

Supporting Information

Nanocapsules formed by interactions between chondroitin sulfate and egg white protein for encapsulating hydrophilic ingredients

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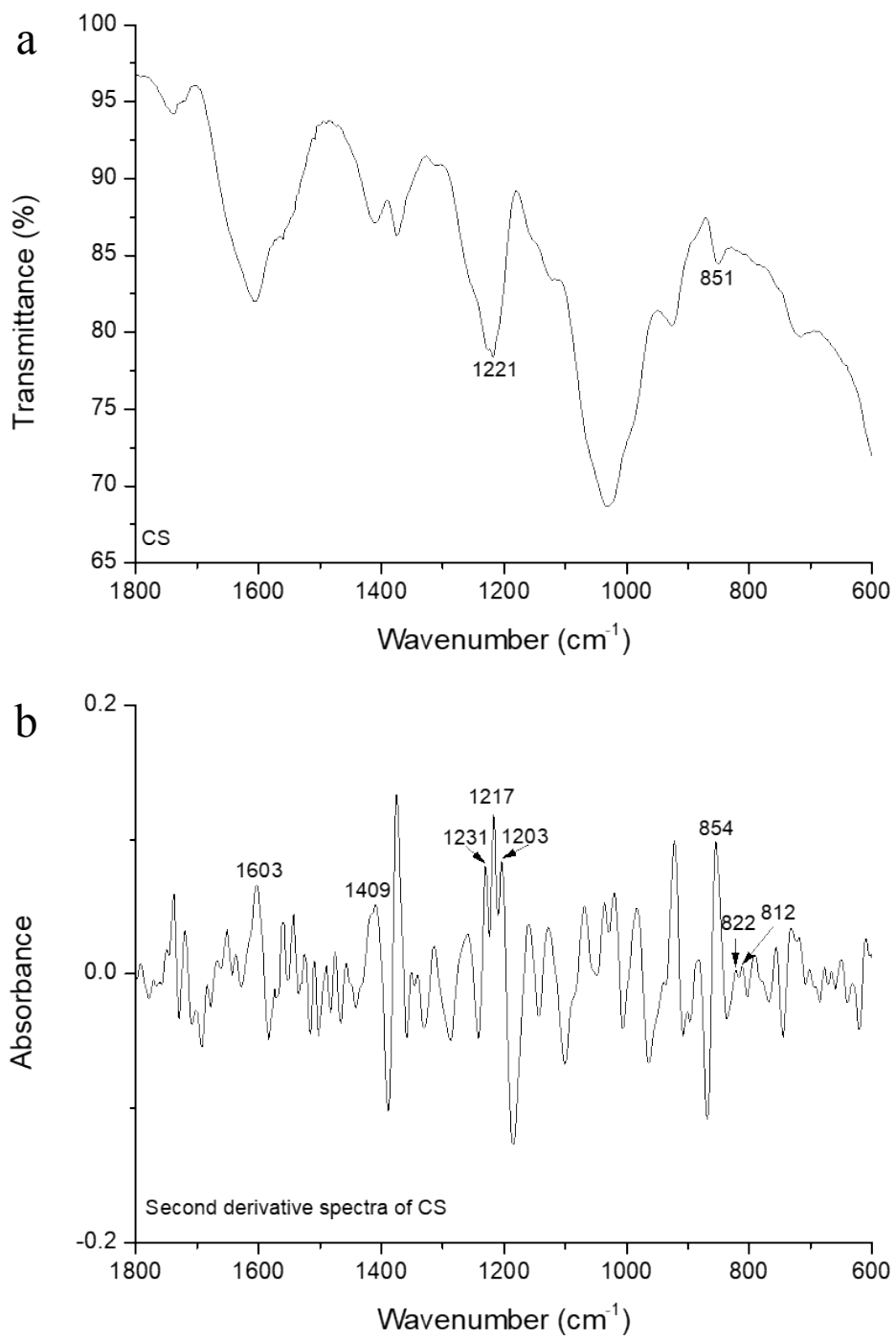


Figure 1 FTIR spectra of CS (a) and its second derivative spectra (b) from 1800 to 600 cm⁻¹.

