Supporting Information

Evaluating metal-free quaternized boronate esters as efficient catalysts for the fixation of CO_2 with epoxide to form cyclic carbonates under suitable conditions

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Contents of Supporting Information

Synthesis of the quaternized boronate esters (QBE_1-QBE_8)

The eight new quaternized boronate esters **(QBE_1-QBE_8)** were synthesized with some slight modifications to the original literature [35, 36]. The synthesis method is given below: 10.0 mmol (2.15 g) 3-(bromomethyl)phenylboronic acid was dissolved homogeneously in 40 mL of toluene in different reaction flasks and then 10 mmol of different catechol derivatives such as 3,5-di-*tert*-butylcatechol, 3,5-Diisopropyl catechol, 4-*tert*-butyl catechol, 4-methyl catechol, Dopamine hydrochloride, Protocatechuic acid ethyl ester, Caffeic acid, and 1,3-dioxane-5,5-dimethanol were added to these solutions. The Dean-Stark system was used to remove the H_2O formed during the esterification reactions with continuous stirring at room temperature, and onwards, all mixtures were stirred for 10 h at reflux conditions. After the completion of the reactions was determined by the TLC technique (a retention factor (Rf) of compounds are found to be 0.73 in chloroform-methanol (7:3) as mobile phase systems), the excess solvents were evaporated with a rotary evaporator. Then, 10.0 mmol trimethylamine (Et_3N) dissolved in 30 mL of ethanol was slowly added to each reaction in a nitrogen atmosphere. Subsequently, the mixtures were mixed for a certain period of time under room conditions and then refluxed for 24 hours. After it was determined by TLC that the reactions were completed, the mixtures were brought to room conditions, and the excess solvent was evaporated. The obtained pure products were washed three times with hexane. Then, the pure quaternized boronate esters **(QBE_1-QBE_8)** were dried in a vacuum for spectroscopic and CO_2 fixation studies.

(QBE_1): Yield (%): 82, M.p. = 159 ^oC, Elemental Analysis (calculated for $C_{27}H_{41}BBrNO_2$) (F.W: 502.34 g/mol) (%): C, 64.56; H, 8.23; N, 2.79. Found: C, 64.52; H, 8.20; N, 2.84. FT-IR (ATR, υ_{max}-cm^{-1}): 3050 υ(Ar-CH), 2949-2675 υ(Aliph-CH), 1477-1428 υ(C=C), 1359 υ(B-O), 1233 υ(C-N), 1156 υ(C-O), and 1030 υ(B-C). LC-MS/MS (Scan ESI^+): m/z = 502.35 $[M]^+$ and 503.34 $[M+1]^+$. ^{1}H-NMR (400 MHz; $CDCl_3$): δ (ppm) 7.80 (s, 1H, Ar-C*H*), 6.91-6.78 (m, 3H, Ar-C*H*), 6.56 (s, 1H, Ar-C*H*), 6.41 (s, 1H, Ar-C*H*), 4.54 (s, 2H, Ar-CH_2), 3.00-2.94 (q, 6H, $^2J_{a,b}$

= 8.0 Hz, N-C$\underline{H}_2$-CH_3), 1.41 (s, 9H, C-(C$\underline{H}_3$)$_3$), 1.27 (t, 9H, $^2J_{a,b}$ = 8.0 Hz, N-CH_2-C$\underline{H}_3$), and 1.20 (s, 9H, C-(C$\underline{H}_3$)$_3$). {^{1}H}^{13}C NMR (100 MHz; $CDCl_3$): δ (ppm) 150.28, 146.93, 139.41, 134.85, 135.51, 130.09, 129.21, 127.88, 124.25, 111.94, and 103.89 (Ar-$\underline{C}$H), 45.90 (N-$\underline{C}H_2$-CH_3), 35.37 ($\underline{C}$-$(CH_3)_3$), 32.01 (-$\underline{C}H_2$-Ar), 29.58 (C-($\underline{C}H_3$)$_3$), and 8.63 (N-CH_2-$\underline{C}H_3$). ^{11}B NMR ($CDCl_3$, 192.5 MHz, 23 °C, δ ppm): 14.14. UV-Vis (λ_{max}/(nm)): 206, 223, and 268 (in CH_3CN); 210, 222, and 286 (in C_2H_5OH).

(QBE$_2$): Yield (%): 84, M.p. = 171 °C, Elemental Analysis (calculated for $C_{25}H_{37}BBrNO_2$) (F.W: 474.29 g/mol) (%): C, 63.31; H, 7.86; N, 2.95. Found: C, 63.28; H, 7.83; N, 3.02. FT-IR (ATR, υ_{max}-cm^{-1}): 3043 υ(Ar-CH), 2958-2868 υ(Aliph-CH), 1477-1438 υ(C=C), 1327 υ(B-O), 1237 υ(C-N), 1157 υ(C-O), and 1065 υ(B-C). LC-MS/MS (Scan ESI$^+$): m/z = 474.30 [M]$^+$ and 475.30 [M+1]$^+$. ^{1}H-NMR (400 MHz; $CDCl_3$): δ (ppm) 8.10 (s, 1H, Ar-C$\underline{H}$), 8.02 (d, 1H, $^3J_{ortho}$ = 8.0 Hz, Ar-C$\underline{H}$), 7.56 (t, 1H, $^3J_{ortho}$ = 8.0 Hz, Ar-C$\underline{H}$), 7.48 (d, 1H, $^3J_{ortho}$ = 8.0 Hz, Ar-C$\underline{H}$), 7.00 (s, 1H, Ar-C$\underline{H}$), 6.82 (s, 1H, Ar-C$\underline{H}$), 4.50 (s, 2H, Ar-C$\underline{H}_2$), 3.36-3.33 (q, 6H, $^2J_{a,b}$ = 4.0 Hz, N-C$\underline{H}_2$-CH_3), 3.17-3.11 (m, 1H, C$\underline{H}$-$(CH_3)_2$), 2.89-2.82 (m, 1H, C$\underline{H}$-$(CH_3)_2$), 1.38 (d, 6H, $^2J_{gem}$ = 4.0 Hz, CH-(C$\underline{H}_3$)$_2$), 1.24 (d, 6H, $^2J_{gem}$ = 8.0 Hz, CH-(C$\underline{H}_3$)$_2$), and 1.05 (t, 9H, $^2J_{a,b}$ = 8.0 Hz, N-CH_2-C$\underline{H}_3$). {^{1}H}^{13}C NMR (100 MHz; $CDCl_3$): δ (ppm) 148.18, 143.35, 138.38, 137.31, 135.21, 134.33, 133.94, 129.43, 119.41, 114.56 and 107.69 (Ar-$\underline{C}$H), 45.68 (N-$\underline{C}H_2$-CH_3), 34.16 ($\underline{C}$H-$(CH_3)_2$), 27.35 (-$\underline{C}H_2$-Ar), 24.72 and 22.81 (CH-($\underline{C}H_3$)$_2$), and 7.39 (N-CH_2-$\underline{C}H_3$). ^{11}B NMR ($CDCl_3$, 192.5 MHz, 23 °C, δ ppm): 16.39. UV-Vis (λ_{max}/(nm)): 216, 282, and 346 (in CH_3CN); 212, 280, and 334 (in C_2H_5OH).

(QBE$_3$): Yield (%): 93, M.p. = 187 °C, Elemental Analysis (calculated for $C_{17}H_{18}BBrO_2$) (F.W: 446.24 g/mol) (%): C, 61.91; H, 7.45; N, 3.14. Found: C, 61.88; H, 7.41; N, 3.23. FT-IR (ATR, υ_{max}-cm^{-1}): 3055 υ(Ar-CH), 2949-2676 υ(Aliph-CH), 1491-1432 υ(C=C), 1393 υ(B-O), 1237 υ(C-N), 1158 υ(C-O), and 1008 υ(B-C). LC-MS/MS (Scan ESI$^+$): m/z = 446.24 [M]$^+$ and 447.25 [M+1]$^+$. ^{1}H-NMR (400 MHz; $CDCl_3$): δ (ppm) 7.72 (s, 1H, Ar-C$\underline{H}$), 7.48 (d, 1H, *J* = 8.0

Hz, Ar-C*H*), 7.15 (s, 1H, Ar-C*H*), 6.86-6.60 (m, 3H, Ar-C*H*), 6.52 (d, 1H, $^{3}J_{ortho}$ = 8.0 Hz, Ar-C*H*), 4.45 (s, 2H, Ar-CH_2), 2.83-2.77 (q, 6H, $^{2}J_{a,b}$ = 8.0 Hz, N-CH_2-CH_3), 1.31 (s, 9H, C-(CH_3)$_3$), and 0.94 (t, 9H, $^{2}J_{a,b}$ = 8.0 Hz, N-CH_2-CH_3). {^{1}H}^{13}C NMR (100 MHz; $CDCl_3$): δ (ppm) 152.17, 149.90, 145.18, 141.36, 135.29, 129.40, 127.84, 124.27, 118.13, 114.04, and 111.53 (Ar-*C*H), 45.98 (N-*C*H_2-CH_3), 34.25 (*C*-(CH_3)$_3$), 31.91 (-*C*H_2-Ar), 31.47 (C-(*C*H_3)$_3$), and 8.62 (N-CH_2-*C*H_3). ^{11}B NMR ($CDCl_3$, 192.5 MHz, 23 ^{o}C, δ ppm): 19.02. UV-Vis (λ_{max}/(nm)): 212, 224, and 288 (in CH_3CN); 210, 228, and 286 (in C_2H_5OH).

(QBE$_4$): Yield (%): 89, M.p. = 101 ^{o}C, Elemental Analysis (calculated for $C_{20}H_{27}BBrNO_2$) (F.W: 404.16 g/mol) (%): C, 59.44; H, 6.73; N, 3.47. Found: C, 59.41; H, 6.71; N, 3.53. FT-IR (ATR, υ_{max}-cm^{-1}): 3069 υ(Ar-CH), 2974-2684 υ(Aliph-CH), 1492-1450 υ(C=C), 1354 υ(B-O), 1242 υ(C-N), 1153 υ(C-O), and 1051 υ(B-C). LC-MS/MS (Scan ESI^{+}): m/z = 404.15 [M]$^{+}$ and 405.16 [M+1]$^{+}$. ^{1}H-NMR (400 MHz; $CDCl_3$): δ (ppm) 7.21 (s, 1H, Ar-C*H*), 6.91-6.43 (m, 6H, Ar-C*H*), 4.45 (s, 2H, Ar-CH_2), 3.09-3.03 (q, 6H, $^{2}J_{a,b}$ = 8.0 Hz, N-CH_2-CH_3), 2.21 (s, 3H, C-CH_3), and 1.36 (t, 9H, $^{2}J_{a,b}$ = 8.0 Hz, N-CH_2-CH_3). {^{1}H}^{13}C NMR (100 MHz; $CDCl_3$): δ (ppm) 148.20, 137.84, 135.31, 134.35, 134.24, 132.88, 131.37, 128.48, 128.11, 123.20, 113.05, and 111.85 (Ar-*C*H), 45.97 (N-*C*H_2-CH_3), 33.23 (-*C*H_2-Ar), 21.37 (C-*C*H_3), and 8.67 (N-CH_2-*C*H_3). ^{11}B NMR ($CDCl_3$, 192.5 MHz, 23 ^{o}C, δ ppm): 23.28. UV-Vis (λ_{max}/(nm)): 224, 282, and 348 (in CH_3CN); 210, 282, and 346 (in C_2H_5OH).

(QBE$_5$): Yield (%): 81, M.p. = 169 ^{o}C, Elemental Analysis (calculated for $C_{21}H_{31}BBrClN_2O_2$) (F.W: 469.66 g/mol) (%): C, 53.71; H, 6.65; N, 5.96. Found: C, 53.68; H, 6.62; N, 5.99. FT-IR (ATR, υ_{max}-cm^{-1}): 3382 υ(stretching-NH_2), 3141 υ(Ar-CH), 2975-2676 υ(Aliph-CH), 1600 υ(bending-NH_2), 1489-1436 υ(C=C), 1396 υ(B-O), 1224 υ(C-N), 1145 υ(C-O), and 1057 υ(B-C). LC-MS/MS (Scan ESI^{+}): m/z = 469.66 [M]$^{+}$ and 470.65 [M+1]$^{+}$. ^{1}H-NMR (400 MHz; DMSO-d_6): δ (ppm) 7.84 (s, 2H, Ar-C*H*), 6.89 (s, 1H, Ar-C*H*), 6.60 (d, 2H, $^{3}J_{ortho}$ = 8.0 Hz, Ar-C*H*), 6.38 (s, 2H, Ar-C*H*), 4.36 (s, 2H, Ar-CH_2), 3.13 (s, 4H, NH_2-CH_2-CH_2), 3.03

(s, 6H, N-C<u>*H*</u>$_2$-CH$_3$), 2.92 (s, 4H, NH$_2$-CH$_2$-C<u>*H*</u>$_2$), 2.67 (s, 4H, NH$_2$-C<u>*H*</u>$_2$-CH$_2$), 1.26 (s, 2H, -N<u>*H*</u>$_2$), and 1.16 (s, 9H, N-CH$_2$-C<u>*H*</u>$_3$). {^{1}H}^{13}C NMR (100 MHz; DMSO-d_6): δ (ppm) 152.25, 150.92, 144.52, 130.49, 128.28, 126.15, 123.37, 119.61, 117.73, 116.45, 116.14, 108.55, and 107.63 (Ar-<u>*C*</u>H), 52.35 (N-<u>*C*</u>H$_2$-CH$_2$), 46.00 (N-<u>*C*</u>H$_2$-CH$_3$), 41.12 (N-CH$_2$-<u>*C*</u>H$_2$), 33.66 (-<u>*C*</u>H$_2$-Ar), and 9.06 (N-CH$_2$-<u>*C*</u>H$_3$). ^{11}B NMR (DMSO-d_6, 192.5 MHz, 23 ^{o}C, δ ppm): 19.64. UV-Vis (λ_{max}/(nm)): 218 and 280 (in CH$_3$CN); 208, 225, and 282 (in C$_2$H$_5$OH).

(QBE$_6$): Yield (%): 86, M.p. = 139 ^{o}C, Elemental Analysis (calculated for C$_{22}$H$_{29}$BBrNO$_4$) (F.W: 462.19 g/mol) (%): C, 57.17; H, 6.32; N, 3.03. Found: C, 57.14; H, 6.21; N, 3.09. FT-IR (ATR, υ_{max}-cm^{-1}): 3032 υ(Ar-CH), 2976-2676 υ(Aliph-CH), 1693 υ(C=O), 1496-1445 υ(C=C), 1366 υ(B-O), 1267 υ(C-N), 1161 υ(C-O), and 1083 υ(B-C). LC-MS/MS (Scan ESI$^+$): m/z = 462.19 [M]$^+$ and 463.20 [M+1]$^+$. ^{1}H-NMR (400 MHz; CDCl$_3$): δ (ppm) 7.79 (d, 1H, $^3J_{ortho}$ = 4.0 Hz, Ar-C<u>*H*</u>), 7.78-7.42 (m, 2H, Ar-C<u>*H*</u>), 7.36 (d, 1H, $^3J_{ortho}$ = 8.0 Hz, Ar-C<u>*H*</u>), 6.88 (s, 1H, Ar-C<u>*H*</u>), 6.78 (d, 1H, $^3J_{ortho}$ = 8.0 Hz, Ar-C<u>*H*</u>), 6.70 (d, 1H, $^3J_{ortho}$ = 8.0 Hz, Ar-C<u>*H*</u>), 4.42 (s, 2H, Ar-C<u>*H*</u>$_2$), 4.28-4.24 (q, 2H, $^2J_{a,b}$ = 4.0 Hz, O-C<u>*H*</u>$_2$), 3.05-3.00 (q, 6H, $^2J_{a,b}$ = 8.0 Hz, N-C<u>*H*</u>$_2$-CH$_3$), 1.33 (t, 3H, $^2J_{a,b}$ = 8.0 Hz O-CH$_2$-C<u>*H*</u>$_3$), and 1.07 (t, 9H, $^2J_{a,b}$ = 8.0 Hz, N-CH$_2$-C<u>*H*</u>$_3$). {^{1}H}^{13}C NMR (100 MHz; CDCl$_3$): δ (ppm) 167.45 (C=O), 157.60, 153.24, 150.71, 145.42, 135.10, 129.53, 128.39, 123.88, 122.58, 122.00, 120.37, 114.84, 113.95, and 108.53 (Ar-<u>*C*</u>H), 60.20 (O-<u>*C*</u>H$_2$-CH$_3$), 45.91 (N-<u>*C*</u>H$_2$-CH$_3$), 33.93 (-<u>*C*</u>H$_2$-Ar), 14.45 (O-CH$_2$-<u>*C*</u>H$_3$), and 8.52 (N-CH$_2$-<u>*C*</u>H$_3$). ^{11}B NMR (CDCl$_3$, 192.5 MHz, 23 ^{o}C, δ ppm): 11.26. UV-Vis (λ_{max}/(nm)): 216, 234, 262, and 304 (in CH$_3$CN); 206, 222, 264, and 302 (in C$_2$H$_5$OH).

(QBE$_7$): Yield (%): 81, M.p. = 154 ^{o}C, Elemental Analysis (calculated for C$_{22}$H$_{27}$BBrNO$_4$) (F.W: 460.18 g/mol) (%): C, 57.42; H, 5.91; N, 3.04. Found: C, 57.40; H, 5.88; N, 3.10. FT-IR (ATR, υ_{max}-cm^{-1}): 3569-2584 υ(-COOH), 3076 υ(Ar-CH), 2987-2901 υ(Aliph-CH), 1690 υ(C=O), 1491-1439 υ(C=C), 1380 υ(B-O), 1248 υ(C-N), 1156 υ(C-O), and 1074 υ(B-C). LC-MS/MS (Scan ESI$^+$): m/z = 460.18 [M]$^+$ and 461.18 [M+1]$^+$. ^{1}H-NMR (400 MHz; CDCl$_3$): δ

(ppm) 12.05 (s, 1H, -COO$\underline{H}$), 7.83-6.66 (m, 7H, Ar-C$\underline{H}$), 7.50 (d, 1H, $^{3}J_{ortho}$ = 16.0 Hz, C$\underline{H}$=CH), 6.20 (d, 1H, $^{3}J_{ortho}$ = 16.0 Hz, CH=C$\underline{H}$), 4.50 (s, 2H, Ar-C$\underline{H_2}$), 2.98-2.93 (q, 6H, $^{2}J_{a,b}$ = 8.0 Hz, N-C$\underline{H_2}$-CH_3), and 1.27 (t, 9H, $^{2}J_{a,b}$ = 6.0 Hz, N-CH_2-C$\underline{H_3}$). $\{^{1}H\}^{13}C$ NMR (100 MHz; $CDCl_3$): δ (ppm) 169.45 (C=O), 147.15, 144.86, 135.29, 134.30, 134.23, 134.20, 130.92, 127.85, 127.42, 121.30, 116.26, and 115.15 (Ar-$\underline{C}$H and $\underline{C}$H=$\underline{C}$H), 45.76 (N-$\underline{C}H_2$-CH_3), 34.26 (-$\underline{C}H_2$-Ar), and 8.60 (N-CH_2-$\underline{C}H_3$). ^{11}B NMR ($CDCl_3$, 192.5 MHz, 23 ^{o}C, δ ppm): 19.94. UV-Vis (λ_{max}/(nm)): 220, 268, 310, and 362 (in CH_3CN); 206, 238, 270, 284, and 340 (in C_2H_5OH).

(QBE$_8$): Yield (%): 92, M.p. = 138 ^{o}C, Elemental Analysis (calculated for $C_{19}H_{31}BBrNO_4$) (F.W: 428.17 g/mol) (%): C, 53.30; H, 7.30; N, 3.27. Found: C, 53.27; H, 7.26; N, 3.32. FT-IR (ATR, υ_{max}-cm^{-1}): 3048 υ(Ar-CH), 2979-2678 υ(Aliph-CH), 1480-1434 υ(C=C), 1314 υ(B-O), 1211 υ(C-N), 1162 υ(C-O), and 1035 υ(B-C). LC-MS/MS (Scan ESI^{+}): m/z = 428.17 $[M]^{+}$ and 429.17 $[M+1]^{+}$. ^{1}H-NMR (400 MHz; $CDCl_3$): δ (ppm) 7.85 (d, 1H, $^{3}J_{ortho}$ = 8.0 Hz, Ar-C$\underline{H}$), 7.71 (s, 1H, Ar-C$\underline{H}$), 7.60 (d, 1H, $^{3}J_{ortho}$ = 8.0 Hz, Ar-C$\underline{H}$), 7.42 (t, 1H, $^{3}J_{ortho}$ = 8.0 Hz, Ar-C$\underline{H}$), 4.84 (s, 2H, O-C$\underline{H_2}$-O), 4.61 (s, 2H, Ar-C$\underline{H_2}$), 4.03 (s, 4H, O-C$\underline{H_2}$), 3.75 (s, 4H, O-C$\underline{H_2}$), 3.14-3.08 (q, 6H, $^{2}J_{a,b}$ = 8.0 Hz, N-C$\underline{H_2}$-CH_3), and 1.40 (t, 9H, $^{2}J_{a,b}$ = 6.0 Hz, N-CH_2-C$\underline{H_3}$). $\{^{1}H\}^{13}C$ NMR (100 MHz; $CDCl_3$): δ (ppm) 134.47, 133.96, 133.86, 131.61, 130.95, 128.13, and 127.60 (Ar-$\underline{C}$H), 69.80 (O-CH_2-$\underline{C}$), 65.45 and 64.93 (C-$\underline{C}H_2$), 45.90 (N-$\underline{C}H_2$-CH_3), 35.22 (-$\underline{C}H_2$-Ar), and 33.70 (Cyc-$\underline{C}H_2$), and 8.63 (N-CH_2-$\underline{C}H_3$). ^{11}B NMR ($CDCl_3$, 192.5 MHz, 23 ^{o}C, δ ppm): 19.14. UV-Vis (λ_{max}/(nm)): 208, 226, and 270 (in CH_3CN); 216, 223, and 276 (in C_2H_5OH).

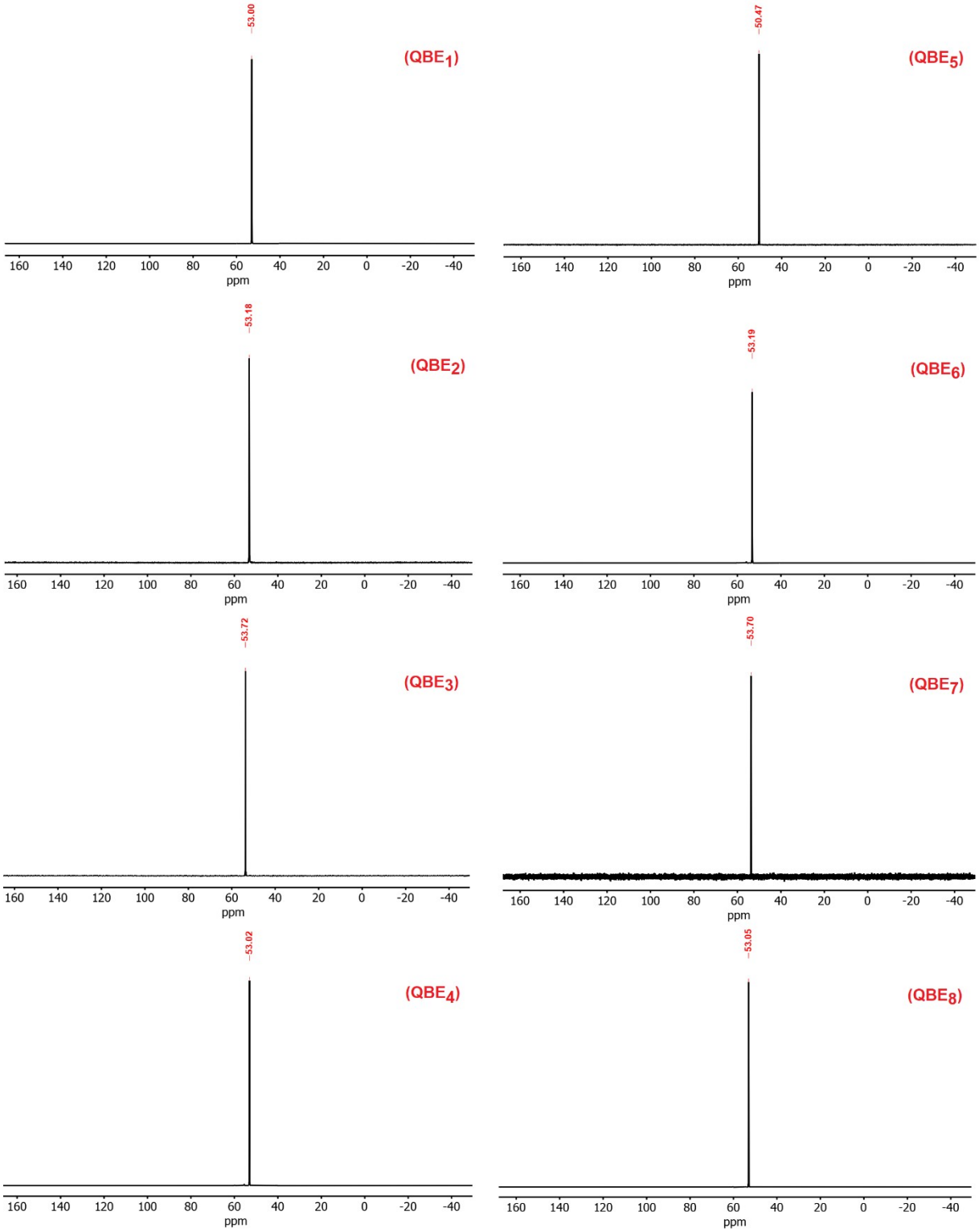


Figure 1. ^{31}P NMR spectra determining the Lewis acidity of compounds **(QBE_1-QBE_8)** by the Gutmann-Beckett method in $CDCl_3$

