

## Supporting information

Correlations between molecular structure and biological activity in "logical series" of dietary  
chromone derivatives

Short title: Structure and biological activity of chromone derivatives

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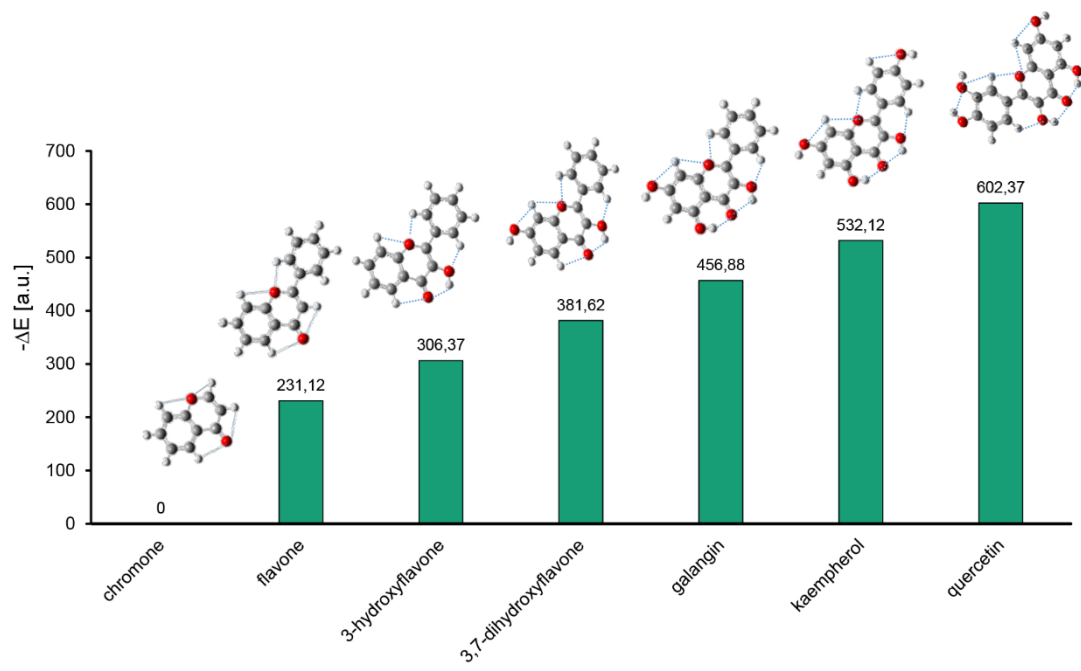


Fig S1. The energy of the most stable conformers of the studied compounds in relation to the energy of chromone.

