Role of hydroxy substitution on the conformation and excited state dynamics of Chalcone
Supplementary Information

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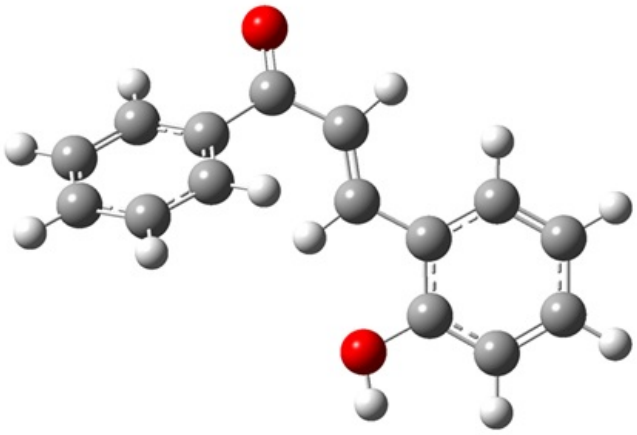

Figure 1 (a) Optimized structure of s-*trans* 2-hydroxychalcone at CAM-B3LYP/6-311++G** level of theory in acetonitrile with CPCM model. The relative energy with respect to the most stable conformer (C_1) is 1.2 kcal mol^{-1}, with a Boltzmann population of 10%.

Table 1 Optimized Cartesian coordinates of unsubstituted Chalcone (s-*cis* conformer) at the CAM-B3LYP/6-311++G** level of theory in gas phase (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-5.201216	0.788595	-0.070438
C	-4.990573	-0.559241	0.179156
C	-3.698625	-1.062471	0.217473
C	-2.595367	-0.231335	0.010525
C	-2.824843	1.125231	-0.242653
C	-4.112784	1.628688	-0.282402
C	-1.256372	-0.820097	0.065801
C	-0.082845	-0.192185	-0.048479
C	1.181156	-0.965021	0.012964
O	1.176930	-2.180853	0.048163
C	2.483023	-0.222533	0.012437
C	2.586548	1.133641	0.317775
C	3.825871	1.758822	0.327287
C	4.970234	1.037479	0.019373
C	4.875849	-0.315577	-0.286278
C	3.641600	-0.941848	-0.282149
H	3.896916	2.810635	0.576633
H	1.706829	1.709506	0.573707
H	3.547673	-1.997174	-0.503876
H	5.768415	-0.881349	-0.524843
H	5.936546	1.527814	0.020461
H	-0.028476	0.876445	-0.204672
H	-1.214274	-1.895276	0.218911
H	-5.832487	-1.220811	0.343423
H	-4.272741	2.681631	-0.481244
H	-6.208485	1.186092	-0.102527
H	-3.535355	-2.116564	0.411481
H	-1.989941	1.792979	-0.415110

Table 2 Optimized Cartesian coordinates of unsubstituted Chalcone (s-*cis* conformer) at the CAM-B3LYP/6-311++G** level of theory in hexane with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	5.194860	0.795689	0.082159
C	4.990772	-0.554420	-0.163381
C	3.700496	-1.062187	-0.209593
C	2.593214	-0.232842	-0.013774
C	2.815467	1.126308	0.234790
C	4.101978	1.633829	0.281908
C	1.256805	-0.826441	-0.075768
C	0.080993	-0.202336	0.044921
C	-1.181916	-0.972348	-0.023827
O	-1.181396	-2.190346	-0.071068
C	-2.480822	-0.227121	-0.015143
C	-2.579576	1.127121	-0.333017
C	-3.815943	1.758563	-0.337043
C	-4.961462	1.046624	-0.009855
C	-4.871583	-0.303845	0.309895
C	-3.640500	-0.937046	0.299346
H	-3.883560	2.808030	-0.596621
H	-1.699584	1.696101	-0.602619
H	-3.553916	-1.990053	0.534350
H	-5.764410	-0.861836	0.564869
H	-5.924974	1.542279	-0.006175
H	0.024534	0.864325	0.211936
H	1.222540	-1.900099	-0.240001
H	5.836061	-1.213793	-0.318577
H	4.257126	2.688244	0.476343
H	6.200531	1.196673	0.119901
H	3.542438	-2.117569	-0.400595
H	1.977685	1.793176	0.396022

Table 3 Optimized Cartesian coordinates of unsubstituted Chalcone (s-*cis* conformer) at the CAM-B3LYP/6-311++G** level of theory in acetonitrile with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	5.185399	0.805646	0.096317
C	4.990001	-0.545946	-0.151541
C	3.702265	-1.060186	-0.206506
C	2.589981	-0.235065	-0.016396
C	2.802757	1.125974	0.234012
C	4.087085	1.639228	0.289361
C	1.257325	-0.835002	-0.086703
C	0.078097	-0.216218	0.041407
C	-1.182975	-0.982178	-0.036731
O	-1.187534	-2.203577	-0.098280
C	-2.477500	-0.233528	-0.019152
C	-2.570395	1.116168	-0.360578
C	-3.802559	1.756125	-0.358581
C	-4.948572	1.059185	-0.000104
C	-4.864244	-0.285787	0.345392
C	-3.637855	-0.928659	0.327476
H	-3.866056	2.800899	-0.636841
H	-1.690673	1.674124	-0.652840
H	-3.560109	-1.976725	0.586410
H	-5.756829	-0.831042	0.627043
H	-5.908026	1.562377	0.009266
H	0.018602	0.848018	0.220786
H	1.233346	-1.906567	-0.264954
H	5.839610	-1.200756	-0.302013
H	4.236011	2.694345	0.484311
H	6.188802	1.211581	0.140406
H	3.551200	-2.116179	-0.399701
H	1.961517	1.790012	0.388315

