

Supplementary material

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6-Gingerol ameliorates ulcerative colitis by inhibiting ferroptosis based on the integrative analysis of plasma metabolomics and network pharmacology

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1. Supplementary tables

Table S1 Assessment of DAI

Score	Weight loss (%)	Stool	Bleeding
0	<1	Normal	Normal
1	1 ≤ ~ <5	Softer stool	Weak hemocult
2	5 ≤ ~ <10	Loose stool	hemocult
3	10 ≤ ~ <15	Moderate diarrhoea	Visual bleeding
4	≥15	Diarrhoea	Gross bleeding

Table S2 Assessment of histopathological scores

Score	Extent of inflammation	Infiltration neutrophils +lymphohistiocytes	Extent of crypt damage	Crypt abscesses	Submucosal oedema	Loss of goblet cells	Reactive epithelial hyperplasia
0	None	None	None	None	None	None	None
1	Mucosa	Focal	Basal one third	Focal	Focal	Focal	Focal
2	Mucosa+submucosa	Multifocal	Basal two third	Multifocal	Multifocal	Multifocal	Multifocal
3	Mucosa+submucosa +muscle layer	Diffuse	Entire crypt damage	Diffuse	Diffuse	Diffuse	Diffuse
4	Transmura	-	Crypt damage +ulceration	-	-	-	-

Table S3 Results from Pathway Analysis

Metabolic pathways	Total	Expected	Hits	Raw p	-log10 (p)	Holm adjust	FDR	Impact
Linoleic acid metabolism	5	0.04	3	3.36E-06	5.47	2.68E-04	2.68E-04	1
Biosynthesis of unsaturated fatty acids	36	0.27	4	1.00E-04	4.00	7.91E-03	4.00E-03	0.00
Arachidonic acid metabolism	44	0.34	3	3.76E-03	2.43	2.93E-01	1.00E-01	0.36
Glycerophospholipid metabolism	36	0.27	2	2.90E-02	1.54	1.00	5.81E-01	0.13
α -Linolenic acid metabolism	13	0.10	1	9.50E-02	1.02	1.00	1.00	0.00
Primary bile acid biosynthesis	46	0.35	1	3.00E-01	0.52	1.00	1.00	0.00

