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The ferric chloride-catalyzed Ritter amidation of norbornane-type dienes

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^{1}H and ^{13}C NMR spectra were measured on a Bruker Avance-III 500 Ascend instrument (400.13 MHz for ^{1}H and 100.62 MHz for ^{13}C in $CDCl_3$). Mass spectra were run on a Shimadzu GCMS-QP2010Plus mass spectrometer (SPB-5 capillary column, 30 m × 0.25 mm, helium as the carrier gas, temperature programming from 40 to 300 °C at 8 °C min^{-1}, evaporation temperature of 280 °C, ion source temperature of 200 °C, and ionization energy of 70 eV). IR spectra were measured on a Bruker Vertex-70v instrument. The elemental composition of the samples was determined on a Carlo Erba 1106 elemental analyzer. The course of the reaction and the purity of the products were monitored by gas liquid chromatography on a Shimadzu GC-9A, GC-2014 instrument [2 m × 3 mm column, SE-30 silicone (5%) on Chromaton N-AW-HMDS as the stationary phase, temperature programming from 50 to 270ºC at 8 °C min^{-1}, helium as the carrier gas (47 ml min^{-1})].

The X-ray diffraction analysis of amides **4'a** and *endo-trans-exo*-**8** was carried out on a XCalibur Eos automated four-circle diffractometer (graphite monochromator, MoKα radiation, λ = 0.71073 Å, ω-scanning, 2θmax = 62°). The data were collected and processed using a CrysAlisPro Oxford Diffraction Ltd program [S1]. The structures were solved by direct methods and refined by full-matrix least-squares method in the anisotropic approximation for non-hydrogen atoms. The hydrogen atoms were located using difference Fourier maps and included in the refinement with fixed thermal and positional parameters. Structures determinations were carried out with the OLEX2 program [S2]. The structures were solved by direct methods and refined by the full-matrix least-squares method in the anisotropic approximation for non-hydrogen atoms. All hydrogen atoms are generated using the proper HFIX command and refined isotropically using the riding model. The calculations were performed using the SHELX program package [S3].

General procedure for the diene amidation. Diene **1**, **3**, **5,** or **7** (0.5 g, **1**: 5.43 mmol, **3**: 3.95 mmol, **5**: 3.16 mmol, **7**: 2.71 mmol), the catalyst (0.022-0.044 g, for **1**: 0.16 mmol, for **3**: 0.12 mmol, for **5**: 0.096 mmol; for **7**: 0.081 mmol), EtCN (27.1-54.3 mmol), and water (0.049-0.098 g, 2.71-5.43 mmol) were placed into a glass ampoule (V= 10 mL). The ampoule was sealed, placed in a steel microautoclave, and heated at 145 °C for 6 hours. After completion the reaction, the microautoclave (ampoule) was cooled down to room temperature, the reaction mixture was filtered

through an Al_2O_3 layer ($CHCl_3$ as the eluent), the solvent was evaporated, and the residue was recrystallized from MeCN.

Reaction of 2-chlorobicyclo[2.2.1]hexa-2,5-diene 3 with MeCN. Diene **3** (0.5 g, 3.95 mmol), the catalyst (0.032 g, 0.12 mmol), MeCN (1.62 g, 39.5 mmol), and water (0.072 g, 3.95 mmol) were placed into a 10 ml glass ampoule. The ampoule was sealed, placed in a steel microautoclave, and heated at 145 °C for 6 hours. After completion the reaction, the microautoclave (ampoule) was cooled down to room temperature, the reaction mixture was filtered through an Al_2O_3 layer ($CHCl_3$ as the eluent), the solvent was evaporated, and the residue was recrystallized from MeCN.

Mixture of 3-*exo*-propioamidotricyclo[2.2.1.0^{2,6}]heptane 2a and **2-*exo*-propioamidobicyclo[2.2.1]hept-5-ene 2b**. Total yield 80% (0.72 g), white crystals, m.p. 68-73.5°C (MeCN.). ^{1}H NMR (400.13 MHz, $CDCl_3$): 0.97-0.98 (m, 1H), 1.01-1.09 (m, 7H), 1.16-1.18 (m, 1H), 1.33-1.81 (m, 8H), 2.07-2.11 (m, 4H), 2.66 (s, 1H, **2a**), 2.74 (s, 1H, **2a**), 3.43 (s, 1H, **2b**), 3.66 (d, 1H, CHNH, **2a**, *J* 6.8 Hz), 3.74 (s, 1H, CHNH, **2b**) 5.74 (br.s, 2H, NH), 5.97-6.04 (m, 2H, CH=CH). ^{13}C NMR (100.62 MHz, $CDCl_3$), **2a**: 9.83 (C^{10}), 10.31 (C^1), 11.80(C^6), 14.14 (C^2), 29.43(C^9), 29.57(C^7), 31.67(C^5), 33.62(C^4), 55.13 (C^3), 173.76 (C^8). ^{13}C NMR (100.62 MHz, $CDCl_3$), **2b**: 10.44 (C^{10}), 29.19 (C^3), 30.43(C^9), 40.81 (C^7), 45.81(C^4), 47.79(C^2), 49.61(C^1), 134.63(C^6), 138.47 (C^5), 173.67 (C^8). MS (EI, 70eV), **2a**, *m/z*, 165(23) [M]$^+$, 150(4), 136(3), 108(47), 98(100), 94(59), 74(51), 71(6), 57(49), 43(54). MS (EI, 70eV), **2b**, *m/z*, 165(1) [M]$^+$, 136(1), 108(2), 100(83), 91(9), 67(56), 57(39), 43(100).

Mixture of 3-*exo*-propioamido-1-chlorotricyclo[2.2.1.0^{2,6}]heptane 4a and **2-*exo*-propioamido-1-chlorotricyclo[2.2.1.0^{2,6}]heptane 4b**. Total yield 82% (0.65 g), white crystals, m.p. 148.5-149.5 °C (MeCN). ^{1}H NMR (400.13 MHz, $CDCl_3$): 1.05-1.12 (m, 7H) 2CH_3), 1.48-1.50 (m, 3H), 1.55-1.60 (m, 5H), 1.64-1.69 (m, 1H), 1.76-1.78 (m, 1H), 2.08-2.09 (m, 4H), 2.11-2.20 (m, 4H), 3.79 (d, 1H, CHNH, **4b**, *J* 6.8 Hz), 3.99 (d, 1H, CHNH, **4a**, *J* 7.2 Hz), 5.71 (s, 1H, NH, **4a**), 6.08 (s, 1H, NH, **4b**). ^{13}C NMR (100.62 MHz, $CDCl_3$), **4a**: 9.87 (C^{10}), 20.79 (C^6), 23.94 (C^2), 29.61 (C^9), 30.67 (C^7), 36.81 (C^4), 39.71 (C^5), 42.61 (C^1), 54.96 (C^3), 173.77 (C^8). ^{13}C NMR (100.62 MHz, $CDCl_3$), **4b**: 9.92 (C^{10}), 22.15 (C^6), 23.82 (C^5), 29.61 (C^9), 32.61 (C^4), 36.42 (C^7), 37.24 (C^3), 42.32 (C^1), 56.30 (C^2), 174.13 (C^8). MS (EI, 70eV), **4a**, *m/z*, 199(7) [M]$^+$, 184(51), 164(3), 163(3), 143(22), 108(54), 98(100), 91(63), 74 (28), 57(47), 43(20). MS (EI, 70eV), **4b**, *m/z*, 199(12) [M]$^+$, 184(1), 164(2), 143(16), 127(4), 108(45), 98(100), 91(60), 74(20), 57(48), 43(25).

3-*exo*-Acetamido-1-chlorotricyclo[2.2.1.0^{2,6}]heptane 4'a. Yield 35% (0.26 g), light brown crystals, m.p. 139.5-140.5 °C. ^{1}H NMR (400.13 MHz, $CDCl_3$): 1.51-1.53 (m, 1H), 1.56-1.62 (m, 3H), 1.70-1.72 (m, 1H), 1.93 (s, 3H), 2.11 (s, 1H), 4.02 (d, 1H, CHNH, *J* 7.2 Hz), 5.64 (s, 1H, NH). ^{13}C NMR (100.62 MHz, $CDCl_3$): 20.84 (C^6), 23.43 (C^9), 23.99 (C^2), 30.77 (C^7), 36.87 (C^4),

39.78 (C^5), 42.61 (C^1), 55.16 (C^3), 170.01 (C^8). MS (EI, 70eV), *m/z*, 185(6) $[M]^+$, 170(1), 150(4), 143(15), 126(12), 108(55), 91(65), 84(78), 77(19), 60(31), 43(100). IR (Nujol): ν_{max} 3276, 1639, 1554 cm^{-1}. Found (%): C 58.26; H 6.58; Cl 19.06; N 7.50. $C_9H_{12}ClNO$. Calculated (%): C 58.23; H 6.52; Cl 19.10; N 7.54.

Crystal data for **4'a**: crystals of $C_9H_{12}ClNO$ (M = 185.65) are orthorhombic, space group Pbca, a = 10.6925(6), b = 9.6385(7) and c = 17.2215(13) Å, V = 1774.8(2) $Å^3$, d_{calc} = 1.390 $g \cdot cm^{-3}$, Z = 8, μ = 0.379 mm^{-1}, $2\theta_{max}$ = 58.204°, 5267 reflections were measured, from which 2110 were independent, 1432 reflections with I > 2σ(I). The refinement converged to R_1 = 0.0686, wR_2 = 0.1608, GOF = 1.112. CCDC 1847560 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk.