Table 4 Optimized Cartesian coordinates of unsubstituted Chalcone (s-*trans* conformer) at the CAM-B3LYP/6-311++G** level of theory in gas phase (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	4.930672	-0.622925	-0.092091
C	4.018864	-1.571857	-0.548078
C	2.657506	-1.285968	-0.541041
C	2.182537	-0.048265	-0.084556
C	3.111422	0.897273	0.375444
C	4.470461	0.610999	0.370658
C	0.743963	0.195047	-0.104842
C	0.124241	1.356394	0.186818
C	-1.326328	1.575491	0.045985
O	-1.760877	2.713755	-0.108802
C	-2.258026	0.409352	0.064401
C	-2.074308	-0.680630	0.922137
C	-3.007424	-1.714473	0.945827
C	-4.114614	-1.677009	0.100773
C	-4.301058	-0.590216	-0.753981
C	-3.384954	0.455298	-0.762035
H	-2.871181	-2.546114	1.623318
H	-1.223203	-0.702782	1.588676
H	-3.525269	1.317104	-1.399773
H	-5.162605	-0.557226	-1.406464
H	-4.832366	-2.485647	0.113396
H	0.684999	2.248627	0.434997
H	0.131500	-0.645346	-0.413080
H	4.366610	-2.530774	-0.906677
H	5.174210	1.349233	0.729802
H	5.989590	-0.840958	-0.094199
H	1.946960	-2.022480	-0.895009
H	2.770054	1.855259	0.742914

Table 5 Optimized Cartesian coordinates of unsubstituted Chalcone (s-*trans* conformer) at the CAM-B3LYP/6-311++G** level of theory in hexane with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	4.955289	-0.619329	-0.086292
C	4.047898	-1.580068	-0.508544
C	2.689757	-1.296720	-0.508243
C	2.214398	-0.051893	-0.088978
C	3.141168	0.906742	0.334153
C	4.496177	0.624724	0.335210
C	0.767512	0.187513	-0.109714
C	0.137219	1.323459	0.205464
C	-1.315378	1.547522	0.064180
O	-1.731525	2.685137	-0.072398
C	-2.276085	0.399233	0.065618
C	-2.119964	-0.703522	0.903752
C	-3.073990	-1.712337	0.915486
C	-4.178702	-1.635098	0.078604
C	-4.340183	-0.536858	-0.758720
C	-3.400830	0.481246	-0.754854
H	-2.954727	-2.558241	1.581622
H	-1.267315	-0.763060	1.568078
H	-3.525554	1.352020	-1.386195
H	-5.203893	-0.472459	-1.409404
H	-4.918036	-2.427168	0.082591
H	0.682545	2.216601	0.489539
H	0.173163	-0.658502	-0.440237
H	4.396439	-2.551180	-0.838525
H	5.200872	1.377993	0.666248
H	6.016754	-0.835715	-0.084414
H	1.982788	-2.049474	-0.838896
H	2.803447	1.880409	0.666024

Table 6 Optimized Cartesian coordinates of unsubstituted Chalcone (s-*trans* conformer) at the CAM-B3LYP/6-311++G** level of theory in acetonitrile with CPCM model (Charge = 0, Multiplicity = 1)

Atom	x (Å)	y (Å)	z (Å)
C	-5.195072	0.796111	-0.085917
C	-4.993097	-0.564754	0.100156
C	-3.702235	-1.072466	0.149791
C	-2.593181	-0.231541	0.014845
C	-2.811950	1.138959	-0.173685
C	-4.099916	1.645185	-0.222818
C	-1.258932	-0.830579	0.076648
C	-0.079817	-0.205454	-0.020990
C	1.181370	-0.973186	0.043807
O	1.184698	-2.194316	0.103416
C	2.480029	-0.228428	0.017684
C	2.574899	1.137214	0.290325
C	3.811566	1.769400	0.281946
C	4.961290	1.049060	-0.013040
C	4.875269	-0.311482	-0.291540
C	3.644178	-0.945484	-0.269118
H	3.875123	2.827711	0.505760
H	1.692783	1.717004	0.528264
H	3.567912	-2.005132	-0.477773
H	5.770374	-0.876045	-0.525027
H	5.924476	1.545996	-0.025877
H	-0.021123	0.864234	-0.164246
H	-1.241173	-1.907777	0.218522
H	-5.840178	-1.232251	0.206541
H	-4.254031	2.707983	-0.368997
H	-6.201180	1.197176	-0.125284
H	-3.543608	-2.135443	0.295160
H	-1.973349	1.815744	-0.282923

Table 7 Vertical excitation energies, dominant orbital contributions, and oscillator strengths of the 10 lowest electronic states of unsubstituted chalcone (s-*cis* conformer) computed at the TD-CAM-B3LYP/6-311++G(d,p) in gas phase.

