# Supplementary Materials

# Plasma-Induced Oxidation Products of (–)-Epigallocatechin Gallate with Digestive Enzymes Inhibitory Effects

**Gyeong Han Jeong and Tae Hoon Kim ***

Department of Food Science and Biotechnology, Daegu University, Gyeongsan 38453, Korea; jkh4598@hanmail.net

* Correspondence: skyey7@daegu.ac.kr; Tel.: +82-53-850-6533

# Contents

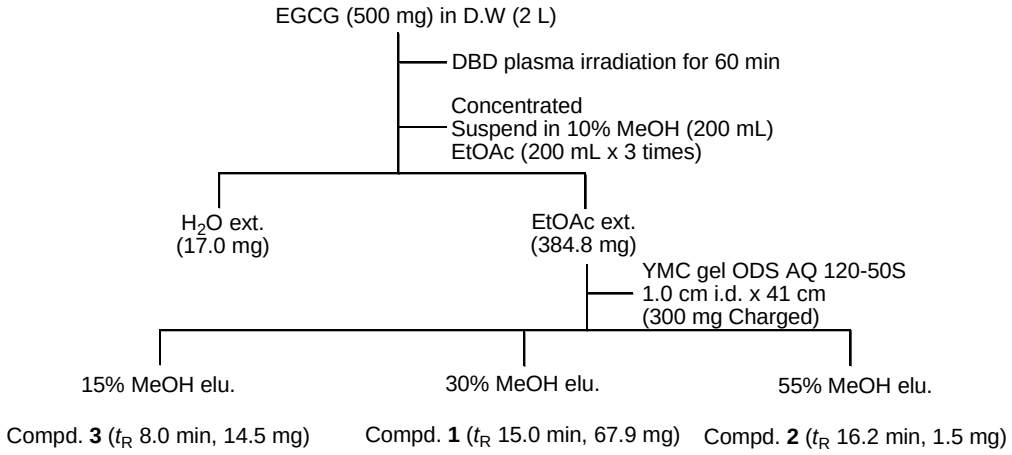
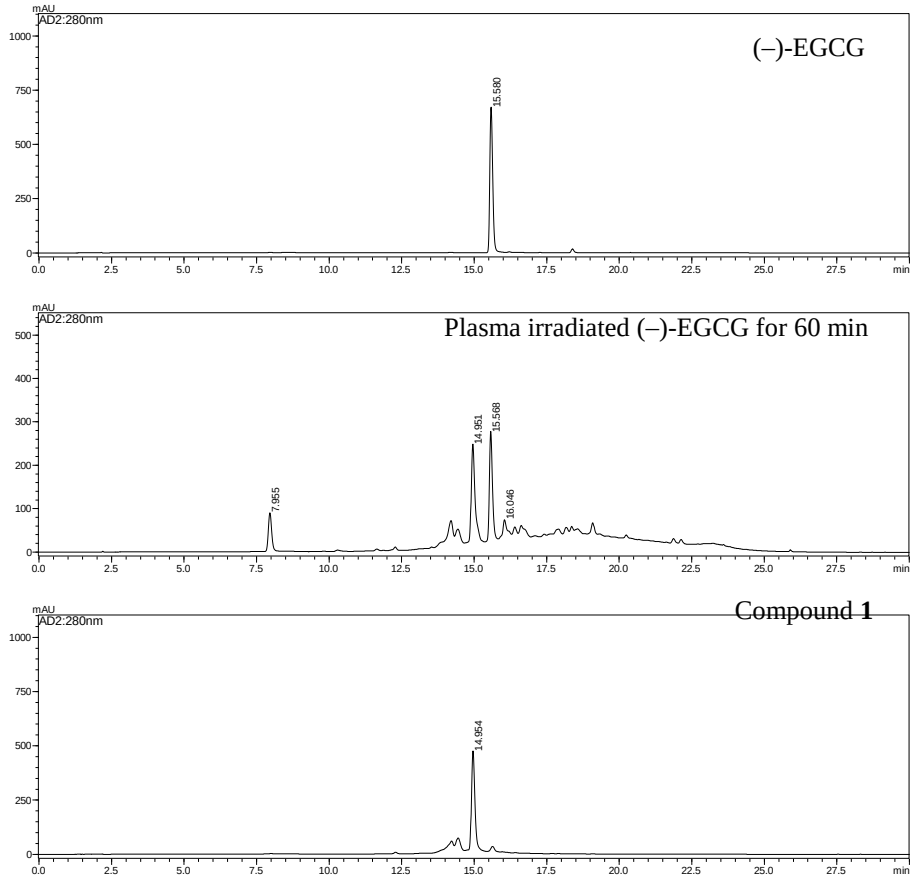



