|  |  |  |  |
| --- | --- | --- | --- |
|  | Optimal Structures | HOMO | LUMO |
| Clobetasol |  | C:\Users\ariasystem\Desktop\clo homo.jpg | C:\Users\ariasystem\Desktop\clo LUMO 1.jpg |
| Clobetasol-C60 |  | C:\Users\ariasystem\Desktop\FCLO HOMO.jpg | C:\Users\ariasystem\AppData\Roaming\Microsoft\Windows\Network Shortcuts\FCLO LUMO.jpg |
| Beclometasone |  | C:\Users\ariasystem\Desktop\bclo homo.jpg | C:\Users\ariasystem\Desktop\bclo lumo.jpg |
| Beclometasone-C60 |  | C:\Users\ariasystem\Desktop\fbclo homo.jpg | C:\Users\ariasystem\Desktop\fbclolumo.jpg |  |
| Prednisolone |  | C:\Users\ariasystem\Desktop\pred homo.jpg | C:\Users\ariasystem\Desktop\pred lumo.jpg |  |
| Prednisolone-C60 |  | C:\Users\ariasystem\Desktop\Fpred homo.jpg | C:\Users\ariasystem\Desktop\Fpred lumo.tif |  |
| Methylprednisolone |  | C:\Users\ariasystem\Desktop\mpred homo.tif | C:\Users\ariasystem\Desktop\mpred lumo.tif |  |
| Methylprednisolone-C60 |  | C:\Users\ariasystem\Desktop\Fmpred homo.tif | C:\Users\ariasystem\Desktop\Fmp lumo.tif |  |

**S1.** Schematic of optimal structures and HOMO/ LUMO of drugs and drug-nanocarriers.