

Supplementary information for

Biom mineralization through a symmetry-controlled oligomeric peptide

Tatsuya Sakaguchi ^{1,2,†}, Natsumi Nakagawa ^{1,†}, Kenta Mine ¹, Jose Isagani B. Janairo ³, Rui Kamada ¹, James G. Omichinski ^{4*}, and Kazuyasu Sakaguchi ^{1,*}

1. Laboratory of Biological Chemistry, Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo 060-0810, Japan; sakaguchi_tatsuya@kurume-u.ac.jp (T.S.); n-nakagawa@sci.hokudai.ac.jp (N.N.); kenta.mine@outlook.com (K.M.), kamadar@sci.hokudai.ac.jp (R.K.)
2. Department of Chemistry, Kurume University School of Medicine, Kurume 830-0011, Japan.
3. Biology Department, De La Salle University, 2401 Taft Avenue, 0922 Manila, Philippines.
4. Département de Biochimie et Médecine Moléculaire, Université de Montréal, H3C 3J7 QC, Canada; jg.omichinski@umontreal.ca

* Correspondence: jg.omichinski@umontreal.ca (J.G.O.); kazuyasu@sci.hokudai.ac.jp (K.S.)

† These authors contributed equally to this work.

Content:

- **Table S1:** Peptide sequences of TBP-CC peptides.
- **Table S2:** DNA sequences of frame strands.
- **Figure S1:** HPLC profiles of the synthesized peptides.
- **Figure S2:** MALDI-TOF MS spectra of the synthesized peptides.
- **Figure S3:** Change in ellipticity at 222 nm as a function of temperature for TBP-CC peptides
- **Figure S4:** Change in ellipticity at 275 nm as a function of temperature for TBP-DNA oligomers.
- **Figure S5:** Histogram and Kernel Density Estimate (KDE) plot of silver nanoparticle sizes produced by TBP-DNAs.

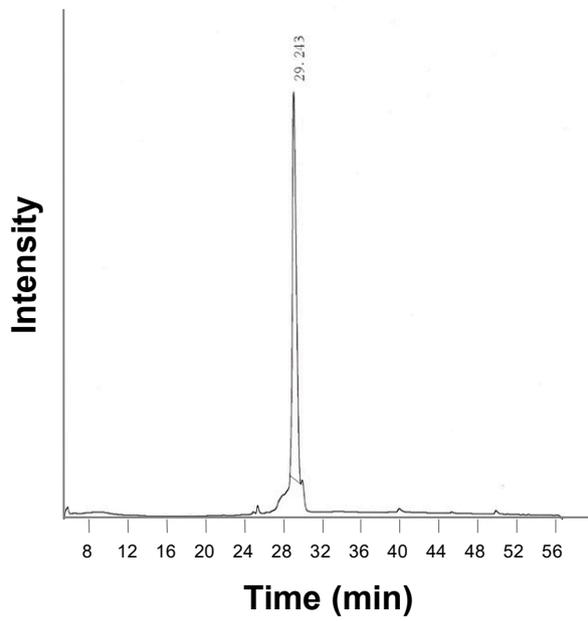
Table S1. Peptide sequences of TBP-CC peptides

| Name | Sequence |
|-------------|--|
| TBP-CC(Di) | H-RKLPDAGGRMKQLEDKVEELLSKKNYHLENEVARLKKLVGER-NH ₂ |
| TBP-CC(Tri) | H-RKLPDAGGSGIDQEQQNLTRLIEAQIHELQLTQWKIKQLLARIL-NH ₂ |
| TBP-CC(Tet) | H-RKLPDAGGGELAAIKQELAAIKKELAAIKWELAAIKQGAG-NH ₂ |

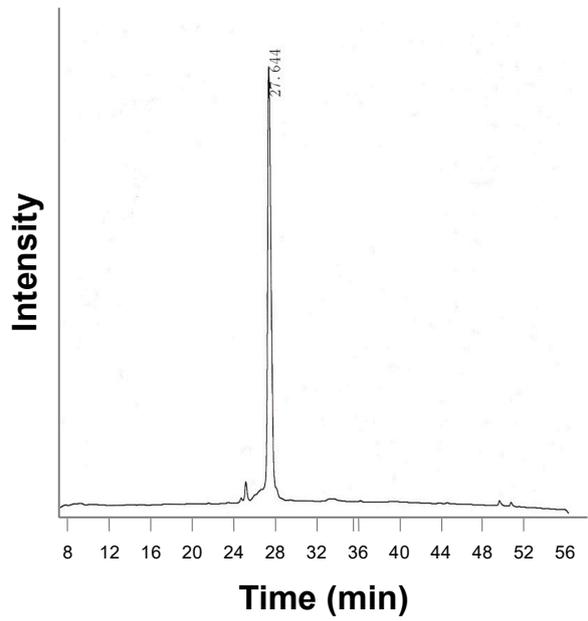
Table S2. DNA sequences of frame strands used in TBP-DNA constructs

