A crystallographic, computational study and Hirshfeld surface analysis of how aryl-bound substituents influence the nature of hydrogen bonds, N–H···N and N–H···O, in the crystal structures of 1-(arylamino)-1,2,3-triazole-4-carbohydrazides†

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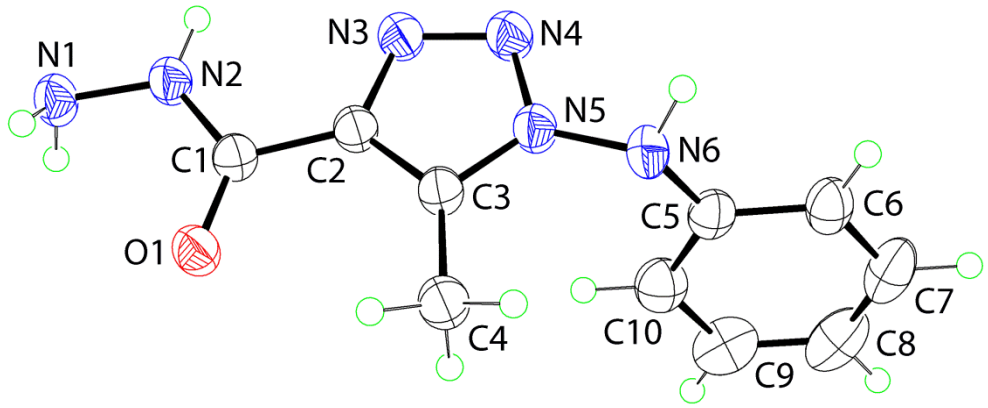
Table S(1). Natural Charge for **1–5** calculated on geometry optimised structures and experimental (crystallographic) structures.

