The Clash of the Synthons: Crystal Structures of Benzimidazole-alcohol
-carboxylic acids

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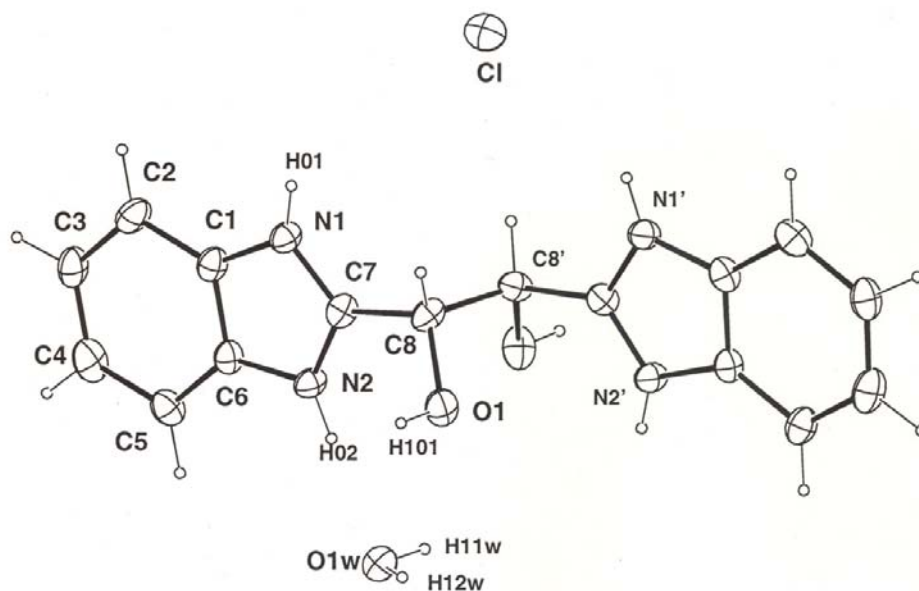Williams*[a]

Supplementary material

Figure S1 ORTEP plot of RR-$\mathbf{1}$H$_2$Cl$_2$2H$_2$O (ellipsoids at 50% probability)

Figure S2 ORTEP plot of (RR,SS)-$\mathbf{1}$H$_2$Cl$_2$H$_2$OetOH (ellipsoids at 50% probability)
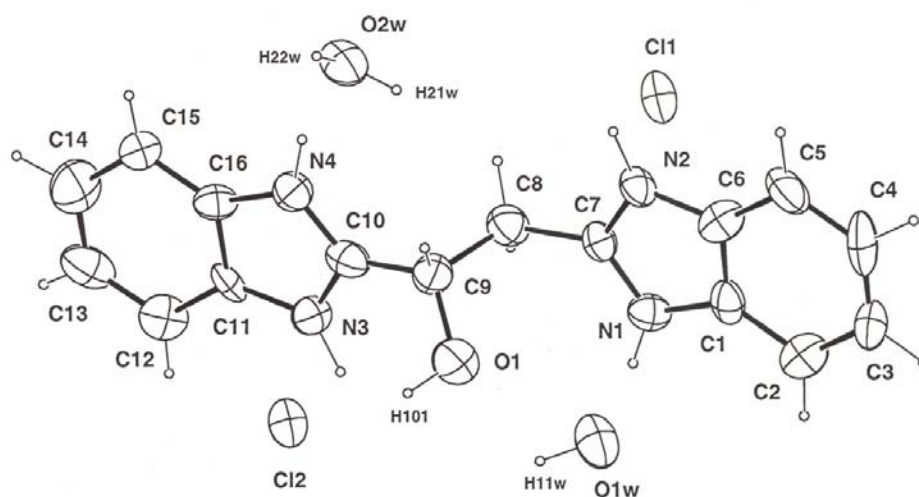
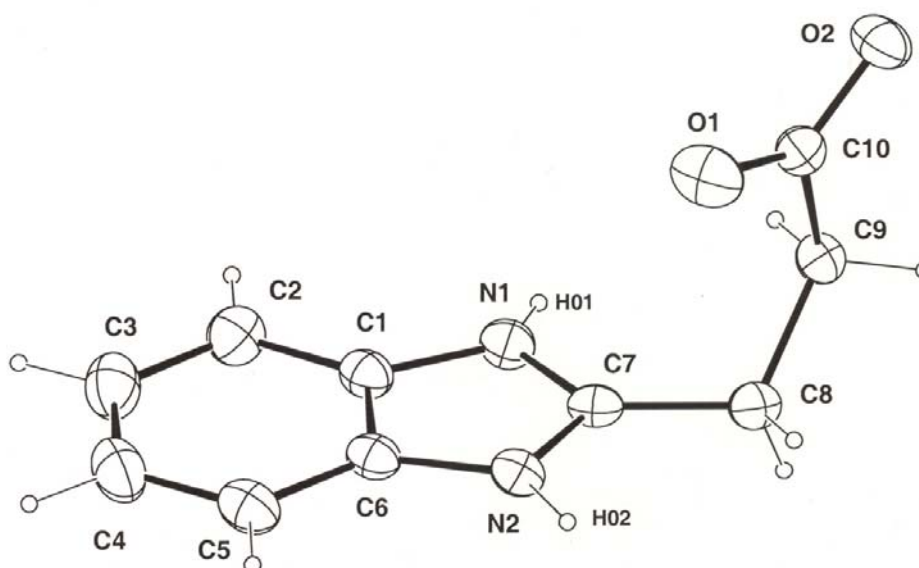Figure S3 ORTEP plot of *S*-**3**$H_2Cl_2 2H_2O$ (ellipsoids at 50% probability)

