Supporting Information

A Simple Array Integrating Machine Learning for Identification of Flavonoids in Red Wines

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1. General Information

Machine learning algorithms: Eight machine learning algorithms, including Support Vector Machine (SVM), Decision Tree (DT), K-nearest Neighbor (KNN), Random Forest (RF), Gaussian Process Classifier (GPC), Naïve Bayes (NB), Logistic Regression (LR) and Linear Discriminant Analysis (LDA), were built in Python using the scikit-learn package, which is an open-source tool for data analysis and machine learning (https://github.com/scikit-learn/scikit-learn).

Linear discriminant analysis: Linear discriminant analysis was carried out using classical linear discriminant analysis (LDA) in SYSTAT (version 13.0). In LDA, all variables were used in the model (complete model) and the tolerance was set as 0.001. The fluorescence response patterns were transformed into canonical patterns. The Mahalanobis distances of each individual pattern to the centroid of each group in a multidimensional space were calculated and the assignment of the case was based on the shortest Mahalanobis distance.

2. The Information of Flavonoids

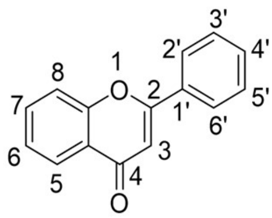
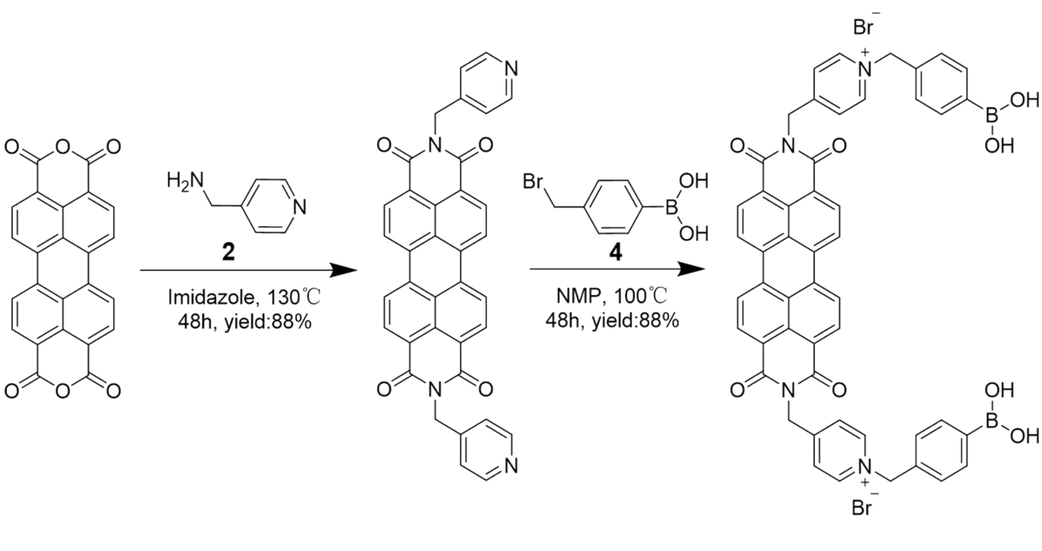


Fig. S1 Basic skeleton structure of flavonoids

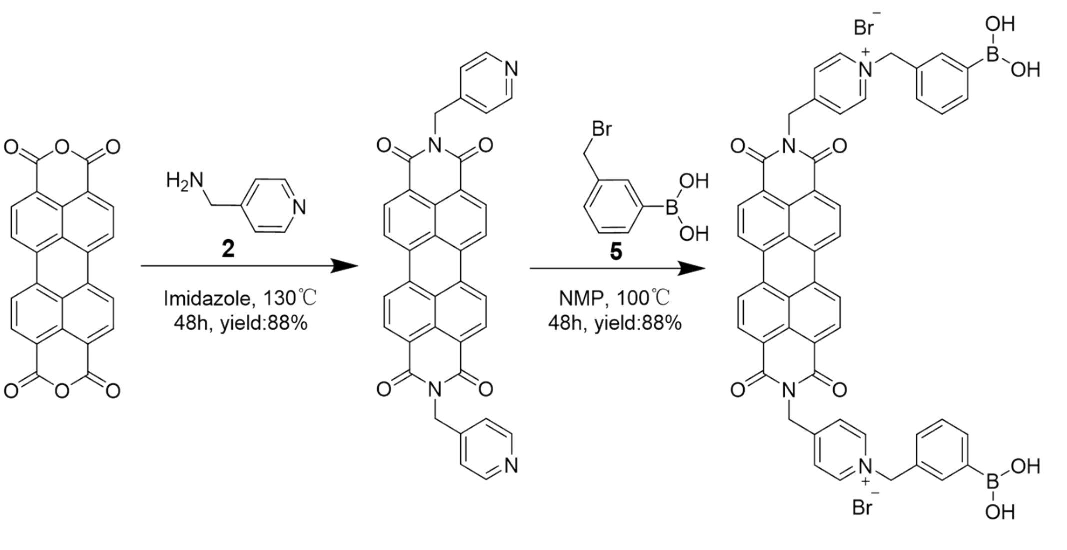
Flavonoids use C6-C3-C6 as the basic skeleton and are composed of two aromatic rings connected to each other through a central three-carbon chain.

3. Synthesized procedure of PDIs



1 **3** **PDI-1**

Fig. S2 Synthetic routes of PDI-1.



1 **3** **PDI-2**

Fig. S3 Synthetic routes of PDI-2.

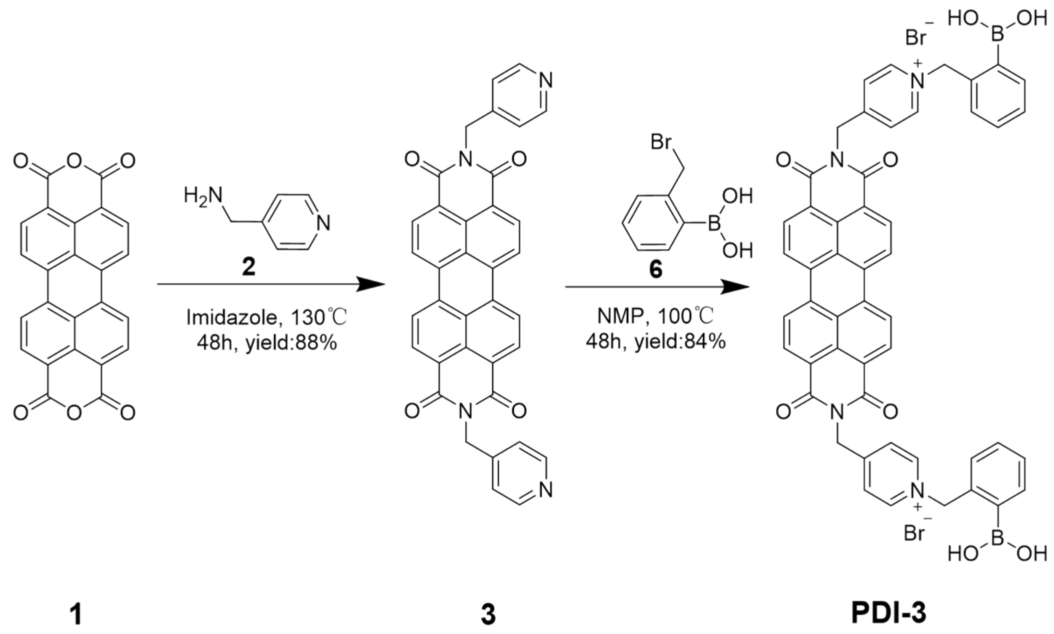


Fig. S4 Synthetic routes of PDI-3.

4. [1]H NMR Spectrum of PDIs

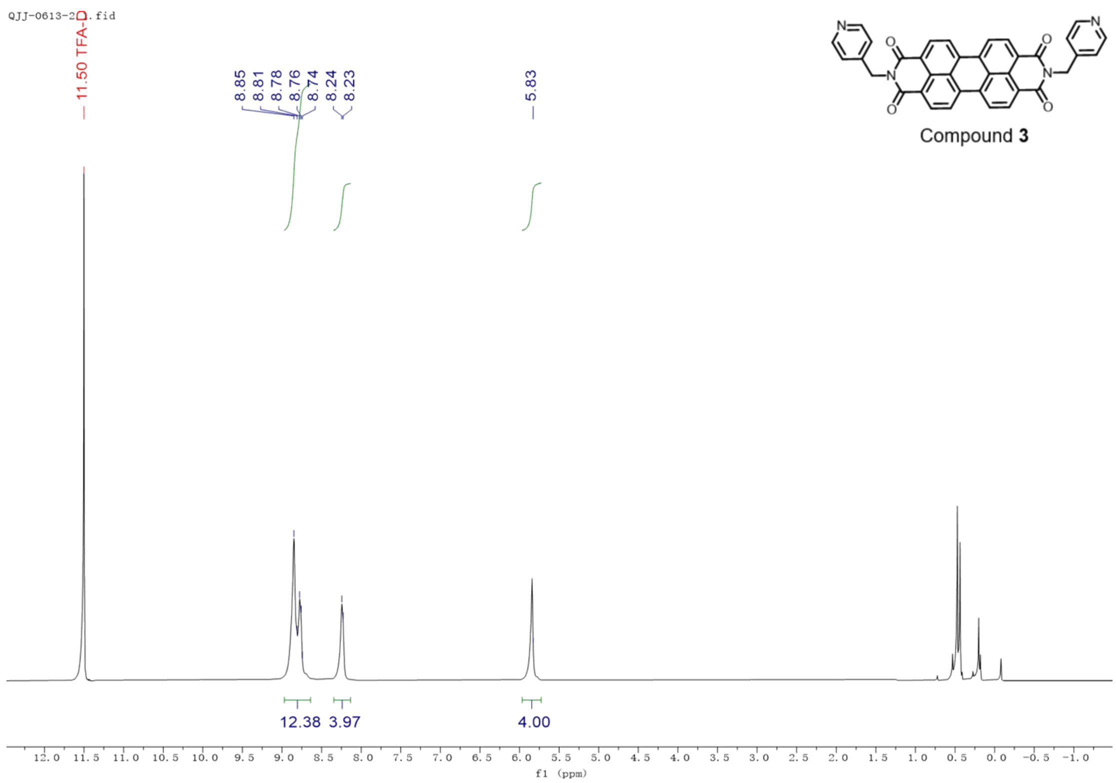


Fig. S5 ^{1}H NMR spectrum of compound **3** in CF_3COOD (300 MHz). The nuclear magnetic peak near 0.5ppm is the residual solvent peak in CF_3COOD.

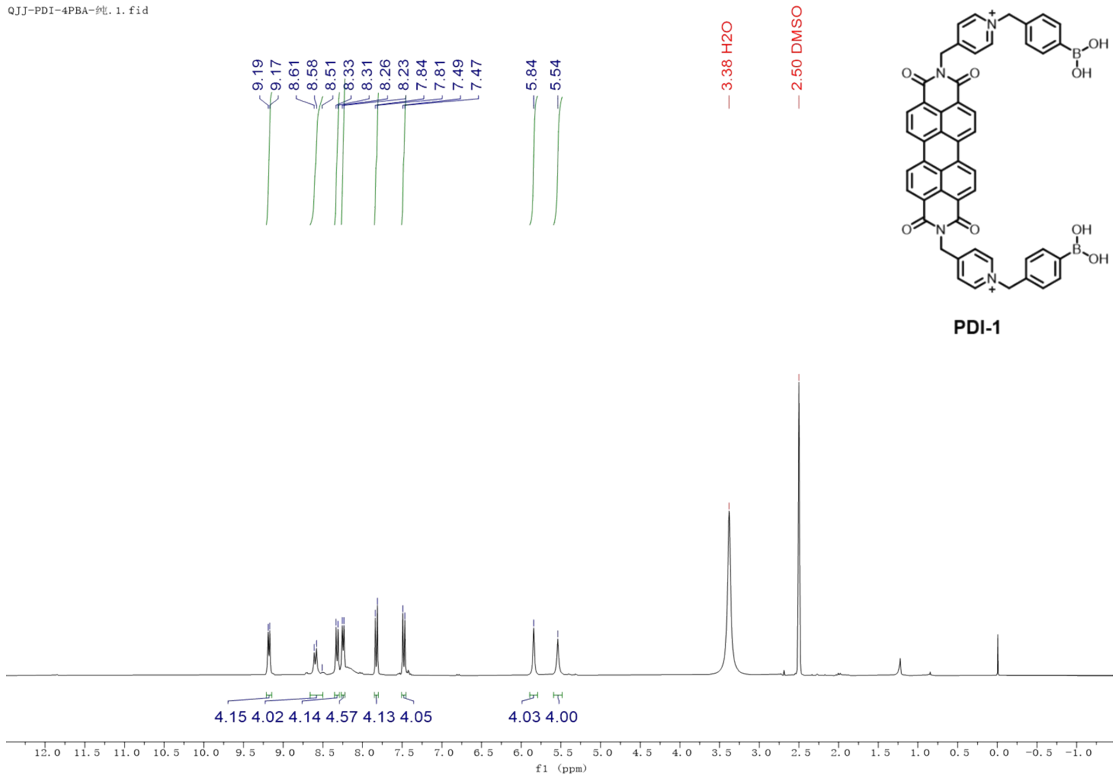


Fig. S6 [1]H NMR spectrum of PDI-1 in DMSO-d_6 (300 MHz).

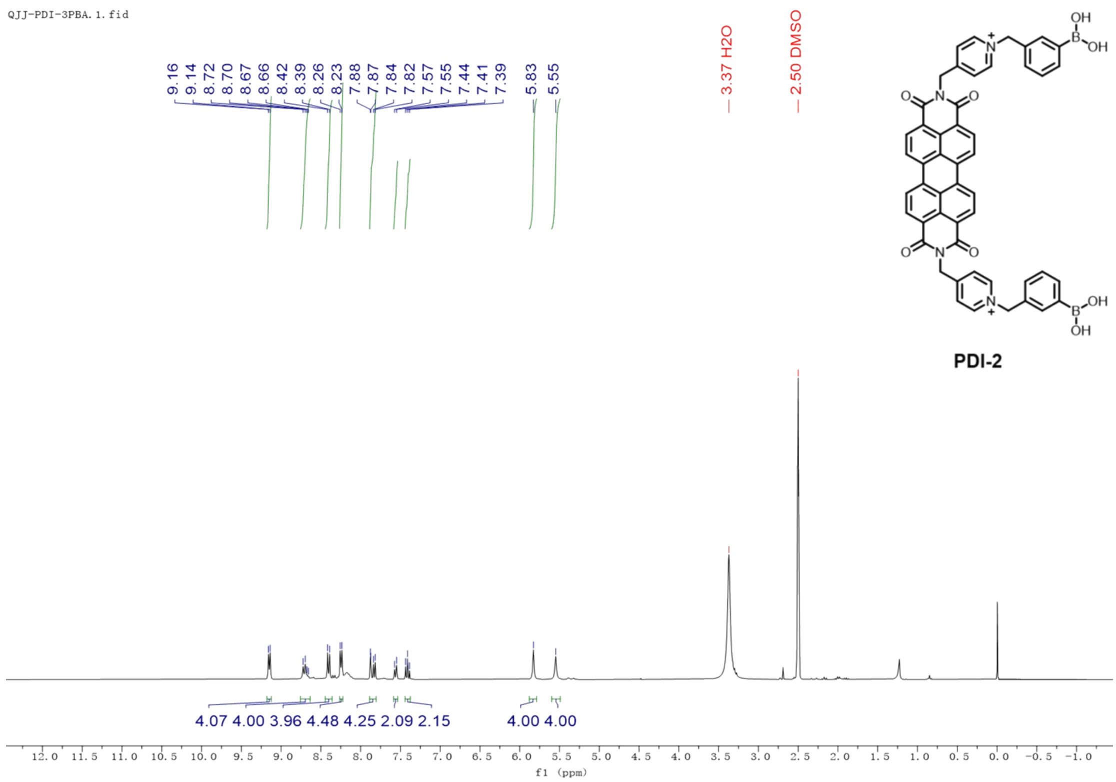


Fig. S7 [1]H NMR spectrum of PDI-2 in DMSO-d_6 (300 MHz).

