Supplementary Materials

(3-(4-chlorophenyl)-4,5-dihydroisoxazol-5-yl)methyl benzenesulfonate

Loubna Mokhi [1], Karim Chkirate [2], Xiaodong Zhang [3], Mohsine Driowya [1,4] and Khalid Bougrin [1,5,*]

[1] *Equipe de Chimie des Plantes et de Synthèse Organique et Bioorganique, URAC23, Faculty of Science, B.P. 1014, Geophysics, Natural Patrimony and Green Chemistry (GEOPAC) Research Center, Mohammed V University in Rabat, Rabat 10010, Morocco*

[2] *Laboratory of Heterocyclic Organic Chemistry URAC 21, Pharmacochemistry Competence Center, Av. Ibn Battouta, BP 1014, Faculty of Sciences, Mohammed V University in Rabat, Rabat 10010, Morocco*

[3] *Department of Chemistry, Tulane University, New Orleans, LA 70118, USA*

[4] *Higher School of Technology, Sultan Moulay Slimane University, B.P. 170, Khenifra 54006, Morocco.*

[5] *Chemical & Biochemical Sciences Green-Process Engineering (CBS), Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid, Ben Guerir 43150, Morocco*

* Corresponding author:

Prof. Khalid Bougrin

Email address: kbougrin@yahoo.fr or k.bougrin@um5.ac.ma

Table of contents

1. Copies of characteristic ^{1}H NMR and ^{13}C NMR spectra

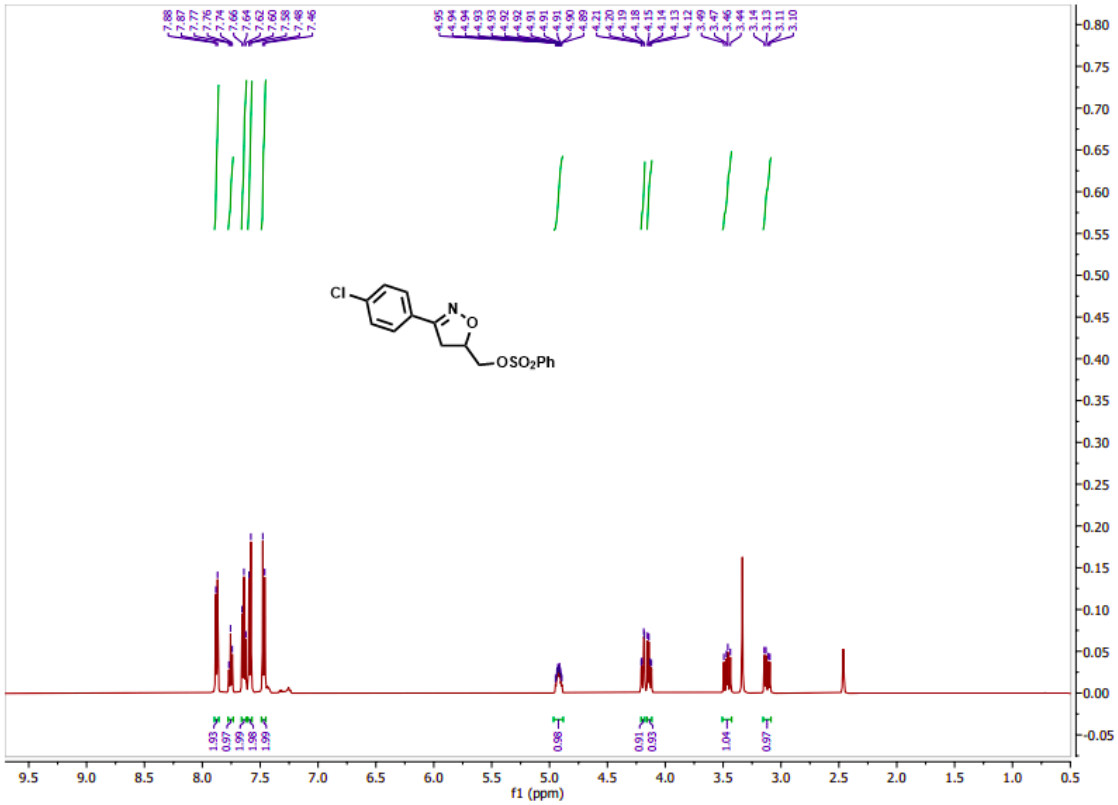

Figure S1. ^{1}H NMR spectrum of **(5)**

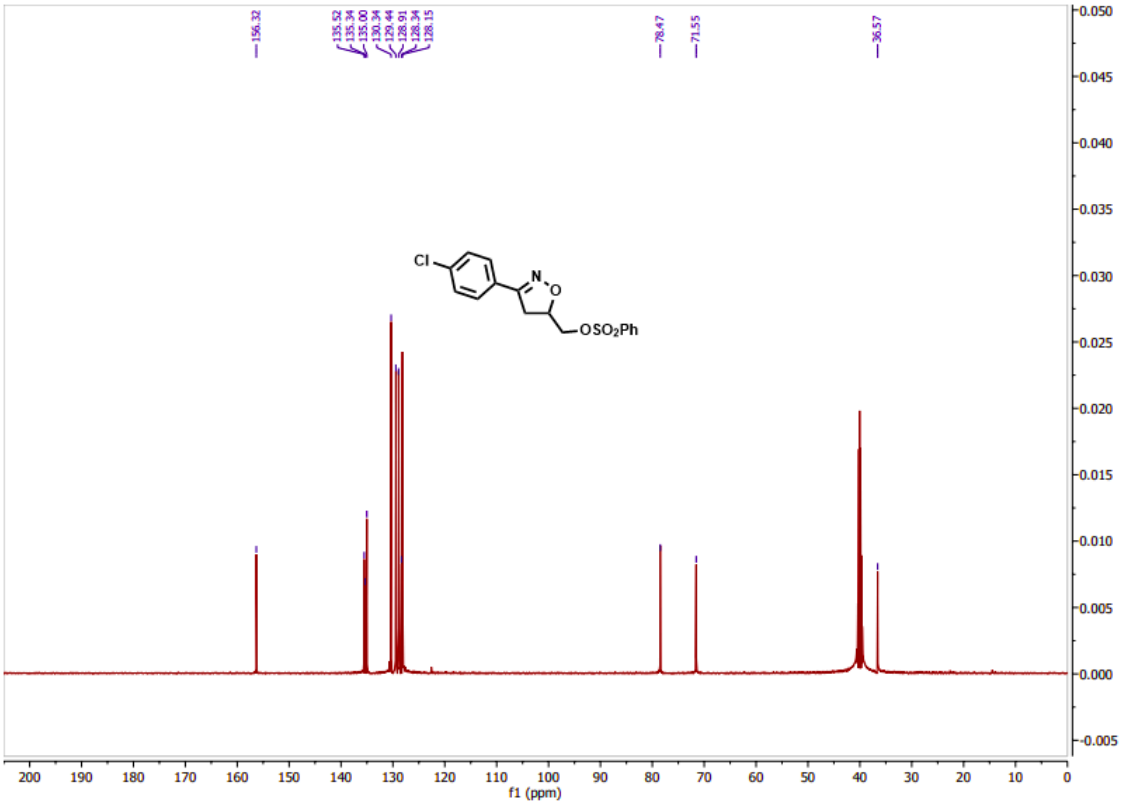

Figure S2. ^{13}C NMR spectrum of **(5)**

2. Copy of characteristic ESI-MS spectra

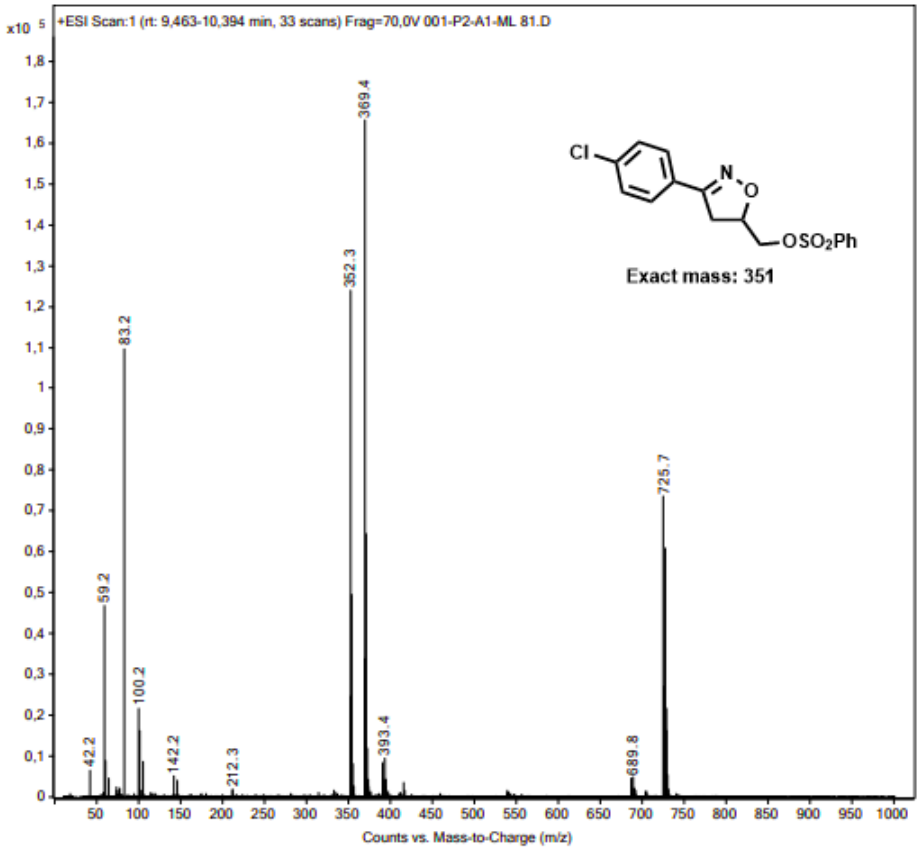

Figure S3. ESI^{+}-MS spectrum of **(5)**

