176800	-1.19295800	2.21452500
H	2.57206400	-1.95544500	1.67109200
O	-0.21236400	-1.41273000	0.24652700
H	-1.06658500	-1.49109200	0.69074500
H	0.48890600	-2.42539000	-0.78498400
H	1.66279400	-1.58441500	2.93086200
C	-5.12476800	-1.03635500	1.44920700
C	-3.96638200	-0.29068700	1.52228500
C	-3.41811500	0.29913100	0.34968300
C	-4.08727600	0.10927400	-0.90373000
C	-5.28075400	-0.66187300	-0.94367900
C	-5.78838700	-1.22354400	0.20916000
H	-5.53982100	-1.48686000	2.35418500
H	-3.44790200	-0.13198500	2.47031700
C	-3.50374100	0.71111000	-2.04919300
H	-5.78665200	-0.80424200	-1.90234100
H	-6.70484100	-1.81709300	0.17200200
C	-2.34464100	1.44231700	-1.92057700
C	-1.74756300	1.57671500	-0.63649900
H	-3.98242000	0.58843800	-3.02464800
H	-1.87945300	1.91591000	-2.78774500
N	-2.27164800	1.02864100	0.44479600
O	0.05354300	0.80178100	2.03132400
H	-0.87843500	0.93581400	1.73228000
C	-0.46302200	2.35779400	-0.45055600
H	-0.51412900	2.90208600	0.50338000
H	-0.36852500	3.11311900	-1.25300700
C	0.80266200	1.52612700	-0.49151700
H	0.96136100	0.93347400	-1.40248900
C	2.05539100	2.19897800	-0.01121700
O	2.74498800	1.69194700	0.85072500
O	2.30818400	3.36721900	-0.58833600
C	3.50161100	4.05107600	-0.16817300
H	4.38688400	3.43253900	-0.37378300
H	3.53570600	4.97961300	-0.74944600
H	3.45852200	4.26801800	0.90879900

G

Fe	1.47386200	0.10628500	1.23197500
O	4.82913500	-1.15315900	-1.21923600
O	3.26174400	-0.18386100	0.46081600
S	3.56554900	-1.33424700	-0.53971600
O	2.41437700	-1.15598800	-1.66304600
O	3.31979800	-2.62062900	0.16165200
O	1.71734200	-1.87428400	2.10465300
H	2.40899400	-2.29990800	1.51413800
O	0.36831200	-0.64510000	-0.07208700
H	-0.56310000	-0.32103200	-0.15542300
H	1.52108800	-1.06380000	-1.20352600
H	0.89605400	-2.32061500	1.84531000
C	-3.87285900	-2.87246300	-1.01005400
C	-2.90322300	-1.93005700	-0.73861900
C	-3.27592800	-0.62742100	-0.30407500
C	-4.66556200	-0.31436200	-0.14489100
C	-5.63902000	-1.30954600	-0.43391200
C	-5.24965700	-2.56211900	-0.85939000
H	-3.58067400	-3.87100900	-1.34433500
H	-1.83950300	-2.15439300	-0.84132900
C	-4.98760100	0.99327500	0.30205600
H	-6.69783500	-1.06560100	-0.31268400
H	-6.00120200	-3.32358000	-1.08084500
C	-3.98013200	1.89575500	0.56128100
C	-2.62595500	1.50093800	0.37450400
H	-6.03613200	1.27279000	0.43797300
H	-4.20631500	2.90534300	0.91021400
N	-2.30230100	0.29124500	-0.04642800
O	0.74370700	0.78129500	2.76167400
H	0.85531000	0.30133300	3.59355100
C	-1.48207900	2.46927900	0.65457500
H	-0.83935700	2.06101700	1.45356900
H	-1.90828500	3.41743300	1.02978900
C	-0.67771900	2.75143600	-0.56777400
H	-1.15876700	3.15761000	-1.46144200
C	0.73906800	2.47260900	-0.65042600
O	1.40794700	2.01045100	0.28463900
O	1.27351200	2.76907700	-1.82643600
C	2.65858800	2.42933900	-2.03448300
H	2.77852800	1.33698400	-2.03401700
H	2.91967300	2.84700800	-3.01324400
H	3.28390400	2.86383800	-1.24239700

TS3$_{C2}$

Fe	1.48696600	0.10180100	1.05029000
O	5.20116100	-1.32217900	-0.65871200
O	3.36408000	-0.26900800	0.65996100
S	3.81590200	-1.43589700	-0.26684600
O	2.94017200	-1.19713300	-1.60686900
O	3.35753600	-2.70331600	0.35754200
O	1.42555000	-1.89871800	1.94332300
H	2.23247900	-2.33462500	1.53566400
O	0.59606800	-0.60076100	-0.43884400
H	-0.35914700	-0.43634200	-0.58087000
H	1.97559000	-1.10577300	-1.36091500
H	0.70101400	-2.32435800	1.45767600
C	-4.59012600	-2.50262900	-1.45100100
C	-3.48227600	-1.70289600	-1.25959600
C	-3.57849100	-0.50889400	-0.49119200
C	-4.84548100	-0.15797300	0.08408200
C	-5.96649100	-1.00293400	-0.13132400
C	-5.84257500	-2.15276100	-0.88469700
H	-4.50518900	-3.41548700	-2.04597600
H	-2.51270400	-1.95932800	-1.69168500
C	-4.89928300	1.03423300	0.85751700
H	-6.92851500	-0.72753400	0.30969800
H	-6.70898000	-2.79819800	-1.04758800
C	-3.76803800	1.79783800	1.01679500
C	-2.55028700	1.38305200	0.39549100
H	-5.84648900	1.33529900	1.31430800
H	-3.78847700	2.72300600	1.59678900
N	-2.46972500	0.25978100	-0.31360500
O	0.13116900	0.75255000	2.26843800
H	-0.42099000	0.11768400	2.74826900
C	-1.28591400	2.13514000	0.54948200
H	-0.60078500	1.42922000	1.48495500
H	-1.31313800	3.03158400	1.19145500
C	-0.47869900	2.22365100	-0.63535000
H	-0.92553000	2.02013200	-1.61312900
C	0.94792600	2.38076100	-0.63470300
O	1.68117500	2.01866400	0.31971500
O	1.47920600	2.83551900	-1.75976000
C	2.90618600	2.72673400	-1.90741200
H	3.21469600	1.67506300	-1.81702100
H	3.12917100	3.11062700	-2.90943500

H	3.42187700	3.32321000	-1.14185900

H

Fe	2.76909000	-0.48252400	-0.79739800
O	5.69361900	0.40383300	2.31763200
O	3.61525200	0.22251300	0.92289000
S	5.12110700	-0.07062600	1.07635500
O	5.79160200	0.77784100	-0.11319800
O	5.33272000	-1.52432300	0.75805800
O	3.93115200	0.44122800	-1.96709600
H	4.16982300	0.17768400	-2.86370200
H	5.19451000	0.70214900	-0.92577000
C	-7.73147600	1.37248900	0.50404400
C	-6.37026500	1.51077900	0.34695700
C	-5.54307000	0.36220200	0.17262800
C	-6.15603700	-0.93963100	0.16312800
C	-7.56380100	-1.04600300	0.32768100
C	-8.33400700	0.08554100	0.49466800
H	-8.35853700	2.25742800	0.63804500
H	-5.88381700	2.48807200	0.35146100
C	-5.30054000	-2.05777600	-0.01236000
H	-8.02461100	-2.03740600	0.32029700
H	-9.41572300	-0.00305800	0.62128200
C	-3.94710800	-1.85937900	-0.16259800
C	-3.43183800	-0.52841800	-0.13798000
H	-5.72482200	-3.06536200	-0.02557200
H	-3.26529200	-2.70186900	-0.29713200
N	-4.20943700	0.53286300	0.02309400
O	3.21472600	-2.43800600	-0.28572600
H	4.08492300	-2.22893700	0.22624800
C	-1.98610500	-0.31488600	-0.29283600
H	3.45088100	-3.09223700	-0.95688200
H	-1.36352500	-1.20325300	-0.43604300
C	-1.38931900	0.89360900	-0.26078700
H	-1.97602900	1.80099000	-0.10991200
C	0.06246700	1.03705700	-0.40587900
O	0.82405400	0.07923500	-0.60944300
O	0.46400500	2.28526200	-0.30155900
C	1.86961100	2.61050000	-0.37084400
H	2.31340600	2.24358300	-1.30862700
H	1.91289700	3.70448000	-0.32986600
H	2.40981800	2.16615900	0.47780500

$TS1_{C8}$

Fe	-0.71702900	-1.08543900	0.40247000
O	-1.42124000	1.33046200	-1.34492700
O	-2.44248700	-0.74032400	-0.55139900
S	-2.74163400	0.78847700	-0.74566400
O	-2.88147600	1.34261600	0.66434700
O	-3.88211900	1.02591300	-1.60921700
O	-1.96070600	-2.79166800	1.01120500
H	-2.67532400	-2.44250700	0.43751700
O	-1.50131200	-0.15172700	2.10965800
H	-0.91576300	0.42445000	2.62035900
H	-2.16884600	0.50716700	1.61332300
H	-2.25268100	-2.56382700	1.90813900
C	0.78509100	2.11689200	0.56507400
C	0.71803000	0.82373100	0.04578600
C	1.97000700	0.18089000	-0.14353200
C	3.22847700	0.83474000	0.04695400
C	3.20975400	2.15858900	0.56458400
C	2.00757800	2.77286800	0.84967300
H	-0.15632200	2.66139700	0.69049400
H	-0.41431400	0.85800300	-0.69136700
C	4.42742100	0.14769500	-0.27544800
H	4.15946800	2.67404700	0.72683600
H	1.99581300	3.78837700	1.25377300
C	4.36833900	-1.15089900	-0.73879100
C	3.12816500	-1.80126600	-0.82589100
H	5.38739100	0.65430800	-0.15069000
H	5.26788700	-1.70682800	-1.00656300
H	3.00053500	-2.84704000	-1.10556900
N	1.99252700	-1.16747400	-0.51070800
O	0.87386300	-1.85638300	-0.50283300

$TS2_{C8}$

Fe	0.69154100	0.24560200	0.76058900
O	4.30005100	-1.03412300	-1.47593000
O	2.09076100	-0.24155000	-0.64199600
S	3.55433100	-0.64574900	-0.29742600
O	3.36761900	-1.96155200	0.60016300
O	4.13242300	0.42404000	0.56268400
O	2.03708400	1.79833300	1.13065000
H	2.97263400	1.43444300	1.03153700
O	1.31903700	-1.09677800	1.91365000
H	0.95840700	-1.19770100	2.80371700
H	2.64139500	-1.76017500	1.27414200
H	1.95301800	2.35053700	1.91841400
C	-0.12174400	-2.08296800	-1.01795600
C	-0.81698600	-0.98535300	-0.55253600
C	-2.17708100	-1.09257000	-0.11958600
C	-2.78627000	-2.39714400	-0.16711400
C	-2.03471400	-3.51797600	-0.61423500
C	-0.72824300	-3.36504200	-1.02181700
H	0.90781400	-1.96707400	-1.36042900
C	-4.14350800	-2.50190200	0.23757900
H	-2.51479600	-4.49975900	-0.63629400
H	-0.14585600	-4.22327700	-1.36482200
C	-4.82591300	-1.37953600	0.65107700
C	-4.13176500	-0.14646100	0.67815300
H	-4.63078200	-3.48069000	0.21374500
H	-5.87051200	-1.42693700	0.96462600
N	-2.87271600	-0.01066000	0.31551700
O	-0.69006100	1.12870200	1.51829200
H	-1.59306800	1.03887700	1.14176200
C	-0.53269300	0.75229300	-1.89414500
H	-1.61275000	0.78081500	-2.04239600
H	0.06143000	0.10031000	-2.53361900
C	0.09402200	1.86728600	-1.36073000
H	1.18170100	1.95213200	-1.38215700
C	-0.59419500	3.04802300	-0.78466200
O	-0.00704900	4.01751600	-0.36405100
O	-1.93618400	2.94606400	-0.82265800
C	-2.66061900	4.03445500	-0.25350700
H	-2.40071200	4.98210300	-0.74892700
H	-3.72355600	3.80621600	-0.40110800
H	-2.43478100	4.12782600	0.81996100
H	-4.64110200	0.75946700	1.02716000

H_2O

O	0.00000000	0.00000000	0.12020700
H	0.00000000	0.75703900	-0.48082800
H	0.00000000	-0.75703900	-0.48082800

2a

C	2.17230200	-0.77179700	0.00001200
H	1.65351500	-1.73343200	0.00056700
H	3.26567200	-0.78260300	0.00009700
C	1.49228000	0.37995800	-0.00013800
H	1.99813600	1.34914500	-0.00020500
C	0.00980700	0.48977200	0.00003700
O	-0.58403500	1.54335400	0.00009000
O	-0.60995100	-0.70801100	-0.00006400
C	-2.03530400	-0.67738600	-0.00002500
H	-2.41761000	-0.15683100	-0.89156600
H	-2.36485400	-1.72387400	-0.00092800
H	-2.41748500	-0.15843300	0.89250800

TS$_{[3+2]}$

C	-4.24167900	-2.83194300	-0.72113500
C	-3.23944100	-1.92106100	-0.41136100
C	-3.58609500	-0.70274700	0.20029300
C	-4.93949700	-0.39002200	0.50184900
C	-5.92665300	-1.34687500	0.18695000
C	-5.58680100	-2.55031900	-0.41802600
H	-3.97810100	-3.77777500	-1.20010400
H	-2.19173900	-2.12778600	-0.62894900
C	-5.24359100	0.88515700	1.11103900
H	-6.97019700	-1.12195300	0.42169600
H	-6.36365800	-3.27959900	-0.65799400
C	-4.26802300	1.80340300	1.31178700
C	-2.89634600	1.54149500	0.87229200
H	-6.27424100	1.08852800	1.41226700
H	-4.48062300	2.77213900	1.76869600
H	-2.09661800	1.99620400	1.46574200
N	-2.58950000	0.20743600	0.57627500
O	-1.37986300	0.05505900	0.16964200
C	-2.51317100	2.34808500	-0.73823500
H	-3.45141800	2.26539100	-1.29601500
H	-2.30480600	3.36532100	-0.39247300
C	-1.40771500	1.65185000	-1.30301800
H	-1.53967600	0.94171800	-2.11885100
C	-0.01720500	1.95436900	-0.98579000
O	0.14617100	2.89298300	-0.06552800
O	0.92848200	1.34616200	-1.50021100
C	1.48962600	3.19453300	0.37587700
H	1.90137300	2.34740200	0.94558700
H	2.13369700	3.39849700	-0.49119000
H	1.39481000	4.08646500	1.00569100
Fe	2.24579700	-0.11808700	-0.84352800
O	3.17783400	-1.97173500	0.44226400
O	2.52995400	0.25510100	1.08103000
S	3.61458000	-0.84857700	1.43423000
O	3.52296500	-1.26034600	2.82653700
O	4.93804600	-0.30435000	0.98808100
O	0.68659500	-1.62623700	-0.48640300
H	1.30125600	-2.04144800	0.16463600
O	4.16905900	0.82617400	-1.25187400
H	4.64051300	0.35924700	-1.95700800
O	3.04618300	-1.69314700	-2.12352300
H	2.34522900	-2.31254600	-2.37746900
H	-0.04678900	-1.20922100	0.00694500
H	3.38922100	-2.05520200	-1.25447700
H	4.63040400	0.52721000	-0.40185600

TS$_{[3+2]U}$

C	-2.03928200	-2.18592100	0.80341200
C	-1.05563300	-1.27044200	1.15061900
C	-1.08469100	0.01906800	0.58974500
C	-2.11171300	0.39952400	-0.31435900
C	-3.10074700	-0.55576600	-0.63753200
C	-3.06764400	-1.83132000	-0.09214300
H	-2.01720900	-3.18961500	1.23526100
H	-0.25485700	-1.51511000	1.84800000
C	-2.10646300	1.73812900	-0.85158300
H	-3.89653100	-0.27128300	-1.33111700
H	-3.83988900	-2.55873200	-0.35268500
C	-1.11771700	2.60731200	-0.52127200
C	-0.00933400	2.19049100	0.32357200
H	-2.92378100	2.04325300	-1.50995700
H	-1.10830400	3.62983700	-0.90507600
H	0.44722800	2.94815900	0.96490500
N	-0.13327900	0.97130000	0.98013500
O	0.90719200	0.62902200	1.65124500
C	1.61491300	1.82438400	-0.68710400
H	1.21141900	1.39381400	-1.60660000
H	1.97338900	2.85298700	-0.79049300
C	2.37295400	0.96616100	0.13831000
C	2.55219800	-0.47426600	-0.12625700
O	3.40995200	-1.16925500	0.36908200
O	1.64223200	-0.94983000	-1.01566200
C	1.71777900	-2.34124800	-1.30190200
H	0.96385200	-2.53949600	-2.07436300
H	2.72004700	-2.61609300	-1.66446400
H	1.50008800	-2.93949900	-0.40293000
H	3.09476600	1.36654900	0.85021000

[$FeSO_4(H_2O)_4$]

Fe	1.05288100	-0.05528600	-0.02181400
O	-0.56820700	-0.55361700	1.11539000
O	-0.84103900	-0.30534200	-1.24612200
S	-1.65439800	-0.08202500	0.06982100
O	-2.87303200	-0.86728500	0.14072700
O	-1.81636900	1.40356000	0.25968200
O	1.13377000	-2.02847800	-0.91156200
H	1.02755300	-2.75056500	-0.27519000
O	0.63297900	2.07690600	0.39083000
H	0.81970600	2.53573600	1.22054200
O	1.89930900	-0.53969000	1.94908000
H	2.30828400	0.10412900	2.54412500
O	1.45948900	0.92226300	-1.89881800
H	0.55022900	0.68465000	-2.19422800
H	0.22529000	-1.84695600	-1.25713300
H	1.36752700	1.84837300	-1.61073500
H	0.98036300	-0.66238800	2.27286000
H	-0.39868500	1.97033700	0.35612700

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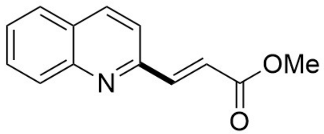
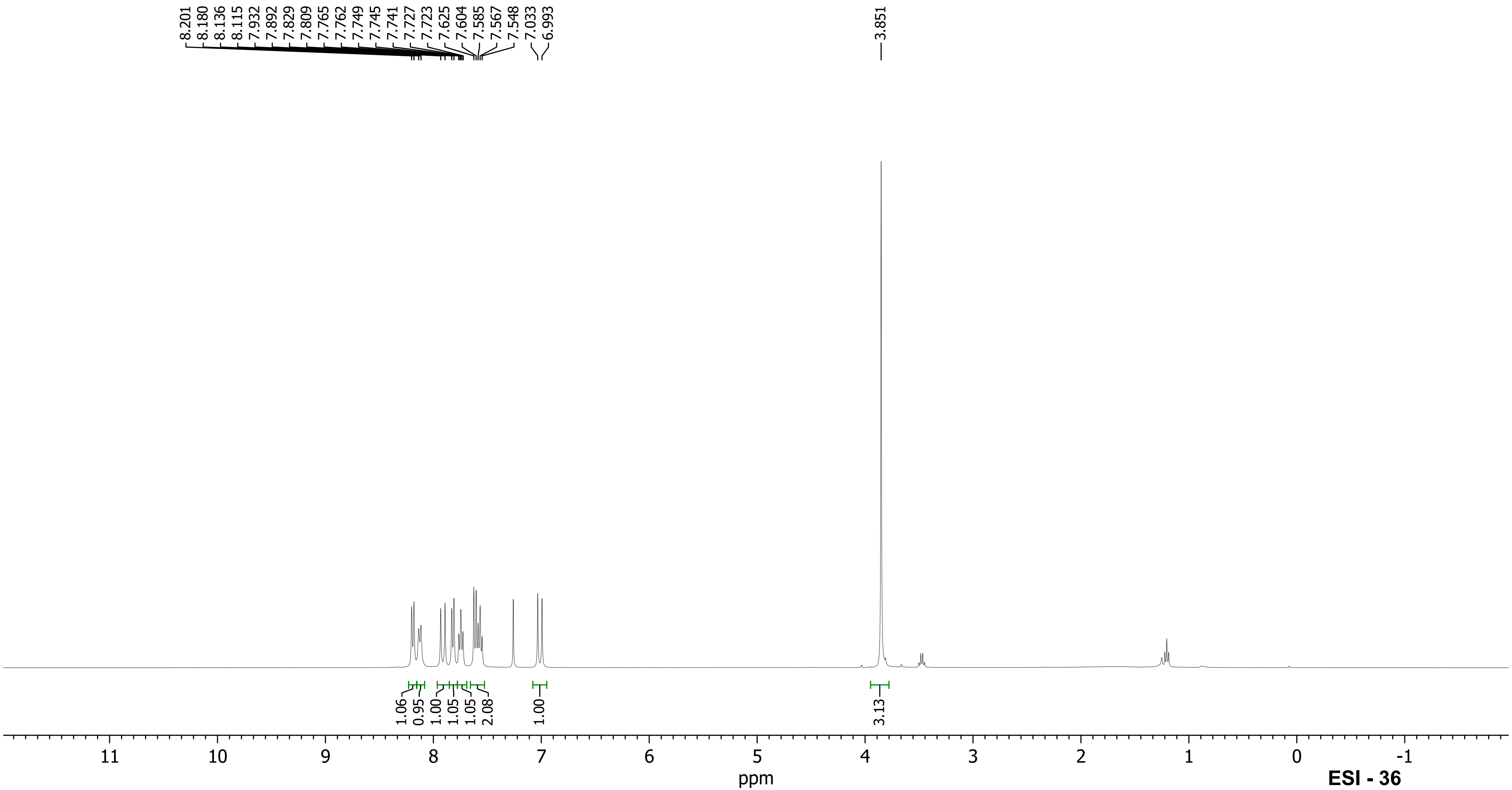
Methyl (E)-3-(quinolin-2-yl)acrylate (3a)





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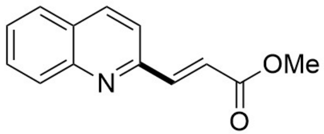

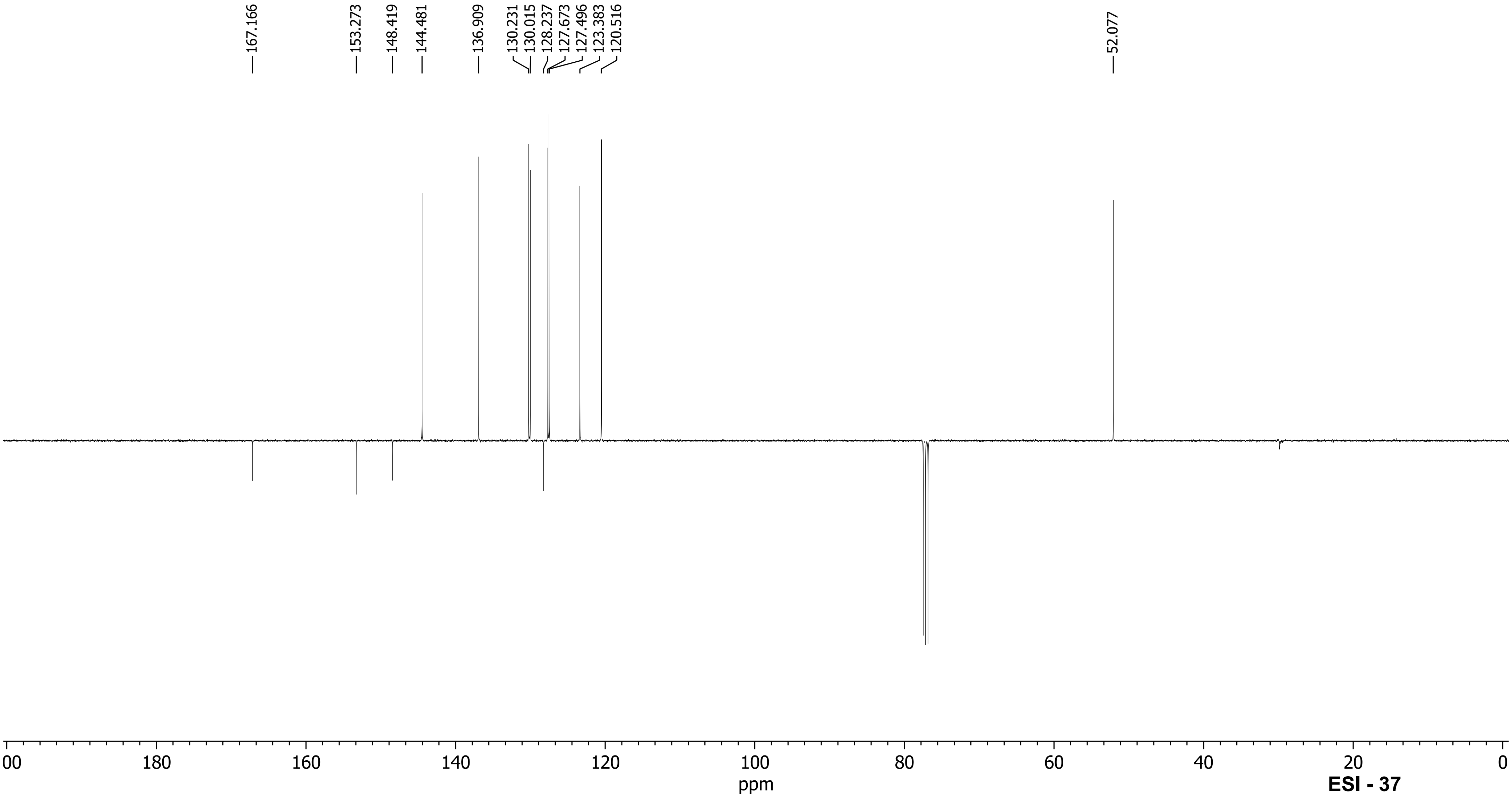

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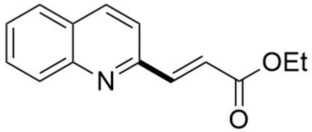

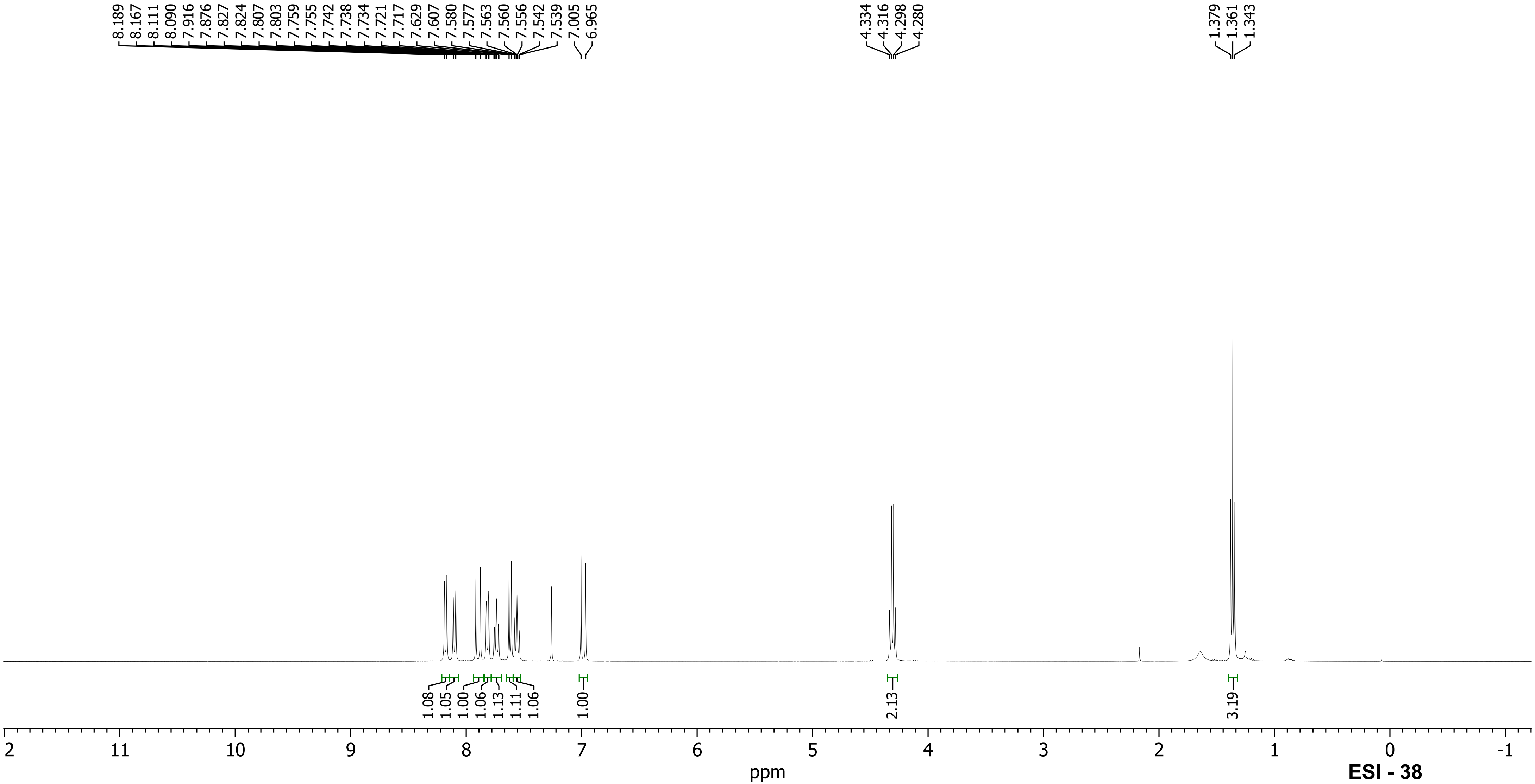

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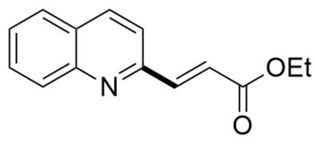

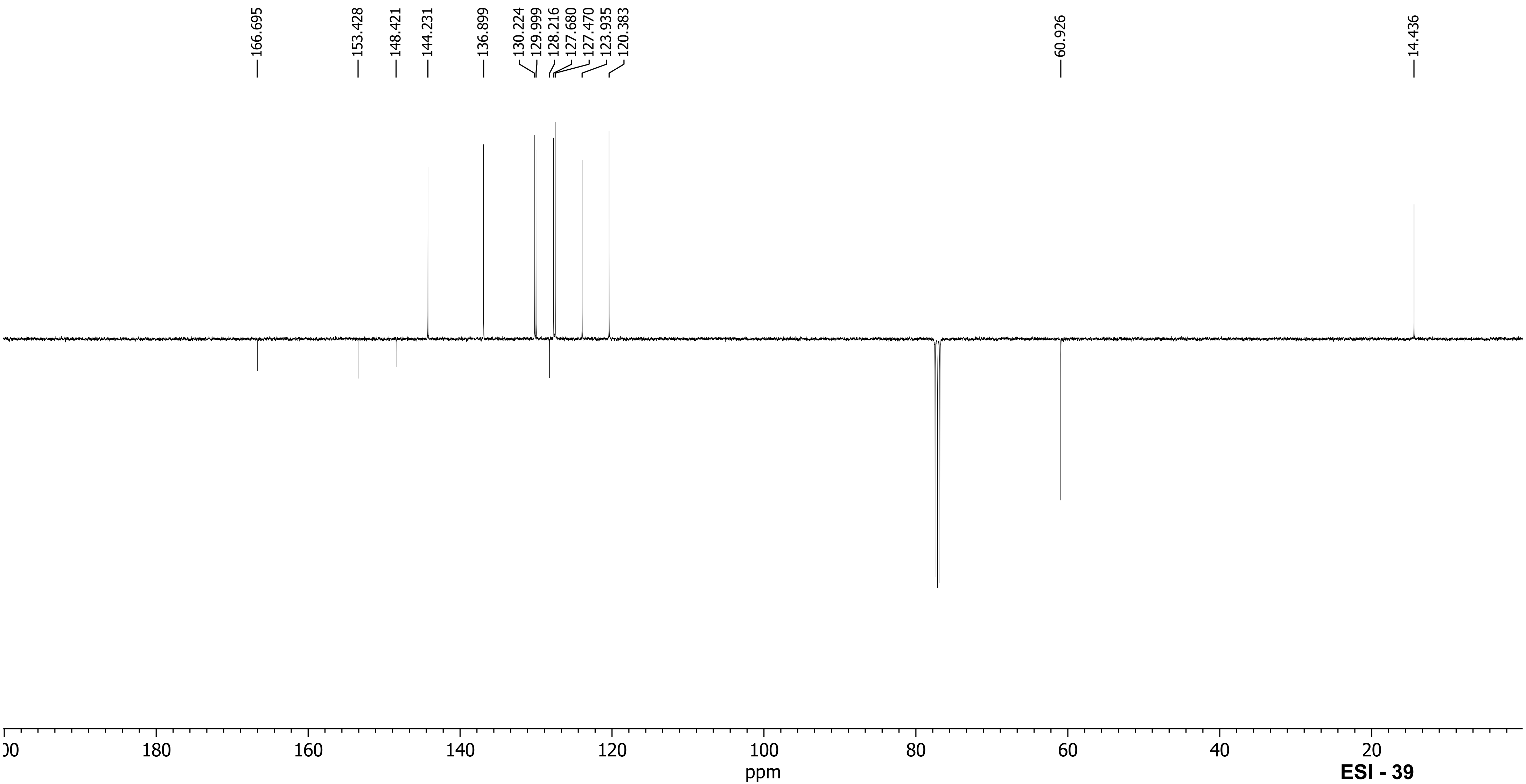

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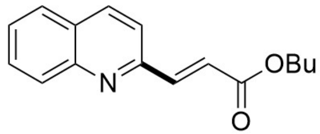

