

Supplementary Information

Spectroscopic and electrochemical studies on the evaluation of the radical scavenging activities of luteolin by chelating iron

Ai-Hong Yang^{a*}, Xue-Ying Shi^b, Xue Li^a, Fang-Fang Li^b, Qin-Qin Zhang^b, Shu-Xin Jiang^b, Jian-Zhong Cui^b and Hong-Ling Gao^b

^a Tianjin Key Laboratory of Chemistry and Analysis of Chinese Materia Medica, College of Chinese Materia Medica, Tianjin University of Traditional Chinese Medicine, Tianjin 300193, P. R. China

^b Department of Chemistry, School of Science, Tianjin University, and Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Tianjin 300072, P. R. China

*Author to whom correspondance should be addressed. Email:yah408@163.com

S1 Luteolin recovery from luteolin-Fe(III) complex by EDTA (1: complex + 0.2 mmol·L⁻¹ EDTA; 2: complex +0.15 mmol·L⁻¹ EDTA; 3: complex + 0.1 mmol·L⁻¹ EDTA; 4: luteolin-Fe(III) complex without EDTA.)

S2 The IR spectrum of luteolin.

S3 The IR spectrum of luteolin- Fe(III) complex.

S4 ESI-MS spectrum in the positive mode of luteolin:Fe(III) 1:1 in ethanol solution.

S5 ESI-MS spectrum in the positive mode of luteolin:Fe(III) 1:2 in ethanol solution.

S6 Absorbance of malonaldehyde-TBA complex at 532 nm at various Fe(II) concentrations in the presence or absence of EDTA and luteolin.

S7 Decay of the visible absorbance (518 nm) of DPPH induced by different concentrations of luteolin.

S8 Decay of the visible absorbance (518 nm) of DPPH induced by different concentrations of luteolin-Fe(III) complex.

S9 Decay of the visible absorbance (518 nm) of DPPH induced by luteolin-Fe(III) complex(mole ratio 4:1).

S10 Complex absorbance at 391 nm versus [Fe³⁺]/[Lu] concentrations.

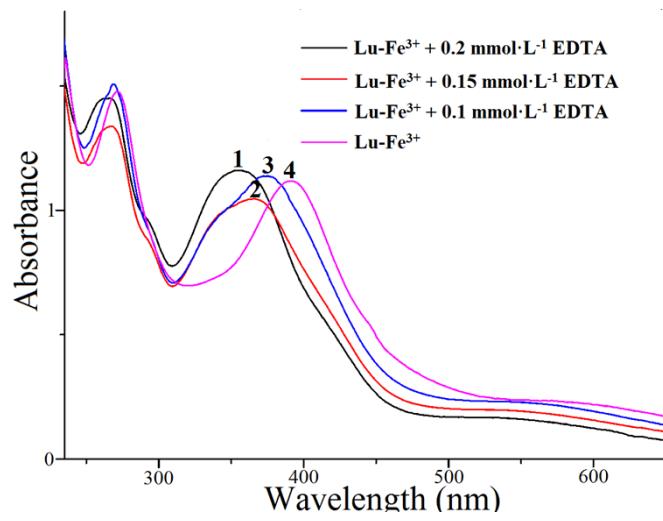


Fig.S1 Luteolin recovery from luteolin-Fe(III) complex by EDTA (1: complex + 0.2 mmol·L⁻¹ EDTA; 2: complex + 0.15 mmol·L⁻¹ EDTA; 3: complex + 0.1 mmol·L⁻¹ EDTA; 4: luteolin-Fe(III) complex without EDTA.)