**Figure S1.** Isolation procedure of plasma irradiated EGCG in aqueous solution.



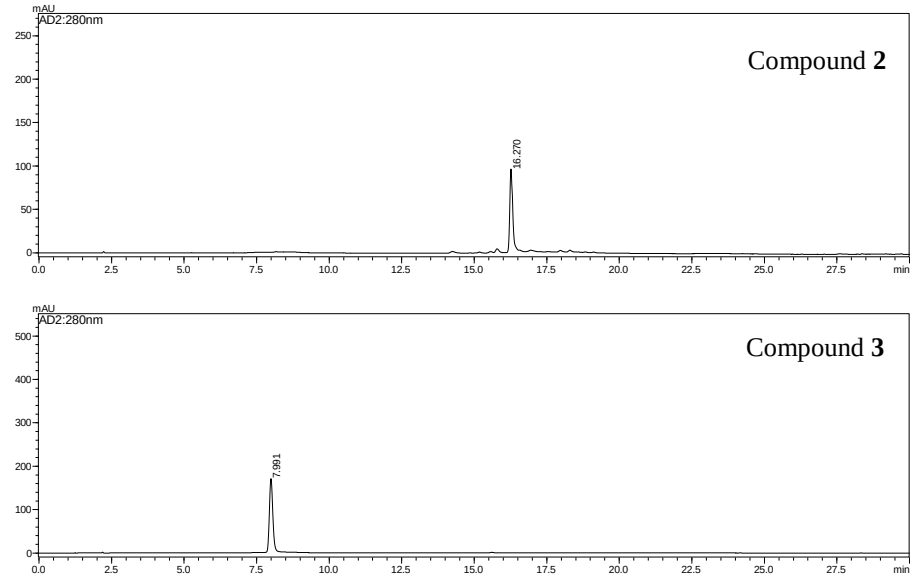



**Figure S2.** HPLC chromatograms of isolated compounds **1**-**3**.

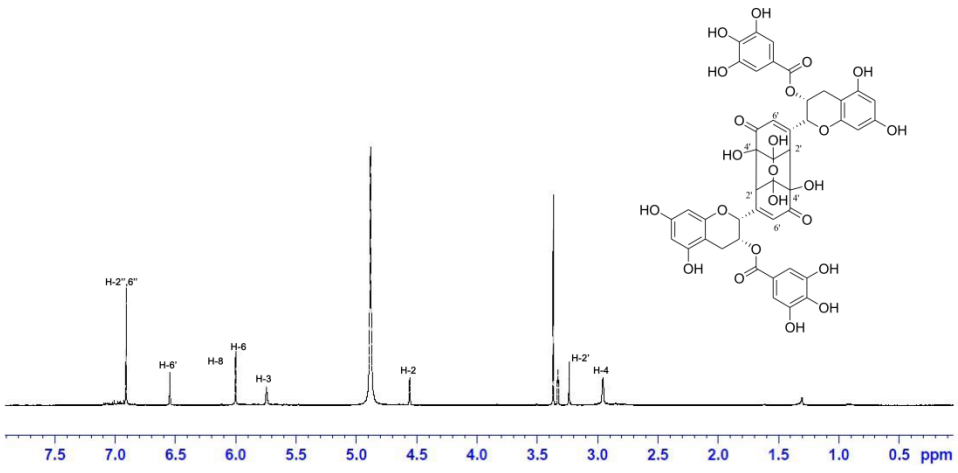



**Figure S3.** $^{1}$H NMR spectrum of compound **1** in $CD_3OD$.

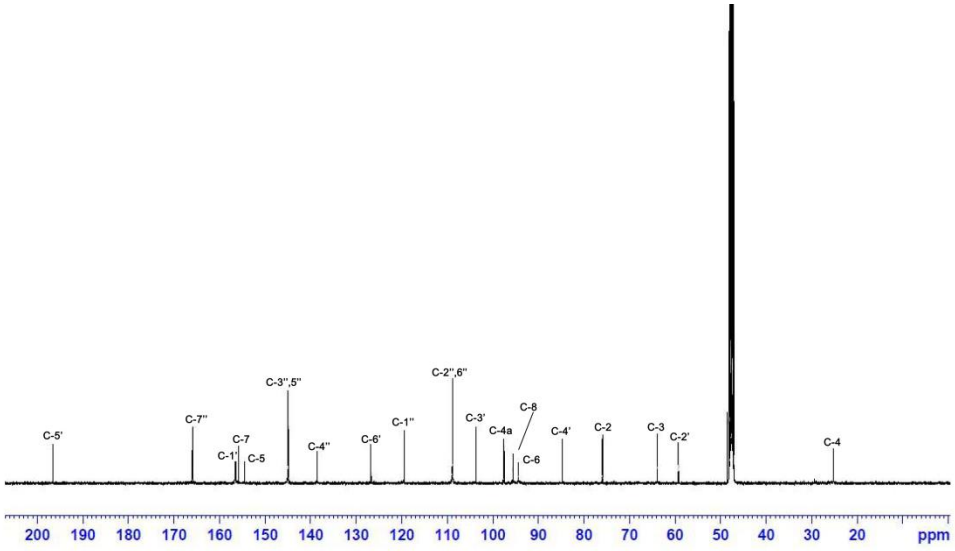



