**Influence of End-Capped Engineering on 3-Dimenional Star-Shaped Triphenylamine-Based Donor Materials for Efficient Organic Solar Cells**

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|  |  |
| Reference | STRO1 |
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| STRO2 | STRO3 |
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| STRO4 | STRO5 |
|  |  |
| STRO6 | STRO7 |
|  |  |
| STRO8 |  |

 **Figure S1**: Chemical structure of STRO (R) along-with eight newly proposed star-shaped molecules (STRO1-STRO8).

**Hole Electrons Overlap Heat Maps**

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| Chart  Description automatically generated**Reference** |
| **Chart  Description automatically generatedSTRO1** |
| Chart  Description automatically generated**STRO2** |
| Chart  Description automatically generated**STRO3** |
| Chart  Description automatically generated**STRO4** |

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| A picture containing graphical user interface  Description automatically generated**STRO5** |
| Chart  Description automatically generated**STRO6** |
| Chart  Description automatically generated**STRO7** |
| A picture containing diagram  Description automatically generated**STRO8** |

**Figure S2**: The hole/electrons overlap heat mapsof STRO (R) along-with eight newly proposed star-shaped molecules (STRO1-STRO8).