

Unraveling the similarity of the photoabsorption of the deprotonated *p*-coumaric acid in the gas phase and within the photoactive yellow protein

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Supplementary Information

Geometries

The geometries of the pCTM⁺ chromophores used in the present study in XYZ format (Å):

Vacuum	X	Y	Z
C	-5.251210	0.014316	-0.000229
S	-3.735636	-0.985874	-0.000351
H	-5.843343	-0.193824	-0.889577
H	-4.930079	1.056791	-0.000927
H	-5.842898	-0.192755	0.889677
C	-2.455605	0.376041	0.000112
O	-2.812578	1.542479	0.000105
C	-1.134811	-0.160209	0.000480
C	-0.028400	0.658002	0.000343
C	1.341268	0.318789	0.000421
C	2.325289	1.348575	0.000051
C	3.664922	1.089879	-0.000283
C	4.188431	-0.264418	-0.000413
C	3.166302	-1.302048	0.000281
C	1.833482	-1.019420	0.000616
O	5.408746	-0.523277	-0.000586
H	-1.041910	-1.237788	0.000536
H	-0.247144	1.722362	0.000209
H	1.977394	2.377640	0.000093
H	4.390853	1.894238	-0.000510
H	3.519114	-2.326724	0.000536
H	1.120842	-1.836616	0.001155

In-protein	X	Y	Z
C	9.847	4.760	-19.710
S	10.643	3.689	-18.507
H	8.892	5.058	-19.275
H	9.611	4.176	-20.594
H	10.427	5.676	-19.821
C	11.841	2.820	-19.484
O	11.989	3.050	-20.704
C	12.652	1.939	-18.722
C	13.516	1.1020	-19.305
C	14.579	0.3930	-18.673
C	15.427	-0.4280	-19.430
C	16.5110	-1.046	-18.8780
C	16.789	-0.8980	-17.5250
C	15.950	-0.07900	-16.755
C	14.8820	0.53400	-17.3320
O	17.7970	-1.5080	-16.9420
H	12.6080	2.0210	-17.649
H	13.4420	1.020	-20.3800
H	15.2450	-0.5490	-20.4870
H	17.1490	-1.6610	-19.4940
H	16.1560	0.07000	-15.7060
H	14.2930	1.17800	-16.7