**Supporting information**

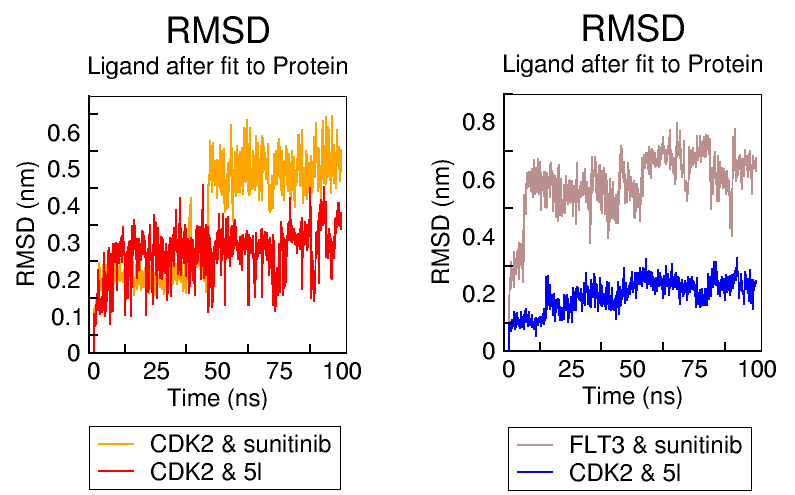
**Discovery and anticancer screening of novel oxindole-based derivative bearing pyridyl group as potent and selective dual FLT3/CDK2 kinase inhibitor**

Aya Soudi 1, Onur Bender 2,\*, Ismail Celik 3,4, Amer Ali Abd El-Hafeez 5, Rumeysa Dogan 2, Arzu Atalay 2, Eslam B. Elkaeed 6, Aisha A. Alsfouk 7, El-Shimaa M. N. Abdelhafez 1, Omar M. Aly 8, Wolfgang Sippl 4, Taha F. S. Ali 1,\*

\*Correspondence: [taha.ali@mu.edu.eg](mailto:taha.ali@mu.edu.eg) (Taha F.S. Ali), [onur.bender@ankara.edu.tr](mailto:onur.bender@ankara.edu.tr) (Onur Bender)

**Contents:**

* **Figure S1:** RMSD profiles for compound **5l** and sunitinib for each target CDK2 and FLT3 complexes, indicating deviations from initial conformations.
* **Figure S2-34:** 1H and 13C NMR spectrums of compounds **5a-p**



**Figure S1.** RMSD profiles for compound **5l** and sunitinib for each target CDK2 and FLT3 complexes, indicating deviations from initial conformations.

A graph of a chemical reaction

Description automatically generated

Figure S2. 1H NMR spectrum of compound (***E/Z***)-**5a**

A graph of a chemical reaction

Description automatically generated

Figure S3. 13C NMR spectrum of compound (***E/Z***)-**5a**.

