

## **Anti-breast cancer sinomenine derivatives via mechanisms of apoptosis induction and metastasis reduction**

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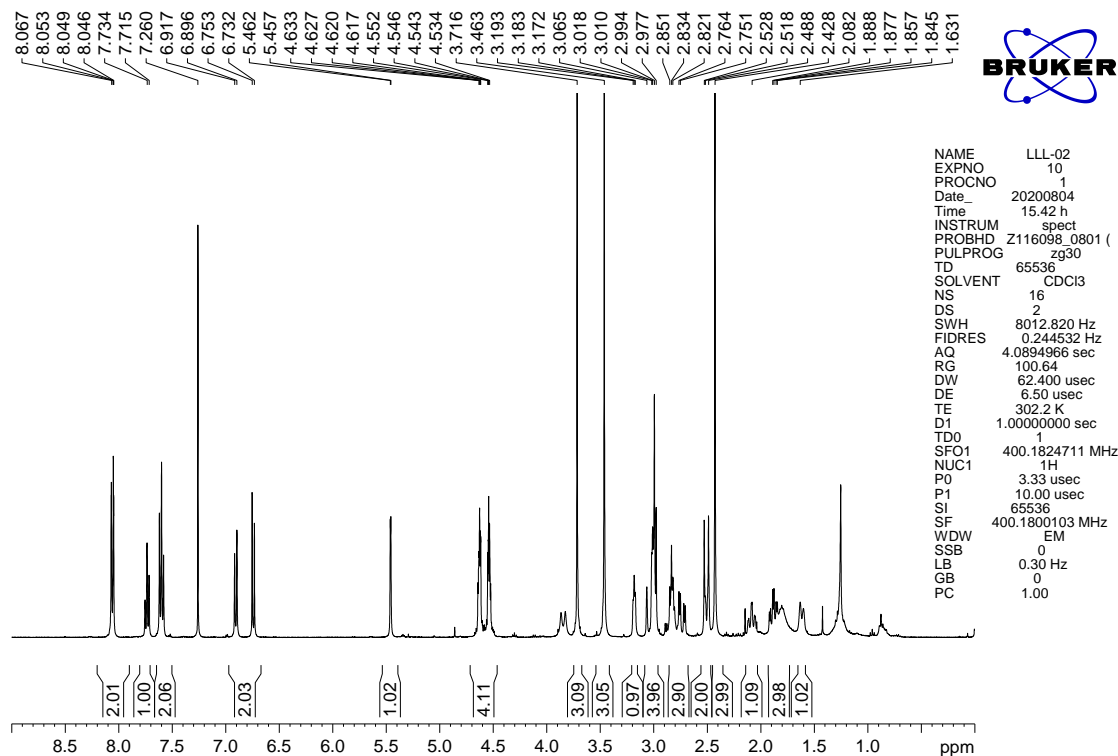


