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# Plant growth promoting N-alkyltropinium bromides enhance seed germination, biomass accumulation and photosynthesis parameters of maize (*Zea mays*)

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## 1. NMR spectra of the synthesized compounds

*N-ethylacetyltropinium bromide (QTS Ethy)* (m.p. 195°C); <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 1.26 (t, *J*=7.09 Hz, 3H CH<sub>3</sub>-CH<sub>2</sub>-OOC-), 1.84 (d, *J*=16.38 Hz, 4H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.21 – 2.30 (m, 4H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.44 (d, *J*=8.07 Hz, 4H, CH<sub>2</sub>-CH-OH), 3.17 (s, 3H, CH<sub>3</sub>-N<sup>+</sup>), 3.92 (br.s, 1H, CH-OH), 4.16 (br.s, 2H, CH-N<sup>+</sup>), 4.24 (q, *J*=7.25 Hz, 2H, CH<sub>3</sub>-CH<sub>2</sub>-OOC-), 4.31 (s, 2H, -OOC-CH<sub>2</sub>-N<sup>+</sup>), 5.03 (s, 1H, CH-OH); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 13.79, 24.32, 34.02, 39.30, 39.72, 58.63, 58.71, 58.71, 61.99, 67.26, 165.27

*N-benzyltropinium bromide (QTS Benz)* (m.p. 243-245°C); <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 1.83 (d, *J*=16.14 Hz, 4H CH<sub>2</sub>-CH-N<sup>+</sup>), 2.30 – 2.243 (m, 4H, CH<sub>2</sub>-CH-OH), 2.88 (br.s, 3H, N<sup>+</sup>-CH<sub>3</sub>), 3.81 (s, 2H, CH-N<sup>+</sup>), 3.92 (s, 1H, CH-OH), 4.48 (s, 2H, Ph-CH<sub>2</sub>-N<sup>+</sup>), 5.02 (d, *J*=2.45 Hz, 1H, CH-OH), 7.53 (m, 5H, Ph); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 24.32, 34.02, 39.30, 39.72, 54.00, 58.63, 58.71, 58.71, 61.99, 128.40, 129.20, 137.80

*N-decanyltropinium bromide (QTS C10)* (m.p. 215-216°C); <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 0.77 – 0.91 (m, 3H, CH<sub>3</sub>-CH<sub>2</sub>), 1.17 – 1.33 (m, 16H, -CH<sub>2</sub>-), 1.65 (br.s, 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 1.79 (d, *J*=16.14 Hz, 4H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.21 (br.s., 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.33 – 2.45 (m, 4H, CH<sub>2</sub>-CH-OH), 2.91 – 3.02 (m, 3H, N<sup>+</sup>-CH<sub>3</sub>), 3.11 – 3.21 (m, 2H, -CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 3.82 (br.s, 2H, CH-N<sup>+</sup>), 3.92 (br.s, 1H, CH-OH), 4.97 (br.s., 1H, CH-OH); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 13.95, 21.65, 22.08, 24.68, 25.92, 28.60, 28.90, 31.26, 31.26, 34.33, 34.33, 39.11, 39.74, 59.00, 60.27, 60.27, 65.42.

*N-dodecyltropinium bromide (QTS C12)* (m.p. 228-229°C); <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 0.86 (t, *J*=6.60 Hz, 3H, CH<sub>3</sub>-CH<sub>2</sub>), 1.25 (m, 20 H, -CH<sub>2</sub>-), 1.65 (br.s, 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 1.79 (d, *J*=16.14 Hz, 4H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.08-2.24 (m, 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.31 – 2.45 (m, 4H, CH<sub>2</sub>-CH-OH), 2.98 (s, 3H, N<sup>+</sup>-CH<sub>3</sub>), 3.10 – 3.23 (m, 2H, -CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 3.82 (br.s, 2H, CH-N<sup>+</sup>), 3.92 (br.s, 1H, CH-OH), 4.97 (br.s., 1H, CH-OH); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 14.39, 22.07, 22.52, 25.12, 26.35, 29.03, 29.13, 29.26, 29.37, 29.42, 29.45, 31.72, 34.78, 39.35, 39.55, 39.76, 39.98, 40.18, 40.39, 40.59, 59.44, 60.73, 65.87, 66.44.

*N-tetradecyltropinium bromide (QTS C14)* (m.p. 244-245°C); <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 0.86 (t, *J*=6.60 Hz, 3H, CH<sub>3</sub>-CH<sub>2</sub>), 1.19 – 1.34 (m, 24H, -CH<sub>2</sub>-), 1.65 (br.s, 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 1.79 (d, *J*=15.89 Hz, 4H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.14 – 2.23 (m, 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.37 (d, 4H, CH<sub>2</sub>-CH-OH), 2.96 (m, 3H, N<sup>+</sup>-CH<sub>3</sub>), 3.15 (m, 2H, -CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 3.81 (br.s, 2H, CH-N<sup>+</sup>), 3.92 (br.s, 1H, CH-OH), 4.97 (s., 1H, CH-OH); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 14.40, 22.10, 22.58, 25.16, 26.39, 29.09, 29.15, 29.30, 29.41, 29.43, 29.50, 31.74, 34.80, 39.52, 39.89, 40.10, 40.11, 40.19, 40.27, 40.35, 59.50, 65.90.

