Supplementary Materials

Experimental and DFT Study of Photoluminescent Green Emission Band of Halogenated (–F, –Cl and –Br) Imines

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Table S1. X-ray data and calculated Cartesian coordinates for (a) **I,** (b) **I**–**F,** (c) **I**–**Cl** and (d) **I**–**Br** compounds. Theory level of calculations is PBE1PBE/6-311G(d,p).

X-ray data structures				Calculated structures			
(a) **I**							
N	8.623128	3.301477	13.108582	N	-1.23458800	-0.47606600	0.70496700
C	8.965310	3.123539	15.472294	C	1.11319800	-0.38926600	0.20143700
C	8.823896	2.333036	16.579164	C	2.16122100	-1.00019700	-0.44808700
H	8.403266	1.507667	16.496879	H	1.99185300	-1.92056500	-1.00180800
C	9.301314	2.743617	17.848283	C	3.46495300	-0.45550600	-0.41545400
C	9.192952	1.924259	18.989660	C	4.55486700	-1.06831700	-1.07729000
H	8.766750	1.100092	18.925623	H	4.38266100	-1.98812700	-1.62829400
C	9.703774	2.328227	20.178152	C	5.80722600	-0.51294400	-1.02637200
H	9.625362	1.777580	20.923033	H	6.63587700	-0.99120500	-1.53785700
C	10.350690	3.562975	20.296934	C	6.02563300	0.68187100	-0.31036800
H	10.712755	3.817258	21.115474	H	7.02090200	1.11257300	-0.27720900
C	10.452948	4.400968	19.218267	C	4.98810300	1.29881600	0.34150400
H	10.864637	5.229944	19.313824	H	5.15469100	2.21896500	0.89347500
C	9.934254	4.009023	17.958107	C	3.68602500	0.75144000	0.30823100
C	10.043350	4.820566	16.808767	C	2.58946400	1.36116900	0.97105400
H	10.437675	5.659761	16.875126	H	2.76156000	2.28048600	1.52308600
C	9.580729	4.391350	15.598376	C	1.34112800	0.81134200	0.92218800
H	9.670113	4.937187	14.851173	H	0.49860400	1.26971100	1.42695500
C	8.521657	2.620983	14.163692	C	-0.22316500	-0.98734500	0.13922400
H	8.150355	1.769765	14.114586	H	-0.29731100	-1.92346000	-0.43872100
C	8.186797	2.682901	11.854063	C	-2.50123300	-1.16919900	0.58582900
H	7.903097	1.760147	12.020956	H	-2.40273100	-2.05494700	-0.06522800
C	7.011901	3.494444	11.311577	C	-2.93550500	-1.63640500	1.97716400
H	6.707693	3.106707	10.488060	H	-3.90371400	-2.14084700	1.92498600
H	6.295478	3.487832	11.951279	H	-2.19844800	-2.32684000	2.39664900
H	7.291808	4.399164	11.154969	H	-3.02686600	-0.77797600	2.64721500
C	9.340822	2.695525	10.860003	C	-3.54878500	-0.25901100	-0.02332700
C	9.557591	1.648334	10.017242	C	-4.52251400	-0.78714700	-0.86817400
H	9.005221	0.901715	10.063362	H	-4.49639600	-1.84424200	-1.11962500
C	10.590166	1.675987	9.092196	C	-5.52151100	0.02289900	-1.39514100
H	10.727695	0.943795	8.537102	H	-6.27110400	-0.40376500	-2.05393200
C	11.403327	2.762853	8.988344	C	-5.55428000	1.37695100	-1.08600800
H	12.087807	2.785096	8.357932	H	-6.32999600	2.01270900	-1.50006200
C	11.192744	3.814252	9.823473	C	-4.58207100	1.91294500	-0.24887600
H	11.743453	4.562074	9.764746	H	-4.59717800	2.97135200	-0.00863800
C	10.181382	3.789605	10.753828	C	-3.58648600	1.10139500	0.27963700
H	10.059102	4.517590	11.320867	H	-2.81788900	1.51769800	0.92120800

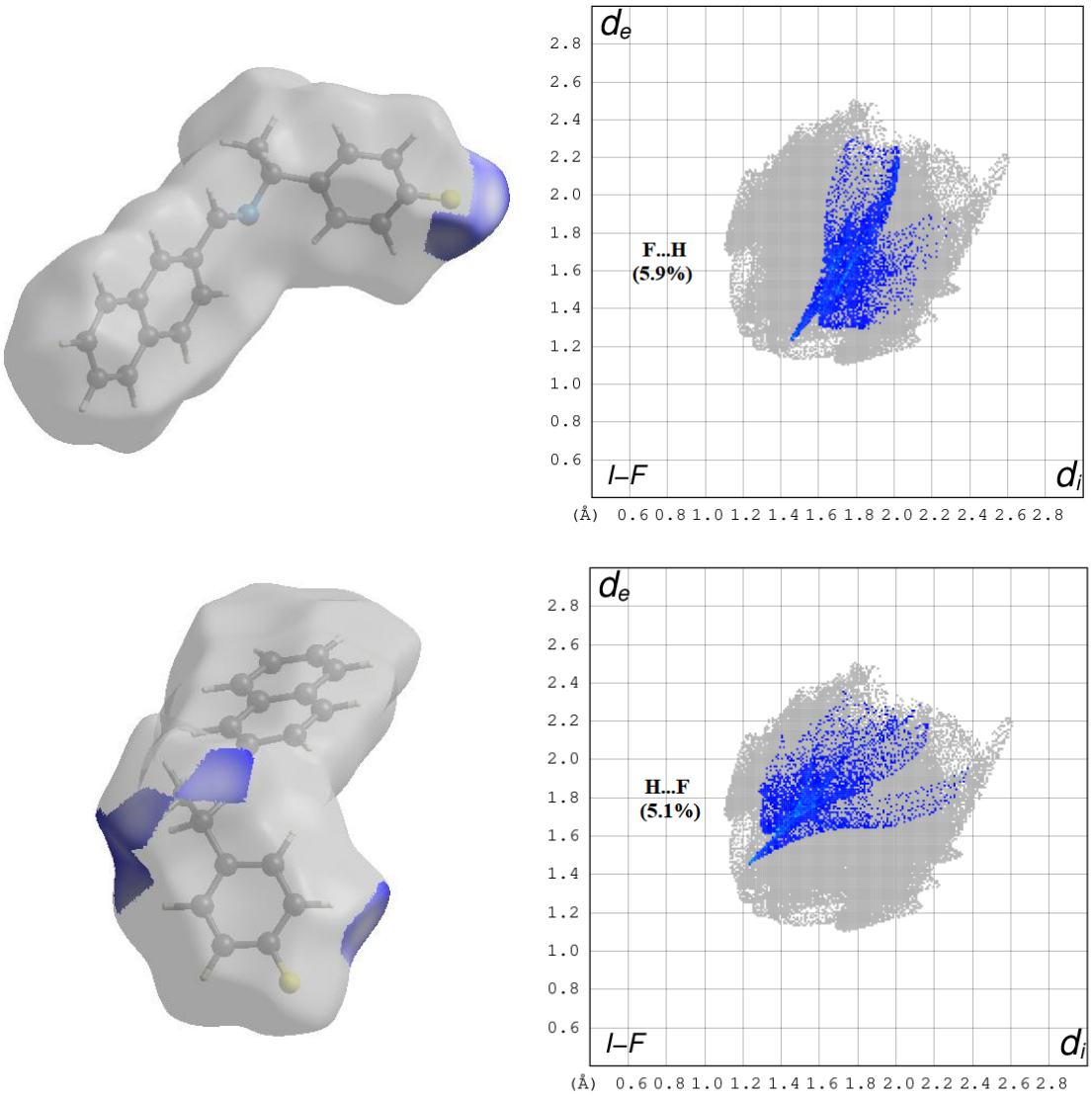
(b) **I–F**							
F	-0.614355	3.356929	8.125196	F	-6.27134400	-2.02521400	-0.77280100
N	3.252291	3.723301	13.096556	N	-0.82186100	0.83518500	0.61900500
C	3.231898	3.767548	15.499240	C	1.50219000	0.49325500	0.11551000
C	3.513608	3.104422	16.657826	C	2.55162500	0.83759300	-0.70532500
H	3.952033	2.285544	16.610879	H	2.40425600	1.57434500	-1.49136900
C	3.162244	3.621236	17.928750	C	3.82794400	0.24992900	-0.55330200
C	3.403379	2.926841	19.125901	C	4.91837600	0.58860200	-1.38862300
H	3.863176	2.119172	19.105781	H	4.76852500	1.32494700	-2.17260500
C	2.967595	3.427726	20.319698	C	6.14360300	-0.00128100	-1.21451300
H	3.124019	2.951030	21.102708	H	6.97278700	0.26548600	-1.86121200
C	2.289018	4.651323	20.376705	C	6.33321600	-0.95715100	-0.19555700
H	1.987976	4.978167	21.193248	H	7.30721900	-1.41750600	-0.06700100
C	2.072934	5.355158	19.248298	C	5.29450100	-1.30548700	0.63009700
H	1.639194	6.176396	19.303629	H	5.43912400	-2.04158900	1.41514000
C	2.486983	4.879052	17.984081	C	4.01985300	-0.71596500	0.47603200
C	2.256557	5.574627	16.781901	C	2.92290500	-1.05175300	1.31118000
H	1.860407	6.415334	16.812081	H	3.07306200	-1.78710500	2.09613900
C	2.598034	5.046603	15.579720	C	1.70107900	-0.46805300	1.13981000
H	2.417231	5.520939	14.801740	H	0.85891300	-0.71782900	1.77466900
C	3.528953	3.147490	14.203165	C	0.19407800	1.12337100	-0.08076100
H	3.931231	2.309143	14.186398	H	0.14517000	1.87392000	-0.88684800
C	3.561763	2.994098	11.867548	C	-2.05817700	1.53783200	0.34476300
H	3.738538	2.054866	12.083840	H	-1.94220900	2.21111000	-0.52223700
C	4.813704	3.614156	11.220350	C	-2.42102400	2.38279400	1.56837400
H	5.023734	3.140410	10.412189	H	-3.36601600	2.90689300	1.40415800
H	4.644855	4.536279	11.015794	H	-2.52801100	1.74119900	2.44655000
H	5.553494	3.551029	11.828985	H	-1.63865500	3.11953300	1.77056900
C	2.394641	3.076104	10.918547	C	-3.16618800	0.55478500	0.02360800
C	2.141892	2.054276	10.024876	C	-4.18010700	0.91343000	-0.86209500
H	2.667294	1.287315	10.053380	H	-4.14665800	1.88216900	-1.35294000
C	1.129559	2.140411	9.085935	C	-5.23494700	0.05167600	-1.13552700
H	0.972637	1.445427	8.489036	H	-6.02673300	0.31917900	-1.82563000
C	0.375750	3.257224	9.060784	C	-5.25947500	-1.18232800	-0.51205300
C	0.563151	4.289672	9.922598	C	-4.26575100	-1.57413300	0.36702700
H	0.016077	5.040704	9.887388	H	-4.31781200	-2.55368400	0.82842800
C	1.584749	4.201766	10.851480	C	-3.22090500	-0.69875500	0.63137300
H	1.730150	4.907370	11.439995	H	-2.42462400	-0.99059800	1.30624700
(c) **I–Cl**							
Cl	5.732667	6.914944	9.272675	Cl	6.37897200	-1.83480400	-0.51225300
N	2.488698	2.627557	13.047962	N	0.39651900	1.01112100	0.56834600
C	2.267628	3.112562	15.391266	C	-1.90281300	0.51601200	0.07552700
C	2.876327	3.095050	16.617422	C	-2.96754500	0.77187800	-0.75794900
H	3.702461	2.676286	16.703070	H	-2.85618400	1.47892500	-1.57654700
C	2.294278	3.688935	17.759961	C	-4.21406800	0.13120100	-0.57676200
C	2.932654	3.730050	19.020308	C	-5.32010900	0.38140900	-1.42266900

