Supporting information

In depth quantum chemical investigation of electro-optical and charge transport properties of trans-3-(3,4-Dimethoxyphenyl)-2-(4-nitrophenyl)prop-2-enenitrile

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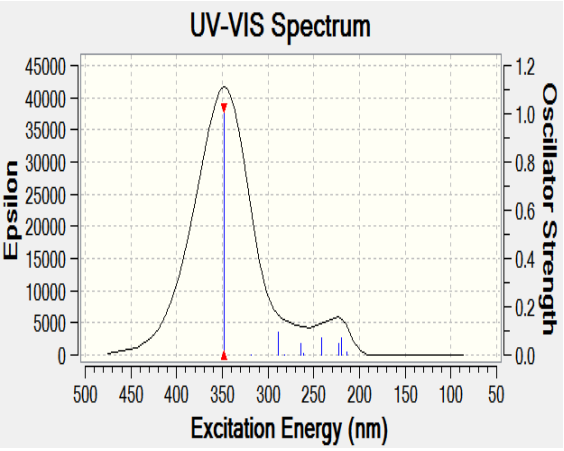
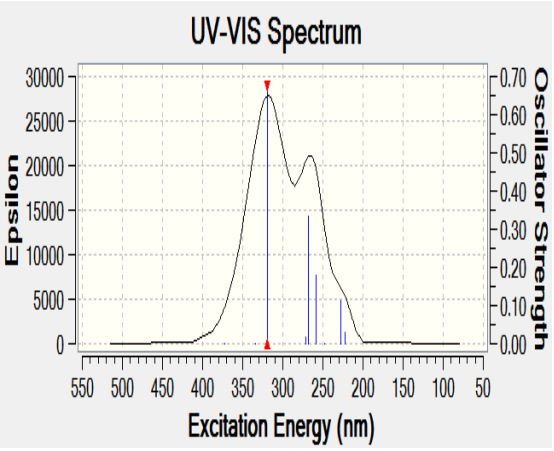
TD-CAM-B3LYP-absorption



TD-CAM-B3LYP- fluorescence emission



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TD-LC-BLYP-absorption TD-LC-BLYP-fluorescence emission

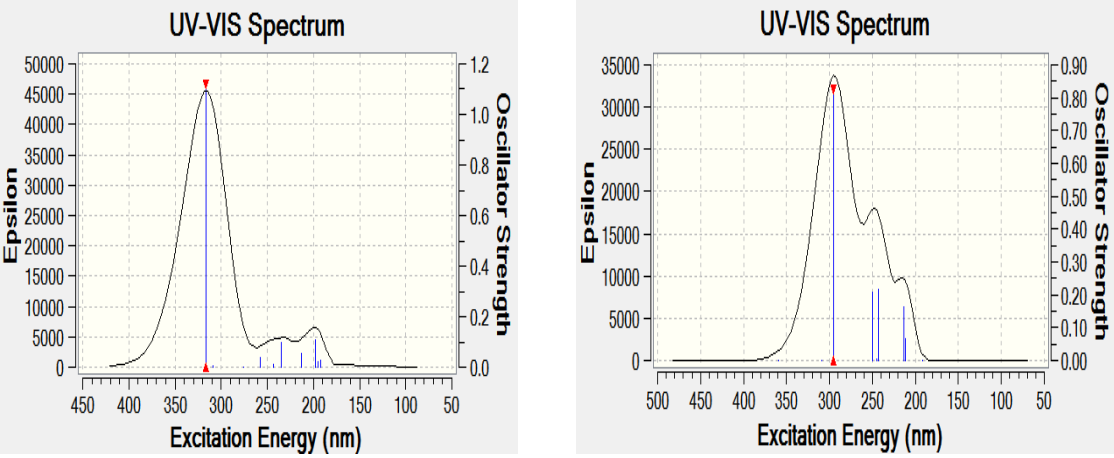

Fig. S1. The absorption and fluorescence emsission spectra calculated at TD-CAM-B3LYP/6-31G** and TD-LC-BLYP/6-31G** levels of theory.