Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Functionalized cellulose nanocrystals as nanocarriers for sustained fragrance release

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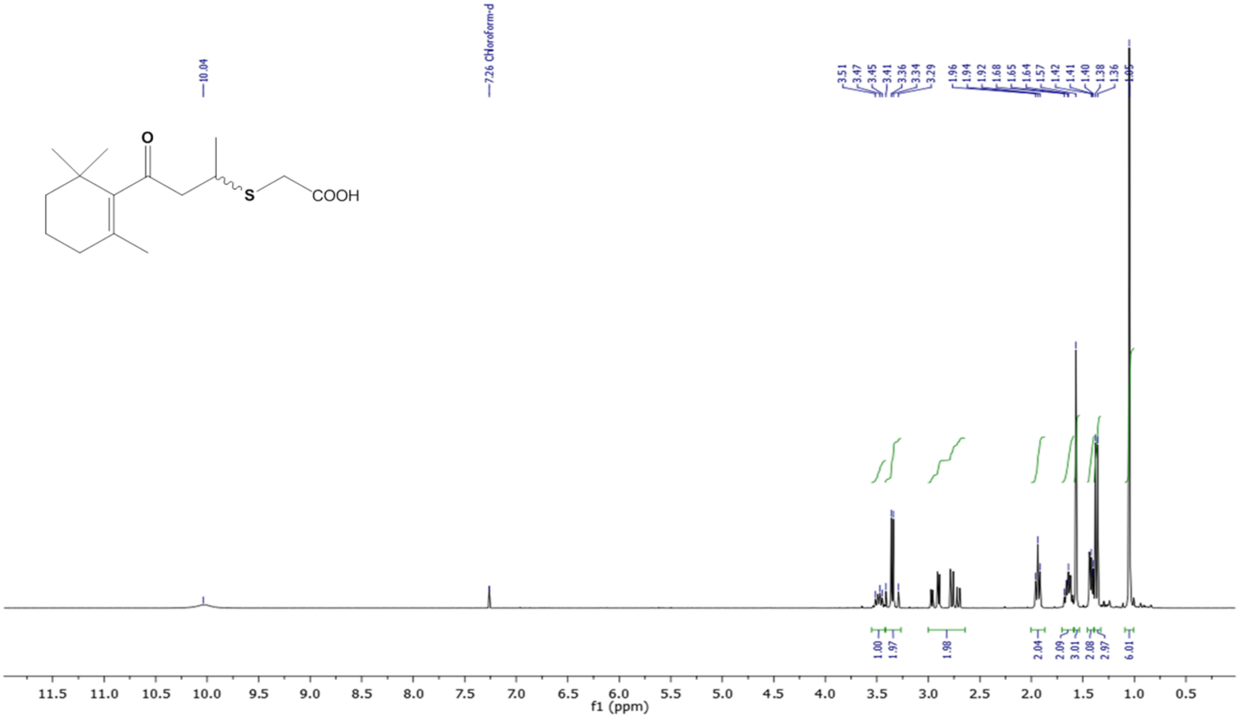

Fig. S1 ^{1}H NMR spectrum of 2-((4-oxo-4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-yl)thio)acetic acid (1) in $CDCl_3$ at 300 MHz.

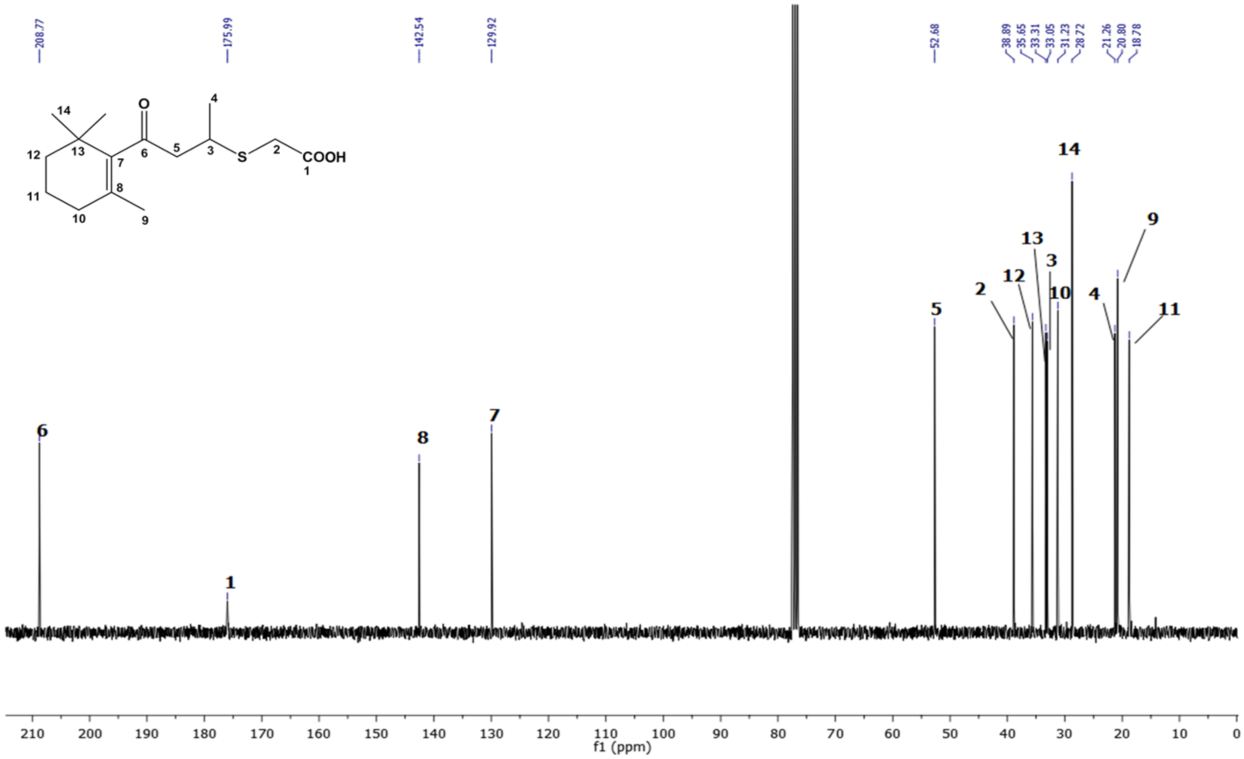

Fig. S2 ^{13}C NMR spectrum of 2-((4-oxo-4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-yl)thio)acetic acid (**1**) in $CDCl_3$ at 300 MHz.

