Impact of Crystal Habit on solubility of Ticagrelor

Yan Ren, Jie Shen, Kaxi Yu, Chi Uyen Phan, Guanxi Chen, Jiyong Liu, Xiurong Hu *, Jianyue Feng*

Department of Chemistry, Zhejiang University, Hangzhou 310028, China

* *Corresponding author: huxiurong@zju.edu.cn, jyfeng@zju.edu.cn*

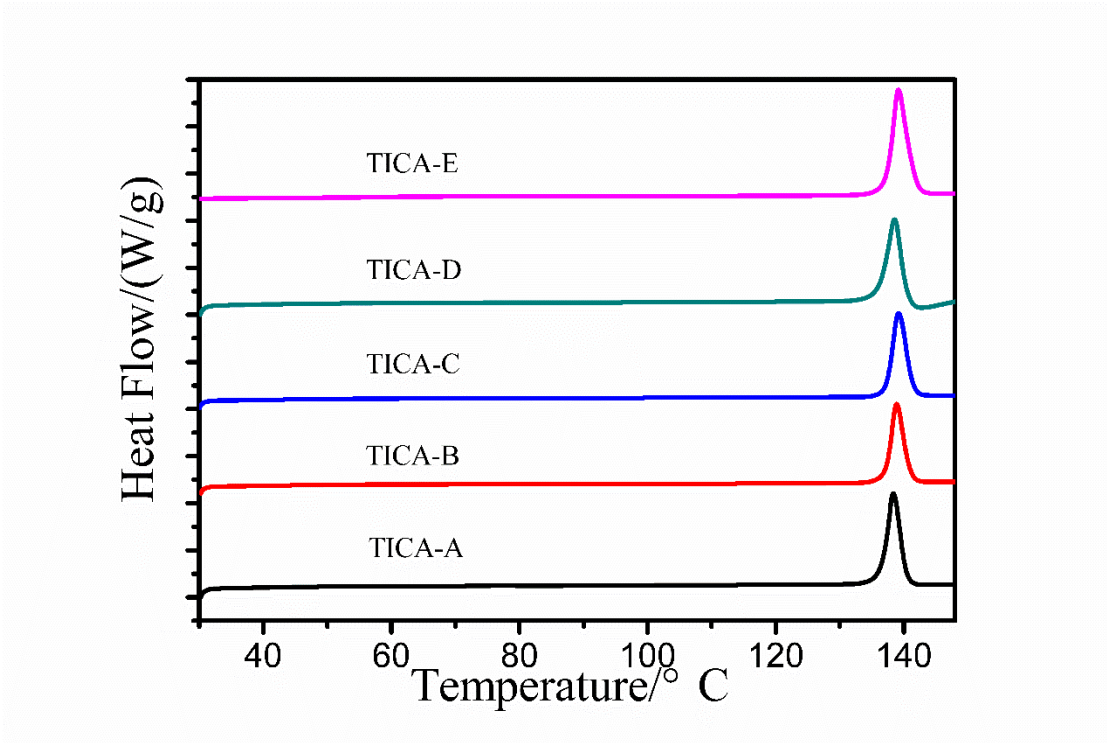

Figure S1 The DSC curve of TICA crystal habits

Table S1 Preparation method for TICA crystal habits

Sample name	preparation method	solvent	Concentration (m/v)	anti-solvent (ratio of solvent: antisolvent)	aspect ratio
TICA-A	rapid-cooling crystallization	acetonitrile	1:8		1:1~2:1
TICA-B	antisolvent crystallization	ethyl acetate	1:15	1:1	10:1
TICA-C	rapid-cooling crystallization	ethyl acetate	1:20		5:1~8:1
TICA-D	antisolvent crystallization	butyl acetate	1:10	1:1	1:1~3:1
TICA-E	antisolvent crystallization	ethyl acetate	1:10	1:1.5	more than10:1

