

# Co-assembly of C<sub>13</sub>-dipeptides: gelations from solutions and precipitations

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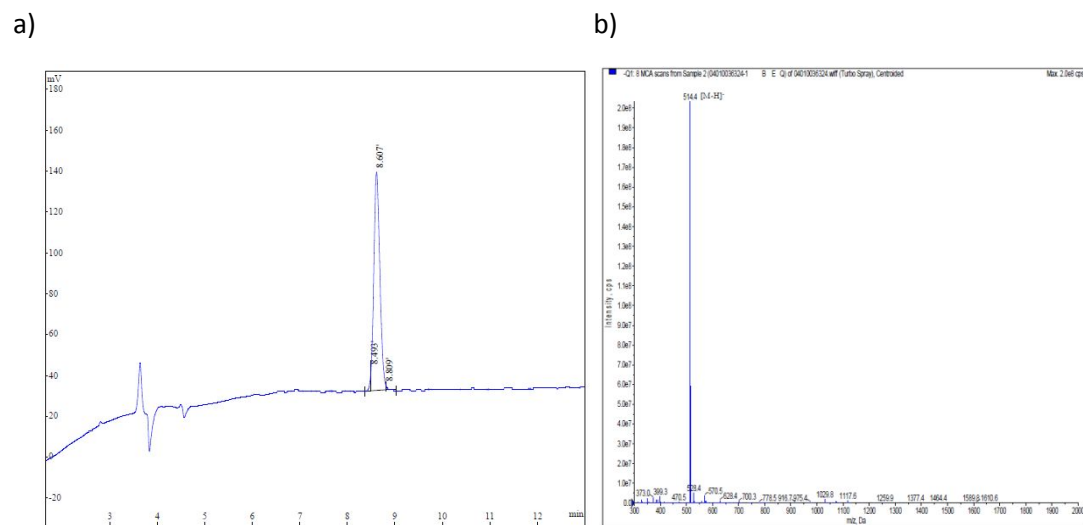
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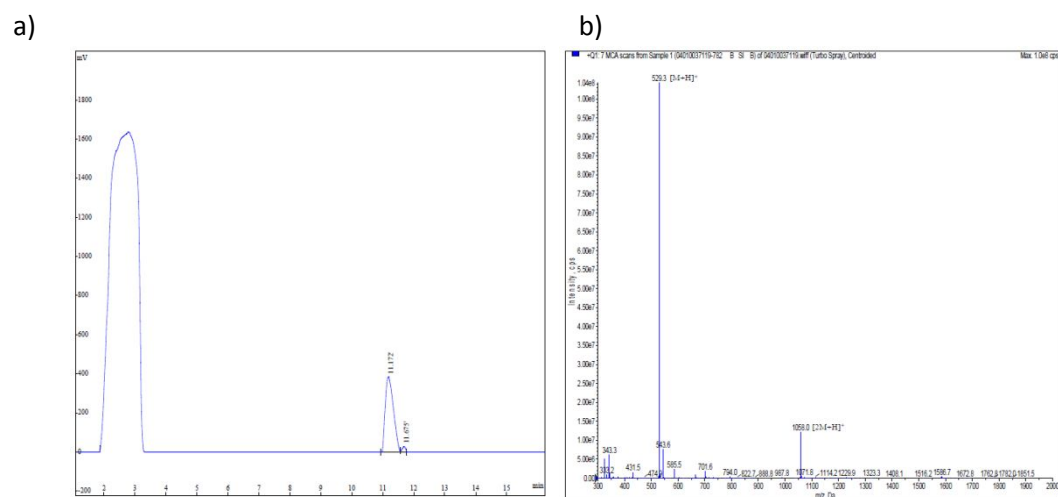
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<sup>1</sup> Tan Hu and Zhuo Zhang contributed equally.