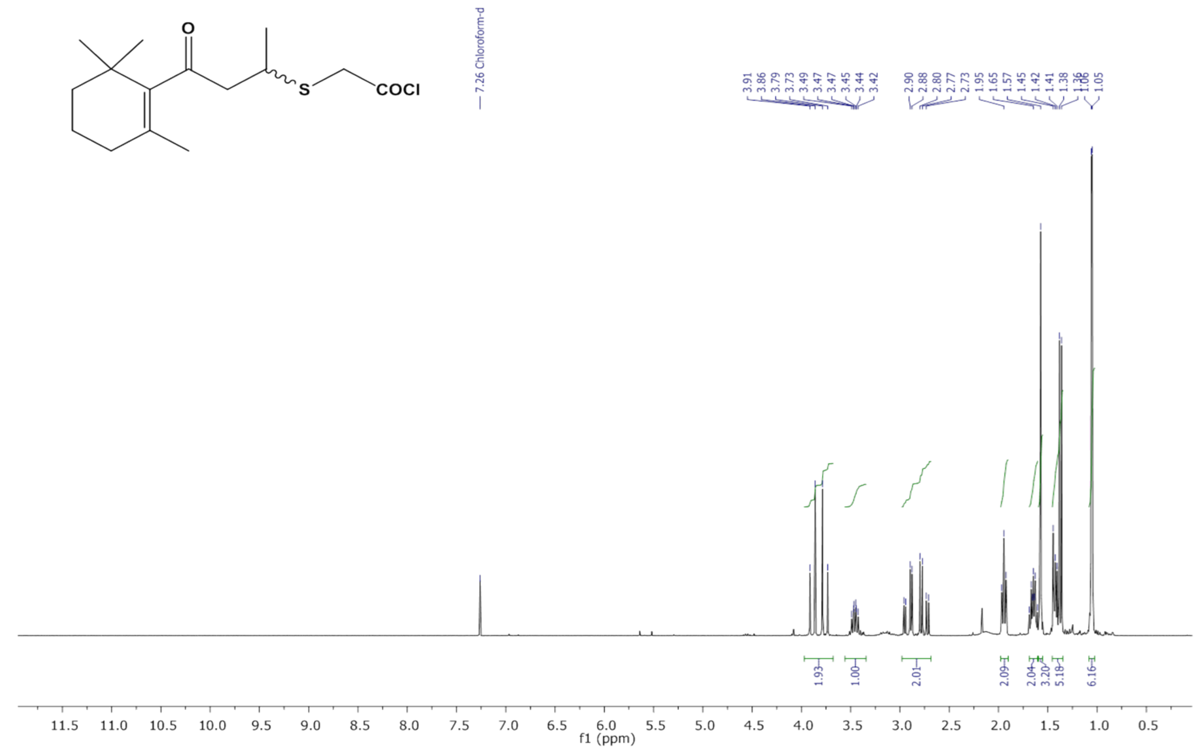

Fig. S3 ^{1}H NMR spectrum of 2-((4-oxo-4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-yl)thio)acetyl chloride (**2**) in $CDCl_3$ at 300 MHz.

