Ellagitannins with a glucopyranose core have higher affinity to proteins than acyclic ellagitannins by isothermal titration calorimetry

Article

Supplemental Material

Supporting Information

Ellagitannins with a Glucopyranose Core Have Higher Affinity to Proteins than Acyclic Ellagitannins by Isothermal Titration Calorimetry

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List of Supporting Information

Figure S1. Examples of thermograms for the interaction of cyclic monomeric ellagitannins with BSA (raw heat data, no control experiments subtracted): A) tellimagrandin I into 30 μM BSA, B) tellimagrandin II into 30 μM BSA and C) geraniin into 40 μM BSA.

Figure S2. Examples of thermograms for the interaction of cyclic dimeric and trimeric ellagitannins with BSA (raw heat data, no control experiments subtracted): A) agrimoniin into 30 μM BSA, B) gemin A into 30 μM BSA, C) sanguiin H-6 into 30 μM BSA and D) lambertianin C into 30 μM BSA.

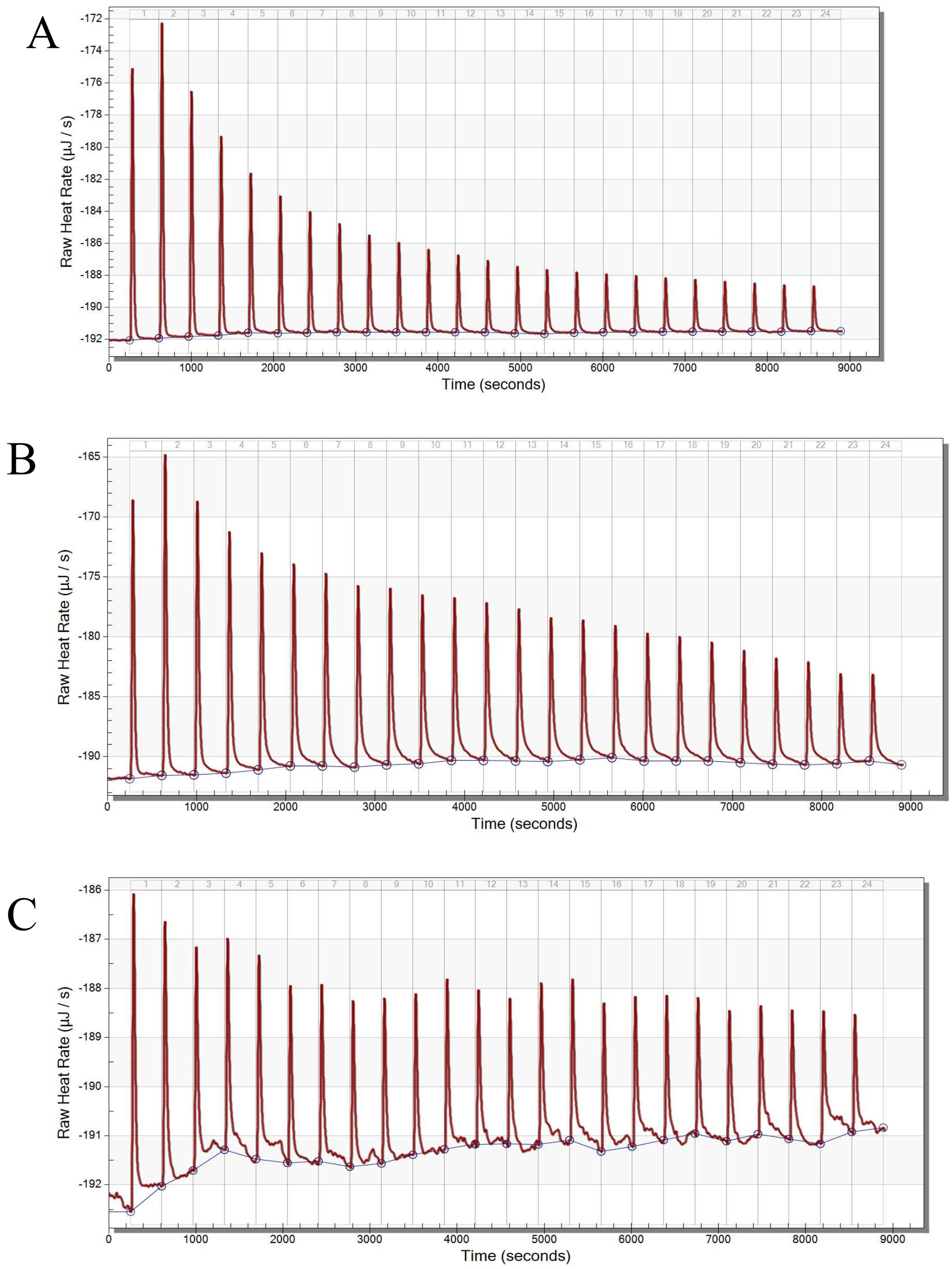
Figure S3. Examples of thermograms for the interaction of acyclic monomeric ellagitannins with BSA (raw heat data, no control experiments subtracted): A) castalagin into 30 μM BSA, B) vescalagin into 30 μM BSA, C) castavaloninic acid into 30 μM BSA and D) vescavaloninic acid into 30 μM BSA.