Figure S1.  $^1\text{H}$  NMR of compound **7Aa**

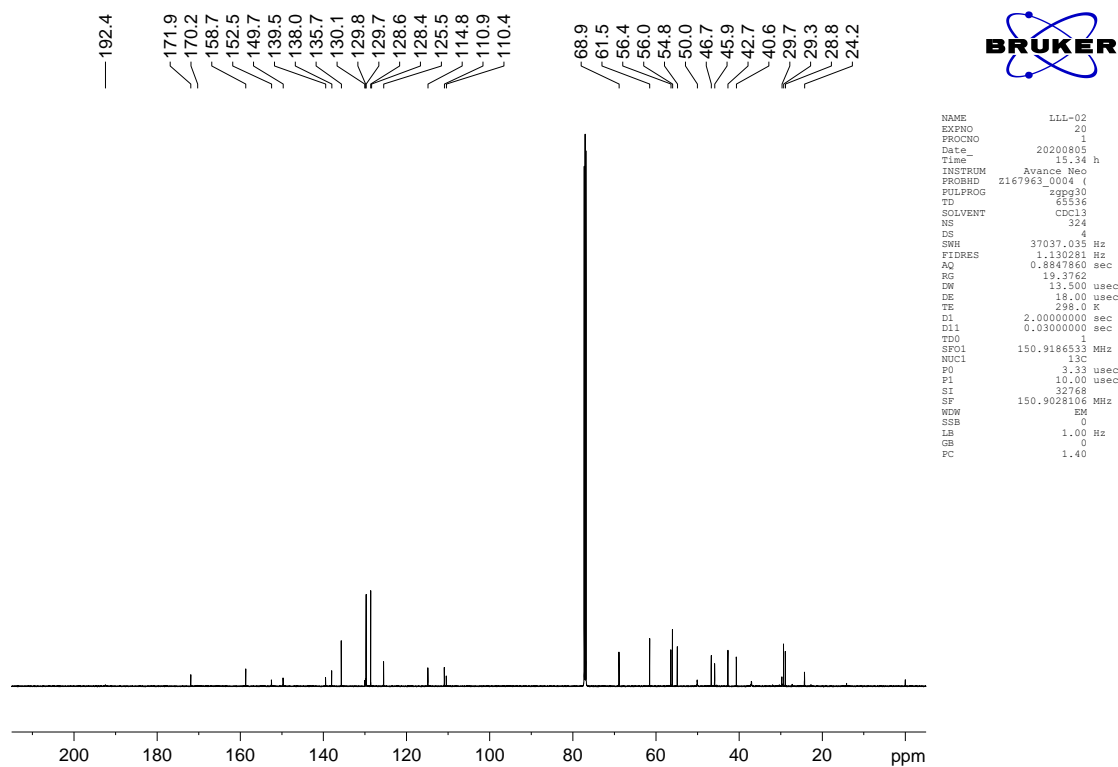


Figure S2.  $^{13}\text{C}$  NMR of compound **7Aa**

+MS, 0.7min #86

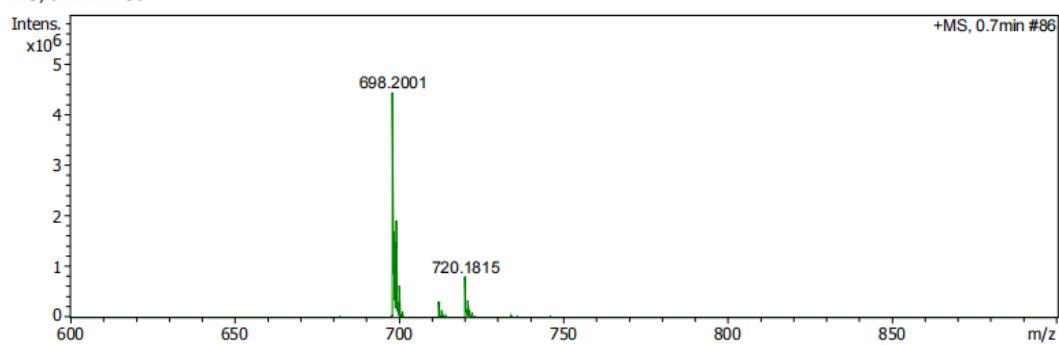


Figure S3. HRESIMS of compound 7Aa

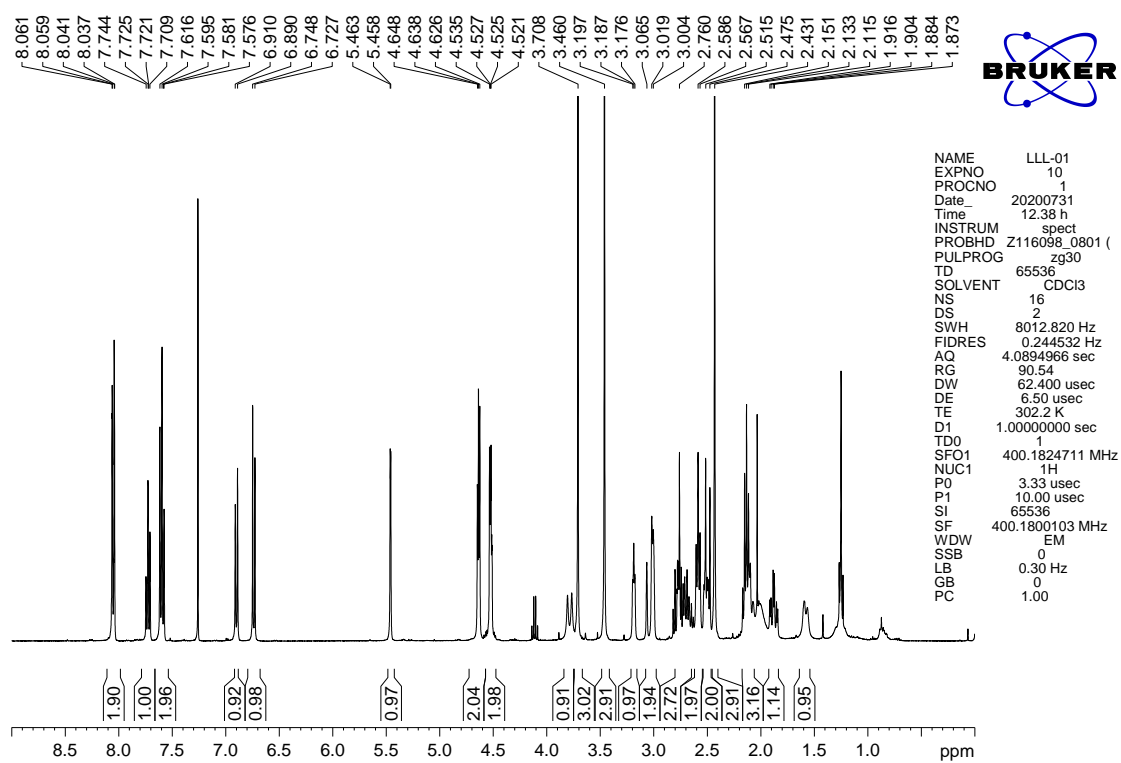


Figure S4. <sup>1</sup>H NMR of compound 7Ab

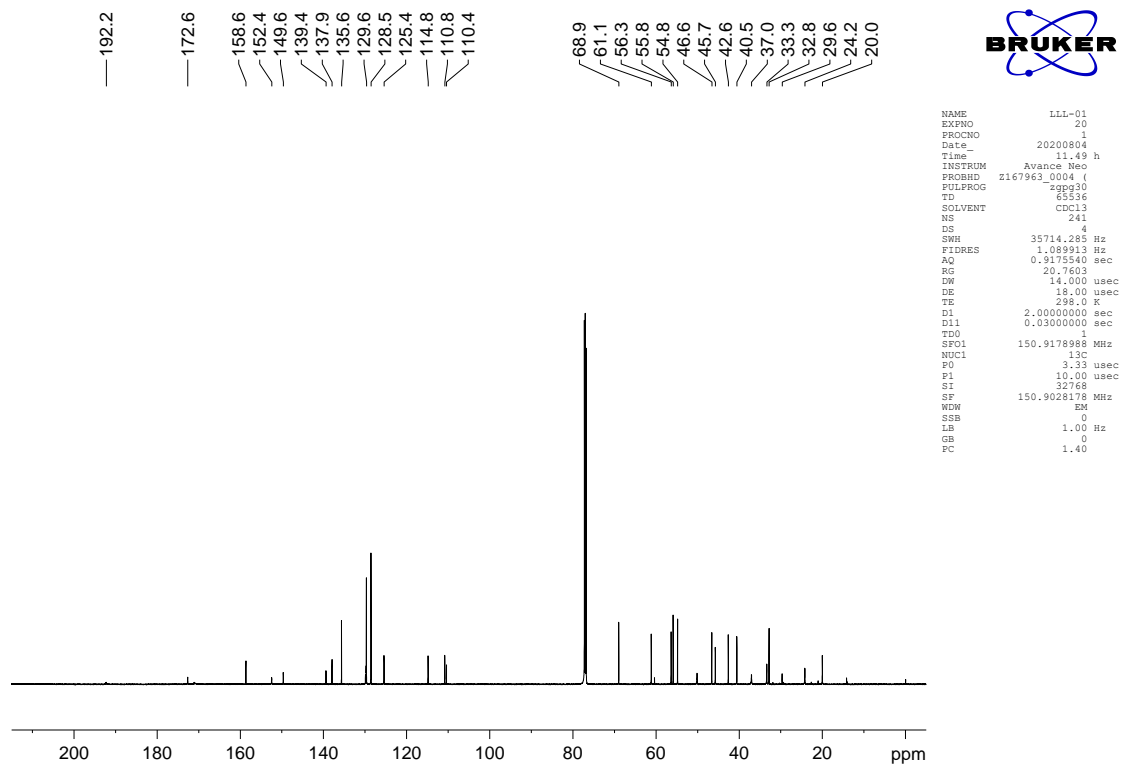


Figure S5. <sup>13</sup>C NMR of compound **7Ab**

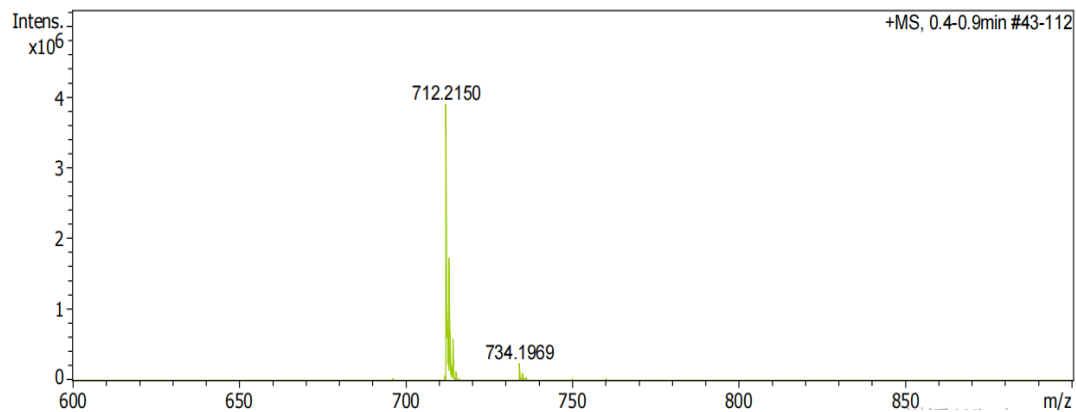


Figure S6. HRESIMS of compound **7Ab**

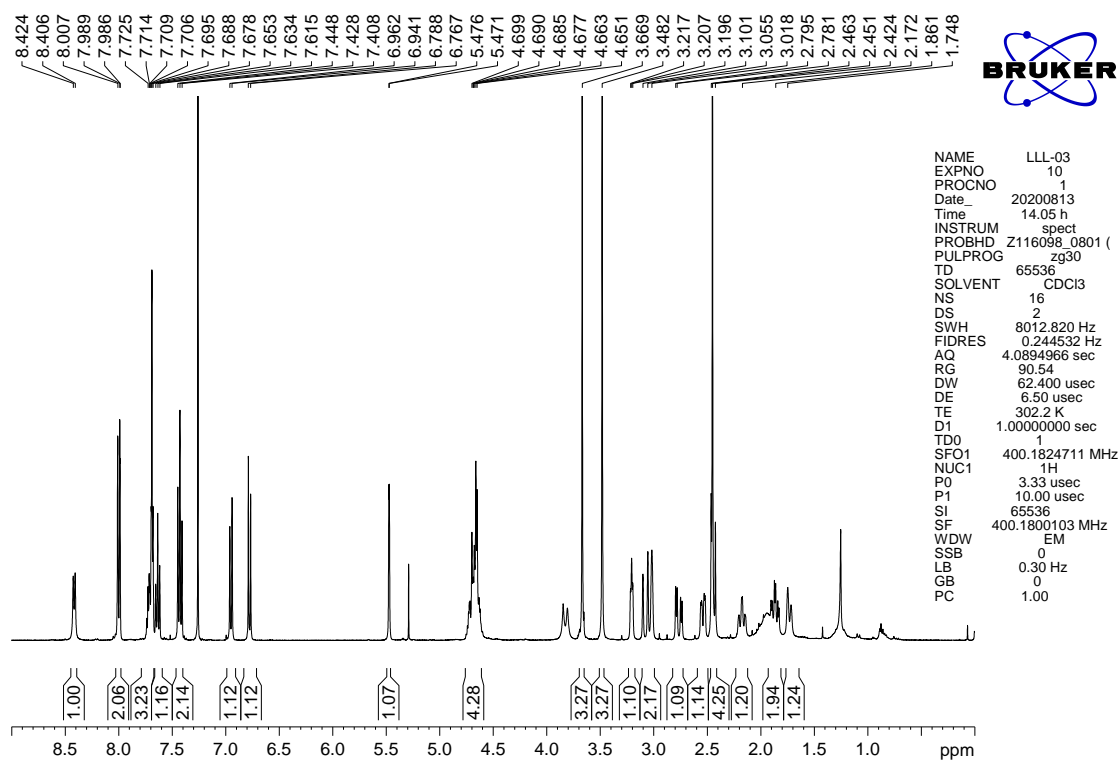


Figure S7.  $^1\text{H}$  NMR of compound **7Ac**

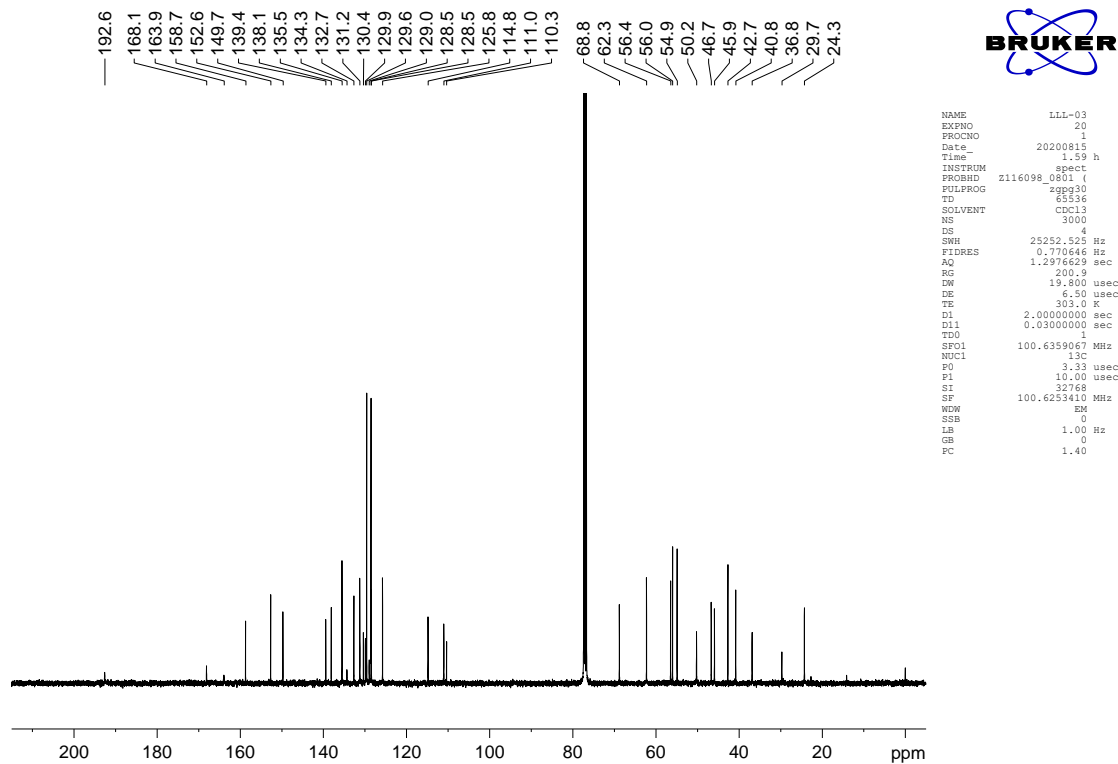


