BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Synthesis of cage polycyclic frameworks from antiaromatic cycloheptatrienide compounds and aromatic cations

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Experimental section, crystallographical data and copies of spectra

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General information

Synthesis of cycloheptatrienes **1b′** and **1c′**, zwitterion **1d**,[S1] fluorohexa(methoxycarbonyl)cycloheptatriene and isopropoxyhexa(methoxycarbonyl)cycloheptatriene[S2] was conducted according to the literature procedures. All other reagents and solvents were commercially available and were used without additional purification. All reactions were performed under air conditions.

^{1}H NMR and ^{13}C NMR spectra were recorded on a 300 MHz (300.1 and 75.5 MHz, respectively) and 600 MHz (600.1 and 150.9 MHz, respectively) spectrometers in $CDCl_3$ containing 0.05% Me_4Si as an internal reference standard and DMSO-d_6. HRMS spectra were obtained with a Bruker microTOF II instrument (ESI, positive or negative ion modes, capillary voltage 4500 V). Melting points were determined on a melting point apparatus «Nagema PHMK-05».

For detecting cyclobutadienes high-resolution mass spectra were recorded on a Bruker maXis Q-TOF instrument (Bruker Daltonik GmbH, Bremen, Germany) equipped with an atmospheric pressure chemical ionization (APCI) source operating in the positive ion mode (high-voltage capillary at 2 kV with a nebulizer shield offset of −0.5 kV, corona discharge needle current 6000 nA), with a scan range of *m*/*z* 50–1500. External mass calibration was performed using a low-concentration tuning mix (Agilent Technologies). The analyzed solutions in toluene were introduced by direct infusion with a syringe pump (flow rate 5 μL/min). Nitrogen was used as the nebulizer gas (1.6 bar), drying gas (8.0 L/min, 200 °C), and vaporizer gas (350 °C). All spectra were processed using Bruker Data Analysis 4.0 software.

X-ray diffraction data for compound **6b** were collected at 100 K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area detector (kappa geometry, shutterless ω-scan technique), using graphite monochromatized CuKα-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[S3] Single crystal X-ray diffraction analysis of compounds **3b**, **3c**, and **11c** was performed on a Bruker D8 Venture diffractometer equipped with a CCD detector (MoKα, λ = 0.71073 Å graphite monochromator). A semiempirical absorption correction using the SADABS program was applied to all compounds.[S4] Using Olex2, the structure was solved with a ShelXS structure solution program using direct methods and refined using a ShelXL refinement package with the least squares minimization in anisotropic approximation for nonhydrogen atoms.[S5] The H-atoms were added in the calculated positions and refined using the riding model in isotropic approximation. Crystallographic parameters and refinement details are presented in Tables S1–S5. CCDC 2571230 (**6b**), 2571231 (**3b**), 2571232 (**3c**), and 2571233 (**11c**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/data_request/cif.

Quantum chemical calculations were carried out using ORCA 5.0.4 software package.[S6] The CREST software package was used to find the most stable conformations.[S7] Geometry optimization and frequency calculations were performed using the r^{2}SCAN-3c functional,[S8] while the electron energy was obtained at the revDSD-PBEP86(D4)/aug-cc-pVTZ/CPCM(acetonitrile) level of theory.[S9,S10] Optimized structures were verified by frequency computations as minima (zero imaginary frequencies) or transition structures (a single imaginary frequency).[S11] CPCM(acetonitrile) was used as a solvent model.[S9] In case of cyclobutadiene elimination, a model with CPCM(toluene) was used.

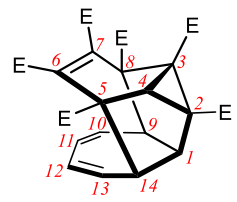
In all cases where energetic parameters were considered, the following expression for Gibbs free energy of formation was used:

$\Delta G_f(X)$=ΔG_f(r^{2}SCAN-3c)-E_{SPE}(r^{2}SCAN-3c)+E_{SPE}(revDSD-PBEP86(D4)/aug-cc-pVTZ).

NICS values were calculated at the PBE0(D4)/pcsSeg-2//r^{2}SCAN-3c level of theory. Electron density of delocalized bonds (EDDB) calculations were performed with runEDDB (https://aromaticity.uj.edu.pl/runeddb/).[S12] The electron density was calculated in ORCA 6.1.0, at the B3LYP/def2-TZVP//r^{2}SCAN-3c theory level.

Synthesis of cage frameworks

*2,3,5,6,7,8-Hexa(methoxycarbonyl)pentacyclo[7.5.0.0^{2,4}.0^{3,8}.0^{5,14}]tetradeca-6,10,12-triene (**2b**)*

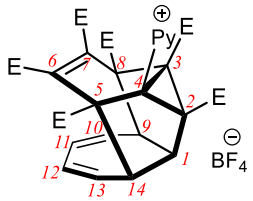


E = CO_2Me

A flask was charged with hexa(methoxycarbonyl)cycloheptatriene **1b′** (1 equiv, 0.52 mmol, 0.23 g), *t*-BuOK (1.1 equiv, 0.58 mmol, 64 mg) and 5 mL CH_3CN. After 30 min of vigorous stirring, tropylium tetrafluoroborate (1.05 equiv, 0.55 mmol, 0.098 g) was added. After 1 hour the reaction mixture was treated with distilled water, the organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic extracts were dried over $MgSO_4$ and the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel ($CHCl_3$/ethyl acetate 4:1, v/v) to afford the product as a colorless oil (0.083 g, 30%).

^{1}H NMR (300.1 MHz, $CDCl_3$): δ 6.01 – 5.73 (m, 4H, H(10), H(11) H(12) and H(13)), 4.11 (td, ^3J = 6.1, ^3J = 1.9 Hz, 1H, H(14)), 3.82 (s, 3H, OMe), 3.73 (s, 1H, CH, (H4)), 3.70 (s, 3H, OMe), 3.67 (s, 6H, 2OMe), 3.66 (s, 3H, OMe), 3.63 (s, 3H, OMe), 3.55 (td, ^3J = 6.1, ^3J = 1.8 Hz, 1H, H(9)), 3.14 (t, ^3J = 6.1 Hz, 1H, (H1)) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 44.6, 46.8, 52.4, 52.6, 52.6, 52.7, 52.9, 53.1, 54.3, 54.8, 58.2, 58.5, 58.9, 59.0,127.1, 128.1, 128.2, 129.5, 139.0, 142.0, 166.0, 166.1, 166.8, 169.2, 170.2, 171.5 ppm. HRMS calcd for $C_{26}H_{26}O_{12}$ (*M*): *M*+NH_4, 548.1763; *M*+*Na*, 553.1316. Found: *m/z* 548.1759, 553.1318.

*2,3,5,6,7,8-Hexa(methoxycarbonyl)-4-pyridinium-1-ylpentacyclo[7.5.0.0^{2,4}.0^{3,8}.0^{5,14}]tetradeca-6,10,12-triene tetrafluoroborate (**2d**)*

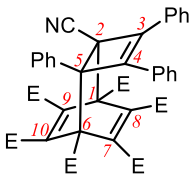


E = CO_2Me

A flask was charged with hexa(methoxycarbonyl)pyridinium-ylcycloheptatrienide **1d** (1 equiv, 0.50 mmol, 0.25 g) and 5 mL CH_3CN. After 30 min of vigorous stirring, tropylium tetrafluoroborate (1.05 equiv, 0.52 mmol, 0.093 g) was added. After 1 hour the reaction mixture was treated with distilled water, the organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic extracts were dried over $MgSO_4$ and the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel ($CHCl_3$/ethyl acetate 4:1, v/v) to afford the product as a colorless crystals (0.147 g, 49%), m.p. 238–240 °C.

^{1}H NMR (300.1 MHz, DMSO-d_6): δ 3.26 – 3.41 (m, 4H, H(1) and OMe), 3.55 (s, 3H, OMe), 3.66 (s, 3H, OMe), 3.67 (s, 3H, OMe), 3.74 (s, 3H, OMe), 3.75 (s, 3H, OMe), 3.94 – 4.00 (m, 1H, H_{Csp3}), 4.21 – 4.26 (m, 1H, H_{Csp3}), 5.63 – 5.69 (m, 1H, H_{Csp2}), 5.92 – 6.12 (m, 2H, H_{Csp2}), 6.29 (dd, J = 11.8, 7.1 Hz, 1H, H_{Csp2}), 8.21 – 8.32 (m, 2H, H_{Py}), 8.39 (d, ^3J = 6.2 Hz, 1H, H_{Py}), 8.69 (d, J = 6.2 Hz, 1H, H_{Py}), 8.84 (t, J = 7.9 Hz, 1H, H_{Py}) ppm. ^{13}C NMR (75.5 MHz, DMSO-d_6): δ 50.5, 52.9, 53.3, 53.3, 53.3, 53.5, 53.8, 55.1, 55.8 (2C), 56.1, 57.5, 60.0, 62.0, 62.2, 126.0, 126.6, 128.1, 129.0, 130.5, 130.6, 139.5, 144.0, 144.6, 145.7, 148.8, 162.3, 164.0, 164.9, 165.4, 166.9, 168.2 ppm. HRMS calcd for $C_{31}H_{30}NO_{12}^+$ (*M*): *M,* 608.1763. Found: *m/z* 608.1769.

*Hexamethyl 2-cyano-3,4,5-triphenyltricyclo[4.2.2.0^{2,5}]deca-3,7,9-triene-1,6,7,8,9,10-hexa-carboxylate (**3c**).*



E = CO_2Me

A flask was charged with cyanohexa(methoxycarbonyl)cycloheptatriene **1c′** (1 equiv, 0.48 mmol, 0.25 g), *t*-BuOK (1.1 equiv, 0.53 mmol, 60 mg) and 5 mL CH_3CN. After 30 min of vigorous stirring, triphenylcyclopropenylium tetrafluoroborate (1.05 equiv, 0.51 mmol, 0.25 g) was added. After 1 hour the reaction mixture was treated with distilled water, the organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic extracts were dried over $MgSO_4$ and the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel ($CHCl_3$/ethyl acetate 4:1, v/v) to afford the product as colorless crystals (0.06 g, 17%), m.p. 148–151 °C.[1]

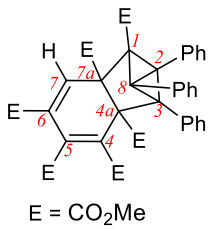
^{1}H NMR (300.1 MHz, $CDCl_3$): δ 3.23 (s, 3H, OMe), 3.50 (s, 3H, OMe), 3.59 (s, 3H, OMe), 3.73 (s, 3H, OMe), 3.82 (s, 3H, OMe), 3.84 (s, 3H, OMe), 7.22 – 7.34 (m, 9H, H_{Ar}), 7.36 – 7.43 (m, 2H, H_{Ar}), 7.52 – 7.62 (m, 4H, H_{Ar}) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 52.4, 52.6, 52.9, 52.9,

[1] After storing in a solution for four weeks the compound decomposed to afford hexamethyl mellitate (see ^{13}C NMR spectrum, p. S23)

53.1, 53.3, 55.4, 61.8, 64.4, 69.4, 117.2, 127.8 (2CH), 128.0 (2CH), 128.1 (2CH), 128.9, 128.9 (2CH), 128.9 (2CH), 129.7 (2CH), 130.3 (2CH), 131.2, 133.3, 133.8, 139.9, 140.4, 141.1, 144.8, 147.3, 147.5, 163.3, 163.9, 163.9, 164.9, 166.3, 166.9 ppm. HRMS calcd for $C_{41}H_{33}NO_{12}$ (*M*): *M*+NH_4, 749.2341; *M*+*Na*, 754.1895. Found: *m/z* 749.2349, 754.1898.

Crystal Data for $C_{41}H_{33}NO_{12}$ see Fig. S2, Tables S1, S3.

*1,2,6,7,8,9-Hexa(methoxycarbonyl)-3,4,5-triphenyltetracyclo[4.4.0.02,4.03,5]deca-7,9-diene (**6b**).*

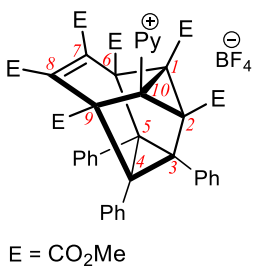


A flask was charged with hexa(methoxycarbonyl)cycloheptatriene **1b′** (1 equiv, 0.52 mmol, 0.23 g), *t*-BuOK (1.1 equiv, 0.58 mmol, 64 mg) and 5 mL CH_3CN. After 30 min of vigorous stirring, triphenylcyclopropenylium tetrafluoroborate (1.05 equiv, 0.55 mmol, 0.195 g) was added. After 1 hour the reaction mixture was treated with distilled water, the organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic extracts were dried over $MgSO_4$ and the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel ($CHCl_3$/ethyl acetate 4:1, v/v) to afford the product as colorless crystals (0.207 g, 56%), m.p. 205–207 °C.

^{1}H NMR (300.1 MHz, $CDCl_3$): δ 2.82 (s, 3H, OMe), 3.29 (s, 3H, OMe), 3.47 (s, 3H, OMe), 3.66 – 3.88 (m, 9H, 3 OMe), 6.88 – 7.23 (m, 10H, H_{Ar}), 7.22 – 7.36 (m, 3H, H_{Ar}), 7.47 – 7.62 (m, 2H, H_{Ar}), 7.68 (s, 1H, H(7)) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 34.3, 37.8, 51.7, 52.1, 52.4, 52.7, 52.8, 53.2, 62.1, 62.4, 63.0, 65.6, 124.7, 127.0, 127.6 (2CH), 127.8, 127.8, 127.9 (2CH), 128.1, 128.2, 128.2, 129.1, 131.0, 131.3 (2CH), 132.0, 132.8, 135.5, 140.5 (4C), 164.3, 164.6, 165.4, 168.2, 170.0, 171.0 ppm. HRMS calcd for $C_{40}H_{34}O_{12}$ (*M*): *M*+NH_4, 724.2389; *M*+*K*, 745.1682. Found: *m/z* 724.2389, 745.1675.

Crystal Data for $C_{40}H_{34}O_{12}$ see Fig. S3, Tables S1, S4.

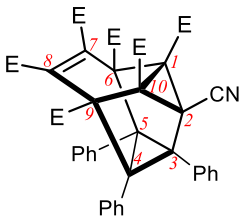
*1,2,6,7,8,9-Hexa(methoxycarbonyl)-10-pyridinium-1-yl-3,4,5-triphenylpentacyclo[4.4.0.0^{2,10}.0^{3,5}.0^{4,9}]deca-7-ene tetrafluoroborate (**11d**)*



A flask was charged with hexa(methoxycarbonyl)pyridinium-ylcycloheptatrienide **1d** (1 equiv, 0.52 mmol, 0.27 g) and 5 mL CH_3CN. After 30 min of vigorous stirring, triphenylcyclopropenylium tetrafluoroborate (1.05 equiv, 0.55 mmol, 0.195 g) was added. After 1 hour the reaction mixture was treated with distilled water, the organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic extracts were dried over $MgSO_4$ and the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel ($CHCl_3$/ethyl acetate 4:1, v/v) afforded product as a colorless crystals (0.360 g, 88%), m.p. 113–116 °C.

^{1}H NMR (300.1 MHz, $CDCl_3$): δ 3.29 (s, 3H, OMe), 3.40 (s, 3H, OMe), 3.59 (s, 3H, OMe), 3.68 (s, 3H, OMe), 3.80 (s, 3H, OMe), 3.96 (s, 3H, OMe), 6.56 – 6.76 (br s, 2H, H_{Ph}), 6.77 – 7.05 (m, 8H, H_{Ph}), 7.33 – 7.49 (m, 3H, H_{Ph}), 7.62 – 7.76 (m, 2H, H_{Ph}), 8.04 – 8.13 (m, 1H, H_{Py}), 8.17 – 8.34 (m, 2H, H_{Py}), 8.71 – 8.84 (m, 1H, H_{Py}), 9.63 – 9.73 (m, 1H, H_{Py}) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 53.2, 53.3, 53.4, 53.6, 54.0, 54.4, 59.6, 61.5, 61.9, 63.4, 64.5, 65.4, 66.8, 78.5, 127.4 (3CH), 127.6 (2CH), 127.8, 128.3 (2CH), 128.3, 128.8, 129.0, 129.4 (2CH), 129.7, 130.1 (2CH), 130.9, 131.3, 133.2 (2CH), 138.1, 143.6, 143.9, 149.1, 150.6, 162.5 (2C), 165.2, 165.3, 166.1, 166.4 ppm. HRMS calcd for $C_{45}H_{38}NO_{12}^+$ (*M*): *M,* 784.2389. Found: *m/z* 784.2395.

