Estrogenic Effect Mechanism and Influencing Factors for Transformation Product Dimer Formed in Preservative Parabens Photolysis

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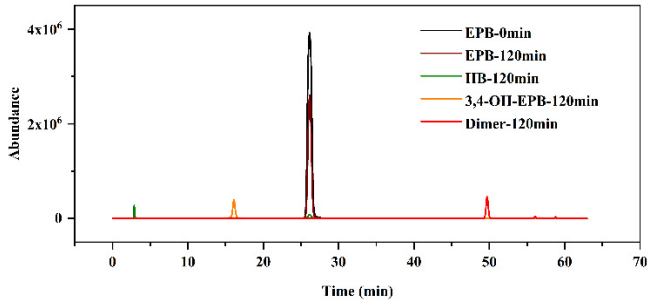

Figure S1. The extracted ion chromatograms (EICs) chromatograms of the 300 μM EPB photochemical degradation under 500W high-pressure mercury lamp irradiation.

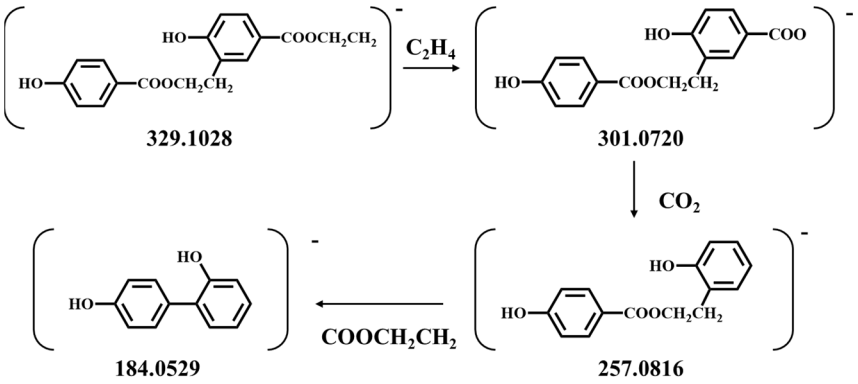

Figure S2. The MS/MS fragmentation scheme of product dimer.

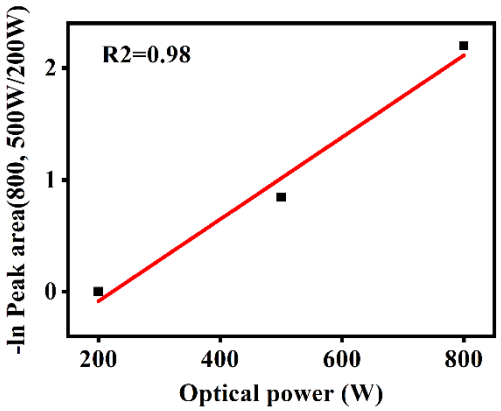

Figure S3. A plot of pseudo-first order rate constant vs. optical power.

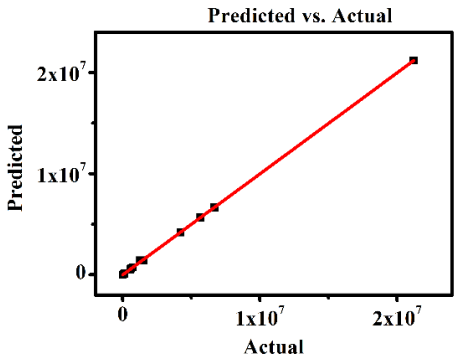

Figure S4. Predicted versus actual values plot for the formation of product dimer

