Supporting Information

Elucidate the Mechanism of Changes in Emission Properties after Powder Compression into Tablets

Xiaoping, Lei[a], Qingfeng Wu[a], Xiangxi Zhang[a], Qing Zhou[a,b,c]* and Lingmin Yi[a]*

[a] X. Lei, Q. Wu, X. Zhang, Prof. Q. Zhou and Prof. L. Yi

Engineering Research Center for Eco-Dyeing and Finishing of Textiles, Key Laboratory of Advanced Textile Materials and Manufacturing Technology, Ministry of Education, College of Textile Science and Engineering (International Institute of Silk), Zhejiang Sci-Tech University, Hangzhou 310018, People's Republic of China

[b] Prof. Q. Zhou

Zhejiang Sci-Tech University Shaoxing-Keqiao Research Institute, Building 8, Cross border E-commerce Park, Huashe Street, Keqiao District, Shaoxing City, Zhejiang, 312030, China

[c] Prof. Q. Zhou

MOE Key Laboratory of Macromolecular Synthesis and Functionalization, Departmentof Polymer Science and Engineering, Zhejiang University, Hangzhou, 310058, China

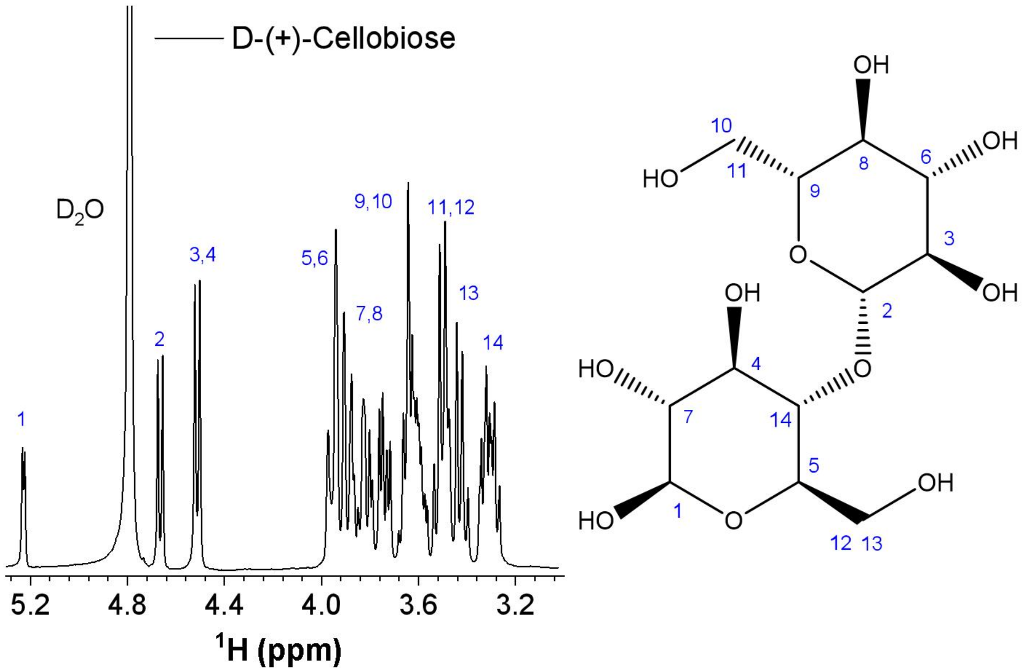

Figure S1. ^{1}H NMR of D-Cbs powder.

