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Supporting information for article:

Crystal structures, thermal stabilities, and dissolution behaviours of tinidazole and tinidazole–vanillic acid cocrystal: insights from energy frameworks

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Table S1 Intermolecular interaction energy values (kJ mol^{-1}) for the **TNZ**–**VA** cocrystal.

R is the distance between molecular centroids (mean atomic position) in Å. Each line corresponds to different intermolecular interactions.

Symop	*R*	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
–	8.72	−133.3	−29.1	−12.6	161.2	−73.8
–	6.54	−43.2	−13.2	−38.2	41.9	−62.8
–	9.15	−65.4	−15.9	−14.6	78.4	−45.2
–	4.95	−15.6	−3.7	−55.7	41.8	−41.9
–	5.54	−27.5	−7.7	−37.2	42.7	−40.8
–	4.72	−17.0	−5.7	−41.0	31.0	−38.7
−*x*, −*y*, −*z*	5.27	−10.1	−9.0	−35.4	22.8	−34.0
–	7.14	−6.6	−2.8	−25.0	11.7	−23.5
−*x*, −*y*, −*z*	6.23	−10.0	−1.3	−25.2	19.4	−21.5
–	6.91	−9.7	−4.1	−18.2	14.2	−20.4
–	5.33	−1.6	−2.1	−27.2	12.8	−19.0
–	8.44	−10.3	−3.3	−11.5	10.3	−17.0
–	9.19	−10.0	−2.9	−8.8	11.1	−13.5
–	10.20	−12.0	−1.7	−7.8	14.8	−11.6
–	7.36	−5.1	−2.2	−11.7	9.4	−11.4
–	7.50	−4.2	−1.7	−10.7	6.8	−10.8
−*x*, −*y*, −*z*	9.92	−5.0	−1.9	−7.0	4.3	−10.1
–	7.20	−0.7	−1.2	−5.6	0.9	−6.0
–	10.67	−3.7	−0.2	−1.6	0.0	−5.5
–	8.36	1.9	−0.8	−7.9	2.1	−4.2
–	9.26	0.7	−0.2	−4.6	1.5	−2.6
–	12.56	−1.0	−0.1	−1.3	0.0	−2.2
–	10.77	−1.1	−0.0	−0.7	0.0	−1.8
–	10.26	1.3	−0.4	−4.2	1.5	−1.6

–	10.17	1.0	−0.4	−3.4	0.9	−1.6
−*x*, −*y*, −*z*	11.26	−1.1	−0.0	−0.4	0.0	−1.5
–	13.18	−1.1	−0.0	−0.3	0.0	−1.5
−*x*, −*y*, −*z*	11.67	0.9	−0.4	−3.1	0.9	−1.5

Table S2 Hydrogen-bonding geometries of **TNZ–VA** cocrystal.

Donor (D)–H···acceptor (A)	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠D–H···A (°)
O6—H6···O14	0.88	1.74	2.6236 (16)	177
O8—H8···N2	0.87	1.88	2.7517 (18)	172
O13—H13*A*···O5	0.90	1.72	2.6177 (16)	174
O16—H16···N5	0.90	1.87	2.7489 (18)	167
C2—H2···O9^{i}	0.95	2.36	3.288 (2)	166
C8—H8*B*···O5^{i}	0.98	2.44	3.413 (2)	173
C13—H13···O9^{i}	0.95	2.60	3.352 (2)	137
C5—H5*B*···O11^{ii}	0.99	2.57	3.2830 (19)	129
C5—H5*A*···O16^{iii}	0.99	2.58	3.240 (2)	125
C6—H6*B*···O12^{iv}	0.99	2.23	3.2212 (18)	178
C21—H21*B*···O1^{iv}	0.99	2.65	3.358 (2)	129
C16—H16*A*···O7^{v}	0.98	2.62	3.352 (2)	132
C16—H16*B*···O16^{vi}	0.98	2.60	3.5684 (19)	169
C24—H24*B*···O14^{vii}	0.98	2.37	3.319 (2)	162
C18—H18···O1^{vii}	0.95	2.55	3.476 (2)	164
C29—H29···O1^{vii}	0.95	2.65	3.370 (2)	133
C22—H22*B*···O3^{viii}	0.99	2.45	3.342 (2)	149

Symmetry codes: (i) *x* − 1, *y* + 1, *z*; (ii) *x* − 2, *y* + 1, *z* − 1; (iii) −*x*, −*y* + 1, −*z* + 1; (iv) −*x* + 1, −*y* + 1, −*z* + 1; (v) −*x*, −*y* + 1, −*z*; (vi) *x* − 1, *y*, *z* − 1; (vii) *x* + 1, *y* − 1, *z*; (viii) *x* + 2, *y* − 1, *z* + 1.