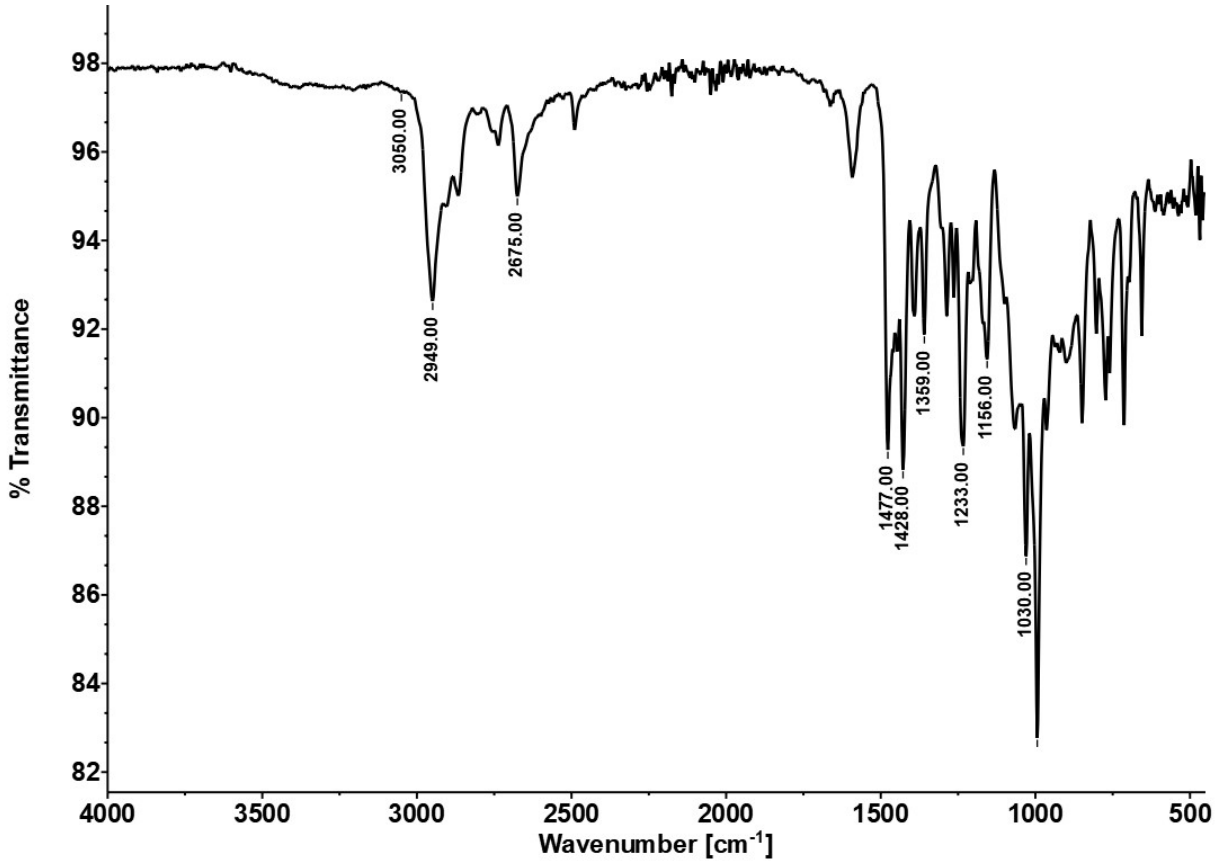


Figure S2. FT-IR spectra of the quaternized boronate ester **(QBE_1)**

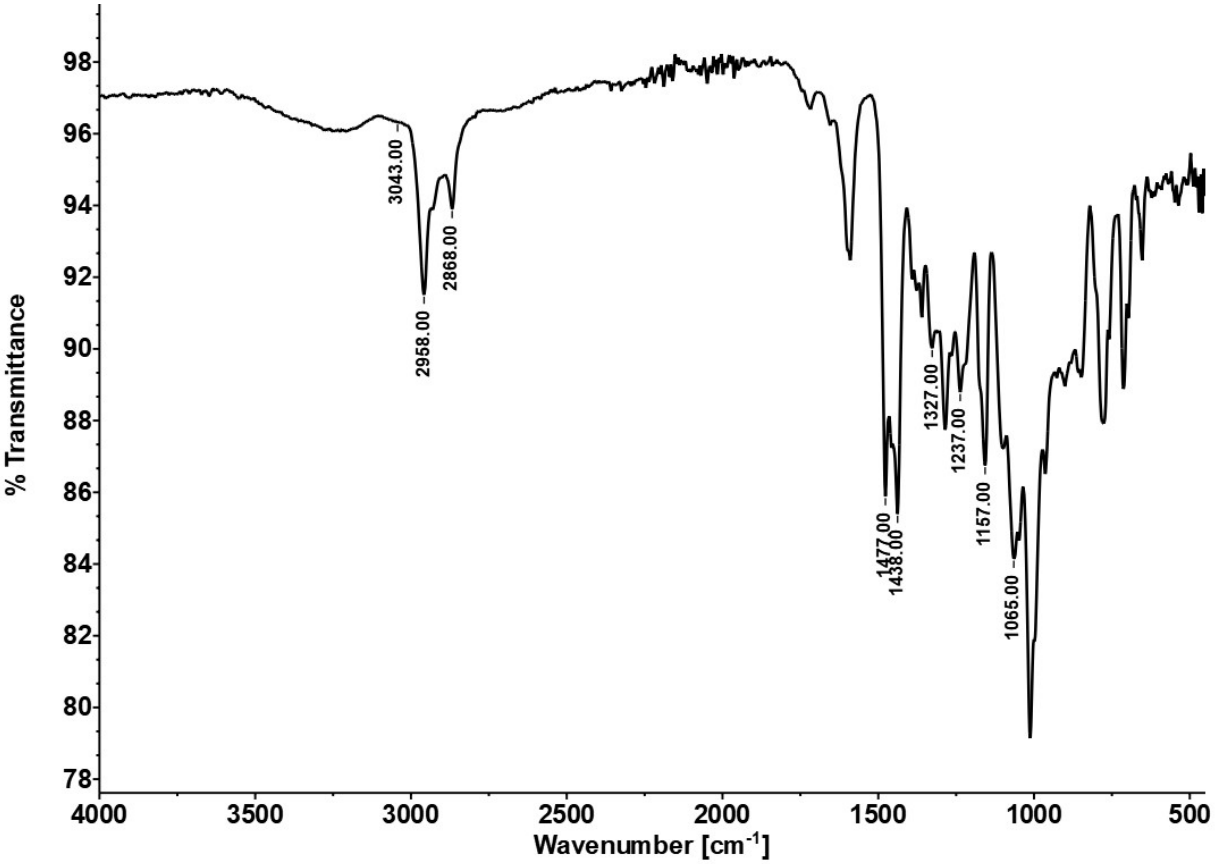


Figure S3. FT-IR spectra of the quaternized boronate ester **(QBE_2)**

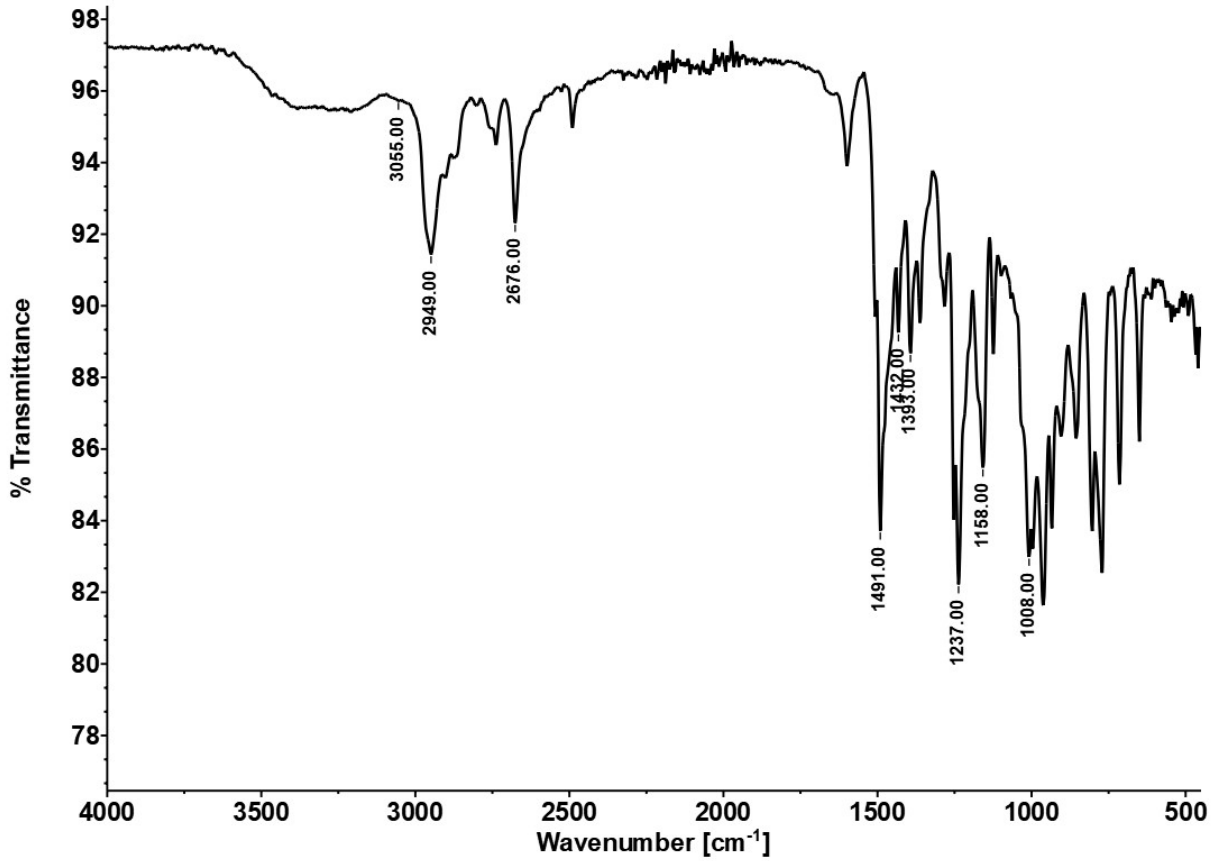


Figure S4. FT-IR spectra of the quaternized boronate ester **(QBE_3)**

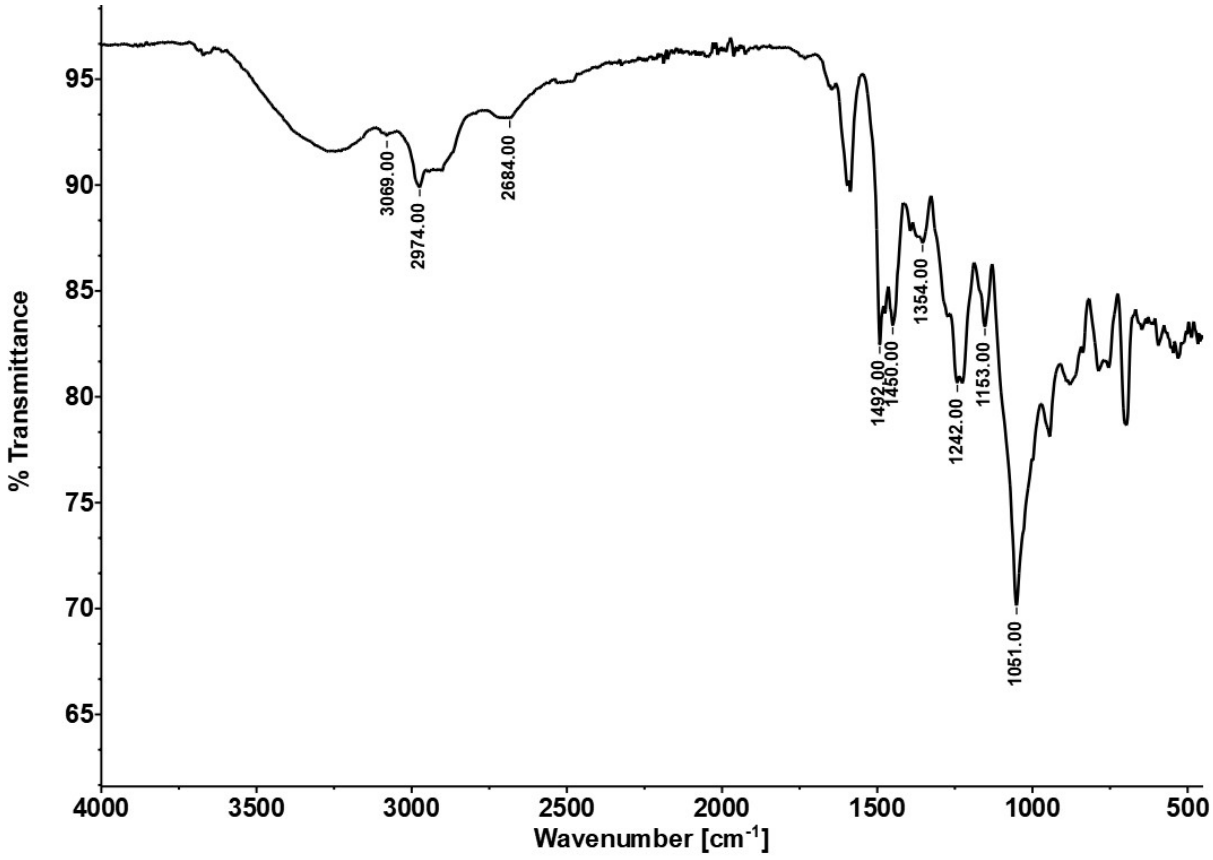


Figure S5. FT-IR spectra of the quaternized boronate ester **(QBE_4)**

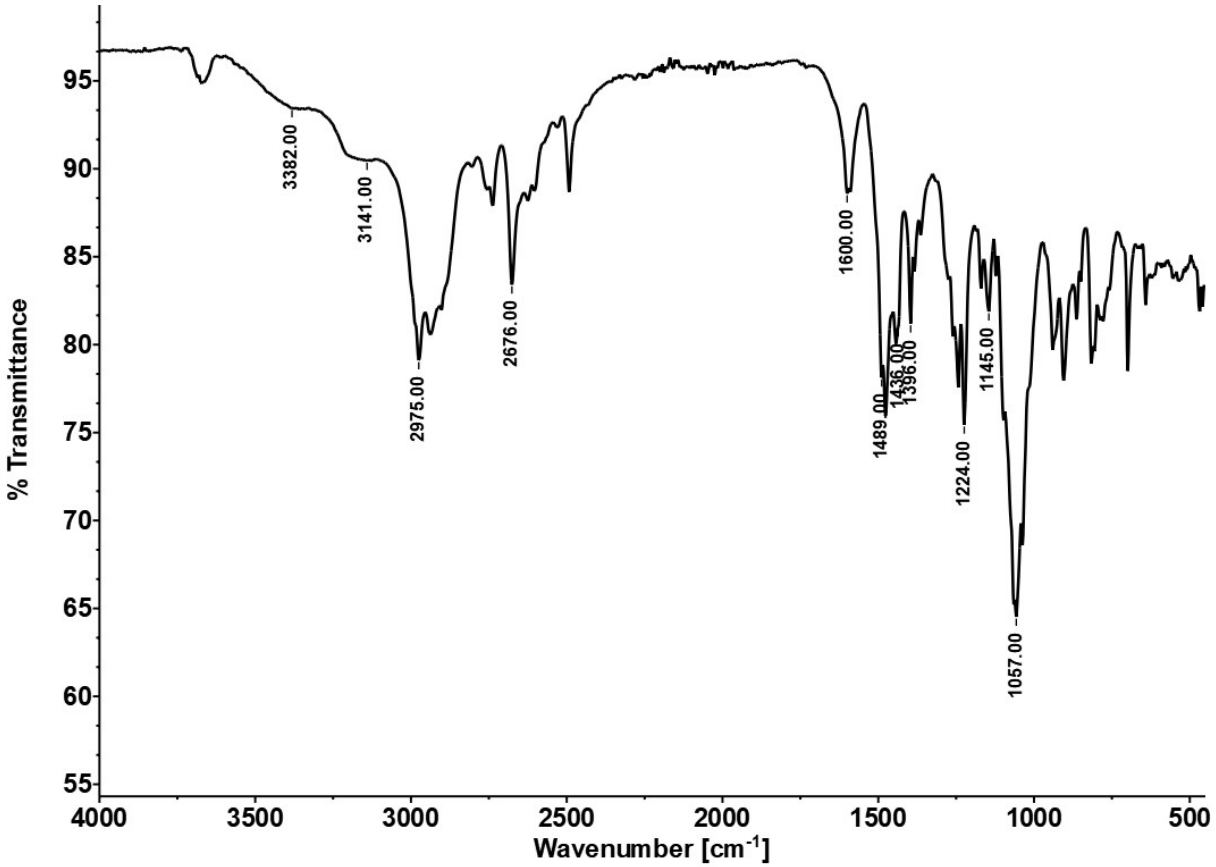


Figure S6. FT-IR spectra of the quaternized boronate ester **(QBE_5)**

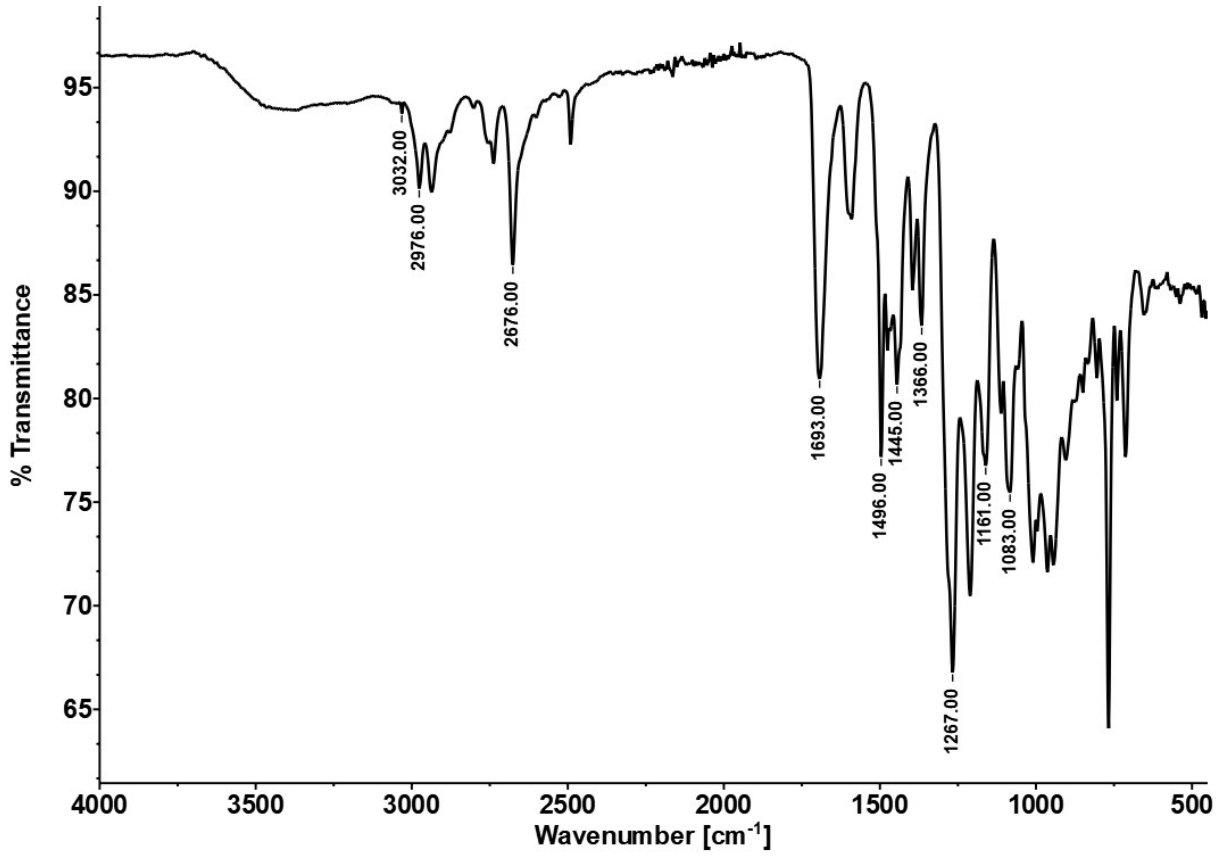


Figure S7. FT-IR spectra of the quaternized boronate ester **(QBE_6)**

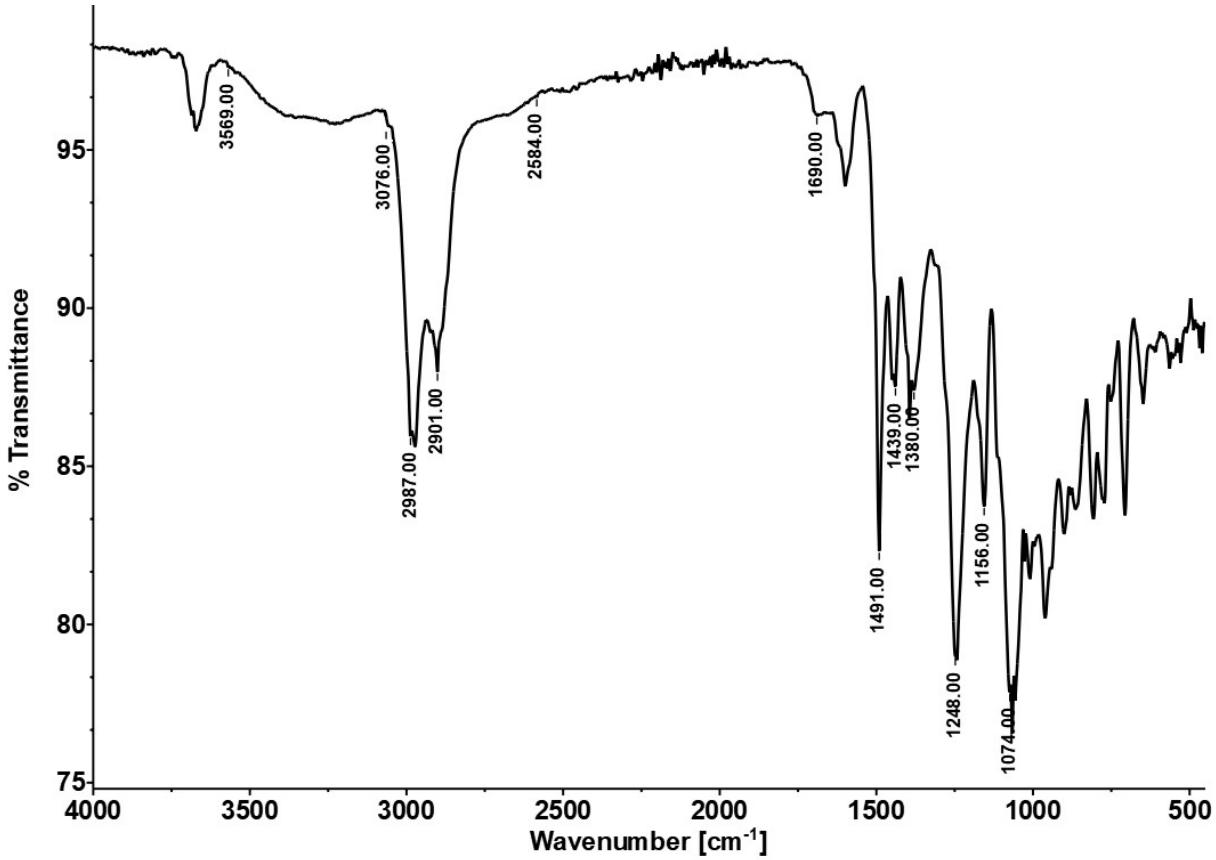


Figure S8. FT-IR spectra of the quaternized boronate ester **(QBE_7)**

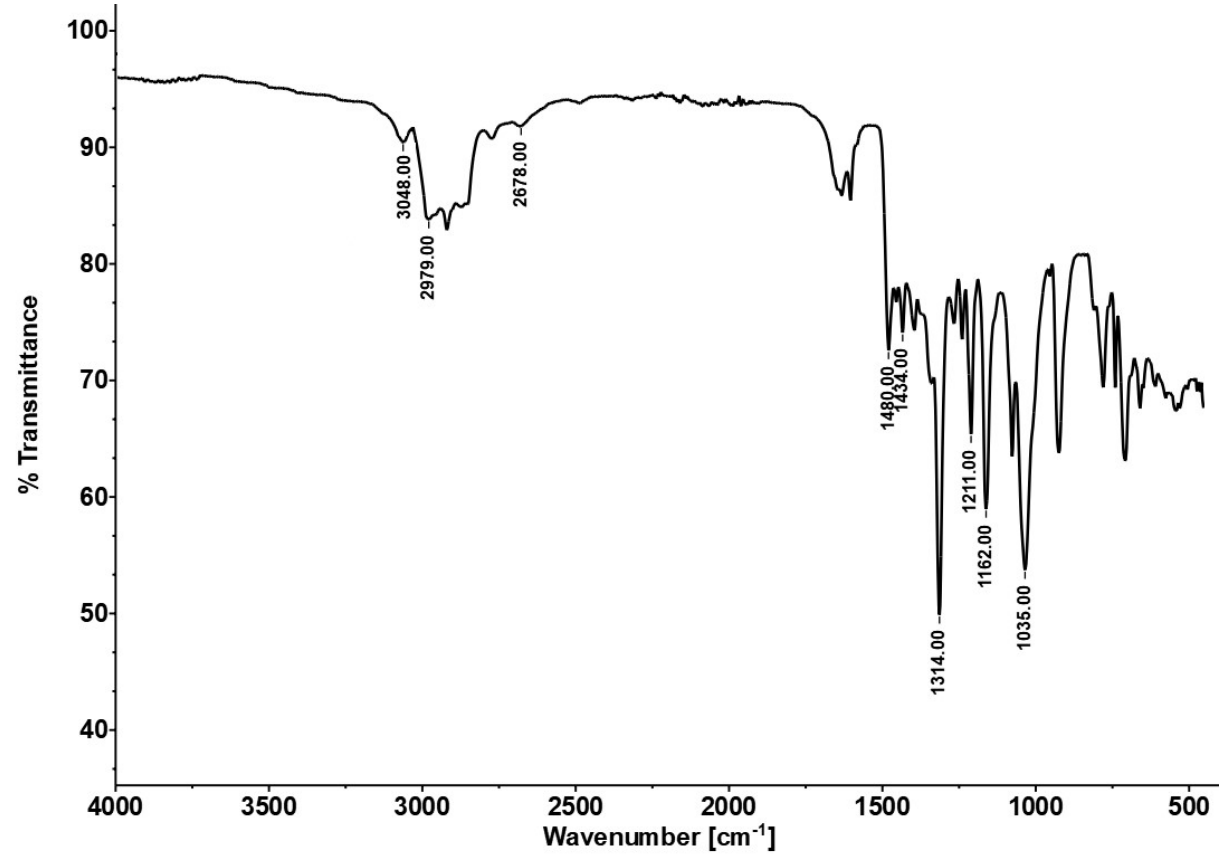


Figure S9. FT-IR spectra of the quaternized boronate ester **(QBE_8)**

