

Supplementary material

Ketoprofen poly(lactide-co-glycolide) physical interaction studied by Brillouin spectroscopy and molecular dynamics

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Table S1. Melting enthalpy (ΔH_m) of KET, and glass transition temperature (T_g) of PLGA, KET and PLGA/KET samples containing different amounts of KET.

KET % (w/w)	First heating scan ^(c)	Second heating scan ^(d)	
	ΔH_m (J/g) \pm SE	PLGA/KET T_g ($^{\circ}$ C) \pm SE	KET T_g ($^{\circ}$ C) \pm SE
0 ^(a)	-	45.4 \pm 0.3	-
5	-	39.0 \pm 1.0	-
10	-	36.0 \pm 0.4	-
15	-	31.4 \pm 0.2	-
25	-	23.6 \pm 0.6	-
35	- 20.8 \pm 0.8	23.9 \pm 0.4	- 6.8 \pm 1.6
50	- 25.2 \pm 0.5	23.2 \pm 0.1	- 5.1 \pm 0.2
100 ^(b)	- 111.4 \pm 0.5	-	- 4.8 \pm 0.3

(a) The sample is pure PLGA Resomer[®] RG 504.

(b) The sample is pure KET.

(c) Polymer T_g was not estimated in the first heating ramp because of the thermo-mechanical history.

(d) Endothermic events ascribable to KET melting were not detected in the second heating ramp.

Table S2. Melting enthalpy (ΔH_m) of KET, and glass transition temperature (T_g) of PLGA, KET and PLGA/KET samples containing different amount of KET, after two months of storage in dry chamber (P_2O_5) at room temperature.

KET % (w/w)	First heating scan ^(c)	Second heating scan ^(d)	
	ΔH_m (J/g) \pm SE	PLGA/KET T_g ($^{\circ}$ C) \pm SE	KET T_g ($^{\circ}$ C) \pm SE
0^(a)	-	44.9 \pm 0.9	-
5	-	40.0 \pm 0.3	-
10	-	35.8 \pm 0.1	-
15	-	30.6 \pm 0.2	-
25	-	22.9 \pm 0.2	-
35	-	22.0 \pm 0.0	- 4.6 \pm 0.3
50	-	22.2 \pm 0.2	- 4.9 \pm 0.2
100^(b)	-	-	- 4.2 \pm 0.1

(a) The sample is pure PLGA Resomer[®] RG 504.

(b) The sample is pure KET.

(c) Polymer T_g was not estimated in the first heating ramp because of the thermo-mechanical history. Endothermic events ascribable to KET melting were not detected.

(d) Endothermic events ascribable to KET melting were not detected in the second heating ramp.

Table S3. Glass transition temperature (T_g) of PLGA, KET and PLGA/KET samples containing different amount of KET, determined from temperature-scanning Brillouin light scattering spectroscopy.

	Cooling scan @ 1°/min
KET % (w/w)	T_g (°C)
0 ^(a)	41.7 ± 0.8
5	35.0 ± 0.8
10	31.2 ± 0.8
15	27.8 ± 0.8
25	20.0 ± 0.8
35	---
50	---
100 ^(b)	-12.2 ± 0.8

(a) The sample is pure PLGA Resomer[®] RG 504.

(b) The sample is pure KET.

Figure S1

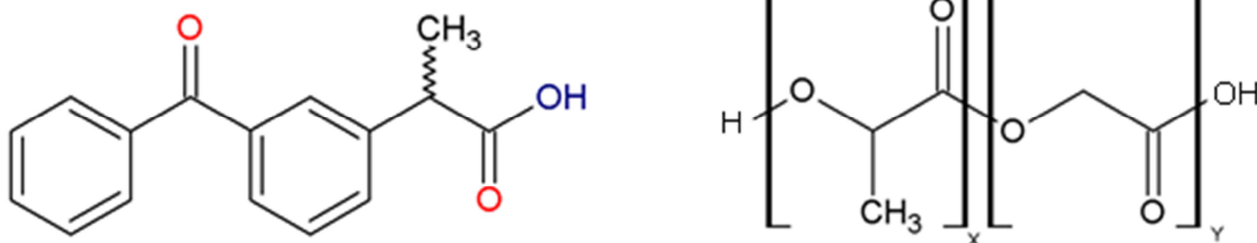


Figure S1. Structure of KET (left) and PLGA (right). In the PLGA structure x is the number of units of lactic acid while y is the number of units of glycolic acid.

