

## Supplementary Information for

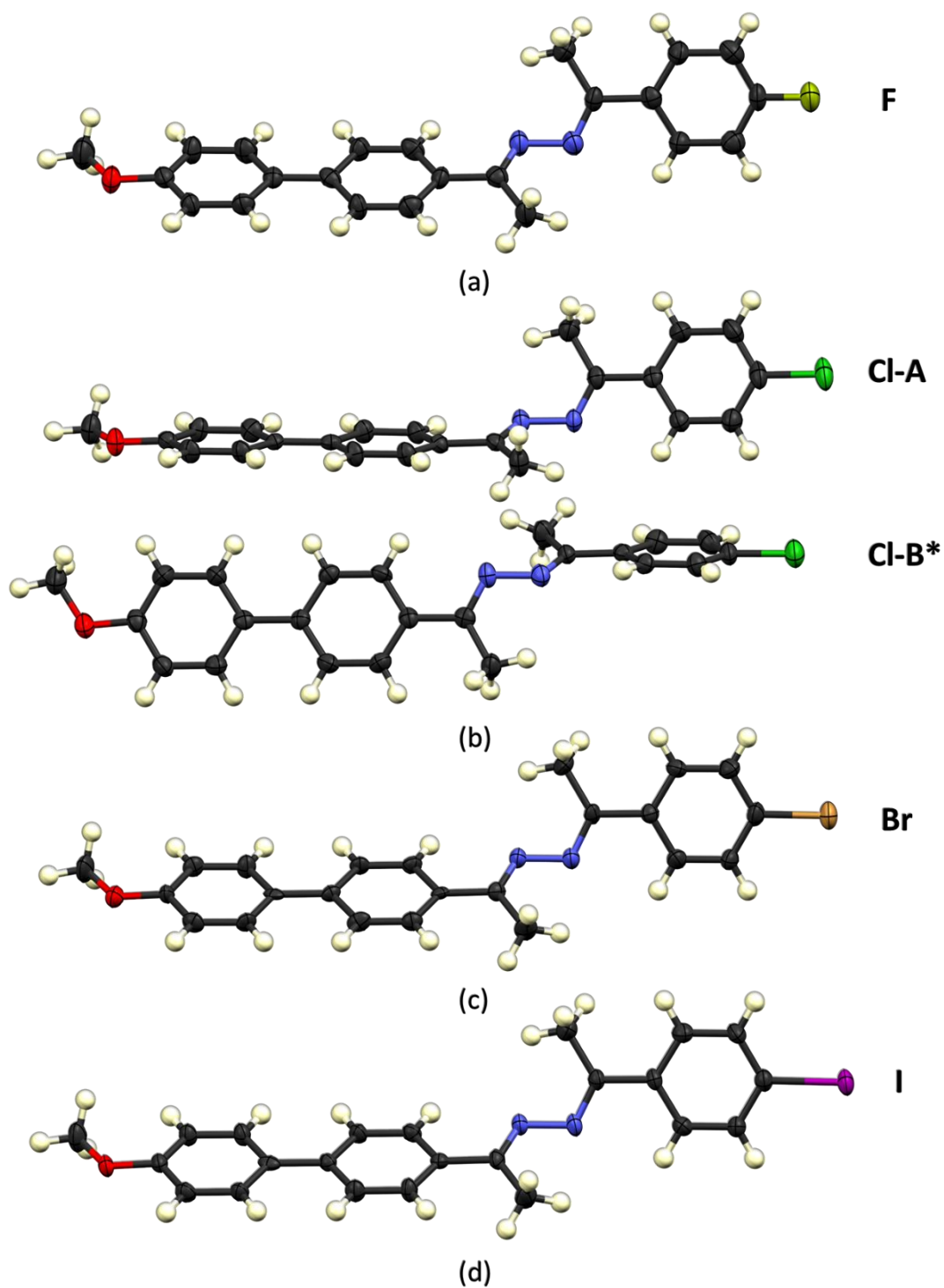
# Perfect Polar Alignment of Parallel Beloamphiphile Layers: Improved Structural Design Bias Realized in Ferroelectric Crystals of the Novel “Methoxyphenyl Series of Acetophenone Azines”

Harmeet Bhoday, Nathan Knotts and Rainer Glaser\*

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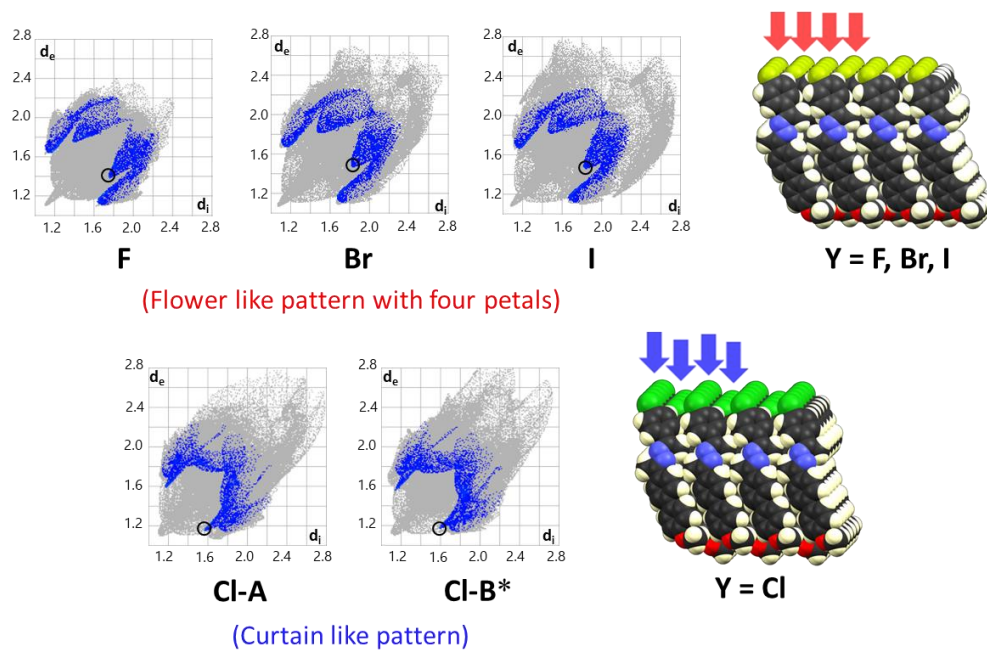
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## Crystal Structure of (MeO-Ph, Y)-azines 1-4

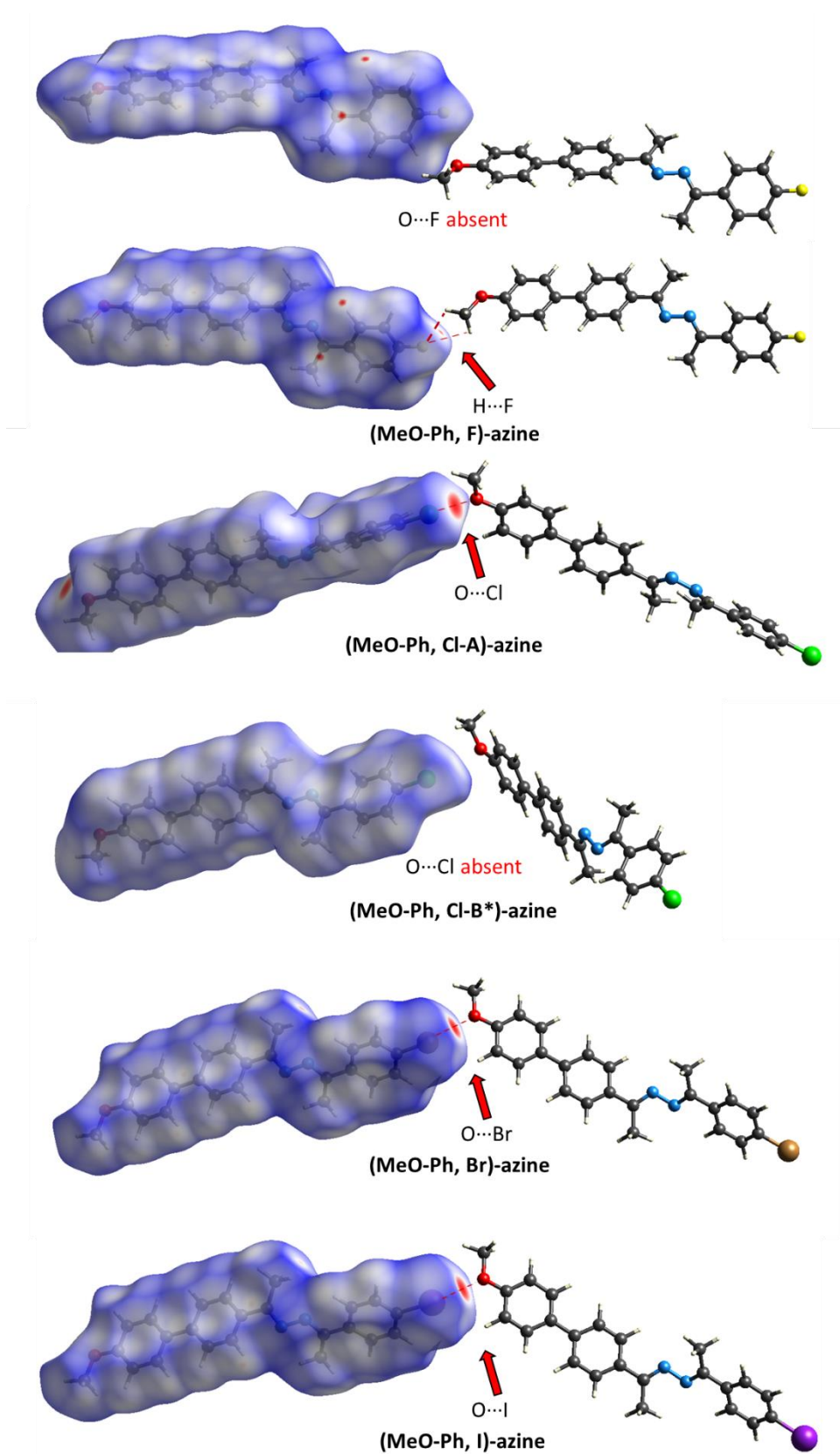


**Supplementary Fig. 1.** ORTEP diagrams of the unique (MeO-Ph, Y)-azine molecules with Y = F, Cl, Br, and I in their crystals. The unique molecules are shown with *M*-helicity for Y = F, Br, and I. For Y = Cl, the **A** and **B\*** molecules have *M*- and *P*-helicity, respectively.