State	Transition orbital (% contribution)	Energy/eV	Oscillator strength
T_1	HOMO $\rightarrow$ LUMO (77)	2.42	0.000
T_2	HOMO-4 $\rightarrow$ LUMO (34)	3.13	0.000
	HOMO-1 $\rightarrow$ LUMO (41)		
T_3	HOMO-4 $\rightarrow$ LUMO (37)	3.33	0.000
S_1	HOMO-4 $\rightarrow$ LUMO (62)	3.62	0.000
T_4	HOMO-5 $\rightarrow$ LUMO (25)	3.84	0.000
	HOMO-3 $\rightarrow$ LUMO+4 (32)		
T_5	HOMO-2 $\rightarrow$ LUMO (45)	4.24	0.000
T_6	HOMO-3 $\rightarrow$ LUMO (60)	4.27	0.000
S_2	HOMO $\rightarrow$ LUMO (93)	4.31	0.81
T_7	HOMO-2 $\rightarrow$ LUMO+5 (27)	4.45	0.000
T_8	HOMO-3 $\rightarrow$ LUMO+4 (39)	4.67	0.000

Table 8 Vertical excitation energies, dominant orbital contributions, and oscillator strengths of the 10 lowest electronic states of unsubstituted chalcone (s-*cis* conformer) computed at the TD-CAM-B3LYP/6-311++G(d,p) in hexane.

State	Transition orbital (% contribution)	Energy/eV	Oscillator strength
T_1	HOMO → LUMO (77)	2.34	0.000
T_2	HOMO-4 → LUMO (39)	3.16	0.000
	HOMO-1 → LUMO (41)		
T_3	HOMO-4 → LUMO (44)	3.32	0.000
S_1	HOMO-4 → LUMO (69)	3.65	0.000
T_4	HOMO-5 → LUMO (25)	3.84	0.000
	HOMO-3 → LUMO+4 (26)		
S_2	HOMO → LUMO (93)	4.15	0.92
T_5	HOMO-2 → LUMO (36)	4.20	0.000
T_6	HOMO-3 → LUMO (50)	4.23	0.000
T_7	HOMO-2 → LUMO+5 (35)	4.45	0.000
T_8	HOMO-3 → LUMO+4 (34)	4.67	0.000

Table 9 Vertical excitation energies, dominant orbital contributions, and oscillator strengths of the 10 lowest electronic states of unsubstituted chalcone (s-*cis* conformer) computed at the TD-CAM-B3LYP/6-311++G(d,p) in acetonitrile.

State	Transition orbital (% contribution)	Energy/eV	Oscillator strength
T_1	HOMO → LUMO (76)	2.38	0.000
T_2	HOMO-4 → LUMO (20)	3.20	0.000
	HOMO-1 → LUMO (38)		
T_3	HOMO-4 → LUMO (59)	3.36	0.000
S_1	HOMO-4 → LUMO (75)	3.72	0.000
T_4	HOMO-5 → LUMO (25)	3.83	0.000
	HOMO-3 → LUMO+4 (26)		
S_2	HOMO → LUMO (93)	4.09	0.92
T_5	HOMO-3 → LUMO (46)	4.15	0.000
T_6	HOMO-2 → LUMO (65)	4.17	0.000
T_7	HOMO-3 → LUMO+3 (33)	4.45	0.000
T_8	HOMO-2 → LUMO+4 (24)	4.66	0.000

Table 10 Tentative assignment of Raman modes of unsubstituted chalcone (s-*cis* conformer) in acetonitrile.

Experiment (cm^{-1})	Computed (cm^{-1})	Tentative Assignments
1665	1664	C=O stretch
1608	1605	C=C stretch
1596	1597	C=C stretch
1575	1574	C=C stretch
1493	1478	CCH + CCC bend
1331	1315	C-C stretch + CCH bend
1205	1208	C-C stretch + CCH bend
1178	1191	C-C stretch
1158	1162	C-C + C-C-H bend
997	987	phenyl ring breathing

