Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Controlled fragrance release from galactose-based pro-fragrances

Tobias Kuhnt[a], Andreas Herrmann[b], Daniel Benczédi[b], Christoph Weder[a]* and E. Johan Foster[a,c]*

[a]Adolphe Merkle Institute, University of Fribourg, Chemin des Verdiers 4, CH-1700 Fribourg, Switzerland

[b]Firmenich SA, Division Recherche et Développement, B.P. 239, CH-1211 Genève 8, Switzerland

[c]Virginia Tech, Department of Materials Science & Engineering, 445 Old Turner Street, 213 Holden Hall, Blacksburg VA 24061, USA

NMR-Spectra:

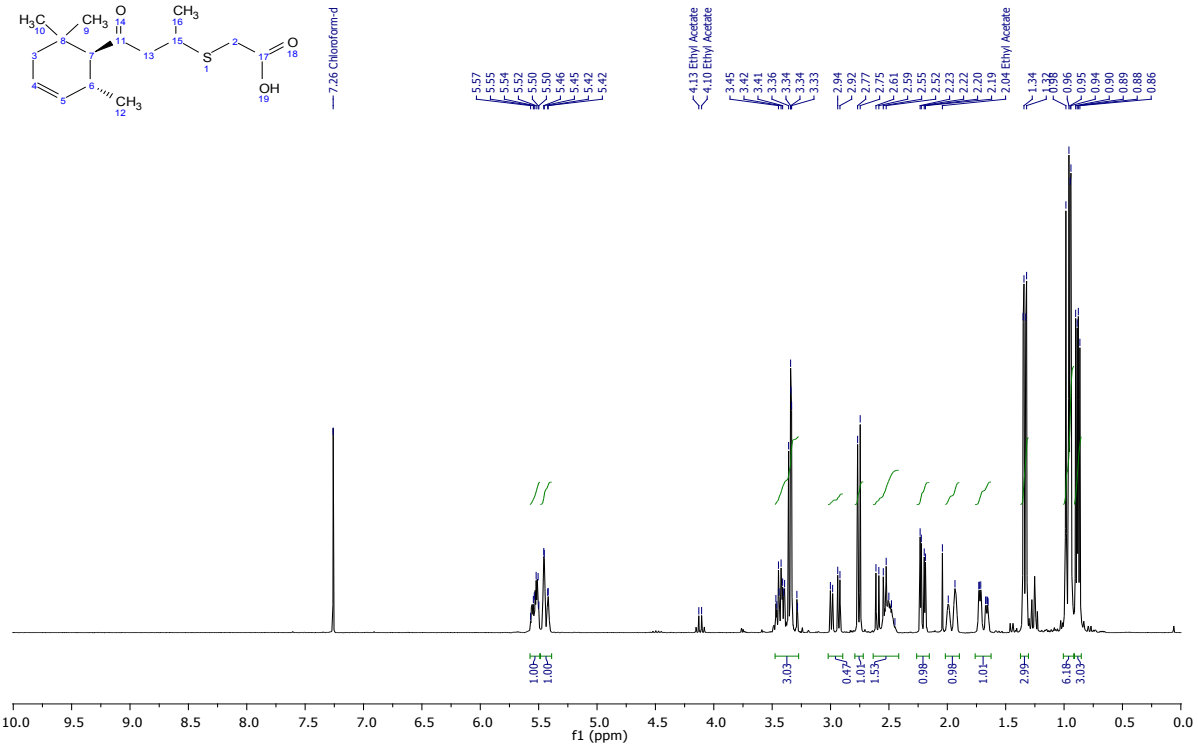

Figure S 1. ^{1}H-NMR of (±)-2-((4-Oxo-4-((1*RS*,2*SR*)-2,6,6-trimethylcyclohex-3-en-1-yl)butan-2-yl)thio)acetic acid (**1**) in $CDCl_3$ at 300 MHz.