Figure S8.  $^{13}\text{C}$  NMR of compound **7Ac**

+MS, 0.8min #91

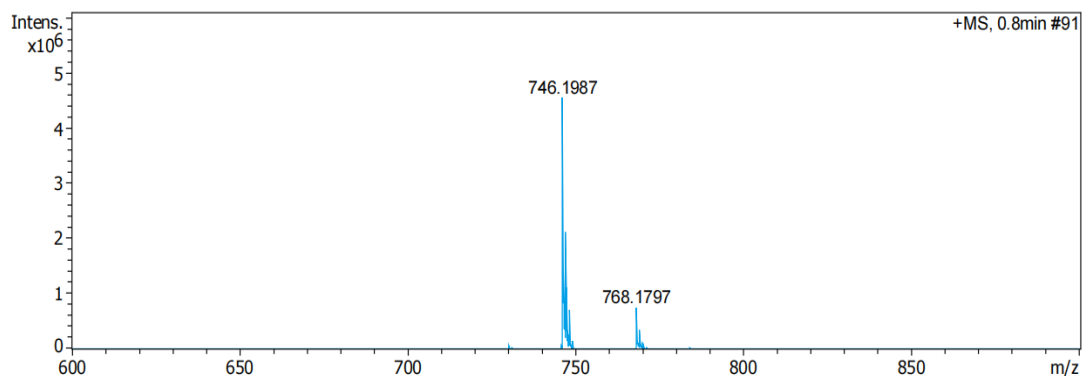


Figure S9. HRESIMS of compound 7Ac

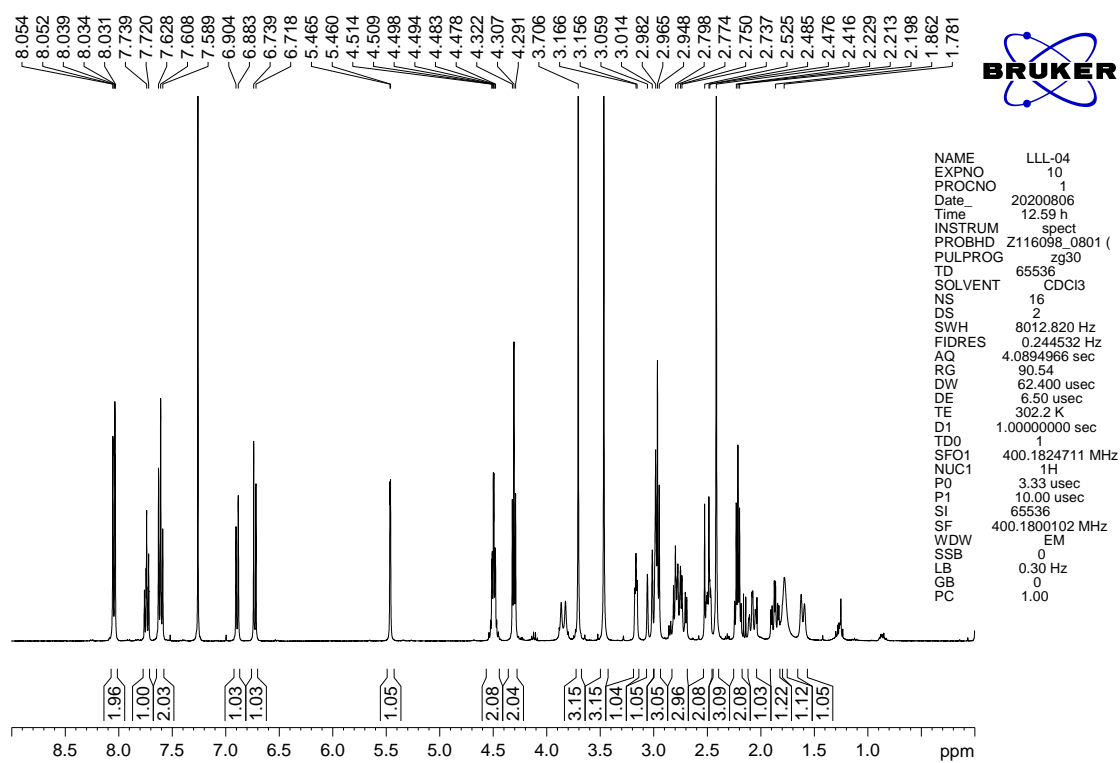


Figure S10. <sup>1</sup>H NMR of compound 7Ba

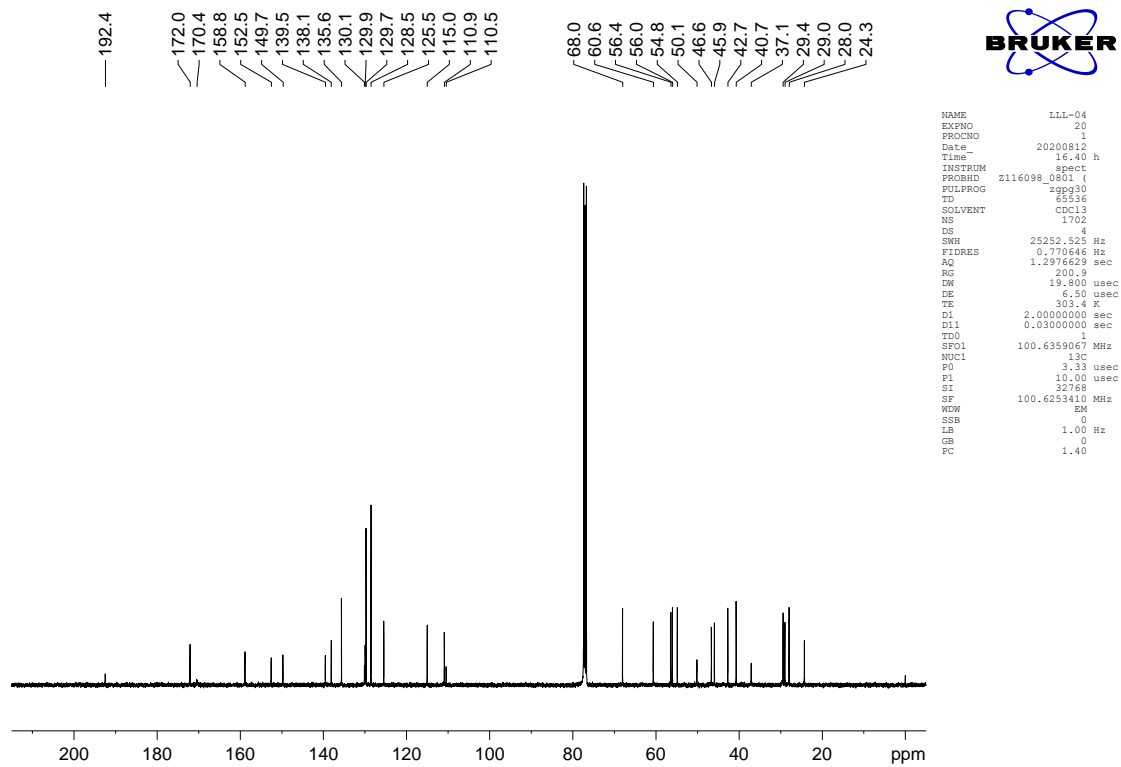


Figure S11.  $^{13}\text{C}$  NMR of compound **7Ba**

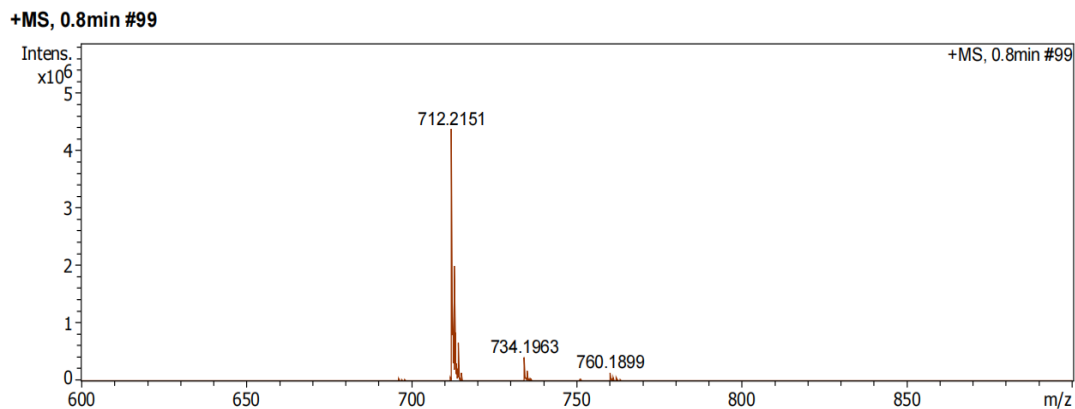


Figure S12. HRESIMS of compound **7Ba**

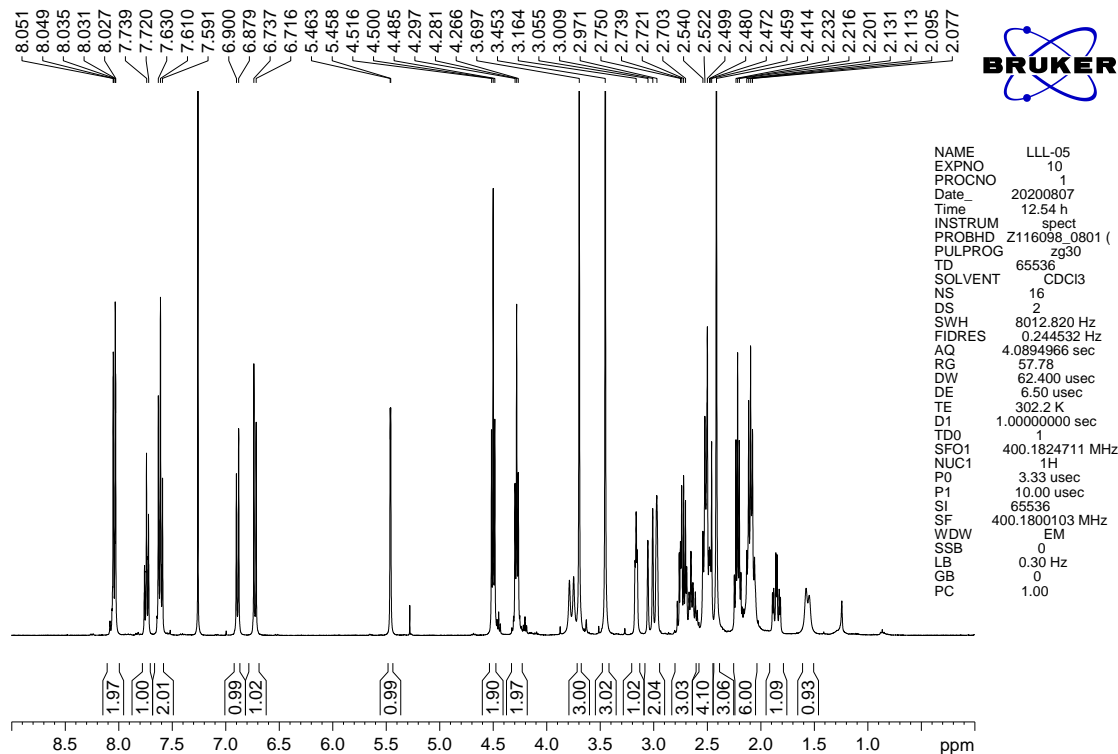


Figure S13. <sup>1</sup>H NMR of compound 7Bb

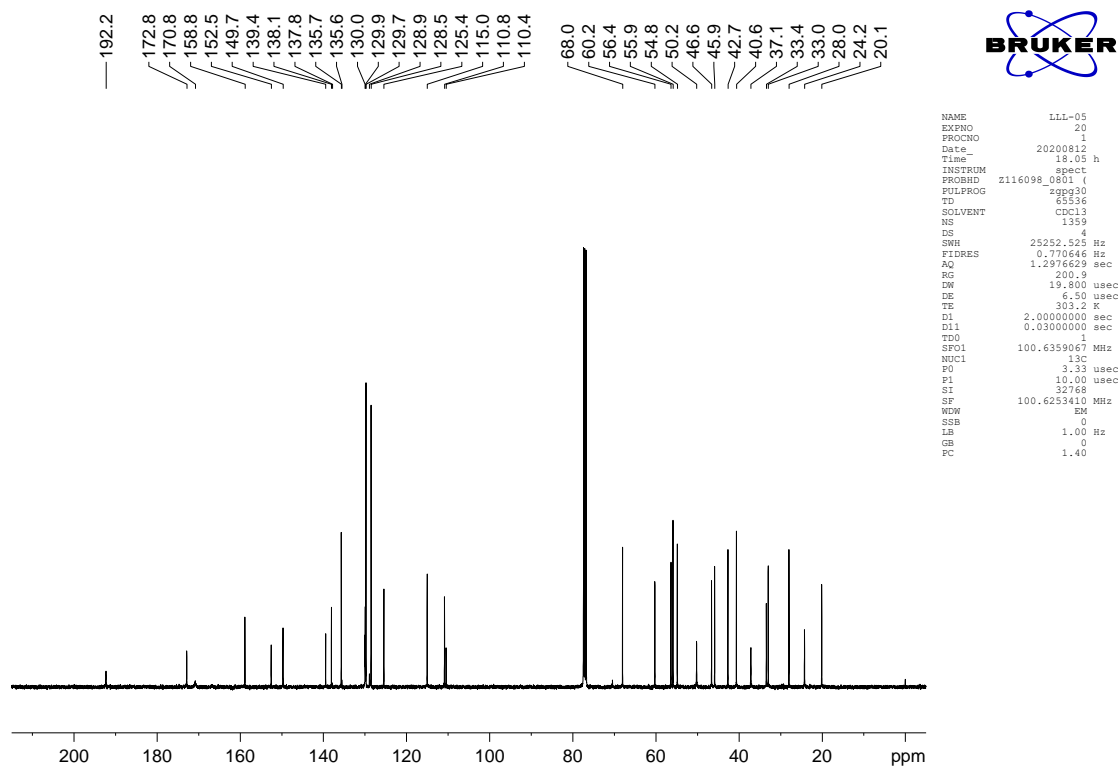


Figure S14. <sup>13</sup>C NMR of compound 7Bb



+MS, 0.8min #98

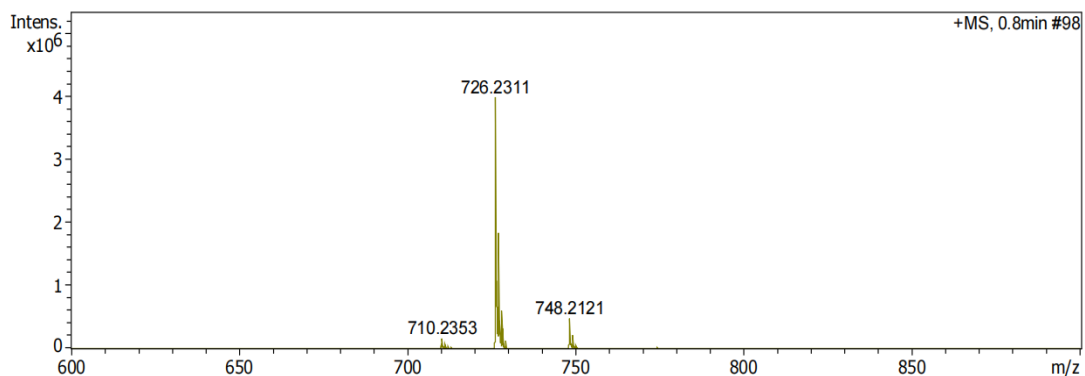


