

New barbituric acid derivatives for data encryption and decryption based on mechanochromic fluorescence effect

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1. Characterization spectrum of CB-Ph

^1H NMR (400 MHz, Chloroform-*d*) δ 9.32 (s, 1H), 8.95 (s, 1H), 8.49 (d, $J = 9.6$ Hz, 1H), 8.23 (d, $J = 7.7$ Hz, 1H), 7.69 – 7.61 (m, 3H), 7.53 (d, $J = 11.4$ Hz, 6H), 7.47 (t, $J = 7.6$ Hz, 4H), 7.37 (d, $J = 8.0$ Hz, 6H)

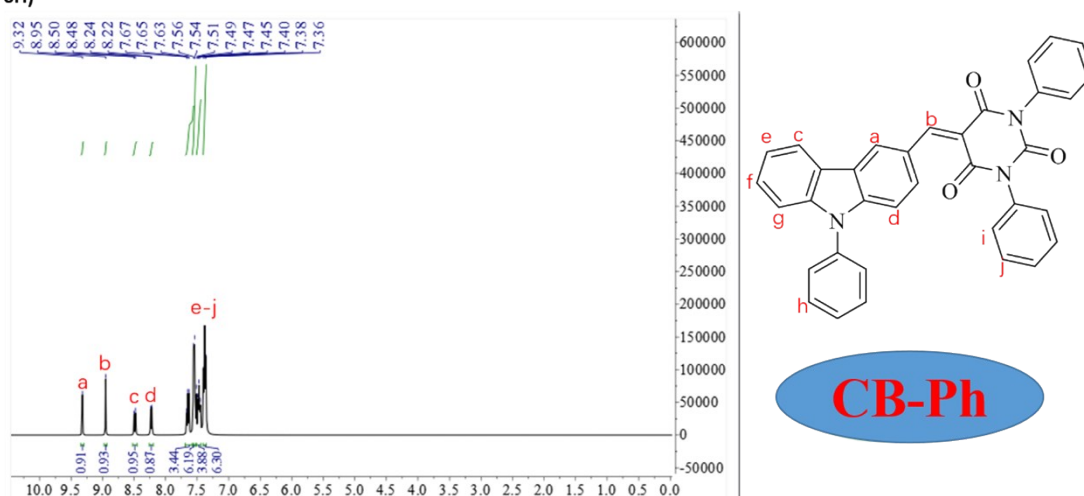


Fig. S1. ^1H NMR of **CB-Ph** in Chloroform-*d*

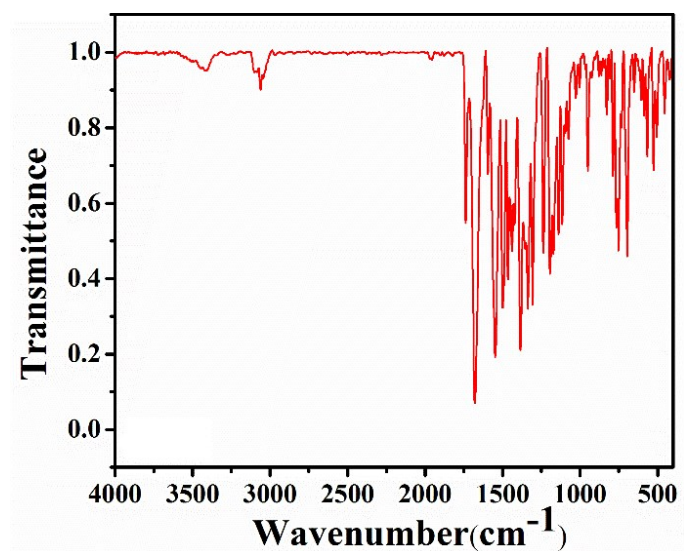


Fig. S2. FT-IR spectra of **CB-Ph**

Mass Spectrum List Report

Analysis Info

Analysis Name D:\Data\HYMBS_002041.d
Method 4_19_MassAccuNeg
Sample Name 58
Comment