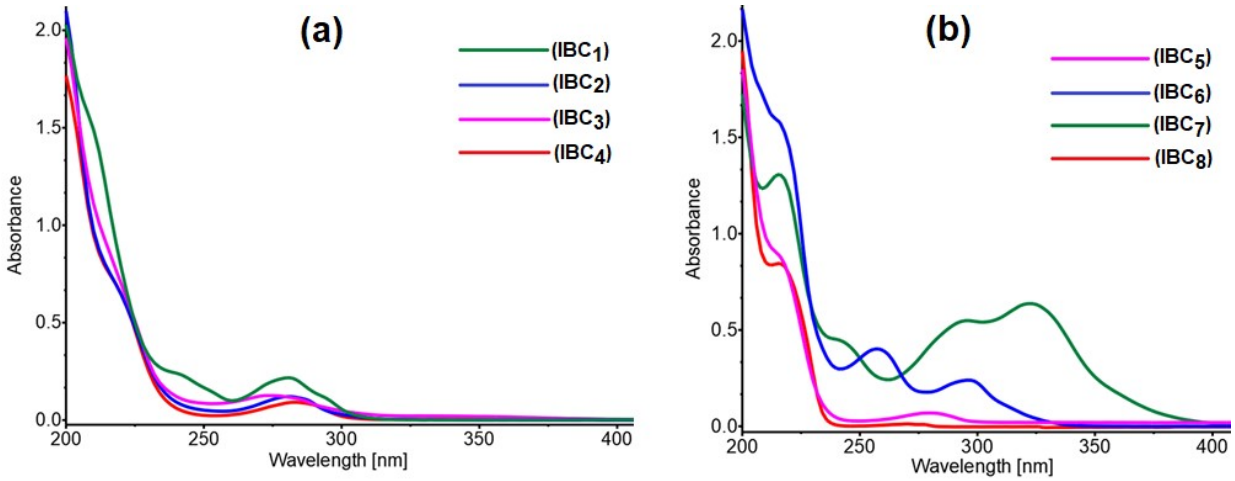
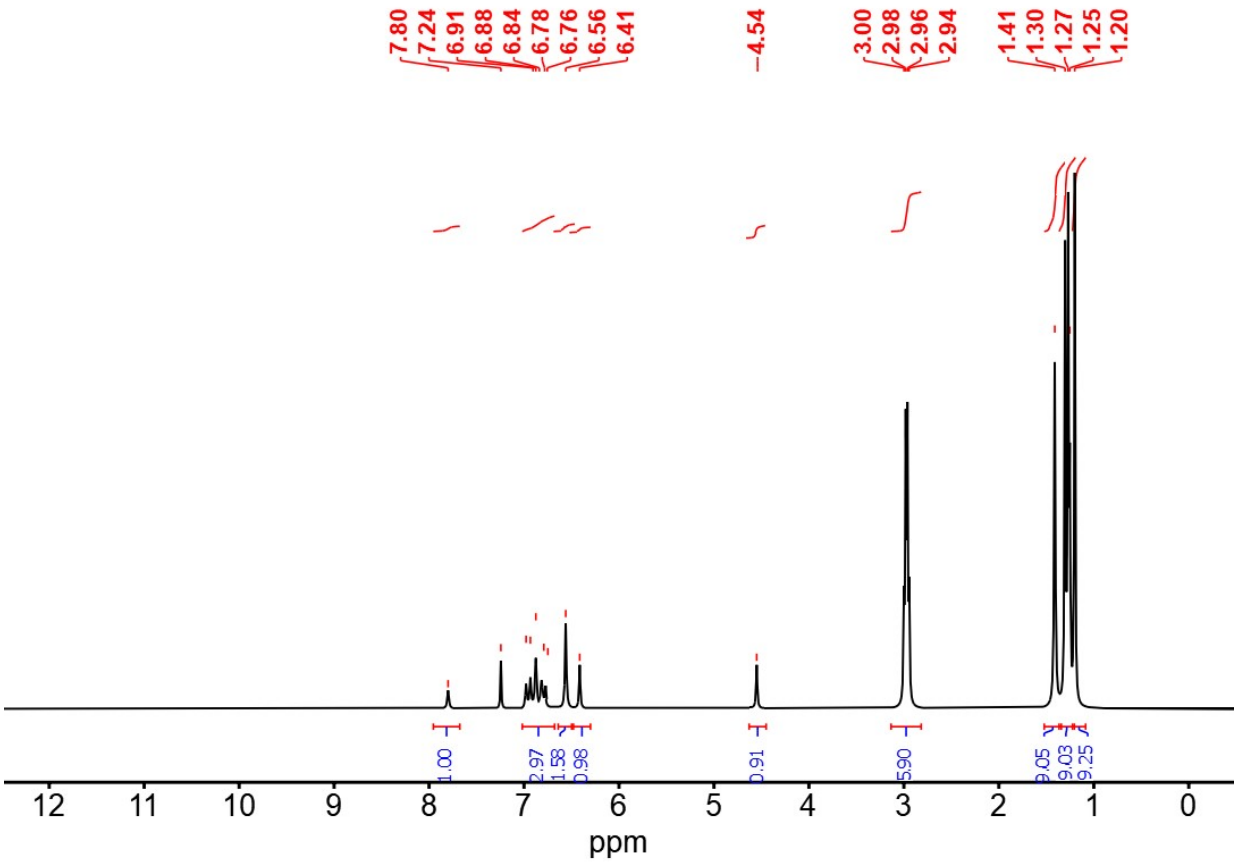


Figure S10. UV-Vis spectra of the quaternized boronate esters **(QBE_1-QBE_4) (a)** and **(QBE_5-QBE_8) (b)** in C_2H_5OH



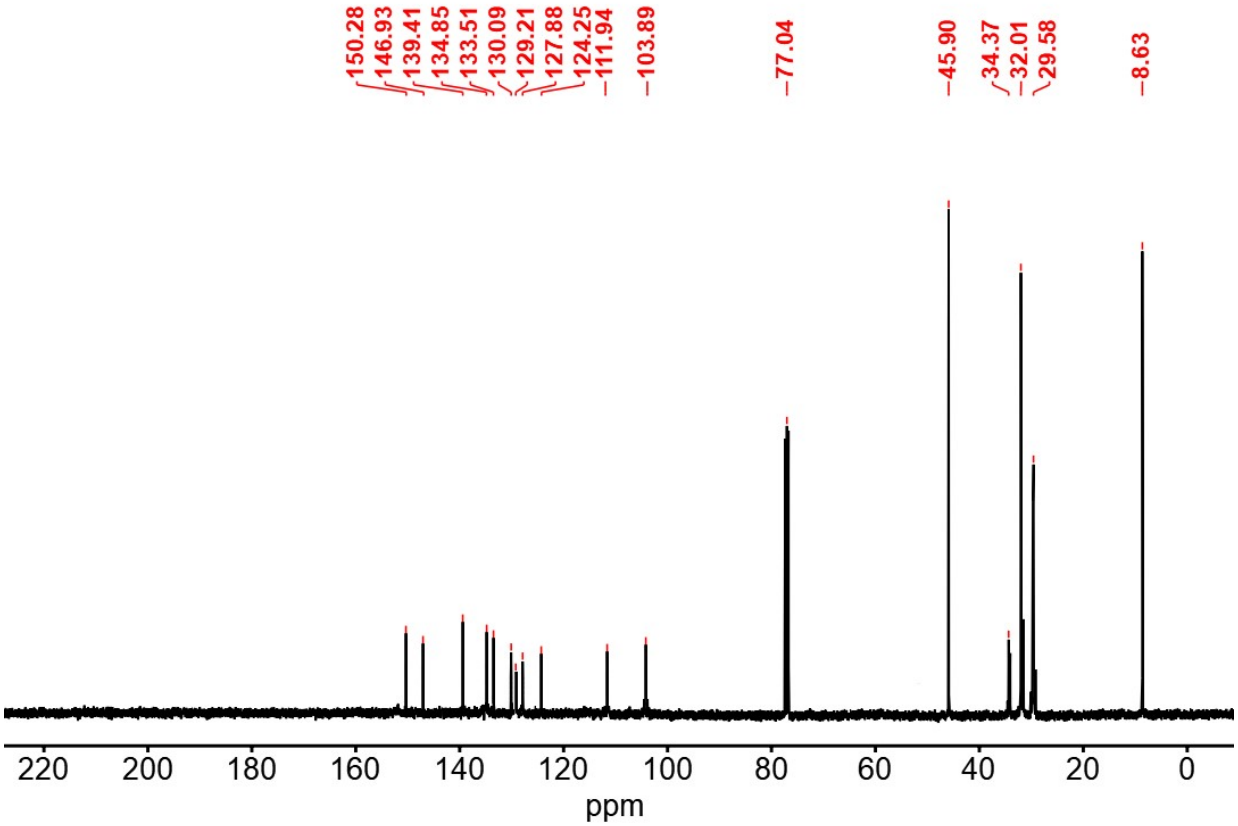


Figure S11. ^{1}H and ^{13}C-NMR spectra of the quaternized boronate ester **(QBE_1)**

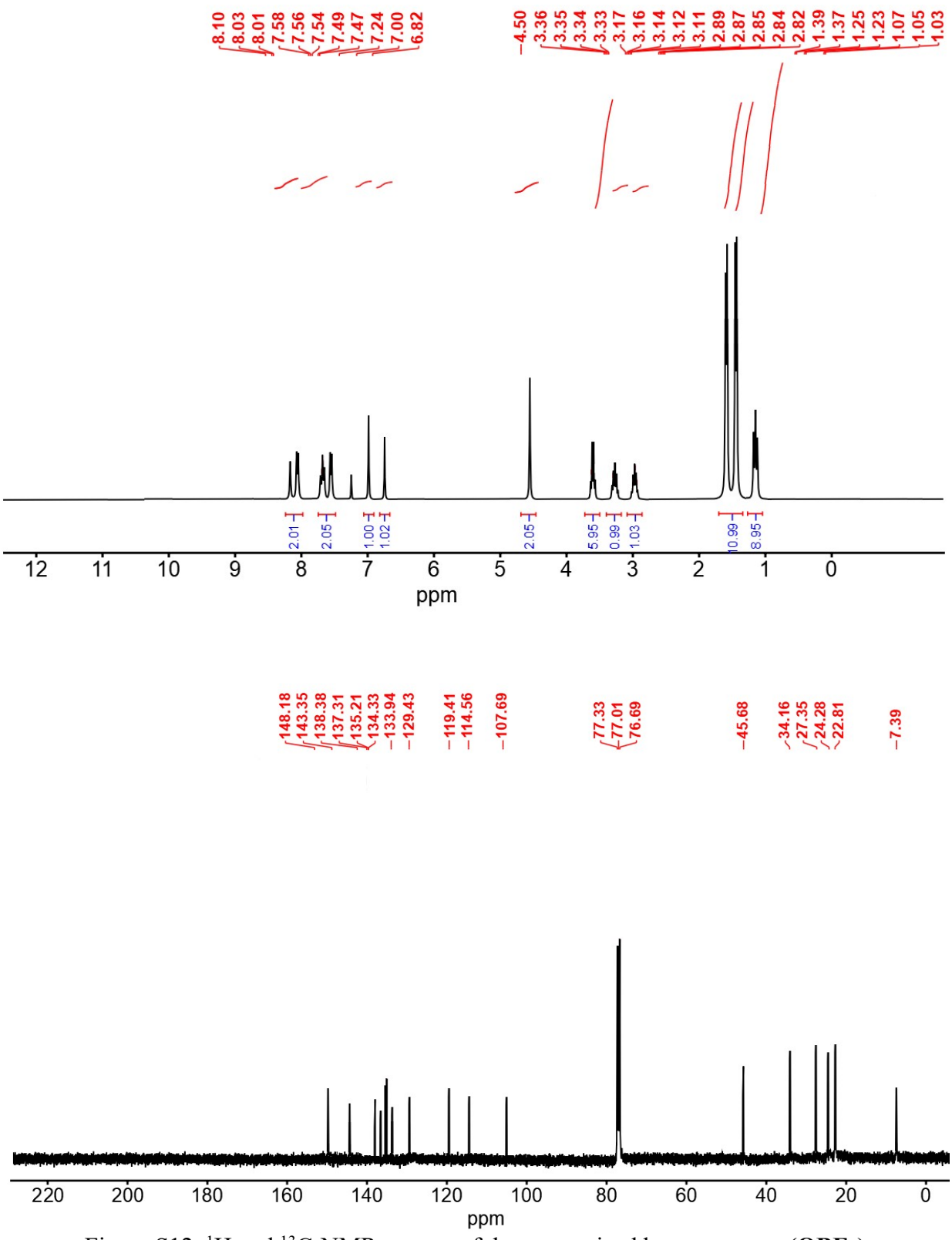


Figure S12. ^{1}H and ^{13}C-NMR spectra of the quaternized boronate ester **(QBE_2)**

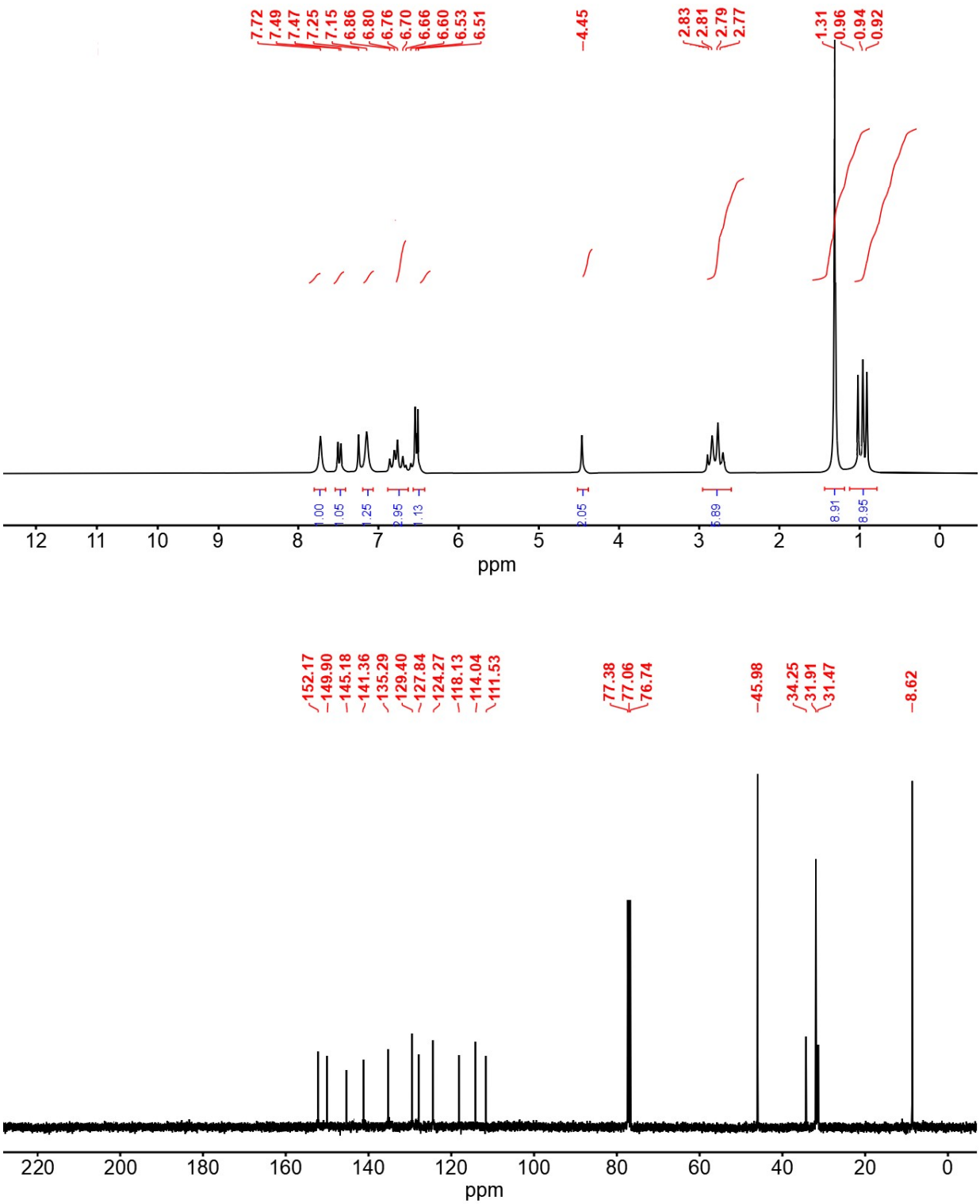


Figure S13. ^{1}H and ^{13}C-NMR spectra of the quaternized boronate ester **(QBE_3)**

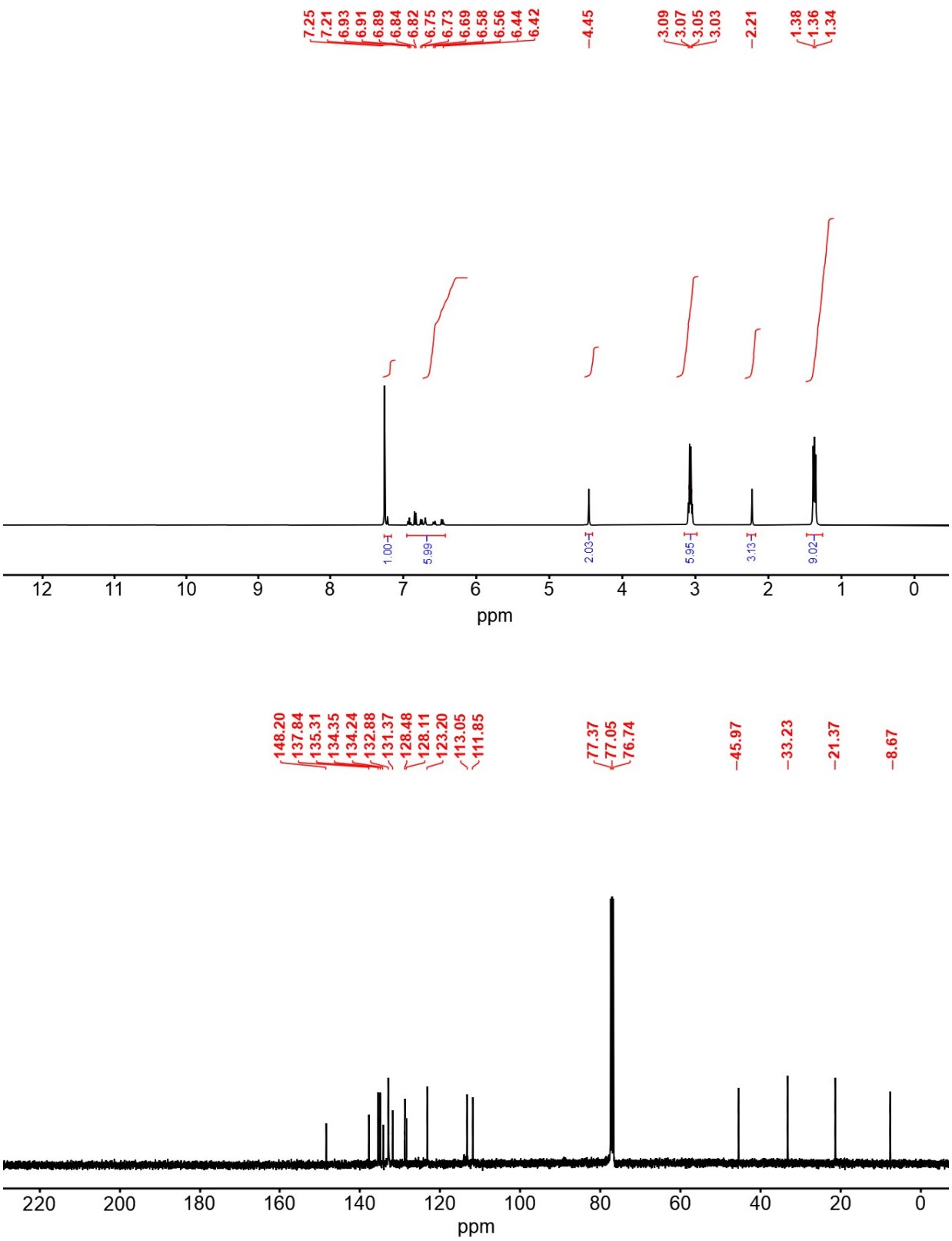


Figure S14. ^{1}H and ^{13}C-NMR spectra of the quaternized boronate ester **(QBE_4)**

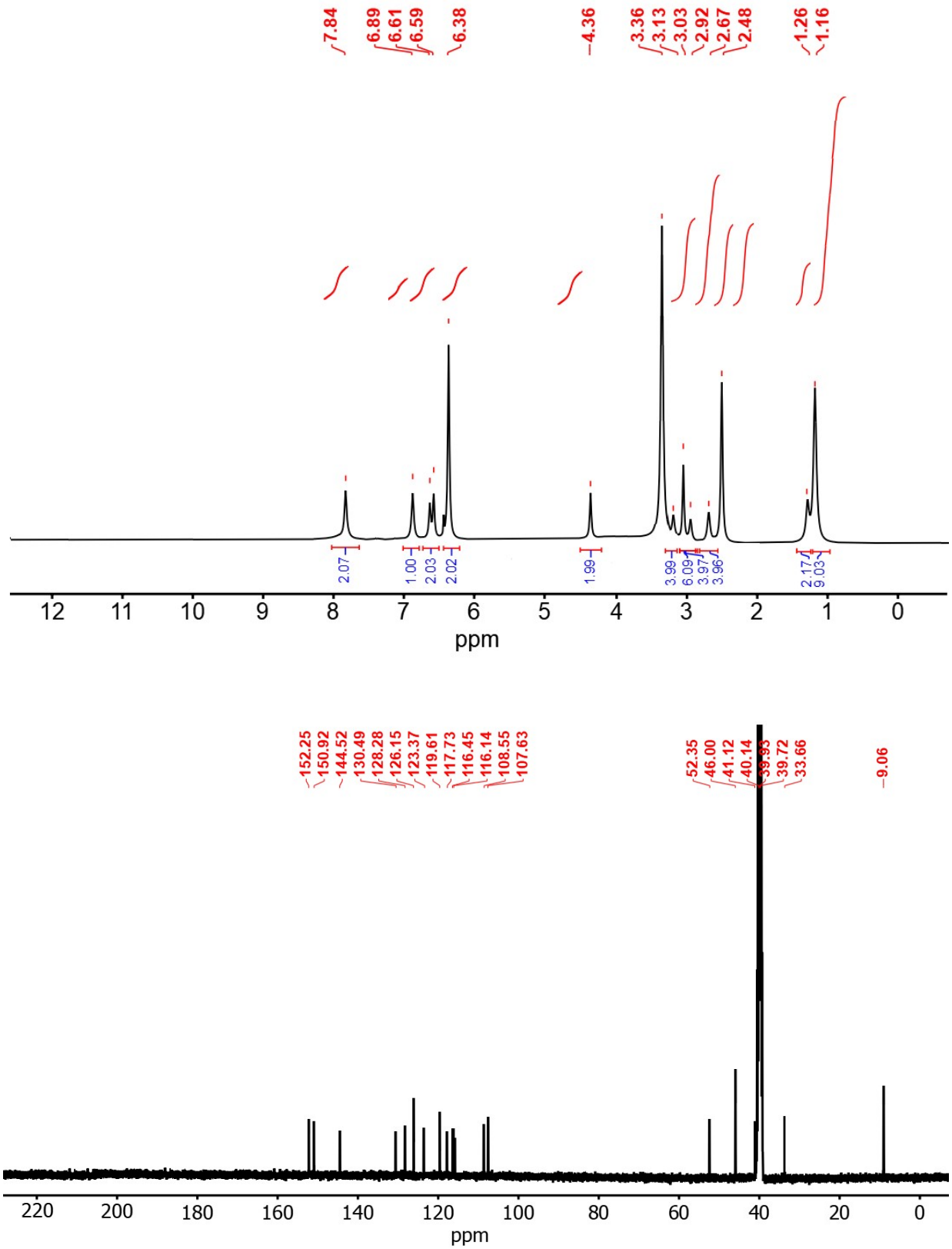


Figure S15. ^{1}H and ^{13}C-NMR spectra of the quaternized boronate ester **(QBE_5)**