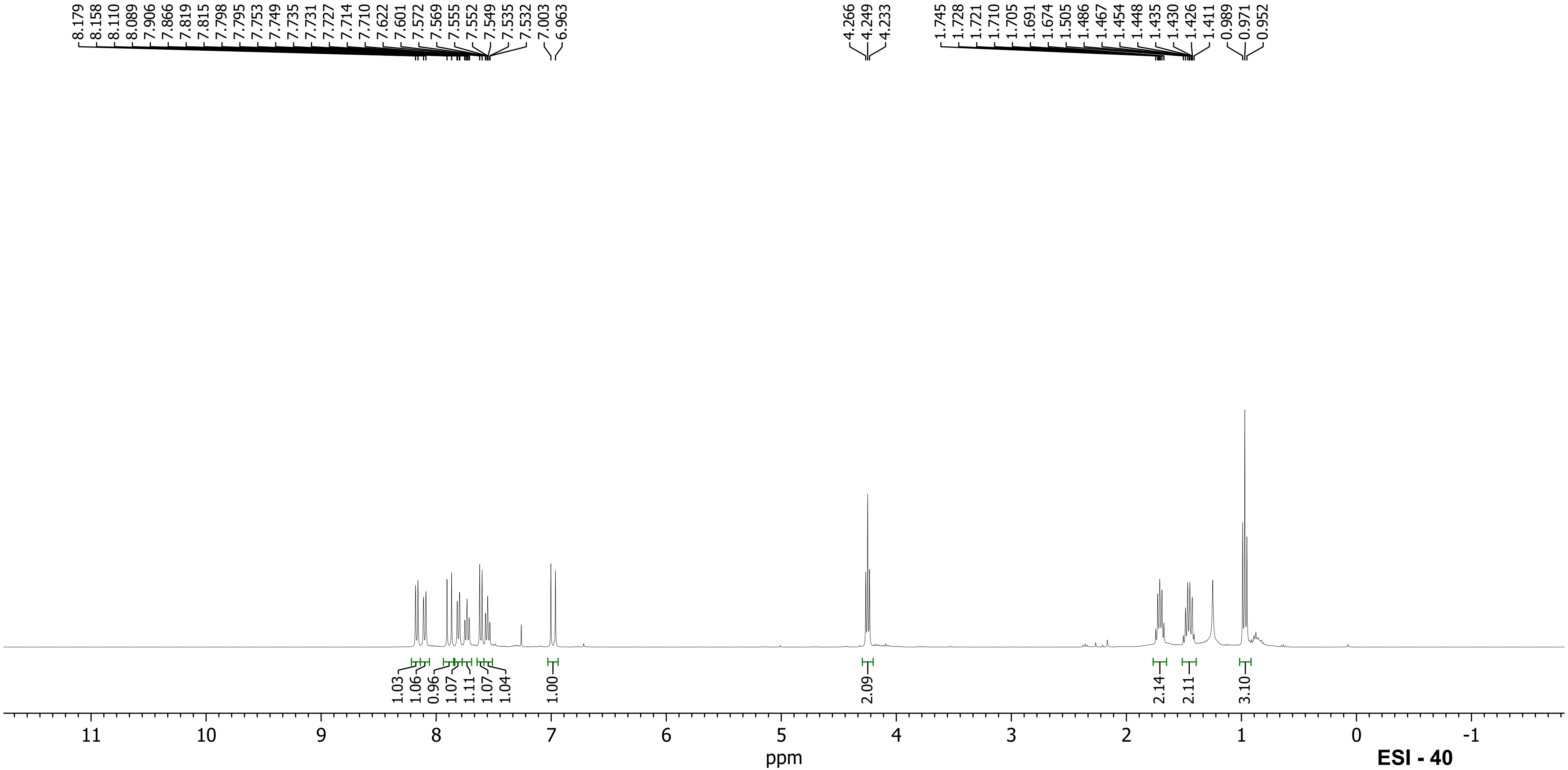

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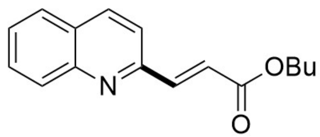
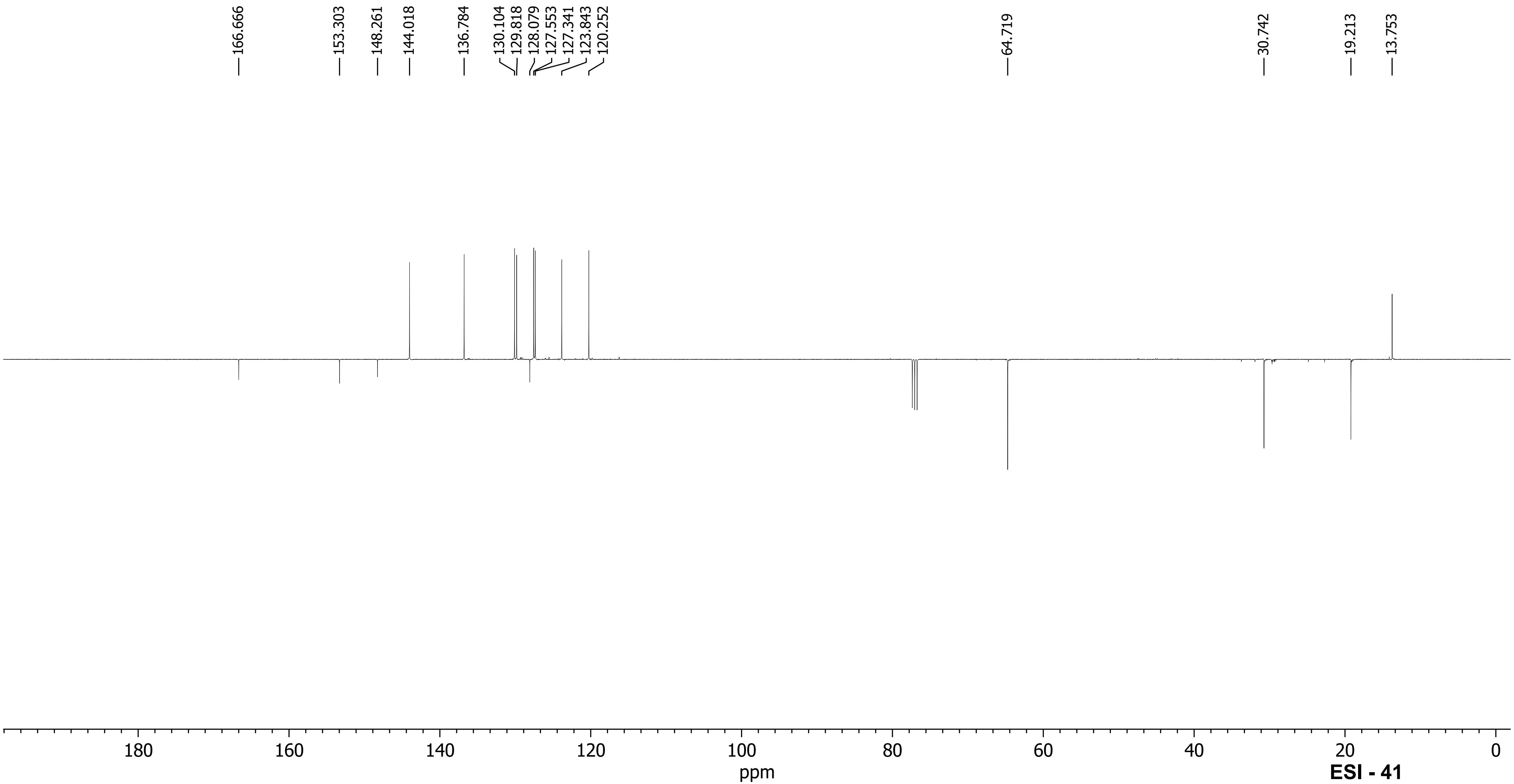
Butyl (E)-3-(quinolin-2-yl)acrylate (3c)





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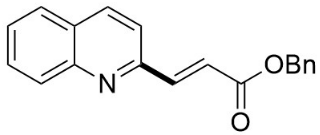

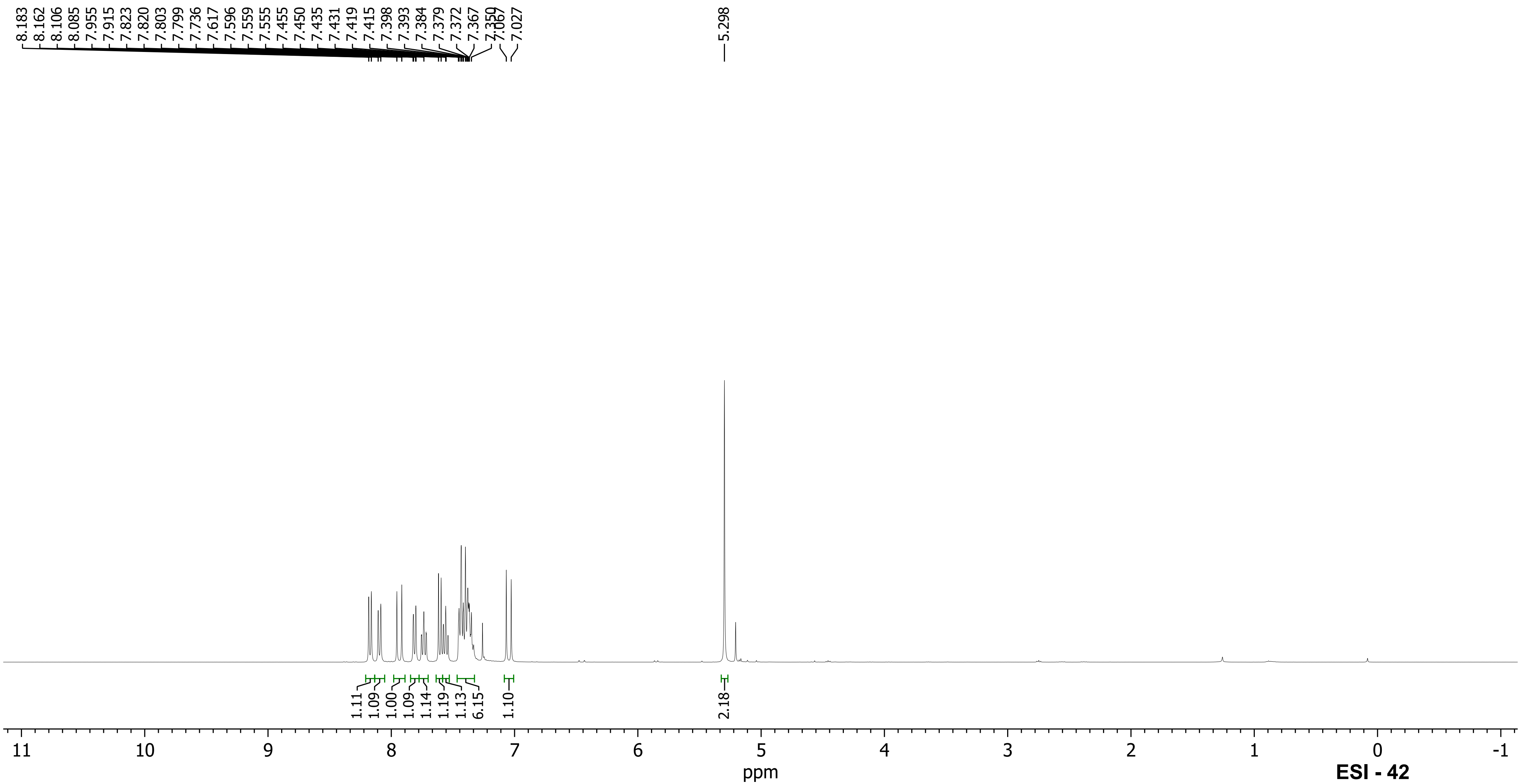

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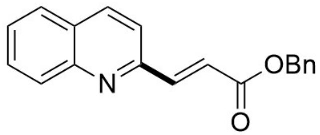

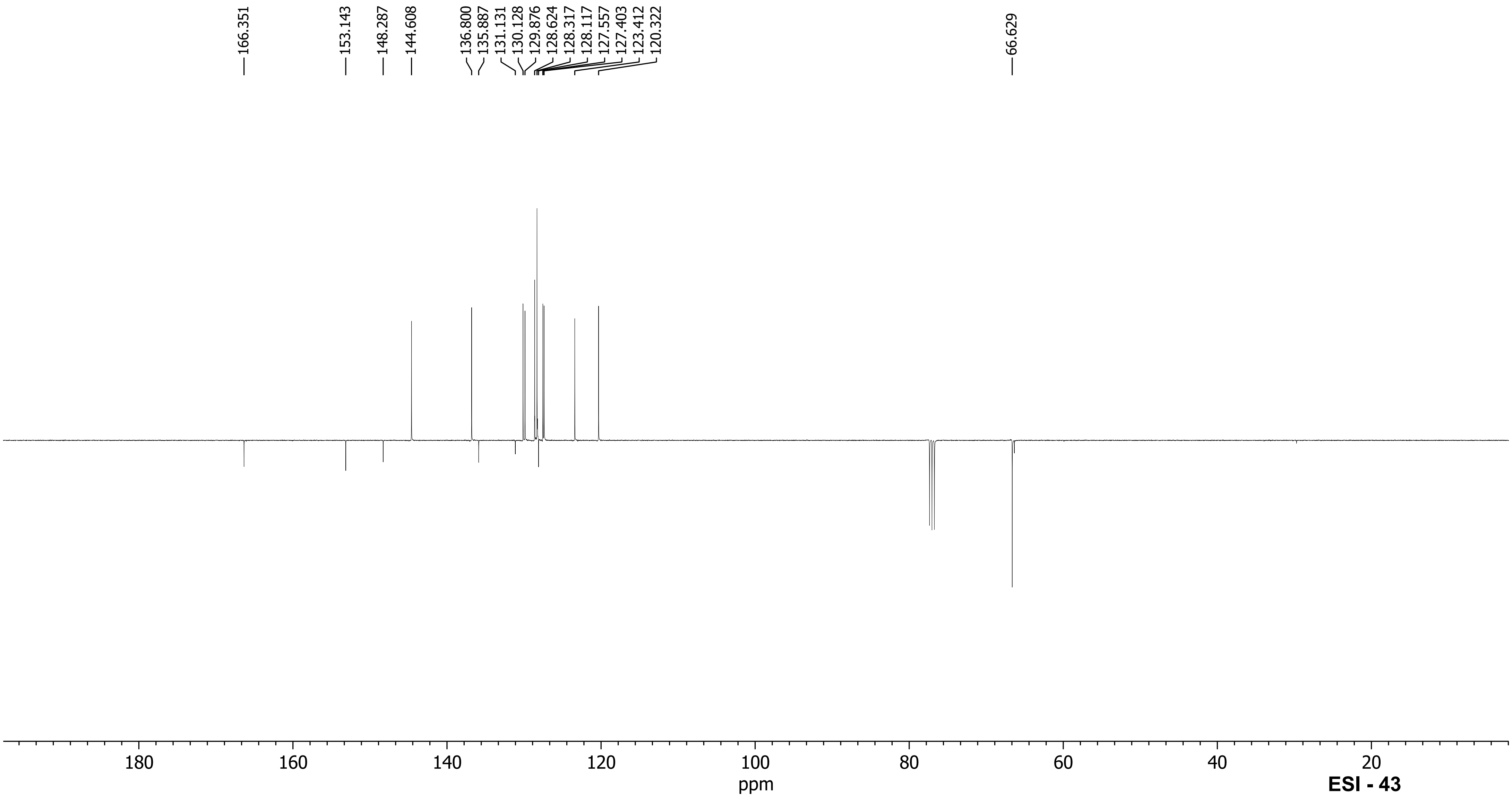

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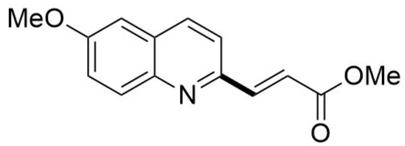
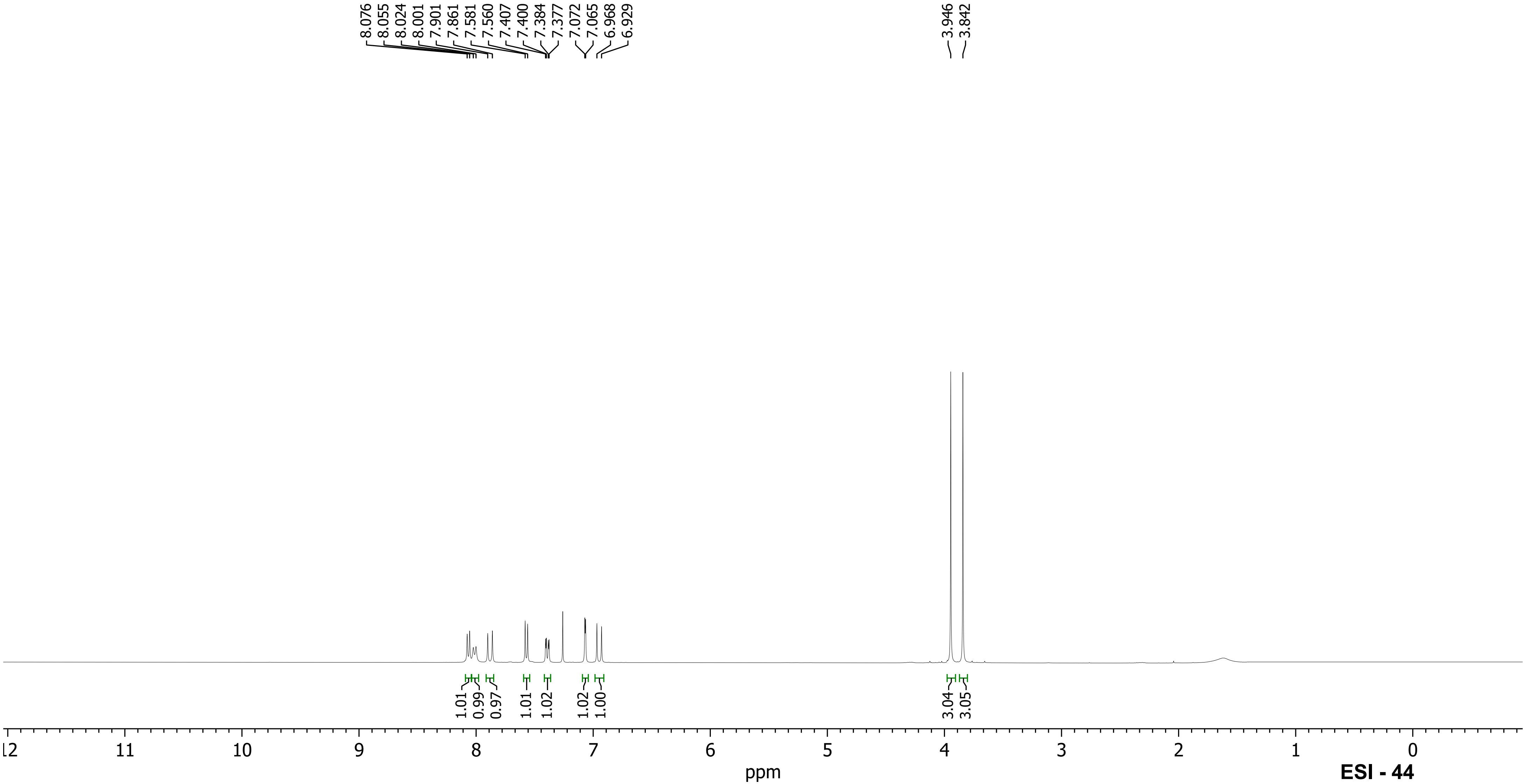
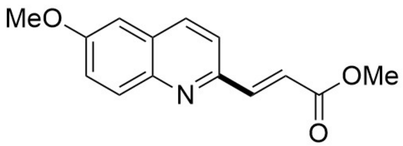
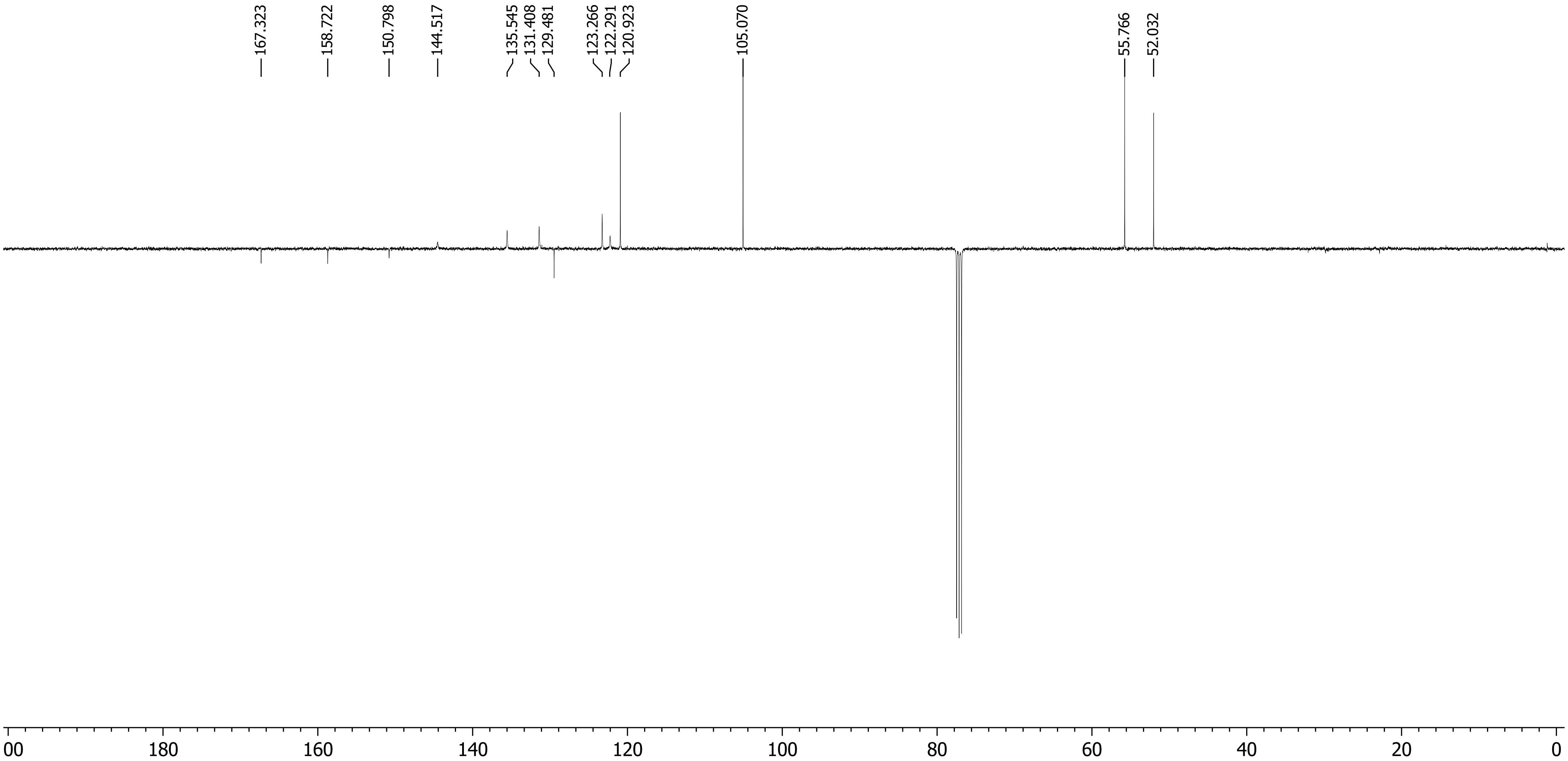




Methyl (E)-3-(6-methoxyquinolin-2-yl)acrylate(3e)





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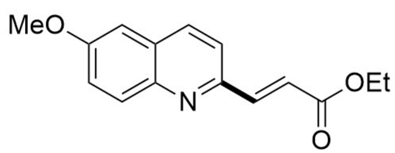

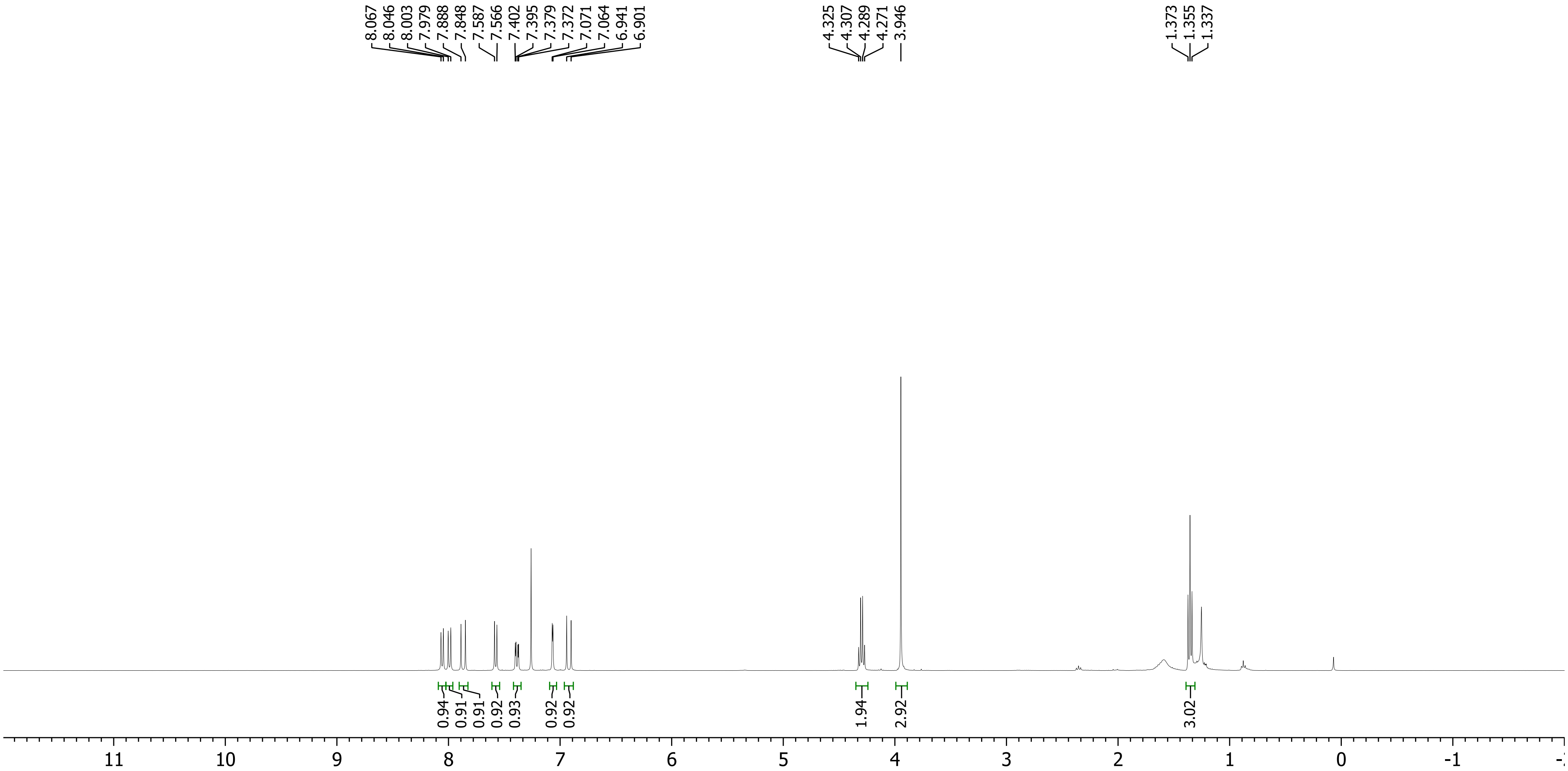

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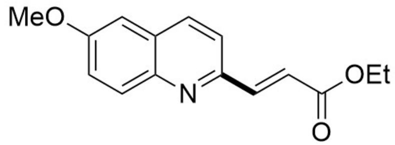

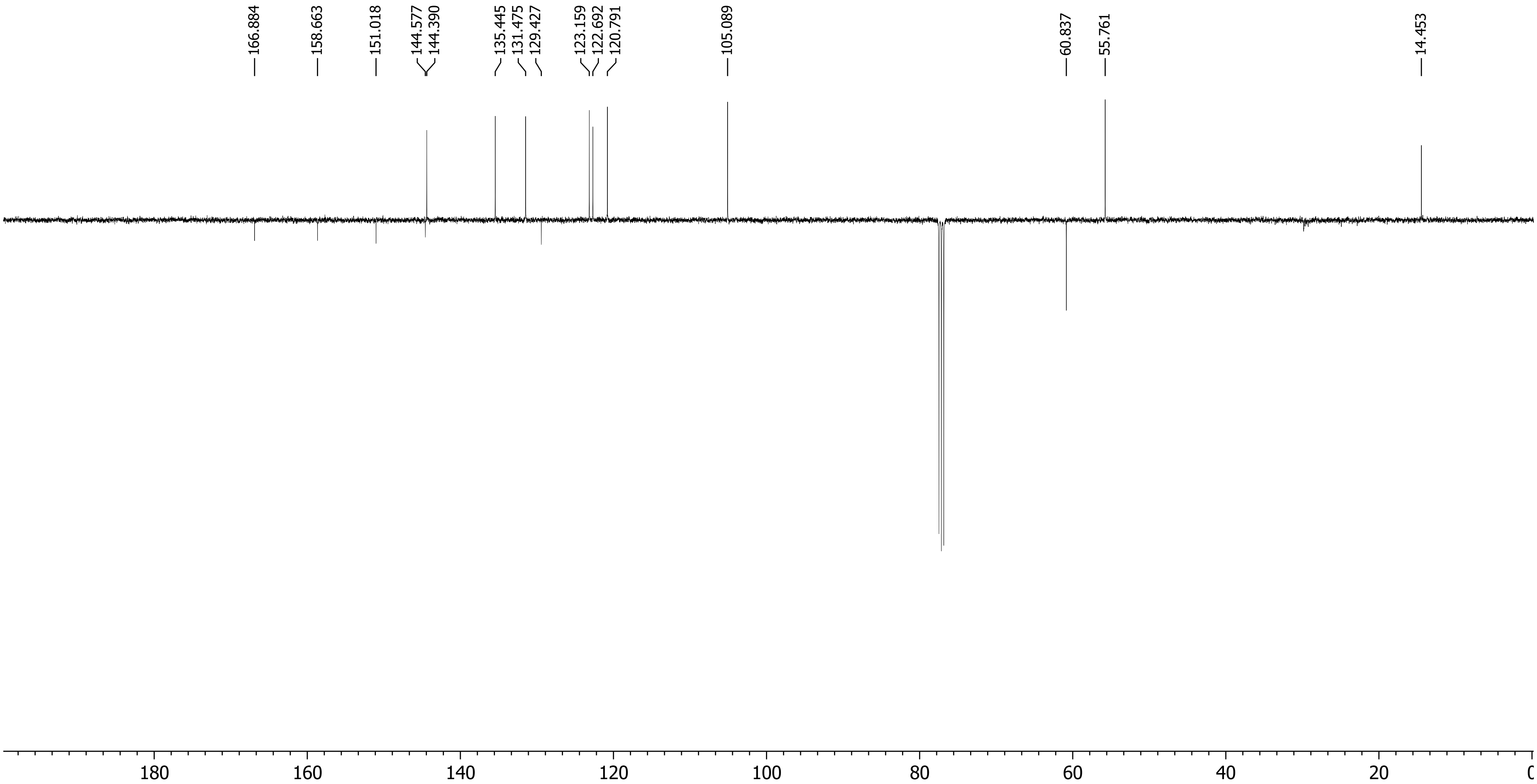

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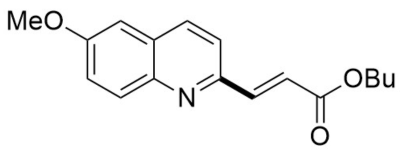

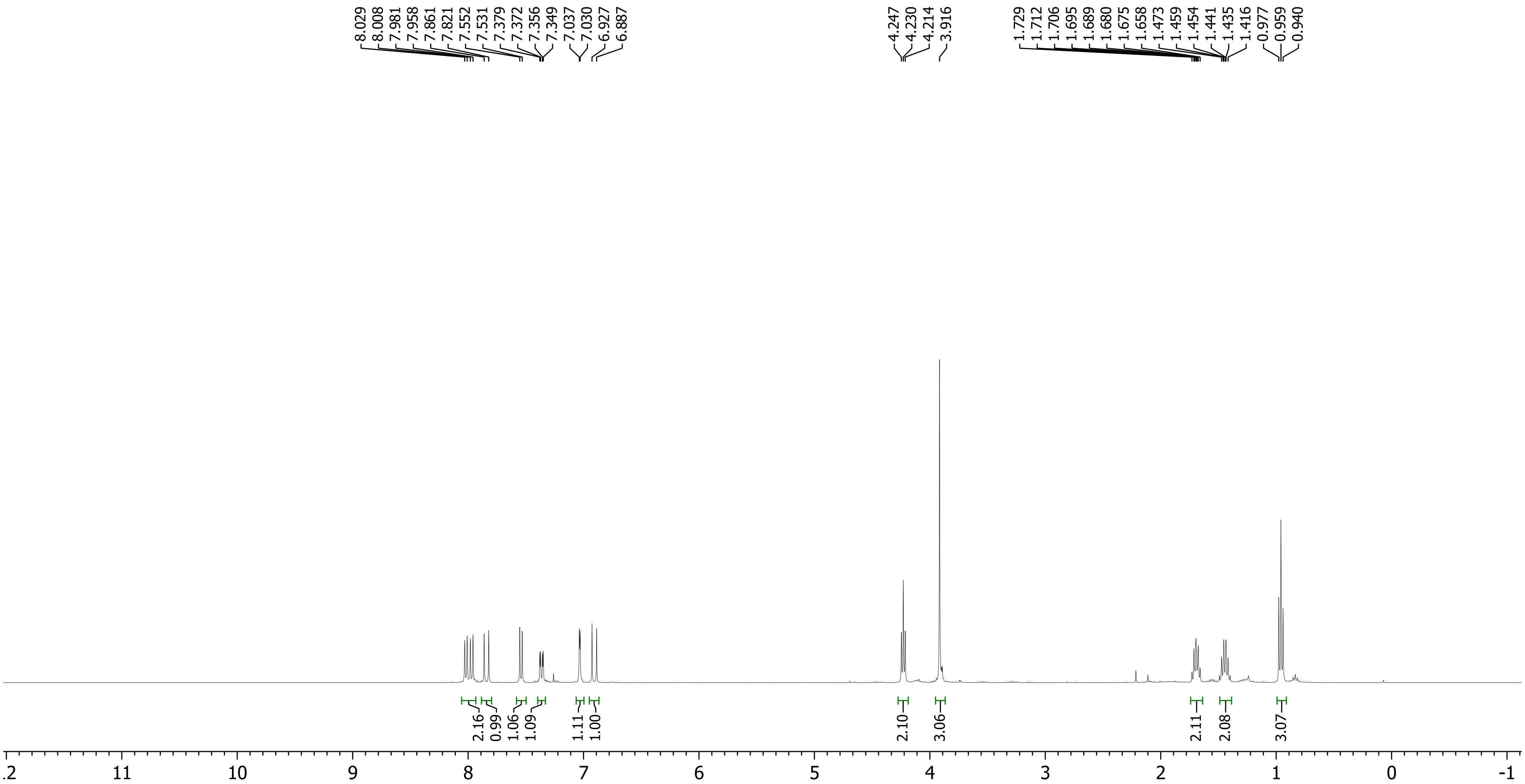

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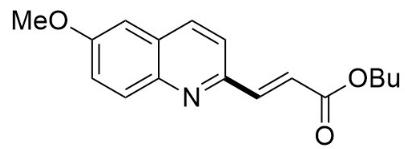