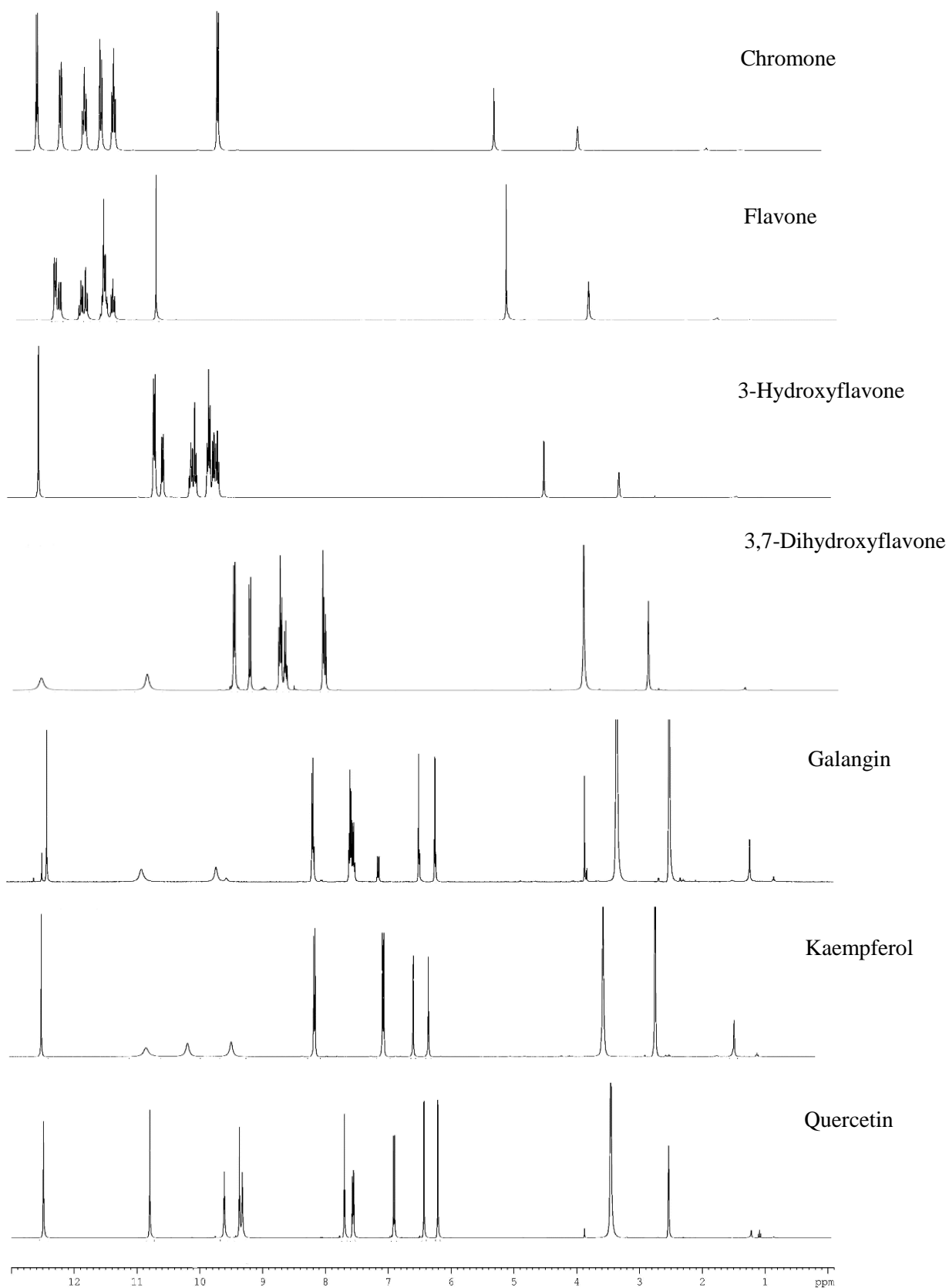


Fig S2. The <sup>1</sup>H NMR spectra of chromone derivatives.