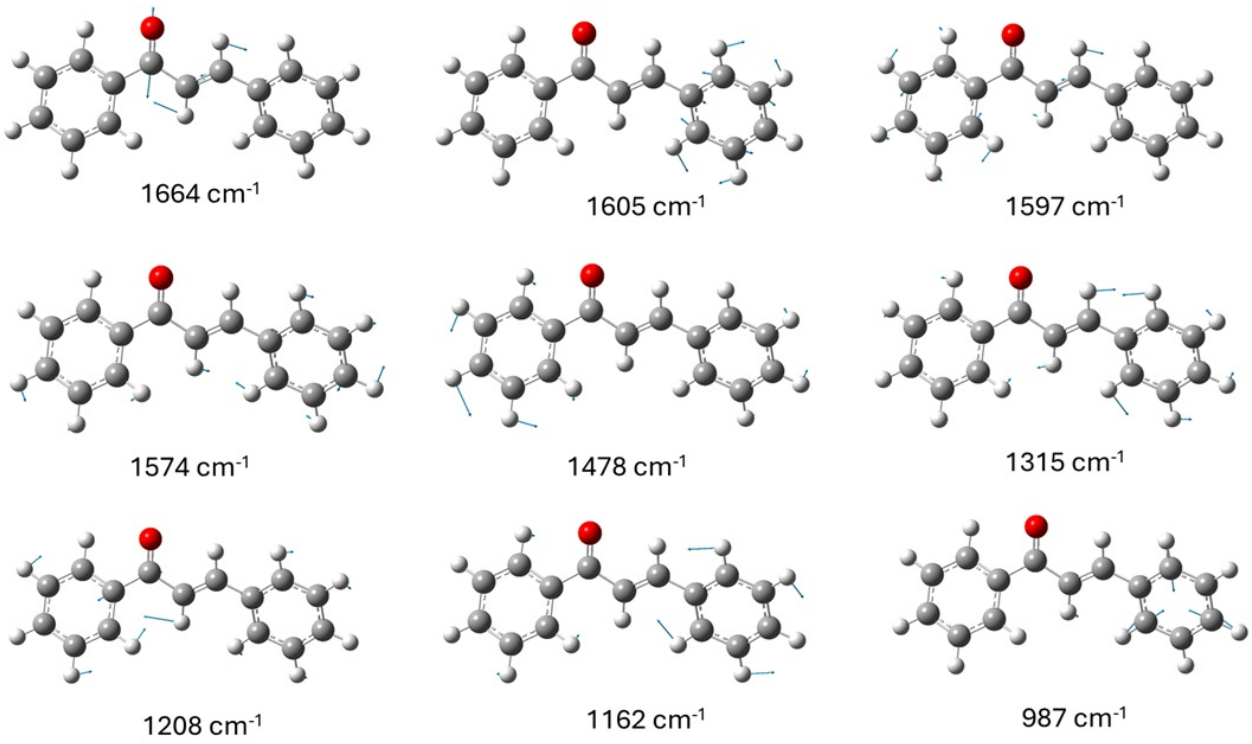

Figure 2 Vector diagram of the computed Raman mode for unsubstituted chalcone in acetonitrile.

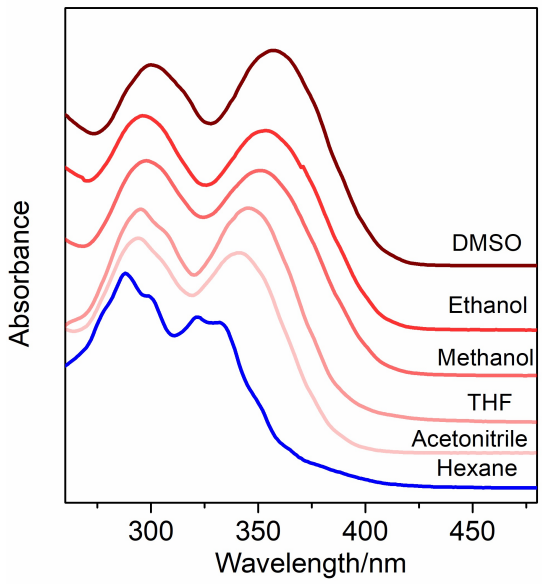

Figure 3 Solvent-dependent UV–Vis spectra of 2HyC presented as a stacked plot.

Table 11 Optimized Cartesian coordinates of 2-hydroxychalcone Chalcone (C_1 conformer) at the CAM-B3LYP/6-311++G** level of theory in gas phase (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-3.978351	1.697433	0.298964
C	-2.739179	1.071759	0.281641
C	-2.641898	-0.292674	0.012956
C	-3.806777	-1.018547	-0.238115
C	-5.041159	-0.392627	-0.232611
C	-5.129297	0.968544	0.037029
H	-4.043895	2.756408	0.518031
H	-1.853617	1.654436	0.497836
H	-3.716613	-2.079329	-0.433841
H	-5.938533	-0.964630	-0.436011
H	-6.095486	1.459214	0.045188
C	-1.339409	-1.036492	0.004230
C	-0.076530	-0.260414	-0.038230
H	-0.114127	0.808425	-0.161346
C	1.090359	-0.908691	0.056844
H	1.019955	-1.987655	0.170161
C	2.454421	-0.391522	0.029344
C	3.501400	-1.313750	0.150202
C	2.806565	0.961225	-0.109619
C	4.831467	-0.934706	0.135145
C	4.140319	1.349612	-0.125173
C	5.150013	0.408944	-0.003854
H	5.612063	-1.678301	0.230740
H	4.385529	2.401664	-0.233573
H	6.184485	0.729802	-0.018376
O	-1.340028	-2.253555	0.020305
H	3.243990	-2.361125	0.258160
O	1.813601	1.884912	-0.228073
H	2.195995	2.761674	-0.327343

