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Supplementary Information

DFT Study for Substitution Patterns of $C_{20}H_{18}X_2$ Regioisomers (X = F, Cl, Br, or OH)

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Here each unit of bond distance and angle is angstrom and degree.

Table S1. The bond distance between carbon and substituent in *cis*-1 isomer

	C1-X1	C2-X2
$C_{20}H_{18}F_2$	1.393	1.393
$C_{20}H_{18}Cl_2$	1.830	1.830
$C_{20}H_{18}Br_2$	1.994	1.994
$C_{20}H_{18}(OH)_2$	1.427	1.427

Table S2. The bond distance between carbon and substituent in *trans*-1 isomer

	C1-X1	C20-X2
$C_{20}H_{18}F_2$	1.405	1.405
$C_{20}H_{18}Cl_2$	1.851	1.851
$C_{20}H_{18}Br_2$	2.011	2.011
$C_{20}H_{18}(OH)_2$	1.431	1.431

Table S3. The bond distance between the carbon (C1 and C2) with each substituent and the nearest neighbor carbon (C3, C4, C5, and C6) in *cis*-1 isomer

	C1-C2	C1-C3	C1-C4	C2-C5	C2-C6
$C_{20}H_{18}F_2$	1.561	1.544	1.544	1.544	1.544
$C_{20}H_{18}Cl_2$	1.585	1.558	1.558	1.558	1.558
$C_{20}H_{18}Br_2$	1.576	1.557	1.557	1.557	1.557
$C_{20}H_{18}(OH)_2$	1.577	1.546	1.555	1.555	1.546

Table S4. The bond distance between the carbon (C1 and C20) with each substituent and the nearest neighbor carbon (C2, C3, C4, C17, C18 and C19) in *trans*-1 isomer

	C1-C2	C1-C3	C1-C4	C20-C17	C20-C18	C20-C19
$C_{20}H_{18}F_2$	1.545	1.545	1.545	1.545	1.545	1.545
$C_{20}H_{18}Cl_2$	1.554	1.554	1.554	1.554	1.554	1.554
$C_{20}H_{18}Br_2$	1.552	1.552	1.552	1.552	1.552	1.552
$C_{20}H_{18}(OH)_2$	1.55	1.560	1.559	1.559	1.559	1.55

Table S5. The angle around the substituted carbon in *cis*-1 isomer

	C2-C1-X1	C3-C1-X1	C4-C1-X1	C1-C2-X2	C5-C2-X2	C6-C2-X2
$C_{20}H_{18}F_2$	110.2	111.0	111.0	110.2	111.0	111.0
$C_{20}H_{18}Cl_2$	114.9	109.6	109.6	114.9	109.6	109.6
$C_{20}H_{18}Br_2$	115.7	108.8	108.8	115.7	108.8	108.8
$C_{20}H_{18}(OH)_2$	111.1	108.5	113.8	111.1	113.8	108.5

Table S6. The angle around the substituted carbon in *trans*-1 isomer

	C2-C1-X1	C3-C1-X1	C4-C1-X1	C17-C20-X2	C18-C20-X2	C19-C20-X2
$C_{20}H_{18}F_2$	110.2	110.2	110.2	110.2	110.2	110.2
$C_{20}H_{18}Cl_2$	110.5	110.5	110.5	110.5	110.5	110.5
$C_{20}H_{18}Br_2$	110.1	110.2	110.2	110.2	110.2	110.1
$C_{20}H_{18}(OH)_2$	107.5	113.1	113.1	113.1	113.1	107.5

Table S7. The dihedral angle around the substituted carbon in *cis*-1 isomer

$C_{20}H_{18}F_2$	X1	X2
C-C-C-X	-121.3	121.3
	121.3	-121.3
	120.9	-120.9
	-122.4	122.4
	-120.9	120.9
	122.4	-122.3
H-C-C-X	-0.7	0.7
	0.7	-0.7
$C_{20}H_{18}Cl_2$		
C-C-C-X	122.1	-122.1
	-122.1	122.1
	-125.2	125.2
	117.9	-117.9
	-117.9	-125.2
	125.2	117.9
H-C-C-X	-3.7	3.7
	3.7	-3.7
$C_{20}H_{18}Br_2$		
C-C-C-X	121.9	-121.9
	-121.9	121.9
	-126.1	126.1
	117.2	-117.2
	-117.2	-126.1
	126.1	117.2
H-C-C-X	-4.5	4.5
	4.5	-4.5
$C_{20}H_{18}(OH)_2$		
C-C-C-X	-118.4	125.4
	125.4	-118.4
	119.9	-123.4
	-123.0	119.8
	-123.4	119.9
	119.8	-123.0
H-C-C-X	-1.5	-1.4
	-1.4	-1.5
X-C-C-X	6.5	

Here the dihedral angle of X-C-C-X in each dihalo- substituent is zero

Table S8. The dihedral angle around the substituted carbon in *trans*-1 isomer

$C_{20}H_{18}F_2$	X1	X2
C-C-C-X	-121.6	121.6
	121.6	-121.6
	121.6	121.6
	-121.6	-121.6
	-121.6	-121.6
	121.6	121.6
H-C-C-X	0.0	0.0
	0.0	0.0
	0.0	0.0
$C_{20}H_{18}Cl_2$		
C-C-C-X	121.8	121.8
	-121.8	-121.8
	-121.8	121.8
	121.8	-121.8
	-121.8	-121.8
	121.8	121.8
H-C-C-X	0.0	0.0
	0.0	0.0
	0.0	0.0
$C_{20}H_{18}Br_2$		
C-C-C-X	-121.9	121.9
	121.9	-121.9
	121.9	121.9
	-121.9	-121.9
	121.9	-121.9
	-121.9	121.9
H-C-C-X	0.0	0.0
	0.0	0.0
	0.0	0.0
$C_{20}H_{18}(OH)_2$		
C-C-C-X	-121.4	117.9
	121.4	-125.1
	117.9	125.1
	-125.1	-117.9
	-117.9	-121.4
	125.1	121.4
H-C-C-X	0.0	-3.0
	-3.0	3.0
	3.0	0.0

Table S9. The bond distance, angle, and dihedral angles for $C_{20}H_{20}$

	Distance and angles
C-C	1.556
C-H	1.094
C-C-H	110.9
C-C-C	108.0
C-C-C-C	0.0
	116.6
C-C-C-H	121.7
H-C-C-H	0.0