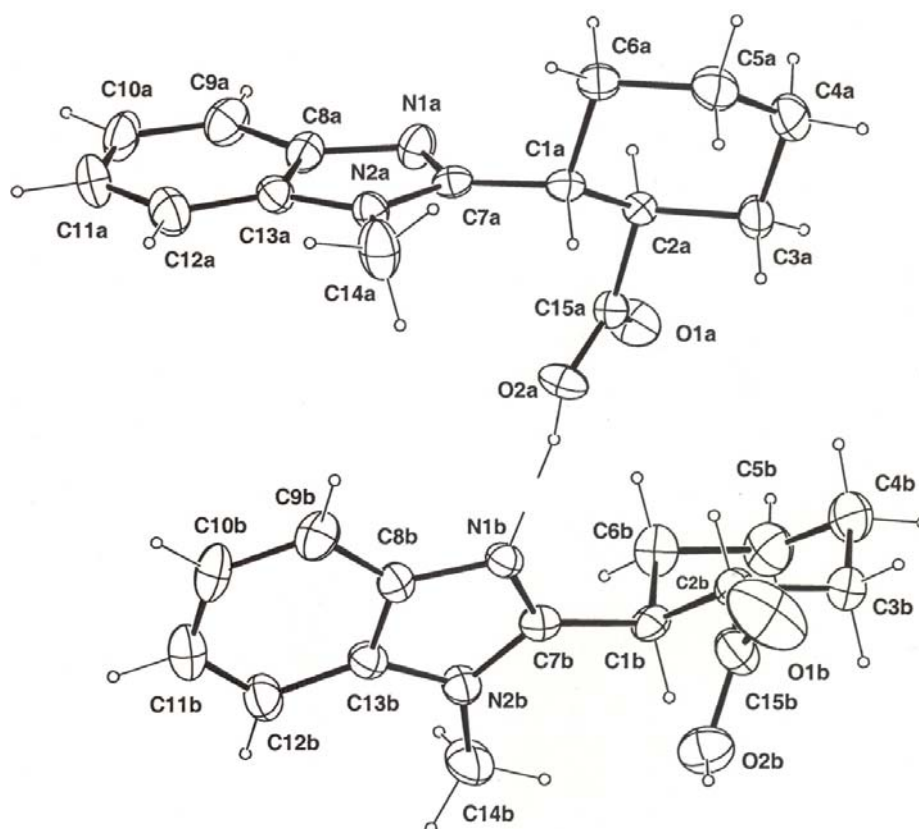Figure S4 ORTEP plot of **4** (ellipsoids at 50% probability)

