Supporting Information

Synthesis, Characterizations, and Quantum Chemical Investigations on Imidazo[1,2-a]pyrimidine-Schiff base derivative : (E)-2-phenyl-N-(thiophen-2-ylmethylene)imidazo[1,2-a]pyrimidin-3-amine

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^{1}H-NMR , ^{13}C-NMR , ^{13}C-NMR (DEPT 135), **FT-IR** and **LC-MS**(ESI^{+}) **of** (E)-2-phenyl-N-(thiophen-2-ylmethylene)imidazo[1,2-a]pyrimidin-3-amine **(3)**

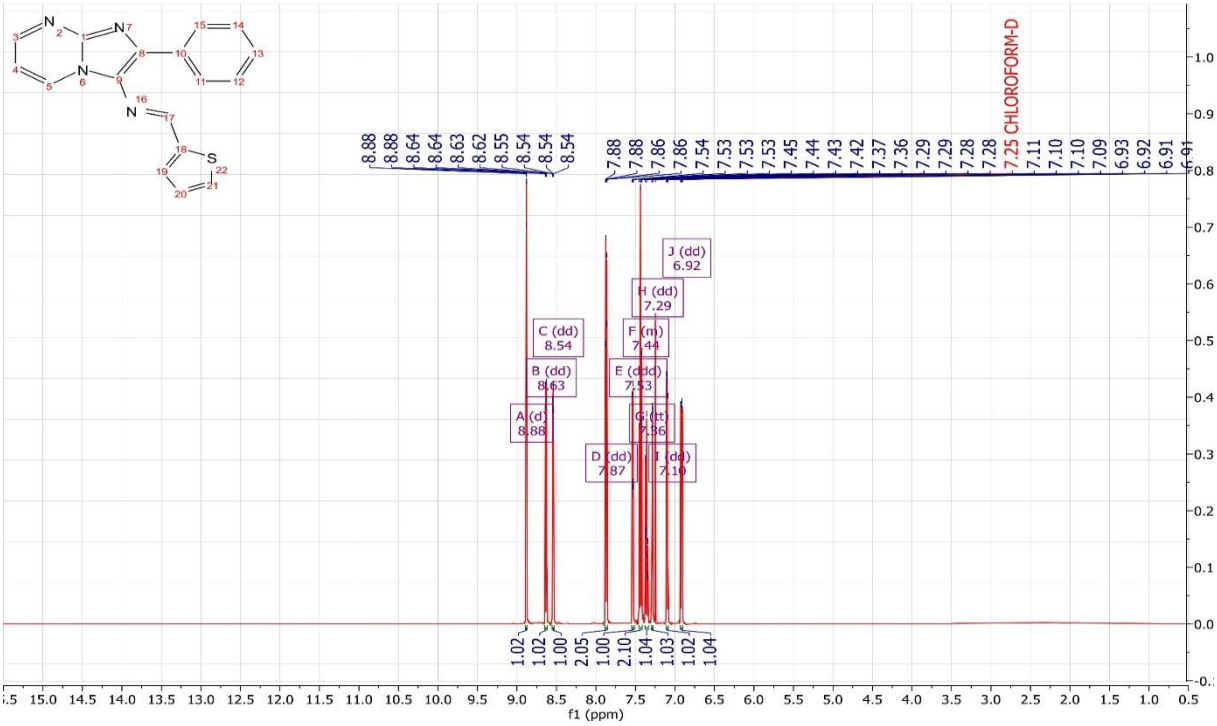


Figure S1. Experimental ^{1}H NMR spectra of compound **(3)**

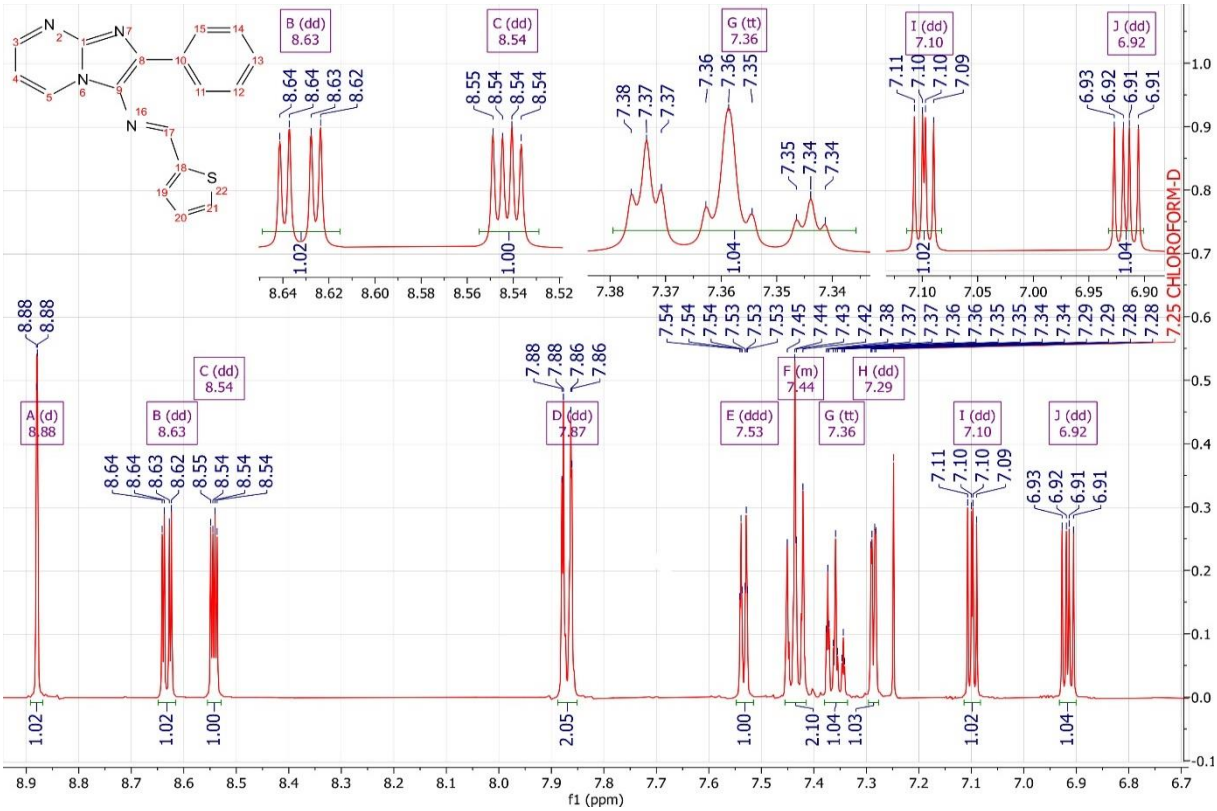


Figure S2. Experimental ^{1}H NMR spectra of compound **(3)**

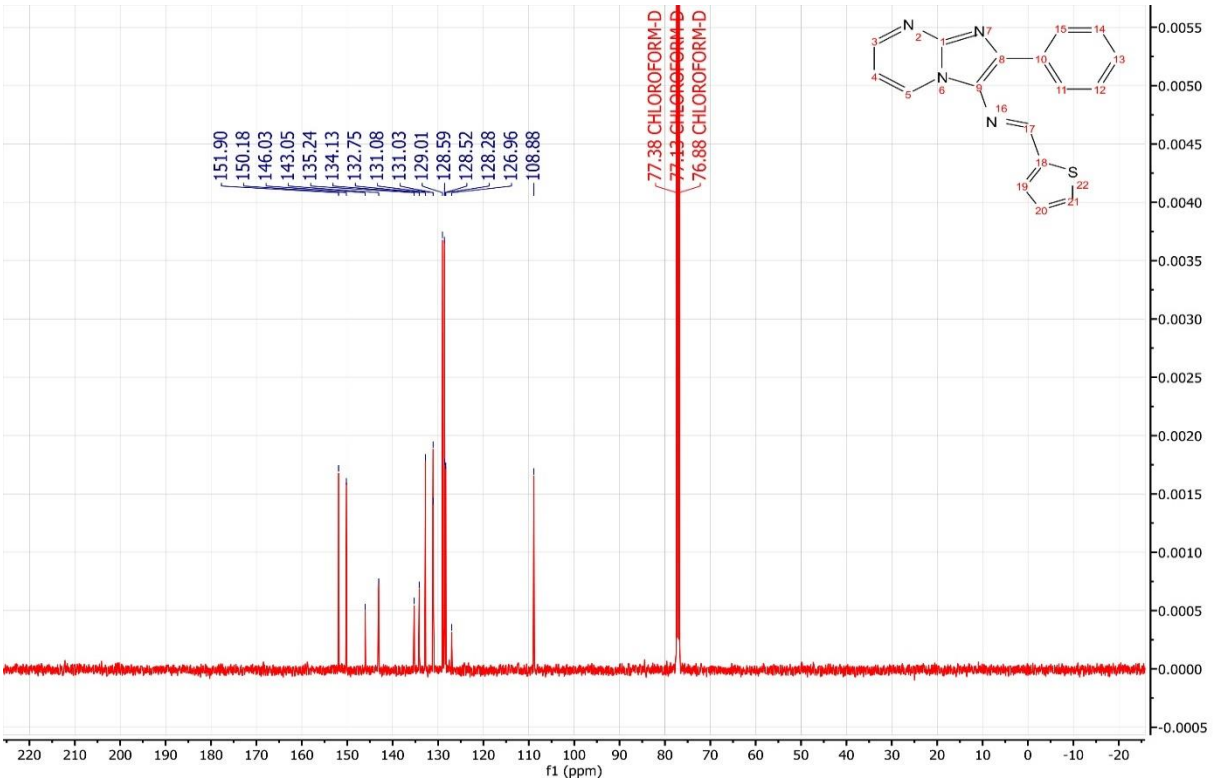


