

Supporting information

Supramolecular Self-Assembly Built by Weak Hydrogen, Chalcogen and Unorthodox Nonbonded Motifs in 4-(4-chlorophenyl)-3-[(4-fluorobenzyl)sulfanyl]-5-(thiophen-2-yl)-4H-1,2,4-triazole, a Selective COX-2 Inhibitor: Insights from X-ray and Theoretical Studies

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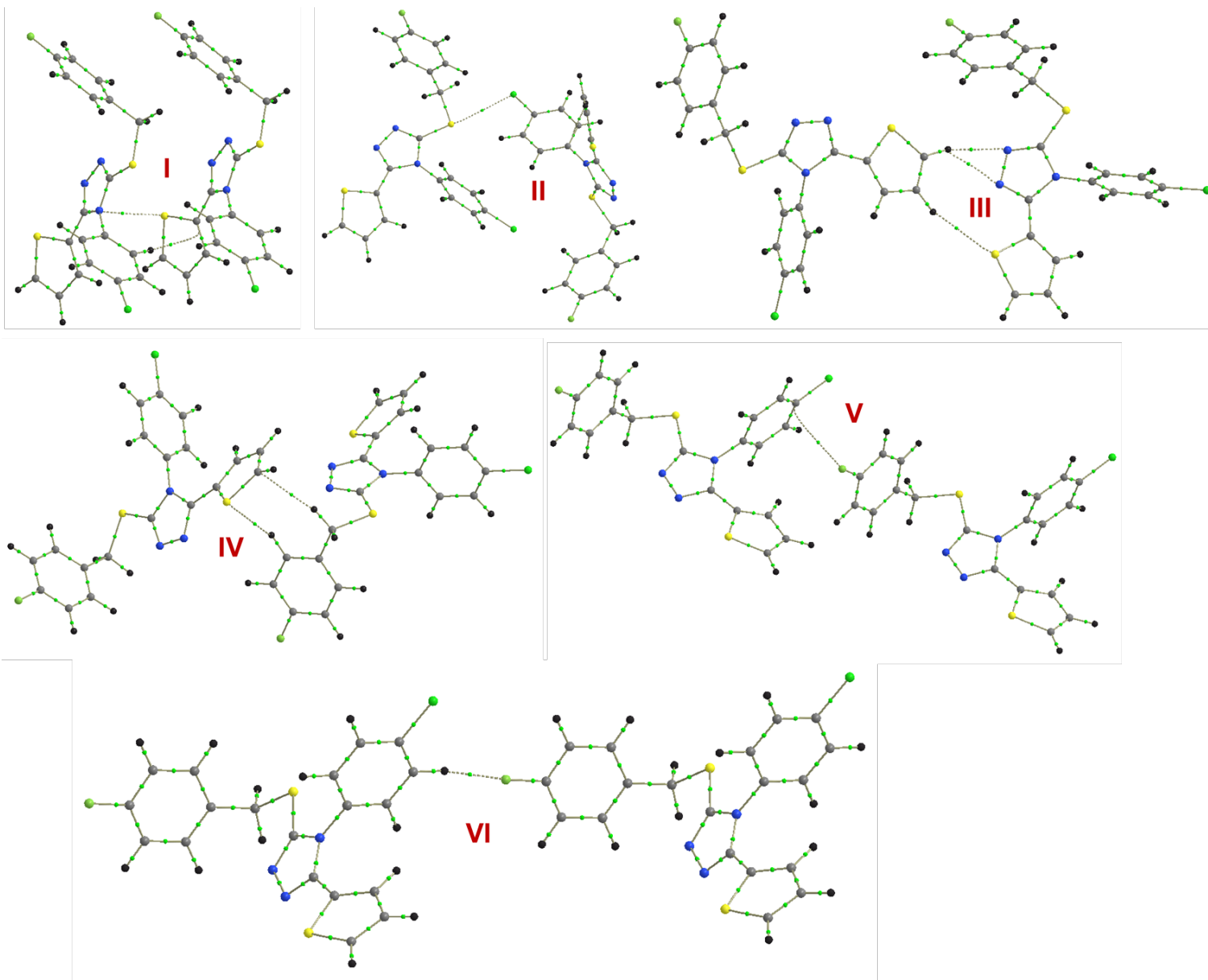


Figure S1. Molecular graphs showing the intermolecular interactions in different molecular pairs (I-VI) of the title compound.