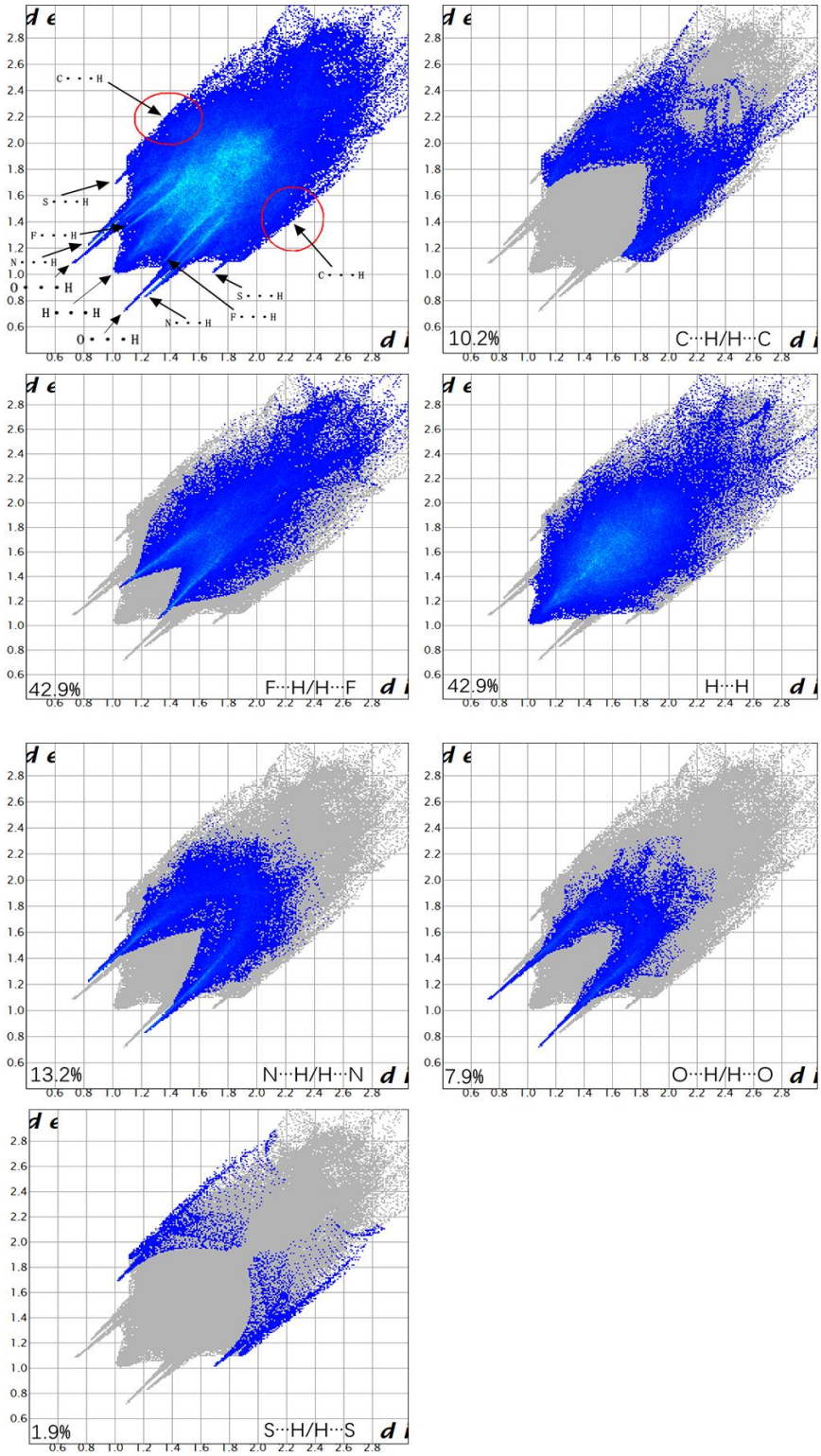

Figure S2 The Hirshfeld surfaces of TICA-Ⅱ

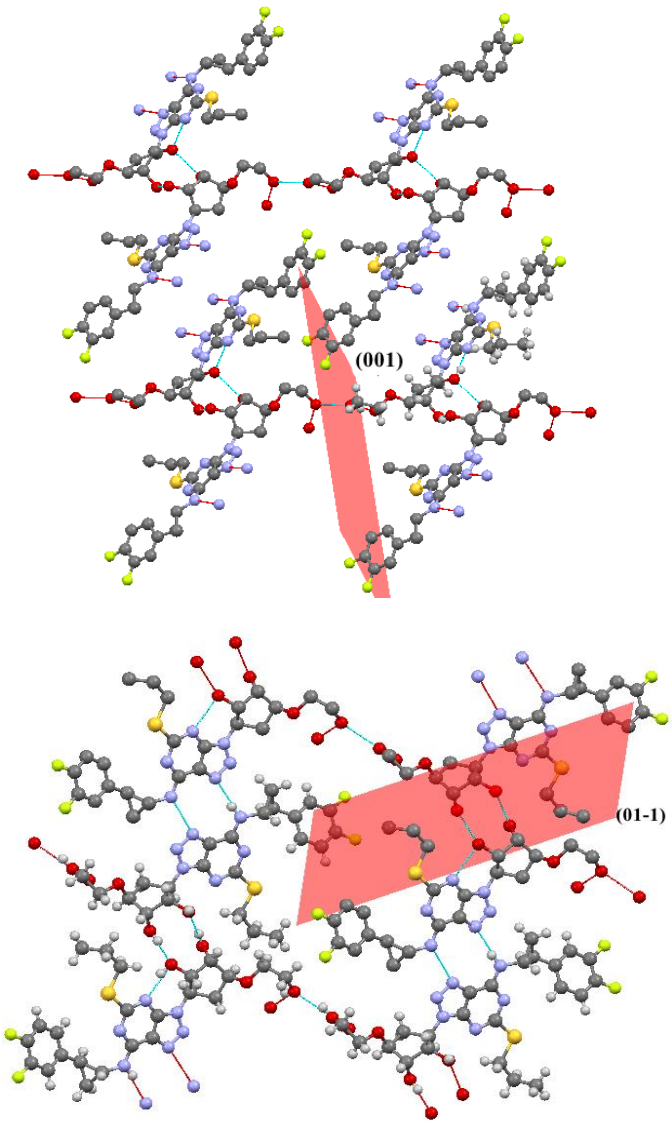

Figure S3 Different screenshots of (001) face and (01-1) face using Mercury 2.3 software.