

Therapeutic Targets and Mechanism of Banxia Xiexin Decoction on Precancerous Lesions of Gastric Cancer: Network Pharmacology

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SUPPLEMENTARY MATERIAL

Herb	NO.	MOL ID	Molecular Name	OB(%)	DL
BanXia	A	MOL000358	beta-sitosterol	36.91391	0.75123
BanXia	B	MOL000449	Stigmasterol	43.82985	0.75665
BanXia	BX1	MOL000519	coniferin	31.11	0.32308
BanXia	BX2	MOL001755	24-Ethylcholest-4-en-3-one	36.08361	0.75703
BanXia	BX3	MOL002670	Cavidine	35.64183	0.80513
BanXia	E	MOL002714	baicalein	33.51892	0.20888
BanXia	BX4	MOL002776	Baicalin	40.12361	0.75264
BanXia	BX5	MOL003578	Cycloartenol	38.68566	0.78093
BanXia	BX6	MOL005030	gondoic acid	30.70294	0.19743
BanXia	BX7	MOL006936	10,13-eicosadienoic	39.99355	0.20012
BanXia	BX8	MOL006937	12,13-epoxy-9-hydroxynonadeca-7,10-dienoic acid	42.15218	0.24248
BanXia	BX9	MOL006957	(3S,6S)-3-(benzyl)-6-(4-hydroxybenzyl)piperazine-2,5-quinone	46.8889	0.26989
BanXia	BX10	MOL006967	beta-D-Ribofuranoside, xanthine-9	44.71879	0.20816
HuangQin	HQ1	MOL000073	ent-Epicatechin	48.96	0.24
HuangQin	HQ2	MOL000173	wogonin	30.68457	0.22942

HuangQin	HQ3	MOL000228	(2R)-7-hydroxy-5-methoxy-2-phenylchroman-4-one	55.23317	0.20163
HuangQin	A	MOL000358	beta-sitosterol	36.91391	0.75123
HuangQin	D	MOL000359	sitosterol	36.91391	0.7512
HuangQin	B	MOL000449	Stigmasterol	43.83	0.76
HuangQin	HQ4	MOL000525	Norwogonin	39.40397	0.20723
HuangQin	HQ5	MOL000552	5,2'-Dihydroxy-6,7,8-trimethoxyflavone	31.71246	0.35462
HuangQin	H1	MOL001458	coptisine	30.67	0.86
HuangQin	HQ6	MOL001490	bis[(2S)-2-ethylhexyl] benzene-1,2-dicarboxylate	43.59	0.35
HuangQin	HQ7	MOL001689	acacetin	34.97357	0.24082
HuangQin	E	MOL002714	baicalein	33.51892	0.20888
HuangQin	K	MOL002879	Diop	43.59	0.39
HuangQin	H2	MOL002897	epiberberine	43.09	0.78
HuangQin	HQ9	MOL002910	Carthamidin	41.15096	0.24189
HuangQin	HQ10	MOL002913	Dihydrobaicalin_qt	40.03778	0.20722
HuangQin	HQ11	MOL002914	Eriodictiol (flavanone)	41.35043	0.2436
HuangQin	HQ12	MOL002915	Salvigenin	49.06593	0.33279
HuangQin	HQ13	MOL002917	5,2',6'-Trihydroxy-7,8-dimethoxyflavone	45.04743	0.33057
HuangQin	HQ14	MOL002925	5,7,2',6'-Tetrahydroxyflavone	37.01349	0.24382
HuangQin	HQ15	MOL002927	Skullcapflavone II	69.51043	0.4379
HuangQin	HQ16	MOL002928	oroxylin a	41.36757	0.23233
HuangQin	HQ17	MOL002932	Panicolin	76.25705	0.2915
HuangQin	HQ18	MOL002933	5,7,4'-Trihydroxy-8-methoxyflavone	36.562	0.26666
HuangQin	HQ19	MOL002934	NEOBAICALEIN	104.3446	0.43917
HuangQin	HQ20	MOL002937	DIHYDROOROXYLIN	66.06174	0.23057
HuangQin	HQ21	MOL008206	Moslosoolflavone	44.09	0.25
HuangQin	HQ22	MOL010415	11,13-Eicosadienoic acid, methyl ester	39.28	0.23
HuangQin	HQ23	MOL012245	5,7,4'-trihydroxy-6-methoxyflavanone	36.63	0.27