Acquisition Date 8/4/2019 8:54:27 PM

Operator
Instrument solariX

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 Ip
Broadband Low Mass	53.8 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Fri Feb 21 02:36:54 2014
Source Accumulation	0.020 sec	n/a	n/a	Data Acquisition Size	1048576
Ion Accumulation Time	0.200 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec	n/a	n/a	Apodization	Apodization

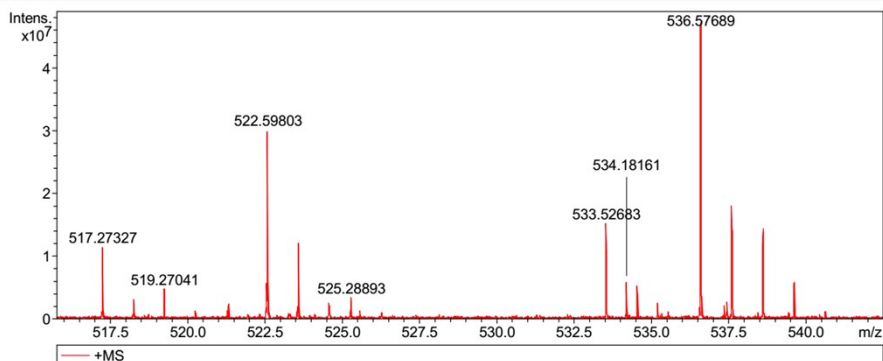


Fig. S3. HRMS spectra of **CB-Ph**

2. Characterization spectrum of CB-Me

^1H NMR (400 MHz, Chloroform- d) δ 9.28 (s, 1H), 8.81 (s, 1H), 8.55 (d, J = 8.9 Hz, 1H), 8.21 (d, J = 7.8 Hz, 1H), 7.62 – 7.33 (m, 4H), 4.35 (t, J = 7.3 Hz, 2H), 3.47 (s, 6H), 2.06 – 1.77 (m, 2H), 1.48 – 1.24 (m, 6H), 0.88 (t, J = 6.9 Hz, 3H).