H	3.759394	3.318138	19.123560	H	-5.20619100	1.08935800	-2.23821000
C	2.361507	4.360481	20.088032	C	-6.51571800	-0.25773400	-1.21939600
H	2.808492	4.390936	20.904228	H	-7.35751200	-0.05869200	-1.87413000
C	1.099291	4.961979	19.956005	C	-6.65834200	-1.17699400	-0.15996700
H	0.711057	5.386073	20.687568	H	-7.60914600	-1.67725600	-0.00878900
C	0.437294	4.928477	18.760656	C	-5.60339600	-1.43996800	0.67670900
H	-0.399137	5.328207	18.690241	H	-5.71196600	-2.14750700	1.49321700
C	1.004201	4.295762	17.629627	C	-4.35860700	-0.79721800	0.49383000
C	0.379755	4.270637	16.361832	C	-3.24643200	-1.04265600	1.34033800
H	-0.463338	4.650570	16.266367	H	-3.36049900	-1.74952100	2.15690100
C	0.975129	3.711015	15.286322	C	-2.05467400	-0.40763600	1.14168400
H	0.537229	3.714822	14.465387	H	-1.20189200	-0.58748400	1.78594300
C	2.950824	2.559032	14.225031	C	-0.62868800	1.20237400	-0.15112800
H	3.768479	2.134938	14.353672	H	-0.61426900	1.90739900	-0.99857400
C	3.323311	2.074026	11.967713	C	1.59227900	1.76691400	0.25951500
H	4.042847	1.546383	12.373272	H	1.45609800	2.35786100	-0.66269800
C	2.475373	1.149699	11.103784	C	1.87373000	2.73140200	1.41491500
H	2.168299	0.409628	11.631891	H	1.04283000	3.43128100	1.53863400
H	3.003518	0.822301	10.372559	H	2.78865000	3.29865100	1.22579200
H	1.720708	1.633943	10.761869	H	1.99769000	2.17265500	2.34584300
C	3.946546	3.250374	11.225655	C	2.76825300	0.83587100	0.04573100
C	3.223981	3.999582	10.308916	C	2.88085300	-0.36216200	0.74826400
H	2.357873	3.741470	10.088194	H	2.08323000	-0.65427200	1.42151500
C	3.771507	5.130246	9.711072	C	3.98590100	-1.18562400	0.58191800
H	3.274858	5.625911	9.099686	H	4.06915600	-2.11889600	1.12625300
C	5.036752	5.501804	10.026920	C	4.99054200	-0.80538400	-0.29641800
C	5.788388	4.785336	10.931134	C	4.90121100	0.38017000	-1.01058200
H	6.652074	5.053345	11.147793	H	5.68979100	0.65928100	-1.69916700
C	5.231777	3.655433	11.513744	C	3.78747200	1.19083000	-0.83463400
H	5.739329	3.159007	12.115989	H	3.71294900	2.11594300	-1.39967000

(d) **I**–**Br**

Br	5.785741	3.166512	26.255661	Br	5.86998800	-1.39951500	-0.22953100
N	2.458566	-1.191467	30.126340	N	-0.38595000	1.31978100	0.50409000
C	2.229173	-0.700773	32.458802	C	-2.62549100	0.58946900	0.03234400
C	2.847143	-0.714574	33.680067	C	-3.66569100	0.61704700	-0.86822200
H	3.673323	-1.133964	33.760579	H	-3.56847000	1.18610100	-1.78969300
C	2.267909	-0.110406	34.828293	C	-4.86801900	-0.08472100	-0.62457400
C	2.914932	-0.068237	36.078434	C	-5.94726700	-0.07159800	-1.53914600
H	3.745349	-0.473060	36.182725	H	-5.84718700	0.49721500	-2.45874700
C	2.332672	0.560465	37.132560	C	-7.09992100	-0.76394300	-1.27180600
H	2.769670	0.581933	37.952625	H	-7.92140900	-0.74736000	-1.98018300
C	1.088257	1.173833	37.000072	C	-7.22464800	-1.50071600	-0.07612000
H	0.709970	1.612391	37.728415	H	-8.14143300	-2.04509300	0.12461200
C	0.420656	1.136264	35.808362	C	-6.19502300	-1.53184700	0.82984300
H	-0.415208	1.537254	35.734305	H	-6.28975800	-2.09944800	1.75065400
C	0.990205	0.493761	34.687992	C	-4.99427000	-0.82941900	0.58337500
C	0.349840	0.466160	33.424264	C	-3.90872200	-0.83962000	1.49706100