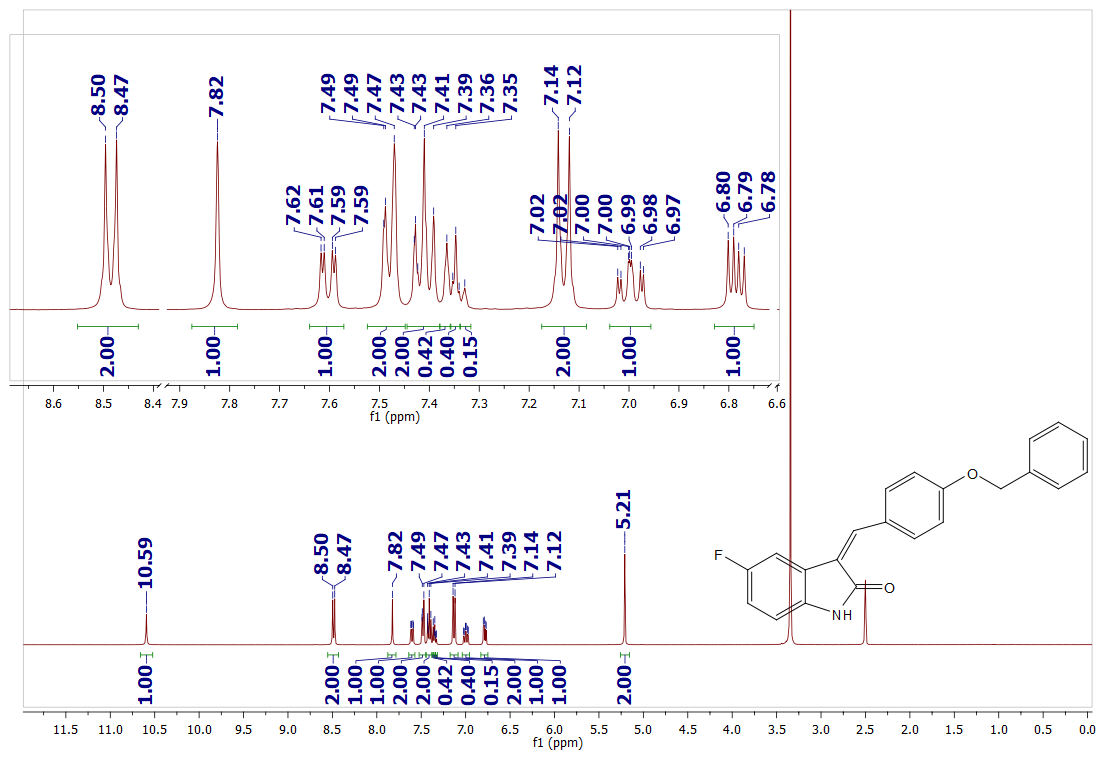


Figure S4. 1H NMR spectrum of compound (***E/Z***)-**5b**.

A graph of a chemical reaction

Description automatically generated

Figure S5. 13C NMR spectrum of compound (***E/Z***)-**5b.**

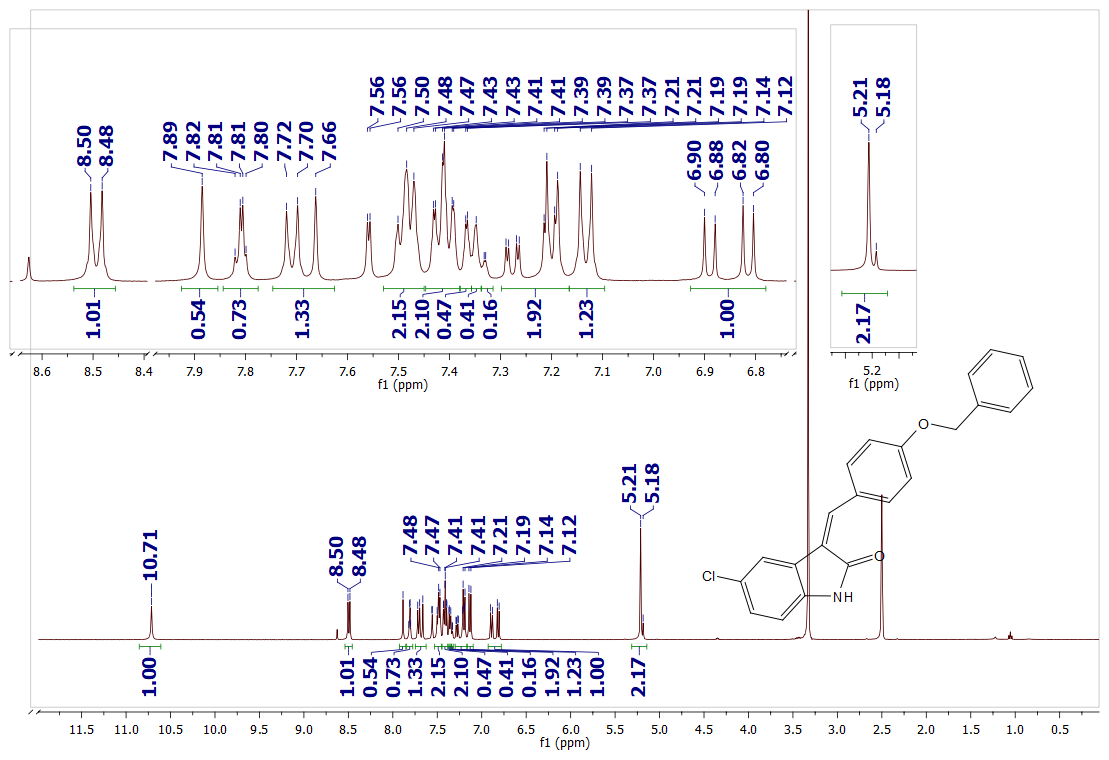


Figure S6. 1H NMR spectrum of compound (***E/Z***)-**5c**.

A graph of a chemical reaction

Description automatically generated with medium confidence

Figure S7. 13C NMR spectrum of compound (***E/Z***)-**5c.**

A screenshot of a graph

Description automatically generated

Figure S8. 1H NMR spectrum of compound (***E/Z***)-**5d**.

A graph of a chemical reaction

Description automatically generated

Figure S9. 13C NMR spectrum of compound (***E/Z***)-**5d.**

A screenshot of a graph

Description automatically generated

Figure S10. 1H NMR spectrum of compound (***E/Z***)-**5e**.

