Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information

Thermodynamic, Energetic, and Topological Properties of Crystal Packing of Pyrazolo[1,5-*a*]pyrimidines Governed by Weak Electrostatic Intermolecular Interactions

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Summary

Figures……

Tables……

Figures

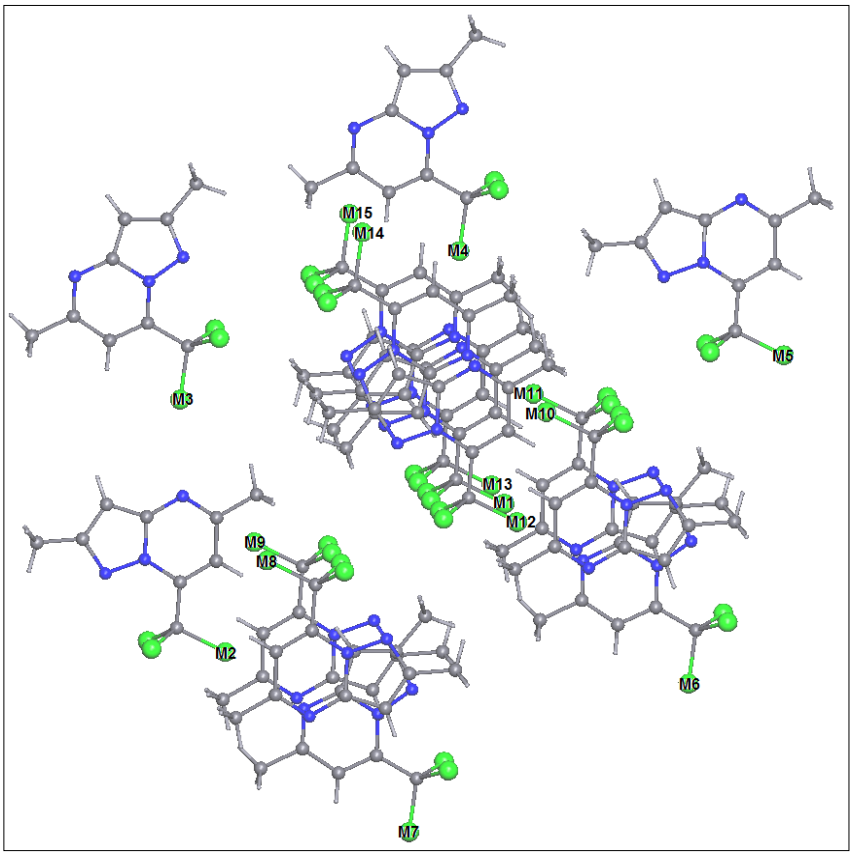

Figure S1. Supramolecular cluster that forms the first coordination sphere for Compound **1**.

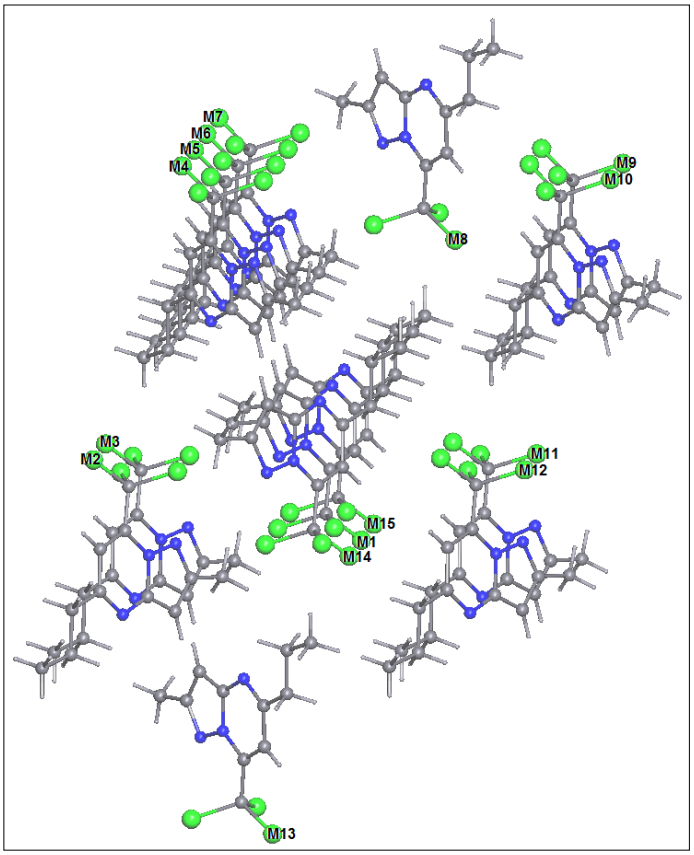

Figure S2. Supramolecular cluster that forms the first coordination sphere for Compound **2**.

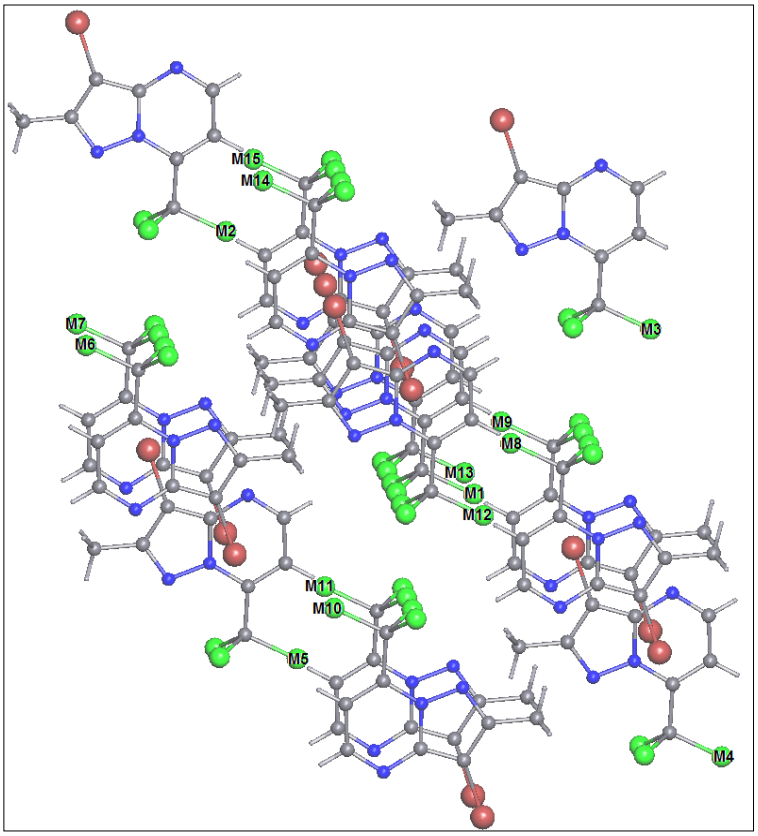

Figure S3. Supramolecular cluster that forms the first coordination sphere for Compound **3**.

