

SUPPORTING INFORMATION

New Taste-Active 3-(*O*- β -D-Glucosyl)-2-oxoindole-3-acetic Acids and Diarylheptanoids in *Cimiciato*-Infected Hazelnuts

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- Figure S1.** RP-HPLC chromatogram of MPLC fraction II-4 at $\lambda=254$ nm.
- Figure S2.** RP-HPLC chromatogram of MPLC fraction II-6 at $\lambda=254$ nm.
- Figure S3.** RP-HPLC chromatogram of MPLC fraction II-7 at $\lambda=254$ nm.
- Figure S4.** RP-HPLC chromatogram of MPLC fraction II-10 at $\lambda=254$ nm.
- Figure S5.** Excerpts of the COSY spectrum (500 MHz, MeOD- d_4) of purified 2-(3-hydroxy-2-oxoindolin-3-yl) acetic acid-3-O-6'-galacto-pyranosyl-2''-(2''oxoindolin-3''yl)acetate **2** showing $^3J_{H,H}$ coupling of the aromatic protons.
- Figure S6.** Excerpts of the HMBC spectrum (400 MHz, MeOD- d_4) of purified **3** showing 2J and 3J coupling of C(3) and 2J coupling of C(9).
- Figure S7.** Excerpts of the HMBC spectrum (500 MHz, DMSO- d_5) of purified **5** showing 2J and 3J coupling of C(7) and C(13).
- Figure S8.** Excerpts of the HMBC spectrum (500 MHz, DMSO- d_5) of purified **5** showing 2J , 3J and 4J coupling of C(9), C(11) and C(10).
- Figure S9.** Excerpts of the COSY spectrum (500 MHz, MeOD- d_4) of purified **6** showing $^3J_{H,H}$ coupling between the protons of the alkyl chain.
- Figure S10.** Excerpts of the HMBC spectrum (500 MHz, MeOD- d_4) of purified **6** showing ^{2-4}J coupling of C(1) and C(2) and 3J coupling of C(13).
- Table S1.** Monitored Mass Transitions and Optimized MS/MS Parameters of the Quantitative Analysis of compounds **1-4** and **6** and the Internal Standards IS1 and IS2.

Figure S1 (Singldinger et al.)

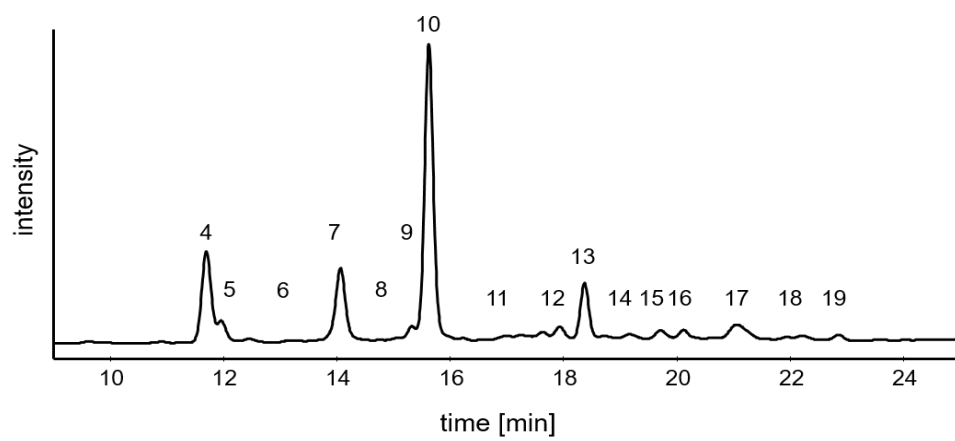


Figure S2 (Singldinger et al.)

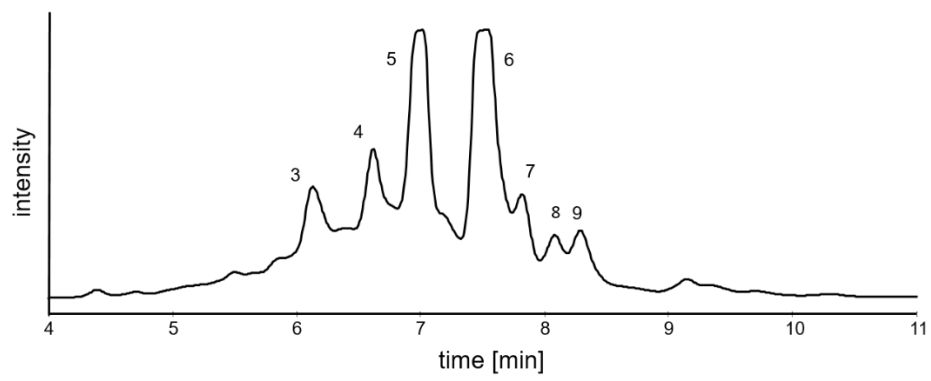


Figure S3 (Singldinger et al.)

