Electronic Supplementary Material (ESI) for Soft Matter.
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Supporting Materials

Folic acid/polydopamine nanofibers show enhanced ordered-stacking via π-π interaction

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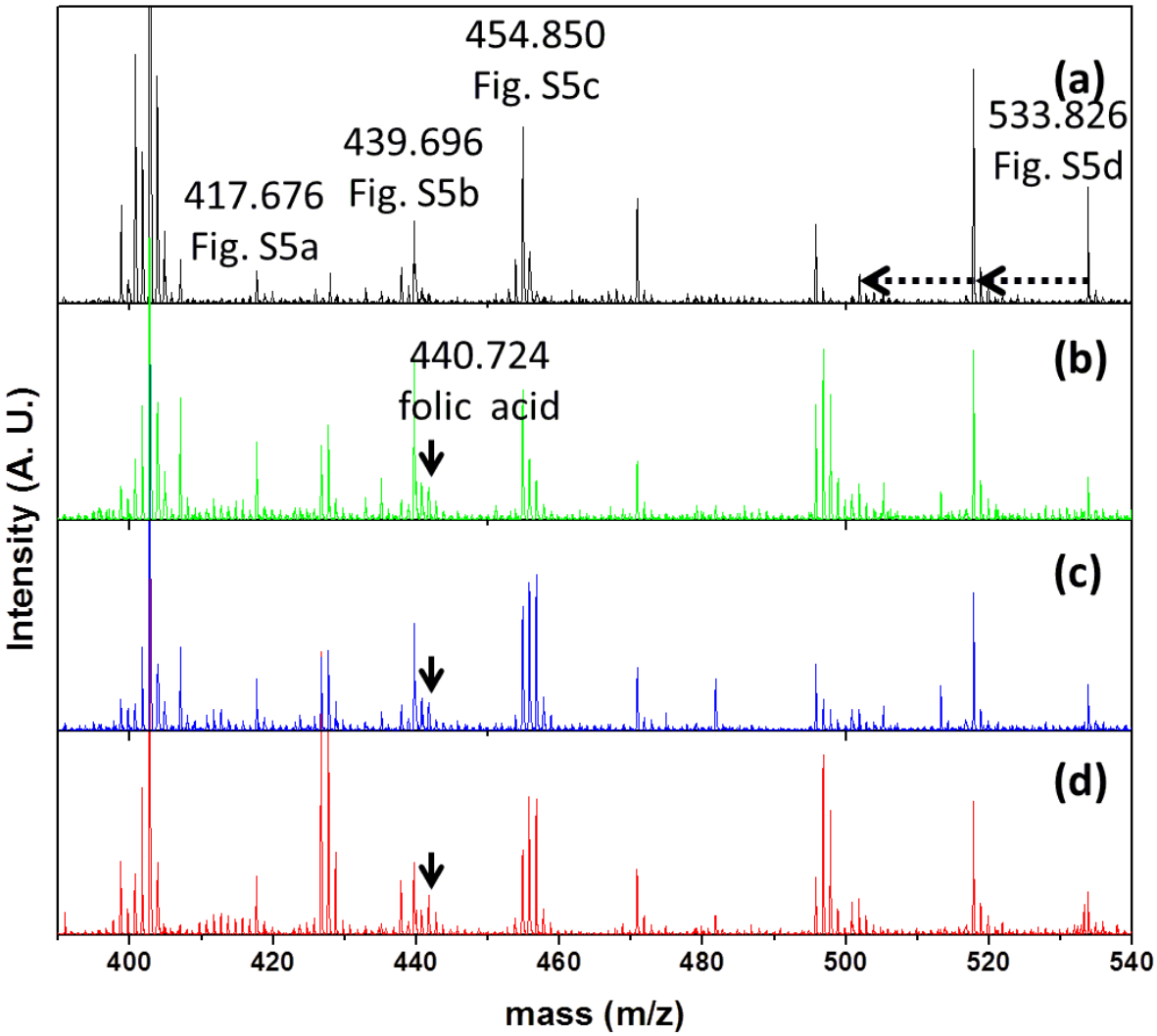

Fig. S1 Segmental spectrum of MALDI-TOF (m/z: 380-540 Da) characterizations of (a) PDA nanoparticles, (b) FA/PDA nanoparticles, (c) FA/PDA nanofibers (NaOH), and (d) FA/PDA nanofibers (tris-HCl buffer), respectively. These m/z values correspond to trimers and tetramers structures.