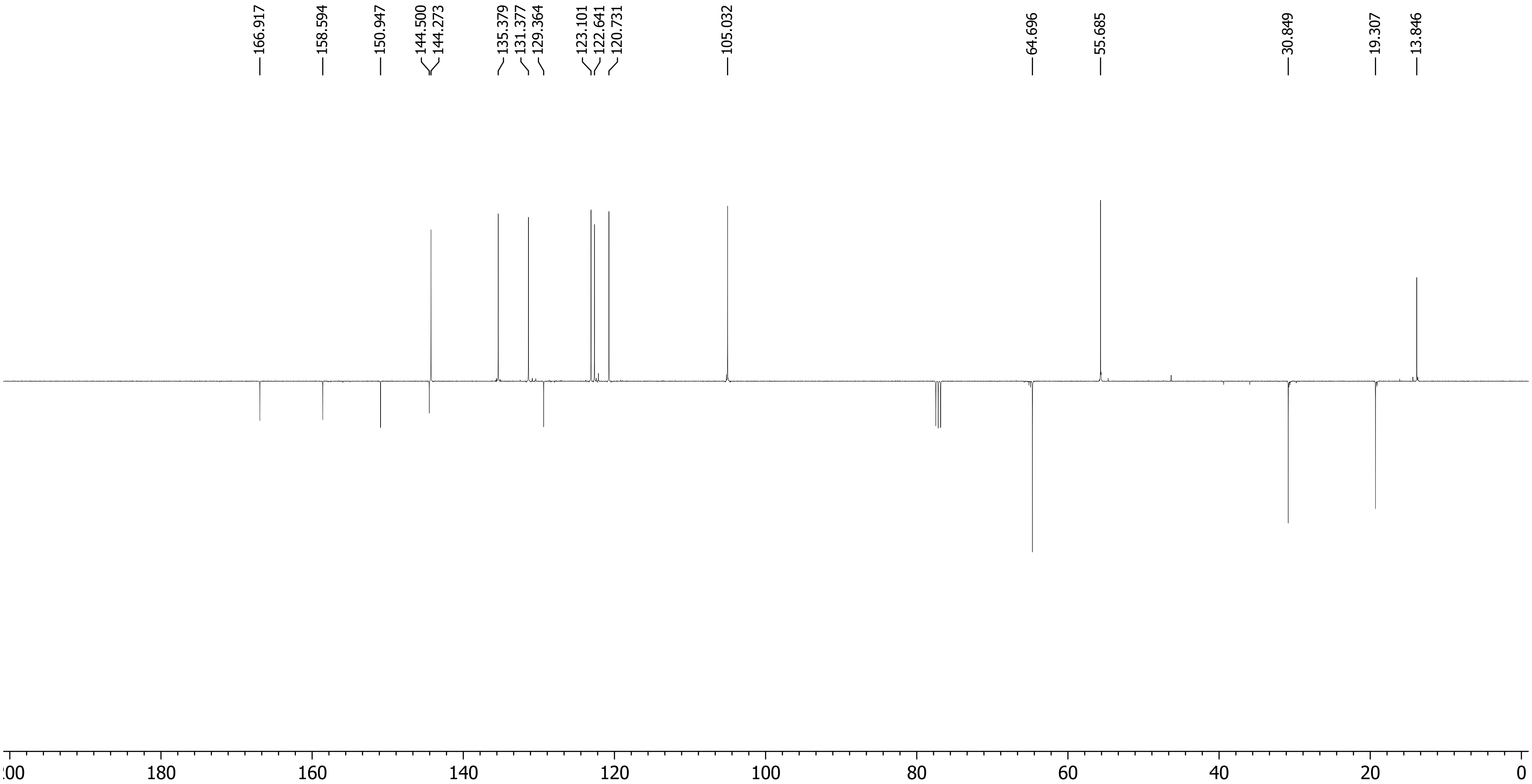

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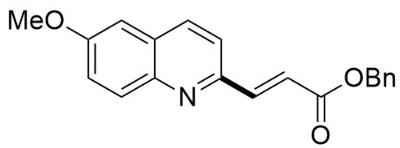

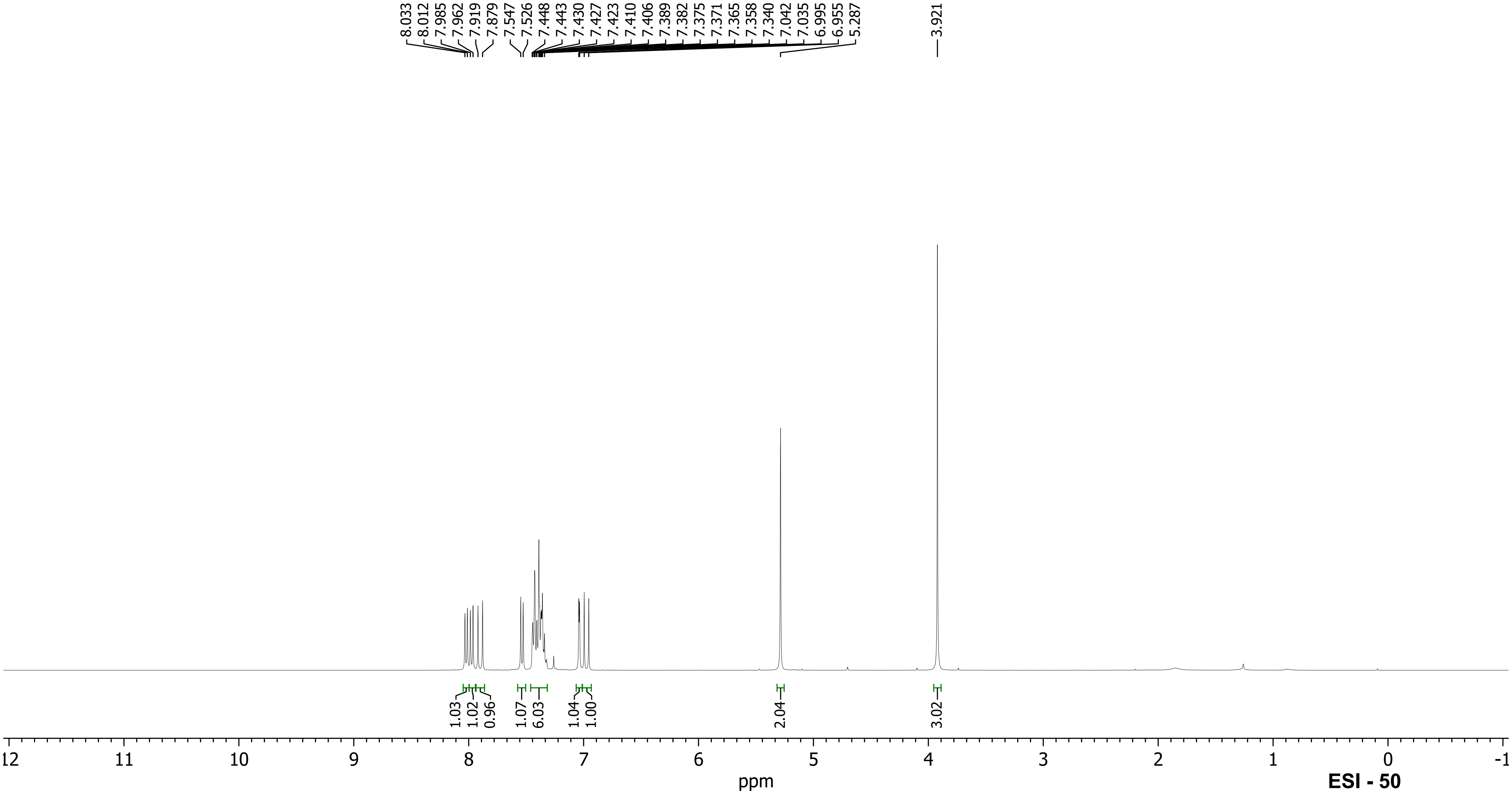

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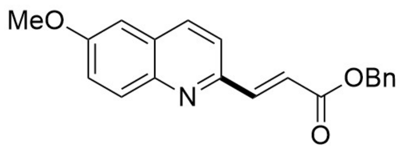

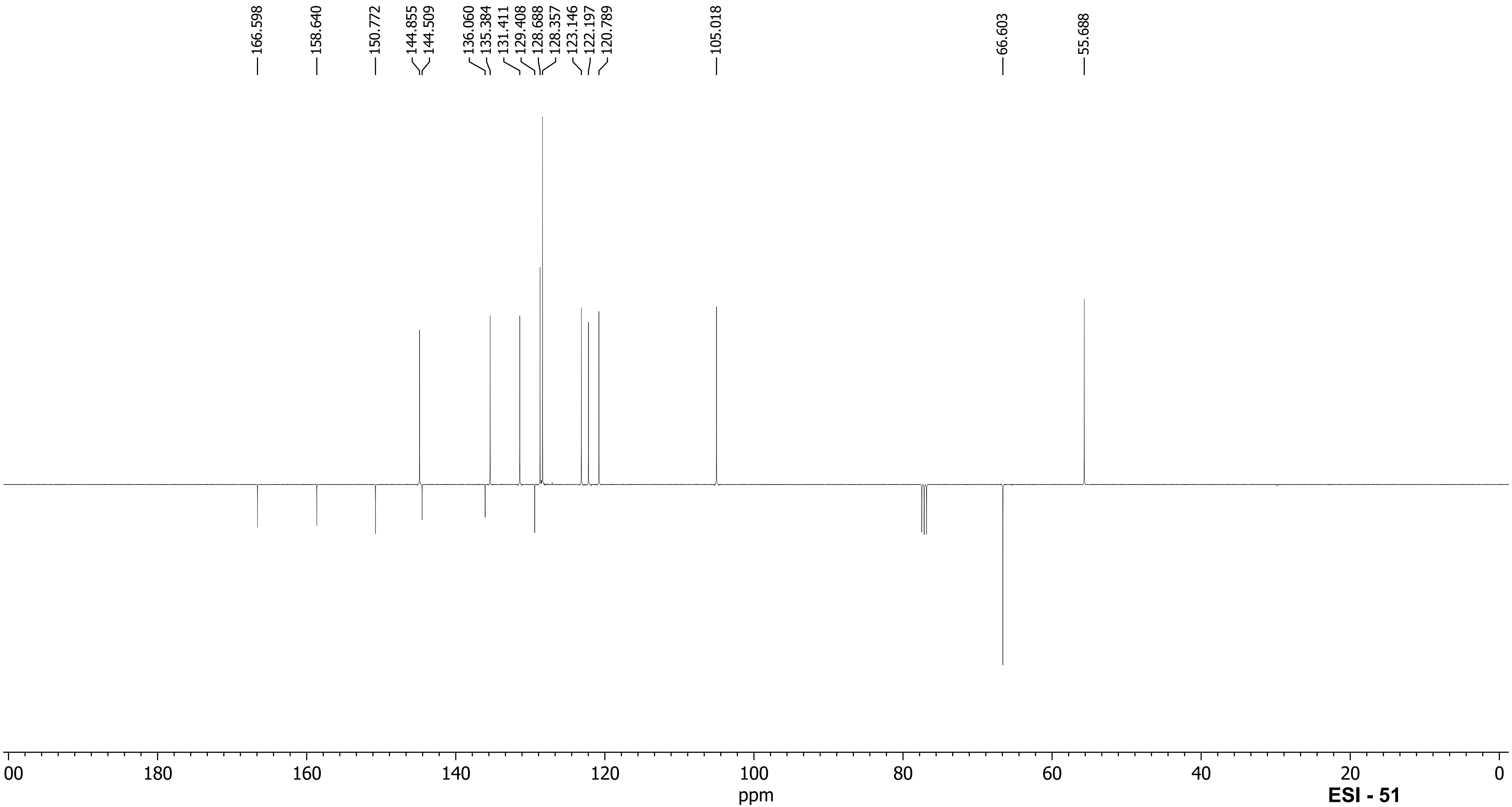

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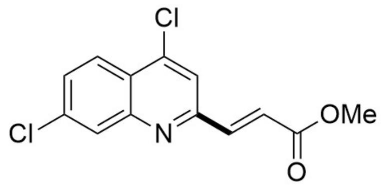
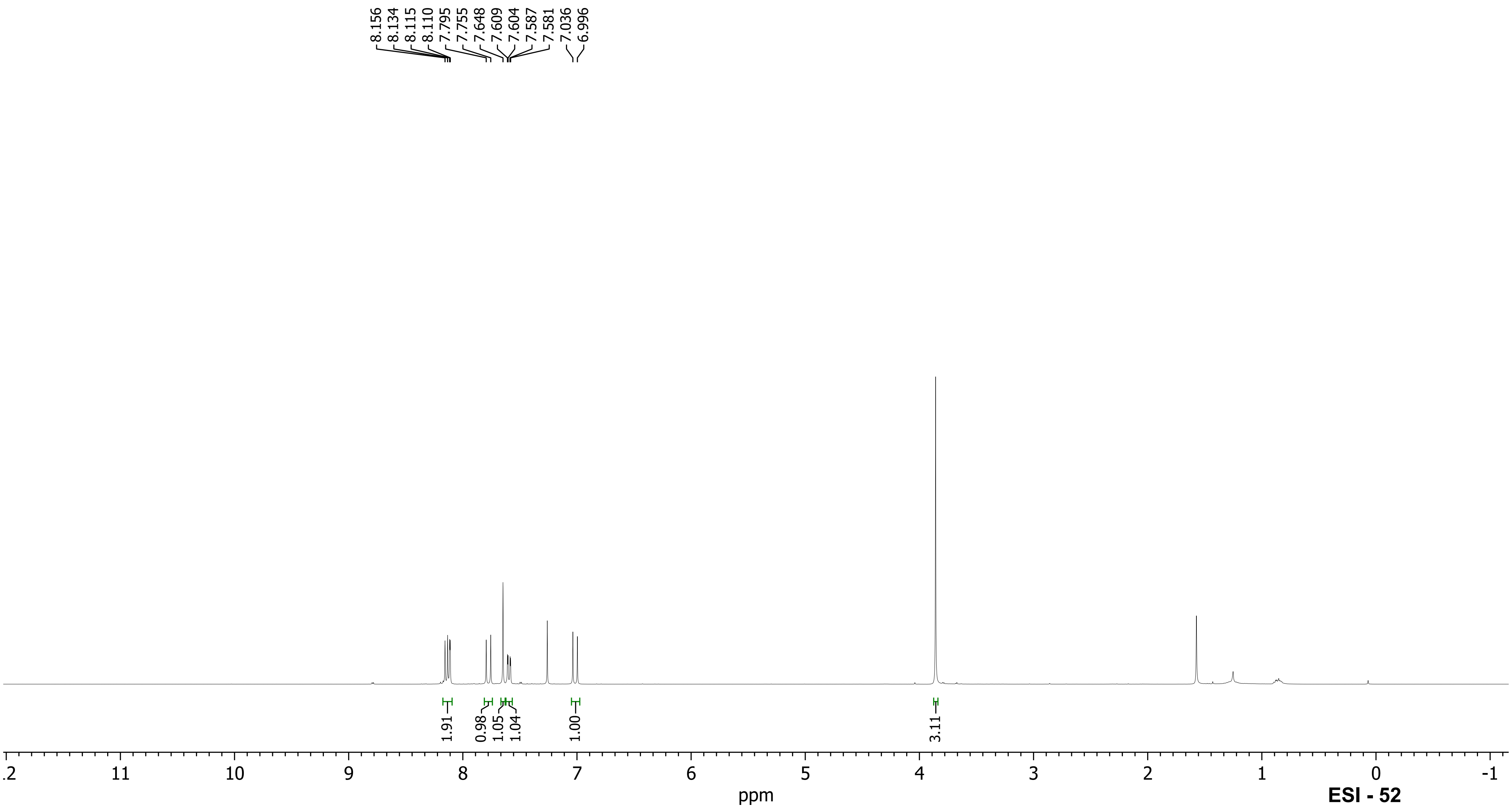
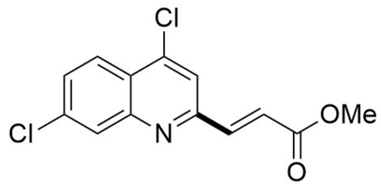
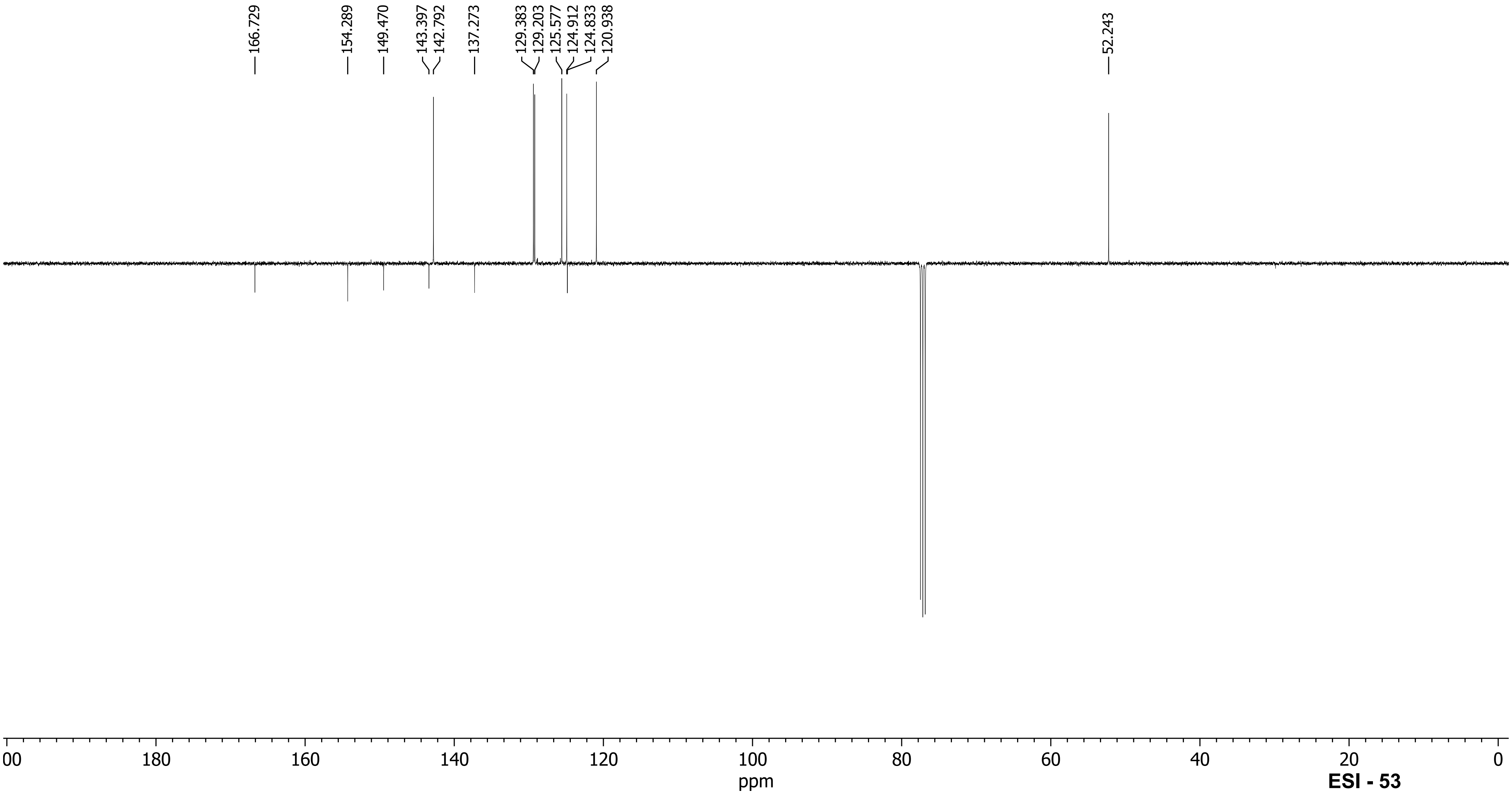




Methyl (E)-3-(4,7-dichloroquinolin-2-yl)acrylate (3i)





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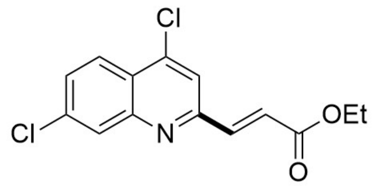
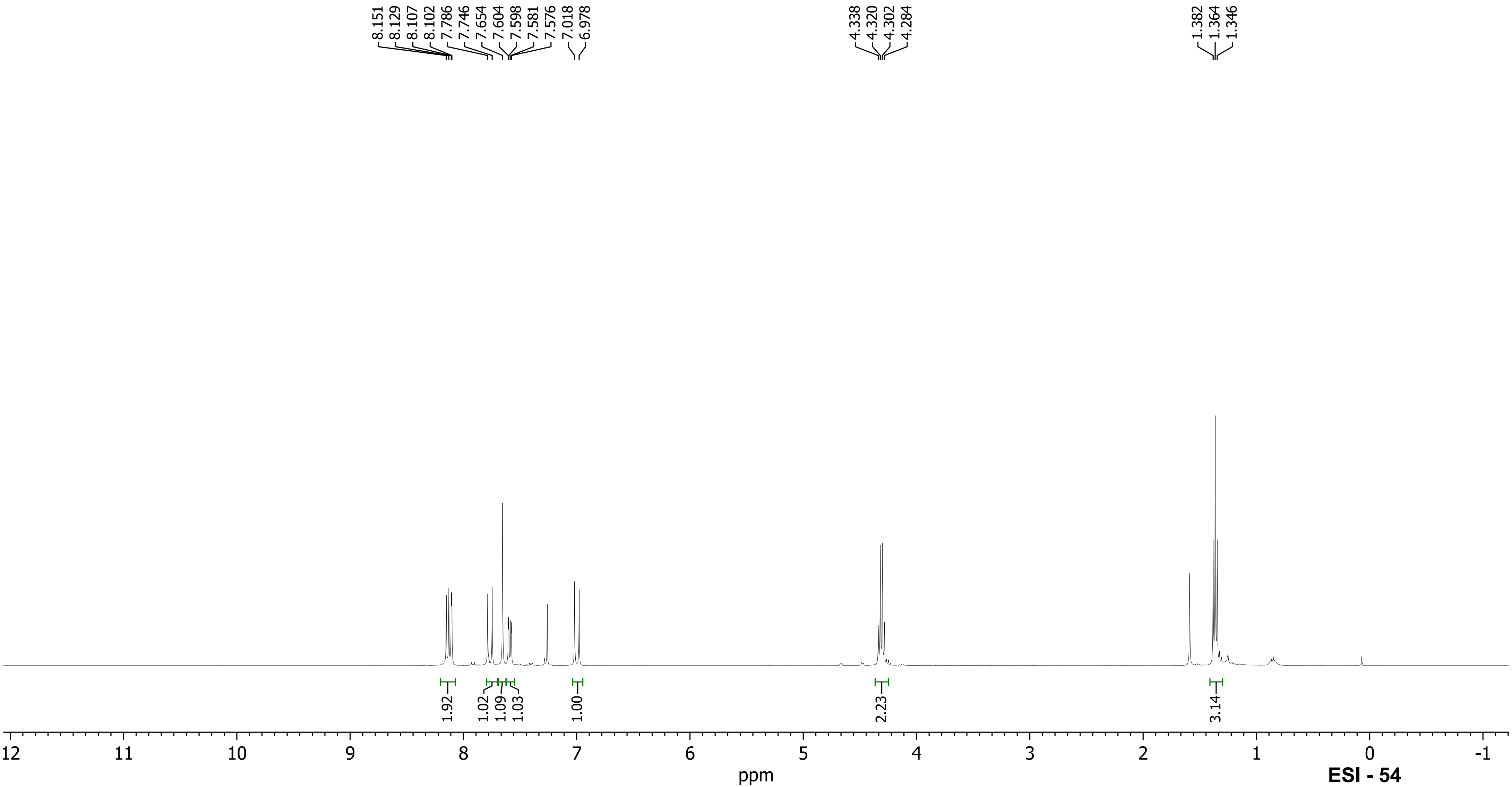
Ethyl (E)-3-(4,7-dichloroquinolin-2-yl)acrylate (3j)





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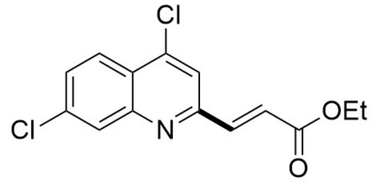

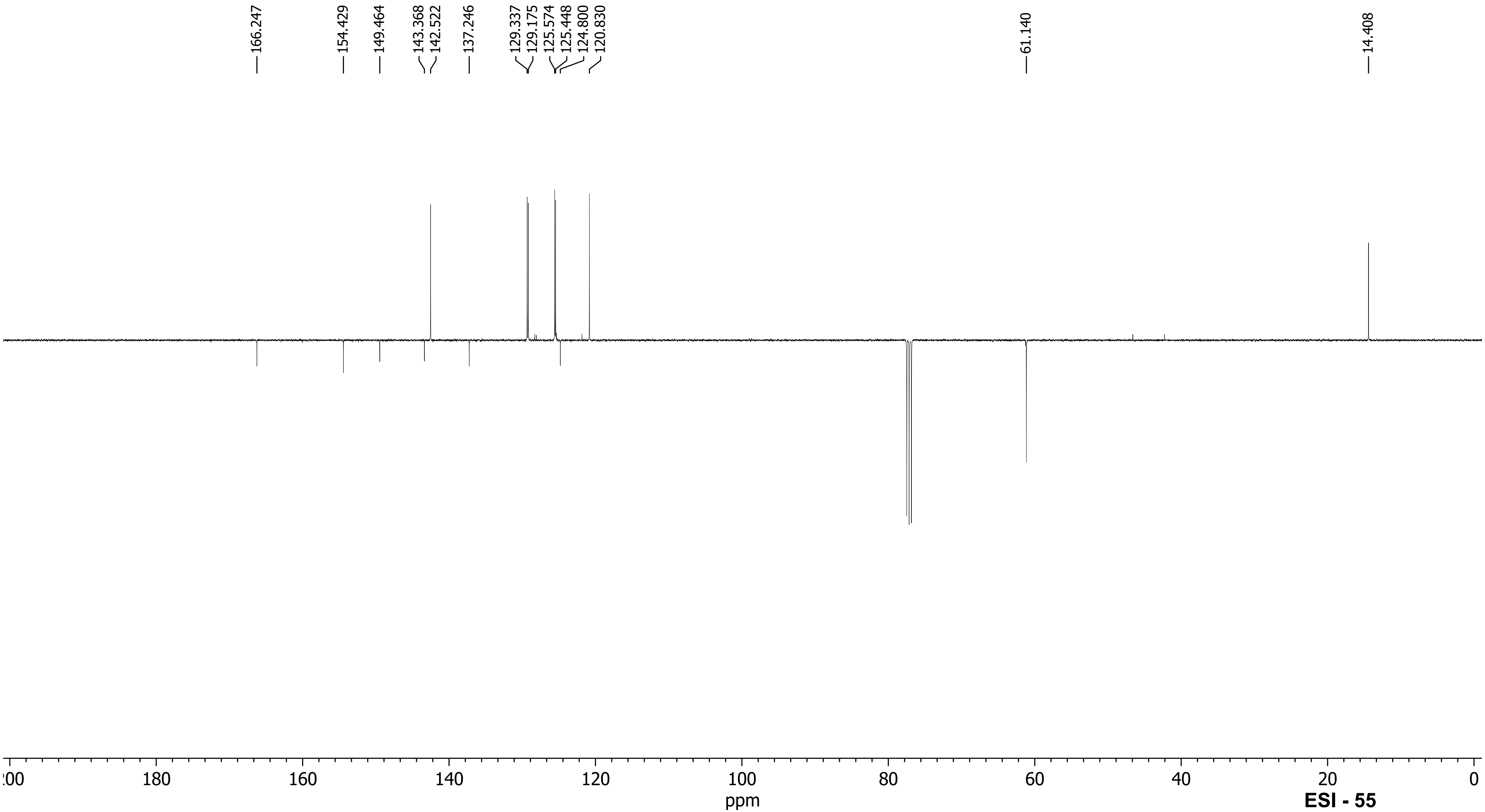

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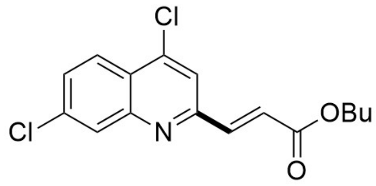

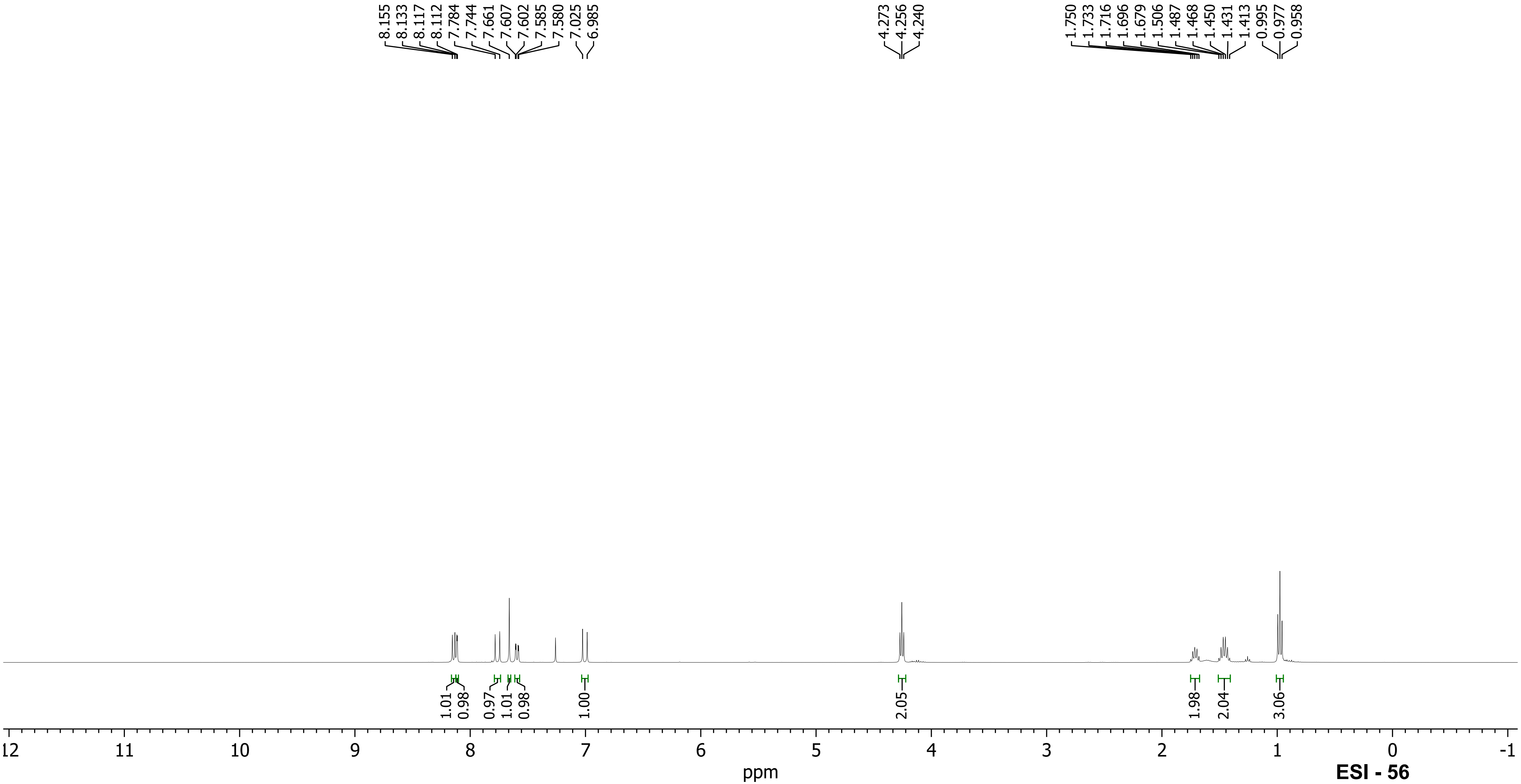

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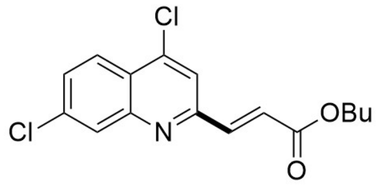