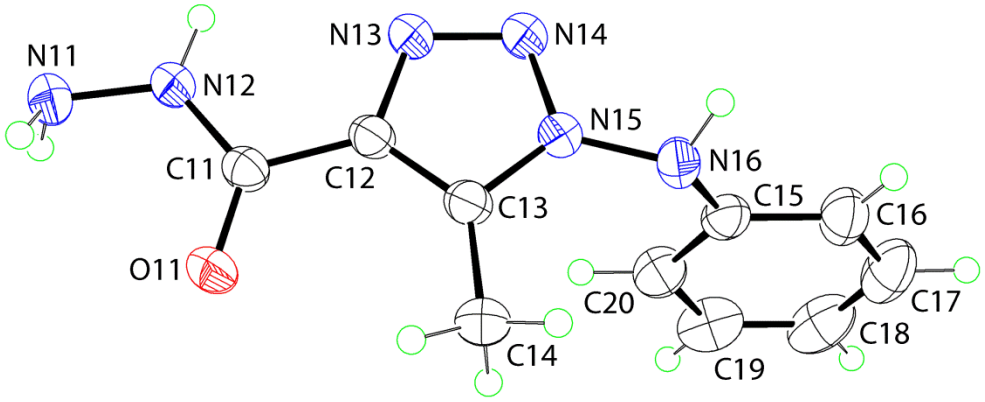
Natural Charge	1a			1b			2			3		
Atom	Optimised	Unoptimised	Diff (Opt-Unopt)	Optimised	Unoptimised	Diff (Opt-Unopt)	Optimised	Unoptimised	Diff (Opt-Unopt)	Optimised	Unoptimised	Diff (Opt-Unopt)
C1	0.62979	0.61778	0.01201	0.6295	0.62057	0.00893	0.62948	0.62079	0.00869	0.62876	0.61679	0.01197
H1	0.35299	0.32568	0.02731	0.35294	0.33219	0.02075	0.35378	0.32743	0.02635	0.35404	0.32874	0.0253
H2	0.35281	0.329	0.02381	0.35274	0.32394	0.0288	0.35265	0.32734	0.02531	0.35256	0.32328	0.02928
H3	0.40383	0.36506	0.03877	0.40373	0.36654	0.03719	0.40368	0.36803	0.03565	0.40368	0.36349	0.04019
C2	-0.01797	-0.02191	0.00394	-0.01805	-0.01963	0.00158	-0.01726	-0.01849	0.00123	-0.01717	-0.01922	0.00205
H4	0.38429	0.35493	0.02936	0.38457	0.35562	0.02895	0.38463	0.3551	0.02953	0.38587	0.34961	0.03626
H5	0.22697	0.21631	0.01066	0.22567	0.20998	0.01569	0.22683	0.22268	0.00415	0.22551	0.20981	0.0157
O1	-0.64653	-0.66382	0.01729	-0.64625	-0.66242	0.01617	-0.64556	-0.65635	0.01079	-0.64509	-0.65751	0.01242
C3	0.2219	0.23703	-0.01513	0.2218	0.23333	-0.01153	0.22194	0.23192	-0.00998	0.2224	0.23399	-0.01159
C4	-0.62149	-0.57465	-0.04684	-0.6211	-0.57594	-0.04516	-0.62159	-0.57341	-0.04818	-0.6205	-0.57753	-0.04297
H6	0.25682	0.23037	0.02645	0.25565	0.23104	0.02461	0.25747	0.22236	0.03511	0.22865	0.21383	0.01482
H7	0.22572	0.2102	0.01552	0.22793	0.21599	0.01194	0.22599	0.21025	0.01574	0.2556	0.23418	0.02142
H8, Cl1 of Cl2	0.20565	0.17602	0.02963	0.2058	0.1761	0.0297	0.21	0.1786	0.0314	0.21065	0.18029	0.03036
N1	-0.62855	-0.57057	-0.05798	-0.62853	-0.57189	-0.05664	-0.62841	-0.57662	-0.05179	-0.62836	-0.56844	-0.05992
N2	-0.45348	-0.40402	-0.04946	-0.45361	-0.40223	-0.05138	-0.45299	-0.4044	-0.04859	-0.4529	-0.39886	-0.05404
N3	-0.25604	-0.24958	-0.00646	-0.25578	-0.25672	0.00094	-0.25468	-0.24918	-0.0055	-0.25318	-0.24946	-0.00372
N4	-0.06651	-0.08012	0.01361	-0.06767	-0.07709	0.00942	-0.06869	-0.08068	0.01199	-0.06886	-0.07399	0.00513
H9	0.2073	0.1739	0.0334	0.20734	0.17359	0.03375	0.22557	0.19351	0.03206	0.2237	0.18937	0.03433
C7	0.15868	0.17247	-0.01379	0.15851	0.17074	-0.01223	0.14375	0.15621	-0.01246	0.15595	0.16507	-0.00912
C8	-0.23774	-0.21463	-0.02311	-0.23752	-0.21387	-0.02365	-0.21736	-0.19011	-0.02725	-0.22003	-0.1941	-0.02593
H10, Cl1, F1, Br1	0.20814	0.17469	0.03345	0.20818	0.17537	0.03281						
C9	-0.17865	-0.14198	-0.03667	-0.1788	-0.14175	-0.03705	-0.24166	-0.21313	-0.02853	-0.20041	-0.17305	-0.02736
H11, Cl2	0.20762	0.17319	0.03443	0.20766	0.17316	0.0345	0.22595	0.19371	0.03224	0.22396	0.18933	0.03463
C10	-0.22585	-0.1933	-0.03255	-0.22569	-0.19554	-0.03015	0.39218	0.4033	-0.01112	-0.05775	-0.04544	-0.01231
C11	-0.17445	-0.13548	-0.03897	-0.17459	-0.13409	-0.0405	-0.23898	-0.20875	-0.03023	-0.19694	-0.16927	-0.02767
H12	0.21557	0.18134	0.03423	0.21561	0.1823	0.03331	0.21982	0.18569	0.03413	0.22051	0.18344	0.03707
C12	-0.24658	-0.22387	-0.02271	-0.24636	-0.2245	-0.02186	-0.22647	-0.199	-0.02747	-0.22866	-0.19014	-0.03852
F1							-0.35385	-0.35875	0.0049			
Cl1										0.00247	0.00567	-0.0032
N5	-0.06982	-0.06241	-0.00741	-0.06914	-0.06275	-0.00639	-0.07122	-0.06481	-0.00641	-0.07111	-0.06593	-0.00518
N6	-0.4344	-0.40163	-0.03277	-0.43454	-0.40203	-0.03251	-0.43499	-0.40324	-0.03175	-0.43335	-0.40397	-0.02938

