Electronic Supporting information file for

Energetic and Topological Supramolecular Study and Nucleation Proposal of Halogenated Aryl Amides

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Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	N2-H2A···O1 N1-H1A..O2	-15,09	-14,56	13,43	4,25	0,97	I
m1···m3	F2···H26-C26	-0,18	-0,07	2,74	0,02	0,20	III
m1···m4	F2···H16-C16	-1,63	-1,36	15,69	0,40	1,14	IV
m1···m5	C24-H24···F1	-1,53	-1,25	11,63	0,37	0,84	III
m1···m6	C26-H26-F2	-0,18	-0,07	2,74	0,02	0,20	III
m1···m7	C27-H27···π1	-3,04	-2,60	20,89	0,76	1,52	IV
m1···m8	O2···H26-C26	-1,99	-1,70	15	0,50	1,09	IV
m1···m9	π2···H15-C15	-2,74	-2,54	14,3	0,74	1,04	III
m1···m10	C24-H24···O1	-3,22	-3,00	8,62	0,87	0,63	III
m1···m11	O2···H2B-N2 π2···π2	-8,73	-8,28	23,41	2,42	1,70	II
m1···m12	N1-H1B···H1A-N1	0,82	0,98	4,57	0,29	0,33	III
m1···m13	N2-H2B···O2 π2···π2	-8,73	-8,28	23,41	2,42	1,70	II
m1···m14	C26-H26···O2	-1,99	-1,70	15	0,50	1,09	IV
m1···m15	C16-H16···π2	-3,90	-3,53	21,48	1,03	1,56	II

Table S1. Energy and contact surface of the interactions on compound 1A supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	N1-H1A···O2 O1···H2A-N2	-15,09	-14,56	13,43	3,67	0,91	I
m1···m3	F1···H24-C24	-1,60	-1,25	11,63	0,32	0,78	III
m1···m4	F1···H14-C14 C14-H14···F1	-2,20	-1,78	13,89	0,45	0,94	III
m1···m5	C15-H15···π2	-2,81	-2,54	14,3	0,64	0,97	III
m1···m6	C16-H16···F2	-1,71	-1,35	15,69	0,34	1,06	IV
m1···m7	C16-H16···π2	-3,90	-3,53	21,84	0,89	1,47	IV
m1···m8	O1···H25-C25	-3,29	-3,00	8,62	0,76	0,58	III
m1···m9	π1···π2	-4,73	-4,20	16,99	1,06	1,15	II
m1···m10	O1···H2B-N2 π1···π2	-8,10	-7,47	22,31	1,88	1,51	II
m1···m11	N1-H1B···H1A-N1	0,82	0,98	4,57	0,25	0,31	III
m1···m12	N1-H1B···O1 π1···π1	-8,10	-7,47	22,31	1,88	1,51	II
m1···m13	π1···H27-C27	-3,04	-2,60	20,89	0,66	1,41	IV
m1···m14	O1···H1A-N1 N1-H1A···O1	-3,14	-2,75	6,13	0,69	0,41	III

Table S2. Energy and contact surface of the interactions on compound 1B supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N1 N1-H1A···O1	-13,29	-12,72	12,38	3,21	0,85	I
m1···m3	C7-H7···π	-4,85	-3,97	19,64	1,00	1,35	II
m1···m4	C6-H6···H6-C6	-0,78	-0,16	14,01	0,04	0,96	IV
m1···m5	C5-H5···O1	-3,34	-2,86	11,61	0,72	0,80	III
m1···m6	C4-H4···O1	-4,90	-4,20	14,9	1,06	1,02	II
m1···m7	O1···H5-C5	-3,71	-2,85	11,61	0,72	0,80	III
m1···m8	O1···H4-C4	-4,83	-4,20	14,9	1,06	1,02	II
m1···m9	Others	-2,02	-1,54	7,68	0,39	0,53	III
m1···m10	C4-H4···H1A-N1	-0,55	0,16	8,73	0,04	0,60	IV
m1···m11	O1···H1B-N1 π···π	-11,12	-10,06	28,58	2,54	1,97	II
m1···m12	N1-H1A···H1B-N1	0,49	0,82	2,57	0,21	0,18	III
m1···m13	N1-H1B···O1 π···π	-10,91	-10,06	28,58	2,54	1,97	II
m1···m14	π···H7-C7	-4,93	-3,96	19,64	1,00	1,35	II
m1···m15	C4-H4···H1A-N1	-0,30	0,16	8,73	0,04	0,60	IV

Table S3. Energy and contact surface of the interactions on compound 2 supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N1 N1-H1A···O1	-12,36	-12,12	11,95	2,93	0,82	I
m1···m3	C7-H7···H5-C5	-0,22	-0,32	12,7	0,08	0,88	IV
m1···m4	C6-H6···N1	-4,23	-4,21	18,11	1,02	1,25	II
m1···m5	C5-H5···O1	-2,35	-2,40	8,94	0,58	0,62	III
m1···m6	C4-H4···Br1 Br1···H4-C4	-2,33	-2,32	11,49	0,56	0,79	III
m1···m7	Br1···π	-2,69	-2,67	8,84	0,64	0,61	III
m1···m8	O1···H5-C5	-2,47	-2,40	8,94	0,58	0,62	III
m1···m9	π···Br1	-2,72	-2,67	8,84	0,64	0,61	III
m1···m10	Others	-0,02	-0,32	12,7	0,08	0,88	IV
m1···m11	O1···H1B-N π···π	-10,61	-10,41	27,91	2,51	1,92	II
m1···m12	N1-H1A···H1B-N1	0,98	0,86	5,3	0,21	0,37	III
m1···m13	N-H1B···O1 π···π	-10,64	-10,41	27,91	2,51	1,92	II
m1···m14	Br1···H5-C5 C5-H5···Br1	-4,37	-4,40	21,37	1,06	1,47	II
m1···m15	O1···H6-C6	-4,20	-4,21	18,11	1,02	1,25	II

Table S4. Energy and contact surface of the interactions on compound 3 supramolecular cluster

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N N-H1A···O1	-13.19	-12.68	12.23	2.95	0.82	I
m1···m3	N-H1B···H5-C5	-0.64	-0.33	13.12	0.08	0.88	IV
m1···m4	C6-H6···O1	-4.61	-4.21	18.65	0.98	1.25	III
m1···m5	C5-H5···O1	-3.02	-2.38	9.31	0.56	0.62	III
m1···m6	C4-H4···I1 I1···H4-C4	-2.24	-2.26	11.13	0.53	0.75	III
m1···m7	I1···π	-3.28	-2.89	8.95	0.67	0.60	III
m1···m8	O1···H5-C5	-2.76	-2.39	9.31	0.56	0.62	III
m1···m9	π···I1	-3.31	-2.89	8.95	0.67	0.60	III
m1···m10	C5-H5···H1B-N1	-0.90	-0.33	13.12	0.08	0.88	IV
m1···m11	O1···H1B-N π···π	-11.76	-11.18	29.25	2.60	1.96	II
m1···m12	N1-H1A···H1B-N1	0.91	1.09	5.53	0.25	0.37	III
m1···m13	N-H1B···O1 π···π	-11.76	-11.18	29.25	2.60	1.96	II
m1···m14	C5-H5···I1 I1···H5-C5	-4.17	-4.28	21.39	1.00	1.43	III
m1···m15	O1···H6-C6	-4.58	-4.21	18.65	0.98	1.25	III

Table S5. Energy and contact surface of the interactions on compound 4 supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N N-H1A···O1	-19,66	-19,20	15,02	4,77	1,11	II
m1···m3	N-H1B···H7-C7 C7-H7···H1B-N	-1,91	-1,71	12,42	0,43	0,92	III
m1···m4	C6-H6···H3-C3	-1,73	-1,55	7,74	0,38	0,57	III
m1···m5	C5-H5···π	-2,34	-2,12	12,24	0,53	0,91	III
m1···m6	F1···H5-C5	-1,34	-0,99	12,6	0,25	0,93	IV
m1···m7	C3-H3···H6-C6	-1,73	-1,55	7,74	0,38	0,57	III
m1···m8	O1···H1A-N N-H1A···O1	-6,75	-6,31	13,86	1,57	1,03	II
m1···m9	Others	-1,95	-1,62	16,98	0,40	1,26	IV
m1···m10	C5-H5···F1	-1,34	-0,99	12,6	0,25	0,93	IV
m1···m11	O1···H1B-N π···π	-10,33	-9,84	22,14	2,44	1,64	II
m1···m12	N1-H1A···H1B-N1 N1-H1B···H1A-N1	2,96	3,04	4,05	0,75	0,30	III
m1···m13	N-H1B···O1 π···π	-10,33	-9,84	22,14	2,44	1,64	II
m1···m14	π···H5-C5	-2,34	-2,12	12,24	0,53	0,91	III
m1···m15	Others	-1,95	-1,62	16,98	0,40	1,26	IV

Table S6. Energy and contact surface of the interactions on compound 5 supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N N-H1A···O1	-17,14	-16,80	15,81	4,08	1,07	II
m1···m3	N-H1B···H1A-N	0,71	0,69	6,45	0,17	0,44	III
m1···m4	C6-H6···π	-3,07	-3,01	17,22	0,73	1,17	III
m1···m5	C5-H5···H5-C5	-0,38	-0,45	3,19	0,11	0,22	III
m1···m6	Cl1···Cl1	-0,58	-0,62	2,63	0,15	0,18	III
m1···m7	C3-H3···π O1···H1B-N	-10,67	-10,35	24,19	2,51	1,64	II
m1···m8	O1···H1A-N N-H1A···O1	-4,91	-4,73	10,97	1,15	0,74	I
m1···m9	π···π	-3,58	-3,31	28,26	0,80	1,91	IV
m1···m10	Cl1···Cl1	-0,58	-0,62	5,92	0,15	0,40	III
m1···m11	π···H6-C6	-3,07	-3,01	17,22	0,73	1,17	III
m1···m12	N-H1B···H1A-N	0,71	0,69	6,45	0,17	0,44	III
m1···m13	π···H3-C3 N-H1B···O1	-10,67	-10,35	24,19	2,51	1,64	II
m1···m14	Cl1···H5-C5 C5-H5···Cl1	-2,57	-2,48	16,1	0,60	1,09	III
m1···m15	π···π	-3,58	-3,31	28,26	0,80	1,91	IV

Table S7. Energy and contact surface of the interactions on compound 6 supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N1 N1-H1A···O1	-13.02	-12.64	15.74	3.28	1.05	II
m1···m3	N1-H1B···H1A-N1	0.45	0.56	5.89	0.15	0.39	III
m1···m4	C6-H6···π	-3.00	-3.30	17.37	0.85	1.16	III
m1···m5	C5-H5···Br1 Br1···H5-C5	-2.12	-2.41	15.63	0.62	1.05	III
m1···m6	Br1···Br1	-0.46	-0.84	5.68	0.22	0.38	III
m1···m7	O1···H1B-N1 C3-H3···π	-9.51	-9.56	24.25	2.48	1.62	II
m1···m8	O1···H1A-N1 N1-H1A···O1	-5.00	-4.74	10.11	1.23	0.68	I
m1···m9	π···π	-3.82	-3.72	29.74	0.96	1.99	IV
m1···m10	C5-H5···H5-C5	-0.31	-0.54	1.84	0.14	0.12	III
m1···m11	Br1···Br1	-0.46	-0.84	5.68	0.22	0.38	III
m1···m12	π···H5-C5	-3.00	-3.30	17.37	0.85	1.16	III
m1···m13	N1-H1A···H1B-N1	0.45	0.56	5.89	0.15	0.39	III
m1···m14	π···H3-C3 N-H1B···O1	-9.51	-9.56	24.25	2.48	1.62	II
m1···m15	π···π	-3.82	-3.72	29.74	0.96	1.99	IV