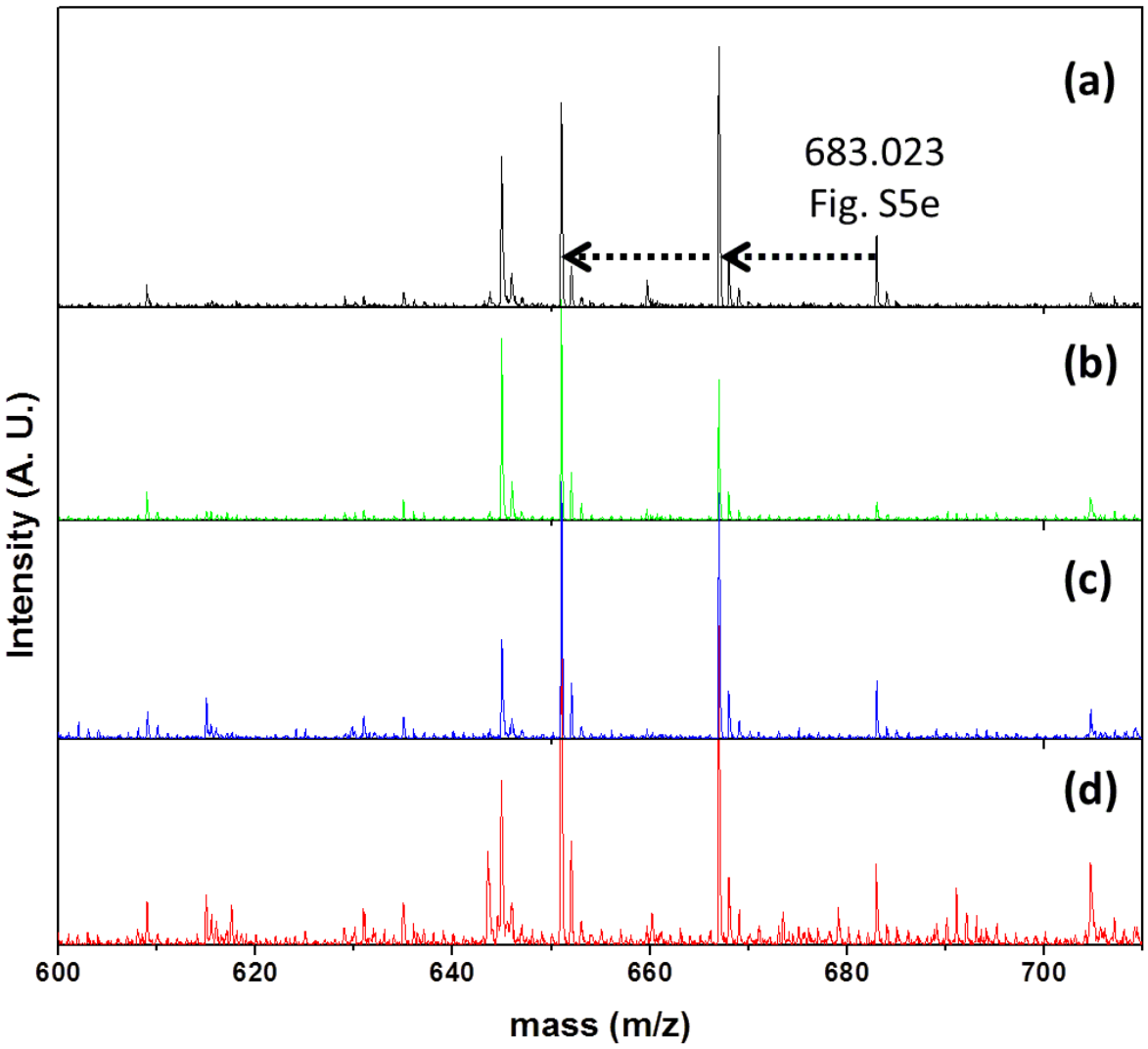

Fig. S2 Segmental spectrum of MALDI-TOF (m/z: 600-710 Da) characterizations of (a) PDA nanoparticles, (b) FA/PDA nanoparticles, (c) FA/PDA nanofibers (NaOH), and (d) FA/PDA nanofibers (tris-HCl buffer), respectively. These m/z values correspond to possible pentamers.