| Strand ID | Sequence |
|------------------|----------------------------|
| S1 | 5'-AACCTG CGAAGT ctatcg-3' |
| S2 | 5'-ACTTCG CAGGTT ctatcg-3' |
| S3 | 5'-ACTTCG GATGCA ctatcg-3' |
| S4 | 5'-TGCATC CAGGTT ctatcg-3' |
| S5 | 5'-TGCATC GACCAT ctatcg-3' |
| S6 | 5'-ATGGTC CAGGTT ctatcg-3' |

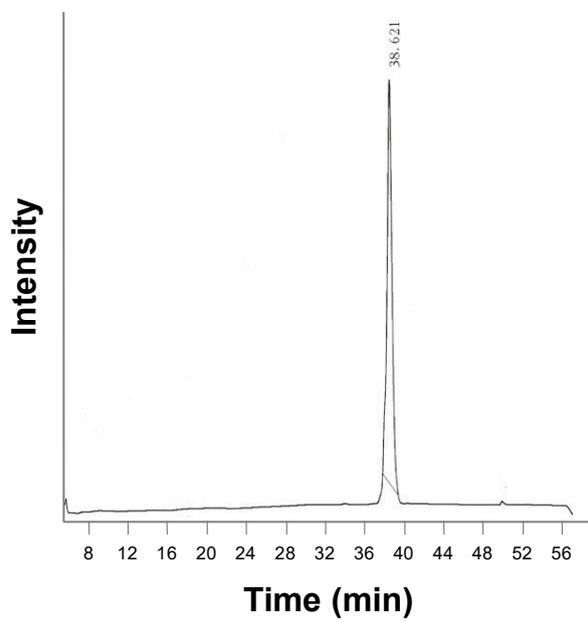
(a)



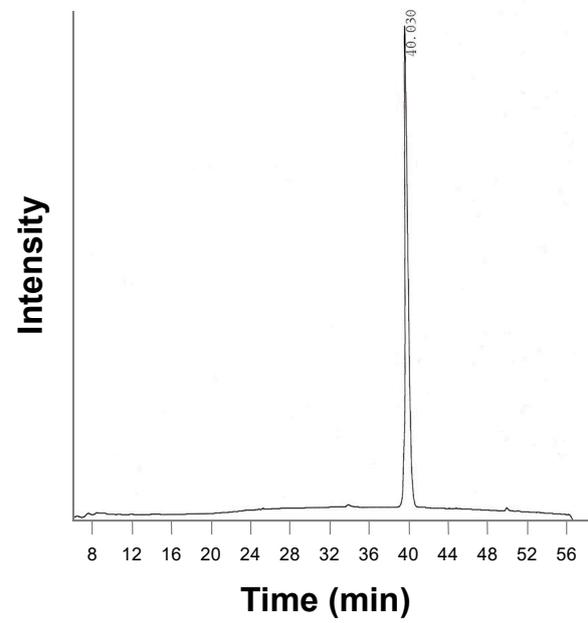
(b)



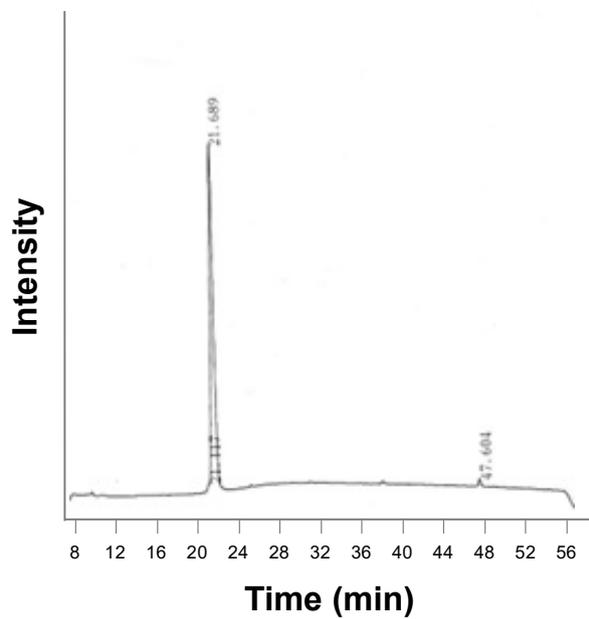
(c)