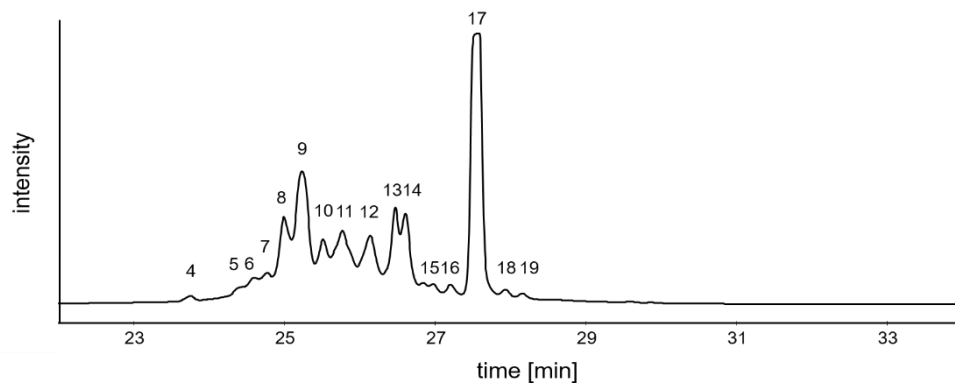


Figure S4 (Singldinger et al.)

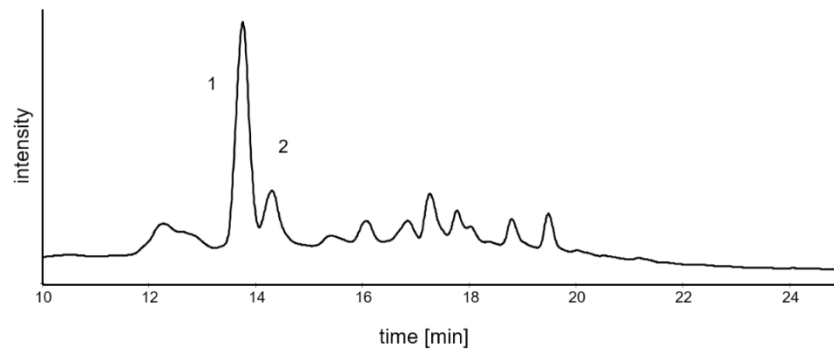


Figure S5 (Singldinger et al.)

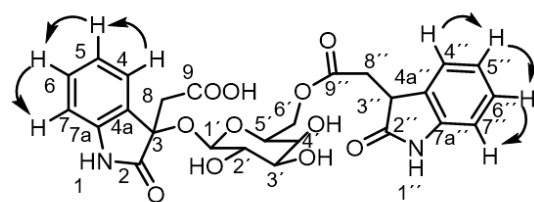
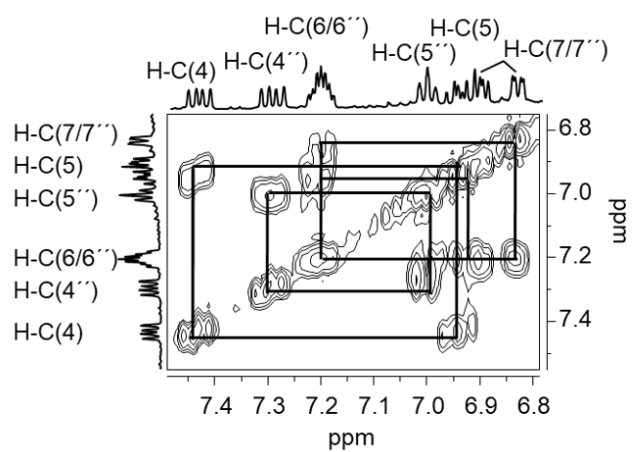


Figure S6 (Singldinger et al.)