Table 12 Optimized Cartesian coordinates of 2-hydroxychalcone Chalcone (C_1 conformer) at the CAM-B3LYP/6-311++G** level of theory in hexane with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-3.971003	1.691348	0.338236
C	-2.734380	1.060277	0.322114
C	-2.639634	-0.297147	0.016703
C	-3.804064	-1.009704	-0.273877
C	-5.035704	-0.377512	-0.271087
C	-5.121419	0.976052	0.036712
H	-4.034836	2.743746	0.586940
H	-1.849993	1.632331	0.569087
H	-3.720062	-2.064696	-0.500710
H	-5.932108	-0.938444	-0.506561
H	-6.085160	1.471352	0.043241
C	-1.339525	-1.042747	0.011314
C	-0.078608	-0.268134	-0.035995
H	-0.120537	0.799638	-0.167107
C	1.091815	-0.911825	0.064336
H	1.028377	-1.989898	0.188147
C	2.453751	-0.391251	0.031916
C	3.502857	-1.310845	0.164321
C	2.801056	0.961811	-0.122877
C	4.831512	-0.927575	0.146070
C	4.134282	1.353994	-0.141880
C	5.145503	0.416512	-0.008453
H	5.614614	-1.667278	0.250895
H	4.376214	2.404850	-0.263140
H	6.179090	0.740118	-0.025845
O	-1.342997	-2.262341	0.032325
H	3.248696	-2.357737	0.284129
O	1.805116	1.878312	-0.253150
H	2.180123	2.758734	-0.357807

Table 13 Optimized Cartesian coordinates of 2-hydroxychalcone Chalcone (C_1 conformer) at the CAM-B3LYP/6-311++G** level of theory in acetonitrile with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-3.960335	1.681218	0.392500
C	-2.727616	1.042300	0.377890
C	-2.635859	-0.303814	0.022275
C	-3.798775	-0.995812	-0.322116
C	-5.026076	-0.354280	-0.322785
C	-5.108975	0.986961	0.037226
H	-4.022230	2.723231	0.681366
H	-1.845311	1.597889	0.666467
H	-3.722050	-2.041054	-0.592404
H	-5.920487	-0.897712	-0.602253
H	-6.068972	1.489188	0.041363
C	-1.339387	-1.051787	0.020289
C	-0.081720	-0.279687	-0.034044
H	-0.129062	0.786869	-0.173981
C	1.094068	-0.916832	0.072343
H	1.039871	-1.993738	0.209183
C	2.452273	-0.391243	0.034098
C	3.505172	-1.306195	0.182802
C	2.792030	0.962404	-0.141357
C	4.831238	-0.916147	0.161859
C	4.124284	1.360549	-0.163517
C	5.137974	0.428690	-0.012927
H	5.618498	-1.649405	0.279791
H	4.361213	2.409935	-0.301175
H	6.170017	0.756942	-0.032819
O	-1.347175	-2.275374	0.047888
H	3.256003	-2.352456	0.318107
O	1.791744	1.867743	-0.288191
H	2.156171	2.753401	-0.398428

Table 14 Optimized Cartesian coordinates of 2-hydroxychalcone Chalcone (C_2 conformer) at the CAM-B3LYP/6-311++G** level of theory in gas phase (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-4.106454	1.651526	0.641618
C	-2.848419	1.081281	0.502782
C	-2.709302	-0.198749	-0.031152
C	-3.851154	-0.898379	-0.421920
C	-5.104539	-0.324601	-0.296586
C	-5.234551	0.952811	0.236707
H	-4.204810	2.642467	1.068187
H	-1.980832	1.635234	0.836896
H	-3.728870	-1.897093	-0.821139
H	-5.984232	-0.873156	-0.611188
H	-6.215667	1.401272	0.339190
C	-1.383652	-0.884001	-0.180183
C	-0.150087	-0.064139	-0.141412
H	-0.247002	1.013290	-0.141778
C	1.049332	-0.653417	-0.112037
H	1.066878	-1.737241	-0.077601
C	2.346285	0.021343	-0.109174
C	2.508544	1.358702	-0.480711
C	3.493757	-0.694168	0.262957
C	3.747770	1.973063	-0.474662
C	4.742802	-0.084010	0.271690
C	4.869031	1.245297	-0.094598
H	3.843366	3.009024	-0.773534
H	5.616209	-0.655666	0.568821
H	5.846804	1.711438	-0.087285
O	-1.340262	-2.088343	-0.343164
H	1.640064	1.920552	-0.801436
O	3.333514	-1.995629	0.623320
H	4.185910	-2.393701	0.819709