Table S8. Energy and contact surface of the interactions on compound 7 supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N1 N1-H1A···O1	-17,09	-16,73	15,4	3,62	0,90	I
m1···m3	N1-H1B···H1A-N1	0,58	0,66	6,76	0,14	0,40	III
m1···m4	C6-H6···π	-3,49	-3,38	19,24	0,73	1,13	III
m1···m5	C5-H5···I1 I1···H5-C5	-2,34	-2,35	16,65	0,51	0,98	III
m1···m6	I1···I1	-1,40	-1,37	6,05	0,30	0,35	III
m1···m7	C3-H3···π O1···H1B-N1	-11,72	-11,40	26,28	2,46	1,54	II
m1···m8	O1···H1B-N1 N-H1B···O1	-4,91	-4,73	11,39	1,02	0,67	I
m1···m9	π···π	-4,11	-3,83	30,99	0,83	1,82	IV
m1···m10	I1···I1	-1,40	-1,37	6,05	0,30	0,35	III
m1···m11	π···H6-C6	-3,49	-3,38	19,24	0,73	1,13	III
m1···m12	N1-H1B···H1A-N1	0,58	0,66	6,76	0,14	0,40	III
m1···m13	π···H3-C3 N-H1B···O1	-11,74	-11,39	26,28	2,46	1,54	II
m1···m14	I1···H5-C5 C5-H5···I1	-2,34	-2,35	16,65	0,51	0,98	III
m1···m15	π···π	-4,11	-3,83	30,99	0,83	1,82	IV

Table S9. Energy and contact surface of the interactions on compound 8 supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N1 N1-H1A···O1	-16.97	-16.56	13.75	4.90	1.16	II
m1···m3	N1-H1A···H3-C3	0.43	0.52	8.50	0.15	0.72	IV
m1···m4	C4-H4···π	-2.18	-1.95	12.59	0.58	1.06	III
m1···m5	F1···F1	-0.02	0.20	5.42	0.06	0.46	III
m1···m6	F1···H6-C6	-1.89	-1.66	16.19	0.49	1.37	IV
m1···m7	O1···H1B-N1	-10.12	-9.74	15.03	2.88	1.27	II
m1···m8	O1···H4-C4 C4-H4···O1	-9.05	-8.59	25.76	2.54	2.18	II
m1···m9	C7-H7···H1A-N1	0.43	0.52	8.50	0.15	0.72	IV
m1···m10	Others	-0.66	-0.46	8.81	0.14	0.74	IV
m1···m11	π···H4-C4	-2.15	-1.95	12.59	0.58	1.06	III
m1···m12	N1-H1B···O1	-10.14	-9.72	15.03	2.88	1.27	II
m1···m13	π···π	-4.91	-4.39	24.33	1.30	2.06	II
m1···m14	C6-H6···F1	-1.89	-1.66	16.19	0.49	1.37	IV
m1···m15	Others	-0.65	-0.46	8.81	0.14	0.74	IV

Table S10. Energy and contact surface of the interactions on compound 9 supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N1 N1-H1A···O1	-8,96	-9,23	13,47	2,42	0,93	I
m1···m3	N1···H3-C3 C3-H3···N1	-0,86	-1,10	12,90	0,29	0,89	IV
m1···m4	C4-H4···O1	-3,32	-3,73	14,52	0,98	1,00	III
m1···m5	Br1···Br1	-1,44	-1,32	8,83	0,35	0,61	III
m1···m6	C6-H6···Br1	-1,10	-1,23	9,67	0,32	0,67	III
m1···m7	O1···H4-C4	-3,23	-3,73	14,52	0,98	1,00	III
m1···m8	O1···H1B-N1 N1-H1B···O1	-6,62	-6,85	12,02	1,80	0,83	I
m1···m9	Others	-2,72	-2,82	22,17	0,74	1,53	IV
m1···m10	Br1···H6-C6	-1,11	-1,23	9,67	0,32	0,67	III
m1···m11	O1···H1B-N1 π···π	-9,03	-9,33	25,51	2,45	1,76	II
m1···m12	N1-H1A···H1B-N1	1,03	0,65	2,56	0,17	0,18	III
m1···m13	N1-H1B···O1 π···π	-9,11	-9,32	25,51	2,44	1,76	II
m1···m14	Br1···Br1	-1,44	-1,32	8,83	0,35	0,61	III
m1···m15	Others	-2,73	-2,82	22,17	0,74	1,53	IV

Table S11. Energy and contact surface of the interactions on compound 11 supramolecular cluster.

Dimer	Interaction	GM1···Mn	GcM1···Mn	CM1···Mn	NG	NC	Type
m1···m2	O1···H1A-N1 N1-H1A···O1	-13.19	-12.83	14.39	3.57	1.07	II
m1···m3	C3-H3···H1B-N1	-0.45	-0.23	15.96	0.06	1.19	IV
m1···m4	C4-H4···O1	-4.04	-3.92	17.00	1.09	1.26	II
m1···m5	I1···I1	-1.85	-1.81	7.10	0.50	0.53	III
m1···m6	I1···H6-C6	-1.34	-1.33	9.56	0.37	0.71	III
m1···m7	O1···H4-C4	-4.04	-3.92	17.00	1.09	1.26	II
m1···m8	N1-H1B···O1 O1···H1B-N1	-7.42	-7.06	13.67	1.97	1.02	II
m1···m9	Others	-3.86	-3.56	23.18	0.99	1.72	IV
m1···m10	O1···H1B-N1 π···π	-8.99	-8.62	27.76	2.40	2.06	II
m1···m11	N1-H1A···H1B-N1	-0.42	-0.32	2.75	0.09	0.20	III
m1···m12	N1-H1B···O1 π···π	-8.99	-8.62	27.76	2.40	2.06	II
m1···m13	I1···I1	-1.85	-1.81	7.10	0.50	0.53	III
m1···m14	C6-H6···I1	-1.34	-1.33	9.56	0.37	0.71	III
m1···m15	Others	-3.86	-3.56	23.18	0.99	1.72	IV

Table S12. Energy and contact surface of the interactions on compound 12 supramolecular cluster.

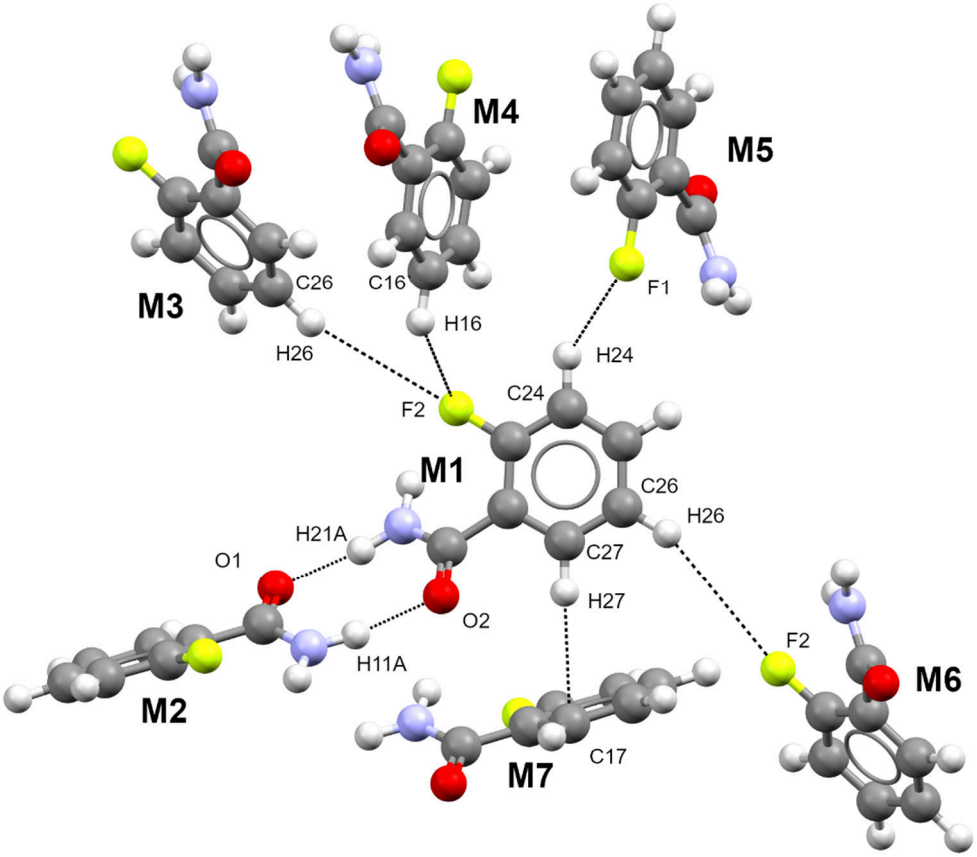

Figure S1. Central molecule with neighboring molecules in the same plane for compound 1A.

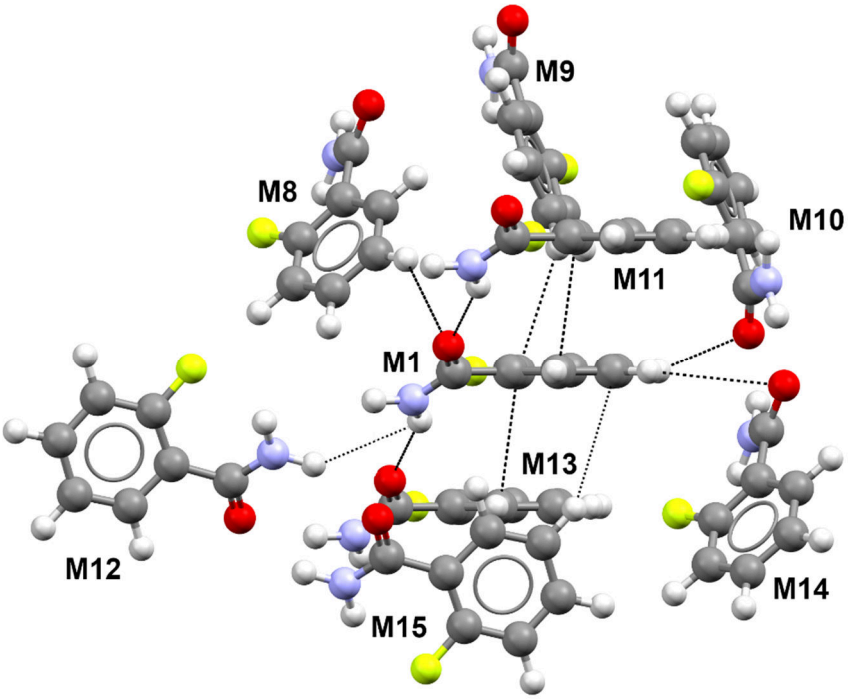

Figure S2. Central Molecule with neighboring molecules in upper and lower planes for compound 1A.