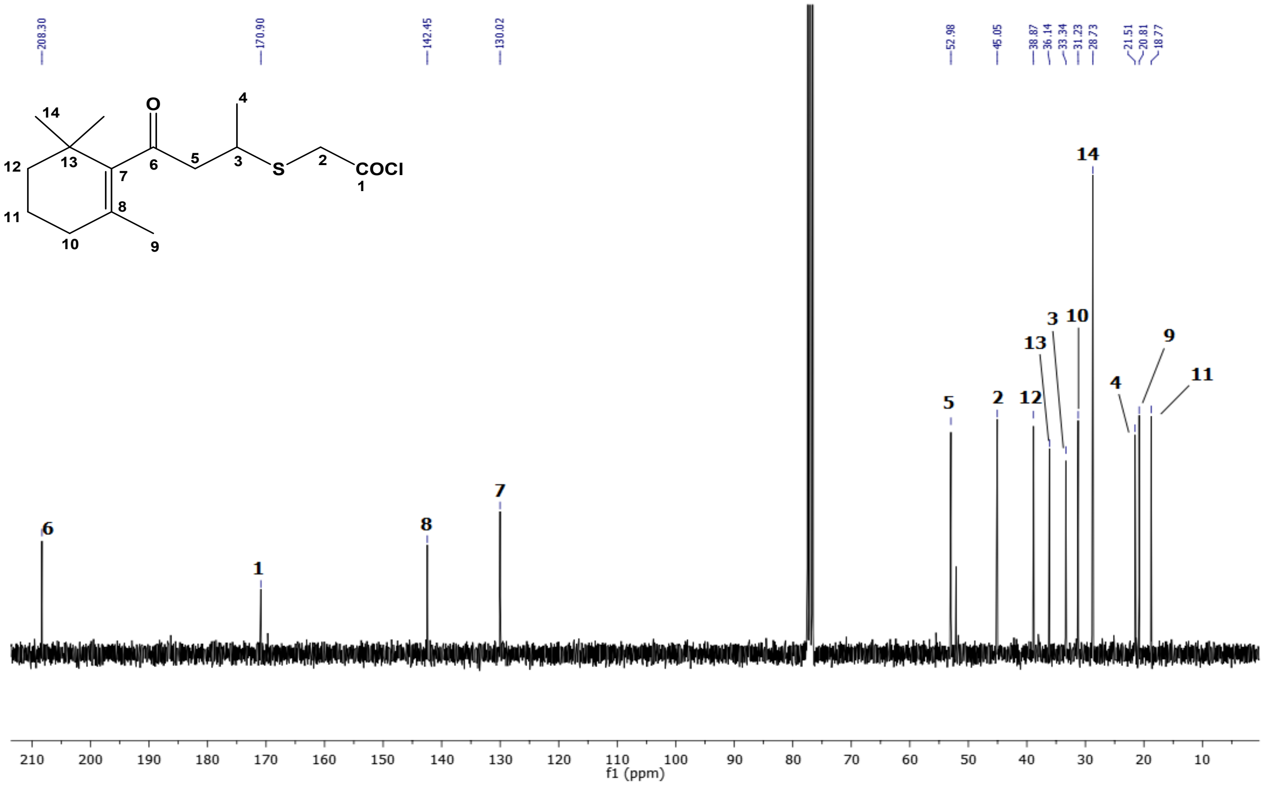

Fig. S4 ^{13}C NMR spectrum of 2-((4-oxo-4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-yl)thio)acetyl chloride (**2**) in $CDCl_3$ at 300 MHz.

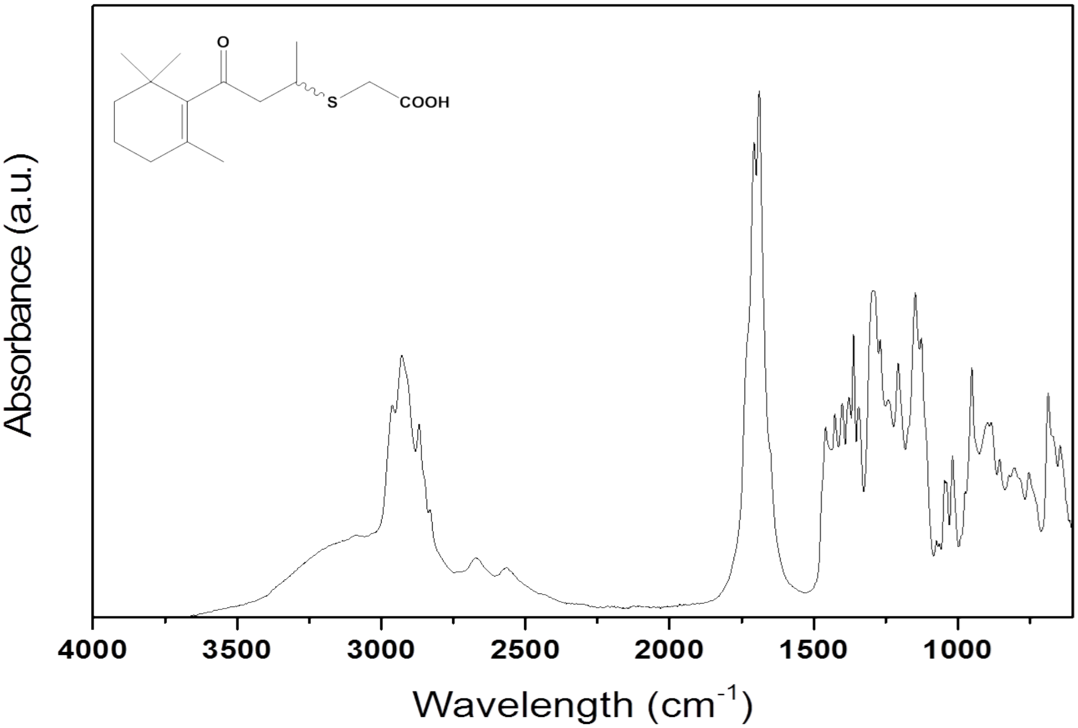

Fig. S5 IR spectrum of 2-((4-oxo-4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-yl)thio)acetic acid (**1**).