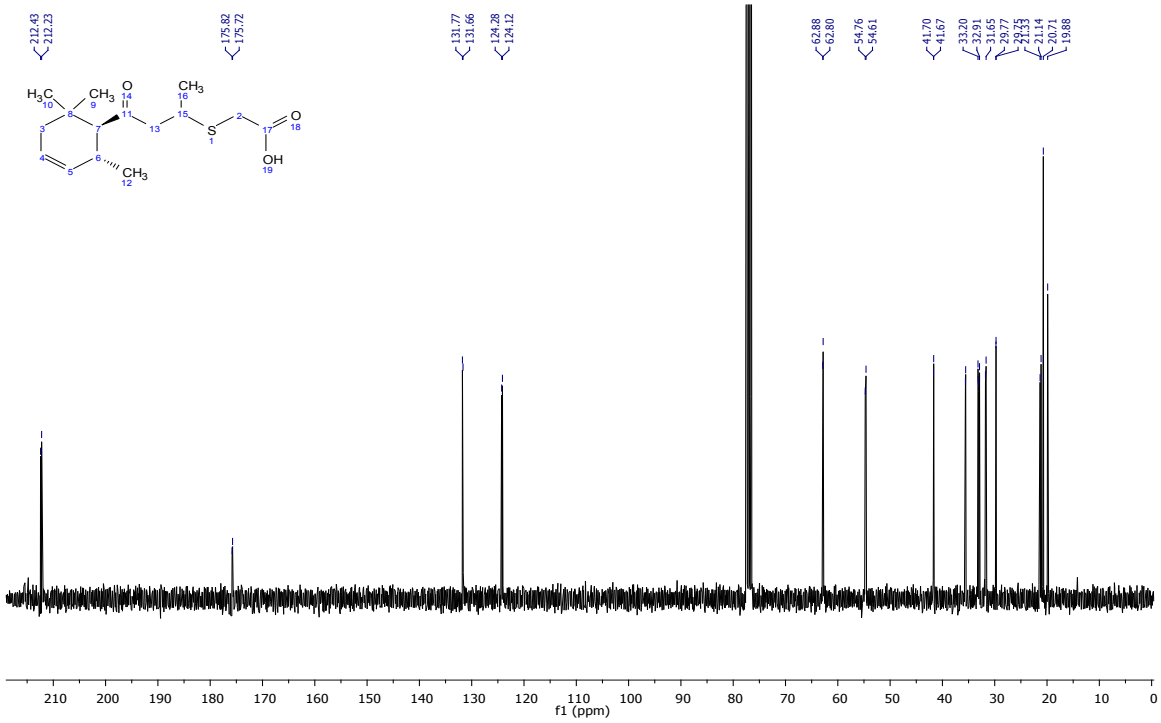

Figure S 2. ^{13}C-NMR of (±)-2-((4-Oxo-4-((1*RS*,2*SR*)-2,6,6-trimethylcyclohex-3-en-1-yl)butan-2-yl)thio)acetic acid (**1**) in $CDCl_3$ at 300 MHz.