Table S(1) continued

Natural Charge	4			5		
Atom	Optimised	Unoptimised	Diff (Opt-Unopt)	Optimised	Unoptimised	Diff (Opt-Unopt)
C1	0.62946	0.61954	0.00992	0.62974	0.61927	0.01047
H1	0.35326	0.33038	0.02288	0.35359	0.32553	0.02806
H2	0.35331	0.32054	0.03277	0.35344	0.32597	0.02747
H3	0.4038	0.36508	0.03872	0.40404	0.36457	0.03947
C2	-0.01674	-0.01865	0.00191	-0.01564	-0.01785	0.00221
H4	0.38578	0.34639	0.03939	0.40269	0.36579	0.0369
H5	0.22583	0.21064	0.01519	0.22722	0.21792	0.0093
O1	-0.64524	-0.66083	0.01559	-0.64423	-0.65683	0.0126
C3	0.22196	0.23513	-0.01317	0.22298	0.2365	-0.01352
C4	-0.6218	-0.57784	-0.04396	-0.62175	-0.57555	-0.0462
H6	0.22703	0.21212	0.01491	0.22651	0.21071	0.0158
H7	0.25791	0.23652	0.02139	0.25922	0.23107	0.02815
H8, Cl1 of Cl2	0.21078	0.18016	0.03062			
N1	-0.62832	-0.56623	-0.06209	-0.62806	-0.56711	-0.06095
N2	-0.4526	-0.40098	-0.05162	-0.45181	-0.40353	-0.04828
N3	-0.25374	-0.25018	-0.00356	-0.24926	-0.24937	0.00011
N4	-0.06689	-0.07166	0.00477	-0.0631	-0.08169	0.01859
H9	0.22396	0.18908	0.03488	0.2275	0.19224	0.03526
C7	0.15816	0.16762	-0.00946	0.15295	0.14933	0.00362
C8	-0.22046	-0.19525	-0.02521	-0.0715	-0.07207	0.00057
H10, Cl1, F1, Br1				0.22803	0.19314	0.03489
C9	-0.20159	-0.17125	-0.03034	-0.187	-0.15761	-0.02939
H11, Cl2	0.22421	0.18914	0.03507			
C10	-0.12315	-0.11018	-0.01297	-0.23487	-0.19663	-0.03824
C11	-0.19808	-0.17194	-0.02614	-0.01771	-0.01174	-0.00597
H12	0.22082	0.18339	0.03743	0.23476	0.20366	0.0311
C12	-0.2293	-0.18699	-0.04231	-0.25317	-0.22759	-0.02558
Br1	0.06608	0.0671	-0.00102			
Cl1				0.00632	0.02189	-0.01557
Cl2				0.0176	0.02243	-0.00483
N5	-0.07192	-0.06956	-0.00236	-0.07952	-0.06668	-0.01284
N6	-0.43251	-0.40127	-0.03124	-0.42898	-0.39577	-0.03321



(a)



(b)

Figure S(1). Molecular structures of the two independent molecules comprising the asymmetric unit of (**1**), showing atom labelling and displacement ellipsoids at the 50% probability level.

