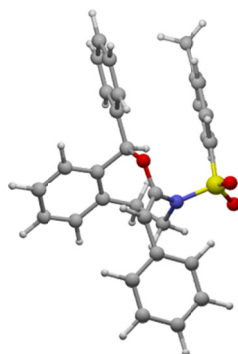
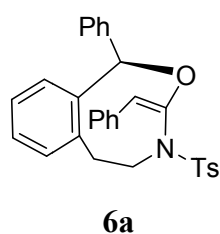
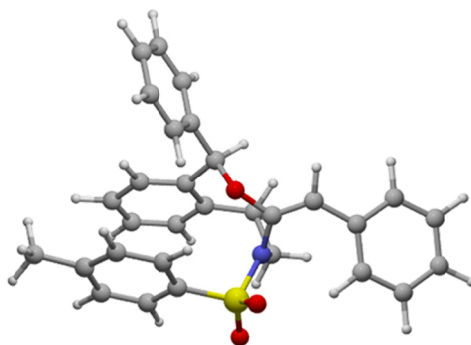
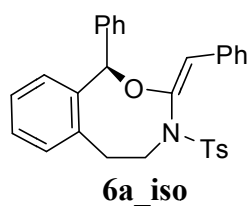


Energy and imaginary vibrational frequency of calculated structures using  
B3LYP-D3 method.



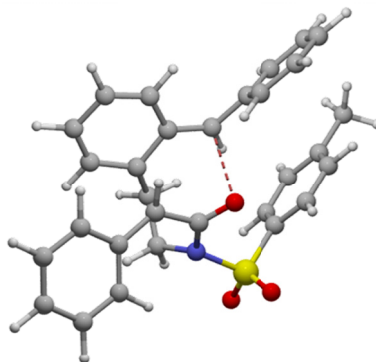
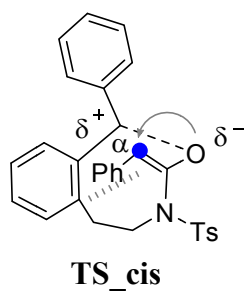
E= -1838.109717 Hartree

E<sub>SMD</sub>=-1838.720846 Hartree



E= -1838.102423 Hartree

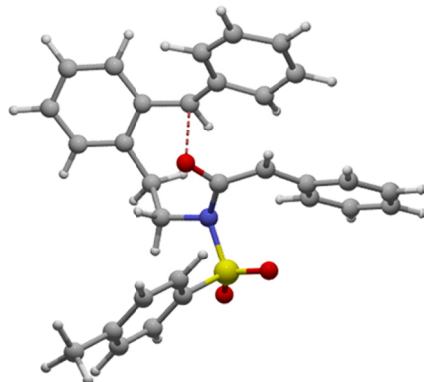
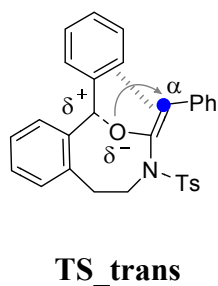
E<sub>SMD</sub>= -1838.71482 Hartree



E=-1838.064467 Hartree

E<sub>SMD</sub>= -1838.677033 Hartree

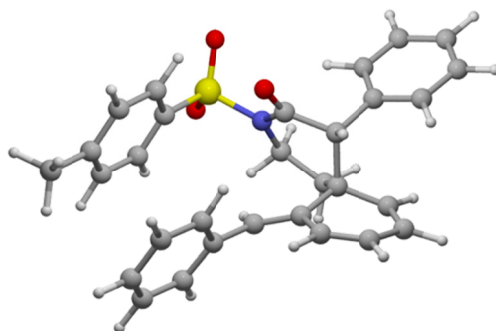
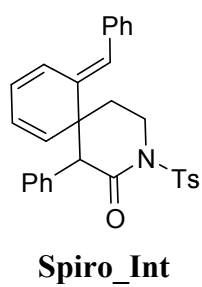
Frequency= -205.64 cm<sup>-1</sup>



E= -1838.042421 Hartree

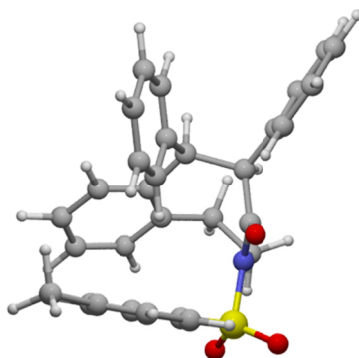
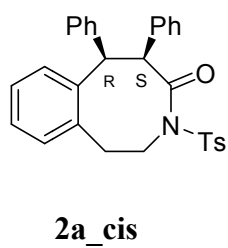
E<sub>SMD</sub>= -1838.660252 Hartree

Frequency= -203.95 cm<sup>-1</sup>



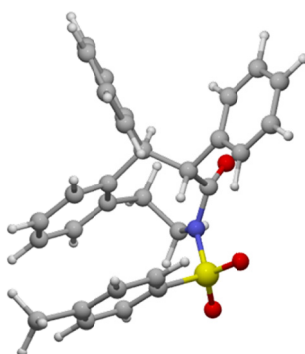
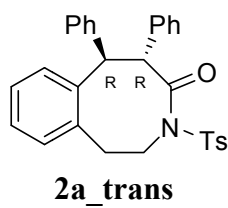
E=-1838.090101 Hartree

E<sub>SMD</sub>= -1838.702537 Hartree



E= -1838.133234 Hartree

E<sub>SMD</sub>= -1838.742115 Hartree



E= -1838.128214 Hartree

E<sub>SMD</sub>=-1838.742451 Hartree