Figure S3. Experimental ^{13}C NMR spectra of compound **(3)**

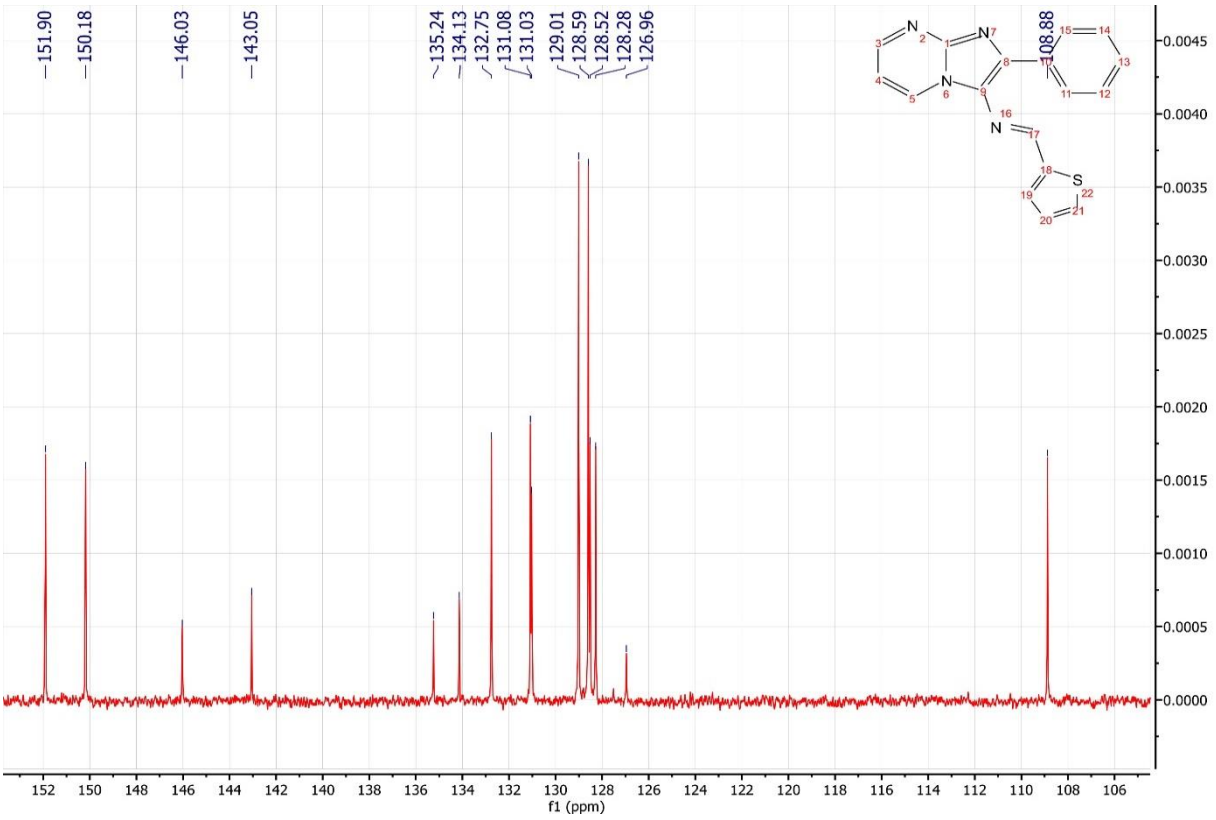


Figure S4. Experimental ^{13}C NMR spectra of compound **(3)**

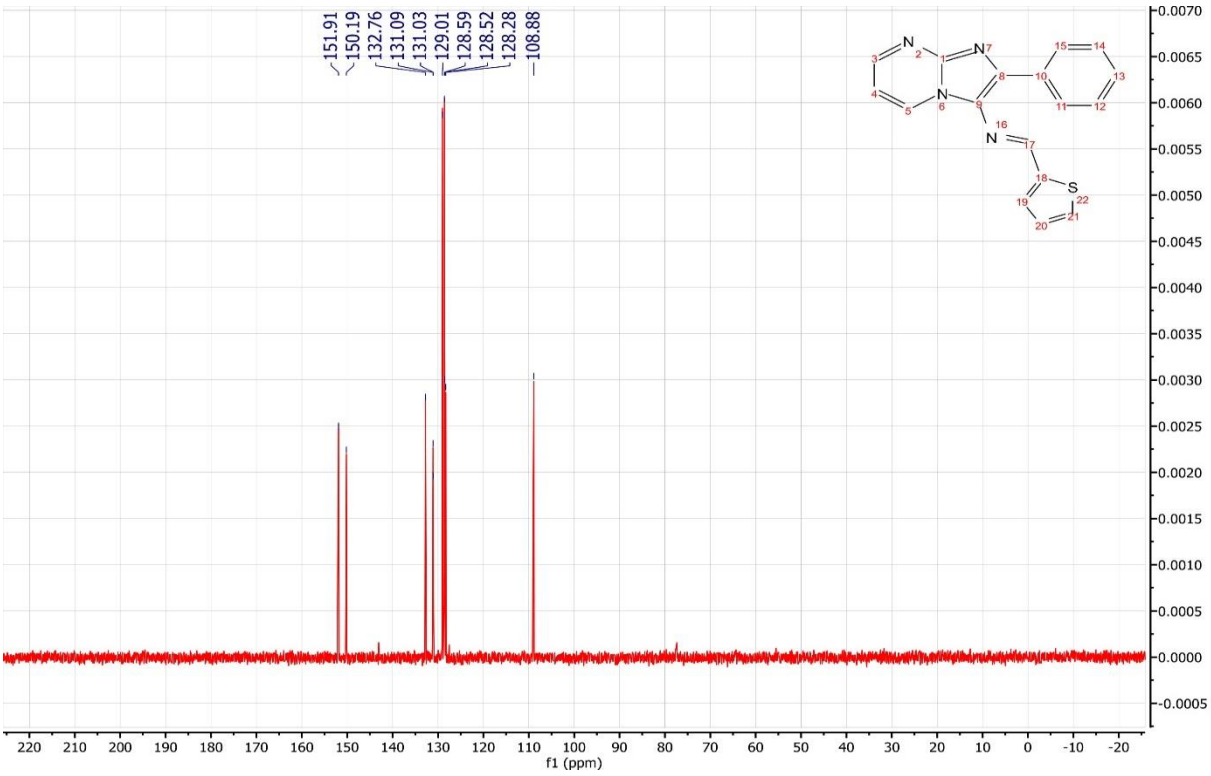


Figure S5. Experimental ^{13}C NMR DEPT 135 spectra of compound **(3)**

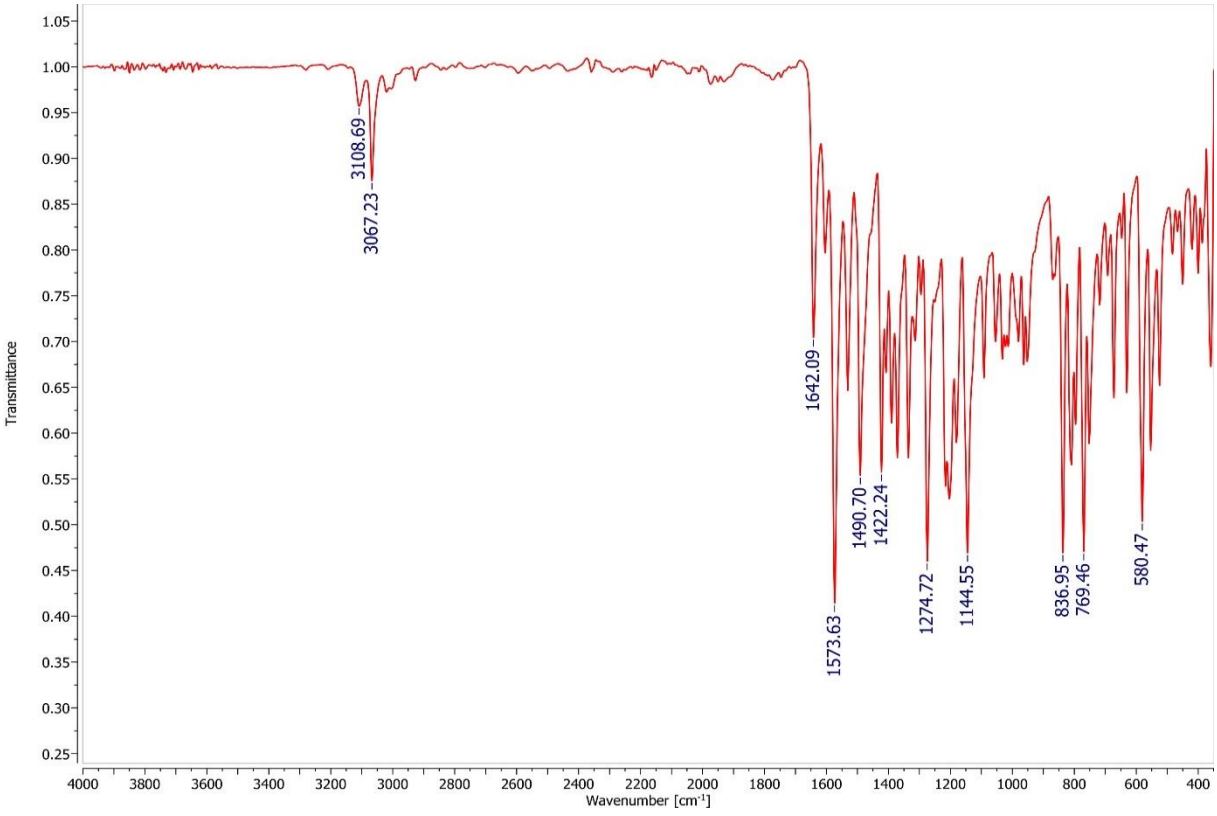


