

Supporting Material

Synthesis of *N-p*-fluorothiosemicarbazone and of bis(*N-p*-fluorophenylthiourea). Crystal structure and conformational analysis of *N,N'*-bis(4-fluorophenyl)hydrazine-1,2-bis(carbothioamide).

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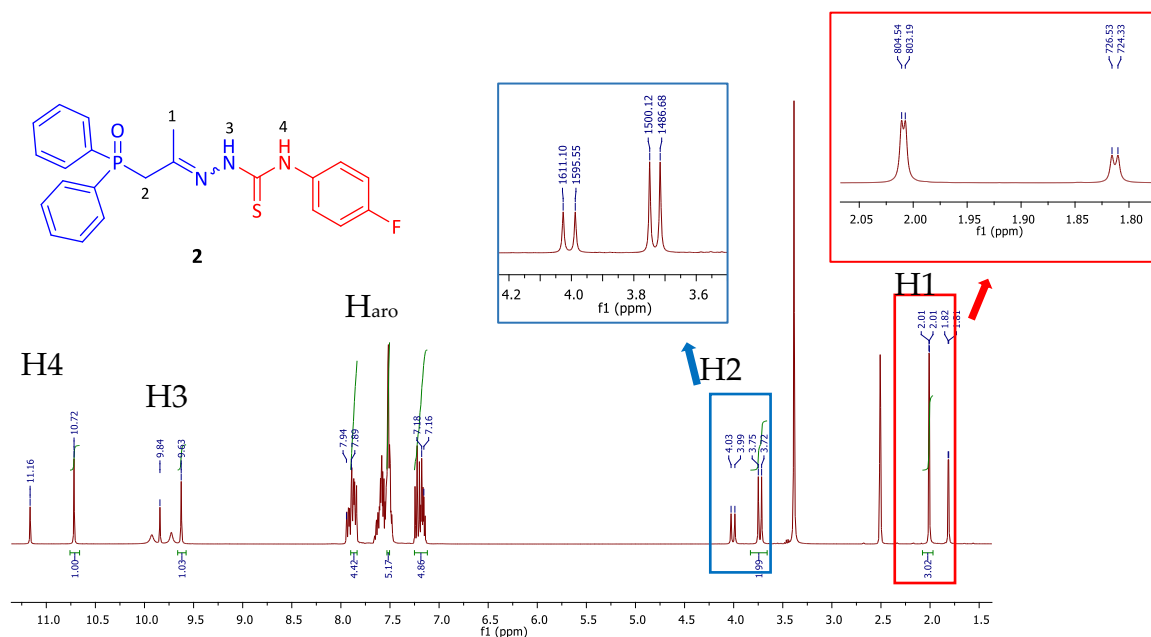


Figure S1. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound **2** at 298 K.