Table S1. **Bond lengths for 4'a**

Bond	Length (Å)	Bond	Length (Å)
Cl^1-C^1	1.748(3)	C^2-C^6	1.522(5)
N^1-C^8	1.341(4)	C^2-C^3	1.510(5)
N^1-C^3	1.449(4)	C^4-C^3	1.532(5)
O^1-C^8	1.229(4)	C^4-C^7	1.529(4)
C^1-C^2	1.495(5)	C^5-C^4	1.535(4)
C^1-C^6	1.491(4)	C^5-C^6	1.509(5)
C^1-C^7	1.507(5)	C^8-C^9	1.498(5)

Table S2. Bond angles for 4'a

Angle	Value (°)	Angle	Value (°)
$C^8N^1C^3$	122.8(3)	$C^7C^4C^5$	101.9(3)
$N^1C^8C^9$	115.5(3)	$C^7C^4C^3$	101.6(3)
$O^1C^8N^1$	122.4(3)	$C^1C^2C^6$	59.2(2)
$O^1C^8C^9$	122.1(3)	$C^1C^2C^3$	105.6(3)
$C^6C^5C^4$	96.7(3)	$C^3C^2C^6$	106.6(3)
$C^2C^1Cl^1$	122.3(3)	$C^5C^6C^2$	107.0(3)
$C^2C^1C^7$	108.3(3)	$C^1C^6C^5$	106.1(3)
$C^6C^1Cl^1$	121.9(2)	$C^1C^6C^2$	59.5(2)
$C^6C^1C^2$	61.3(2)	$N^1C^3C^4$	115.9(3)
$C^6C^1C^7$	108.2(3)	$N^1C^3C^2$	113.1(3)
$C^7C^1Cl^1$	120.5(2)	$C^2C^3C^4$	97.1(3)
$C^3C^4C^5$	102.7(3)	$C^1C^7C^4$	95.5(3)

5-*exo*-Propioamido-*exo,exo*-tetracyclo[6.2.1.1^{3,6}.0^{2,7}]dodec-9-ene 6a. Yield 62% (0.45 g), yellow oil. ^{1}H NMR (400.13 MHz, $CDCl_3$): 1.09-1.12 (m, 3H), 1.30-2.01 (m, 9H), 2.05-2.19 (m,

2H), 2.67 (d, 1H, *J* 2.4 Hz), 3.53-3.66 (m, 1H), 3.94-3.96 (m, 1H, CHNH), 5.91 (s, 1H, NH), 6.09 (s, CH=CH). ^{13}C NMR (100.62 MHz, $CDCl_3$): 10.03 (C^{15}), 29.78 (C^{14}), 33.07 (C^{2}), 36.38 (C^{3}), 38.27 (C^{11}), 42.64 (C^{6}), 45.11 (C^{1}), 45.34 (C^{8}), 45.50 (C^{12}), 46.89 (C^{7}), 49.02 (C^{4}), 53.65 (C^{5}), 139.47 (C^{9}), 139.58 (C^{10}), 173.05 (C^{13}). MS (EI, 70eV), *m/z*, 231(2) $[M]^+$, 216 (1), 202 (1), 174(1), 158(100), 100(90), 91(45), 74(43), 66(82), 57(51), 43(81). IR (Nujol): ν_{max} 3270, 1643, 1546 cm^{-1}. Found (%): C 77.84; H 9.17; N 6.07. $C_{15}H_{21}NO$. Calculated (%): C 77.88; H 9.15; N 6.05.

5-*exo*-Propioamido-*endo,trans,exo*-pentacyclo[8.2.1.1^{4,7}.0^{2,9}.0^{3,8}]tetradec-11-ene

endo,trans,exo-**8**. Yield 87% (0.61 g), white crystals, m.p. 174-175 °C (MeCN). ^{1}H NMR (400.13 MHz, $CDCl_3$): 0.94-1.04 (m, 2H), 1.07-1.11 (m, 3H), 1.22-1.49 (m, 2H), 1.86-1.88 (m, 2H), 1.95-1.99 (m, 2H), 2.01-2.14 (m, 5H), 2.78 (s, 1H), 3.35-3.39 (m, 1H, CH), 5.52-5.53 (m, 2H, CH=CH), 6.25 (s, 1H). ^{13}C NMR (100.62 MHz, $CDCl_3$): 10.05 (C^{17}), 29.83 (C^{16}), 33.03 (C^{2}), 38.58 (C^{13}), 38.64 (C^{8}), 41.27 (C^{7}), 41.73 (C^{6}), 42.36 (C^{9}), 43.37 (C^{1}), 45.28 (C^{10}), 45.33 (C^{14}), 45.36 (C^{3}), 135. 87 (C^{12}), 135.99 (C^{11}), 173.09 (C^{15}). MS (EI, 70eV), *m/z*, 257(9) $[M]^+$, 239 (1), 228 (2), 200 (3), 192(6), 185(8), 169(2), 158(15), 143(13), 130(16), 118(39), 100(31), 91(100), 79(32), 66(47), 57(39), 44(48). IR (Nujol): ν_{max} 3309, 1643, 1545 cm^{-1}. Found (%): C 79.28; H 9.06; N 5.40. $C_{15}H_{21}NO$. Calculated (%): C 79.33; H 9.01; N 5.44.

Crystal data for *endo,trans,exo*-**8**: crystals of $C_{17}H_{23}NO$ (M = 257.36) are monoclinic, space group $P2_1/c$, a = 9.4127(6), b = 15.7092(14) and c = 19.6191(16) Å, b = 92.115(7)°, V = 2899.0(4) $Å^3$, D_{calc} = 1.179 g cm^{-3}, Z = 8, μ = 0.072 mm^{-1}, 13282 reflections were measured, from which 6681 were independent, 2167 reflections with I > 2s(I). The refinement converged to R1 = 0.0775, wR2 = 0.2134, GOF = 0.876.

CCDC 1853228 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk.

Table S3. Bond lengths for *endo,trans,exo*-8

Bond	Length (Å)	Bond	Length (Å)
C^3-C^8	1.551(4)	C^9-C^{10}	1.552(5)
C^3-C^4	1.536(4)	C^2-C^1	1.556(5)
C^3-C^2	1.543(4)	C^{15}-C^{16}	1.493(5)
O^1-C^{15}	1.238(4)	C^1-C^{12}	1.511(5)
C^5-N^1	1.464(5)	C^1-C^{13}	1.524(5)
C^5-C^4	1.518(4)	C^7-C^6	1.535(5)
C^5-C^6	1.542(5)	C^7-C^{14}	1.527(4)
N^1-C^{15}	1.322(4)	C^{10}-C^{11}	1.495(5)
C^8-C^9	1.547(5)	C^{10}-C^{13}	1.550(5)
C^8-C^7	1.517(5)	C^{11}-C^{12}	1.300(5)
C^4-C^{14}	1.524(4)	C^{16}-C^{17}	1.428(6)
C^9-C^2	1.532(4)		

Table S4. Bond angles for *endo,trans,exo*-**8**

Angle	Value (°)	Angle	Value (°)
$C^4C^3C^8$	103.7(3)	$O^1C^{15}N^1$	120.9(3)
$C^4C^3C^2$	118.4(3)	$O^1C^{15}C^{16}$	122.1(4)
$C^2C^3C^8$	89.6(2)	$N^1C^{15}C^{16}$	117.0(3)
$N^1C^5C^4$	112.4(3)	$C^{12}C^1C^2$	107.5(3)
$N^1C^5C^6$	111.7(3)	$C^{12}C^1C^{13}$	99.6(3)
$C^4C^5C^6$	103.4(3)	$C^{13}C^1C^2$	98.7(3)
$C^{15}N^1C^5$	123.1(3)	$C^8C^7C^6$	107.1(3)
$C^9C^8C^3$	89.7(3)	$C^8C^7C^{14}$	102.9(3)
$C^7C^8C^3$	102.9(3)	$C^{14}C^7C^6$	100.2(3)
$C^7C^8C^9$	118.3(3)	$C^{11}C^{10}C^9$	108.8(3)
$C^5C^4C^3$	105.6(2)	$C^{11}C^{10}C^{13}$	99.1(4)
$C^5C^4C^{14}$	101.9(3)	$C^{13}C^{10}C^9$	98.0(3)
$C^{14}C^4C^3$	101.6(3)	$C^7C^6C^5$	103.5(3)
$C^8C^9C^{10}$	119.4(3)	$C^4C^{14}C^7$	95.2(2)
$C^2C^9C^8$	90.1(3)	$C^{12}C^{11}C^{10}$	109.2(4)
$C^2C^9C^{10}$	102.8(3)	$C^{11}C^{12}C^1$	107.5(4)
$C^3C^2C^1$	121.1(3)	$C^{17}C^{16}C^{15}$	116.7(4)
$C^9C^2C^3$	90.6(3)	$C^1C^{13}C^{10}$	93.9(3)
$C^9C^2C^1$	103.8(3)		

5-*exo*-Propioamido-*exo,trans,exo*-pentacyclo[8.2.1.1^{4,7}.0^{2,9}.0^{3,8}]tetradec-11-ene

exo,trans,exo-**8**. Yield 70% (0.49 g), white crystals, m.p. 179-181^{o}C (CH_3CN). ^{1}H NMR (400.13 MHz, $CDCl_3$): 1.09-1.13 (m, 3H), 1.13-1.17 (m, 2H), 1.21-1.24 (m, 2H), 1.31 (m, 2H), 1.41-1.78 (m, 4H), 2.05-2.17 (m, 5H,), 3.46 (s, 1H), 5.49 (s, 1H, NH), 5.92 (s, 2H, CH=CH). ^{13}C NMR (100.62 MHz, $CDCl_3$): 10.06 (C^{17}), 29.88 (C^{16}), 31.21 (C^2), 38.59 (C^{14}), 38.97 (C^8), 39.28 (C^7), 40.15 (C^6), 40.39 (C^{13}), 41.56 (C^3), 41.87 (C^9), 44.15 (C^1), 44.22 (C^{10}), 45.32 (C^4), 51.04 (C^5), 135.39 (C^{12}), 135.49 (C^{11}), 173.12 (C^{15}). MS (EI, 70eV), *m/z*, 257(22) $[M]^+$, 242 (1), 228 (1), 200 (3), 192(82), 185(56), 169(9), 158(35), 143(10), 129(15), 118(46), 100(34), 91(100), 79(33), 66(54), 57(46), 44(41). IR (vaseline oil): ν_{max} 3440, 1644, 1538 cm^{-1}. Found (%): C 79.35; H 9.06; N 5.47. $C_{15}H_{21}NO$. Calculated (%): C 79.33; H 9.01; N 5.44.

