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Supporting information for article:

Involvement of conformational isomerism in the complexity of the crystal network of 1-(4-nitrophenyl)-1*H*-1,3-benzimidazole derivatives driven by C—H···*A* (*A* = NO2, Npy and π) and orthogonal Npy···NO2 and ONO···C*sp*^{2} interactions

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Supporting information

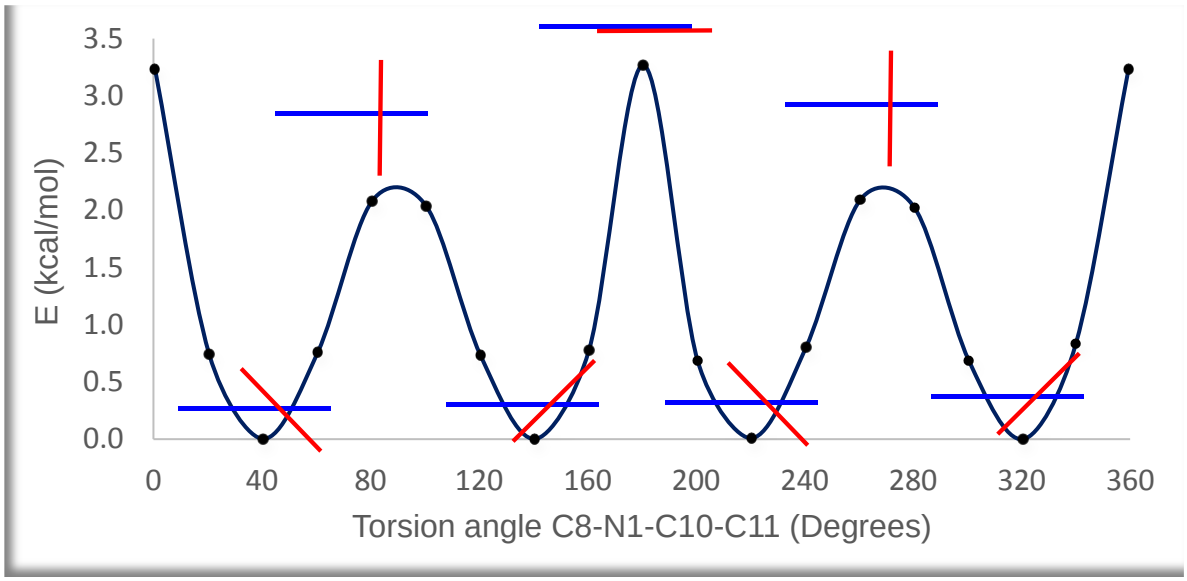

Figure S1 Theoretical rotation profile of the C8-N1-C10-C11 torsion angle in compound (I). Bz heterocycle in blue and *N*-nitroBz ring in red.

