

Figure S1. <sup>1</sup>H spectrum of Th4CN.

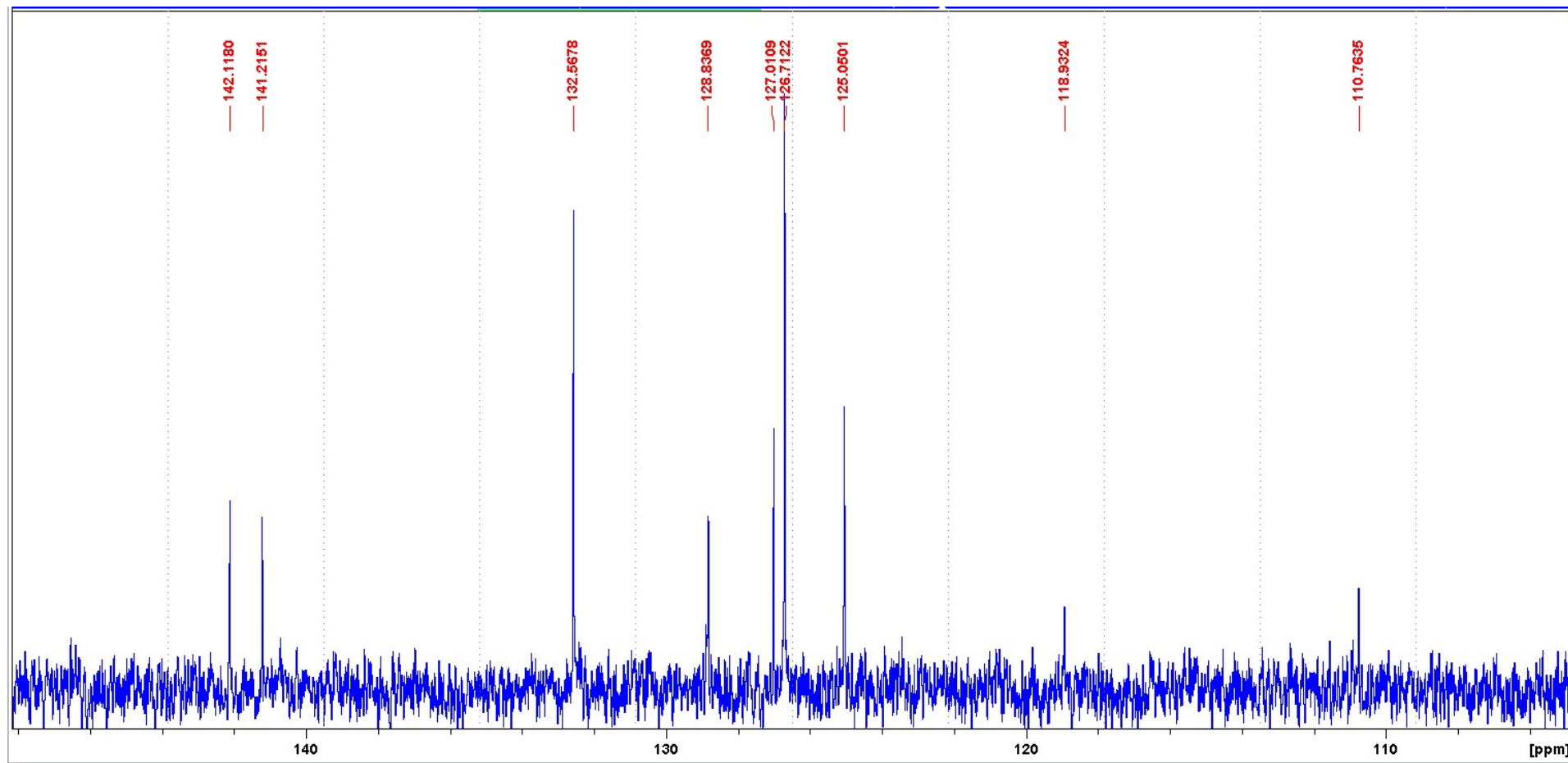
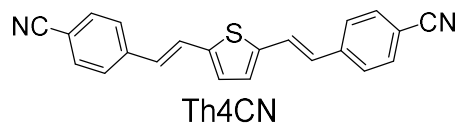


Figure S2.  $^{13}\text{C}$  spectrum of Th4CN.

