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Intermolecular Interactions in Crystalline 1-(Adamantane-1-carbonyl)-3-substituted Thioureas with Hirshfeld Surface Analysis

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Electronic supplementary information (ESI)

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Table S1. Experimental and computed [B3LYP/6-311++G(d,p)] geometric parameters of the central 1-acyl-thioamide group for compound **(1)** (Å, ^{o}).

Parameter	Experimental	Calculated
C1—S1	1.669(1)	1.673
C2—O1	1.218(2)	1.227
C1—N1	1.326(2)	1.341
C1—N2	1.393(2)	1.409
C2—N2	1.366(2)	1.379
N1—C11	1.438(1)	1.437
C2—C21	1.527(2)	1.534
C2—N2—C1	130.5(1)	129.6
N1—C1—N2	117.8(1)	115.3
C1—N1—C11	120.4(1)	124.9
N1—C1—S1	125.14(9)	126.5
N2—C2—O1	121.5(1)	122.3

Table S2. The ring puckering parameters of the adamantane group for compound **1**.

Ring	Atoms	q(2) (Å)	q(3) (Å)	ϕ(2) (°)	QT (Å)	θ(°)
A	C21/C22/C23/C24/C25/C26	0.016(1)	-0.621(1)	27.8(1)	0.621(1)	178.5(1)
B	C21/C22/C23/C28/C27/C30	0.011(1)	0.631(1)	107.9(4)	0.631(1)	1.0(1)
C	C21/C25/C26/C27/C29/C30	0.007(1)	-0.628(1)	157.4(8)	0.628(1)	179.4(1)
D	C23/C24/C25/C28/C29/C30	0.009(1)	0.621(1)	-177.5(6)	0.621(1)	0.8(1)

Table S3. Hirshfeld contact surfaces C_{XY} (%)*, proportion of chemical type on the molecular surface *S*x (%) and random contacts R_{XY} (%) of the main intermolecular interactions for compounds **1-6**.

Contact C_{XY}	**1**	**2**	**3**	**4**	**5**	**6**
H···H	72.0	42.9	45.9	41.2	33.9	38.0
C···H	10.4	8.3	12.7	13.4	14.2	12.7
N···H	1.0	4.6	3.6	0.5	-	1.5
O···H	5.5	26.4	17.9	4.3	4.3	11.9
S···H	10.5	11.8	11.8	9.5	10.2	12.8
F···H	-	-	-	-	18.3	19.6
Cl···H	-	-	-	19.6	-	-
Br···H	-	-	-	-	7.9	-
C···C	-	3.4	0.5	0.7	-	1.2
C···O	-	1.4	3.0	-	-	-
N···O	-	0.8	2.2	-	-	-
O···O	-	-	2.4	-	-	-
C···F	-	-	-	-	-	0.5
N···F	-	-	-	-	-	0.6
O···F	-	-	-	-	-	0.8
Surface *S*x						
H	85.6	68.5	68.9	64.9	61.4	67.3
C	5.2	8.3	8.3	9.2	8.5	7.9
N	0.7	2.8	2.9	2.0	1.3	1.0
O	2.8	14.4	14.0	3.2	3.0	6.5
S	5.5	6.0	5.9	6.4	7.0	6.4
F	-	-	-	-	10.3	10.8
Cl	-	-	-	14.2	-	-
Br	-	-	-	-	8.4	-
Random contacts R_{XY}						
H···H	73.3	46.9	47.5	42.1	37.7	45.3
C···H	8.9	11.4	11.5	12.0	10.4	10.6
N···H	1.2	3.8	4.0	2.6	1.6	1.3
O···H	4.8	19.6	19.2	4.2	3.7	8.7
S···H	9.4	8.2	8.1	8.3	8.6	8.6
F···H	-	-	-	-	12.7	14.5
Cl···H	-	-	-	18.4	-	-
Br···H	-	-	-	-	10.3	-
C···C	-	0.7	0.7	0.7	-	0.6
C···O	-	2.4	2.3	-	-	-
N···O	-	0.8	0.8	-	-	-
O···O	-	-	2.0	-	-	-
C···F	-	-	-	-	-	1.7
N···F	-	-	-	-	-	0.2
O···F	-	-	-	-	-	1.4

*Data obtained from CrystalExplorer3.1, including reciprocal contacts. C_{XY} lower than 0.5% were not included.