

## Transformation of Herbicides into Dual Function Quaternary Tropinium Salts

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The following abbreviations were used in the description of NMR spectra: s – singlet, d – doublet, dd – doublet of doublets, t – triplet, q – quintet, m – multiplet; br – broad; H<sub>a</sub> – axial position of proton, H<sub>e</sub> – equatorial position of proton.

**N-octyltropinium 4-chloro-2-methylphenoxyacetate [QTS-C<sub>8</sub>][MCPA]** <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 0.85 (t, J=6.5 Hz, 3H, CH<sub>3</sub>-CH<sub>2</sub>), 1.27 (m, 10H, CH<sub>3</sub>-(CH<sub>2</sub>)<sub>5</sub>-), 1.66 (q, J=4.2 Hz, 2H, -(CH<sub>2</sub>)<sub>5</sub>-CH<sub>2</sub>-), 1.81 (d, J=15.9 Hz, 2H, HO-CH-(CH<sub>a</sub>H<sub>e</sub>-CH-)<sub>2</sub>), 2.12 (s, 3H, CH<sub>3</sub>-Ar), 2.14 (t, J=5.5 Hz, 2H, -CH<sub>e</sub>H<sub>a</sub>-CH<sub>2</sub>-N<sup>+</sup>), 2.32 (d, J=16.3 Hz, 2H, -CH<sub>e</sub>H<sub>a</sub>-CH<sub>2</sub>-N<sup>+</sup>), 2.39 (d, J=8.2 Hz, 2H, HO-CH-(CH<sub>a</sub>H<sub>e</sub>-CH-)<sub>2</sub>), 2.96 (s, 3H, N<sup>+</sup>-CH<sub>3</sub>), 3.14 (t, J=8.3 Hz, 2H, alkyl-CH<sub>2</sub>N<sup>+</sup>), 3.78 (s, 2H, -CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 3.89 (t, J=4.9 Hz, 1H, -CH<sub>2</sub><sub>2</sub>-CH-OH), 4.08 (s, 2H, OCH<sub>2</sub>COO<sup>-</sup>), 6.63 (d, J=8.8 Hz, 1H, CIC=HCCH=CO), 7.05 (dd, J<sup>1,2</sup>=2.4 Hz, J<sup>1,3</sup>=8.7 Hz, 1H, CIC=HCCH=CO), 7.10 (d, J=2.2 Hz, 1H, CICCH=CCH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 14.34 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>7</sub>-N<sup>+</sup>), 16.43 (CH<sub>3</sub>-Ar), 22.04, (CH<sub>3</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>6</sub>-N<sup>+</sup>), 22.46 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>4</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>2</sub>-N<sup>+</sup>), 25.05 (-CH-CH<sub>2</sub>-CH<sub>2</sub>-CH-), 26.36, (CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>5</sub>-N<sup>+</sup>), 28.91, (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>3</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>3</sub>-N<sup>+</sup>), 28.98, (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>2</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>4</sub>-N<sup>+</sup>), 31.59 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>5</sub>-CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 34.66 (-CH<sub>2</sub>-CH(OH)-CH<sub>2</sub>-), 59.24 (CH<sub>3</sub>-N<sup>+</sup>(CH-)<sub>2</sub>), 60.59 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>6</sub>-CH<sub>2</sub>-N<sup>+</sup>), 65.90 (-CH<sub>2</sub>-CH(OH)-CH<sub>2</sub>-), 68.87 (OCH<sub>2</sub>COO<sup>-</sup>), 113.24 (CIC=HCCH=CO), 122.74 (CICCH=CCH<sub>3</sub>), 126.21, (CICCH=CCH<sub>3</sub>), 128.12 (CIC=HCCH=CO), 129.68 (CICCH=CCH<sub>3</sub>), 156.69 (CIC=HCCH=CO), 169.70 (OCH<sub>2</sub>COO<sup>-</sup>).

**N-decyltropinium 4-chloro-2-methylphenoxyacetate [QTS-C<sub>10</sub>][MCPA]** <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 0.84 (t, J=6.5 Hz, 3H, CH<sub>3</sub>-CH<sub>2</sub>), 1.24 (m, 14H, CH<sub>3</sub>-(CH<sub>2</sub>)<sub>5</sub>-), 1.63 (q, J=4.2 Hz, 2H, -(CH<sub>2</sub>)<sub>5</sub>-CH<sub>2</sub>-), 1.81 (d, J=15.9 Hz, 2H, HO-CH-(CH<sub>a</sub>H<sub>e</sub>-CH-)<sub>2</sub>), 2.12 (s, 3H, CH<sub>3</sub>-Ar), 2.14 (t, J=5.1 Hz, 2H, -CH<sub>e</sub>H<sub>a</sub>-CH<sub>2</sub>-N<sup>+</sup>), 2.33 (d, J=16.3 Hz, 2H, -CH<sub>e</sub>H<sub>a</sub>-CH<sub>2</sub>-N<sup>+</sup>), 2.39 (d, J=8.3 Hz, 2H, HO-CH-(CH<sub>a</sub>H<sub>e</sub>-CH-)<sub>2</sub>), 2.96 (s, 3H, N<sup>+</sup>-CH<sub>3</sub>), 3.14 (t, J=8.3 Hz, 2H, alkyl-CH<sub>2</sub>N<sup>+</sup>), 3.78 (s, 2H, -CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 3.89 (t, J=4.7 Hz, 1H, -CH<sub>2</sub><sub>2</sub>-CH-OH), 4.07 (s, 2H, OCH<sub>2</sub>COO<sup>-</sup>), 6.62 (d, J=8.7 Hz, 1H, CIC=HCCH=CO), 7.05 (dd, J<sup>1,2</sup>=2.3 Hz, J<sup>1,3</sup>=8.7 Hz, 1H, CIC=HCCH=CO), 7.10 (d, J=2.3 Hz, 1H, CICCH=CCH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 14.34 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>9</sub>-N<sup>+</sup>), 16.44 (CH<sub>3</sub>-Ar), 22.04 (CH<sub>3</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>8</sub>-N<sup>+</sup>), 22.49 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>6</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>2</sub>-N<sup>+</sup>), 25.05 (-CH-CH<sub>2</sub>-CH<sub>2</sub>-CH-), 26.35 (CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>7</sub>-N<sup>+</sup>), 29.02 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>5</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>3</sub>-N<sup>+</sup>), 29.08 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>2</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>6</sub>-N<sup>+</sup>), 29.25 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>4</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>4</sub>-N<sup>+</sup>), 29.31 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>3</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>5</sub>-N<sup>+</sup>), 31.67, (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>7</sub>-CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 34.67 (-CH<sub>2</sub>-CH(OH)-CH<sub>2</sub>-), 59.24 (CH<sub>3</sub>-N<sup>+</sup>(CH-)<sub>2</sub>), 60.60 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>8</sub>-CH<sub>2</sub>-N<sup>+</sup>), 65.89 (-CH<sub>2</sub>-CH(OH)-CH<sub>2</sub>-), 68.93 (OCH<sub>2</sub>COO<sup>-</sup>), 113.25 (CIC=HCCH=CO), 122.70 (CICCH=CCH<sub>3</sub>), 126.20 (CICCH=CCH<sub>3</sub>), 128.09 (CIC=HCCH=CO), 129.66 (CICCH=CCH<sub>3</sub>), 156.72 (CIC=HCCH=CO), 169.60 (OCH<sub>2</sub>COO<sup>-</sup>).

**N-dodecyltropinium 4-chloro-2-methylphenoxyacetate [QTS-C<sub>12</sub>][MCPA]** <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 0.84 (t, J=6.6 Hz, 3H, CH<sub>3</sub>-CH<sub>2</sub>), 1.23 (m, 18H, CH<sub>3</sub>-(CH<sub>2</sub>)<sub>5</sub>-), 1.63 (q, J=4.2 Hz, 2H, -(CH<sub>2</sub>)<sub>5</sub>-CH<sub>2</sub>-), 1.80 (d, J=15.8 Hz, 2H, HO-CH-(CH<sub>a</sub>H<sub>e</sub>-CH-)<sub>2</sub>), 2.12 (s, 3H, CH<sub>3</sub>-Ar), 2.16 (t, J=4.7 Hz, 2H, -CH<sub>e</sub>H<sub>a</sub>-CH<sub>2</sub>-N<sup>+</sup>), 2.32 (d, J=16.3 Hz, 2H, -CH<sub>e</sub>H<sub>a</sub>-CH<sub>2</sub>-N<sup>+</sup>), 2.38 (d, J=8.4 Hz, 2H, HO-CH-(CH<sub>a</sub>H<sub>e</sub>-CH-)<sub>2</sub>), 2.96 (s, 3H, N<sup>+</sup>-CH<sub>3</sub>), 3.14 (t, J=8.5 Hz, 2H, alkyl-CH<sub>2</sub>N<sup>+</sup>), 3.34 (br. s, 1H, CH-OH + H<sub>2</sub>O), 3.79 (s, 2H, -CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 3.90 (t, J=4.7 Hz, 1H, -CH<sub>2</sub><sub>2</sub>-CH-OH), 4.05 (s, 2H, OCH<sub>2</sub>COO<sup>-</sup>), 6.62 (d, J=8.7 Hz, 1H, CIC=HCCH=CO), 7.04 (dd, J<sup>1,2</sup>=2.7 Hz, J<sup>1,3</sup>=8.7 Hz, 1H, CIC=HCCH=CO), 7.09 (d, J=2.1 Hz, 1H, CICCH=CCH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 14.33 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>11</sub>-N<sup>+</sup>), 16.43 (CH<sub>3</sub>-Ar), 22.03 (CH<sub>3</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>10</sub>-N<sup>+</sup>), 22.48 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>8</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>2</sub>-N<sup>+</sup>), 25.07 (-CH-CH<sub>2</sub>-CH<sub>2</sub>-CH-), 26.54 (CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>9</sub>-N<sup>+</sup>), 28.99 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>7</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>3</sub>-N<sup>+</sup>), 29.09 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>2</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>8</sub>-N<sup>+</sup>), 29.22 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>6</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>4</sub>-N<sup>+</sup>), 29.33 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>3</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>7</sub>-N<sup>+</sup>), 29.39 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>5</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>5</sub>-N<sup>+</sup>), 29.41 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>4</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>6</sub>-N<sup>+</sup>), 31.68 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>9</sub>-CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 34.71 (-CH<sub>2</sub>-CH(OH)-CH<sub>2</sub>-), 59.31 (CH<sub>3</sub>-N<sup>+</sup>(CH-)<sub>2</sub>), 60.67 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>10</sub>-CH<sub>2</sub>-N<sup>+</sup>), 65.90 (-CH<sub>2</sub>-CH(OH)-CH<sub>2</sub>-)

$\underline{\text{CH}}(\text{OH})\text{-CH}_2$ -), 69.00 ( $\text{OCH}_2\text{COO}^-$ ), 113.31 ( $\text{ClC=HCCH=CO}$ ), 122.66 ( $\text{ClCCH=CCH}_3$ ), 126.19 ( $\text{ClCCH=CCH}_3$ ), 128.09 ( $\text{ClC=HCCH=CO}$ ), 129.64 ( $\text{ClC=HCCH=CO}$ ), 156.76 ( $\text{ClC=HCCH=CO}$ ), 169.47 ( $\text{OCH}_2\text{COO}^-$ ).

**N-tetradecyltropinium 4-chloro-2-methylphenoxyacetate [QTS-C<sub>14</sub>][MCPA]** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ ppm = 0.84 (t, *J*=6.5 Hz, 3H,  $\text{CH}_3\text{-CH}_2$ ), 1.23 (m, 22H,  $\text{CH}_3\text{-}(\text{CH}_2)_{5-}$ ), 1.63 (q, *J*=4.2 Hz, 2H, -( $\text{CH}_2)_5\text{-CH}_2$ -), 1.79 (d, *J*=16.1 Hz, 2H, HO-CH-( $\text{CH}_a\text{H}_e\text{-CH-}_2$ )), 2.12 (s, 3H,  $\text{CH}_3\text{-Ar}$ ), 2.17 (t, *J*=4.4 Hz, 2H, - $\text{CH}_e\text{H}_a\text{-CH}_2$ -N<sup>+</sup>), 2.33 (d, *J*=16.0 Hz, 2H, - $\text{CH}_e\text{H}_a\text{-CH}_2$ -N<sup>+</sup>), 2.38 (d, *J*=7.5 Hz, 2H, HO-CH-( $\text{CH}_a\text{H}_e\text{-CH-}_2$ )), 2.96 (s, 3H, N<sup>+</sup>- $\text{CH}_3$ ), 3.14 (t, *J*=8.3 Hz, 2H, alkyl- $\text{CH}_2$ N<sup>+</sup>), 3.33 (br. s, 1H, CH-OH + H<sub>2</sub>O), 3.79 (s, 2H, - $\text{CH}_2\text{-CH}_2$ -N<sup>+</sup>), 3.90 (t, *J*=4.9 Hz, 1H, - $\text{CH}_2\text{-CH}_2$ -OH), 4.05 (s, 2H,  $\text{OCH}_2\text{COO}^-$ ), 6.62 (d, *J*=8.7 Hz, 1H, ClC=HCCH=CO), 7.04 (dd, *J*<sup>1,2</sup>=2.1 Hz, *J*<sup>1,3</sup>=8.5 Hz, 1H, ClC=HCCH=CO), 7.09 (d, *J*=2.2 Hz, 1H, CICCH=CCH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz): δ ppm = 14.34 ( $\text{CH}_3\text{-}(\text{CH}_2)_{13}\text{-N}^+$ ), 16.43 ( $\text{CH}_3\text{-Ar}$ ), 22.03 ( $\text{CH}_3\text{-CH}_2\text{-}(\text{CH}_2)_{12}\text{-N}^+$ ), 22.47 ( $\text{CH}_3\text{-}(\text{CH}_2)_{10}\text{-CH}_2\text{-}(\text{CH}_2)_2\text{-N}^+$ ), 25.07 (-CH- $\text{CH}_2\text{-CH}_2$ -CH-), 26.53 ( $\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-}(\text{CH}_2)_{11}\text{-N}^+$ ), 28.99 ( $\text{CH}_3\text{-}(\text{CH}_2)_9\text{-CH}_2\text{-}(\text{CH}_2)_3\text{-N}^+$ ), 29.09 ( $\text{CH}_3\text{-}(\text{CH}_2)_2\text{-CH}_2\text{-}(\text{CH}_2)_{10}\text{-N}^+$ ), 29.22 ( $\text{CH}_3\text{-}(\text{CH}_2)_8\text{-CH}_2\text{-}(\text{CH}_2)_4\text{-N}^+$ ), 29.33 ( $\text{CH}_3\text{-}(\text{CH}_2)_3\text{-CH}_2\text{-}(\text{CH}_2)_9\text{-N}^+$ ), 29.40 ( $\text{CH}_3\text{-}(\text{CH}_2)_7\text{-CH}_2\text{-}(\text{CH}_2)_5\text{-N}^+$ ), 29.43, ( $\text{CH}_3\text{-}(\text{CH}_2)_4\text{-CH}_2\text{-}(\text{CH}_2)_9\text{-N}^+$ ), 29.44 ( $\text{CH}_3\text{-}(\text{CH}_2)_5\text{-CH}_2\text{-}(\text{CH}_2)_6\text{-N}^+$ ), 31.68 ( $\text{CH}_3\text{-}(\text{CH}_2)_9\text{-CH}_2\text{-CH}_2\text{-N}^+$ ), 34.71 (- $\text{CH}_2\text{-CH(OH)}$ - $\text{CH}_2$ ), 59.32 ( $\text{CH}_3\text{-N}^+(\text{CH-})_2$ ), 60.67 ( $\text{CH}_3\text{-}(\text{CH}_2)_{12}\text{-CH}_2\text{-N}^+$ ), 65.89 (- $\text{CH}_2\text{-CH(OH)}$ - $\text{CH}_2$ ), 69.02 ( $\text{OCH}_2\text{COO}^-$ ), 113.31 (ClC=HCCH=CO), 122.63 (CICCH=CCH<sub>3</sub>), 126.19 (ClCCH=CCH<sub>3</sub>), 128.07 (ClC=HCCH=CO), 129.63 (ClC=HCCH=CO), 156.77 (ClC=HCCH=CO), 169.39 (OCH<sub>2</sub>COO<sup>-</sup>).

**N-hexadecyltropinium 4-chloro-2-methylphenoxyacetate [QTS-C<sub>16</sub>][MCPA]** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ ppm = 0.86 (t, *J*=6.2 Hz, 3H,  $\text{CH}_3\text{-CH}_2$ ), 1.24 (m, 26H,  $\text{CH}_3\text{-}(\text{CH}_2)_{5-}$ ), 1.65 (q, *J*=4.2 Hz, 2H, -( $\text{CH}_2)_5\text{-CH}_2$ -), 1.81 (d, *J*=15.9 Hz, 2H, HO-CH-( $\text{CH}_a\text{H}_e\text{-CH-}_2$ )), 2.13 (s, 3H,  $\text{CH}_3\text{-Ar}$ ), 2.18 (t, *J*=5.5 Hz, 2H, - $\text{CH}_e\text{H}_a\text{-CH}_2$ -N<sup>+</sup>), 2.34 (d, *J*=16.0 Hz, 2H, - $\text{CH}_e\text{H}_a\text{-CH}_2$ -N<sup>+</sup>), 2.38 (d, *J*=8.0 Hz, 2H, HO-CH-( $\text{CH}_a\text{H}_e\text{-CH-}_2$ )), 2.98 (s, 3H, N<sup>+</sup>- $\text{CH}_3$ ), 3.15 (t, *J*=7.0 Hz, 2H, alkyl- $\text{CH}_2$ N<sup>+</sup>), 3.36 (br. s, 1H, CH-OH + H<sub>2</sub>O), 3.80 (s, 2H, - $\text{CH}_2\text{-CH}_2$ -N<sup>+</sup>), 3.91 (t, *J*=4.9 Hz, 1H, - $\text{CH}_2\text{-CH}_2$ -OH), 4.06 (s, 2H,  $\text{OCH}_2\text{COO}^-$ ), 6.63 (d, *J*=8.9 Hz, 1H, ClC=HCCH=CO), 7.05 (dd, *J*<sup>1,2</sup>=2.2 Hz, *J*<sup>1,3</sup>=8.7 Hz, 1H, ClC=HCCH=CO), 7.10 (d, *J*=2.2 Hz, 1H, CICCH=CCH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz): δ ppm = 13.91 ( $\text{CH}_3\text{-}(\text{CH}_2)_{13}\text{-N}^+$ ), 16.01 ( $\text{CH}_3\text{-Ar}$ ), 21.61 ( $\text{CH}_3\text{-CH}_2\text{-}(\text{CH}_2)_{14}\text{-N}^+$ ), 22.06 ( $\text{CH}_3\text{-}(\text{CH}_2)_{12}\text{-CH}_2\text{-}(\text{CH}_2)_2\text{-N}^+$ ), 24.64 (-CH- $\text{CH}_2\text{-CH}_2$ -CH-), 25.91 ( $\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-}(\text{CH}_2)_{11}\text{-N}^+$ ), 28.58 ( $\text{CH}_3\text{-}(\text{CH}_2)_{11}\text{-CH}_2\text{-}(\text{CH}_2)_3\text{-N}^+$ ), 28.68 ( $\text{CH}_3\text{-}(\text{CH}_2)_2\text{-CH}_2\text{-}(\text{CH}_2)_{12}\text{-N}^+$ ), 28.81 ( $\text{CH}_3\text{-}(\text{CH}_2)_{10}\text{-CH}_2\text{-}(\text{CH}_2)_4\text{-N}^+$ ), 28.87 ( $\text{CH}_3\text{-}(\text{CH}_2)_3\text{-CH}_2\text{-}(\text{CH}_2)_{11}\text{-N}^+$ ), 28.92 ( $\text{CH}_3\text{-}(\text{CH}_2)_9\text{-CH}_2\text{-}(\text{CH}_2)_5\text{-N}^+$ ), 28.98 ( $\text{CH}_3\text{-}(\text{CH}_2)_4\text{-CH}_2\text{-}(\text{CH}_2)_{10}\text{-N}^+$ ), 28.99 ( $\text{CH}_3\text{-}(\text{CH}_2)_8\text{-CH}_2\text{-}(\text{CH}_2)_6\text{-N}^+$ ), 29.02 ( $\text{CH}_3\text{-}(\text{CH}_2)_5\text{-CH}_2\text{-}(\text{CH}_2)_9\text{-N}^+$ ), 29.09 ( $\text{CH}_3\text{-}(\text{CH}_2)_6\text{-}(\text{CH}_2)_2\text{-}(\text{CH}_2)_7\text{-N}^+$ ), 31.26 ( $\text{CH}_3\text{-}(\text{CH}_2)_{13}\text{-CH}_2\text{-CH}_2\text{-N}^+$ ), 34.27 (- $\text{CH}_2\text{-CH(OH)}$ - $\text{CH}_2$ ), 58.88 ( $\text{CH}_3\text{-N}^+(\text{CH-})_2$ ), 60.22 ( $\text{CH}_3\text{-}(\text{CH}_2)_{14}\text{-CH}_2\text{-N}^+$ ), 65.45 (- $\text{CH}_2\text{-CH(OH)}$ - $\text{CH}_2$ ), 68.55 ( $\text{OCH}_2\text{COO}^-$ ), 112.85 (ClC=HCCH=CO), 122.21 (CICCH=CCH<sub>3</sub>), 125.76 (ClCCH=CCH<sub>3</sub>), 127.64 (ClC=HCCH=CO), 129.21 (ClC=HCCH=CO), 156.32 (ClC=HCCH=CO), 169.02 (OCH<sub>2</sub>COO<sup>-</sup>).