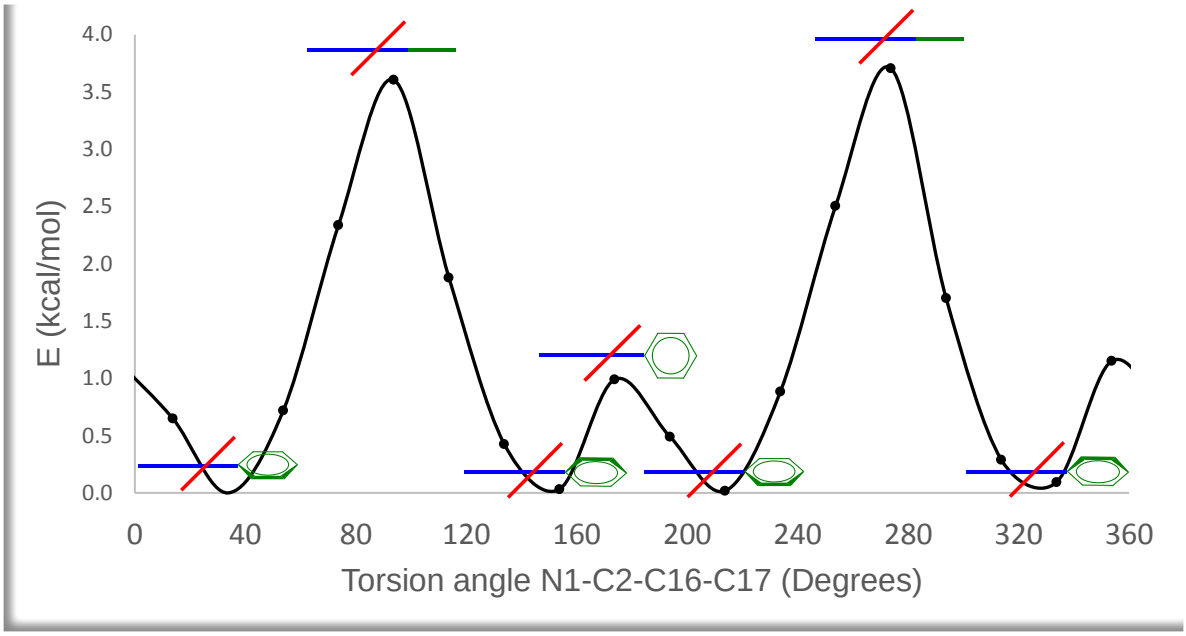

Figure S2 Theoretical rotation profile of the N1-C2-C16-C17 torsion angle in compound (II). Bz heterocycle in blue, N-nitroBz ring in red and C-Ph ring in green.

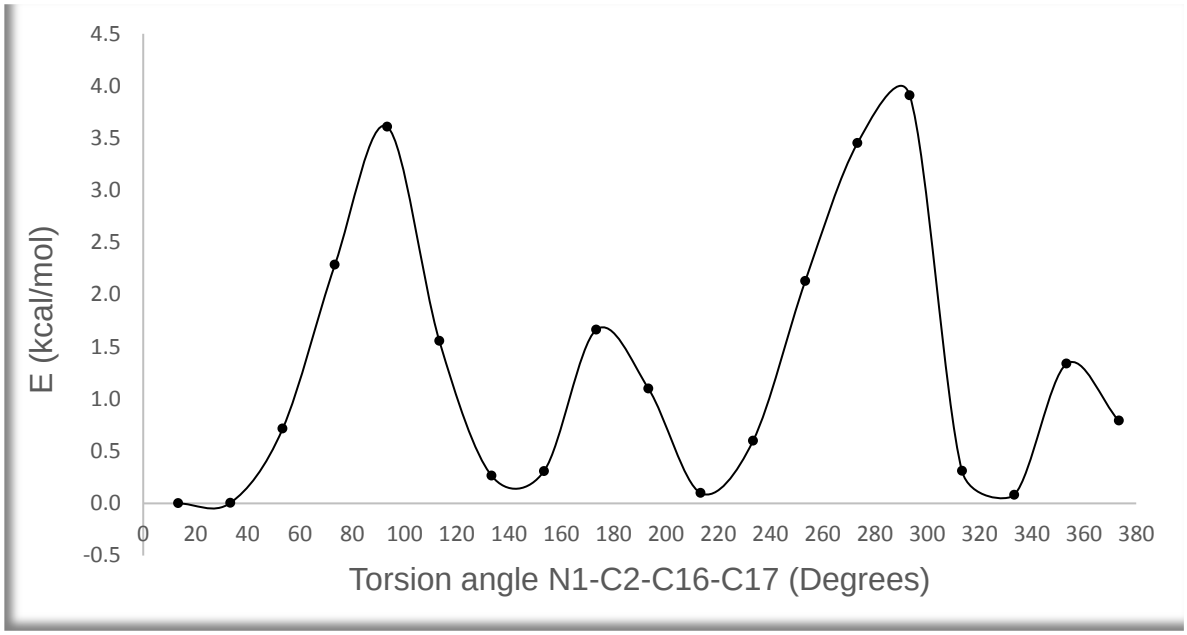

Figure S3 Theoretical rotation profile of the N1-C2-C16-C17 torsion angle in compound (III).