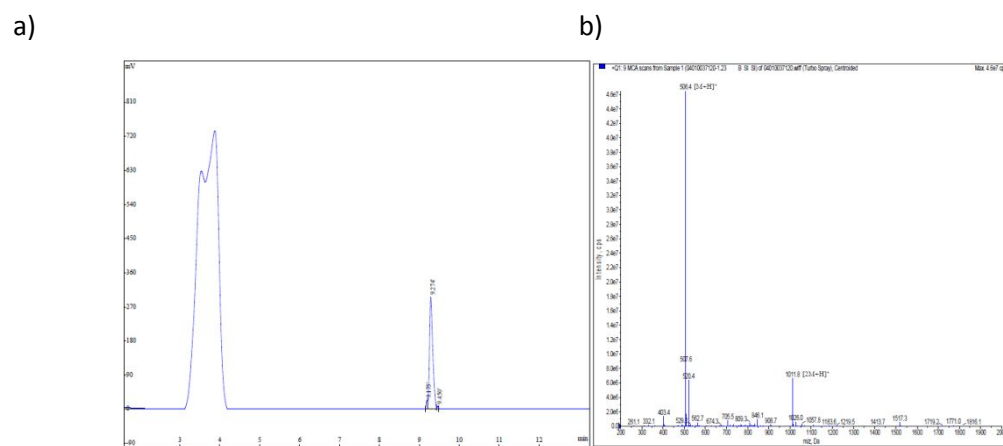
## HPLC analysis and Mass analysis of C<sub>13</sub>-dipeptides



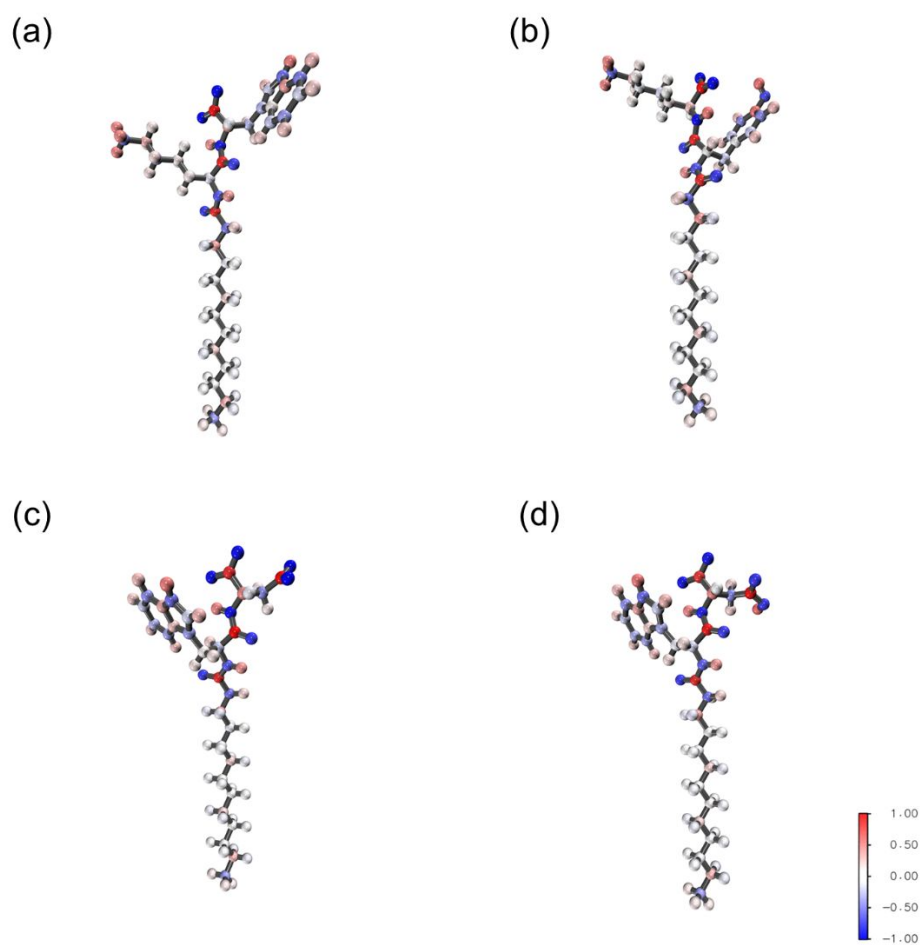
**Figure S1** HPLC (a) and mass spectroscopy (b) of synthesized C<sub>13</sub>-WD.



