
Supporting information

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Figure S1 Correlation analysis between molecular characteristic values of FECs and DAI scores in colitis.

Figure S2 Correlation analysis between molecular characteristic values of FECs and pro-inflammatory cytokines in colon.

Figure S3 Correlation analysis between molecular characteristic values of FECs and oxidative indicators in colon.

Figure S4 Correlation analysis between molecular characteristic values of FECs and the protein expression levels of Nrf2, NQO1 and HO-1 in colon.

Table S1 Analysis of the interaction between FECs and BTB domain of Keap1.

Compound name	amino acid	Interaction force
FMA	Tyr85	Hydrogen bond
	His129	Hydrogen bond
	His154	Hydrogen bond
	Asn157	Hydrogen bond
	Gln86	Van der Waals
	Gly127	Van der Waals
	Ile128	Van der Waals
	Val132	Van der Waals
	Val155	Van der Waals
	Gly158	Van der Waals
ISO	Lys131	Hydrogen bond
	Arg135	Hydrogen bond
	Cys151	Hydrogen bond, Pi-alkyl
	Tyr85	Van der Waals
	Val132	Van der Waals
	Gly148	Van der Waals
	His129	Pi-cation
CA	His154	Pi-Pi stacked
	Tyr85	Hydrogen bond
	His154	Hydrogen bond, Pi-Pi stacked
	Val132	Van der Waals
	His129	Pi-cation
	Lys131	Pi-alkyl
	Cys151	Pi-alkyl

FA	Glu149	Hydrogen bond
	Lys150	Van der Waals
	Val152	Van der Waals
	His154	Van der Waals
	Leu175	Van der Waals
	Leu153	Pi-alkyl

SFN	His129	Hydrogen bond
	Tyr85	Van der Waals
	Gly127	Van der Waals
	Ile128	Van der Waals
	Val132	Van der Waals
	Leu153	Van der Waals
	Asn157	Van der Waals
	Gly158	Van der Waals
	His154	Pi-sulfur

CGA	Lys131	Hydrogen bond
	Arg135	Hydrogen bond
	Gly148	Hydrogen bond
	Tyr85	Van der Waals
	Val132	Van der Waals
	Met147	Van der Waals
	Lys150	Van der Waals
	His129	Pi-cation
	His154	Pi-Pi stacked
	Cys151	Pi-alkyl

Table S2 The data of correlation analysis between molecular characteristic values of FECs and DAI scores in colitis.

	<u>DAI score</u>	<u>logP</u>	<u>Keap1 affinity</u>	<u>Electrophilic index</u>
<u>DAI score</u>	<u>1</u>	<u>-0.738*</u>	<u>-0.592</u>	<u>0.392</u>
<u>logP</u>	<u>-0.738*</u>	<u>1</u>	<u>-0.12</u>	<u>0.278</u>
<u>Keap1 affinity</u>	<u>-0.592</u>	<u>-0.12</u>	<u>1</u>	<u>-0.754*</u>
<u>Electrophilic index</u>	<u>0.392</u>	<u>0.278</u>	<u>-0.754*</u>	<u>1</u>

* **P < 0.05**

Table S3 The data of correlation analysis between molecular characteristic values of FECs and pro-inflammatory cytokines in colitis.

	<u>logP</u>	<u>Keap1 affinity</u>	<u>Electrophilic index</u>	<u>TNF-α</u>	<u>IL-1β</u>	<u>IL-6</u>
<u>logP</u>	<u>1</u>	<u>-0.012</u>	<u>0.278</u>	<u>-0.544</u>	<u>-0.618</u>	<u>-0.577</u>
<u>Keap1 affinity</u>	<u>-0.012</u>	<u>1</u>	<u>-0.754*</u>	<u>-0.45</u>	<u>-0.181</u>	<u>-0.803*</u>
<u>Electrophilic index</u>	<u>0.278</u>	<u>-0.754*</u>	<u>1</u>	<u>0.561</u>	<u>0.179</u>	<u>0.442</u>
<u>TNF-α</u>	<u>-0.544</u>	<u>-0.45</u>	<u>0.561</u>	<u>1</u>	<u>0.785*</u>	<u>0.646</u>
<u>IL-1β</u>	<u>-0.618</u>	<u>-0.181</u>	<u>0.179</u>	<u>0.785*</u>	<u>1</u>	<u>0.429</u>
<u>IL-6</u>	<u>-0.577</u>	<u>-0.803*</u>	<u>0.442</u>	<u>0.646</u>	<u>0.439</u>	<u>1</u>