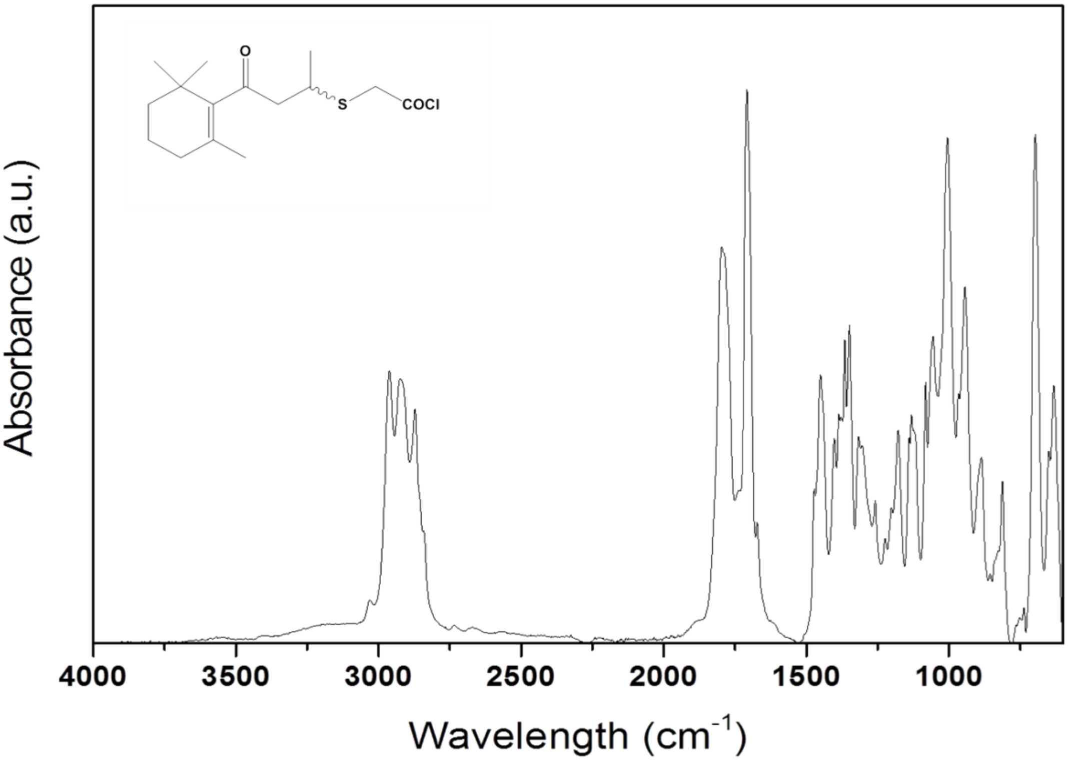

Fig. S6 IR spectrum of 2-((4-oxo-4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-yl)thio)acetyl chloride (**2**).

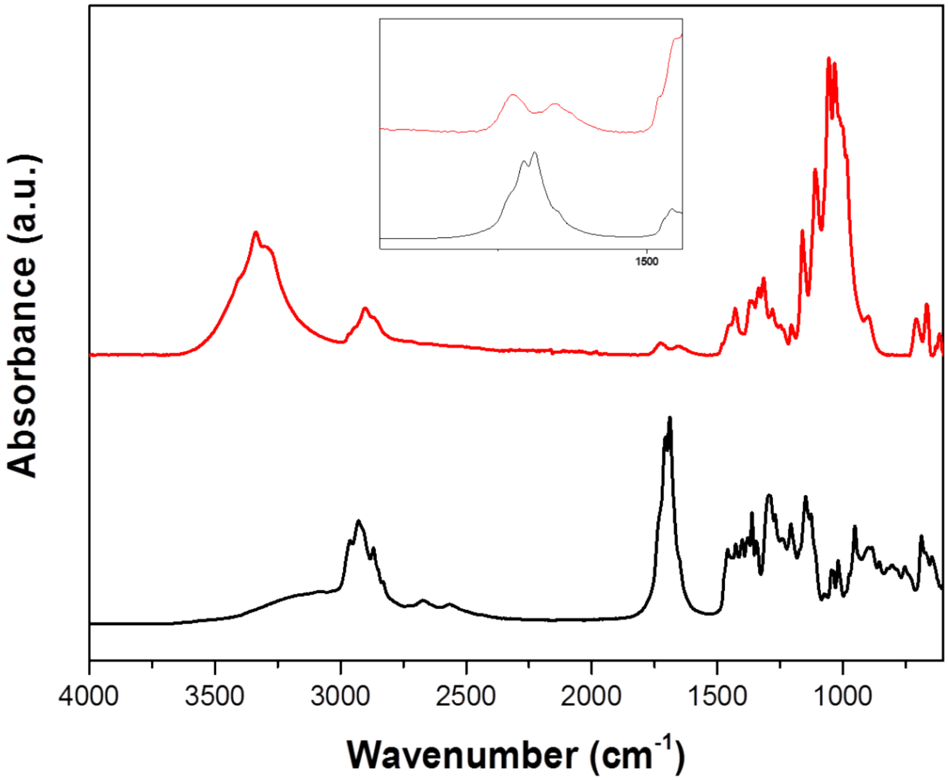

Fig. S7 IR spectra of modified CNCs (red) and acid 3 (black). A magnification of the carbonyl region is shown as inset..