Figure S4. Examples of thermograms for the interaction of cyclic monomeric ellagitannins with gelatin (raw heat data, no control experiments subtracted): A) tellimagrandin I into 15 μM gelatin, B) tellimagrandin II into 20 μM gelatin and C) geraniin into 20 μM gelatin.

Figure S5. Examples of thermograms for the interaction of cyclic dimeric and trimeric ellagitannins with gelatin (raw heat data, no control experiments subtracted): A) agrimoniin into 30 μM gelatin, B) gemin A into 30 μM gelatin, C) sanguiin H-6 into 30 μM gelatin and D) lambertianin C into 30 μM gelatin.

Figure S6. Examples of thermograms for the interaction of acyclic monomeric ellagitannins with gelatin (raw heat data, no control experiments subtracted): A) castalagin into 20 μM gelatin, B) vescalagin into 20 μM gelatin, C) castavaloninic acid into 20 μM gelatin and D) vescavaloninic acid into 20 μM gelatin.

Table S1. Estimated Entropies for the Interaction of Ellagitannins with BSA and Gelatin Fitted by Two-Site and One-Site Binding Models



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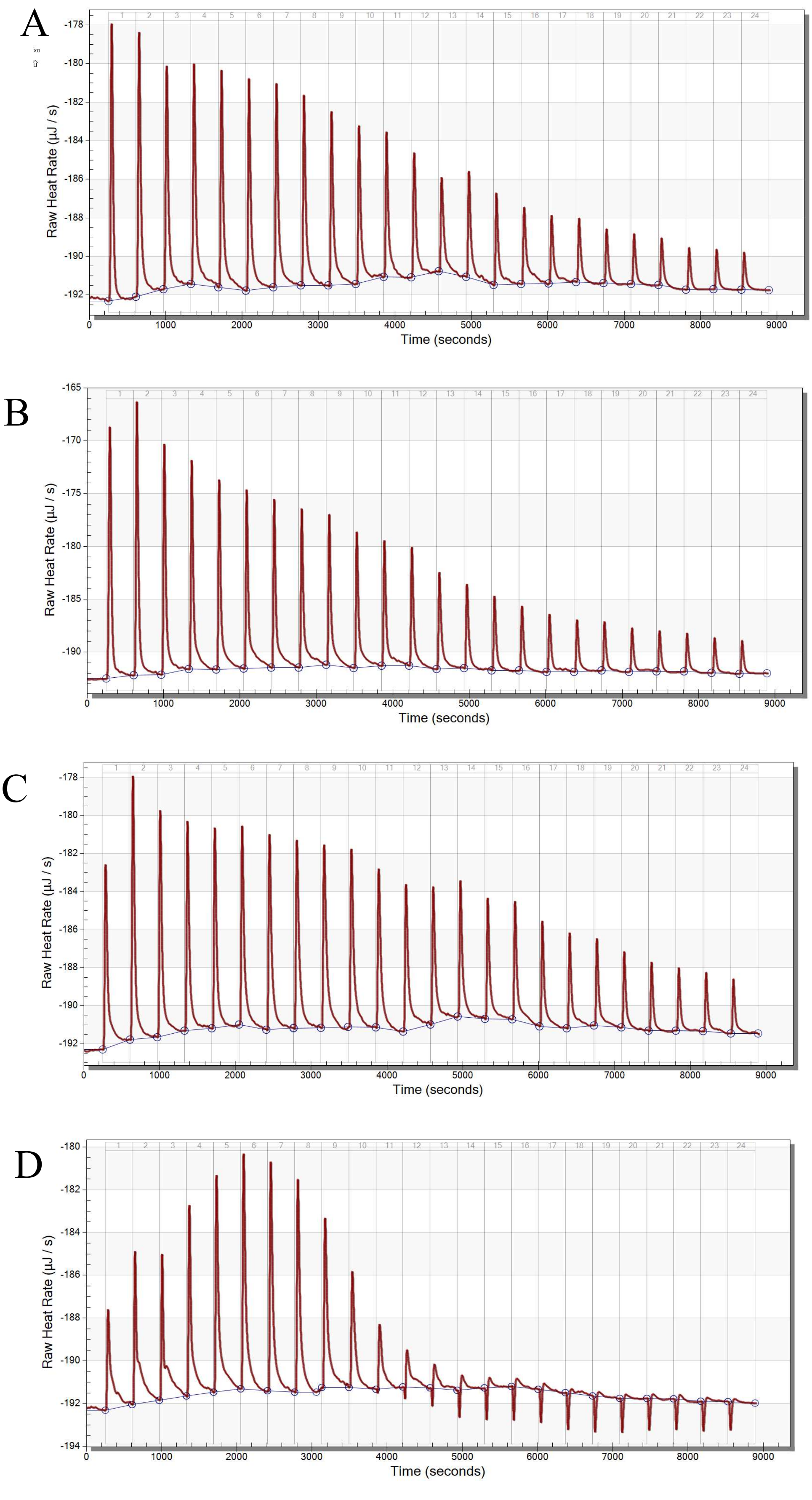