3. Copy of characteristic FT-IR spectra

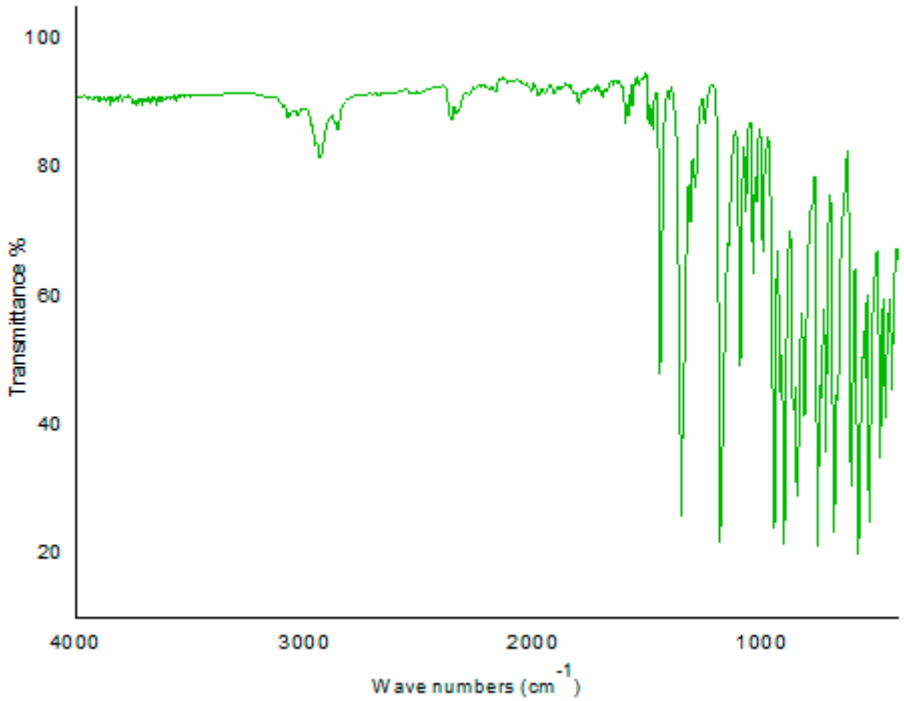

Figure S4. FT-IR spectrum of **(5)**

4. Figures S5–S7 and Figures S8–S10

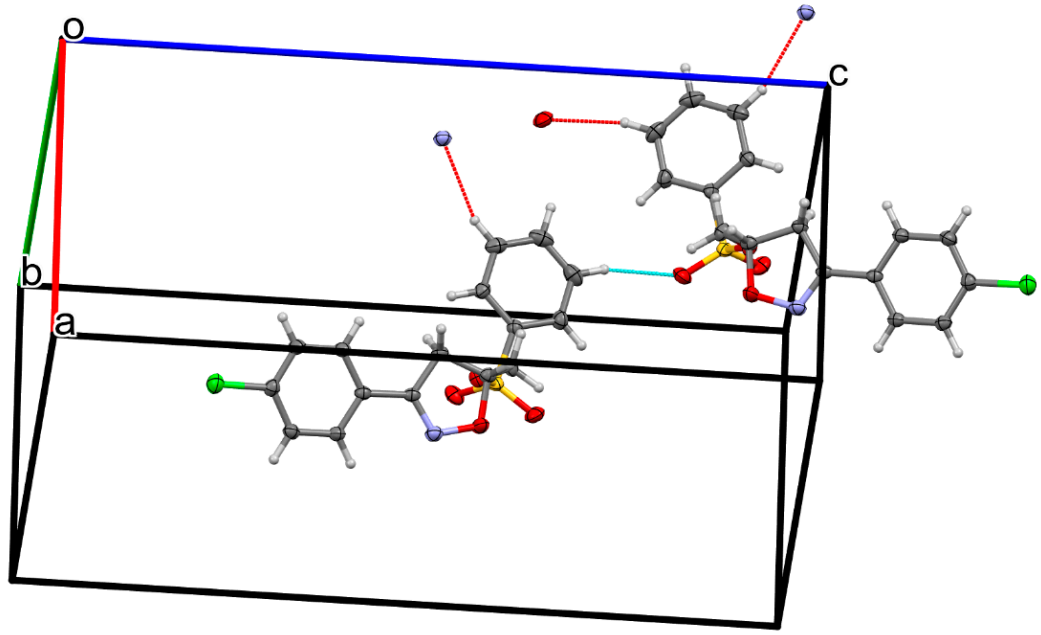

Figure S5. This picture shows two molecules connected through C—H···O short contact to form a pair.

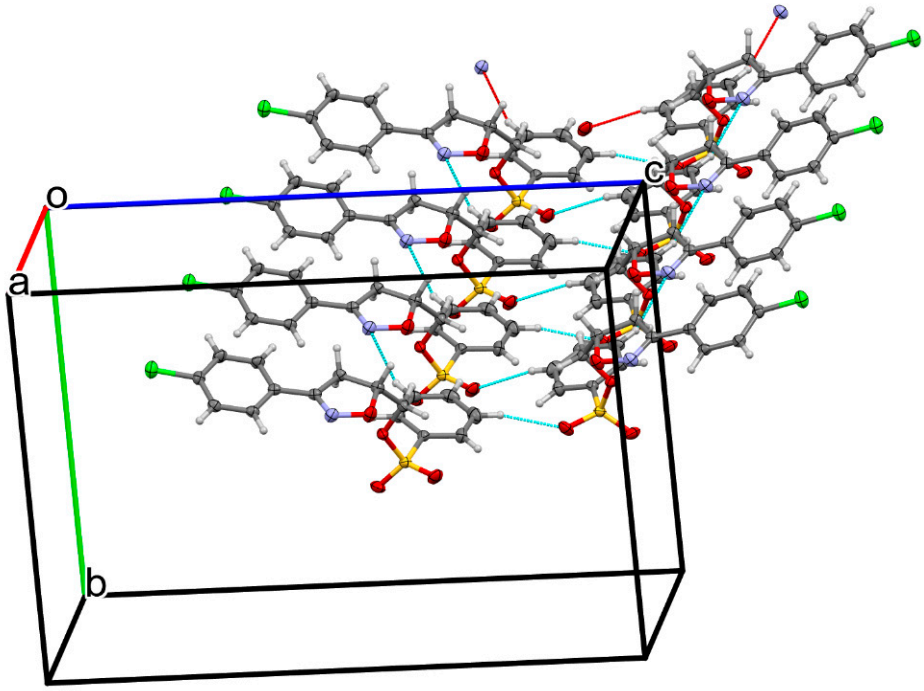

Figure S6. This picture shows many pairs of molecules are connected through C—H···N short contacts to form a long chain along a-axis.

