

Food & Function

Electronic Supplementary Information

Corn cob and corn silk-based ingredients exhibit bioaccessible and antioxidant phenolic compounds displaying anti-inflammatory effects in vitro

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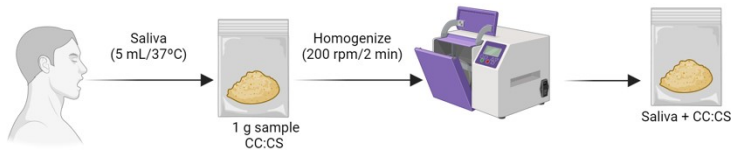
Supplementary Table S1. Binding energies between selected phenolic compounds and a model 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC), 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanoamine (POPE), and cholesterol membrane.

Phenolic compounds	Gibbs' Free energy (ΔG)
<i>Hydroxybenzoic acids</i>	
Gallic acid	-6.30
2,3-dihydroxybenzoic acid	-6.40
Syringic acid	-6.40
<i>Hydroxycinnamic acids</i>	
<i>p</i> -Coumaric acid	-8.10
Chlorogenic acid	-8.60
Ferulic acid	-7.30
<i>Flavanols</i>	
(+)-Catechin	-9.40

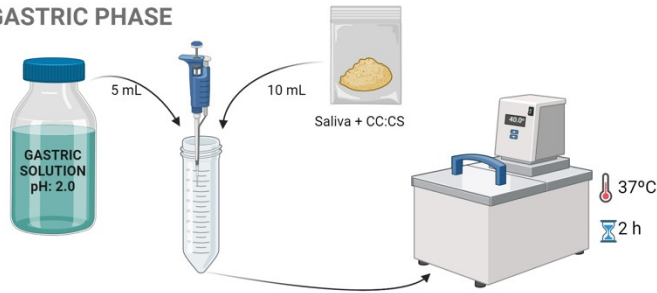
Supplementary Table S2. Main energy binding values between selected (poly)-phenols and inflammation targets at two experimental pH values (5.7 and 7.0) in a model of membrane instability.

Compounds	PGE ₂		COX-2		PPAR _γ		PAF-R	
	pH	pH	pH	pH	pH	pH	pH	pH
	5.7	7.0	5.7	7.0	5.7	7.0	5.7	7.0
<i>Hydroxybenzoic acids</i>								
Gallic acid	-5.20	-6.20	-6.80	-6.30	-6.10	-6.10	-6.50	-6.70
2,3-dihydroxybenzoic acid	-5.80	-4.90	-6.40	-6.30	-6.70	-5.80	-6.30	-6.40
Syringic acid	-5.20	-5.20	-6.30	-6.0	-5.50	-5.70	-6.70	-5.10
<i>Hydroxycinnamic acids</i>								
<i>p</i> -Coumaric acid	-6.80	-6.00	-6.70	-6.70	-7.10	-6.70	-7.30	-7.20
Chlorogenic acid	-6.20	-5.90	-7.90	-8.60	-7.80	-7.10	-7.30	-6.20
Ferulic acid	-6.80	-6.80	-6.90	-6.40	-6.80	-6.80	-6.30	-6.90
<i>Flavanols</i>								
(+)-Catechin	-6.90	-6.80	-9.30	-9.20	-8.50	-8.50	-7.80	-7.40

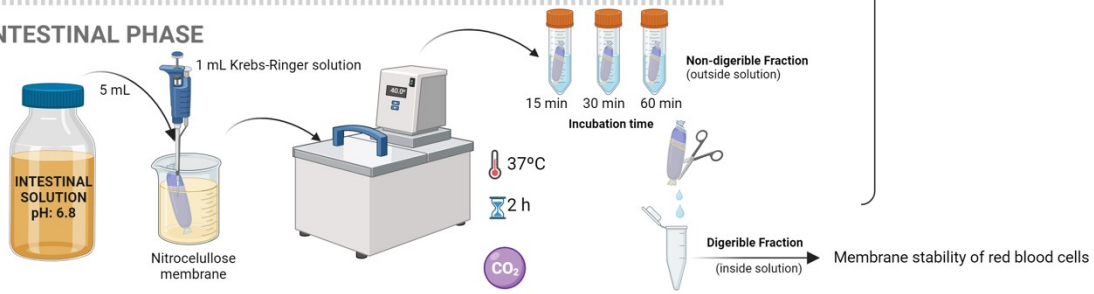
ORAL PHASE



GASTRIC PHASE



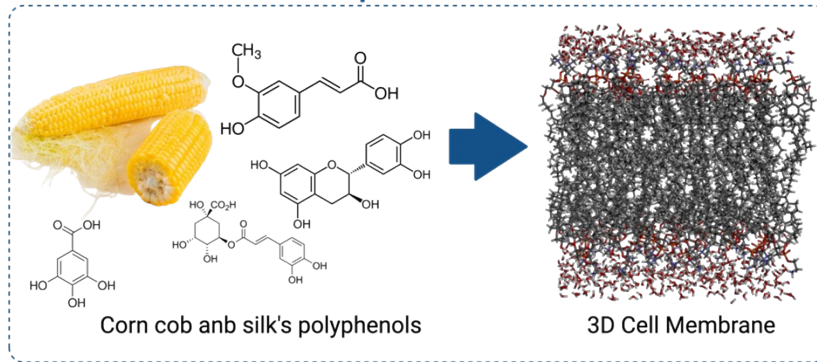
INTESTINAL PHASE



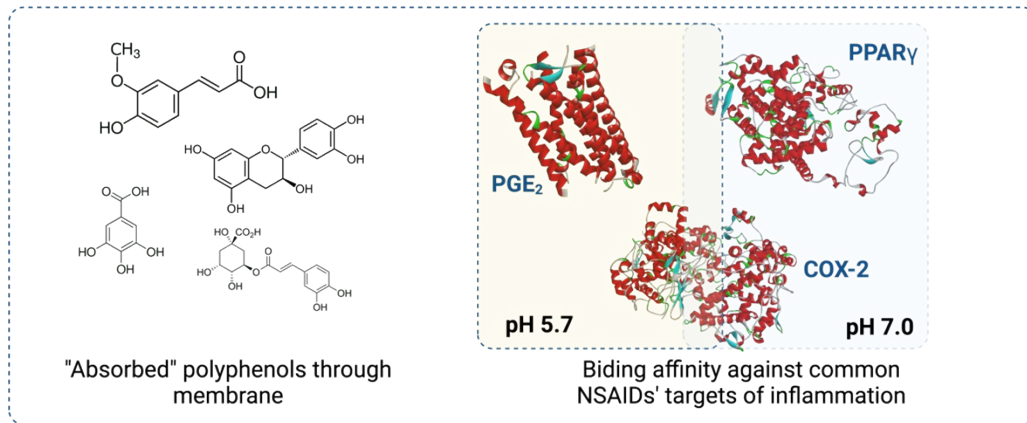
- Identification and quantification of phenolic compounds by HPLC-DAD.
- Antioxidant capacity:
 - ABTS
 - DPPH
 - FRAP

Supplementary Fig. S1. Schematic diagram *in vitro* gastrointestinal digestion

***In silico* cellular absorption in 3D-model membrane**



***In silico* docking between inflammation targets and absorbed polyphenols**



Supplementary Fig. S2. *In silico* analysis procedure