Article

Synthesis, Single Crystal X-ray Structure, DFT Computations, Hirshfeld Surface Analysis and Molecular Docking Simulations on ({[(1*E*)-1-(1,3-Benzodioxol-5-yl)-3-(1*H*-imidazol-1-yl)propylidene]amino}oxy)(furan-2-yl)methanone: A New Antifungal Agent

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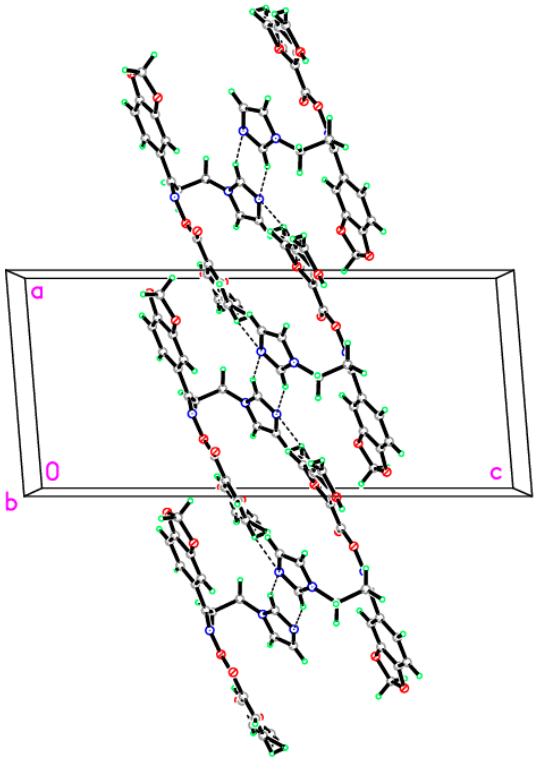

Figure S1. Molecular packing of the oximino ester **5** manifesting hydrogen bonds, which are drawn as dashed lines.

Table S1. Hydrogen-bond geometry (Å, °) of the oximino ester **5**.

D-H···A	D-H	H···A	D···A	D-H···A
C13-H13A···N3i	0.950	2.550	3.384 (3)	147
C18-H18A···N3ii	0.950	2.590	3.428 (3)	147
Symmetry code: (i) −x+1, −y+1, −z+1; (ii) −x+2, −y+1, −z+1.				

Table S2: Second-order perturbation theory analysis of the Fock matrix in an NBO basis for the oximino ester **5**.

Donor (i)		Acceptor (j)		E(2)[a] kcal/mol	E(j)-E(i)[b] (a.u.)	F(i,j)[c] (a.u.)
NBO	Occupancy	NBO	Occupancy			
π(C4-C5)	1.80680	σ*(C1-O2)	0.01452	19.86	0.30	0.070
		π*(C6-C7)	0.26111	15.18	0.29	0.061
π(C6-C7)	1.82771	π*(C4-C5)	0.30866	17.66	0.30	0.067
σ(O8-C9)	1.98254	σ*(C10-C24)	0.03309	3.87	1.25	0.062
σ(C11-C12)	1.96757	π*(N9-C10)	0.17309	3.24	0.64	0.042
		σ*(C10-C24)	0.03309	0.79	1.07	0.026
		σ*(C13-N17)	0.02825	1.47	1.08	0.036
π(C13-N14)	1.86630	π*(C15-C16)	0.30339	21.73	0.32	0.078
π(C15-C16)	1.85698	π*(C13-N14)	0.38136	14.92	0.28	0.061
π(C21-C23)	1.70108	π*(C22-C26)	0.36332	20.89	0.29	0.071
		π*(C24-C25)	0.38236	17.76	0.30	0.066
π(C22-C26)	1.68748	π*(C21-C23)	0.32406	18.21	0.30	0.066

		π*(C24-C25)	0.38236	19.66	0.30	0.070
π(C24-C25)	1.69244	π*(N9-C10)	0.17309	18.10	0.28	0.065
		π*(C21-C23)	0.32406	17.04	0.29	0.063
		π*(C22-C26)	0.36332	17.20	0.28	0.063
n1(O8)	1.97266	σ*(C1-O2)	0.01452	5.38	1.28	0.074
		σ*(O3-C4)	0.02723	0.64	0.99	0.022
		σ*(C10-C24)	0.03309	0.69	1.09	0.025
n1(N9)	1.95415	σ*(C23-H39)	0.01337	0.65	1.04	0.023
n1(N14)	1.92284	σ*(C13-N17)	0.03973	7.41	0.81	0.070
		σ*(C15-C16)	0.01827	5.10	0.95	0.063
n1(N17)	1.55704	σ*(C10-C11)	0.03381	0.54	0.65	0.019
		σ*(C11-C12)	0.02091	5.28	0.61	0.057
		π*(C13-N14)	0.38136	46.08	0.28	0.102
		π*(C15-C16)	0.30339	30.39	0.29	0.087
n1(O20)	1.96239	σ*(O18-C19)	0.03073	2.83	0.84	0.044
		σ*(C21-C22)	0.03960	2.83	0.84	0.044