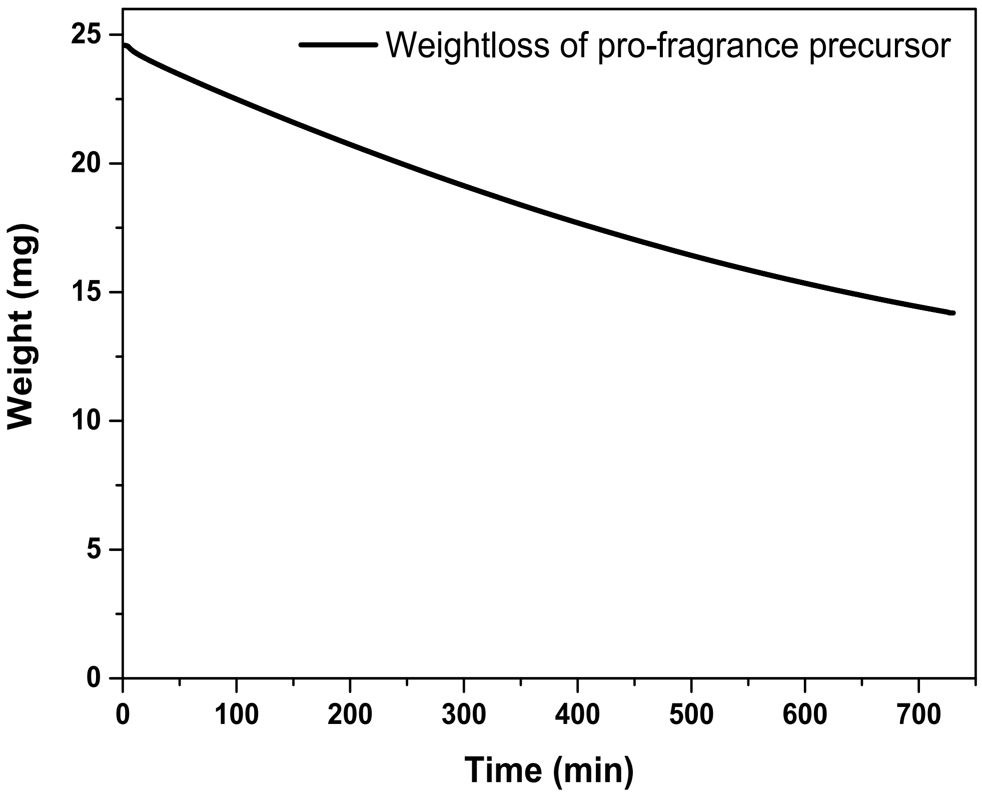

Fig. S8 Isothermal TGA, the sample was kept at 130 °C for 12 h showing the breaking of the thioether bond and the evaporation of the mercaptoacetic acid (bp. 95°C).

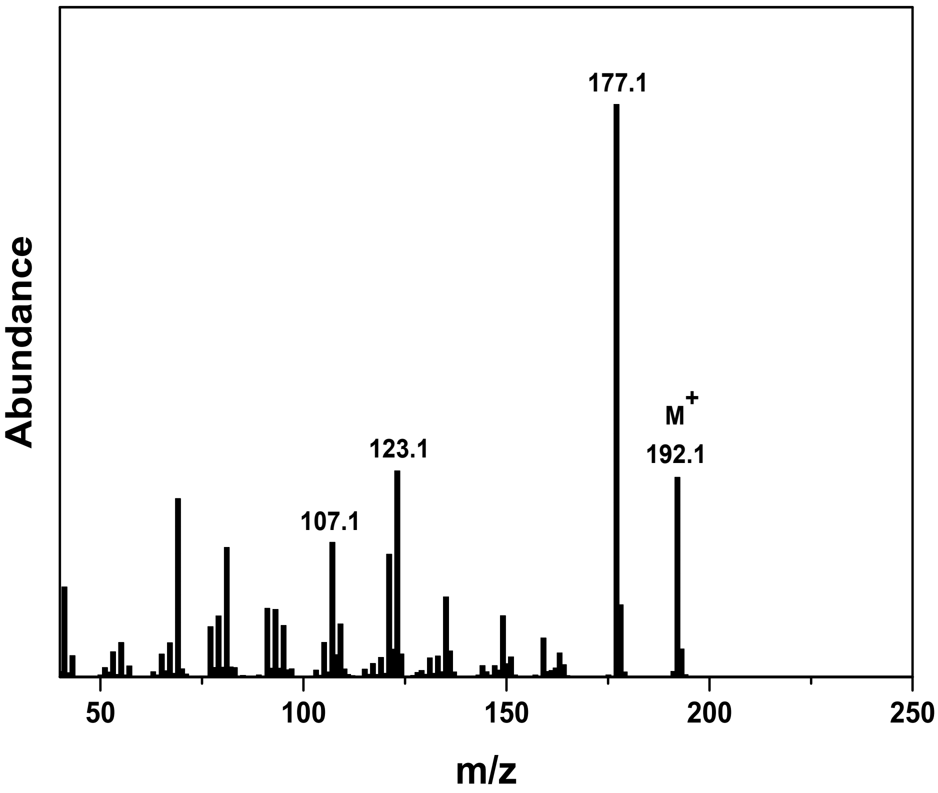

Fig. S9 Mass spectrum of β-damascone showing the characteristic m/z peaks that were used for the selecting ion monitoring (SIM).

