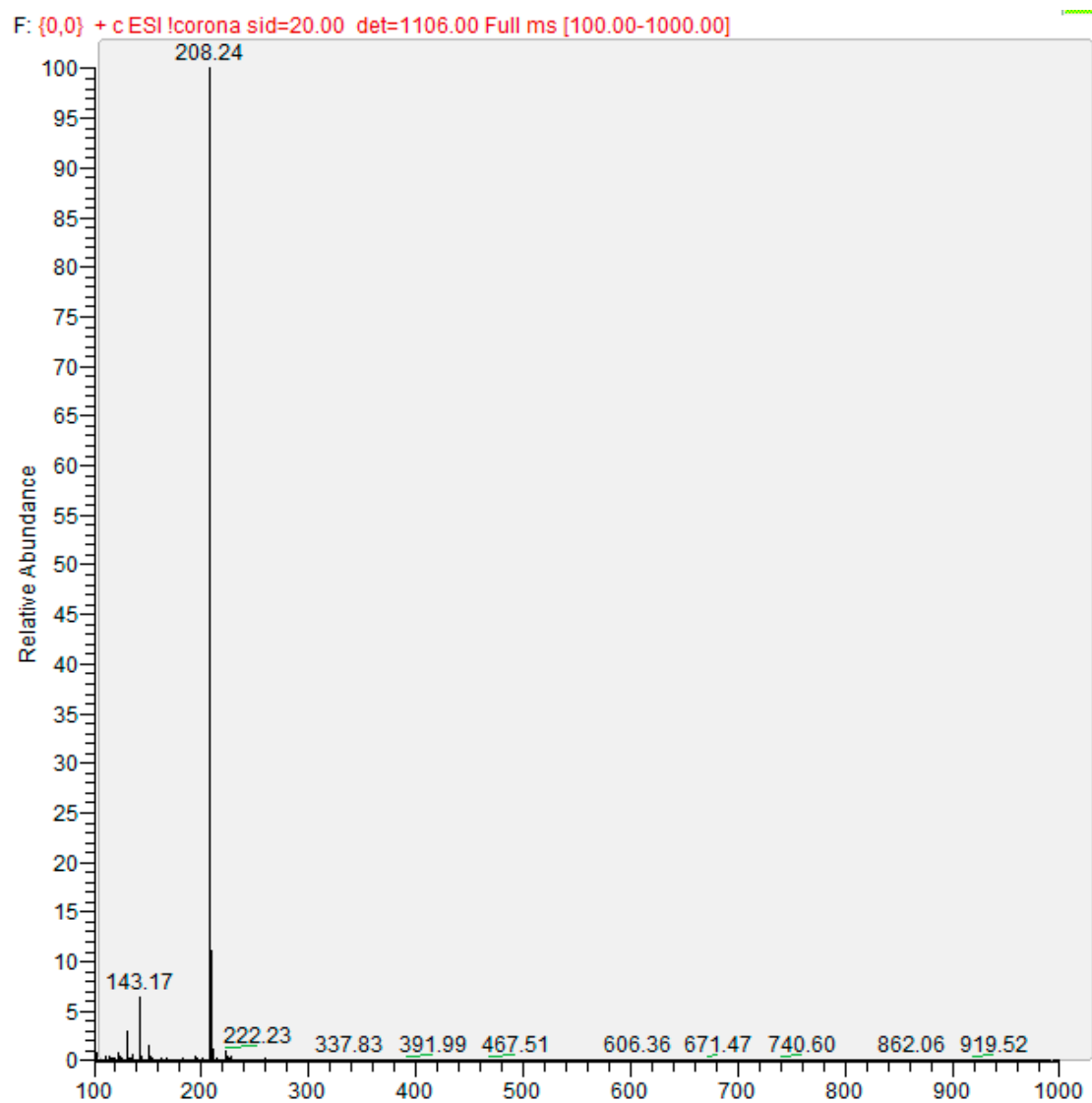
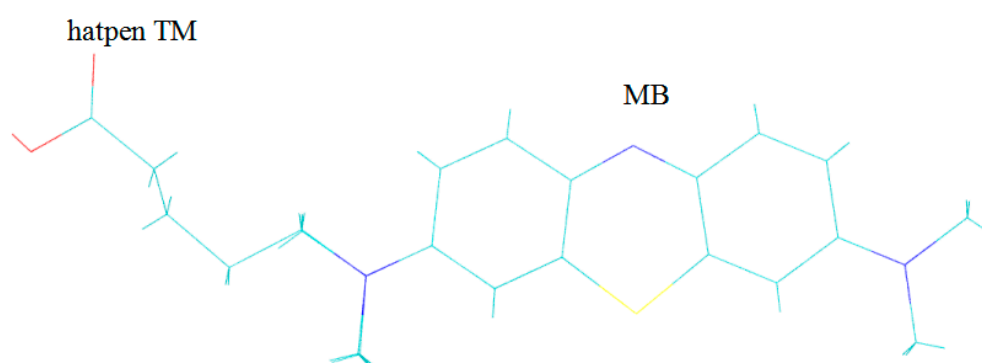


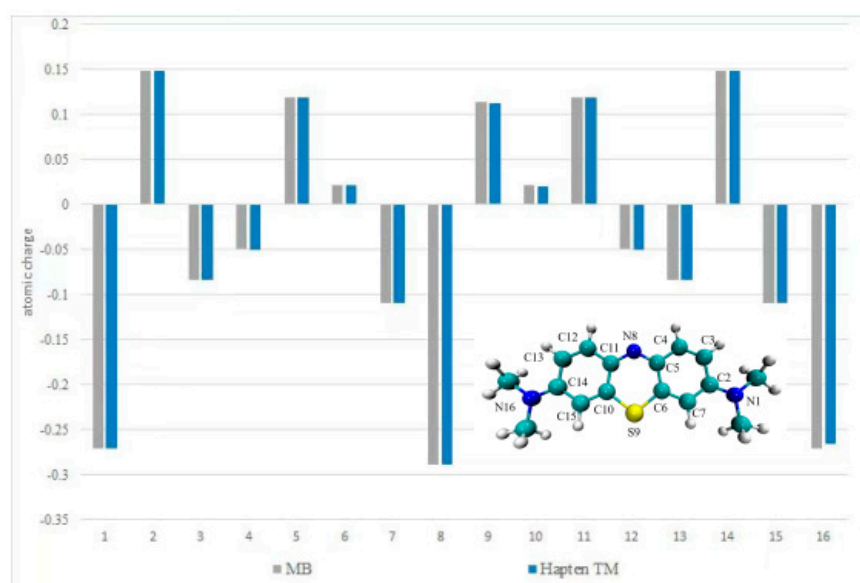
Figure S1. The MS spectrogram for Intermediate I.



**Figure S2.** The MS spectrogram for Intermediate II.



**Figure S3.** The alignment of the lowest energy conformations of MB and hapten TM. Color scheme: C, cyan; N, blue; S, yellow; O, red, and hydrogen is omitted for brevity.



**Figure S4.** Calculated partial atomic charges of common structure atoms of MB and hapten TM.