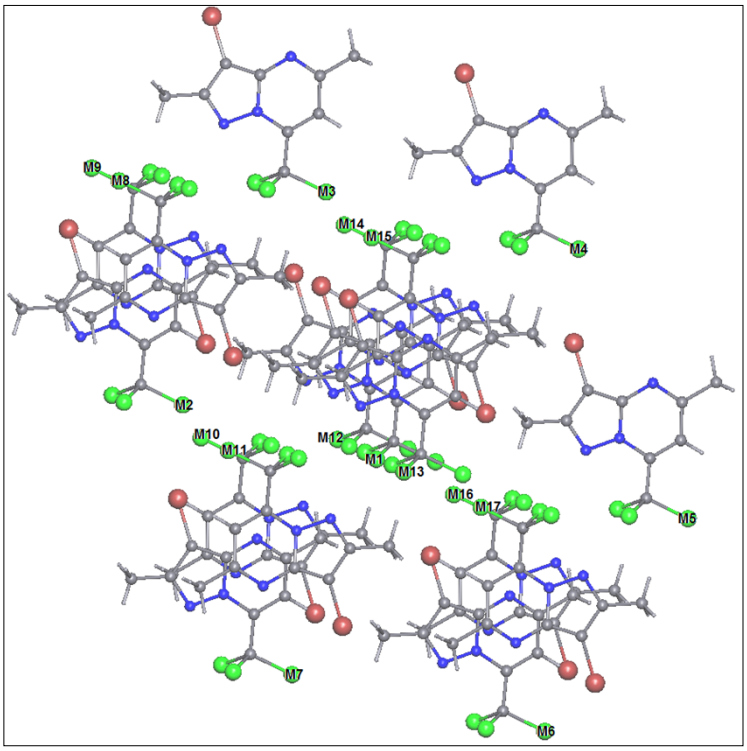

Figure S4. Supramolecular cluster that forms the first coordination sphere for Compound **4**.

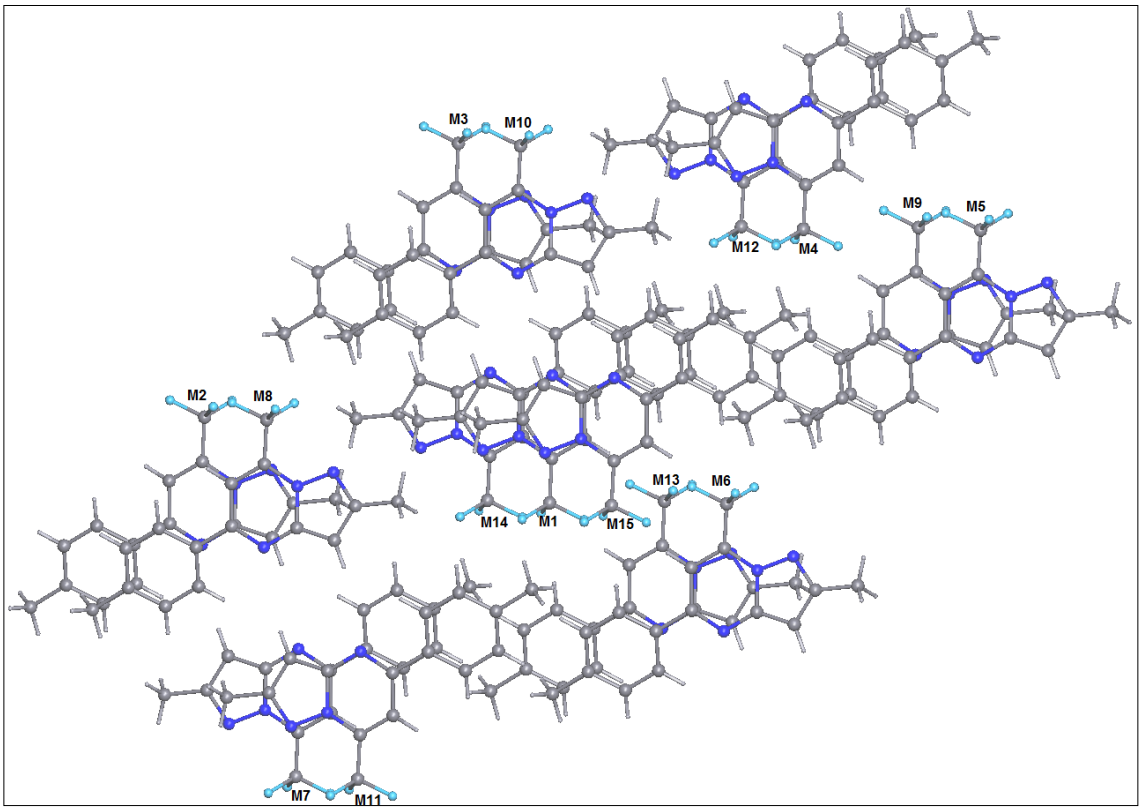

Figure S5. Supramolecular cluster that forms the first coordination sphere for Compound **5**.

