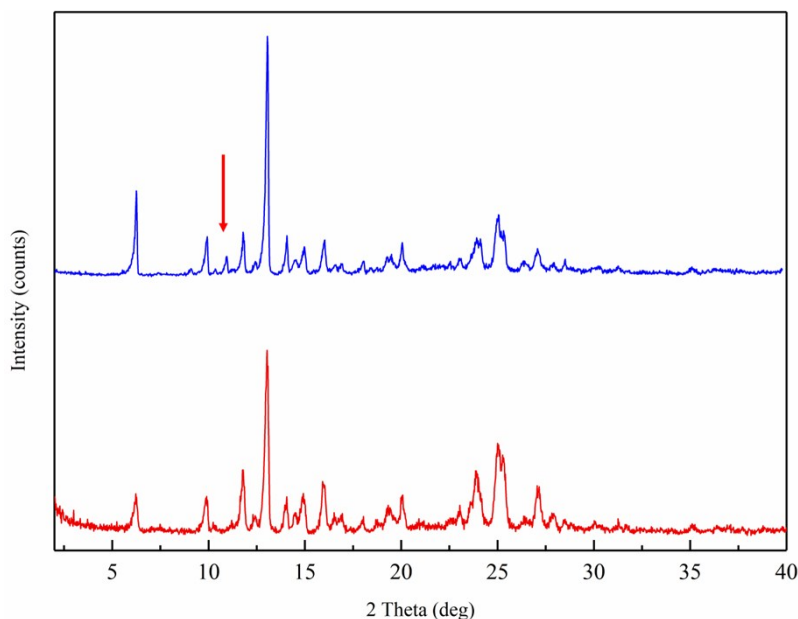


## Supporting information

### Relationship between form III and the form reported in patent CN107954984

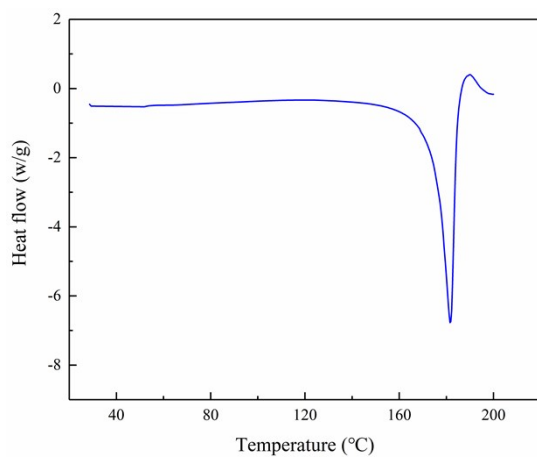
The form claimed in patent CN107954984 is the form III reported in this research. A figure of the comparison of PXRD patterns was shown in figure S1. The high similarity explains they are the same form. However, one small peak was seen in the “patent form” but not in “form III” reported here. This tiny disagreement may be due to the different content of impurity. The purity of the form reported in patent is about 92%, but the form reported in this research is about 99%. The “patent form” were found in our earlier study and then we applied for a patent. During the later study, we found nicosulfuron is easy to decomposition in the crystallization process. Therefore, the crystallization conditions were controlled strictly to prevent decomposition, and the purity of all the product were detected using HPLC to inhibit the influence of impurity. And the purity of all the forms declared in this research is above 98%.



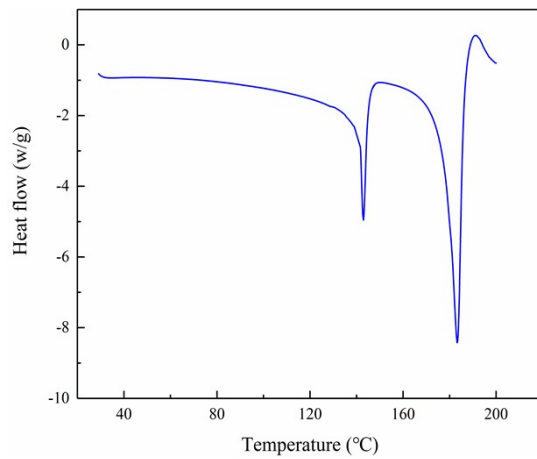
**Fig. S1** The comparison of form III reported in this research (bottom) and the form reported in patent CN107954984 (top).