* **P < 0.05**

Table S4 Correlation analysis between molecular characteristic values of FECs and oxidative indicators in colon.

	<u>logP</u>	<u>Keap1</u> <u>affinity</u>	<u>Electrophilic</u> <u>index</u>	<u>T-AOC</u>	<u>MPO</u>	<u>GSH-</u> <u>px</u>	<u>SOD</u>	<u>MDA</u>
<u>logP</u>	<u>1</u>	<u>-0.012</u>	<u>0.278</u>	<u>0.607</u>	<u>-0.371</u>	<u>0.621</u>	<u>0.517</u>	<u>-0.402</u>
<u>Keap1</u> <u>affinity</u>	<u>-0.012</u>	<u>1</u>	<u>-0.754*</u>	<u>0.693</u>	<u>-0.631</u>	<u>0.59</u>	<u>0.509</u>	<u>-0.221</u>
<u>Electrophilic</u> <u>index</u>	<u>0.278</u>	<u>-0.754*</u>	<u>1</u>	<u>-0.385</u>	<u>0.747</u>	<u>-0.31</u>	<u>-0.476</u>	<u>0.377</u>
<u>T-AOC</u>	<u>0.607</u>	<u>0.693</u>	<u>-0.385</u>	<u>1</u>	<u>-0.797*</u>	<u>0.711*</u>	<u>0.486</u>	<u>-0.588</u>
<u>MPO</u>	<u>-0.371</u>	<u>-0.631</u>	<u>0.747*</u>	<u>-0.797*</u>	<u>1</u>	<u>0.565</u>	<u>-0.611</u>	<u>0.714</u>
<u>GSH-px</u>	<u>0.621</u>	<u>0.59</u>	<u>-0.31</u>	<u>0.711</u>	<u>-0.565</u>	<u>1</u>	<u>0.817*</u>	<u>-0.563</u>
<u>SOD</u>	<u>0.517</u>	<u>0.509</u>	<u>-0.476</u>	<u>0.486</u>	<u>-0.611</u>	<u>0.817*</u>	<u>1</u>	<u>-0.332</u>
<u>MDA</u>	<u>-0.402</u>	<u>-0.221</u>	<u>0.377</u>	<u>-0.588</u>	<u>0.714</u>	<u>-0.563</u>	<u>-0.332</u>	<u>1</u>

* P < 0.05

Table S5 The data of correlation analysis between molecular characteristic values of FECs and the protein expression levels of Nrf2, NQO1 and HO-1 in colitis.

	<u>logP</u>	<u>Keap1</u> <u>affinity</u>	<u>Electrophilic</u> <u>index</u>	<u>Nrf2</u>	<u>NQO1</u>	<u>HO-1</u>
<u>logP</u>	<u>1</u>	<u>-0.012</u>	<u>0.278</u>	<u>0.922**</u>	<u>0.737*</u>	<u>0.759*</u>
<u>Keap1</u> <u>affinity</u>	<u>-0.012</u>	<u>1</u>	<u>-0.754*</u>	<u>0.173</u>	<u>0.468</u>	<u>0.266</u>
<u>Electrophilic</u> <u>index</u>	<u>0.278</u>	<u>-0.754*</u>	<u>1</u>	<u>-0.069</u>	<u>-0.382</u>	<u>-0.18</u>