Figure S15. HRESIMS of compound **7Bb**

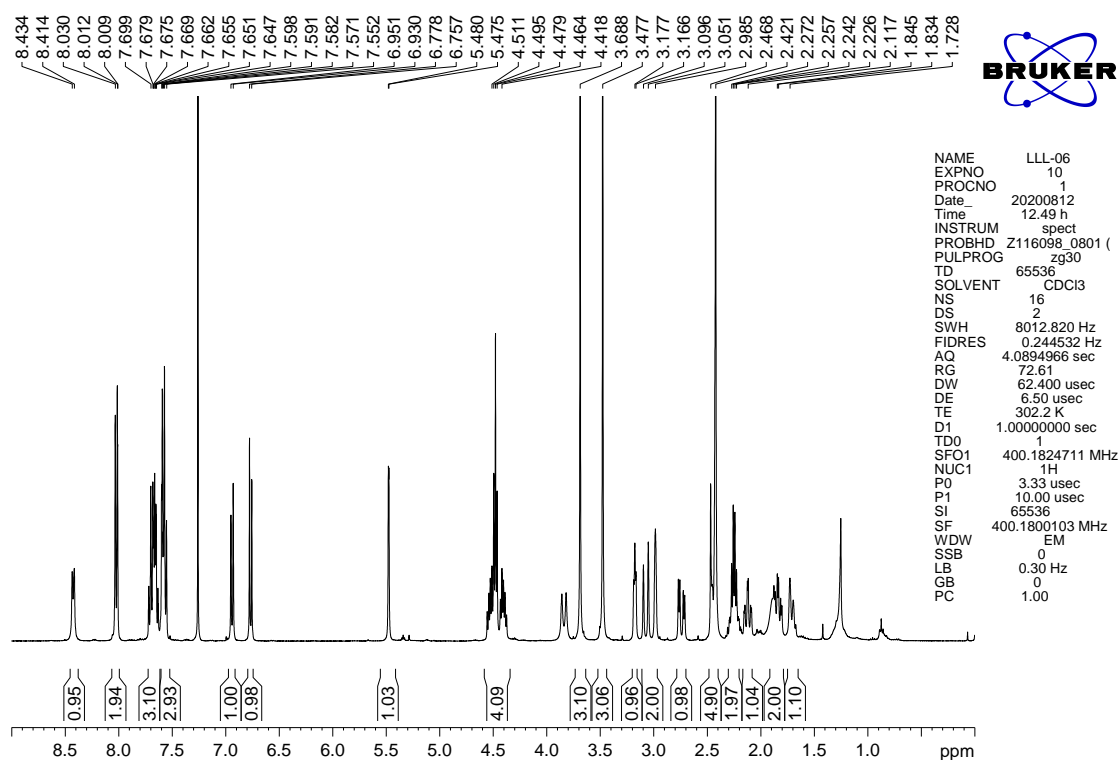


Figure S16. <sup>1</sup>H NMR of compound **7Bc**

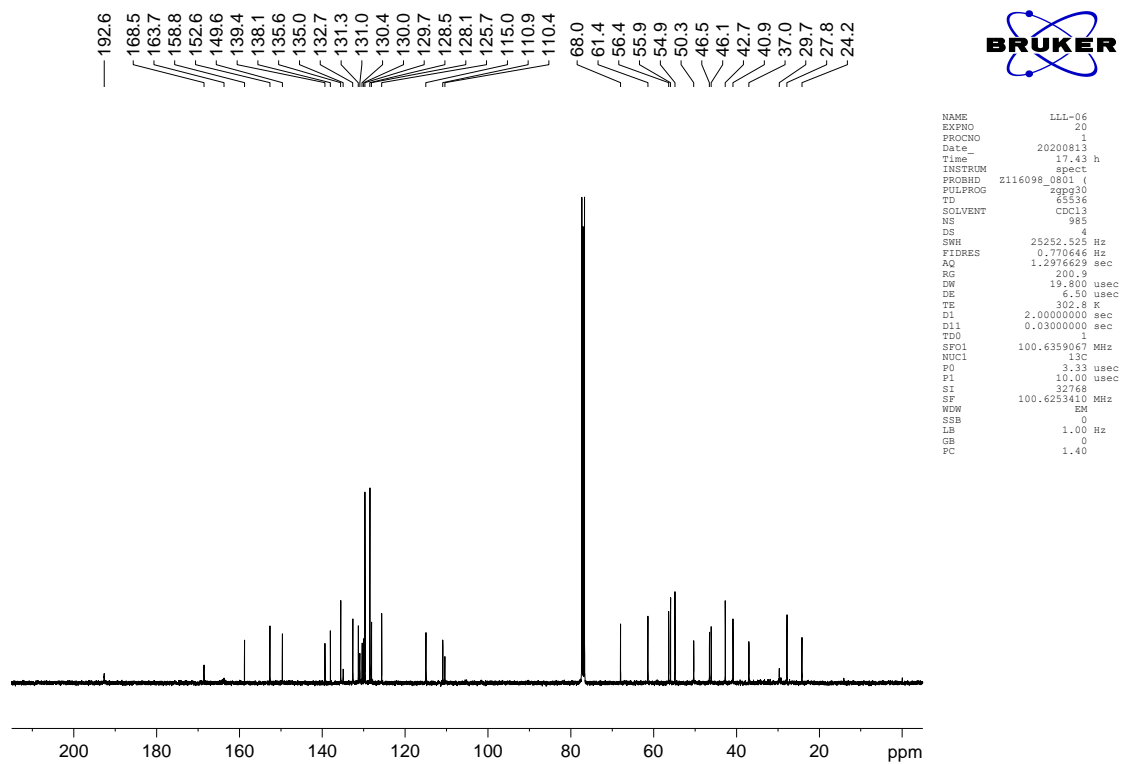


Figure S17. <sup>13</sup>C NMR of compound **7Bc**

+MS, 0.9min #103

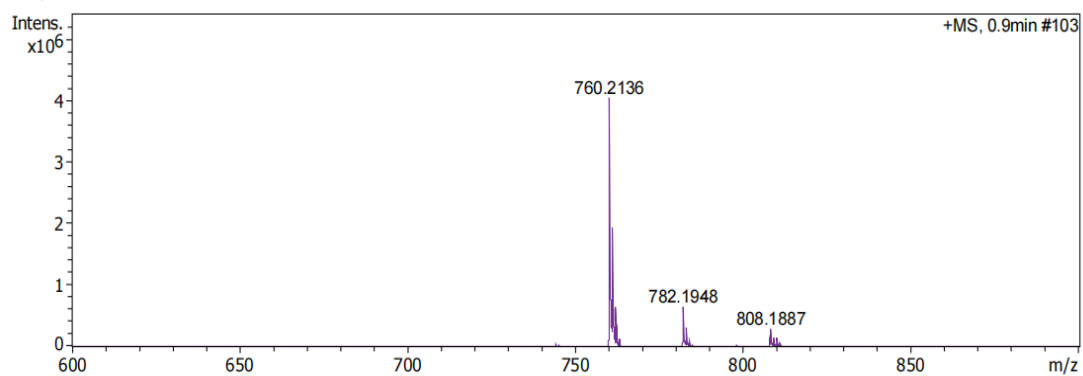


Figure S18. HRESIMS of compound **7Bc**

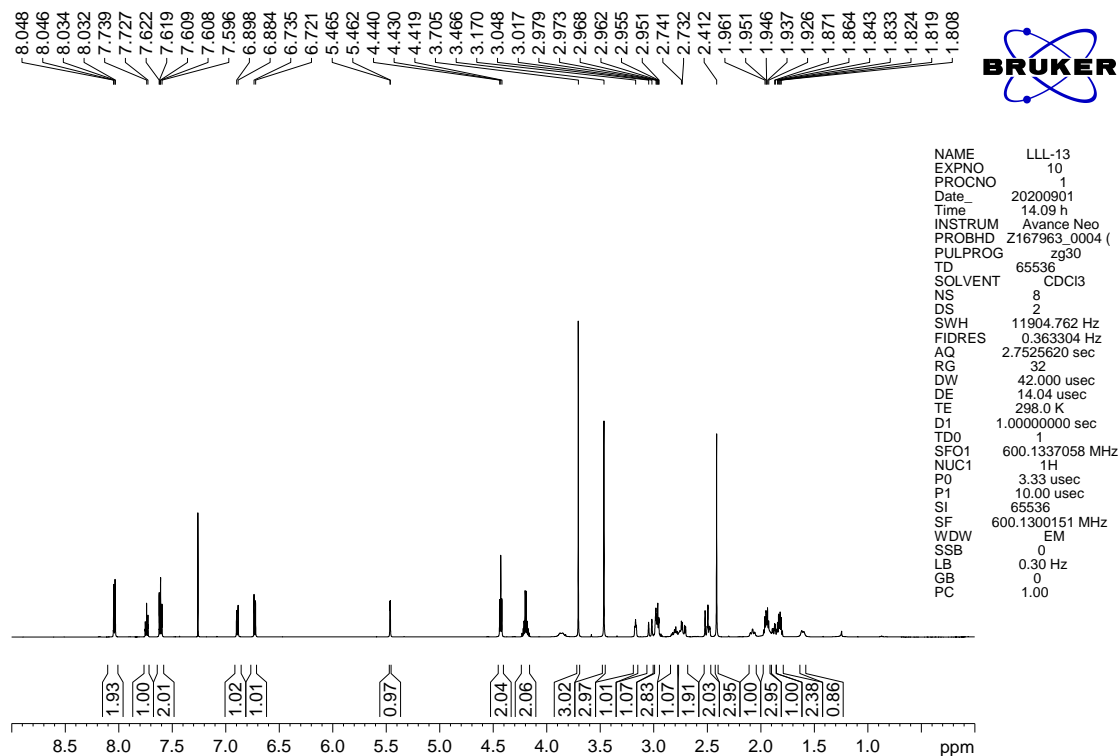


Figure S19. <sup>1</sup>H NMR of compound 7Ca

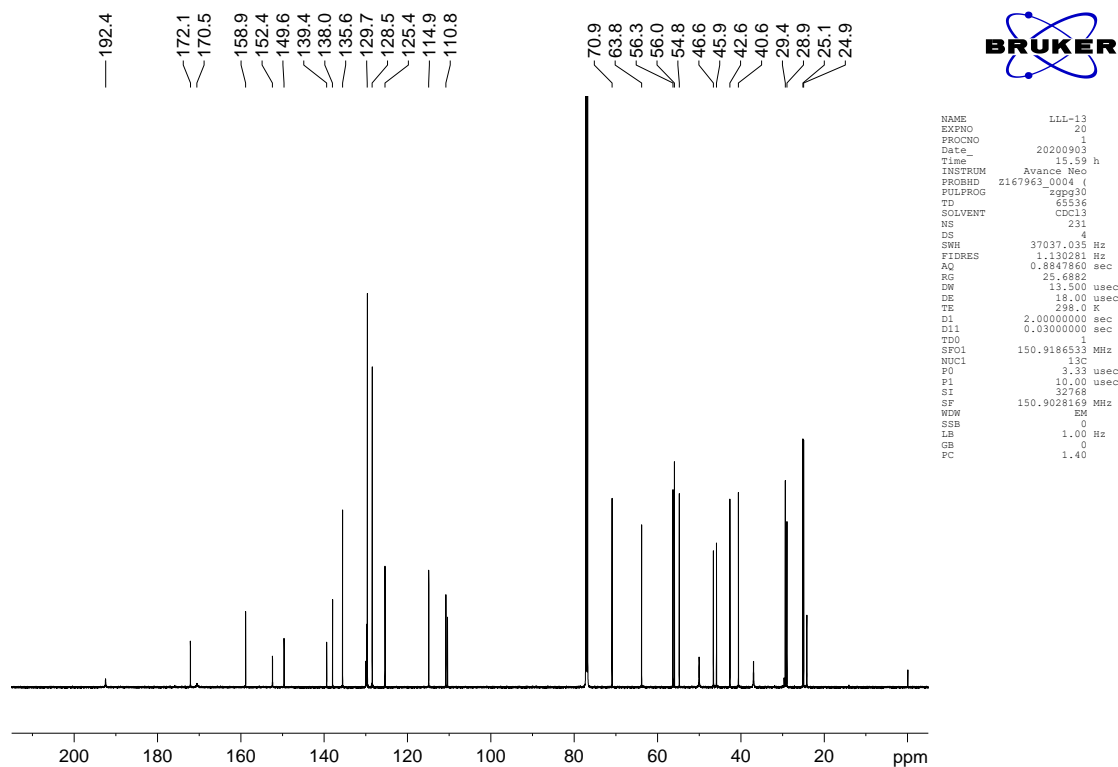


Figure S20. <sup>13</sup>C NMR of compound 7Ca

+MS, 0.9min #104

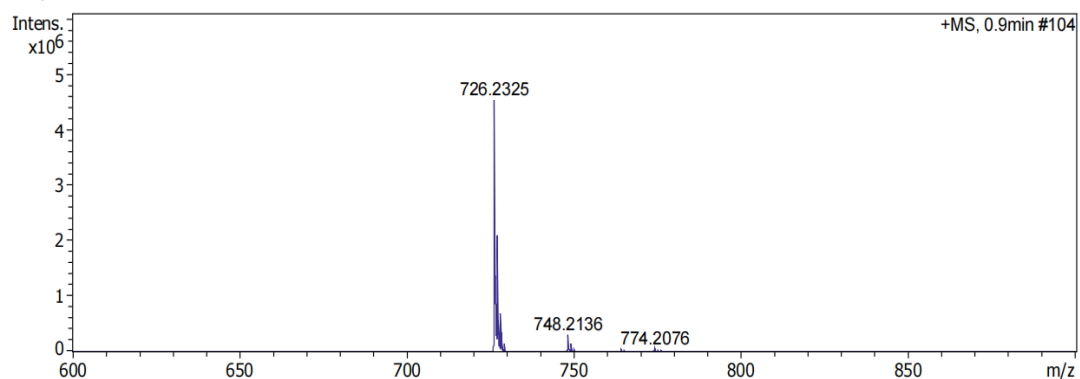


Figure S21. HRESIMS of compound 7Ca

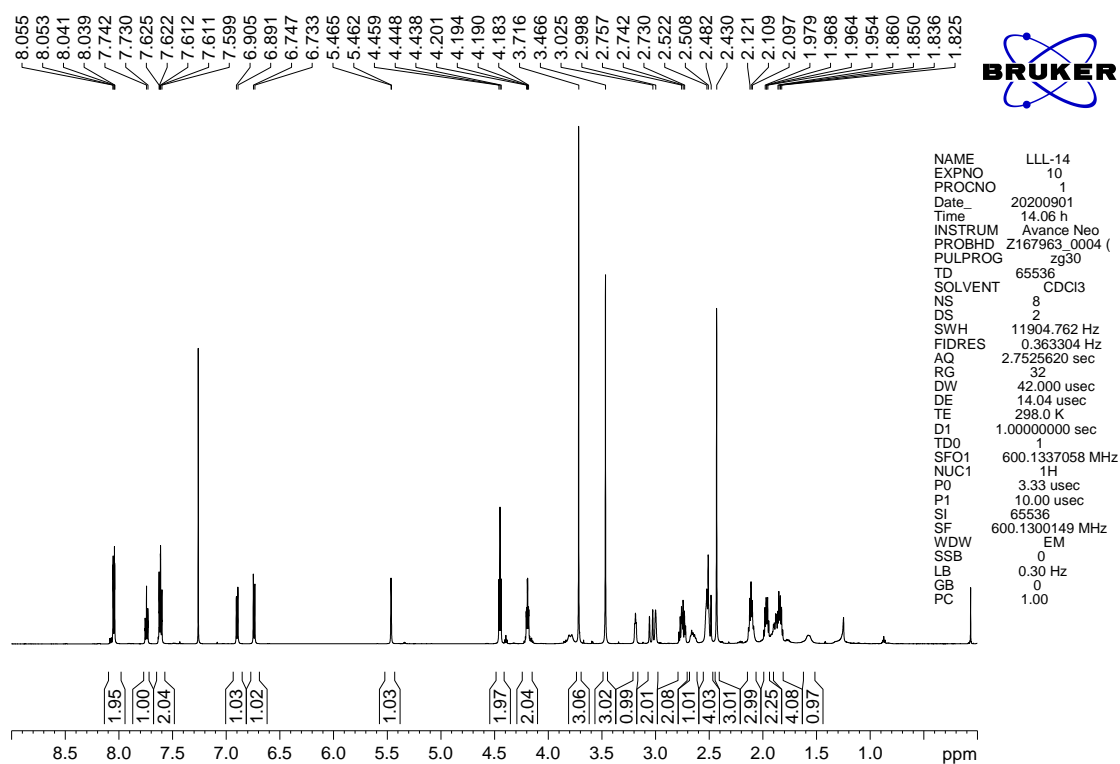