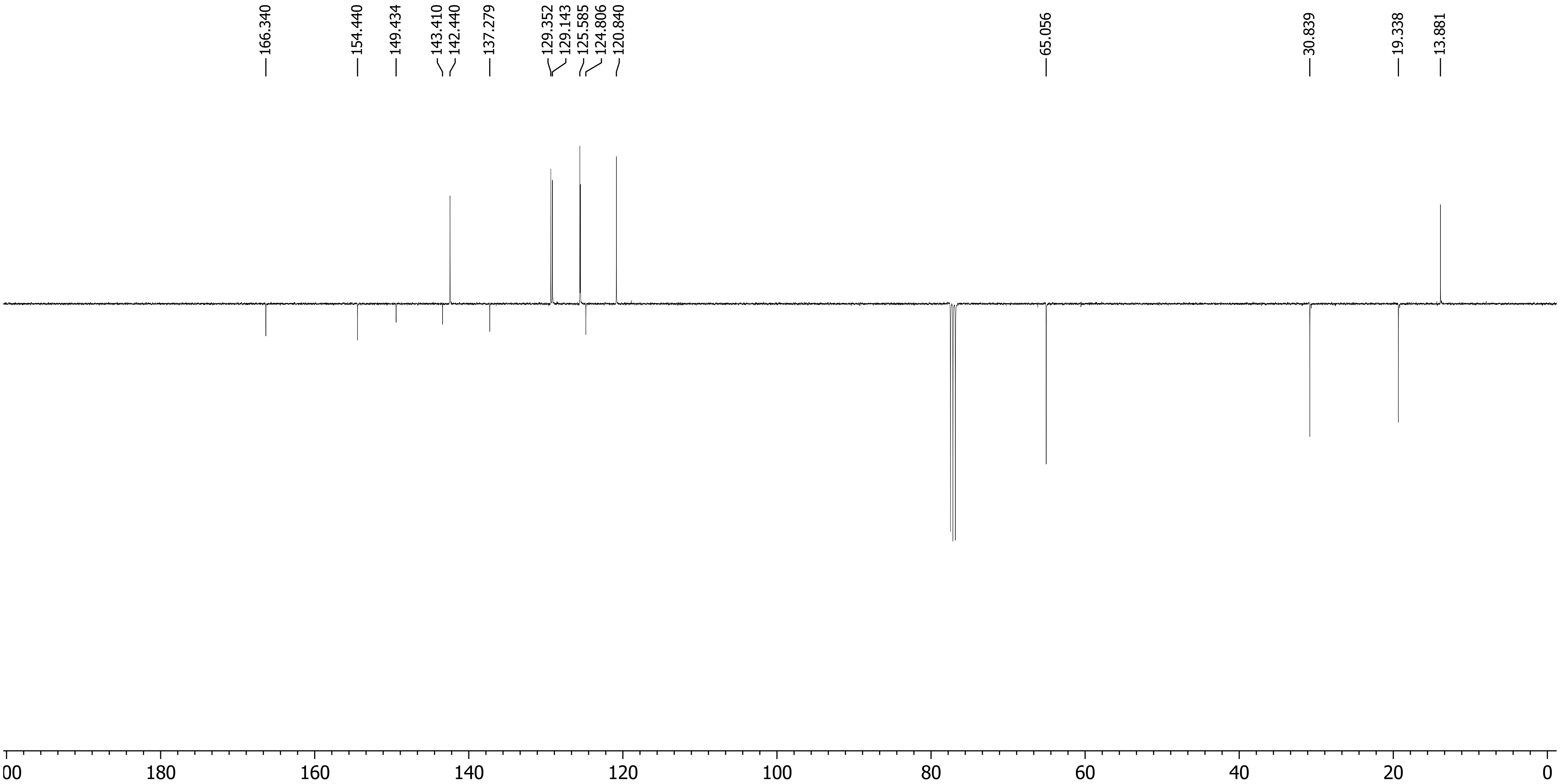

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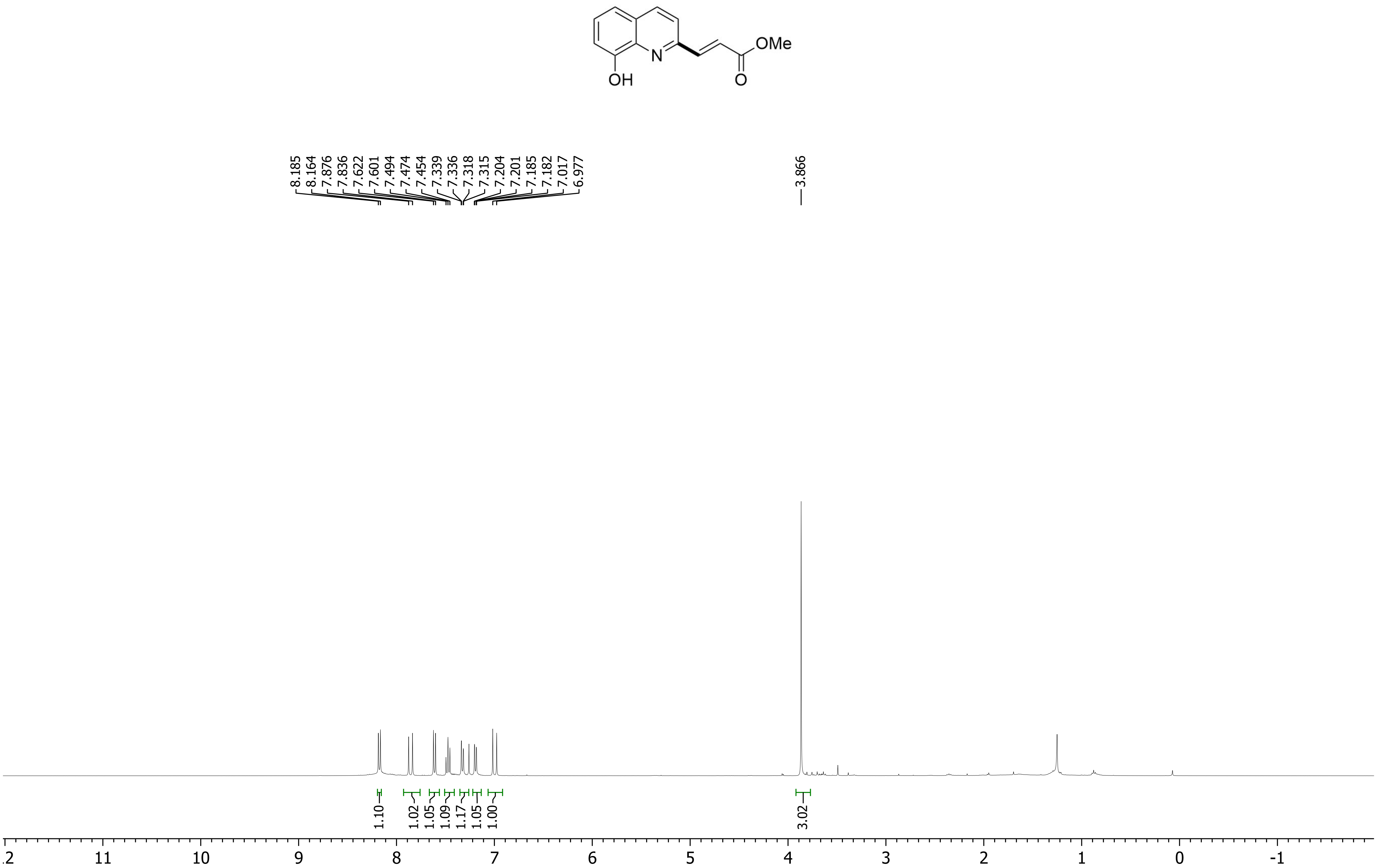
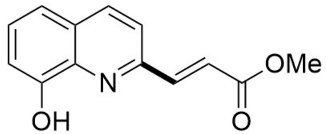
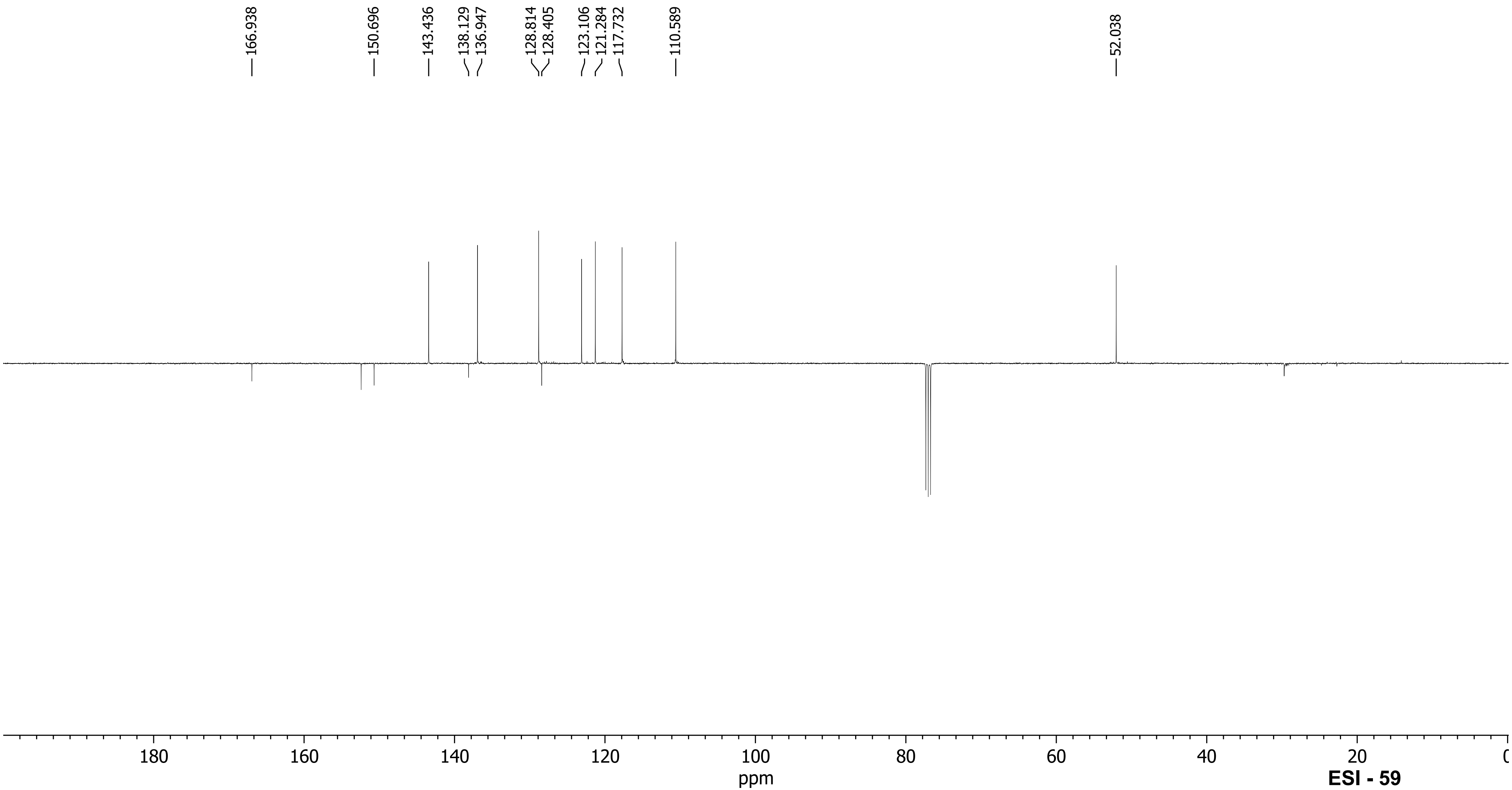
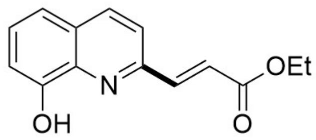


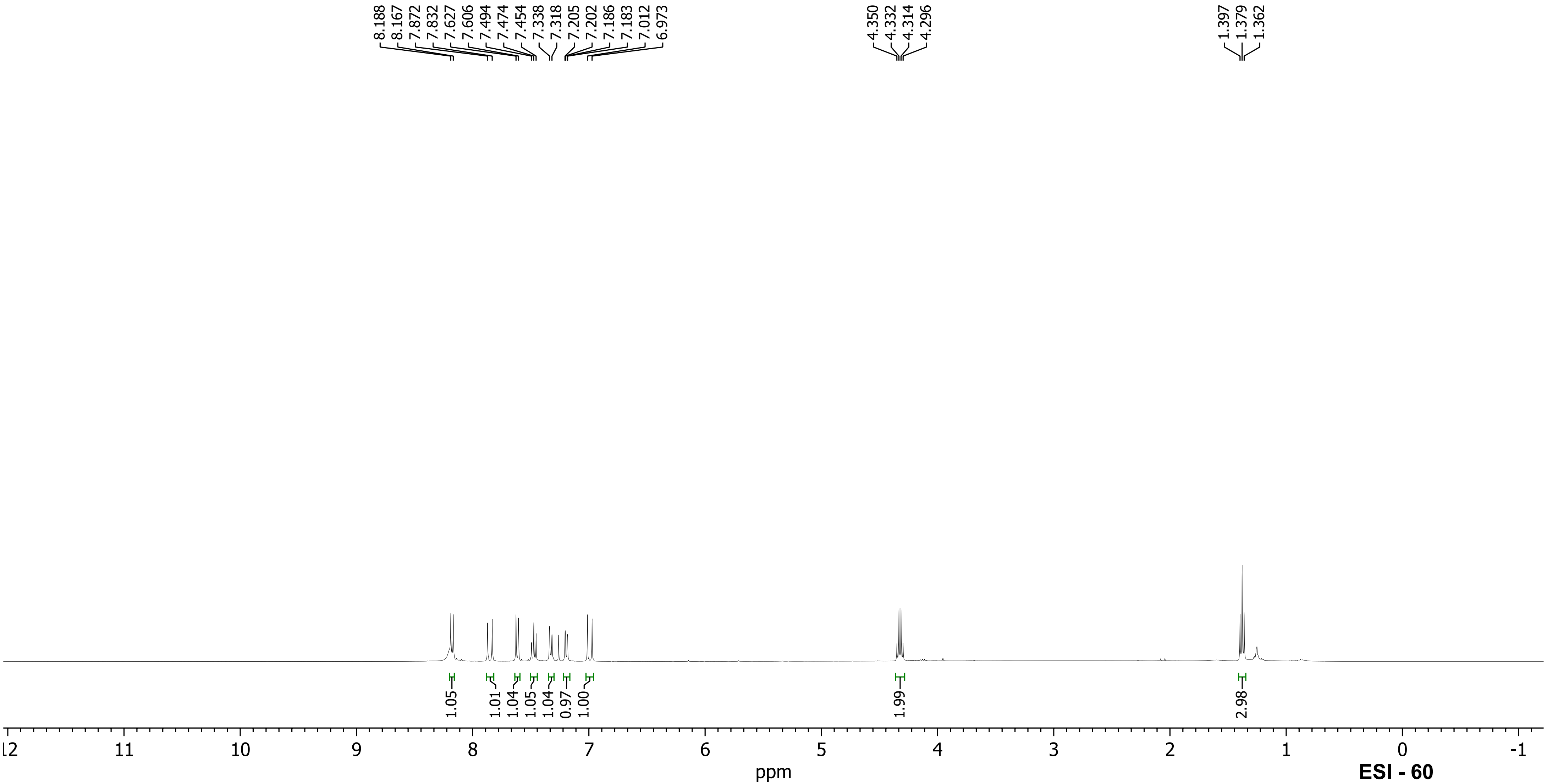
Methyl (E)-3-(8-hydroxyquinolin-2-yl)acrylate (3l)



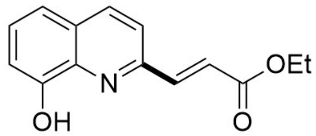


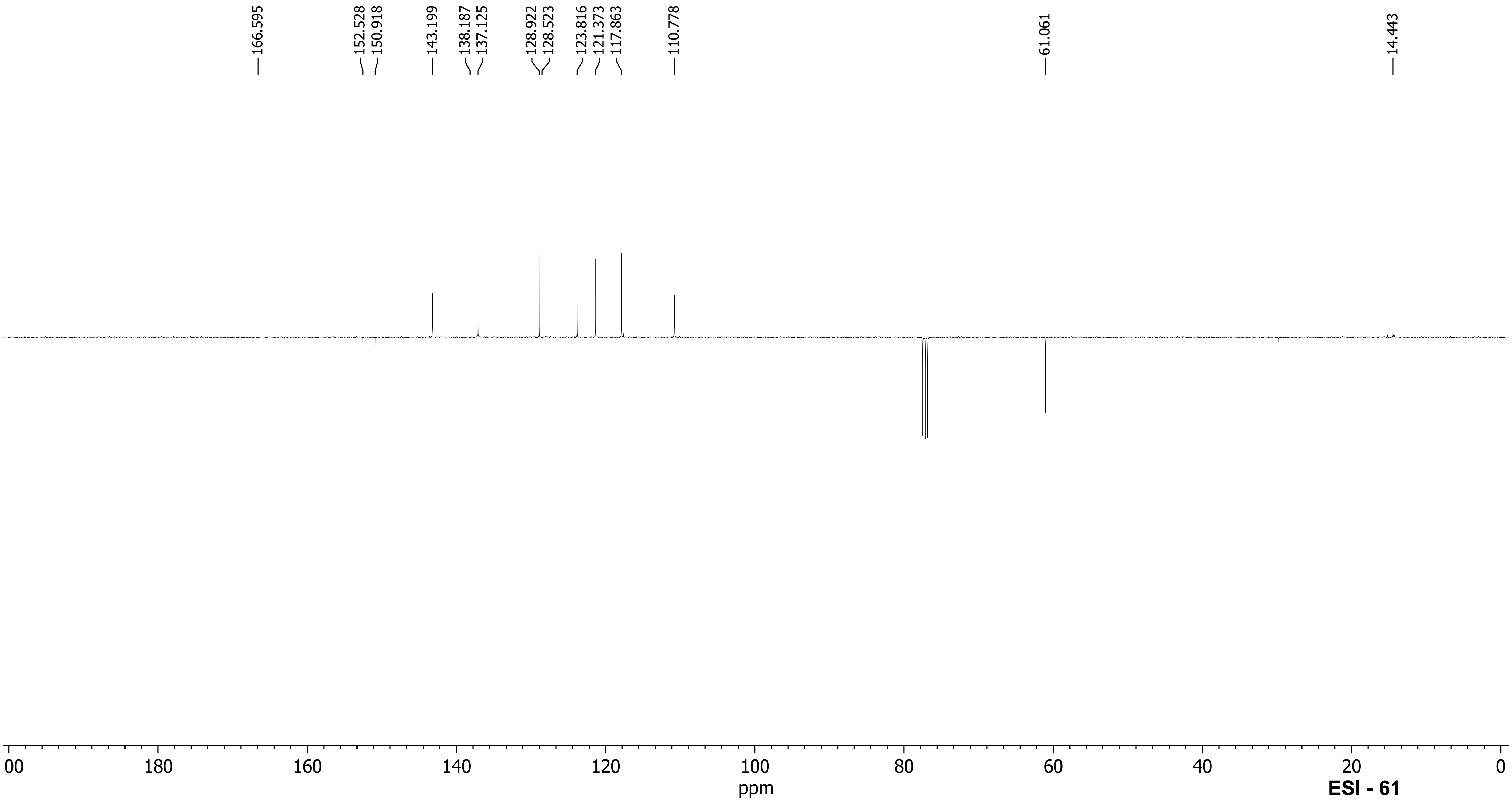
Ethyl (E)-3-(8-hydroxyquinolin-2-yl)acrylate (3m)



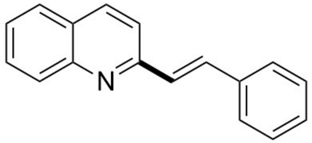


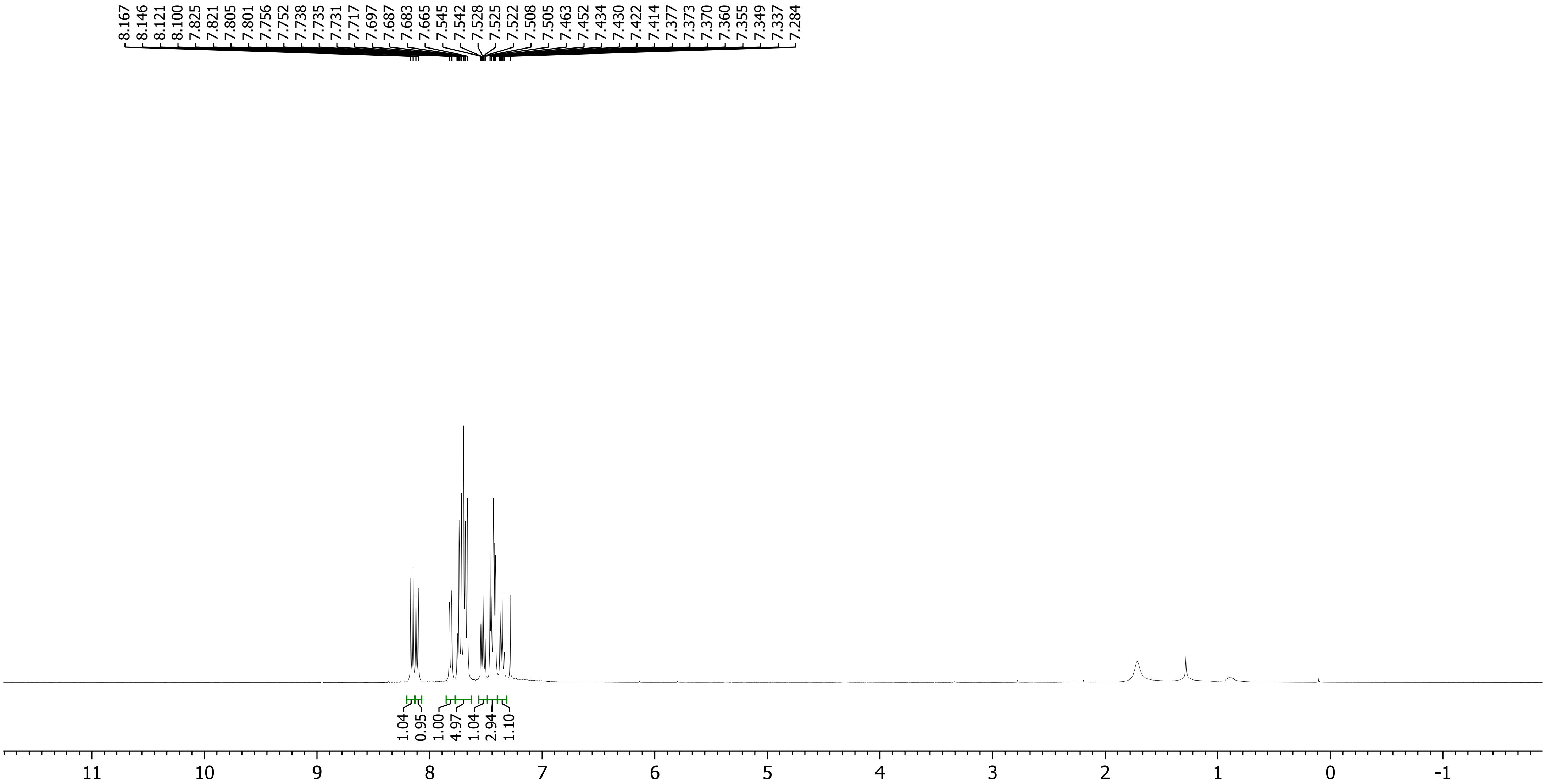
Ethyl (E)-3-(8-hydroxyquinolin-2-yl)acrylate (3m)



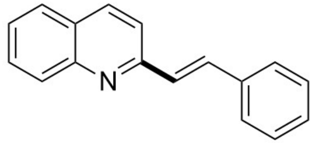


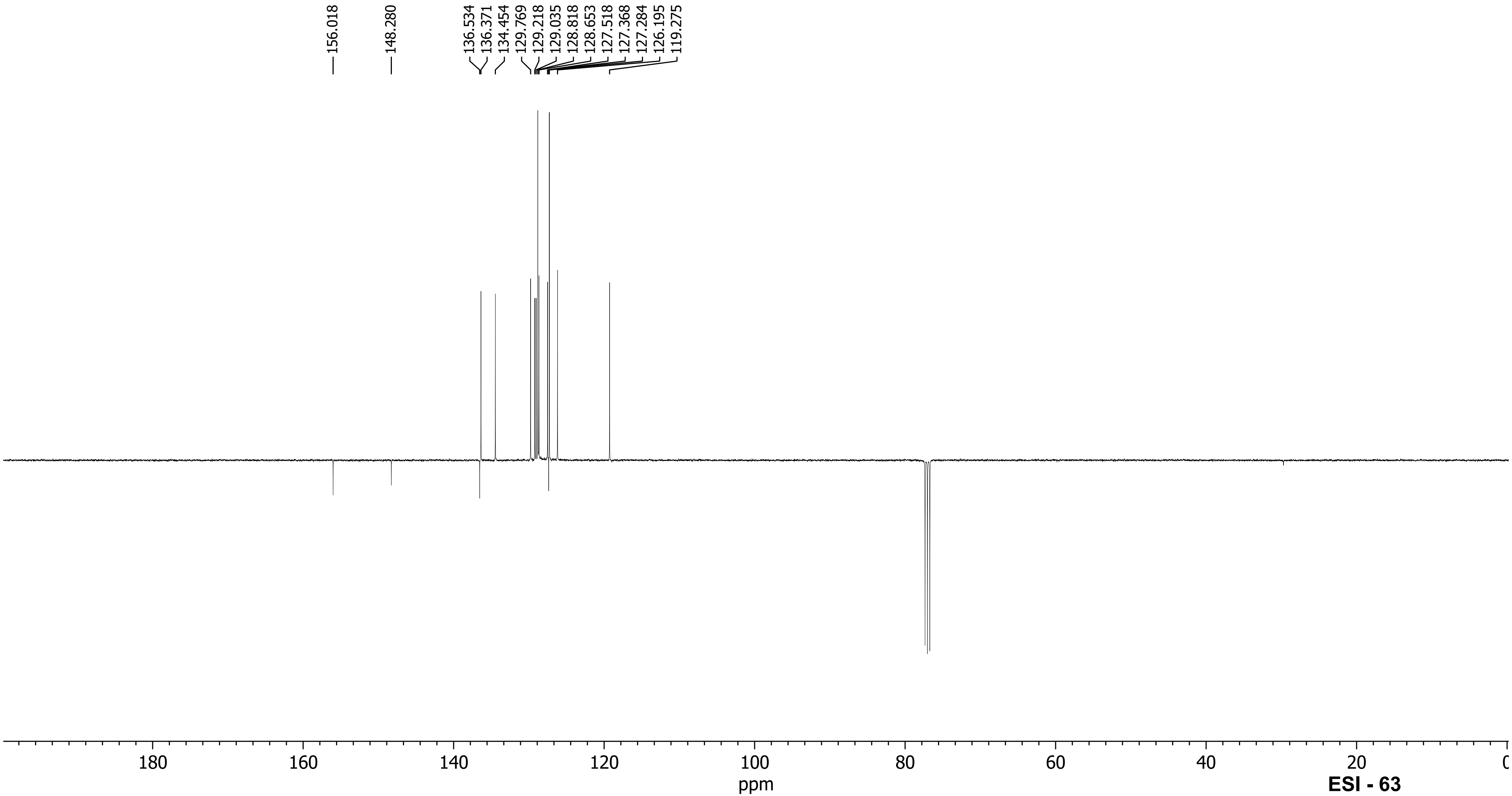
(E)-2-styrylquinoline (6a)



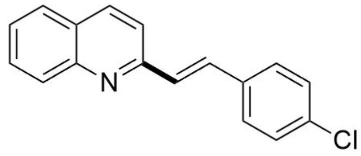


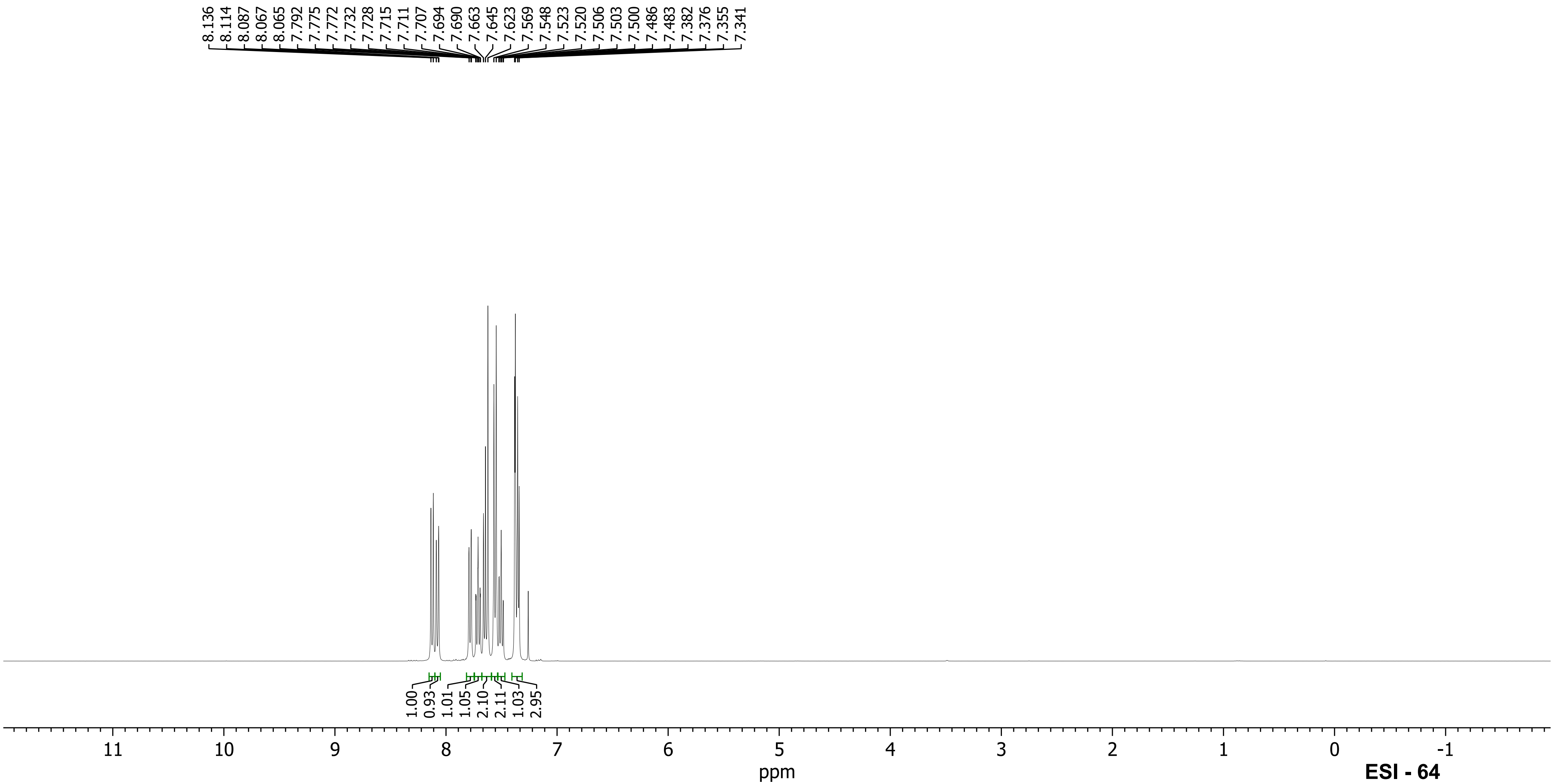
(E)-2-styrylquinoline (6a)



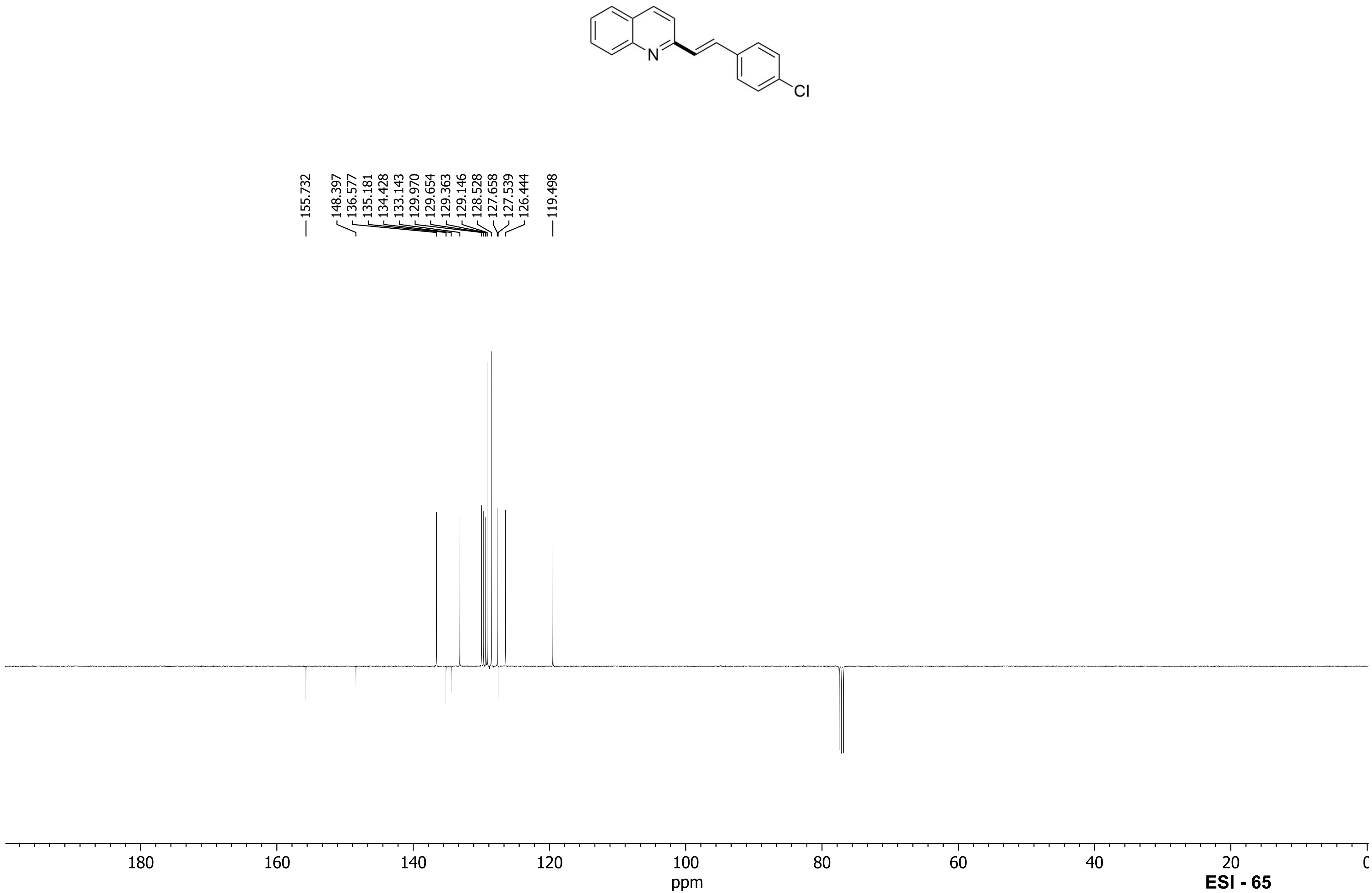


(E)-2-(4-chlorostyryl)quinoline (6b)

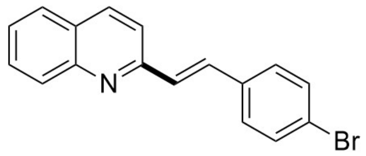


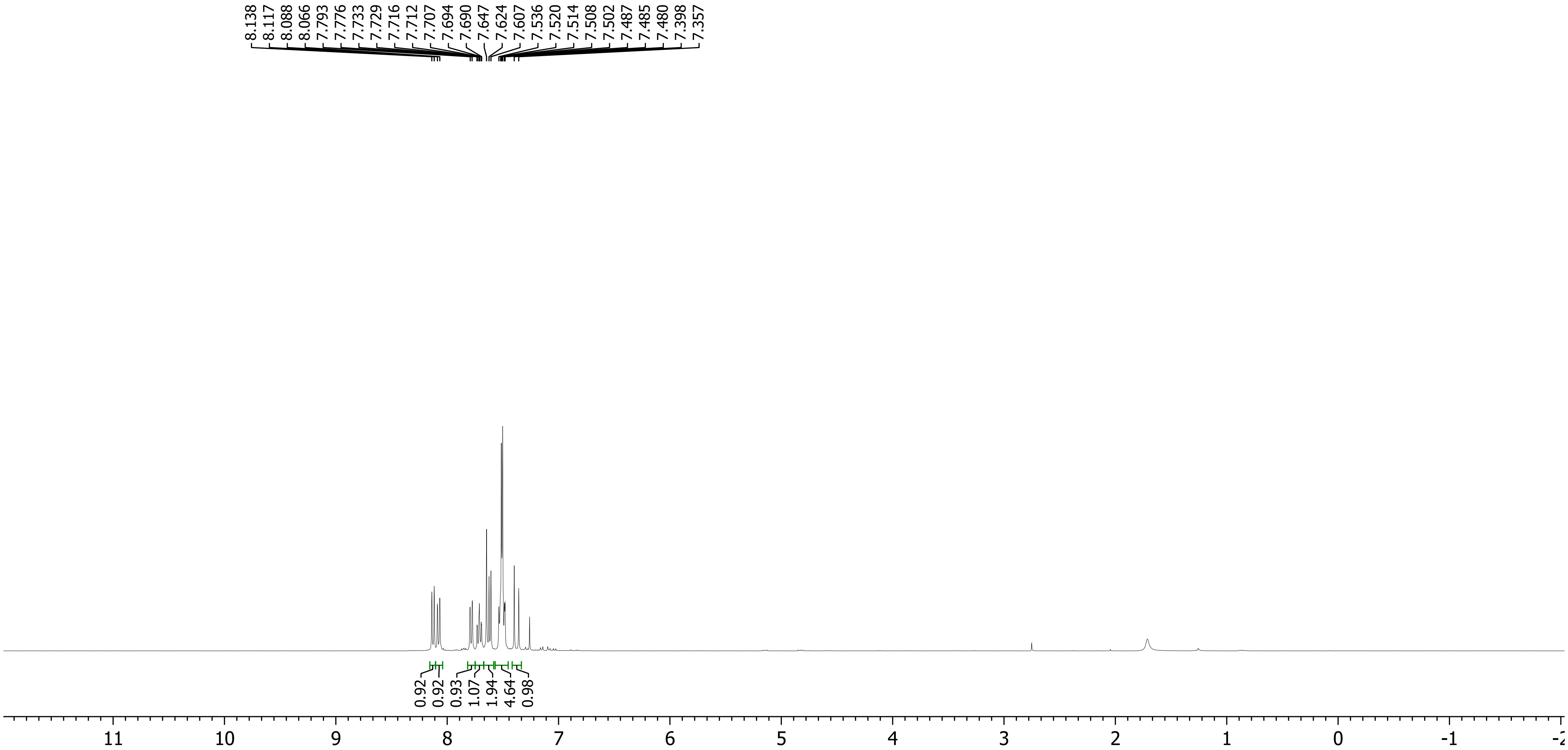


(E)-2-(4-chlorostyryl)quinoline (6b)