**N-octadecyltropinium 4-chloro-2-methylphenoxyacetate [QTS-C<sub>18</sub>][MCPA]** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ ppm = 0.84 (t, *J*=6.3 Hz, 3H,  $\text{CH}_3\text{-CH}_2$ ), 1.22 (m, 30H,  $\text{CH}_3\text{-}(\text{CH}_2)_{5-}$ ), 1.63 (q, *J*=4.2 Hz, 2H, -( $\text{CH}_2)_5\text{-CH}_2$ -), 1.81 (d, *J*=15.9 Hz, 2H, HO-CH-( $\text{CH}_a\text{H}_e\text{-CH-}_2$ )), 2.12 (s, 3H,  $\text{CH}_3\text{-Ar}$ ), 2.17 (t, *J*=5.0 Hz, 2H, - $\text{CH}_e\text{H}_a\text{-CH}_2$ -N<sup>+</sup>), 2.32 (d, *J*=16.0 Hz, 2H, - $\text{CH}_e\text{H}_a\text{-CH}_2$ -N<sup>+</sup>), 2.38 (d, *J*=8.0 Hz, 2H, HO-CH-( $\text{CH}_a\text{H}_e\text{-CH-}_2$ )), 2.96 (s, 3H, N<sup>+</sup>- $\text{CH}_3$ ), 3.14 (t, *J*=8.5 Hz, 2H, alkyl- $\text{CH}_2$ N<sup>+</sup>), 3.35 (br. s, 1H, CH-OH + H<sub>2</sub>O), 3.79 (s, 2H, - $\text{CH}_2\text{-CH}_2$ -N<sup>+</sup>), 3.90 (t, *J*=4.9 Hz, 1H, - $\text{CH}_2\text{-CH}_2$ -OH), 4.06 (s, 2H,  $\text{OCH}_2\text{COO}^-$ ), 6.63 (d, *J*=8.7 Hz, 1H, ClC=HCCH=CO), 7.04 (dd, *J*<sup>1,2</sup>=2.2 Hz, *J*<sup>1,3</sup>=8.7 Hz, 1H, ClC=HCCH=CO), 7.08 (d, *J*=2.2 Hz, 1H, CICCH=CCH<sub>3</sub>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz): δ ppm = 14.31 ( $\text{CH}_3\text{-}(\text{CH}_2)_{15}\text{-N}^+$ ), 16.42 ( $\text{CH}_3\text{-Ar}$ ), 22.04 ( $\text{CH}_3\text{-CH}_2\text{-}(\text{CH}_2)_{16}\text{-N}^+$ ), 22.49 ( $\text{CH}_3\text{-}(\text{CH}_2)_{14}\text{-CH}_2\text{-}(\text{CH}_2)_2\text{-N}^+$ ), 24.84 (-CH- $\text{CH}_2\text{-CH}_2$ -CH-), 25.06 ( $\text{CH}_3\text{-CH}_2\text{-}(\text{CH}_2)_{15}\text{-N}^+$ ), 26.36 ( $\text{CH}_3\text{-}(\text{CH}_2)_{13}\text{-CH}_2\text{-}(\text{CH}_2)_3\text{-N}^+$ ), 28.92 ( $\text{CH}_3\text{-}(\text{CH}_2)_2\text{-CH}_2\text{-}(\text{CH}_2)_{14}\text{-N}^+$ ), 28.98 ( $\text{CH}_3\text{-}(\text{CH}_2)_{12}\text{-N}^+$ ),

$\underline{\text{CH}_2}-(\text{CH}_2)_4-\text{N}^+$ ), 28.99 ( $\text{CH}_3-(\text{CH}_2)_3-\underline{\text{CH}_2}-(\text{CH}_2)_{13}-\text{N}^+$ ), 29.01 ( $\text{CH}_3-(\text{CH}_2)_{11}-\underline{\text{CH}_2}-(\text{CH}_2)_5-\text{N}^+$ ), 29.02 ( $\text{CH}_3-(\text{CH}_2)_4-\underline{\text{CH}_2}-(\text{CH}_2)_{12}-\text{N}^+$ ), 29.09 ( $\text{CH}_3-(\text{CH}_2)_{10}-\underline{\text{CH}_2}-(\text{CH}_2)_6-\text{N}^+$ ), 29.10 ( $\text{CH}_3-(\text{CH}_2)_5-\underline{\text{CH}_2}-(\text{CH}_2)_{11}-\text{N}^+$ ), 29.25 ( $\text{CH}_3-(\text{CH}_2)_9-\underline{\text{CH}_2}-(\text{CH}_2)_7-\text{N}^+$ ), 29.44 ( $\text{CH}_3-(\text{CH}_2)_6-\underline{(\text{CH}_2)_3}-(\text{CH}_2)_8-\text{N}^+$ ), 31.69 ( $\text{CH}_3-(\text{CH}_2)_{15}-\underline{\text{CH}_2}-\text{CH}_2-\text{N}^+$ ), 34.70 ( $-\underline{\text{CH}_2}-\text{CH}(\text{OH})-\underline{\text{CH}_2}$ ), 59.29 ( $\underline{\text{CH}_3}-\text{N}^+(\underline{\text{CH}}_2)_2$ ), 60.64 ( $\text{CH}_3-(\text{CH}_2)_{16}-\underline{\text{CH}_2}-\text{N}^+$ ), 65.91 ( $-\text{CH}_2-\underline{\text{CH}}(\text{OH})-\text{CH}_2$ ), 68.98 ( $\text{O}\underline{\text{CH}_2}\text{COO}^-$ ), 113.28 ( $\text{ClC}=\text{HC}\underline{\text{CH}}=\text{CO}$ ), 122.68 ( $\text{ClC}\underline{\text{CH}}=\underline{\text{CCH}}_3$ ), 126.18 ( $\text{Cl}\underline{\text{CCH}}=\text{CCH}_3$ ), 128.09 ( $\text{ClC}=\underline{\text{H}}\underline{\text{CCH}}=\text{CO}$ ), 129.63 ( $\text{ClC}=\text{H}\underline{\text{CCH}}=\text{CO}$ ), 156.76 ( $\text{ClC}=\text{HC}\underline{\text{CH}}=\text{CO}$ ), 169.15 ( $\text{OCH}_2\underline{\text{COO}}^-$ ).

**N-octyltropinium 3,6-dichloro-2-methoxybenzoate [QTS-C<sub>8</sub>][dicamba]** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  ppm = 0.85 (t, *J*=6.7 Hz, 3H,  $\underline{\text{CH}_3}-\text{CH}_2$ ), 1.26 (m, 10H,  $\text{CH}_3-(\underline{\text{CH}_2})_5-$ ), 1.63 (q, *J*=4.2 Hz, 2H,  $-(\text{CH}_2)_5-\underline{\text{CH}_2}$ ), 1.79 (d, *J*=15.9 Hz, 2H, HO-CH-( $\underline{\text{CH}_a}\text{H}_e-\text{CH}-$ )<sub>2</sub>), 2.16 (t, *J*=4.9 Hz, 2H,  $-\underline{\text{CH}_e}\text{H}_a-\text{CH}$ )<sub>2</sub>-N<sup>+</sup>), 2.34 (d, *J*=16.0 Hz, 2H,  $-\text{CH}_e\text{H}_a-\text{CH}$ )<sub>2</sub>-N<sup>+</sup>), 2.36 (d, *J*=8.0 Hz, 2H, HO-CH-( $\text{CH}_a\text{H}_e-\text{CH}-$ )<sub>2</sub>), 2.97 (s, 3H,  $\text{N}^+-\underline{\text{CH}_3}$ ), 3.14 (t, *J*=8.3 Hz, 2H, alkyl- $\underline{\text{CH}_2}\text{N}^+$ ), 3.36 (br. s, 1H, CH-OH + H<sub>2</sub>O), 3.77 (s, 3H,  $\underline{\text{CH}_3}-\text{O}-\text{Ar}$ ), 3.78 (s, 2H,  $-\text{CH}_2-\underline{\text{CH}}$ )<sub>2</sub>-N<sup>+</sup>), 3.90 (t, *J*=5.0 Hz, 1H,  $-\text{CH}_2$ )<sub>2</sub>-CH-OH), 7.00 (d, *J*=8.5 Hz, 1H, CICCH=CHC(Cl)=CCOO<sup>-</sup>), 7.13 (d, *J*=8.5 Hz, 1H, CICCH=CHC(Cl)=CCOO<sup>-</sup>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz):  $\delta$  ppm = 14.34 ( $\underline{\text{CH}_3}-(\text{CH}_2)_7-\text{N}^+$ ), 22.04 ( $\text{CH}_3-\underline{\text{CH}_2}-(\text{CH}_2)_6-\text{N}^+$ ), 22.45 ( $\text{CH}_3-(\text{CH}_2)_4-\underline{\text{CH}_2}-(\text{CH}_2)_2-\text{N}^+$ ), 25.06 ( $-\text{CH}-\underline{\text{CH}_2}-\underline{\text{CH}_2}-\text{CH}-$ ), 26.33 ( $\text{CH}_3-\text{CH}_2-\underline{\text{CH}_2}-(\text{CH}_2)_5-\text{N}^+$ ), 28.89 ( $\text{CH}_3-(\text{CH}_2)_3-\underline{\text{CH}_2}-(\text{CH}_2)_3-\text{N}^+$ ), 28.95 ( $\text{CH}_3-(\text{CH}_2)_2-\underline{\text{CH}_2}-(\text{CH}_2)_4-\text{N}^+$ ), 31.57 ( $\text{CH}_3-(\text{CH}_2)_5-\underline{\text{CH}_2}-\text{CH}_2-\text{N}^+$ ), 34.69 ( $-\underline{\text{CH}_2}-\text{CH}(\text{OH})-\underline{\text{CH}_2}$ ), 59.34 ( $\underline{\text{CH}_3}-\text{N}^+(\underline{\text{CH}}_2)_2$ ), 60.64 ( $\text{CH}_3-(\text{CH}_2)_6-\underline{\text{CH}_2}-\text{N}^+$ ), 61.22 ( $\underline{\text{CH}_3}-\text{O}-\text{Ar}$ ), 65.85 ( $-\text{CH}_2-\underline{\text{CH}}(\text{OH})-\text{CH}_2$ ), 125.35 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 125.51 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 126.61 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 127.91, (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 141.69 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 151.48 ( $\underline{\text{CH}_3}-\text{O}-\underline{\text{C}}=\text{CCl}$ ), 165.23 (-COO<sup>-</sup>).

**N-decyltropinium 3,6-dichloro-2-methoxybenzoate [QTS-C<sub>10</sub>][dicamba]** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  ppm = 0.84 (t, *J*=6.6 Hz, 3H,  $\underline{\text{CH}_3}-\text{CH}_2$ ), 1.23 (m, 14H,  $\text{CH}_3-(\underline{\text{CH}_2})_5-$ ), 1.62 (q, *J*=4.2 Hz, 2H,  $-(\text{CH}_2)_5-\underline{\text{CH}_2}$ ), 1.80 (d, *J*=15.9 Hz, 2H, HO-CH-( $\underline{\text{CH}_a}\text{H}_e-\text{CH}-$ )<sub>2</sub>), 2.15 (t, *J*=4.8 Hz, 2H,  $-\underline{\text{CH}_e}\text{H}_a-\text{CH}$ )<sub>2</sub>-N<sup>+</sup>), 2.32 (d, *J*=16.0 Hz, 2H,  $-\text{CH}_e\text{H}_a-\text{CH}$ )<sub>2</sub>-N<sup>+</sup>), 2.37 (d, *J*=8.5 Hz, 2H, HO-CH-( $\text{CH}_a\text{H}_e-\text{CH}-$ )<sub>2</sub>), 2.97 (s, 3H,  $\text{N}^+-\underline{\text{CH}_3}$ ), 3.15 (t, *J*=8.3 Hz, 2H, alkyl- $\underline{\text{CH}_2}\text{N}^+$ ), 3.43 (br. s, 1H, CH-OH + H<sub>2</sub>O), 3.78 (s, 3H,  $\underline{\text{CH}_3}-\text{O}-\text{Ar}$ ), 3.78 (s, 2H,  $-\text{CH}_2-\underline{\text{CH}}$ )<sub>2</sub>-N<sup>+</sup>), 3.90 (t, *J*=4.8 Hz, 1H,  $-\text{CH}_2$ )<sub>2</sub>-CH-OH), 7.01 (d, *J*=8.5 Hz, 1H, CICCH=CHC(Cl)=CCOO<sup>-</sup>), 7.13 (d, *J*=8.6 Hz, 1H, CICCH=CHC(Cl)=CCOO<sup>-</sup>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz):  $\delta$  ppm = 14.34 ( $\underline{\text{CH}_3}-(\text{CH}_2)_9-\text{N}^+$ ), 22.05 ( $\text{CH}_3-\underline{\text{CH}_2}-(\text{CH}_2)_8-\text{N}^+$ ), 22.49 ( $\text{CH}_3-(\text{CH}_2)_6-\underline{\text{CH}_2}-(\text{CH}_2)_2-\text{N}^+$ ), 25.05 ( $-\text{CH}-\underline{\text{CH}_2}-\underline{\text{CH}_2}-\text{CH}-$ ), 26.34 ( $\text{CH}_3-\text{CH}_2-\underline{\text{CH}_2}-(\text{CH}_2)_7-\text{N}^+$ ), 29.01 ( $\text{CH}_3-(\text{CH}_2)_5-\underline{\text{CH}_2}-(\text{CH}_2)_3-\text{N}^+$ ), 29.09 ( $\text{CH}_3-(\text{CH}_2)_2-\underline{\text{CH}_2}-(\text{CH}_2)_6-\text{N}^+$ ), 29.26 ( $\text{CH}_3-(\text{CH}_2)_4-\underline{\text{CH}_2}-(\text{CH}_2)_4-\text{N}^+$ ), 29.31 ( $\text{CH}_3-(\text{CH}_2)_3-\underline{\text{CH}_2}-(\text{CH}_2)_5-\text{N}^+$ ), 31.68 ( $\text{CH}_3-(\text{CH}_2)_7-\underline{\text{CH}_2}-\text{CH}_2-\text{N}^+$ ), 34.66 ( $-\underline{\text{CH}_2}-\text{CH}(\text{OH})-\underline{\text{CH}_2}$ ), 59.32 ( $\underline{\text{CH}_3}-\text{N}^+(\underline{\text{CH}}_2)_2$ ), 60.58 ( $\text{CH}_3-(\text{CH}_2)_8-\underline{\text{CH}_2}-\text{N}^+$ ), 61.24 ( $\underline{\text{CH}_3}-\text{O}-\text{Ar}$ ), 65.84 ( $-\text{CH}_2-\underline{\text{CH}}(\text{OH})-\text{CH}_2$ ), 125.40 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 125.54 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 126.74 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 127.89 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 141.52 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 151.50 ( $\underline{\text{CH}_3}-\text{O}-\underline{\text{C}}=\text{CCl}$ ), 165.43 (-COO<sup>-</sup>).

**N-dodecyltropinium 3,6-dichloro-2-methoxybenzoate [QTS-C<sub>12</sub>][dicamba]** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  ppm = 0.84 (t, *J*=6.7 Hz, 3H,  $\underline{\text{CH}_3}-\text{CH}_2$ ), 1.23 (m, 18H,  $\text{CH}_3-(\underline{\text{CH}_2})_5-$ ), 1.63 (q, *J*=4.2 Hz, 2H,  $-(\text{CH}_2)_5-\underline{\text{CH}_2}$ ), 1.80 (d, *J*=15.9 Hz, 2H, HO-CH-( $\underline{\text{CH}_a}\text{H}_e-\text{CH}-$ )<sub>2</sub>), 2.16 (t, *J*=5.0 Hz, 2H,  $-\underline{\text{CH}_e}\text{H}_a-\text{CH}$ )<sub>2</sub>-N<sup>+</sup>), 2.34 (d, *J*=16.0 Hz, 2H,  $-\text{CH}_e\text{H}_a-\text{CH}$ )<sub>2</sub>-N<sup>+</sup>), 2.37 (d, *J*=7.9 Hz, 2H, HO-CH-( $\text{CH}_a\text{H}_e-\text{CH}-$ )<sub>2</sub>), 2.97 (s, 3H,  $\text{N}^+-\underline{\text{CH}_3}$ ), 3.15 (t, *J*=8.3 Hz, 2H, alkyl- $\underline{\text{CH}_2}\text{N}^+$ ), 3.37 (br. s, 1H, CH-OH + H<sub>2</sub>O), 3.78 (s, 3H,  $\underline{\text{CH}_3}-\text{O}-\text{Ar}$ ), 3.80 (s, 2H,  $-\text{CH}_2-\underline{\text{CH}}$ )<sub>2</sub>-N<sup>+</sup>), 3.90 (t, *J*=4.9 Hz, 1H,  $-\text{CH}_2$ )<sub>2</sub>-CH-OH), 7.00 (d, *J*=8.6 Hz, 1H, CICCH=CHC(Cl)=CCOO<sup>-</sup>), 7.13 (d, *J*=8.5 Hz, 1H, CICCH=CHC(Cl)=CCOO<sup>-</sup>); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz):  $\delta$  ppm = 14.32 ( $\underline{\text{CH}_3}-(\text{CH}_2)_{11}-\text{N}^+$ ), 22.04 ( $\text{CH}_3-\underline{\text{CH}_2}-(\text{CH}_2)_{10}-\text{N}^+$ ), 22.48 ( $\text{CH}_3-(\text{CH}_2)_8-\underline{\text{CH}_2}-(\text{CH}_2)_2-\text{N}^+$ ), 25.06 ( $-\text{CH}-\underline{\text{CH}_2}-\underline{\text{CH}_2}-\text{CH}-$ ), 26.33 ( $\text{CH}_3-\text{CH}_2-\underline{\text{CH}_2}-(\text{CH}_2)_9-\text{N}^+$ ), 28.99 ( $\text{CH}_3-(\text{CH}_2)_7-\underline{\text{CH}_2}-(\text{CH}_2)_3-\text{N}^+$ ), 29.09 ( $\text{CH}_3-(\text{CH}_2)_2-\underline{\text{CH}_2}-(\text{CH}_2)_8-\text{N}^+$ ), 29.23 ( $\text{CH}_3-(\text{CH}_2)_6-\underline{\text{CH}_2}-(\text{CH}_2)_4-\text{N}^+$ ), 29.33 ( $\text{CH}_3-(\text{CH}_2)_3-\underline{\text{CH}_2}-(\text{CH}_2)_7-\text{N}^+$ ), 29.39 ( $\text{CH}_3-(\text{CH}_2)_5-\underline{\text{CH}_2}-(\text{CH}_2)_5-\text{N}^+$ ), 29.41 ( $\text{CH}_3-(\text{CH}_2)_4-\underline{\text{CH}_2}-(\text{CH}_2)_6-\text{N}^+$ ), 31.69 ( $\text{CH}_3-(\text{CH}_2)_9-\underline{\text{CH}_2}-\text{CH}_2-\text{N}^+$ ), 34.71 ( $-\underline{\text{CH}_2}-\text{CH}(\text{OH})-\underline{\text{CH}_2}$ ), 59.34 ( $\underline{\text{CH}_3}-\text{N}^+(\underline{\text{CH}}_2)_2$ ), 60.64 ( $\text{CH}_3-$