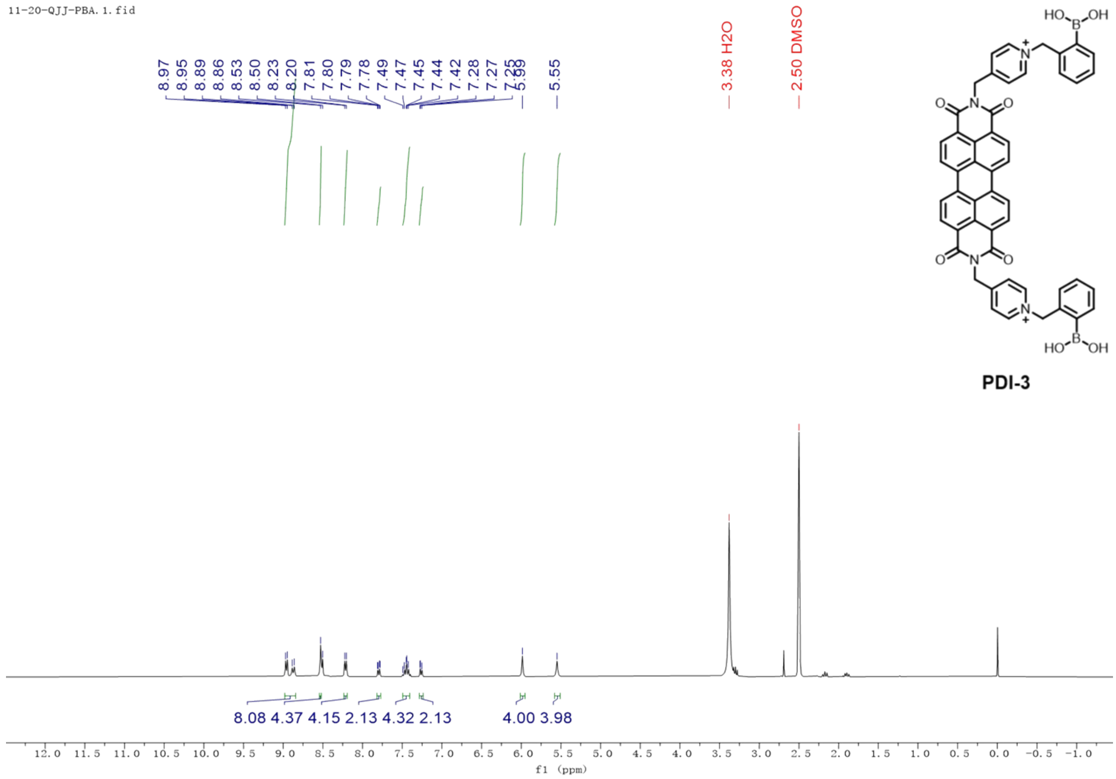


Fig. S8 ^{1}H NMR spectrum of PDI-3 in DMSO-d_6 (300 MHz).

5. ^{13}C NMR Spectrum of PDIs

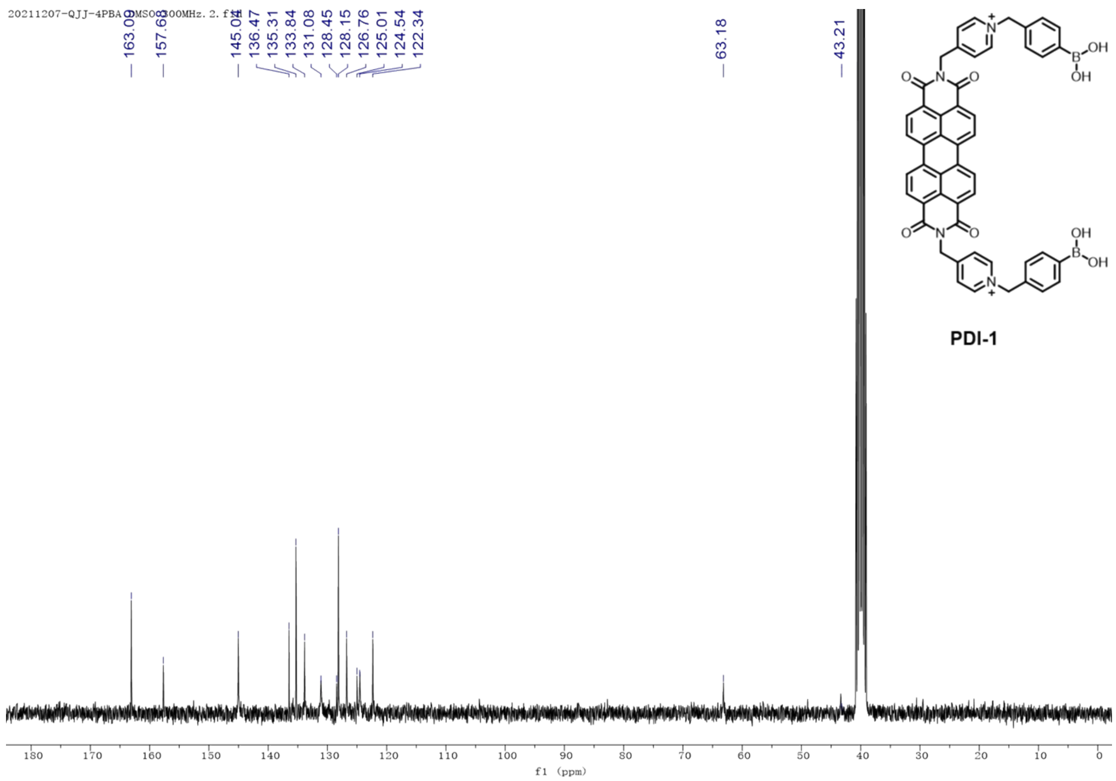


Fig. S9 ^{13}C NMR spectrum of PDI-1 in DMSO-d_6 (75 MHz).

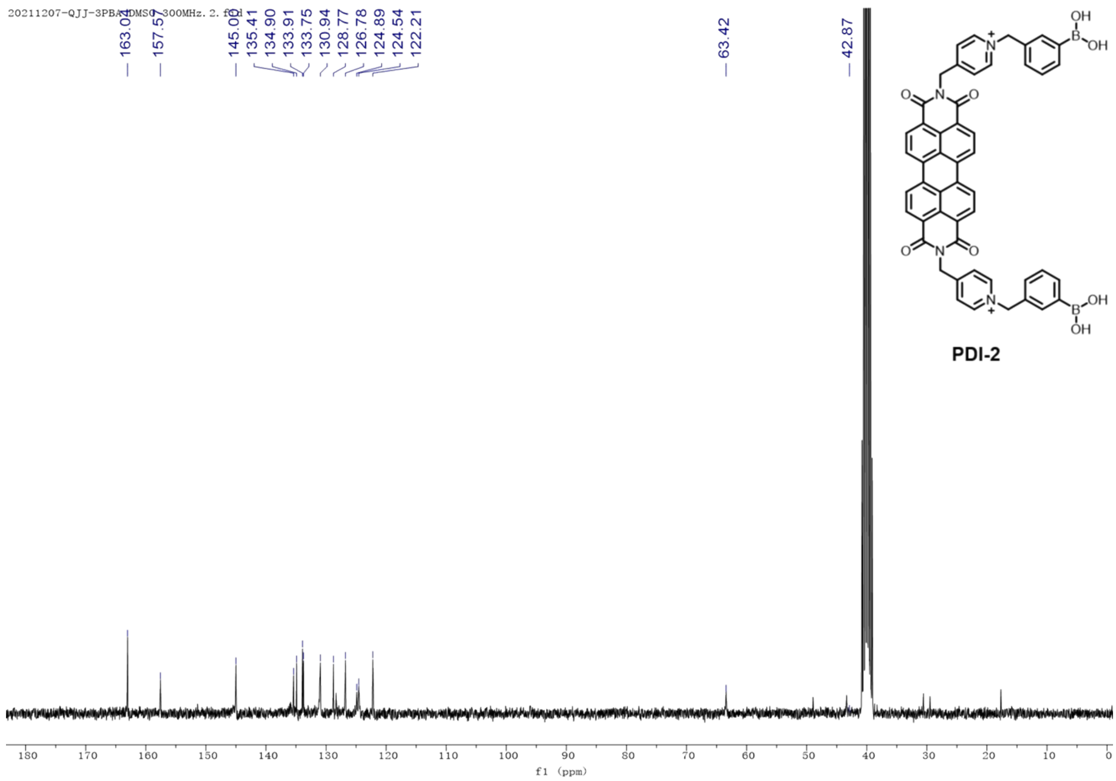


Fig. S10 ^{13}C NMR spectrum of PDI-2 in DMSO-d_6 (75 MHz).

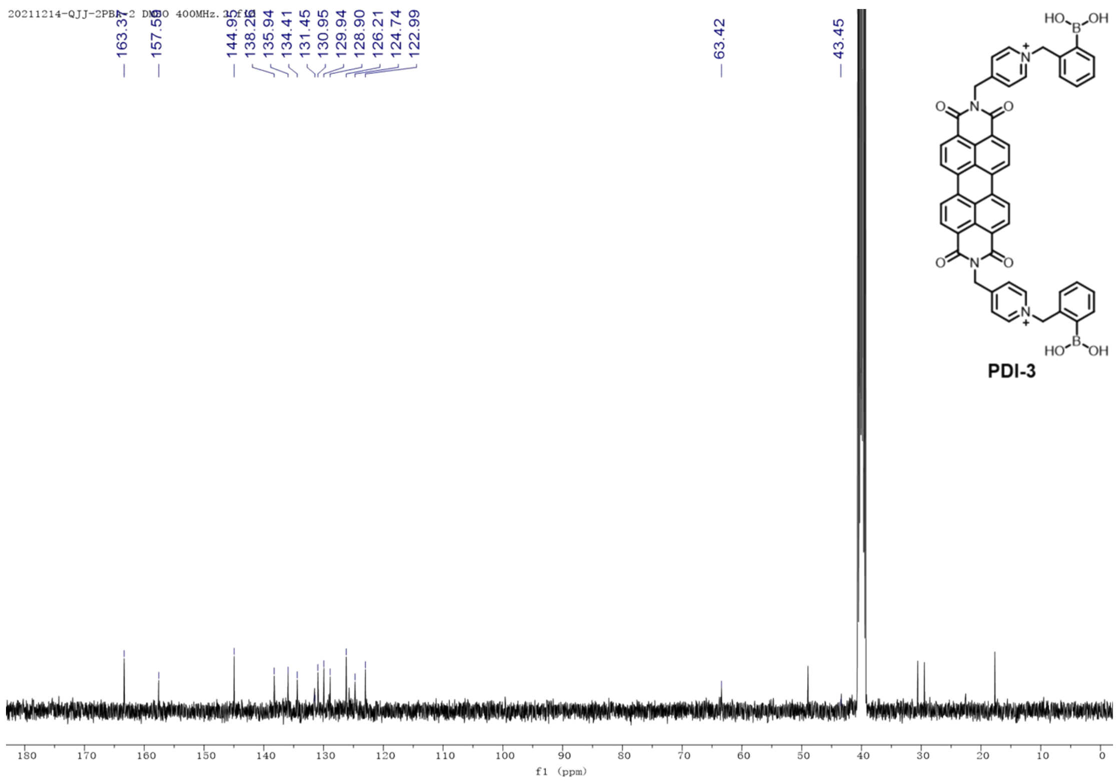


Fig. S11 ^{13}C NMR spectrum of PDI-3 in DMSO-d_6 (100 MHz).

6. MS Data for PDIs

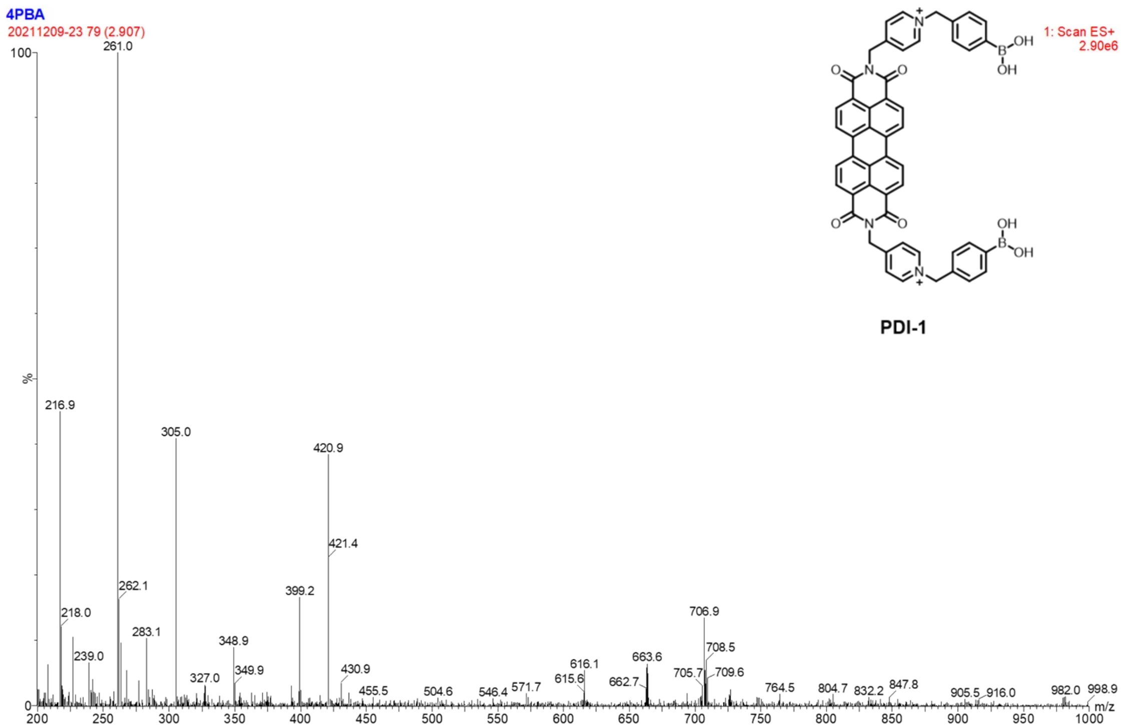


Fig. S12 MS Data for PDI-1.

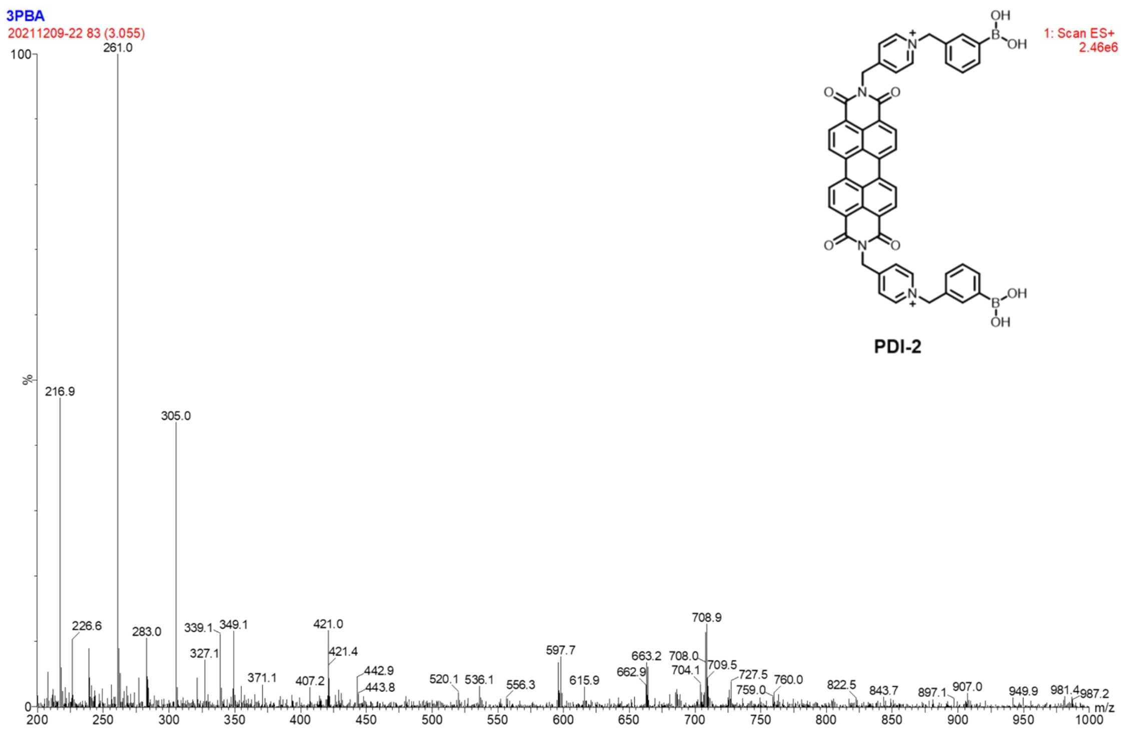


Fig. S13 MS Data for PDI-2.

