Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Information

β-Cyclodextrin-Resveratrol inclusion complex and the role of geometrical and electronic effects on its electronic induced circular dichroism

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NMR spectra

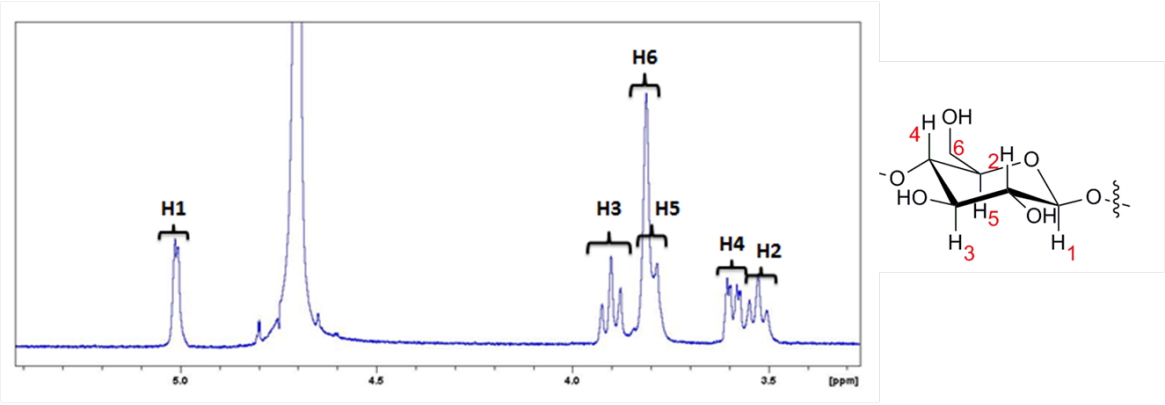


Fig. 1 1D ^{1}H annotated spectrum of β-cyclodextrin (D_2O, 400 MHz).

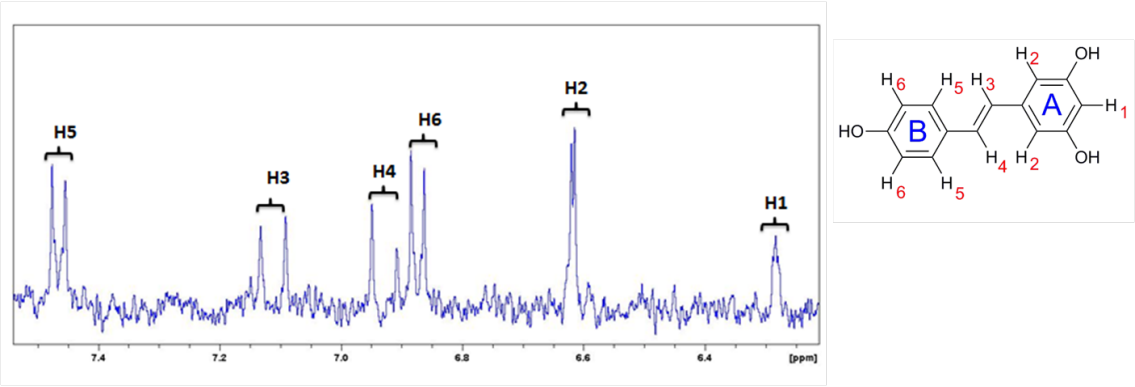


Fig. 2 1D ^{1}H annotated spectrum of resveratrol (D_2O, 400 MHz).

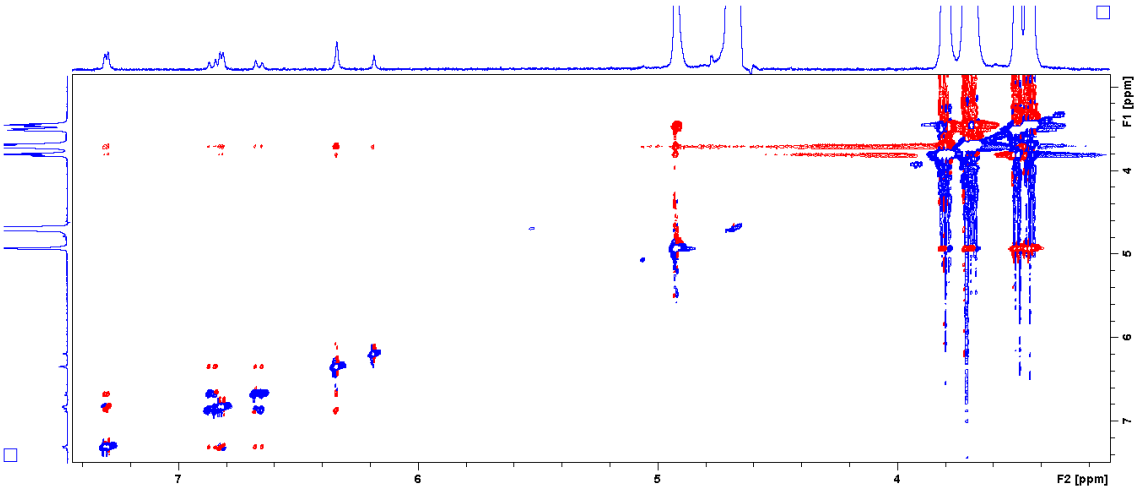


Fig. 3 2D T-ROESY spectrum (D_2O, 600 MHz).

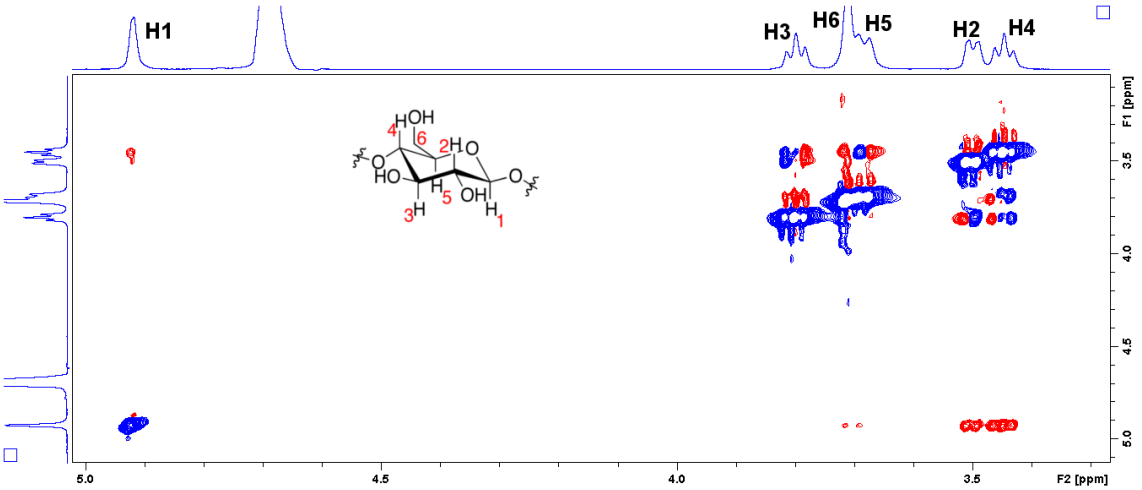


Fig. 4 2D T-ROESY annotated spectrum in the β-cyclodextrin region.