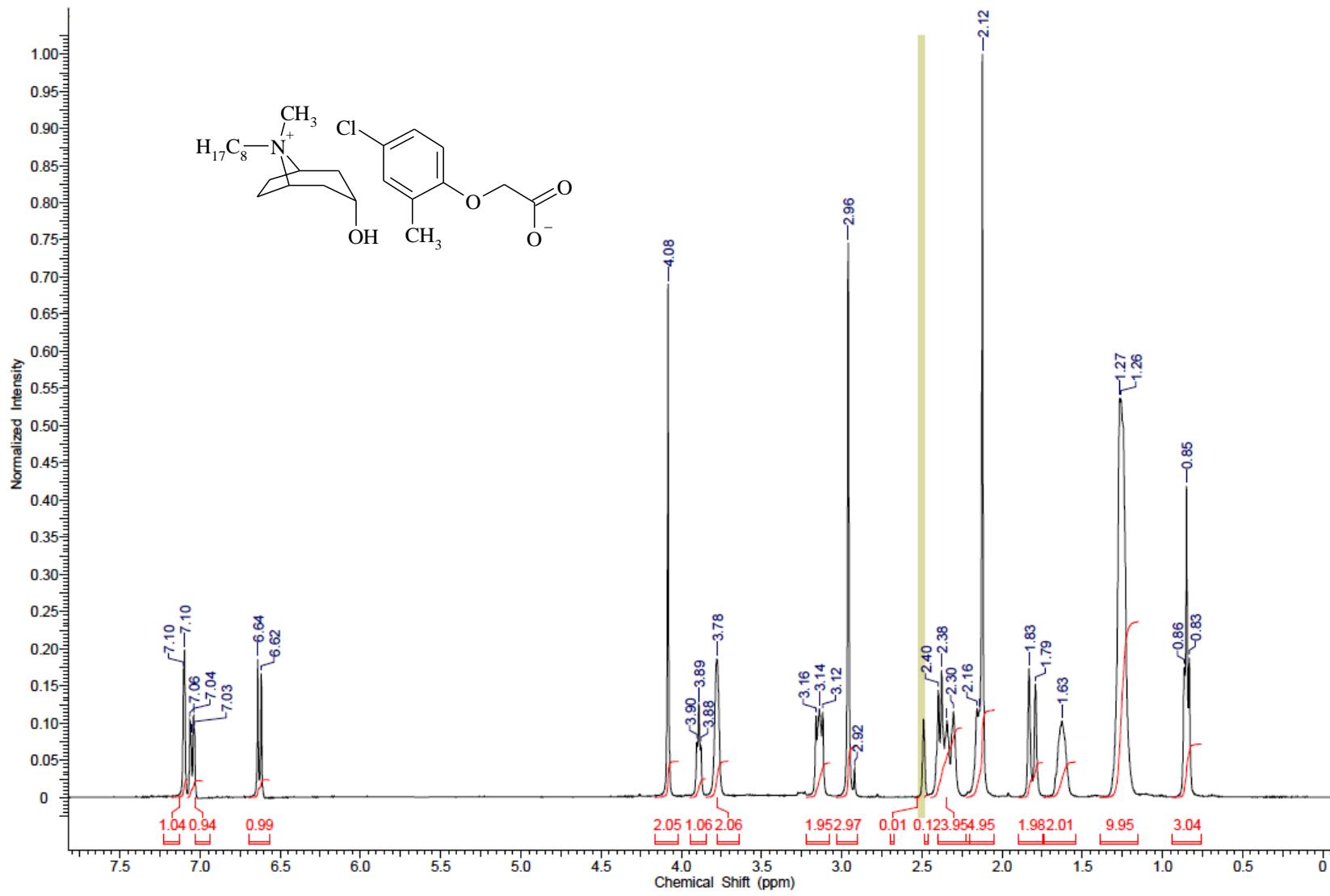
$(\text{CH}_2)_{10}-\underline{\text{CH}_2-\text{N}^+}$ ), 61.22 ( $\underline{\text{CH}_3-\text{O-Ar}}$ ), 65.87 ( $-\text{CH}_2-\underline{\text{CH(OH)-CH}_2-}$ ), 125.36 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 125.49 ( $\underline{\text{CICCH=CHC(Cl)=CCOO}^-}$ ), 126.66 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 127.92 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 141.60 ( $\underline{\text{CICCH=CHC(Cl)=CCOO}^-}$ ), 151.51 ( $\underline{\text{CH}_3-\text{O-C=CCI}}$ ), 165.31 ( $-\underline{\text{COO}^-}$ ).

**N-tetradecyltropinium 3,6-dichloro-2-methoxybenzoate [QTS-C<sub>14</sub>][dicamba]** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ ppm = 0.84 (t, *J*=6.7 Hz, 3H,  $\underline{\text{CH}_3-\text{CH}_2}$ ), 1.23 (m, 22H,  $\text{CH}_3-(\underline{\text{CH}_2})_5^-$ ), 1.63 (q, *J*=4.2 Hz, 2H,  $-(\text{CH}_2)_5-\underline{\text{CH}_2-}$ ), 1.79 (d, *J*=15.9 Hz, 2H,  $\text{HO-CH-(CH}_a\underline{\text{H}_e-\text{CH}})_2$ ), 2.17 (t, *J*=4.7 Hz, 2H,  $-\underline{\text{CH}_e\text{H}_a-\text{CH}})_2-\text{N}^+$ ), 2.34 (d, *J*=16.0 Hz, 2H,  $-\underline{\text{CH}_e\text{H}_a-\text{CH}})_2-\text{N}^+$ ), 2.37 (d, *J*=8.0 Hz, 2H,  $\text{HO-CH-(CH}_a\underline{\text{H}_e-\text{CH}})_2$ ), 2.96 (s, 3H,  $\text{N}^+-\underline{\text{CH}_3}$ ), 3.14 (t, *J*=8.5 Hz, 2H, alkyl- $\underline{\text{CH}_2}\text{N}^+$ ), 3.31 (br. s, 1H,  $\text{CH-OH} + \text{H}_2\text{O}$ ), 3.77 (s, 3H,  $\underline{\text{CH}_3-\text{O-Ar}}$ ), 3.80 (s, 2H,  $-\text{CH}_2-\underline{\text{CH}_2}\text{N}^+$ ), 3.90 (t, *J*=4.7 Hz, 1H,  $-\text{CH}_2)_2-\underline{\text{CH-OH}}$ ), 6.99 (d, *J*=8.5 Hz, 1H,  $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 7.11 (d, *J*=8.6 Hz, 1H,  $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz): δ ppm = 14.33 ( $\underline{\text{CH}_3-(\text{CH}_2)_{13}\text{N}^+}$ ), 22.04 ( $\text{CH}_3-\underline{\text{CH}_2-(\text{CH}_2)_{12}\text{N}^+}$ ), 22.47  $\text{CH}_3-(\text{CH}_2)_{10}-\underline{\text{CH}_2-(\text{CH}_2)_2\text{N}^+}$ , 25.07 ( $-\text{CH-CH}_2-\underline{\text{CH}_2-\text{CH}}$ ), 26.32 ( $\text{CH}_3-\text{CH}_2-\underline{\text{CH}_2-(\text{CH}_2)_{11}\text{N}^+}$ ), 28.98 ( $\text{CH}_3-(\text{CH}_2)_9-\underline{\text{CH}_2-(\text{CH}_2)_3\text{N}^+}$ ), 29.09 ( $\text{CH}_3-(\text{CH}_2)_2-\underline{\text{CH}_2-(\text{CH}_2)_{10}\text{N}^+}$ ), 29.22 ( $\text{CH}_3-(\text{CH}_2)_8-\underline{\text{CH}_2-(\text{CH}_2)_4\text{N}^+}$ ), 29.27 ( $\text{CH}_3-(\text{CH}_2)_3-\underline{\text{CH}_2-(\text{CH}_2)_9\text{N}^+}$ ), 29.33 ( $\text{CH}_3-(\text{CH}_2)_7-\underline{\text{CH}_2-(\text{CH}_2)_5\text{N}^+}$ ), 29.40 ( $\text{CH}_3-(\text{CH}_2)_4-\underline{\text{CH}_2-(\text{CH}_2)_9\text{N}^+}$ ), 29.42 ( $\text{CH}_3-(\text{CH}_2)_6-\underline{\text{CH}_2-(\text{CH}_2)_6\text{N}^+}$ ), 29.44 ( $\text{CH}_3-(\text{CH}_2)_5-\underline{\text{CH}_2-(\text{CH}_2)_7\text{N}^+}$ ), 31.68 ( $\text{CH}_3-(\text{CH}_2)_9-\underline{\text{CH}_2-\text{CH}_2\text{N}^+}$ ), 34.73 ( $-\underline{\text{CH}_2-\text{CH(OH)-CH}_2-}$ ), 59.37 ( $\underline{\text{CH}_3-\text{N}^+(\text{CH}-)_2}$ ), 60.68 ( $\text{CH}_3-(\text{CH}_2)_{12}-\underline{\text{CH}_2\text{N}^+}$ ), 61.18 ( $\underline{\text{CH}_3-\text{O-Ar}}$ ), 65.87 ( $-\text{CH}_2-\underline{\text{CH(OH)-CH}_2-}$ ), 125.31 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 125.45 ( $\underline{\text{CICCH=CHC(Cl)=CCOO}^-}$ ), 126.46 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 127.93 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 141.90 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 151.48 ( $\underline{\text{CH}_3-\text{O-C=CCI}}$ ), 165.09 ( $-\underline{\text{COO}^-}$ ).

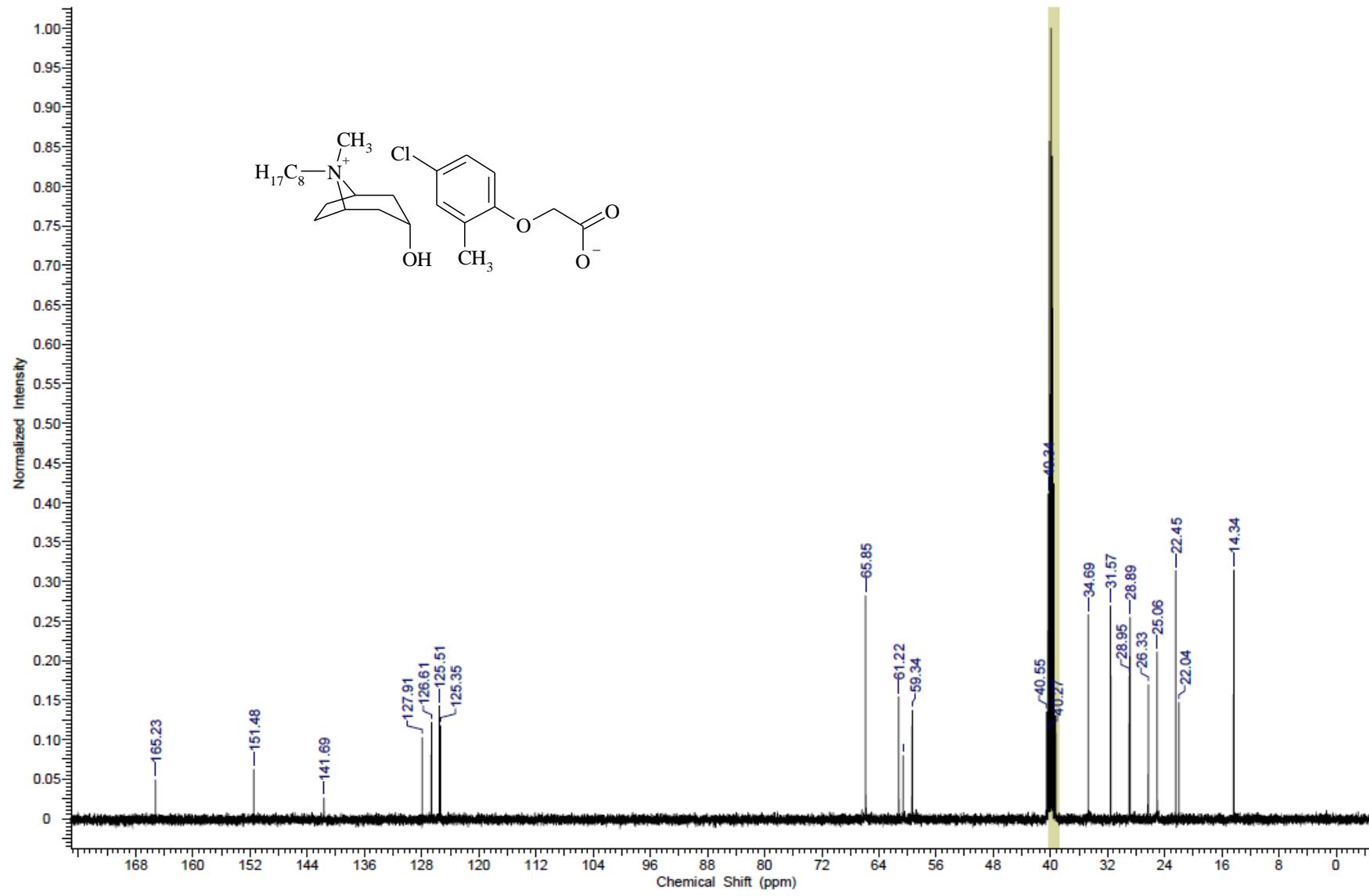
**N-hexadecyltropinium 3,6-dichloro-2-methoxybenzoate [QTS-C<sub>16</sub>][dicamba]** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ ppm = 0.85 (t, *J*=6.7 Hz, 3H,  $\underline{\text{CH}_3-\text{CH}_2}$ ), 1.24 (m, 26H,  $\text{CH}_3-(\underline{\text{CH}_2})_5^-$ ), 1.64 (q, *J*=4.2 Hz, 2H,  $-(\text{CH}_2)_5-\underline{\text{CH}_2-}$ ), 1.80 (d, *J*=16.3 Hz, 2H,  $\text{HO-CH-(CH}_a\underline{\text{H}_e-\text{CH}})_2$ ), 2.19 (t, *J*=4.9 Hz, 2H,  $-\underline{\text{CH}_e\text{H}_a-\text{CH}})_2-\text{N}^+$ ), 2.34 (d, *J*=16.3 Hz, 2H,  $-\underline{\text{CH}_e\text{H}_a-\text{CH}})_2-\text{N}^+$ ), 2.38 (d, *J*=8.0 Hz, 2H,  $\text{HO-CH-(CH}_a\underline{\text{H}_e-\text{CH}})_2$ ), 2.98 (s, 3H,  $\text{N}^+-\underline{\text{CH}_3}$ ), 3.16 (t, *J*=8.1 Hz, 2H, alkyl- $\underline{\text{CH}_2}\text{N}^+$ ), 3.34 (s, 1H,  $\text{CH-OH} + \text{H}_2\text{O}$ ), 3.79 (s, 3H,  $\underline{\text{CH}_3-\text{O-Ar}}$ ), 3.81 (s, 2H,  $-\text{CH}_2-\underline{\text{CH}})_2-\text{N}^+$ ), 3.91 (t, *J*=5.0 Hz, 1H,  $-\text{CH}_2)_2-\underline{\text{CH-OH}}$ ), 7.01 (d, *J*=8.7 Hz, 1H,  $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 7.13 (d, *J*=8.4 Hz, 1H,  $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz): δ ppm = 13.95 ( $\underline{\text{CH}_3-(\text{CH}_2)_{13}\text{N}^+}$ ), 21.66 ( $\text{CH}_3-\underline{\text{CH}_2-(\text{CH}_2)_{14}\text{N}^+}$ ), 22.10 ( $\text{CH}_3-(\text{CH}_2)_{12}-\underline{\text{CH}_2-(\text{CH}_2)_2\text{N}^+}$ ), 24.67 ( $-\text{CH-CH}_2-\underline{\text{CH}_2-\text{CH}}$ ), 26.15 ( $\text{CH}_3-\text{CH}_2-\underline{\text{CH}_2-(\text{CH}_2)_{11}\text{N}^+}$ ), 28.63 ( $\text{CH}_3-(\text{CH}_2)_{11}-\underline{\text{CH}_2-(\text{CH}_2)_3\text{N}^+}$ ), 28.65 ( $\text{CH}_3-(\text{CH}_2)_2-\underline{\text{CH}_2-(\text{CH}_2)_{12}\text{N}^+}$ ), 28.72 ( $\text{CH}_3-(\text{CH}_2)_{10}-\underline{\text{CH}_2-(\text{CH}_2)_4\text{N}^+}$ ), 28.87 ( $\text{CH}_3-(\text{CH}_2)_3-\underline{\text{CH}_2-(\text{CH}_2)_{11}\text{N}^+}$ ), 29.92 ( $\text{CH}_3-(\text{CH}_2)_9-\underline{\text{CH}_2-(\text{CH}_2)_5\text{N}^+}$ ), 28.97 ( $\text{CH}_3-(\text{CH}_2)_4-\underline{\text{CH}_2-(\text{CH}_2)_{10}\text{N}^+}$ ), 29.04 ( $\text{CH}_3-(\text{CH}_2)_8-\underline{\text{CH}_2-(\text{CH}_2)_6\text{N}^+}$ ), 29.07 ( $\text{CH}_3-(\text{CH}_2)_5-\underline{\text{CH}_2-(\text{CH}_2)_3-\text{N}^+}$ ), 31.31, ( $\text{CH}_3-(\text{CH}_2)_{13}-\underline{\text{CH}_2-\text{CH}_2\text{N}^+}$ ), 34.30 ( $-\underline{\text{CH}_2-\text{CH(OH)-CH}_2-}$ ), 58.96 ( $\underline{\text{CH}_3-\text{N}^+(\text{CH}-)_2}$ ), 60.23 ( $\text{CH}_3-(\text{CH}_2)_{14}-\underline{\text{CH}_2\text{N}^+}$ ), 60.81 ( $\underline{\text{CH}_3-\text{O-Ar}}$ ), 65.45 ( $-\text{CH}_2-\underline{\text{CH(OH)-CH}_2-}$ ), 124.96 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 125.10 ( $\underline{\text{CICCH=CHC(Cl)=CCOO}^-}$ ), 126.17 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 127.51 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 141.39 ( $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 151.07 ( $\underline{\text{CH}_3-\text{O-C=CCI}}$ ), 164.86 ( $-\underline{\text{COO}^-}$ ).