<u>Nrf2</u>	<u>0.922**</u>	<u>0.173</u>	<u>-0.069</u>	<u>1</u>	<u>0.888**</u>	<u>0.842*</u>
<u>NQO1</u>	<u>0.737*</u>	<u>0.468</u>	<u>-0.382</u>	<u>0.888**</u>	<u>1</u>	<u>0.953**</u>
<u>HO-1</u>	<u>0.759*</u>	<u>0.266</u>	<u>-0.18</u>	<u>0.842*</u>	<u>0.953**</u>	<u>1</u>

* P < 0.05, ** P < 0.01

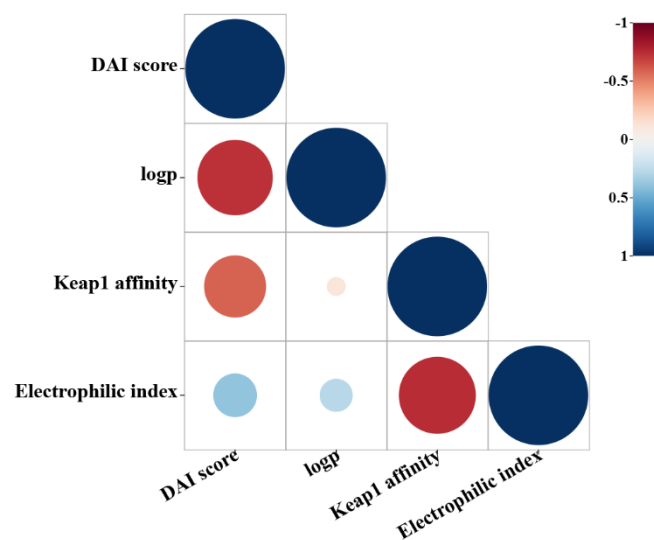


Figure S1 Correlation analysis between molecular characteristic values of FECs and DAI scores in colitis.

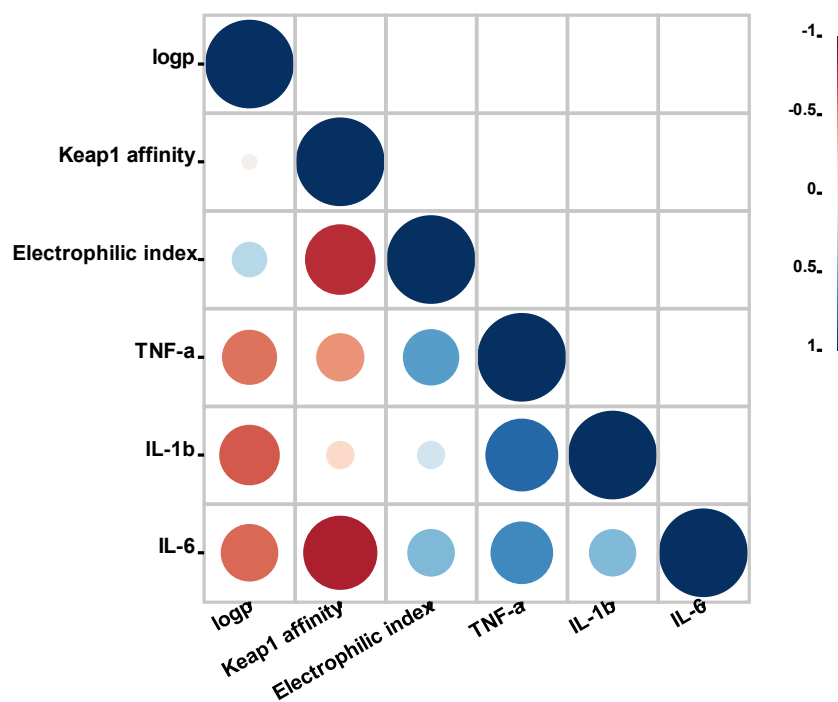


Figure S2 Correlation analysis between molecular characteristic values of FECs and pro-inflammatory cytokines scores in colitis.