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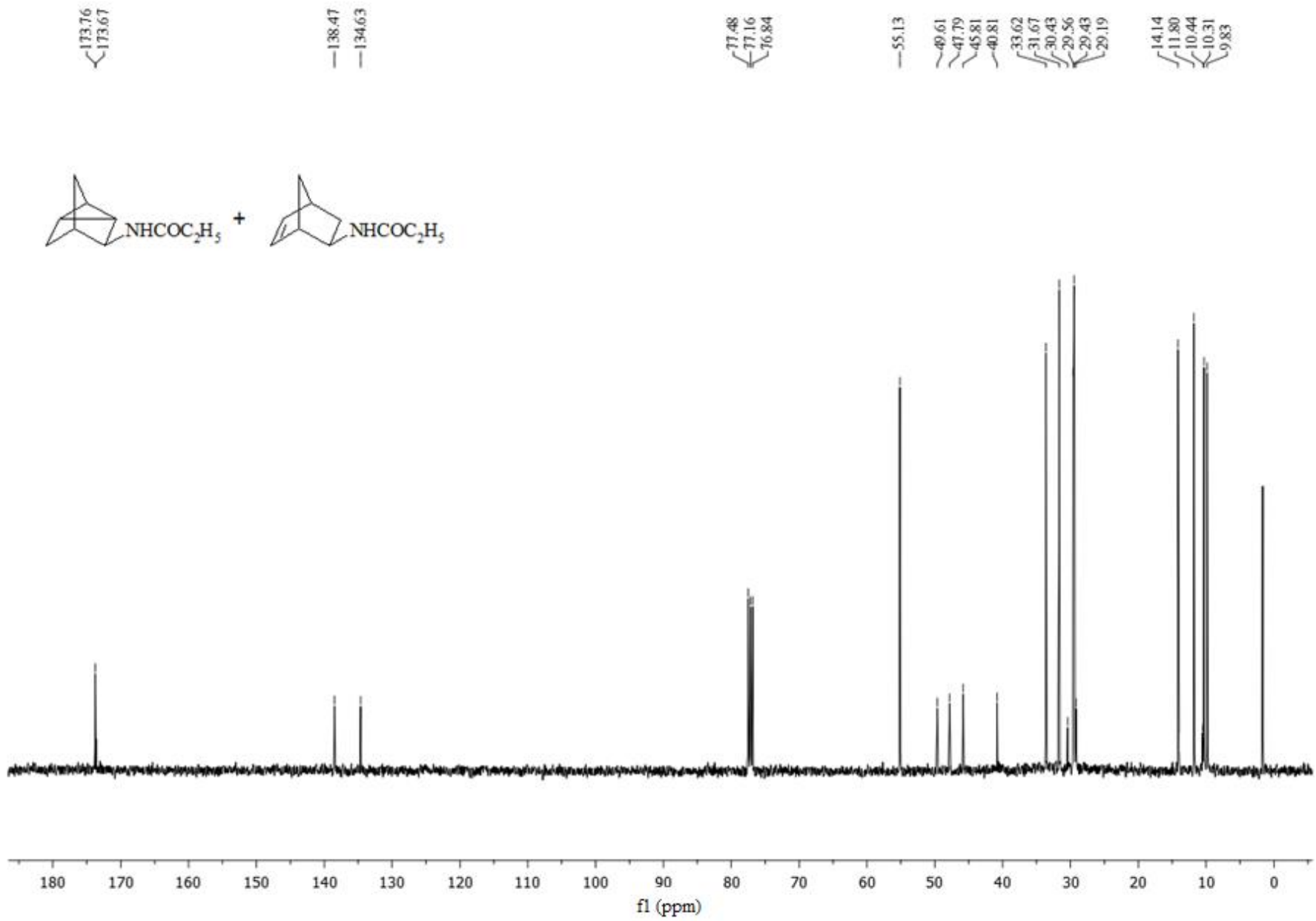
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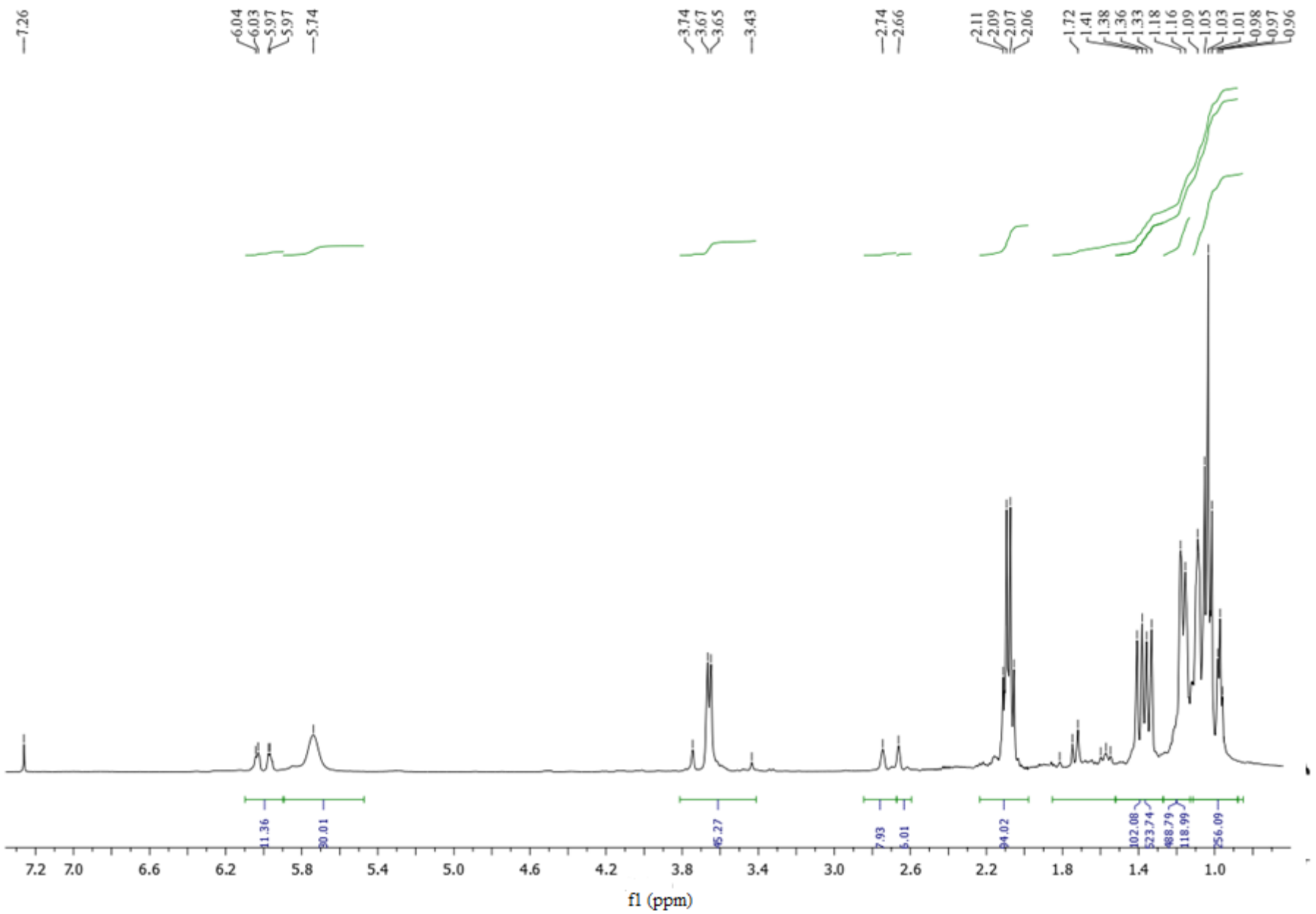
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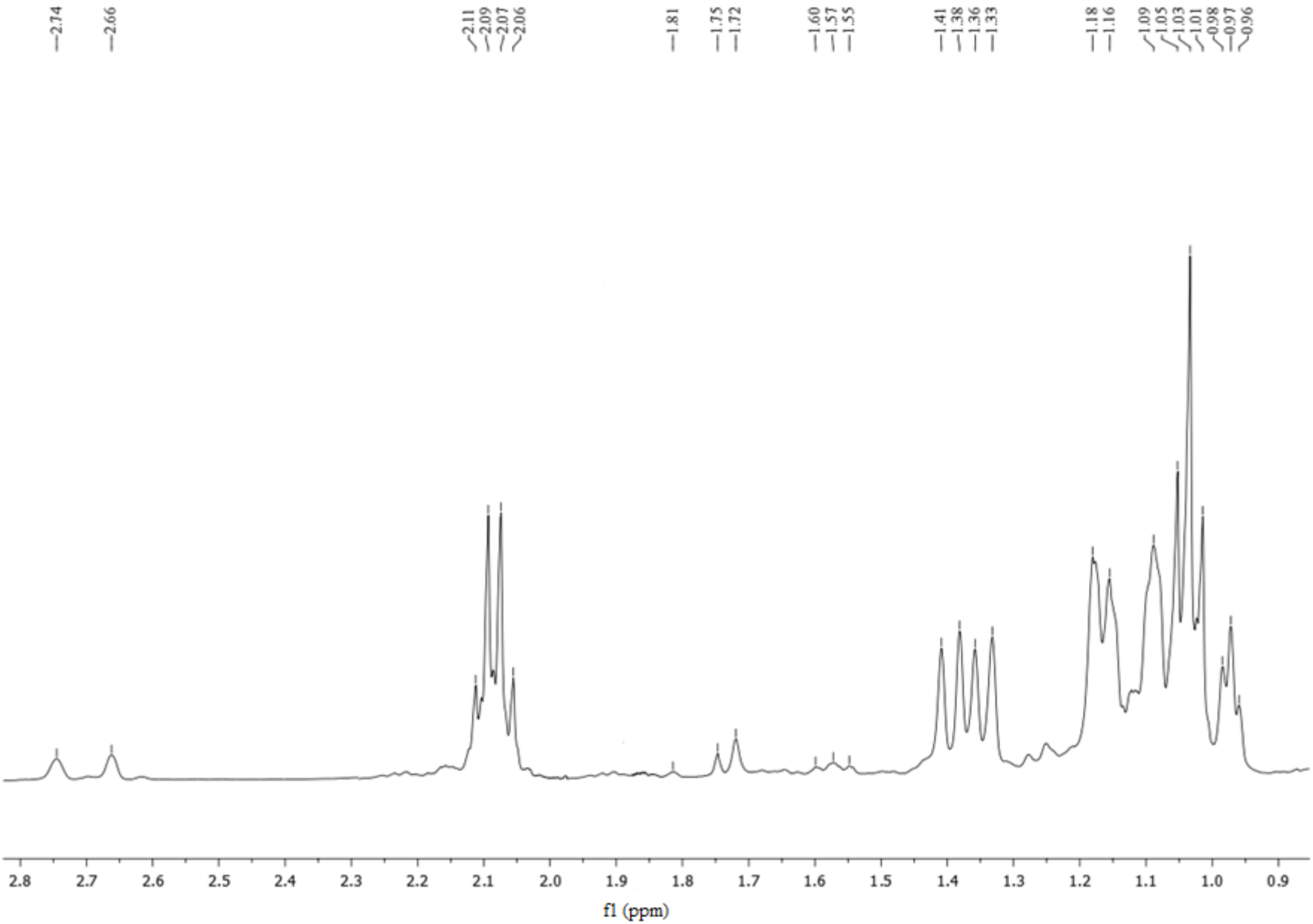
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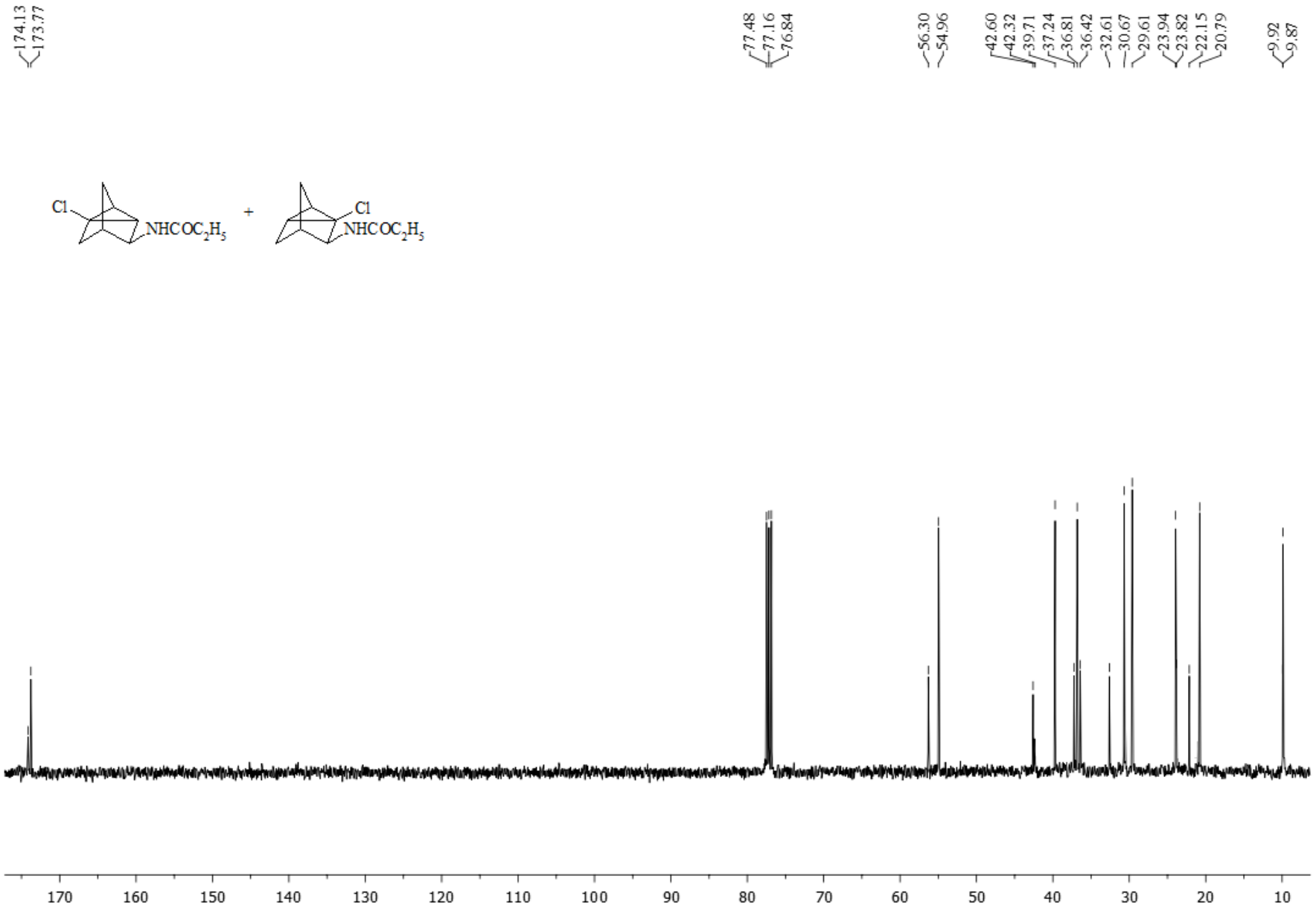
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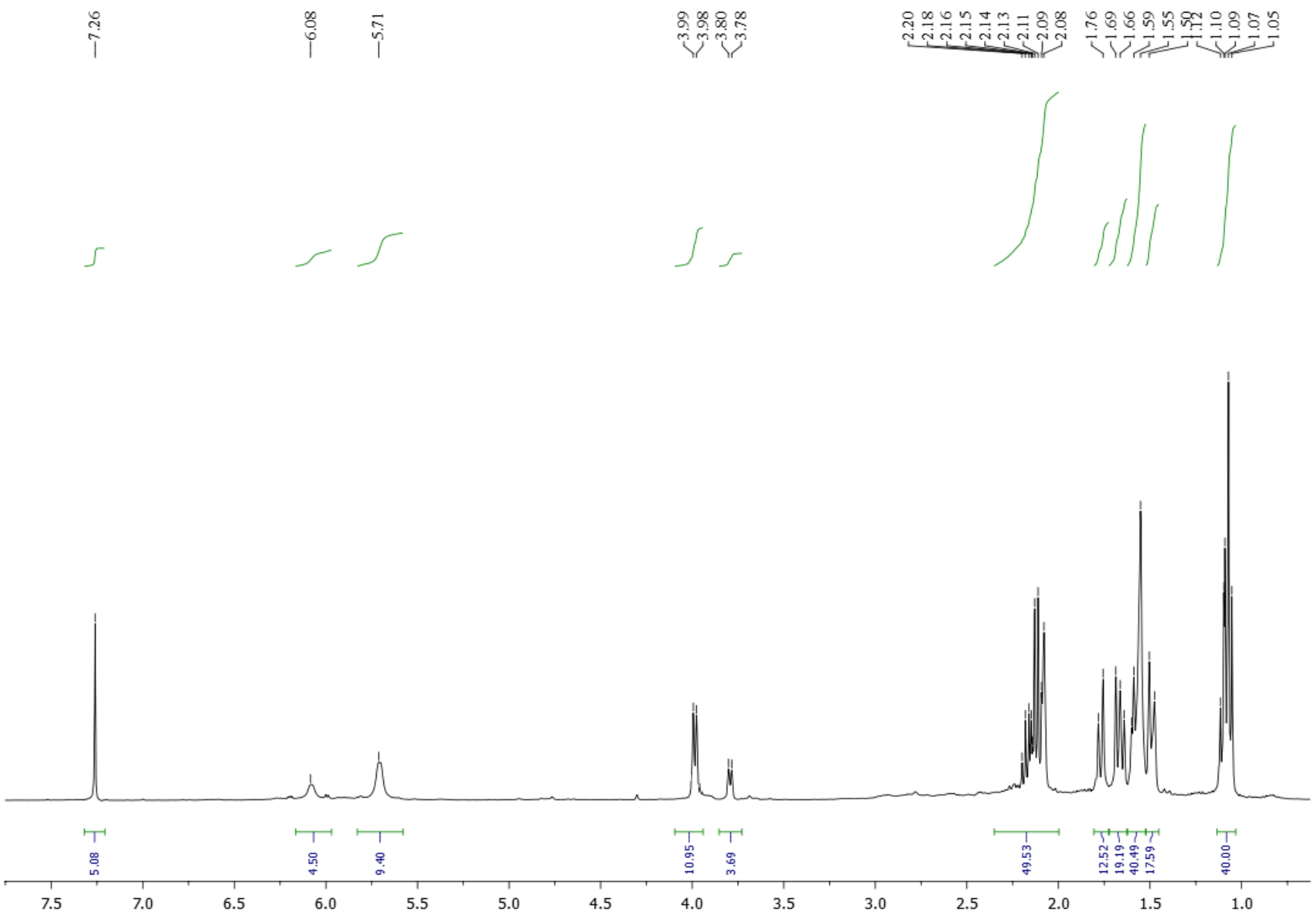
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2.13
2.11
2.09
2.08
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1.69
1.66