H	-0.496313	0.839547	33.332541	H	-4.00925300	-1.40773100	2.41712600
C	0.951469	-0.095839	32.351793	C	-2.75860700	-0.15356700	1.23368600
H	0.519313	-0.084338	31.528671	H	-1.92551200	-0.15554500	1.92696800
C	2.922801	-1.258938	31.303442	C	-1.39456500	1.32683900	-0.26269900
H	3.739902	-1.682928	31.436948	H	-1.39711500	1.89623800	-1.20672900
C	3.296851	-1.748866	29.046395	C	0.76966500	2.10055300	0.11407300
H	4.017111	-2.274829	29.453030	H	0.61165800	2.57155000	-0.87145900
C	2.442224	-2.683485	28.193378	C	0.98746900	3.20540200	1.15076500
H	2.959721	-3.001670	27.448730	H	1.87085300	3.79800400	0.89956000
H	1.674754	-2.206591	27.866575	H	1.13421700	2.76523600	2.14016500
H	2.154120	-3.428727	28.726047	H	0.11767000	3.86666000	1.19149200
C	3.916032	-0.578099	28.312278	C	1.99470000	1.21461100	0.01351500
C	5.201604	-0.174043	28.603411	C	2.98258600	1.49205800	-0.92791100
H	5.705181	-0.666271	29.211835	H	2.85070100	2.32059700	-1.61843900
C	5.759654	0.942287	28.015030	C	4.13822200	0.72471100	-1.00676200
H	6.624571	1.206802	28.233464	H	4.89996900	0.94642100	-1.74457700
C	5.013369	1.663761	27.096788	C	4.30018500	-0.33820200	-0.13026300
C	3.741112	1.278106	26.768966	C	3.32783700	-0.64094500	0.81305800
H	3.246615	1.762666	26.147633	H	3.46460000	-1.47913000	1.48592900
C	3.200615	0.152575	27.376031	C	2.18073600	0.13847800	0.87921600
H	2.339935	-0.118073	27.149783	H	1.40749500	-0.09669500	1.60167000


d_e
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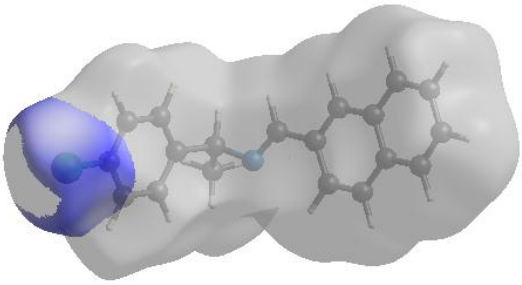
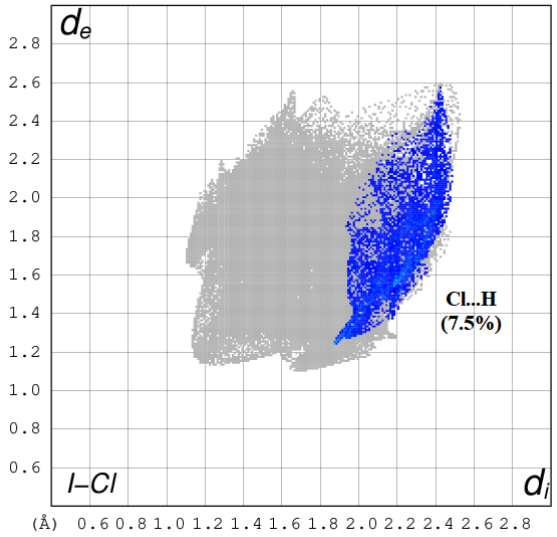
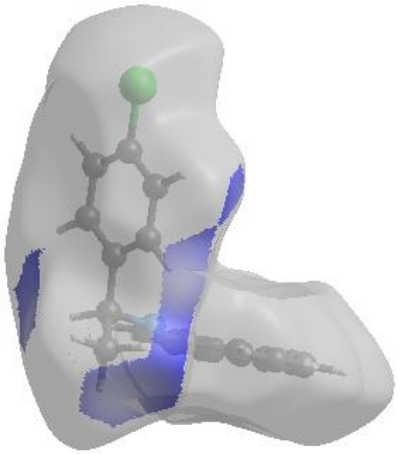
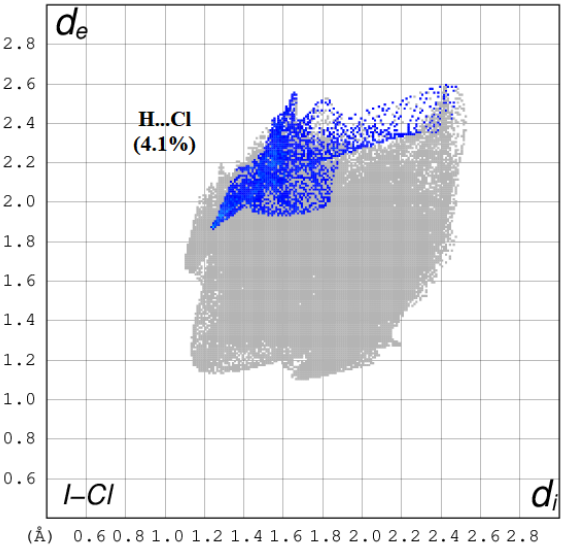
(5.9%)
I–F
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8
d_e
H...F
(5.1%)
I–F
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

(a)




d_e
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
Cl...H
(7.5%)
I–Cl
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8




d_e
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
H...Cl
(4.1%)
I–Cl
d_i
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

(b)

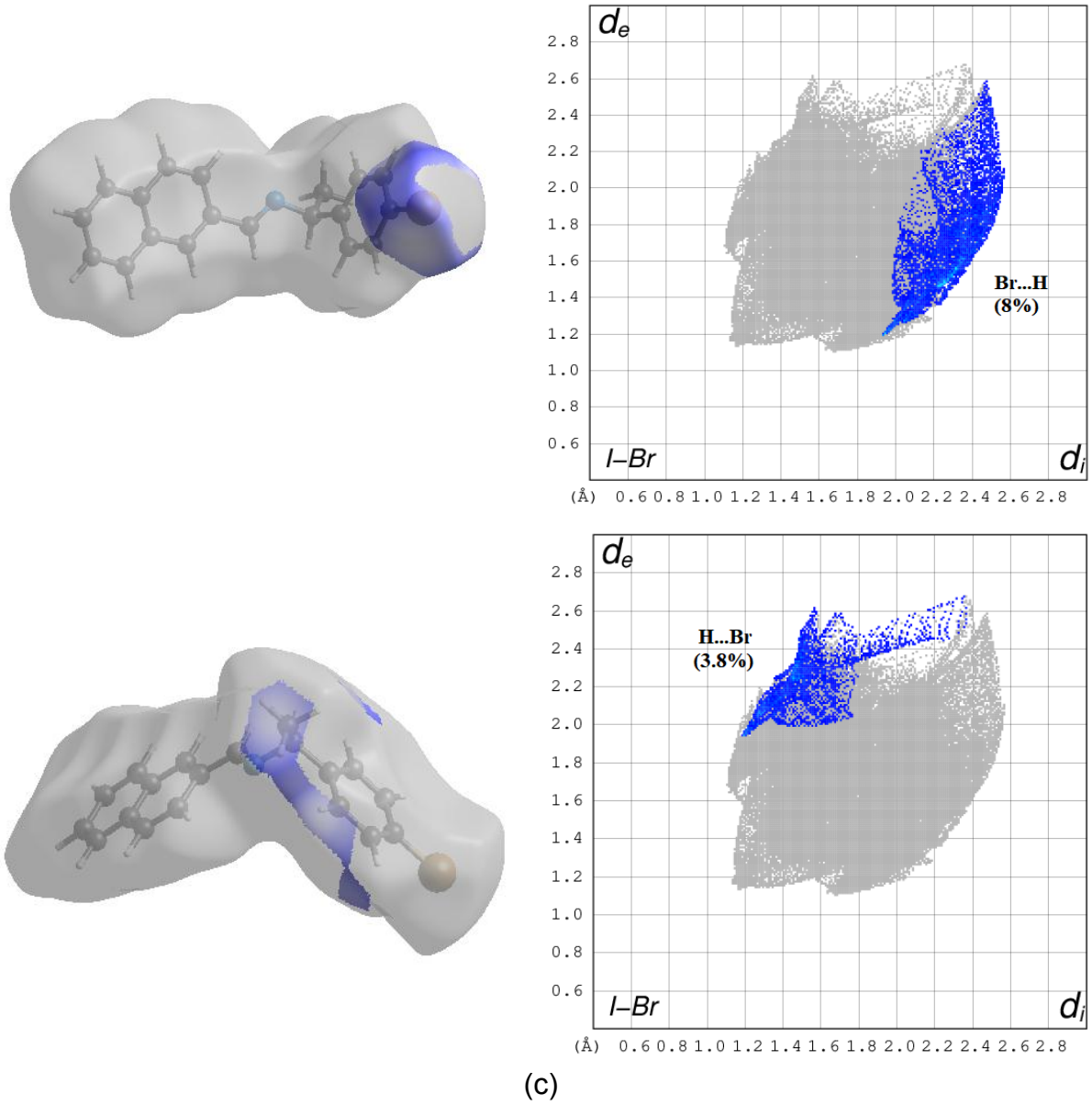


Figure S1. Hirshfeld surfaces (d_{norm} mapping) (left) and fingerprint plots (right) of halogen bonds C–X···H for (a) **I–F,** (b) **I–Cl** and (c) **I–Br** compounds.