**N-octadecyltropinium 3,6-dichloro-2-methoxybenzoate [QTS-C<sub>18</sub>][dicamba]** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ ppm = 0.84 (t, *J*=6.7 Hz, 3H,  $\underline{\text{CH}_3-\text{CH}_2}$ ), 1.22 (m, 30H,  $\text{CH}_3-(\underline{\text{CH}_2})_5^-$ ), 1.63 (q, *J*=4.2 Hz, 2H,  $-(\text{CH}_2)_5-\underline{\text{CH}_2-}$ ), 1.79 (d, *J*=16.1 Hz, 2H,  $\text{HO-CH-(CH}_a\underline{\text{H}_e-\text{CH}})_2$ ), 2.18 (t, *J*=4.9 Hz, 2H,  $-\underline{\text{CH}_e\text{H}_a-\text{CH}})_2-\text{N}^+$ ), 2.36 (d, *J*=16.7 Hz, 2H,  $-\underline{\text{CH}_e\text{H}_a-\text{CH}})_2-\text{N}^+$ ), 2.37 (d, *J*=7.6 Hz, 2H,  $\text{HO-CH-(CH}_a\underline{\text{H}_e-\text{CH}})_2$ ), 2.97 (s, 3H,  $\text{N}^+-\underline{\text{CH}_3}$ ), 3.14 (t, *J*=8.3 Hz, 2H, alkyl- $\underline{\text{CH}_2}\text{N}^+$ ), 3.32 (s, 1H,  $\text{CH-OH} + \text{H}_2\text{O}$ ), 3.77 (s, 3H,  $\underline{\text{CH}_3-\text{O-Ar}}$ ), 3.78 (s, 2H,  $-\text{CH}_2-\underline{\text{CH}})_2-\text{N}^+$ ), 3.90 (t, *J*=5.0 Hz, 1H,  $-\text{CH}_2)_2-\underline{\text{CH-OH}}$ ), 6.99 (d, *J*=8.6 Hz, 1H,  $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ), 7.11 (d, *J*=8.5 Hz, 1H,  $\text{CICCH}=\underline{\text{CHC(Cl)=CCOO}^-}$ ); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz): δ ppm = 14.32 ( $\underline{\text{CH}_3-(\text{CH}_2)_{15}\text{N}^+}$ ), 22.04 ( $\text{CH}_3-\underline{\text{CH}_2-(\text{CH}_2)_{16}\text{N}^+}$ ), 22.48 ( $\text{CH}_3-(\text{CH}_2)_{14}-\underline{\text{CH}_2-(\text{CH}_2)_2\text{N}^+}$ ), 24.84 ( $-\text{CH-CH}_2-\underline{\text{CH}_2-\text{CH}}$ ), 25.07 ( $\text{CH}_3-\text{CH}_2-\underline{\text{CH}_2-(\text{CH}_2)_{15}\text{N}^+}$ ), 26.33 ( $\text{CH}_3-(\text{CH}_2)_{13}-\underline{\text{CH}_2-(\text{CH}_2)_3\text{N}^+}$ ), 29.00 ( $\text{CH}_3-(\text{CH}_2)_2-\underline{\text{CH}_2-(\text{CH}_2)_{14}\text{N}^+}$ ), 29.09 ( $\text{CH}_3-(\text{CH}_2)_{12}-\underline{\text{CH}_2-(\text{CH}_2)_4\text{N}^+}$ ), 29.24 ( $\text{CH}_3-(\text{CH}_2)_3-\underline{\text{CH}_2-(\text{CH}_2)_{13}\text{N}^+}$ ), 29.29 ( $\text{CH}_3-(\text{CH}_2)_{11}-\underline{\text{CH}_2-(\text{CH}_2)_5\text{N}^+}$ ), 29.34 ( $\text{CH}_3-(\text{CH}_2)_4-$

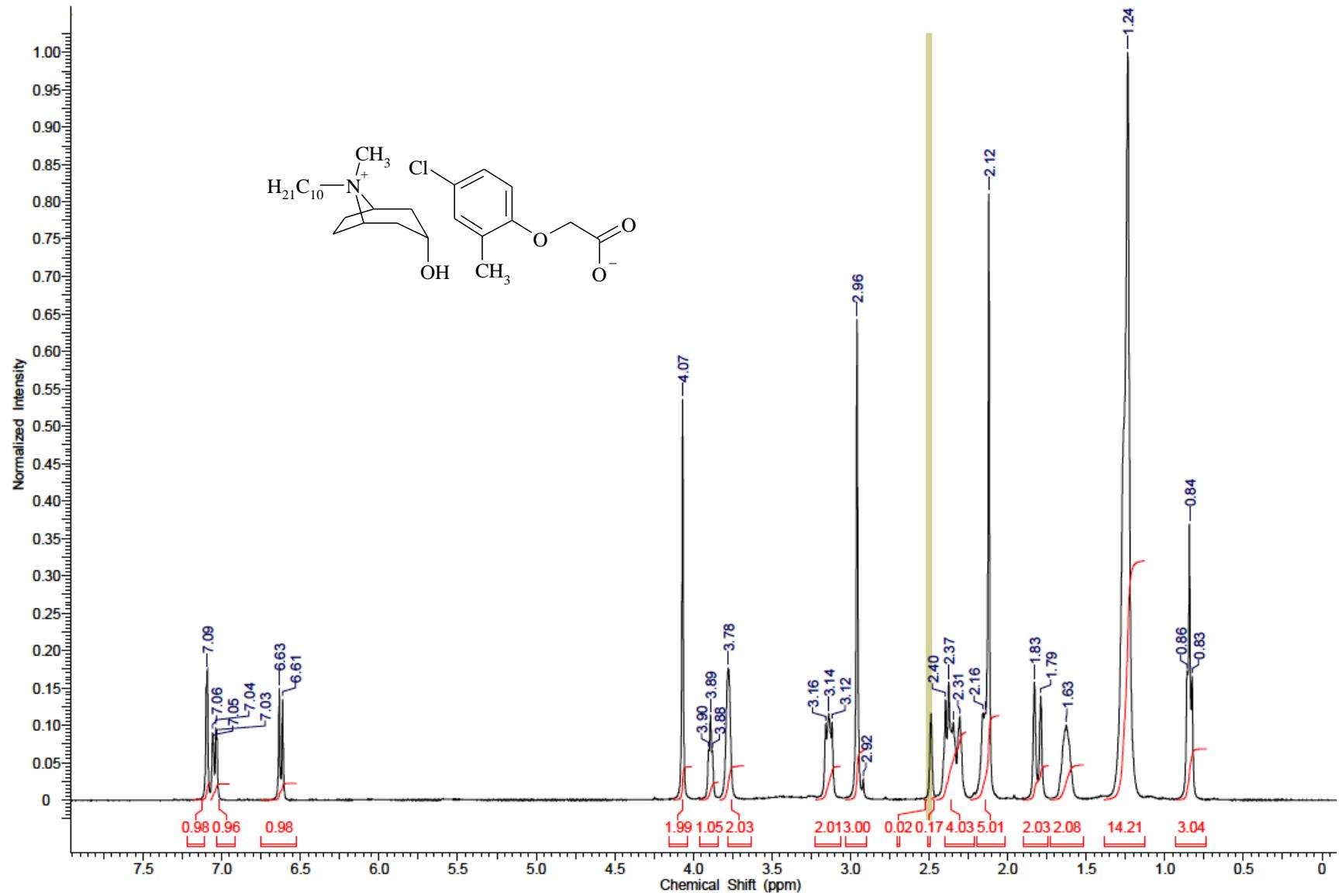
CH<sub>2</sub>-(CH<sub>2</sub>)<sub>12</sub>-N<sup>+</sup>), 29.39 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>5</sub>-CH<sub>2</sub>-(CH<sub>2</sub>)<sub>3</sub>-(CH<sub>2</sub>)<sub>2</sub>-(CH<sub>2</sub>)<sub>6</sub>-N<sup>+</sup>), 29.44 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>6</sub>-(CH<sub>2</sub>)<sub>3</sub>-(CH<sub>2</sub>)<sub>8</sub>-N<sup>+</sup>), 31.68 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>15</sub>-CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 34.72 (-CH<sub>2</sub>-CH(OH)-CH<sub>2</sub>-), 59.37 (CH<sub>3</sub>-N<sup>+</sup>(CH-)<sub>2</sub>), 60.66 (CH<sub>3</sub>-(CH<sub>2</sub>)<sub>16</sub>-CH<sub>2</sub>-N<sup>+</sup>), 61.18 (CH<sub>3</sub>-O-Ar), 65.86 (-CH<sub>2</sub>-CH(OH)-CH<sub>2</sub>-), 125.31 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 125.45 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 126.45 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 127.93 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 141.91 (CICCH=CHC(Cl)=CCOO<sup>-</sup>), 151.46 (CH<sub>3</sub>-O-C=CCl), 165.01 (-COO<sup>-</sup>).



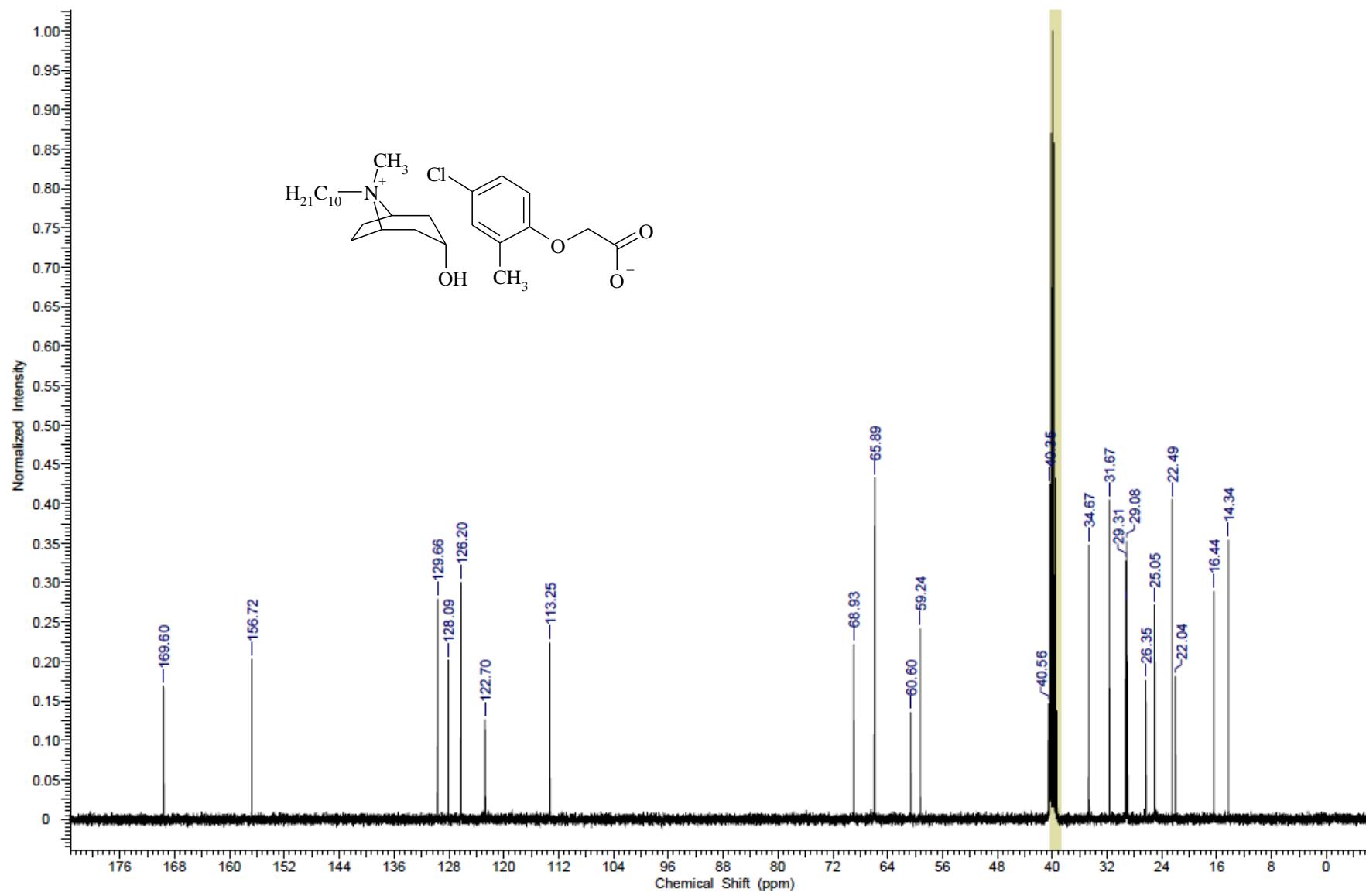
**Fig. S1** <sup>1</sup>H NMR spectrum of [QTS-C<sub>8</sub>][MCPA].



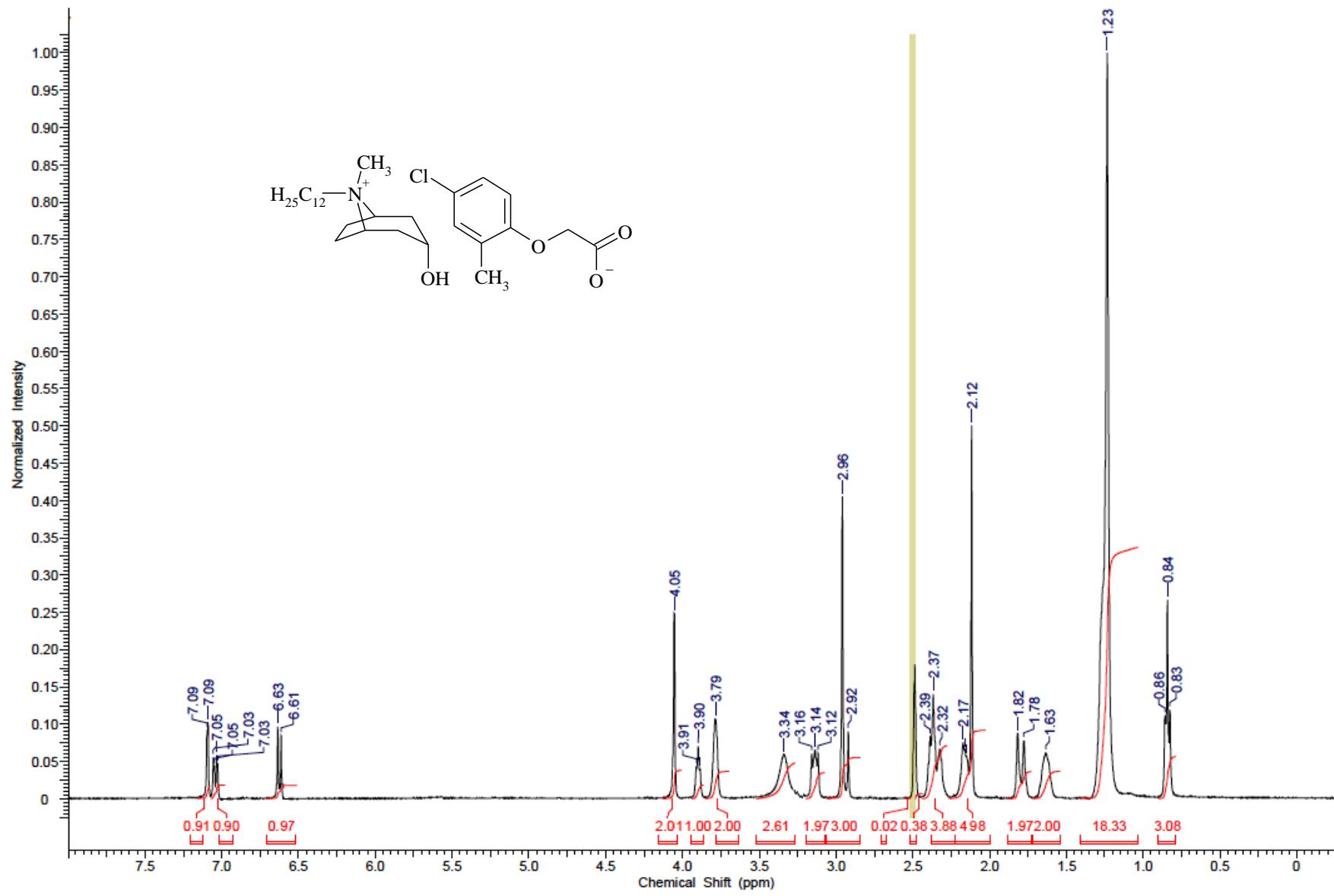
**Fig. S2**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_8][\text{MCPA}]$ .



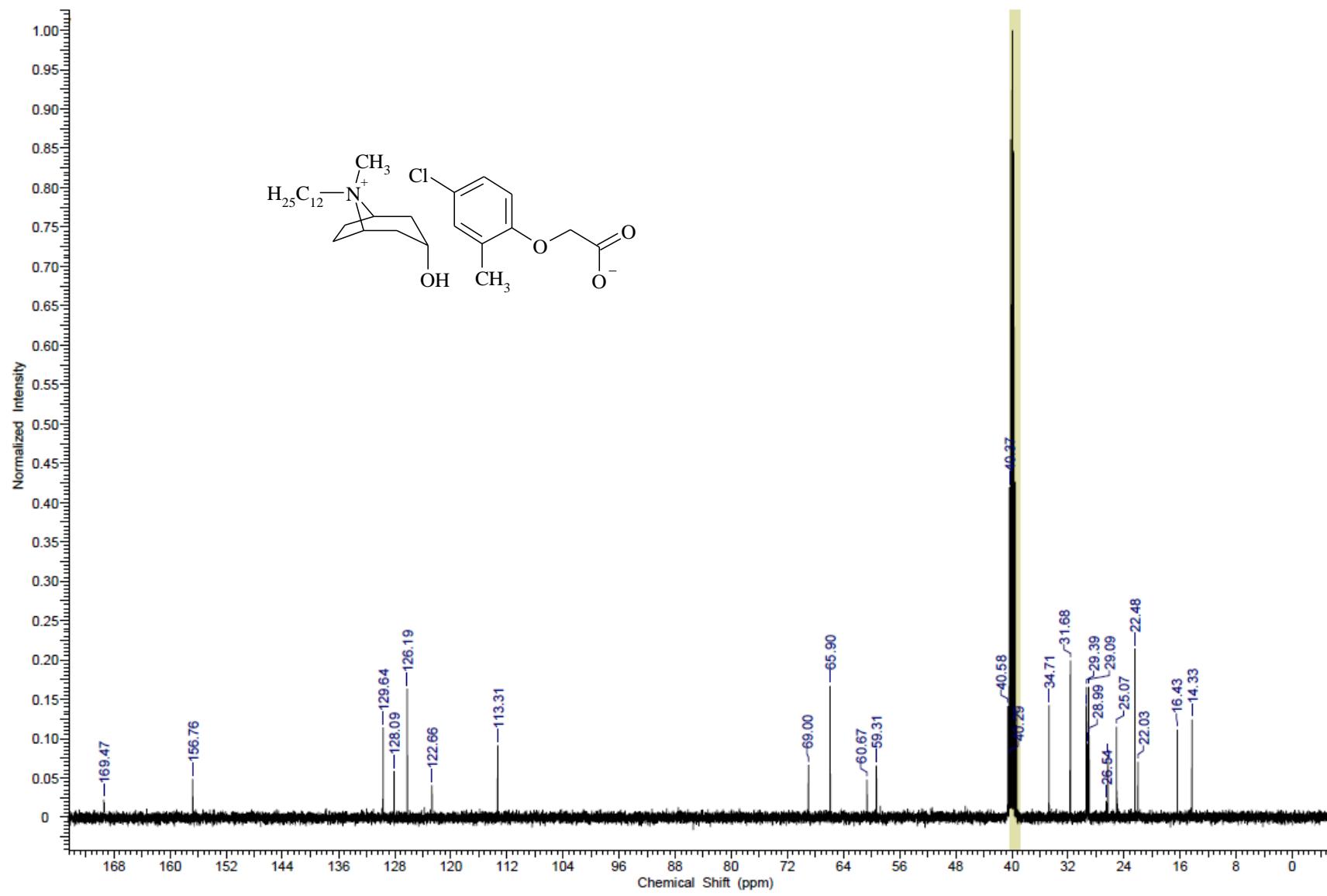
**Fig. S3**  $^1\text{H}$  NMR spectrum of  $[\text{QTS-C}_{10}][\text{MCPA}]$ .



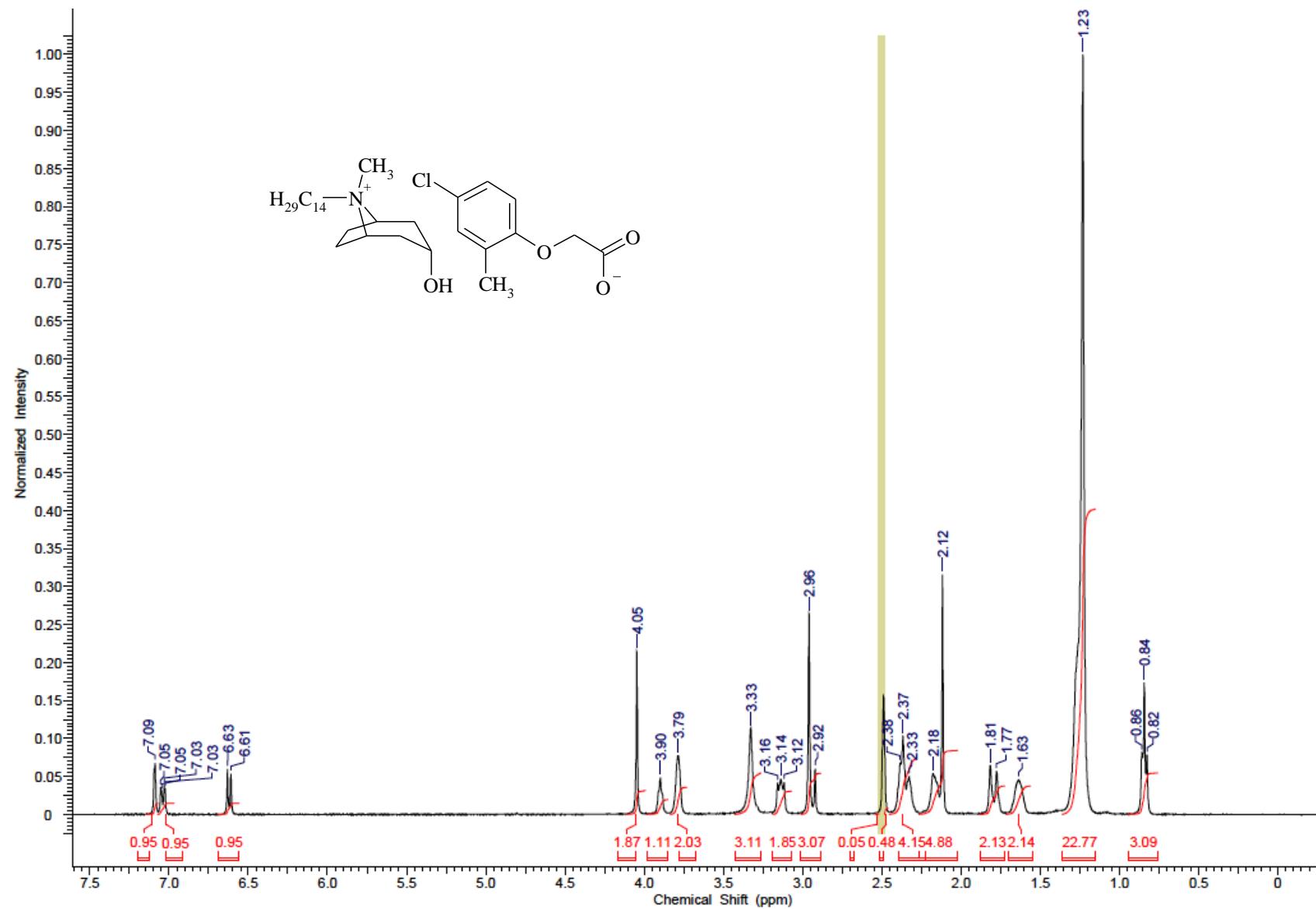
**Fig. S4**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_{10}][\text{MCPA}]$ .