2. Supplementary figures

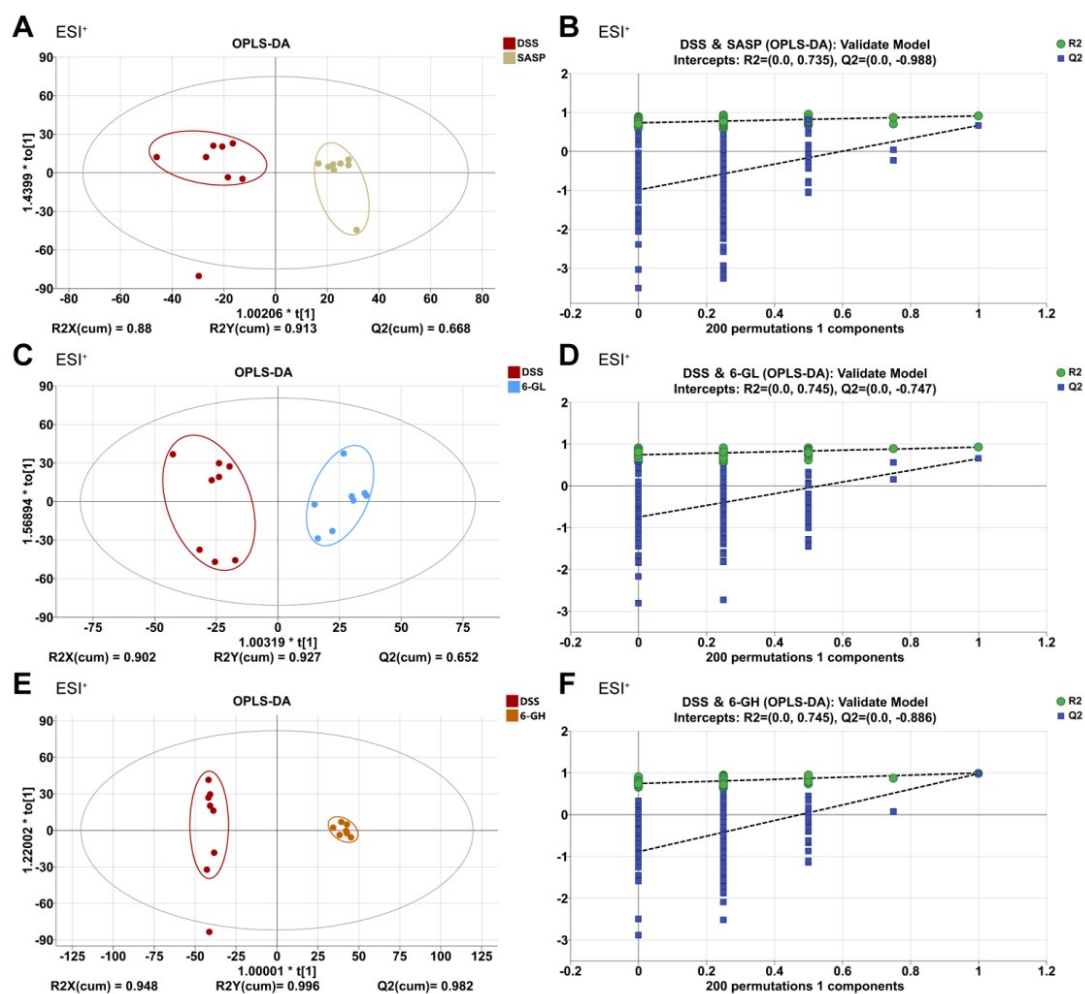


Fig. S1 Multivariate statistical analysis of plasma metabolic profiles in positive mode. (A, C, E) PCA score plots for the DSS and SASP, 6-GL, 6-GH, respectively; (B, D, F) validation plot of the OPLS-DA model obtained from 200 permutation tests for the DSS and SASP, 6-GL, 6-GH, respectively.