Table 1. The nomenclature of all the nicosulfuron polymorphs mentioned in this research

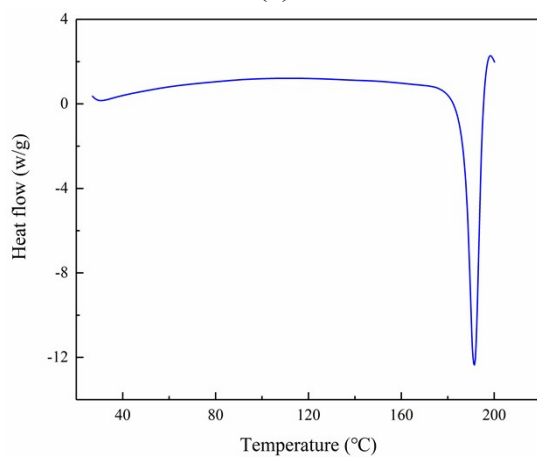
Reported in literature	New forms	Details	Designated in this research
Ia		Solvent-free form	Ia
Ib		Solvent-free form	Ib
II		monohydrate	II
	III	Solvent-free form	III
	IV	Solvent-free form	IV
	V	Solvent-free form	V
	VI	Solvent-free form	VI
	S1	Methanol solvate	S1
	S2	Ethanol solvate	S2
	S3	Acetonitrile solvate	S3
	S4	1,4-dioxane solvate	S4
	S5	1,4-dioxane solvate	S5



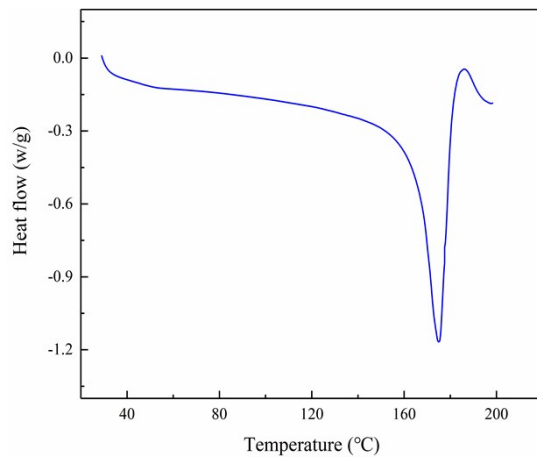
(a)



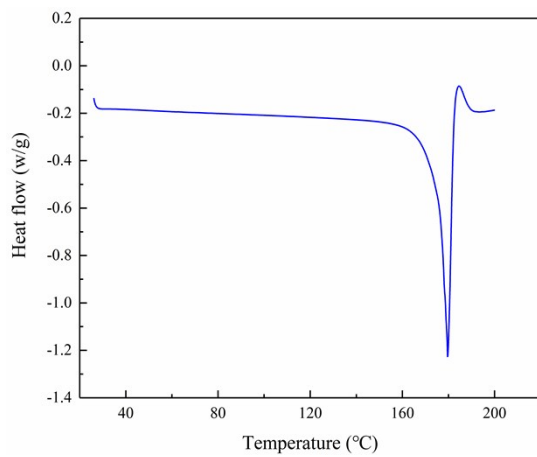
(b)



(c)

