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Supporting information for article:

Crystal packing and theoretical analysis of halogen- and hydrogen-bonded hydrazones from pharmaceuticals. Evidence of type I and II halogen bonds in infinite chains of dichloromethane

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S1. Crystal data and structure refinement details

Identification code	HyI	HyBr	HyOH	IsI	IsBr
Empirical formula	C15 H11 I N4	C15 H11 Br N4	C16 H14 Cl2 N4 O	C13 H10 I N3 O	C13 H10 Br N3 O
Formula weight	374.18	327.19	349.21	351.14	304.15
Temperature			297(2) K		
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Tetragonal	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	$I4_1$	$P2_1/c$	$P2_1/c$	P-1	$P2_1/c$
Unit cell dimensions	a = 15.0197(4) Å	a = 14.8761(7) Å	a = 9.51859(16) Å	a = 10.0223(9) Å	a = 18.763(3) Å
	b = 15.0197(4) Å	b = 4.0269(2) Å	b = 15.70955(19) Å	b = 11.1984(3) Å	b = 6.5126(7) Å
	c = 12.8791(6) Å	c = 23.1830(12) Å	c = 21.6869(3) Å	c = 12.4505(10) Å	c = 10.1237(15) Å
	α = 90°.	α = 90°.	α = 90°.	α = 109.836(6)°.	α = 90°.
	β = 90°.	β = 105.810(5)°.	β = 98.0651(15)°.	β = 101.250(7)°.	β = 95.458(15)°.
	γ = 90°.	γ = 90°.	γ = 90°.	γ = 97.494(6)°.	γ = 90°.
Volume	2905.40(19) $Å^3$	1336.24(12) $Å^3$	3210.83(8) $Å^3$	1259.58(17) $Å^3$	1231.5(3) $Å^3$
Z	8	4	8	4	4
ρ (calculated) g/cm³	1.711	1.626	1.445	1.852	1.640
Absorption coefficient mm⁻¹	2.199	3.071	0.414	2.533	3.328
F(000)	1456	656	1440	680	608
Crystal size mm³	0.50 x 0.02 x 0.02	0.50 x 0.12 x 0.07	0.5 x 0.5 x 0.32	0.50 x 0.20 x 0.10	0.18 x 0.18 x 0.03
Theta range for data collection	3.421 to 25.258°.	3.541 to 26.177°.	3.070 to 26.190°.	3.025 to 25.904°.	3.272 to 25.381°.
Reflections collected	13780	12533	22125	18494	8113
Independent reflections	2616 [$R_{(int)}$ = 0.0396]	2600 [$R_{(int)}$ = 0.0489]	6290 [$R_{(int)}$ = 0.0196]	4823 [$R_{(int)}$ = 0.0379]	2245 [$R_{(int)}$ = 0.0590]
Completeness to □ = 25.242°	99.5 %	98.3 %	98.2 %	98.3 %	99.5 %
Absorption correction	Semi-empirical from equivalents				

Max. and min. transmission	1.00000 and 0.90524	1.00000 and 0.37783	1.00000 and 0.87464	1.00000 and 0.50646	1.00000 and 0.53317
Refinement method	Full-matrix least-squares on F^2				
Data / restraints / parameters	2616 / 1 / 181	2600 / 0 / 181	6290 / 0 / 417	4823 / 0 / 325	2245 / 0 / 163
Goodness-of-fit on F^2	1.058	1.079	1.016	1.046	1.043
Final R indices [I>2sigma(I)]	R_1 = 0.0353, wR_2 = 0.0799	R_1 = 0.0384, wR_2 = 0.1073	R_1 = 0.0526, wR_2 = 0.1329	R_1 = 0.0285, wR_2 = 0.0783	R_1 = 0.0475, wR_2 = 0.1160
R indices (all data)	R_1 = 0.0408, wR_2 = 0.0830	R_1 = 0.0433, wR_2 = 0.1112	R_1 = 0.0566, wR_2 = 0.1361	R_1 = 0.0300, wR_2 = 0.0795	R_1 = 0.0613, wR_2 = 0.1250
Largest diff. peak and hole e.Å^{-3}	1.169 and -0.598	0.409 and -0.491	1.237 and -1.132	0.612 and -0.487	0.431 and -0.571

S2. Crystal structures

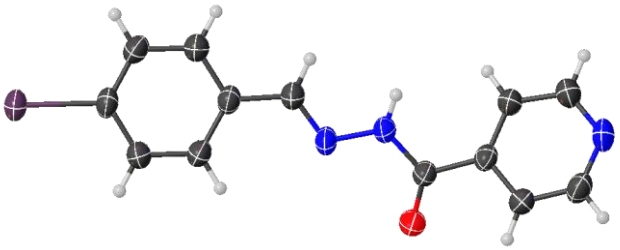

Figure S1 X-ray structure of IsI (ellipsoids drawn at the 50% probability level).

