Electronic supplementary information

Fluorine Substitution Effects of Halide Anion Receptors Based on Combination of Distinct Hydrogen Bond and Anion-π Noncovalent Interactions: A Theoretical Investigation

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eigenvalue (Right) of **1**@F^-, **2**@F^-, **4**@F^- and **6**@F^-.

Table S1 Cartesian coordinates of **1**@Cl^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-4.78342400	-4.34340700	0.36662800
C	-6.06896900	-3.96966300	0.25243900
H	-4.57442100	-5.38297100	0.62460200
H	-6.36428200	-2.95495300	-0.00104300
H	-6.87197200	-4.68356300	0.41308600
C	-1.22399500	-1.97954900	-0.14612800
C	-2.50046700	-1.37892900	-0.30184600
C	-3.64693100	-2.14590400	-0.14012000
C	-3.58730800	-3.51295500	0.18578500
C	-2.31708400	-4.08454300	0.34651400
C	-1.15102300	-3.34106600	0.18498700
N	-0.08680100	-1.18143100	-0.34097000
C	-2.58274900	0.09984900	-0.60428100
H	-4.60393500	-1.65376700	-0.26619500
H	-2.23531400	-5.13922900	0.60221100
H	-0.18143400	-3.79780300	0.32285000
H	-0.19652500	-0.30045700	-0.85834800
C	1.21110300	-1.47277500	0.03660900
N	2.08039700	-0.46965900	-0.37385000
O	1.55625200	-2.47605000	0.65912500
H	1.65327900	0.31077100	-0.90683600
C	5.44387300	0.95554500	-0.50709300
C	4.08551400	0.76826200	-0.68107200
C	3.43728500	-0.37608000	-0.15221900
C	4.20060400	-1.33129700	0.55846300
C	5.56344100	-1.13793800	0.72952800
C	6.18516000	-0.00099600	0.20131800
H	5.94205100	1.82921000	-0.90927700
H	3.49374800	1.49803700	-1.22691500
H	3.70885500	-2.20448600	0.96232400
H	6.15715000	-1.86299900	1.27315900
N	7.60653500	0.18994500	0.38828600
O	8.13251700	1.20877300	-0.08539400
O	8.24184100	-0.67236100	1.01466600
O	-3.95873600	0.48669200	-0.77469200
H	-2.12151400	0.67280600	0.20551200
H	-2.04829200	0.35522600	-1.52466700
C	-4.51457300	1.58899800	-0.21698300
O	-5.72793300	1.63694300	-0.13520600
C	-1.72732700	4.18364000	0.06560200
C	-2.16253600	4.89870900	1.18247000
C	-3.34698900	4.52905700	1.83161300
C	-4.08911600	3.44712500	1.36383800
C	-3.64416200	2.71255400	0.25230500
C	-2.46431600	3.09388800	-0.40125500
H	-0.80391100	4.44201300	-0.44349600
H	-1.58028700	5.73940900	1.55190700
H	-3.68946800	5.08354300	2.70175000
H	-5.01653500	3.15568700	1.84666000
H	-2.08544000	2.55592500	-1.26233700
Cl	0.37469100	1.63991100	-1.92293000

Table S2 Cartesian coordinates of **2**@Cl^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-4.28624500	-4.84488800	0.47016200
C	-5.59129200	-4.59336200	0.27334700
H	-4.00373100	-5.84319900	0.80841500
H	-5.95857900	-3.62746900	-0.06334800
H	-6.33816000	-5.36273300	0.44785300
C	-0.91455100	-2.22102900	-0.05685700
C	-2.22884300	-1.74273500	-0.29951800
C	-3.31396500	-2.59326900	-0.13213600
C	-3.15641000	-3.92730700	0.28439500
C	-1.85165800	-4.37642400	0.53236200
C	-0.74501800	-3.54799800	0.36739600
N	0.16071100	-1.34398400	-0.26332500
C	-2.42154500	-0.29876400	-0.70317700
H	-4.30206700	-2.19465800	-0.32828400
H	-1.69384600	-5.40219800	0.85982600
H	0.25169000	-3.91146700	0.57183700
H	-0.00370600	-0.50115600	-0.82689400
C	1.47266300	-1.52163100	0.13861900
N	2.27281000	-0.48158300	-0.31642600
O	1.88157900	-2.46467900	0.81402300
H	1.79862100	0.23773000	-0.89278200
C	5.54184000	1.13753000	-0.55259700
C	4.19683400	0.85782500	-0.70565600
C	3.62196400	-0.29070400	-0.10628400
C	4.44408900	-1.15273000	0.65559900
C	5.79312400	-0.86647500	0.80606200
C	6.34233400	0.27207300	0.20625100
H	5.98444000	2.01390800	-1.01004900
H	3.56027200	1.51578600	-1.29093400
H	4.00902000	-2.02943700	1.11332900
H	6.43168800	-1.51990700	1.38831100
N	7.75061600	0.55994600	0.37061800
O	8.21171800	1.57642100	-0.17042400
O	8.43889100	-0.22088000	1.04557300
O	-3.81651400	-0.04829600	-0.96134700
H	-2.05484400	0.36393300	0.08633300
H	-1.86561800	-0.05534500	-1.61391600
C	-4.49063400	1.04038900	-0.52736800
O	-5.70590700	0.99260400	-0.50325700
C	-1.95038900	3.88894800	-0.33621900
C	-2.50764100	4.66449100	0.68123100
C	-3.68818300	4.22427300	1.27155200
C	-4.32471100	3.05544400	0.89401000
C	-3.74330900	2.27410000	-0.11869100
C	-2.56244100	2.70028700	-0.73987100
H	-1.02114700	4.18358900	-0.81332100
H	-2.04472600	5.58546500	1.02140900
H	-5.25306600	2.75029400	1.36322500
H	-2.08444200	2.12603600	-1.52382100
F	-4.24120000	4.98014700	2.26573200
Cl	0.44563600	1.42348400	-1.99041700

Table S3 Cartesian coordinates of **3**@Cl^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	4.37754800	-4.67393900	-0.40788900
C	5.67663600	-4.40010200	-0.20092000
H	4.10896200	-5.69491700	-0.68439000
H	6.03077400	-3.41117000	0.07806700
H	6.43146400	-5.17441000	-0.30565700
C	0.98220600	-2.04460600	-0.14905000
C	2.28020900	-1.54857500	0.13521400
C	3.37466400	-2.40088600	0.04271800
C	3.23766300	-3.75521500	-0.30925200
C	1.94272400	-4.23033700	-0.56300900
C	0.83036700	-3.39792100	-0.48785700
N	-0.09713000	-1.15111500	-0.10315400
C	2.45122800	-0.10466300	0.55447400
H	4.35190900	-1.99647700	0.27694400
H	1.80039100	-5.27547900	-0.83104000
H	-0.16082800	-3.78360700	-0.68057400
H	0.09542800	-0.15048900	-0.25784200
C	-1.43620500	-1.47958700	-0.00862200
N	-2.23081000	-0.34551500	-0.12560000
O	-1.87295300	-2.61660500	0.16518700
H	-1.72365300	0.54213700	-0.30578100
C	-5.52889500	1.22841500	-0.17131600
C	-4.16165000	1.03516000	-0.22750500
C	-3.60284600	-0.25615200	-0.05292500
C	-4.46628100	-1.35179500	0.18219700
C	-5.83747800	-1.15137900	0.23833100
C	-6.37005500	0.13090800	0.06257800
H	-5.95857200	2.21371900	-0.30471700
H	-3.49321700	1.87259100	-0.40788400
H	-4.04313800	-2.33718400	0.31451900
H	-6.50749800	-1.98349400	0.41842200
N	-7.80116900	0.32679300	0.12316900
O	-8.24735200	1.47382600	-0.03484800
O	-8.52538000	-0.65936100	0.33064400
O	3.79873500	0.08363700	1.03866600
H	2.24456200	0.58292400	-0.27183600
H	1.76376300	0.15123800	1.36540600
C	4.55145700	1.15507100	0.72155300
O	5.75333500	1.10443300	0.89783200
C	2.21505600	4.14421000	0.23039800
C	2.73000300	4.67418800	-0.95071100
C	3.83000000	4.07635700	-1.57575600
C	4.40849700	2.93757600	-1.02177900
C	3.88824900	2.36983100	0.15144300
C	2.80873100	3.00847100	0.75988200
F	2.32963000	2.51079900	1.92772100
H	1.34482500	4.56341300	0.72049600
H	2.25772800	5.54681200	-1.39237800
H	5.26608900	2.46310600	-1.48874000
H	4.22726900	4.49164300	-2.49745300
Cl	-0.26124900	2.00551200	-0.66170400