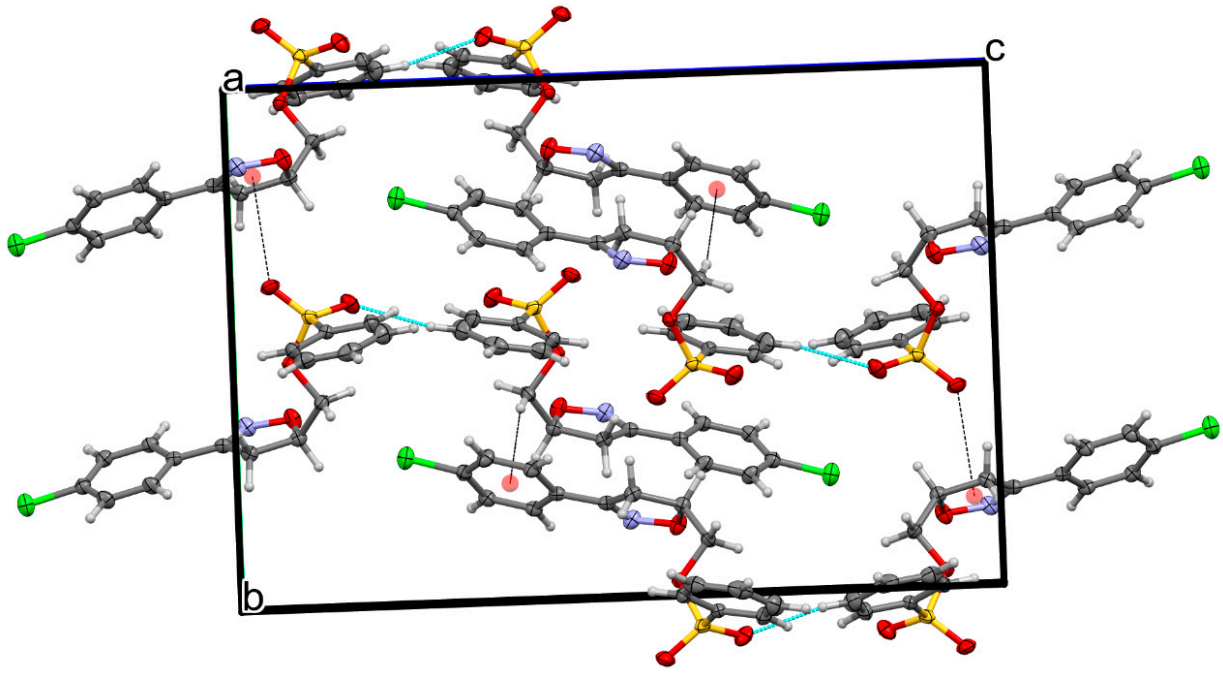

Figure S7. This picture shows eight crystallographic symmetry related molecules in one-unit cell.