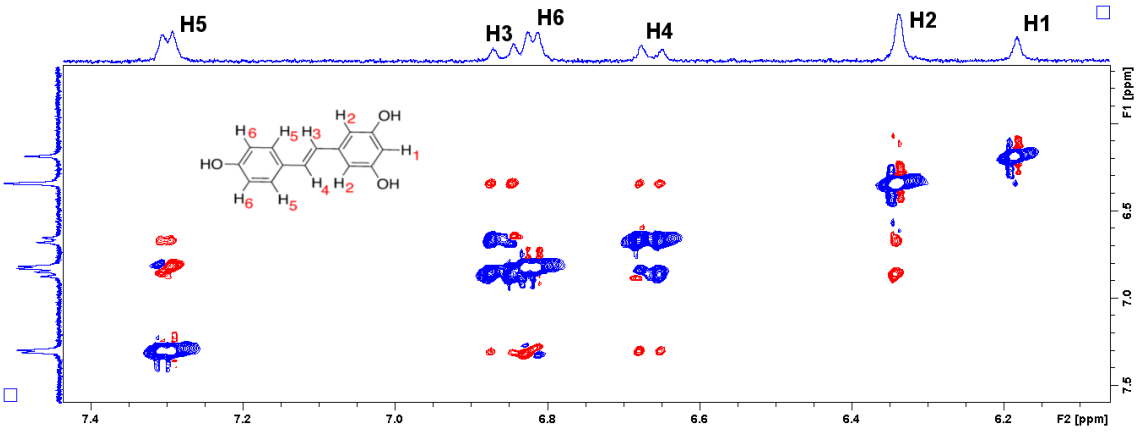


Fig. 5 2D T-ROESY annotated spectrum in the resveratrol region.

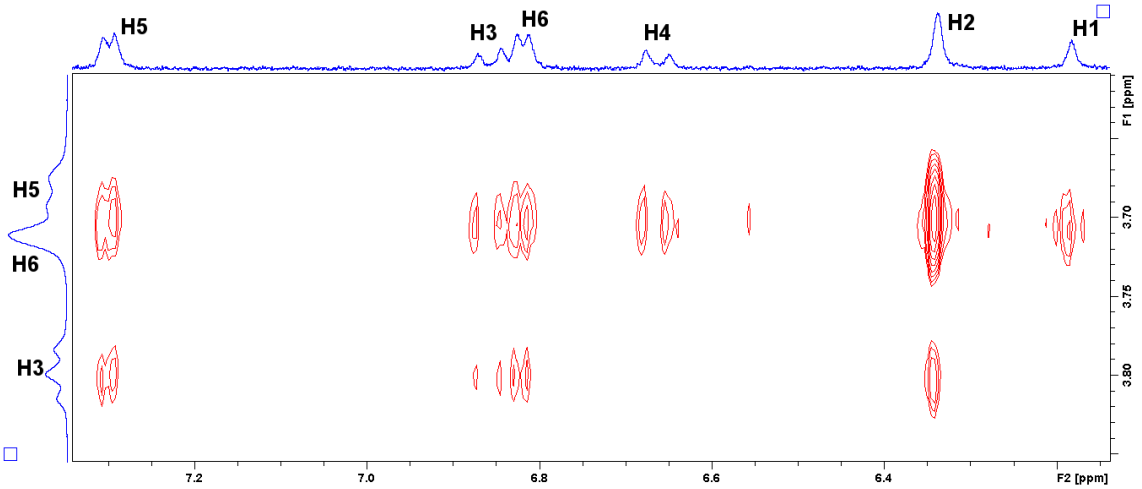


Fig. 6 2D T-ROESY annotated spectrum in the cross-peaks region between resveratrol (F2 dimension) and β-cyclodextrin (F1 dimension).