Table S4 Cartesian coordinates of **4**@Cl^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-3.99836500	-5.20615000	0.53852100
C	-5.31277300	-5.01294400	0.33836500
H	-3.67392100	-6.18621000	0.89205800
H	-5.72053700	-4.06846400	-0.01221400
H	-6.02652700	-5.81048500	0.52446800
C	-0.74075900	-2.44895400	-0.02709300
C	-2.07355100	-2.03361500	-0.28454200
C	-3.12165600	-2.92690100	-0.10518500
C	-2.90845300	-4.24423000	0.33876800
C	-1.58663800	-4.63083800	0.60127800
C	-0.51608700	-3.75854300	0.42464000
N	0.29596200	-1.52989300	-0.24722000
C	-2.32611900	-0.60788900	-0.71833900
H	-4.12495500	-2.57576500	-0.31440600
H	-1.38600900	-5.64203300	0.94992700
H	0.49435900	-4.07430900	0.64064100
H	0.09621500	-0.70473800	-0.82464700
C	1.61437100	-1.64381500	0.15790400
N	2.36924200	-0.57814900	-0.31415200
O	2.06260600	-2.55723400	0.84861800
H	1.86556400	0.11140000	-0.90040800
C	5.56891700	1.16970700	-0.58613300
C	4.23640100	0.83175800	-0.73173400
C	3.71000300	-0.32729300	-0.10920100
C	4.56685500	-1.13917100	0.66889100
C	5.90307400	-0.79446400	0.81209600
C	6.40446600	0.35322300	0.18870100
H	5.97455200	2.05442800	-1.06143000
H	3.57320900	1.45172900	-1.32878900
H	4.16865000	-2.02377900	1.14465800
H	6.56833700	-1.40899100	1.40665000
N	7.80042300	0.70171500	0.34505100
O	8.21922100	1.72405600	-0.21832800
O	8.51987700	-0.03599900	1.03551800
O	-3.72928700	-0.42209200	-0.98709900
H	-1.99223400	0.08523500	0.05967400
H	-1.77677300	-0.35974600	-1.63176400
C	-4.45241400	0.64388400	-0.57835800
O	-5.66398100	0.53789200	-0.54200500
C	-2.04168300	3.61379600	-0.47001800
C	-2.67677400	4.38777700	0.48800300
C	-3.85500100	3.94478500	1.09125100
C	-4.40999200	2.72733300	0.74538300
C	-3.76706100	1.92495000	-0.21287900
C	-2.59112000	2.38011400	-0.82335300
F	-4.45190500	4.72827500	2.02255800
H	-1.11519200	3.94835500	-0.92467800
H	-5.33612700	2.40114300	1.20530700
H	-2.06090800	1.79901300	-1.56777100
F	-2.16508800	5.58337200	0.85698000
Cl	0.45556000	1.22674000	-2.01378200

Table S5 Cartesian coordinates of **5**@Cl^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-3.99921500	-5.02394600	0.50582300
C	-5.30595500	-4.82836400	0.26210200
H	-3.68406200	-6.01564500	0.83452400
H	-5.70507900	-3.87251500	-0.06697400
H	-6.02183000	-5.63580500	0.38763300
C	-0.74109700	-2.23161000	0.19257600
C	-2.05433200	-1.82394600	-0.15477200
C	-3.10456900	-2.72803600	-0.04519400
C	-2.90687900	-4.05133200	0.38683400
C	-1.59708600	-4.43999100	0.70354200
C	-0.52853100	-3.55346500	0.61258200
N	0.29074700	-1.28513600	0.12245000
C	-2.28597000	-0.41710300	-0.66065300
H	-4.09403100	-2.39176000	-0.33015700
H	-1.40802300	-5.45929700	1.03458600
H	0.47525000	-3.87315100	0.85459300
H	0.04190500	-0.28912300	0.20897800
C	1.64744400	-1.54569000	0.07398600
N	2.37791500	-0.36525300	0.13425100
O	2.14711000	-2.66583700	-0.02010600
H	1.82140600	0.50294200	0.24559500
C	5.58415200	1.38920800	0.11340400
C	4.22875400	1.12410200	0.16598400
C	3.74466600	-0.20513500	0.07451800
C	4.67034900	-1.26452000	-0.07174000
C	6.02941400	-0.99217000	-0.12449100
C	6.48763100	0.32687800	-0.03298800
H	5.95700600	2.40379900	0.18301800
H	3.51292200	1.93369400	0.27892600
H	4.30429900	-2.27883600	-0.14036200
H	6.74695000	-1.79605600	-0.23714700
N	7.90701500	0.59787400	-0.09017800
O	8.28651700	1.77621500	-0.00798200
O	8.68723000	-0.35824400	-0.21918200
O	-3.63157000	-0.32199600	-1.17910800
H	-2.13001200	0.32694800	0.12685100
H	-1.59581000	-0.17498100	-1.47345800
C	-4.43402900	0.73336000	-0.95153600
O	-5.62722500	0.62875600	-1.15548500
C	-2.23577800	3.84575200	-0.59753000
C	-2.78887000	4.42794900	0.54009200
C	-3.86515500	3.79877900	1.15611300
C	-4.40264200	2.61207100	0.68923300
C	-3.83234600	2.00863200	-0.44188400
C	-2.77208100	2.65699000	-1.07194200
F	-4.41205100	4.37376600	2.26548000
F	-2.25043600	2.11365500	-2.19984300
H	-1.37387300	4.27401600	-1.09369300
H	-2.38071000	5.34072700	0.95986300
H	-5.24788400	2.15133100	1.18799400
Cl	0.27002900	1.90899500	0.47019800

Table S6 Cartesian coordinates of **6**@Cl^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-3.89477200	-5.27617500	0.55395200
C	-5.20703000	-5.09486400	0.33065200
H	-3.57005600	-6.24704900	0.93156900
H	-5.61500400	-4.16045700	-0.04568500
H	-5.91911300	-5.89238600	0.52288600
C	-0.64324600	-2.51663400	-0.02795700
C	-1.97535100	-2.10842600	-0.29771000
C	-3.02235800	-3.00197800	-0.11370600
C	-2.80728400	-4.31221000	0.35015100
C	-1.48624400	-4.68995700	0.62982000
C	-0.41707500	-3.81721500	0.44684500
N	0.39171300	-1.59899300	-0.26250900
C	-2.22313600	-0.68838700	-0.74672400
H	-4.02587000	-2.65806600	-0.33376700
H	-1.28545500	-5.69500000	0.99556300
H	0.59301800	-4.12615300	0.67501600
H	0.20221200	-0.80763000	-0.88889500
C	1.70135700	-1.68815400	0.17455300
N	2.46358100	-0.64637900	-0.33813700
O	2.13590100	-2.56230800	0.92216000
H	1.97196500	0.00518800	-0.97489800
C	5.66209700	1.10097000	-0.62901400
C	4.33504600	0.74796500	-0.78856700
C	3.79804800	-0.37712600	-0.11521300
C	4.63811700	-1.13951200	0.72829100
C	5.96902300	-0.78025500	0.88481800
C	6.48104200	0.33363200	0.21088100
H	6.07610400	1.95968000	-1.14320100
H	3.68473300	1.32981400	-1.43603500
H	4.23131200	-1.99791500	1.24322000
H	6.62180400	-1.35702600	1.52895000
N	7.87151800	0.69773000	0.38173800
O	8.29932300	1.69073600	-0.22546800
O	8.57702600	0.00182100	1.12756300
O	-3.62308500	-0.50499500	-1.03781500
H	-1.90199900	0.01274800	0.02999200
H	-1.66047600	-0.44631600	-1.65378000
C	-4.30056500	0.63677000	-0.79367000
O	-5.50227800	0.65207600	-0.95392600
C	-1.77436500	3.50731300	-0.69774400
C	-2.27584700	4.24313200	0.36457700
C	-3.39246000	3.80870400	1.07632400
C	-4.01844800	2.62282000	0.70667100
C	-3.54065400	1.85791800	-0.36324400
C	-2.41303000	2.32152900	-1.05556400
F	-1.68477900	5.39479900	0.74855700
F	-3.85756100	4.52294800	2.11931200
F	-5.07488300	2.22239000	1.43620000
H	-0.87941800	3.82702700	-1.21958000
H	-1.98587500	1.75017400	-1.87113900
Cl	0.56924400	1.04222600	-2.18794700