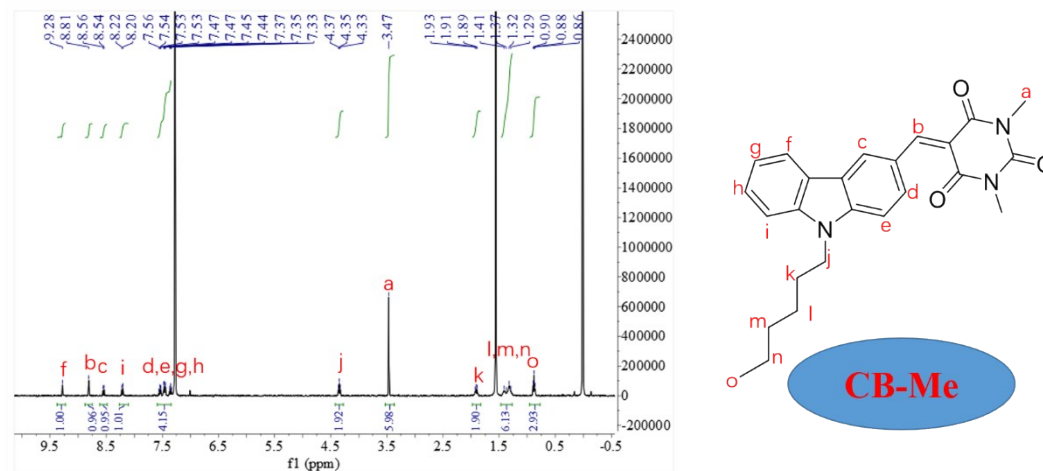


Fig. S4. ^1H NMR of CB-Me in Chloroform- d

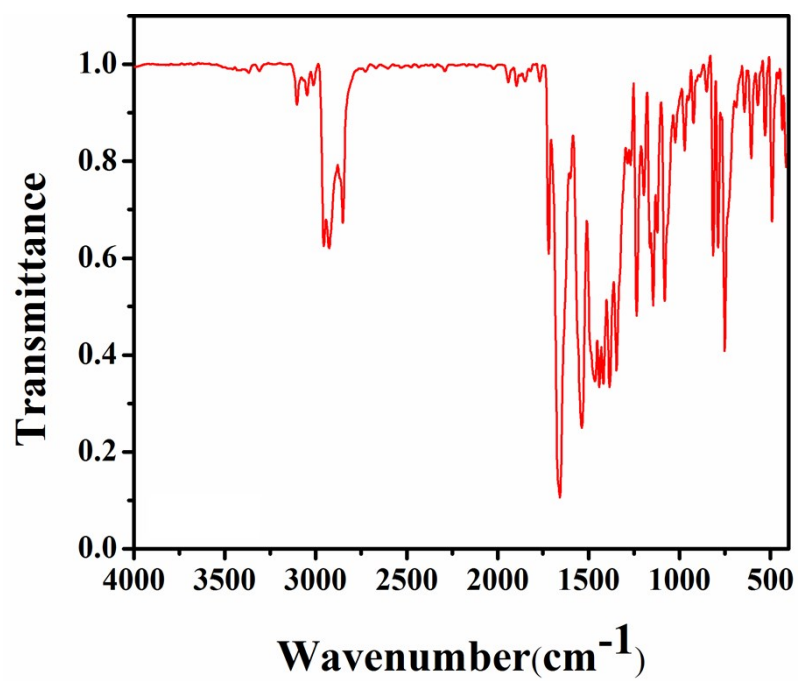


Fig. S5. FT-IR spectra of **CB-Me**

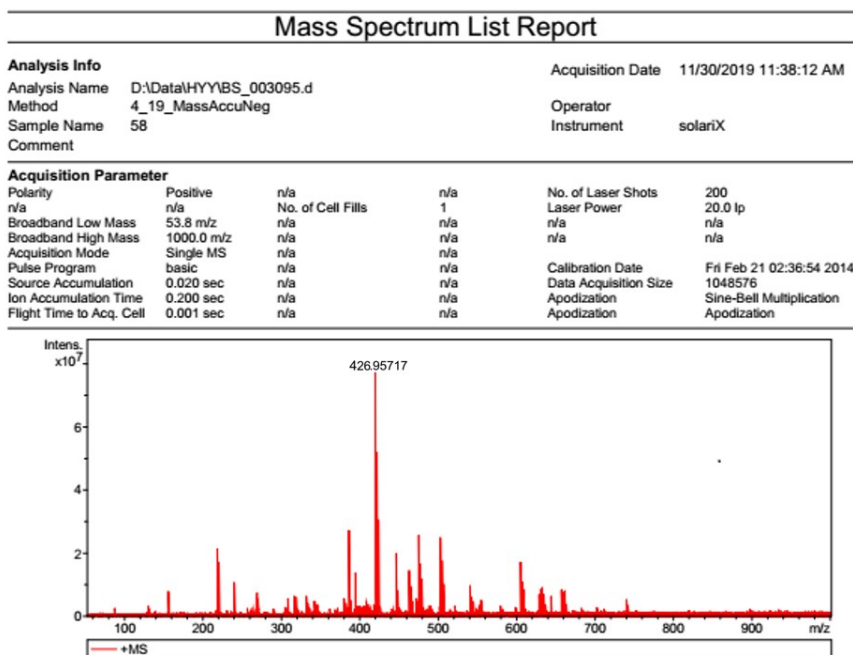


Fig. S6. HRMS spectra of **CB-Me**