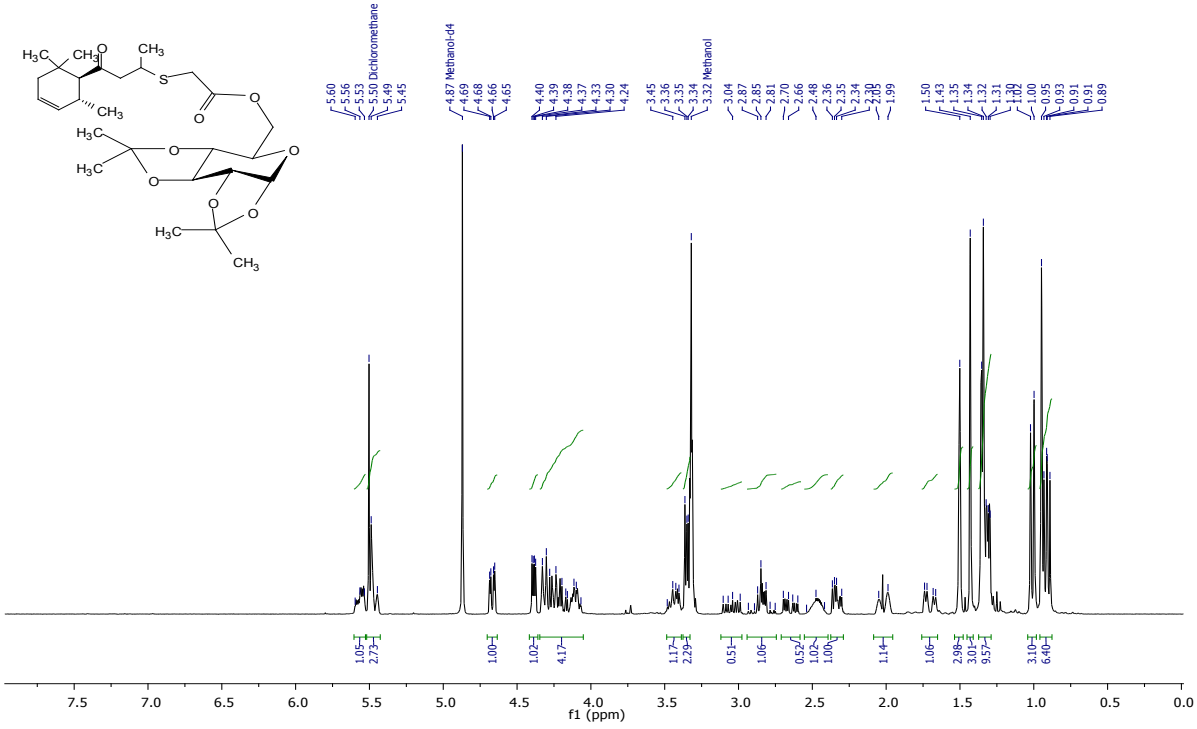

Figure S 3. ^{1}H-NMR of ((3a*R*,5*R*,5a*R*,8a*S*,8b*R*)-2,2,7,7-Tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)methyl 2-((4-oxo-4-((1*RS*,2*SR*)-2,6,6-trimethylcyclohex-3-en-1-yl)butan-2-yl)thio)acetate (**2**) in MeOH-D_4 at 300 MHz.