## Hirshfeld Surface Analysis and 2-D Fingerprint Plots

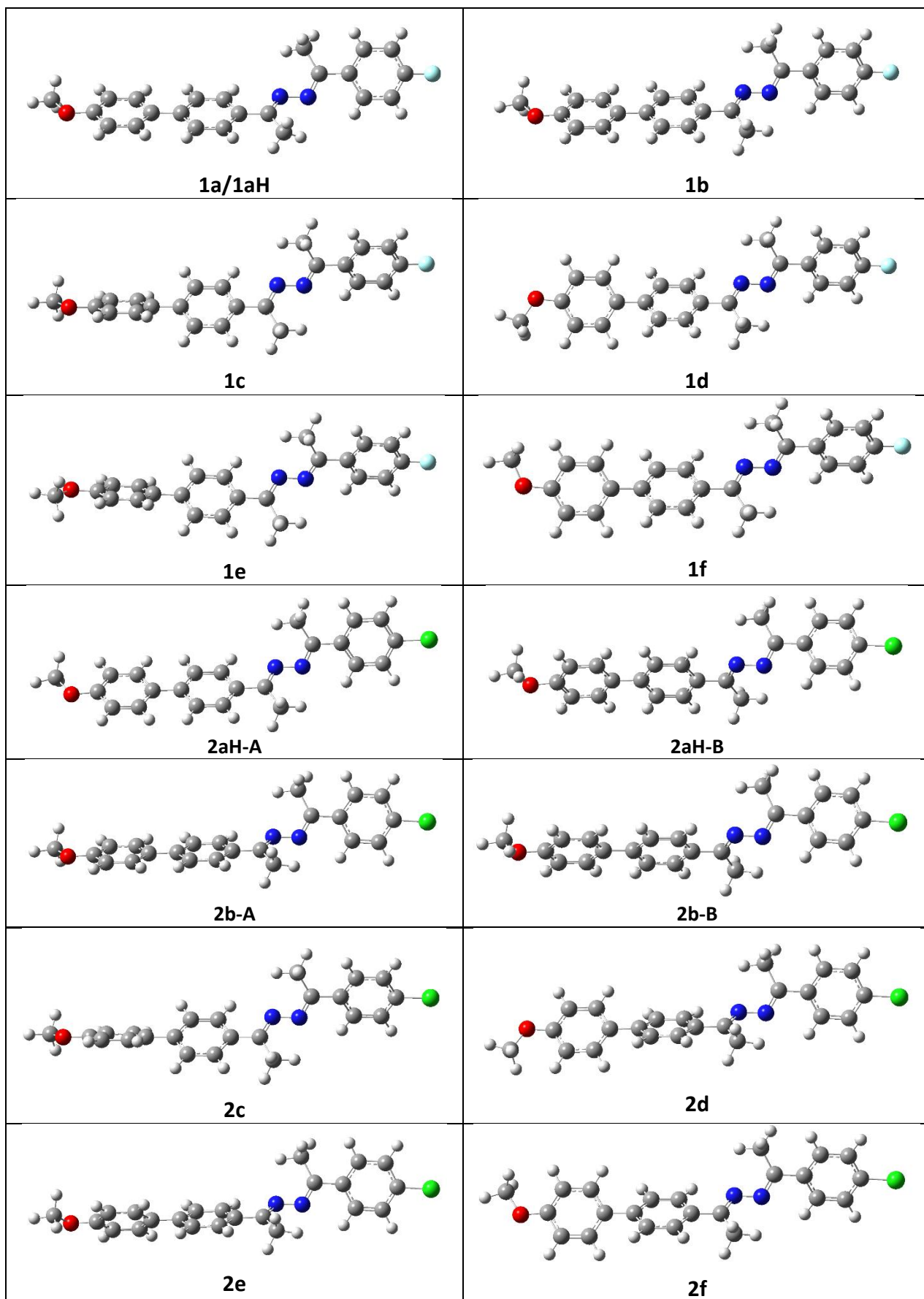


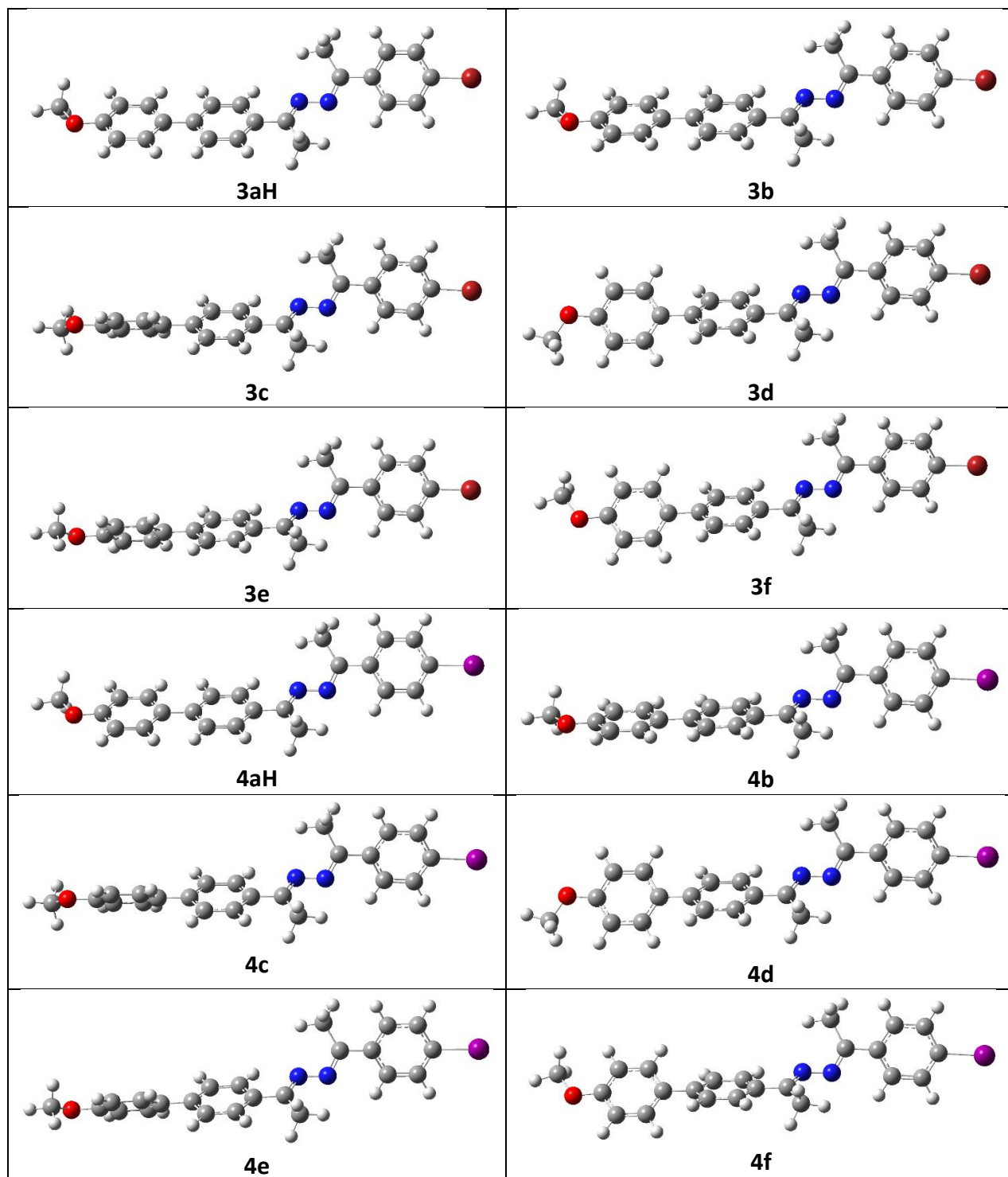
**Supplementary Fig. 2. Hirshfeld 2-D fingerprint plots resolved into  $N\cdots H$  contacts in the crystals of 1-4.** Open circles mark  $N\cdots H$  contacts involving arene edge-hydrogens and they are very different for chloroazine **2** as compared to all others.



**Supplementary Fig. 3.** Hirshfeld surfaces for (MeO-Ph, Y)-azines **1-4**. The red color represents the places of significant interactions where the distance is less than the sum of the vdW radii. The *interlayer* pairs are shown for **1-4**.

## Molecular Geometry Data





**Supplementary Fig. 4.** Molecular structures of optimized (MeO-Ph, Y)-azines 1-4.

## Cartesian Coordinates and Models of Stationary Structures of Optimized Free (MeO-Ph, Y)-Azines

Supplementary Table 1. Cartesian coordinates of optimized **1aH**.

F	-1	-8.44870000	5.38680000	4.48200000
O	-1	9.59010000	5.34060000	1.61640000
N	-1	-2.21910000	5.79670000	3.83740000
N	-1	-0.88130000	5.80610000	3.43690000
C	-1	-3.05470000	5.42500000	2.93580000
C	-1	-4.49270000	5.43510000	3.32220000
C	-1	-5.46100000	4.78920000	2.54300000
H	0	-5.17638600	4.27759600	1.62945000
C	-1	-6.79520000	4.78050000	2.92750000
H	0	-7.55376300	4.27697800	2.33754900
C	-1	-7.14800000	5.41560000	4.08980000
C	-1	-6.23600000	6.06080000	4.88960000
H	0	-6.56874100	6.54672000	5.80092400
C	-1	-4.90660000	6.06230000	4.51040000
H	0	-4.16008800	6.55768400	5.12091700
C	-1	-2.65670000	4.98330000	1.56030000
H	0	-2.69362900	3.89137500	1.47319200
H	0	-1.63588700	5.29678600	1.34984500
H	0	-3.33032800	5.39366500	0.80355900
C	-1	-0.04520000	5.43660000	4.33840000
C	-1	1.37710000	5.43370000	3.95200000
C	-1	2.37860000	4.85920000	4.74540000
H	0	2.11735600	4.39212000	5.69077400
C	-1	3.70530000	4.85630000	4.35900000
H	0	4.42651200	4.39726200	5.02588400
C	-1	4.12030000	5.42140000	3.14640000
C	-1	3.11750000	6.00170000	2.35630000
H	0	3.36820200	6.46075200	1.40625000
C	-1	1.79650000	6.01250000	2.74330000
H	0	1.04899100	6.47335600	2.10638900
C	-1	-0.44010000	4.99630000	5.70810000
H	0	-0.37623400	3.90618300	5.80226500
H	0	-1.46742300	5.28732300	5.91791800
H	0	0.22240800	5.42408500	6.46513800
C	-1	5.53960000	5.40700000	2.72590000
C	-1	6.53880000	4.78270000	3.47940000
H	0	6.28334700	4.27558100	4.40402300
C	-1	7.86570000	4.77120000	3.10130000
H	0	8.62024900	4.27829600	3.70543500
C	-1	8.25360000	5.40050000	1.92160000
C	-1	7.29090000	6.02760000	1.13980000
H	0	7.55231300	6.52565900	0.21332300
C	-1	5.96500000	6.01680000	1.54680000
H	0	5.25011600	6.52390800	0.90776500
C	-1	10.02300000	6.00600000	0.43600000
H	0	9.80919800	7.07962700	0.48034400
H	0	9.56060200	5.57607900	-0.45949700
H	0	11.09989400	5.85413300	0.39257800

**Supplementary Table 2. Cartesian coordinates of optimized 1b.**

F	-9.43623600	-0.11539300	-0.57420900
O	8.74653700	-0.43564500	0.25676400
N	-3.16530000	0.11269100	-0.32768800
N	-1.83023900	-0.06592100	-0.18254700
C	-3.94518300	-0.59367500	0.41073600
C	-5.39353800	-0.47524400	0.15569500
C	-6.33283500	-0.93019100	1.08670000
H	-6.00501300	-1.37531500	2.02047000
C	-7.69737700	-0.80953600	0.85084300
H	-8.43180900	-1.15494400	1.57090800
C	-8.11952500	-0.23188300	-0.33384500
C	-7.21650400	0.23012400	-1.28249800
H	-7.58680600	0.67244500	-2.20168400
C	-5.86078300	0.10880700	-1.03041900
H	-5.13494300	0.46239000	-1.75430000
C	-3.45577000	-1.49941200	1.50252000
H	-3.56342500	-1.02698400	2.48551200
H	-2.39664800	-1.71365900	1.35606300
H	-4.01625700	-2.43706100	1.52466200
C	-1.08984300	0.98409700	-0.12224100
C	0.36843000	0.77224500	-0.08162600
C	1.24169000	1.79641100	0.29841800
H	0.85269300	2.77361800	0.56744900
C	2.61311400	1.58675700	0.34334500
H	3.27024400	2.40744600	0.61705600
C	3.16506100	0.34765700	0.00642600
C	2.28672200	-0.67789400	-0.37340900
H	2.68753600	-1.65877400	-0.61387300
C	0.92003000	-0.47277500	-0.41452600
H	0.24982300	-1.27638400	-0.70041200
C	-1.63853100	2.38034600	-0.07551000
H	-1.62935600	2.77304000	0.94749600
H	-2.67324000	2.38317200	-0.41953400
H	-1.04828700	3.06082100	-0.69363600
C	4.62063700	0.12629300	0.04729000
C	5.40881700	0.66775000	1.07343000
H	4.93353900	1.23554700	1.86842000
C	6.77478800	0.46233500	1.11531600
H	7.38259000	0.87044900	1.91676400
C	7.40547900	-0.29520200	0.12373700
C	6.63949700	-0.84238700	-0.90769900
H	7.09817200	-1.42513200	-1.69866600
C	5.26516200	-0.62824800	-0.93347100
H	4.68701000	-1.03675600	-1.75765700
C	9.43261600	-1.19874800	-0.70890700
H	9.33911800	-0.76084300	-1.70942500
H	9.07526000	-2.23475600	-0.73161400
H	10.47947900	-1.18776600	-0.41041300



