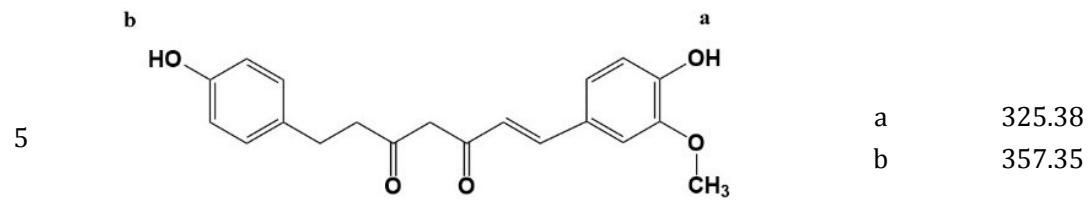


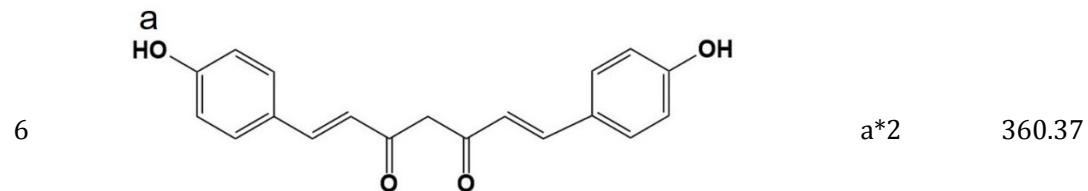
Supporting Information

Table S1. Molecular structure of 18 natural phenolic antioxidants and the free energies of dissociation of ArO-H bonds at different positions.

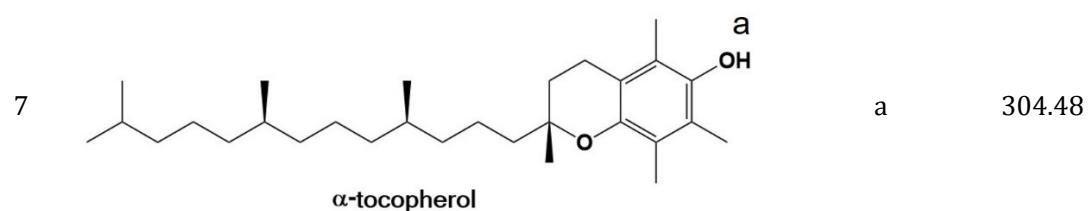
Number	Molecular Structure and the corresponding position	Dissociation positions	ΔG^{298K} (kJ/mol)
1		a b c d e	362.01 404.86 413.34 355.00 315.15
Dihydromyricetin			
2		a b c d e	353.46 315.37 410.77 407.54 366.16
Quercetin			
3		a b c d e	367.55 387.77 407.15 348.61 421.55
Silymarin			
4		a b c	328.46 328.77 404.00
Curcumin			



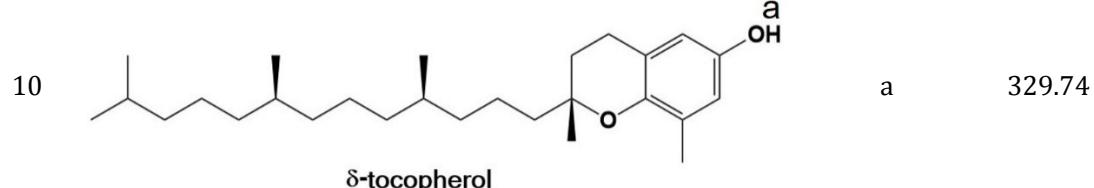
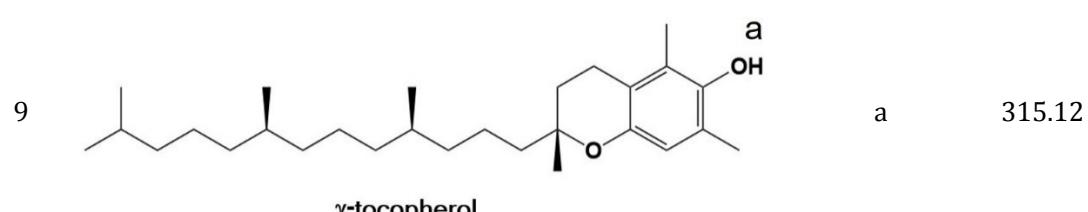
Demethoxycurcumin