Titrations

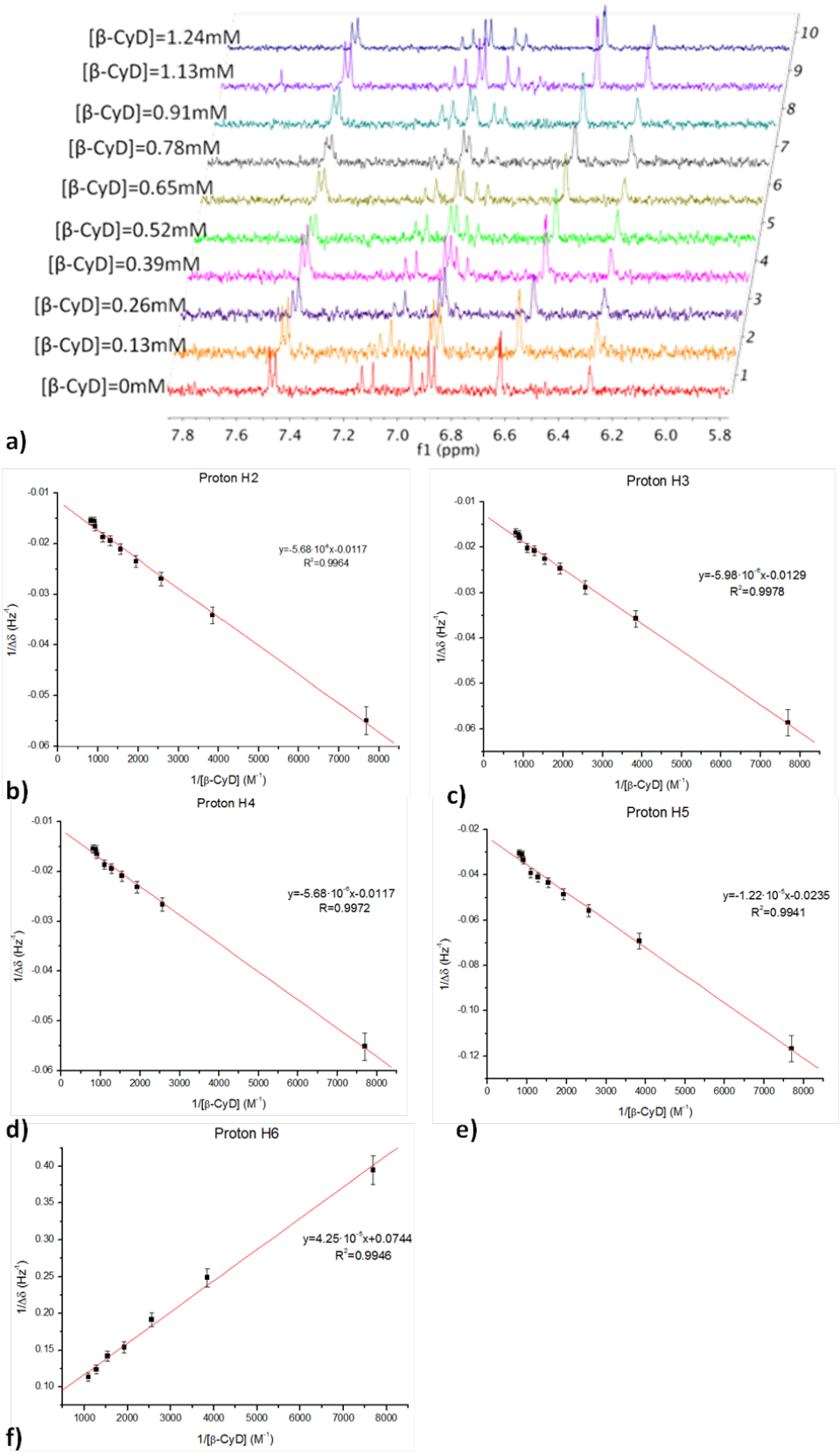


Fig. 7 a) NMR titration of the β-cyclodextrin-resveratrol inclusion complex (D_2O, 400 MHz), and individual plots for protons b) H2, c) H3, d) H4, e) H5 and f) H6 of resveratrol, along with the equations for each fitting (error bars were estimated as a 5% of error for each measurement).

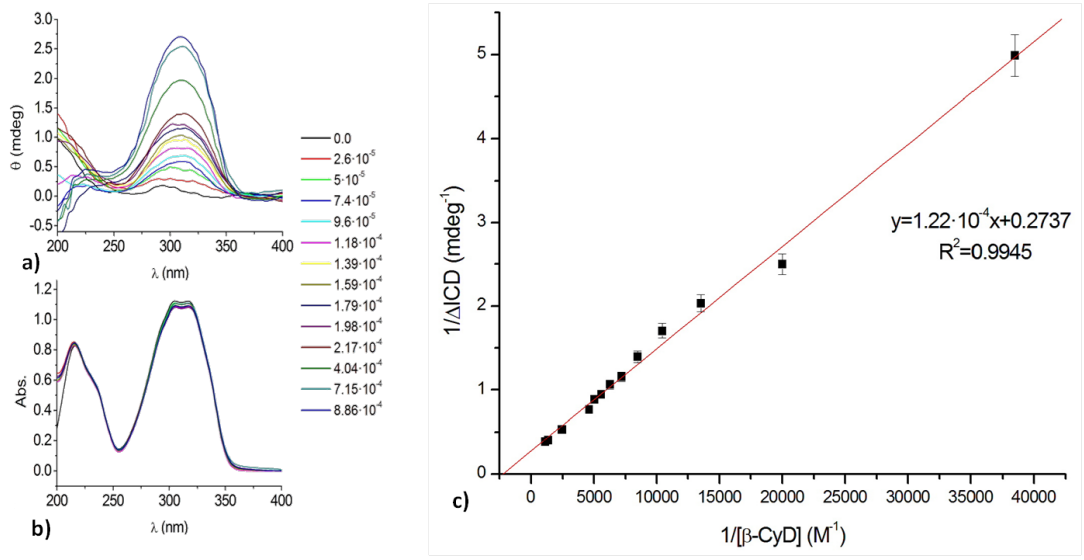


Fig. 8 a) Circular Dichroism titration of the β-cyclodextrin-resveratrol inclusion complex, b) UV-vis spectra for each solution and c) plot of the inverse of the CD intensity at 308 nm vs. the inverse of the β-CyD concentration (error bars were estimated as a 5% of error for each measurement).

β-CyD crystallization

Crystal data and structure refinement

Identification code	an14581s	
Empirical formula	C42 H70 O45	
Formula weight	1294.98	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 15.1815(18) Å	α= 90°
	b = 10.2073(12) Å	β= 110.803(2)°
	c = 21.019(2) Å	γ = 90°
Volume	3044.8(6) $Å^3$	
Z	2	
Density (calculated)	1.412 Mg/m^3	
Absorption coefficient	0.131 mm^{-1}	
F(000)	1364	
Crystal size	0.52 x 0.48 x 0.36 mm^3	
Theta range for data collection	1.43 to 27.95°.	
Index ranges	-19<=h<=19, -13<=k<=13, -19<=l<=27	
Reflections collected	19843	
Independent reflections	13372 [R(int) = 0.0206]	

Completeness to theta = 27.95°	98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. Transmission	1.0000 and 0.9545
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13372 / 1 / 805
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0711, wR2 = 0.1980
R indices (all data)	R1 = 0.0956, wR2 = 0.2280
Largest diff. peak and hole	1.593 and -0.504 e.Å^{-3}

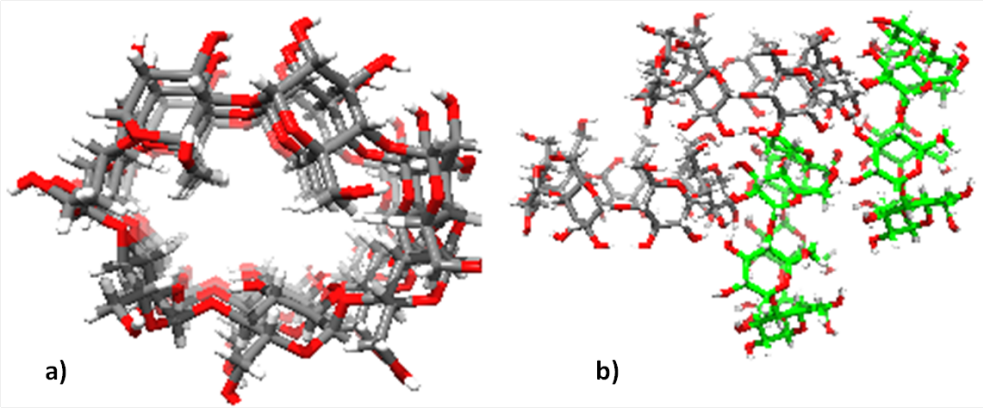


Fig. 9 β-CyD channels and the two perpendicular arrangements.