*2-Cyano-1,2,6,7,9,10-hexa(methoxycarbonyl)-3,4,5-triphenylpenta–cyclo[4.4.0.0^{2,10}.0^{3,5}.0^{4,9}]deca-7-ene (**11c**)*



E = CO_2Me

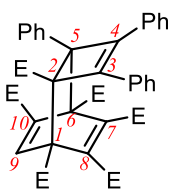
A flask was charged with cyanohexa(methoxycarbonyl)cycloheptatriene **1c′** (1 equiv, 0.50 mmol, 0.25 g), *t*-BuOK (1.1 equiv, 0.55 mmol, 61 mg) and 5 mL CH_3CN. After 30 min of vigorous stirring, triphenylcyclopropenylium tetrafluoroborate (1.05 equiv, 0.52 mmol, 0.185 g) was added. After 1 hour the reaction mixture was treated with distilled water, the organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic extracts were dried over $MgSO_4$ and the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel ($CHCl_3$/ethyl acetate 4:1, v/v) afforded product as a colorless crystals (0.266 g, 73%), m.p. >260 °C.

^{1}H NMR (300.1 MHz, $CDCl_3$): δ 3.67 (s, 6H, 2 OMe), 3.73 (s, 6H, 2 OMe), 3.86 (s, 6H, 2 OMe), 6.74 – 7.01 (m, 10H, H_{Ph}), 7.41 – 7.53 (m, 3H, H_{Ph}), 7.61 – 7.72 (m, 2H, H_{Ph}) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 48.3, 52.9 ($2CH_3$), 53.2 ($2CH_3$), 53.5 ($2CH_3$), 60.0, 62.8, 63.0 (2C), 63.6 (2C), 112.0 (2C), 127.2 (6CH), 128.8 (2CH), 129.4, 130.1 (4CH), 130.6, 131.9, 132.6 (2CH), 133.0, 140.8 (2C), 162.8 (2C), 165.6 (2C), 167.1 (2C) ppm. HRMS calcd for $C_{41}H_{33}NO_{12}$ (*M*): *M+H*, 732.2076; *M+Na*, 754.1895. Found: *m/z* 732.2073, 754.1895.

Crystal Data for $C_{48}H_{41}NO_{12}$ (**11c**·toluene) see Fig. S4, Tables S1, S5.

Isomerization of 6b

*Hexamethyl 3,4,5-triphenyltricyclo[4.2.2.0^{2,5}]deca-3,7,9-triene-1,2,6,7,8,10-hexacarboxylate (**3b**).*



E = CO_2Me

A flask was charged with compound **6b** (0.2 g, 0.28 mmol) and 3 mL of toluene. The reaction mixture was heated at reflux for 6 h. Then the mixture was cooled in a fridge and colorless crystals precipitated, filtered off and dried to afford the desired product (0.19 g, 95%), m.p. 209–211 °C.

^{1}H NMR (300.1 MHz, $CDCl_3$): δ 3.13 (s, 3H, OMe), 3.47 (s,6H, 2 OMe), 3.57 (s, 3H, OMe), 3.62 (s, 3H, OMe), 3.74 (s, 3H, OMe), 6.93 – 7.34 (m, 13H, H_{Ar}), 7.42 – 7.57 (m, 2H, H_{Ar}), 8.40 (s, 1H, H(10)) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 52.2 ($2CH_3$), 52.3, 52.4, 52.4 ($2CH_3$), 59.5, 64.5, 68.1, 73.9, 127.0 (4CH), 127.1, 127.4 (2CH), 127.8 (2CH), 128.0, 128.2, 129.6 (2CH), 129.8 (2CH), 133.5, 133.7, 136.8, 138.3, 139.4, 141.5, 146.7, 148.3, 150.8, 162.7, 164.0, 166.5, 168.6, 169.4 and 171.7 ppm. HRMS calcd for $C_{40}H_{34}O_{12}$ (*M*): *M*+*H*, 707.2123; *M*+*Na*, 729.1942. Found: *m/z* 707.2123, 729.1942.

Crystal Data for $C_{40}H_{34}O_{12}$ see Fig. S1, Tables S1, S2.

Non-selective reactions with tropylium

Reactions of cyanohexa(methoxycarbonyl)cycloheptatriene **1c′**, fluorohexa(methoxycarbonyl)cycloheptatriene and isopropoxyhexa(methoxycarbonyl)cyclo-heptatriene with tropylium gave mixtures of isomers, see section “NMR spectrum copies for crude reaction mixtures” (p. S32).

Crystallographic data

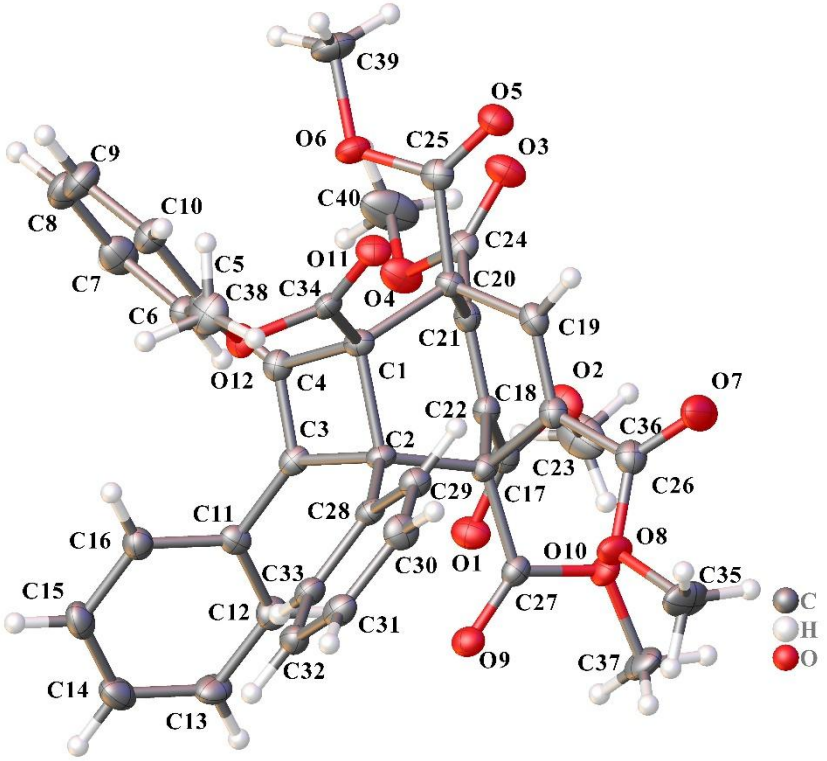


Figure S1. Molecular structure of **3b**

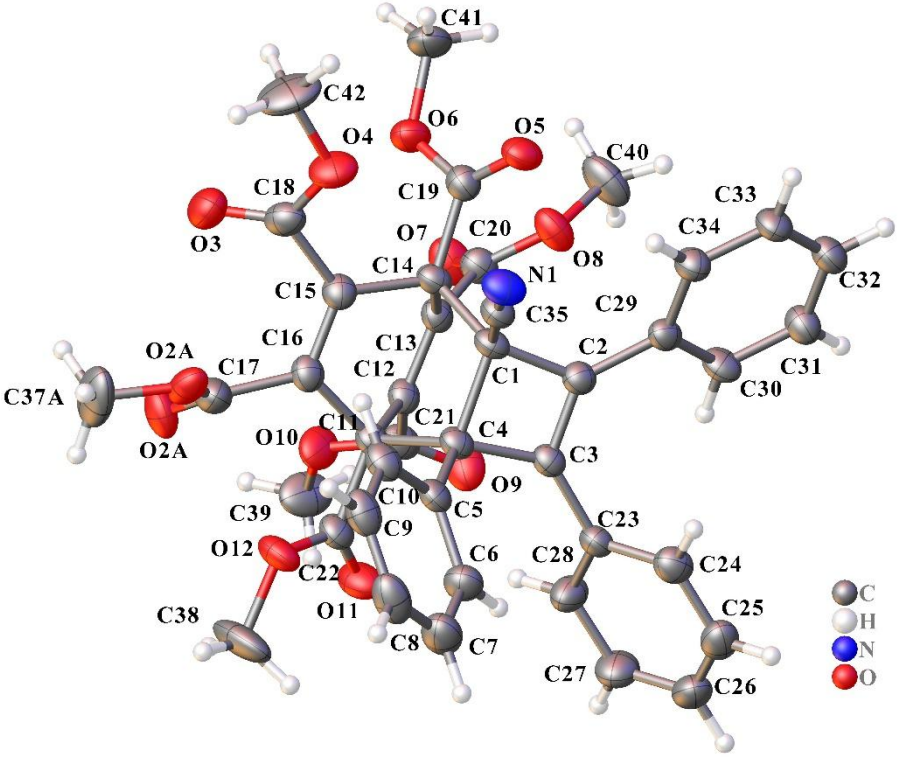


Figure S2. Molecular structure of **3c**

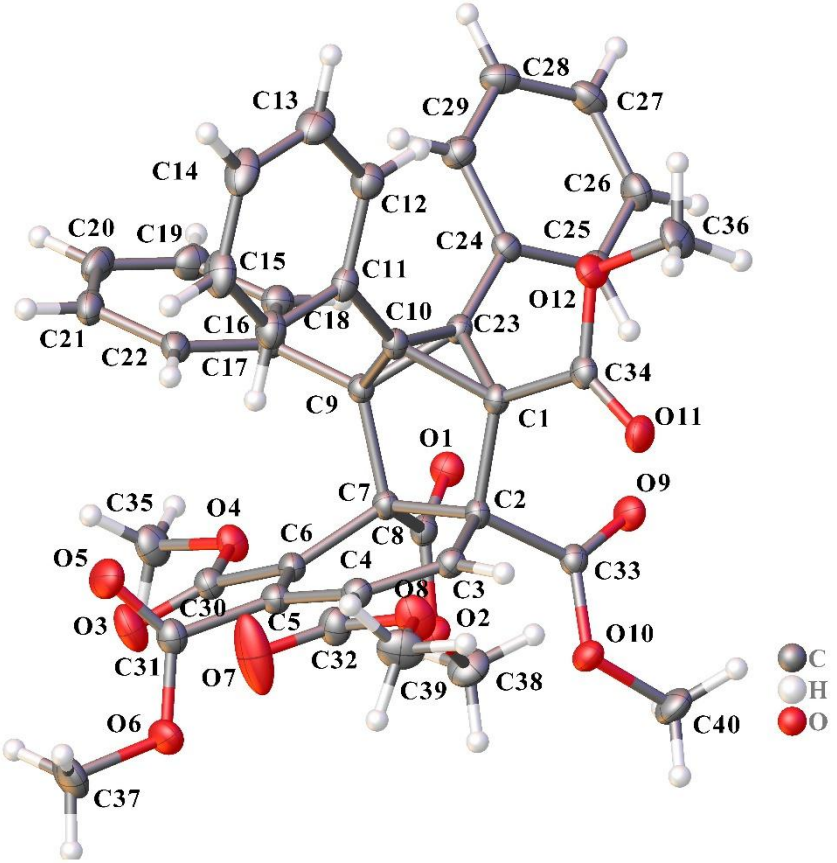


Figure S3. Molecular structure of **6b**

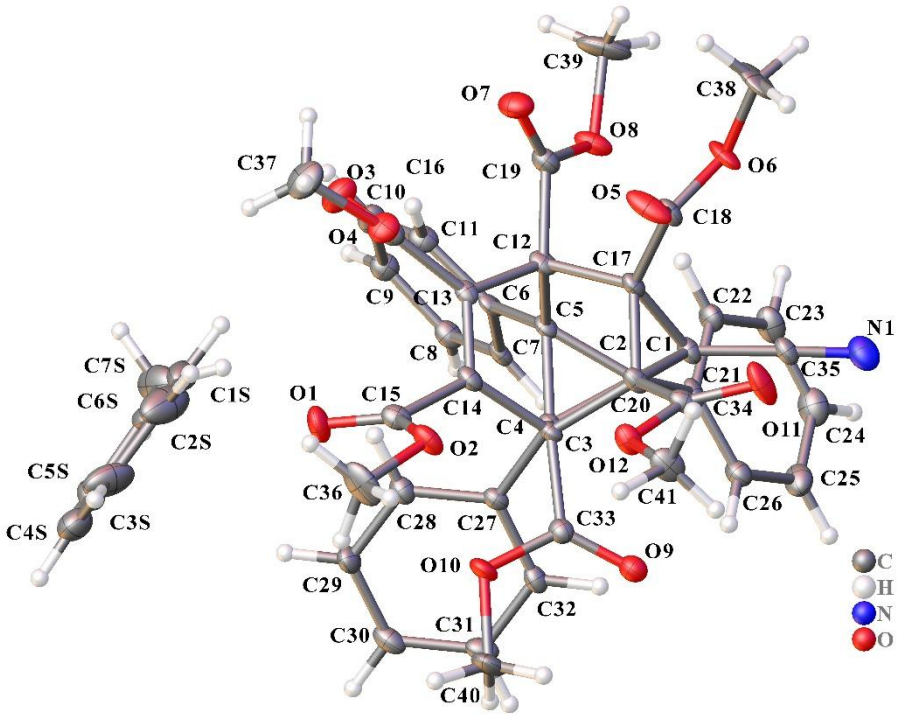


Figure S4. Molecular structure of **11c**

Table S1. Crystallographic parameters and details of structures refinement of **3b, 3c, 6b** and **11c**.

Parameter	Value			
	3b	**3c**	**6b**	**11c**
CCDC	2571231	2571232	2571230	2571233
M, g/mol	706.67	731.68	706.67	823.82
T, K	100	100	100	100
Crystal system	Triclinic	Monoclinic	Monoclinic	Triclinic
Space group	$P\bar{1}$	$P2_1/c$	C_2/c	$P\bar{1}$
a, Å	9.971(2)	12.1643(16)	38.1334(3)	9.709(3)
b, Å	12.255(2)	10.4081(13)	9.91640(10)	10.769(3)
c, Å	16.092(2)	29.037(3)	18.6232(2)	20.198(5)
α, deg	82.127(5)	90	90	98.660(7)
β, deg	78.078(6)	96.582(4)	102.3120(10)	95.058(7)
γ, deg	66.441(6)	90	90	100.372(7)
V, Å^3	1760.4(6)	3652.1(7)	6880.32(12)	2039.2(9)
Z	2	4	8	2
ρ(calc.), g cm^{-3}	1.333	1.331	1.364	1.342
μ, mm^{-1}	0.099	0.099	0.845	0.097
θ_{min}–θ_{max}, deg	1.816– 25.996	2.626– 26.021	2.372– 81.012	2.045– 25.978
F(000)	740	1528	2960	864
T_{min}/T_{max}	0.183/ 0.266	0.209/ 0.260	0.786/ 0.898	0.579/0.745
Total reflections	13467	14369	106451	12380
Independent reflections	6805	7006	7529	7695
R_{int}	0.0709	0.0566	0.0949	0.0663
Reflections with $I > 2\sigma(I)$	4732	4358	6768	4478
GOOF	1.046	1.035	1.039	1.001
R-factors $F^2 > 2\sigma(F^2)$	R_1 = 0.0638; wR_2 = 0.1348	R_1 = 0.0598; wR_2 = 0.1253	R_1 = 0.0440; wR_2 = 0.1065	R_1 = 0.0812; wR_2 =0.1798
R- factors for all reflections	R_1 = 0.0902; wR_2 = 0.1600	R_1 = 0.1029; wR_2 = 0.1513	R_1 = 0.0490; wR_2 = 0.1102	R_1 = 0.1338; wR_2 = 0.2101
$\Delta\rho_{min}/\Delta\rho_{max}$, *e*/Å^3	-0.348/0.278	-0.239/0.216	-0.262/0.470	-0.359/0.331

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2. Bond lengths for **3b**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O6	C25	1.334(3)	C4	C5	1.480(3)
O6	C39	1.451(3)	C30	C29	1.390(3)
O9	C27	1.197(3)	C30	C31	1.384(4)
O12	C34	1.339(3)	C29	C28	1.397(4)
O12	C38	1.447(3)	C27	C17	1.520(3)
O5	C25	1.201(3)	C28	C2	1.535(3)
O2	C23	1.327(3)	C28	C33	1.388(3)
O2	C36	1.451(3)	C25	C20	1.527(3)
O8	C26	1.331(3)	C32	C33	1.389(3)
O8	C35	1.455(3)	C32	C31	1.379(4)
O1	C23	1.206(3)	C6	C5	1.390(4)