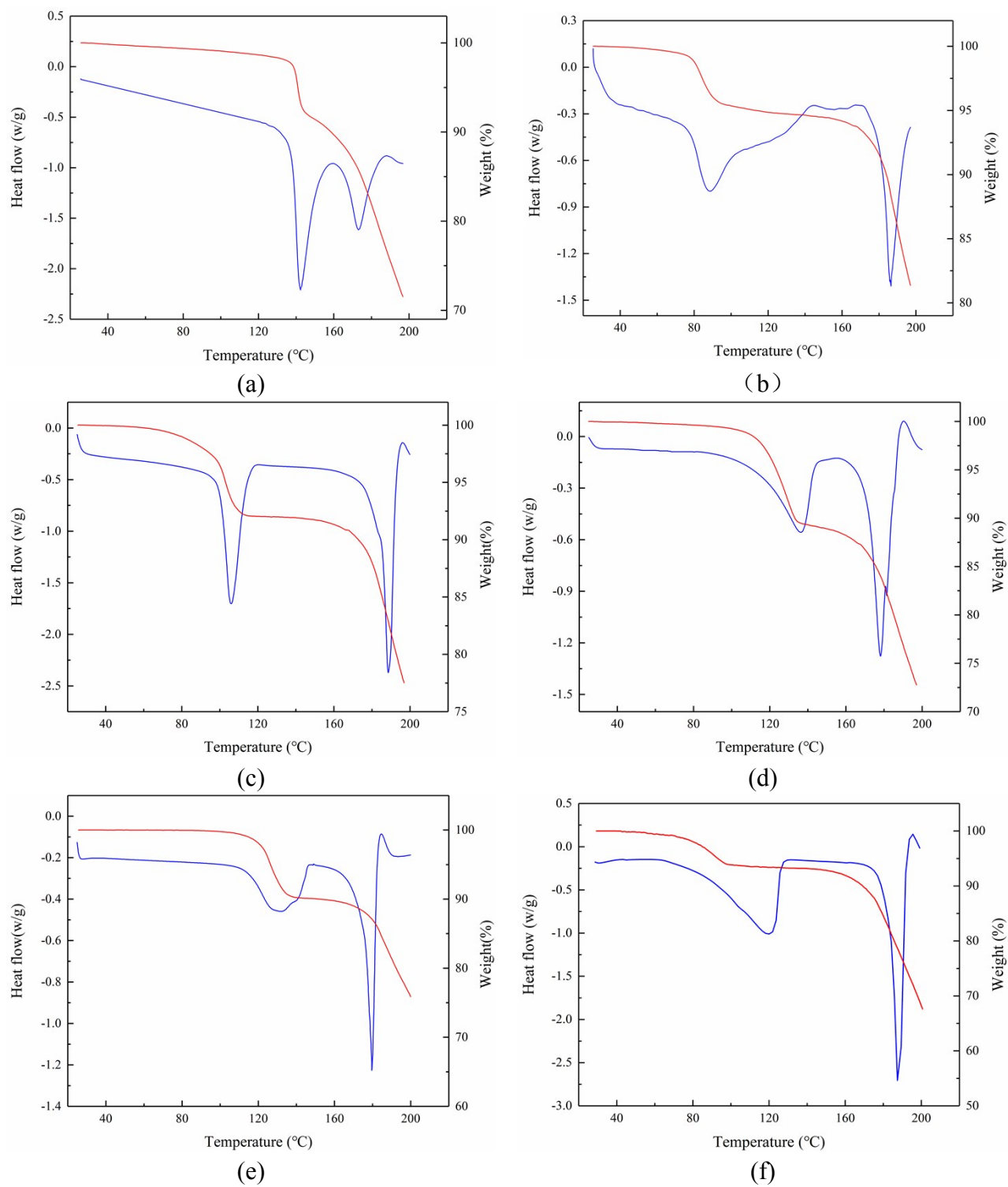


(d)