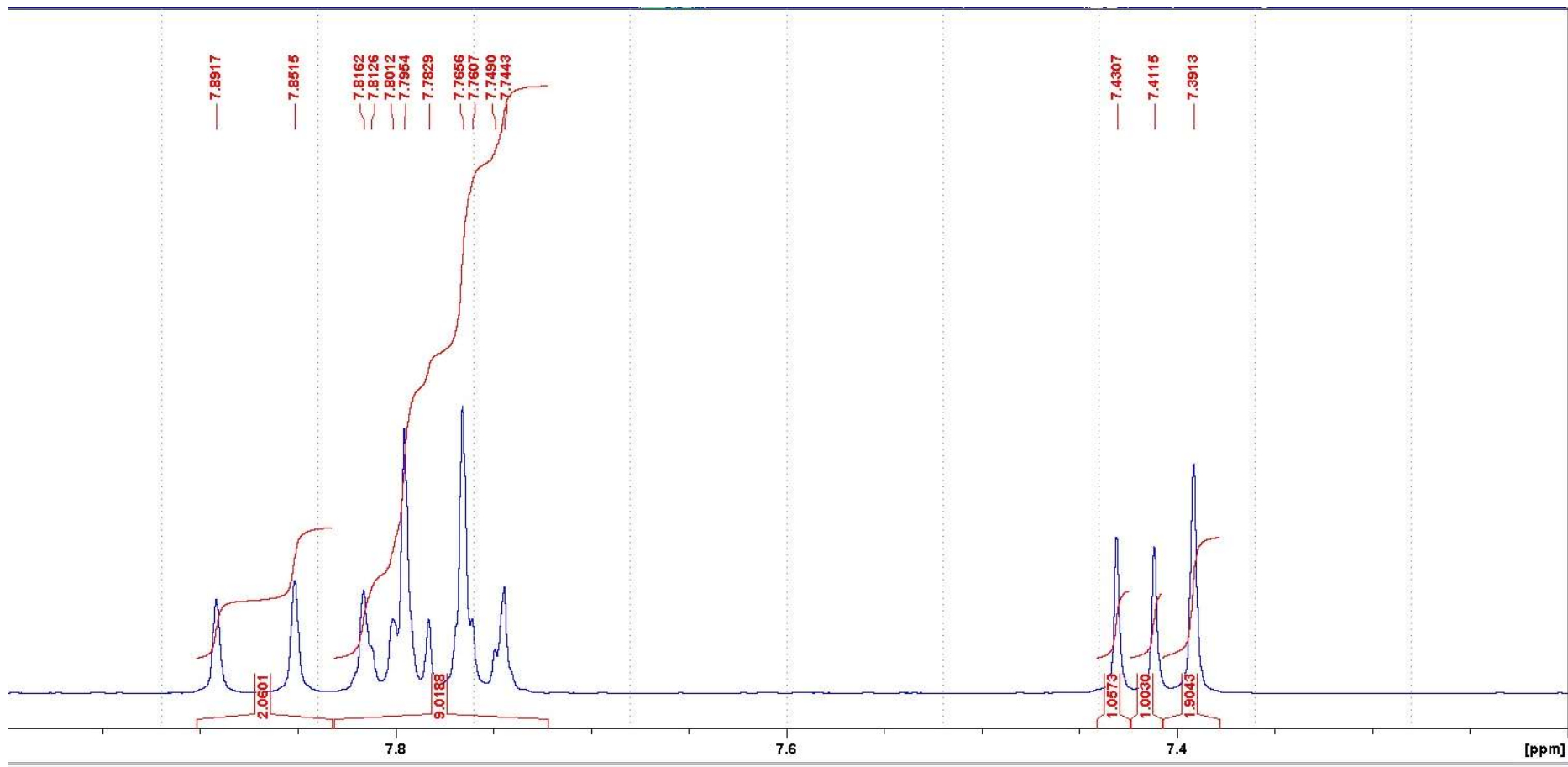
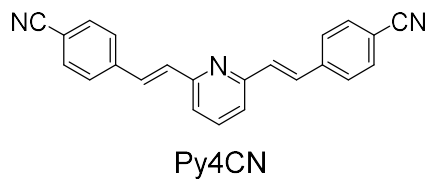
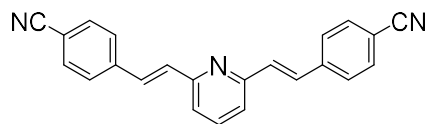


Figure S3. <sup>1</sup>H spectrum of Py4CN.