**Figure S4.** $^{13}C$ NMR spectrum of compound **1** in $CD_3OD$.

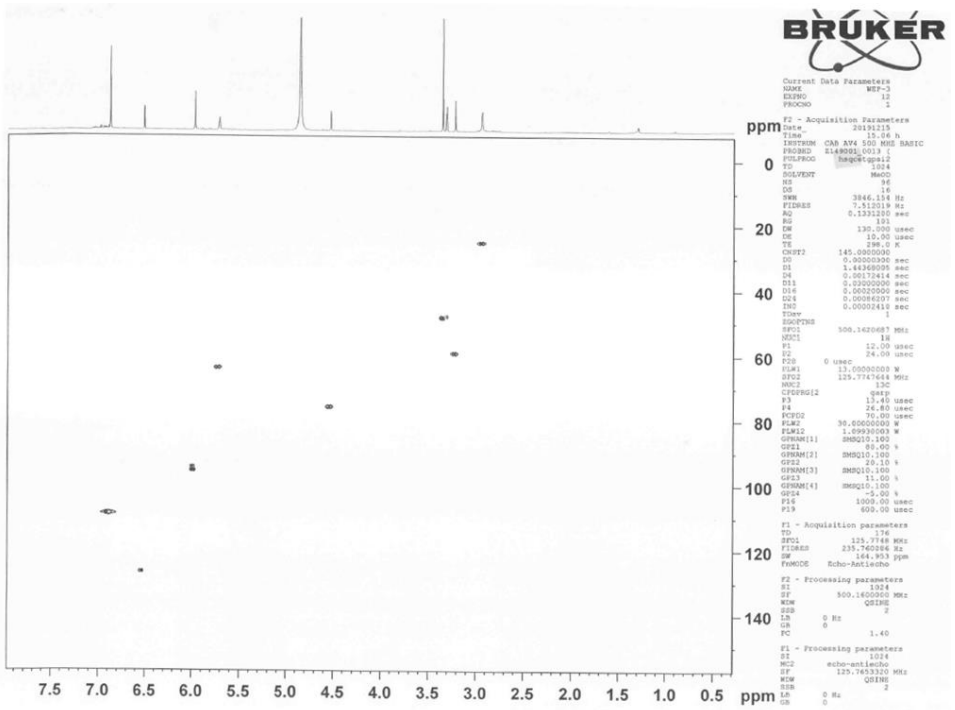



**Figure S5.** HSQC spectrum of compound **1** in $CD_3OD$.

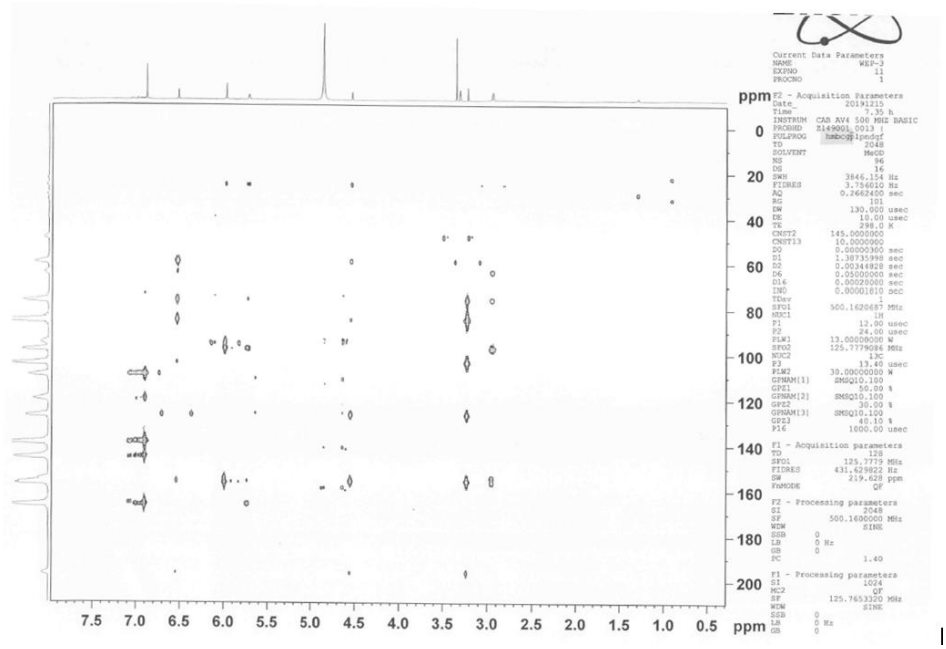



**Figure S6.** HMBC spectrum of compound **1** in $CD_3OD$.

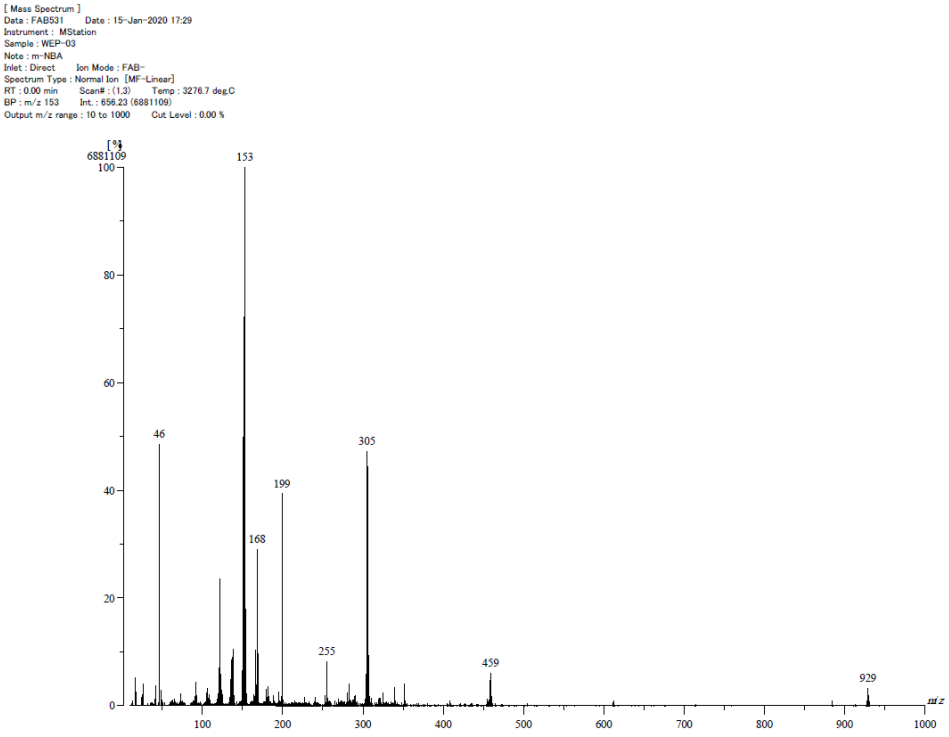