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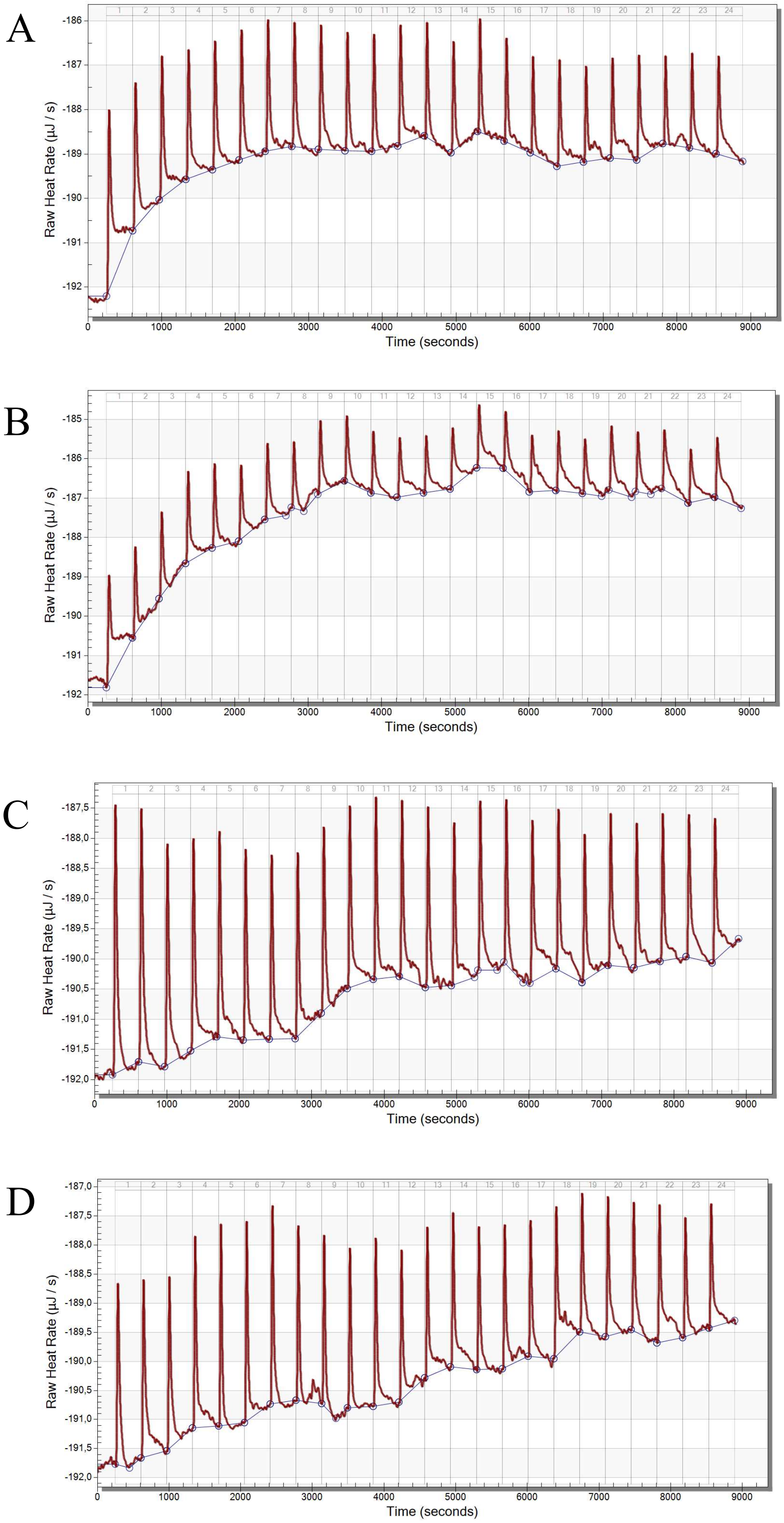