HuangQin	HQ24	MOL012246	5,7,4'-trihydroxy-8-methoxyflavanone	74.24	0.26
HuangQin	HQ25	MOL012266	rivularin	37.94	0.37
HuangLian	C	MOL000098	quercetin	46.43335	0.27525
HuangLian	HL1	MOL000622	Magnograndiolide	63.70888	0.18833
HuangLian	HL2	MOL000785	palmatine	64.60111	0.64524
HuangLian	G	MOL001454	berberine	36.86125	0.77665
HuangLian	H1	MOL001458	coptisine	30.67	0.86
HuangLian	HL3	MOL002668	Worenine	45.83	0.87
HuangLian	HL4	MOL002894	berberrubine	35.73551	0.7269
HuangLian	H2	MOL002897	epiberberine	43.09233	0.7761
HuangLian	HL5	MOL002903	(R)-Canadine	55.36687	0.77465
HuangLian	HL6	MOL002904	Berlambine	36.6809	0.81596
HuangLian	HL7	MOL002907	Corchoroside A_qt	104.9542	0.77599
GanJiang	A	MOL000358	beta-sitosterol	36.91391	0.75123
GanJiang	D	MOL000359	sitosterol	36.91391	0.7512
GanJiang	GJ1	MOL002464	1-Monolinolein	37.17663	0.30249
GanJiang	GJ2	MOL002501	[[(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	62.51583	0.30983
GanJiang	GJ3	MOL002514	Sexangularetin	62.85792	0.2968
RenShen	A	MOL000358	beta-sitosterol	36.91391	0.75123
RenShen	J	MOL000422	kaempferol	41.88225	0.24066
RenShen	B	MOL000449	Stigmasterol	43.82985	0.75665
RenShen	I1	MOL000787	Fumarine	59.2625	0.82694
RenShen	K	MOL002879	Diop	43.59333	0.39247
RenShen	RS1	MOL003648	Inermin	65.83093	0.53754
RenShen	RS2	MOL005308	Aposiopolamine	66.64691	0.21999
RenShen	RS3	MOL005317	Deoxyharringtonine	39.27444	0.8116

RenShen	RS4	MOL005318	Dianthramine	40.44641	0.19676
RenShen	RS5	MOL005320	arachidonate	45.57325	0.20491
RenShen	RS6	MOL005321	Frutinone A	65.90373	0.34184
RenShen	RS7	MOL005344	ginsenoside rh2	36.31951	0.55868
RenShen	RS8	MOL005348	Ginsenoside-Rh4_qt	31.11215	0.77829
RenShen	RS9	MOL005356	Girinimbin	61.2153	0.31484
RenShen	I2	MOL005360	malkangunin	57.71384	0.62642
RenShen	RS10	MOL005376	Panaxadiol	33.08796	0.79404
RenShen	RS11	MOL005384	suchilactone	57.51882	0.55573
RenShen	RS12	MOL005399	alexandrin_qt	36.91391	0.75268
DaZao	DZ1	MOL000096	(-)catechin	49.67639	0.24162
DaZao	C	MOL000098	quercetin	46.43335	0.27525
DaZao	F	MOL000211	Mairin	55.37707	0.7761
DaZao	A	MOL000358	beta-sitosterol	36.91391	0.75123
DaZao	B	MOL000449	Stigmasterol	43.82985	0.75665
DaZao	DZ2	MOL000492	(+)-catechin	54.82643	0.24164
DaZao	DZ3	MOL000627	Stepholidine	33.10625	0.54083
DaZao	I1	MOL000787	Fumarine	59.2625	0.82694
DaZao	G	MOL001454	berberine	36.86125	0.77665
DaZao	DZ4	MOL001522	(S)-Coclaurine	42.35064	0.23518
DaZao	DZ5	MOL002773	beta-carotene	37.18433	0.58358
DaZao	DZ6	MOL003410	Ziziphin_qt	66.94529	0.61926
DaZao	DZ7	MOL004350	Ruvoside_qt	36.12102	0.75671
DaZao	I2	MOL005360	malkangunin	57.71384	0.62642
DaZao	DZ8	MOL007213	Nuciferin	34.43103	0.40475
DaZao	DZ9	MOL008034	21302-79-4	73.52245	0.7661
DaZao	DZ10	MOL012921	stepharine	31.54787	0.33376