Table 15 Optimized Cartesian coordinates of 2-hydroxychalcone Chalcone (C_2 conformer) at the CAM-B3LYP/6-311++G** level of theory in hexane with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-4.116123	1.659922	0.591896
C	-2.856178	1.087118	0.482438
C	-2.710658	-0.205048	-0.021211
C	-3.847593	-0.912703	-0.413590
C	-5.102694	-0.336012	-0.318476
C	-5.239240	0.952651	0.186257
H	-4.219719	2.659875	0.995355
H	-1.993380	1.649010	0.815339
H	-3.724213	-1.918926	-0.792919
H	-5.977912	-0.890523	-0.634856
H	-6.221418	1.403388	0.265339
C	-1.382520	-0.889487	-0.134094
C	-0.155460	-0.063237	-0.121299
H	-0.261640	1.012268	-0.158356
C	1.048666	-0.644194	-0.073752
H	1.071600	-1.726408	-0.011620
C	2.344456	0.030383	-0.087626
C	2.496125	1.382673	-0.411052
C	3.502370	-0.699528	0.222244
C	3.735829	1.994947	-0.421858
C	4.752833	-0.090688	0.212907
C	4.868238	1.251430	-0.106417
H	3.823498	3.042258	-0.680955
H	5.633778	-0.674161	0.458926
H	5.846466	1.716664	-0.112869
O	-1.334171	-2.102170	-0.248164
H	1.619225	1.960200	-0.675663
O	3.354493	-2.013544	0.537688
H	4.212835	-2.417303	0.697894

Table 16 Optimized Cartesian coordinates of 2-hydroxychalcone Chalcone (C_2 conformer) at the CAM-B3LYP/6-311++G** level of theory in acetonitrile with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-4.131952	1.677342	0.490247
C	-2.868924	1.103314	0.434212
C	-2.711896	-0.212022	-0.003976
C	-3.839988	-0.939612	-0.388080
C	-5.097757	-0.361448	-0.347622
C	-5.245886	0.949323	0.094292
H	-4.244748	2.695013	0.843358
H	-2.014429	1.683480	0.756595
H	-3.712458	-1.961237	-0.722072
H	-5.965183	-0.930863	-0.658638
H	-6.229801	1.401453	0.130780
C	-1.380348	-0.892755	-0.052384
C	-0.162346	-0.060132	-0.086649
H	-0.280233	1.009207	-0.191095
C	1.048017	-0.628330	-0.005244
H	1.077137	-1.706039	0.107357
C	2.342365	0.043526	-0.048034
C	2.482613	1.416754	-0.284483
C	3.512062	-0.708893	0.148575
C	3.723148	2.024325	-0.323500
C	4.764319	-0.103279	0.109725
C	4.867874	1.256848	-0.124477
H	3.802756	3.087579	-0.509890
H	5.653542	-0.704386	0.264744
H	5.846824	1.719624	-0.153355
O	-1.325075	-2.114823	-0.078196
H	1.596716	2.017548	-0.446858
O	3.377565	-2.041369	0.379857
H	4.242146	-2.451616	0.490175

Table 17 Optimized Cartesian coordinates of 2-hydroxychalcone Chalcone (C_1 conformer) at the CAM-B3LYP/aug-cc-pvdz level of theory in acetonitrile with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-3.980129	1.731761	0.000037
C	-2.736497	1.104398	-0.000012
C	-2.646636	-0.292692	-0.000050
C	-3.828066	-1.046256	-0.000035
C	-5.068264	-0.421596	0.000015
C	-5.146925	0.971936	0.000051
H	-4.036342	2.819335	0.000065
H	-1.842873	1.722315	-0.000022
H	-3.753942	-2.131364	-0.000063
H	-5.978819	-1.019688	0.000025
H	-6.119073	1.464232	0.000090
C	-1.340703	-1.031385	-0.000106
C	-0.077086	-0.262786	-0.000057
H	-0.111561	0.817945	-0.000032
C	1.099322	-0.918076	-0.000045
H	1.038776	-2.008432	-0.000071
C	2.462943	-0.397249	-0.000004
C	2.811873	0.969305	0.000036
C	3.514681	-1.331434	-0.000003
C	4.150058	1.362453	0.000073
C	4.847427	-0.948154	0.000034
H	3.259497	-2.391031	-0.000033
C	5.162493	0.410686	0.000072
H	4.393024	2.425407	0.000103
H	5.635521	-1.698897	0.000033
H	6.202575	0.734894	0.000101
O	-1.343496	-2.260362	-0.000072
O	1.815213	1.894855	0.000036
H	2.192525	2.783873	0.000066

Table 18 Optimized Cartesian coordinates of 2-hydroxychalcone Chalcone (C_2 conformer) at the CAM-B3LYP/aug-cc-pvdz level of theory in acetonitrile with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-4.166171	1.749790	-0.000121
C	-2.889835	1.191975	-0.000242
C	-2.722930	-0.198068	-0.000070
C	-3.861124	-1.015602	0.000260
C	-5.133817	-0.460264	0.000419
C	-5.289219	0.926775	0.000221
H	-4.282205	2.832595	-0.000278
H	-2.032965	1.859796	-0.000462
H	-3.727153	-2.094968	0.000442
H	-6.010009	-1.107629	0.000707
H	-6.287004	1.364725	0.000325
C	-1.379606	-0.866056	-0.000227
C	-0.155909	-0.037147	-0.000217
H	-0.258076	1.043387	-0.000158
C	1.055432	-0.621126	-0.000216
H	1.075971	-1.709995	-0.000209
C	2.355958	0.045903	-0.000102
C	2.499385	1.443280	-0.000087
C	3.529631	-0.731979	0.000048
C	3.746264	2.048519	0.000063
C	4.789308	-0.130456	0.000210
C	4.895433	1.253812	0.000216
H	3.828491	3.133796	0.000068
H	5.683515	-0.754541	0.000341
H	5.881921	1.716158	0.000346
O	-1.316291	-2.093148	-0.000340
H	1.608720	2.068682	-0.000195
O	3.393673	-2.087072	0.000062
H	4.262943	-2.506377	0.000373

