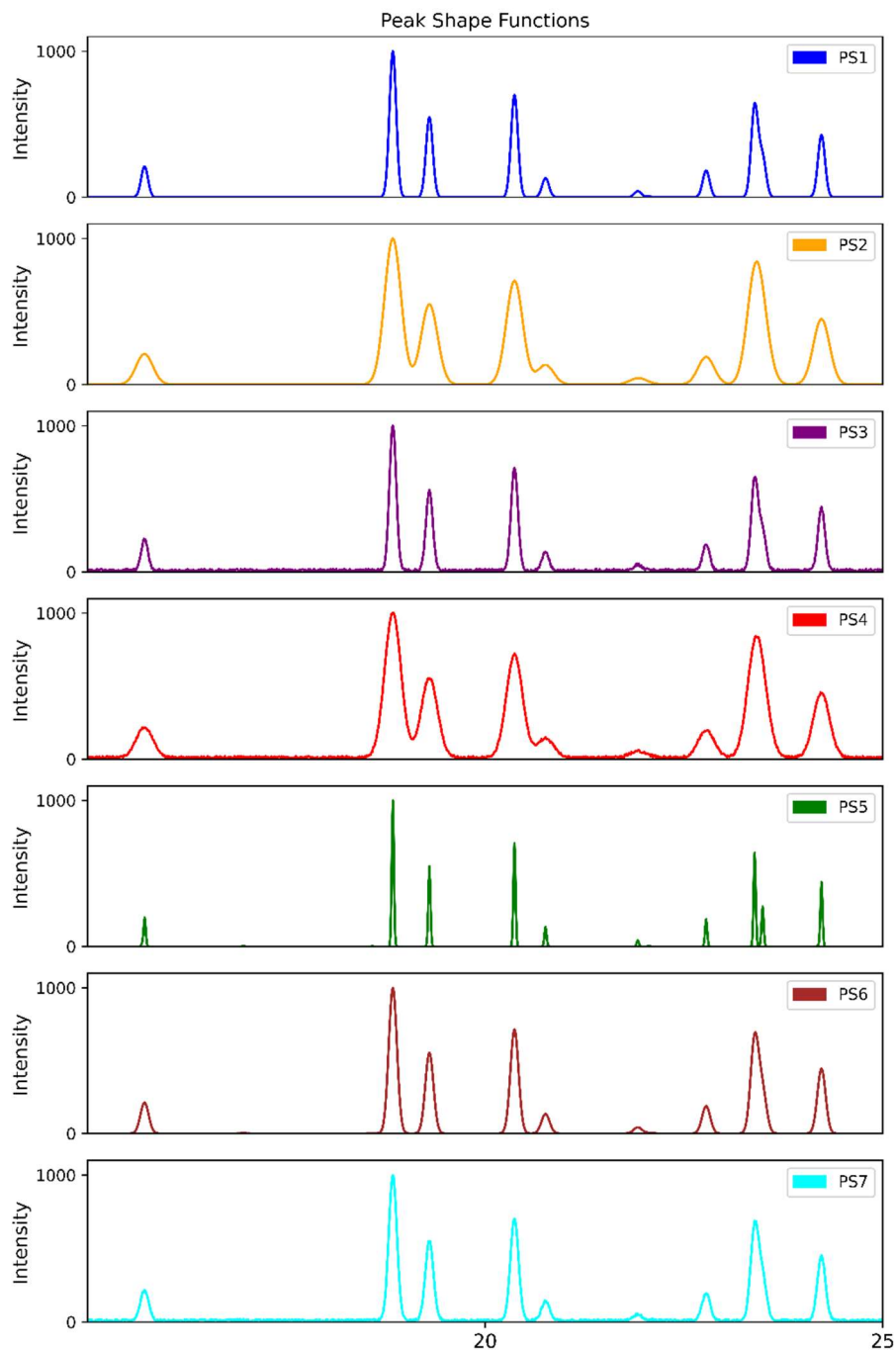# Supplementary materials

Peak Shape Function Comparison

In the main paper, we discuss the use of several peak shape functions to add variety to our patterns. The following figure shows the effect of peak shapes functions on the first ICSD entry "icsd_000001".

The next figure reiterates our peak shape function Caglioti parameters:

Dataset Name (#)	U	V	W	Noise*
Peak Shape 1 (1)	0.05	-0.06	0.07	No
Peak Shape 2 (2)	0.05	-0.01	0.01	No
Peak Shape 1 + Noise (3)	0.05	-0.06	0.07	Yes
Peak Shape 2 + Noise (4)	0.05	-0.01	0.01	Yes
Peak Shape 3 (5)	0	0	0.01	No
Peak Shape 4 (6)	0	0	0.001-0.1**	No
Peak Shape 4 + Noise (7)	0	0	0.001-0.1**	Yes

RRUFF Comparison

We have discussed how removing pooling layers affects classification, showing that they are responsible for extracting fine-grained features that incorporate spatial properties. To better visualize this property, we present three specific examples to further explore the model properties. All three examples have what would be considered a large number of peaks for highly symmetric crystals (Cubic and Tetragonal). The NPCNN model correctly identified these cases are the highly symmetric tetragonal and cubic crystal systems.

The SCNN model incorrectly predicted that these were instead low symmetry classes such as monoclinic and orthorhombic. This leads us to believe that the SCNN's draws less relationships between the peaks, making it unable to decipher whether all the atoms have symmetry. However, the NPCNN can detect symmetry as it can account for a large number of peaks since the extracted features are highly contextualized with other peaks. For example, these features could be relative peak intensity or position, both of which are important for crystal system and space group classification. Ultimately, these highly symmetric cases show evidence that the removal of pooling layers can benefit classification.