Figure S22. <sup>1</sup>H NMR of compound 7Cb

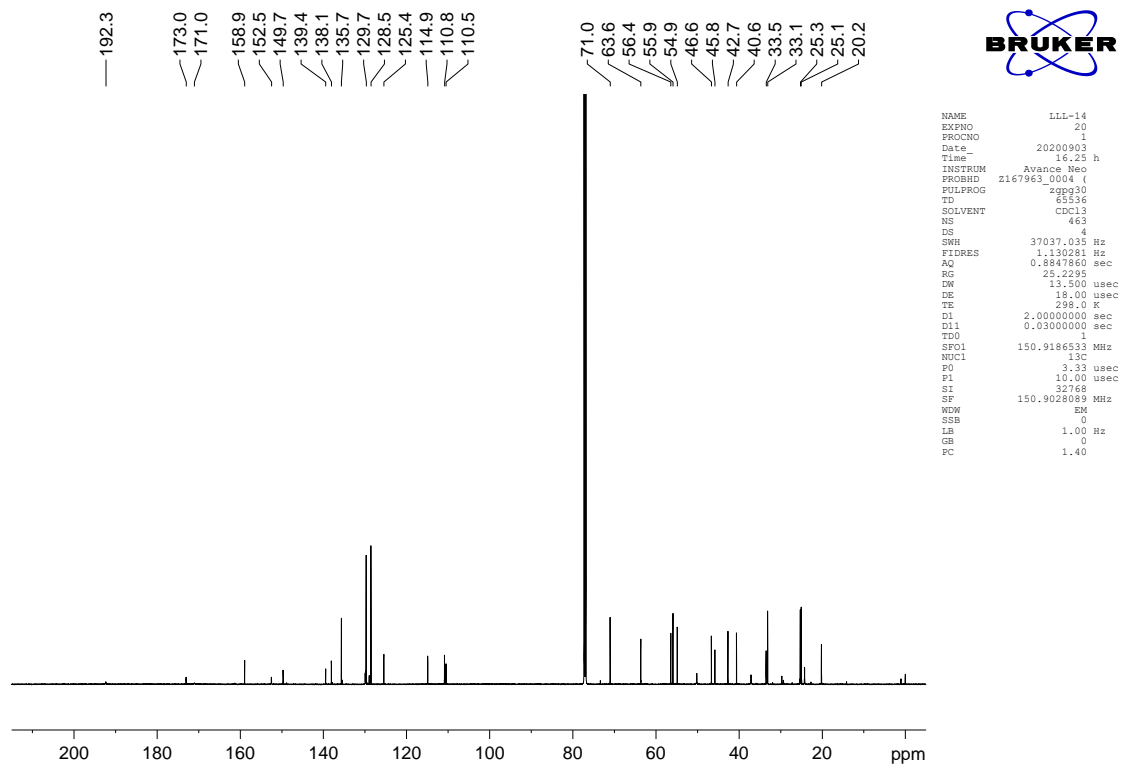


Figure S23.  $^{13}\text{C}$  NMR of compound **7Cb**

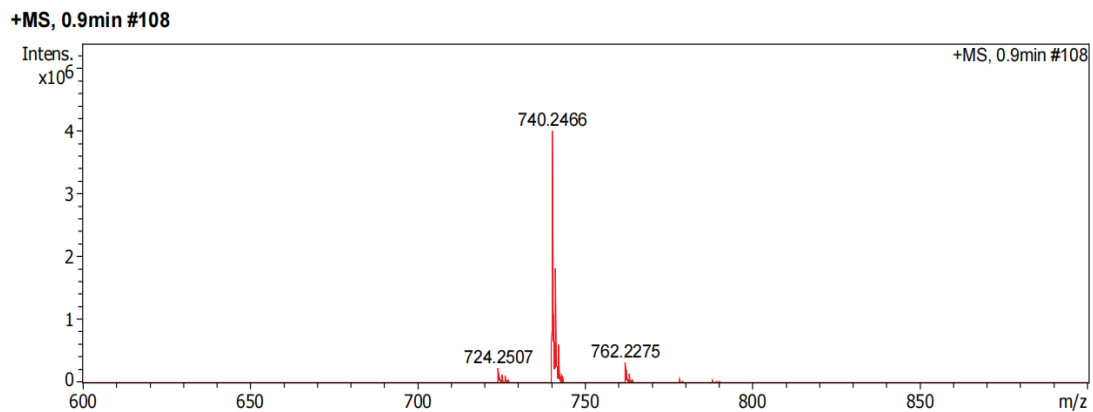


Figure S24. HRESIMS of compound **7Cb**

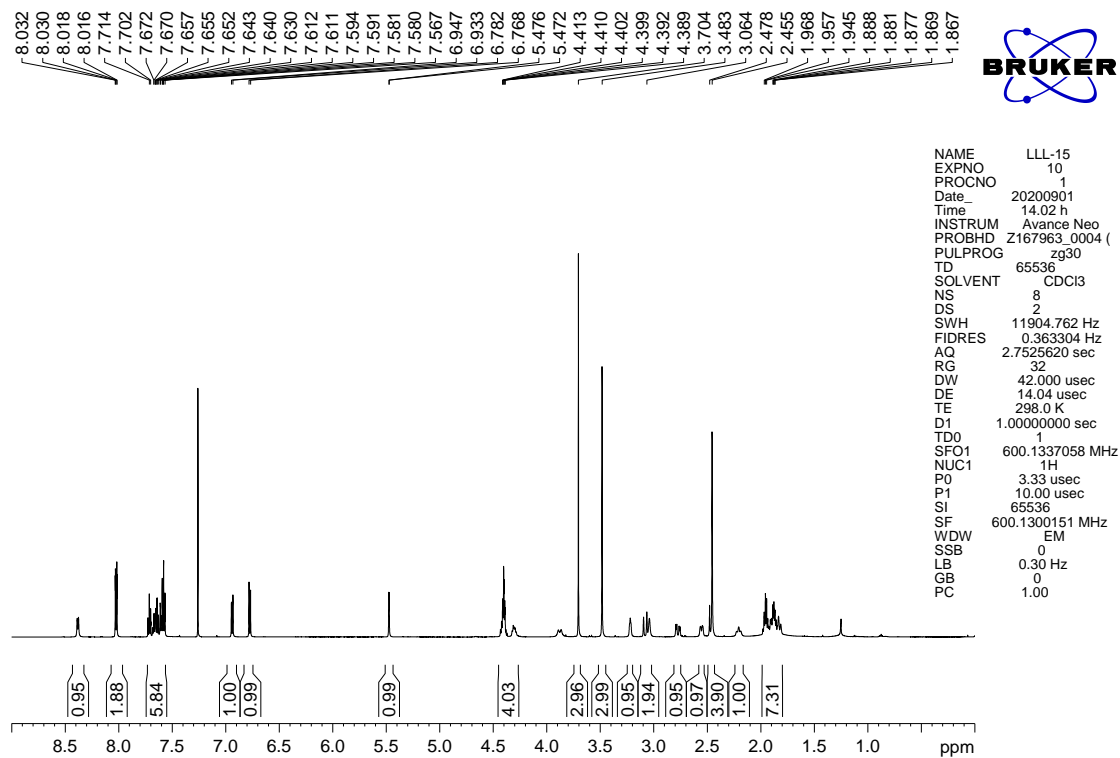


Figure S25. <sup>1</sup>H NMR of compound 7Cc

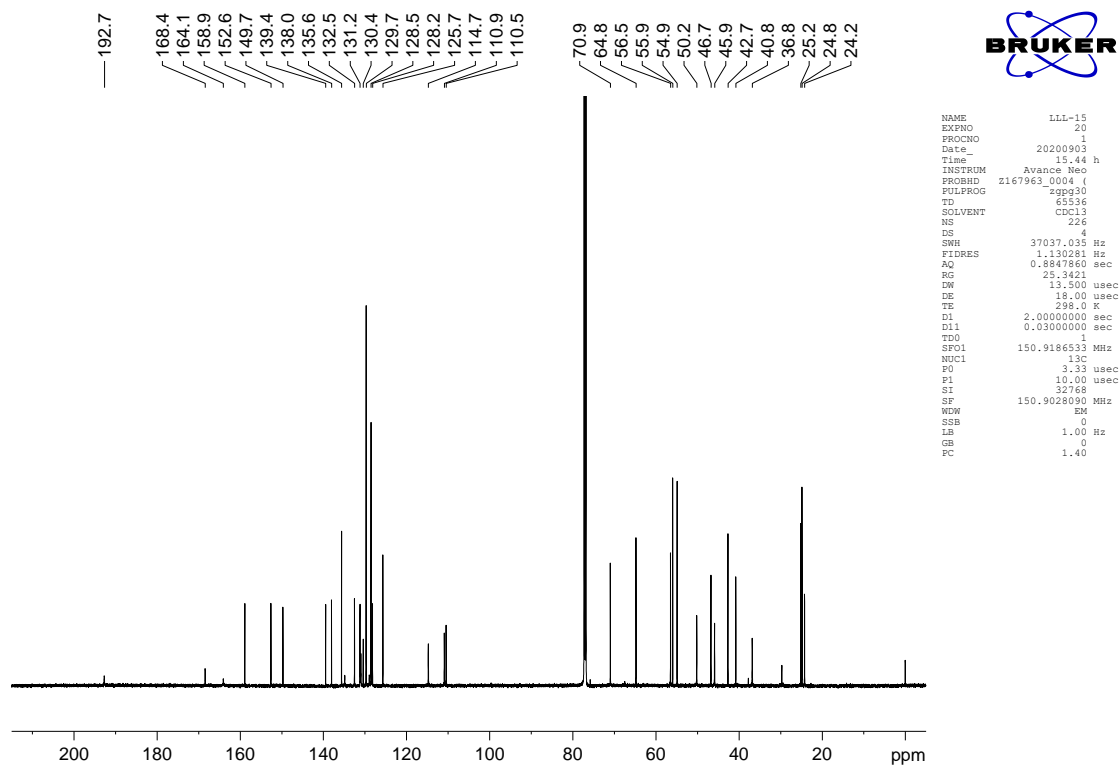


Figure S26. <sup>13</sup>C NMR of compound 7Cc

+MS, 0.9min #102

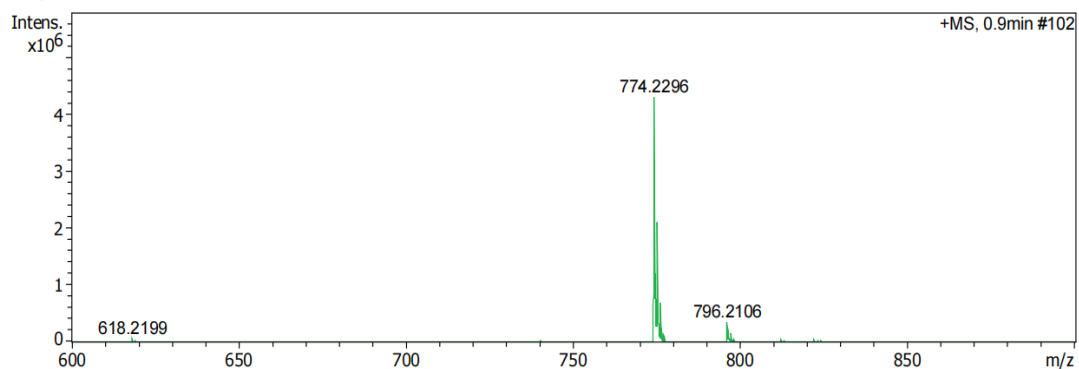


Figure S27. HRESIMS of compound 7Cc

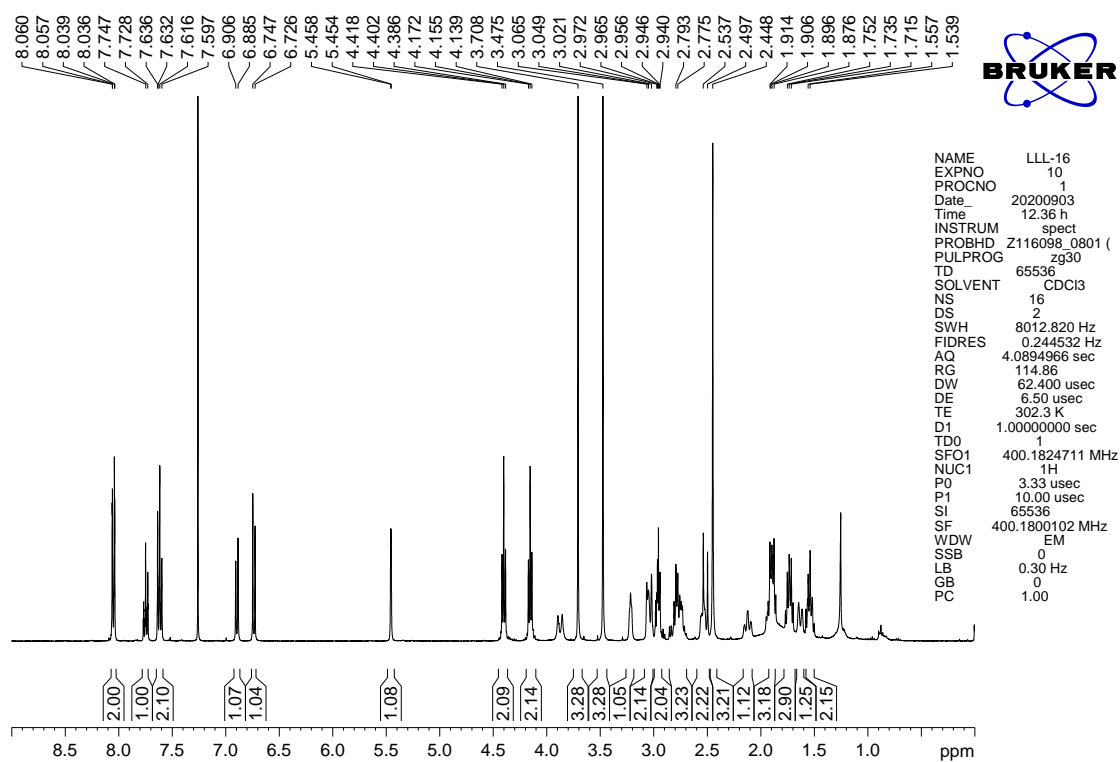


Figure S28. <sup>1</sup>H NMR of compound 7Da

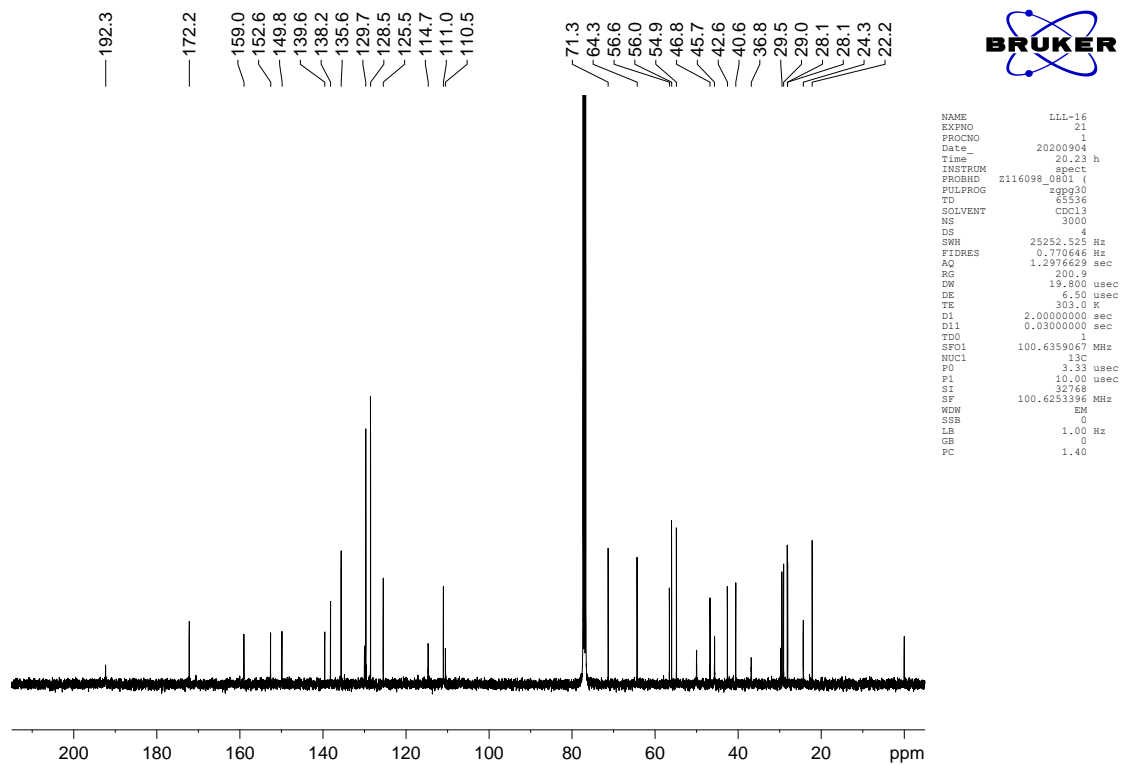


Figure S29. <sup>13</sup>C NMR of compound **7Da**