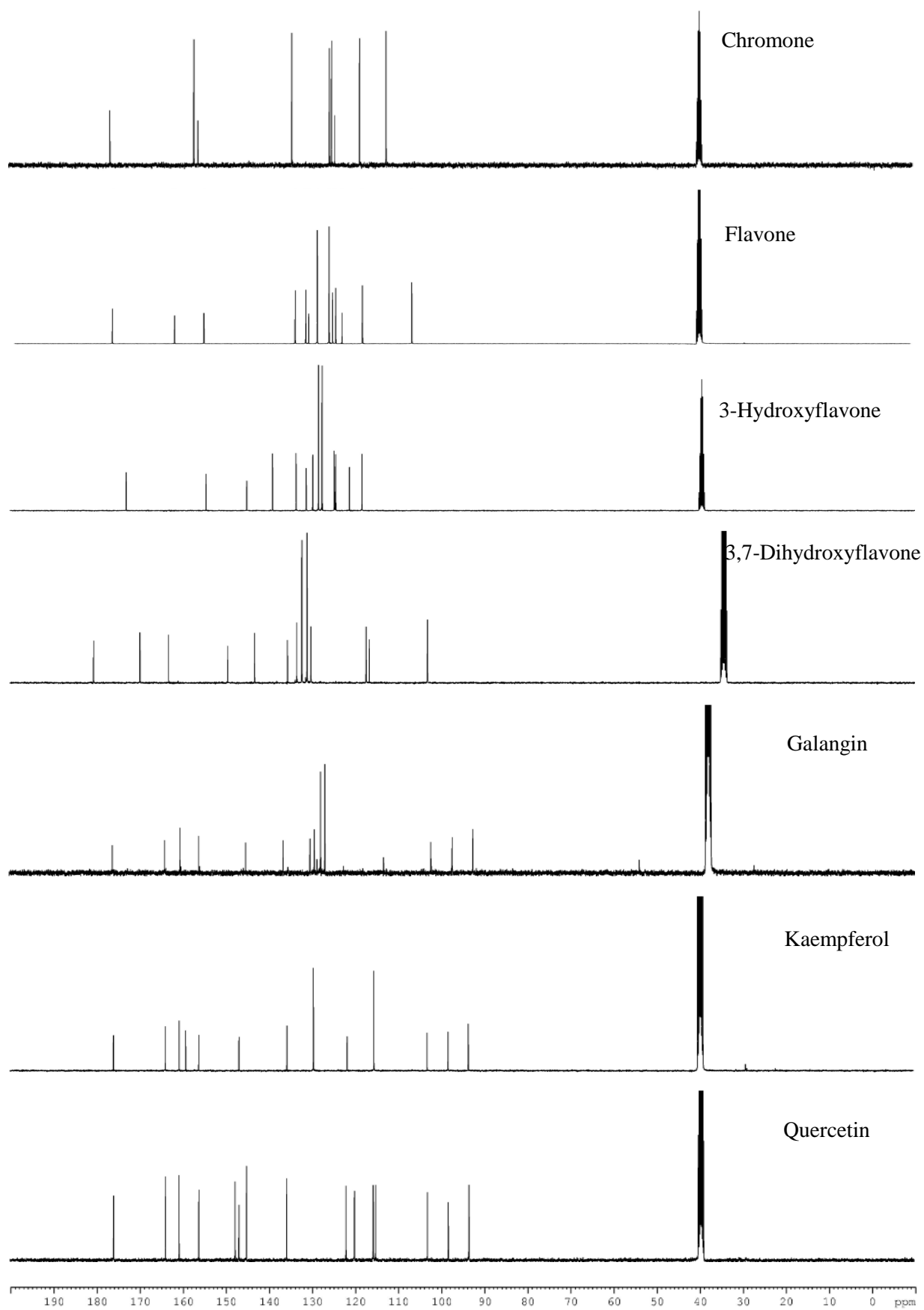


Fig S3. The  $^{13}\text{C}$  NMR spectra of chromone derivatives.

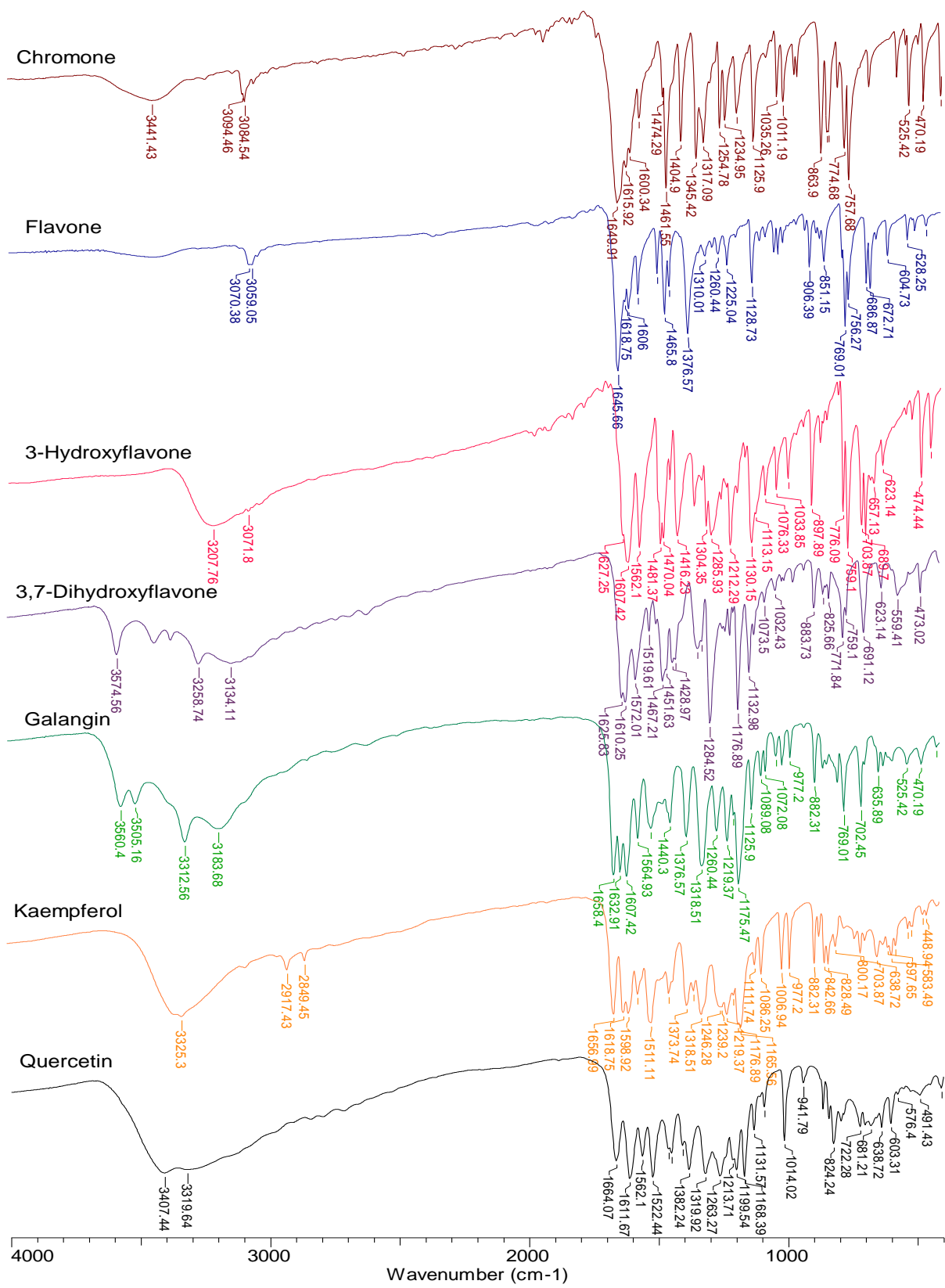


Fig S4. The IR spectra of chromone derivatives registered in the range of 400-4000  $\text{cm}^{-1}$ .