A graph of a chemical reaction

Description automatically generated

Figure S11. 13C NMR spectrum of compound (***E/Z***)-**5e.**

A graph of a chemical formula

Description automatically generated

Figure S12. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5e.**

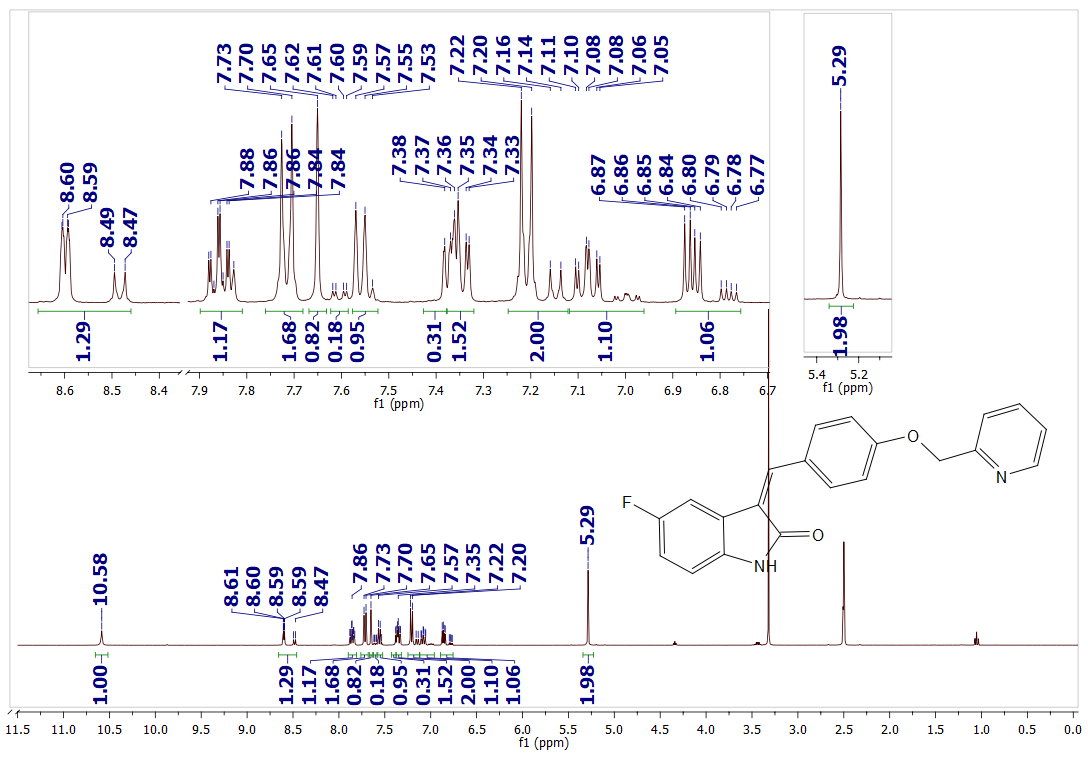


Figure S13. 1H NMR spectrum of compound (***E/Z***)-**5f**

A graph of a chemical formula

Description automatically generated

Figure S14. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5f.**

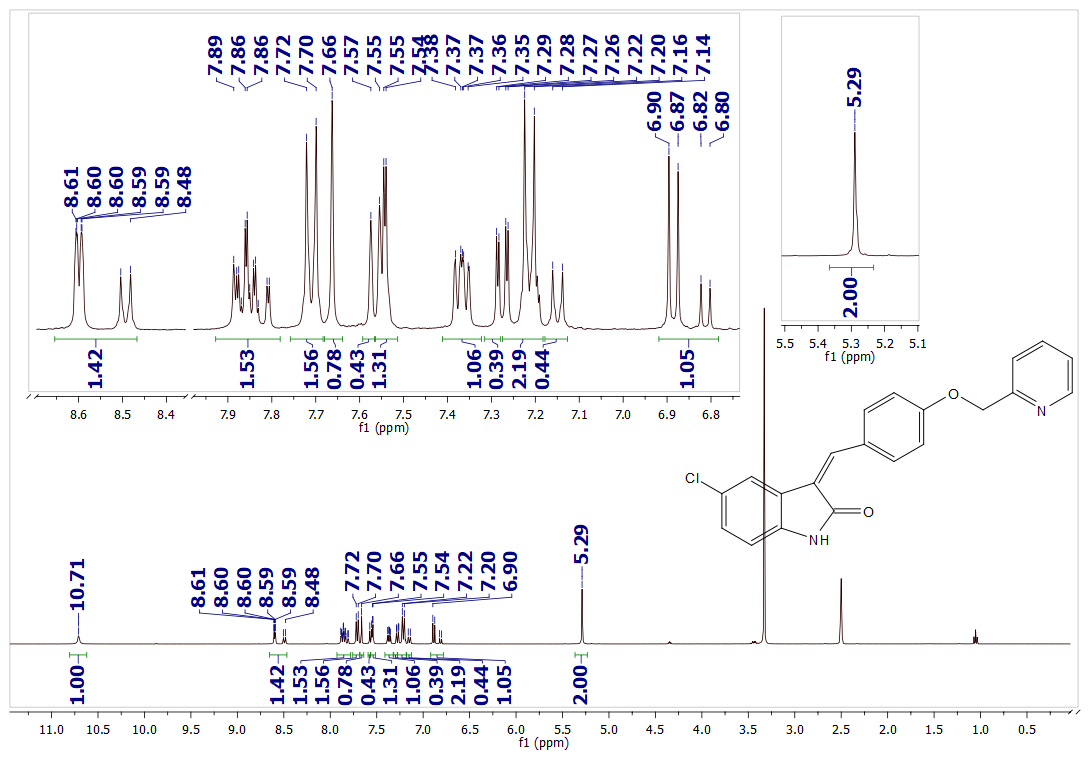


Figure S15. 1H NMR spectrum of compound (***E/Z***)-**5g**

A graph of a chemical formula

Description automatically generated

Figure S16. 13C NMR spectrum of compound (***E/Z***)-**5g.**

A screenshot of a graph

Description automatically generated

