

Figure S1. The MS spectrogram for Intermediate I.

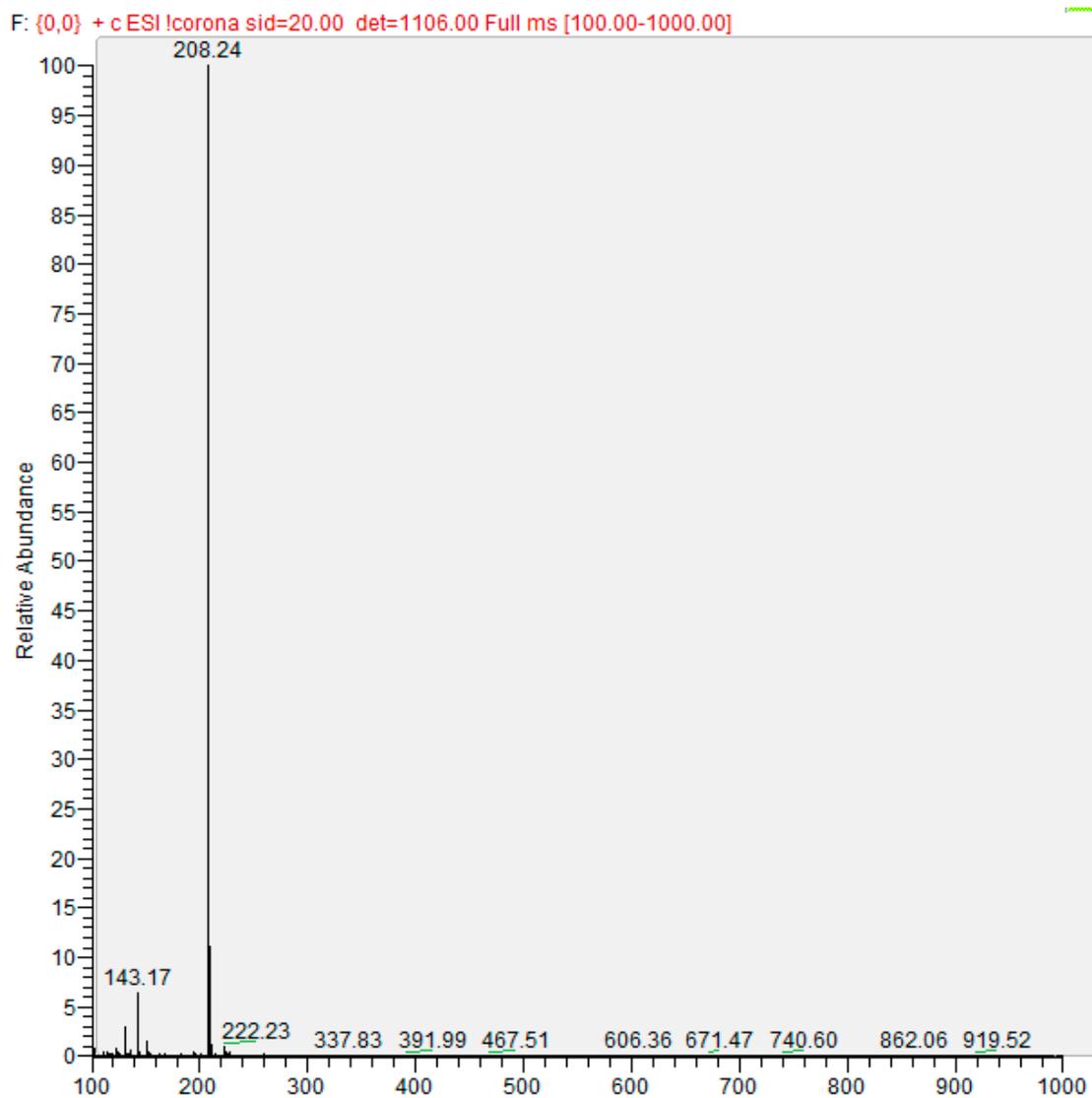


Figure S2. The MS spectrogram for Intermediate II.

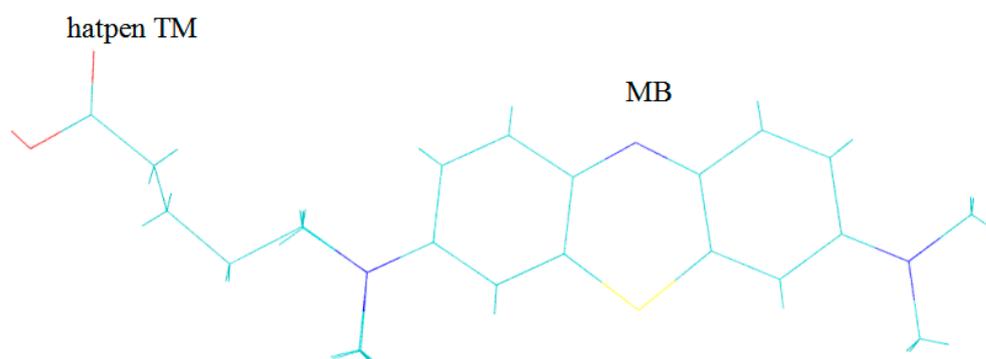


Figure S3. The alignment of the lowest energy conformations of MB and hatpen TM. Color scheme: C, cyan; N, blue; S, yellow; O, red, and hydrogen is omitted for brevity.

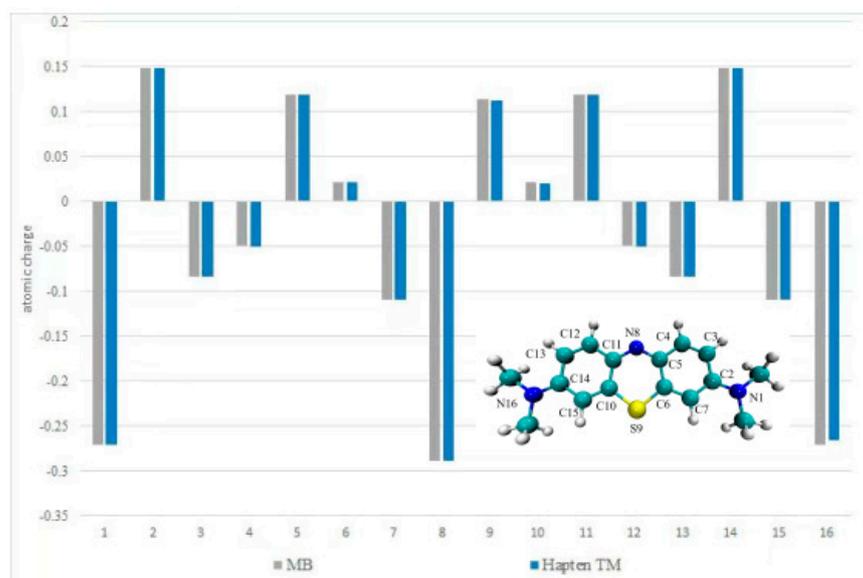


Figure S4. Calculated partial atomic charges of common structure atoms of MB and hapten TM.