










Experimental, DFT study, and *in silico* molecular docking investigations of dichlorodiphenyltrichloroethane against human estrogen receptor alpha

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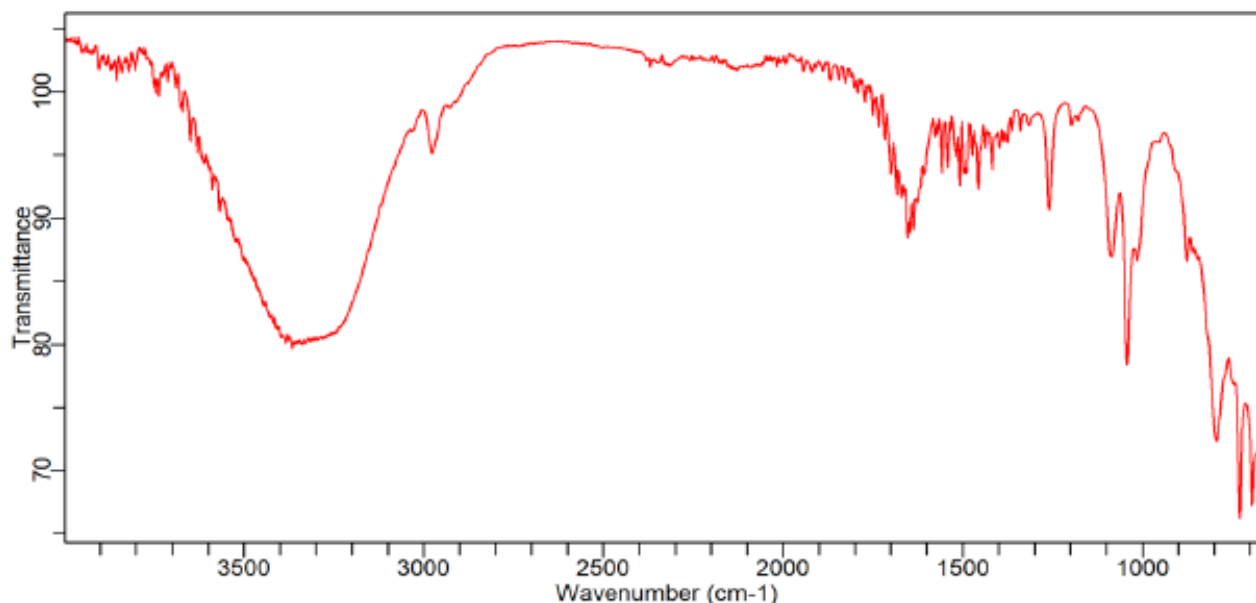


Figure S1. The ESI-Mass spectrum of dichlorodiphenyltrichloroethane (DDT).

Table S1. ADCH, HPA, BPA and MPA result of DDT.

Atoms	ADCH	HPA	BPA	MPA
C	0.0957	0.1321	0.6365	-0.2842
C	0.1777	-0.0175	-1.1844	-0.2833
H	0.0929	0.0392	0.0717	0.1909
C	-0.4344	-0.0101	1.8669	0.1801
C	-0.2849	-0.0315	0.4992	-0.1513
C	0.1021	-0.0369	-0.9841	-0.1694
C	-0.0902	-0.0414	0.3357	-0.1334
H	0.3078	0.0409	-0.7734	0.1491
C	-0.1675	-0.0429	-0.1831	-0.1292
H	0.1019	0.0435	0.1667	0.1465
C	0.1569	0.0293	0.2059	-0.0629
H	0.1153	0.0531	-0.1346	0.1607
H	0.1457	0.0531	0.0220	0.1602
C	-0.2301	-0.0048	1.1507	0.1756
C	-0.1779	-0.0341	0.2824	-0.1718
C	0.5055	0.0408	-3.6223	-0.1747
C	-0.0821	0.0409	-0.1093	-0.1254
H	0.1251	0.0479	0.0671	0.1417
C	-0.2409	-0.0407	0.3509	-0.1330
H	-0.1773	0.0332	1.9935	0.1603
C	0.0014	0.0278	0.3894	-0.0635
H	0.1409	0.0536	0.0787	0.1607
H	0.1367	0.0532	0.1088	0.1611
Cl	-0.0631	-0.0517	-0.2071	0.0373
Cl	-0.0569	-0.0520	-0.2055	0.0475
Cl	-0.0343	-0.0332	-0.2737	0.0418
Cl	-0.0664	-0.0619	-0.2387	-0.0157
Cl	-0.0971	-0.0616	-0.3100	-0.0157