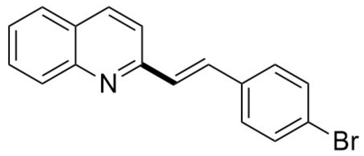


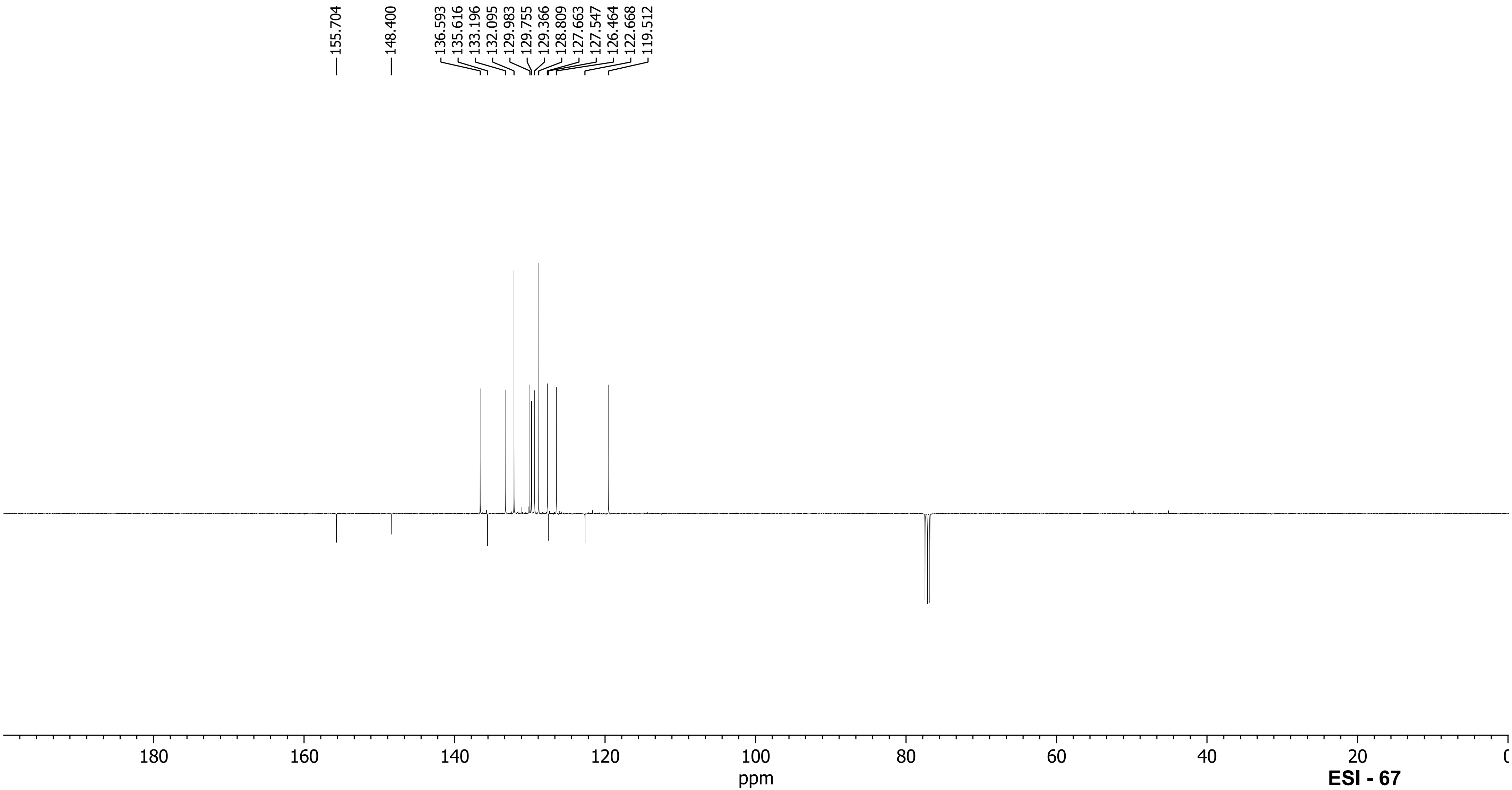
(E)-2-(4-bromostyryl)quinoline (6c)



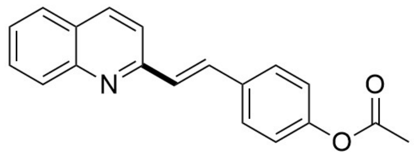


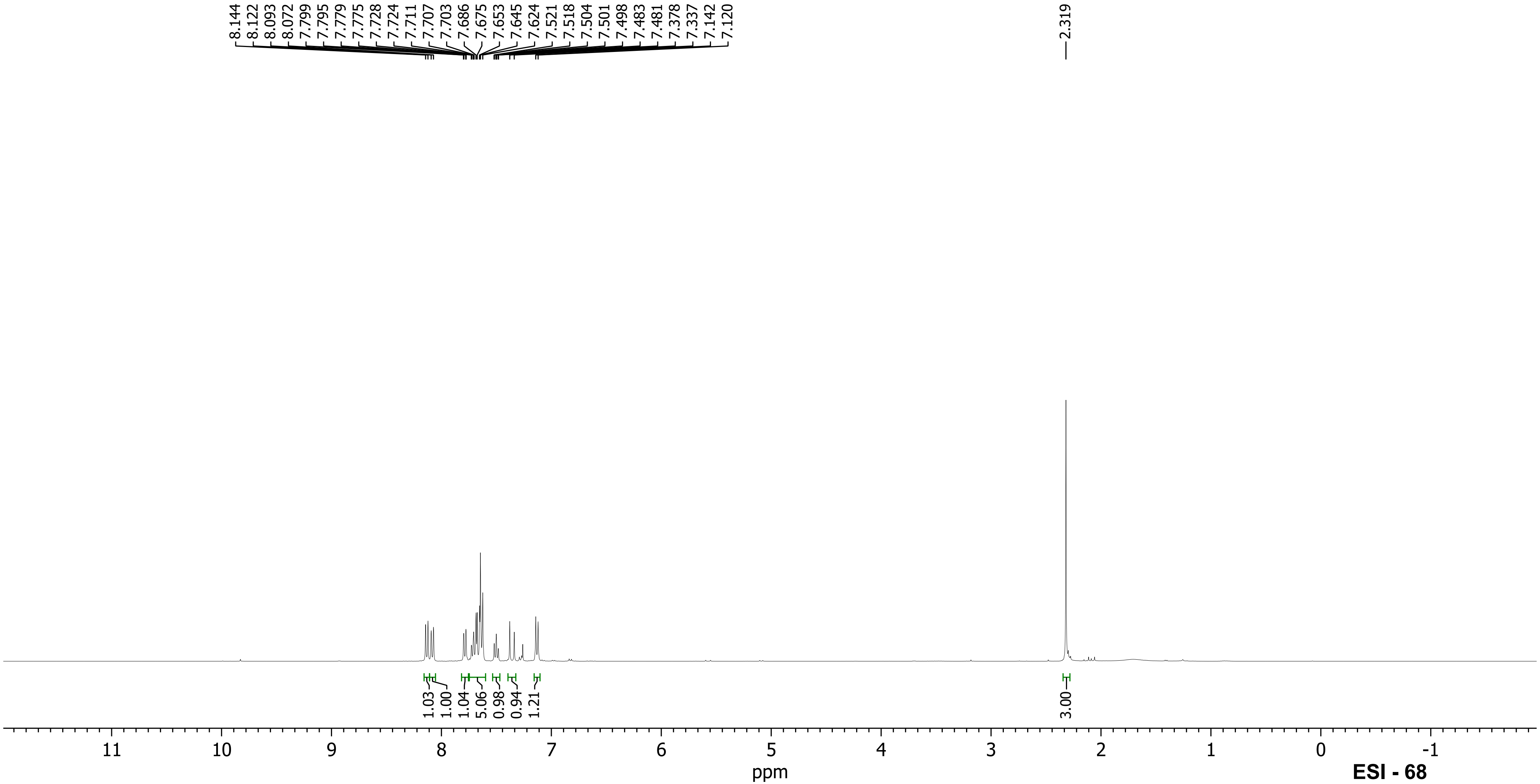
(E)-2-(4-bromostyryl)quinoline (6c)



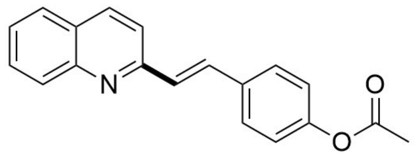


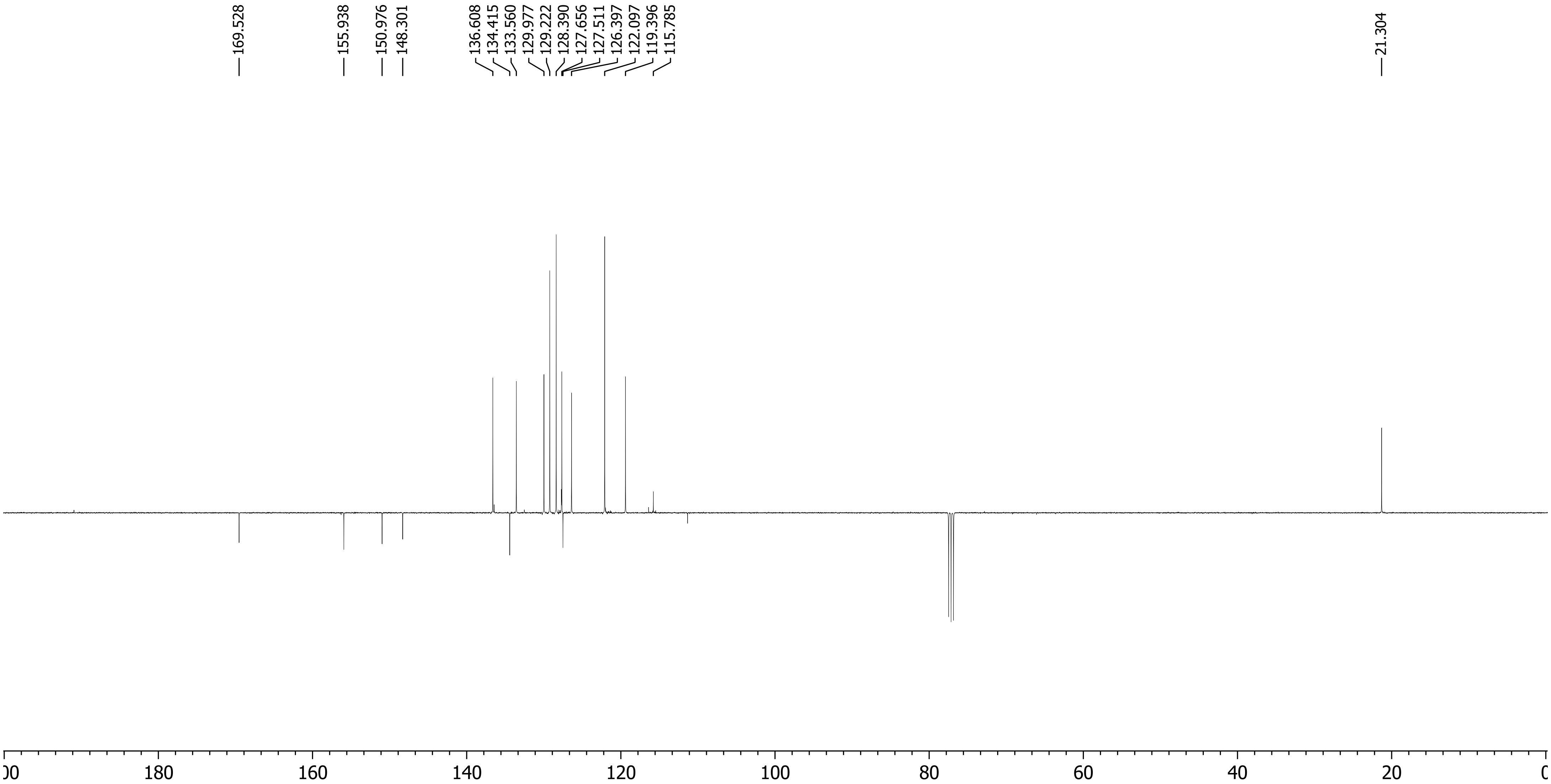
(E)-4-(2-(quinolin-2-yl)vinyl)phenyl acetate (6d)



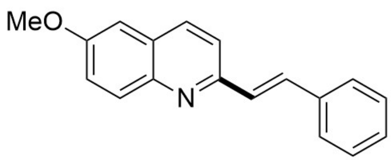


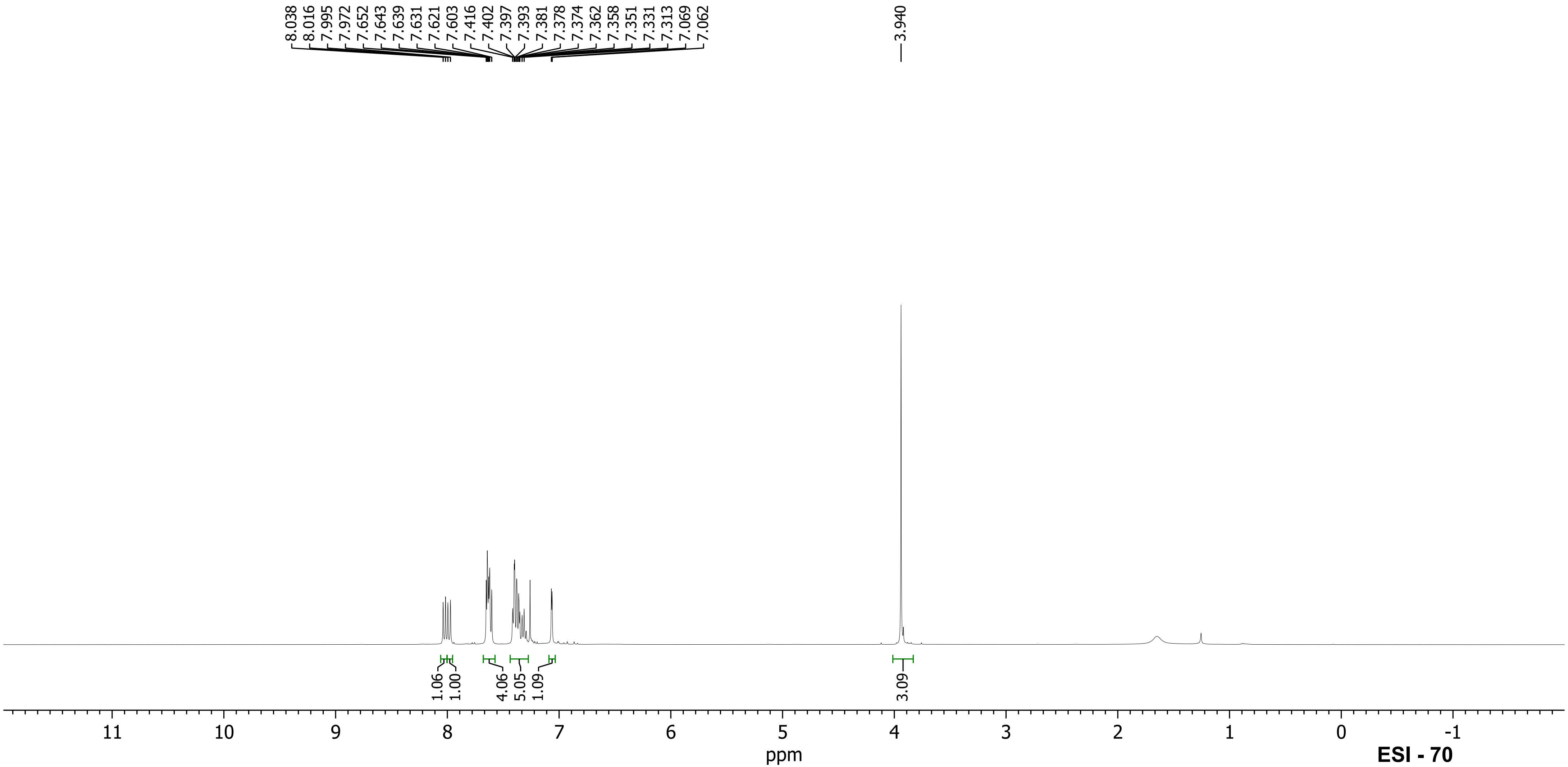
(E)-4-(2-(quinolin-2-yl)vinyl)phenyl acetate (6d)





(E)-6-methoxy-2-styrylquinoline (6e)





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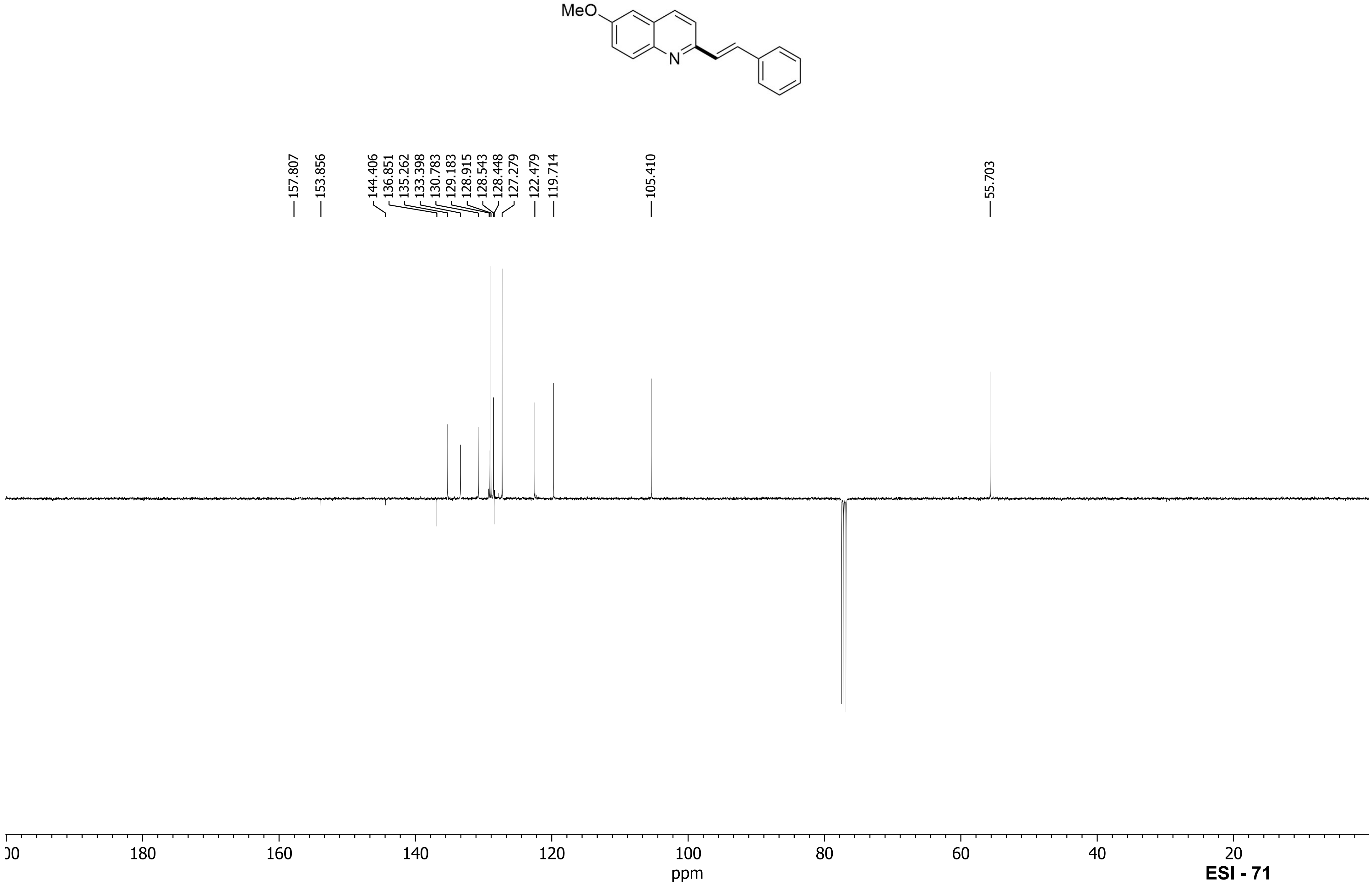
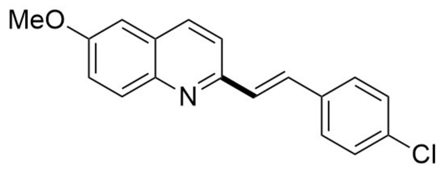
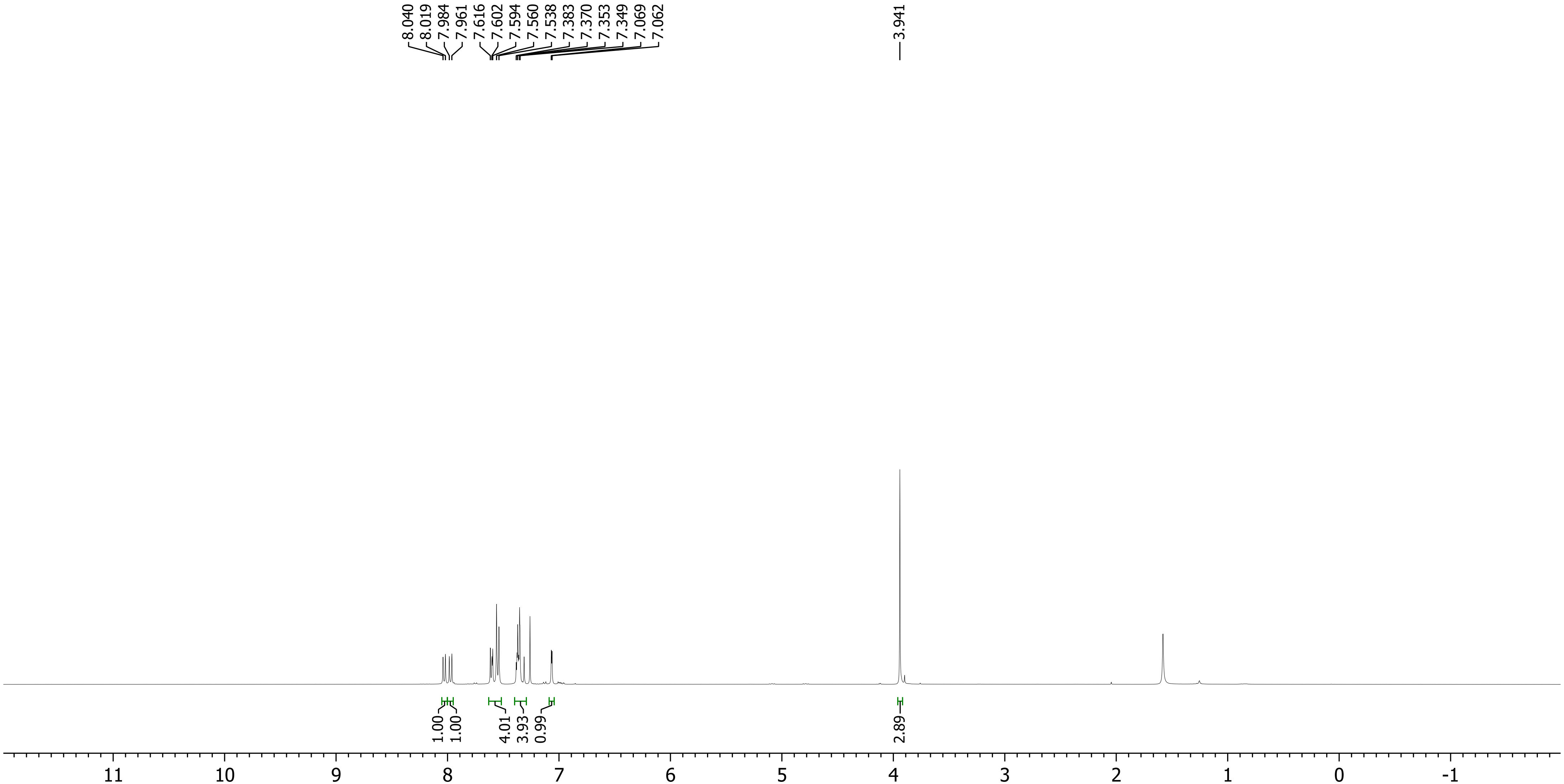
(E)-6-methoxy-2-styrylquinoline (6e)

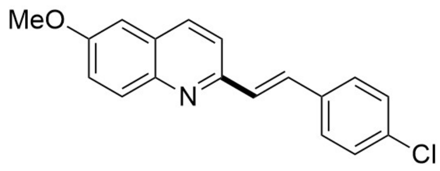


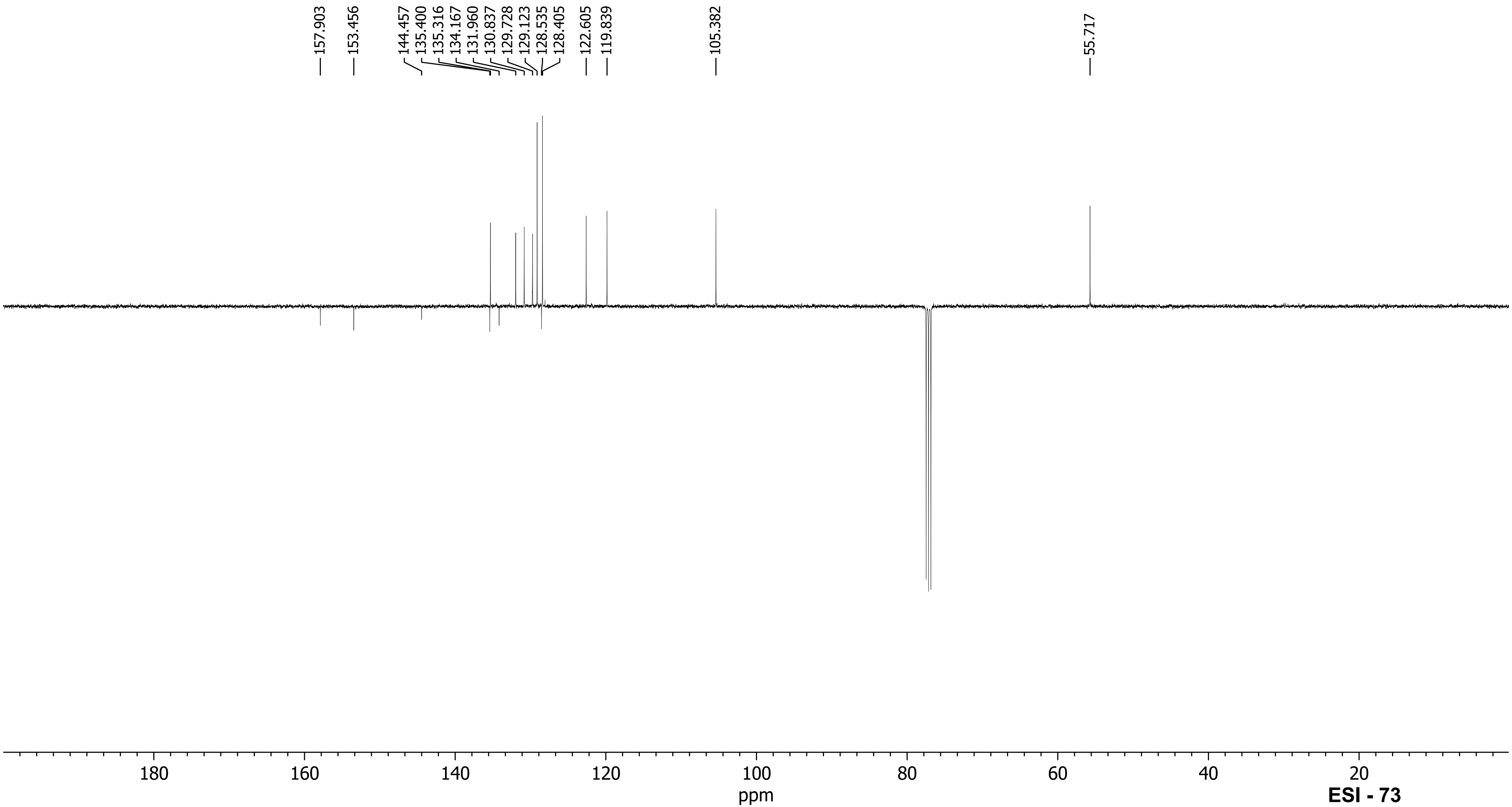
(E)-2-(4-chlorostyryl)-6-methoxyquinoline (6f)



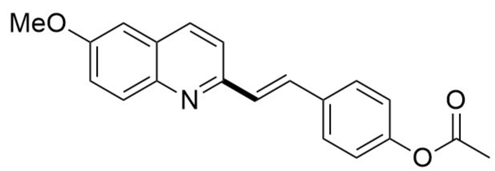


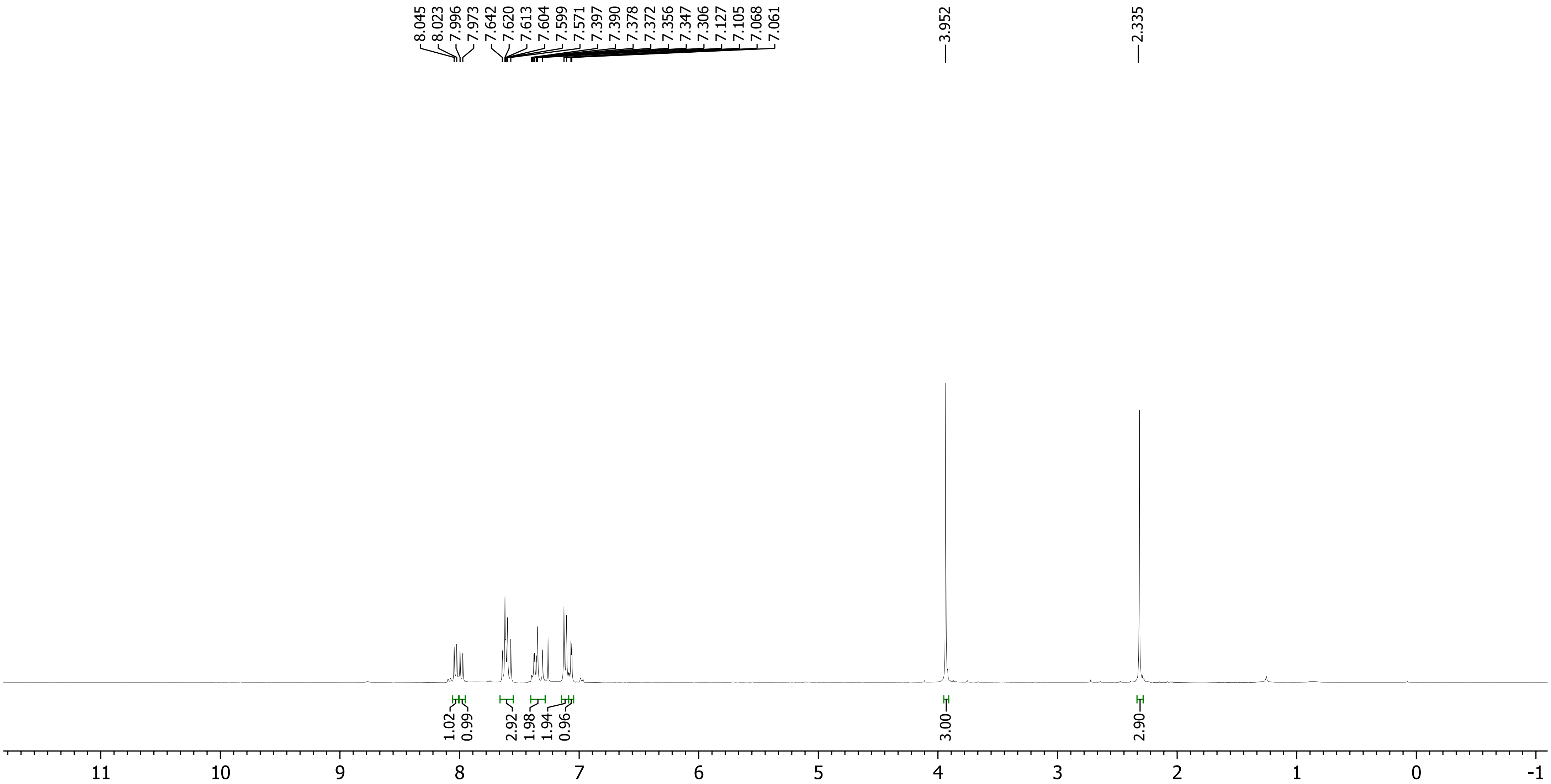
(E)-2-(4-chlorostyryl)-6-methoxyquinoline (6f)



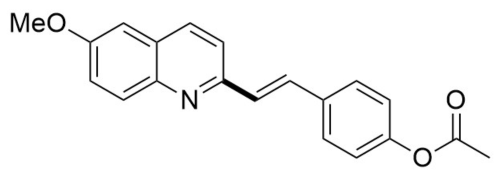


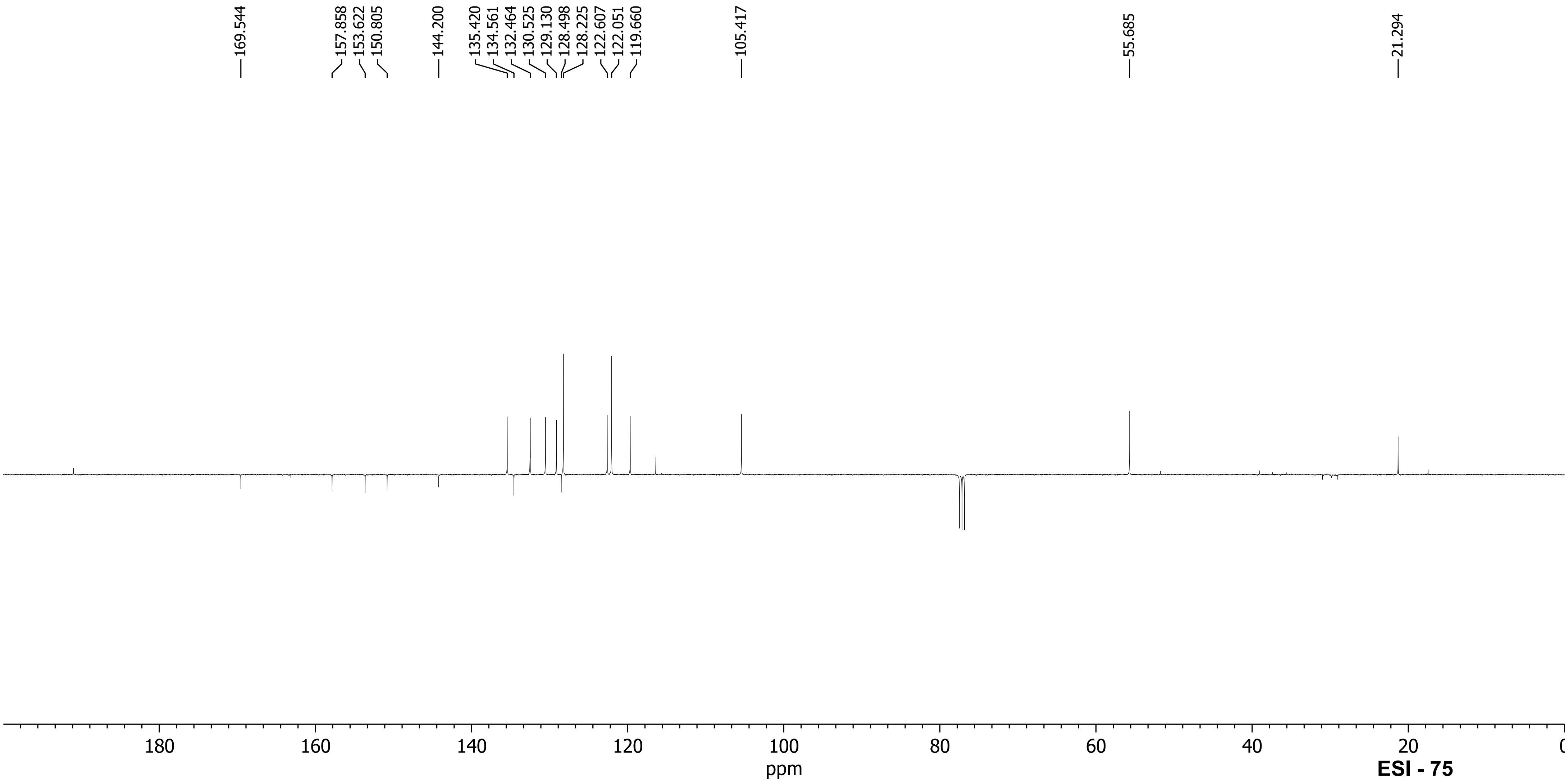
(E)-4-(2-(6-methoxyquinolin-2-yl)vinyl)phenyl acetate (6g)