Figure S2

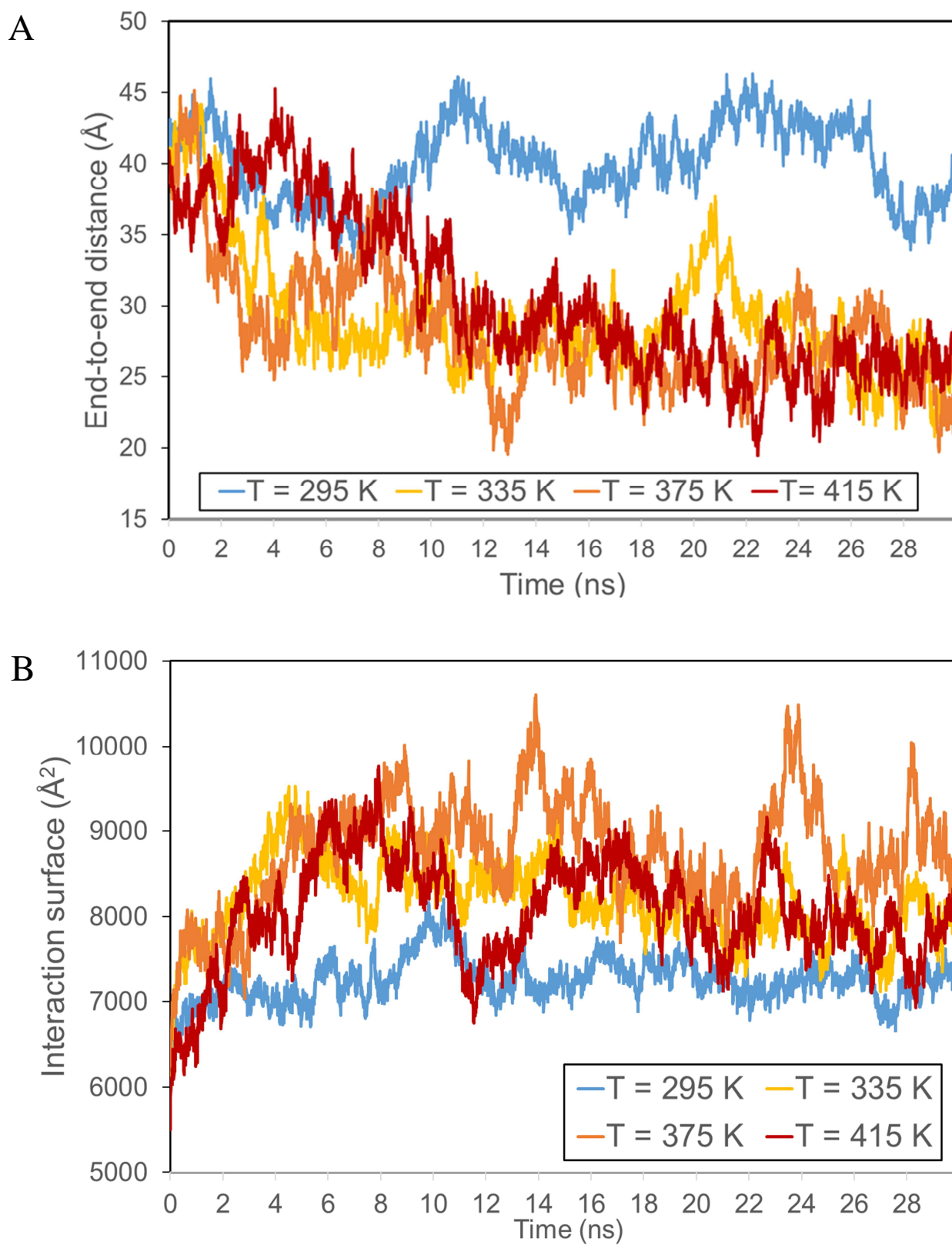


Figure S2. Molecular dynamics runs of the PLGA- CCl_4 system: (A) dynamic profiles of the PLGA end-to-end distance and (B) of the PLGA- CCl_4 interaction surfaces.