Molecular Dynamics

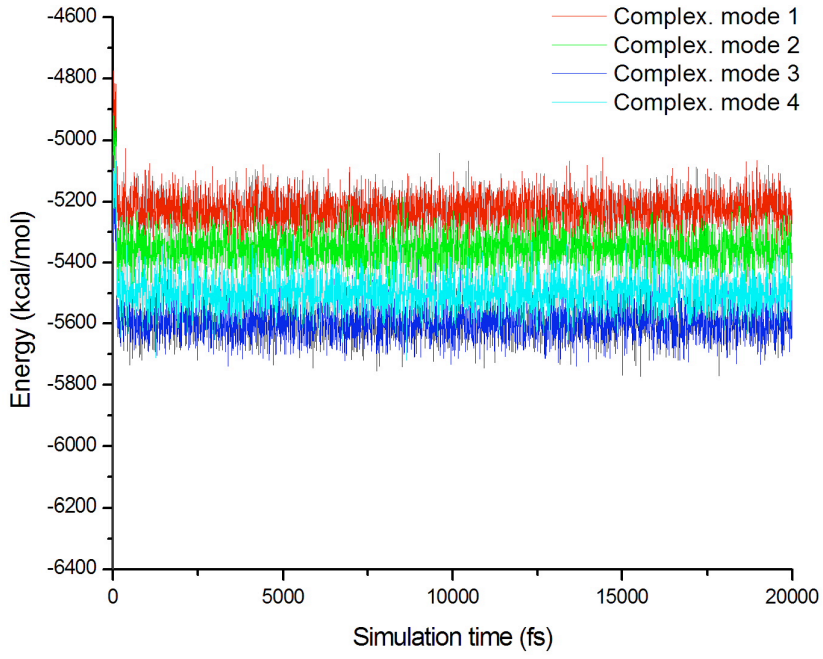


Fig. 10 Comparison of the total Energy (kcal/mol) over the 20 ns of MD simulation for each of the possible inclusion modes.

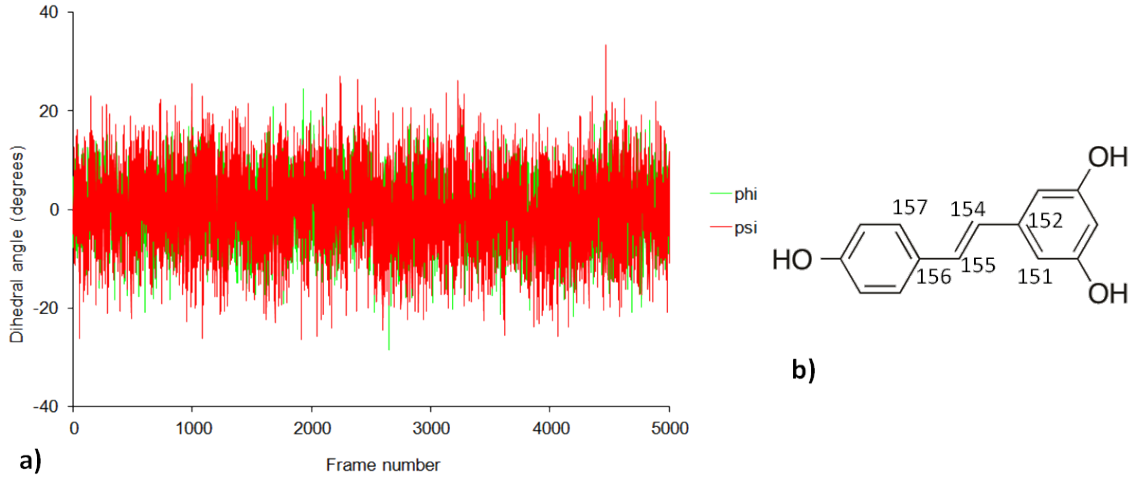


Fig. 11 Variation of the dihedral angles of the alkene bond of resveratrol with each of the aromatic moieties where the phi angle is the one formed by atoms: 151, 152, 154 and 155 and psi is the one formed by: 157, 156, 155 and 154.

Table 1 Most representative families of structures extracted from their MD runs by clustering them (in parenthesis the step number of the simulation), and their relative energies calculated at the CAM-B3LYP/SVP theory level.

Shaded conformations are depicted in the manuscript (Figure 6).

Structure	ΔE	Structure	ΔE
a(411)	7.1	**b**(436)	30.4
a(1976)	4.6	**b**(756)	19.2
a(2381)	14.3	**b**(1366)	31.2
a(2716)	21.3	**b**(1466)	34.9
a(3116)	23.2	**b**(2691)	23.3
a(3661)	6.5	**b**(4111)	5.8
a(4591)	50.8	**b**(4376)	14.3
c(336)	12.7	**d**(126)	13.6
c(846)	26.0	**d**(296)	1.5
c(2926)	0.0	**d**(816)	17.0
c(3236)	9.4	**d**(1051)	5.9
c(3551)	16.7	**d**(2041)	25.5
c(3816)	22.8	**d**(3051)	40.7
c(4641)	18.3	**d**(4356)	15.1

Details of TD-DFT electronic circular dichroism computations for the functional comparison

Rotatory strengths were computed using the 6-31+G* level and the IEFPCM solvation model with water parameters on CAM-B3LYP/6-31+G* geometries. ECD spectrum was simulated by convoluting transitions with gaussian bands of 0.5 eV half-height full linewidth.

CAM-B3LYP

Transition	λ (nm)	Rotatory strength (length)[a]
1	304.88	70.3821
2	272	-7.0984
3	257.8	10.5935
4	226.17	-4.8249
5	222.72	6.5274
6	216.12	23.4063
7	212.43	15.7362
8	210.74	-36.4473
9	207.59	42.8367
10	205.61	2.9915

a) 10^{-40} erg.esu.cm/Gauss

B3LYP

Transition	λ (nm)	Rotatory strength (length)[a]
1	332.9	66.0404
2	308.58	-7.1342
3	279.14	9.2196
4	258.48	5.561
5	253.23	2.884
6	248.24	-4.0155
7	245.46	3.5776
8	243.75	-1.4229
9	243.06	1.983
10	241.82	-0.0874

OPBE

Transition	λ (nm)	Rotatory strength (length)[a]
1	363.53	1.8354
2	354.84	60.3365
3	343.02	-0.1252
4	336.40	-0.5909
5	326.33	-0.0383
6	325.12	-0.1607
7	317.62	-0.4211
8	313.75	0.3506
9	312.29	0.0459
10	307.72	0.6043

M05

Transition	λ (nm)	Rotatory strength (length)[a]
1	330.72	71.1038
2	297.83	-7.2459
3	273.98	9.8375
4	249.78	7.0704
5	249.07	1.6106
6	243.05	-5.598
7	239.27	6.4393
8	236.52	30.8278
9	234.81	-27.4561
10	233.12	4.5192