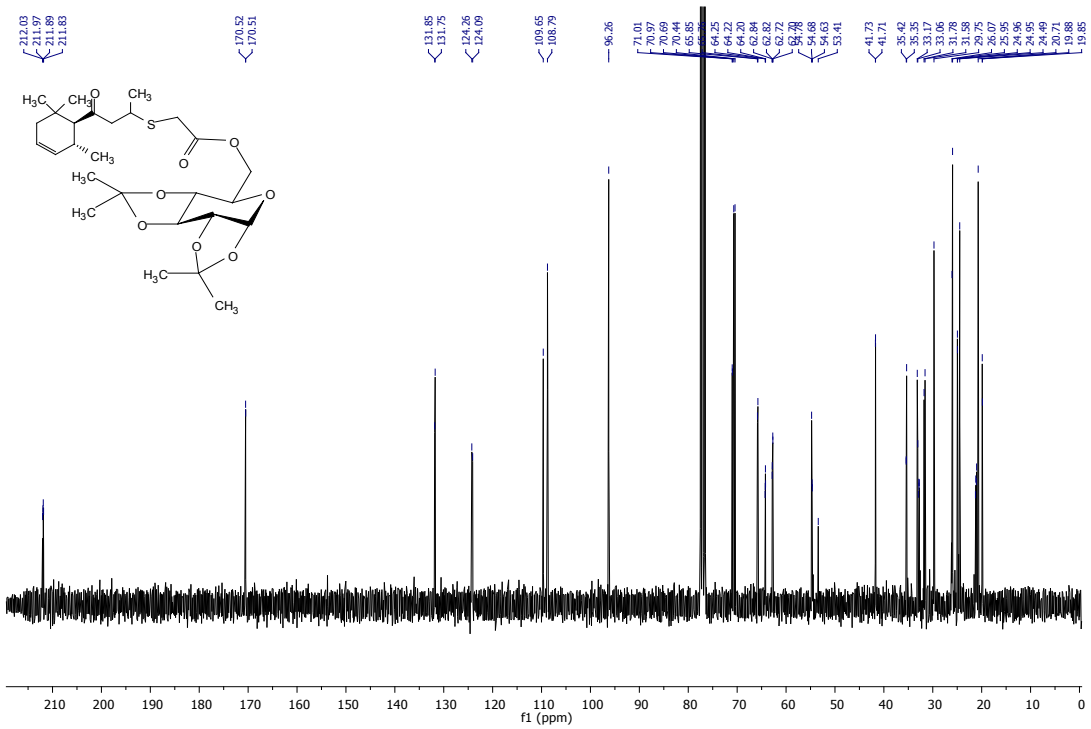

Figure S 4. ^{13}C-NMR of ((3a*R*,5*R*,5a*R*,8a*S*,8b*R*)-2,2,7,7-Tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)methyl 2-((4-oxo-4-((1*RS*,2*SR*)-2,6,6-trimethylcyclohex-3-en-1-yl)butan-2-yl)thio)acetate (**2**) in $CDCl_3$ at 300 MHz.