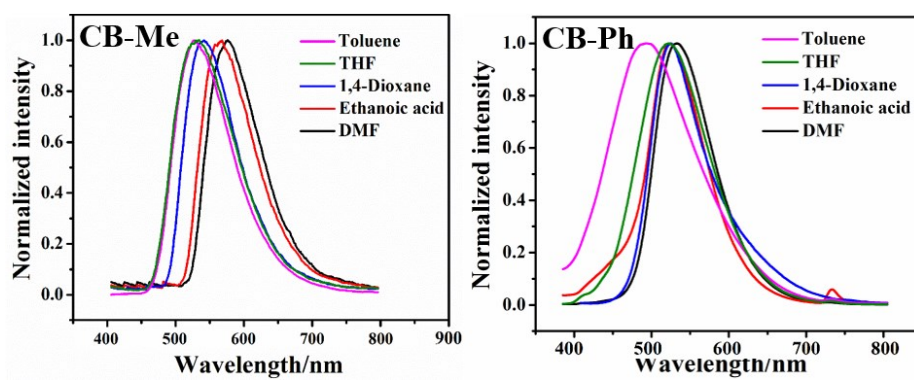


Fig. S7. Solvation effects of CB-Me and CB-Ph.

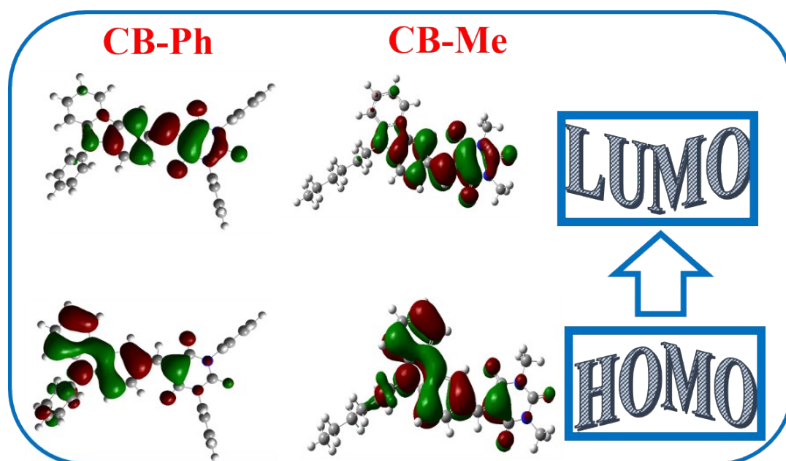


Fig. S8. LUMO and HOMO molecular orbitals of **CB-Me**, **CB-Ph** electron density distributions.