1.59
1.55
1.50
1.12
1.10
1.09
1.07
1.05
5.08
4.50
9.40
10.95
3.69
49.53
12.52
19.19
40.49
17.59
40.00
7.5
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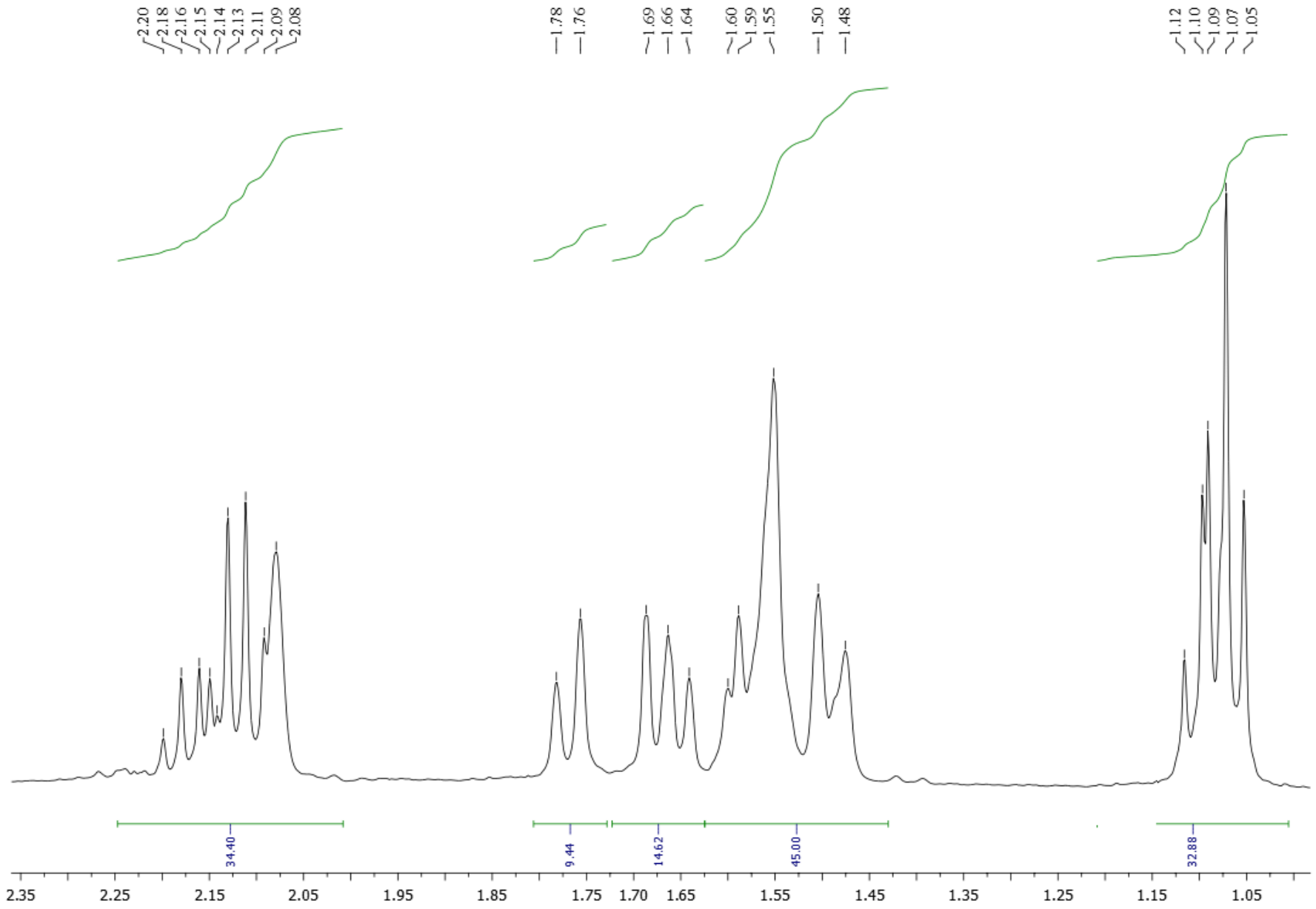
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1.55
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1.12
1.10
1.09
1.07
1.05
34.40
9.44
14.62
45.00
32.88
2.35
2.25
2.15
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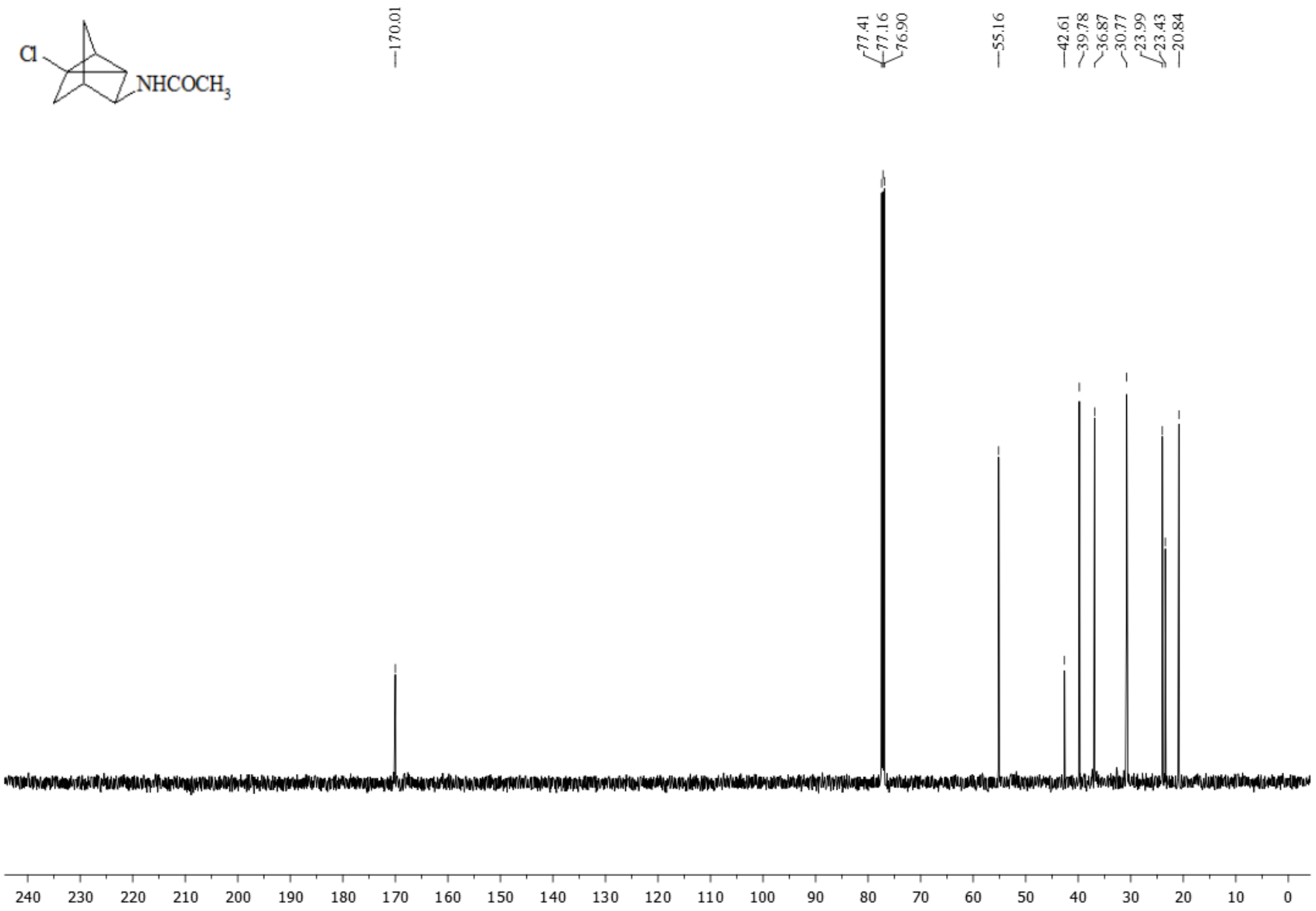
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20.84
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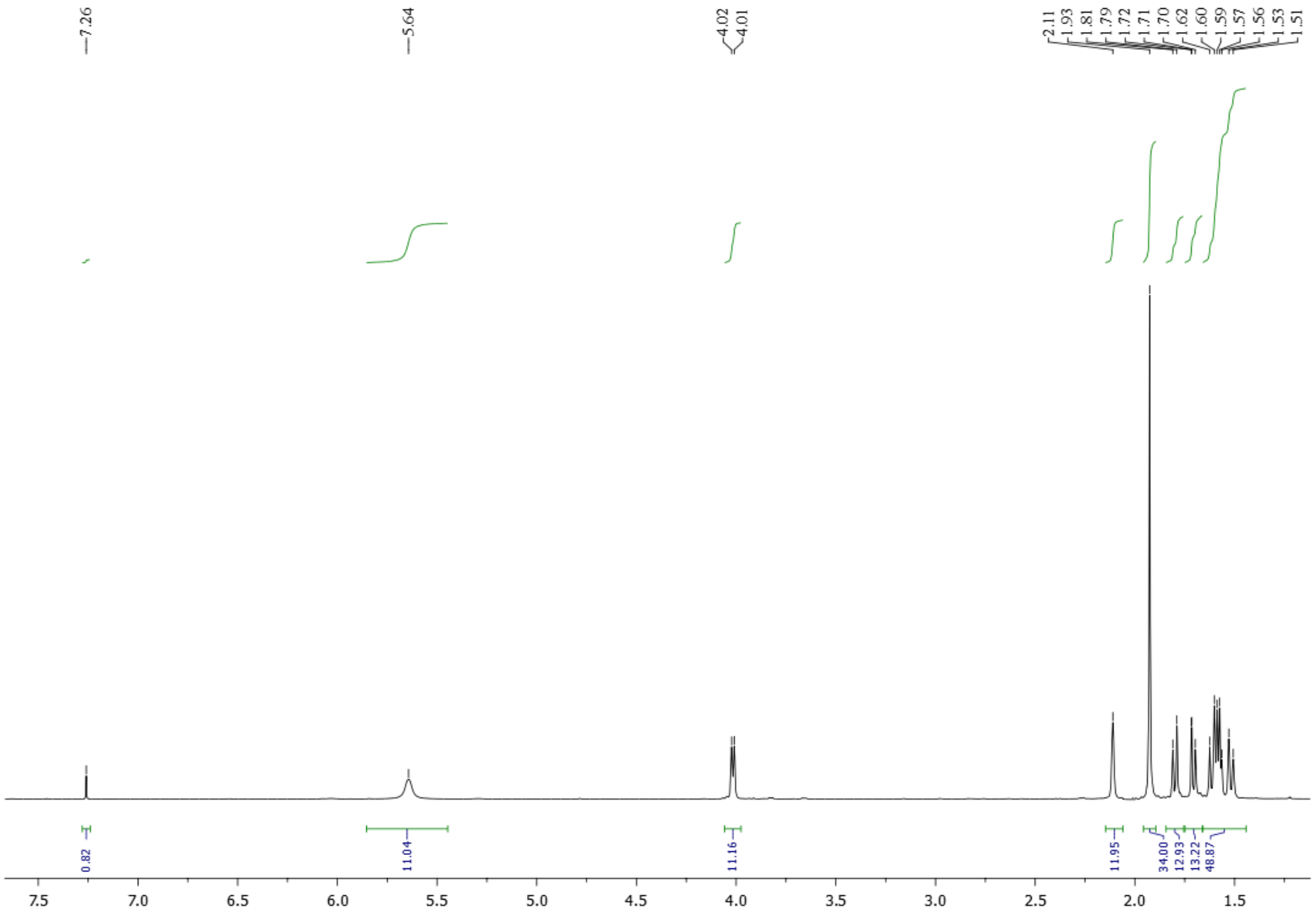
