

Supplementary Materials

Supplementary Information.

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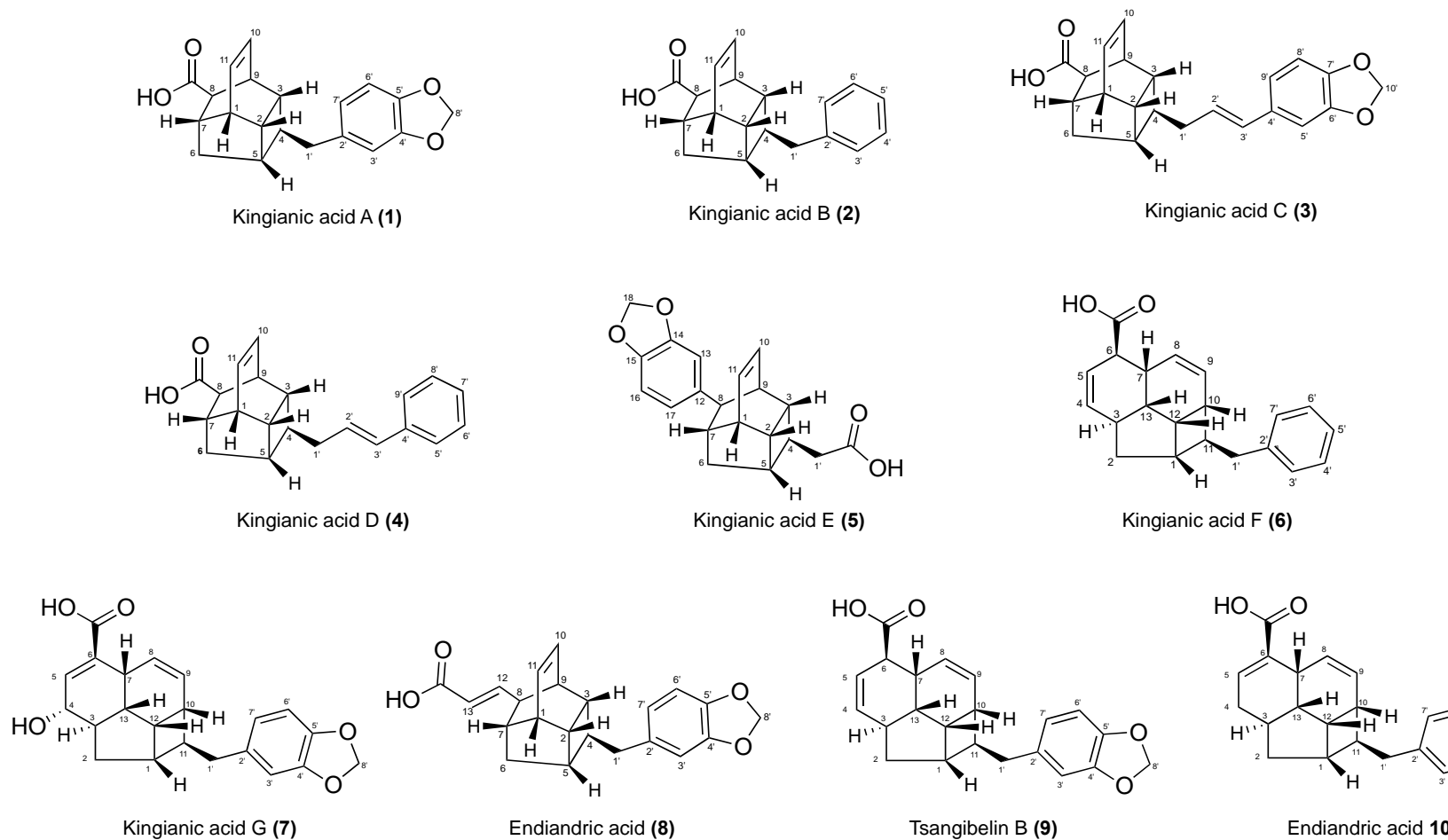
Figure S1. Structures of kingianic acids A-G (1–7), endiandric acid M (8), tsangibeilin B (9) and endiandric acid 10.

Figure S2. X-ray crystallographic analysis of endiandric acid **10**: A colourless crystal was obtained from MeOH, crystallized in the monoclinic crystal system with P21/c space group. Cell parameters: $a = 7.9900(2) \text{ \AA}$; $b = 21.9056(6) \text{ \AA}$; $c = 10.8257(3) \text{ \AA}$; $V = 1834.58(8) \text{ \AA}^3$, T 100 K. In the crystal structure, two molecules are linked by hydrogen bonds across a centre of inversion (**A**) and adjacent pairs are further linked by the double CH- π interactions that occur between the phenyl and the dioxole ring (**B**). The overall crystal packing gives rise to a 2-D layered structure as shown in **C**. Supplementary crystallographic data have been deposited at the CCDC; CCDC 918161. ORTEP plot of endiandric acid **10** with the displacement ellipsoids drawn at the 50% probability level.

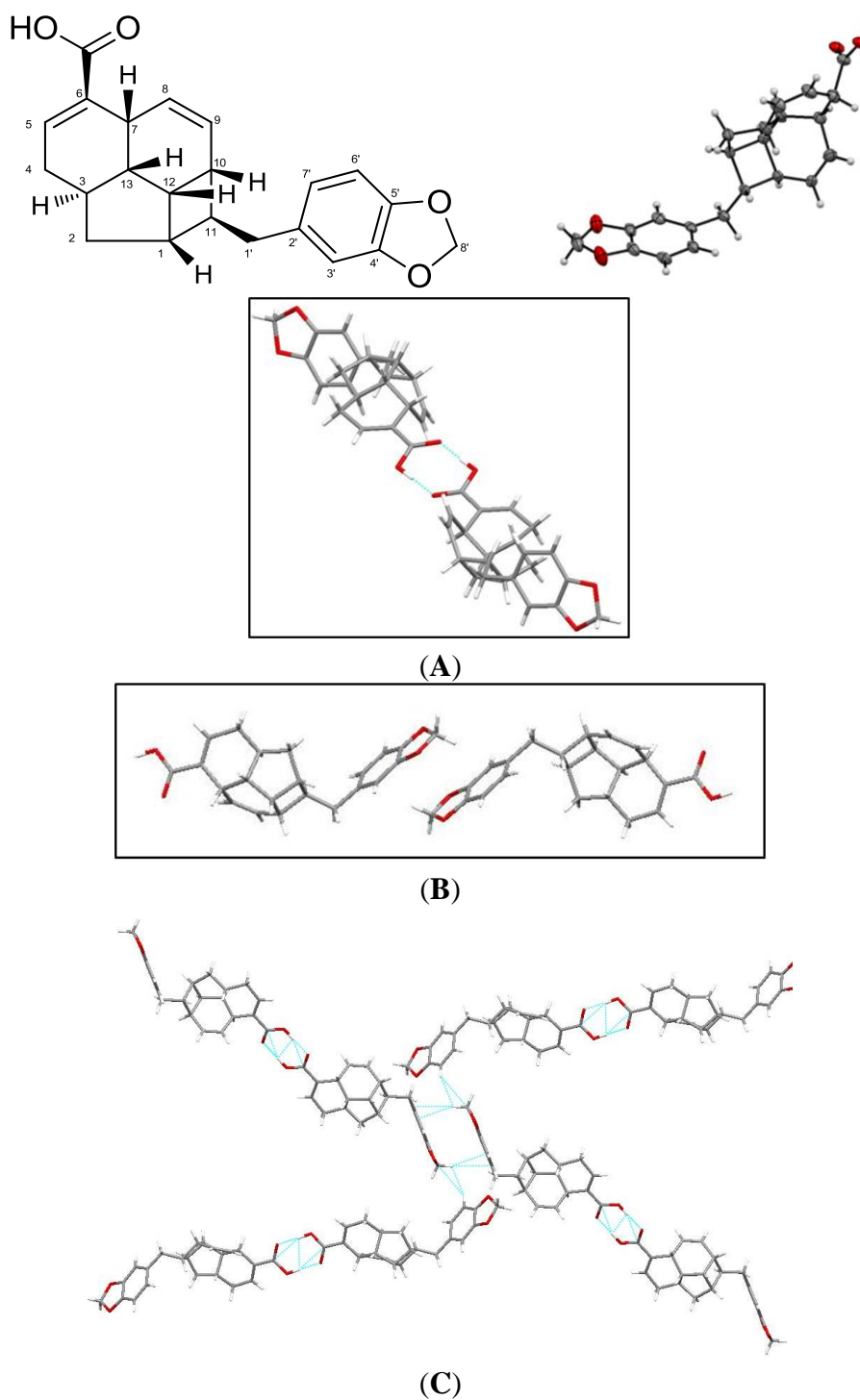


Figure S3. X-Ray Crystallographic Data of *tsangibeilin B* (**9**). A colorless crystal was obtained from MeOH, crystallized in the monoclinic crystal system with C2/c space group. Cell parameters: $a = 41.694(9) \text{ \AA}$; $b = 6.8688(15) \text{ \AA}$; $c = 12.282(3) \text{ \AA}$; $\beta = 101.742(4)^\circ$; $V = 1834.58(8) \text{ \AA}^3$, , $T 100 \text{ K}$.

ORTEP plot of *tsangibeilin B* (**9**) with the displacement ellipsoids drawn at the 50% probability level.

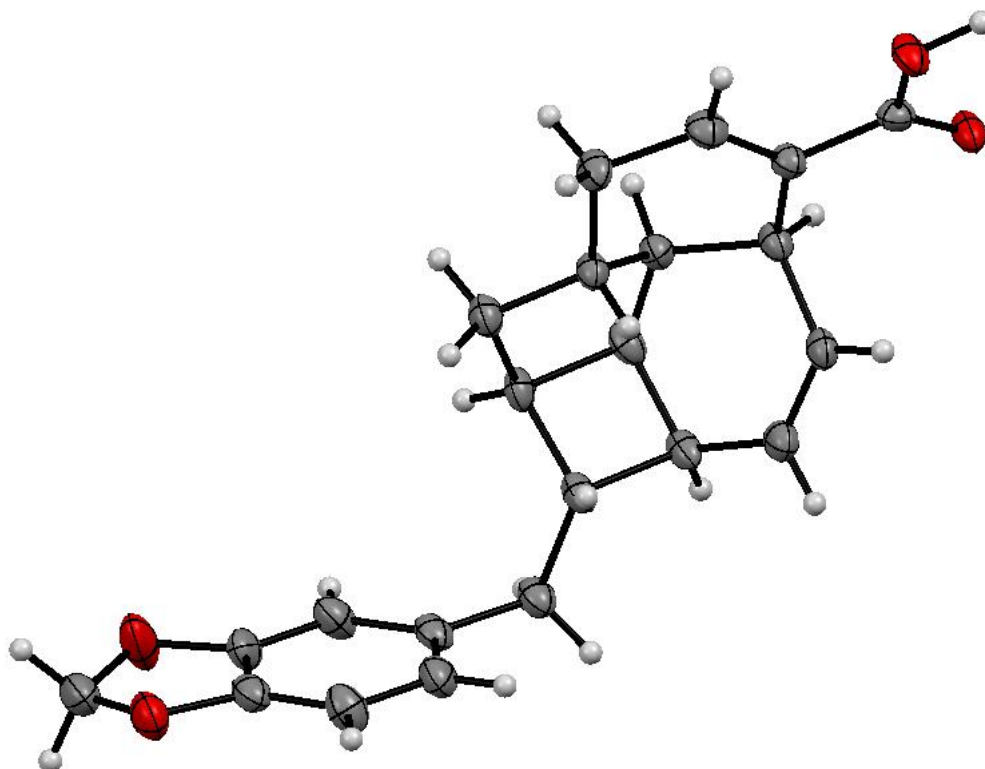


Figure S4. HRESIMS of kingianic acid A (1).

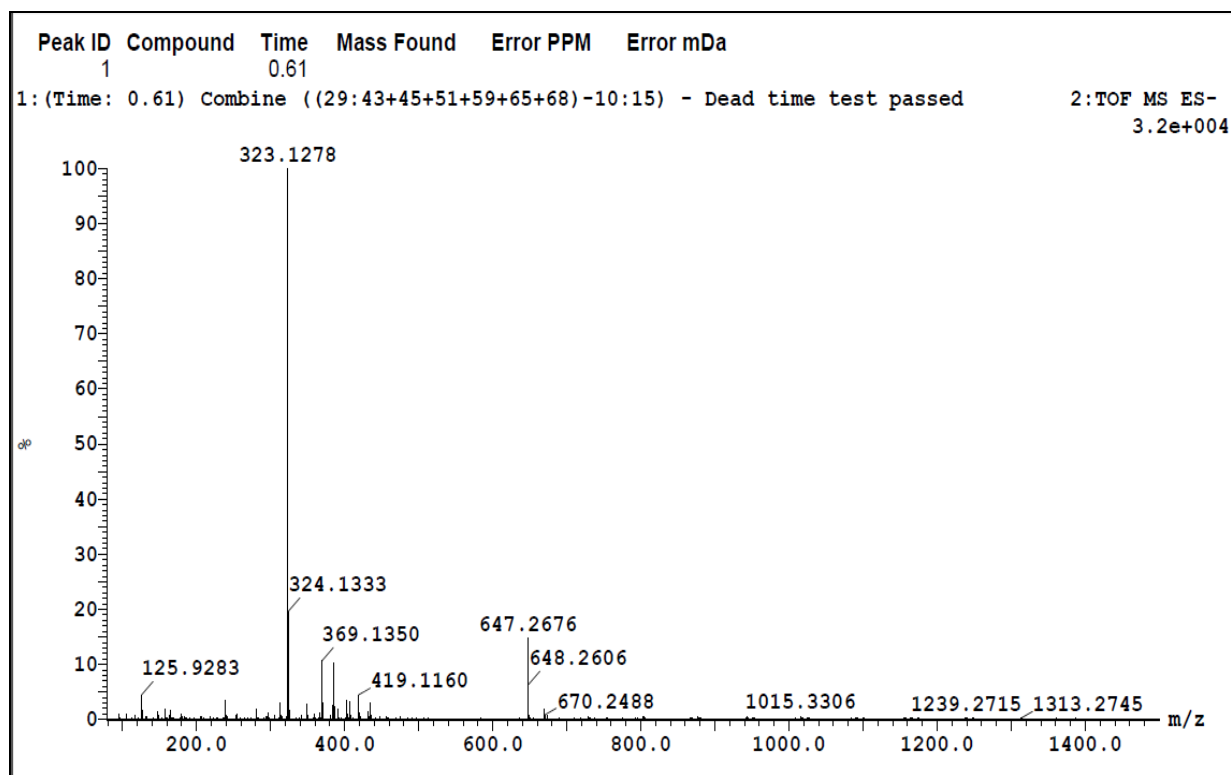
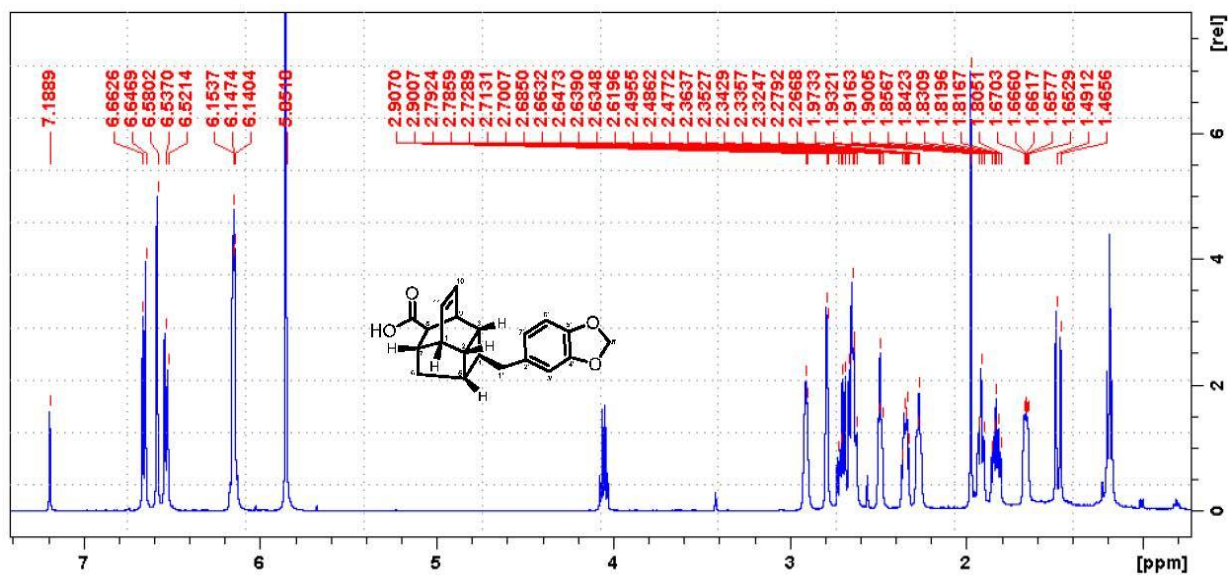
Figure S5. $^1\text{H-NMR}$ kingianic acid A (1) in CDCl_3 at 600 MHz.