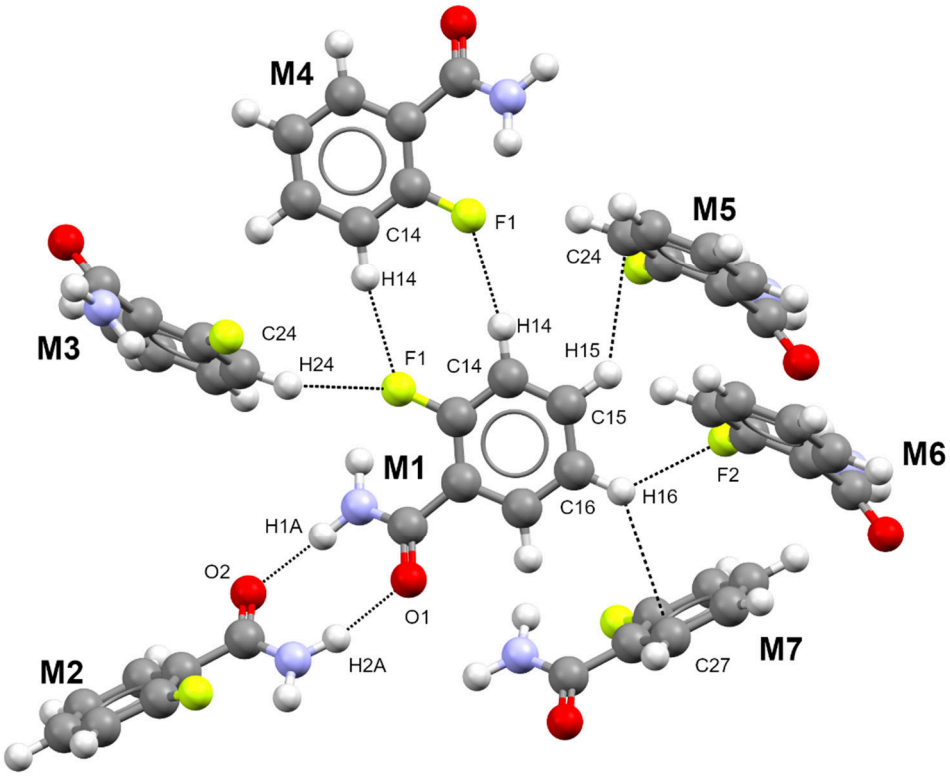

Figure S3. Central molecule with neighboring molecules in the same plane for compound 1B.

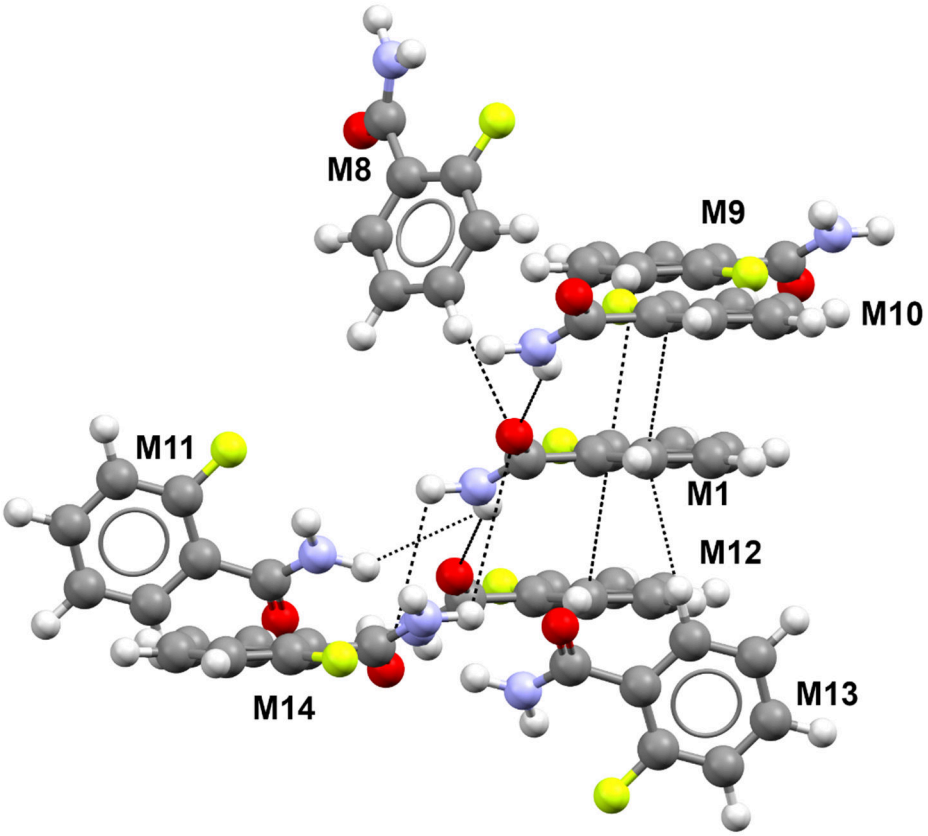

Figure S4. Central Molecule with neighboring molecules in upper and lower planes for compound 1B.

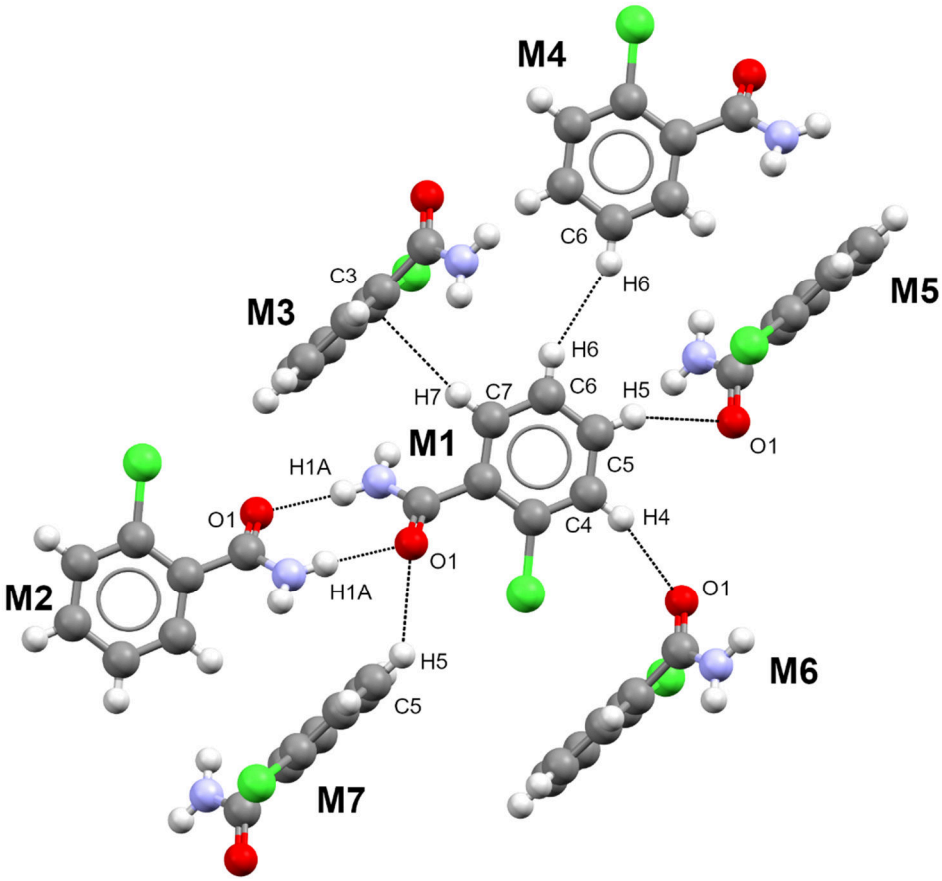

Figure S5. Central molecule with neighboring molecules in the same plane for compound 2.

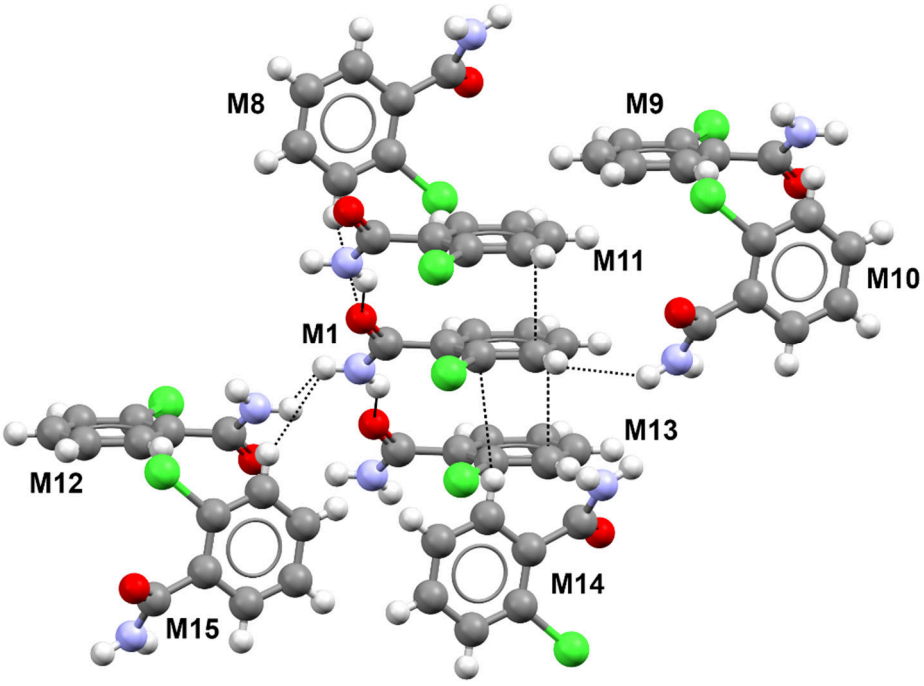

Figure S6. Central Molecule with neighboring molecules in upper and lower planes for compound 2.

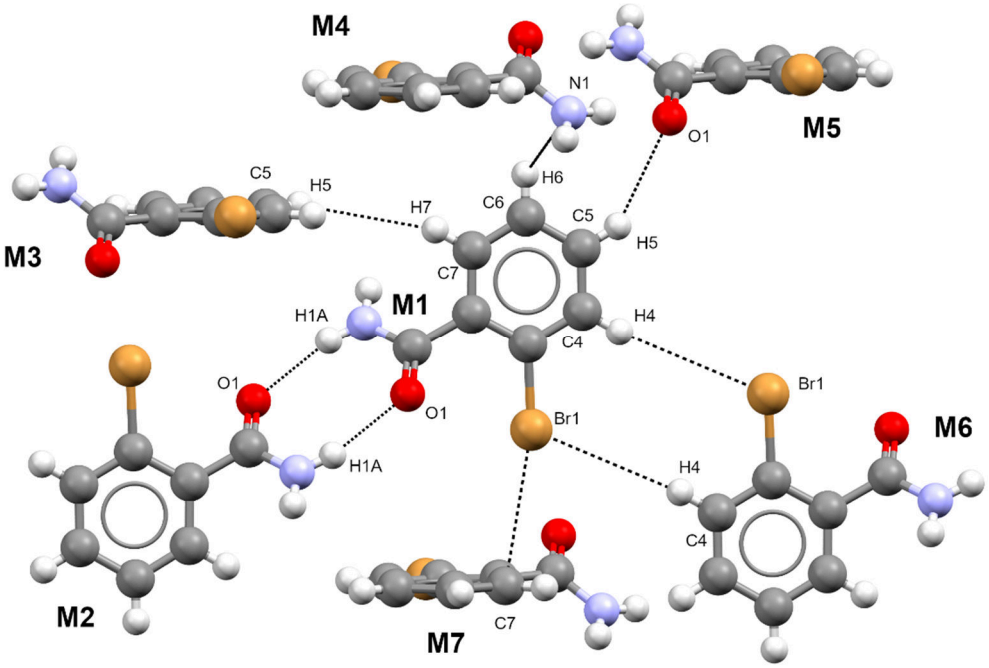

Figure S7. Central molecule with neighboring molecules in the same plane for compound 3.

