

Supplementary Material

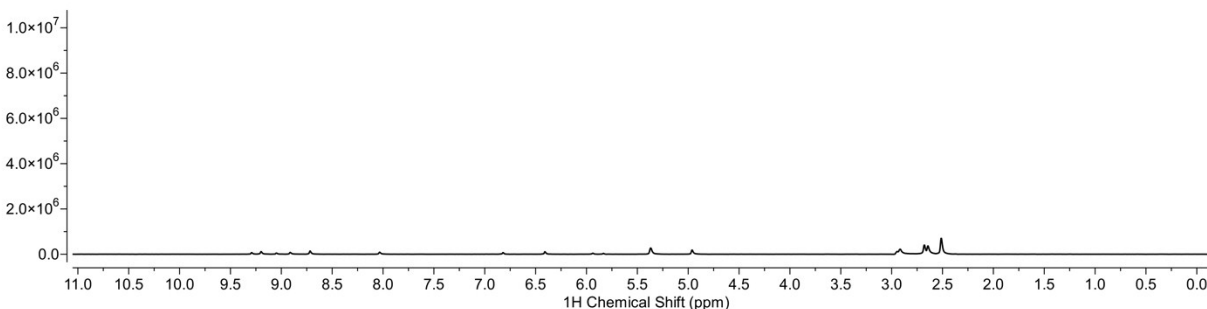


Figure S1 Difference Spectra of EGCG. A STD-NMR experiment on EGCG at 25 mM acquired in DMSO- d_6 in the absence of peptide receptor α_2 -gliadin (57-89) result in very small ligand signal in the difference spectra. This negative control demonstrates that the presence of ligand signal in the difference spectra. This negative control demonstrates that the presence of ligand signal in the experiments run in the presence of α_2 -gliadin (57-89) appear as a result of peptide-ligand interaction and saturation transfer rather than direct saturation of the ligand. In STD-NMR experiments, the control difference spectra acquired with EGCG alone was subtracted from the experimental difference spectra.

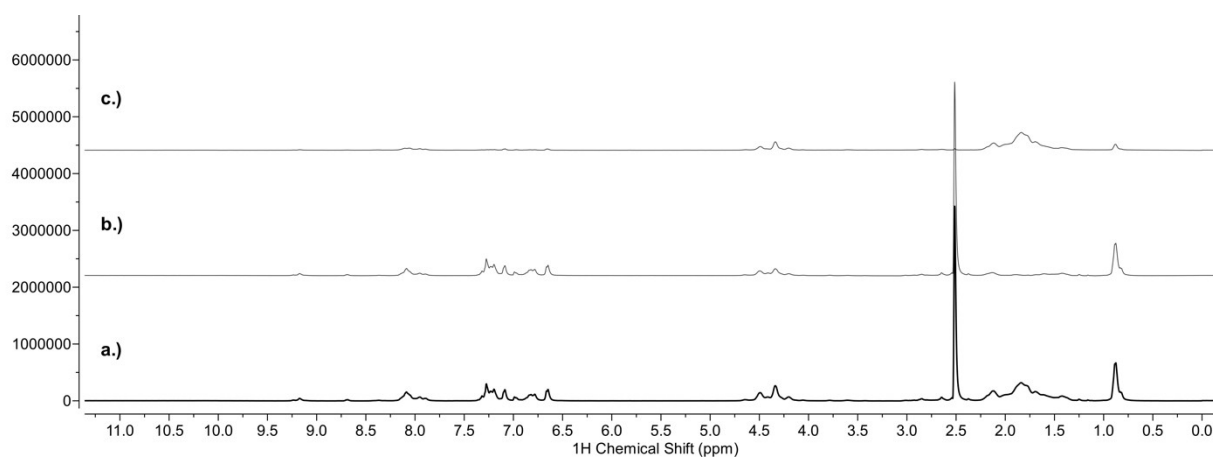


Figure S2 STD-NMR of α_2 -gliadin (57-89) in the Absence of Ligands. Off-resonance (reference) (a), on-resonance (b) and difference (c) spectra of α_2 -gliadin (57-89) at a

concentration of 0.25 mM in DMSO-d₆. Spectra are presented at 1:1:1 ratio. The presence of peptide signal in (c) results from the attenuation at the saturation point (1.8 ppm) and spin diffusion for the remaining signals.