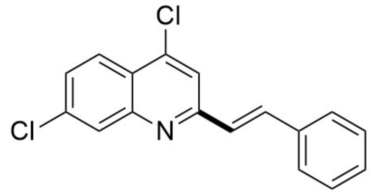


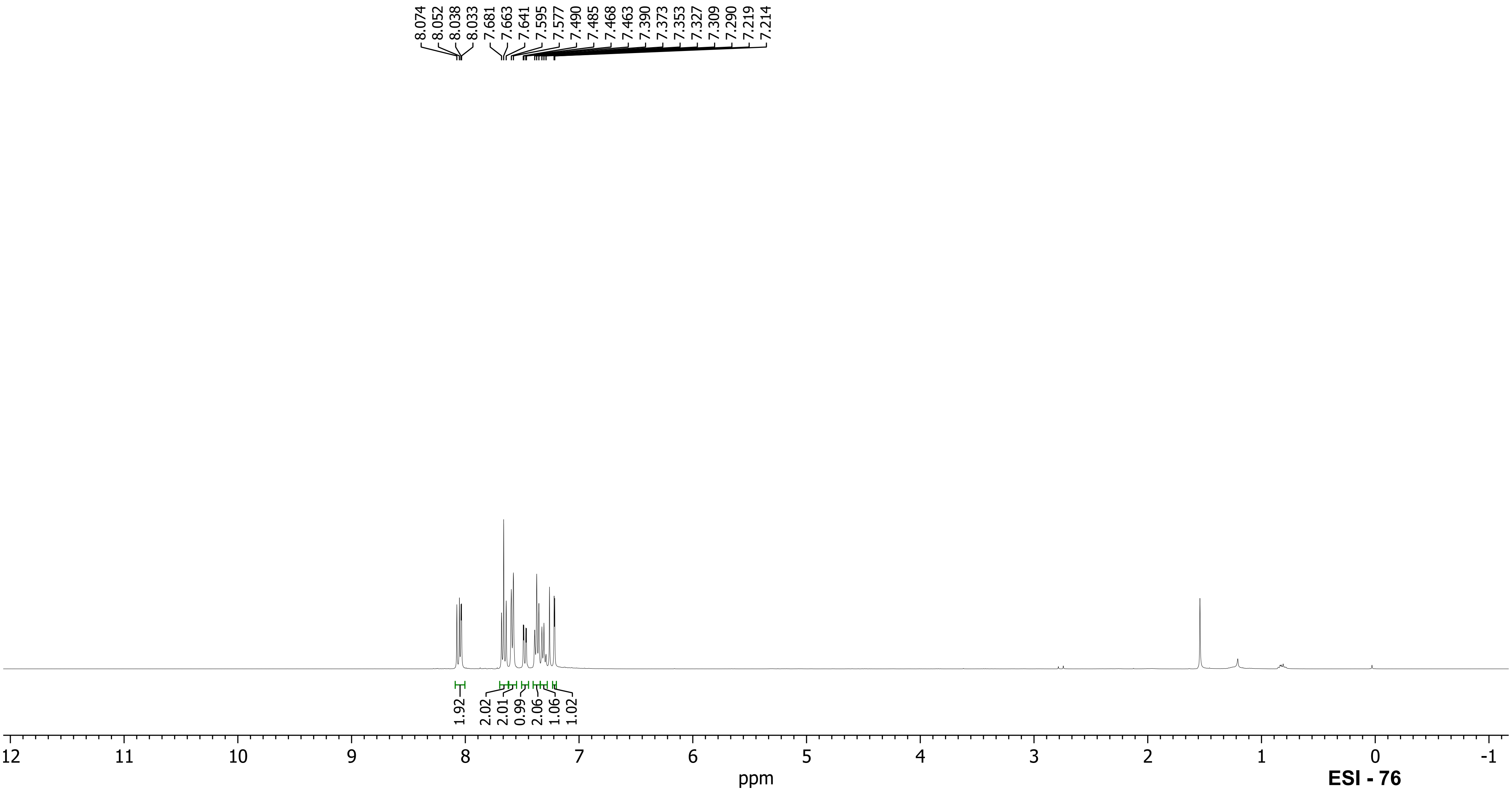
(E)-4-(2-(6-methoxyquinolin-2-yl)vinyl)phenyl acetate (6g)



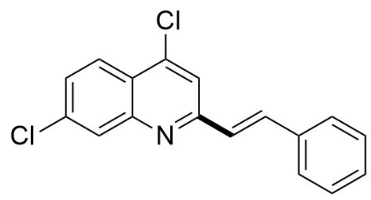


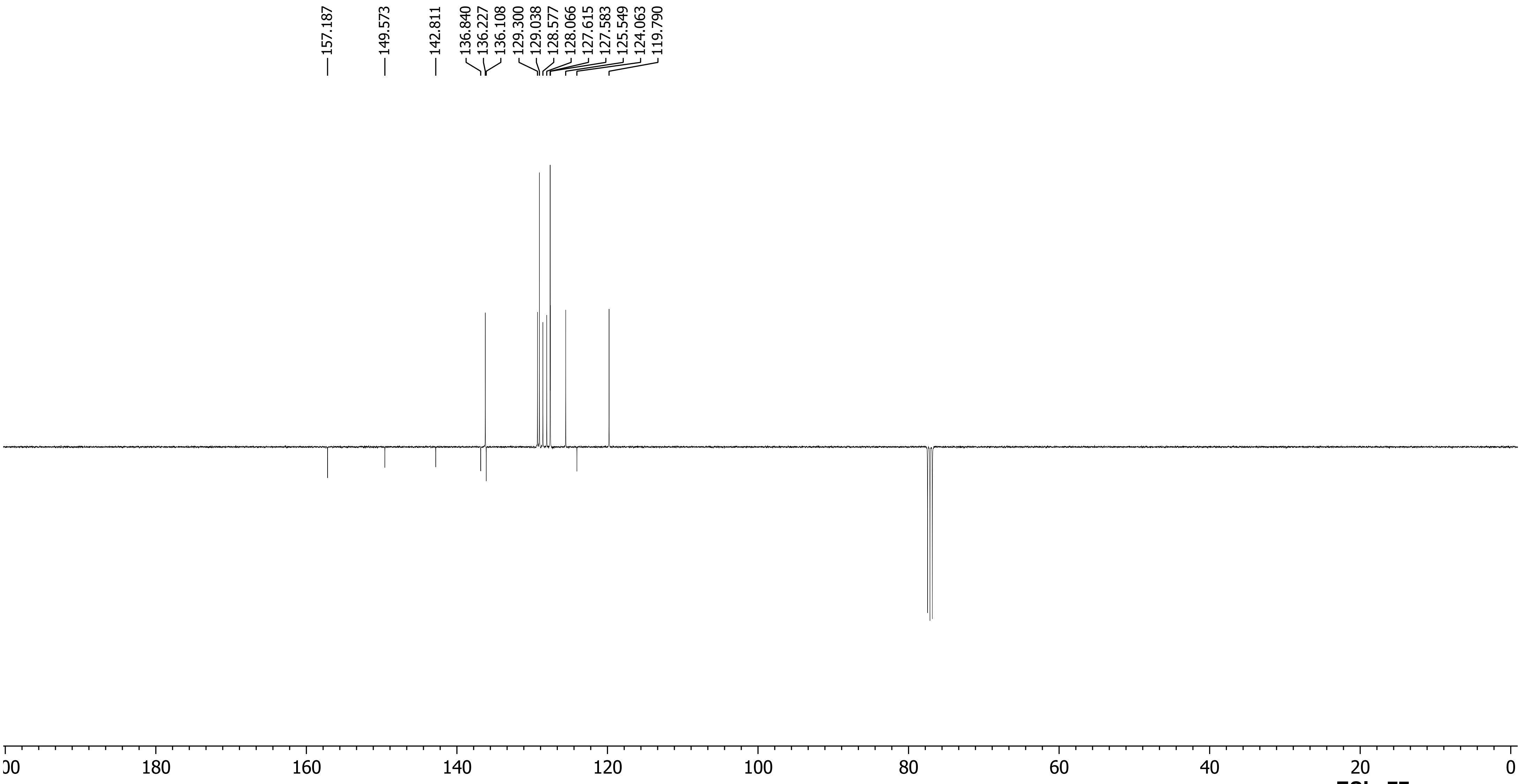
(E)-4,7-dichloro-2-styrylquinoline (6h)



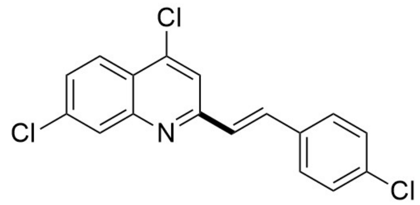


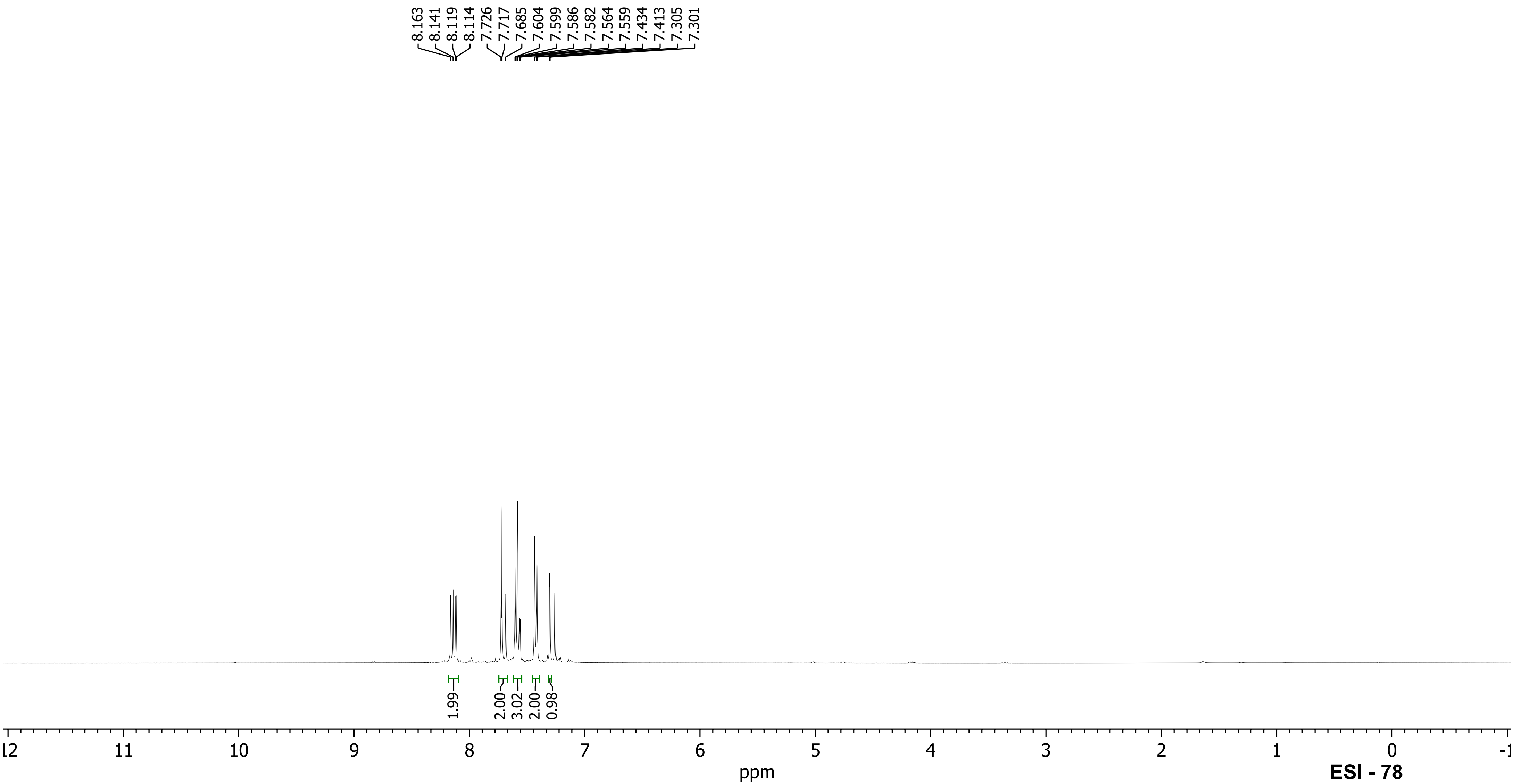
(E)-4,7-dichloro-2-styrylquinoline (6h)



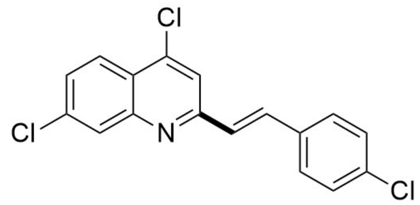


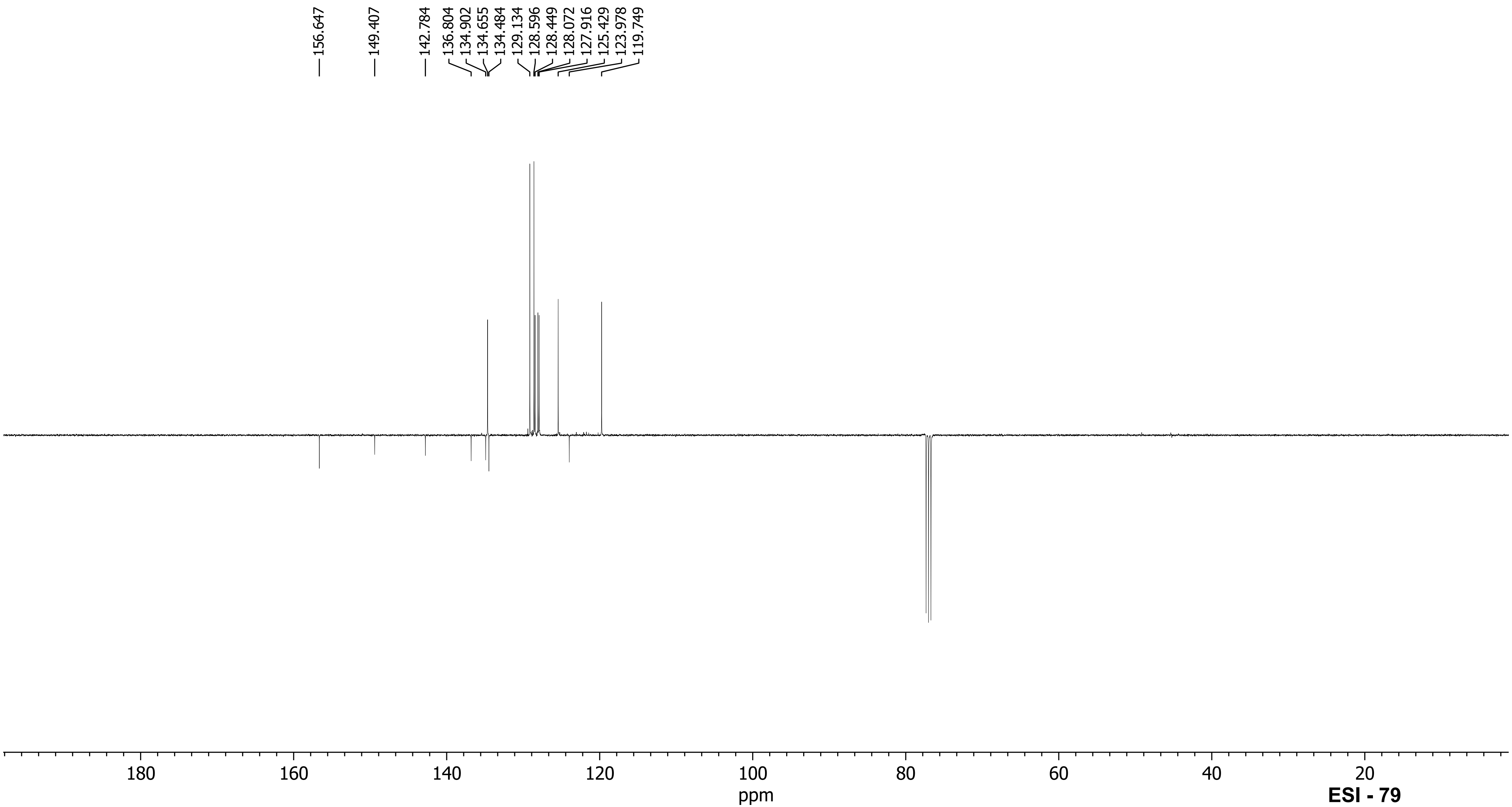
(E)-4,7-dichloro-2-(4-chlorostyryl)quinoline (6i)



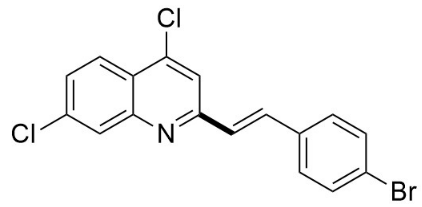


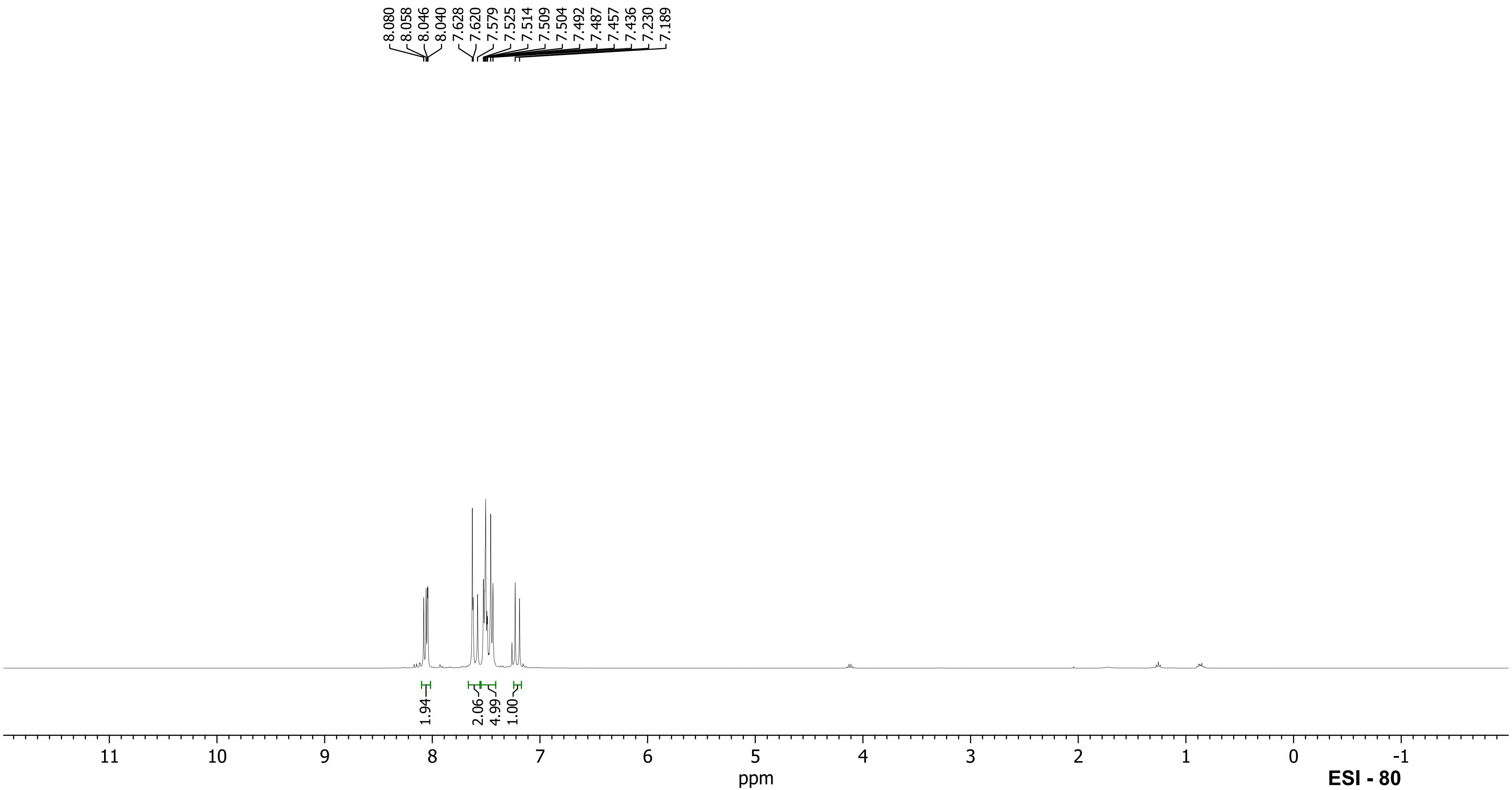
(E)-4,7-dichloro-2-(4-chlorostyryl)quinoline (6i)



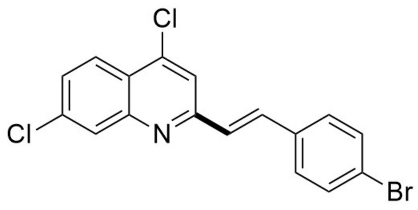


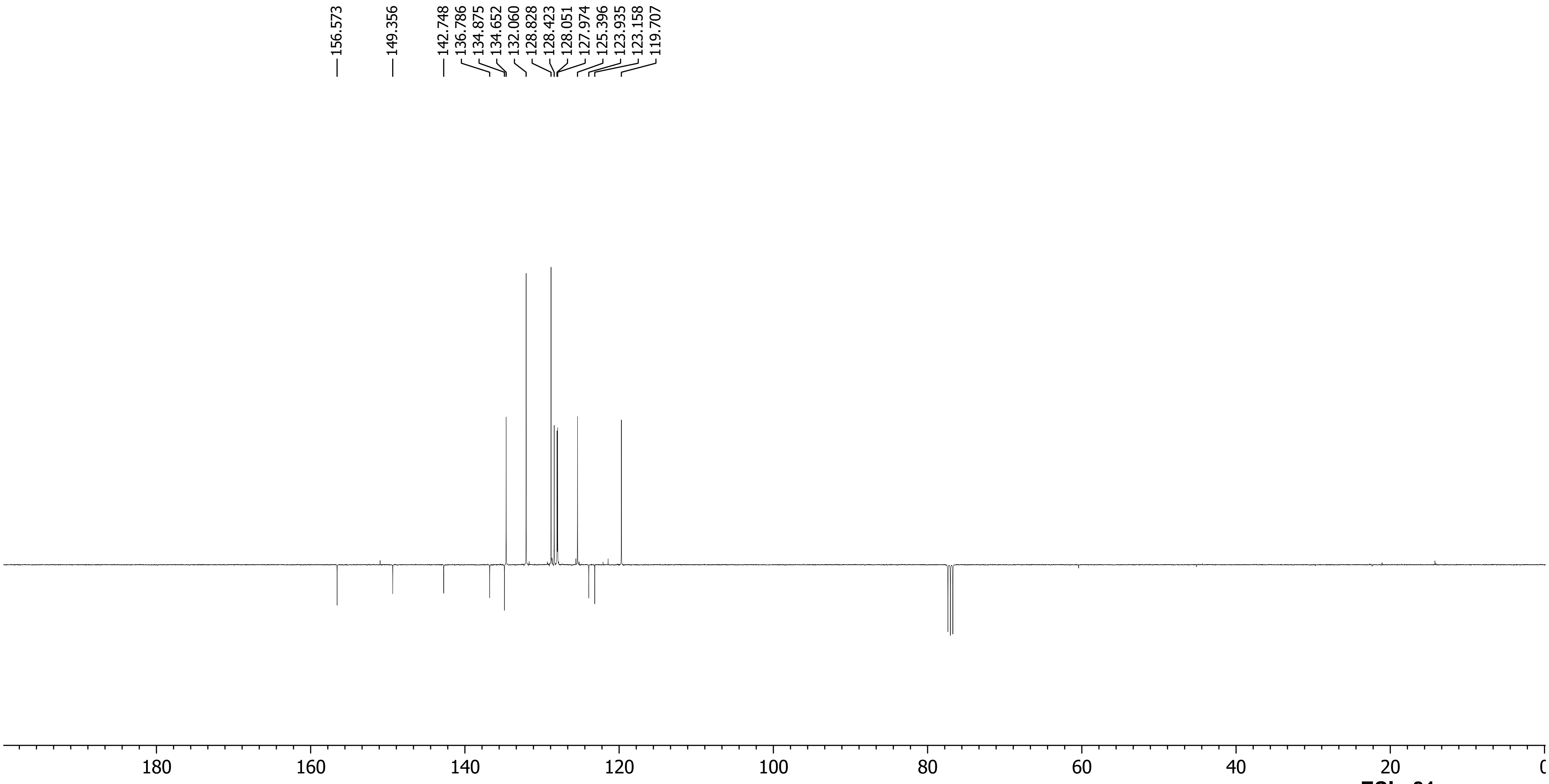
(E)-2-(4-bromostyryl)-4,7-dichloroquinoline (6j)



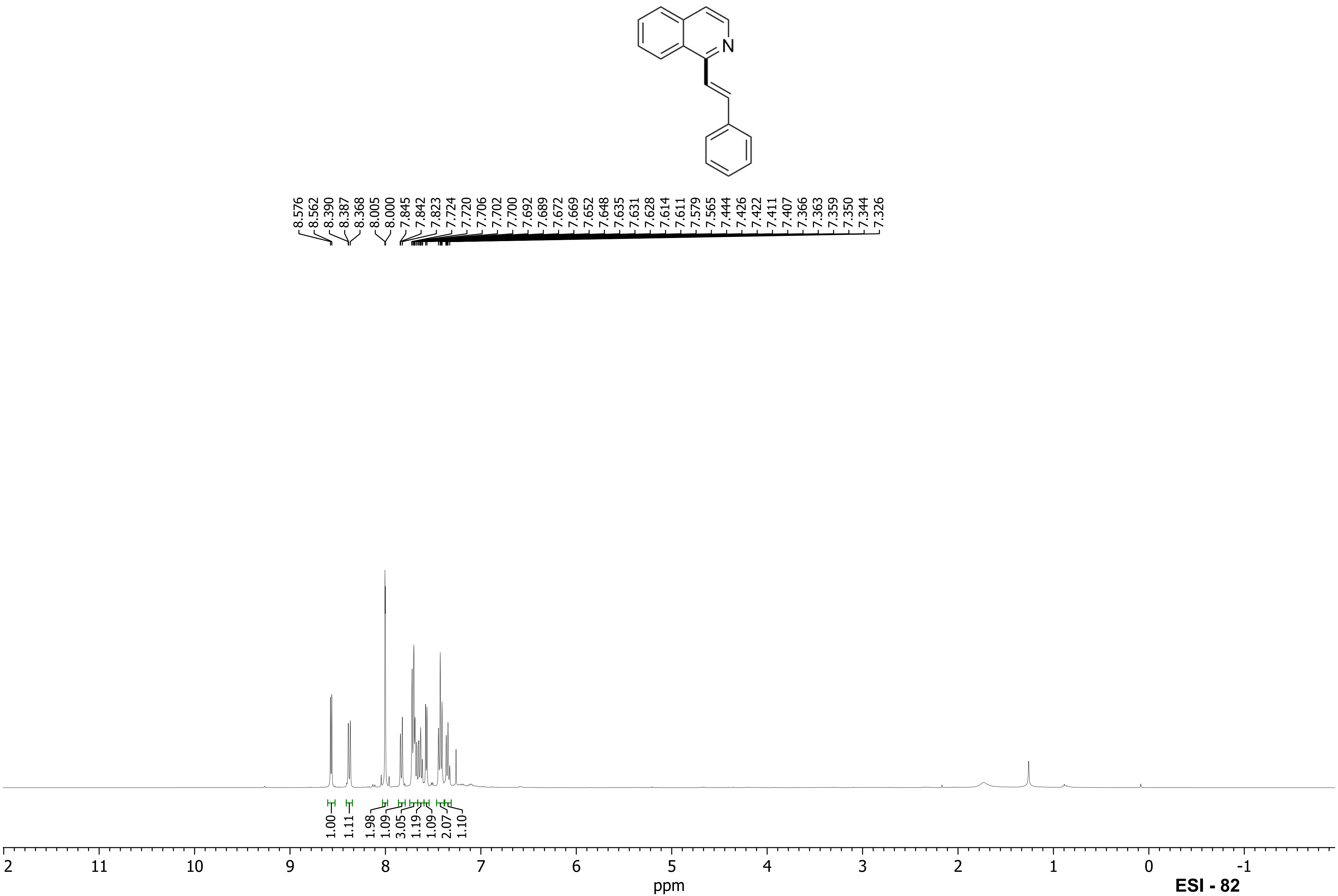


(E)-2-(4-bromostyryl)-4,7-dichloroquinoline (6j)

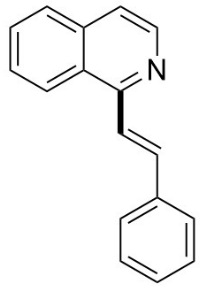


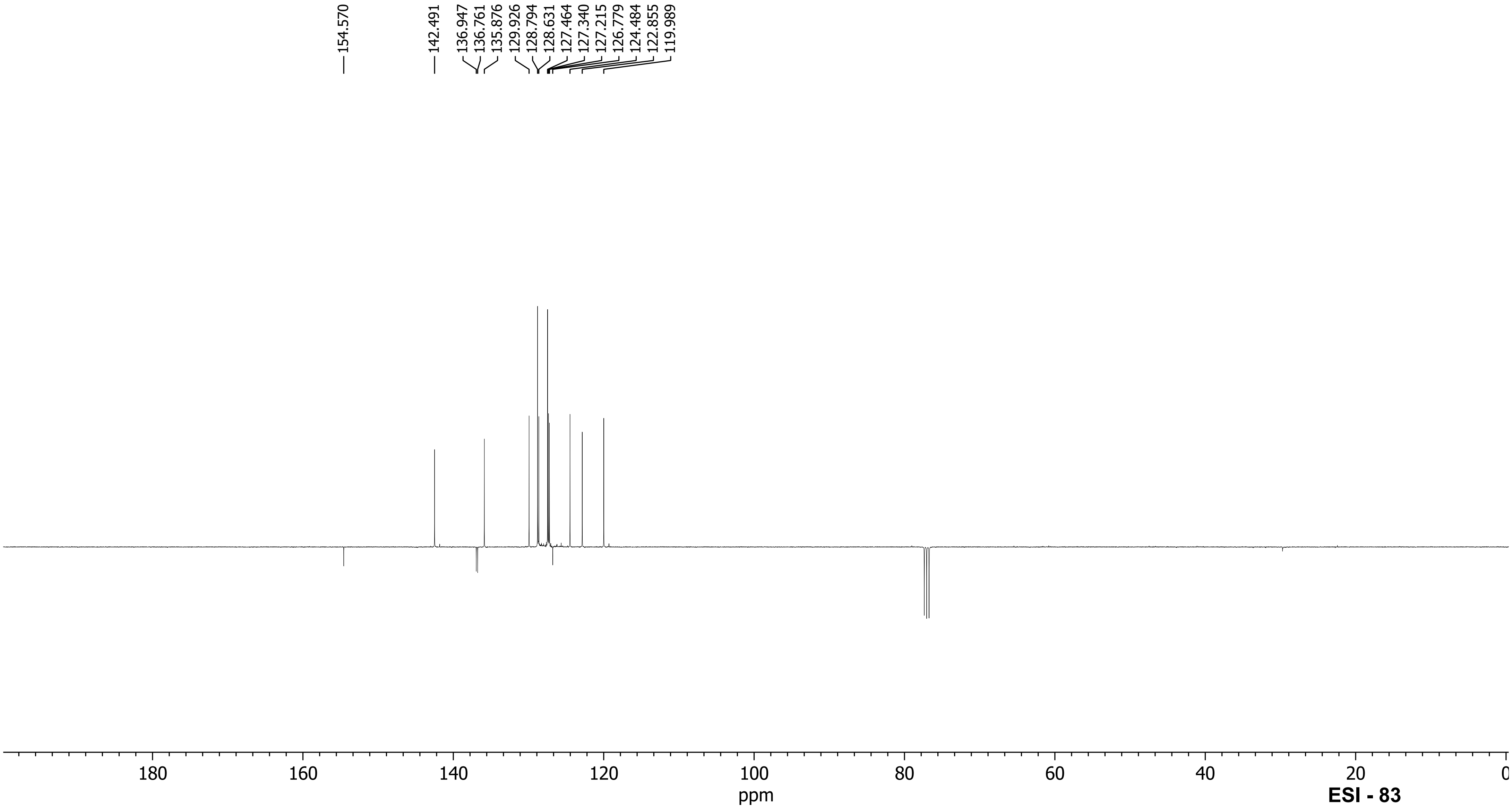


(E)-1-styrylisoquinoline (6k)

