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Supporting information for article:

Preparation, spectroscopic, X-ray crystallographic, DFT, antimicrobial and ADMET studies of *N*-[(4-flourophenyl)sulfanyl]phthalimide

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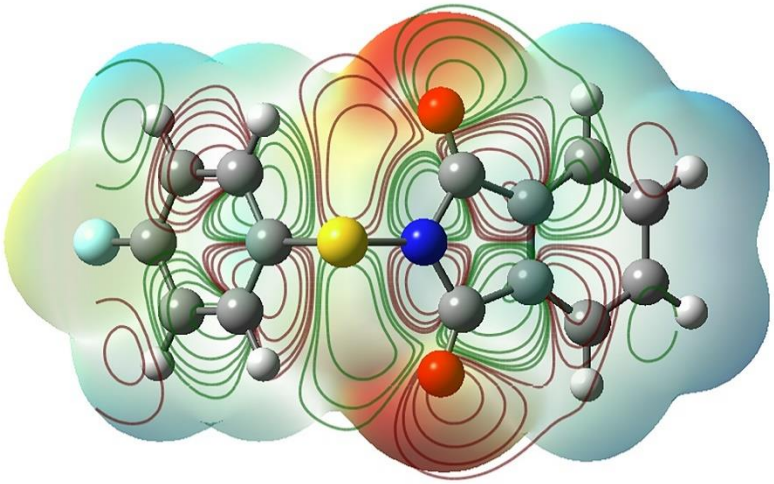

Figure S1. Total electron density and contour mapped for **FP** compound.

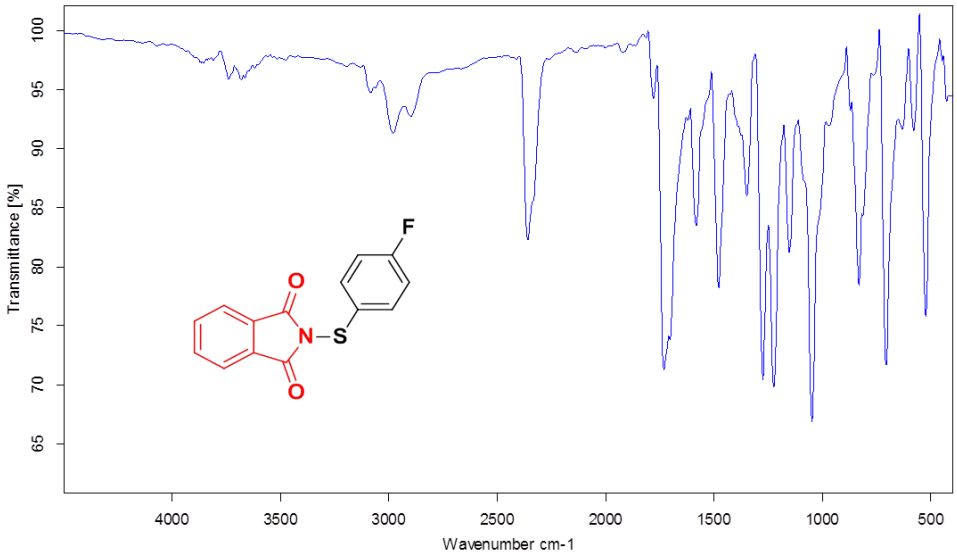

Figure S2. Experimental IR spectrum of the **FP** compound.