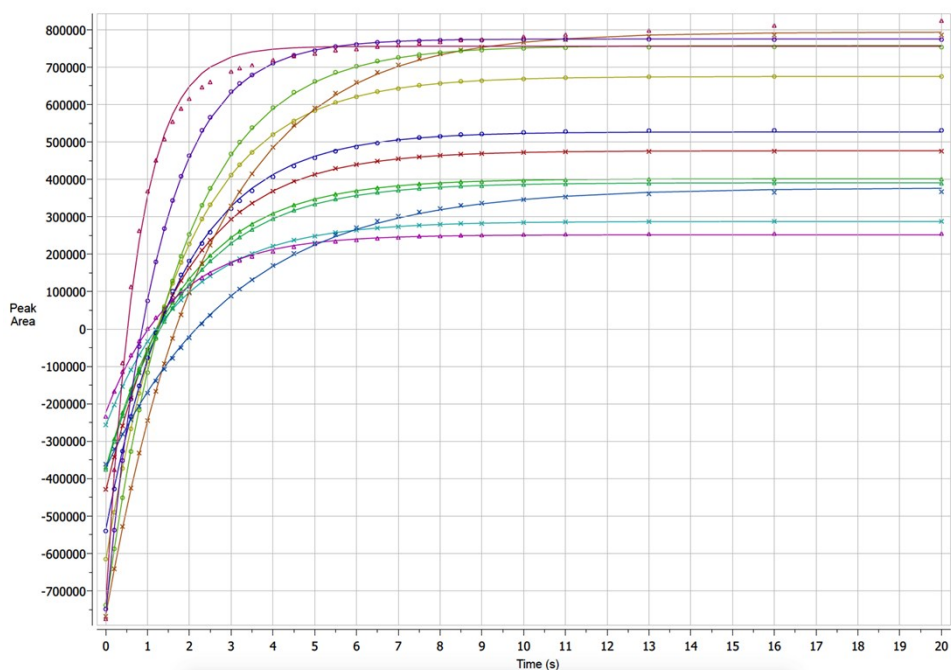


Figure S3 Calculation of T₁ Proton Relaxation Time for Ligand EGCG. Inversion-Recovery was used to measure the relaxation time of EGCG signal in a sample of EGCG and α₂-gliadin (57-89) at a 100:1 molar ratio in DMSO-d₆.

Signal	T ₁ (s)
H-2	1.27
H-4	0.76
H-5	1.60
H-6	1.93
H-7	1.89
H-8	3.14
H-9,13	1.83
H-9',13'	2.47
H-10,12	1.89
H-10',12'	1.79
H-11	1.88
H-11'	1.87

Table S1 T1 Proton Relaxation Times for Ligand EGCG. Values were calculated from Inversion-Recovery experiments (Figure S4). The 0.5-3 second relaxation rates of the EGCG protons ensure full relaxation of all of the protons within the 14-second recycle delay of the experiment.

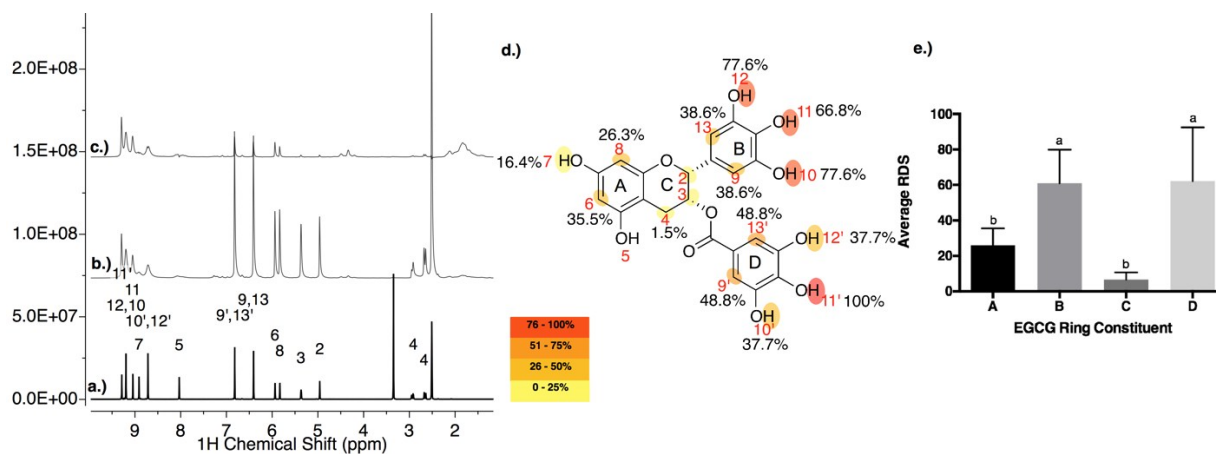


Figure S4 EGCG/ α_2 g interactions are localized to galloyl moieties on EGCG. The following descriptions corresponds to spectra a-c, which were recorded in DMSO-d₆: (a) ¹H NMR spectrum of EGCG (25 mM). (b) Reference spectrum of EGCG and α_2 -gliadin (57-89) in a

100:1 molar ratio and (c) corresponding difference spectrum, shown at a 1:4 ratio. (d) Relative degree of saturation of EGCG hydrogens upon interaction with α_2 -gliadin (57-89) normalized to that of H-11'. The following hydrogens that produced detectable STD signals that are not listed are H-2, 6.7%; H-3, 6.0%. Saturation signals for H-10,12; H-9',13' and H-9,13 are quantified as averages due to overlapping signals. STD signal from H-5 could not be measured due to overlap with α_2 -gliadin (57-89) signal. (e) Average relative degrees of saturation per EGCG ring constituent. Different letters denote significant differences in relative degree of saturation between ring constituents ($p \leq 0.05$).