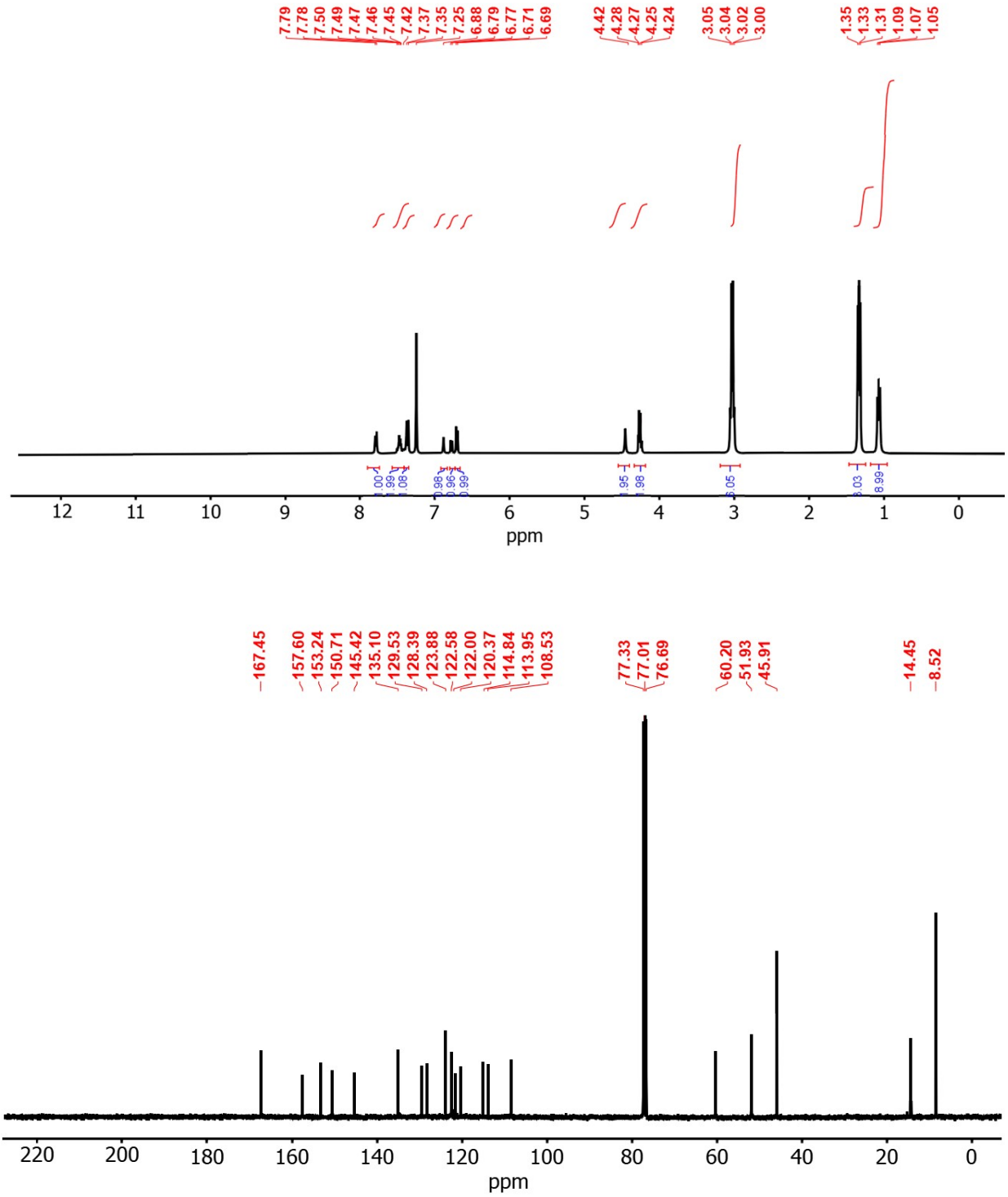


Figure S16. ^{1}H and ^{13}C-NMR spectra of the quaternized boronate ester **(QBE_6)**

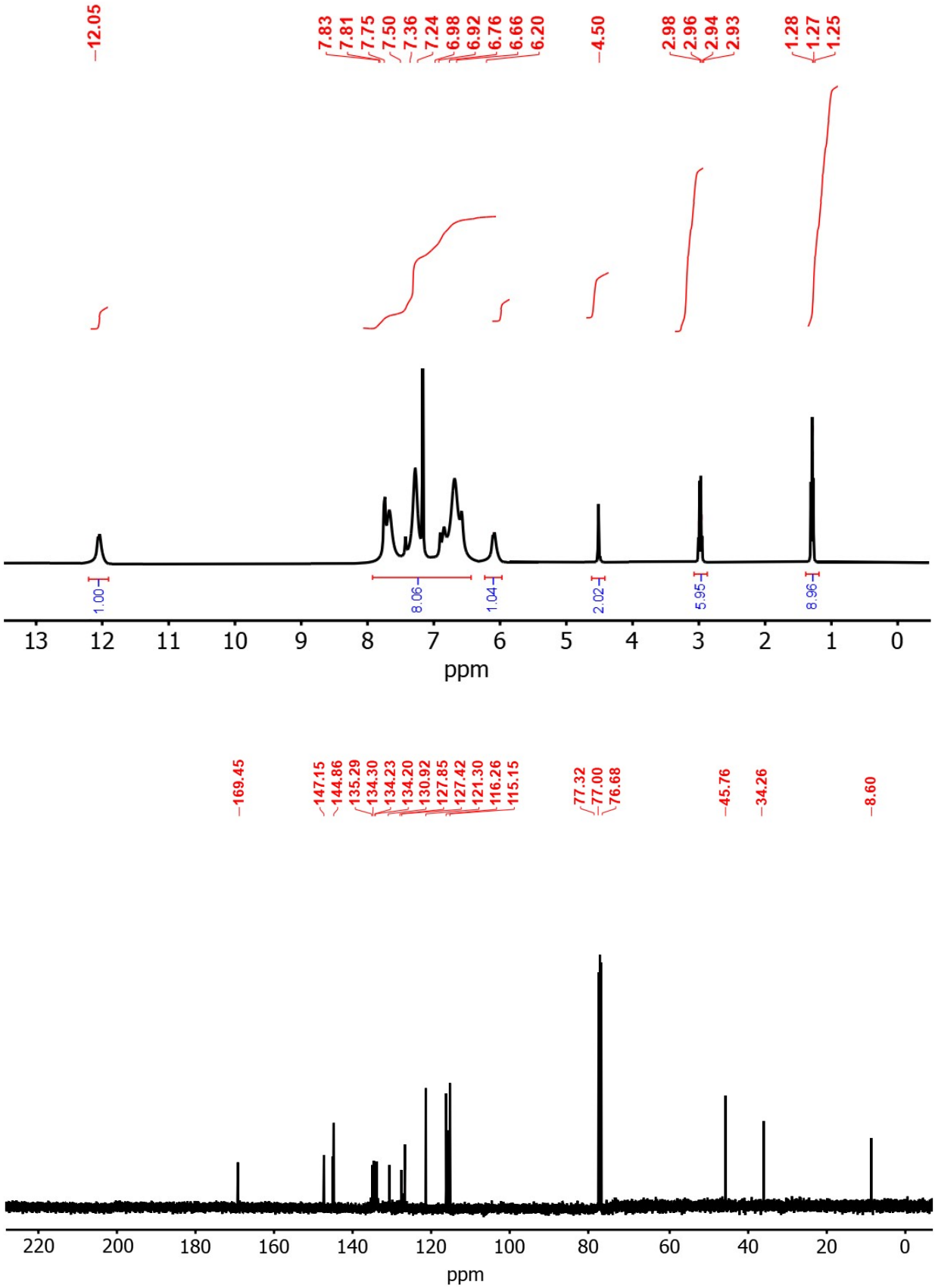


Figure S17. ^{1}H and ^{13}C-NMR spectra of the quaternized boronate ester **(QBE_7)**

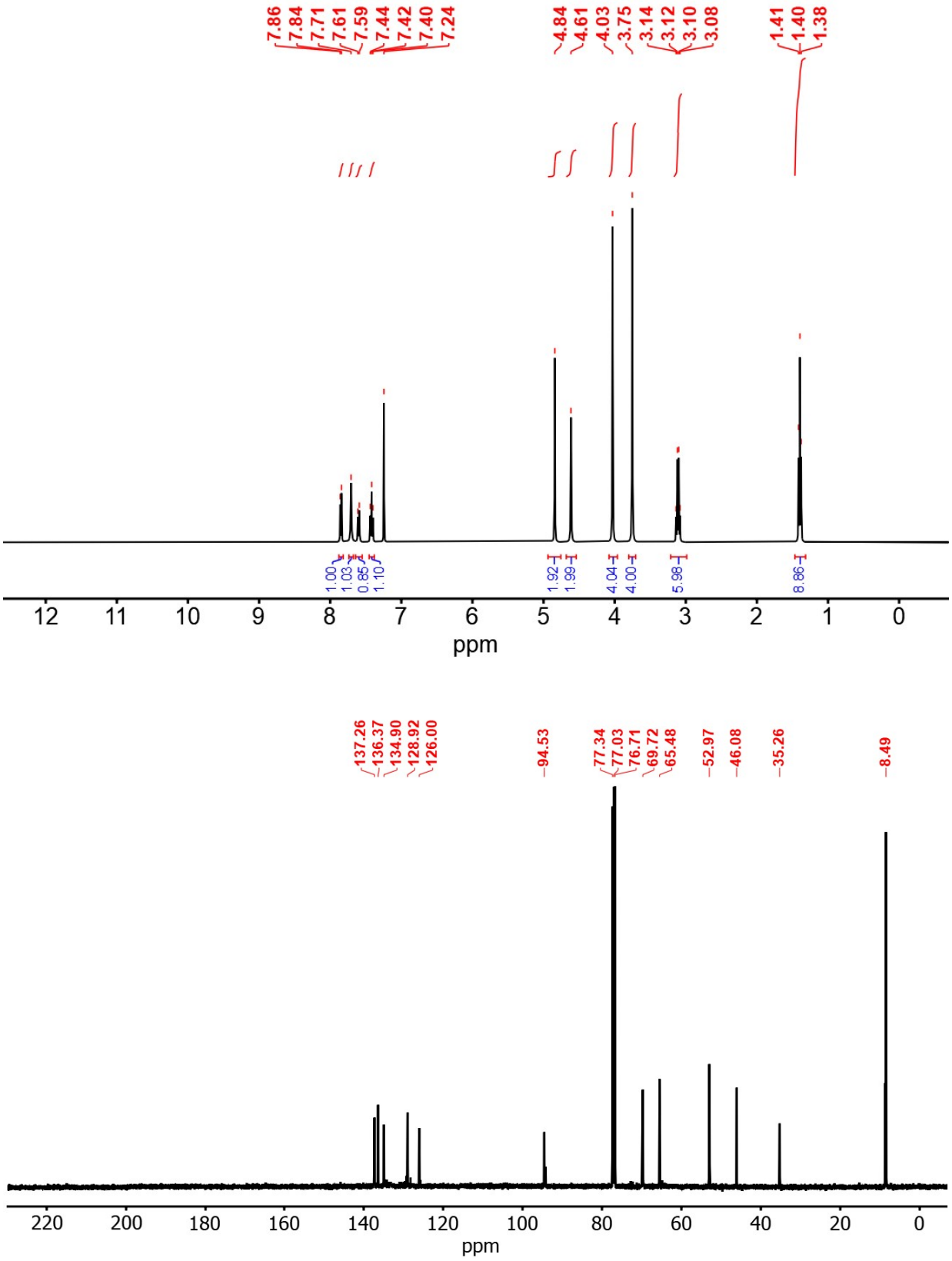


Figure S18. ^{1}H and ^{13}C-NMR spectra of the quaternized boronate ester **(QBE_8)**

