Electronic Supplementary Information for:

Photoprotective Properties of Eumelanin: Computational Insights into the Photophysics of a Catechol:Quinone Heterodimer Model System

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Cartesian coordinates associated with

a) Ground state optimized parent C:Q heterodimer

Atom	X	Y	Z
C	-2.302152	-1.463135	-0.029785
C	-2.361266	-0.084422	-0.162334
C	-1.522786	0.724499	0.613029
C	-0.647346	0.153228	1.527472
C	-0.583542	-1.23156	1.65119
C	-1.406419	-2.033542	0.870464
H	-2.953534	-2.075146	-0.642513
H	-0.019095	0.798969	2.131866
H	0.106323	-1.676185	2.358302
H	-1.364401	-3.112318	0.96855
C	0.686213	0.147927	-1.602996
C	0.987913	-1.156665	-1.667019
C	2.007228	-1.770904	-0.816293
C	2.698115	-1.073597	0.095141
C	2.436875	0.362091	0.288016
C	1.350437	1.013593	-0.62145
H	-0.074245	0.599282	-2.229371
H	0.465463	-1.796389	-2.369453
H	2.193945	-2.831776	-0.943697
H	3.453818	-1.524766	0.727298
O	1.078384	2.185563	-0.474726
O	3.007171	1.035372	1.108938
O	-3.199122	0.481608	-1.061512
O	-1.638659	2.072017	0.408046
H	-3.08764	1.437259	-0.991602
H	-0.76245	2.459515	0.272031

b) The optimized geometry of the biradical tautomer

Atom	X	Y	Z
C	-4.061963	-0.239459	-0.719075
C	-3.251965	0.587891	0.047399
C	-1.92416	0.160192	0.481477
C	-1.484484	-1.15174	0.094089
C	-2.301592	-1.941794	-0.658313
C	-3.586164	-1.490052	-1.066422
H	-5.041041	0.104762	-1.02756
H	-0.505728	-1.481184	0.422484
H	-1.974981	-2.931991	-0.952698
H	-4.207918	-2.146457	-1.663976
C	1.671963	1.152915	-0.392762
C	2.507015	1.340431	-1.484185
C	3.696955	0.592046	-1.632533
C	4.042826	-0.338402	-0.695764
C	3.214763	-0.596143	0.465405
C	1.994635	0.213812	0.584166
H	0.767169	1.741239	-0.28504
H	2.243167	2.078844	-2.232832
H	4.331186	0.764984	-2.494549
H	4.947775	-0.929169	-0.779117
O	1.243836	-0.01729	1.652137
O	3.503279	-1.454447	1.309991
O	-3.634968	1.79716	0.419083
O	-1.257634	0.977407	1.160824
H	-2.902376	2.164549	0.944584
H	0.399674	0.47359	1.591535

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(Harmonic) normal mode wavenumbers (in cm^{-1}) of the C:Q heterodimer and the C monomer at the respective minimum energy geometries. The O–H stretch normal modes are indicated in red, and labelled to indicate the free, intra- or inter-chromophore nature of the motion.

C:Q Heterodimer		C Monomer	
mode	cm^{-1}	mode	cm^{-1}
1	21.56	1	156.38
2	39.34	2	193.02
3	58.08	3	298.87
4	69.28	4	299.74
5	80.52	5	417.28
6	107.96	6	455.93
7	143.41	7	462.16
8	213.41	8	566.25
9	236.81	9	576.72
10	312.72	10	595.6
11	325.01	11	719.89
12	356.65	12	762.13
13	400.07	13	794.08
14	411.99	14	858.73
15	443.04	15	870.03
16	459.01	16	944.06
17	468.99	17	988.81
18	480.1	18	1064.26
19	545.2	19	1121.17
20	553.23	20	1175.38
21	565.57	21	1185.21
22	576.77	22	1213.3
23	581.16	23	1288.59
24	593.04	24	1320.12
25	686.04	25	1365.94
26	741.95	26	1399.32
27	743.07	27	1520.89
28	777.21	28	1567.91
29	785.95	29	1686.25
30	799.73	30	1688.99
31	875.57	31	3176.18
32	882.29	32	3198.5
33	886.46	33	3212.46
34	891.27	34	3222.21
35	965.52	35(intra)	3867.87
36	969.57	36(free)	3935.24
37	999.82		
38	1022.14		
39	1030.95		

40	1061.55
41	1126.18
42	1142.47
43	1171.99
44	1183.36
45	1198.06
46	1212.47
47	1245.78
48	1292.68
49	1303.89
50	1318.43
51	1363.7
52	1396.76
53	1407.5
54	1445.32
55	1516.82
56	1562.23
57	1661.83
58	1672.14
59	1684.63
60	1714.53
61	1784.97
62	1817.49
63	3190.97
64	3191.53
65	3198.41
66	3202.35
67	3211.31
68	3217.42
69	3219.51
70	3221.96
71	3755.75(inter)
72	3821.59(intra)