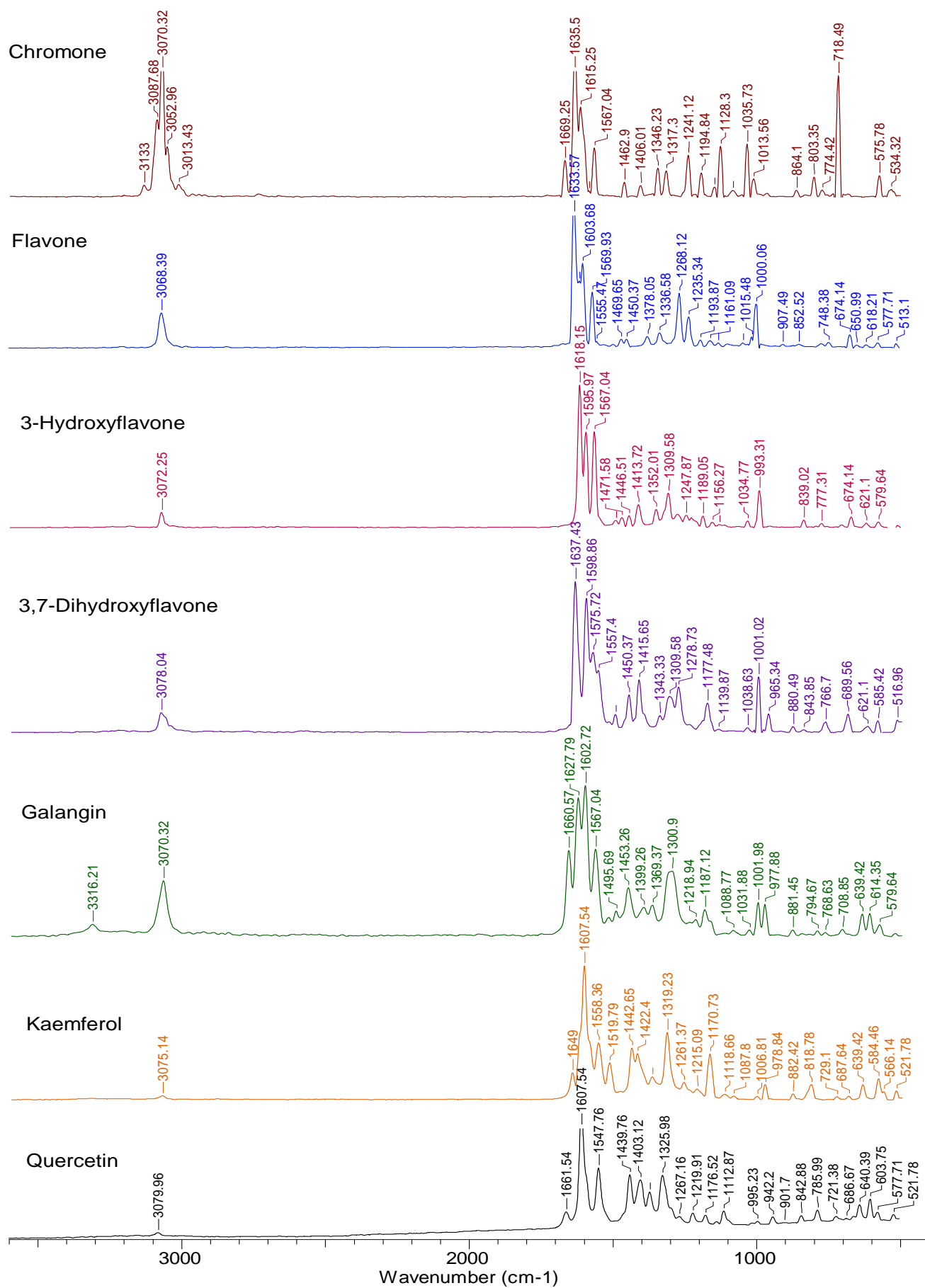


Fig S5. The Raman spectra of chromone derivatives registered in the range of 400-4000  $\text{cm}^{-1}$ .

