

Supporting Information

Synthesis of New trans-Ferulic Acid Derivatives as Potential Anticancer Agents and VEGFR-2 Inhibitors

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Supporting Information

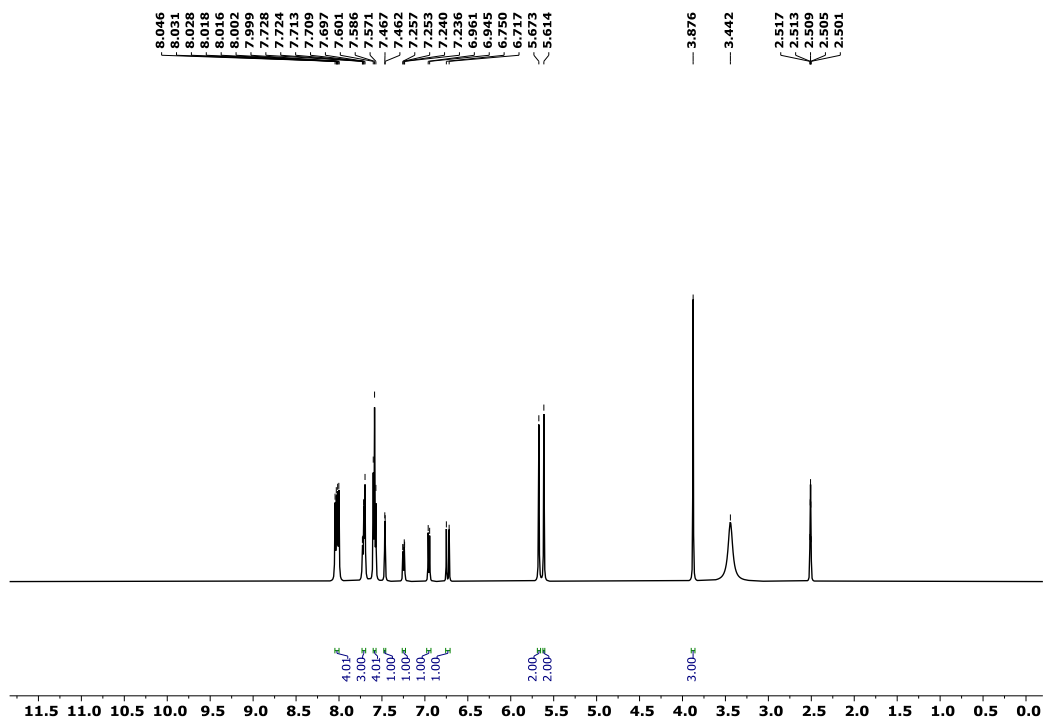


Figure S1. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound **4a**

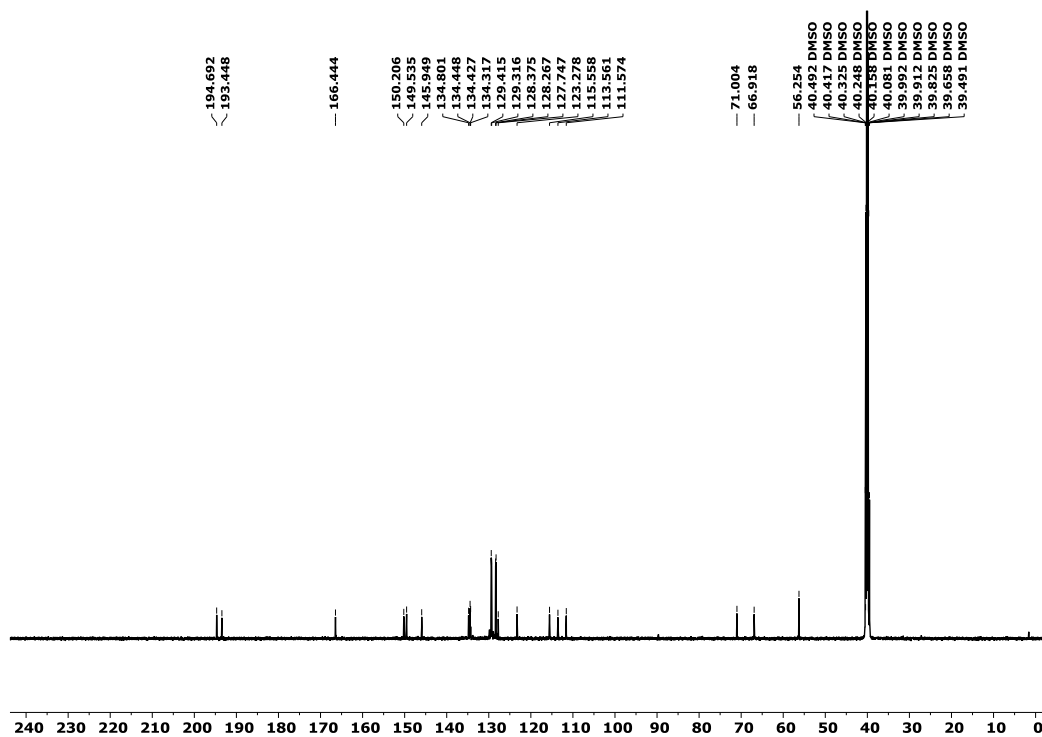


Figure S2. ¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of compound **4a**

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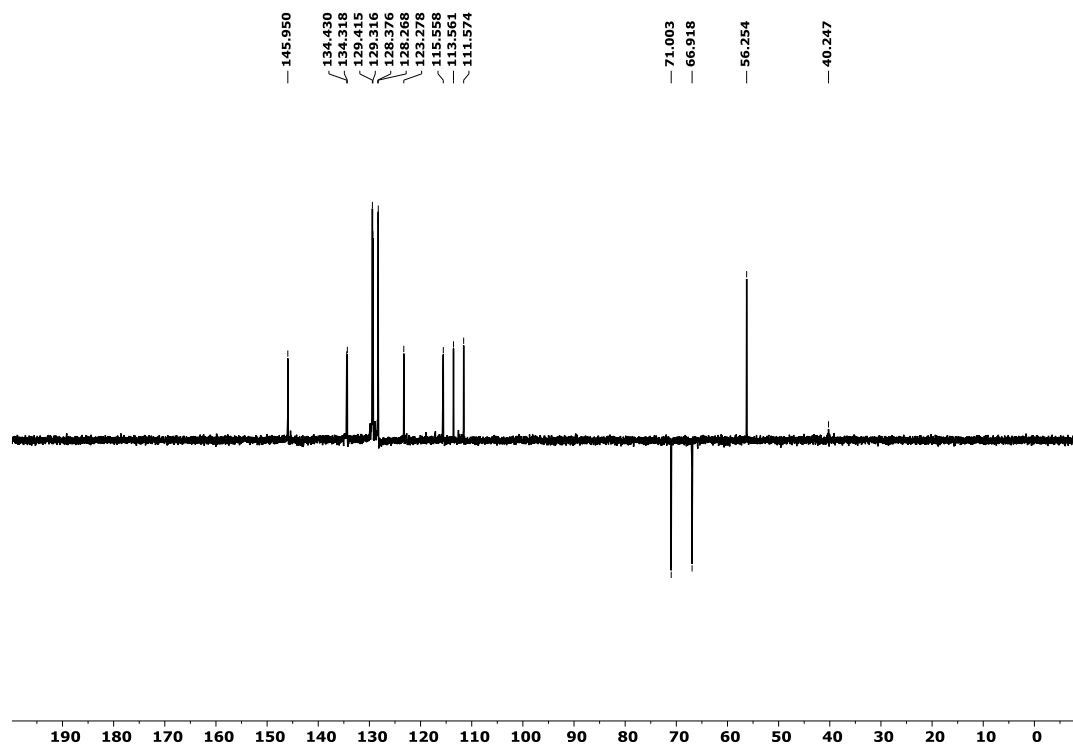