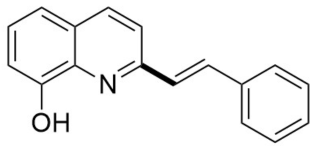


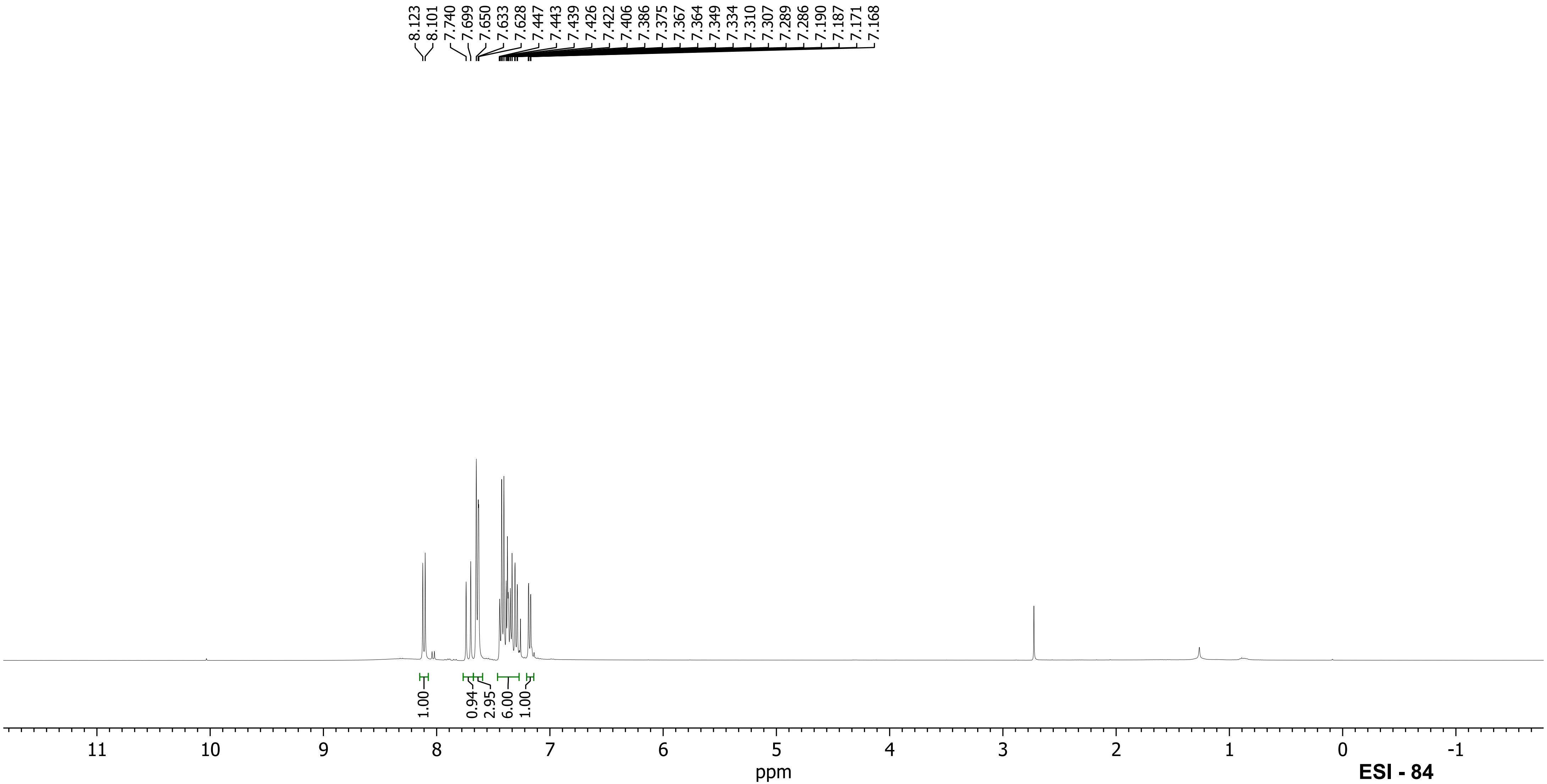
(E)-1-styrylisoquinoline (6k)



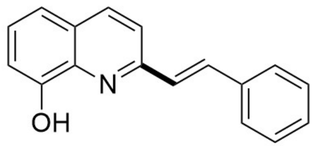


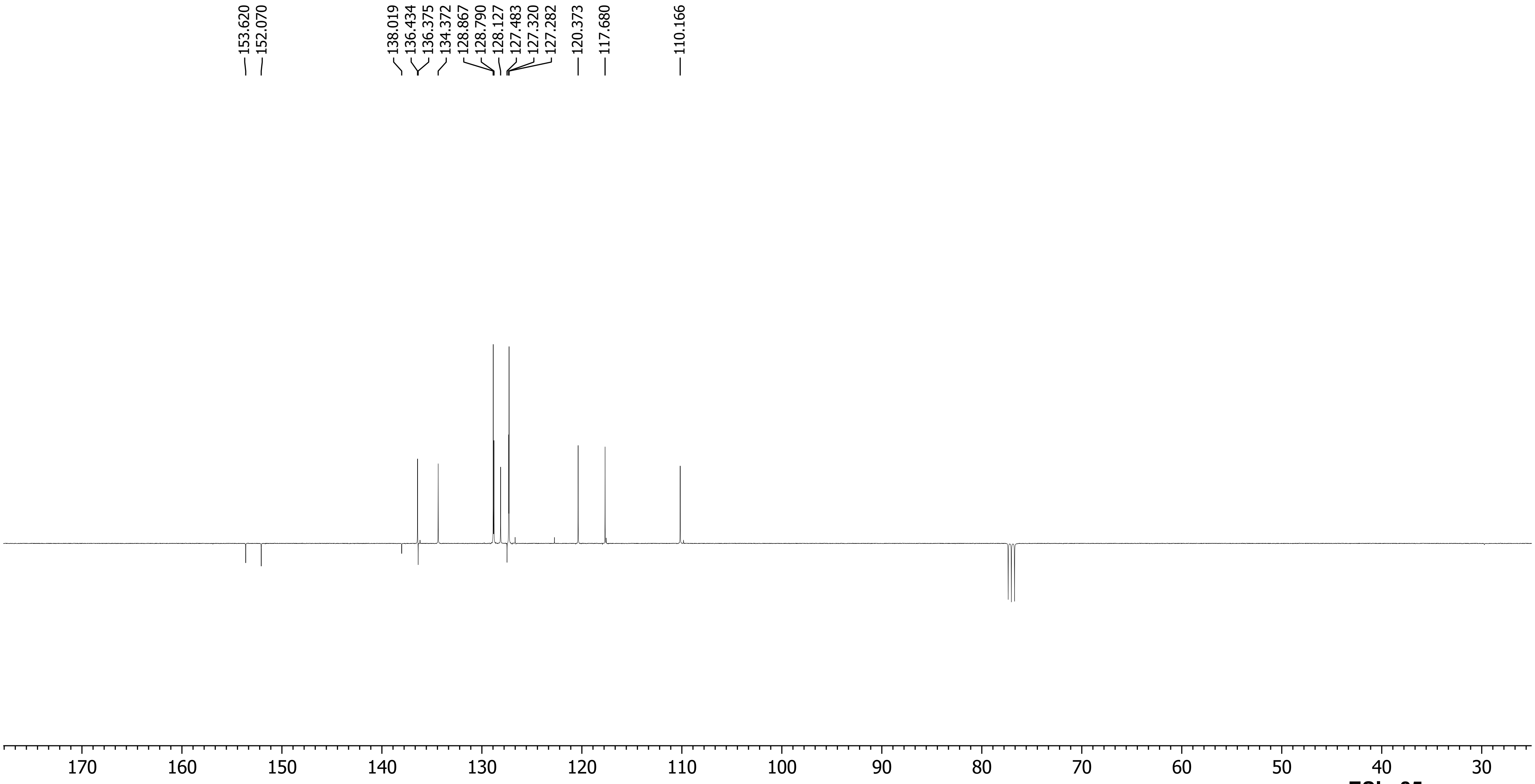
(E)-2-styrylquinolin-8-ol (6l)



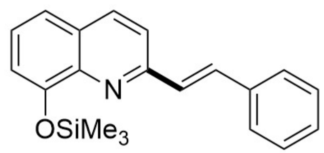


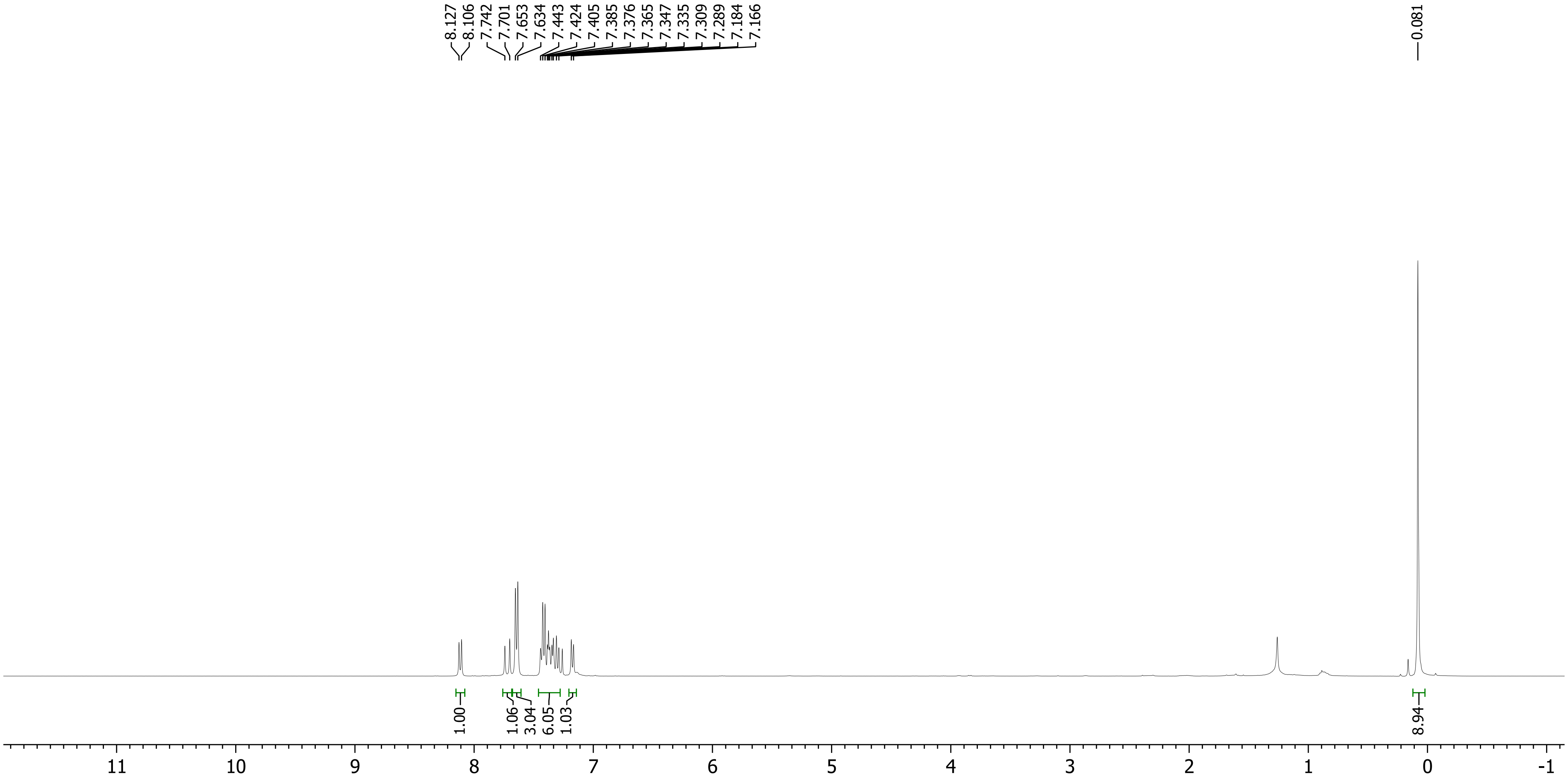
(E)-2-styrylquinolin-8-ol (6l)



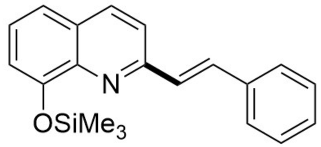


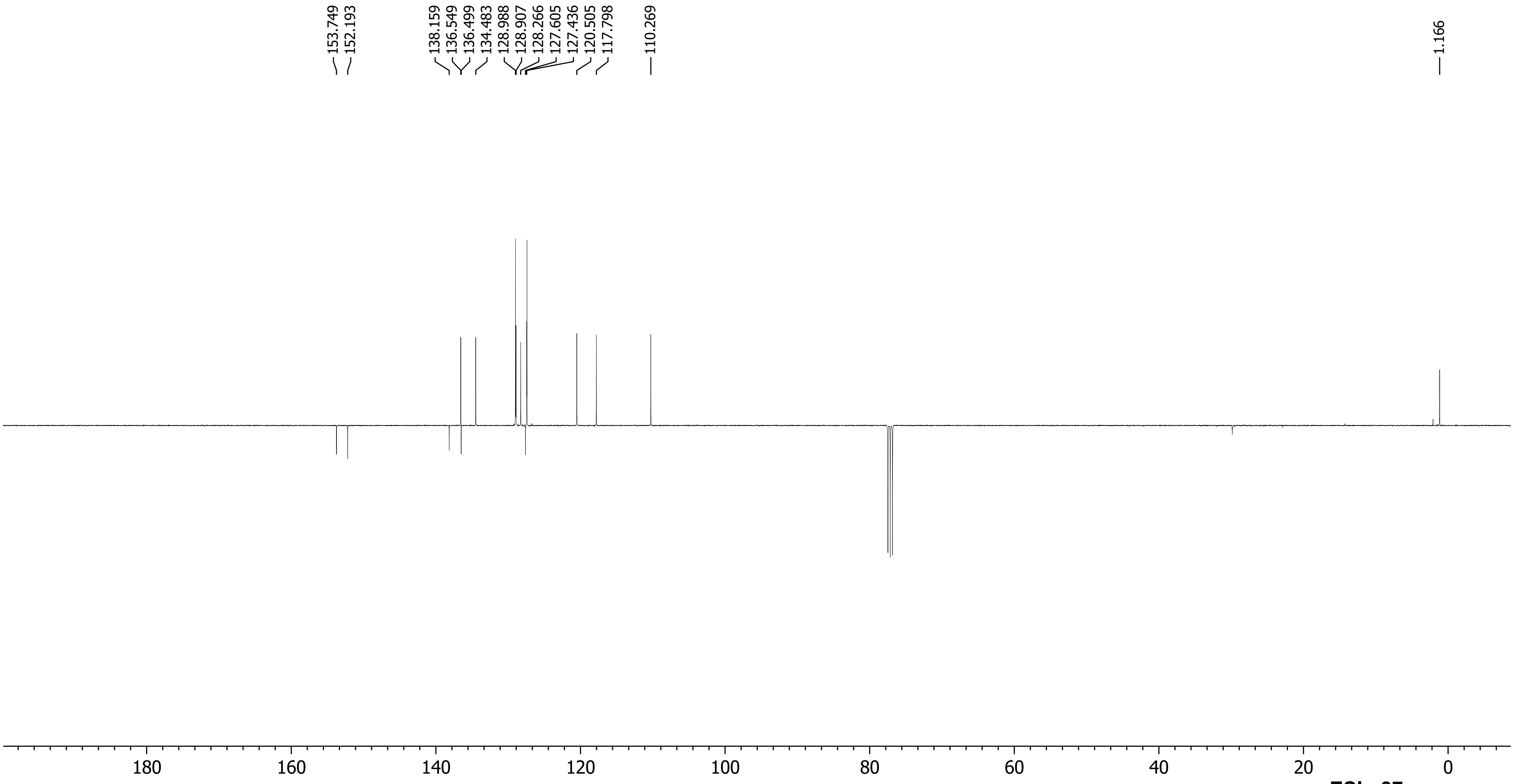
(E)-2-styryl-8-((trimethylsilyl)oxy)quinoline (6m)



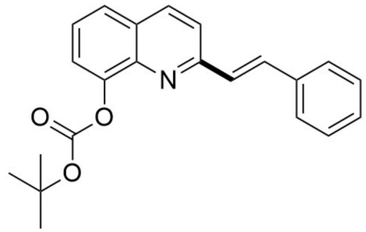


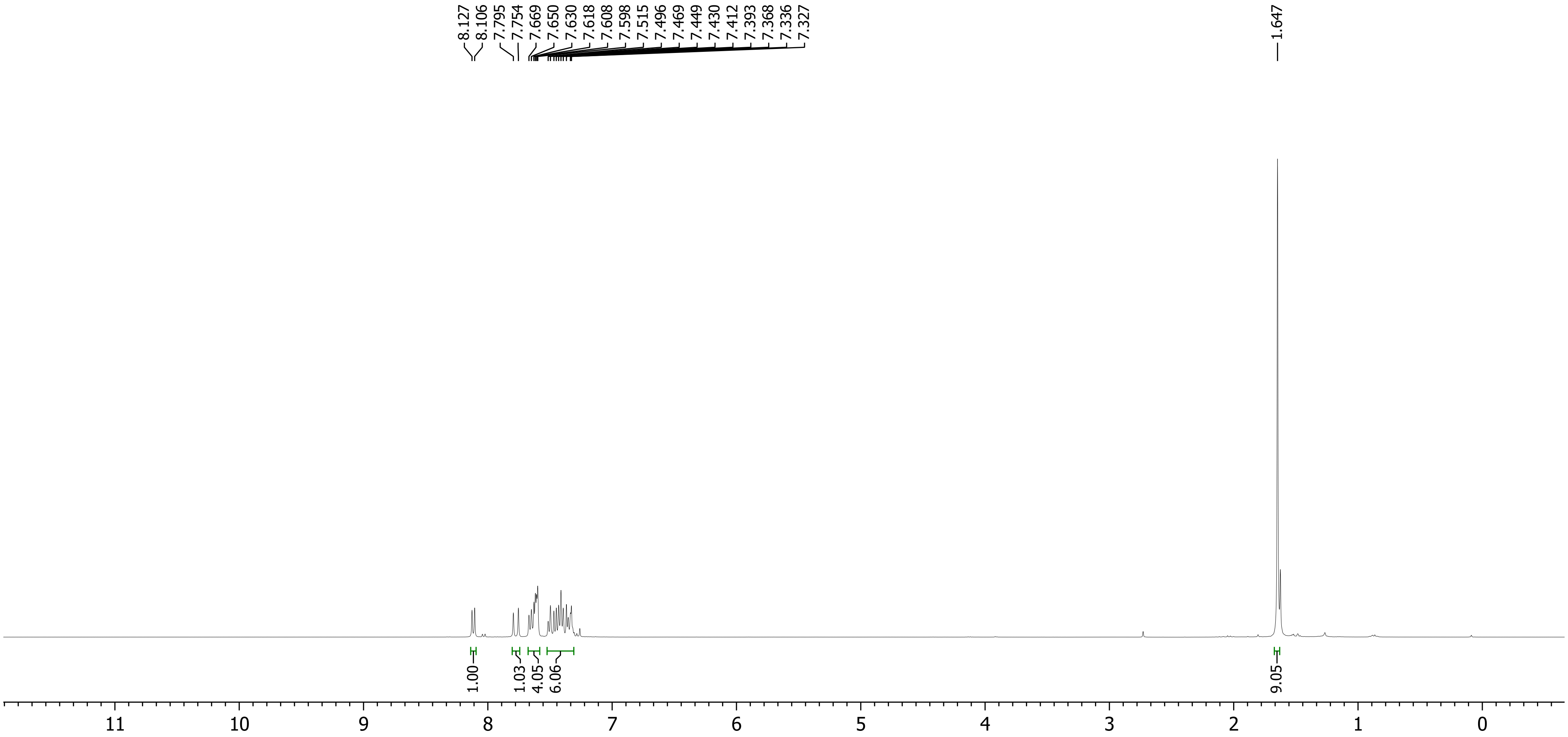
(E)-2-styryl-8-((trimethylsilyl)oxy)quinoline (6m)



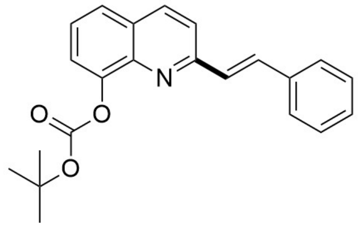


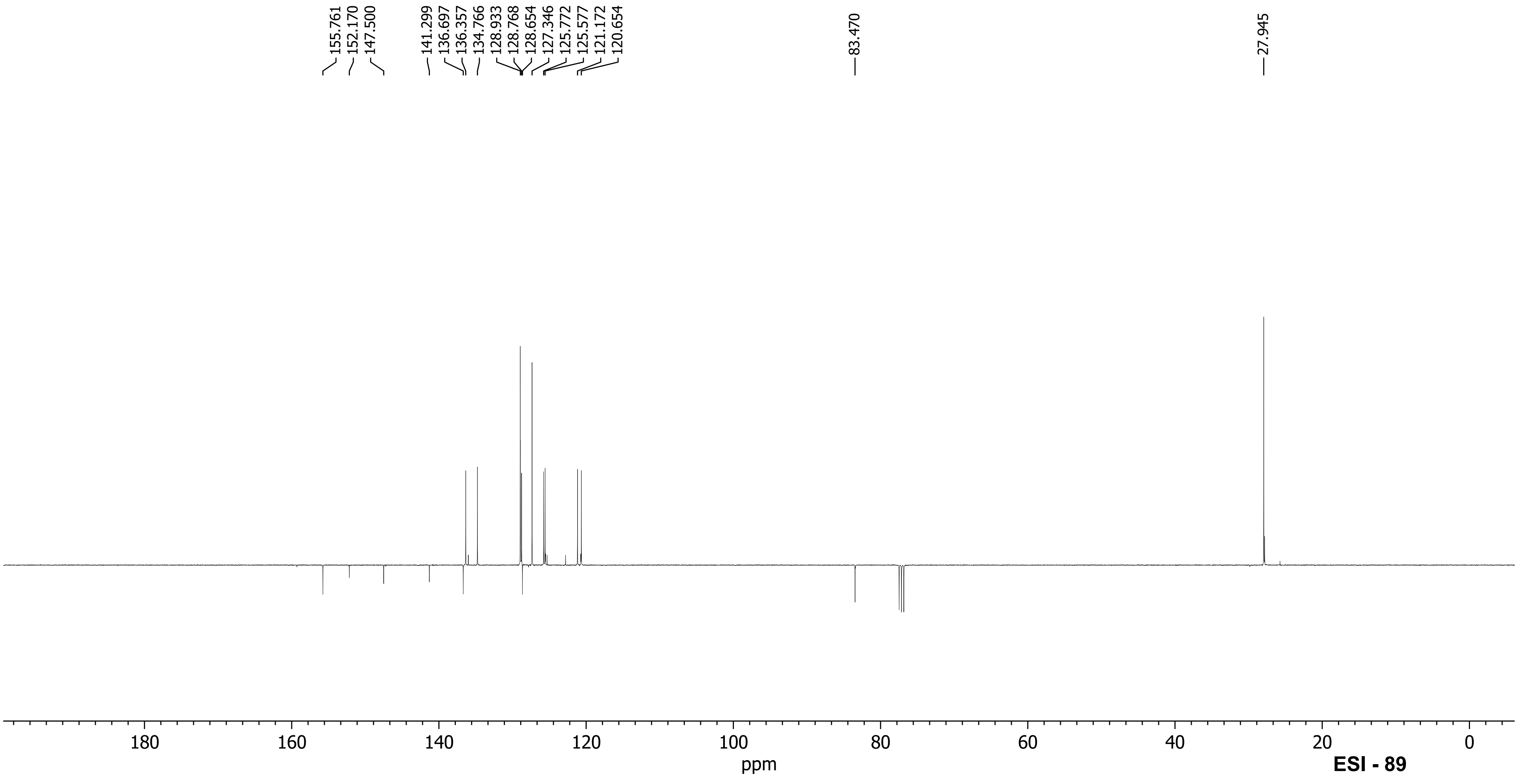
(E)-tert-butyl (2-styrylquinolin-8-yl) carbonate (6n)



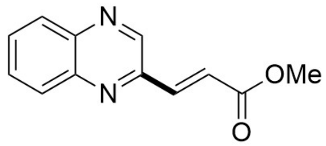


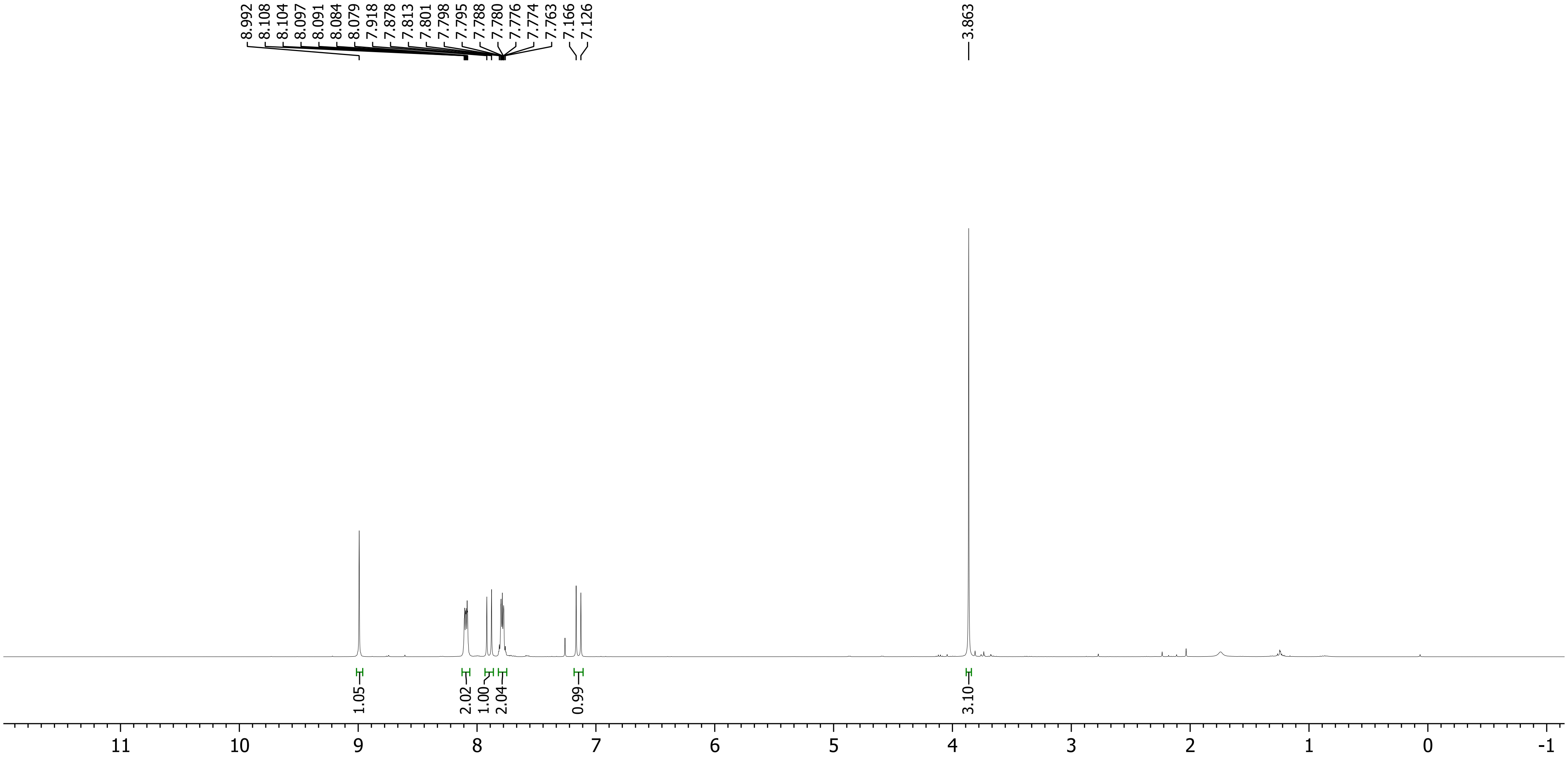
(E)-tert-butyl (2-styrylquinolin-8-yl) carbonate (6n)



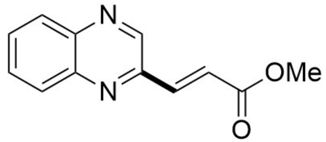


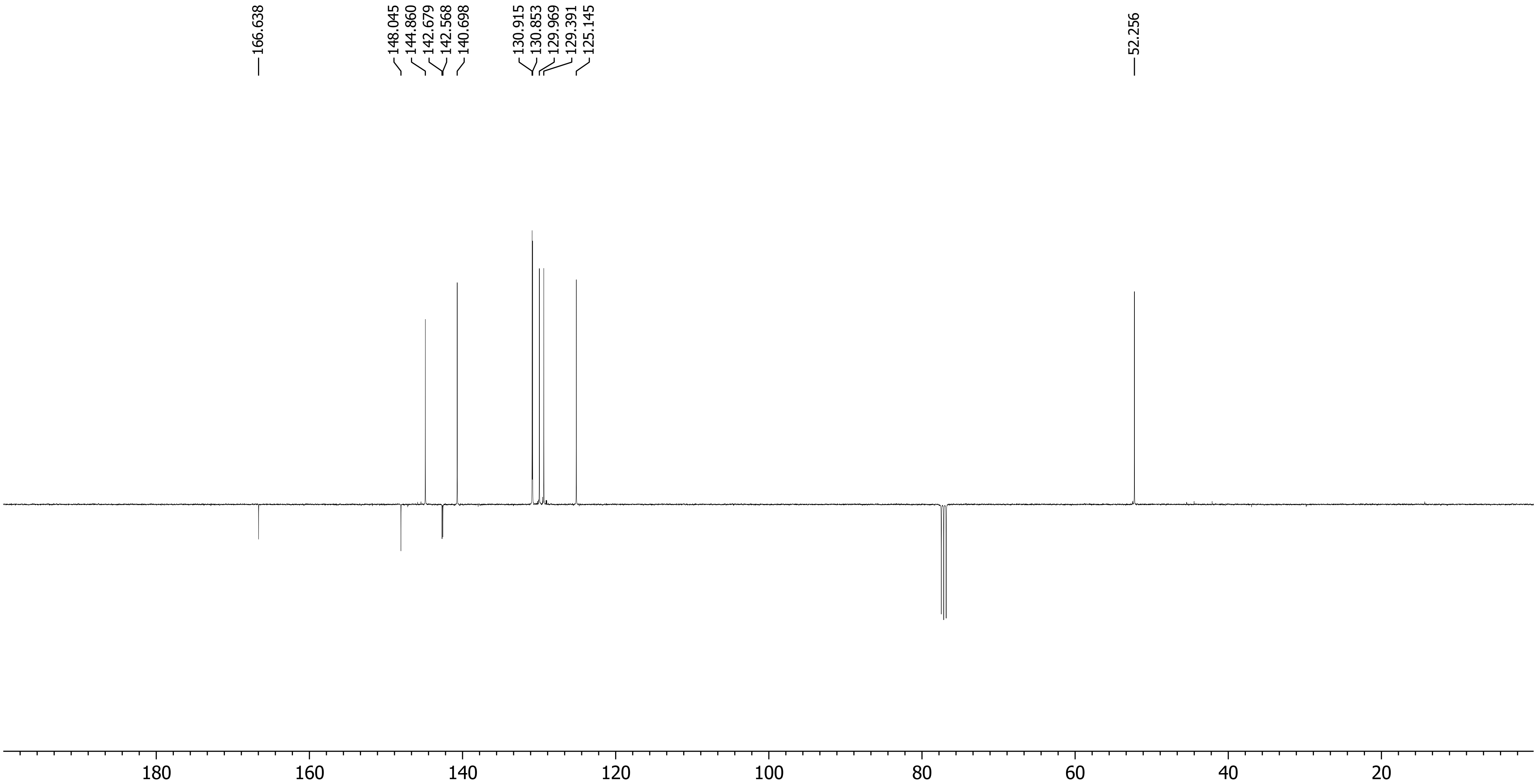
Methyl (E)-3-(quinoxalin-2-yl)acrylate (8a)



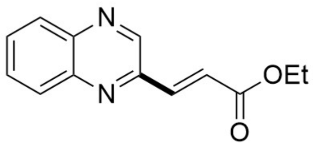


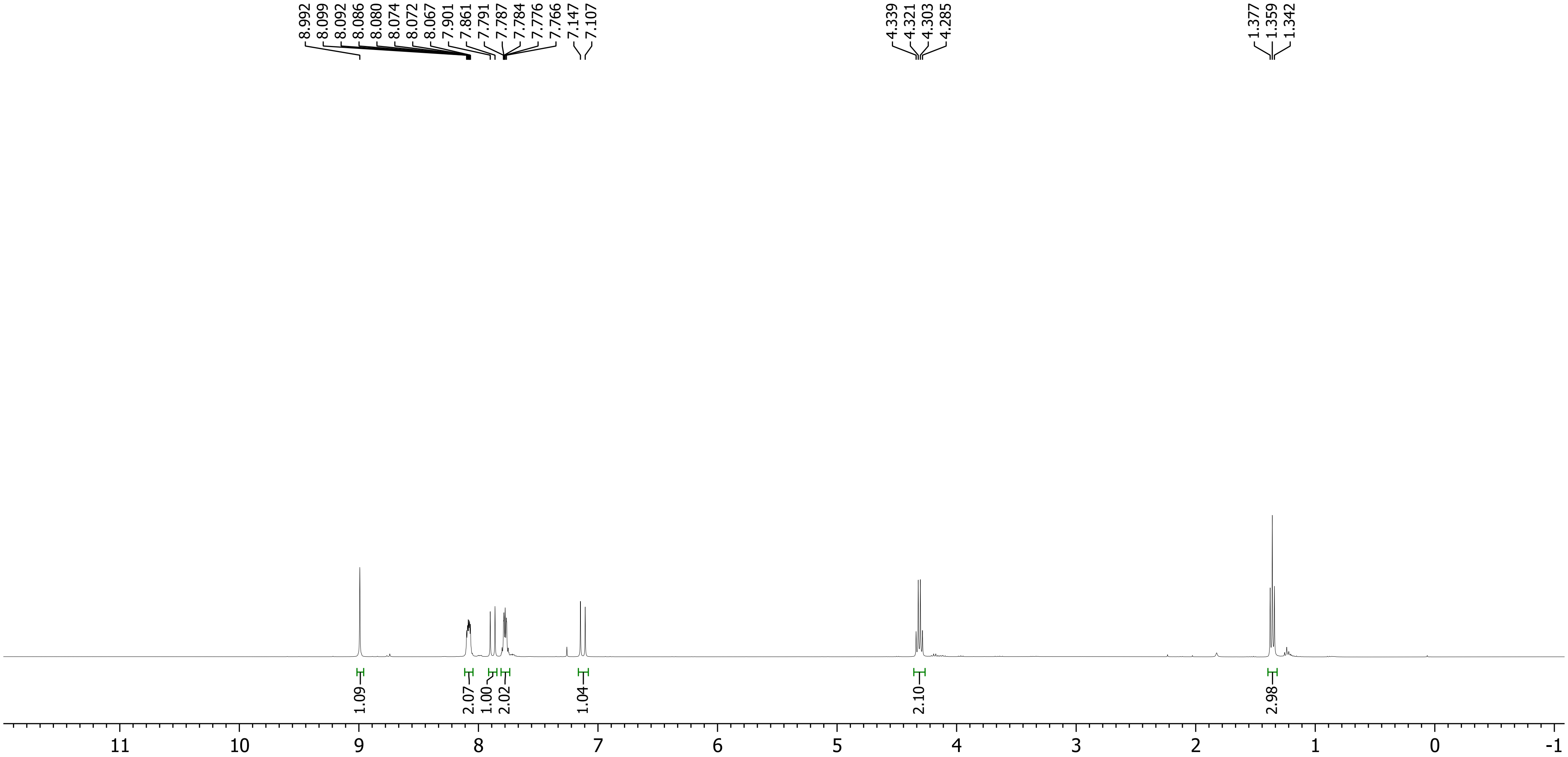
Methyl (E)-3-(quinoxalin-2-yl)acrylate (8a)