The used numbering of atoms is as shown in Figure 2. a: E(2) means energy of stabilization interactions; b: Energy difference between donor-to-acceptor, *i* and *j* NBO orbitals; c: F(*i*,*j*) is the Fock matrix element between *i* and *j* NBO orbitals.

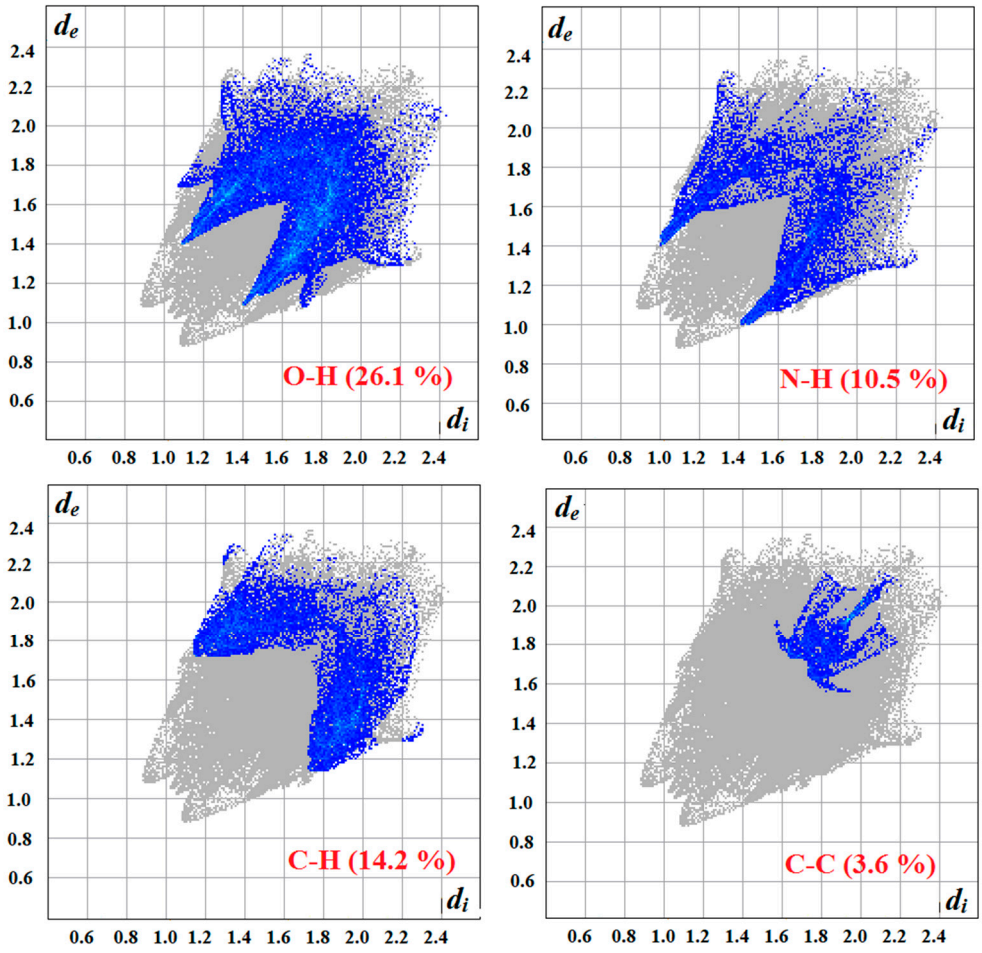

Figure S2: 2-D fingerprint plots showing various intermolecular contacts in the oximino ester **5**.