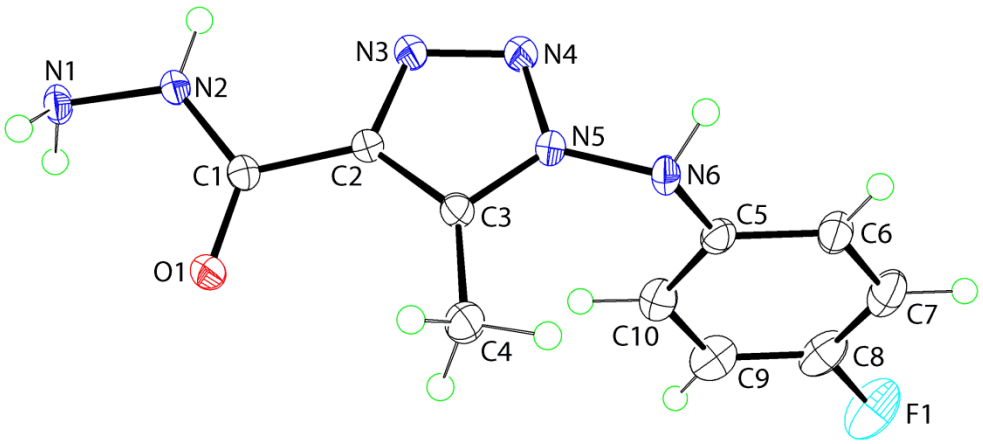


Figure S(2). Molecular structure of (**2**), showing atom labelling and displacement ellipsoids at the 50% probability level.

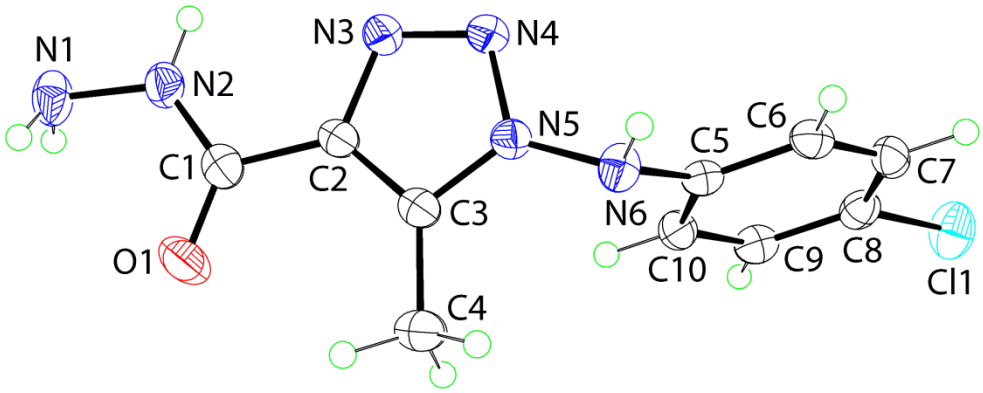


Figure S(3). Molecular structure of (**3**), showing atom labelling and displacement ellipsoids at the 50% probability level.

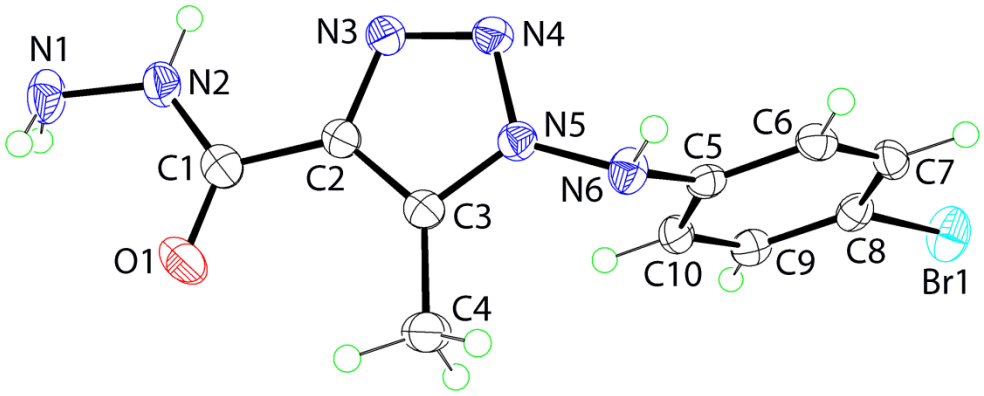


Figure S(4). Molecular structure of (**4**), showing atom labelling and displacement ellipsoids at the 50% probability level.

