SUPPLEMENTARY INFORMATION

# Protonation of Patented Blue V in aqueous solutions: Theoretical and experimental studies

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**Table S1.** The structures of different forms of Patented Blue V that were considered in this study.

The geometry was optimized with B97-D3/6-31+G** method, and single point energies were calculated at B97-D3/6-311++G** level of theory. Form I corresponds to dicationic state, form II – monocationic, form III – neutral, IV – monoanionic state, form V – dianionic state, form VI corresponds to hydroxylation of central carbon. The most stable geometry marked only with number (**I,II,…**), whereas letters (**a,b,…**) were added to the less stable geometries. For each form, the difference in total energies between the considered geometry and the most stable one is shown in brackets.

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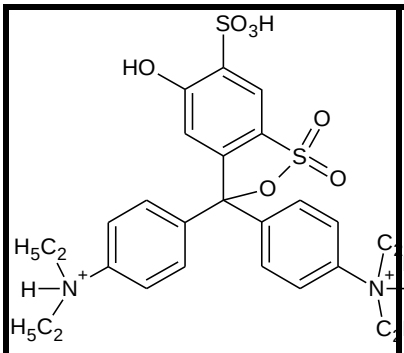
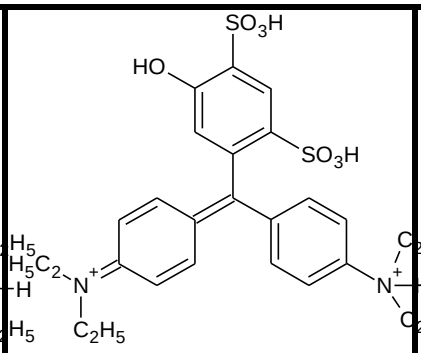
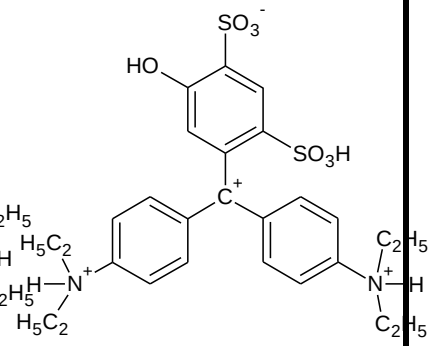
<td>  <br>I (0.00)</td>
<td>  <br>Ia (2.37)</td>
<td>  <br>Ib (7.94)</td>
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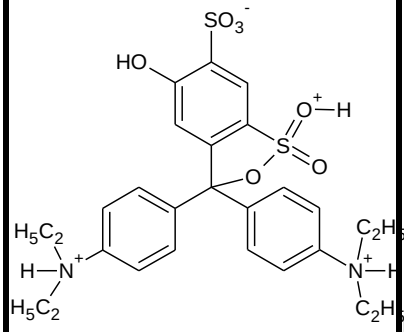
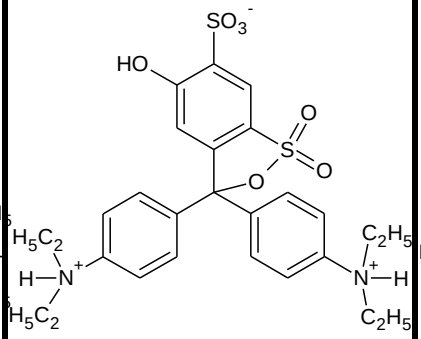
