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Supporting information for article:

Insulin polymorphism induced by two polyphenols: new crystal forms and advances in macromolecular powder diffraction

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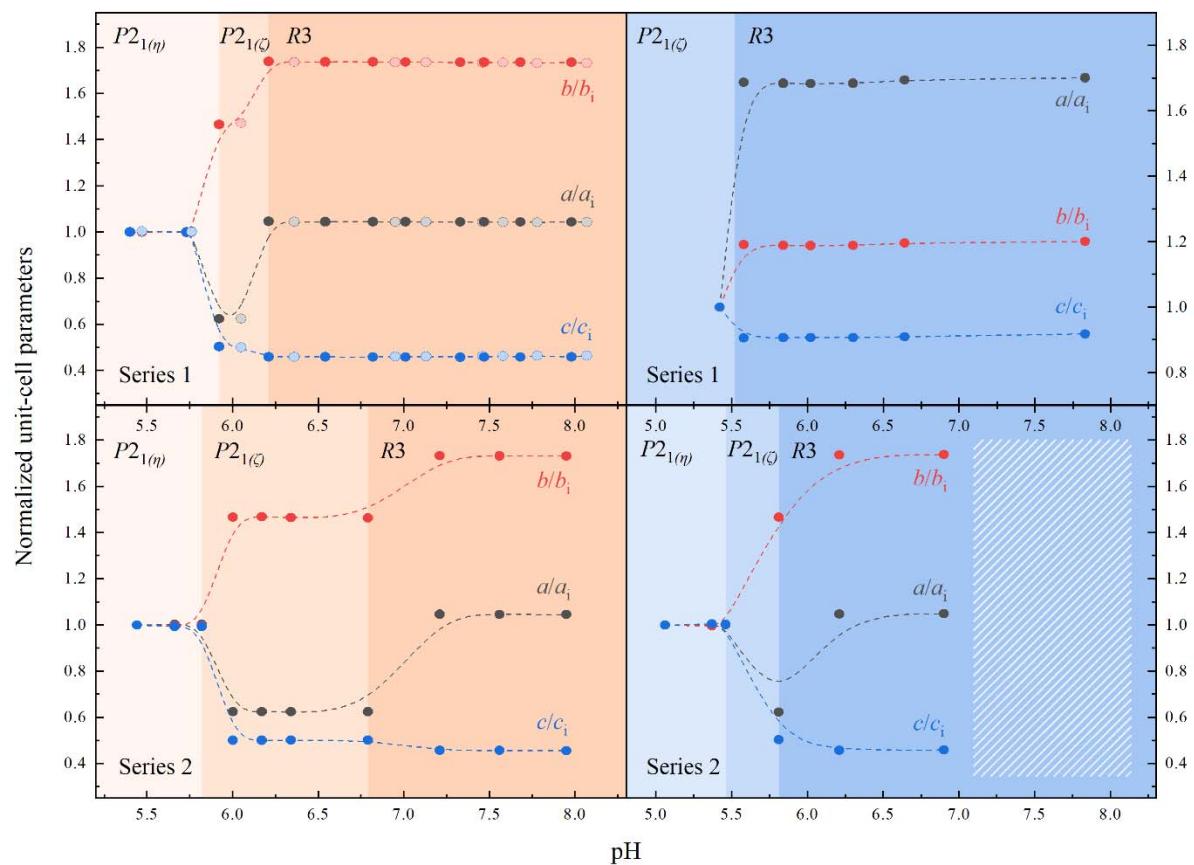


Figure S1 Evolution of normalized unit-cell parameters of HI co-crystallized with pcm (left) and rsv (right) (Series 1: top; Series 2: bottom). The values were extracted from XRPD data collected at ID22-ESRF. Bold and dim circles correspond to first and second measurement, respectively. The different background colors correspond to different crystalline phases. Samples that lie on the border of two regions are mixtures of the adjacent phases. The white hatched region corresponds to degraded resveratrol samples. The lines serve as a guide to the eye.