Table S7 Cartesian coordinates of **7**@Cl^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	4.10091500	5.42569200	-0.27090400
C	5.42143300	5.18702000	-0.20396000
H	3.77452100	6.46037200	-0.38752900
H	5.83205000	4.18677400	-0.09355200
H	6.13753400	6.00196200	-0.26037800
C	0.83477300	2.62777600	-0.12891900
C	2.16693300	2.16778400	0.03908900
C	3.21898200	3.07384600	-0.01251400
C	3.00673900	4.44992400	-0.21099500
C	1.68143200	4.88706300	-0.34726100
C	0.60898300	4.00064300	-0.31057300
N	-0.19712200	1.67986200	-0.12449900
C	2.40488300	0.70056500	0.30848000
H	4.22356400	2.69297500	0.12342900
H	1.48160500	5.94676500	-0.49335000
H	-0.40613900	4.35675400	-0.41407500
H	0.04549300	0.70222800	-0.33661300
C	-1.55277500	1.92386700	-0.00207900
N	-2.27974000	0.75191800	-0.17038000
O	-2.05310300	3.02246700	0.23335600
H	-1.72620900	-0.09403500	-0.39491200
C	-5.48304700	-1.00764700	-0.27433500
C	-4.12903800	-0.73363900	-0.32520700
C	-3.64576400	0.57892700	-0.09817800
C	-4.56864000	1.61214500	0.18438100
C	-5.92615000	1.33125200	0.23438500
C	-6.38407800	0.02902100	0.00649700
H	-5.85587300	-2.00975900	-0.44737700
H	-3.41561700	-1.52409600	-0.54165500
H	-4.20224000	2.61373100	0.35735400
H	-6.64208100	2.11536600	0.44961800
N	-7.80270500	-0.25113100	0.06091600
O	-8.18230600	-1.41372000	-0.14495500
O	-8.58028800	0.68258400	0.31091000
O	3.82258300	0.48362000	0.50563600
H	1.87257100	0.38988100	1.21282900
H	2.05007900	0.06826800	-0.51153500
C	4.38352100	-0.71878800	0.29641800
O	5.59010600	-0.81538800	0.21029000
C	2.78685800	-3.82401500	-1.13539600
C	1.91987700	-4.22084100	-0.12047800
C	1.84532000	-3.46623500	1.04364900
C	2.62551600	-2.32270700	1.17294800
C	3.48833900	-1.91899900	0.15970500
C	3.57703900	-2.69707600	-1.00167400
F	2.84956500	-4.57213700	-2.25757500
F	1.16435500	-5.31827500	-0.25578500
F	1.02489300	-3.84189200	2.03282600
F	2.53593500	-1.61826200	2.32191800
H	4.25424200	-2.41592100	-1.79982400
Cl	-0.15926500	-1.45827600	-0.84338300

Table S8 Cartesian coordinates of **8**@Cl^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	3.92128300	5.57125400	0.16758100
C	5.24574300	5.35354000	0.10936800
H	3.57654200	6.60341500	0.24753600
H	5.67391900	4.35748100	0.03345500
H	5.94752200	6.18223000	0.13778600
C	0.70392700	2.71220800	0.11807600
C	2.04577600	2.27008800	-0.02064500
C	3.08166600	3.19584300	0.00067700
C	2.84453000	4.57476400	0.14135700
C	1.51095900	4.99292100	0.25287200
C	0.45409400	4.08746200	0.24433500
N	-0.31247600	1.74830200	0.13807900
C	2.31346600	0.79731100	-0.21683400
H	4.09404600	2.82835300	-0.11139400
H	1.29158000	6.05383000	0.35552300
H	-0.56746300	4.42976200	0.32698800
H	-0.05208300	0.77499400	0.34658900
C	-1.67337100	1.96613800	0.01428700
N	-2.37788500	0.78109700	0.18193000
O	-2.19471500	3.05486400	-0.22070900
H	-1.80867300	-0.05694700	0.39532600
C	-5.54638300	-1.04097500	0.27726500
C	-4.19782500	-0.74096600	0.32779900
C	-3.74095000	0.58252300	0.11071700
C	-4.68412500	1.59991400	-0.16110300
C	-6.03612300	1.29301000	-0.21071400
C	-6.46786700	-0.01975300	0.00692500
H	-5.89924700	-2.05155900	0.44266500
H	-3.46869600	-1.51917600	0.53610500
H	-4.33773700	2.60979200	-0.32689600
H	-6.76768600	2.06478100	-0.41779700
N	-7.88118500	-0.32719600	-0.04696300
O	-8.23727300	-1.49855600	0.15020300
O	-8.67716300	0.59314900	-0.28776200
O	3.73212600	0.60496900	-0.43637700
H	1.99549400	0.20286700	0.64546000
H	1.76736200	0.42204800	-1.08854600
C	4.27223300	-0.62113000	-0.41589900
O	5.46873100	-0.76913200	-0.51740800
C	1.77940800	-3.38617400	-1.24862000
C	1.75255300	-4.10007200	-0.05553400
C	2.51211500	-3.67426800	1.02916300
C	3.29890900	-2.53589600	0.90866000
C	3.34164100	-1.80215300	-0.27379200
C	2.56795400	-2.24758300	-1.34111800
F	1.03991800	-3.79211700	-2.29061200
F	0.98723800	-5.19218500	0.05245400
F	2.47232700	-4.35682700	2.18305800
F	4.01404100	-2.12944900	1.97369000
F	2.57809100	-1.55937700	-2.50204200
Cl	-0.22352500	-1.40577100	0.80731900

Table S9 Cartesian coordinates of **1**@Br^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-4.891811	-4.408434	0.286998
C	-6.171971	-4.010005	0.201279
C	-1.302018	-2.076791	-0.139006
C	-2.568471	-1.448755	-0.250264
C	-3.725984	-2.205211	-0.118186
C	-3.684384	-3.587742	0.137033
C	-2.422130	-4.186721	0.257457
C	-1.246345	-3.453461	0.121970
N	-0.151340	-1.288563	-0.307134
C	-2.626956	0.045142	-0.472494
C	1.129246	-1.595854	0.113059
N	2.031177	-0.614291	-0.279072
O	1.435162	-2.597238	0.757644
C	5.428040	0.739156	-0.321830
C	4.071625	0.579294	-0.535717
C	3.383789	-0.545378	-0.016314
C	4.103145	-1.509113	0.727007
C	5.464174	-1.343234	0.938272
C	6.125842	-0.225565	0.418316
N	7.545550	-0.063497	0.646921
O	8.107413	0.938691	0.179940
O	8.141982	-0.933108	1.300306
O	-3.998537	0.473107	-0.560992
C	-4.504766	1.534363	0.112437
O	-5.710474	1.594869	0.263911
C	-1.659375	4.058667	0.418197
C	-2.000122	4.678225	1.621818
C	-3.141800	4.268491	2.321254
C	-3.936960	3.241873	1.816776
C	-3.586024	2.602293	0.616996
C	-2.448456	3.023351	-0.085293
H	-4.696879	-5.462306	0.492311
H	-6.453245	-2.979776	-0.000078
H	-6.984852	-4.718477	0.333710
H	-4.675994	-1.691929	-0.207001
H	-2.355104	-5.254094	0.458688
H	-0.282923	-3.931591	0.228576
H	-0.240119	-0.416529	-0.841401
H	-2.115743	0.562428	0.344575
H	-2.127388	0.337461	-1.402024
H	1.642747	0.166854	-0.834214
H	5.956863	1.597722	-0.717306
H	3.513612	1.316309	-1.106937
H	3.580439	-2.367212	1.124196
H	6.025128	-2.075174	1.506838
H	-0.769982	4.350040	-0.132141
H	-1.376919	5.475733	2.019049
H	-3.409929	4.748947	3.258832
H	-4.833009	2.921279	2.338843
H	-2.145316	2.554957	-1.014952
Br	0.378195	1.650620	-2.023418

Table S10 Cartesian coordinates of **2**@Br^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-4.399913	-4.907711	0.439026
C	-5.702975	-4.629225	0.268266
C	-0.997782	-2.316013	-0.030864
C	-2.306168	-1.806890	-0.231071
C	-3.402354	-2.647448	-0.083508
C	-3.258613	-3.999952	0.273725
C	-1.957604	-4.479654	0.482021
C	-0.841247	-3.661280	0.333454
N	0.091346	-1.448969	-0.219729
C	-2.479508	-0.343391	-0.566853
C	1.383627	-1.632383	0.237747
N	2.219833	-0.617922	-0.210882
O	1.748797	-2.561843	0.954756
C	5.527884	0.934215	-0.360855
C	4.183925	0.676817	-0.558155
C	3.564932	-0.445291	0.045983
C	4.339348	-1.303547	0.859440
C	5.687505	-1.039865	1.054139
C	6.281232	0.072506	0.448286
N	7.688902	0.336623	0.658466
O	8.189941	1.330469	0.111737
O	8.335219	-0.441582	1.376079
O	-3.876920	-0.052691	-0.760816
C	-4.509096	1.026441	-0.246697
O	-5.722317	0.999821	-0.165901
C	-1.910002	3.820252	-0.076104
C	-2.391178	4.556766	1.007264
C	-3.542515	4.108979	1.647331
C	-4.222766	2.969295	1.256273
C	-3.716965	2.226476	0.176724
C	-2.566965	2.661199	-0.494356
F	-4.021258	4.826879	2.705684
H	-4.128519	-5.922219	0.735432
H	-6.059136	-3.645888	-0.027284
H	-6.459604	-5.393231	0.423104
H	-4.387122	-2.225424	-0.243971
H	-1.811345	-5.520697	0.763100
H	0.152637	-4.048261	0.507456
H	-0.048302	-0.625199	-0.815626
H	-2.068441	0.276056	0.235930
H	-1.952140	-0.073612	-1.487705
H	1.787364	0.092501	-0.824482
H	6.004828	1.790194	-0.822356
H	3.583986	1.332680	-1.183249
H	3.869477	-2.159596	1.321697
H	6.290433	-1.690995	1.675593
H	-1.006647	4.123620	-0.595817
H	-1.892036	5.453943	1.359504
H	-5.127562	2.658208	1.765956
H	-2.151010	2.115739	-1.332946
Br	0.446266	1.397056	-2.137560

