Electronic Supplementary Material (ESI) for Materials Advances.

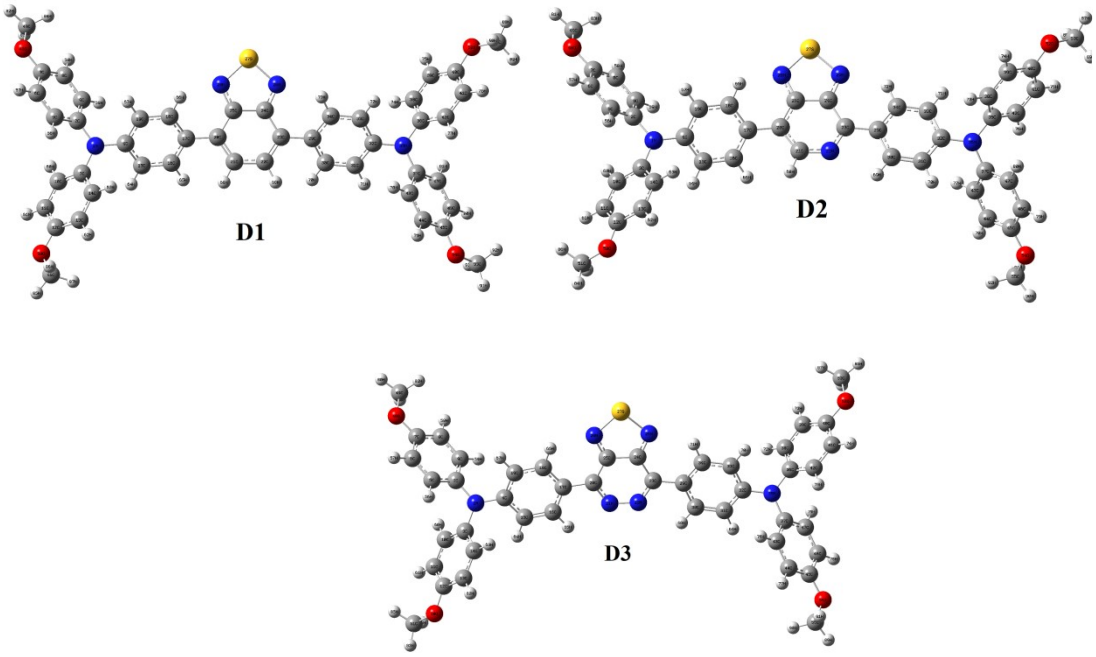
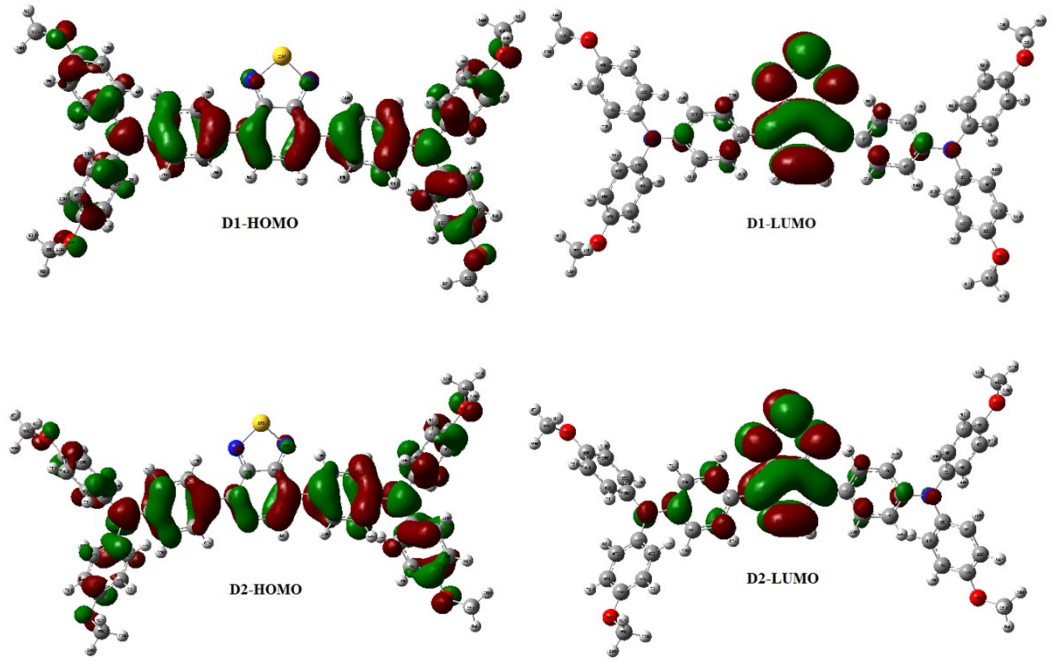


Figure S1. Optimized geometric structures of designed donors(D1,D2 and D3) in solvent phase.