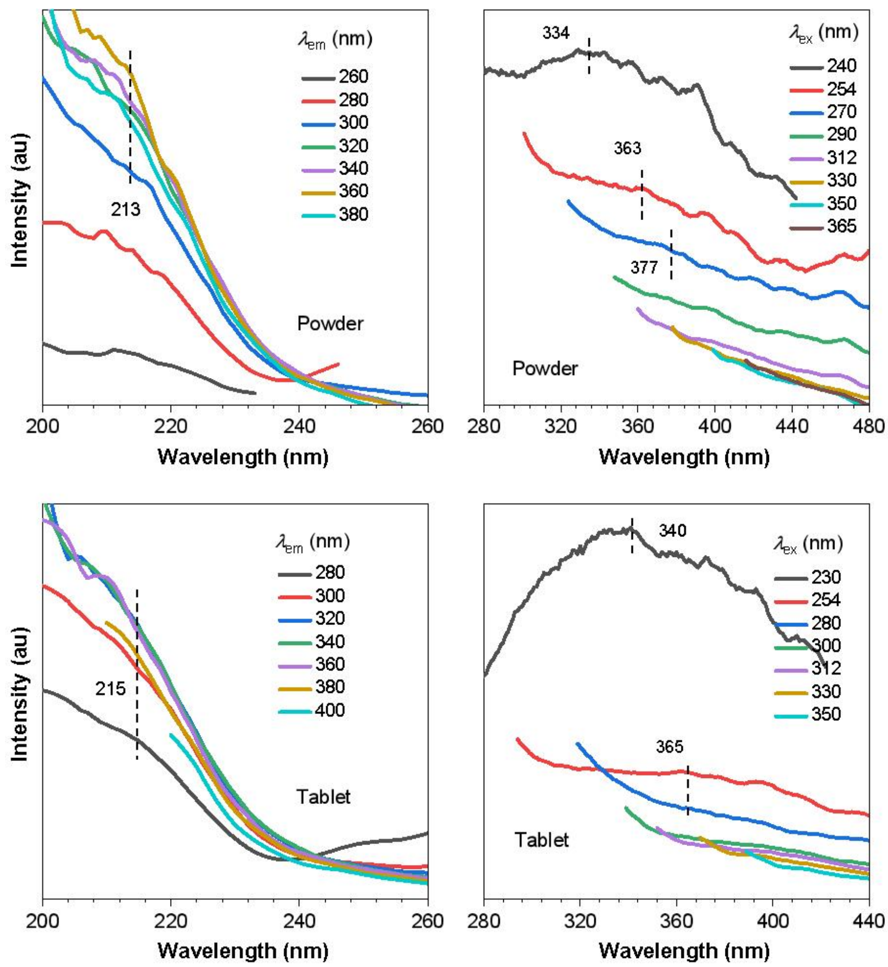

Figure S2. Excitation and emission spectra of powders and flakes at different excitation and emission wavelengths.