Figure S3. DEPT-135 (125 MHz, DMSO- d_6) spectrum of compound **4a**

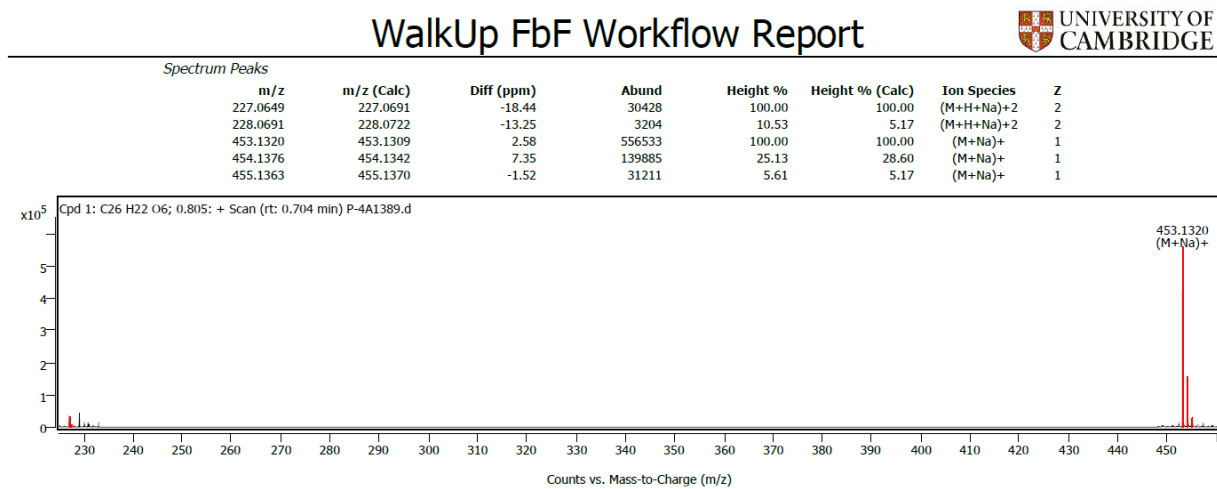


Figure S4. High-resolution mass spectrum of compound **4a**

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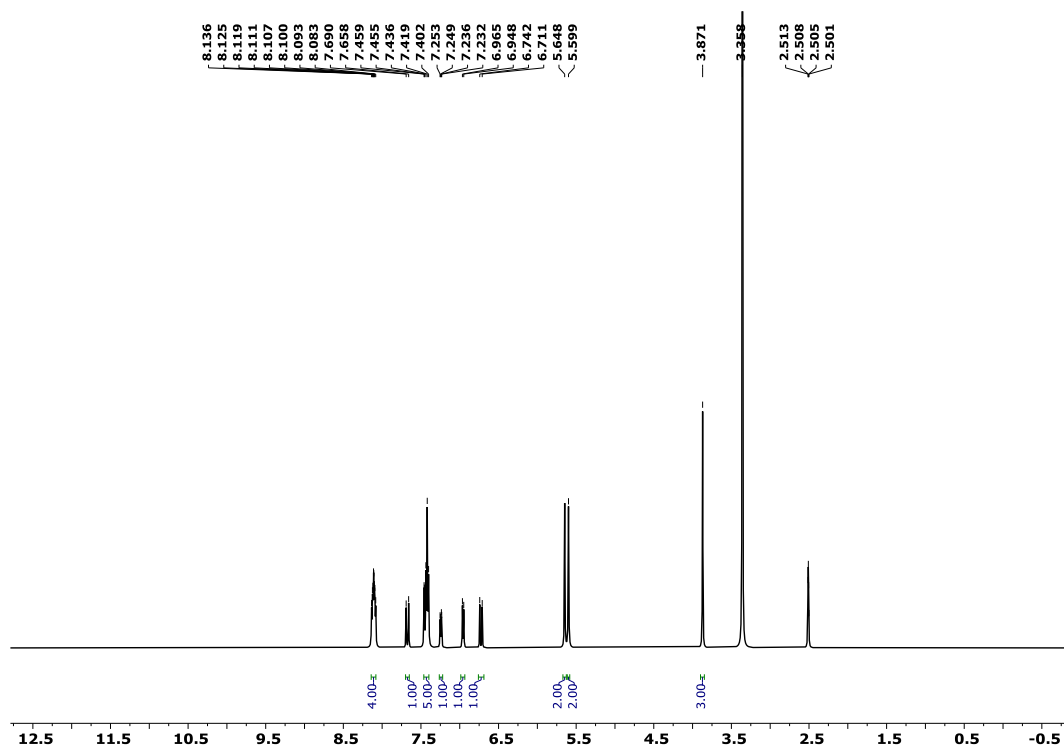


Figure S5. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound **4b**

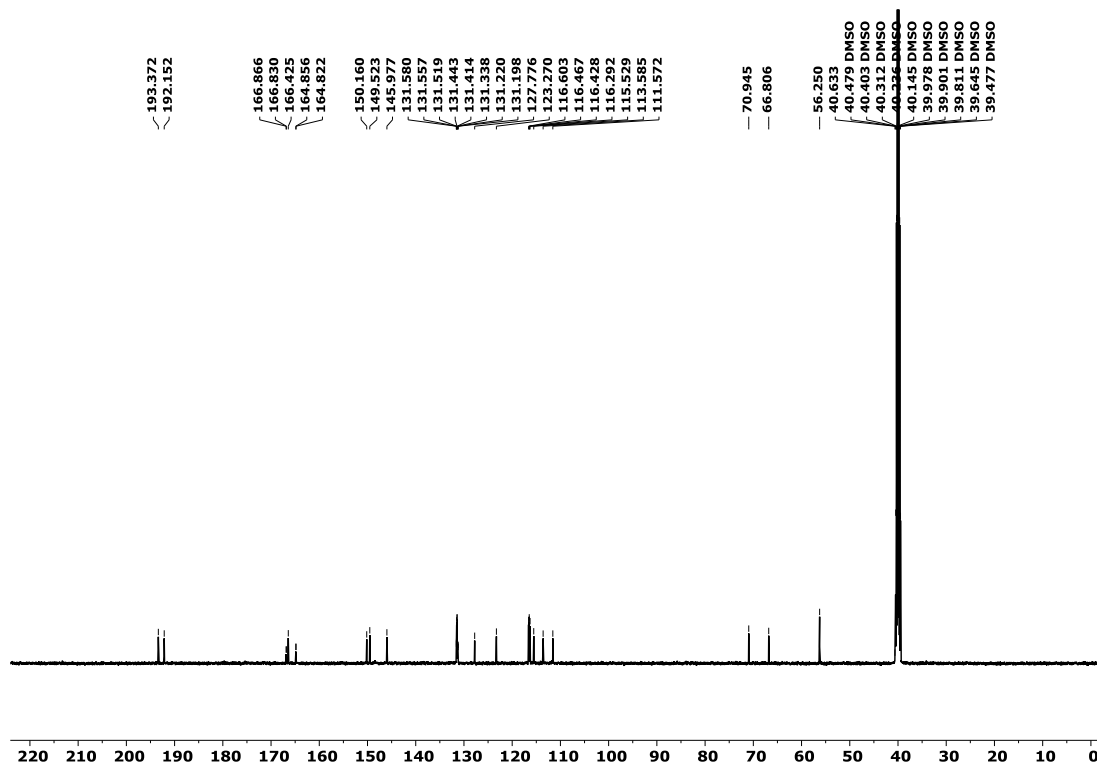


Figure S6. ¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of compound **4b**

