Kinetics and mechanism of photooxygenation of 4'-diethylamino-3-hydroxyflavone

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Electronic Supporting Information (ESI)

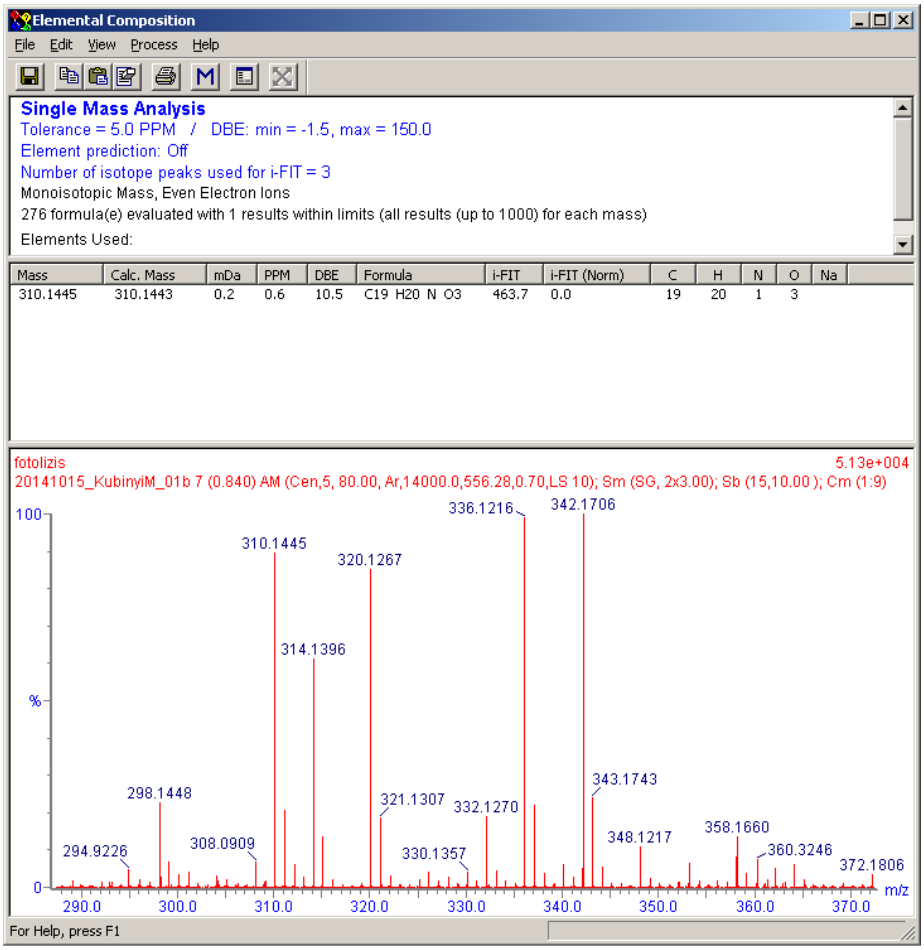

Fig. S1. High resolution positive electrospray mass spectrum of photolysis reaction mixture. 310.1445 - $[D+H]^+$, 332.1270 - $[D+Na]^+$, 314.1396 - $[P+H]^+$, 336.1216 - $[P+Na]^+$.

Table S1. Stability constants of alkaline earth metal complexes of 4'-diethylamino-3-hydroxyflavone (D).

Complex	K_S /M^{-1}/
MgD^{2+}	110
CaD^{2+}	17
SrD^{2+}	5,6
BaD^{2+}	11

Table S2. Theoretically calulated Gibbs free energies /Hartree/.

Species	S_0	S_1	T_1
D	-1015.237726	-1015.13004	
T	-1015.217948	-1015.13637	-1015.175567
T-O_2	-1165.511091	-1165.505880	
TS1	-1165.429035		
TS2	-1165.480667	-1165.501203	
P	-1052.382106	-1052.241846	
O_2			-150.279963
CO	-113.291676		
TS(rearr.)	-1015.050586		

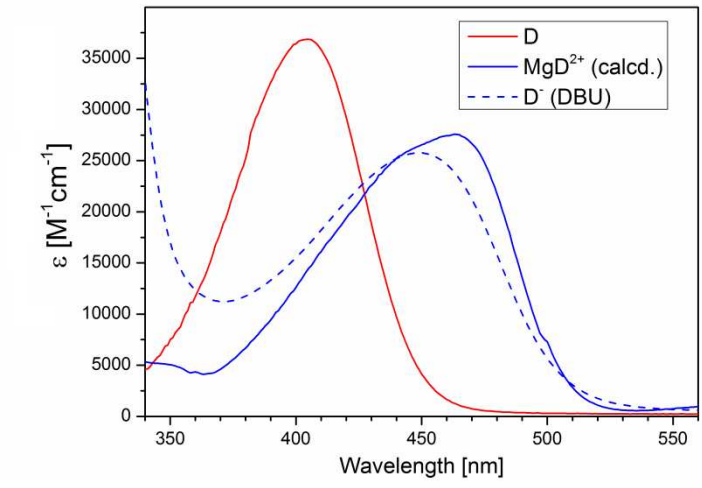

Fig. S2. Absorption spectra of the neutral 4'-diethylamino-3-hydroxyflavone (D), its anionic form (D^-) and Mg complex (MgD^{2+}) in acetonitrile solution. The spectrum of D^- measured in presence of 3M DBU. The spectrum MgD^{2+} was calculated by least square fitting from the spectra in Fig. 1a in the paper.