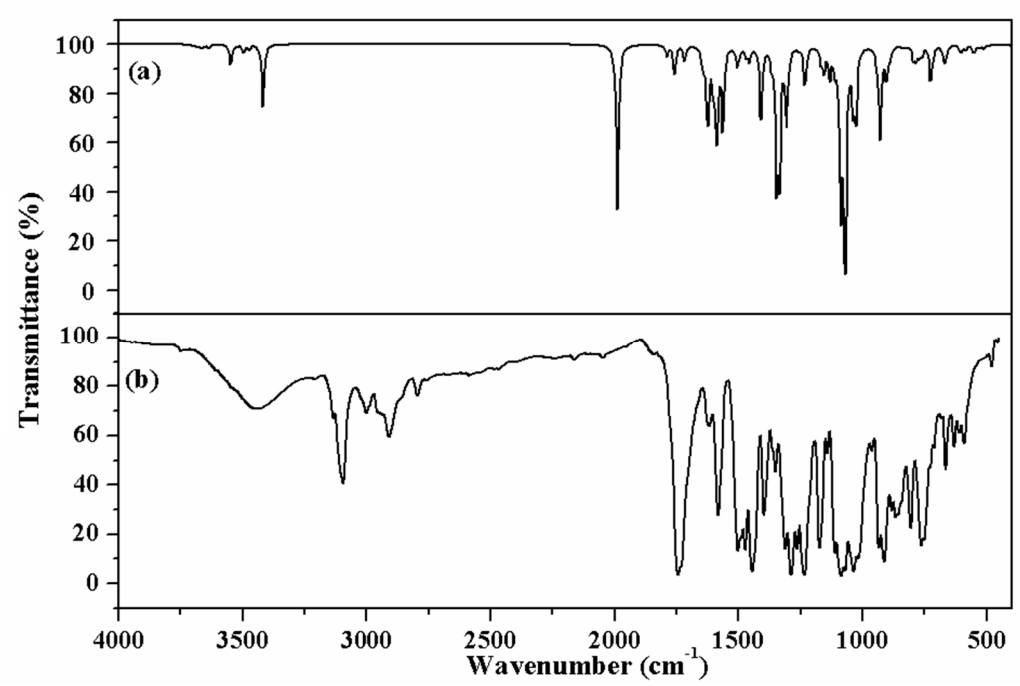

Figure S3: Comparison of (**a**) calculated, and (**b**) observed FT-IR spectra of the oximino ester **5**.

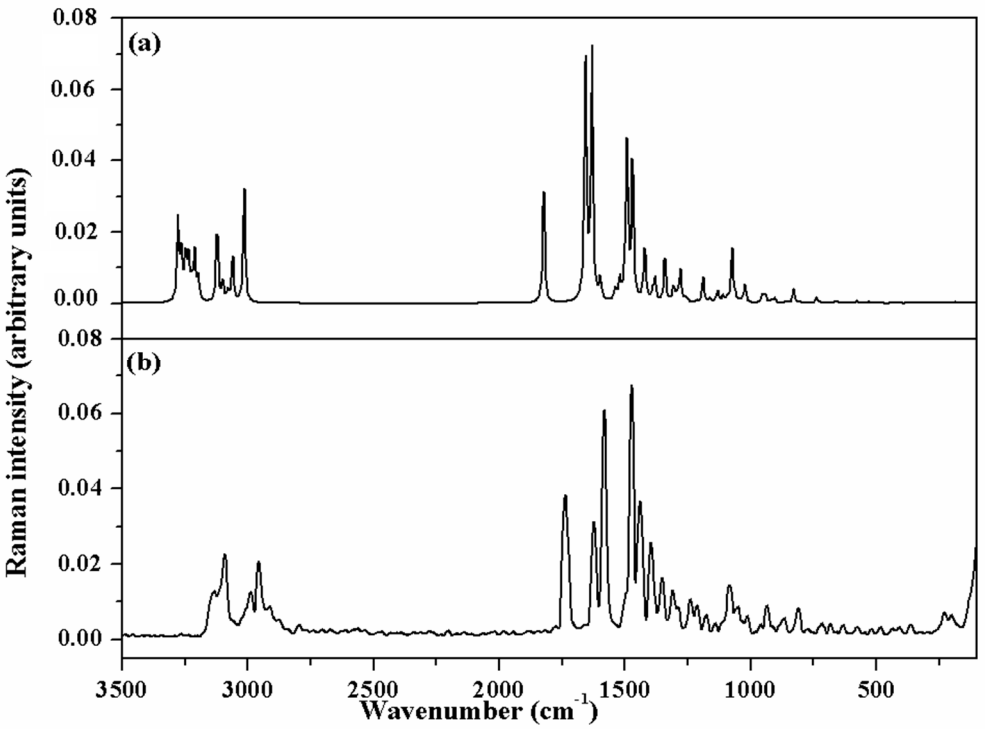

Figure S4: Comparison of (**a**) calculated, and (**b**) observed FT-Raman spectra of the oximino ester **5**.