Supporting Information

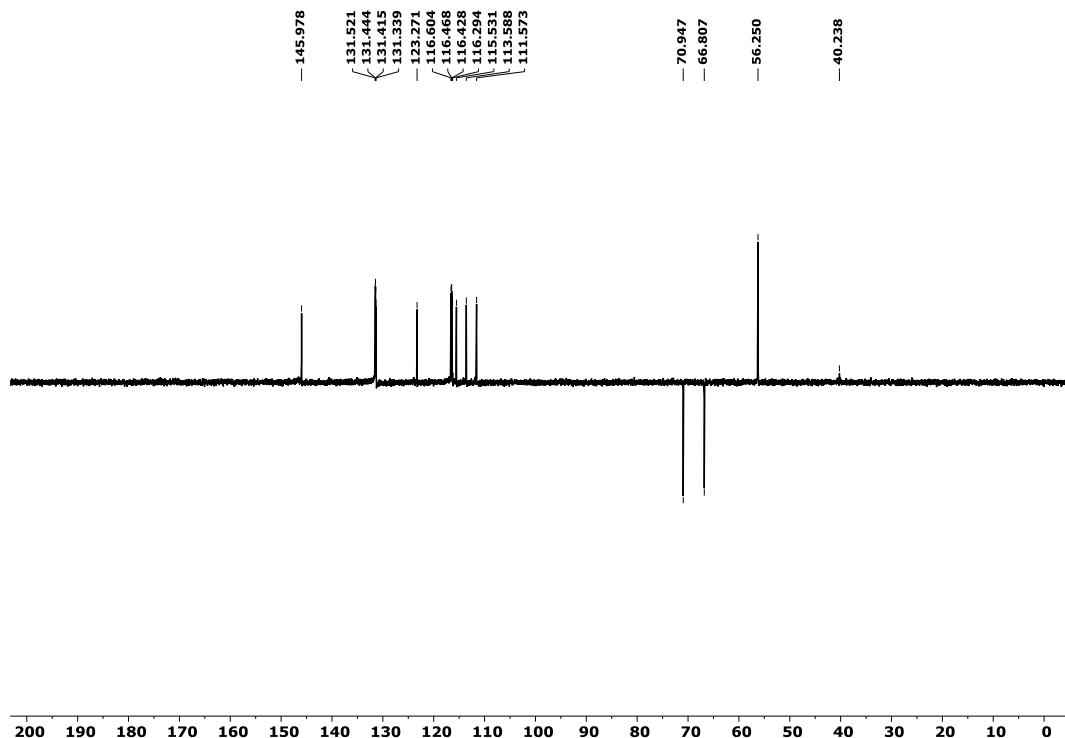


Figure S7. DEPT-135 (125 MHz, DMSO- d_6) spectrum of compound **4b**

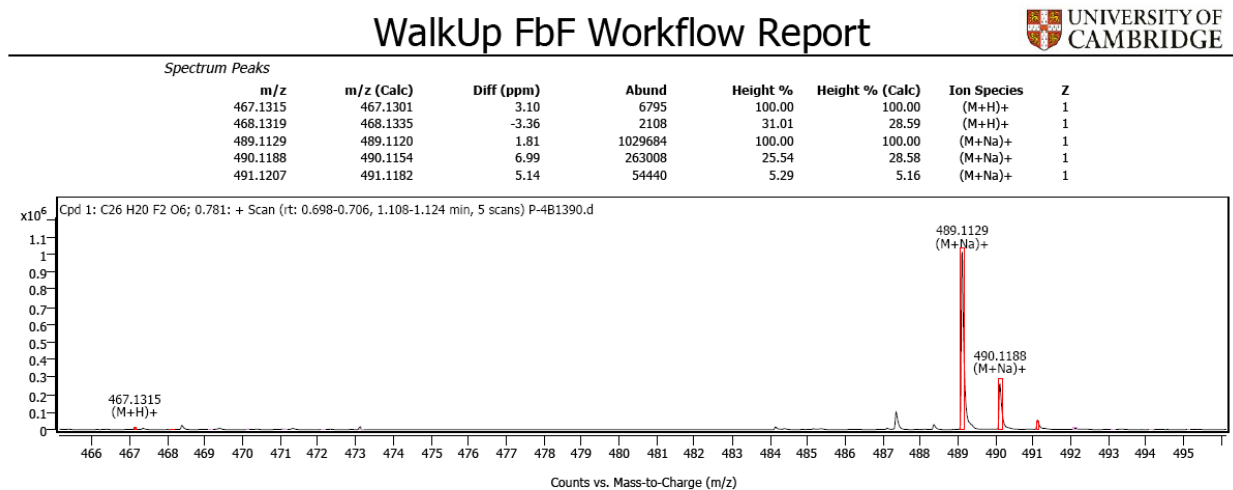


Figure S8. High-resolution mass spectrum of compound **4b**

Supporting Information

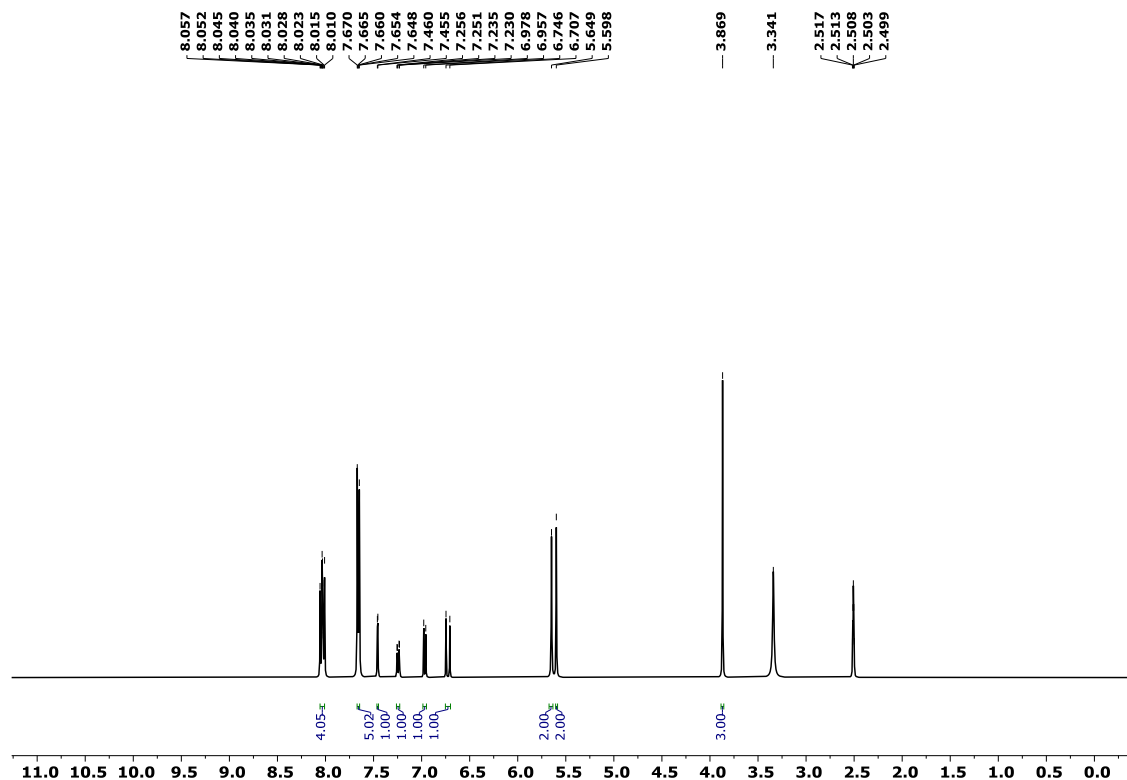


Figure S9. ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of compound **4c**