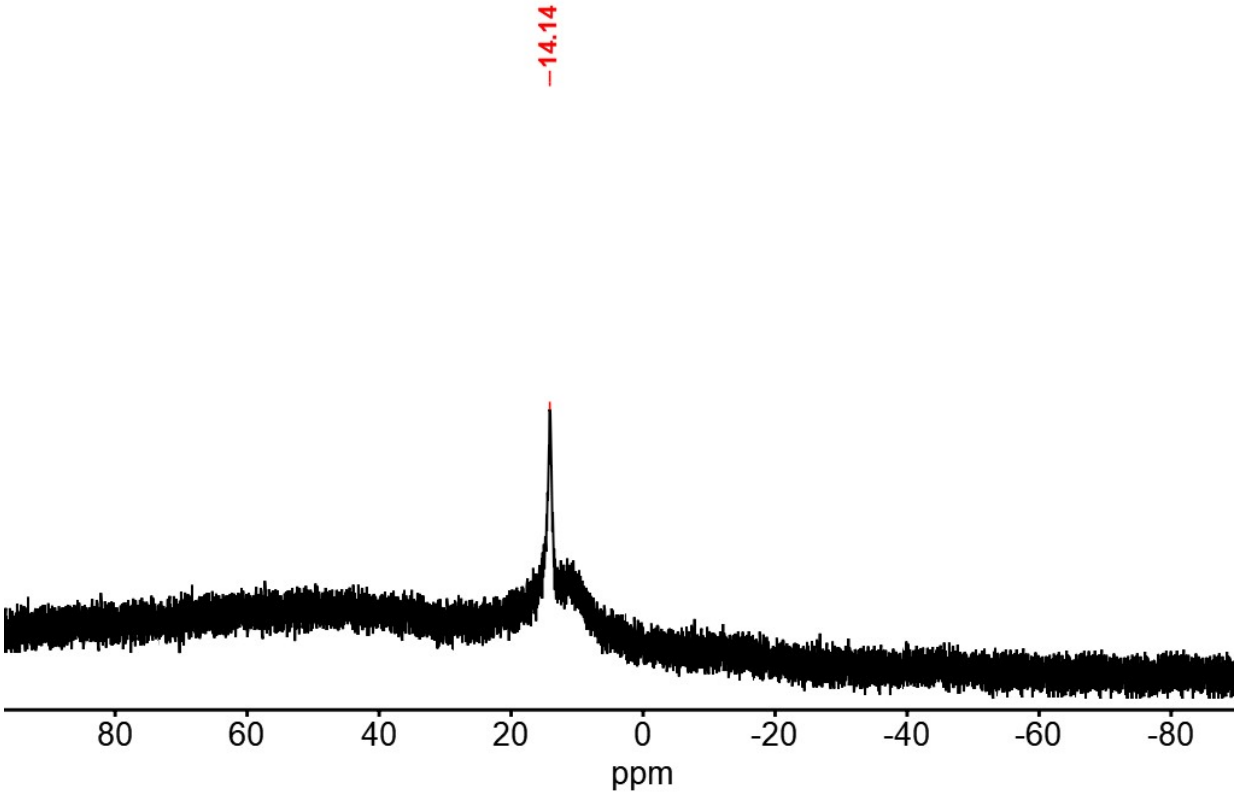


Figure S19. ^{11}B-NMR spectra of the quaternized boronate ester **(QBE_1)**

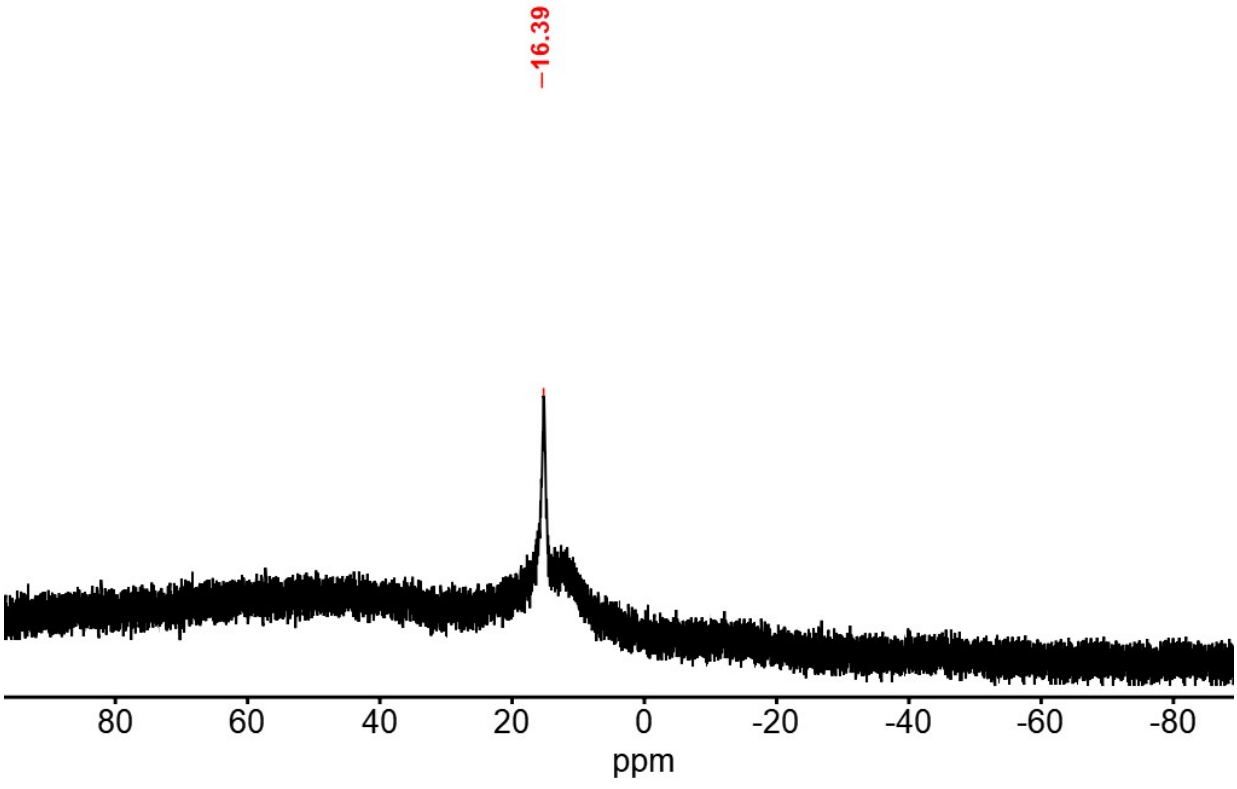


Figure S20. ^{11}B-NMR spectra of the quaternized boronate ester **(QBE_2)**

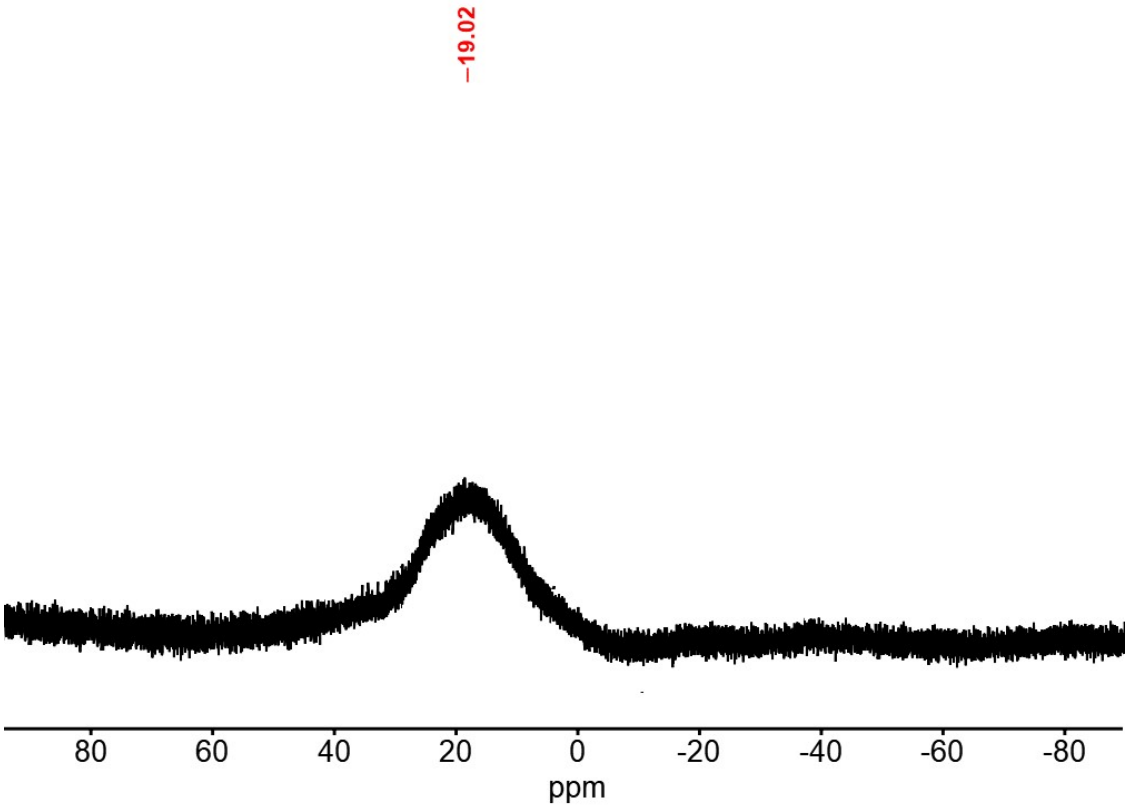


Figure S21. ^{11}B-NMR spectra of the quaternized boronate ester **(QBE_3)**

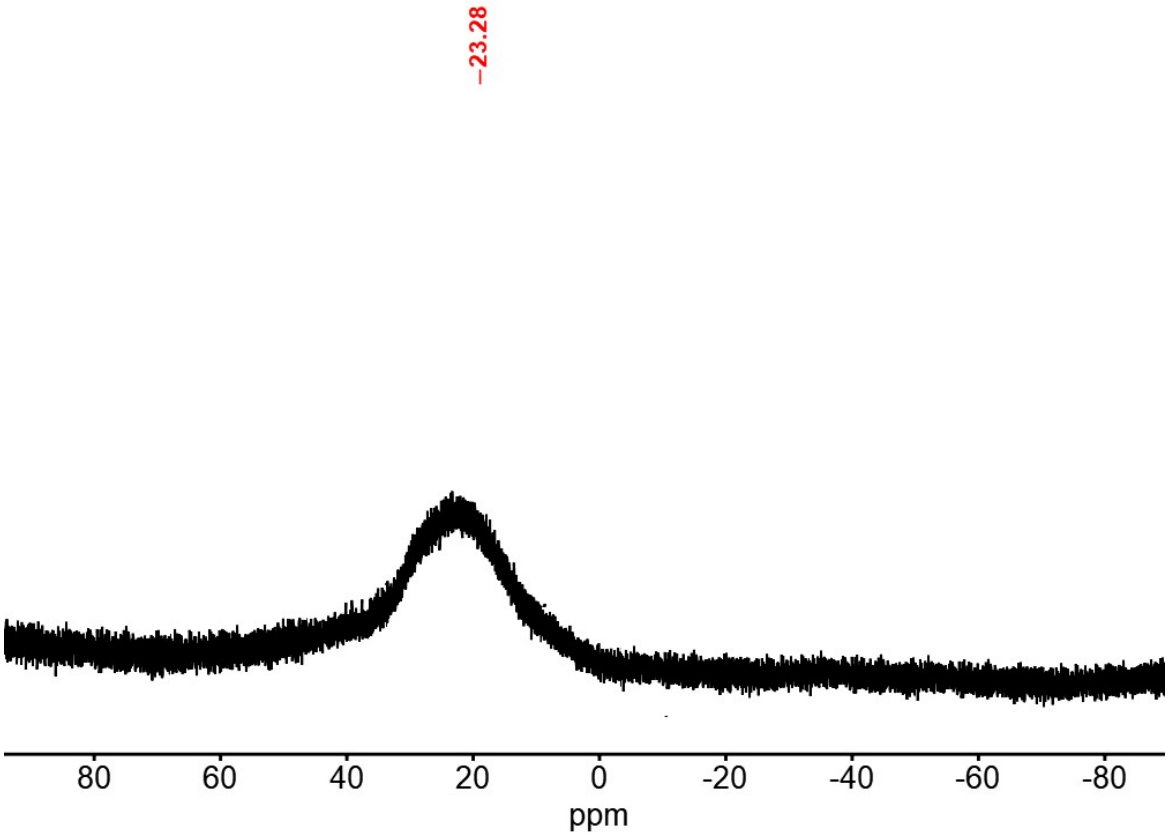


Figure S22. ^{11}B-NMR spectra of the quaternized boronate ester **(QBE_4)**

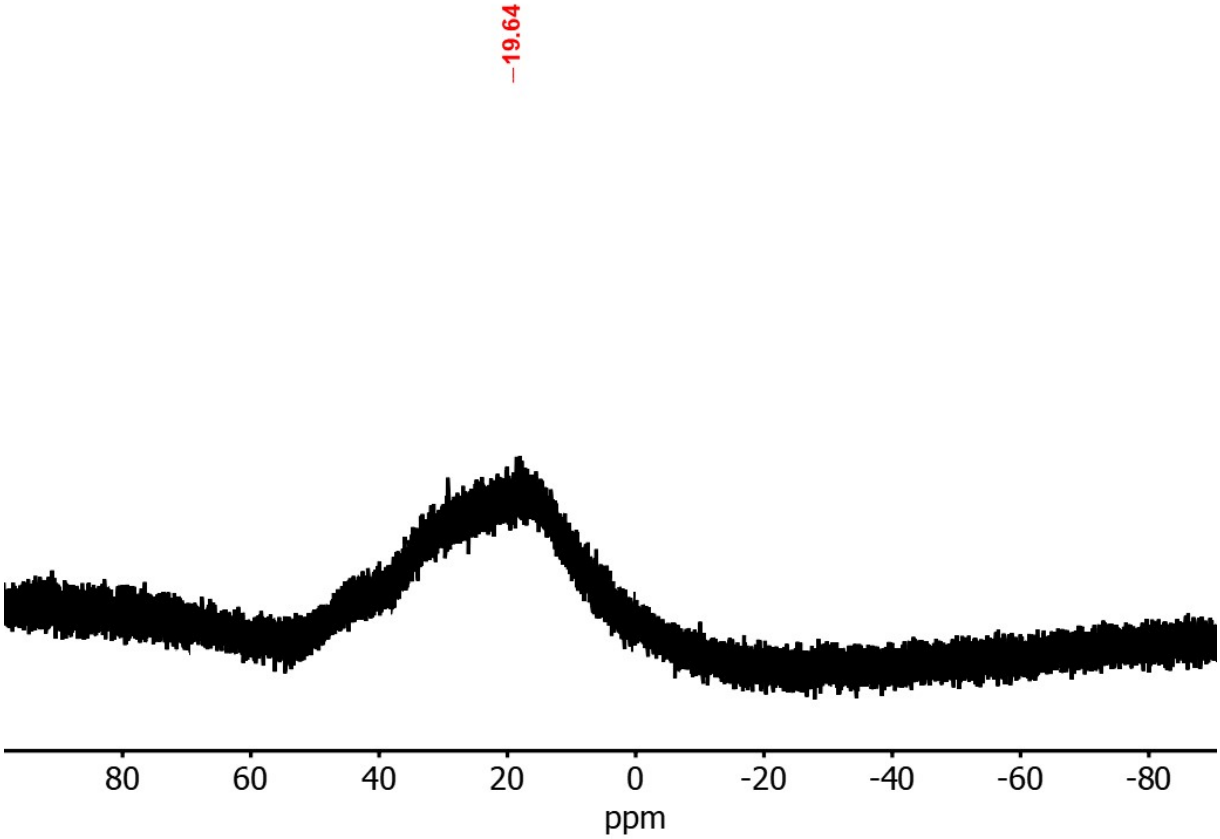


Figure S23. ^{11}B-NMR spectra of the the quaternized boronate ester **(QBE_5)**

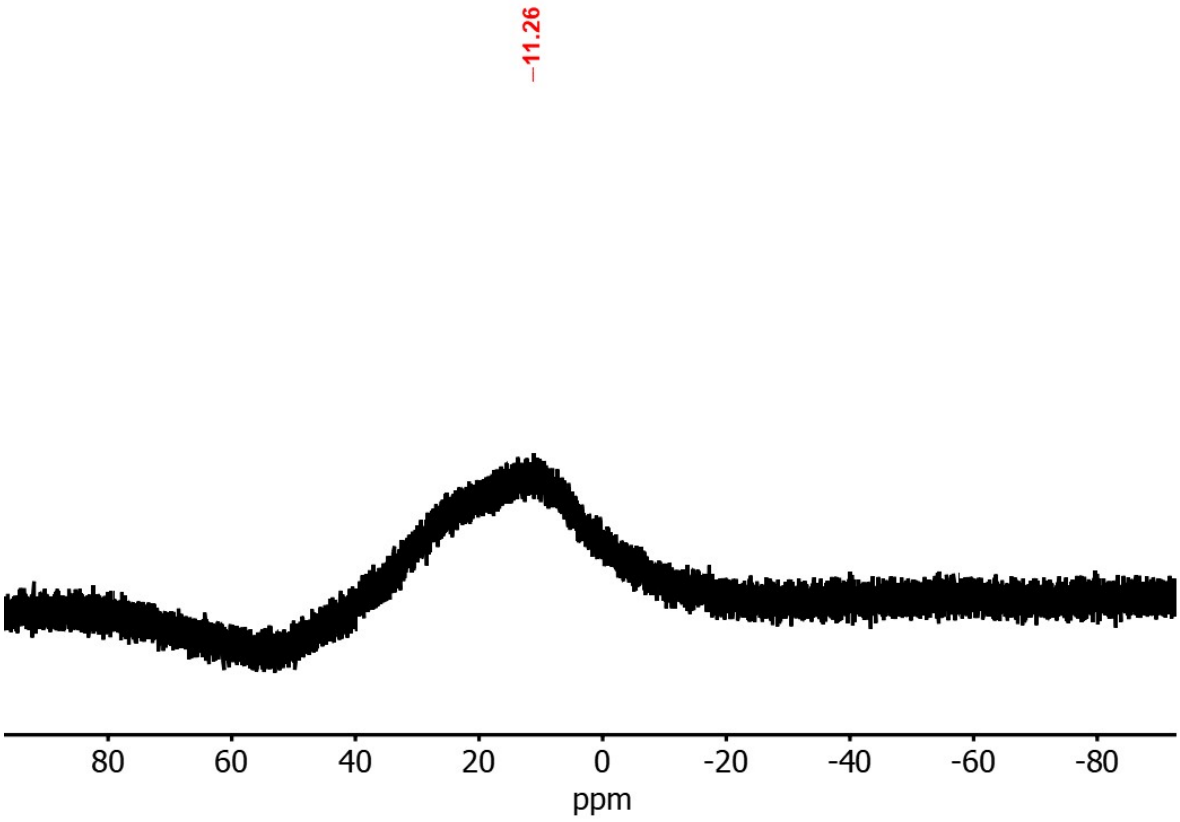


Figure S24. ^{11}B-NMR spectra of the quaternized boronate ester **(QBE_6)**

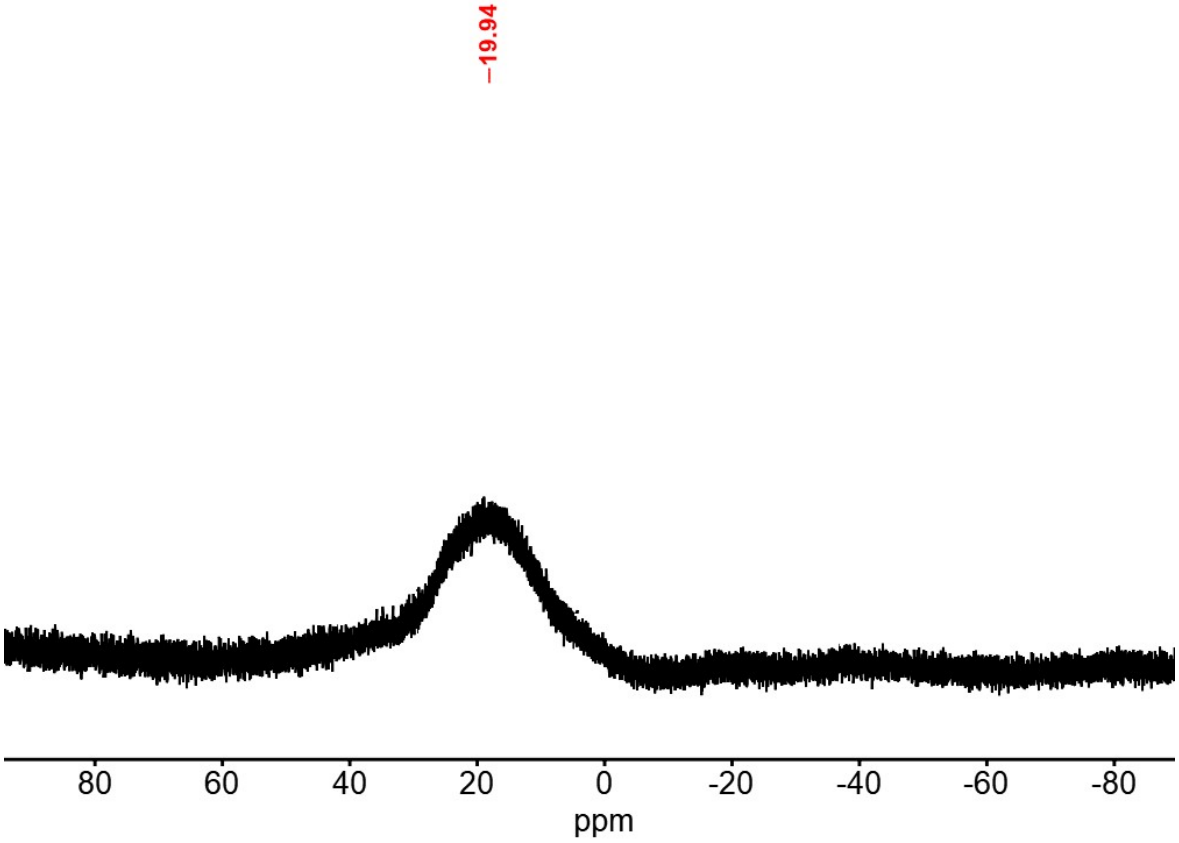


Figure S25. ^{11}B-NMR spectra of the quaternized boronate ester **(QBE_7)**

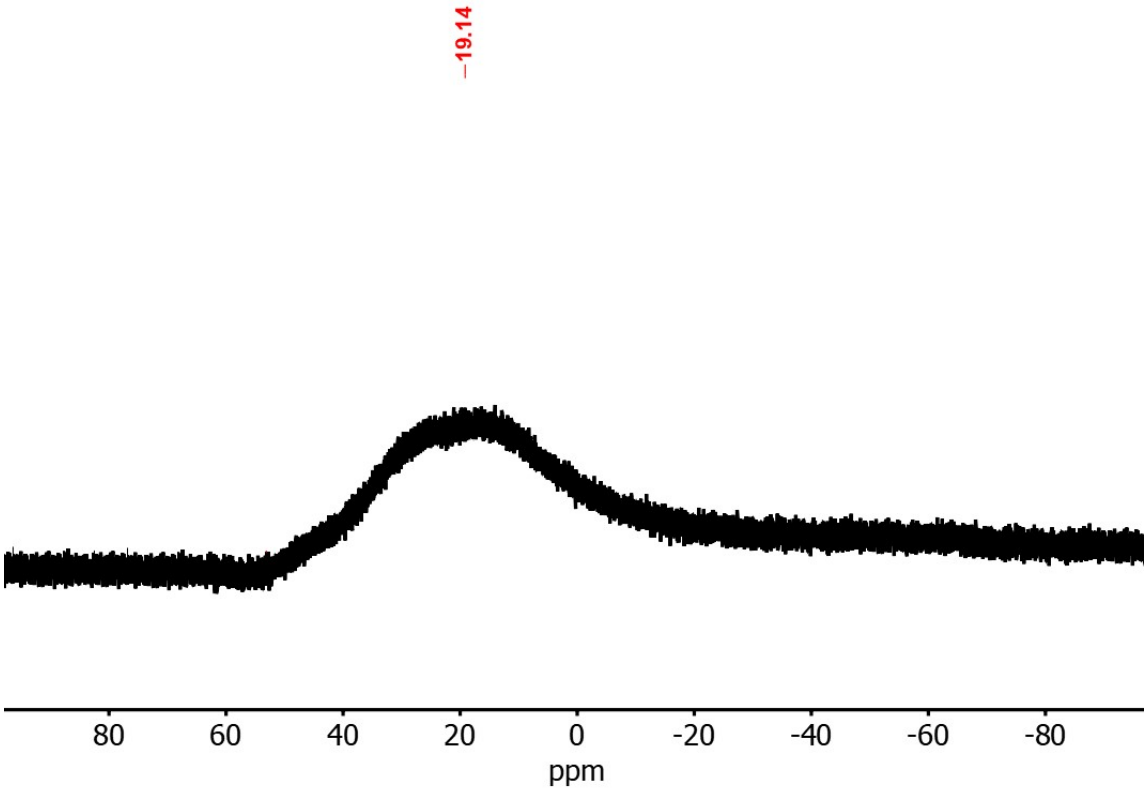


Figure S26. ^{11}B-NMR spectra of the quaternized boronate ester **(QBE_8)**

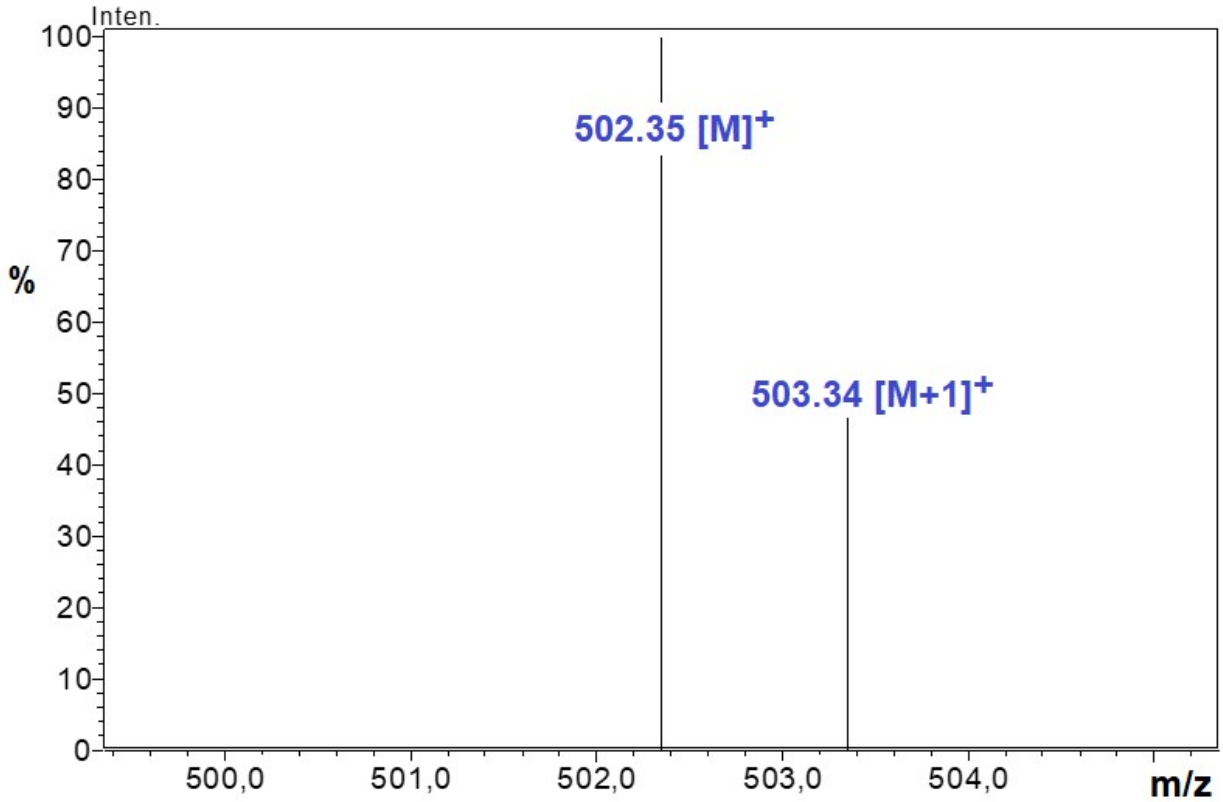


Figure S27. LC-MS/MS spectra of the quaternized boronate ester **(QBE_1)**

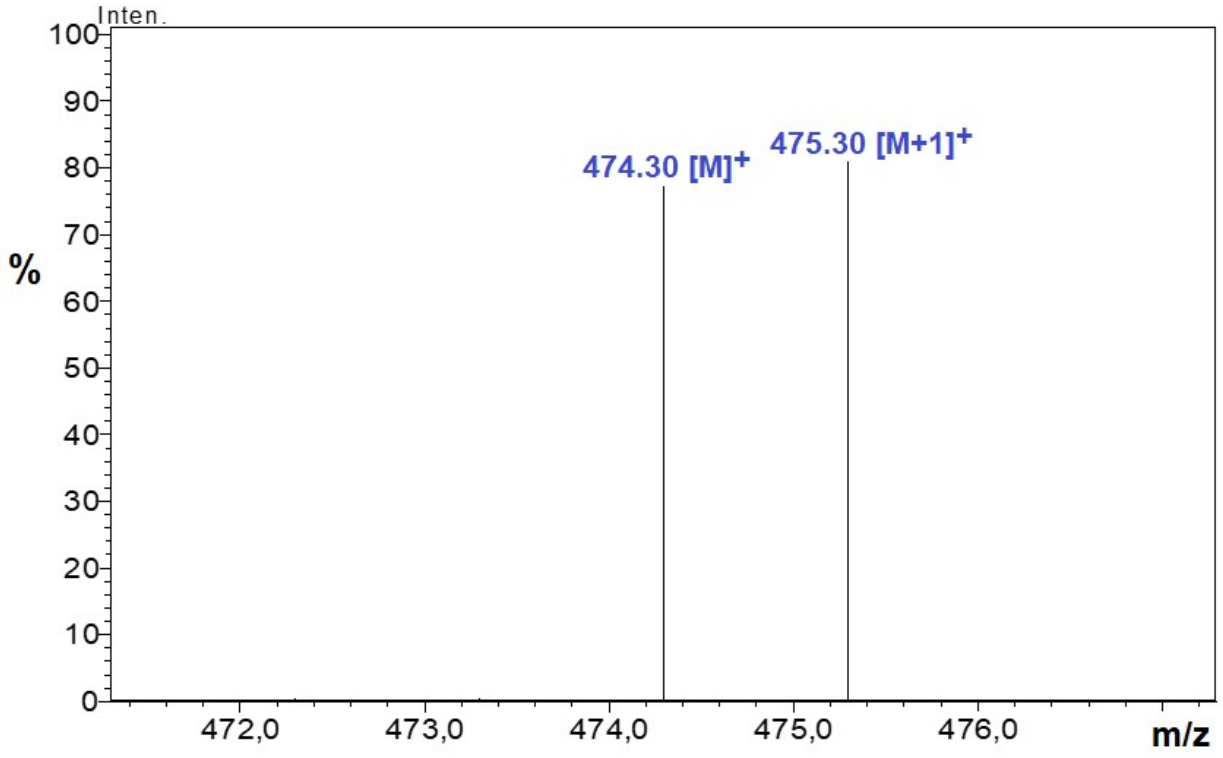


Figure S28. LC-MS/MS spectra of the quaternized boronate ester **(QBE_2)**

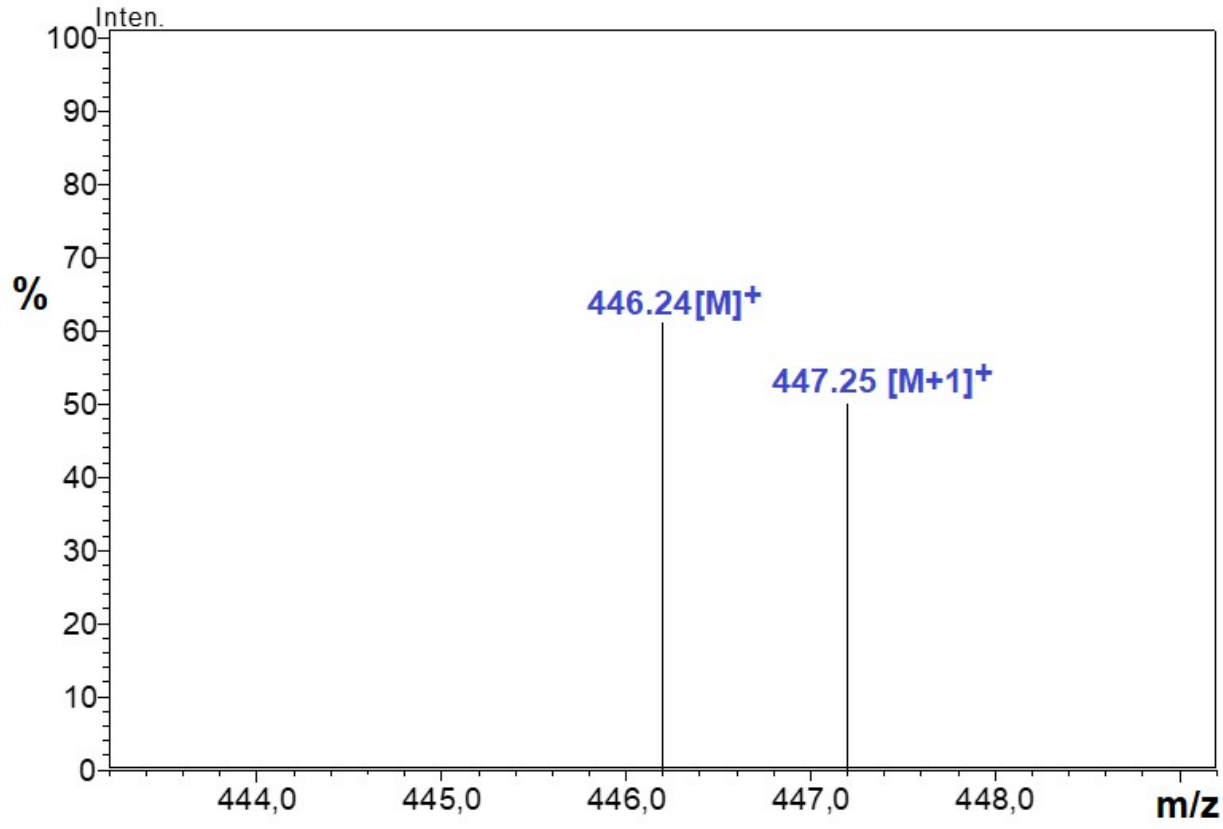


Figure S29. LC-MS/MS spectra of the quaternized boronate ester **(QBE_3)**

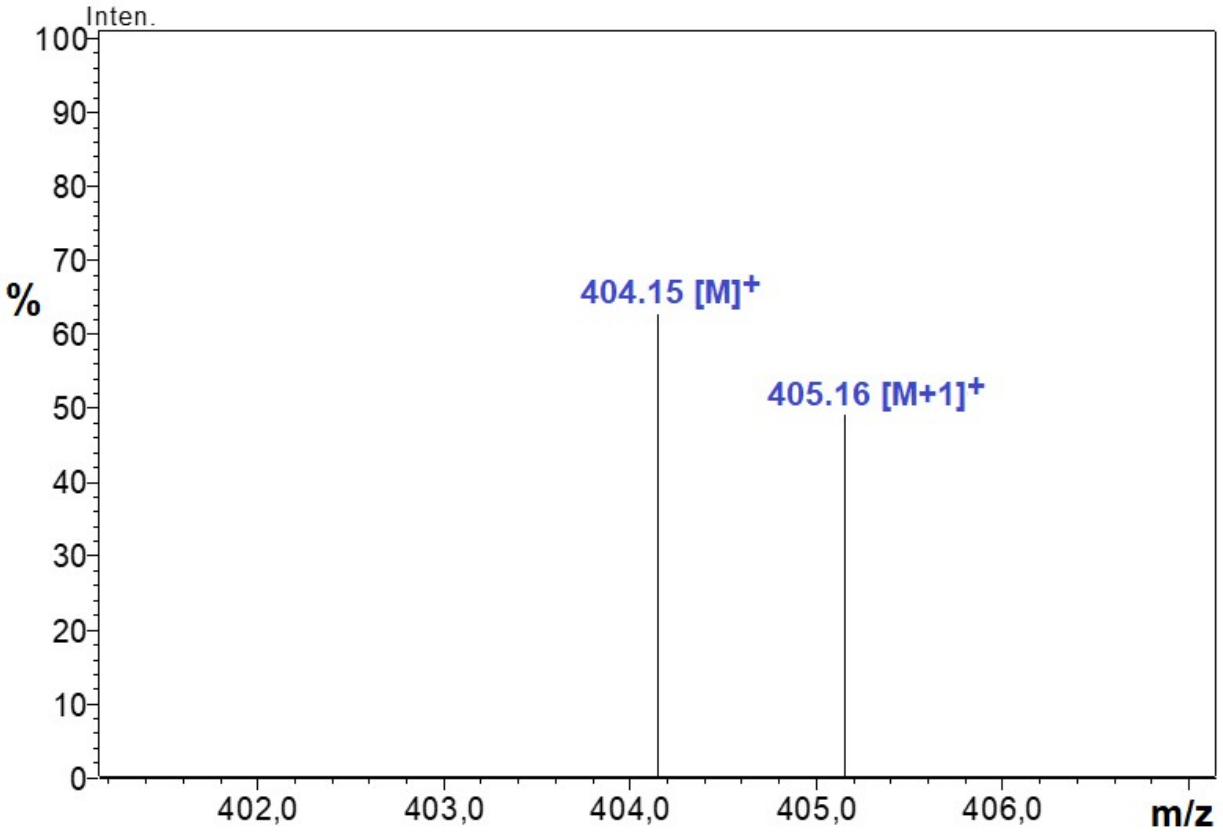