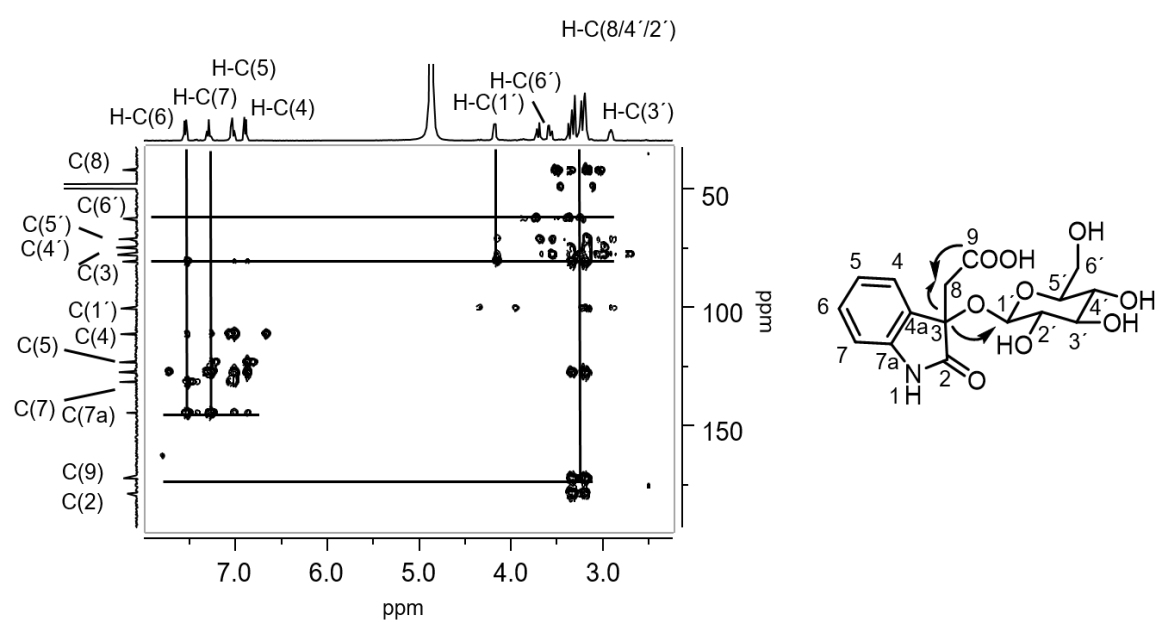


Figure S7 (Singldinger et al.)

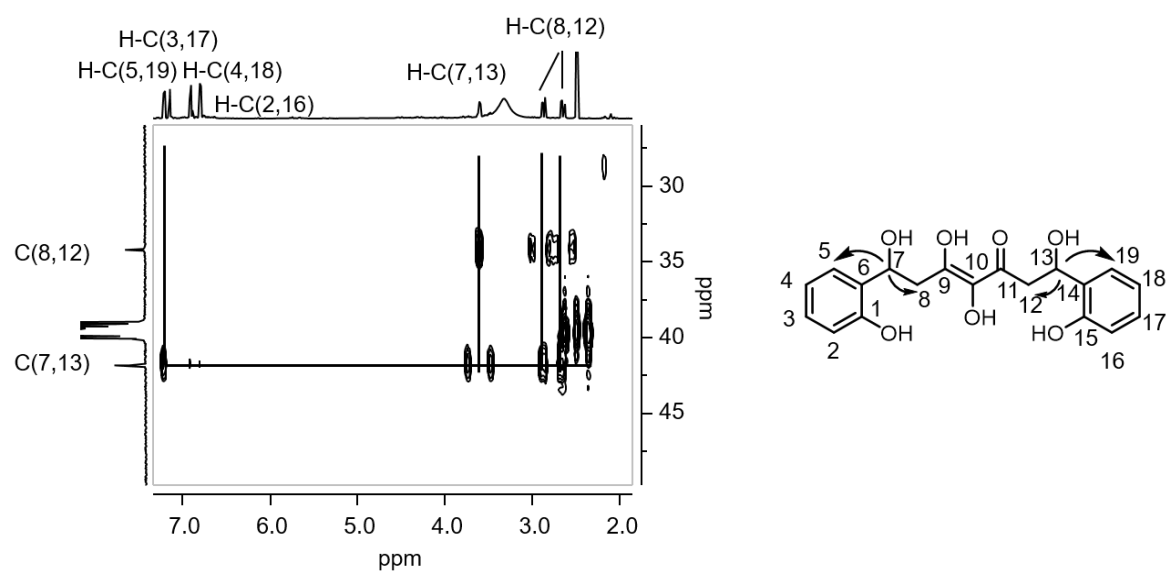


Figure S8 (Singldinger et al.)

