Electronic Supplementary Material (ESI) for RSC Advances.

A combined experimental and theoretical investigation of noncovalent interactions in 1,3,4-oxadiazole-2-thione-*N*-Mannich derivatives: *in vitro* bioactivity and molecular docking

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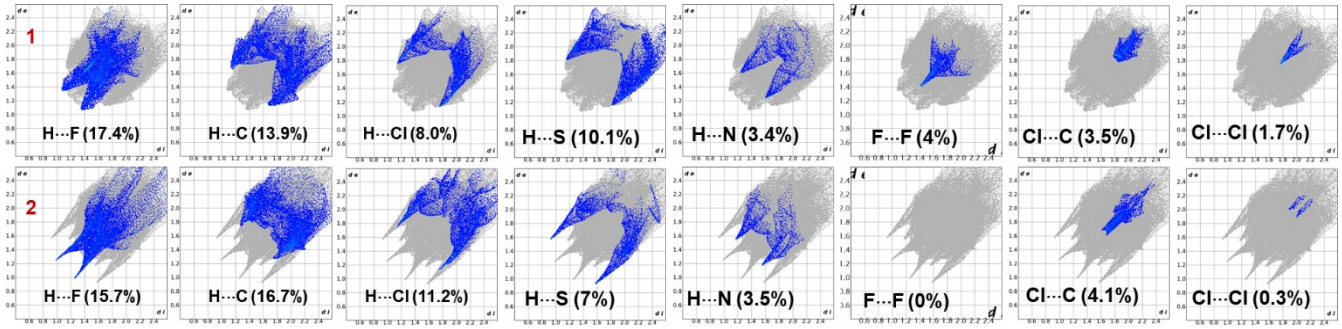

Fig. S1 2D-fingerprint plots showing the relative contribution of selected intermolecular interactions observed in **1** and **2**.