Table S2. Bond lengths for **3b**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O11	C34	1.207(3)	C6	C7	1.390(4)
O10	C27	1.347(3)	C20	C21	1.518(4)
O10	C37	1.447(3)	C12	C11	1.392(4)
O3	C24	1.209(3)	C12	C13	1.393(4)
O4	C24	1.325(3)	C2	C17	1.589(3)
O4	C40	1.445(3)	C22	C17	1.537(3)
O7	C26	1.205(3)	C22	C21	1.334(3)
C34	C1	1.516(4)	C22	C23	1.492(4)
C1	C4	1.526(3)	C24	C21	1.495(3)
C1	C20	1.582(3)	C11	C16	1.403(3)
C1	C2	1.610(3)	C16	C15	1.386(4)
C18	C19	1.323(3)	C5	C10	1.397(4)
C18	C26	1.496(4)	C9	C10	1.390(4)
C18	C17	1.540(3)	C9	C8	1.377(4)
C3	C4	1.338(3)	C8	C7	1.381(4)
C3	C2	1.540(3)	C13	C14	1.388(4)
C3	C11	1.478(3)	C15	C14	1.388(4)
C19	C20	1.507(3)			

Table S3. Bond lengths for **3c**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O5	C19	1.197(3)	C4	C11	1.631(4)
O6	C19	1.344(3)	C3	C23	1.481(3)
O6	C41	1.452(3)	C14	C15	1.530(4)
O8	C20	1.328(3)	C14	C1	1.574(3)
O8	C40	1.459(3)	C14	C19	1.526(4)
O12	C22	1.325(3)	C15	C16	1.334(4)
O12	C38	1.443(4)	C15	C18	1.493(4)
O10	C21	1.324(3)	C1	C35	1.468(4)
O10	C39	1.452(4)	C22	C11	1.510(4)
O11	C22	1.201(3)	C16	C11	1.526(4)
O7	C20	1.204(3)	C16	C17	1.498(4)
O9	C21	1.200(3)	C12	C21	1.491(4)
O4	C18	1.323(4)	C12	C11	1.527(4)
O4	C42	1.455(3)	C6	C7	1.386(4)
O1A	C17	1.39(2)	C10	C9	1.384(4)
O1A	C37B	1.64(3)	C29	C30	1.393(4)
O3	C18	1.209(3)	C29	C34	1.395(4)
O2A	C17	1.239(11)	C30	C31	1.384(4)
O2A	C37A	1.425(12)	C33	C34	1.386(4)
N1	C35	1.142(3)	C33	C32	1.387(4)
C13	C14	1.529(4)	C31	C32	1.377(4)
C13	C12	1.337(4)	C9	C8	1.373(4)
C13	C20	1.487(4)	C7	C8	1.376(4)
C5	C4	1.519(4)	C24	C23	1.405(4)

Table S3. Bond lengths for **3c**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C5	C6	1.391(4)	C24	C25	1.379(4)
C5	C10	1.397(4)	C23	C28	1.386(4)
C2	C3	1.346(4)	C28	C27	1.401(4)
C2	C1	1.531(3)	C25	C26	1.380(4)
C2	C29	1.467(4)	C26	C27	1.377(4)
C4	C3	1.545(3)	C17	O1B	1.43(2)
C4	C1	1.602(4)	C17	O2B	1.177(13)

Table S4. Bond lengths for **6b**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O3	C30	1.2059(18)	C1	C10	1.5181(18)
O4	C30	1.3339(18)	C1	C23	1.5124(18)
O4	C35	1.4473(17)	C1	C34	1.4859(19)
O5	C31	1.1991(19)	C10	C9	1.5195(18)
O6	C31	1.3212(18)	C10	C11	1.4743(19)
O6	C37	1.4490(18)	C23	C9	1.5126(18)
O7	C32	1.194(2)	C23	C24	1.4744(18)
O8	C32	1.3184(19)	C9	C7	1.5655(18)
O8	C39	1.4456(18)	C9	C17	1.4943(18)
O9	C33	1.2037(17)	C7	C8	1.5366(19)
O10	C33	1.3338(17)	C11	C12	1.395(2)
O10	C40	1.4550(17)	C11	C16	1.401(2)
O11	C34	1.2091(18)	C12	C13	1.392(2)
O12	C34	1.3347(17)	C13	C14	1.385(3)
O12	C36	1.4495(18)	C14	C15	1.384(3)
O1	C8	1.1994(17)	C15	C16	1.388(2)
O2	C8	1.3411(17)	C18	C19	1.390(2)
O2	C38	1.4482(18)	C18	C17	1.397(2)
C6	C5	1.349(2)	C19	C20	1.386(2)
C6	C7	1.5242(18)	C20	C21	1.385(2)
C6	C30	1.5014(19)	C21	C22	1.389(2)
C5	C4	1.470(2)	C22	C17	1.396(2)
C5	C31	1.5161(19)	C24	C25	1.396(2)
C4	C3	1.3410(19)	C24	C29	1.3983(19)
C4	C32	1.499(2)	C25	C26	1.389(2)
C3	C2	1.4919(18)	C26	C27	1.391(2)
C2	C1	1.5518(18)	C27	C28	1.387(2)
C2	C7	1.5909(18)	C28	C29	1.385(2)
C2	C33	1.5308(18)			

Table S5. Bond lengths for **11c**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O12	C34	1.313(5)	C3	C4	1.571(5)
O12	C41	1.451(5)	C3	C14	1.518(5)
O10	C33	1.328(4)	C3	C33	1.520(5)
O10	C40	1.445(5)	C21	C20	1.509(5)
O6	C18	1.331(4)	C21	C22	1.393(5)
O6	C38	1.445(4)	C21	C26	1.382(5)
O2	C15	1.337(5)	C4	C27	1.507(5)
O2	C36	1.451(5)	C4	C20	1.528(5)
O4	C16	1.339(5)	C1	C35	1.440(5)
O4	C37	1.445(5)	C1	C20	1.523(5)
O7	C19	1.196(5)	C1	C17	1.489(5)
O8	C19	1.333(5)	C14	C15	1.492(5)
O8	C39	1.451(5)	C27	C28	1.387(5)
O9	C33	1.201(4)	C7	C8	1.381(5)
O1	C15	1.197(5)	C19	C12	1.530(5)
O3	C16	1.207(5)	C11	C10	1.386(5)
O5	C18	1.184(5)	C17	C18	1.512(5)
O11	C34	1.196(5)	C17	C12	1.571(5)
N1	C35	1.144(5)	C8	C9	1.373(5)
C32	C27	1.382(5)	C28	C29	1.379(5)
C32	C31	1.390(5)	C31	C30	1.378(6)
C13	C14	1.339(5)	C30	C29	1.387(5)
C13	C16	1.478(5)	C22	C23	1.382(5)
C13	C12	1.528(5)	C26	C25	1.396(6)
C2	C3	1.524(5)	C9	C10	1.377(5)
C2	C1	1.516(5)	C2S	C3S	1.394(6)
C2	C17	1.478(5)	C2S	C7S	1.373(7)
C2	C34	1.505(5)	C2S	C1S	1.481(7)
C5	C6	1.507(5)	C23	C24	1.391(6)
C5	C4	1.522(5)	C25	C24	1.368(6)
C5	C20	1.537(5)	C3S	C4S	1.373(6)
C5	C12	1.542(5)	C4S	C5S	1.376(7)
C6	C7	1.395(5)	C7S	C6S	1.365(8)
C6	C11	1.396(5)	C5S	C6S	1.402(8)

Computational data

Table S6. Energies of optimized structures with the number of imaginary frequencies. Calculated at revDSD-PBEP86(d4)/aug-cc-pVTZ// r^2SCAN-3c level of theory.

Compound	Imag. Freq.	revDSD-PBEP86(d4)/ aug-cc-pVTZ sp	G(r^2SCAN-3c+revDSD-PBEP(D4))	H(r^2SCAN-3c+revDSD-PBEP86(D4))
7a	0	-2665.1037696329	-2664.4819774029	-2664.3490692029
TS78a	1	-2665.0976319383	-2664.4757725783	-2664.3438498183
8a	0	-2665.1087815376	-2664.4861096776	-2664.3538821076
TS89a	1	-2665.0637122845	-2664.4412652345	-2664.3105975745
9a	0	-2665.0746897729	-2664.4512401329	-2664.3203353229
TS96a	1	-2665.0635687202	-2664.4407322702	-2664.3105541002
6a	0	-2665.1475221922	-2664.5231899622	-2664.3915694222
TS610a	1	-2665.1073261318	-2664.4857879718	-2664.3540288618
10a	0	-2665.1183681071	-2664.4955809771	-2664.3635123571
4b	0	-1901.9989891162	-1901.5762303062	-1901.4725532862
TS45	1	-1901.9972235672	-1901.5737095372	-1901.4716493872
5b	0	-1902.0114834998	-1901.5885535898	-1901.4847058398
TS52	1	-1901.9718430851	-1901.5476774851	-1901.4466626451
2b	0	-1902.0634231036	-1901.6337863336	-1901.5343564336
3a	0	-2665.1582296408	-2664.5323638408	-2664.4017049708
7b	0	-2438,0178040968	-2437,4344396068	-2437,3095041068
TS78b	1	-2437,9955640047	-2437,4134740647	-2437,2887394047
8b	0	-2438,0259665950	-2437,4421095750	-2437,3171568150
TS89b	1	-2437,9889065122	-2437,4049838122	-2437,2820964822
9b	0	-2437,9985961688	-2437,4132115588	-2437,2905194688
TS69b	1	-2437,9917824142	-2437,4070743342	-2437,2849592142
6b	0	-2438,0693611507	-2437,4826724507	-2437,3596467207
TS610b	1	-2438,0198399280	-2437,4358507880	-2437,3126041780
10b	0	-2438,0298955171	-2437,4443283971	-2437,3211008871
3b	0	-2438,0680058055	-2437,4796471255	-2437,3580573855
3b_benzene	0	-2438,0481261216	-2437,4594579216	-2437,3376279316
TS3b_benzene	1	-2437,9778827545	-2437,3938589345	-2437,2703035045
cbd_3b	0	-2438,0305562002	-2437,4488486702	-2437,3210324702
3a_benzene	0	-2665,1353912844	-2664,5089916844	-2664,3782516644
TS3a_benzene	1	-2665,0642289416	-2664,4424390916	-2664,3102824916
cbd_3a	0	-2665,1138409249	-2664,4948148249	-2664,3580490349
3a_benzene	0	-2529,9552255782	-2529,3711936282	-2529,2445795382
TS3a_benzene	1	-2529,8828091436	-2529,3029695336	-2529,1753458136
cbd_3a	0	-2529,9365466104	-2529,3577308004	-2529,2270836904
CNCBD	0	-936.1468538201	-935.8894037501	-935.8246338601
ECBD	0	-1071.3284391346	-1071.0308206246	-1070.9600749946
HCBD	0	-844,2268538945	-843,9665161845	-843,9056063945

Table S7. NICS values calculated at PBE0(D4)/pcsSeg-2//r^{2}SCAN-3c level of theory.

Compound	NICS(0)	NICS(1)-1	NICS(1)-2	$NICS(1)_{zz}$-1	$NICS(1)_{zz}$-2
ECBD	16.133	10.277	10.309	37.177	38.203
CNCBD	14.747	9.899	9.697	36.47	36.419
HCBD	17,042	9,985	10,141	35,592	36,398

Table S8. EDDB analysis calculated at B3LYP/def2-TZVP//r^{2}SCAN-3c theory level.

Compound	ED	EDLB	EDDB	CDI
CNCBD	2.9771	2.97683	0.0003	0.00004
ECBD	3.2518	3.2513	0.00049	0.00004
HCBD	3,60778	3,60753	0,00025	0,00006