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1.59
1.57
1.56
1.53
1.51
0.82
11.04
11.16
11.95
34.00
12.93
13.22
48.87
7.5
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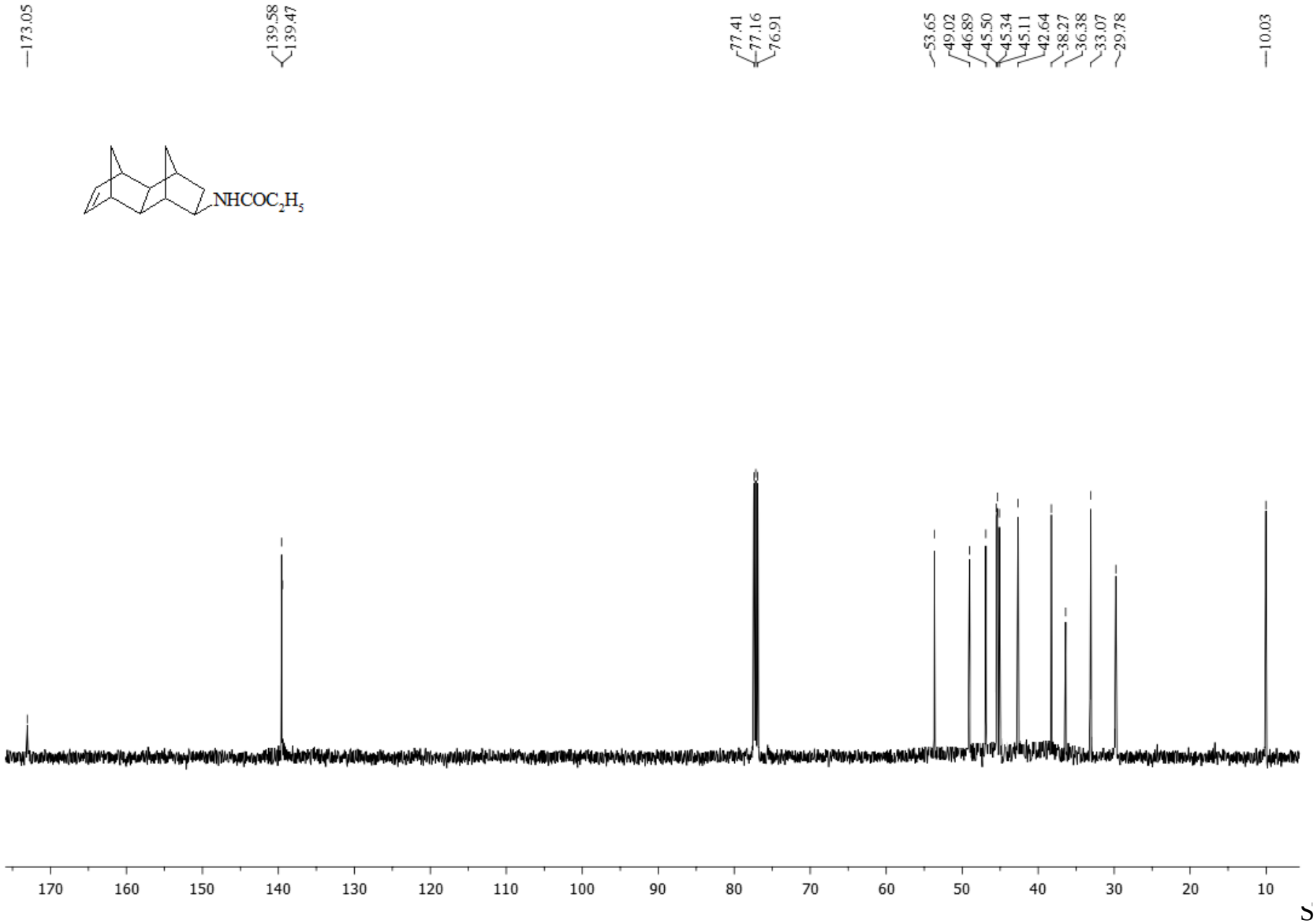
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49.02
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42.64
38.27
36.38
33.07
29.78
10.03
NHCOC2H5
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160
150
140
130
120
110
100
90
80
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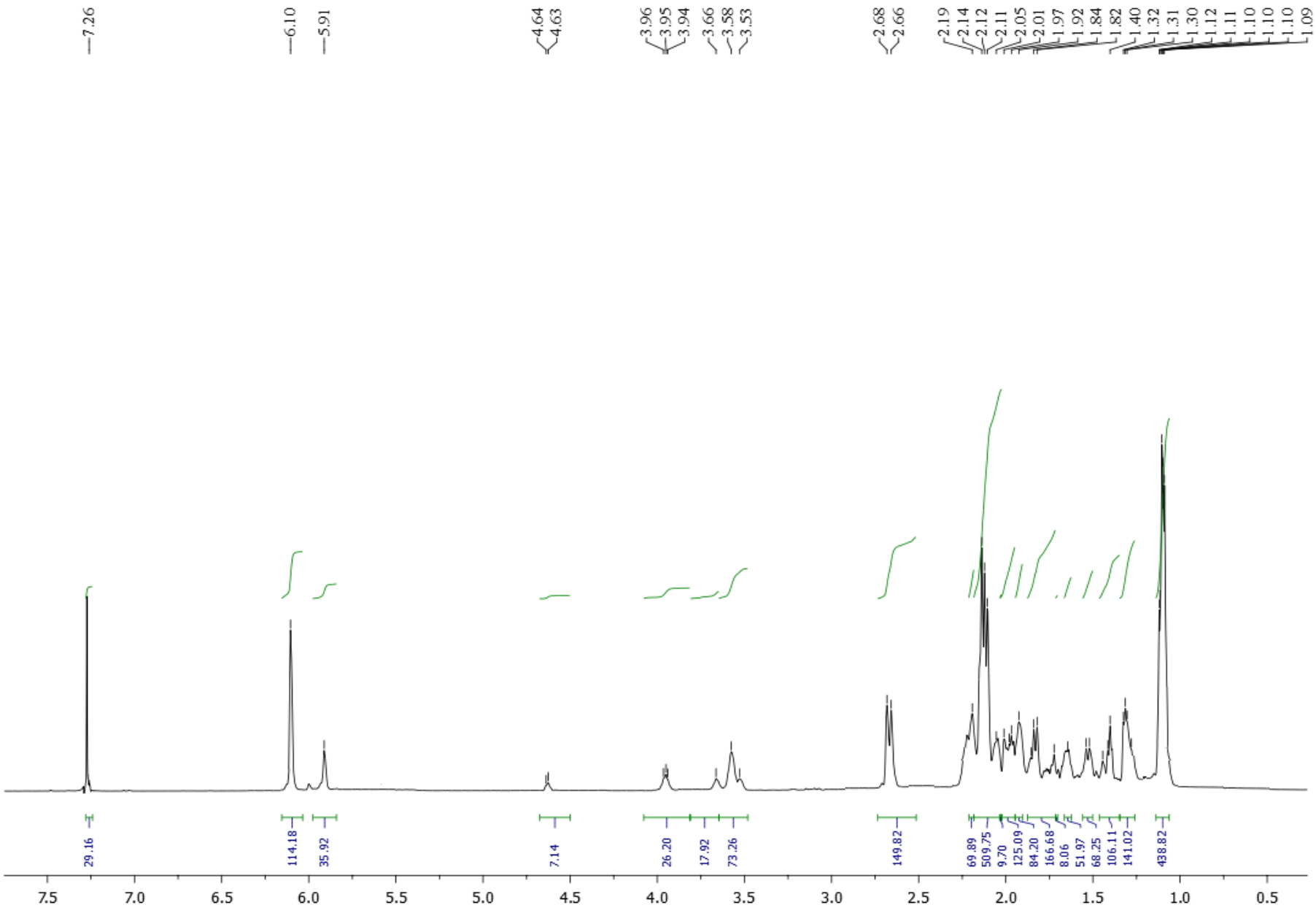
30
20
