**S31 Fig:** Chemical structures of molecules optimized with DFT-B3LYP (6-31G, d) level of theory

|  |  |
| --- | --- |
| Epalrestat | C10H9NO2S (4) |
| C18H15NO3S (7a) | C17H12NO2SCl (7b) |
| C17H12N2O4S (7c) | C17H13NO3S (7d) |
| C17H12NO2SCl (7e) |  |