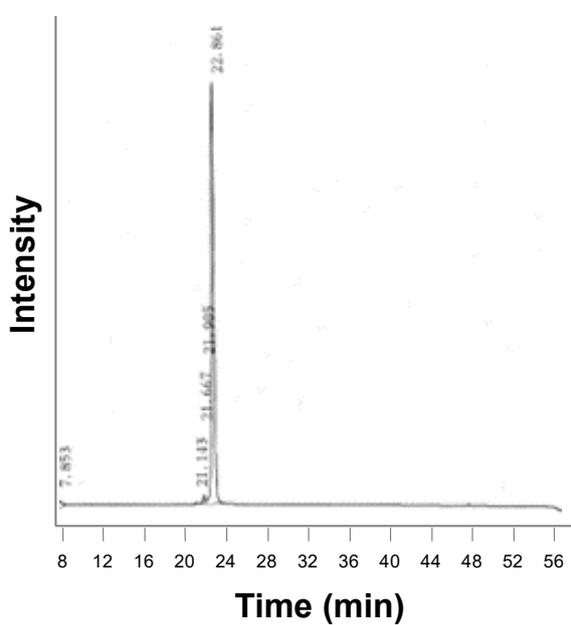
(d)



(e)



(f)



(g)

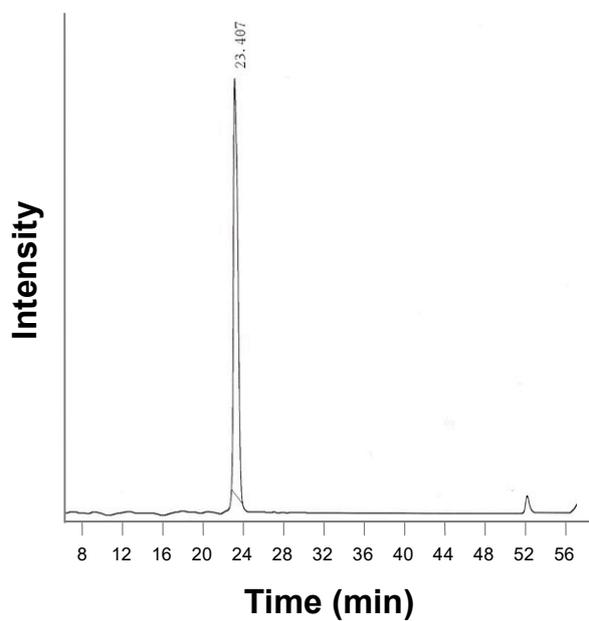
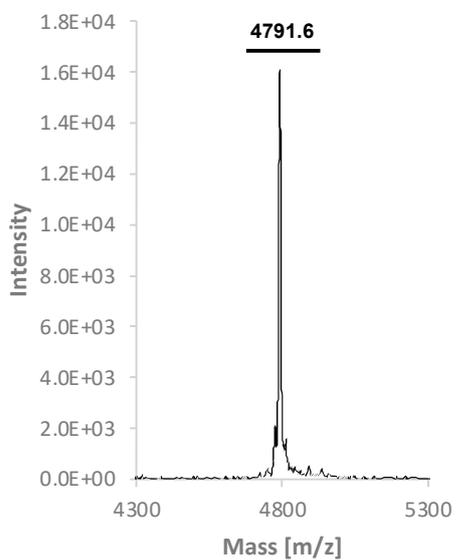
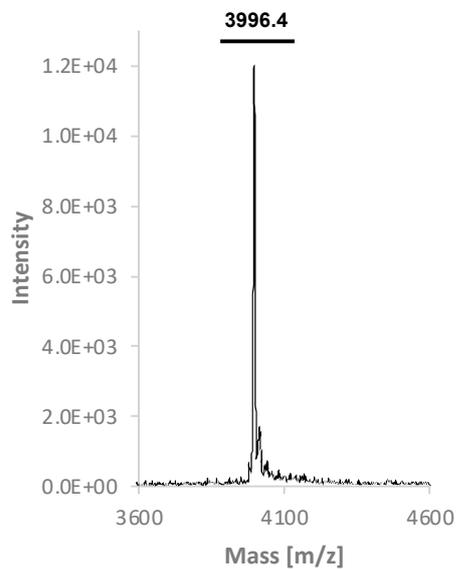