Figure S6. Experimental FT-IR spectra of **(3)**

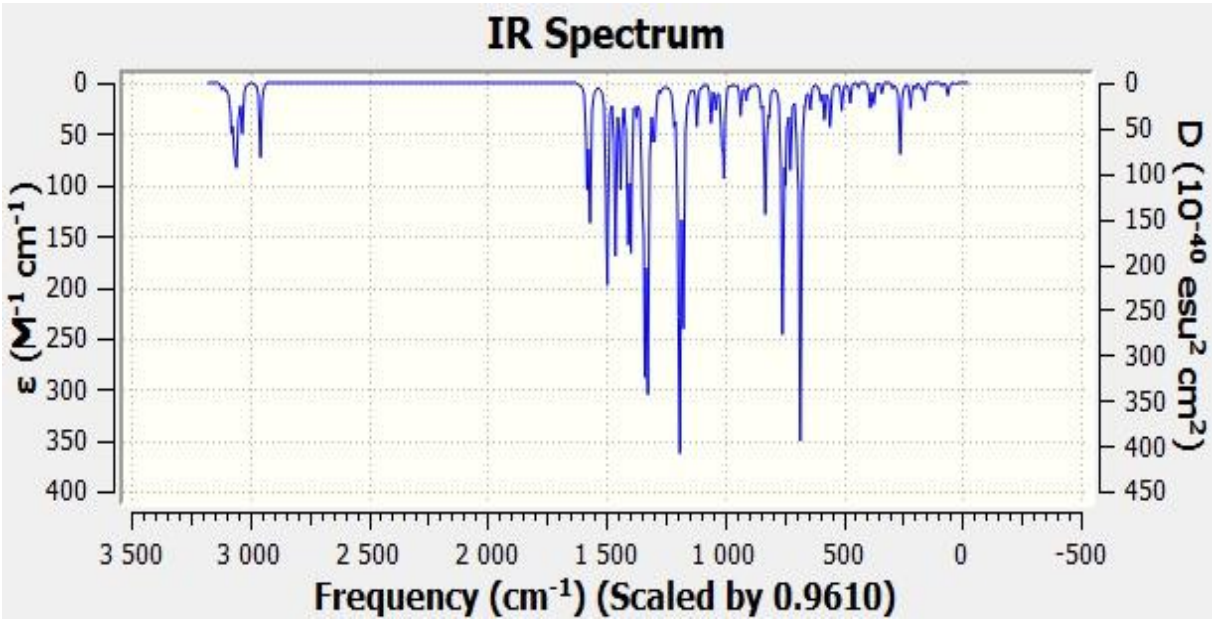


Figure S7. Theoretical FT-IR spectra of (**3)**

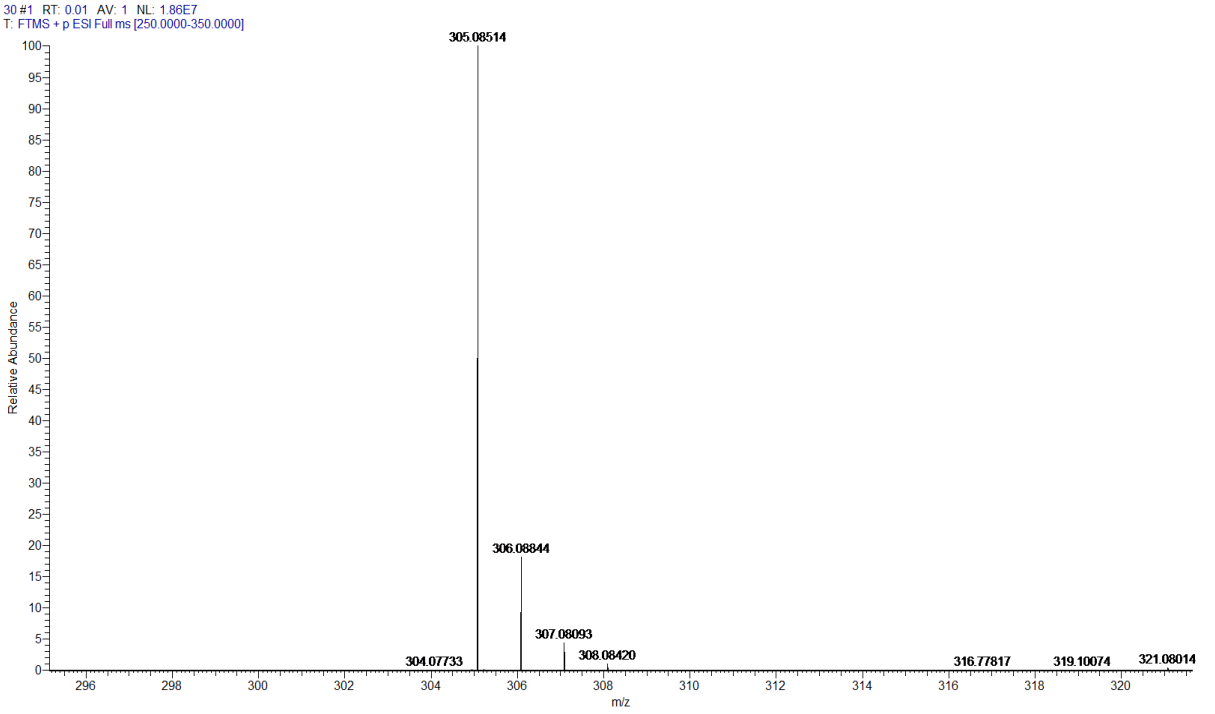
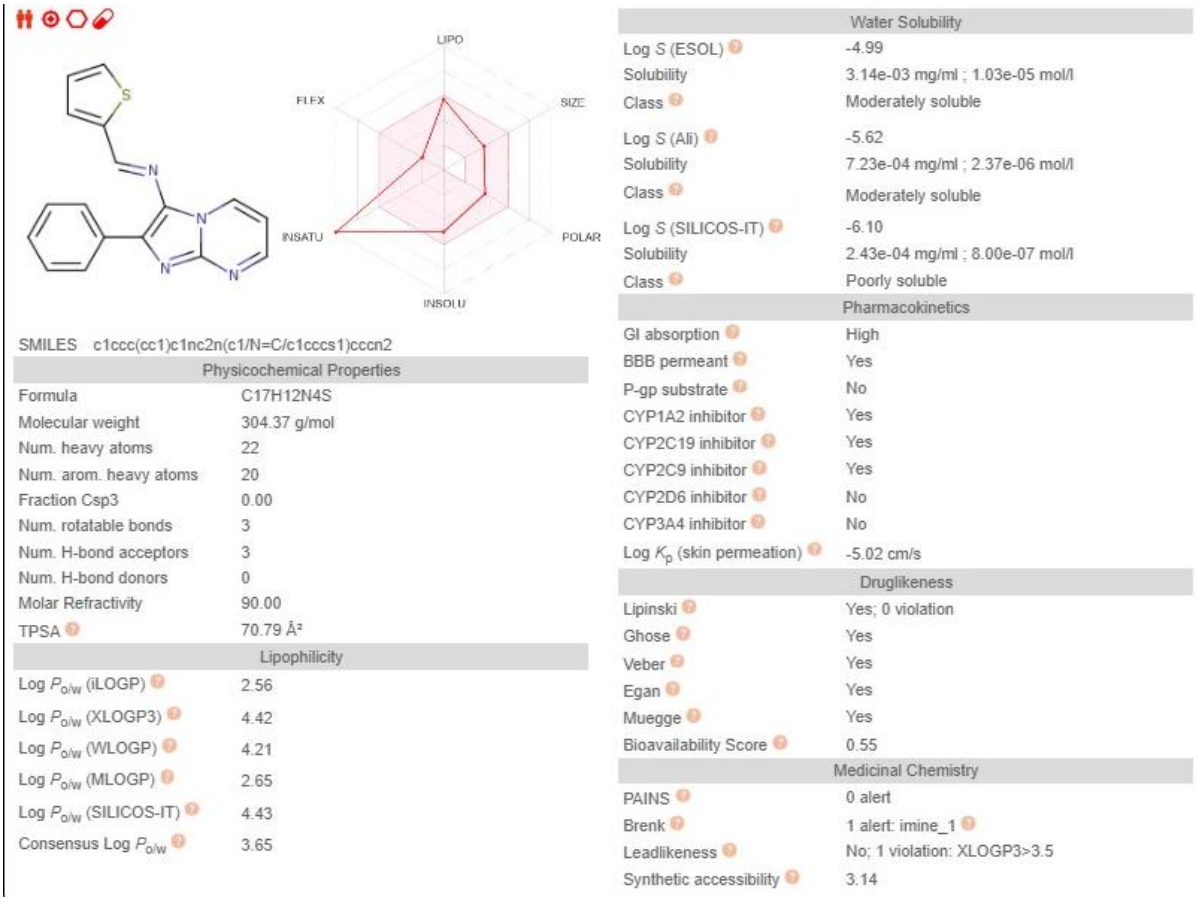


Figure S8. ESI^{+}-MS spectra of (**3)**



SMILES c1ccc(cc1)c1nc2n(c1/N=C/c1cccs1)cccn2

Physicochemical Properties	
Formula	C17H12N4S
Molecular weight	304.37 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	20
Fraction Csp3	0.00
Num. rotatable bonds	3
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	90.00
TPSA	70.79 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.56
Log $P_{o/w}$ (XLOGP3)	4.42
Log $P_{o/w}$ (WLOGP)	4.21
Log $P_{o/w}$ (MLOGP)	2.65
Log $P_{o/w}$ (SILICOS-IT)	4.43
Consensus Log $P_{o/w}$	3.65

Water Solubility	
Log *S* (ESOL)	-4.99
Solubility	3.14e-03 mg/ml ; 1.03e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-5.62
Solubility	7.23e-04 mg/ml ; 2.37e-06 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-6.10
Solubility	2.43e-04 mg/ml ; 8.00e-07 mol/l
Class	Poorly soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.02 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: imine_1
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	3.14

Figure S9. Pharmacokinetics and drug-likeness properties of **(3)** predicted through SwissADME server.