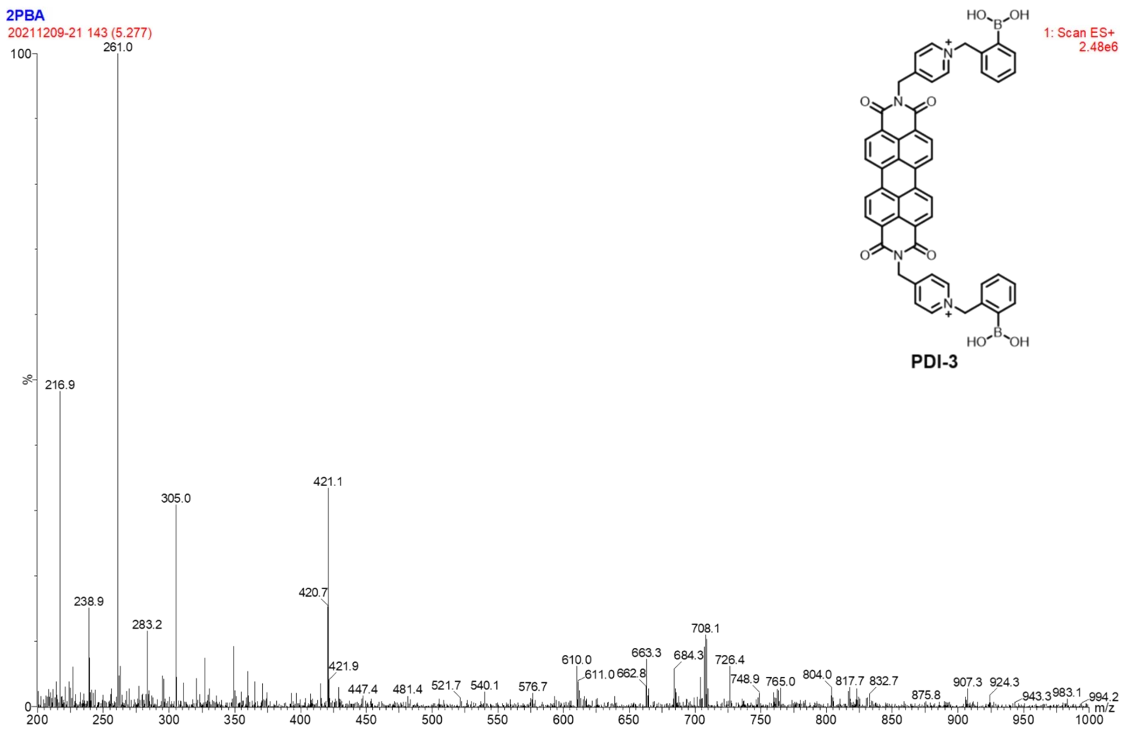


Fig. S14 MS Data for PDI-3.

7. Absorption and fluorescence spectra

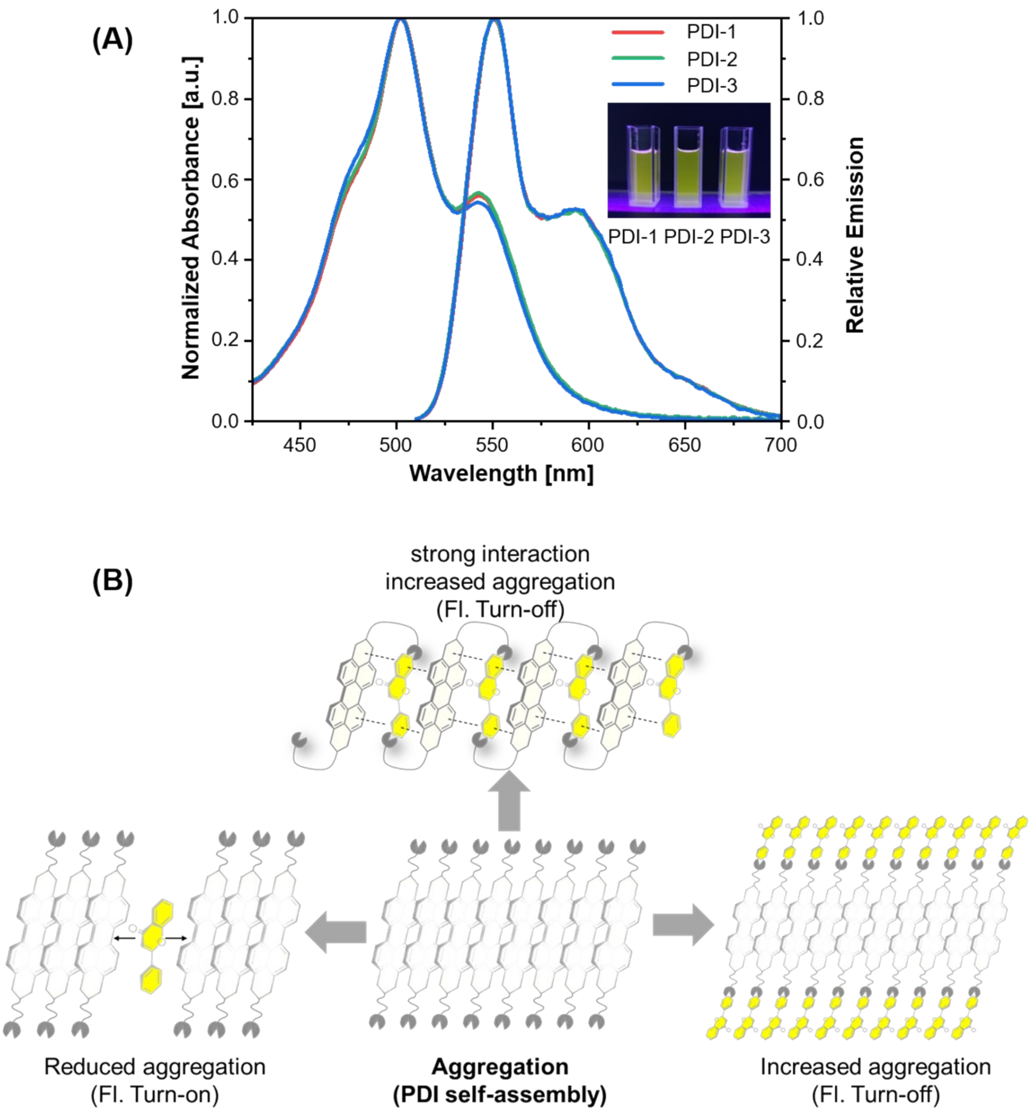


Fig. S15 (A) Normalized absorption and fluorescence spectra of the sensing array in aqueous solution, (B) Putative PDI assembly pattern with flavonoids.

8. Fluorescence changes for PDIs against tangeretin and hesperidin in different concentrations

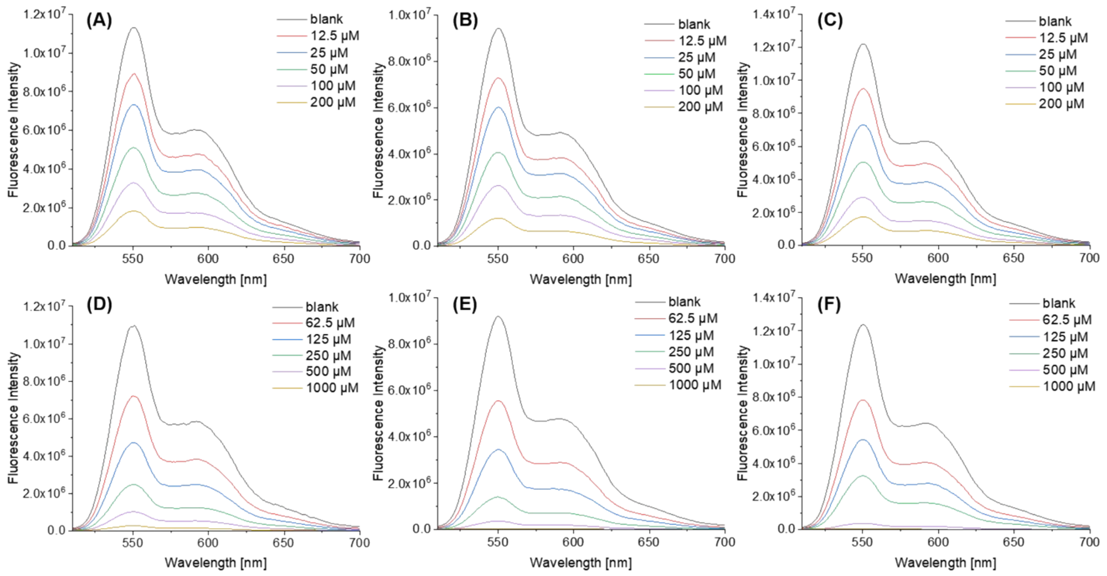


Fig. S16 Fluorescence change of PDIs (10 μM, aqueous solution) after adding tangeretin hesperidin in different concentrations, PDI-1-Tangeretin. (A) PDI-2- Tangeretin, (B) PDI-3-Tangeretin, (C) PDI-1-Hesperidin, (D) PDI-2- Hesperidin, (E) PDI-3- Hesperidin, (F) The fluorescence value changes were recorded on a SpectraMaxR ID3 Multi-Mode Microplate Reader (Molecular Devices, California, USA) at room temperature, (λex = 470 nm, λem = 550 nm).

9. Discrimination of the flavonoids in carbohydrates and carboxylic acids

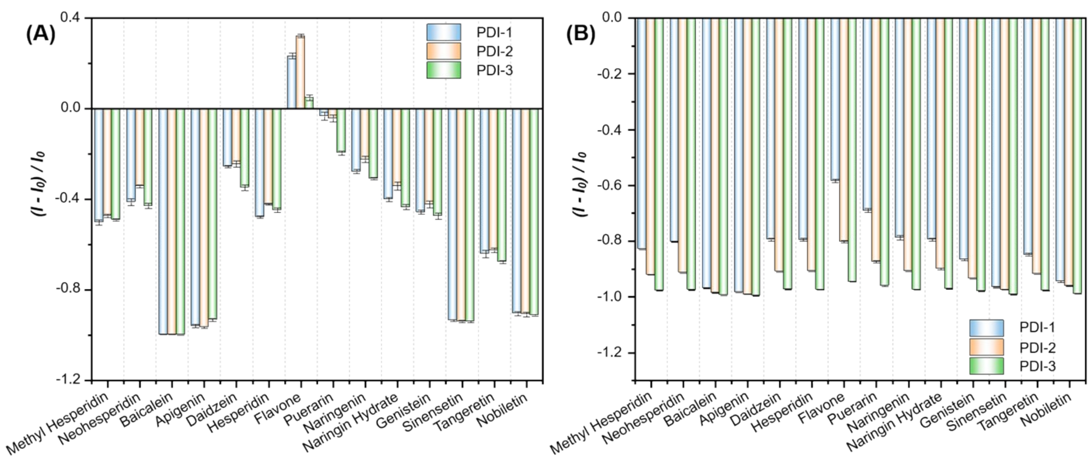


Fig. S17 Fluorescence response pattern ($(I-I_0)/I_0$) obtained by PDIs (10 μM, aqueous solution) treated with flavonoids in carbohydrates (A) and natural acid (B). Each value is the average of six independent measurements; each error bar shows the standard error (SE) of these measurements.

10. Wine sample analysis

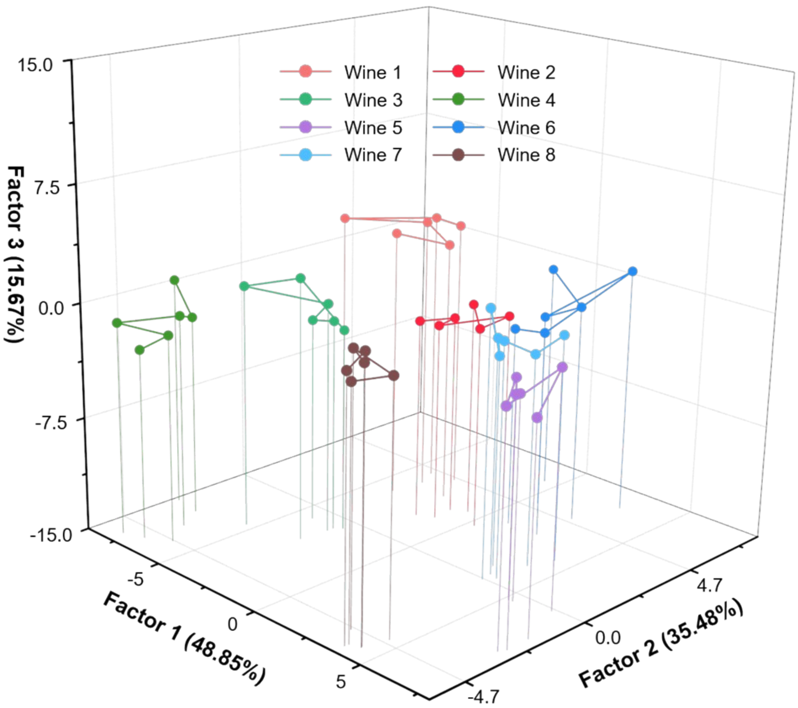


Fig. S18 3D canonical score plot of simplified fluorescence-response patterns obtained with an array of the PDIs (10 μM, aqueous solution). Each point represents the response pattern for a single wine to the array.

11. Fluorescence Response Pattern *$(I-I_0)/I_0$* and Linear Discriminant Analysis

The flavonoids were dissolved in DMSO and mixed into a 1mM solution. To the constructed new fluorescent array sensor, 10 μL of different flavonoids were added. The final concentration of flavonoids was 50 μM, the 96-well plate was placed in a microplate reader and shaken for 10 seconds, and each group of flavonoids was tested repeatedly six times, and the fluorescence intensity data were recorded. For convenience of record, abbreviations in the table refer to Methyl Hesperidin (MH), Neohesperidin (Neo), Baicalein (Bai), Apigenin (Api), Daidzein (Dai), Hesperidin (Hes), Flavone (Fla), Puerarin (Pue), Naringenin (Nar), Naringin hydrate (NH), Genistein (Gen), Sinensetin (Sin), Tangeretin (Tan), Nobiletin (Nob).

Table S1 Data matrix for the fluorescence response of the array sensor to different flavonoids (the concentration of 14 flavonoids was 50 μM).