Table S1. Selected bond lengths [Å] and angles [°] of 3-dihydroxyflavone conformers (atom numbering in Fig. 4)

<b>Bond lengths [Å]</b>	<b>Conformers of 3-dihydroxyflavone</b>	
	<b>1</b>	<b>2</b>
C2-C1'	1,476	1,472
C2-C3	1,363	1,363
C3-O3	1,360	1,355
O3-H3	0,965	0,975
C3-C4	1,472	1,458
C4=O4	1,222	1,232
C4-C10	1,475	1,463
C9-C10	1,398	1,400
C8-C9	1,399	1,399
C7-C8	1,384	1,384
C6-C7	1,405	1,406
C5-C6	1,382	1,382
C1'-C2'	1,404	1,403
C2'-C3'	1,490	1,391
C3'-C4'	1,395	1,394
C4'-C5'	1,393	1,394
C5'-C6'	1,404	1,391
C6'-C1'	1,404	1,402
C6-O1	1,363	1,393
O1-C5	1,370	1,369
<b>Hydrogen bonds [Å]</b>		
O1...H2'	2,591	2,469
O1...H8	2,557	2,556
O4...H5	2,565	2,633
O3...H3	-	2,057
O2-H6'	2,691	2,397

Table S2. The NBO atomic charges [e] calculated for 3-dihydroxyflavone conformers (atom numbering in Fig. 4)

		<b>Conformers of 3-dihydroxyflavone</b>	
<b>Ring</b>	<b>Atom</b>	<b>1</b>	<b>2</b>
<b>A</b>	C8	-0,235	-0,233
	C9	0,341	0,346
	C10	-0,182	-0,183
	C5	-0,144	-0,144
	C6	-0,214	-0,213
	C7	-0,171	-0,169
	<b>Total charge</b>		-0,605
<b>C</b>	O1	-0,489	-0,481
	C2	0,270	0,303
	C3	0,203	0,200
	C4	0,466	0,455
	C10	-0,182	-0,183
	C9	0,341	0,346
	<b>Total charge</b>		0,609
<b>B</b>	3'C	-0,199	-0,209
	4'C	-0,189	-0,188
	5'C	-0,201	-0,207
	6'C	-0,198	-0,151
	C1'	-0,099	-0,097
	C2'	-0,157	-0,159
	<b>Total charge</b>		-1,043
	O1	-0,489	-0,481
	O3	-0,652	-0,674
	O4	-0,564	-0,619

$$e = 1,602 \cdot 10^{-19} \text{ C}$$



Table S3. Selected bond lengths [Å] and angles [°] of 3,7-dihydroxyflavone conformers (atom numbering in Fig. 4)

<b>Bond lengths [Å]</b>	<b>Conformers of 3,7-dihydroxyflavone</b>			
	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>
C1'-C7	1,475	1,468	1,468	1,475
C2-C3	1,361	1,366	1,365	1,361
C3-O3	1,360	1,353	1,352	1,359
O3-H3	0,965	0,979	0,978	0,965
C2-C4	1,474	1,462	1,463	1,475
C4=O4	1,223	1,238	1,238	1,223
C4-C10	1,470	1,451	1,450	1,470
C9-C10	1,401	1,403	1,400	1,397
C8-C9	1,395	1,395	1,398	1,398
C7-C8	1,387	1,387	1,388	1,388
C7-O7	1,363	1,362	1,361	1,363
O7-H7	0,963	0,963	0,963	0,963
C6-C7	1,409	1,410	1,410	1,408
C5-C6	1,380	1,378	1,376	1,377
C5-C10	1,405	1,406	1,410	1,408
C1'-C2'	1,404	1,408	1,408	1,404
C2'-C3'	1,390	1,389	1,390	1,390
C3'-C4'	1,395	1,394	1,394	1,396
C4'-C5'	1,393	1,393	1,393	1,393
C5'-C6'	1,393	1,391	1,391	1,393
C6'-C1'	1,404	1,408	1,408	1,404
C9-O1	1,361	1,356	1,356	1,361
O1-C2	1,373	1,376	1,377	1,374
<b>Hydrogen bonds [Å]</b>				
O4...H3	-	1,978	1,974	-
O3...H6'	2,678	2,157	2,157	2,688
O1...H2'	2,578	2,309	2,313	2,590
H8...O7	2,581	2,576	2,702	2,704
O1...H8	2,569	2,571	2,551	2,550
O4...H5	2,572	2,653	2,658	2,577

Table S4. The NBO atomic charges [e] calculated for 3,7-dihydroxyflavone conformers (atom numbering in Fig. 4)

		<b>Conformers of 3,7-dihydroxyflavone</b>			
<b>Ring</b>	<b>Atom</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>
<b>A</b>	C8	-0,291	-0,295	-0,322	-0,324
	C9	0,363	0,376	0,377	0,364
	C10	-0,208	-0,208	-0,222	-0,208
	C5	-0,123	-0,122	-0,110	-0,124
	C6	-0,285	-0,284	-0,261	-0,255
	C7	0,344	0,347	0,350	0,347
	<b>Total charge</b>		-0,200	-0,186	-0,188
<b>C</b>	O1	-0,489	-0,485	-0,488	-0,492
	C2	0,266	0,311	0,312	0,268
	C3	0,205	0,210	0,198	0,207
	C4	0,467	0,448	0,461	0,465
	C10	-0,208	-0,208	-0,222	-0,208
	C9	0,363	0,376	0,377	0,364
	<b>Total charge</b>		0,604	0,652	0,638
<b>B</b>	C3'	-0,199	-0,201	-0,201	-0,199
	C4'	-0,190	-0,189	-0,190	-0,190
	C5'	-0,201	-0,206	-0,205	-0,201
	C6'	-0,199	-0,159	-0,159	-0,199
	C1'	-0,093	-0,115	-0,114	-0,098
	C2'	-0,157	-0,174	-0,176	-0,158
	<b>Total charge</b>		-1,039	-1,044	-1,045
	O3	-0,652	-0,679	-0,679	-0,652
	O4	-0,570	-0,634	-0,631	-0,569
	7O	-0,663	-0,660	-0,659	-0,662