M06L

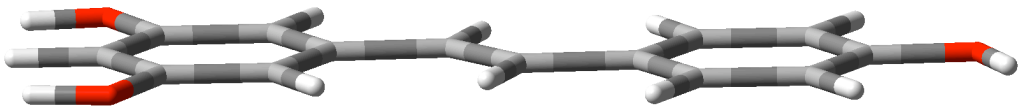
Transition	λ (nm)	Rotatory strength (length)[a]
1	346.61	62.3773
2	339.31	-5.4645
3	308.99	-0.0859
4	301.8	0.225
5	294.93	-0.419
6	294.03	2.7184
7	292.38	-0.0593
8	288.12	1.2921
9	285.84	0.7738
10	284.05	0.0654

M06-2X

Transition	λ (nm)	Rotatory strength (length)[a]
1	306.04	72.3112
2	271.81	-6.9806
3	256.86	14.7474
4	231.71	2.2888
5	225.18	0.3401
6	221.2	-16.2248
7	217.93	71.929
8	213.81	-24.8837
9	212.67	23.5498
10	210.91	-22.2782

Fig. 12 3D Cartesian coordinate of the DFT optimized[1] structures

Planar resveratrol (PL):



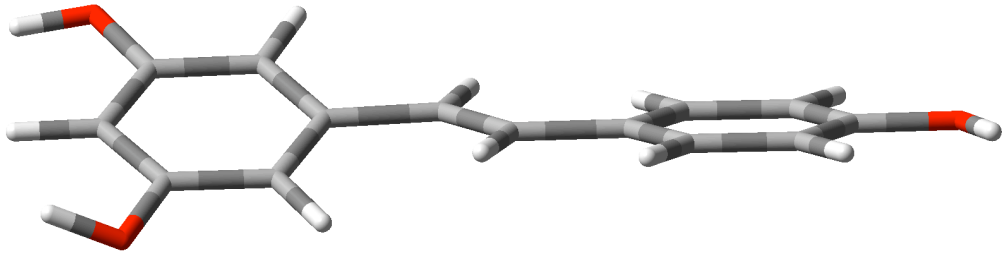
29

C	3.960321	-1.110575	0.150174
C	4.487548	0.171669	0.007507
C	3.609465	1.246547	-0.165402
C	2.234190	1.039040	-0.218137
C	1.711360	-0.249178	-0.066560
C	2.585469	-1.325914	0.113790
C	0.265347	-0.512902	-0.101171
C	-0.695564	0.395647	0.115871
C	-2.144997	0.181220	0.060723
C	-2.734896	-1.024845	-0.349727
C	-4.109562	-1.175472	-0.385624
C	-4.938997	-0.116113	-0.011166
C	-4.376739	1.091584	0.394110
C	-2.995638	1.230990	0.425373
O	-6.281447	-0.322910	-0.066999
O	4.063473	2.514007	-0.318911
O	4.753018	-2.203956	0.329872
H	2.210061	-2.332794	0.258139
H	-0.006553	-1.542872	-0.317206
H	-0.403117	1.412299	0.372034
H	-2.565369	2.177622	0.742886
H	-5.017255	1.920823	0.682216
H	-4.560807	-2.108743	-0.705870
H	-2.116070	-1.863352	-0.653897
H	1.589652	1.894655	-0.382647
H	5.560350	0.339670	0.031747
H	-6.746316	0.480285	0.213277
H	4.944232	2.626323	0.114137
H	5.686992	-1.951239	0.274917

SCF energy= -766.0248901 u.a.

[1] Both geometry optimizations and excited states TD-DFT calculations were performed at the theory level CAM-B3LYP/6-31+G*.

Twisted resveratrol (TW):

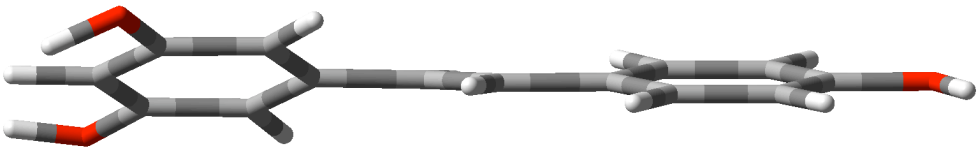


29

C	3.960321	-1.110575	0.150174
C	4.487548	0.171669	0.007507
C	3.609465	1.246547	-0.165402
C	2.234190	1.039040	-0.218137
C	1.711360	-0.249178	-0.066560
C	2.585469	-1.325914	0.113790
C	0.265347	-0.512902	-0.101171
C	-0.695564	0.395647	0.115871
C	-2.144997	0.181220	0.060723
C	-2.734896	-1.024845	-0.349727
C	-4.109562	-1.175472	-0.385624
C	-4.938997	-0.116113	-0.011166
C	-4.376739	1.091584	0.394110
C	-2.995638	1.230990	0.425373
O	-6.281447	-0.322910	-0.066999
O	4.063473	2.514007	-0.318911
O	4.753018	-2.203956	0.329872
H	2.210061	-2.332794	0.258139
H	-0.006553	-1.542872	-0.317206
H	-0.403117	1.412299	0.372034
H	-2.565369	2.177622	0.742886
H	-5.017255	1.920823	0.682216
H	-4.560807	-2.108743	-0.705870
H	-2.116070	-1.863352	-0.653897
H	1.589652	1.894655	-0.382647
H	5.560350	0.339670	0.031747
H	-6.746316	0.480285	0.213277
H	4.944232	2.626323	0.114137
H	5.686992	-1.951239	0.274917

SCF energy =-766.0233507 u.a.

Mirror twisted resveratrol (TWm):