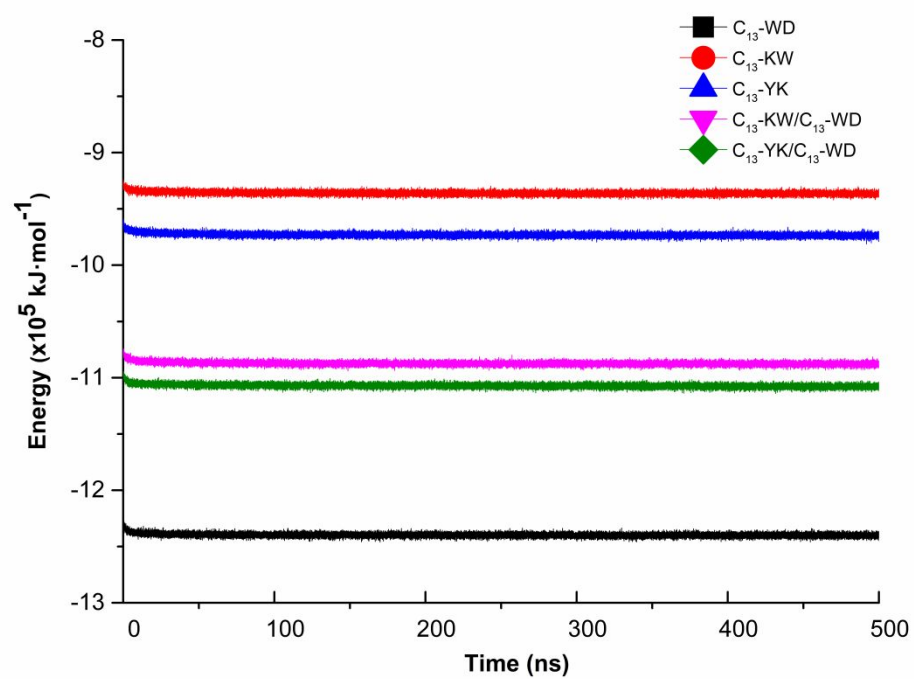
**Figure S2** HPLC (a) and mass spectroscopy (b) of synthesized C<sub>13</sub>-KW.



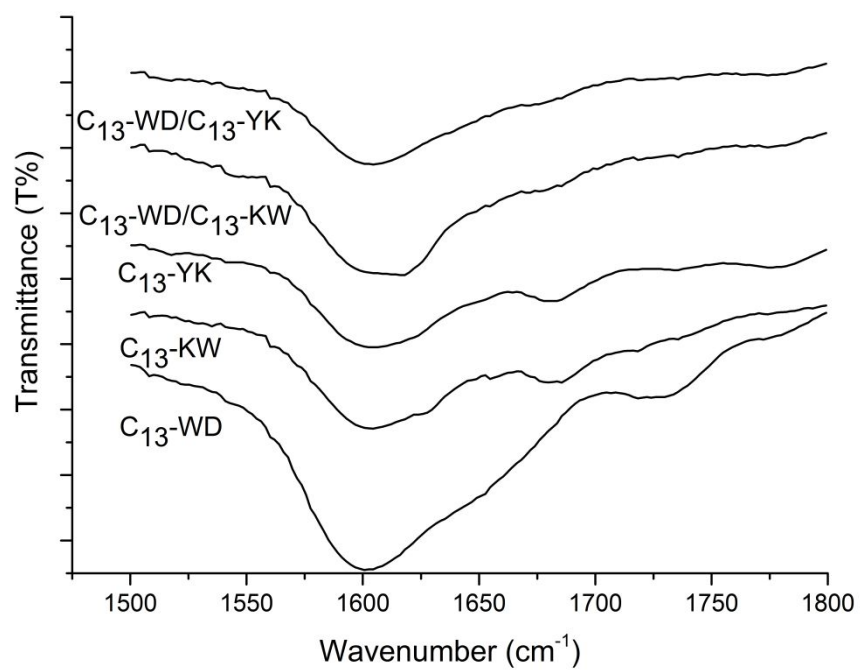
**Figure S3.** HPLC (a) and mass spectroscopy (b) of synthesized C<sub>13</sub>-YK.