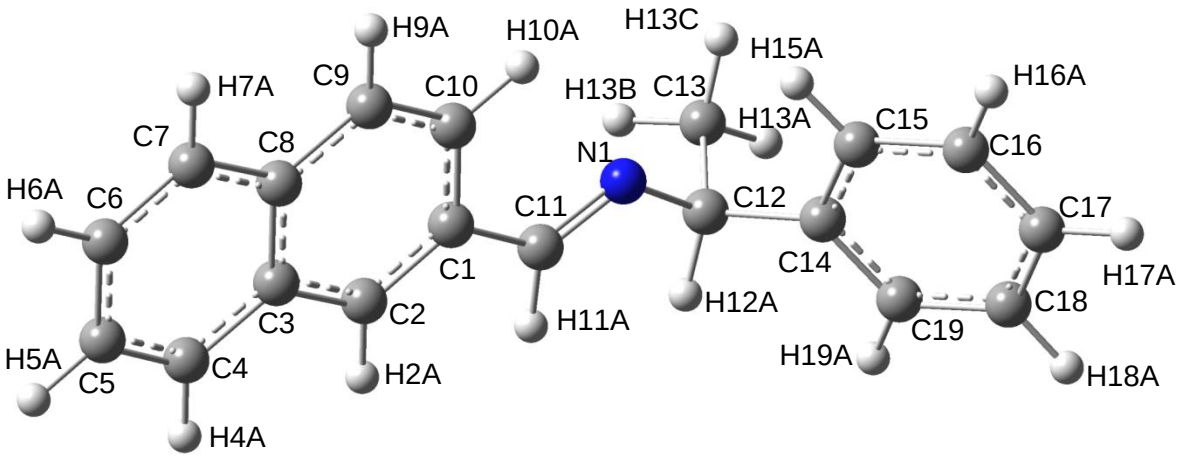


Figure S2. Numbering convention used in the theoretical calculations PBE1PBE/6-311G(d,p) for (a) **I,** (b) **I–F,** (c) **I–Cl** and (d) **I–Br** compounds. For compound (b) **I–F** atom H17A is substituted by F1, for (c) by Cl1 and for (d) by Br1.

Table S2. RMSD parameter between X-ray experimental and calculated structures for internal coordinates of (a) **I,** (b) **I–F,** (c) **I–Cl** and (d) **I–Br** compounds. Theory level of calculations is PBE1PBE/6-311G(d,p). RMSD is calculated from standard equation $\sqrt{\frac{1}{n}\sum_{i=1}^{n}|v_i - w_i|^2}$ for n data for internal coordinate: Bond length, valence angle or dihedral angle for w_i predicted values respect to v_i experimental values. Numbering convention is shown in Figure S2.

Parameter	X-ray	Calculated	RMSD
(a) **I**			
N1 C11	1.260(5)	1.26667	
N1 C12	1.465(5)	1.44880	
C1 C2	1.368(5)	1.37603	
C1 C10	1.415(5)	1.41876	
C1 C11	1.470(5)	1.46541	
C2 C3	1.417(5)	1.41332	
C2 H2A	0.9300	1.08737	
C3 C4	1.409(5)	1.41474	
C3 C8	1.420(5)	1.42454	
C4 C5	1.356(6)	1.37092	
C4 H4A	0.9300	1.08596	
C5 C6	1.399(7)	1.40995	
C5 H5A	0.9300	1.08490	

C6 C7	1.370(6)	1.37187	
C6 H6A	0.9300	1.08497	
C7 C8	1.418(5)	1.41285	
C7 H7A	0.9300	1.08586	
C8 C9	1.411(5)	1.41900	
C9 C10	1.365(5)	1.36493	
C9 H9A	0.9300	1.08605	
C10 H10A	0.9300	1.08385	
C11 H11A	0.9300	1.10265	
C12 C14	1.523(5)	1.51555	
C12 C13	1.528(8)	1.53058	
C12 H12A	0.9800	1.10369	
C13 H13A	0.9600	1.09298	
C13 H13B	0.9600	1.09358	
C13 H13C	0.9600	1.09280	
C14 C19	1.362(6)	1.39314	
C14 C15	1.384(6)	1.39324	
C19 C18	1.386(7)	1.38892	
C19 H19A	0.9300	1.08690	
C18 C17	1.361(9)	1.38928	
C18 H18A	0.9300	1.08533	
C17 C16	1.359(9)	1.39042	
C17 H17A	0.9300	1.08506	
C16 C15	1.375(6)	1.38893	
C16 H16A	0.9300	1.08543	
C15 H15A	0.9300	1.08428	0.10031687
C11 N1 C12	117.7(4)	117.92149	
C2 C1 C10	119.4(3)	119.54771	
C2 C1 C11	119.5(3)	119.55857	
C10 C1 C11	121.1(3)	120.89371	
C1 C2 C3	121.5(3)	121.36997	
C1 C2 H2A	119.2	119.83684	
C3 C2 H2A	119.2	118.79311	
C4 C3 C2	122.1(3)	122.20318	
C4 C3 C8	119.3(3)	119.01892	
C2 C3 C8	118.6(3)	118.77789	
C5 C4 C3	120.5(4)	120.72507	
C5 C4 H4A	119.7	120.45308	
C3 C4 H4A	119.7	118.82185	
C4 C5 C6	120.8(4)	120.24279	
C4 C5 H5A	119.6	120.10912	
C6 C5 H5A	119.6	119.64808	
C7 C6 C5	120.5(4)	120.34756	
C7 C6 H6A	119.7	120.04741	
C5 C6 H6A	119.7	119.60503	
C6 C7 C8	120.2(4)	120.76875	
C6 C7 H7A	119.9	120.43730	
C8 C7 H7A	119.9	118.79395	

C9 C8 C7	122.4(3)	122.32437	
C9 C8 C3	118.9(3)	118.89691	
C7 C8 C3	118.6(3)	118.77871	
C10 C9 C8	121.0(3)	121.12773	
C10 C9 H9A	119.5	120.27189	
C8 C9 H9A	119.5	118.60038	
C9 C10 C1	120.5(3)	120.39783	
C9 C10 H10A	119.7	121.59480	
C1 C10 H10A	119.7	118.00735	
N1 C11 C1	122.4(3)	122.98867	
N1 C11 H11A	118.8	121.53967	
C1 C11 H11A	118.8	115.47166	
N1 C12 C14	109.3(3)	110.48918	
N1 C12 C13	108.0(4)	108.62314	
C14 C12 C13	110.3(3)	110.64504	
N1 C12 H12A	109.8	110.75846	
C14 C12 H12A	109.8	107.85234	
C13 C12 H12A	109.8	108.45600	
C12 C13 H13A	109.5	110.41535	
C12 C13 H13B	109.5	110.49827	
H13A C13 H13B	109.5	108.90309	
C12 C13 H13C	109.5	109.95650	
H13A C13 H13C	109.5	108.52731	
H13B C13 H13C	109.5	108.48740	
C19 C14 C15	117.6(4)	118.86666	
C19 C14 C12	121.3(4)	121.15422	
C15 C14 C12	121.1(4)	119.94637	
C14 C19 C18	121.1(5)	120.75355	
C14 C19 H19A	119.4	119.48535	
C18 C19 H19A	119.4	119.7607	
C17 C18 C19	120.8(5)	120.04072	
C17 C18 H18A	119.6	120.12752	
C19 C18 H18A	119.6	119.83032	
C16 C17 C18	118.6(4)	119.55063	
C16 C17 H17A	120.7	120.24876	
C18 C17 H17A	120.7	120.19959	
C17 C16 C15	121.0(5)	120.33516	
C17 C16 H16A	119.5	119.96136	
C15 C16 H16A	119.5	119.70312	
C16 C15 C14	120.9(5)	120.45194	
C16 C15 H15A	119.6	120.59206	
C14 C15 H15A	119.6	118.94916	1.54509014
C10 C1 C2 C3	-1.2(5)	-0.10803	
C11 C1 C2 C3	176.6(3)	179.88347	
C1 C2 C3 C4	-178.3(3)	-179.96561	
C1 C2 C3 C8	0.3(4)	-0.00751	
C2 C3 C4 C5	177.6(3)	179.95329	
C8 C3 C4 C5	-1.0(5)	-0.01231	

