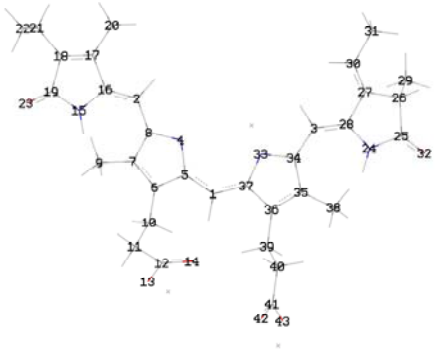
Supporting Information Available: Optimized geometrical parameters for Model I-III.

Table S1. Comparison between the bond lengths of PCB molecule from the crystal structure and the optimization at B3LYP/6-31G* level.



Geom Param	α-84 PCB Crystal Strucure	α-84 PCB Optimizated in Gas phase	α-84 PCBH$^+$ Optimizated in Gas phase	α-84 PCBH$^+$+Asp87 Optimizated in Protein
B21-18	1.5077	1.4978	1.4961	1.4974
B18-17	1.4238	1.3579	1.3562	1.3586
B17-16	1.4363	1.4761	1.4805	1.4779
B16-15	1.3811	1.3925	1.3793	1.3909
B15-19	1.3507	1.3933	1.4055	1.3980
B19-18	1.4941	1.4902	1.4954	1.4891
B16-2	1.4063	1.3593	1.3657	1.3615
B2-8	1.4054	1.4504	1.4384	1.4452
B8-4	1.3797	1.3341	1.3753	1.3608
B4-5	1.4148	1.3865	1.3956	1.3835
B5-6	1.4110	1.4542	1.4207	1.4312
B6-7	1.4356	1.3777	1.4065	1.3973
B7-8	1.4296	1.4655	1.4193	1.4276
B5-1	1.4076	1.3844	1.3995	1.4031
B1-37	1.4097	1.4114	1.3897	1.3916
B37-33	1.4079	1.3785	1.3996	1.3839
B33-34	1.4075	1.3629	1.3763	1.3595
B34-35	1.4408	1.4203	1.4263	1.4374
B35-36	1.4262	1.4098	1.4005	1.3893
B36-37	1.4059	1.4155	1.4259	1.4392
B34-3	1.4251	1.4482	1.4306	1.4379
B3-28	1.4041	1.3573	1.3724	1.3627
B28-27	1.5139	1.4820	1.4794	1.4823
B27-26	1.5517	1.5224	1.5218	1.5221
B26-25	1.5327	1.5334	1.5286	1.5307
B25-24	1.3249	1.3830	1.4016	1.3864
B24-28	1.4184	1.3968	1.3777	1.3921
B27-30	1.6041	1.3424	1.3442	1.3430