

1 **An Intelligent Extraction Approach of Feature Information from**
2 **Three-Dimensional DAD Chromatogram for Integrated Quality**
3 **Control of Traditional Chinese Medicine: *Gardenia Jasminoides* root**
4 **as an example**

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Table S1 Sample information of *Gardenia Jasminoides* root

No.	Batches	Geographical regions
S1	ZZG-R2006001	Yunhe, Zhejiang
S2	ZZG-R2006002	Jingning, Zhejiang
S3	ZZG-R2006003	Jingning, Zhejiang
S4	ZZG-R2006004	Qingtian, Zhejiang
S5	ZZG-R2006005	Qingtian, Zhejiang
S6	ZZG-R2006006	Jingning, Zhejiang
S7	ZZG-R2006007	Jingning, Zhejiang
S8	ZZG-R2006008	Lishui, Zhejiang
S9	ZZG-R2006009	Yunhe, Zhejiang
S10	ZZG-R2006010	Qingtian, Zhejiang
S11	ZZG-R2006011	Lishui, Zhejiang
S12	ZZG-R2006012	Lishui, Zhejiang
S13	ZZG-R2006013	Lishui, Zhejiang
S14	ZZG-R2006014	Sanming, Fujian
S15	ZZG-R2006015	Sanming, Fujian
S16	ZZG-R2006016	Sanming, Fujian
S17	ZZG-R2006017	Meizhou, Guangdong
S18	ZZG-R2006018	Meizhou, Guangdong
S19	ZZG-R2006019	Meizhou, Guangdong
S20	ZZG-R2006020	Meizhou, Guangdong
S21	ZZG-R2006021	Yulin, Guangxi
S22	ZZG-R2006022	Yulin, Guangxi
S23	ZZG-R2006023	Yulin, Guangxi
S24	ZZG-R2006024	Jiujiang, Jiangxi
S25	ZZG-R2006025	Jiujiang, Jiangxi
S26	ZZG-R2006026	Jiujiang, Jiangxi
S27	ZZG-R2006027	Bozhou, Anhui

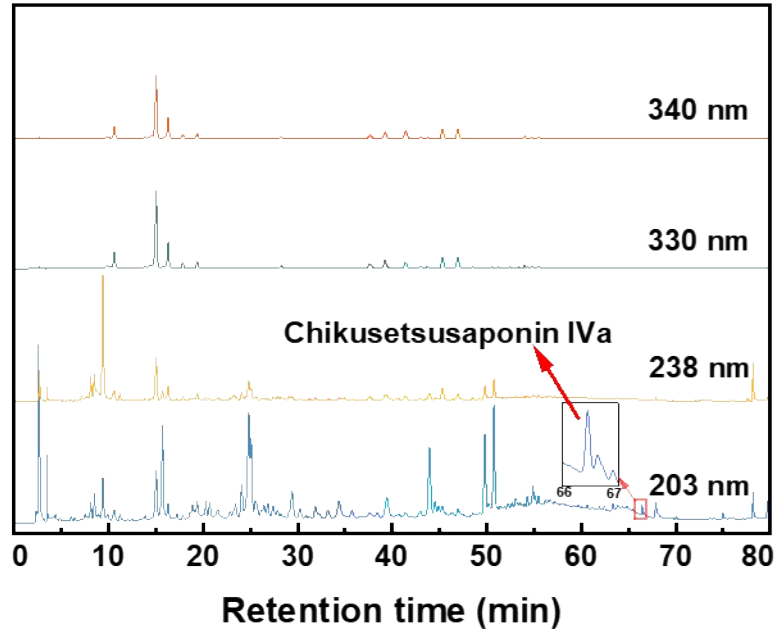


Fig. S1. Chromatograms in different wavelengths with *Gardenia Jasminoides* root.