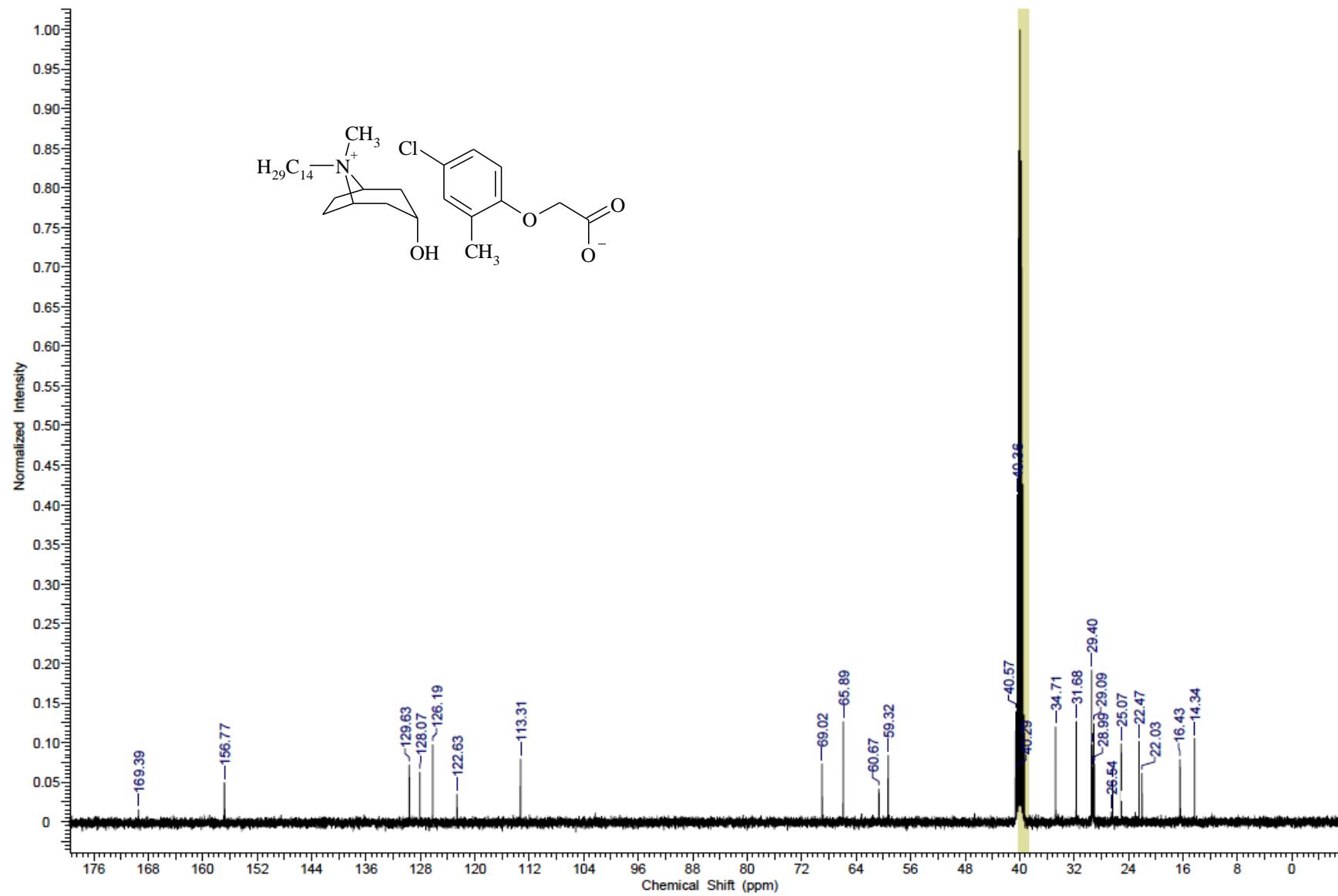
**Fig. S5**  $^1\text{H}$  NMR spectrum of [QTS-C<sub>12</sub>][MCPA].



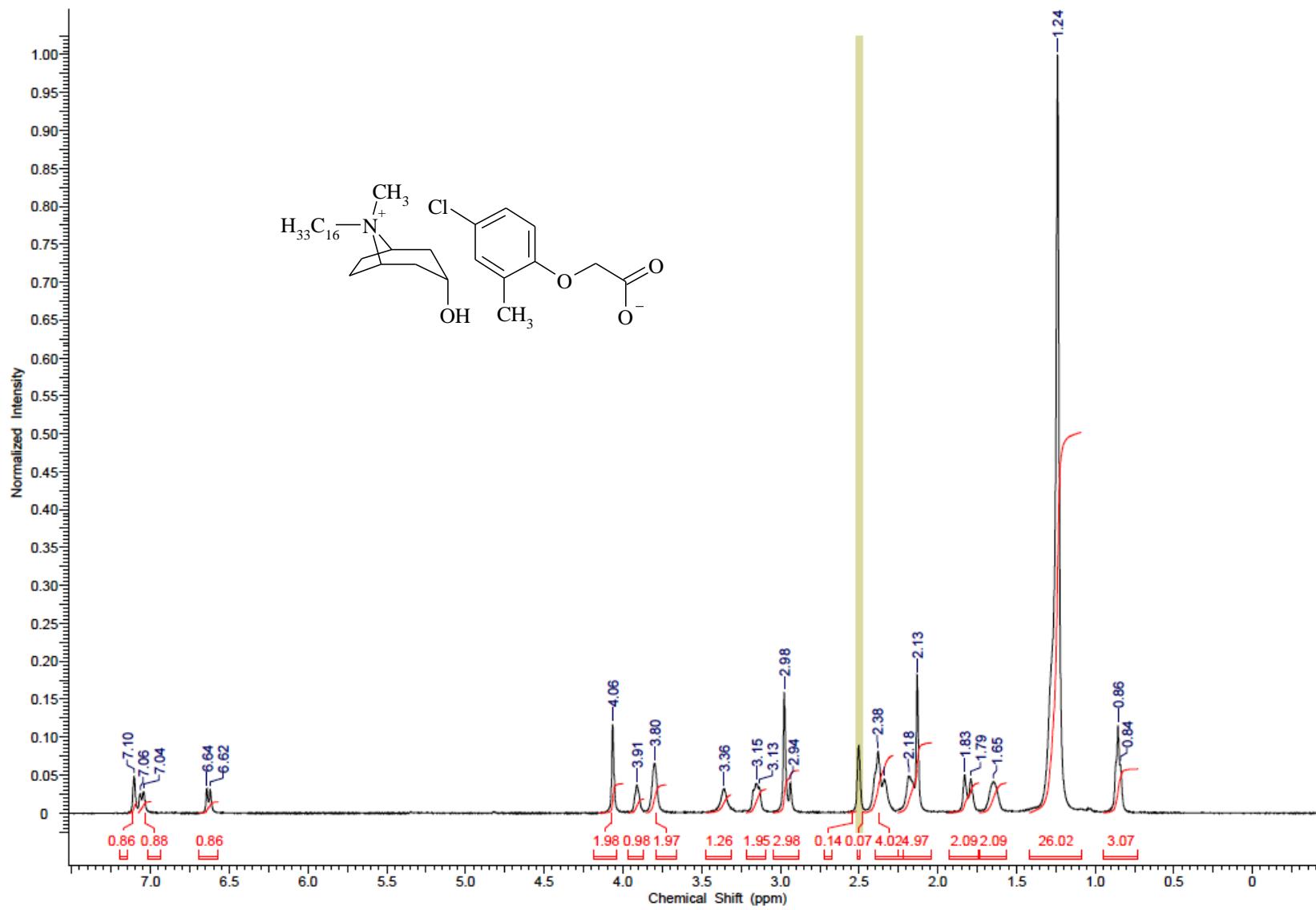
**Fig. S6**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_{12}][\text{MCPA}]$ .



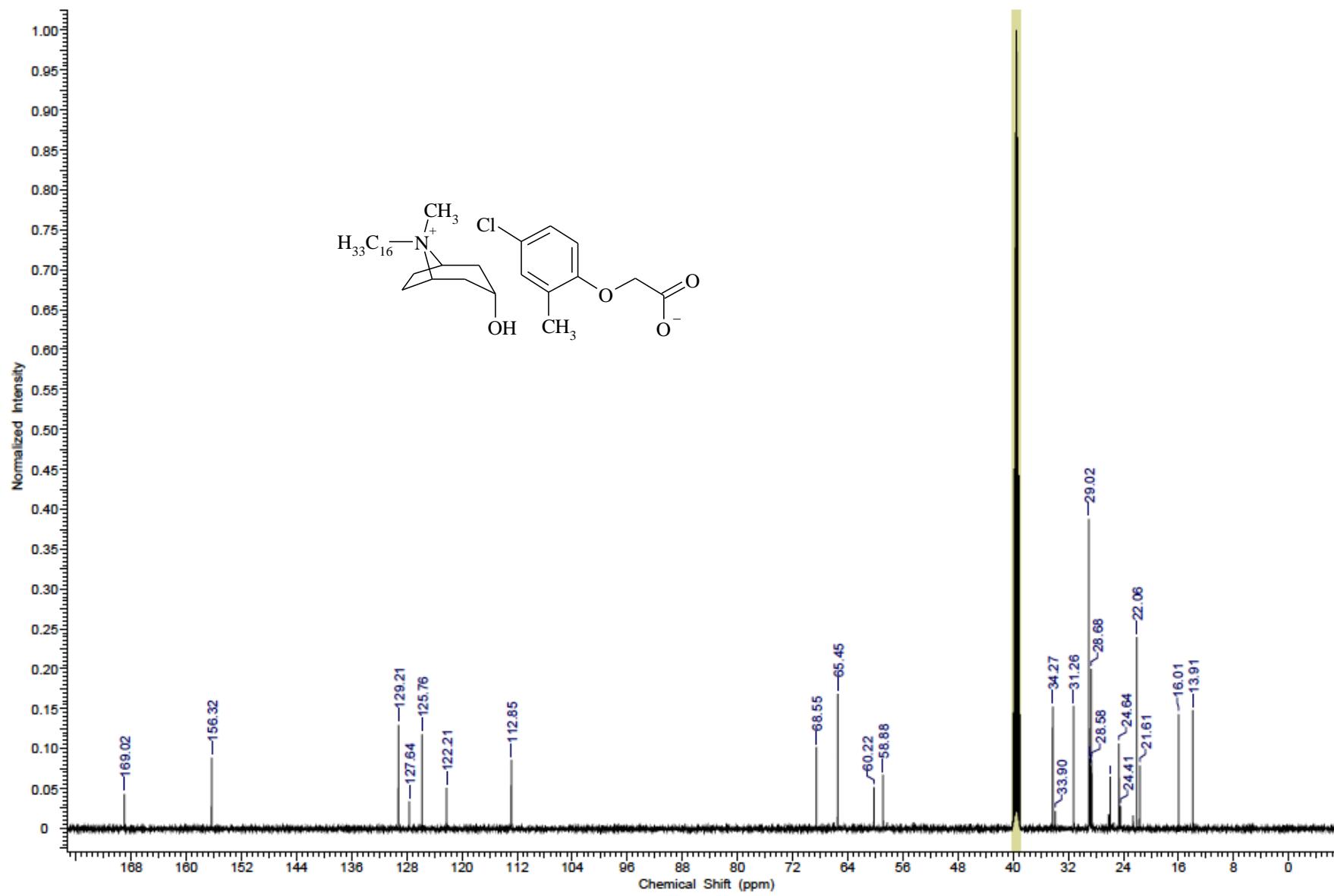
**Fig. S7** <sup>1</sup>H NMR spectrum of [QTS-C<sub>14</sub>][MCPA].



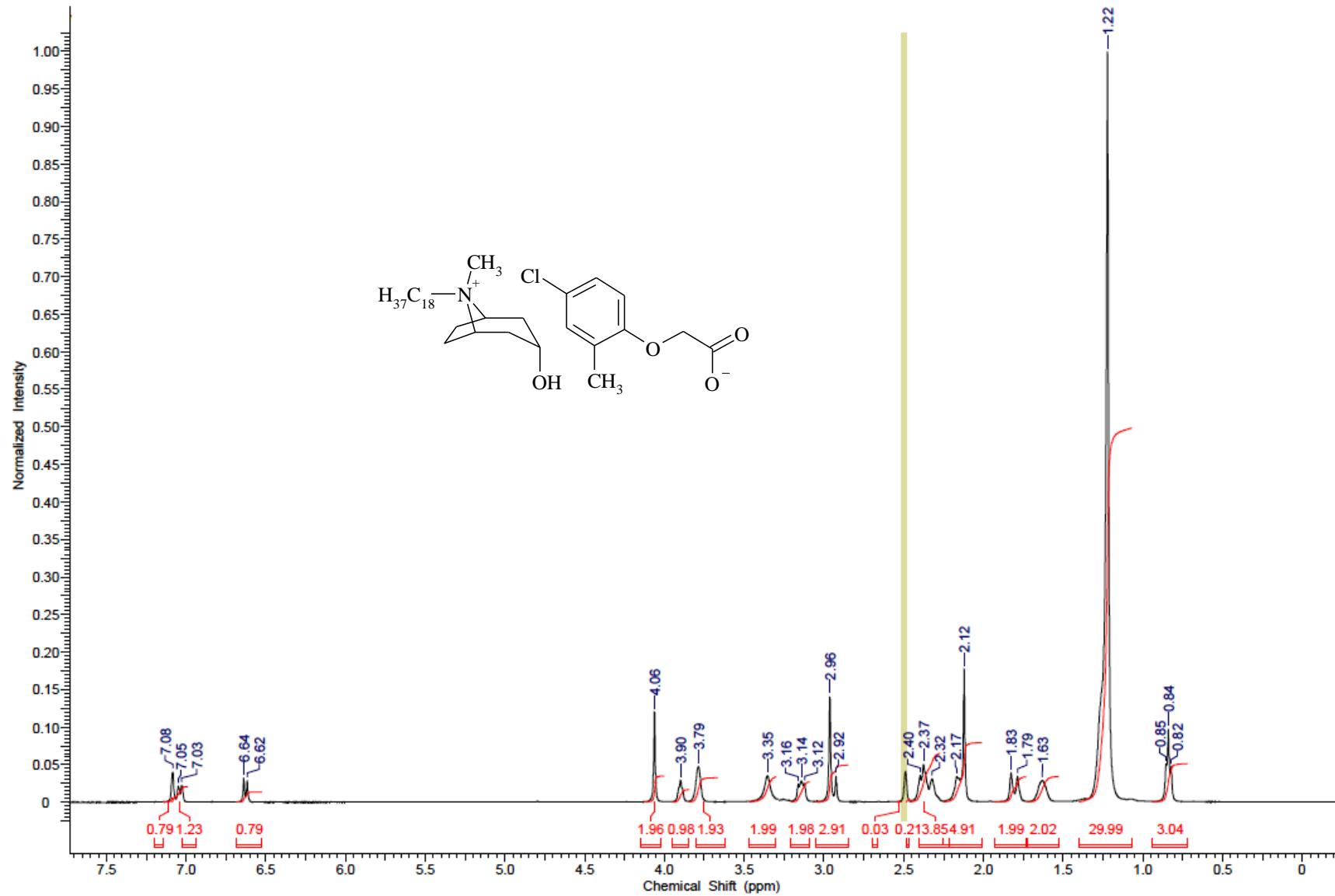
**Fig. S8**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_{14}][\text{MCPA}]$ .



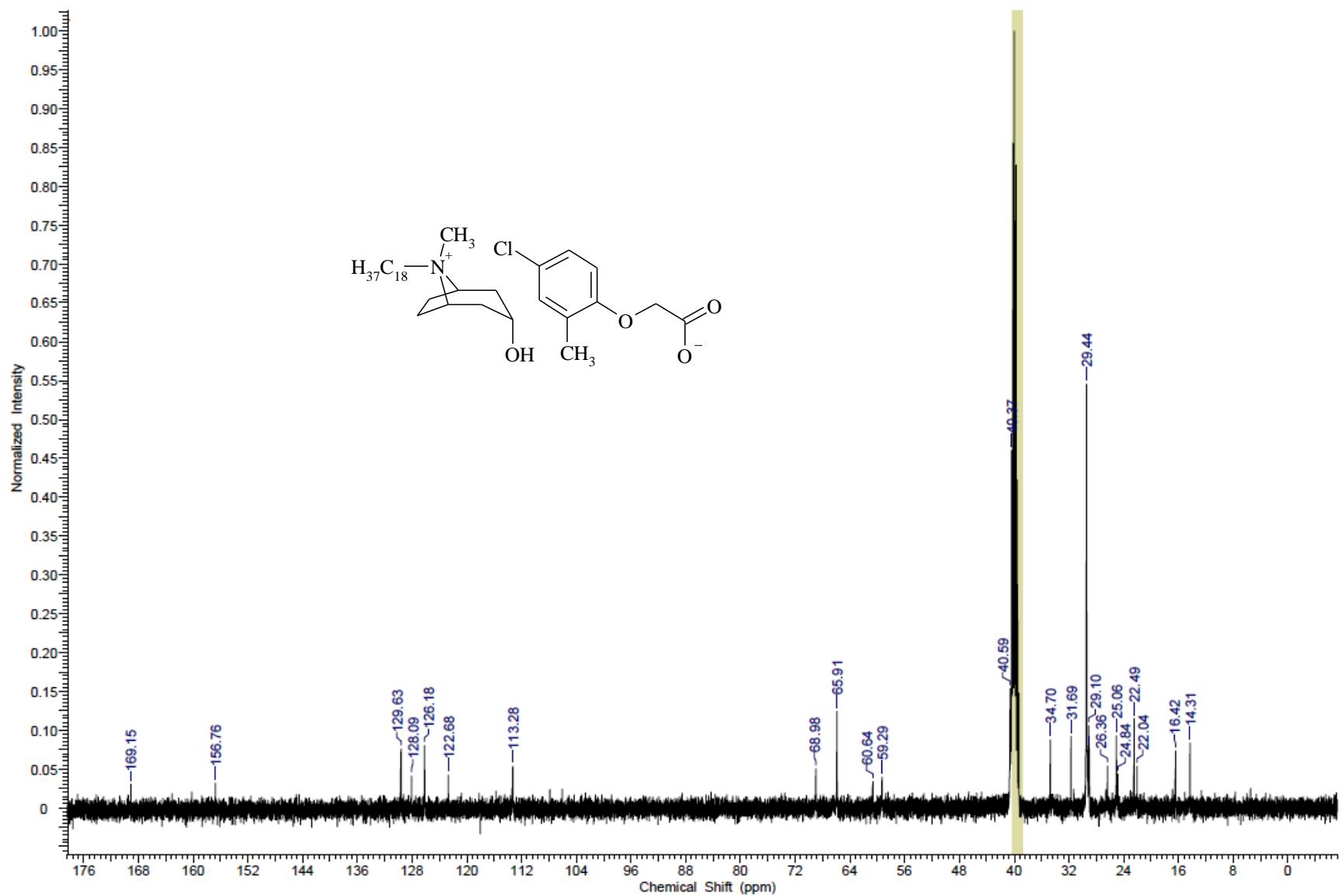
**Fig. S9**  $^1\text{H}$  NMR spectrum of [QTS-C<sub>16</sub>][MCPA].