DaZao	DZ11	MOL012946	zizyphus saponin I_qt	32.69114	0.61923
DaZao	DZ12	MOL012961	jujuboside A_qt	36.6657	0.61915
DaZao	DZ13	MOL012976	coumestrol	32.48703	0.33733
DaZao	DZ14	MOL012981	Daechuine S7	44.81774	0.82806
DaZao	DZ15	MOL012986	Jujubasaponin V_qt	36.98963	0.63448
DaZao	DZ16	MOL012989	Jujuboside C_qt	40.26243	0.61911
DaZao	DZ17	MOL012992	Mauritine D	89.12509	0.45286
DaZao	DZ18	MOL013357	(3S,6R,8S,9S,10R,13R,14S,17R)-17-[(1R,4R)-4-ethyl-1,5-dimethylhexyl]-10,13-dimethyl-2,3,6,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[al]phenanthrene-3,6-diol	34.37	0.78
GanCao	C	MOL000098	quercetin	46.43335	0.27525
GanCao	F	MOL000211	Mairin	55.37707	0.7761
GanCao	GC1	MOL000239	Jaranol	50.82882	0.29148
GanCao	GC2	MOL000354	isorhamnetin	49.60438	0.306
GanCao	D	MOL000359	sitosterol	36.91391	0.7512
GanCao	GC3	MOL000392	formononetin	69.67388	0.21202
GanCao	GC4	MOL000417	Calycosin	47.75183	0.24278
GanCao	J	MOL000422	kaempferol	41.88225	0.24066
GanCao	GC5	MOL000497	licochalcone a	40.78965	0.28517
GanCao	GC6	MOL000500	Vestitol	74.65519	0.20935
GanCao	GC7	MOL001484	Inermine	75.18306	0.53754
GanCao	GC8	MOL001792	DFV	32.76272	0.18316
GanCao	GC9	MOL002311	Glycyrol	90.77578	0.66819
GanCao	GC10	MOL002565	Medicarpin	49.21982	0.3351
GanCao	GC11	MOL003656	Lupiwighteone	51.63569	0.36739
GanCao	GC12	MOL003896	7-Methoxy-2-methyl isoflavone	42.56474	0.19946
GanCao	GC13	MOL004328	naringenin	59.2939	0.21128
GanCao	GC14	MOL004805	(2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-	31.78703	0.72403

			dihydropyrano[2,3-f]chromen-4-one		
GanCao	GC15	MOL004806	euchrenone	30.28726	0.57386
GanCao	GC16	MOL004808	glyasperin B	65.22439	0.43851
GanCao	GC17	MOL004810	glyasperin F	75.8368	0.53514
GanCao	GC18	MOL004811	Glyasperin C	45.56381	0.39947
GanCao	GC19	MOL004814	Isotrifoliol	31.94479	0.42422
GanCao	GC20	MOL004815	(E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one	39.61686	0.35077
GanCao	GC21	MOL004820	kanzonols W	50.48008	0.51704
GanCao	GC22	MOL004824	(2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one	60.25041	0.63433
GanCao	GC23	MOL004827	Semilicoisoflavone B	48.77755	0.54732
GanCao	GC24	MOL004828	Glepidotin A	44.72187	0.34685
GanCao	GC25	MOL004829	Glepidotin B	64.46292	0.34485
GanCao	GC26	MOL004833	Phaseolinisoflavan	32.00811	0.44538
GanCao	GC27	MOL004835	Glypallichalcone	61.59706	0.18993
GanCao	GC28	MOL004838	8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol	58.43728	0.38106
GanCao	GC29	MOL004841	Licochalcone B	76.75735	0.1935
GanCao	GC30	MOL004848	licochalcone G	49.25496	0.32325
GanCao	GC31	MOL004849	3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin	59.62247	0.42894
GanCao	GC32	MOL004855	Licoricone	63.57846	0.4712
GanCao	GC33	MOL004856	Gancaonin A	51.07519	0.40378
GanCao	GC34	MOL004857	Gancaonin B	48.7944	0.44924
GanCao	GC35	MOL004863	3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl)chromone	66.37125	0.41392
GanCao	GC36	MOL004864	5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone	30.48878	0.41002
GanCao	GC37	MOL004866	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-	44.15196	0.41482

