Supplementary Material

Molecular Dynamics Simulation Studies on the Aggregation of Amyloid-β Peptides and Their Disaggregation by Ultrasonic Wave and Infrared Laser Irradiation

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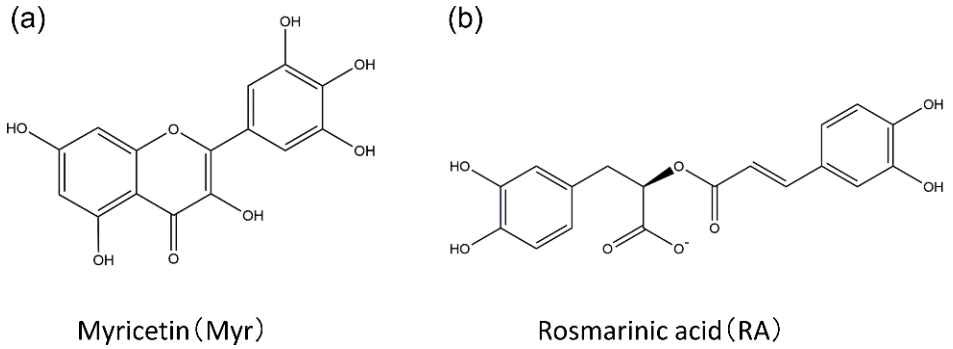

Figure S1. The chemical structures of (a) myricetin (Myr) and (b) rosmarinic acid (RA). Reprinted with permission from Ref. [1]. Copyright 2020 Elsevier.

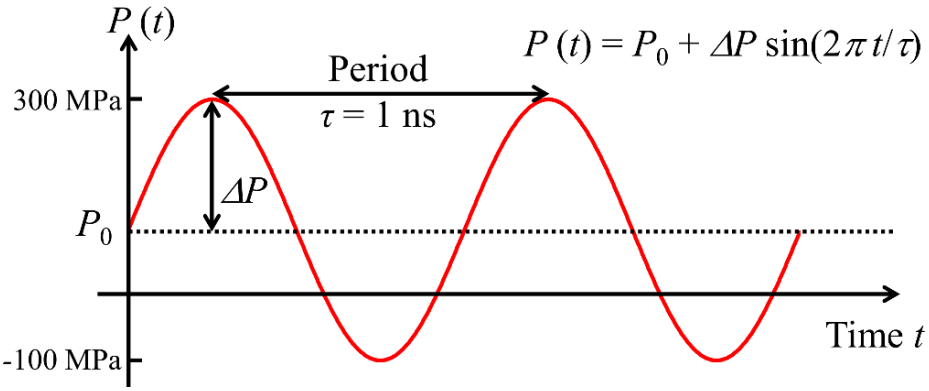

Figure S2. Time series of the set pressure, which varies sinusoidally. Reprinted with permission from Ref. [2]. Copyright 2014 American Chemical Society.

References

1. Ngoc, L.L.N.; Itoh, S.G.; Sompornpisut, P.; Okumura, H. Replica-permutation molecular dynamics simulations of an amyloid-β(16–22) peptide and polyphenols. *Chem. Phys. Lett.* **2020**, *758*, 137913.
2. Okumura, H.; Itoh, S.G. Amyloid Fibril Disruption by Ultrasonic Cavitation: Nonequilibrium Molecular Dynamics Simulations. *J. Am. Chem. Soc.* **2014**, *136*, 10549–10552.