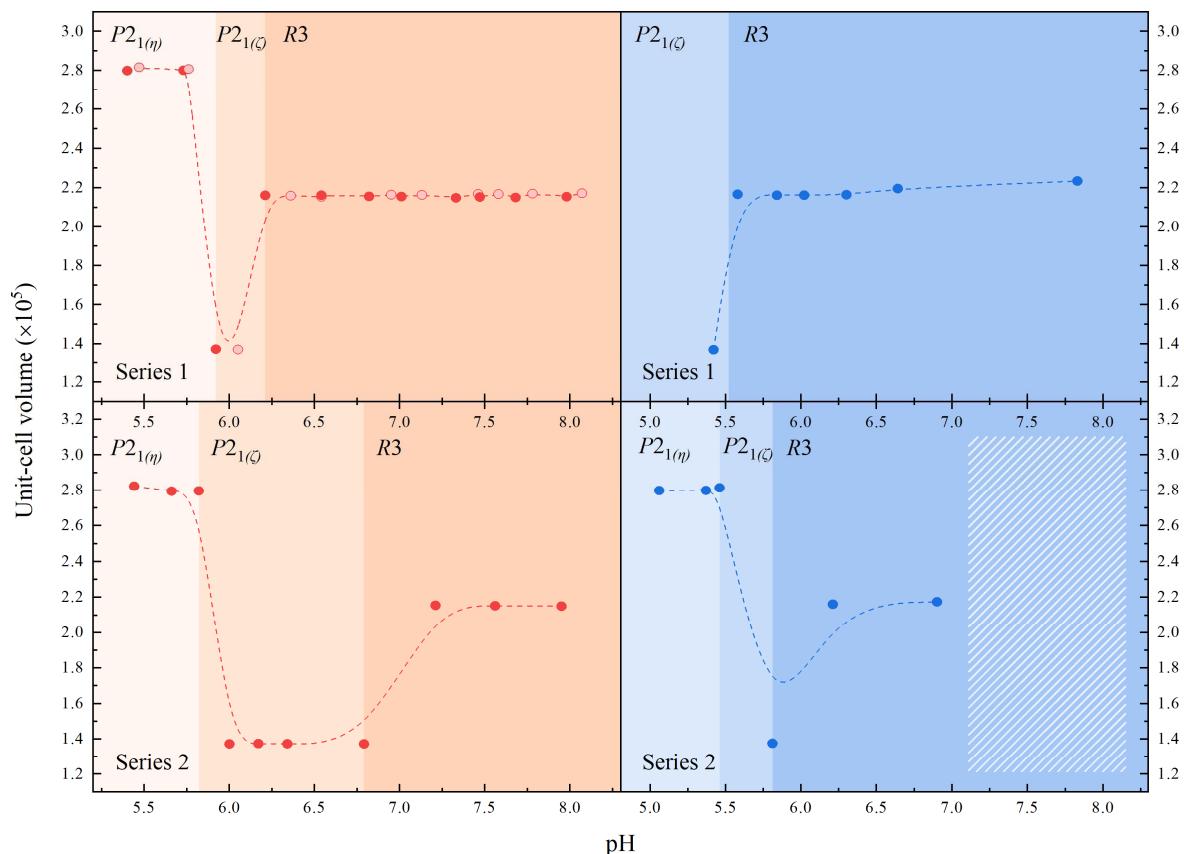


Figure S2 Evolution of normalized unit-cell volume of HI co-crystallized with pcm (left) and rsv (right) (Series 1: top; Series 2: bottom). The values were extracted from XRPD data collected at ID22-ESRF. Bold and dim circles correspond to first and second measurement, respectively. The different background colors correspond to different crystalline phases. Samples that lie on the border of two regions are mixtures of the adjacent phases. The white hatched region corresponds to degraded resveratrol samples. The lines serve as a guide to the eye.

Table S1 Unit-cell parameters and volume with errors for every sample of p-coumaric acid and resveratrol (Series 1: $\lambda = 1.30003(3)$ Å; Series 2: $\lambda = 1.30017(2)$ Å), measured at ESRF (ID22).

Sample code	pH	Space group	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β (°)	<i>V</i> ($\times 10^5$ Å ³)
pcm11	4.90	amorphous	-	-	-	-	-
pcm12	5.40	<i>P</i> 2 ₁ (η)	77.51(1)	46.636(4)	82.69(1)	110.56(2)	2.7988(7)
pcm13	5.73	<i>P</i> 2 ₁ (η)	77.60(1)	46.616(4)	82.697(1)	110.59(1)	2.8008(5)
pcm14	5.92	<i>P</i> 2 ₁ (ζ)	48.401(6)	68.397(9)	41.644(5)	95.205(9)	1.3730(3)
pcm15	6.21	<i>R</i> 3	81.082(3)	81.082(3)	37.964(1)	90.00(0)	2.1616(2)
pcm16	6.54	<i>R</i> 3	81.062(5)	81.062(5)	37.996(1)	90.00(0)	2.1623(3)
pcm17	6.82	<i>R</i> 3	81.014(5)	81.014(6)	37.937(2)	90.00(0)	2.1564(3)
pcm18	7.01	<i>R</i> 3	81.008(3)	81.008(4)	37.931(2)	90.00(0)	2.1557(2)
pcm19	7.33	<i>R</i> 3	80.937(4)	80.937(4)	37.884(2)	90.00(0)	2.1493(3)
pcm110	7.47	<i>R</i> 3	80.956(2)	80.956(3)	37.9348(8)	90.00(0)	2.1532(2)
pcm111	7.68	<i>R</i> 3	80.924(4)	80.924(4)	37.928(1)	90.00(0)	2.1510(2)
pcm112	7.98	<i>R</i> 3	80.945(4)	80.945(3)	37.975(1)	90.00(0)	2.1548(2)