### Supplementary Table 3. Cartesian coordinates of optimized 1c.

F (Fragment=1)	0	-9.44942100	-0.10267300	-0.54378600
O (Fragment=1)	0	8.79631800	-0.34187200	0.07587000
N (Fragment=1)	0	-3.17872300	0.14329400	-0.31402500
N (Fragment=1)	0	-1.84183000	-0.03802000	-0.19290600
C (Fragment=1)	0	-3.94973700	-0.62851500	0.36599000
C (Fragment=1)	0	-5.40027400	-0.49818300	0.13006100
C (Fragment=1)	0	-6.33123200	-1.03779500	1.02346100
H (Fragment=1)	0	-5.99510200	-1.55959600	1.91353800
C (Fragment=1)	0	-7.69787300	-0.90605000	0.80639200
H (Fragment=1)	0	-8.42588400	-1.31698900	1.49800200
C (Fragment=1)	0	-8.13059700	-0.23104600	-0.32166200
C (Fragment=1)	0	-7.23607500	0.31685900	-1.23186200
H (Fragment=1)	0	-7.61452700	0.83448400	-2.10736900
C (Fragment=1)	0	-5.87817100	0.18295400	-0.99867700
H (Fragment=1)	0	-5.15882900	0.60237800	-1.69330100
C (Fragment=1)	0	-3.44813300	-1.62024400	1.37432800
H (Fragment=1)	0	-3.55475600	-1.23433400	2.39450400
H (Fragment=1)	0	-2.38810800	-1.81255000	1.20571500
H (Fragment=1)	0	-4.00128300	-2.56089000	1.31868200
C (Fragment=1)	0	-1.10749900	1.00891400	-0.05108700
C (Fragment=1)	0	0.35069600	0.80482700	-0.03876600
C (Fragment=1)	0	1.22675900	1.79954300	0.40374900
H (Fragment=1)	0	0.84090400	2.75129800	0.75585400
C (Fragment=2)	-1	2.59798900	1.59313300	0.41953700
H (Fragment=1)	0	3.22687600	2.40285000	0.77289000
C (Fragment=2)	-1	3.17154500	0.38953200	-0.00981100
C (Fragment=2)	-1	2.28127700	-0.59970900	-0.45189400
H (Fragment=1)	0	2.65636700	-1.55750200	-0.79570400
C (Fragment=1)	0	0.91336200	-0.40510800	-0.46403500
H (Fragment=1)	0	0.25195900	-1.19189700	-0.81072400
C (Fragment=1)	0	-1.66408900	2.39282800	0.11530100
H (Fragment=1)	0	-1.64626300	2.70020700	1.16698900
H (Fragment=1)	0	-2.70222800	2.41724600	-0.21725100
H (Fragment=1)	0	-1.08419300	3.12560500	-0.45064400
C (Fragment=2)	-1	4.63655000	0.17724700	0.00183100
C (Fragment=2)	-1	5.52940200	1.13554800	0.49212700
H (Fragment=1)	0	5.15745500	2.07448200	0.88848600
C (Fragment=1)	0	6.89681600	0.94264300	0.50663200
H (Fragment=1)	0	7.56531900	1.70435100	0.89514300
C (Fragment=1)	0	7.44787200	-0.24454000	0.02050200
C (Fragment=1)	0	6.58609300	-1.22263800	-0.47605900
H (Fragment=1)	0	6.96387400	-2.16093200	-0.86646500
C (Fragment=2)	-1	5.21468300	-0.99759200	-0.47630500
H (Fragment=1)	0	4.58922700	-1.78668400	-0.87963200
C (Fragment=1)	0	9.39472400	-1.52485000	-0.40352000
H (Fragment=1)	0	9.18348900	-1.67947000	-1.46779800
H (Fragment=1)	0	9.06254500	-2.40178500	0.16381800
H (Fragment=1)	0	10.46675700	-1.39470800	-0.26649400

### Supplementary Table 4. Cartesian coordinates of optimized 1d.

F	-9.45137200	0.21798200	-0.49982600
O	8.69426600	-0.87277200	-0.18405900
N	-3.17534700	0.21683300	-0.28003200
N	-1.84420800	-0.02702400	-0.22160400
C	-3.96790800	-0.67877900	0.19092500
C	-5.41444700	-0.45135600	0.01031100
C	-6.35873700	-1.16861300	0.75178700
H	-6.03605800	-1.90494500	1.48063800
C	-7.72131400	-0.94691900	0.58927300
H	-8.45949400	-1.49536400	1.16501800
C	-8.13647800	-0.00024300	-0.33095400
C	-7.22833100	0.73025900	-1.08624000
H	-7.59336900	1.46007100	-1.80163200
C	-5.87446600	0.50279400	-0.90847200
H	-5.14469200	1.06043500	-1.48496900
C	-3.49382600	-1.90711900	0.91091300
H	-3.57953800	-1.78632800	1.99678800
H	-2.44222200	-2.08434000	0.68299400
H	-4.07929300	-2.78578000	0.62995600
C	-1.07990400	0.92247200	0.18873500
C	0.37327700	0.68181000	0.13447800
C	1.27007200	1.48680300	0.84418700
H	0.90147200	2.29827900	1.46422400
C	2.63639900	1.24676800	0.79822900
H	3.30768100	1.86261100	1.39018800
C	3.15998600	0.20070300	0.03317900
C	2.25822700	-0.60352500	-0.67933400
H	2.64101900	-1.40227300	-1.30862600
C	0.89593500	-0.37268000	-0.62698400
H	0.20879000	-0.99589000	-1.18926900
C	-1.59702600	2.22644300	0.72256700
H	-1.58707000	2.23526600	1.81836200
H	-2.62919700	2.37363800	0.40279300
H	-0.98734400	3.06628500	0.38158500
C	4.61029800	-0.04944300	-0.02451500
C	5.12138200	-1.35565900	-0.02188800
H	4.43725000	-2.19635200	0.05172900
C	6.48135900	-1.59549400	-0.07409200
H	6.87714100	-2.60614500	-0.05919200
C	7.38437700	-0.52977300	-0.13461800
C	6.89656400	0.77867300	-0.14053200
H	7.56852600	1.62757500	-0.19930600
C	5.52465600	1.00259200	-0.08480500
H	5.15898200	2.02512200	-0.11987200
C	9.64928700	0.16178400	-0.23867700
H	9.59536800	0.80672300	0.64604500
H	9.53012800	0.77293700	-1.14080800
H	10.62074300	-0.32884000	-0.26513500

**Supplementary Table 5. Cartesian coordinates of optimized 1e.**

F	9.45713800	0.06736900	0.40657100
O	-8.71068500	-0.70553700	0.38094100
N	3.17911000	0.17283900	0.30176200
N	1.84374600	-0.04518700	0.23214500
C	3.95089100	-0.65585700	-0.30661200
C	5.40327600	-0.47382700	-0.12147700
C	6.32538100	-1.09408000	-0.97062200
H	5.98068900	-1.71905500	-1.78800600
C	7.69344400	-0.91435200	-0.80247900
H	8.41448700	-1.38774200	-1.46065200
C	8.13671200	-0.10880700	0.23192700
C	7.25122100	0.52218100	1.09599000
H	7.63800700	1.14184000	1.89854100
C	5.89158600	0.33863000	0.91187900
H	5.17910800	0.82070800	1.57205400
C	3.44821800	-1.76306000	-1.18599500
H	3.52565800	-1.49219900	-2.24509200
H	2.39612500	-1.95413100	-0.97237500
H	4.02138400	-2.68149900	-1.03831100
C	1.08526000	0.96608500	-0.00560500
C	-0.36996300	0.73454600	0.03682400
C	-1.26933900	1.65776100	-0.50609400
H	-0.90335800	2.56995500	-0.96719600
C	-2.63789600	1.42860300	-0.47013700
H	-3.31567600	2.17497700	-0.87492400
C	-3.16062300	0.27053300	0.11220300
C	-2.25630800	-0.65326500	0.65650900
H	-2.63455700	-1.57352400	1.09310400
C	-0.89246800	-0.42941200	0.61765200
H	-0.20214700	-1.15579100	1.03297600
C	1.61002100	2.33361500	-0.33306600
H	1.56920100	2.52321900	-1.41160000
H	2.65279900	2.41348800	-0.02451800
H	1.02449800	3.11317400	0.15982300
C	-4.61266000	0.02710700	0.15422700
C	-5.43178400	0.34589100	-0.92923500
H	-4.98627600	0.75449000	-1.83206500
C	-6.80410100	0.11920800	-0.90188000
H	-7.39874100	0.37128300	-1.77278500
C	-7.38997300	-0.43990800	0.23574000
C	-6.58318400	-0.76457100	1.33050800
H	-7.05563000	-1.18791200	2.21133300
C	-5.22106800	-0.53550900	1.28592200
H	-4.61538100	-0.76959800	2.15686300
C	-9.57228900	-0.39011000	-0.68837600
H	-9.31572200	-0.95428100	-1.59251300
H	-9.55818400	0.68250000	-0.91398200
H	-10.57117700	-0.67388500	-0.36151800

**Supplementary Table 6. Cartesian coordinates of optimized 1f.**

F	-9.44033900	0.01973500	-0.49135300
O	8.76319000	-0.28393000	-0.18465800
N	-3.16690600	0.21326200	-0.28357800
N	-1.82881900	0.01118700	-0.22296300
C	-3.93120800	-0.69685300	0.20591400
C	-5.38424300	-0.51699700	0.02377300
C	-6.30538000	-1.24956100	0.77927600
H	-5.95960700	-1.96273400	1.52045500
C	-7.67427800	-1.07247700	0.61512400
H	-8.39471700	-1.63296200	1.20165000
C	-8.11921300	-0.15524000	-0.32086900
C	-7.23463500	0.58927000	-1.09031700
H	-7.62256900	1.29499700	-1.81772400
C	-5.87426700	0.40638300	-0.91082900
H	-5.16252900	0.97588300	-1.49817200
C	-3.41901600	-1.89625100	0.94828700
H	-3.50834000	-1.75802200	2.03178600
H	-2.36245700	-2.04483600	0.72285800
H	-3.97694500	-2.79776400	0.68412300
C	-1.09334200	0.99230400	0.16524600
C	0.36642000	0.79515600	0.11279200
C	1.23924900	1.64143600	0.80409200
H	0.84700900	2.45388100	1.40812600
C	2.61226000	1.44282800	0.75966000
H	3.26500000	2.09177300	1.33677100
C	3.16643600	0.39769800	0.01511700
C	2.28867600	-0.44695400	-0.68038700
H	2.69523000	-1.24461100	-1.29603100
C	0.91999700	-0.25736900	-0.62928500
H	0.25141800	-0.91182300	-1.17831300
C	-1.64927600	2.29096300	0.67227100
H	-1.63808800	2.32342300	1.76761100
H	-2.68591500	2.39974200	0.35158600
H	-1.06599800	3.14155900	0.31232000
C	4.62365600	0.19019800	-0.03730600
C	5.17300400	-1.09198100	-0.00855300
H	4.51508800	-1.95193800	0.08129100
C	6.54757900	-1.30121300	-0.05388100
H	6.92904000	-2.31545900	-0.01648100
C	7.41142300	-0.20689300	-0.13318500
C	6.87698600	1.08471500	-0.16464000
H	7.56140200	1.92396000	-0.23903500
C	5.50906700	1.27515900	-0.11619400
H	5.11211700	2.28500100	-0.17031600
C	9.35591600	-1.56215200	-0.16710300
H	9.03970800	-2.16445300	-1.02662400
H	9.12375500	-2.10129300	0.75863600
H	10.43012300	-1.39464800	-0.22331500