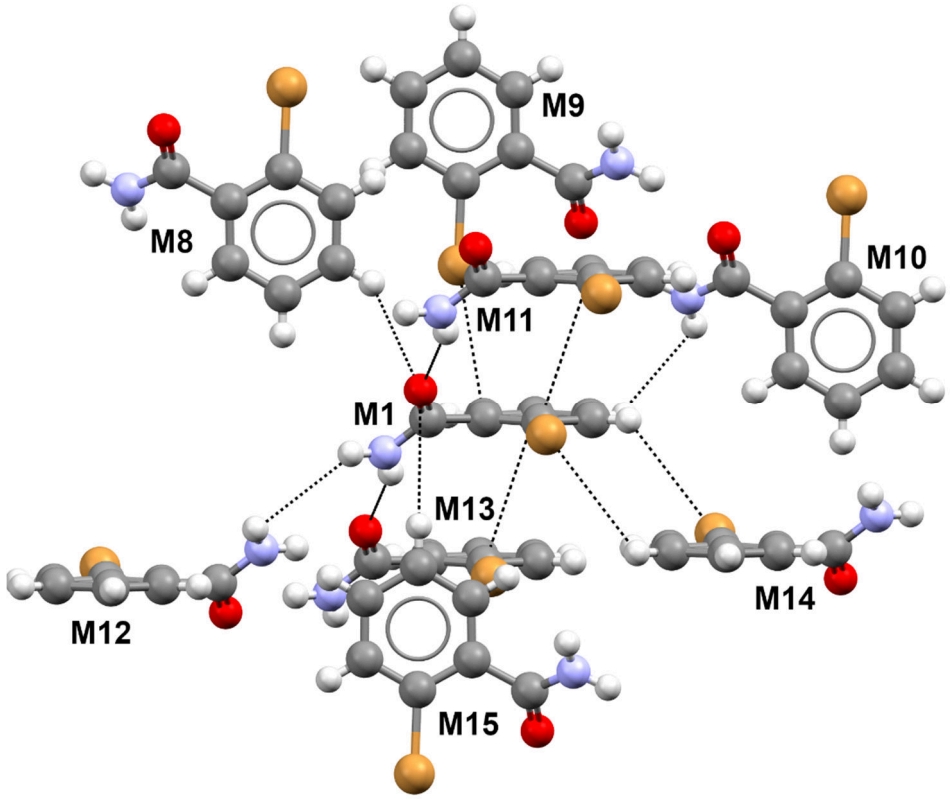

Figure S8. Central Molecule with neighboring molecules in upper and lower planes for compound 3.

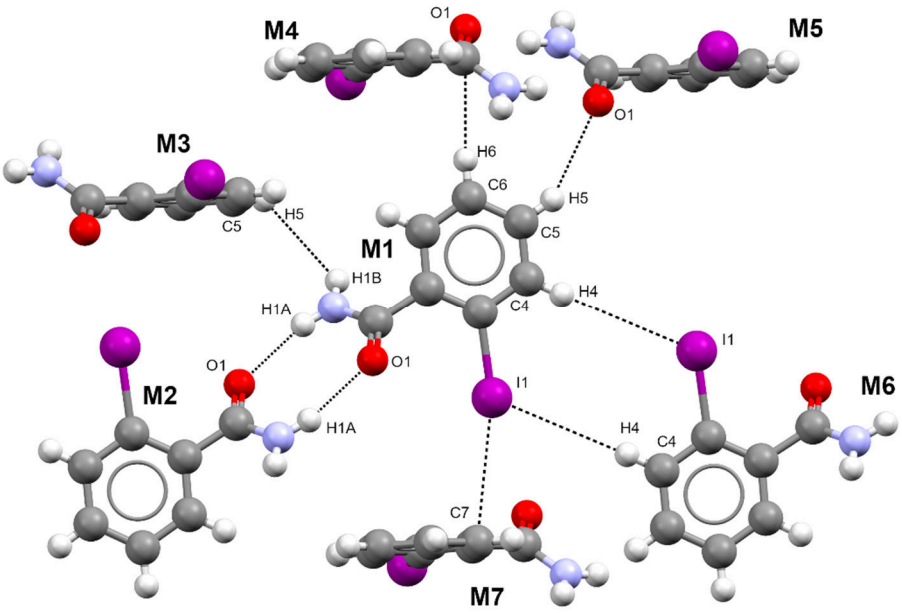

Figure S9. Central molecule with neighboring molecules in the same plane for compound 4.

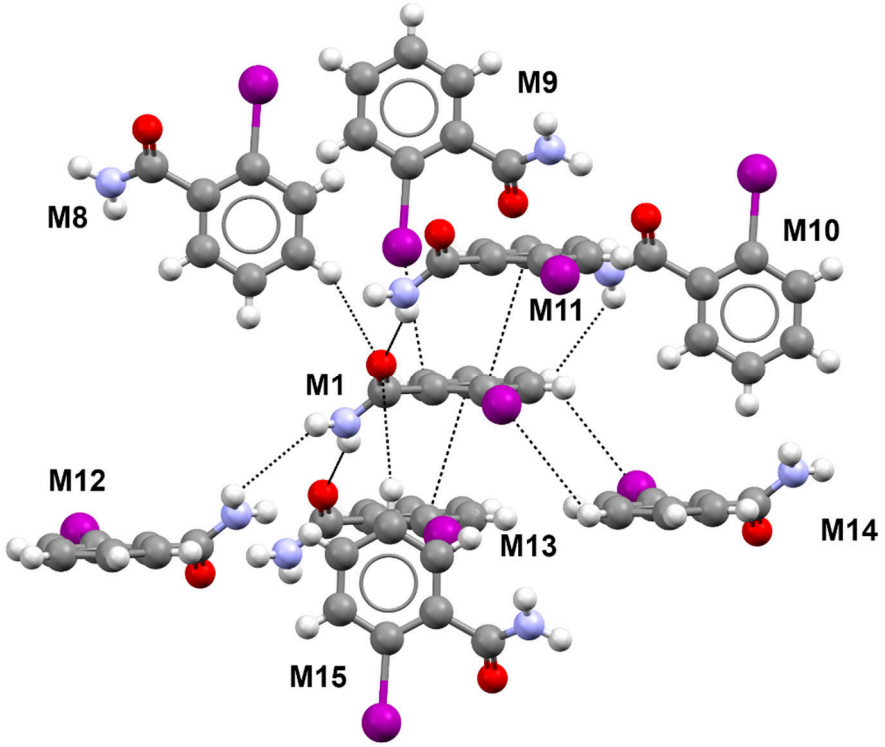

Figure S10. Central Molecule with neighboring molecules in upper and lower planes for compound 4.

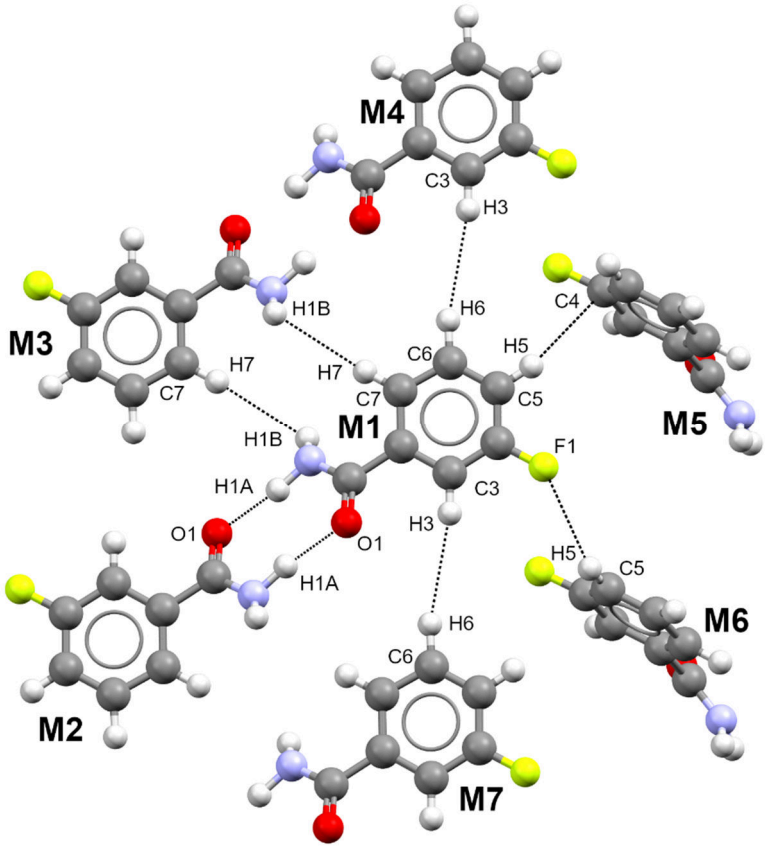

Figure S11. Central molecule with neighboring molecules in the same plane for compound 5.

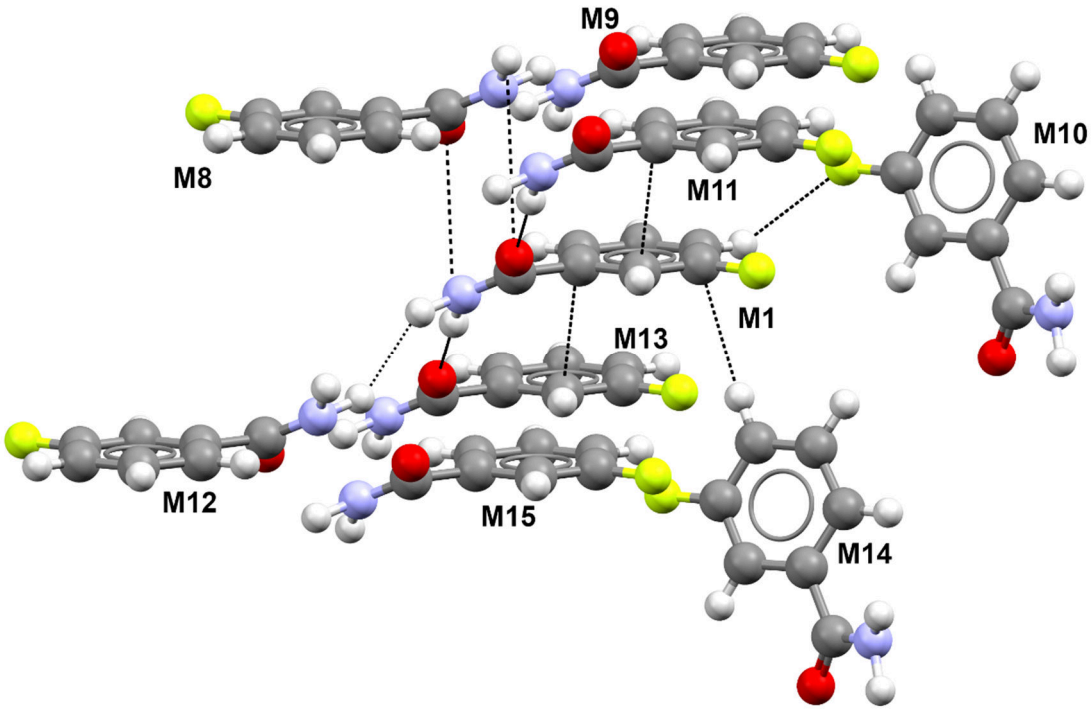

Figure S12. Central Molecule with neighboring molecules in upper and lower planes for compound 5.