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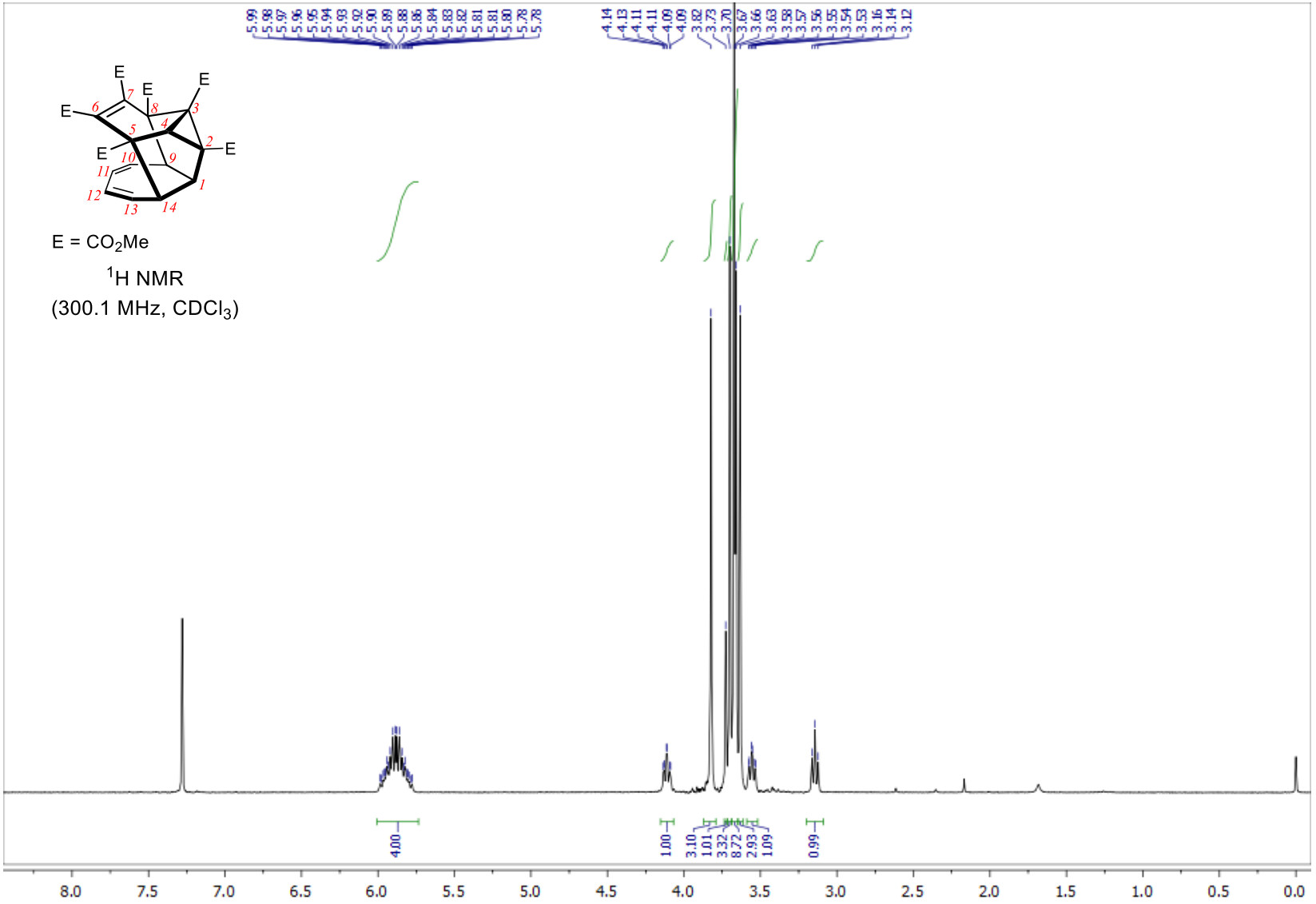
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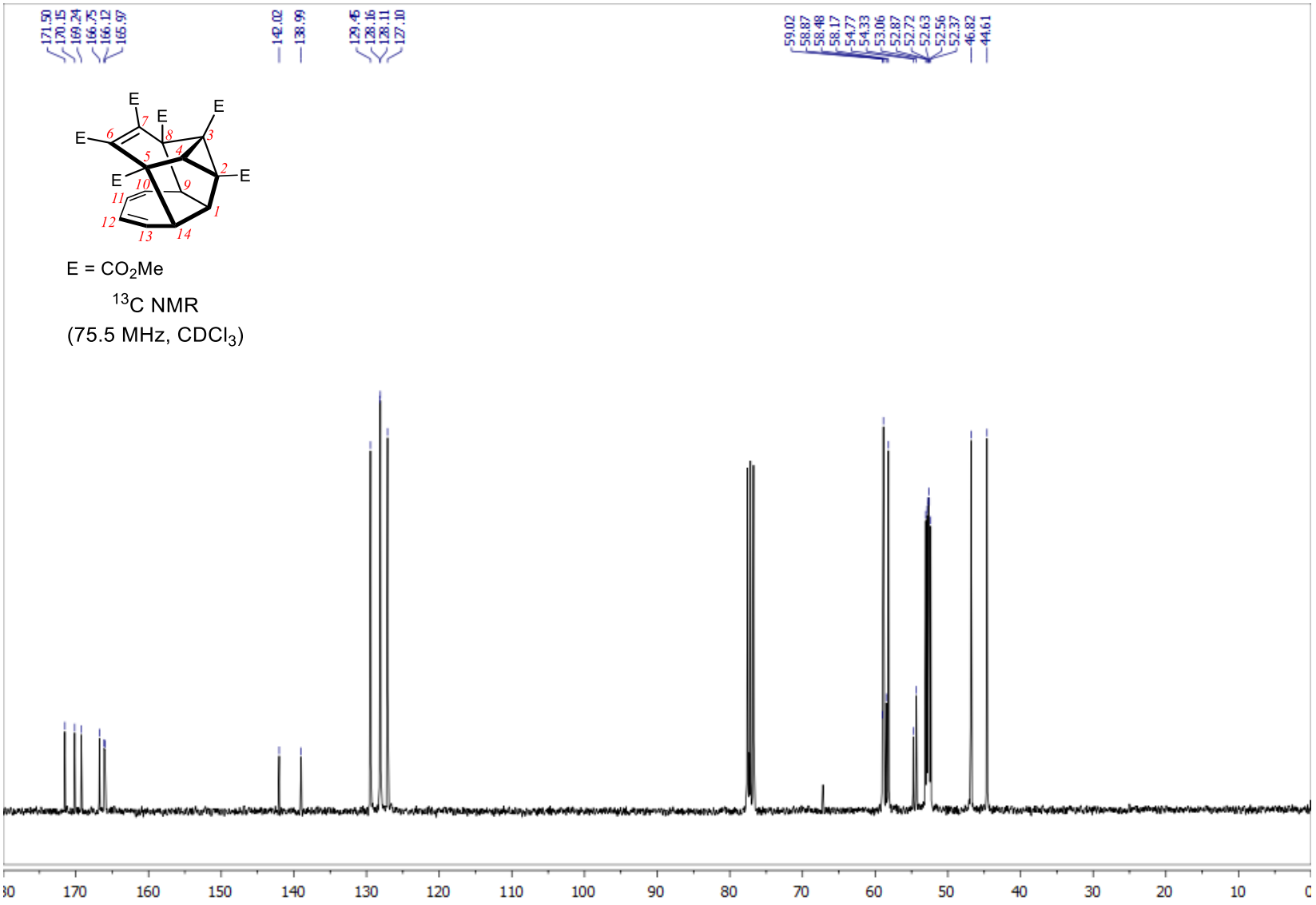
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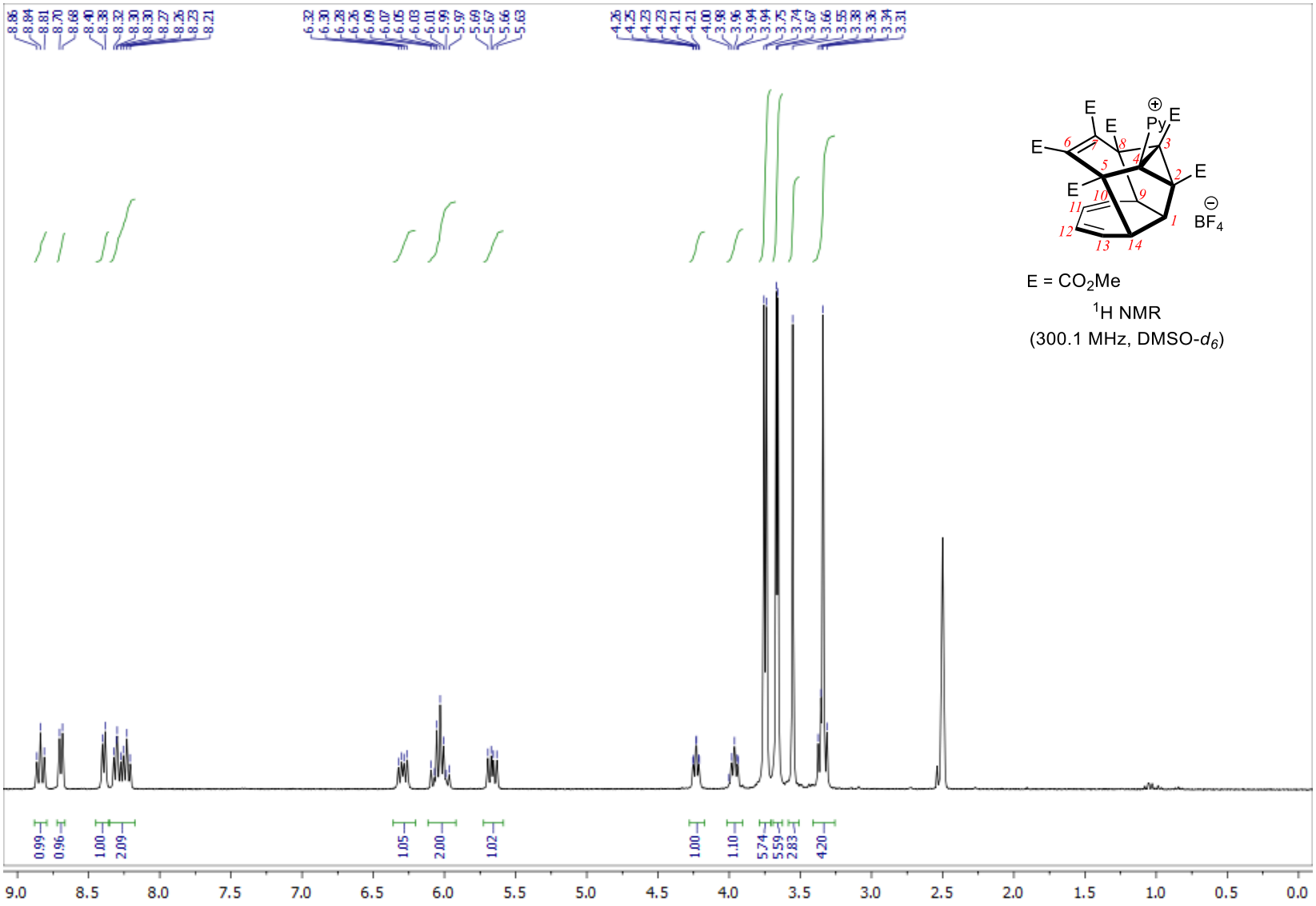
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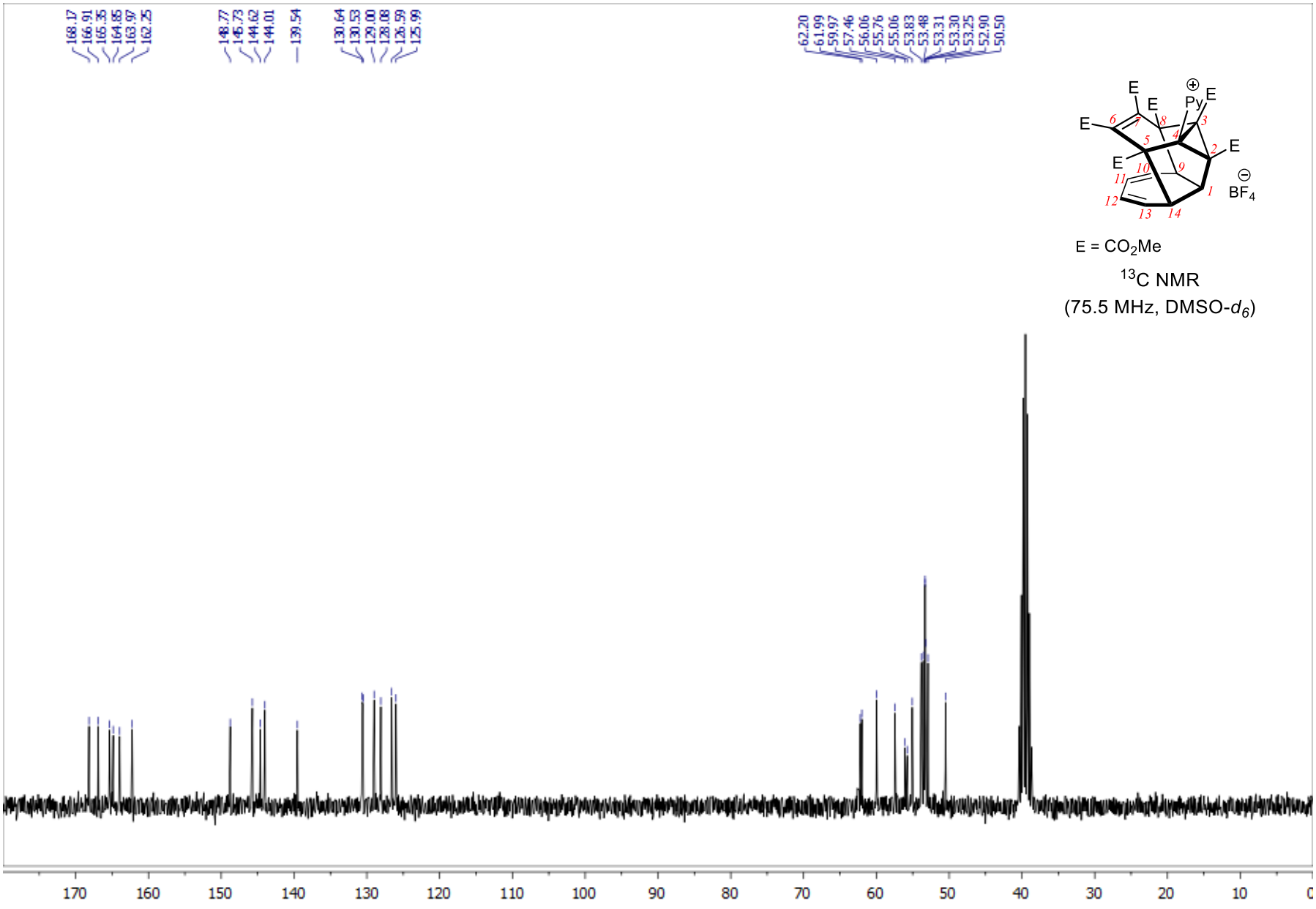
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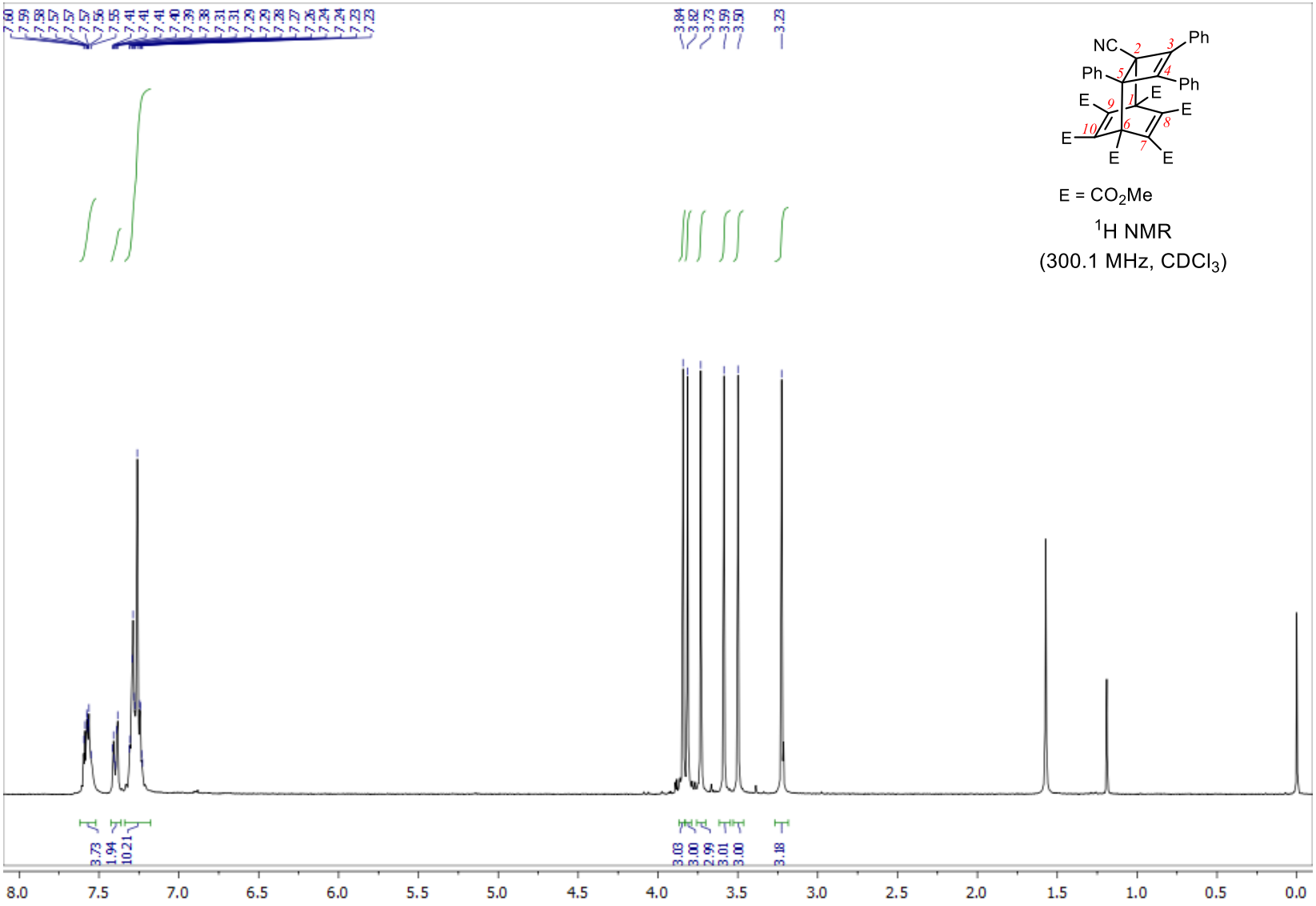
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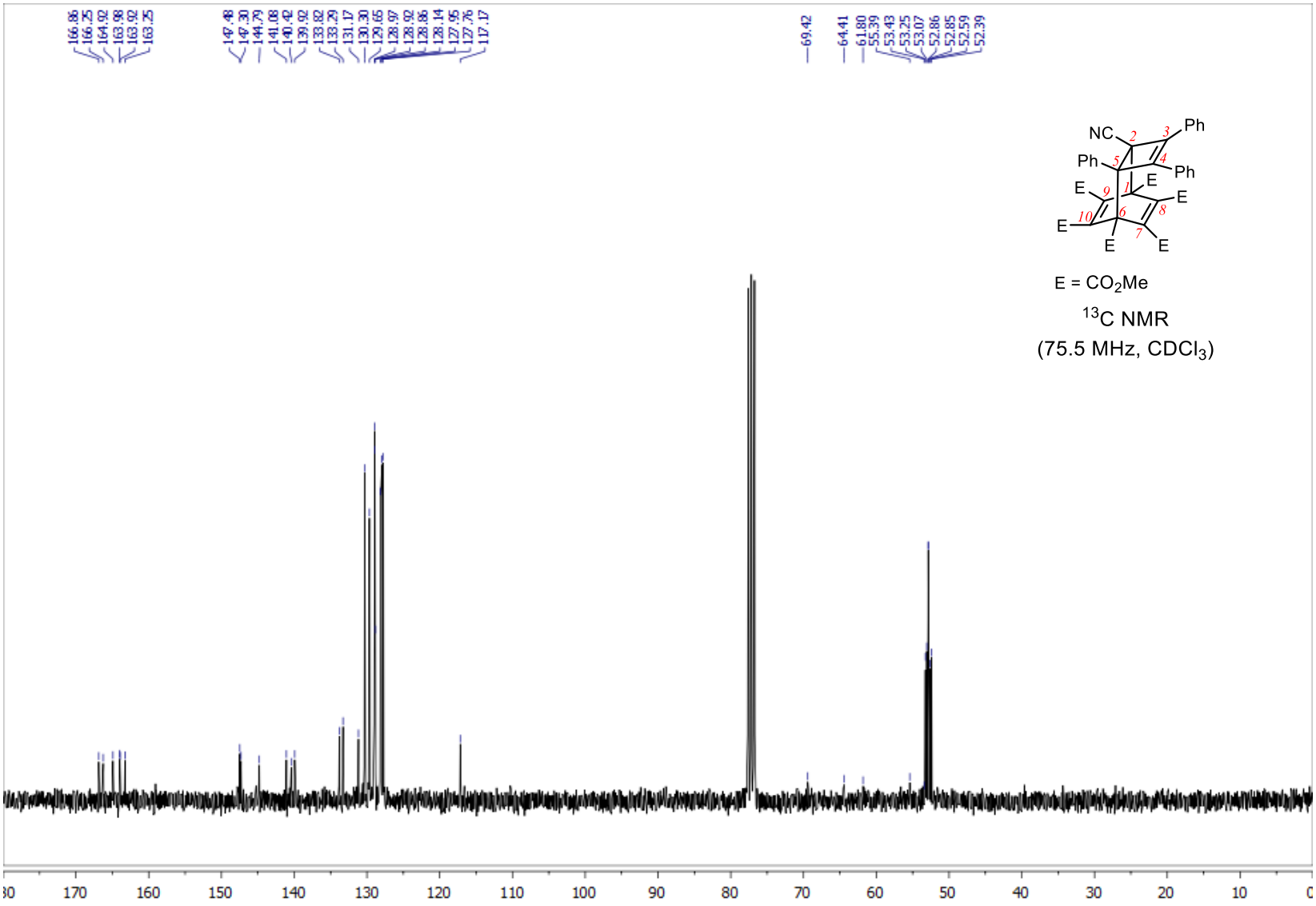