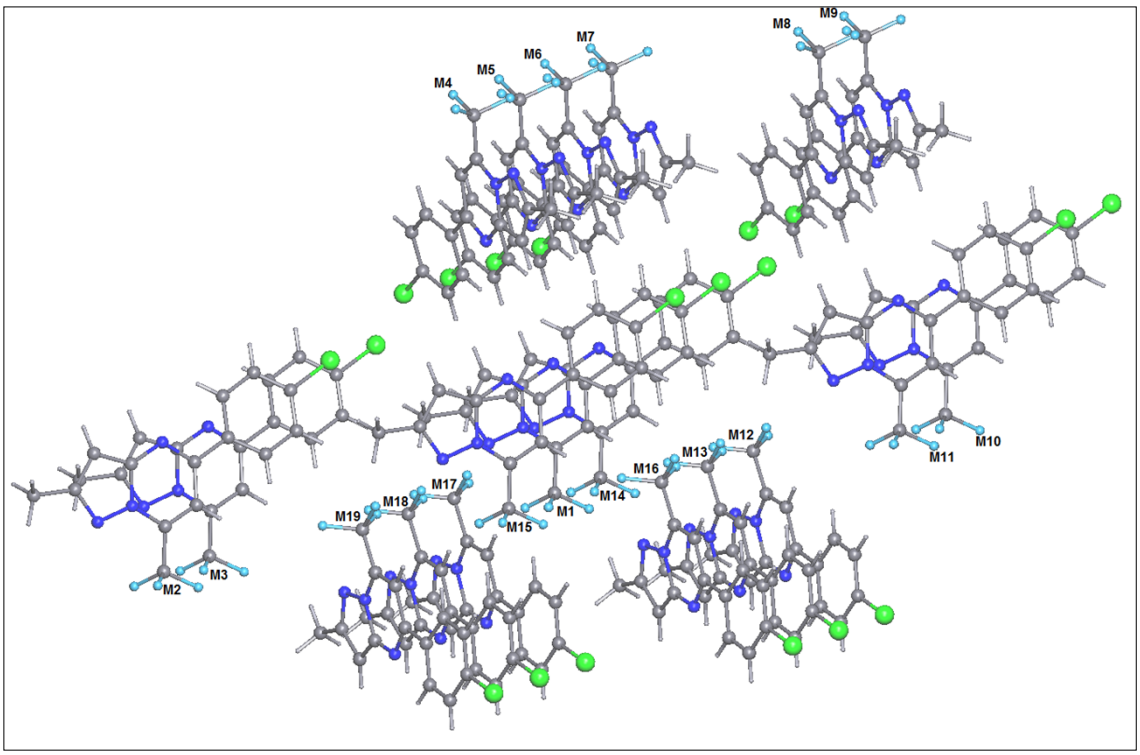

Figure S6. Supramolecular cluster that forms the first coordination sphere for Compound **6**.

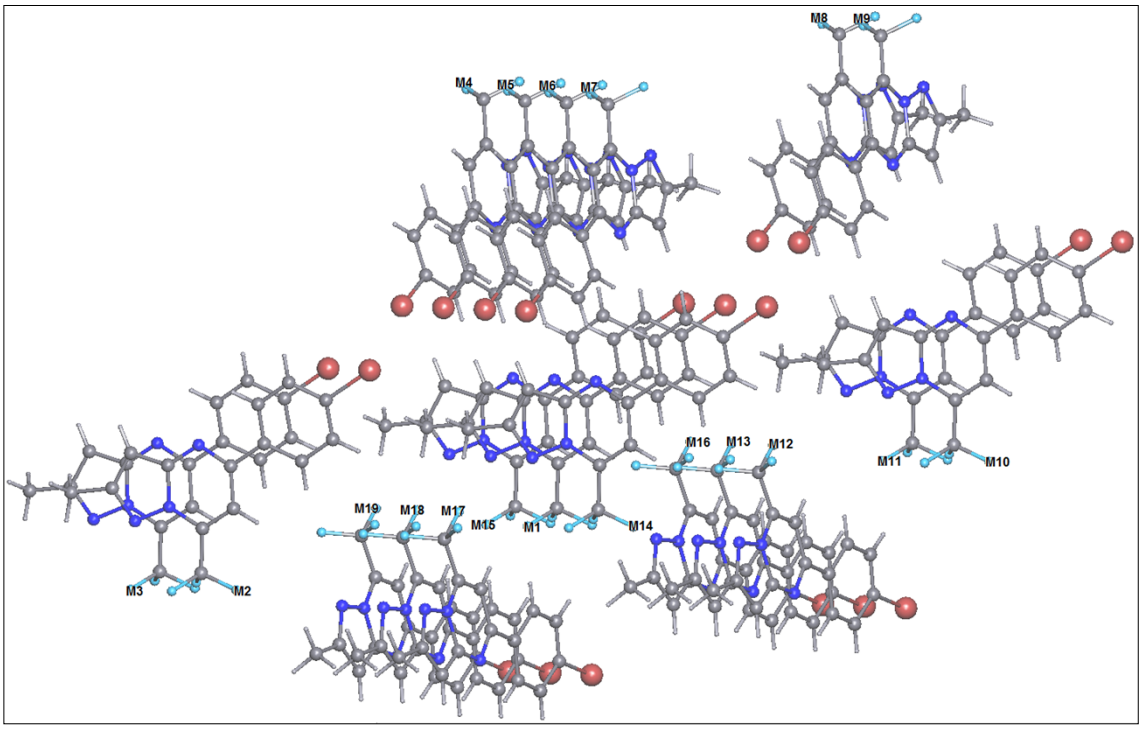

Figure S7. Supramolecular cluster that forms the first coordination sphere for Compound **7**.

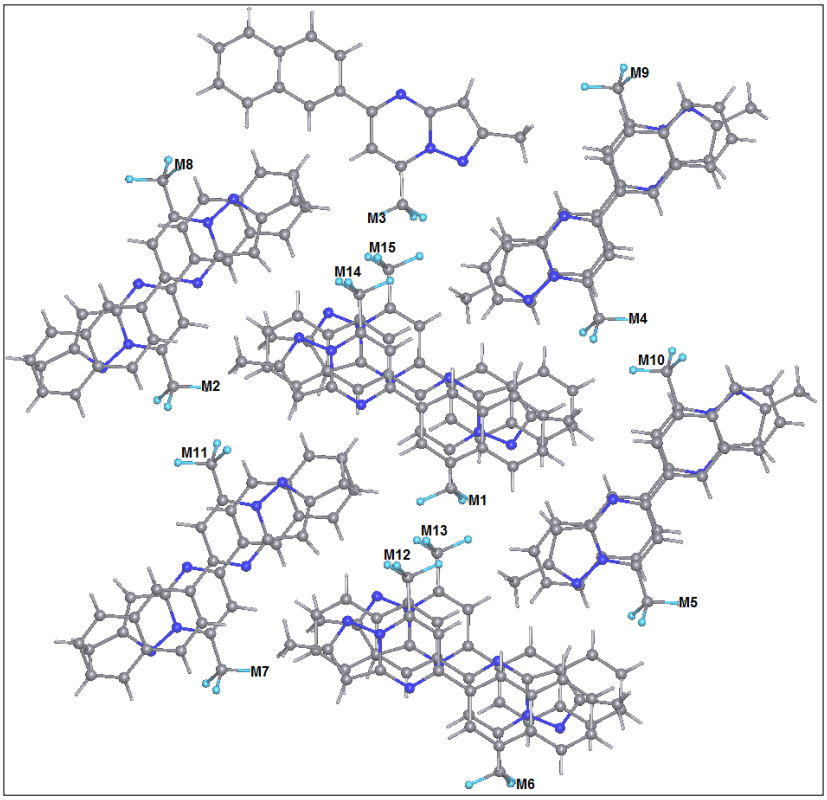

Figure S8. Supramolecular cluster that forms the first coordination sphere for Compound **8**.