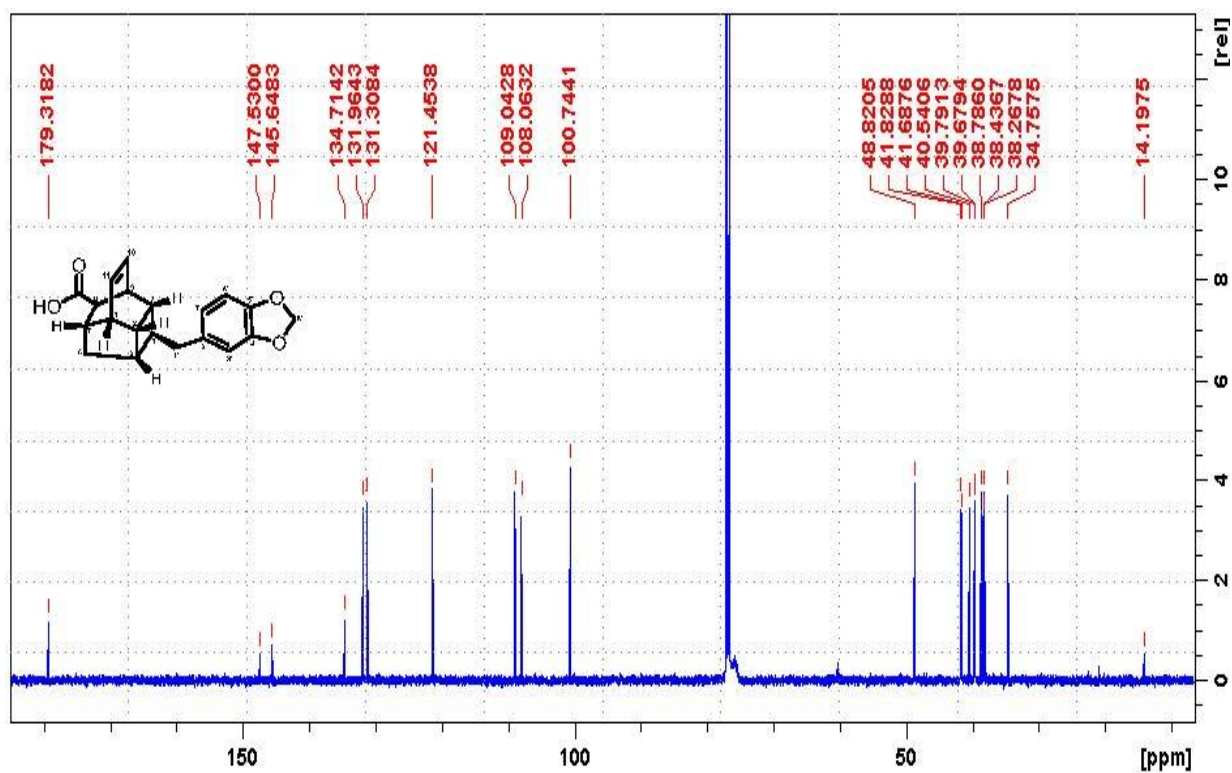
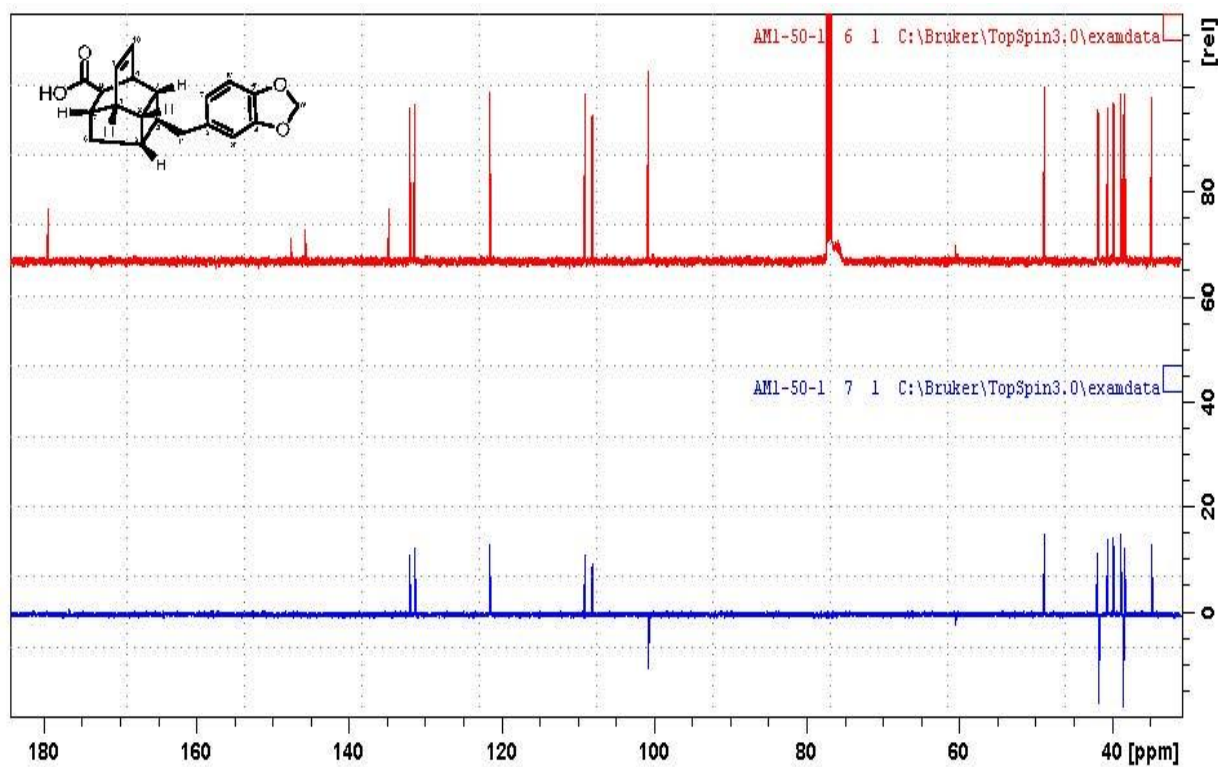
Figure S6. ^{13}C -NMR kingianic acid A (1) in CDCl_3 at 150 MHz.Figure S7. DEPT135 kingianic acid A (1) in CDCl_3 .

Figure S8. HRESIMS of kingianic acid B (2).

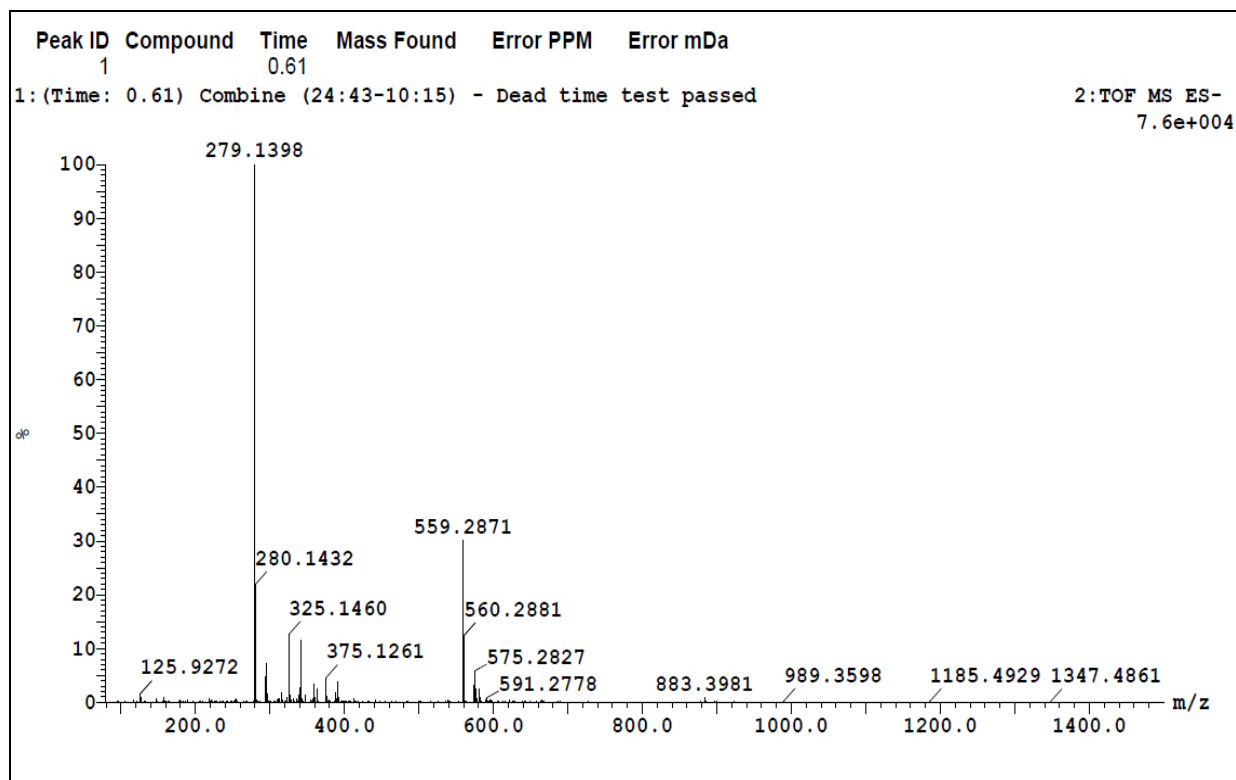
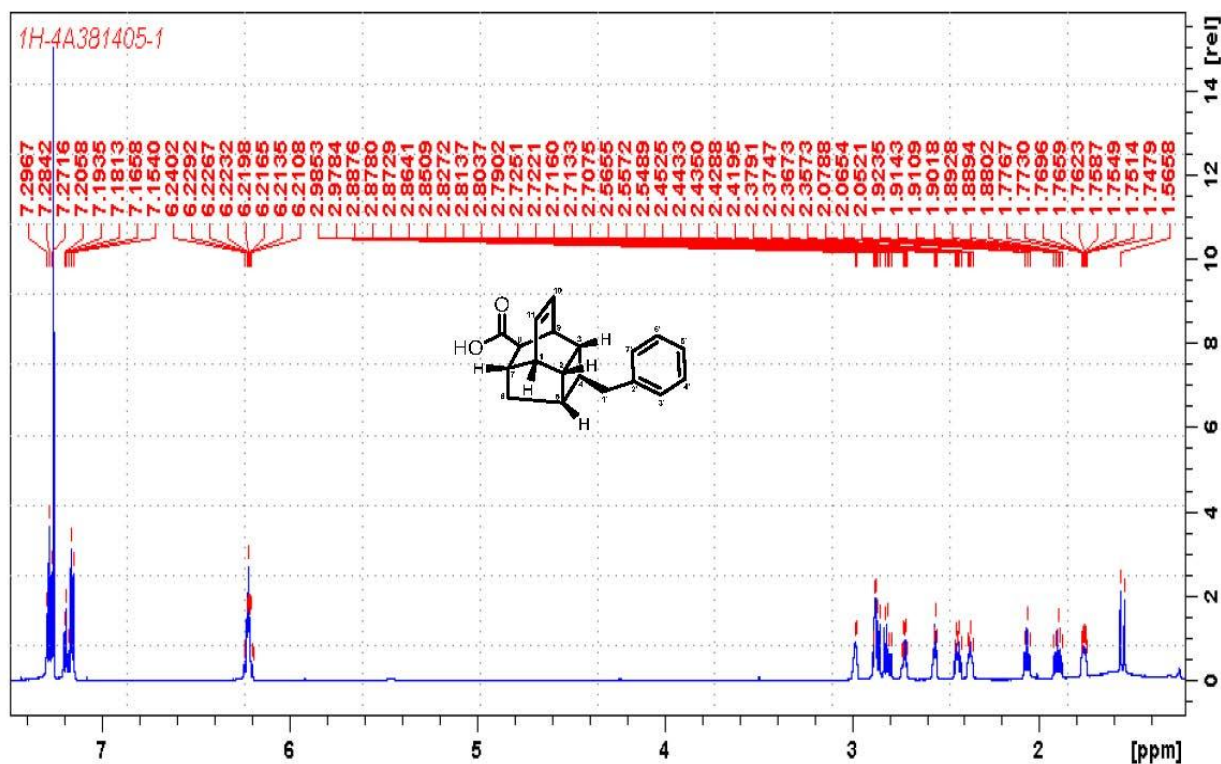
Figure S9. $^1\text{H-NMR}$ kingianic acid B (2) in CDCl_3 at 600 MHz.