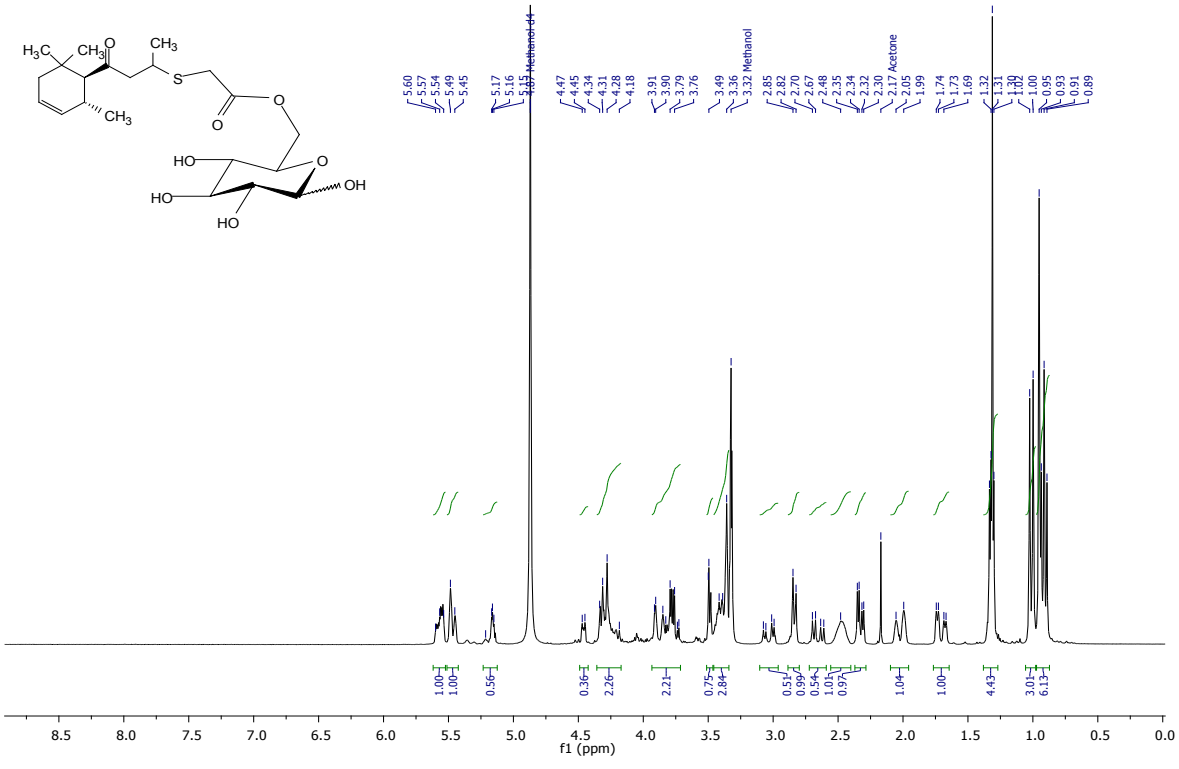

Figure S 5. ^{1}H-NMR of ((2*R*,3*S*,4*S*,5*R*,6*S*)-3,4,5,6-Tetrahydroxytetrahydro-2*H*-pyran-2-yl)methyl 2-((4-oxo-4-((1*RS*,2*SR*)-2,6,6 trimethylcyclohex-3-en-1-yl)butan-2-yl)thio)acetate (**3**) in MeOH-D_4 at 300 MHz.

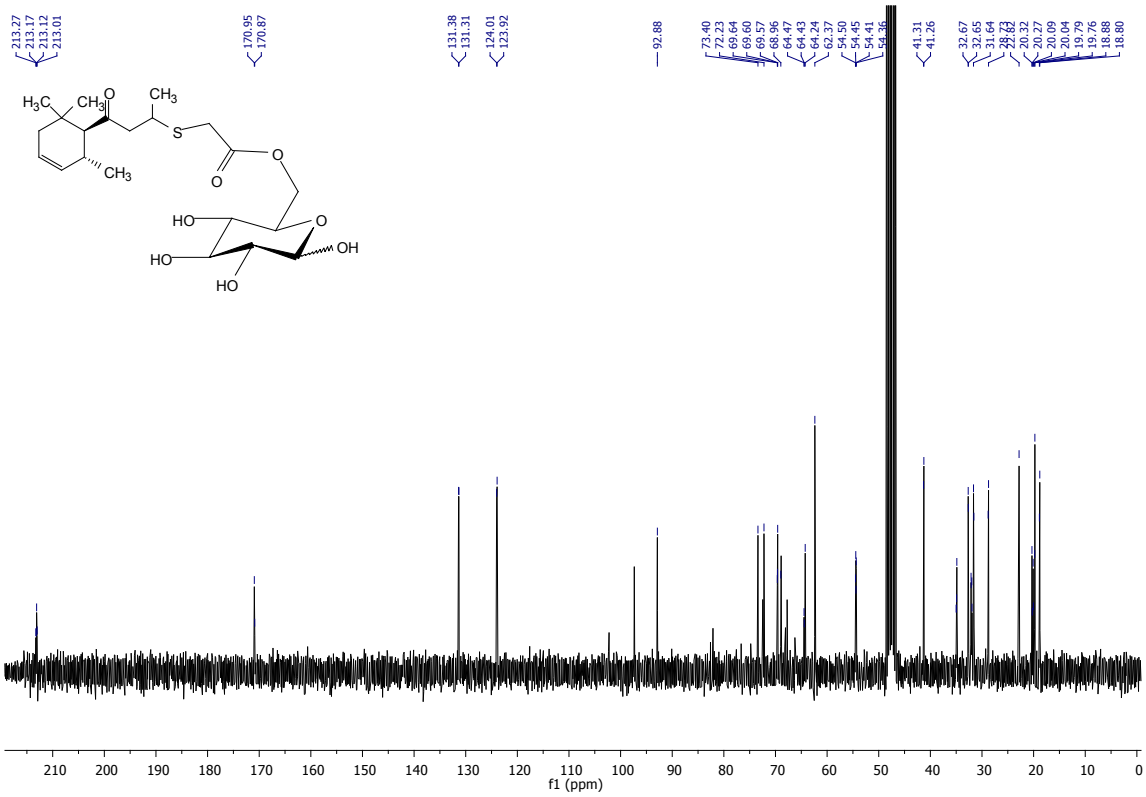

Figure S 6. ^{13}C-NMR of ((2*R*,3*S*,4*S*,5*R*,6*S*)-3,4,5,6-Tetrahydroxytetrahydro-2*H*-pyran-2-yl)methyl 2-((4-oxo-4-((1*RS*,2*SR*)-2,6,6 trimethylcyclohex-3-en-1-yl)butan-2-yl)thio)acetate (**3**) in MeOH-D_4 at 300 MHz.