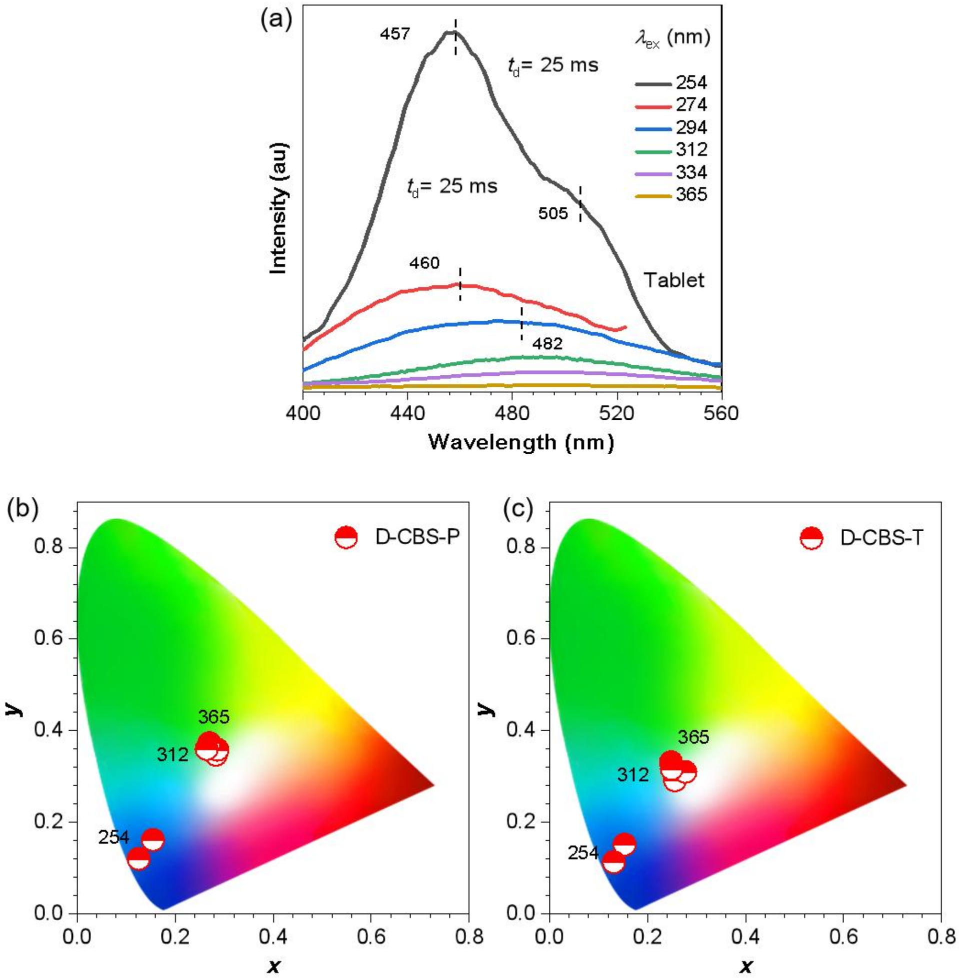

Figure S3. (a) Emission spectra of D-Cbs tablet under different excitations. (b) and (c) CIE coordinate diagram of the PL of emission under different excitations.

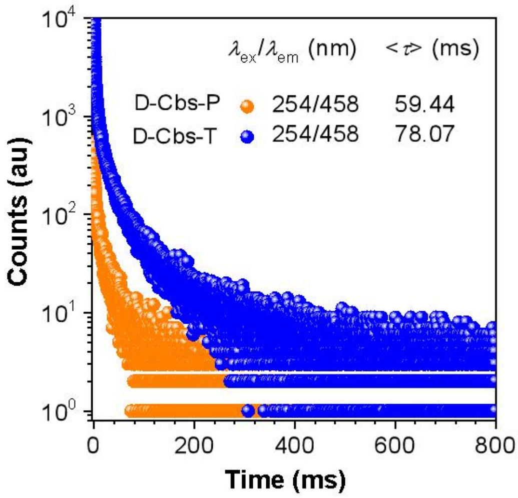

Figure S4. Lifetimes of D-Cbs powder and tablet at different excitation and emission wavelengths.

Table S2. Summary of the ns lifetimes of samples.[a]

	τ_1 [ns]	A_1 [%]	τ_2 [ns]	A_2 [%]	τ_3 [ns]	A_3 [%]	τ [nds]	λ_{ex} [nm]	λ_{em} [nm]
D-Cbs-P	1.39	17.79	14.24	47.82	59.44	34.39	27.50	254	458
D-Cbs-T	1.50	28.03	13.14	42.00	78.07	29.98	29.34	254	458

[a] All measurements were conducted at ambient conditions. λ_{ex} = excitation wavelength used for the lifetime measurement; λ_{em} = monitored emission wavelength. $\tau = (A_1\tau_1^2 + A_2\tau_2^2 + A_3\tau_2^3)/(A_1\tau_1 + A_2\tau_2 + A_3\tau_3)$.