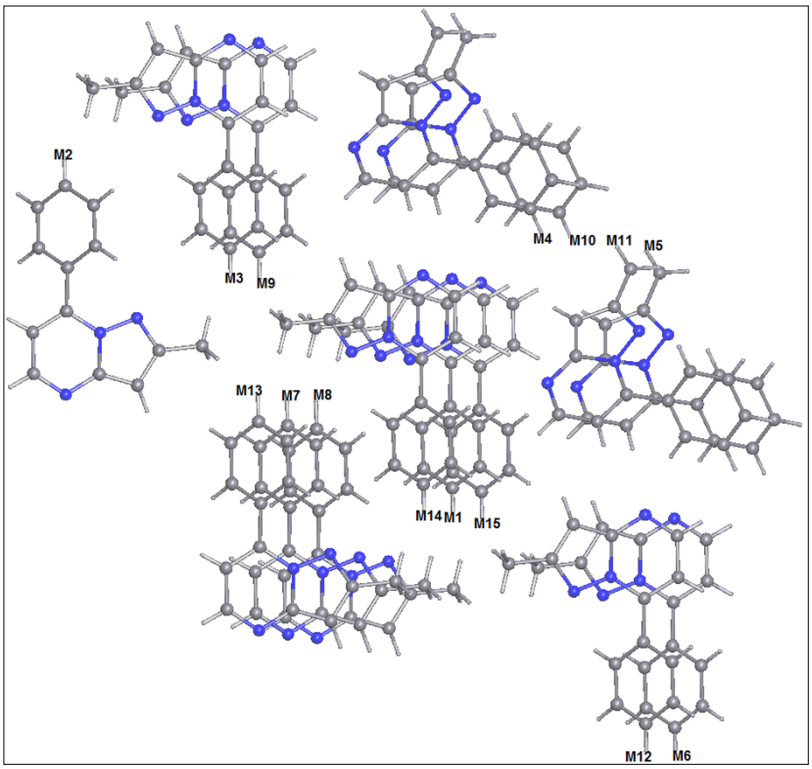

Figure S9. Supramolecular cluster that forms the first coordination sphere for Compound **9**.

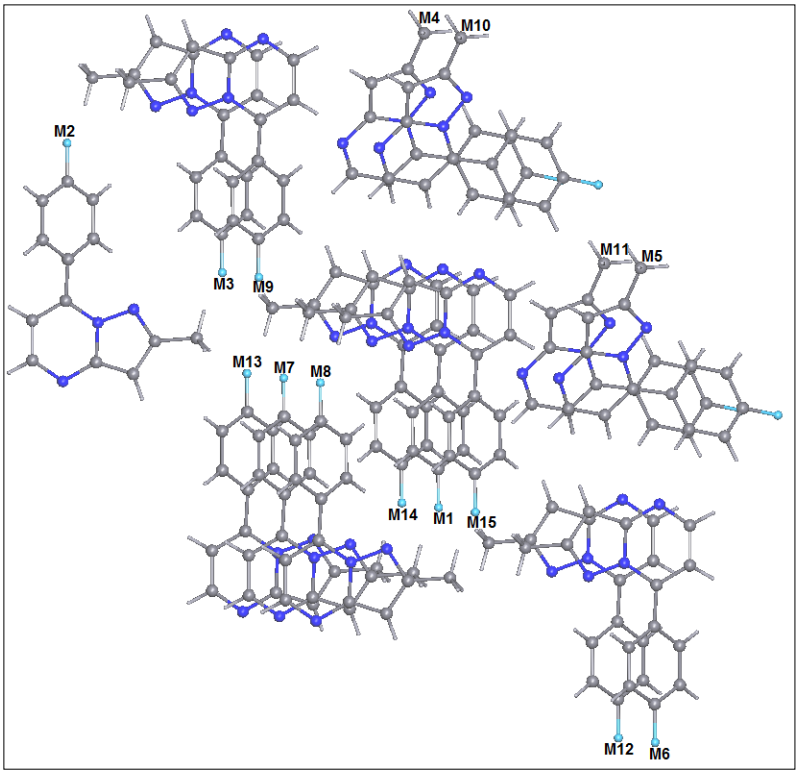

Figure S10. Supramolecular cluster that forms the first coordination sphere for Compound **10**.

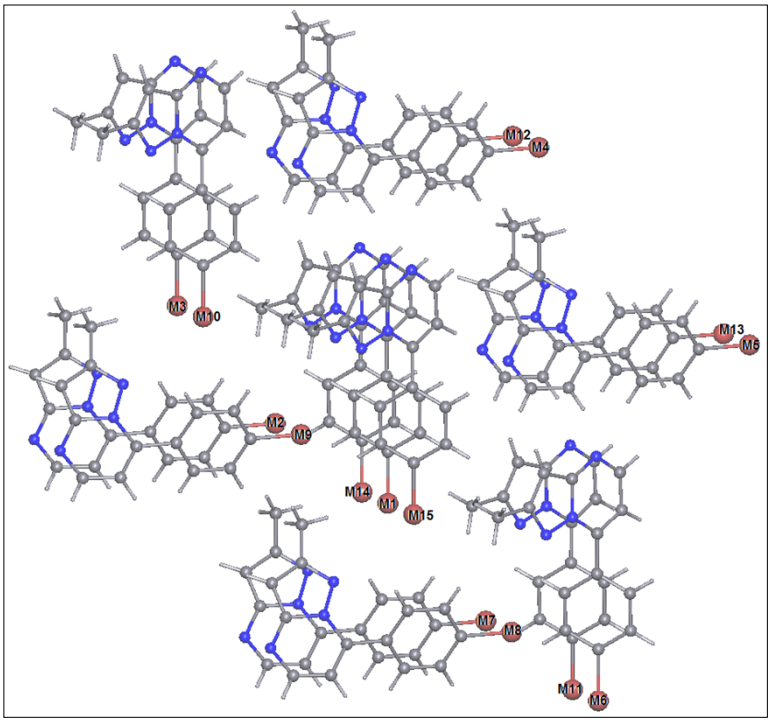

Figure S11. Supramolecular cluster that forms the first coordination sphere for Compound **11**.