**Supplementary Table 7. Cartesian coordinates of optimized 2aH-A.**

Cl	-1	2.12640000	6.55740000	-1.99380000
O	-1	-3.54990000	23.72530000	2.64600000
N	-1	0.34820000	12.59640000	0.24420000
N	-1	-0.24190000	13.81520000	0.58600000
C	-1	-0.34400000	11.83600000	-0.53710000
C	-1	0.25430000	10.51480000	-0.87440000
C	-1	-0.38380000	9.64440000	-1.75490000
H	0	-1.33540800	9.90996900	-2.20251500
C	-1	0.17820000	8.42130000	-2.08520000
H	0	-0.32950500	7.75347100	-2.77330100
C	-1	1.39090000	8.07210000	-1.55340000
C	-1	2.04580000	8.91140000	-0.67220000
H	0	3.00232500	8.62135100	-0.25065900
C	-1	1.47070000	10.12160000	-0.34180000
H	0	1.97538700	10.78890300	0.34878700
C	-1	-1.64960000	12.21970000	-1.13230000
H	0	-2.01068400	13.14765500	-0.69248000
H	0	-2.40180700	11.44062200	-0.97650000
H	0	-1.55946000	12.36738700	-2.21433900
C	-1	0.52520000	14.84490000	0.48600000
C	-1	-0.06290000	16.15160000	0.85150000
C	-1	0.55220000	17.35900000	0.49140000
H	0	1.49846200	17.35440000	-0.04047800
C	-1	-0.03010000	18.57190000	0.79430000
H	0	0.49944200	19.46982300	0.49345500
C	-1	-1.26080000	18.67350000	1.44660000
C	-1	-1.86730000	17.45710000	1.79530000
H	0	-2.82182900	17.45271100	2.31068400
C	-1	-1.28750000	16.23910000	1.51680000
H	0	-1.78785200	15.32006200	1.80406000
C	-1	1.92120000	14.77390000	-0.02820000
H	0	2.30198400	13.75692600	0.05993800
H	0	2.58329700	15.45594600	0.51032300
H	0	1.96272300	15.04804500	-1.08876200
C	-1	-1.88410000	19.97940000	1.76400000
C	-1	-1.27940000	21.19740000	1.39630000
H	0	-0.33378700	21.20435800	0.86596600
C	-1	-1.85910000	22.40680000	1.69230000
H	0	-1.38251700	23.34018000	1.40854500
C	-1	-3.07500000	22.46730000	2.37670000
C	-1	-3.69520000	21.29400000	2.73150000
H	0	-4.64385300	21.29389100	3.25722500
C	-1	-3.10320000	20.07870000	2.42550000
H	0	-3.62971000	19.18139000	2.73220400
C	-1	-4.82030000	23.83400000	3.28840000
H	0	-5.61149300	23.37102800	2.68856800
H	0	-5.00995600	24.90181100	3.37742000
H	0	-4.80365700	23.38316000	4.28680000

**Supplementary Table 8. Cartesian coordinates of optimized 2aH-B\*.**

Cl	-1	4.55440000	7.62350000	2.01130000
O	-1	-1.06560000	24.83190000	6.73940000
N	-1	2.73590000	13.90820000	3.37240000
N	-1	2.11940000	15.12110000	3.71490000
C	-1	1.98140000	12.87230000	3.45940000
C	-1	2.59130000	11.56990000	3.07790000
C	-1	1.99410000	10.34720000	3.41510000
H	0	1.05072800	10.34107000	3.95310300
C	-1	2.57600000	9.13390000	3.10990000
H	0	2.09830400	8.19960300	3.38321800
C	-1	3.79050000	9.13350000	2.43920000
C	-1	4.41650000	10.32050000	2.08900000
H	0	5.36377300	10.29704500	1.56082200
C	-1	3.81270000	11.52200000	2.39420000
H	0	4.29057800	12.45686400	2.12086000
C	-1	0.57720000	12.91190000	3.97360000
H	0	0.53872200	12.60501900	5.02507600
H	0	-0.07514800	12.23868500	3.41198600
H	0	0.18713800	13.92702000	3.91411500
C	-1	2.81060000	15.88870000	4.48250000
C	-1	2.19950000	17.19610000	4.81590000
C	-1	2.82080000	18.07940000	5.70790000
H	0	3.77034000	17.81886900	6.16407400
C	-1	2.25400000	19.29470000	6.02980000
H	0	2.79742500	19.93631300	6.71490100
C	-1	1.02630000	19.70790000	5.50410000
C	-1	0.40520000	18.80810000	4.61600000
H	0	-0.54998400	19.05580800	4.16588000
C	-1	0.97870000	17.59680000	4.28410000
H	0	0.47249100	16.93308300	3.59068700
C	-1	4.14770000	15.54100000	5.05700000
H	0	4.07965300	15.39098900	6.13976200
H	0	4.86778100	16.34579300	4.88596200
H	0	4.52836200	14.62475000	4.60955800
C	-1	0.43300000	21.03300000	5.82840000
C	-1	1.05140000	21.90180000	6.73630000
H	0	1.96743200	21.61393000	7.23916200
C	-1	0.52100000	23.15280000	7.02860000
H	0	1.00957200	23.82296000	7.72810600
C	-1	-0.64320000	23.56750000	6.40290000
C	-1	-1.29230000	22.71410000	5.53160000
H	0	-2.21632500	23.00381700	5.04404500
C	-1	-0.75230000	21.46780000	5.25620000
H	0	-1.28658500	20.83661700	4.55461400
C	-1	-2.24780000	25.30510000	6.10770000
H	0	-2.13405800	25.33965300	5.01845600
H	0	-2.39964800	26.31460400	6.48556600
H	0	-3.11613400	24.68872300	6.36634200

### Supplementary Table 9. Cartesian coordinates of optimized 2b-A.

C1 (Fragment=1)	0	-9.43744900	-0.05620900	-0.51104200
O (Fragment=1)	0	9.21544900	-0.33333300	0.02402800
N (Fragment=1)	0	-2.76622200	0.13847200	-0.26976500
N (Fragment=1)	0	-1.42930300	-0.04091100	-0.16007800
C (Fragment=1)	0	-3.53170900	-0.62841600	0.42167000
C (Fragment=1)	0	-4.98382100	-0.49559700	0.19618300
C (Fragment=1)	0	-5.90913200	-1.02679800	1.09941800
H (Fragment=1)	0	-5.56875300	-1.54421900	1.99057600
C (Fragment=1)	0	-7.27686300	-0.89285900	0.89203700
H (Fragment=1)	0	-7.98704100	-1.30322100	1.60174500
C (Fragment=1)	0	-7.72718100	-0.22417800	-0.23674300
C (Fragment=1)	0	-6.82944300	0.31411300	-1.15462100
H (Fragment=1)	0	-7.19788600	0.82993000	-2.03495400
C (Fragment=1)	0	-5.47003700	0.17888500	-0.93201700
H (Fragment=1)	0	-4.75708100	0.59303100	-1.63651000
C (Fragment=1)	0	-3.02344200	-1.61492800	1.43141300
H (Fragment=1)	0	-1.96580500	-1.81204000	1.25327900
H (Fragment=1)	0	-3.57995300	-2.55420100	1.38757500
H (Fragment=1)	0	-3.11824800	-1.22208500	2.45009700
C (Fragment=1)	0	-0.69400000	1.00450800	-0.01224500
C (Fragment=1)	0	0.76382700	0.80084200	-0.01438700
C (Fragment=1)	0	1.64479800	1.78974300	0.42849600
H (Fragment=1)	0	1.26499800	2.73901600	0.79350900
C (Fragment=2)	-1	3.01614900	1.58118300	0.42924500
H (Fragment=1)	0	3.64415000	2.38912900	0.78919500
C (Fragment=2)	-1	3.59178100	0.38736300	-0.01107400
C (Fragment=2)	-1	2.69302600	-0.59412400	-0.45603200
H (Fragment=1)	0	3.06496700	-1.54665300	-0.81845700
C (Fragment=1)	0	1.32513100	-0.40382700	-0.45561800
H (Fragment=1)	0	0.66396400	-1.18897300	-0.80639800
C (Fragment=1)	0	-1.25025400	2.38572800	0.17533500
H (Fragment=1)	0	-2.29048600	2.41438300	-0.15052000
H (Fragment=1)	0	-0.67426400	3.12593700	-0.38476700
H (Fragment=1)	0	-1.22593900	2.67956900	1.23072600
C (Fragment=2)	-1	5.05726300	0.17088100	-0.02196500
C (Fragment=2)	-1	5.95431400	1.15290300	0.44206100
H (Fragment=1)	0	5.58128500	2.10053500	0.81458300
C (Fragment=1)	0	7.32038300	0.95958700	0.44483800
H (Fragment=1)	0	7.99496200	1.72951000	0.80591300
C (Fragment=1)	0	7.86623400	-0.24058000	-0.01909200
C (Fragment=1)	0	7.00273900	-1.23306300	-0.48123300
H (Fragment=1)	0	7.38019000	-2.18035500	-0.84952700
C (Fragment=2)	-1	5.62921500	-1.01351100	-0.47333300
H (Fragment=1)	0	5.00072800	-1.81624800	-0.84365000
C (Fragment=1)	0	9.81231200	-1.52586400	-0.43314300
H (Fragment=1)	0	9.48986000	-2.38953000	0.15957600
H (Fragment=1)	0	10.88540200	-1.38890400	-0.31207900
H (Fragment=1)	0	9.58895000	-1.70726200	-1.49068400

**Supplementary Table 10. Cartesian coordinates of optimized 2b-B\*.**

Cl	0	9.43669300	-0.04932900	-0.52675500
O	0	-9.21651300	-0.31023800	0.00811900
N	0	2.76570800	0.13106200	-0.26707400
N	0	1.42960000	-0.05049400	-0.15018600
C	0	3.53544600	-0.62399000	0.43265800
C	0	4.98647900	-0.49047800	0.20071100
C	0	5.91606000	-1.00683600	1.10817000
H	0	5.57989700	-1.51286700	2.00743100
C	0	7.28276900	-0.87223100	0.89458400
H	0	7.99626600	-1.27098600	1.60757200
C	0	7.72775100	-0.21793800	-0.24469100
C	0	6.82569100	0.30538900	-1.16697700
H	0	7.18998200	0.81003400	-2.05547600
C	0	5.46735700	0.16971600	-0.93818200
H	0	4.75108700	0.57229900	-1.64600500
C	0	3.03311500	-1.59760200	1.45776800
H	0	3.13041100	-1.19037100	2.47055100
H	0	3.59188300	-2.53599200	1.42508400
H	0	1.97539200	-1.79980000	1.28603700
C	0	0.69167500	0.99510900	-0.01728900
C	0	-0.76564900	0.78710600	-0.01111300
C	0	-1.64719900	1.78114800	0.41854700
H	0	-1.26752000	2.73782600	0.76389900
C	-1	-3.01870600	1.57108700	0.42827700
H	0	-3.64677000	2.38590100	0.77141200
C	-1	-3.59189300	0.36522000	0.01393100
C	-1	-2.69012100	-0.62356300	-0.42566400
H	0	-3.06189500	-1.58298400	-0.76948900
C	0	-1.32357600	-0.42678900	-0.43226500
H	0	-0.65967400	-1.21375600	-0.77377900
C	0	1.24457700	2.38082600	0.14556700
H	0	1.22151100	2.69264700	1.19580800
H	0	0.66552300	3.10980900	-0.42599600
H	0	2.28406500	2.40663400	-0.18283300
C	-1	-5.06437500	0.15405000	-0.00245800
C	-1	-5.94341900	1.13865700	0.46588300
H	0	-5.56232300	2.07557800	0.85582000
C	0	-7.31235300	0.95928700	0.45791800
H	0	-7.98251500	1.73044800	0.82449900
C	0	-7.86596300	-0.23000100	-0.02478400
C	0	-7.00938700	-1.22583500	-0.49422200
H	0	-7.39420800	-2.16387200	-0.87820400
C	-1	-5.63383200	-1.01837500	-0.47419900
H	0	-5.00697500	-1.81791200	-0.85362900
C	0	-9.82174900	-1.49121900	-0.46741400
H	0	-9.59373200	-1.66171200	-1.52579900
H	0	-10.89423100	-1.34555900	-0.35113400
H	0	-9.51120400	-2.36527800	0.11640200