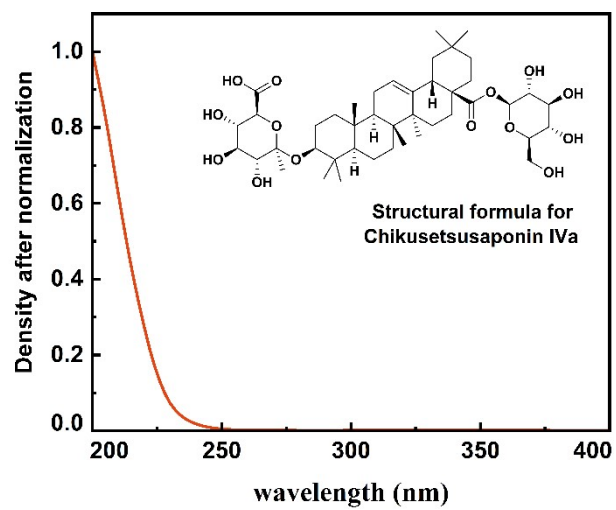


Fig. S2. The UV absorption spectrum and structural formula of Chikusetsusaponin IVa.

Table S2 Linear regression equation

Approach	Regression equation	R ²
Single-wavelength fingerprint	$y = 3.7659x + 6.199$	0.9999
BFD	$y = 0.0699x + 0.152$	0.9999

Table S3 The results of RT and peak area from single-wavelength fingerprint and BFD

No.	Single-wavelength fingerprint (n=6)		BFD (n=6)	
	RT (min)	S	RT (min)	S
1	65.78	559.60	65.78	10.59
2	65.89	543.00	65.89	10.85
3	66.03	566.90	66.03	11.02
4	65.92	578.00	65.92	10.89
5	66.00	577.10	66.00	11.37
6	66.12	562.90	66.12	10.74
Average	65.96	564.58	65.96	10.91
RSD (%)	0.18	2.29	0.18	2.46