Figure S5 ORTEP plot of *RR*-**5** (ellipsoids at 50% probability)
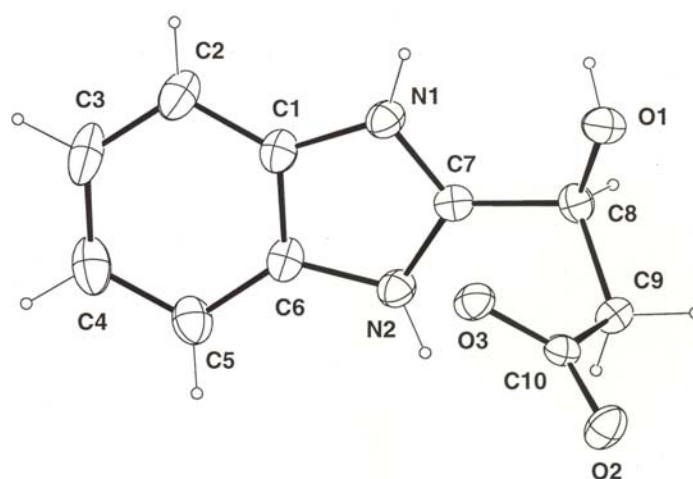

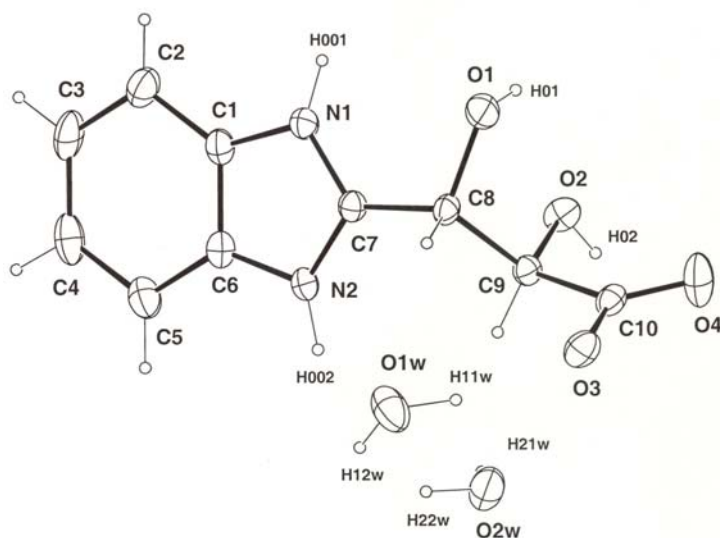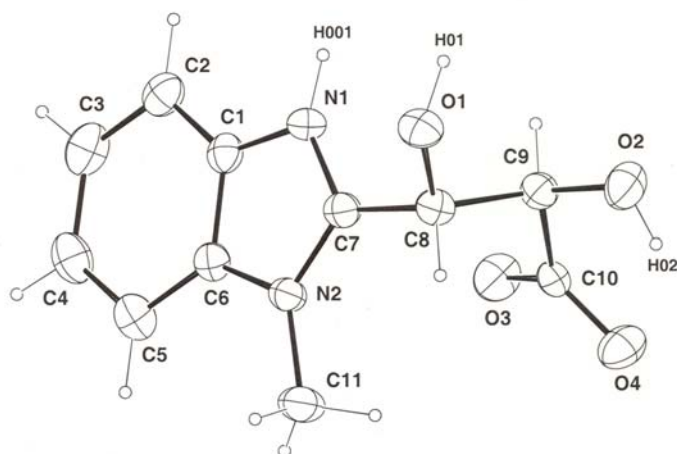Figure S6 ORTEP plot of *S*-**6** (ellipsoids at 50% probability)

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Figure S7 ORTEP plot of *RS*-**7**.2H$_2$O (ellipsoids at 50% probability)

Figure S8 ORTEP plot of *RS*-**8** (ellipsoids at 50% probability)