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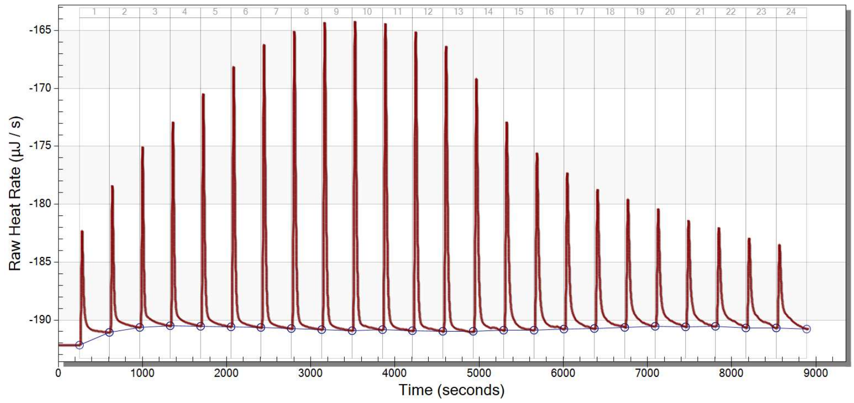
A



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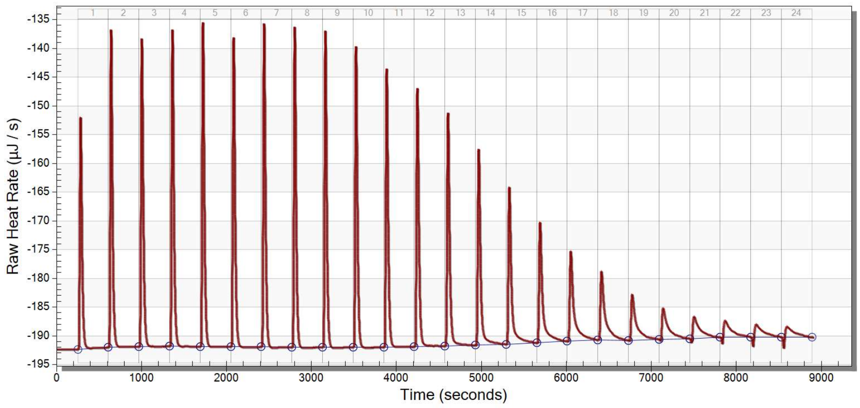

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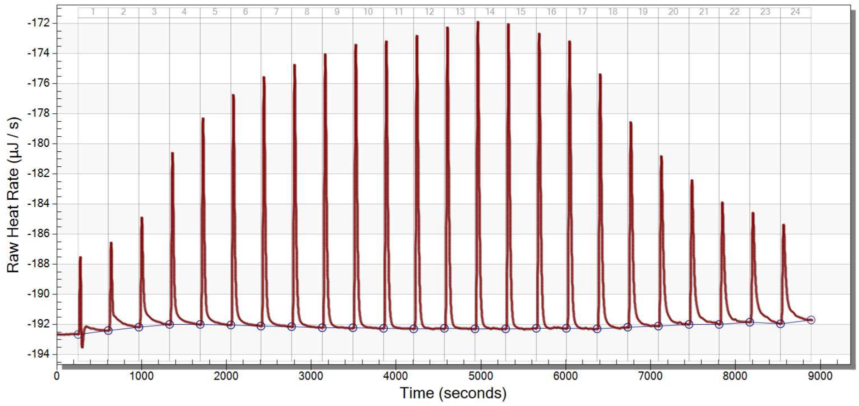

