Supporting Information

Thermal Azide-Alkene Cycloaddition Reactions: Straightforward Multi-gram Access to Δ^2-1,2,3-Triazolines in Deep Eutectic Solvents

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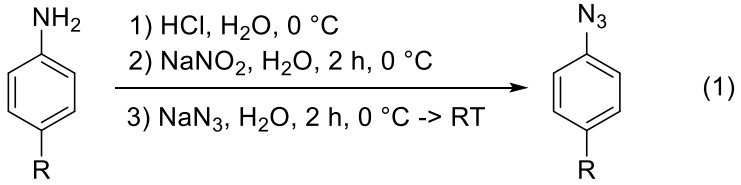
1. General Considerations

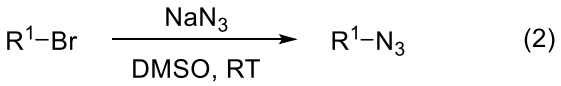
All chemicals were obtained from commercial sources and used without further purification. All Deep Eutectic Solvents in this work, including DES (choline chloride/urea = 1:2) were prepared following a reported procedure.[1] Column chromatography and TLC were performed on silica gel (Kieselgel 60), using UV light and $KMnO_4$, or vanillin dip to visualise the products. Basified silica was prepared by submerging silica gel into petroleum ether containing 2% v/v NEt_3 overnight.

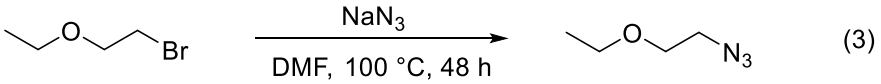
Melting points were determined on an Electrothermal Gallenhamp apparatus and are uncorrected. Infrared spectra were recorded using a Perkin Elmer 100 series FT-IR spectrometer, equipped with a beam-condensing accessory (samples were sandwiched between diamond compressor cells). NMR spectra were measured on Bruker AVANCE 400 spectrometers (^{1}H: 400 MHz, ^{13}C: 101 MHz, ^{19}F: 377 MHz) at 20 °C. The chemical shifts (δ) are given in ppm relatively to a tetramethylsilane or 1-fluorobenzene standard or the residual solvent signal. The multiplicity is given in br, s, d, t, q, sept, and m for broad, singlet, doublet, triplet, quartet, septet, and multiplet. Assignments of some ^{1}H and ^{13}C NMR signals rely on COSY, HSQC, HMBC and/or DEPT-135 experiments. Single crystal X-ray diffraction data was collected using Xcalibur PX Ultra A (**3aa**, **3dd** and **5du'**) and Agilent Xcalibur 3 E (**4aa**, **4dq** and **5du**) diffractometers, and the structures were refined using the SHELXTL[2] and SHELX-2013[3] program systems. Mass spectra (MS) were recorded on a Micromass Autospec Premier, Micromass LCT Premier or a VG Platform II spectrometer using EI, CI or ESI techniques at the Mass Spectrometry Service of Imperial College London. Elemental analyses were carried out by the Science Technical Support Unit at London Metropolitan University (UK).

2. Synthesis of Azides

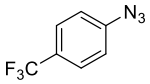
Aryl azides (Eq. 1)[4] were prepared following a modified literature procedure: The chosen aniline was added to HCl (1 mL per 1 mmol of aniline; 12 M) in water (1 mL per 1 mmol of aniline) at 0 °C. A solution of $NaNO_2$ (1.2 equiv) in water (1 mL per 1 mmol of aniline) was added portion-wise and the solution was stirred at 0 °C for 2 h. A solution of NaN_3 (1.5 equiv) in water (0.5 mL per 1 mmol of aniline) was added dropwise at 0 °C (CAUTION: vigorous release of N_2) and the reaction was stirred for 2 h and allowed to warm to room temperature. The aqueous layer was extracted twice with diethyl ether and the combined organic layers were washed with water, sodium bicarbonate, brine, dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield the corresponding pure aryl azide. Benzylic azides were synthesised at room temperature from the corresponding bromides by nucleophilic substitution with sodium azide in DMSO (Alvarez procedure, Eq. 2).[5] 1-Azido-2-ethoxyethane (Eq. 3),[6] and 4-azidopyridine[7] were prepared following previously reported procedures. 1-(Azidomethyl)-4-trifluoromethylbenzene was prepared by a modified literature procedure.[8]







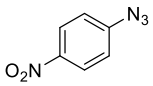
1-Azido-4-trifluoromethylbenzene (1a)



Following the general procedure for preparation of aryl azides from 4-trifluoromethylaniline (15.0 mL, 119.5 mmol), the title compound was obtained as an orange oil (21.1 g, 95%). Spectroscopic data for this compound is in accordance with the literature.[9]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.5 Hz, 2H), 7.12 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 127.1 (q, *J* = 33 Hz), 127.0 (q, *J* = 3 Hz), 124.0 (q, *J* = 272 Hz), 119.2.

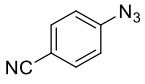
1-Azido-4-nitrobenzene (1b)



Following the general procedure for preparation of aryl azides from 4-nitroaniline (10.0 g, 72.4 mmol), the title compound was obtained as a yellow solid (11.8 g, 99%). Spectroscopic data for this compound is in accordance with the literature.[10]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 9.0 Hz, 2H), 7.14 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.9, 144.6, 125.6, 119.4.

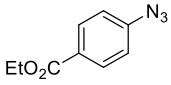
4-Azidobenzonitrile (1c)



Following the general procedure for preparation of aryl azides from 4-aminobenzonitrile (10.0 g, 84.7 mmol), the title compound was obtained as an off-white solid (11.7 g, 96%). Spectroscopic data for this compound is in accordance with the literature.[10]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.5 Hz, 2H), 7.10 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 133.8, 119.8, 118.4, 108.3.

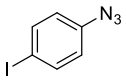
4-Ethylazidobenzoate (1d)



Following the general procedure for preparation of aryl azides from 4-ethylaminobenzoate (10.0 g, 60.5 mmol), the title compound was obtained as a yellow oil (11.2 g, 97%). Spectroscopic data for this compound is in accordance with the literature.[11]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.5 Hz, 2H), 7.04 (d, *J* = 8.5 Hz, 2H), 4.36 (q, *J* = 7.0 Hz, 2H), 1.39 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 144.6, 131.3, 127.1, 118.7, 61.0, 14.3.

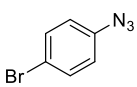
1-Azido-4-iodobenzene (1e)



Following the general procedure for preparation of aryl azides from 4-iodoaniline (10.0 g, 45.7 mmol), the title compound was obtained as a dark brown oily solid (10.0 g, 89%). Spectroscopic data for this compound is in accordance with the literature.[12]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 9.0 Hz, 2H), 6.76 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.0, 138.7, 121.1, 88.3.

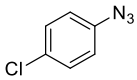
1-Azido-4-bromobenzene (1f)



Following the general procedure for preparation of aryl azides from 4-bromoaniline (10.0 g, 58.1 mmol), the title compound was obtained as an orange oil (11.1 g, 97%). Spectroscopic data for this compound is in accordance with the literature.[13]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 9.0 Hz, 2H), 6.88 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.2, 132.8, 120.7, 117.8.

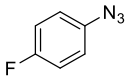
1-Azido-4-chlorobenzene (1g)



Following the general procedure for preparation of aryl azides from 4-chloroaniline (10.0 g, 78.4 mmol), the title compound was obtained as a dark orange oil (8.0 g, 66%). Spectroscopic data for this compound is in accordance with the literature.[14]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.5 Hz, 2H), 6.95 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.7, 130.2, 129.8, 120.3.

1-Azido-4-fluorobenzene (1h)



Following the general procedure for preparation of aryl azides from 4-fluoroaniline (8.53 mL, 90.0 mmol), the title compound was obtained as an orange oil (10.3 g, 84%). Spectroscopic data for this compound is in accordance with the literature.[15]

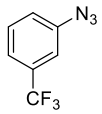
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07–7.03 (m, 2H), 7.00–6.96 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0 (d, *J* = 244 Hz), 135.8, 120.3 (d, *J* = 8 Hz), 116.6 (d, *J* = 23 Hz).

1-Azidobenzene (1i)

Following the general procedure for preparation of aryl azides from aniline (9.8 mL, 107.5 mmol), the title compound was obtained as a brown oil (7.5 g, 58%). Spectroscopic data for this compound is in accordance with the literature.[16]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31–7.25 (m, 2H), 7.11–7.05 (m, 1H), 6.99–6.93 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.1, 129.8, 124.9, 119.1.

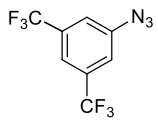
1-Azido-3-trifluoromethylbenzene (1j)



Following the general procedure for preparation of aryl azides from 3-trifluoromethylaniline (5.0 mL, 40.0 mmol), the title compound was obtained as an orange oil (6.7 g, 89%). Spectroscopic data for this compound is in accordance with the literature.[17]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48–7.44 (m, 1H), 7.39–7.37 (m, 1H), 7.24 (s, 1H), 7.20–7.18 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 132.4 (q, *J* = 33 Hz), 130.3, 123.5 (q, *J* = 273 Hz), 122.1, 121.5 (q, *J* = 4 Hz), 116.0 (q, *J* = 4 Hz).

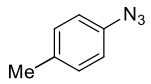
1-Azido-3,5-bis(trifluoromethyl)benzene (1k)



Following the general procedure for preparation of aryl azides from 3,5-bis(trifluoromethyl)aniline (3.4 mL, 21.8 mmol), the title compound was obtained as a yellow oil (5.5 g, 98%). Spectroscopic data for this compound is in accordance with the literature.[18]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.44 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6, 133.6 (q, *J* = 34 Hz), 122.9 (q, *J* = 273 Hz), 119.3 (q, *J* = 2 Hz), 118.6 (sept, *J* = 4 Hz).

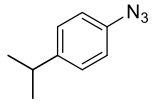
4-Azidotoluene (1l)



Following the general procedure for preparation of aryl azides from *p*-toluidine (10.0 g, 93.4 mmol), the title compound was obtained as a brown solid (11.0 g, 89%). Spectroscopic data for this compound is in accordance with the literature.[12]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.2, 134.6, 130.4, 118.9, 20.9.

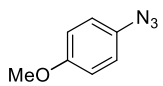
1-Azido-4-isopropylbenzene (1m)



Following the general procedure for preparation of aryl azides from 4-isopropylaniline (10.0 mL, 73.1 mmol), the title compound was obtained as a red liquid (11.1 g, 94%). Spectroscopic data for this compound is in accordance with the literature.[19]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.5 Hz, 2H), 6.96 (d, *J* = 8.5 Hz, 2H), 2.89 (sept, *J* = 7.0 Hz, 1H), 1.23 (d, *J* = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.7, 137.4, 127.7, 118.9, 33.6, 24.0.

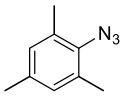
4-Azidoanisole (1n)



Following the general procedure for preparation of aryl azides from *p*-anisidine (10.0 g, 81.2 mmol), the title compound was obtained as a brown solid (11.3 g, 93%). Spectroscopic data for this compound is in accordance with the literature.[14]

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (d, *J* = 9.0 Hz, 2H), 6.88 (d, *J* = 9.0 Hz, 2H), 3.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0, 132.3, 120.0, 115.1, 55.5.

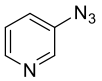
Mesityl azide (1o)



Following the general procedure for preparation of aryl azides from mesidine (10.0 g, 74.0 mmol), the title compound was obtained as an orange oil (9.3 g, 78%). Spectroscopic data for this compound is in accordance with the literature.[20]

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (s, 2H), 2.36 (s, 6H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.3, 134.4, 131.9, 129.5, 20.7, 18.1.

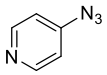
3-Azidopyridine (1p)



Following the general procedure for preparation of aryl azides from 3-aminopyridine (5.0 g, 53.2 mmol), the title compound was obtained as an orange oil (3.7 g, 59%). Spectroscopic data for this compound is in accordance with the literature.[10]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41–8.36 (m, 2H), 7.38–7.34 (m, 1H), 7.32–7.28 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0, 141.3, 137.1, 125.9, 124.1.

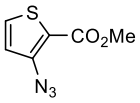
4-Azidopyridine (1q)



A solution of 4-chloropyridine hydrochloride (7.2 g, 47.7 mmol) in water (20 mL) was neutralised with aqueous solution of NaOH (1 M) to pH 7 before adding MeOH (40 mL). Subsequently, a solution of NaN_3 (6.2 g, 95.3 mmol) in water (20 mL) was added and the mixture was heated under reflux overnight, cooled to room temperature, concentrated under reduced pressure and neutralised with saturated aqueous solution of K_2CO_3. The aqueous layer was extracted twice with diethyl ether and the combined organic layers were washed with water, brine, dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield the title compound as a red oil (4.7 g, 75%). Spectroscopic data for this compound is in accordance with the literature.[21]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55–8.51 (m, 2H), 6.97–6.93 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.1, 148.7, 114.1.

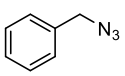
Methyl 3-azidothiophene-2-carboxylate (1r)



Following the general procedure for preparation of aryl azides from methyl 3-aminothiophene-2-carboxylate (7.5 g, 47.7 mmol), the title compound was obtained as a yellow solid (8.0 g, 91%). Spectroscopic data for this compound is in accordance with the literature.[22]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, J = 5.5 Hz, 1H), 6.93 (d, J = 5.5 Hz, 1H), 3.88 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3, 142.2, 131.2, 122.1, 117.1, 52.1.

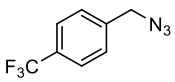
Benzyl azide (1s)



From benzyl bromide (7.0 mL, 58.5 mmol) and NaN_3 (4.2 g, 64.4 mmol) and following the Alvarez procedure[5] (16 h, RT), the title compound was obtained as a yellow oil (7.6 g, 98%). Spectroscopic data for this compound is in accordance with the literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46–7.34 (m, 5H), 4.36 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.4, 128.8, 128.3, 128.2, 54.8.

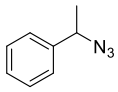
1-(Azidomethyl)-4-trifluoromethylbenzene (1t)



1-Bromomethyl-4-trifluoromethylbenzene (4.5 g, 18.8 mmol) was dissolved in DMF (40 mL) and NaN_3 (1.5 g, 22.6 mmol) was added. The reaction mixture was stirred at 65 °C for 16 h, then allowed to cool down to room temperature. Water (100 mL) was added and the aqueous layer was extracted twice with diethyl ether. The combined organic layers were thoroughly washed with water, brine, dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield the title compound as a colourless oil (3.7 g, 97%). Spectroscopic data for this compound is in accordance with the literature.[23]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 4.40 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 130.4 (q, *J* = 33 Hz), 128.3, 125.8 (q, *J* = 4 Hz), 124.0 (q, *J* = 272 Hz), 54.0.

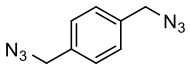
(1-Azidoethyl)benzene (1u)



From 1-phenylethylbromide (3.4 mL, 24.9 mmol) and NaN_3 (1.8 g, 27.4 mmol) and following the Alvarez procedure[5] (12 h, RT), the title compound was obtained as a pale yellow oil (3.4 g, 93%). Spectroscopic data for this compound is in accordance with the literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.27 (m, 5H), 4.59 (q, *J* = 7.0 Hz, 1H), 1.51 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 128.8, 128.1, 126.4, 61.1, 21.6.

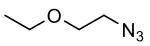
1,4-Bis-(azidomethyl)benzene (1v)



From 1,4-bis(bromomethyl)benzene (10.0 g, 37.9 mmol) and NaN_3 (5.4 g, 83.4 mmol) and following the Alvarez procedure[5] (16 h, RT), the title compound was obtained as a pale yellow oil (6.2 g, 87%). Spectroscopic data for this compound is in accordance with the literature.[24]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (s, 4H), 4.34 (s, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.4, 128.6, 54.3.

1-Azido-2-ethoxyethane (1w)



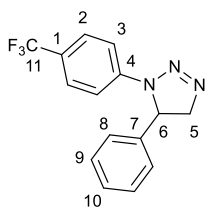
1-Bromo-2-ethoxyethane (10.0 mL, 88.7 mmol) was dissolved in DMF (100 mL) and NaN_3 (8.7 g, 133.0 mmol) was added. The reaction mixture was stirred at 100 °C for 48 h behind a safety screen, then allowed to cool down to room temperature. Brine (40 mL) was added and the aqueous layer was extracted four times with diethyl ether. The combined organic layers were thoroughly washed with water, brine, dried over $MgSO_4$, filtered and carefully concentrated under reduced pressure (150 mm Hg, 30 °C) to yield the title compound as a yellow oil (7.4 g, 72%).

IR: ν_{max} 2978, 2932, 2870, 2092 (s, N_3), 1444, 1379, 1346, 1284 (m), 1116 (s), 1046, 1030, 933, 852, 825 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.61 (t, *J* = 5.0 Hz, 2H), 3.55 (q, *J* = 7.0 Hz, 2H), 3.38 (t, *J* = 5.0 Hz, 2H), 1.23 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 69.2, 66.7, 50.8, 15.2; HRMS (EI+) calculated for C_4H_9O 73.0653, found 73.0658 ($[M - N_3]^+$)

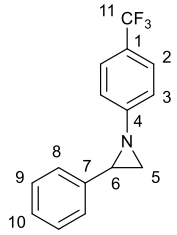
3. Dipolar Cycloadditions in DES

General procedure for the dipolar cycloadditions: Azide (1.0 equiv.) and alkene (2.0 equiv.) were stirred in deep eutectic solvent (choline chloride/urea = 1:2; 0.5 M) at 80 °C for 16 h, unless stated otherwise. The reaction mixture was cooled down to room temperature, diluted with water (2 mL per mmol of azide) and pentane/Et_2O (3:1; 1 mL per mmol of azide) and stored at -18 °C overnight. If triazoline precipitated overnight, this was triturated at room temperature, collected by filtration, washed three times with ice cold pentane/Et_2O and recrystallised from boiling ethanol if necessary. Occasionally, the washings and/or filtrate from this recrystallisation were further purified by column chromatography as described next, either to improve the triazoline recovery, or to isolate the corresponding aziridine. If no solid precipitated at -18 °C, the mixture was extracted with EtOAc, the combined organic phases were washed with water and brine, dried over $MgSO_4$, filtered, concentrated under reduced pressure and purified by column chromatography on basified silica (eluent: petroleum ether/EtOAc 0→25% gradient basified with 2% v/v NEt_3 unless stated otherwise; reaction crude was dry-loaded onto stationary phase). Occasionally, the product recovered after column chromatography required washing with ice-cold pentane/Et_2O (1:1).

5-Phenyl-1-[4-(trifluoromethyl)phenyl]-Δ^2-1,2,3-triazoline (3aa): Following the general procedure from 1-azido-4-trifluoromethylbenzene (5.00 g, 26.7 mmol) and styrene (6.18 mL, 53.4 mmol), the title compound was isolated as a white solid (3.68 g after recrystallisation, 0.82 g after column: 58% overall). From this reaction, 2-phenyl-1-[4-(trifluoromethyl)phenyl]aziridine **4aa** was also isolated as a white solid (1.28 g, 18%) after column chromatography and recrystallisation from pentane at -18 °C.



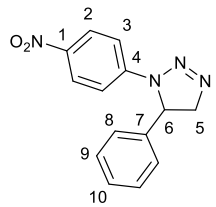
3aa: Single crystals for X-ray diffraction were grown from Et_2O, CCDC 1843142; Mp 88.0–90.0 °C; R_f = 0.49 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 1612 (m), 1523 (m), 1502 (m), 1458, 1431, 1365 (m), 1316 (m), 1193, 1153 (m), 1111 (s), 1067 (s), 1010 (m), 990 (m), 963 (m), 926 (m), 841 (m), 820 (s), 751 (s), 698 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.45 (d, *J* = 8.5 Hz, 2H, H^2), 7.35–7.24 (m, 5H, H^{Ar}), 7.15 (d, *J* = 8.5 Hz, 2H, H^3), 4.94 (dd, *J* = 12.5; 8.0 Hz, 1H, H^6), 4.88 (dd, *J* = 17.5; 12.5 Hz, 1H, H^5), 4.37 (dd, *J* = 17.5; 8.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 142.9 (C^4), 139.5 (C^7), 129.5 (C^9), 128.4 (C^{10}), 126.5 (q, *J* = 3 Hz, C^2), 125.9 (C^8), 124.3 (q, *J* = 269 Hz, C^{11}), 124.0 (q, *J* = 33 Hz, C^1), 114.4 (C^3), 76.1 (C^5), 57.4 (C^6); ^{19}F NMR ($CDCl_3$, 377 MHz): δ -61.9 (s); HRMS (ES+) calculated for $C_{15}H_{13}N_3F_3$ 292.1062, found 292.1058 ($[M + H]^+$); Elemental analysis calculated for $C_{15}H_{12}N_3F_3$: C, 61.85; H, 4.15; N, 14.43, found: C, 61.95; H, 4.27; N, 14.27.



4aa: Single crystals for X-ray diffraction were grown from Et_2O, CCDC 1843144; Mp 85.0–87.0 °C; R_f = 0.83 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3053, 1614 (m), 1516, 1464, 1418, 1389, 1327 (s), 1279 (s), 1185, 1163 (m), 1127 (m), 1101 (s), 1076 (m), 1065 (s), 1010 (m), 981 (m), 914, 867, 843 (s), 790, 767 (m), 758 (s), 714 (s), 698 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.50 (d, *J* = 8.5 Hz, 2H, H^2), 7.38–7.36 (m, 4H, H^{Ar}), 7.34–7.29 (m, 1H, H^{Ar}), 7.11 (d, *J* = 8.5 Hz, 2H, H^3), 3.16 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.49 (dd, *J* = 6.5; 1.0 Hz, 1H, H^5), 2.47 (dd, *J* = 3.5; 1.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 157.6

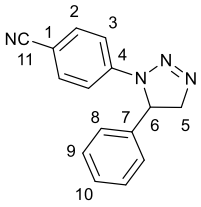
(C^4), 138.6 (C^7), 128.6 (C^9), 127.7 (C^{10}), 126.3 (q, J = 3 Hz, C^2), 126.2 (C^8), 124.6 (q, J = 32 Hz, C^1), 124.4 (q, J = 269 Hz, C^{11}), 120.7 (C^3), 41.7 (C^6), 37.7 (C^5); ^{19}F NMR ($CDCl_3$, 377 MHz): δ -61.8 (s); HRMS (ES+) calculated for $C_{15}H_{13}NF_3$ 264.1000, found 264.0988 ([M + H]$^+$); Elemental analysis calculated for $C_{15}H_{12}NF_3$: C, 68.44; H, 4.59; N, 5.32, found: C, 68.39; H, 4.69; N, 5.29.

1-(4-Nitrophenyl)-5-phenyl-Δ^2-1,2,3-triazoline (3ba): Following the general procedure at 80 °C for 8 h from 1-azido-4-nitrobenzene (3.00 g, 18.3 mmol) and styrene (4.22 mL, 36.6 mmol), the title compound was isolated as an orange solid (3.21 g after recrystallisation, 0.10 g after column: 67% overall).

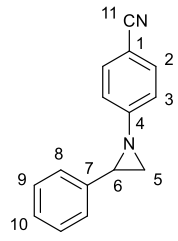


3ba: Mp 128.7–130.9 °C; R_f = 0.22 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3032, 1597 (s, NO_2), 1517 (m), 1496 (s), 1455, 1435, 1372 (w, NO_2), 1324 (s), 1304 (m), 1284 (m), 1203, 1187, 1127, 1115, 1080, 1061 (s), 984, 959, 920 (m), 906 (m), 843 (s), 810, 750 (s), 711, 695, 688 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.10 (d, J = 9.5 Hz, 2H, H^2), 7.38–7.31 (m, 3H, H^{Ar}), 7.26 (d, J = 9.5 Hz, 2H, H^3), 7.16–7.14 (m, 2H, H^{Ar}), 4.99 (dd, J = 12.0; 7.5 Hz, 1H, H^6), 4.96 (dd, J = 18.0; 12.0 Hz, 1H, H^5), 4.47 (dd, J = 18.0; 7.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 145.2 (C^1), 142.1 (C^4), 139.0 (C^7), 129.7 (C^9), 128.7 (C^{10}), 125.8 (C^8), 125.6 (C^2), 114.1 (C^3), 76.8 (C^5), 57.0 (C^6); HRMS (ES+) calculated for $C_{14}H_{13}N_4O_2$ 269.1039, found 269.1048 ([M + H]$^+$).

4-(5-Phenyl-Δ^2-1,2,3-triazolin-1-yl)benzonitrile (3ca): Following the general procedure from 4-azidobenzonitrile (3.00 g, 20.8 mmol) and styrene (4.81 mL, 41.6 mmol), the title compound was isolated as a white solid (2.97 g, 57%) after column chromatography. From this reaction, 4-(2-phenylaziridin-1-yl)benzonitrile **4ca** was also isolated as a white solid (0.19 g, 4%) after column chromatography and recrystallisation from pentane at -18 °C.



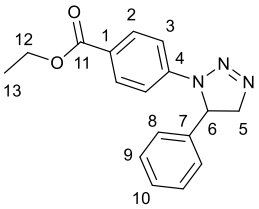
3ca: Mp 94.0–96.0 °C; R_f = 0.26 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2224 (s, CN), 1605 (s), 1505 (s), 1494 (s), 1456, 1435, 1367 (m), 1354 (m), 1316, 1281, 1180, 1131, 1116, 1081 (m), 1064 (s), 986, 961, 920 (s), 905 (m), 873, 839 (s), 816 (s), 758 (s), 697 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.50 (d, J = 9.0 Hz, 2H, H^2), 7.37–7.29 (m, 3H, H^{Ar}), 7.24 (d, J = 9.0 Hz, 2H, H^3), 7.15–7.13 (m, 2H, H^{Ar}), 4.95 (dd, J = 12.5; 4.5 Hz, 1H, H^6), 4.92 (dd, J = 17.0; 12.0 Hz, 1H, H^5), 4.43 (dd, J = 17.0; 4.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 143.5 (C^4), 139.1 (C^7), 133.5 (C^2), 129.6 (C^9), 128.6 (C^{10}), 125.7 (C^8), 119.1 (C^{11}), 114.7 (C^3), 104.9 (C^1), 76.5 (C^5), 57.1 (C^6); HRMS (ES+) calculated for $C_{15}H_{13}N_4$ 249.1140, found 249.1141 ([M + H]$^+$).



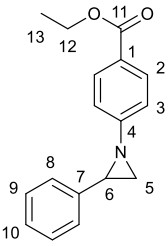
4ca: Mp 69.0–70.2 °C; R_f = 0.61 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3057, 2984, 2222 (s, CN), 1598 (s), 1505 (s), 1496 (s), 1459 (m), 1450, 1417, 1386 (s), 1314 (m), 1297 (m), 1282 (m), 1179, 1151 (s), 1134, 1115, 1101 (m), 990, 913, 896 (m), 835 (s), 821 (m), 767, 755 (s), 696 (s), 663 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53 (d, J = 8.5 Hz, 2H, H^2), 7.40–7.29 (m, 5H, H^{Ar}), 7.08 (d, J = 8.5 Hz, 2H, H^3), 3.19 (dd, J = 6.5; 3.5 Hz, 1H, H^6), 2.52 (dd, J = 6.5; 0.5 Hz, 1H, H^5), 2.50 (dd, J = 3.5; 0.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 158.5 (C^4), 138.1 (C^7), 133.3 (C^2), 128.6 (C^9), 127.8 (C^{10}), 126.1 (C^8), 121.1 (C^3),

119.2 (C^{11}), 105.4 (C^{1}), 41.8 (C^{6}), 37.7 (C^{5}); HRMS (ES+) calculated for $C_{15}H_{13}N_2$ 221.1079, found 221.1086 ($[M + H]^+$).

Ethyl 4-(5-phenyl-Δ²-1,2,3-triazolin-1-yl)benzoate (3da): Following the general procedure from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and styrene (3.63 mL, 31.4 mmol), the title compound was isolated as a white solid (2.51 g after recrystallisation, 0.14 g after column: 57% overall). From this reaction, ethyl 4-(2-phenylaziridin-1-yl)benzoate **4da** was also isolated as a white solid (0.45 g, 11%) after column chromatography and recrystallisation from pentane at -18 °C.

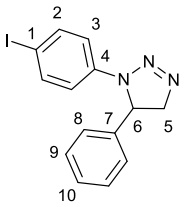


3da: Mp 123.0–127.0 °C; R_f = 0.35 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2971, 1702 (s, C=O), 1608 (s), 1518, 1502 (s), 1455, 1422, 1365 (m), 1307, 1271 (s), 1176 (s), 1106 (s), 1066 (s), 1025 (m), 988, 963 (s), 925 (s), 872, 851 (m), 830 (m), 764 (s), 748 (s), 691 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 9.0 Hz, 2H, H^2), 7.35–7.28 (m, 5H, H^{Ar}), 7.22 (d, *J* = 9.0 Hz, 2H, H^3), 4.98 (dd, *J* = 12.5; 7.5 Hz, 1H, H^6), 4.89 (dd, *J* = 17.5; 12.5 Hz, 1H, H^5), 4.39 (dd, *J* = 17.5; 7.5 Hz, 1H, H^5), 4.32 (q, *J* = 7.0 Hz, 2H, H^{12}), 1.35 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{11}), 143.7 (C^4), 139.6 (C^7), 131.1 (C^2), 129.4 (C^9), 128.3 (C^{10}), 125.8 (C^8), 124.0 (C^1), 114.1 (C^3), 76.0 (C^5), 60.6 (C^{12}), 57.3 (C^6), 14.3 (C^{13}); HRMS (ES+) calculated for $C_{17}H_{18}N_3O_2$ 296.1399, found 296.1385 ($[M + H]^+$); Elemental analysis calculated for $C_{17}H_{17}N_3O_2$: C, 69.14; H, 5.80; N, 14.23, found: C, 68.97; H, 5.70; N, 14.06.



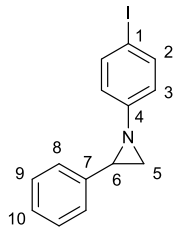
4da: Mp 32.0–33.3 °C; R_f = 0.67 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3052, 2991, 1698 (s, C=O), 1601 (s), 1499, 1466, 1390, 1367, 1310, 1267 (s), 1174, 1154, 1129, 1109 (s), 1096 (s), 1065, 1015, 1003, 983, 914, 860 (s), 838, 783, 771 (s), 760, 728, 699 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.95 (d, *J* = 8.5 Hz, 2H, H^2), 7.37–7.29 (m, 5H, H^{Ar}), 7.06 (d, *J* = 8.5 Hz, 2H, H^3), 4.34 (q, *J* = 7.0 Hz, 2H, H^{12}), 3.16 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.50 (dd, *J* = 6.5; 1.0 Hz, 1H, H^5), 2.47 (dd, *J* = 3.5; 1.0 Hz, 1H, H^5), 1.37 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 166.4 (C^{11}), 158.7 (C^4), 138.7 (C^7), 130.8 (C^2), 128.5 (C^9), 127.6 (C^{10}), 126.1 (C^8), 124.6 (C^1), 120.2 (C^3), 60.7 (C^{12}), 41.6 (C^6), 37.7 (C^5), 14.4 (C^{13}); HRMS (ES+) calculated for $C_{17}H_{18}NO_2$ 268.1338, found 268.1327 ($[M + H]^+$).

1-(4-Iodophenyl)-5-phenyl-Δ²-1,2,3-triazoline (3ea): Following the general procedure from 1-azido-4-iodobenzene (3.25 g, 13.3 mmol) and styrene (3.07 mL, 26.6 mmol), the title compound was isolated as a brown solid (2.20 g after recrystallisation, 0.31 g after column: 54% overall). From this reaction, 1-(4-iodophenyl)-2-phenylaziridine **4ea** was also isolated as a yellow solid (0.87 g, 20%) after column chromatography and recrystallisation from pentane at -18 °C.



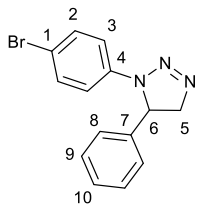
3ea: Mp 128.0–130.5 °C; R_f = 0.49 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 1583 (m), 1480 (s), 1456 (s), 1425, 1397, 1352 (m), 1304 (m), 1275 (m), 1205, 1121 (m), 1101 (m), 1070 (m), 1027 (m), 999 (m), 986 (m), 962 (m), 924 (m), 909 (m), 838 (m), 827, 801 (s), 759 (s), 722, 693 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.50 (d, *J* = 9.0 Hz, 2H, H^2), 7.35–7.28 (m, 3H, H^{Ar}), 7.15–7.13 (m, 2H, H^{Ar}), 6.96 (d, *J* = 9.0 Hz, 2H, H^3), 4.90 (dd, *J* = 12.5; 9.5 Hz, 1H, H^6),

4.87 (dd, *J* = 18.5; 12.5 Hz, 1H, H^5), 4.33 (dd, *J* = 18.5; 9.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 140.0 (C^4), 139.7 (C^7), 138.0 (C^2), 129.4 (C^9), 128.3 (C^{10}), 125.9 (C^8), 116.8 (C^3), 85.0 (C^1), 75.8 (C^5), 57.7 (C^6); HRMS (ES+) calculated for $C_{14}H_{13}N_3I$ 350.0154, found 350.0154 ($[M + H]^+$).

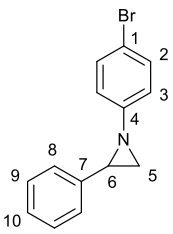


4ea: Mp 75.7–76.5 °C; R_f = 0.84 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3045, 2985, 1575 (m), 1480 (s), 1463 (s), 1397 (m), 1387 (m), 1313 (m), 1303 (m), 1283 (m), 1268 (m), 1228, 1154 (m), 1125, 1104, 1091, 1073, 1058, 998 (m), 983 (m), 915, 871, 825 (s), 773 (m), 759 (m), 721 (s), 691 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53 (d, *J* = 8.5 Hz, 2H, H^2), 7.36–7.35 (m, 4H, H^{Ar}), 7.32–7.27 (m, 1H, H^{Ar}), 6.81 (d, *J* = 8.5 Hz, 2H, H^3), 3.07 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.42 (dd, *J* = 6.5; 0.5 Hz, 1H, H^5), 2.41 (dd, *J* = 3.5; 0.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 154.3 (C^4), 138.8 (C^7), 137.8 (C^2), 128.5 (C^9), 127.5 (C^{10}), 126.1 (C^8), 122.8 (C^3), 85.3 (C^1), 41.7 (C^6), 37.6 (C^5); HRMS (ES+) calculated for $C_{14}H_{13}NI$ 322.0093, found 322.0088 ($[M + H]^+$).

1-(4-Bromophenyl)-5-phenyl-Δ²-1,2,3-triazoline (3fa): Following the general procedure from 1-azido-4-bromobenzene (3.00 g, 15.2 mmol) and styrene (3.50 mL, 30.4 mmol), the title compound was isolated as a pale yellow solid (2.39 g after recrystallisation, 0.22 g after column: 56% overall). From this reaction, 1-(4-bromophenyl)-2-phenylaziridine **4fa** was also isolated as a pale yellow solid (0.99 g, 24%) after column chromatography and recrystallisation from pentane at -18 °C.



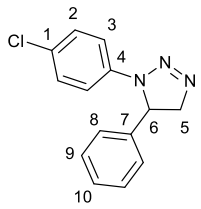
3fa: Mp 139.0–140.6 °C; R_f = 0.50 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3086, 3025, 2938, 1592 (m), 1484 (s), 1456 (m), 1432 (m), 1411, 1359 (s), 1307, 1274, 1253, 1204, 1124 (m), 1102, 1085 (s), 1071 (s), 1029, 1003 (m), 968 (m), 927 (s), 906, 869, 834 (s), 801 (s), 754 (s), 711, 695 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35–7.26 (m, 3H, H^{Ar}), 7.32 (d, *J* = 9.0 Hz, 2H, H^2), 7.16–7.14 (m, 2H, H^{Ar}), 7.07 (d, *J* = 9.0 Hz, 2H, H^3), 4.90 (dd, *J* = 12.5; 10.0 Hz, 1H, H^6), 4.87 (dd, *J* = 19.0; 12.5 Hz, 1H, H^5), 4.33 (dd, *J* = 19.0; 10.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 139.7 (C^7), 139.4 (C^4), 132.1 (C^2), 129.4 (C^9), 128.3 (C^{10}), 125.9 (C^8), 116.4 (C^3), 114.8 (C^1), 75.8 (C^5), 57.8 (C^6); HRMS (ES+) calculated for $C_{14}H_{13}N_3Br$ 302.0293, found 302.0288 ($[M + H]^+$).



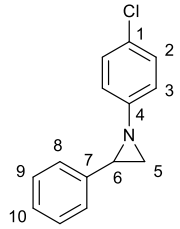
4fa: Mp 58.2–59.4 °C; R_f = 0.85 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3035, 2978, 1581 (m), 1482 (s), 1462 (s), 1400 (m), 1390 (m), 1313 (m), 1300 (m), 1283 (m), 1272 (m), 1225, 1156 (m), 1126, 1105, 1093, 1066 (m), 1002 (m), 984 (m), 915, 871, 828 (s), 775 (m), 760, 726 (s), 692 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36–7.32 (m, 4H, H^{Ar}), 7.34 (d, *J* = 8.5 Hz, 2H, H^2), 7.32–7.26 (m, 1H, H^{Ar}), 6.92 (d, *J* = 8.5 Hz, 2H, H^3), 3.07 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.43 (dd, *J* = 6.5; 1.0 Hz, 1H, H^5), 2.41 (dd, *J* = 3.5; 1.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 153.6 (C^4), 138.8 (C^7), 131.9 (C^2), 128.5 (C^9), 127.4 (C^{10}), 126.1 (C^8), 122.3 (C^3), 115.0 (C^1), 41.7 (C^6), 37.7 (C^5); HRMS (ES+) calculated for $C_{14}H_{13}NBr$ 274.0231, found 274.0230 ($[M + H]^+$).

1-(4-Chlorophenyl)-5-phenyl-Δ²-1,2,3-triazoline (3ga): Following the general procedure from 1-azido-4-chlorobenzene (3.00 g, 19.5 mmol) and styrene (4.51 mL, 39.0 mmol), the title

compound was isolated as an off-white solid (2.80 g after recrystallisation, 0.10 g after column: 58% overall). From this reaction, 1-(4-chlorophenyl)-2-phenylaziridine **4ga** was also isolated as a pale yellow solid (0.94 g, 21%) after column chromatography and recrystallisation from pentane at -18 °C.

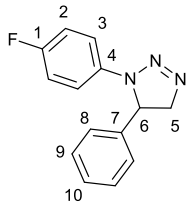


3ga: Mp 125.0–129.0 °C; R_f = 0.48 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2938, 1597, 1496 (m), 1485 (s), 1456, 1413, 1354 (m), 1305, 1273, 1124, 1096, 1088, 1071 (s), 1008, 992, 967, 931 (m), 913 (m), 824 (s), 807 (m), 763 (s), 728, 701 (m), 696 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35–7.26 (m, 3H, H^{Ar}), 7.18–7.10 (m, 6H, H^{Ar}), 4.90 (dd, *J* = 12.5; 11.0 Hz, 1H, H^6), 4.86 (dd, *J* = 20.0; 12.5 Hz, 1H, H^5), 4.32 (dd, *J* = 20.0; 11.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 139.8 (C^7), 139.0 (C^4), 129.4 (C^9), 129.2 (C^2), 128.3 (C^{10}), 127.4 (C^1), 125.9 (C^8), 116.0 (C^3), 75.7 (C^5), 57.9 (C^6); HRMS (ES+) calculated for $C_{14}H_{13}N_3Cl$ 258.0798, found 258.0804 ($[M + H]^+$).

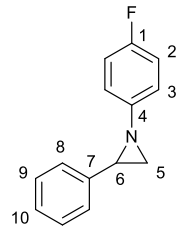


4ga: Mp 42.5–43.0 °C; R_f = 0.81 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3030, 2924, 1594, 1488 (s), 1463, 1388, 1315, 1300, 1282, 1271, 1224, 1155, 1089 (m), 1033, 1009, 912, 830 (s), 741 (s), 697 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37–7.35 (m, 4H, H^{Ar}), 7.33–7.27 (m, 1H, H^{Ar}), 7.20 (d, *J* = 9.0 Hz, 2H, H^2), 6.97 (d, *J* = 9.0 Hz, 2H, H^3), 3.07 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.43 (dd, *J* = 6.5; 1.0 Hz, 1H, H^5), 2.41 (dd, *J* = 3.5; 1.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 153.1 (C^4), 138.9 (C^7), 128.9 (C^2), 128.5 (C^9), 127.4 (C^{10}), 127.3 (C^1), 126.1 (C^8), 121.8 (C^3), 41.8 (C^6), 37.7 (C^5); HRMS (ES+) calculated for $C_{14}H_{13}NCl$ 230.0737, found 230.0744 ($[M + H]^+$).

1-(4-Fluorophenyl)-5-phenyl-Δ^2-1,2,3-triazoline (3ha): Following the general procedure from 1-azido-4-fluorobenzene (3.00 g, 21.9 mmol) and styrene (5.06 mL, 43.8 mmol), the title compound was isolated as a pale yellow solid (2.84 g after recrystallisation, 0.10 g after column: 56% overall). From this reaction, 1-(4-fluorophenyl)-2-phenylaziridine **4ha** was also isolated as a yellow solid (0.70 g, 15%) after column chromatography and recrystallisation from pentane at -18 °C.

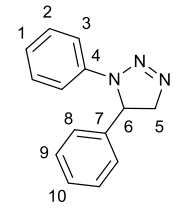


3ha: Mp 117.1–119.5 °C; R_f = 0.47 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 1508 (m), 1490 (s), 1455, 1429 (m), 1362, 1306, 1277, 1225 (m), 1165, 1111 (s), 1084 (m), 1074 (s), 1028, 1011, 994 (m), 964 (m), 929 (m), 921, 912 (m), 873, 852, 830 (s), 811 (s), 750 (s), 696 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36–7.29 (m, 3H, H^{Ar}), 7.18–7.12 (m, 4H, H^{Ar}), 6.95–6.91 (m, 2H, H^{Ar}), 4.90 (dd, *J* = 12.5; 10.0 Hz, 1H, H^6), 4.87 (dd, *J* = 18.5; 12.5 Hz, 1H, H^5), 4.31 (dd, *J* = 18.5; 10.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 158.5 (d, *J* = 242 Hz, C^1), 140.0 (C^7), 136.8 (C^4), 129.3 (C^9), 128.2 (C^{10}), 126.0 (C^8), 116.2 (d, *J* = 7 Hz, C^3), 115.8 (d, *J* = 22 Hz, C^2), 75.6 (C^5), 58.5 (C^6); ^{19}F NMR ($CDCl_3$, 377 MHz): δ -121.4 (s); HRMS (ES+) calculated for $C_{14}H_{13}N_3F$ 242.1094, found 242.1095 ($[M + H]^+$).

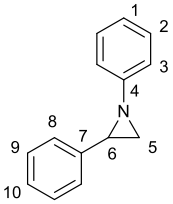


4ha: Mp 31.5–33.0 °C; R_f = 0.79 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3045, 2985, 1498 (s), 1462 (m), 1451, 1415, 1389, 1316, 1296, 1277, 1235, 1209 (s), 1176, 1161 (m), 1148, 1128, 1103, 1093 (m), 1076, 985, 911, 839 (s), 814 (m), 766 (s), 760 (s), 699 (s), 676 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.36–7.31 (m, 4H, H^{Ar}), 7.31–7.25 (m, 1H, H^{Ar}), 6.97–6.90 (m, 4H, H^{Ar}), 3.05 (dd, *J* = 6.0; 3.0 Hz, 1H, H^6), 2.41 (dd, *J* = 6.0; 0.5 Hz, 1H, H^5), 2.39 (dd, *J* = 3.0; 0.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 158.5 (d, *J* = 241 Hz, C^1), 150.5 (C^4), 139.1 (C^7), 128.5 (C^9), 127.4 (C^{10}), 126.1 (C^8), 121.5 (d, *J* = 8 Hz, C^3), 115.5 (d, *J* = 22 Hz, C^2), 41.9 (C^5), 37.8 (C^6); ^{19}F NMR ($CDCl_3$, 377 MHz): δ -121.5 (s); HRMS (ES+) calculated for $C_{14}H_{13}NF$ 214.1032, found 214.1036 ($[M + H]^+$).

1,5-Diphenyl-Δ^2-1,2,3-triazoline (3ia): Following the general procedure from 1-azidobenzene (3.00 g, 25.2 mmol) and styrene (5.81 mL, 50.4 mmol), the title compound was isolated as a pale yellow solid (2.90 g after recrystallisation, 0.11 g after column: 54% overall). From this reaction, 1,2-diphenylaziridine **4ia** was also isolated as a yellow oil (1.12 g, 23%) after column chromatography.

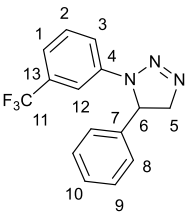


3ia: Mp 129.0–132.0 °C; R_f = 0.51 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3032, 2965, 2938, 1672, 1599 (m), 1503, 1489 (s), 1455 (m), 1358 (m), 1329, 1276, 1113 (m), 1097 (s), 1064 (s), 1029 (m), 1000 (m), 985, 964 (m), 928 (m), 914, 882, 871, 755 (m), 744 (s), 707, 697 (m), 687 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.34–7.17 (m, 9H, H^{Ar}), 6.97–6.94 (m, 1H, H^1), 4.94 (dd, *J* = 12.5; 8.5 Hz, 1H, H^6), 4.85 (dd, *J* = 17.0; 12.5 Hz, 1H, H^5), 4.31 (dd, *J* = 17.0; 8.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 140.4 (C^4), 140.3 (C^7), 129.3 (C^9), 129.2 (C^2), 128.1 (C^{10}), 126.0 (C^8), 122.4 (C^1), 115.0 (C^3), 75.5 (C^5), 58.0 (C^6); HRMS (ES+) calculated for $C_{14}H_{14}N_3$ 224.1188, found 224.1186 ($[M + H]^+$).



4ia: R_f = 0.79 (petroleum ether/EtOAc = 80:20); ^1H NMR ($CDCl_3$, 400 MHz) δ 7.40–7.34 (m, 4H, H^{Ar}), 7.30–7.23 (m, 3H, H^{Ar}), 7.06–7.04 (m, 2H, H^{Ar}), 7.00–6.97 (m, 1H, H^{Ar}), 3.09 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.44 (dd, *J* = 6.5; 1.0 Hz, 1H, H^5), 2.39 (dd, *J* = 3.5; 1.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 154.5 (C^4), 139.4 (C^7), 129.0 (C^2), 128.4 (C^9), 127.3 (C^{10}), 126.1 (C^8), 122.5 (C^1), 120.5 (C^3), 41.5 (C^6), 37.5 (C^5). Spectroscopic data for this compound is in accordance with the literature.[25]

5-Phenyl-1-[3-(trifluoromethyl)phenyl]-Δ^2-1,2,3-triazoline (3ja):
Following the general procedure from 1-azido-3-trifluoromethylbenzene (3.00 g, 16.0 mmol) and styrene (3.70 mL, 32.0 mmol), the title compound was isolated after column chromatography as an orange oil (3.52 g, 76%).

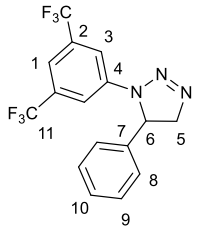


3ja: R_f = 0.44 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3034, 1615, 1594, 1490 (m), 1451 (m), 1431, 1360 (m), 1318 (m), 1288 (m), 1165 (m), 1120 (s), 1107 (s), 1085, 1070 (s), 1029, 1000 (m), 965, 926 (m), 910, 882, 862, 787 (m), 758 (m), 695 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.56 (s, 1H, H^{12}), 7.37–7.17 (m, 8H, H^{Ar}), 4.95 (dd, *J* = 12.5; 10.0 Hz, 1H, H^6), 4.91 (dd, *J* = 19.5; 12.5 Hz, 1H, H^5), 4.39 (dd, *J* = 19.5; 10.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 140.9 (C^4), 139.6 (C^7), 131.6 (q, *J* = 32 Hz, C^{13}), 129.8 (C^2), 129.5 (C^9), 128.4

(C^{10}), 126.0 (C^{8}), 124.0 (q, J = 272 Hz, C^{11}), 118.7 (q, J = 4 Hz, C^{12}), 117.6 (C^{3}), 111.7 (q, J = 4 Hz, C^{1}), 76.0 (C^{5}), 57.7 (C^{6}); ^{19}F NMR ($CDCl_3$, 377 MHz): δ -63.0 (s); HRMS (ES+) calculated for $C_{15}H_{13}N_3F_3$ 292.1062, found 292.1064 ($[M + H]^+$).

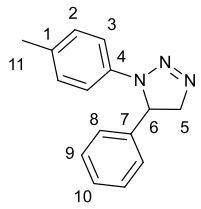
1-[3,5-Bis(trifluoromethyl)phenyl]-5-phenyl-Δ^2-1,2,3-triazoline (3ka):

Following the general procedure from 1-azido-3,5-bis(trifluoromethyl)benzene (3.00 g, 11.8 mmol) and styrene (2.70 mL, 23.6 mmol), the title compound was isolated after column chromatography as an orange solid (2.87 g, 68%).

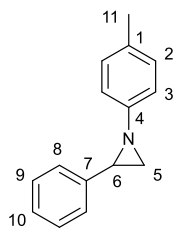


3ka: R_f = 0.70 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3034, 1621, 1519, 1495, 1477, 1466, 1403 (m), 1358, 1308, 1274 (s), 1171 (m), 1125 (s), 1088, 1074, 1046, 1028, 1008 (m), 964, 925 (m), 909, 871 (m), 782, 757, 698 (s), 681 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.60 (s, 2H, H^3), 7.42 (s, 1H, H^1), 7.39–7.30 (m, 3H, H^{Ar}), 7.19–7.17 (m, 2H, H^{Ar}), 4.98 (dd, J = 12.5; 7.0 Hz, 1H, H^6), 4.96 (dd, J = 12.5; 12.0 Hz, 1H, H^5), 4.48 (dd, J = 12.0; 7.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 141.7 (C^4), 138.8 (C^7), 132.7 (q, J = 33 Hz, C^2), 129.8 (C^9), 128.9 (C^{10}), 126.1 (C^8), 123.3 (q, J = 274 Hz, C^{11}), 115.4 (sept, J = 3 Hz, C^1), 114.5 (q, J = 3 Hz, C^3), 76.7 (C^5), 57.7 (C^6); ^{19}F NMR ($CDCl_3$, 377 MHz): δ -63.3 (s); HRMS (ES+) calculated for $C_{16}H_{12}N_3F_6$ 360.0935, found 360.0930 ($[M + H]^+$).

5-Phenyl-1-(*p*-tolyl)-Δ^2-1,2,3-triazoline (3la): Following the general procedure from 4-azidotoluene (3.00 g, 22.5 mmol) and styrene (5.20 mL, 45.0 mmol), the title compound was isolated as an off-white solid (2.30 g after recrystallisation, 0.30 g after column: 48% overall). From this reaction, 2-phenyl-1-(*p*-tolyl)aziridine **4la** was also isolated as a white solid (1.34 g, 28%) after column chromatography and recrystallisation from pentane at -18 °C.

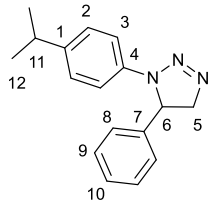


3la: Mp 105.0–108.0 °C; R_f = 0.56 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3031, 2917, 2863, 1612, 1518 (s), 1486 (s), 1457, 1429, 1415, 1351 (m), 1317, 1275, 1206, 1128, 1114, 1091 (s), 1074 (s), 1027, 1017, 996, 967, 932 (m), 914 (m), 867, 829 (m), 807 (s), 763 (s), 699 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35–7.25 (m, 3H, H^{Ar}), 7.20–7.16 (m, 2H, H^{Ar}), 7.09 (d, J = 8.5 Hz, H^3), 7.03 (d, J = 8.5 Hz, H^2), 4.92 (dd, J = 12.5; 7.5 Hz, 1H, H^6), 4.82 (dd, J = 16.5; 12.5 Hz, 1H, H^5), 4.28 (dd, J = 16.5; 7.5 Hz, 1H, H^5), 2.25 (s, 3H, H^{11}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 140.4 (C^7), 138.1 (C^4), 131.8 (C^1), 129.7 (C^2), 129.2 (C^9), 128.0 (C^{10}), 126.0 (C^8), 114.9 (C^3), 75.2 (C^5), 58.3 (C^6), 20.6 (C^{11}); HRMS (ES+) calculated for $C_{15}H_{16}N_3$ 238.1344, found 238.1332 ($[M + H]^+$).

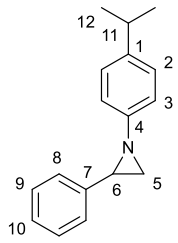


4la: Mp 50.0–51.0 °C; R_f = 0.82 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3061, 3032, 2991, 2924, 2870, 1606, 1577, 1508 (s), 1496 (m), 1462 (m), 1449, 1385 (m), 1313 (m), 1292, 1276 (m), 1215, 1155 (m), 1127, 1113, 1091, 1071, 1028, 979 (m), 906, 889, 827 (s), 819 (s), 761 (s), 699 (s), 687 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37–7.30 (m, 4H, H^{Ar}), 7.27–7.23 (m, 1H, H^{Ar}), 7.03 (d, J = 8.0 Hz, 2H, H^2), 6.92 (d, J = 8.0 Hz, 2H, H^3), 3.02 (dd, J = 6.5; 3.0 Hz, 1H, H^6), 2.38 (dd, J = 6.5; 1.0 Hz, 1H, H^5), 2.35 (dd, J = 3.0; 1.0 Hz, 1H, H^5), 2.26 (s, 3H, C^{11}); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 152.1 (C^4), 139.5 (C^7), 131.8 (C^1), 129.5 (C^2), 128.4 (C^9), 127.2 (C^{10}), 126.2 (C^8), 120.4 (C^3), 41.6 (C^6), 37.6 (C^5), 20.7 (C^{11}); HRMS (ES+) calculated for $C_{15}H_{16}N$ 210.1283, found 210.1293 ($[M + H]^+$).

1-(4-Isopropylphenyl)-5-phenyl-Δ^2-1,2,3-triazoline (3ma):
Following the general procedure from 1-azido-4-isopropylbenzene (3.00 g, 18.6 mmol) and styrene (4.30 mL, 37.2 mmol), the title compound was isolated as a yellow solid (2.09 g after recrystallisation, 0.25 g after column: 46% overall). From this reaction, 1-(4-isopropylphenyl)-2-phenylaziridine **4ma** was also isolated as a pink solid (1.27 g, 27%) after column chromatography and recrystallisation from pentane at -18 °C. Aziridine **4ma** melted to a red oil at room temperature.

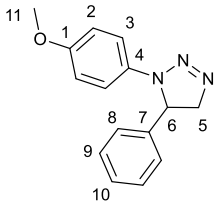


3ma: Mp 102.5–104.5 °C; R_f = 0.58 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2953 (m), 1613, 1515 (m), 1489 (s), 1466, 1456, 1432, 1361 (m), 1340 (m), 1308, 1275, 1117 (s), 1086 (s), 1077 (s), 1055 (m), 1015, 996 (m), 970 (m), 930 (m), 915 (m), 842 (m), 818 (s), 760 (m), 747 (s), 697 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.35–7.26 (m, 3H, H^{Ar}), 7.21–7.19 (m, 2H, H^{Ar}), 7.13 (d, *J* = 9.0 Hz, H^3), 7.09 (d, *J* = 9.0 Hz, H^2), 4.91 (dd, *J* = 12.5; 9.0 Hz, 1H, H^6), 4.84 (dd, *J* = 17.0; 12.5 Hz, 1H, H^5), 4.27 (dd, *J* = 17.0; 9.0 Hz, 1H, H^5), 2.82 (sept, *J* = 7.0 Hz, H^{11}), 1.19 (d, *J* = 7.0 Hz, 3H, H^{12}), 1.18 (d, *J* = 7.0 Hz, 3H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 143.0 (C^1), 140.6 (C^7), 138.4 (C^4), 129.3 (C^9), 128.0 (C^{10}), 127.1 (C^2), 126.0 (C^8), 114.9 (C^3), 75.4 (C^5), 58.4 (C^6), 33.4 (C^{11}), 24.0 (C^{12}); HRMS (ES+) calculated for $C_{17}H_{20}N_3$ 266.1657, found 266.1658 ($[M + H]^+$).



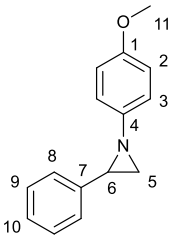
4ma: R_f = 0.83 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3028, 2958 (m), 2869, 1608 (m), 1509 (s), 1462 (m), 1390 (m), 1362, 1313 (m), 1299, 1273 (m), 1224, 1155 (m), 1128, 1094, 1052, 1013, 987, 913, 834 (s), 784, 753 (s), 736, 698 (s), 670 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.39–7.33 (m, 4H, H^{Ar}), 7.30–7.25 (m, 1H, H^{Ar}), 7.11 (d, *J* = 8.5 Hz, 2H, H^2), 6.98 (d, *J* = 8.5 Hz, 2H, H^3), 3.07 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.85 (sept, *J* = 7.0 Hz, H^{11}), 2.44 (dd, *J* = 6.5; 1.0 Hz, 1H, H^5), 2.37 (dd, *J* = 3.5; 1.0 Hz, 1H, H^5), 1.22 (d, *J* = 7.0 Hz, 6H, C^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 152.3 (C^4), 143.0 (C^1), 139.6 (C^7), 128.4 (C^9), 127.2 (C^{10}), 126.9 (C^2), 126.2 (C^8), 120.3 (C^3), 41.5 (C^6), 37.6 (C^5), 33.4 (C^{11}), 24.1 (C^{12}); HRMS (ES+) calculated for $C_{17}H_{20}N$ 238.1596, found 238.1609 ($[M + H]^+$).

1-(4-Methoxyphenyl)-5-phenyl-Δ^2-1,2,3-triazoline (3na): Following the general procedure from 4-azidoanisole (3.00 g, 20.1 mmol) and styrene (4.64 mL, 40.2 mmol), the title compound was isolated as an off-white solid (1.99 g after recrystallisation, 0.59 g after column: 51% overall). From this reaction, 1-(4-methoxyphenyl)-2-phenylaziridine **4na** was also isolated after the filtrate from recrystallisation was treated with $NaBH_4$ (0.15 g, 4.0 mmol) in EtOH (6 mL) at 60 °C for 6 h to reduce the imine by-product. Aziridine **4na** was isolated as an orange oil (1.33 g, 29%) after column chromatography on basified silica (eluent: petroleum ether/toluene 0→5% gradient basified with 2% NEt_3).



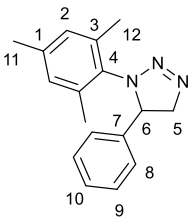
3na: Mp 100.5–102.0 °C; R_f = 0.38 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3025, 2931, 2837, 1586, 1510 (s), 1482 (s), 1454, 1442, 1430, 1422, 1349, 1302, 1245 (s), 1178 (m), 1120 (m), 1086 (s), 1071 (s), 1041 (m), 1028 (s), 992, 961, 928 (m), 906, 870, 826 (s), 802 (m), 754 (s), 696 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.35–7.26 (m, 3H, H^{Ar}), 7.19–7.17 (m, 2H, H^{Ar}), 7.12 (d, *J* = 9.0 Hz, H^3), 6.78 (d, *J* = 9.0 Hz, H^2), 4.90 (dd, *J* = 12.5; 9.0 Hz, 1H, H^6), 4.83 (dd, *J* = 17.0; 12.5 Hz, 1H, H^5), 4.26 (dd, *J* = 17.0; 9.0 Hz, 1H, H^5), 3.73

(s, 3H, H^{11}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 155.4 (C^1), 140.4 (C^7), 134.4 (C^4), 129.3 (C^9), 128.1 (C^{10}), 126.1 (C^8), 116.5 (C^3), 114.5 (C^2), 75.2 (C^5), 59.0 (C^6), 55.5 (C^{11}); HRMS (ES+) calculated for $C_{15}H_{16}N_3O$ 254.1293, found 254.1287 ($[M + H]^+$).

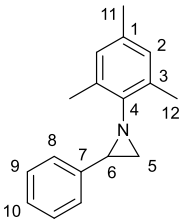


4na: R_f = 0.69 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3036, 2950, 2833, 1606, 1586, 1505 (s), 1463 (m), 1441, 1390, 1293, 1269, 1238 (s), 1179 (m), 1156, 1128, 1109, 1095, 1074, 1034 (m), 985, 912, 830 (m), 802, 761 (m), 699 (m), 681 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.37–7.32 (m, 4H, H^{Ar}), 7.28–7.25 (m, 1H, H^{Ar}), 6.97 (d, *J* = 8.5 Hz, 2H, H^3), 6.79 (d, *J* = 8.5 Hz, 2H, H^2), 3.74 (s, 3H, H^{11}), 3.01 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.39 (dd, *J* = 6.5; 0.5 Hz, 1H, H^5), 2.35 (dd, *J* = 3.5; 0.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 155.2 (C^1), 147.9 (C^4), 139.5 (C^7), 128.4 (C^9), 127.2 (C^{10}), 126.2 (C^8), 121.3 (C^3), 114.3 (C^2), 55.5 (C^{11}), 41.9 (C^6), 37.8 (C^5); HRMS (ES+) calculated for $C_{15}H_{16}NO$ 226.1232, found 226.1230 ($[M + H]^+$).

1-Mesityl-5-phenyl-Δ²-1,2,3-triazoline (3oa): Following the general procedure from mesityl azide (3.00 g, 18.6 mmol) and styrene (4.30 mL, 37.2 mmol), the title compound was isolated as a pale yellow solid (2.65 g after recrystallisation, 0.11 g after column: 56% overall). From this reaction, 1-mesityl-2-phenylaziridine **4oa** was also isolated as a pale yellow solid (0.50 g, 11%) after column chromatography and recrystallisation from pentane at -18 °C. Aziridine **4oa** melted to a pale yellow oil at room temperature.

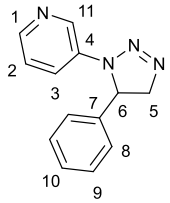


3oa: Mp 126.6–128.6 °C; R_f = 0.47 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2952, 2925, 1605, 1585, 1491, 1477 (s), 1456 (m), 1433, 1378, 1361, 1327, 1295, 1277, 1262, 1204, 1158, 1090 (s), 1074 (s), 1032 (s), 990, 927 (m), 906 (m), 860 (m), 772 (m), 757, 734, 701 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.26–7.25 (m, 3H, H^{Ar}), 7.15–7.13 (m, 2H, H^{Ar}), 6.79 (s, 2H, H^2), 4.86 (dd, *J* = 15.5; 12.0 Hz, 1H, H^5), 4.73 (dd, *J* = 12.0; 9.0 Hz, 1H, H^6), 4.62 (dd, *J* = 15.5; 9.0 Hz, 1H, H^5), 2.22 (s, 3H, H^{11}), 1.97 (s, 6H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 139.3 (C^7), 137.8 (C^1), 136.8 (C^3), 134.4 (C^4), 129.5 (C^2), 128.6 (C^9), 128.2 (C^{10}), 128.0 (C^8), 72.6 (C^5), 61.4 (C^6), 20.9 (C^{11}), 18.5 (C^{12}); HRMS (ES+) calculated for $C_{17}H_{20}N_3$ 266.1657, found 266.1663 ($[M + H]^+$).

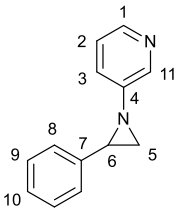


4oa: R_f = 0.82 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3032, 2980, 1598 (m), 1488 (s), 1464 (m), 1451, 1393 (m), 1314 (m), 1298, 1275 (m), 1222, 1152 (m), 1129, 1101, 1078, 1058, 1025, 1001, 986, 912, 895, 855, 758 (s), 721 (m), 694 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.41–7.34 (m, 4H, H^{Ar}), 7.30–7.26 (m, 1H, H^{Ar}), 6.77 (s, 2H, H^2), 3.04 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.45 (dd, *J* = 3.5; 0.5 Hz, 1H, H^5), 2.41 (dd, *J* = 6.5; 0.5 Hz, 1H, H^5), 2.26 (s, 6H, H^{12}), 2.22 (s, 3H, H^{11}); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 148.6 (C^4), 140.0 (C^7), 131.2 (C^1), 129.8 (C^2), 129.0 (C^3), 128.6 (C^9), 127.4 (C^{10}), 126.2 (C^8), 43.2 (C^6), 41.1 (C^5), 20.7 (C^{11}), 19.4 (C^{12}); HRMS (ES+) calculated for $C_{17}H_{20}N$ 238.1596, found 238.1596 ($[M + H]^+$).

3-(5-Phenyl-Δ²-1,2,3-triazolin-1-yl)pyridine (3pa): Following the general procedure at 70 °C for 24 h from 3-azidopyridine (1.50 g, 12.5 mmol) and styrene (2.89 mL, 25.0 mmol), the title compound was isolated as an orange solid (1.70 g after recrystallisation, 0.03 g after column: 62% overall). From this reaction, 3-(2-phenylaziridin-1-yl)pyridine **4pa** was also isolated as an orange oil (0.34 g, 14%) after column chromatography.

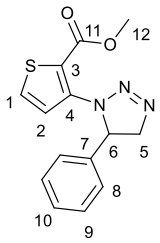


3pa: Mp 119.3–121.2 °C; R_f = 0.08 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2984, 1585 (m), 1572, 1489 (s), 1455, 1429 (s), 1400, 1363 (m), 1339, 1241, 1194, 1130, 1110 (m), 1085 (s), 1073 (s), 1047 (m), 1028, 1018, 984, 962 (m), 927 (m), 913 (m), 804 (s), 756 (s), 707 (s), 696 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.44 (d, *J* = 2.5 Hz, 1H, H^{11}), 8.22 (dd, *J* = 4.5; 1.5 Hz, 1H, H^1), 7.60 (ddd, *J* = 8.5; 2.5; 1.5 Hz, 1H, H^3), 7.38–7.27 (m, 3H, H^{Ar}), 7.19–7.17 (m, 3H, H^1), 4.95 (dd, *J* = 12.5; 9.0 Hz, 1H, H^6), 4.92 (dd, *J* = 18.0; 12.5 Hz, 1H, H^5), 4.39 (dd, *J* = 18.0; 9.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 143.7 (C^1), 139.2 (C^7), 136.8 (C^4), 136.4 (C^{11}), 129.5 (C^9), 128.5 (C^{10}), 126.0 (C^8), 123.7 (C^2), 121.8 (C^3), 76.0 (C^5), 57.5 (C^6); HRMS (ES+) calculated for $C_{13}H_{13}N_4$ 225.1140, found 225.1137 ($[M + H]^+$).



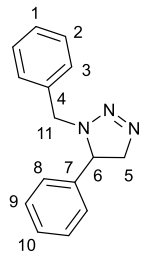
4pa: R_f = 0.17 (petroleum ether/EtOAc = 80:20); ν_{max} 3030, 2982, 1580 (m), 1573 (m), 1476 (s), 1463 (m), 1420 (s), 1392 (m), 1316 (m), 1298 (m), 1282 (m), 1224, 1160, 1099, 1041, 1033, 1018, 911, 807 (m), 778, 763, 734 (s), 709 (s), 697 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.40 (d, *J* = 2.5 Hz, 1H, H^{11}), 8.25 (d, *J* = 4.5 Hz, 1H, H^1), 7.39–7.36 (m, 4H, H^{Ar}), 7.32–7.28 (m, 2H, H^{Ar}), 7.16 (dd, *J* = 8.0; 4.5 Hz, 1H, H^2), 3.12 (dd, *J* = 6.0; 3.5 Hz, 1H, H^6), 2.48 (dd, *J* = 6.5; 0.5 Hz, 1H, H^5), 2.47 (dd, *J* = 3.5; 0.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 150.5 (C^4), 143.9 (C^1), 143.2 (C^{11}), 138.5 (C^7), 128.6 (C^9), 127.7 (C^{10}), 127.7 (C^3), 126.2 (C^8), 123.5 (C^2), 41.5 (C^6), 37.4 (C^5); HRMS (ES+) calculated for $C_{13}H_{13}N_2$ 197.1079, found 197.1084 ($[M + H]^+$).

Methyl 3-(5-phenyl-Δ²-1,2,3-triazolin-1-yl)thiophene-2-carboxylate (3ra):
Following the general procedure at 60 °C for 32 h from methyl 3-azido-2-thiophenecarboxylate (3.00 g, 16.4 mmol) and styrene (3.77 mL, 32.8 mmol), the title compound was isolated as a pale yellow solid (1.55 g, 33%) after column chromatography.

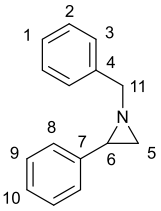


3ra: Mp 95.6–98.1 °C; R_f = 0.38 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3119, 3092, 3012, 2951, 1692 (s, C=O), 1575, 1545 (m), 1502 (s), 1430 (s), 1410 (m), 1309, 1298, 1281 (m), 1245 (s), 1204 (m), 1114 (m), 1091 (m), 1069 (m), 1023 (s), 1002, 969, 958 (m), 928 (m), 904 (m), 834, 779 (s), 769, 754 (s), 742 (m), 700 (s), 650 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.38 (d, *J* = 5.5 Hz, 1H, H^1), 7.33 (d, *J* = 5.5 Hz, 1H, H^2), 7.22–7.16 (m, 3H, H^{Ar}), 6.95–6.92 (m, 2H, H^{Ar}), 5.85 (dd, *J* = 12.0; 5.5 Hz, 1H, H^6), 4.79 (dd, *J* = 17.0; 12.0 Hz, 1H, H^5), 4.60 (dd, *J* = 17.0; 5.5 Hz, 1H, H^5), 3.82 (s, 3H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 161.4 (C^{11}), 143.6 (C^4), 139.4 (C^7), 130.4 (C^1), 128.8 (C^9), 128.1 (C^{10}), 126.5 (C^8), 124.2 (C^2), 112.1 (C^3), 76.0 (C^5), 58.3 (C^6), 52.0 (C^{12}); HRMS (ES+) calculated for $C_{14}H_{14}N_3O_2S$ 288.0807, found 288.0810 ($[M + H]^+$).

1-Benzyl-5-phenyl-Δ²-1,2,3-triazoline (3sa): Following the general procedure at 85 °C for 16 h from benzyl azide (3.00 g, 22.5 mmol) and styrene (5.21 mL, 45.0 mmol), the title compound was isolated as a dark yellow oil (1.51 g, 28%) after column chromatography. From this reaction, 1-benzyl-2-phenylaziridine **4sa** was also isolated as a yellow oil (1.37 g, 29%) after column chromatography.

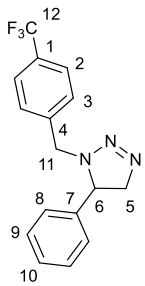


3sa: R_f = 0.45 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3030, 2913, 1602, 1491 (m), 1455 (m), 1431, 1355, 1329, 1262, 1219, 1157, 1090, 1057 (m), 1028 (m), 1002, 969, 934 (m), 911, 845, 818, 756 (s), 698 (s), 663 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.37–7.28 (m, 6H, H^{Ar}), 7.20–7.16 (m, 4H, H^{Ar}), 5.17 (d, *J* = 15.0 Hz, 1H, H^{11}), 4.61 (dd, *J* = 15.5; 11.5 Hz, 1H, H^5), 4.13 (d, *J* = 15.0 Hz, 1H, H^{11}), 4.13 (dd, *J* = 12.0; 11.5 Hz, 1H, H^6), 4.01 (dd, *J* = 15.5; 12.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 138.9 (C^7), 135.5 (C^4), 128.9 (CH^{Ar}), 128.8 (CH^{Ar}), 128.6 (CH^{Ar}), 128.2 (CH^{Ar}), 127.8 (CH^{Ar}), 127.3 (CH^{Ar}), 74.1 (C^5), 60.3 (C^6), 51.9 (C^{11}); HRMS (CI+) calculated for $C_{15}H_{16}N_3$ 238.1339, found 238.1328 ($[M + H]^+$); Elemental analysis calculated for $C_{15}H_{15}N_3$: C, 75.92; H, 6.37; N, 17.71, found: C, 75.72; H, 6.22; N, 17.53.

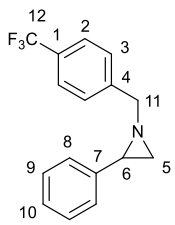


4sa: R_f = 0.62 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3030, 2978, 2829, 1603, 1495 (m), 1452 (m), 1388, 1356, 1325, 1310, 1263, 1212, 1196, 1143, 1085, 1065, 1028 (m), 949, 911, 827, 749 (m), 731 (s), 696 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.37–7.19 (m, 10H, H^{Ar}), 3.69 (d, *J* = 14.0 Hz, 1H, H^{11}), 3.60 (d, *J* = 14.0 Hz, 1H, H^{11}), 2.50 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 1.98 (d, *J* = 3.5 Hz, 1H, H^5), 1.84 (d, *J* = 6.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.1 (C^4), 139.1 (C^7), 128.3 (CH^{Ar}), 128.2 (CH^{Ar}), 127.8 (CH^{Ar}), 126.9 (CH^{Ar}), 126.8 (CH^{Ar}), 126.2 (C^{Ar}), 64.7 (C^{11}), 41.5 (C^6), 37.9 (C^5); HRMS (ES+) calculated for $C_{15}H_{16}N$ 210.1283, found 210H.1290 ($[M + H]^+$). Spectroscopic data for this compound is in accordance with the literature.[26]

5-Phenyl-1-[4-(trifluoromethyl)benzyl]-Δ^2-1,2,3-triazoline (3ta): Following the general procedure at 85 °C for 24 h from 1-(azidomethyl)-4-(trifluoromethyl)benzene (3.00 g, 14.9 mmol) and styrene (3.45 mL, 29.8 mmol), the title compound was isolated as an orange oil after column chromatography and solidified when triturated with pentane/Et_2O (6:1) at -18 °C to give a pale yellow solid (1.90 g, 42%). From this reaction, 2-phenyl-1-[4-(trifluoromethyl)benzyl]aziridine **4ta** was also isolated as a pale yellow solid (0.91 g, 22%) after column chromatography and recrystallisation from pentane at -18 °C. Aziridine **4ta** melted to a pale yellow oil at room temperature.

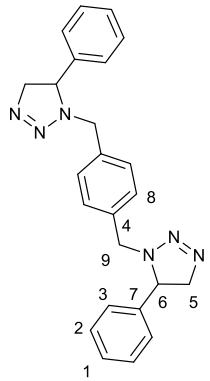


3ta: Mp 55.2–56.6 °C; R_f = 0.44 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 1619, 1510, 1493, 1422, 1321 (s), 1272, 1166 (m), 1153 (m), 1120 (s), 1110 (s), 1065 (s), 1034, 1017 (s), 1002, 928 (s), 910, 883, 857 (m), 848, 842, 827 (m), 789, 752 (s), 731, 697 (s), 668 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.56 (d, *J* = 8.0 Hz, 2H, H^2), 7.37–7.31 (m, 3H, H^{Ar}), 7.29 (d, *J* = 8.0 Hz, 2H, H^3), 7.18–7.15 (m, 2H, H^{Ar}), 5.11 (d, *J* = 15.0 Hz, 1H, H^{11}), 4.65 (dd, *J* = 16.0; 11.5 Hz, 1H, H^5), 4.26 (d, *J* = 15.0 Hz, 1H, H^{11}), 4.13 (dd, *J* = 12.0; 11.5 Hz, 1H, H^6), 4.07 (dd, *J* = 16.0; 12.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 139.8 (C^4), 138.4 (C^7), 130.1 (q, *J* = 32 Hz, C^1), 129.1 (C^3), 129.0 (C^9), 128.4 (C^{10}), 127.3 (C^8), 125.6 (q, *J* = 4 Hz, C^2), 124.0 (q, *J* = 273 Hz, C^{12}), 74.3 (C^5), 60.8 (C^6), 51.6 (C^{11}); ^{19}F NMR ($CDCl_3$, 377 MHz): δ -62.7 (s); HRMS (CI+) calculated for $C_{16}H_{15}N_3F_3$ 306.1213, found 306.1200 ($[M + H]^+$).

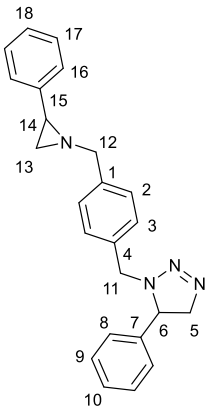


4ta: R_f = 0.67 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3044, 2981, 2828, 1619, 1606, 1497, 1467, 1452, 1418, 1392, 1323 (s), 1258, 1214, 1161 (m), 1119 (s), 1107 (s), 1086, 1065 (s), 1031, 1018 (m), 948, 824, 746 (m), 727, 697 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.54 (d, *J* = 8.0 Hz, 2H, H^2), 7.47 (d, *J* = 8.0 Hz, 2H, H^3), 7.31–7.20 (m, 5H, H^{Ar}), 3.74 (d, *J* = 14.5 Hz, 1H, H^{11}), 3.60 (d, *J* = 14.5 Hz, 1H, H^{11}), 2.47 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.00 (d, *J* = 3.5 Hz, 1H, H^5), 1.82 (d, *J* = 6.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 143.3 (C^4), 139.8 (C^7), 129.2 (q, *J* = 32 Hz, C^1), 128.4 (C^3), 127.9 (C^9), 127.1 (C^{10}), 126.1 (C^8), 125.3 (q, *J* = 3.5 Hz, C^2), 124.3 (q, *J* = 273 Hz, C^{12}), 64.1 (C^{11}), 41.7 (C^6), 38.1 (C^5); ^{19}F NMR ($CDCl_3$, 377 MHz): δ -62.5 (s); HRMS (ES+) calculated for $C_{16}H_{15}NF_3$ 278.1157, found 278.1153 ($[M + H]^+$).

1,4-Bis[(5-phenyl-Δ²-1,2,3-triazolin-1-yl)methyl]benzene (33va): Following the general procedure at 80 °C for 24 h from 1,4-bis(azidomethyl)benzene (0.93 g, 4.9 mmol) and styrene (2.26 mL, 19.6 mmol), the title compound was isolated as a white solid (0.29 g after recrystallisation, 0.09 g after column: 20% overall). From this reaction, 5-phenyl-1-{4-[(2-phenylaziridin-1-yl)methyl]benzyl}-Δ²-1,2,3-triazoline **34va** (orange oil, 0.52 g, 29%), 1-[4-(azidomethyl)benzyl]-5-phenyl-Δ²-1,2,3-triazoline **31va** (yellow oil, 0.08 g, 6%) and 1,4-bis[(2-phenylaziridin-1-yl)methyl]benzene **44va** (yellow oil, 0.02 g, 1%) were also isolated after column chromatography.

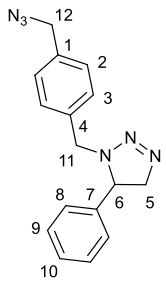


33va: Mp 158.4–160.5 °C; R_f = 0.13 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2911, 1603, 1490 (m), 1457, 1440, 1426, 1363, 1346, 1327, 1257, 1210, 1153, 1113, 1080, 1053 (m), 1032 (m), 1016 (m), 935 (m), 913 (m), 878, 855, 840, 768, 752 (s), 696 (s), 668 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.38–7.32 (m, 6H, H^{Ar}), 7.19–7.17 (m, 4H, H^{Ar}), 7.11 (s, 4H, H^8), 5.08 (d, *J* = 15.0 Hz, 1H, H^9), 4.63 (dd, *J* = 15.5; 11.0 Hz, 1H, H^5), 4.16 (d, *J* = 15.0 Hz, 1H, H^9), 4.13 (dd, *J* = 12.0; 11.0 Hz, 1H, H^6), 4.03 (dd, *J* = 15.5; 12.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 138.8 (C^7), 135.2 (C^4), 129.0 (C^8), 129.0 (C^2), 128.2 (C^1), 127.3 (C^3), 74.2 (C^5), 60.5 (C^6), 51.6 (C^9); HRMS (ES+) calculated for $C_{24}H_{25}N_6$ 397.2141, found 397.2129 ($[M + H]^+$).

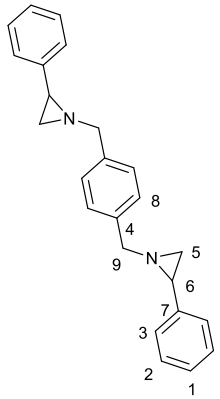


34va: R_f = 0.21 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3030, 2974, 2923, 1604, 1513, 1492 (m), 1455, 1421, 1389, 1349, 1261, 1215, 1156, 1064 (m), 1033 (m), 1019 (m), 970, 935 (m), 911 (m), 830, 751 (s), 731 (s), 698 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.35–7.15 (m, 12H, H^{Ar}), 7.11 (d, *J* = 8.0 Hz, 2H, H^{Ar}), 5.15 (d, *J* = 15.0 Hz, 1H, H^{11}), 4.59 (dd, *J* = 15.5; 11.5 Hz, 1H, H^5), 4.11 (dd, *J* = 12.5; 11.5 Hz, 1H, H^6), 4.09 (dd, *J* = 15.0; 1.5 Hz, 1H, H^{11}), 3.99 (dd, *J* = 15.5; 12.5 Hz, 1H, H^5), 3.68 (dd, *J* = 14.0; 6.0 Hz, 1H, H^{12}), 3.58 (dd, *J* = 14.0; 4.5 Hz, 1H, H^{12}), 2.50 (dt, *J* = 6.5; 3.0 Hz, 1H, H^{14}), 1.99 (d, *J* = 3.0 Hz, 1H, H^{13}), 1.85 (dd, *J* = 6.5; 1.0 Hz, 1H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.0 (C^1), 138.9 (C^7), 138.8 (C^{15}), 134.1 (C^4), 128.9 (CH^{Ar}), 128.8 (CH^{Ar}), 128.3 (CH^{Ar}), 128.1 (CH^{Ar}), 128.0 (CH^{Ar}), 127.3 (CH^{Ar}), 126.9 (CH^{Ar}), 126.2 (CH^{Ar}), 74.0 (C^5), 64.4 (C^{12}), 60.2 (C^6), 51.6 (C^{11}),

41.5 (C^{14}), 38.0 (C^{13}); HRMS (ES+) calculated for $C_{24}H_{25}N_4$ 369.2079, found 369.2084 ($[M + H]^+$).

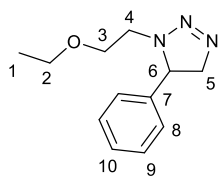


31va: R_f = 0.33 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2923, 2093 (s, N_3), 1720, 1675, 1601, 1514, 1491, 1455, 1421, 1345, 1252 (m), 1066, 1033, 1020, 970, 935, 915, 879, 845, 817, 757 (m), 699 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37–7.30 (m, 3H, H^{Ar}), 7.27–7.25 (m, 2H, H^{Ar}), 7.20–7.17 (m, 4H, H^{Ar}), 5.14 (d, *J* = 15.0 Hz, 1H, H^{11}), 4.63 (dd, *J* = 15.5; 11.0 Hz, 1H, H^5), 4.33 (s, 2H, H^{12}), 4.16 (d, *J* = 15.0 Hz, 1H, H^{11}), 4.14 (dd, *J* = 12.0; 11.0 Hz, 1H, H^6), 4.03 (dd, *J* = 15.5; 12.0 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 138.7 (C^7), 135.7 (C^1), 135.0 (C^4), 129.2 (CH^{Ar}), 129.0 (C^9), 128.4 (CH^{Ar}), 128.2 (C^{10}), 127.3 (C^8), 74.1 (C^5), 60.4 (C^6), 54.4 (C^{12}), 51.5 (C^{11}); HRMS (EI+) calculated for $C_{16}H_{16}N_6$ 292.1436, found 292.1447 ($[M]^+$).