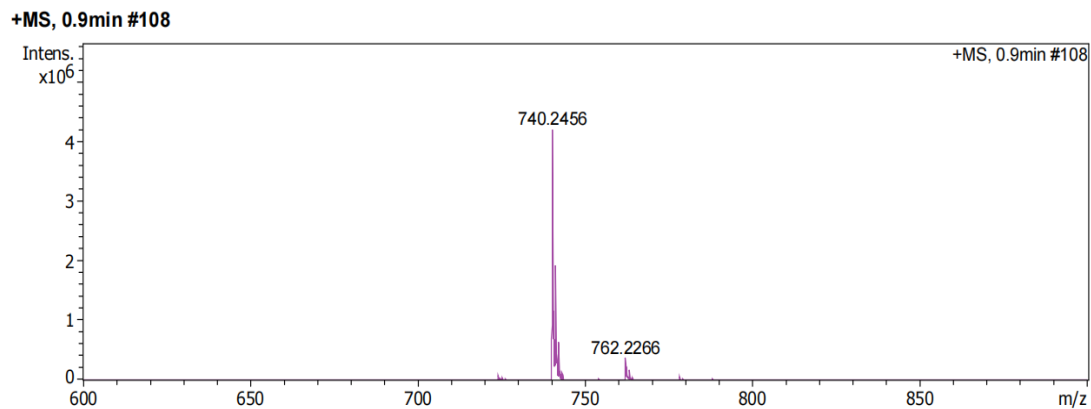


Figure S30. HRESIMS of compound **7Da**



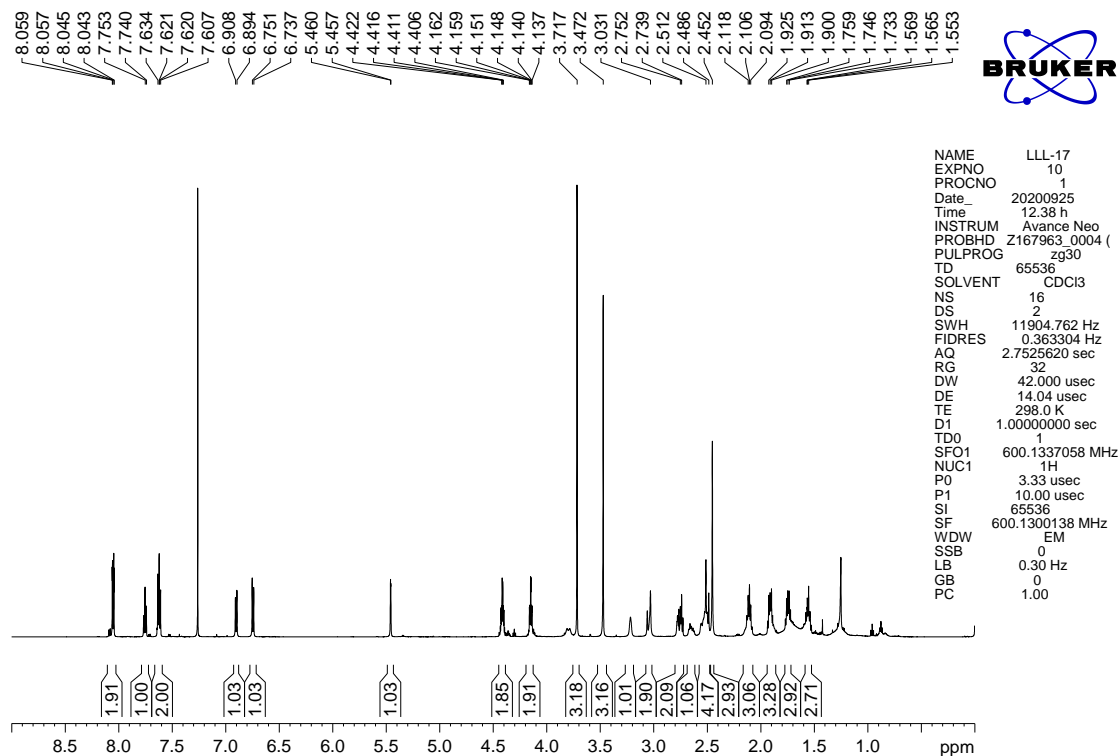


Figure S31. <sup>1</sup>H NMR of compound 7Db

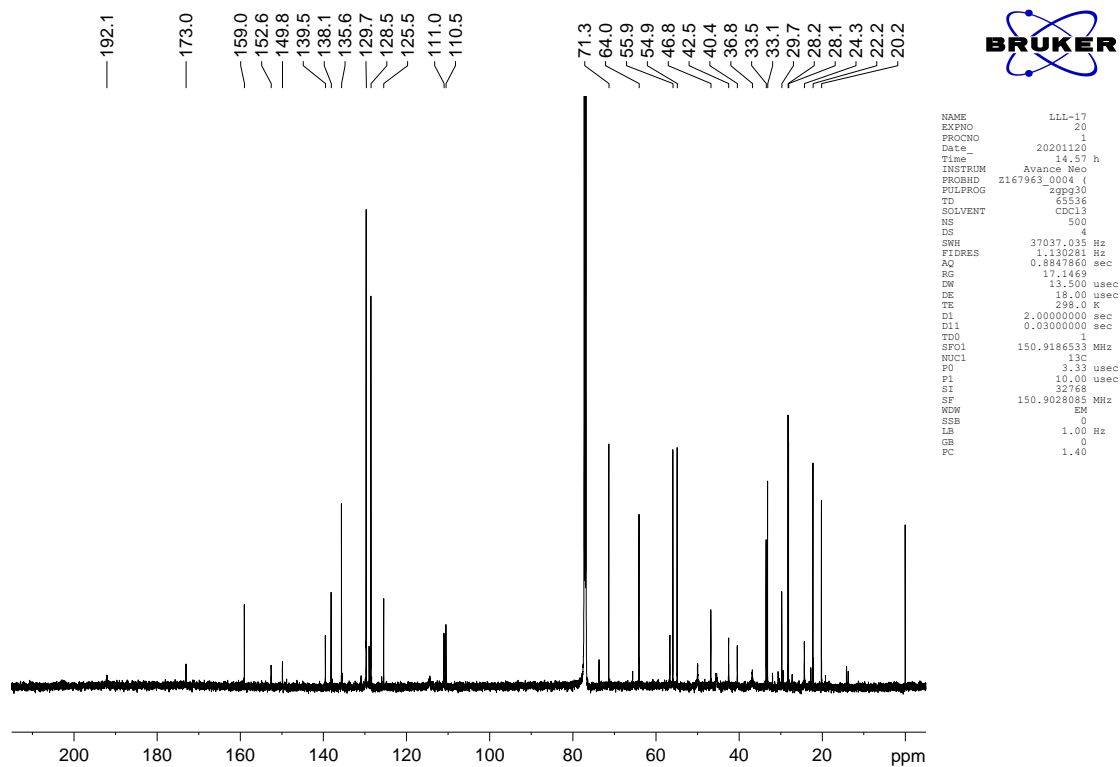


Figure S32. <sup>13</sup>C NMR of compound 7Db

+MS, 0.8min #95

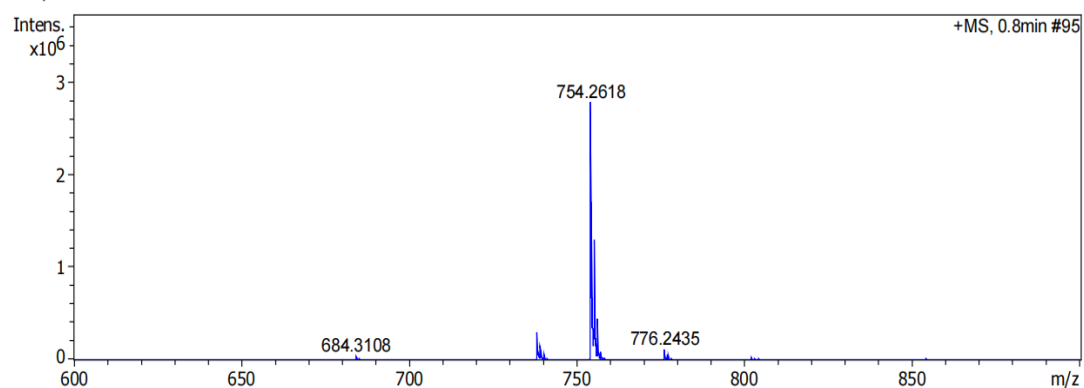


Figure S33. HRESIMS of compound **7Db**

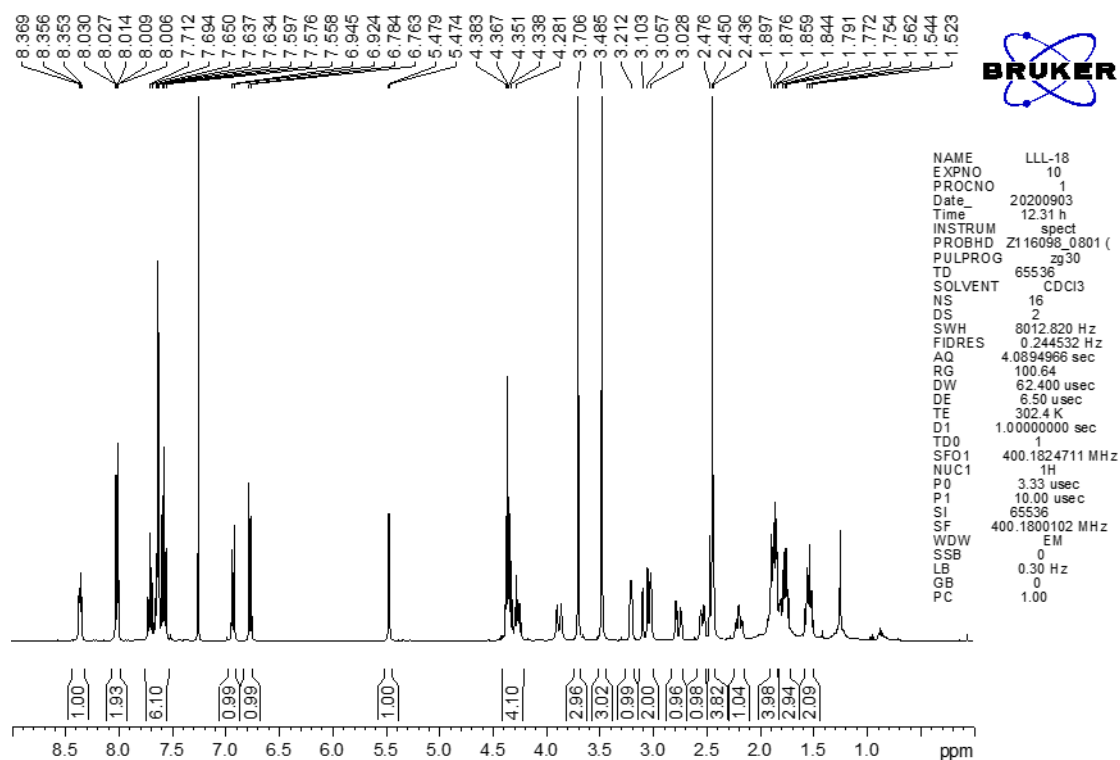


Figure S34. <sup>1</sup>H NMR of compound **7Dc**

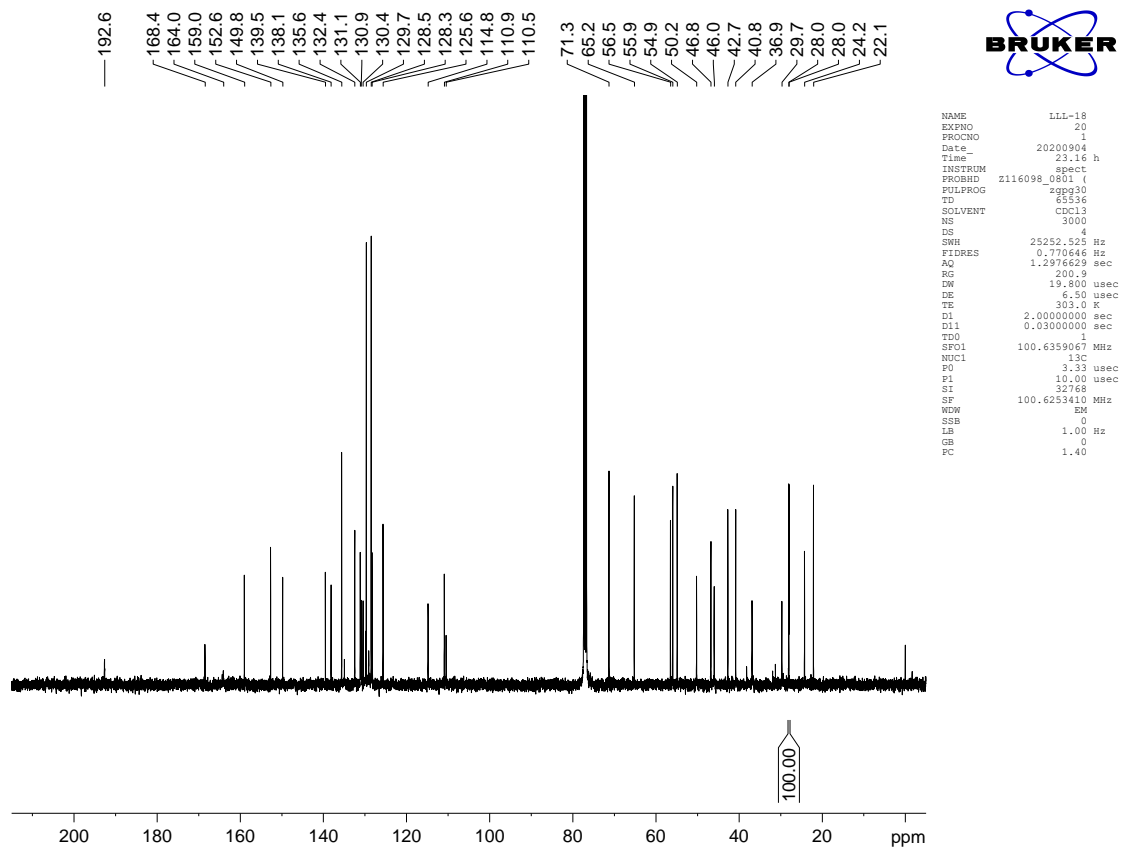


Figure S35. <sup>13</sup>C NMR of compound **7Dc**

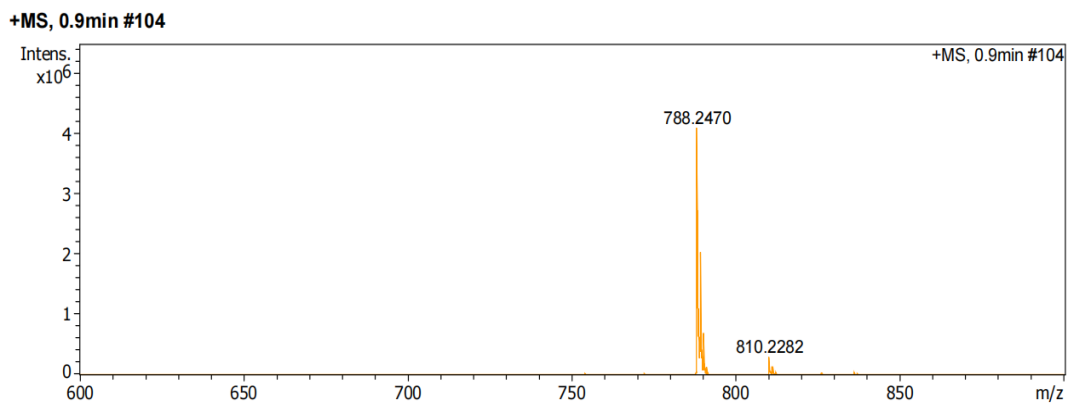


Figure S36. HRESIMS of compound **7Dc**

