# Rationalising the difference in crystallisability of two Sulflowers using efficient in silico methods
# Supplementary Information

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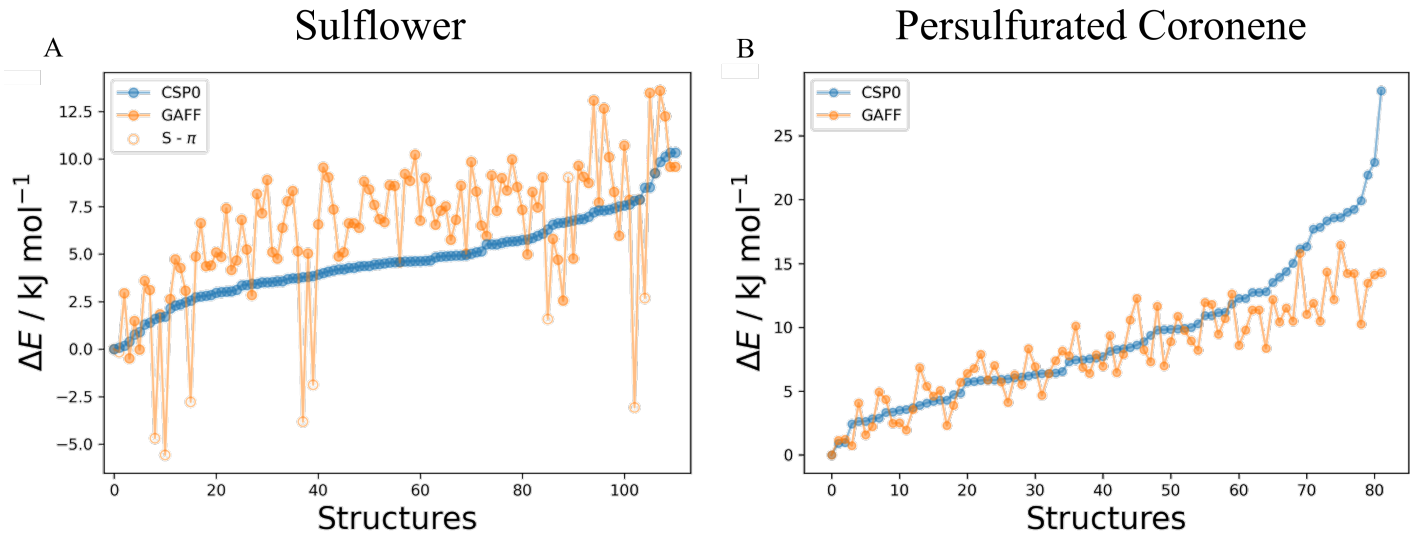


**Fig. 1** Comparison between the CSP_0 (blue) and GAFF (orange) energies for the Sulflower and persulfurated coronene sets. Energies are rescaled with respect to the CSP_0 global minimum. In the Sulflower plot, structures with edge-face interactions are shown with an empty circle.

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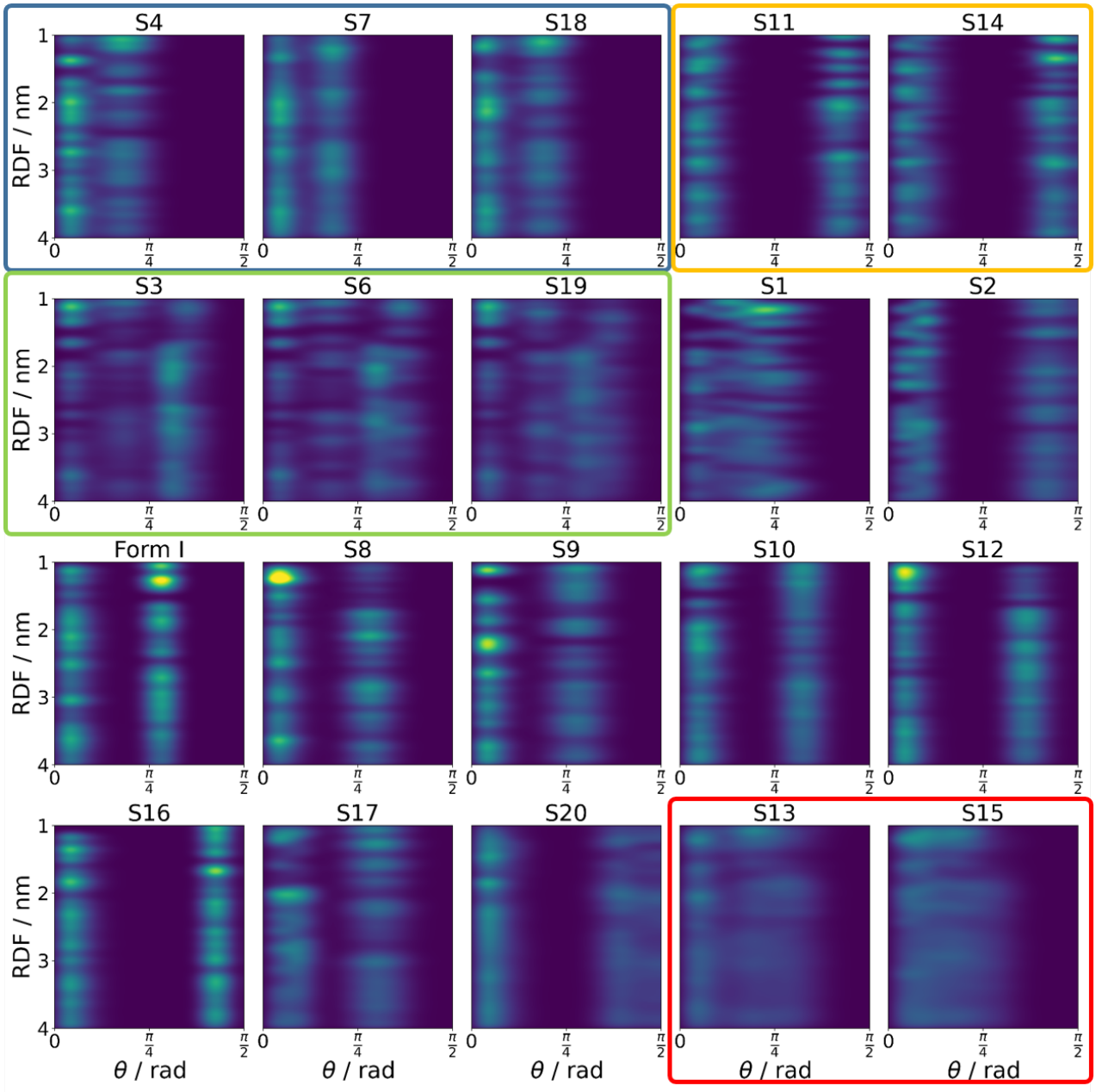