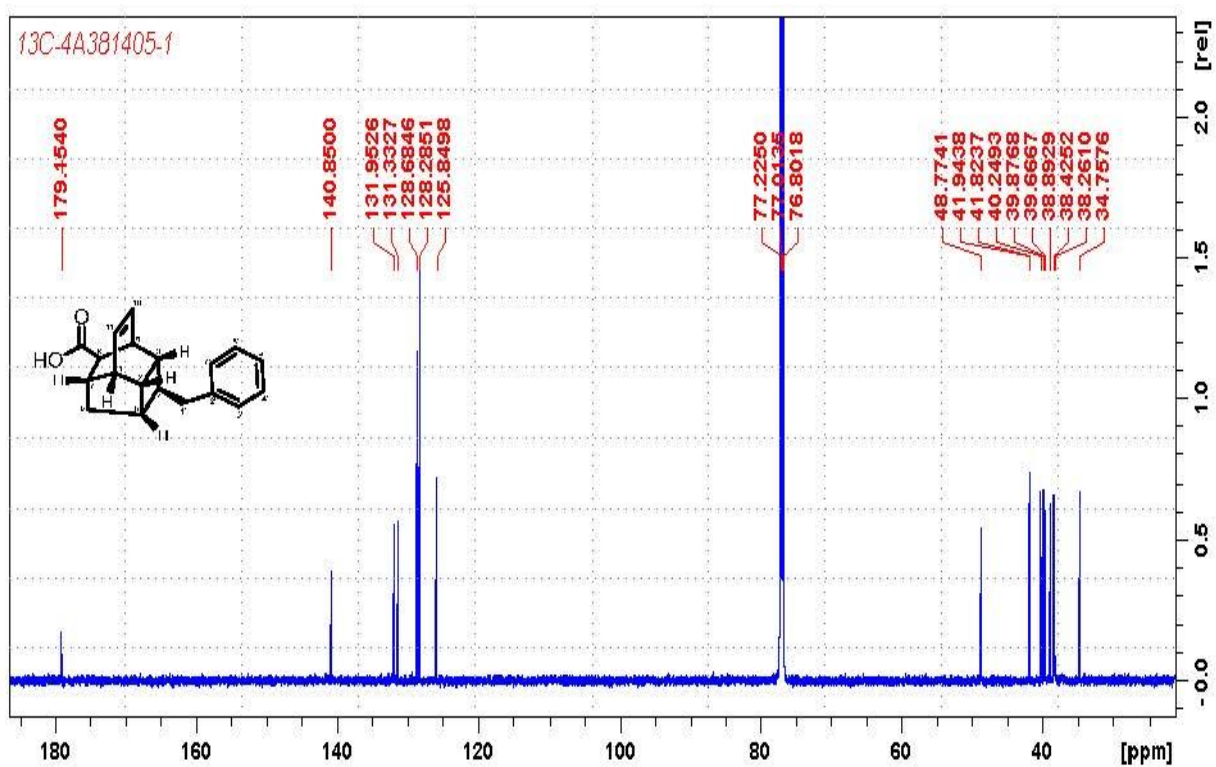
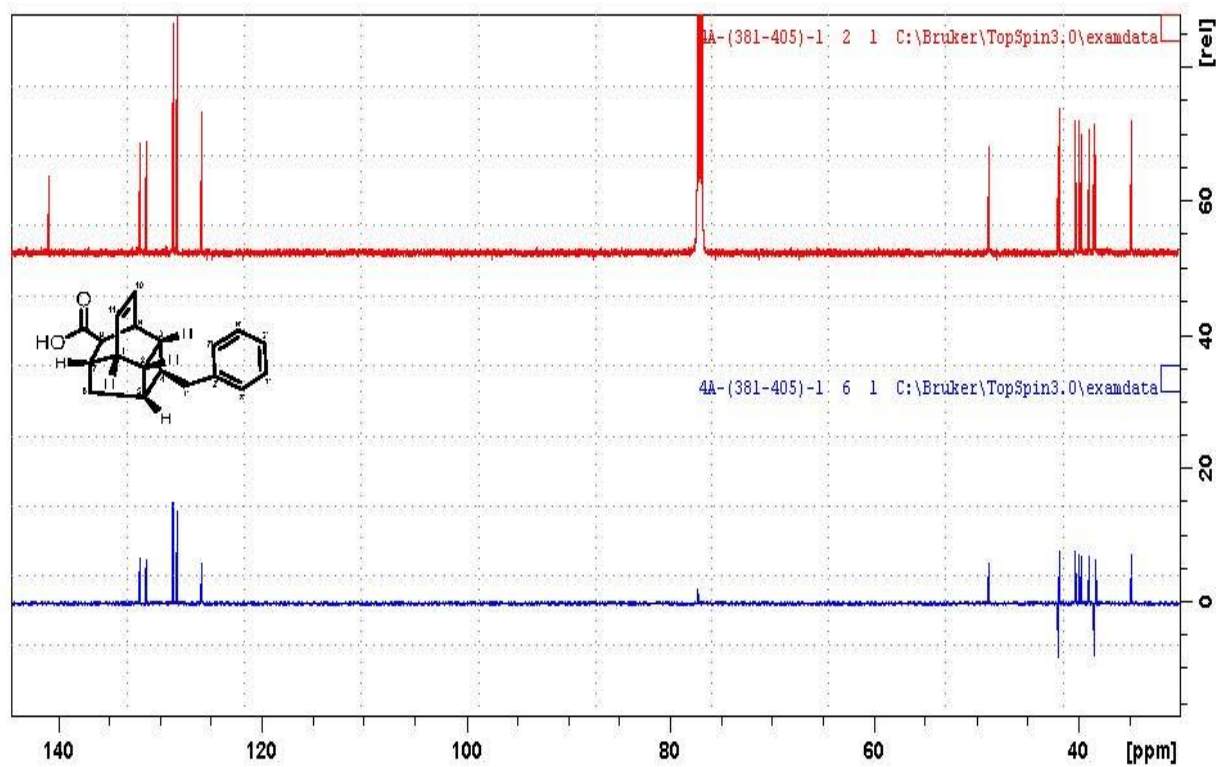
Figure S10. ^{13}C -NMR kingianic acid B (2) in CDCl_3 at 150 MHz.Figure S11. DEPT135 kingianic acid B (2) in CDCl_3 .

Figure S12. HRESIMS of kingianic acid C (3).

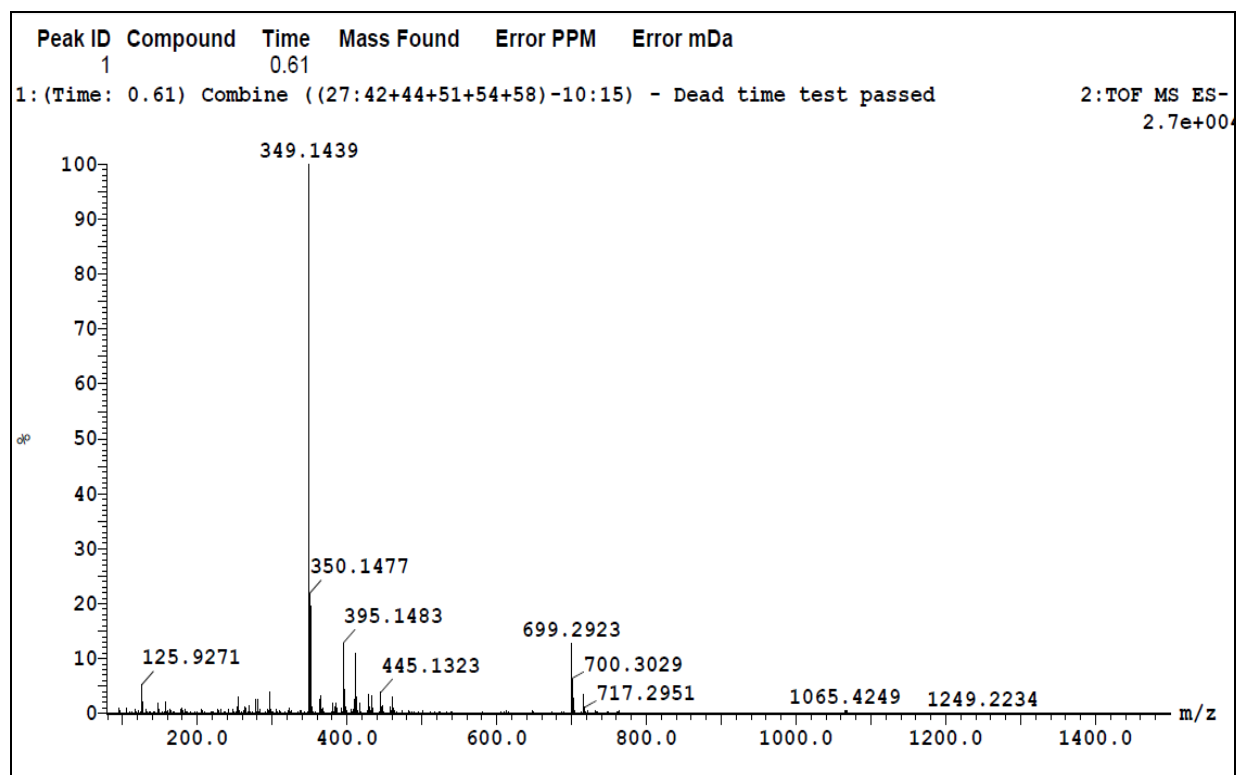
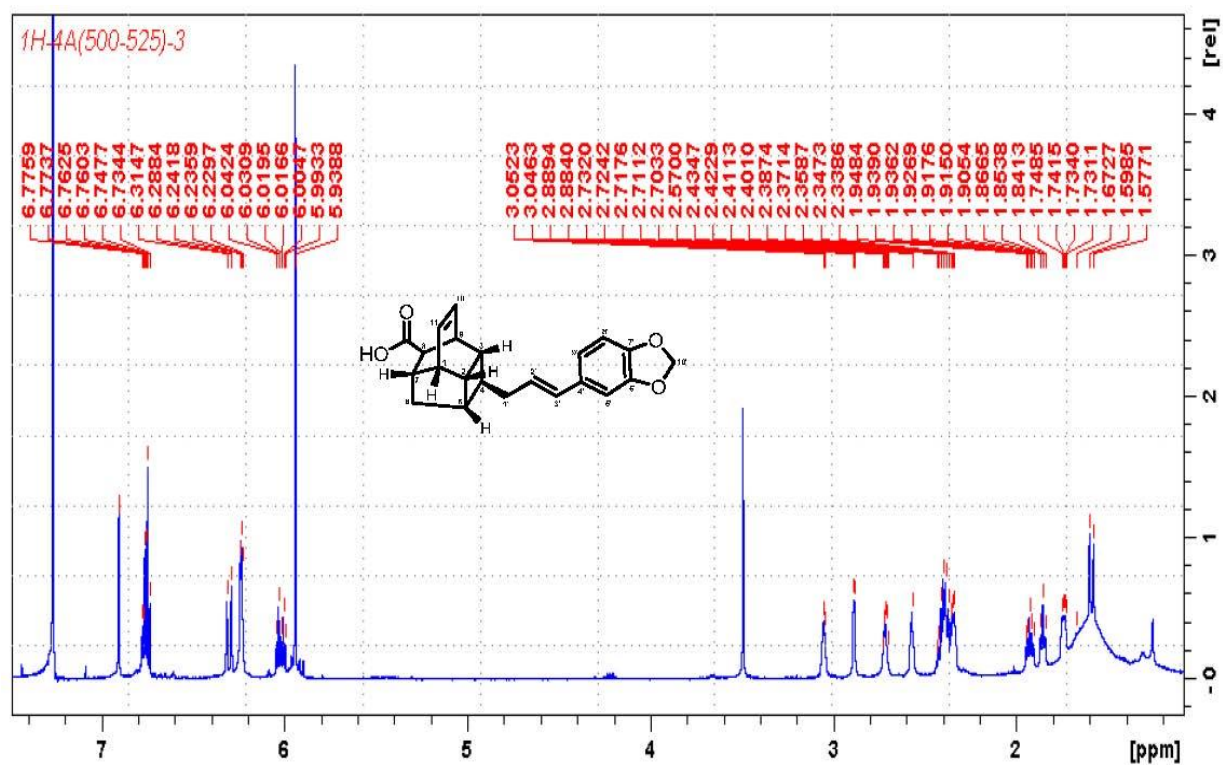
Figure S13. $^1\text{H-NMR}$ kingianic acid C (3) in CDCl_3 at 600 MHz.

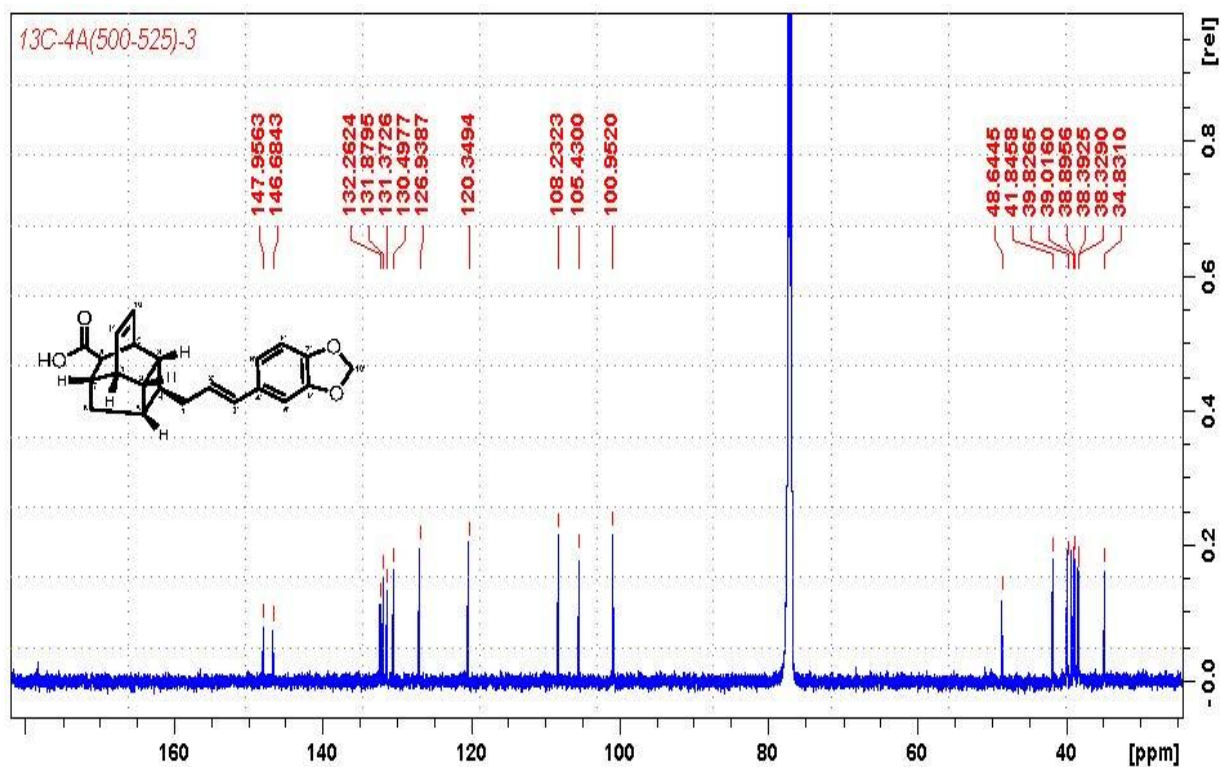
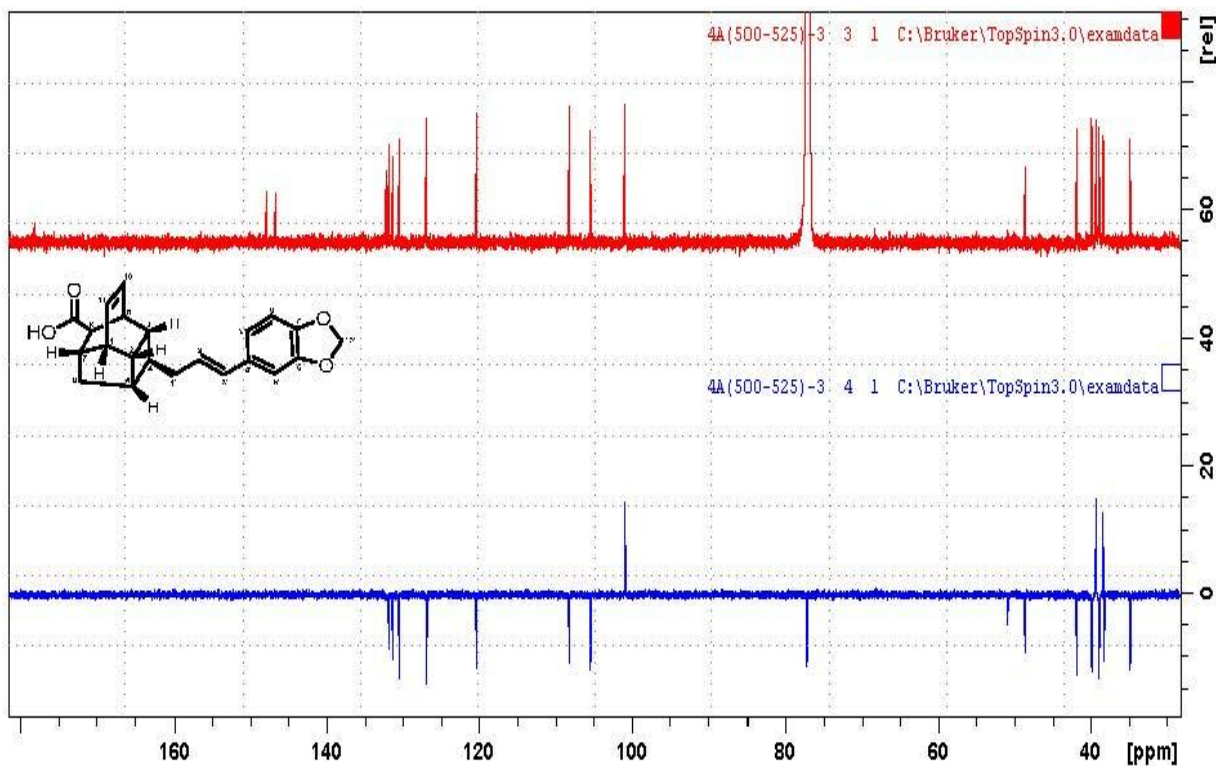
Figure S14. ^{13}C -NMR kingianic acid C (**3**) in CDCl_3 at 150 MHz.**Figure S15.** DEPT135 kingianic acid C (**3**) in CDCl_3 .