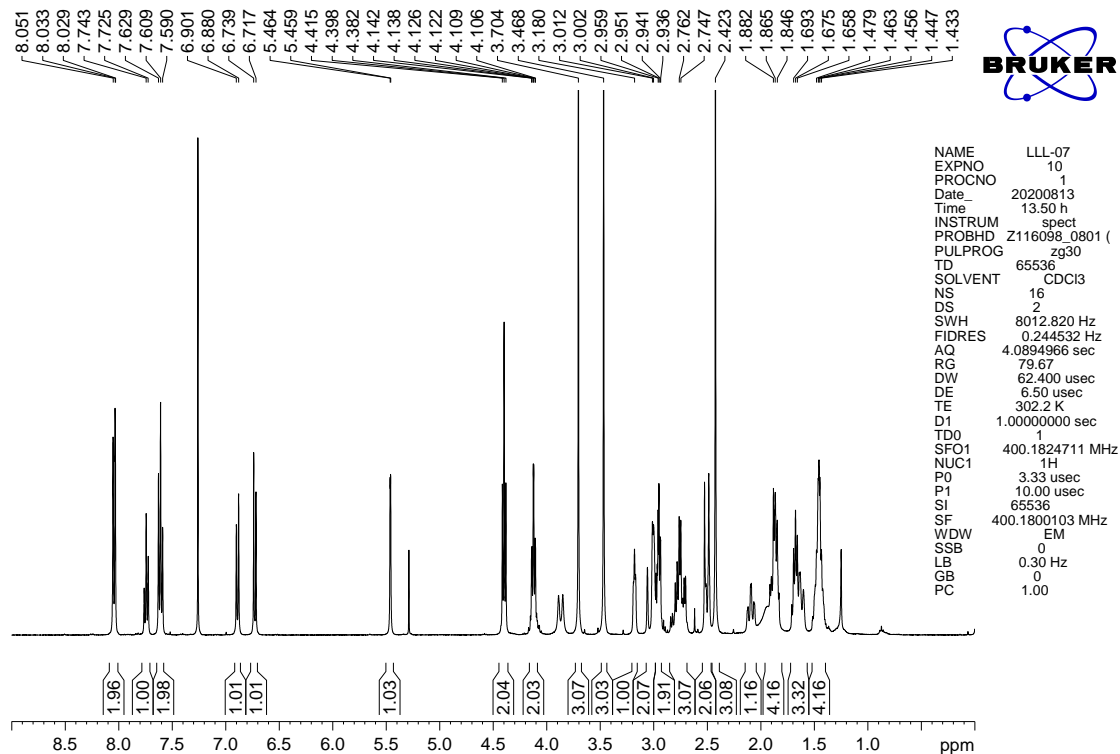


Figure S37. <sup>1</sup>H NMR of compound 7Ea

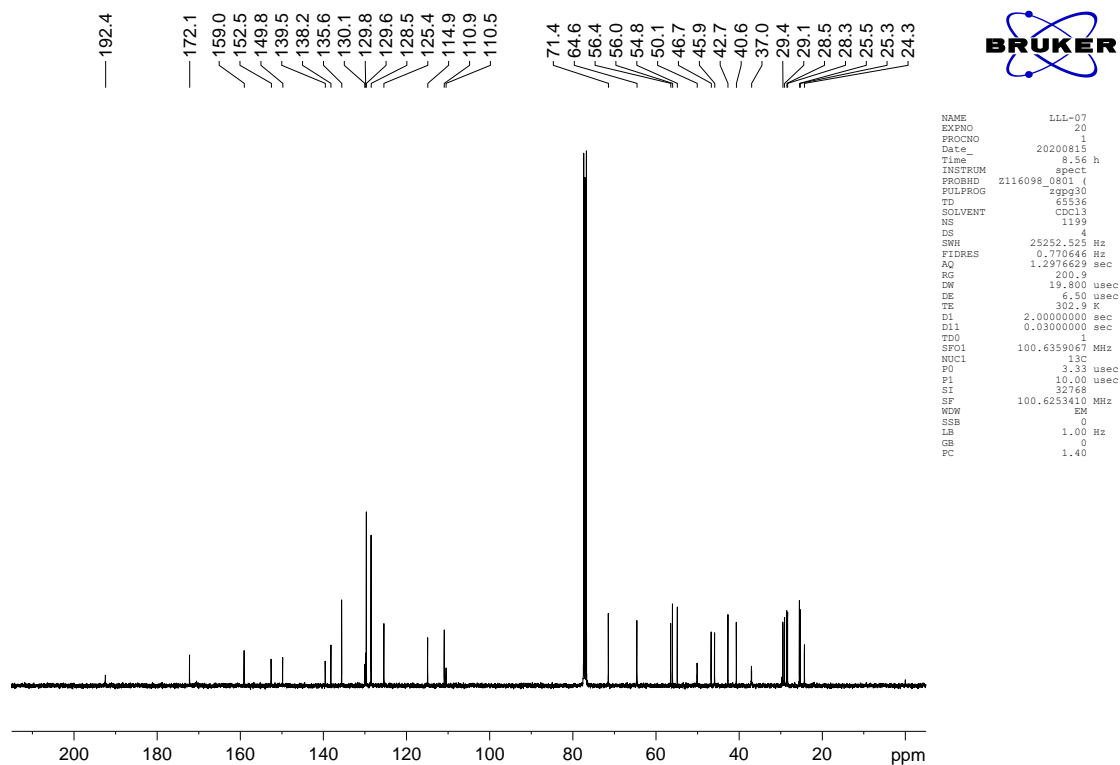


Figure S38. <sup>13</sup>C NMR of compound 7Ea

+MS, 0.9min #101

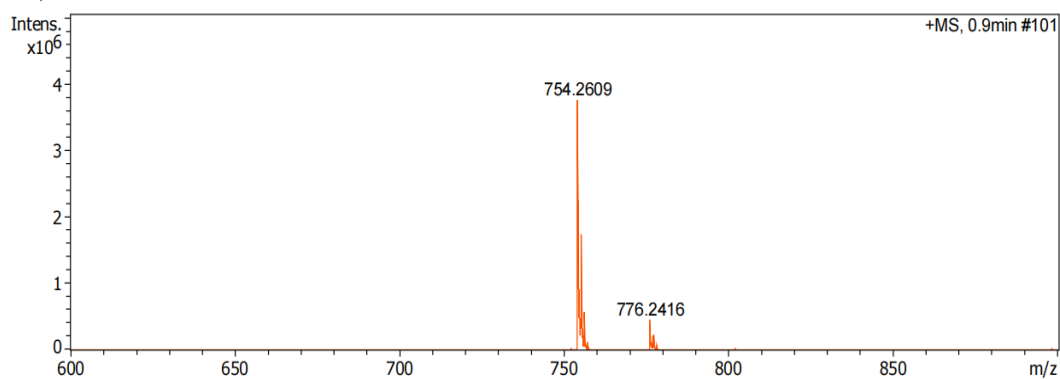


Figure S39. HRESIMS of compound **7Ea**

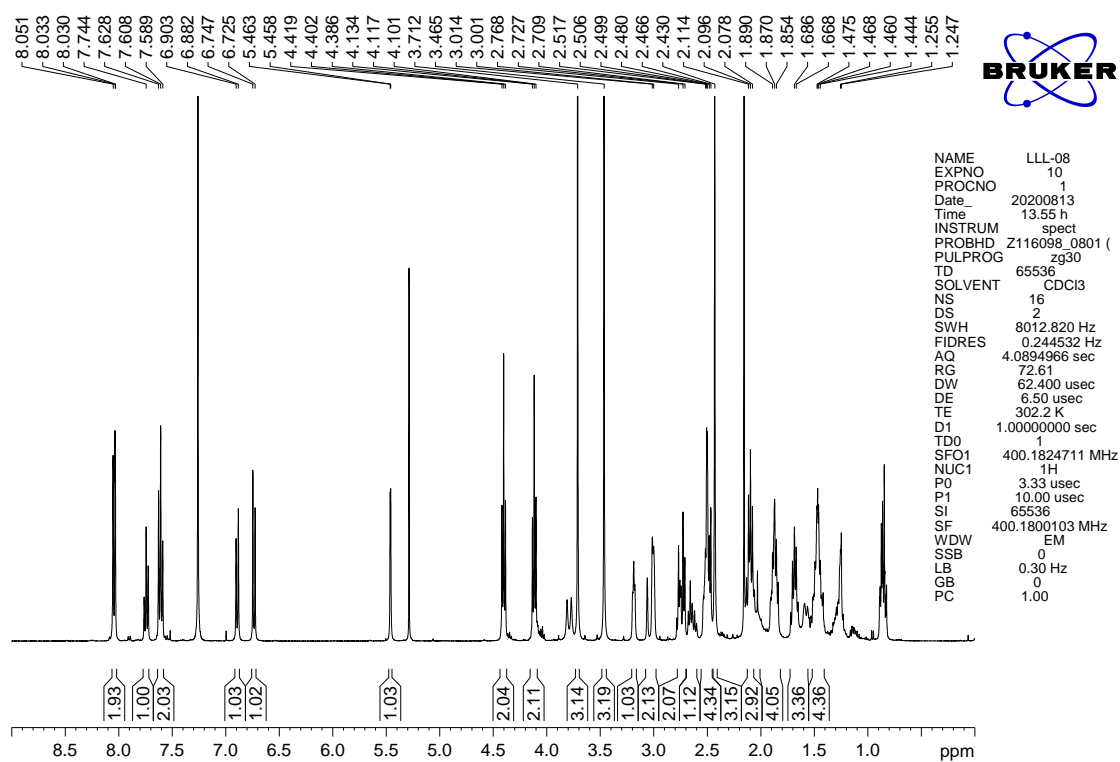


Figure S40. <sup>1</sup>H NMR of compound **7Eb**

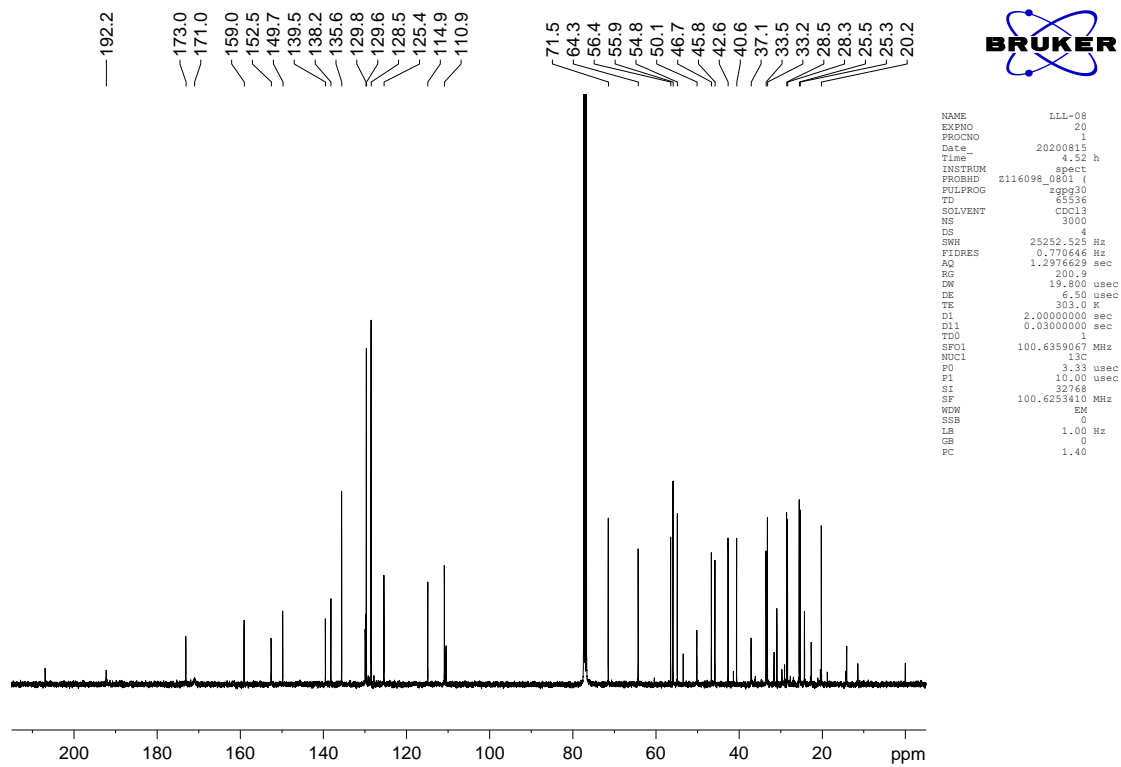


Figure S41.  $^{13}\text{C}$  NMR of compound **7Eb**

+MS, 0.9min #102

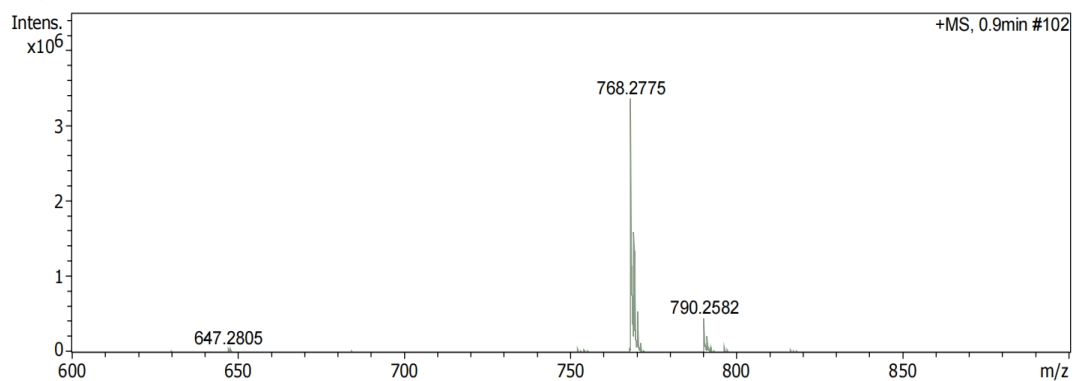


Figure S42. HRESIMS of compound **7Eb**

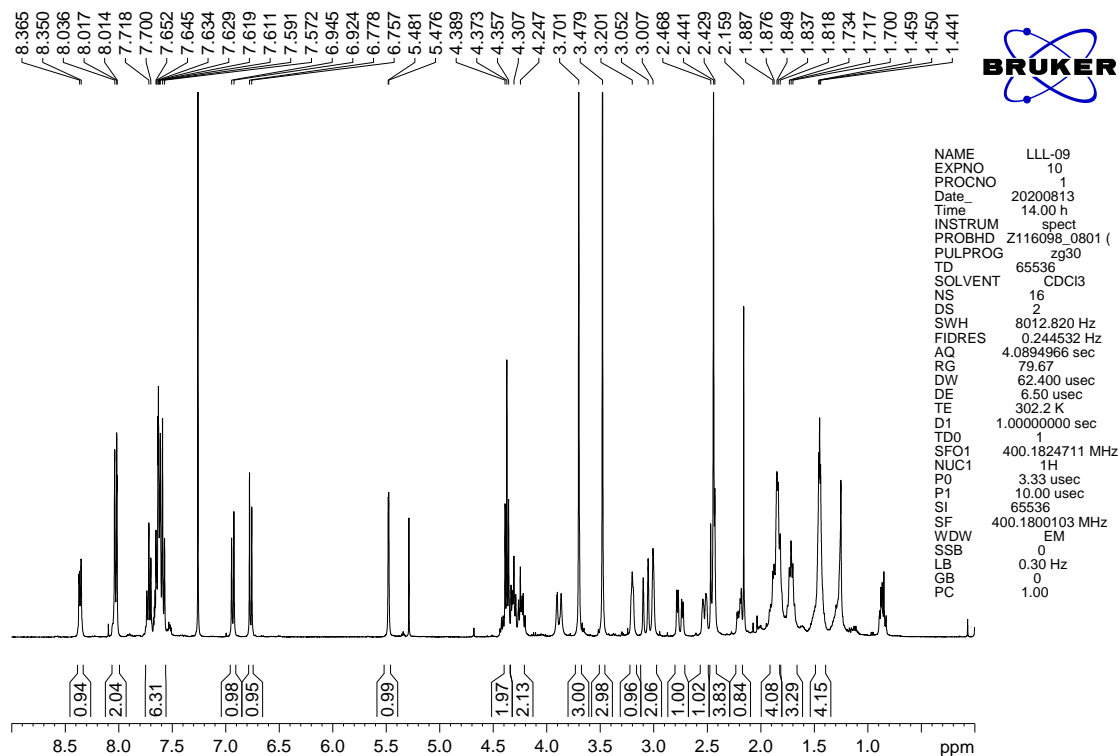


Figure S43.  $^1\text{H}$  NMR of compound **7Ec**