### Supplementary Table 11. Cartesian coordinates of optimized 2c.

Cl	-9.42204600	-0.08171700	-0.54426300
O	9.16402300	-0.43249400	0.21373900
N	-2.75121500	0.10200000	-0.28052700
N	-1.41600400	-0.07193200	-0.14212800
C	-3.52568800	-0.58118000	0.48464900
C	-4.97559500	-0.46564000	0.23632500
C	-5.90956600	-0.88996500	1.18598500
H	-5.57779700	-1.30893200	2.13053600
C	-7.27517100	-0.77198600	0.95612800
H	-7.99212000	-1.09854900	1.70163100
C	-7.71455500	-0.22811600	-0.24187200
C	-6.80800800	0.20178500	-1.20704000
H	-7.16796400	0.62033600	-2.14087700
C	-5.45081700	0.08425900	-0.96194900
H	-4.73108700	0.41502500	-1.70269700
C	-3.02985000	-1.45579300	1.59834500
H	-1.97280300	-1.67830100	1.44890500
H	-3.59304100	-2.39046900	1.65313400
H	-3.12698400	-0.95428000	2.56792000
C	-0.67514200	0.97869000	-0.10075700
C	0.78328900	0.76779500	-0.06931400
C	1.65894400	1.79659200	0.29222100
H	1.27167900	2.77658700	0.55349600
C	3.03072800	1.58795800	0.32838500
H	3.68965300	2.41190200	0.58751000
C	3.58050000	0.34532000	0.00087400
C	2.69962500	-0.68486100	-0.36018700
H	3.09894300	-1.66822100	-0.59276600
C	1.33257200	-0.48078300	-0.39248600
H	0.66060300	-1.28799900	-0.66374800
C	-1.22483400	2.37483900	-0.06651000
H	-2.26105500	2.37348100	-0.40624100
H	-0.63796700	3.04916400	-0.69437300
H	-1.21182200	2.77840600	0.95218700
C	5.03642100	0.12503900	0.03225300
C	5.83282100	0.67894900	1.04532800
H	5.36396900	1.25584900	1.83757300
C	7.19916300	0.47459800	1.07820600
H	7.81343500	0.89235600	1.86967900
C	7.82196000	-0.29427300	0.09031700
C	7.04765800	-0.85391400	-0.92818200
H	7.50002400	-1.44568900	-1.71605700
C	5.67306700	-0.64076900	-0.94493100
H	5.08832500	-1.05920400	-1.75942900
C	9.84263200	-1.20654300	-0.74859900
H	9.48578100	-2.24293100	-0.75611100
H	10.89189600	-1.19142500	-0.45889900
H	9.74055700	-0.78043500	-1.75334600

**Supplementary Table 12. Cartesian coordinates of optimized 2d.**

Cl	-9.43565600	0.23743400	-0.46407900
O	9.11303800	-0.84261100	-0.23363100
N	-2.76105100	0.18554600	-0.24212100
N	-1.42936500	-0.05056800	-0.19265300
C	-3.54658300	-0.71074500	0.23878000
C	-4.99485900	-0.48638000	0.06731500
C	-5.93267600	-1.20127300	0.81800900
H	-5.60501700	-1.93425000	1.54818800
C	-7.29651100	-0.98240200	0.66409000
H	-8.01638600	-1.53773500	1.25554500
C	-7.73025900	-0.04054100	-0.25722000
C	-6.81977000	0.68552400	-1.02011800
H	-7.17548400	1.41490800	-1.74002600
C	-5.46422600	0.46189600	-0.85161900
H	-4.74145100	1.01949500	-1.43712900
C	-3.06399600	-1.93452900	0.96035000
H	-2.01419700	-2.11114600	0.72357900
H	-3.65017400	-2.81569700	0.68891700
H	-3.13985000	-1.80882300	2.04639000
C	-0.66680800	0.89684000	0.22567700
C	0.78698400	0.66428400	0.15919700
C	1.68395500	1.46377100	0.87485800
H	1.31514800	2.26444400	1.50866900
C	3.05109800	1.23134800	0.81713400
H	3.72292800	1.84210400	1.41367700
C	3.57515200	0.19892100	0.03401300
C	2.67306300	-0.59980600	-0.68429400
H	3.05595600	-1.38758200	-1.32717000
C	1.31000000	-0.37677200	-0.62025200
H	0.62266500	-0.99565700	-1.18709200
C	-1.18795000	2.19033600	0.78050700
H	-2.22158100	2.33839700	0.46558100
H	-0.58279800	3.03779900	0.45075200
H	-1.17539900	2.18259400	1.87625900
C	5.02627200	-0.04288300	-0.03626200
C	5.54392300	-1.34637300	-0.05600100
H	4.86460000	-2.19161400	0.00962000
C	6.90471300	-1.57835400	-0.12022400
H	7.30573400	-2.58703600	-0.12258300
C	7.80190900	-0.50717000	-0.17088200
C	7.30742400	0.79871700	-0.15456400
H	7.97468200	1.65183300	-0.20520200
C	5.93482100	1.01469100	-0.08683200
H	5.56378900	2.03573500	-0.10466000
C	10.06259400	0.19749100	-0.27929500
H	9.93449700	0.82105000	-1.17163900
H	11.03624300	-0.28782200	-0.31916600
H	10.01121500	0.82914100	0.61509300

**Supplementary Table 13. Cartesian coordinates of optimized 2e.**

Cl	9.44109400	0.09695800	0.38759800
O	-9.12648100	-0.68545400	0.42241100
N	2.76386800	0.15398100	0.26973300
N	1.42846300	-0.05853200	0.20776500
C	3.52998300	-0.67224300	-0.34873100
C	4.98352300	-0.49141300	-0.17046400
C	5.90077600	-1.10578500	-1.02802600
H	5.55279900	-1.72579100	-1.84795000
C	7.26956500	-0.92724700	-0.86623800
H	7.97331200	-1.40337400	-1.54038900
C	7.72924200	-0.12862400	0.17056100
C	6.83970300	0.49480100	1.04134300
H	7.21557700	1.11217900	1.85027000
C	5.47896700	0.31337900	0.86441700
H	4.77227800	0.79240400	1.53317900
C	3.02089200	-1.77331200	-1.23168600
H	1.97053900	-1.96623600	-1.01100500
H	3.59511300	-2.69274600	-1.09476100
H	3.08974800	-1.49534600	-2.28952600
C	0.67130600	0.95166400	-0.03858400
C	-0.78414200	0.72509700	0.01461000
C	-1.68348400	1.64340300	-0.53658900
H	-1.31726200	2.54790200	-1.01242300
C	-3.05244100	1.41883700	-0.49030300
H	-3.73016300	2.16144400	-0.90199400
C	-3.57545000	0.27056600	0.11098500
C	-2.67102700	-0.64831900	0.66342600
H	-3.04968300	-1.56123400	1.11477400
C	-1.30678600	-0.42917600	0.61427700
H	-0.61656500	-1.15196200	1.03602500
C	1.19926900	2.31283800	-0.38645000
H	2.24268300	2.39473200	-0.08024900
H	0.61656300	3.10101000	0.09578200
H	1.15788500	2.48691700	-1.46755500
C	-5.02789200	0.03207700	0.16402700
C	-5.85182100	0.33846200	-0.91937800
H	-5.41002000	0.73336600	-1.83009000
C	-7.22456500	0.11609300	-0.88168400
H	-7.82313800	0.35787600	-1.75280700
C	-7.80595500	-0.42568200	0.26661500
C	-6.99426700	-0.73764500	1.36149700
H	-7.46323000	-1.14746300	2.25053000
C	-5.63178700	-0.51325800	1.30655600
H	-5.02218300	-0.73716500	2.17743900
C	-9.99301500	-0.38243200	-0.64659900
H	-9.97722600	0.68691400	-0.88702800
H	-10.99085900	-0.65892100	-0.31048700
H	-9.74278900	-0.95977800	-1.54415500

**Supplementary Table 14. Cartesian coordinates of optimized 2f.**

Cl	-9.42591700	0.05620700	-0.45958700
O	9.17803100	-0.27067800	-0.22424300
N	-2.75228700	0.19700100	-0.24638300
N	-1.41439000	-0.00052000	-0.19293800
C	-3.51196600	-0.70850100	0.25823500
C	-4.96611500	-0.52919200	0.08341900
C	-5.88299600	-1.25247300	0.85174200
H	-5.53443600	-1.95857600	1.59852800
C	-7.25255500	-1.07590700	0.69431800
H	-7.95613900	-1.63734200	1.29946100
C	-7.71324500	-0.16850900	-0.24825400
C	-6.82402000	0.56497100	-1.02893600
H	-7.20055600	1.26705100	-1.76521000
C	-5.46262100	0.38371200	-0.85685500
H	-4.75621600	0.94770200	-1.45605300
C	-2.99470200	-1.89974300	1.00966000
H	-1.94009600	-2.05165700	0.77720800
H	-3.55504700	-2.80386300	0.75993700
H	-3.07499600	-1.74967600	2.09228000
C	-0.67831800	0.97981600	0.19615200
C	0.78133300	0.78640800	0.13330500
C	1.65638600	1.63048300	0.82447000
H	1.26609200	2.43813300	1.43614600
C	3.02949000	1.43538500	0.77012000
H	3.68435100	2.08219400	1.34718100
C	3.58135900	0.39625700	0.01544600
C	2.70121800	-0.44616400	-0.67980400
H	3.10573000	-1.23894700	-1.30299900
C	1.33247400	-0.26025100	-0.61878000
H	0.66211400	-0.91303700	-1.16765000
C	-1.23486700	2.27370900	0.71438000
H	-2.27270800	2.38343100	0.39764200
H	-0.65426100	3.12789900	0.35888200
H	-1.22054600	2.29816100	1.80986600
C	5.03864800	0.19258900	-0.04753700
C	5.59109100	-1.08848200	-0.03088200
H	4.93581000	-1.95061100	0.05737000
C	6.96580400	-1.29412700	-0.08623200
H	7.34988100	-2.30767300	-0.05799200
C	7.82658100	-0.19722300	-0.16370400
C	7.28894200	1.09332900	-0.18314700
H	7.97091700	1.93465600	-0.25629800
C	5.92095600	1.28020800	-0.12469900
H	5.52136900	2.28946200	-0.16957300
C	9.77403400	-1.54756200	-0.21902100
H	9.54905900	-2.09341600	0.70453800
H	10.84742600	-1.37694800	-0.28089200
H	9.45386100	-2.14481500	-1.08057400