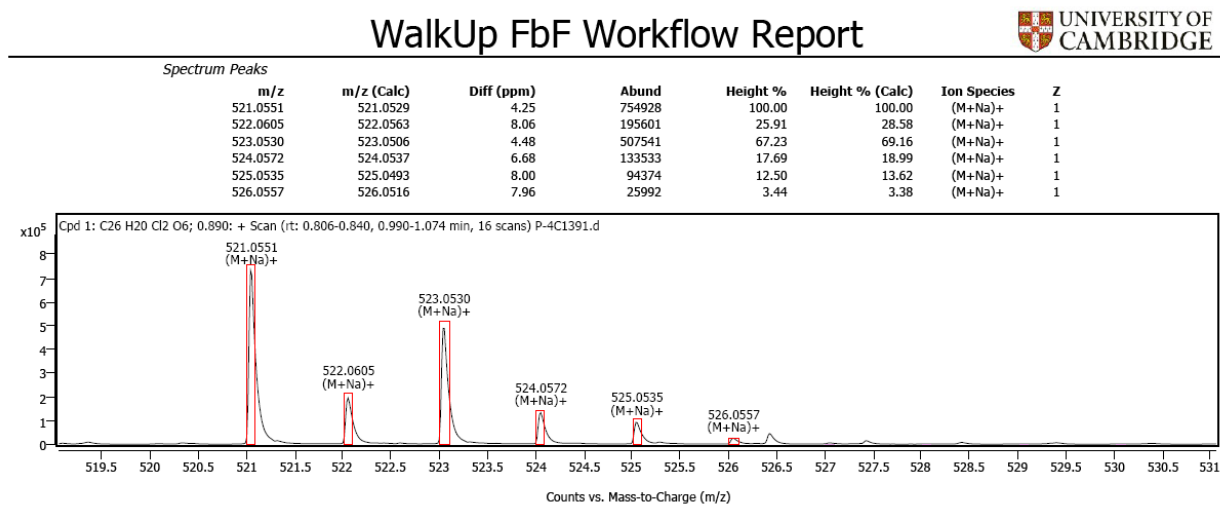


Figure S10. High-resolution mass spectrum of compound **4c**

Supporting Information

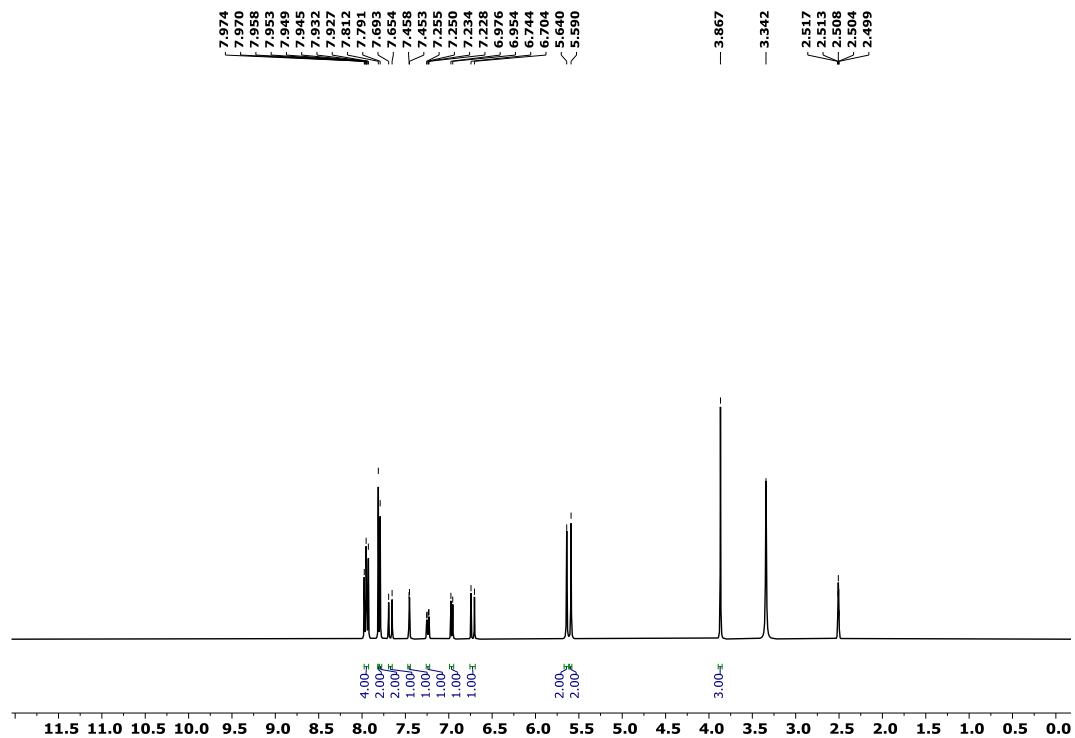


Figure S11. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound **4d**

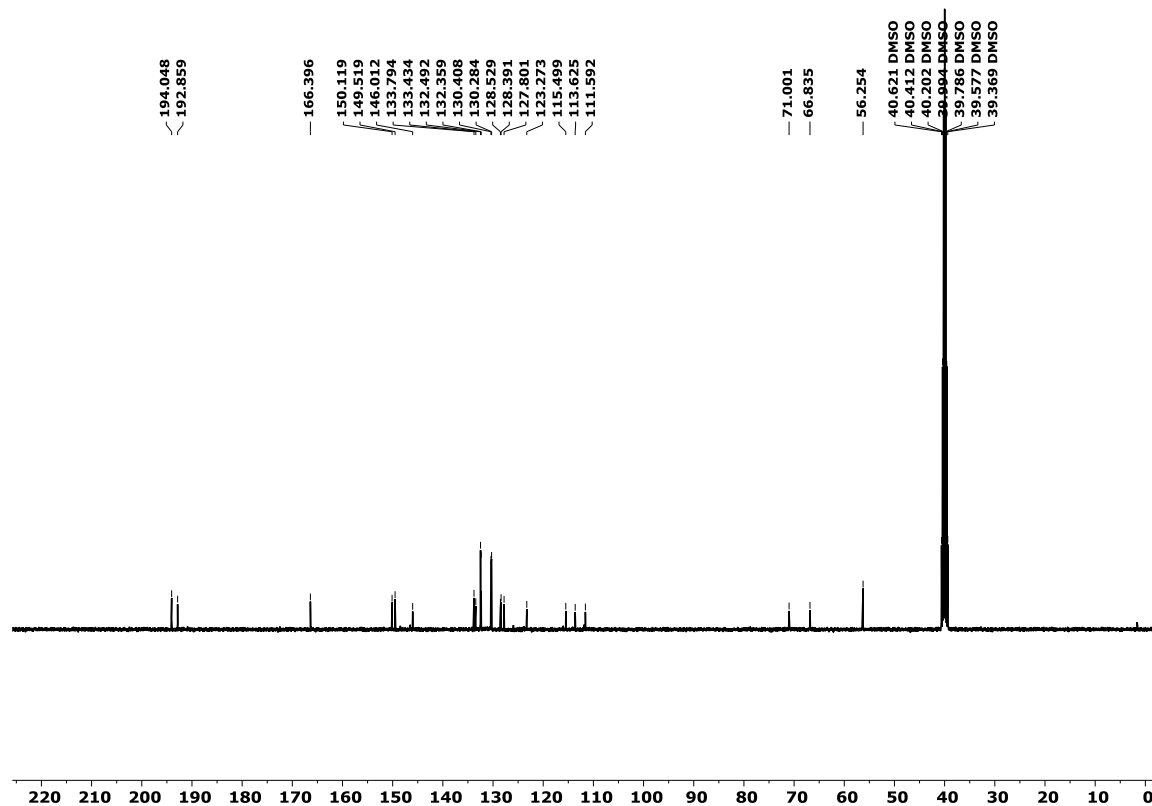


Figure S12. ¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of compound **4d**

