**Supplementary Table 5**. TD-DFT/MM emission for electronic transition between S1 and S0 for the model GBAv-closed-R337L/I351L (resulting from double R337L and I351L mutations in GBAv-closed before MD). The TD-DFT/MM calculations were performed with the 6-311G(2d,p) basis set and the B3LYP functional on a structure optimized at the same level of theory.

|  |  |
| --- | --- |
| Model*a* | TD-DFT/MM  in eV*b* |
| Snapshot (1) [simulation times = 7 ns] | 2.08 (595) |
| Snapshot (2) [simulation times = 9.5 ns] | 2.10 (590) |
| GBAv-closed snapshot (1) of Supplementary Table 2 | 2.32 (535) |
| GBAv double mutant R337L/I351 (experimental value) | 2.13 (580) |

*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.