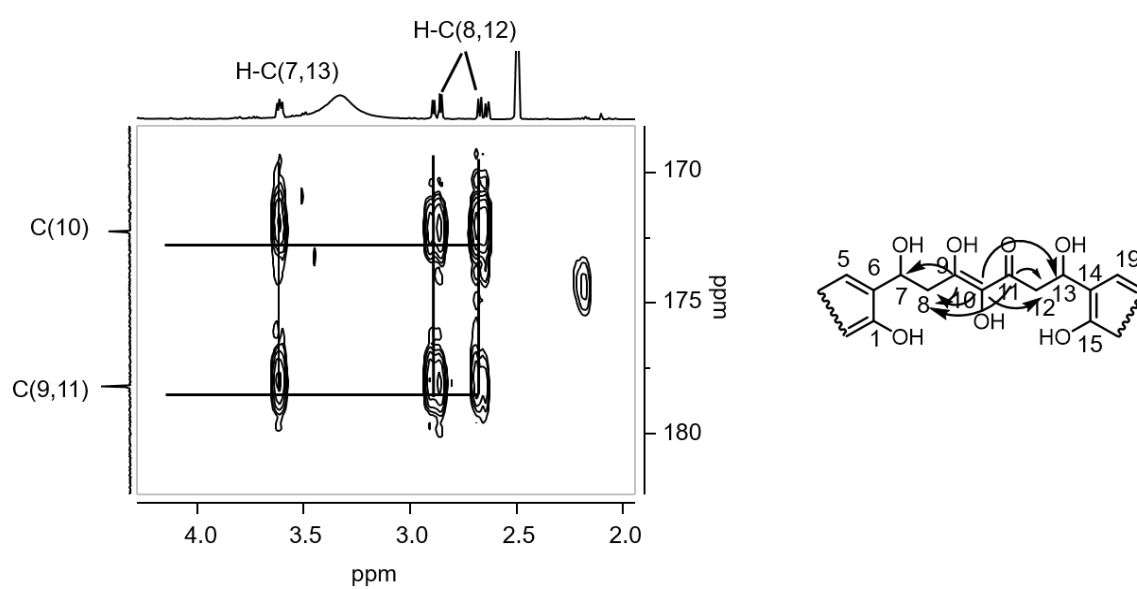


Figure S9 (Singldinger et al.)

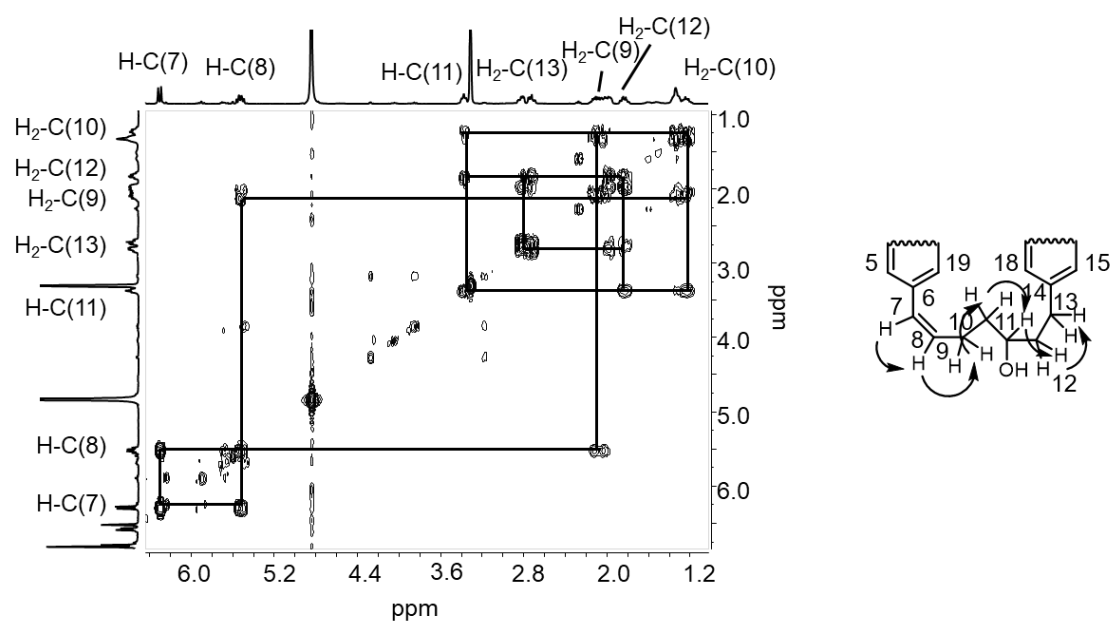


Figure S10 (Singldinger et al.)