C3 C4 C5 C6	0.0(6)	-0.00751	
C4 C5 C6 C7	1.4(7)	0.01588	
C5 C6 C7 C8	-1.6(6)	-0.00389	
C6 C7 C8 C9	-178.4(3)	179.95585	
C6 C7 C8 C3	0.5(5)	-0.01588	
C4 C3 C8 C9	179.7(3)	-179.94897	
C2 C3 C8 C9	1.1(4)	0.08424	
C4 C3 C8 C7	0.8(4)	0.02377	
C2 C3 C8 C7	-177.9(3)	-179.94302	
C7 C8 C9 C10	177.4(3)	179.9674	
C3 C8 C9 C10	-1.6(5)	-0.06084	
C8 C9 C10 C1	0.6(5)	-0.04741	
C2 C1 C10 C9	0.8(5)	0.13252	
C11 C1 C10 C9	-177.0(3)	-179.85886	
C12 N1 C11 C1	178.1(3)	-179.25575	
C2 C1 C11 N1	179.9(3)	-179.53596	
C10 C1 C11 N1	-2.4(5)	0.45542	
C11 N1 C12 C14	-123.3(4)	-123.00938	
C11 N1 C12 C13	116.7(4)	115.44974	
N1 C12 C14 C19	142.0(4)	145.33193	
C13 C12 C14 C19	-99.5(6)	-94.33065	
N1 C12 C14 C15	-40.0(6)	-36.77324	
C13 C12 C14 C15	78.6(5)	83.56419	
C15 C14 C19 C18	0.3(7)	-0.42354	
C12 C14 C19 C18	178.5(5)	177.51931	
C14 C19 C18 C17	-1.0(8)	0.27325	
C19 C18 C17 C16	0.9(8)	-0.05056	
C18 C17 C16 C15	-0.2(8)	-0.21736	
C17 C16 C15 C14	-0.5(8)	0.06291	
C19 C14 C15 C16	0.4(7)	0.25526	
C12 C14 C15 C16	-177.8(5)	-177.66183	1.99251267
$RMSD_{tot}$			1.46403028
(b) **I–F**			
F1 C17	1.367(6)	1.34251	
N1 C11	1.277(6)	1.26683	
N1 C12	1.462(7)	1.44824	
C1 C2	1.364(7)	1.37610	
C1 C10	1.430(7)	1.41875	
C1 C11	1.467(7)	1.46517	
C2 C3	1.417(7)	1.41331	
C2 H2A	0.9300	1.08738	
C3 C4	1.405(7)	1.41474	
C3 C8	1.428(7)	1.42454	
C4 C5	1.365(7)	1.37093	
C4 H4A	0.9300	1.08595	
C5 C6	1.400(9)	1.40993	

C5 H5A	0.9300	1.08486	
C6 C7	1.347(8)	1.37185	
C6 H6A	0.9300	1.08496	
C7 C8	1.413(7)	1.41280	
C7 H7A	0.9300	1.08584	
C8 C9	1.408(7)	1.41899	
C9 C10	1.356(7)	1.36489	
C9 H9A	0.9300	1.08603	
C10 H10A	0.9300	1.08383	
C11 H11A	0.9300	1.10249	
C12 C14	1.507(7)	1.51566	
C12 C13	1.540(8)	1.53063	
C12 H12A	0.9800	1.10383	
C13 H13A	0.9600	1.09300	
C13 H13B	0.9600	1.09283	
C13 H13C	0.9600	1.09351	
C14 C15	1.381(7)	1.39324	
C14 C19	1.389(7)	1.39418	
C15 C16	1.383(8)	1.38927	
C15 H15A	0.9300	1.08651	
C16 C17	1.348(9)	1.38278	
C16 H16A	0.9300	1.08385	
C17 C18	1.357(9)	1.38339	
C18 C19	1.384(8)	1.38848	
C18 H18A	0.9300	1.08403	
C19 H19A	0.9300	1.08383	0.09710186
C11 N1 C12	117.2(5)	118.01050	
C2 C1 C10	118.6(5)	119.55712	
C2 C1 C11	120.2(5)	119.56088	
C10 C1 C11	121.2(5)	120.88197	
C1 C2 C3	122.3(5)	121.36489	
C1 C2 H2A	118.9	119.82686	
C3 C2 H2A	118.9	118.80807	
C4 C3 C2	122.8(5)	122.20854	
C4 C3 C8	118.9(5)	119.02009	
C2 C3 C8	118.2(5)	118.77136	
C5 C4 C3	120.6(5)	120.72073	
C5 C4 H4A	119.7	120.44878	
C3 C4 H4A	119.7	118.83048	
C4 C5 C6	120.7(6)	120.24396	
C4 C5 H5A	119.7	120.10426	
C6 C5 H5A	119.7	119.65178	
C7 C6 C5	120.0(6)	120.34974	
C7 C6 H6A	120.0	120.04493	
C5 C6 H6A	120.0	119.60533	
C6 C7 C8	121.7(6)	120.76647	
C6 C7 H7A	119.1	120.42534	
C8 C7 H7A	119.1	118.80819	

C9 C8 C7	123.3(5)	122.31227	
C9 C8 C3	118.7(5)	118.78872	
C7 C8 C3	118.0(5)	118.89901	
C10 C9 C8	121.5(5)	121.12619	
C10 C9 H9A	119.2	120.27063	
C8 C9 H9A	119.2	118.60317	
C9 C10 C1	120.7(5)	120.39144	
C9 C10 H10A	119.7	121.56613	
C1 C10 H10A	119.7	118.04233	
N1 C11 C1	122.0(5)	122.96731	
N1 C11 H11A	119.0	121.54447	
C1 C11 H11A	119.0	115.48818	
N1 C12 C14	109.8(5)	110.45749	
N1 C12 C13	109.0(5)	108.59162	
C14 C12 C13	110.1(5)	110.74057	
N1 C12 H12A	109.3	110.79209	
C14 C12 H12A	109.3	107.81728	
C13 C12 H12A	109.3	108.42669	
C12 C13 H13A	109.5	110.45985	
C12 C13 H13B	109.5	109.96850	
H13A C13 H13B	109.5	108.51806	
C12 C13 H13C	109.5	110.49556	
H13A C13 H13C	109.5	108.86260	
H13B C13 H13C	109.5	108.48187	
C15 C14 C19	117.6(5)	118.68640	
C15 C14 C12	120.6(6)	119.98365	
C19 C14 C12	121.7(5)	121.29797	
C14 C15 C16	121.8(6)	121.19824	
C14 C15 H15A	119.1	119.62378	
C16 C15 H15A	119.1	119.17751	
C17 C16 C15	118.3(6)	118.57310	
C17 C16 H16A	120.8	119.62889	
C15 C16 H16A	120.8	121.79618	
C16 C17 C18	122.8(6)	121.77065	
C16 C17 F1	118.6(7)	119.08388	
C18 C17 F1	118.6(7)	119.14448	
C17 C18 C19	118.7(6)	118.87949	
C17 C18 H18A	120.7	119.46526	
C19 C18 H18A	120.7	121.65480	
C18 C19 C14	120.9(6)	120.89056	
C18 C19 H19A	119.5	120.10912	
C14 C19 H19A	119.5	118.99383	0.95965786
C10 C1 C2 C3	2.0(7)	0.19337	
C11 C1 C2 C3	-175.6(4)	-179.75204	
C1 C2 C3 C4	177.6(4)	179.87004	
C1 C2 C3 C8	0.1(7)	-0.10212	
C2 C3 C4 C5	-175.7(5)	-179.95739	
C8 C3 C4 C5	1.7(7)	0.01470	