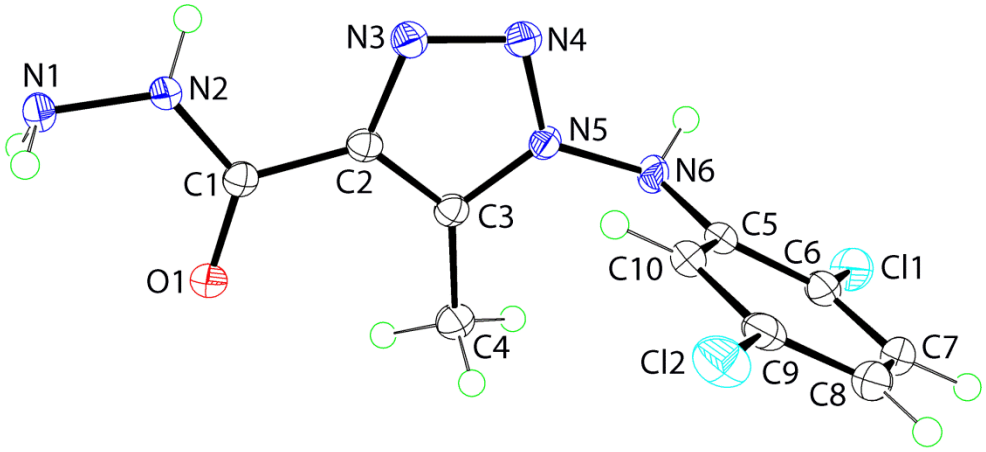


Figure S(5). Molecular structure of (**5**), showing atom labelling and displacement ellipsoids at the 50% probability level.

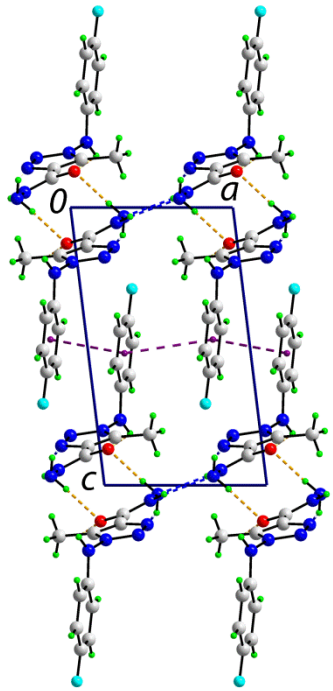


Figure S(6). Crystal packing in **2**: view in projection down the *b*-axis of the unit cell contents highlighting the inter-digitation of layers. The N–H...O, N–H...N and π...π interactions are shown as orange, blue and purple dashed lines, respectively.