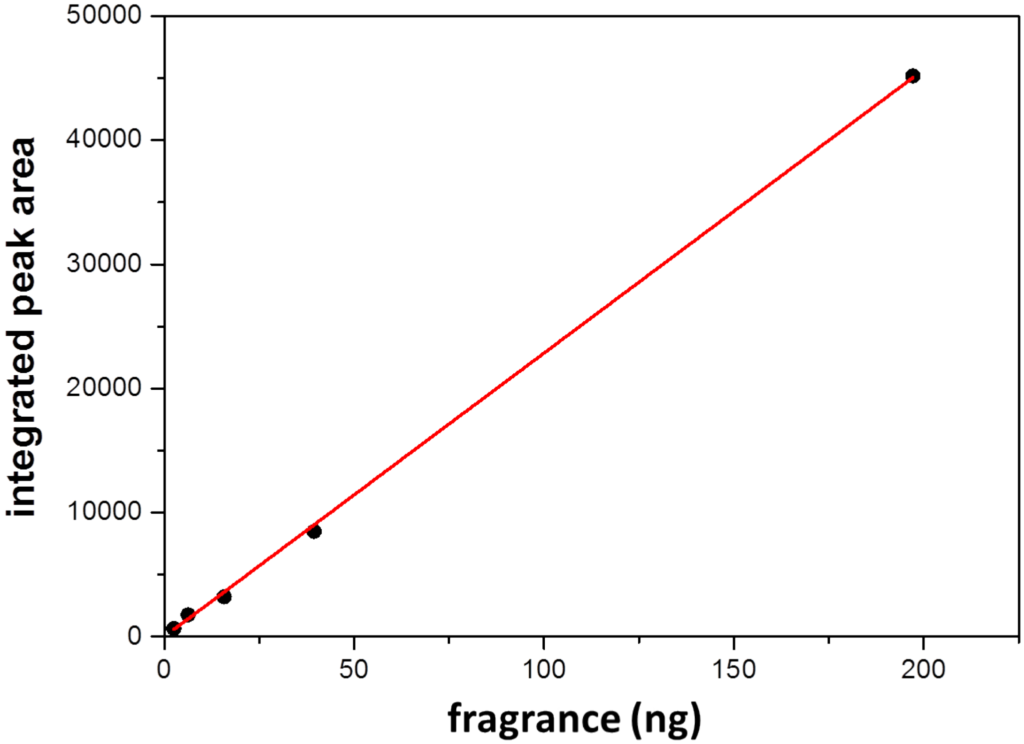

Fig. S10 Gas chromatography calibration curve constructed from measurements of 5 β-damascone solutions with different concentration. The β-damascone (197.12, 39.4, 15.77, 6.31, 2.52 ng) was dissolved in ethanol (1 mL) and 2 µL of each solution were manually injected into the GC-MS. The recorded chromatograms (Figure S11) were integrated and the peak areas were plotted against the amount of β-damascone injected. The calibration curve was established by a linear least square fit that was forced through the origin.

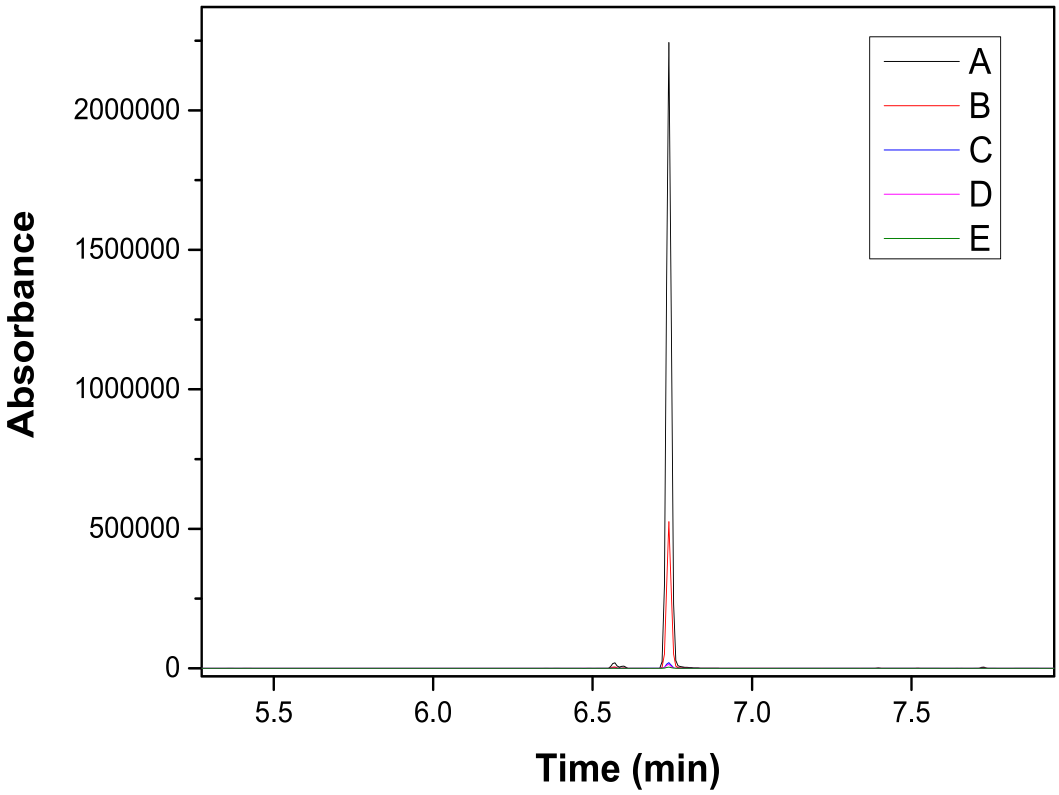

Fig. S11 Gas chromatograms of 5 different concentrations of β-damascone (197.12, 39.4, 15.77, 6.31, 2.52 ng) dissolved in ethanol (1 mL). The recorded chromatograms were integrated and the peak areas were used to construct the calibration curve shown in Figure S10.