Table S11 Cartesian coordinates of **3**@Br^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-4.652121	4.749315	-0.254260
C	-5.949683	4.411695	-0.168688
C	-1.185155	2.209427	-0.165554
C	-2.472739	1.645964	0.016617
C	-3.592188	2.469451	-0.020418
C	-3.486573	3.858447	-0.213660
C	-2.200438	4.398290	-0.361536
C	-1.064390	3.594857	-0.342401
N	-0.079601	1.344673	-0.185287
C	-2.591504	0.164047	0.287671
C	1.236701	1.689778	0.049508
N	2.083616	0.617059	-0.205856
O	1.615201	2.791613	0.443167
C	5.441137	-0.827718	-0.284907
C	4.074602	-0.665082	-0.414734
C	3.450774	0.552442	-0.044230
C	4.245907	1.605622	0.464001
C	5.616445	1.435908	0.593264
C	6.214381	0.226596	0.221480
N	7.644704	0.062450	0.361077
O	8.150132	-1.019478	0.025048
O	8.307426	1.009851	0.811120
O	-3.969703	-0.136639	0.603002
C	-4.455974	-1.390988	0.529163
O	-5.658448	-1.562089	0.549847
C	-1.648227	-3.888763	1.241686
C	-1.767091	-4.729109	0.135871
C	-2.753546	-4.494244	-0.824706
C	-3.617344	-3.411290	-0.684462
C	-3.495106	-2.534275	0.402046
C	-2.511318	-2.810677	1.348575
F	-2.401392	-1.999799	2.439324
H	-4.406261	5.806000	-0.371727
H	-6.281925	3.383164	-0.055116
H	-6.725754	5.170721	-0.211482
H	-4.562550	2.012487	0.129639
H	-2.084699	5.471059	-0.503019
H	-0.080245	4.028540	-0.454504
H	-0.231017	0.384352	-0.524298
H	-2.270380	-0.439510	-0.568635
H	-1.960077	-0.110257	1.137718
H	1.632479	-0.236249	-0.579226
H	5.921213	-1.756340	-0.568519
H	3.458503	-1.470488	-0.805326
H	3.772356	2.535020	0.746058
H	6.234871	2.235667	0.982621
H	-0.885192	-4.037880	1.997669
H	-1.073268	-5.555565	0.016639
H	-2.835316	-5.141513	-1.692435
H	-4.389533	-3.217424	-1.422460
Br	0.178918	-1.813060	-1.357613

Table S12 Cartesian coordinates of **4**@Br^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-4.134019	-5.244042	0.543602
C	-5.446246	-5.024513	0.357963
C	-0.838139	-2.527731	0.020608
C	-2.164814	-2.080781	-0.205937
C	-3.226600	-2.961214	-0.041543
C	-3.030065	-4.294643	0.359483
C	-1.712231	-4.712255	0.594237
C	-0.629363	-3.853011	0.429312
N	0.214938	-1.621854	-0.188516
C	-2.394589	-0.637040	-0.589569
C	1.512096	-1.737917	0.278191
N	2.307902	-0.704813	-0.199601
O	1.911437	-2.629163	1.024621
C	5.556708	0.962299	-0.407810
C	4.222881	0.649110	-0.593466
C	3.646160	-0.473396	0.049871
C	4.451419	-1.273481	0.891756
C	5.789221	-0.953944	1.074771
C	6.341361	0.157283	0.429170
N	7.739336	0.479162	0.626505
O	8.203375	1.470010	0.043403
O	8.413750	-0.249475	1.369578
O	-3.801365	-0.407334	-0.797723
C	-4.478319	0.661078	-0.321377
O	-5.688808	0.583254	-0.229248
C	-1.995994	3.570470	-0.263515
C	-2.551976	4.325389	0.757120
C	-3.700712	3.888239	1.418646
C	-4.305926	2.695967	1.068596
C	-3.742335	1.912573	0.047173
C	-2.595296	2.361388	-0.620147
F	-4.219323	4.652467	2.410521
F	-1.990512	5.496613	1.130822
H	-3.823007	-6.237807	0.869723
H	-5.840859	-4.065161	0.033755
H	-6.171721	-5.814670	0.529595
H	-4.226412	-2.586174	-0.224047
H	-1.525469	-5.736890	0.909487
H	0.377995	-4.192510	0.623914
H	0.044983	-0.823830	-0.810489
H	-2.012269	0.023066	0.194963
H	-1.873758	-0.376865	-1.516891
H	1.849444	-0.031064	-0.834380
H	6.001503	1.818593	-0.899798
H	3.599218	1.260916	-1.239636
H	4.013642	-2.129438	1.384746
H	6.415976	-1.560301	1.717558
H	-1.093247	3.901904	-0.766063
H	-5.209944	2.375250	1.574149
H	-2.129289	1.793210	-1.416405
Br	0.454573	1.182151	-2.189110

Table S13 Cartesian coordinates of **5**@Br^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	3.933548	5.188791	0.564330
C	5.241600	5.014831	0.312388
C	0.714717	2.359110	0.210691
C	2.028919	1.977438	-0.156009
C	3.067737	2.893555	-0.032398
C	2.853926	4.203441	0.430767
C	1.541029	4.567372	0.764635
C	0.485379	3.667020	0.661675
N	-0.307085	1.399521	0.130618
C	2.275388	0.587629	-0.701334
C	-1.661907	1.654847	0.036588
N	-2.397526	0.479228	0.126366
O	-2.156520	2.769917	-0.118080
C	-5.611053	-1.264913	0.104621
C	-4.256069	-1.002232	0.181534
C	-3.764183	0.318783	0.036976
C	-4.679434	1.372653	-0.188236
C	-6.038009	1.102814	-0.265111
C	-6.504510	-0.208201	-0.119961
N	-7.923900	-0.476883	-0.202745
O	-8.310871	-1.647968	-0.071555
O	-8.694969	0.474323	-0.401526
O	3.608331	0.536287	-1.256854
C	4.451130	-0.492434	-1.055232
O	5.637994	-0.339120	-1.265252
C	2.383497	-3.700101	-0.774769
C	2.980695	-4.300381	0.330817
C	4.037969	-3.647390	0.954305
C	4.516559	-2.422375	0.523478
C	3.902435	-1.802243	-0.574978
C	2.857973	-2.471035	-1.210345
F	4.627440	-4.237814	2.032603
F	2.288120	-1.907559	-2.305548
H	3.606436	6.169706	0.912910
H	5.651930	4.070528	-0.035638
H	5.947365	5.829104	0.450307
H	4.059421	2.579277	-0.334187
H	1.340382	5.576332	1.119439
H	-0.521256	3.966991	0.917892
H	-0.050142	0.412888	0.270594
H	2.155907	-0.178987	0.071382
H	1.568694	0.353283	-1.502228
H	-1.853460	-0.383094	0.298948
H	-5.990476	-2.273421	0.214872
H	-3.548247	-1.808144	0.355517
H	-4.306496	2.380875	-0.296999
H	-6.748171	1.902517	-0.437932
H	1.535264	-4.149904	-1.275742
H	2.618813	-5.244721	0.721967
H	5.350908	-1.945147	1.024977
Br	-0.224945	-1.934062	0.694294

Table S14 Cartesian coordinates of **6**@Br^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	4.070963	5.279701	0.576936
C	5.380438	5.065182	0.368259
C	0.767518	2.580063	0.026366
C	2.091432	2.133405	-0.213089
C	3.156740	3.007916	-0.040330
C	2.964537	4.334569	0.384925
C	1.649148	4.750159	0.637464
C	0.563282	3.896638	0.462479
N	-0.287934	1.681027	-0.200608
C	2.308490	0.694717	-0.615994
C	-1.574231	1.774379	0.298233
N	-2.383007	0.770375	-0.219382
O	-1.954159	2.623857	1.101112
C	-5.637524	-0.884903	-0.438269
C	-4.309349	-0.559077	-0.642362
C	-3.714207	0.522621	0.051707
C	-4.494713	1.268878	0.963350
C	-5.826837	0.936931	1.164599
C	-6.397465	-0.133618	0.468444
N	-7.789596	-0.468675	0.685462
O	-8.270203	-1.423071	0.056899
O	-8.442179	0.213007	1.489882
O	3.712311	0.458234	-0.842287
C	4.339180	-0.695427	-0.528741
O	5.546640	-0.752883	-0.619105
C	1.726173	-3.486561	-0.524972
C	2.125708	-4.200041	0.594551
C	3.200681	-3.774192	1.372480
C	3.889455	-2.620624	1.011757
C	3.514520	-1.879192	-0.113599
C	2.425681	-2.332357	-0.871572
F	1.472851	-5.320480	0.969807
F	3.565823	-4.465321	2.469150
F	4.903263	-2.226099	1.802523
H	3.764317	6.265438	0.930210
H	5.770802	4.114242	0.015430
H	6.108262	5.851058	0.549088
H	4.155290	2.635099	-0.234118
H	1.467211	5.769060	0.973241
H	-0.442481	4.234365	0.669357
H	-0.132569	0.920322	-0.871726
H	1.931679	0.026692	0.164946
H	1.775392	0.447168	-1.540039
H	-1.941571	0.137338	-0.905194
H	-6.096553	-1.710058	-0.968894
H	-3.704711	-1.129608	-1.342147
H	-4.042536	2.093736	1.494894
H	-6.434947	1.501998	1.860673
H	0.862683	-3.799388	-1.101458
H	2.079434	-1.775573	-1.734836
Br	-0.555154	-0.982343	-2.366823