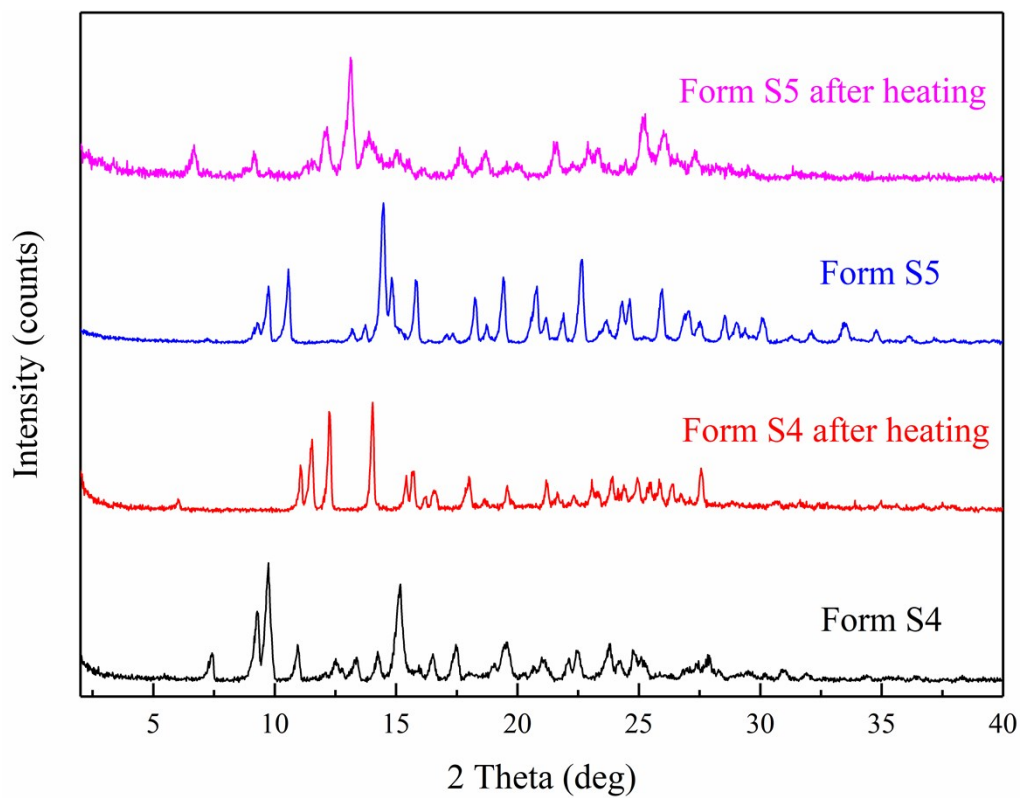
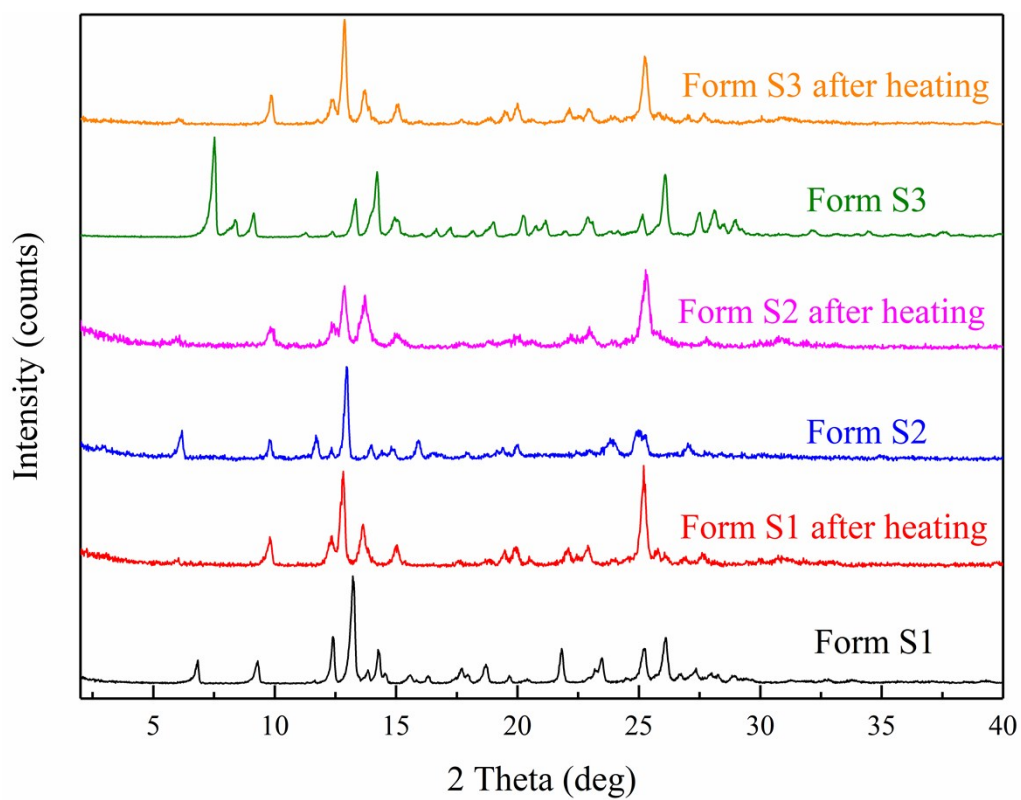