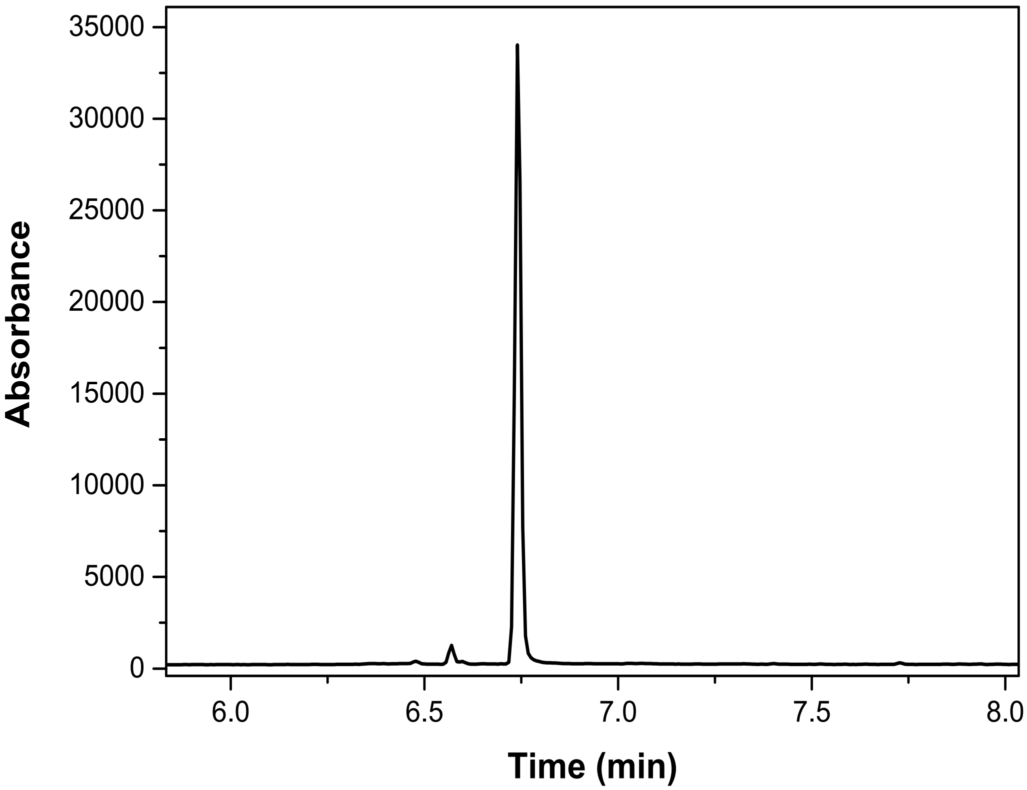

Fig. S12 Gas chromatogram of β-damascone released from βD-CNCs (10 mg) after heating them for 24 h at 130 °C in DMF (5 mL). The suspension was subsequently centrifuged, and 2 µL of the supernatant were injected into the GC-MS. The chromatogram was integrated and used to determine the amount of attached fragrance, using the calibration curve shown in Figure S10.

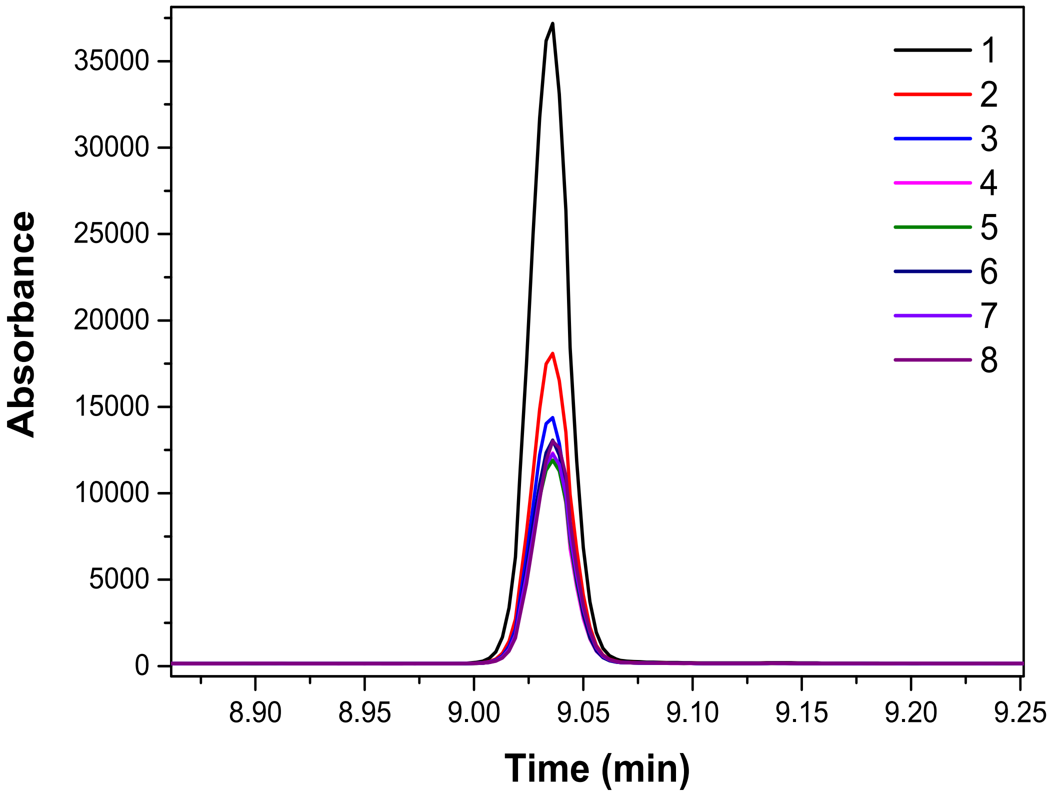

Fig. S13 Example of a series of 8 different gas chromatograms showing the release of β-damascone after deposition of βD-CNCs onto ceramic tiles. βD-CNCs were dispersed in an aqueous all-purpose cleaner solution (2.75 mg·mL^{-1}) and a portion (0.75 mL) was deposited onto ceramic tiles. After 3 days of drying, the amount of fragrance released was analyzed *via* dynamic headspace analysis followed by GC. Measurements 1-8 were made in 1 h intervals.