Sample code	pH	Space group	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β (°)	<i>V</i> ($\times 10^5$ Å ³)
pcm21	5.18	amorphous	-	-	-	-	-
pcm22	5.44	<i>P</i> 2 ₁ (η)	77.337(4)	46.708(2)	83.154(4)	109.985(5)	2.823(5)
pcm23	5.66	<i>P</i> 2 ₁ (η)	77.578(3)	46.587(1)	82.630(3)	110.668(4)	2.794(4)
pcm24	5.82	<i>P</i> 2 ₁ (η)	77.618(3)	46.590(1)	82.630(3)	110.648(4)	2.796(4)
pcm25	6.00	<i>P</i> 2 ₁ (ζ)	48.2711(8)	68.513(1)	41.6667(8)	95.030(1)	1.3727(2)
pcm26	6.17	<i>P</i> 2 ₁ (ζ)	48.301(1)	68.570(1)	41.654(1)	95.018(2)	1.3745(3)
pcm27	6.34	<i>P</i> 2 ₁ (ζ)	48.2870(8)	68.461(1)	41.6974(9)	95.034(2)	1.3731(2)
pcm28	6.79	<i>P</i> 2 ₁ (ζ)	48.2996(9)	68.388(1)	41.7071(9)	94.995(2)	1.3724(2)
pcm29	7.21	<i>R</i> 3	80.937(2)	80.937(2)	37.9891(7)	90.00(0)	2.1552(1)
pcm210	7.56	<i>R</i> 3	80.904(2)	80.904(2)	37.9731(6)	90.00(0)	2.1525(1)

pcm211	7.95	<i>R</i> 3	80.885(3)	80.885(3)	37.9582(9)	90.00(0)	2.1507(2)
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Sample code	pH	Space group	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β (°)	<i>V</i> ($\times 10^5$ Å ³)
rsv11	5.42	<i>P</i> 2 ₁ (η)	48.211(2)	68.305(2)	41.770(2)	95.108(3)	1.37011(5)
rsv12	5.58	<i>R</i> 3	81.342(7)	81.342(7)	37.826(2)	90.00(0)	2.1675(4)
rsv13	5.84	<i>R</i> 3	81.201(2)	81.201(2)	37.870(1)	90.00(0)	2.1625(1)
rsv14	6.02	<i>R</i> 3	81.164(5)	81.164(5)	37.907(1)	90.00(0)	2.1626(2)
rsv15	6.30	<i>R</i> 3	81.208(4)	81.208(4)	37.905(1)	90.00(0)	2.1649(2)
rsv16	6.64	<i>R</i> 3	81.706(4)	81.706(4)	37.994(1)	90.00(0)	2.1964(3)
rsv17	7.83	<i>R</i> 3	82.02(1)	82.02(1)	38.353(4)	90.00(0)	2.2348(8)
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Sample code	pH	Space group	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β (°)	<i>V</i> ($\times 10^5$ Å ³)
rsv21	5.06	<i>P</i> 2 ₁ (η)	77.4454(1)	46.7230(7)	82.864(1)	111.068(2)	2.798217(8)
rsv22	5.20	amorphous	-	-	-	-	-
rsv23	5.27	amorphous	-	-	-	-	-
rsv24	5.37	<i>P</i> 2 ₁ (η)	77.527(9)	46.544(3)	83.268(8)	111.33(1)	2.79889(4)
rsv25	5.46	<i>P</i> 2 ₁ (η)	77.544(5)	46.861(3)	83.150(4)	111.376(7)	2.814(2)
rsv26	5.81	<i>P</i> 2 ₁ (η)	48.262(3)	68.531(4)	41.758(2)	95.050(5)	1.3758(1)
rsv27	6.21	<i>R</i> 3	81.116(5)	81.116(5)	37.9356(1)	90.00(0)	2.1616(2)
rsv28	6.90	<i>R</i> 3	81.204(3)	81.204(3)	38.088(1)	90.00(0)	2.1750(2)
rsv29	7.58	amorphous	-	-	-	-	-

Table S2 Unit-cell parameters and volume with errors for sample of *p*-coumaric acid and resveratrol (Series 2: $\lambda = 1.3004392(8)$ Å), measured at SLS (X04SA).

Sample code	pH	Space group	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β (°)	<i>V</i> ($\times 10^5$ Å ³)
rsv21	5.06	<i>P</i> 2 ₁ (η)	77.41(3)	46.728(2)	82.96(3)	111.148(6)	2.794(2)
pcm25	6.00	<i>P</i> 2 ₁ (ζ)	48.2704(2)	68.6564(2)	41.5914(2)	94.9412(3)	1.37324(4)
pcm210	7.56	<i>R</i> 3	80.958(2)	80.958(1)	37.9731(6)	90.00(0)	2.1554(1)