Figure S16. HRESIMS of kingianic acid D (4).

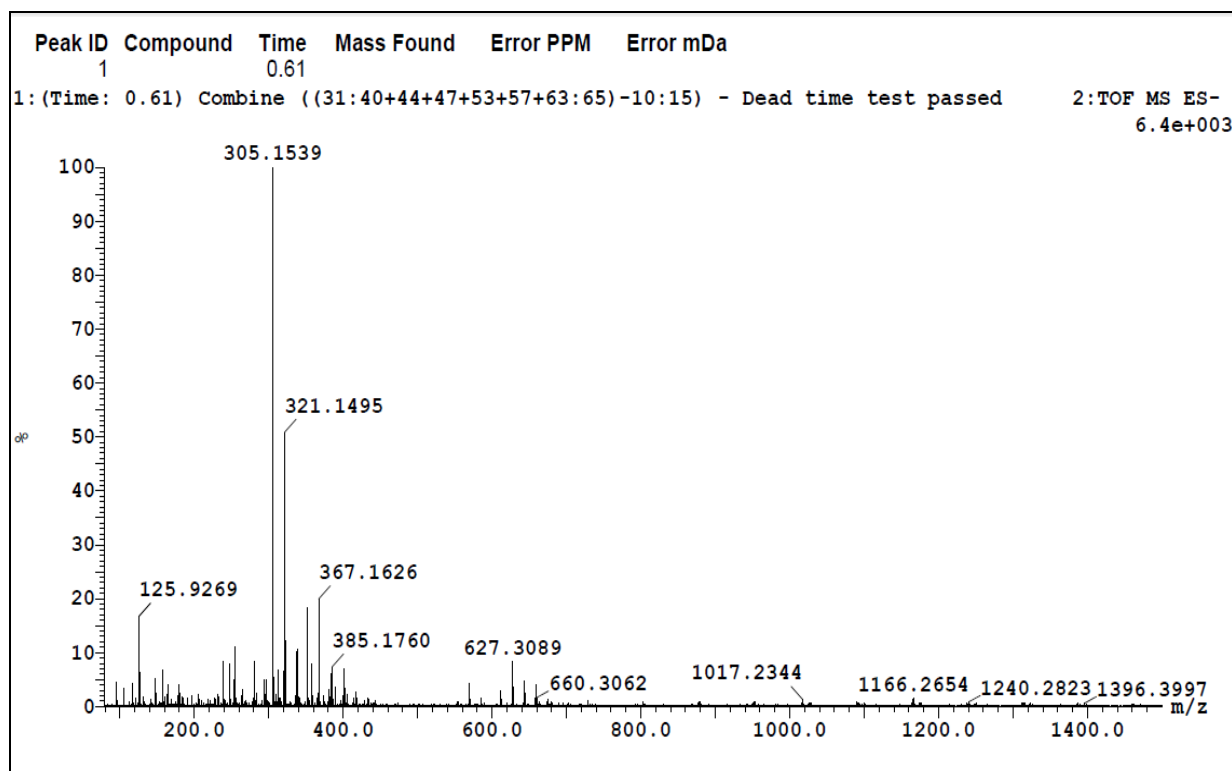
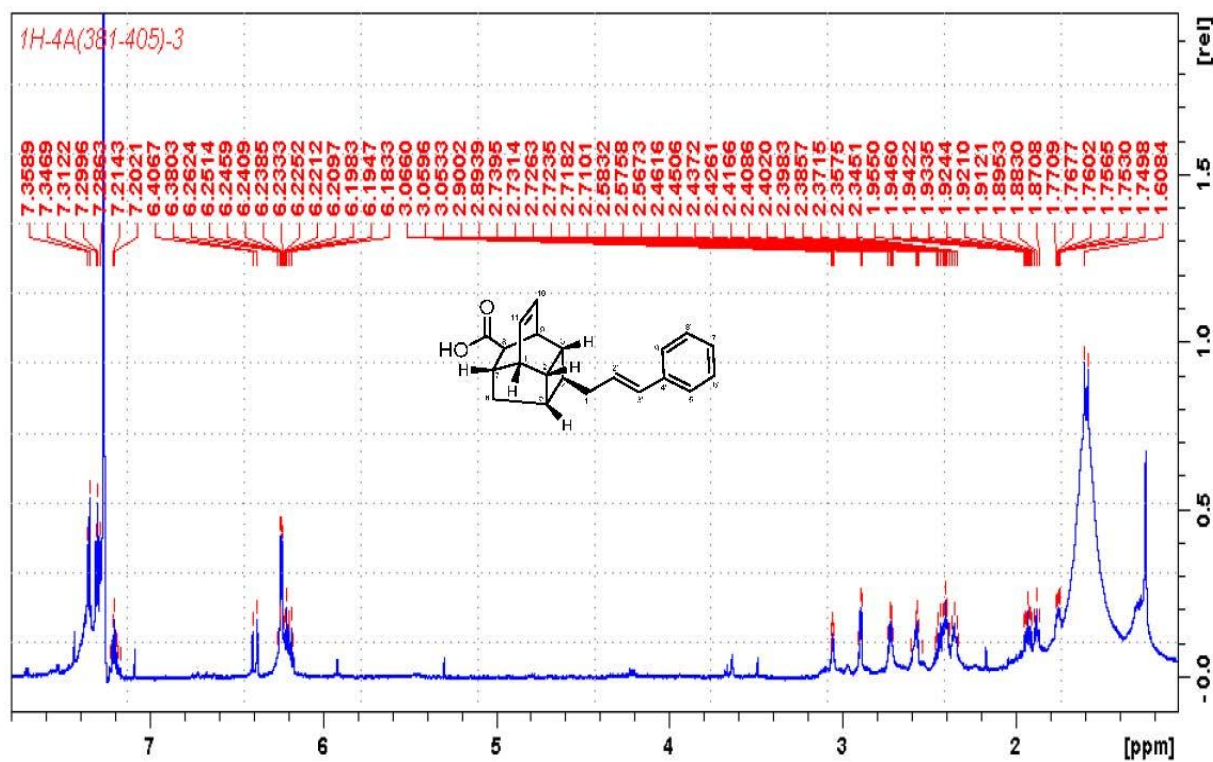
Figure S17. $^1\text{H-NMR}$ kingianic acid D (4) in CDCl_3 at 600 MHz.

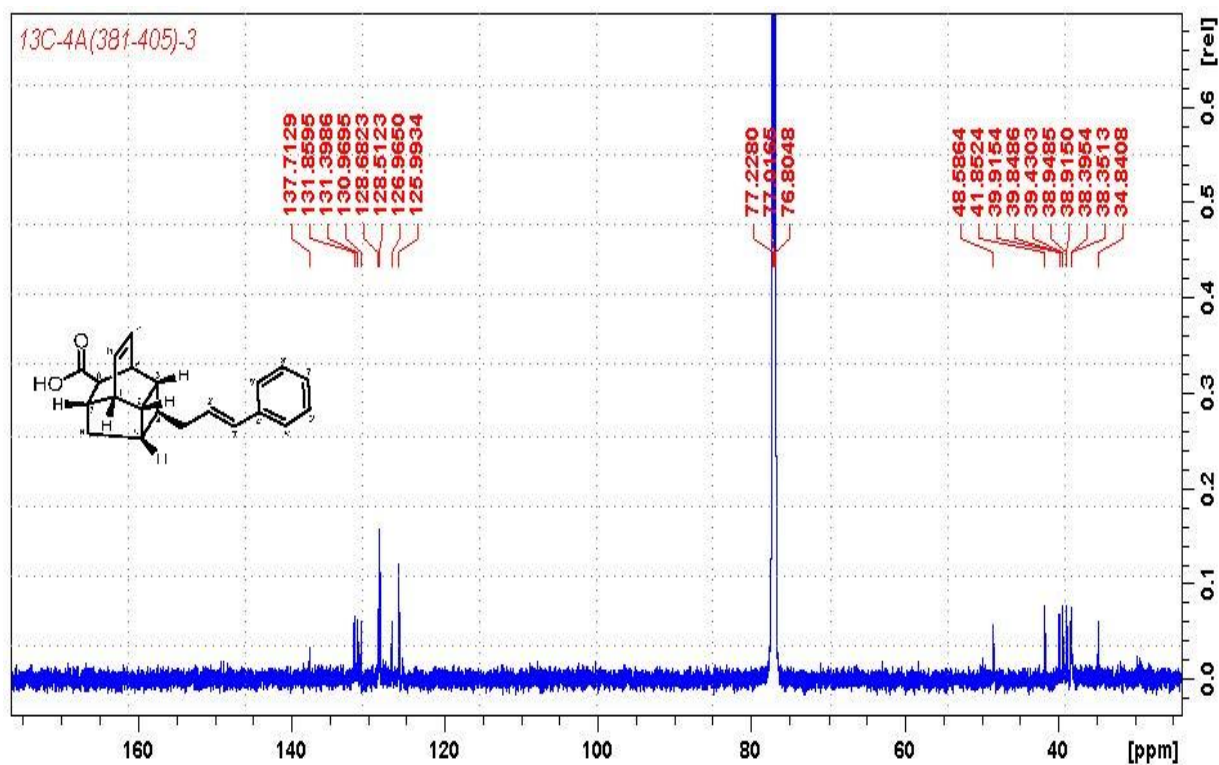
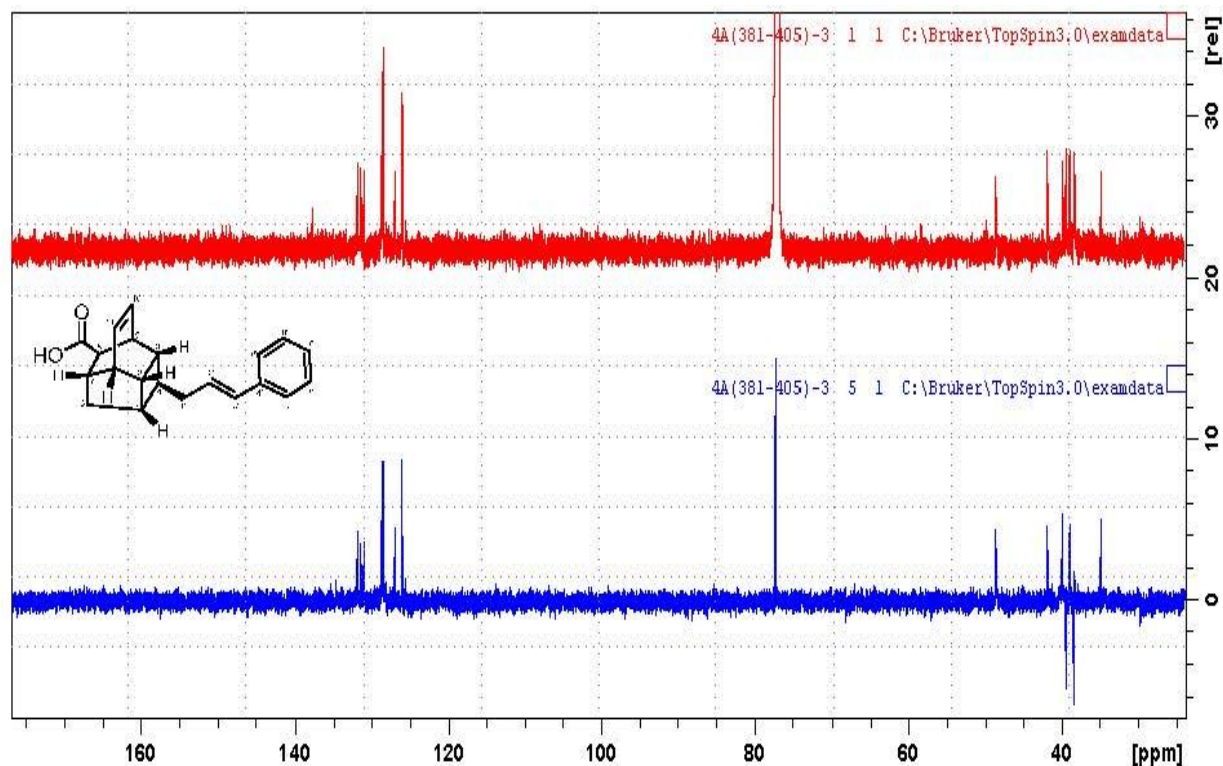
Figure S18. ^{13}C -NMR kingianic acid D (4) in CDCl_3 at 150 MHz.Figure S19. DEPT135 kingianic acid D (4) in CDCl_3 .

Figure S20. HRESIMS of kingianic acid E (5).