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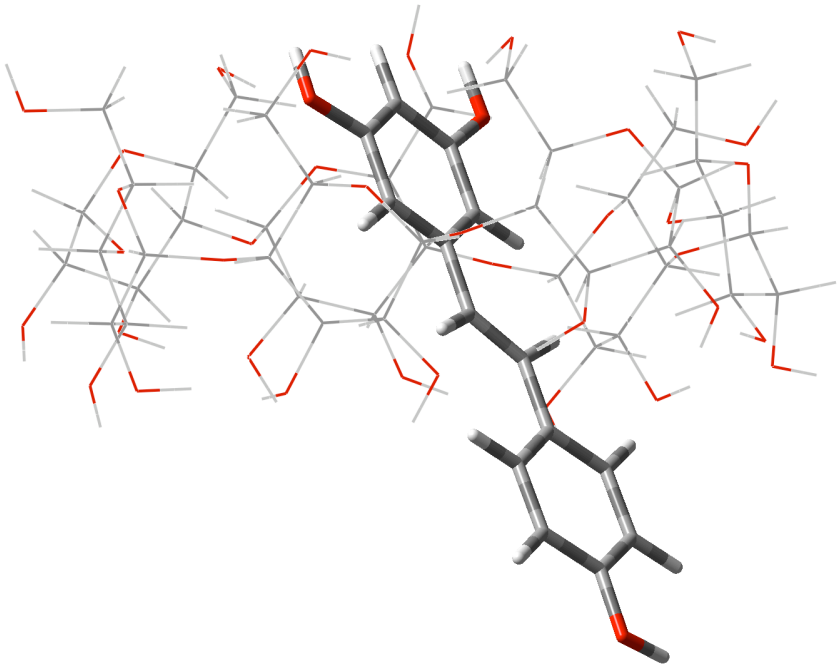
C	-3.96032	1.11058	-0.15017
C	-4.48755	-0.17167	-0.00751
C	-3.60947	-1.24655	0.1654
C	-2.23419	-1.03904	0.21814
C	-1.71136	0.24918	0.06656
C	-2.58547	1.32591	-0.11379
C	-0.26535	0.5129	0.10117
C	0.69556	-0.39565	-0.11587
C	2.145	-0.18122	-0.06072
C	2.7349	1.02485	0.34973
C	4.10956	1.17547	0.38562
C	4.939	0.11611	0.01117
C	4.37674	-1.09158	-0.39411
C	2.99564	-1.23099	-0.42537
O	6.28145	0.32291	0.067
O	-4.06347	-2.51401	0.31891
O	-4.75302	2.20396	-0.32987
H	-2.21006	2.33279	-0.25814
H	0.00655	1.54287	0.31721
H	0.40312	-1.4123	-0.37203
H	2.56537	-2.17762	-0.74289
H	5.01725	-1.92082	-0.68222
H	4.56081	2.10874	0.70587
H	2.11607	1.86335	0.6539
H	-1.58965	-1.89466	0.38265
H	-5.56035	-0.33967	-0.03175
H	6.74632	-0.48029	-0.21328
H	-4.94423	-2.62632	-0.11414
H	-5.68699	1.95124	-0.27492

SCF energy =-766.0233507 u.a.

Inclusion complex with planar resveratrol (CPL):



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176
C       2.546391    5.565248    0.200379
C       1.811706    6.127357    1.412393
O       2.623379    5.950854    2.559721
C       0.473312    5.436826    1.576291
O      -0.171339    6.030106    2.680939
C      -0.340740    5.557481    0.293028
O      -1.496662    4.747734    0.439885
C       0.473529    5.036557   -0.894685
O       1.742830    5.702539   -0.955740
C      -0.198750    5.260987   -2.229619
O       0.383593    4.352984   -3.171926
C      -2.748387    5.363671    0.591060
C      -3.482422    4.696601    1.753492
O      -2.694741    4.818645    2.926763
C      -3.769954    3.242312    1.427104
O      -4.525032    2.697095    2.491072
C      -4.504212    3.151298    0.099864
O      -4.604243    1.765647   -0.202980
C      -3.739520    3.895646   -0.996041
O      -3.516476    5.251586   -0.579395
C      -4.469745    3.923467   -2.319401
O      -5.811617    4.334240   -2.111256
C      -5.815912    1.264354   -0.708615
C      -6.340316    0.195451    0.260899
O      -6.397986    0.718607    1.584817
C      -5.427840   -1.017148    0.266603
O      -6.045744   -2.060897    0.983941
C      -5.098093   -1.471997   -1.153647
O      -4.073582   -2.443370   -0.995281
C      -4.634317   -0.315913   -2.032019
O      -5.629434    0.715019   -1.987454
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C	-4.468812	-0.662490	-3.501063
O	-4.148508	0.496275	-4.250943
C	-4.139502	-3.645736	-1.706969
C	-3.985936	-4.800024	-0.721359
O	-4.965754	-4.678186	0.295745
C	-2.591727	-4.806206	-0.123086
O	-2.510451	-5.954817	0.696005
C	-1.535219	-4.785730	-1.223625
O	-0.253765	-4.642690	-0.616243
C	-1.797476	-3.602332	-2.158431
O	-3.127527	-3.717870	-2.677545
C	-0.867418	-3.524857	-3.355419
O	-1.004055	-2.299309	-4.054600
C	0.514852	-5.800816	-0.458067
C	1.067424	-5.861329	0.967534
O	-0.007035	-5.766410	1.885056
C	2.070775	-4.744272	1.203948
O	2.619542	-4.825520	2.515542
C	3.144923	-4.703098	0.122541
O	3.865019	-3.498278	0.315540
C	2.485948	-4.716112	-1.257483
O	1.592250	-5.830509	-1.362884
C	3.450974	-4.861360	-2.416888
O	2.750439	-4.821557	-3.645427
C	5.278125	-3.515702	0.343804
C	5.722470	-2.905560	1.666141
O	5.201889	-3.591787	2.785362
C	5.351922	-1.427877	1.729270
O	5.862744	-0.874516	2.924805
C	5.901879	-0.686063	0.522693
O	5.376461	0.634705	0.577428
C	5.461596	-1.404223	-0.767499
O	5.819776	-2.795853	-0.724139
C	6.083087	-0.842823	-2.027481
O	7.493226	-0.774894	-1.864839
C	6.104394	1.685637	0.000893
C	6.254392	2.824127	1.010413
O	6.943647	2.373543	2.153456
C	4.884381	3.374496	1.364972
O	5.078502	4.468831	2.239110
C	4.171291	3.789426	0.091200
O	2.861832	4.228530	0.438042
C	4.107272	2.636794	-0.904033
O	5.448303	2.189558	-1.148002
C	3.472219	3.032627	-2.236106
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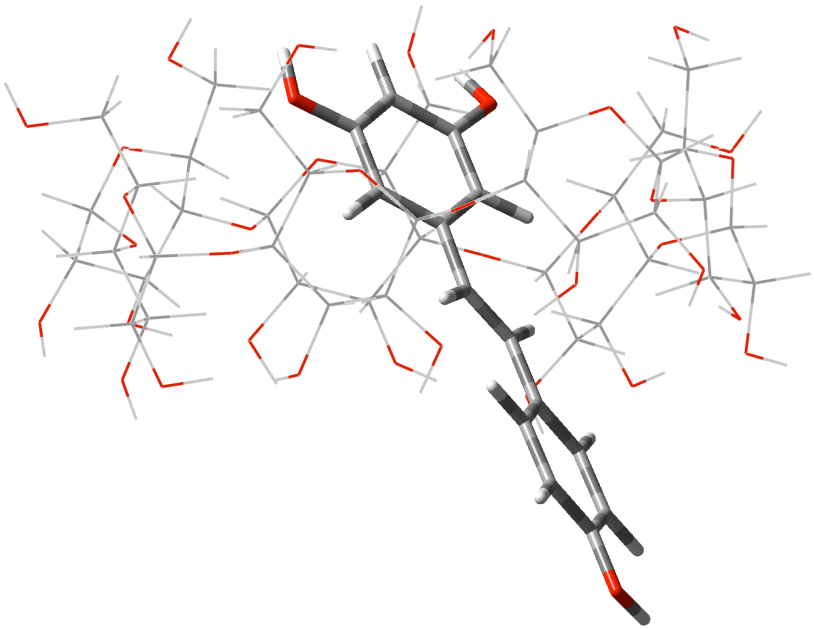
Inclusion complex with twisted resveratrol (CTW):