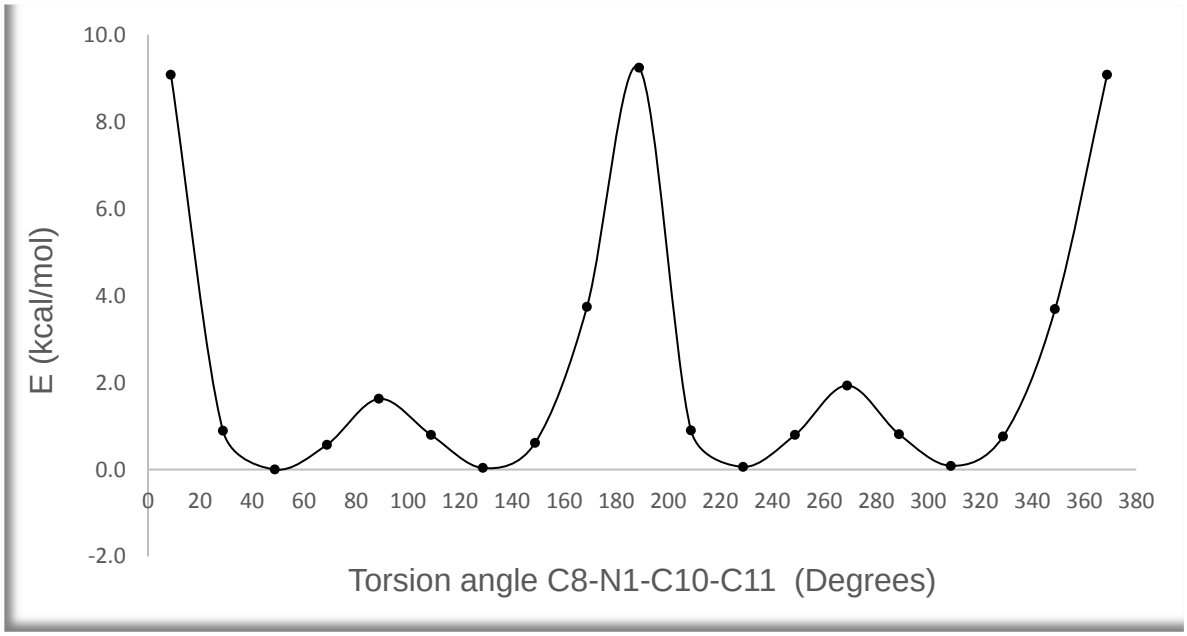

Figure S4 Theoretical rotation profile of the C8-N1-C10-C11 torsion angle in compound (III).

Table S1 Calculated rotation barriers (E_R in kcal mol^{-1}) at B3LYP/6-31G (*d*, *p*) level of theory in the rotation of C8-N1-C10-C11 (torsion angle 1), compounds (I)-(III), or N1-C2-C16-C17 (torsion angle 2), compounds (II) and (III)

Parameter	Compound

	(I)	(II)		(III)	
Fixed (°)		N1-C2-C16-C17 = 33.73	C8-N1-C10-C11 = 58.60	N1-C2-C16-C17 = 33.31	C8-N1-C10-C11 = 58.72
Rotating (°)	C8-N1-C10-C11	C8-N1-C10-C11	N1-C2-C16-C17	C8-N1-C10-C11	N1-C2-C16-C17
E_{R1} (kcal mol^{-1}) at (°)	3.27 180.57	8.95 8.57, 188.57	3.60 93.73, 273.73	9.20 188.81, 368.81.	3.75 93.35, 293.35
E_{R2} (kcal mol^{-1}) at (°)	2.10 90.57	1.60 88.57, 188.57	0.99 173.73, 353.73	1.78 88.81, 268.81	1.54 173.4, 353.4