C3 C4 C5 C6	-0.9(9)	-0.02024	
C4 C5 C6 C7	-0.8(9)	0.00650	
C5 C6 C7 C8	1.5(9)	0.01274	
C6 C7 C8 C9	178.8(5)	-179.99932	
C6 C7 C8 C3	-0.6(8)	-0.01785	
C4 C3 C8 C9	179.6(5)	179.98637	
C2 C3 C8 C9	-2.8(6)	-0.04057	
C4 C3 C8 C7	-1.0(7)	0.00423	
C2 C3 C8 C7	176.6(5)	179.97729	
C7 C8 C9 C10	-176.0(5)	-179.92749	
C3 C8 C9 C10	3.4(7)	0.09102	
C8 C9 C10 C1	-1.3(8)	-0.00096	
C2 C1 C10 C9	-1.5(7)	-0.14170	
C11 C1 C10 C9	176.1(5)	179.80298	
C12 N1 C11 C1	-178.4(4)	179.16131	
C2 C1 C11 N1	178.4(4)	178.53447	
C10 C1 C11 N1	0.9(7)	-1.41019	
C11 N1 C12 C14	134.2(5)	123.17434	
C11 N1 C12 C13	-105.2(6)	-115.20676	
N1 C12 C14 C15	-150.1(5)	-148.48630	
C13 C12 C14 C15	90.0(7)	91.17412	
N1 C12 C14 C19	33.7(7)	33.59768	
C13 C12 C14 C19	-86.2(7)	-86.74190	
C19 C14 C15 C16	0.4(8)	0.43953	
C12 C14 C15 C16	-175.9(5)	-177.53065	
C14 C15 C16 C17	-0.2(9)	-0.25738	
C15 C16 C17 C18	-0.6(9)	-0.11017	
C15 C16 C17 F1	179.1(5)	-179.74501	
C16 C17 C18 C19	1.0(9)	0.28169	
F1 C17 C18 C19	-178.6(5)	179.91631	
C17 C18 C19 C14	-0.8(8)	-0.09029	
C15 C14 C19 C18	0.1(8)	-0.26208	
C12 C14 C19 C18	176.3(5)	177.68031	3.04837903
$RMSD_{tot}$			1.72332805
(c) **I–Cl**			
Cl1 C17	1.746(6)	1.74185	
N1 C11	1.266(5)	1.26699	
N1 C12	1.473(6)	1.44791	
C1 C2	1.369(5)	1.37616	
C1 C10	1.428(5)	1.41876	
C1 C11	1.461(5)	1.46488	
C2 C3	1.413(5)	1.41319	
C2 H2A	0.9300	1.08739	
C3 C4	1.413(5)	1.41474	
C3 C8	1.432(5)	1.42444	
C4 C5	1.365(6)	1.37088	

C4 H4A	0.9300	1.08594	
C5 C6	1.405(7)	1.40988	
C5 H5A	0.9300	1.08486	
C6 C7	1.367(6)	1.37189	
C6 H6A	0.9300	1.08496	
C7 C8	1.415(5)	1.41282	
C7 H7A	0.9300	1.08586	
C8 C9	1.413(5)	1.41907	
C9 C10	1.351(5)	1.36492	
C9 H9A	0.9300	1.08602	
C10 H10A	0.9300	1.08381	
C11 H11A	0.9300	1.10247	
C12 C13	1.523(7)	1.53114	
C12 C14	1.524(7)	1.51508	
C12 H12A	0.9800	1.10374	
C13 H13A	0.9600	1.09340	
C13 H13B	0.9600	1.09299	
C13 H13C	0.9600	1.09279	
C14 C19	1.378(7)	1.39278	
C14 C15	1.387(6)	1.39338	
C15 C16	1.391(7)	1.38813	
C15 H15A	0.9300	1.08388	
C16 C17	1.356(8)	1.38757	
C16 H16A	0.9300	1.08362	
C17 C18	1.377(8)	1.38692	
C18 C19	1.388(8)	1.38872	
C18 H18A	0.9300	1.08347	
C19 H19A	0.9300	1.08658	0.09681894
C11 N1 C12	117.0(4)	117.92634	
C2 C1 C10	118.3(4)	119.56175	
C2 C1 C11	120.1(3)	119.48036	
C10 C1 C11	121.6(4)	120.95788	
C1 C2 C3	122.4(3)	121.36634	
C1 C2 H2A	118.8	119.84149	
C3 C2 H2A	118.8	118.79210	
C2 C3 C4	123.2(3)	122.19172	
C2 C3 C8	118.4(3)	118.77379	
C4 C3 C8	118.4(3)	119.03449	
C5 C4 C3	121.5(4)	120.71234	
C5 C4 H4A	119.3	120.45037	
C3 C4 H4A	119.3	118.83728	
C4 C5 C6	120.0(4)	120.24080	
C4 C5 H5A	120.0	120.11344	
C6 C5 H5A	120.0	119.64576	
C7 C6 C5	120.5(4)	120.36237	
C7 C6 H6A	119.8	120.03453	
C5 C6 H6A	119.8	119.60310	
C6 C7 C8	121.1(4)	120.75471	

C6 C7 H7A	119.5	120.43805	
C8 C7 H7A	119.5	118.80723	
C9 C8 C7	123.2(4)	122.31830	
C9 C8 C3	118.2(4)	118.78638	
C7 C8 C3	118.5(4)	118.89529	
C10 C9 C8	121.8(4)	121.13266	
C10 C9 H9A	119.1	120.26196	
C8 C9 H9A	119.1	118.60534	
C9 C10 C1	120.9(4)	120.37885	
C9 C10 H10A	119.5	121.55349	
C1 C10 H10A	119.5	118.06756	
N1 C11 C1	123.4(4)	123.03896	
N1 C11 H11A	118.3	121.49693	
C1 C11 H11A	118.3	115.46410	
N1 C12 C13	109.2(5)	108.64251	
N1 C12 C14	107.4(4)	110.50786	
C13 C12 C14	114.8(4)	110.54207	
N1 C12 H12A	108.4	110.84220	
C13 C12 H12A	108.4	108.41609	
C14 C12 H12A	108.4	107.87159	
C12 C13 H13A	109.5	110.41999	
C12 C13 H13B	109.5	110.50069	
H13A C13 H13B	109.5	108.87436	
C12 C13 H13C	109.5	109.97462	
H13A C13 H13C	109.5	108.48711	
H13B C13 H13C	109.5	108.53061	
C19 C14 C15	117.7(5)	118.59954	
C19 C14 C12	120.5(5)	120.03805	
C15 C14 C12	121.7(5)	121.32850	
C14 C15 C16	121.2(5)	120.92809	
C14 C15 H15A	119.4	119.04067	
C16 C15 H15A	119.4	120.02558	
C17 C16 C15	119.3(5)	119.31906	
C17 C16 H16A	120.3	119.89160	
C15 C16 H16A	120.3	120.78905	
C16 C17 C18	121.3(6)	120.90135	
C16 C17 Cl1	119.5(5)	119.57806	
C18 C17 Cl1	119.2(5)	119.51971	
C17 C18 C19	118.7(5)	119.03920	
C17 C18 H18A	120.6	120.03852	
C19 C18 H18A	120.6	120.92084	
C14 C19 C18	121.7(5)	121.21146	
C14 C19 H19A	119.1	119.70210	
C18 C19 H19A	119.1	119.08597	1.128413162
C10 C1 C2 C3	-2.5(5)	-0.09970	
C11 C1 C2 C3	176.0(3)	179.92696	
C1 C2 C3 C4	-177.3(3)	179.97899	
C1 C2 C3 C8	1.9(5)	-0.03985	

C2 C3 C4 C5	177.4(4)	179.97641	
C8 C3 C4 C5	-1.8(5)	-0.00470	
C3 C4 C5 C6	1.4(6)	-0.01907	
C4 C5 C6 C7	-0.4(6)	0.01802	
C5 C6 C7 C8	-0.3(6)	0.00731	
C6 C7 C8 C9	-177.9(4)	179.89938	
C6 C7 C8 C3	-0.1(6)	-0.03072	
C2 C3 C8 C9	-0.2(5)	0.11487	
C4 C3 C8 C9	179.0(3)	-179.90336	
C2 C3 C8 C7	-178.1(3)	-179.95253	
C4 C3 C8 C7	1.1(5)	0.02924	
C7 C8 C9 C10	176.9(4)	-179.98091	
C3 C8 C9 C10	-0.8(5)	-0.05073	
C8 C9 C10 C1	0.2(6)	-0.08990	
C2 C1 C10 C9	1.4(5)	0.16596	
C11 C1 C10 C9	-177.1(4)	-179.86110	
C12 N1 C11 C1	177.4(4)	-178.92816	
C2 C1 C11 N1	-174.8(4)	-179.50971	
C10 C1 C11 N1	3.6(6)	0.51732	
C11 N1 C12 C13	130.7(5)	113.39712	
C11 N1 C12 C14	-104.2(5)	-125.16520	
N1 C12 C14 C19	97.9(5)	149.24992	
C13 C12 C14 C19	-140.5(5)	-90.44341	
N1 C12 C14 C15	-77.9(6)	-32.89788	
C13 C12 C14 C15	43.8(6)	87.40879	
C19 C14 C15 C16	-0.7(7)	0.25166	
C12 C14 C15 C16	175.2(4)	-177.63062	
C14 C15 C16 C17	0.3(8)	0.06701	
C15 C16 C17 C18	-0.2(8)	-0.24603	
C15 C16 C17 Cl1	179.7(4)	-179.90243	
C16 C17 C18 C19	0.6(8)	0.09903	
Cl1 C17 C18 C19	-179.3(4)	179.75562	
C15 C14 C19 C18	1.1(7)	-0.40311	
C12 C14 C19 C18	-174.9(4)	177.50730	
C17 C18 C19 C14	-1.0(8)	0.23114	16.04746053
$RMSD_{tot}$			8.444173096
(d) **I–Br**			
Br1 C17	1.887(6)	1.89750	
N1 C11	1.267(6)	1.26701	
N1 C12	1.477(6)	1.44816	
C1 C2	1.369(6)	1.37615	
C1 C10	1.418(6)	1.41882	
C1 C11	1.459(6)	1.46490	
C2 C3	1.421(6)	1.41331	
C2 H2A	0.9300	1.08737	
C3 C4	1.408(6)	1.41471	