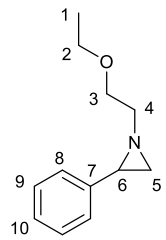


44va: R_f = 0.30 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3030, 2972, 2923, 1668, 1605, 1514, 1495, 1451, 1419, 1389, 1351, 1257, 1197, 1143, 1108, 1084, 1064, 1033 (m), 1019 (m), 950, 913, 798, 748 (s), 697 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.34–7.19 (m, 14H, H^{Ar}), 3.64 (d, *J* = 14.0 Hz, 1H, H^9), 3.59 (d, *J* = 14.0 Hz, 1H, H^9), 2.48 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 1.96 (d, *J* = 3.5 Hz, 1H, H^5), 1.82 (d, *J* = 6.5 Hz, 1H, H^5); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.2 (C^4), 137.8 (C^7), 128.3 (C^8), 127.9 (C^2), 126.8 (C^1), 126.2 (C^3), 64.5 (C^9), 41.5 (C^6), 38.0 (C^5); HRMS (ES+) calculated for $C_{24}H_{25}N_2$ 341.2018, found 341.2023 ($[M + H]^+$).

1-(2-Ethoxyethyl)-5-phenyl-Δ^2-1,2,3-triazoline (3wa): Following the general procedure at 70 °C for 16 h from 1-azido-2-ethoxyethane (3.00 g, 26.1 mmol) and styrene (6.03 mL, 52.2 mmol), the title compound was isolated as an orange oil (0.91 g, 16%) after column chromatography (eluent: petroleum ether/EtOAc 0→10% gradient basified with 2% v/v NEt_3). From this reaction, 1-(2-ethoxyethyl)-2-phenylaziridine **4wa** was also isolated as a yellow oil (0.25 g, 5%) after column chromatography.



3wa: R_f = 0.51 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3032, 2974, 2865, 1602, 1489 (m), 1456, 1378, 1351, 1323, 1266, 1113 (s), 1079 (m), 1027 (m), 972, 935 (m), 847, 817, 756 (m), 699 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37–7.27 (m, 3H, H^{Ar}), 7.25–7.20 (m, 2H, H^{Ar}), 4.67 (dd, *J* = 16.0; 12.0 Hz, 1H, H^5), 4.50 (dd, *J* = 12.0; 11.0 Hz, 1H, H^6), 4.05 (dd, *J* = 16.0; 11.0 Hz, 1H, H^5), 3.78 (dt, *J* = 14.0; 5.0 Hz, 1H, H^4), 3.65–3.55 (m, 2H, H^3 + H^4), 3.51–3.36 (m, 3H, H^2 + H^3), 1.16 (t, *J* = 7.0 Hz, 3H, H^1); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 139.6 (C^7), 128.9 (C^9), 128.1 (C^{10}), 127.2 (C^8), 74.1 (C^5), 68.7 (C^3), 66.3 (C^2), 62.3 (C^6), 47.8 (C^4), 15.2 (C^1); HRMS (ES+) calculated for $C_{12}H_{18}N_3O$ 220.1450, found 220.1453 ($[M + H]^+$).



4wa: R_f = 0.69 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3032, 2975, 2930, 2864, 1606, 1496, 1451, 1379, 1350, 1311, 1247, 1208, 1114 (s), 1086 (m), 1064, 1029, 931, 832, 793, 738 (s), 696 (s) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.31–7.18 (m, 5H, H^{Ar}), 3.65 (td, *J* = 6.0; 1.5 Hz, 2H, H^3), 3.52 (qd, *J* = 7.0; 2.5 Hz, 1H, H^2), 3.49 (qd, *J* = 7.0; 2.5 Hz, 1H, H^2), 2.70 (dt, *J* = 12.0; 6.0 Hz, 1H, H^4), 2.56 (dt, *J* = 12.0; 6.0 Hz, 1H, H^4), 2.41 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 1.93 (d, *J* = 3.5 Hz, 1H, H^5), 1.74 (d, *J* = 6.5 Hz, 1H, H^5), 1.18 (t, *J* = 7.0 Hz, 3H, H^1); ^{13}C NMR

($CDCl_3$, 101 MHz): δ 140.2 (C^7), 128.2 (C^9), 126.8 (C^{10}), 126.3 (C^8), 70.1 (C^3), 66.6 (C^2), 60.9 (C^4), 41.1 (C^6), 37.3 (C^5), 15.2 (C^1); HRMS (ES+) calculated for $C_{12}H_{18}NO$ 192.1388, found 192.1388 ($[M + H]^+$).

Ethyl 4-[5-(4-chlorophenyl)-Δ²-1,2,3-triazolin-1-yl]benzoate (3db): Following the general procedure at 80 °C for 24 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and 4-chlorostyrene (3.79 mL, 31.4 mmol), the title compound was isolated as a pale yellow solid (1.65 g after recrystallisation, 0.35 g after column: 39% overall).

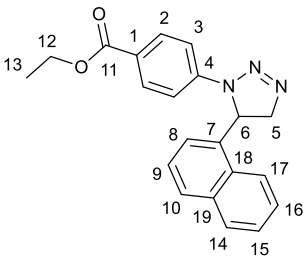
3db: Mp 126.4–128.6 °C; R_f = 0.30 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2976, 1699 (s, C=O), 1605 (s), 1508 (s), 1488 (m), 1475, 1450, 1410, 1366, 1351 (m), 1308, 1275 (s), 1201, 1181 (m), 1131 (m), 1116 (s), 1104 (s), 1089 (m), 1063 (s), 1025 (m), 1013 (m), 979 (m), 959, 951, 945 (m), 919 (s), 870, 847 (m), 842, 821 (s), 766 (s), 692 (m), 632, 604 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.94 (d, *J* = 9.0 Hz, 2H, H^2), 7.31 (d, *J* = 8.5 Hz, 2H, H^9), 7.19 (d, *J* = 9.0 Hz, 2H, H^3), 7.09 (d, *J* = 8.5 Hz, 2H, H^8), 4.97 (dd, *J* = 12.5; 7.5 Hz, 1H, H^6), 4.89 (dd, *J* = 17.5; 12.5 Hz, 1H, H^5), 4.37 (dd, *J* = 17.5; 7.5 Hz, 1H, H^5), 4.32 (q, *J* = 7.0 Hz, 2H, H^{12}), 1.35 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.1 (C^{11}), 143.4 (C^4), 138.1 (C^7), 134. 2 (C^{10}), 131.1 (C^2), 129.7 (C^9), 127.2 (C^8), 124.2 (C^1), 114.1 (C^3), 75.9 (C^5), 60.7 (C^{12}), 56.7 (C^6), 14.4 (C^{13}); HRMS (ES+) calculated for $C_{17}H_{17}N_3O_2Cl$ 330.1009, found 330.1017 ($[M + H]^+$).

Ethyl 4-[5-(4-methoxyphenyl)-Δ²-1,2,3-triazolin-1-yl]benzoate (3dc):

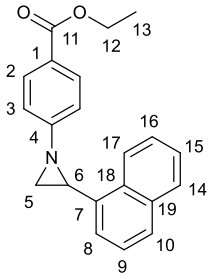
Following the general procedure from 4-ethylazidobenzoate (1.00 g, 5.2 mmol) and 4-vinylanisole (1.38 mL, 10.4 mmol), the title compound was isolated as a pale yellow solid (1.19 g, 70%) after recrystallisation.

3dc: Mp 72.3–76.5 °C; R_f = 0.20 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2977, 1702 (s, C=O), 1607 (s), 1512 (s), 1499 (s), 1466 (m), 1446, 1361 (m), 1307, 1278 (s), 1247 (s), 1175 (s), 1123 (s), 1111 (s), 1077 (s), 1023 (s), 988 (m), 960, 941, 922 (s), 846 (m), 837 (m), 825, 814 (s), 765 (s), 693 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 9.0 Hz, 2H, H^2), 7.23 (d, *J* = 9.0 Hz, 2H, H^3), 7.06 (d, *J* = 8.5 Hz, 2H, H^8), 6.85 (d, *J* = 8.5 Hz, 2H, H^9), 4.95 (dd, *J* = 12.5; 7.5 Hz, 1H, H^6), 4.88 (dd, *J* = 17.5; 12.5 Hz, 1H, H^5), 4.37 (dd, *J* = 17.5; 7.5 Hz, 1H, H^5), 4.31 (q, *J* = 7.0 Hz, 2H, H^{12}), 3.77 (s, 3H, H^{14}), 1.35 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{11}), 159.5 (C^{10}), 143.7 (C^4), 131.5 (C^7), 131.1 (C^2), 127.1 (C^8), 123.9 (C^1), 114.8 (C^9), 114.1 (C^3), 76.0 (C^5), 60.7 (C^{12}), 56.8 (C^6), 55.3 (C^{14}), 14.4 (C^{13}); HRMS (ES+) calculated for $C_{18}H_{20}N_3O_3$ 326.1505, found 326.1491 ($[M + H]^+$).

Ethyl 4-[5-(4-chlorophenyl)-Δ²-1,2,3-triazolin-1-yl]benzoate (3dd): Following the general procedure at 80 °C for 24 h from 4-ethylazidobenzoate (1.50 g, 7.8 mmol) and 1-vinylnaphthalene (2.32 mL, 15.6 mmol), the title compound was isolated as a yellow solid (1.14 g, 42%) after column chromatography. From this reaction, ethyl 4-[2-(naphthalen-1-yl)aziridin-1-yl]benzoate **4dd** was also isolated as an orange oil (0.35 g, 14%) after column chromatography.

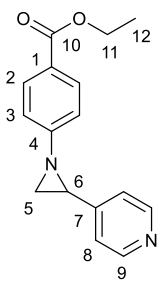


3dd: Single crystals for X-ray diffraction were grown from Et_2O, CCDC 1843143 Mp 122.6–126.8 °C; R_f = 0.30 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2983, 1704 (s, C=O), 1606 (s), 1507 (s), 1472, 1366 (m), 1312, 1273 (s), 1232, 1182 (m), 1107 (s), 1089 (m), 1075 (m), 1033 (m), 1017 (s), 988, 955, 928 (s), 876, 846 (m), 796 (s), 765 (s), 734 (m), 717, 693 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.95–7.92 (m, 2H, H^{Ar}), 7.90 (d, *J* = 9.0 Hz, 2H, H^2), 7.79 (d, *J* = 8.0 Hz, 1H, H^{Ar}), 7.65–7.55 (br m, 2H, H^{Ar}), 7.34 (t, *J* = 8.0 Hz, 1H, H^{Ar}), 7.20 (d, *J* = 9.0 Hz, 2H, H^3), 7.10 (br s, 1H, H^{Ar}), 5.67 (br s, 1H, H^6), 5.08 (dd, *J* = 17.0; 12.5 Hz, 1H, H^5), 4.40 (br dd, *J* = 17.0; 5.0 Hz, 1H, H^5), 4.30 (q, *J* = 7.0 Hz, 2H, H^{12}), 1.33 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.1 (C^{11}), 143.8 (C^4), 134.2 (C^{Ar}), 133.9 (C^{Ar}), 131.1 (C^2), 129.8 (C^{Ar}), 129.4 (CH^{Ar}), 128.7 (CH^{Ar}), 126.9 (CH^{Ar}), 126.2 (CH^{Ar}), 125.7 (CH^{Ar}), 124.0 (C^1), 122.7 (C^{Ar}), 122.1 (CH^{Ar}), 114.0 (C^3), 75.1 (C^5), 60.7 (C^{12}), 53.4 (C^6), 14.3 (C^{13}); HRMS (ES+) calculated for $C_{21}H_{20}N_3O_2$ 346.1556, found 346.1548 ($[M + H]^+$).



4dd: R_f = 0.54 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3048, 2981, 1704 (s, C=O), 1601 (s), 1508 (m), 1463, 1416, 1366 (m), 1345, 1306, 1268 (s), 1166 (s), 1150 (s), 1099 (s), 1016 (m), 983, 908, 855 (m), 800 (m), 773 (s), 734, 701 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.11 (d, *J* = 9.0 Hz, 1H, H^{Ar}), 7.97 (d, *J* = 8.5 Hz, 2H, H^2), 7.88–7.84 (m, 1H, H^{Ar}), 7.77 (d, *J* = 8.0 Hz, 1H, H^{Ar}), 7.72 (d, *J* = 7.0 Hz, 1H, H^{Ar}), 7.54–7.46 (m, 2H, H^{Ar}), 7.45 (t, *J* = 7.5 Hz, 1H, H^{Ar}), 7.10 (d, *J* = 8.5 Hz, 2H, H^3), 4.33 (q, *J* = 7.0 Hz, 2H, H^{12}), 3.69 (dd, *J* = 6.5; 3.5 Hz, 1H, H^6), 2.61 (dd, *J* = 6.5; 1.5 Hz, 1H, H^5), 2.41 (dd, *J* = 3.5; 1.5 Hz, 1H, H^5), 1.36 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{11}), 159.0 (C^4), 134.5 (C^{Ar}), 133.3 (C^{Ar}), 131.4 (C^{Ar}), 130.9 (C^2), 128.7 (C^{Ar}), 127.8 (CH^{Ar}), 126.2 (CH^{Ar}), 125.8 (CH^{Ar}), 125.6 (CH^{Ar}), 124.5 (C^1), 123.6 (CH^{Ar}), 122.9 (CH^{Ar}), 120.1 (C^3), 60.6 (C^{12}), 39.8 (C^6), 37.1 (C^5), 14.3 (C^{13}); HRMS (ES+) calculated for $C_{21}H_{20}NO_2$ 318.1494, found 318.1504 ($[M + H]^+$).

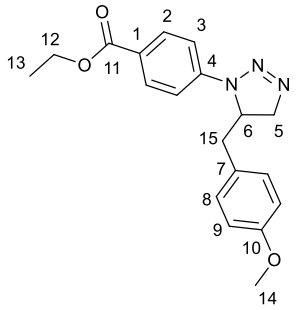
Ethyl 4-[2-(pyridin-4-yl)aziridin-1-yl]benzoate (4de): Following the general procedure from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and 4-vinylpyridine (3.41 mL, 31.4 mmol), the title compound was isolated as a yellow solid (1.33 g, 31%) after column chromatography (eluent: petroleum ether/EtOAc 0→75% gradient basified with 2% v/v NEt_3).



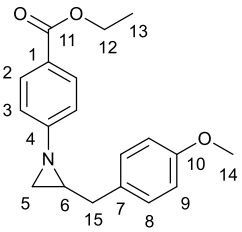
4de: Mp 121.2–122.5 °C; R_f = 0.08 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2980, 1698 (s, C=O), 1599 (s), 1557, 1509, 1474, 1421, 1392, 1368, 1330 (m), 1312 (m), 1278 (s), 1210, 1176, 1154 (m), 1122, 1102 (s), 1071, 1023, 998, 989 (m), 962, 923, 890, 875, 857 (m), 826 (s), 772 (s), 753, 732, 704 (m), 668, 620 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.59 (d, *J* = 5.5 Hz, 2H, H^9), 7.96 (d, *J* = 8.5 Hz, 2H, H^2), 7.31 (d, *J* = 5.5 Hz, 2H, H^8), 7.04 (d, *J* = 8.5 Hz, 2H, H^3), 4.35 (q, *J* = 7.0 Hz, 2H, H^{11}), 3.13 (dd, *J* = 6.5; 3.0 Hz, 1H, H^6), 2.57 (dd, *J* = 6.5; 1.0 Hz, 1H, H^5), 2.46 (dd, *J* = 3.0; 1.0 Hz, 1H, H^5), 1.38 (t, *J* = 7.0 Hz, 3H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{10}), 157.8 (C^4), 150.0 (C^9), 147.9 (C^7), 130.9 (C^2), 125.2 (C^1), 121.2 (C^8), 120.2 (C^3), 60.8 (C^{11}), 40.3 (C^6), 38.0 (C^5), 14.4 (C^{12}); HRMS (ES+) calculated for $C_{16}H_{17}N_2O_2$ 269.1290, found 269.1309 ($[M + H]^+$).

Ethyl 4-[5-(4-methoxybenzyl)-Δ^2-1,2,3-triazolin-1-yl]benzoate (3df):

Following the general procedure at 80 °C for 24 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and 4-allylanisole (4.82 mL, 31.4 mmol), the title compound was isolated as a pale yellow solid (2.01 g after recrystallisation, 0.19 g after column: 41% overall). From this reaction, ethyl 4-[2-(4-methoxybenzyl)aziridin-1-yl]benzoate **4df** was also isolated as a yellow oil (0.13 g, 3%) after column chromatography.



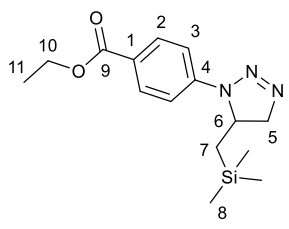
3df: Mp 94.7–96.4 °C; R_f = 0.20 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2991, 2944, 2837, 1693 (s, C=O), 1602 (s), 1585, 1510 (s), 1497 (s), 1366 (s), 1305, 1273 (s), 1242 (s), 1212 (m), 1176 (s), 1130 (m), 1109 (m), 1079 (s), 1062 (s), 1032 (s), 991 (m), 941 (s), 922 (s), 851 (s), 818 (m), 809 (m), 769 (s), 743 (m), 698 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.08 (d, *J* = 9.0 Hz, 2H, H^2), 7.39 (d, *J* = 9.0 Hz, 2H, H^3), 7.02 (d, *J* = 8.5 Hz, 2H, H^8), 6.84 (d, *J* = 8.5 Hz, 2H, H^9), 4.43 (dd, *J* = 15.5; 2.5 Hz, 1H, H^5), 4.38 (q, *J* = 7.0 Hz, 2H, H^{12}), 4.36–4.30 (m, 1H, H^6), 4.24 (dd, *J* = 15.5; 11.0 Hz, 1H, H^5), 3.79 (s, 3H, H^{14}), 3.00 (dd, *J* = 14.0; 3.0 Hz, 1H, H^{15}), 2.55 (dd, *J* = 14.0; 8.5 Hz, 1H, H^{15}), 1.41 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{11}), 158.7 (C^{10}), 143.5 (C^4), 131.5 (C^2), 130.3 (C^8), 127.3 (C^7), 124.0 (C^1), 114.3 (C^9), 114.0 (C^3), 70.3 (C^5), 60.8 (C^{12}), 55.3 (C^{14}), 53.7 (C^6), 35.9 (C^{15}), 14.4 (C^{13}); HRMS (ES+) calculated for $C_{19}H_{22}N_3O_3$ 340.1661, found 340.1660 ([M + H]$^+$).



4df: R_f = 0.40 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2982, 2836, 1706 (s, C=O), 1602 (s), 1509 (s), 1463, 1443, 1417, 1397, 1366, 1307, 1268 (s), 1245 (s), 1166 (s), 1100 (s), 1033 (m), 856, 838, 804, 775 (s), 757, 729, 702 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.85 (d, *J* = 8.5 Hz, 2H, H^2), 7.25 (d, *J* = 8.5 Hz, 2H, H^8), 6.90 (d, *J* = 8.5 Hz, 2H, H^9), 6.79 (d, *J* = 8.5 Hz, 2H, H^3), 4.31 (q, *J* = 7.0 Hz, 2H, H^{12}), 3.82 (s, 3H, H^{14}), 2.90 (dd, *J* = 14.0; 5.0 Hz, 1H, H^{15}), 2.75 (dd, *J* = 14.0; 7.5 Hz, 1H, H^{15}), 2.36–2.31 (m, 1H, H^6), 2.28 (d, *J* = 3.5 Hz, 1H, H^5), 2.16 (d, *J* = 6.0 Hz, 1H, H^5), 1.35 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 166.4 (C^{11}), 159.1 (C^{10}), 158.4 (C^4), 131.0 (C^7), 130.7 (C^2), 129.9 (C^8), 124.2 (C^1), 120.2 (C^3), 114.0 (C^9), 60.6 (C^{12}), 55.3 (C^{14}), 41.8 (C^6), 38.6 (C^5), 34.0 (C^{15}), 14.4 (C^{13}); HRMS (ES+) calculated for $C_{19}H_{22}NO_3$ 312.1600, found 312.1600 ([M + H]$^+$).

Ethyl 4-{5-[(trimethylsilyl)methyl]-Δ^2-1,2,3-triazolin-1-yl}benzoate (3dg):

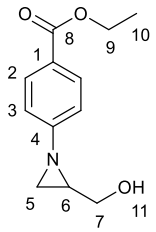
Following the general procedure at 80 °C for 24 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and allyltrimethylsilane (4.98 mL, 31.4 mmol), the title compound was isolated as a yellow solid (2.16 g after recrystallisation, 0.80 g after column: 62% overall).



3dg: Mp 65.6–67.6 °C; R_f = 0.54 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2964, 2910, 1698 (s, C=O), 1603 (s), 1515 (m), 1495 (s), 1475, 1360 (s), 1339, 1310 (m), 1273 (s), 1249 (s), 1214, 1176 (s), 1128 (m), 1106 (s), 1063 (m), 1046 (s), 1026 (m), 1003 (m), 923 (s), 876 (m), 845 (s), 829 (s), 767 (s), 695 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.05 (d, *J* = 9.0 Hz, 2H, H^2), 7.27 (d, *J* = 9.0 Hz, 2H, H^3), 4.41–4.34 (m, 1H, H^5), 4.36 (q, *J* = 7.0 Hz, 2H, H^{10}), 4.22–4.14 (m, 2H, H^5; H^6), 1.39 (t, *J* =

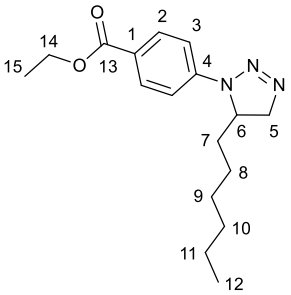
7.0 Hz, 3H, H^{11}), 1.19 (dd, *J* = 14.5; 1.5 Hz, 1H, H^7), 0.71 (dd, *J* = 14.5; 11.0 Hz, 1H, H^7), 0.10 (s, 9H, H^8); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.3 (C^9), 143.3 (C^4), 131.3 (C^2), 123.9 (C^1), 114.2 (C^3), 72.4 (C^5), 60.7 (C^{10}), 50.5 (C^6), 20.6 (C^7), 14.4 (C^{11}), -1.1 (C^8); HRMS (ES+) calculated for $C_{15}H_{24}N_3O_2Si$ 306.1638, found 306.1640 ($[M + H]^+$).

Ethyl 4-[2-(hydroxymethyl)aziridin-1-yl]benzoate (4dh): Following the general procedure at 80 °C for 24 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and allyl alcohol (2.13 mL, 31.4 mmol), the title compound was isolated as a yellow solid (0.56 g, 16%) after column chromatography (eluent: petroleum ether/EtOAc 0→50% gradient basified with 2% v/v NEt_3).

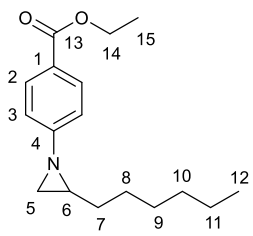


4dh: Mp 43.5–45.9 °C; R_f = 0.05 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3321 (br, OH), 2986, 2926, 2905, 1702 (s, C=O), 1601 (s), 1506, 1477, 1467, 1451, 1407, 1368, 1347, 1308 (m), 1272 (s), 1203, 1164 (s), 1124 (m), 1098 (s), 1038 (s), 1024 (m), 975, 939 (m), 884, 870, 863 (m), 853, 810, 779 (s), 742, 704 (s), 632, 614 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.93 (d, *J* = 8.5 Hz, 2H, H^2), 7.03 (d, *J* = 8.5 Hz, 2H, H^3), 4.34 (q, *J* = 7.0 Hz, 2H, H^9), 4.03 (ddd, *J* = 12.0; 5.0; 3.0 Hz, 1H, H^7), 3.63 (dt, *J* = 12.0; 6.0 Hz, 1H, H^7), 2.46 (dq, *J* = 6.0; 3.0 Hz, 1H, H^6), 2.38 (d, *J* = 3.0 Hz, 1H, H^5), 2.21–2.11 (br m, 1H, H^{11}), 2.16 (d, *J* = 6.0 Hz, 1H, H^5), 1.37 (t, *J* = 7.0 Hz, 3H, H^{10}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.4 (C^8), 158.3 (C^4), 130.8 (C^2), 124.8 (C^1), 120.5 (C^3), 62.9 (C^7), 60.7 (C^9), 41.0 (C^6), 31.4 (C^5), 14.4 (C^{10}); HRMS (ES+) calculated for $C_{12}H_{16}NO_3$ 222.1130, found 222.1133 ($[M + H]^+$).

Ethyl 4-(5-hexyl-Δ²-1,2,3-triazolin-1-yl)benzoate (3di): Following the general procedure at 85 °C for 24 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and 1-octene (4.92 mL, 31.4 mmol), the title compound was isolated as an off-white solid (1.06 g after recrystallisation, 0.99 g after column: 43% overall). From this reaction, ethyl 4-(2-hexylaziridin-1-yl)benzoate **4di** was also isolated as an orange oil (0.71 g, 16%) after column chromatography (eluent: petroleum ether/EtOAc 0→15% gradient basified with 2% v/v NEt_3).

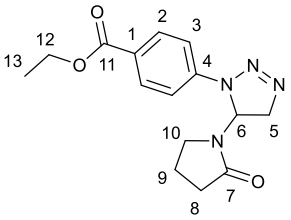


3di: Mp 58.5–60.7 °C; R_f = 0.46 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2956, 2923, 2854, 1711 (s, C=O), 1605 (s), 1505 (s), 1479, 1466, 1425, 1365 (s), 1313, 1272 (s), 1176 (s), 1123 (m), 1108 (s), 1085 (m), 1062 (s), 1024 (m), 989, 922 (s), 880, 844 (s), 763 (s), 728, 695 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.04 (d, *J* = 9.0 Hz, 2H, H^2), 7.31 (d, *J* = 9.0 Hz, 2H, H^3), 4.42 (dd, *J* = 17.0; 11.5 Hz, 1H, H^5), 4.36 (q, *J* = 7.0 Hz, 2H, H^{14}), 4.31 (dd, *J* = 17.0; 5.5 Hz, 1H, H^5), 4.10 (dddd, *J* = 11.5; 8.5; 5.5; 2.5 Hz, 1H, H^6), 1.74–1.65 (m, 1H, H^7), 1.49–1.38 (m, 1H, H^7), 1.39 (t, *J* = 7.0 Hz, 3H, H^{15}), 1.32–1.12 (br m, 8H, H^8 + H^9 + H^{10} + H^{11}), 0.86 (t, *J* = 7.0 Hz, 3H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.3 (C^{13}), 143.6 (C^4), 131.3 (C^2), 123.9 (C^1), 113.9 (C^3), 71.0 (C^5), 60.7 (C^{14}), 52.6 (C^6), 31.6 (C^7), 31.3 (C^8), 28.9 (C^9), 24.3 (C^{10}), 22.5 (C^{11}), 14.4 (C^{15}), 14.0 (C^{12}); HRMS (ES+) calculated for $C_{17}H_{26}N_3O_2$ 304.2025, found 304.2029 ($[M + H]^+$); Elemental analysis calculated for $C_{17}H_{25}N_3O_2$: C, 67.30; H, 8.31; N, 13.85, found: C, 67.17; H, 8.47; N, 13.68.



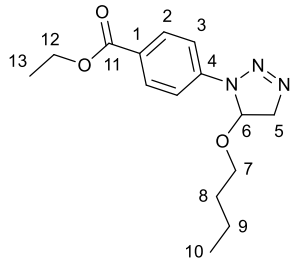
4di: R_f = 0.66 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2957, 2927, 2856, 1710 (s, C=O), 1603 (s), 1508 (m), 1463, 1406, 1366, 1307 (m), 1268 (s), 1199, 1166 (s), 1101 (s), 1018, 944, 897, 854 (m), 774 (m), 725, 702 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 8.5 Hz, 2H, H^2), 6.98 (d, *J* = 8.5 Hz, 2H, H^3), 4.34 (q, *J* = 7.0 Hz, 2H, H^{14}), 2.16–2.08 (m, 3H, H^5; H^6), 1.66–1.50 (br m, 4H, H^7; H^8), 1.44–1.25 (br m, 6H, H^9; H^{10}; H^{11}), 1.37 (t, *J* = 7.0 Hz, 3H, H^{15}), 0.91 (t, *J* = 7.0 Hz, 3H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 166.4 (C^{13}), 159.4 (C^4), 130.7 (C^2), 124.1 (C^1), 120.3 (C^3), 60.6 (C^{14}), 40.4 (C^5), 34.1 (C^6), 33.1 (C^7), 31.8 (C^8), 29.2 (C^9), 27.6 (C^{10}), 22.6 (C^{11}), 14.4 (C^{15}), 14.1 (C^{12}); HRMS (ES+) calculated for $C_{17}H_{26}NO_2$ 276.1964, found 276.1969 ($[M + H]^+$).

Ethyl 4-[5-(2-oxopyrrolidin-1-yl)-Δ²-1,2,3-triazolin-1-yl]benzoate (3dj):
Following the general procedure at 75 °C for 24 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and N-vinyl-2-pyrrolidinone (3.35 mL, 31.4 mmol), the title compound was isolated as an off-white solid (3.14 g, 66%) after recrystallisation.



3dj: Mp 109.8–111.0 °C; R_f = 0.05 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2984, 1701 (s, C=O), 1678 (s, C=O), 1605 (s), 1501 (m), 1463, 1427 (m), 1416 (m), 1357 (m), 1314, 1262 (s), 1236 (s), 1184 (s), 1170 (m), 1110 (s), 1075, 1045 (s), 1020 (s), 1004 (m), 985, 932 (s), 919 (s), 865, 848 (s), 769 (s), 695 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.05 (d, *J* = 8.5 Hz, 2H, H^2), 7.40 (d, *J* = 8.5 Hz, 2H, H^3), 6.38 (dd, *J* = 9.0; 3.5 Hz, 1H, H^6), 4.42 (dd, *J* = 18.0; 3.5 Hz, 1H, H^5), 4.35 (q, *J* = 7.0 Hz, 2H, H^{12}), 4.34 (dd, *J* = 18.0; 9.0 Hz, 1H, H^5), 2.94 (td, *J* = 9.0; 5.0 Hz, 1H, H^{10}), 2.62 (td, *J* = 9.0; 6.5 Hz, 1H, H^{10}), 2.38 (ddd, *J* = 17.0; 9.5; 6.0 Hz, 1H, H^8), 2.27 (ddd, *J* = 17.0; 9.5; 7.5 Hz, 1H, H^8), 2.00–1.88 (m, 1H, H^9), 1.87–1.75 (m, 1H, H^9), 1.39 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 175.3 (C^7), 166.1 (C^{11}), 142.0 (C^4), 131.5 (C^2), 125.2 (C^1), 114.3 (C^3), 68.9 (C^5), 60.8 (C^{12}), 58.8 (C^6), 41.4 (C^{10}), 30.4 (C^8), 17.5 (C^9), 14.4 (C^{13}); HRMS (ES+) calculated for $C_{15}H_{19}N_4O_3$ 303.1457, found 303.1467 ($[M + H]^+$).

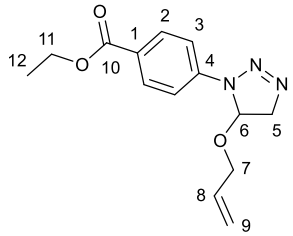
Ethyl 4-(5-butoxy-Δ²-1,2,3-triazolin-1-yl)benzoate (3dk): Following the general procedure at 65 °C for 16 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and butyl vinyl ether (4.06 mL, 31.4 mmol), the title compound was isolated as a white solid (3.64 g after recrystallisation, 0.22 g after column: 85% overall).



3dk: Mp 67.1–68.9 °C; R_f = 0.41 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2957, 2870, 1706 (s, C=O), 1607 (s), 1579, 1518, 1503 (m), 1426, 1367 (m), 1315, 1267 (s), 1235, 1192, 1182 (m), 1130, 1121, 1107 (m), 1066 (s), 1025 (s), 986 (m), 947 (s), 907, 881, 849 (s), 823, 766 (s), 693 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.06 (d, *J* = 9.0 Hz, 2H, H^2), 7.49 (d, *J* = 9.0 Hz, 2H, H^3), 5.66 (dd, *J* = 8.5; 2.0 Hz, 1H, H^6), 4.52 (dd, *J* = 18.5; 2.0 Hz, 1H, H^5), 4.37 (q, *J* = 7.0 Hz, 2H, H^{12}), 4.21 (dd, *J* = 18.5; 8.5 Hz, 1H, H^5), 3.08 (dt, *J* = 8.5; 6.5 Hz, 1H, H^7), 2.97 (dt, *J* = 8.5; 6.5 Hz, 1H, H^7), 1.47–1.40 (m, 2H, H^8), 1.40 (t, *J* = 7.0 Hz, 3H, H^{13}), 1.31–1.17 (m, 2H, H^9), 0.81 (t, *J* = 7.5 Hz, 3H, H^{10}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{11}), 142.9 (C^4), 131.2 (C^2), 125.0 (C^1), 114.4 (C^3), 81.0 (C^6), 70.0 (C^5), 63.2 (C^7), 60.8 (C^{12}), 31.3 (C^8), 19.2 (C^9),

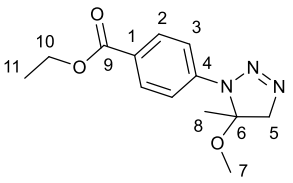
14.4 (C^{13}), 13.7 (C^{10}); HRMS (ES+) calculated for $C_{15}H_{22}N_3O_3$ 292.1661, found 292.1665 ([M + H]$^+$).

Ethyl 4-[5-(allyloxy)-Δ^2-1,2,3-triazolin-1-yl]benzoate (3dl):
Following the general procedure at 60 °C for 24 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and allyl vinyl ether (3.41 mL, 31.4 mmol), the title compound was isolated as a white solid (1.60 g, 37%) after column chromatography.



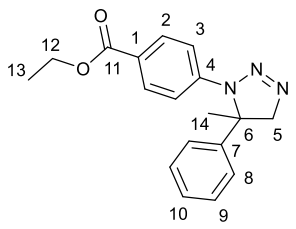
3dl: Mp 56.0–57.3 °C; R_f = 0.29 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2984, 1709 (s, C=O), 1607 (s), 1578, 1519, 1505 (m), 1462, 1426, 1367 (m), 1336, 1317, 1274 (s), 1184 (m), 1171 (m), 1129, 1108 (m), 1084 (m), 1063 (s), 1022 (s), 983 (m), 948 (s), 929 (s), 879, 848 (s), 824, 781, 767 (s), 695 (m), 659, 631 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.07 (d, *J* = 9.0 Hz, 2H, H^2), 7.49 (d, *J* = 9.0 Hz, 2H, H^3), 5.77 (ddt, *J* = 16.0; 11.0; 5.5 Hz, 1H, H^8), 5.69 (dd, *J* = 8.0; 2.0 Hz, 1H, H^6), 5.21 (ddd, *J* = 16.0; 1.5; 1.0 Hz, 1H, H^9), 5.15 (dd, *J* = 11.0; 1.5 Hz, 1H, H^9), 4.57 (dd, *J* = 18.5; 2.0 Hz, 1H, H^5), 4.37 (q, *J* = 7.0 Hz, 2H, H^{11}), 4.25 (dd, *J* = 18.5; 8.0 Hz, 1H, H^5), 3.67 (ddt, *J* = 12.0; 5.5; 1.0 Hz, 1H, H^7), 3.61 (ddt, *J* = 12.0; 5.5; 1.0 Hz, 1H, H^7), 1.40 (t, *J* = 7.0 Hz, 3H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{10}), 142.8 (C^4), 132.9 (C^8), 131.3 (C^2), 125.1 (C^1), 117.9 (C^9), 114.5 (C^3), 80.8 (C^6), 70.5 (C^5), 65.2 (C^7), 60.8 (C^{11}), 14.4 (C^{12}); HRMS (ES+) calculated for $C_{14}H_{18}N_3O_3$ 276.1348, found 276.1347 ([M + H]$^+$).

Ethyl 4-(5-methoxy-5-methyl-Δ^2-1,2,3-triazolin-1-yl)benzoate (3dm):
4-Ethylazidobenzoate (1.00 g, 5.2 mmol) and 2-methoxypropene (2.02 mL, 20.8 mmol) were stirred in DES (5 mL) in a vial fitted with a screw cap at 75 °C for 96 h. The reaction mixture was cooled down to room temperature, diluted with water (3 mL) and left at -18 °C overnight. The precipitate was collected, triturated with cold acetone and dried under reduced pressure to give the title compound as a white solid (1.20 g, 87%).



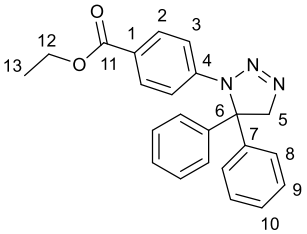
3dm: Mp 53.1–55.3 °C; R_f = 0.29 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2983, 1706 (s, C=O), 1606 (s), 1513, 1496 (m), 1473, 1378, 1351 (m), 1309, 1291, 1269 (s), 1240 (m), 1211 (m), 1174 (m), 1141, 1115 (m), 1102 (s), 1043 (s), 999 (m), 934 (m), 877, 858 (s), 829 (s), 767 (s), 695 (m) cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.06 (d, *J* = 9.0 Hz, 2H, H^2), 7.56 (d, *J* = 9.0 Hz, 2H, H^3), 4.57 (d, *J* = 19.0 Hz, 1H, H^5), 4.38 (q, *J* = 7.0 Hz, 2H, H^{10}), 4.17 (d, *J* = 19.0 Hz, 1H, H^5), 2.94 (s, 3H, H^7), 1.79 (s, 3H, H^8), 1.40 (t, *J* = 7.0 Hz, 3H, H^{11}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^9), 142.5 (C^4), 131.0 (C^2), 125.6 (C^1), 115.9 (C^3), 90.1 (C^6), 75.0 (C^5), 60.8 (C^{10}), 50.5 (C^7), 23.7 (C^8), 14.4 (C^{11}); HRMS (ES+) calculated for $C_{13}H_{18}N_3O_3$ 264.1348, found 264.1350 ([M + H]$^+$).

Ethyl 4-(5-phenyl-Δ^2-1,2,3-triazolin-1-yl)benzoate (3dn): Following the general procedure at 90 °C for 16 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and isopropenylbenzene (4.07 mL, 31.4 mmol), the title compound was isolated as an off-white solid (1.96 g after recrystallisation, 0.52 g after column: 51% overall).

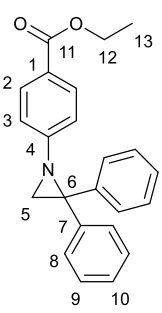


3dn: Mp 88.7–90.2 °C; R_f = 0.38 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2997, 1696 (s, C=O), 1604 (s), 1573, 1496 (s), 1462, 1447, 1390, 1367, 1346 (m), 1307, 1267 (s), 1179 (s), 1157, 1101 (s), 1073, 1028 (s), 952, 925, 908 (m), 870, 850 (m), 818, 761 (s), 693 (s), 667 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.86 (d, *J* = 9.0 Hz, 2H, H^2), 7.41–7.36 (m, 2H, H^{Ar}), 7.33–7.29 (m, 3H, H^{Ar}), 7.14 (d, *J* = 9.0 Hz, 2H, H^3), 4.64 (d, *J* = 17.0 Hz, 1H, H^5), 4.42 (d, *J* = 17.0 Hz, 1H, H^5), 4.31 (q, *J* = 7.0 Hz, 2H, H^{12}), 1.78 (s, 3H, H^{14}), 1.34 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{11}), 143.1 (C^4), 142.9 (C^7), 130.8 (C^2), 129.3 (C^9), 127.9 (C^{10}), 125.3 (C^8), 124.1 (C^1), 114.9 (C^3), 84.8 (C^5), 63.0 (C^6), 60.6 (C^{12}), 22.3 (C^{14}), 14.4 (C^{13}); HRMS (ES+) calculated for $C_{18}H_{20}N_3O_2$ 310.1556, found 310.1558 ($[M + H]^+$).

Ethyl 4-(5,5-diphenyl-Δ²-1,2,3-triazolin-1-yl)benzoate (3do): Following the general procedure at 100 °C for 72 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and 1,1-diphenylethylene (5.88 mL, 31.4 mmol), the title compound was isolated as a white solid (1.41 g, 24%) after column chromatography. From this reaction, ethyl 4-(2,2-diphenylaziridin-1-yl)benzoate **4do** was also isolated as a white solid (0.60 g, 11%) after column chromatography.

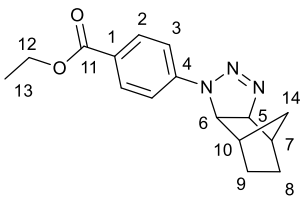


3do: Mp 99.6–102.8 °C; R_f = 0.41 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2975, 1703 (s, C=O), 1604 (s), 1505 (s), 1446, 1421, 1390, 1367, 1338 (m), 1275 (s), 1180 (m), 1172 (m), 1106 (s), 1068 (m), 1047 (s), 1014 (m), 1002, 980 (s), 950 (s), 854, 844 (m), 767 (s), 760 (s), 698 (s), 673, 627 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.78 (d, *J* = 8.5 Hz, 2H, H^2), 7.36–7.25 (m, 10H, H^{Ar}), 7.20 (d, *J* = 8.5 Hz, 2H, H^3), 5.09 (s, 2H, H^5), 4.27 (q, *J* = 7.0 Hz, 2H, H^{12}), 1.31 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{11}), 144.0 (C^4), 141.0 (C^7), 130.5 (C^2), 128.8 (C^9), 128.0 (C^{10}), 127.8 (C^8), 124.1 (C^1), 115.7 (C^3), 88.6 (C^5), 70.3 (C^6), 60.6 (C^{12}), 14.4 (C^{13}); HRMS (ES+) calculated for $C_{23}H_{22}N_3O_2$ 372.1712, found 372.1703 ($[M + H]^+$).



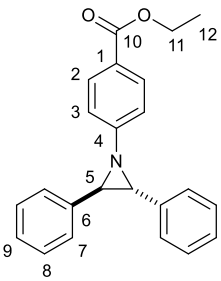
4do: Mp 71.1–73.8 °C; R_f = 0.53 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 3057, 2979, 1706 (s, C=O), 1599 (s), 1506 (m), 1462, 1445, 1416, 1365, 1348, 1308, 1269 (s), 1170 (s), 1103 (s), 1045, 1019 (m), 953, 916, 855 (m), 775 (s), 732 (m), 695 (s), 638, 628, 617 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.76 (d, *J* = 8.5 Hz, 2H, H^2), 7.28–7.18 (m, 10H, H^{Ar}), 6.81 (d, *J* = 8.5 Hz, 2H, H^3), 4.27 (q, *J* = 7.0 Hz, 2H, H^{12}), 3.01 (s, 2H, H^5), 1.31 (t, *J* = 7.0 Hz, 3H, H^{13}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.5 (C^{11}), 153.9 (C^4), 139.1 (C^7), 130.3 (C^2), 128.9 (C^9), 128.2 (C^8), 127.6 (C^{10}), 123.9 (C^1), 120.8 (C^3), 60.6 (C^{12}), 52.6 (C^6), 40.2 (C^5); 14.4 (C^{13}); HRMS (ES+) calculated for $C_{23}H_{22}NO_2$ 344.1651, found 344.1637 ($[M + H]^+$).

Ethyl 4-(3a,4,5,6,7,7a-hexahydro-1*H*-4,7-methano-benzo-Δ²-1,2,3-triazolin-1-yl)benzoate (3dp): 4-Ethylazidobenzoate (1.00 g, 5.2 mmol) and 2-norbornene (0.54 g, 5.7 mmol) were stirred in DES (10 mL) at room temperature for 16 h. The mixture was diluted with water (10 mL) and the precipitate was washed with water and dried under reduced pressure to give the title compound as a white solid (1.48 g, 99%).



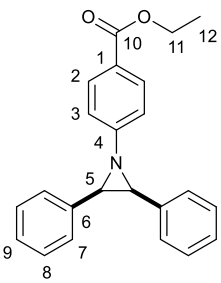
3dp: Mp 87.6–89.2 °C; R_f = 0.40 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2976, 2959, 2872, 1699 (s, C=O), 1604 (s), 1575, 1513 (m), 1488 (m), 1453, 1422, 1367 (s), 1311 (m), 1299, 1274 (s), 1216, 1174 (s), 1161, 1126 (m), 1106 (s), 1087 (s), 1047 (m), 1035, 1023 (m), 1010 (m), 978 (s), 964, 954 (s), 913 (s), 891, 871, 844 (s), 766 (s), 754 (s), 711, 695 (s), 633 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.02 (d, *J* = 9.0 Hz, 2H, H^2), 7.30 (d, *J* = 9.0 Hz, 2H, H^3), 4.63 (d, *J* = 9.0 Hz, 1H, H^5), 4.36 (q, *J* = 7.0 Hz, 2H, H^{12}), 3.73 (d, *J* = 9.0 Hz, 1H, H^6), 2.81 (s, 1H, H^7), 2.65 (s, 1H, H^{10}), 1.70–1.58 (m, 2H, H^8), 1.43–1.31 (m, 2H, H^9), 1.39 (t, *J* = 7.0 Hz, 3H, H^{13}), 1.19 (d, *J* = 11.0 Hz, 1H, H^{14}), 1.09 (d, *J* = 11.0 Hz, 1H, H^{14}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.2 (C^{11}), 143.7 (C^4), 131.3 (C^2), 123.5 (C^1), 113.1 (C^3), 86.8 (C^5), 60.7 (C^{12}), 59.7 (C^6), 41.1 (C^7), 39.8 (C^{10}), 32.1 (C^{14}), 25.4 (C^8), 24.8 (C^9), 14.4 (C^{13}); HRMS (ES+) calculated for $C_{16}H_{20}N_3O_2$ 286.1556, found 286.1553 ($[M + H]^+$).

Ethyl 4-(*trans*-2,3-diphenylaziridin-1-yl)benzoate (4dq): Following the general procedure at 100 °C for 48 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and *trans*-stilbene (5.65 g, 31.4 mmol), the title compound was isolated as a white solid (2.90 g, 53%) after column chromatography (eluent: petroleum ether/EtOAc 0→10% gradient basified with 2% v/v NEt_3).



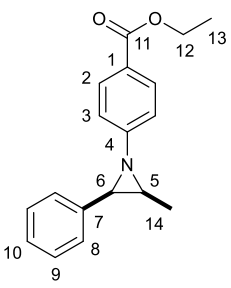
4dq: Single crystals for X-ray diffraction were grown from Et_2O, CCDC 1843145 Mp 121.3–123.1 °C; R_f = 0.58 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2977, 1698 (s, C=O), 1601 (s), 1499 (m), 1461 (m), 1454, 1406, 1362 (m), 1308 (m), 1271 (s), 1214, 1169 (s), 1144 (m), 1113 (m), 1101 (s), 1072, 1014, 898, 851 (s), 773 (s), 760 (m), 748 (m), 718 (m), 706 (s), 693 (s), 664 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.83 (d, *J* = 8.5 Hz, 2H, H^2), 7.33–7.28 (m, 6H, H^{Ar}), 7.20–7.16 (m, 4H, H^{Ar}), 6.75 (d, *J* = 8.5 Hz, 2H, H^3), 4.31 (q, *J* = 7.0 Hz, 2H, H^{11}), 3.68 (s, 2H, H^5), 1.35 (t, *J* = 7.0 Hz, 3H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.6 (C^{10}), 152.8 (C^4), 135.7 (C^6), 130.5 (C^2), 128.4 (C^8), 127.8 (C^9), 127.2 (C^7), 123.9 (C^1), 120.3 (C^3), 60.6 (C^{11}), 50.2 (C^5), 14.4 (C^{12}); HRMS (ES+) calculated for $C_{23}H_{22}NO_2$ 344.1651, found 344.1654 ($[M + H]^+$).

Ethyl 4-(*cis*-2,3-diphenylaziridin-1-yl)benzoate (4dr): Following the general procedure at 110 °C for 16 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and *cis*-stilbene (5.64 mL, 31.4 mmol), the title compound was isolated as a white solid (1.97 g, 36%) after column chromatography (eluent: petroleum ether/EtOAc 0→2% gradient basified with 2% v/v NEt_3).



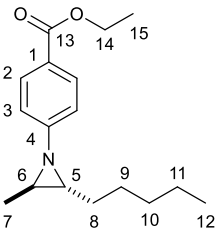
4dr: Mp 79.7–83.2 °C; R_f = 0.66 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2975, 1704 (s, C=O), 1602 (s), 1506, 1495, 1477, 1455, 1413 (m), 1364, 1308, 1274 (s), 1167 (m), 1141 (m), 1104 (m), 1071, 1039, 1027 (m), 922, 899, 859 (m), 794, 771 (m), 752 (m), 727, 693 (s), 658, 647, 622, 613 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.98 (d, *J* = 8.5 Hz, 2H, H^2), 7.29–7.25 (m, 4H, H^{Ar}), 7.23–7.13 (m, 8H, H^{Ar}), 4.36 (q, *J* = 7.0 Hz, 2H, H^{11}), 3.70 (s, 2H, H^5), 1.39 (t, *J* = 7.0 Hz, 3H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.4 (C^{10}), 158.9 (C^4), 135.2 (C^6), 131.0 (C^2), 127.9 (C^7), 127.7 (C^8), 127.2 (C^9), 124.9 (C^1), 119.6 (C^3), 60.7 (C^{11}), 49.2 (C^5), 14.4 (C^{12}); HRMS (ES+) calculated for $C_{23}H_{22}NO_2$ 344.1651, found 344.1660 ($[M + H]^+$).

Ethyl 4-(*cis*-2-methyl-3-phenylaziridin-1-yl)benzoate (4ds): Following the general procedure at 90 °C for 32 h from 4-ethylazidobenzoate (1.50 g, 7.8 mmol) and *cis*-propenylbenzene (2.04 mL, 15.6 mmol), the title compound was isolated as a yellow oil (0.46 g, 21%) after column chromatography (eluent: petroleum ether/EtOAc 0→2% gradient basified with 2% v/v NEt_3).



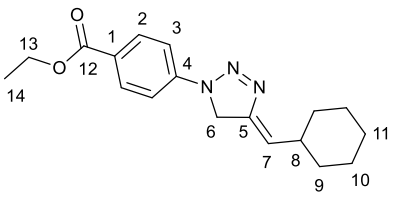
4ds: R_f = 0.64 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2982, 2925, 1707 (s, C=O), 1602 (s), 1508 (m), 1450, 1417 (m), 1366, 1308, 1267 (s), 1165 (s), 1144 (m), 1099 (s), 1046, 1018 (m), 904, 856 (m), 774 (m), 729 (m), 699 (s) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.94 (d, *J* = 8.5 Hz, 2H, H^2), 7.43–7.34 (m, 4H, H^{Ar}), 7.33–7.27 (m, 1H, H^{Ar}), 7.05 (d, *J* = 8.5 Hz, 2H, H^3), 4.34 (q, *J* = 7.0 Hz, 2H, H^{12}), 3.35 (d, *J* = 6.5 Hz, 1H, H^6), 2.59 (dq, *J* = 6.5; 6.0 Hz, 1H, H^5), 1.37 (t, *J* = 7.0 Hz, 3H, H^{13}), 1.16 (d, *J* = 6.0 Hz, 3H, H^{14}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.4 (C^{11}), 159.5 (C^4), 136.2 (C^7), 130.9 (C^2), 128.2 (C^9), 127.6 (C^8), 127.2 (C^{10}), 124.4 (C^1), 119.7 (C^3), 60.6 (C^{12}), 46.5 (C^6), 42.1 (C^5), 14.4 (C^{13}), 13.4 (C^{14}); HRMS (ES+) calculated for $C_{18}H_{20}NO_2$ 282.1494, found 282.1497 ($[M + H]^+$).

Ethyl 4-(*trans*-2-methyl-3-pentylaziridin-1-yl)benzoate (4dt): Following the general procedure at 95 °C for 32 h from 4-ethylazidobenzoate (3.00 g, 15.7 mmol) and *trans*-2-octene (4.90 mL, 31.4 mmol), the title compound was isolated as a pale yellow oil (0.90 g, 21%) after column chromatography (eluent: petroleum ether/EtOAc 0→2% gradient basified with 2% v/v NEt_3).

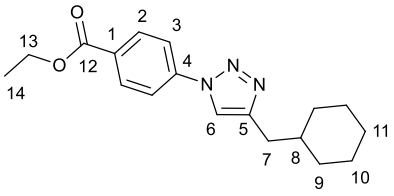


4dt: R_f = 0.60 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2958, 2929, 2857, 1709 (s, C=O), 1602 (s), 1507 (m), 1459, 1416, 1381, 1366, 1307, 1268 (s), 1197, 1165 (s), 1100 (s), 1020, 854 (m), 775 (m), 726, 705 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 8.5 Hz, 2H, H^2), 6.90 (d, *J* = 8.5 Hz, 2H, H^3), 4.34 (q, *J* = 7.0 Hz, 2H, H^{14}), 2.27 (qd, *J* = 5.5; 3.0 Hz, 1H, H^6), 2.00 (td, *J* = 6.0; 3.0 Hz, 1H, H^5), 1.64–1.46 (m, 3H, H^8; H^{10}), 1.43–1.28 (m, 5H, H^8; H^9; H^{11}), 1.37 (t, *J* = 7.0 Hz, 3H, H^{15}), 1.14 (d, *J* = 5.5 Hz, 3H, H^7), 0.90 (t, *J* = 7.0 Hz, 3H, H^{12}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 166.6 (C^{13}), 155.2 (C^4), 130.6 (C^2), 123.7 (C^1), 120.5 (C^3), 60.5 (C^{14}), 46.5 (C^5), 40.3 (C^6), 31.7 (C^8), 31.7 (C^9), 27.3 (C^{10}), 22.6 (C^{11}), 15.6 (C^7), 14.4 (C^{15}), 14.0 (C^{12}); HRMS (ES+) calculated for $C_{17}H_{26}NO_2$ 276.1964, found 276.1972 ($[M + H]^+$).

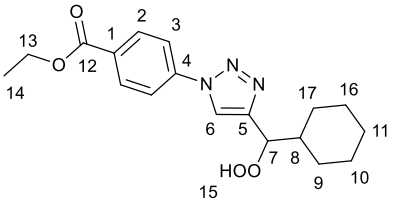
Ethyl *cis*-4-[4-(cyclohexylmethylene)-Δ^2-1,2,3-triazolin-1-yl]benzoate (3du): Following the general procedure at 95 °C for 96 h from 4-ethylazidobenzoate (0.33 g, 1.7 mmol) and cyclohexylallene (0.50 mL, 3.4 mmol), the title compound was isolated as a yellow solid (0.04 g, 7%) after column chromatography (eluent: petroleum ether/EtOAc 0→10% gradient basified with 2% v/v NEt_3). From this reaction, ethyl 4-[4-(cyclohexylmethyl)-1*H*-1,2,3-triazol-1-yl]benzoate **5du** was also isolated as a white solid (0.12 g, 23%) after column chromatography (eluent: petroleum ether/EtOAc 10→25% gradient basified with 2% v/v NEt_3). Attempted recrystallisation of triazoline **(3du)** from boiling MeOH yielded ethyl ethyl 4-{4-[cyclohexyl(hydroperoxy)methyl]-1*H*-1,2,3-triazol-1-yl}benzoate **5du'** as a white solid (0.01 g, 2%).



3du: IR: ν_{max} 2921 (m), 2850 (m), 1697 (s, C=O), 1607 (s), 1517 (m), 1448 (m), 1436 (s), 1384 (s), 1365 (m), 1313 (m), 1275 (s), 1180 (m), 1172 (m), 1129 (m), 1105 (s), 1081 (s), 1018 (s), 992 (m), 973 (m), 915 (m), 892 (m), 850 (s), 825 (m), 767 (s), 691 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.06 (d, *J* = 9.0 Hz, 2H, H^2), 7.30 (d, *J* = 9.0 Hz, 2H, H^3), 6.17 (dt, *J* = 10.0; 4.0 Hz, 1H, H^7), 4.37 (q, *J* = 7.0 Hz, 2H, H^{13}), 4.35 (dd, *J* = 4.0; 1.0 Hz, 2H, H^6), 2.13–2.00 (m, 1H, H^{Cy}), 1.83–1.73 (m, 4H, H^{Cy}), 1.73–1.66 (m, 1H, H^{Cy}), 1.40 (t, *J* = 7.0 Hz, 3H, H^{14}), 1.36–1.19 (m, 5H, H^{Cy}).



5du: Single crystals for X-ray diffraction were grown from TBME/Et_2O, CCDC 1843146 Mp 110.4–112.1 °C; R_f = 0.38 (petroleum ether/EtOAc = 80:20); IR: ν_{max} 2980, 2920 (m), 2851 (m), 1713 (s, C=O), 1608 (m), 1519 (m), 1446 (m), 1412 (m), 1366 (m), 1312, 1275 (s), 1232 (m), 1198, 1177 (m), 1109 (s), 1044 (s), 1027 (m), 992 (m), 960, 893, 851 (m), 828, 786, 768 (s), 689 (m) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.20 (d, *J* = 9.0 Hz, 2H, H^2), 7.84 (d, *J* = 9.0 Hz, 2H, H^3), 7.78 (s, 1H, H^6), 4.42 (q, *J* = 7.0 Hz, 2H, H^{13}), 2.68 (d, *J* = 7.0 Hz, 2H, H^7), 1.80–1.63 (m, 6H, H^{Cy}), 1.43 (t, *J* = 7.0 Hz, 3H, H^{14}), 1.31–1.11 (m, 3H, H^{Cy}), 1.07–0.95 (m, 2H, H^{Cy}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 165.5 (C^{12}), 148.1 (C^5), 140.2 (C^4), 131.2 (C^2), 130.2 (C^1), 119.6 (C^3), 119.1 (C^6), 61.4 (C^{13}), 38.1 (C^7), 33.4 (C^8), 33.1 (C^9), 26.4 (C^{11}), 26.2 (C^{10}), 14.3 (C^{14}); HRMS (ES+) calculated for $C_{18}H_{24}N_3O_2$ 314.1869, found 314.1874 ($[M + H]^+$).



5du': Single crystals for X-ray diffraction were grown from MeOH, CCDC 1843147. R_f = 0.08 (petroleum ether/EtOAc = 80:20); ^1H NMR ($CDCl_3$, 400 MHz) δ 8.43 (br s, 1H, H^{15}), 8.21 (d, *J* = 9.0 Hz, 2H, H^2), 8.04 (s, 1H, H^6), 7.86 (d, *J* = 9.0 Hz, 2H, H^3), 5.03 (d, *J* = 7.0 Hz, 1H, H^7), 4.43 (q, *J* = 7.0 Hz, 2H, H^{13}), 2.04–1.96 (m, 2H, H^{Cy}), 1.81–1.62 (m, 3H, H^{Cy}), 1.44 (t, *J* = 7.0 Hz, 3H, H^{14}), 1.30–1.07 (m, 6H, H^{Cy}); ^{13}C NMR ($CDCl_3$, 101 MHz): δ 165.4 (C^{12}), 148.2 (C^5), 139.9 (C^4), 131.3 (C^2), 130.6 (C^1), 120.2 (C^6), 119.8 (C^3), 84.7 (C^7), 61.5 (C^{13}), 40.8 (C^8), 29.1 (C^{Cy}), 28.8 (C^{Cy}), 26.2 (C^{Cy}), 25.9 (C^{Cy}), 25.8 (C^{Cy}), 14.3 (C^{14}); HRMS (ES+) calculated for $C_{18}H_{24}N_3O_4$ 346.1767, found 346.1758 ($[M + H]^+$).

4. Crystallographic Data

Tables S1 and S2 provide a summary of the crystallographic data for the structures of **3aa**, **3dd**, **4aa**, **4dq**, **5du** and **5du'**. The absolute structures of **4aa**, **4dq** and **5du'** could not be reliably determined [Flack parameters 0.0(10), 0.2(7) and 0.1(3) respectively]. CCDC 1843142 to 1843147.

Table S1. Crystal data, data collection and refinement parameters for the structures of **3aa**, **3dd** and **4aa**.

Data	**3aa**	**3dd**	**4aa**
formula	$C_{15}H_{12}F_3N_3$	$C_{21}H_{19}N_3O_2$	$C_{15}H_{12}F_3N$
solvent	$0.25(C_4H_{10}O)$	—	—
formula weight	309.81	345.39	263.26
colour, habit	colourless blocky	colourless blocky	colourless blocks
temperature / K	173	173	173
crystal system	Monoclinic	monoclinic	orthorhombic
space group	$P2_1/c$ (no. 14)	$P2_1/c$ (no. 14)	$Pna2_1$ (no. 33)
a / Å	5.6803(5)	12.8553(5)	27.0703(18)
b / Å	22.150(2)	5.5968(2)	5.7522(4)
c / Å	23.2022(16)	24.4632(9)	8.0156(5)
α / deg	90	90	90
β / deg	90.281(7)	92.110(3)	90
γ / deg	90	90	90
V / Å^3	2919.2(5)	1758.90(12)	1248.14(14)
Z	8[a]	4	4
D_c / g cm^{-3}	1.410	1.304	1.401
radiation used	Cu-Kα	Cu-Kα	Mo-Kα
μ / mm^{-1}	0.969	0.688	0.113
2θ max / deg	148	147	57
no. of unique reflns			
measured (R_{int})	5581 (0.0666)	3371 (0.0265)	1611 (0.0219)
obs, $\|F_o\| >$	2632	2566	1477
no. of variables	424	245	172
R_1(obs), wR_2(all)[b]	0.0915, 0.2987	0.0421, 0.1185	0.0489, 0.1228

[a] There are two crystallographically independent molecules; [b] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$; $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$.

Table S2. Crystal data, data collection and refinement parameters for the structures of **4dq**, **5du** and **5du'**.

Data	**4dq**	**5du**	**5du'**
formula	$C_{23}H_{21}NO_2$	$C_{18}H_{23}N_3O_4$	$C_{18}H_{23}N_3O_2$
solvent	—	—	—
formula weight	343.41	345.39	313.39
colour, habit	colourless blocks	colourless plates	colourless blocky
temperature / K	173	173	173
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1$ (no. 4)	$P2_1$ (no. 4)	$P2_1/c$ (no. 14)
a / Å	5.66625(19)	5.35503(14)	12.8362(5)
b / Å	18.3197(5)	10.1690(2)	11.1053(4)
c / Å	17.6253(6)	32.7300(7)	11.7668(4)
α / deg	90	90	90
β / deg	90.314(3)	92.720(2)	92.584(4)
γ / deg	90	90	90
V / Å^3	1829.55(10)	1780.32(7)	1675.64(11)
Z	4[a]	4[a]	4
D_c / g cm^{-3}	1.247	1.289	1.242
radiation used	Mo-Kα	Cu-Kα	Mo-Kα
μ / mm^{-1}	0.079	0.757	0.082
2θ max / deg	57	147	57
no. of unique reflns			
measured (R_{int})	6266 (0.0226)	4567 (0.0393)	3343 (0.0165)
obs, $\|F_o\| >$	5285	3891	2478
no. of variables	494	492	210
R_1(obs), wR_2(all)[b]	0.0421, 0.0791	0.0493, 0.1355	0.0431, 0.0989

[a] There are two crystallographically independent molecules; [b] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$; $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$.

X-Ray crystal structure of 3aa: Inspection of reciprocal space plots of the diffraction data collected for a crystal of **3aa** revealed substantial twinning, with the initial indexing using only *ca*. 52% of the observed spots. Unfortunately, despite numerous efforts, no attempts at modelling the twinning gave any noticeable improvement over the standard, non-twin, data processing. The consequences of this unresolved twinning can be seen in the elevated final agreement factors, with R_1(obs) in excess of 0.09 and wR_2(all) only just under 0.30. However, despite the evident issues, the structure derived from this data clearly shows both the nature and geometry of the compound.

The structure of **3aa** was found to contain two independent molecules, **3aa-A** and **3aa-B**, in the asymmetric unit. The included diethyl ether solvent molecule was found to be disordered across a centre of symmetry, and this was modelled by using one complete, 50% occupancy orientation. The geometry of the unique orientation was optimised, and all of the non-hydrogen atoms were refined anisotropically.

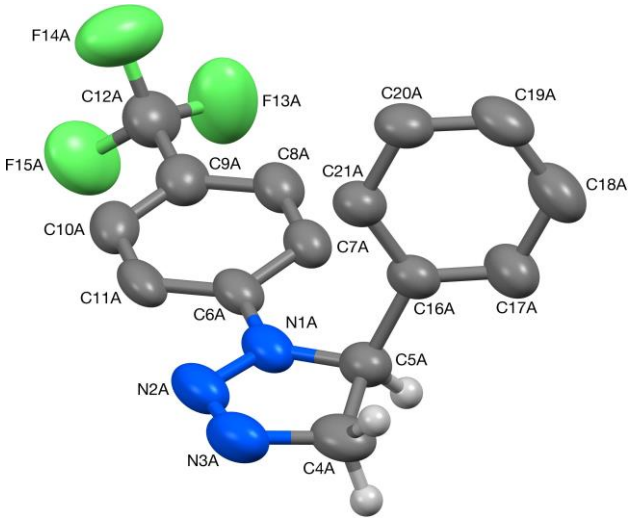


Figure S1. Structure of one (**3aa-A**) of the two independent molecules present in the crystal of **3aa** (50% probability ellipsoids).

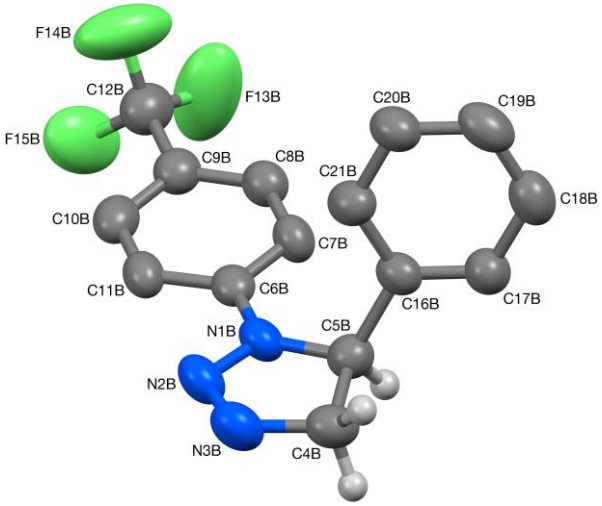


Figure S2. Structure of one (**3aa-B**) of the two independent molecules present in the crystal of **3aa** (50% probability ellipsoids).

X-Ray crystal structure of 3dd: The terminal ethyl unit of the C9-bound ethyl formate moiety in the structure of **3dd** was found to be disordered. Two orientations were identified of *ca*. 87 and 13% occupancy, their geometries were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically).

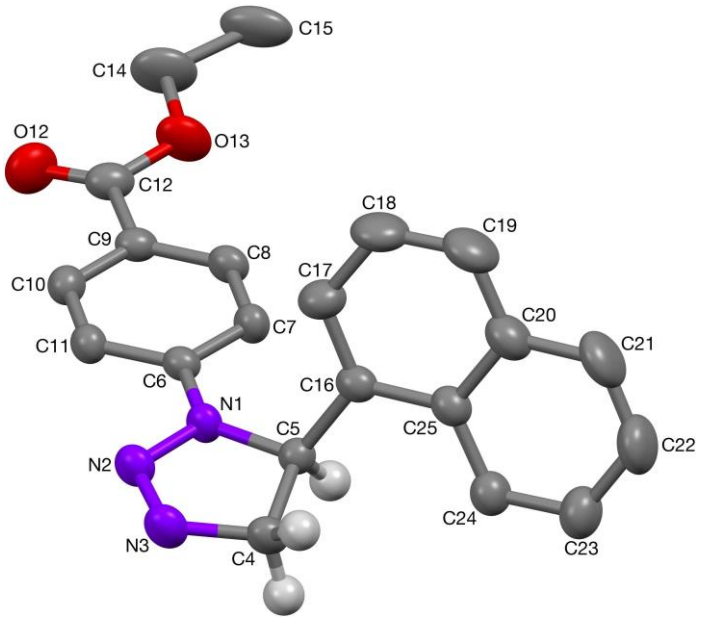


Figure S3. Crystal structure of **3dd** (50% probability ellipsoids).

X-Ray crystal structure of 4aa: The structure of **4aa** was found to crystallise in a polar space group ($Pna2_1$), but the absolute structure could not be reliably determined [Flack parameter x = 0.0(10)].

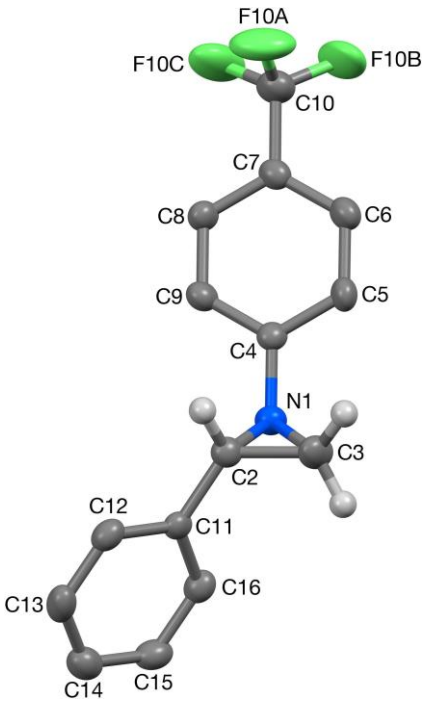


Figure S4. Crystal structure of **4aa** (50% probability ellipsoids).

X-Ray crystal structure of 4dq: The structure of **4dq** was found to crystallise in a chiral space group ($P2_1$), with two crystallographically independent molecules (**4dq-A** and **4dq-B**) of opposite chirality. It is thus unsurprising that the absolute structure could not be reliably determined [Flack parameter x = 0.2(7)]. Attempts to solve the structure in the related centrosymmetric space group $P2_1/m$ proved unsuccessful. The C10B-based ethyl ester moiety

of the second independent molecule was found to be disordered. Two orientations were identified of *ca*. 78 and 22% occupancy, their geometries were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically).

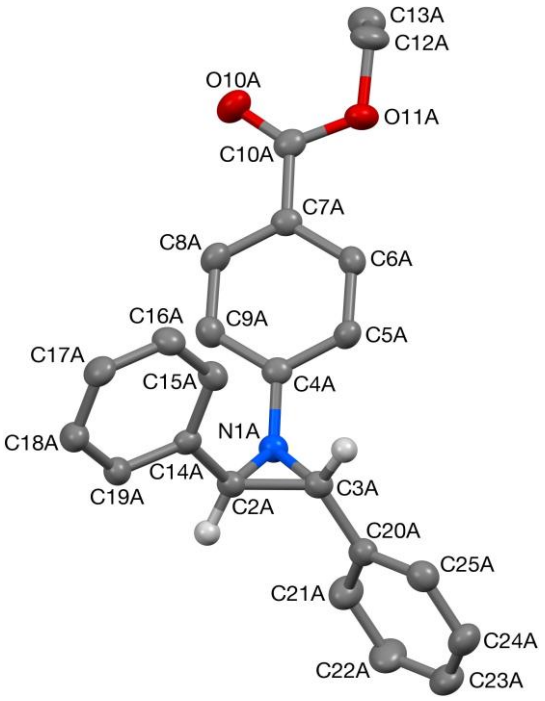


Figure S5. Structure of one (**4dq-A**) of the two independent molecules present in the crystal of **4dq** (50% probability ellipsoids).

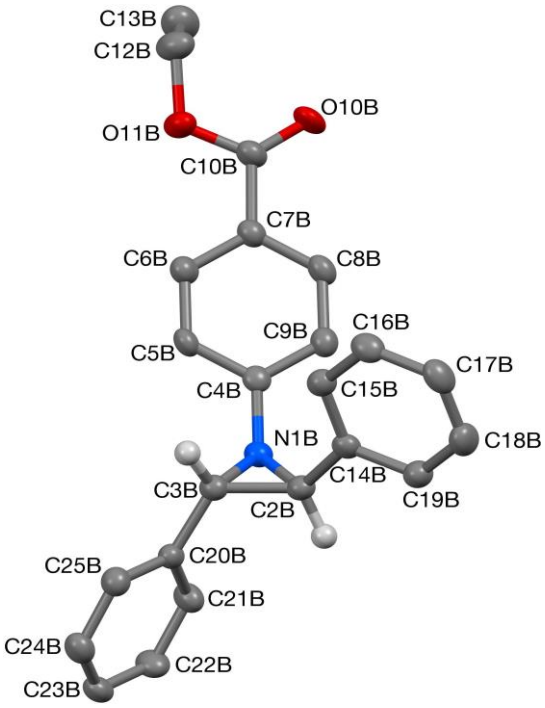


Figure S6. Structure of one (**4dq-B**) of the two independent molecules present in the crystal of **4dq** (50% probability ellipsoids).

X-ray crystal structure of 5du: The structure of **5du** was found to crystallise in the centrosymmetric space group $P2_1/c$.

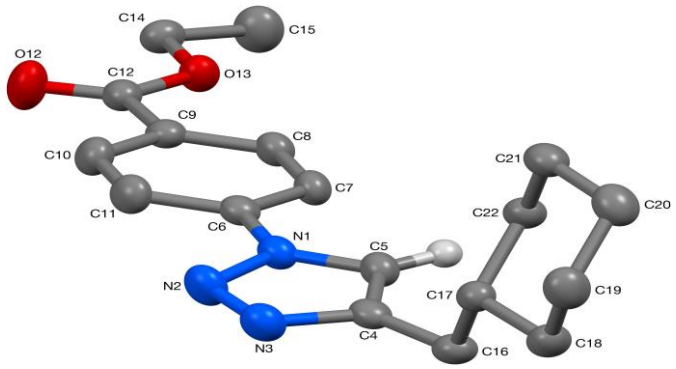


Figure S7. Crystal structure of **5du** (50% probability ellipsoids)

X-Ray crystal structure of 5du': The structure of **5du'** was found to contain two independent molecules, **5du'-A** and **5du'-B**, in the asymmetric unit. The C17B-based cyclohexyl unit and the O23B-based peroxy moiety were both found to be disordered, and two orientations were identified in each case, of *ca*. 67:33 and 69:31% occupancy when treated separately. As both groups bond to the same carbon atom, C16B, and the relative occupancies of the two orientations in each case were so similar, the two disorders were treated as linked with a common occupancy, which refined to *ca*. 68:32%. The geometries of the two orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically). The peroxy hydrogen atom on O24A was located from a ΔF map and refined freely subject to an O–H distance constraint of 0.90 Å. As the peroxy group is disordered in the second independent molecule it is not surprisingly that the associated hydrogen atoms could not be located from a ΔF map and so they were added to the atom list in calculated positions (the SHELX HFIX 147 command) with

a O–H distance of 0.90 Å. The structure was found to crystallise in a chiral space group ($P2_1$), but the absolute structure could not be reliably determined [Flack parameter x = 0.1(3)].

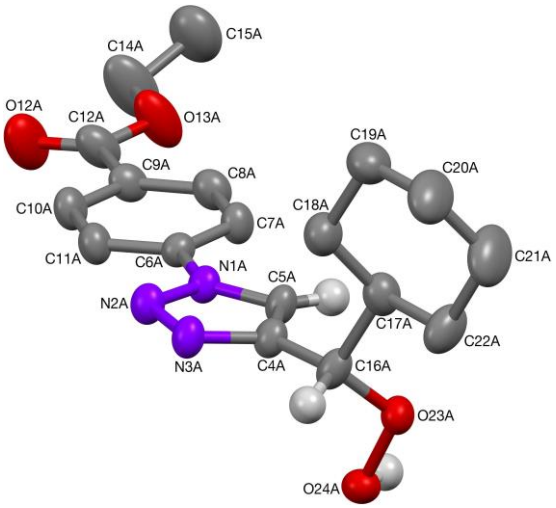


Figure S8. Crystal structure of **5du'** (50% probability ellipsoids).