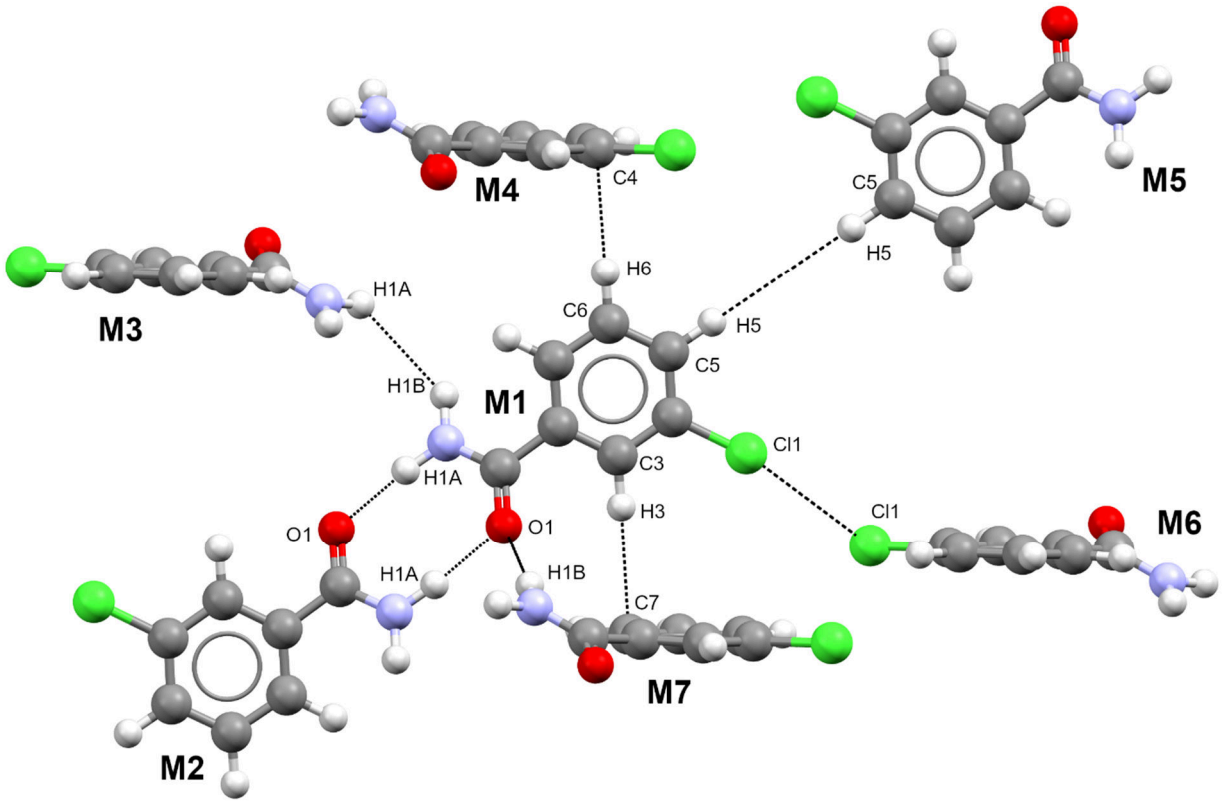

Figure S13. Central molecule with neighboring molecules in the same plane for compound 6.

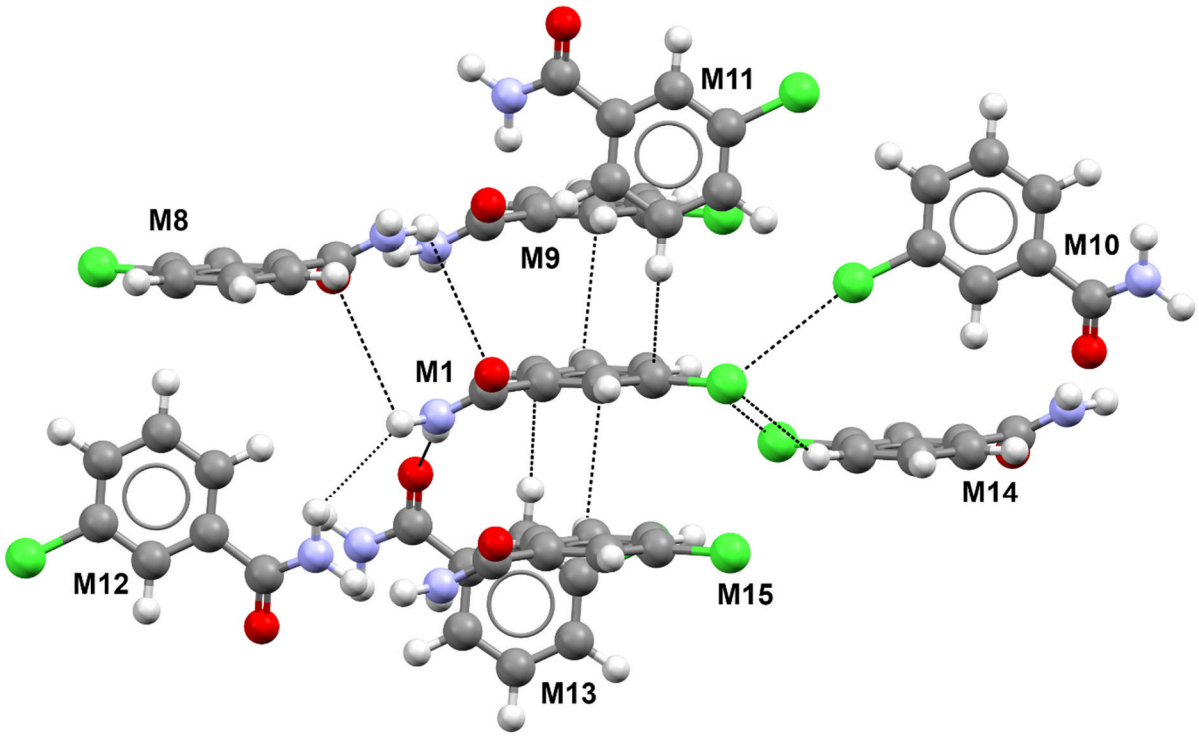

Figure S14. Central Molecule with neighboring molecules in upper and lower planes for compound 6.

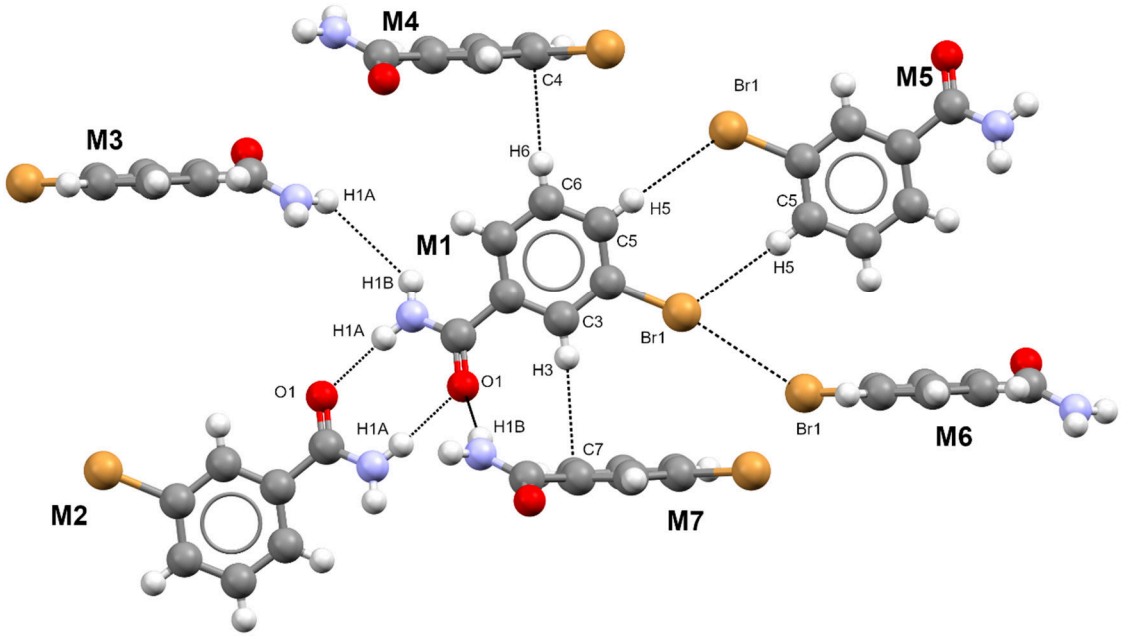

Figure S15. Central molecule with neighboring molecules in the same plane for compound 7.

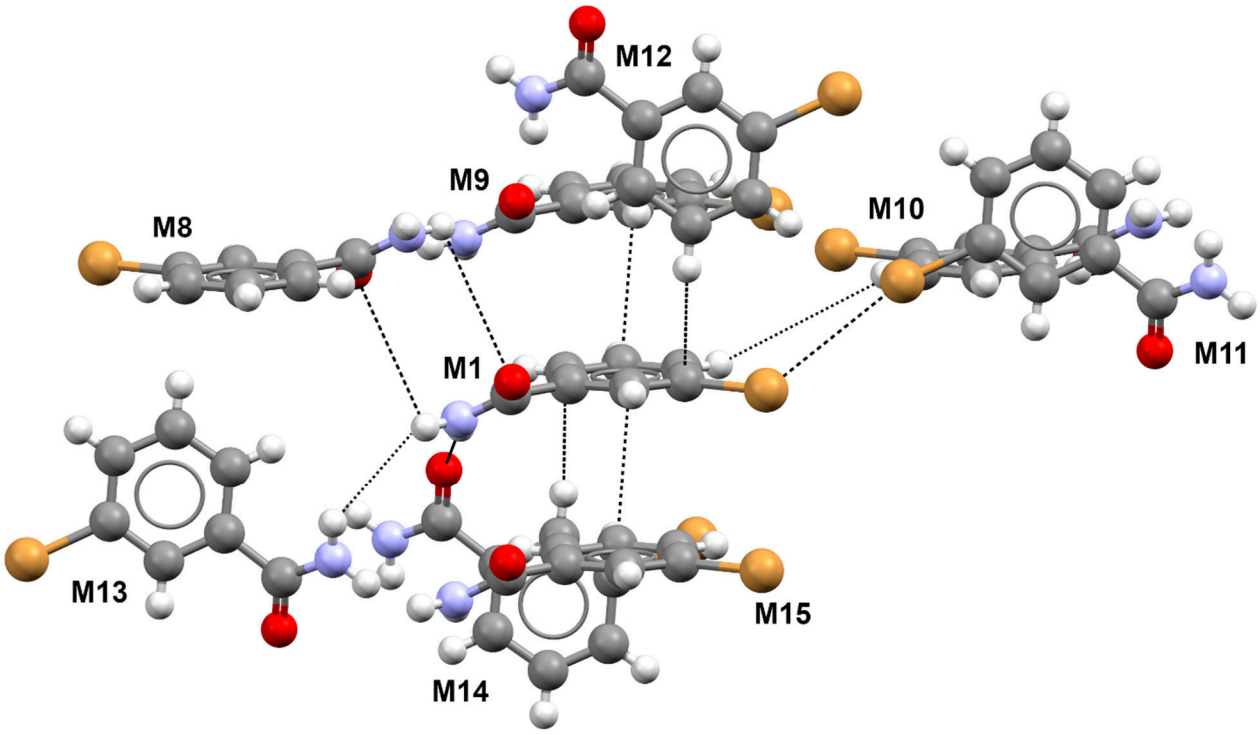

Figure S16. Central Molecule with neighboring molecules in upper and lower planes for compound 7.