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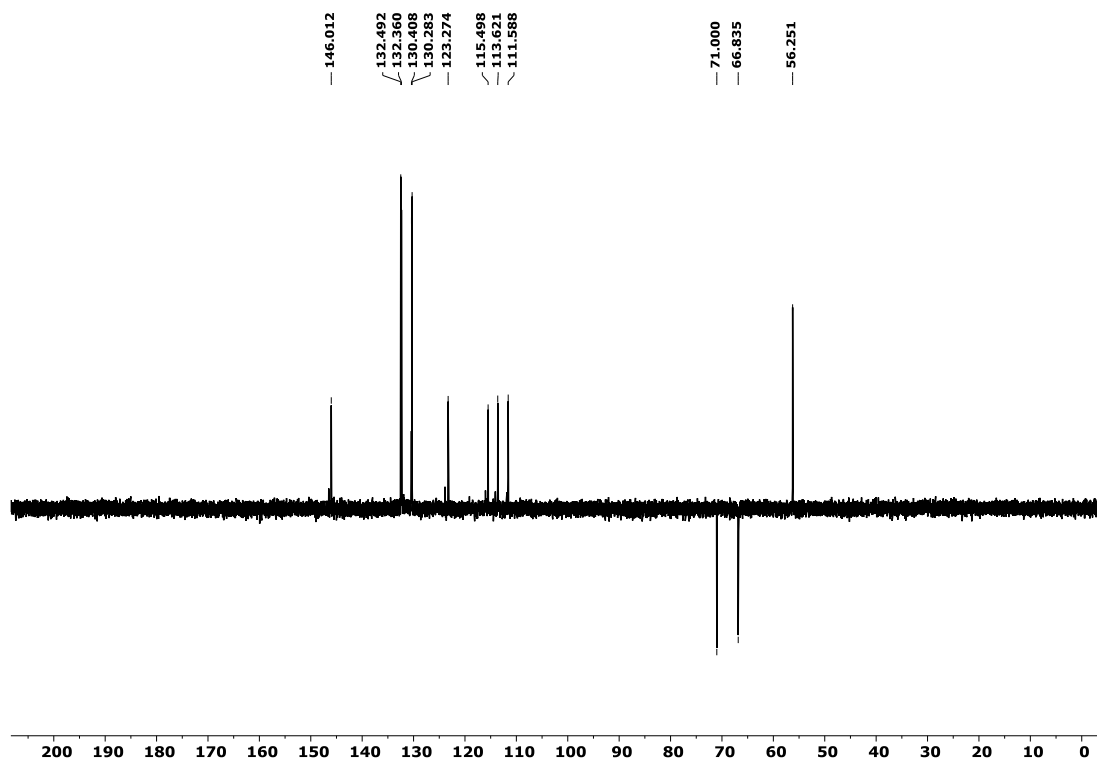


Figure S13. DEPT-135 (125 MHz, DMSO- d_6) spectrum of compound **4d**

WalkUp FbF Workflow Report

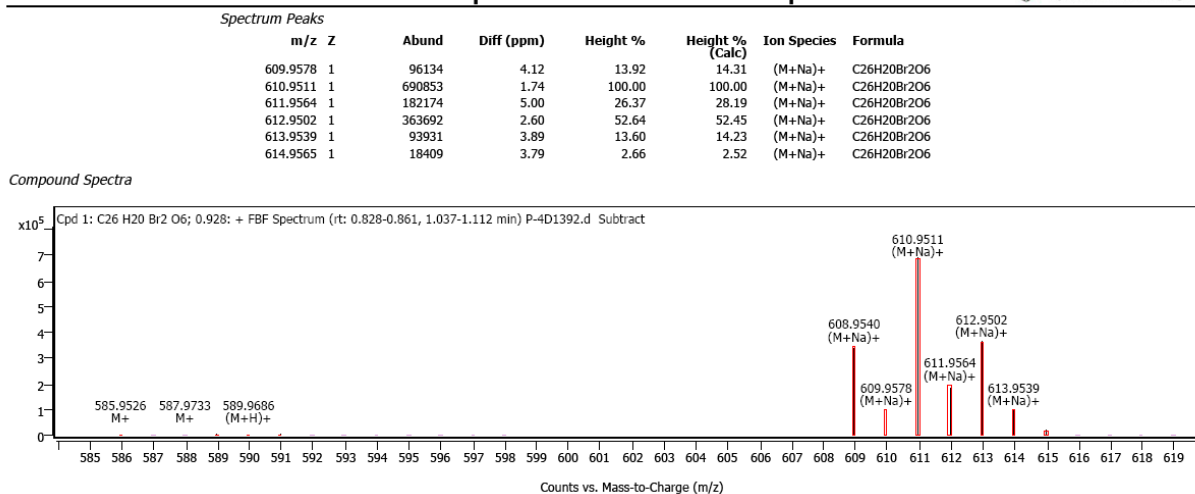


Figure S14. High-resolution mass spectrum of compound **4d**

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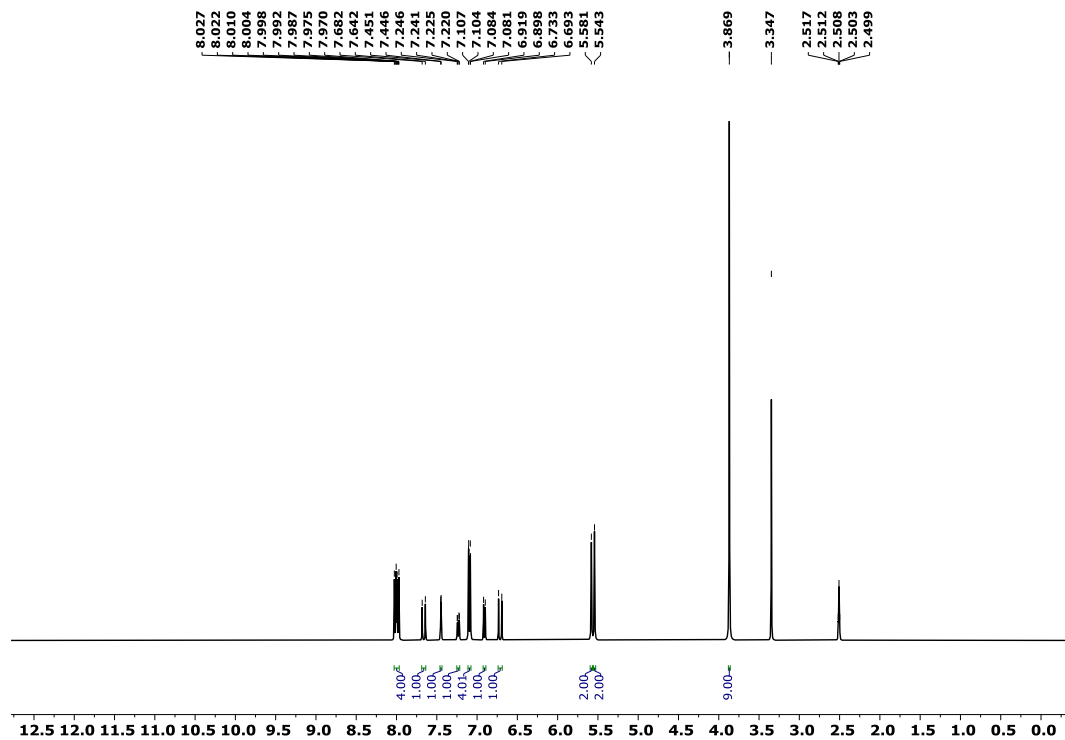