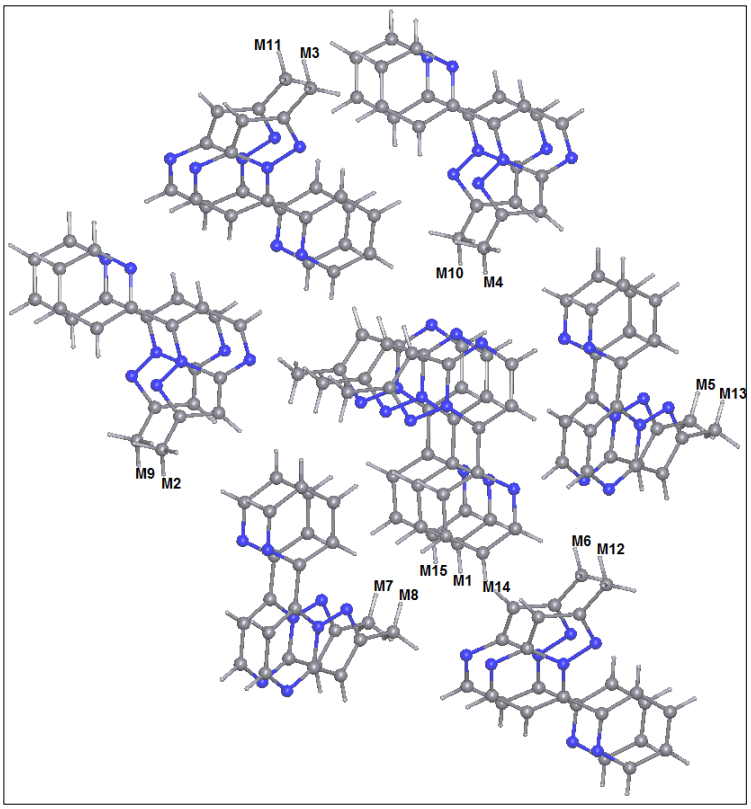

Figure S12. Supramolecular cluster that forms the first coordination sphere for Compound **12**.

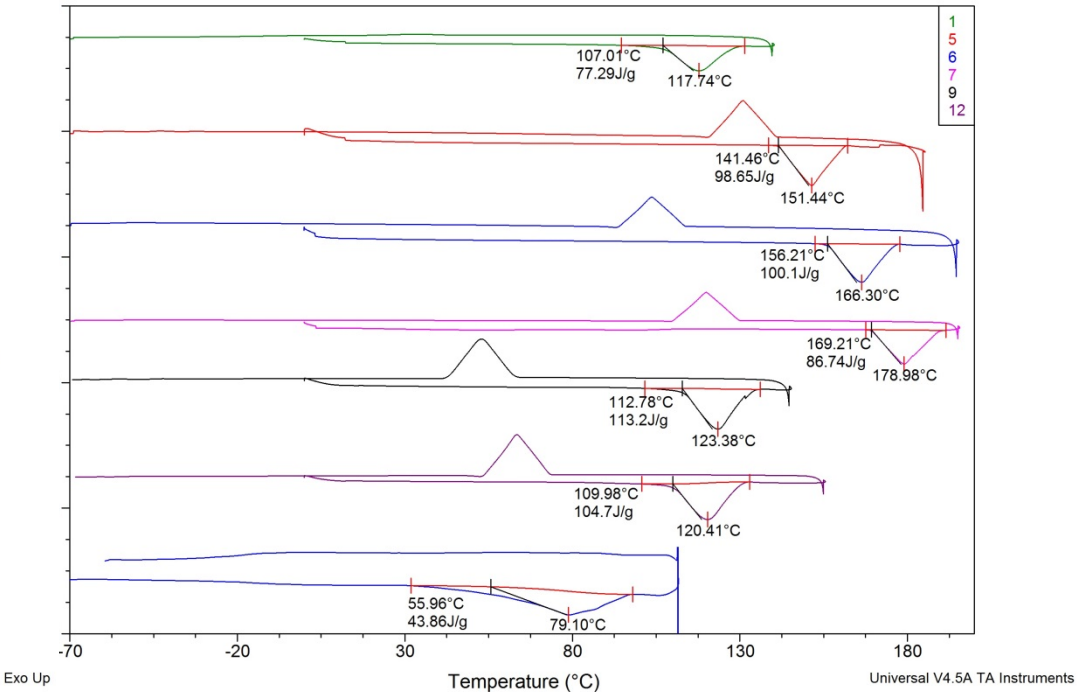

Figure S13. DSC thermograms of compounds **1**, **5**, **6**, **7**, **9**, **12**, and **13**.

Tables

Table S1. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **1**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	NG$_{(M1\cdots Mn)}$	NC$_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-0.60	10.29	0.24	0.52	III
M1···M3	-0.84	10.69	0.34	0.54	III
M1···M4	-2.13	14.15	0.87	0.71	III
M1···M5	-0.60	10.29	0.24	0.52	III
M1···M6	-2.13	14.15	0.87	0.71	III
M1···M7	-0.84	10.69	0.34	0.54	III
M1···M8	-0.79	4.16	0.32	0.21	III
M1···M9	-0.74	8.63	0.30	0.43	III
M1···M10	-3.34	31.76	1.36	1.59	III
M1···M11	-3.48	34.65	1.42	1.74	III
M1···M12	-0.59	2.76	0.24	0.14	III
M1···M13	-0.61	2.76	0.25	0.14	III
M1···M14	-8.82	62.25	3.60	3.12	II
M1···M15	-8.82	62.25	3.60	3.12	II

Table S2. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **2**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	NG$_{(M1\cdots Mn)}$	NC$_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-1.82	30.36	0.76	1.26	III
M1···M3	-3.14	27.15	1.31	1.13	III
M1···M4	-0.47	10.58	0.20	0.44	III
M1···M5	-2.86	22.69	1.19	0.94	III
M1···M6	-2.86	22.69	1.19	0.94	III
M1···M7	-0.47	10.58	0.20	0.44	III
M1···M8	-0.97	14.49	0.41	0.60	III
M1···M9	-0.81	15.44	0.34	0.64	III
M1···M10	-0.81	15.44	0.34	0.64	III
M1···M11	-1.76	23.95	0.73	0.99	III
M1···M12	-4.18	30.50	1.75	1.27	III
M1···M13	-0.94	14.49	0.39	0.60	III
M1···M14	-6.20	49.47	2.59	2.05	II
M1···M15	-6.20	49.47	2.59	2.05	II