Py4CN

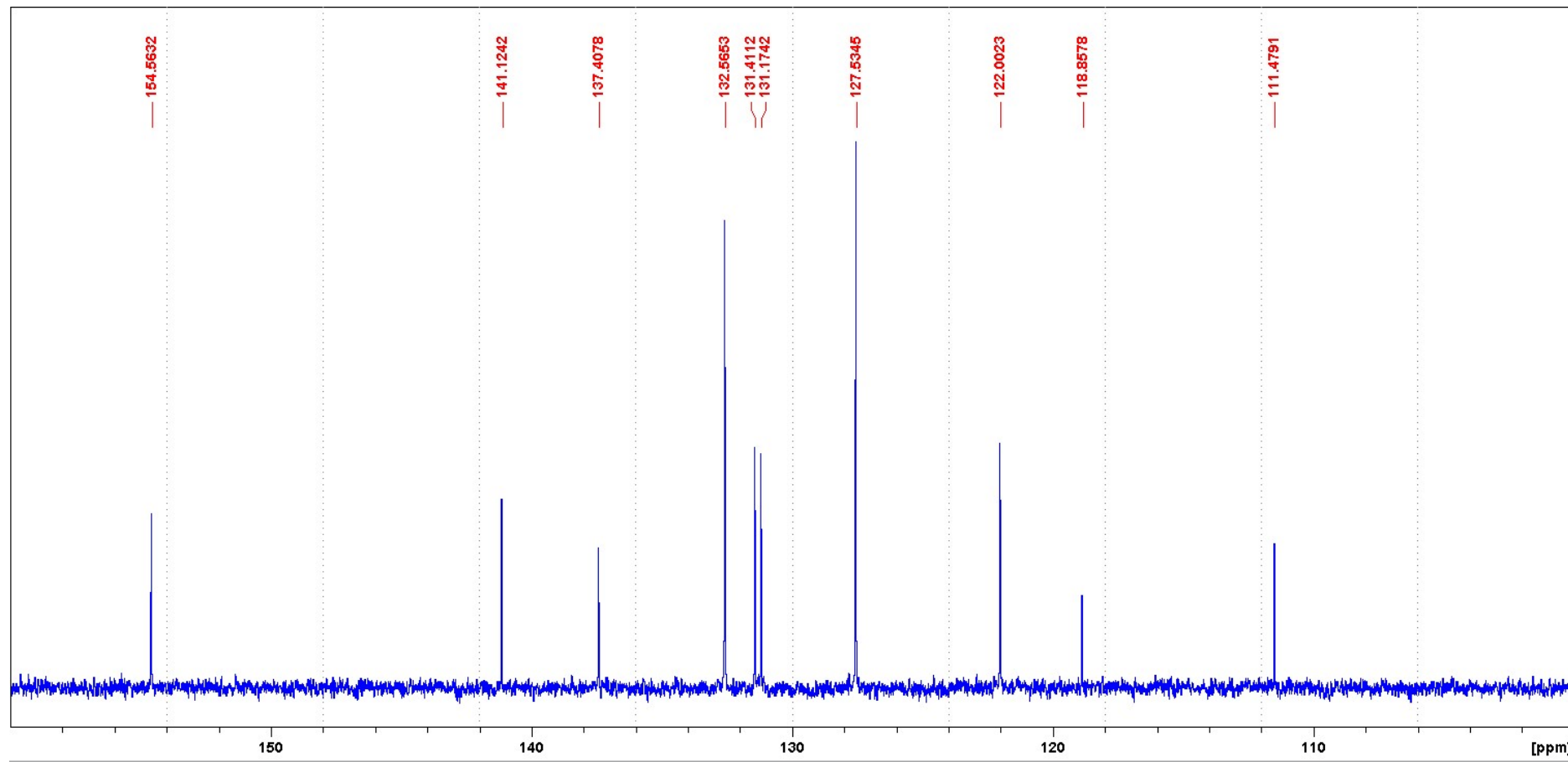


Figure S4.  $^{13}\text{C}$  spectrum of Py4CN.