10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1.92
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1.40
1.32
1.31
1.30
1.12
1.11
1.10
1.10
1.10
1.09
29.16
114.18
35.92
7.14
26.20
17.92
73.26
149.82
69.89
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9.70
125.09
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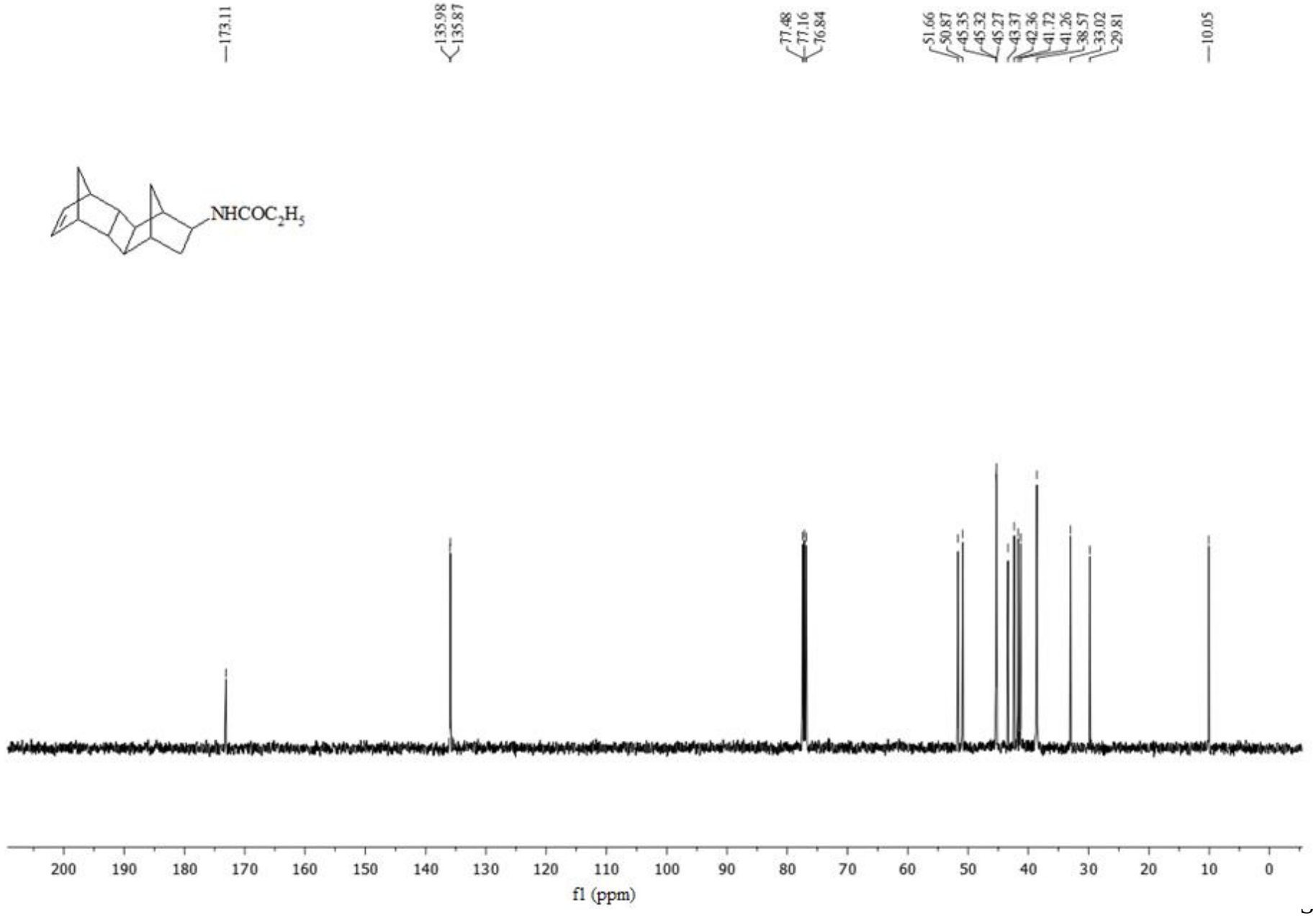
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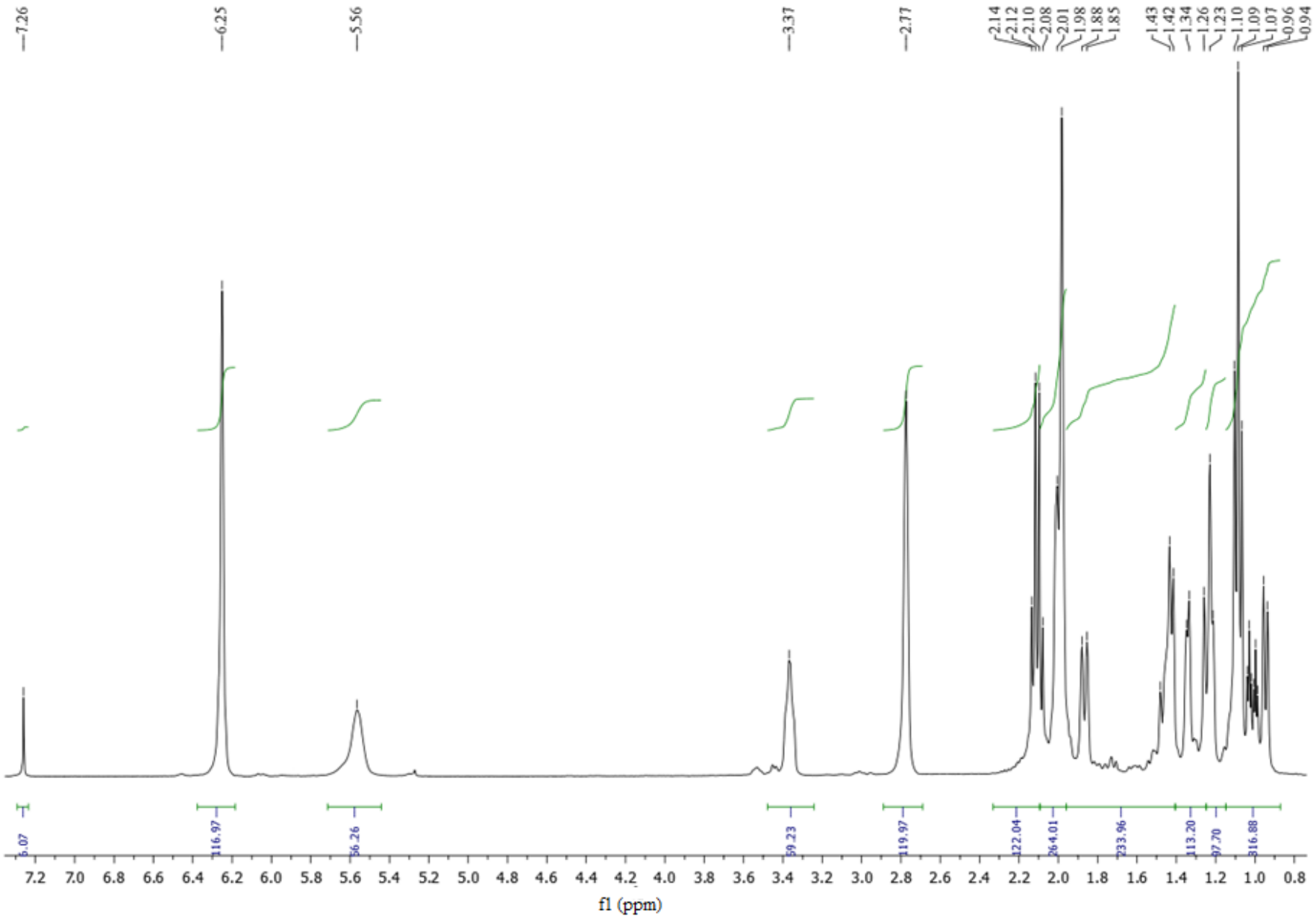
76.84
51.66
50.87
45.35
45.32
45.27
43.37
42.36
41.72
41.26
38.57
33.02
29.81
10.05
NHCOC2H5