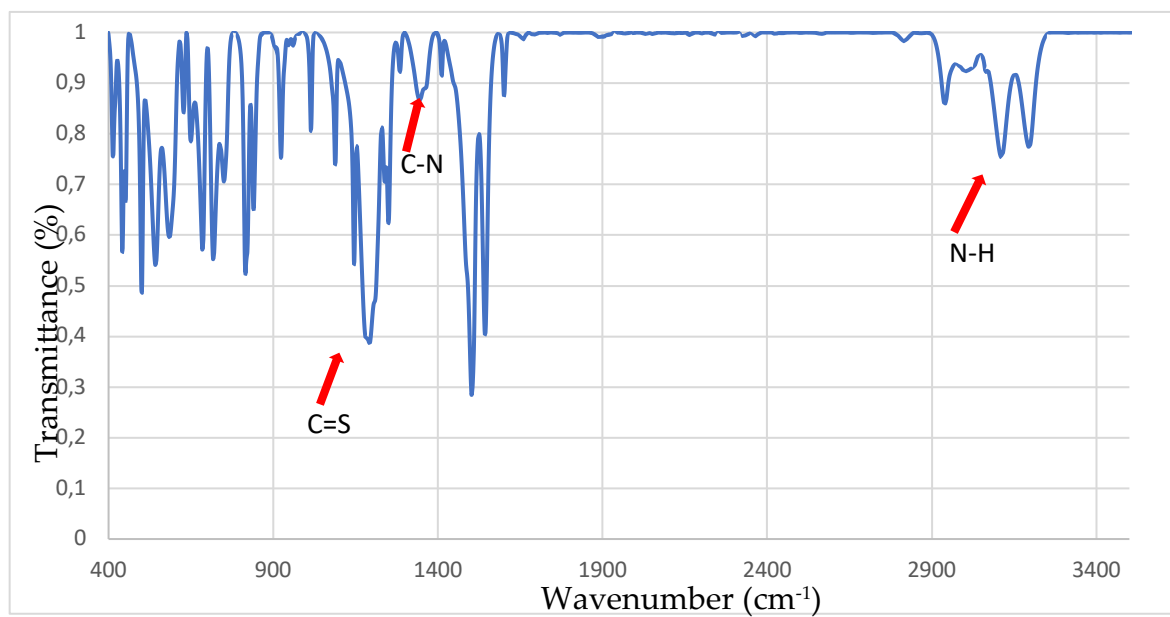


Figure S2. IR-ATR spectrum of compound **3**

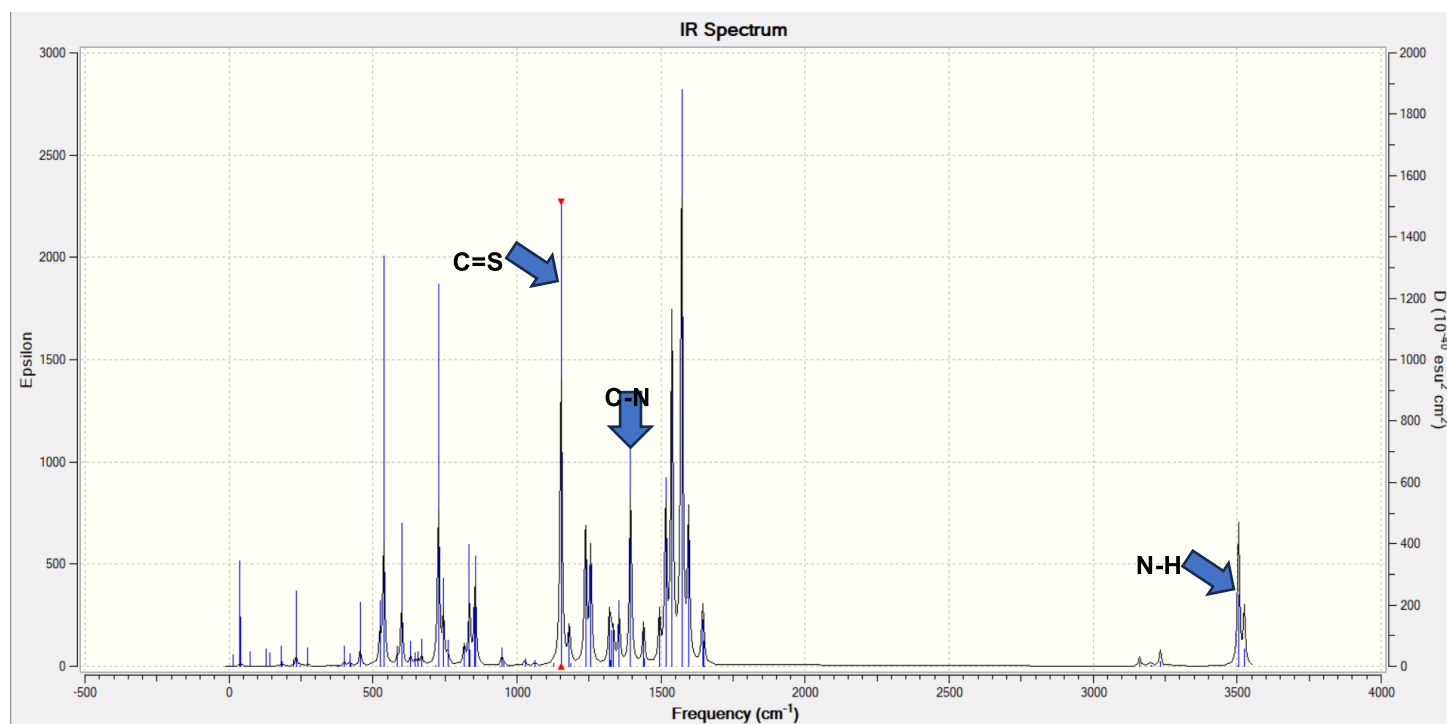


Figure S3. Theoretical IR Spectrum of **3** calculated using Gaussian 09/ B3LYP/ 6-311++ G (d,p).