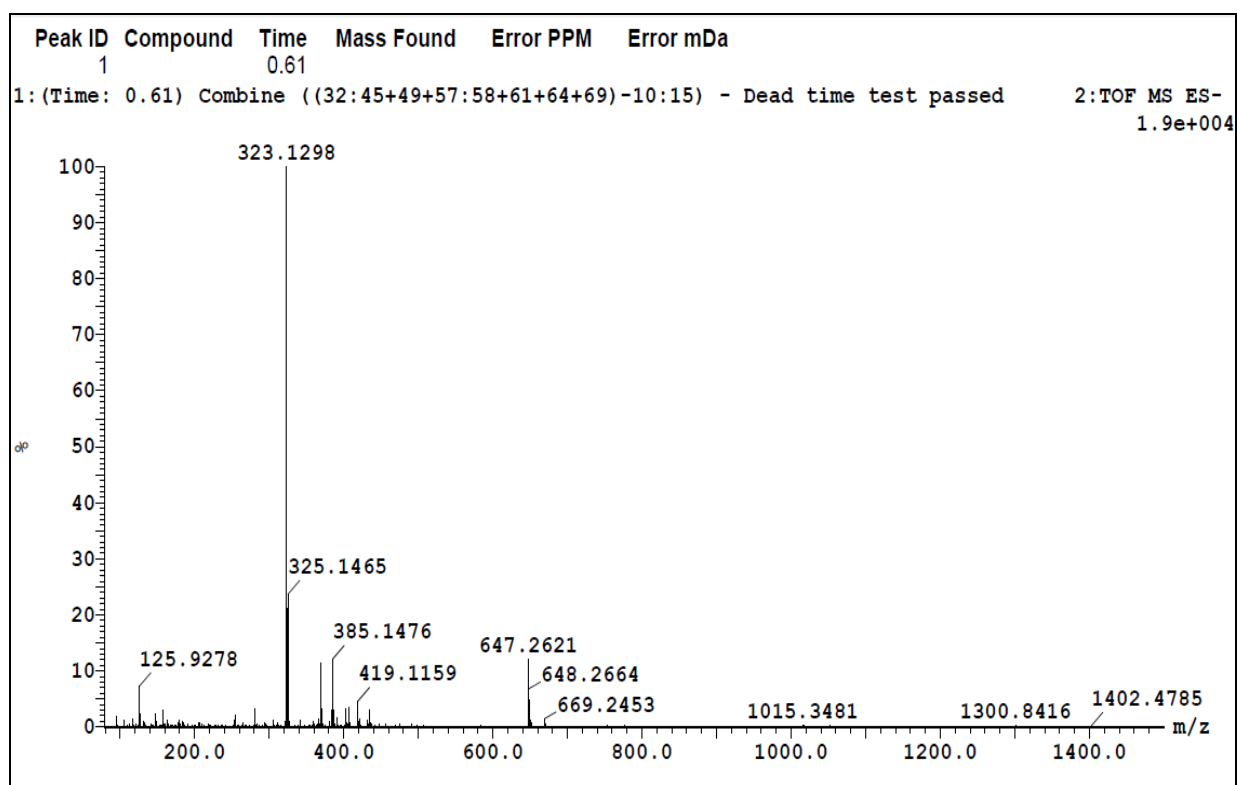
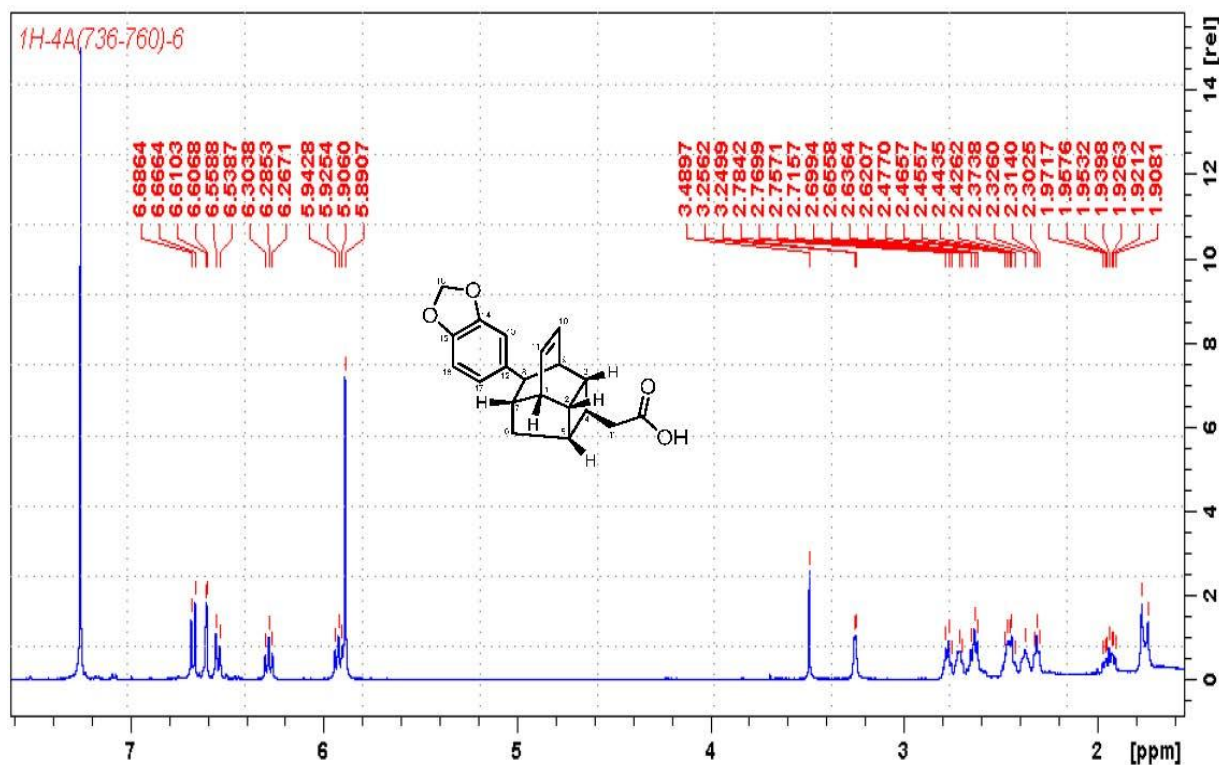
Figure S21. ¹H-NMR kingianic acid E (5) in CDCl₃ at 600 MHz.

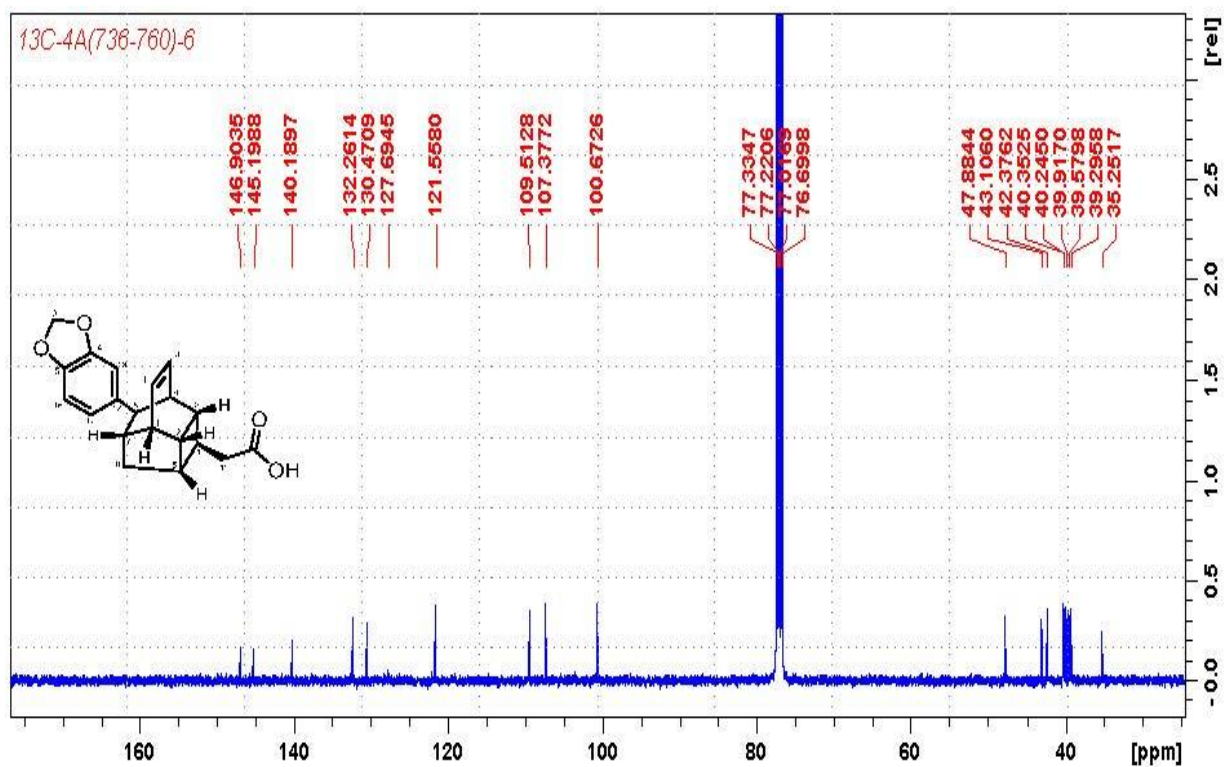
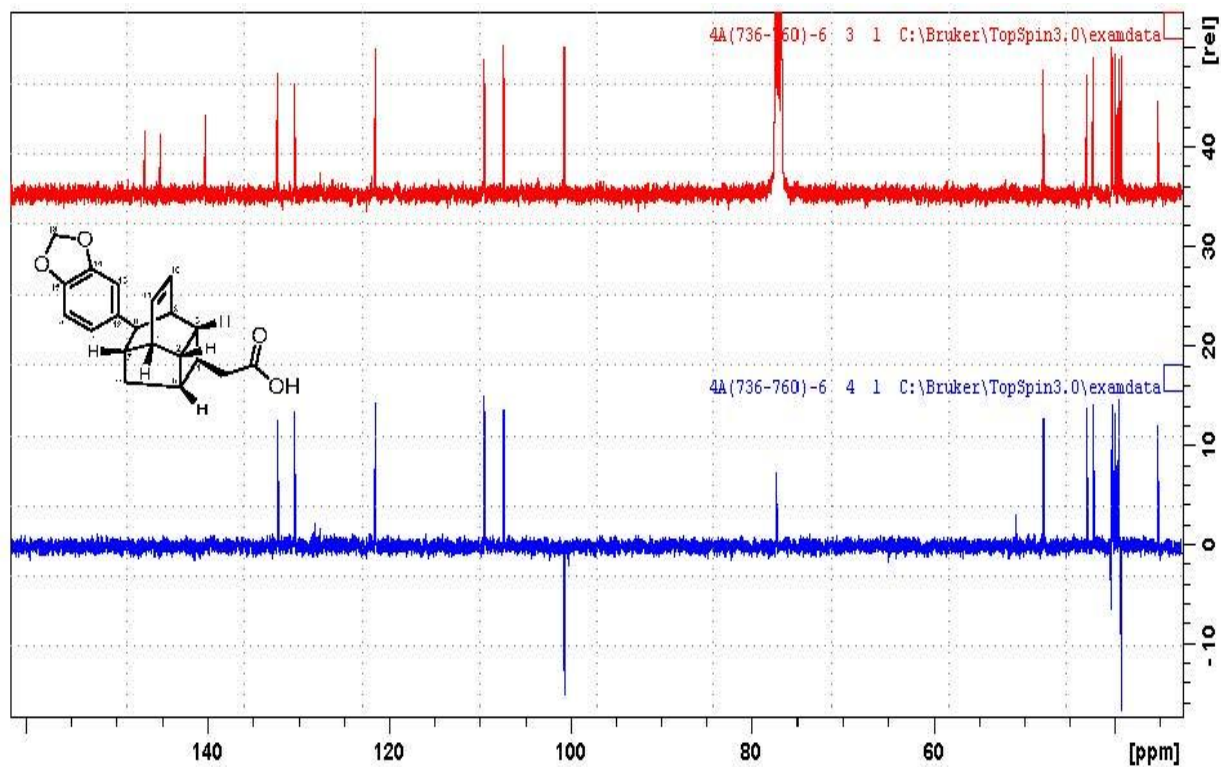
Figure S22. ^{13}C -NMR kingianic acid E (5) in CDCl_3 at 150 MHz.Figure S23. DEPT135 kingianic acid E (5) in CDCl_3 .

Figure S24. HRESIMS of kingianic acid F (6).

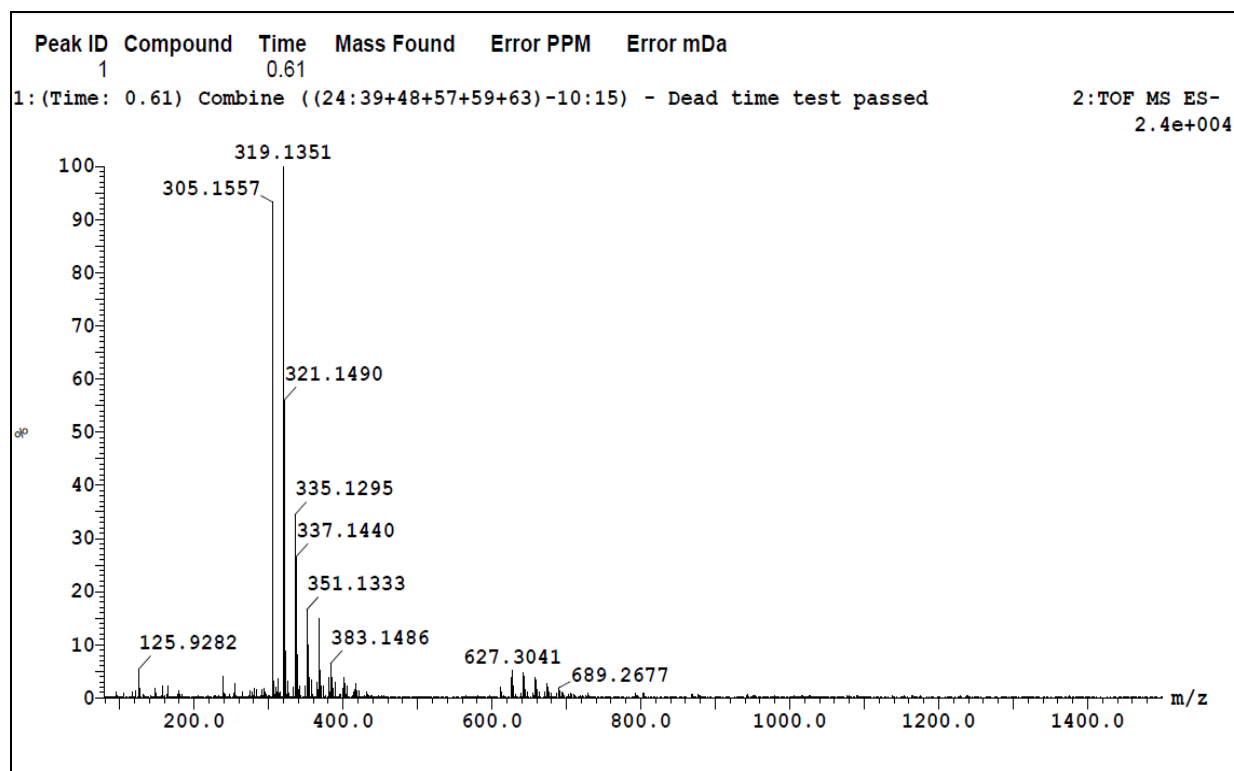
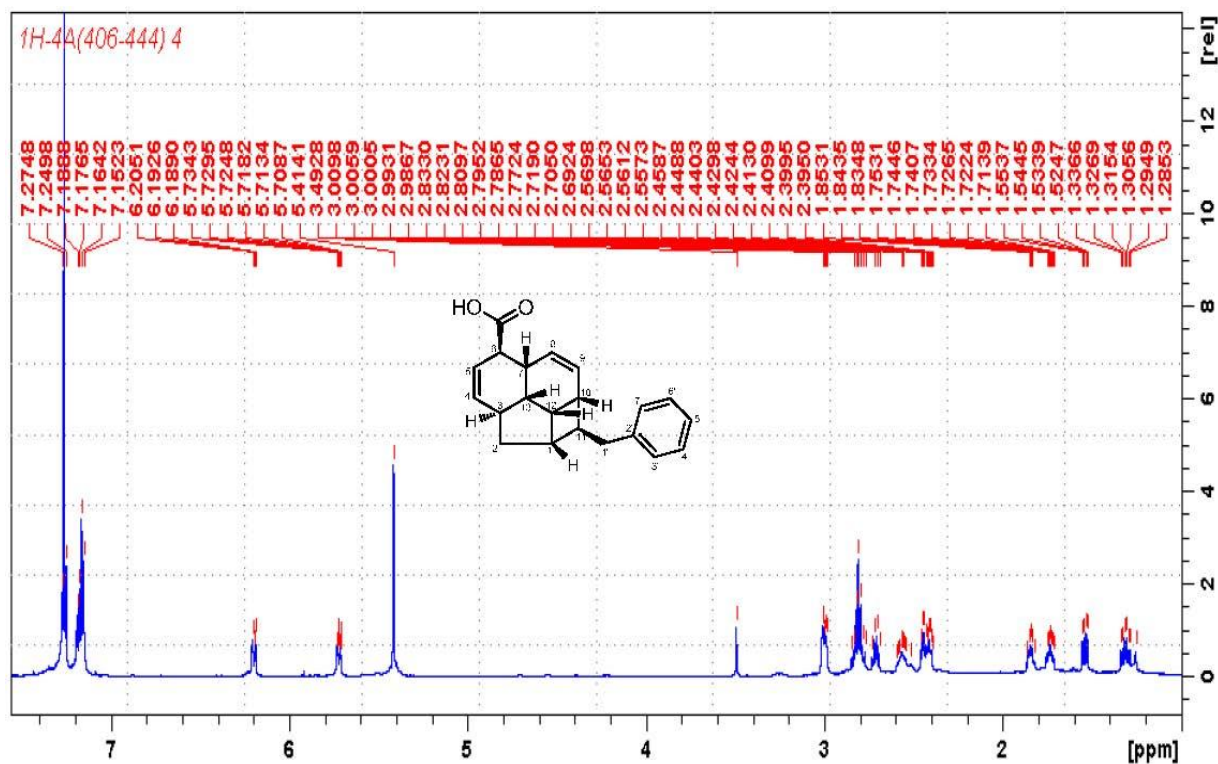
Figure S25. $^1\text{H-NMR}$ kingianic acid F (6) in CDCl_3 at 600 MHz.