$$e = 1,602 \cdot 10^{-19} \text{ C}$$

Table S5. Selected bond lengths [Å] and angles [°] of galangin conformers (atom numbering in Fig. 4)

<b>Bond lengths [Å]</b>	<b>Conformers of galangin</b>							
	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>
C3-OH	1,359	1,360	1,360	1,364	1,359	1,350	1,354	1,354
H3-O3	0,965	0,965	0,965	0,966	0,965	0,982	0,977	0,977
C4=O4	1,242	1,242	1,241	1,233	1,219	1,235	1,255	1,256
C5-OH	1,338	1,338	1,338	1,356	1,352	1,351	1,340	1,341
H5-O5	0,993	0,993	0,991	0,966	0,964	0,964	0,985	0,986
C7-OH	1,361	1,361	1,361	1,358	1,362	1,361	1,360	1,360
C1'-C2	1,475	1,475	1,475	1,475	1,475	1,467	1,467	1,467
C2-C3	1,362	1,362	1,362	1,358	1,356	1,361	1,367	1,367
C3-C4	1,465	1,465	1,466	1,472	1,482	1,471	1,453	1,452
C4-C10	1,448	1,448	1,449	1,465	1,476	1,454	1,432	1,433
C10-C5	1,424	1,424	1,427	1,426	1,420	1,423	1,425	1,422
<b>Hydrogen bonds [Å]</b>								
C4=O...HO-C5	1,702	1,702	1,710	-	-	-	1,778	1,771
C3-OH...O=C4	-	-	-	-	-	1,920	2,006	2,011

Table S6. The NBO atomic charges [e] calculated for galangin conformers (atom numbering in Fig. 4)

		Conformers of galangin							
Ring	Atom	1	2	3	4	5	6	7	8
A	C8	-0,332	-0,332	-0,363	-0,347	-0,323	-0,352	-0,360	-0,329
	C9	0,380	0,380	0,381	0,383	0,381	0,394	0,393	0,391
	C10	-0,265	-0,265	-0,264	-0,257	-0,255	-0,254	-0,269	-0,270
	C5	0,404	0,404	0,403	0,401	0,408	0,389	0,402	0,398
	C6	-0,352	-0,352	-0,352	-0,352	-0,384	-0,334	-0,321	-0,337
	C7	0,369	0,369	0,369	0,368	0,360	0,360	0,372	0,366
	<b>Total charge</b>		-0,265	-0,265	-0,264	-0,257	-0,255	-0,254	-0,269
C	O1	-0,483	-0,483	-0,485	-0,483	-0,489	-0,491	-0,486	-0,481
	C2	0,280	0,280	0,277	0,289	0,261	0,290	0,313	0,327
	C3	0,207	0,206	0,208	0,197	0,210	0,206	0,202	0,198
	C4	0,463	0,463	0,463	0,465	0,463	0,462	0,456	0,455
	C10	-0,265	-0,265	-0,264	-0,257	-0,255	-0,254	-0,269	-0,270
	C9	0,380	0,380	0,381	0,383	0,381	0,394	0,393	0,391
	<b>Total charge</b>		0,582	0,581	0,580	0,594	0,571	0,607	0,609
B	C3'	-0,198	-0,198	-0,199	-0,204	-0,199	-0,200	-0,208	-0,203
	C4'	-0,188	-0,188	-0,188	-0,190	-0,192	-0,192	-0,186	-0,186
	C5'	-0,201	-0,201	-0,201	-0,204	-0,201	-0,206	-0,206	-0,206
	C6'	-0,198	-0,198	-0,197	0,194	-0,196	-0,163	-0,160	-0,157
	C1'	-0,101	-0,101	-0,101	-0,109	-0,112	-0,099	-0,104	-0,118
	C2'	-0,156	-0,156	-0,156	-0,161	-0,156	-0,167	-0,162	-0,172
	<b>Total charge</b>		-1,042	-1,042	-1,042	-1,062	-1,056	-1,027	-1,026
	O1	-0,483	-0,483	-0,485	-0,483	-0,489	-0,491	-0,486	-0,481
	O3	-0,652	-0,652	-0,651	-0,681	-0,652	-0,680	-0,676	-0,676
	O4	-0,621	-0,621	-0,619	-0,635	-0,541	-0,607	-0,685	-0,687
	O5	-0,670	-0,670	-0,667	-0,657	-0,625	-0,628	-0,665	-0,668
	O7	-0,660	-0,660	-0,658	-0,674	-0,660	-0,660	-0,655	-0,657

e = 1,602\*10<sup>-19</sup> C

Table S7. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] of kaempferol conformers (atom numbering in Fig. 4)