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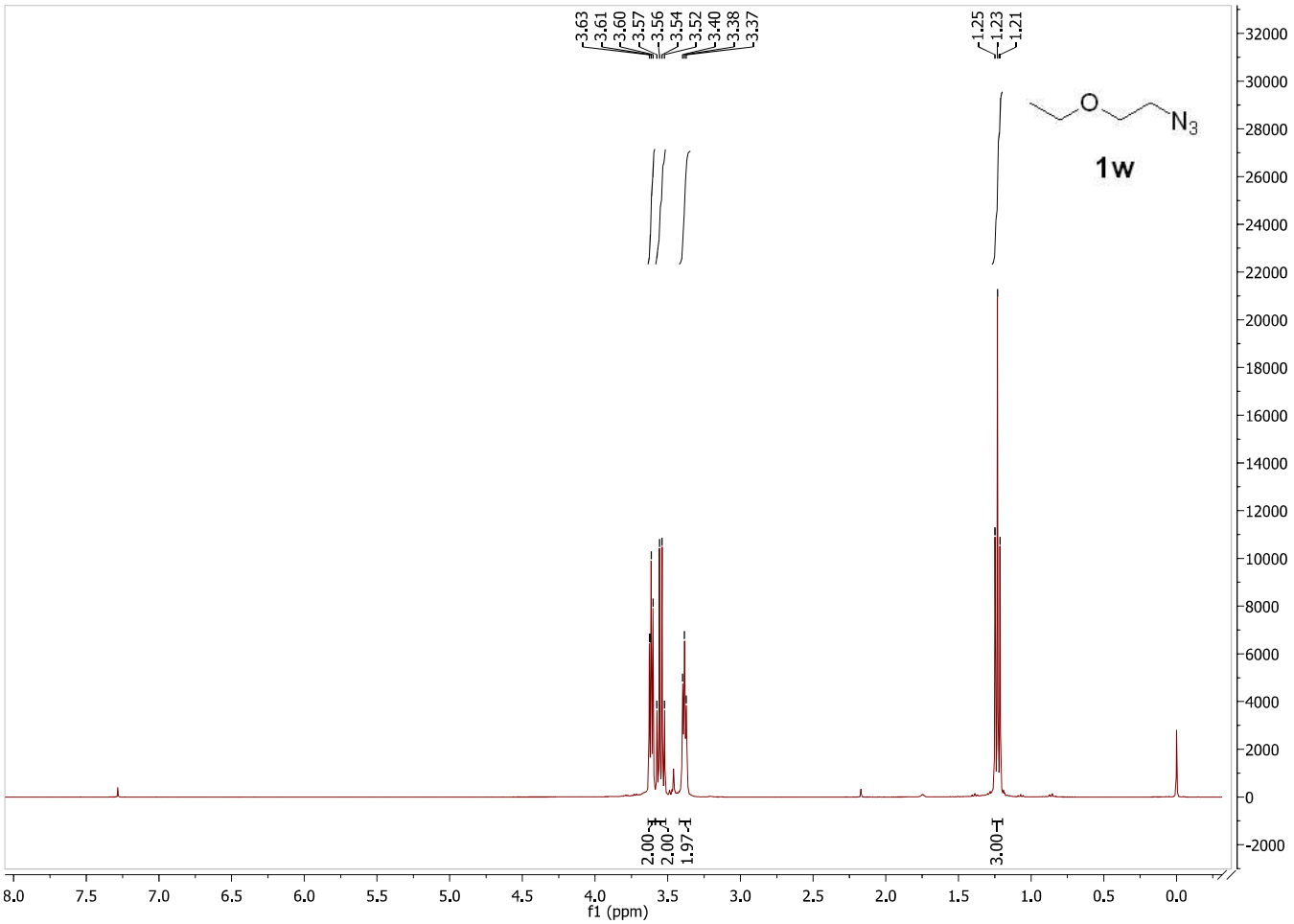
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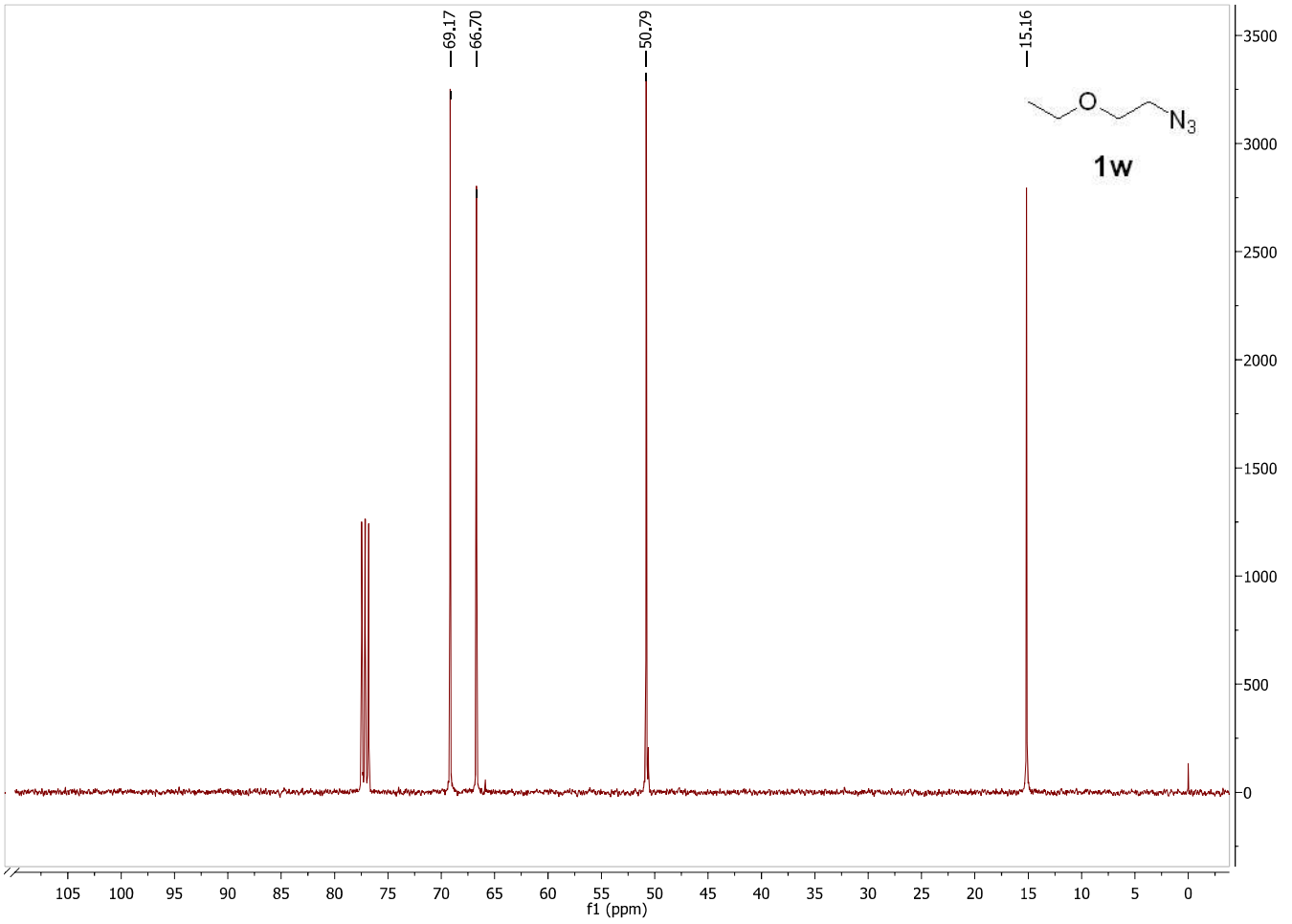
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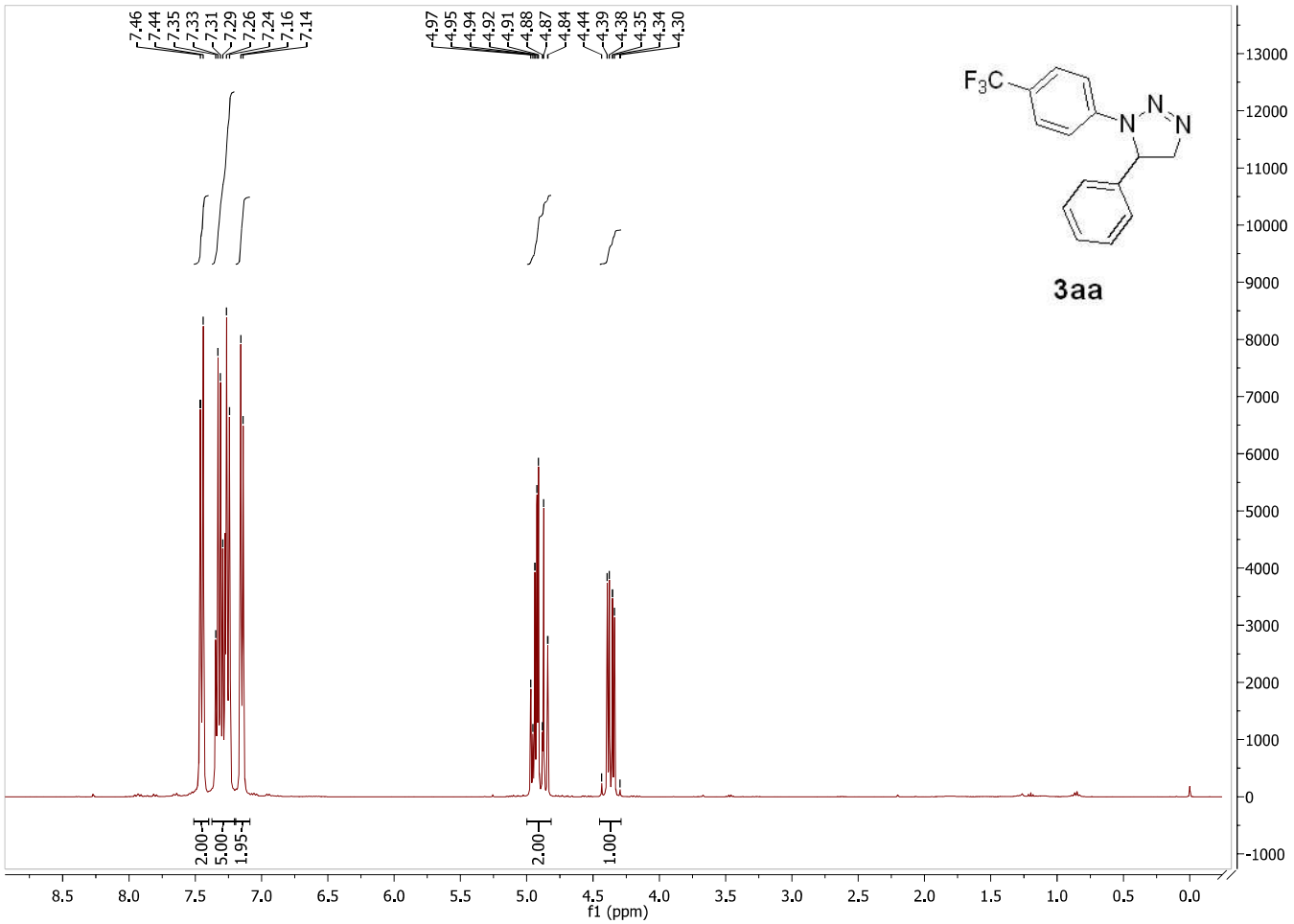
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4.38
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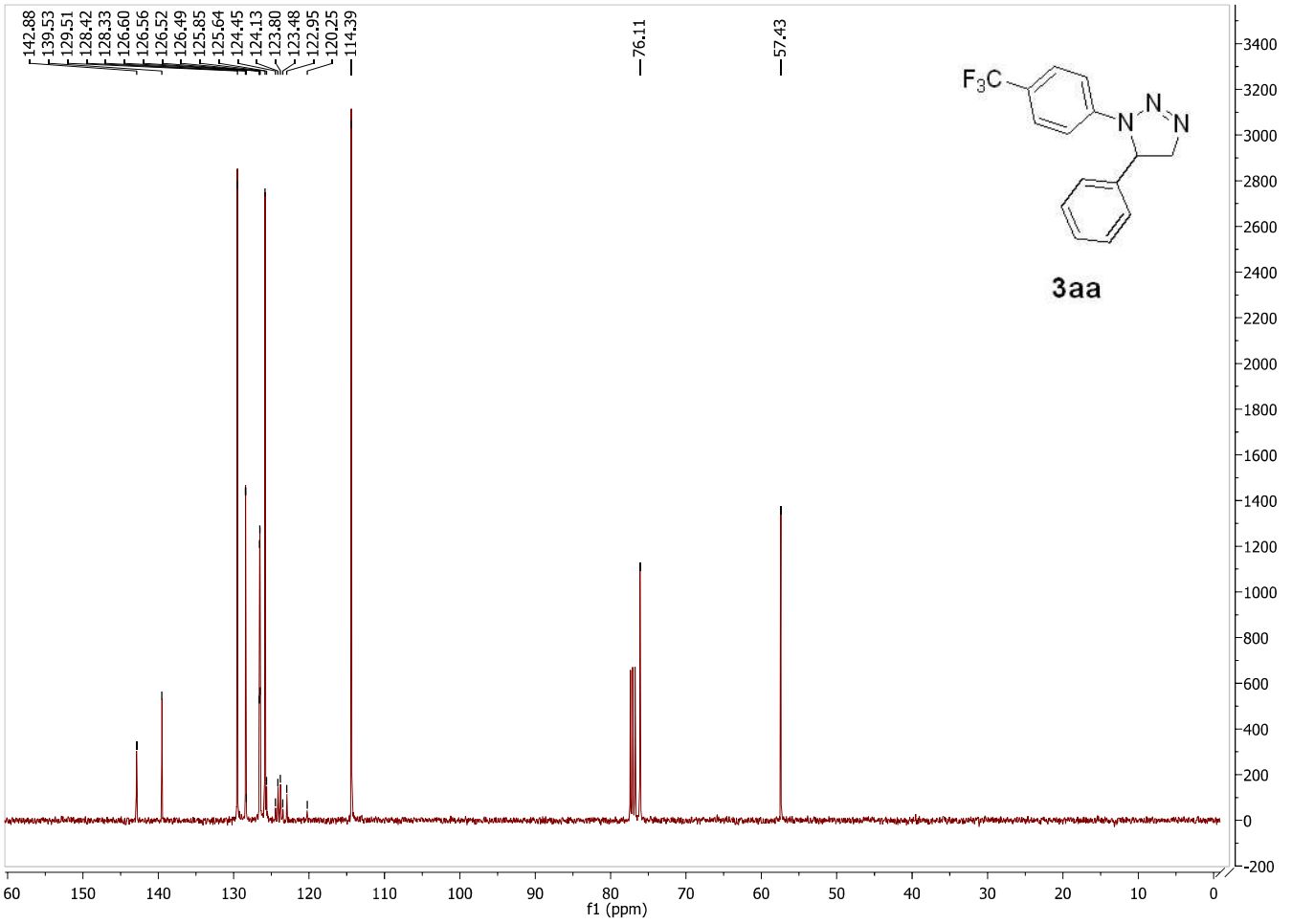
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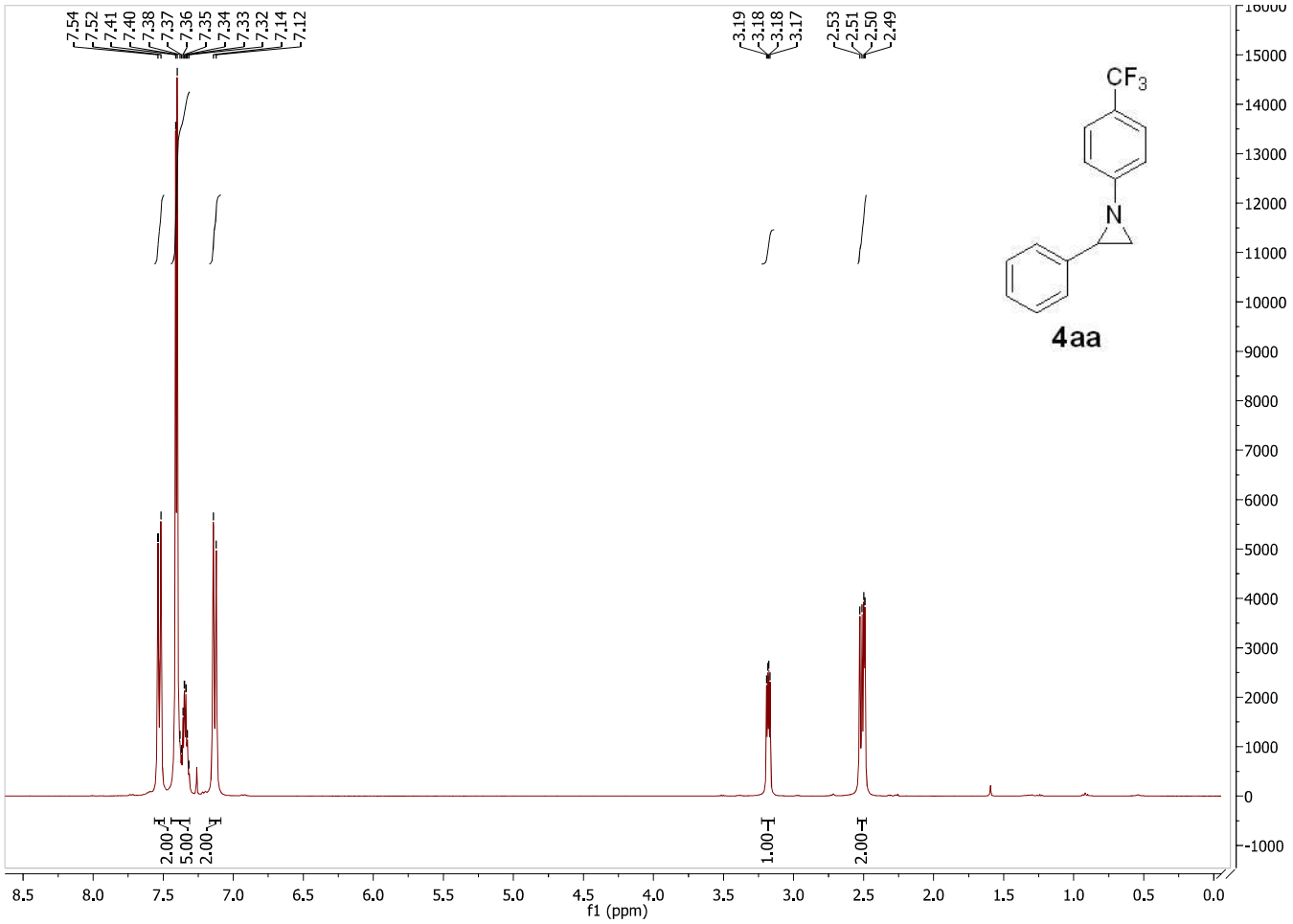
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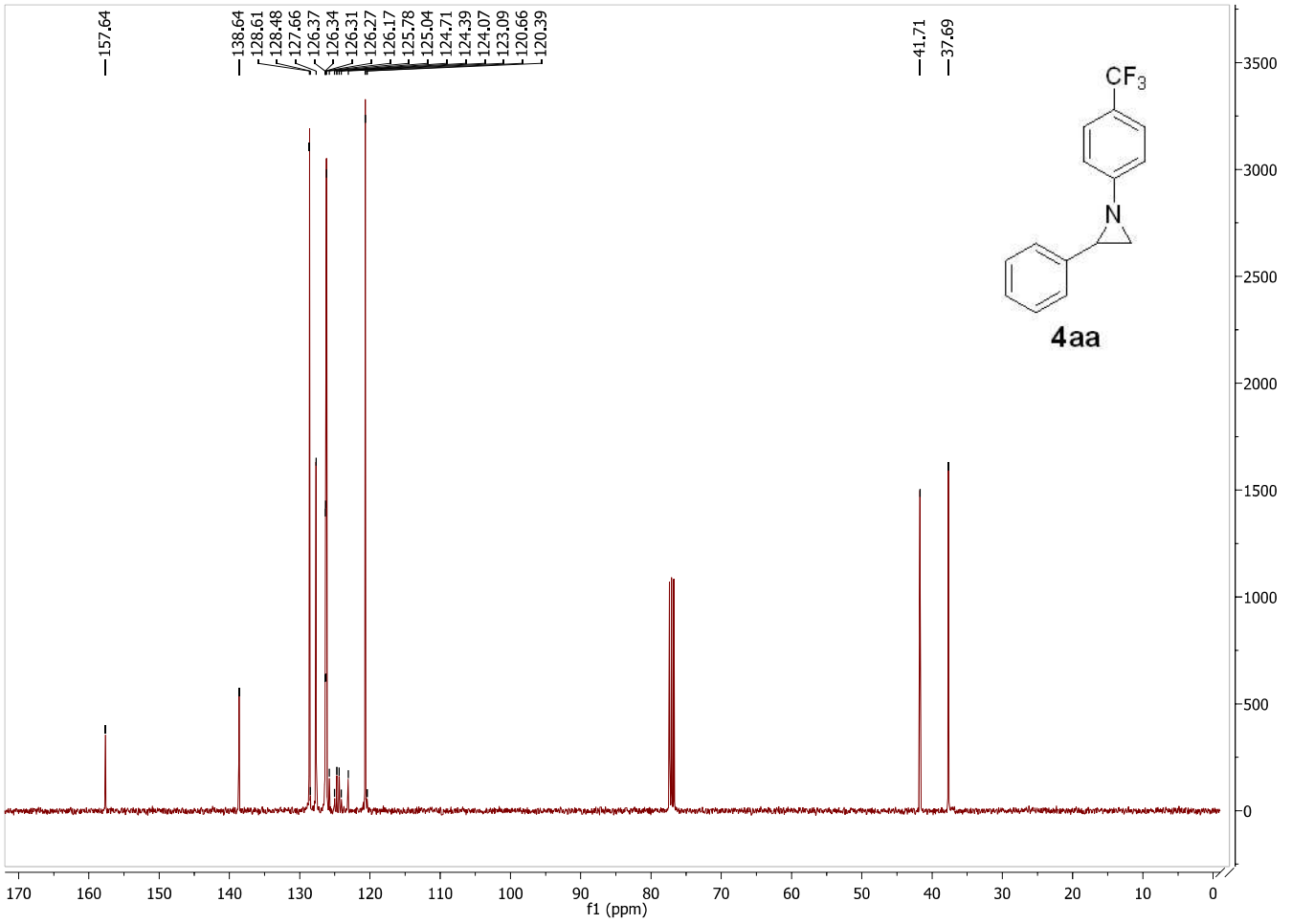
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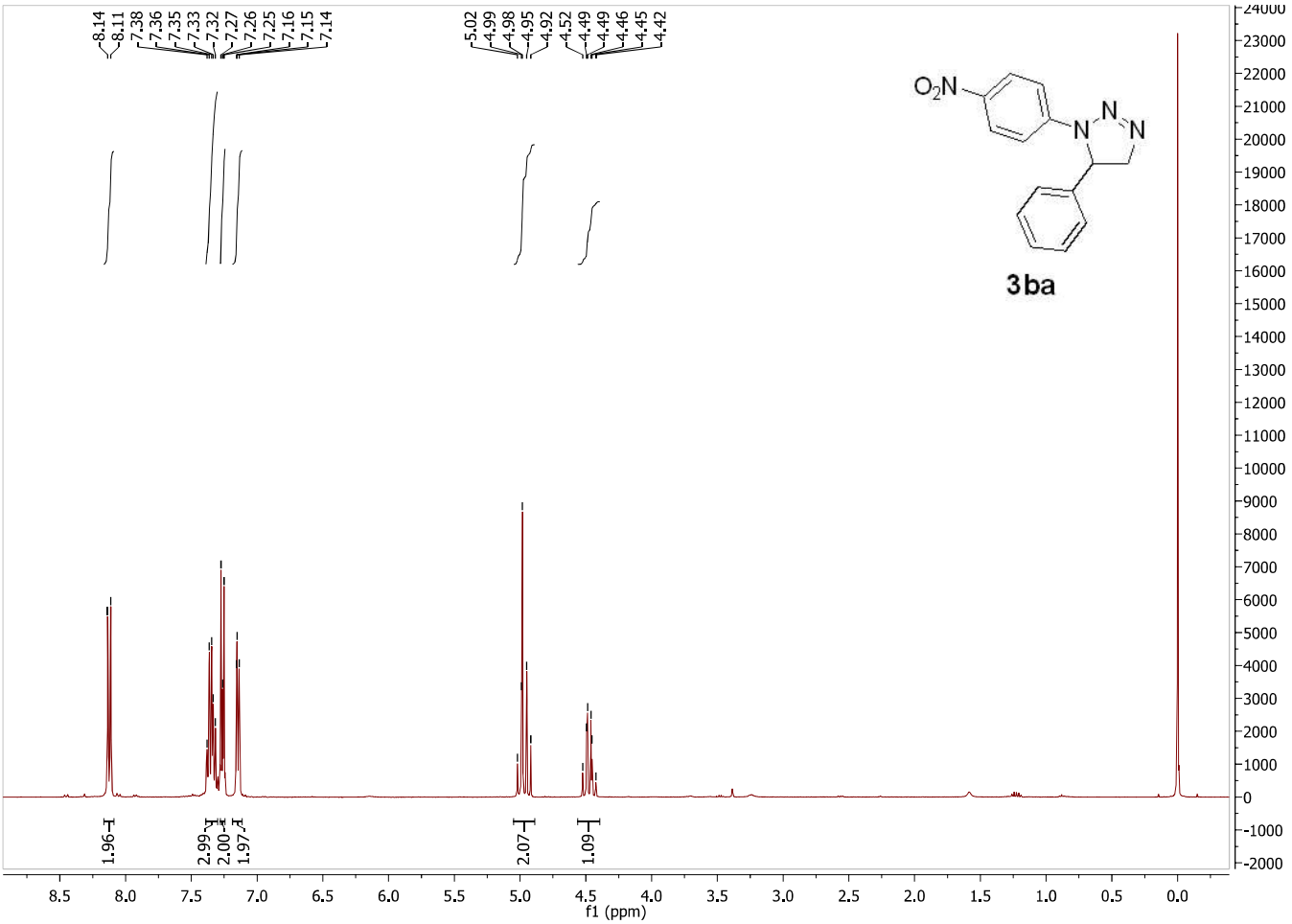
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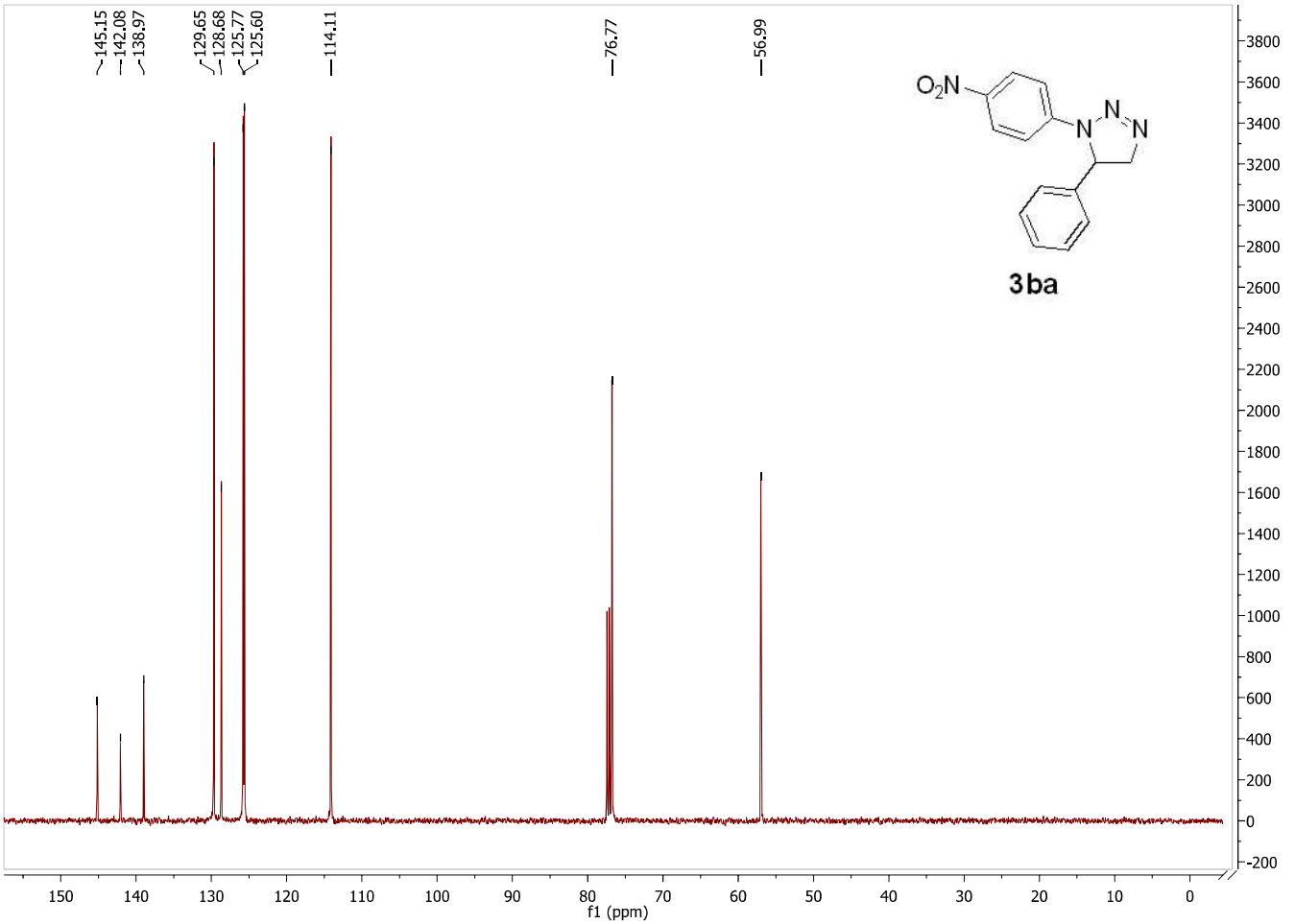
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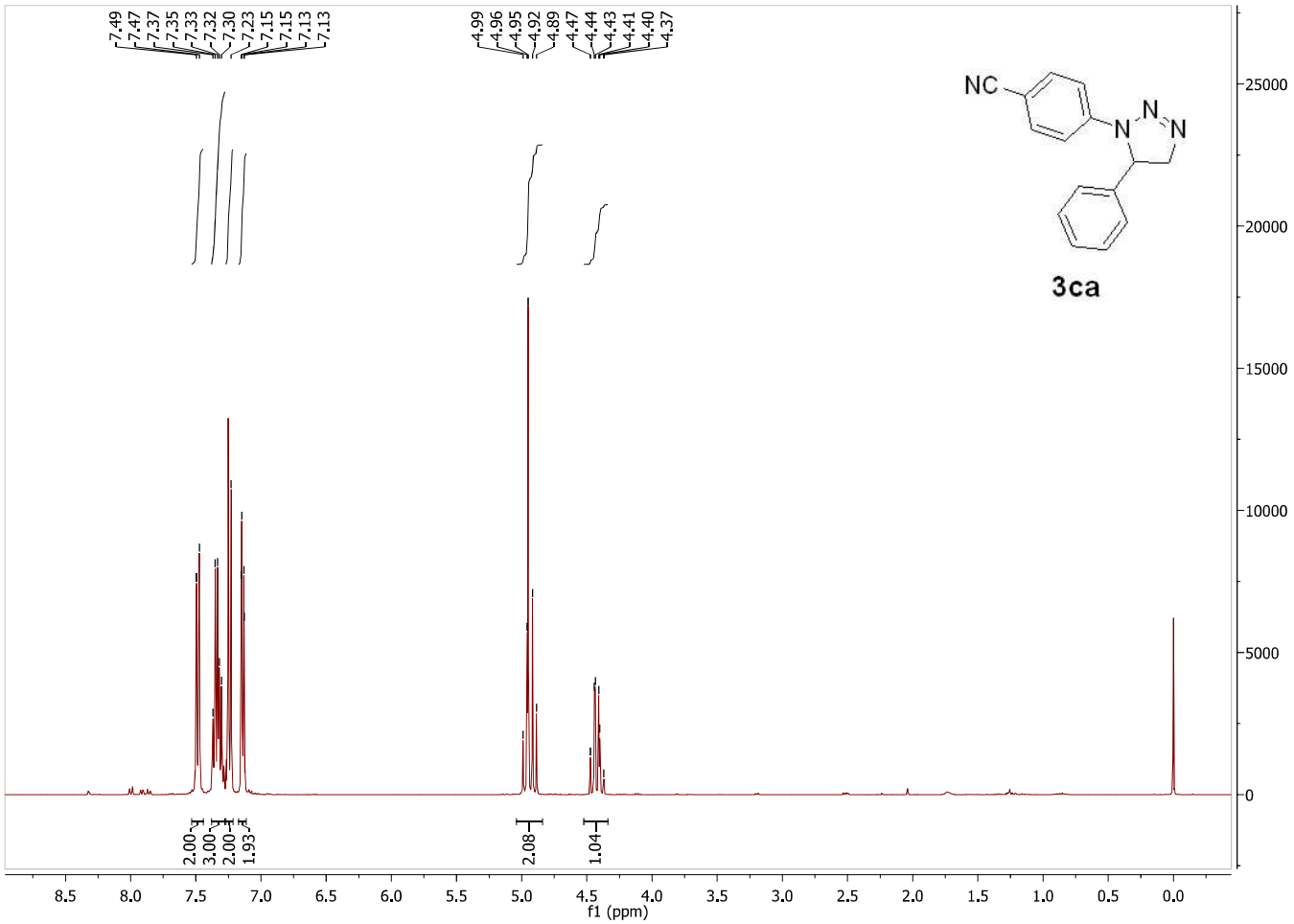
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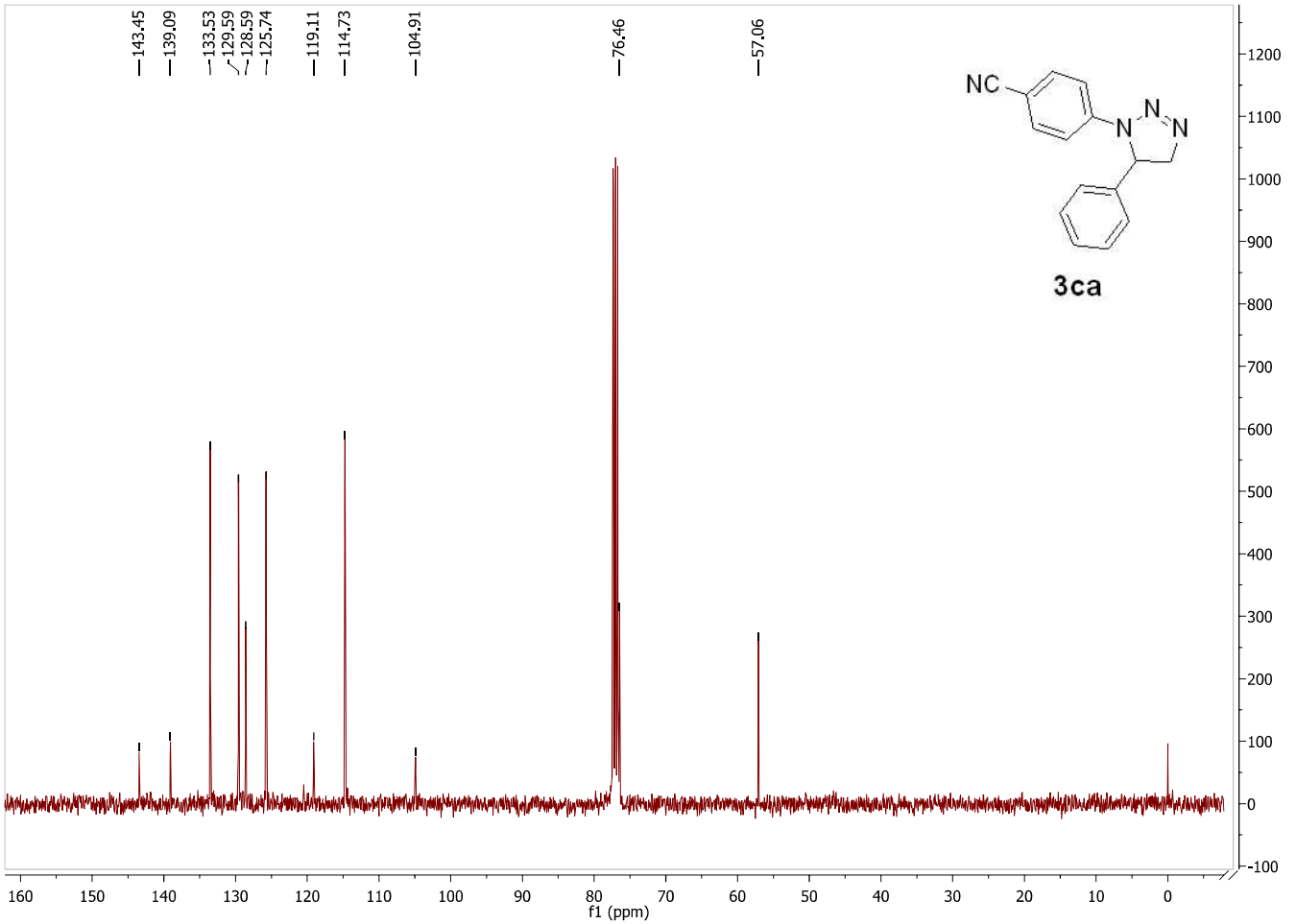
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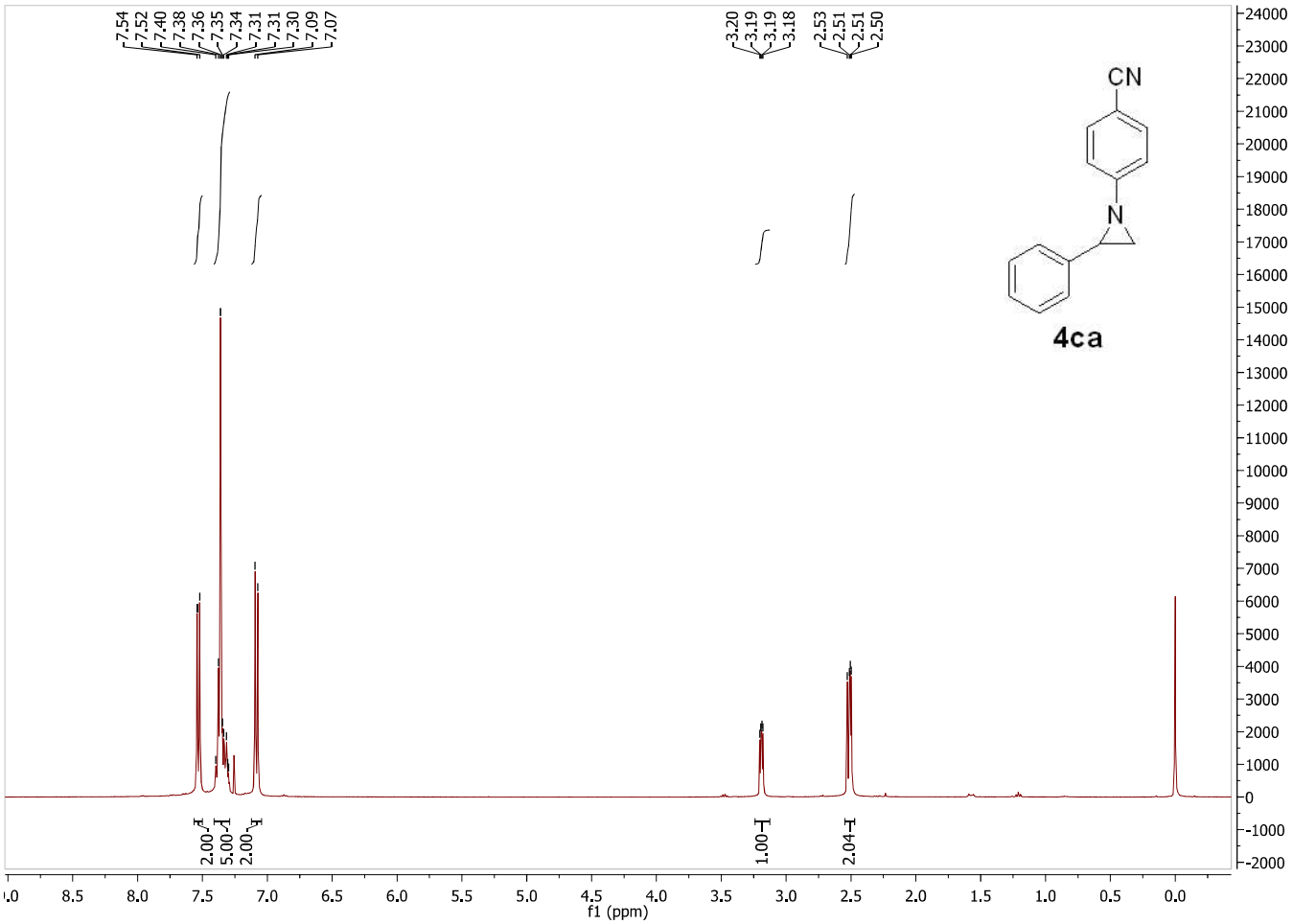
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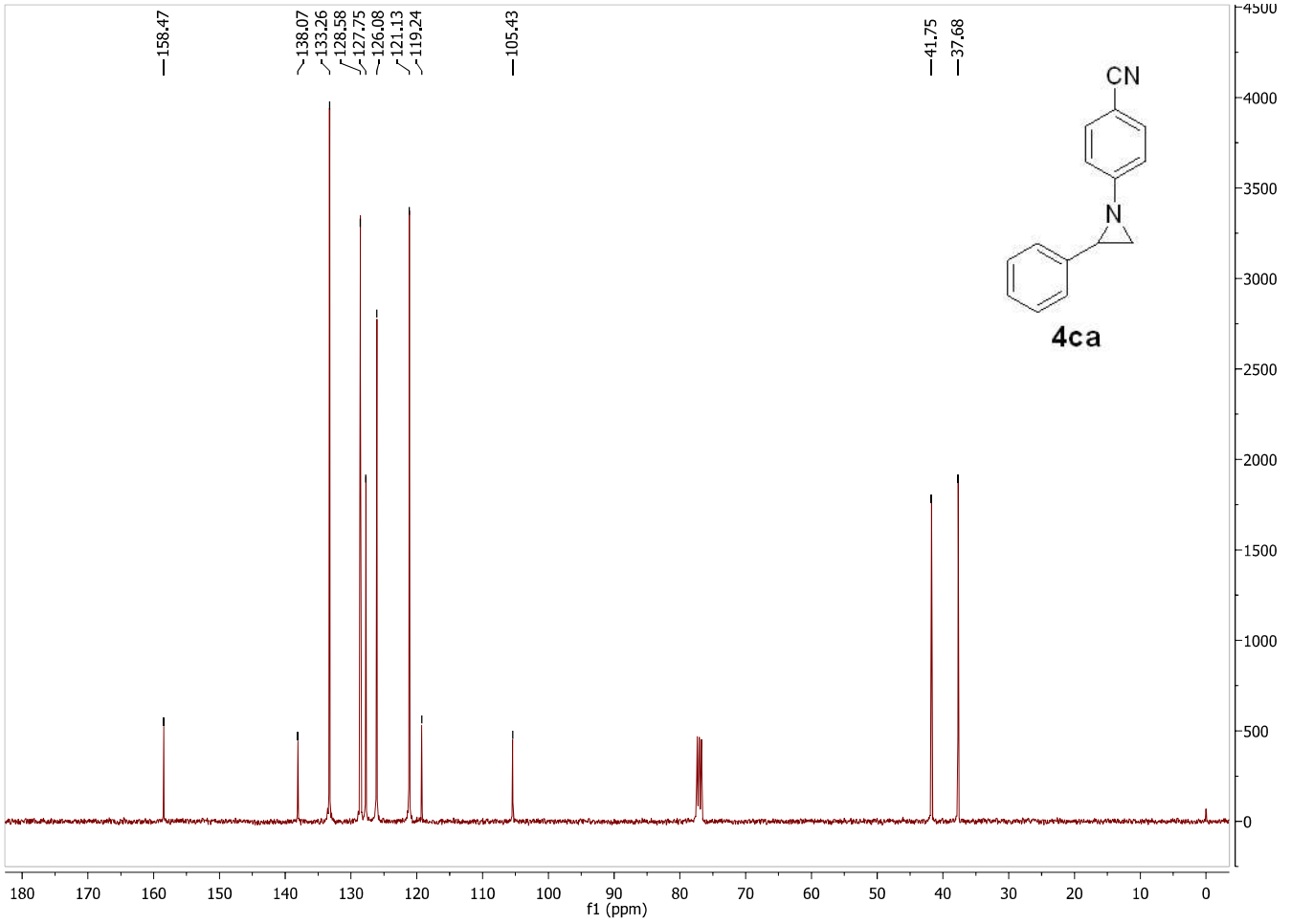
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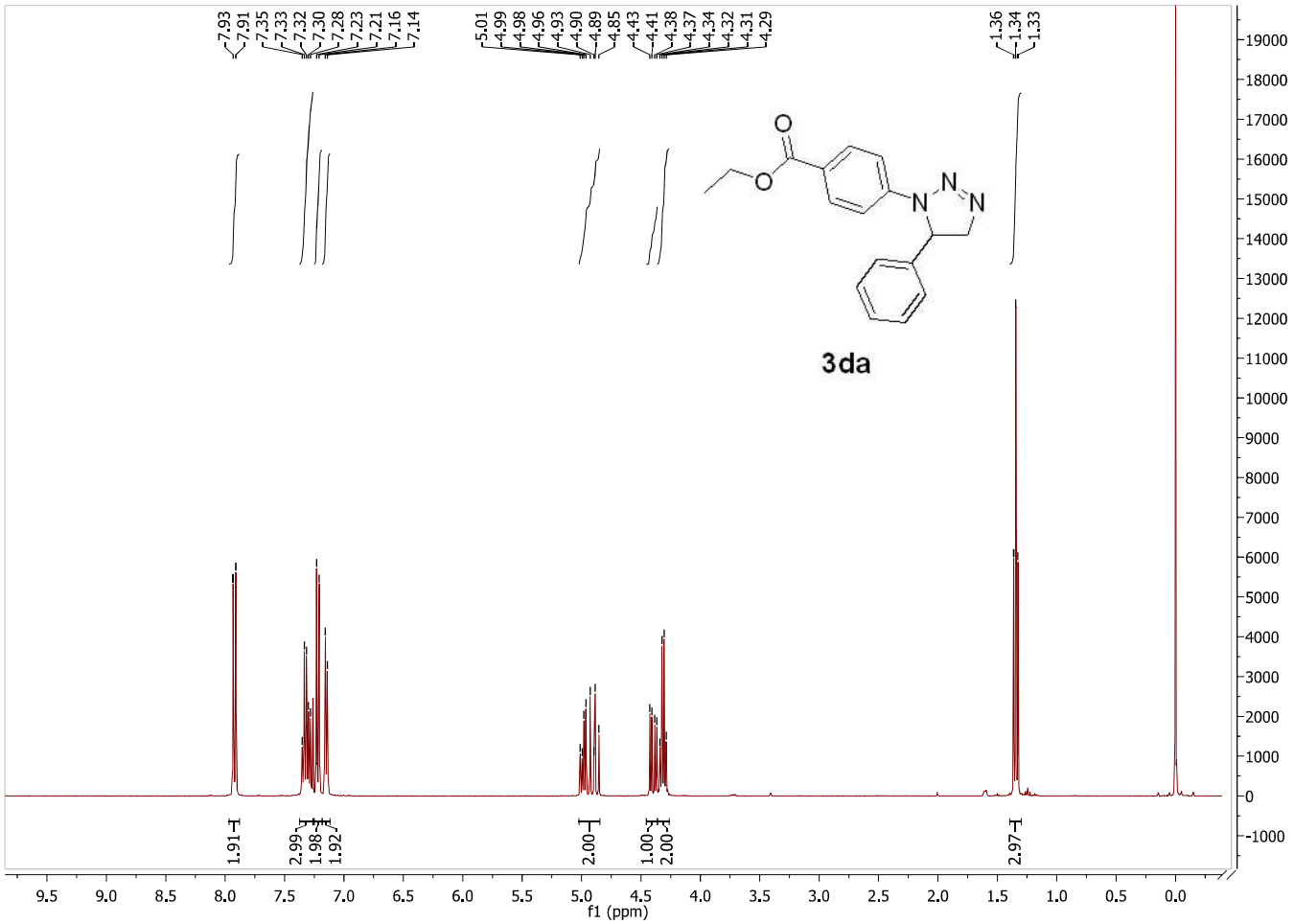
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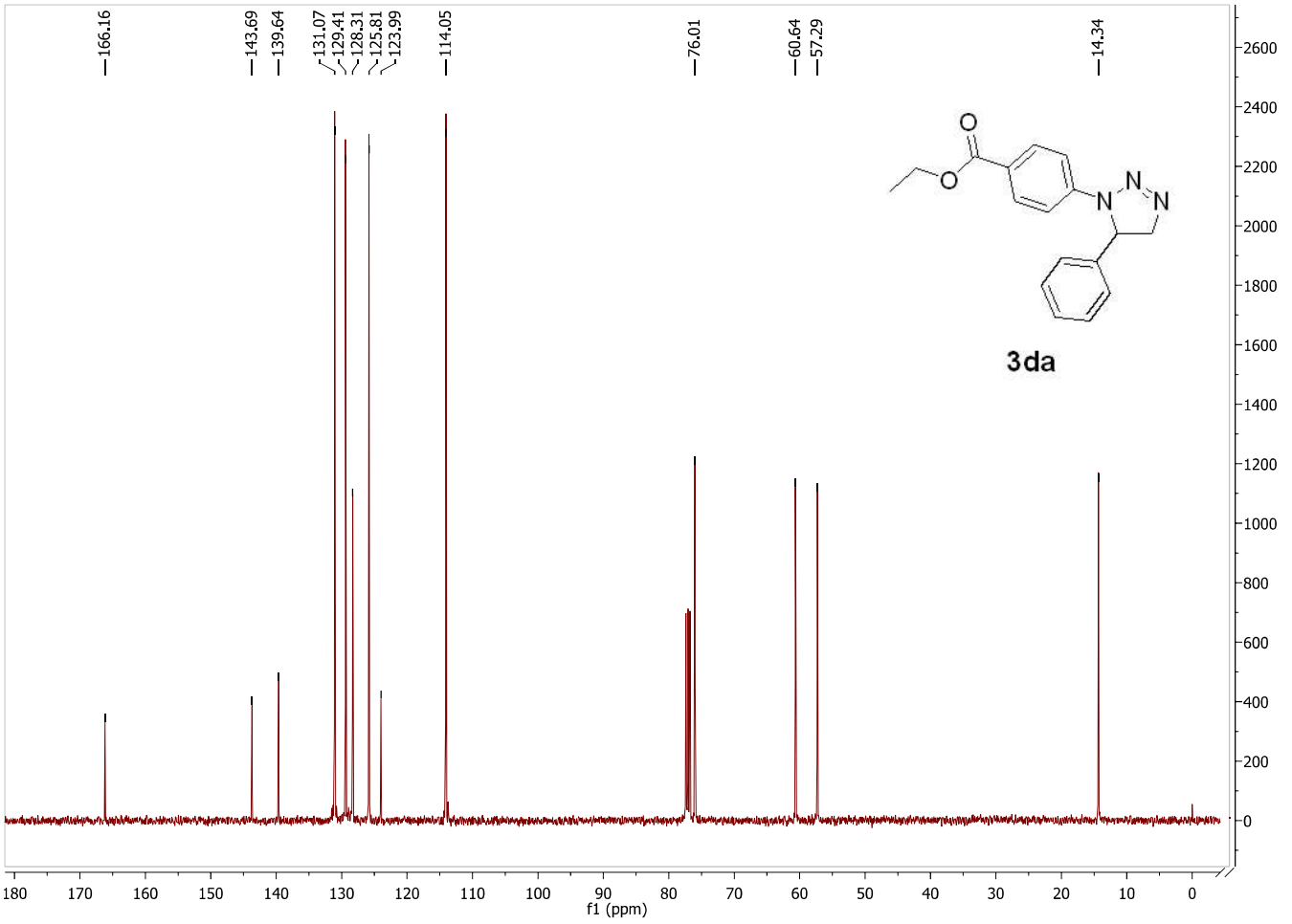
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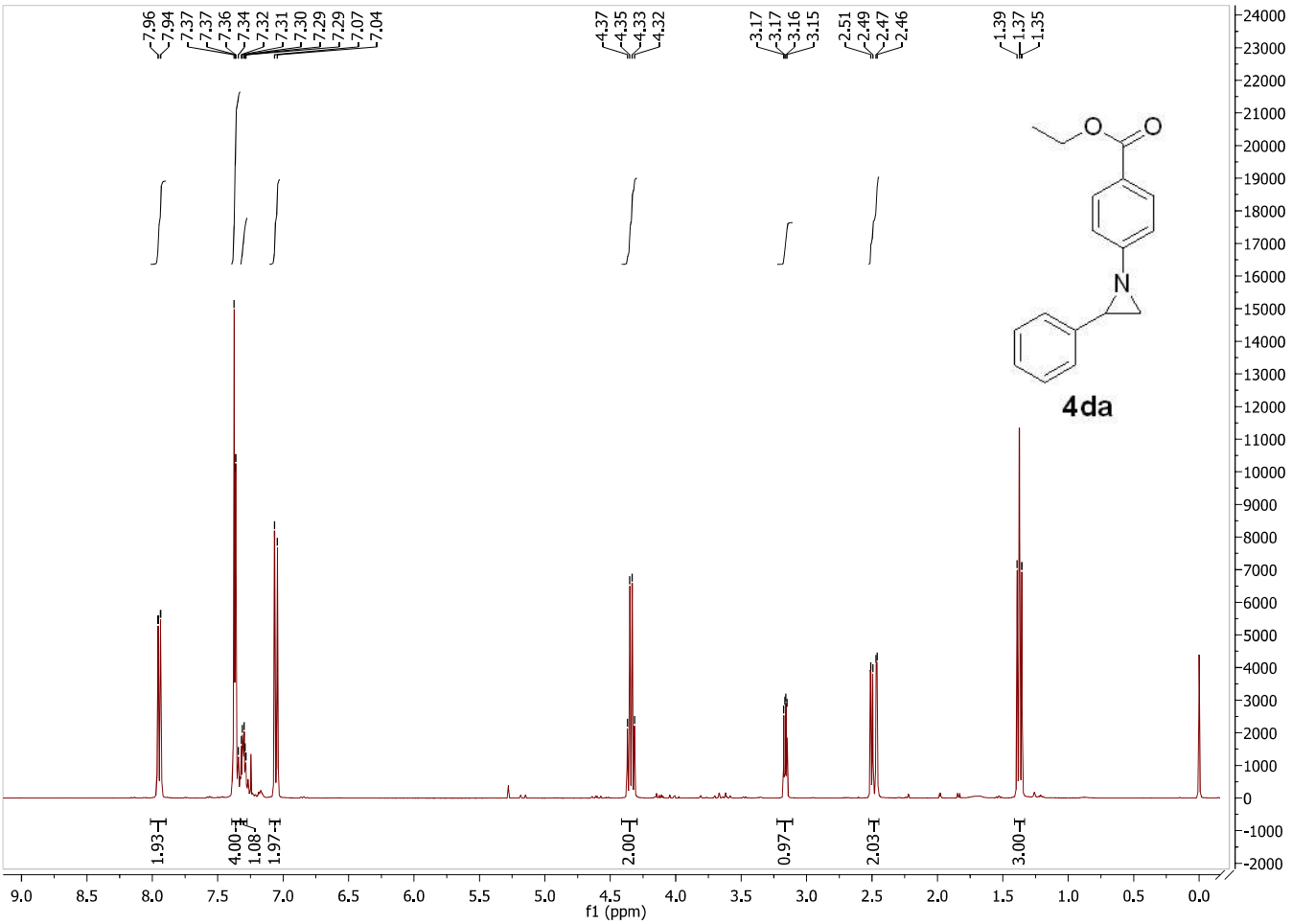
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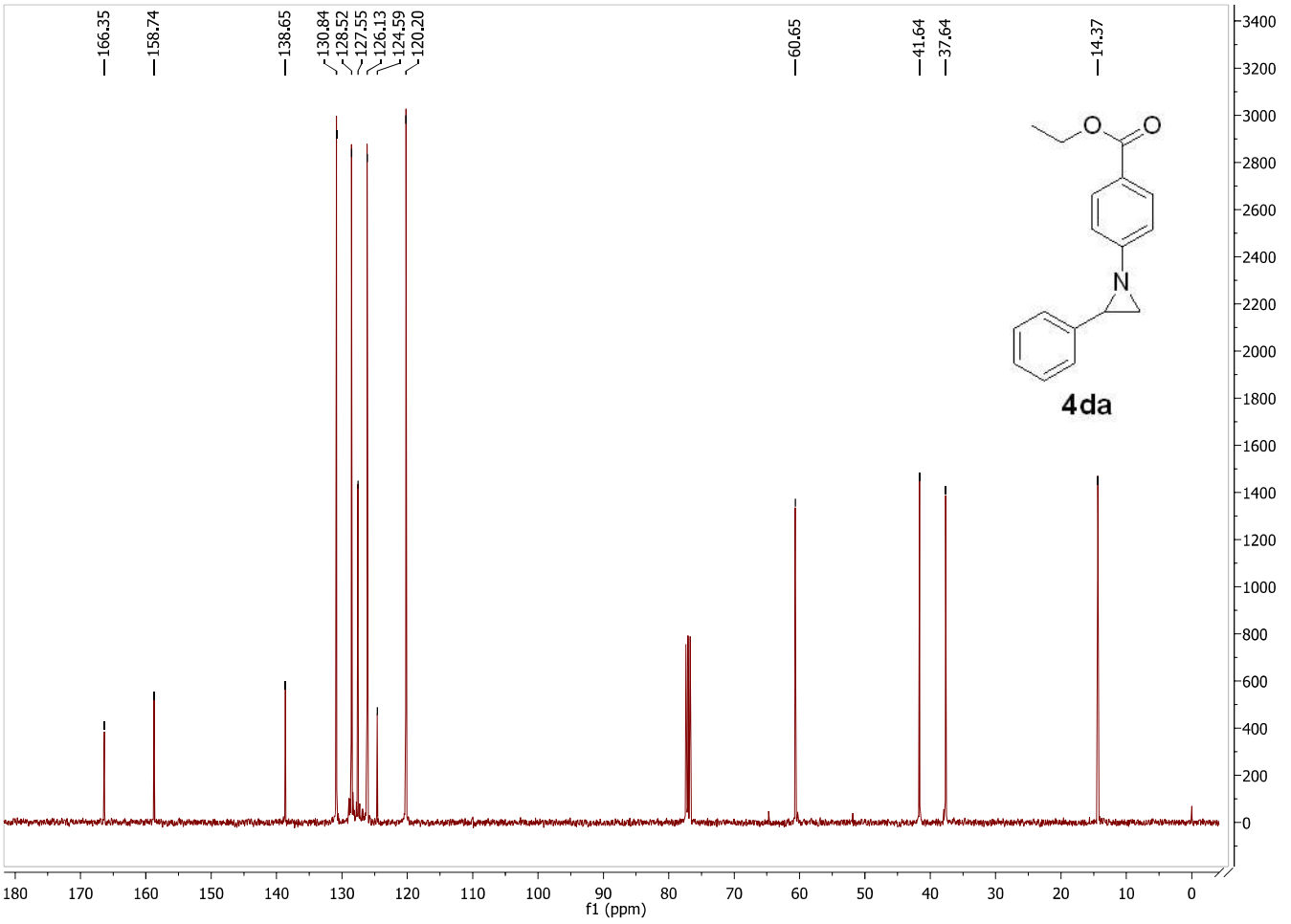
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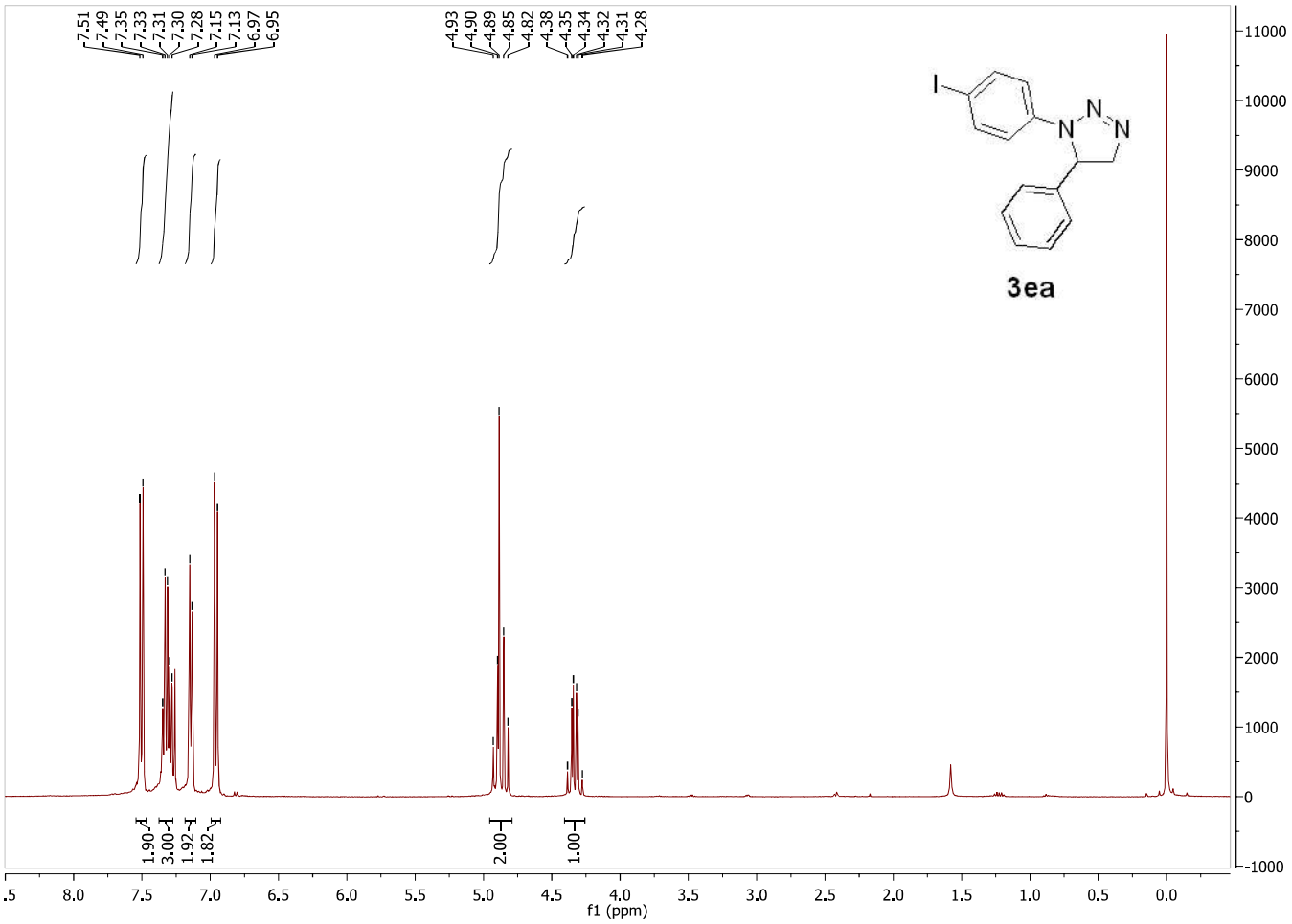
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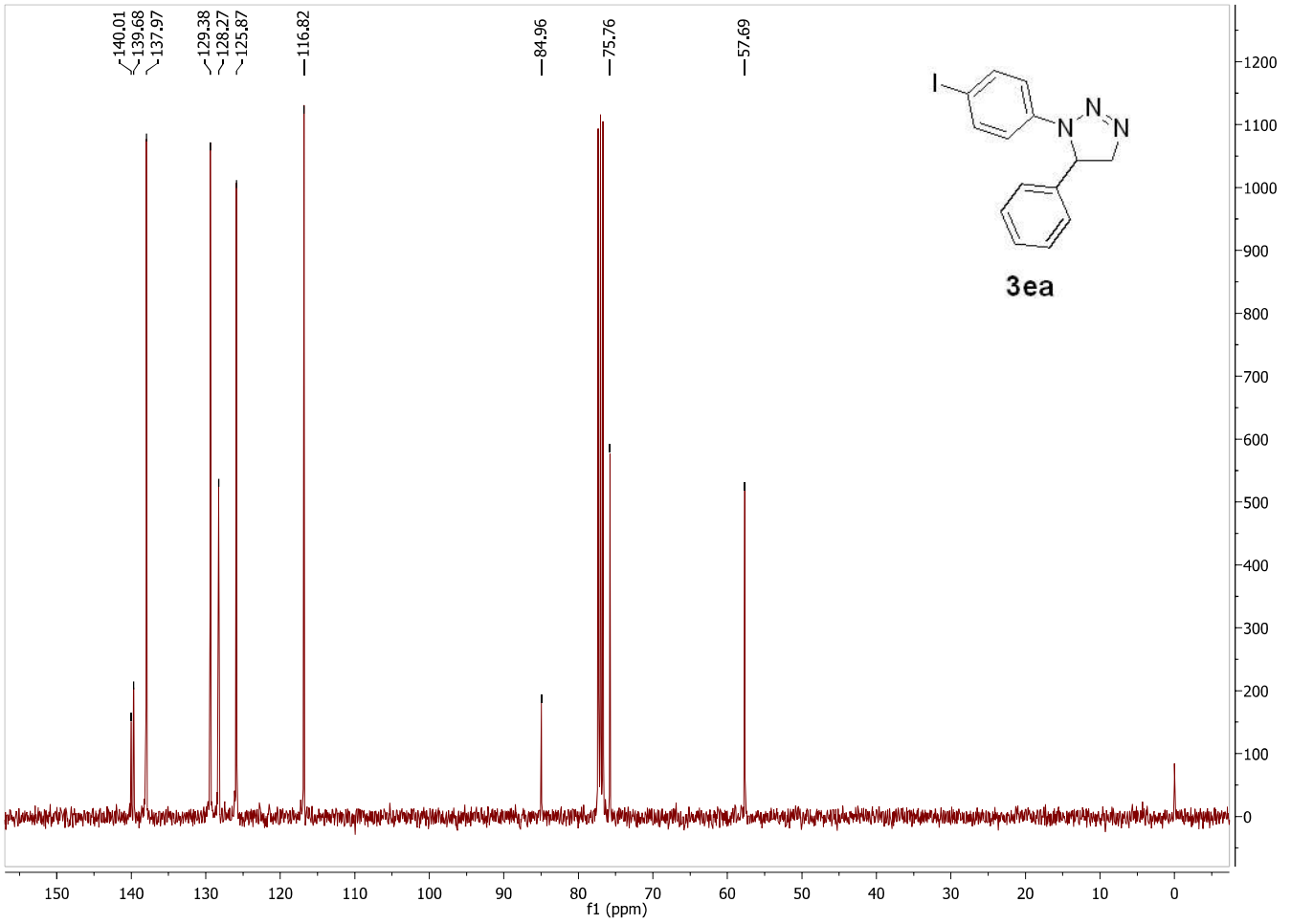
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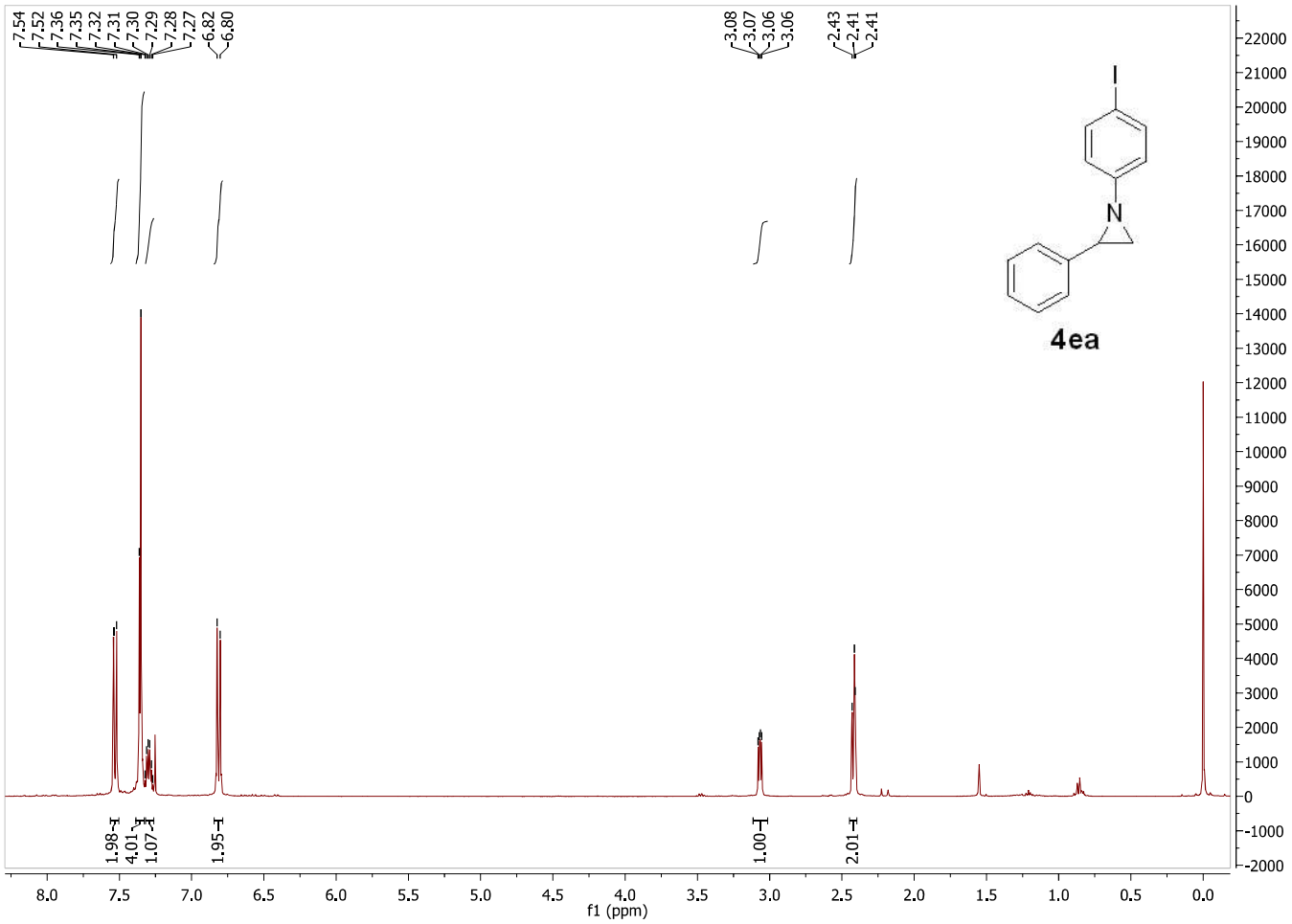
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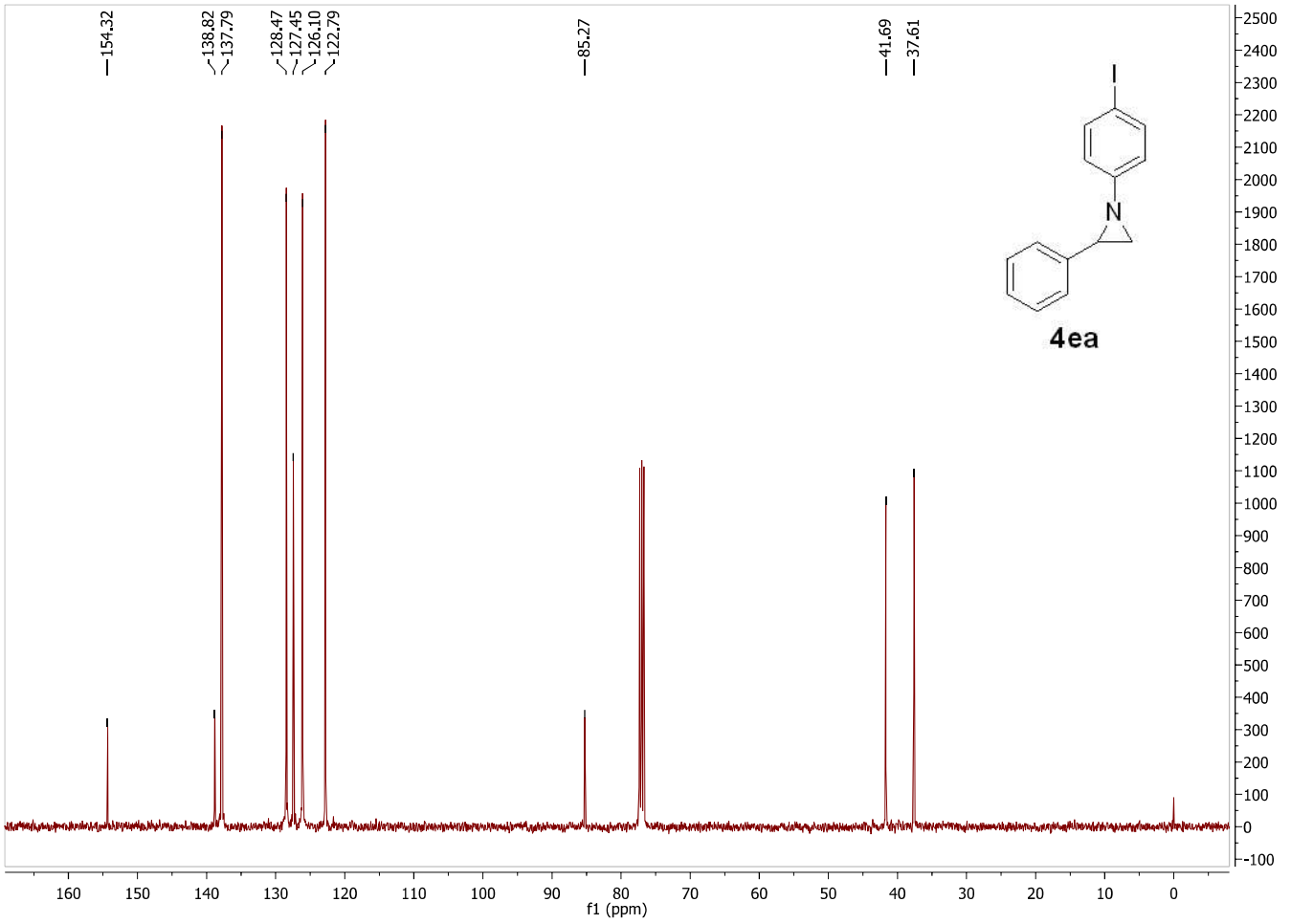
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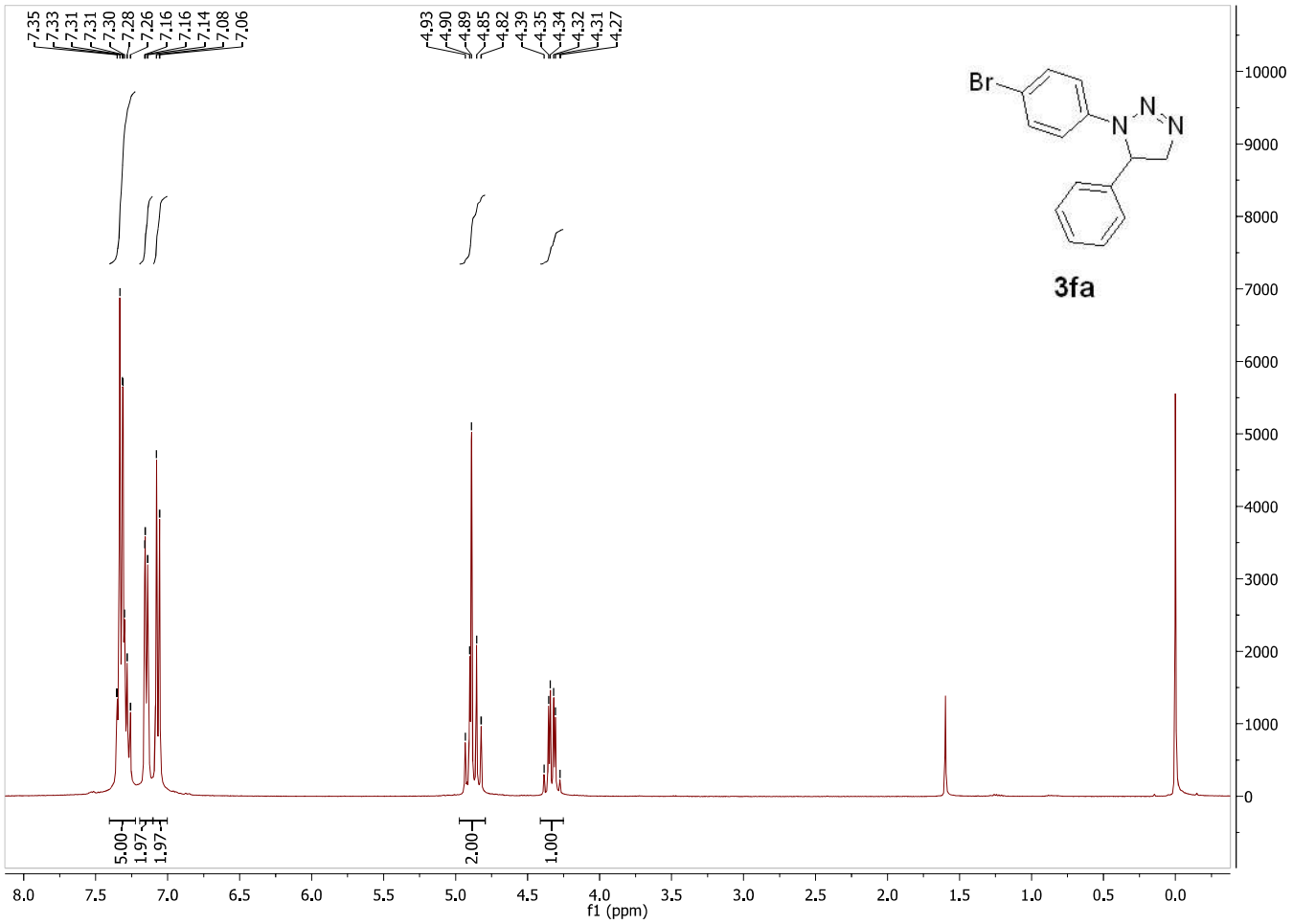
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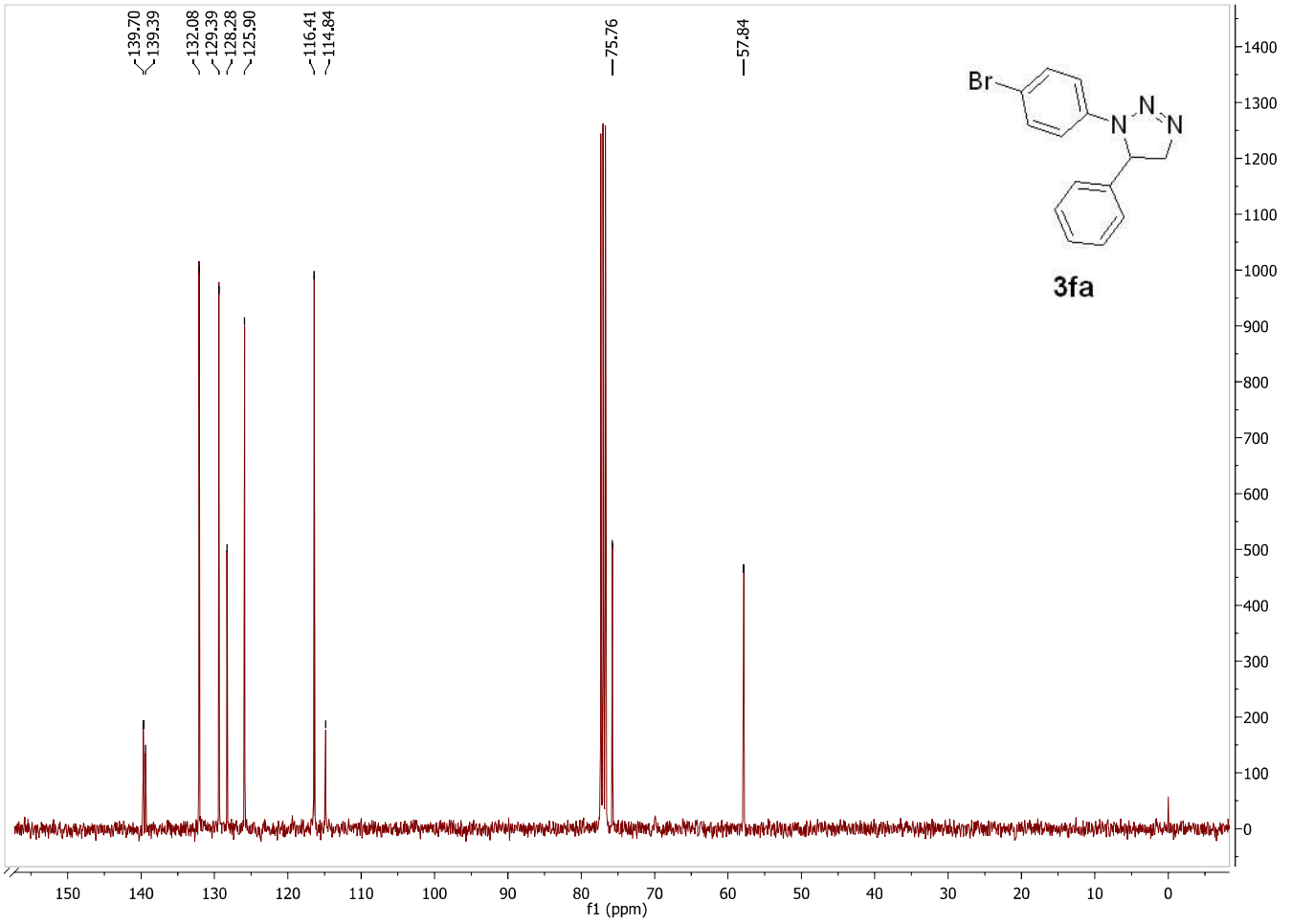
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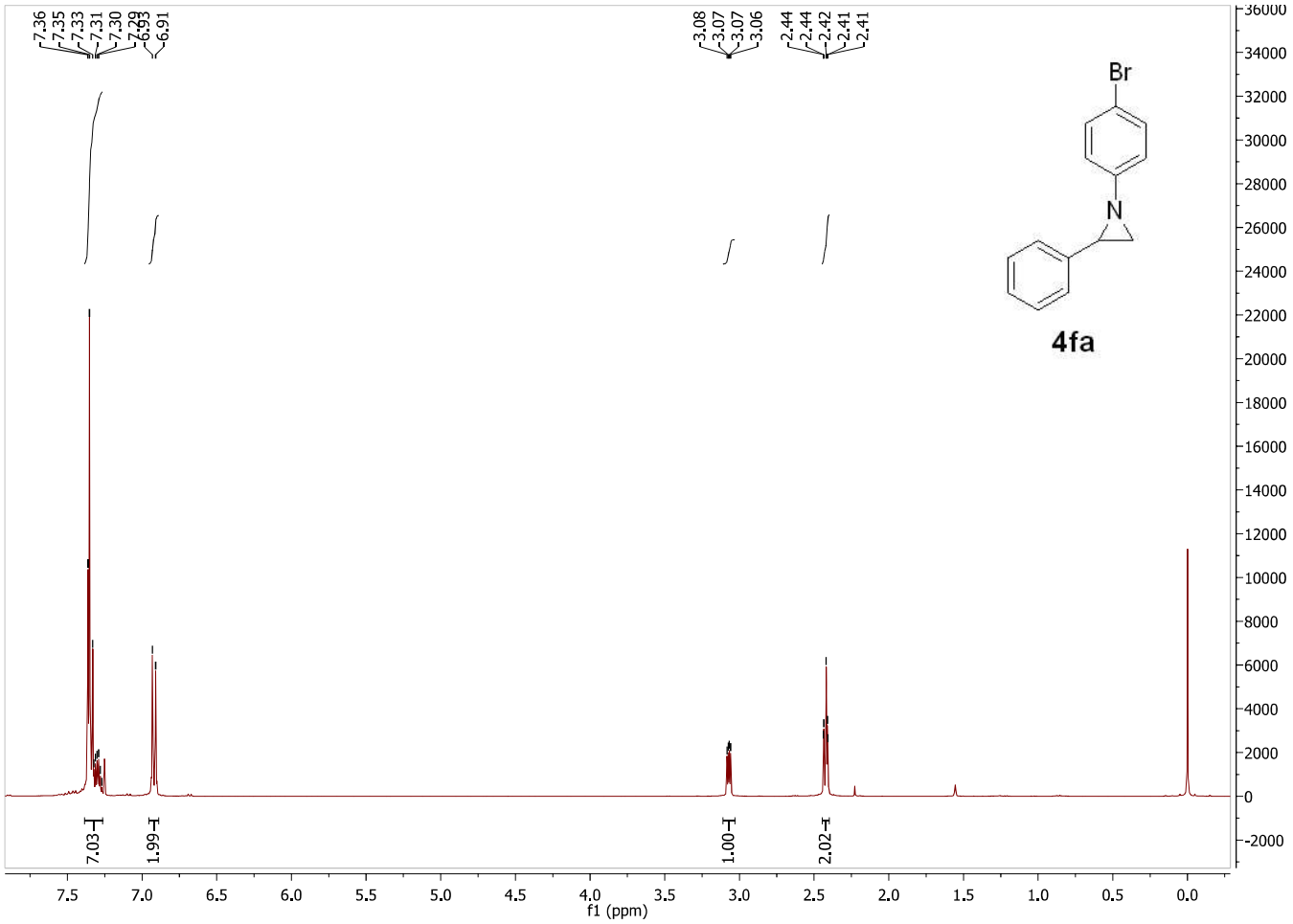
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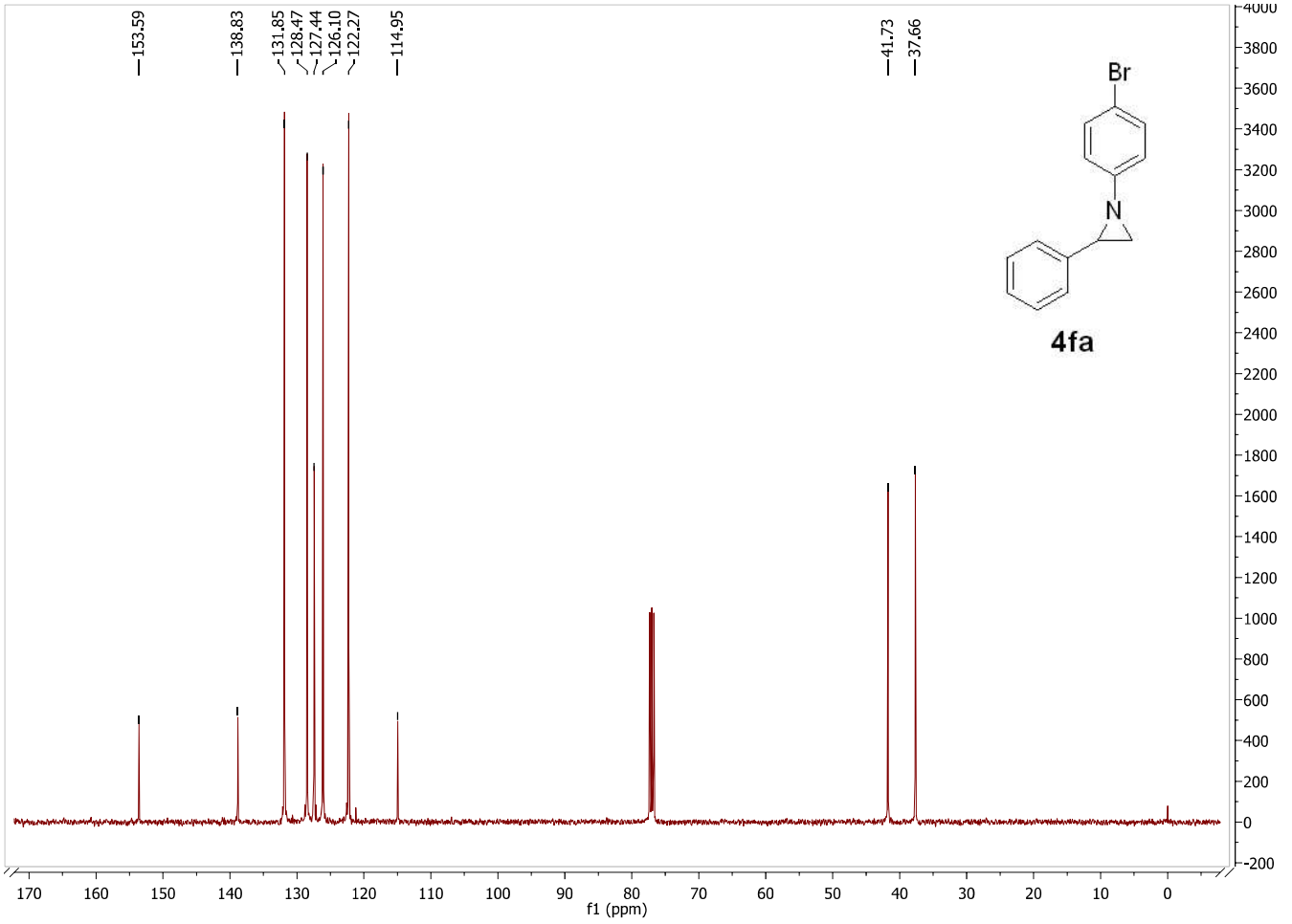
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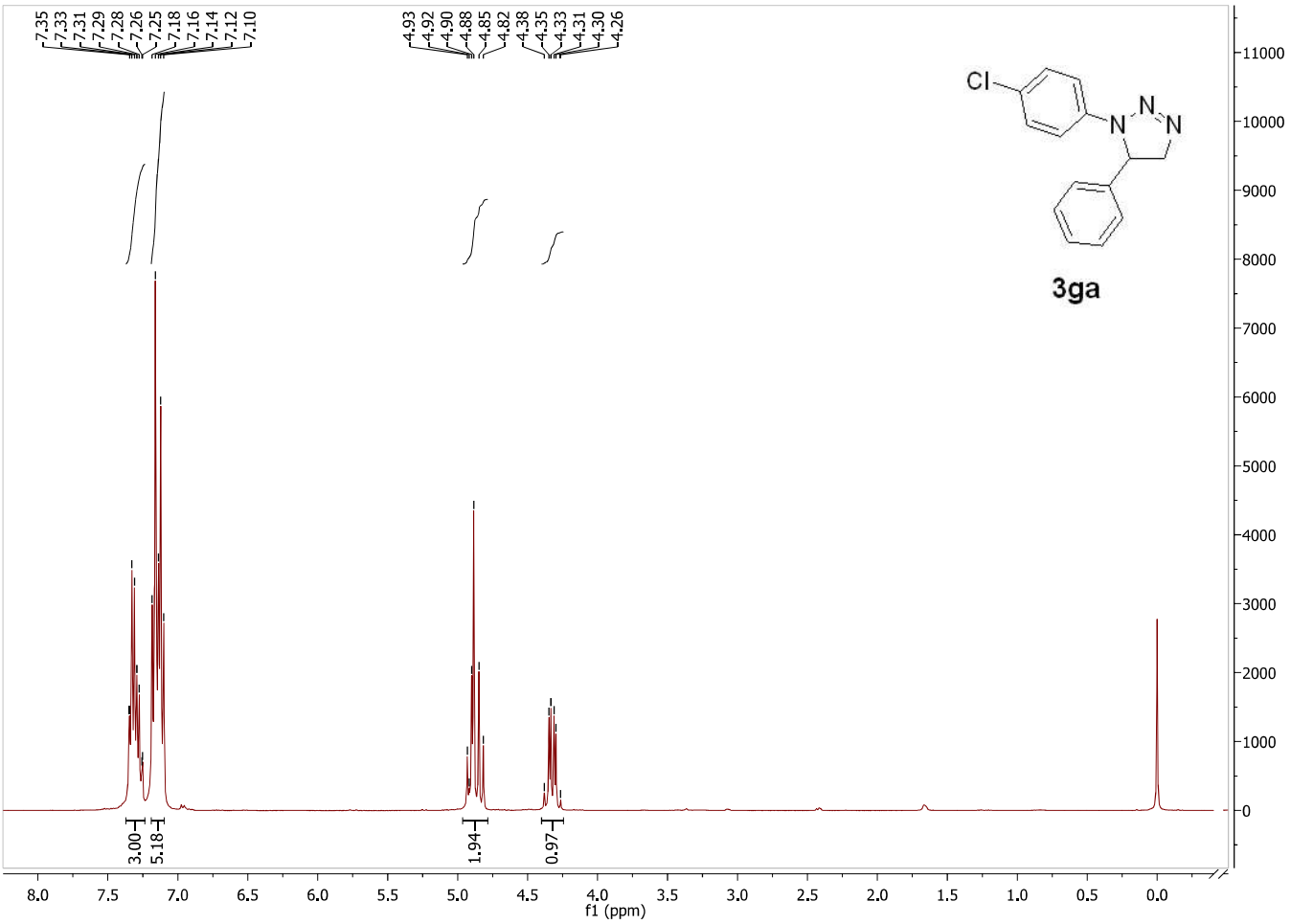
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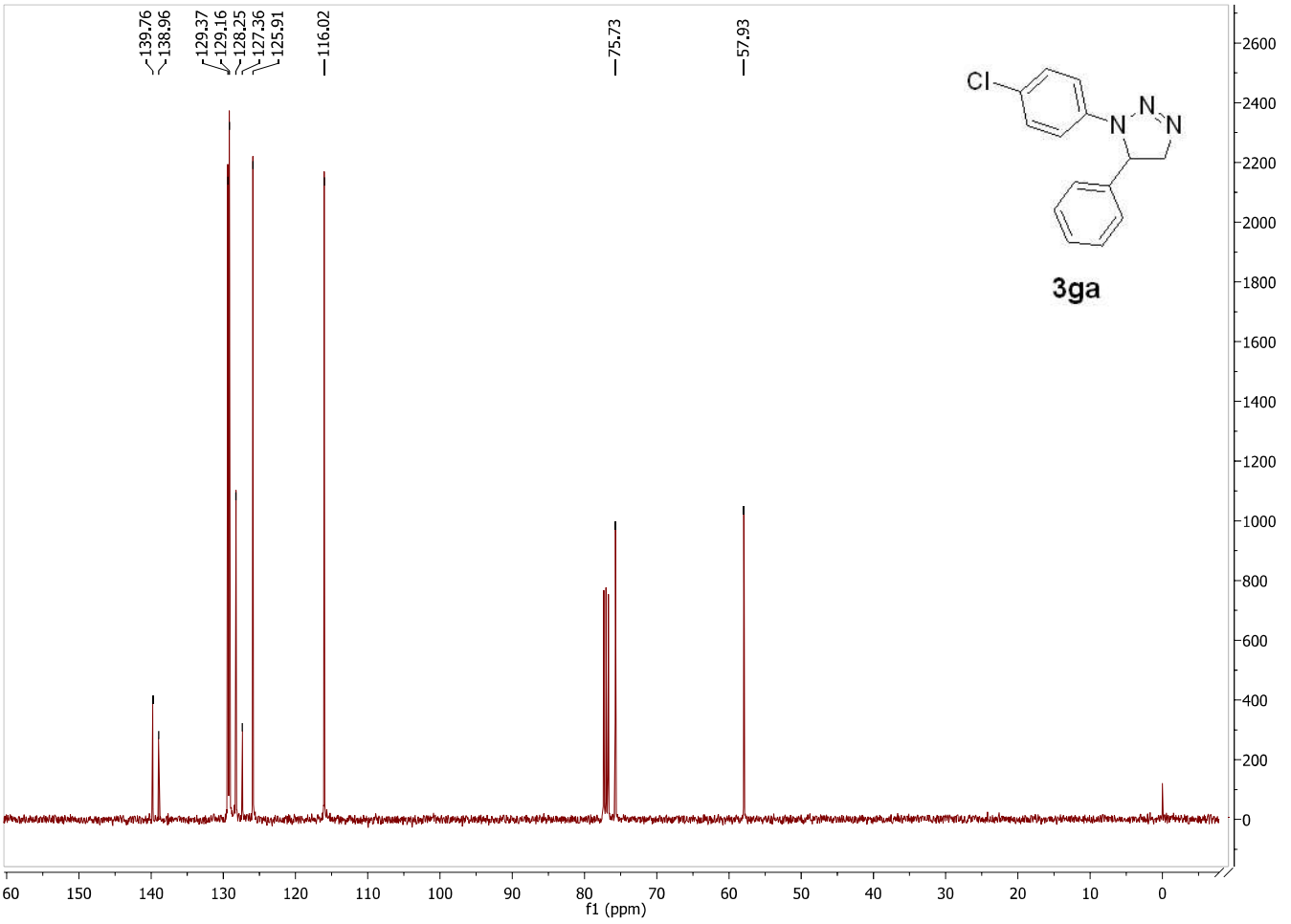
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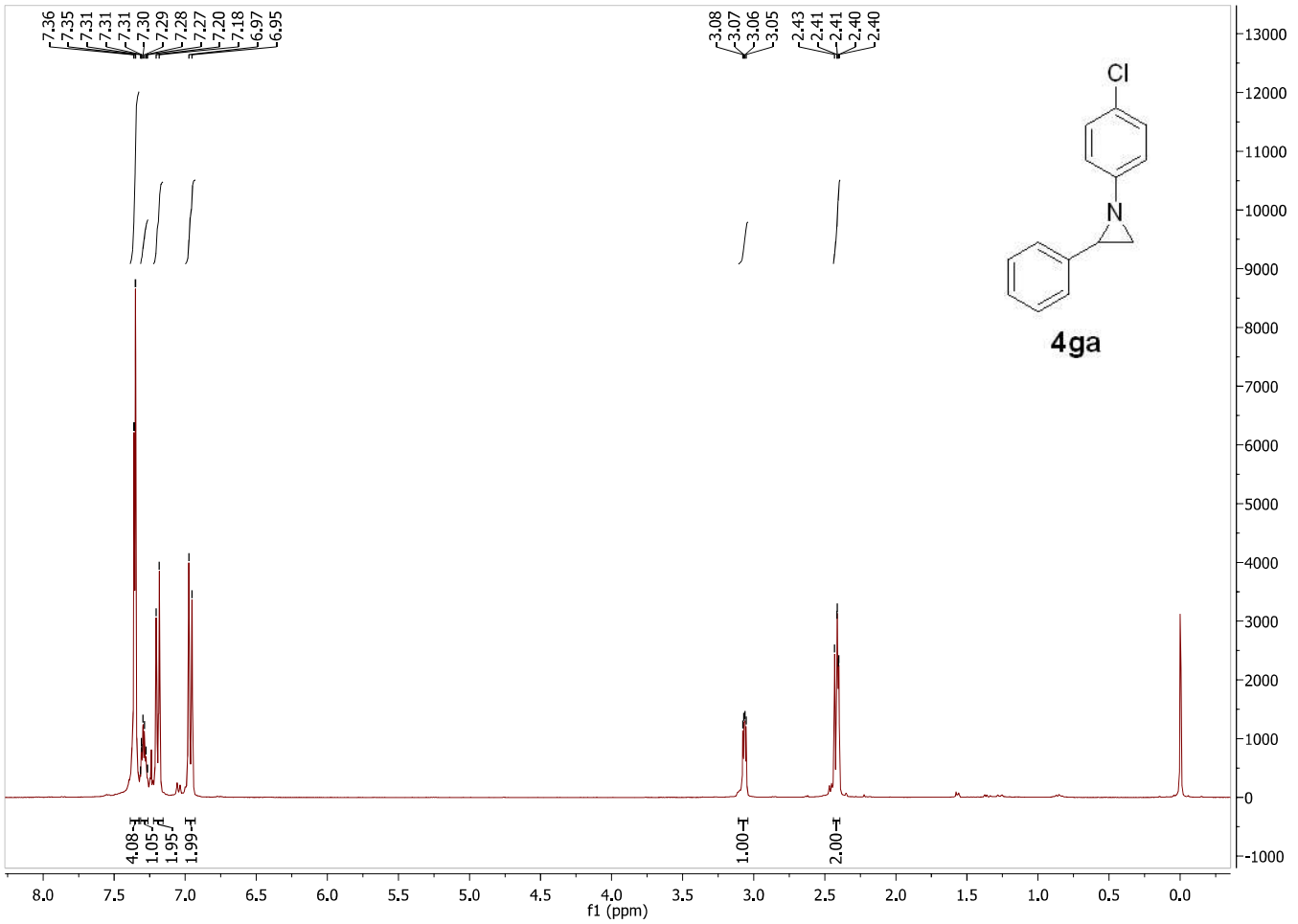
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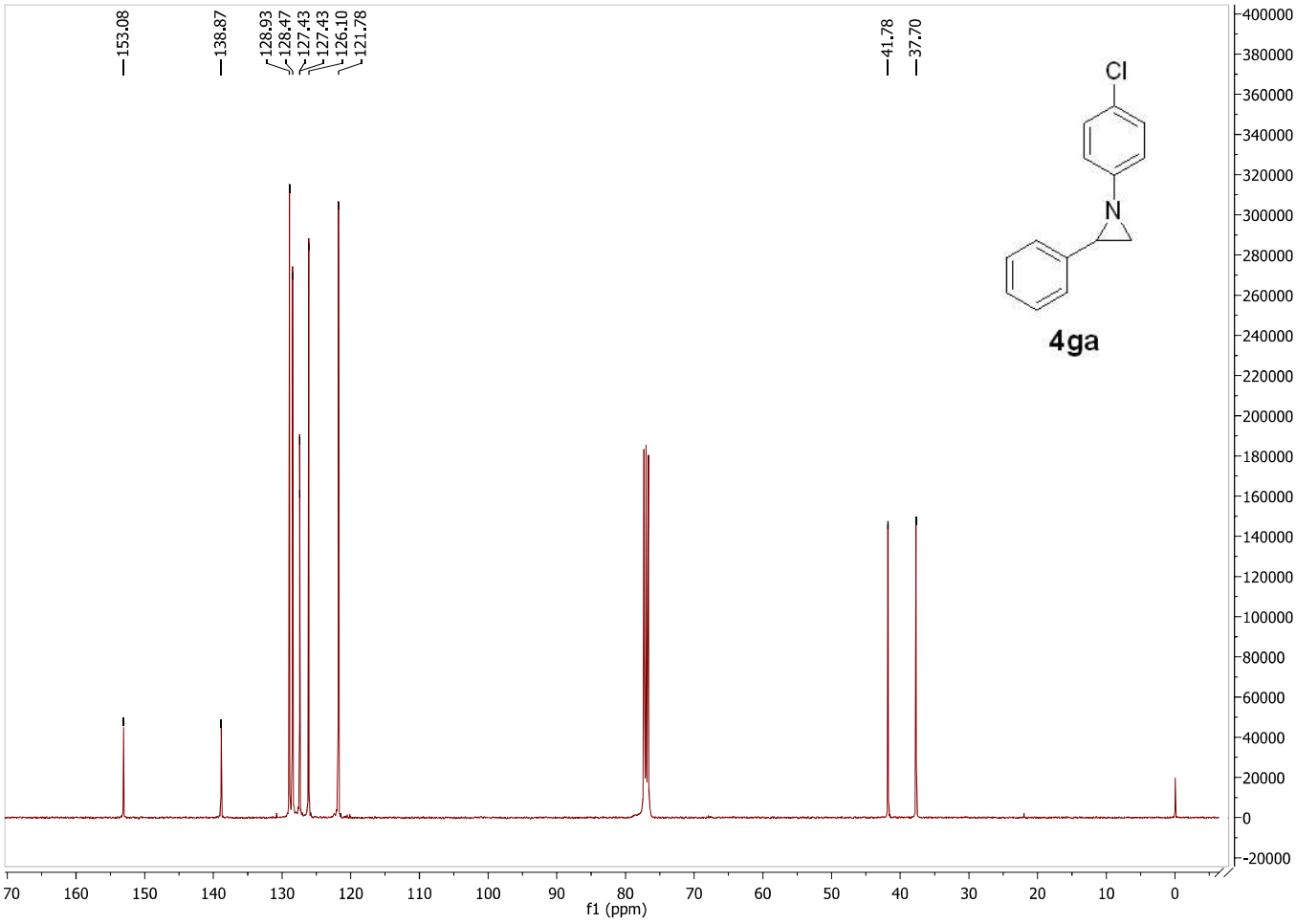
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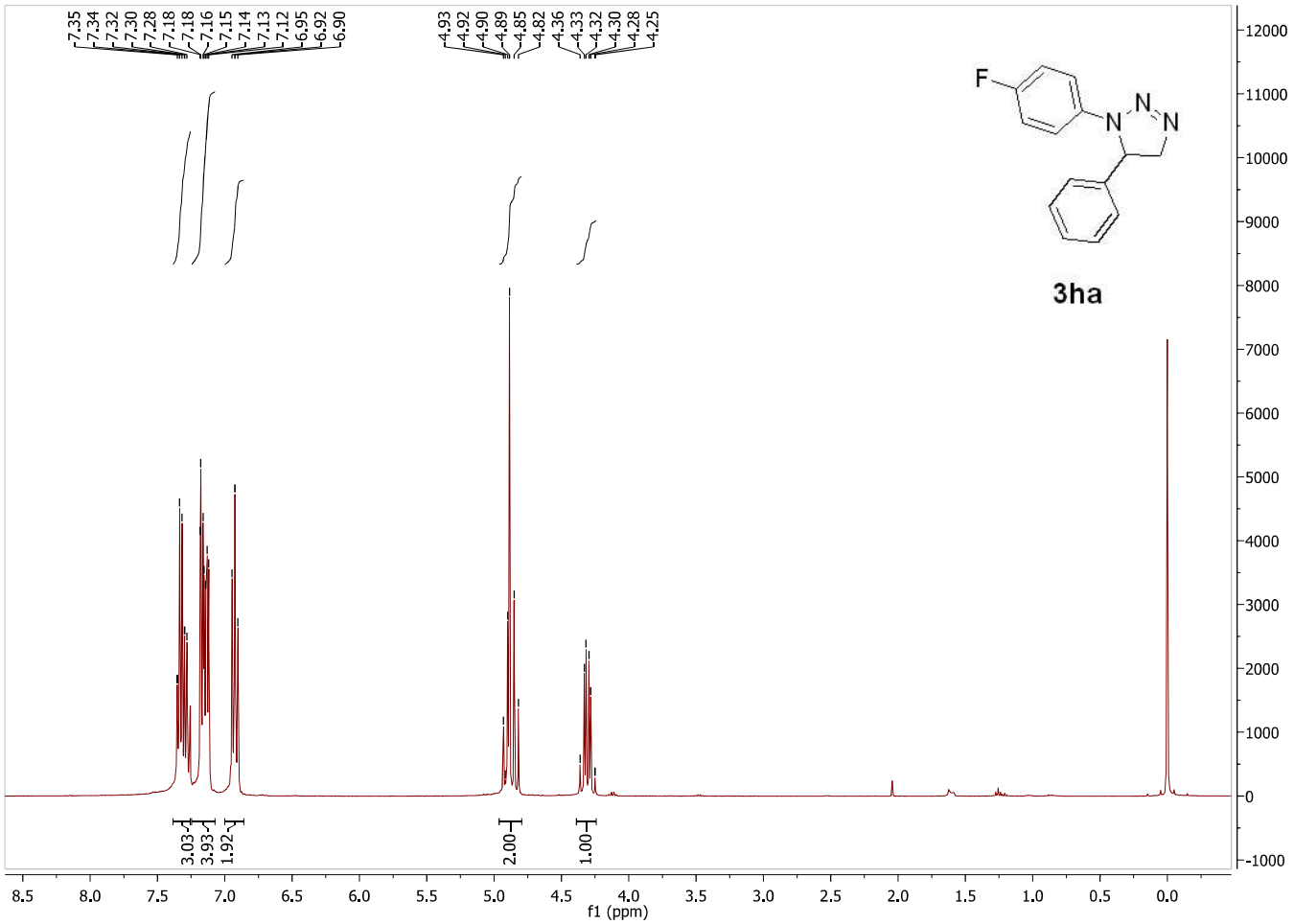
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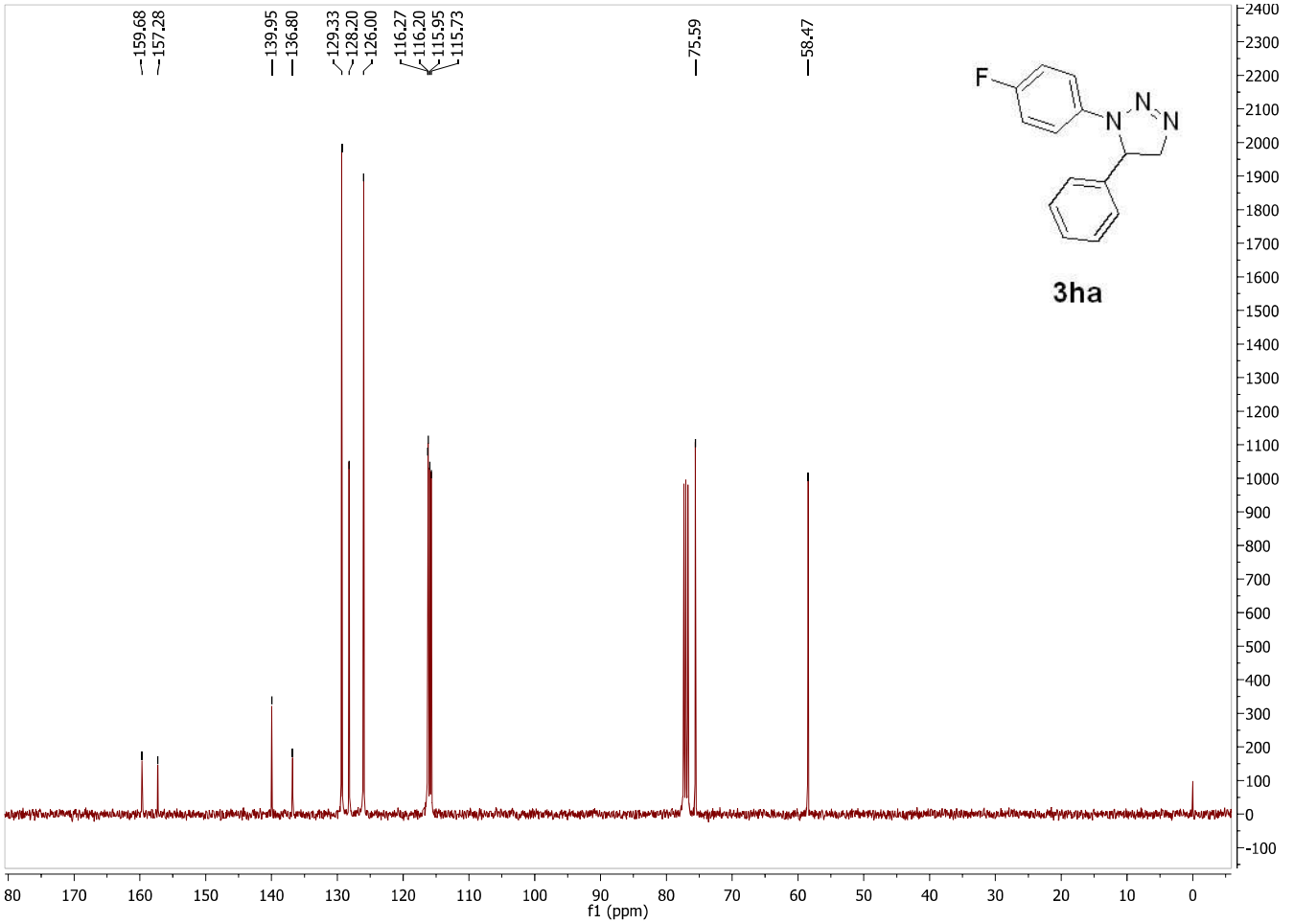
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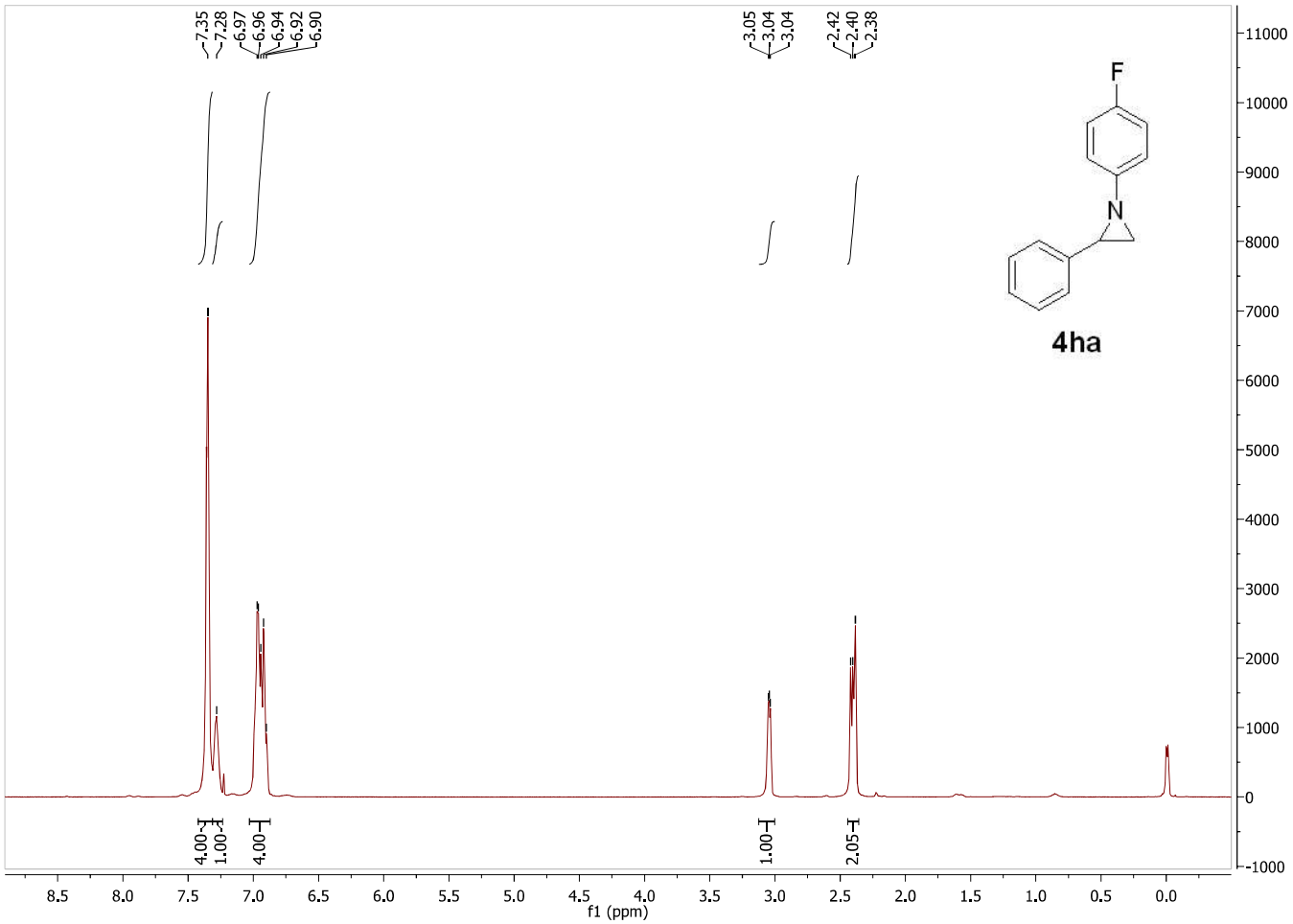
3ha
f1 (ppm)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7.28
6.97
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6.94
6.92
6.90
3.05
3.04
3.04
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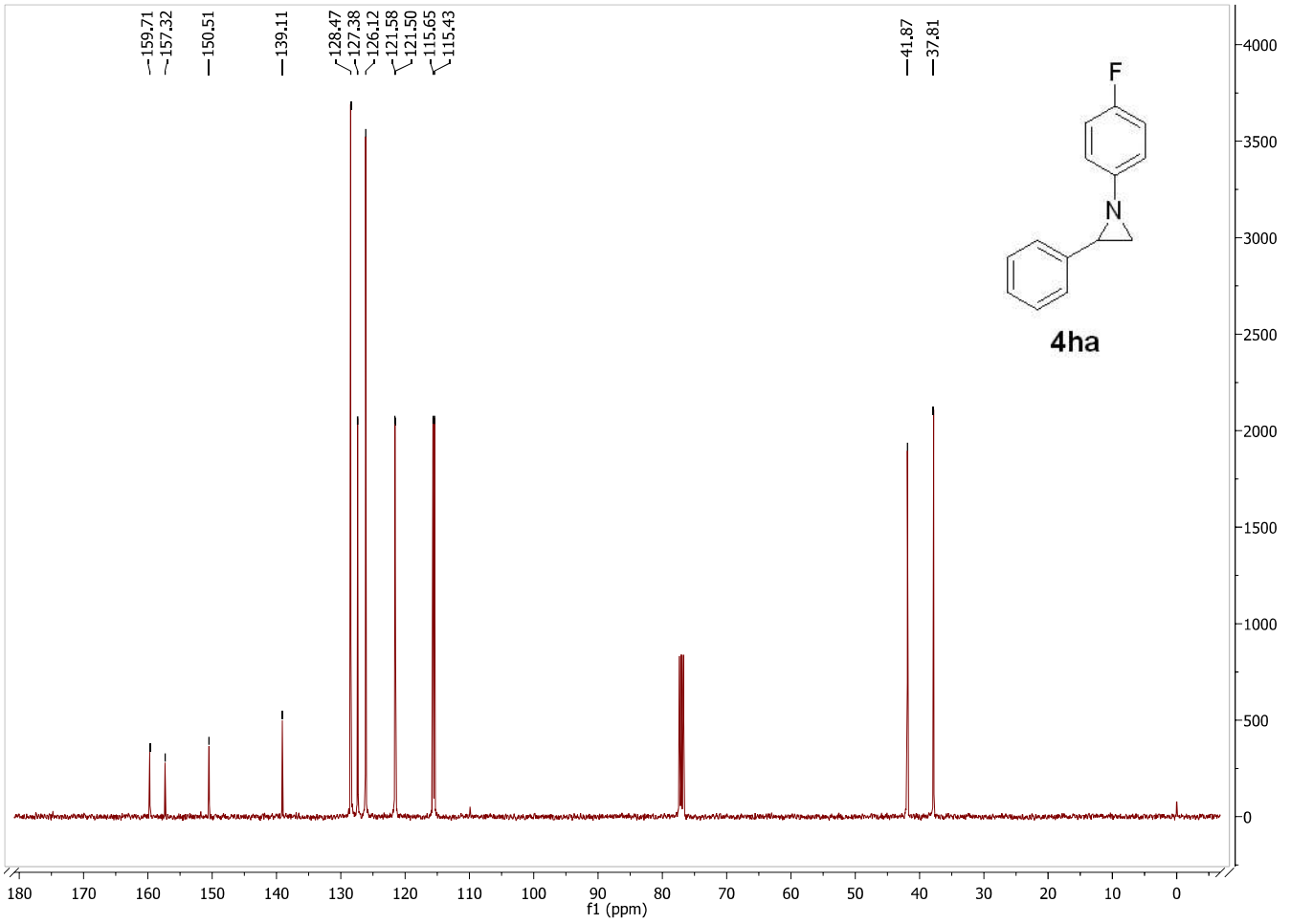
2.38
F
N
4ha
4.00
1.00
4.00
1.00
2.05
f1 (ppm)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121.58
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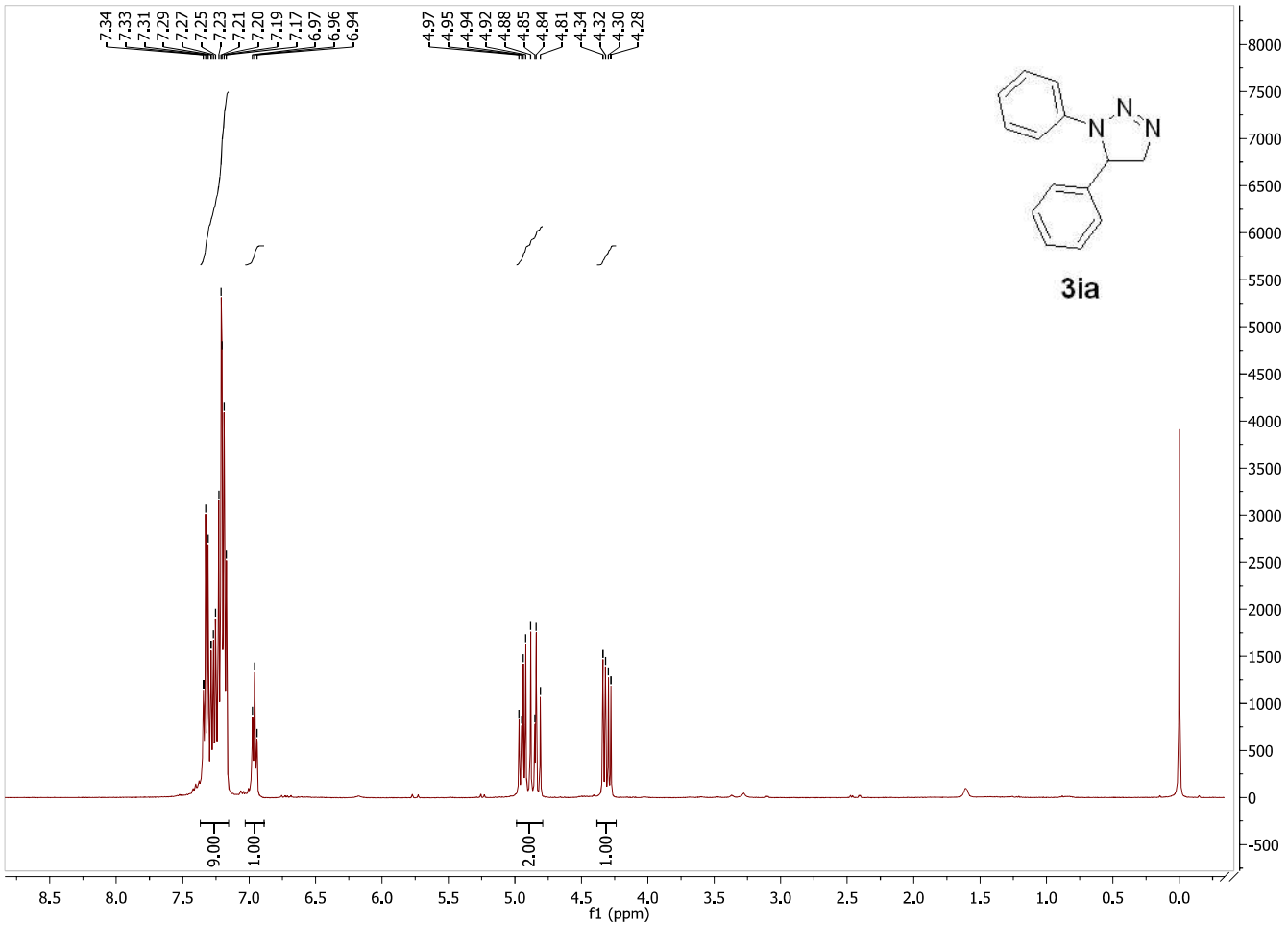
115.65
115.43
41.87
37.81
F
N
4ha
f1 (ppm)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7.17
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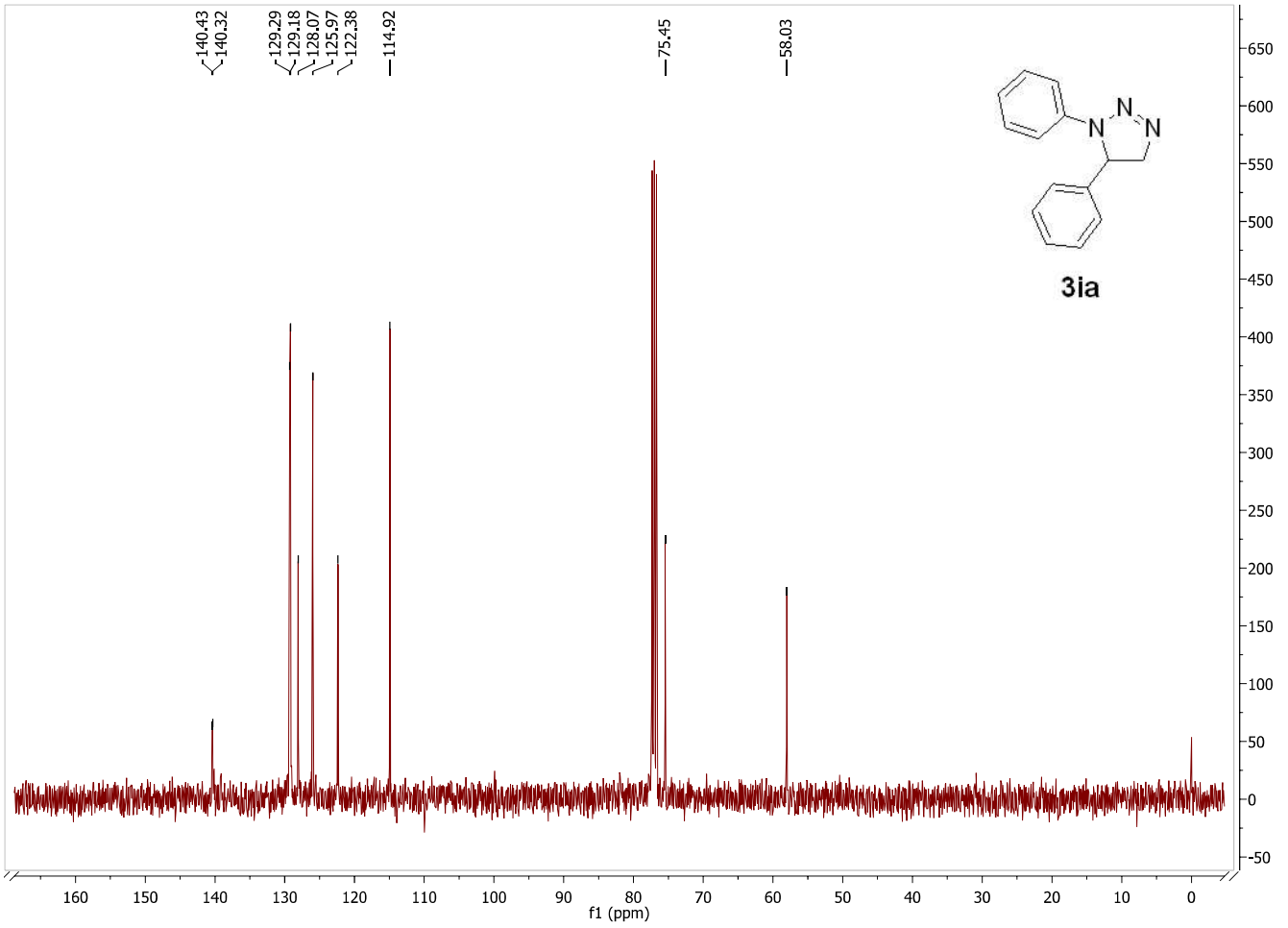
6.94
4.97
4.95
4.94
4.92
4.88
4.85
4.84
4.81
4.34
4.32
4.30
4.28
9.00
1.00
2.00
1.00
f1 (ppm)
3ia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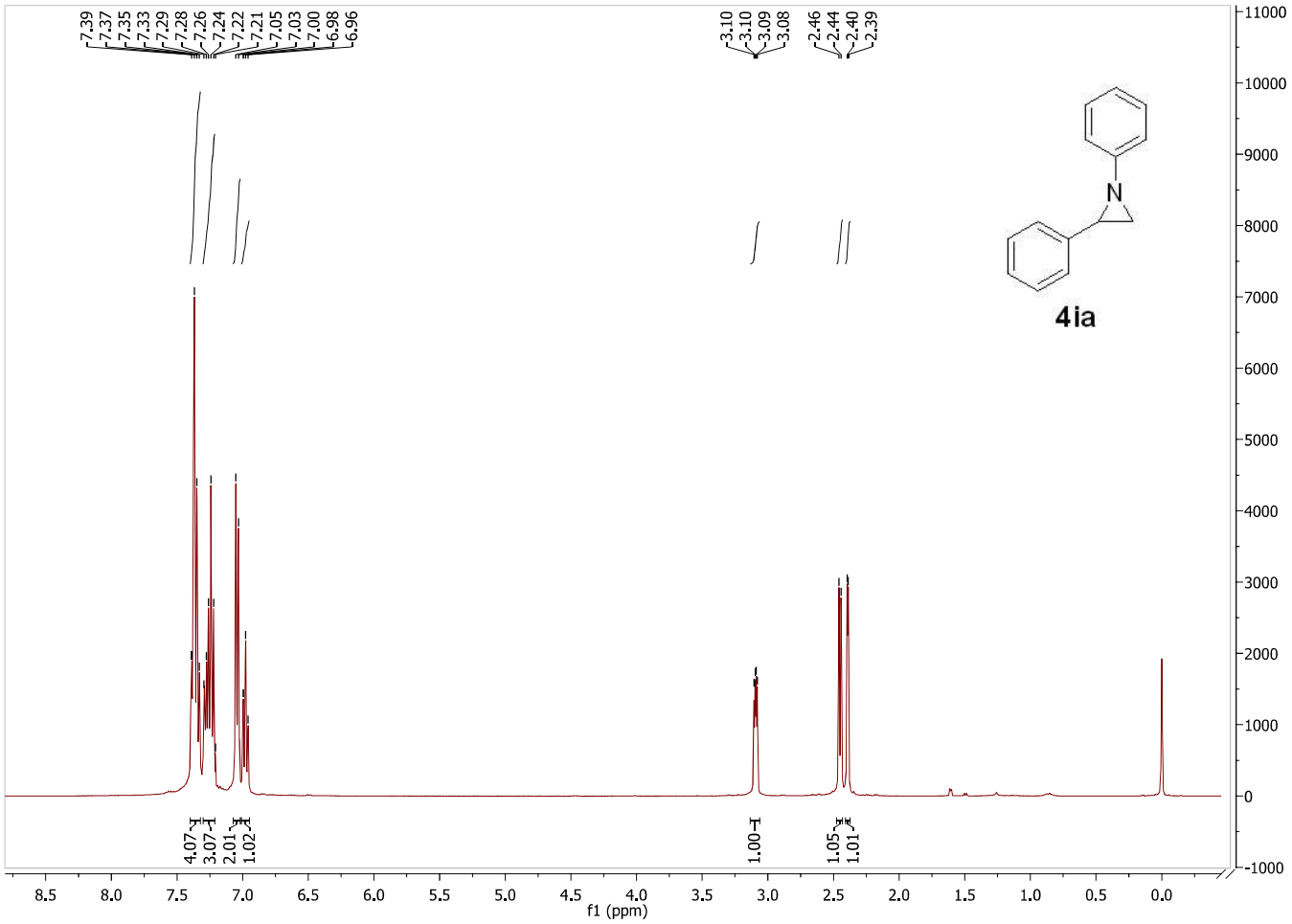
125.97
122.38
114.92
75.45
58.03
f1 (ppm)
3ia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7.03
7.00
6.98
6.96
3.10
3.10
3.09
3.08
2.46
2.44
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N
4ia
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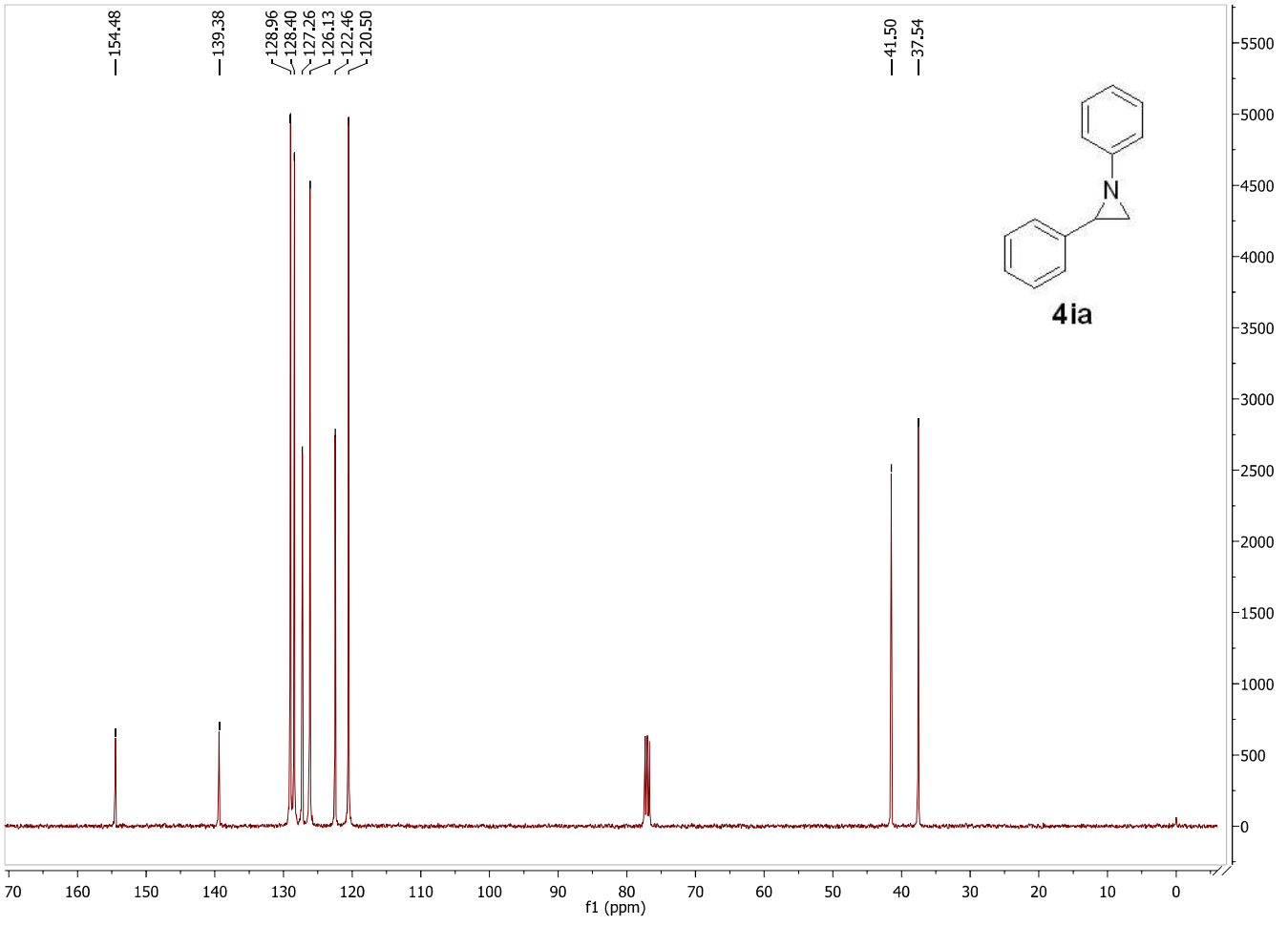
3.07
2.01
1.02
1.00
1.05
1.01
f1 (ppm)


