**Supplementary Table 3**. TD-DFT/MM emission for electronic transition between S1 and S0 for the model GBAv-closed-I351L (resulting from the I351L mutation in GBAv-closed before MD). The TD-DFT/MM calculations were performed with the 6-311G(2d,p) basis set with the B3LYP functional on a structure optimized at the same level of theory.

|  |  |
| --- | --- |
| Model*a* | TD-DFT/MM  in eV*b* |
| Snapshot (1) | 2.35 (528) |
| Snapshot (2) | 2.40 (517) |
| Snapshot (3) | 2.33 (531) |
| GBAv-closed snapshot (1) of Supplementary Table 2 | 2.32 (535) |
| GBAv mutant I351L (experimental value) | 2.30 (538) |

*a*The values in parentheses represent the number of the snapshot extracted from the corresponding MD simulation.

*b*The associated wavelengths in nm are given in parentheses.