Figure S30. LC-MS/MS spectra of the quaternized boronate ester **(QBE_4)**

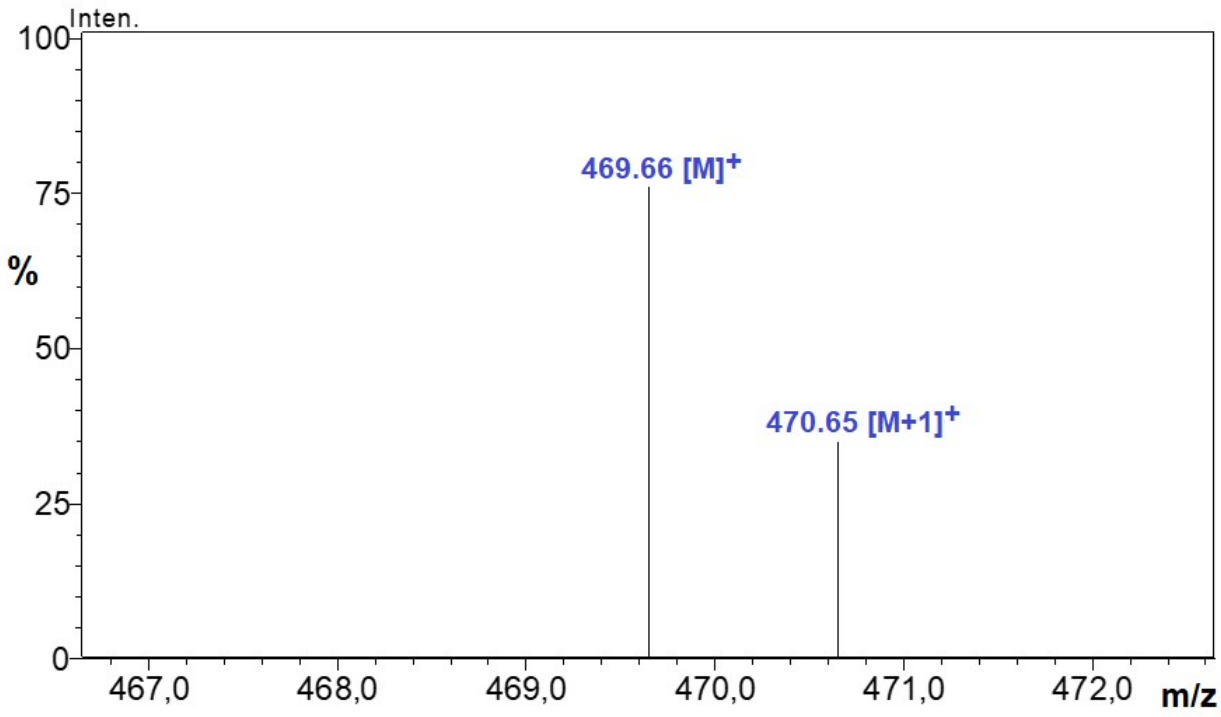


Figure S31. LC-MS/MS spectra of the quaternized boronate ester **(QBE_5)**

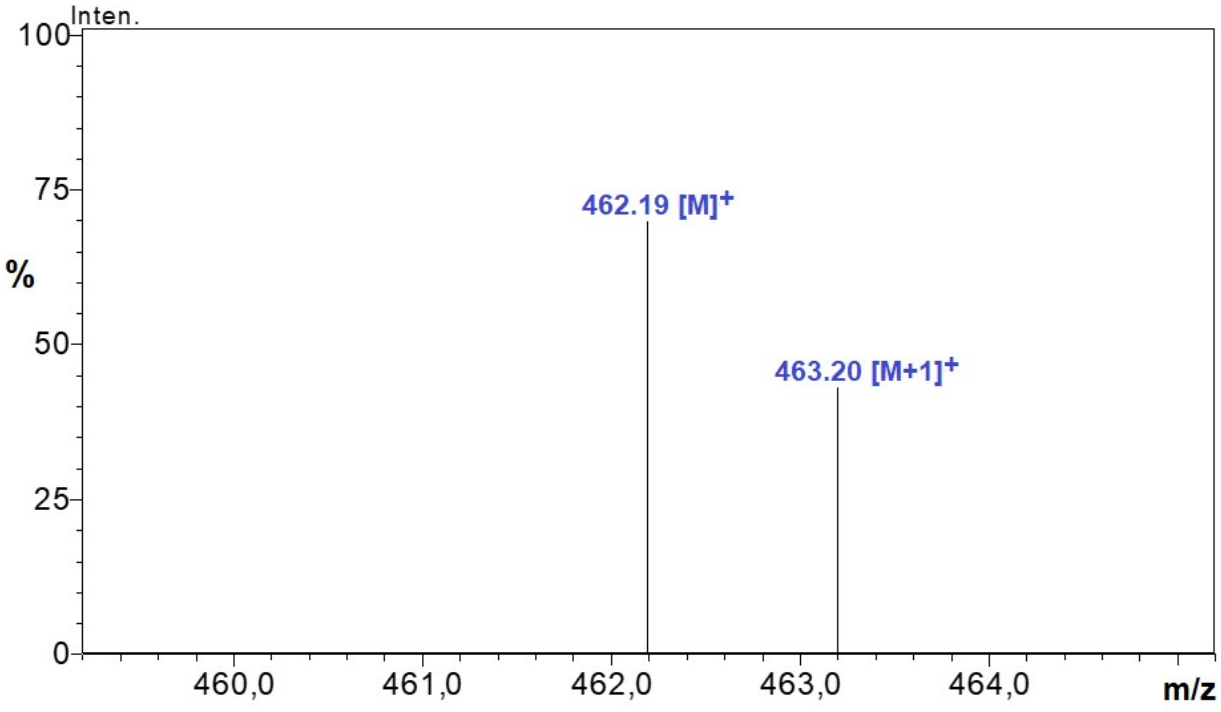


Figure S32. LC-MS/MS spectra of the quaternized boronate ester **(QBE_6)**

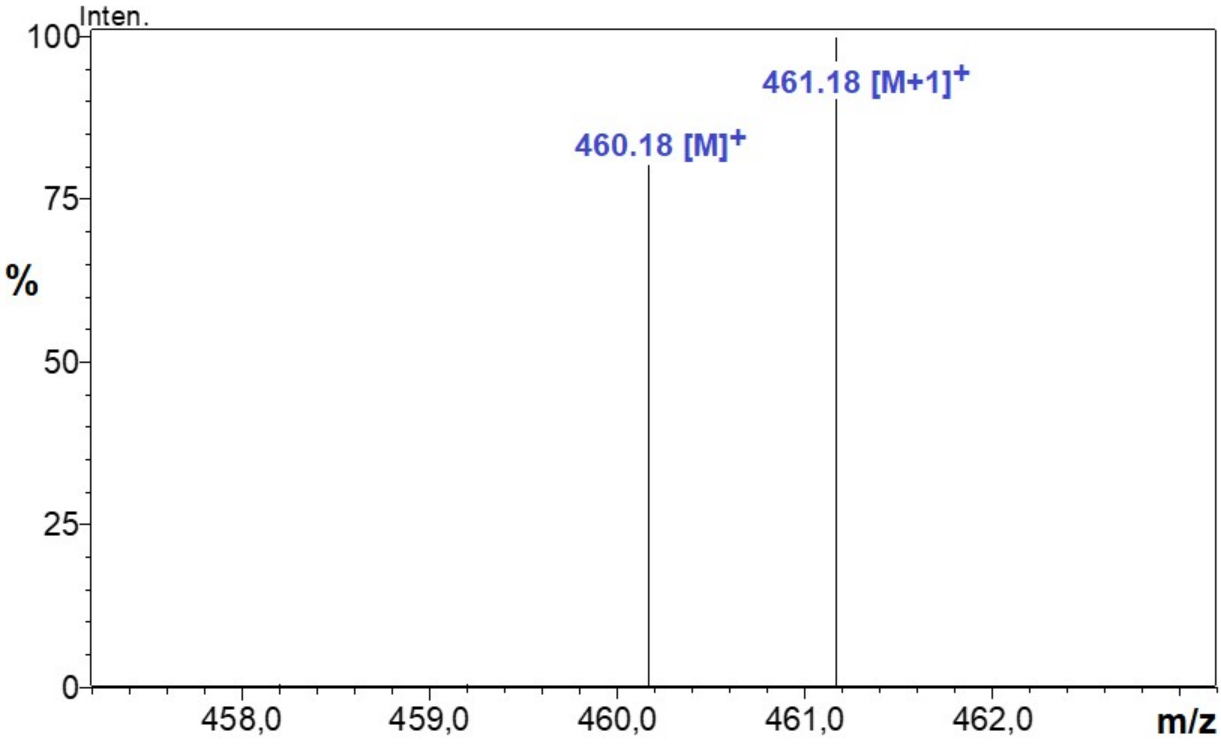


Figure S33. LC-MS/MS spectra of the quaternized boronate ester **(QBE_7)**

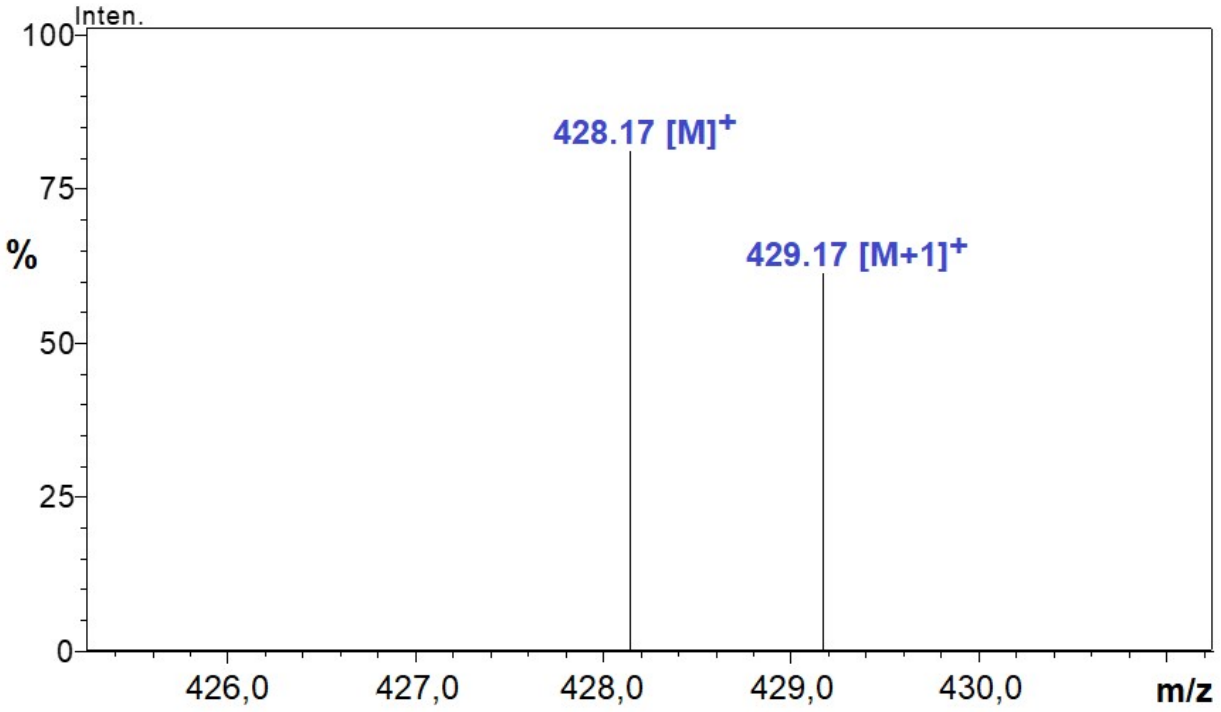


Figure S34. LC-MS/MS spectra of the quaternized boronate ester **(QBE_8)**

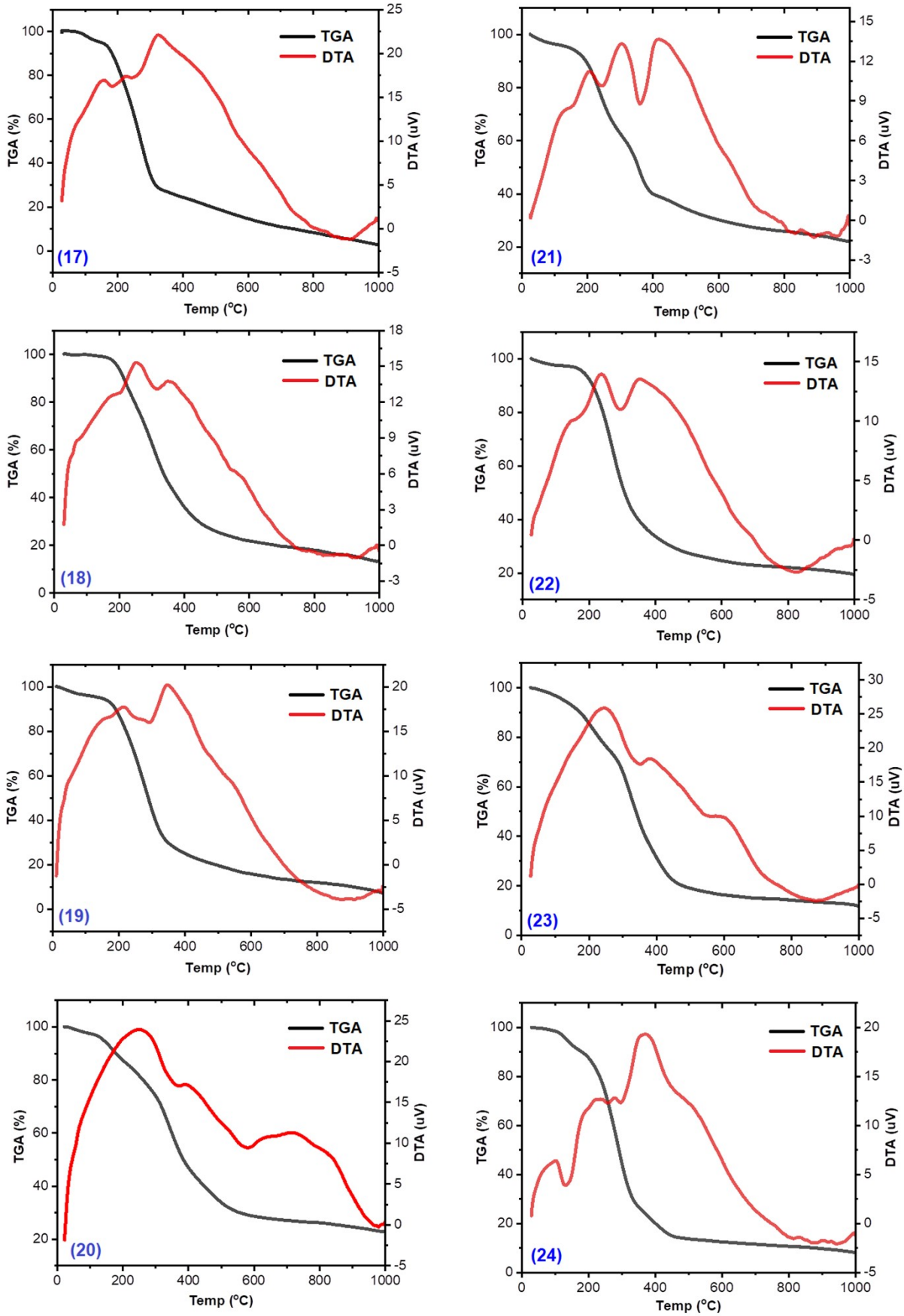
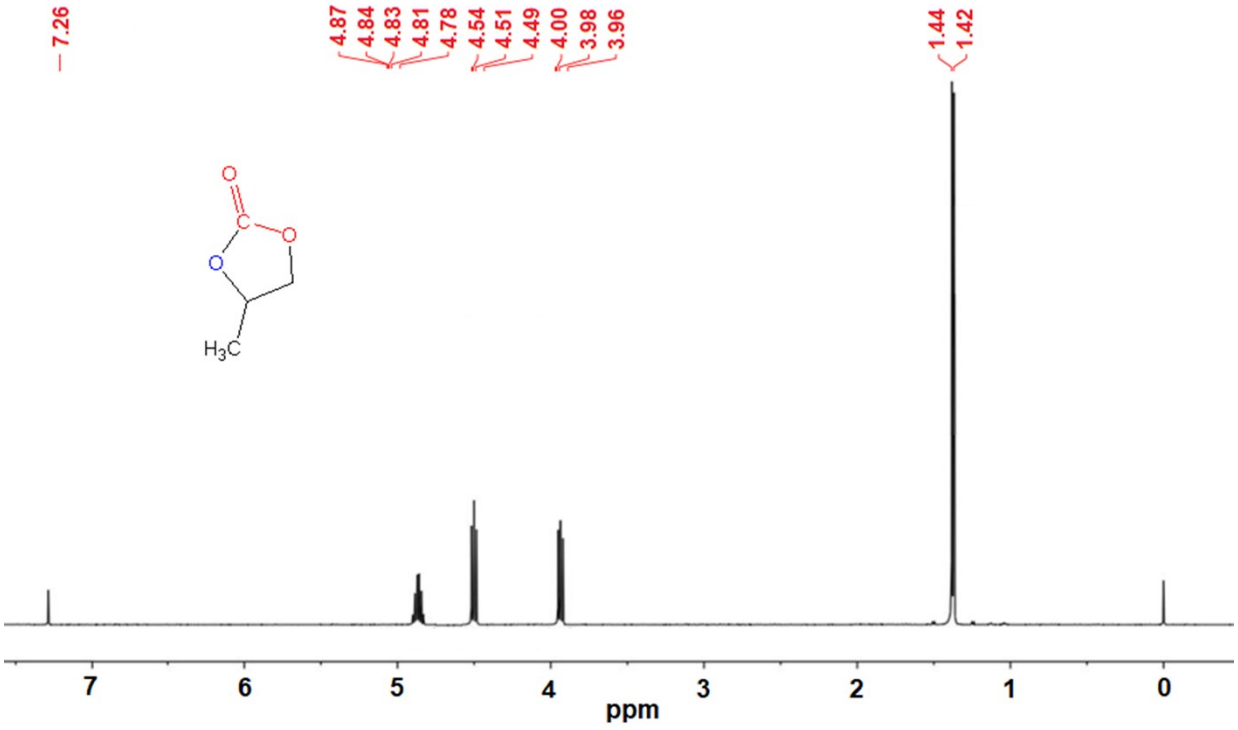
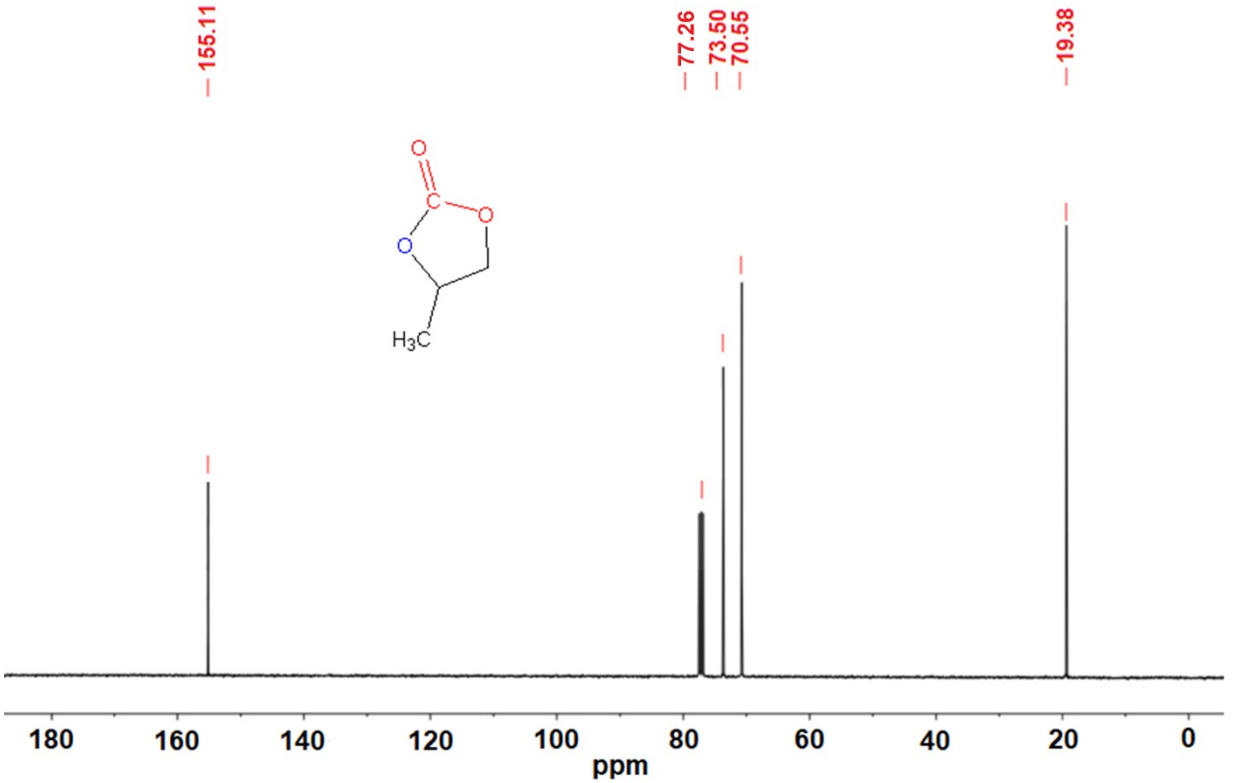


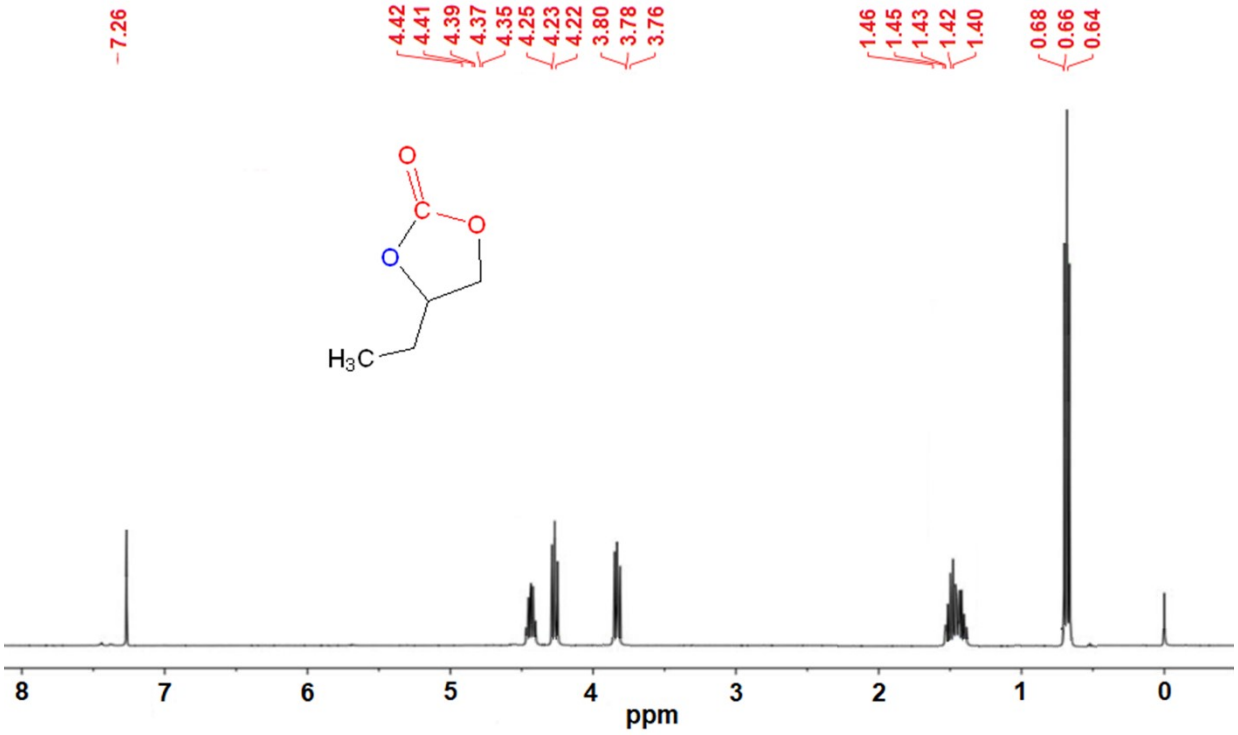
Figure S35. The TGA-DTA curves of the quaternized boronate esters **(QBE_1-QBE_8)** in N_2 atmosphere

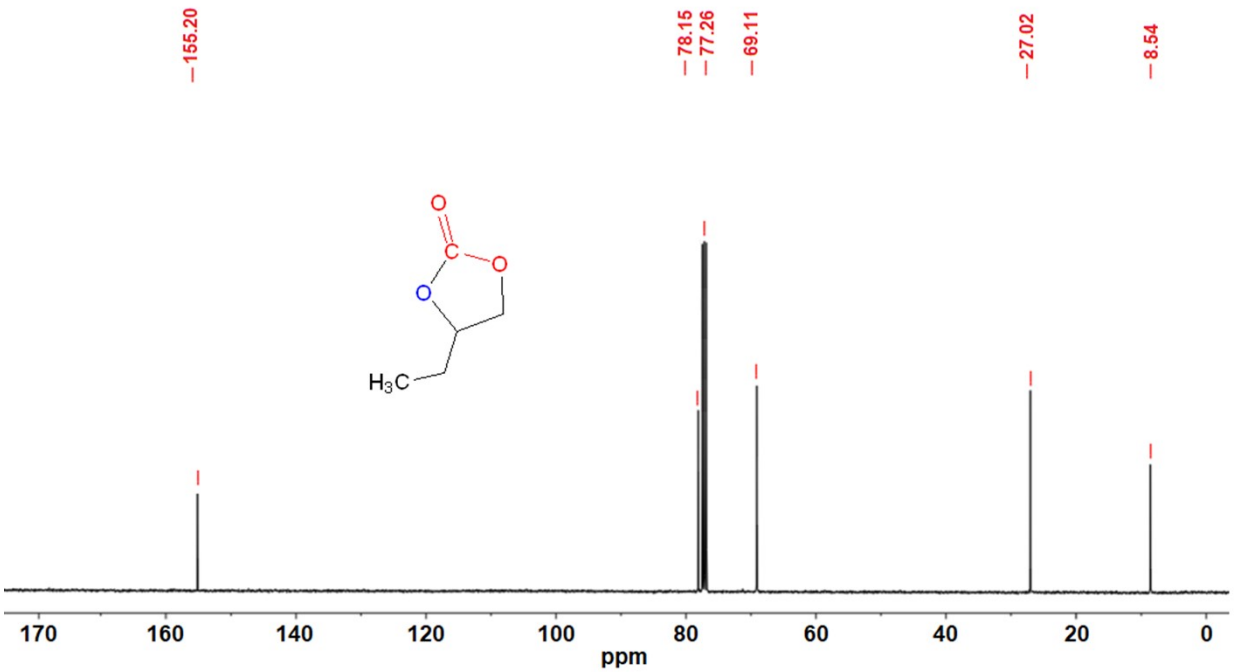
The ^{1}H and ^{13}C NMR spectra of the synthesized cyclic carbonates (1-10) [1-3]



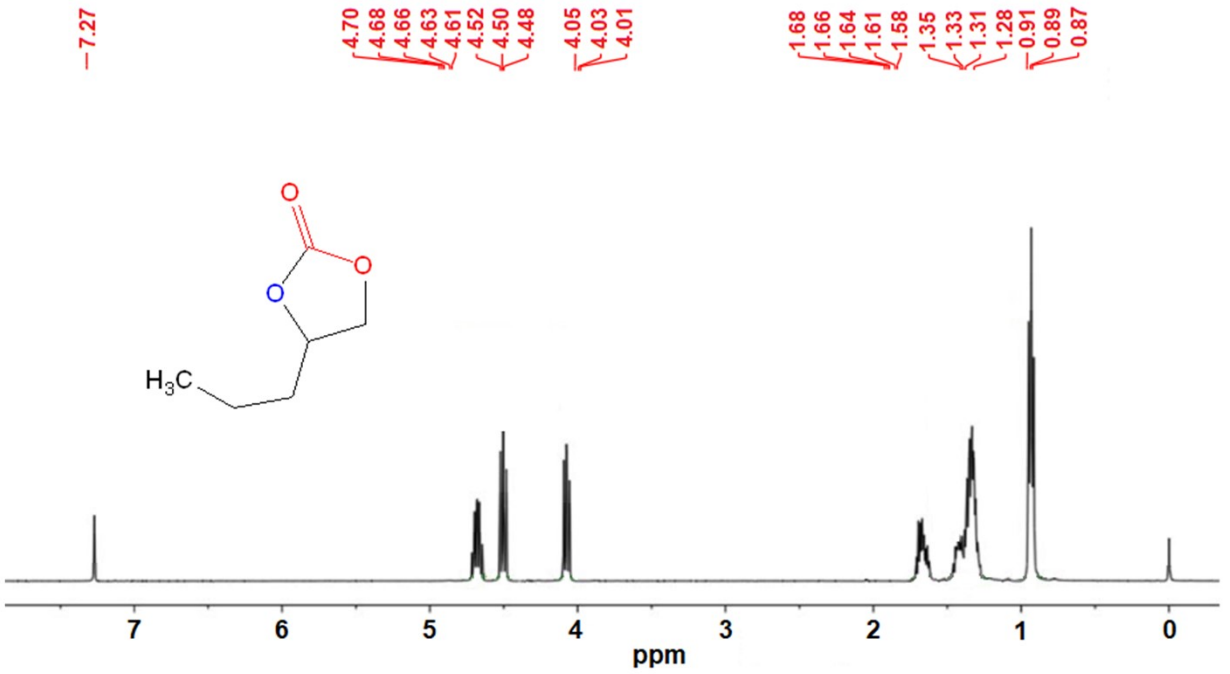


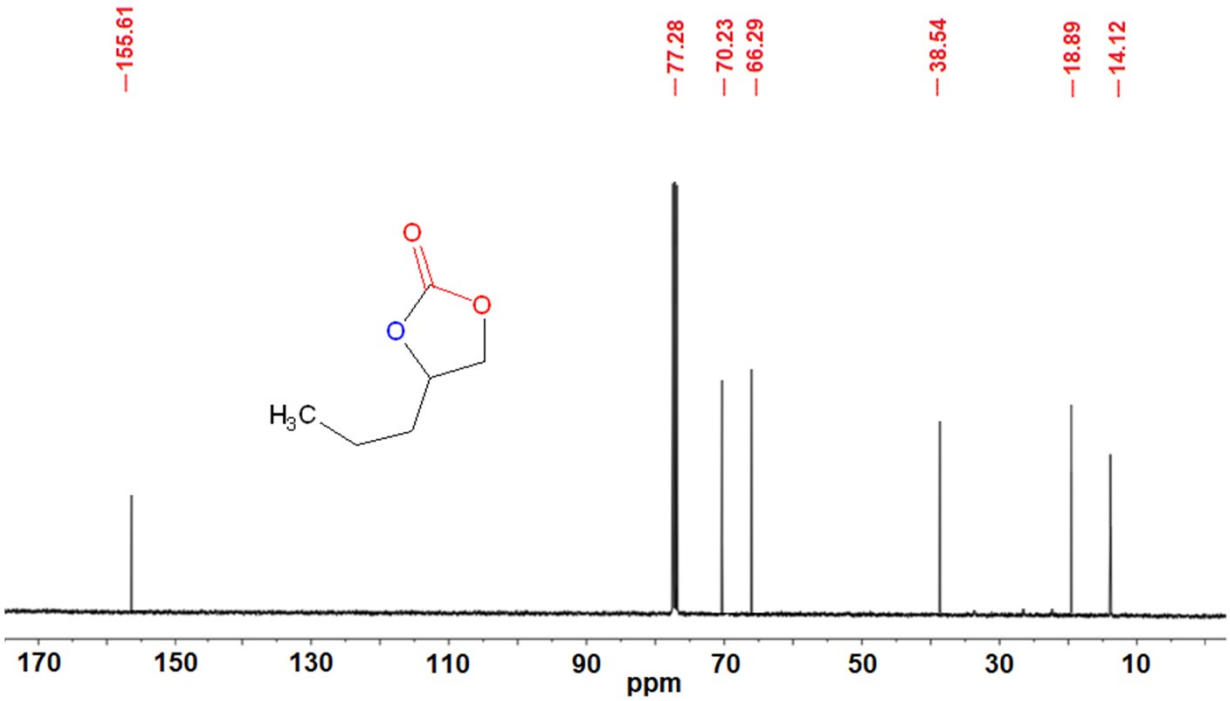
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.87-4.78 (m, 1H, -C*H*), 4.51 (dd, 1H, *J* = 8.4, 7.3 Hz, CH_2), 3.98 (dd, *J* = 8.4, 7.3 Hz, 1H, CH_2), and 1.50 (d, 3H, *J* = 8.0 Hz, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 155.11 (*C*=O), 73.50 (-*C*H), 70.55 (-*C*H_2), and 19.38 (-*C*H_3).