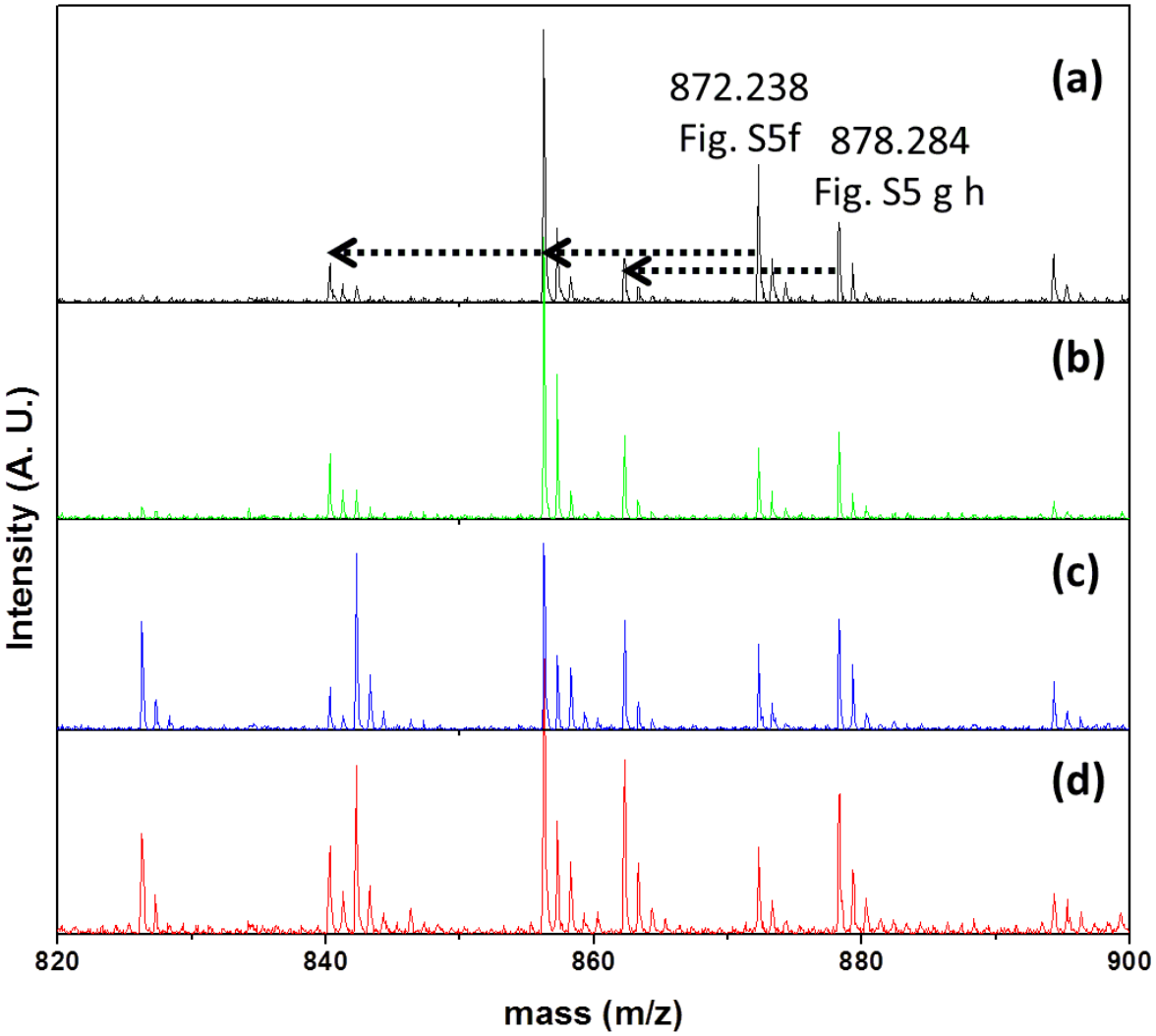

Fig. S3 Segmental spectrum of MALDI-TOF (m/z: 820-900 Da) characterizations of (a) PDA nanoparticles, (b) FA/PDA nanoparticles, (c) FA/PDA nanofibers (NaOH), and (d) FA/PDA nanofibers (tris-HCl buffer), respectively. This part represents to possible hexamer's structures.