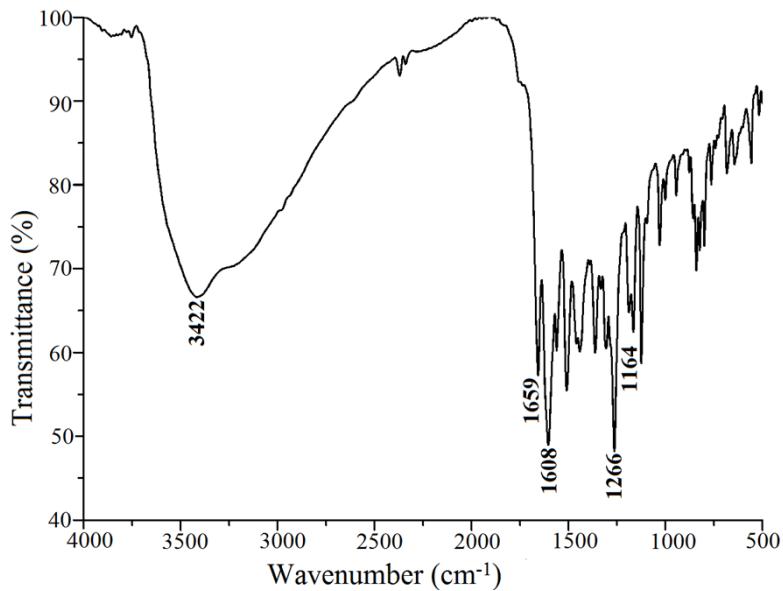


Fig.S2 The IR spectrum of luteolin.

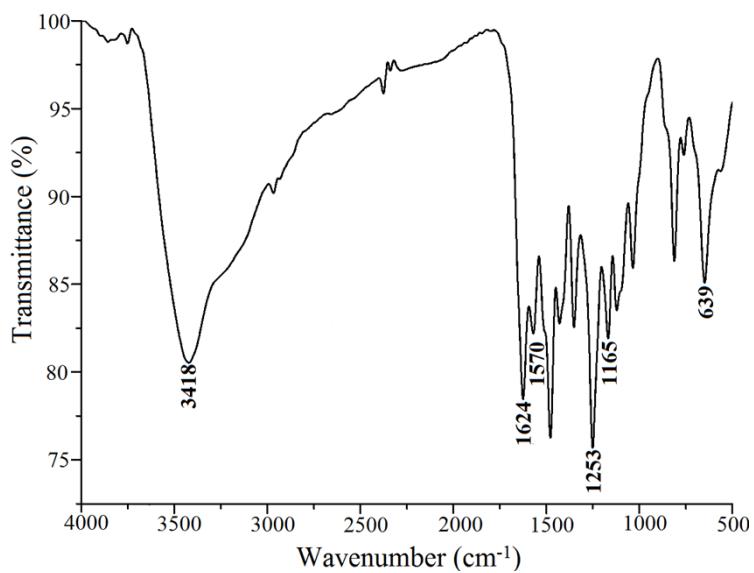


Fig.S3 The IR spectrum of luteolin-Fe(III) complex.

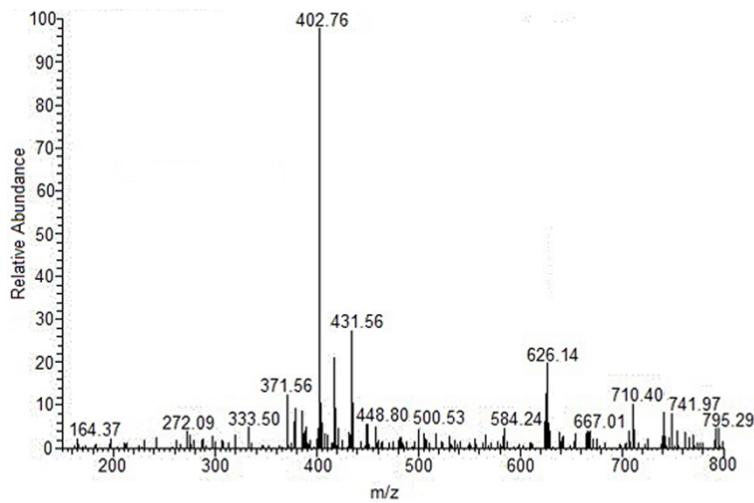


Fig. S4 ESI-MS spectrum in the positive mode of luteolin:Fe(III) 1:1 in ethanol solution.