$\Delta I/I_0$	PDI-1	PDI-2	PDI-3	Factor 1	Factor 2	Factor 3
MH	-0.45748	-0.45975	-0.45734	9.80468	-2.83683	3.35062

MH	-0.45447	-0.47836	-0.46935	8.99230	-2.32981	5.35348
MH	-0.45496	-0.47748	-0.47679	8.53588	-1.68611	5.15975
MH	-0.45721	-0.46713	-0.47925	8.41585	-1.21493	3.91567
MH	-0.45950	-0.47181	-0.48643	7.85048	-0.87022	4.08842
MH	-0.46541	-0.47947	-0.49059	7.30478	-1.05508	4.22126
Neo	-0.35116	-0.30017	-0.49528	13.05381	10.87193	-2.06758
Neo	-0.36240	-0.28909	-0.50455	12.20680	11.54011	-4.31534
Neo	-0.36261	-0.30463	-0.51100	11.64587	11.53428	-2.87919
Neo	-0.36850	-0.32408	-0.51629	10.90741	11.03182	-1.60950
Neo	-0.41150	-0.33753	-0.52113	8.91886	9.00958	-4.54017
Neo	-0.39175	-0.33369	-0.51755	9.88891	9.74084	-2.95594
Bai	-0.99877	-0.99879	-0.99908	-48.12919	-0.27657	-1.55498
Bai	-0.99883	-0.99888	-0.99908	-48.13253	-0.28194	-1.55233
Bai	-0.99881	-0.99880	-0.99908	-48.13074	-0.27871	-1.55814
Bai	-0.99878	-0.99886	-0.99913	-48.13333	-0.27500	-1.54892
Bai	-0.99881	-0.99883	-0.99909	-48.13144	-0.27852	-1.55435
Bai	-0.99886	-0.99890	-0.99913	-48.13697	-0.27993	-1.55353
Api	-0.97581	-0.97522	-0.98857	-46.41558	0.70410	-1.51531
Api	-0.97469	-0.97559	-0.98825	-46.35988	0.71497	-1.36845
Api	-0.97654	-0.97607	-0.98880	-46.46510	0.66066	-1.50615
Api	-0.97615	-0.97602	-0.98935	-46.48328	0.72707	-1.47768
Api	-0.97780	-0.97459	-0.98927	-46.52302	0.69498	-1.77684
Api	-0.97629	-0.97711	-0.98900	-46.47872	0.65190	-1.38222
Dai	-0.33963	-0.26877	-0.33290	23.58971	-1.35483	-2.67512
Dai	-0.36141	-0.28186	-0.34849	21.72399	-1.47933	-3.65807
Dai	-0.36250	-0.28929	-0.35674	21.10838	-1.08647	-3.11045
Dai	-0.36402	-0.28855	-0.36142	20.77961	-0.73061	-3.36851
Dai	-0.36581	-0.30359	-0.36039	20.61733	-1.42968	-2.07397
Dai	-0.35823	-0.29457	-0.36027	20.99463	-0.77646	-2.20830
Hes	-0.49696	-0.47786	-0.43937	9.26792	-6.80871	1.39976
Hes	-0.49476	-0.48246	-0.42946	9.89583	-7.71650	2.14004
Hes	-0.49905	-0.48097	-0.43719	9.29109	-7.20038	1.51442
Hes	-0.49474	-0.47484	-0.44093	9.28600	-6.46828	1.31007
Hes	-0.48932	-0.50463	-0.44512	8.91402	-6.91299	4.69677
Hes	-0.48817	-0.49464	-0.44141	9.28501	-6.82496	3.86961
Fla	0.12925	0.25585	0.19442	77.88350	-6.49540	-3.55726
Fla	0.13523	0.23429	0.21366	79.03054	-8.62406	-0.72577
Fla	0.12792	0.22501	0.21200	78.56755	-9.14265	-0.55203
Fla	0.12424	0.23027	0.21277	78.53730	-9.19138	-1.41531
Fla	0.11496	0.22574	0.23869	79.71571	-11.98622	-1.67207
Fla	0.11801	0.25596	0.20171	77.91765	-7.62667	-4.60633
Pue	-0.06380	-0.01714	-0.29849	38.30413	17.15279	0.10702
Pue	-0.06294	-0.00928	-0.31697	37.30502	19.04552	-0.72225
Pue	-0.08354	-0.00964	-0.31274	36.81116	17.73248	-2.66422

Pue	-0.09761	-0.05474	-0.33312	34.59603	17.24213	0.17522
Pue	-0.14013	-0.09359	-0.34028	32.21556	14.54481	-0.26273
Pue	-0.12722	-0.07256	-0.32476	33.84052	14.55044	-0.91843
Nar	-0.38163	-0.33342	-0.33087	21.50790	-5.72116	-0.48511
Nar	-0.39863	-0.33076	-0.34648	19.98070	-5.07018	-2.52839
Nar	-0.40121	-0.32924	-0.36546	18.75995	-3.51448	-3.08140
Nar	-0.36430	-0.34004	-0.37552	19.37413	-1.35342	1.48975
Nar	-0.38520	-0.32648	-0.38365	18.27182	-1.13544	-1.93349
Nar	-0.37224	-0.33433	-0.37392	19.24322	-1.65063	0.17273
NH	-0.41247	-0.43412	-0.54302	6.54037	7.43191	4.56379
NH	-0.41545	-0.45955	-0.54662	5.94598	6.70724	6.71191
NH	-0.41598	-0.45577	-0.55502	5.46096	7.53349	6.22528
NH	-0.43408	-0.47124	-0.55276	4.77859	5.96962	5.97784
NH	-0.41506	-0.47469	-0.56462	4.71483	7.72825	8.07370
NH	-0.42042	-0.47948	-0.55023	5.33795	6.08665	8.13318
Gen	-0.62702	-0.58596	-0.53893	-2.58023	-8.05208	-1.61177
Gen	-0.62652	-0.59189	-0.54957	-3.26647	-7.32914	-1.07260
Gen	-0.62544	-0.60263	-0.55223	-3.50145	-7.43192	0.05350
Gen	-0.63753	-0.60816	-0.56281	-4.63503	-7.27506	-0.67570
Gen	-0.63557	-0.60632	-0.56243	-4.52132	-7.15328	-0.65985
Gen	-0.63055	-0.60176	-0.54763	-3.39995	-8.02629	-0.49255
Sin	-0.95427	-0.95341	-0.95234	-43.22194	-0.63731	-1.23684
Sin	-0.95475	-0.95381	-0.95385	-43.33476	-0.54479	-1.25766
Sin	-0.95154	-0.95571	-0.95552	-43.33960	-0.32263	-0.77356
Sin	-0.95583	-0.95366	-0.95238	-43.28354	-0.71436	-1.36567
Sin	-0.95414	-0.95475	-0.95593	-43.44850	-0.37204	-1.12395
Sin	-0.95258	-0.95574	-0.95468	-43.32702	-0.44231	-0.86519
Tan	-0.64479	-0.64641	-0.61724	-8.58326	-4.30754	1.88854
Tan	-0.64868	-0.64898	-0.61744	-8.76301	-4.55940	1.75652
Tan	-0.65355	-0.65275	-0.62606	-9.49885	-4.17760	1.57757
Tan	-0.65787	-0.67001	-0.63777	-10.54358	-3.98327	2.73643
Tan	-0.64959	-0.66667	-0.64496	-10.64228	-2.87436	3.16177
Tan	-0.66094	-0.66466	-0.65039	-11.35835	-2.85802	1.81435
Nob	-0.90895	-0.90667	-0.90164	-38.03255	-1.25111	-0.93913
Nob	-0.91010	-0.90449	-0.90145	-38.03940	-1.24313	-1.26136
Nob	-0.90948	-0.90617	-0.90154	-38.04036	-1.26615	-1.03840
Nob	-0.90601	-0.90577	-0.90099	-37.87759	-1.14097	-0.73488
Nob	-0.90462	-0.90614	-0.90199	-37.89187	-1.00461	-0.57129
Nob	-0.90747	-0.90475	-0.90680	-38.26952	-0.67563	-1.02275

Table S2 Canonical scores of group means.

	Factor 1	**Factor 2**	**Factor 3**
Api	-46.454	0.692	-1.504

Bai	-48.132	-0.278	-1.554
Dai	21.469	-1.143	-2.849
Fla	78.609	-8.844	-2.088
Gen	-3.651	-7.545	-0.743
Hes	9.323	-6.989	2.488
MH	8.484	-1.665	4.348
NH	5.463	6.91	6.614
Nar	19.523	-3.074	-1.061
Neo	11.104	10.621	-3.061
Nob	-38.025	-1.097	-0.928
Pue	35.512	16.711	-0.714
Sin	-43.326	-0.506	-1.104
Tan	-9.898	-3.793	2.156

Table S3 Jackknifed classification matrix.

Jackknifed classification matrix showed the 100% correct classification.

	Api	Bai	Dai	Fla	Gen	Hes	MH	NH	Nar	Neo	Nob	Pue	Sin	Tan	**%correct**
Api	6	0	0	0	0	0	0	0	0	0	0	0	0	0	100
Bai	0	6	0	0	0	0	0	0	0	0	0	0	0	0	100
Dai	0	0	6	0	0	0	0	0	0	0	0	0	0	0	100
Fla	0	0	0	6	0	0	0	0	0	0	0	0	0	0	100
Gen	0	0	0	0	6	0	0	0	0	0	0	0	0	0	100
Hes	0	0	0	0	0	6	0	0	0	0	0	0	0	0	100
MH	0	0	0	0	0	0	6	0	0	0	0	0	0	0	100
NH	0	0	0	0	0	0	0	6	0	0	0	0	0	0	100
Nar	0	0	0	0	0	0	0	0	6	0	0	0	0	0	100
Neo	0	0	0	0	0	0	0	0	0	6	0	0	0	0	100
Nob	0	0	0	0	0	0	0	0	0	0	6	0	0	0	100
Pue	0	0	0	0	0	0	0	0	0	0	0	6	0	0	100
Sin	0	0	0	0	0	0	0	0	0	0	0	0	6	0	100
Tan	0	0	0	0	0	0	0	0	0	0	0	0	0	6	100
Total	6	6	6	6	6	6	6	6	6	6	6	6	6	6	**100**

Table S4 Data matrix for the fluorescence response of the array sensor to unknown samples.

Fluorescence Response Pattern			**Results LDA**				**Analyte**	
PDI-1	**PDI-2**	**PDI-3**	**Factor1**	**Factor2**	**Factor3**	**Group**	**Identification**	**Verification**
-0.44529	-0.46514	-0.48332	8.62267	-0.25278	4.85356	7	MH	MH
-0.43956	-0.45379	-0.48130	9.07173	0.23621	4.32804	7	MH	MH
-0.44673	-0.45217	-0.48065	8.86904	-0.08957	3.47611	7	MH	MH
-0.44119	-0.47648	-0.47241	9.30778	-1.39650	6.44257	7	MH	MH
-0.36680	-0.31865	-0.51663	11.00654	11.32957	-1.97258	10	Neo	Neo

-0.36505	-0.30658	-0.50938	11.63408	11.21604	-2.91563	10	Neo	Neo
-0.36615	-0.29882	-0.51837	11.13531	12.20603	-3.84801	10	Neo	Neo
-0.35723	-0.30965	-0.50455	12.17570	11.05240	-1.81469	10	Neo	Neo
-0.99878	-0.99882	-0.99908	-48.13020	-0.27745	-1.55358	2	Bai	Bai
-0.99885	-0.99879	-0.99911	-48.13378	-0.27746	-1.56327	2	Bai	Bai
-0.99882	-0.99885	-0.99909	-48.13233	-0.27922	-1.55362	2	Bai	Bai
-0.99883	-0.99889	-0.99907	-48.13148	-0.28379	-1.55093	2	Bai	Bai
-0.97707	-0.97675	-0.98888	-46.49602	0.61912	-1.49289	1	Api	Api
-0.97746	-0.97536	-0.98894	-46.49947	0.65562	-1.66626	1	Api	Api
-0.97541	-0.97421	-0.98927	-46.43287	0.81809	-1.58062	1	Api	Api
-0.97581	-0.97427	-0.99008	-46.49652	0.86612	-1.62037	1	Api	Api
-0.35608	-0.28713	-0.35330	21.57097	-1.01156	-2.66514	3	Dai	Dai
-0.35808	-0.29077	-0.33955	22.28865	-2.40395	-2.39562	3	Dai	Dai
-0.34716	-0.28488	-0.34493	22.42163	-1.23960	-1.94433	3	Dai	Dai
-0.36079	-0.27753	-0.34705	21.87868	-1.42126	-4.00628	3	Dai	Dai
-0.49803	-0.48577	-0.44052	9.07613	-7.03858	2.05272	6	Hes	Hes
-0.47981	-0.50697	-0.43227	10.00705	-7.65808	5.95679	6	Hes	Hes
-0.48068	-0.46953	-0.42363	10.89326	-7.11634	2.30730	6	Hes	Hes
-0.48481	-0.48402	-0.42549	10.47860	-7.65644	3.29502	6	Hes	Hes
0.11930	0.25496	0.21083	78.50323	-8.38118	-4.31051	4	Fla	Fla
0.14298	0.25364	0.23227	80.63758	-9.17703	-1.69641	4	Fla	Fla
0.14788	0.22485	0.25995	82.17744	-12.32986	1.80089	4	Fla	Fla
0.13119	0.24920	0.23340	80.23221	-9.96846	-2.40749	4	Fla	Fla
-0.08930	-0.02680	-0.32785	35.51070	18.15489	-1.68279	12	Pue	Pue
-0.11107	-0.03443	-0.31695	35.29970	15.96304	-2.97947	12	Pue	Pue
-0.09836	-0.00683	-0.31921	35.91506	17.70829	-4.43648	12	Pue	Pue
-0.09111	-0.02798	-0.30910	36.56240	16.43028	-1.59359	12	Pue	Pue
-0.38171	-0.33565	-0.38176	18.41481	-1.46041	-0.68820	9	Nar	Nar
-0.39395	-0.29147	-0.37671	18.74462	-0.89289	-6.12976	3	Nar	Dai
-0.35534	-0.29856	-0.37944	19.90111	0.85057	-1.69459	3	Nar	Dai
-0.36588	-0.31384	-0.35614	20.76222	-2.15571	-1.05169	9	Nar	Nar
-0.41938	-0.47191	-0.54943	5.50391	6.33234	7.50523	8	NH	NH
-0.40936	-0.47349	-0.54871	5.89276	6.67264	8.64291	8	NH	NH
-0.41371	-0.44729	-0.54484	6.24664	7.06653	5.70685	8	NH	NH
-0.42276	-0.44543	-0.54105	6.16717	6.39542	4.67294	8	NH	NH
-0.62270	-0.59756	-0.54736	-3.05540	-7.54365	-0.13138	5	Gen	Gen
-0.62783	-0.60215	-0.55025	-3.46369	-7.69272	-0.21087	5	Gen	Gen
-0.63003	-0.59365	-0.55717	-3.86975	-6.90336	-1.30572	5	Gen	Gen
-0.62704	-0.59565	-0.54856	-3.26424	-7.57260	-0.75036	5	Gen	Gen
-0.95123	-0.95303	-0.95564	-43.30721	-0.20380	-1.00425	13	Sin	Sin
-0.94936	-0.95348	-0.95450	-43.17613	-0.23129	-0.76865	13	Sin	Sin
-0.95123	-0.95235	-0.95274	-43.12518	-0.42731	-1.04634	13	Sin	Sin
-0.95069	-0.95540	-0.95378	-43.20075	-0.42132	-0.70602	13	Sin	Sin
-0.65001	-0.65454	-0.63147	-9.71534	-3.61828	2.05356	14	Tan	Tan

-0.64486	-0.65332	-0.64487	-10.32377	-2.19652	2.32826	14	Tan	Tan
-0.64701	-0.66295	-0.63861	-10.12687	-3.16760	3.10453	14	Tan	Tan
-0.65513	-0.65920	-0.64555	-10.79856	-2.81433	1.89156	14	Tan	Tan
-0.90477	-0.90238	-0.90799	-38.21892	-0.36717	-0.99840	11	Nob	Nob
-0.90550	-0.90516	-0.90915	-38.34432	-0.39967	-0.81003	11	Nob	Nob
-0.90949	-0.90751	-0.90395	-38.20053	-1.10746	-0.92917	11	Nob	Nob
-0.91001	-0.90929	-0.90911	-38.54888	-0.75433	-0.84842	11	Nob	Nob

Table S5 Data matrix for the fluorescence response of the array sensor to tangeretin in different concentrations.