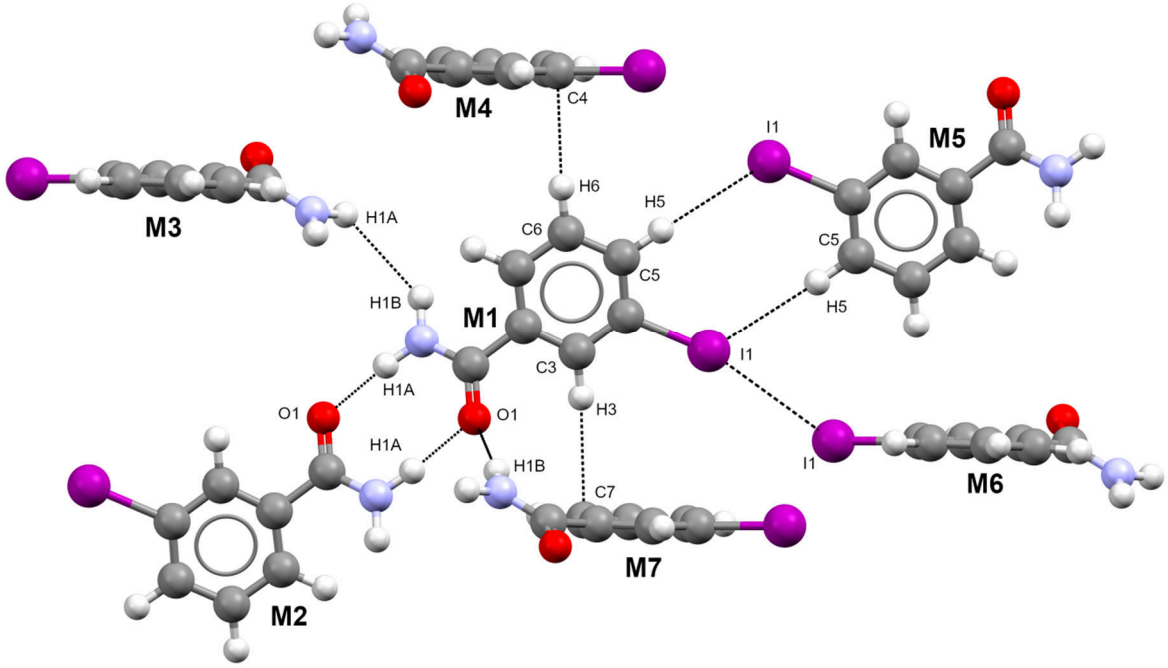

Figure S17. Central molecule with neighboring molecules in the same plane for compound 8.

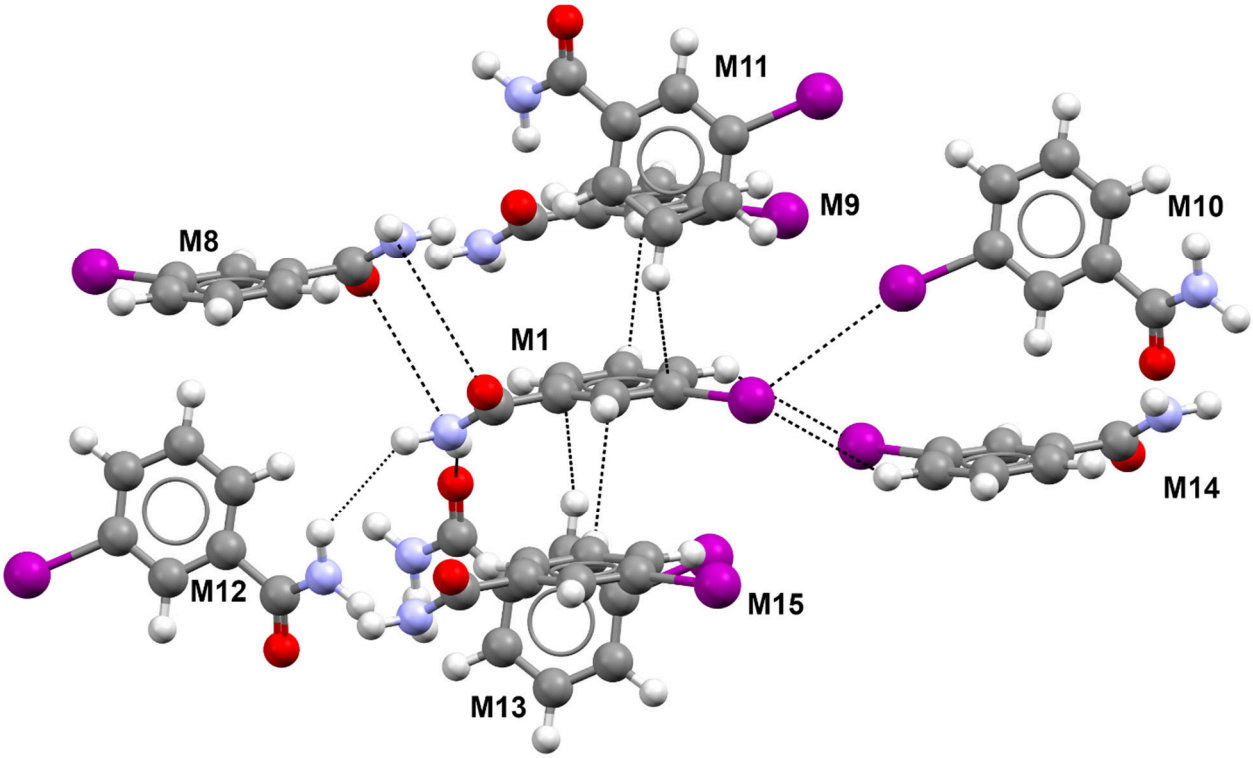

Figure S18. Central Molecule with neighboring molecules in upper and lower planes for compound 8.

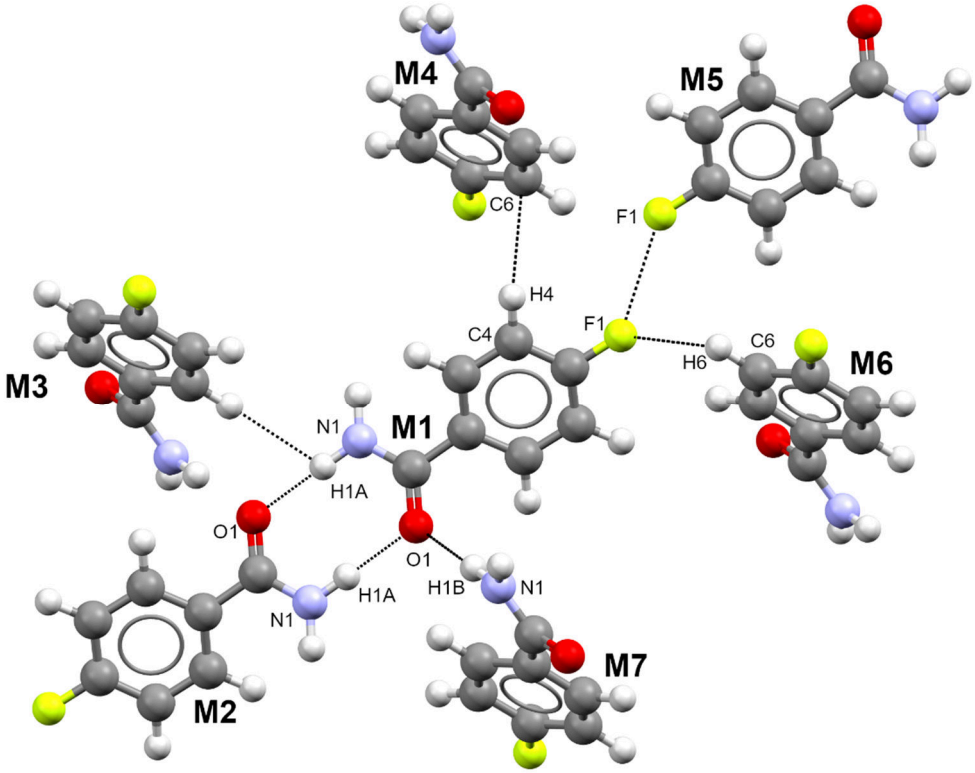

Figure S19. Central molecule with neighboring molecules in the same plane for compound 9.

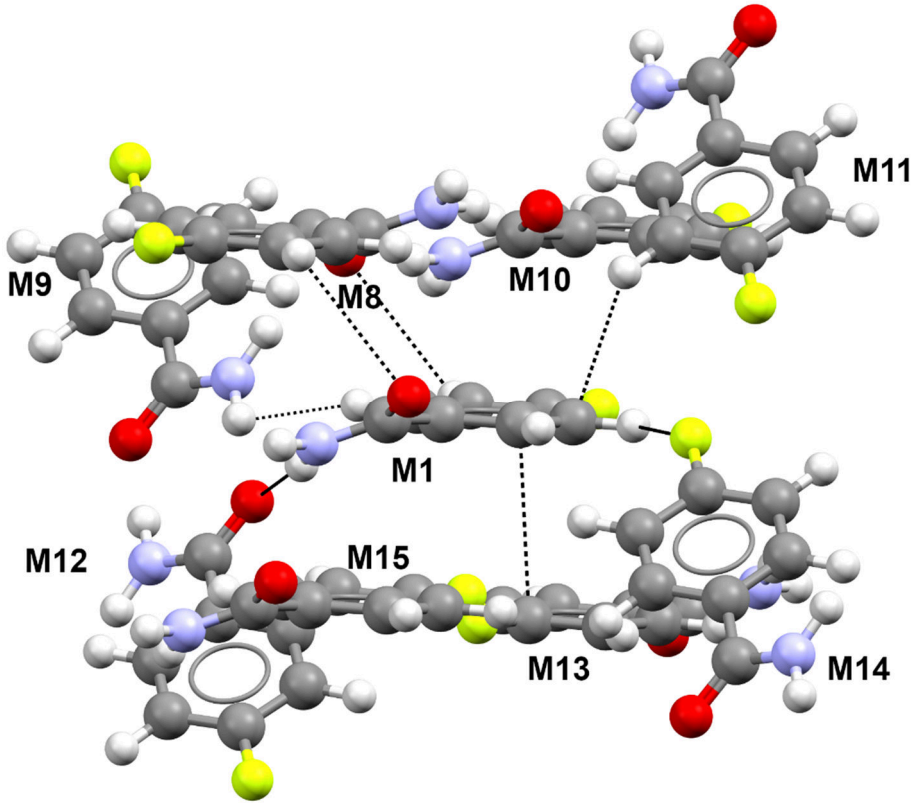

Figure S20. Central Molecule with neighboring molecules in upper and lower planes for compound 9.