Table S15 Cartesian coordinates of **7**@Br^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	4.009793	5.587512	-0.27579
C	5.332653	5.373	-0.18221
C	0.791751	2.737843	-0.13739
C	2.127082	2.301986	0.05605
C	3.165095	3.224614	0.004479
C	2.931597	4.593616	-0.21662
C	1.601126	5.007302	-0.37628
C	0.543937	4.102752	-0.34151
N	-0.22635	1.772193	-0.13822
C	2.382622	0.842986	0.352466
C	-1.57908	1.997143	0.036293
N	-2.30625	0.831244	-0.17047
O	-2.07701	3.07804	0.344706
C	-5.50494	-0.93963	-0.2653
C	-4.15473	-0.65442	-0.3499
C	-3.66917	0.64416	-0.05943
C	-4.58386	1.651907	0.321968
C	-5.93752	1.359867	0.405659
C	-6.39829	0.071675	0.113917
N	-7.81344	-0.22032	0.204194
O	-8.1956	-1.37002	-0.05927
O	-8.58409	0.691276	0.54092
O	3.794766	0.660205	0.612042
C	4.391148	-0.53269	0.453514
O	5.601862	-0.59982	0.404978
C	2.958702	-3.74836	-0.90477
C	2.060797	-4.1308	0.088704
C	1.907547	-3.32755	1.212081
C	2.640685	-2.15108	1.322405
C	3.534537	-1.76199	0.33006
C	3.701669	-2.588	-0.78878
F	3.097257	-4.5423	-1.98685
F	1.350721	-5.25973	-0.02767
F	1.056818	-3.68872	2.181618
F	2.477656	-1.40338	2.43559
H	3.667657	6.614032	-0.41642
H	5.758522	4.382334	-0.04616
H	6.035532	6.199163	-0.24143
H	4.173873	2.863313	0.161133
H	1.386082	6.061311	-0.54025
H	-0.47582	4.440286	-0.46283

H	0.026091	0.814081	-0.41368
H	1.817301	0.534023	1.237006
H	2.077299	0.194537	-0.47568
H	-1.76245	0.003702	-0.46403
H	-5.87982	-1.93132	-0.48701
H	-3.44754	-1.4258	-0.64256
H	-4.21507	2.64296	0.543651
H	-6.64768	2.124505	0.696643
H	4.403303	-2.31747	-1.56918
Br	-0.1193	-1.47094	-1.11762

Table S16 Cartesian coordinates of **8**@Br^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	3.807422	5.728216	-0.21185
C	5.131975	5.540689	-0.09021
C	0.645298	2.812977	-0.15794
C	1.986692	2.401209	0.044973
C	3.007005	3.344746	0.020597
C	2.749042	4.711803	-0.18301
C	1.412701	5.100944	-0.35544
C	0.373363	4.175611	-0.34679
N	-0.3545	1.829049	-0.18137
C	2.269656	0.942378	0.311421
C	-1.711659	2.025381	-0.00334
N	-2.414553	0.844661	-0.20807
O	-2.231315	3.095596	0.305843
C	-5.572643	-0.999305	-0.27151
C	-4.229818	-0.683785	-0.36646
C	-3.772637	0.627543	-0.08827
C	-4.707797	1.617029	0.290771
C	-6.05396	1.294635	0.384935
C	-6.486549	-0.005951	0.105774
N	-7.894241	-0.329949	0.207249
O	-8.251092	-1.489906	-0.04601
O	-8.683395	0.565888	0.542896
O	3.669223	0.796052	0.65319
C	4.25338	-0.408919	0.68961
O	5.44244	-0.510223	0.889715
C	2.791903	-3.582291	-0.82547
C	1.939	-4.010776	0.186607
C	1.800353	-3.256498	1.346866
C	2.520379	-2.077071	1.480735
C	3.385581	-1.628113	0.487255

C	3.506692	-2.40201	-0.66442
F	2.910593	-4.303055	-1.94977
F	1.242688	-5.143083	0.038909
F	0.971944	-3.665213	2.31828
F	2.375315	-1.355822	2.611994
F	4.314766	-1.997163	-1.66033
H	3.446922	6.748336	-0.35278
H	5.575751	4.558473	0.049853
H	5.818458	6.381684	-0.12872
H	4.021066	3.00225	0.185053
H	1.178885	6.152698	-0.50752
H	-0.651232	4.494856	-0.47604
H	-0.081472	0.875982	-0.45417
H	1.662329	0.584288	1.149138
H	2.037457	0.31269	-0.55398
H	-1.853505	0.026223	-0.4931
H	-5.925935	-2.001	-0.48344
H	-3.506888	-1.441201	-0.65711
H	-4.360574	2.617813	0.503423
H	-6.779715	2.044949	0.674703
Br	-0.174726	-1.424435	-1.11103

Table S17 Cartesian coordinates of **1**@I^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	6.134492	2.251858	-1.41922
C	7.259763	1.782891	-0.855
C	2.130815	0.669179	-1.18144
C	3.204875	-0.04821	-0.60123
C	4.498645	0.467341	-0.69634
C	4.783367	1.684118	-1.33117
C	3.701074	2.375022	-1.90242
C	2.403828	1.88383	-1.8363
N	0.826805	0.160394	-1.10756
C	3.029421	-1.33981	0.168545
C	-0.335723	0.906451	-1.11725
N	-1.454358	0.096376	-0.9612
O	-0.38636	2.12801	-1.24273
C	-5.003027	-0.23216	-0.13396
C	-3.683012	-0.53346	-0.41707
C	-2.750305	0.493686	-0.70326
C	-3.183908	1.839746	-0.69091
C	-4.5088	2.13614	-0.40381
C	-5.415857	1.107514	-0.12641

N	-6.795509	1.430809	0.171822
O	-7.580639	0.500899	0.40883
O	-7.134048	2.624155	0.178007
O	3.650254	-1.24878	1.483791
C	3.242918	-0.29266	2.360414
O	4.022755	0.096215	3.206939
C	-0.55243	-0.17747	2.187142
C	-0.774665	1.200595	2.169967
C	0.309566	2.083979	2.199446
C	1.611459	1.590808	2.262779
C	1.836794	0.207566	2.264083
C	0.750582	-0.67639	2.224118
H	6.201426	3.165623	-2.01168
H	7.276718	0.889702	-0.23596
H	8.20705	2.296717	-0.9915
H	5.29933	-0.09744	-0.22806
H	3.880826	3.31976	-2.4117
H	1.5857	2.439903	-2.27129
H	0.710171	-0.84581	-0.95517
H	1.995008	-1.66584	0.258657
H	3.579759	-2.15646	-0.30374
H	-1.277952	-0.91795	-0.88433
H	-5.717576	-1.01564	0.086994
H	-3.342355	-1.56559	-0.41907
H	-2.473917	2.624994	-0.90582
H	-4.85175	3.163747	-0.39153
H	-1.384693	-0.87246	2.132136
H	-1.787939	1.586315	2.100782
H	0.138923	3.155731	2.152619
H	2.461184	2.266063	2.286417
H	0.908989	-1.74995	2.207125
I	-0.418158	-3.30041	-0.61773

Table S18 Cartesian coordinates of **2**@I^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	6.119528	1.941389	-1.67164
C	7.246825	1.511025	-1.08157
C	2.118889	0.371379	-1.3363
C	3.18198	-0.26646	-0.65355
C	4.476272	0.241432	-0.78055
C	4.769054	1.378872	-1.54533
C	3.696108	1.995284	-2.21202
C	2.400154	1.505203	-2.11924

N	0.813215	-0.13107	-1.23167
C	2.987296	-1.45884	0.256855
C	-0.34214	0.62553	-1.29253
N	-1.46884	-0.15067	-1.05067
O	-0.37672	1.83165	-1.52301
C	-5.01265	-0.34044	-0.15658
C	-3.70003	-0.68841	-0.42135
C	-2.75688	0.290759	-0.81872
C	-3.17049	1.637772	-0.93586
C	-4.48818	1.981269	-0.6669
C	-5.40609	0.999065	-0.27973
N	-6.77875	1.371055	-0.00245
O	-7.57292	0.481232	0.335738
O	-7.10086	2.563146	-0.11489
O	3.598257	-1.2275	1.560415
C	3.220526	-0.16463	2.313717
O	3.997511	0.282049	3.133516
C	-0.56353	0.136103	2.041792
C	-0.7161	1.515425	1.895105
C	0.427936	2.30574	1.876153
C	1.703525	1.781199	2.003861
C	1.841768	0.392123	2.130391
C	0.708393	-0.43041	2.151232
F	0.288491	3.651945	1.729722
H	6.184267	2.813913	-2.32331
H	7.268637	0.656355	-0.41046
H	8.192326	2.018076	-1.25139
H	5.268455	-0.25831	-0.23099
H	3.882751	2.878699	-2.81918
H	1.589174	2.004201	-2.63039
H	0.691719	-1.11409	-0.97042
H	1.948239	-1.75922	0.375701
H	3.530543	-2.33151	-0.11204
H	-1.30378	-1.15223	-0.86297
H	-5.73547	-1.08706	0.148865
H	-3.37387	-1.72054	-0.32278
H	-2.45226	2.387842	-1.23335
H	-4.81576	3.010365	-0.75267
H	-1.43533	-0.51031	2.037027
H	-1.69161	1.972692	1.768613
H	2.572056	2.429965	1.990158
H	0.802495	-1.50765	2.237644
I	-0.46214	-3.47605	-0.25528