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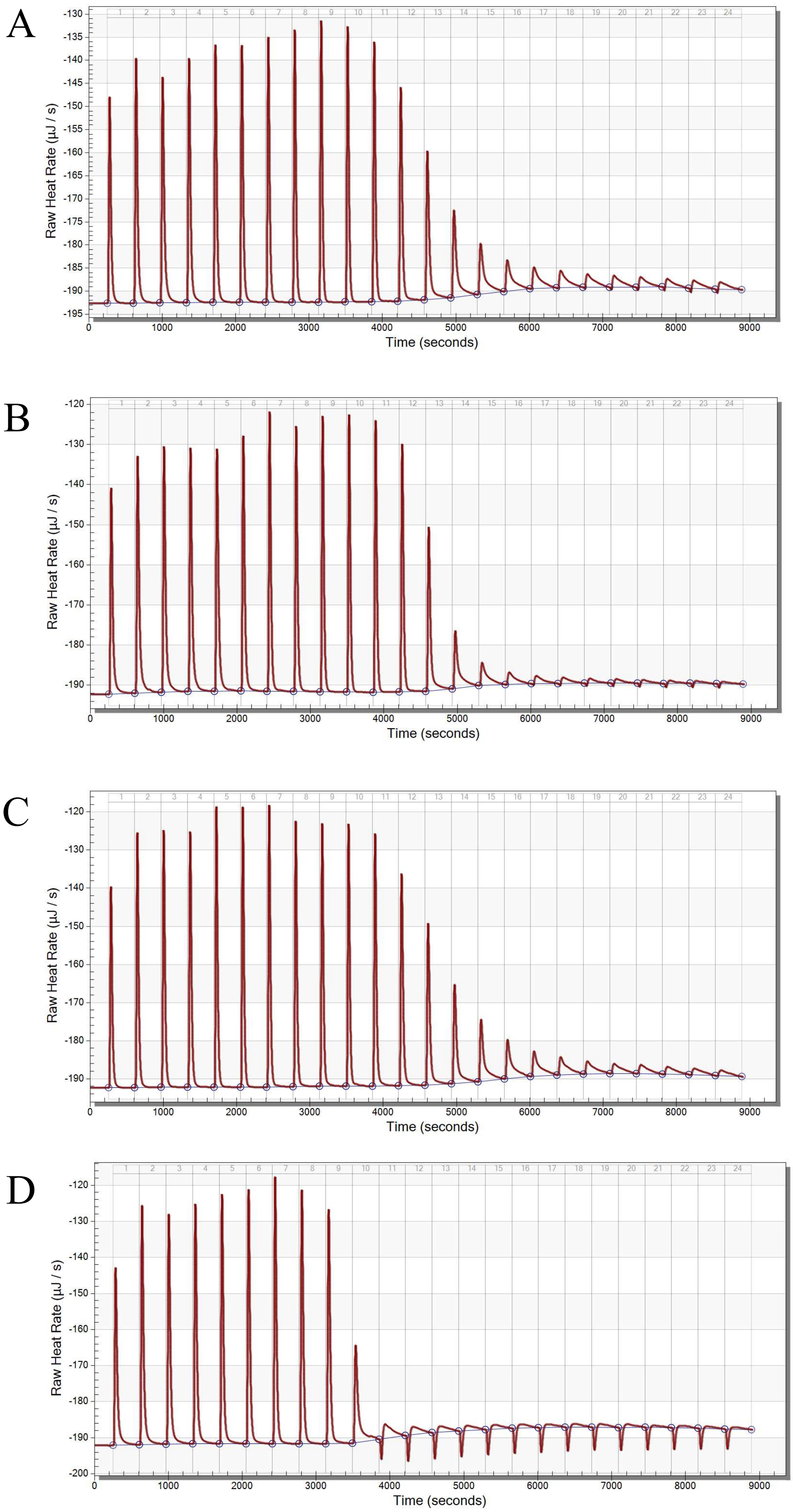

