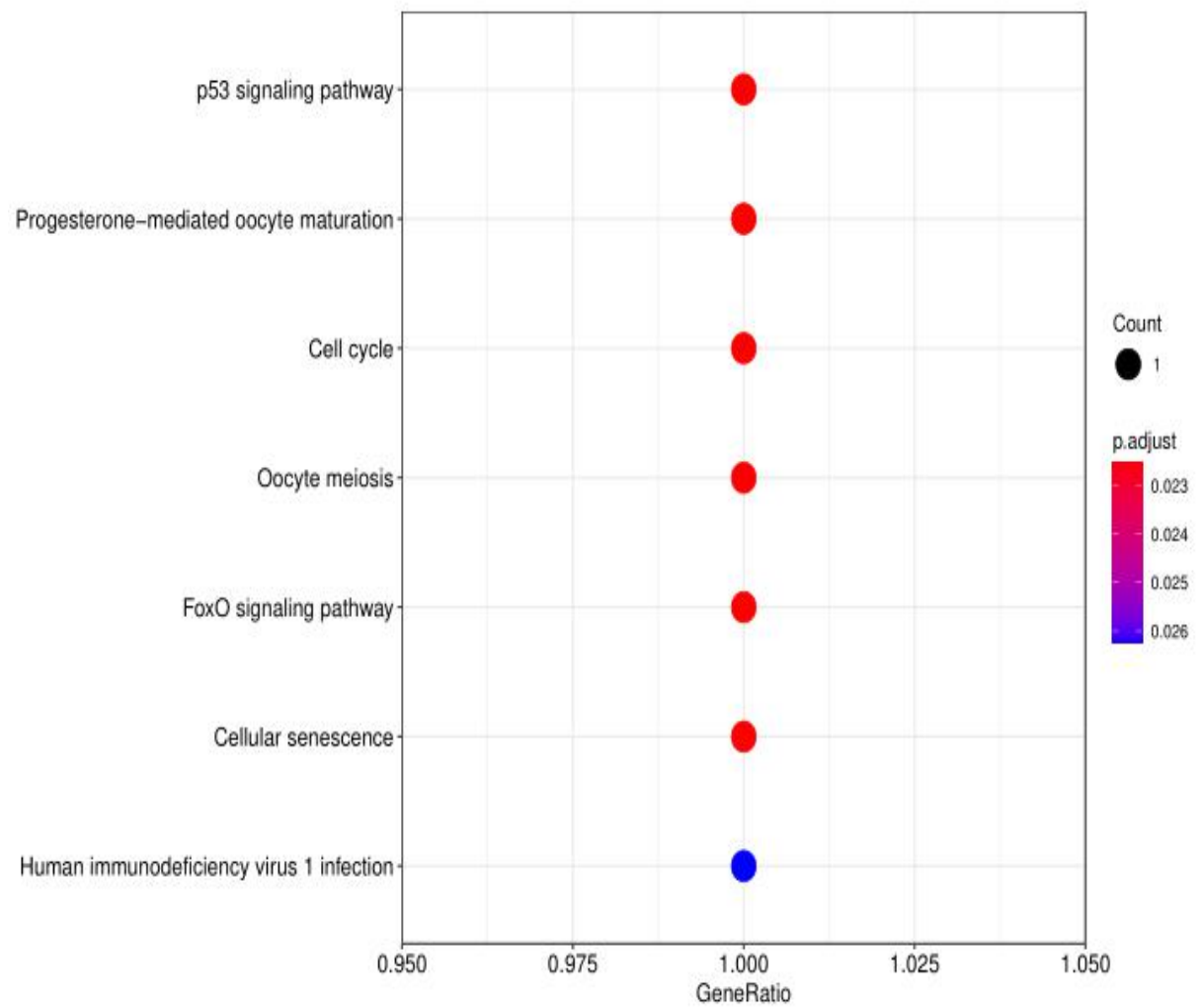


**Supplementary Figure 1 GO analysis results.**



**Supplementary Figure 2 KEGG analysis results.**

**Supplementary Table 1 Composition in huanglian decoction**

<b>Drug</b>	<b>MolId</b>	<b>Compounds name</b>
Folium Artemisiae Argyi	MOL000098	Quercetin
Coptidis Rhizoma	MOL000098	Quercetin
Mume Fructus	MOL000098	Quercetin
Folium Artemisiae Argyi	MOL000358	Beta-sitosterol
Zingiberis Rhizoma	MOL000358	Beta-sitosterol
Mume Fructus	MOL000358	Beta-sitosterol
Zingiberis Rhizoma	MOL000359	Sitosterol
Mume Fructus	MOL000422	Kaempferol
Folium Artemisiae Argyi	MOL000449	Stigmasterol
Mume Fructus	MOL000449	Stigmasterol
Coptidis Rhizoma	MOL000622	Magnograndiolide
Coptidis Rhizoma	MOL000785	palmatine
Mume Fructus	MOL000953	CLR
Folium Artemisiae Argyi	MOL001040	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl) chroman-4-one
Coptidis Rhizoma	MOL001454	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl) chroman-4-one
Coptidis Rhizoma	MOL001458	Berberine
Folium Artemisiae Argyi	MOL001494	Coptisine
Zingiberis Rhizoma	MOL002464	Mandenol
Zingiberis Rhizoma	MOL002501	1-Monolinolein
Zingiberis Rhizoma	MOL002514	[(1S)-3-[(E)-but-2-enyl]-2-methyl-4-oxo-1-cyclopent-2-enyl](1R,3R)-3-[(E)-3-methoxy-2-methyl-3-oxoprop-1-enyl]-2,2-dimethylcyclopropane-1-carboxylate