**Supplementary Table 15. Cartesian coordinates of optimized 3aH.**

Br	-1	8.36710000	3.82480000	44.92560000
O	-1	2.69240000	3.49440000	26.98280000
N	-1	6.56230000	4.01110000	38.33750000
N	-1	5.96470000	4.00820000	37.08270000
C	-1	5.80230000	3.61530000	39.30630000
C	-1	6.41080000	3.64710000	40.68140000
C	-1	5.76780000	3.06670000	41.75780000
H	0	4.81145500	2.56954500	41.63306200
C	-1	6.33600000	3.10580000	43.00610000
H	0	5.83151000	2.64807600	43.85131500
C	-1	7.56270000	3.73680000	43.20250000
C	-1	8.22430000	4.31280000	42.13840000
H	0	9.18175400	4.80201200	42.28276400
C	-1	7.65480000	4.24990000	40.87790000
H	0	8.15777900	4.69458900	40.02660800
C	-1	4.39980000	3.14560000	39.12620000
H	0	4.03993300	3.41289400	38.13432800
H	0	3.73817200	3.57846600	39.88172200
H	0	4.33270300	2.05582700	39.22375700
C	-1	6.72150000	3.63120000	36.12630000
C	-1	6.14170000	3.62760000	34.77160000
C	-1	6.76430000	3.04000000	33.68290000
H	0	7.72729000	2.55215600	33.80787400
C	-1	6.19610000	3.04210000	32.42240000
H	0	6.74508700	2.55921500	31.62192000
C	-1	4.94440000	3.62470000	32.17270000
C	-1	4.32570000	4.24050000	33.27770000
H	0	3.36502900	4.73023000	33.15740300
C	-1	4.88630000	4.23830000	34.52600000
H	0	4.37771100	4.71803900	35.35530400
C	-1	4.34290000	3.61890000	30.81800000
C	-1	4.97000000	3.01610000	29.73350000
H	0	5.93231700	2.53162100	29.85695300
C	-1	4.40050000	2.99080000	28.47290000
H	0	4.89538100	2.50799700	27.63696200
C	-1	3.16610000	3.59350000	28.26420000
C	-1	2.52300000	4.22670000	29.31600000
H	0	1.56365000	4.71253400	29.17542500
C	-1	3.10410000	4.23470000	30.57250000
H	0	2.56983100	4.73243200	31.37332700
C	-1	8.13930000	3.20640000	36.32680000
H	0	8.50424300	3.55472200	37.29102000
H	0	8.78334500	3.59088100	35.53204800
H	0	8.22866700	2.11396700	36.31522100
C	-1	1.43120000	4.09790000	26.70080000
H	0	0.63089600	3.64928600	27.29960000
H	0	1.24417500	3.90565400	25.64608200
H	0	1.45795500	5.17939100	26.87389100

**Supplementary Table 16. Cartesian coordinates of optimized 3b.**

Br	0	-8.78872100	-0.02799000	-0.41332000
O	0	10.02669300	-0.31072100	-0.07487800
N	0	-1.95435700	0.13269800	-0.19392300
N	0	-0.61736100	-0.04919400	-0.09073200
C	0	-2.71740200	-0.62269600	0.51270100
C	0	-4.17059100	-0.48796100	0.29501300
C	0	-5.09139700	-1.00327000	1.21169500
H	0	-4.74691600	-1.50933900	2.10788600
C	0	-6.46055100	-0.86798700	1.01230800
H	0	-7.16363500	-1.26748900	1.73500900
C	0	-6.91792300	-0.21320800	-0.12359800
C	0	-6.02272800	0.30930600	-1.05530000
H	0	-6.39090900	0.81467200	-1.94164000
C	0	-4.66209400	0.17219800	-0.83907200
H	0	-3.95271200	0.57410300	-1.55430600
C	0	-2.20554700	-1.59757200	1.53183400
H	0	-1.14997600	-1.80108300	1.34867900
H	0	-2.76591900	-2.53516900	1.50460900
H	0	-2.29141700	-1.19080500	2.54583600
C	0	0.12218200	0.99587200	0.03781700
C	0	1.57939400	0.78803100	0.02784300
C	0	2.46548500	1.78077900	0.45286000
H	0	2.08879500	2.73514400	0.80789700
C	-1	3.83623300	1.57121200	0.44668400
H	0	4.46870400	2.38175300	0.79156200
C	-1	4.40731700	0.36355200	0.01779300
C	-1	3.49932600	-0.62201700	-0.41490600
H	0	3.86474400	-1.57906900	-0.77161300
C	0	2.13265700	-0.42353600	-0.40459100
H	0	1.46486200	-1.20862800	-0.74284500
C	-1	5.87624200	0.16719700	-0.00966600
C	-1	6.76165300	1.15311000	0.41079300
H	0	6.39313200	2.10350000	0.78034200
C	0	8.13225200	0.96991000	0.37952900
H	0	8.80988500	1.75000000	0.71170600
C	0	8.67561400	-0.22972600	-0.08324300
C	0	7.81057600	-1.23951200	-0.51288100
H	0	8.19132000	-2.18596200	-0.88029800
C	-1	6.43820800	-1.03442100	-0.47271300
H	0	5.80020000	-1.84063900	-0.81572700
C	0	-0.42909700	2.38101600	0.21084100
H	0	-1.47148700	2.40809900	-0.10820500
H	0	0.14487700	3.11215000	-0.36306100
H	0	-0.39678900	2.68885300	1.26201600
C	0	10.62330500	-1.50263500	-0.53372300
H	0	10.32528700	-2.36270100	0.07679700
H	0	11.69770900	-1.35372800	-0.44179300
H	0	10.37529000	-1.69861600	-1.58316200

**Supplementary Table 17. Cartesian coordinates of optimized 3c.**

Br	-8.77690300	-0.05842100	-0.42169400
O	9.97726100	-0.43631000	0.15286600
N	-1.94224500	0.10418900	-0.21033400
N	-0.60588300	-0.06922800	-0.08510600
C	-2.70868700	-0.56706900	0.57319800
C	-4.16121000	-0.45252500	0.33973500
C	-5.08471000	-0.86077800	1.30626300
H	-4.74295700	-1.26619600	2.25326500
C	-6.45318200	-0.74389300	1.09116800
H	-7.15839900	-1.05913500	1.85242400
C	-6.90709700	-0.21675800	-0.11061900
C	-6.00912700	0.19702200	-1.09291200
H	-6.37463600	0.60279700	-2.03008700
C	-4.64919200	0.08022700	-0.86088400
H	-3.93766900	0.39859300	-1.61499500
C	-2.20131000	-1.42675800	1.69325700
H	-1.14666000	-1.65399600	1.53415400
H	-2.76591800	-2.35914700	1.76839900
H	-2.28538100	-0.91111100	2.65661600
C	0.13638900	0.98096800	-0.06282500
C	1.59487400	0.76897100	-0.04586800
C	2.47541500	1.80029300	0.29605200
H	2.09195200	2.78305900	0.55249100
C	3.84733700	1.59068900	0.31864500
H	4.50986100	2.41639800	0.56252000
C	4.39229900	0.34450200	-0.00339800
C	3.50651600	-0.68820200	-0.34470700
H	3.90233600	-1.67408400	-0.57251800
C	2.13935900	-0.48313400	-0.36342600
H	1.46368200	-1.29224600	-0.61940900
C	5.84829900	0.12317700	0.01342900
C	6.65667800	0.68582400	1.01210100
H	6.19739000	1.27052800	1.80422700
C	8.02314600	0.48056900	1.03125500
H	8.64676600	0.90516300	1.81170200
C	8.63399000	-0.29806000	0.04354300
C	7.84762800	-0.86652500	-0.96073300
H	8.29046500	-1.46606600	-1.74814500
C	6.47310700	-0.65231900	-0.96375400
H	5.87876500	-1.07782700	-1.76756700
C	-0.41184800	2.37785200	-0.03645300
H	-1.45145500	2.37413800	-0.36573400
H	0.16913100	3.04563000	-0.67664100
H	-0.38836300	2.79116300	0.97813900
C	10.64420800	-1.21991100	-0.80990500
H	10.28649000	-2.25600600	-0.80364900
H	11.69673000	-1.20301600	-0.53237600
H	10.53097700	-0.80310600	-1.81735500

**Supplementary Table 18. Cartesian coordinates of optimized 3d.**

Br	8.78869500	-0.19572400	-0.35534400
O	-9.92793100	0.80611300	-0.29776500
N	1.95129300	-0.15122300	-0.18188100
N	0.61803800	0.07735000	-0.14761800
C	2.72715500	0.75420200	0.29750700
C	4.17822300	0.53572500	0.14223800
C	5.10472200	1.26191200	0.89579900
H	4.76629700	1.99971400	1.61627200
C	6.47160700	1.04905900	0.75810300
H	7.17911400	1.61542800	1.35381800
C	6.92092500	0.10053200	-0.15107500
C	6.01987300	-0.63700100	-0.91697100
H	6.38191900	-1.37188100	-1.62790200
C	4.66140300	-0.41807300	-0.76337200
H	3.94749700	-0.98464700	-1.35129900
C	2.23103600	1.98246700	1.00202200
H	1.18301500	2.15172100	0.75225200
H	2.81592600	2.86382000	0.72847000
H	2.29567100	1.86755300	2.08997900
C	-0.14295900	-0.86848800	0.27702000
C	-1.59736700	-0.64551300	0.19384200
C	-2.49627800	-1.44002500	0.91259300
H	-2.12873200	-2.22937800	1.56116800
C	-3.86414600	-1.21655500	0.83895600
H	-4.53793700	-1.82271300	1.43796600
C	-4.38687000	-0.19852400	0.03633600
C	-3.48279000	0.59523700	-0.68497000
H	-3.86425600	1.37150100	-1.34252700
C	-2.11911200	0.38123100	-0.60518800
H	-1.43015400	0.99606800	-1.17446400
C	-5.83864700	0.03362200	-0.05082200
C	-6.36364700	1.33360000	-0.09408500
H	-5.68989600	2.18371800	-0.03427400
C	-7.72509800	1.55653300	-0.17431200
H	-8.13194400	2.56267100	-0.19488900
C	-8.61553400	0.47941300	-0.21796100
C	-8.11364600	-0.82314900	-0.17828000
H	-8.77542300	-1.68085600	-0.22289700
C	-6.74051100	-1.02995800	-0.09465200
H	-6.36339900	-2.04892800	-0.09437600
C	0.38068000	-2.15081500	0.85493400
H	1.41771800	-2.29761700	0.55073100
H	-0.21694100	-3.00641600	0.53258600
H	0.35900900	-2.12720500	1.95031400
C	-10.87094800	-0.24017200	-0.33744400
H	-10.73073800	-0.87564400	-1.21950200
H	-11.84697800	0.23871800	-0.39344700
H	-10.82439700	-0.85865100	0.56636300