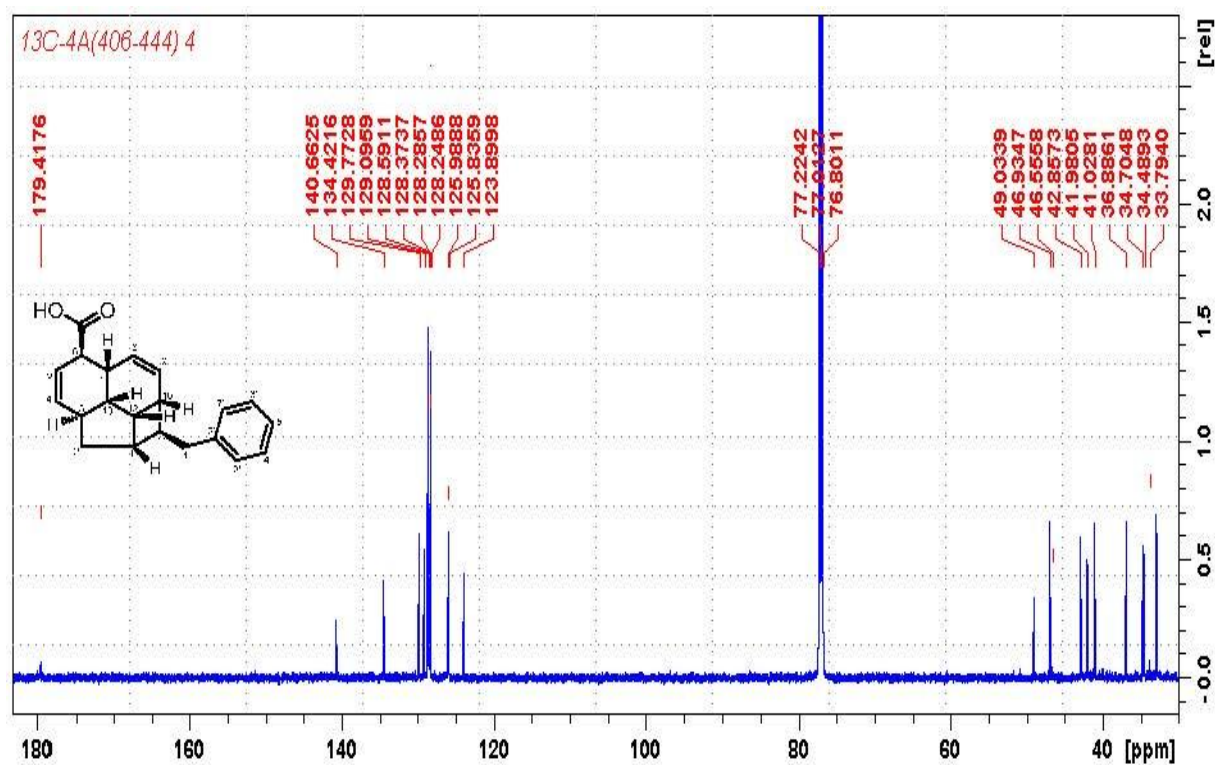
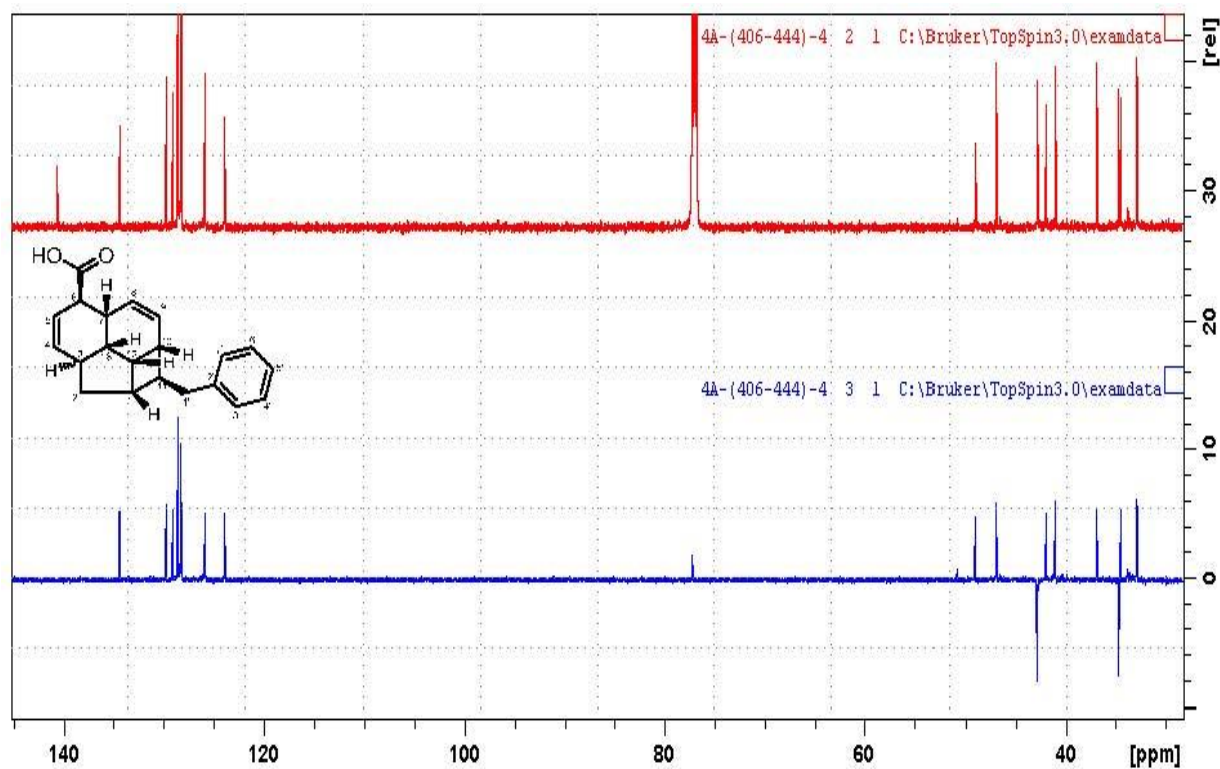
Figure S26. ^{13}C -NMR kingianic acid F (6) in CDCl_3 at 150 MHz.Figure S27. DEPT135 kingianic acid F (6) in CDCl_3 .

Figure S28. HRESIMS of kingianic acid G (7).

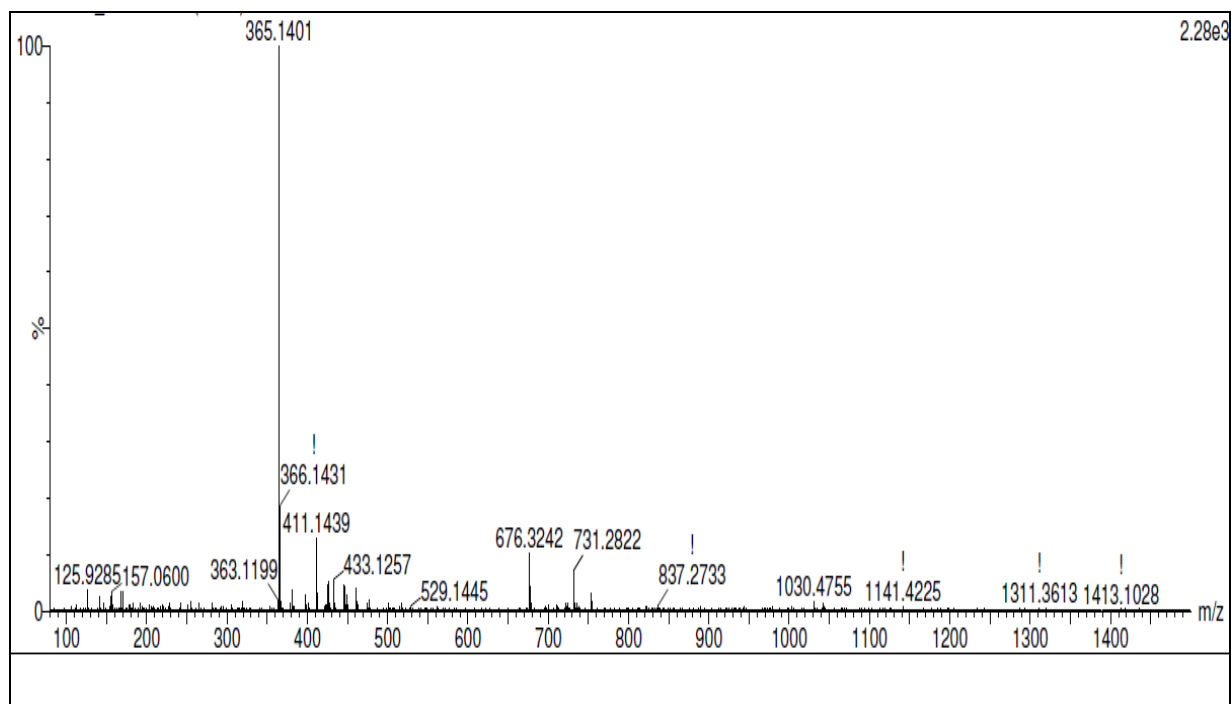
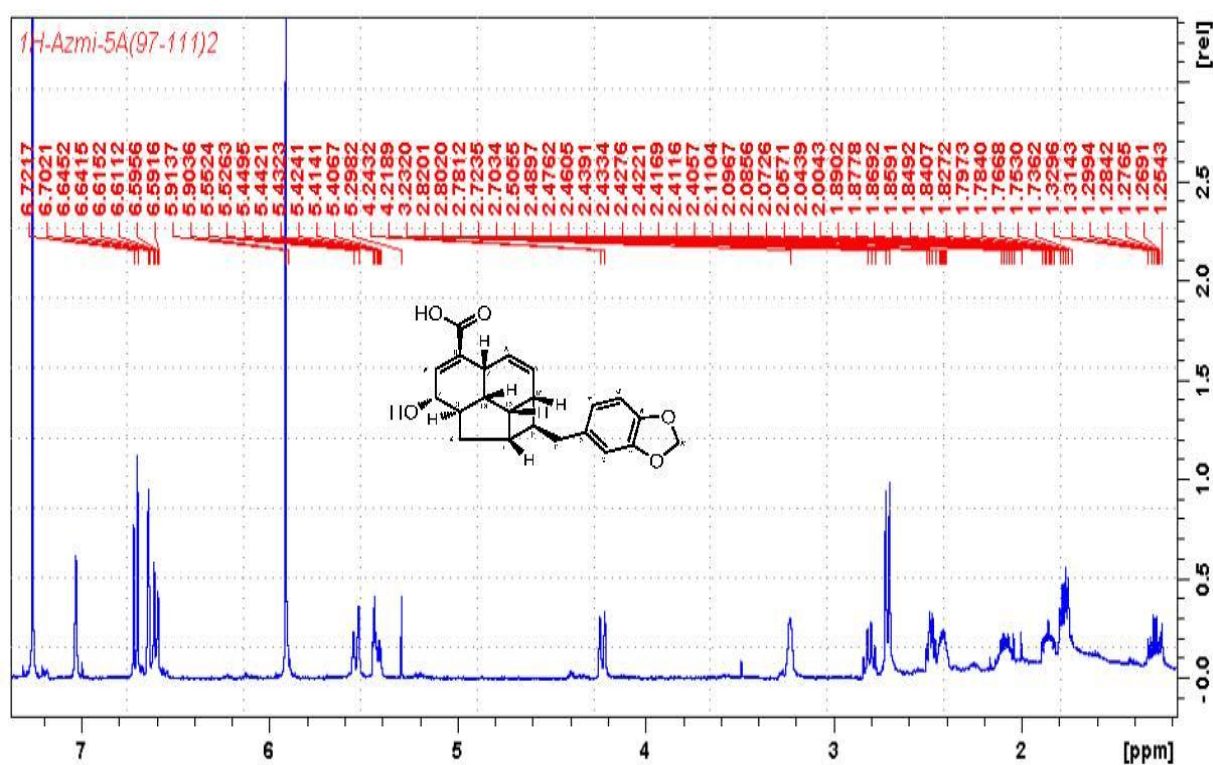
Figure S29. $^1\text{H-NMR}$ kingianic acid G (7) in CDCl_3 at 600 MHz.

