Supporting Information

Table S1. Polychlorinated dibenzofurans with identity number (ID) representing the substitution pattern.

ID	X_1	X_2	X_3	X_4	X_6	X_7	X_8	X_9
1	H	Cl	H	H	H	H	H	H
2	H	H	H	Cl	H	H	H	H
3	H	Cl	H	H	Cl	H	H	H
4	H	Cl	H	H	H	H	Cl	H
5	Cl	H	Cl	H	Cl	H	H	H
6	Cl	H	Cl	H	H	H	Cl	H
7	H	Cl	Cl	Cl	H	H	H	H
8	H	Cl	Cl	H	H	H	Cl	H
9	H	Cl	H	H	Cl	Cl	H	H
10	H	Cl	Cl	Cl	Cl	H	H	H
11	H	Cl	Cl	Cl	H	H	Cl	H
12	H	Cl	Cl	H	H	Cl	Cl	H
13	Cl	Cl	H	Cl	Cl	Cl	H	H
14	Cl	Cl	Cl	Cl	H	H	Cl	H
15	Cl	Cl	Cl	H	H	Cl	Cl	H
16	H	Cl	Cl	Cl	H	Cl	Cl	H
17	Cl	Cl	Cl	Cl	H	Cl	Cl	H
18	H	Cl	Cl	Cl	Cl	Cl	Cl	H
19	H	Cl	Cl	H	Cl	H	Cl	H
20	Cl	Cl	Cl	H	Cl	H	H	H
21	Cl	Cl	Cl	H	H	Cl	H	H
22	Cl	H	Cl	Cl	H	Cl	Cl	H
23	H	Cl	Cl	Cl	H	Cl	H	Cl
24	Cl	Cl	Cl	H	H	Cl	H	Cl
25	Cl	Cl	Cl	H	H	Cl	H	H
26	Cl	H	Cl	Cl	H	Cl	Cl	H
27	H	Cl	Cl	Cl	H	Cl	H	Cl

Table S2. Polyhalogenated dibenzo-*p*-dioxins with identity number (ID) representing the substitution pattern

ID	X_1	X_2	X_3	X_4	X_6	X_7	X_8	X_9
28	Cl	Cl	Cl	H	H	Cl	Cl	H
29	H	Cl	Cl	H	Cl	Cl	H	H
30	H	Cl	Cl	H	Cl	H	H	H
31	Cl	Cl	Cl	Cl	H	Cl	Cl	H
32	Cl	H	Cl	H	H	Cl	Cl	H
33	Cl	Cl	H	Cl	H	Cl	Cl	H
34	Cl	Cl	Cl	Cl	H	H	H	H
35	H	Cl	Cl	H	H	Cl	H	H
36	H	Cl	H	H	H	H	Cl	H
37	Cl	Cl	Cl	Cl	Cl	Cl	Cl	Cl
38	Cl	H	H	H	H	H	H	H
39	H	Br	Br	H	H	Br	Br	H
40	H	Br	Br	H	H	Cl	Cl	H
41	H	Br	Cl	H	H	Cl	Br	H
42	H	Br	Cl	H	H	Cl	Cl	H
43	Br	H	Br	H	H	Br	Br	H
44	Br	Br	H	Br	H	Br	Br	H
45	H	Br	Br	H	H	Br	H	H
46	H	Br	H	H	H	Br	H	H

Table S3. Polychlorinated biphenyls with identity number (ID) representing the substitution pattern

ID	X_2	X_3	X_4	X_5	X_6	$X_{2'}$	$X_{3'}$	$X_{4'}$	$X_{5'}$	$X_{6'}$
47	H	Cl	Cl	H	H	H	Cl	Cl	H	H
48	H	Cl	Cl	Cl	H	H	Cl	Cl	H	H
49	Cl	H	H	H	H	H	Cl	Cl	Cl	H
50	Cl	Cl	Cl	H	H	H	Cl	Cl	H	H
51	Cl	H	Cl	Cl	H	H	Cl	Cl	H	H
52	Cl	Cl	Cl	Cl	H	H	Cl	Cl	H	H
53	Cl	Cl	Cl	Cl	H	H	Cl	Cl	Cl	H
54	Cl	H	Cl	H	H	Cl	H	Cl	H	H
55	Cl	H	Cl	Cl	H	Cl	H	Cl	Cl	H
56	Cl	Cl	Cl	Cl	H	H	H	H	H	H
57	Cl	H	Cl	H	Cl	H	Cl	Cl	Cl	H