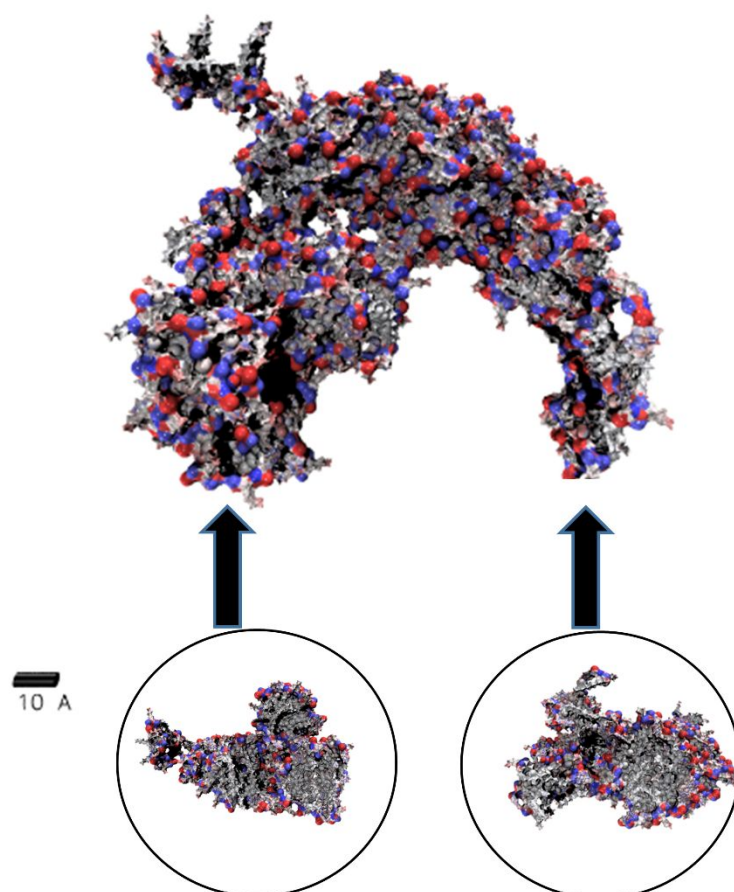
**Figure S4.** The atomic charges at pH=4.6 of (a) C<sub>13</sub>-KW, (b) C<sub>13</sub>-YK, (c) C<sub>13</sub>-WD<sup>2-</sup>, and (d) C<sub>13</sub>-WD<sup>-</sup>.



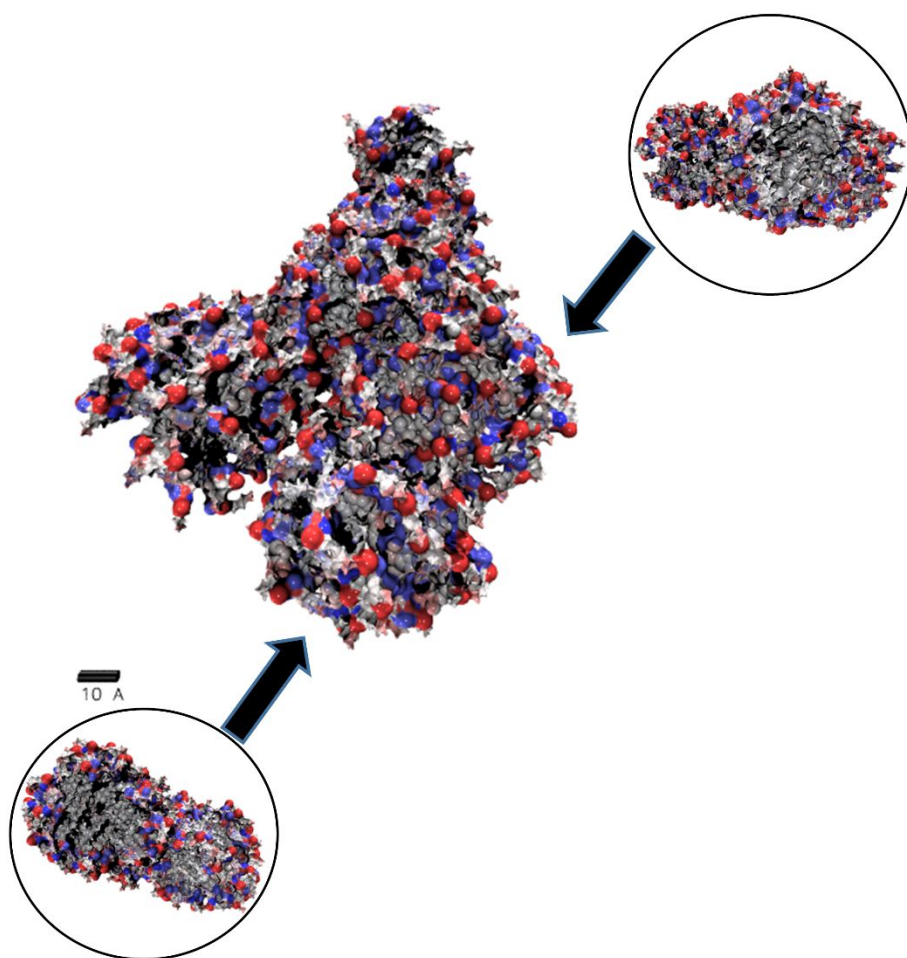
**Figure S5.** The total energies of the individual systems for the 500 ns trajectories.