<b>Bond lengths [<math>\text{\AA}</math>]</b>	<b>Conformers of kaempferol</b>				
	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>
C4'-OH	1,363	1,364	1,364	1,364	1,364
C3-OH	1,361	1,357	1,356	1,356	1,356
C4=O	1,243	1,257	1,256	1,256	1,256
C5-OH	1,338	1,341	1,341	1,340	1,340
C7-OH	1,361	1,360	1,360	1,361	1,361
C1'-C2	1,472	1,463	1,463	1,463	1,463
<b>Hydrogen bonds [<math>\text{\AA}</math>]</b>					
C4=O...HO-C5	1,700	1,768	1,771	1,767	1,774
C3-OH...O=C4	-	2,017	2,012	2,018	2,014

Table S8. The NBO atomic charges [e] calculated for kaempherol conformers (atom numbering in Fig. 4)

Ring	Atom	Conformers of kaempherol				
		1	2	3	4	5
<b>A</b>	C8	-0.223	-0.334	-0.349	-0.330	-0.361
	C9	0.380	0.390	0.386	0.390	0.392
	C10	-0.265	-0.262	-0.261	-0.269	-0.268
	C5	0.404	0.396	0.401	0.403	0.402
	C6	-0.353	-0.337	-0.321	-0.351	-0.321
	C7	0.368	0.365	0.367	0.370	0.371
	<b>Total charge</b>		0.311	0.218	0.223	0.213
<b>C</b>	O1	-0.484	-0.484	-0.488	-0.484	-0.489
	C2	0.286	0.330	0.326	0.333	0.318
	C3	0.200	0.204	0.205	0.190	0.194
	C4	0.464	0.438	0.439	0.453	0.454
	C9	0.380	0.390	0.386	0.390	0.392
	C10	-0.265	-0.262	-0.261	-0.269	-0.268
	<b>Total charge</b>		0.581	0.616	0.607	0.613
<b>B</b>	C1'	-0.133	-0.147	-0.147	-0.146	-0.133
	C2'	-0.133	-0.149	-0.150	-0.159	-0.138
	C3'	-0.246	-0.247	-0.247	-0.262	-0.287
	C4'	0.329	0.332	0.332	0.327	0.331
	C5'	-0.283	-0.285	-0.285	-0.253	-0.254
	C6'	-0.171	-0.134	-0.134	-0.135	-0.137
	<b>Total charge</b>		-0.637	-0.630	-0.631	-0.628
	O1	-0.484	-0.484	-0.488	-0.484	-0.489
	O3	-0.656	-0.682	-0.680	-0.680	-0.679
	O4	-0.626	-0.692	-0.690	-0.690	-0.688
	O5	-0.670	-0.669	-0.665	-0.668	-0.666
	O7	-0.660	-0.658	-0.657	-0.658	-0.656
	O4'	-0.663	-0.664	-0.664	-0.664	-0.664

$$e = 1,602 \cdot 10^{-19} \text{ C}$$

Table S9. Selected bond lengths [Å] and angles [°] of quercetin conformers (atom numbering Fig. 4)

<b>Bond lengths [Å]</b>	<b>Conformers of quercetin</b>					
	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>
O3-H3	0,977	0,977	0,977	0,966	0,982	0,965
O3-C3	1,355	1,356	1,355	1,360	1,352	1,359
C3-C4	1,449	1,450	1,450	1,463	1,467	1,481
C4=O4	1,256	1,257	1,256	1,246	1,236	1,220
C4-C10	1,434	1,433	1,434	1,449	1,456	1,476
C10-C5	1,422	1,422	1,425	1,424	1,420	1,420
C5-O5	1,340	1,341	1,340	1,338	1,352	1,352
O5-H5	0,987	0,987	0,986	0,993	0,964	0,964
<b>Hydrogen bonds [Å]</b>						
H3...O4	2,019	2,012	2,014	-	1,929	-
O4...H5	1,766	1,769	1,772	1,699	-	-
H6...O5	2,589	2,590	2,608	2,582	2,641	2,629
H6...O7	2,684	2,682	2,560	2,685	2,673	2,673

Table S10. The NBO atomic charges [e] calculated for quercetin conformers (atom numbering Fig. 4)