Figure S17. 1H NMR spectrum of compound (***E/Z***)-**5g**

A graph of a chemical formula

Description automatically generated with medium confidence

Figure S18. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5h.**

A screenshot of a graph

Description automatically generated

Figure S19. 1H NMR spectrum of compound (***E/Z***)-**5i.**

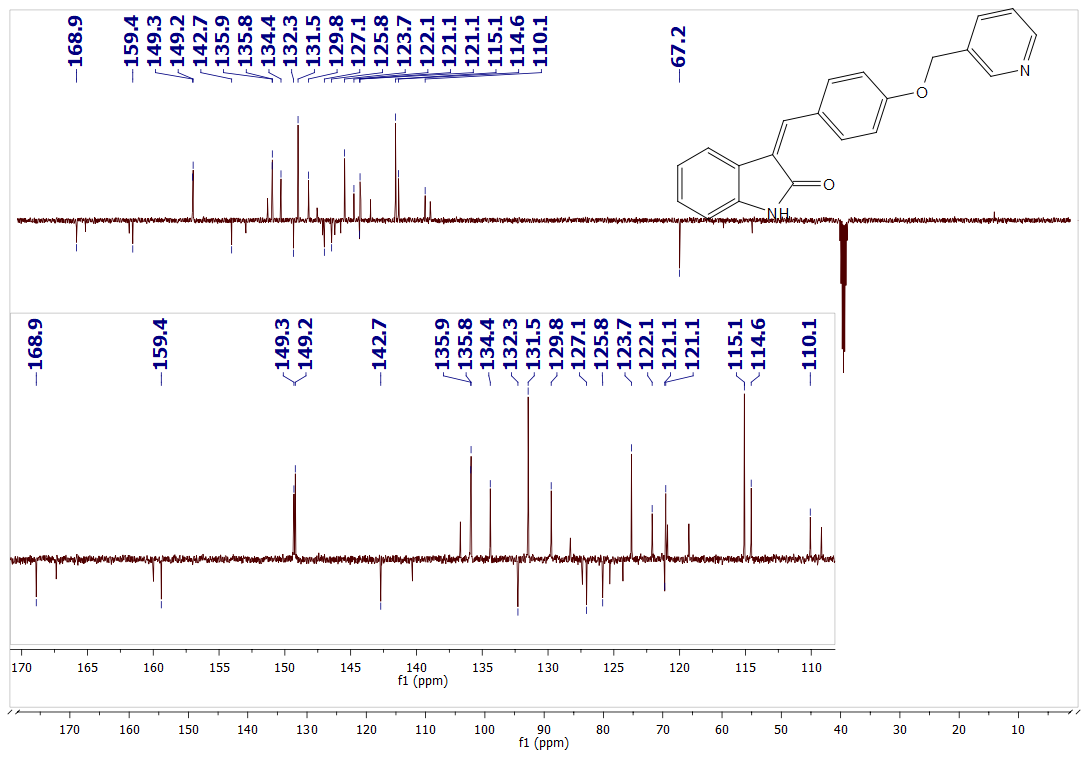


Figure S20. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5i.**

A screenshot of a graph

Description automatically generated

Figure S21. 1H NMR spectrum of compound (***E/Z***)-**5j.**

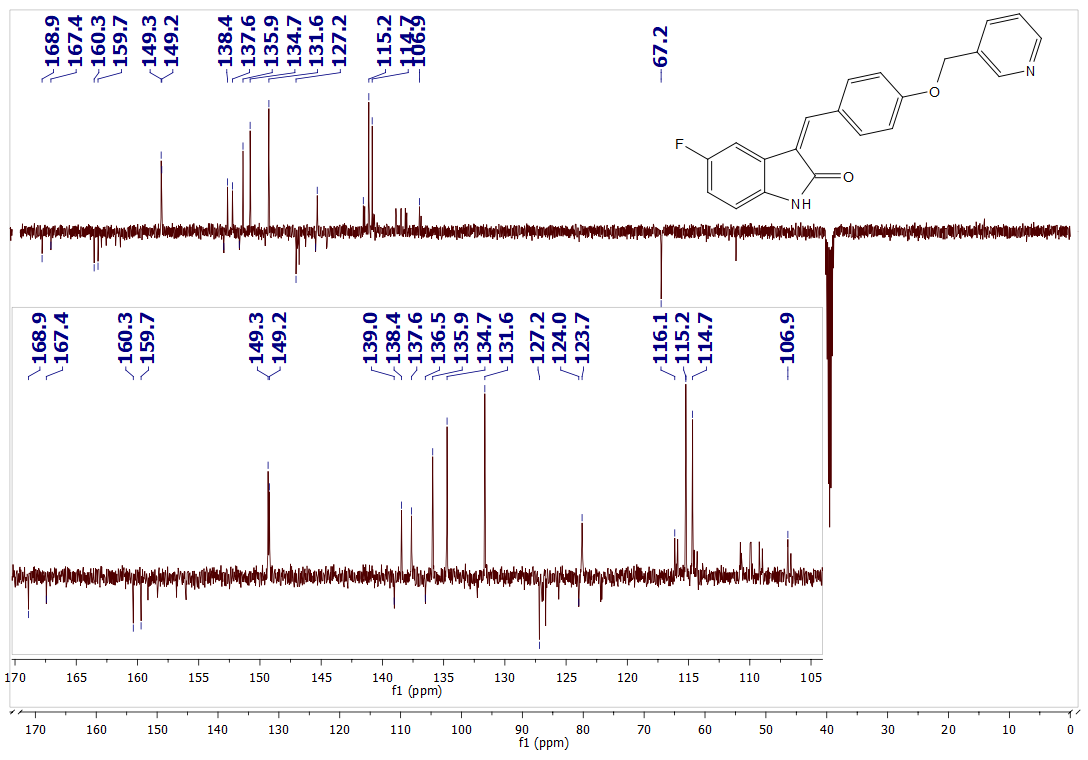


Figure S22. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5j.**

A screenshot of a graph

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Figure S23. 1H NMR spectrum of compound (***E/Z***)-**5k.**