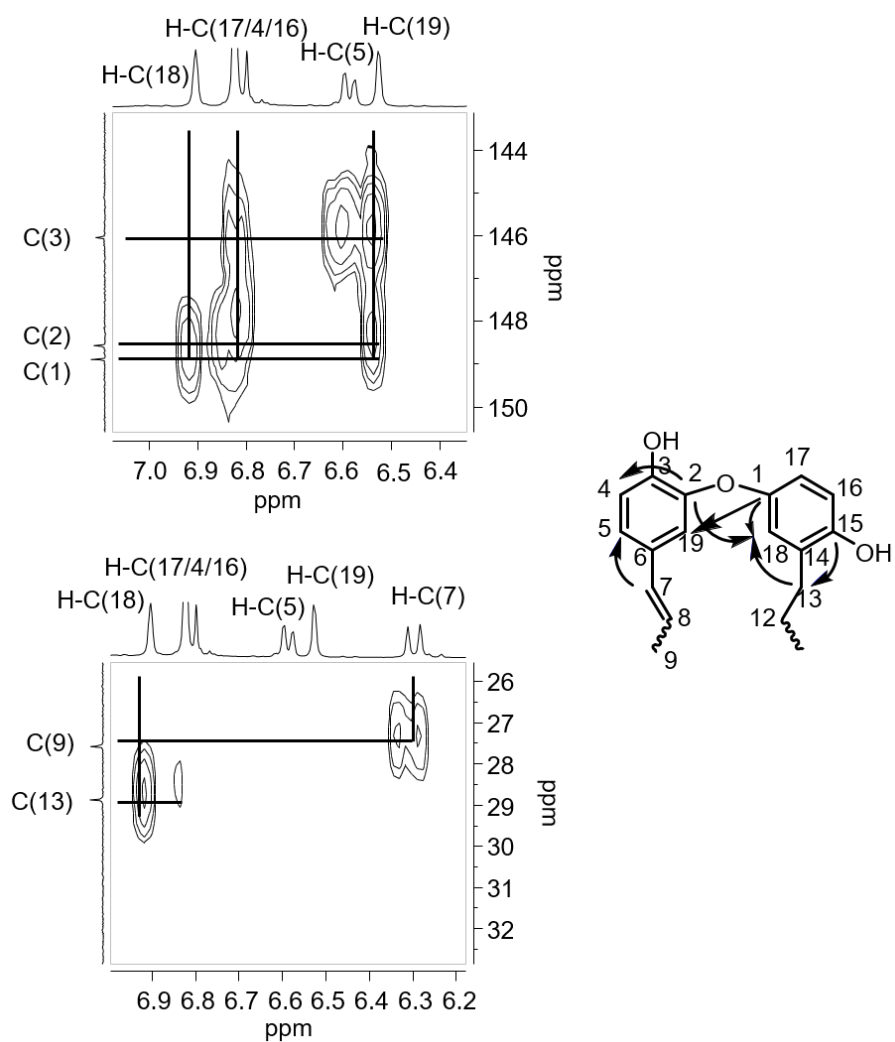


Table S1: Monitored Mass Transitions and Optimized MS/MS Parameters of the Quantitative Analysis of compounds **1-4** and **6** and the Internal Standards IS1 and IS2.

analyte/standard no. ^a	Q1	Q3	DP ^b	CE ^c	CXP ^d
asadanin (1)	343.0	211.0	-35	-38	-25
2-(3-hydroxy-2-oxoindolin-3-yl) acetic acid-3-O-6'-galactopyranosyl-2''-(2''oxoindolin-3''yl) acetate (2)	541.0	189.9	-110	-42	-23
3-(-O-β-D-glycosyl)dioxindol-3-acetic acid (3)	368.0	144.1	-20	-22	-3
Giffonin P (4)	361.1	241.0	-5	-40	-23
4,12,16-trihydroxy-2-oxatricyclo[13.3.1.1 ^{3,7}]-nonadeca-1(18),3,5,7(20),8,15,17-heptaene (6)	311.1	161.1	-55	-26	-13
L-tryptophane- <i>d</i> ₅ (IS1)	208.0	120.9	-85	-24	-21
myricanol (IS2)	357.1	327.0	-15	-30	-9

^aChemical structures of the individual compounds **1-4** and **6** are given in **Figure 1**, structures of the internal standards are given in **Figure 5B**. ^bdeclustering potential [V], ^ccollision energy [V], ^dcollision cell exit potential [V].