$\Delta I/I_0$	PDI-1	PDI-2	PDI-3	Factor 1	Factor 2	Factor 3
200 μM	-0.86451	-0.88513	-0.80877	-30.79666	0.14400	0.64479
200 μM	-0.86437	-0.88314	-0.86490	-31.05852	1.42545	0.55702
200 μM	-0.87720	-0.89385	-0.85646	-32.17034	0.95330	0.45838
200 μM	-0.88111	-0.88341	-0.82316	-31.90035	0.03291	-0.35055
200 μM	-0.87355	-0.85496	-0.84784	-30.67195	0.64813	-1.52904
200 μM	-0.87181	-0.88792	-0.86599	-31.69414	1.28171	0.42144
100 μM	-0.71340	-0.75426	-0.65378	-16.04183	-0.15880	1.46698
100 μM	-0.74642	-0.74409	-0.64924	-17.83081	-1.17582	-0.90054
100 μM	-0.74657	-0.73053	-0.74493	-17.98570	0.94548	-1.64235
100 μM	-0.74613	-0.75745	-0.55873	-17.69137	-3.17554	-0.16076
100 μM	-0.73250	-0.74402	-0.66755	-17.03809	-0.39350	-0.14218
100 μM	-0.75510	-0.74313	-0.72821	-18.82981	0.40538	-1.40319
50 μM	-0.54708	-0.56860	-0.53792	1.16958	0.54726	0.05167
50 μM	-0.58434	-0.60716	-0.58106	-2.69388	0.76737	0.20317
50 μM	-0.56694	-0.60375	-0.52840	-1.15172	-0.00550	0.94226
50 μM	-0.56182	-0.59688	-0.43494	-0.05269	-2.05248	0.80797
50 μM	-0.56167	-0.58701	-0.42723	0.31041	-2.27675	0.25996
50 μM	-0.58744	-0.62363	-0.45651	-2.66864	-2.08545	0.92333
25 μM	-0.38297	-0.41463	-0.37010	17.55940	0.16820	0.28021
25 μM	-0.39400	-0.43115	-0.39057	16.21113	0.43696	0.61433
25 μM	-0.38563	-0.40992	-0.40563	17.32355	0.88976	-0.11871
25 μM	-0.36988	-0.42414	-0.40568	17.89718	1.37501	1.53592
25 μM	-0.38845	-0.41694	-0.38753	17.03005	0.43742	0.11667
25 μM	-0.37369	-0.38161	-0.39466	19.04190	0.80153	-1.06203
12.5 μM	-0.25628	-0.25800	-0.21176	31.55934	-0.98144	-1.67224
12.5 μM	-0.23271	-0.29347	-0.22053	31.92423	0.01812	1.60251
12.5 μM	-0.22873	-0.28521	-0.24840	32.27347	0.71834	1.36385
12.5 μM	-0.23846	-0.25128	-0.23836	32.76141	0.05791	-1.07346
12.5 μM	-0.24053	-0.26118	-0.24283	32.29290	0.15826	-0.62854
12.5 μM	-0.23939	-0.24337	-0.24273	32.92193	0.09276	-1.56685

Table S6 Jackknifed classification matrix for the fluorescence response of the array sensor to tangeretin in different concentrations.

Jackknifed classification matrix showed the 100% correct classification.

	200 μM	100 μM	50 μM	25 μM	12.5 μM	**%correct**
200 μM	6	0	0	0	0	100
100 μM	0	6	0	0	0	100
50 μM	0	0	6	0	0	100
25 μM	0	0	0	6	0	100
12.5 μM	0	0	0	0	6	100
Total	6	6	6	6	6	**100**

Table S7 Data matrix for the fluorescence response of the array sensor to unknown samples (tangeretin in different concentrations).

Fluorescence Response Pattern			**Results LDA**				**Analyte**	
PDI-1	**PDI-2**	**PDI-3**	**Factor1**	**Factor2**	**Factor3**	**Group**	**Identification**	**Verification**
-0.87610	-0.88875	-0.80856	-31.65683	-0.14369	0.21777	3	200 μM	200 μM
-0.87329	-0.88441	-0.78462	-31.19778	-0.64230	0.12040	3	200 μM	200 μM
-0.86783	-0.88498	-0.84937	-31.24733	0.98826	0.46737	3	200 μM	200 μM
-0.87288	-0.84577	-0.73798	-29.69113	-1.90319	-2.04051	3	200 μM	200 μM
-0.75395	-0.69969	-0.71079	-17.29885	-0.19056	-3.78462	1	100 μM	100 μM
-0.72903	-0.73126	-0.71646	-16.70682	0.75272	-0.65628	1	100 μM	100 μM
-0.72037	-0.75783	-0.65661	-16.61998	-0.25660	1.28919	1	100 μM	100 μM
-0.74712	-0.74154	-0.60185	-17.51538	-2.29466	-1.09502	1	100 μM	100 μM
-0.58825	-0.59680	-0.47385	-1.98779	-1.84829	-0.62186	5	50 μM	50 μM
-0.56266	-0.59249	-0.42789	0.07159	-2.25890	0.51395	5	50 μM	50 μM
-0.55945	-0.59704	-0.51928	-0.40480	-0.05457	0.97055	5	50 μM	50 μM
-0.56901	-0.59302	-0.57321	-1.21653	0.91316	0.24059	5	50 μM	50 μM
-0.40237	-0.44112	-0.40538	15.27168	0.61049	0.72272	4	25 μM	25 μM
-0.38994	-0.41761	-0.40635	16.80154	0.83405	0.07901	4	25 μM	25 μM
-0.37204	-0.41546	-0.40103	18.05609	1.16687	0.92968	4	25 μM	25 μM
-0.39502	-0.41235	-0.40206	16.66275	0.57604	-0.49383	4	25 μM	25 μM
-0.23610	-0.24437	-0.24422	33.09471	0.21786	-1.33130	2	12.5 μM	12.5 μM
-0.24112	-0.25918	-0.23378	32.37100	-0.07523	-0.77560	2	12.5 μM	12.5 μM
-0.22900	-0.27361	-0.25239	32.59362	0.74248	0.69915	2	12.5 μM	12.5 μM
-0.22988	-0.29167	-0.26319	31.91030	1.06147	1.66842	2	12.5 μM	12.5 μM

Table S8 Data matrix for the fluorescence response of the array sensor to hesperidin in different concentrations.

ΔI/I₀	**PDI-1**	**PDI-2**	**PDI-3**	**Factor 1**	**Factor 2**	**Factor 3**

1000 μM	-0.98211	-0.99538	-0.99653	-26.64627	-1.95459	0.70503
1000 μM	-0.99331	-0.99396	-0.99520	-26.72482	-2.35876	0.02096
1000 μM	-0.98917	-0.99353	-0.99617	-26.64355	-2.27297	0.25545
1000 μM	-0.99406	-0.99491	-0.99349	-26.75589	-2.29353	-0.03541
1000 μM	-0.99288	-0.99515	-0.99094	-26.67611	-2.18832	-0.03474
1000 μM	-0.99427	-0.99386	-0.97427	-26.13358	-1.94775	-0.61299
500 μM	-0.92553	-0.97074	-0.93747	-22.14561	-0.28021	1.28978
500 μM	-0.94837	-0.97796	-0.89966	-21.99690	0.20903	-0.74233
500 μM	-0.94880	-0.97977	-0.89495	-21.99569	0.39713	-0.83592
500 μM	-0.94581	-0.97525	-0.89025	-21.48883	0.33946	-0.95521
500 μM	-0.92276	-0.98126	-0.85893	-20.56076	2.07076	-0.38786
500 μM	-0.89966	-0.96114	-0.90387	-20.01314	0.71885	1.42950
250 μM	-0.80716	-0.86724	-0.79920	-8.69615	0.64323	0.39146
250 μM	-0.80815	-0.87487	-0.74492	-7.68192	2.19668	-0.91174
250 μM	-0.82079	-0.85212	-0.76254	-6.85187	0.15389	-1.85320
250 μM	-0.82559	-0.88357	-0.76015	-9.06046	1.80562	-1.13851
250 μM	-0.78539	-0.88108	-0.75068	-7.84108	3.13761	0.67238
250 μM	-0.78671	-0.87742	-0.81356	-9.42322	1.54862	2.22105
125 μM	-0.59362	-0.68268	-0.60405	13.85351	1.26921	0.34336
125 μM	-0.60608	-0.68171	-0.59760	13.86623	0.96011	-0.53479
125 μM	-0.53662	-0.63852	-0.59900	18.16306	0.71578	1.80106
125 μM	-0.58569	-0.65916	-0.60687	15.55872	0.14882	0.06990
125 μM	-0.57856	-0.69295	-0.51211	16.07741	4.28068	-1.05465
125 μM	-0.56596	-0.64928	-0.58845	17.15452	0.61484	0.29198
62.5 μM	-0.34862	-0.45046	-0.41880	40.03308	0.02150	0.68266
62.5 μM	-0.35879	-0.43733	-0.41272	40.92457	-0.90101	-0.46457
62.5 μM	-0.35035	-0.44689	-0.43500	39.78117	-0.57783	0.92005
62.5 μM	-0.37052	-0.42956	-0.44070	40.43308	-2.30157	-0.57557
62.5 μM	-0.36606	-0.42555	-0.43649	40.91830	-2.29434	-0.58521
62.5 μM	-0.36480	-0.43179	-0.43432	40.57219	-1.86093	-0.37195

Table S9 Jackknifed classification matrix for the fluorescence response of the array sensor to hesperidin in different concentrations.

Jackknifed classification matrix showed the 100% correct classification.

	1000 μM	500 μM	250 μM	125 μM	62.5 μM	**%correct**
1000 μM	6	0	0	0	0	100
500 μM	0	6	0	0	0	100
250 μM	0	0	6	0	0	100
125 μM	0	0	0	6	0	100
62.5 μM	0	0	0	0	6	100
Total	6	6	6	6	6	**100**

Table S10 Data matrix for the fluorescence response of the array sensor to unknown samples (hesperidin in different concentrations).

Fluorescence Response Pattern			Results LDA				Analyte	
PDI-1	PDI-2	PDI-3	Factor1	Factor2	Factor3	Group	Identification	Verification
-0.99444	-0.99422	-0.97119	-26.07316	-1.86697	-0.69547	1	1000 μM	1000 μM
-0.98822	-0.99512	-0.97348	-26.08219	-1.66958	-0.26901	1	1000 μM	1000 μM
-0.99031	-0.99404	-0.96060	-25.67647	-1.52056	-0.77277	1	1000 μM	1000 μM
-0.99054	-0.99483	-0.99160	-26.62833	-2.14660	0.09829	1	1000 μM	1000 μM
-0.94246	-0.98269	-0.90239	-22.29113	0.60077	-0.19403	4	500 μM	500 μM
-0.91762	-0.97462	-0.88938	-20.87739	1.21257	0.51106	4	500 μM	500 μM
-0.93076	-0.97518	-0.89790	-21.41493	0.64758	0.06135	4	500 μM	500 μM
-0.94353	-0.97235	-0.83384	-19.61857	1.45517	-2.48941	4	500 μM	500 μM
-0.76973	-0.86585	-0.73455	-6.01746	3.12777	0.56255	3	250 μM	250 μM
-0.79342	-0.86724	-0.72131	-6.18827	2.74052	-1.02825	3	250 μM	250 μM
-0.81378	-0.82974	-0.72701	-4.13914	-0.11289	-3.19974	3	250 μM	250 μM
-0.80925	-0.86405	-0.78005	-7.96340	0.80859	-0.35611	3	250 μM	250 μM
-0.56750	-0.61878	-0.60751	18.69532	-1.54036	-0.27078	2	125 μM	125 μM
-0.59919	-0.65308	-0.62147	15.30042	-0.92740	-0.45041	2	125 μM	125 μM
-0.59908	-0.65102	-0.64414	14.79236	-1.52315	0.11492	2	125 μM	125 μM
-0.57380	-0.62235	-0.61027	18.24615	-1.59911	-0.41407	2	125 μM	125 μM
-0.36847	-0.43747	-0.38641	41.48645	-0.63635	-1.70685	5	62.5 μM	62.5 μM
-0.36850	-0.43394	-0.39628	41.44654	-1.04517	-1.55199	5	62.5 μM	62.5 μM
-0.35831	-0.44456	-0.38807	41.14203	0.04346	-0.88212	5	62.5 μM	62.5 μM
-0.35262	-0.45968	-0.41083	39.54539	0.57935	0.55178	5	62.5 μM	62.5 μM

Table S11 Data matrix for the fluorescence response of the array sensor to tangeretin and hesperidin in different volume ratio.

$\Delta I/I_0$	PDI-1	PDI-2	PDI-3	Factor 1	Factor 2	Factor 3
100:0	-0.57162	-0.54978	-0.87269	-25.66638	0.90020	3.94973
100:0	-0.58648	-0.56039	-0.88738	-24.81398	1.16068	1.86073
100:0	-0.58812	-0.57248	-0.88630	-25.52394	2.39614	2.06950
100:0	-0.58196	-0.56414	-0.88697	-24.52992	1.78867	2.13211
100:0	-0.59803	-0.56589	-0.89953	-23.94065	1.05896	0.12104
100:0	-0.59765	-0.57392	-0.88789	-26.25757	2.07185	1.53573
75:25	-0.52668	-0.49773	-0.91546	-11.72734	-3.00253	0.29153
75:25	-0.53858	-0.48196	-0.91505	-12.58510	-5.27577	-0.33000
75:25	-0.55018	-0.47951	-0.91921	-12.95225	-6.14764	-1.28046
75:25	-0.52037	-0.48830	-0.92108	-9.77936	-3.77490	-0.20646
75:25	-0.54626	-0.48827	-0.93200	-10.45603	-5.15510	-2.44214

75:25	-0.54602	-0.49991	-0.93438	-10.32416	-3.91502	-2.55179
50:50	-0.47549	-0.51149	-0.95158	-0.22100	0.56398	-1.55101
50:50	-0.46141	-0.53156	-0.95338	0.99423	3.38931	-0.94477
50:50	-0.48040	-0.53538	-0.95817	-0.19904	2.82777	-2.17745
50:50	-0.47806	-0.53434	-0.95551	-0.41523	2.85829	-1.80139
50:50	-0.47625	-0.54519	-0.95705	-0.25330	4.09855	-1.76532
50:50	-0.48086	-0.54158	-0.96269	0.40477	3.42332	-2.62098
25:75	-0.38676	-0.46272	-0.96722	13.18484	-0.56177	-0.42043
25:75	-0.40734	-0.47860	-0.96472	10.15300	0.17908	-0.75121
25:75	-0.40082	-0.48382	-0.97152	11.92305	0.98238	-1.18714
25:75	-0.40199	-0.49214	-0.96563	10.48728	1.88787	-0.47055
25:75	-0.41256	-0.49394	-0.97302	10.69697	1.48702	-1.68782
25:75	-0.40500	-0.50048	-0.96952	10.65330	2.59829	-0.91786
0:100	-0.26887	-0.39937	-0.96089	25.99620	-1.60199	4.12286
0:100	-0.28746	-0.41700	-0.97634	26.40437	-0.77372	1.89076
0:100	-0.29018	-0.42398	-0.97454	25.59690	-0.13379	2.07300
0:100	-0.31134	-0.41920	-0.97858	24.28565	-1.71933	0.73027
0:100	-0.30332	-0.41934	-0.97771	24.95024	-1.30600	1.14396
0:100	-0.30857	-0.43090	-0.97679	23.91442	-0.30479	1.18558

Table S12 Jackknifed classification matrix.

Jackknifed classification matrix showed the 100% correct classification.

	100:0	75:25	50:50	25:75	0:100	**%correct**
100:0	6	0	0	0	0	100
75:25	0	6	0	0	0	100
50:50	0	0	6	0	0	100
25:75	0	0	0	6	0	100
0:100	0	0	0	0	6	100
Total	6	6	6	6	6	**100**

Table S13 Data matrix for the fluorescence response of the array sensor to unknown samples.