Table S4. Energy, hardness, chemical potential, electrophilicity and local electrophilicity (MPA and HPA) for different polychlorinated dibenzofurans (solvent phase)

Molecule	Energy (a.u.)	h (eV)	m (eV)	w (eV)	w^{+}_{max} (eV) MPA	Observed pIC_{50}[a]	Calculated pIC_{50}
1	–996·9274	2·507	–3·743	2·794	0·434	4·061	3·729
2	–996·9253	2·537	–3·742	2·760	0·439	3·429	3·670
3	–1456·5199	2·474	–3·902	3·077	0·461	4·125	4·763
4	–1456·5221	2·475	–3·930	3·121	0·457	4·103	4·860
5	–1916·1125	2·456	–4·048	3·336	0·508	6·123	5·947
6	–1916·1148	2·410	–4·029	3·367	0·503	4·653	6·002
7	–1916·1040	2·443	–4·025	3·315	0·524	5·396	6·082
8	–1916·1114	2·430	–4·053	3·380	0·524	6·858	6·309
9	–2375·6956	2·423	–4·170	3·587	0·553	7·255	7·086
10	–2375·6978	2·404	–4·176	3·626	0·549	7·379	7·176
11	–2375·7050	2·409	–4·200	3·661	0·553	7·657	7·358
12	–2375·7004	2·369	–4·142	3·620	0·525	8·444	6·862
13	–2375·7011	2·415	–4·310	3·846	0·596	5·715	8·239
14	–2835·2884	2·350	–4·260	3·860	0·598	8·194	8·314
15	–2835·2848	2·345	–4·251	3·854	0·558	7·911	7·779
16	–2835·2882	2·361	–4·270	3·860	0·558	8·147	7·810
17	–2835·2866	2·322	–4·360	4·094	0·610	8·943	8·975
18	–3294·8734	2·361	–4·399	4·097	0·574	7·587	8·530
19	–3294·8723	2·422	–4·213	3·665	0·542	8·376	7·231
20	–2375·7017	2·425	–4·168	3·583	0·561	7·610	7·181
21	–2375·6970	2·367	–4·109	3·567	0·545	7·379	6·920
22	–2375·6995	2·339	–4·245	3·853	0·565	7·954	7·870
23	–2835·2904	2·358	–4·266	3·86	0·571	7·657	7·964
24	–2835·2899	2·339	–4·272	3·900	0·562	7·657	8·001
25	–2835·2805	2·367	–4·109	3·567	0·545	7·313	6·920
26	–2375·6980	2·339	–4·245	3·853	0·565	8·689	7·870
27	–2375·6995	2·358	–4·266	3·860	0·571	7·954	7·963

[a]Experimental data as given in ref. [31]

Table S5. Energy, hardness, chemical potential, electrophilicity and local electrophilicity (MPA and HPA) for different polychlorinated biphenyls (solvent phase).

Molecule	Energy (Hartree)	h (eV)	m (eV)	w (eV)	w^{+}_{max} (eV) HPA	Observed pIC_{50}[a]	Calculated pIC_{50}
1	–2301·6832	2·508	–4·033	3·242	0·188	7·028	6·949
3	–2761·2718	2·494	–4·181	3·504	0·255	7·871	7·165
4	–2301·6767	2·674	–4·062	3·085	0·241	5·584	5·685
5	–2761·2667	2·641	–4·107	3·194	0·240	6·134	5·602
6	–2761·2711	2·610	–4·131	3·269	0·202	5·762	6·305
8	–3220·8544	2·618	–4·229	3·415	0·293	6·057	5·704
10	–3680·4426	2·619	–4·364	3·635	0·280	5·885	6·315
11	–2301·6823	2·886	–3·972	2·733	0·163	4·442	4·381
12	–3220·8605	2·765	–4·206	3·198	0·187	4·689	5·351
13	–2301·6686	2·657	–4·033	3·060	0·312	4·405	5·003
14	–3220·8591	2·991	–4·223	2·981	0·213	4·577	3·966