Figure S1. HPLS profiles of the synthesized peptides. (a) TBP-CC(Di), (b) CC(Di), (c) TBP-CC(Tri), (d) CC(Tri), HPLS profiles of the synthesized peptides. (e) TBP-CC(Tet), (f) CC(Tet), (g) TBP-GlyGlyCys

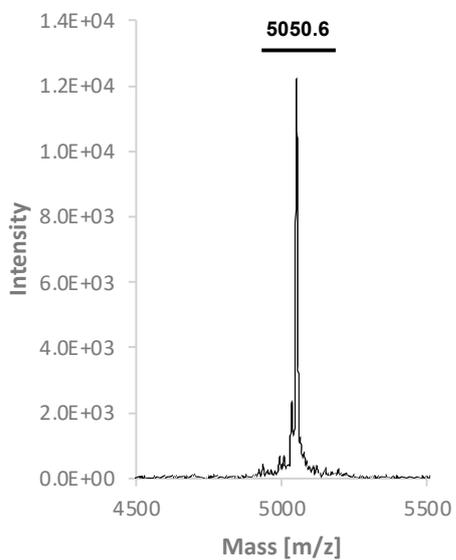
(a) [MH]⁺(ave, calc): 4791.61



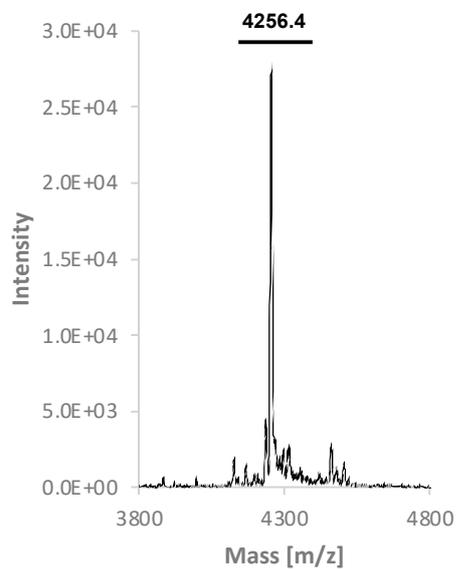
(b) [MH]⁺(ave, calc): 3996.70



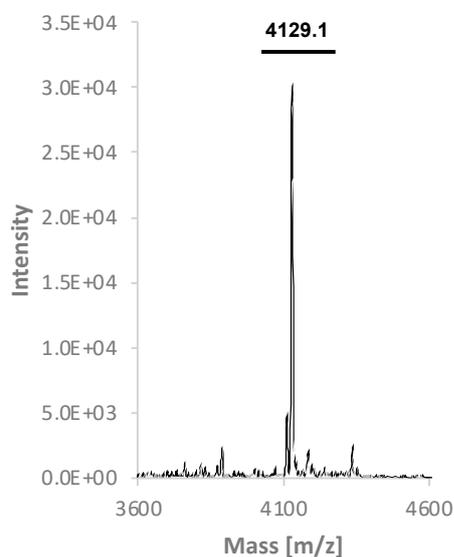
(c) [MH]⁺(ave, calc): 5050.90



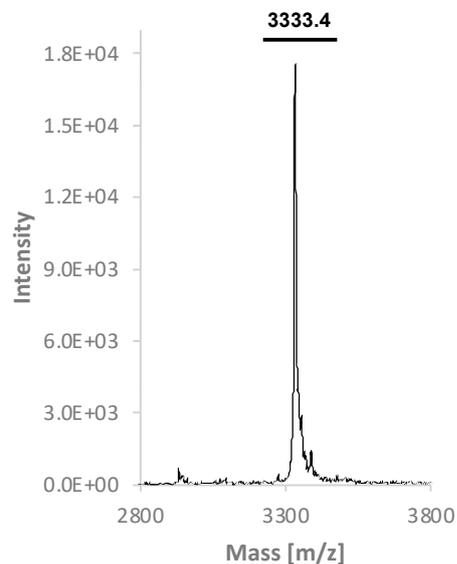
(d) [MH]⁺(ave, calc): 4255.99



(e) $[MH]^+$ (ave,calc): 4128.93



(f) $[MH]^+$ (ave, calc): 3334.01



(g) $[MH]^+$ (ave, calc): 916.1

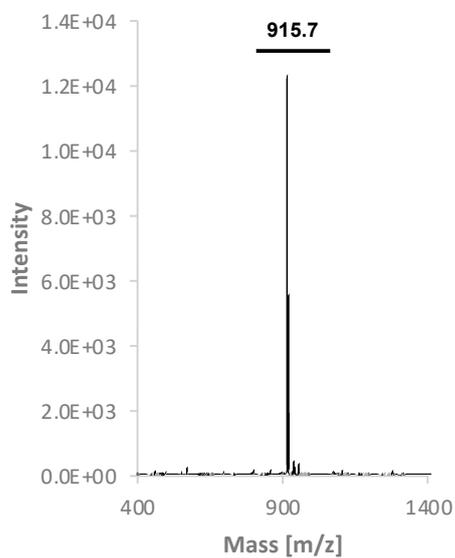