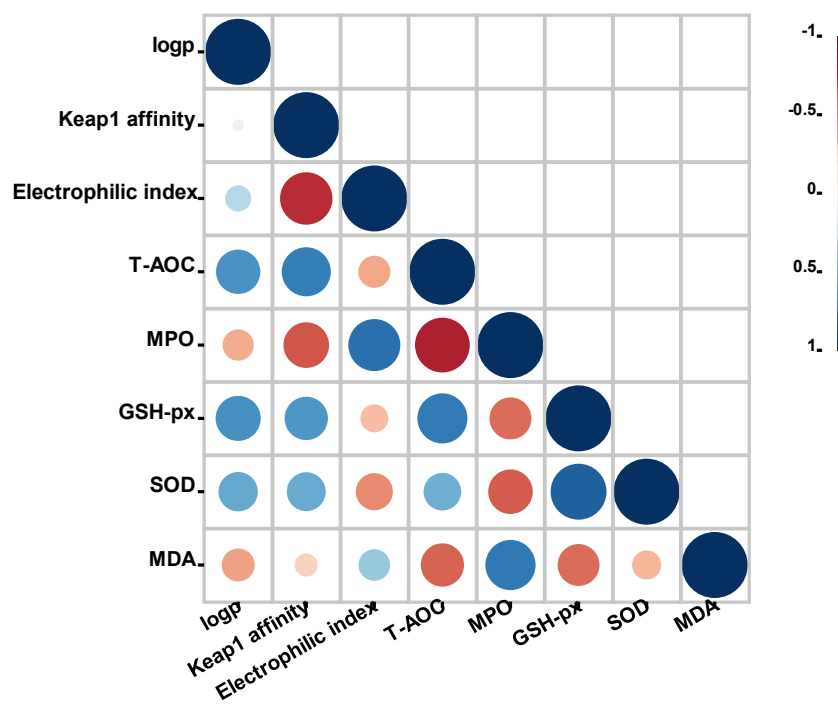


Figure S3 Correlation analysis between molecular characteristic values of FECs and oxidative indicators in colon.

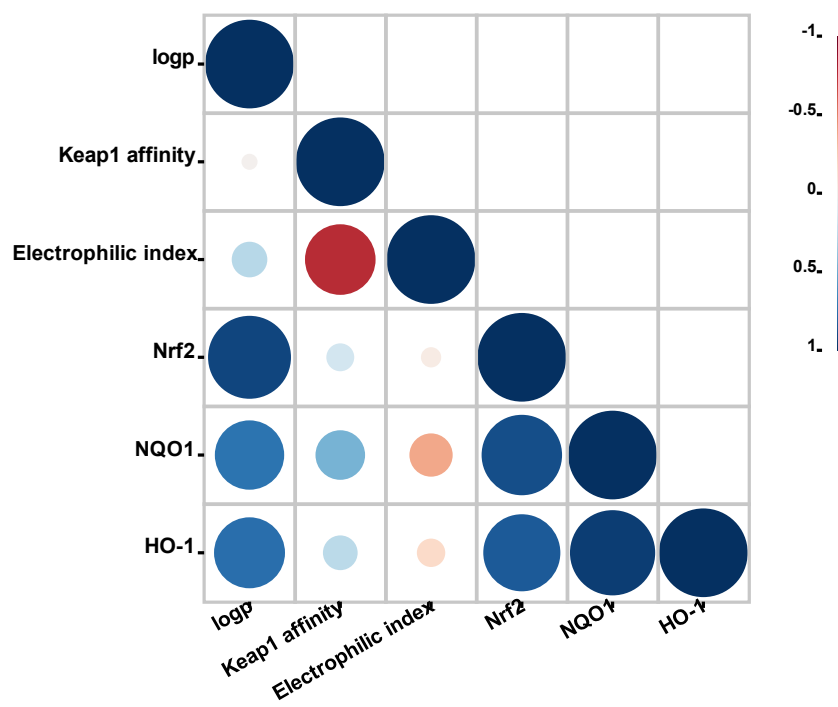


Figure S4 Correlation analysis between molecular characteristic values of FECs and the protein expression levels of Nrf2, NQO1 and HO-1 in colon.