*N-hexadecyltropinium bromide (QTS C16)* (m.p. 241-242°C); <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 0.85 (t, *J*=6.72 Hz, 3H, CH<sub>3</sub>-CH<sub>2</sub>), 1.24 (s, 28H, -CH<sub>2</sub>-), 1.65 (br.s, 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 1.79 (d, *J*=15.89 Hz, 4H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.20 (d, *J*=5.14 Hz, 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.32-2.45 (m, 4H, CH<sub>2</sub>-CH-OH), 2.98 (s, 3H, N<sup>+</sup>-CH<sub>3</sub>), 3.11- 3.20 (m, 2H, -CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 3.82 (br.s, 2H, CH-N<sup>+</sup>), 3.92 (br.s, 1H, CH-OH), 4.97 (s., 1H, CH-OH); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 14.44, 22.13, 22.58, 25.17, 26.40, 29.09, 29.18, 29.32, 29.43, 29.49, 29.53, 31.78, 34.83, 39.52, 39.69, 39.86, 40.02, 40.11, 40.19, 40.28, 40.35, 40.44, 40.52, 59.50, 60.79, 65.92.

*N-octadecyltropinium bromide (QTS C18)* (m.p. 238-239°C); <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ ppm = 0.85 (t, *J*=6.60 Hz, 3H, CH<sub>3</sub>-CH<sub>2</sub>), 1.24 (s, 32H, -CH<sub>2</sub>-), 1.65 (br.s, 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 1.79 (d, *J*=15.89 Hz, 4H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.20 (d, *J*=5.38 Hz, 2H, CH<sub>2</sub>-CH-N<sup>+</sup>), 2.30-2.45 (m, 4H, CH<sub>2</sub>-CH-OH), 2.98 (s, 3H, N<sup>+</sup>-CH<sub>3</sub>), 3.10- 3.21 (m, 2H, -CH<sub>2</sub>-CH<sub>2</sub>-N<sup>+</sup>), 3.82 (br.s, 2H, CH-N<sup>+</sup>), 3.92 (br.s, 1H, CH-OH), 4.96 (s., 1H, CH-OH); <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100 MHz): δ ppm = 14.44, 22.58, 25.17, 29.09, 29.18, 29.31, 29.43, 29.52, 31.77, 34.84, 39.52, 39.68, 39.85, 40.02, 40.19, 40.27, 40.35, 40.43, 40.52, 59.50, 65.94.

## 2. Crystallographic parameters of the synthesized compounds

Table S1. Crystallographic data.

Compound	QTS Benz	QTS C10	QTS Ethy
Space group	Pbca	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c
Z	8	4	4
<i>a</i> [Å]	9.788(1)	25.460(1)	14.081(1)
<i>b</i> [Å]	9.698(1)	9.951(1)	10.117(1)
<i>c</i> [Å]	29.266(1)	9.9512(10)	9.705(1)
$\beta$ [°]	90.0	101.16	107.67
R <sub>int</sub>	0.057 (0.082)	0.114 (0.204)	0.071 (0.119)
Resolution [Å]	0.78	0.80	0.81
Wavelength [Å]	0.82650	0.8950	0.88561
I/ $\sigma$ (I)	57 (32)	37 (8)	42 (23)
% completeness	95.2 (90.4)	90.7 (82.2)	94.8 (90.6)
Av. data redundancy	12.8 (12.2)	6.3 (5.4)	6.5 (5.4)
Independent reflections	2944	4600	2475
R-factor	0.0302	0.0637	0.0345
CCDC deposition number	1872985	1872984	1872986

\* Values in brackets are for the highest resolution shell.