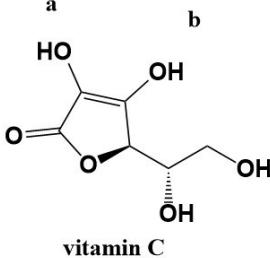
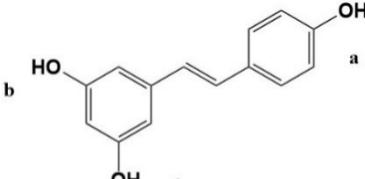
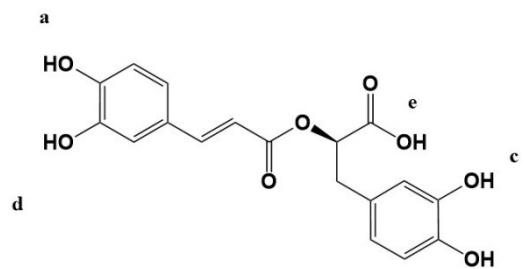
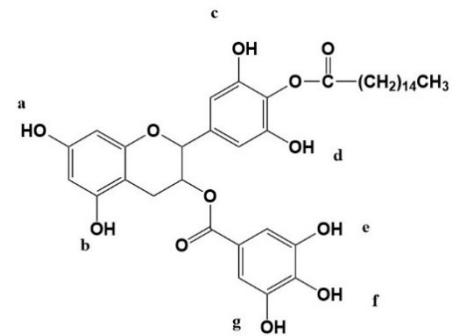
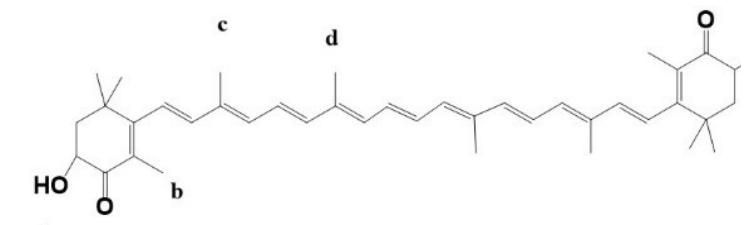
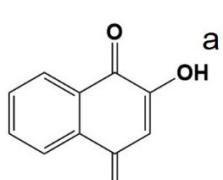


Bilemethoxycurcumin



β-tocopherol



11	 <p>vitamin C</p>	<table border="0"> <tr> <td>a</td> <td>328.54</td> </tr> <tr> <td>b</td> <td>322.46</td> </tr> </table>	a	328.54	b	322.46										
a	328.54															
b	322.46															
12	 <p>Resveratrol</p>	<table border="0"> <tr> <td>a</td> <td>327.08</td> </tr> <tr> <td>b</td> <td>349.94</td> </tr> <tr> <td>c</td> <td>350.30</td> </tr> </table>	a	327.08	b	349.94	c	350.30								
a	327.08															
b	349.94															
c	350.30															
13	 <p>Rosmarinic acid</p>	<table border="0"> <tr> <td>a</td> <td>295.67</td> </tr> <tr> <td>b</td> <td>301.95</td> </tr> <tr> <td>c</td> <td>331.56</td> </tr> <tr> <td>d</td> <td>342.67</td> </tr> <tr> <td>e</td> <td>402.06</td> </tr> </table>	a	295.67	b	301.95	c	331.56	d	342.67	e	402.06				
a	295.67															
b	301.95															
c	331.56															
d	342.67															
e	402.06															
14	 <p>lipid-soluble EGCG</p>	<table border="0"> <tr> <td>a</td> <td>353.78</td> </tr> <tr> <td>b</td> <td>327.34</td> </tr> <tr> <td>c</td> <td>329.69</td> </tr> <tr> <td>d</td> <td>321.54</td> </tr> <tr> <td>e</td> <td>304.29</td> </tr> <tr> <td>f</td> <td>261.51</td> </tr> <tr> <td>g</td> <td>329.86</td> </tr> </table>	a	353.78	b	327.34	c	329.69	d	321.54	e	304.29	f	261.51	g	329.86
a	353.78															
b	327.34															
c	329.69															
d	321.54															
e	304.29															
f	261.51															
g	329.86															
15	 <p>Astaxanthin</p>	<table border="0"> <tr> <td>a*2</td> <td>384.00</td> </tr> <tr> <td>b*2</td> <td>307.16</td> </tr> <tr> <td>c*2</td> <td>341.24</td> </tr> <tr> <td>d*2</td> <td>362.73</td> </tr> </table>	a*2	384.00	b*2	307.16	c*2	341.24	d*2	362.73						
a*2	384.00															
b*2	307.16															
c*2	341.24															
d*2	362.73															
16	 <p>Lawsone</p>	<table border="0"> <tr> <td>a</td> <td>355.32</td> </tr> </table>	a	355.32												
a	355.32															