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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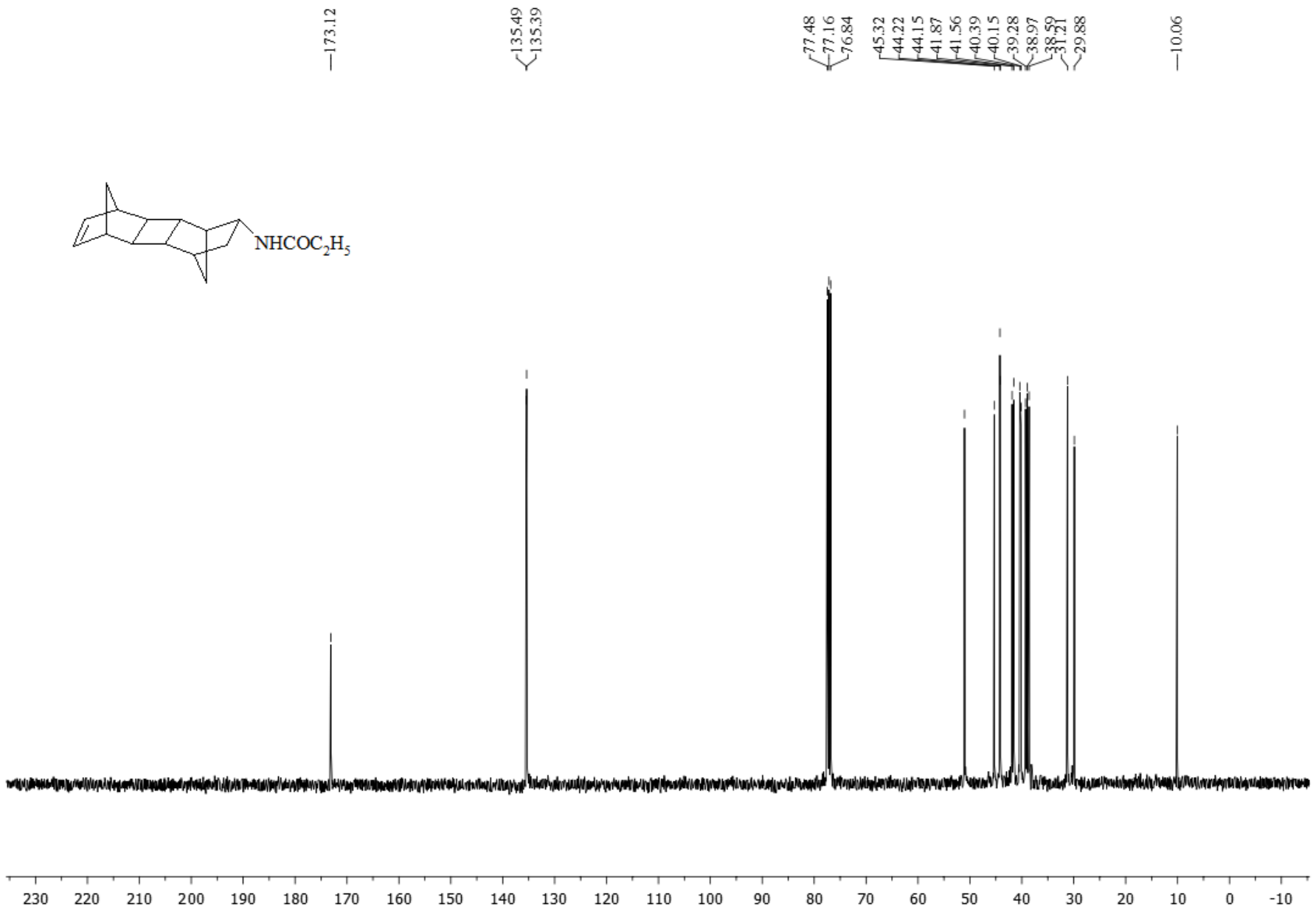
2.10
2.08
2.01
1.98
1.88
1.85
1.43
1.42
1.34
1.26
1.23
1.10
1.09
1.07
0.96
0.94
6.07
16.97
6.26
9.23
19.97
22.04
64.01
33.96
13.20
7.70
16.88
7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
f1 (ppm)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76.84
45.32
44.22
44.15
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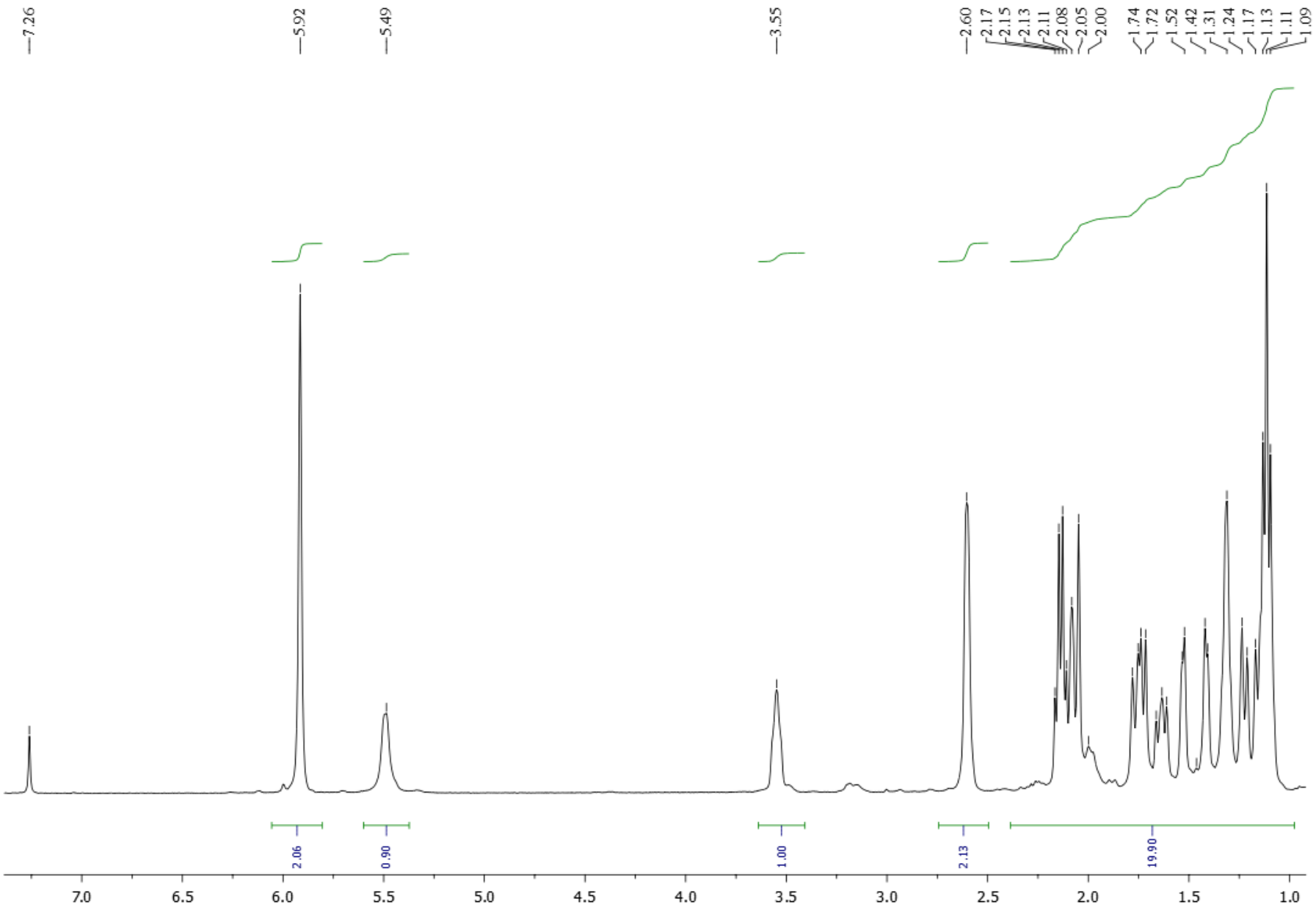
41.56
40.39
40.15
39.28
38.97
38.59
31.21
29.88
10.06
NHCOC2H5
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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2.11