### 3. MS spectra

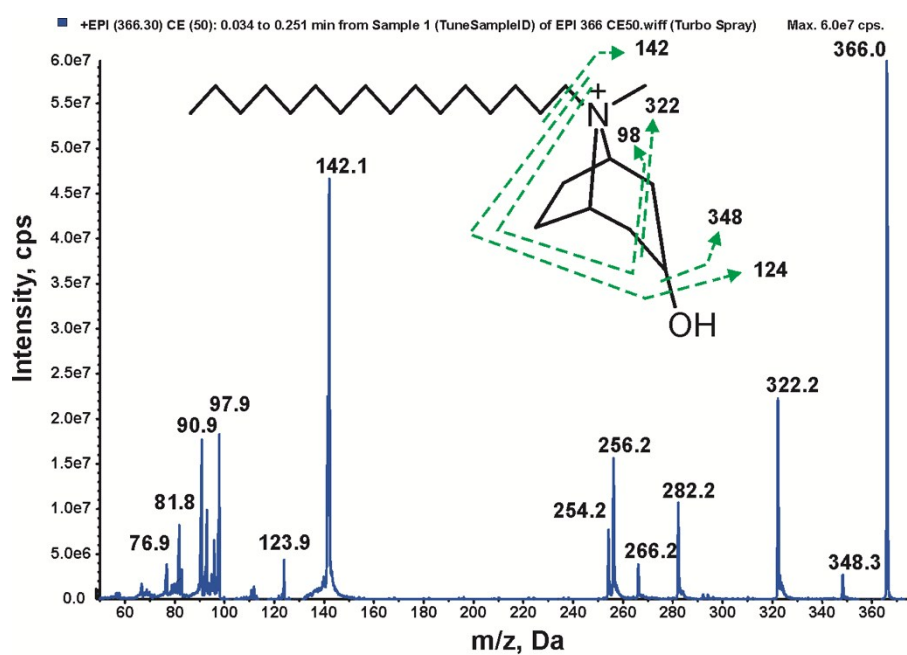


Fig. S1. MS spectrum of QTS-C16.

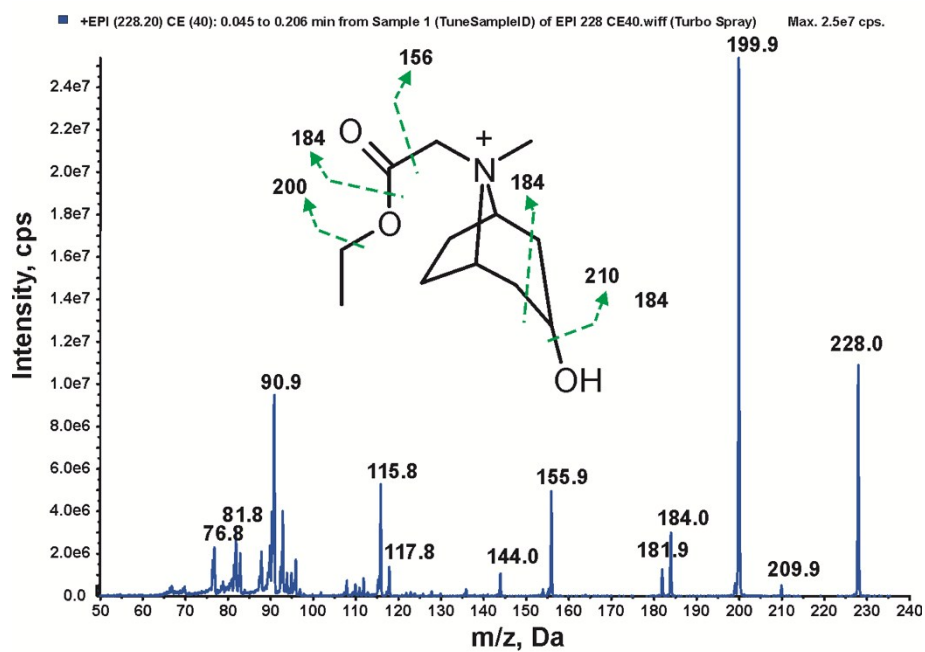


Fig. S2. MS spectrum of QTS-Ethy.

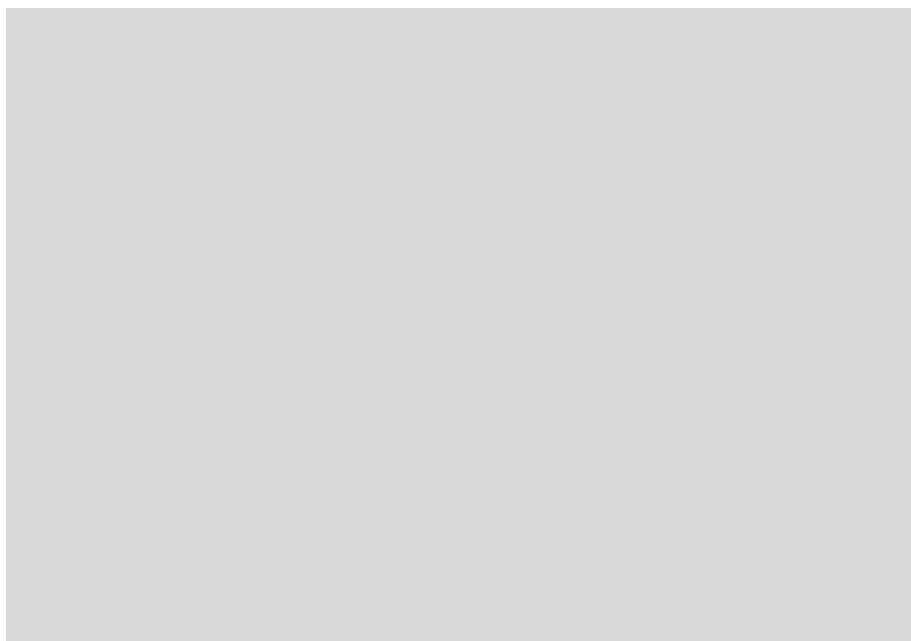


Fig. S3. MS spectrum of QTS-Benz.