Figure S15. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound 4e

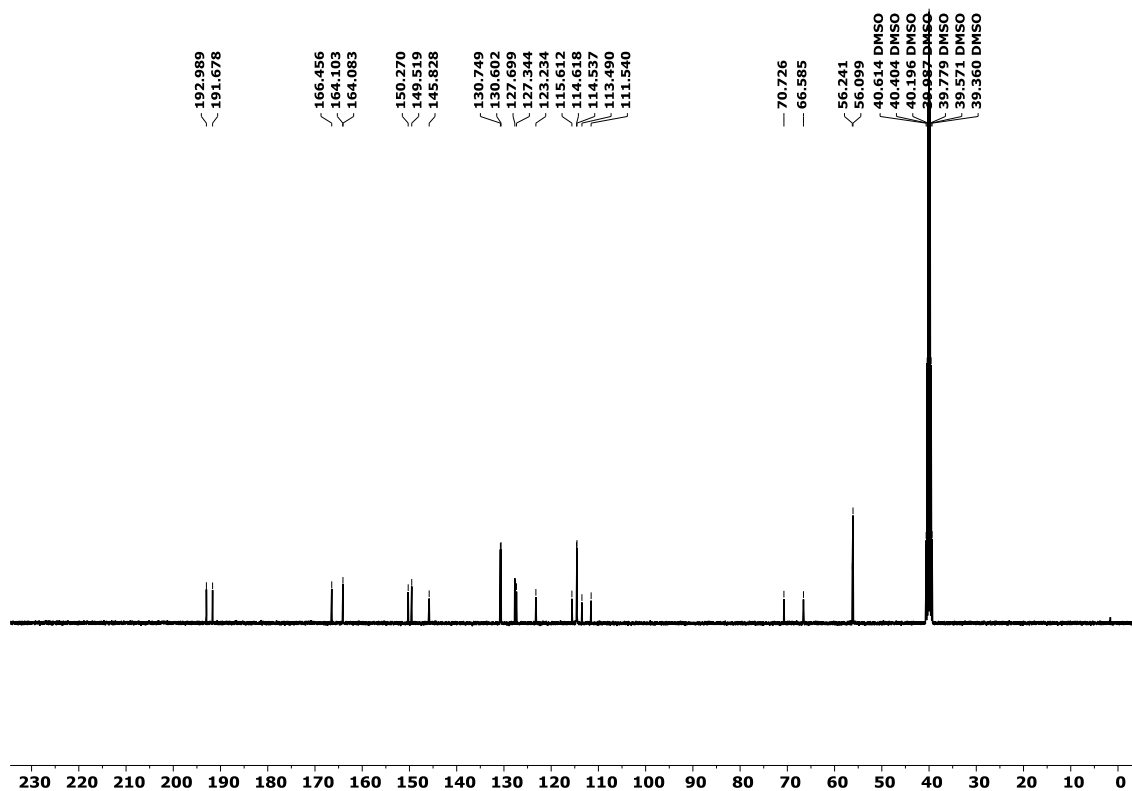


Figure S16. ¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of compound 4e

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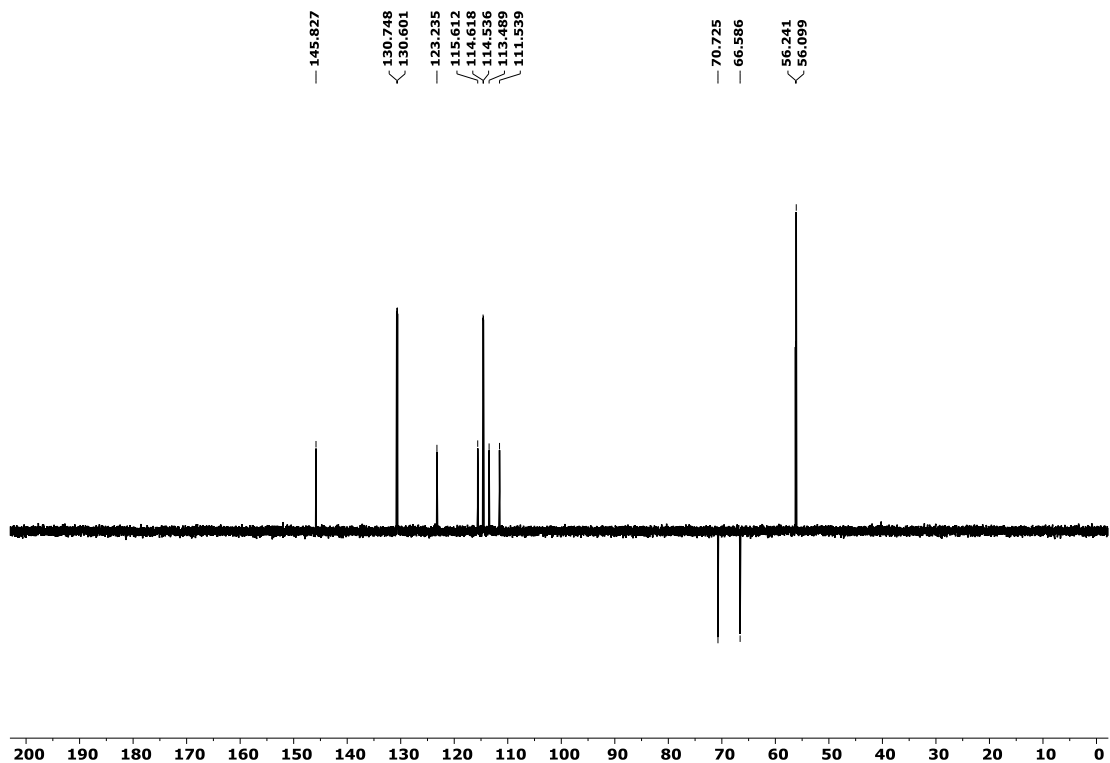


Figure S17. DEPT-135 (125 MHz, DMSO- d_6) spectrum of compound **4e**

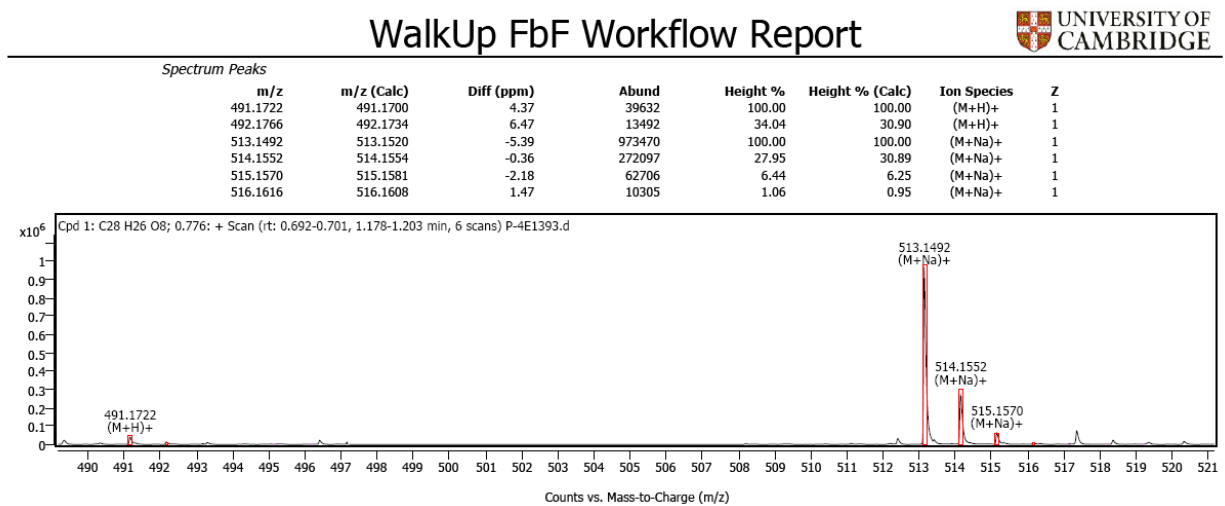


Figure S18. High-resolution mass spectrum of compound **4e**

¹³C NMR spectrum (DMSO-d₆) of compound 10. The x-axis represents the chemical shift in ppm, ranging from 0 to 220. The spectrum shows several sharp peaks. A large peak is at 39.903 ppm, labeled as DMSO. Other peaks are labeled with their chemical shifts: 166.848, 150.476, 149.743, 145.482, 137.215, 136.814, 128.934, 128.912, 128.581, 128.517, 128.412, 128.309, 127.596, 123.360, 115.948, 113.524, 111.183, 70.265, 65.917, and 56.151. The peak at 56.151 ppm is also labeled as DMSO.