Figure S2. MALDI-TOF MS spectra of the synthesized peptides. (a) TBP-CC(Di), (b) CC(Di), (c) TBP-CC(Tri), (d) CC(Tri), MALDI-TOF MS spectra of the synthesized peptides. (e) TBP-CC(Tet), (f) CC(Tet), (g) TBP-GlyGlyCys

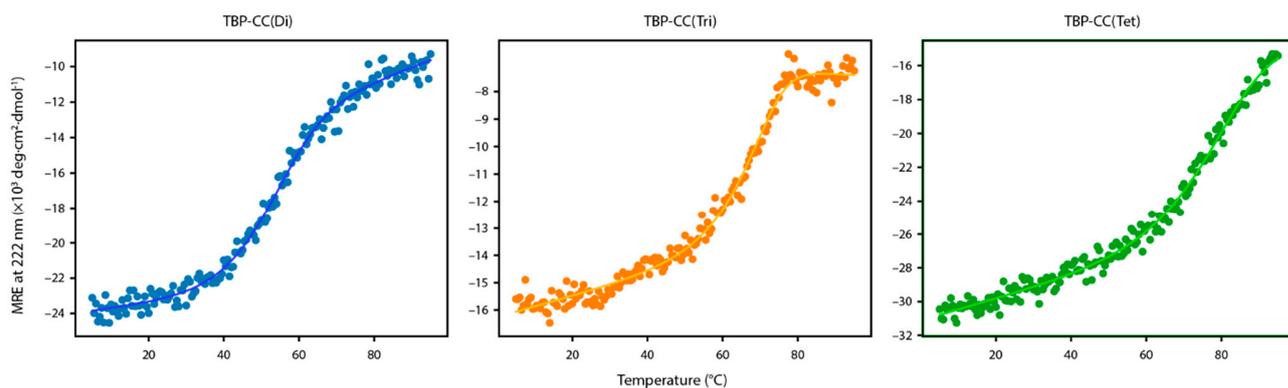


Figure S3. Change in ellipticity at 222 nm as a function of temperature for TBP-CC peptides. The temperature-dependent curves are shown for the TBP-CC(Di) peptide (**left panel**), the TBP-CC(Tri) peptide (**center panel**), and the TBP-CC(Tet) peptide (**right panel**). Peptide solutions were prepared at a concentration of 10 μM in a 20 mM phosphate buffer (pH 7.4). Temperature variation was monitored from 4°C to 96°C, with a scanning rate of 1°C per minute.

