Intermolecular interactions in antipyrine-like derivatives 2-halo-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1-*H*-pyrazol-4-yl)benzamides: X-ray structure, Hirshfeld surface analysis and DFT calculations

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ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Scheme S1. General mechanism for synthesis of benzamide derivatives of 4-aminophenazone.

Figure S1. Optimized molecular structures of compounds 1 and 2 calculated at B3LYP/6-311++G(d,p) level of theory.

Figure S2. Energy frameworks along a-axis (above), b-axis (middle), c-axis (botton) for compound **2**, showing separate electrostatic (left, red), and dispersion (middle, green) components, and total energy interactions (right, blue). The tube size (scale factor) used in all energy frameworks was 90 and the cut-off was 5.00 kJ/mol.

Table S1. Hirshfeld contact surfaces C_{XY}(%)*, proportion of chemical type on the molecular surface S_Y(%) and random contacts R_{XY} and contacts R_{XY} (%) of the main intermolecular interactions for compounds **1-2**.

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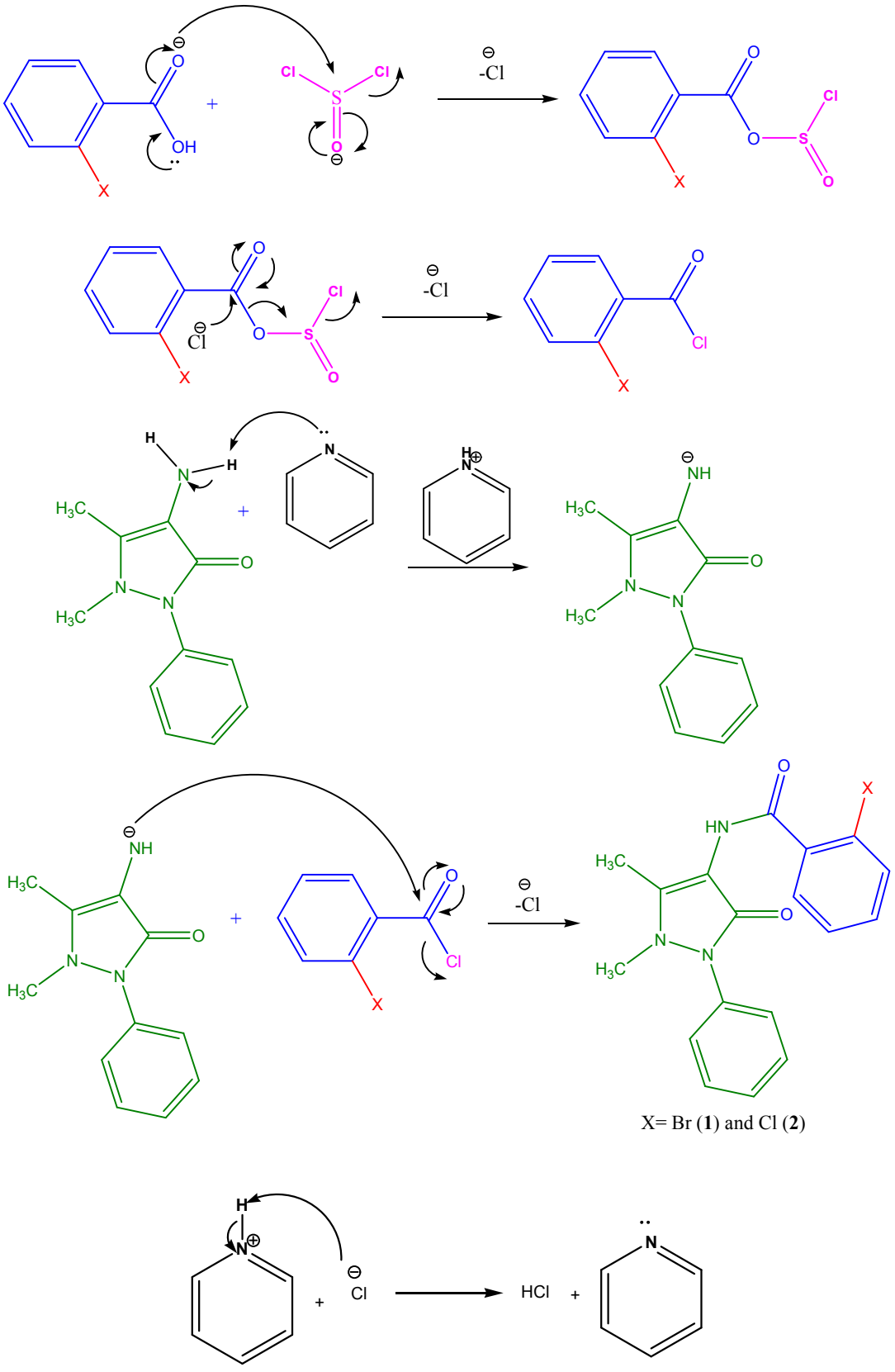
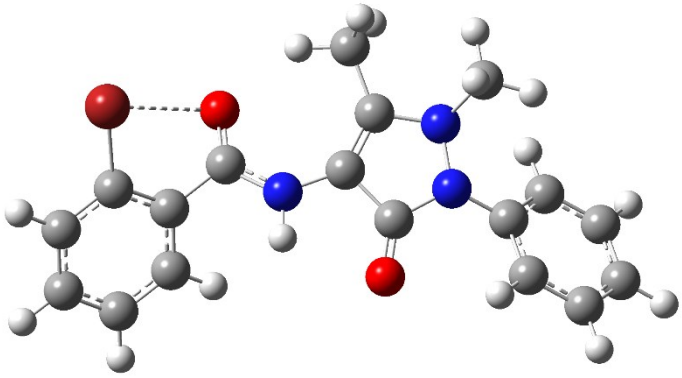
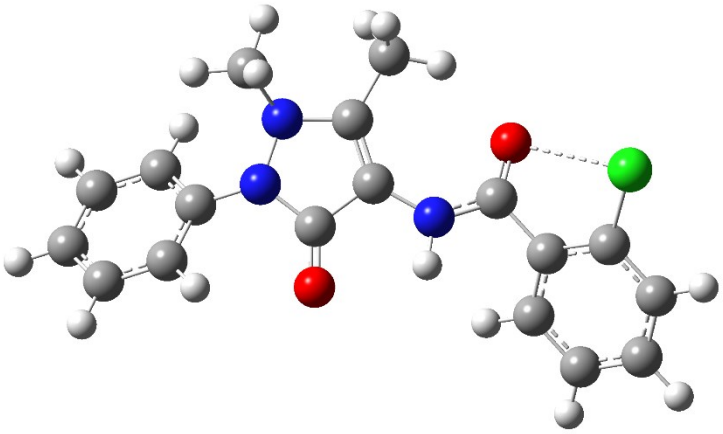


