Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information

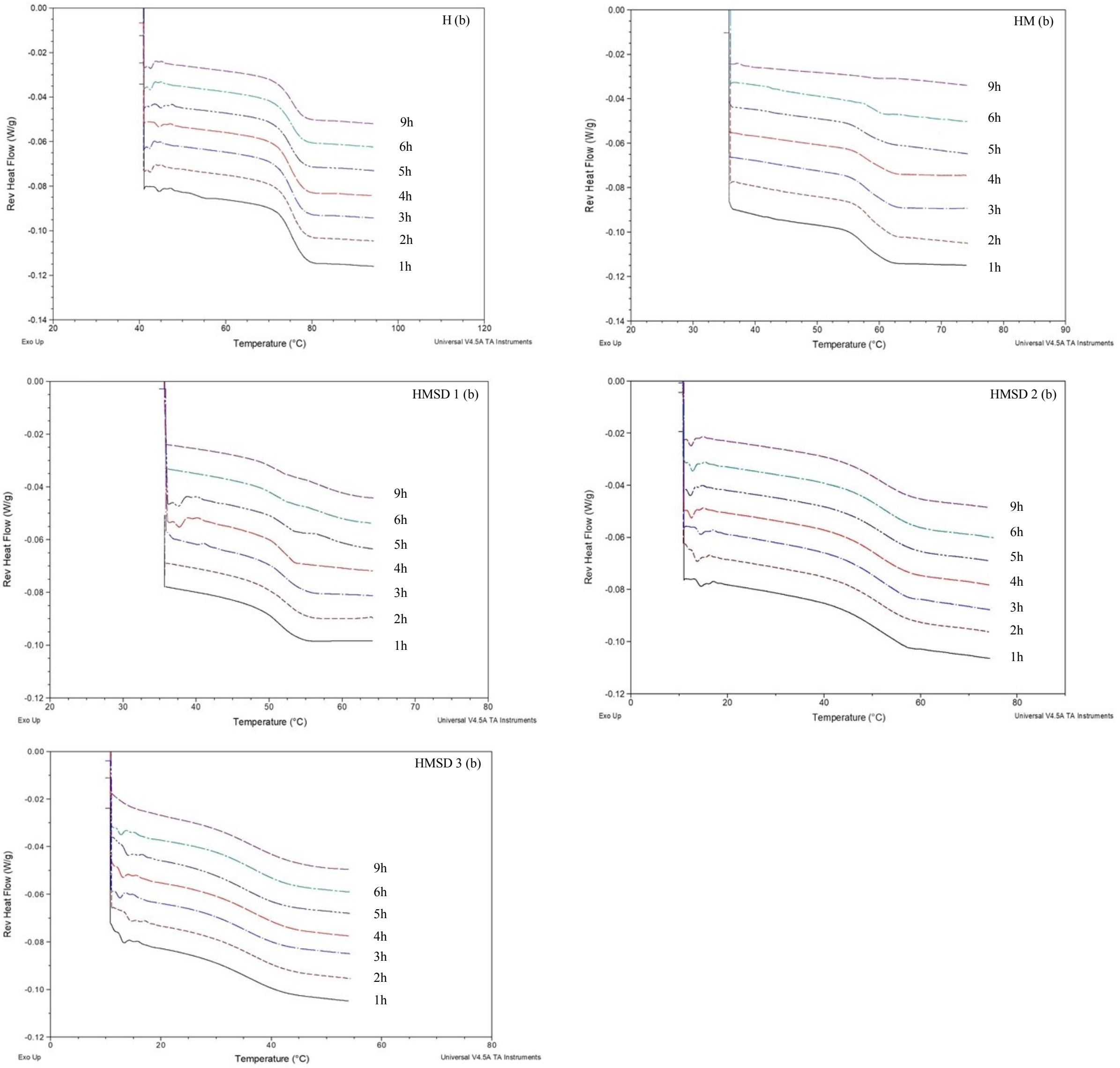

Fig. S1. mDSC heating curves of samples H (b), HM (b), HMSD 1 (b), HMSD 2 (b) and, HMSD 3 (b) at all time points. The step change in the reversing heat flow (vertical axis) shows the T_g of hesperetin.