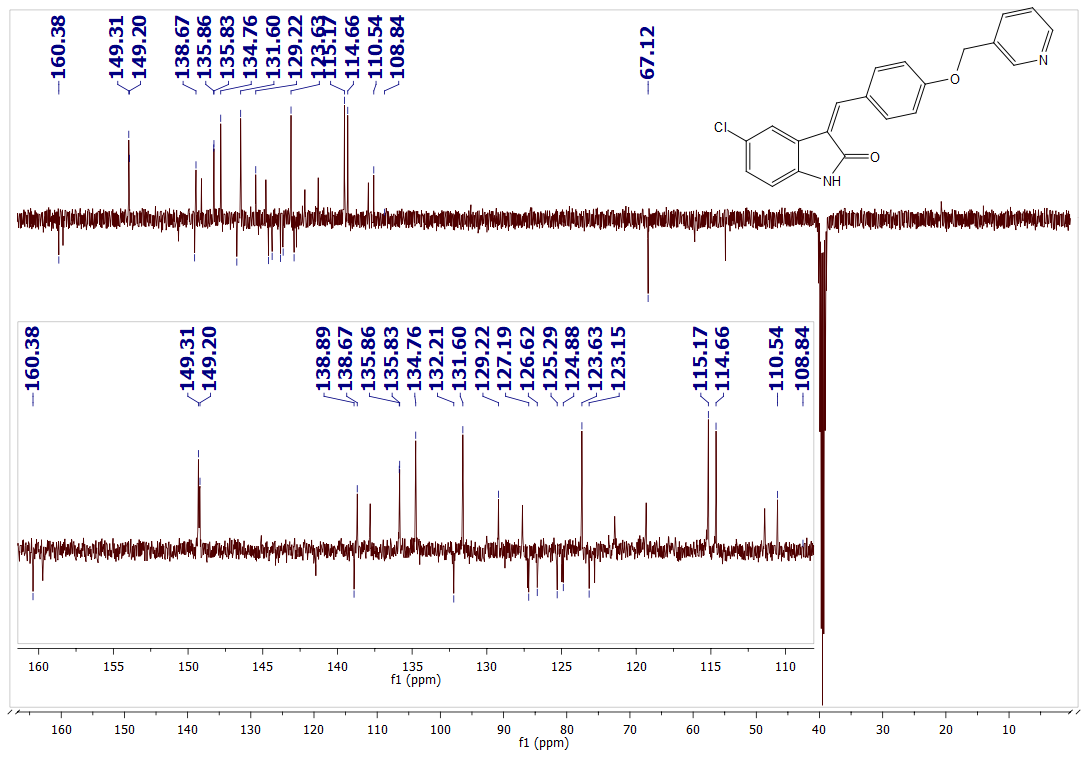


Figure S24. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5k.**

A graph of a chemical reaction

Description automatically generated with medium confidence

Figure S25. 1H NMR spectrum of compound (***E/Z***)-**5l.**

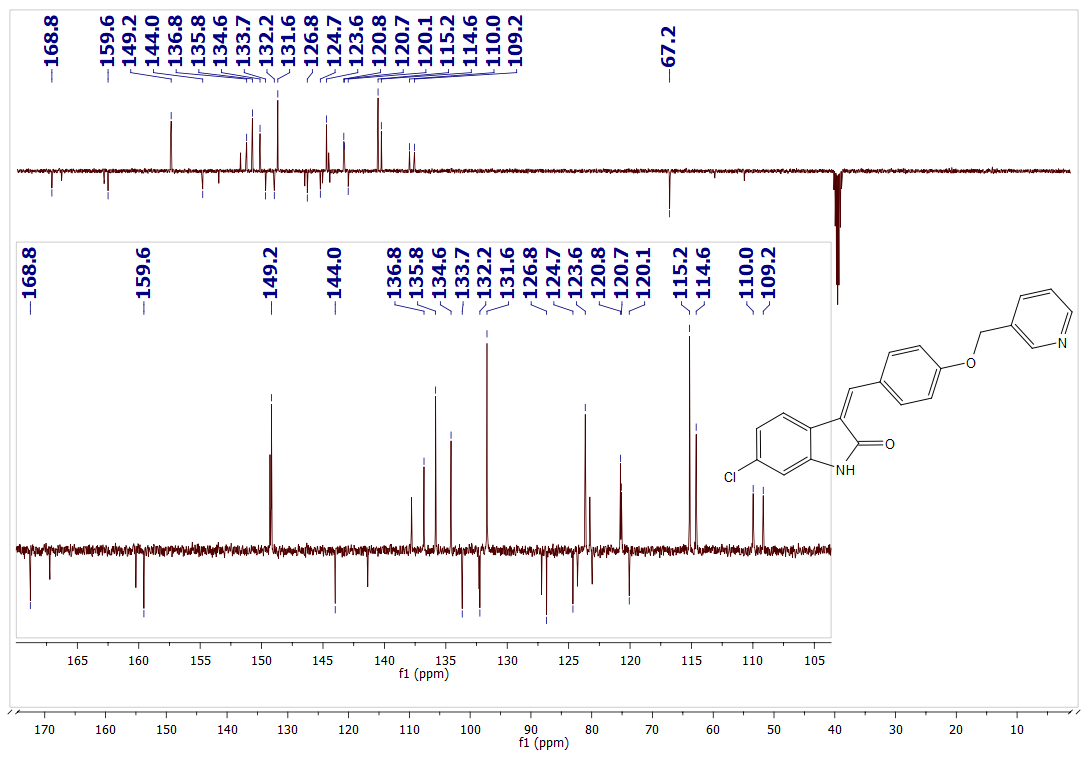


Figure S26. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5l.**