Table S3. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **3**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	NG$_{(M1\cdots Mn)}$	NC$_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-0.43	9.46	0.17	0.46	IV
M1···M3	-3.98	26.22	1.60	1.27	III
M1···M4	-0.41	9.46	0.16	0.46	III
M1···M5	-3.98	26.22	1.60	1.27	III
M1···M6	-2.37	23.98	0.95	1.17	III
M1···M7	-2.37	23.98	0.95	1.17	III
M1···M8	-2.54	24.36	1.02	1.18	III
M1···M9	-2.54	24.36	1.02	1.18	III
M1···M10	-0.22	10.44	0.09	0.51	IV
M1···M11	-0.22	10.44	0.09	0.51	IV
M1···M12	-0.69	5.24	0.28	0.25	III
M1···M13	-0.69	5.24	0.28	0.25	III
M1···M14	-7.22	44.34	2.90	2.15	II
M1···M15	-7.22	44.34	2.90	2.15	II

Table S4. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **4**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	NG$_{(M1\cdots Mn)}$	NC$_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-1.10	22.61	0.50	1.15	IV
M1···M3	-0.59	8.78	0.27	0.45	III
M1···M4	-0.92	11.17	0.42	0.57	III
M1···M5	-1.08	22.61	0.49	1.15	IV
M1···M6	-0.57	8.78	0.26	0.45	III
M1···M7	-0.92	11.17	0.42	0.57	III
M1···M8	-1.12	13.8	0.51	0.70	III
M1···M9	-1.12	13.8	0.51	0.70	III
M1···M10	-2,48	23,64	1,13	1,20	III
M1···M11	-2.48	23.64	1.13	1.20	III
M1···M12	-0.64	2.42	0.29	0.12	III
M1···M13	-0.64	2.42	0.29	0.12	III
M1···M14	-9.86	68.42	4.50	3.48	II
M1···M15	-9.86	68.42	4.50	3.48	II
M1···M16	-0.85	6.4	0.39	0.33	III
M1···M17	-0.85	6.4	0.39	0.33	III

Table S5. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **5**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	NG$_{(M1\cdots Mn)}$	NC$_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-0.41	9.08	0.14	0.36	III
M1···M3	-4.03	39.16	1.40	1.56	III
M1···M4	-0.87	13.9	0.30	0.55	III
M1···M5	-0.44	14.61	0.15	0.58	III
M1···M6	-1.97	21.63	0.69	0.86	III
M1···M7	-0.88	13.9	0.30	0.55	III
M1···M8	-1.91	18.78	0.66	0.75	III
M1···M9	-1.97	19.58	0.68	0.78	III
M1···M10	-3.23	34.74	1.12	1.39	III
M1···M11	-0.56	8.47	0.19	0.34	III
M1···M12	-0.55	8.47	0.19	0.34	III
M1···M13	-2.48	21.17	0.86	0.84	III
M1···M14	-10.48	63.63	3.65	2.54	II
M1···M15	-10.49	63.63	3.65	2.54	II

Table S6. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **6**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	$NG_{(M1\cdots Mn)}$	$NC_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-0.49	11.04	0.21	0.57	III
M1···M3	-1.22	12.52	0.52	0.65	III
M1···M4	-1.33	15.8	0.56	0.82	III
M1···M5	-3.19	19.57	1.35	1.02	III
M1···M6	-3.19	19.57	1.35	1.02	III
M1···M7	-1.33	15.8	0.56	0.82	III
M1···M8	-0.49	5.72	0.21	0.30	III
M1···M9	-0.49	5.72	0.21	0.30	III
M1···M10	-0.49	11.04	0.21	0.57	III
M1···M11	-1.22	12.52	0.52	0.65	III
M1···M12	-1.02	13.32	0.43	0.69	III
M1···M13	-2.59	21.78	1.10	1.13	III
M1···M14	-10.33	65.93	4.38	3.42	II
M1···M15	-10.33	62.65	4.38	3.25	II
M1···M16	-0.57	9.46	0.24	0.49	III
M1···M17	-1.02	13.32	0.43	0.69	III
M1···M18	-2.59	21.78	1.10	1.13	III
M1···M19	-0.57	9.46	0.24	0.49	III

Table S7. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **7**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	$NG_{(M1\cdots Mn)}$	$NC_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-1.22	11.85	0.51	0.97	III
M1···M3	-0.45	10.24	0.19	0.84	III
M1···M4	-1.39	16.3	0.58	1.33	IV
M1···M5	-3.21	19.81	1.34	1.62	III
M1···M6	-3.21	19.81	1.34	1.62	III
M1···M7	-1.39	16.3	0.58	1.33	IV
M1···M8	-0.62	5.74	0.26	0.47	III
M1···M9	-0.62	5.74	0.26	0.47	III
M1···M10	-0.45	10.24	0.19	0.84	IV
M1···M11	-1.22	11.85	0.51	0.97	III
M1···M12	-0.98	13.54	0.41	1.11	IV
M1···M13	-2.62	22.53	1.09	1.84	IV
M1···M14	-10.47	65.16	4.37	5.32	II
M1···M15	-10.47	64.95	4.37	5.31	II
M1···M16	-0.62	10.14	0.26	0.83	IV
M1···M17	-0.98	13.54	0.41	1.11	IV

M1···M18	-2.62	22.53	1.09	1.84	IV
M1···M19	-0.62	10.14	0.26	0.83	IV

Table S8. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **8**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	$NG_{(M1\cdots Mn)}$	$NC_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-2.77	26.43	0.73	0.98	III
M1···M3	-0.71	6.84	0.19	0.25	III
M1···M4	-3.39	27.29	0.89	1.01	III
M1···M5	-3.39	27.29	0.89	1.01	III
M1···M6	-0.71	6.84	0.19	0.25	III
M1···M7	-2.77	26.43	0.73	0.98	III
M1···M8	-2.05	19.75	0.54	0.73	III
M1···M9	-2.08	19.75	0.55	0.73	III
M1···M10	-2.55	29.96	0.67	1.11	III
M1···M11	-2.55	29.96	0.67	1.11	III
M1···M12	-0.71	7.85	0.19	0.29	III
M1···M13	-0.47	4.87	0.12	0.18	III
M1···M14	-14.53	80.83	3.83	2.99	II
M1···M15	-14.45	64.45	3.81	2.38	II

Table S9. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **9**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	$NG_{(M1\cdots Mn)}$	$NC_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-0.36	5.75	0.12	0.29	III
M1···M3	-0.69	12.3	0.23	0.61	III
M1···M4	-2.68	18.75	0.90	0.93	III
M1···M5	-3.14	17.85	1.05	0.89	III
M1···M6	-0.69	12.3	0.23	0.61	III
M1···M7	-4.52	34.5	1.51	1.71	III
M1···M8	-0.99	11.86	0.33	0.59	III
M1···M9	-0.93	7.48	0.31	0.37	III
M1···M10	-3.14	17.58	1.05	0.87	III
M1···M11	-2.68	18.75	0.90	0.93	III
M1···M12	-0.93	7.48	0.31	0.37	III
M1···M13	-1.02	9.77	0.34	0.48	III
M1···M14	-10.05	54	3.36	2.68	II
M1···M15	-10.05	54	3.36	2.68	II

