Description of DOI XXXXX content, related to

**Digital Navigation of Energy–Structure–Function Maps for Hydrogen-Bonded Porous Molecular Crystals**

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Computational data related to landscapes of predicted crystal structures (Table D1) and energy–structure–function (ESF) maps (Table D2) have been deposited in a series of files that can be accessed via DOI XXXXX. Further description of the deposited data can be found within the individual files.

Table D1. Predicted crystal structures of molecules **TH1**, **TH2**, **TH3**, **TH4**, **TH5**, **T2**, **SH1**, **SH2** and **S2** with relative lattice energies (Erel) within 100 or 150 kJ mol-1 from the corresponding global minimum.

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| File name | File content description |
| TH1\_Predicted\_Structures.cif | **TH1** predicted crystal structures with Erel below 100 kJ mol-1. |
| TH2\_Predicted\_Structures.cif | **TH2** predicted crystal structures with Erel below 100 kJ mol-1. |
| TH3\_Predicted\_Structures.cif | **TH3** predicted crystal structures with Erel below 100 kJ mol-1. |
| TH4\_Predicted\_Structures.cif | **TH4** predicted crystal structures with Erel below 100 kJ mol-1. |
| TH5\_Predicted\_Structures.cif | **TH5** predicted crystal structures with Erel below 100 kJ mol-1. |
| T2\_Predicted\_Structures.cif | **T2** predicted crystal structures with Erel below 100 kJ mol-1. |
| SH1\_Predicted\_Structures.cif | **SH1** predicted crystal structures with Erel below 150 kJ mol-1. |
| SH2\_Predicted\_Structures.cif | **SH2** predicted crystal structures with Erel below 150 kJ mol-1. |
| S2\_Predicted\_Structures.cif | **S2** predicted crystal structures with Erel below 150 kJ mol-1. |

Table D2. ESF maps. Calculated properties of predicted crystal structures listed in Table D1.

|  |  |
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| File name | File content description |
| TH1\_ESF\_data.txt | Crystal density (ρ), lattice energy (Elatt), number of hydrogen bonds per molecule (HB) and number of 𝜋–𝜋 stacking modes per molecule (𝜋–𝜋) of **TH1** predicted crystal structures. |
| TH2\_ESF\_data.txt | ρ, Elatt, HB and 𝜋–𝜋 of **TH2** predicted crystal structures. |
| TH3\_ESF\_data.txt | ρ, Elatt, HB and 𝜋–𝜋 of **TH3** predicted crystal structures. |
| TH4\_ESF\_data.txt | ρ, Elatt, HB and 𝜋–𝜋 of **TH4** predicted crystal structures. |
| TH5\_ESF\_data.txt | ρ, Elatt, HB and 𝜋–𝜋 of **TH5** predicted crystal structures. |
| T2\_ESF\_data.txt | ρ, Elatt, HB and 𝜋–𝜋 of **T2** predicted crystal structures. |
| SH1\_ESF\_data.txt | ρ, Elatt, HB and 𝜋–𝜋 of **TH1** predicted crystal structures. |
| SH2\_ESF\_data.txt | ρ, Elatt, HB and 𝜋–𝜋 of **SH2** predicted crystal structures. |
| S2\_ESF\_data.txt | ρ, Elatt, HB and 𝜋–𝜋 of **S2** predicted crystal structures. |