A screenshot of a graph

Description automatically generated

Figure S27. 1H NMR spectrum of compound (***E/Z***)-**5m.**

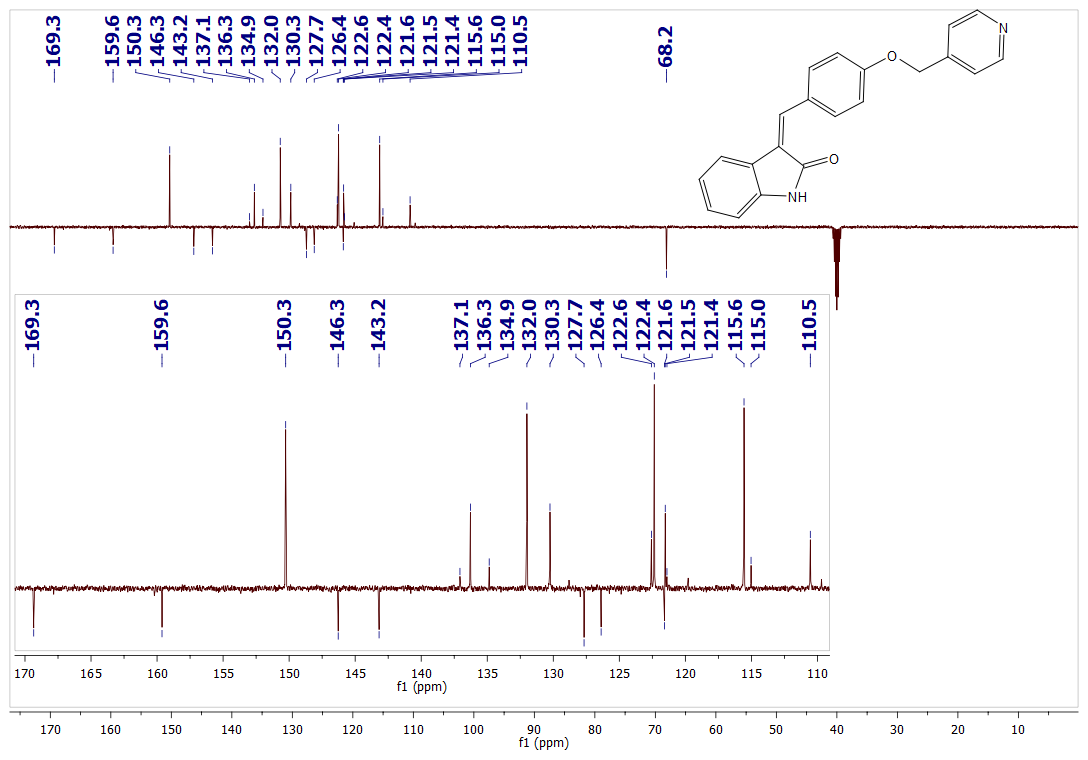


Figure S28. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5m.**

A graph of a chemical formula

Description automatically generated with medium confidence