Table S10. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **10**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	$NG_{(M1\cdots Mn)}$	$NC_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-0.16	3.38	0.05	0.17	III
M1···M3	-0.65	12.26	0.21	0.61	III
M1···M4	-3	19.02	0.99	0.94	III
M1···M5	-3.31	17.53	1.09	0.87	III
M1···M6	-0.65	12.26	0.21	0.61	III
M1···M7	-3.42	33.65	1.12	1.66	III
M1···M8	-0.65	12.57	0.21	0.62	III
M1···M9	-0.86	7.48	0.28	0.37	III
M1···M10	-3.31	17.53	1.09	0.87	III
M1···M11	-3	19.02	0.99	0.94	III
M1···M12	-0.86	7.48	0.28	0.37	III
M1···M13	-1.01	9.82	0.33	0.48	III
M1···M14	-10.86	55.75	3.57	2.75	II
M1···M15	-10.86	55.75	3.57	2.75	II

Table S11. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **11**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	$NG_{(M1\cdots Mn)}$	$NC_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-1.49	21.44	0.49	1.02	IV
M1···M3	-0.79	11.22	0.26	0.53	III
M1···M4	-2.98	19.18	0.98	0.91	III
M1···M5	-2.98	19.18	0.98	0.91	III
M1···M6	-0.79	11.22	0.26	0.53	III
M1···M7	-1.49	21.44	0.49	1.02	IV
M1···M8	-1.05	3.1	0.34	0.15	III
M1···M9	-1.05	3.1	0.34	0.15	III
M1···M10	-0.71	7.78	0.23	0.37	III
M1···M11	-0.71	7.78	0.23	0.37	III
M1···M12	-3.44	20.99	1.13	1.00	III
M1···M13	-3.44	20.99	1.13	1.00	III
M1···M14	-10.92	63.91	3.58	3.03	II
M1···M15	-10.92	63.91	3.58	3.03	II

Table S12. Energy of M1···Mn and contact surface of M1···Mn for the supramolecular cluster of compound **12**.

	$G_{M1\cdots Mn}$ (kcal.mol^{-1})	$C_{M1\cdots Mn}$ (Å^2)	NG$_{(M1\cdots Mn)}$	NC$_{(M1\cdots Mn)}$	Inter. Type
M1···M2	-0.82	7.62	0.28	0.40	III
M1···M3	-2.25	12.58	0.76	0.67	III
M1···M4	-0.82	7.62	0.27	0.40	III
M1···M5	-3.50	23.19	1.17	1.23	III
M1···M6	-1.20	12.49	0.40	0.66	III
M1···M7	-2.62	22.44	0.88	1.19	III
M1···M8	-2.62	22.44	0.88	1.19	III
M1···M9	-0.94	6.83	0.32	0.36	III
M1···M10	-0.94	6.83	0.32	0.36	III
M1···M11	-1.2	12.49	0.40	0.66	III
M1···M12	-2.25	12.58	0.75	0.67	III
M1···M13	-3.50	23.19	1.17	1.23	III
M1···M14	-9.53	47.04	3.20	2.49	II
M1···M15	-9.53	47.04	3.20	2.49	II

Table S13. Data collection and structure refinement for compounds **1-3**.

Compound	**1**	**2**	**3**
Empirical formula	$C_9H_8Cl_3N_3$	$C_{11}H_{12}Cl_3N_3$	$C_8H_5BrCl_3N_3$
Molecular weight	264.53	292.59	329.41
CCDC	1056486	1056487	1056488
Temperature (K)	293(2) K	293(2) K	293(2) K
Wavelenght (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1$
a (Å)	10.3016(7)	11.2451(8)	7.4329(2)
b (Å)	16.0564(11)	5.8697(4)	6.7756(2)
c (Å)	6.8555(6)	20.9201(16)	11.1667(3)
α (deg)	90	90	90
β (deg)	93.098(5)	104.896(5)	90.2760(10)
γ (deg)	90	90	90
Volume (Å^3)	1132.29(15)	1334.43(17)	562.37(3)
Z/density (calcd)(mg/m^3)	4/ 1.552	4/ 1.456	2/ 1.945
Absorption coefficient (mm^{-1})	0.778	0.667	4.334
F(000)	536	600	320
Crystal size (mm)	0.28 x 0.04 x 0.02	0.880 x 0.328 x 0.158	0.340 x 0.337 x 0.162
θ range for data collection (deg)	3.96 to 28.80	1.87 to 28.40	2.74 to 28.40
Reflections collected/unique	12894 / 2780 [R(int) = 0.0662]	13171 / 3314 [R(int) = 0.0292]	5503 / 2653 [R(int) = 0.0197]
Completeness to θ (%)	94	99.6 %	99.6
Absorption correction	Gaussian	Gaussian	Gaussian
Max. and min. transmission	1.000000 and 0.503699	0.92276 and 0.79327	0.496 and 0.250
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	2421 / 0 / 167	3314 / 0 / 154	2653 / 1 / 136
Goodness-of-fit on F^2	1.069	1.100	1.063
Final R indices [$I \geq 2\sigma(I)$][a]	R1 = 0.0686, wR2 = 0.2105	R1 = 0.0361, wR2 = 0.1069	R1 = 0.0362, wR2 = 0.0954
R_1 (all data)[a]	R1 = 0.0974, wR2 = 0.2401	R1 = 0.0576, wR2 = 0.1361	R1 = 0.0482, wR2 = 0.1008
Larges diff. peak and hole (e A^{-3})	0.340 and -0.334	0.512 and -0.460	0.460 and -0.808

Table S14. Data collection and structure refinement for compounds **4**-**6**.