RT: retention time

S: peak area

RSD: relative standard deviation

Table S4 RT and common peak areas of 27 batches in 203nm HPLC fingerprints

No.	RT (min)	S1	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26	S27
1	2.35	13.7	13.0	22.2	23.5	21.4	19.8	14.4	14.2	32.6	30.6	24.2	19.4	23.1	13.7	8.9	14.6	18.6	18.0	15.9	6.1	3.4	7.1	0.0	37.1	34.0	30.9	21.5	2.35
2	2.58	83.9	42.0	43.7	48.2	52.0	45.8	43.6	38.3	51.6	46.7	43.9	36.9	48.1	25.1	21.7	30.3	45.0	31.1	46.6	27.0	12.1	14.4	65.9	37.5	33.2	28.9	25.7	2.58
3	2.71	92.8	60.0	61.3	60.7	60.9	55.0	49.9	56.1	70.6	66.2	63.0	66.9	58.7	48.3	41.4	64.3	49.6	77.6	46.3	46.0	44.0	44.8	72.5	61.2	55.4	56.1	65.4	2.71
4	3.49	28.4	16.5	17.5	17.0	16.6	16.5	15.0	16.3	20.4	19.8	17.6	15.5	16.7	9.2	7.2	10.9	13.4	17.2	7.9	6.8	11.0	5.5	13.1	13.0	12.9	7.3	13.6	3.49
5	10.63	17.9	15.6	19.1	15.6	15.7	14.6	13.9	16.4	19.3	15.8	17.4	16.2	18.1	14.8	10.4	20.0	18.5	20.5	16.2	13.2	20.8	24.1	39.3	26.4	20.2	19.9	9.0	10.63
6	11.22	7.6	6.5	7.1	6.3	6.6	7.2	6.2	7.4	7.1	5.6	6.9	5.8	6.4	2.4	5.8	2.2	17.4	1.6	0.6	1.0	8.6	1.5	5.1	8.3	8.8	7.2	0.0	11.22
7	15.04	62.9	45.7	49.0	53.7	51.8	45.8	36.4	50.2	78.2	60.3	50.4	47.2	49.8	47.5	31.8	44.9	20.8	36.5	22.7	29.0	33.5	28.5	36.0	22.8	22.6	31.1	24.5	15.04
8	15.71	102.6	81.5	85.2	93.2	88.4	84.4	85.2	81.4	108.3	102.5	81.5	75.1	88.0	67.9	43.5	47.6	79.5	80.0	70.5	50.7	59.4	91.9	73.3	47.2	40.1	53.1	82.7	15.71
9	16.31	16.9	10.8	13.8	15.0	12.2	10.9	10.9	15.0	23.4	12.0	11.8	14.2	15.5	13.2	10.6	23.8	15.3	21.8	12.5	12.8	11.1	7.1	4.2	10.8	12.2	12.3	6.4	16.31
10	24.09	41.3	26.1	25.5	32.8	22.6	25.8	27.5	19.6	26.2	22.9	25.1	21.5	24.0	13.3	29.9	42.0	30.3	30.9	23.0	18.9	5.8	3.5	41.2	28.5	21.6	41.3	5.4	24.09