2.08
2.05
2.00
1.74
1.72
1.52
1.42
1.31
1.24
1.17
1.13
1.11
1.09
2.06
0.90
1.00
2.13
19.90
7.0
6.5
6.0
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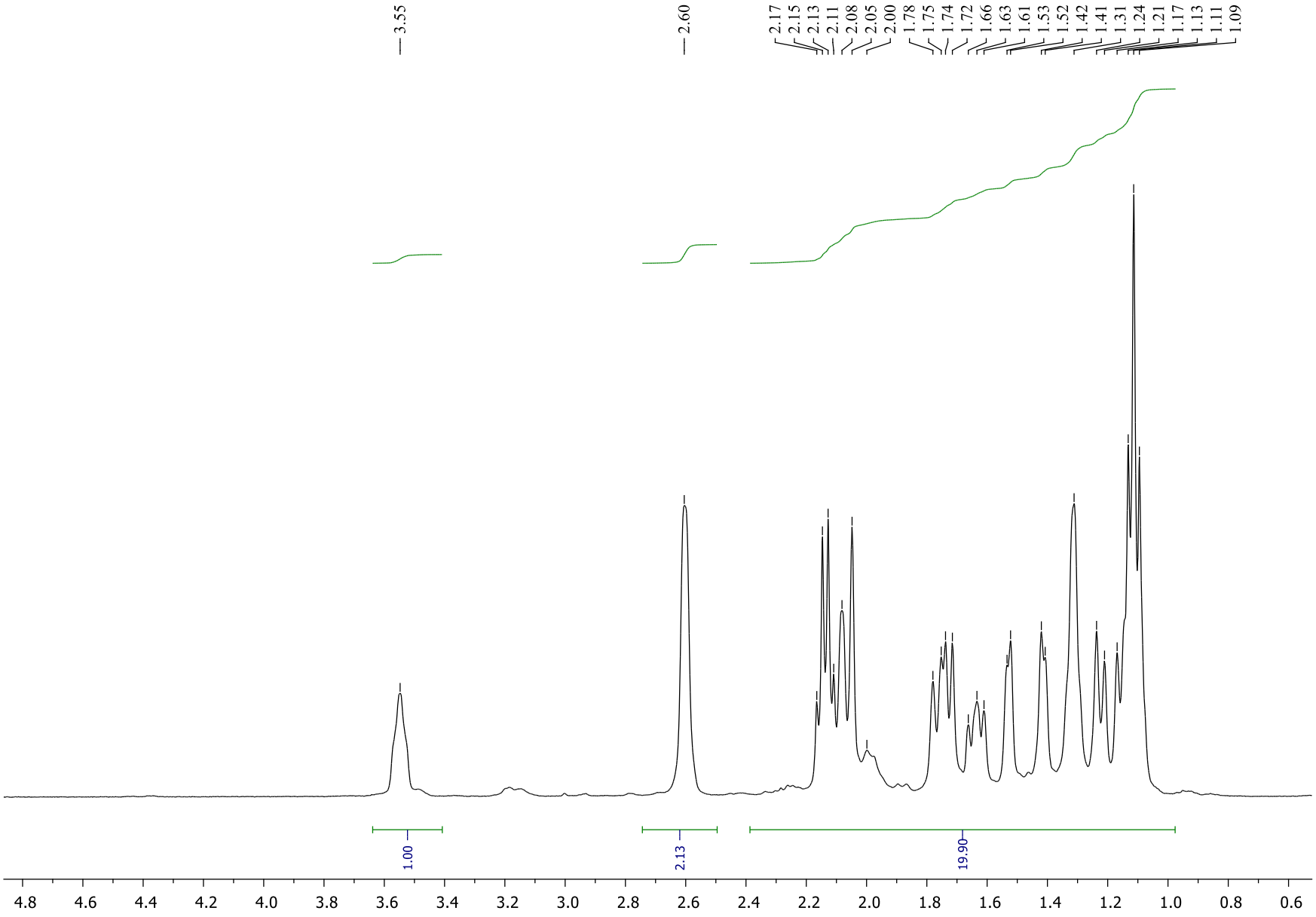
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0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2.00
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1.75
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1.72
1.66
1.63
1.61
1.53
1.52
1.42
1.41
1.31
1.24
1.21
1.17
1.13
1.11
1.09
1.00
2.13
19.90
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6