Figure S29. 1H NMR spectrum of compound (***E/Z***)-**5n.**

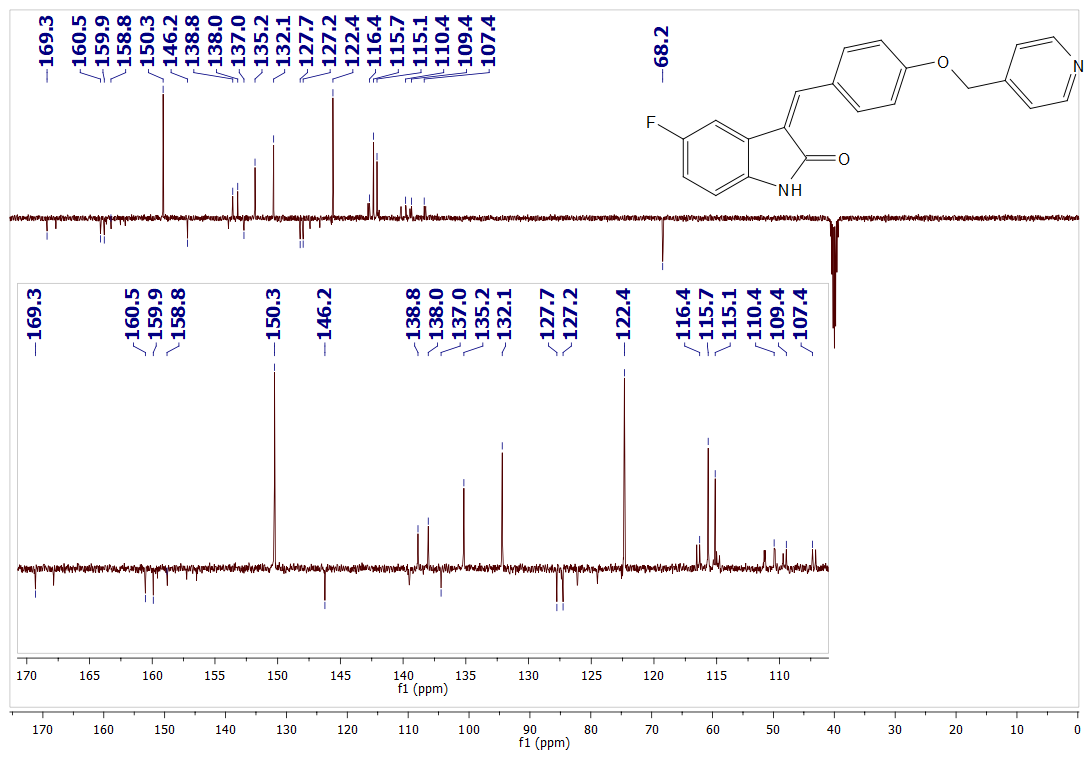


Figure S30. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5n.**

A screenshot of a graph

Description automatically generated

Figure S31. 1H NMR spectrum of compound (***E/Z***)-**5o.**

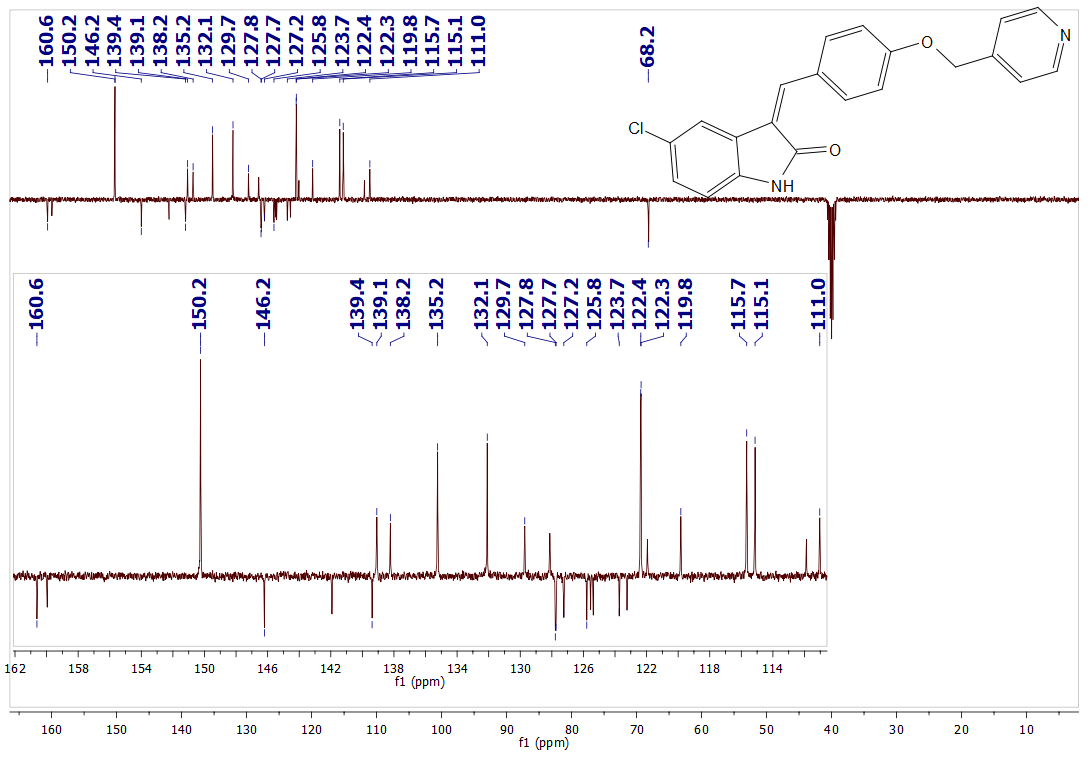