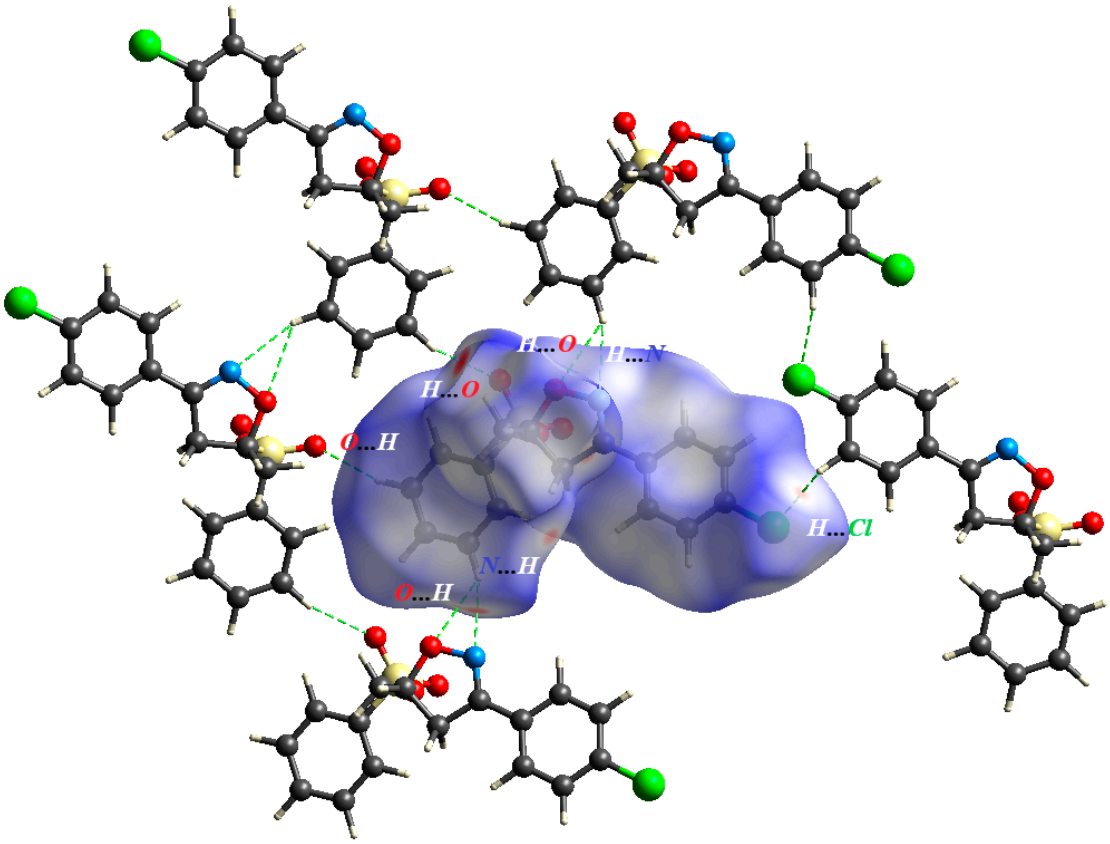

Figure S8. Principal non-covalent interactions and the Hirshfeld surface are plotted over dnorm in the crystal packing of [3-(4-chlorophenyl)-4,5-dihydroisoxazol-5-yl]methyl benzenesulfonate .