[a]Experimental data as given in ref. [31]

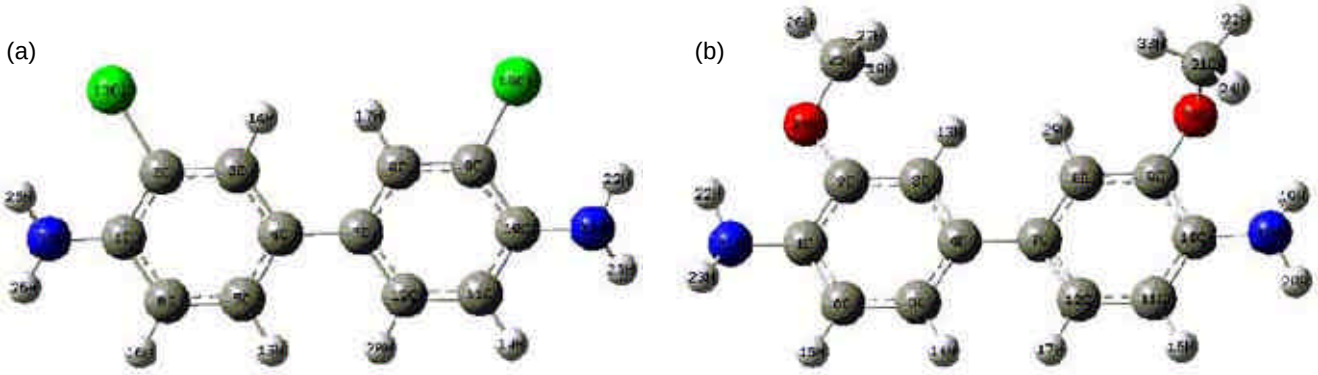

Figure S1. The geometries of (**a**) 3,3′-dichlorobenzidine (**b**) 3,3′-dimethoxybenzidine with the atom numbering.

