**S32 Fig: HOMO and LUMO structures of the optimized molecules.**

|  |  |  |
| --- | --- | --- |
| Compounds | HOMO | LUMO |
| Epalrestat |  |  |
| 4 |  |  |
| 7a |  |  |
| 7b |  |  |
| 7c |  |  |
| 7d |  |  |
| 7e |  |  |