Photophysical properties of NIR-emitting fluorescence probes: insights from TD-DFT

Éric Brémond, Marta E. Alberto, Nino Russo, Gino Ricci, Ilaria Ciofini, Carlo Adamo

SUPPLEMENTARY INFORMATION

Figure SI.1 Computed HOMO and LUMO for the neutral (N2) and anionic forms of SNAFR-x (x=1,6). Isocontour value=0.02 a.u..
**Figure SI.2** Computed HOMO and LUMO for the neutral (N$_1$) of SNAFR-1. Isocontour value=0.02 a.u.