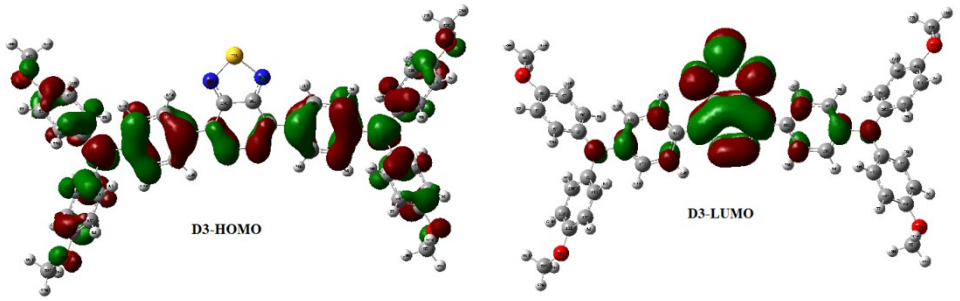
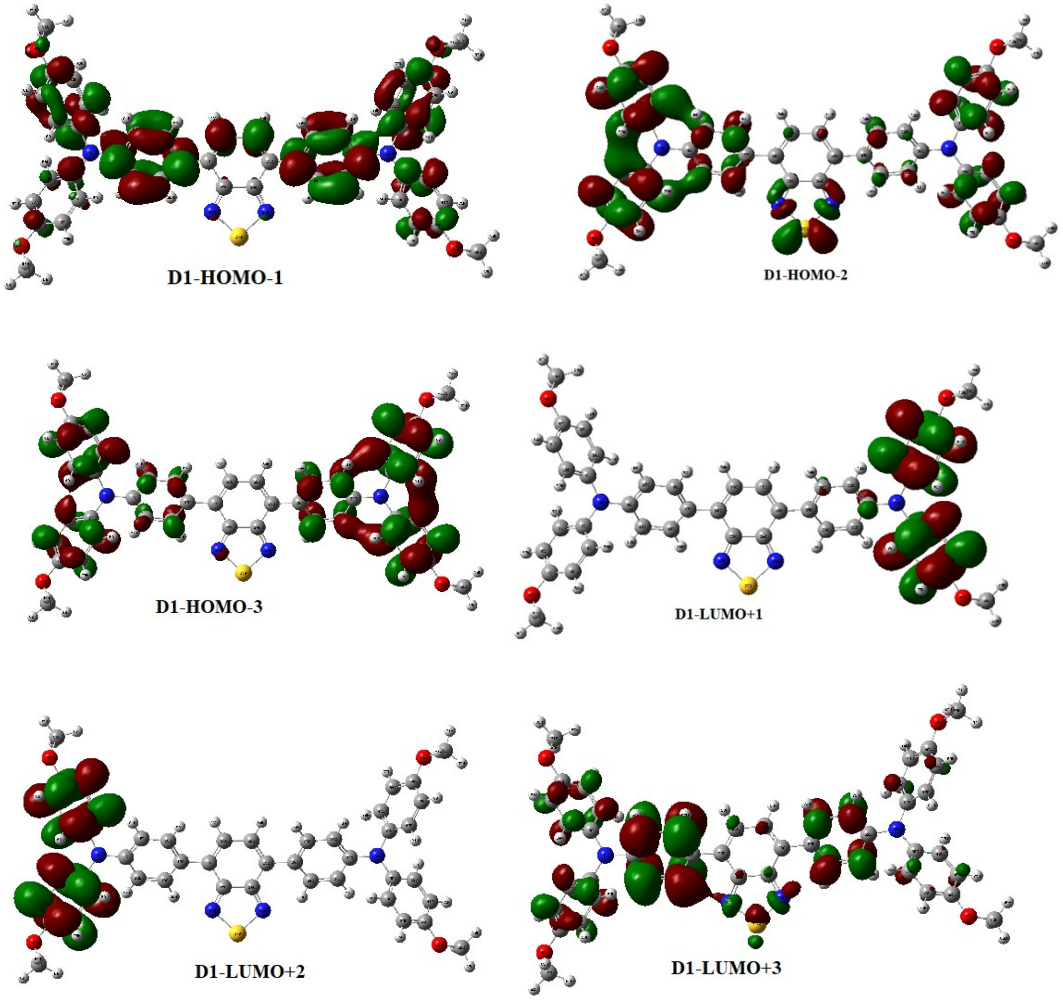
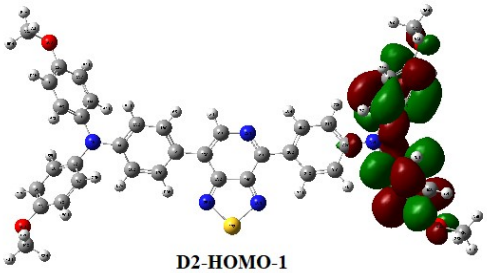
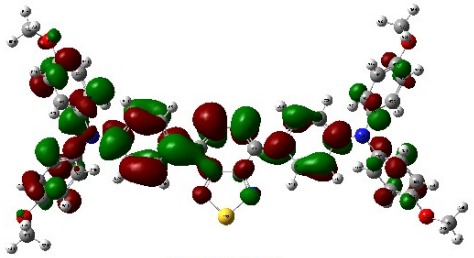