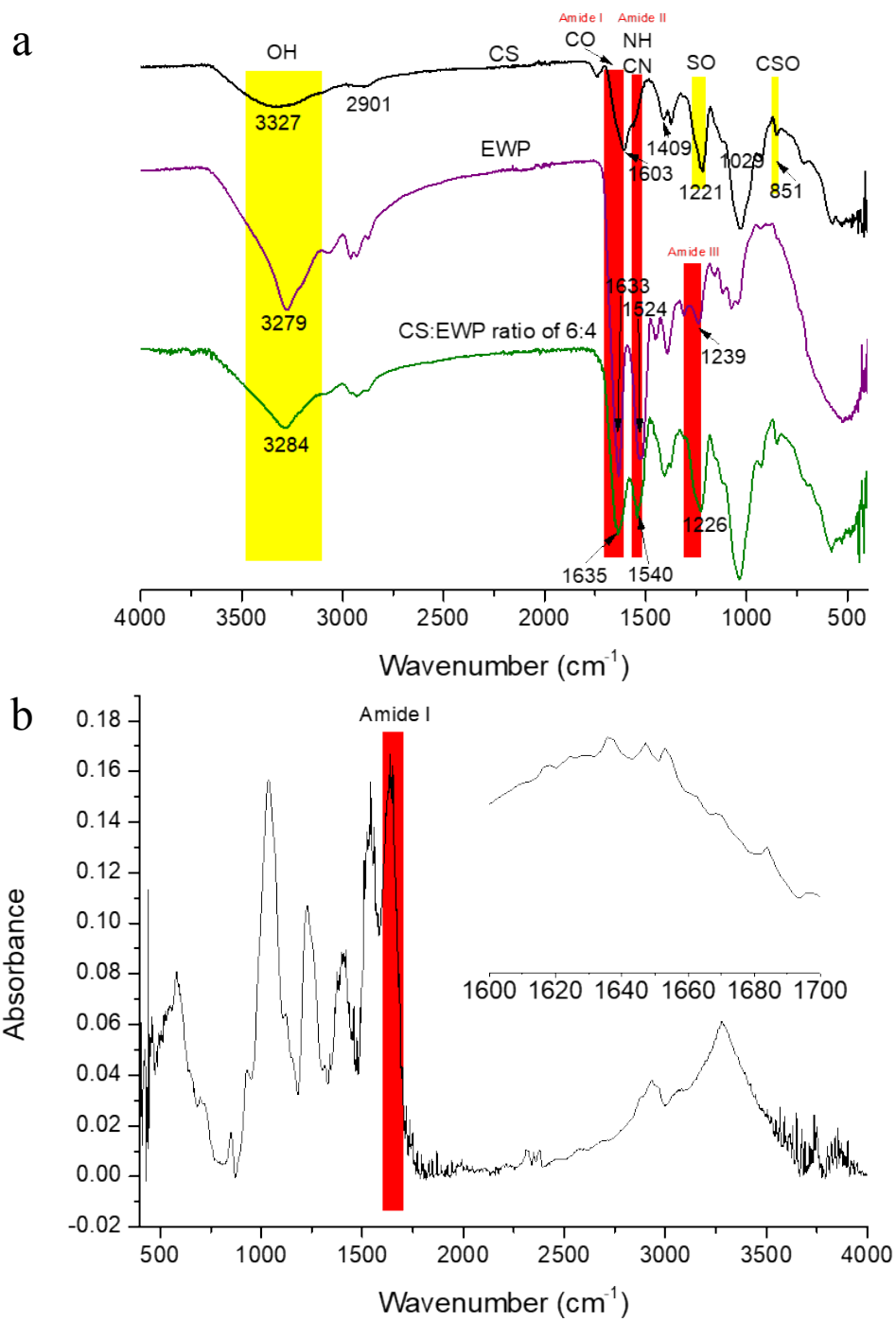


Figure 2 The FTIR spectra of CS, EWP, nanocapsules synthesized at the CS:EWP ratio of 6:4 (a), and the absorption spectra of nanocapsules synthesized at the CS:EWP ratio of 6:4 (b).