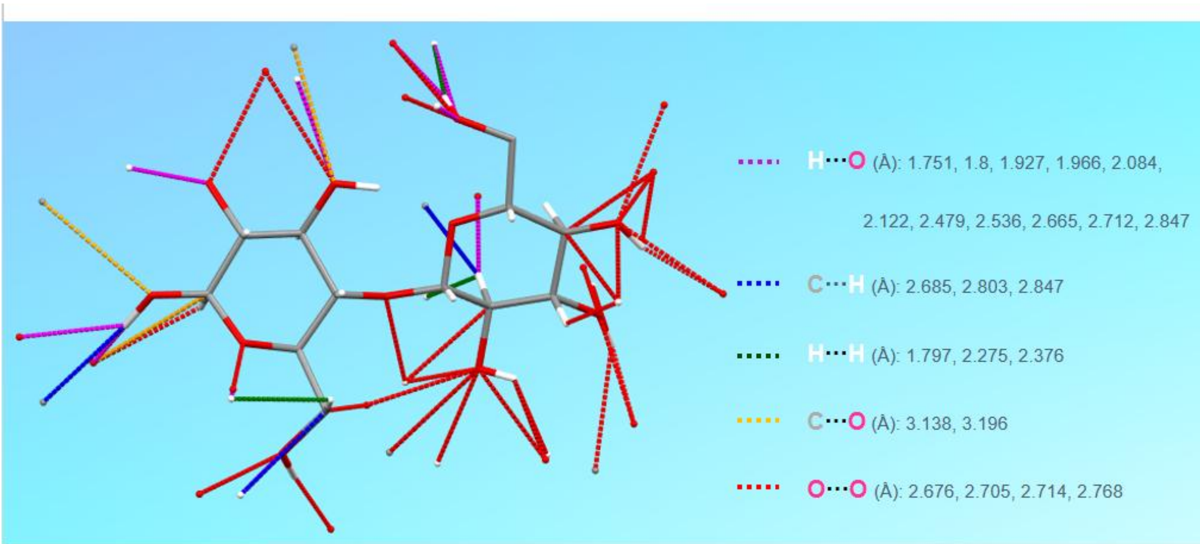

Figure S5. Intermolecular interaction of the D-Cbs molecule (numerical unit:Å).