C3 C8	1.420(6)	1.42466	
C4 C5	1.358(7)	1.37092	
C4 H4A	0.9300	1.08592	
C5 C6	1.393(8)	1.40998	
C5 H5A	0.9300	1.08486	
C6 C7	1.366(7)	1.37181	
C6 H6A	0.9300	1.08496	
C7 C8	1.412(7)	1.41278	
C7 H7A	0.9300	1.08584	
C8 C9	1.417(6)	1.41892	
C9 C10	1.352(6)	1.36484	
C9 H9A	0.9300	1.08599	
C10 H10A	0.9300	1.08383	
C11 H11A	0.9300	1.10246	
C12 C14	1.515(8)	1.51516	
C12 C13	1.527(8)	1.53064	
C12 H12A	0.9800	1.10367	
C13 H13A	0.9600	1.09300	
C13 H13B	0.9600	1.09279	
C13 H13C	0.9600	1.09338	
C14 C15	1.379(7)	1.39254	
C14 C19	1.386(7)	1.39360	
C15 C16	1.380(8)	1.38944	
C15 H15A	0.9300	1.08660	
C16 C17	1.386(8)	1.38718	
C16 H16A	0.9300	1.08341	
C17 C18	1.369(8)	1.38815	
C18 C19	1.388(8)	1.38842	
C18 H18A	0.9300	1.08352	
C19 H19A	0.9300	1.08404	0.09679236
C11 N1 C12	116.8(5)	117.98573	
C2 C1 C10	118.6(4)	119.58264	
C2 C1 C11	119.2(4)	119.55475	
C10 C1 C11	122.2(4)	120.86259	
C1 C2 C3	122.2(4)	121.35039	
C1 C2 H2A	118.9	119.83271	
C3 C2 H2A	118.9	118.81677	
C4 C3 C8	119.2(4)	119.03745	
C4 C3 C2	122.9(4)	122.20433	
C8 C3 C2	117.9(4)	118.75821	
C5 C4 C3	120.4(5)	120.70826	
C5 C4 H4A	119.8	120.47492	
C3 C4 H4A	119.8	118.81681	
C4 C5 C6	120.8(5)	120.24106	
C4 C5 H5A	119.6	120.10709	
C6 C5 H5A	119.6	119.65185	
C7 C6 C5	120.5(5)	120.36480	
C7 C6 H6A	119.8	120.04282	

C5 C6 H6A	119.8	119.59238	
C6 C7 C8	120.5(5)	120.75838	
C6 C7 H7A	119.8	120.42591	
C8 C7 H7A	119.8	118.81568	
C7 C8 C9	122.3(4)	122.29783	
C7 C8 C3	118.6(4)	118.89004	
C9 C8 C3	119.1(4)	118.81213	
C10 C9 C8	121.0(4)	121.11873	
C10 C9 H9A	119.5	120.29479	
C8 C9 H9A	119.5	118.58648	
C9 C10 C1	121.2(4)	120.37761	
C9 C10 H10A	119.4	121.55875	
C1 C10 H10A	119.4	118.06355	
N1 C11 C1	122.7(5)	122.97102	
N1 C11 H11A	118.6	121.52993	
C1 C11 H11A	118.6	115.49901	
N1 C12 C14	107.1(4)	110.35360	
N1 C12 C13	108.8(5)	108.68175	
C14 C12 C13	115.5(5)	110.60745	
N1 C12 H12A	108.4	110.87513	
C14 C12 H12A	108.4	107.81956	
C13 C12 H12A	108.4	108.48926	
C12 C13 H13A	109.5	110.53016	
C12 C13 H13B	109.5	109.97307	
H13A C13 H13B	109.5	108.53821	
C12 C13 H13C	109.5	110.40028	
H13A C13 H13C	109.5	108.88145	
H13B C13 H13C	109.5	108.46377	
C15 C14 C19	118.0(6)	118.62726	
C15 C14 C12	120.4(5)	120.12852	
C19 C14 C12	121.6(5)	121.21309	
C14 C15 C16	121.6(6)	121.22305	
C14 C15 H15A	119.2	119.69878	
C16 C15 H15A	119.2	119.07780	
C15 C16 C17	119.1(5)	118.97484	
C15 C16 H16A	120.5	120.69175	
C17 C16 H16A	120.5	120.33219	
C18 C17 C16	120.8(6)	120.97775	
C18 C17 Br1	119.9(5)	119.54187	
C16 C17 Br1	119.3(4)	120.97775	
C17 C18 C19	119.1(6)	119.25286	
C17 C18 H18A	120.5	120.15238	
C19 C18 H18A	120.5	120.59437	
C14 C19 C18	121.4(5)	120.94282	
C14 C19 H19A	119.3	119.09743	
C18 C19 H19A	119.3	119.95288	1.1739708
C10 C1 C2 C3	-1.9(7)	-0.20027	
C11 C1 C2 C3	175.8(4)	179.74200	

C1 C2 C3 C4	-177.3(4)	-179.83897	
C1 C2 C3 C8	1.5(6)	0.15722	
C8 C3 C4 C5	-1.0(7)	-0.01243	
C2 C3 C4 C5	177.9(5)	179.98375	
C3 C4 C5 C6	0.0(8)	0.02209	
C4 C5 C6 C7	1.0(8)	-0.00766	
C5 C6 C7 C8	-1.0(8)	-0.01651	
C6 C7 C8 C9	-178.1(5)	-179.96544	
C6 C7 C8 C3	0.0(7)	0.02566	
C4 C3 C8 C7	0.9(6)	-0.01124	
C2 C3 C8 C7	-178.0(4)	179.99246	
C4 C3 C8 C9	179.1(4)	179.98018	
C2 C3 C8 C9	0.2(6)	-0.01613	
C7 C8 C9 C10	176.5(5)	179.91106	
C3 C8 C9 C10	-1.7(7)	-0.08005	
C8 C9 C10 C1	1.4(7)	0.03905	
C2 C1 C10 C9	0.4(7)	0.10118	
C11 C1 C10 C9	-177.2(4)	-179.84032	
C12 N1 C11 C1	177.4(5)	-179.28507	
C2 C1 C11 N1	-174.6(5)	-178.23575	
C10 C1 C11 N1	3.0(7)	1.70576	
C11 N1 C12 C14	-104.2(5)	-122.39017	
C11 N1 C12 C13	130.3(5)	116.16230	
N1 C12 C14 C15	98.1(6)	147.12127	
C13 C12 C14 C15	-140.6(6)	-92.58109	
N1 C12 C14 C19	-79.2(6)	-34.93602	
C13 C12 C14 C19	42.1(7)	85.36163	
C19 C14 C15 C16	1.7(8)	-0.41535	
C12 C14 C15 C16	-175.7(5)	177.58014	
C14 C15 C16 C17	-0.8(8)	0.21654	
C15 C16 C17 C18	-0.2(8)	0.12882	
C15 C16 C17 Br1	-178.5(4)	179.77812	
C16 C17 C18 C19	0.3(8)	-0.26360	
Br1 C17 C18 C19	178.6(4)	-179.91268	
C15 C14 C19 C18	-1.6(7)	0.27630	
C12 C14 C19 C18	175.7(5)	-177.69656	
C17 C18 C19 C14	0.6(8)	0.05686	15.4142874
$RMSD_{tot}$			8.1166585