**Supplementary Table 19. Cartesian coordinates of optimized 3e.**

Br	8.79236700	0.08732600	0.29800200
O	-9.93765400	-0.66337200	0.47707400
N	1.95311500	0.13982100	0.21794800
N	0.61676800	-0.06933400	0.16999300
C	2.71161000	-0.69684700	-0.39581600
C	4.16711600	-0.51739800	-0.23227300
C	5.07522600	-1.14519000	-1.08956600
H	4.71883700	-1.77491900	-1.89850700
C	6.44629600	-0.96858100	-0.94258700
H	7.13930700	-1.45714600	-1.61879400
C	6.91860700	-0.15713700	0.08048000
C	6.03631100	0.48005900	0.95112400
H	6.41624400	1.10776500	1.74998800
C	4.67341900	0.29935600	0.78756100
H	3.97392600	0.78901400	1.45632400
C	2.19214100	-1.80830600	-1.25944100
H	1.14341000	-1.99586500	-1.02670200
H	2.76558700	-2.72714700	-1.11554800
H	2.25196600	-1.54454800	-2.32145700
C	-0.13954400	0.93918300	-0.08566000
C	-1.59512200	0.71770800	-0.01732400
C	-2.49627100	1.62992700	-0.57562800
H	-2.13136100	2.52588600	-1.06832500
C	-3.86541900	1.40996800	-0.51515100
H	-4.54435300	2.14800100	-0.93301500
C	-4.38677000	0.27261600	0.10793900
C	-3.48052100	-0.64013500	0.66751700
H	-3.85808500	-1.54486900	1.13592500
C	-2.11612500	-0.42564400	0.60428400
H	-1.42458100	-1.14379000	1.03175900
C	-5.83937400	0.03898700	0.17592700
C	-6.67090500	0.33079900	-0.90569500
H	-6.23519200	0.71034100	-1.82582400
C	-8.04388100	0.11275300	-0.85393700
H	-8.64859200	0.34260700	-1.72405200
C	-8.61772000	-0.40960500	0.30709000
C	-7.79835400	-0.70677400	1.40037000
H	-8.26144500	-1.10152400	2.29924300
C	-6.43576800	-0.48696500	1.33141000
H	-5.81998600	-0.69903000	2.20091000
C	0.38954500	2.29324300	-0.45862900
H	1.43546300	2.37691100	-0.16154100
H	-0.18731900	3.09048600	0.01563200
H	0.34055600	2.45062900	-1.54196900
C	-10.81163700	-0.37474200	-0.58986100
H	-10.79505000	0.69069600	-0.84700400
H	-11.80754600	-0.64339000	-0.24186700
H	-10.56973400	-0.96660700	-1.48021000

**Supplementary Table 20. Cartesian coordinates of optimized 3f.**

Br	-8.77929200	0.05397400	-0.35415300
O	9.98796400	-0.25827500	-0.27873300
N	-1.94273900	0.18468200	-0.18718100
N	-0.60415800	-0.00995600	-0.14681200
C	-2.69580800	-0.72290900	0.32348800
C	-4.15190200	-0.54564300	0.16279900
C	-5.05997900	-1.27052600	0.93969200
H	-4.70326600	-1.97646600	1.68289800
C	-6.43176200	-1.09641500	0.79637600
H	-7.12488100	-1.66118500	1.41024700
C	-6.90468800	-0.18864900	-0.14197200
C	-6.02235400	0.54668400	-0.93141700
H	-6.40264800	1.24953200	-1.66485200
C	-4.65884300	0.36674200	-0.77205400
H	-3.95935100	0.93217600	-1.37811400
C	-2.16930600	-1.91423200	1.06827600
H	-1.11696000	-2.06455600	0.82473700
H	-2.73106800	-2.81880200	0.82345200
H	-2.23852700	-1.76540000	2.15182800
C	0.13358700	0.97020000	0.23953600
C	1.59295000	0.78011700	0.16214700
C	2.47270200	1.62297400	0.84881300
H	2.08650000	2.42711900	1.46766500
C	3.84562500	1.43094700	0.78076800
H	4.50455100	2.07656400	1.35452500
C	4.39250000	0.39627200	0.01639400
C	3.50759900	-0.44490400	-0.67431500
H	3.90786300	-1.23410300	-1.30475400
C	2.13911600	-0.26210200	-0.59966200
H	1.46498400	-0.91388700	-1.14509700
C	5.84953400	0.19585300	-0.06111300
C	6.40463000	-1.08416900	-0.05545200
H	5.75191400	-1.94801200	0.03502400
C	7.77916200	-1.28678900	-0.12462100
H	8.16548800	-2.29967300	-0.10458600
C	8.63701000	-0.18781200	-0.20518200
C	8.09667100	1.10173300	-0.21370900
H	8.77626900	1.94475400	-0.28942900
C	6.72893000	1.28558900	-0.14158400
H	6.32695400	2.29423000	-0.17813200
C	-0.42087200	2.26061100	0.76855400
H	-1.46167400	2.36977600	0.46143000
H	0.15491400	3.11755700	0.41188400
H	-0.39701100	2.28009500	1.86397100
C	10.58651000	-1.53397000	-0.28497700
H	10.37130000	-2.08450000	0.63813200
H	11.65893300	-1.36090600	-0.35613300
H	10.25943300	-2.12790800	-1.14622800

**Supplementary Table 21. Cartesian coordinates of optimized 4aH.**

I	-1	1.09860000	0.23870000	0.10830000
O	-1	6.98980000	-0.12410000	18.20830000
N	-1	3.07170000	0.40220000	6.85410000
C	-1	3.81640000	0.00800000	5.87020000
C	-1	2.01220000	0.14230000	1.99100000
N	-1	3.67440000	0.38550000	8.10850000
C	-1	3.20160000	0.04070000	4.52920000
C	-1	3.83690000	-0.52780000	3.41050000
H	0	4.79961200	-1.01742000	3.51564500
C	-1	3.25080000	-0.47700000	2.16730000
H	0	3.75634100	-0.92152500	1.31576800
C	-1	1.36150000	0.69690000	3.08240000
H	0	0.39586400	1.17707500	2.96287100
C	-1	1.94440000	0.63450000	4.33550000
H	0	1.44110200	1.06975200	5.19168700
C	-1	5.20540000	-0.49660000	6.05310000
H	0	5.24186000	-1.58813400	5.95849300
H	0	5.57087600	-0.23652700	7.04472800
H	0	5.88208600	-0.08577900	5.29845100
C	-1	2.91360000	0.02400000	9.07080000
C	-1	3.50350000	0.01740000	10.42090000
C	-1	2.87590000	-0.58010000	11.52310000
H	0	1.91576700	-1.07180800	11.39290600
C	-1	3.44720000	-0.58880000	12.77910000
H	0	2.90471300	-1.07756000	13.58022000
C	-1	4.69490000	0.01090000	13.02500000
C	-1	5.31990000	0.62290000	11.91880000
H	0	6.27930600	1.11403800	12.04030500
C	-1	4.74860000	0.63230000	10.67150000
H	0	5.25688900	1.11664300	9.84420700
C	-1	1.49780000	-0.42470000	8.87540000
H	0	1.43061800	-1.51838400	8.89630200
H	0	1.12792700	-0.09014300	7.90802700
H	0	0.84758200	-0.04405900	9.66674900
C	-1	5.31420000	-0.00070000	14.38390000
C	-1	4.68460000	-0.61850000	15.46990000
H	0	3.71947300	-1.09719800	15.35044200
C	-1	5.25980000	-0.62940000	16.72380000
H	0	4.76938100	-1.10949400	17.56467800
C	-1	6.50870000	-0.03780000	16.93450000
C	-1	7.14590000	0.60110000	15.87590000
H	0	8.10823900	1.08314200	16.00736000
C	-1	6.55920000	0.59600000	14.62330000
H	0	7.09008300	1.09025700	13.81762300
C	-1	8.25850000	0.46610000	18.47710000
H	0	8.24131300	1.54725000	18.30091700
H	0	9.04822000	0.00736400	17.87208800
H	0	8.45276400	0.27490700	19.53063300

**Supplementary Table 22. Cartesian coordinates of optimized 4b.**

I	0	-8.28261200	-0.01661800	-0.32546000
O	0	10.75123300	-0.32331500	-0.07457500
N	0	-1.23217500	0.13347200	-0.15805800
C	0	-1.98499300	-0.62814700	0.55271200
C	0	-6.19777000	-0.22067100	-0.03026700
N	0	0.10607500	-0.04578600	-0.07287100
C	0	-3.44097500	-0.49407000	0.35350900
C	0	-4.34962600	-1.01553600	1.27846800
H	0	-3.99369400	-1.52603500	2.16776600
C	0	-5.72157500	-0.88091300	1.09643900
H	0	-6.40929700	-1.28778300	1.82974000
C	0	-5.31113400	0.30753200	-0.96910600
H	0	-5.68386800	0.81837400	-1.85038600
C	0	-3.94735900	0.17137100	-0.77057100
H	0	-3.24771000	0.57833600	-1.49265300
C	0	-1.45908400	-1.60906000	1.55872800
H	0	-1.53133200	-1.20873100	2.57634600
H	0	-0.40597000	-1.81088700	1.36005600
H	0	-2.01928200	-2.54679600	1.53322800
C	0	0.84493800	0.99900100	0.06139600
C	0	2.30261400	0.79501200	0.03085700
C	0	3.18949500	1.78371500	0.46494400
H	0	2.81146600	2.72859300	0.84327500
C	-1	4.56116200	1.58115000	0.44159400
H	0	5.19698100	2.38407200	0.79705300
C	-1	5.12613200	0.38046500	-0.02319400
C	-1	4.21813600	-0.60663000	-0.45912400
H	0	4.58425800	-1.55573900	-0.83516700
C	0	2.85153500	-0.40883500	-0.42896300
H	0	2.17915900	-1.18857600	-0.77065900
C	0	0.29186400	2.37996300	0.26035500
H	0	0.85943000	3.12146200	-0.30649100
H	0	0.33119000	2.67144900	1.31594300
H	0	-0.75310900	2.40925200	-0.05014300
C	-1	6.60459200	0.17190200	-0.05373200
C	-1	7.49222000	1.15855100	0.38911000
H	0	7.12191600	2.10715500	0.76044300
C	0	8.86055800	0.96568900	0.36952400
H	0	9.54137600	1.73763100	0.71424400
C	0	9.40059700	-0.23545000	-0.09685600
C	0	8.53593100	-1.23780100	-0.54195500
H	0	8.91661600	-2.18394500	-0.91015400
C	-1	7.16271200	-1.02760900	-0.51532000
H	0	6.52447300	-1.82941200	-0.86840700
C	0	11.34682800	-1.51503400	-0.53504100
H	0	11.10855900	-1.70299300	-1.58821000
H	0	11.03838900	-2.37757400	0.06676900
H	0	12.42093600	-1.37195500	-0.43116200

**Supplementary Table 23. Cartesian coordinates of optimized 4c.**

I	-8.26996600	-0.04233400	-0.34851100
O	10.70183300	-0.43650000	0.10759100
N	-1.21983500	0.10116900	-0.16196600
C	-1.97970000	-0.56009600	0.63623900
C	-6.18762700	-0.21491600	-0.01782400
N	0.11725600	-0.07055100	-0.04634000
C	-3.43409200	-0.44723600	0.41328700
C	-4.34971600	-0.84241300	1.39235300
H	-4.00066300	-1.23608600	2.34175800
C	-5.72011700	-0.72709800	1.18684800
H	-6.41337200	-1.03409800	1.96233700
C	-5.29388100	0.18523300	-1.01162400
H	-5.65984700	0.58029300	-1.95318500
C	-3.93175500	0.07051600	-0.78962000
H	-3.22663200	0.37891600	-1.55396000
C	-1.46331800	-1.40624300	1.76238600
H	-1.53797600	-0.87843300	2.71991300
H	-0.41041400	-1.63689200	1.59661800
H	-2.02829300	-2.33688700	1.85439200
C	0.85970500	0.97970100	-0.03695100
C	2.31824200	0.76784800	-0.03068700
C	3.20141600	1.80111600	0.29829900
H	2.81997900	2.78530200	0.55230900
C	4.57347000	1.59162000	0.31104000
H	5.23791200	2.41866700	0.54492700
C	5.11585600	0.34361600	-0.00835500
C	4.22740900	-0.69100700	-0.33669400
H	4.62142300	-1.67815500	-0.56211100
C	2.86014200	-0.48605200	-0.34552700
H	2.18248900	-1.29664500	-0.59142500
C	0.31130300	2.37657800	-0.01486100
H	0.34136500	2.79566600	0.99718000
H	-0.73050300	2.37082000	-0.33719800
H	0.88775400	3.04083800	-0.66271200
C	6.57193800	0.12236000	-0.00195900
C	7.38825300	0.69054200	0.98707900
H	6.93531400	1.27966100	1.77959000
C	8.75482300	0.48533000	0.99646700
H	9.38465400	0.91422200	1.76953900
C	9.35776300	-0.29880600	0.00824400
C	8.56340200	-0.87281600	-0.98654700
H	8.99993600	-1.47674300	-1.77412000
C	7.18890600	-0.65859600	-0.97977500
H	6.58817600	-1.08854500	-1.77644400
C	11.36110900	-1.22546700	-0.85610600
H	11.23986200	-0.81424200	-1.86491300
H	11.00345400	-2.26149300	-0.84124300
H	12.41580000	-1.20706700	-0.58705100