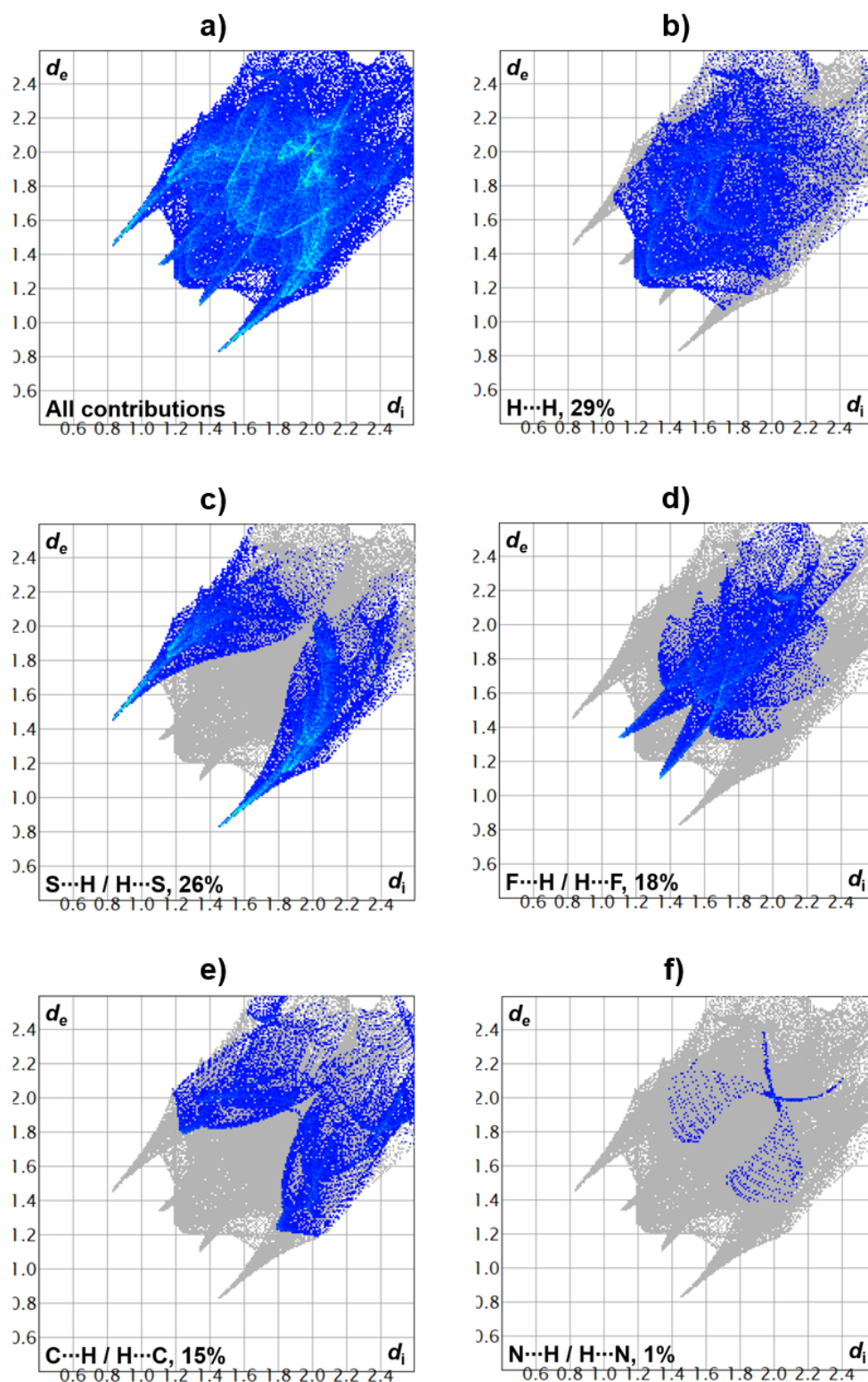


Figure S4. Fingerprint plots from the Hirshfeld analysis of compound 3. The respective interactions are highlighted in the corresponding two-dimensional diagrams: All contributions (a), H...H contacts (b), S...H / H...S contacts (c), F...H / H...F contacts (d), C...H / H...C contacts (e), N...H / H...N contacts (f) showing the percentages participations to the total Hirshfeld surface area.

DFT Calculation study of bis(*N*-p-fluorophenylthiourea) **3**

Table S1. DFT summary results of **3** in gaseous phase

Title Card Required		
File Name	OPT1 B3367	
File Type	.log	
Calculation Type	FREQ	
Calculation Method	RB3LYP	
Basis Set	6-311++G(d,p)	
Charge	0	
Spin	Singlet	
E(RB3LYP)	-1756.09346211	a.u.
RMS Gradient Norm	0.00000189	a.u.
Imaginary Freq	0	
Dipole Moment	0.3136	Debye
Point Group	C1	
Job cpu time: 0 days 7 hours 38 minutes 17.0 seconds.		

Table S2. DFT summary results of **3** in ethanol

Title Card Required		
File Name	OPT1 B3367 ETHANOL	
File Type	.log	
Calculation Type	FREQ	
Calculation Method	RB3LYP	
Basis Set	6-311++G(d,p)	
Charge	0	
Spin	Singlet	
E(RB3LYP)	-1756.11462516	a.u.
RMS Gradient Norm	0.00000469	a.u.
Imaginary Freq	0	
Dipole Moment	0.1078	Debye
Point Group	C1	
Job cpu time: 0 days 13 hours 41 minutes 40.0 seconds.		

Table S3. Selected torsion angles (°) from X-ray diffraction and DFT optimization of **3**

Torsion angles (°)	Exp SCXRD	Calc. in gas	Calc. in EtOH
C5-N4-N21-C22	-125.65	-127.52	-119.95
H16-N4-N21-H33	-54.93	-52.58	-57.81
S1-C5-N4-N21	-166.61	-163.61	-167.07
N3-C5-N4-N21	15.25	18.12	13.94
C6-N3-C5-N4	174.83	177.02	176.02

*The atom numbering is shown in the optimized structure of **3**