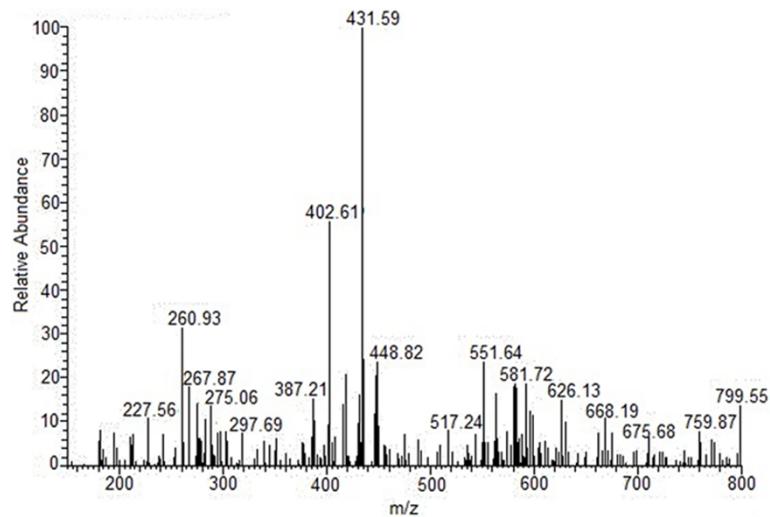


Fig. S5 ESI-MS spectrum in the positive mode of luteolin:Fe(III) 1:2 in ethanol solution.

Table.S6 Absorbance of malonaldehyde-TBA complex at 532 nm at various Fe(II) concentrations in the presence or absence of EDTA and luteolin.

The concentration of Fe ²⁺	Absorbance	Absorbance after the addition of EDTA of 0.4 mmol·L ⁻¹	Absorbance after the addition of luteolin of 0.4 mmol·L ⁻¹	Absorbance after the addition of EDTA and luteolin of 0.4 mmol·L ⁻¹
0.05	0.354	0.045	0.142	0.026
0.1	0.392	0.067	0.169	0.028
0.15	0.402	0.126	0.215	0.025
0.2	0.461	0.173	0.258	0.023
0.25	0.462	0.176	0.278	0.028
0.3	0.465	0.202	0.284	0.026
0.35	0.469	0.191	0.296	0.068
0.4	0.512	0.186	0.328	0.087
0.45	0.517	0.229	0.338	0.106
0.5	0.525	0.251	0.357	0.119
0.05	0.351	0.042	0.140	0.025
0.1	0.396	0.071	0.165	0.026
0.15	0.405	0.121	0.213	0.027
0.2	0.458	0.170	0.255	0.025
0.25	0.463	0.175	0.273	0.031
0.3	0.467	0.206	0.280	0.026
0.35	0.472	0.195	0.299	0.065
0.4	0.510	0.181	0.325	0.089
0.45	0.516	0.225	0.334	0.105
0.5	0.528	0.248	0.359	0.121
0.05	0.357	0.045	0.145	0.027
0.1	0.391	0.069	0.163	0.029
0.15	0.407	0.123	0.215	0.024
0.2	0.457	0.169	0.259	0.022
0.25	0.465	0.179	0.275	0.027
0.3	0.468	0.200	0.286	0.029
0.35	0.470	0.197	0.293	0.066
0.4	0.515	0.184	0.323	0.085
0.45	0.519	0.223	0.333	0.108
0.5	0.529	0.255	0.354	0.115

Table.S7 Decay of the visible absorbance (518 nm) of DPPH induced by different concentrations of luteolin.

Time (s)	Absorbance at Lu/DPPH=0.15	Absorbance at Lu/DPPH=0.25	Absorbance at Lu/DPPH=0.75	Absorbance at Lu/DPPH=1.0	Absorbance at Lu/DPPH=1.5
0	0.798	0.798	0.798	0.798	0.798
60	0.647	0.546	0.373	0.26	0.204

