**Supplementary Table 2**. TD-DFT/MM emission for electronic transition between S1 and S0 for the model GBAv-closed-insert-R356 (resulting from the insertion of Arg 356). TD-DFT/MM done with 6-311G(2d,p) basis set and B3LYP functional on structure optimized at the same level of theory.

|  |  |
| --- | --- |
| Model*a* | TD-DFT/MMin eV*b* |
| Snapshot (1) | 2.25 (550) |
| Snapshot (2) | 2.25 (550) |
| Snapshot (3) | 2.23 (553) |
| GBAv-closed snapshot (1) of Supplementary Table 2 | 2.32 (535) |

*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.