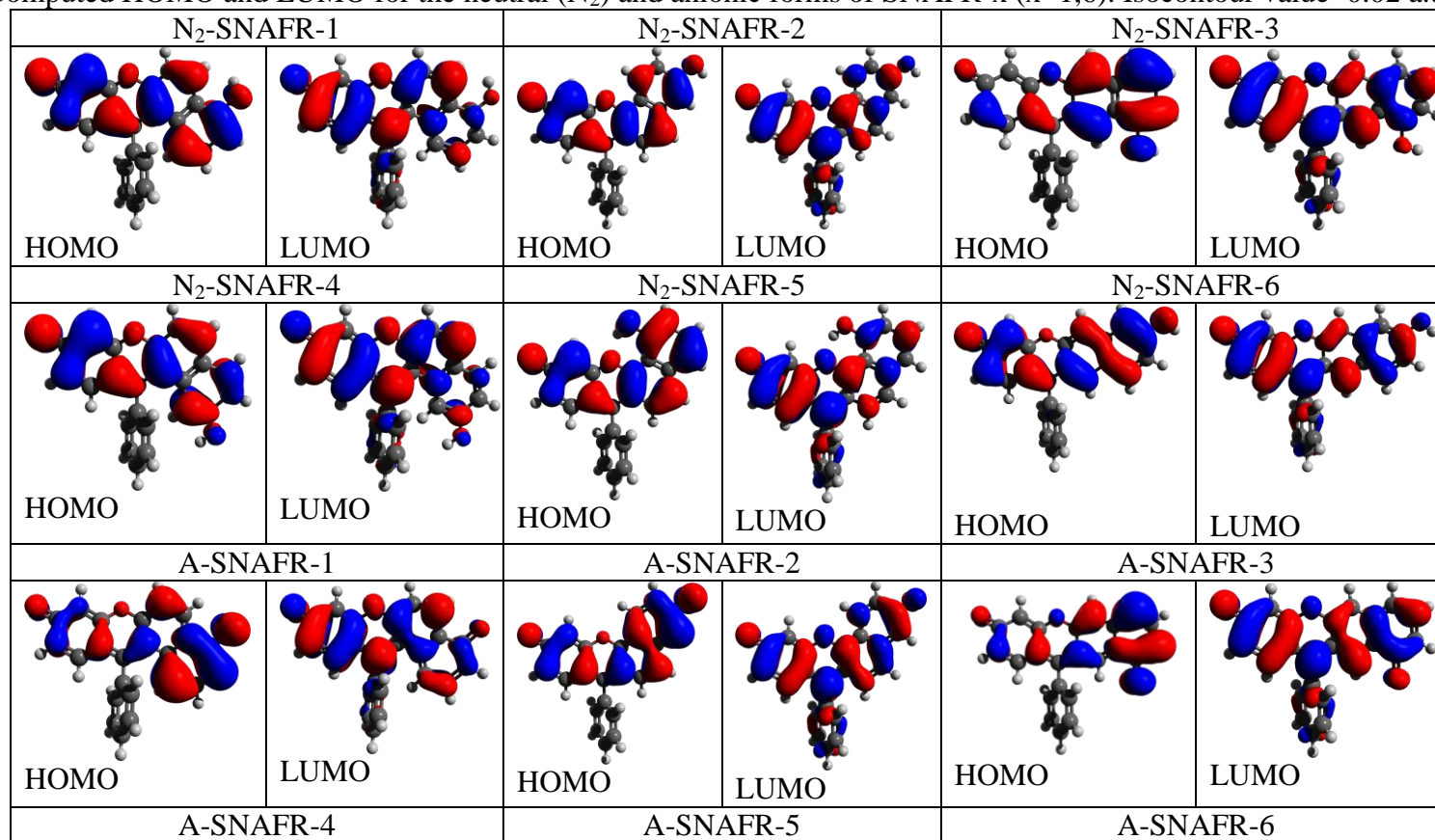


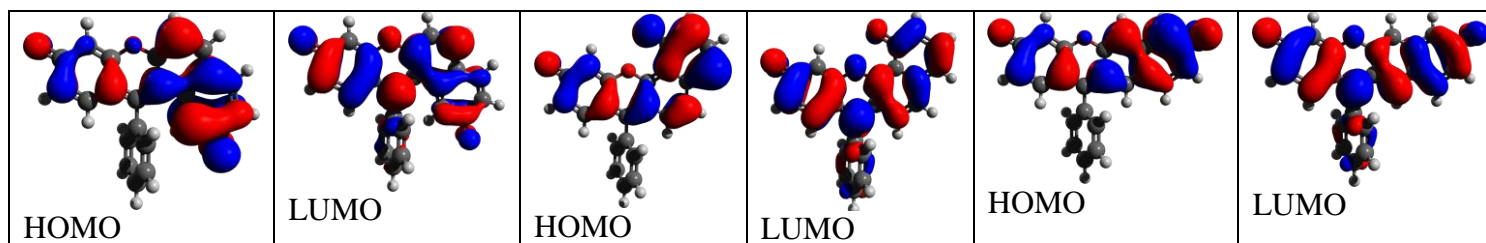
## Photophysical properties of NIR-emitting fluorescence probes: insights from TD-DFT

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### SUPPLEMENTARY INFORMATION

**Figure SI.1** Computed HOMO and LUMO for the neutral ( $N_2$ ) 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..