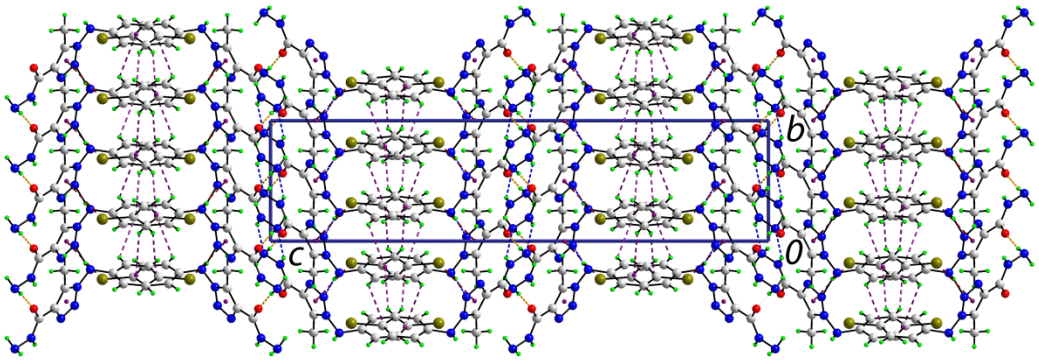


Figure S(7). Crystal packing in **4**: view in projection down the *a*-axis of the unit cell contents highlighting the inter-digitation of layers. The N–H...O, N–H...N, N–H...π, C–Br...π and π...π interactions are shown as orange, blue, purple, brown and pink dashed lines, respectively.

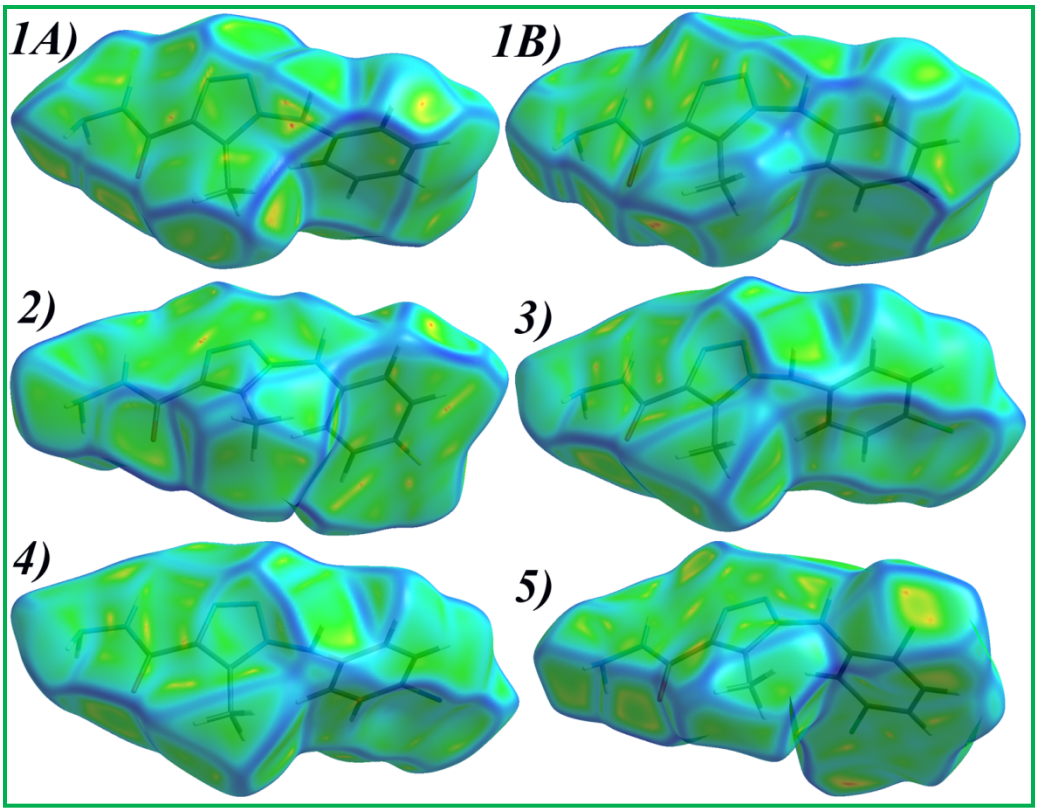


Figure S(8) Hirshfeld surfaces mapped with curvedness for **1**–**5**. For compound **1**, with two molecules in the asymmetric unit, these are denoted by '***A***' and '***B***'.