Fluorescence Response Pattern			**Results LDA**				**Analyte**	
PDI-1	**PDI-2**	**PDI-3**	**Factor1**	**Factor2**	**Factor3**	**Group**	**Identification**	**Verification**
-0.59065	-0.57338	-0.88654	-25.76696	2.36754	1.95468	2	100:0	100:0
-0.59515	-0.58037	-0.88297	-27.08311	2.94231	2.26371	2	100:0	100:0
-0.58670	-0.56475	-0.89429	-23.69548	1.54299	1.13632	2	100:0	100:0
-0.59289	-0.55083	-0.90649	-21.70945	-0.39237	-0.64304	2	100:0	100:0
-0.55308	-0.51166	-0.92172	-13.70290	-2.85057	-1.26885	5	75:25	75:25
-0.54966	-0.50399	-0.92749	-12.07611	-3.57652	-1.87585	5	75:25	75:25
-0.54811	-0.48806	-0.93177	-10.68138	-5.26515	-2.49276	5	75:25	75:25
-0.54308	-0.47465	-0.91739	-12.41316	-6.30761	-0.86008	5	75:25	75:25

-0.48790	-0.52898	-0.95421	-1.51678	1.81769	-2.11151	4	50:50	50:50
-0.48401	-0.54059	-0.95240	-1.77518	3.27741	-1.61025	4	50:50	50:50
-0.48941	-0.52673	-0.95674	-1.14650	1.47346	-2.48134	4	50:50	50:50
-0.49366	-0.53703	-0.95365	-2.44225	2.41295	-2.17338	4	50:50	50:50
-0.39959	-0.50221	-0.97175	11.57108	3.02234	-0.93186	3	25:75	25:75
-0.41009	-0.49246	-0.97394	11.16268	1.43827	-1.71145	3	25:75	25:75
-0.40693	-0.48996	-0.97000	10.83991	1.36448	-1.18022	3	25:75	25:75
-0.41825	-0.49321	-0.97196	9.93777	1.14435	-1.80321	3	25:75	25:75
-0.29600	-0.43566	-0.97698	25.11228	0.81604	1.71879	1	0:100	0:100
-0.30430	-0.42641	-0.97869	24.82809	-0.60305	1.08537	1	0:100	0:100
-0.30256	-0.42419	-0.97948	25.21644	-0.76584	1.03714	1	0:100	0:100
-0.30031	-0.43837	-0.97762	24.70574	0.89220	1.51292	1	0:100	0:100

Table S14 Data matrix for the fluorescence response of the array sensor to 14 flavonoids in carbohydrates (the concentration of 14 flavonoids was 50 μM).

$\Delta I/I_0$	PDI-1	PDI-2	PDI-3	Factor 1	Factor 2	Factor 3
MH	-0.48513	-0.46429	-0.48566	4.41742	-3.79843	1.71453
MH	-0.51003	-0.47450	-0.49107	2.28491	-4.79674	0.83094
MH	-0.51492	-0.46785	-0.49627	2.02425	-4.36288	-0.15662
MH	-0.50966	-0.48112	-0.49497	1.76538	-4.61477	1.28748
MH	-0.49575	-0.48300	-0.48082	3.26214	-5.29469	2.69305
MH	-0.49874	-0.46925	-0.49490	2.90850	-3.75180	1.01390
Neo	-0.41311	-0.33388	-0.41510	18.53896	-3.00215	-2.46225
Neo	-0.43695	-0.33765	-0.41707	16.96735	-4.07688	-3.70993
Neo	-0.40222	-0.34464	-0.43892	17.21080	-0.61272	-1.53583
Neo	-0.40320	-0.34592	-0.44445	16.77061	-0.19184	-1.64074
Neo	-0.39731	-0.34970	-0.43036	17.74548	-1.30744	-0.58811
Neo	-0.41727	-0.34243	-0.43087	16.98272	-2.00849	-2.44884
Bai	-0.99682	-0.99773	-0.99850	-78.28039	3.01709	-0.84618
Bai	-0.99679	-0.99730	-0.99835	-78.24949	3.01678	-0.87488
Bai	-0.99723	-0.99761	-0.99844	-78.29257	2.99500	-0.87996
Bai	-0.99730	-0.99749	-0.99842	-78.28994	2.99357	-0.89374
Bai	-0.99682	-0.99735	-0.99852	-78.26372	3.02925	-0.87706
Bai	-0.99683	-0.99729	-0.99852	-78.26111	3.03088	-0.88300
Api	-0.96559	-0.96115	-0.94337	-71.63319	0.53862	-0.38224
Api	-0.96125	-0.97126	-0.93064	-71.11747	-0.71076	1.05133
Api	-0.96491	-0.96684	-0.92982	-71.05946	-0.83316	0.48349
Api	-0.95098	-0.96142	-0.93343	-70.27327	0.32346	0.82499
Api	-0.94859	-0.96217	-0.93513	-70.28072	0.57253	0.99092
Api	-0.96475	-0.96479	-0.92295	-70.54844	-1.39423	0.50949
Dai	-0.25070	-0.23321	-0.34024	36.37946	0.87979	1.58642
Dai	-0.25955	-0.23085	-0.32947	36.65255	-0.46183	1.12368
Dai	-0.25500	-0.24974	-0.35569	34.46293	1.60584	2.24654

Dai	-0.25078	-0.23304	-0.35223	35.67275	1.97798	1.24883
Dai	-0.26085	-0.25656	-0.34560	34.42852	0.20456	2.70029
Dai	-0.26026	-0.26087	-0.36713	32.98415	2.07675	2.51511
Hes	-0.47929	-0.42277	-0.43048	9.93461	-7.35803	0.17778
Hes	-0.47151	-0.41465	-0.45168	9.47466	-4.80954	-0.55448
Hes	-0.48234	-0.42291	-0.44741	8.76148	-5.95987	-0.45308
Hes	-0.48139	-0.42771	-0.45041	8.41103	-5.78047	-0.08319
Hes	-0.47899	-0.41872	-0.44964	9.00461	-5.47382	-0.64157
Hes	-0.46950	-0.42184	-0.45986	8.76270	-4.17345	-0.06175
Fla	0.25247	0.33492	0.06359	113.77725	4.63117	-2.10680
Fla	0.23293	0.32444	0.05915	111.97788	3.79441	-2.60481
Fla	0.23766	0.31438	0.05002	111.22183	4.56425	-1.73229
Fla	0.22746	0.32204	0.04402	110.67576	4.84577	-3.15704
Fla	0.21523	0.31459	0.04597	109.78779	3.86355	-3.27062
Fla	0.22861	0.31788	0.02722	109.54842	6.31670	-3.19423
Pue	-0.04094	-0.01912	-0.18912	66.56379	3.35922	1.43608
Pue	0.00076	-0.04287	-0.21070	66.41580	6.64597	5.41781
Pue	-0.04606	-0.06219	-0.20429	63.38293	3.24835	4.20755
Pue	-0.03805	-0.03158	-0.19079	66.03949	3.28852	2.58568
Pue	-0.02442	-0.04996	-0.18955	65.98715	3.29655	4.97008
Pue	-0.04573	-0.05140	-0.18803	64.86734	2.09179	3.78442
Nar	-0.27364	-0.20770	-0.30955	38.15588	-2.28701	-1.11389
Nar	-0.26239	-0.22448	-0.31402	37.71256	-1.82547	0.83837
Nar	-0.27991	-0.20875	-0.30978	37.75655	-2.59856	-1.42992
Nar	-0.28355	-0.22417	-0.30583	37.07733	-3.58251	-0.30220
Nar	-0.28189	-0.23871	-0.30154	36.74266	-4.31723	1.09750
Nar	-0.28283	-0.24150	-0.31014	36.05224	-3.65719	1.03622
NH	-0.39799	-0.32196	-0.41681	19.80402	-1.77321	-2.52264
NH	-0.38503	-0.33291	-0.42567	19.46482	-0.65858	-1.05300
NH	-0.40268	-0.34579	-0.43592	17.31045	-0.94337	-1.39053
NH	-0.41254	-0.35039	-0.44441	16.06356	-0.77444	-1.86465
NH	-0.41032	-0.37038	-0.43536	15.78753	-2.07566	0.13873
NH	-0.39634	-0.32982	-0.44837	17.65693	0.96411	-2.61921
Gen	-0.45411	-0.44695	-0.46957	7.84302	-3.27578	2.68815
Gen	-0.45192	-0.40477	-0.45753	10.63907	-3.04581	-0.27885
Gen	-0.47518	-0.41997	-0.47101	7.88470	-3.37210	-0.86848
Gen	-0.44919	-0.42646	-0.47078	8.98960	-2.33375	1.30215
Gen	-0.45720	-0.42222	-0.47363	8.58903	-2.33417	0.37738
Gen	-0.45318	-0.40995	-0.49938	7.85089	0.57034	-1.05098
Sin	-0.92921	-0.94363	-0.94064	-68.70348	2.54649	0.55962
Sin	-0.93571	-0.93726	-0.94102	-68.77748	2.45351	-0.37717
Sin	-0.93531	-0.93864	-0.93905	-68.70420	2.25218	-0.18758
Sin	-0.93518	-0.93580	-0.93940	-68.58526	2.37331	-0.41915
Sin	-0.93904	-0.93138	-0.94275	-68.78519	2.62307	-1.11105

Sin	-0.93638	-0.94623	-0.93320	-68.76847	1.44520	0.51693
Tan	-0.66170	-0.61163	-0.67549	-23.16966	0.79656	-2.49447
Tan	-0.62143	-0.61627	-0.67289	-21.07113	2.35956	0.48850
Tan	-0.62740	-0.63183	-0.67528	-22.25837	1.83855	1.31268
Tan	-0.65489	-0.63265	-0.67471	-23.73756	0.44210	-0.33754
Tan	-0.63027	-0.63360	-0.67081	-22.22961	1.24082	1.39458
Tan	-0.65436	-0.62094	-0.68911	-24.01641	2.12427	-1.63832
Nob	-0.91126	-0.90755	-0.91603	-64.60141	2.20611	-0.58480
Nob	-0.89020	-0.91506	-0.90826	-63.36013	2.28934	1.55838
Nob	-0.90577	-0.91412	-0.90922	-64.20908	1.65664	0.47571
Nob	-0.89732	-0.89851	-0.91773	-63.53255	3.29348	-0.48587
Nob	-0.91183	-0.89449	-0.91049	-63.69468	2.05123	-1.53430
Nob	-0.90718	-0.91714	-0.91351	-64.67980	1.89362	0.51854

Table S15 Jackknifed classification matrix.

Jackknifed classification matrix showed the 93% correct classification.

	Api	Bai	Dai	Fla	Gen	Hes	MH	NH	Nar	Neo	Nob	Pue	Sin	Tan	**%correct**
Api	6	0	0	0	0	0	0	0	0	0	0	0	0	0	100
Bai	0	6	0	0	0	0	0	0	0	0	0	0	0	0	100
Dai	0	0	6	0	0	0	0	0	0	0	0	0	0	0	100
Fla	0	0	0	6	0	0	0	0	0	0	0	0	0	0	100
Gen	0	0	0	0	6	0	0	0	0	0	0	0	0	0	100
Hes	0	0	0	0	0	6	0	0	0	0	0	0	0	0	100
MH	0	0	0	0	0	0	6	0	0	0	0	0	0	0	100
NH	0	0	0	0	0	0	0	3	0	3	0	0	0	0	50
Nar	0	0	0	0	0	0	0	0	6	0	0	0	0	0	100
Neo	0	0	0	0	0	0	0	3	0	3	0	0	0	0	50
Nob	0	0	0	0	0	0	0	0	0	0	6	0	0	0	100
Pue	0	0	0	0	0	0	0	0	0	0	0	6	0	0	100
Sin	0	0	0	0	0	0	0	0	0	0	0	0	6	0	100
Tan	0	0	0	0	0	0	0	0	0	0	0	0	0	6	100
Total	6	6	6	6	6	6	6	6	6	6	6	6	6	6	**93**

Table S16 Data matrix for the fluorescence response of the array sensor to unknown samples.

Fluorescence Response Pattern			**Results LDA**				**Analyte**	
PDI-1	**PDI-2**	**PDI-3**	**Factor1**	**Factor2**	**Factor3**	**Group**	**Identification**	**Verification**
-0.49933	-0.48132	-0.48953	2.63201	-4.62119	2.09903	7	MH	MH
-0.48896	-0.47201	-0.49997	3.00377	-2.89783	1.71911	7	MH	MH
-0.48474	-0.47136	-0.48696	4.03145	-3.86676	2.27837	7	MH	MH
-0.50902	-0.47565	-0.50529	1.44301	-3.48095	0.60953	7	MH	MH
-0.40606	-0.35991	-0.42589	17.06496	-2.43354	-0.19069	10	Neo	Neo
-0.39889	-0.33900	-0.42941	18.21498	-1.15884	-1.53079	8	NH	Neo

-0.41025	-0.33951	-0.42893	17.61046	-1.76325	-2.19266	10	Neo	Neo
-0.41051	-0.35913	-0.43643	16.23835	-1.66016	-0.81494	10	Neo	Neo
-0.99683	-0.99720	-0.99855	-78.25898	3.03675	-0.89099	2	Bai	Bai
-0.99718	-0.99738	-0.99850	-78.28323	3.00940	-0.89650	2	Bai	Bai
-0.99665	-0.99736	-0.99852	-78.25528	3.03787	-0.86589	2	Bai	Bai
-0.99659	-0.99738	-0.99838	-78.24424	3.02773	-0.85622	2	Bai	Bai
-0.95108	-0.96483	-0.94584	-71.17315	1.35498	0.76486	1	Api	Api
-0.95803	-0.96792	-0.92346	-70.36377	-1.11539	1.17292	1	Api	Api
-0.95913	-0.96635	-0.95317	-72.10978	1.59462	0.18641	1	Api	Api
-0.95559	-0.96746	-0.93218	-70.72808	-0.18666	1.05781	1	Api	Api
-0.25972	-0.22609	-0.37180	34.35734	3.54035	-0.39975	3	Dai	Dai
-0.24515	-0.23800	-0.36749	34.83906	3.49966	1.60012	3	Dai	Dai
-0.25254	-0.24681	-0.35125	34.99471	1.40339	2.28212	3	Dai	Dai
-0.25686	-0.24096	-0.37107	33.86068	3.17838	1.00789	3	Dai	Dai
-0.48746	-0.42949	-0.46045	7.40787	-5.20535	-0.58848	6	Hes	Hes
-0.49132	-0.42699	-0.46312	7.15897	-5.07390	-1.10567	6	Hes	Hes
-0.48154	-0.41712	-0.46167	8.22992	-4.44973	-1.25200	6	Hes	Hes
-0.49230	-0.42777	-0.46336	7.05594	-5.12176	-1.10949	6	Hes	Hes
0.23206	0.32566	0.04884	111.37673	4.73051	-3.03294	4	Fla	Fla
0.23046	0.33896	0.04384	111.61418	5.49787	-4.34684	4	Fla	Fla
0.22383	0.32800	0.02852	109.84015	6.26160	-4.28236	4	Fla	Fla
0.22295	0.31524	0.03810	109.76625	4.97215	-3.04625	4	Fla	Fla
-0.04643	-0.06373	-0.22097	62.30337	4.71229	3.86514	12	Pue	Pue
-0.06046	-0.03202	-0.19994	64.27466	3.03546	0.96564	12	Pue	Pue
-0.04514	-0.02979	-0.20823	64.70923	4.59448	1.52929	12	Pue	Pue
-0.04512	-0.04325	-0.21966	63.40499	5.24974	2.31980	12	Pue	Pue
-0.25850	-0.23545	-0.32798	36.58280	-0.68127	1.60345	3	Dai	Nar
-0.28351	-0.22282	-0.32045	36.27620	-2.20459	-0.79790	9	Nar	Nar
-0.26588	-0.23495	-0.32398	36.44757	-1.38682	1.20405	9	Nar	Nar
-0.25527	-0.23086	-0.32532	37.12759	-0.63546	1.50514	3	Dai	Nar
-0.40718	-0.34517	-0.45451	15.99604	0.55822	-2.21968	8	NH	NH
-0.39407	-0.35992	-0.45899	15.74673	1.16960	-0.31526	8	NH	NH
-0.38950	-0.38078	-0.46333	14.76293	1.18044	1.55149	8	NH	NH
-0.39672	-0.34785	-0.44575	16.95146	0.18195	-1.10975	8	NH	NH
-0.47156	-0.41425	-0.46393	8.76505	-3.68041	-0.91680	5	Gen	Gen
-0.47181	-0.43005	-0.48988	6.47785	-1.77817	-0.33901	5	Gen	Gen
-0.46022	-0.44588	-0.50325	5.56899	-0.45834	1.32034	5	Gen	Gen
-0.46730	-0.44020	-0.49383	6.01255	-1.49487	0.66397	5	Gen	Gen
-0.94687	-0.94604	-0.94597	-70.07906	2.11521	-0.49951	13	Sin	Sin
-0.94395	-0.93382	-0.94416	-69.24585	2.44465	-1.25913	13	Sin	Sin
-0.92334	-0.93822	-0.93643	-67.88698	2.60017	0.60154	13	Sin	Sin
-0.93062	-0.93582	-0.94103	-68.43823	2.74108	-0.17348	13	Sin	Sin
-0.64639	-0.63608	-0.68048	-23.78320	1.27855	0.32261	14	Tan	Tan
-0.65523	-0.62009	-0.68114	-23.55149	1.37852	-1.55068	14	Tan	Tan

-0.66275	-0.63385	-0.69322	-25.31235	1.72202	-1.22779	14	Tan	Tan
-0.63162	-0.63816	-0.69200	-23.77059	2.98110	1.11590	14	Tan	Tan
-0.89080	-0.88688	-0.91172	-62.28500	3.39574	-0.85975	11	Nob	Nob
-0.91631	-0.91839	-0.91433	-65.27577	1.49297	0.02279	11	Nob	Nob
-0.89414	-0.91580	-0.91338	-63.90961	2.54720	1.23392	11	Nob	Nob
-0.90271	-0.90916	-0.91282	-64.02710	2.27657	0.16957	11	Nob	Nob

Table S17 Data matrix for the fluorescence response of the array sensor to 14 flavonoids in natural acids (the concentration of 14 flavonoids was 50 μM).