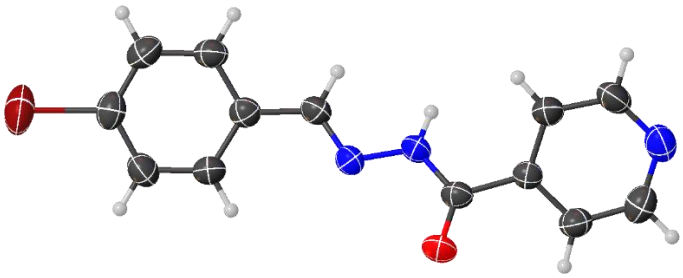

Figure S2 X-ray structure of IsBr (ellipsoids drawn at the 50% probability level).

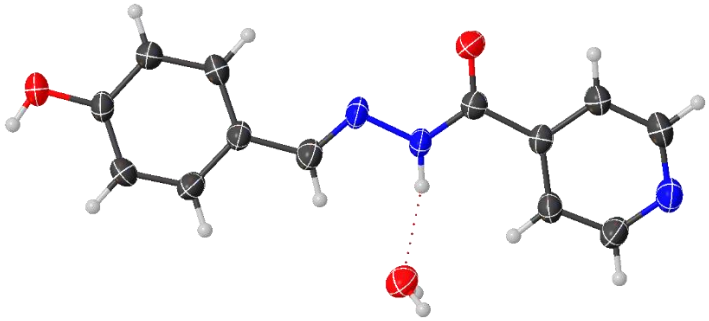

Figure S3 X-ray structure of IsOH (ellipsoids drawn at the 50% probability level).

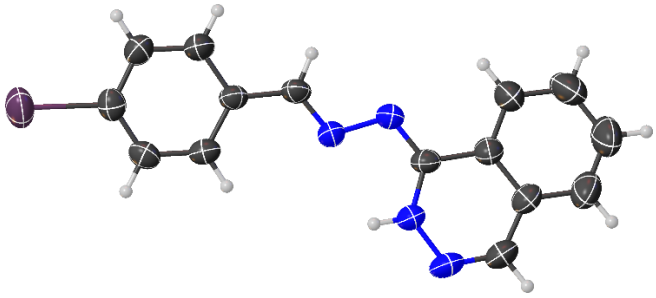

Figure S4 X-ray structure of HyI (ellipsoids drawn at the 50% probability level).

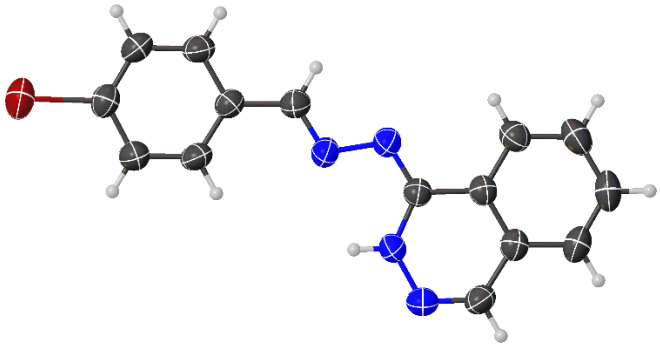

Figure S5 X-ray structure of HyBr (ellipsoids drawn at the 50% probability level).

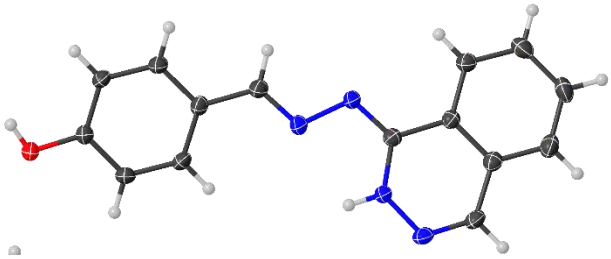

Figure S6 X-ray structure of HyOH (ellipsoids drawn at the 50% probability level).

S3. Gaussian full reference

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato,

X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowskiand, D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.