IR spectra:

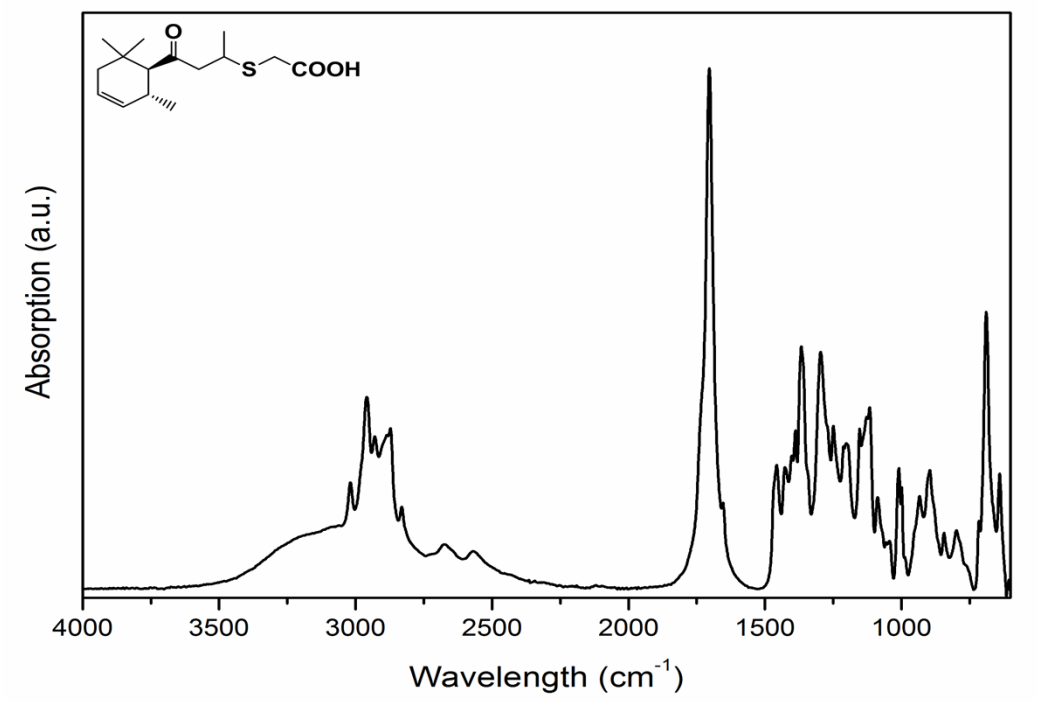

Figure S 7. IR spectra of (±)-2-((4-Oxo-4-((1*RS*,2*SR*)-2,6,6-trimethylcyclohex-3-en-1-yl)butan-2-yl)thio)acetic acid (**1**).