$\Delta I/I_0$	**PDI-1**	**PDI-2**	**PDI-3**	**Factor 1**	**Factor 2**	**Factor 3**
MH	-0.82883	-0.92038	-0.97759	0.25836	0.59309	0.91148
MH	-0.82652	-0.92154	-0.97768	0.19525	1.70499	0.95343
MH	-0.82911	-0.91981	-0.97761	0.33811	0.25518	1.03805
MH	-0.82462	-0.91960	-0.97821	0.44466	1.29266	2.28086
MH	-0.83264	-0.92114	-0.97859	-0.94198	0.24416	1.86987
MH	-0.82917	-0.92190	-0.97739	0.04529	1.21471	0.25316
Neo	-0.80004	-0.91136	-0.97416	7.34238	2.33427	0.17733
Neo	-0.80367	-0.91185	-0.97501	6.30704	1.87055	1.01398
Neo	-0.80282	-0.91139	-0.97537	6.25614	1.90540	1.68484
Neo	-0.80400	-0.91176	-0.97588	5.72046	1.89396	2.24532
Neo	-0.80393	-0.91408	-0.97517	5.70957	2.91653	0.72860
Neo	-0.80140	-0.91440	-0.97423	6.52083	3.50285	-0.49579
Bai	-0.96737	-0.98619	-0.99441	-38.66507	3.08033	-0.15180
Bai	-0.96813	-0.98426	-0.99462	-38.47677	2.00550	0.51771
Bai	-0.96825	-0.98517	-0.99455	-38.63109	2.40424	0.20088
Bai	-0.96963	-0.98465	-0.99434	-38.52868	1.80319	-0.07895
Bai	-0.96836	-0.98506	-0.99439	-38.51389	2.29820	-0.00825
Bai	-0.96984	-0.98588	-0.99432	-38.79409	2.34309	-0.39401
Api	-0.98191	-0.99146	-0.99599	-42.28588	2.51702	-0.16374
Api	-0.98228	-0.99165	-0.99569	-42.16274	2.47191	-0.66703
Api	-0.98259	-0.99115	-0.99562	-42.04781	2.14988	-0.67284
Api	-0.98200	-0.99100	-0.99631	-42.41140	2.32769	0.39320
Api	-0.98499	-0.99098	-0.99586	-42.41919	1.55567	-0.46853
Api	-0.98509	-0.99151	-0.99615	-42.72353	1.83183	-0.19053
Dai	-0.79238	-0.90761	-0.97401	9.00281	2.27391	1.37303
Dai	-0.78429	-0.90516	-0.97238	11.40999	2.69478	0.21030
Dai	-0.79297	-0.90808	-0.97326	9.33849	2.23923	0.15764
Dai	-0.79768	-0.90909	-0.97352	8.47622	1.68114	-0.05002
Dai	-0.79695	-0.90828	-0.97431	8.19796	1.58752	1.31080
Dai	-0.79748	-0.91143	-0.97441	7.42408	3.00411	0.70880
Hes	-0.78871	-0.90430	-0.97336	10.48976	1.41717	1.46764
Hes	-0.79249	-0.90514	-0.97351	9.83029	0.97551	1.20993
Hes	-0.79575	-0.90639	-0.97411	8.84647	0.91753	1.53471

Hes	-0.79944	-0.90820	-0.97454	7.80517	1.01477	1.47543
Hes	-0.80188	-0.90906	-0.97488	7.15791	0.91362	1.57855
Hes	-0.79392	-0.90977	-0.97430	8.20409	3.00672	1.19610
Fla	-0.57806	-0.80139	-0.94471	72.28569	-4.23541	-0.66368
Fla	-0.57873	-0.79874	-0.94483	72.69084	-5.65528	0.04514
Fla	-0.58809	-0.80220	-0.94696	69.61357	-5.79979	1.60398
Fla	-0.58026	-0.79736	-0.94505	72.67756	-6.63958	0.54884
Fla	-0.58906	-0.80649	-0.94656	68.88611	-4.01847	0.00712
Fla	-0.59152	-0.80739	-0.94664	68.39118	-4.13773	-0.25921
Pue	-0.68116	-0.87187	-0.95899	37.69517	8.28903	-3.74023
Pue	-0.69863	-0.86988	-0.95926	36.13991	3.32871	-4.21414
Pue	-0.69011	-0.87699	-0.95917	35.59703	8.71839	-5.29772
Pue	-0.68121	-0.87129	-0.96038	36.89591	8.22598	-1.63728
Pue	-0.69318	-0.87741	-0.96156	33.62528	8.60545	-2.22184
Pue	-0.69508	-0.87724	-0.96134	33.60924	8.04733	-2.63625
Nar	-0.77552	-0.90279	-0.97518	10.96069	4.03378	5.37945
Nar	-0.78379	-0.90631	-0.97515	9.39950	3.82082	3.93453
Nar	-0.78845	-0.90909	-0.97465	8.67212	4.00317	2.25514
Nar	-0.79873	-0.90830	-0.97433	8.00058	1.18772	1.19747
Nar	-0.79337	-0.90557	-0.97530	8.47749	1.27036	3.59025
Nar	-0.78798	-0.90825	-0.97456	8.95722	3.69084	2.34556
NH	-0.78900	-0.89811	-0.97108	13.24910	-2.01491	-0.42853
NH	-0.79860	-0.89909	-0.97009	12.71090	-3.91894	-2.77060
NH	-0.79523	-0.89535	-0.97229	12.38857	-4.59289	1.44636
NH	-0.79823	-0.90206	-0.97003	12.17169	-2.41035	-3.49047
NH	-0.79696	-0.90051	-0.97101	11.97877	-2.70593	-1.65415
NH	-0.78832	-0.90063	-0.97035	13.27603	-0.75789	-1.97706
Gen	-0.86760	-0.93177	-0.97962	-7.41335	-2.54270	-1.62961
Gen	-0.86956	-0.93394	-0.98108	-9.02707	-1.70757	-0.18215
Gen	-0.86849	-0.93141	-0.98083	-8.22126	-2.72661	0.09533
Gen	-0.86701	-0.93497	-0.97978	-8.12411	-0.83165	-2.07108
Gen	-0.86662	-0.93318	-0.97925	-7.36189	-1.69626	-2.40193
Gen	-0.85971	-0.93326	-0.98082	-7.69941	0.20041	0.32254
Sin	-0.96410	-0.97480	-0.99154	-34.07640	-2.13442	-1.45362
Sin	-0.96663	-0.97444	-0.99173	-34.38642	-2.86354	-1.29144
Sin	-0.96377	-0.97364	-0.99222	-34.24505	-2.50752	-0.21057
Sin	-0.96755	-0.97503	-0.99216	-34.88529	-2.71912	-0.88080
Sin	-0.96671	-0.97408	-0.99270	-34.95266	-2.89945	0.15469
Sin	-0.96663	-0.97503	-0.99250	-35.01160	-2.45341	-0.33590
Tan	-0.84263	-0.91467	-0.97780	-0.10392	-5.32588	1.45115
Tan	-0.84343	-0.91699	-0.97751	-0.47602	-4.43525	0.45474
Tan	-0.85040	-0.91614	-0.97826	-1.50759	-6.33609	1.19021
Tan	-0.85413	-0.91962	-0.97703	-1.80519	-5.71757	-1.61169
Tan	-0.85340	-0.91999	-0.97750	-2.11615	-5.29547	-0.96513

Tan	-0.84617	-0.91573	-0.97752	-0.50503	-5.67472	0.55376
Nob	-0.94068	-0.96079	-0.98847	-26.74643	-3.98665	-0.95936
Nob	-0.94544	-0.95957	-0.98826	-26.84066	-5.71313	-1.34106
Nob	-0.94709	-0.96230	-0.98935	-28.29488	-4.59463	-0.51972
Nob	-0.94660	-0.96188	-0.98892	-27.87525	-4.75833	-1.00006
Nob	-0.94809	-0.96245	-0.98827	-27.71867	-4.93156	-2.16221
Nob	-0.93993	-0.96227	-0.98953	-27.67508	-2.92619	0.28109

Table S18 Jackknifed classification matrix.

Jackknifed classification matrix showed the 92% correct classification.

	Api	Bai	Dai	Fla	Gen	Hes	MH	NH	Nar	Neo	Nob	Pue	Sin	Tan	**%correct**
Api	6	0	0	0	0	0	0	0	0	0	0	0	0	0	100
Bai	0	6	0	0	0	0	0	0	0	0	0	0	0	0	100
Dai	0	0	4	0	0	1	0	0	0	1	0	0	0	0	67
Fla	0	0	0	6	0	0	0	0	0	0	0	0	0	0	100
Gen	0	0	0	0	6	0	0	0	0	0	0	0	0	0	100
Hes	0	0	2	0	0	3	0	0	0	1	0	0	0	0	50
MH	0	0	0	0	0	0	6	0	0	0	0	0	0	0	100
NH	0	0	0	0	0	0	0	6	0	0	0	0	0	0	100
Nar	0	0	0	0	0	2	0	0	4	0	0	0	0	0	67
Neo	0	0	0	0	0	0	0	0	0	6	0	0	0	0	100
Nob	0	0	0	0	0	0	0	0	0	0	6	0	0	0	100
Pue	0	0	0	0	0	0	0	0	0	0	0	6	0	0	100
Sin	0	0	0	0	0	0	0	0	0	0	0	0	6	0	100
Tan	0	0	0	0	0	0	0	0	0	0	0	0	0	6	100
Total	6	6	6	6	6	6	6	6	4	8	6	6	6	6	**92**

Table S19 Data matrix for the fluorescence response of the array sensor to unknown samples.

Fluorescence Response Pattern			**Results LDA**				**Analyte**	
PDI-1	**PDI-2**	**PDI-3**	**Factor1**	**Factor2**	**Factor3**	**Group**	**Identification**	**Verification**
-0.83603	-0.91896	-0.97870	-0.91499	-1.57569	2.27171	7	MH	MH
-0.83609	-0.92181	-0.97693	-0.34333	-0.50307	-0.90116	7	MH	MH
-0.83469	-0.92095	-0.97736	-0.30682	-0.52369	0.01491	7	MH	MH
-0.83675	-0.92040	-0.97709	-0.22592	-1.30948	-0.40360	7	MH	MH
-0.80150	-0.91347	-0.97472	6.38615	3.10731	0.39648	10	Neo	Neo
-0.80215	-0.91015	-0.97456	7.11210	1.32714	0.86429	10	Neo	Neo
-0.80590	-0.91329	-0.97500	5.78881	2.04704	0.50491	10	Neo	Neo
-0.80571	-0.91313	-0.97559	5.45345	2.11037	1.39607	10	Neo	Neo
-0.96912	-0.98547	-0.99455	-38.78560	2.35145	0.07542	2	Bai	Bai
-0.96947	-0.98508	-0.99446	-38.67954	2.06525	0.00264	2	Bai	Bai
-0.96909	-0.98493	-0.99388	-38.22797	1.98649	-0.75961	2	Bai	Bai
-0.96742	-0.98423	-0.99429	-38.18536	2.10257	0.11237	2	Bai	Bai

-0.98390	-0.99212	-0.99598	-42.61826	2.37404	-0.47664	1	Api	Api
-0.98439	-0.99176	-0.99606	-42.64836	2.09898	-0.31589	1	Api	Api
-0.98403	-0.99155	-0.99595	-42.49311	2.06449	-0.40476	1	Api	Api
-0.98195	-0.99132	-0.99609	-42.32694	2.45908	0.00262	1	Api	Api
-0.78284	-0.90732	-0.97315	10.60458	4.19879	0.92825	3	Dai	Dai
-0.79285	-0.90809	-0.97378	9.00588	2.36081	0.90272	3	Dai	Dai
-0.79119	-0.90636	-0.97407	9.34489	1.95285	1.82923	6	Hes	Dai
-0.79331	-0.90881	-0.97393	8.71004	2.62449	0.92551	3	Dai	Dai
-0.78977	-0.91003	-0.97516	8.01297	4.23080	2.66359	9	Nar	Hes
-0.79272	-0.90853	-0.97468	8.33462	2.75011	2.09972	9	Nar	Hes
-0.80152	-0.90683	-0.97517	7.46462	-0.03014	2.52137	6	Hes	Hes
-0.79433	-0.90405	-0.97375	9.71627	0.05765	1.64882	6	Hes	Hes
-0.58370	-0.80283	-0.94691	69.96364	-4.48782	1.72470	4	Fla	Fla
-0.58247	-0.80168	-0.94802	69.59971	-4.57944	3.65295	4	Fla	Fla
-0.59012	-0.80687	-0.94616	68.95890	-4.14588	-0.72066	4	Fla	Fla
-0.59376	-0.80403	-0.94701	68.62154	-6.21822	0.84021	4	Fla	Fla
-0.68466	-0.87452	-0.96023	35.96975	8.96285	-2.82680	12	Pue	Pue
-0.69110	-0.87388	-0.96068	35.15115	7.23483	-2.53330	12	Pue	Pue
-0.68593	-0.87433	-0.96019	35.90847	8.56878	-2.94479	12	Pue	Pue
-0.70328	-0.87233	-0.96096	34.03663	3.71703	-2.68754	12	Pue	Pue
-0.79125	-0.90817	-0.97455	8.64885	2.89200	2.09970	9	Nar	Nar
-0.79028	-0.90480	-0.97505	9.11545	1.57225	3.64483	9	Nar	Nar
-0.79336	-0.90825	-0.97447	8.46677	2.42850	1.81375	6	Hes	Nar
-0.79719	-0.90403	-0.97434	9.03510	-0.51745	2.28702	6	Hes	Nar
-0.79203	-0.90113	-0.97131	12.16269	-1.21959	-1.00289	8	NH	NH
-0.79462	-0.90184	-0.97163	11.53405	-1.42005	-0.89374	8	NH	NH
-0.79058	-0.90124	-0.97150	12.15794	-0.79833	-0.63772	8	NH	NH
-0.79635	-0.89764	-0.97087	12.73179	-3.97565	-1.16911	8	NH	NH
-0.85945	-0.93148	-0.98013	-6.84948	-0.71460	-0.24131	5	Gen	Gen
-0.86868	-0.93471	-0.98059	-8.76944	-1.21568	-0.99170	5	Gen	Gen
-0.86958	-0.93423	-0.98087	-8.94854	-1.60584	-0.55222	5	Gen	Gen
-0.86911	-0.93484	-0.97986	-8.36369	-1.36909	-2.08800	5	Gen	Gen
-0.96919	-0.97507	-0.99178	-34.80802	-3.14436	-1.55945	13	Sin	Sin
-0.96908	-0.97536	-0.99235	-35.23289	-2.88518	-0.79951	13	Sin	Sin
-0.96755	-0.97547	-0.99189	-34.79894	-2.55292	-1.36311	13	Sin	Sin
-0.96691	-0.97509	-0.99191	-34.66423	-2.58702	-1.20507	13	Sin	Sin
-0.85446	-0.91726	-0.97729	-1.52048	-6.89284	-0.73544	14	Tan	Tan
-0.85286	-0.91850	-0.97690	-1.35471	-5.98949	-1.45367	14	Tan	Tan
-0.85581	-0.91968	-0.97715	-2.07115	-6.05683	-1.57208	14	Tan	Tan
-0.84402	-0.91677	-0.97763	-0.57400	-4.65857	0.64236	14	Tan	Tan
-0.94701	-0.96123	-0.98860	-27.57501	-5.21477	-1.33924	11	Nob	Nob
-0.94222	-0.95969	-0.98912	-27.10387	-4.76967	0.10348	11	Nob	Nob
-0.94506	-0.96226	-0.98950	-28.17963	-4.12155	-0.14263	11	Nob	Nob
-0.94511	-0.96216	-0.98942	-28.10945	-4.19725	-0.23874	11	Nob	Nob

Table S20 Data matrix for the fluorescence response of the array sensor to 8 red grape wines.