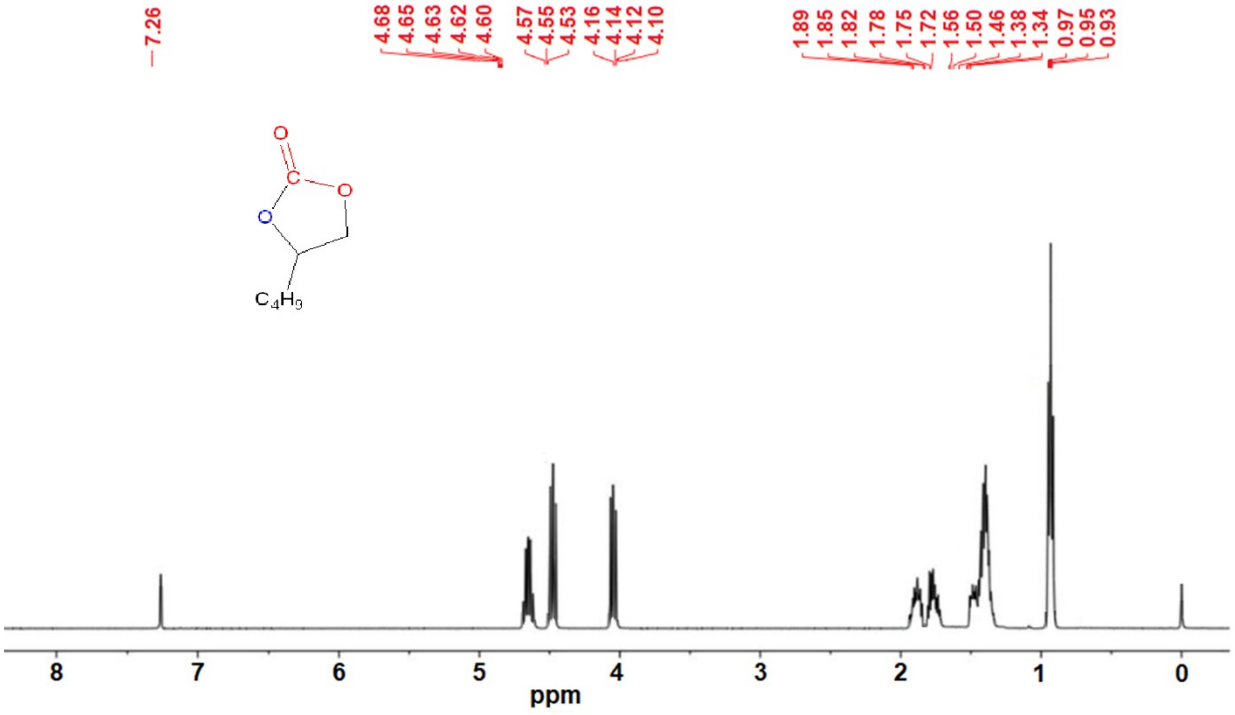


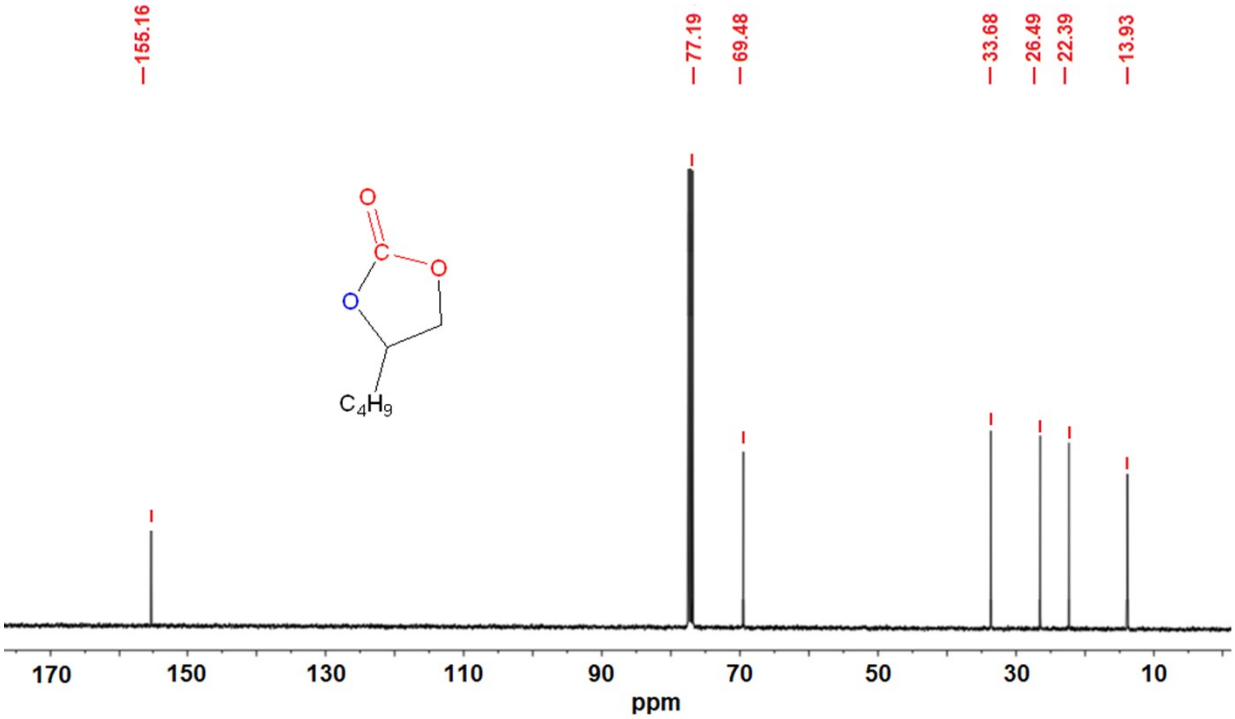
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.42-4.35 (m, 1H, -C<u>*H*</u>), 4.23 (dd, 1H, *J* = 8.2, 6.4 Hz, C<u>*H*</u>$_2$), 3.78 (dd, *J* = 8.2, 6.4 Hz, 1H, CH-C<u>*H*</u>$_2$), 1.46-1.40 (m, 2H, C<u>*H*</u>$_2$-CH_3), and 0.66 (t, 3H, *J* = 8.0 Hz, CH_2-C<u>*H*</u>$_3$). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 155.20 (<u>*C*</u>=O), 78.15 (-<u>*C*</u>H), 69.11 (CH-<u>*C*</u>H_2), 27.02 (<u>*C*</u>H_2-CH_3), and 8.54 (CH_2-<u>*C*</u>H_3).



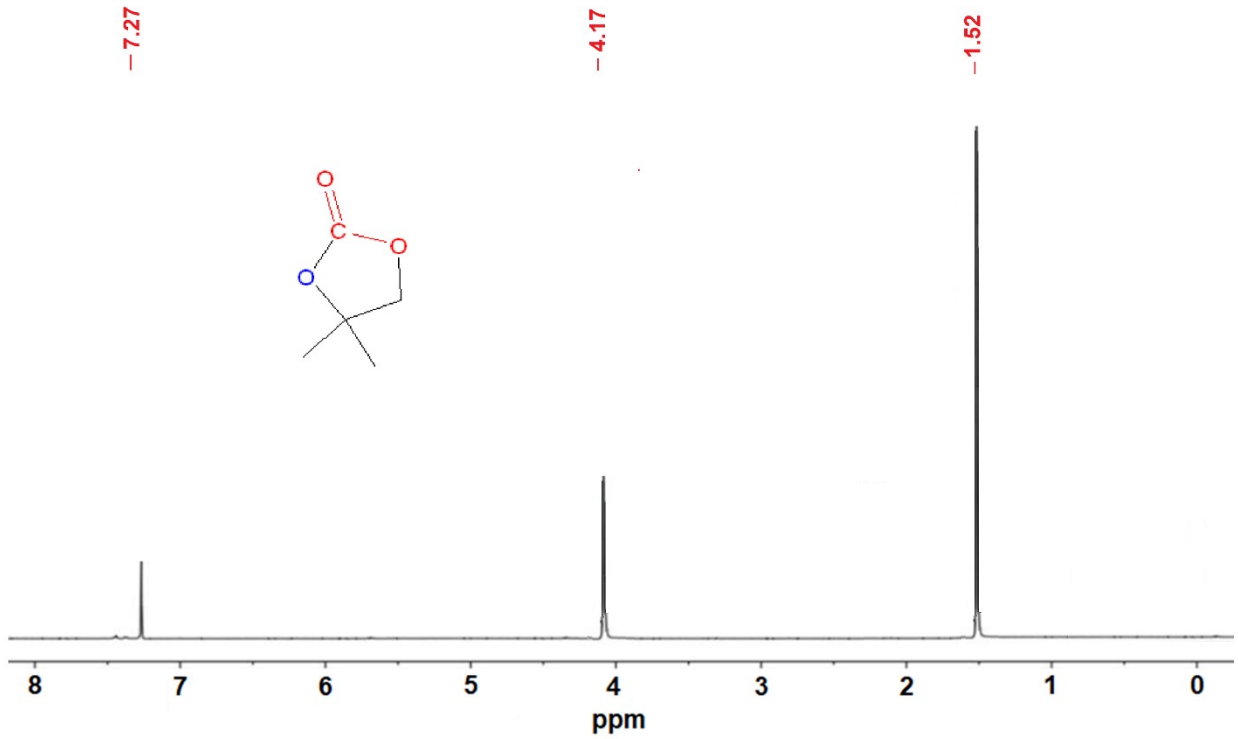


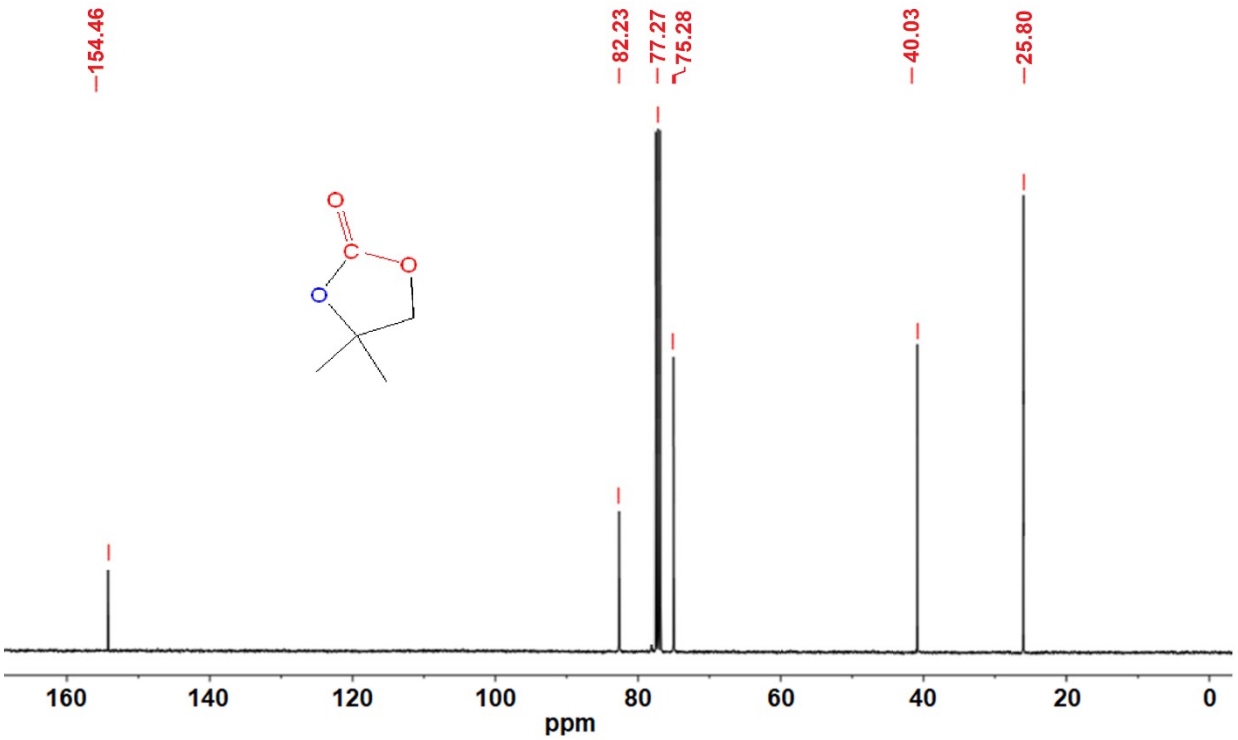
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.70-4.61 (m, 1H, -C*H*), 4.50 (dd, 1H, *J* = 8.2, 6.4 Hz, -CH_2), 4.03 (dd, *J* = 8.2, 6.4 Hz, 1H, -CH_2), 1.68-1.58 (m, 2H, -CH_2-CH_2-CH_3), 1.35-1.28 (m, 2H, -CH_2-CH_2-CH_3), and 0.89 (t, 3H, *J* = 8.0 Hz, CH_2-CH_2-CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 155.61 (*C*=O), 70.23 (-*C*H), 66.29 (-CH-*C*H_2), 38.54 (-*C*H_2-CH_2-CH_3), 18.89 (CH_2-*C*H_2-CH_3), and 14.12 (-CH_2-CH_2-*C*H_3).



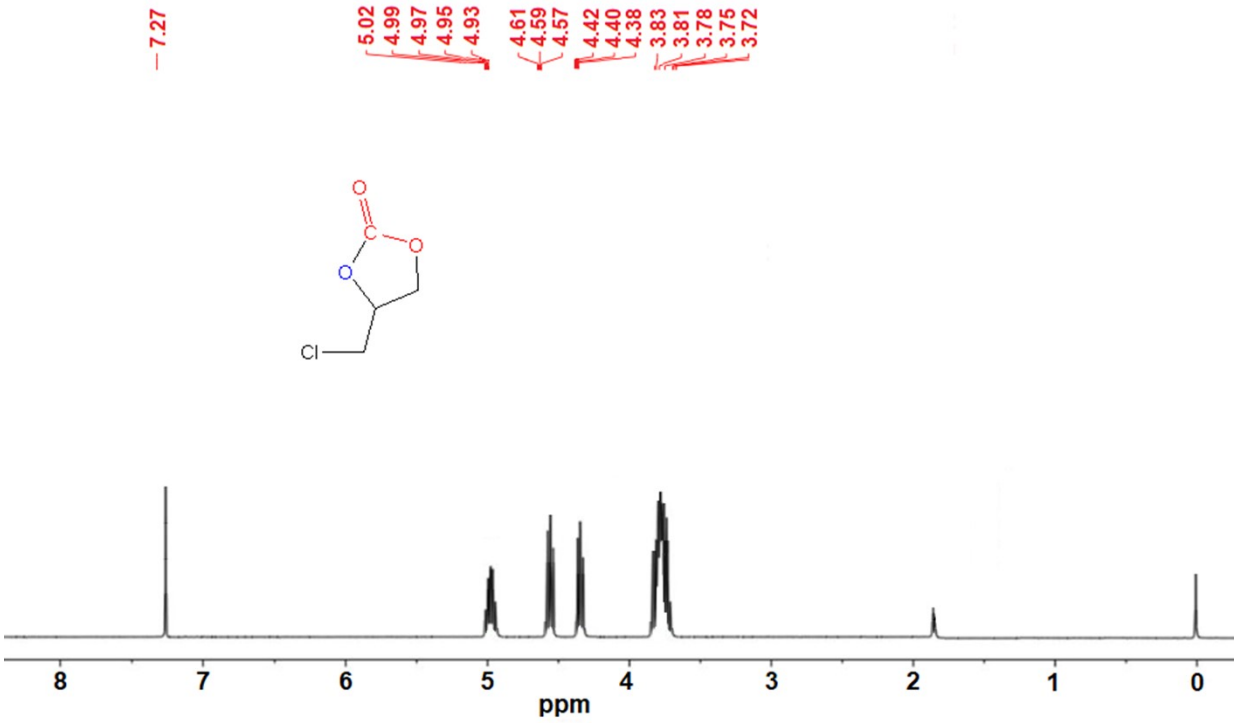


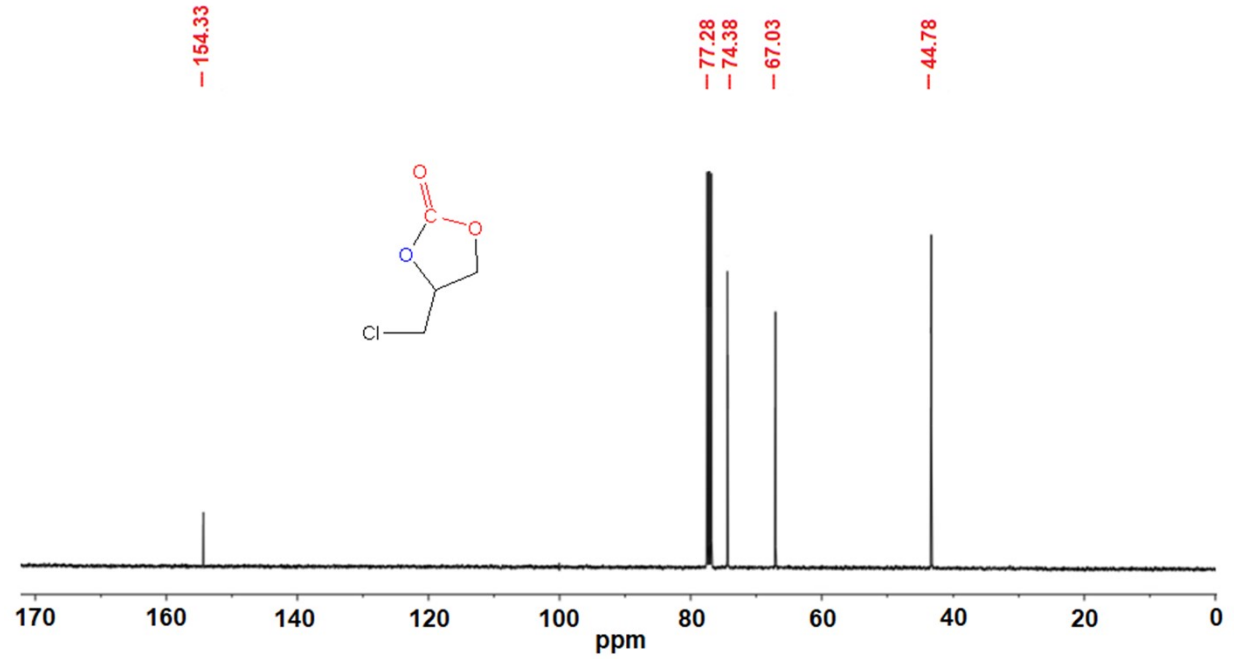
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.68-4.60 (m, 1H, -C<u>*H*</u>), 4.55 (t, 1H, *J* = 8.1 Hz, C<u>*H*$_2$</u>), 4.16-4.10 (dd, *J* = 8.3, 7.3 Hz, 1H, -C<u>*H*$_2$</u>), 1.89-1.72 (m, 2H, -C<u>*H*$_2$</u>-CH_2-CH_2-CH_3), 1.56-1.34 (m, 4H, -CH_2-C<u>*H*$_2$</u>-C<u>*H*$_2$</u>-CH_3), and 0.95 (t, 3H, *J* = 8.0 Hz, -$(CH_2)_3$-C<u>*H*$_3$</u>). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 155.61 (<u>*C*</u>=O), 70.23 (-<u>*C*</u>H), 66.29 (-CH-<u>*C*</u>H_2), 38.54 (-<u>*C*</u>H_2-CH_2-CH_3), 18.89 (CH_2-<u>*C*</u>H_2-CH_3), and 14.12 (-CH_2-CH_2-<u>*C*</u>H_3).



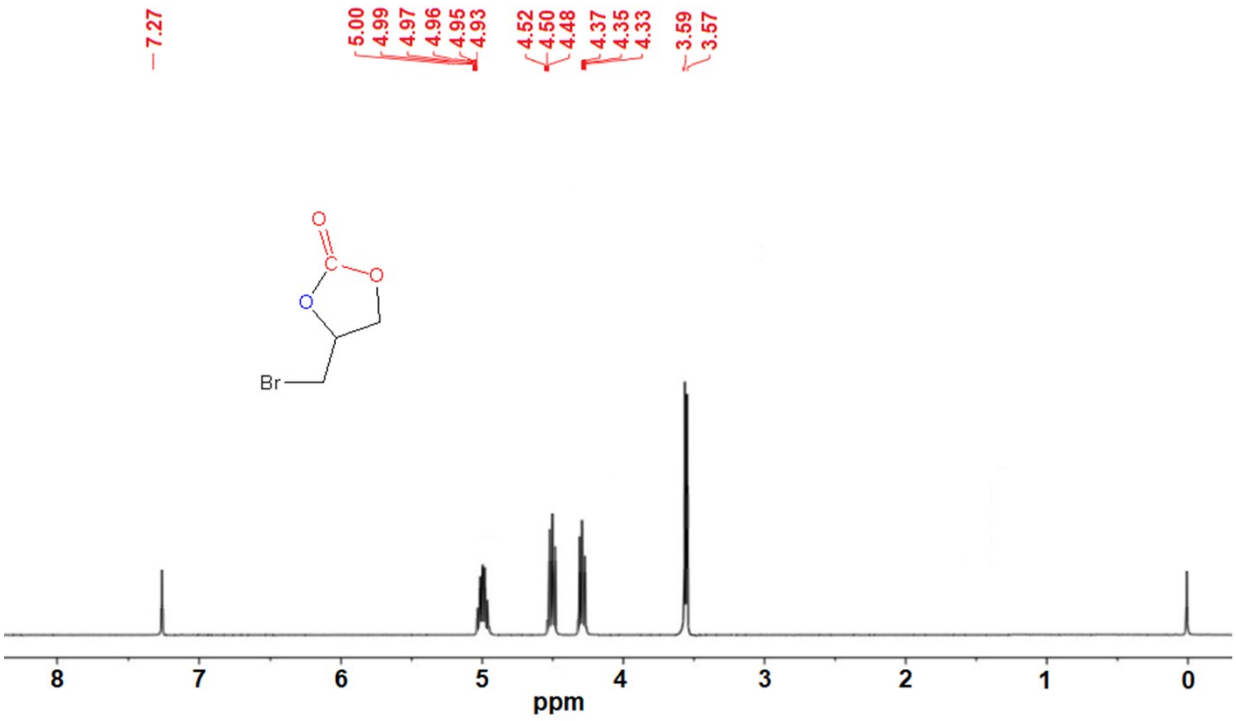


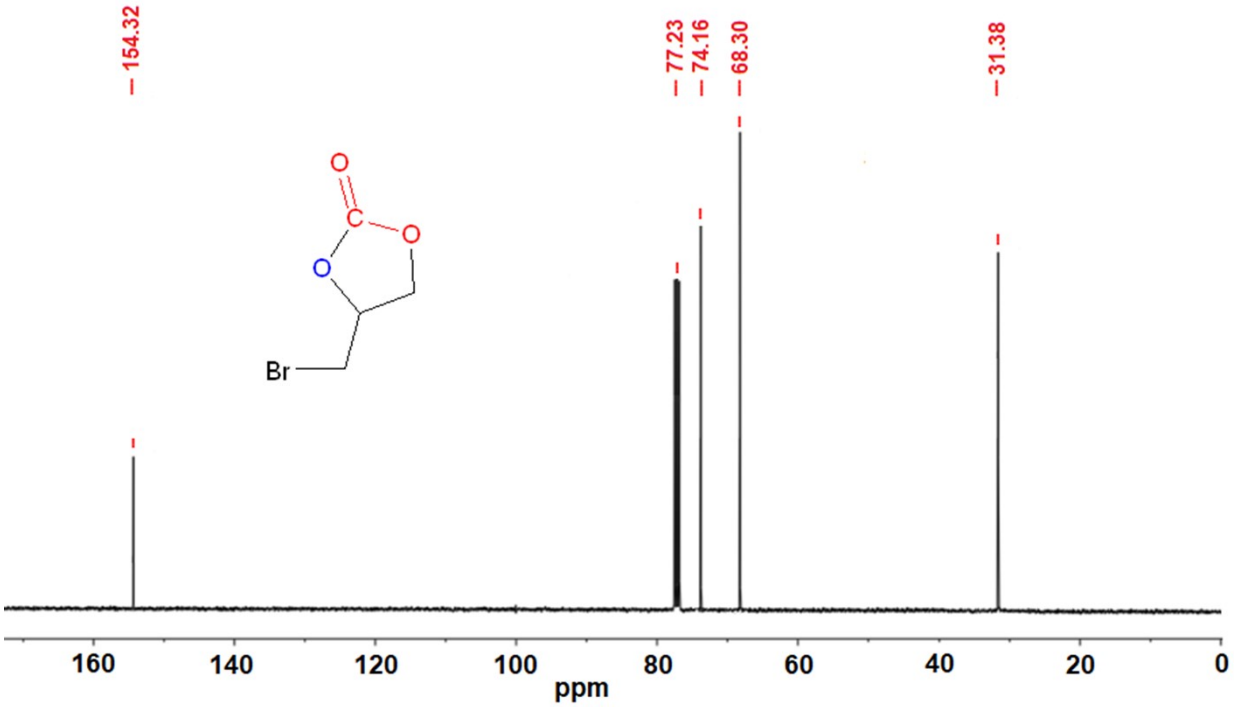
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.17 (s, 2H, -C-C$\underline{H_2}$) and 1.52 (s, 6H, (-C-C$\underline{H_3}_{)2}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 154.46 ($\underline{C}$=O), 82.23 (-$\underline{C}$H), 75.28 (-CH-$\underline{C}H_2$), 40.03 (C-$\underline{C}H_3$), and 25.80 (C-$\underline{C}H_3$).