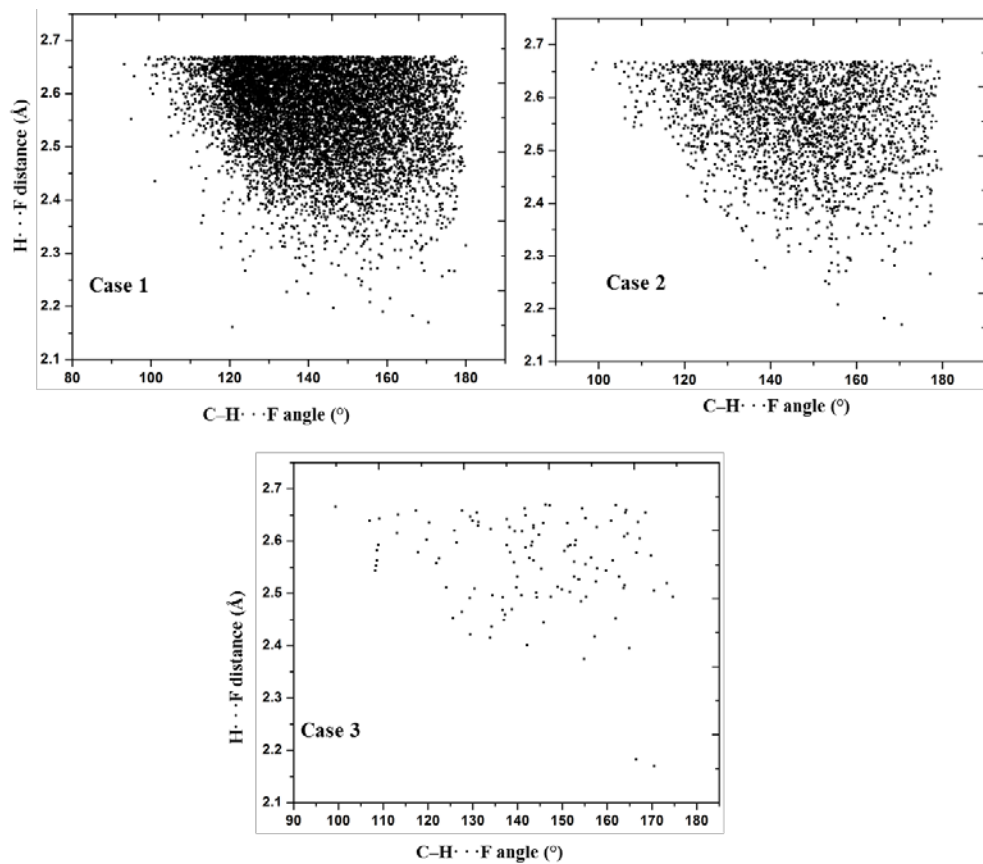


Figure S2. The distribution of C–H...F contacts (distance and angle) for three different cases (see Scheme 2).

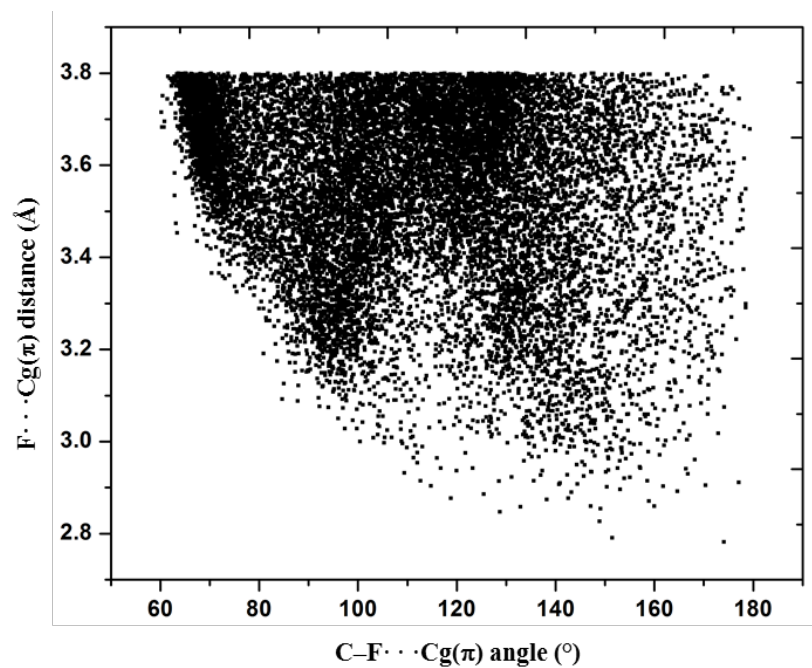


Figure S3. The distribution of C-F...Cg(π) contacts

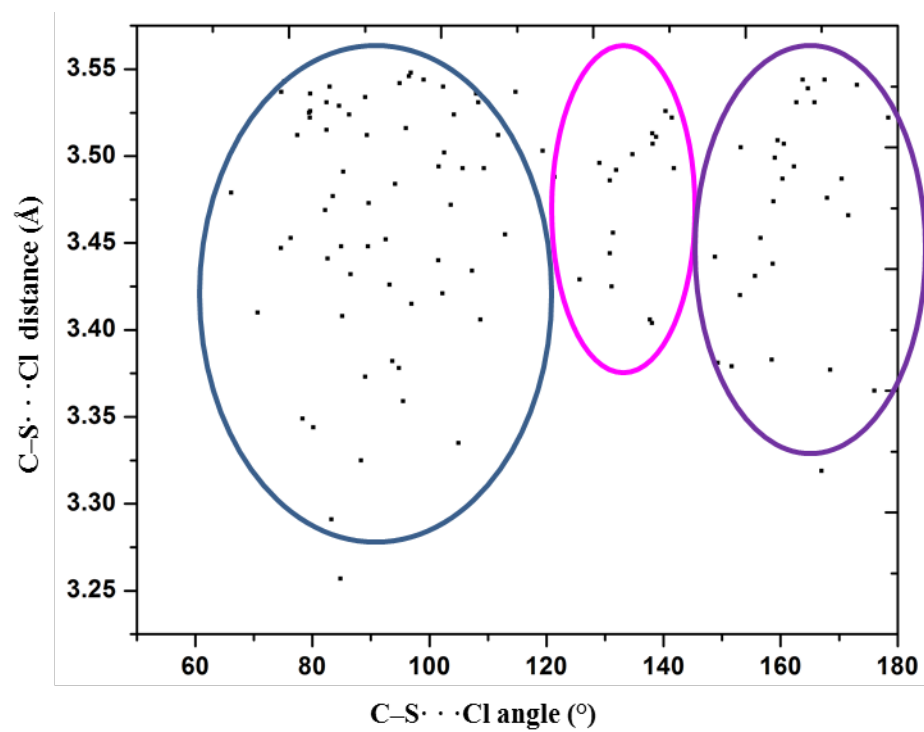


Figure S4. The distribution of C-S...Cl contacts.