Figure S2. Contours of the HOMO and LUMO of D-A-D in the solvent phase.

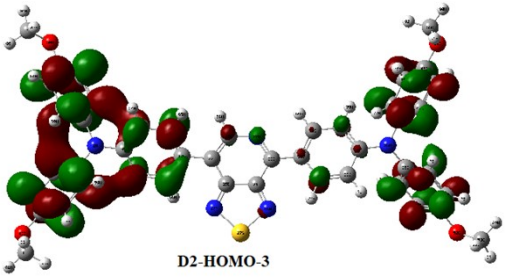




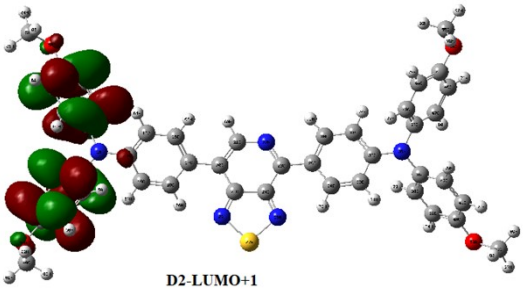
D2-HOMO-1



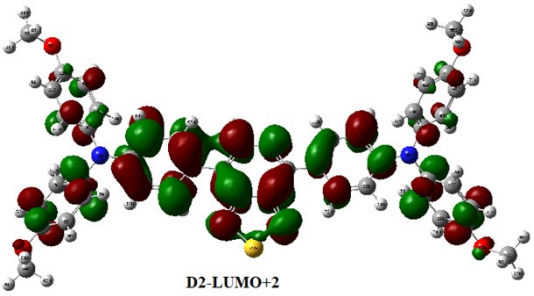
D2-HOMO-2



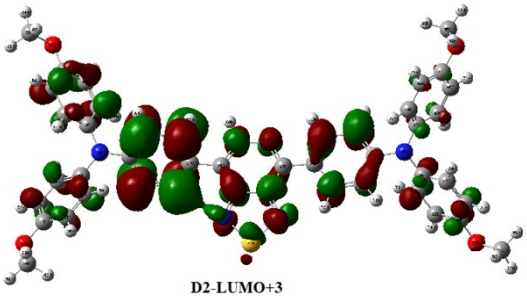
D2-HOMO-3



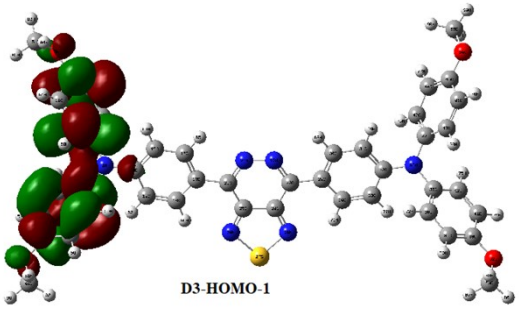
D2-LUMO+1



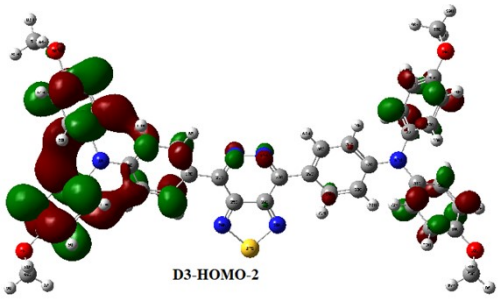
D2-LUMO+2



D2-LUMO+3



D3-HOMO-1