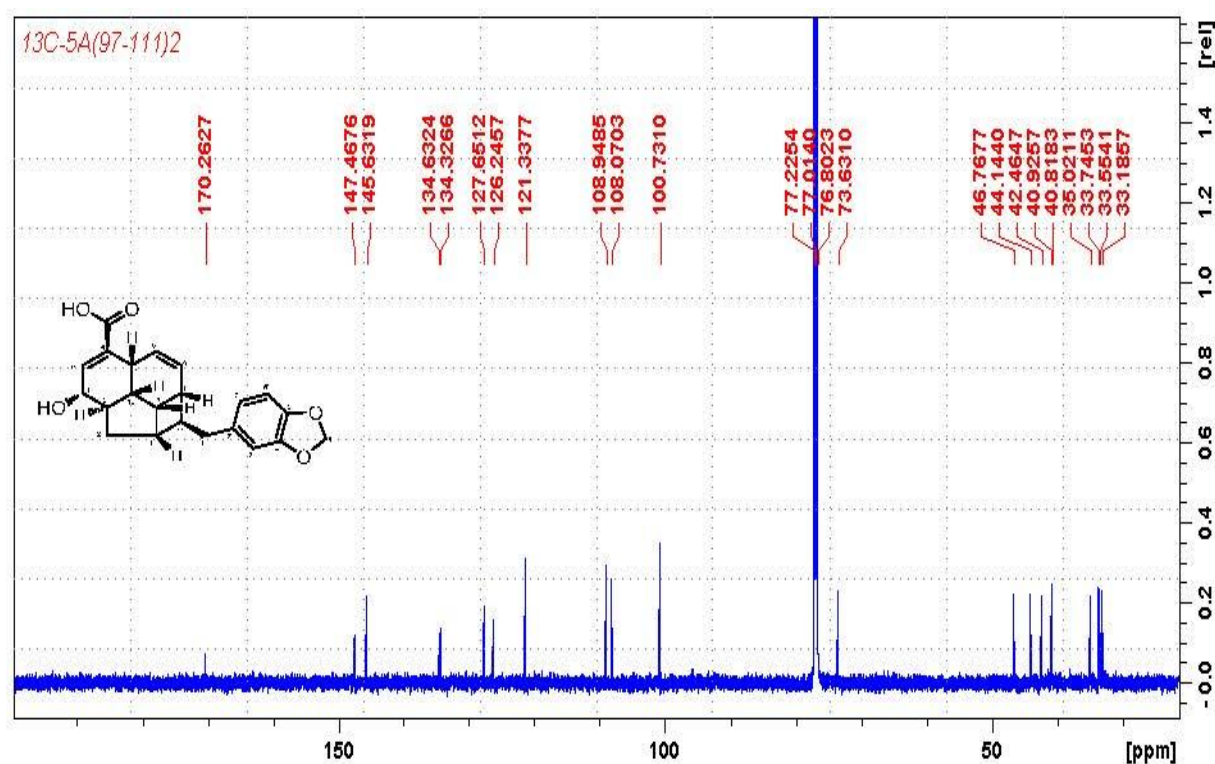
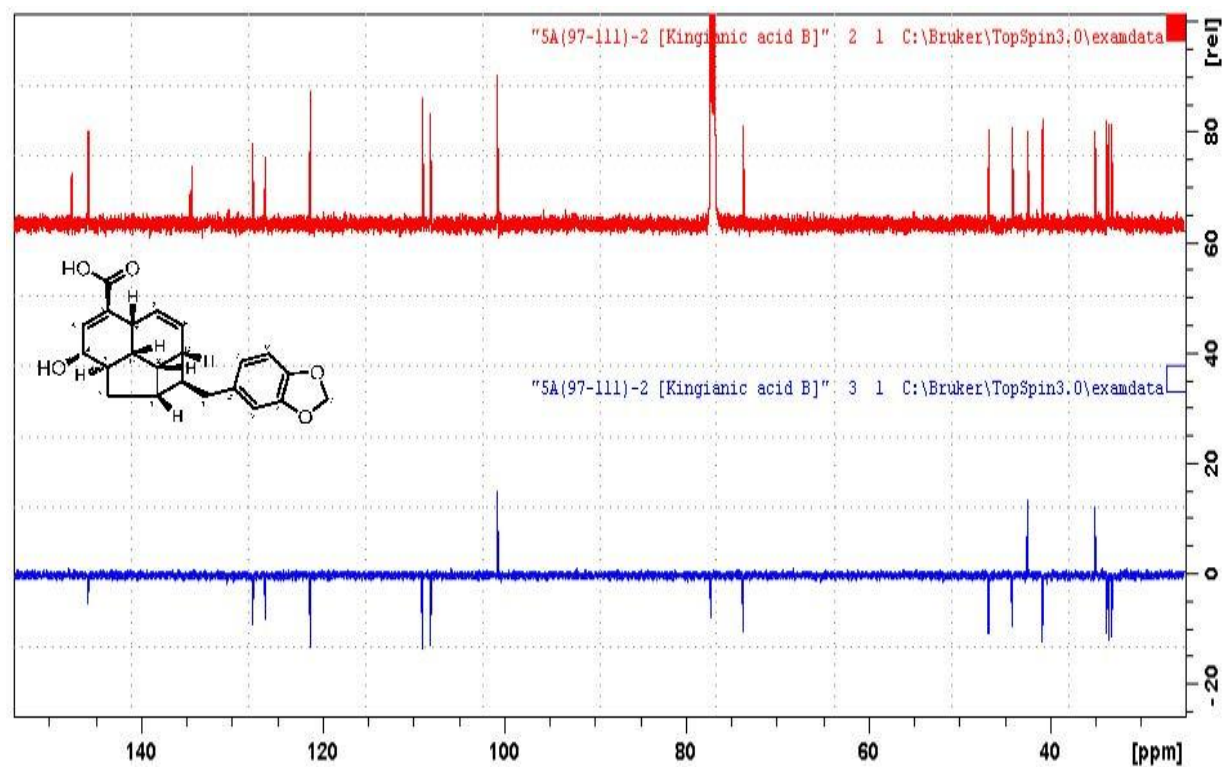
Figure S30. ^{13}C -NMR kingianic acid G (7) in CDCl_3 at 150 MHz.Figure S31. DEPT135 kingianic acid G (7) in CDCl_3 .

Figure S32. HRESIMS of endiandric acid M (8).

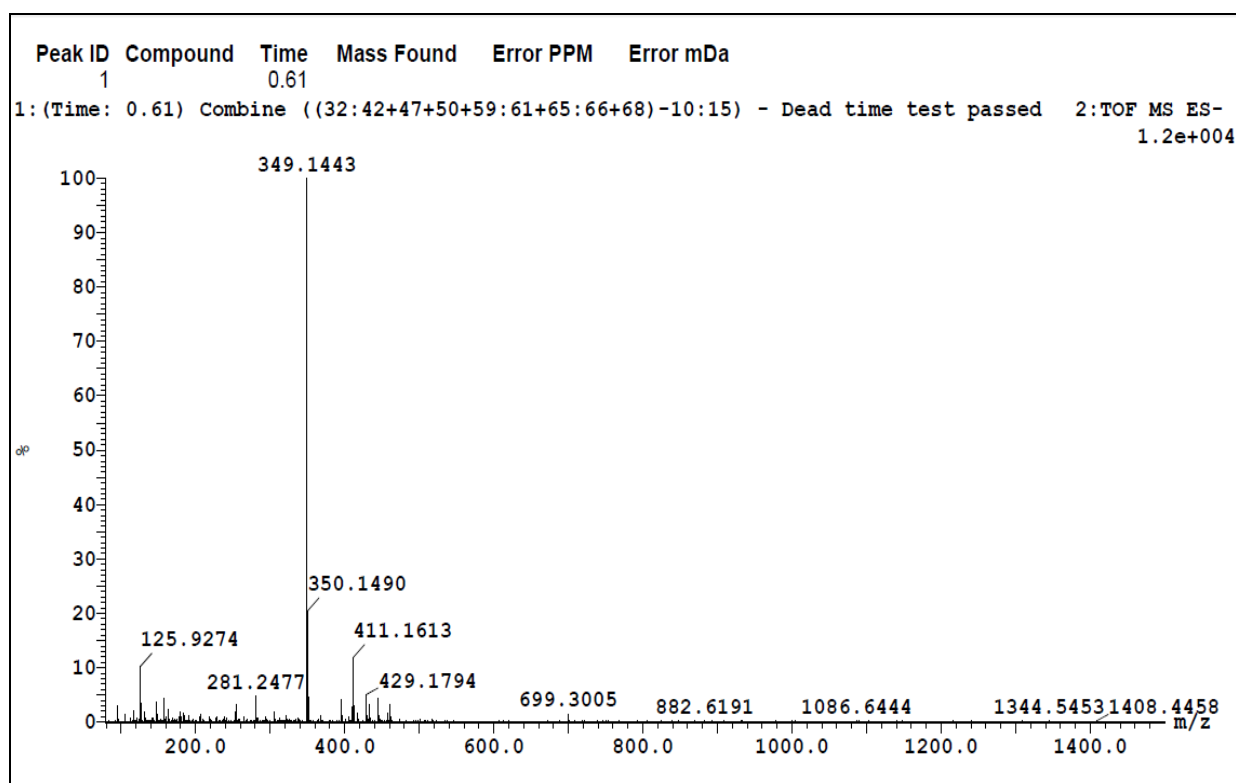
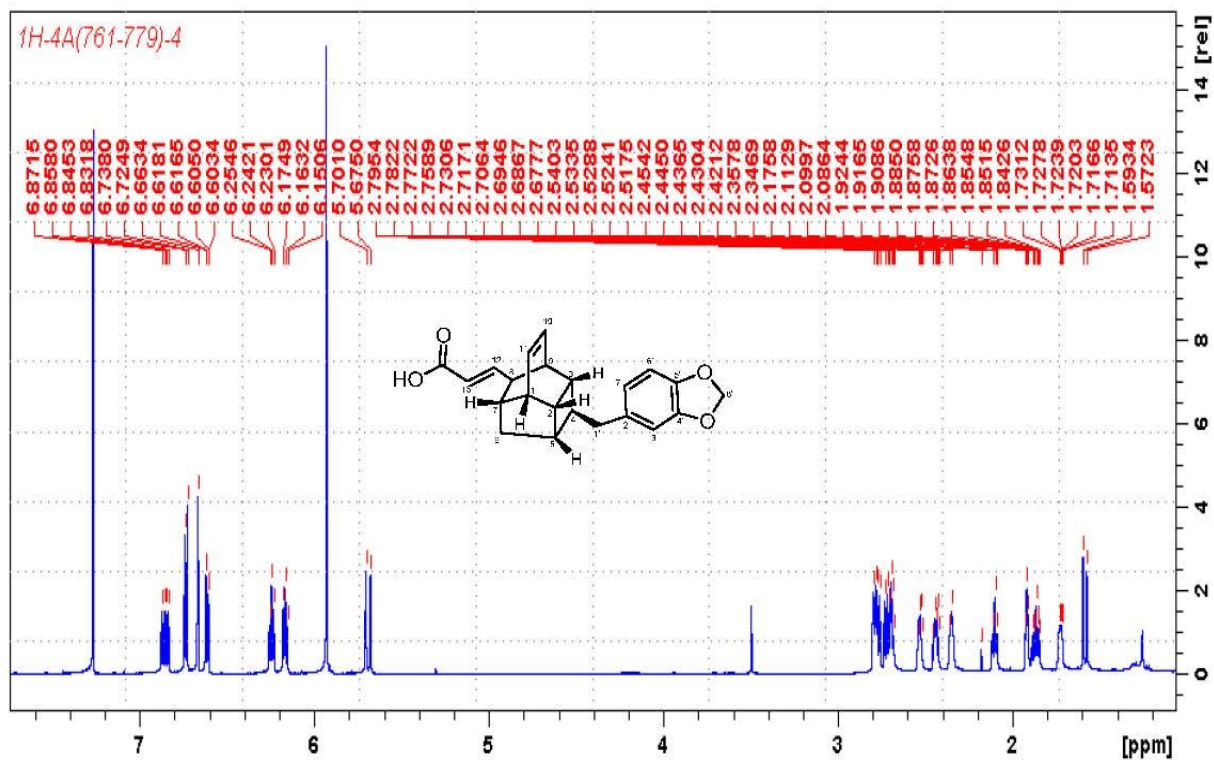
Figure S33. $^1\text{H-NMR}$ endiandric acid M (8) in CDCl_3 at 600 MHz.

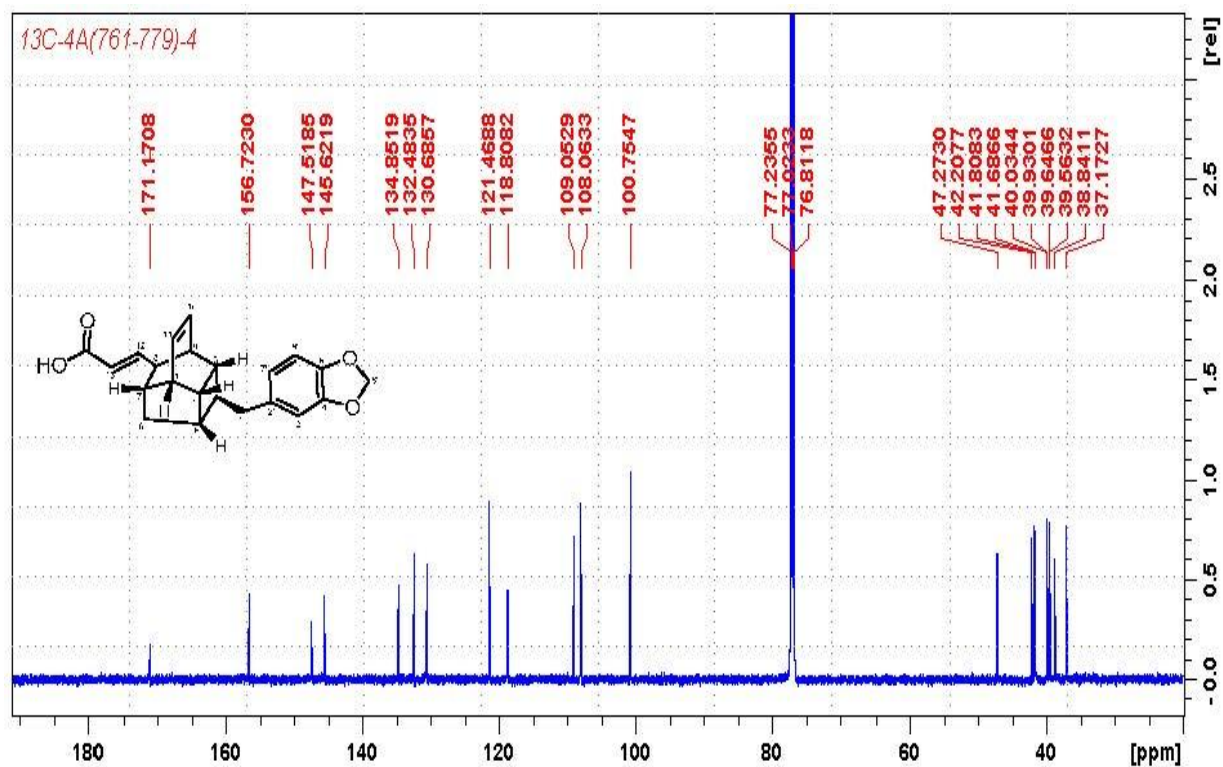
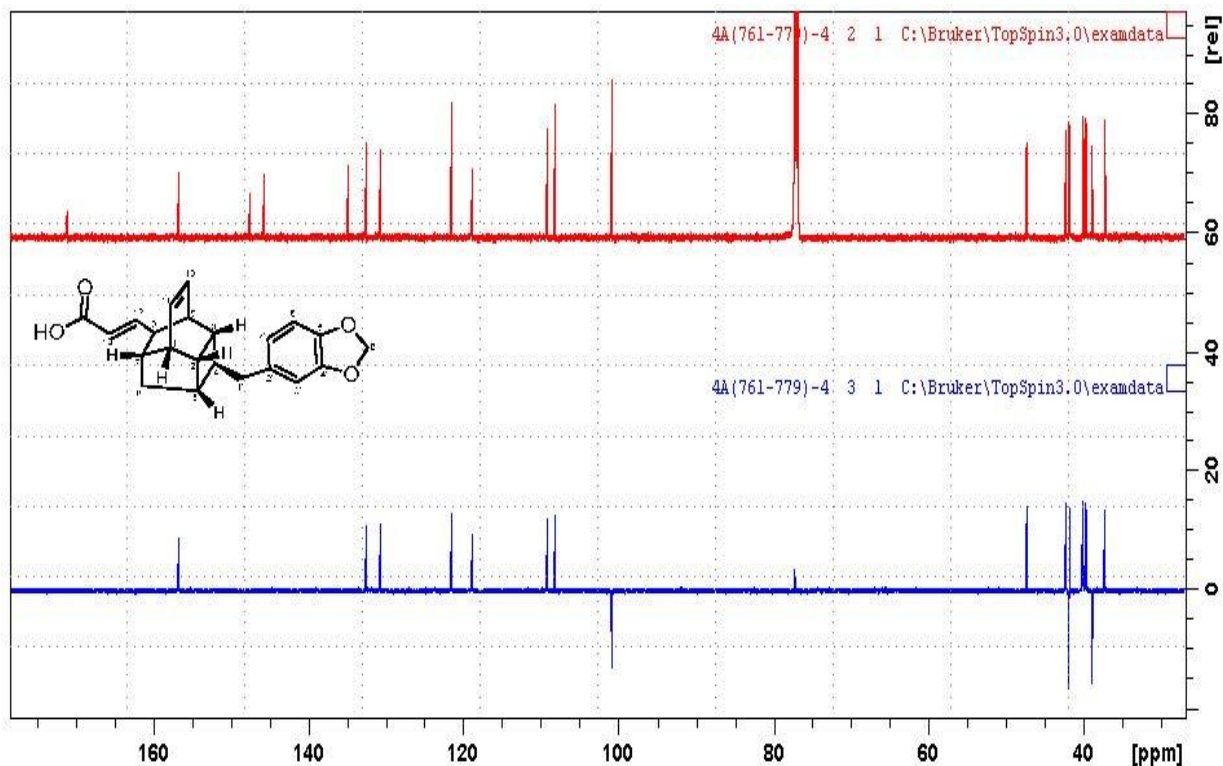
Figure S34. ^{13}C -NMR endiandric acid M (8) in CDCl_3 at 150 MHz.Figure S35. DEPT135 endiandric acid M (8) in CDCl_3 .

