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CORRECTION

Correction to: Molecular modeling as a design tool for sunscreen candidates: a case study of bemotrizinol

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Correction to: Journal of Molecular Modeling (2019) 25:362
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The original version of this article unfortunately contained mistakes. Table 1 was missing and the presentation of Table 2 was incorrect. In Table 2, the second [λexp (nm)] and last [MAD[a]] columns, many values are wrongly in the same cell/line. For example, in column 2, line 2, the first number (342) should be above the other (318). In the version published, these values are together (342318). This error repeats in column 2, lines 3-4 and last column, lines 2-4. The corrected tables are given below.

The original article has been corrected.

The online version of the original article can be found at https://doi.org/10.1007/s00894-019-4237-7

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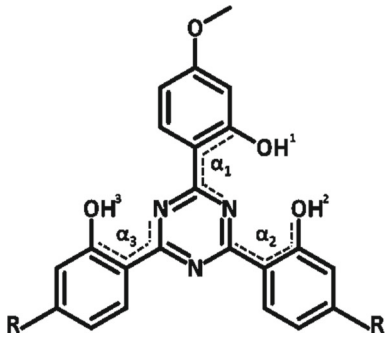
Table 1 Total energy (eV) and structural parameters[a] of the three lower energy geometries (conf 1–3) of each triazine derivatives (A–D) obtained by ground-stated optimization at DFT/B3LYP/6-31G(d)



Derivatives	Data	Conformers		
		conf1	conf2	conf3
A	eV	-49748.65	-49748.65	-49748.67
	α_1	0.74	-0.46	0.85
	α_2	-0.44	-0.91	-0.97
	α_3	-1.28	-1.09	-0.75
B	eV	-52865.47	-52865.34	-52865.32
	$OH^1\cdots N$	1.708	1.705	1.715
	α_1	-2.56	-2.6	-3.63
	α_2	-9.19	-10.65	-11.03
	α_3	-1.86	-0.56	-2.53
C	eV	-56959.44	-56959.41	-56959.41
	$OH^1\cdots N$	1.711	1.708	1.705
	$OH^2\cdots N$	1.707	1.705	1.711
	$OH^3\cdots N$	1.703	1.722	1.720
	α_1	-7.27	7.06	6.8
	α_2	-7.76	7.57	7.95
	α_3	-6.86	8.38	8.03
D (BEMT)	eV	-54912.45	-54912.36	-54912.41
	$OH^2\cdots N$	1.710	1.709	1.712
	$OH^3\cdots N$	1.704	1.704	1.700
	α_1	-10.73	18.46	10.34
	α_2	-2.84	3.33	2.65
	α_3	-7.19	1.9	6.87

[a]The H bond lengths are in Å and dihedral angles α between the benzene and triazine rings in ° (degrees).

Table 2 Transitions (eV/nm) and oscillator strength (f) calculated for the ten lowest states in gas phase, the experimental absorption maxima (λexp) in ethanol [17] and the mean absolute deviation (MAD)[a] between the experimental (λexp) and calculated (λcalc)[b] absorptions maxima for the UVA and UVB ranges of derivatives A-D

Derivative	λexp (nm)	conf1			conf2			conf3			MAD[a]
		eV	nm	f	eV	nm	f	eV	nm	f	
A	310	3.775	328	0.000	3.775	328	0.000	3.775	328	0.000	2.00
		3.964	313	0.003	3.957	313	0.008	3.962	313	0.017	
		3.981	311	0.041	3.986	311	0.020	3.983	311	0.003	
		4.017	**309**	**1.062**	4.017	309	0.924	**4.016**	**309**	**1.010**	
		4.044	307	0.816	**4.046**	**306**	**0.966**	4.044	307	0.881	
		4.151	299	0.001	4.151	299	0.001	4.150	299	0.003	
		4.216	294	0.000	4.212	294	0.001	4.214	294	0.001	
		4.219	294	0.000	4.218	294	0.000	4.217	294	0.000	
		4.227	293	0.005	4.233	293	0.004	4.228	293	0.004	
		4.302	288	0.025	4.298	288	0.010	4.300	288	0.017	
B	342	3.400	365	0.002	3.404	364	0.002	3.492	355	0.003	5.00
	318	**3.662**	**339**	**0.481**	**3.680**	**337**	**0.465**	**3.700**	**335**	**0.347**	12.67
		3.837	323	0.180	3.830	324	0.212	3.817	325	0.107	
		3.981	311	0.299	3.977	312	0.161	3.894	318	0.106	
		4.007	**309**	**0.465**	**4.000**	**310**	**0.698**	3.966	313	0.358	
		4.087	303	0.017	4.093	303	0.033	3.984	311	0.410	
		4.131	300	0.055	4.120	301	0.006	**4.042**	**307**	**0.630**	
		4.146	299	0.473	4.149	299	0.374	4.132	300	0.003	
		4.280	290	0.005	4.294	289	0.006	4.258	291	0.012	
		4.295	289	0.003	4.309	288	0.027	4.279	290	0.004	
C	362	3.426	362	0.002	3.433	361	0.006	3.430	361	0.007	17.33
	305	3.474	357	0.124	3.478	356	0.109	3.480	356	0.113	4.00
		3.485	356	0.215	3.521	352	0.319	3.519	352	0.352	
		3.580	346	0.442	**3.592**	**345**	**0.418**	**3.600**	**344**	**0.417**	
		3.590	**345**	**0.463**	3.608	344	0.281	3.602	344	0.245	
		3.766	329	0.001	3.733	332	0.037	3.733	332	0.038	
		4.084	304	0.041	3.894	318	0.008	3.895	318	0.004	
		4.090	**303**	**0.378**	**3.971**	**312**	**0.471**	**3.969**	**312**	**0.501**	
		4.108	302	0.356	4.094	303	0.189	4.088	303	0.004	
		4.124	301	0.055	4.101	302	0.220	4.095	303	0.367	
D (BEMT)	343	3.167	391	0.152	3.373	368	0.012	3.384	366	0.030	9.67
	310	3.405	364	0.033	3.387	366	0.001	3.467	358	0.019	3.00
		3.416	**363**	**0.391**	**3.558**	**348**	**0.811**	**3.574**	**347**	**0.615**	
		3.536	351	0.056	3.719	333	0.146	3.724	333	0.337	
		3.725	333	0.339	3.986	311	0.082	3.964	313	0.068	
		3.812	325	0.007	4.014	309	0.092	**4.028**	**308**	**0.313**	
		3.977	**312**	**0.496**	4.085	304	0.228	4.069	305	0.237	
		4.024	308	0.000	**4.118**	**301**	**0.567**	4.109	302	0.138	
		4.099	302	0.193	4.138	300	0.099	4.159	298	0.250	
		4.340	286	0.025	4.298	288	0.004	4.243	292	0.010	

[a] $\sum |\lambda exp - \lambda calc|$

[b] The calculated absorption maxima (λcalc) at UVA and UVB ranges is in bold