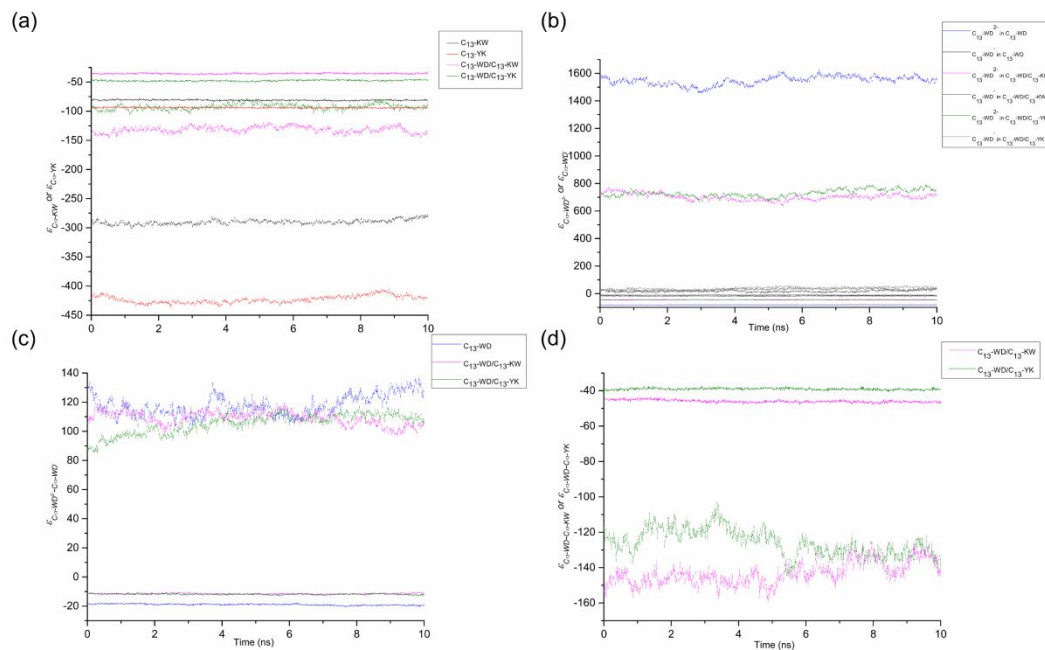
**Figure S6.** The details of FT-IR in 1500cm<sup>-1</sup>~1800cm<sup>-1</sup> of C<sub>13</sub>-WD, C<sub>13</sub>-KW, C<sub>13</sub>-YK, C<sub>13</sub>-WD/C<sub>13</sub>-KW and C<sub>13</sub>-WD/C<sub>13</sub>-YK.



**Figure S7.** The charge distribution of C<sub>13</sub>-KW at pH=4.6.



**Figure S8.** The charge distribution of C<sub>13</sub>-YK at pH=4.6.



**Figure S9.** Molecular contributions to the hydrophobic (as revealed by Lennard-Jones potentials, solid lines) and electrostatic (as revealed by Coulomb potentials, dashed lines) interactions,  $\epsilon$ , for various molecules and systems.



**Table S1.** Lennard-Jones potentials and the Coulomb potentials averaged from the last 100 ns of the trajectories for a single C<sub>13</sub>-dipeptide molecule.

Name	C <sub>13</sub> -KW	C <sub>13</sub> -YK	C <sub>13</sub> -WD <sup>2-</sup>	C <sub>13</sub> -WD <sup>-</sup>
Lennard-Jones potential (kJ/mol)	-54.82±5.09	-32.11±4.54	-34.26±6.06	-35.98±5.98
Coulomb potential (kJ/mol)	-799.75±25.48	-951.29±25.91	-521.54±21.16	-640.55±48.33