11	24.82	139.7	160.2	129.9	138.1	128.5	120.4	120.2	155.9	160.2	141.2	164.8	142.2	147.1	131.7	105.7	140.6	106.5	147.6	122.1	128.3	183.5	120.6	46.2	80.7	68.6	54.6	33.1	24.82
12	39.47	48.6	37.8	42.5	43.1	35.1	32.0	34.1	40.8	46.3	40.6	36.4	38.8	37.8	25.6	23.4	16.6	14.0	13.2	27.5	26.8	12.8	20.6	13.5	12.3	27.4	18.5	16.1	39.47
13	43.96	112.1	87.6	95.9	112.0	90.6	93.2	97.6	86.2	111.9	105.6	89.0	82.4	91.9	138.5	87.7	159.1	56.2	43.5	53.2	107.0	58.8	27.0	32.5	54.4	45.3	50.0	39.9	43.96
14	46.97	12.5	13.1	24.1	22.9	12.9	10.5	11.6	20.7	18.0	22.0	21.0	21.7	15.2	28.7	10.0	18.7	6.2	17.4	9.2	8.4	23.4	3.6	9.7	13.1	17.0	19.8	12.4	46.97
15	49.81	105.0	88.6	98.1	107.7	95.2	91.4	92.4	86.1	103.1	96.6	85.5	87.5	89.4	103.8	46.5	120.8	32.9	50.0	27.4	75.3	65.2	27.9	26.8	46.5	37.9	36.0	3.9	49.81
16	50.77	117.6	83.2	82.1	107.5	88.2	78.5	88.5	73.6	103.2	107.1	76.4	70.1	82.9	99.8	45.7	90.5	52.0	54.9	25.7	87.3	54.7	18.3	29.1	37.6	34.5	32.9	1.3	50.77
17	54.90	22.9	20.0	17.3	18.7	18.1	17.6	14.6	17.4	10.0	20.7	18.4	16.8	17.5	20.0	11.2	23.7	16.7	15.1	13.5	19.5	8.4	9.3	10.7	16.9	14.8	9.2	2.5	54.90
18	66.45	5.5	3.7	4.3	4.7	3.4	3.6	4.6	3.9	3.9	3.4	4.7	3.6	4.0	11.9	7.8	6.0	14.8	10.0	10.1	11.9	1.2	2.2	9.4	8.8	8.6	8.1	6.5	66.45
19	67.88	27.9	29.2	29.4	30.4	28.2	27.8	26.8	28.1	28.4	28.6	28.1	29.1	28.2	0.5	1.1	1.3	0.8	1.2	0.9	1.2	1.9	0.6	1.5	0.8	1.3	0.6	12.4	67.88
20	70.08	2.3	1.6	1.7	2.0	1.4	1.3	1.8	1.6	1.7	1.5	2.1	1.6	1.6	2.2	1.4	1.5	2.1	1.9	2.6	2.7	0.4	0.6	3.5	1.8	1.4	3.2	2.4	70.08
21	75.01	5.6	6.1	6.0	1.4	5.5	5.3	5.2	5.2	5.1	5.2	5.2	5.2	5.2	0.5	0.5	0.8	1.2	2.9	2.0	1.0	0.7	0.2	1.5	1.0	1.6	1.3	0.9	75.01
22	78.19	31.4	30.1	29.1	29.3	28.5	29.5	29.1	30.0	40.6	31.2	29.6	29.7	30.2	8.3	7.6	7.4	22.8	4.1	7.7	8.6	25.0	9.9	8.4	24.9	24.7	8.1	12.9	78.19