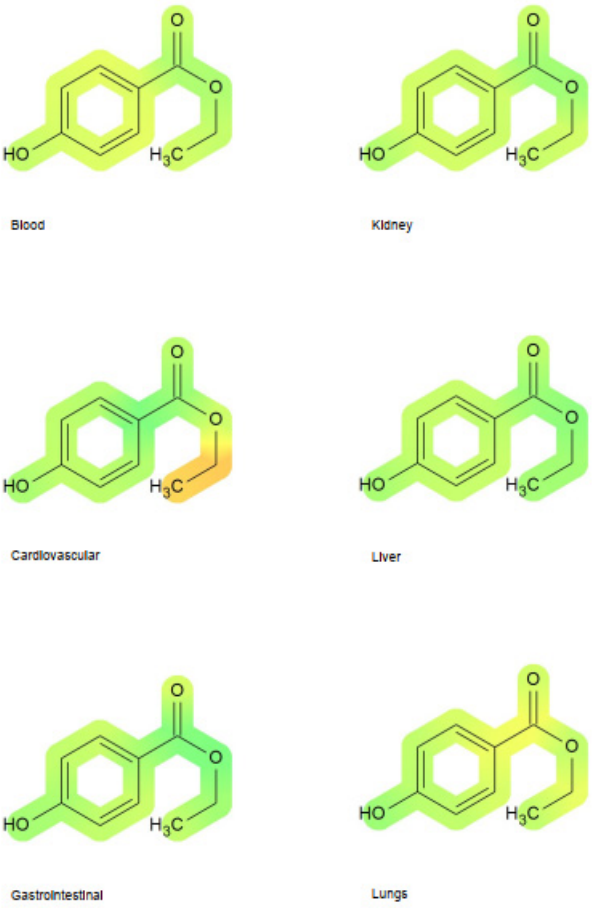

Figure S5. The atomic/functional group contributions to the calculated parameter values are highlighted on EPB

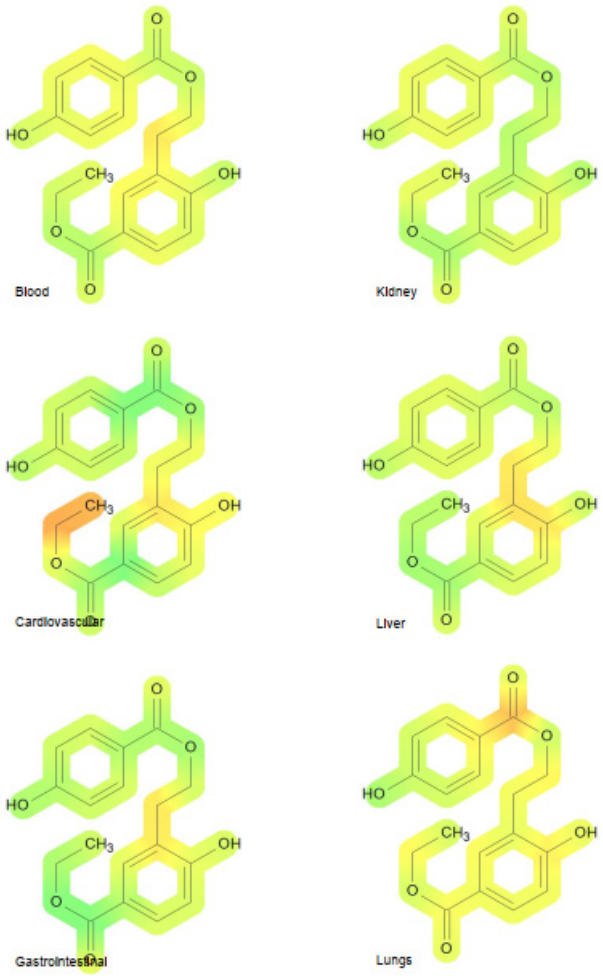

Figure S6. The atomic/functional group contributions to the calculated parameter values are highlighted on product dimer

Table S1. Experimental design matrix and values of response

Run number	Symbols			Response value	
	A	B	C	Actual values	Predicted values
1	0	0	1	131846	131800
2	0	-1	0	559681	559700
3	0	1	0	1427760	1428000
4	-1	-1	1	13020	13020
5	1	1	-1	21179027	21180000
6	1	-1	-1	5656710	5657000
7	1	-1	1	137301	137300
8	0	0	0	1272934	1273000
9	-1	1	-1	72145	72145
10	1	1	1	744156	744200
11	0	0	-1	6687576	6688000
12	-1	1	1	0	0
13	-1	0	0	0	0
14	0	0	0	1272934	1273000
15	0	0	0	1542319	1542000
16	0	0	0	1542319	1542000
17	-1	-1	-1	623926	623900
18	1	0	0	4210574	4211000

Table S2. The $[M-H]^-$, retention times and mass error of product dimer

Product	$[M-H]^-$	Retention times (min)	Mass Error (ppm)
Dimer	329.1028	49.50	0.9