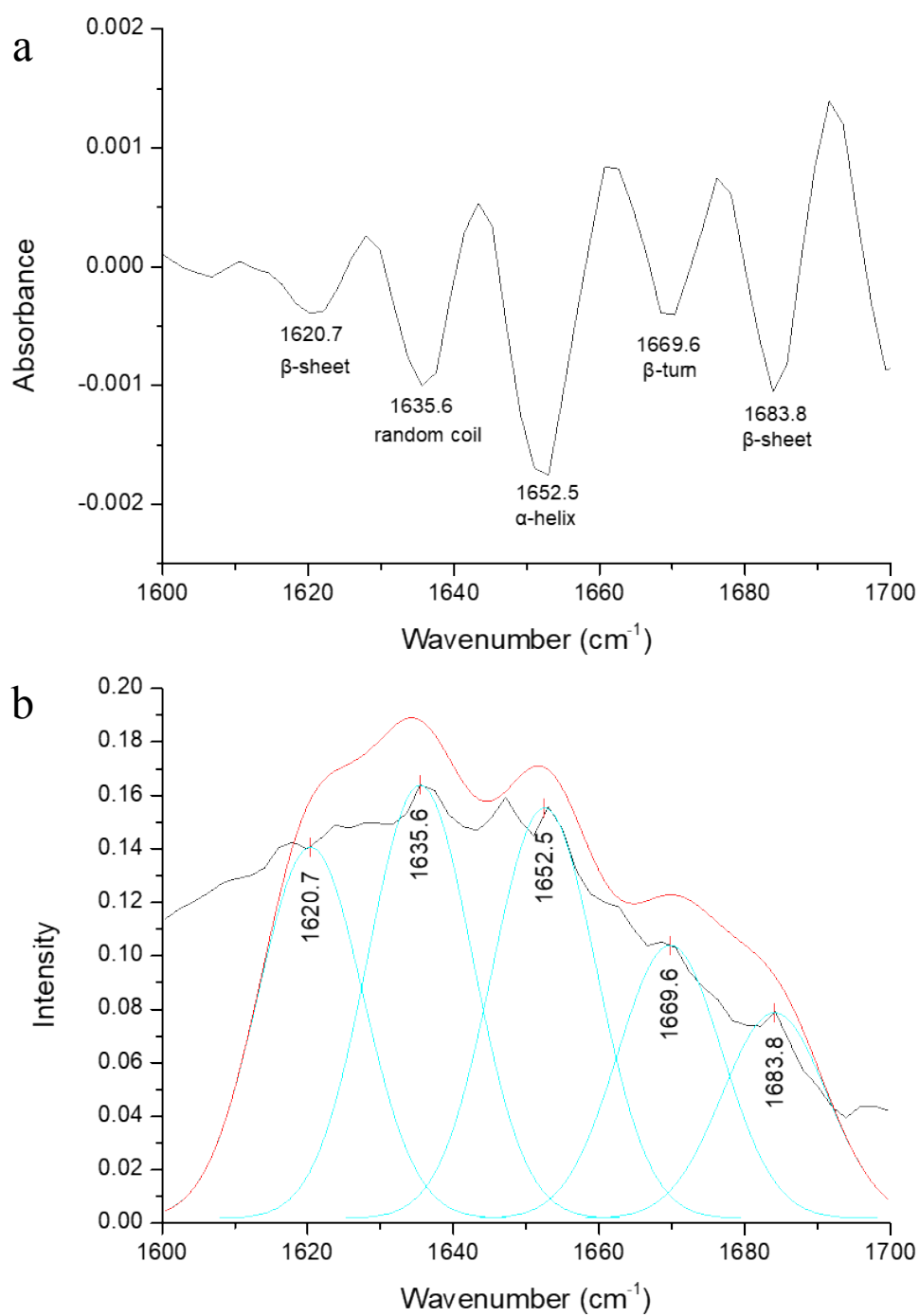


Figure 3 The secondary structural analysis of EWP by the amide I band (1600-1700 cm⁻¹). Results showed the definitions and peak areas of β -sheet, random coil, α -helix, and β -turn according to (a) the secondary derivative and (b) the deconvolution of EWP.