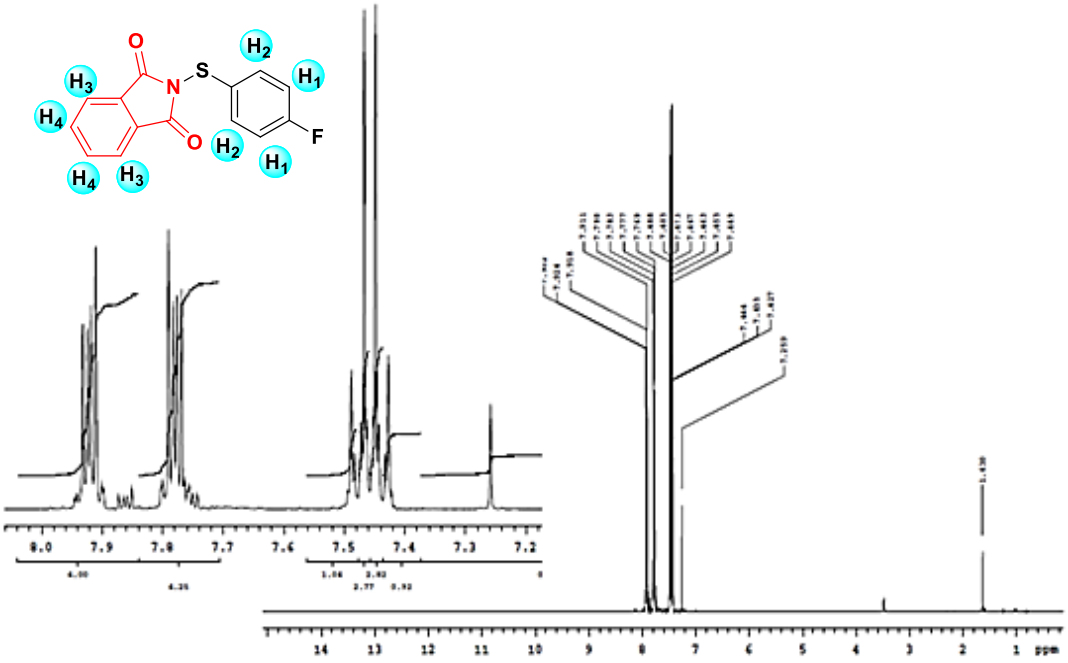

Figure S3. ^{1}H NMR spectrum of the **FP** compound.

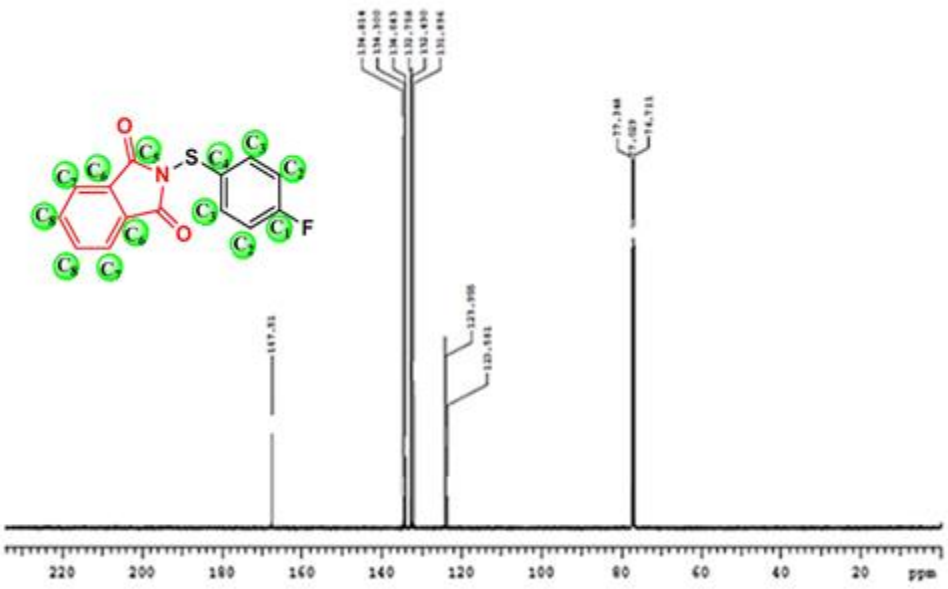

Figure S4. ^{13}C NMR spectrum of the **FP** compound.

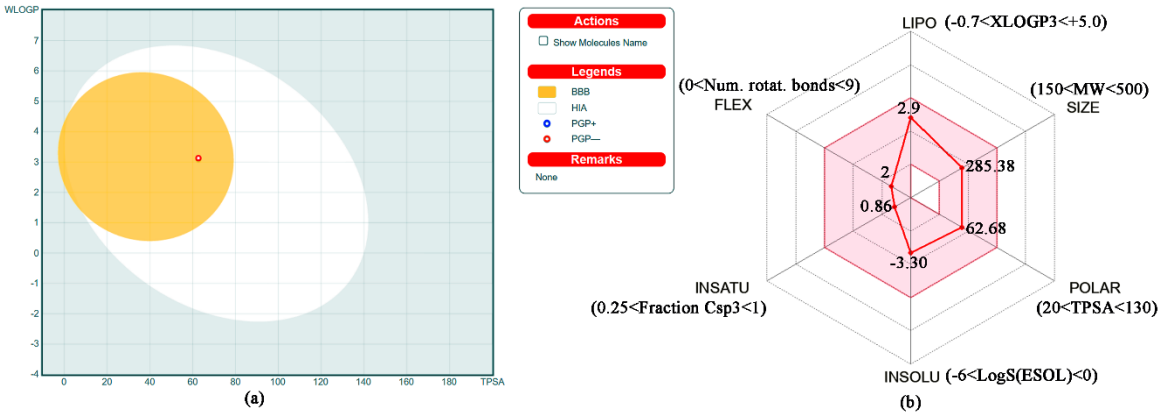

Figure S5. BOILED-Egg radar (a) and Radar graph (b) of the **FP** compounds (LIPO: Lipophilicity, SIZE: Molecular Weight, POLAR: Polarity, INSOLU: Insolubility, INSATU: Insaturation, FLEX: Flexibility)

