

Table S1

S₁-S₀ Transition-Energies(TE) and the Oscillator-Strengths (OS) of bare *cis*- and *trans*-estrone. They were calculated by M05-2X/6-311++G** level of theory and a scaling factor of 0.8432 is multiplied. TEs are shown in cm⁻¹ unit.

	bare-estriol	
	TE	OS
<i>trans</i>	35157	0.0445
<i>cis</i>	35072	0.0513

Table S2

S₁-S₀ Transition-Energies (TE) and the Oscillator-Strengths (OS) of bare estriol, estriol-(*D*)-H₂O and estriol-(*A*)-H₂O. They were calculated by M05-2X/6-311++G** level of theory and a scaling factor of 0.8432 is multiplied. TEs are shown in cm⁻¹ unit.

	bare-estriol		Estriol-(<i>D</i>)-H ₂ O		Estriol-(<i>A</i>)-H ₂ O	
	TE	OS	TE	OS	TE	OS
3 <i>t</i> _16 <i>g</i> _-17 <i>g</i> +	35155	0.0447	35156	0.0447	34732	0.0504
3 <i>t</i> _16 <i>g</i> +_17 <i>g</i> -	35140	0.0451	35136	0.045	34722	0.0506
3 <i>t</i> _16 <i>g</i> _-17 <i>a</i>	35151	0.0447	35152	0.0447	34722	0.0503
3 <i>t</i> _16 <i>a</i> _17 <i>g</i> -	35146	0.0448	35140	0.0448	34718	0.0506
3 <i>t</i> _16 <i>g</i> +_17 <i>g</i> +	35145	0.0449	35158	0.0444	34726	0.0504
3 <i>t</i> _16 <i>g</i> +_17 <i>a</i>	35142	0.0449	-	-	34721	0.0505
3 <i>t</i> _16 <i>a</i> _17 <i>a</i>	35149	0.0446	-	-	34716	0.0507
3 <i>t</i> _16 <i>a</i> _17 <i>g</i> +	35154	0.0445	35164	0.0441	34728	0.0502
3 <i>c</i> _16 <i>g</i> _-17 <i>g</i> +	35066	0.0518	35069	0.0519	34664	0.0522
3 <i>c</i> _16 <i>g</i> +_17 <i>g</i> -	35051	0.0522	35047	0.0521	34657	0.0524
3 <i>c</i> _16 <i>g</i> _-17 <i>a</i>	35061	0.0518	35062	0.0518	34658	0.0521
3 <i>c</i> _16 <i>a</i> _17 <i>g</i> -	35059	0.0519	35054	0.0519	34652	0.0523
3 <i>c</i> _16 <i>g</i> +_17 <i>g</i> +	35057	0.0520	35072	0.0515	34659	0.0522
3 <i>c</i> 16 <i>g</i> +_17 <i>a</i>	35054	0.0519	-	-	34657	0.0523
3 <i>c</i> 16 <i>a</i> _17 <i>g</i> +	35067	0.0516	35082	0.0513	34651	0.0525
3 <i>c</i> _16 <i>a</i> _17 <i>a</i>	35061	0.0517	-	-	34662	0.0521