11

Supporting Information

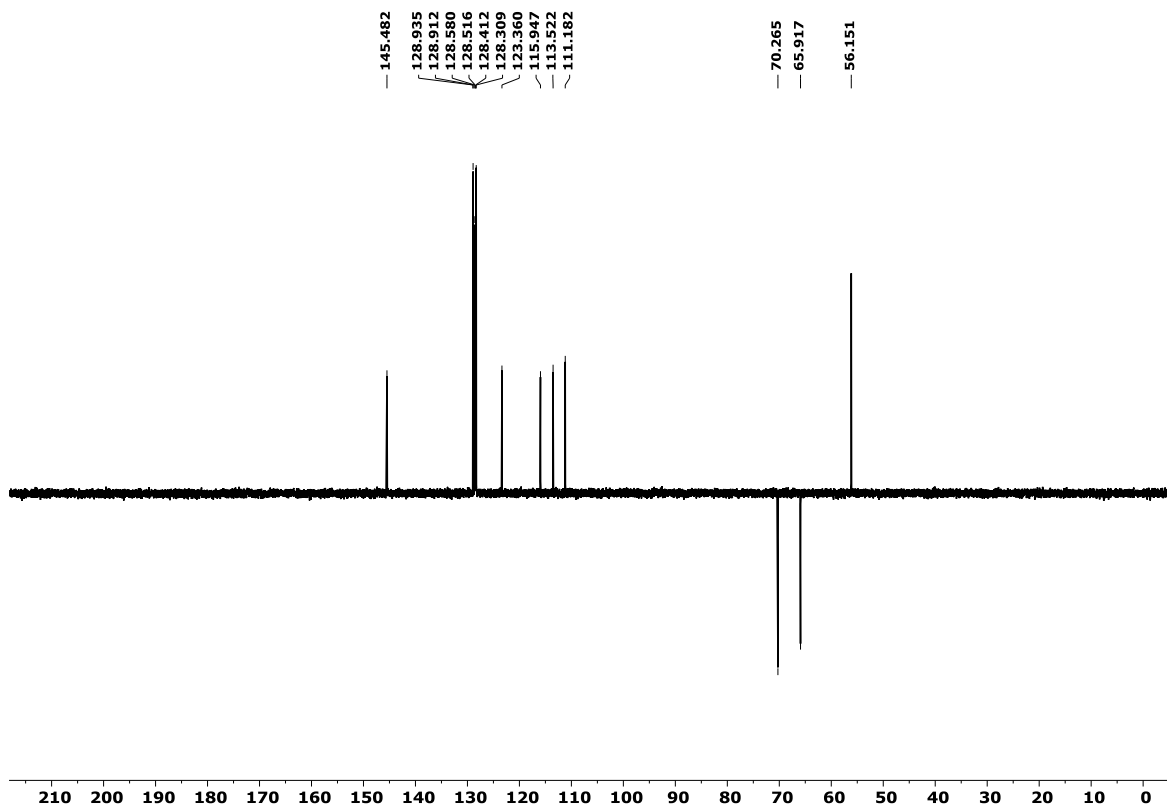


Figure S21. DEPT-135 (125 MHz, DMSO- d_6) spectrum of compound 6

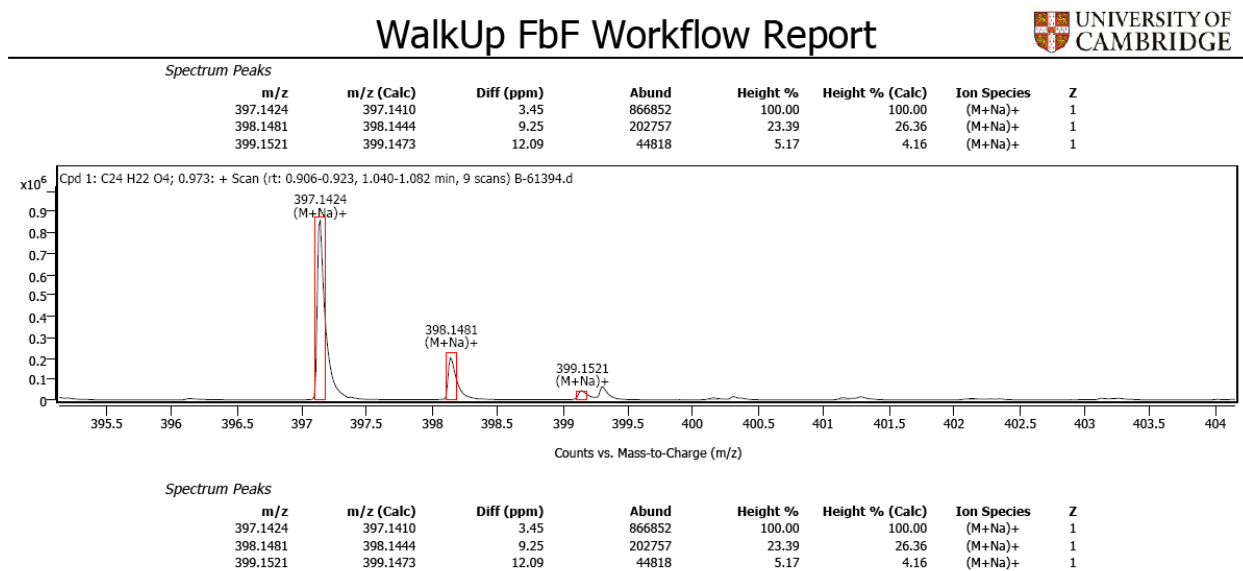


Figure S22. High-resolution mass spectrum of compound 6

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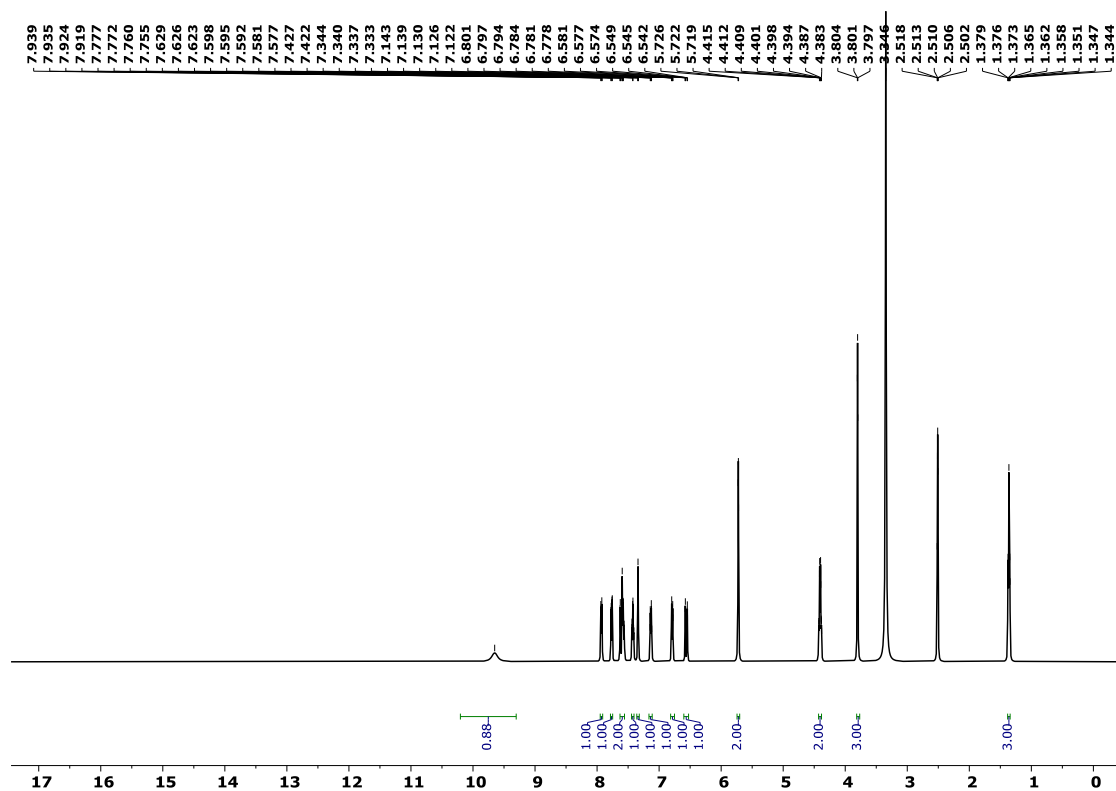