**Figure S7.** FABMS spectrum of compound **1**.

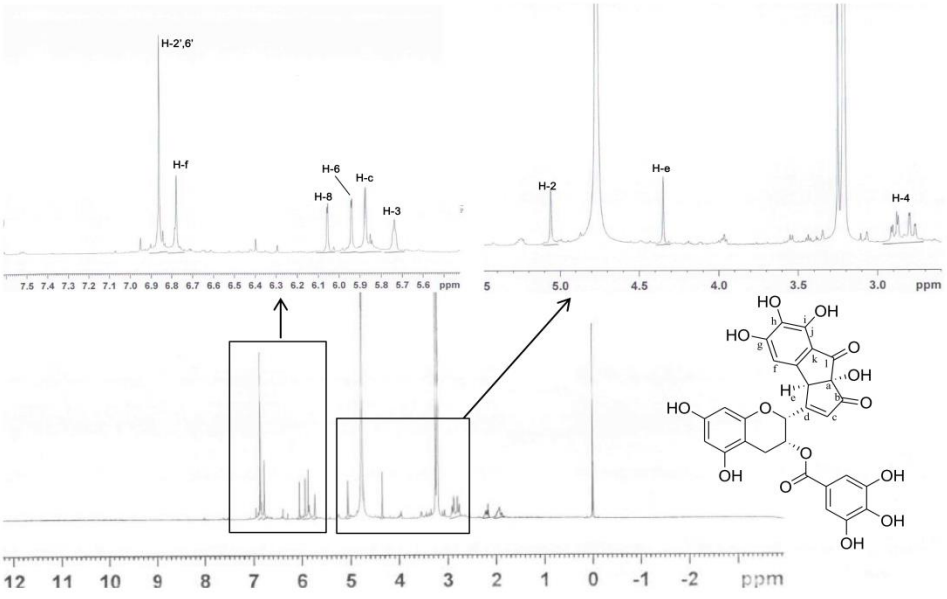



**Figure S8.** $^{1}$H NMR spectrum of compound **2** in $CD_3OD$.

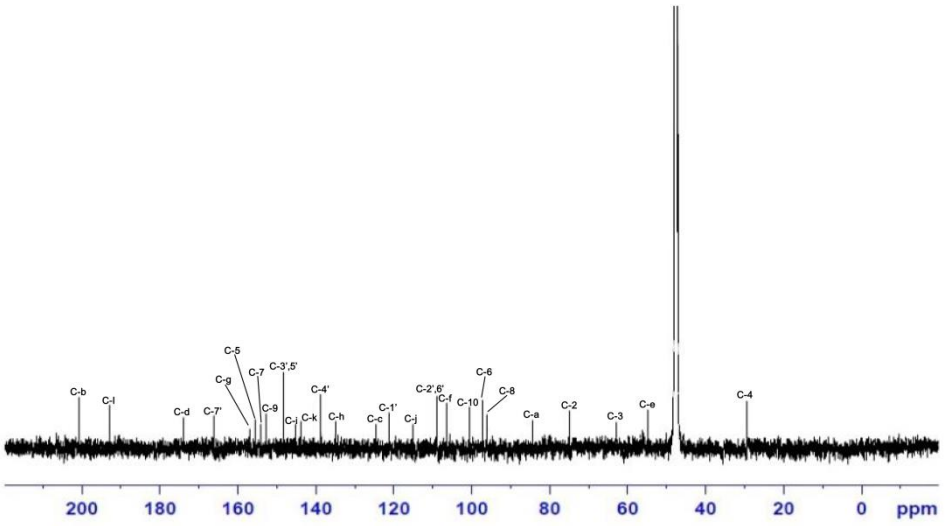



**Figure S9.** $^{13}$C NMR spectrum of compound **2** in $CD_3OD$.

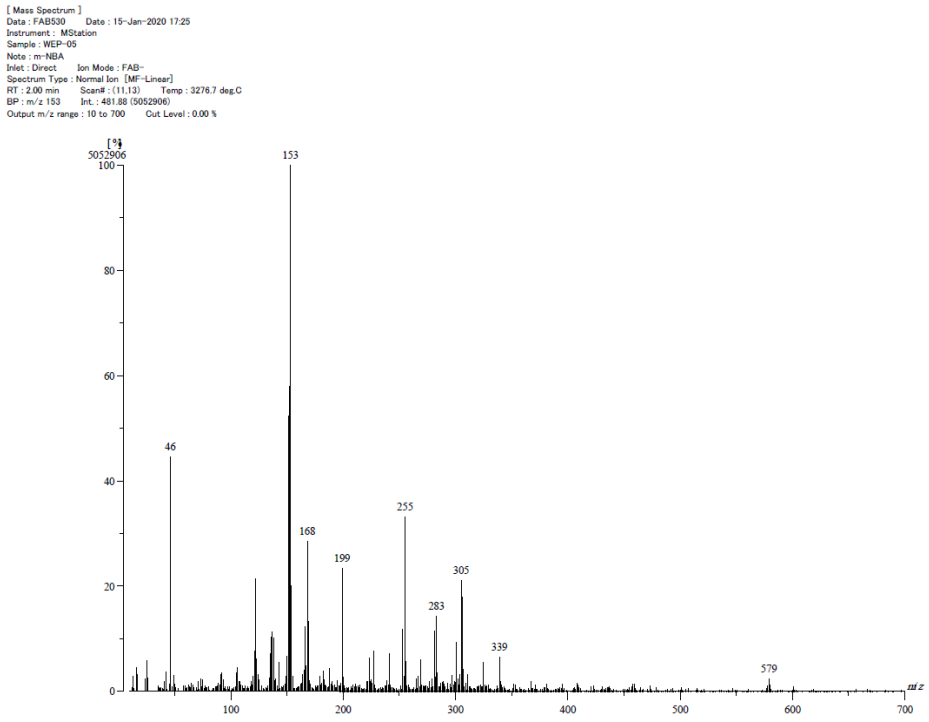