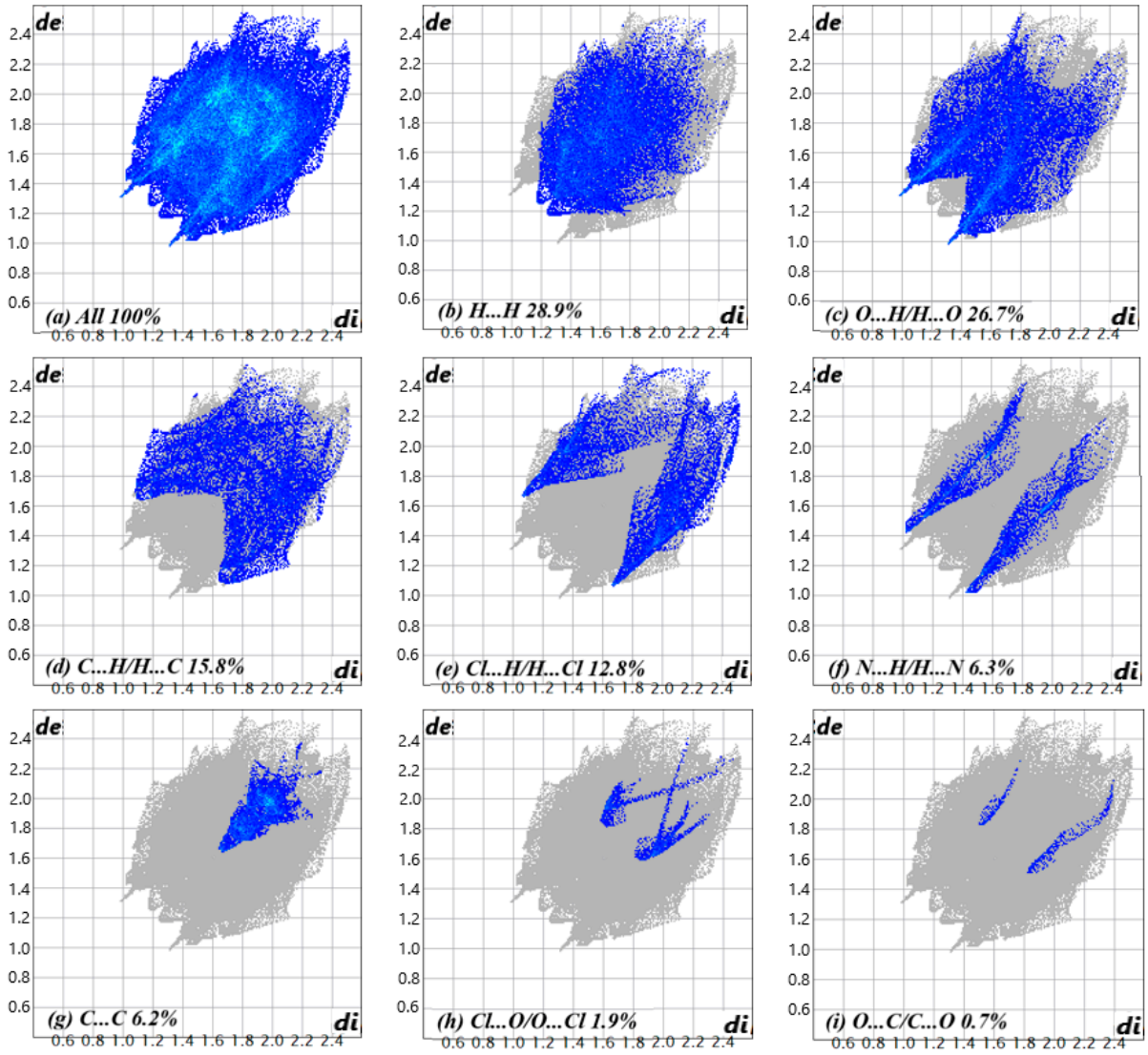

Figure S9. Two-dimensional fingerprint plots for the title compound, showing (a) all interactions, and delineated into (b) H···H, (c) H···O/O···H, (d) C···H/H···C, (e) Cl···H/H···Cl, (f) N···H/H···N, (g) C···C, (h) Cl···O/O···Cl and (i) O···C/C···O interactions. The d_e and d_i values are the closest external and internal distances (in Å) from given points on the HS.

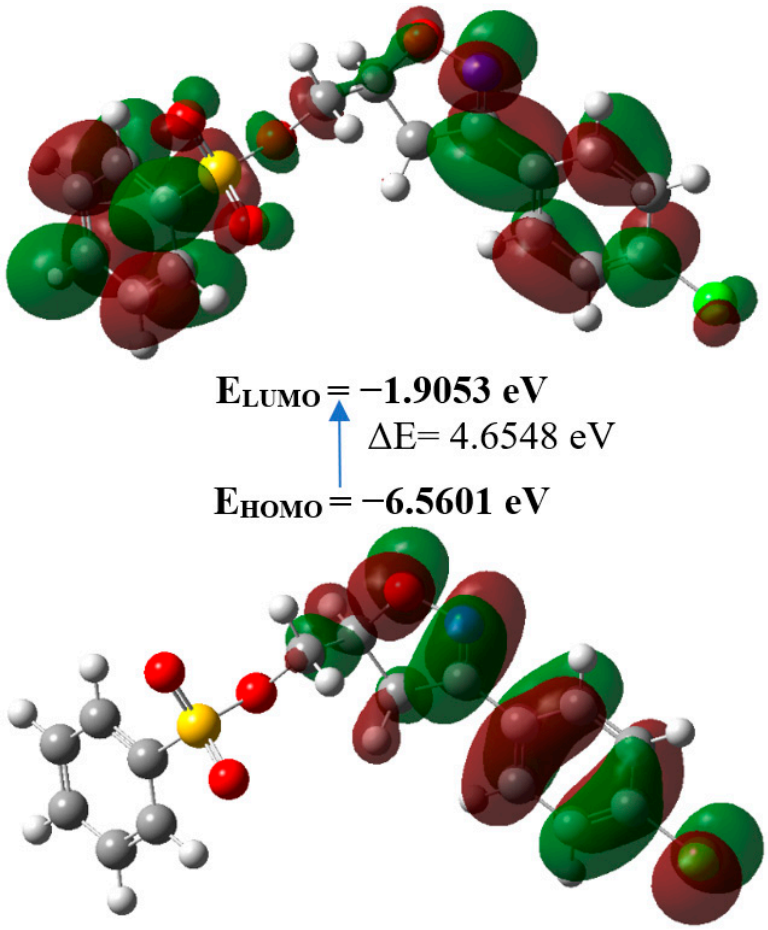

Figure S10. The energy band gap of [3-(4-chlorophenyl)-4,5-dihydroisoxazol-5-yl]methyl benzenesulfonate.

5. Tables S1 – S4

Table S1. Hydrogen bond geometries (Å, °) for [3-(4-chlorophenyl)-4,5-dihydroisoxazol-5-yl]methyl benzenesulfonate.