Table S19 Cartesian coordinates of **3**@I^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-4.70846	4.826666	-0.35884
C	-6.00201	4.487332	-0.22903
C	-1.2301	2.310668	-0.20795
C	-2.508	1.751013	0.028769
C	-3.63399	2.565448	-0.02911
C	-3.5373	3.943358	-0.29389
C	-2.2566	4.48273	-0.49083
C	-1.11674	3.684771	-0.45462
N	-0.11878	1.448114	-0.21311
C	-2.60426	0.28569	0.382054
C	1.180111	1.8022	0.088664
N	2.059795	0.755598	-0.17034
O	1.519095	2.893098	0.543061
C	5.449804	-0.62156	-0.12404
C	4.087109	-0.48276	-0.31478
C	3.420467	0.710384	0.058455
C	4.166437	1.763796	0.635893
C	5.532671	1.617052	0.829325
C	6.173865	0.432053	0.451394
N	7.599972	0.29249	0.656753
O	8.14422	-0.76777	0.313317
O	8.218668	1.238552	1.167613
O	-3.95513	0.007399	0.813691
C	-4.41686	-1.25298	0.925
O	-5.61181	-1.43829	1.043404
C	-1.51558	-3.61032	1.746677
C	-1.69009	-4.58166	0.761242
C	-2.74372	-4.47897	-0.15023
C	-3.617	-3.39627	-0.08537
C	-3.44121	-2.39041	0.875271
C	-2.39331	-2.53809	1.781695
F	-2.2321	-1.60257	2.760473
H	-4.47098	5.876481	-0.53787
H	-6.32522	3.464789	-0.05289
H	-6.78362	5.238798	-0.29694
H	-4.59913	2.113612	0.164278
H	-2.15034	5.547656	-0.6873
H	-0.13627	4.115883	-0.60708
H	-0.25293	0.509871	-0.61289
H	-2.35053	-0.36058	-0.46654

H	-1.90763	0.05835	1.193367
H	1.651747	-0.082	-0.613
H	5.962605	-1.53133	-0.41133
H	3.509737	-1.28862	-0.76011
H	3.660143	2.674795	0.920722
H	6.113717	2.416907	1.272327
H	-0.7056	-3.66009	2.46626
H	-0.99046	-5.40929	0.697624
H	-2.86971	-5.22885	-0.9248
H	-4.43828	-3.30297	-0.78891
I	0.156468	-1.84016	-1.74935

Table S20 Cartesian coordinates of **4**@I^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	-6.08916	-1.88787	-1.92839
C	-7.24282	-1.46095	-1.38908
C	-2.1076	-0.32129	-1.39077
C	-3.20687	0.330451	-0.78203
C	-4.49375	-0.17584	-0.97532
C	-4.74637	-1.32585	-1.73535
C	-3.63873	-1.95526	-2.32904
C	-2.34847	-1.46736	-2.16987
N	-0.80901	0.181405	-1.22323
C	-3.06255	1.535236	0.120683
C	0.351844	-0.57229	-1.237
N	1.466892	0.208974	-0.97418
O	0.393236	-1.78285	-1.44498
C	5.052151	0.467718	-0.28121
C	3.717925	0.787228	-0.46187
C	2.776763	-0.2095	-0.81417
C	3.210643	-1.54434	-0.97105
C	4.549557	-1.85956	-0.78848
C	5.466922	-0.86006	-0.44752
N	6.863274	-1.20192	-0.26295
O	7.654157	-0.29936	0.048444
O	7.208152	-2.38157	-0.42544
O	-3.7331	1.316687	1.398275
C	-3.42371	0.234931	2.154162
O	-4.25551	-0.20741	2.921251
C	0.365178	-0.15606	2.080398
C	0.462681	-1.53525	1.975099
C	-0.68548	-2.3244	1.900085
C	-1.94179	-1.74772	1.949212

C	-2.05133	-0.35281	2.042125
C	-0.89807	0.438681	2.103783
F	-0.55513	-3.66529	1.788954
F	1.671303	-2.13408	1.940881
H	-6.1226	-2.75756	-2.58615
H	-7.29586	-0.61117	-0.71356
H	-8.17934	-1.96656	-1.60627
H	-5.31471	0.336791	-0.48261
H	-3.79283	-2.84811	-2.93151
H	-1.51181	-1.97711	-2.62582
H	-0.69928	1.167257	-0.96878
H	-2.0327	1.84611	0.285613
H	-3.5941	2.399328	-0.28364
H	1.293919	1.207678	-0.78154
H	5.775412	1.227717	-0.0122
H	3.375813	1.810854	-0.33357
H	2.491405	-2.31012	-1.22104
H	4.893588	-2.88036	-0.90243
H	1.266145	0.446867	2.113168
H	-2.82587	-2.37388	1.903274
H	-0.9607	1.519863	2.163967
I	0.420803	3.514083	-0.13377

Table S21 Cartesian coordinates of **5**@I^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	3.96752	5.391161	0.563945
C	5.275335	5.220676	0.308015
C	0.771252	2.531263	0.306747
C	2.083278	2.147163	-0.05647
C	3.118404	3.072276	0.037352
C	2.895066	4.392964	0.463842
C	1.580274	4.75957	0.792131
C	0.531397	3.848161	0.720688
N	-0.2464	1.560896	0.262918
C	2.323438	0.747644	-0.57407
C	-1.58387	1.808622	0.0294
N	-2.34505	0.654738	0.186243
O	-2.04474	2.901889	-0.29217
C	-5.57204	-1.06313	0.016616
C	-4.22637	-0.80309	0.201646
C	-3.69997	0.49223	-0.02577
C	-4.56892	1.523429	-0.45065
C	-5.91746	1.255683	-0.63941

C	-6.41912	-0.02961	-0.40687
N	-7.82834	-0.29563	-0.60659
O	-8.24697	-1.44374	-0.39571
O	-8.55792	0.635253	-0.98013
O	3.613036	0.720091	-1.22804
C	4.36962	-0.38821	-1.3064
O	5.537434	-0.28845	-1.62821
C	2.100152	-3.47642	-1.29946
C	2.76296	-4.2828	-0.37711
C	3.922988	-3.79965	0.216615
C	4.438425	-2.54607	-0.06605
C	3.763192	-1.72073	-0.97778
C	2.61439	-2.2206	-1.58889
F	4.579549	-4.59002	1.110732
F	1.978487	-1.46317	-2.5216
H	3.6345	6.378503	0.887502
H	5.690786	4.270596	-0.01742
H	5.975446	6.043936	0.418642
H	4.110644	2.757484	-0.26233
H	1.375365	5.777478	1.117304
H	-0.47723	4.147321	0.973007
H	-0.00146	0.603658	0.548232
H	2.294389	0.002013	0.228694
H	1.555044	0.477973	-1.30254
H	-1.83958	-0.18208	0.512972
H	-5.97767	-2.05204	0.191841
H	-3.55493	-1.59218	0.529581
H	-4.16955	2.512079	-0.6248
H	-6.59222	2.037714	-0.96616
H	1.178952	-3.79623	-1.77146
H	2.3764	-5.25749	-0.10174
H	5.352028	-2.20425	0.406902
I	-0.12455	-1.8915	1.394288

Table S22 Cartesian coordinates of **6**@I^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	4.402403	5.141097	0.726319
C	5.703554	4.850412	0.561988
C	0.974919	2.62564	0.098132
C	2.275804	2.097082	-0.07997
C	3.384544	2.911674	0.115714
C	3.251125	4.255927	0.508235
C	1.953402	4.753074	0.703013