Scheme S1. General mechanism for synthesis of benzamide derivatives of 4-aminophenazone.



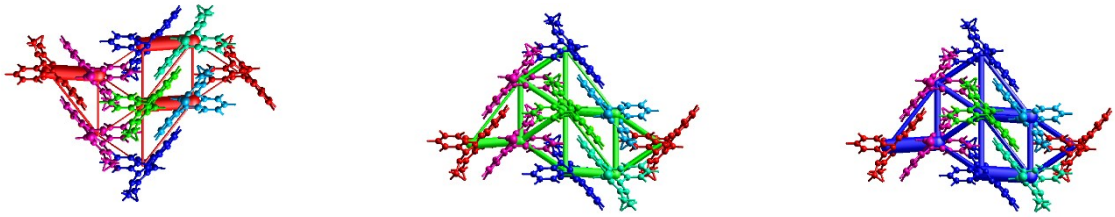
Compound 1



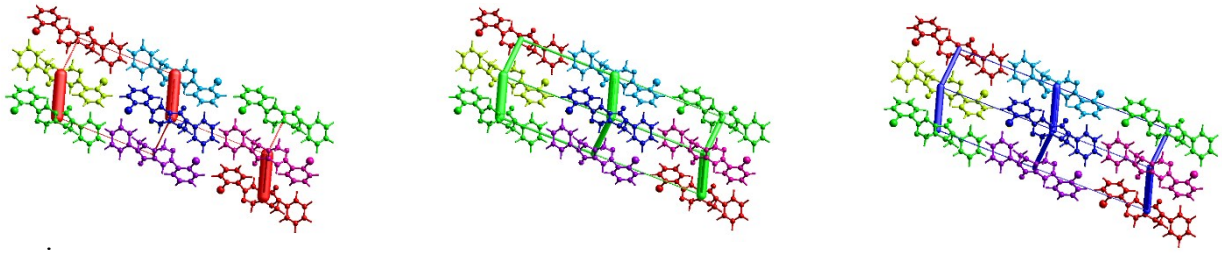
Compound 2

Figure S1

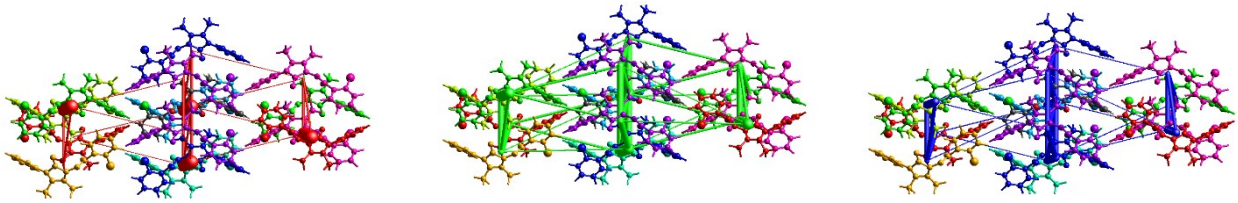
Compound 2



a-axis



b-axis



c-axis

Figure S2

Table S1: Hirshfeld contact surfaces C_{XY}(%)*, proportion of chemical type on the molecular surface S_Y(%) and random contacts R_{XY} and contacts R_{XY} (%) of the main intermolecular interactions for compounds **1-2**.

Contacts C_{XY}	**1**	**2**
H···H/ H···H	39.2	40.6
H···C/ C···H	26.7	25.8
H···O/ O···H	16.8	17.4
H···N/ N···H	1.6	1.4
H···Br/ Br···H	12.5	-
H···Cl/ Cl···H	-	12.3
C···C	0.2	0.2
C···N/ N···C	0.7	0.8
N···O/ O···N	0.3	0.3
C···Br/ Br···C	1.9	-
C···Cl/ Cl···C	-	1.33
Surface S_X		
H	68	69
C	14.9	14.2
O	8.6	8.9
N	1.3	1.2
Br	7.2	-
Cl	-	6.8
Random contacs R_{XY}		
H···H	46.2	47.6
C···H	20.3	19.6
O···H	11.7	12.3
N···H	1.77	1.6
C···C	2.22	2
C···N	0.4	0.34
N···O	0.22	0.2
H···Br	9.8	-
H···Cl	-	9.4
C···Br	1.2	-
C···Cl	-	1.9