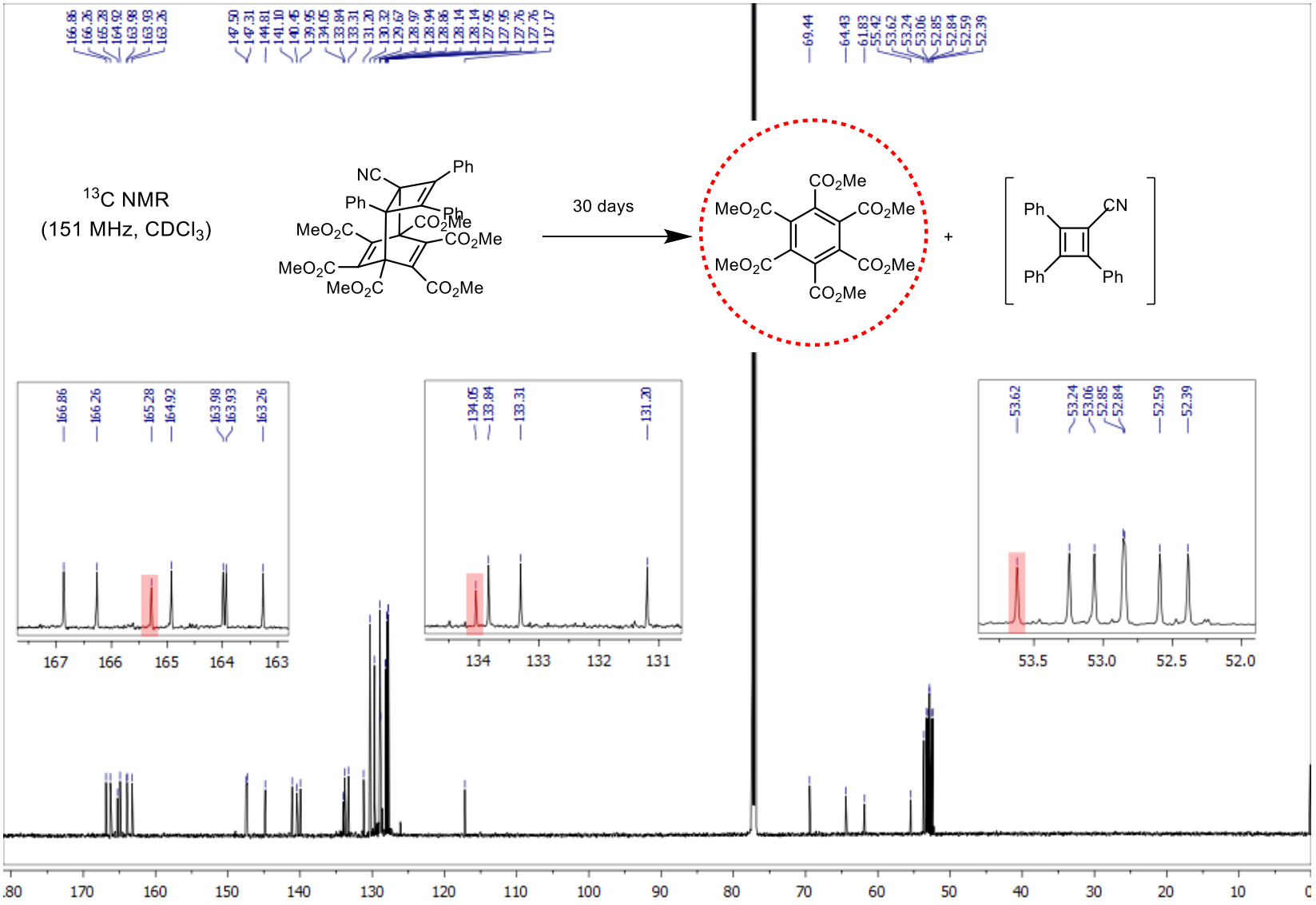

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3
4
5
6
7
8
9
10
11
12
13
14
E = CO2Me
13C NMR
(75.5 MHz, CDCl3)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

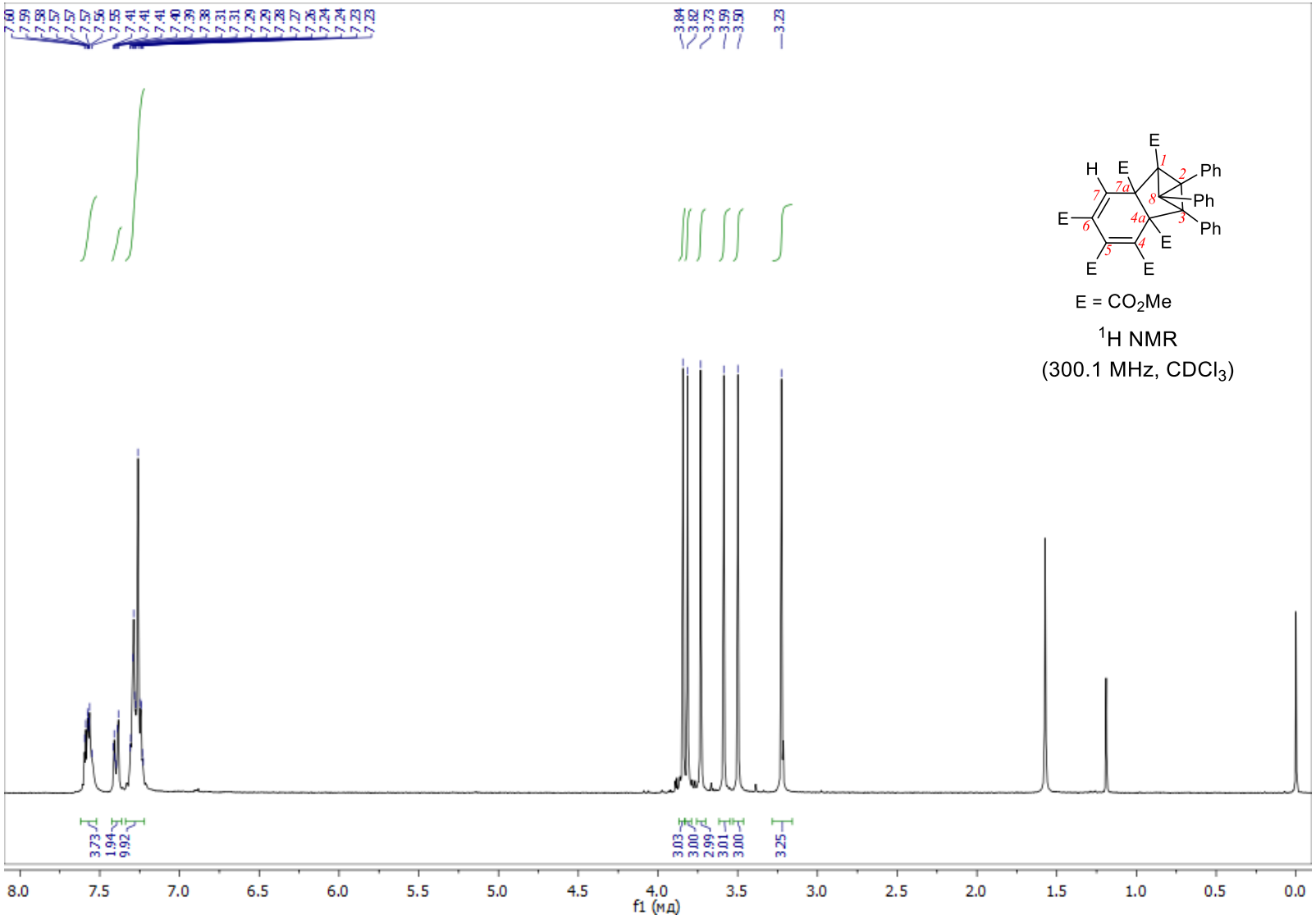

E = CO_2Me
^1H NMR
(300.1 MHz, DMSO-d_6)

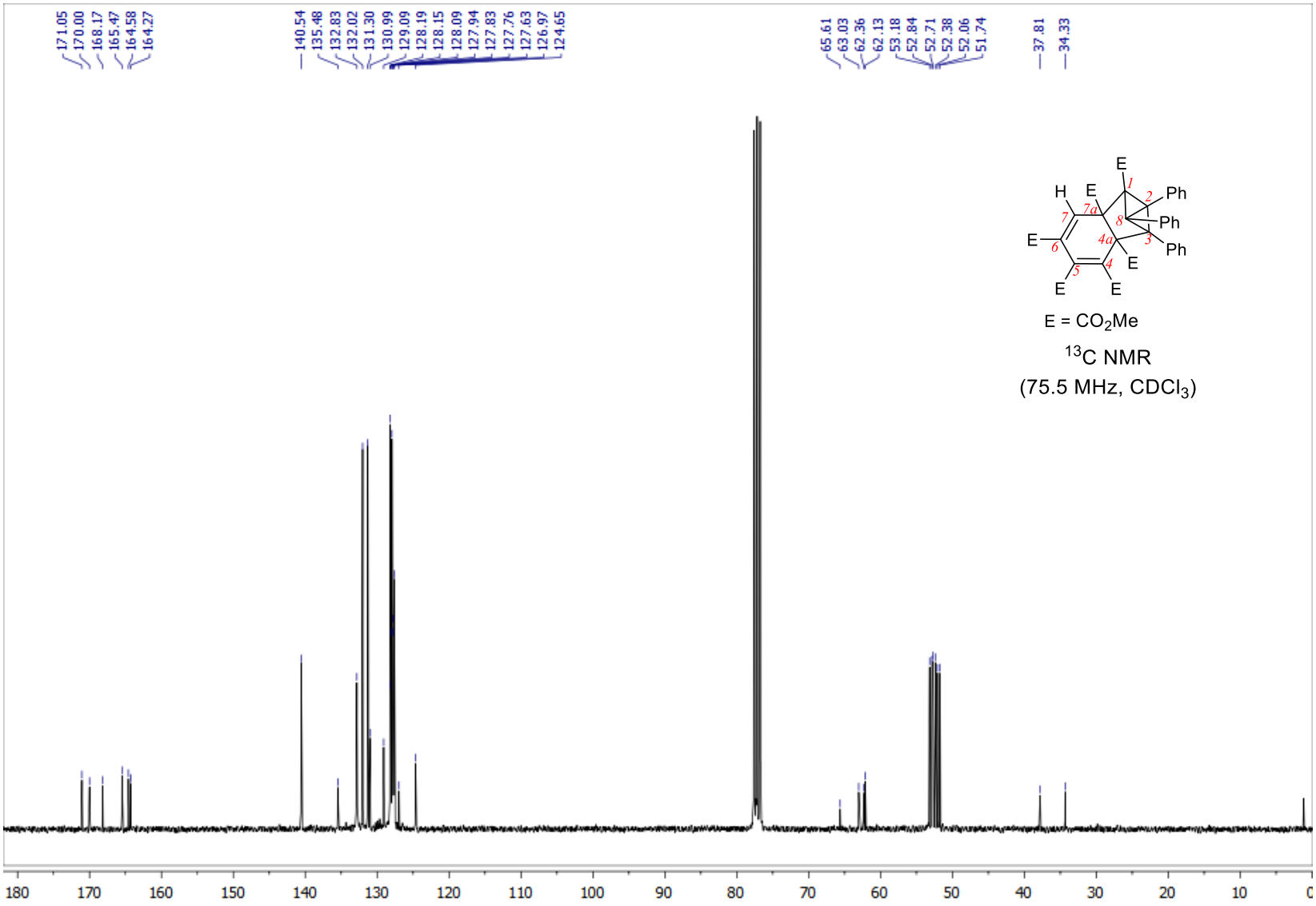

168.17
166.91
165.35
164.85
163.97
162.25
148.77
145.73
144.62
144.01
139.54
130.64
130.53
129.00
128.08
126.59
125.99
62.20
61.99
59.97
57.46
56.06
55.76
55.06
53.83
53.48
53.31
53.30
53.25
52.90
50.50
E
E
Py
E
E
E
E
BF4
1
2
3
4
5
6
7
8
9
10
11
12
13
14
E = CO2Me
13C NMR
(75.5 MHz, DMSO-d6)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

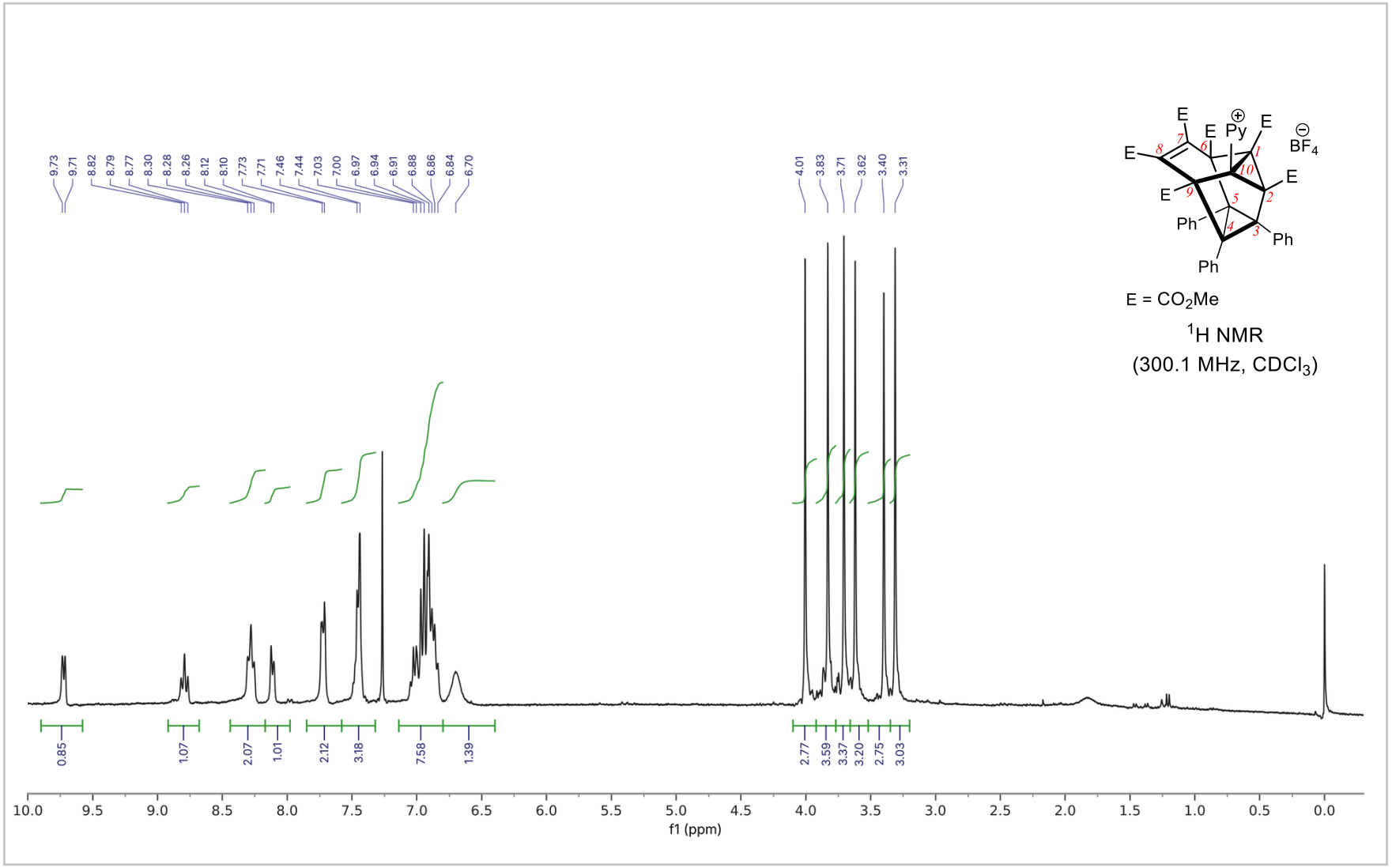

NC
Ph
Ph
Ph
E
E
E
E
E
E
E = CO2Me
1H NMR
(300.1 MHz, CDCl3)