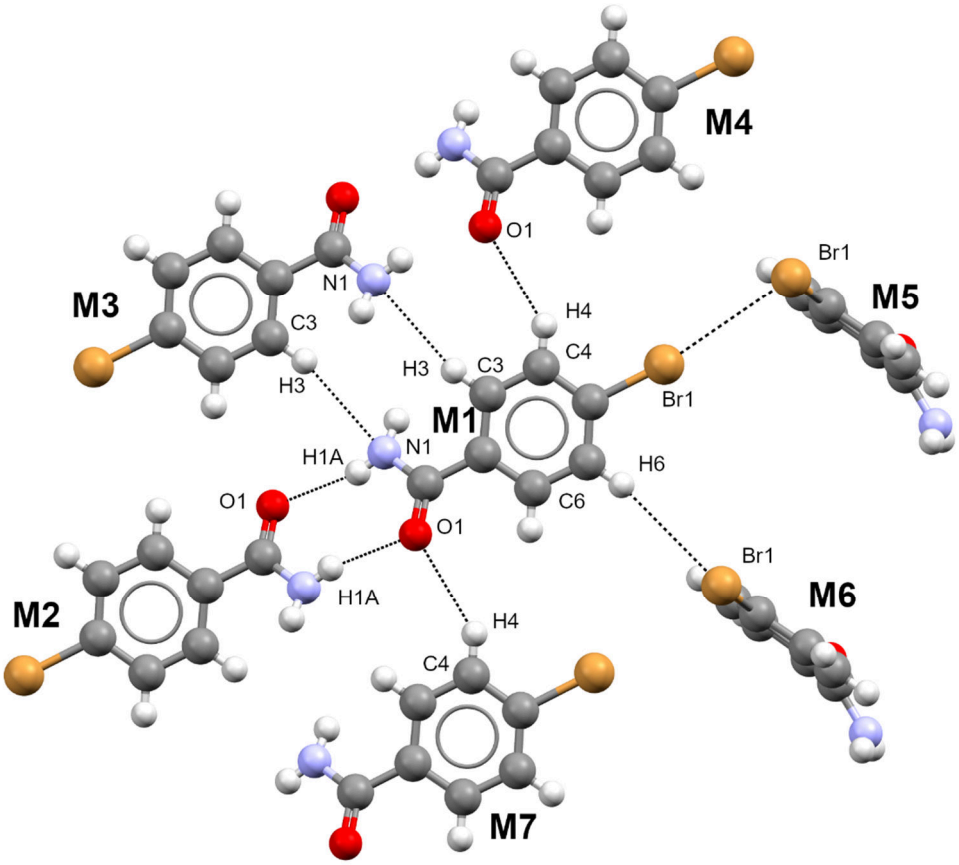

Figure S21. Central molecule with neighboring molecules in the same plane for compound 11.

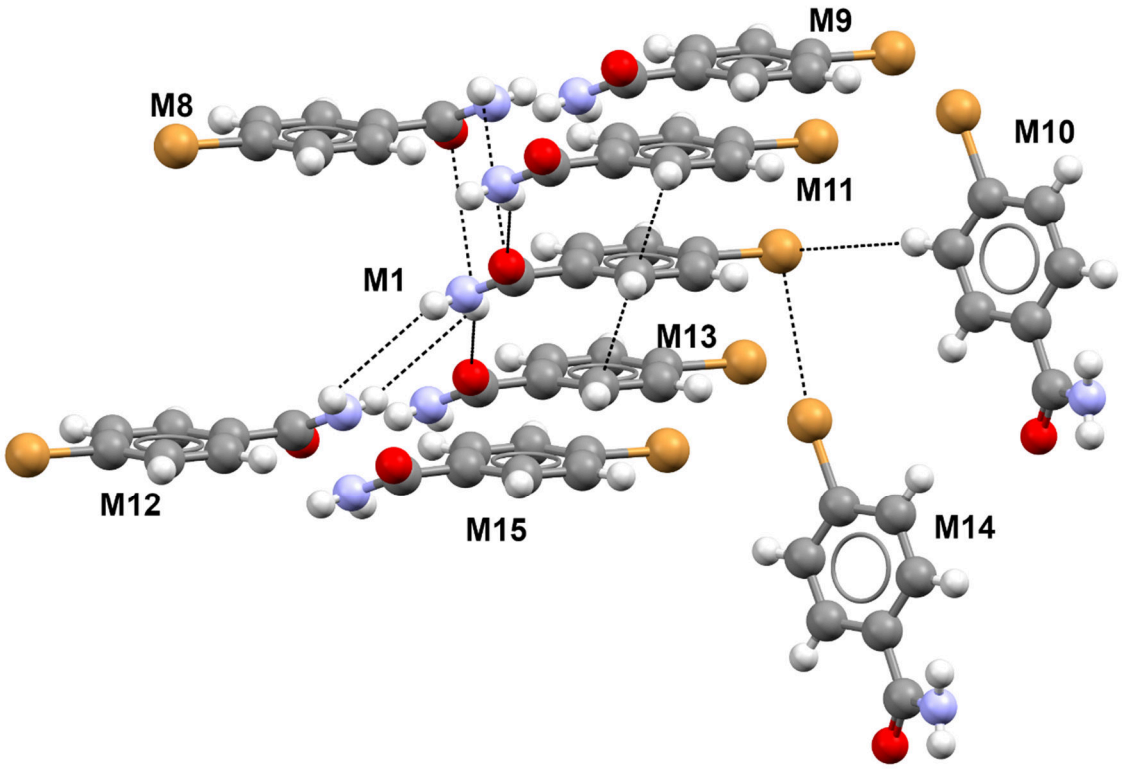

Figure S22. Central Molecule with neighboring molecules in upper and lower planes for compound 11.

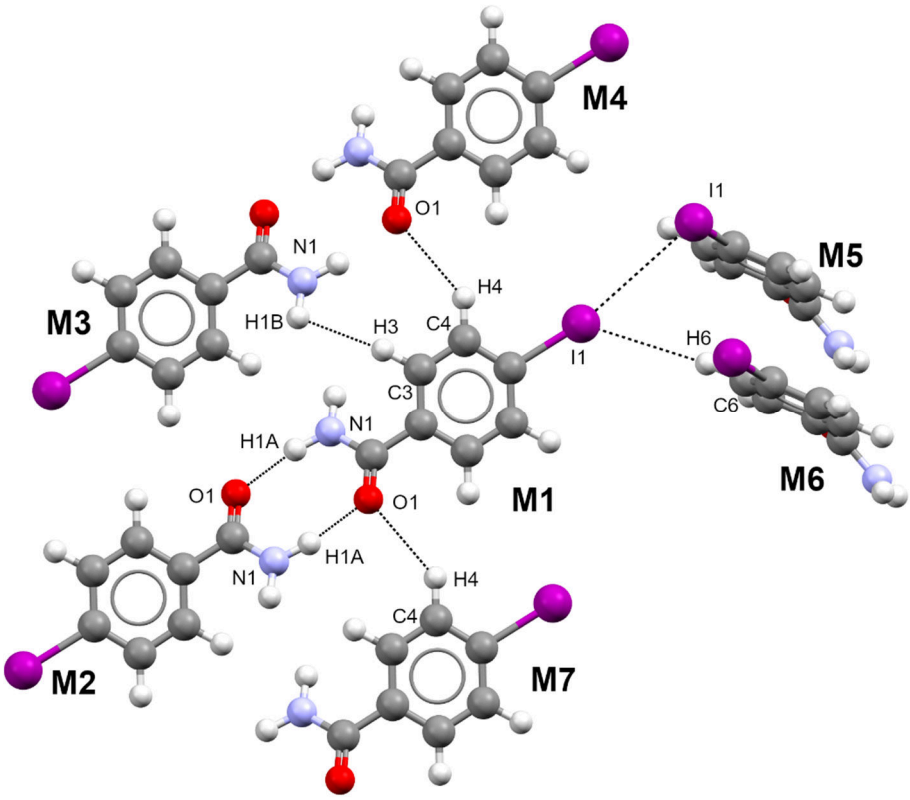

Figure S23. Central molecule with neighboring molecules in the same plane for compound 12

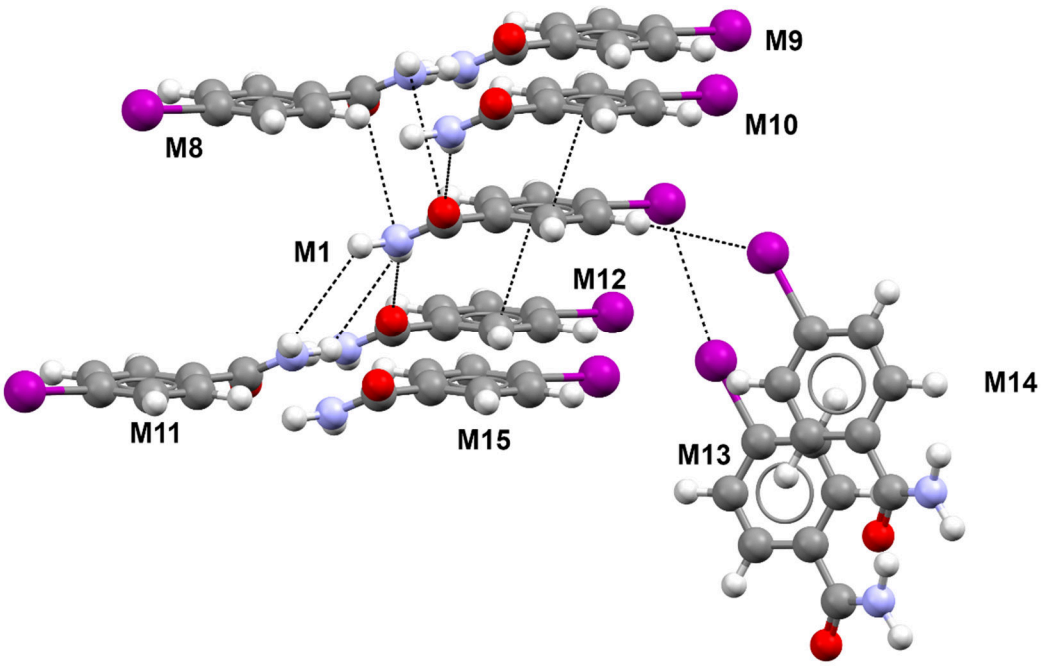

Figure S24. Central Molecule with neighboring molecules in upper and lower planes for compound 12