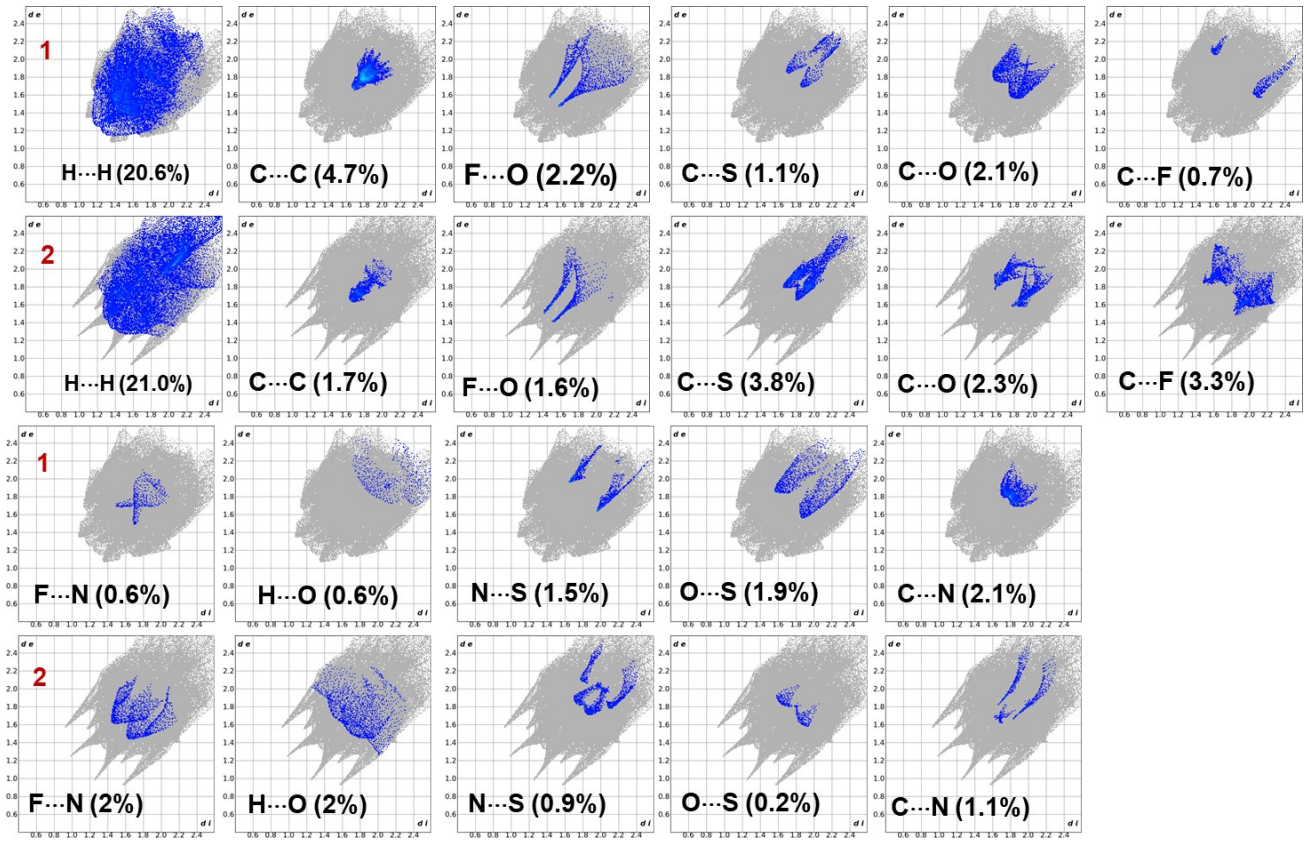

Fig. S2 2D-fingerprint plots showing the relative contribution of selected intermolecular interactions observed in **1** and **2**.

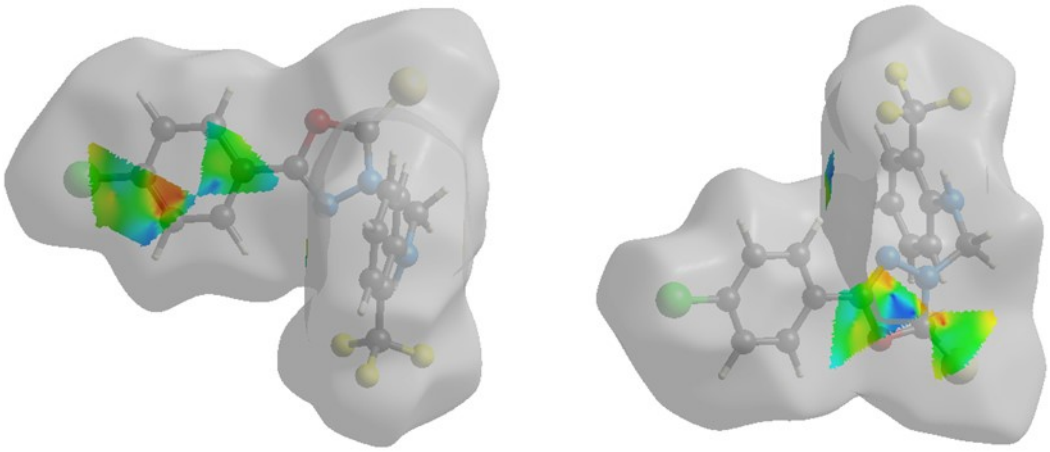

Fig. S3 Two different views of shape index diagram showing the red-blue triangles over the surface of the rings A and B in **1**.