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O      -2.307957    5.849012   -0.358136
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O      -6.270021   -0.830688    1.039360
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O      -4.522308   -1.490147   -1.083236
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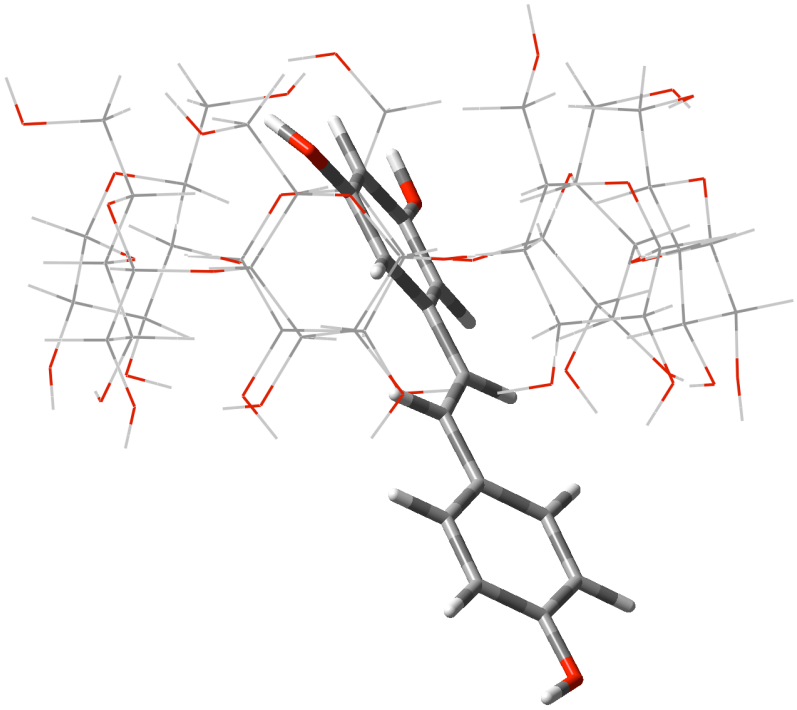
SCF energy=-5039.8457118 u.a.

Inclusion complex with "mirror" twisted resveratrol (CTWm):



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O	0.798559	5.183489	2.615245
C	0.484301	5.312566	0.197578
O	-0.800137	4.696011	0.259979
C	1.179313	4.992916	-1.129419
O	2.511161	5.525552	-1.111977
C	0.461507	5.582705	-2.322543
O	0.252880	6.969769	-2.102597
C	-1.927384	5.515349	0.075593
C	-2.752459	5.558907	1.361395
O	-1.912601	5.924096	2.445249
C	-3.422616	4.225789	1.627482
O	-4.230413	4.396250	2.770109
C	-4.224086	3.802516	0.405491
O	-4.785216	2.530457	0.683029
C	-3.305725	3.750046	-0.819735
O	-2.721098	5.049197	-0.987401
C	-4.013691	3.435746	-2.138241
O	-3.893670	2.061545	-2.487788
H	-6.649731	3.385729	0.878034
H	-7.580093	1.489208	2.123752
H	-4.826905	0.243270	1.816919
H	-7.408150	-0.769840	0.588603
H	-5.047836	0.651305	-0.718386
H	-6.224413	-0.841397	-2.285857
H	-7.778877	-0.079822	-1.874216
H	-7.088675	-2.802242	-0.161387
H	-6.047662	-4.834112	0.715299
H	-3.637288	-3.113485	1.394880
H	-3.939326	-5.235217	-0.769183
H	-3.683630	-2.196238	-0.962607
H	-4.274698	-2.822315	-3.414436
H	-2.597157	-2.798129	-2.867215
H	-2.192988	-6.244583	-1.017527
H	-0.056437	-6.877912	-0.102942
H	0.289250	-3.987111	0.766338
H	1.640911	-5.632084	-1.418733
H	3.607964	-5.225288	-1.587141
H	5.608262	-4.322607	-0.573056
H	3.882905	-2.043665	0.446265
H	6.093224	-1.897160	-1.635099
H	6.968462	0.009427	-1.394553
H	7.185553	1.948638	0.115030
H	4.250499	1.418699	0.705015
H	5.537691	3.878400	-0.521769
H	4.298356	5.525050	-0.210241
H	1.225191	3.906838	-1.264833
H	-0.492810	5.056171	-2.441738
H	1.070443	5.408331	-3.219244
H	0.383254	6.396592	0.296248
H	-1.614222	6.519277	-0.221600
H	-2.513627	3.009534	-0.658855
H	-5.070561	3.715295	-2.079553
H	-3.543563	4.050397	-2.913878
H	-5.020299	4.534007	0.218637

H	-2.646422	3.468284	1.807449
H	-3.535427	6.318445	1.230459
H	1.341123	3.686768	1.289821
H	2.669209	6.422445	1.363658
H	3.819178	1.785570	-1.918287
H	3.743425	3.931781	-2.945528
H	4.691254	2.818479	-3.960108
H	3.057551	-1.676823	-1.967211
H	5.201829	-1.946386	-4.098963
H	4.496462	-0.393341	-3.588836
H	-0.263548	-3.250027	-1.490671
H	1.014675	-2.759787	-3.339970
H	-0.169926	-3.882835	-4.011666
H	-2.506928	-4.933209	-3.032062
H	-4.771823	1.714928	-2.769470
H	-6.946530	1.860972	-2.686508
H	6.538284	0.818796	2.104881
H	5.986050	-1.361135	1.189033
H	2.442933	-5.001757	1.239119
H	-2.834199	-5.300783	1.840778
H	-0.452288	-6.213438	2.156426
H	-5.920923	1.506278	3.886077
H	-5.663817	-4.052314	2.918970
H	2.552824	-4.162309	-3.668062
H	4.631861	3.331868	2.053855
H	-4.666060	3.542199	2.977758
H	-0.179711	5.227993	2.563740
H	3.350623	-1.456197	-5.385768
H	-0.280677	7.308982	-2.835384
H	4.748678	-4.141342	1.696815
H	-2.431800	5.756445	3.250785
H	3.017039	4.849891	3.112225
H	5.689032	4.945225	-3.581290
H	-6.061649	-1.551605	2.774969

SCF energy=-5039.8457118 u.a.