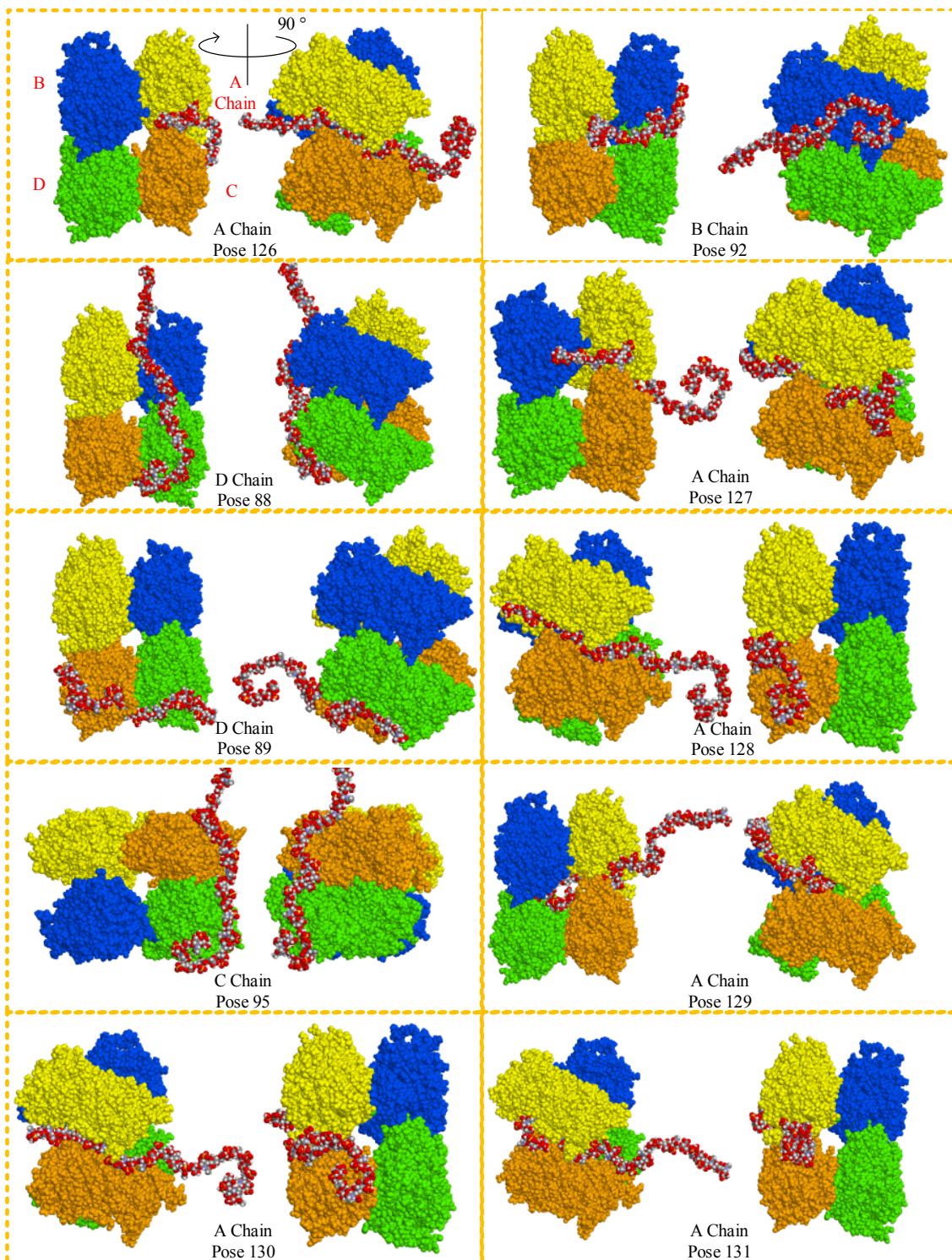


Figure 4 The best 10 conformations ranked by ZDOCK scores of protein poses in Corey-Pauling-Koltun models. The four chains of EWP were marked as yellow (A Chain), blue (B Chain), orange (C Chain), and green (D Chain), respectively.