3. Process of mchanochromic fluorescence

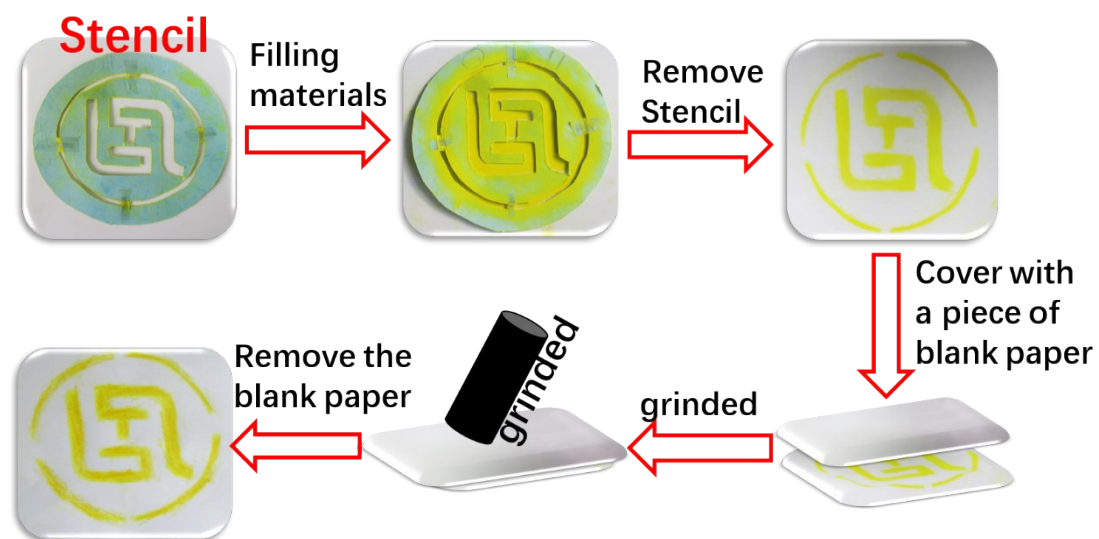


Fig. S9. The detailed preparation process of mchanochromic fluorescence

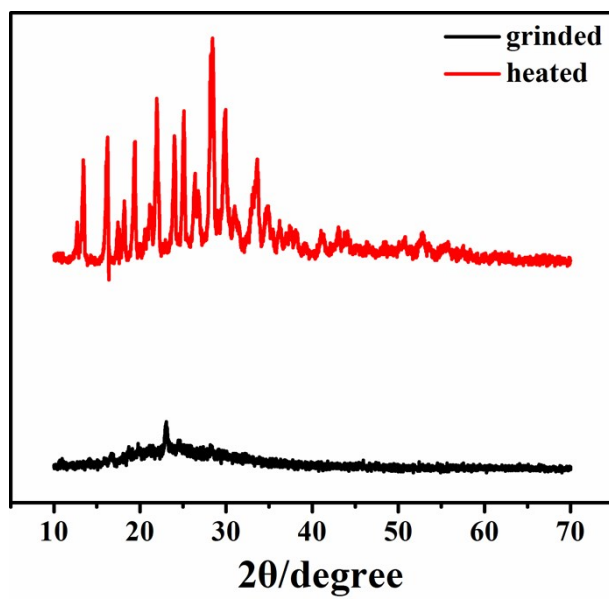


Fig. S10. XRD patterns of the **CB-Ph** of solid powder in grinded and heated;

4. Process of information encryption and decryption

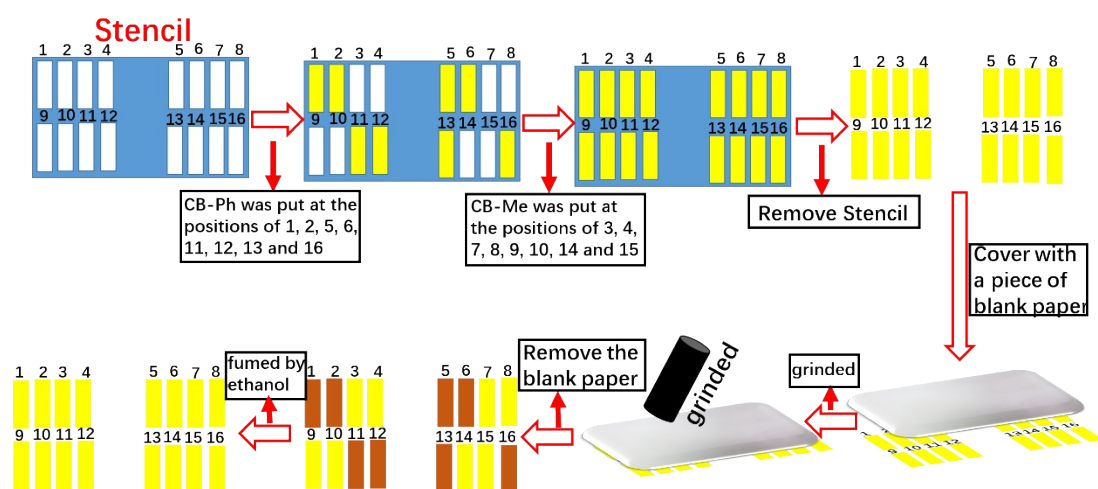


Fig. S11. The detailed preparation process of information encryption and decryption.