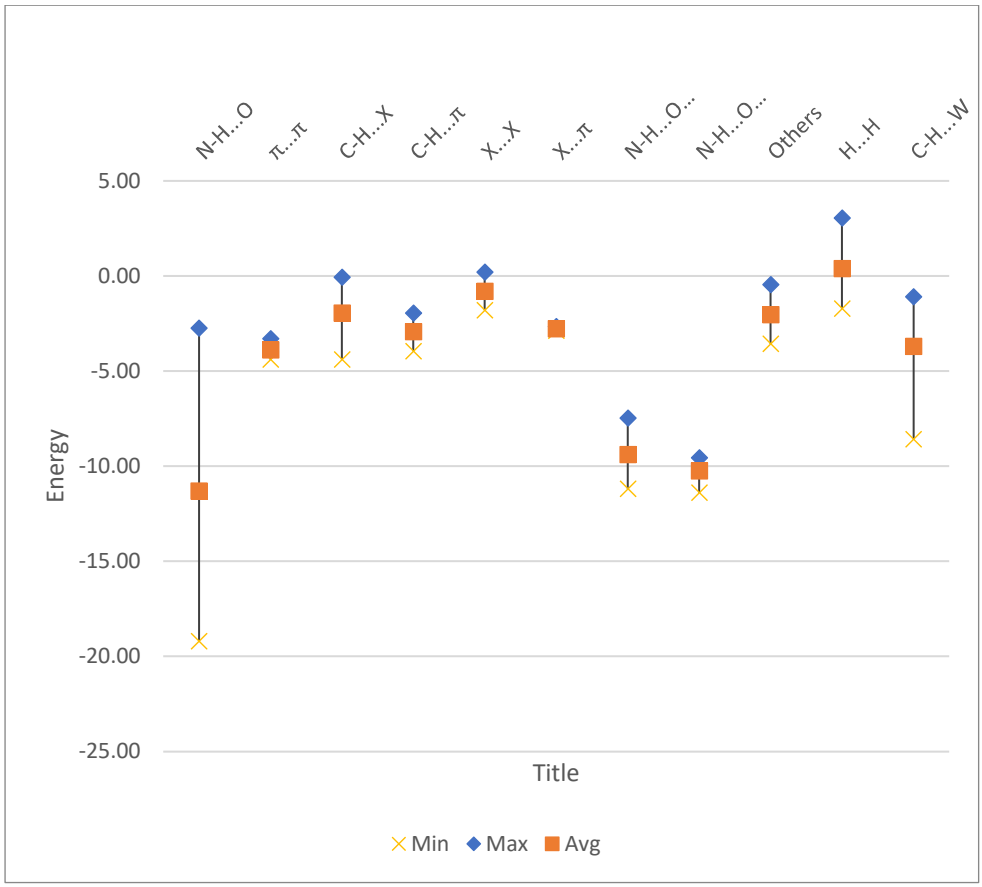

Figure S25 - energy range by interaction Class

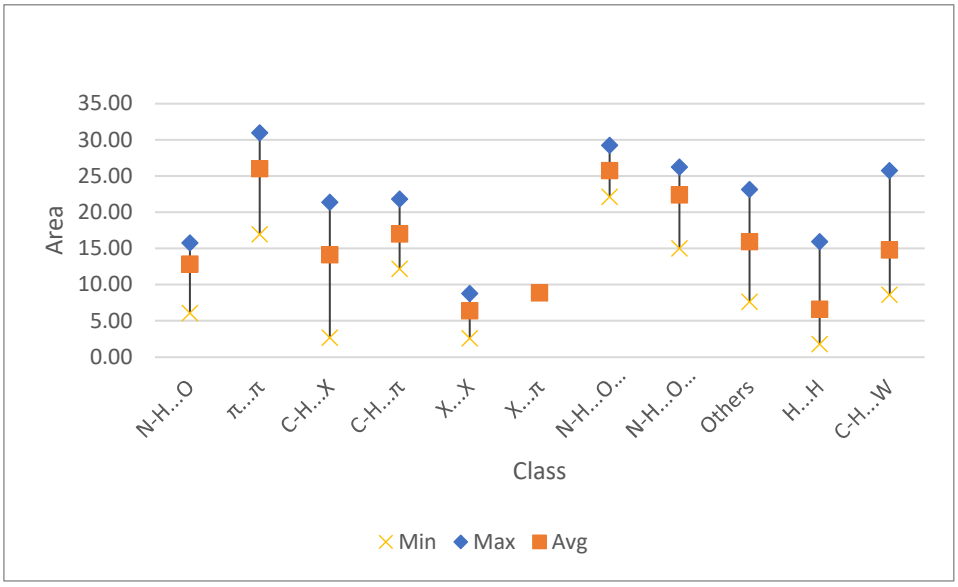

Figure S26 - Area range by interaction class

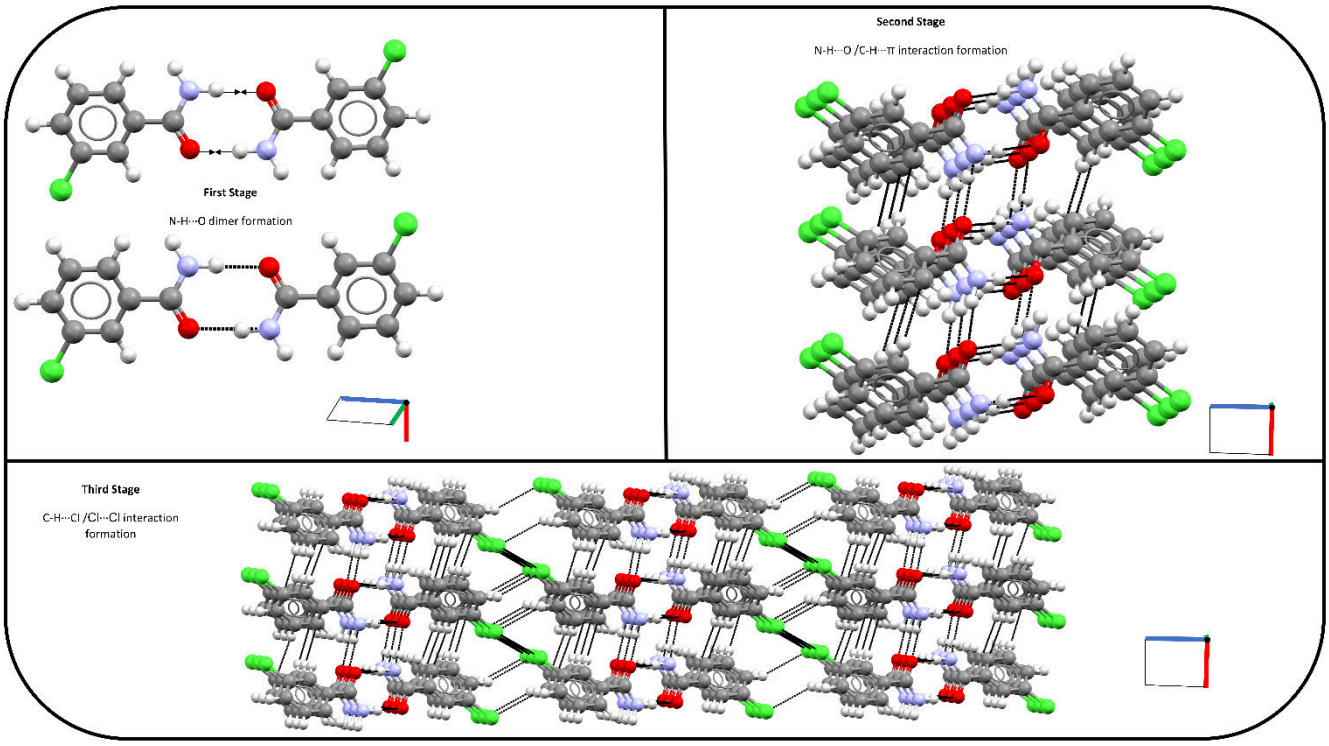

Figure S27 - *Nucleation proposal for compound* 6.

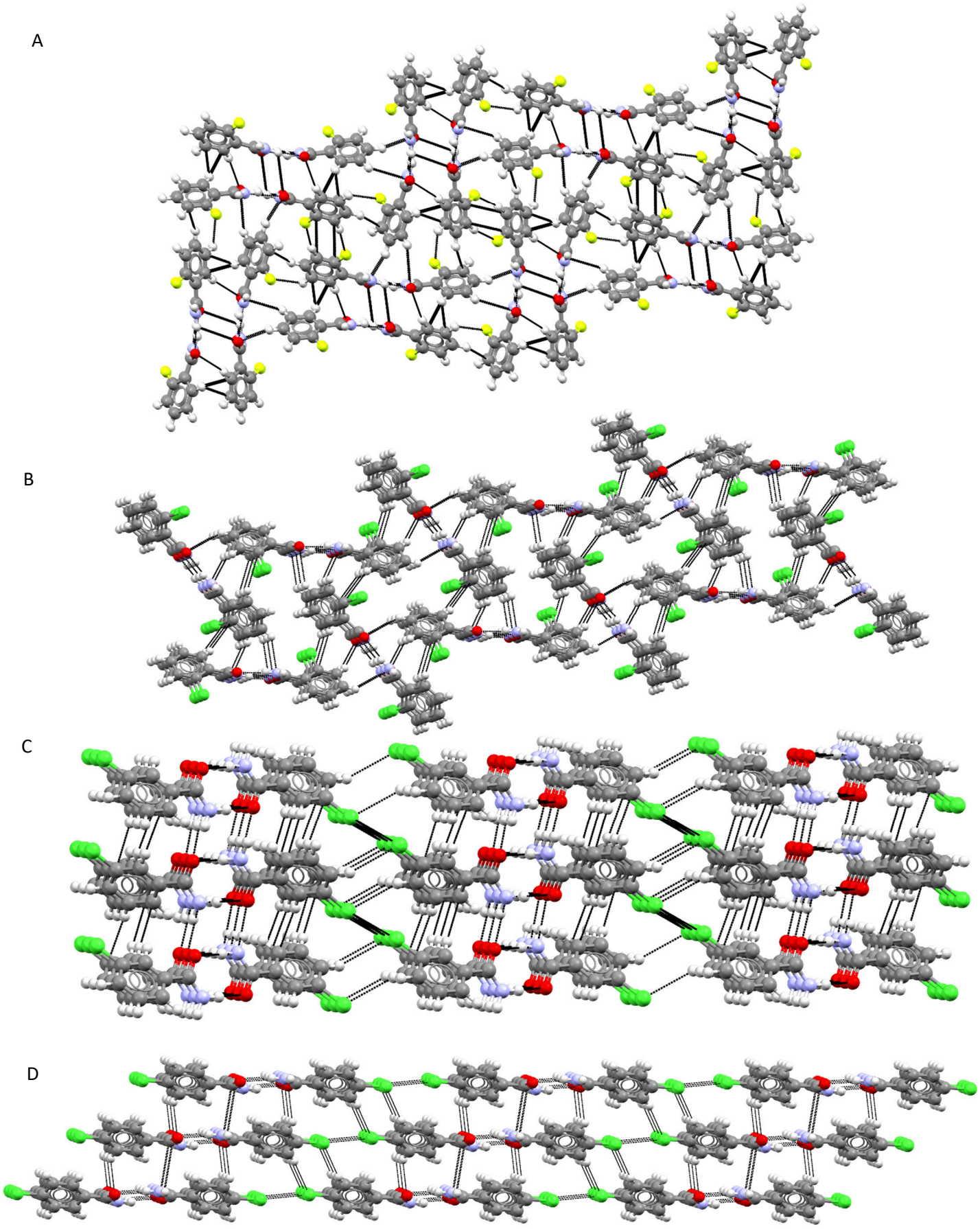

Figure S28 – *last stage of the nucleation for compound 1 (a), 2 – 3 (b), 6 – 9(C) and 5, 10 - 12(d)*