**Fig. 2** Fingerprints of the finite-temperature structures of Sulflower. Disordered structures are delimited with a red box. The different groups from the clustering analysis are shown in boxes of different colours.

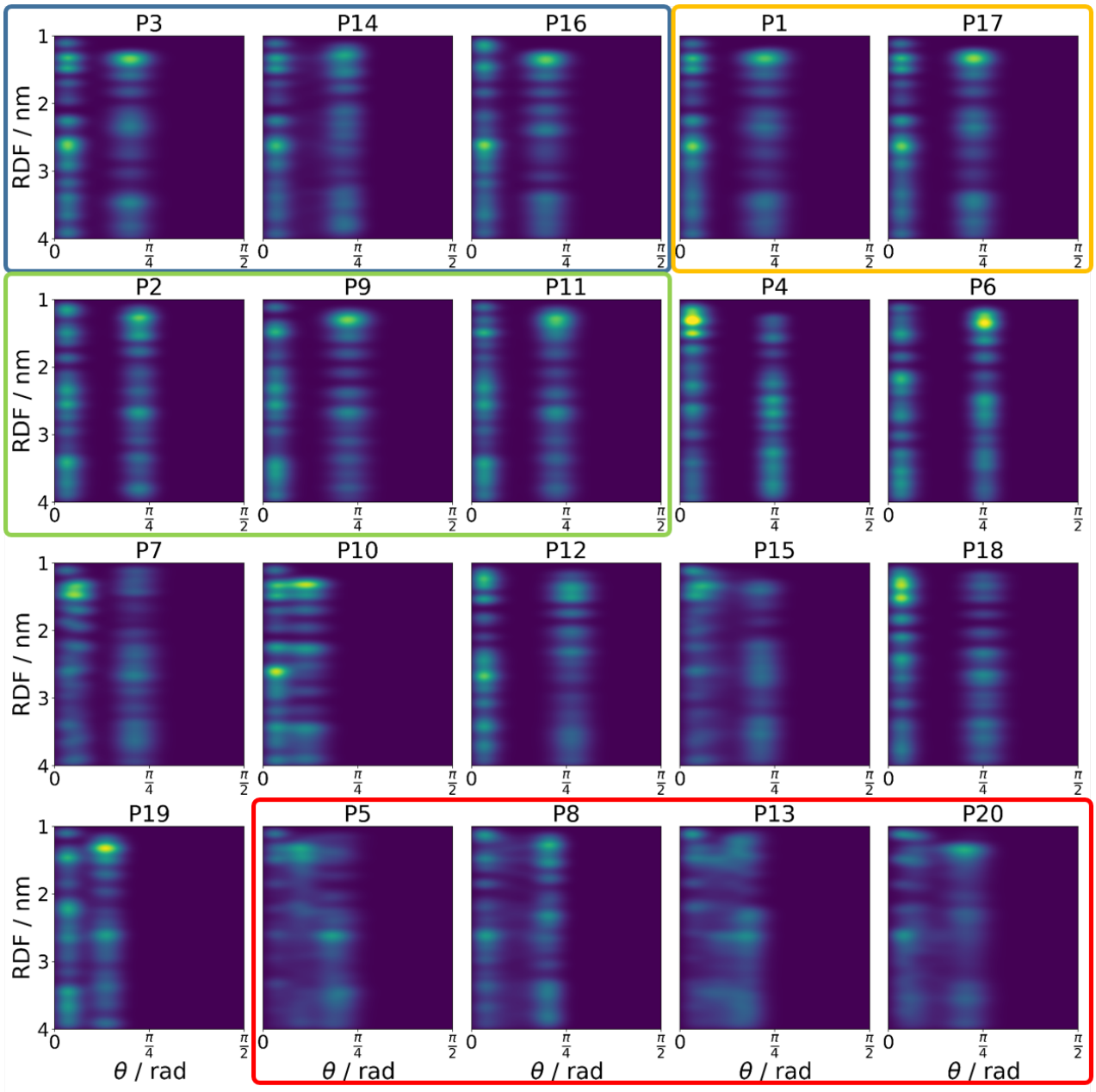


**Fig. 3** Fingerprints of the finite-temperature structures of persulfurated coronene. Disordered structures are delimited with a red box. The different groups from the clustering analysis are shown in boxes of different colours