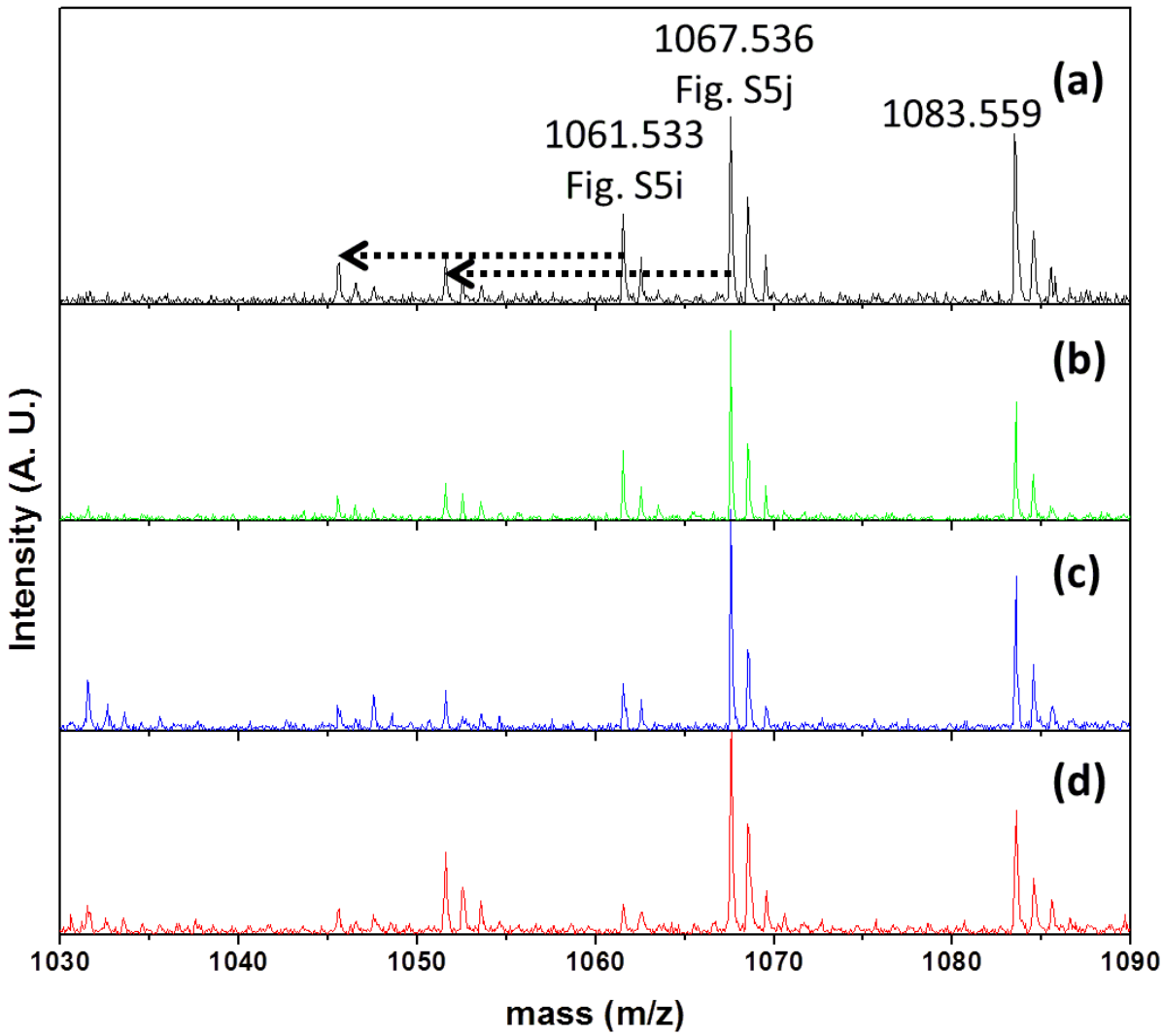

Fig. S4 Segmental spectrum of MALDI-TOF (m/z: 1030-1090 Da) characterizations of (a) PDA nanoparticles, (b) FA/PDA nanoparticles, (c) FA/PDA nanofibers (NaOH), and (d) FA/PDA nanofibers (tris-HCl buffer), respectively. This part corresponds to possible octamers' structure.