Table 1 The best 10 protein poses ranked by ZDOCK scores in different chains of EWP

| NO. | Chain | Pose | ZDOCK Score |
|-----|---------|---------|-------------|
| 1 | A chain | Pose126 | 17.66 |
| 2 | B Chain | Pose92 | 17.6 |
| 3 | D Chain | Pose88 | 17.42 |
| 4 | A chain | Pose127 | 17.3 |
| 5 | D Chain | Pose89 | 17.28 |
| 6 | A chain | Pose128 | 17.1 |
| 7 | C Chain | Pose95 | 17.08 |
| 8 | A chain | Pose129 | 16.88 |
| 9 | A chain | Pose130 | 16.54 |
| 10 | A chain | Pose131 | 16.12 |

Table 2 The non-bonds between EWP and CS at the highest ZDOCK scores (A Chain Pose 126)

| Types | H-Donor | H-Acceptor | distance |
|----------------------------|---------------|--------------|----------|
| Conventional Hydrogen Bond | A:LYS296:HZ3 | CS:O611 | 3.006 |
| Conventional Hydrogen Bond | C:ALA28:HN | CS:O471 | 2.872 |
| Conventional Hydrogen Bond | C:GLN87G:HE22 | CS:O612 | 2.092 |
| Conventional Hydrogen Bond | C:ASN91:HD21 | CS:O520 | 2.221 |
| Conventional Hydrogen Bond | C:HIS376:HD1 | CS:O516 | 2.610 |
| Conventional Hydrogen Bond | C:ASN380:HD21 | CS:O482 | 2.607 |
| Conventional Hydrogen Bond | CS:H462 | C:ASN380:OD1 | 2.683 |
| Conventional Hydrogen Bond | CS:H603 | A:GLU295:OE1 | 2.594 |
| Conventional Hydrogen Bond | CS:H604 | A:GLU295:OE2 | 2.554 |
| Carbon Hydrogen Bond | A:SER215:HB2 | CS:O389 | 2.516 |
| Carbon Hydrogen Bond | A:LYS296:HE1 | CS:O611 | 2.300 |
| Carbon Hydrogen Bond | A:SER301:HA | CS:O659 | 1.957 |
| Carbon Hydrogen Bond | C:SER278:HB1 | CS:O336 | 1.542 |
| Carbon Hydrogen Bond | C:THR379:HB | CS:O481 | 2.779 |
| Carbon Hydrogen Bond | CS:H404 | C:ASN279:OD1 | 2.702 |
| Carbon Hydrogen Bond | CS:H452 | A:SER215:O | 2.376 |
| Carbon Hydrogen Bond | CS:H501 | C:ALA378:O | 2.428 |
| Carbon Hydrogen Bond | CS:H507 | C:ALA378:O | 2.352 |
| Carbon Hydrogen Bond | CS:H550 | C:ASP98:OD2 | 2.054 |
| Carbon Hydrogen Bond | CS:H553 | C:ASP98:OD2 | 3.094 |
| Carbon Hydrogen Bond | CS:H592 | A:LYS296:O | 2.251 |
| Carbon Hydrogen Bond | CS:H594 | A:LYS296:O | 2.526 |
| Pi-Sulfur | CS:S468 | C:PHE269 | 5.293 |
| Pi-Sulfur | CS:S515 | C:HIS376 | 4.313 |

Example: A:LYS296:HZ3 means the HZ3 of the 296th Lysine (LYS296) from the A Chain of egg white protein (EWP). CS:O611 means the 611th O atom from chondroitin sulfate (CS).