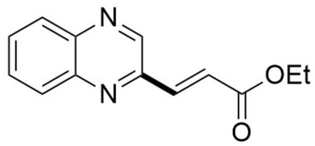


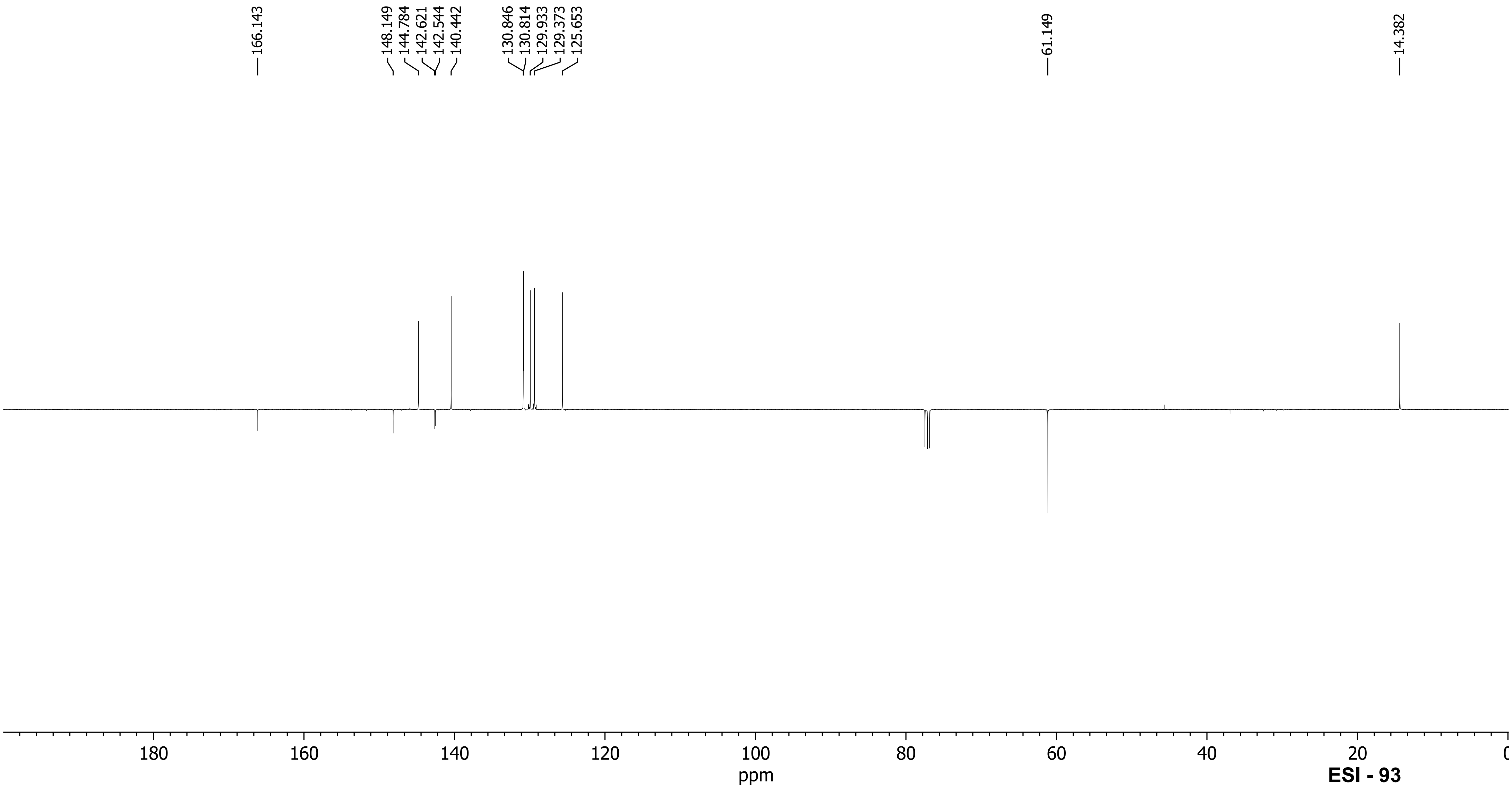
Ethyl (E)-3-(quinoxalin-2-yl)acrylate (8b)



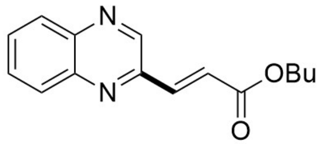


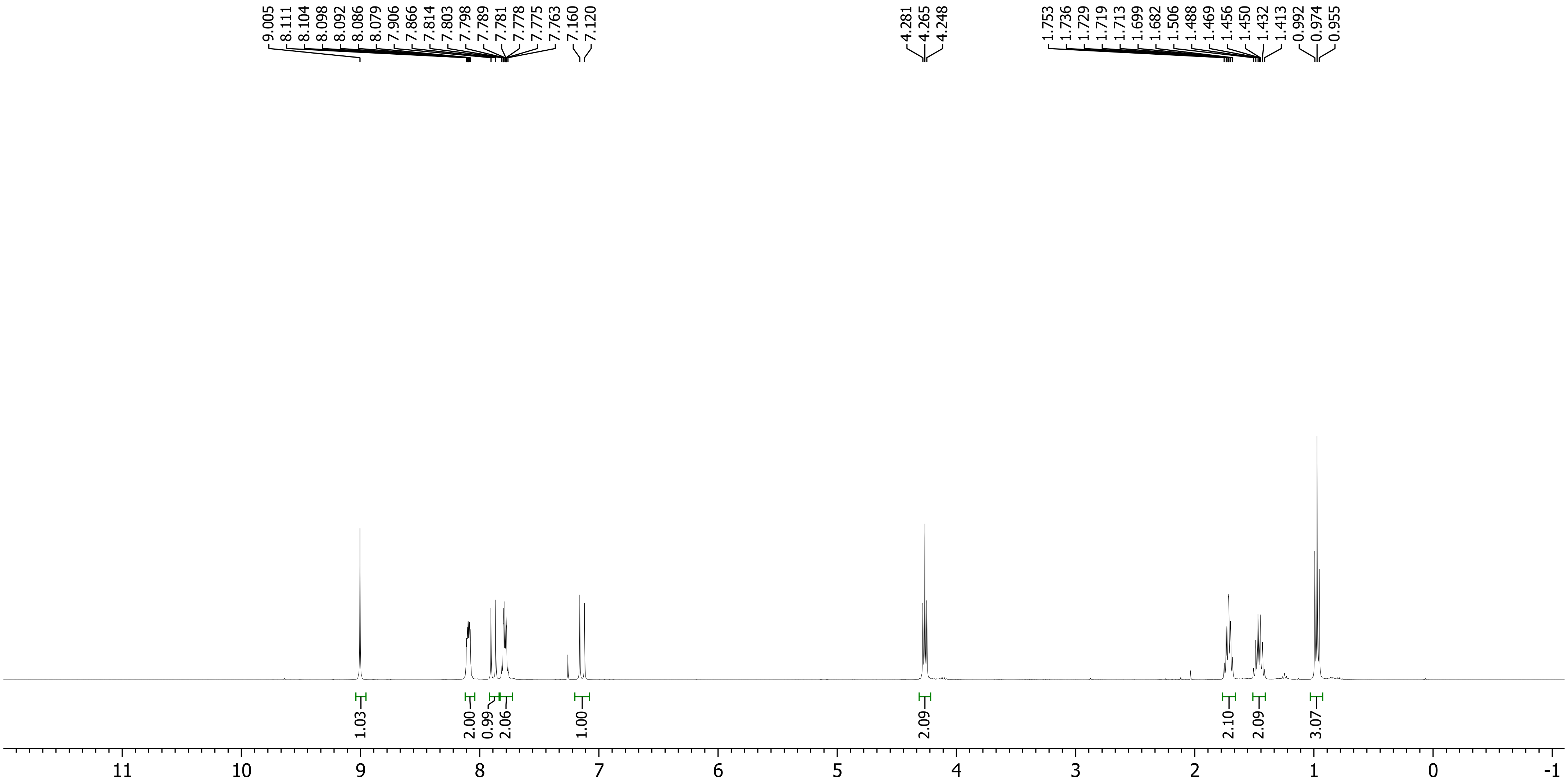
Ethyl (E)-3-(quinoxalin-2-yl)acrylate (8b)



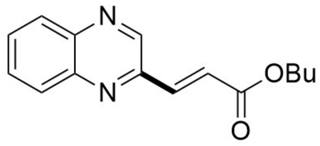


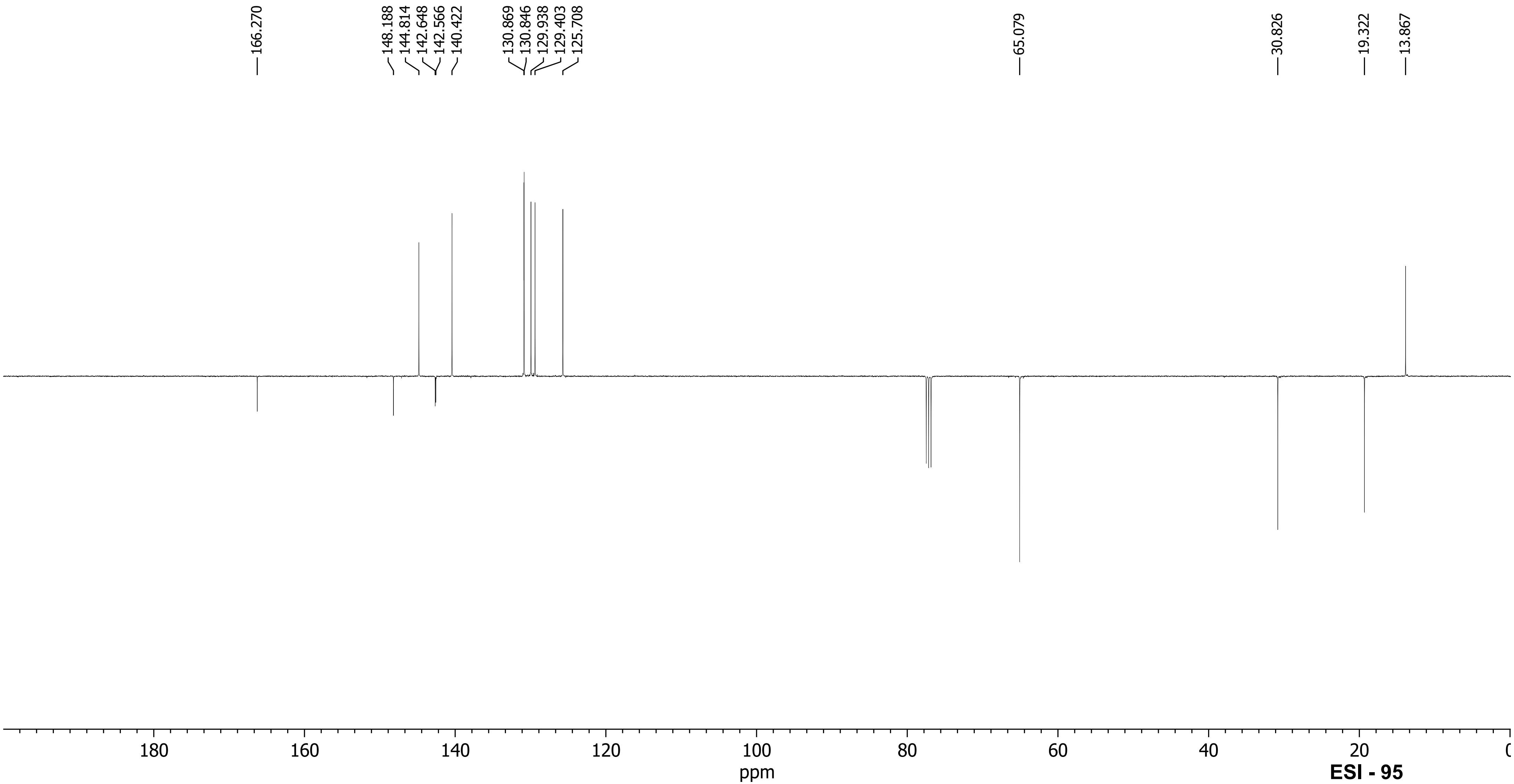
Butyl (E)-3-(quinoxalin-2-yl)acrylate (8c)



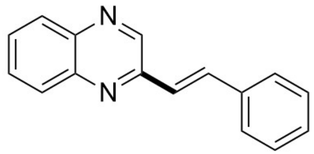


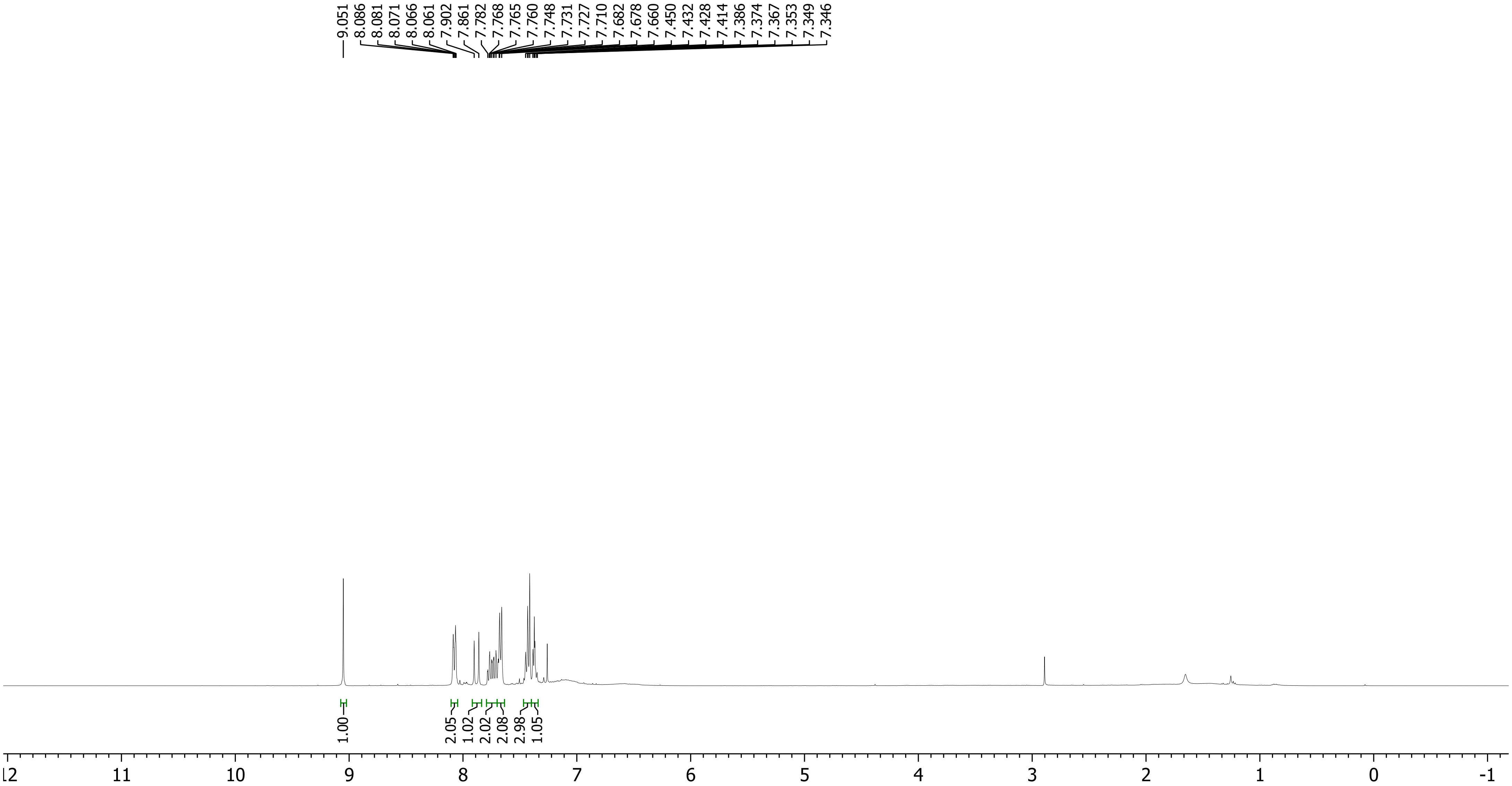
Butyl (E)-3-(quinoxalin-2-yl)acrylate (8c)



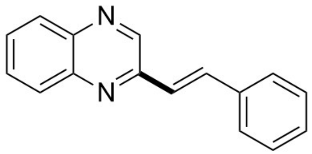


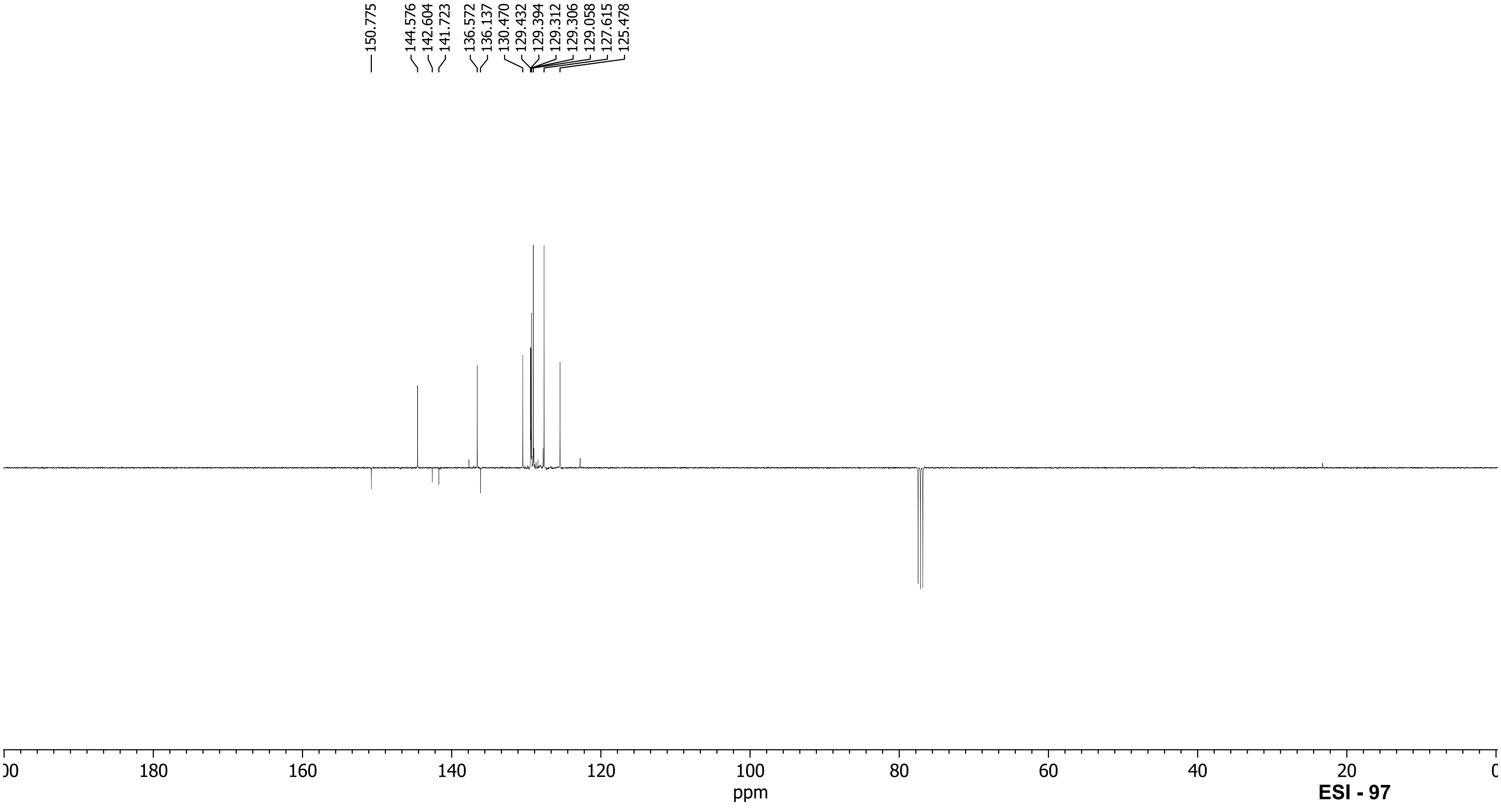
(E)-2-styrylquinoxaline (8d)



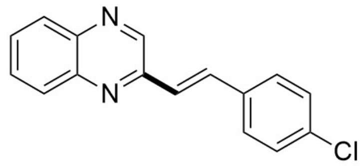


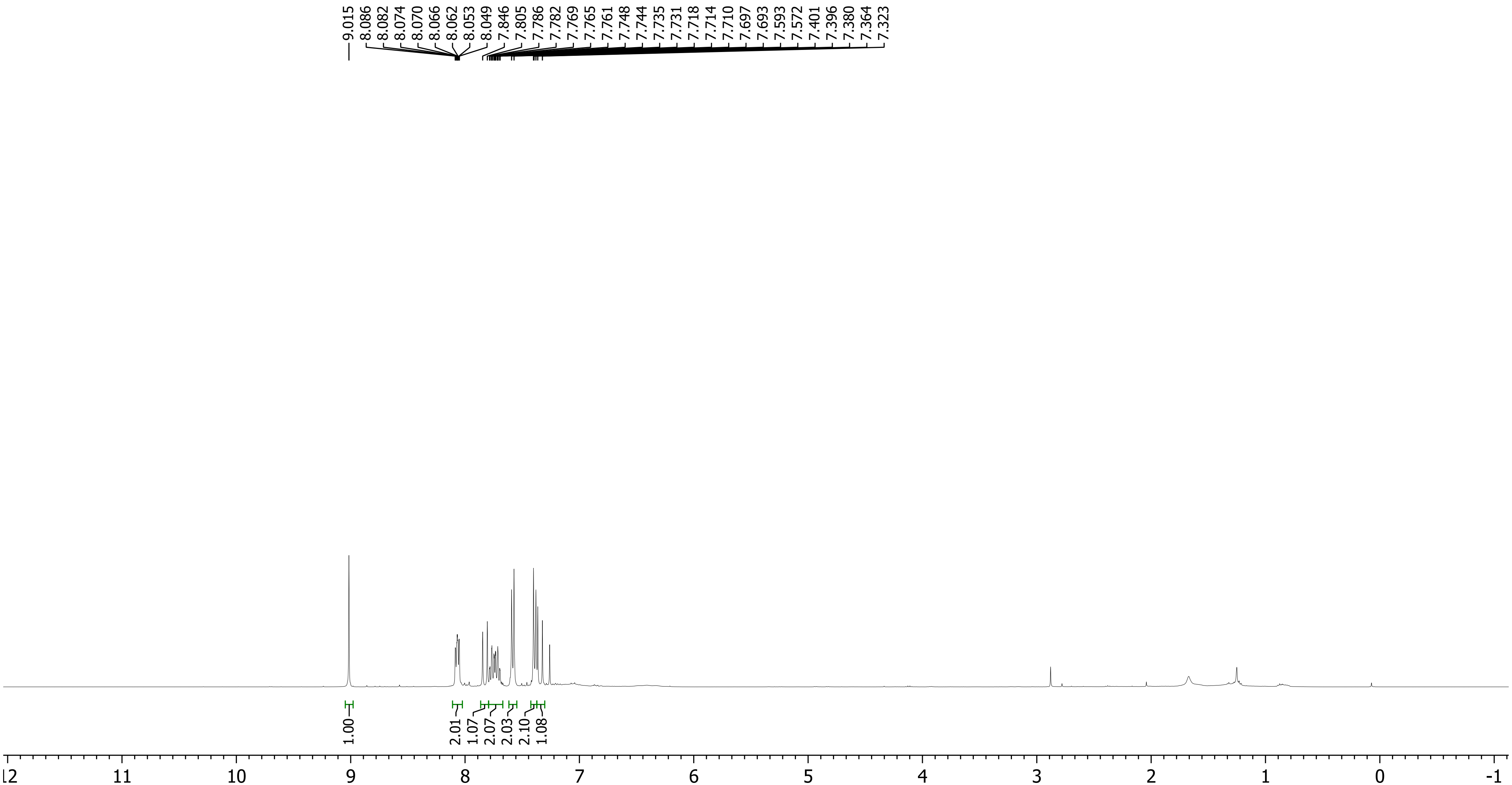
(E)-2-styrylquinoxaline (8d)



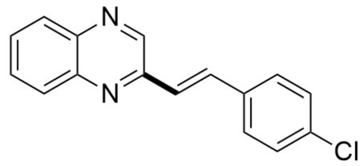


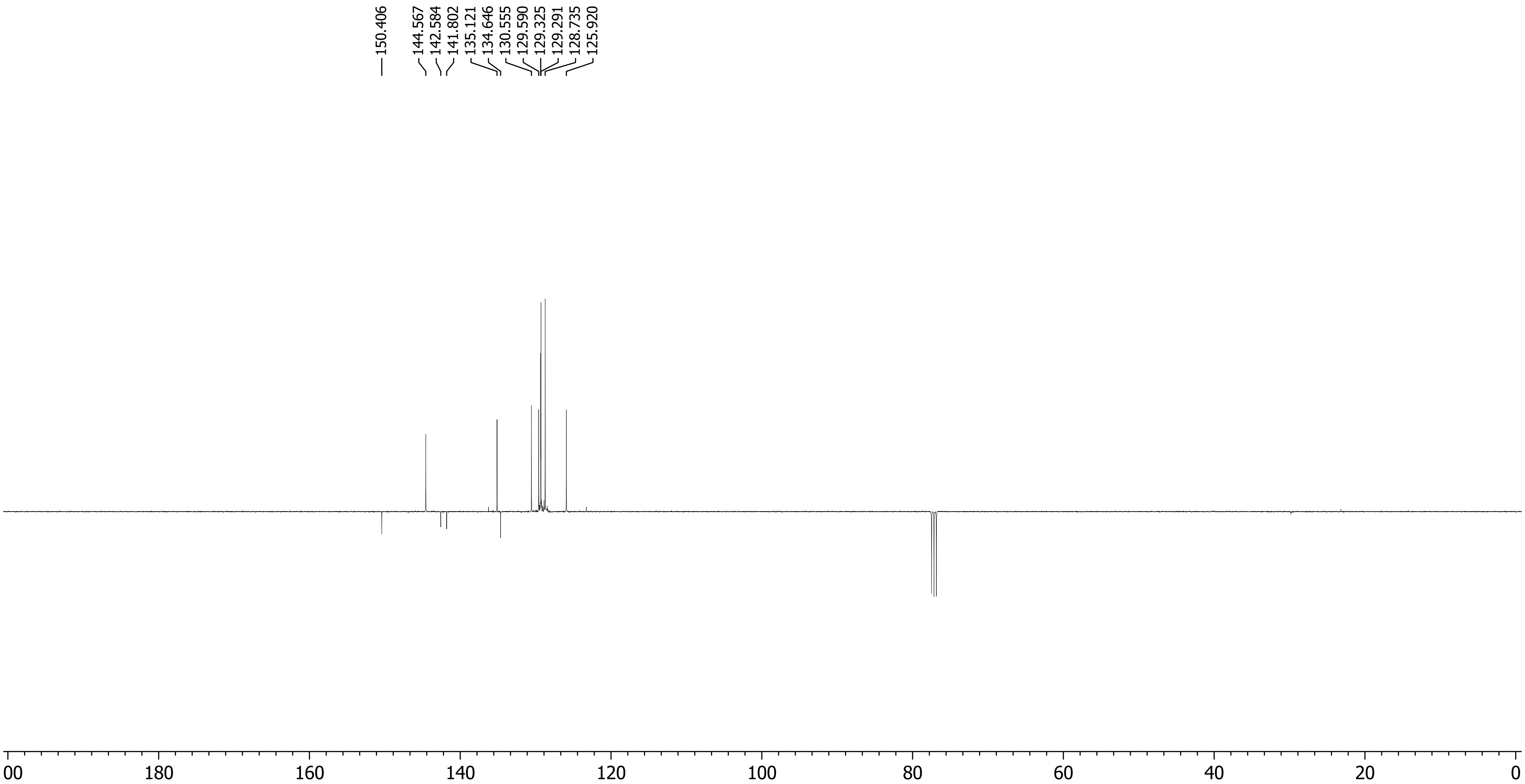
(E)-2-(4-chlorostyryl)quinoxaline (8e)



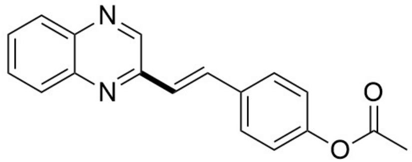


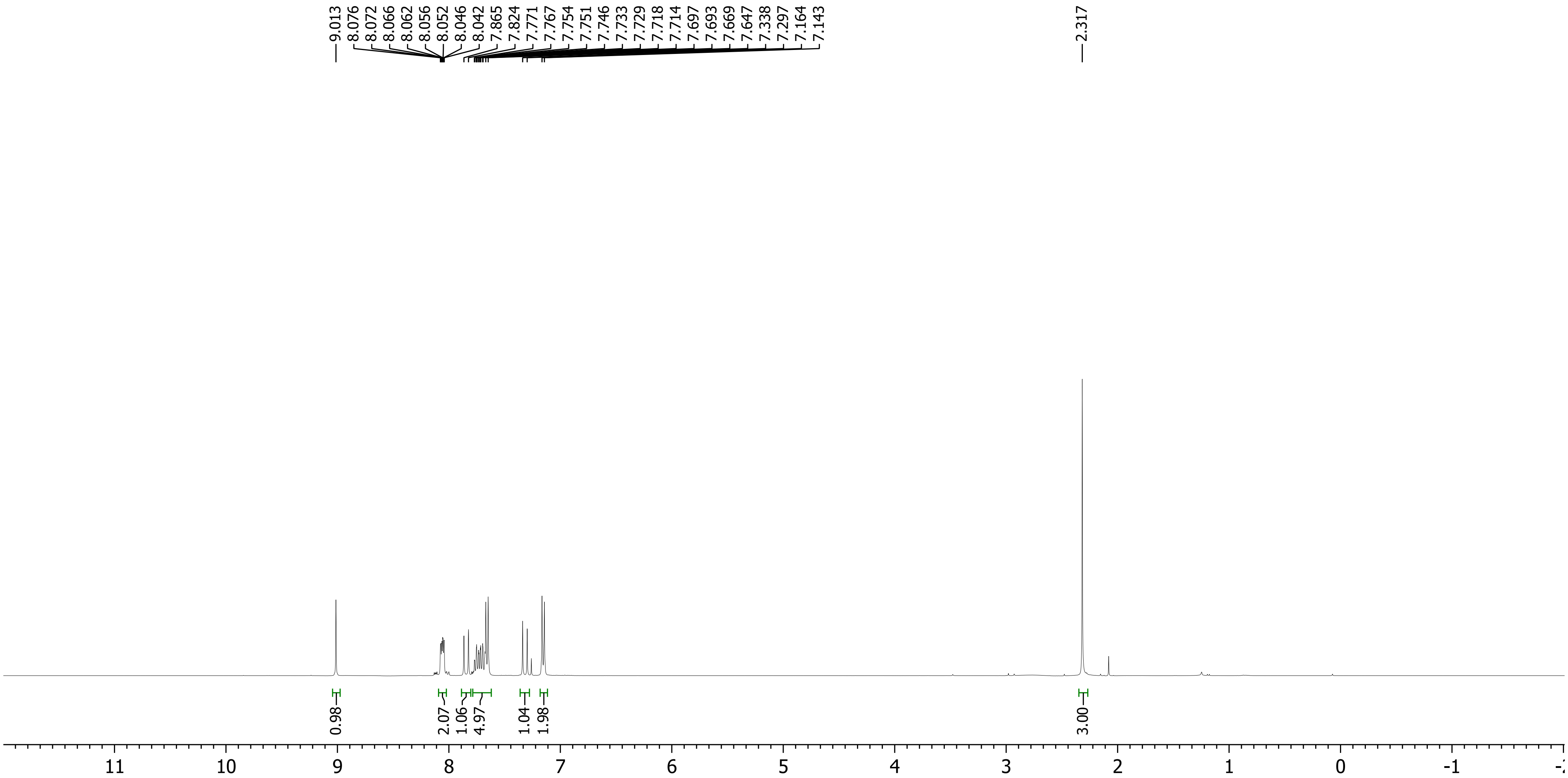
(E)-2-(4-chlorostyryl)quinoxaline (8e)





(E)-4-(2-(quinoxalin-2-yl)vinyl)phenyl acetate (8f)





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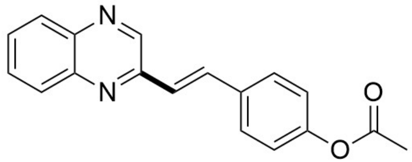
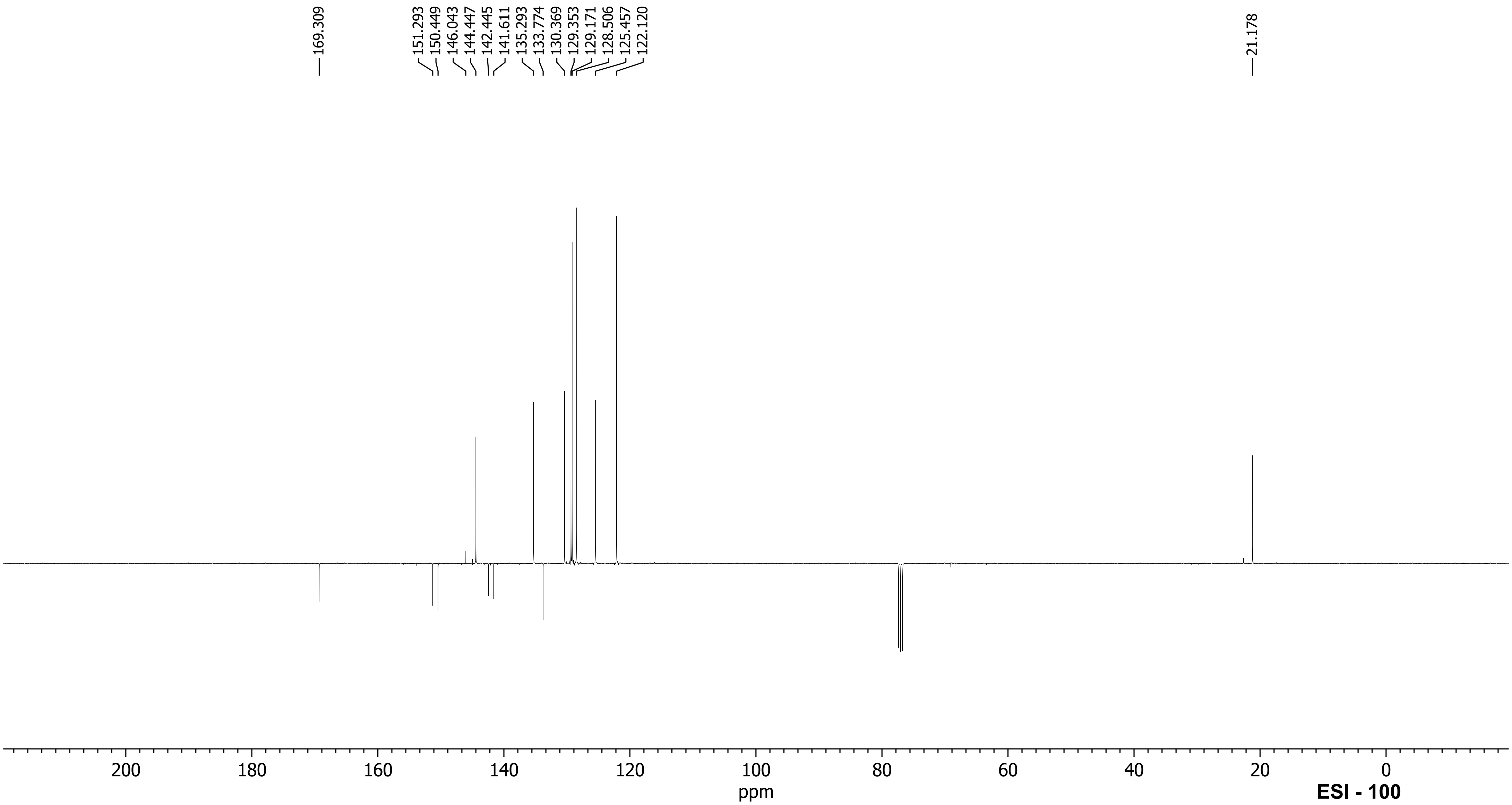
(E)-4-(2-(quinoxalin-2-yl)vinyl)phenyl acetate (8f)





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