Figure S32. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5o.**

A graph of a chemical reaction

Description automatically generated with medium confidence

Figure S33. 1H NMR spectrum of compound (***E/Z***)-**5p.**

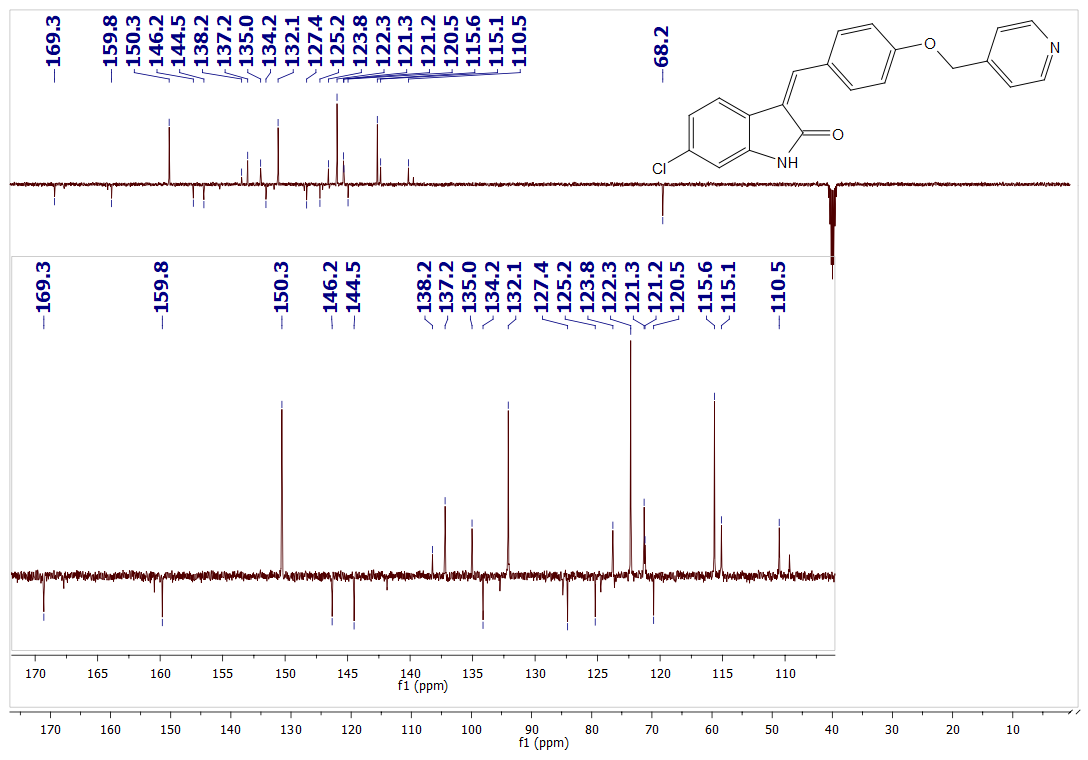


Figure S34. DEPTQ 13C NMR spectrum of compound (***E/Z***)-**5p.**