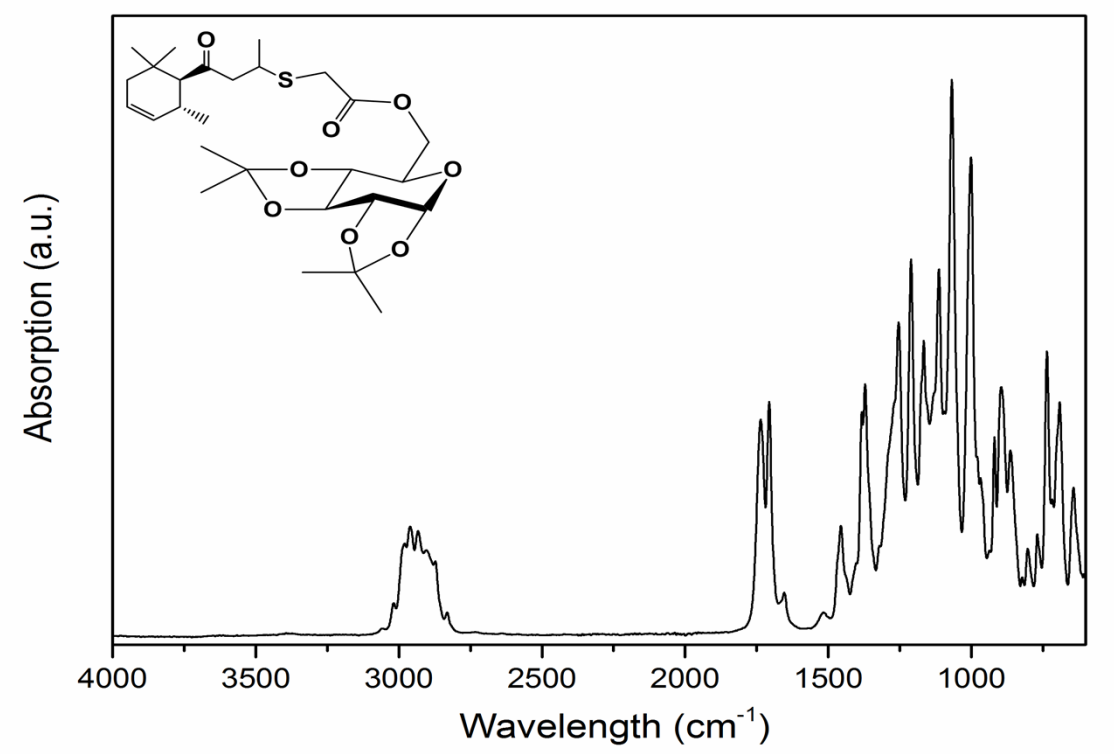

Figure S 8. IR spectra of ((3a*R*,5*R*,5a*R*,8a*S*,8b*R*)-2,2,7,7-Tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)methyl 2-((4-oxo-4-((1*RS*,2*SR*)-2,6,6-trimethylcyclohex-3-en-1-yl)butan-2-yl)thio)acetate (**2**).