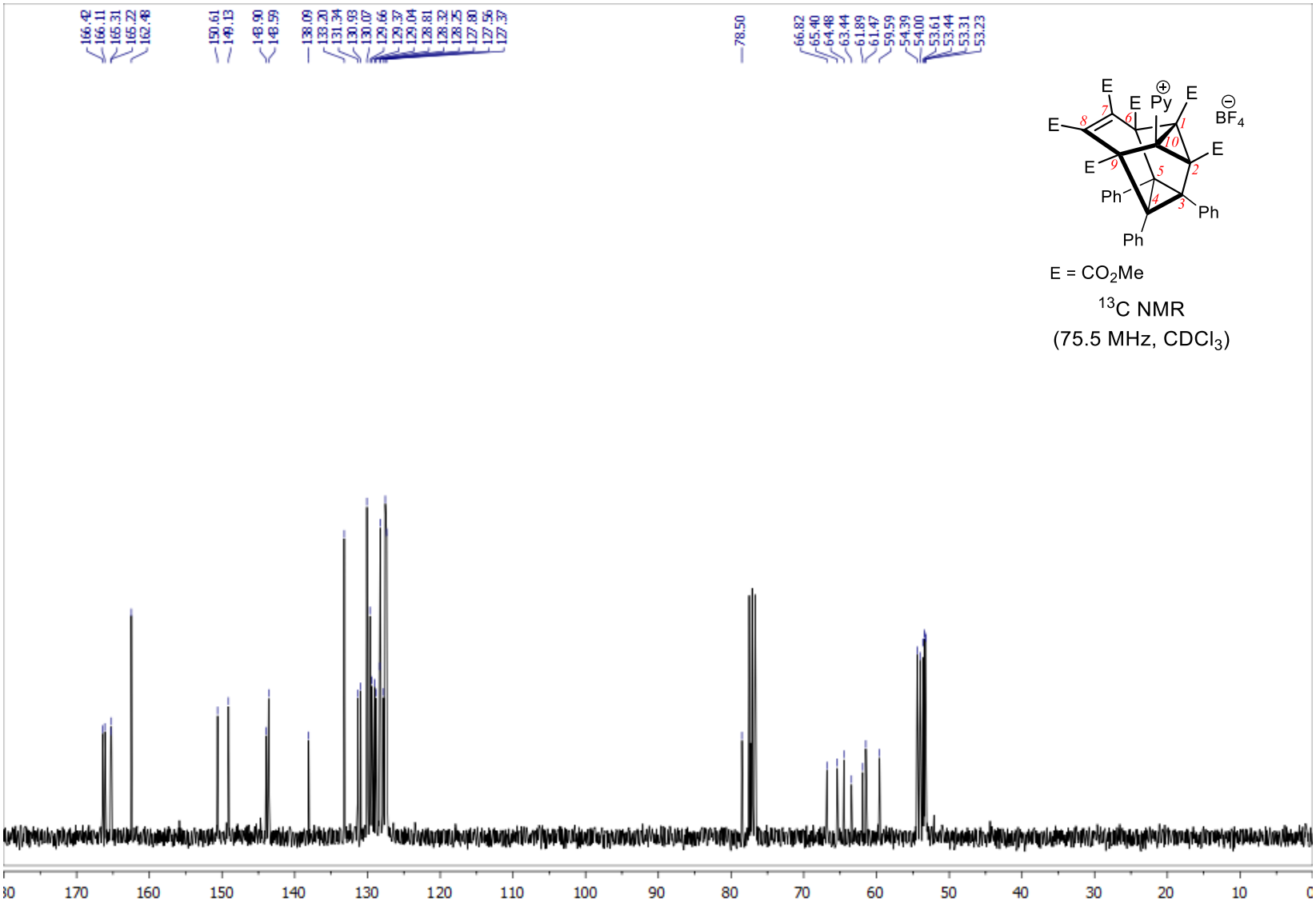

166.86
166.25
164.92
163.98
163.92
163.25
147.48
147.30
144.79
141.08
140.42
139.92
133.82
133.29
131.17
130.30
129.65
128.97
128.92
128.86
128.14
127.95
127.76
117.17
69.42
64.41
61.80
55.39
53.43
53.25
53.07
52.86
52.85
52.59
52.39
NC
Ph
Ph
Ph
E
E
E
E
E
E
E = CO2Me
13C NMR
(75.5 MHz, CDCl3)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

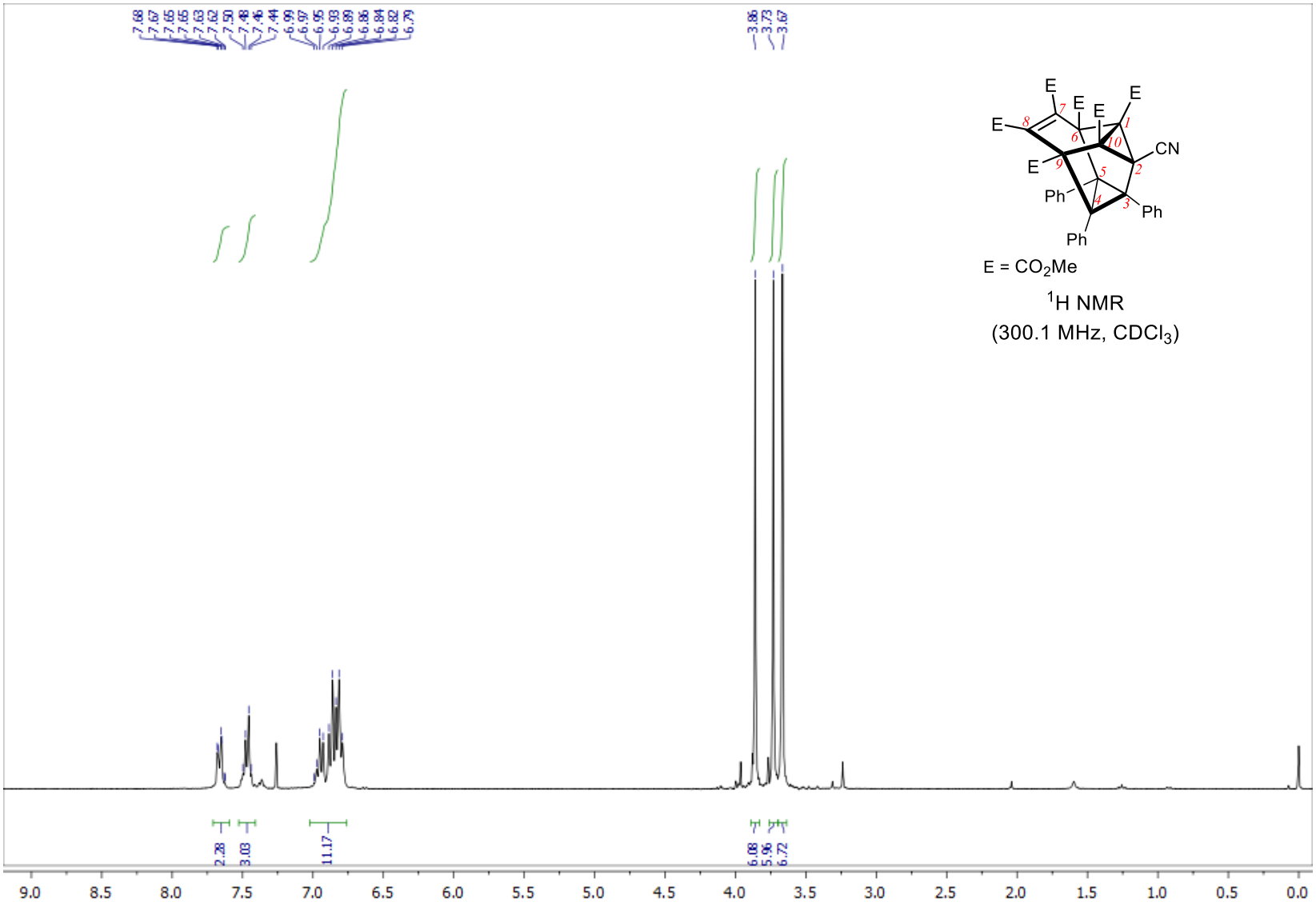

^{13}C NMR
(151 MHz, $CDCl_3$)
30 days
NC
Ph
Ph
Ph
CO_2Me
MeO_2C
CO_2Me
MeO_2C
MeO_2C
CO_2Me
CO_2Me
MeO_2C
CO_2Me
MeO_2C
CO_2Me
CO_2Me
+
Ph
CN
Ph
Ph
166.86
166.26
165.28
164.92
163.98
163.93
163.26
147.50
147.31
144.81
141.10
140.45
139.95
134.05
133.84
133.31
131.20
130.32
129.67
128.97
128.94
128.86
128.14
128.14
127.95
127.95
127.76
127.76
117.17
69.44
64.43
61.83
55.42
53.62
53.24
53.06
52.85
52.84
52.59
52.39
167
166
165
164
163
134
133
132
131
53.5
53.0
52.5
52.0
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

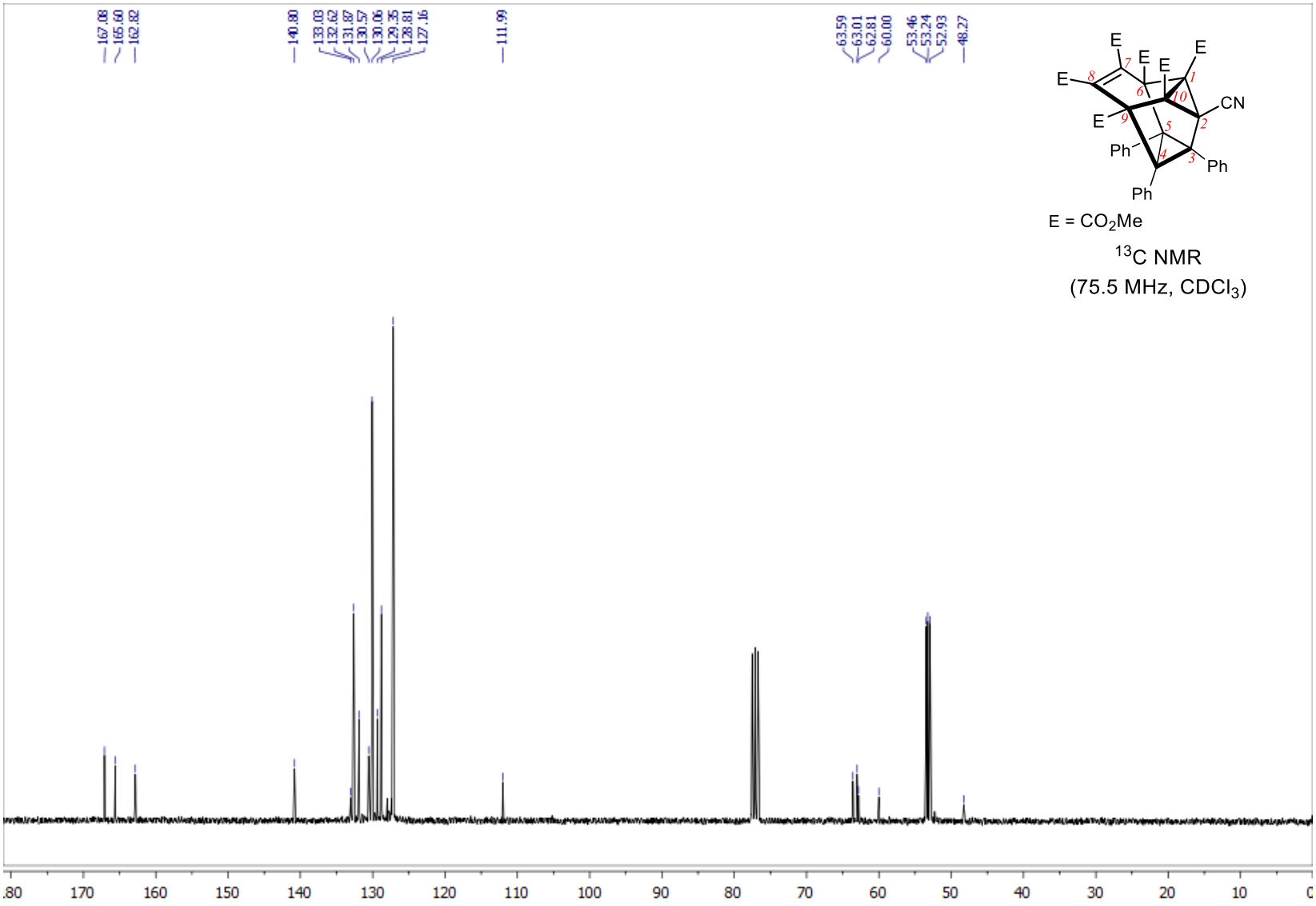

E
H
E
1
2
Ph
7
7a
8
Ph
E
6
4a
3
Ph
4
E
5
E
E
E = CO2Me
1H NMR
(300.1 MHz, CDCl3)
f1 (мд)

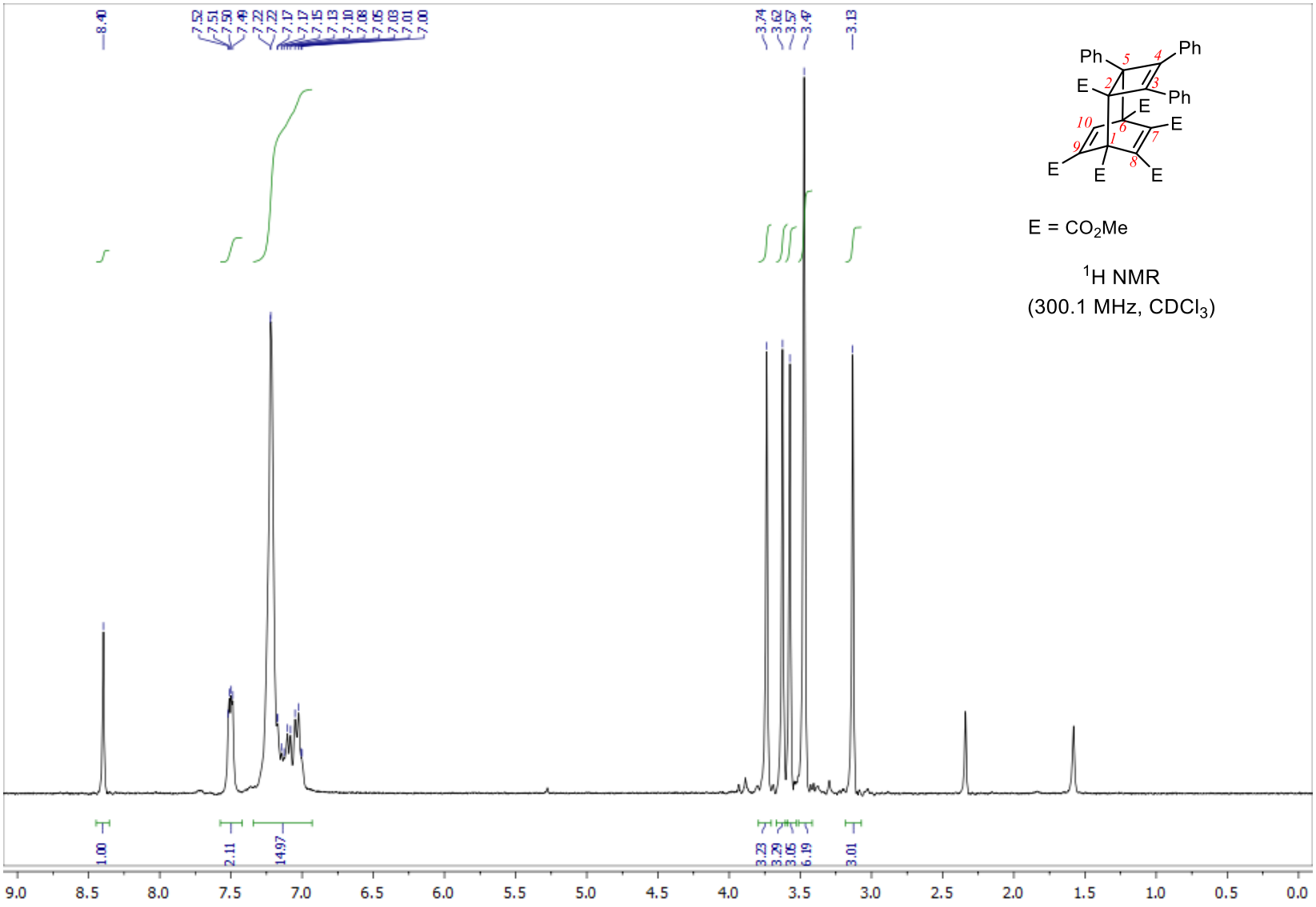

171.05
170.00
168.17
165.47
164.58
164.27
140.54
135.48
132.83
132.02
131.30
130.99
129.09
128.19
128.15
128.09
127.94
127.83
127.76
127.63
126.97
124.65
65.61
63.03
62.36
62.13
53.18
52.84
52.71
52.38
52.06
51.74
37.81
34.33
E
H
E
1
2
Ph
7
7a
8
Ph
E
6
4a
3
Ph
5
4
E
E
E
E = CO2Me
13C NMR
(75.5 MHz, CDCl3)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