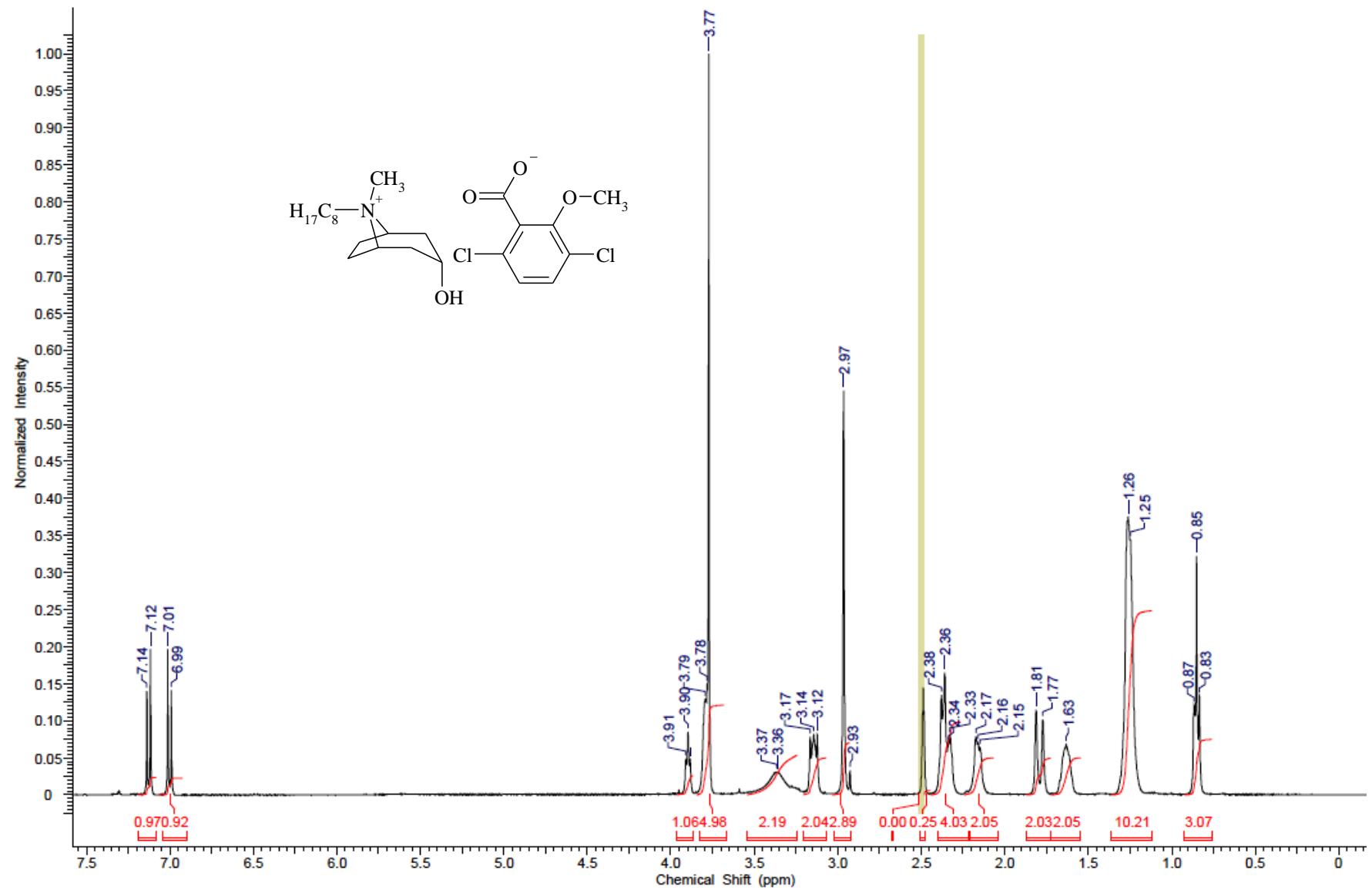
**Fig. S10**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_{16}][\text{MCPA}]$ .



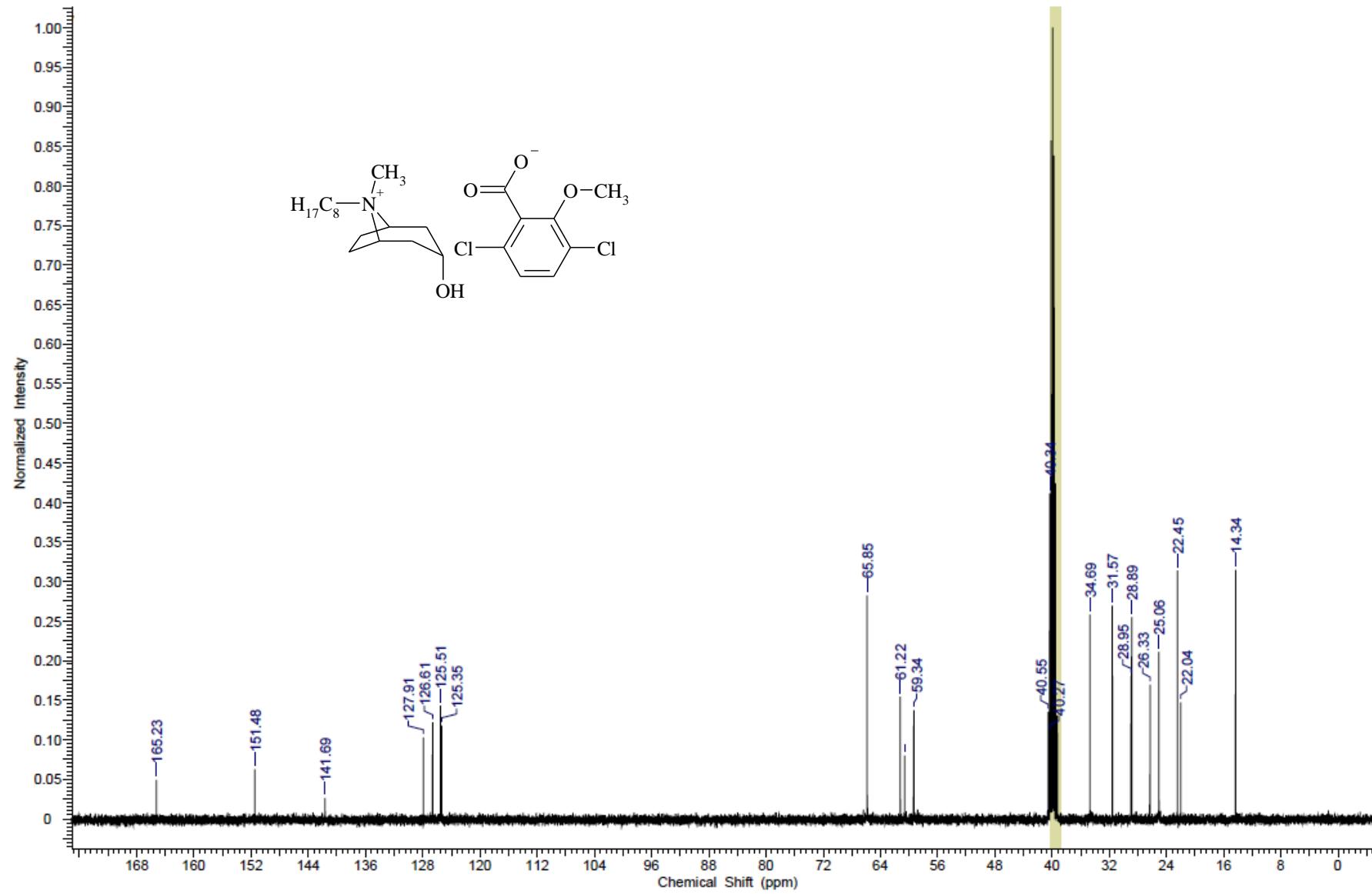
**Fig. S11**  $^1\text{H}$  NMR spectrum of  $[\text{QTS-C}_{18}][\text{MCPA}]$ .



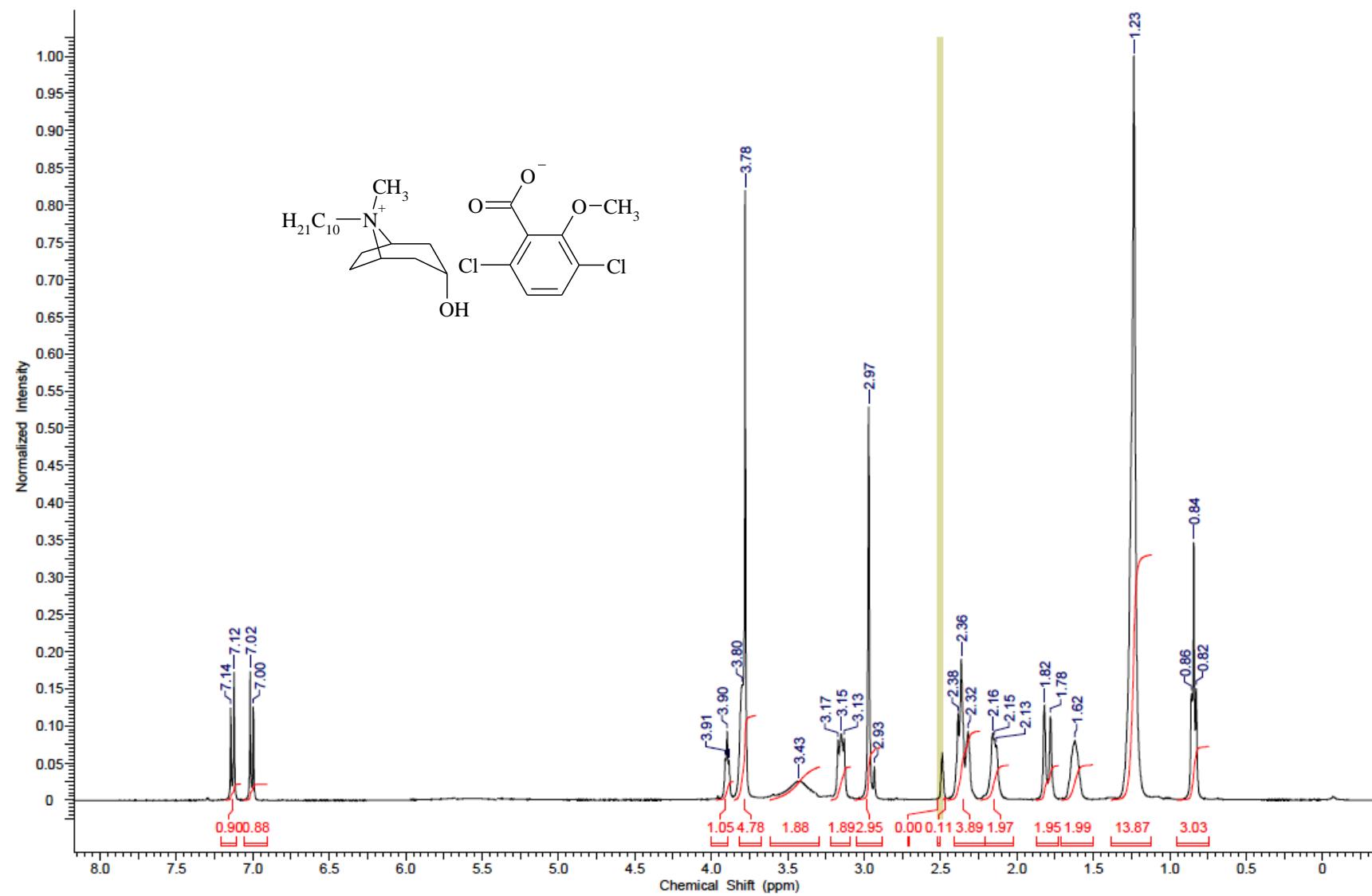
**Fig. S12**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_{18}][\text{MCPA}]$ .



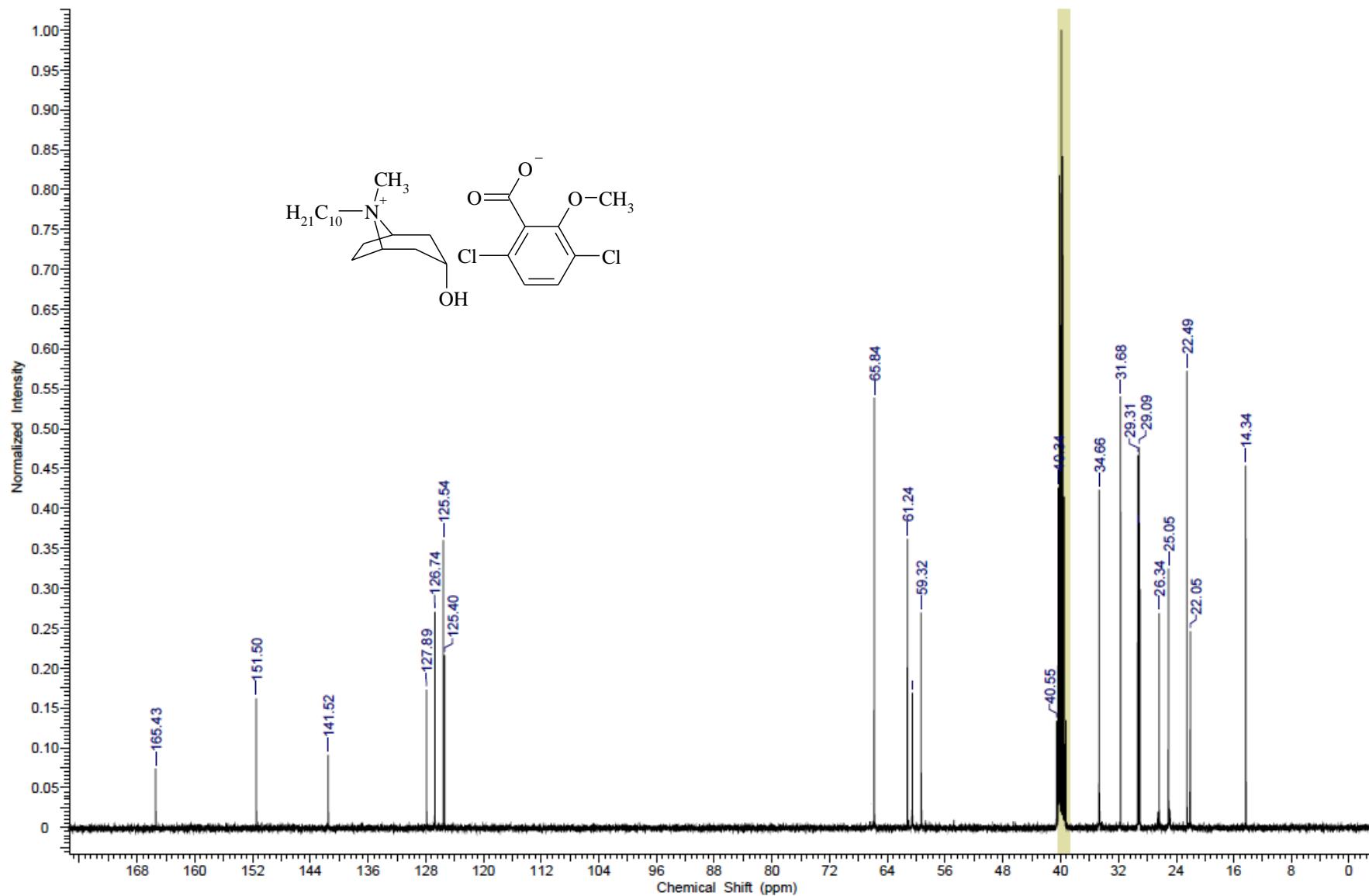
**Fig. S13** <sup>1</sup>H NMR spectrum of [QTS-C<sub>8</sub>][dicamba].



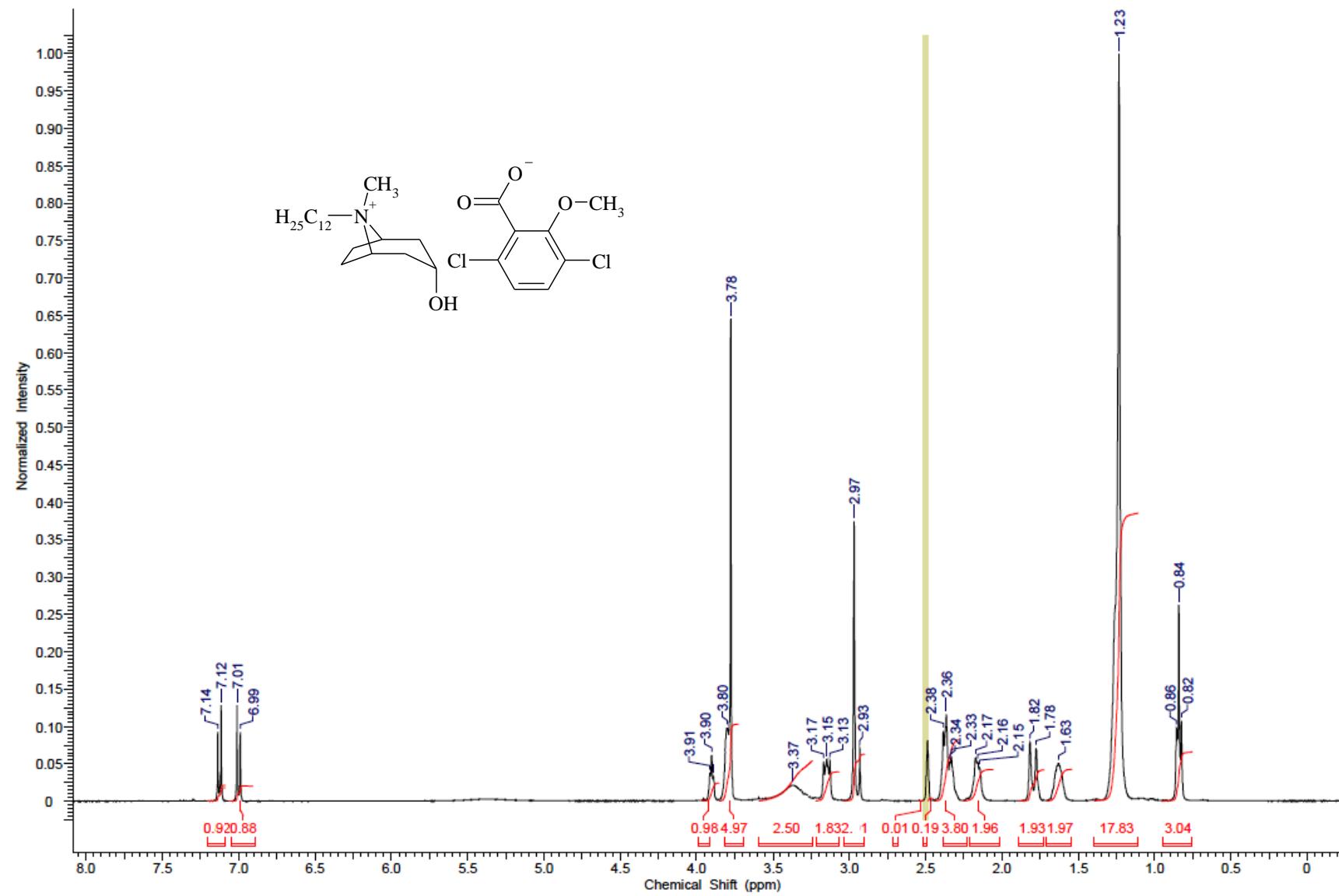
**Fig. S14**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_8][\text{dicamba}]$ .