Section S1. Modelling and statistical analysis

One-way analysis of variance (ANOVA) with post-hoc Tukey's HSD test was used to compare the significant differences of α(t) values of all samples at the same time points. Here, ANOVA was used because there were more than two independent (categorical) variables i.e. amorphous samples [H (b), HM (b), HMSD 1-3 (b)] and one dependent (continuous) variable i.e., time. ANOVA test only suggested that one or more samples or variables were significantly different. The post-hoc test identifies which of the pairs of samples or variables are significantly different from each other. Tukey's HSD (Honest significant difference) test is one of the ANOVA post-hoc tests to identify the significant difference amongst samples. Table 1S shows the pair-wise analysis of α(t) values of all samples at all time points. Maximum differences were observed at 4h amongst the samples. The data for sample H (b) and HM (b) are significantly different than all other samples (Table S1). However, HMSD 1-3 (b) samples are significantly different from each other only at some of the time points.

Table S1. A pair-wise comparison of α(t) of all samples at all time points using ANOVA with post-hoc tukey's test.

Time points (h)	H (b) vs. HM (b)	H (b) vs. HMSD 1 (b)	H (b) vs. HMSD 2 (b)	H (b) vs. HMSD 3 (b)	HM (b) vs. HMSD 1 (b)	HM (b) vs. HMSD 2 (b)	HM (b) vs. HMSD 3 (b)	HMSD 1 (b) vs. HMSD 2 (b)	HMSD 1 (b) vs. HMSD 3 (b)	HMSD 2 (b) vs. HMSD 3 (b)
0	–	–	–	–	–	–	–	–	–	–
1	**	*	**	**	**	–	**	–	–	–
2	**	*	*	*	*	**	*	–	**	–
3	**	*	**	*	**	**	*	–	*	**
4	**	**	**	**	**	**	**	**	**	–
5	*	*	**	*	**	–	–	–	–	–
6	**	*	**	**	**	*	**	–	–	–
9	*	*	*	*	*	*	*	–	*	*

*Significance level is ≤0.01

**Significance level is ≤0.05

– No significant difference

Nucleation models are based on certain mechanistic assumptions of solid-state reactions. Avrami-Erofeyev (A) models assumes that nucleation is a uniform and random process and nuclei growth occurs continuously considering certain restrictions such as ingestion and coalescence. Avrami-Erofeyev (A) models are commonly known as JMAK (John-Mehl-Avrami-Kolmogorov) models. Prout-Trompkins (B1) models are autocatlayitc models which mean the products catalyze the reaction and this occurs when the reactants are regenerated during the reaction (called as 'branching'). Table S2 shows the entire data fitted to various nucleation models including Avrami-Erofeyev (A) and Prout-Trompkins (B1) models. All the Avrami plots generated from this data passed the normality test (p value > 0.05).

Table S2. Model fitting of the isothermal crystallization kinetics data for H (b), HM (b) and HMSD 1-3 (b) samples.

	H (b)				HM (b)				HMSD 1 (b)				HMSD 2 (b)				HMSD 3 (b)			
	(A2)	(A3)	(A4)	(B1)	(A2)	(A3)	(A4)	(B1)	(A2)	(A3)	(A4)	(B1)	(A2)	(A3)	(A4)	(B1)	(A2)	(A3)	(A4)	(B1)
R^2	0.98	0.96	0.96	0.96	0.87	0.86	0.85	0.87	0.94	0.92	0.92	0.95	0.92	0.90	0.90	0.93	0.96	0.97	0.98	0.93
Adj R^2	0.97	0.96	0.95	0.96	0.84	0.83	0.82	0.85	0.93	0.91	0.90	0.94	0.90	0.88	0.88	0.92	0.95	0.97	0.97	0.91
Normality test	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed
PRESS	0.05	0.04	0.03	0.86	0.51	0.25	0.14	5.46	0.34	0.16	0.09	3.02	0.51	0.22	0.13	4.72	0.19	0.04	0.02	4.85
Power	1.00	1.00	0.99	1.00	0.92	0.90	0.89	0.92	0.99	0.98	0.97	0.99	0.97	0.96	0.95	0.98	0.98	0.99	0.99	0.93
AICc	-41.72	-43.61	-45.79	-21.48	-24.47	-29.68	-33.45	-8.01	-27.47	-33.04	-36.92	-12.08	-24.39	-30.50	-34.70	-8.44	-30.16	-40.55	-46.39	-7.73
BIC	-42.58	-44.46	-46.65	-22.33	-25.32	-30.54	-34.31	-8.87	-28.32	-33.89	-37.78	-12.94	-25.25	-31.35	-35.55	-9.29	-31.01	-41.41	-47.25	-8.59