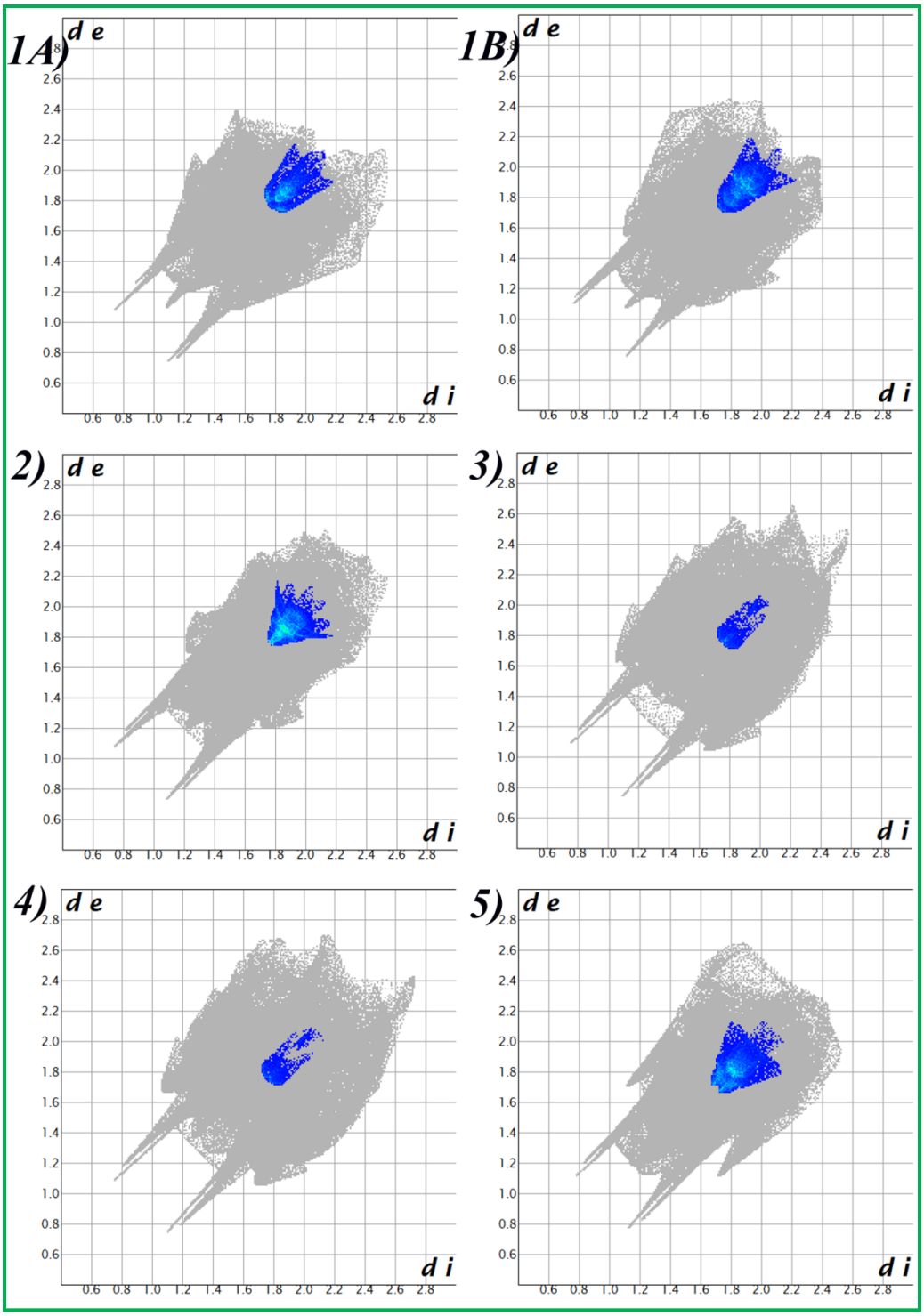


Figure S(9) Fingerprint plots resolved into $C_\pi \cdots C_\pi$ contacts for **1**–**5**. For compound **1**, with two molecules in the asymmetric unit, these are denoted by '***A***' and '***B***'.