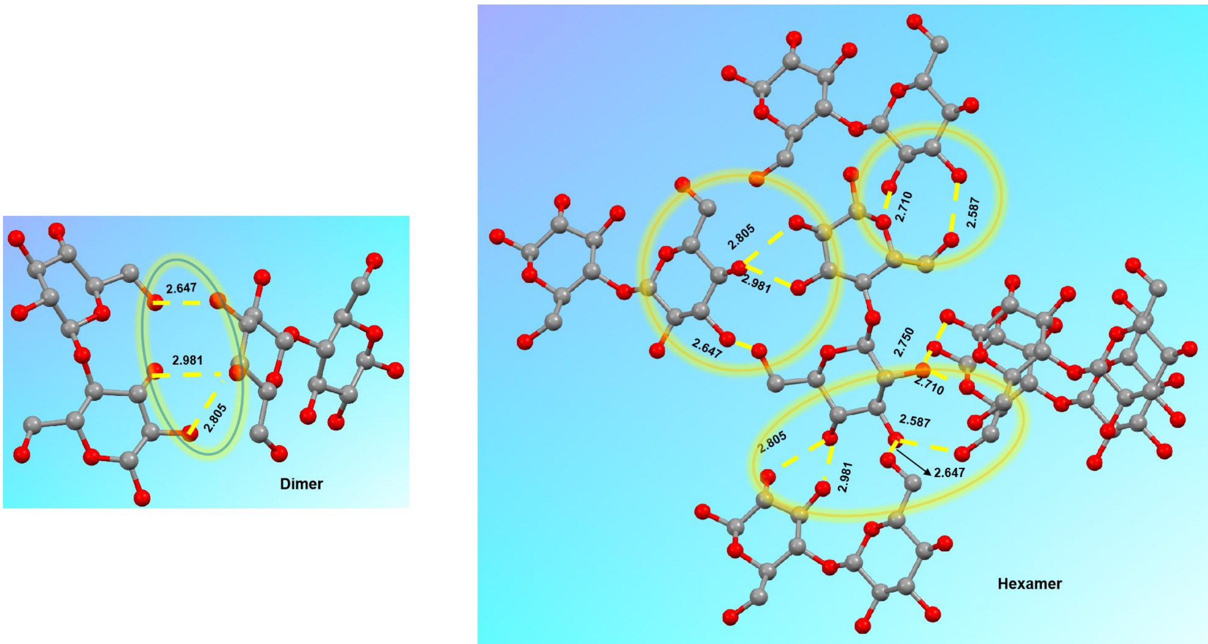

Figure 6. O···O interaction between dimer-p and hexamer-p coupling (numerical unit:Å).

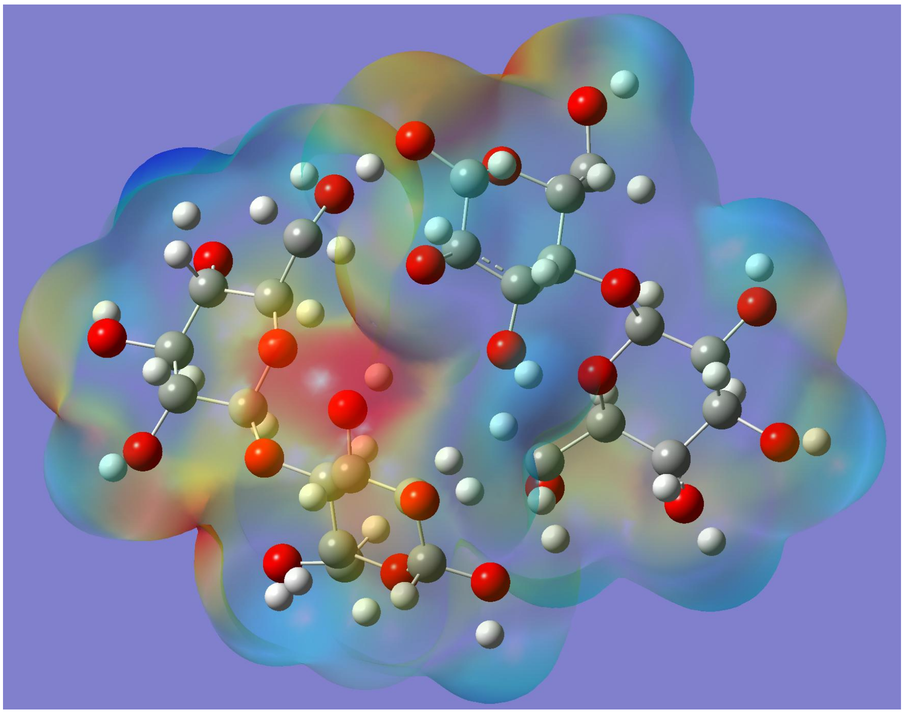

Figure S7. Electrostatic potential analysis of dimer-2-P of D-Cbs powder.