Details of TD-DFT electronic circular dichroism computations

Planar resveratrol (PL)

Transition	λ (nm)	Rotatory strength (length)[a]
1	313.49	0.0057
2	275.68	0.0015
3	260.9	-0.0023
4	227.69	0.0098
5	221.27	-0.0003
6	216.27	-0.0019
7	214.64	0.0005
8	213.28	-0.0049
9	211.23	-0.0006
10	210.21	-0.0129

Twisted resveratrol (TW)

Transition	λ (nm)	Rotatory strength (length)[a]
1	302.37	45.9596
2	269.57	-8.7952
3	257.78	1.3439
4	225.22	-10.2019
5	220.64	1.0663
6	215.08	54.0411
7	213.83	17.4163
8	212.31	0.7012
9	210.21	-35.6106
10	207.68	-60.8537

Mirror image of twisted resveratrol (TWm)

Transition	λ (nm)	Rotatory strength (length)[a]
1	302.37	-45.9596
2	269.57	8.7951
3	257.78	-1.3437
4	225.22	10.2025
5	220.64	-1.0662
6	215.08	-54.0421
7	213.83	-17.4157
8	212.31	-0.7011
9	210.21	35.6112
10	207.68	60.8538

Inclusion complex with planar resveratrol (CPL)

Transition	λ (nm)	Rotatory strength (length)[a]
1	310.78	31.6071
2	274.59	0.6021
3	258.67	9.8039
4	228.09	5.1736
5	223.84	15.7318
6	219.01	-56.026
7	214.58	-10.8757
8	211.05	55.7326
9	209.15	67.0325
10	207.7	-3.0549

Inclusion complex with twisted resveratrol (CTW)

Transition	λ (nm)	Rotatory strength (length)[a]
1	304.88	70.3821
2	272	-7.0984
3	257.8	10.5935
4	226.17	-4.8249
5	222.72	6.5274
6	216.12	23.4063
7	212.43	15.7362
8	210.74	-36.4473
9	207.59	42.8367
10	205.61	2.9915

Inclusion complex of the mirror image of twisted resveratrol (CTWm)

Transition	λ (nm)	Rotatory strength (length)[a]
1	303.95	-91.4705
2	274.98	9.7889
3	258.39	-10.4871
4	227.41	11.3318
5	223.45	-6.9053
6	216.08	-24.2487
7	213.05	-94.2795
8	209.66	83.654
9	209.35	-3.4615
10	208.18	8.2437

Charge comparison between PL, TW, CPL, CTW in ground and excited states

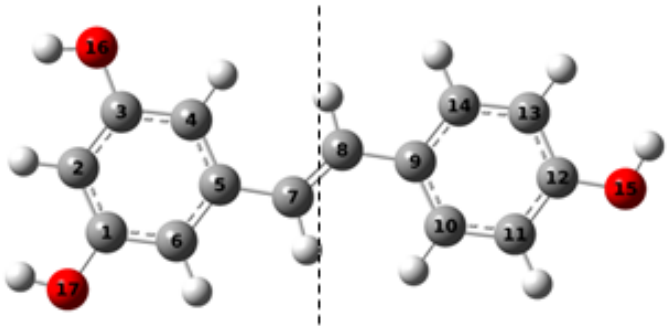

Fig. 12 Labelled resveratrol

Table 2. NPA (Natural Population Analysis) charges of resveratrol atoms in free resveratrol (PL and TW) and in the complexes (CPL and CTW) in their ground (S_0) and first excited (S_1) electronic states.

	PL		TW		CPL		CTW	
	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1
C1	0.3354	0.3246	0.3345	0.3281	0.3217	0.30486	0.3278	0.3130
C2	-0.3962	-0.4082	-0.3911	-0.4089	-0.4083	-0.40933	-0.3993	-0.4025
C3	0.3363	0.3332	0.3356	0.3312	0.3777	0.36982	0.3382	0.3297
C4	-0.3236	-0.3431	-0.3227	-0.3432	-0.3244	-0.33452	-0.3338	-0.3421
C5	-0.0311	-0.0515	-0.0280	-0.0338	-0.0351	-0.06602	0.0112	-0.0197
C6	-0.3201	-0.3025	-0.3192	-0.3085	-0.3205	-0.30978	-0.3382	-0.3308
C7	-0.2264	-0.2402	-0.2398	-0.2563	-0.2320	-0.21987	-0.2455	-0.2311
C8	-0.2063	-0.2315	-0.1903	-0.2118	-0.1898	-0.24512	-0.1938	-0.2491
C9	-0.1143	-0.0780	-0.1243	-0.0995	-0.1305	-0.07688	-0.1301	-0.0724
C10	-0.2058	-0.2309	-0.2020	-0.2287	-0.1944	-0.23416	-0.1988	-0.2417
C11	-0.2948	-0.2751	-0.2932	-0.2785	-0.2959	-0.27996	-0.2954	-0.2779
C12	0.3162	0.3143	0.3153	0.3240	0.3175	0.33308	0.3172	0.3341
C13	-0.3249	-0.3233	-0.3185	-0.3227	-0.3201	-0.31848	-0.3202	-0.3202
C14	-0.1915	-0.1778	-0.2013	-0.1850	-0.1928	-0.16613	-0.1938	-0.1651
O15	-0.7311	-0.7077	-0.7299	-0.7052	-0.7290	-0.69866	-0.7293	-0.6970
O16	-0.7324	-0.7317	-0.7426	-0.7431	-0.7800	-0.78114	-0.7598	-0.7613
O17	-0.7316	-0.7326	-0.7322	-0.7347	-0.7276	-0.72894	-0.7273	-0.7288
$\sum q_{H(2,4,6,7,16,17)}$	2.0539	2.0438	2.0641	2.0567	2.0398	2.0315	2.0551	2.0453
$\sum q_{H(10,11,13,14,15)}$	1.7882	1.8183	1.7855	1.8198	1.7747	1.7974	1.7794	1.8024
q(2OH)	-0.0358	-0.1083	-0.0414	-0.1124	-0.0887	-0.1434	-0.0714	-0.1283
q(1OH)	0.0358	0.1083	0.0415	0.1124	0.0397	0.1111	0.0352	0.1131
q_{TOTAL}	0.0000	0.0000	0.0000	0.0000	-0.0490	-0.0323	-0.0362	-0.0152

To help the interpretation of the charge distribution both in the ground and excited states, we have added charges dividing the molecule as represented in the figure above and according to the expressions:

$$q(2OH) = \sum q(C1,C2,C3,C4,C5,C7,O16,O17) + \sum q(H_{C2},H_{C4},H_{C3},H_{C4},H_{C5},H_{C7},H_{O16},H_{O17})$$

$$q(1OH) = \sum q(C8,C9,C10,C11,C12,C13,C14,O15) + \sum q(H_{C8},H_{C9},H_{C10},H_{C11},H_{C12},H_{C13},H_{C14},H_{O15})$$

q_{TOTAL} represents the total charge of the resveratrol unit: Zero values correspond to free resveratrol and the negative values in the complexes indicate the existence of charge transfer from the β-CyD towards resveratrol.