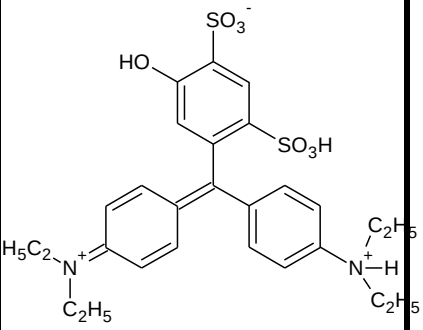
<td>  <br>during the optimization the geometry transformed to Ib</td>
<td>  <br>II (0.00)</td>
<td>  <br>IIa (1.65)</td>
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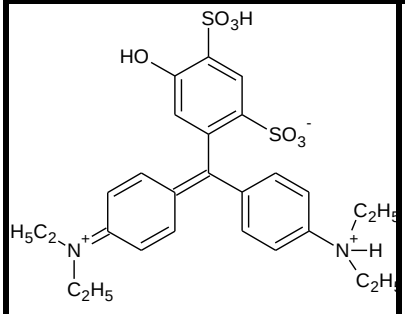
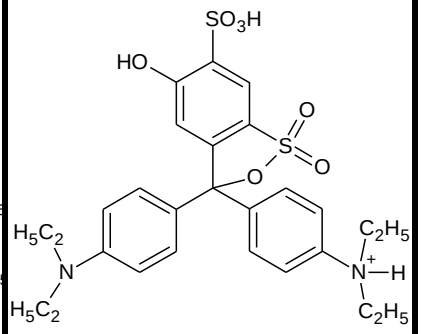
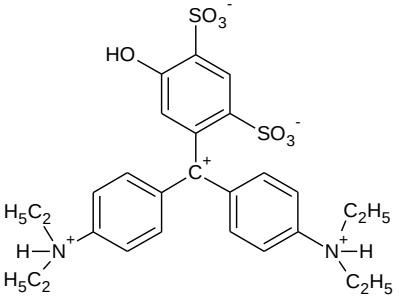
<td>  <br>IIb (5.71)</td>
<td>  <br>IIc (17.07)</td>
<td>  <br>during the optimization the geometry transformed to II</td>
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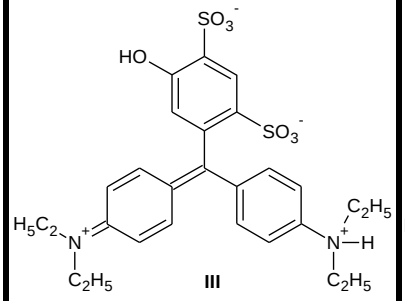
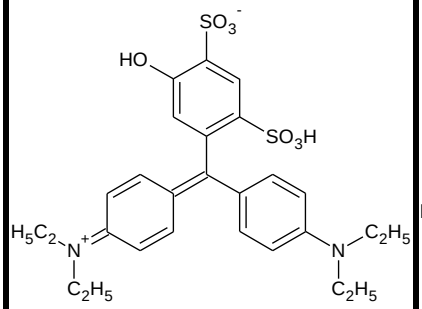
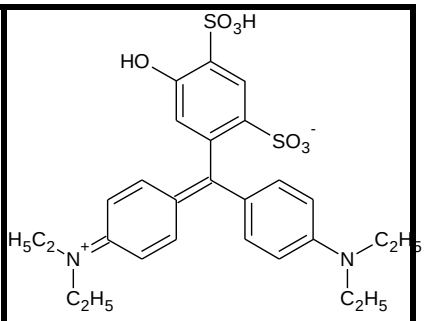
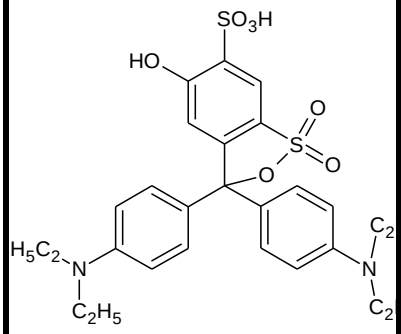
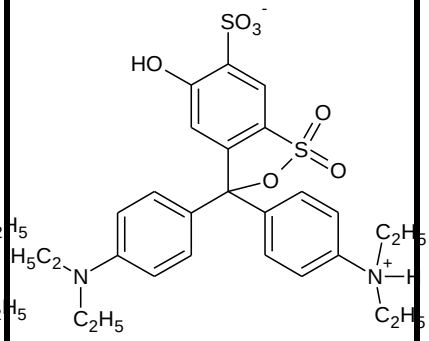
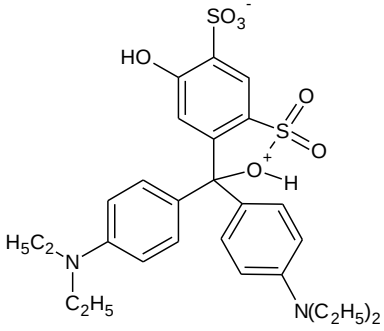
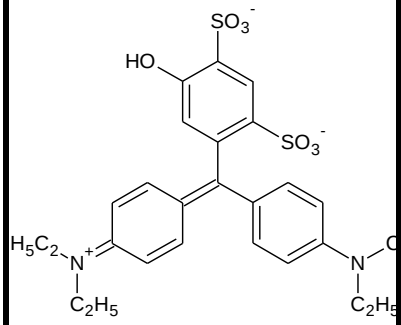
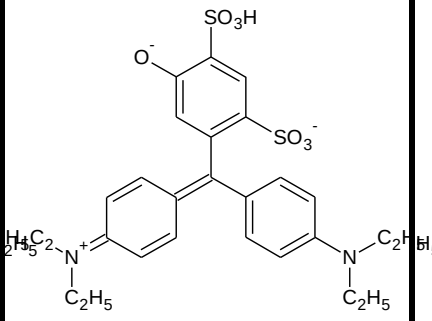
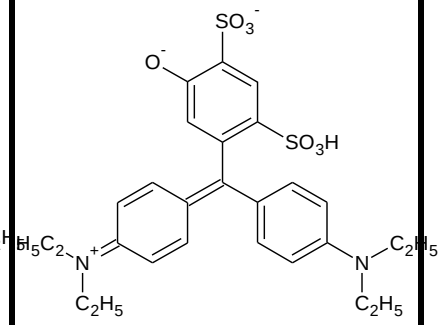
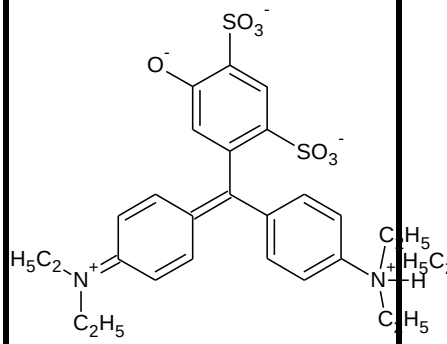
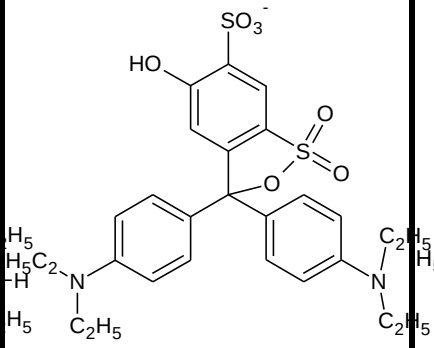
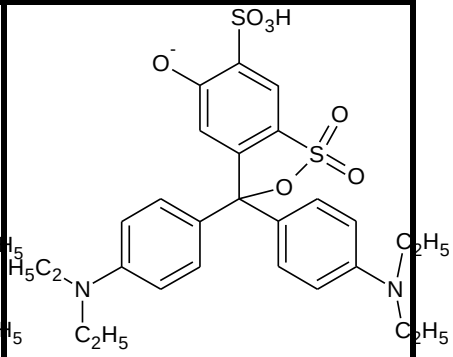
|  **III (0.00)** |  **IIIa (2.13)** |  **IIIb (8.63)** |
|  **IIIc (28.12)** |  **IIId (9.22)** |  **during the optimization the geometry transformed to IIIa** |
|  **IV (0.00)** |  **IVa (22.93)** |  **IVb (18.77)** |
|  **IVc (23.56)** |  **IVd (18.50)** |  **IVe (38.37)** |