(e)

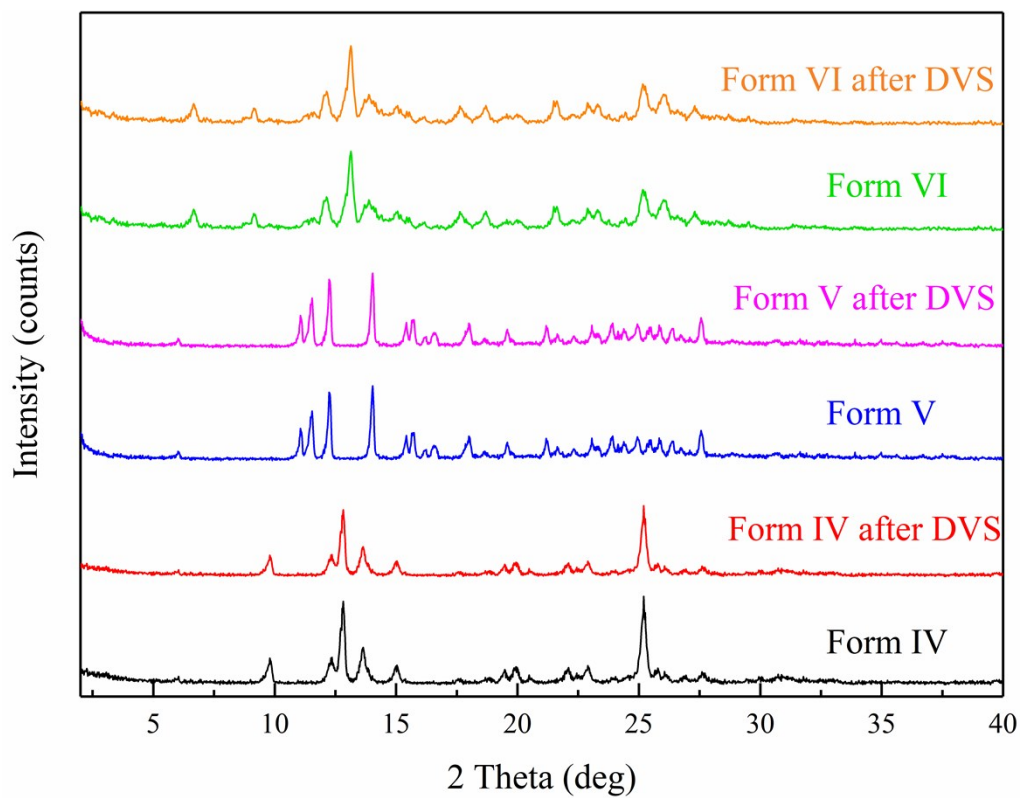
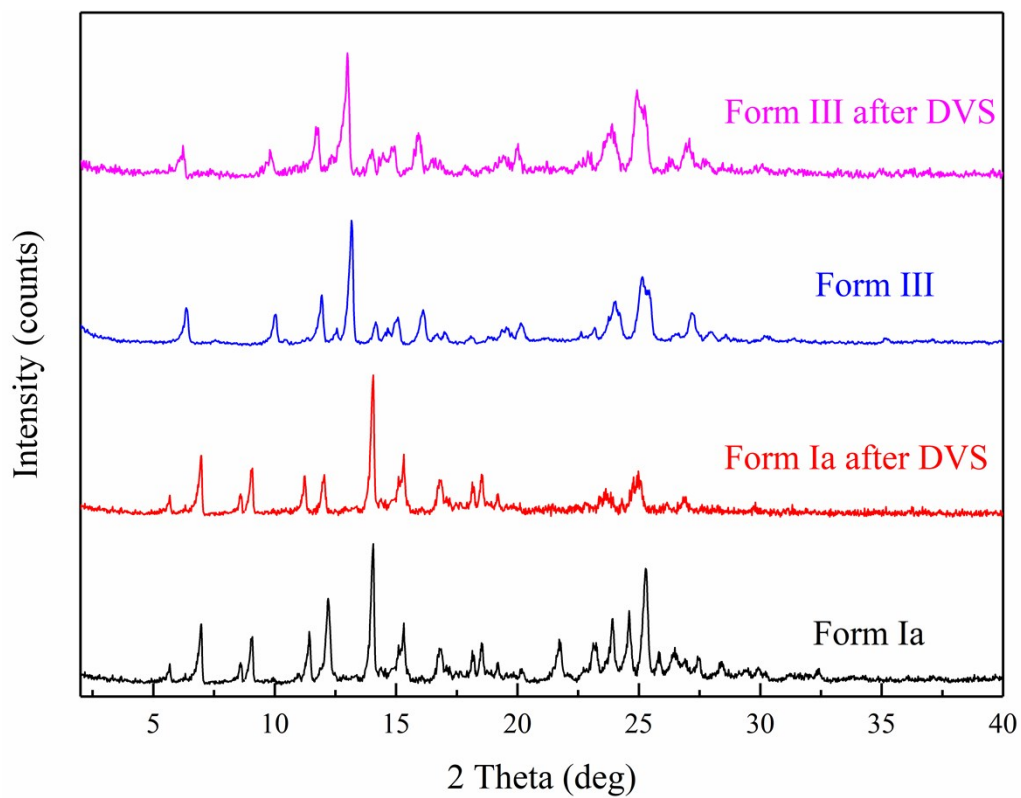
**Fig. S2** The DSC curves of (a) Ia, (b) III, (c) IV, (d) V, (e) VI

