

Supplementary Material

Multichannel microperfusion cell-capture system for screening anticancer active ingredients in traditional Chinese medicine formulas

Doudou Xu^{a,1}, Yi Tian^{d,1}, Dan Tie^a, Shuang Hu^{a b c}, Rongrong Xing^{a b c}, Xuan Chen^{a b c*}*

^aSchool of Pharmacy, Shanxi Medical University, Taiyuan 030001, China

^bMedicinal Basic Research Innovation Center of Chronic Kidney Disease, Ministry of Education, Shanxi Medical University, Taiyuan 030001, China

^cShanxi Provincial Key Laboratory of Drug Synthesis and Novel Pharmaceutical Preparation Technology, Shanxi Medical University, Taiyuan 030001, China

^dAcademy of Medical Sciences, Shanxi Medical University, Taiyuan 030001, China

¹These authors contributed equally to this work.

*** Corresponding author.**

Xuan Chen, School of Pharmacy, Shanxi Medical University, No. 56, Xinjian South Road, Yingze District, Taiyuan 030001, P. R. China.

E-mail address: ywfxcx@163.com.

Rongrong Xing, School of Pharmacy, Shanxi Medical University, No. 56, Xinjian South Road, Yingze District, Taiyuan 030001, P. R. China.

E-mail address: rongrongxing@sxmu.edu.cn

Table S1 Reproducibility of screening using multichannel microperfusion system ($n=3$)

Samples	Active ingredients	Parameters	t_R (min) and RPA			HepG2 cells	
			I	II	III	Average value	RSD (%)
Huangqisan	1	t_R	4.40	4.41	4.41	4.41	0.08
		RPA	1176.40	1184.02	1499.10	1286.51	11.6
	X_1	t_R	4.80	4.81	4.81	4.81	0.07
		RPA	192.77	194.21	235.83	207.60	9.62
	X_2	t_R	6.30	6.31	6.31	6.31	0.09
		RPA	330.61	326.45	388.95	348.67	8.18
	X_3	t_R	6.72	6.73	6.73	6.73	0.10
		RPA	54.00	54.23	65.04	57.76	8.92
	2	t_R	8.40	8.40	8.40	8.40	0.03
		RPA	21.99	23.05	25.50	23.51	6.26
	X_4	t_R	12.97	12.97	12.96	12.97	0.03
		RPA	1.45	1.41	1.60	1.49	5.51
	X_5	t_R	13.68	13.69	13.68	13.68	0.03
		RPA	4.24	4.27	4.90	4.47	6.8
	3	t_R	18.73	18.73	18.73	18.73	0.01
		RPA	43.31	44.62	47.91	45.28	4.27
	4	t_R	20.10	20.10	20.10	20.10	0.01
		RPA	2.23	2.29	2.70	2.41	8.59
	X_6	t_R	20.85	20.85	20.85	20.85	0.01
		RPA	188.88	193.58	206.30	196.25	3.75
	X_7	t_R	23.76	23.76	23.76	23.76	0.01
		RPA	19.64	19.62	20.63	19.96	2.36
	5	t_R	24.07	24.08	24.08	24.07	0.01
		RPA	13.17	13.19	13.46	13.27	1.02
	X_8	t_R	27.65	27.65	27.66	27.66	0.01
		RPA	16.07	18.00	18.51	17.53	6.00
Puerariae Lobatae Radix	6	t_R	30.31	30.30	30.31	30.31	0.01
		RPA	45.08	46.55	47.16	46.27	1.88
	7	t_R	32.69	32.69	32.69	32.69	0.01
		RPA	2.26	1.90	2.32	2.16	8.54
	8	t_R	36.40	36.40	36.40	36.40	0.01
		RPA	45.78	43.97	43.42	44.39	2.27
	1	t_R	4.41	4.41	4.41	4.41	0.03
		RPA	653.81	686.21	674.24	671.42	1.99
	X_1	t_R	4.81	4.81	4.81	4.81	0.06
		RPA	133.91	97.83	106.52	112.75	13.6