154.48
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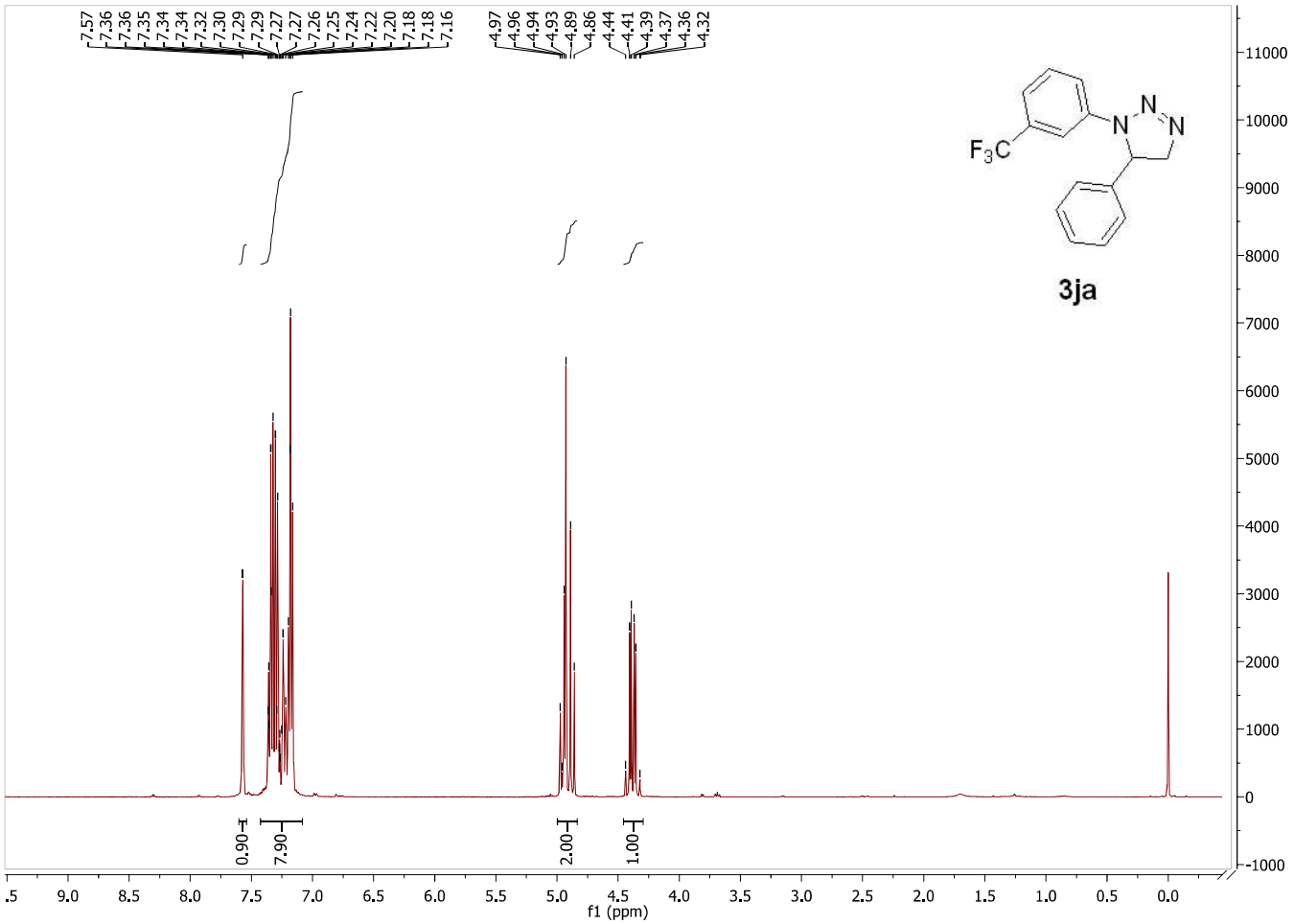
126.13
122.46
120.50
41.50
37.54
N
4ia
f1 (ppm)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7.24
7.22
7.20
7.18
7.18
7.16
4.97
4.96
4.94
4.93
4.89
4.86
4.44
4.41
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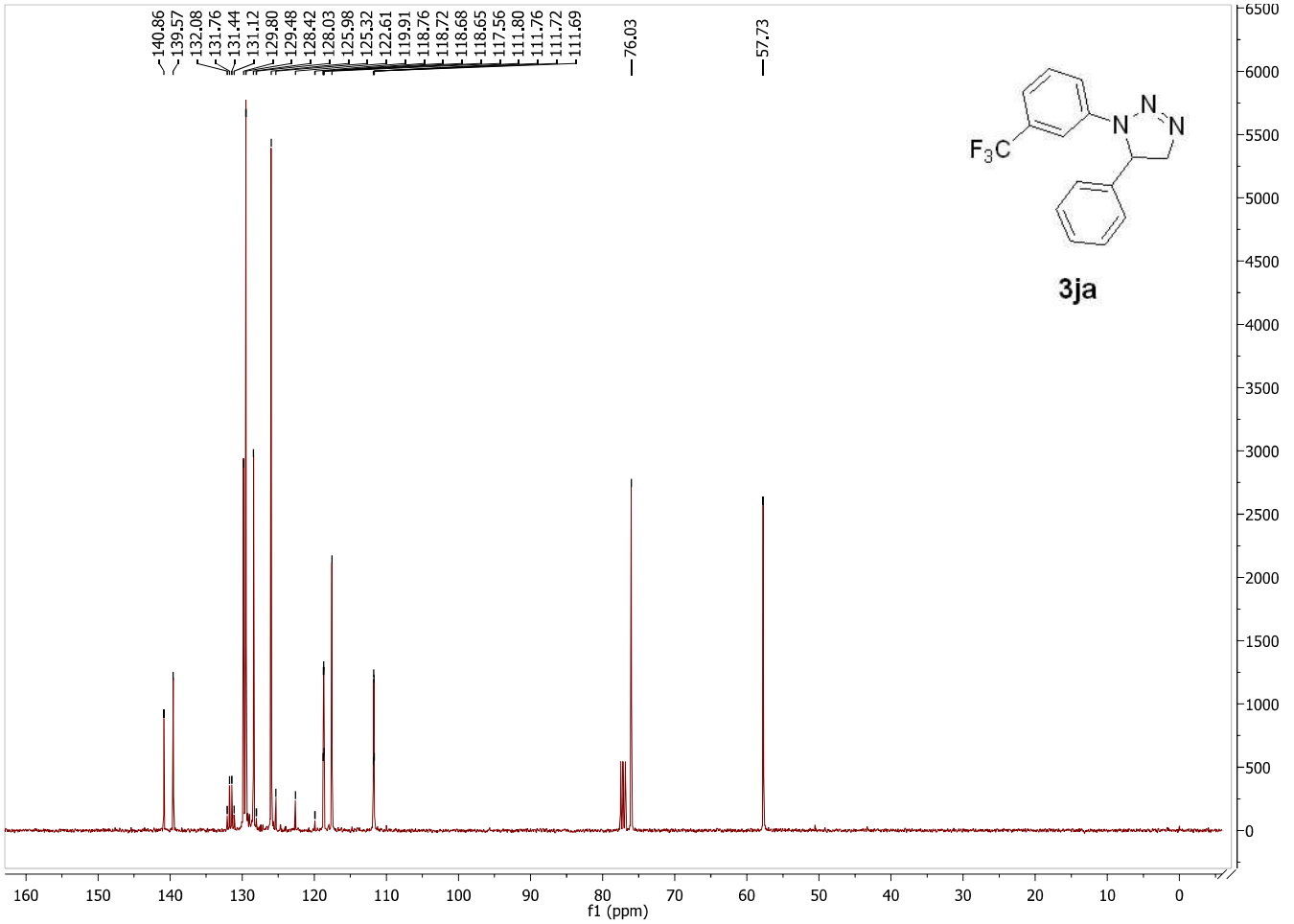
4.37
4.36
4.32
0.90
7.90
2.00
1.00
f1 (ppm)

3ja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122.61
119.91
118.76
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111.76
111.72
111.69
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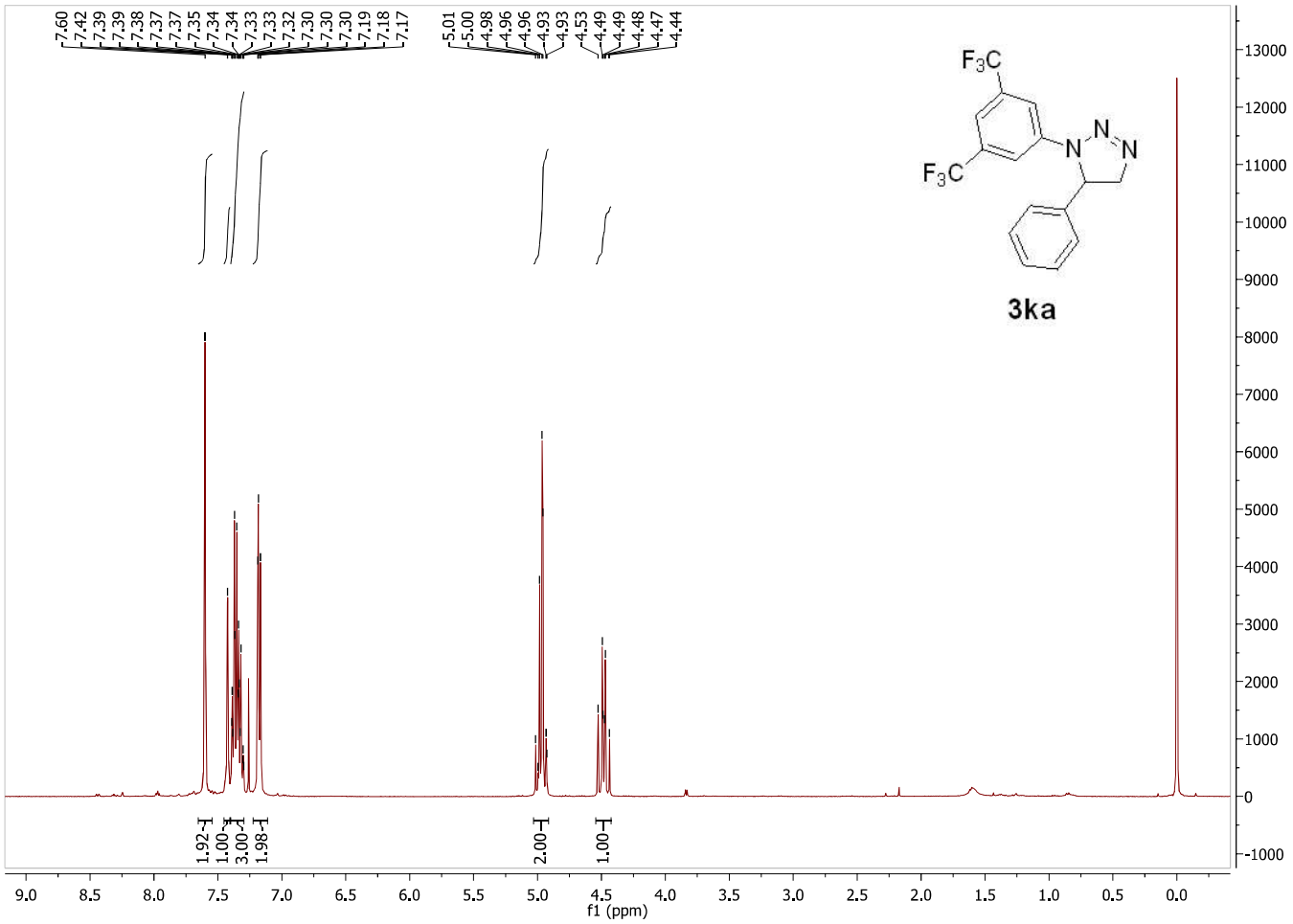
57.73
f1 (ppm)