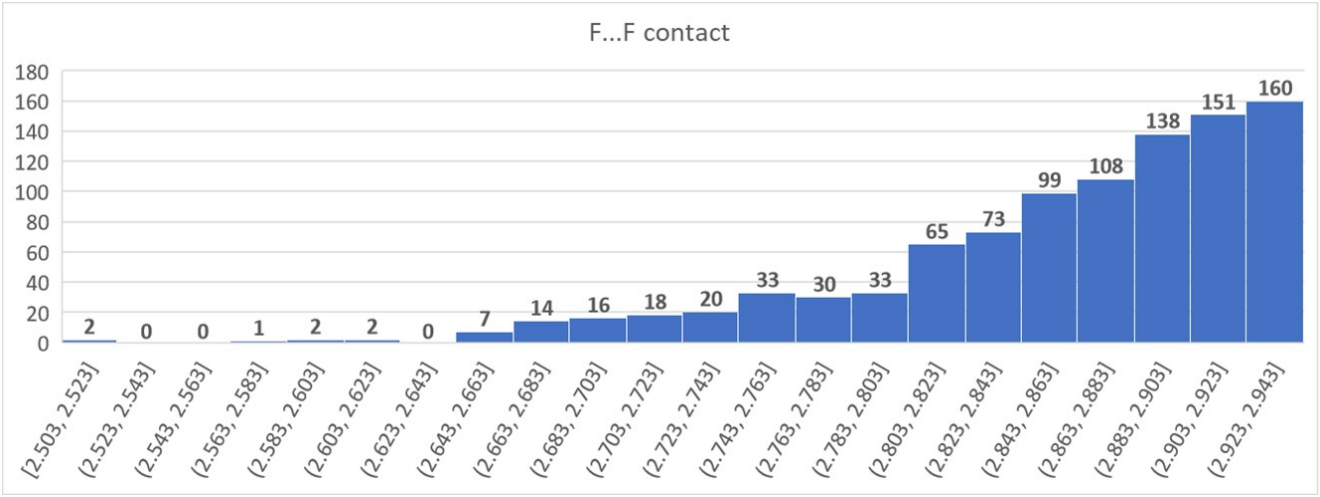

Fig. S4 Distribution of C–F···F–C contacts observed in structures deposited in CSD.

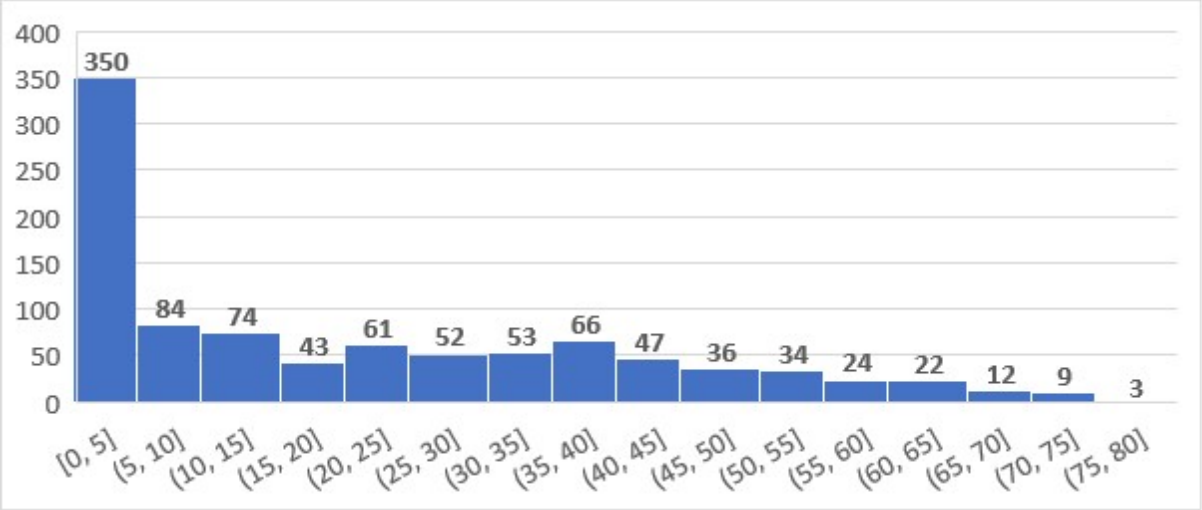

Fig. S5 Distribution of $|\theta_1 - \theta_2|$ angles for the C–F···F–C contacts observed in structures deposited in CSD.