Supplementary Tables

Table S1. The selected molecular structure parameters of the **FP** compound

Bond length	**Exp.**	**Theor.**	(Tanak *et al.*, 2018)
F1—C12	1.357 (2)	1.353	-
S1—N1	1.703 (2)	1.727	1.698(1)
S1—C9	1.774 (2)	1.795	1.775(2)
N1—C4	1.409 (2)	1.422	1.408(2)
N1—C1	1.419 (2)	1.422	1.419(2)
C4—O2	1.204 (2)	1.204	1.197(2)
C1—O1	1.200 (2)	1.204	1.198(2)
Bond angles			
N1—S1—C9	101.48 (7)	101.79	100.89(7)
C4—N1—C1	111.15 (13)	111.84	111.24(1)
C4—N1—S1	124.57 (11)	124.07	124.70(1)
C1—N1—S1	124.18 (12)	124.06	124.04(1)
O1—C1—N1	124.67 (16)	125.86	124.69(2)
F1—C12—C11	118.60 (16)	118.64	-
F1—C12—C13	118.40 (16)	118.64	-
O1—C1—C2	129.59 (16)	128.89	129.75(2)
O2—C4—N1	125.15 (15)	125.86	125.15(2)
O2—C4—C3	129.00 (16)	128.88	129.28(2)
Torsion angles			
N1—S1—C9—C14	−94.43 (14)	-91.20	-
C14—C13—C12—F1	−179.83 (15)	179.97	-
S1—N1—C4—O2	−2.4 (2)	-3.72	-
S1—N1—C1—C2	−177.35 (10)	176.79	-
C9—S1—N1—C4	102.84 (13)	-91.15	-
C3—C8—C7—C6	0.1 (3)	-0.12	-
C8—C3—C4—N1	179.94 (15)	179.60	-

Table S2. Geometric parameters (Å, º) for the intermolecular interactions.

(a) Intermolecular hydrogen bonds

D-H···A	**D-H**	**H···A**	**D···A**	**D-H···A**
C6—H6···O2^{i}	0.93	2.46	3.336 (2)	157
C8—H8···F1^{ii}	0.93	2.53	3.240 (2)	134
C11—H11···O1^{iii}	0.93	2.56	3.304 (2)	137
C13—H13···S1^{iv}	0.93	2.99	3.8823 (19)	162

Symmetry codes: (i) *x*,-1+*y*,*z;* (ii) 1+*x*,*y*,1+*z;* (iii) 1-*x*,1-*y*,-*z;* (iv) 1+*x*, *y*, *z*;

(b) Y—X···π interactions

Y—X···π	**X···Cg(π)**	**X$_{perp}$**	**Y—X···Cg(π)**	**Y···Cg(π)**
C7—H7···π(A)^{i}	2.819	-2.81	153	3.671(2)
C4—O2···π(B)^{ii}	3.5274(18)	3.150	111.70(12)	4.127(2)

Rings A and B have C9-C14 and N1-C4, respectively. Symmetry codes: (i) 1-*x*,1-*y*,1-*z*; (ii) 2-*x*,2-*y*,1-*z*

(c) π··π interactions

Cg(I)···Cg(J)	**Cg···Cg**	***α***	**β**	**γ**	**CgIperp**	**CgJperp**	Slippage
Cg(C)···Cg(D)^{i}	3.5578(14)	0.16(8)	12.9	13.1	3.4657(8)	3.4678(6)	0.795
Cg(D)···Cg(C)^{i}	3.5578(14)	0.16(8)	13.1	12.9	3.4678(6)	3.4656(8)	0.805
Cg(C)···Cg(D)^{ii}	4.1152(16)	0.16(8)	35.3	35.5	3.3508(8)	3.3576(6)	2.379
Cg(D)···Cg(D)^{i}	3.6403(13)	0.00(6)	17.8	17.8	3.4655(6)	3.4655(6)	1.115

Rings A, B C and D have C9-C14, N1-C4, C2-C5 and N1—C1—C2—C5—C6—C7—C8—C3—C4 respectively. Symmetry codes: (i) 1-*x*,1-*y*,1-*z*; (ii) 2-x,1-y,1-z

Table S3. Selected of some experimental and calculated vibrational frequencies (cm^{-1})

Assignments [a]	**Experimental IR with KBr**	**Calculated**
ν (C−H) s R2,R1	2980	3111,3105
ν (C−H) as R2,R1	2899	3097,3078
ν (C=O) s	1778	1790
ν (C=O) as	1718	1748
ν (C=C)R1	1699	1598
ν (C=C)R2	1555	1573
ν (C−F)+γ (C−H)R2	1461	1472
γ (C−H)R1	1348	1452
ν (CCN) + ν (N−S)	1162	1242
θ, R2+ ν (C−S)+ ν (C−F)’	1053	1059
ν (C−N−C)	897	1027
δ (C−H)R1	863	884
ν (CCN)	826	827
ω (C−H)R2,R1	745	804
β (CCC)R2	715	785
τ (CCC) R2 + ν(C−S)	511	522

[a] ν, stretching; γ, rocking; ω, wagging; δ, twisting; β, bending; τ, torsion; θ, breathing; s, symmetric; as, asymmetric. Abbreviations: R1, C2/C3/C5-C8 ring; R2, C9-C14 ring.