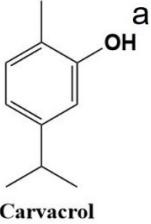
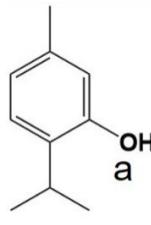
17	 Carvacrol	a	342.00
18	 Thymol	a	335.59

Table S2. Free energy of dissociation for hydrogen in NR.

Dissociation position ¹	a	b	c	d
$\Delta G^{298.15K}$ (kJ/mol)	347.42	437.21	357.91	354.29

¹the structure of NR at different dissociation position was seen in Fig. S1.

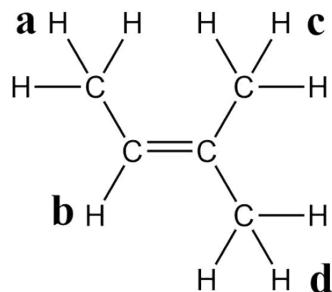


Figure S1. The dissociation positions of NR.

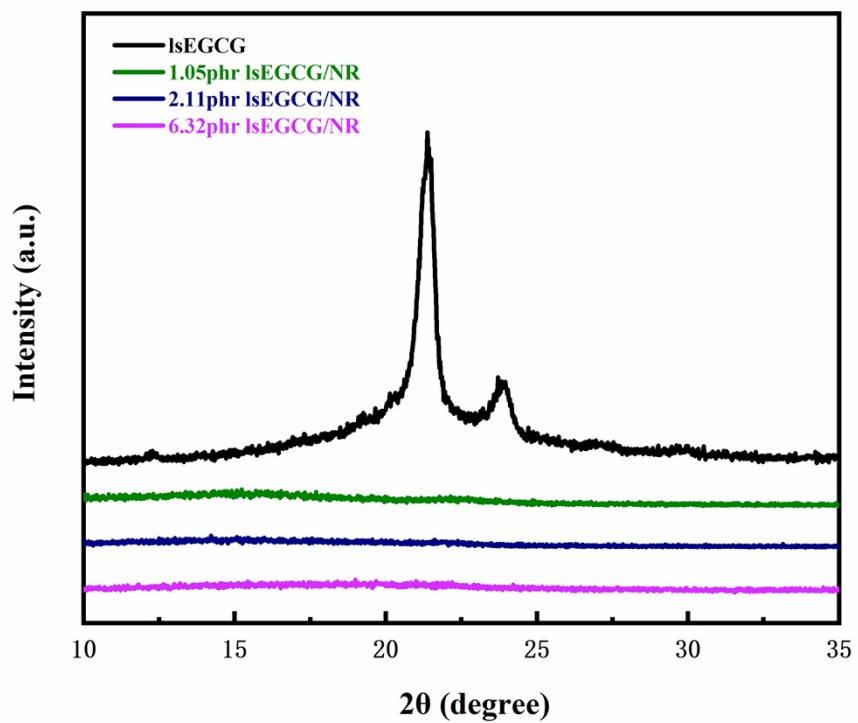


Figure S2. X-ray diffraction patterns of lsEGCG powder and lsEGCG/NR compounds with different contents.