Figure S23. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound 12

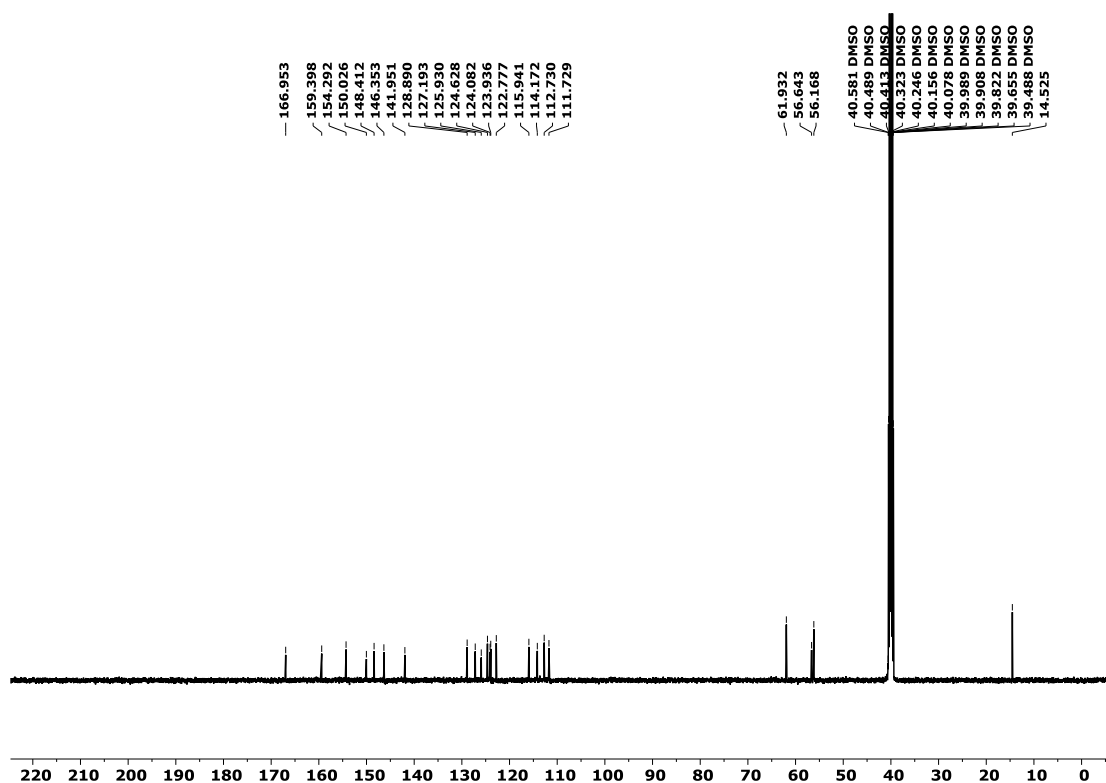


Figure S24. ¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of compound 12

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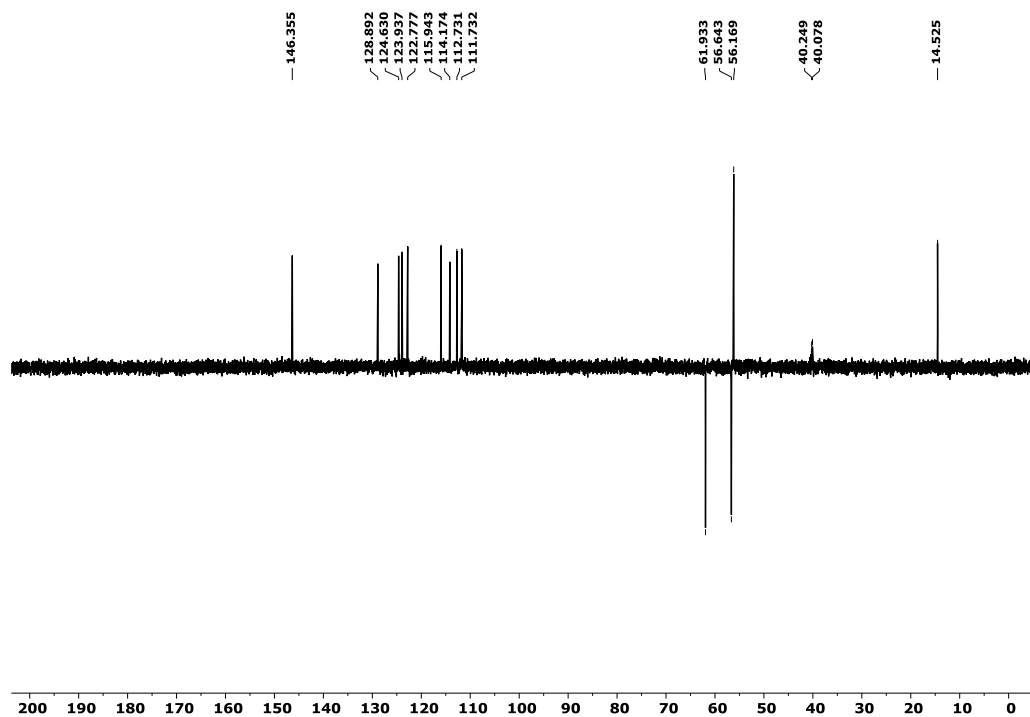


Figure S25. DEPT-135 (125 MHz, DMSO- d_6) spectrum of compound **12**

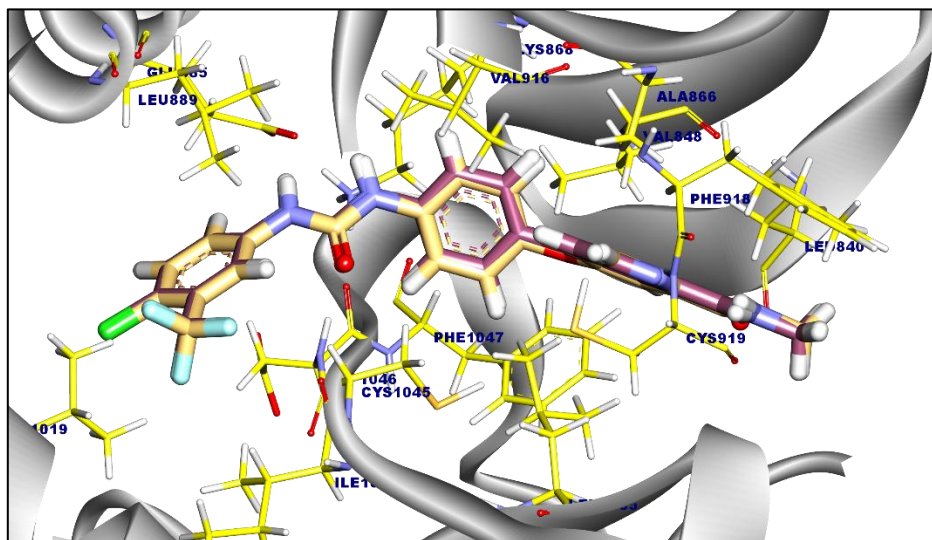


Figure S26. Superimposition of the co-crystallized ligand (sorafenib) complexed with VEGFR-2 TK. Original pose of Sorafenib colored by (dark purple), and the redocked pose colored by (faint brown) with RMSD value equal 0.15 Å.

Supporting Information

References

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