23	79.75	19.4	20.1	20.4	19.8	19.6	19.6	19.7	20.0	19.7	20.0	20.4	20.3	20.9	4.4	4.5	4.9	11.4	3.0	4.8	4.5	11.3	3.4	4.8	10.9	11.0	5.7	4.5	79.75
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Table S5 RT and common peak areas of 27 batches in BFD

No.	RT (min)	S1 to S27																											
		S1	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26	S27
1	2.35	15.1	23.0	26.0	28.2	25.6	24.0	24.3	24.8	40.1	38.3	28.3	22.6	27.1	16.2	10.6	18.0	23.1	20.2	19.1	6.8	4.2	8.7	0.0	49.0	45.0	39.7	26.9	2.35
2	2.58	91.6	50.1	52.5	57.6	60.4	54.8	53.2	46.9	62.3	56.6	53.5	45.1	57.7	35.8	29.6	37.3	28.6	29.9	26.3	36.5	16.7	22.6	20.3	24.0	26.0	26.2	29.7	2.58
3	2.71	83.8	62.7	63.8	62.4	63.4	56.5	51.2	58.5	73.7	68.8	66.5	61.0	61.8	52.7	43.8	68.8	48.7	93.5	48.2	44.6	47.5	47.7	80.4	62.9	56.2	59.8	74.6	2.71
4	3.49	29.2	17.2	18.0	17.5	17.2	17.0	15.7	16.9	20.8	20.0	18.0	15.9	17.1	9.8	7.7	11.4	13.8	18.1	8.0	7.0	11.0	5.9	13.5	12.9	12.8	7.7	13.8	3.49
5	6.06	7.9	6.4	6.3	6.4	6.2	6.0	7.1	5.6	7.6	7.1	7.2	5.6	7.4	3.6	0.0	4.8	0.0	11.8	5.3	4.8	0.0	3.2	9.6	8.9	6.5	7.0	16.2	6.06
6	6.43	4.9	0.0	0.0	0.0	0.0	0.0	5.0	0.0	5.7	5.3	5.2	0.0	5.6	0.0	0.0	0.0	0.0	4.6	3.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.43
7	9.41	133.5	68.7	77.8	74.5	62.6	65.5	59.5	65.8	79.5	62.5	85.3	64.2	72.8	53.1	58.5	40.7	21.3	41.1	118.0	73.1	267.0	274.5	180.3	192.5	166.2	205.0	26.2	9.41
8	11.21	6.3	7.7	8.5	8.5	9.4	8.7	8.2	8.5	8.8	7.0	9.0	7.3	8.2	0.0	0.0	0.0	0.0	0.0	6.3	4.2	10.5	0.0	7.5	8.8	9.3	9.2	7.9	11.21
9	15.04	90.9	52.6	56.7	57.5	62.0	53.5	41.7	60.8	95.2	71.1	58.5	56.1	60.2	63.4	40.2	49.3	29.5	49.2	28.0	38.3	48.6	37.7	32.4	30.6	31.5	44.9	25.0	15.04
10	15.71	102.8	79.2	83.6	89.3	86.0	83.1	84.9	79.5	108.5	103.0	80.4	74.8	84.0	65.6	41.9	43.0	73.4	79.1	69.4	50.5	61.0	87.0	64.8	43.2	37.0	51.0	81.4	15.71
11	16.31	22.1	21.8	25.9	22.4	22.9	21.5	19.9	24.8	33.0	25.0	24.8	23.1	20.7	23.2	17.0	31.9	25.1	35.1	21.8	22.1	20.7	14.7	7.3	17.7	17.8	22.1	9.1	16.31
12	17.25	7.9	6.9	7.3	7.3	4.7	7.0	7.9	5.3	7.1	7.4	6.0	5.1	7.4	8.0	7.1	9.6	8.7	6.9	8.6	6.5	0.0	0.0	12.2	0.0	0.0	0.0	7.7	17.25
13	17.85	7.9	9.7	10.0	10.0	6.3	8.0	8.7	7.9	6.6	6.0	8.4	6.6	9.0	9.4	6.3	8.0	7.4	11.4	12.5	15.6	6.8	0.0	12.5	7.3	6.7	8.0	0.0	17.85
14	20.71	17.2	15.8	16.8	19.9	16.7	15.8	14.9	14.3	18.5	17.8	17.0	14.3	15.2	14.0	7.8	34.6	11.0	14.4	10.9	10.5	24.3	7.5	8.0	8.8	10.8	12.8	17.9	20.71
15	24.09	40.2	25.9	25.3	32.5	22.1	26.6	28.5	20.8	25.0	22.8	25.0	7.7	24.5	18.7	39.1	54.3	34.7	35.1	19.3	25.7	8.2	6.1	43.7	35.4	26.8	42.7	9.7	24.09
16	24.82	137.9	164.0	125.6	138.6	121.7	115.7	115.6	158.6	155.8	138.3	165.5	144.9	152.4	130.2	106.8	141.1	111.3	149.6	124.9	131.1	196.6	122.0	49.8	80.9	69.6	56.5	33.7	24.82
17	25.09	84.1	0.0	38.1	41.8	36.5	38.1	32.9	0.0	54.2	51.8	0.0	0.0	0.0	47.5	39.6	13.1	0.0	20.8	50.0	80.4	0.0	49.4	0.0	0.0	0.0	0.0	0.0	25.09
18	26.45	17.3	14.5	15.7	18.8	15.5	14.8	16.7	12.6	17.8	17.6	14.1	11.1	14.5	17.6	16.0	22.1	11.8	12.9	14.4	17.7	7.7	13.9	14.6	10.8	9.2	14.4	18.5	26.45
19	26.85	21.9	17.2	18.3	21.5	17.3	17.6	19.1	15.2	20.6	19.5	16.2	13.2	16.9	22.8	10.5	6.5	15.2	14.0	15.1	21.8	13.8	11.2	17.4	14.3	11.8	13.5	16.0	26.85
20	29.41	49.8	23.3	33.0	36.6	36.4	28.6	22.3	27.8	49.3	41.7	26.4	21.6	24.6	21.6	17.0	44.7	5.7	42.4	6.1	21.7	23.5	9.4	10.1	15.1	13.9	14.5	6.9	29.41
21	30.26	16.8	20.1	19.5	21.3	18.5	18.9	19.7	18.8	19.1	17.1	20.0	17.6	19.1	13.4	6.9	11.5	14.1	9.3	11.8	16.5	0.0	10.8	7.2	0.0	15.5	0.0	0.0	30.26