3ja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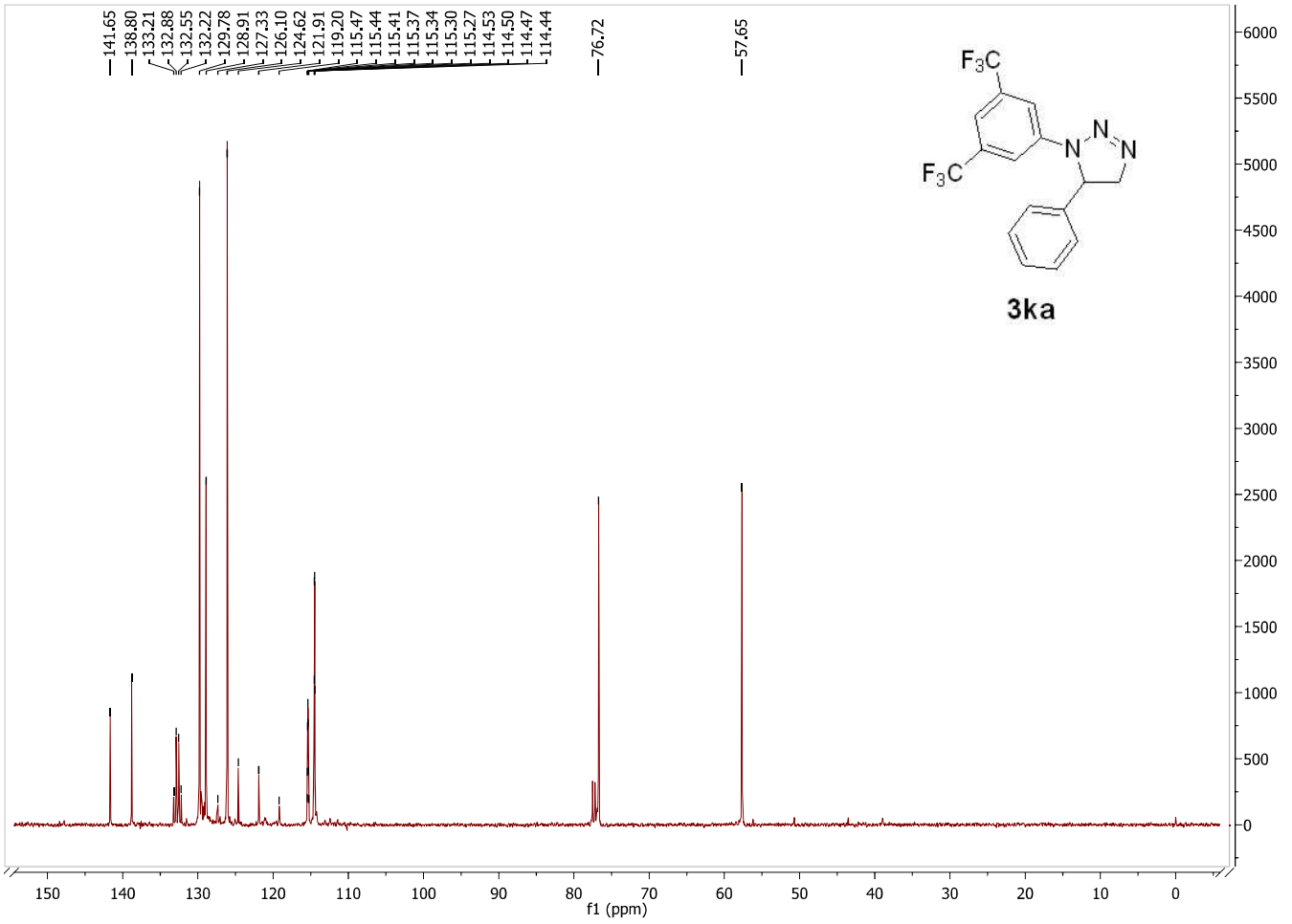
7.30
7.30
7.30
7.19
7.18
7.17
5.01
5.00
4.98
4.96
4.96
4.93
4.93
4.53
4.49
4.49
4.48
4.47
4.44
F3C
F3C
N
N
N
3ka
1.92
1.00
3.00
1.98
2.00
1.00
f1 (ppm)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128.91
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126.10
124.62
121.91
119.20
115.47
115.44
115.41
115.37
115.34
115.30
115.27
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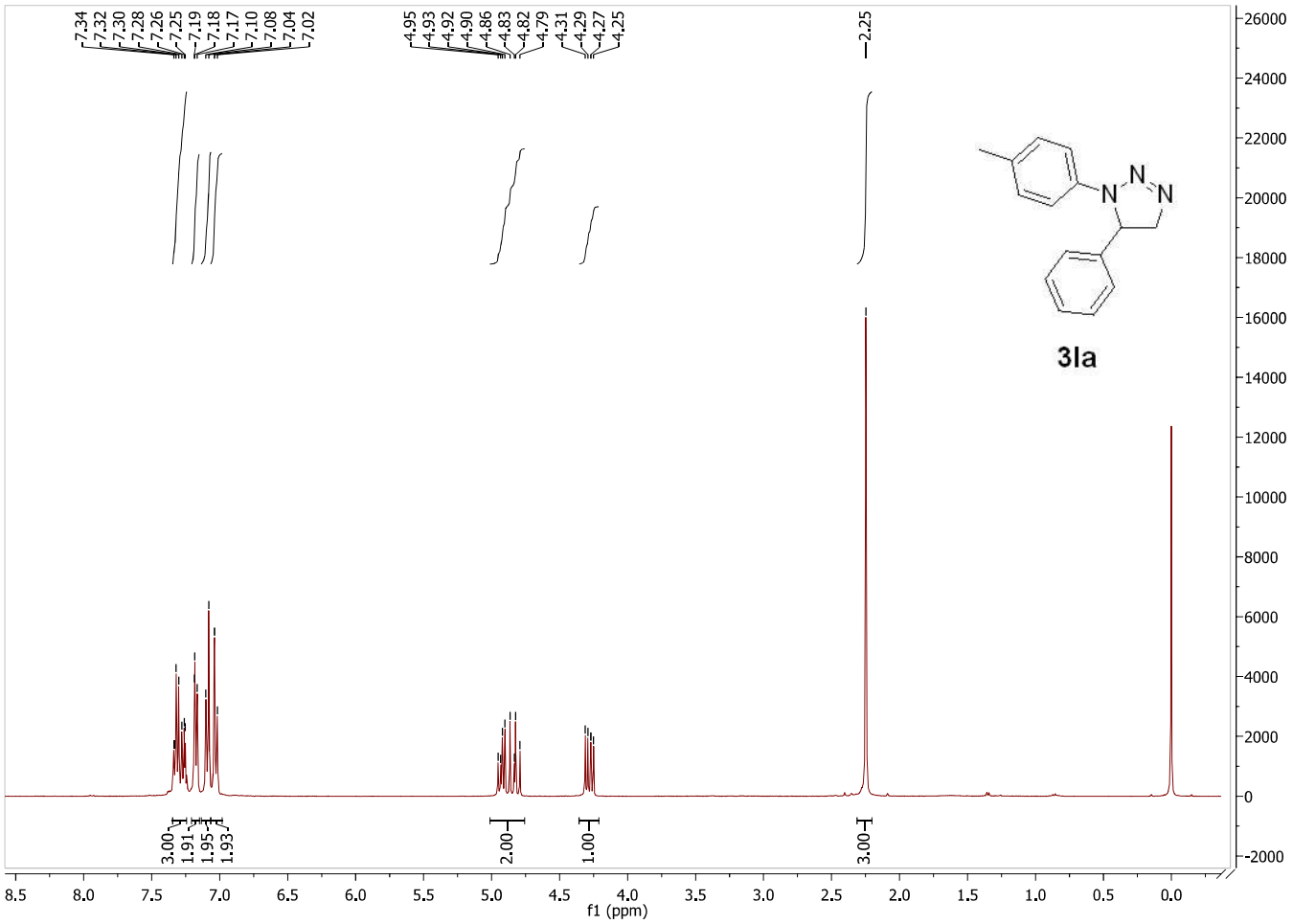
114.47
114.44
76.72
57.65
F3C
F3C
N
N
N
3ka
f1 (ppm)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4.92
4.90
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4.83
4.82
4.79
4.31
4.29
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3.00
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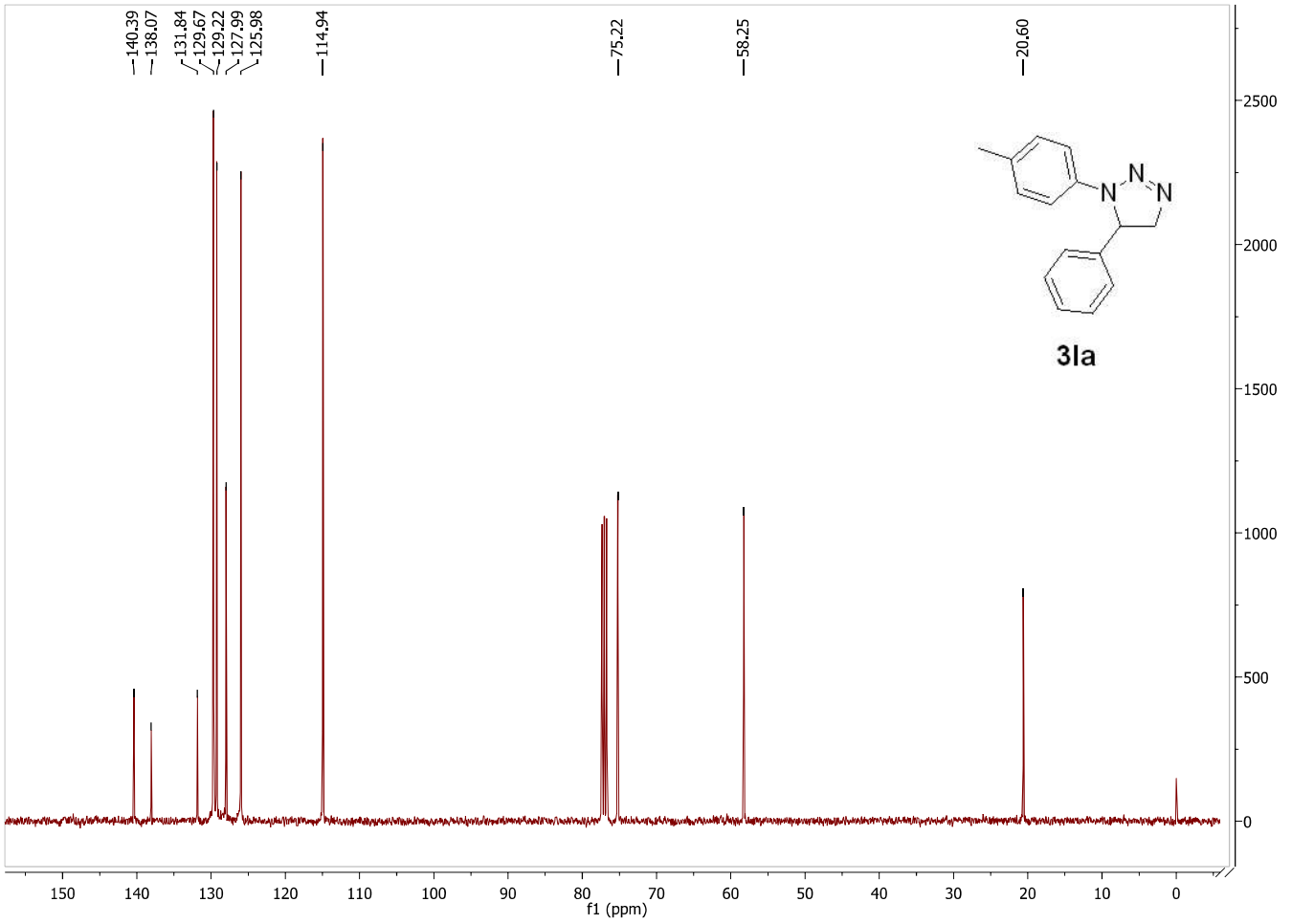
1.95
1.93
2.00
1.00
3.00
f1 (ppm)
3Ia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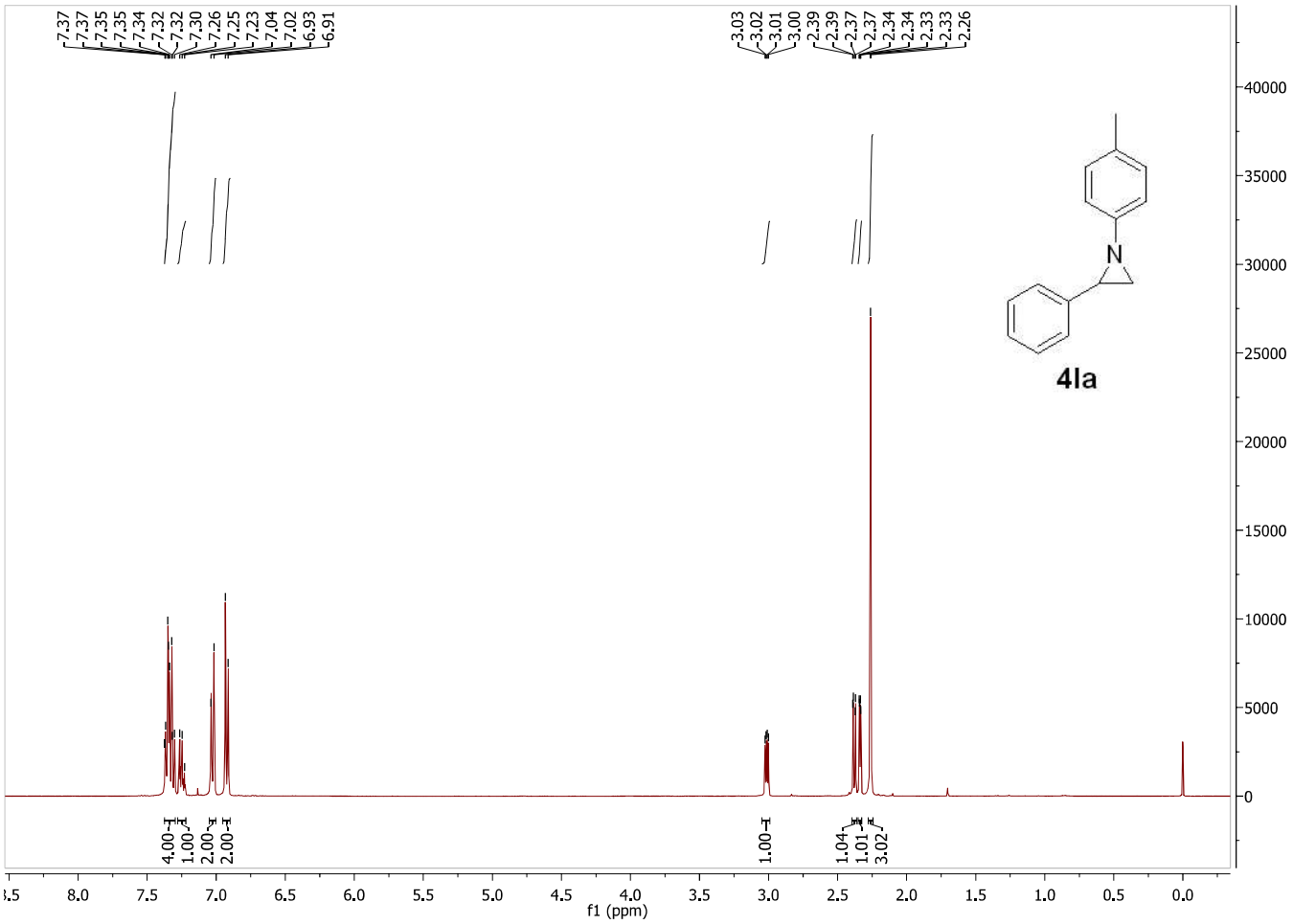
125.98
114.94
75.22
58.25
20.60
f1 (ppm)
3Ia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7.23
7.04
7.02
6.93
6.91
3.03
3.02
3.01
3.00
2.39
2.39
2.37
2.37
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2.34
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2.33
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2.00
2.00
1.00
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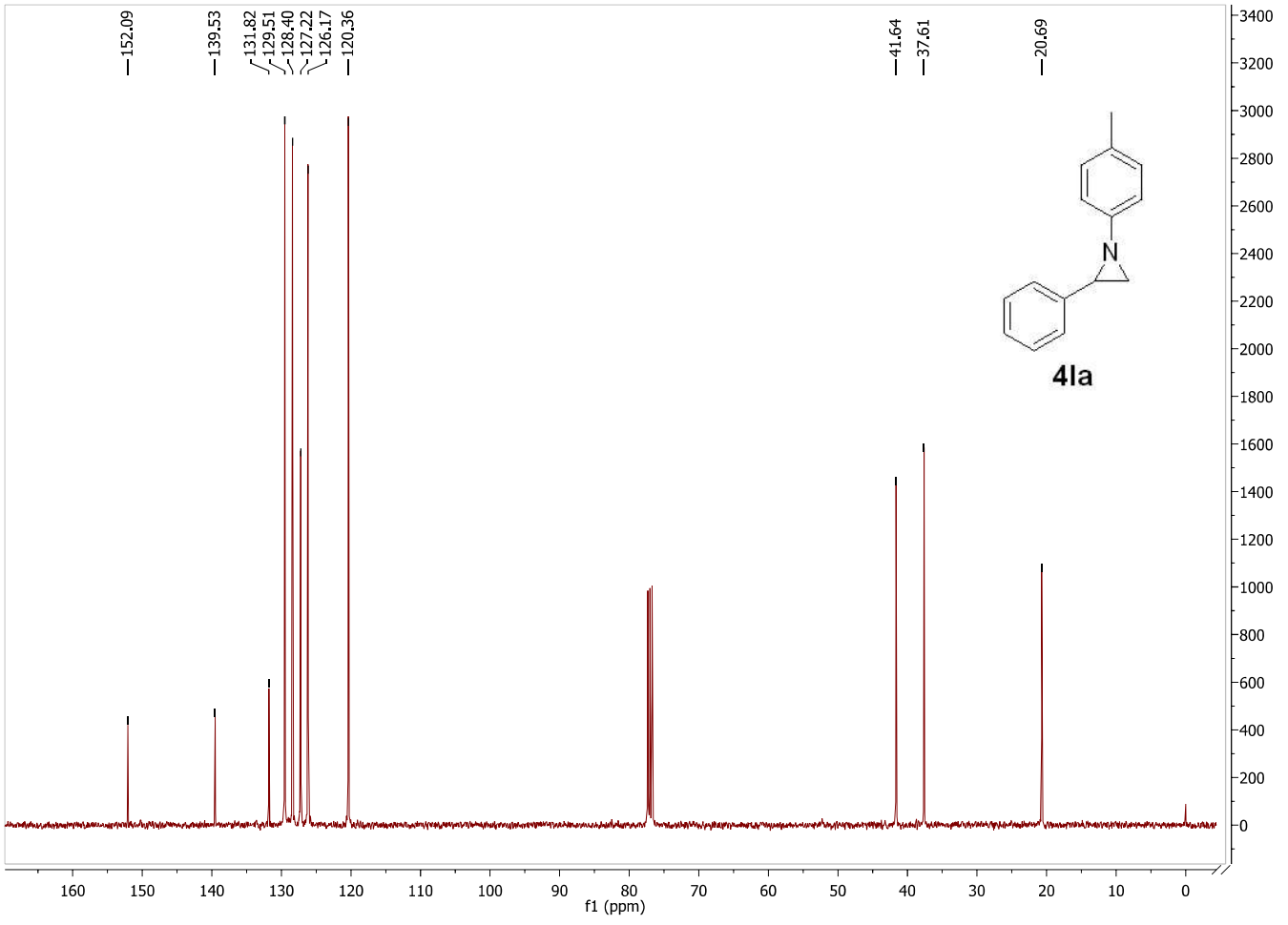
1.01
3.02
N
4la
f1 (ppm)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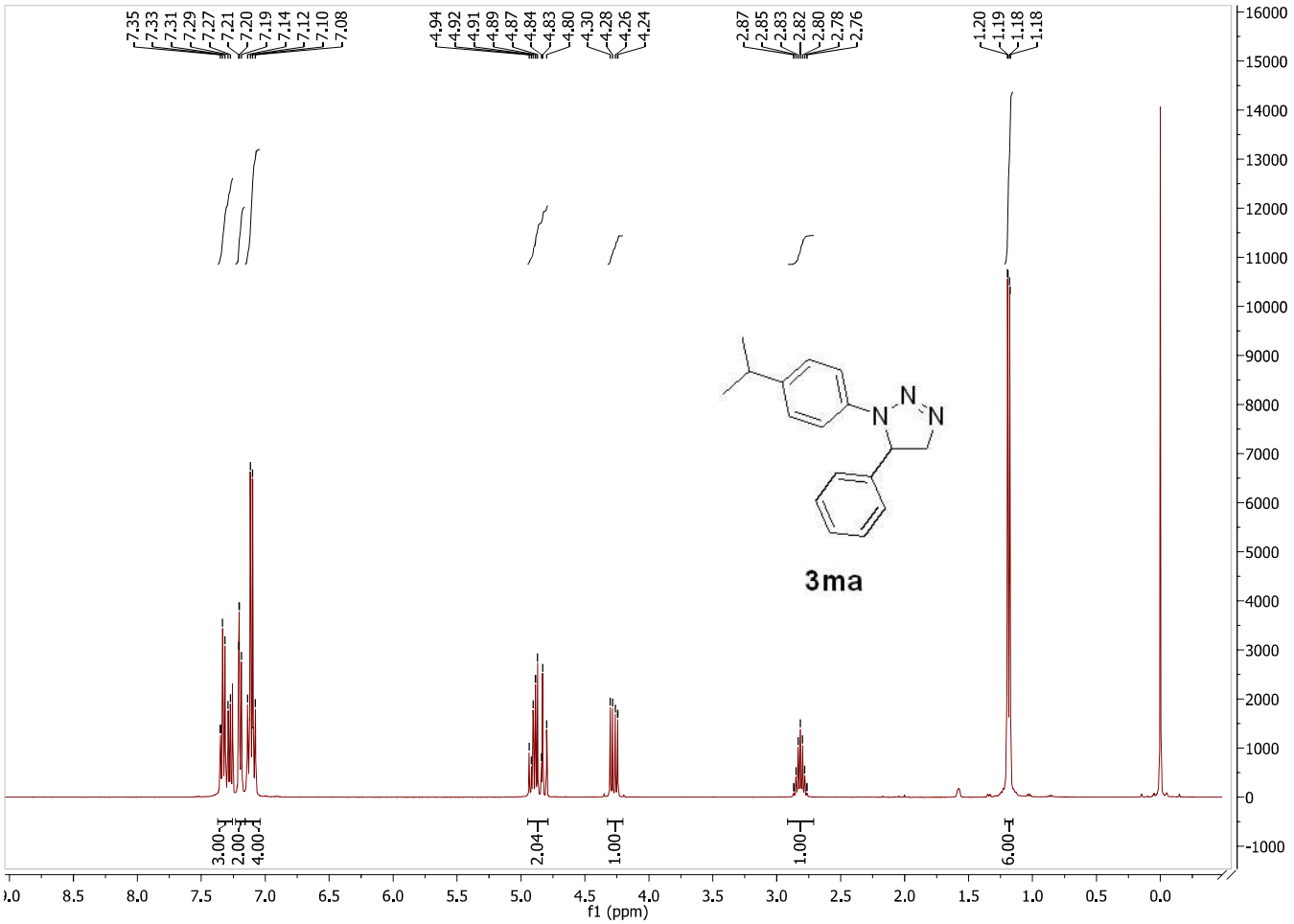
N
4la
f1 (ppm)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4.92
4.91
4.89
4.87
4.84
4.83
4.80
4.30
4.28
4.26
4.24
2.87
2.85
2.83
2.82
2.80
2.78
2.76
1.20
1.19
1.18
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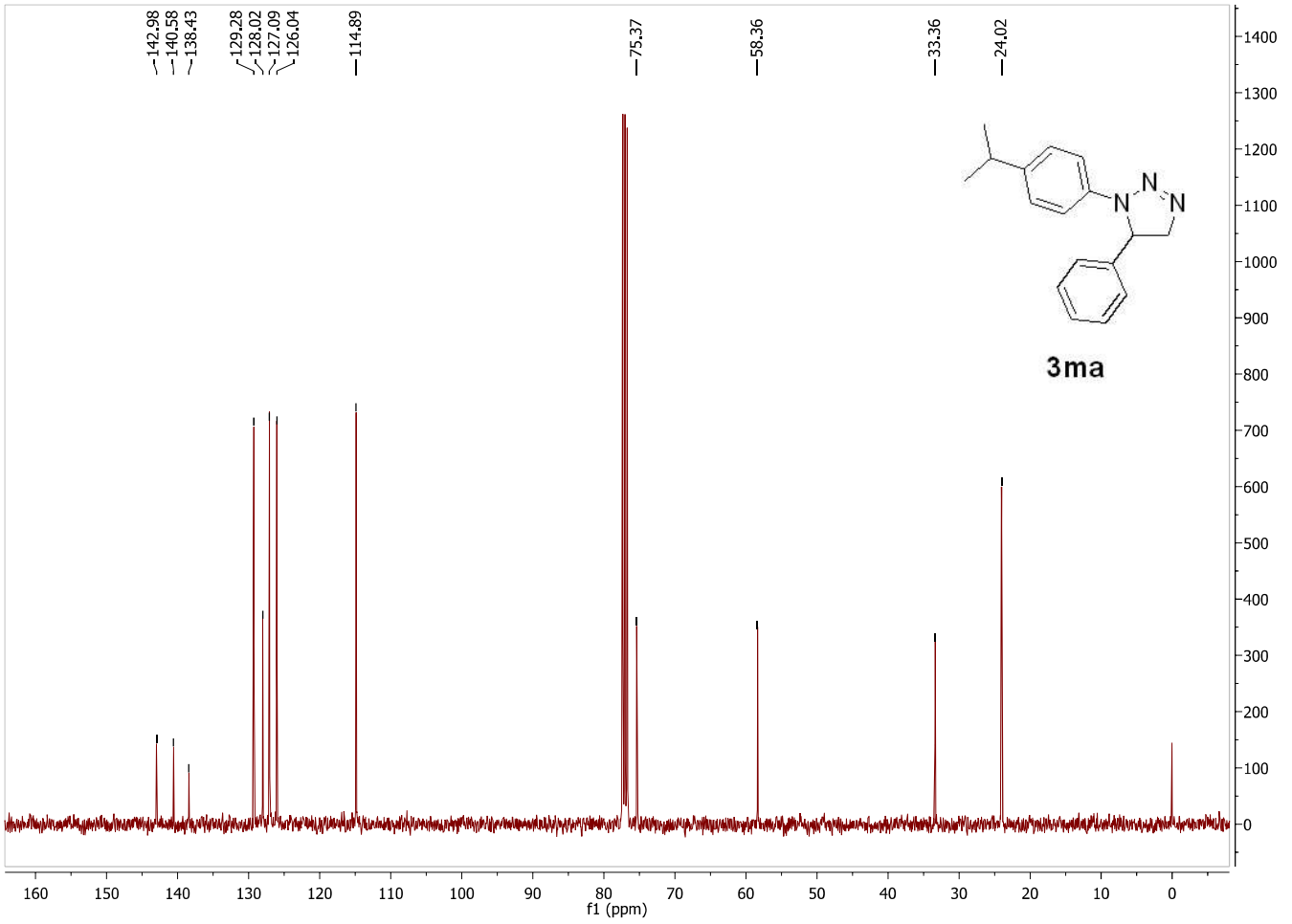
3.00
2.00
4.00
2.04
1.00
1.00
6.00
3ma
f1 (ppm)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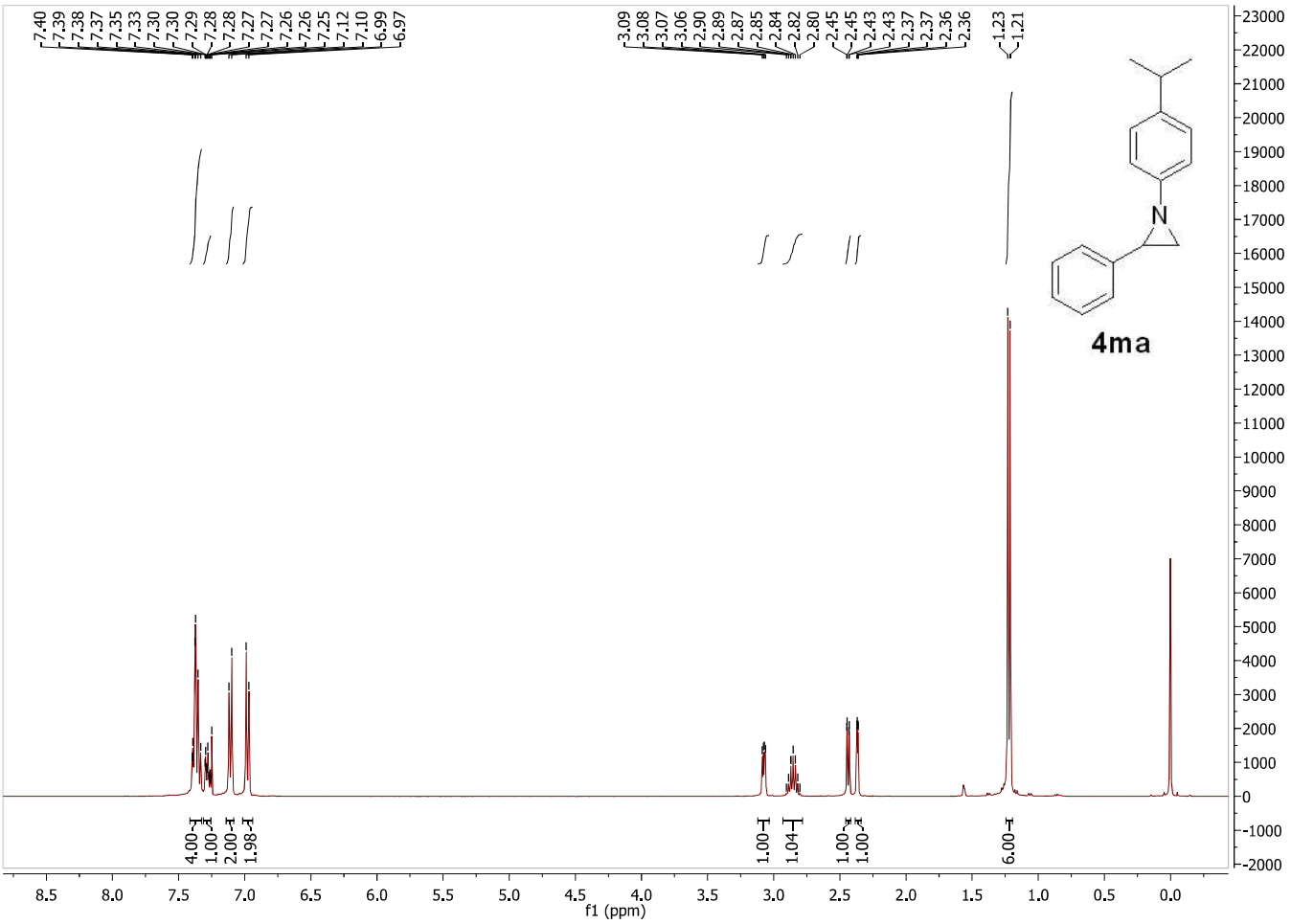
75.37
58.36
33.36
24.02
3ma
f1 (ppm)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7.26
7.26
7.25
7.12
7.10
6.99
6.97
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3.08
3.07
3.06
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2.87
2.85
2.84
2.82
2.80
2.45
2.45
2.43
2.43
2.37
2.37
2.36
2.36
1.23
1.21
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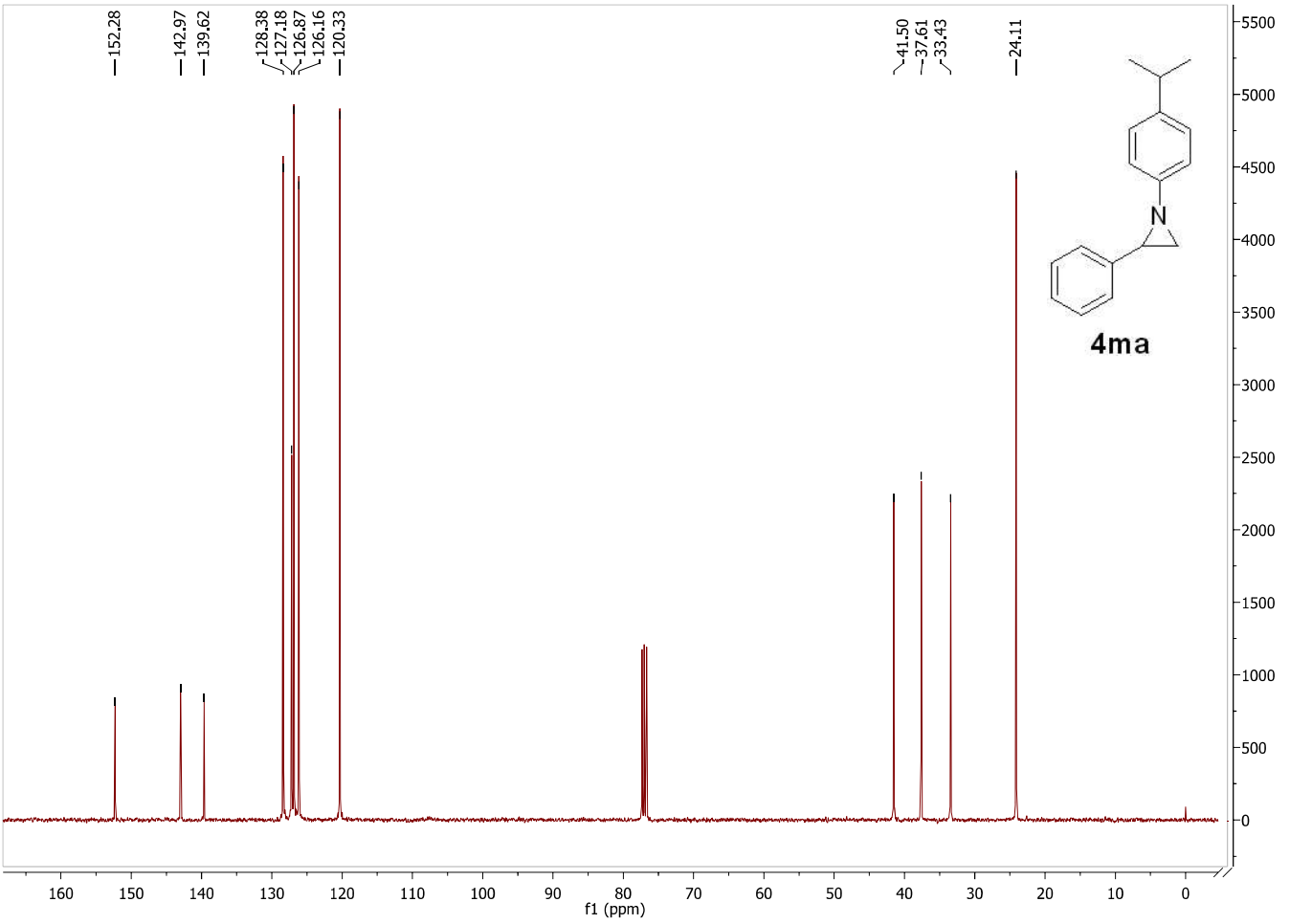
2.00
1.98
1.00
1.04
1.00
1.00
6.00
N
4ma
f1 (ppm)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120.33
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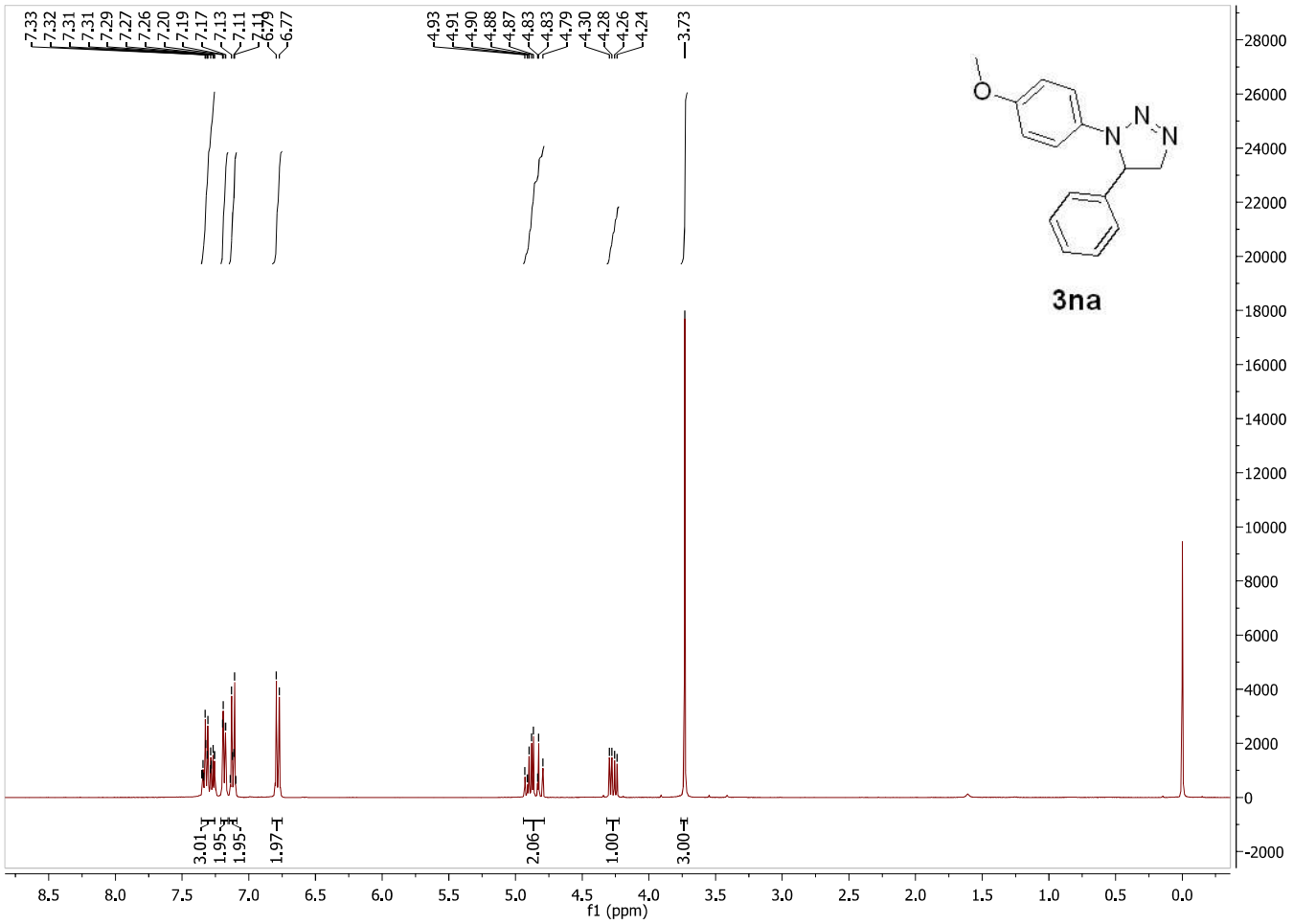
33.43
24.11
N
4ma
f1 (ppm)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6.77
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4.91
4.90
4.88
4.87
4.83
4.83
4.79
4.30
4.28
4.26
4.24
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1.97
2.06
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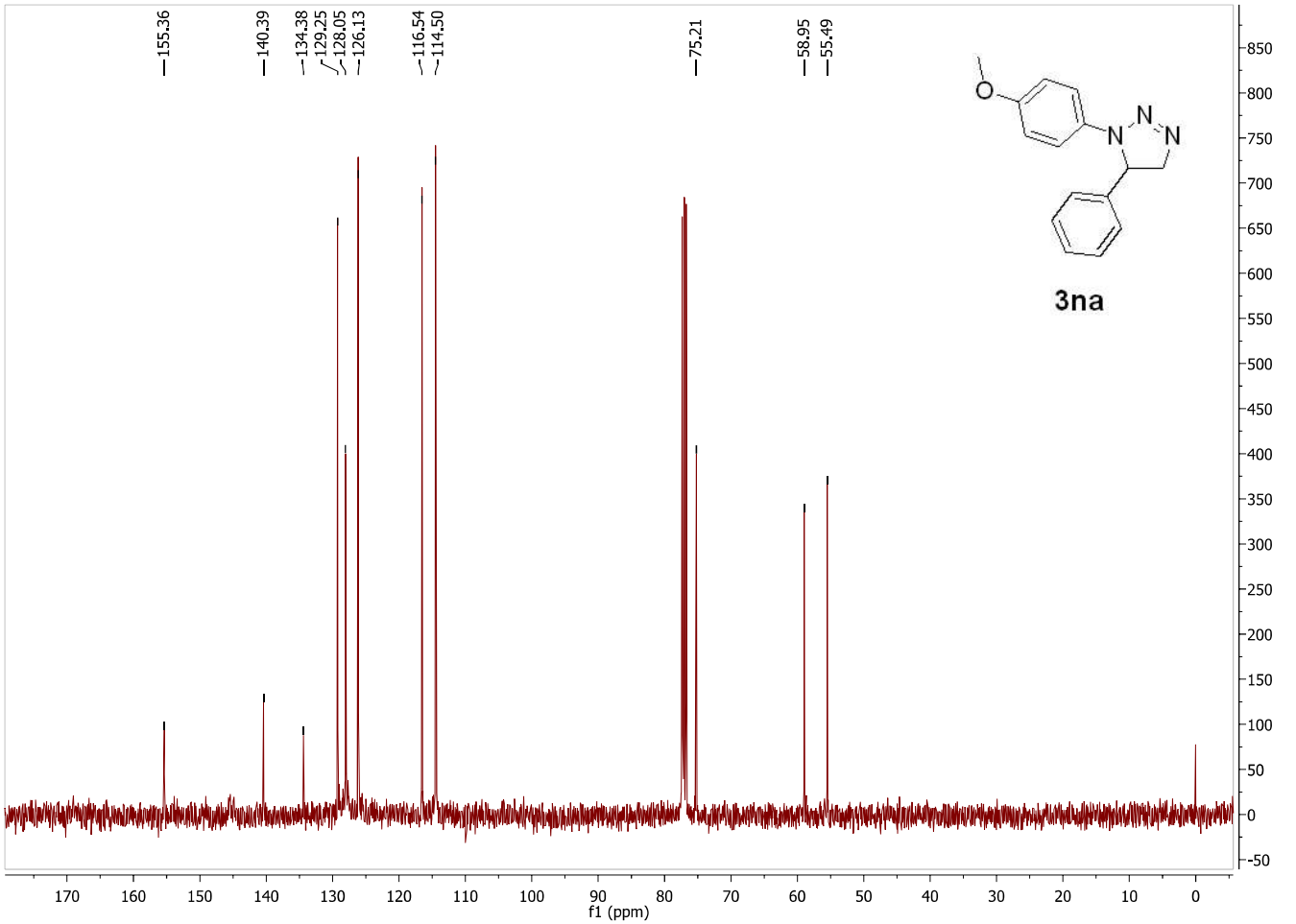
3.00
O
N
N
N
3na
f1 (ppm)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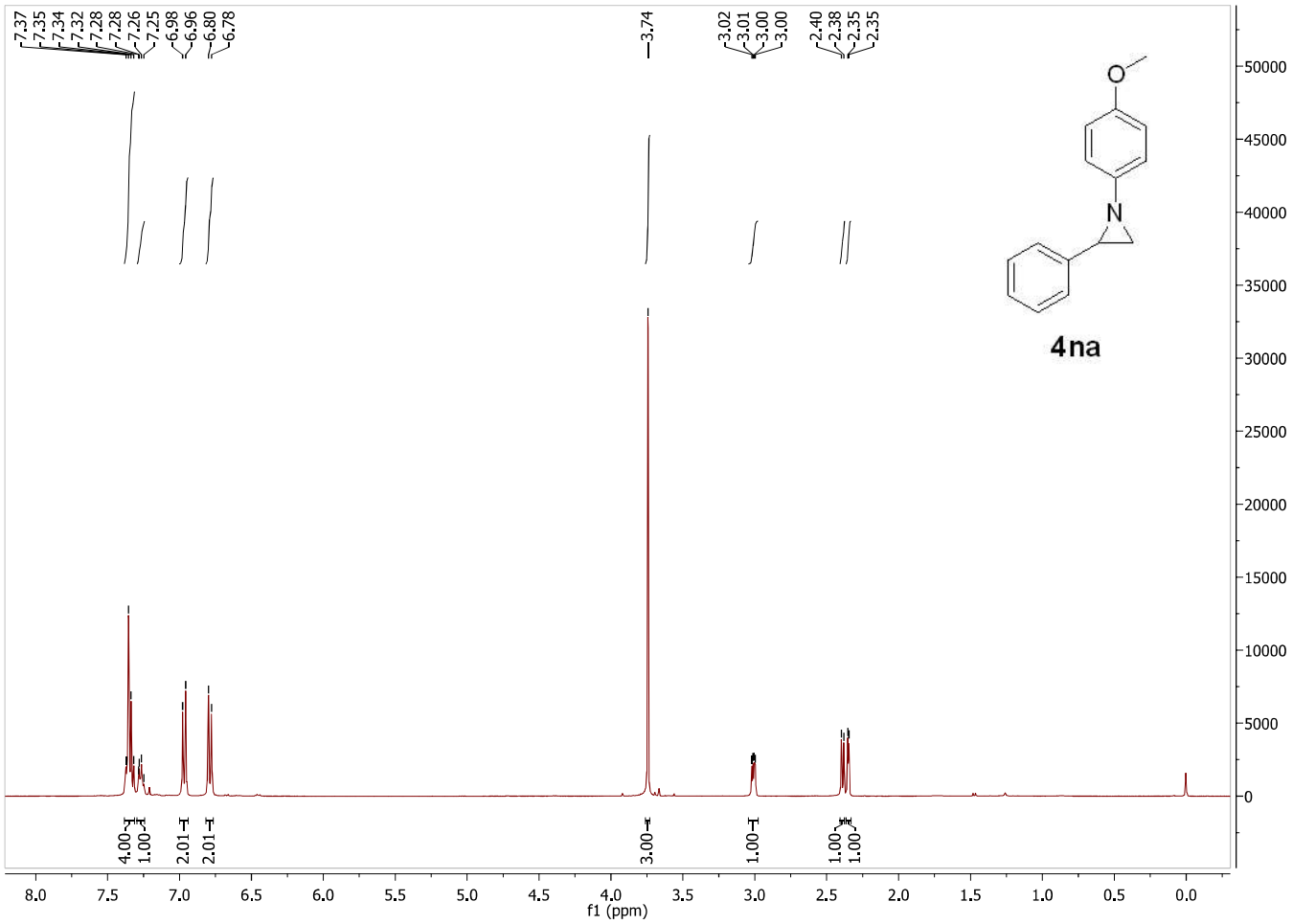
N
3na
f1 (ppm)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2.38
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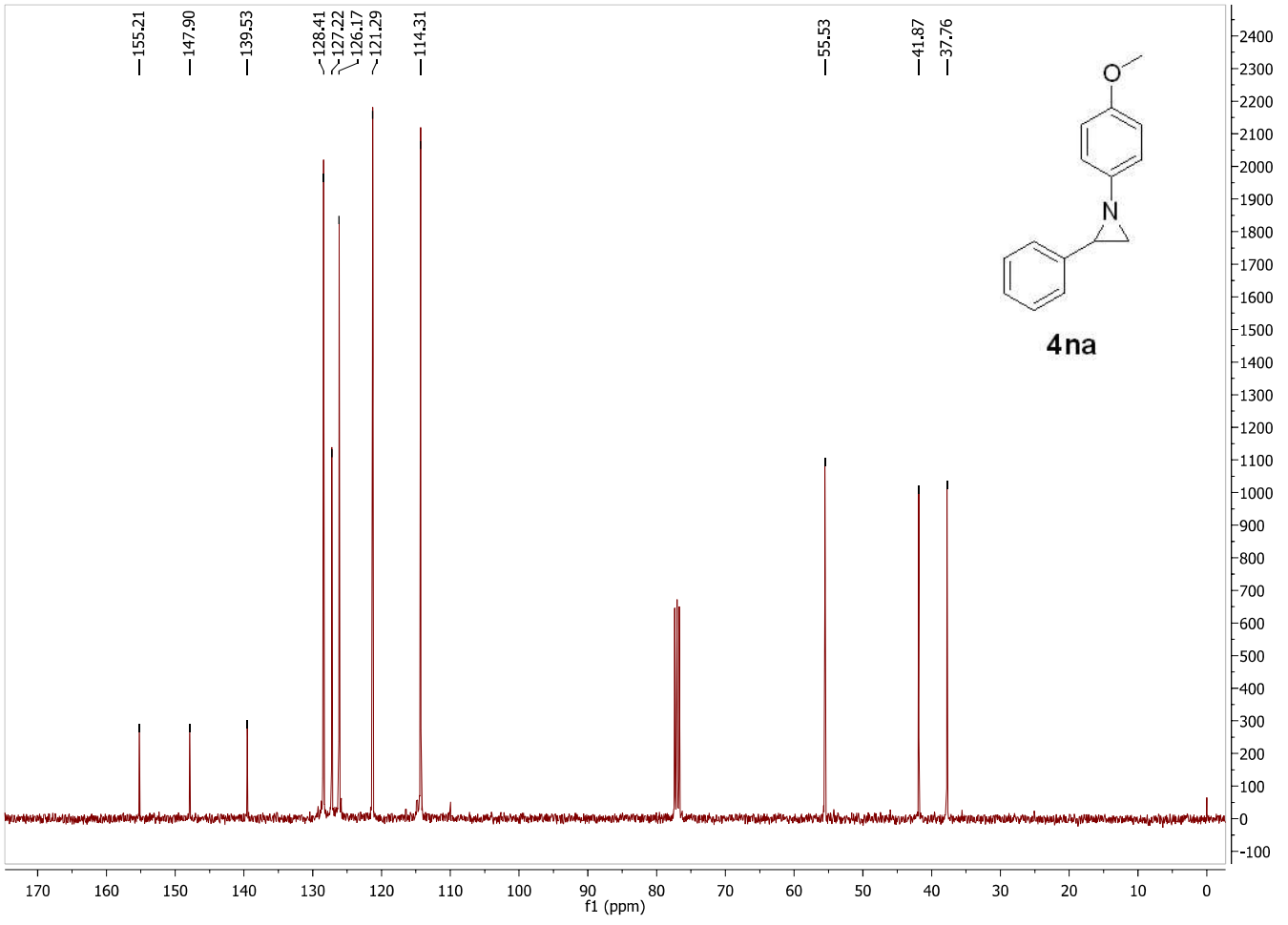
2.01
2.01
3.00
1.00
1.00
1.00
f1 (ppm)
4na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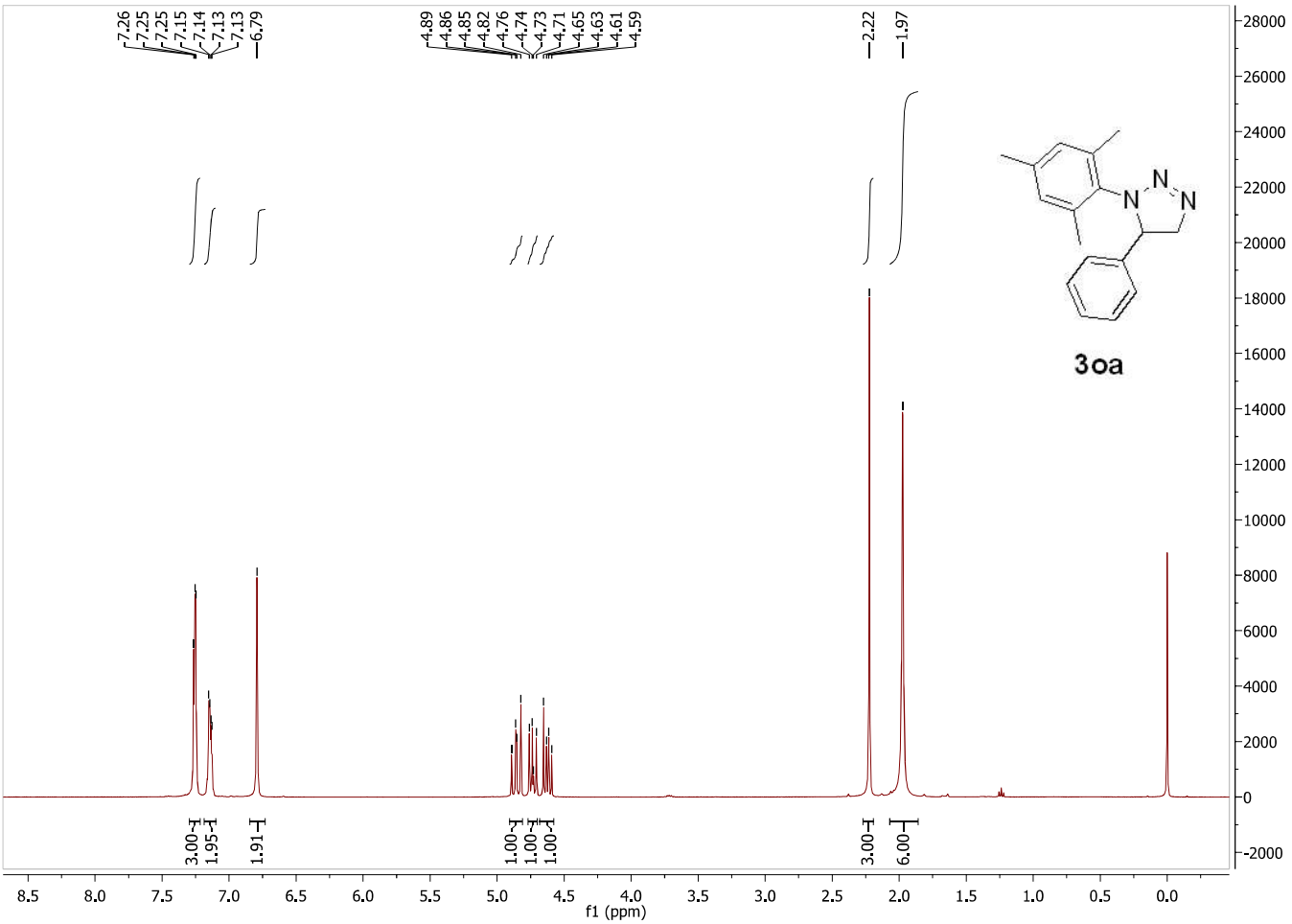
126.17
121.29
114.31
55.53
41.87
37.76
f1 (ppm)
4na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4.76
4.74
4.73
4.71
4.65
4.63
4.61
4.59
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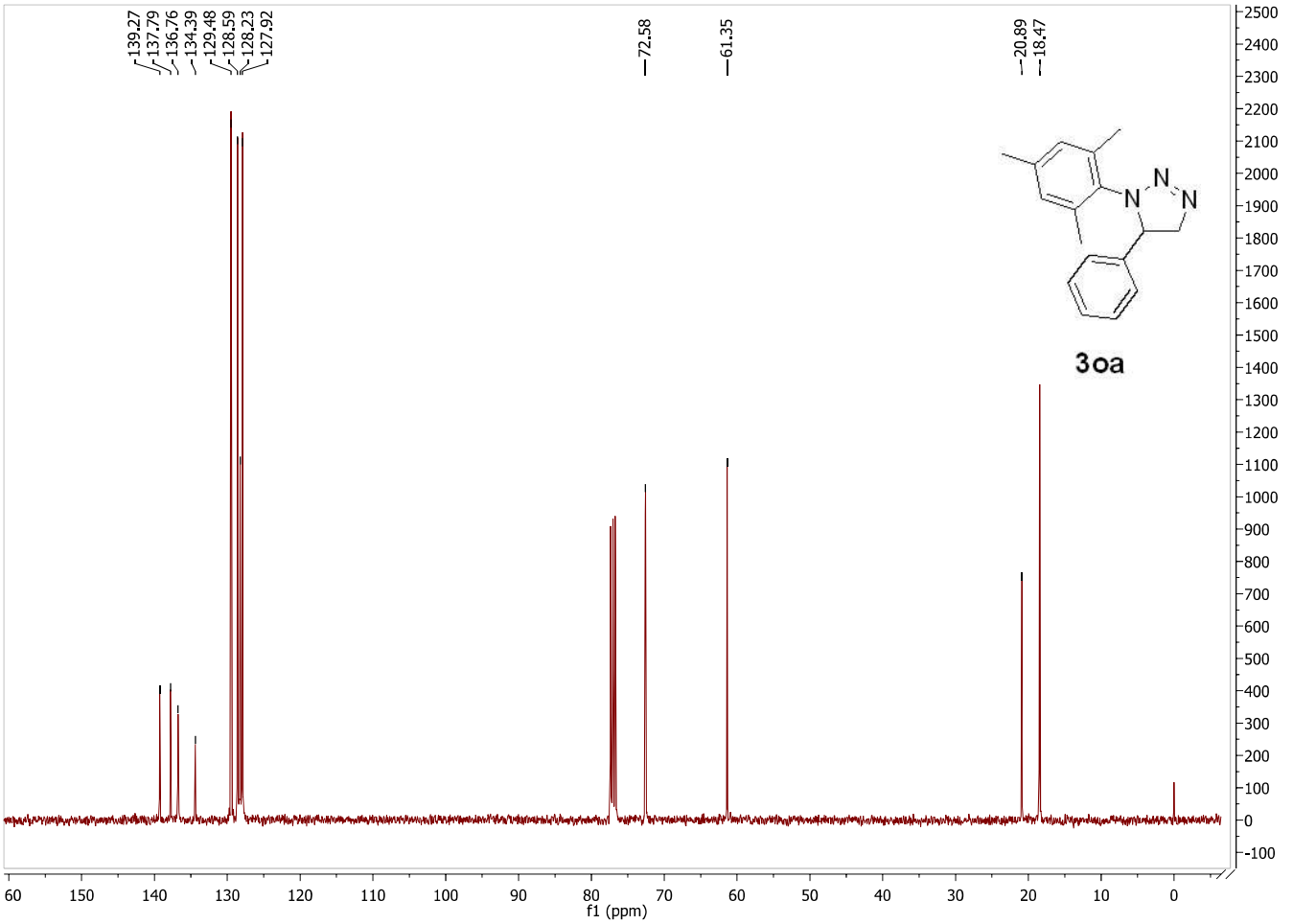
1.95
1.91
1.00
1.00
1.00
3.00
6.00
f1 (ppm)
3oa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127.92
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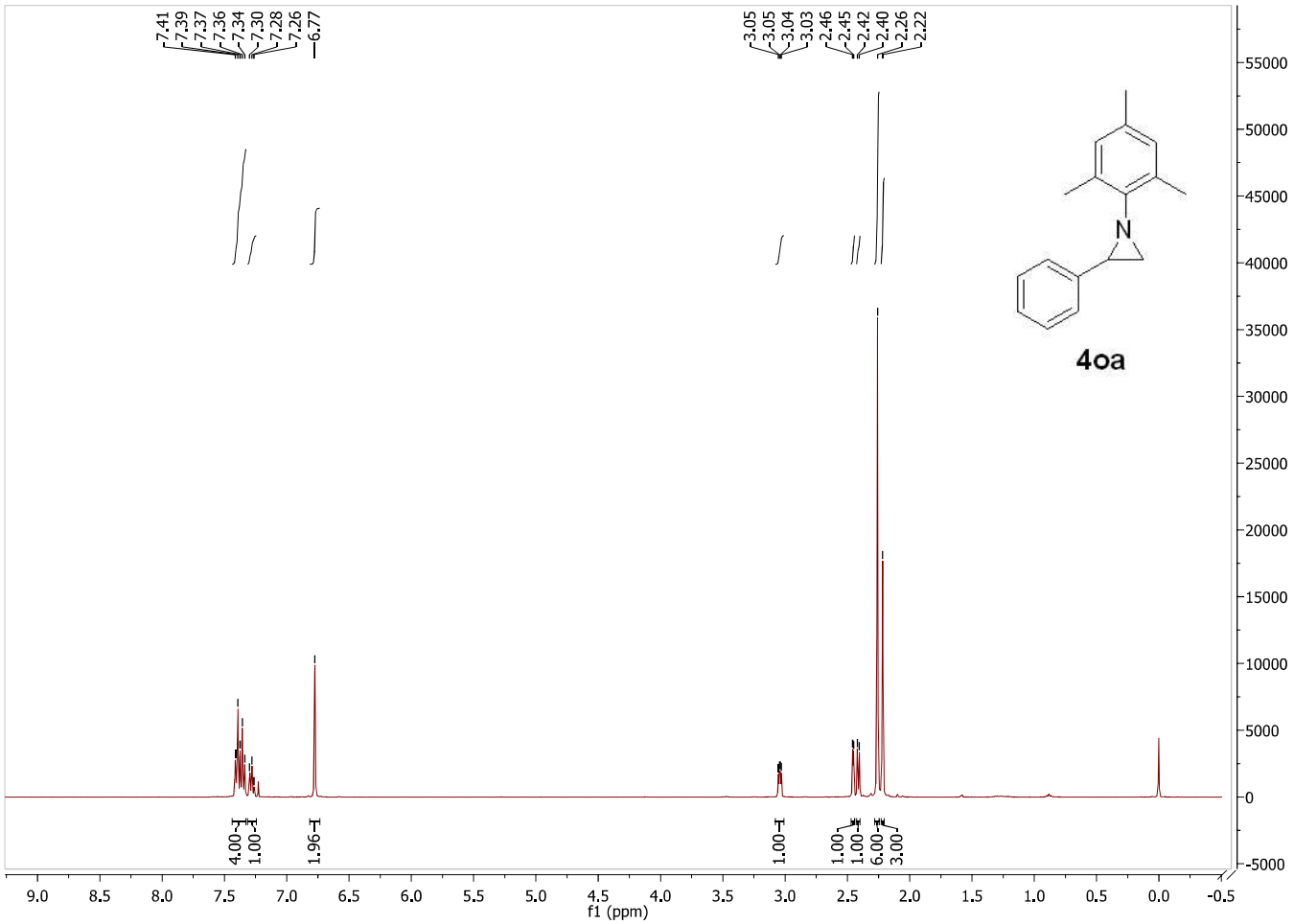
f1 (ppm)
3oa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3.03
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2.42
2.40
2.26
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6.00
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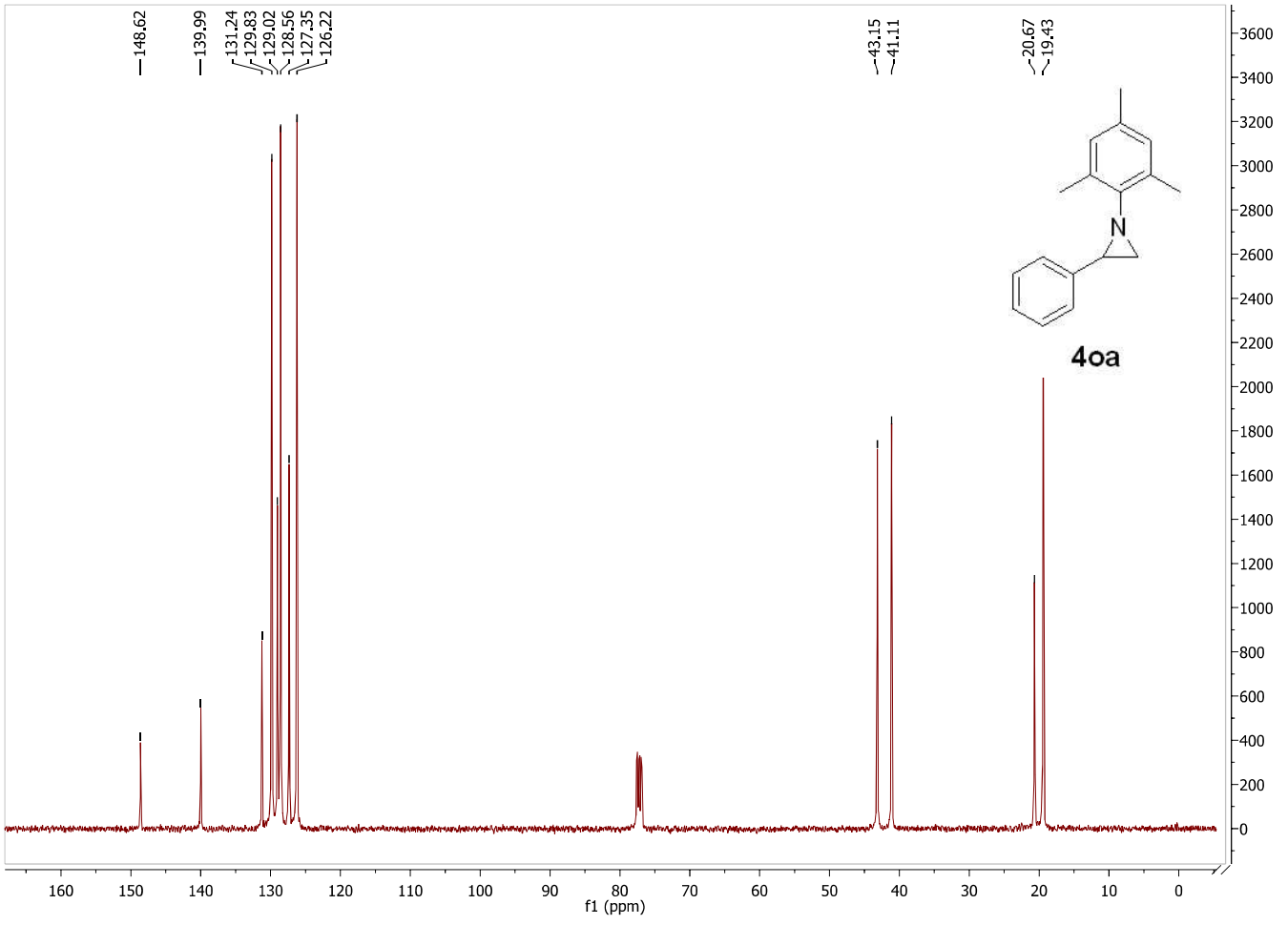
N
4oa
f1 (ppm)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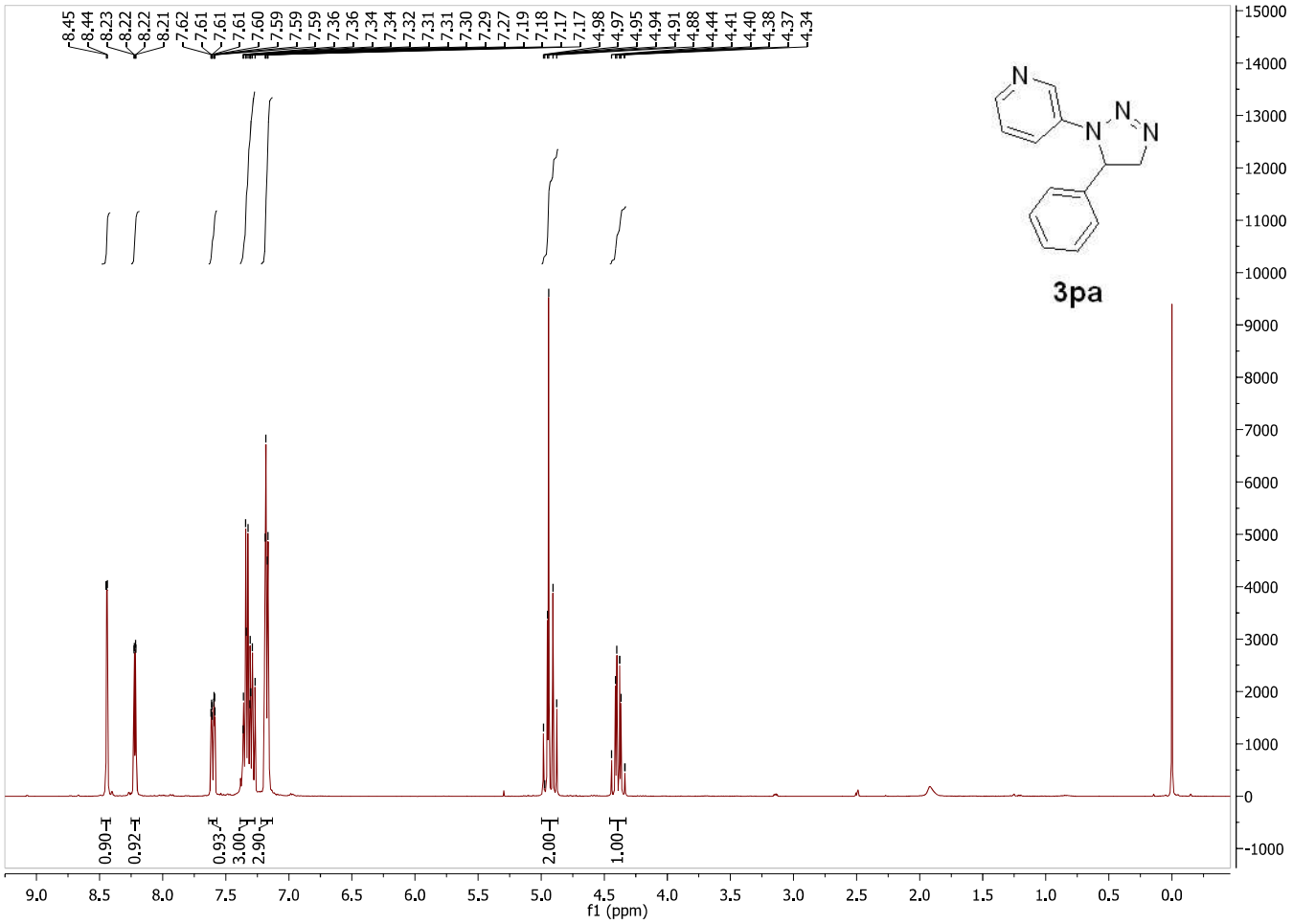
19.43
N
4oa
f1 (ppm)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4.95
4.94
4.91
4.88
4.44
4.41
4.40
4.38
4.37
4.34
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N
3pa
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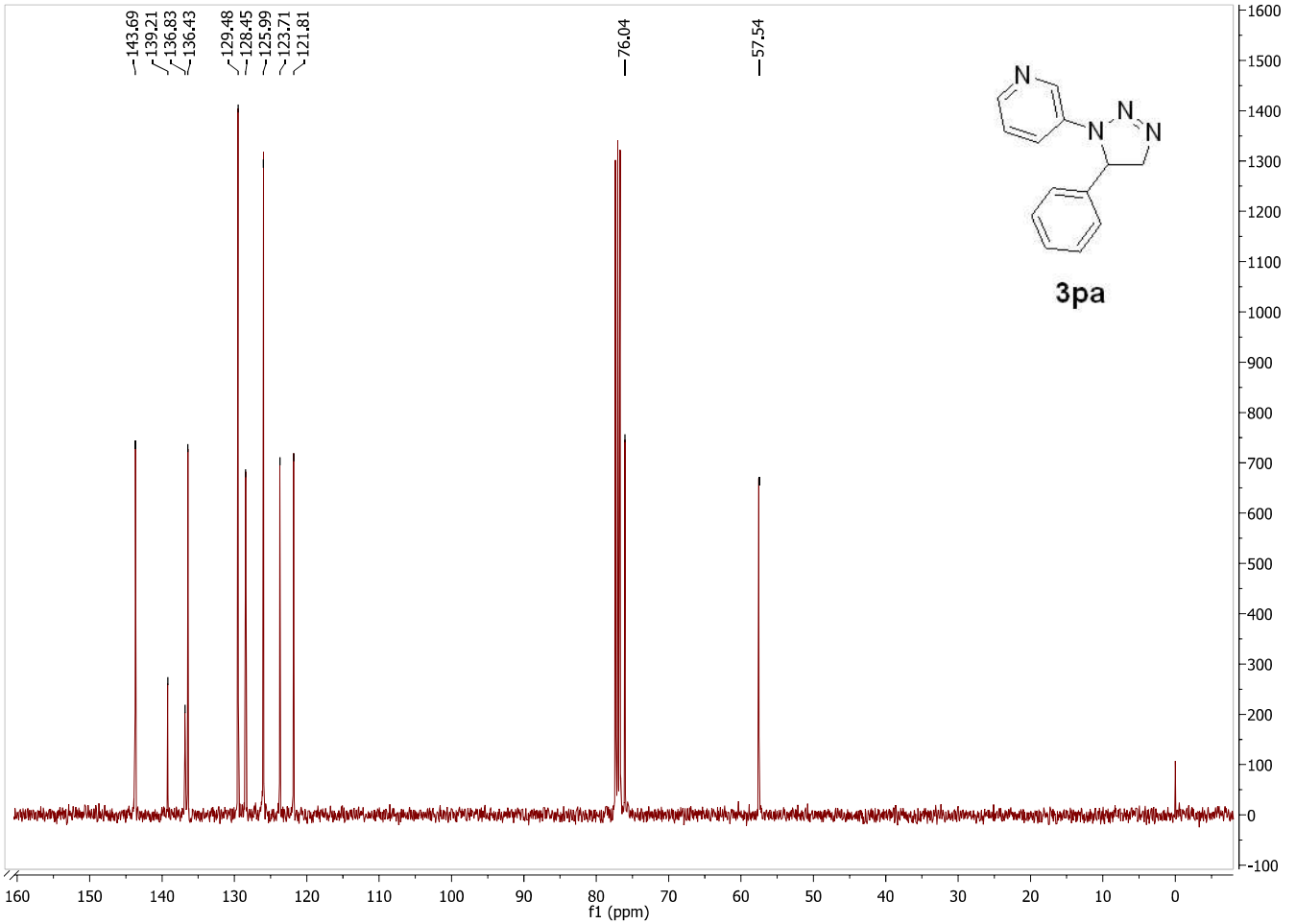
0.92
0.93
3.00
2.90
2.00
1.00
f1 (ppm)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123.71
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N
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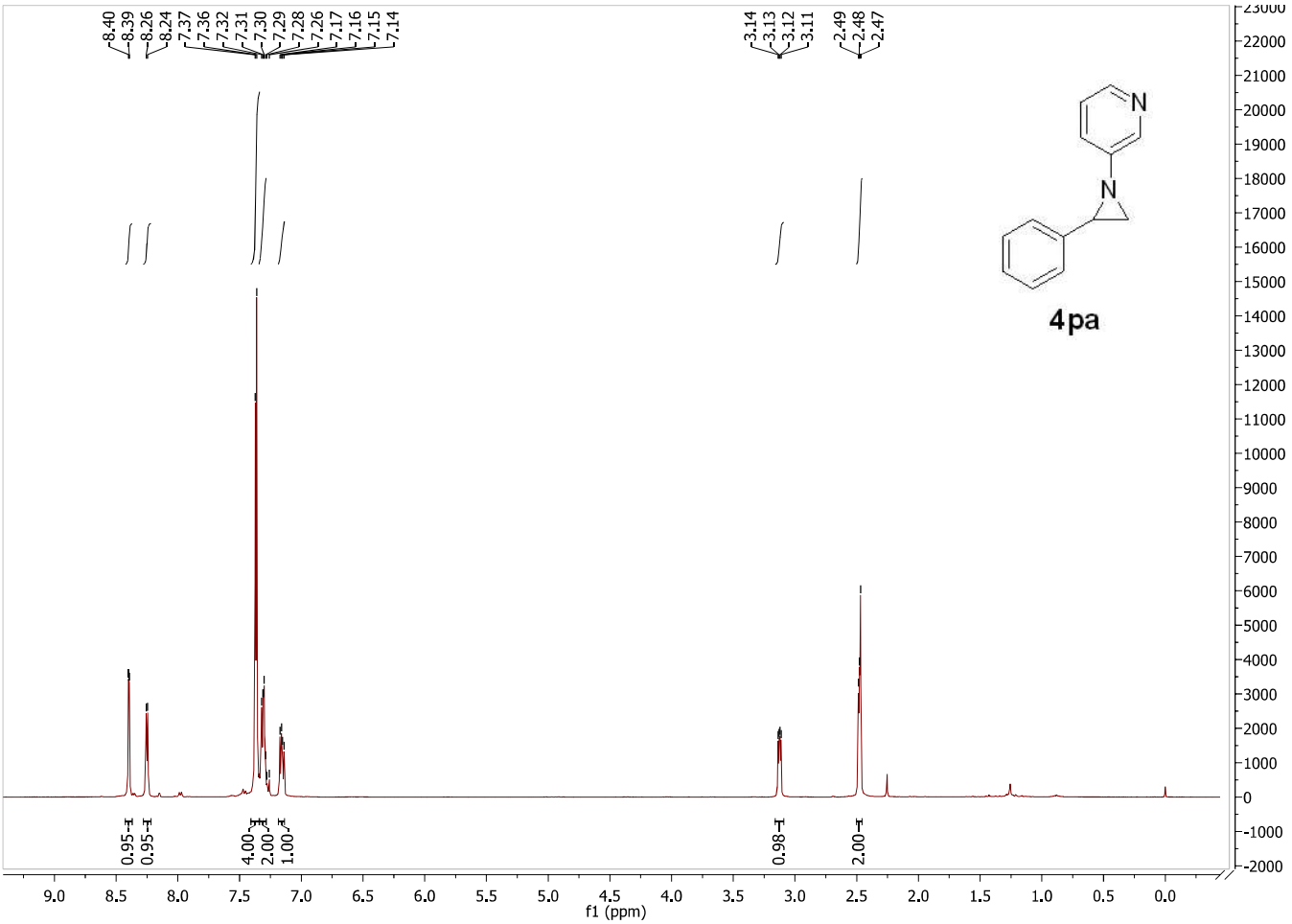
N
N
3pa
f1 (ppm)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7.16
7.15
7.14
3.14
3.13
3.12
3.11
2.49
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2.47
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N
4pa
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0.95
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1.00
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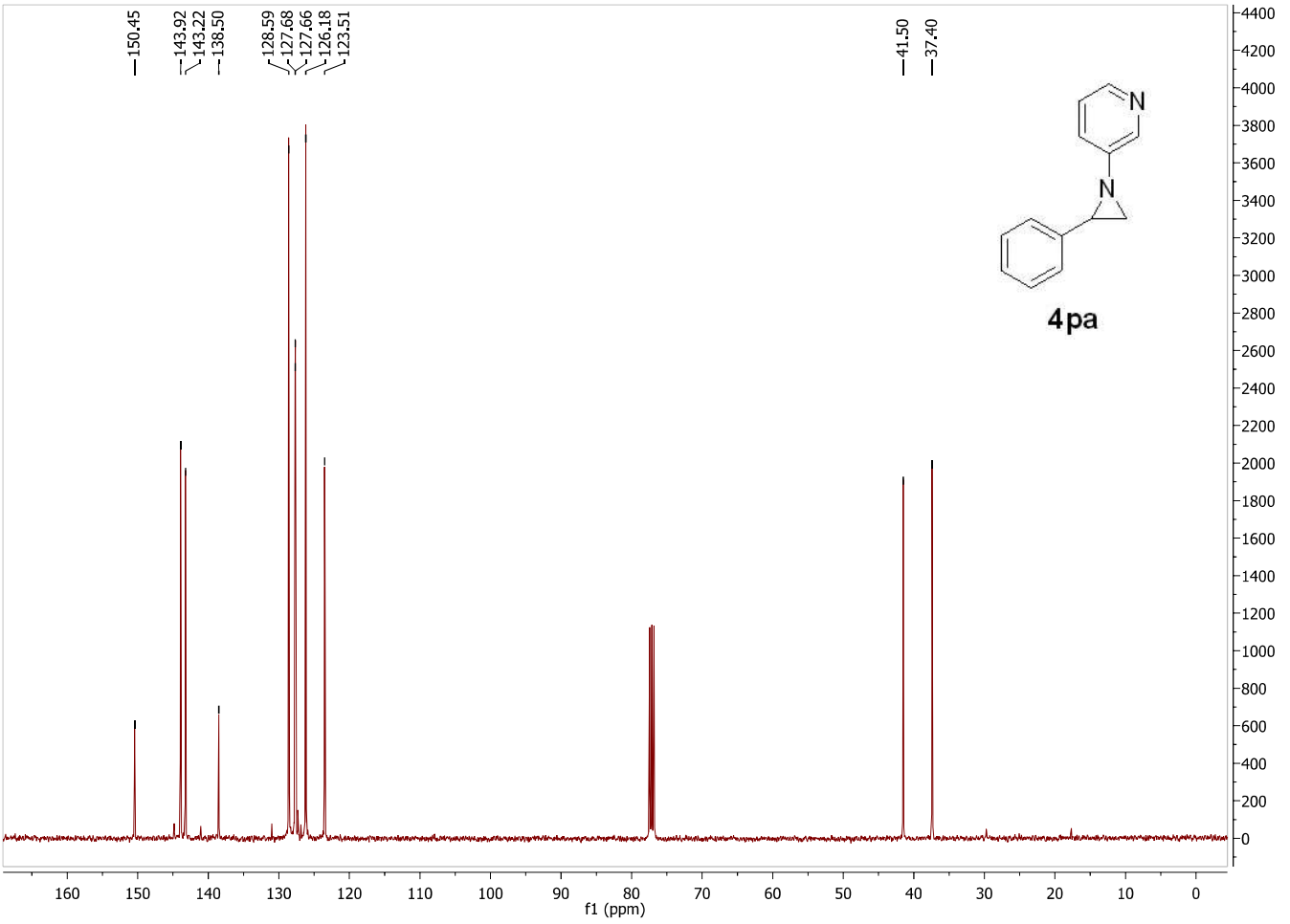
2.00
f1 (ppm)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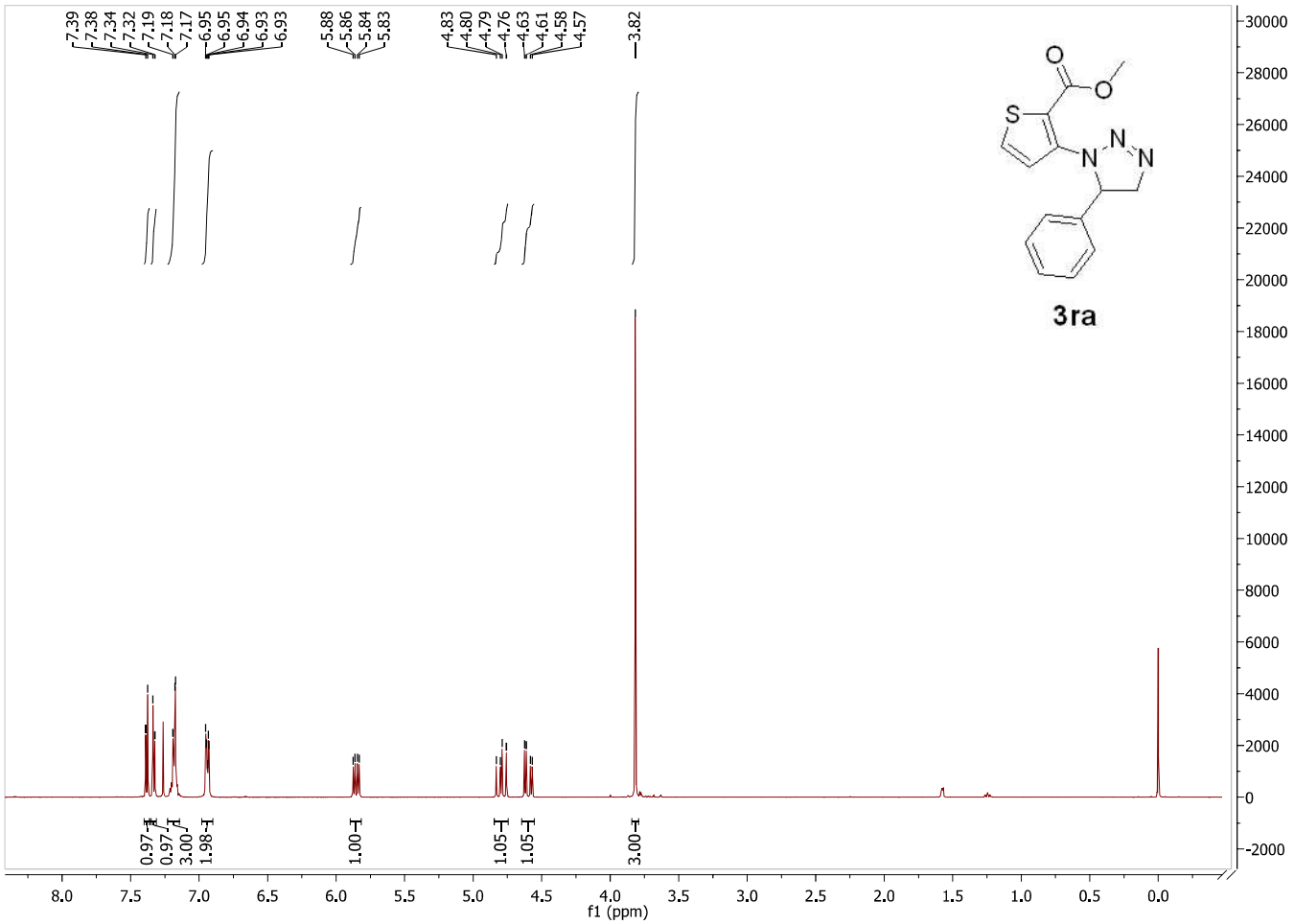
37.40
N
N
4pa
f1 (ppm)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6.93
5.88
5.86
5.84
5.83
4.83
4.80
4.79
4.76
4.63
4.61
4.58
4.57
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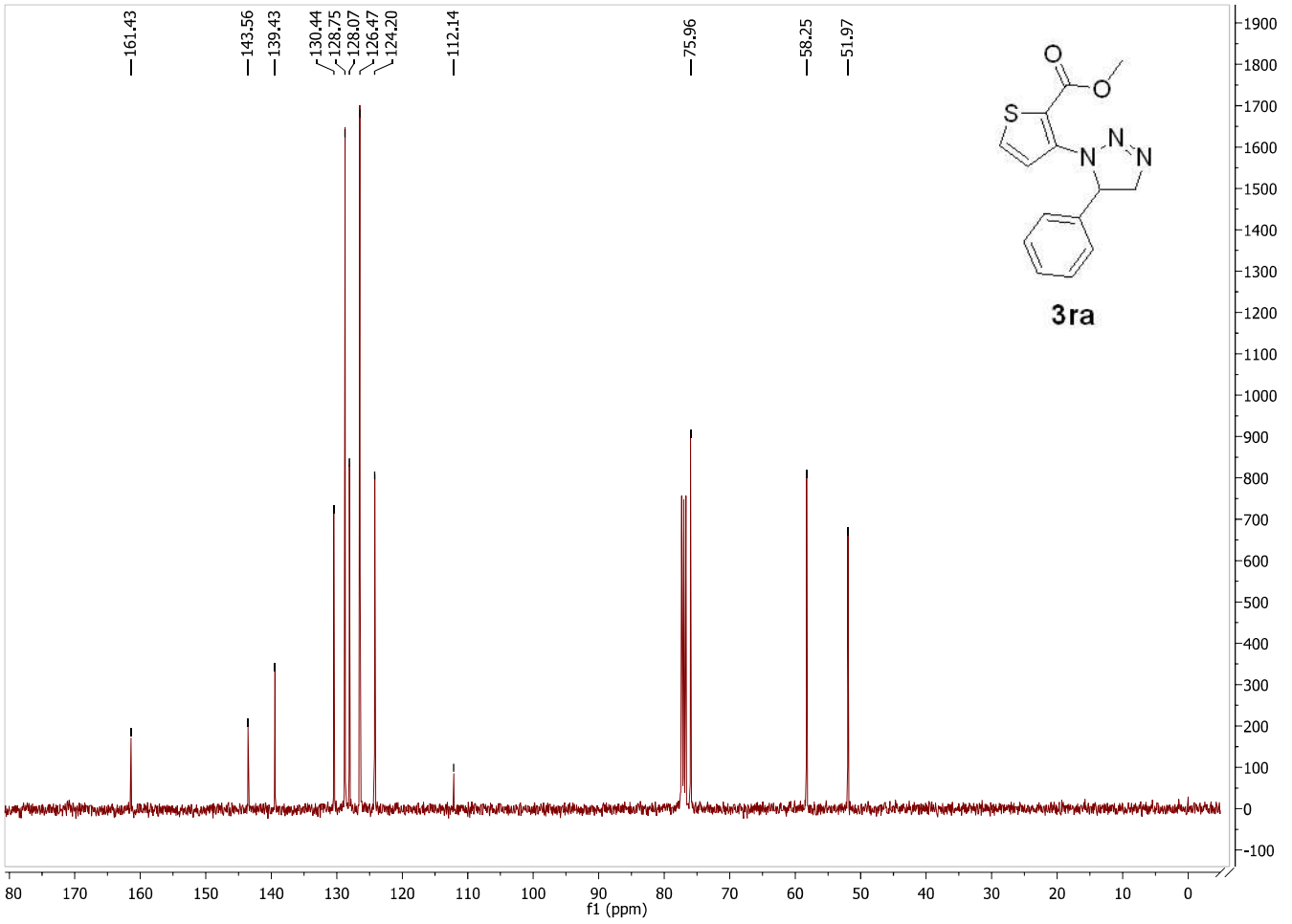
1.00
1.05
1.05
3.00
f1 (ppm)
3ra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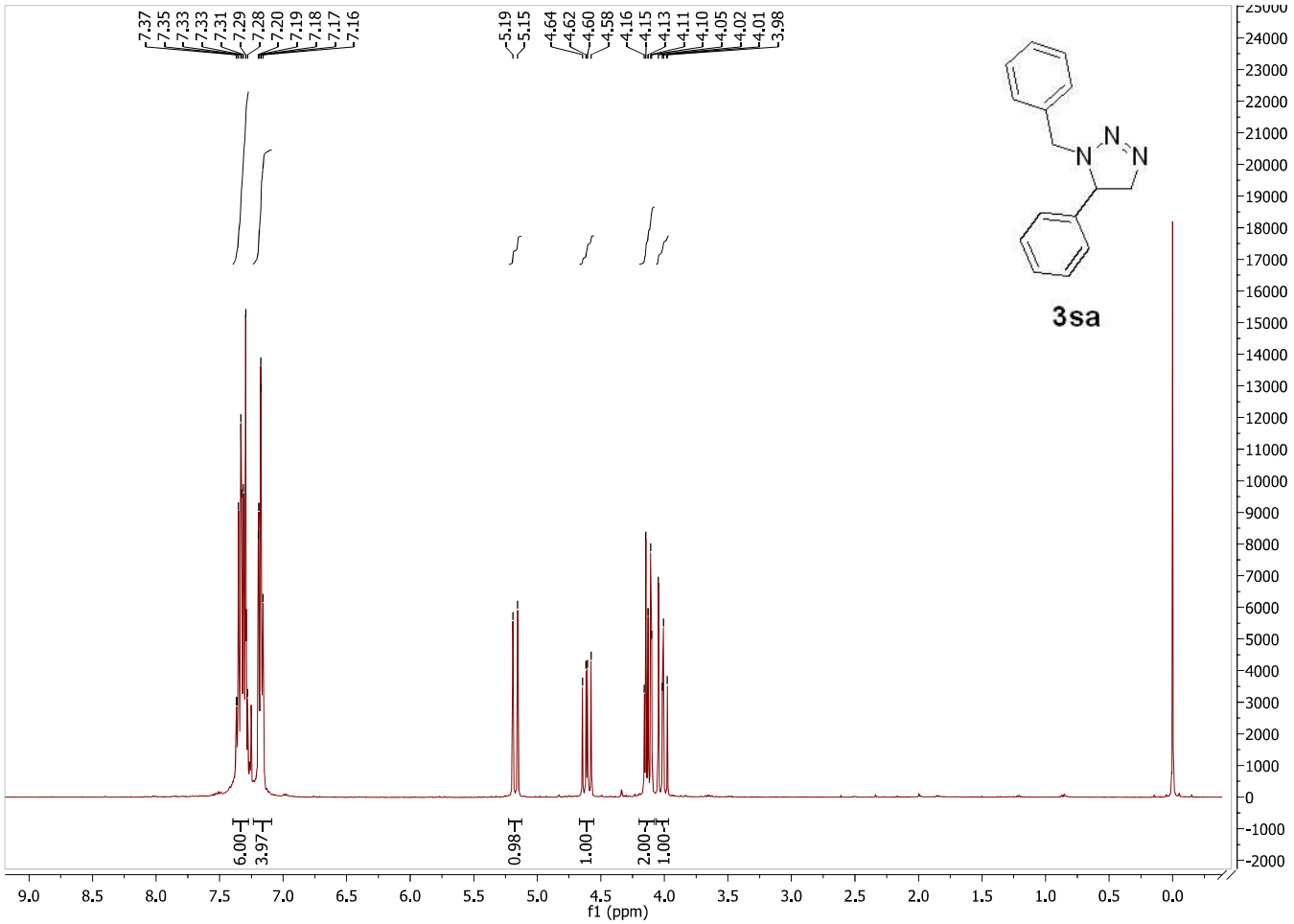
f1 (ppm)
3ra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4.62
4.60
4.58
4.16
4.15
4.13
4.11
4.10
4.05
4.02
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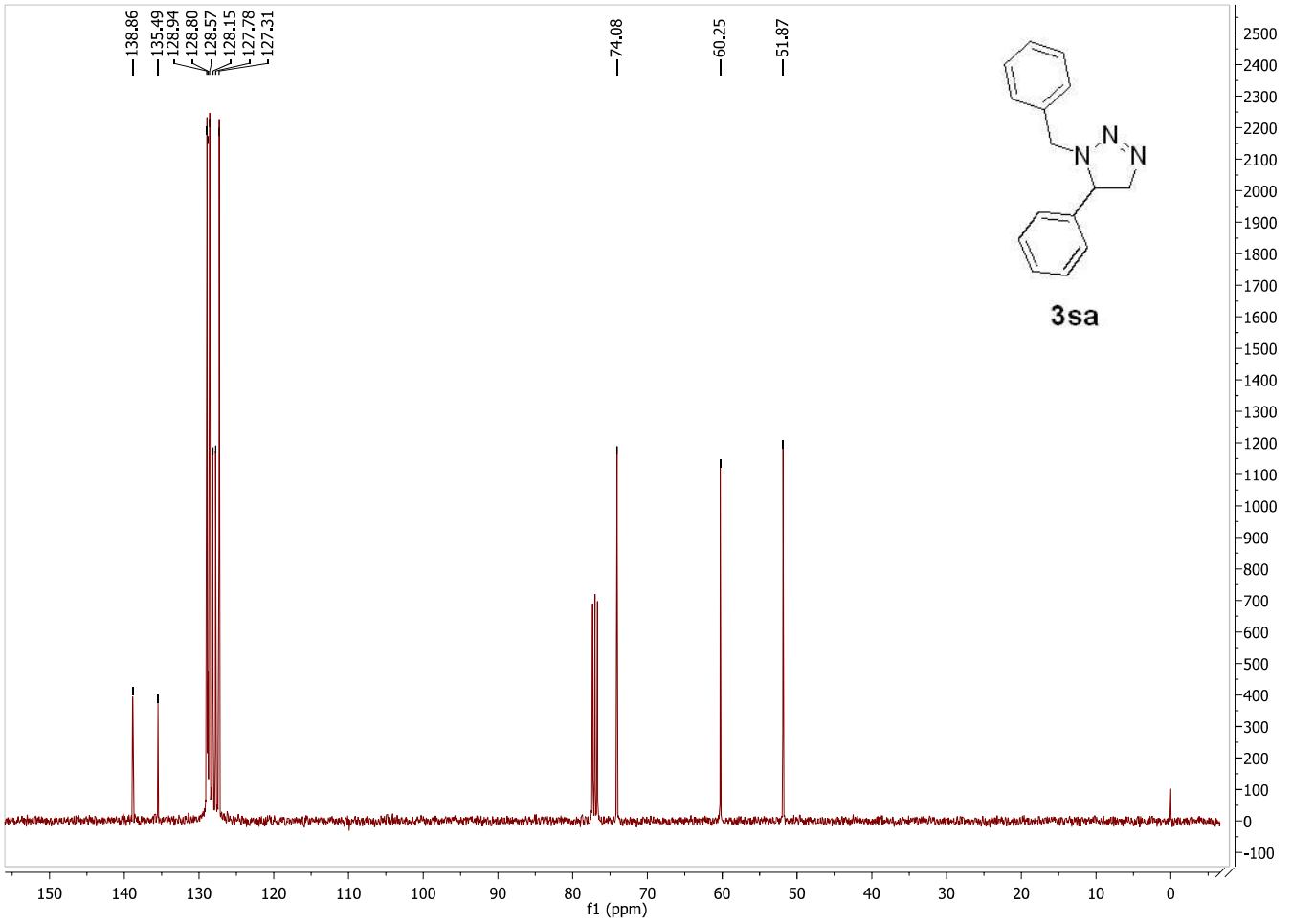
1.00
f1 (ppm)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N
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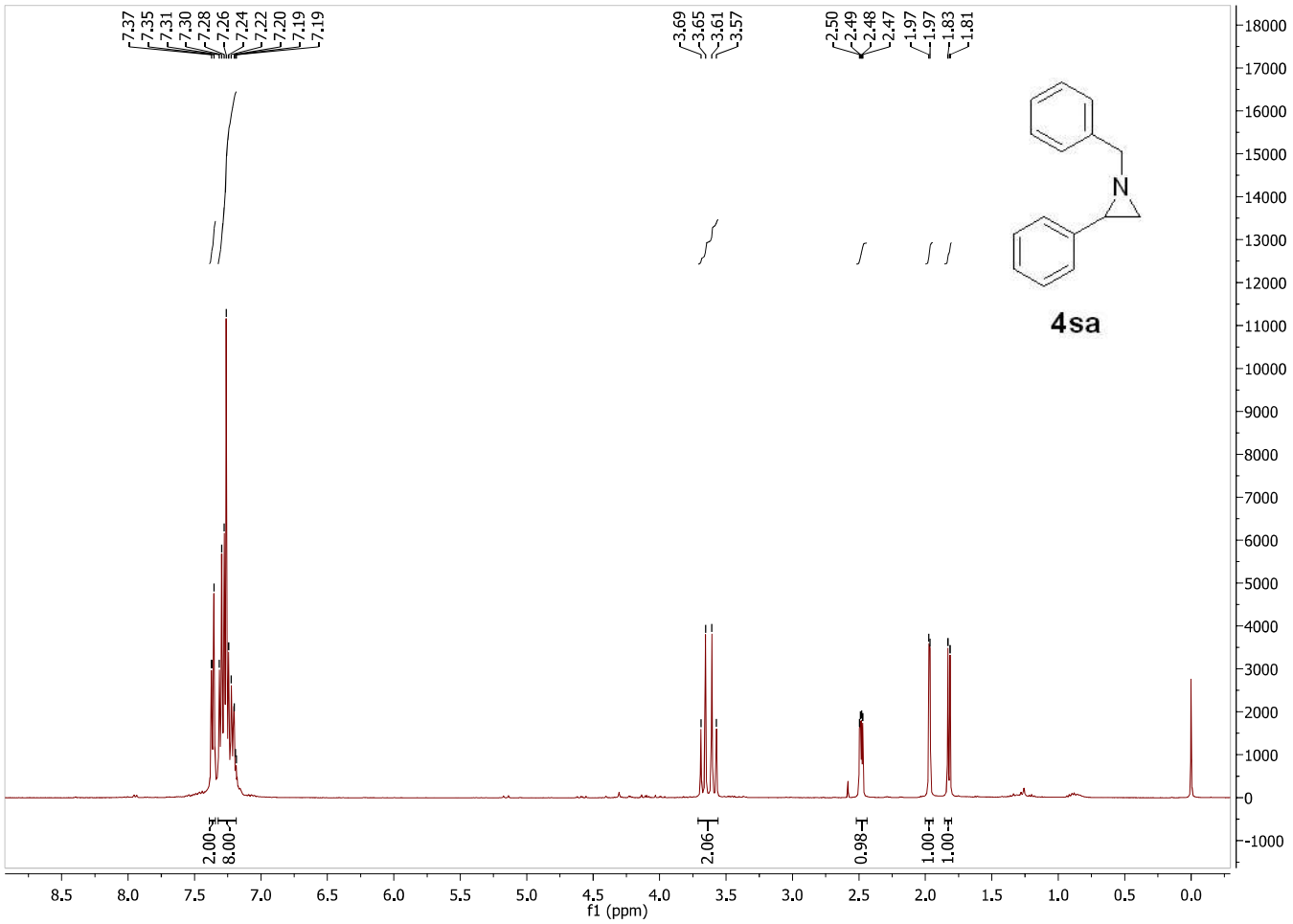
f1 (ppm)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3.57
2.50
2.49
2.48
2.47
1.97
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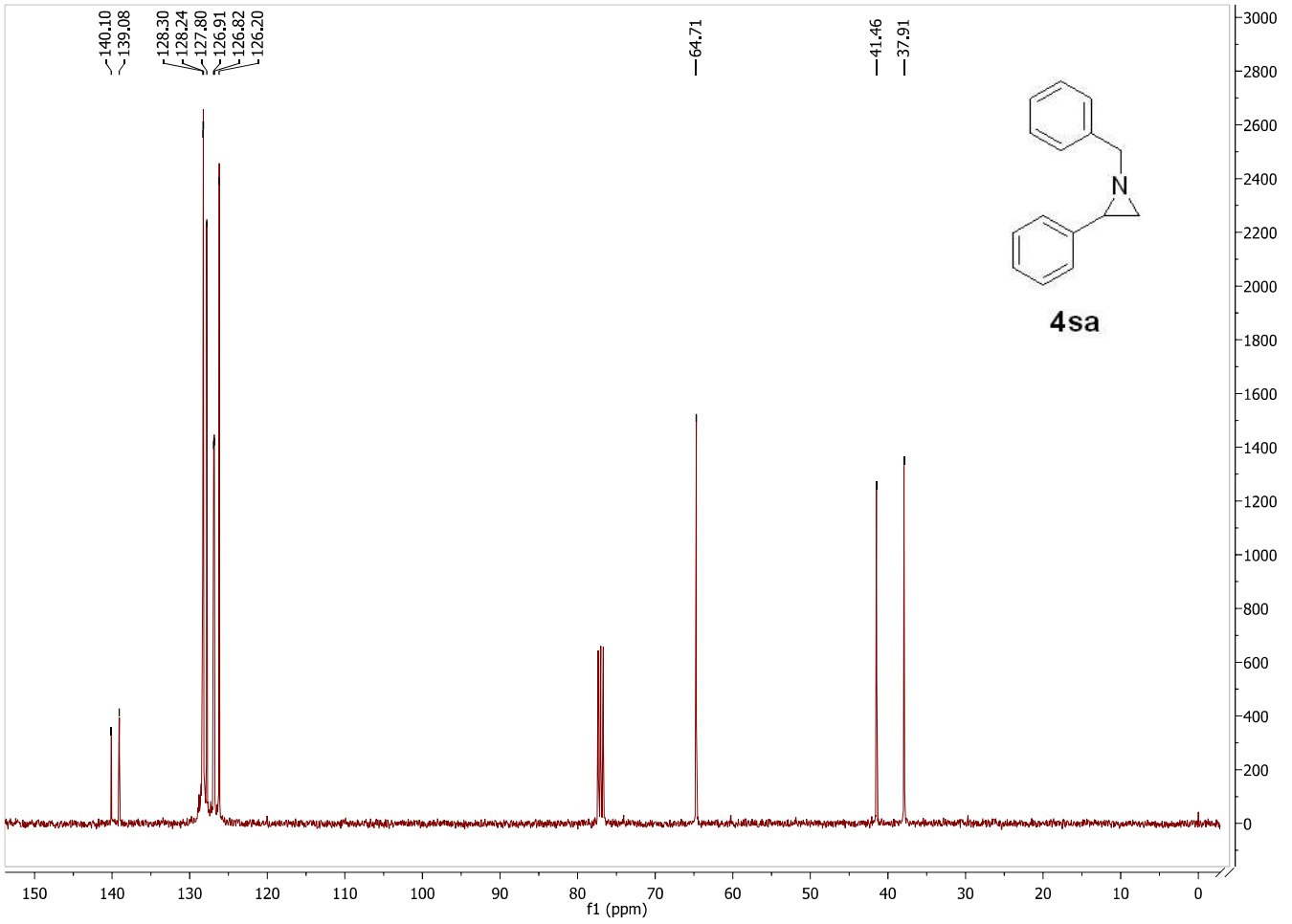
1.00
f1 (ppm)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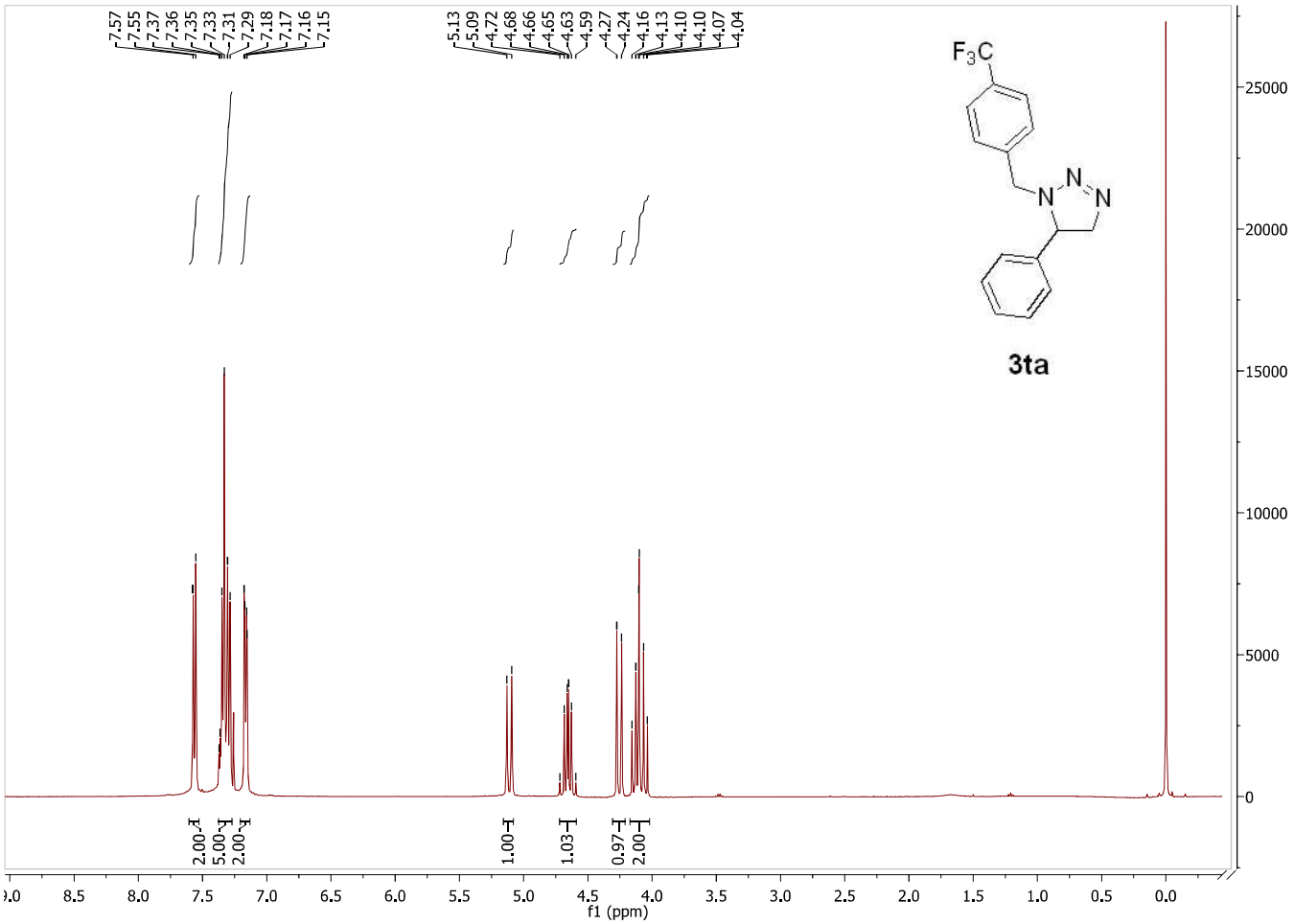
4sa
f1 (ppm)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4.63
4.59
4.27
4.24
4.16
4.13
4.10
4.10
4.07
4.04
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5.00
2.00