Figure S36. HRESIMS of endiandric acid 10.

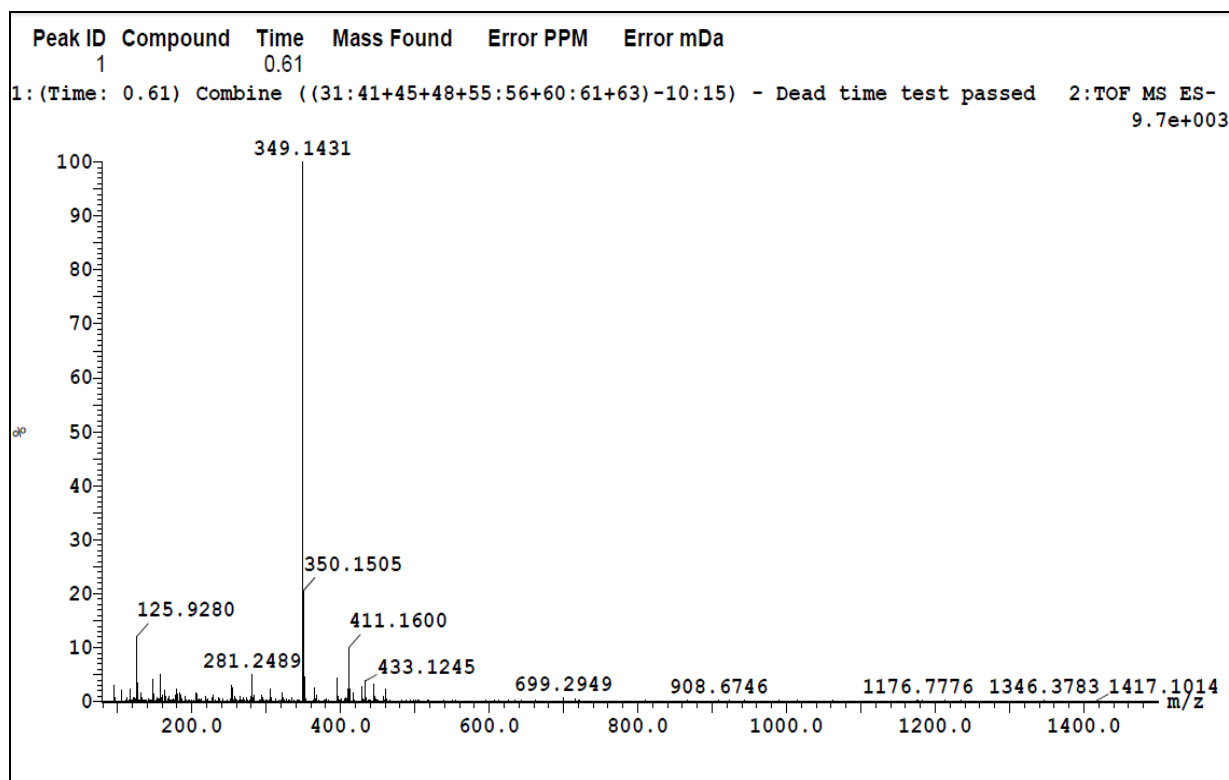
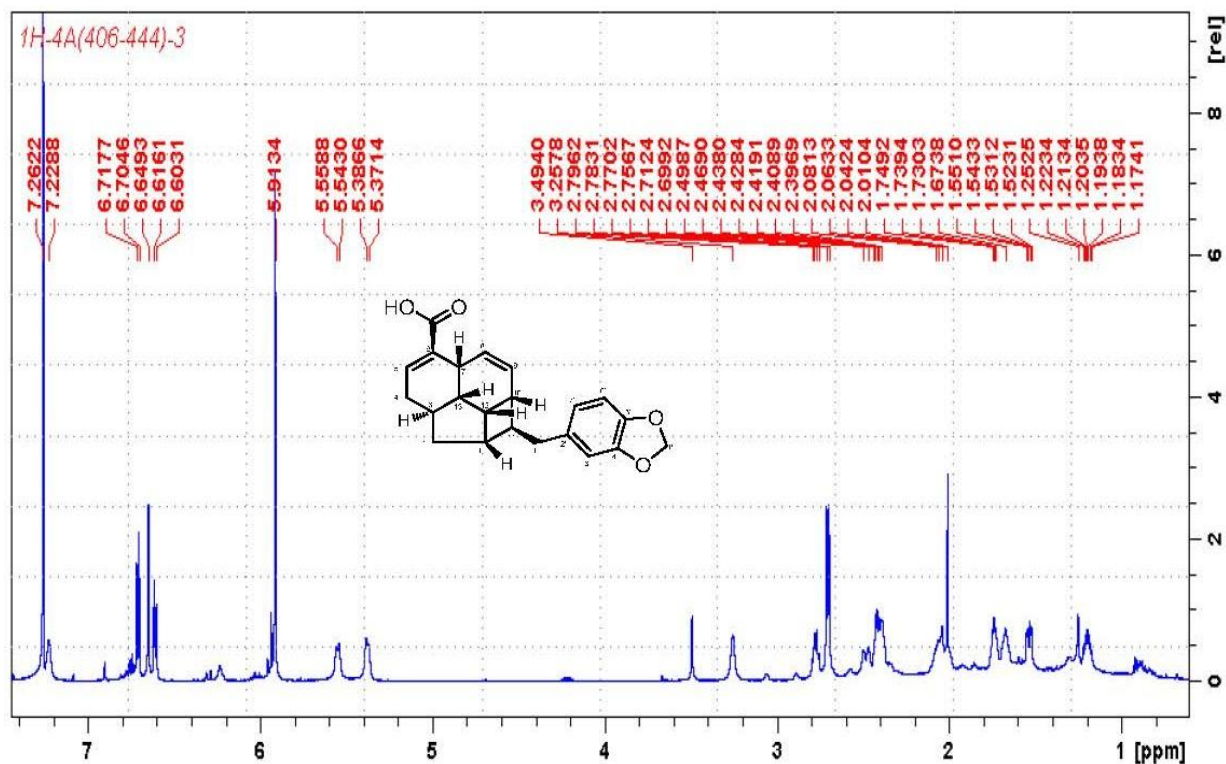
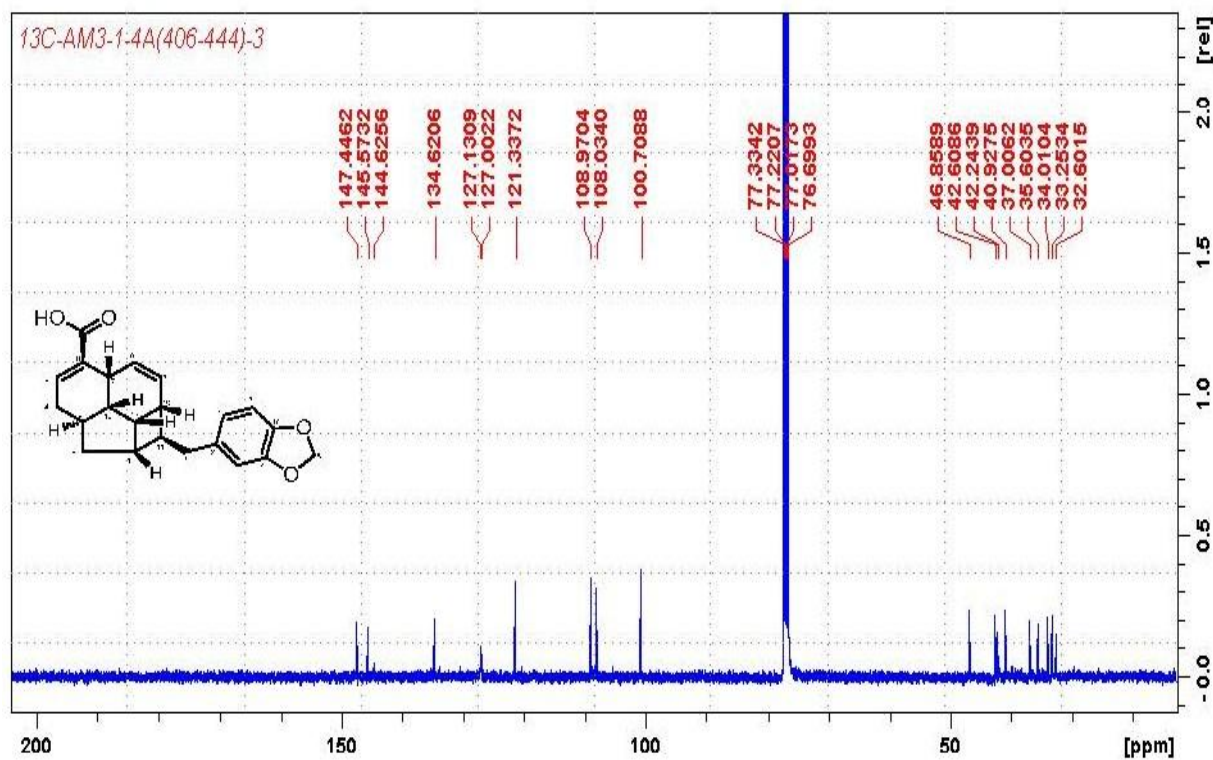
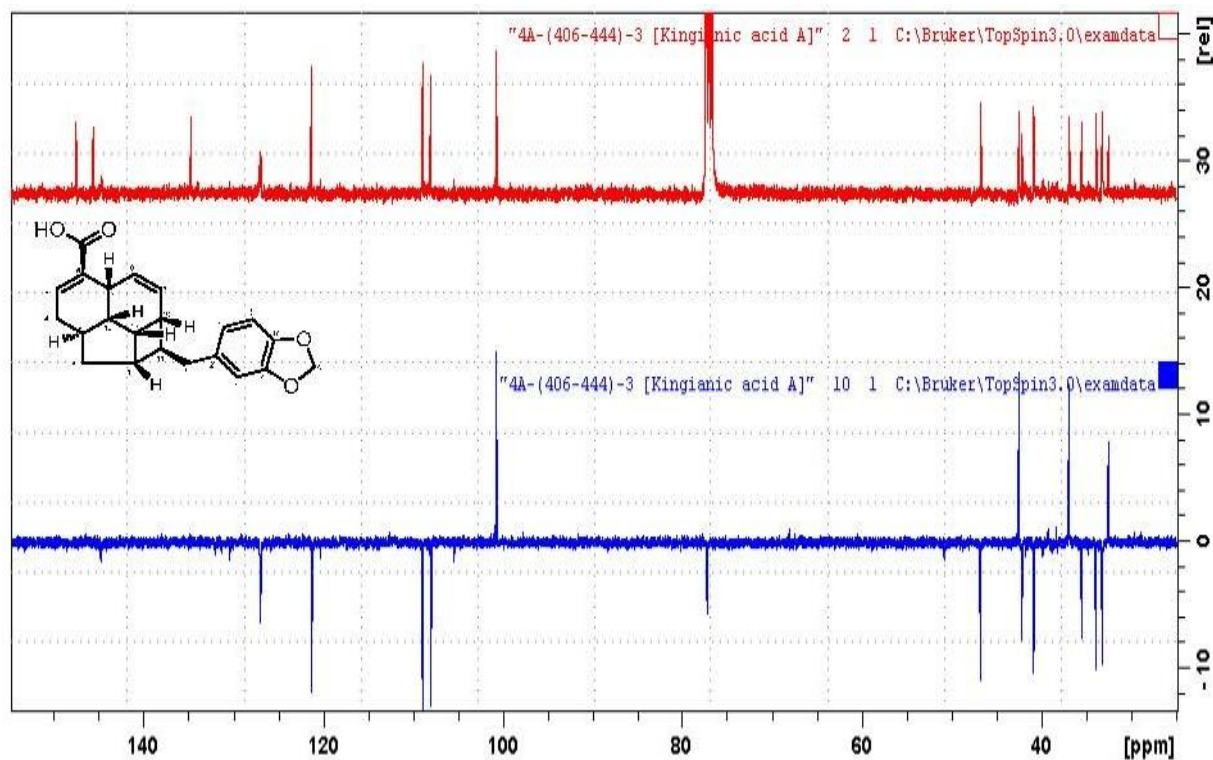
Figure S37. $^1\text{H-NMR}$ endiandric acid 10 in CDCl_3 at 600 MHz.

Figure S38. ^{13}C -NMR endiandric acid **10** in CDCl_3 at 150 MHz.**Figure S39.** DEPT135 endiandric acid **10** in CDCl_3 .

Sequences alignment of Bcl-xL and Mcl-1 with Bak-BH3 and Bid-BH3 peptides, respectively.

Both protein targets include an N-terminal His-tag followed by the thrombin cleavage site, to facilitate purification. Our Bcl-xL construct includes the four homology domains of the human protein, whereas our Mcl-1 construct includes the three homology domains of the mouse protein. Trans-membrane domains have been deleted in both sequences.

Bak (PolyP) →	-----GQ----- 2
Bcl-xL(ICSN)→	MHHHHHHSSGLVPRGSEFMSQ SNRELVVDFLSYKLSQKGYSW SQFSDVEENRTE APEGTE 60
Bak (PolyP) →	--- VGRQLAIGDDINR ----- 16
Bcl-xL(ICSN)→	SEA VKQALREAGDEFELR YRRAFSDLTSQLHITPGTAYQSFEQVNV ELFRDGVNW GRIVA 120
Bak (PolyP) →	-----
Bcl-xL(ICSN)→	FFSFGG ALCVESVYKEMQVLVSRIAAWMATYLN DHLEPWIQENGGWDTFVELY G 174

- BH4 domain
- BH3 domain
- BH1 domain
- BH2 domain

Bid (PolyP) →	-----EDII----- RN I 7
Mcl-1 (ICSN)→	MGSSHHHHHHSSGLVPRGSHMEDDLRQ SLEIISRYLRE QATGSKDSKPLGEAGA AG RR A 60
Bid (PolyP) →	ARHLAQVGDSMDR ----- 20
Mcl-1 (ICSN)→	LETLRRVGDGVQRN HETAFQ GMLRKL DIKNEG DVKSFSRVMVH VFKDGV TNWG RIVTLIS 120
Bid (PolyP) →	-----
Mcl-1 (ICSN)→	FGAFVAKHLKSVNQESFIEPLAETITDVLV RTKR DWL VK QRGW DFVEFF HVQD LE 176

- BH3 domain
- BH1 domain
- BH2 domain