22	32.29	9.3	8.3	9.0	9.5	8.6	7.9	6.9	8.5	8.8	8.8	8.0	7.6	7.7	7.7	14.3	22.3	10.0	14.7	17.5	6.1	0.0	0.0	8.2	0.0	0.0	12.9	0.0	32.29
23	33.19	18.8	13.9	15.7	13.2	15.0	14.9	14.9	14.3	19.0	18.3	15.1	13.9	14.3	21.9	14.4	21.0	14.1	10.1	6.7	16.8	7.1	14.1	7.3	6.0	0.0	5.8	0.0	33.19
24	39.47	43.8	34.0	38.1	42.1	36.0	32.6	33.2	35.8	42.0	39.8	35.3	33.6	35.6	42.5	25.7	28.9	14.8	16.6	29.6	28.7	15.3	24.6	13.9	23.9	26.6	21.2	19.2	39.47
25	41.44	14.0	15.0	18.2	19.4	15.1	12.7	12.8	18.2	18.6	18.7	19.7	20.5	19.7	7.2	12.1	8.4	9.3	7.5	10.4	11.6	9.9	11.1	12.0	11.2	8.1	9.7	0.0	41.44
26	42.98	13.1	14.8	13.4	12.0	15.8	15.8	15.5	13.5	14.4	14.9	12.7	12.3	12.9	10.3	0.0	15.8	8.0	0.0	0.0	0.0	23.1	0.0	9.6	0.0	0.0	0.0	41.8	42.98
27	43.96	105.7	82.2	92.7	112.2	85.4	85.5	91.3	83.3	106.3	101.4	86.0	79.8	85.7	128.8	82.6	152.5	51.3	44.9	50.2	100.9	56.2	54.5	31.0	52.1	42.2	45.9	33.4	43.96
28	45.33	18.3	15.6	22.8	21.8	17.6	18.8	16.4	20.8	21.0	17.4	24.2	20.4	18.0	11.9	20.0	19.0	8.6	25.4	8.1	21.3	22.0	26.3	36.9	25.7	25.0	25.2	10.4	45.33
29	46.96	18.6	19.2	28.5	24.1	19.1	16.2	15.6	22.8	26.2	22.8	23.4	24.9	24.1	47.6	17.1	27.6	8.8	19.3	14.9	15.9	30.0	20.1	13.8	21.1	24.8	23.1	19.0	46.96
30	49.81	101.0	83.8	93.4	104.5	90.3	86.3	87.2	81.7	98.2	92.0	81.4	83.5	84.5	81.6	43.7	123.8	32.1	47.0	24.6	68.5	64.2	25.0	23.9	44.9	35.8	32.9	0.0	49.81
31	50.77	119.9	82.7	82.5	105.4	87.8	79.4	90.8	75.7	104.2	106.0	75.5	69.6	79.5	95.5	46.5	93.4	51.2	54.9	27.5	87.3	56.3	19.9	28.0	37.7	33.8	34.1	0.0	50.77
32	54.31	10.0	6.9	7.5	10.2	6.6	7.0	6.1	7.0	7.5	7.7	6.6	7.3	6.8	6.4	5.2	9.2	5.1	6.6	4.4	9.7	0.0	5.9	0.0	3.8	3.8	3.2	0.0	54.31
33	54.90	21.0	18.6	18.3	19.9	18.5	16.9	15.9	17.0	21.0	20.0	18.5	16.7	17.5	20.0	12.4	18.8	17.9	17.1	13.4	18.5	8.9	9.8	11.6	18.0	16.2	9.9	0.0	54.90
34	55.16	6.9	3.6	5.5	6.6	5.9	4.9	5.1	5.1	5.2	6.4	5.4	4.5	3.7	6.3	3.4	0.0	0.0	0.0	0.0	2.5	5.6	0.0	0.0	0.0	0.0	3.2	0.0	55.16
35	55.49	10.0	9.1	11.0	10.4	8.3	8.3	7.9	9.2	11.0	9.9	9.5	7.7	8.9	10.0	4.6	9.8	0.0	12.6	2.8	5.9	5.6	14.0	0.0	6.8	6.9	4.4	5.1	55.49
36	63.35	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.9	0.0	3.4	3.9	0.0	0.0	5.3	0.0	0.0	4.5	0.0	63.35
37	66.45	7.0	4.8	5.4	6.0	4.7	4.9	6.1	5.0	5.3	4.6	6.2	4.8	5.4	4.4	6.3	9.3	7.8	16.8	13.0	11.7	13.7	7.7	9.2	11.4	10.4	10.1	9.6	66.45
38	77.61	3.6	3.4	3.5	5.3	3.1	0.0	4.4	3.6	3.9	3.7	4.1	3.9	3.4	3.1	3.8	0.0	0.0	0.0	3.7	0.0	0.0	3.4	0.0	0.0	0.0	0.0	0.0	77.61

Table S6 Comparison of different fingerprint processing methods

	Single-wavelength fingerprint	MFCF	BFD
Number of common peaks	23	21	38
Number of wavelength	1	5	all
Processing means	Manual	Manual	computer
Data processing time (per sample)	Second most	Most	4 s
Number of origin classification categories	2	3	3
Classification accuracy	Less accuracy	Accurate	Accurate