Table 19 Optimized Cartesian coordinates of 2-hydroxychalcone Chalcone (C_3 conformer) at the CAM-B3LYP/6-311++G** level of theory in acetonitrile with CPCM model (Charge = 0, Multiplicity = 1).

Atom	x (Å)	y (Å)	z (Å)
C	-4.071451	1.611605	0.772021
C	-2.820852	1.037231	0.588912
C	-2.700425	-0.198536	-0.047887
C	-3.851834	-0.845752	-0.501122
C	-5.097376	-0.265000	-0.332231
C	-5.209064	0.965350	0.307556
H	-4.156007	2.565571	1.277718
H	-1.947359	1.552158	0.966389
H	-3.752156	-1.805900	-0.990620
H	-5.983641	-0.769778	-0.696932
H	-6.183471	1.418903	0.444090
C	-1.384361	-0.879075	-0.240936
C	-0.148505	-0.071569	-0.156133
H	-0.236761	1.004439	-0.101156
C	1.049154	-0.667485	-0.149237
H	1.031748	-1.754482	-0.186809
C	2.350544	-0.004545	-0.120626
C	2.512070	1.312855	-0.573802
C	3.491485	-0.683843	0.336155
C	3.746021	1.932035	-0.581575
C	4.738077	-0.065164	0.324829
C	4.864633	1.233635	-0.130782
H	3.843154	2.946419	-0.946627
H	5.594552	-0.620111	0.686635
H	5.839767	1.705390	-0.135554
O	-1.344224	-2.078752	-0.473671
H	1.647653	1.844107	-0.952326
O	3.460983	-1.956371	0.816370
H	2.559751	-2.276179	0.922741

Table 20 Vertical excitation energies, dominant orbital contributions, and oscillator strengths of the 10 lowest electronic states of C_1 conformer) computed at the TD-CAM-B3LYP/6-311++G(d,p) in acetonitrile.

State	Transition orbital (% contribution)	Energy/eV	Oscillator strength
T_1	HOMO → LUMO (64)	2.4	0.000
T_2	HOMO-2 → LUMO (41)	3.21	0.000
T_3	HOMO-4 → LUMO (61)	3.36	0.000
S_1	HOMO-4 → LUMO (74)	3.73	0.004
T_4	HOMO-1 → LUMO (53)	3.78	0.000
T_5	HOMO-5 → LUMO (14)	3.84	0.000
S_2	HOMO → LUMO (92)	3.95	0.76
T_6	HOMO-3 → LUMO (48)	4.17	0.000
T_7	HOMO-3 → LUMO+2 (21)	4.42	0.000
T_8	HOMO-3 → LUMO+2 (20)	4.52	0.000

Table 21 Vertical excitation energies, dominant orbital contributions, and oscillator strengths of the 10 lowest electronic states of C_2 conformer) computed at the TD-CAM-B3LYP/6-311++G(d,p) in acetonitrile.

State	Transition orbital (% contribution)	Energy/eV	Oscillator strength
T_1	HOMO → LUMO (64)	2.4	0.000
T_2	HOMO-2 → LUMO (41)	3.21	0.000
T_3	HOMO-4 → LUMO (61)	3.36	0.000
S_1	HOMO-4 → LUMO (74)	3.73	0.004
T_4	HOMO-1 → LUMO (53)	3.78	0.000
T_5	HOMO-5 → LUMO (14)	3.84	0.000
S_2	HOMO → LUMO (92)	3.95	0.76
T_6	HOMO-3 → LUMO (48)	4.17	0.000
T_7	HOMO-3 → LUMO+2 (21)	4.42	0.000
T_8	HOMO-3 → LUMO+2 (20)	4.52	0.000