Compound	**4**	**5**	**6**
Empirical formula	$C_9H_7BrCl_3N_3$	$C_{15}H_{12}F_3N_3$	$C_{14}H_9ClF_3N_3$
Molecular weight	343.44	291.28	311.69
CCDC	1056489	1056490	1056491
Temperature (K)	293(2)	293(2)	293(2)
Wavelenght (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Orthorhombic
Space group	$P2_1$	P -1	$P2_12_12_1$
a (Å)	9.6363(3)	4.8715(2)	4.7929(4)
b (Å)	6.9353(2)	11.2655(5)	10.5914(9)
c (Å)	9.8541(3)	13.5584(6)	26.224(2)
α (deg)	90	110.225(3)	90
β (deg)	111.240(2)	96.808(3)	90
γ (deg)	90	99.835(3)	90
Volume (Å^3)	613.82(3)	675.13(5)	1331.22(19)
Z/density (calcd)(mg/m^3)	2/ 1.858	2/ 1.433	4/ 1.555
Absorption coefficient (mm^{-1})	3.975	0.117	0.318
F(000)	336	300	632
Crystal size (mm)	0.858 x 0.295 x 0.166	0.980 x 0.212 x 0.197	0.752 x 0.148 x 0.109
θ range for data collection (deg)	2.22 to 28.26	1.63 to 29.66	1.55 to 27.30
Reflections collected/unique	6092 / 2998 [R(int) = 0.0199]	16787 / 3757 [R(int) = 0.0395]	20143 / 2967 [R(int) = 0.0347]
Completeness to θ (%)	99.9	98.7	99.4
Absorption correction	Gaussian	Gaussian	Gaussian
Max. and min. transmission	0.59927 and 0.26415	1.000000 and 0.894762	0.98976 and 0.9698
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	2998 / 1 / 145	3757 / 0 / 190	2967 / 0 / 190
Goodness-of-fit on F^2	1.073	1.050	1.026
Final R indices [$I \geq 2\sigma(I)$][a]	R1 = 0.0416, wR2 = 0.1250	R1 = 0.0570, wR2 = 0.1815	R1 = 0.0367, wR2 = 0.0766
R_1 (all data)[a]	R1 = 0.0579, wR2 = 0.1356	R1 = 0.0985, wR2 = 0.2270	R1 = 0.0642, wR2 = 0.0878
Larges diff. peak and hole (e A^{-3})	0.510 and -0.792	0.399 and -0.447	0.171 and -0.139

Table S15. Data collection and structure refinement for compounds **7**-**9**.

Compound	**7**	**8**	**9**
Empirical formula	$C_{14}H_9BrF_3N_3$	$C_{18}H_{12}F_3N_3$	$C_{13}H_{11}N_3$
Molecular weight	356.15	327.31	209.25
CCDC	734998	914143	734999
Temperature (K)	293(2)	293(2)	293(2)
Wavelenght (Å)	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group	$P2_12_12_1$	$P2_1/n$	$P2_1/n$
a (Å)	4.7574(7)	7.8462(5)	3.9185(3)
b (Å)	11.0476(17)	11.2089(9)	10.5324(10)
c (Å)	26.177(5)	16.8641(12)	25.539(2)
α (deg)	90	90	90
β (deg)	90	92.389(5)	90.642(3)
γ (deg)	90	90	90
Volume ($Å^3$)	1375.8(4)	1481.86(18)	1053.97(16)
Z/density (calcd)(mg/m^3)	4/ 1.719	4/ 1.467	4/ 1.319
Absorption coefficient (mm^{-1})	3.018	0.115	0.082
F(000)	704	672	440
Crystal size (mm)	0.758 x 0.088 x 0.05	0.42 x 0.08 x 0.08	0.67 x 0.16 x 0.09
θ range for data collection (deg)	2.00 to 27.36	2.18 to 30.08	2.09 to 27.15
Reflections collected/unique	13211 / 3093 [R(int) = 0.0623]	23457 / 4299 [R(int) = 0.0735]	9242 / 2310 [R(int) = 0.0446]
Completeness to θ (%)	99.4	98.8	99.3
Absorption correction	Gaussian	Gaussian	Gaussian
Max. and min. transmission	0.9330 and 0.5595	0.9908 and 0.9531	0.99490 and 0.97605
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	2998 / 1 / 145	4299 / 0 / 217	2310 / 0 / 146
Goodness-of-fit on F^2	1.008	0.954	1.034
Final R indices [$I \geq 2\sigma(I)$][a]	R1 = 0.0442, wR2 = 0.0991	R1 = 0.0535, wR2 = 0.1099	R1 = 0.0515, wR2 = 0.1373
R_1 (all data)[a]	R1 = 0.0905, wR2 = 0.1263	R1 = 0.1910, wR2 = 0.1521	R1 = 0.0931, wR2 = 0.1630
Larges diff. peak and hole (e A^{-3})	0.280 and -0.391	0.200 and -0.161	0.281 and -0.186

Table S16. Data collection and structure refinement for compounds **10**-**12**.

Compound	**10**	**11**	**12**
Empirical formula	$C_{13}H_{10}FN_3$	$C_{13}H_{10}BrN_3$	$C_{12}H_{10}N_4$
Molecular weight	227.24	288.15	210.24
CCDC	735000	735001	735002
Temperature (K)	293(2)	293(2)	296(2)
Wavelenght (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	$P2_1/n$	$P2_1$	$P2_12_12_1$
a (Å)	3.8161(2)	3.91340(10)	4.0774(3)
b (Å)	10.6532(5)	10.8096(2)	12.7591(6)
c (Å)	25.8317(12)	13.8568(3)	19.5223(9)
α (deg)	90	90	90
β (deg)	90.724(3)	96.9070(10)	90
γ (deg)	90	90	90
Volume (Å^3)	1050.07(9)	581.92(2)	1015.63(10)
Z/density (calcd)(mg/m^3)	4/ 1.437	2/ 1.645	4/ 1.375
Absorption coefficient (mm^{-1})	0.101	3.511	0.088
F(000)	472	288	440
Crystal size (mm)	0.22 x 0.12 x 0.09	0.608 x 0.094 x 0.074	0.67 x 0.20 x 0.08
θ range for data collection (deg)	1.58 to 26.72	2.96 to 29.57	3.51 to 29.53
Reflections collected/unique	8925 / 2199 [R(int) = 0.0587]	6214 / 3182 [R(int) = 0.0296]	11517 / 2819 [R(int) = 0.0565]
Completeness to θ (%)	98.6	98.9	98.8
Absorption correction	Gaussian	Gaussian	Gaussian
Max. and min. transmission	0.9909 and 0.9780	0.86209 and 0.48773	0.99490 and 0.97605
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	2199 / 0 / 155	3182 / 1 / 155	2819 / 0 / 146
Goodness-of-fit on F^2	1.038	1.042	0.954
Final R indices [$I \geq 2\sigma(I)$][a]	R1 = 0.0553, wR2 = 0.1472	R1 = 0.0465, wR2 = 0.1056	R1 = 0.0492, wR2 = 0.1217
R_1 (all data)[a]	R1 = 0.1022, wR2 = 0.1941	R1 = 0.0759, wR2 = 0.1173	R1 = 0.1078, wR2 = 0.1458
Larges diff. peak and hole (e A^{-3})	0.394 and -0.356	0.373 and -0.298	0.149 and -0.168