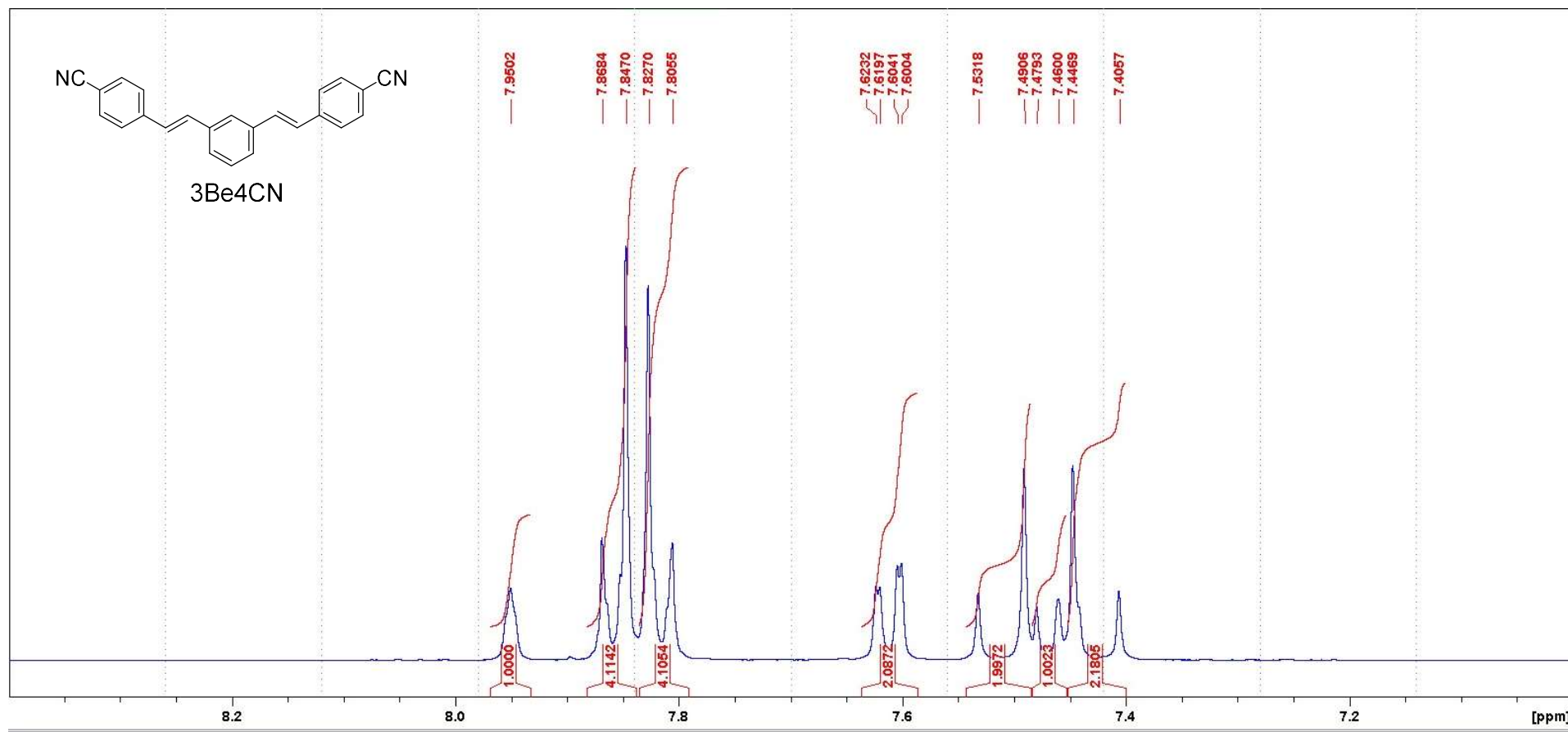
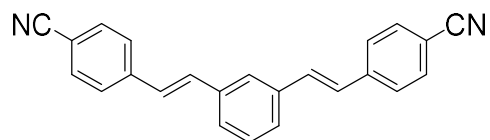


Figure S5.  $^1\text{H}$  spectrum of 3Be4CN.