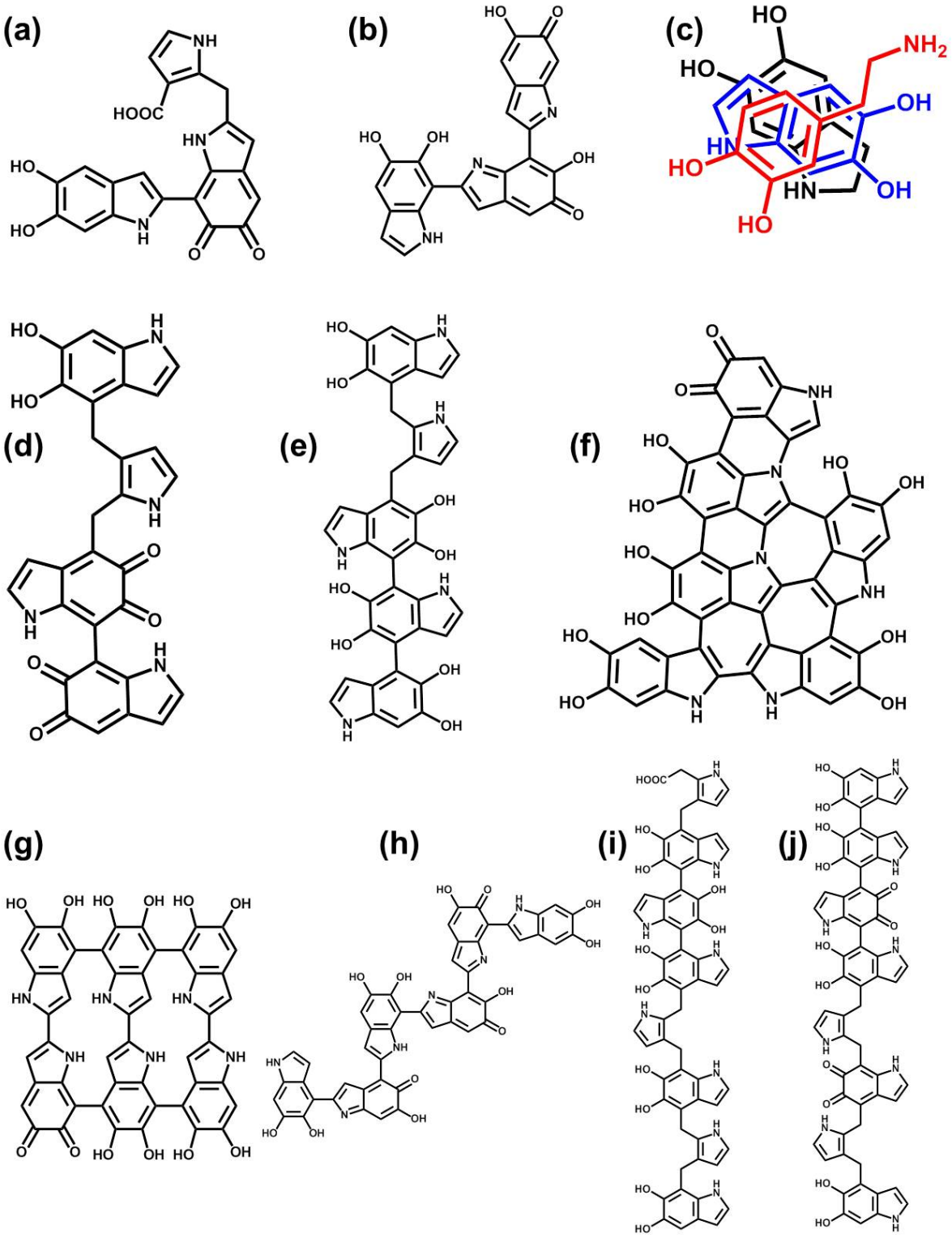

Fig. S5 Possible oligomer structures in PDA and FA/PDA nanoparticles or nanofibers.

Table S1. MALDI-TOF MS common peaks of four samples.

	m/z peak	calculated $[M+H]^+$ or $M\bullet^+$ mass	oligomer*	possible structure**
Trimer (III)	417.676	417.371	H+q+D	a[1]
	439.696	439.377	H+2q	b
	454.850	454.495	DA+2H	c[2]
	470.838		DA+2H +16	
Tetramer (IV)	501.905		IV-16-16	
	517.812		IV-16	
	533.826	533.511	H+2q+D (IV)	d
Pentamer (V)	651.001		V-16-16	
	666.995		V-16	
	683.032	683.202	4H+D (V)	e
Hexamer (VI)	840.306		VI_1-16-16	
	856.257		VI_1-16	
	862.247		VI_2-16	
	872.238	872.114	3H+3q-6 (VI_1)	f[3]
	878.284	878.161	3H+3q (VI_2)	g[4] h
	894.285		VI_2+16	
Octamer (VIII)	1051.566		VIII_2-16	
	1061.533	1061.347	5H+3D (VIII_1)	i
	1067.536	1067.300	4H+2q+2D (VIII_2)	j
	1083.559		VIII_2+16	