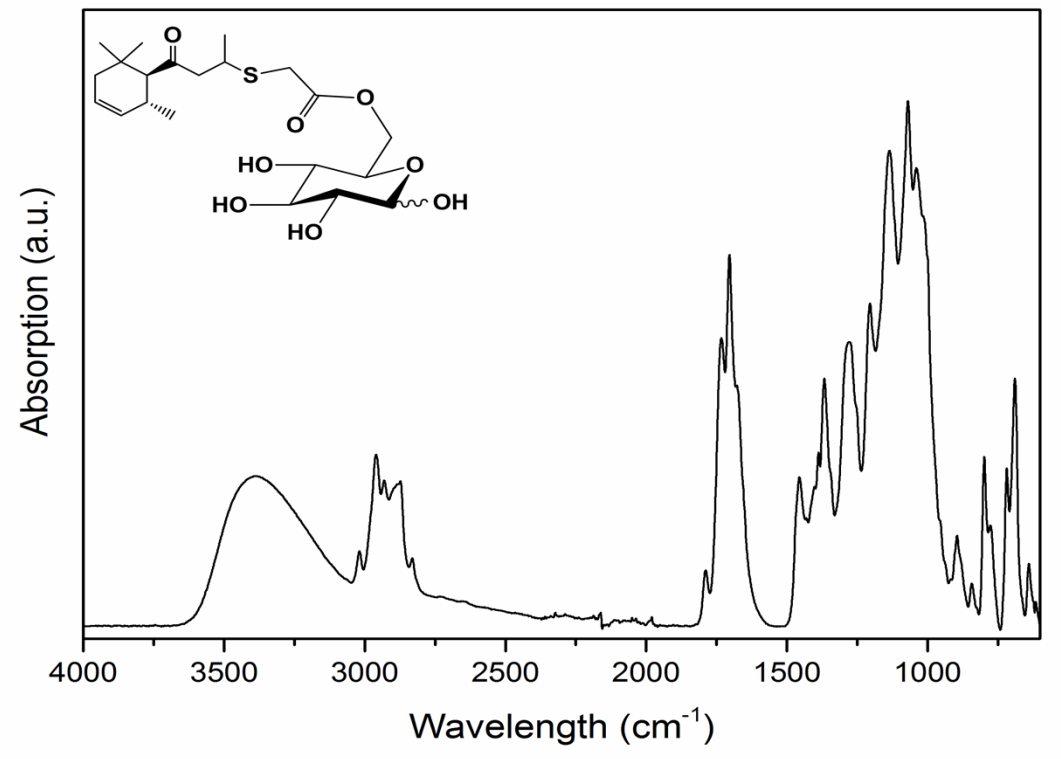

Figure S 9. IR spectra of ((2*R*,3*S*,4*S*,5*R*,6*S*)-3,4,5,6-Tetrahydroxytetrahydro-2H-pyran-2-yl)methyl 2-((4-oxo-4-((1*RS*,2*SR*)-2,6,6 trimethylcyclohex-3-en-1-yl)butan-2-yl)thio)acetate (**3**).

GCMS Spectra:

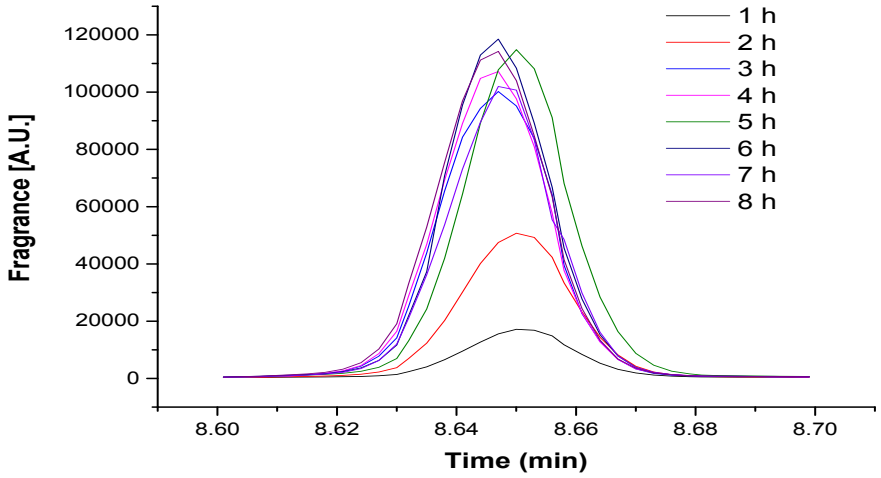

Figure S 10. Overlaid GC traces, showing the released fragrance for the 8 recorded time intervals from the protected pro-fragrance in the softener test.

Buffer preparation:

Buffer solutions (10 mL) were prepared according to previous established protocols[1] using reagent grade chemicals from Sigma-Aldrich: boric acid (anhydrous), citric acid (anhydrous), sodium hydrogen phosphate (Na_2HPO_4), monopotassium phosphate (KH_2PO_4), sodium hydroxide (NaOH) and deuterium oxide (D_2O). A 0.1 M sodium hydroxide solution was prepared by dissolving 0.4 g NaOH in 10 mL of D_2O. A buffer of pH 4 was prepared by dissolving 107.5 mg of citric acid, 25.7 mg NaCl and 0.68 mL $NaOH_{aq}$ (0.1 M) in 10 mL of D_2O. The buffer of pH 7 was prepared by dissolving 35.2 mg KH_2PO_4 and 72.6 mg Na_2HPO_4 in D_2O (10 mL). Buffer of pH 10 was prepared by dissolving 47.7 mg of boric acid and 1.8 mL of $NaOH_{aq}$ (0.1 M) in D2O (10 mL).

1. W. R. Carmody, *Journal of Chemical Education*, 1961, **38**, 559-560.