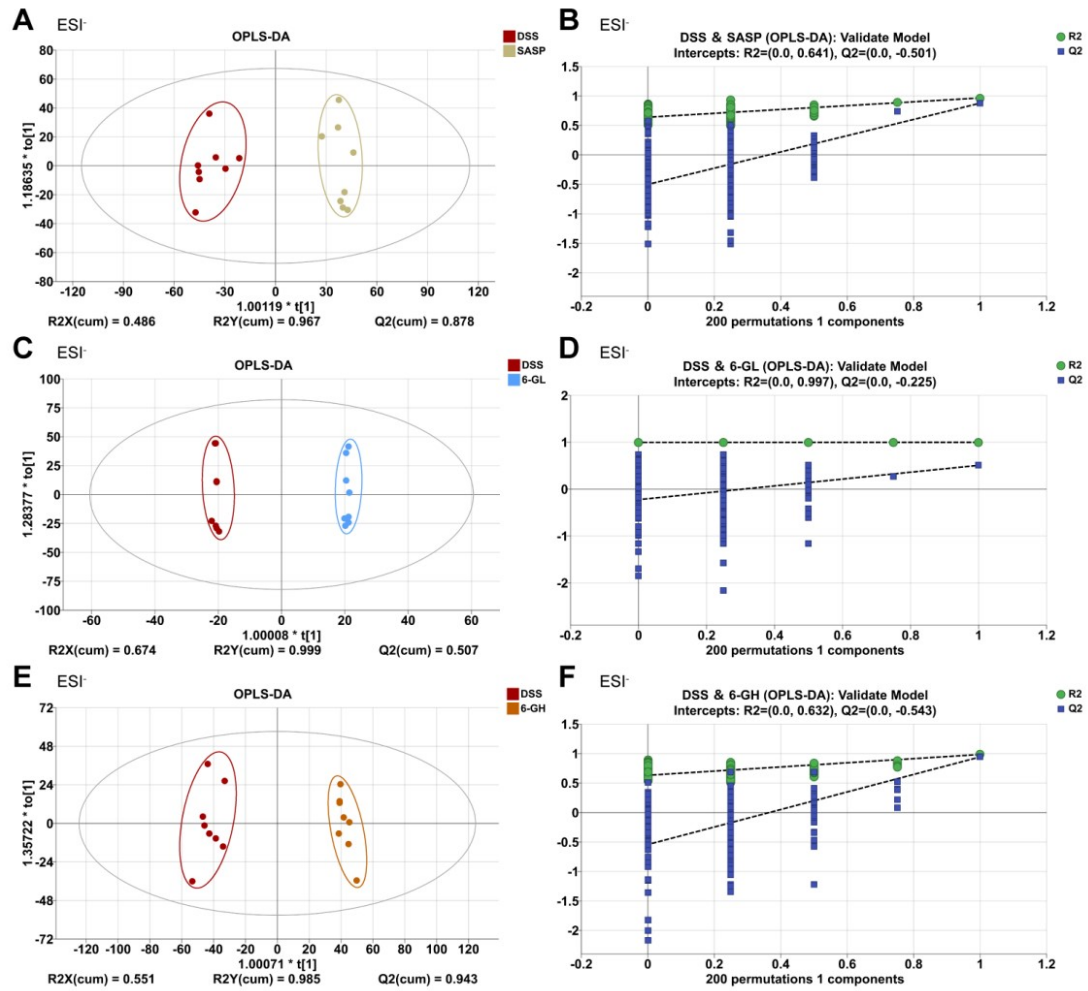


Fig. S2 Multivariate statistical analysis of plasma metabolic profiles in negative mode. (A, C, E) PCA score plots for the DSS and SASP, 6-GL, 6-GH, respectively; (B, D, F) validation plot of the OPLS-DA model obtained from 200 permutation tests for the DSS and SASP, 6-GL, 6-GH, respectively.

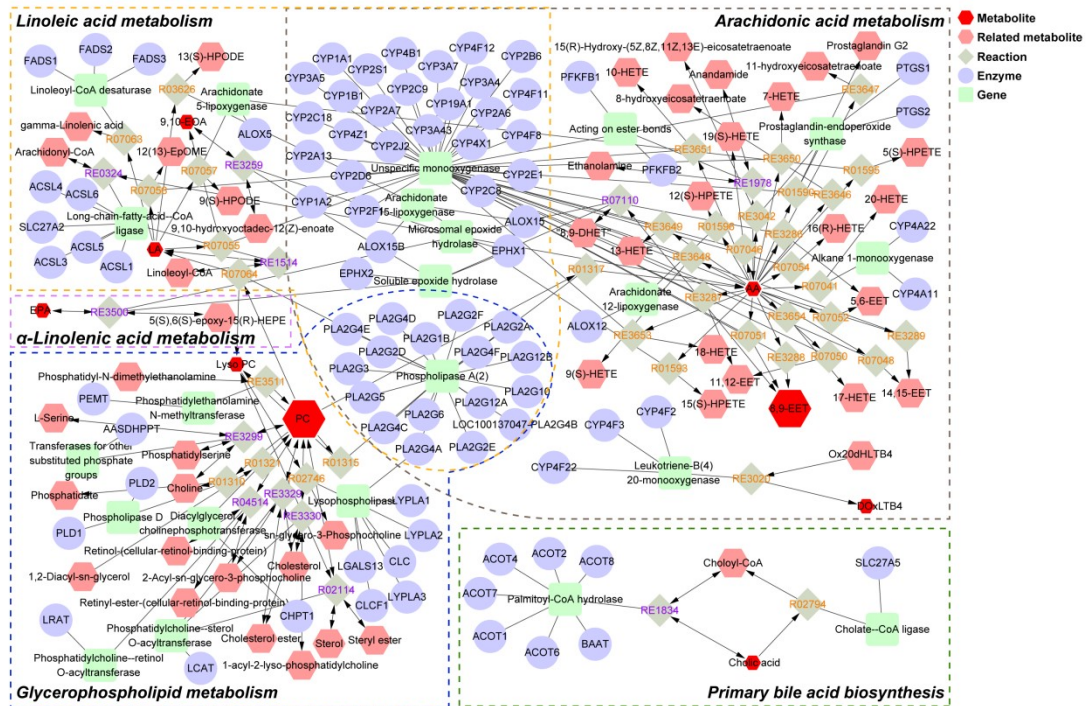


Fig. S3 The network of metabolites-reactions-enzymes-targets.