* DA (dopamine), H (DHI), q (Quinone-methide or Indolequinone), D (partially degradation),[5,6] -16 suggests liberation of one hydroxyl group,[7] +16 suggests add an oxygen group.[8]

** The chemical structures of those oligomers are similar or identical to that in literature.

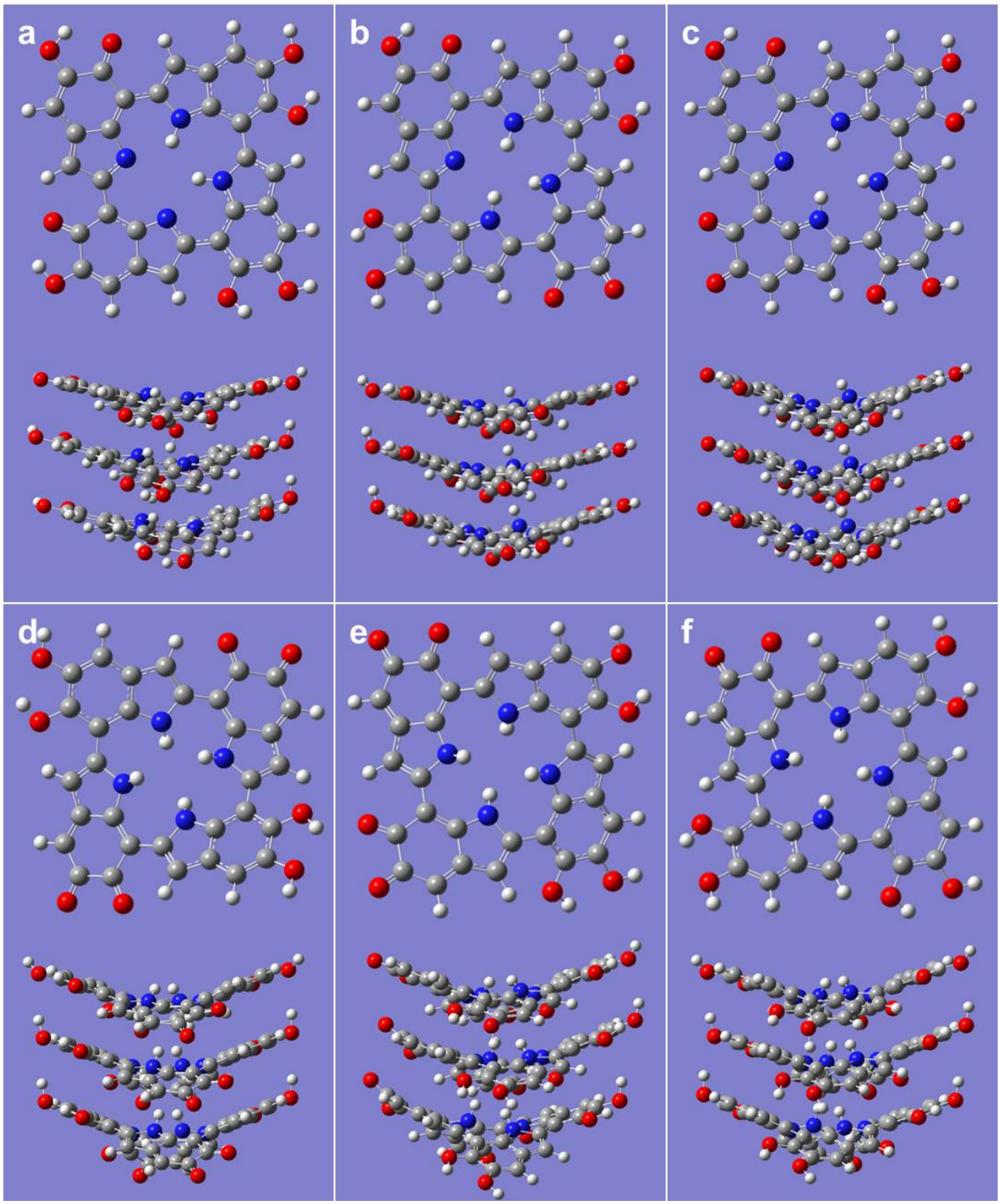

Fig. S6 Optimized molecule structures and three-layer stacked structures of (a) QQHH, (b) QHIH, (c) QIHH, (d) HIHI, (e) HHII, and (f) IHHH, respectively.

References:

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