Astragali Radix	X ₂	<i>t_R</i>	6.31	6.31	6.31	6.31	0.03
		RPA	212.71	166.94	185.85	188.50	9.96
	X ₃	<i>t_R</i>	6.73	6.73	6.73	6.73	0.03
		RPA	39.04	35.04	32.32	35.47	7.78
	2	<i>t_R</i>	8.36	8.36	8.36	8.36	0.02
		RPA	11.38	8.80	8.58	9.59	13.2
	3	<i>t_R</i>	18.73	18.73	18.73	18.73	0.01
		RPA	20.16	17.51	19.04	18.90	5.75
	X ₆	<i>t_R</i>	20.86	20.86	20.86	20.86	0.01
		RPA	88.54	83.73	91.26	87.84	3.54
	6	<i>t_R</i>	30.31	30.32	30.31	30.32	0.01
		RPA	25.59	25.01	23.77	24.79	3.07
	8	<i>t_R</i>	36.40	36.40	36.40	36.40	0
		RPA	10.11	9.71	9.07	9.63	4.46
	2	<i>t_R</i>	8.44	8.44	8.44	8.44	0
		RPA	28.42	30.44	28.42	29.09	3.28
	X ₅	<i>t_R</i>	13.70	13.70	13.70	13.70	0.01
		RPA	8.45	9.29	8.45	8.73	4.55
	3	<i>t_R</i>	18.73	18.72	18.73	18.72	0.03
		RPA	15.94	16.46	15.94	16.11	1.51
	5	<i>t_R</i>	24.08	24.07	24.08	24.08	0.02
		RPA	32.75	33.09	32.75	32.87	0.49
	6	<i>t_R</i>	30.31	30.32	30.31	30.31	0.01
		RPA	1.61	1.55	1.71	1.62	3.99
	7	<i>t_R</i>	32.72	32.72	32.72	32.72	0.01
		RPA	3.33	3.24	2.88	3.15	6.12
	8	<i>t_R</i>	36.40	36.40	36.40	36.40	0
		RPA	51.45	51.30	51.45	51.40	0.13
Mori Cortex	X ₄	<i>t_R</i>	13.03	13.03	13.03	13.03	0.01
		RPA	1.40	1.62	1.62	1.55	6.75
	4	<i>t_R</i>	19.91	19.91	19.91	19.91	0.01
		RPA	0.40	0.44	0.43	0.42	4.15
	X ₇	<i>t_R</i>	23.74	23.75	23.75	23.75	0.02
		RPA	1.00	1.00	1.00	1.00	0
	X ₈	<i>t_R</i>	27.90	27.91	27.91	27.90	0.01
		RPA	1.42	1.63	1.53	1.53	5.46

Table S2 Screening results of HepG2 cells on the active ingredients of TCM ($n=3$)

Samples	Number of ingredients screened	Known ingredients peak number	Unknown ingredients peak number	t_R (min)	Standards	CFF_{HepG2}	Activity grade
Huangqisan	16	1		4.406	Puerarin	3.9	D
			X ₁	4.806	-	3.7	D
			X ₂	6.309	-	4.1	D
			X ₃	6.727	-	3.7	D
		2		8.397	Calycosin glycoside	4.6	D
			X ₄	12.966	-	8.4	C
			X ₅	13.684	-	2.5	D
		3		18.728	Ononin	4.3	D
		4		20.098	Morin	6.4	C
			X ₆	20.851	-	6.4	C
			X ₇	23.76	-	3.9	D
		5		24.073	Calycosin	5.2	C
			X ₈	27.655	-	4.1	D
		6		30.306	Genistein	7.1	C
		7		32.69	Isorhamnetin	7.3	C
		8		36.399	Formononetin	5.7	C
Puerariae Lobatae Radix	9	1		4.41	Puerarin	1.4	D
			X ₁	4.808	-	1.5	D
			X ₂	6.311	-	1.9	D
			X ₃	6.727	-	1.1	D
		2		8.358	Calycosin glycoside	2.0	D
		3		18.728	Ononin	2.0	D
			X ₆	20.857	-	3.7	D
		6		30.315	Genistein	5.4	C
		8		36.402	Formononetin	2.8	D
Astragali Radix	7	2		8.44	Calycosin glycoside	2.7	D
			X ₅	13.697	-	3.0	D
		3		18.722	Ononin	2.8	D
		5		24.08	Calycosin	4.3	D
		6		30.313	Genistein	3.0	D
		7		32.72	Isorhamnetin	5.3	C

Mori Cortex	4	8	36.397	Formononetin	5.3	C
		X ₄	13.032	-	12.2	B
		4	19.911	Morin	19.8	A
		X ₇	23.748	-	4.0	D
		X ₈	27.906	-	9.0	C

Note: Undetermined ingredients are indicated by –.