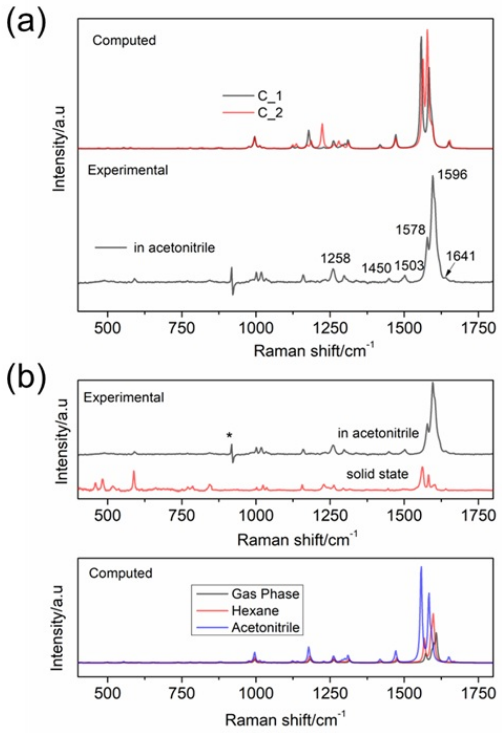

Figure 4 (a) Experimental and computed Raman spectra (CAM-B3LYP/6-311++G** level of theory in acetonitrile using the CPCM solvation model) of two conformers of 2HyC, together with comparison to the experimental Raman spectrum of 2HyC in acetonitrile. (b) Comparison between the solid-state and solution-phase Raman spectra of 2HyC; the computed Raman spectra in different solvents are shown below.

Table 22 Tentative assignment of Raman modes of 2HyC (C_1 conformer) in acetonitrile.

Experiment (cm^{-1})	Computed (cm^{-1})	Tentative Assignments
1641	1650	C=O stretch
1596	1583	C=C stretch
1578	1558	C=C stretch
1503	1471	C=C stretch
1450	1418	ring vibration
1258	1260	C-C stretch + CCH bend
1023	995	ring breathing

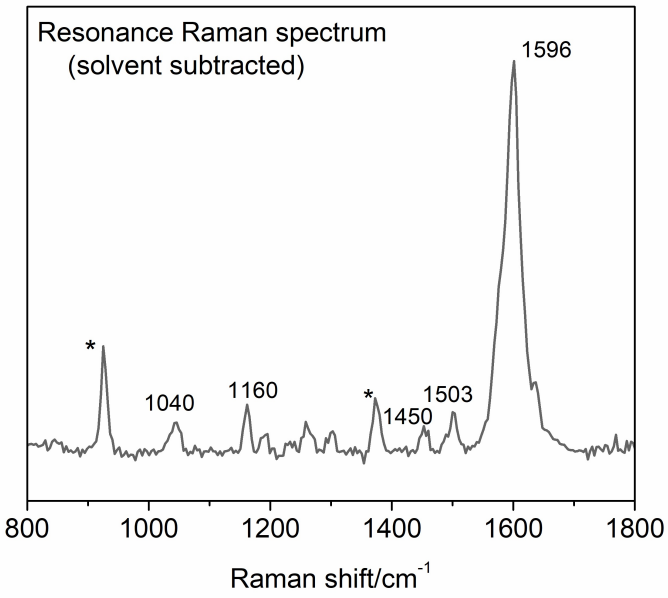

Figure 5 Solvent-subtracted resonance Raman spectrum of 2HyC in acetonitrile collected with 325 nm excitation. Peaks marked with an asterisk (*) indicate artefacts arising from solvent subtraction.

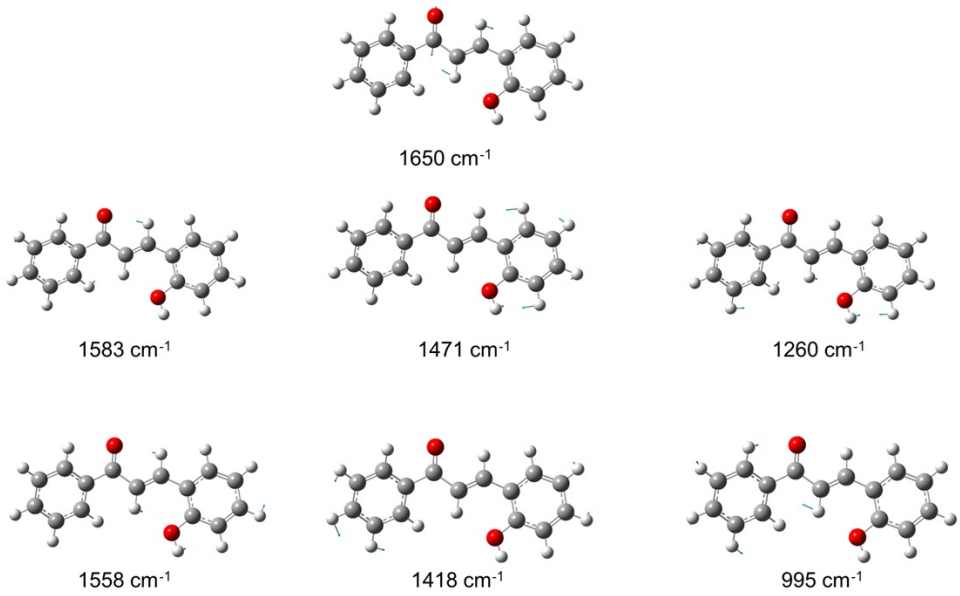

Figure 6 Vector diagrams of the computed Raman vibrational modes of the C_1 conformer of 2HyC (CAM-B3LYP/6-311++G** level of theory in acetonitrile using the CPCM solvation model).