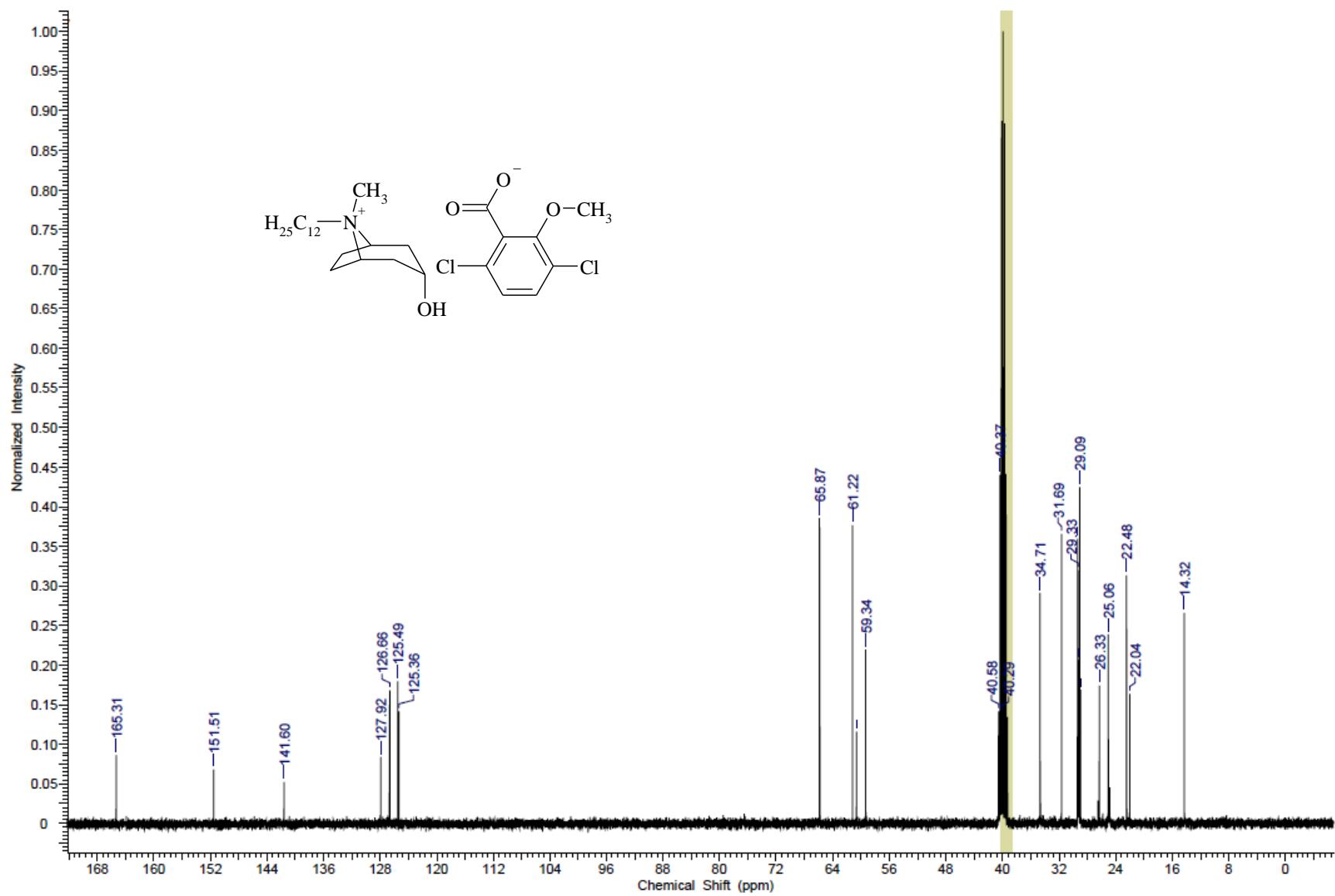
**Fig. S15**  $^1\text{H}$  NMR spectrum of  $[\text{QTS-C}_{10}][\text{dicamba}]$ .



**Fig. S16**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_{10}][\text{dicamba}]$ .



**Fig. S17**  $^1\text{H}$  NMR spectrum of  $[\text{QTS-}\text{C}_{12}][\text{dicamba}]$ .



**Fig. S18**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_{12}][\text{dicamba}]$ .

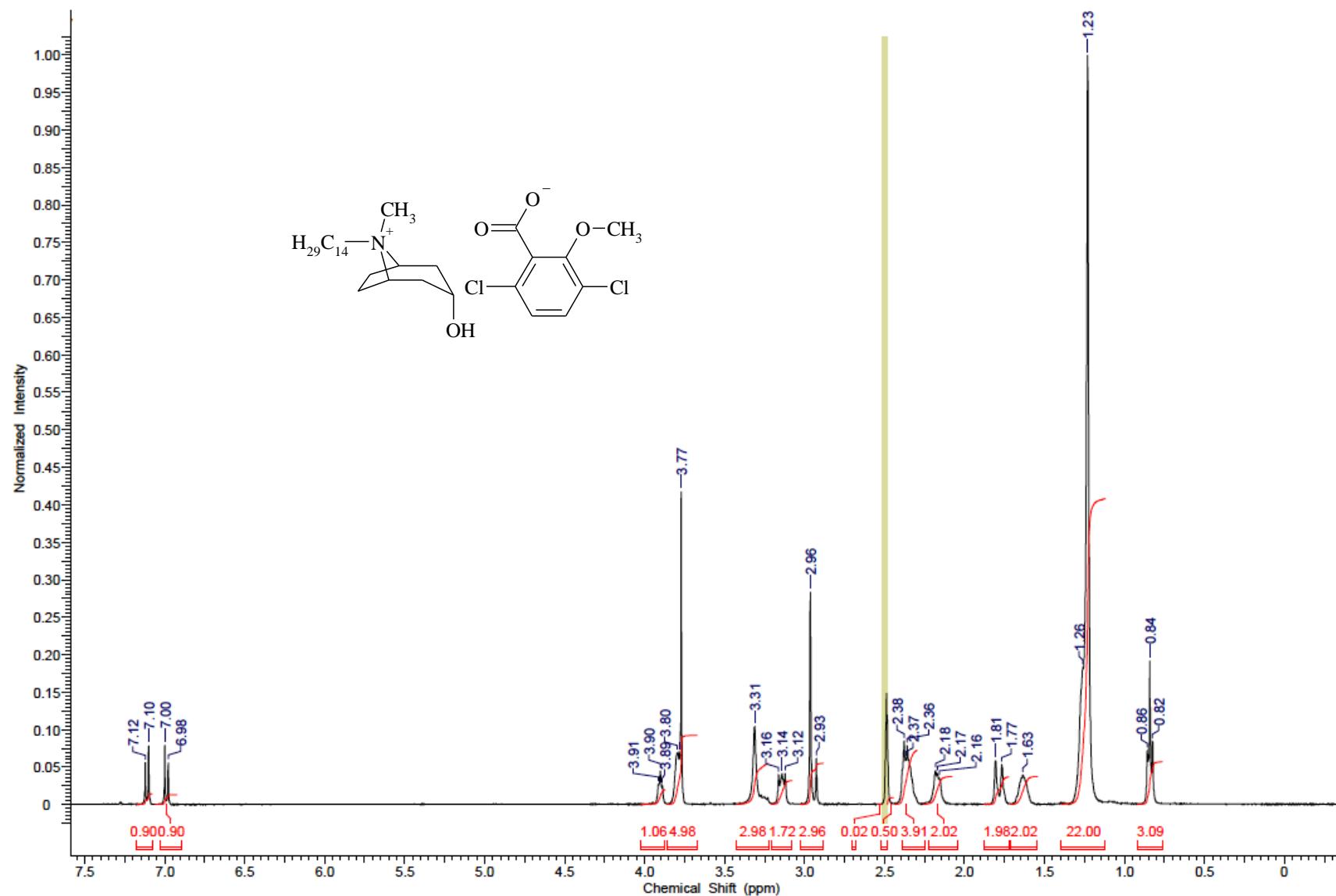
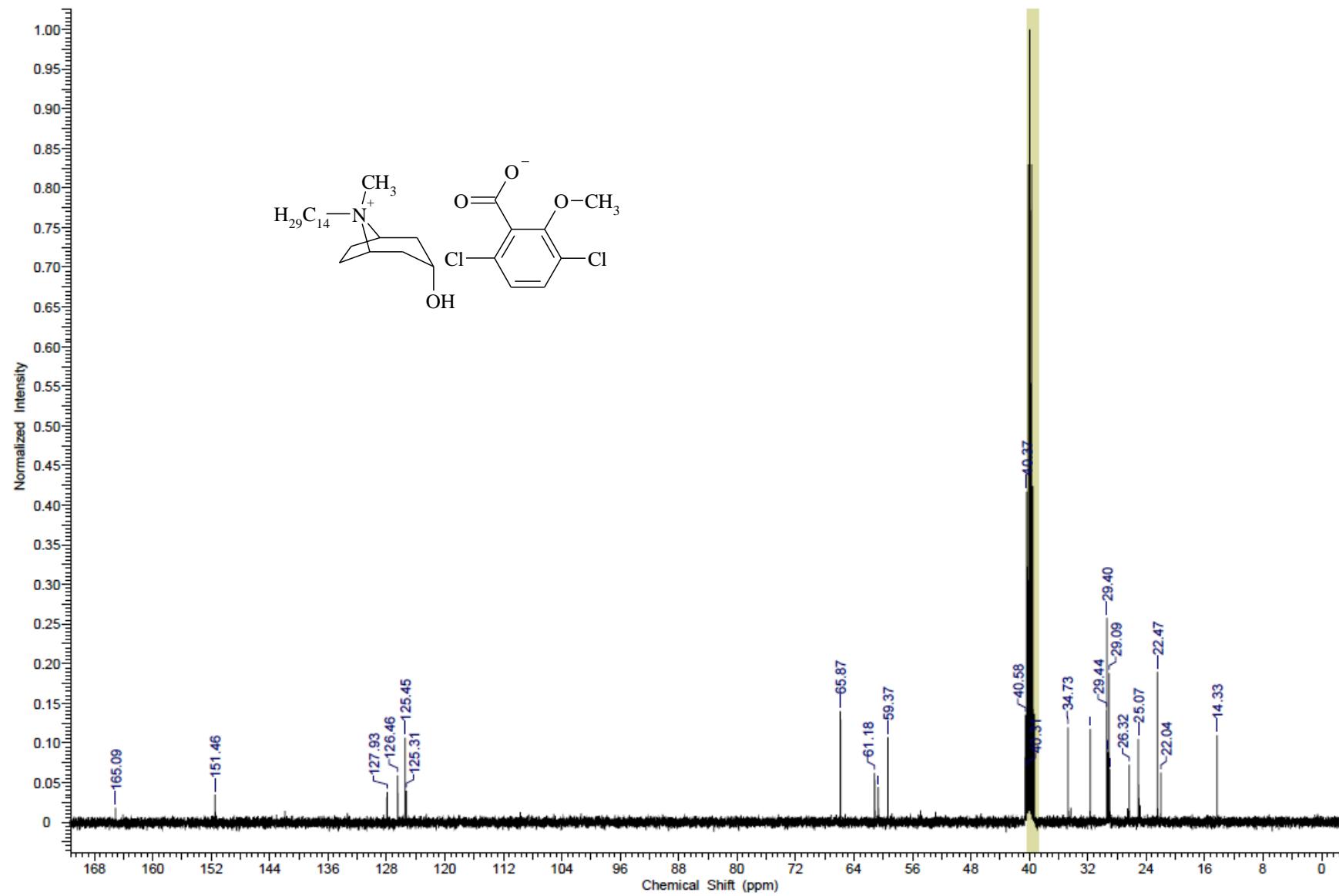
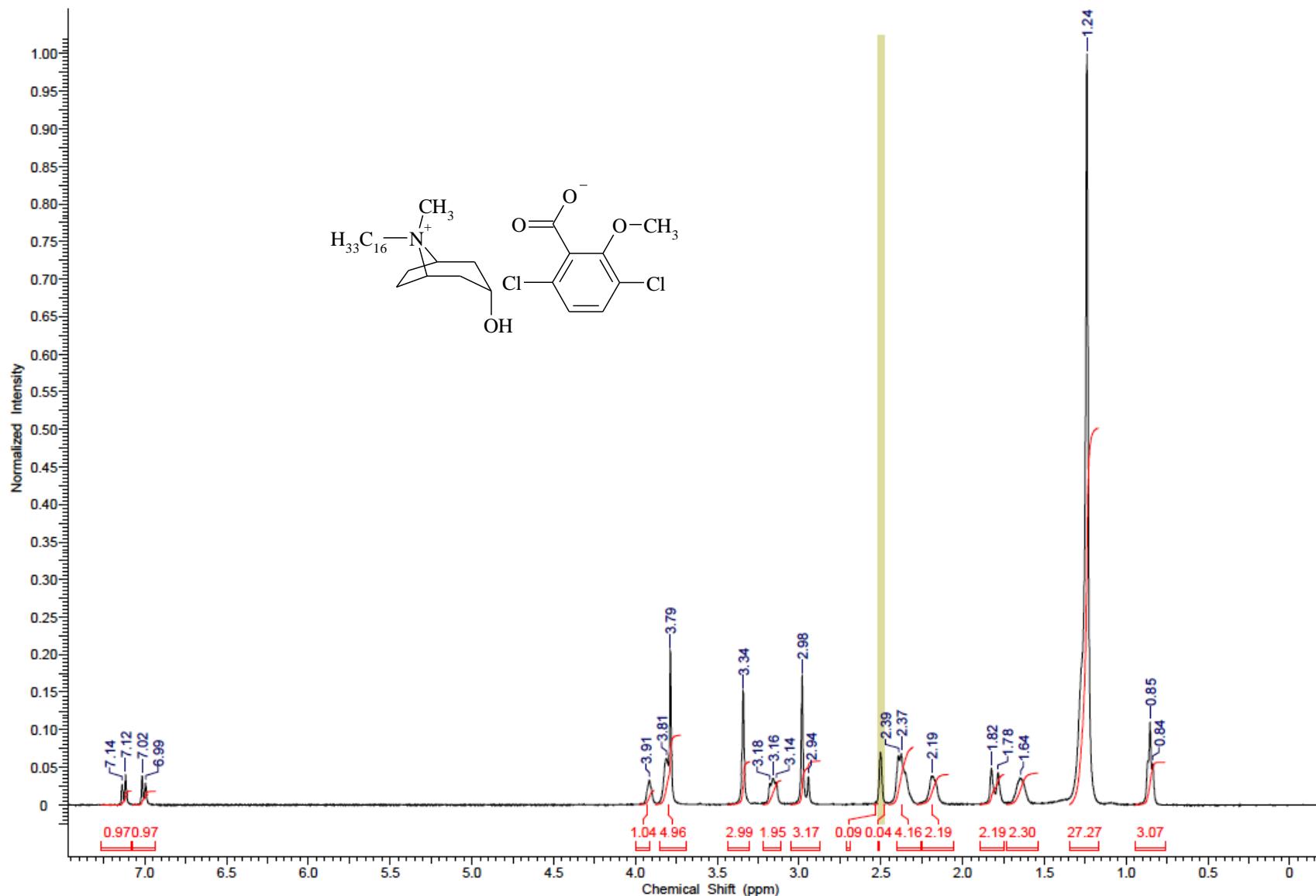


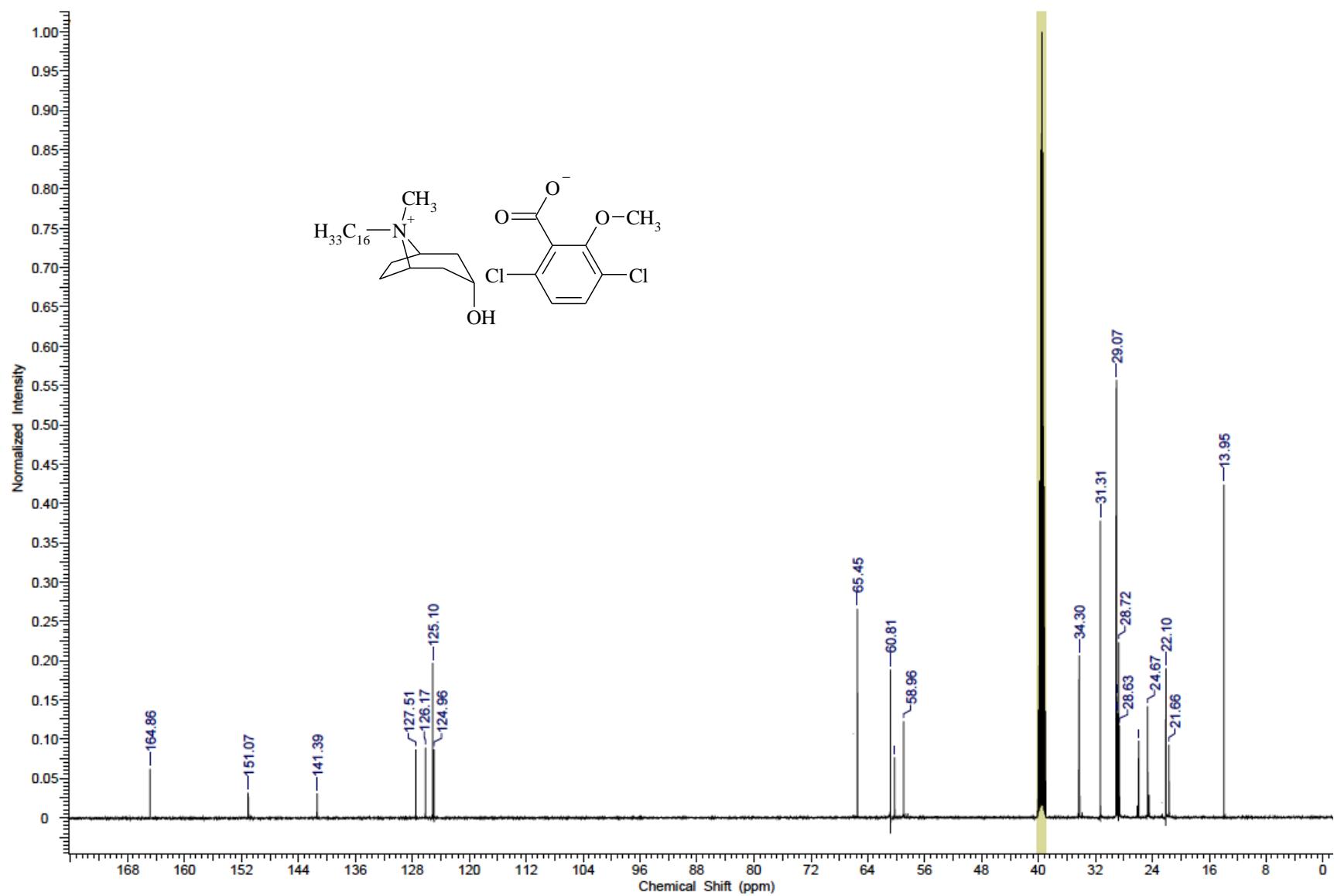
Fig. S19  $^1\text{H}$  NMR spectrum of  $[\text{QTS-C}_{14}][\text{dicamba}]$ .