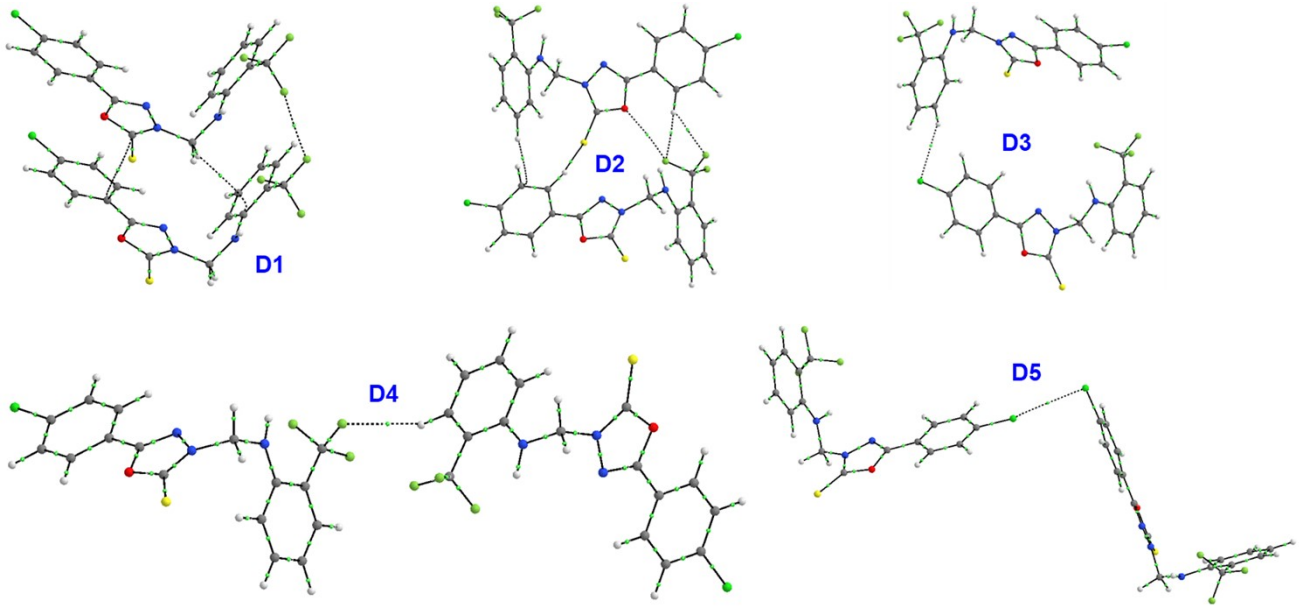

Fig. S6 Molecular graphs of molecular dimers of **1** showing bond critical points for intermolecular interactions.