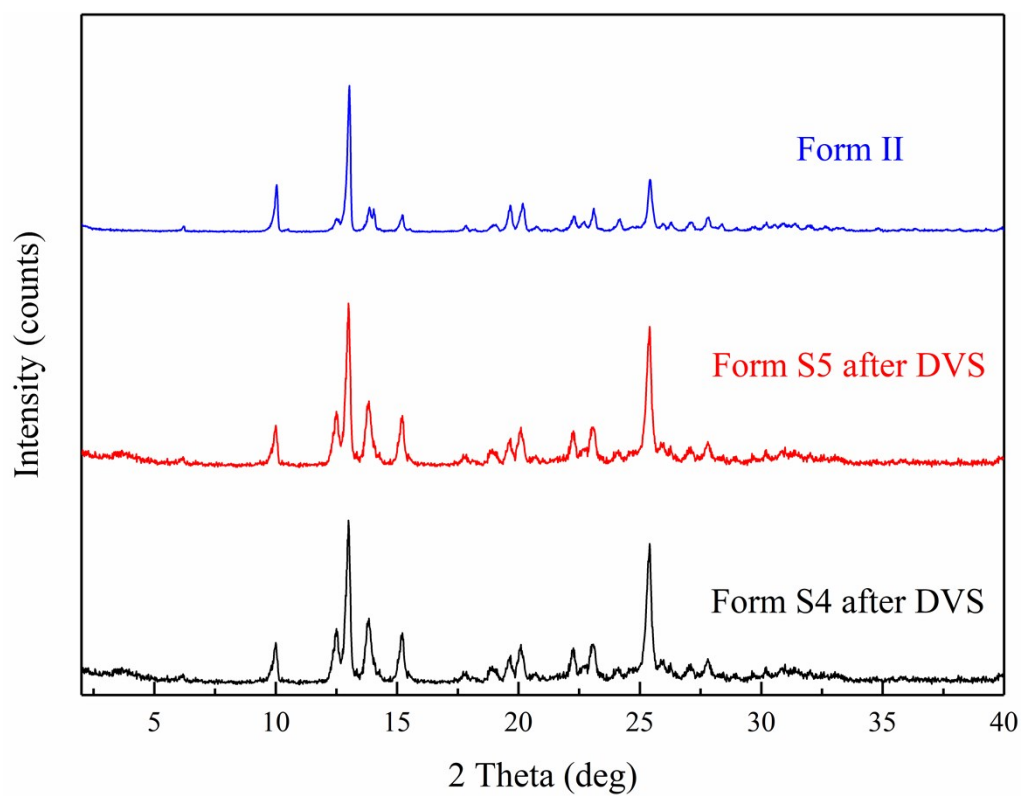
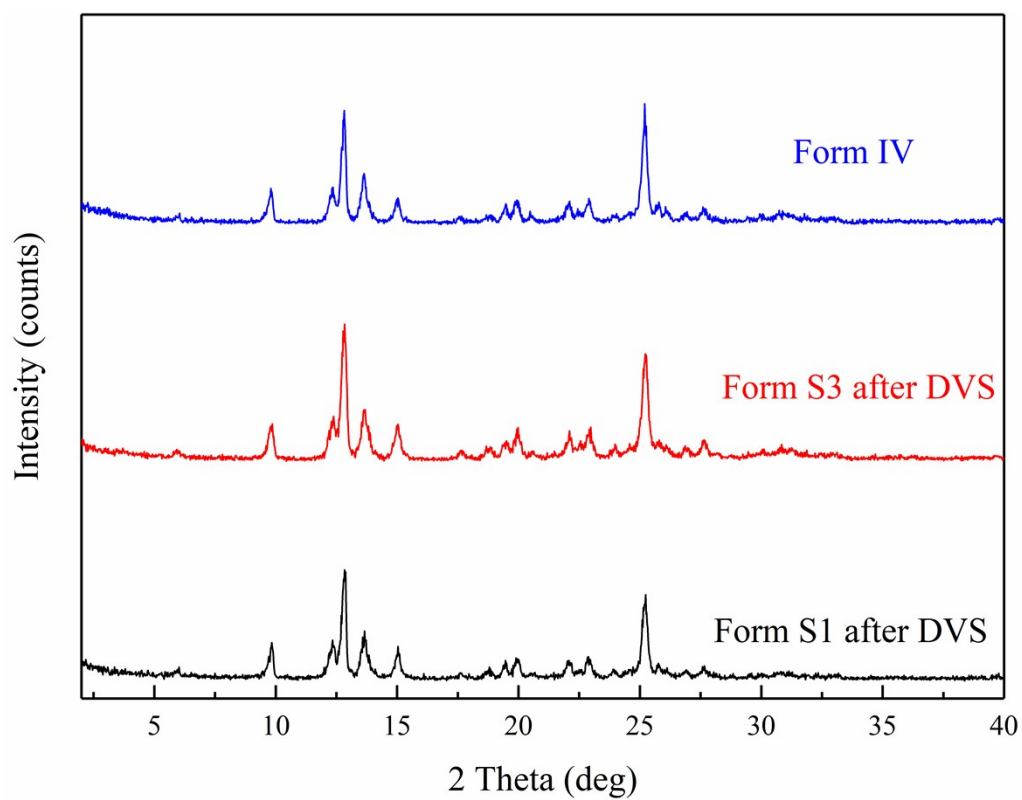


**Fig. S3** The overlaid DSC/TGA curves of (a) S1, (b) S2, (c) S3, (d) S4, (e) S5, (f) II



**Fig. S4** Compared XRPD patterns of nicosulfuron solvates after heating





**Fig. S5** Compared XRPD patterns of nicosulfuron solid forms after DVS experiment