3Be4CN

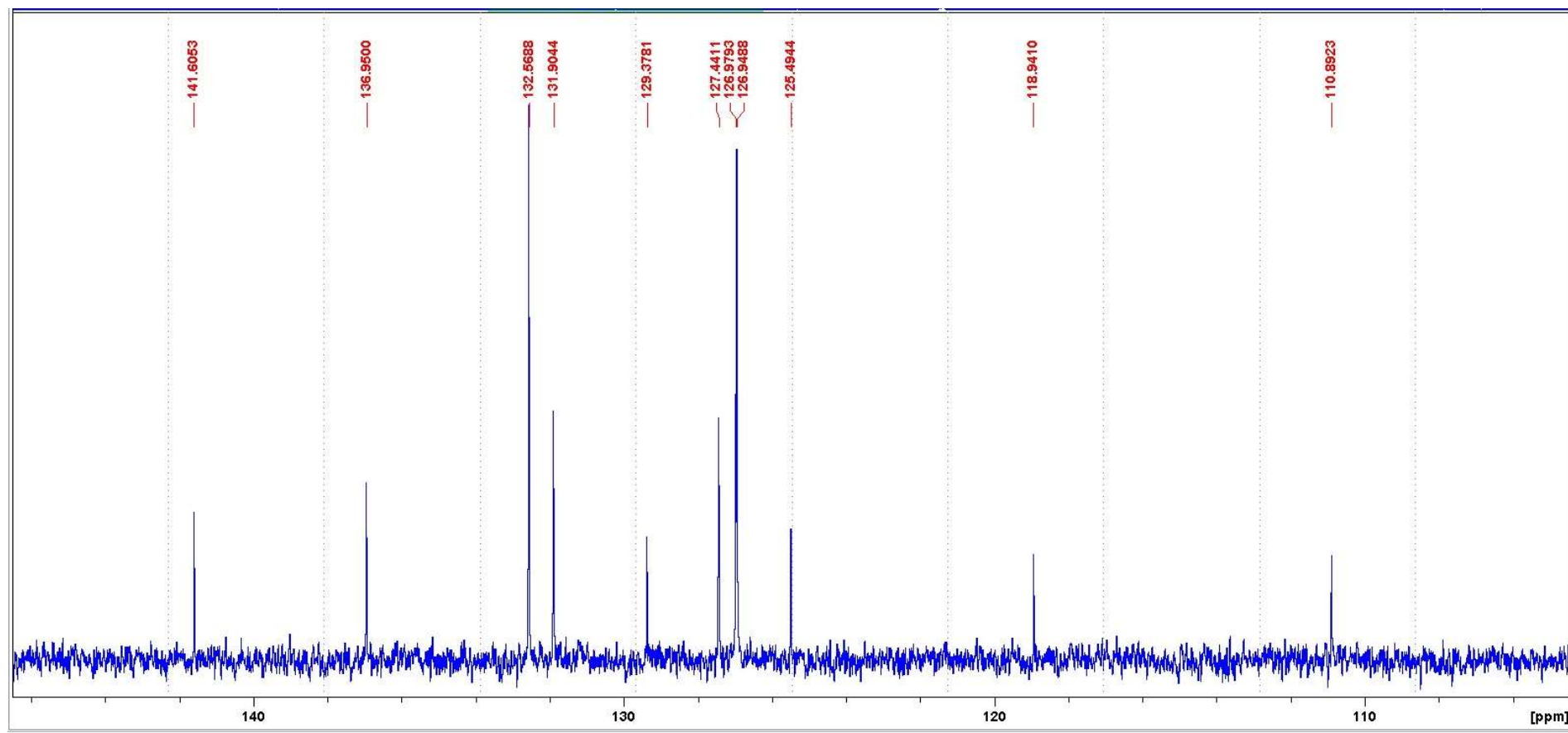


Figure S6.  $^{13}\text{C}$  spectrum of 3Be4CN.