**Figure S10.** FABMS spectrum of compound **2**.

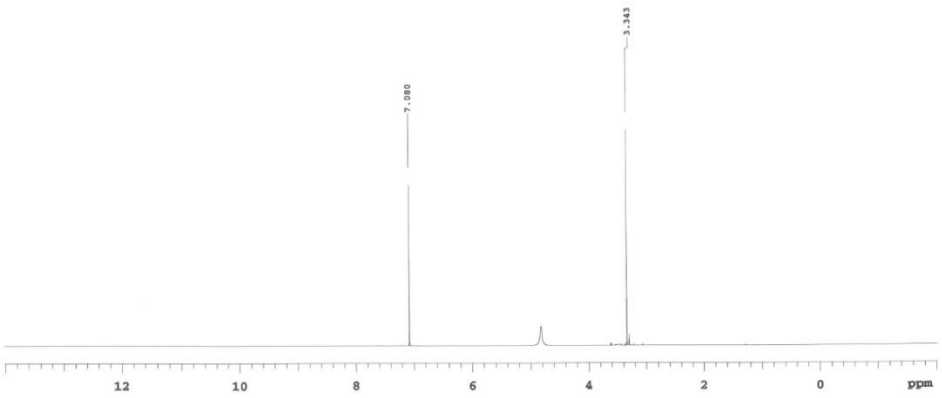


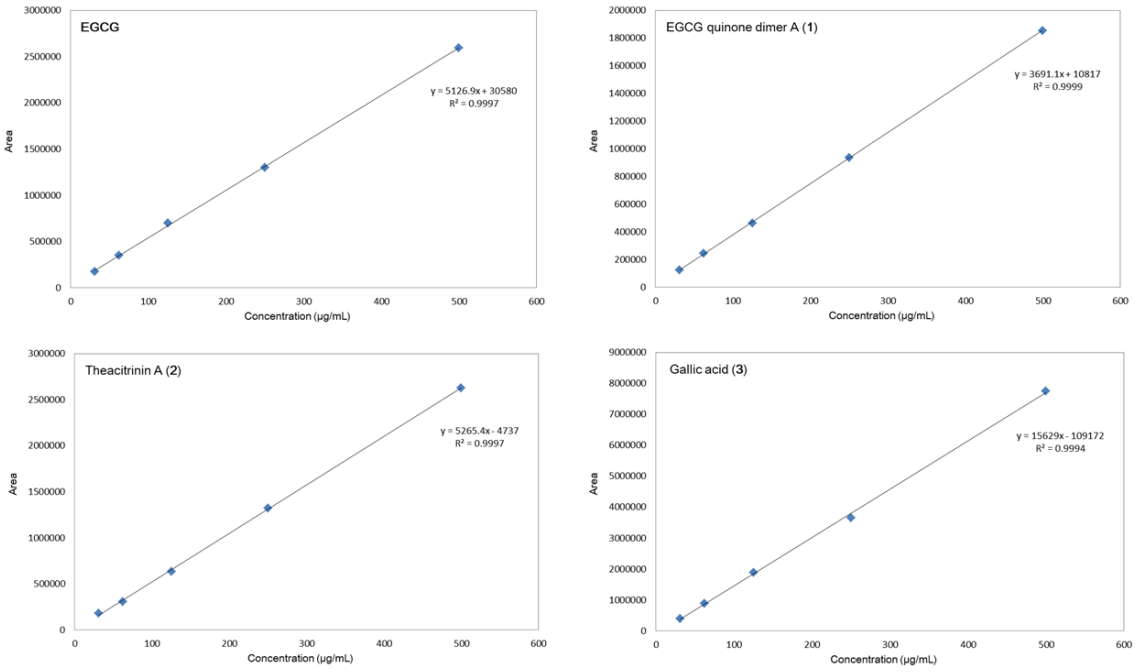

**Figure S11.** $^{1}$H NMR spectrum of compound **3** in $CD_3OD$.

EGCG quinone dimer A (**1**): Brown amorphous powder, $[\alpha]^{25}_{D}$ -62.3 (*c* 