120	0.631	0.515	0.33	0.232	0.182
180	0.617	0.471	0.272	0.196	0.155
240	0.596	0.421	0.226	0.178	0.12
300	0.583	0.411	0.217	0.157	0.12
360	0.571	0.396	0.19	0.157	0.12
420	0.561	0.377	0.19	0.157	0.12
480	0.555	0.377	0.19	0.157	0.12
540	0.555	0.377	0.19	0.157	0.12
600	0.555	0.377	0.19	0.157	0.12
660	0.555	0.377	0.19	0.157	0.12
720	0.555	0.377	0.19	0.157	0.12
780	0.555	0.377	0.19	0.157	0.12
840	0.555	0.377	0.19	0.157	0.12
900	0.555	0.377	0.19	0.157	0.12
960	0.555	0.377	0.19	0.157	0.12
0	0.801	0.801	0.801	0.801	0.801
60	0.653	0.551	0.378	0.267	0.201
120	0.630	0.519	0.335	0.236	0.184
180	0.613	0.477	0.275	0.205	0.158
240	0.599	0.425	0.230	0.180	0.124
300	0.584	0.408	0.221	0.161	0.124
360	0.573	0.392	0.193	0.161	0.124
420	0.564	0.374	0.193	0.161	0.124
480	0.550	0.374	0.193	0.161	0.124
540	0.550	0.374	0.193	0.161	0.124
600	0.550	0.374	0.193	0.161	0.124
660	0.550	0.374	0.193	0.161	0.124
720	0.550	0.374	0.193	0.161	0.124
780	0.550	0.374	0.193	0.161	0.124
840	0.550	0.374	0.193	0.161	0.124
900	0.550	0.374	0.193	0.161	0.124
960	0.550	0.374	0.193	0.161	0.124
0	0.801	0.801	0.801	0.801	0.801
60	0.644	0.545	0.374	0.26	0.205
120	0.626	0.522	0.328	0.232	0.178
180	0.614	0.473	0.270	0.196	0.151
240	0.601	0.419	0.233	0.178	0.118
300	0.583	0.410	0.216	0.157	0.118
360	0.578	0.397	0.189	0.157	0.118
420	0.567	0.379	0.189	0.157	0.118
480	0.560	0.379	0.189	0.157	0.118
540	0.552	0.379	0.189	0.157	0.118
600	0.552	0.379	0.189	0.157	0.118
660	0.552	0.379	0.189	0.157	0.118

720	0.552	0.379	0.189	0.157	0.118
780	0.552	0.379	0.189	0.157	0.118
840	0.552	0.379	0.189	0.157	0.118
900	0.552	0.379	0.189	0.157	0.118
960	0.552	0.379	0.189	0.157	0.118

Table.S8 Decay of the visible absorbance (518 nm) of DPPH induced by different concentrations of luteolin-Fe(III) complex.

Time (s)	Absorbance at (Lu-Fe)/DPPH=1	Absorbance at (Lu-Fe)/DPPH=1	Absorbance at (Lu-Fe)/DPPH=1
0	0.798	0.801	0.801
60	0.739	0.742	0.738
120	0.719	0.722	0.717
180	0.710	0.708	0.713
240	0.701	0.697	0.704
300	0.694	0.692	0.698
360	0.688	0.685	0.691
420	0.683	0.680	0.685
480	0.678	0.675	0.679
540	0.673	0.670	0.675
600	0.670	0.667	0.672
660	0.665	0.663	0.668
720	0.661	0.659	0.664
780	0.657	0.653	0.659
840	0.65	0.649	0.654
900	0.645	0.641	0.650
960	0.64	0.635	0.645

Table.S9 Decay of the visible absorbance (518 nm) of DPPH induced by luteolin-Fe(III) complex(mole ratio 4:1).

Time (s)	Absorbance at (Lu-Fe)/DPPH=4	Absorbance at (Lu-Fe)/DPPH=4	Absorbance at (Lu-Fe)/DPPH=4
0	0.798	0.801	0.801
120	0.729	0.733	0.727
240	0.71	0.708	0.713
360	0.694	0.696	0.697
480	0.683	0.679	0.685
600	0.67	0.667	0.674
720	0.661	0.664	0.657
840	0.657	0.654	0.650
960	0.657	0.654	0.650
1080	0.657	0.654	0.650
1200	0.657	0.654	0.650

Table S10 Complex absorbance at 391 nm versus $[Fe^{3+}]/[Lu]$ concentrations.

$c_{Fe^{3+}}/c_{Lu}$	Absorbance	Absorbance	Absorbance
0.1	0.158	0.162	0.154
0.2	0.208	0.209	0.212
0.3	0.213	0.211	0.216
0.4	0.239	0.242	0.236
0.5	0.284	0.282	0.287
0.6	0.344	0.337	0.341
0.7	0.406	0.401	0.403
0.8	0.439	0.434	0.436
0.9	0.507	0.505	0.511
1	0.557	0.561	0.559
2	0.586	0.584	0.589
3	0.586	0.584	0.589
4	0.586	0.584	0.589
5	0.586	0.584	0.589
6	0.586	0.584	0.589