C	0.827555	3.958954	0.499765
N	-0.12509	1.783312	-0.15343
C	2.41125	0.636868	-0.43506
C	-1.37272	1.882789	0.431148
N	-2.25333	0.944573	-0.09627
O	-1.66509	2.685061	1.314682
C	-5.56632	-0.61321	-0.14795
C	-4.24268	-0.32216	-0.42551
C	-3.57163	0.720922	0.257422
C	-4.26844	1.461824	1.238575
C	-5.59456	1.161514	1.517584
C	-6.24236	0.131514	0.827758
N	-7.62885	-0.16832	1.124456
O	-8.17983	-1.08447	0.497184
O	-8.20481	0.504426	1.992137
O	3.804135	0.291688	-0.56104
C	4.313497	-0.90271	-0.19355
O	5.514555	-1.06556	-0.21999
C	1.486943	-3.47937	-0.25397
C	1.755551	-4.17016	0.91859
C	2.811158	-3.7949	1.747595
C	3.612754	-2.71603	1.386171
C	3.370022	-1.99954	0.209768
C	2.297437	-2.39985	-0.60015
F	0.991989	-5.21761	1.293745
F	3.05059	-4.462	2.892007
F	4.604601	-2.36681	2.224063
H	4.140739	6.146637	1.058993
H	6.050001	3.874991	0.230845
H	6.468854	5.595877	0.758524
H	4.366858	2.477364	-0.02668
H	1.819933	5.787386	1.012923
H	-0.16501	4.357536	0.660403
H	-0.02964	1.085692	-0.89937
H	1.933242	0.023963	0.335435
H	1.92255	0.404622	-1.38806
H	-1.88822	0.347445	-0.85128
H	-6.08354	-1.40773	-0.67172
H	-3.70361	-0.88882	-1.18008
H	-3.75796	2.255936	1.763897
H	-6.13843	1.72241	2.268055
H	0.643842	-3.75602	-0.87785
H	2.057149	-1.8608	-1.51072
I	-0.55475	-0.82006	-2.76129

Table S23 Cartesian coordinates of **7**@I^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	3.909024	5.761324	0.152061
C	5.220883	5.572963	-0.06741
C	0.731727	2.868546	0.182301
C	2.050669	2.457052	-0.1236
C	3.080434	3.391819	-0.12478
C	2.843839	4.750369	0.150312
C	1.52322	5.141443	0.42175
C	0.479092	4.221246	0.443243
N	-0.2735	1.886802	0.235681
C	2.291691	1.009519	-0.4744
C	-1.61503	2.086504	-0.02367
N	-2.35144	0.933209	0.223849
O	-2.09521	3.139707	-0.43684
C	-5.53752	-0.86846	0.164997
C	-4.19842	-0.56512	0.333533
C	-3.703	0.724186	0.021839
C	-4.59443	1.705177	-0.4685
C	-5.93622	1.394234	-0.63992
C	-6.40728	0.115377	-0.32459
N	-7.81053	-0.19614	-0.50758
O	-8.20267	-1.33616	-0.21948
O	-8.5594	0.690471	-0.94431
O	3.618681	0.882548	-1.03736
C	4.226373	-0.31667	-1.12866
O	5.406424	-0.37579	-1.39475
C	1.647337	-3.02556	-1.74266
C	1.9433	-3.94062	-0.73584
C	2.962541	-3.65431	0.165595
C	3.677425	-2.46548	0.049467
C	3.381255	-1.54822	-0.95454
C	2.348804	-1.83804	-1.85639
F	0.658608	-3.31817	-2.61088
F	1.255562	-5.08353	-0.62627
F	3.248932	-4.52244	1.145119
F	4.645851	-2.21344	0.947849
H	3.566144	6.775737	0.360964
H	5.646646	4.595754	-0.27956
H	5.914777	6.408273	-0.03905
H	4.078527	3.050905	-0.37158

H	1.309238	6.187692	0.629851
H	-0.53366	4.539609	0.65128
H	-0.01399	0.962177	0.603852
H	2.195577	0.349677	0.395352
H	1.55053	0.678544	-1.20892
H	-1.82789	0.132167	0.604683
H	-5.91972	-1.8535	0.403184
H	-3.50963	-1.31647	0.710506
H	-4.21821	2.689342	-0.70752
H	-6.62859	2.137454	-1.01655
H	2.091772	-1.14926	-2.65309
I	-0.04209	-1.47523	1.590406

Table S24 Cartesian coordinates of **8**@I^- optimized at B3LYP-D3/6-31+G(D, P) level of theory

Atom	x	y	z
C	3.861215	5.7982	-0.22042
C	5.173179	5.611511	-0.00034
C	0.687165	2.902151	-0.25587
C	2.007657	2.490188	0.042063
C	3.036405	3.425966	0.044884
C	2.797321	4.785896	-0.22102
C	1.475428	5.177055	-0.48585
C	0.432215	4.255942	-0.50846
N	-0.3182	1.920562	-0.30935
C	2.251201	1.040128	0.379517
C	-1.65707	2.116484	-0.03376
N	-2.39289	0.960224	-0.27026
O	-2.13585	3.168937	0.382066
C	-5.57037	-0.85452	-0.16226
C	-4.23521	-0.54576	-0.351
C	-3.74066	0.74602	-0.04862
C	-4.62879	1.724107	0.453109
C	-5.96661	1.407819	0.644728
C	-6.43691	0.12654	0.338316
N	-7.83604	-0.19062	0.54226
O	-8.22729	-1.33297	0.262275
O	-8.58232	0.693734	0.987715
O	3.578824	0.911553	0.943255
C	4.129978	-0.29127	1.153221
O	5.269702	-0.38473	1.550089
C	2.934558	-3.5802	-0.34506
C	1.888302	-3.91837	0.507825
C	1.535029	-3.06593	1.54909

C	2.237935	-1.88122	1.725958
C	3.290298	-1.51847	0.889006
C	3.623473	-2.38974	-0.14667
F	3.263369	-4.39696	-1.35539
F	1.217172	-5.05923	0.322136
F	0.525469	-3.38955	2.368652
F	1.88969	-1.07159	2.74772
F	4.618825	-2.07438	-0.99268
H	3.516928	6.812523	-0.42733
H	5.600208	4.634785	0.211492
H	5.865799	6.447931	-0.02657
H	4.036071	3.085928	0.286472
H	1.259619	6.224264	-0.68702
H	-0.58178	4.574306	-0.71029
H	-0.05975	0.996946	-0.67871
H	1.516116	0.701831	1.115513
H	2.163452	0.392299	-0.49994
H	-1.8721	0.160362	-0.65535
H	-5.95188	-1.84159	-0.39298
H	-3.54903	-1.29517	-0.73646
H	-4.25316	2.710051	0.685617
H	-6.65638	2.148672	1.030676
I	-0.09083	-1.44314	-1.67474

Table S25 The key geometry parameters (defined as Figure 2 showing) of the 8, 8@X$^-$ (X=F, Cl, Br and I) at M06-2X/6-31+G(D,P)

	l_1/Å	l_2/Å	d_1/Å	d_2/Å	θ_1/°	θ_2/°	$d_{penetration}$/Å [b]
8	1.012	1.013	–	–	–	–	–
8@F$^-$	1.051	1.048	1.612	1.609	156.18	159.21	1.31
8@Cl$^-$	1.032	1.026	2.124	2.270	165.21	159.86	1.11
8@Br$^-$	1.030	1.025	2.282	2.463	167.48	159.94	1.18
[a]**8@I$^-$**	1.026	1.025	2.630	2.666	166.10	164.36	1.08

[a] MIDIX basis set used for I atom. [b] Here, the $d_{penetration}$, mutual penetration distance between halide-anion and H atom, is defined as sum of the van der Waals radii of H atom and halide-anion substrate the average of d_1 and d_2, namely $d_{penetration}$=∑vdW-radii 1/2(d_1+d_2).