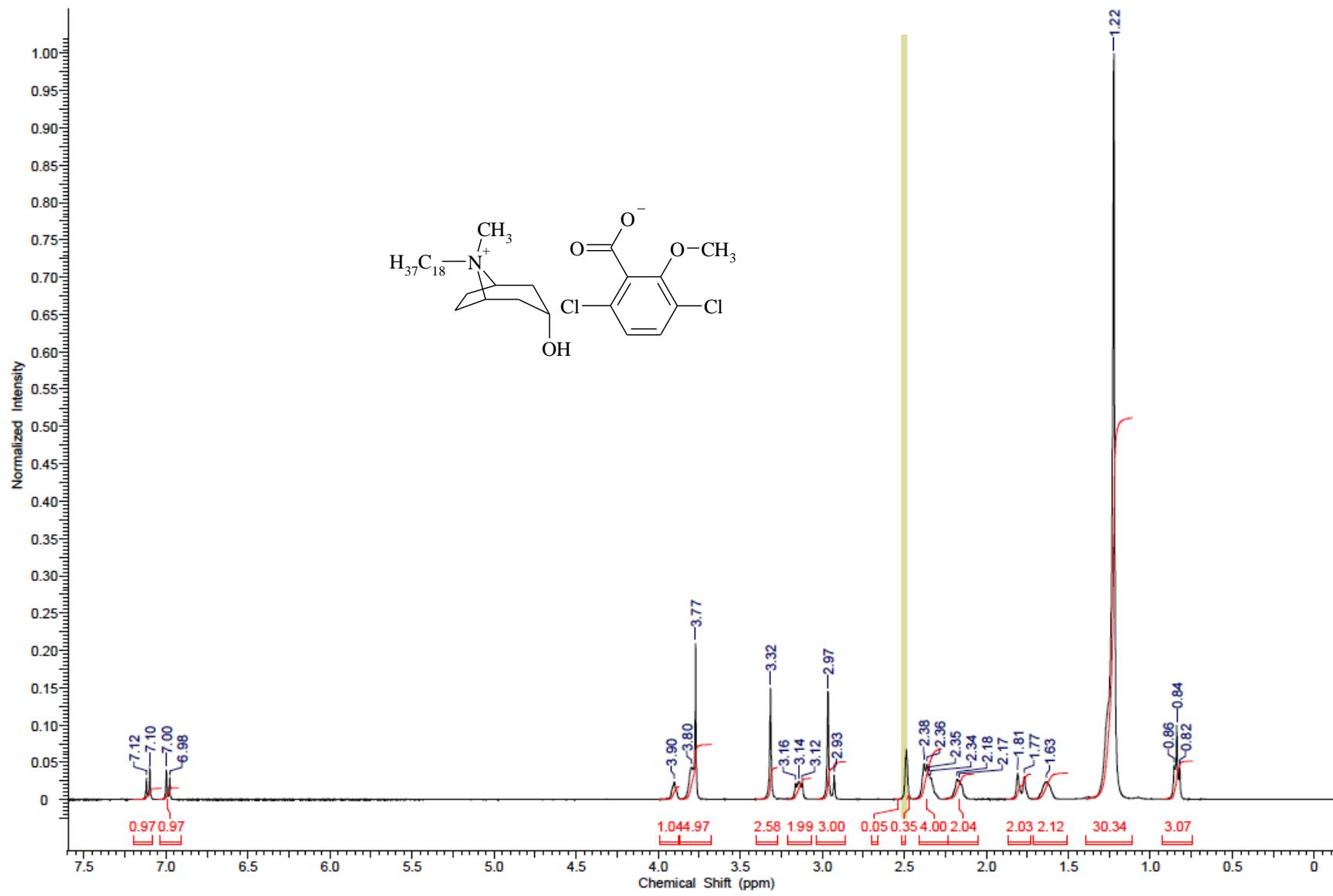
**Fig. S20**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_{14}][\text{dicamba}]$ .



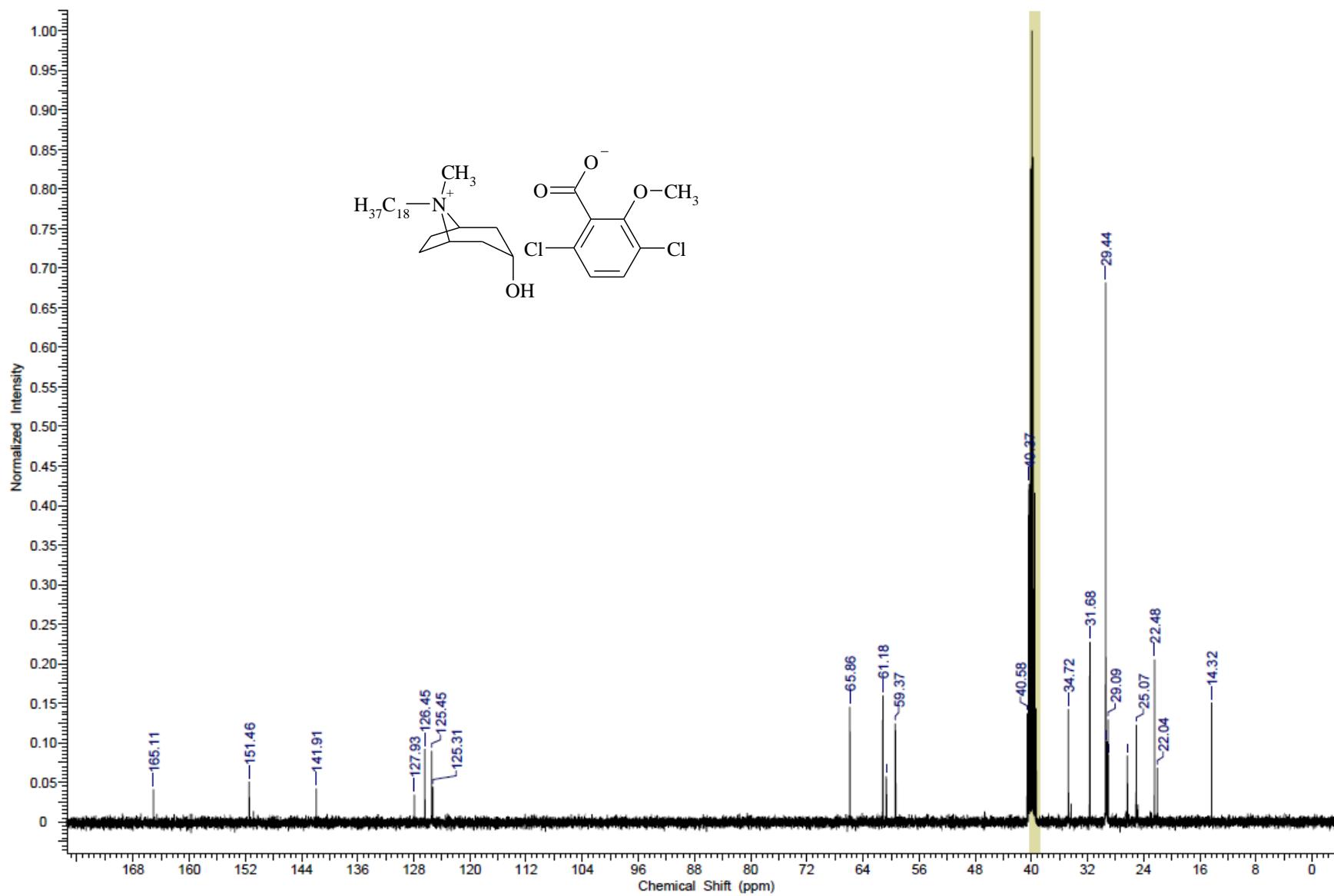
**Fig. S21**  $^1\text{H}$  NMR spectrum of [QTS- $\text{C}_{16}$ ][dicamba].



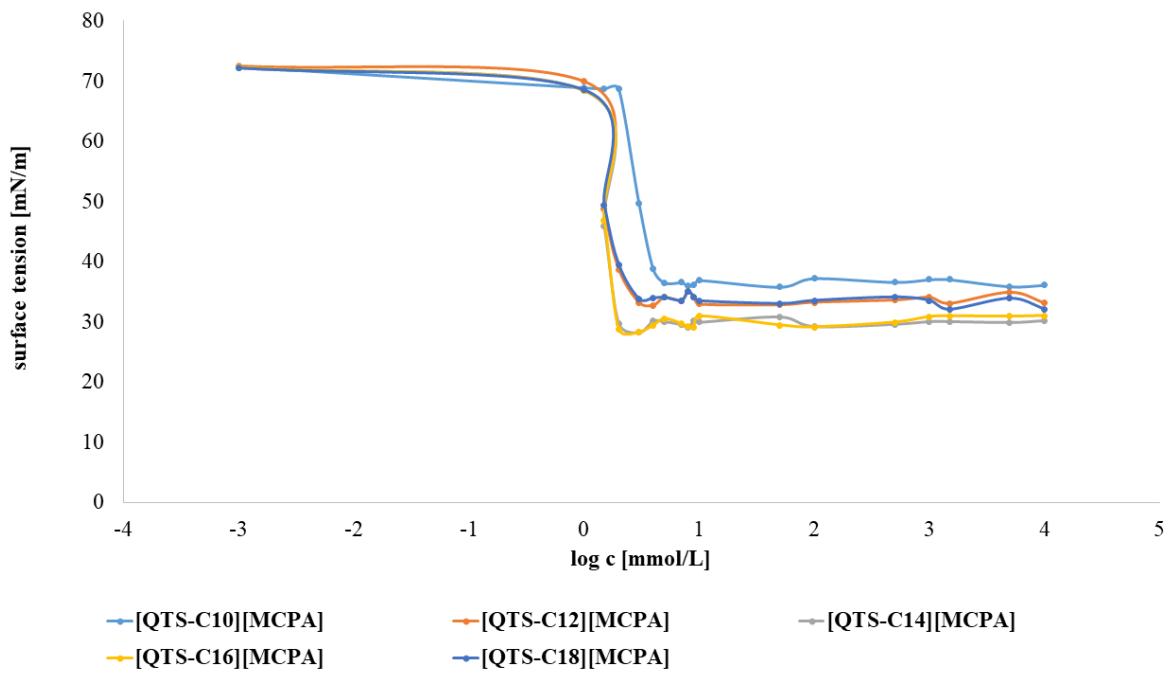
**Fig. S22**  $^{13}\text{C}$  NMR spectrum of  $[\text{QTS-C}_{16}][\text{dicamba}]$ .



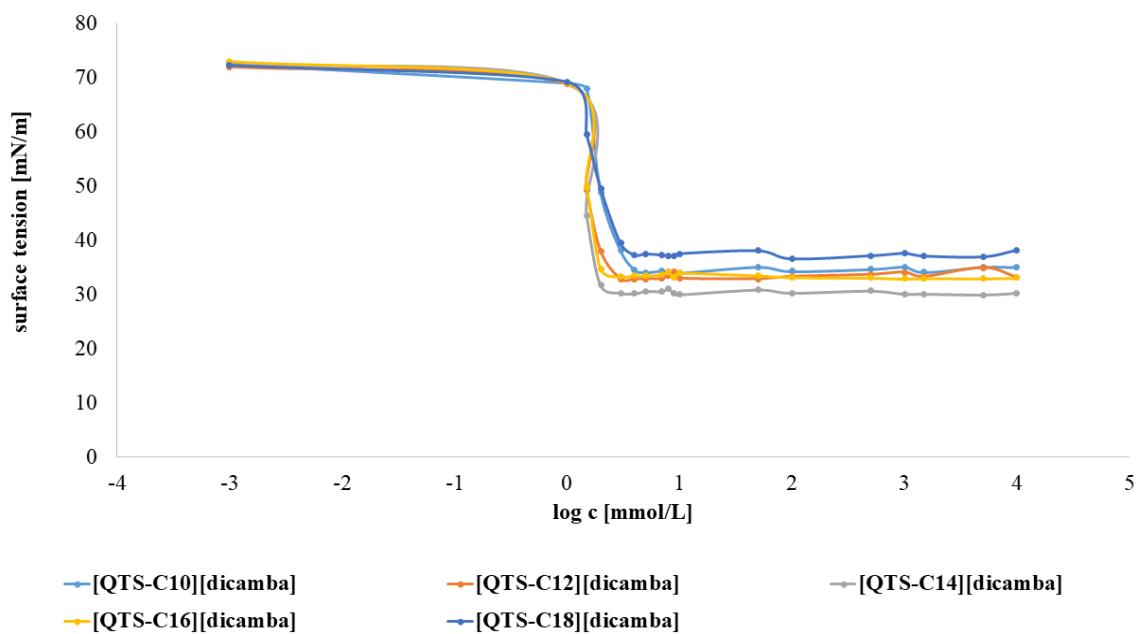
**Fig. S23**  $^1\text{H}$  NMR spectrum of  $[\text{QTS-C}_{18}][\text{dicamba}]$ .



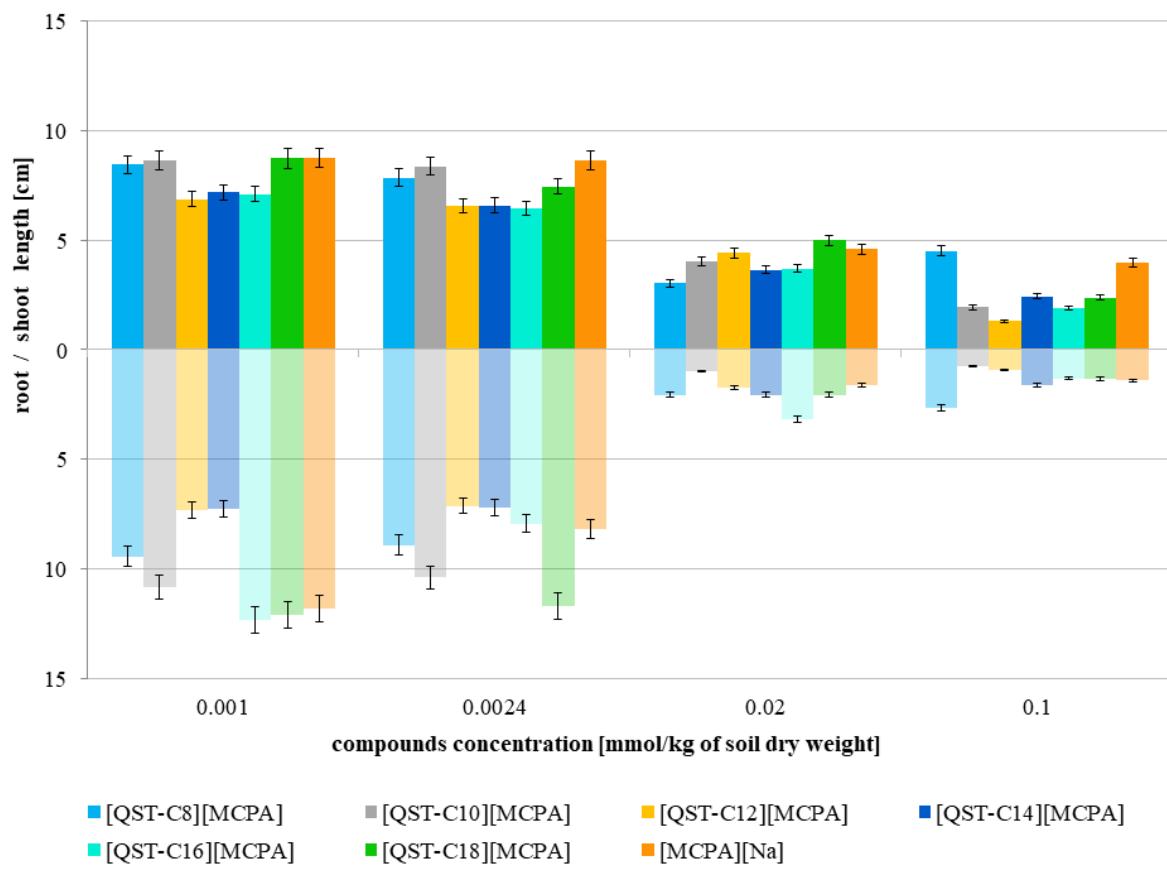
**Fig. S24**  $^{13}\text{C}$  NMR spectrum of **[QTS-C<sub>18</sub>][dicamba]**.



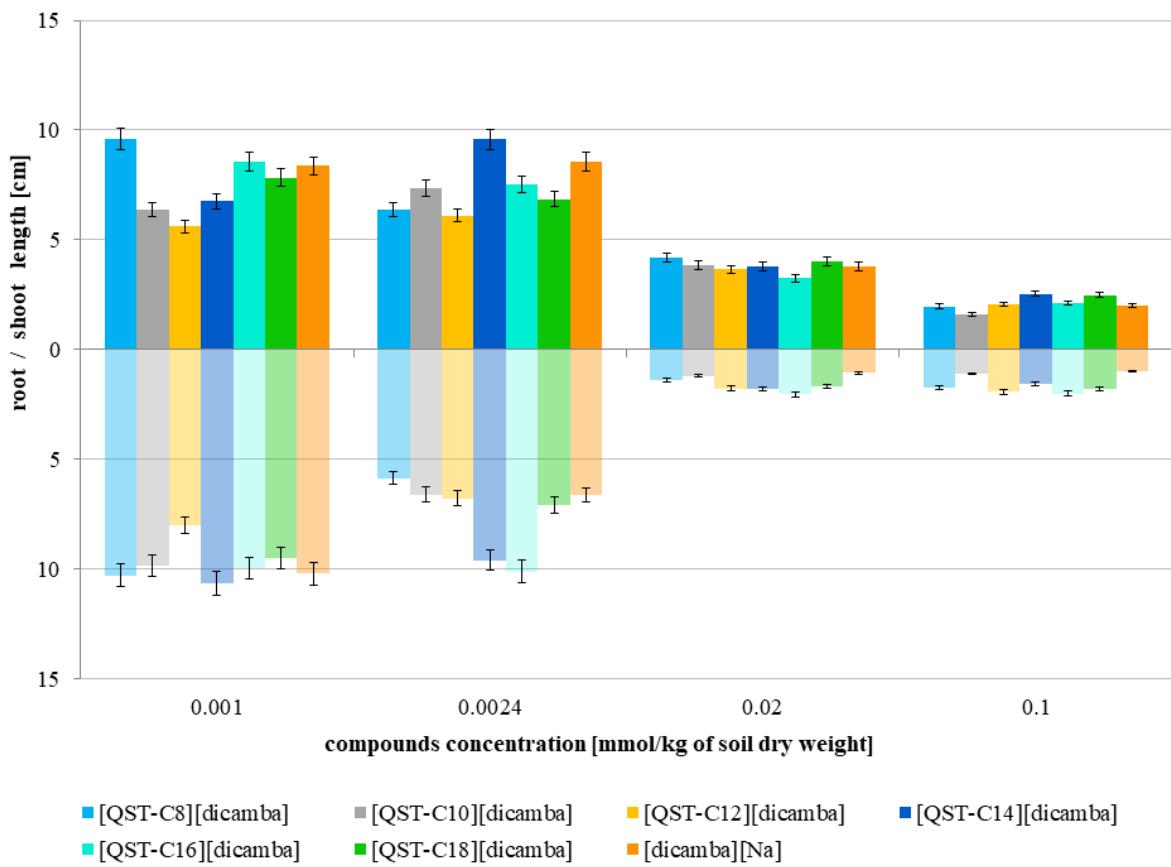
**Fig. S25** Surface tension of *N*-alkyltropinium MCPA salts.



**Fig. S26** Surface tension of *N*-alkyltropinium dicamba salts.



**Fig. S27** The effect of *N*-alkyltropinium MCPA salts concentration on the shoots and roots length of maize.



**Fig. S28** The effect of *N*-alkyltropinium dicamba salts concentration on the shoots and roots length of maize

**Table S1** The effect of *N*-alkyltropinium dicamba and MCPA salts concentration on the germination index of cornflower

		Germination index [%]			
Concentration [mmol/kg of soil d.w.]		0.001	0.0024	0.02	0.1
Quaternary tropinium salt					
[QTS-C <sub>8</sub> ][MCPA]		38.61 ± 2.77	34.71 ± 1.23	8.10 ± 1.87	0.00
[QTS-C <sub>10</sub> ][MCPA]		38.83 ± 2.89	19.31 ± 2.36	3.04 ± 2.36	0.00
[QTS-C <sub>12</sub> ][MCPA]		112.58 ± 4.56	64.49 ± 1.47	0.00 ± 0.00	0.00
[QTS-C <sub>14</sub> ][MCPA]		41.65 ± 1.87	20.39 ± 2.34	0.00 ± 0.00	0.00
[QTS-C <sub>16</sub> ][MCPA]		52.28 ± 2.13	20.61 ± 2.14	0.00 ± 0.00	0.00
[QTS-C <sub>18</sub> ][MCPA]		68.02 ± 3.12	42.30 ± 1.12	8.13 ± 1.86	0.00
[MCPA][Na]		39.91 ± 2.54	41.00 ± 1.57	0.00 ± 0.00	0.00
[QTS-C <sub>8</sub> ][dicamba]		95.41 ± 3.42	106.35 ± 3.45	20.11 ± 3.15	0.00
[QTS-C <sub>10</sub> ][dicamba]		68.61 ± 2.74	55.73 ± 2.42	12.09 ± 2.56	0.00
[QTS-C <sub>12</sub> ][dicamba]		67.27 ± 1.23	75.59 ± 1.89	18.37 ± 1.32	0.00
[QTS-C <sub>14</sub> ][dicamba]		89.42 ± 2.42	72.56 ± 3.48	27.46 ± 2.47	0.00
[QTS-C <sub>16</sub> ][dicamba]		57.60 ± 1.56	61.73 ± 1.56	42.63 ± 1.85	0.00
[QTS-C <sub>18</sub> ][dicamba]		114.08 ± 5.28	132.53 ± 4.02	26.98 ± 1.26	0.00
[dicamba][Na]		113.08 ± 4.63	43.08 ± 2.45	13.10 ± 2.86	0.00

± represents standard error of the mean from three independent samples