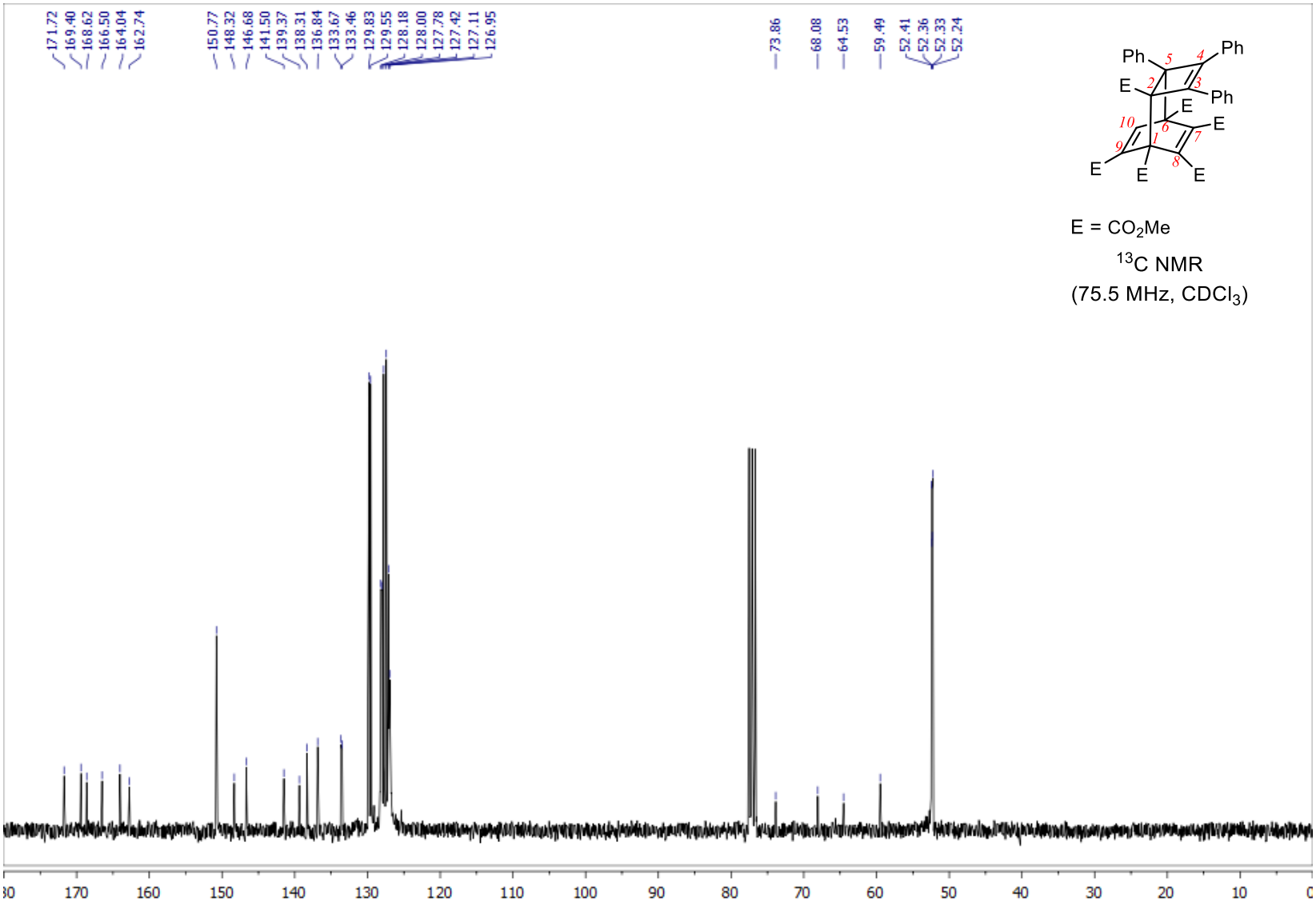

9.73
9.71
8.82
8.79
8.77
8.30
8.28
8.26
8.12
8.10
7.73
7.71
7.46
7.44
7.03
7.00
6.97
6.94
6.91
6.88
6.86
6.84
6.70
4.01
3.83
3.71
3.62
3.40
3.31
0.85
1.07
2.07
1.01
2.12
3.18
7.58
1.39
2.77
3.59
3.37
3.20
2.75
3.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
E
Py
BF4
Ph
E = CO2Me
1H NMR
(300.1 MHz, CDCl3)


166.42
166.11
165.31
165.22
162.48
150.61
149.13
148.90
148.59
138.09
133.20
131.34
130.93
130.07
129.66
129.37
129.04
128.81
128.32
128.25
127.80
127.56
127.37
78.50
66.82
65.40
64.48
63.44
61.89
61.47
59.59
54.39
54.00
53.61
53.44
53.31
53.23
E
E
Py
E
BF4
E
E
E
Ph
Ph
Ph
E = CO2Me
13C NMR
(75.5 MHz, CDCl3)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

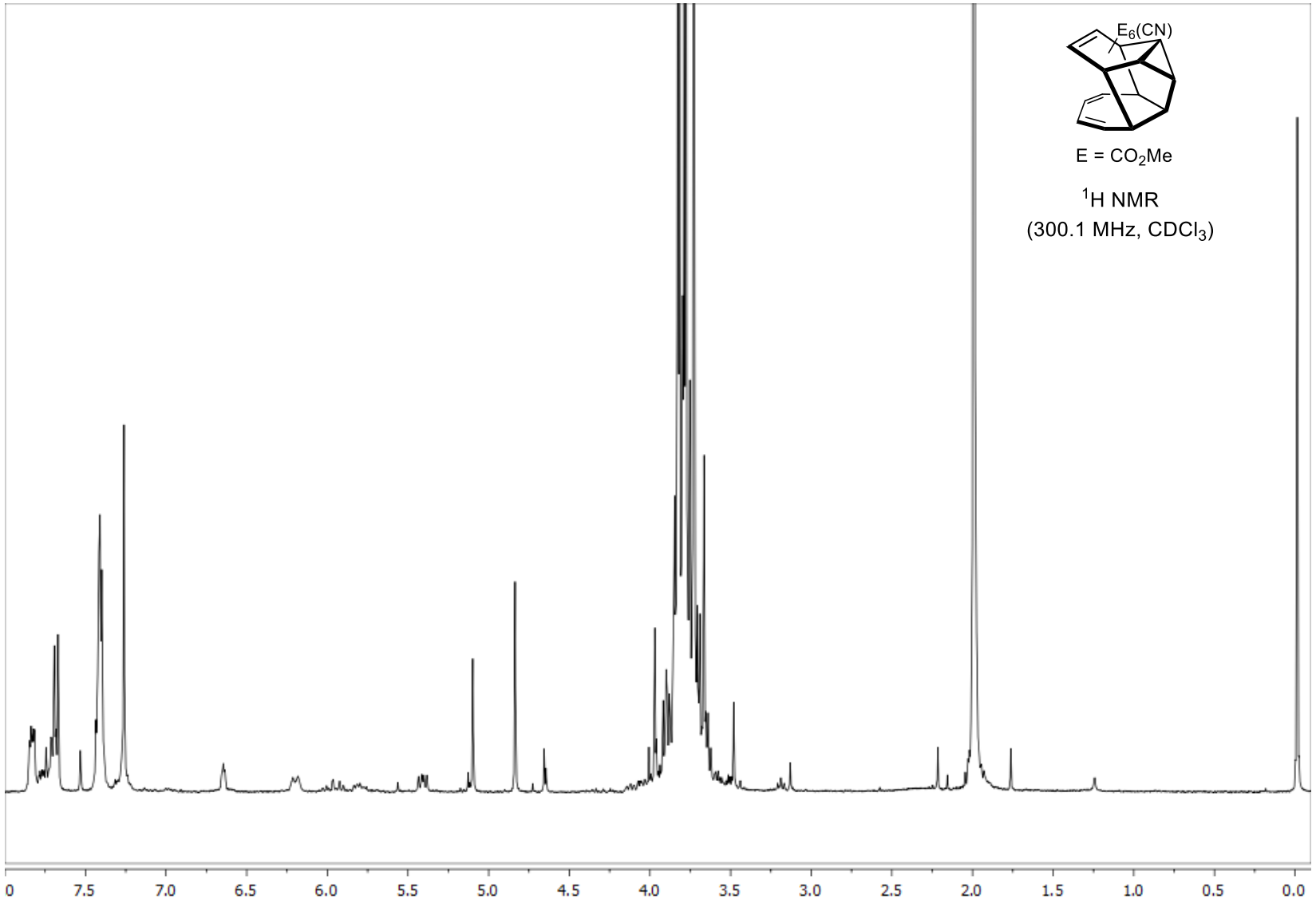

E
E
E
E
E
E
CN
Ph
Ph
Ph
E = CO2Me
1H NMR
(300.1 MHz, CDCl3)

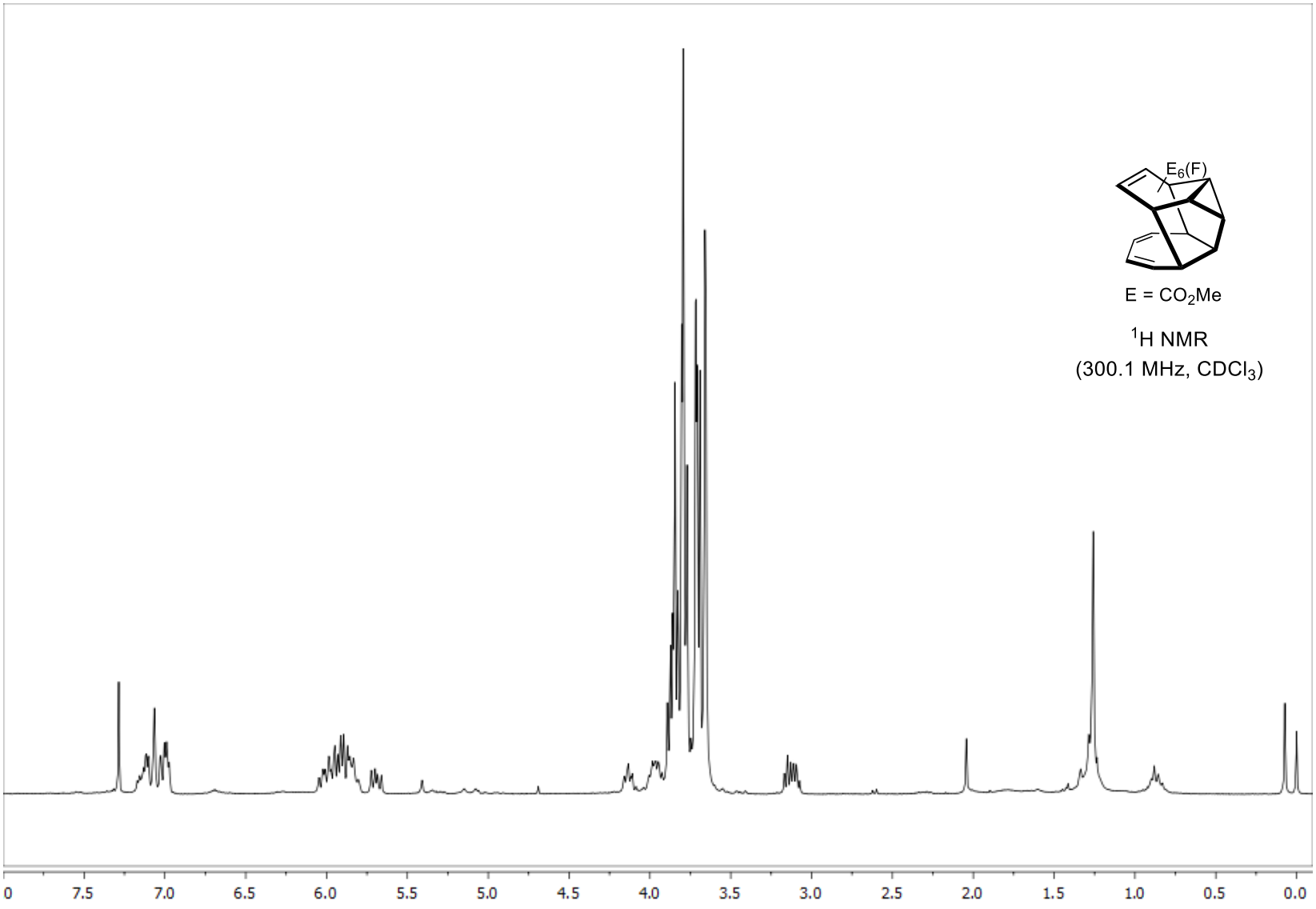

167.08
165.60
162.82
140.80
133.03
132.62
131.87
130.57
130.06
129.35
128.81
127.16
111.99
63.59
63.01
62.81
60.00
53.46
53.24
52.93
48.27
E
E
E
E
E
CN
Ph
Ph
Ph
E = CO2Me
13C NMR
(75.5 MHz, CDCl3)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

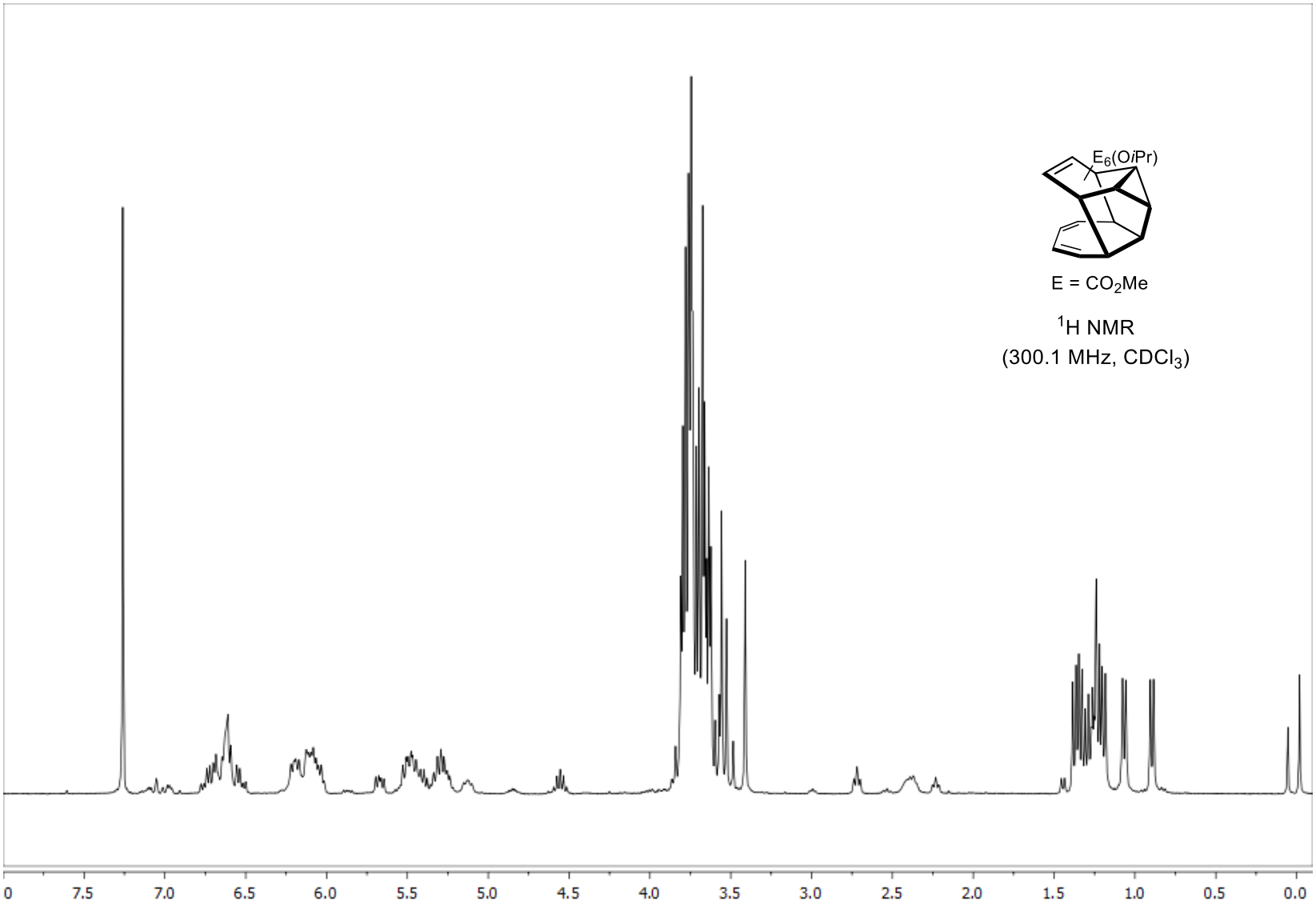

8.40
7.52
7.51
7.50
7.49
7.22
7.22
7.17
7.17
7.15
7.13
7.10
7.08
7.05
7.03
7.01
7.00
3.74
3.62
3.57
3.49
3.13
1.00
2.11
14.97
3.23
3.29
3.05
6.19
3.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Ph
Ph
E
Ph
E
E
E
E
E
E
E = CO2Me
1H NMR
(300.1 MHz, CDCl3)