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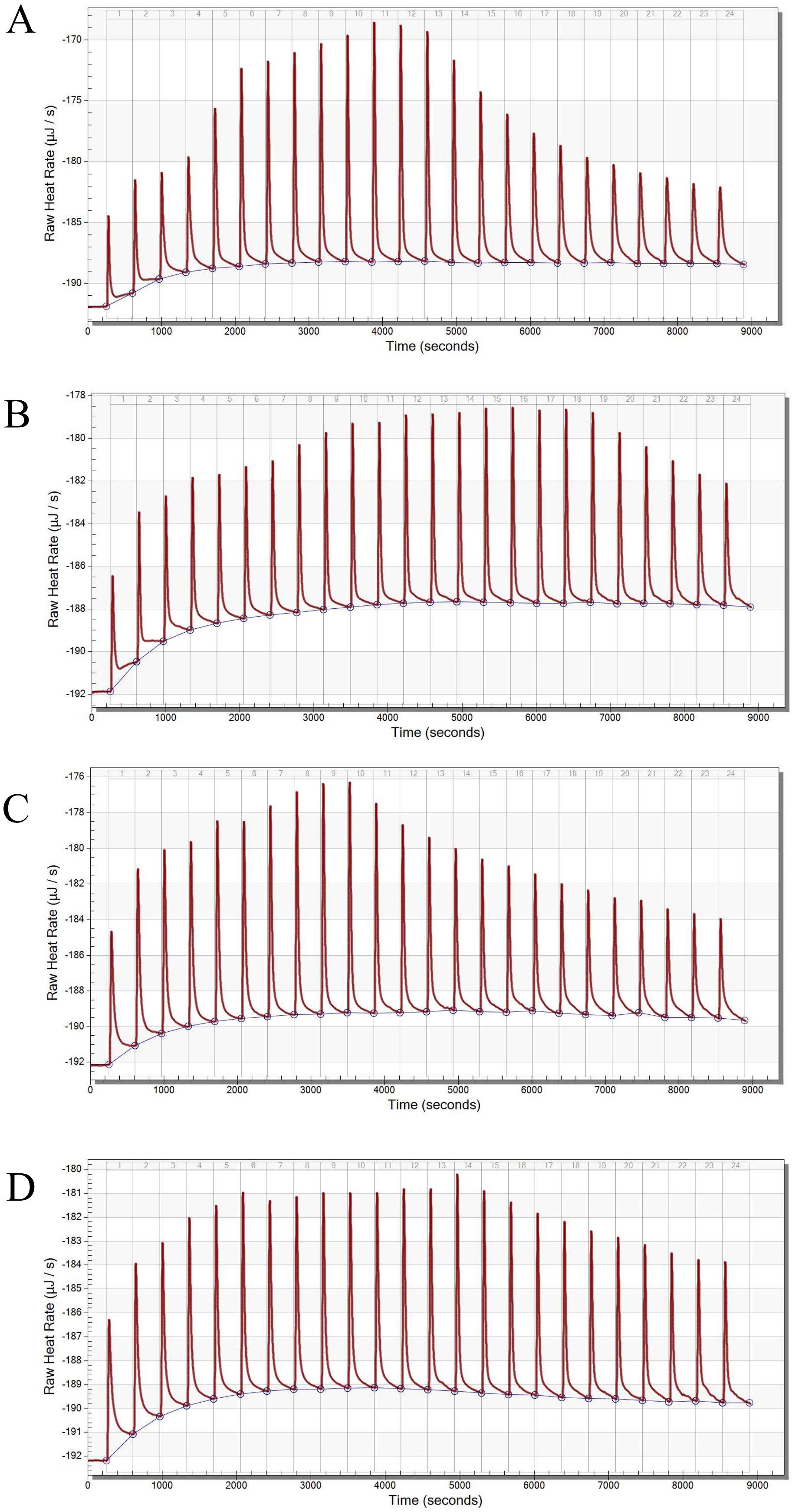

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	Tellimagrandin I	Tellimagrandin II	Agrimoniin	Gemin A	Sanguiin H-6	Roshenin C	Lambertianin C
BSA							
Two-Site							
ΔS_1 (J mol^{-1} K^{-1})	15 ± 14	-38 ± 22	26 ± 17	-45 ± 2	28 ± 4		16 ± 7
ΔS_2 (J mol^{-1} K^{-1})	18 ± 22	-64 ± 23	28 ± 4	29 ± 7	38 ± 7		46 ± 13
One-Site							
ΔS_1 (J mol^{-1} K^{-1})	2 ± 24	-52 ± 25	1 ± 18	-73 ± 14	-8 ± 10		4 ± 7
Gelatin							
Two-Site							
ΔS_1 (J mol^{-1} K^{-1})	53 ± 10	-93 ± 1	-117 ± 17	-99 ± 8	-108 ± 14	-2 ± 13	-185 ± 22
ΔS_2 (J mol^{-1} K^{-1})	55 ± 8	64 ± 2	44 ± 7	32 ± 4	49 ± 2	31 ± 4	-28 ± 34
One-Site							
ΔS_1 (J mol^{-1} K^{-1})	-57 ± 30	-103 ± 7	-163 ± 17	-165 ± 5	-170 ± 9	-112 ± 27	-194 ± 18