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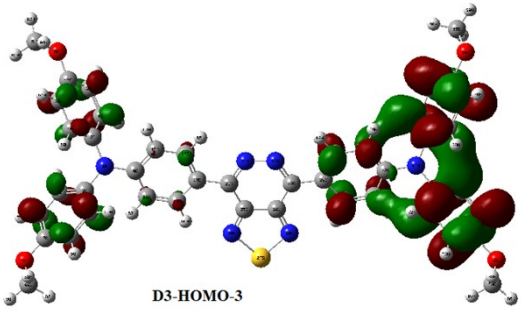
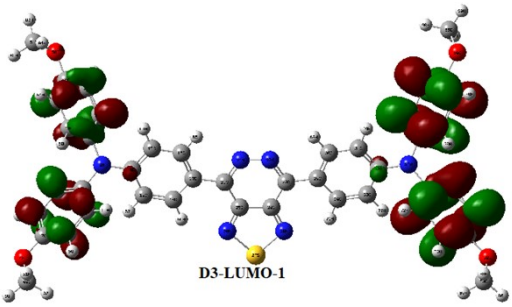


D3-HOMO-3



D3-LUMO-1

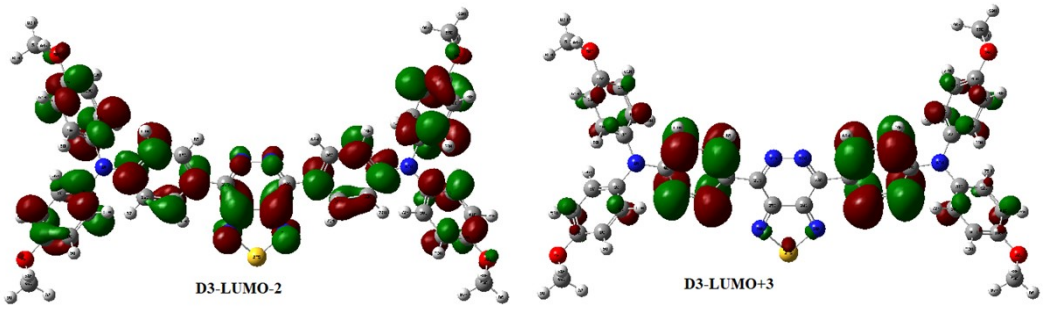


Figure S3. Contours of the HOMO-1, HOMO-2 HOMO-3 and LUMO+1, LUMO+2, LUMO+3 Orbitals for D1,D2 and D3 monomers in the gas phase.

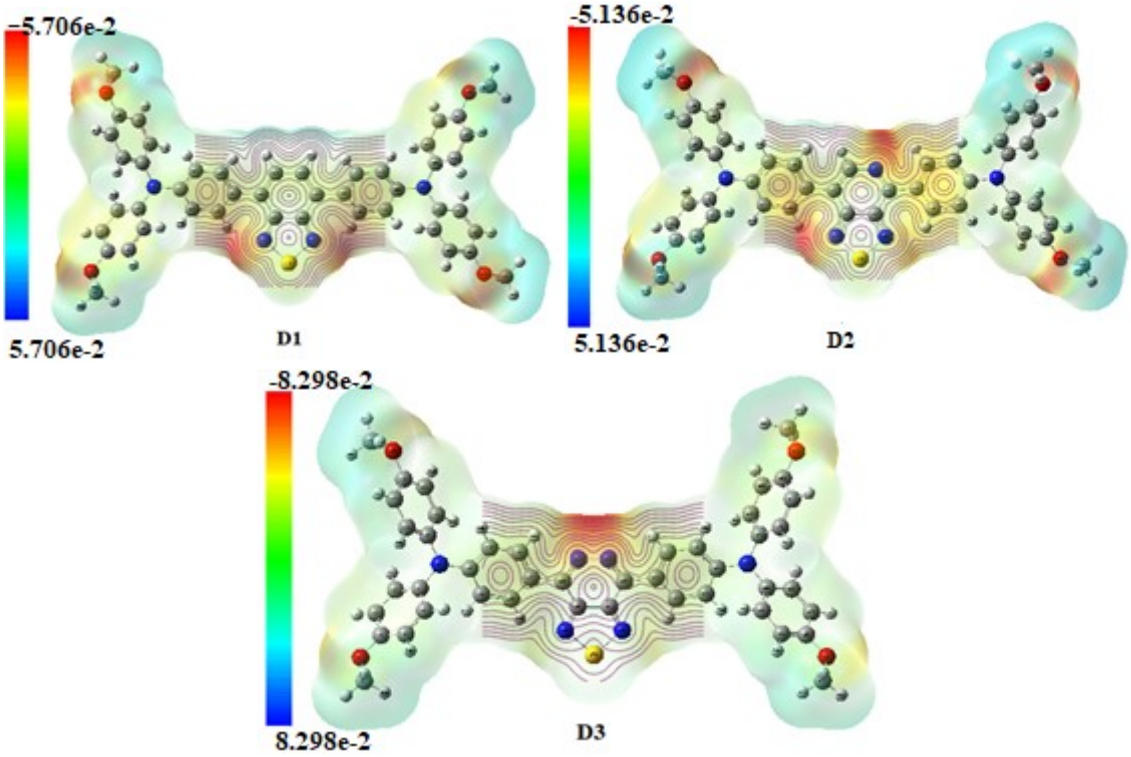


Fig. S4. MEP maps representation of designed molecules (D1-D3)in the gas solvent phase.