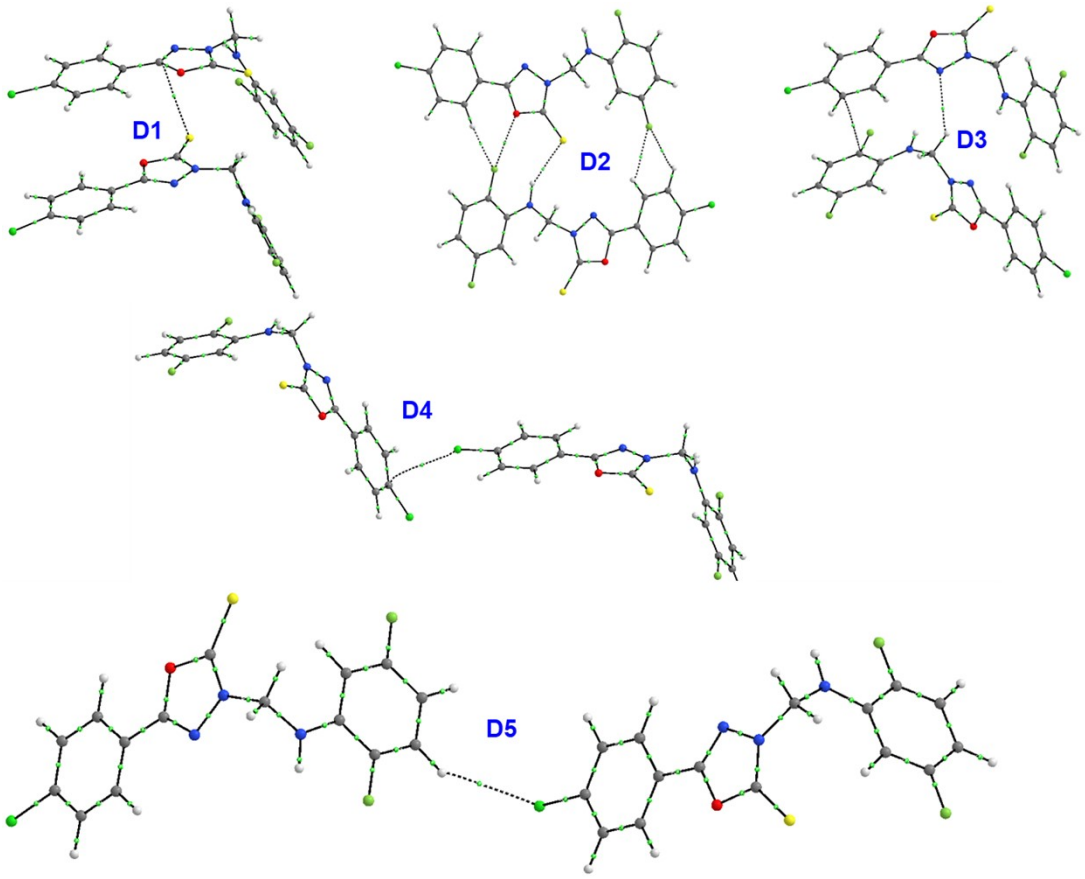

Fig. S7 Molecular graphs of molecular dimers of **2** showing bond critical points for intermolecular interactions.

Table S1 Topological parameters for selected intermolecular interactions in different dimers of compounds **1** and **2**. R_{ij}, Bond path (Å); ρ(r), Electron density (e Å^{-3}); $\nabla^2\rho$(r), Laplacian of electron density (e Å^{-5}); V(r), Potential electron density (kJ mol^{-1} br^{-3}); G(r), Kinetic electron density (kJ mol^{-1} br^{-3}); H(r), Total electronic energy density (kJ mol^{-1} br^{-3}); D_e, Dissociation energy (kcal mol^{-1}).

Interaction	R_{ij}	ρ(r)	$\nabla^2\rho$(r)	V(r)	G(r)	H(r)	$\lvert -V(r)/G(r)\rvert$	D_e
Compound **1**								
D1								
C8···C4	3.447	0.039	0.437	-7.3	9.6	2.3	0.76	0.9
C9–H9B···*Cg*3	3.139	0.039	0.464	-7.6	10.1	2.5	0.75	0.9
C16–F1···F2–C16	2.838	0.042	0.841	-10.9	16.9	6.0	0.65	1.3
D2								
C12–H12···C2(π)	2.988	0.043	0.443	-7.7	9.9	2.2	0.78	0.9
C3–H3···S1	3.017	0.046	0.460	-7.8	10.1	2.4	0.77	0.9
C6–H6···F2	3.057	0.031	0.545	-6.8	10.8	4.0	0.63	0.8
C5–H5···F3	2.442	0.053	0.758	-11.3	16.0	4.7	0.71	1.4
C5–H5···F1	2.462	0.056	0.824	-12.6	17.5	4.9	0.72	1.5
D3								
C12–H12···Cl1	2.932	0.045	0.500	-8.1	10.9	2.8	0.75	1.0
D4								
C14–H14···F1	2.625	0.038	0.543	-8.0	11.4	3.4	0.70	1.0
D5								
C1–Cl1···Cl1	3.532	0.041	0.533	-7.3	10.9	3.6	0.67	0.9
Compound **2**								
D1								
S1···C7	3.513	0.047	0.500	-9.0	11.3	2.3	0.79	1.1
D2								
C3–H3···F1	2.251	0.074	1.162	-17.3	24.5	7.2	0.71	2.1
C11–F1···O1	2.925	0.040	0.764	-10.0	15.4	5.4	0.65	1.2
N3–H3A···S1	2.524	0.105	0.980	-18.6	22.6	4.1	0.82	2.2
C5–H5···F2	2.594	0.040	0.642	-9.3	13.4	4.1	0.69	1.1
C6–H6···F2	2.663	0.035	0.569	-8.1	11.8	3.7	0.69	1.0
D3								
C11···C6	3.358	0.044	0.456	-8.0	10.2	2.2	0.79	1.0
C9–H9A···N1	2.760	0.043	0.476	-8.0	10.5	2.5	0.76	1.0
D4								
C1–Cl1···C6(π)	3.389	0.050	0.626	-9.2	13.5	3.6	0.74	1.2
D5								
C12–H12···Cl1	2.920	0.041	0.450	-7.1	9.7	2.6	0.74	0.9