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1.03
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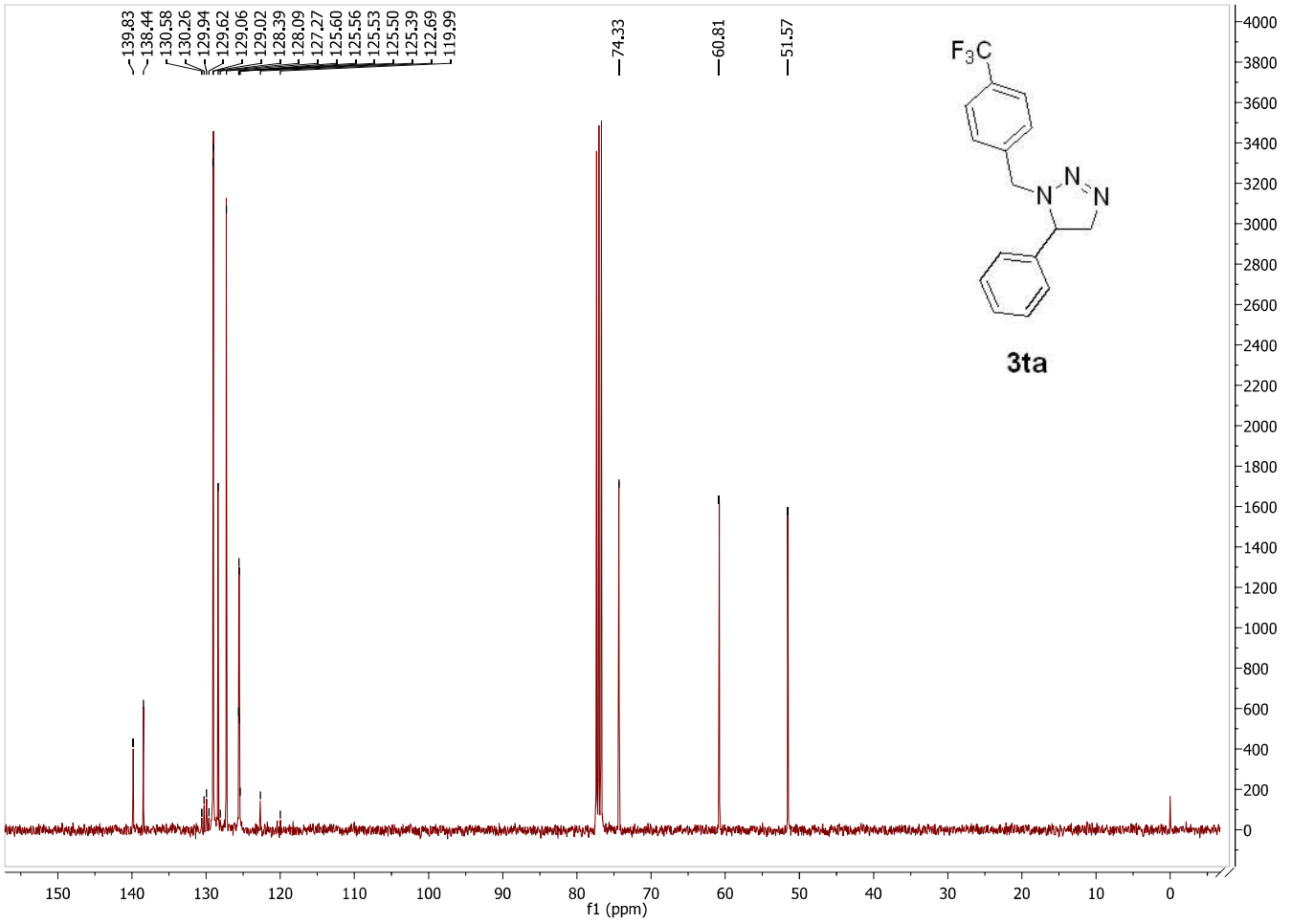
2.00
f1 (ppm)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125.53
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F3C
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N
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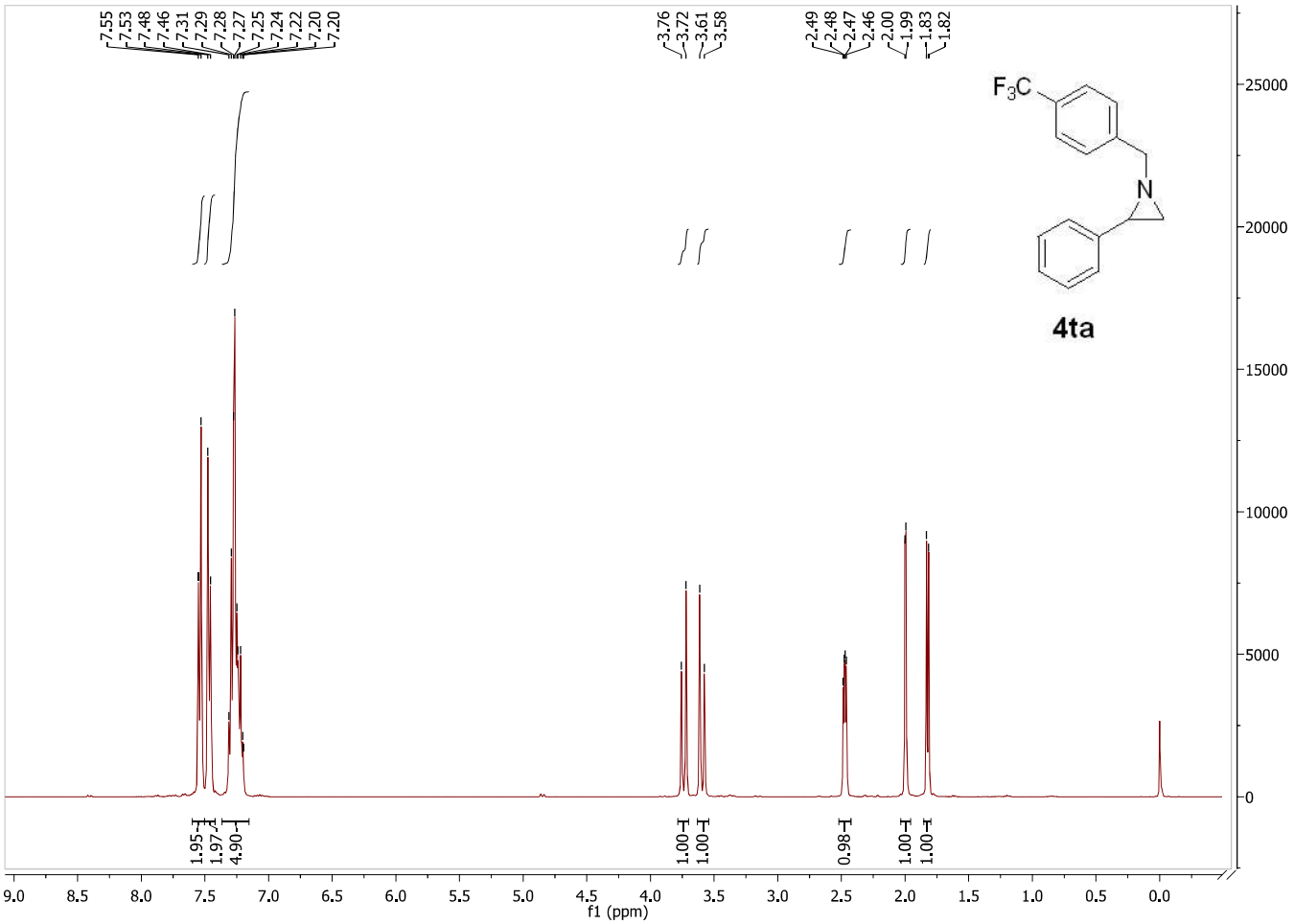
f1 (ppm)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3.72
3.61
3.58
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2.48
2.47
2.46
2.00
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1.83
1.82
F3C
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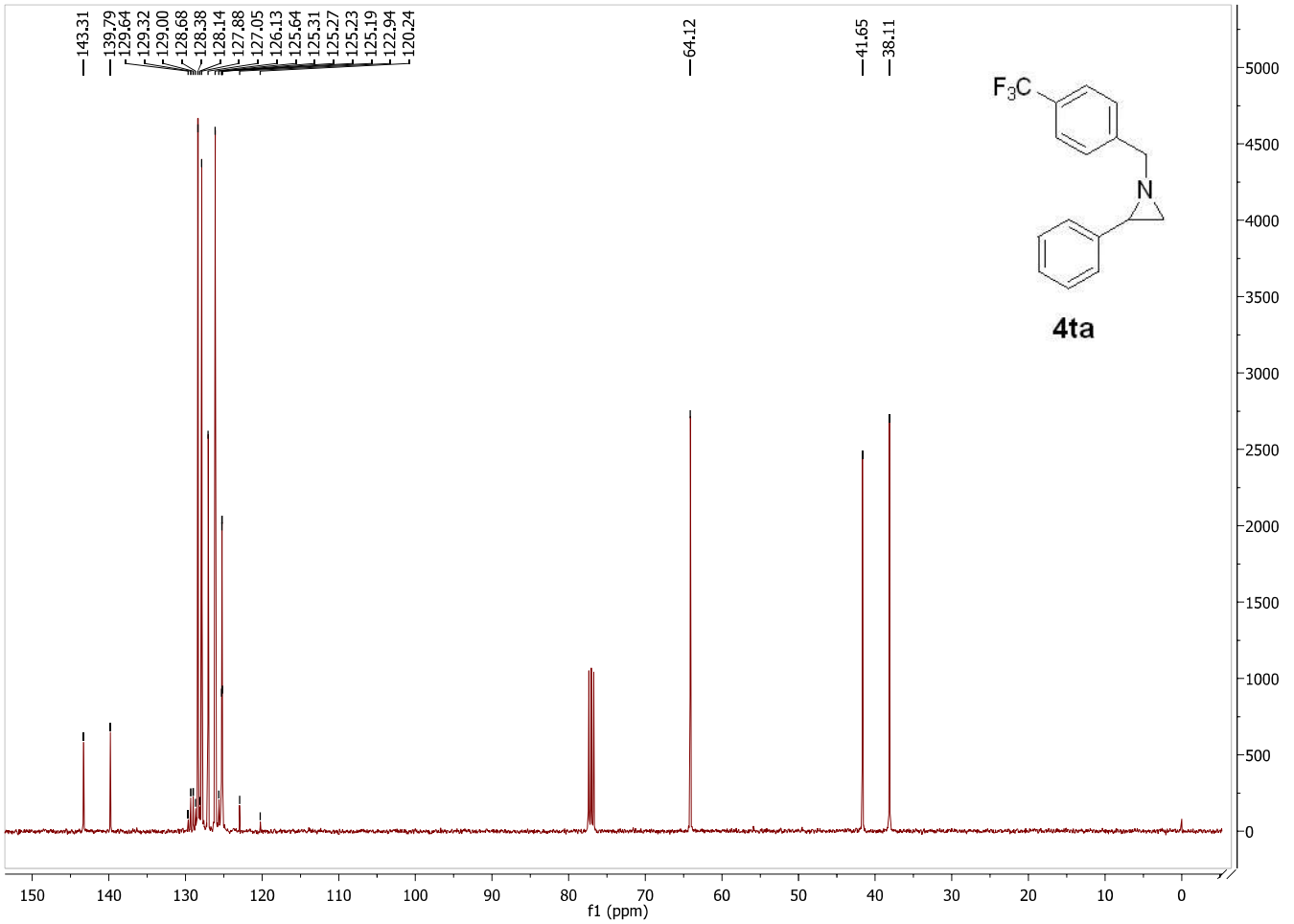
4.90
1.00
1.00
0.98
1.00
1.00
f1 (ppm)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127.05
126.13
125.64
125.31
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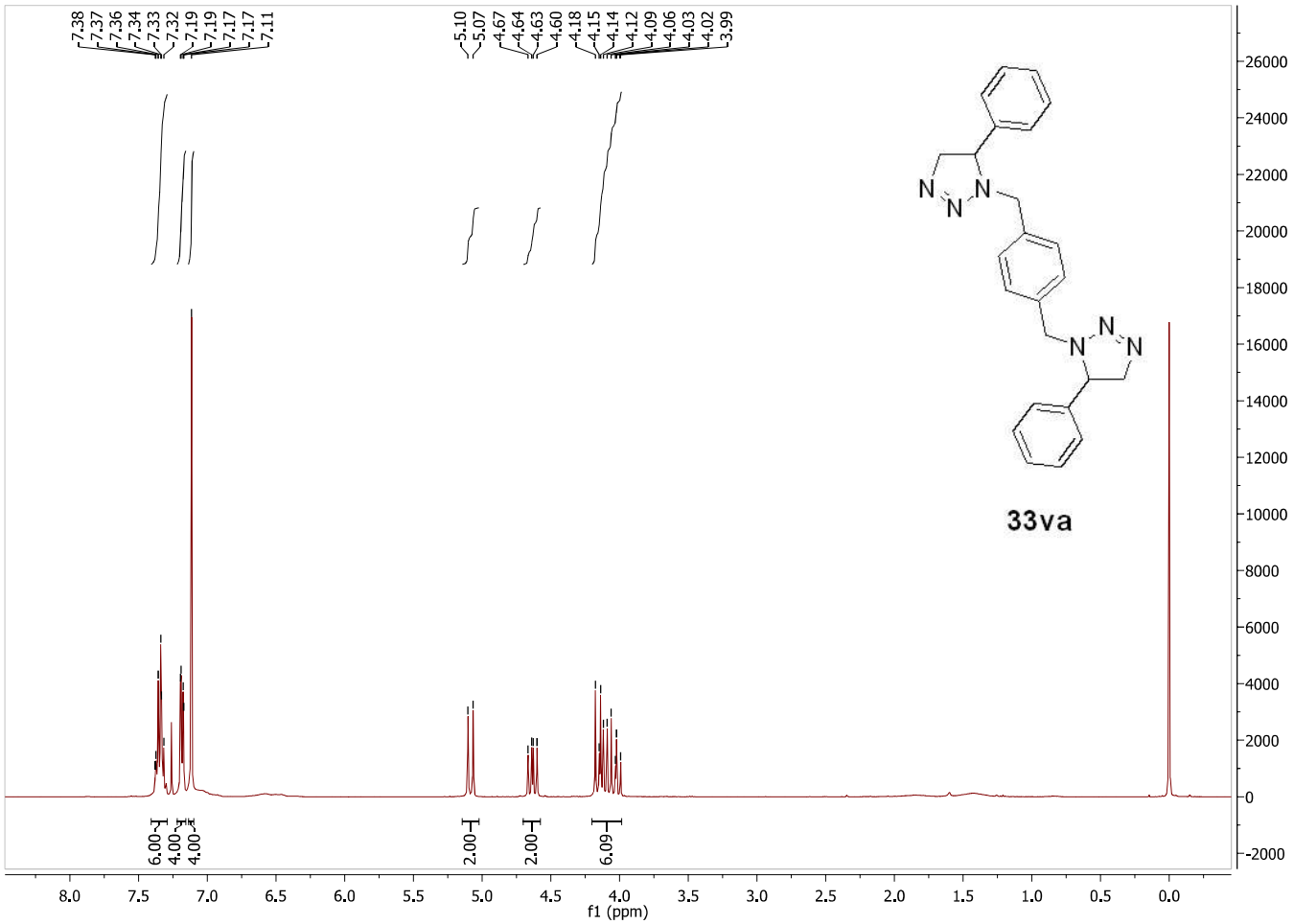
125.19
122.94
120.24
64.12
41.65
38.11
F3C
N
4ta
f1 (ppm)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4.18
4.15
4.14
4.12
4.09
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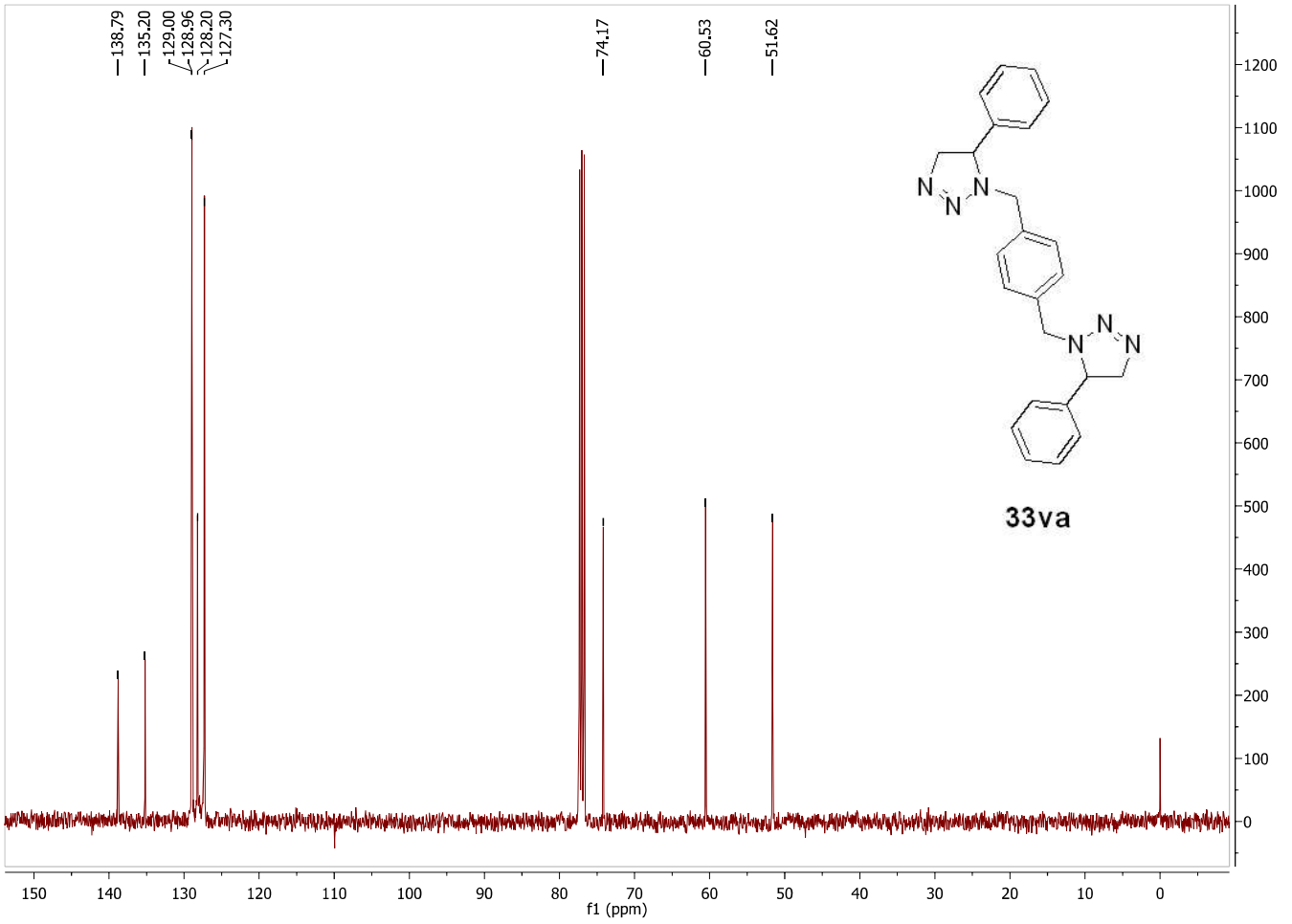
4.00
4.00
2.00
2.00
6.09
33va
f1 (ppm)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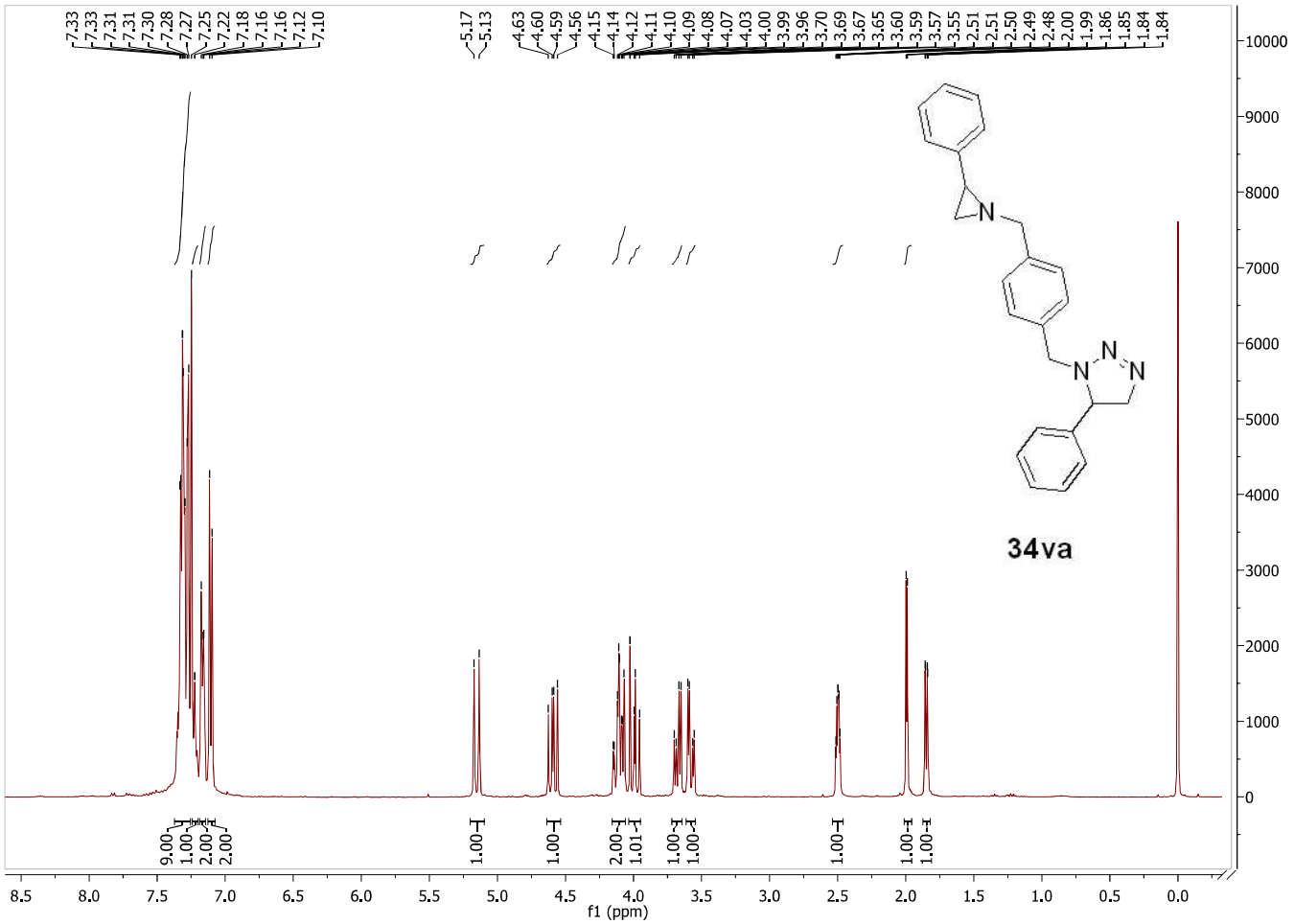
f1 (ppm)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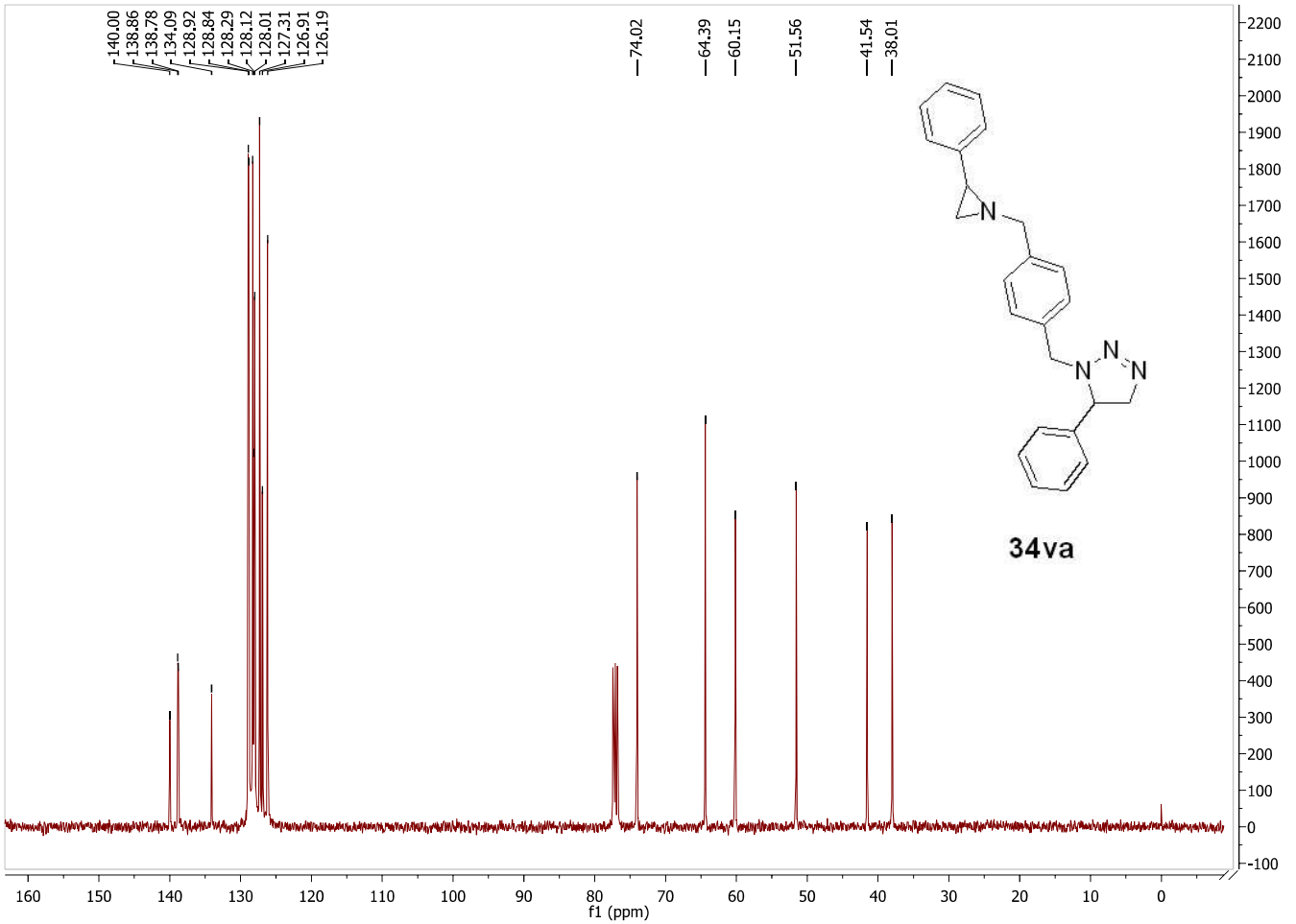
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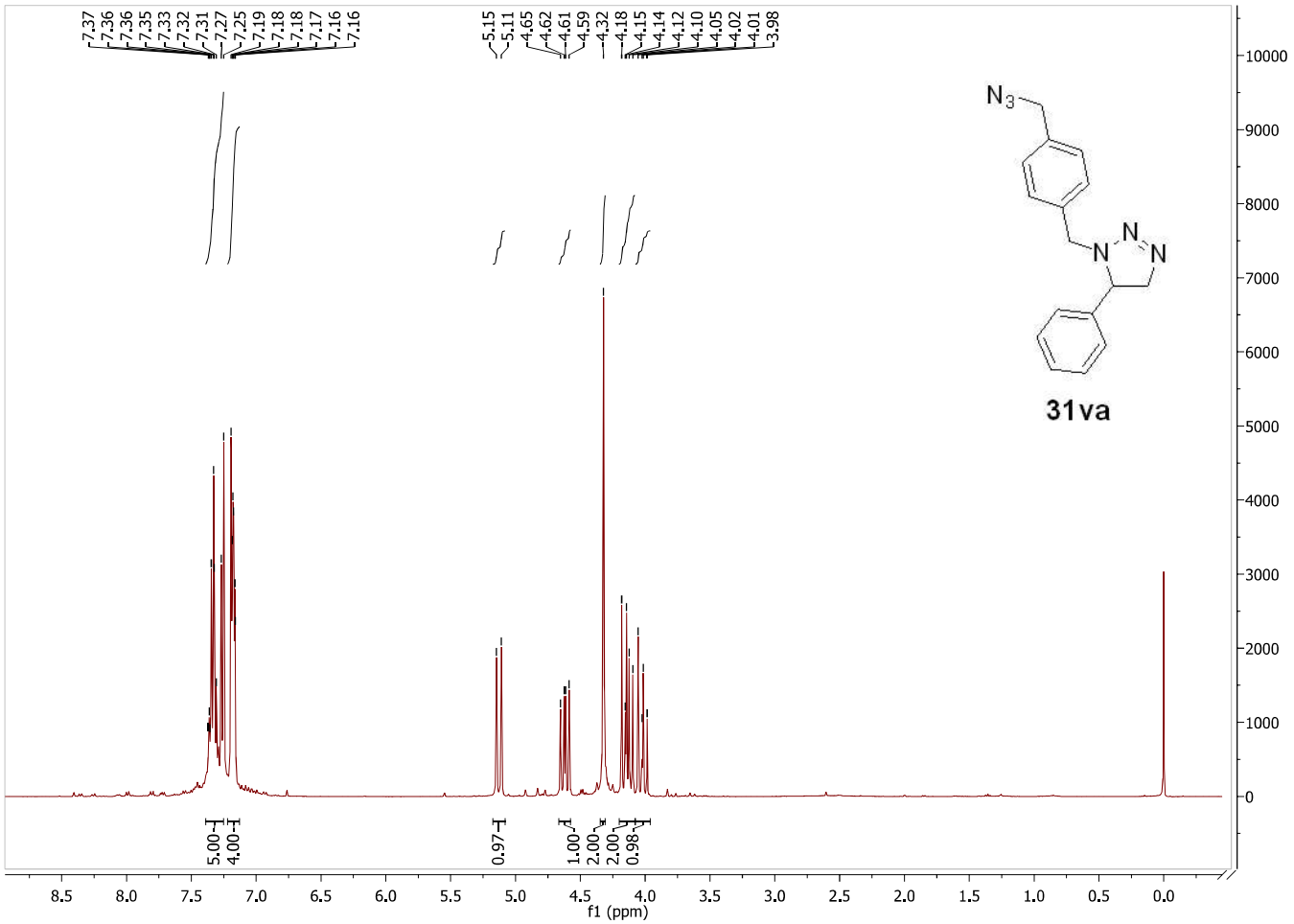
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4.12
4.10
4.05
4.02
4.01
3.98
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31va
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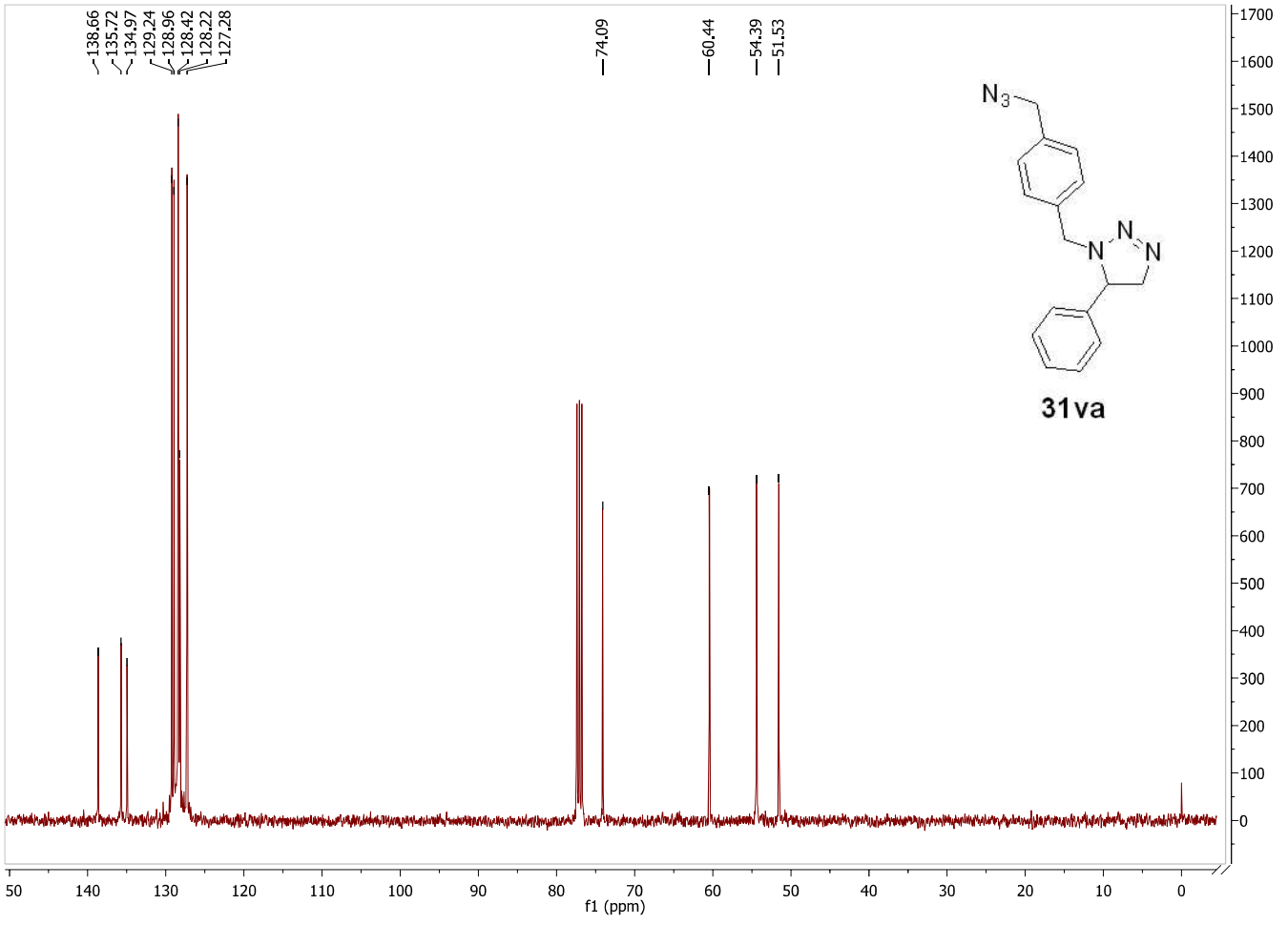
0.98
f1 (ppm)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N3
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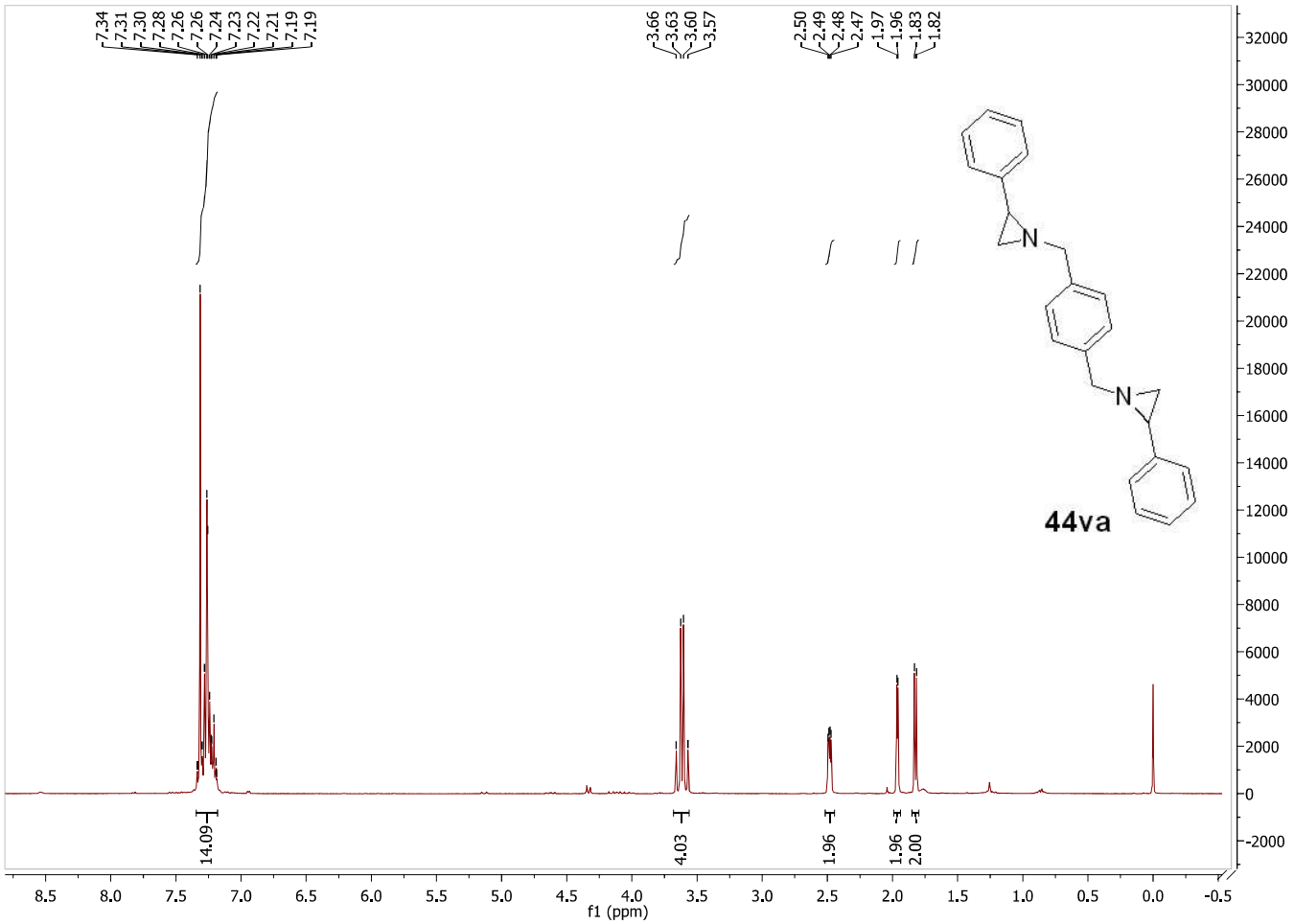
N
N
31va
f1 (ppm)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2.48
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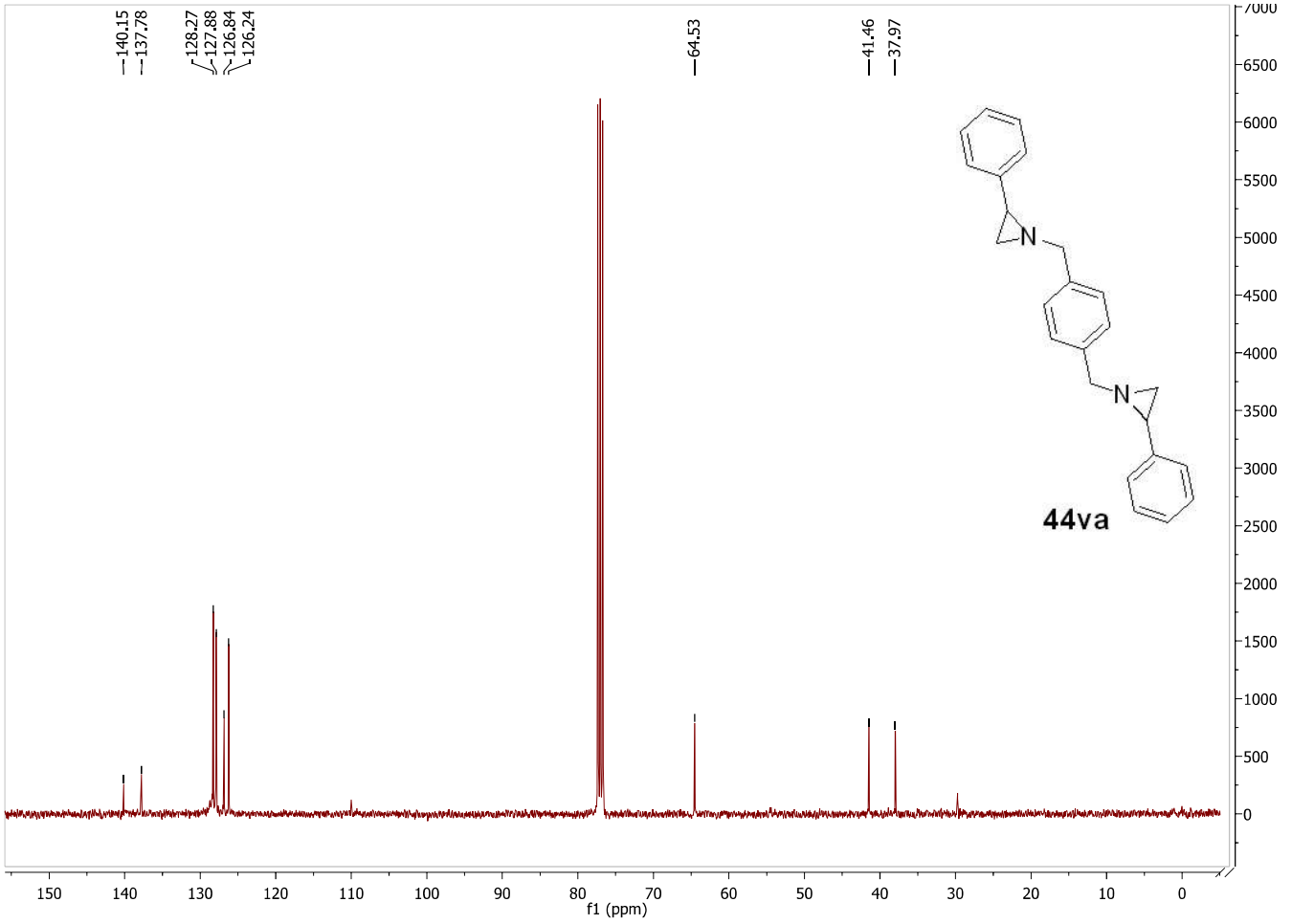
f1 (ppm)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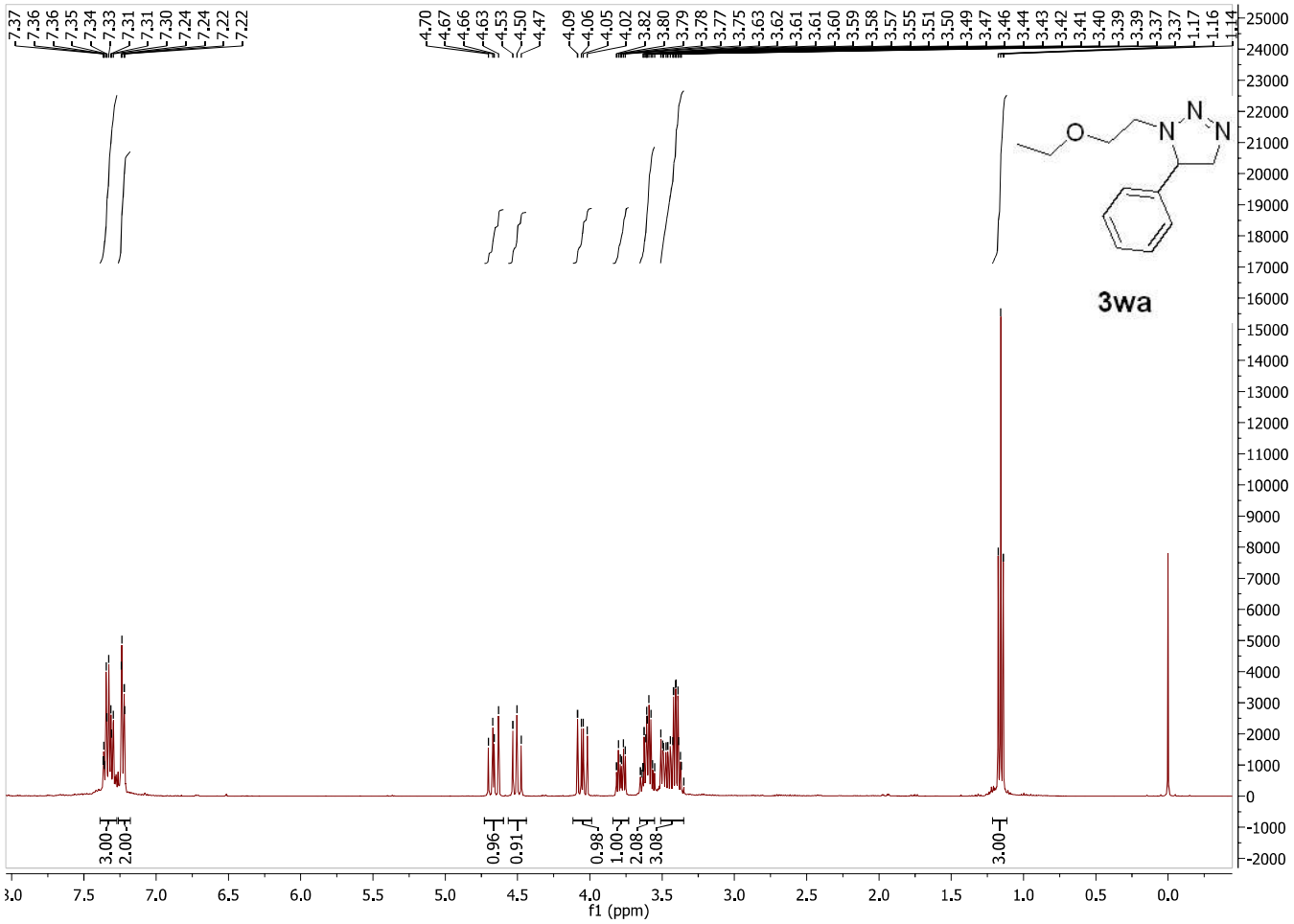
f1 (ppm)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4.66
4.63
4.53
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4.47
4.09
4.06
4.05
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3.40
3.39
3.39
3.37
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1.16
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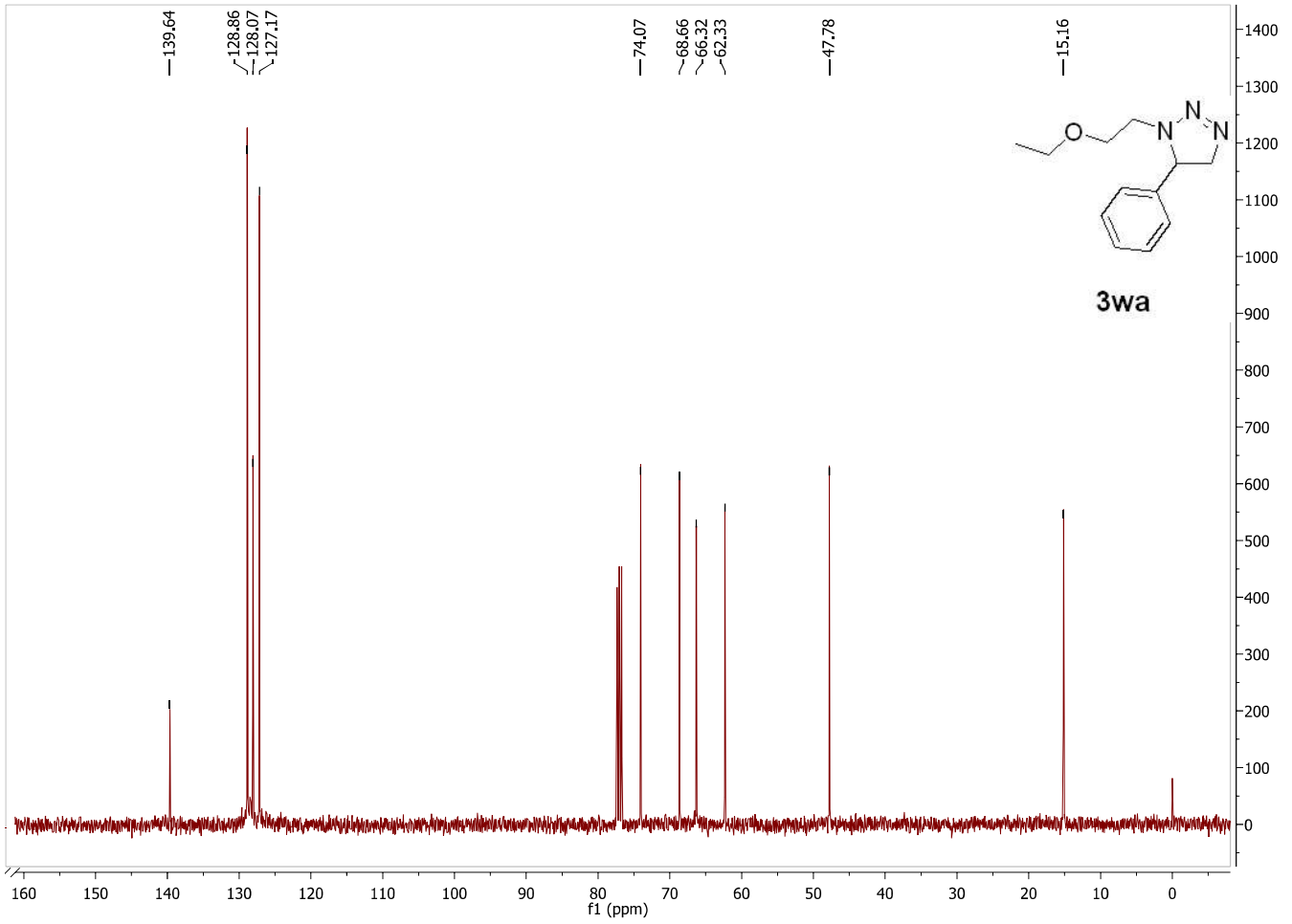
3.00
f1 (ppm)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62.33
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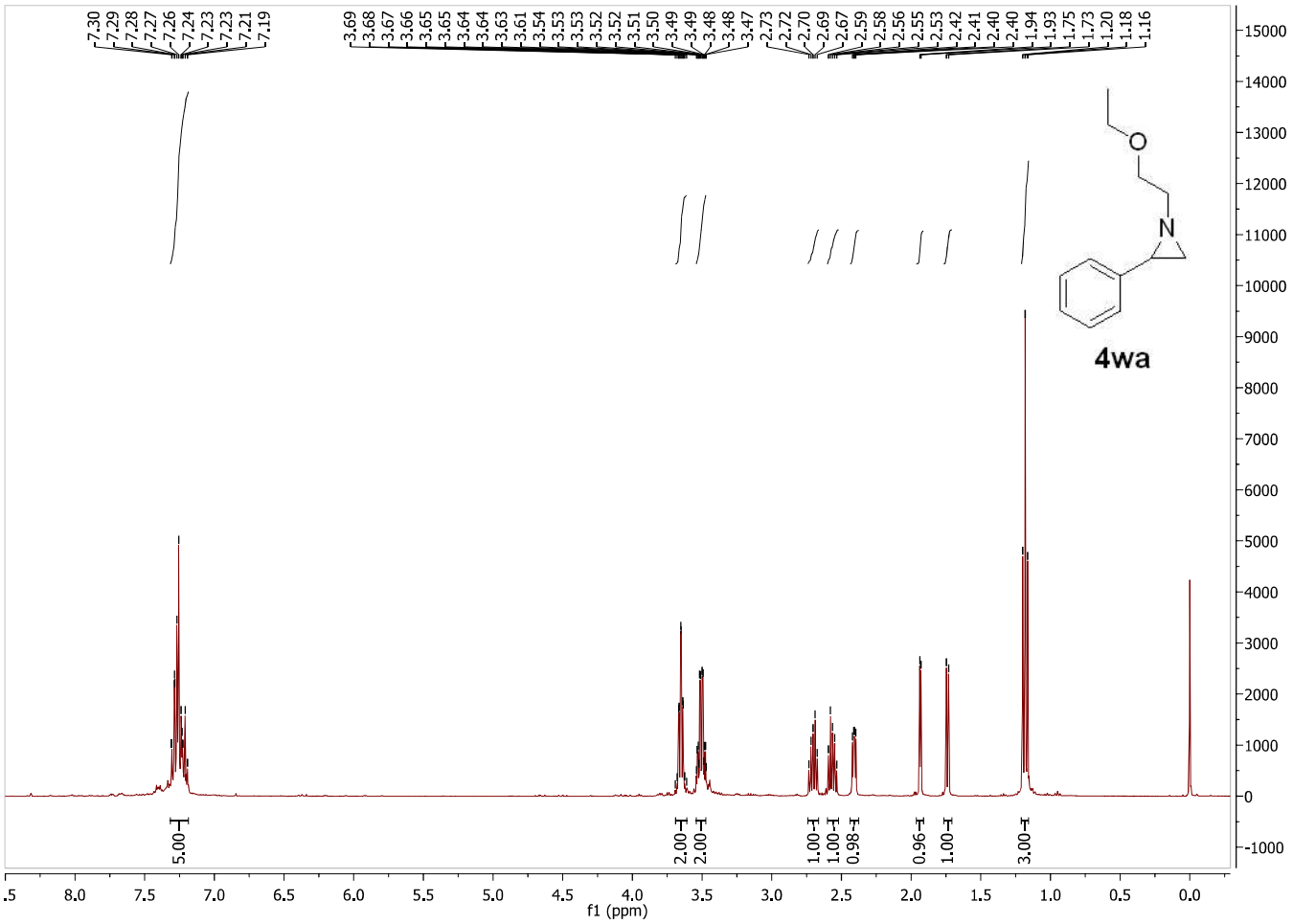
f1 (ppm)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2.73 2.72 2.70 2.69 2.67 2.59 2.58 2.56 2.55 2.53 2.42 2.41 2.40 2.40 1.94 1.93 1.75 1.73 1.20 1.18 1.16
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4wa
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2.00
2.00
1.00
1.00
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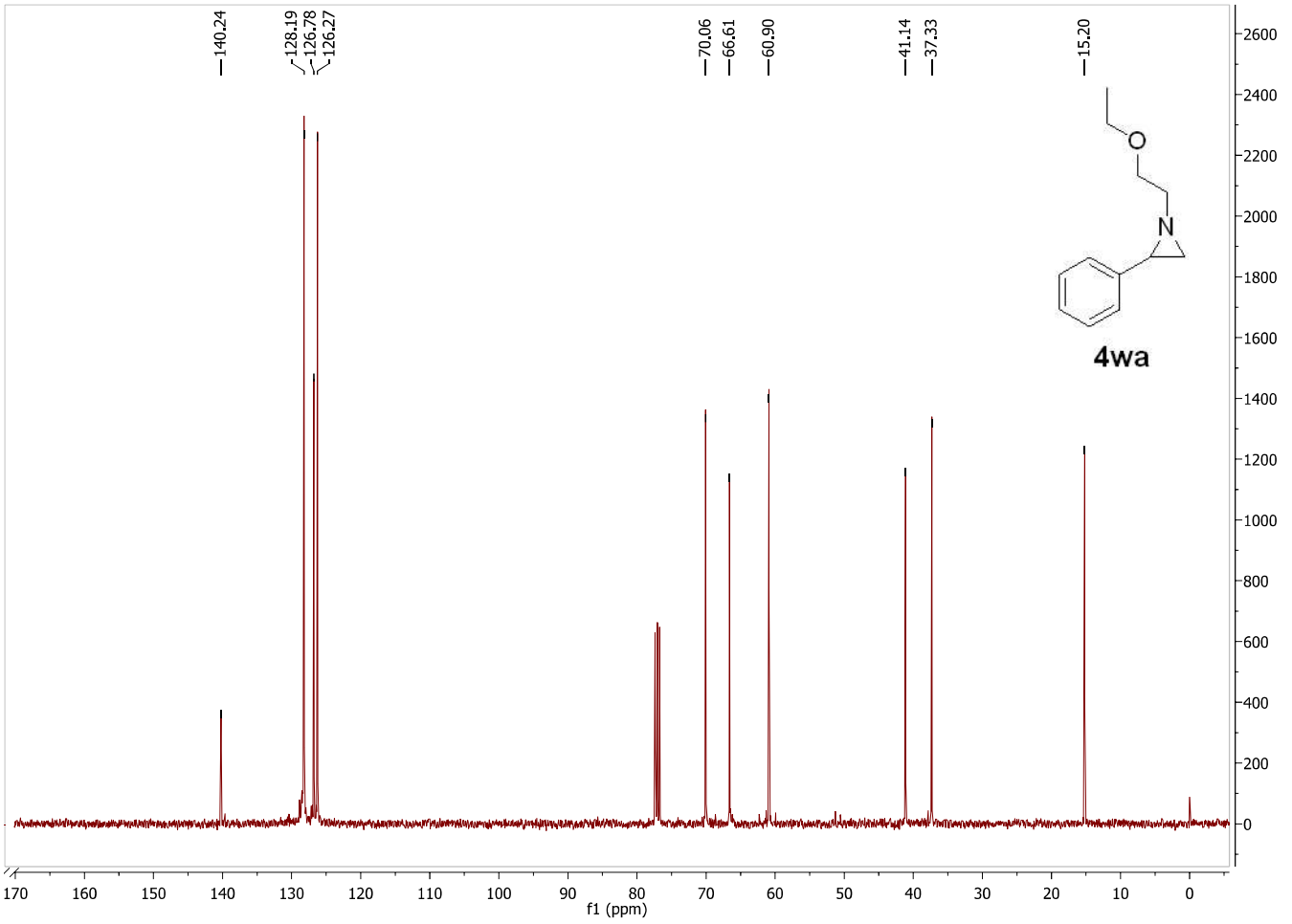
0.96
1.00
3.00
f1 (ppm)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66.61
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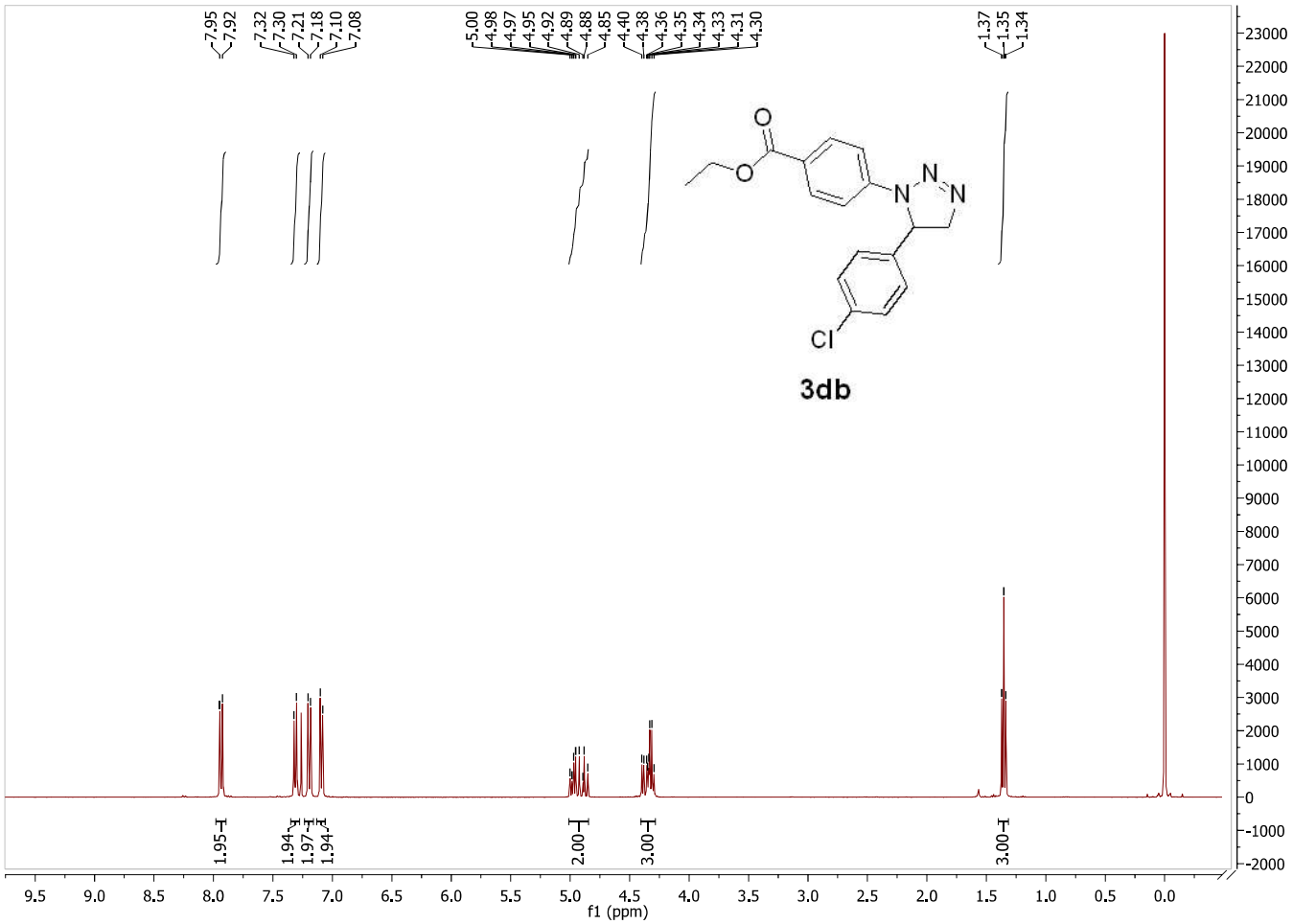
41.14
37.33
15.20
O
N
4wa
f1 (ppm)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4.88
4.85
4.40
4.38
4.36
4.35
4.34
4.33
4.31
4.30
1.37
1.35
1.34
O
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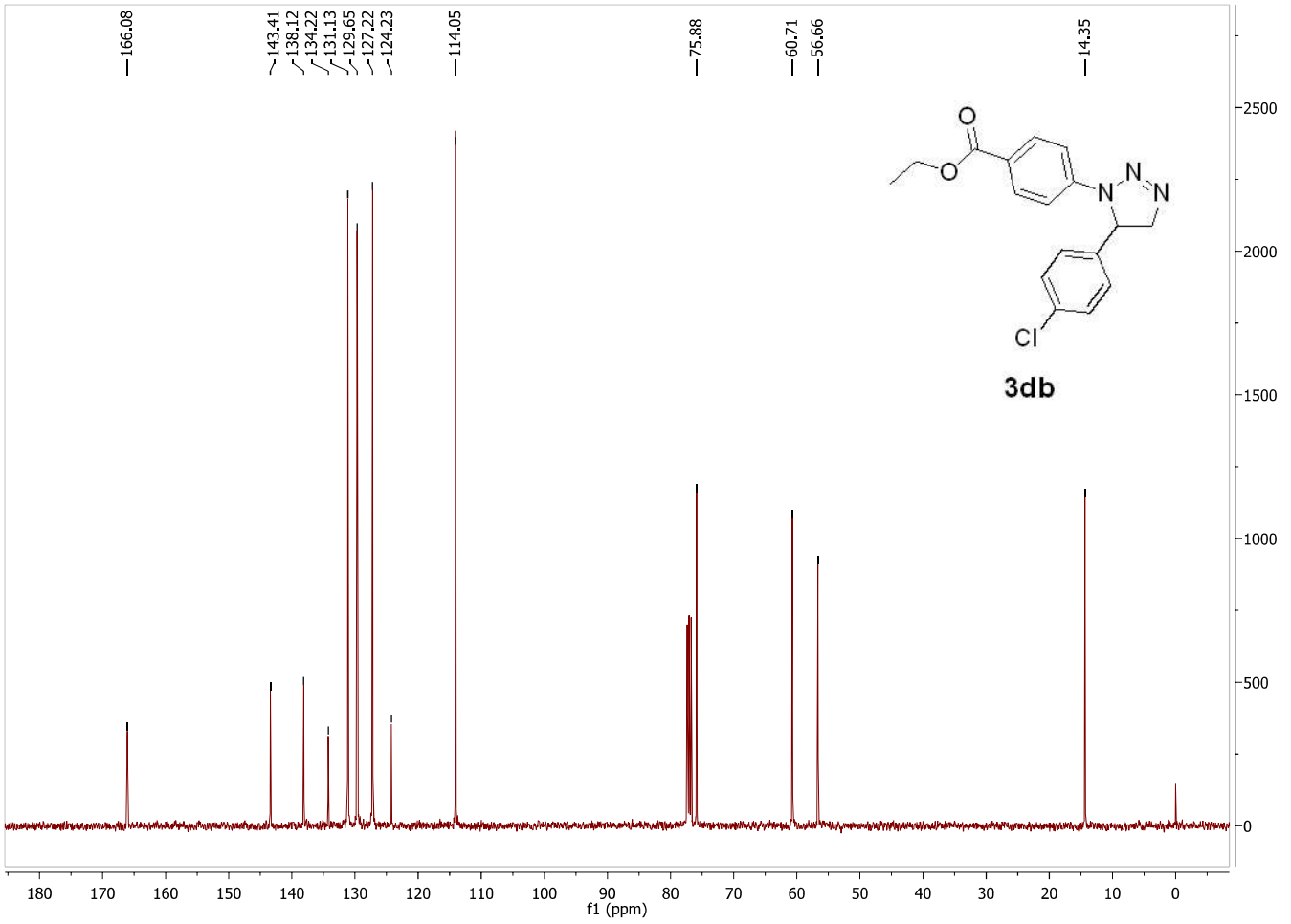
3.00
f1 (ppm)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127.22
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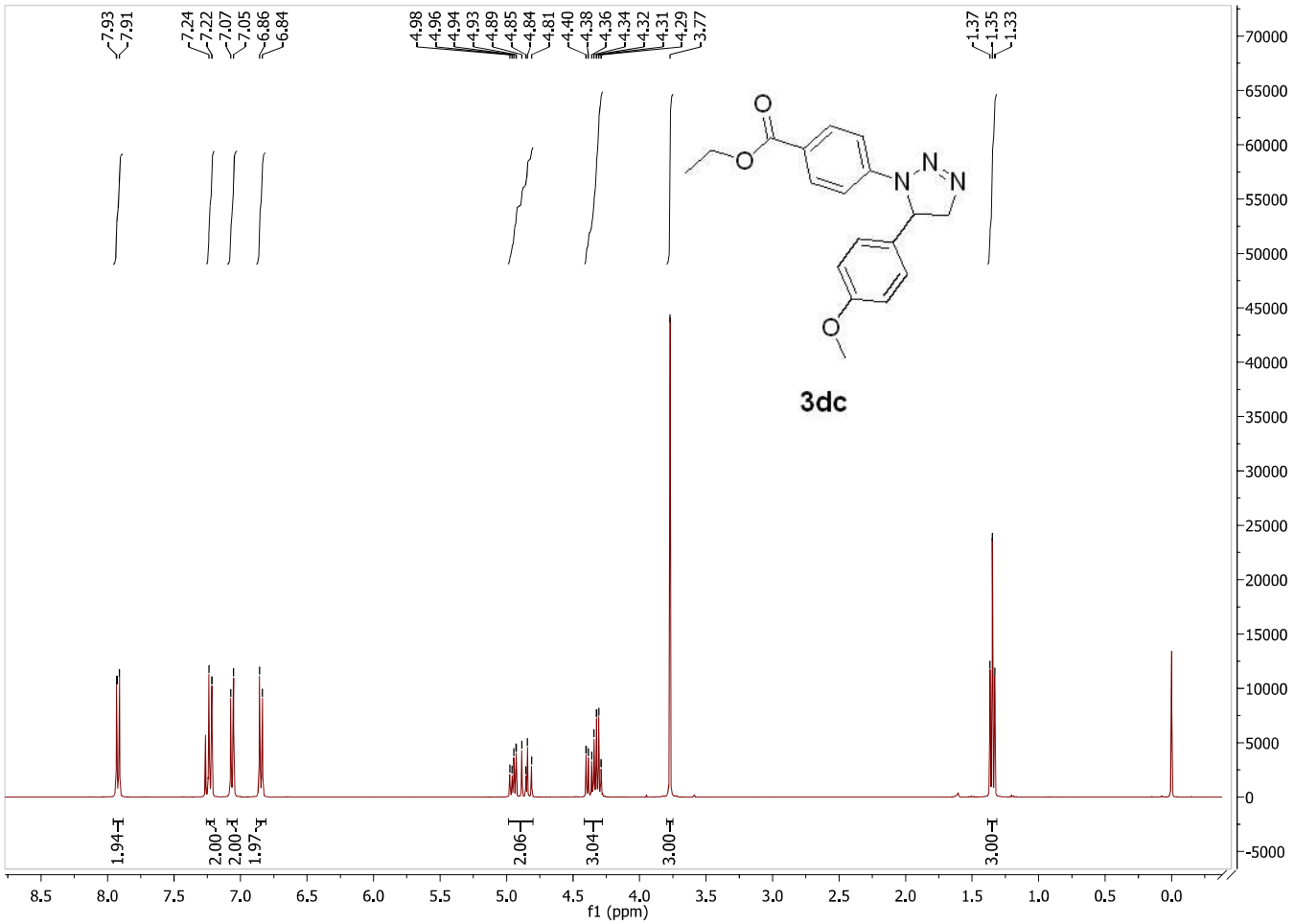
O
N
N
N
Cl
3db
f1 (ppm)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4.89
4.85
4.84
4.81
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4.32
4.31
4.29
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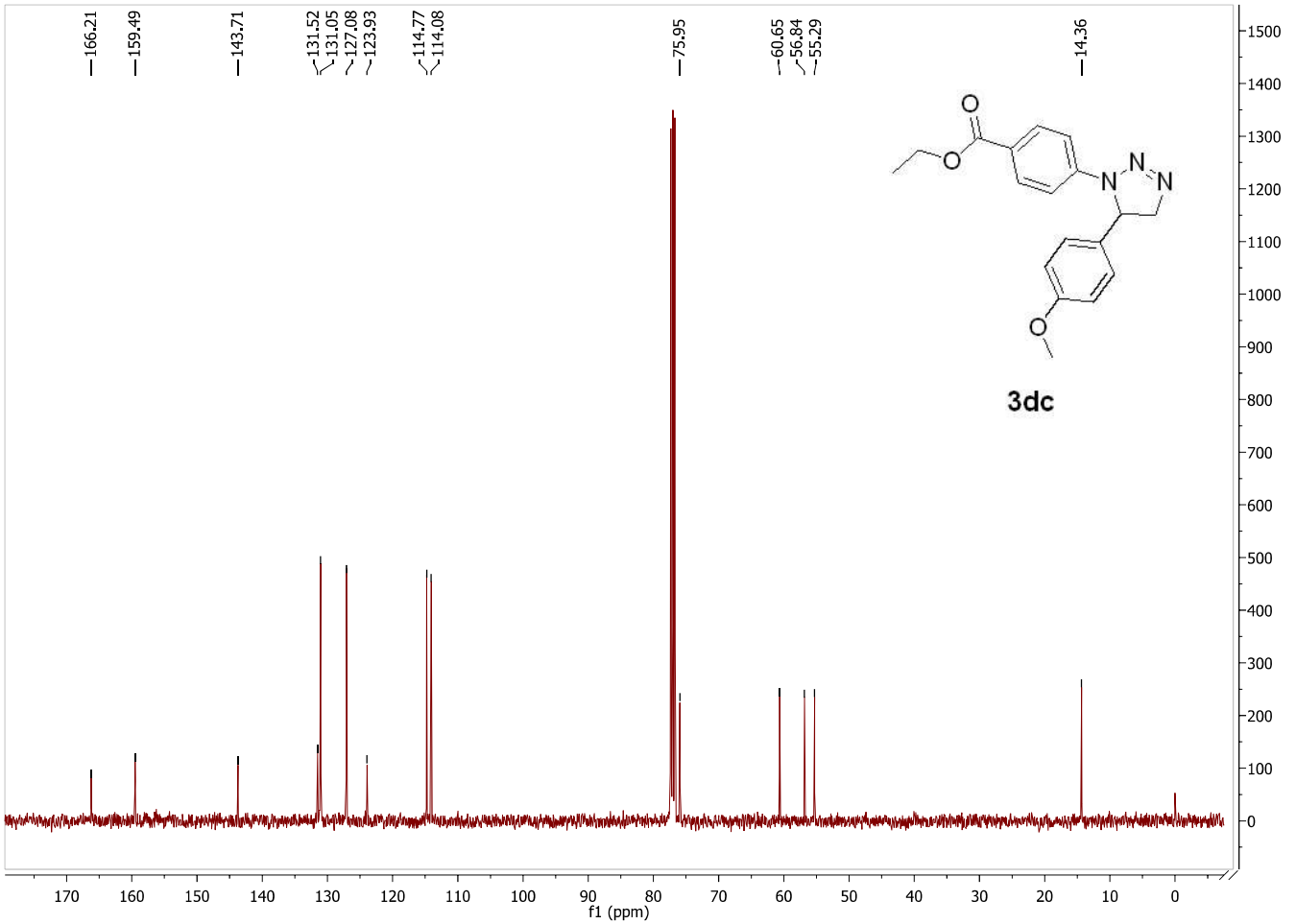
2.06
3.04
3.00
3.00
3dc
f1 (ppm)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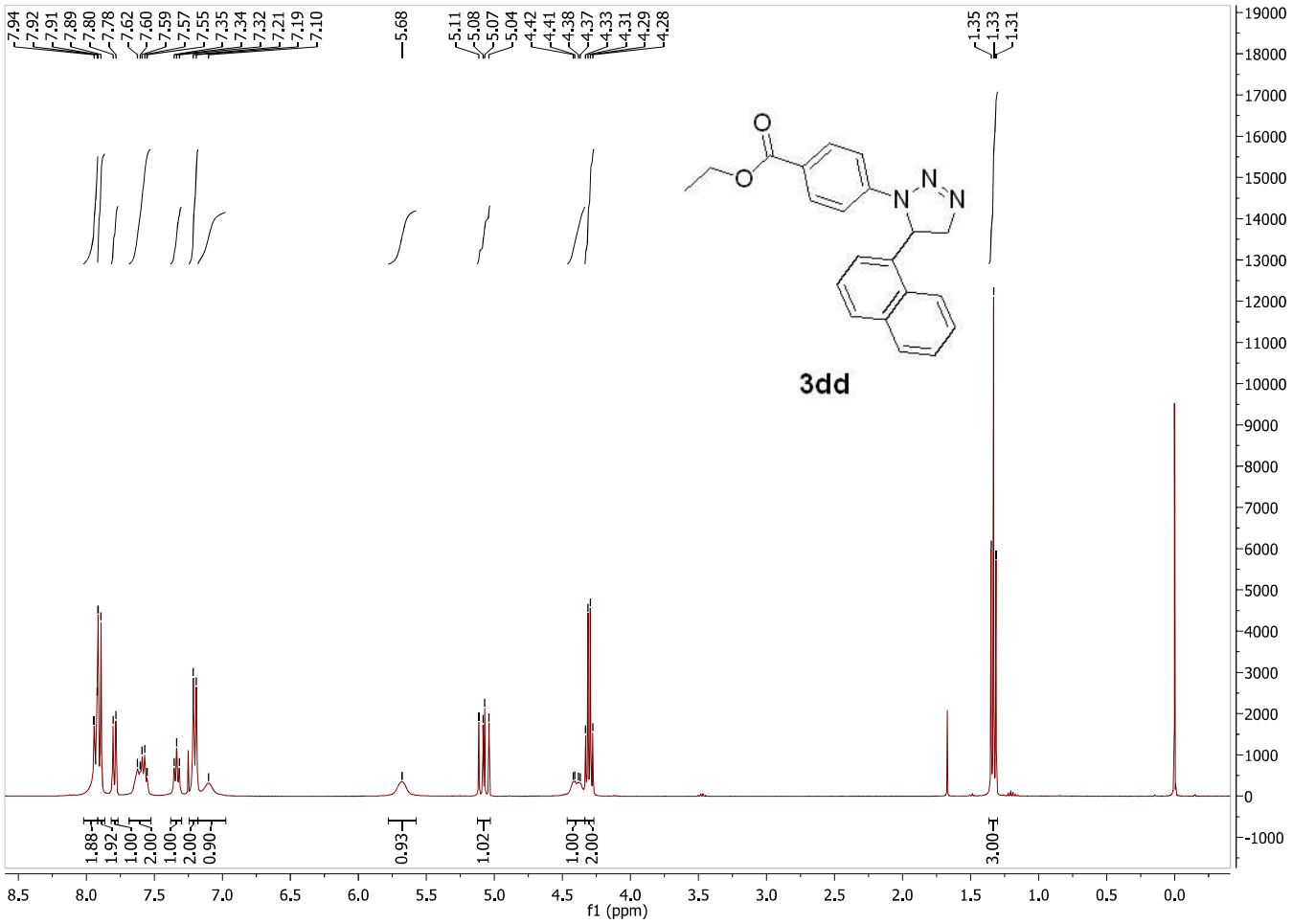
f1 (ppm)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5.07
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4.29
4.28
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1.33
1.31
3dd
1.88
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2.00
0.90
0.93
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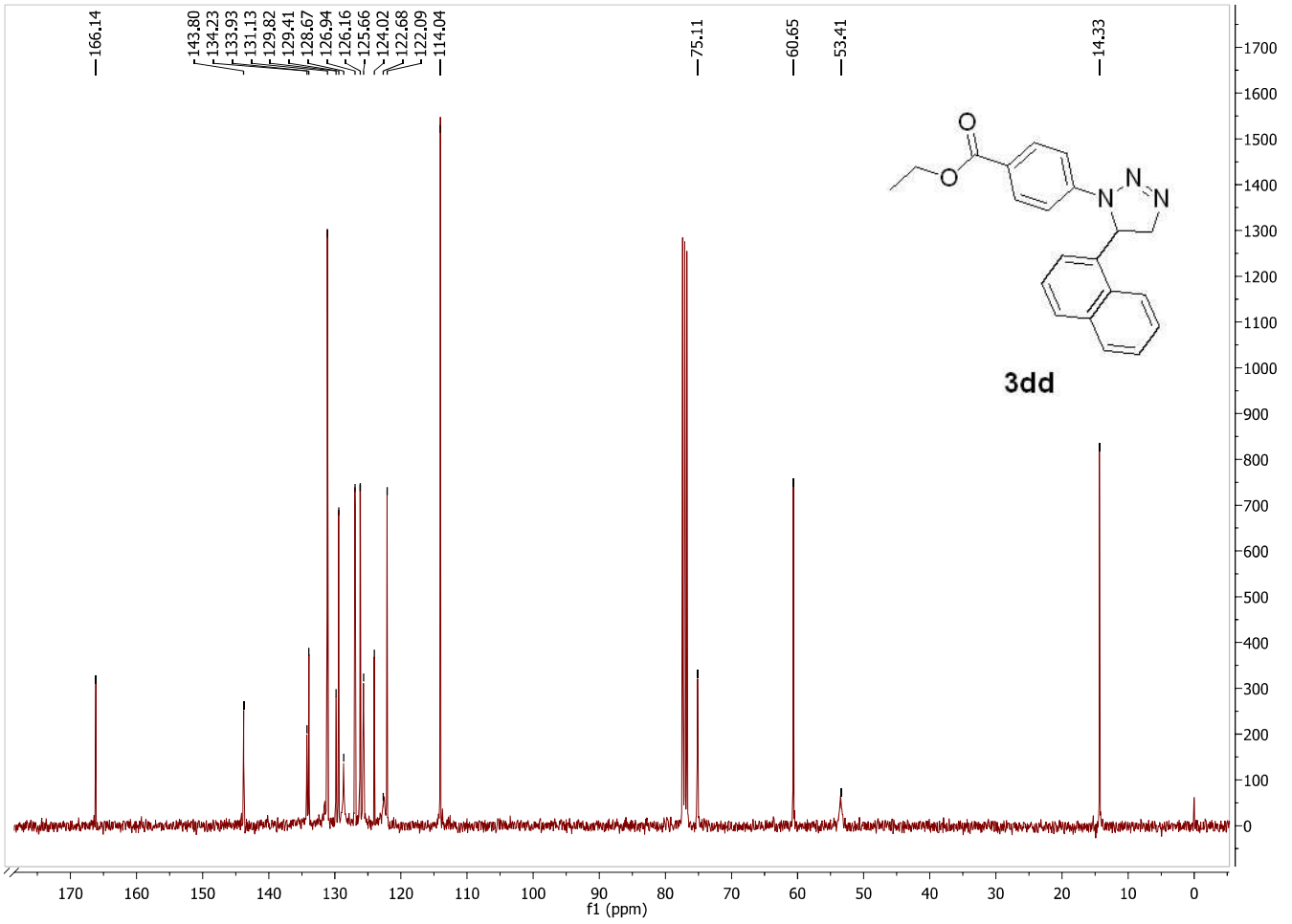
1.00
2.00
3.00
f1 (ppm)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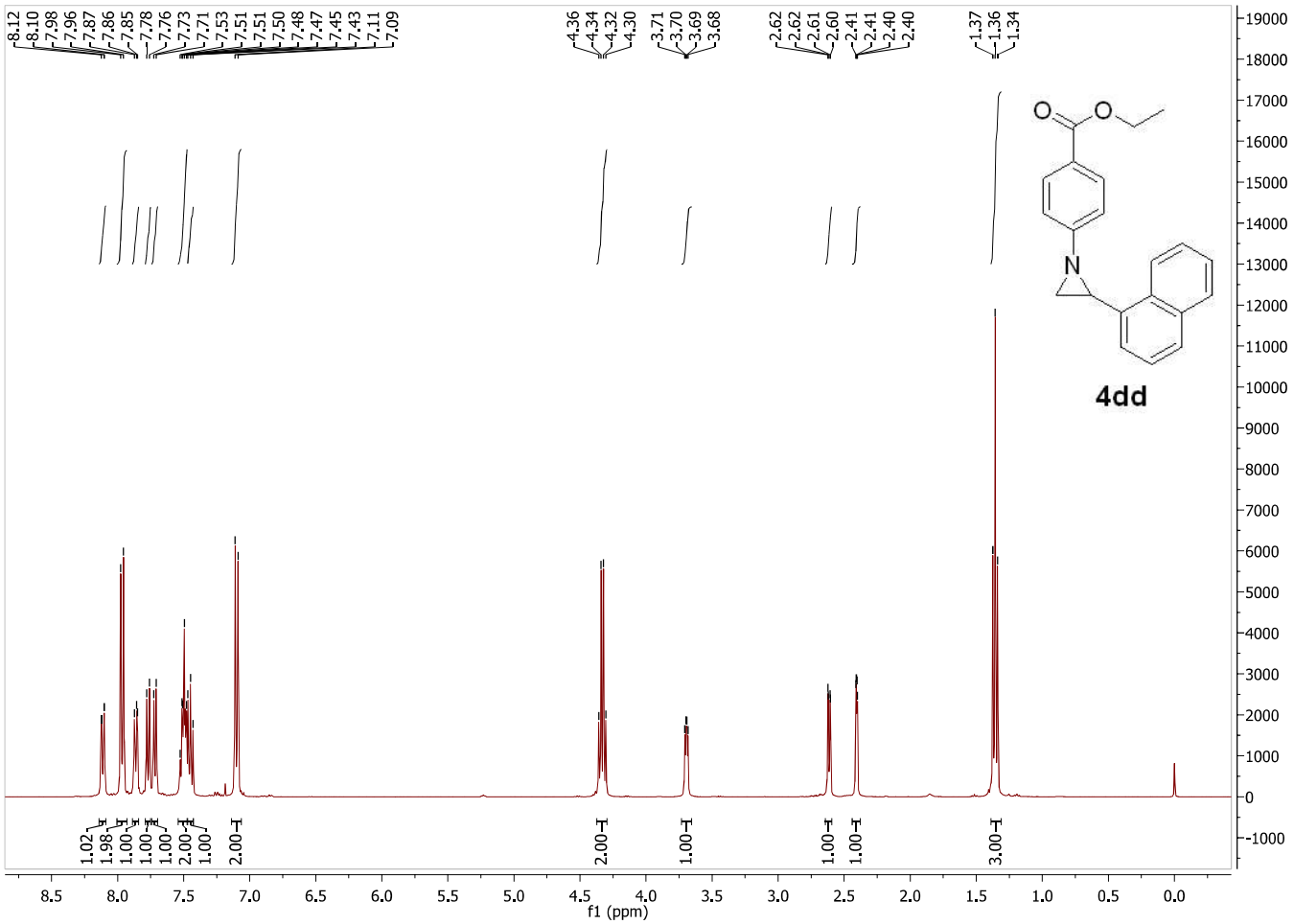
3dd
f1 (ppm)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1.37
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1.34
1.02
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1.00
1.00
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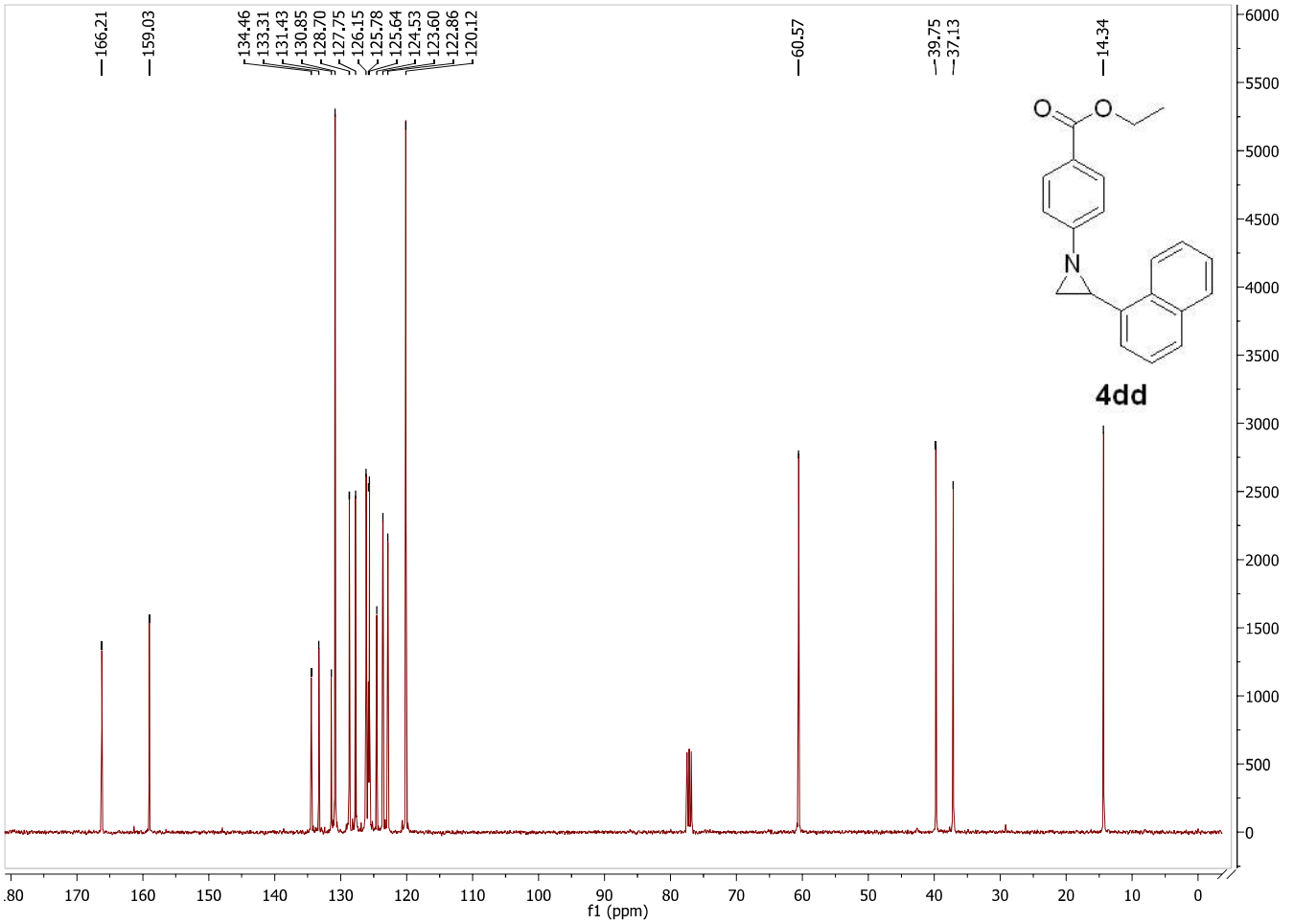
N
4dd
f1 (ppm)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N
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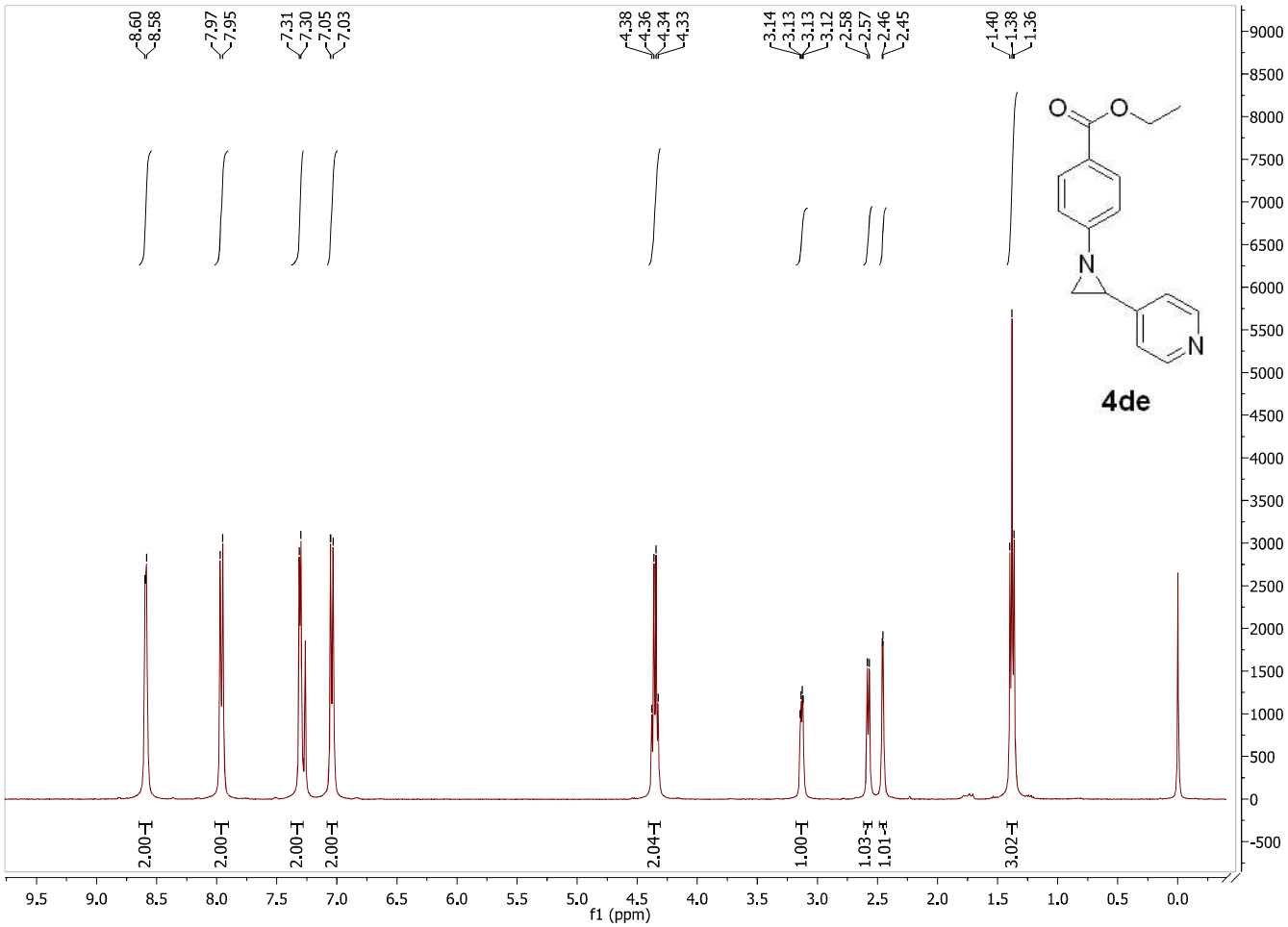
f1 (ppm)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1.00
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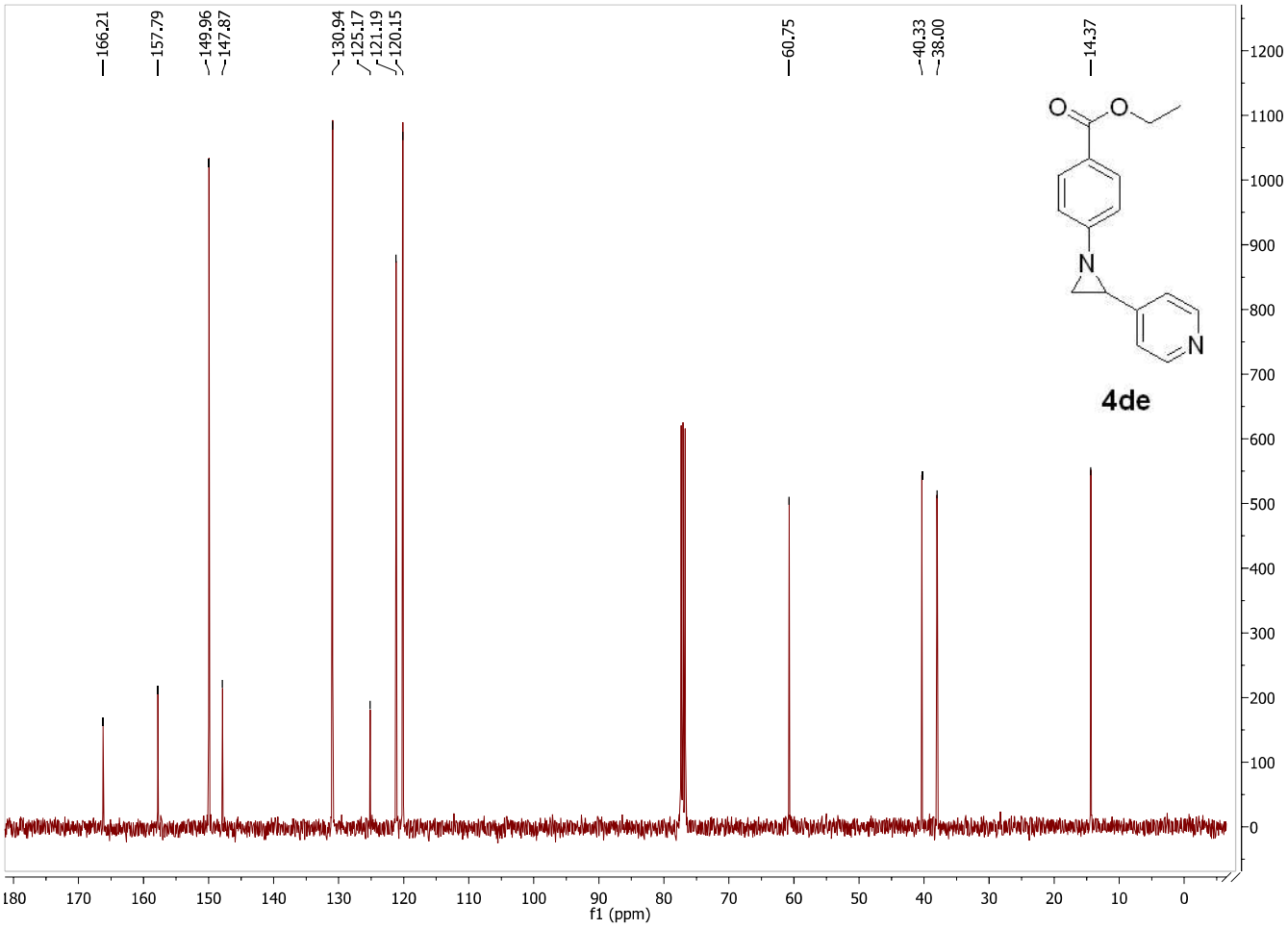
1.01
3.02
f1 (ppm)
4de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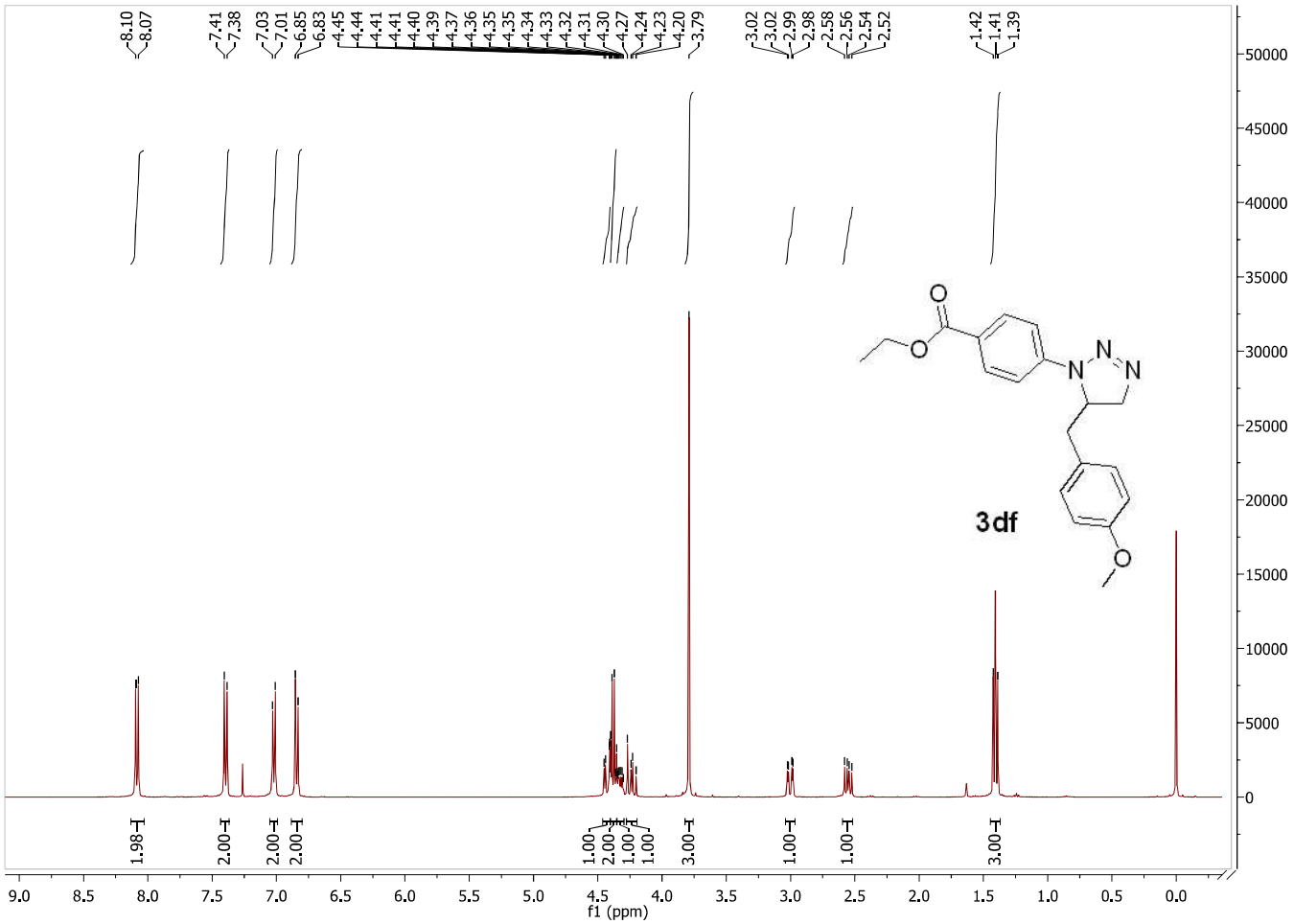
f1 (ppm)
4de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4.37
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4.35
4.35
4.34
4.33
4.32
4.31
4.30
4.27
4.24
4.23
4.20
3.79
3.02
3.02
2.99
2.98
2.58
2.56
2.54
2.52
1.42
1.41
1.39
3df
1.98
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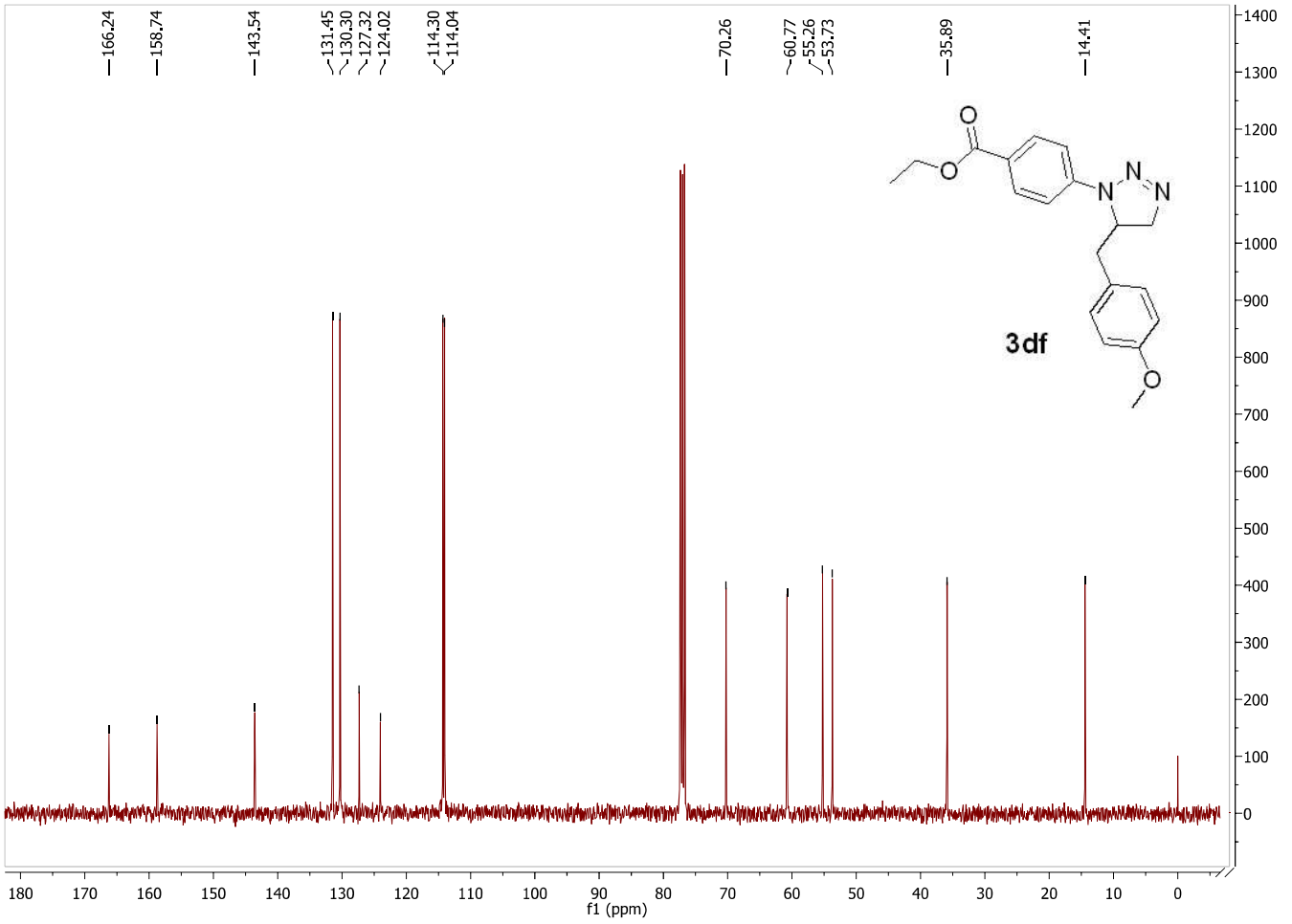
3.00
f1 (ppm)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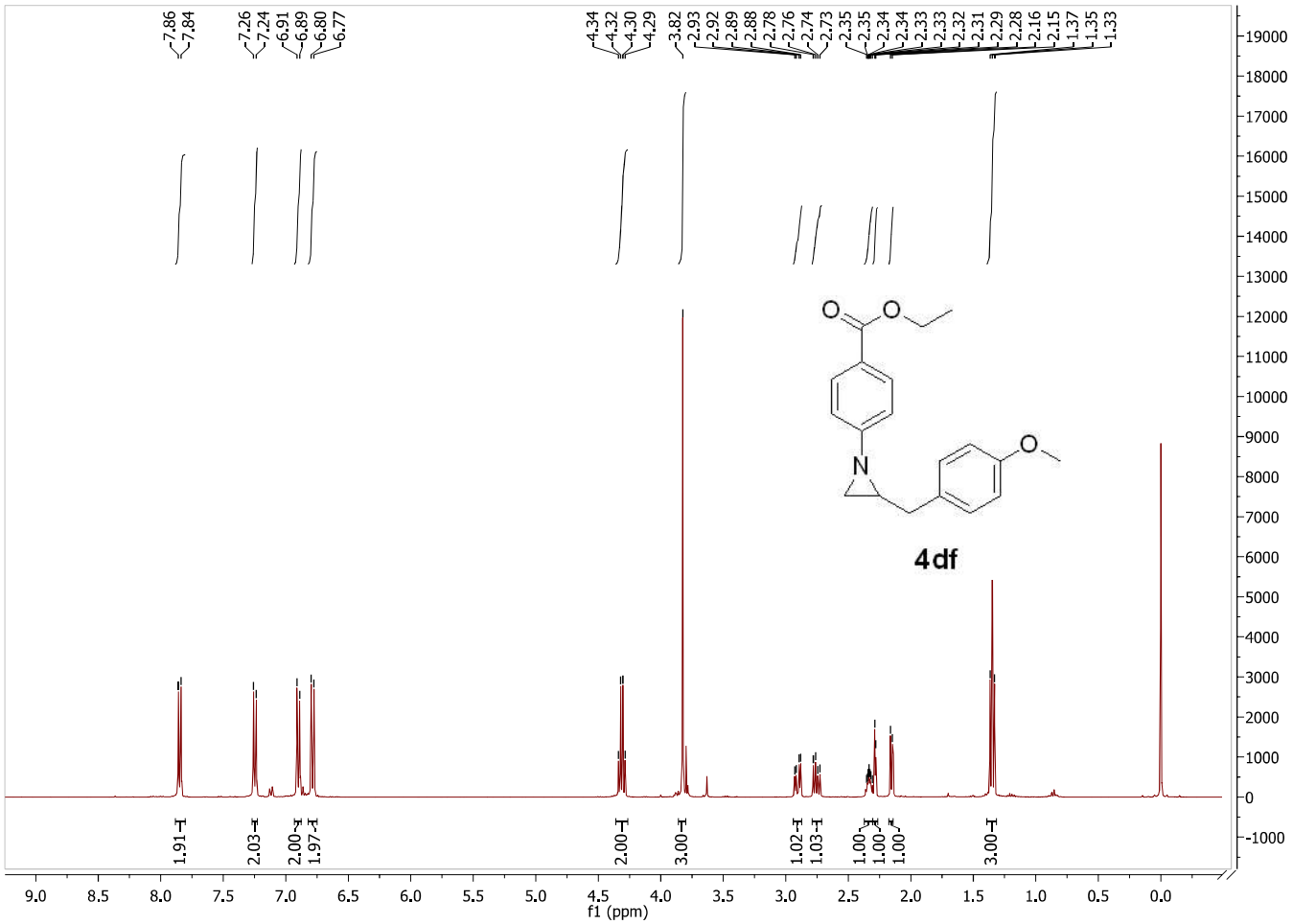
14.41
3df
f1 (ppm)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4.29
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2.92
2.89
2.88
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2.73
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2.35
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2.15
1.37
1.35
1.33
1.91
2.03
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1.00
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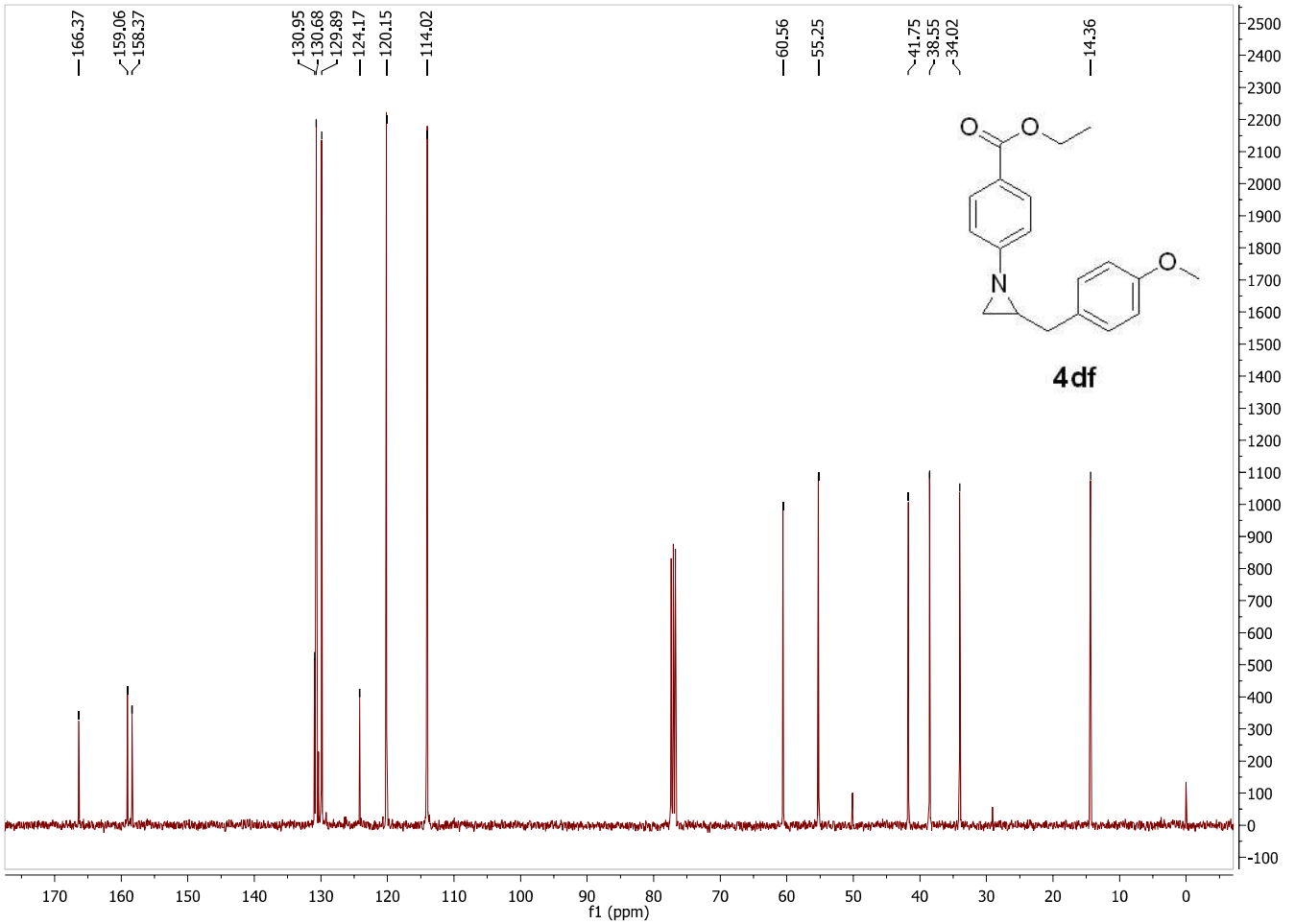
f1 (ppm)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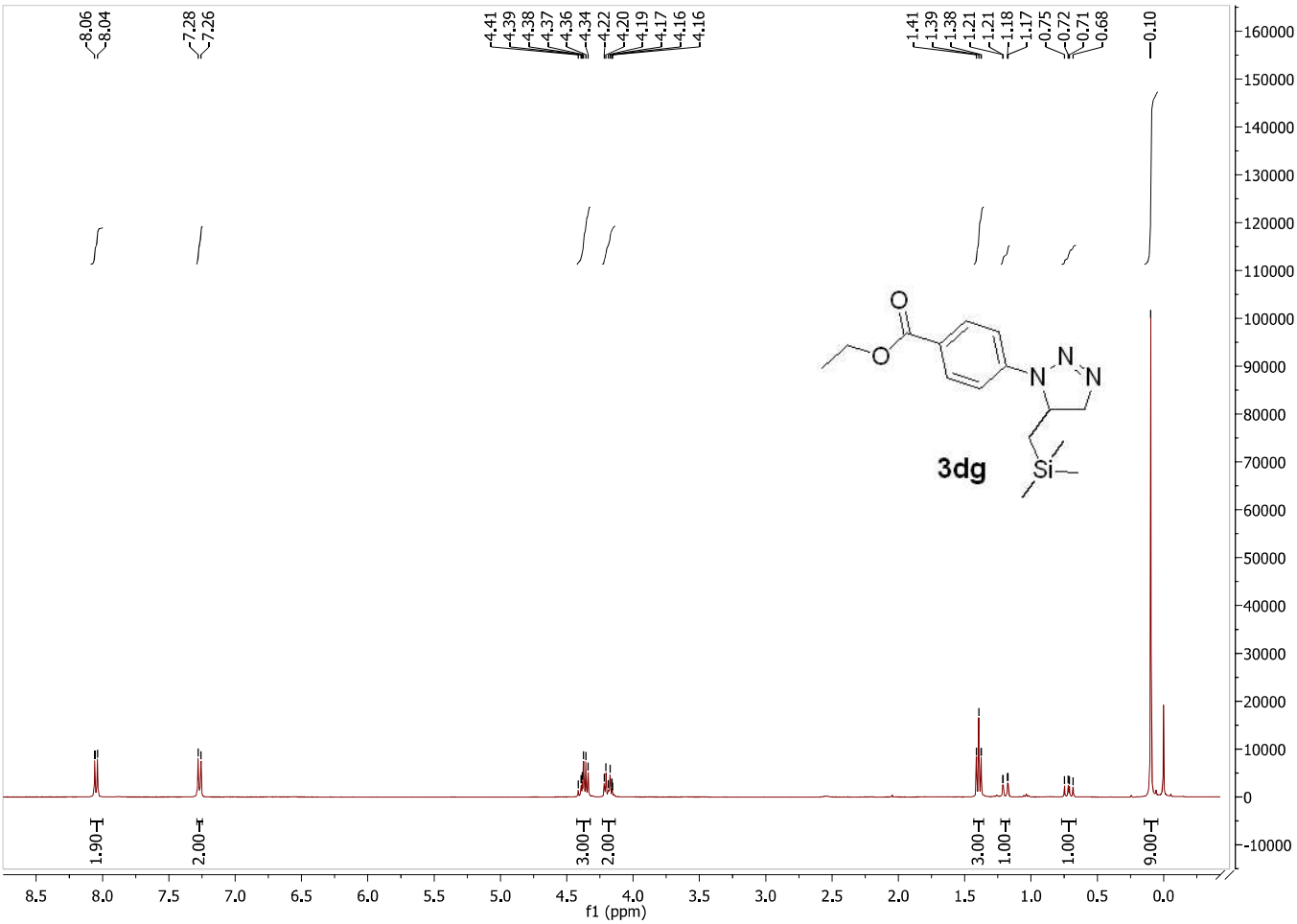
34.02
14.36
4df
f1 (ppm)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4.19
4.17
4.16
4.16
1.41
1.39
1.38
1.21
1.21
1.18
1.17
0.75
0.72
0.71