Electronic Circular Dichroism (ECD) calculations

Structure determination is mostly achieved by interpretation of MS (mass spectrometry), NMR (nuclear magnetic resonance) data [ref1], Theoretical Calculation of Electronic Circular Dichroism [ref2, ref3] and stereochemical assignments are generally the most time consuming step within this procedure. The calculations of electronic circular dichroism (ECD) are altenative to determine absolute configuration of chiral molecules. The quantum chemistry methods including time dependent density functional theory (TD-DFT) can be used to calculate or predict the ECD of chiral molecules. In this study, the calculations showed that both conformations *R* and *S* of the fluorine-containing system (**I**–**F**) have the same Gibbs free energy values. However, theoretical calculation of its ECD by using the TD-PBE1PBE/6-311G(d,p) theory level was employed to calculate rotatory strength R in the dipole velocity form (R_{vel}) and dipole length form (R_{len}) and excitation energy (in nm) to establish the most favored configuration. Thus, we calculated the ECD and UV spectra of conformers of the **I**–**F** compound to verify the assignment of *R*-(**I**–**F**) over *S*-(**I**–**F**) configuration. Experimentally a R chiral compound was prefered in crystalography, it is reasonably perceived that the calculated ECD of the major conformer should reflect when the configuracions are correct and appropriate. The simulated ECD theoretical spectra of R- and *S*-(**I**–**F**) enantiomers are shown in Figure 3. In the ECD curve of *R*-(**I**–**F**), the diagnostic Cotton effects (CEs) were two strong negative signals with Rotational strengths of -59.11 and -46.63 cgs, while for *S*-(**I**–**F**) the ECD spectrum was opposite to that of *R*-(**I**–**F**) with slightly weaker intensities of 59.10 and 46.62 cgs consistent with the optical rotation results and concluded that the *R*-(**I**–**F**) and *S*-(**I**–**F**) absolute configurations assigned to **I**–**F** system may be present crystallographically on theoretical study in gas phas. Table 3 presents the results that the two conformers exist crystallographically since the Gibbs free energies, wavelength, oscillator strength, rotatory strength in velocity form and rotatory strength in length form are practically the same but of the opposite sign.

[ref1] Breton, R.C.; Reynolds, W.F. Using NMR to identify and characterize natural products. *Nat. Prod. Rep.* 2013, *30*, 501–524.

[ref2] Ding, Y.; Li, Xing-Cong; Ferreira D. Theoretical Calculation of Electronic Circular Dichroism of the Rotationally Restricted 3,8-Biflavonoid Morelloflavone. *J. Org. Chem.* **2007**, 72, 24, 9010-9017.

[ref3] Li, L.; Wang, L.; Si, Y. Electronic circular dichroism behavior of chiral Phthiobuzone. *Acta Pharm. Sin. B.* **2014**, 4(2), 167-171.

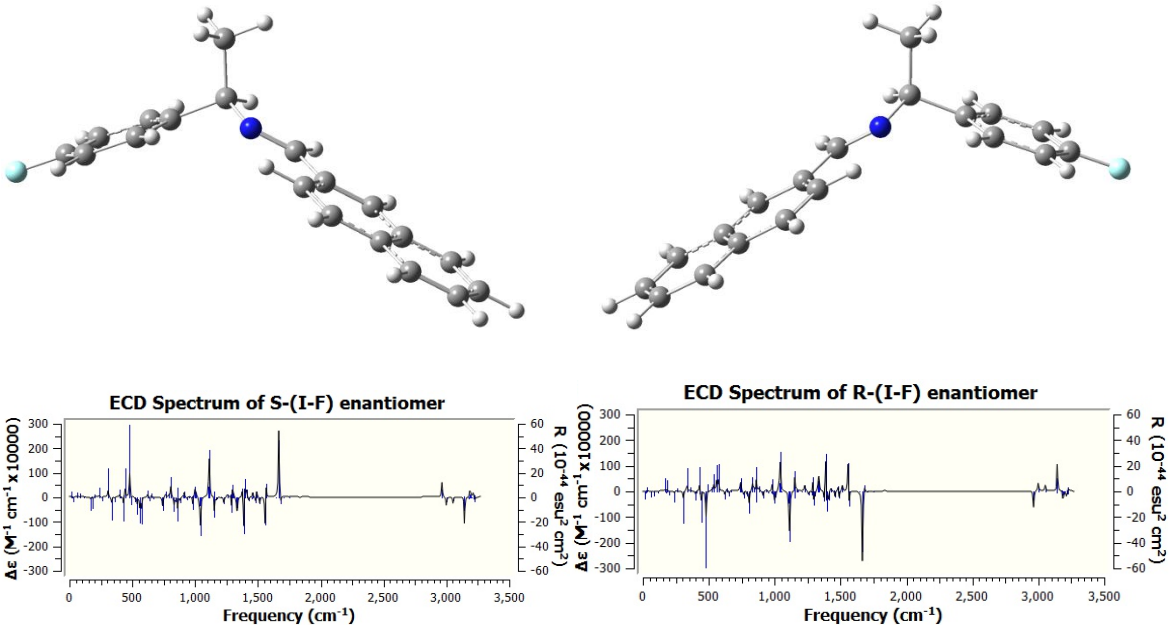


Figure S3. Structures and comparison between calculated ECD spectra of *R*- and *S*-(**I**–**F**) enantiomers at PBE1PBE/6-311G(d,p) theory level.

Table S3. Gibbs free energies, transitions, oscillator strengths and their related rotatory (Rotatory strength in velocity form and Rotatory strength in length form) in the ECD spectra of compound (**I**–**F**) at the PBE1PBE/6-311G(d,p) theory level.

Enantiomer	G^0(u.a.)	Transition	ΔE_g(eV)	λ(nm)	Oscillator strength	R_{vel} (10^{-40}cgs)	R_{len} (10^{-40}cgs)
R-(**I**–**F**)	-887.1774	73 → 74	4.13	300.6	0.076	9.973	8.216
		73 → 75	4.41	281.1	0.145	18.863	14.807
		69 → 74	4.47	277.4	0.004	-10.911	-12.454
		72 → 74	4.61	269.0	0.009	6.424	6.967
		71 → 74	5.13	241.7	1.058	-87.763	-73.342
S-(**I**–**F**)	-887.1774	73 → 74	4.13	300.6	0.076	-9.929	-8.173
		73 → 75	4.41	281.1	0.145	-18.800	-14.739
		69 → 74	4.47	277.4	0.004	10.831	12.369
		72 → 74	4.61	269.0	0.009	-6.425	-6.969
		71 → 74	5.13	241.7	1.058	87.688	73.279

Table S4. Ring tilt angle **(θ_{tilt},** degrees**),** Molecular Orbital Energies (E_{HOMO} and E_{LUMO}, hartrees), gap Energies (ΔE_g, eV), total energy (E_{Tot}, hartrees) and dipole moment (Debyes) for **I**, **I–F, I–Cl** and **I–Br** compounds calculated at PBE1PBE/6-311G(d,p) and PBE1PBE-D3/6-311G(d,p) theory levels.

PBE1PBE/6-311G(d,p)						
Compound	θ_{tilt}	E_{HOMO}	E_{LUMO}	ΔE_g	E_{Tot}	μ
I	145.33 (142.01[a])	-0.2350	-0.0566	4.8535	-788.2530	1.4943
I–F	33.59 (33.72 [a])	-0.2371	-0.0591	4.8431	-887.4288	2.9426
I–Cl	149.25 (97.72 [a])	-0.2382	-0.0605	4.8347	-1247.7157	3.5991
I–Br	147.12 (98.08 [a])	-0.2380	-0.0604	4.8341	-3361.4753	3.4362
PBE1PBE-D3/6-311G(d,p)						
Compound	θ_{tilt}	E_{HOMO}	E_{LUMO}	ΔE_g	E_{Tot}	μ
I	145.89	-0.2349	-0.0565	4.8545	-788.2720	1.4802
I–F	36.42	-0.2369	-0.0589	4.8439	-887.4482	2.9018
I–Cl	148.64	-0.2381	-0.0603	4.8360	-1247.7359	3.5188
I–Br	148.93	-0.2381	-0.0604	4.8349	-3361.4959	3.4611

[a]Ring tilt N-C_{chiral}-C_{ring}-C_{ring} of compounds of X-ray data.

[ref1] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parameterization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, *J. Chem. Phys*., **2010**, *132*, 154104.