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Coptidis Rhizoma	MOL002668	Sexangularetin
Folium Artemisiae Argyi	MOL002883	Worenine
Coptidis Rhizoma	MOL002894	Ethyl oleate (NF)
Coptidis Rhizoma	MOL002897	Berberrubine
Coptidis Rhizoma	MOL002903	Epiberberine (R)-Canadine
Coptidis Rhizoma	MOL002904	Berlambine
Coptidis Rhizoma	MOL002907	Corchoroside A <sub>qt</sub>
Mume Fructus	MOL005043	Campest-5-en-3beta-ol
Mume Fructus	MOL008601	Methyl arachidonate

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**Supplementary Table 2 Composition in huanglian decoction and the target gene**

<b>Drug</b>	<b>MolId</b>	<b>MolName</b>	<b>Target</b>
Aiye	MOL000449	Stigmasterol	ADH1C
Wumei	MOL000449	Stigmasterol	ADH1C
Wumei	MOL000422	kaempferol	AKR1C3
Aiye	MOL000098	quercetin	BIRC5
Huanglian	MOL000098	quercetin	BIRC5
Wumei	MOL000098	quercetin	BIRC5
Aiye	MOL000098	quercetin	CCNB1
Huanglian	MOL000098	quercetin	CCNB1
Wumei	MOL000098	quercetin	CCNB1
Aiye	MOL000098	quercetin	CDK1
Huanglian	MOL000098	quercetin	CDK1
Wumei	MOL000422	kaempferol	CDK1
Wumei	MOL000098	quercetin	CDK1
Huanglian	MOL002668	Worenine	CHEK1
Aiye	MOL000098	quercetin	CHEK2
Huanglian	MOL000098	quercetin	CHEK2
Wumei	MOL000098	quercetin	CHEK2
Aiye	MOL000098	quercetin	CYP1A2
Huanglian	MOL000098	quercetin	CYP1A2
Wumei	MOL000422	kaempferol	CYP1A2
Wumei	MOL000098	quercetin	CYP1A2
Aiye	MOL000098	quercetin	CYP3A4
Huanglian	MOL000098	quercetin	CYP3A4
Wumei	MOL000422	kaempferol	CYP3A4
Wumei	MOL000098	quercetin	CYP3A4

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Aiye	MOL000098	quercetin	E2F1
Huanglian	MOL000098	quercetin	E2F1
Wumei	MOL000098	quercetin	E2F1
Aiye	MOL000098	quercetin	E2F2
Huanglian	MOL000098	quercetin	E2F2
Wumei	MOL000098	quercetin	E2F2
Aiye	MOL000098	quercetin	FOS
Huanglian	MOL000098	quercetin	FOS
Wumei	MOL000098	quercetin	FOS
Aiye	MOL000098	quercetin	HSPB1
Huanglian	MOL000098	quercetin	HSPB1
Wumei	MOL000098	quercetin	HSPB1
Aiye	MOL000098	quercetin	IGFBP3
Huanglian	MOL000098	quercetin	IGFBP3
Wumei	MOL000098	quercetin	IGFBP3
Aiye	MOL000358	beta-sitosterol	MAP2
Ganjiang	MOL000358	beta-sitosterol	MAP2
Wumei	MOL000358	beta-sitosterol	MAP2
Aiye	MOL000098	quercetin	MMP9
Huanglian	MOL000098	quercetin	MMP9
Wumei	MOL000098	quercetin	MMP9
Aiye	MOL000098	quercetin	NQO1
Huanglian	MOL000098	quercetin	NQO1
Wumei	MOL000098	quercetin	NQO1
Aiye	MOL000098	quercetin	PARP1
Huanglian	MOL000098	quercetin	PARP1
Wumei	MOL000098	quercetin	PARP1
Aiye	MOL000098	quercetin	SERPINE1
Huanglian	MOL000098	quercetin	SERPINE1

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Wumei	MOL000098	quercetin	SERPINE1
Aiye	MOL000098	quercetin	TOP2A
Huanglian	MOL000098	quercetin	TOP2A
Wumei	MOL000098	quercetin	TOP2A

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