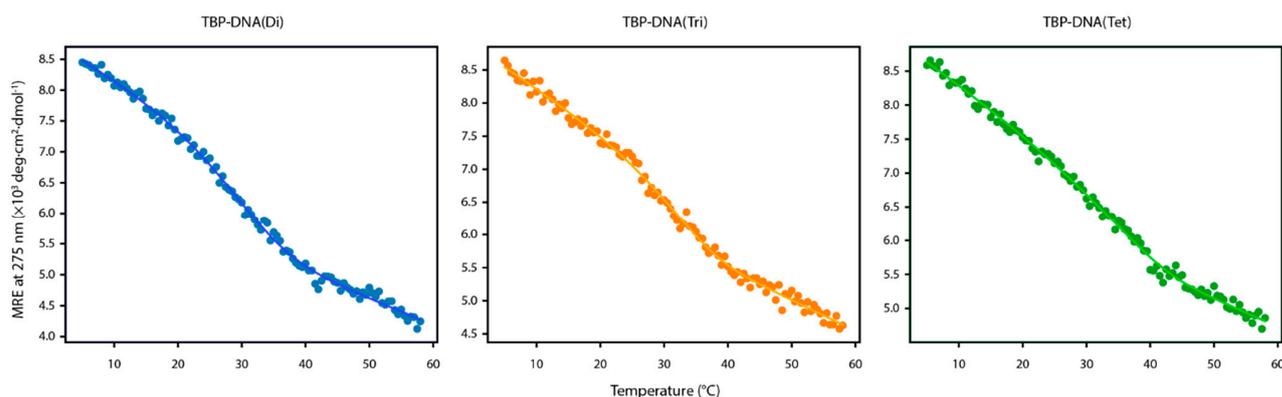


Figure S4. Change in ellipticity at 275 nm as a function of temperature for TBP-DNA oligomers. The temperature-dependent curves are shown for the TBP-DNA(Di) peptide (**left panel**), the TBP-DNA(Tri) peptide (**center panel**), and TBP-DNA(Tet) peptide (**right panel**). The solutions were prepared with a concentration of 20 μM monomer strands in a 20 mM phosphate buffer (pH 7.4). The temperature ranged from 4°C to 58°C, and the scan rate was set at 1°C per minute.

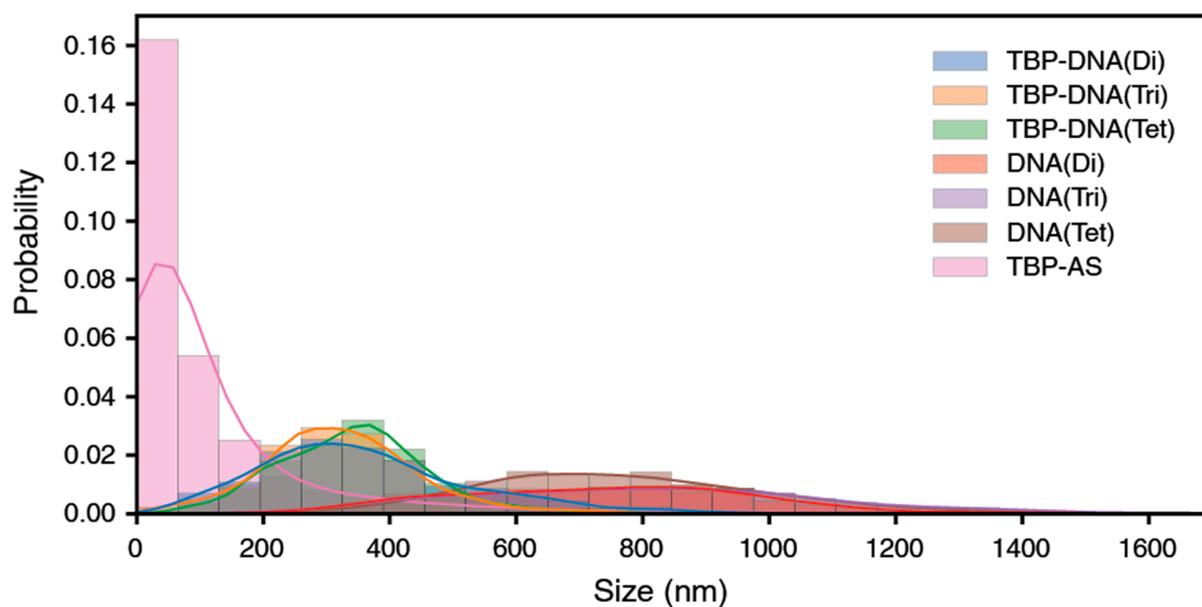


Figure S5. Histogram and Kernel Density Estimate (KDE) plot of silver nanoparticle sizes produced by TBP-DNA(Di) (blue), TBP-DNA(Tri) (orange), TBP-DNA(Tet) (green), DNA(Di) (red), DNA(Tri) (purple), DNA(Tet) (brown), and TBP-AS (pink). The number of particles analyzed for TBP-DNA(Di), TBP-DNA(Tri), TBP-DNA(Tet), DNA(Di), DNA(Tri), DNA(Tet), and TBP-SA were $N=1500$, $N=1397$, $N=1356$, $N=973$, $N=1071$, $N=1304$, and $N=3035$, respectively.