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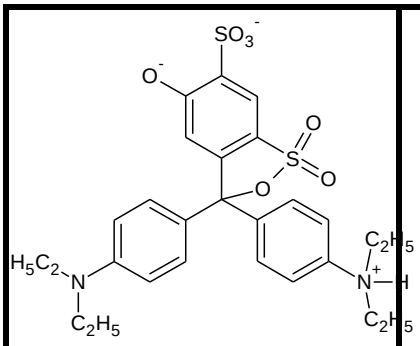
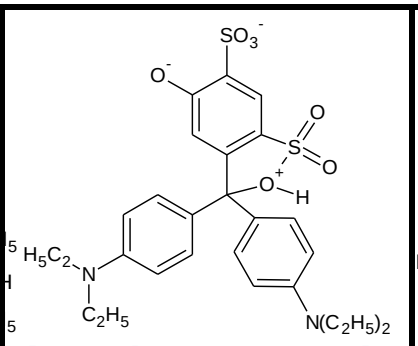
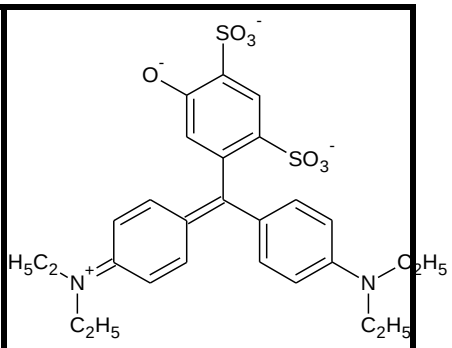
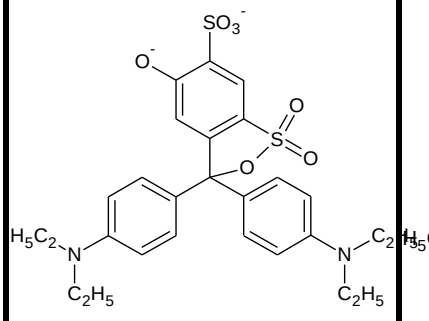
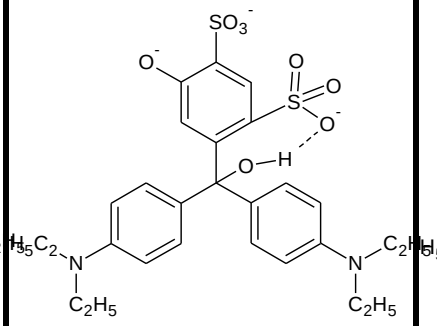
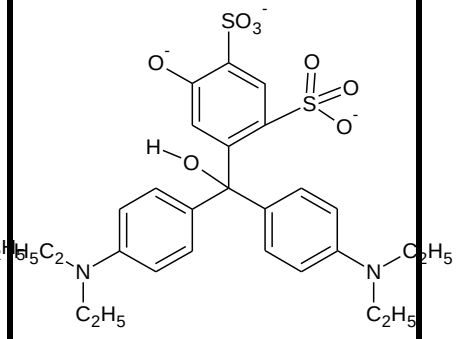
|  **IVf (29.92)** |  **during the optimization the geometry transformed to IVb** |  **V (0.00)** |
|  **Va (15.24)** |  **VI (0.00)** |  **VIa (9.09)** |