		Conformers of quercetin					
Ring		1	2	3	4	5	6
<b>A</b>	C8	-0,318	-0,317	-0,350	-0,334	-0,322	-0,324
	C9	0,385	0,387	0,385	0,380	0,393	0,379
	C10	-0,262	-0,270	-0,261	-0,265	-0,254	-0,247
	C5	0,403	0,403	0,402	0,404	0,390	0,388
	C6	-0,351	-0,351	-0,321	-0,350	-0,362	-0,362
	C7	0,366	0,366	0,366	0,368	0,357	0,354
	<b>Total charge</b>		0,223	0,218	0,221	0,203	0,202
<b>C</b>	O1	-0,491	-0,487	-0,494	-0,490	-0,497	-0,497
	C2	0,314	0,320	0,311	0,283	0,297	0,254
	C3	0,208	0,195	0,210	0,204	0,198	0,214
	C4	0,437	0,453	0,438	0,463	0,460	0,462
	C9	0,385	0,387	0,385	0,380	0,393	0,379
	C10	-0,262	-0,270	-0,261	-0,265	-0,254	-0,247
	<b>Total charge</b>		0,853	0,868	0,850	0,840	0,851
<b>B</b>	C1'	-0,114	-0,109	-0,113	-0,111	-0,109	-0,107
	C2'	-0,229	-0,201	-0,231	-0,225	-0,234	-0,227
	C3'	0,248	0,274	0,248	0,256	0,248	0,255
	C4'	0,295	0,265	0,294	0,291	0,289	0,287
	C5'	-0,243	-0,271	-0,242	-0,238	-0,242	-0,238
	C6'	-0,160	-0,167	-0,161	-0,202	-0,164	-0,203
	<b>Total charge</b>		-0,203	-0,209	-0,205	-0,229	-0,212
	O1	-0,491	-0,487	-0,494	-0,490	-0,497	-0,497
	O3	-0,679	-0,679	-0,679	-0,653	-0,682	-0,652
	O4	-0,688	-0,691	-0,686	-0,622	-0,610	-0,545
	O5	-0,668	-0,669	-0,665	-0,670	-0,627	-0,624
	O7	-0,659	-0,658	-0,657	-0,661	-0,659	-0,661
	O3'	-0,706	-0,671	-0,706	-0,701	-0,707	-0,703
	O4'	-0,663	-0,699	-0,663	-0,662	-0,666	-0,665

e = 1,602\*10<sup>-19</sup> C



**Table S11. The cytotoxic activity of studied compounds in relation to different cancer cell lines**

Compound	Parameters	Cell lines	Ref.	
Chromone	-	-	-	
Flavone	IC50 > 50.000 nM	A549	[1]	
3-Hydroxyflavone	LC50=40.4 μM	TIG-1	[2]	
	LC50= 64.0 μM	HUVEC		
	IC50= 20 ± 2 μM	B16 melanoma cells/ Lewis lung cells	[3]	
3,7-Dihydroxyflavone	GI50=17.4 ± 2.0 μM	MCF-7	[4]	
	GI50=15.4 ± 1.2 μM	NCI-H460		
	GI50=23.0 ± 1.0 μM	A375-C5		
Galangin	IC50= 48 ± 4 μM	B16 melanoma cells/ Lewis lung cells	[3]	
	IC50=275.48 μM	V79	[5]	
	IC50=145.0 μmol/L <sup>a</sup>	B16F10	[6]	
Kaempferol	LC50=221 μM	TIG-1	[2]	
	LC50=167 μM	HUVEC	[3]	
	IC50= 51 ± 5 μM	B16 melanoma cells/ Lewis lung cells		
	IC50= 31 ± 8 μM	EAhy 926 endothelial cells		
	IC50=30.92 ±0.05 μM	HepG2	[7]	
	IC50=88.02 ±001 μM	CT26		
IC50=70.62 ±0.05 μM	B16F1			
Quercetin	LC50=4.45mM	RAW264.7	[8]	
	IC50=118.1±5.55 μM <sup>a</sup>	CT-26	[9]	
	IC50=110.7±4.30 μM <sup>a</sup>	LNCaP		
	IC50>120 μM μM <sup>a</sup>	PC3		
	IC50=99.3±6.11 μM <sup>a</sup>	PC12		
	IC50=105.4±5.2 μM <sup>a</sup>	MCF-7		
	IC50=64.9±3.5 μM <sup>a</sup>	MOLT-4		
	IC50=54.3±4.5 μM <sup>a</sup>	U266B1		
	IC50=66.5±3.57 μM <sup>a</sup>	Raji		
	IC50=>120 μM <sup>a</sup>	CHO		
	IC50=50 μM	PC3		
	IC50=50 μM	LNCaP		[10]
	IC50= 35.5±1.1 μM	HeLa		[11]
	IC50=20.9±0.9 μM	NIH-3T3		
LC50= 303 μM	TIG-1	[2]		
LC50= 61.0 μM	HUVE			
IC50= 26 ± 4 μM	B16 melanoma cells/ Lewis lung cells	[3]		
IC50= 36 ± 2 μM	EAhy 926 endothelial cells			

<sup>a</sup>for 24h

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