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0.10
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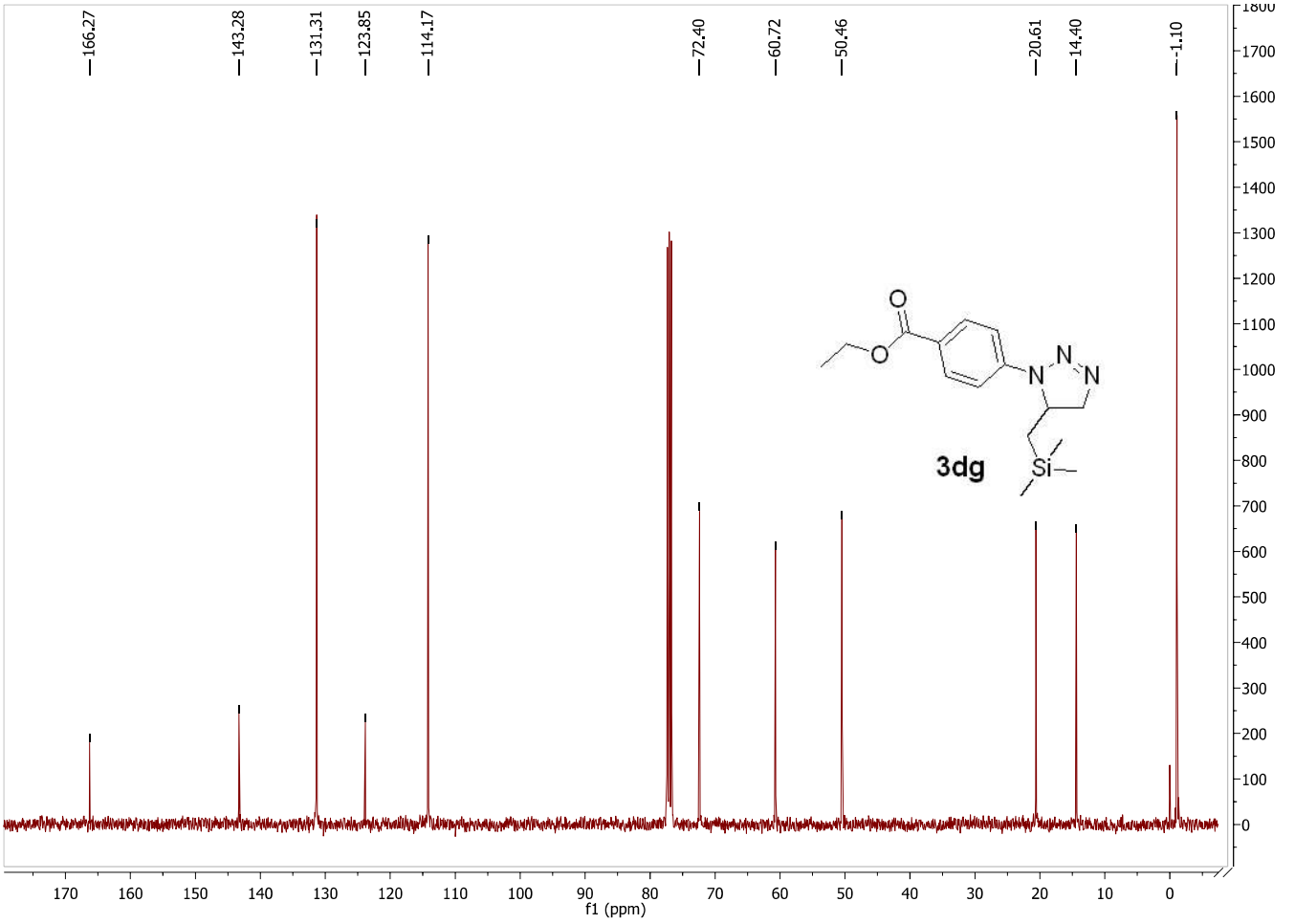
2.00
3.00
1.00
1.00
9.00
3dg
f1 (ppm)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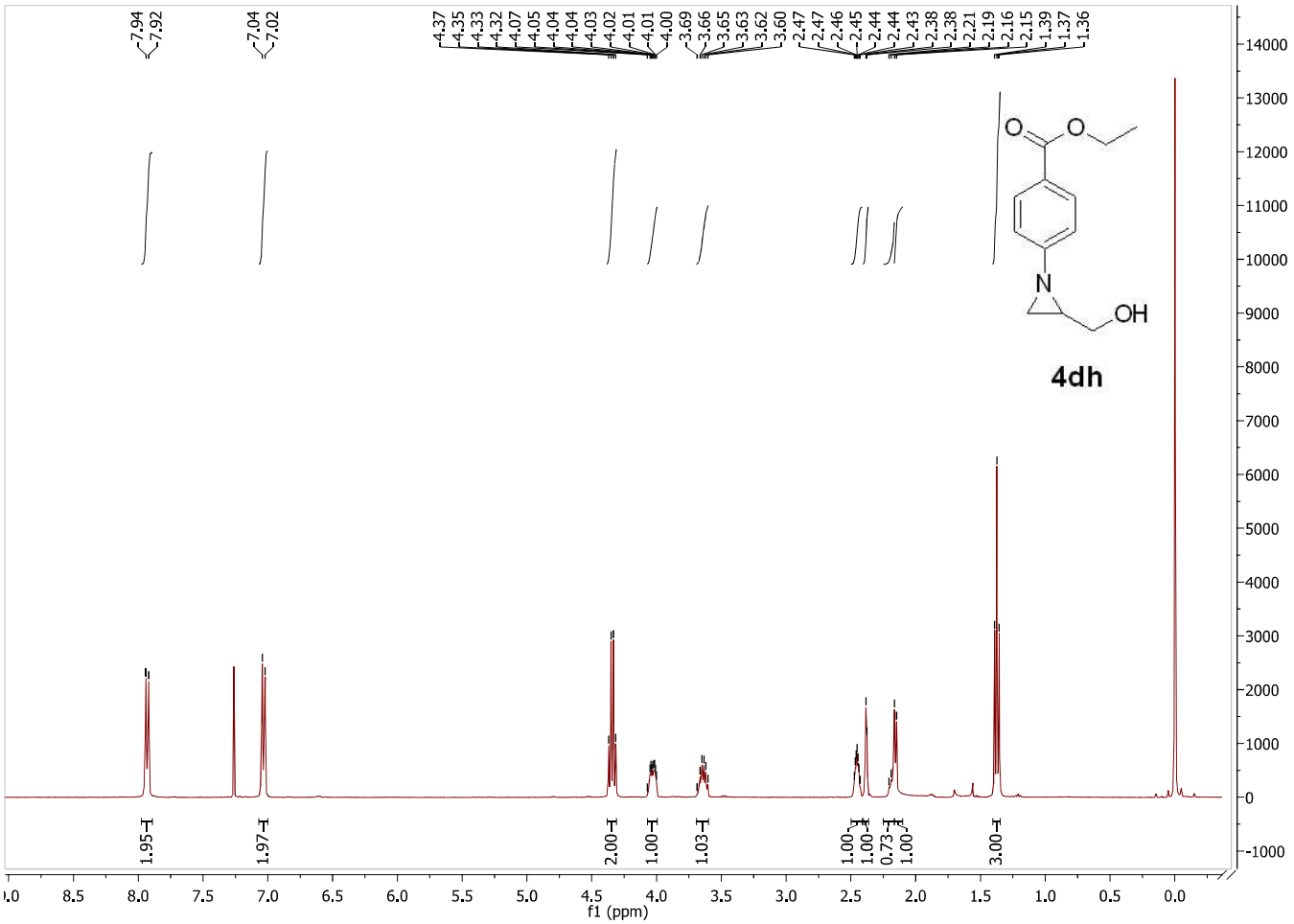
f1 (ppm)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4.04
4.03
4.02
4.01
4.01
4.00
3.69
3.66
3.65
3.63
3.62
3.60
2.47
2.47
2.46
2.45
2.44
2.44
2.43
2.38
2.21
2.19
2.16
2.15
1.39
1.37
1.36
O
O
N
OH
4dh
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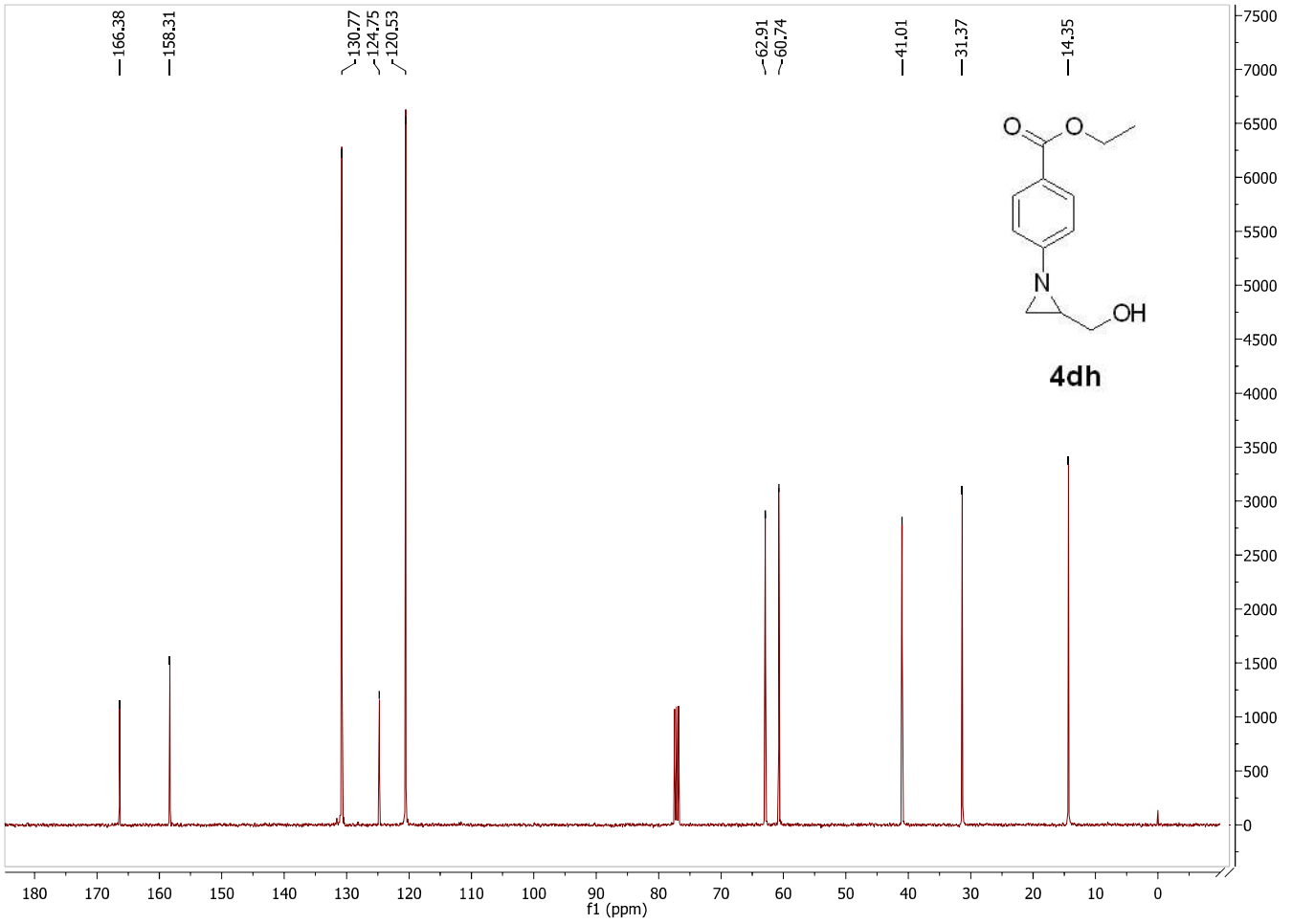
2.00
1.00
1.03
1.00
1.00
0.73
1.00
3.00
f1 (ppm)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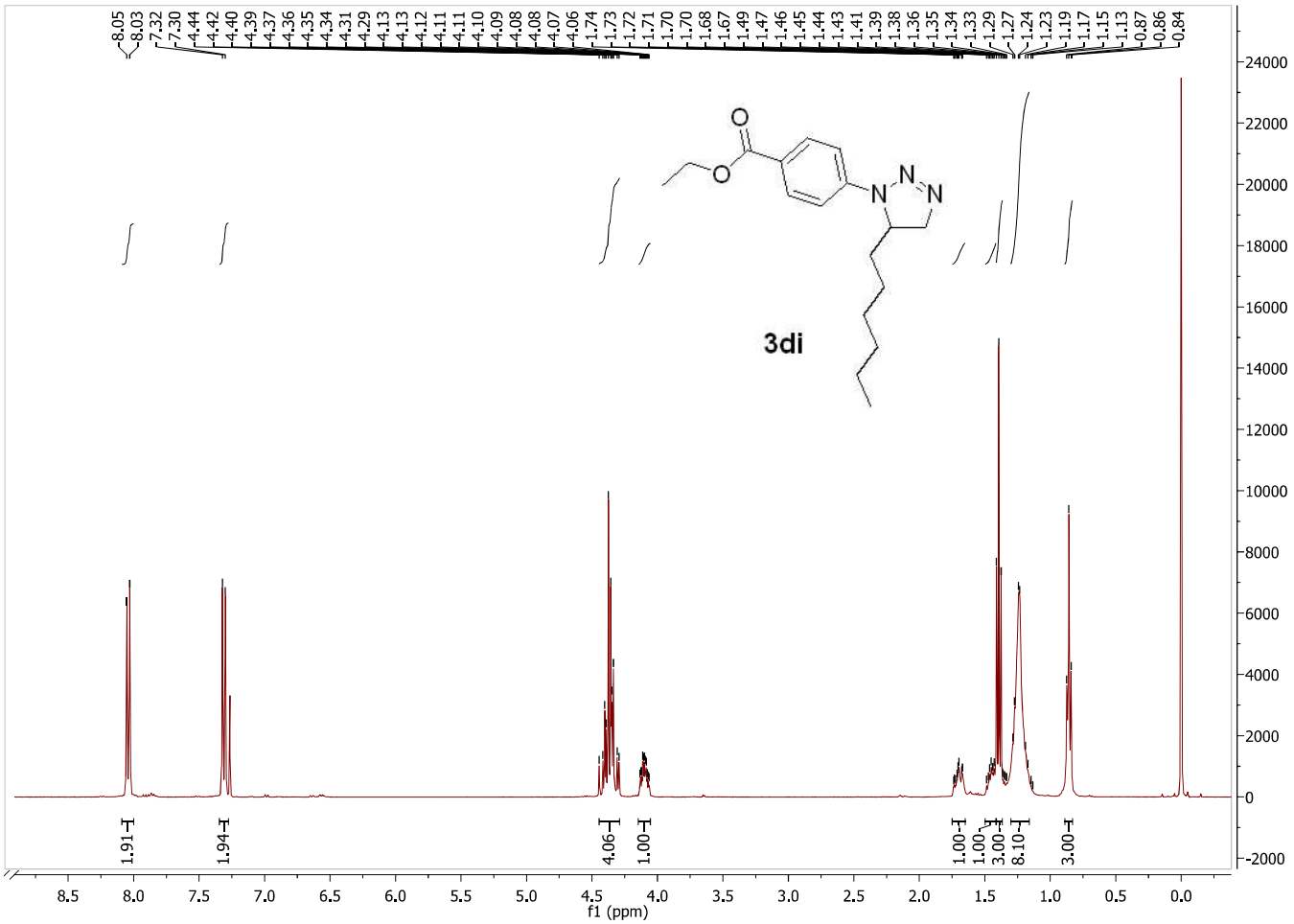
O
O
N
OH
4dh
f1 (ppm)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4.31
4.29
4.13
4.13
4.12
4.11
4.11
4.10
4.09
4.08
4.08
4.07
4.06
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1.72
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1.46
1.45
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1.43
1.41
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1.35
1.34
1.33
1.29
1.27
1.24
1.23
1.19
1.17
1.15
1.13
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0.86
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1.94
4.06
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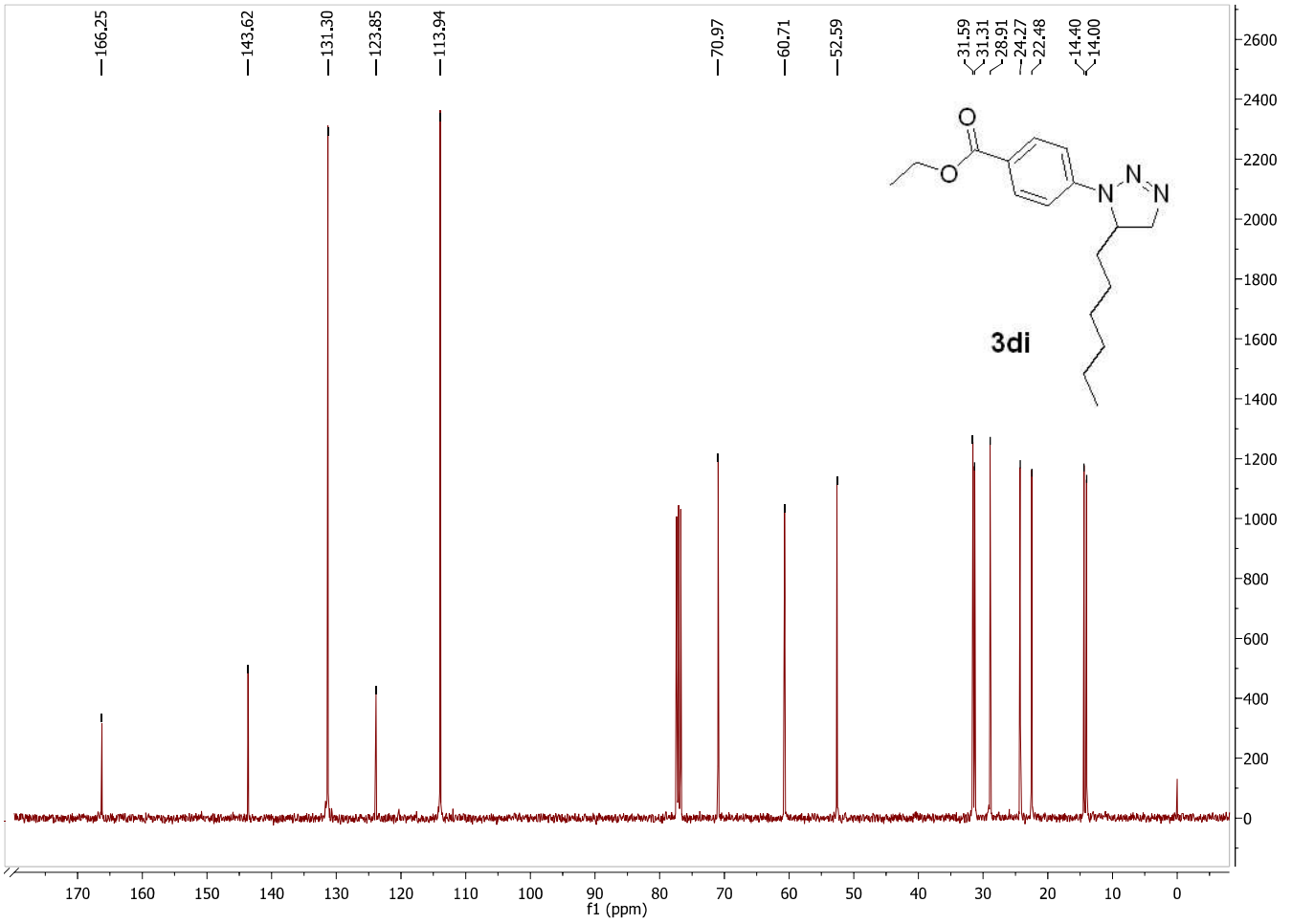
1.00
1.00
3.00
8.10
3.00
f1 (ppm)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24.27
22.48
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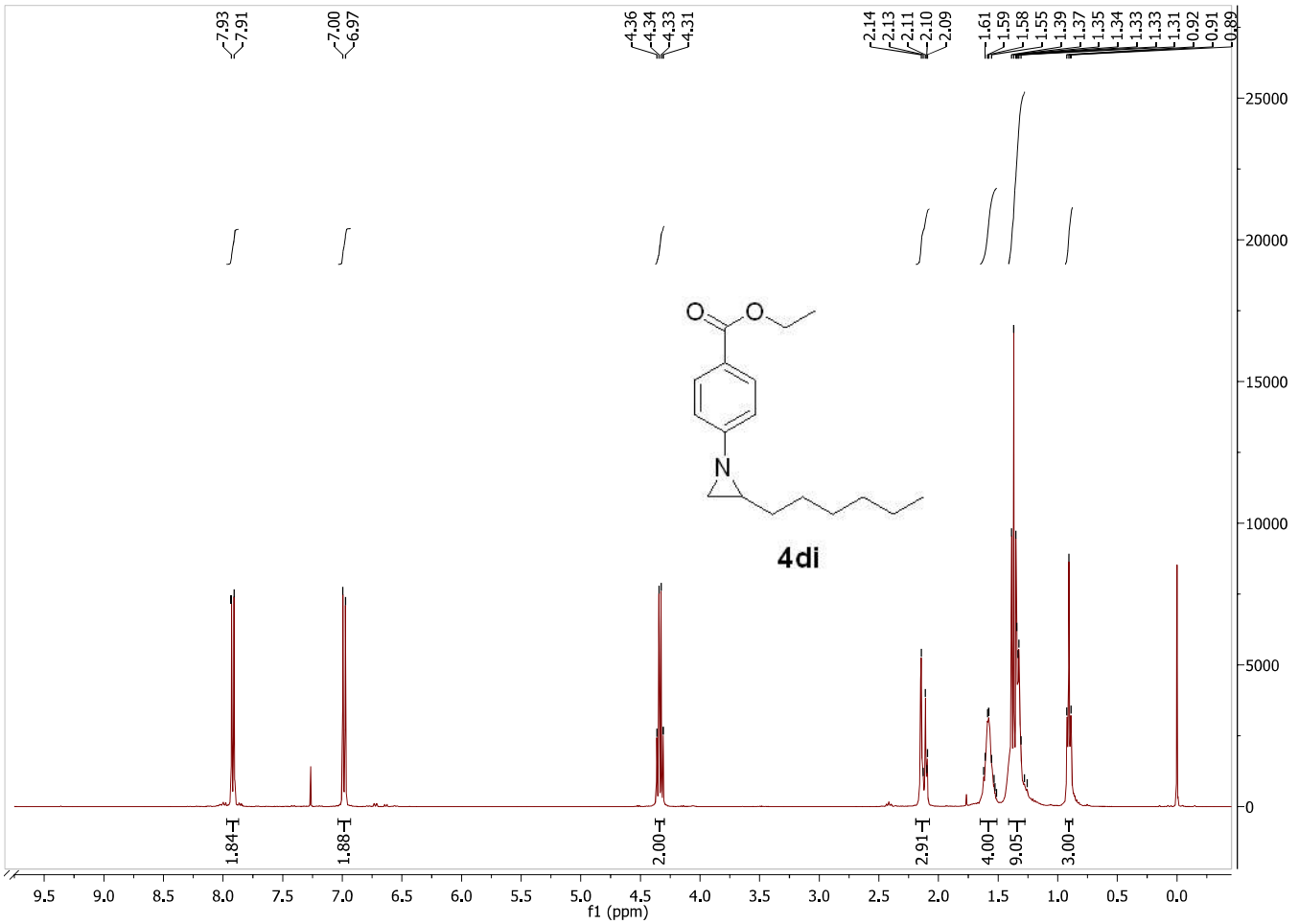
14.00
3di
f1 (ppm)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2.10
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1.61
1.59
1.58
1.55
1.39
1.37
1.35
1.34
1.33
1.33
1.31
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0.91
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O
N
4di
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1.88
2.00
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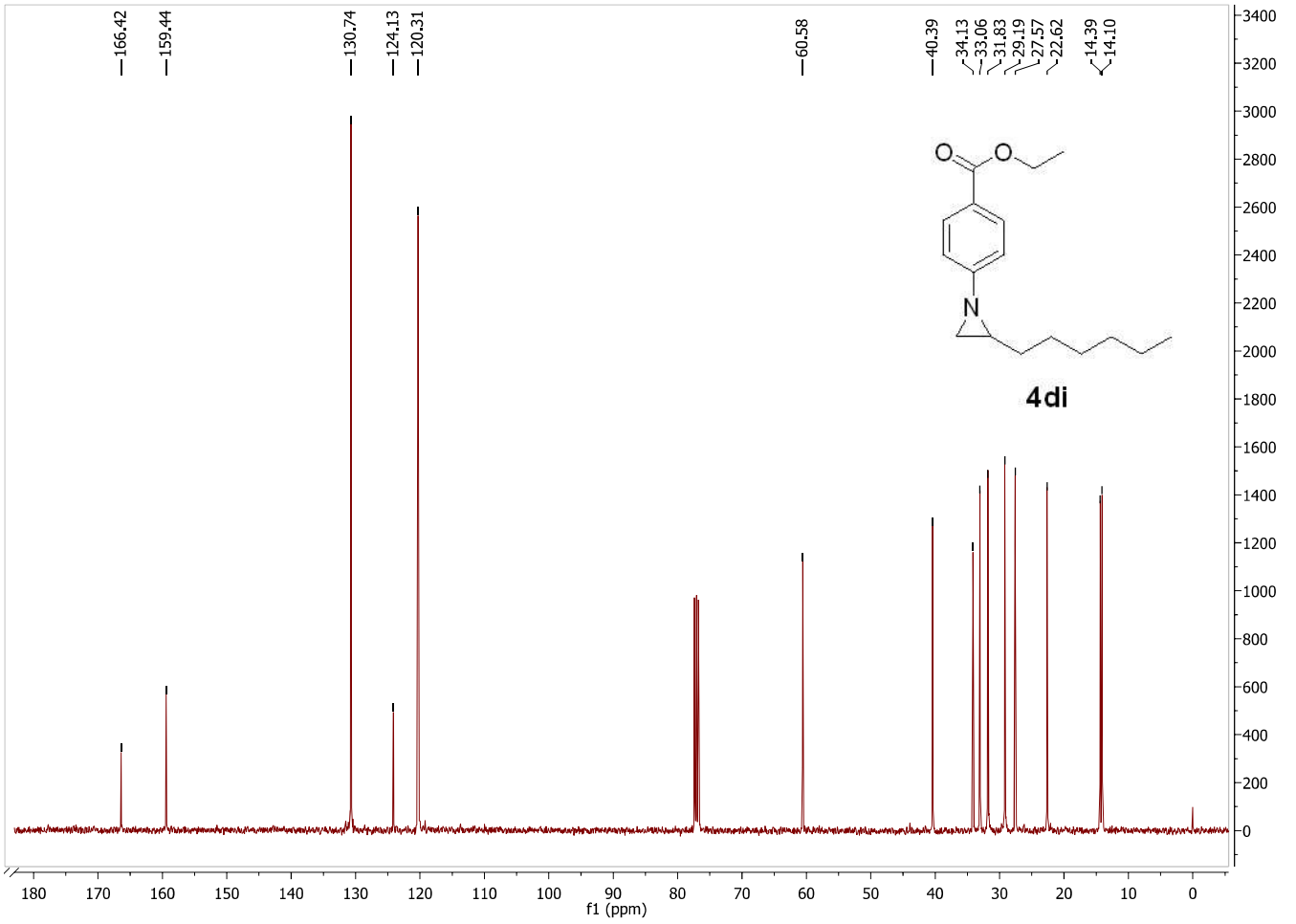
4.00
9.05
3.00
f1 (ppm)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14.10
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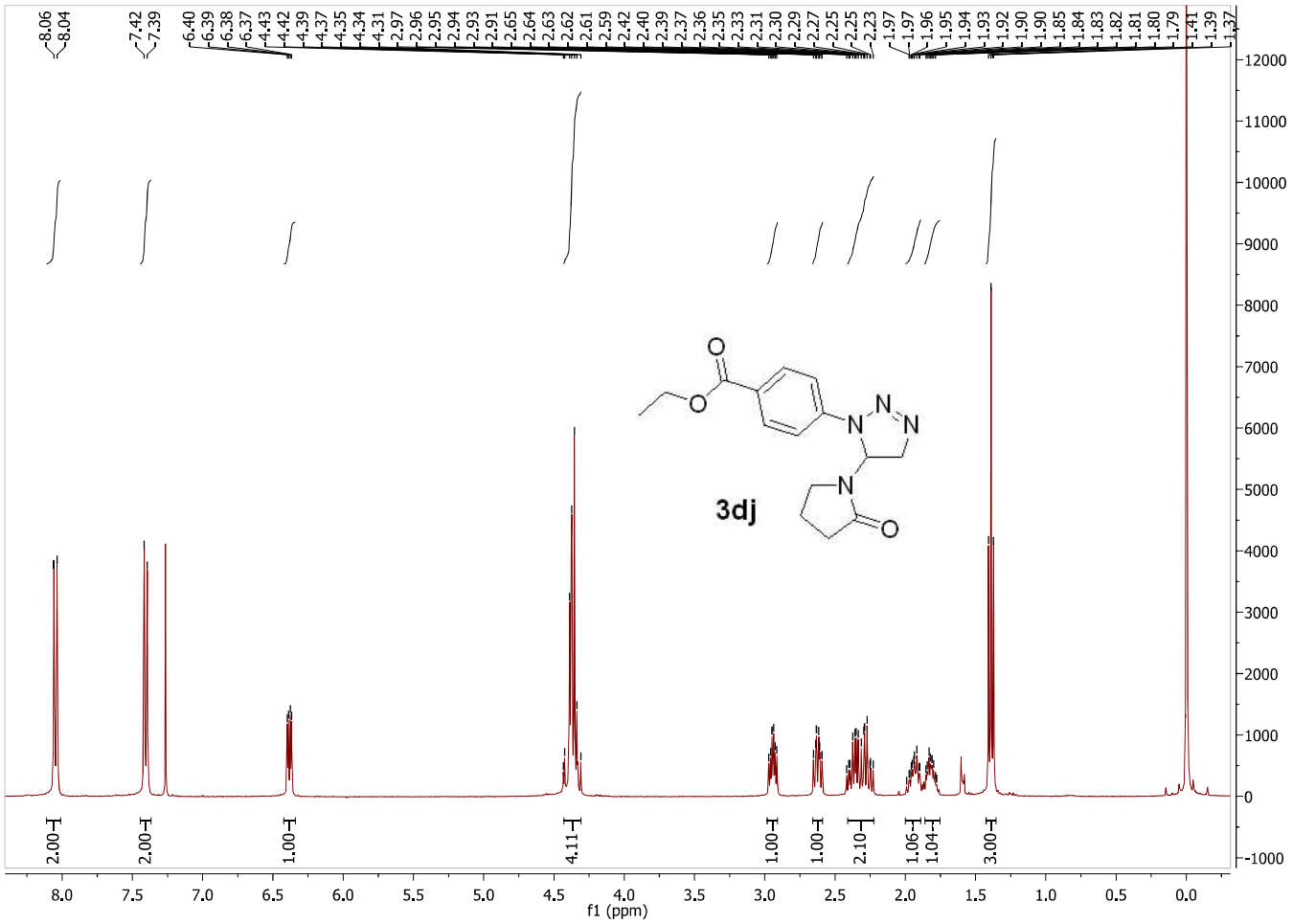
O
N
4di
f1 (ppm)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4.42
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4.34
4.31
2.97
2.96
2.95
2.94
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2.91
2.65
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2.63
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2.36
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2.25
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1.96
1.95
1.94
1.93
1.92
1.90
1.90
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1.84
1.83
1.82
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1.80
1.79
1.41
1.39
1.37
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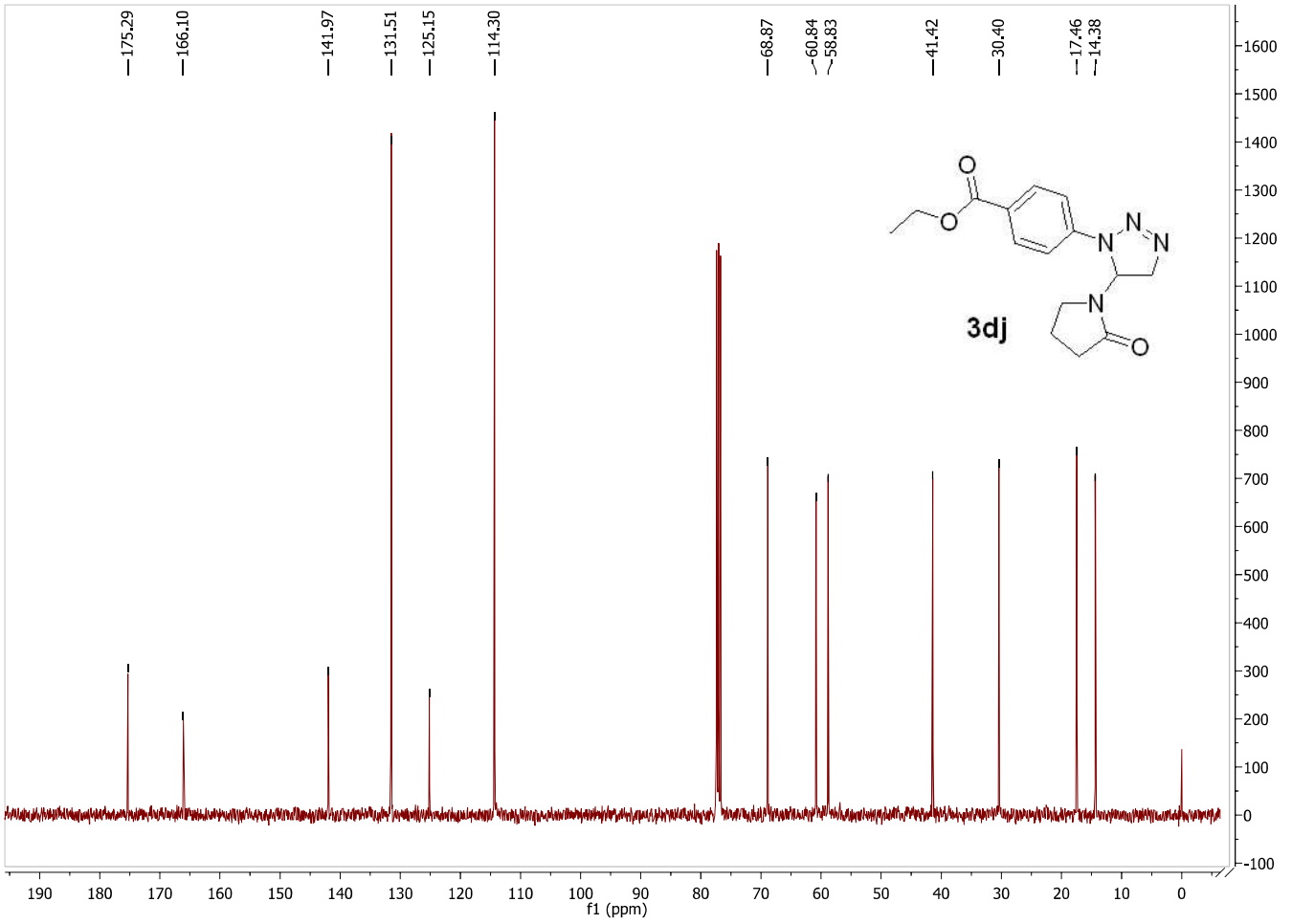
1.00
2.10
1.06
1.04
3.00
f1 (ppm)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17.46
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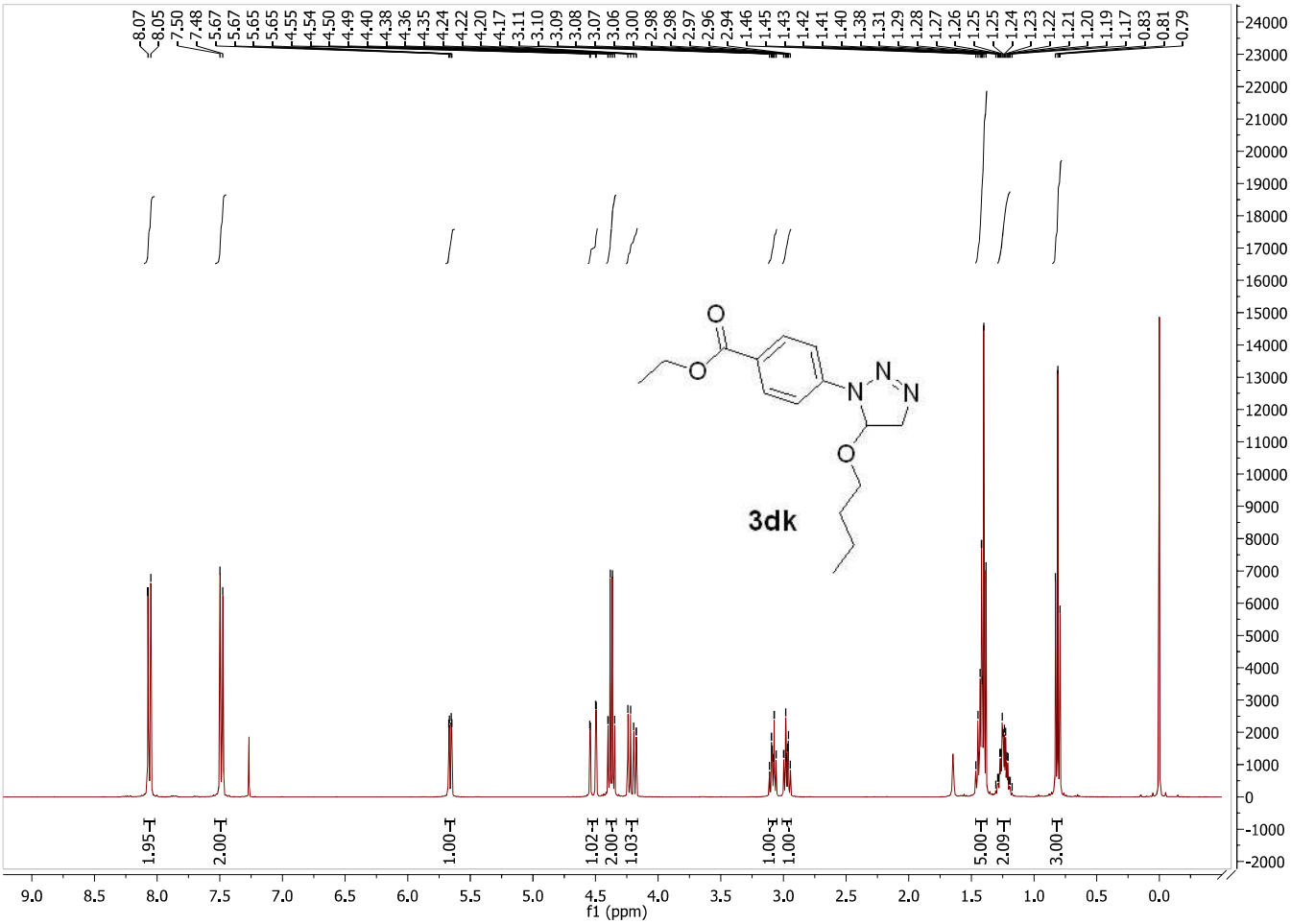
3dj
f1 (ppm)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4.38
4.36
4.35
4.24
4.22
4.20
4.17
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3.10
3.09
3.08
3.07
3.06
3.00
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2.98
2.97
2.96
2.94
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1.45
1.43
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1.41
1.40
1.38
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1.29
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1.26
1.25
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1.24
1.23
1.22
1.21
1.20
1.19
1.17
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0.81
0.79
3dk
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1.03
1.00
1.00
5.00
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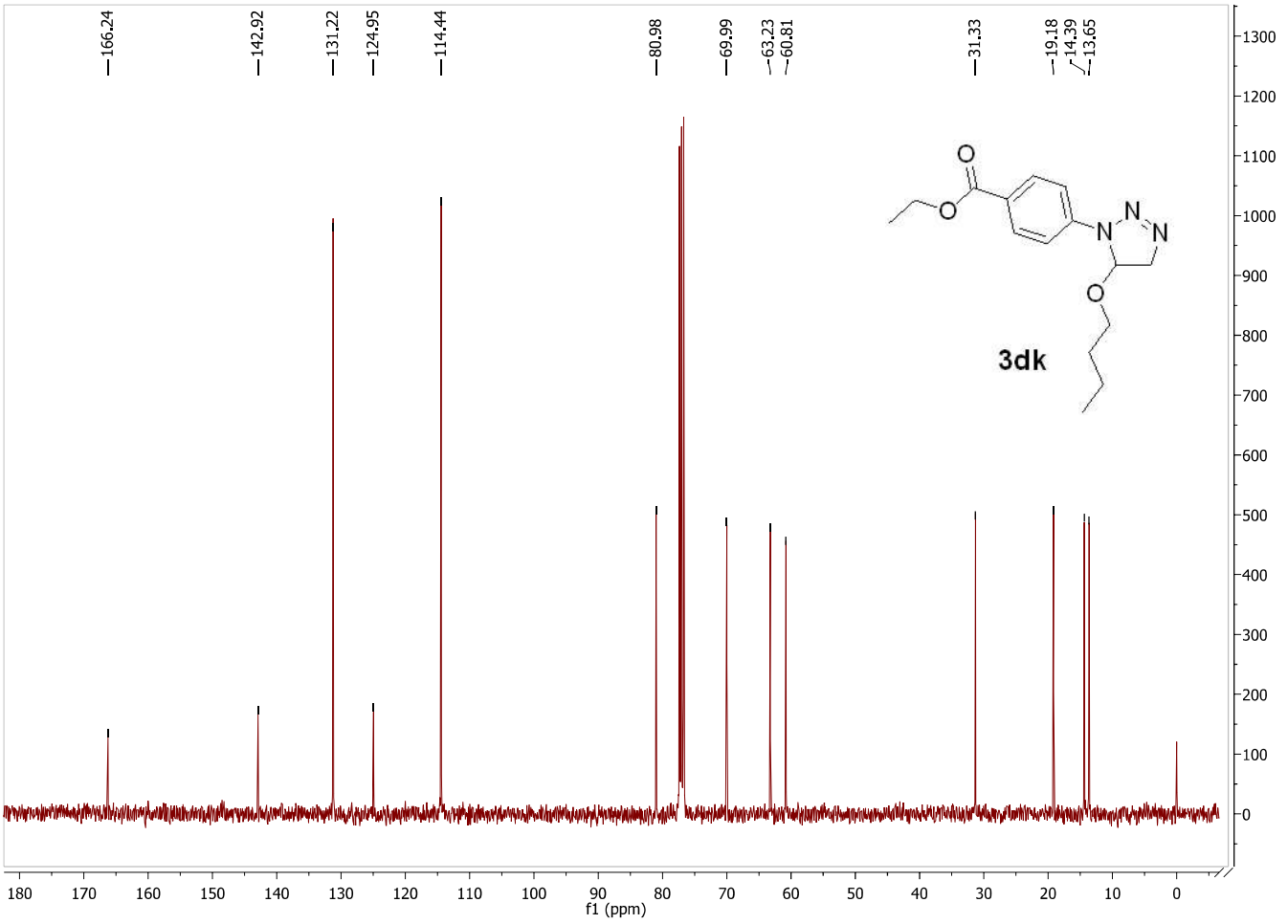
3.00
f1 (ppm)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19.18
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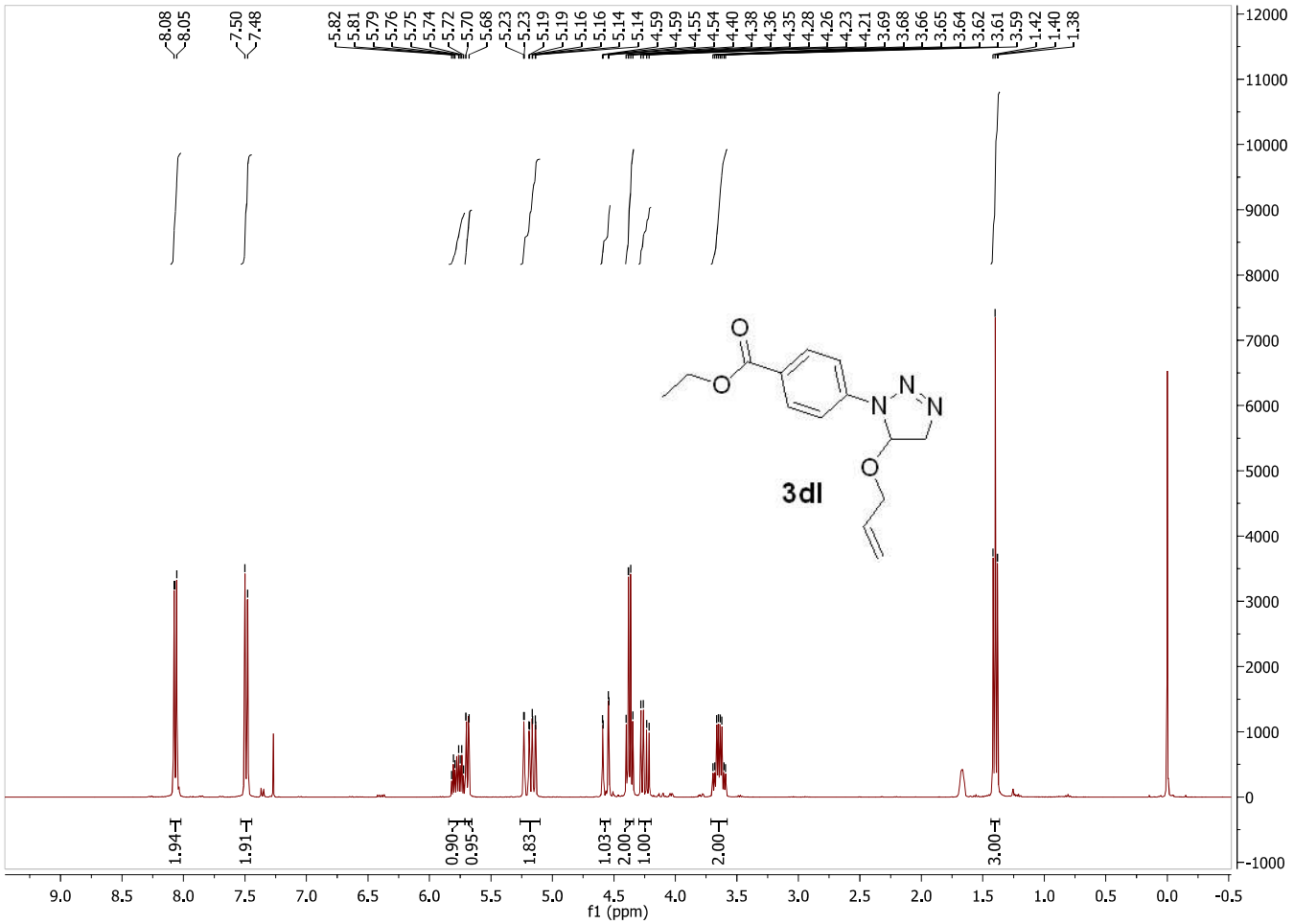
13.65
3dk
f1 (ppm)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5.23
5.19
5.19
5.16
5.16
5.14
5.14
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4.21
3.69
3.68
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3.65
3.64
3.62
3.61
3.59
1.42
1.40
1.38
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1.83
1.03
2.00
1.00
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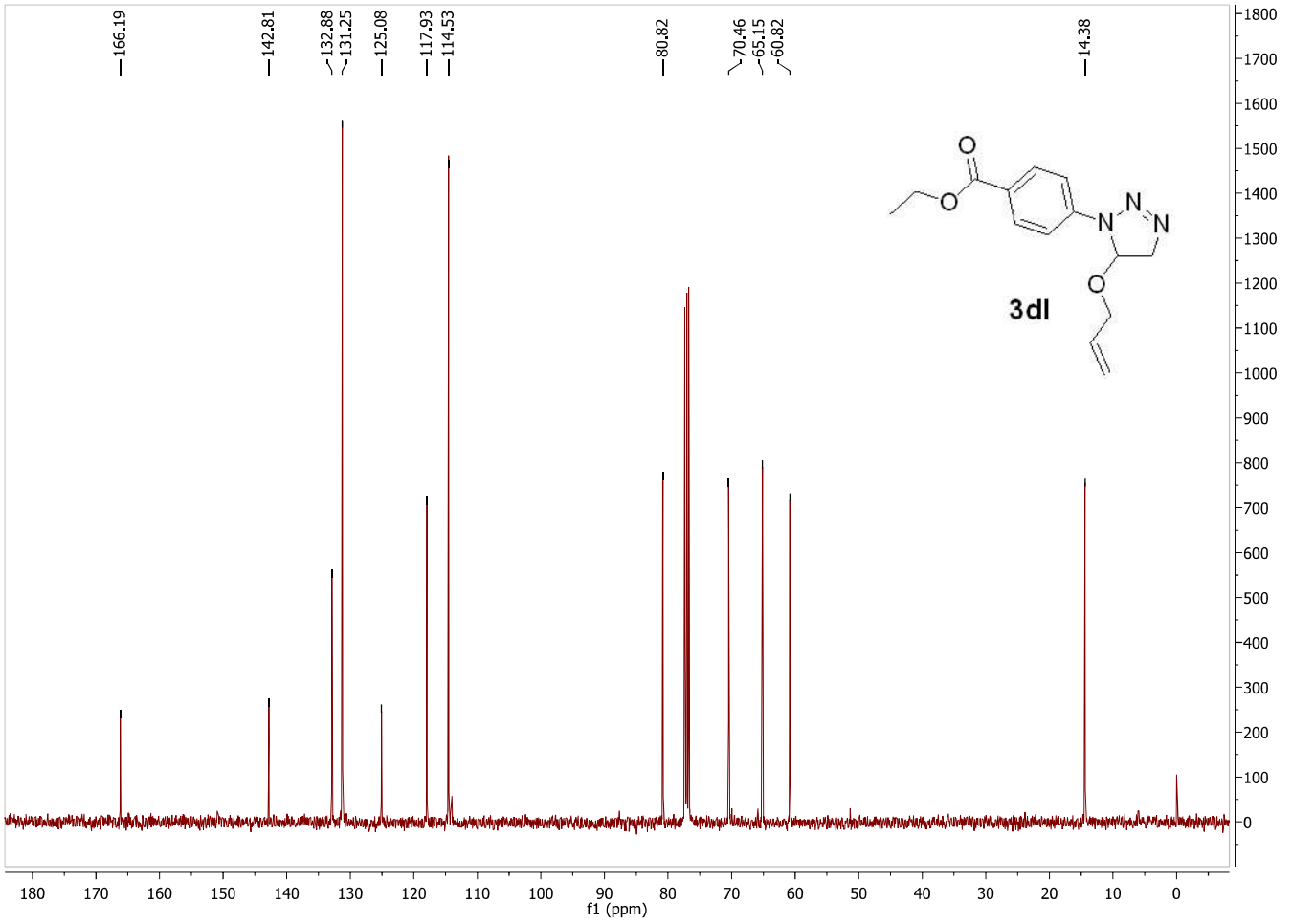
3.00
f1 (ppm)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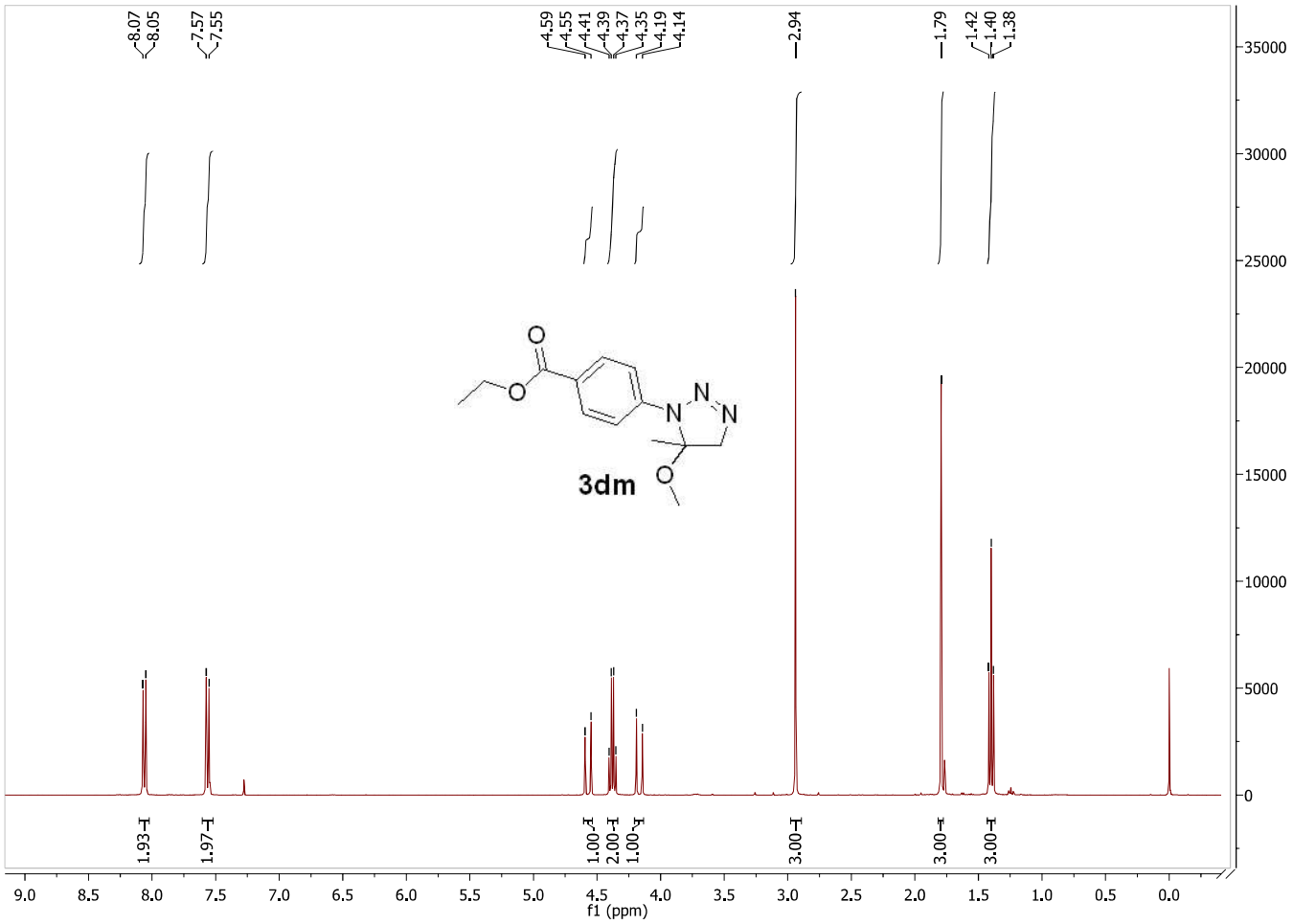
65.15
60.82
14.38
3dl
f1 (ppm)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4.35
4.19
4.14
2.94
1.79
1.42
1.40
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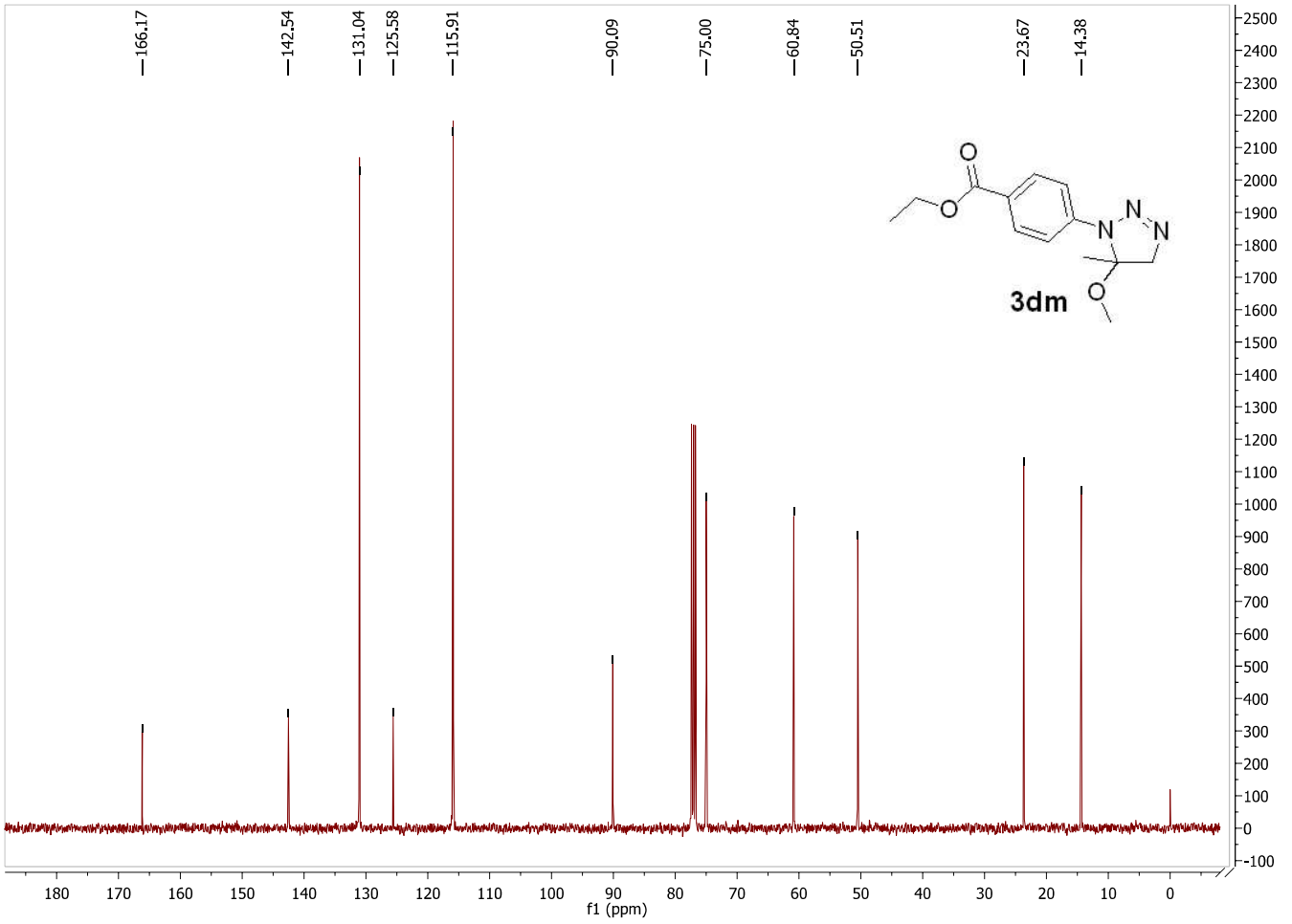
1.97
1.00
2.00
1.00
3.00
3.00
3.00
f1 (ppm)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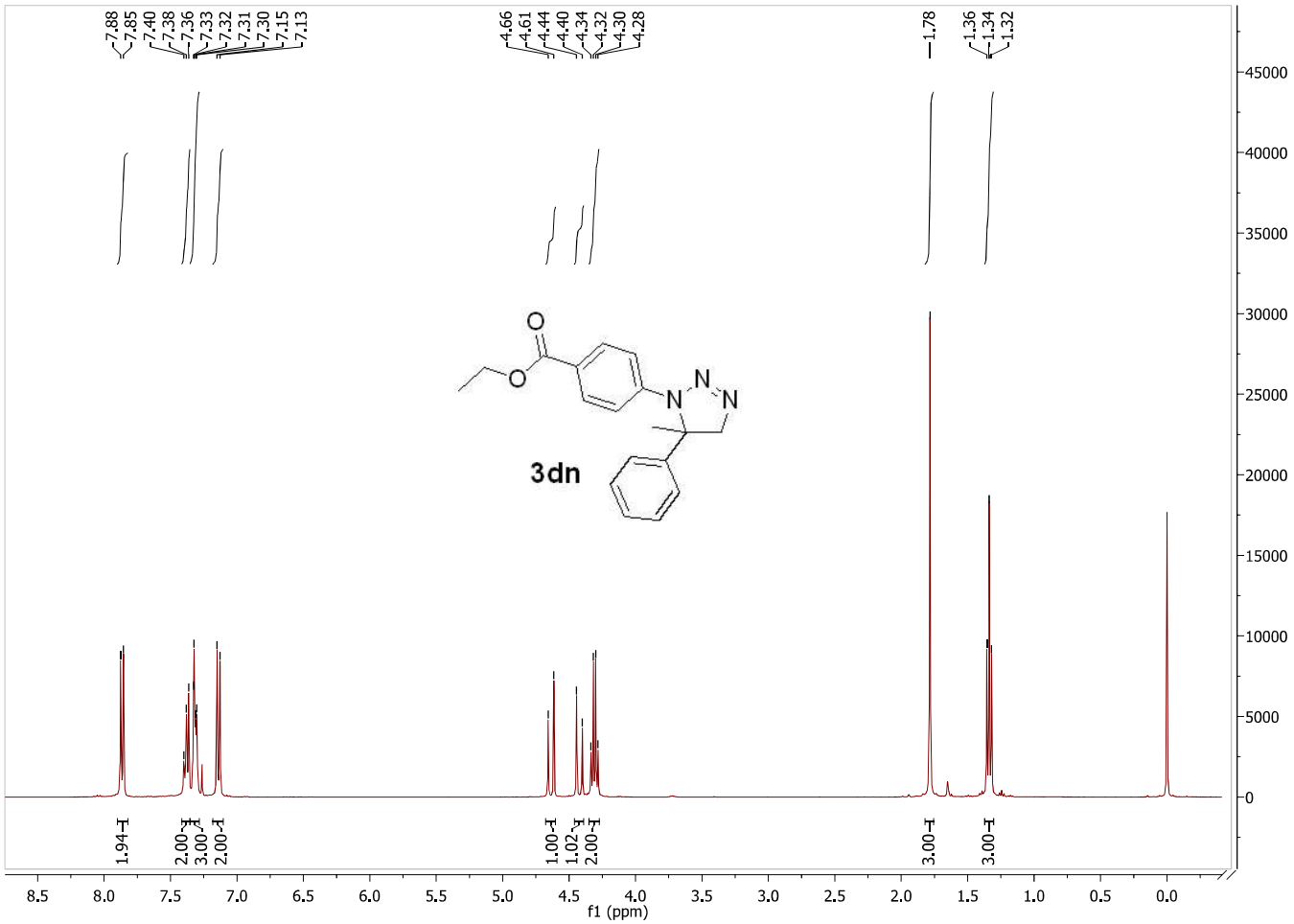
3dm
f1 (ppm)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4.61
4.44
4.40
4.34
4.32
4.30
4.28
1.78
1.36
1.34
1.32
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3.00
2.00
1.00
1.02
2.00
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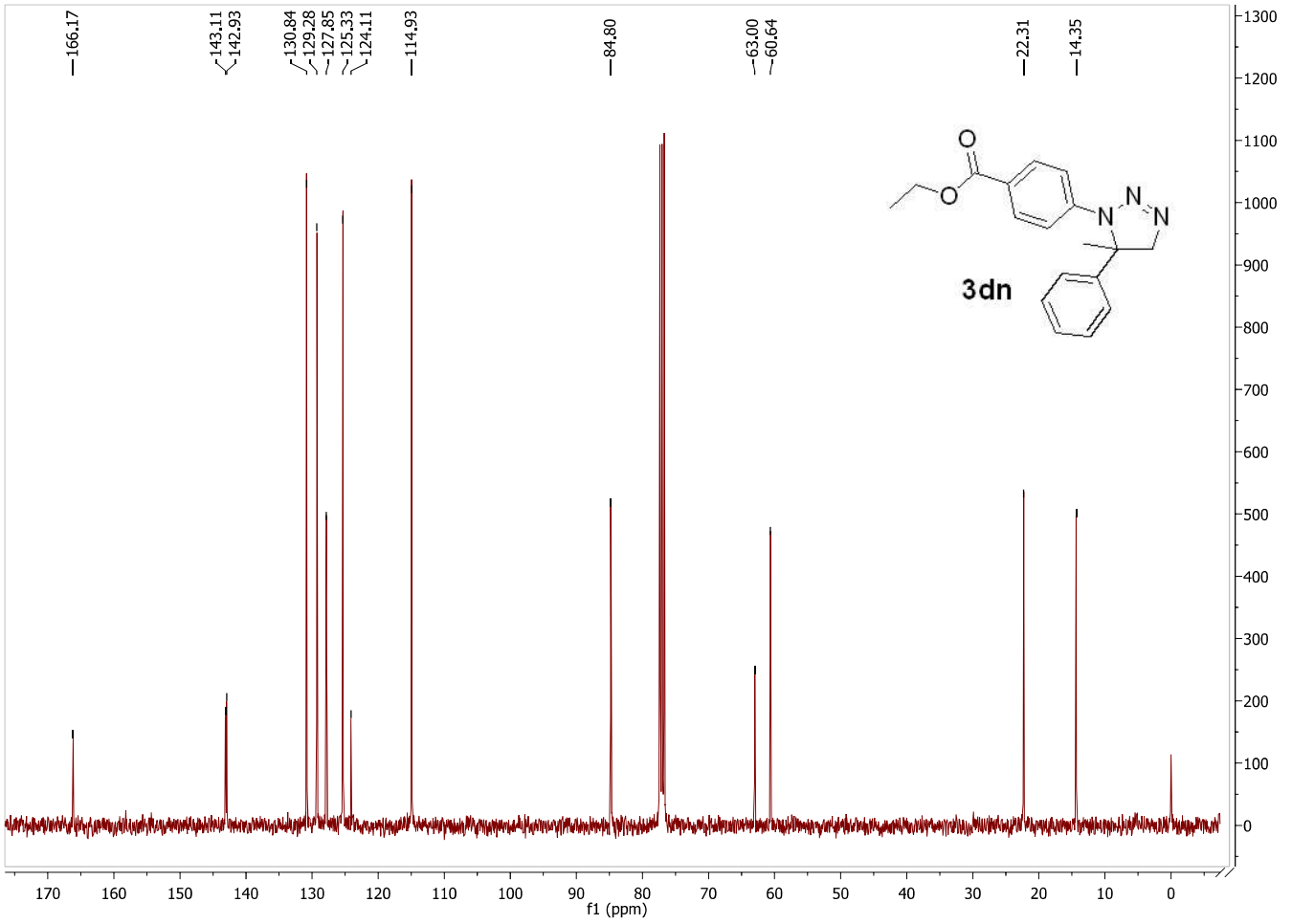
3.00
f1 (ppm)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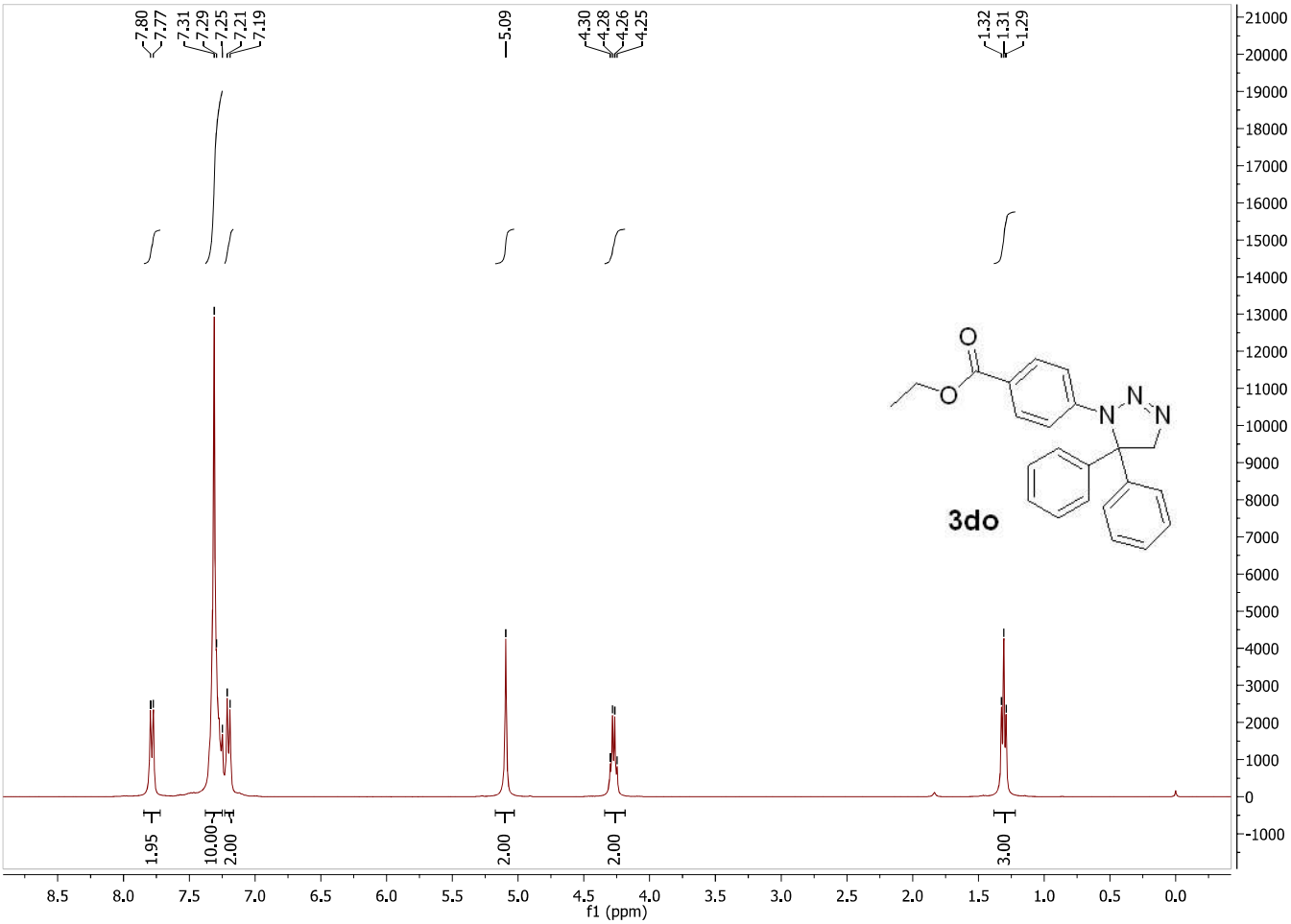
3dn
f1 (ppm)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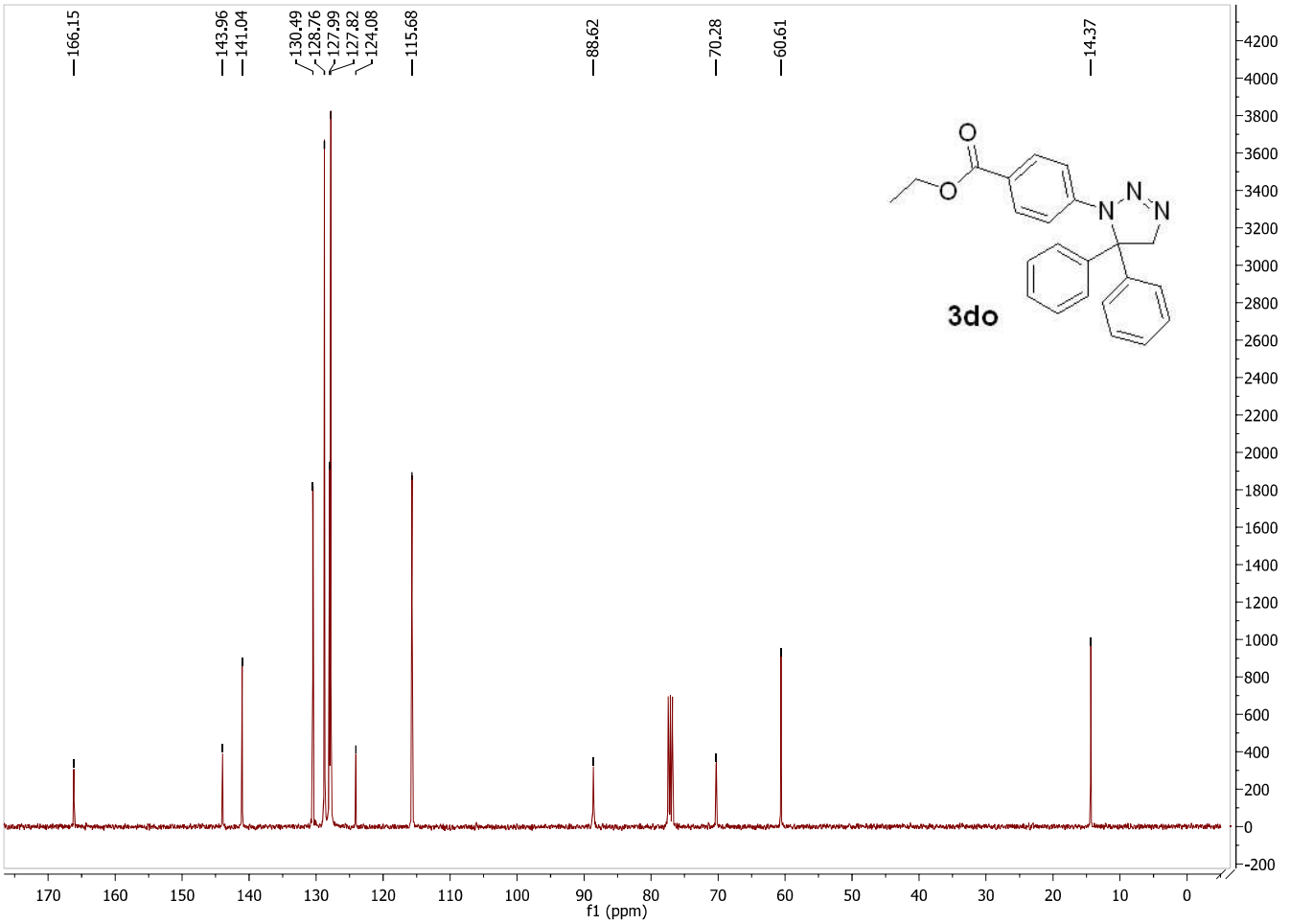
f1 (ppm)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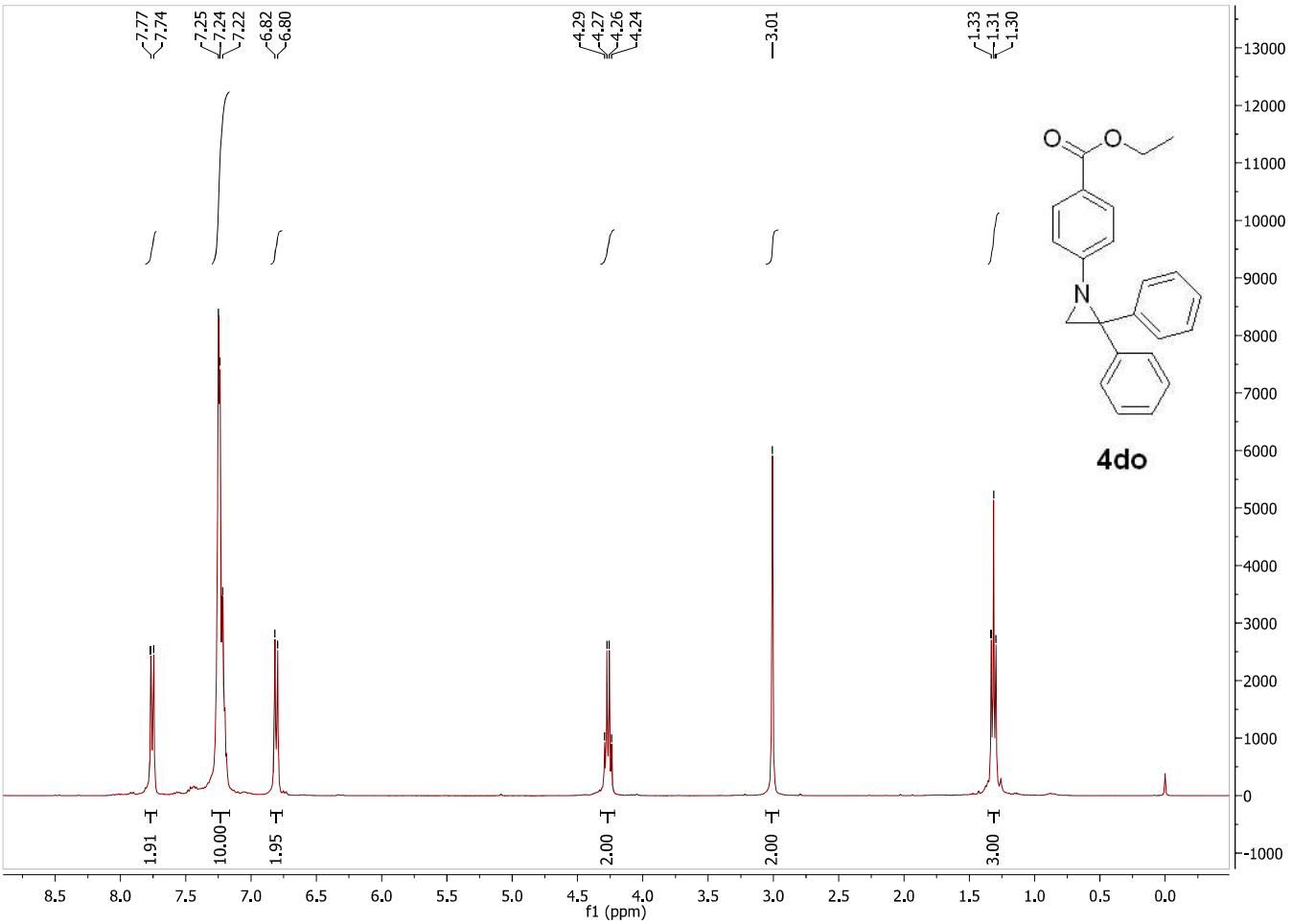
70.28
60.61
14.37
3do
f1 (ppm)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4.27
4.26
4.24
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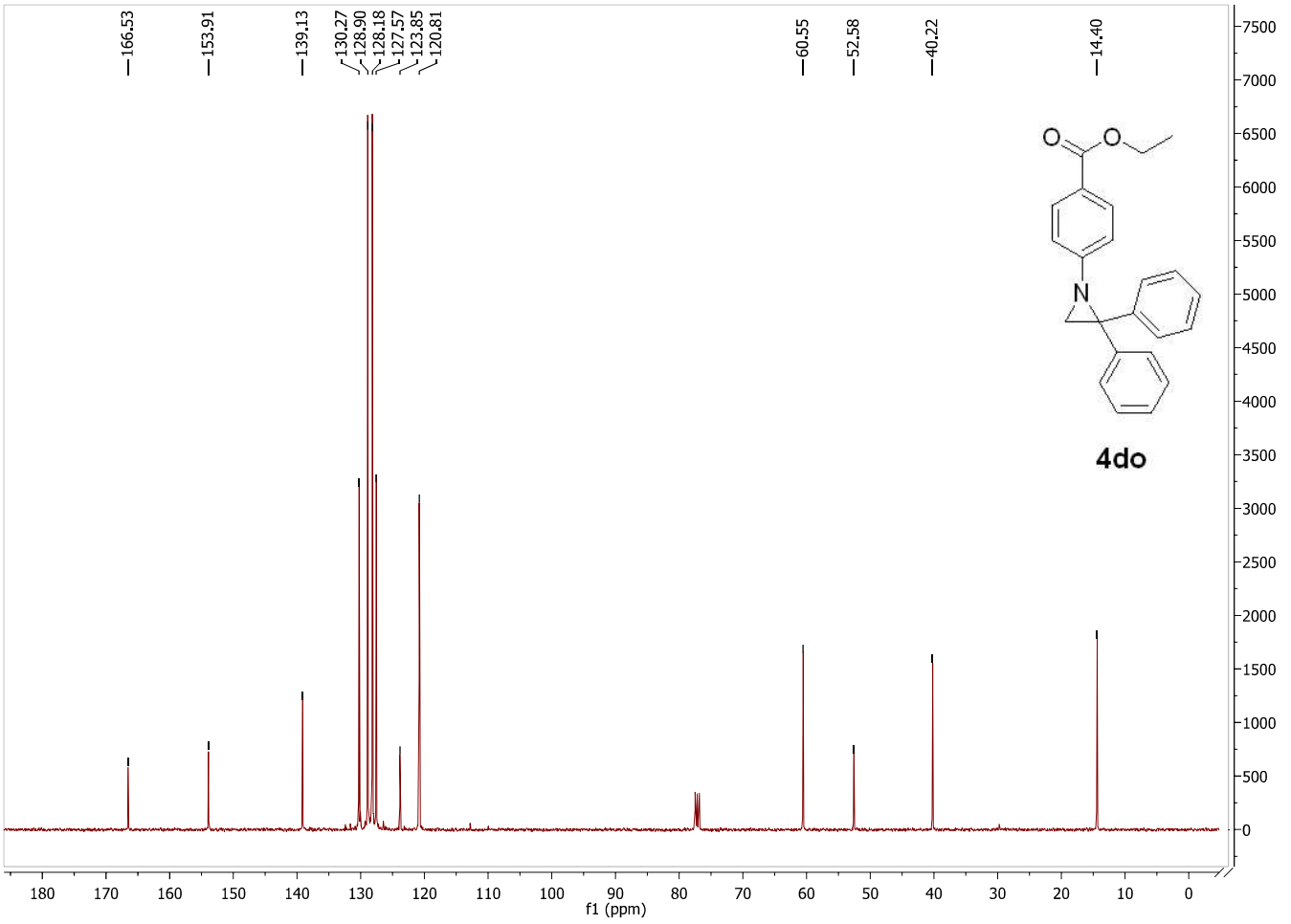
1.30
1.91
10.00
1.95
2.00
2.00
3.00
f1 (ppm)
4do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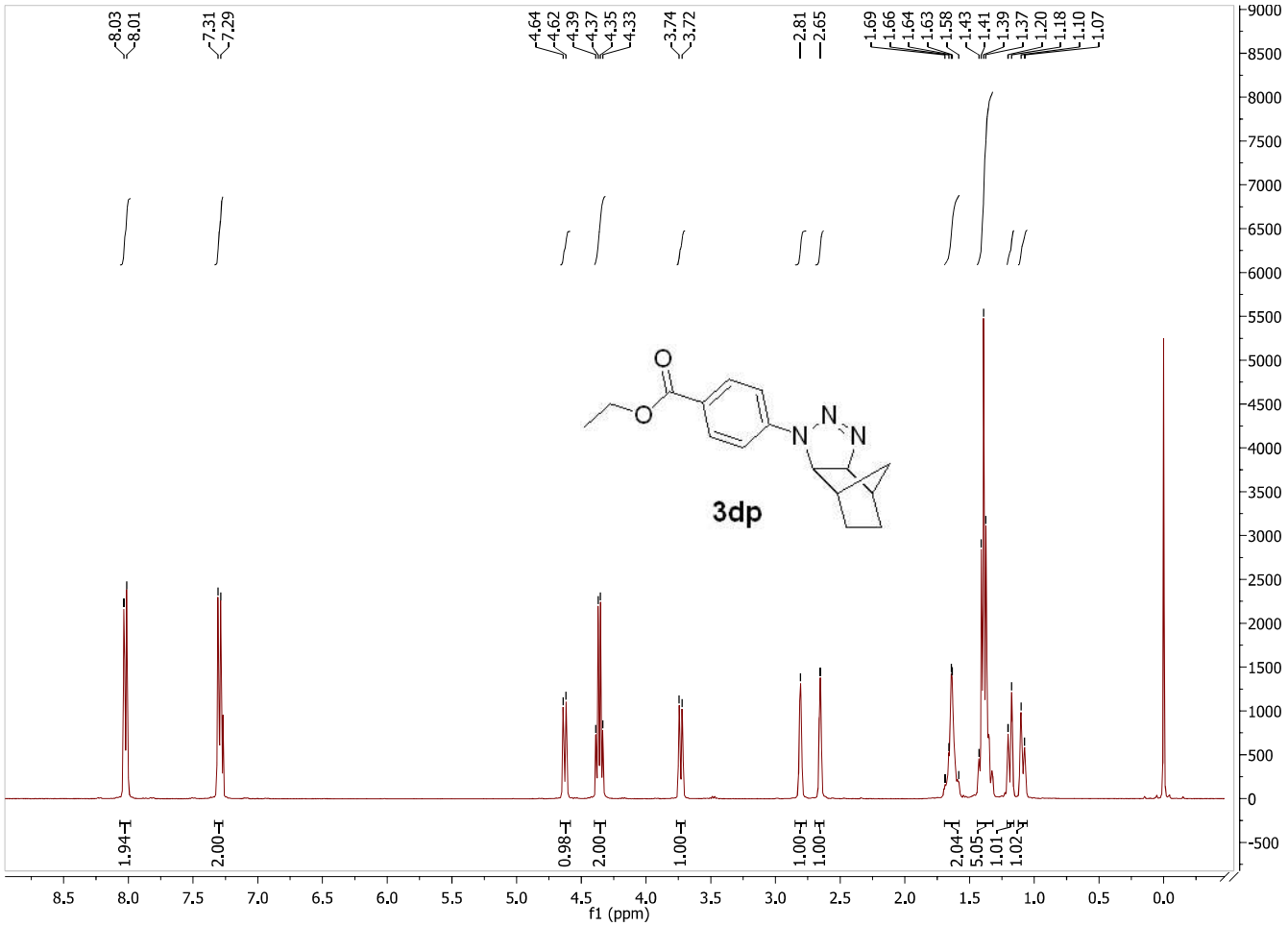
60.55
52.58
40.22
14.40
f1 (ppm)
4do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1.58
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1.00
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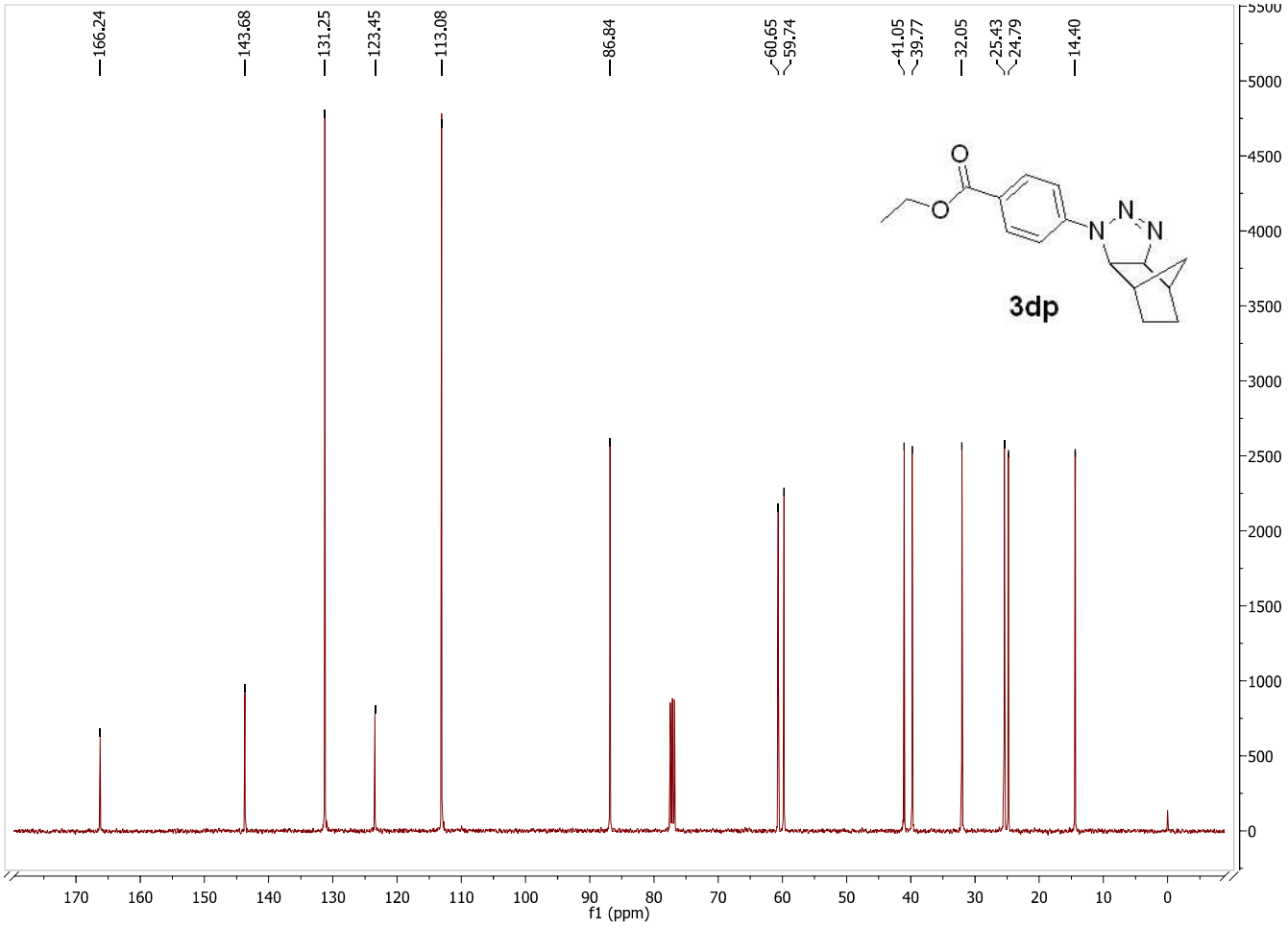
5.05
1.01
1.02
f1 (ppm)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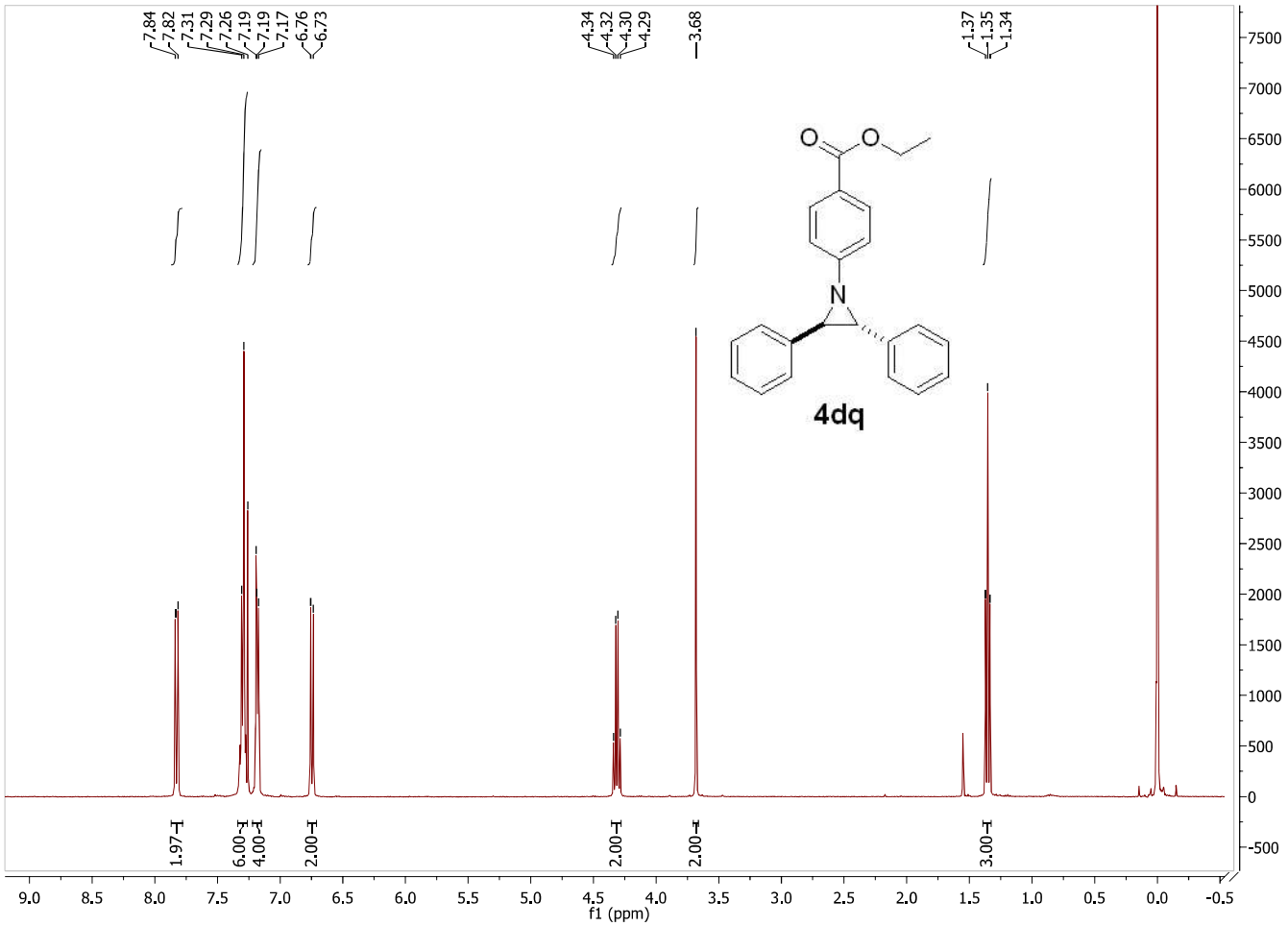
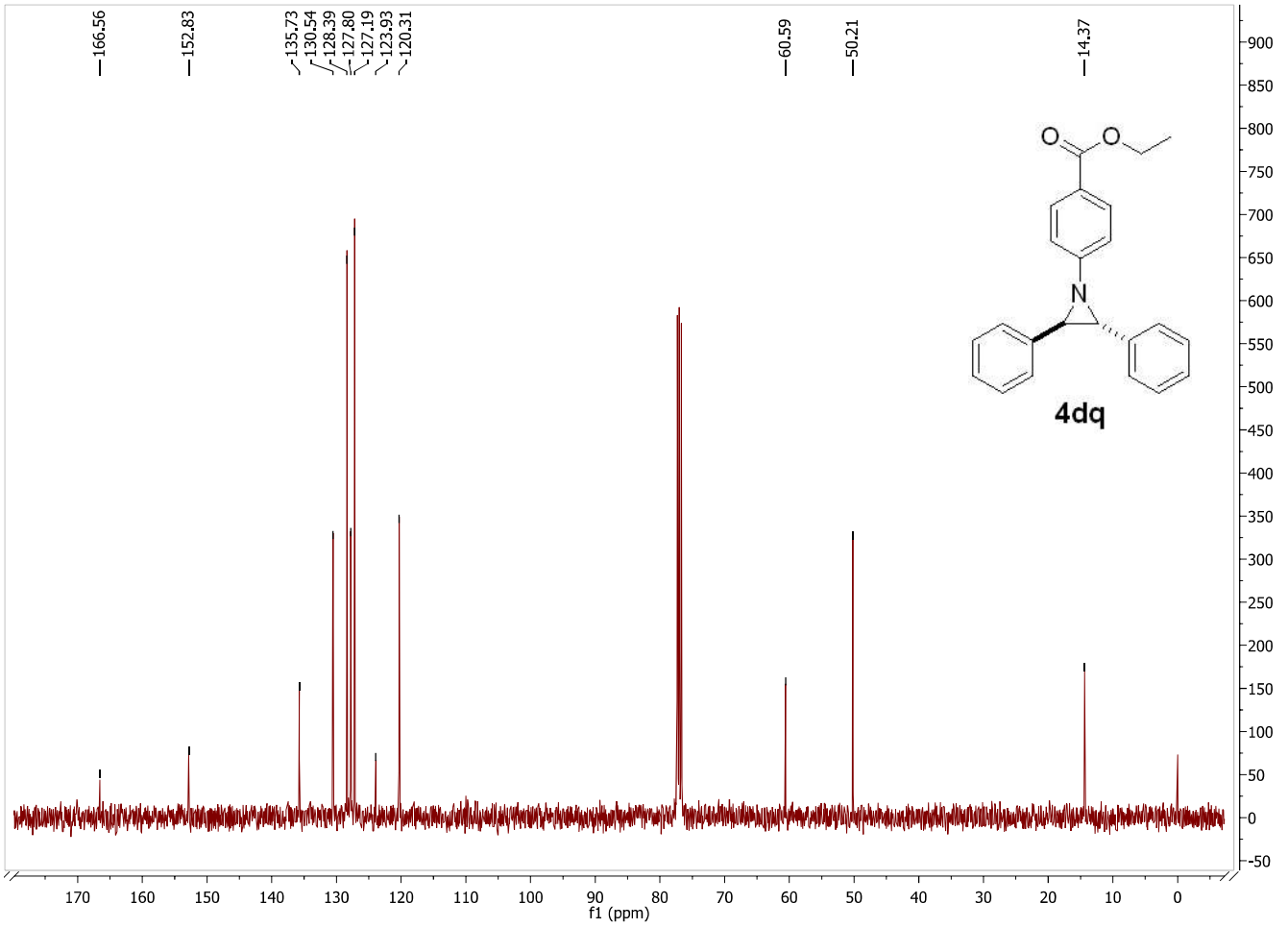
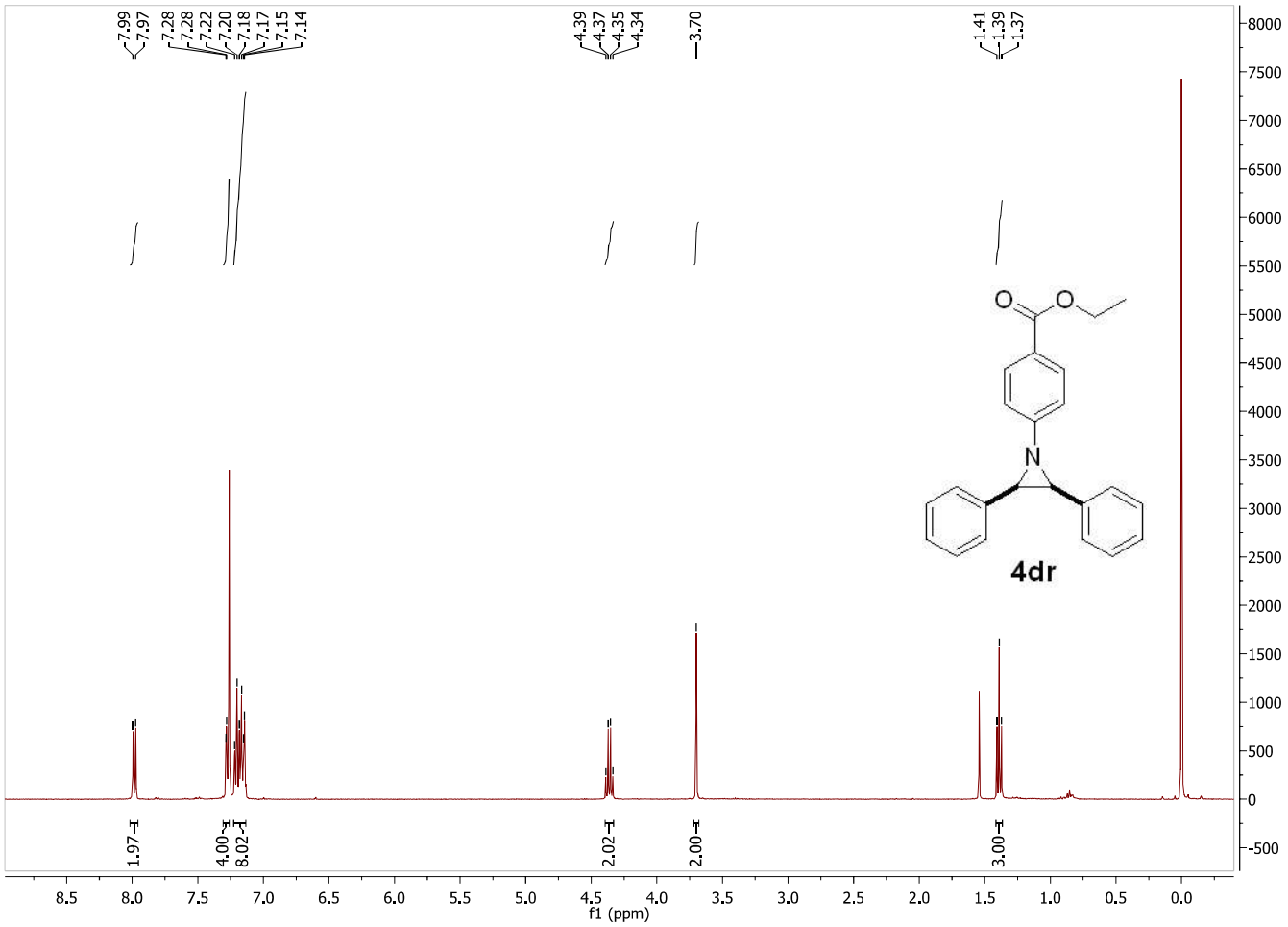
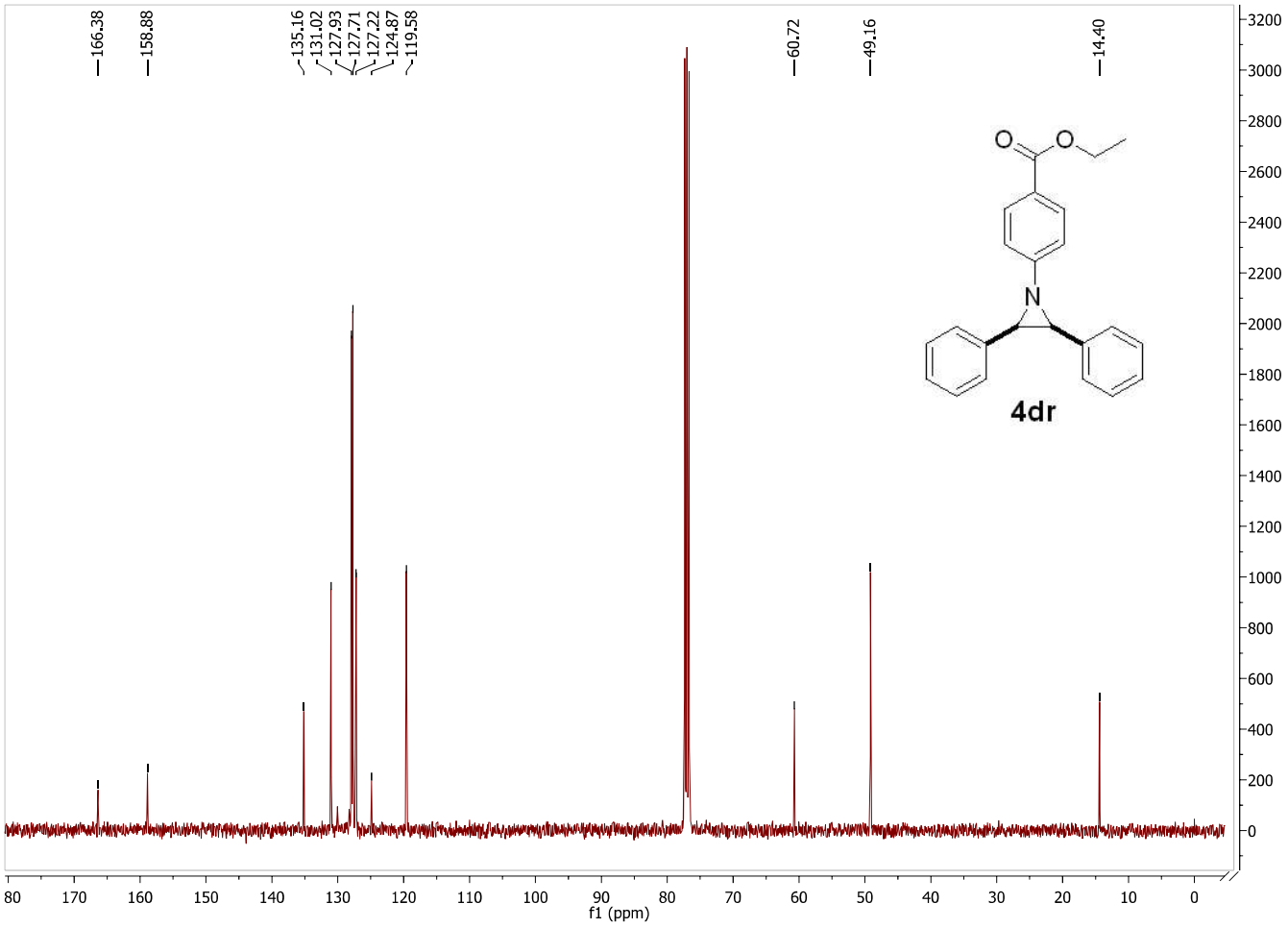
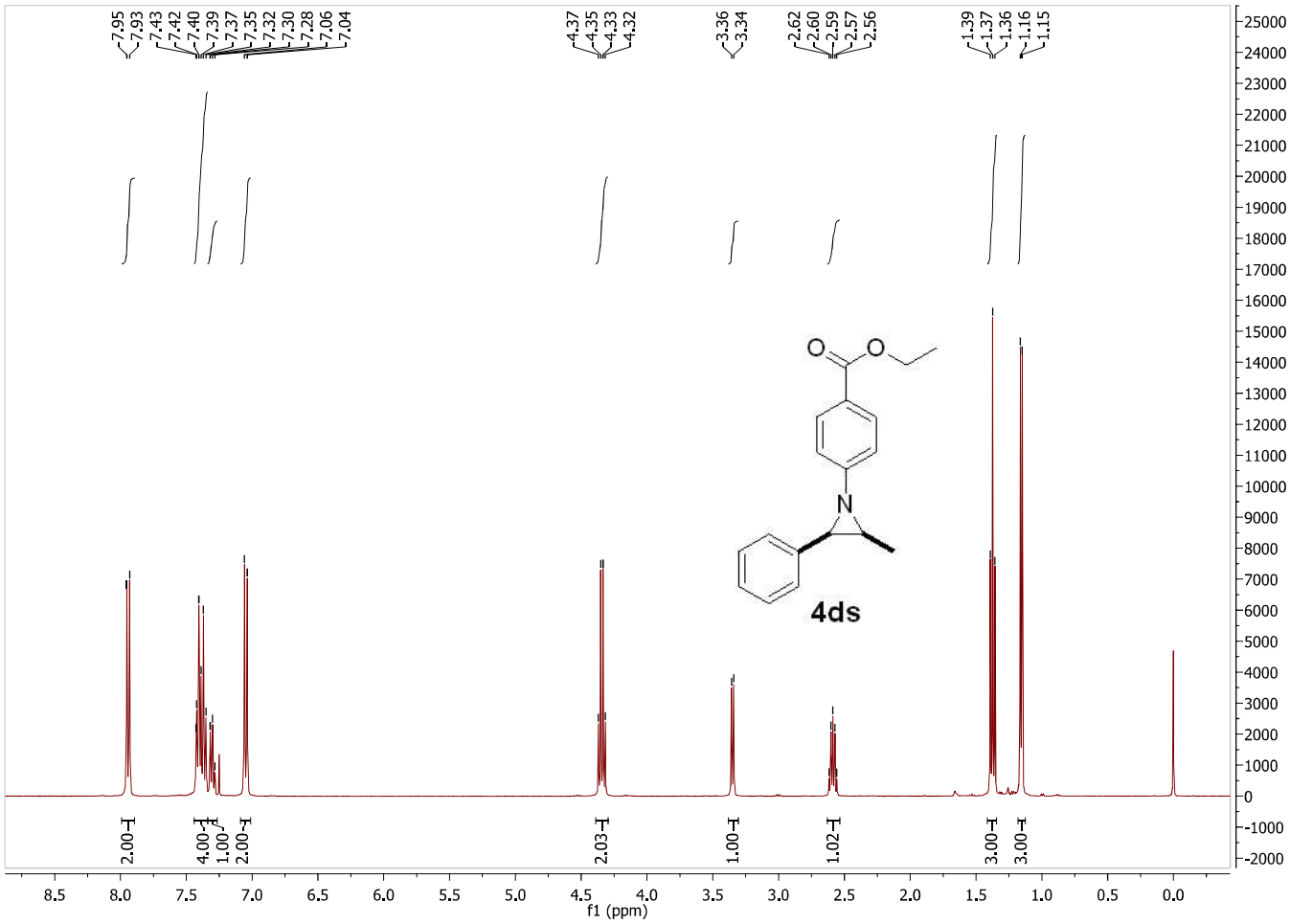
41.05
39.77
32.05
25.43
24.79
14.40
3dp
f1 (ppm)