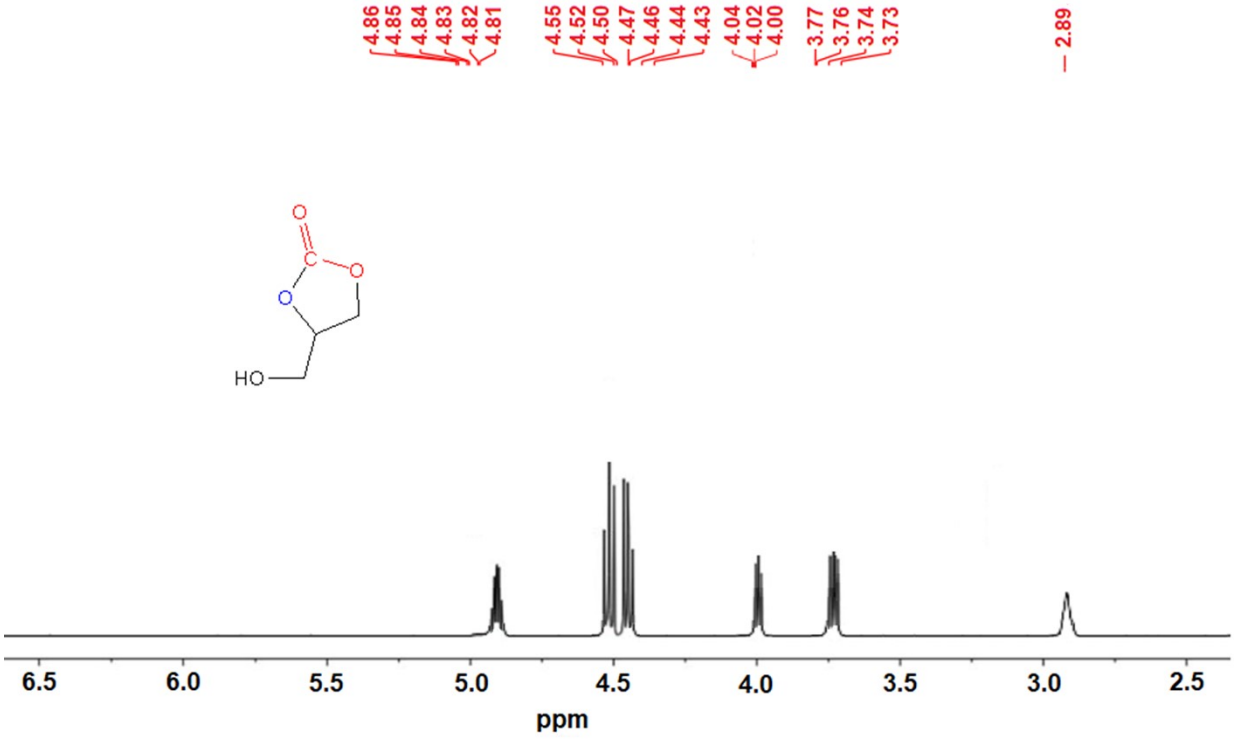


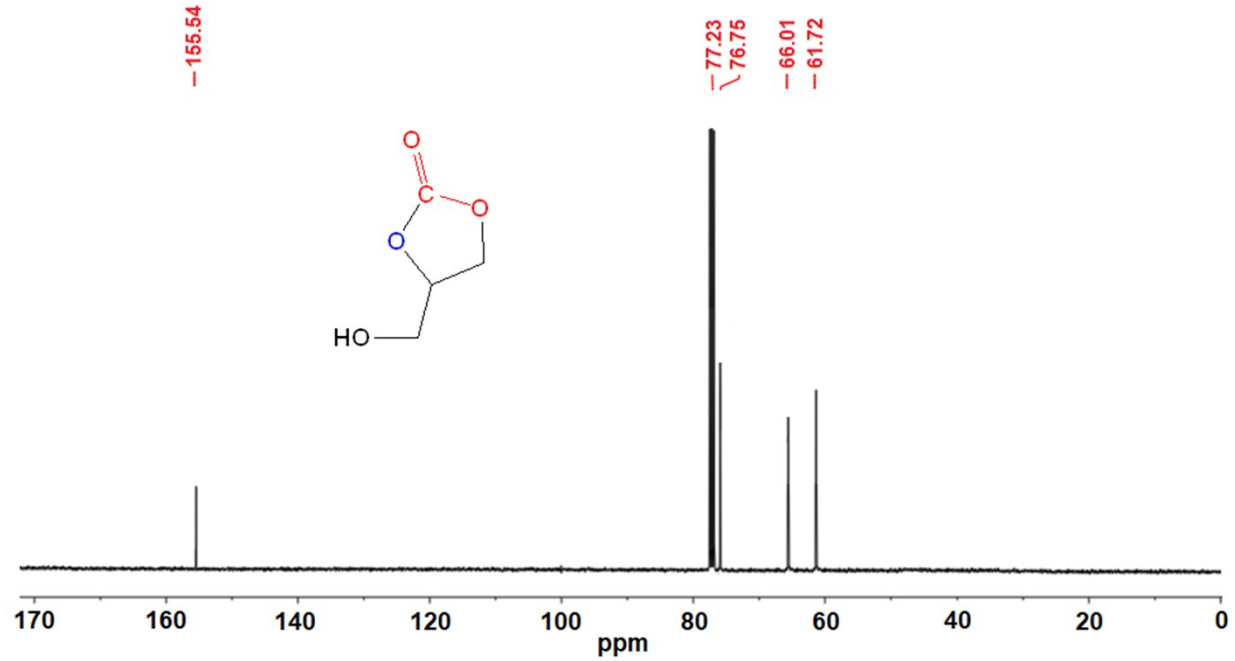
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 5.02-4.93 (m, 1H, -C*H*), 4.59 (t, 1H, *J* = 8.6 Hz, -CH_2), 4.40 (t, 1H, *J* = 8.6 Hz, -CH_2), and 3.83-3.72 (m, 2H, -CH_2-Cl). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 154.33 (*C*=O), 74.38 (-*C*H), 67.03 (-CH-*C*H_2), and 44.78 (-*C*H_2-Cl).



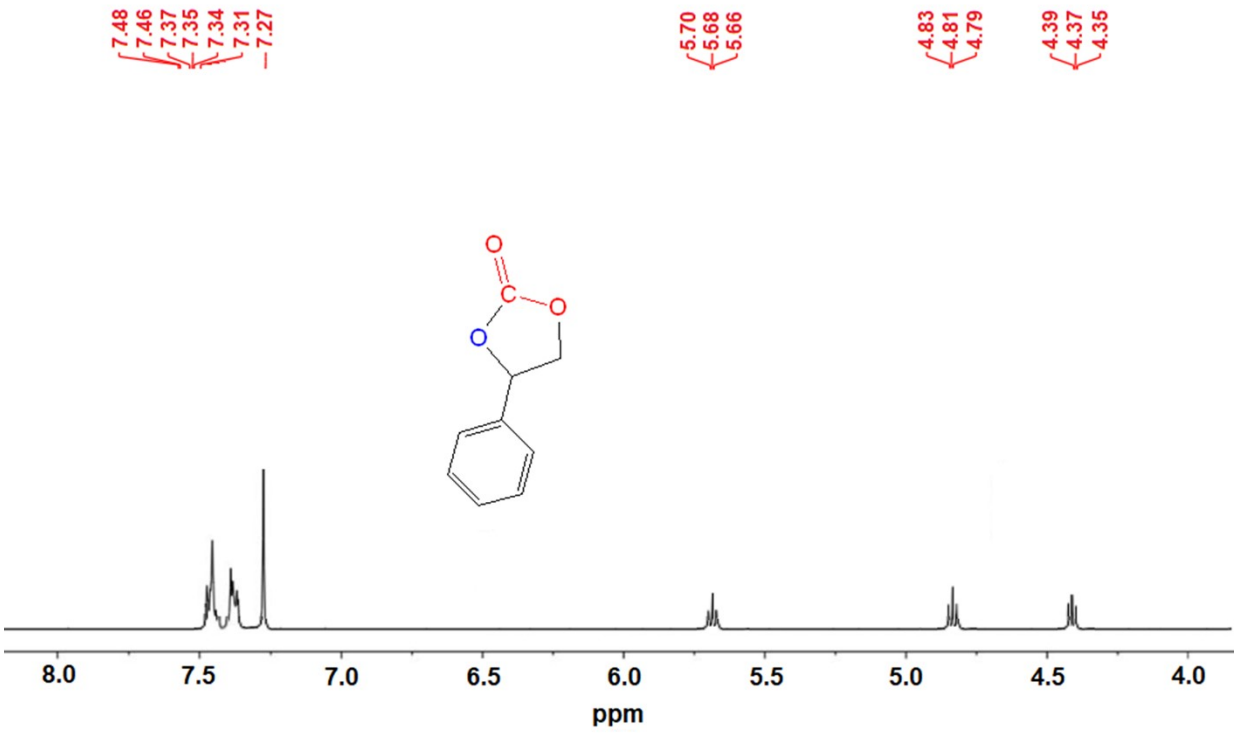


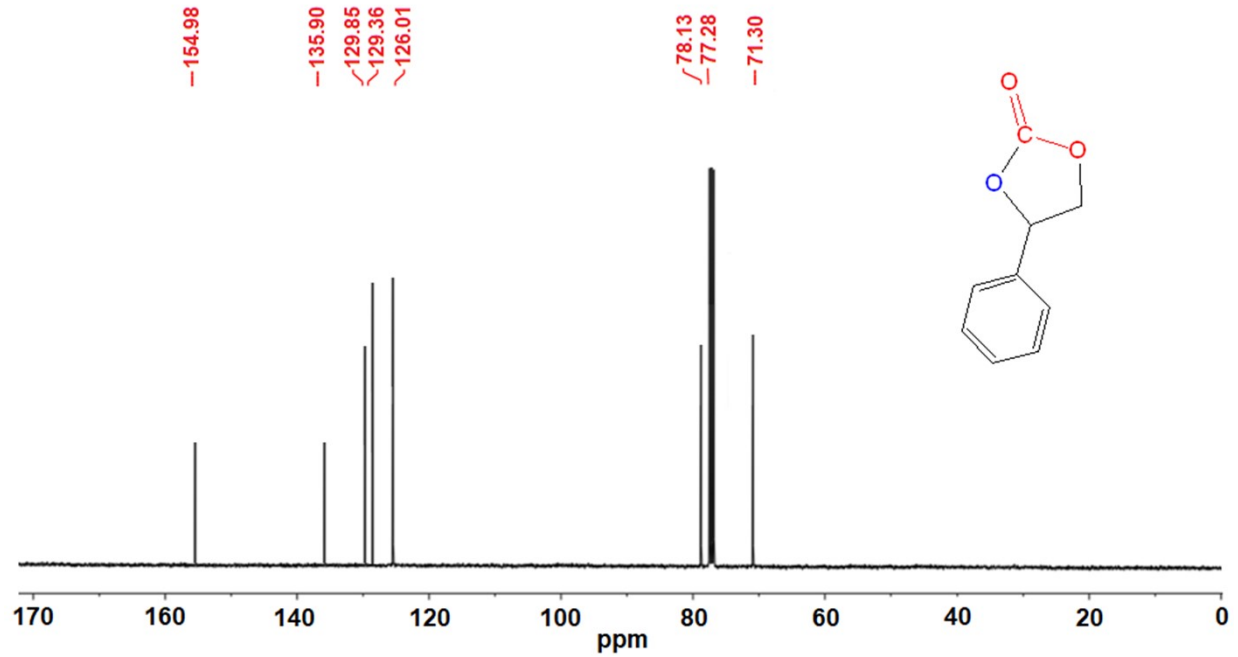
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 5.00-4.93 (m, 1H, -C<u>*H*</u>), 4.50 (t, 1H, *J* = 8.6 Hz, -C<u>*H*$_2$</u>), 4.35 (t, 1H, *J* = 8.6 Hz, -C<u>*H*$_2$</u>), and 3.58 (d, 2H, *J* = 8.0 Hz, -C<u>*H*$_2$</u>-Br). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 154.32 (<u>*C*</u>=O), 74.16 (-<u>C</u>H), 68.30 (-CH-<u>C</u>H$_2$), and 31.38 (-<u>C</u>H$_2$-Br).



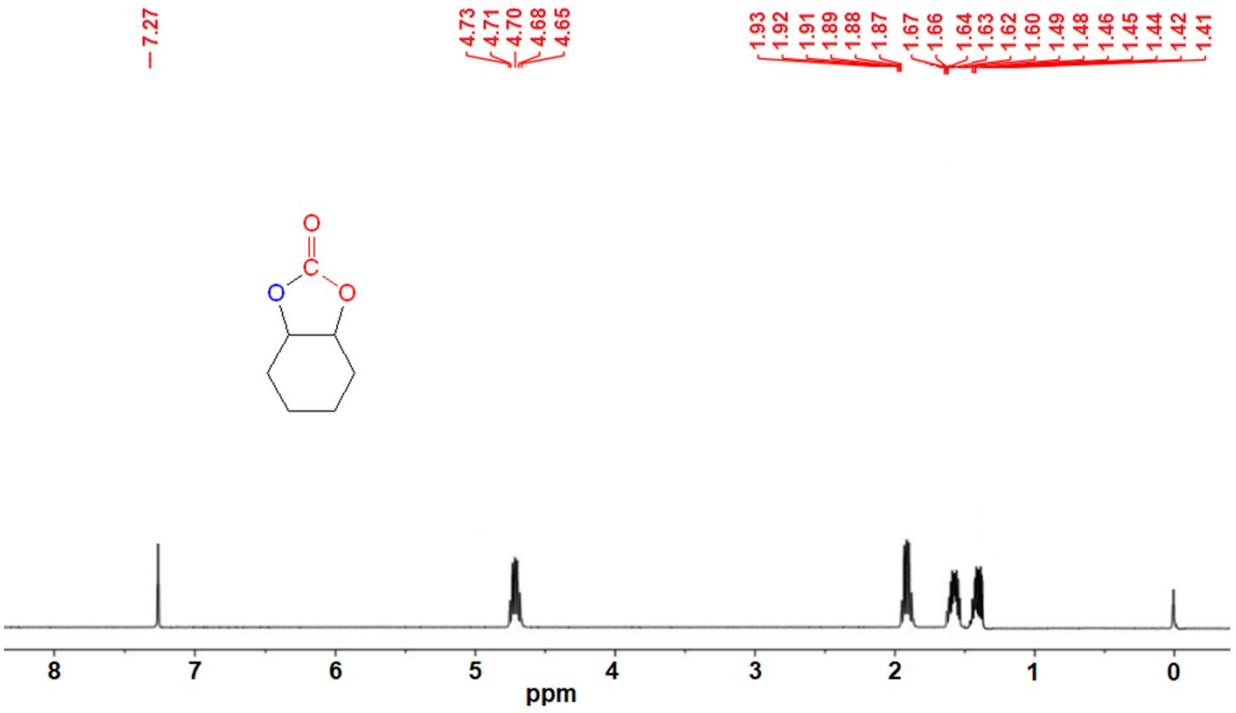


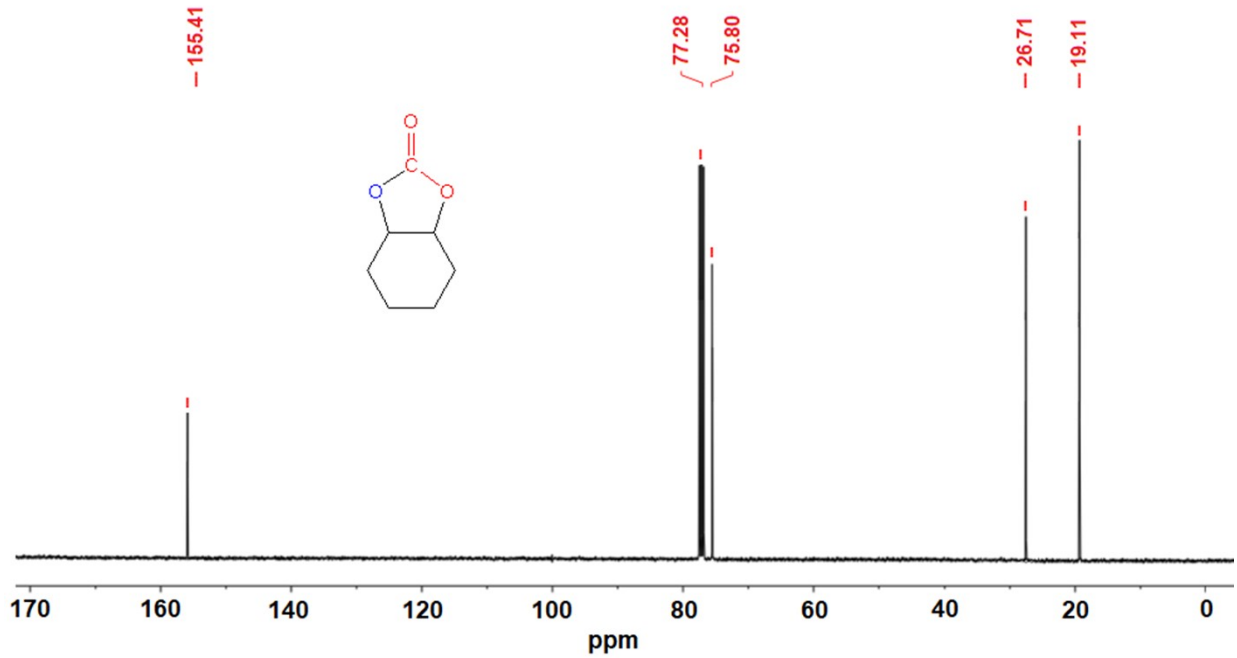
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.86-4.81 (m, 1H, -C*H*), 4.55-4.43 (m, 2H, -CH_2), 4.02 (t, 1H, *J* = 8.0 Hz, -CH_2-OH), 4.02 (dd, 1H, *J* = 4.0 Hz, -CH_2-OH), and 2.89 (bs, 1H, *J* = 8.0 Hz, -CH_2-O*H*). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 155.54 (*C*=O), 76.75 (-*C*H), 66.01 (-CH-CH_2), and 61.72(-CH_2-OH).





^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.48-7.31 (m, 5H, Ar-C*H*), 5.68 (t, 1H, *J* = 8.0 Hz, -C*H*), 4.81 (t, 1H, *J* = 8.0 Hz, -CH_2), and 4.37 (t, 1H, *J* = 8.0 Hz, -C*H*). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 154.98 (*C*=O), 135.90, 129.85, 129.36, 126.01 (Ar-*C*H), 78.13 (-*C*H), and 71.30 (-CH-*C*H_2).





^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.73-4.65 (m, 2H, O-C*H*), 1.93-1.87 (m, 4H, O-CH-C*H*$_2$), 1.67-1.60 (m, 2H, O-CH-CH$_2$-C*H*$_2$), and 1.49-1.41 (m, 2H, O-CH-CH$_2$-C*H*$_2$). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) = 155.41 (*C*=O), 75.80 (O-*C*H), 26.91 (O-CH-*C*H$_2$), and 19.11 (O-CH-CH$_2$-*C*H$_2$).

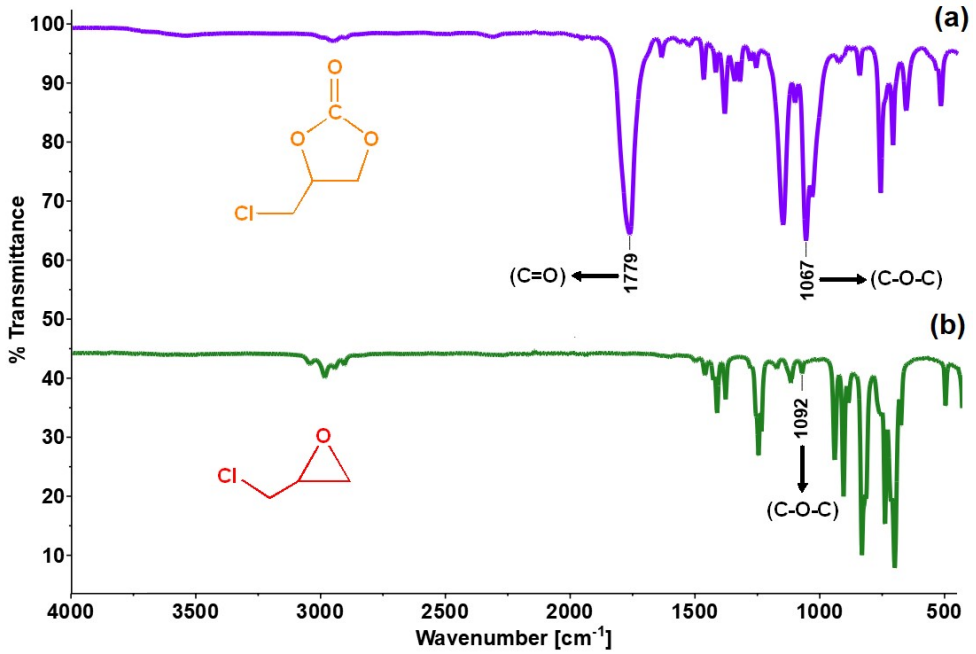


Figure S36. FT-IR spectra of the epichlorohydrin **(b)** and the corresponding cyclic carbonate **(a)**

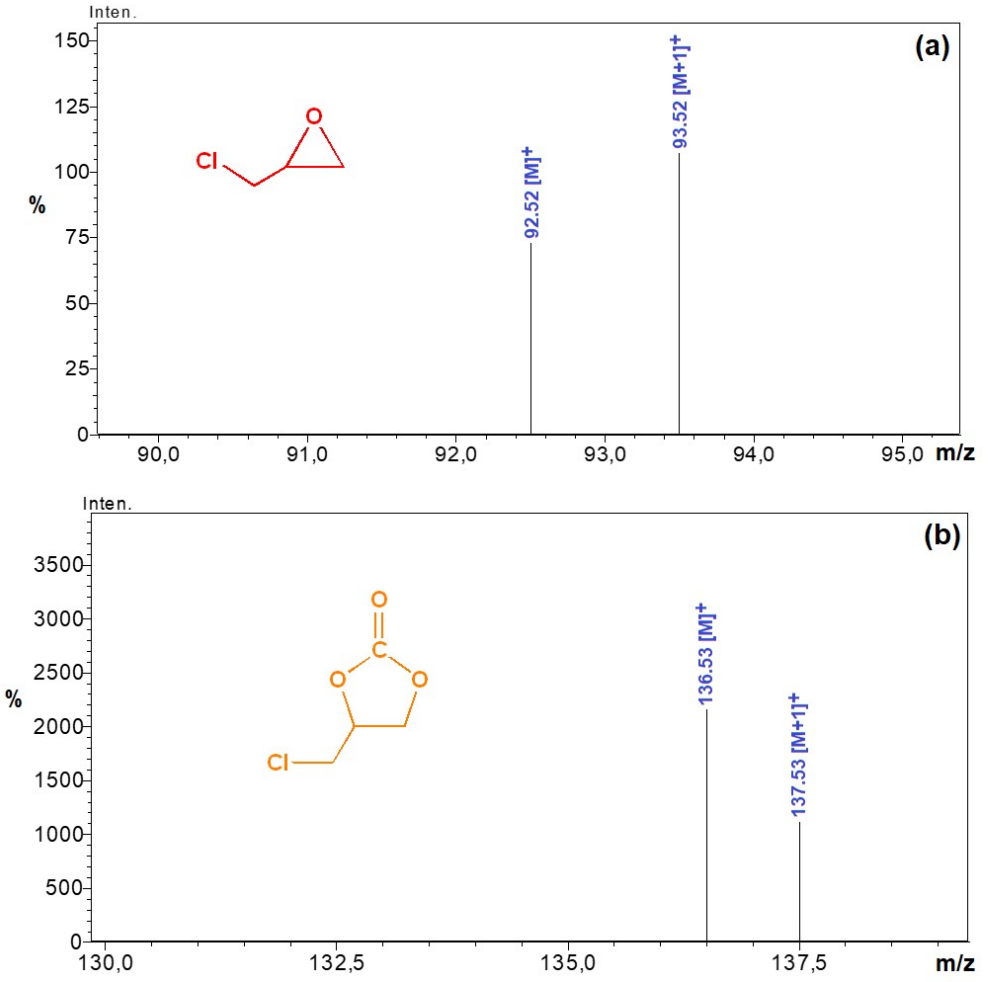


Figure S37. LC-MS/MS spectra of the epichlorohydrin **(a)** and the corresponding cyclic carbonate **(b)**

References

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