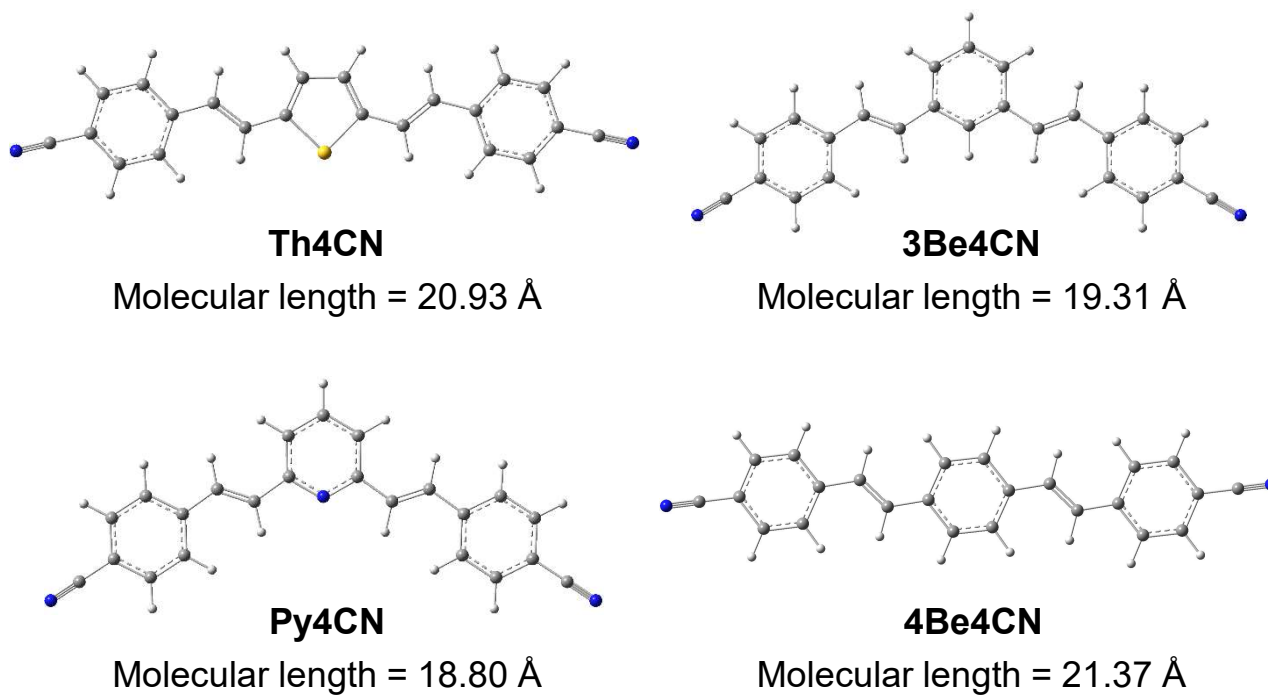


Figure S7. Optimized structures for 4 compounds.

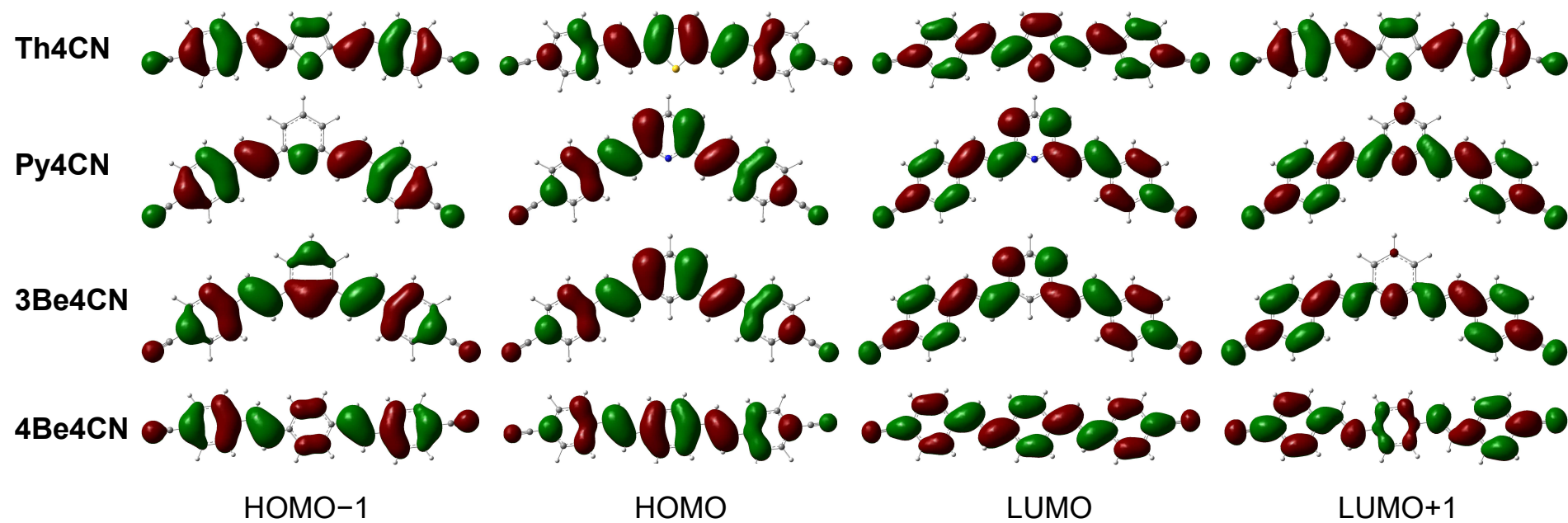


Figure S8. Localization of HOMO and LUMO orbit for 4 compounds.