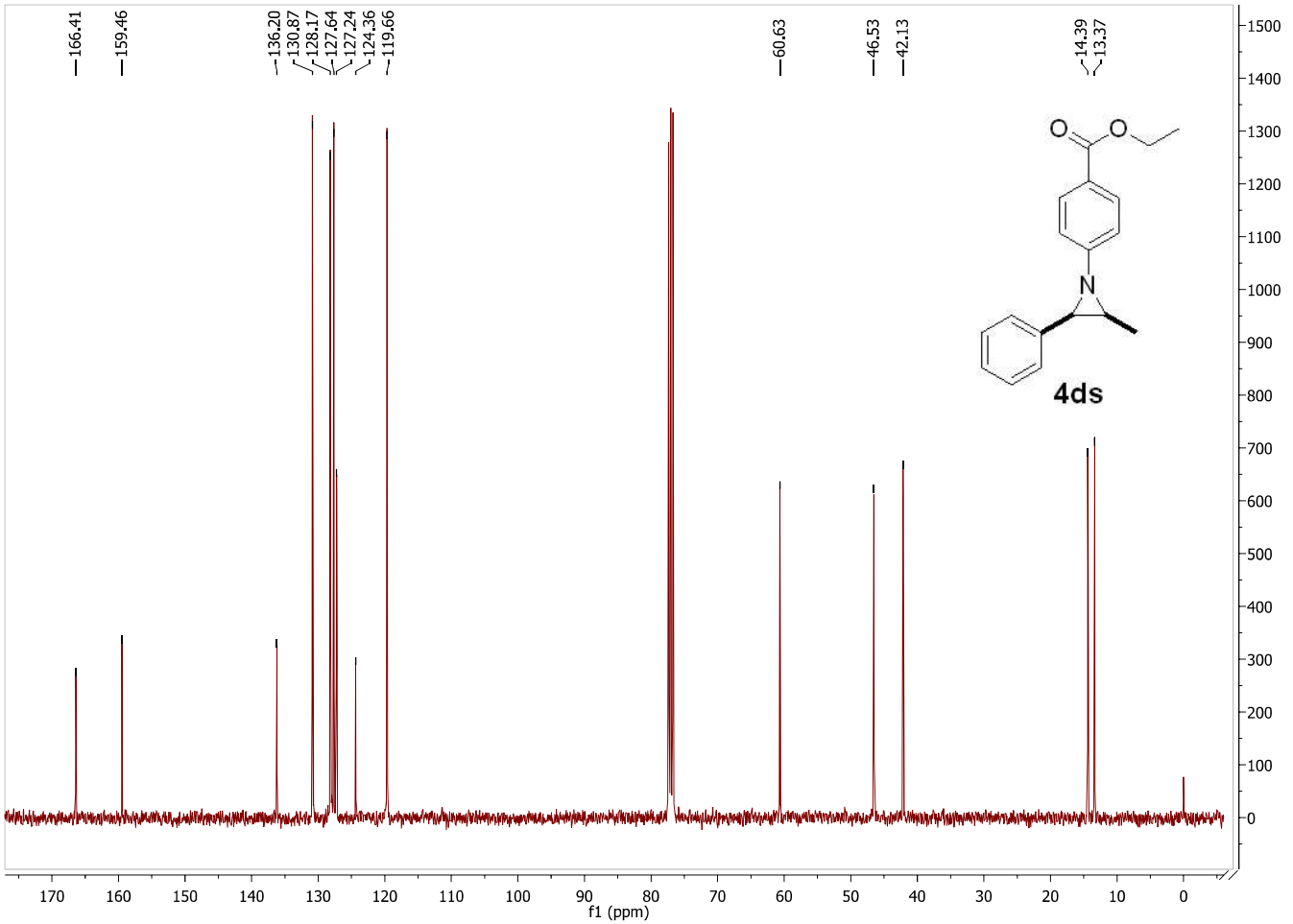

7.84
7.82
7.31
7.29
7.26
7.19
7.19
7.17
6.76
6.73
4.34
4.32
4.30
4.29
3.68
1.37
1.35
1.34
1.97
6.00
4.00
2.00
2.00
2.00
3.00
4dq
f1 (ppm)

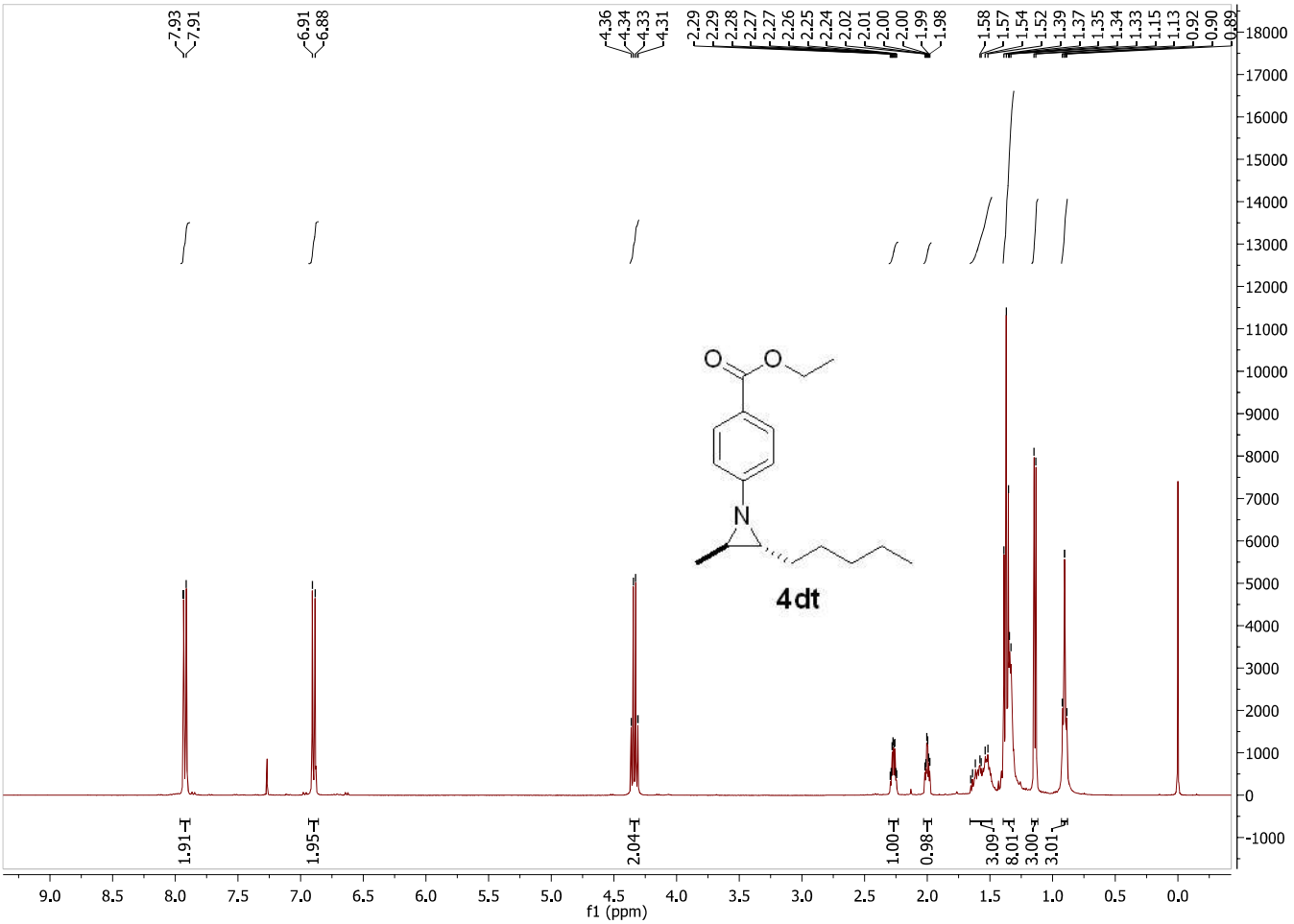

166.56
152.83
135.73
130.54
128.39
127.80
127.19
123.93
120.31
60.59
50.21
14.37
4dq
f1 (ppm)

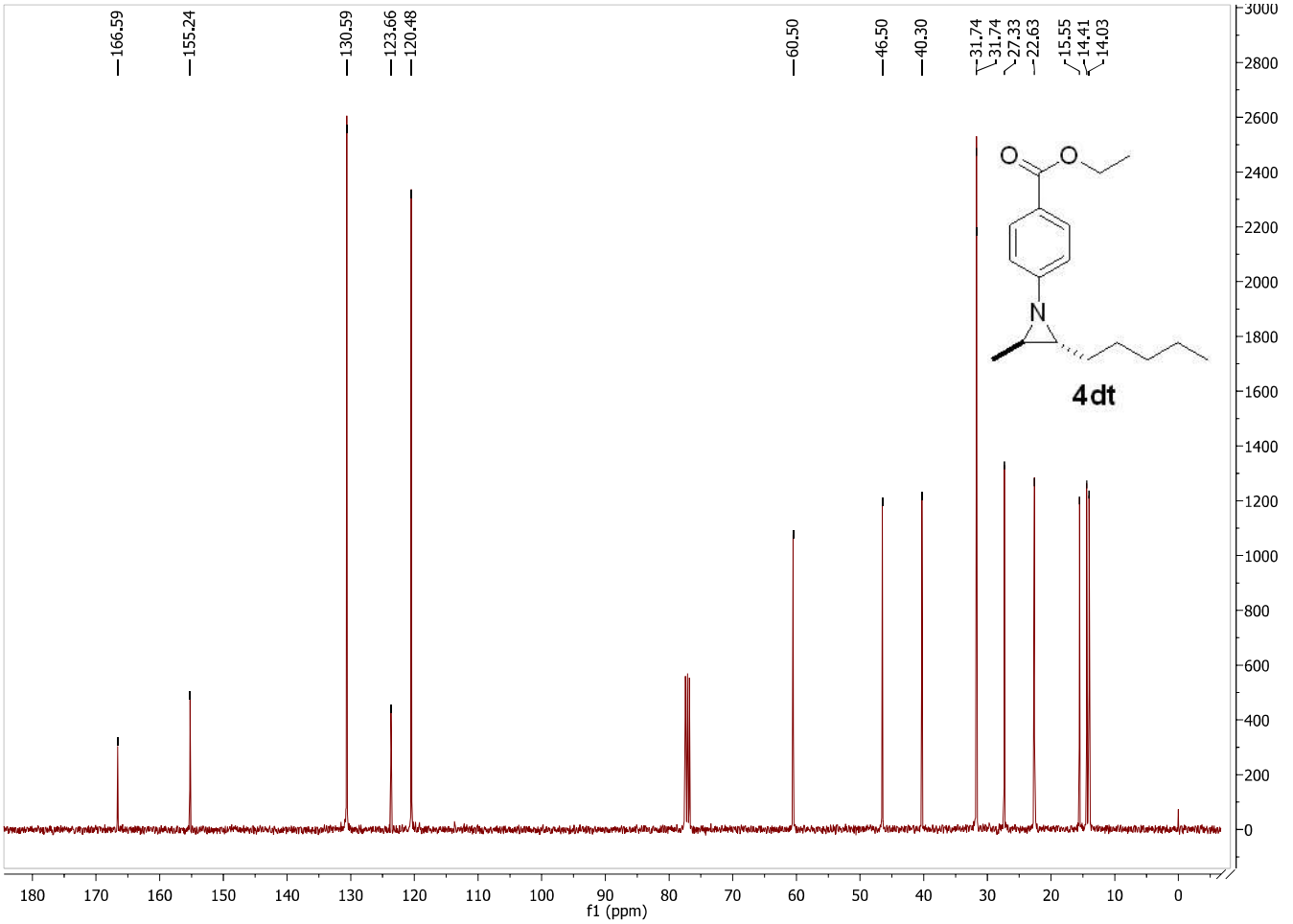

7.99
7.97
7.28
7.28
7.22
7.20
7.18
7.17
7.15
7.14
4.39
4.37
4.35
4.34
3.70
1.41
1.39
1.37
1.97
4.00
8.02
2.02
2.00
3.00
O
O
N
4dr
f1 (ppm)


166.38
158.88
135.16
131.02
127.93
127.71
127.22
124.87
119.58
60.72
49.16
14.40
O
O
N
4dr
f1 (ppm)


7.95
7.93
7.43
7.42
7.40
7.39
7.37
7.35
7.32
7.30
7.28
7.06
7.04
4.37
4.35
4.33
4.32
3.36
3.34
2.62
2.60
2.59
2.57
2.56
1.39
1.37
1.36
1.16
1.15
2.00
4.00
1.00
2.00
2.03
1.00
1.02
3.00
3.00
O
O
N
4ds
f1 (ppm)


166.41
159.46
136.20
130.87
128.17
127.64
127.24
124.36
119.66
60.63
46.53
42.13
14.39
13.37
O
O
N
4ds
f1 (ppm)


7.93
7.91
6.91
6.88
4.36
4.34
4.33
4.31
2.29
2.29
2.28
2.27
2.27
2.26
2.25
2.24
2.02
2.01
2.00
2.00
1.99
1.98
1.58
1.57
1.54
1.52
1.39
1.37
1.35
1.34
1.33
1.15
1.13
0.92
0.90
0.89
4dt
1.91
1.95
2.04
1.00
0.98
3.09
8.01
3.00
3.01
f1 (ppm)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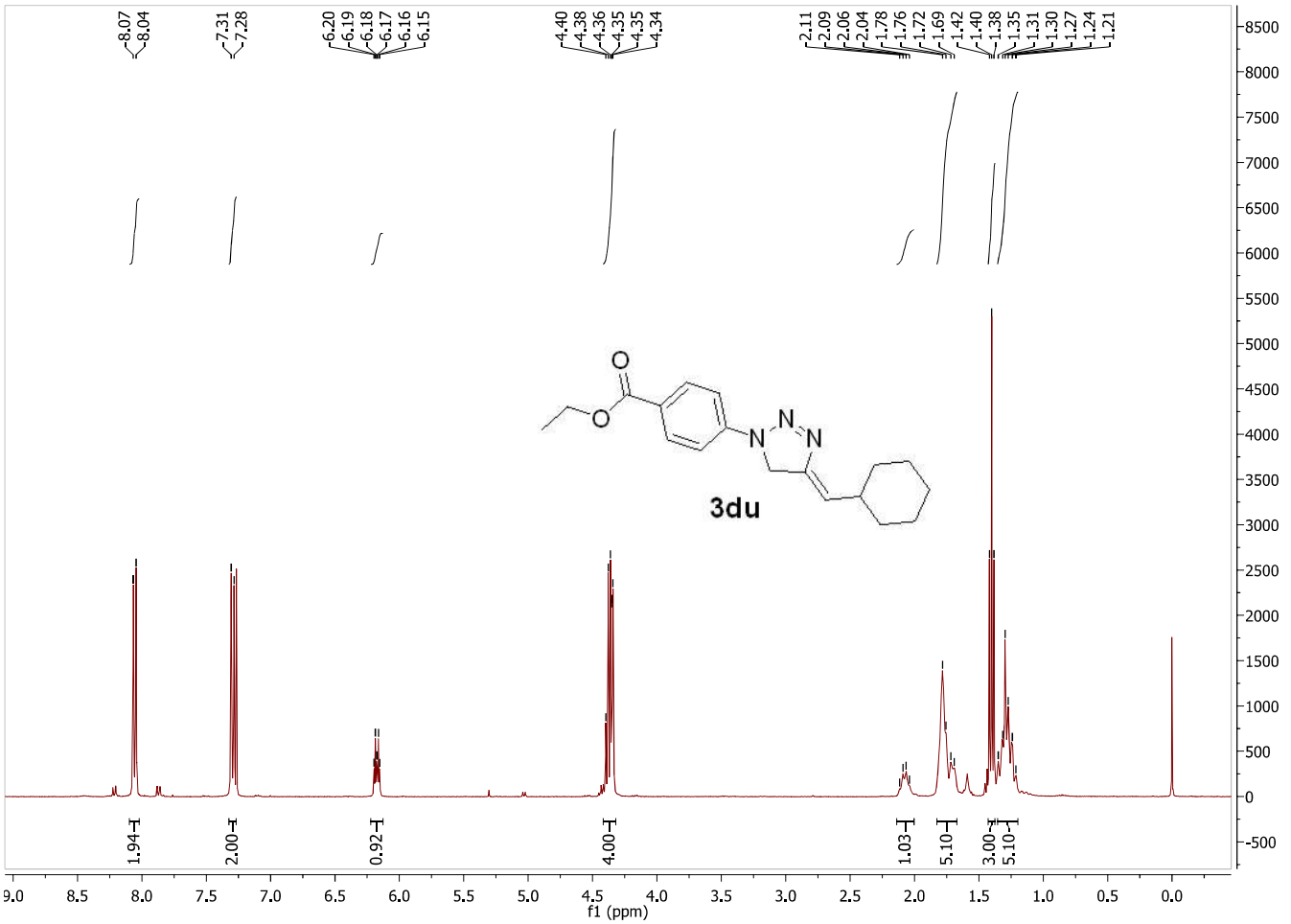
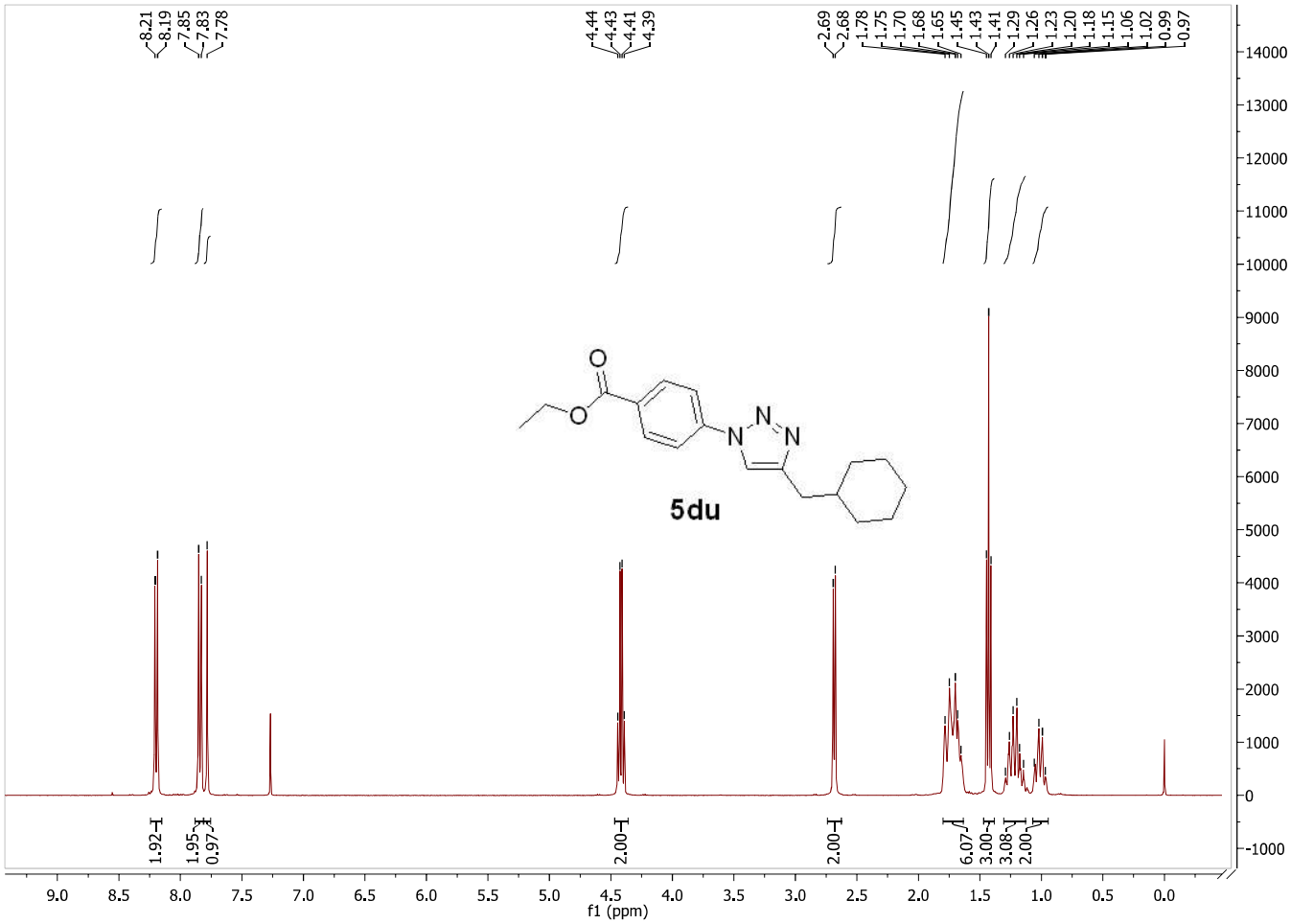
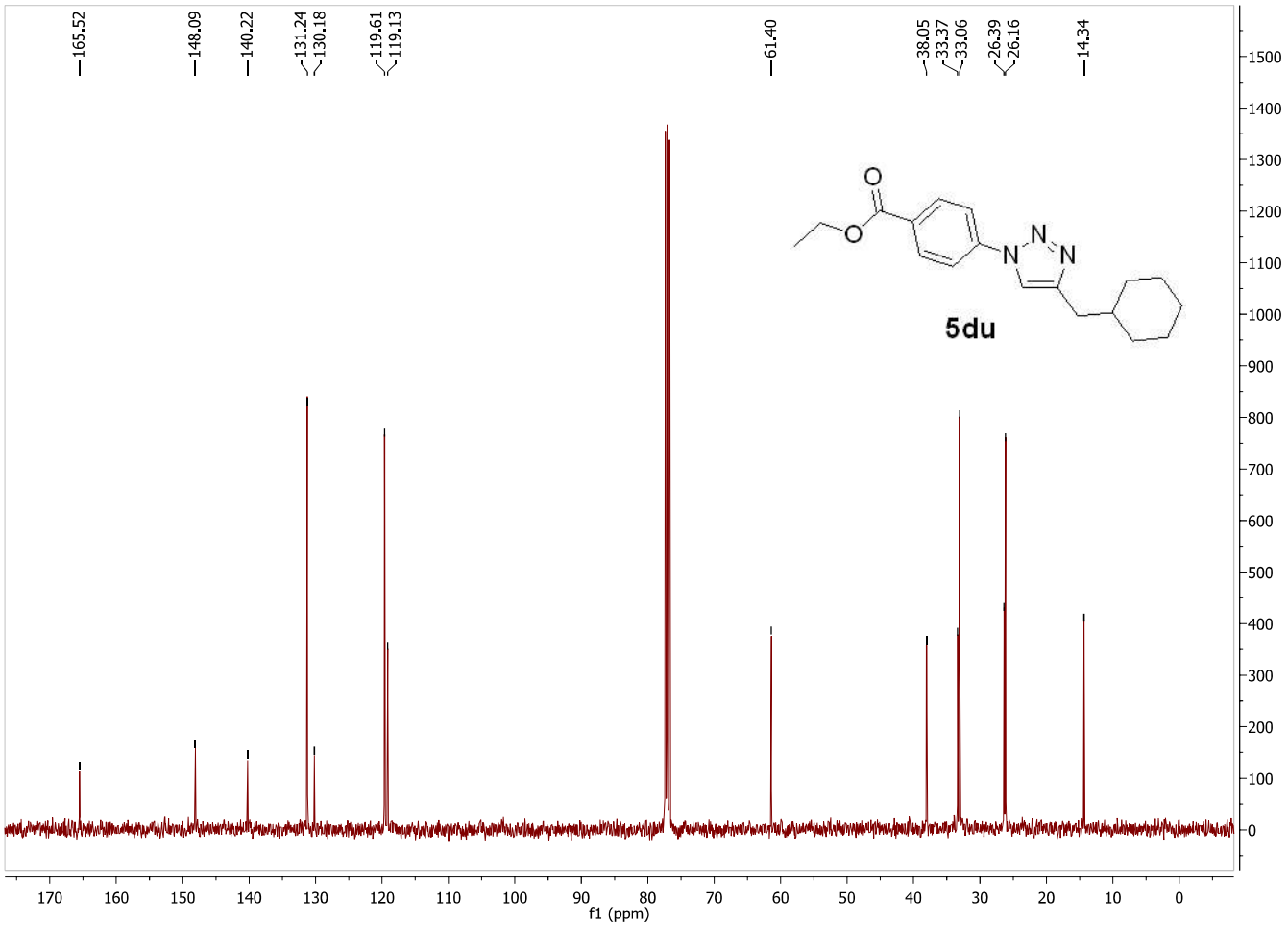
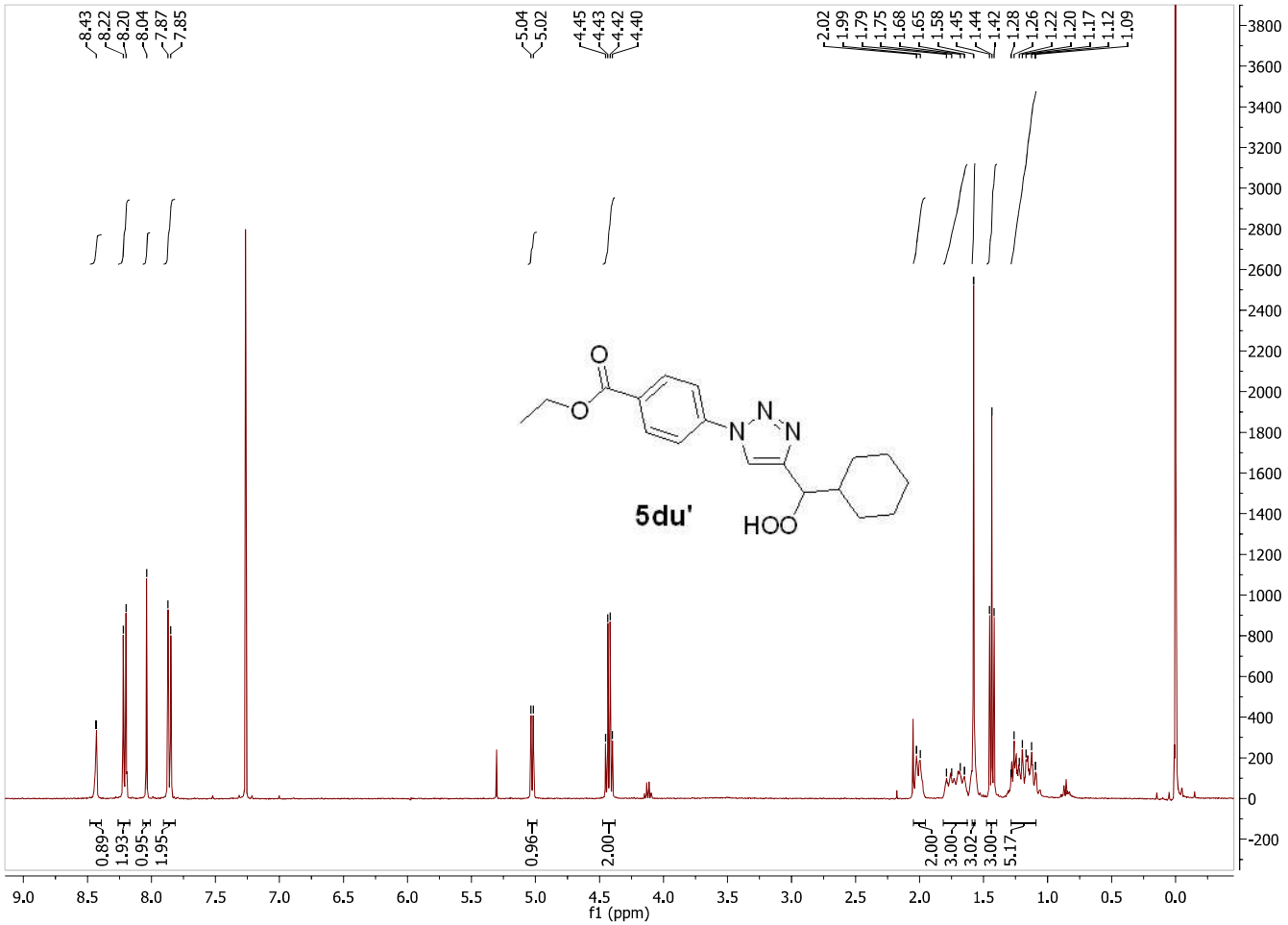
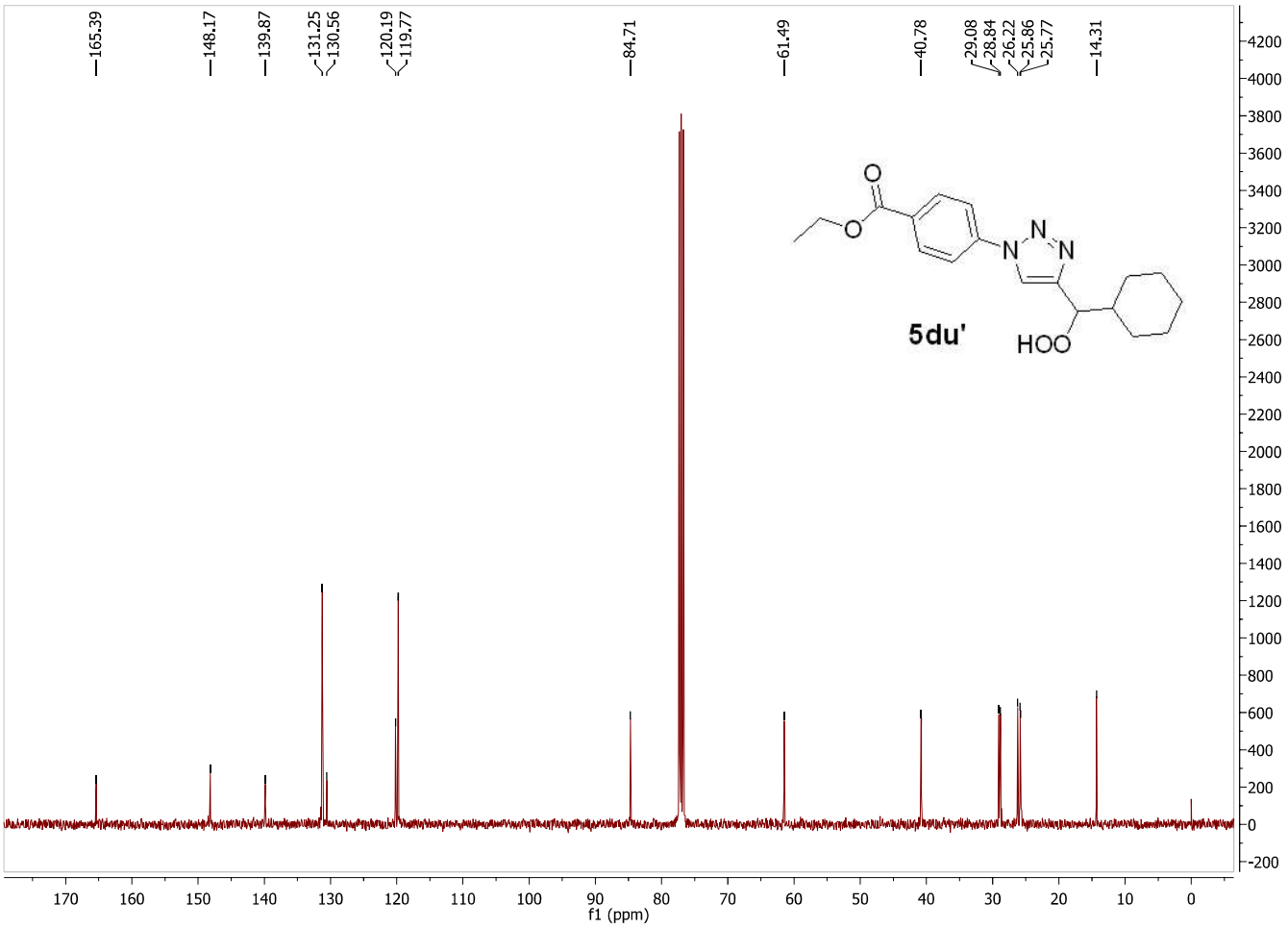
155.24
130.59
123.66
120.48
60.50
46.50
40.30
31.74
31.74
27.33
22.63
15.55
14.41
14.03
4dt
f1 (ppm)


8.07
8.04
7.31
7.28
6.20
6.19
6.18
6.17
6.16
6.15
4.40
4.38
4.36
4.35
4.35
4.34
2.11
2.09
2.06
2.04
1.78
1.76
1.72
1.69
1.42
1.40
1.38
1.35
1.31
1.30
1.27
1.24
1.21
O
O
N
N
N
3du
1.94
2.00
0.92
4.00
1.03
5.10
3.00
5.10
f1 (ppm)


8.21
8.19
7.85
7.83
7.78
4.44
4.43
4.41
4.39
2.69
2.68
1.78
1.75
1.70
1.68
1.65
1.45
1.43
1.41
1.29
1.26
1.23
1.20
1.18
1.15
1.06
1.02
0.99
0.97
O
O
N
N
N
5du
1.92
1.95
0.97
2.00
2.00
6.07
3.00
3.08
2.00
f1 (ppm)


165.52
148.09
140.22
131.24
130.18
119.61
119.13
61.40
38.05
33.37
33.06
26.39
26.16
14.34
5du
f1 (ppm)


8.43
8.22
8.20
8.04
7.87
7.85
5.04
5.02
4.45
4.43
4.42
4.40
2.02
1.99
1.79
1.75
1.68
1.65
1.58
1.45
1.44
1.42
1.28
1.26
1.22
1.20
1.17
1.12
1.09
0.89
1.93
0.95
1.95
0.96
2.00
2.00
3.00
3.02
3.00
5.17
5du'
HOO
f1 (ppm)


165.39
148.17
139.87
131.25
130.56
120.19
119.77
84.71
61.49
40.78
29.08
28.84
26.22
25.86
25.77
14.31
5du'
HOO
f1 (ppm)