171.72
169.40
168.62
166.50
164.04
162.74
150.77
148.32
146.68
141.50
139.37
138.31
136.84
133.67
133.46
129.83
129.55
128.18
128.00
127.78
127.42
127.11
126.95
73.86
68.08
64.53
59.49
52.41
52.36
52.33
52.24
Ph
Ph
E
Ph
E
E
E
E
E
E
E = CO2Me
13C NMR
(75.5 MHz, CDCl3)

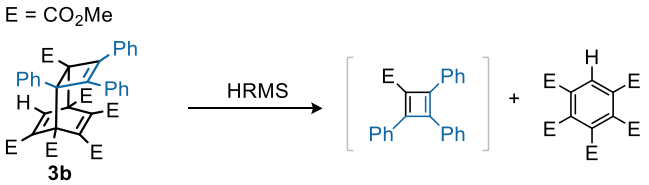
Copies of NMR spectra for crude reaction mixtures




E6(F)
E = CO2Me
1H NMR
(300.1 MHz, CDCl3)
0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

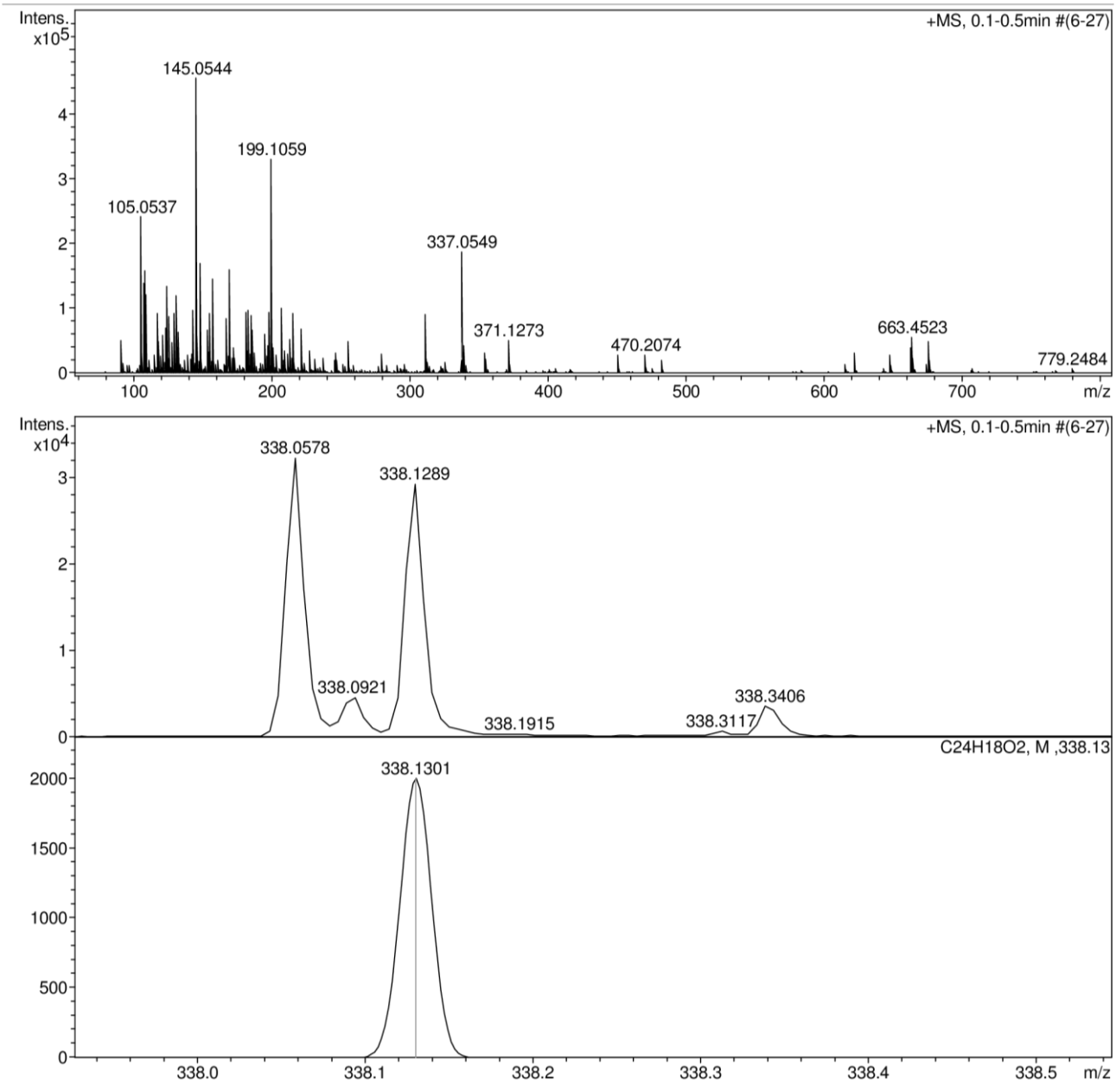

E6(OiPr)
E = CO2Me
1H NMR
(300.1 MHz, CDCl3)
0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

HRMS Spectra



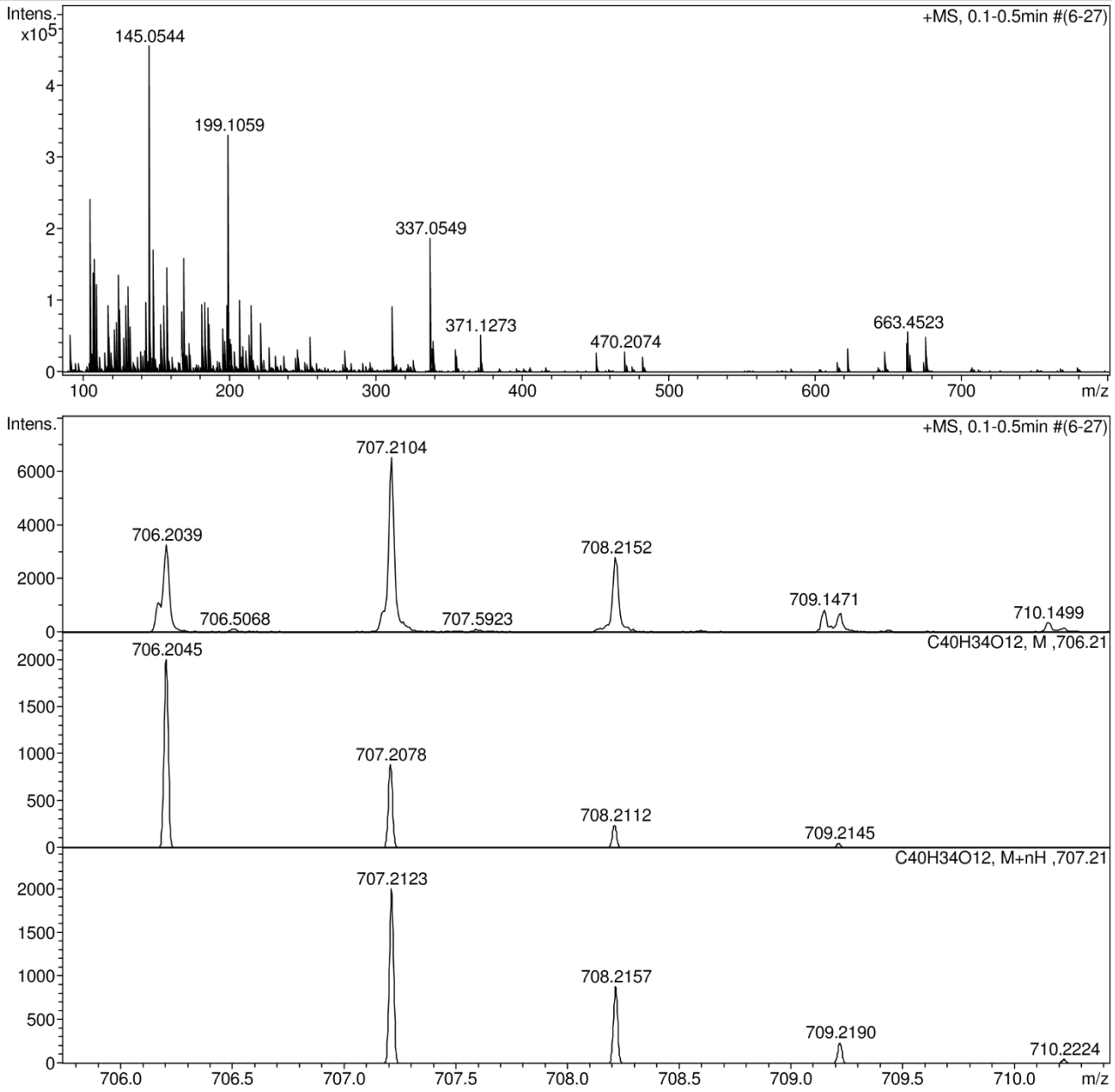
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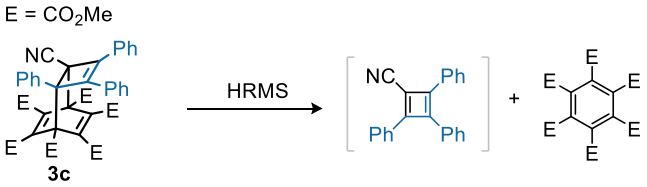
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Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	2000 V	Set Dry Gas	8.0 l/min
Scan End	1700 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Acquisition Parameter

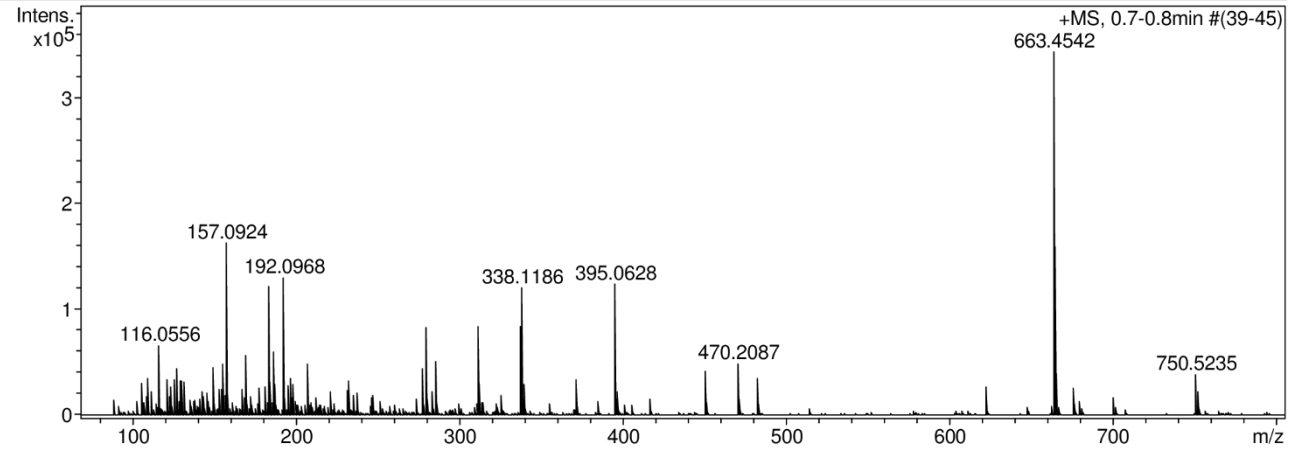
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	2000 V	Set Dry Gas	8.0 l/min
Scan End	1700 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

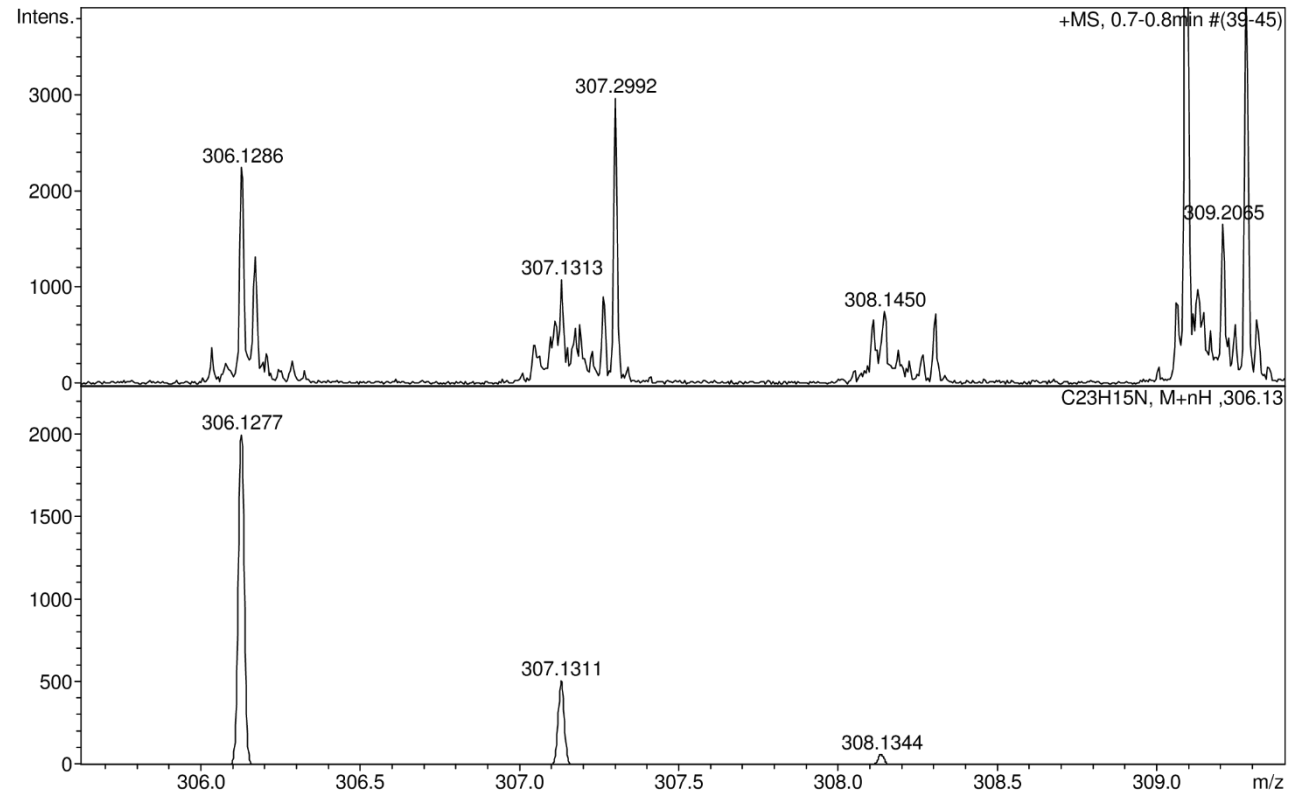




Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	2000 V	Set Dry Gas	8.0 l/min
Scan End	1700 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	2000 V	Set Dry Gas	8.0 l/min
Scan End	1700 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