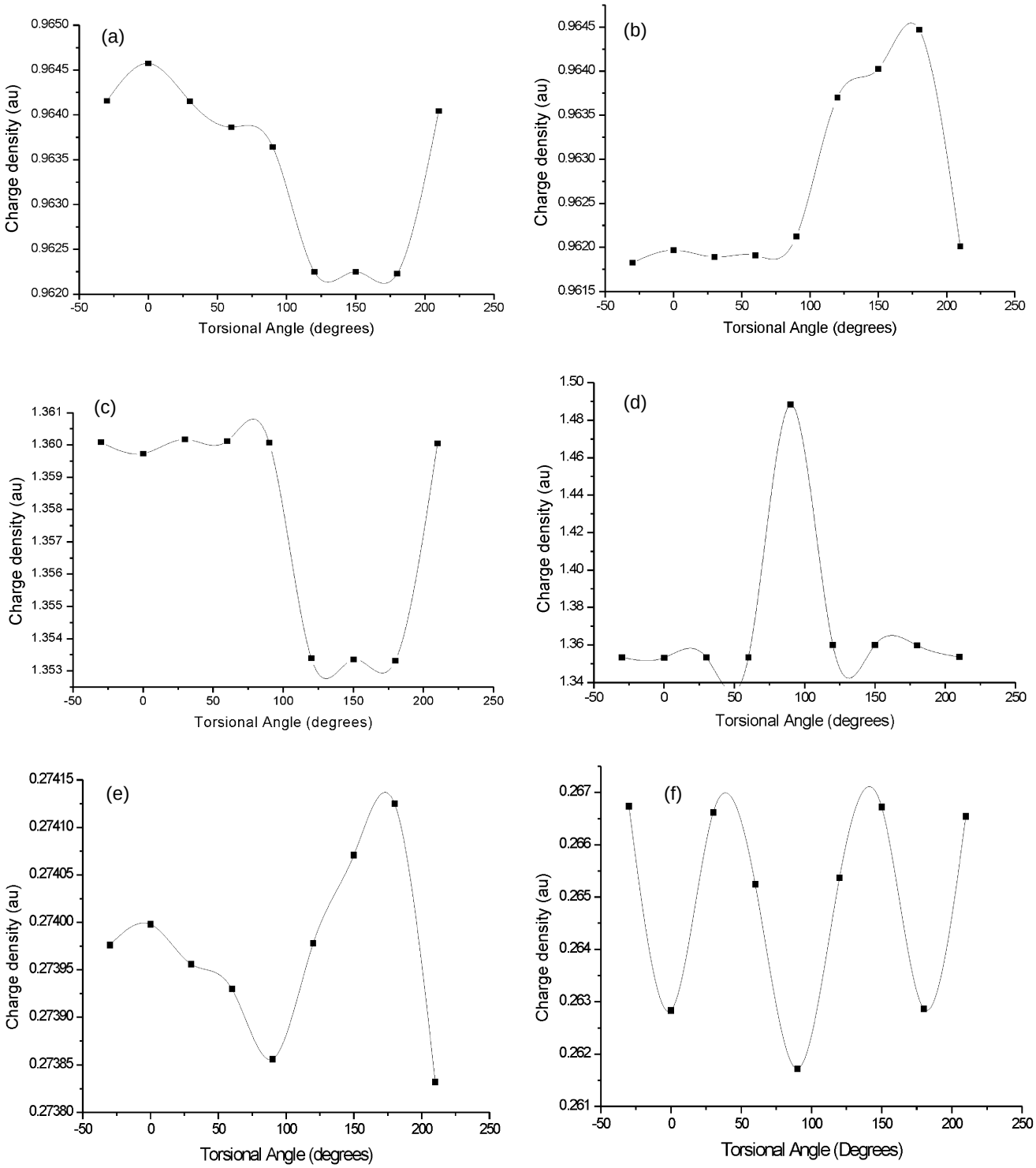

Figure S2. The charge density (r) distribution at the bond critical point of the selected group for 3,3′-dimethoxybenzidine. (**a**) $C_1N_{21}H_{22}H_{23}$, (**b**) $C_{10}N_{18}H_{19}H_{20}$, (**c**) $C_2O_{24}C_{25}H_{26}H_{27}H_{28}$, (**d**) $C_9O_{30}C_{31}H_{32}H_{33}H_{24}$, (**e**) $C_{11}H_{16}$ and (**f**) C_3C_7.

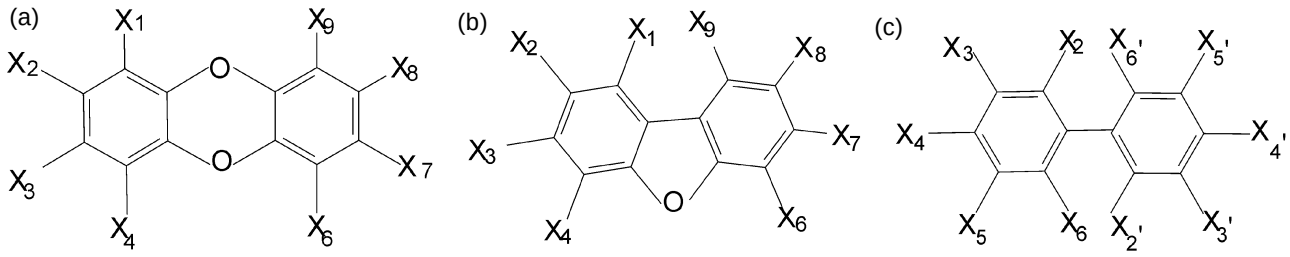

Figure S3. The structural template of (**a**) polychlorinated dibenzofurans, (**b**) polyhalogenated dibenzo-*p*-dioxins and (**c**) polychlorinated biphenyls with required atom numbering.