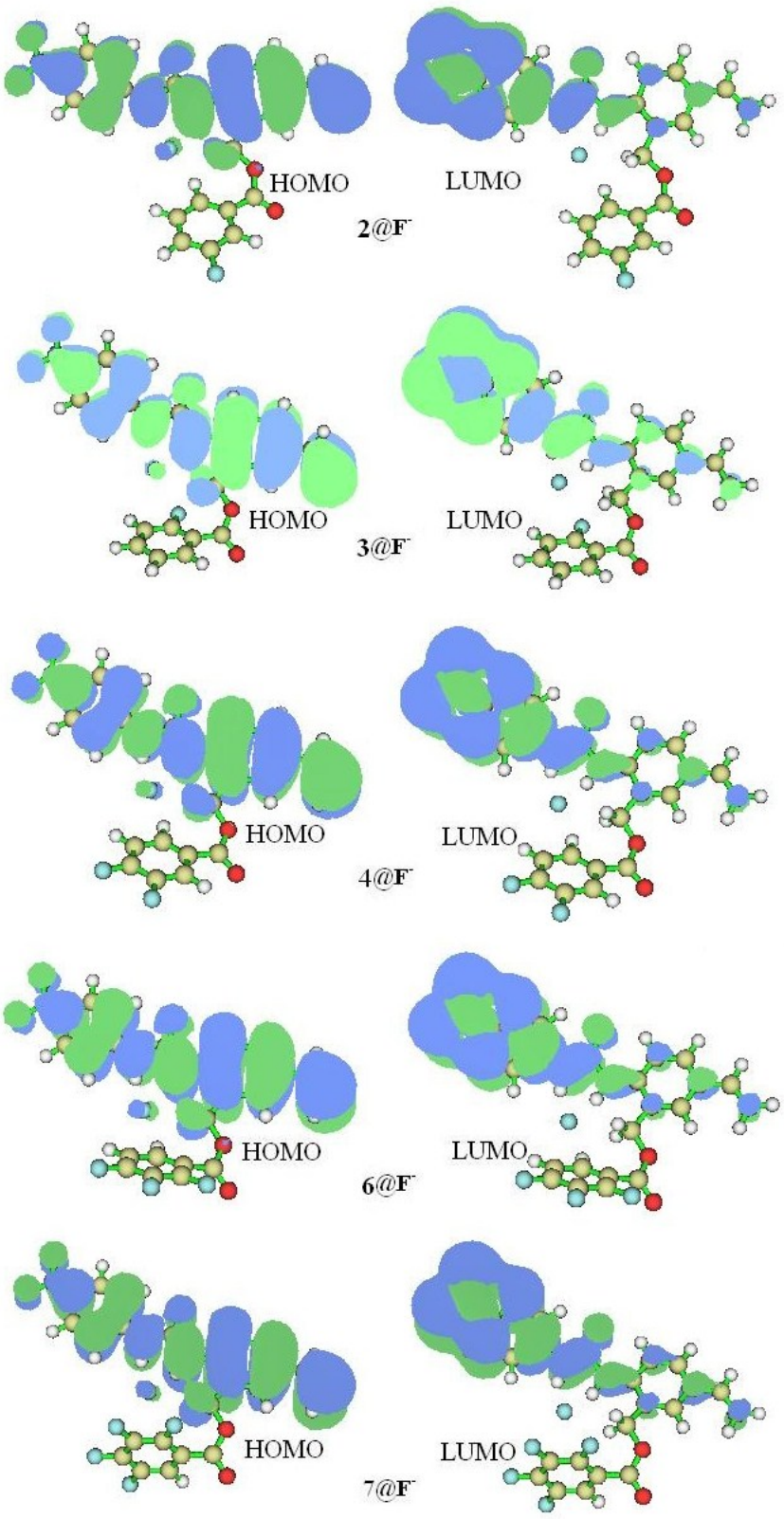

Figure S1 Frontier orbital of the some selected complexes (**2**@F^-, **3**@F^-, **4**@F^-, **6**@F^-, and **7**@F^-).

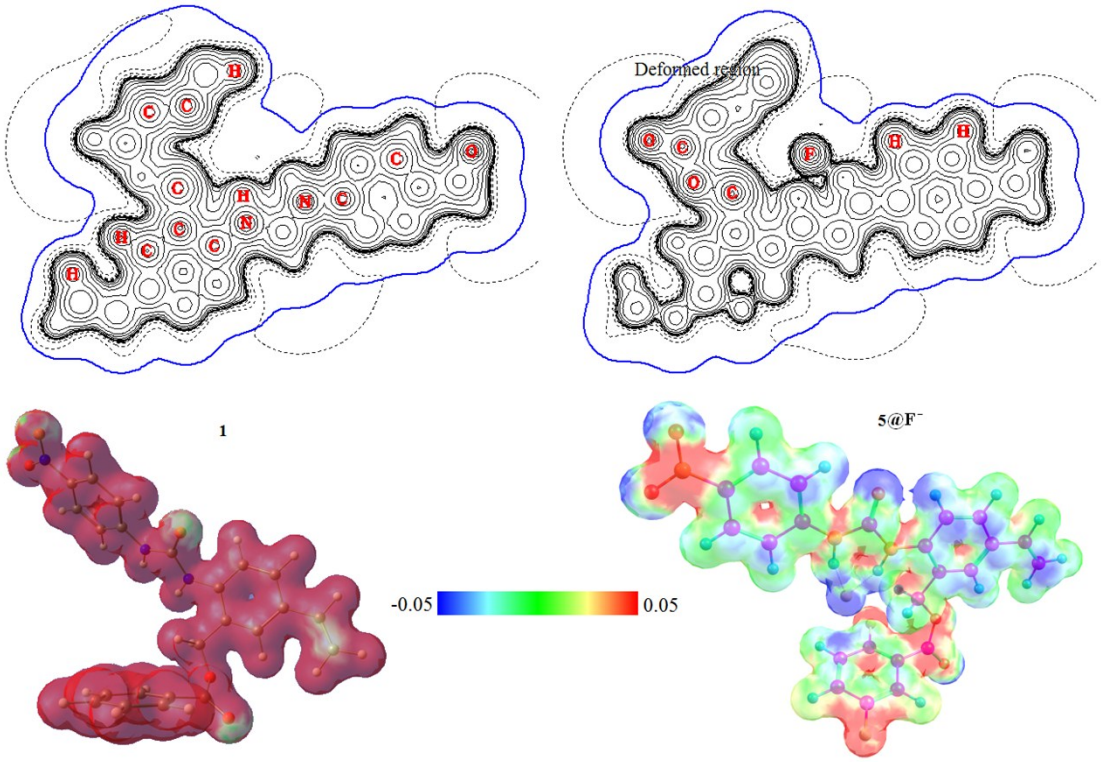

Figure S2 Contour maps (upper) of ESP and van der Waals interfaces (bold blue) and 3D maps (lower) of ESP surfaces of free receptor **1** and **5**@F^- complex.

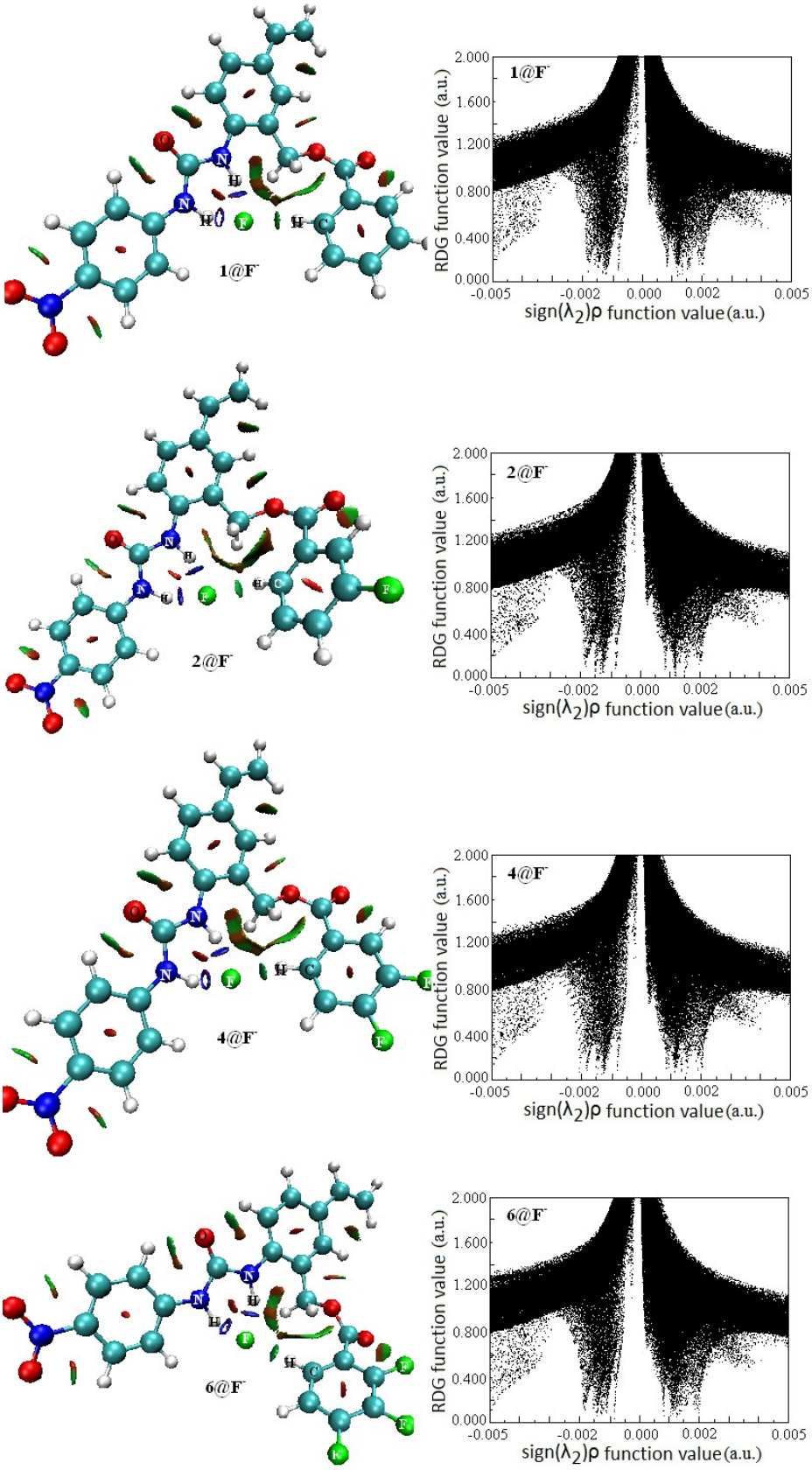

Figure S3 Reduced density gradient iso-surface map (Left) and reduced density gradient versus the electron density multiplied by the sign of the second Hessian eigenvalue (Right) of **1**@F^-, **2**@F^-, **4**@F^- and **6**@F^-.