0.1, MeOH), FABMS *m/z* 929 $[M–H]^–$, $^{1}$H NMR (500 MHz, $CD_3OD$): $\delta$ 6.92 (4H, s, H-2", 6"), 6.54 (2H, d, $J$ = 1.0 Hz, H-6'), 6.03 (2H, d, $J$ = 2.0 Hz, H-8), 5.99 (2H, d, $J$ = 2.0 Hz, H-6), 5.68 (2H, br dd, $J$ = 4.0, 1.0 Hz, H-3), 4.56 (2H, br s, H-2), 3.22 (2H, br s, H-2'), 2.95 (2H, m, H-4), 2.93 (2H, m, H-4), $^{13}$C NMR (125 MHz, $CD_3OD$): $\delta$ 196.5 (C-5'), 165.9 (C-7"), 156.6 (C-7), 156.5 (C-9), 155.8 (C-1'), 154.4 (C-5), 144.9 (C-3", 5"), 138.5 (C-4"), 126.7 (C-6'), 119.6 (C-1"), 108.9 (C-2",

6''), 103.7 (C-3'), 97.7 (C-10), 95.6 (C-8), 94.4 (C-6), 84.7 (C-4'), 75.9 (C-2), 63.8 (C-3), 59.2 (C-2'), 25.2 (C-4).