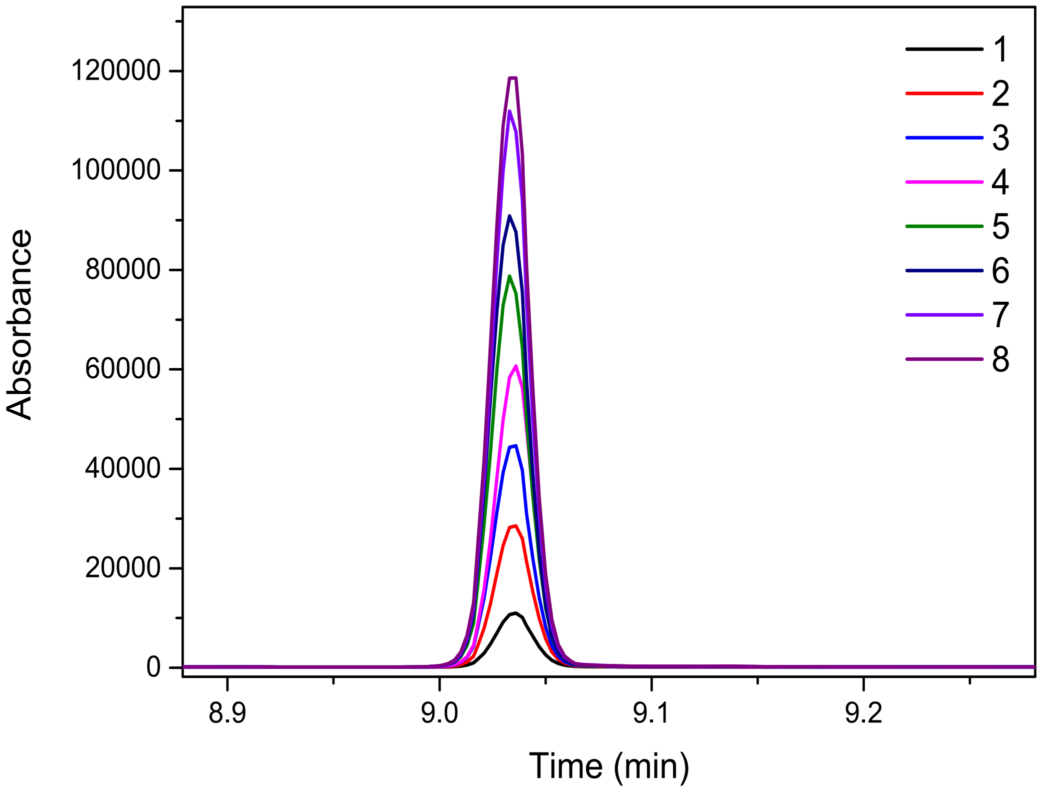

Fig. S14 Example of a series of 8 different gas chromatograms showing the release of β-damascone from cotton tissue. An aqueous washing formulation was prepared by mixing βD-CNCs (100 mg) with a softener emulsion (1.8 g) and deionized water (600 mL). The cotton tissue (12x12 cm, 3.12 g) was washed with the aqueous βD-CNCs mixture (170.0 μg·mL^{-1}) and line dried for 3 days. The amount of fragrance released was then analyzed *via* dynamic headspace analysis followed by GC. Measurements 1-8 were made in 1 h intervals.

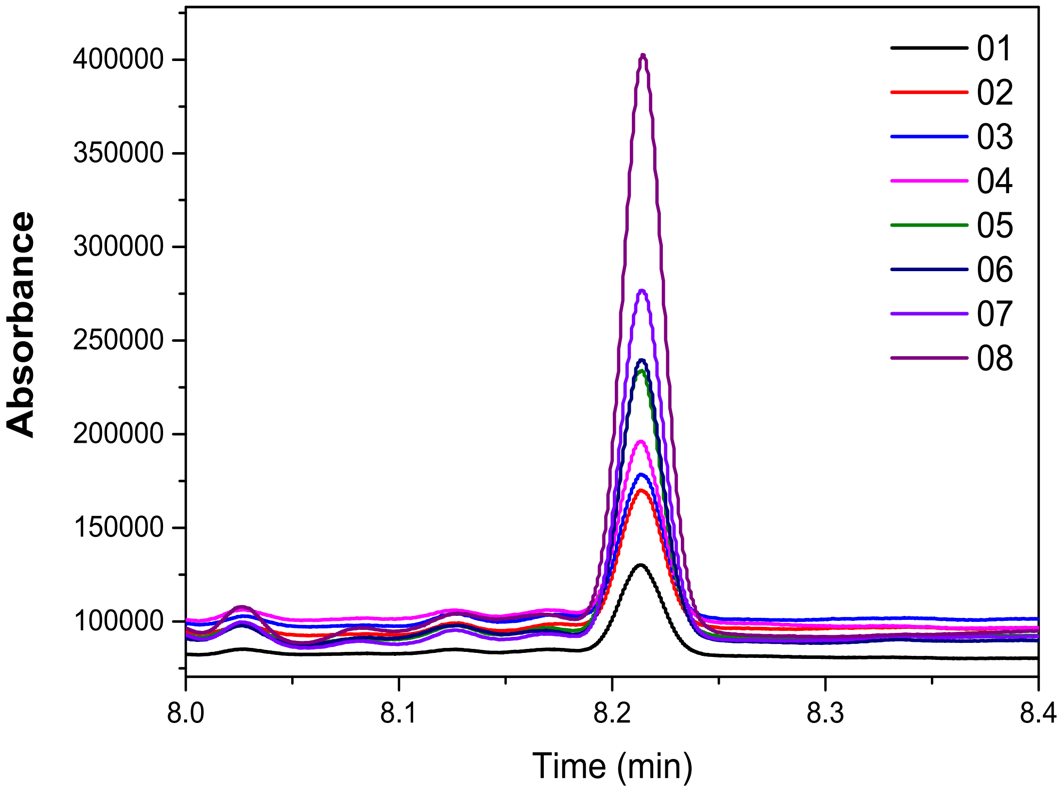

Fig. S15 Example of a series of 8 different gas chromatograms showing the release of β-damascone from cotton tissue after the direct deposition of βD-CNCs. Dispersions of βD-CNCs (100 mg) in dimethyl sulfoxide (200 μL) were directly deposited onto freshly washed cotton tissue and line dried for 3 days. The amount of fragrance released was then analyzed *via* dynamic headspace analysis followed by GC. Measurements 1-8 were made in 1 h intervals.