**Supplementary Table 24. Cartesian coordinates of optimized 4d.**

I	8.28023800	-0.17269200	-0.29018000
O	-10.65420700	0.77294300	-0.34695800
N	1.22829300	-0.12163600	-0.14104000
C	1.99671300	0.79125600	0.33602200
C	6.20015600	0.15022400	-0.07991800
N	-0.10598100	0.10020900	-0.11756200
C	3.44971100	0.57734900	0.19200200
C	4.36818300	1.31279900	0.94601200
H	4.02230700	2.05487000	1.65867500
C	5.73705400	1.10401000	0.81895500
H	6.43251400	1.68131800	1.41836900
C	5.30347900	-0.59567200	-0.84550700
H	5.66612200	-1.33618000	-1.55025300
C	3.94278000	-0.38113600	-0.70286600
H	3.23539100	-0.95527000	-1.29152000
C	1.49065300	2.02301600	1.02707300
H	1.54759800	1.91701300	2.11636100
H	0.44385800	2.18617400	0.76818800
H	2.07408200	2.90450800	0.75088100
C	-0.86516000	-0.84362000	0.31473400
C	-2.32002800	-0.62912500	0.21918600
C	-3.21964300	-1.41865200	0.94252700
H	-2.85245500	-2.19743600	1.60395500
C	-4.58808800	-1.20320000	0.85690600
H	-5.26278500	-1.80481500	1.45945300
C	-5.11057900	-0.19859200	0.03738300
C	-4.20574000	0.59022300	-0.68839300
H	-4.58673900	1.35576100	-1.35866500
C	-2.84157000	0.38430800	-0.59678500
H	-2.15198800	0.99512700	-1.16962700
C	-0.33867700	-2.11533600	0.91310900
H	-0.36643700	-2.07674100	2.00791900
H	0.70071000	-2.26143800	0.61659300
H	-0.93041200	-2.97816100	0.59934900
C	-6.56288400	0.02488700	-0.06248400
C	-7.45901700	-1.04382900	-0.09823100
H	-7.07676200	-2.06075100	-0.08194600
C	-8.83257700	-0.84522500	-0.19378400
H	-9.48968300	-1.70684600	-0.23149200
C	-9.34077400	0.45410500	-0.25405200
C	-8.45611900	1.53629300	-0.21870600
H	-8.86791900	2.53995400	-0.25531900
C	-7.09413400	1.32146700	-0.12646700
H	-6.42512300	2.17576800	-0.07342800
C	-11.59164400	-0.27862100	-0.37922000
H	-11.54815200	-0.88489100	0.53296800
H	-11.44217400	-0.92490100	-1.25185000
H	-12.56966800	0.19447300	-0.44815500

**Supplementary Table 25. Cartesian coordinates of optimized 4e.**

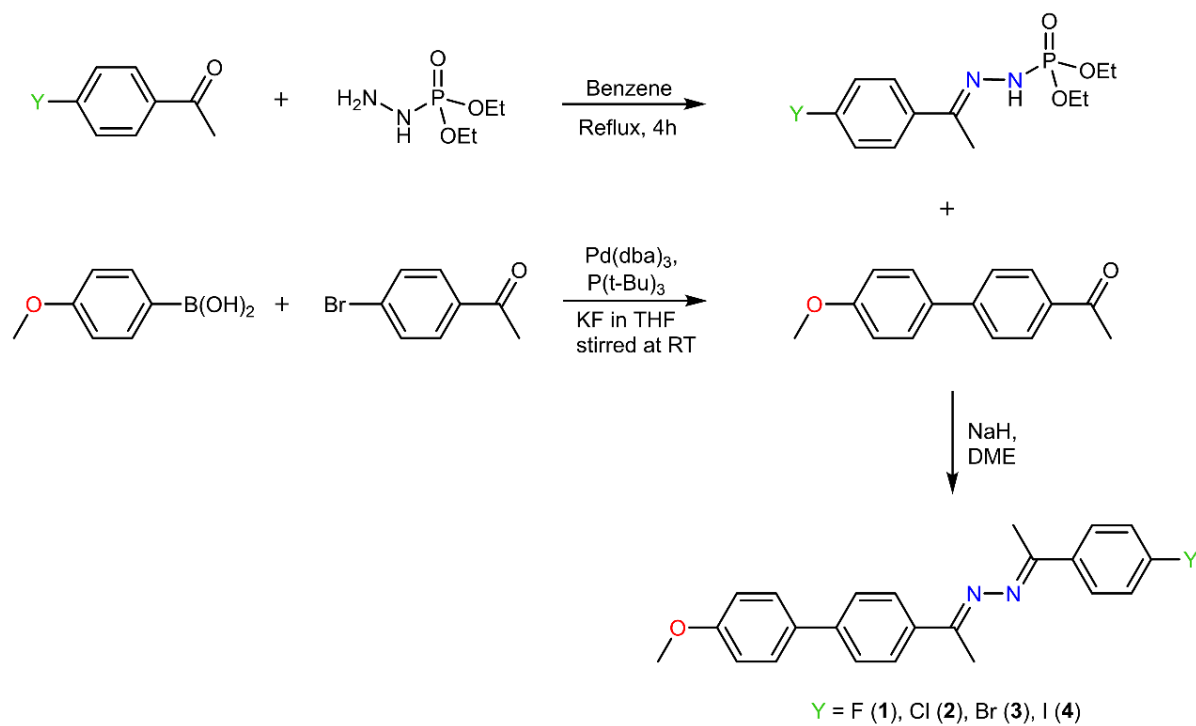
I	8.28314800	0.08494200	0.24442700
O	-10.66159700	-0.63769900	0.52123600
N	1.22956000	0.12391800	0.18233600
C	1.98197400	-0.72303000	-0.42468200
C	6.19716600	-0.18567500	0.01940500
N	-0.10741400	-0.08143600	0.14516800
C	3.43888900	-0.54459200	-0.27215000
C	4.34037000	-1.18550900	-1.12637900
H	3.97805000	-1.82519000	-1.92493900
C	5.71294700	-1.00967400	-0.98988800
H	6.39490200	-1.51175800	-1.66745300
C	5.31781600	0.46398200	0.88615700
H	5.69691100	1.10285100	1.67651700
C	3.95319600	0.28422400	0.73349800
H	3.25916100	0.78440700	1.40031500
C	1.45460800	-1.84464900	-1.27006200
H	1.50784500	-1.59512000	-2.33585700
H	0.40707000	-2.02693900	-1.02788800
H	2.02711300	-2.76273000	-1.11784800
C	-0.86227500	0.92474300	-0.12367900
C	-2.31803700	0.70897600	-0.04330600
C	-3.21952200	1.61372400	-0.61309900
H	-2.85470000	2.49950000	-1.12393400
C	-4.58893800	1.39903200	-0.54120800
H	-5.26799000	2.13144100	-0.96864500
C	-5.11017300	0.27468900	0.10517600
C	-4.20355300	-0.63055200	0.67625200
H	-4.58120300	-1.52550900	1.16300300
C	-2.83890400	-0.42139800	0.60169600
H	-2.14716500	-1.13385200	1.03829400
C	-0.33107600	2.27036400	-0.52318900
H	-0.38445700	2.40852200	-1.60893600
H	0.71642300	2.35637300	-0.23232000
H	-0.90350400	3.07761700	-0.06067800
C	-6.56304500	0.04670300	0.18523700
C	-7.39962200	0.32147000	-0.89696100
H	-6.96787400	0.68300800	-1.82616400
C	-8.77291300	0.10853000	-0.83382200
H	-9.38171700	0.32444700	-1.70465400
C	-9.34190600	-0.39105000	0.33955700
C	-8.51743100	-0.67093300	1.43356700
H	-8.97674100	-1.04801100	2.34191500
C	-7.15461000	-0.45654200	1.35324700
H	-6.53469600	-0.65476100	2.22307800
C	-11.54057300	-0.36574200	-0.54600300
H	-11.30523800	-0.97429400	-1.42680600
H	-11.52230100	0.69483100	-0.82240800
H	-12.53533100	-0.62509100	-0.18782600

**Supplementary Table 26. Cartesian coordinates of optimized 4f.**

I	-8.27146000	0.05591300	-0.29163100
O	10.71045100	-0.24227900	-0.32037300
N	-1.22008300	0.16925600	-0.14625700
C	-1.96790000	-0.74010100	0.36883900
C	-6.18468100	-0.21104100	-0.06965300
N	0.11889600	-0.02192000	-0.11486600
C	-3.42532500	-0.56479100	0.21752900
C	-4.32726300	-1.29083900	1.00008300
H	-3.96503900	-1.99648400	1.74104800
C	-5.70046000	-1.11829400	0.86553000
H	-6.38292200	-1.68742200	1.48729400
C	-5.30478400	0.52463900	-0.86405800
H	-5.68378300	1.22876800	-1.59692000
C	-3.93964700	0.34671200	-0.71376100
H	-3.24521000	0.91338600	-1.32463400
C	-1.43452200	-1.93084800	1.10949100
H	-1.49618500	-1.78248200	2.19356000
H	-0.38372300	-2.07967300	0.85838500
H	-1.99672500	-2.83614500	0.86841100
C	0.85694400	0.95790200	0.27176000
C	2.31616300	0.77183100	0.18370500
C	3.19836700	1.61328500	0.86894200
H	2.81432500	2.41312600	1.49468000
C	4.57126500	1.42515400	0.79058000
H	5.23242500	2.06940000	1.36329500
C	5.11556400	0.39598900	0.01696200
C	4.22814300	-0.44382000	-0.67218900
H	4.62612500	-1.22861400	-1.30952400
C	2.85974600	-0.26497000	-0.58728100
H	2.18362600	-0.91562200	-1.13161500
C	0.30264600	2.24403000	0.81122900
H	0.33265800	2.25736300	1.90658000
H	-0.74014000	2.35268000	0.51063300
H	0.87444000	3.10427900	0.45615600
C	6.57253100	0.19981700	-0.07161400
C	7.44852600	1.29228800	-0.15213300
H	7.04372100	2.30006400	-0.18035800
C	8.81619500	1.11240600	-0.23474500
H	9.49307800	1.95760000	-0.31053300
C	9.35989800	-0.17575800	-0.23707000
C	8.50546100	-1.27740700	-0.15661500
H	8.89453200	-2.28936700	-0.14482300
C	7.13093200	-1.07876900	-0.07684200
H	6.48110100	-1.94480900	0.01338300
C	11.31226700	-1.51634700	-0.33793700
H	10.98072300	-2.10631000	-1.20020600
H	11.10494700	-2.07257900	0.58355300
H	12.38370800	-1.34004100	-0.41559900



### General synthesis of (MeO-Ph, Y)-azines 1-4



**Supplementary Fig. 5.** General synthesis of (MeO-Ph, Y)-azines with Y = F (1), Cl (2), Br (3), and I (4).