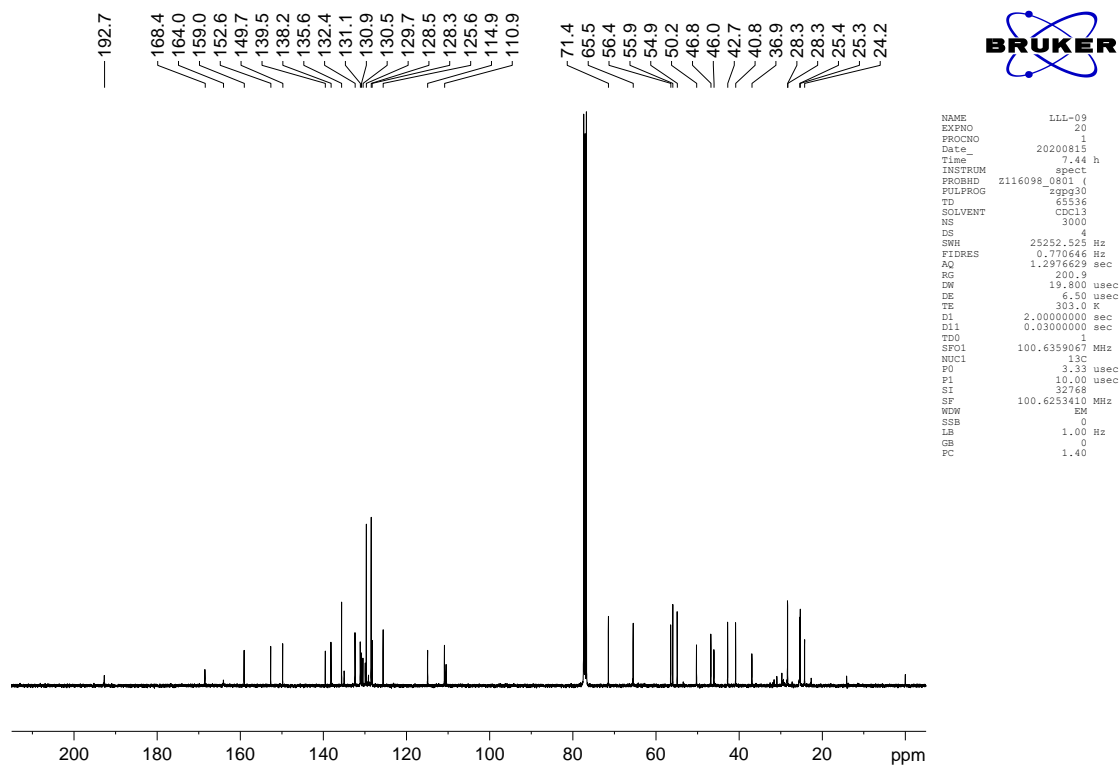


Figure S44.  $^{13}\text{C}$  NMR of compound **7Ec**

+MS, 0.9min #101

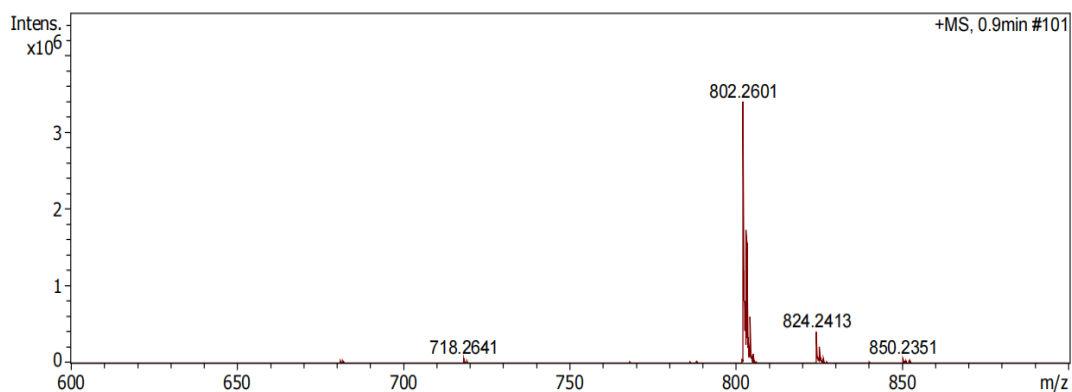
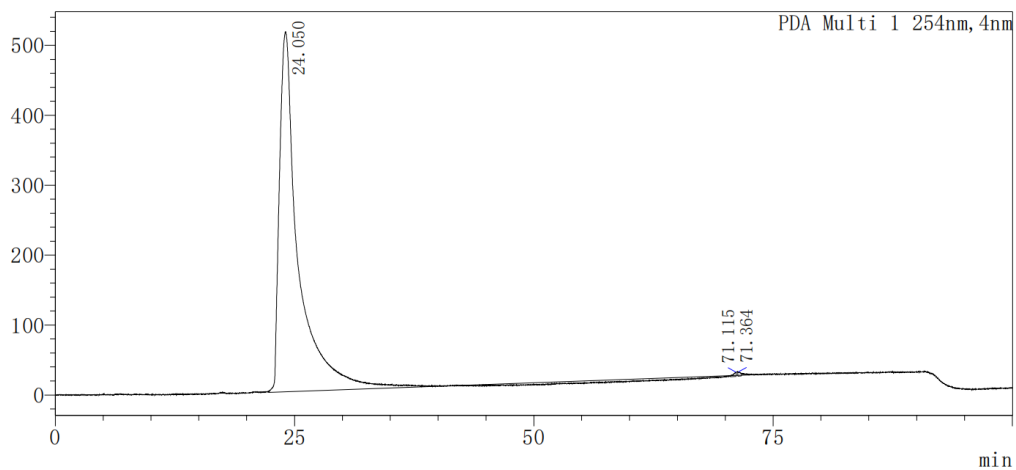


Figure S45. HRESIMS of compound 7Ec

mAU



Results of analytical HPLC analysis of compound 7Cc (254nm)

Peak	tR	S	H	S%
1	24.050	65369726	514335	99.639
2	71.115	125767	6083	0.192
3	71.364	111218	6065	0.170
Total		65606711	526483	

The analytical HPLC was a Shimadzu SPD-20A series equipped with an YMC C18 column (150 × 4.6 mm, 5  $\mu$ m, 0.5 ml/min) using 85% aqueous MeOH as mobile phase to test compound 7Cc.

Figure S46. Purity test of Compound 7Cc