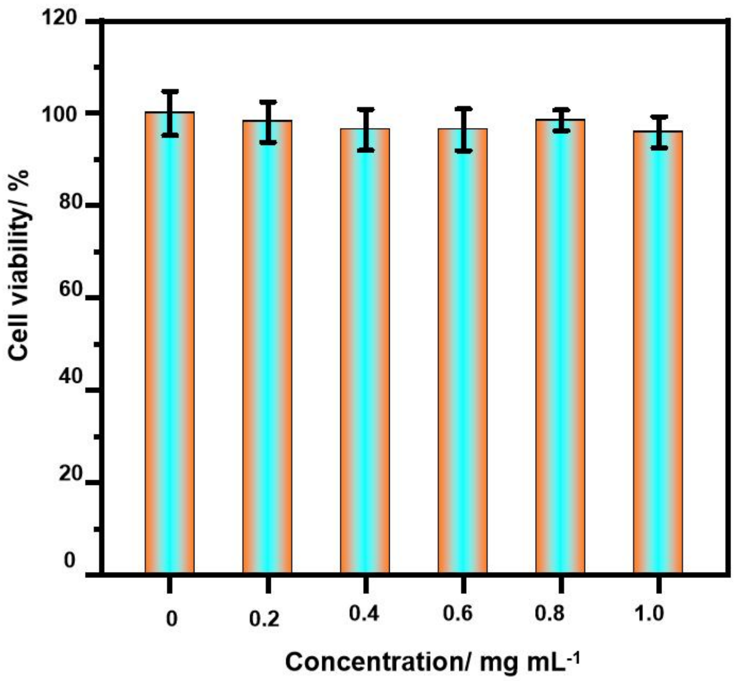

Figure S8. The viability of HeLa cells with the various concentrations of D-Cbs. Error bars±s.d. (n=5)

The original calculation code used:

1) GROMACS software (version: 2020.6-MODIFIED)

```
title        = OPLS Lysozyme MD simulation
; Run parameters
integrator      = md            ; leap-frog integrator
nsteps          = 500000; 2 * 500000 = 1000 ps (1 ns)
dt              = 0.001         ; 2 fs
; Output control
nstxout                 = 50000       ; save coordinates every 10.0 ps
nstvout                 = 50000       ; save velocities every 10.0 ps
nstenergy               = 5000        ; save energies every 10.0 ps
nstlog                  = 5000        ; update log file every 10.0 ps
nstxout-compressed   = 5000           ; save compressed coordinates every 10.0 ps
                                        ; nstxout-compressed replaces nstxtcout
compressed-x-grps     = System       ; replaces xtc-grps
; Bond parameters
continuation            = yes           ; Restarting after NPT
constraint_algorithm      = lincs       ; holonomic constraints
constraints                   = all-bonds   ; all bonds (even heavy atom-H bonds) constrained
lincs_iter                = 1             ; accuracy of LINCS
lincs_order                   = 4             ; also related to accuracy
; Neighborsearching
cutoff-scheme      = Verlet
ns_type              = grid           ; search neighboring grid cells
nstlist              = 10       ; 20 fs, largely irrelevant with Verlet scheme
rcoulomb             = 1.0            ; short-range electrostatic cutoff (in nm)
rvdw                 = 1.0            ; short-range van der Waals cutoff (in nm)
; Electrostatics
coulombtype         = PME          ; Particle Mesh Ewald for long-range electrostatics
pme_order           = 4               ; cubic interpolation
fourierspacing      = 0.16           ; grid spacing for FFT
; Temperature coupling is on
tcoupl          = V-rescale                        ; modified Berendsen thermostat
tc-grps         = system ; two coupling groups - more accurate
tau_t           = 0.1                           ; time constant, in ps
ref_t       = 300                       ; reference temperature, one for each group, in K
; Pressure coupling is on
pcoupl                  = Parrinello-Rahman          ; Pressure coupling on in NPT
pcoupltype              = semiisotropic                     ; uniform scaling of box vectors
tau_p                   = 5.0                              ; time constant, in ps
ref_p                   = 40.0     40.0                          ; reference pressure, in bar
compressibility             = 0     4.5e-5                  ; isothermal compressibility, bar^-1
; Periodic boundary conditions
pbc        = xyz            ; 3-D PBC
; Dispersion correction
DispCorr= EnerPres     ; account for cut-off vdW scheme
; Velocity generation
gen_vel         = no       ; Velocity generation is off
```

2) Orca 4.2 software

```
 !D3 GCP(DFT/SV) b3lyp def2-SVP miniprint
%maxcore    1800
%pal nprocs    20 end
%tddft
nroots 5
dosoc true
tda false
printlevel 3
end
* xyz 0 1
```