			enyl)chromone		
GanCao	GC38	MOL004879	Glycyrin	52.60657	0.47466
GanCao	GC39	MOL004882	Licocoumarone	33.21085	0.3568
GanCao	GC40	MOL004883	Licoisoflavone	41.61022	0.41646
GanCao	GC41	MOL004884	Licoisoflavone B	38.92871	0.54714
GanCao	GC42	MOL004885	licoisoflavanone	52.46625	0.54488
GanCao	GC43	MOL004891	shinpterocarpin	80.29528	0.72746
GanCao	GC44	MOL004898	(E)-3-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-1-(2,4-dihydroxyphenyl)prop-2-en-1-one	46.26792	0.3062
GanCao	GC45	MOL004903	liquiritin	65.69011	0.73893
GanCao	GC46	MOL004904	licopyranocoumarin	80.36001	0.6535
GanCao	GC47	MOL004907	Glyzaglabrin	61.06889	0.35347
GanCao	GC48	MOL004908	Glabridin	53.24514	0.46967
GanCao	GC49	MOL004910	Glabranin	52.89566	0.31208
GanCao	GC50	MOL004911	Glabrene	46.26686	0.43902
GanCao	GC51	MOL004912	Glabrone	52.51217	0.49645
GanCao	GC52	MOL004913	1,3-dihydroxy-9-methoxy-6-benzofurano[3,2-c]chromenone	48.14154	0.42831
GanCao	GC53	MOL004914	1,3-dihydroxy-8,9-dimethoxy-6-benzofurano[3,2-c]chromenone	62.90135	0.52759
GanCao	GC54	MOL004915	Eurycarpin A	43.27728	0.37429
GanCao	GC55	MOL004924	(-)Medicocarpin	40.99397	0.95059
GanCao	GC56	MOL004935	Sigmoidin-B	34.88109	0.41455
GanCao	GC57	MOL004941	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one	71.12299	0.18303
GanCao	GC58	MOL004945	(2S)-7-hydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)chroman-4-one	36.56537	0.32291
GanCao	GC59	MOL004948	Isoglycyrol	44.69923	0.83845
GanCao	GC60	MOL004949	Isolicoflavonol	45.16999	0.41859
GanCao	GC61	MOL004957	HMO	38.36542	0.21067
GanCao	GC62	MOL004959	1-Methoxyphaseollidin	69.98098	0.63739

GanCao	GC63	MOL004961	Quercetin der.	46.44939	0.3343
GanCao	GC64	MOL004966	3'-Hydroxy-4'-O-Methylglabridin	43.71495	0.57406
GanCao	GC65	MOL004974	3'-Methoxyglabridin	46.16151	0.57393
GanCao	GC66	MOL004978	2-[(3R)-8,8-dimethyl-3,4-dihydro-2H-pyrano[6,5-f]chromen-3-yl]-5-methoxyphenol	36.21429	0.52122
GanCao	GC67	MOL004980	Inflacoumarin A	39.7091	0.32613
GanCao	GC68	MOL004985	icos-5-enoic acid	30.70294	0.19725
GanCao	GC69	MOL004988	Kanzonol F	32.46833	0.89364
GanCao	GC70	MOL004989	6-prenylated eriodictyol	39.22383	0.41259
GanCao	GC71	MOL004990	7,2',4'-trihydroxy-5-methoxy-3-arylcoumarin	83.71437	0.27136
GanCao	GC72	MOL004991	7-Acetoxy-2-methylisoflavone	38.92333	0.26217
GanCao	GC73	MOL004993	8-prenylated eriodictyol	53.79476	0.40383
GanCao	GC74	MOL004996	gadelaidic acid	30.70294	0.19725
GanCao	GC75	MOL005000	Gancaonin G	60.43521	0.39404
GanCao	GC76	MOL005001	Gancaonin H	50.10372	0.78416
GanCao	GC77	MOL005003	Licoagrocarpin	58.8139	0.58498
GanCao	GC78	MOL005007	Glyasperins M	72.67081	0.59274
GanCao	GC79	MOL005008	Glycyrrhiza flavonol A	41.27528	0.59512
GanCao	GC80	MOL005012	Licoagroisoflavone	57.28224	0.48679
GanCao	GC81	MOL005013	18 α -hydroxyglycyrrhetic acid	41.16139	0.7091
GanCao	GC82	MOL005016	Odoratin	49.94822	0.30487
GanCao	GC83	MOL005017	Phaseol	78.76622	0.57867
GanCao	GC84	MOL005018	Xambioona	54.84916	0.87419
GanCao	GC85	MOL005020	dehydroglyasperins C	53.82326	0.37006

Table S1: BXD composition details.