Table S1. Data for hydrogen bonds

Donor, D	Hydrogen, H	Acceptor, A	D-H, Å	H…A, Å	D...A, Å	Angle D-H-A (°)	Equivalent position for A
$[RR\text{-}1H_2]Cl_2.$ $2H_2O$							
O1	H101	Cl1	0.82(2)	2.27(2)	3.068(3)	165(5)	x - 1/2 , y - 1/2 , z
N1	H01	O1w	0.85(3)	1.96(3)	2.808(5)	170(5)	x, y + 1, z
N2	H02	O1w	0.86(3)	1.97(3)	2.815(5)	170(5)	x , y , z
O1w	H11w	Cl	0.86(2)	2.23(2)	3.084(3)	172(5)	x, y -1, z
O1w	H12w	Cl	0.85(3)	2.31(3)	3.142(3)	169(5)	1 - x, y - 1, 1 - z
$[RR,SS\text{-}1H_2]$ $Cl_2.H_2OEtOH$							
O1	H001	Cl1	0.80(3)	2.28(3)	3.074(1)	171(3)	1-x, 1-y, 1-z
O2	H002	Cl1	0.82(4)	2.23(4)	3.049(2)	177(2)	-x, 1-y, 1-z
N1	H01	Cl2	0.87(3)	2.31(3)	3.124(2)	156(2)	1-x, 1-y, 1-z
N2	H02	Cl2	0.88(3)	2.20(3)	3.082(2)	173(2)	-x, 1-y, 1-z
N3	H03	O1a	0.87(3)	1.87(3)	2.702(2)	161(3)	1-x, -y, 1-z
N4	H04	O1w	0.84(3)	1.98(3)	2.775(2)	158(3)	1-x, 1-y, 1-z
O1a	H01a	Cl2	0.78(2)	2.31(2)	3.070(2)	166(2)	x, y, z
O1w	H11w	Cl1	0.87(2)	2.30(2)	3.134(2)	160(3)	1-x, 1-y, 1-z
$[S\text{-}3H_2]Cl_2$ $2H_2O$							
O1	H101	Cl2	0.92(5)	2.19(4)	3.051(7)	158(4)	x , y , z
N1	H01	O1W	0.97	1.71	2.673(11)	172	x , y , z
N2	H02	Cl2	0.96	2.14	3.090(7)	172	1 - x , ½ + y , -z
N3	H03	Cl1	1.00	2.10	3.092(7)	175	-x, y-½ ,-z
N4	H04	O2w	1.01	1.70	2.690(11)	166	x ,y, z
O1w	H11w	Cl1	0.90(5)	2.38(4)	3.227(8)	158(6)	-x, y-½ ,-z
O1w	H12w	Cl2	0.90(6)	2.29(5)	3.165(9)	164(5)	x-1, y, z
O2w	H21w	Cl2	0.89(4)	2.60(6)	3.185(7)	125(5)	1 - x , ½ + y , -z
O2w	H22w	Cl1	0.89(4)	2.24(5)	3.079(8)	156(5)	x+1, y, z
4							
N1	H01	O1	0.92(2)	1.78(2)	2.691(2)	174(2)	x , y-1 , z
N2	H02	O2	1.00(2)	1.62(3)	2.621(2)	177(2)	x , 5/2-y, ½+z
RR,SS-**5**							
O2a	H02a	N1b	0.89(8)	1.77(8)	2.638(9)	164(10)	x, y, z
O2b	H02b	N1a	0.86(10)	1.86(10)	2.679(12)	160(9)	x, y-1, z
S-**6**							
O1	H101	O3	0.83(4)	1.82(4)	2.633(4)	165(4)	1-x , y-1/2 , 1-z
N1	H01	O2	0.89	1.81	2.688(5)	169	1-x , y-1/2 , 1-z
N2	H02	O3	0.89	1.88	2.748(5)	166	x-1, y, z
2R,3S-**7**. $2H_2O$							
N1	H001	O2w	0.91(3)	1.84(3)	2.694(4)	156(3)	3/2-x , 2-y , z-½
N2	H002	O3	0.91(2)	1.92(2)	2.765(3)	153(4)	1-x , y -1/2 , 3/2-z
O1	H01	O2	0.90(2)	2.19(5)	2.654(3)	111(5)	x,y,z
O2	H02	O1w	0.88(2)	1.80(2)	2.674(3)	170(3)	x+1, y, z
O1w	H11w	O3	0.91(3)	1.90(3)	2.798(3)	167(4)	x,y,z
O1w	H12w	O4	0.90(3)	1.86(3)	2.752(3)	168(3)	1-x , y -½ , 3/2-z
O2w	H21w	O4	0.90(3)	1.88(2)	2.706(3)	151(3)	2-x, y-½, 3/2-z
O2w	H22w	O3	0.90(3)	1.86(3)	2.759(3)	176(4)	1-x , y -½ , 3/2-z
2R,3S-**8**							

N1	H001	O4	0.91(4)	1.68(4)	2.594(4)	175(4)	x-½, ½-y, 1-z
O1	H01	O3	0.97(4)	1.75(4)	2.700(4)	167(4)	x-½, ½-y, 1-z
O2	H02	O4	0.84(4)	2.05(4)	2.616(4)	124(4)	x, y, z