$\Delta I/I_0$	PDI-1	PDI-2	PDI-3	Factor 1	Factor 2	Factor 3
Wine 1	-0.20014	-0.18520	-0.21420	-3.94701	2.51029	2.85284
Wine 1	-0.18559	-0.18506	-0.19414	-2.28274	3.35954	2.36610
Wine 1	-0.19572	-0.19552	-0.20972	-3.73502	3.63713	3.21454
Wine 1	-0.22463	-0.19241	-0.23064	-6.54427	2.41686	2.93681
Wine 1	-0.19930	-0.20205	-0.20606	-4.11874	4.36464	3.09081
Wine 1	-0.19020	-0.19934	-0.19664	-3.08004	4.53099	2.86458
Wine 2	-0.18363	-0.16320	-0.15358	-0.68672	3.05029	-0.79003
Wine 2	-0.17810	-0.15118	-0.14235	0.32378	2.44146	-1.66541
Wine 2	-0.17974	-0.16449	-0.13399	0.03632	3.97793	-1.70004
Wine 2	-0.19353	-0.15091	-0.15121	-1.15994	2.01011	-1.89252
Wine 2	-0.19320	-0.15773	-0.14821	-1.23703	2.74802	-1.77940
Wine 2	-0.19906	-0.15119	-0.15820	-1.78494	1.73311	-1.73564
Wine 3	-0.20975	-0.13562	-0.17907	-2.75137	-0.55492	-1.64703
Wine 3	-0.19890	-0.14301	-0.23047	-3.14703	-1.95494	2.17484
Wine 3	-0.22579	-0.14000	-0.23368	-5.40238	-2.43659	0.96112
Wine 3	-0.20520	-0.14122	-0.20226	-3.01577	-0.98281	0.15159
Wine 3	-0.22279	-0.13897	-0.18949	-4.15900	-0.71618	-1.52469
Wine 3	-0.21002	-0.13738	-0.18789	-3.01045	-0.75646	-1.07301
Wine 4	-0.25758	-0.10580	-0.22371	-7.00371	-5.20712	-2.50695
Wine 4	-0.24415	-0.11205	-0.22733	-6.11040	-4.75177	-1.40482
Wine 4	-0.25975	-0.11318	-0.24573	-7.85201	-5.44686	-1.02559
Wine 4	-0.24867	-0.12405	-0.23094	-6.86826	-3.83073	-0.92827
Wine 4	-0.25788	-0.12970	-0.22038	-7.55205	-2.91702	-1.75911
Wine 4	-0.26144	-0.14327	-0.24622	-8.75466	-2.75872	0.12709
Wine 5	-0.13345	-0.11147	-0.12914	5.35505	-0.46817	-1.90081
Wine 5	-0.10553	-0.09727	-0.15393	7.51347	-2.67849	0.31215
Wine 5	-0.13114	-0.11598	-0.14006	5.19769	-0.50059	-0.97140
Wine 5	-0.10956	-0.09294	-0.14978	7.37321	-2.91213	-0.29653
Wine 5	-0.11174	-0.11980	-0.14090	6.71463	-0.13356	0.15561
Wine 5	-0.11261	-0.09586	-0.12931	7.49173	-1.82215	-1.52311
Wine 6	-0.17108	-0.15572	-0.13159	1.03528	3.30986	-1.77896
Wine 6	-0.15687	-0.15345	-0.12710	2.38495	3.33070	-1.45547
Wine 6	-0.13732	-0.19161	-0.13197	2.97028	6.63103	1.28884
Wine 6	-0.17510	-0.17036	-0.12028	0.58000	5.08010	-2.04647
Wine 6	-0.15205	-0.17096	-0.12648	2.36680	4.94979	-0.56071
Wine 6	-0.17703	-0.19548	-0.13961	-0.63076	6.55031	-0.00093
Wine 7	-0.13492	-0.14536	-0.13503	4.25822	2.34236	-0.26890
Wine 7	-0.14322	-0.13522	-0.13225	3.87389	1.51732	-1.23299
Wine 7	-0.13882	-0.13176	-0.15575	3.81593	0.25889	0.21356
Wine 7	-0.14238	-0.13337	-0.15704	3.44850	0.34107	0.18356

Wine 7	-0.15225	-0.13121	-0.14015	3.04187	0.80645	-1.36166
Wine 7	-0.13358	-0.13941	-0.18082	3.51854	-0.05970	2.23678
Wine 8	-0.14139	-0.08740	-0.19747	3.79436	-5.45249	0.75698
Wine 8	-0.13369	-0.09401	-0.18922	4.45676	-4.49687	0.90529
Wine 8	-0.14230	-0.10042	-0.21098	3.09745	-4.83185	2.02552
Wine 8	-0.13222	-0.09272	-0.20719	4.22004	-5.34247	1.97590
Wine 8	-0.12993	-0.09610	-0.21352	4.18946	-5.28939	2.59097
Wine 8	-0.13884	-0.08946	-0.20574	3.77611	-5.59630	1.44500

Table S21 Jackknifed classification matrix.

Jackknifed classification matrix showed the 100% correct classification.

	Wine 1	Wine 2	Wine 3	Wine 4	Wine 5	Wine 6	Wine 7	Wine 8	**%correct**
Wine 1	6	0	0	0	0	0	0	0	100
Wine 2	0	6	0	0	0	0	0	0	100
Wine 3	0	0	6	0	0	0	0	0	100
Wine 4	0	0	0	6	0	0	0	0	100
Wine 5	0	0	0	0	6	0	0	0	100
Wine 6	0	1	0	0	0	5	0	0	83
Wine 7	0	0	0	0	0	0	6	0	100
Wine 8	0	0	0	0	0	0	0	6	100
Total	6	7	6	6	6	5	6	6	**98**

Table S22 Data matrix for the fluorescence response of the array sensor to unknown wine samples.

Fluorescence Response Pattern			**Results LDA**				**Analyte**	
PDI-1	**PDI-2**	**PDI-3**	**Factor1**	**Factor2**	**Factor3**	**Group**	**Identification**	**Verification**
-0.20372	-0.21274	-0.22818	-5.23960	4.41241	4.60344	1	Wine 1	Wine 1
-0.21499	-0.18094	-0.18479	-4.44654	3.28319	0.25297	1	Wine 1	Wine 1
-0.21241	-0.18530	-0.23502	-5.43570	1.63253	3.49079	1	Wine 1	Wine 1
-0.19573	-0.17697	-0.18023	-2.62869	3.16769	0.74485	1	Wine 1	Wine 1
-0.18616	-0.15762	-0.13867	-0.43402	3.14807	-2.00714	2	Wine 2	Wine 2
-0.16930	-0.15652	-0.17605	0.19336	1.57314	0.94034	2	Wine 2	Wine 2
-0.17303	-0.16289	-0.15116	0.26506	3.15215	-0.43957	2	Wine 2	Wine 2
-0.17110	-0.14425	-0.13456	1.25497	2.15458	-2.06522	2	Wine 2	Wine 2
-0.20260	-0.14691	-0.17045	-2.24381	0.83620	-1.35888	2	Wine 2	Wine 3
-0.20670	-0.12879	-0.20656	-2.92558	-2.28356	-0.16528	3	Wine 3	Wine 3
-0.20290	-0.14709	-0.22119	-3.38252	-1.21936	1.60459	3	Wine 3	Wine 3
-0.22352	-0.14082	-0.19642	-4.41731	-0.83432	-1.07906	3	Wine 3	Wine 3
-0.24140	-0.16240	-0.23592	-7.32194	-0.55409	1.24480	3	Wine 3	Wine 4
-0.25246	-0.13856	-0.25799	-8.13931	-3.63718	1.05530	4	Wine 4	Wine 4

-0.23366	-0.13232	-0.24658	-6.15408	-3.67903	1.03347	4	Wine 4	Wine 4
-0.24079	-0.13463	-0.23664	-6.59430	-3.08537	0.20470	4	Wine 4	Wine 4
-0.12893	-0.09701	-0.14627	5.72070	-2.45865	-1.26183	5	Wine 5	Wine 5
-0.12372	-0.10805	-0.15350	5.72561	-1.74292	-0.14791	5	Wine 5	Wine 5
-0.11951	-0.10308	-0.16678	5.91269	-2.72046	0.63101	5	Wine 5	Wine 5
-0.11163	-0.09679	-0.14807	7.14095	-2.50056	-0.34051	5	Wine 5	Wine 5
-0.17394	-0.17732	-0.14663	-0.07197	4.63577	-0.17038	6	Wine 6	Wine 6
-0.16362	-0.18135	-0.12382	1.19405	5.96058	-0.85208	6	Wine 6	Wine 6
-0.16073	-0.16811	-0.13864	1.44294	4.17003	-0.37715	6	Wine 6	Wine 6
-0.17343	-0.15182	-0.12820	1.00953	3.09070	-2.24499	2	Wine 2	Wine 6
-0.14343	-0.14653	-0.17363	2.66982	0.84691	1.63106	7	Wine 7	Wine 7
-0.14172	-0.15214	-0.15274	3.13015	2.21093	0.71498	7	Wine 7	Wine 7
-0.15409	-0.15169	-0.16988	1.72762	1.43385	1.11097	7	Wine 7	Wine 7
-0.15110	-0.13928	-0.15465	2.62048	0.94523	-0.13509	7	Wine 7	Wine 7
-0.12299	-0.08724	-0.21616	4.93615	-6.17543	2.72135	8	Wine 8	Wine 8
-0.13359	-0.09023	-0.20285	4.26177	-5.39405	1.55706	8	Wine 8	Wine 8
-0.13222	-0.07455	-0.20643	4.68892	-6.94941	1.20330	8	Wine 8	Wine 8
-0.13142	-0.07648	-0.21974	4.41776	-7.31654	2.09814	8	Wine 8	Wine 8

12. Machine learning algorithm code

```
import matplotlib.pyplot as plt
import pandas as pd
import numpy as np
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.model_selection import cross_val_score
from sklearn.svm import SVC
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis as LDA
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import cross_val_predict
from sklearn.linear_model import LogisticRegression
from sklearn.gaussian_process import GaussianProcessClassifier
from sklearn.naive_bayes import BernoulliNB
from sklearn.metrics import accuracy_score
data=pd.read_csv('',encoding='gb2312')
x=data.iloc[ ].values
y=data.iloc[ ].values
test_size=0.4
seed=4
x_train,x_test,y_train,y_test=train_test_split(x,y,test_size=test_size,random_state=seed,stratify=y)
sc=StandardScaler()
```

```
sc.fit(x_train)
x_train=sc.transform(x_train)
x_test=sc.transform(x_test)
#LDA
lda=LDA(n_components=2)
lda=lda.fit(x_train,y_train)
#RF/DT
clf=DecisionTreeClassifier(random_state=1
                              ,max_depth=6
                              ,min_samples_leaf=2
                              ,criterion='entropy'
                              )
rfc=RandomForestClassifier(random_state=10
                              ,max_depth=3
                              ,min_samples_leaf=1
                              ,criterion='entropy'
                              ,n_estimators=100)
#SVM
for kernel in ["poly"]:
    svr=SVC(kernel=kernel
            #,gamma="auto"
            #,degree=1
            #,cache_size=5000
           ).fit(x_train,y_train)
    result=svr.predict(x_test)
    score=svr.score(x_test,y_test)
#LR
LR=LogisticRegression(random_state=0)
LR.fit(x_train,y_train)
#KNN
KNN = KNeighborsClassifier(n_neighbors=1, algorithm = 'ball_tree')
KNN = KNN.fit(x_train, y_train)
#Naive Bayes
BNB = BernoulliNB()
BNB = BNB.fit(x_train,y_train)
#GPC
gpc = GaussianProcessClassifier(random_state=0)
gpc = gpc.fit(x_train, y_train)
#Naive Bayes_train
score_BNB1 = cross_val_score(BNB,x_train,y_train,cv=6)
BNB_train = score_BNB1.mean()
BNB_train
np.std(score_BNB1 ,ddof = 1)
#Naive Bayes_test
```

```
score_BNB2 = cross_val_score(BNB,x_test,y_test,cv=4)
BNB_test = score_BNB2.mean()
BNB_test
np.std(score_BNB2 ,ddof = 1)
#GCP_train
score_gpc1 = cross_val_score(gpc,x_train,y_train,cv=6)
gpc_train = score_gpc1.mean()
gpc_train
np.std(score_gpc1 ,ddof = 1)
#GCP_test
score_gpc2 = cross_val_score(gpc,x_test,y_test,cv=4)
gpc_test = score_gpc2.mean()
gpc_test
np.std(score_gpc2 ,ddof = 1)
#KNN_train
score_KNN1 = cross_val_score(KNN,x_train,y_train,cv=6)
KNN_train = score_KNN1.mean()
KNN_train
np.std(score_KNN1 ,ddof = 1)
#KNN_test
score_KNN2 = cross_val_score(KNN,x_test,y_test,cv=4)
KNN_test = score_KNN2.mean()
KNN_test
np.std(score_KNN2 ,ddof = 1)
#lda_train
score_lda1 = cross_val_score(lda,x_train,y_train,cv=6)
lda_train = score_lda1.mean()
lda_train
np.std(score_lda1 ,ddof = 1)
#lda_test
score_lda2 = cross_val_score(lda,x_test,y_test,cv=4)
lda_test = score_lda2.mean()
lda_test
np.std(score_lda2 ,ddof = 1)
#RF_train
score_rfc1 = cross_val_score(rfc,x_train,y_train,cv=6)
rfc_train = score_rfc1.mean()
rfc_train
np.std(score_rfc1 ,ddof = 1)
#RF_test
score_rfc2 = cross_val_score(rfc,x_test,y_test,cv=4)
rfc_test = score_rfc2.mean()
rfc_test
np.std(score_rfc2 ,ddof = 1)
```

```
#DT_train
score_clf1 = cross_val_score(clf,x_train,y_train,cv=6)
clf_train = score_clf1.mean()
clf_train
np.std(score_clf1 ,ddof = 1)
#DT_test
score_clf2 = cross_val_score(clf,x_test,y_test,cv=4)
clf_test = score_clf2.mean()
clf_test
np.std(score_clf2 ,ddof = 1)
#SVM_train
score_svm1 = cross_val_score(svr,x_train,y_train,cv=6)
svm_train = score_svm1.mean()
svm_train
np.std(score_svm1 ,ddof = 1)
#SVM_test
score_svm2 = cross_val_score(svr,x_test,y_test,cv=4)
svm_test = score_svm2.mean()
svm_test
np.std(score_svm2 ,ddof = 1)
#LR_train
score_LR1 = cross_val_score(LR,x_train,y_train,cv=6)
LR_train = score_LR1.mean()
LR_train
np.std(score_LR1 ,ddof = 1)
#LR_test
score_LR2 = cross_val_score(LR,x_test,y_test,cv=4)
LR_train = score_LR2.mean()
LR_train
np.std(score_LR2 ,ddof = 1)
```