D—H···*A*	*D*—H	H···*A*	D···*A*	*D*—H···*A*
C2—H2···Cl1^{i}	0.95	2.84	3.5624 (11)	133.2
C4—H4···O4^{ii}	0.95	2.59	3.2807 (12)	129.5
C16—H16···O2^{iii}	0.95	2.61	3.4229 (12)	144.1
C16—H16···O3^{iii}	0.95	2.61	3.4416 (13)	146.5

Symmetry codes: (i) *x*−1/2, *y*, −*z*+1/2; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1.

Table S2. Similarity (DFT and X-ray) of selected Angles and bond lengths (°, Å).

	X-ray	B3LYP/6–311G+(d,p)
S1-O4	1.4318(8)	1.4564
S1-O3	1.4304(8)	1.4566
S1-O2	1.5791(7)	1.6509
S1-C11	1.7534(9)	1.7867
C10-O2	1.4573(11)	1.4522
C9-O1	1.4609(12)	1.4564
N1-O1	1.4126(11)	1.3954
N1-C7	1.2845(12)	1.2827
C3-Cl1	1.7445(10)	1.7562
S1-C11-C12	120.00(7)	118.8948
S1-C11-C16	118.24(7)	118.9752
C11-S1-O4	109.17(5)	110.1399
C11-S1-O3	110.00(5)	109.829
O4-S1-O3	119.42(5)	120.2536
O4-S1-O2	109.46(5)	108.1129
S1-O2-C10	117.55(6)	116.2247
C10-C9-O1	108.18(8)	106.9904
C9-O1-N1	109.36(7)	109.628
O1-N1-C7	109.72(8)	110.3487
N1-C7-C8	114.14(8)	113.2056
N1-C7-C6	121.07(8)	121.4667
C4-C3-Cl1	119.91(7)	119.4282
C2-C3-Cl1	118.44(8)	119.5688

Table S3. Calculated energies.

Molecular Energy	Title Product
Total Energy TE (eV)	-49861.0176
EHOMO (eV)	-6.5601
ELUMO (eV)	-1.9053
Gap, ΔE (eV)	4.6548
Dipole moment, μ (Debye)	6.4787
Ionization potential, I (eV)	6.5601
Electron affinity, A	1.9053
Electronegativity, χ	4.2327
Hardness, η	2.3274
Electrophilicity, index ω	3.8489
Softness, σ	0.4297
Transfer of a fraction of an electron, ΔN	0.5945

Table S4. Details of the experiment.

Crystal Data	
CCDC Number	2288360
Empirical formula	$C_{16}H_{14}ClNO_4S$
Formula weight	351.79
Temperature/K	150
Crystal system and Space group	Orthorhombic, *Pbca*
a, b, c (Å)	9.5722 (11), 15.0133 (17), 21.978 (2)
α, β, γ (°)	90, 90, 90
Volume (Å^3)	3158.5 (6)
Z	8
Radiation type	Mo Kα
μ (mm^{-1})	0.39
Crystal size (mm)	0.30 × 0.25 × 0.16
Data collection	
Diffractometer	diffractometer Bruker D8 QUEST PHOTON 3
Absorption correction	Numerical mu Calculated SADABS [40]
T_{min}, T_{max}	0.89, 0.94
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	68386, 5453, 4943
R_{int}	0.032
(sin θ/λ)max (Å^{-1})	0.748
Refinement	
R[F2 > 2σ(F2)], wR(F2), S	0.032, 0.093, 1.07
No. of reflections	5453
No. of parameters	208
No. of restraints	0
H-atom treatment	H-atom parameters constrained
$\Delta\rho$max, $\Delta\rho$min (e Å^{-3})	0.41, −0.34

Software applications: SHELXTL [28], SAINT [28], APEX4 [28], SHELXT [29], SHELXL [30], DIAMOND [41].

28. Bruker. *APEX4, SAINT & SHELXTL*; Bruker AXS LLC.: Madison, WI, USA, 2021.
29. Sheldrick, G.M. SHELXT—Integrated space-group and crystal-structure determination. *Acta Cryst. A* **2015**, *71*, 3–8.
30. Sheldrick, G.M. Crystal structure refinement with SHELXL. *Acta Cryst. C* **2015**, *71*, 3–8.
40. Krause, L.; Herbst-Irmer, R.; Sheldrick, G.M.; Stalke, D. Comparison of silver and molybdenum microfocus X-ray sources for single-crystal structure determination. *J. Appl. Cryst.* **2015**, *48*, 3–10.
41. Brandenburg, K.; Putz, H. *DIAMOND*; Crystal Impact GbR: Bonn, Germany, 2012.