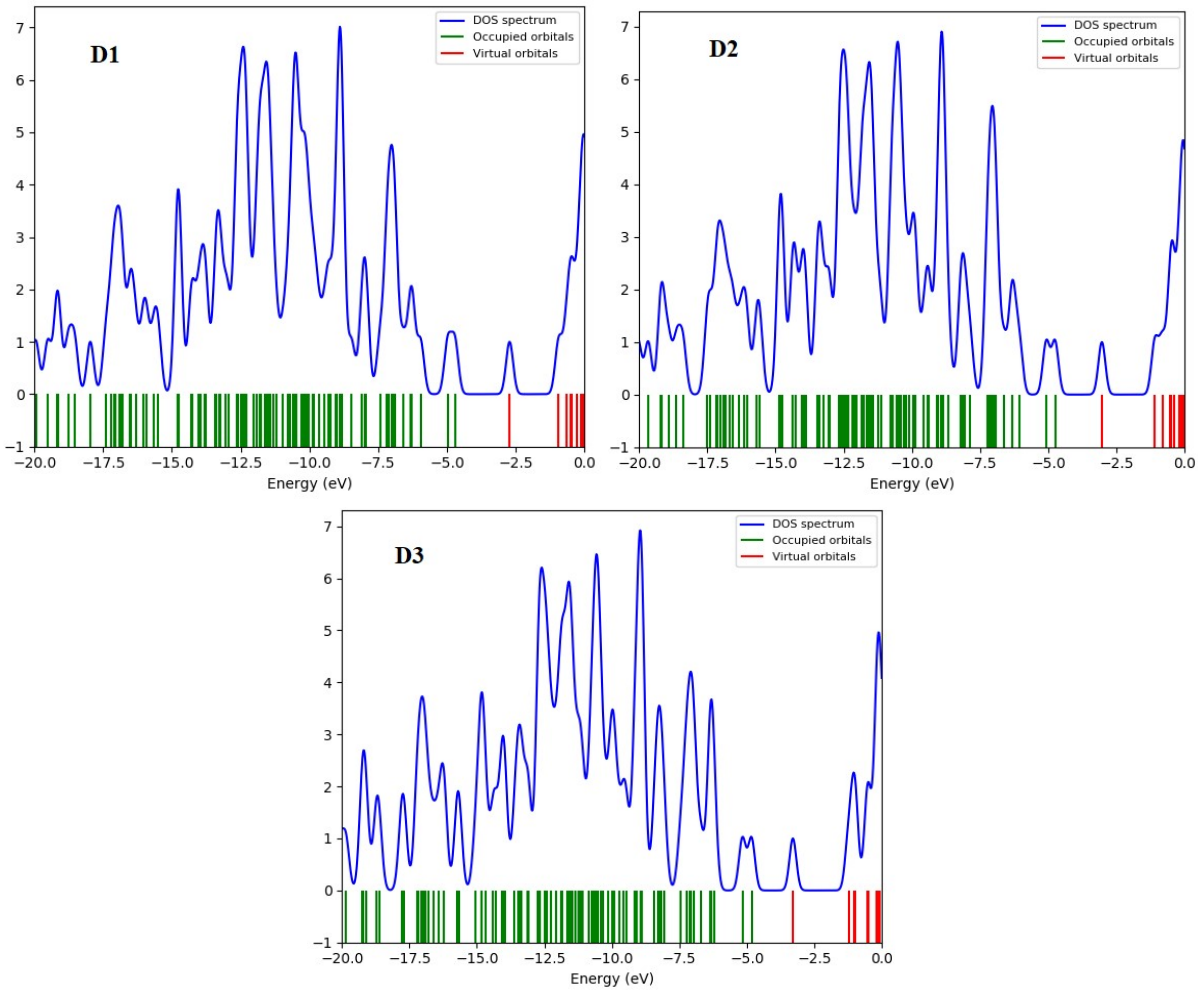


Fig. S5. DOS plots of designed molecules D1-D3 in the solvent phase.