Theacitrinin A (**2**): Brown amorphous powder, $[\alpha]^{25}_{D}$ +104.8 (*c* 0.1, MeOH), FABMS *m/z* 579 $[M–H]^-$, $^1$H NMR (500 MHz, $CD_3OD$): $\delta$ 6.95 (2H, s, H-2', 6'), 6.71 (1H, s, H-f), 6.05 (1H, d, $J$ = 2.0 Hz, H-8), 5.98 (1H, d, $J$ = 2.0 Hz, H-6), 5.85 (1H, br s, H-c), 5.73 (1H, m, H-3), 5.23 (1H, br s, H-2), 4.35 (1H, s, H-e), 2.91 (1H, dd, $J$ = 17.0, 4.0 Hz, H-4), 2.80 (1H, dd, $J$ = 17.0, 1.0 Hz, H-4), $^{13}$C NMR (125 MHz, $CD_3OD$): $\delta$ 200.1 (C-b), 193.9 (C-l), 174.0 (C-d), 166.0 (C-7'), 157.0 (C-g), 156.9 (C-5), 156.1 (C-7), 155.0 (C-9), 148.2 (C-3', 5'), 145.1 (C-i), 143.0 (C-k), 138.9 (C-4'), 134.0 (C-h), 125.0 (C-c), 122.0 (C-1'), 115.0 (C-j), 108.8 (C-2', 6'), 106.1 (C-f), 100.4 (C-10), 97.2 (C-6), 95.9 (C-8), 84.8 (C-a), 73.1 (C-2), 63.0 (C-3), 54.8 (C-e), 29.0 (C-4).

Gallic acid (**3**): White amorphous powder, $^1$H NMR (500 MHz, $CD_3OD$): $\delta$ 7.08 (2H, s, H-2, 6).




| Compounds | $t_R$ (min) | UV $\lambda_{max}$ (nm) | $[M–H]^-$ | Regression equation[a] ($Y$=a$X$+b, $R^2$) | Linear range (μg/mL) |
|---|---|---|---|---|---|
| (-)-EGCG | 15.6 | 224, 280 | 457 | $Y$ = 5126.9$X$+30580, 0.9997 | 500-31.25 |
| **1** | 15.0 | 276 | 929 | $Y$ = 3691.1$X$+10817, 0.999 | 500-31.25 |
| **2** | 16.2 | 277, 345 | 579 | $Y$ = 5265.4$X$-4737, 0.9997 | 500-31.25 |
| **3** | 8.0 | 214, 268 | 169 | $Y$ = 15629$X$-109172, 0.9994 | 500-31.25 |

[a] $Y$ = peak area and $X$ = concentration.

**Figure S12.** Calibration curve of EGCG and oxidation products **1**-**3**.

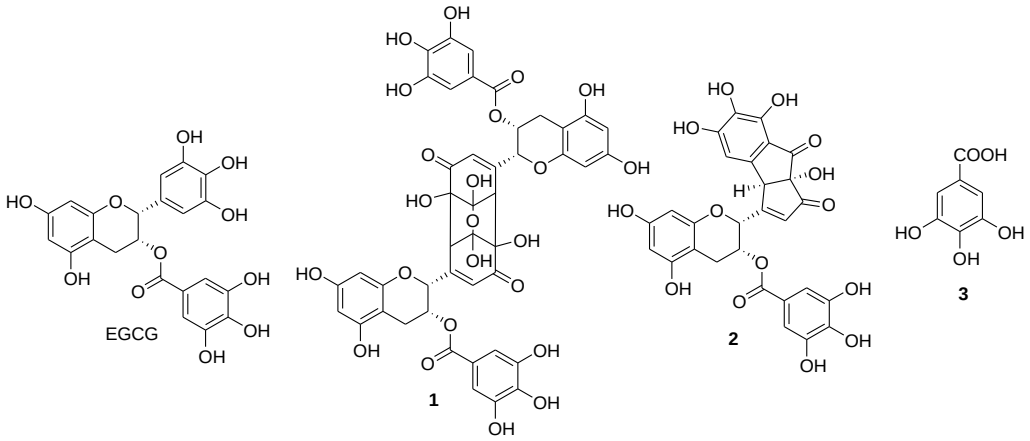



**Figure S13.** Chemical structures of isolated compounds **1**-**3**.