

## Crystal structure, Hirshfeld surface analysis, energy frameworks, and DFT calculations of 1-methyl-3-(trifluoromethyl)-1*H*-pyrazole-4-carboxylic acid

Qing Tian<sup>1</sup>, Rong-Rong Yang<sup>1</sup>, Xue-Mei Wu<sup>1</sup>, Li-Jing Min<sup>2</sup> and Guo-Xiang Sun<sup>1\*</sup>

<sup>1</sup>Department of Pharmaceutical Engineering, School of Chemistry and Chemical Engineering, Yancheng Institute of Technology, Jiangsu, Yancheng, 224051, China

<sup>2</sup>College of Life Science, Key Laboratory of Vector Biology and Pathogen Control of Zhejiang Province, Huzhou University, Huzhou, 31300, China

**ABSTRACT** An organic carboxylic acid (1-methyl-3-(trifluoromethyl)-1*H*-pyrazole-4-carboxylic acid) was synthesized. The structure was confirmed by X-ray single crystal diffraction. The title compound exhibited inter-molecular hydrogen bonds of the type C–H...O, O–H...N and C–H...F. Hirshfeld surface analysis showed that the major intermolecular interaction is mainly due to H...H contacts. Furthermore, energy frameworks, and DFT calculations indicated that pyrazole ring and trifluoromethyl group are important for the bioactivity.

**KEYWORDS** Pyrazole-4-carboxylic acid, X-ray, DFT calculation, Hirshfeld surface analysis.

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