

Supplementary material

CHEMODIVERSITY AND ANTI-LEUKEMIA EFFECT OF METABOLITES FROM *Penicillium setosum*

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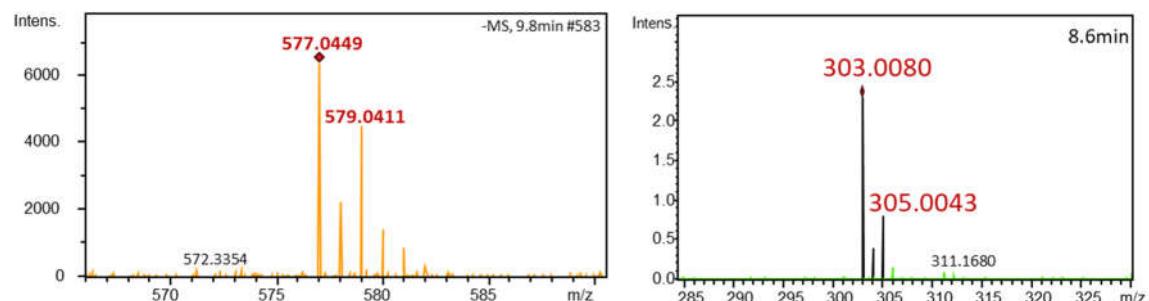


Figure S1: Mass spectrum (ESI-) of some peaks found in the base peak chromatogram obtained from the methanolic extracts of *Penicillium setosum* CMLD 18 (9.8 min.; 8.6 min.).



Figure S2. Macroscopic pictures of *Penicillium setosum* CMLD 18 in PDA and YES growth medium respectively.

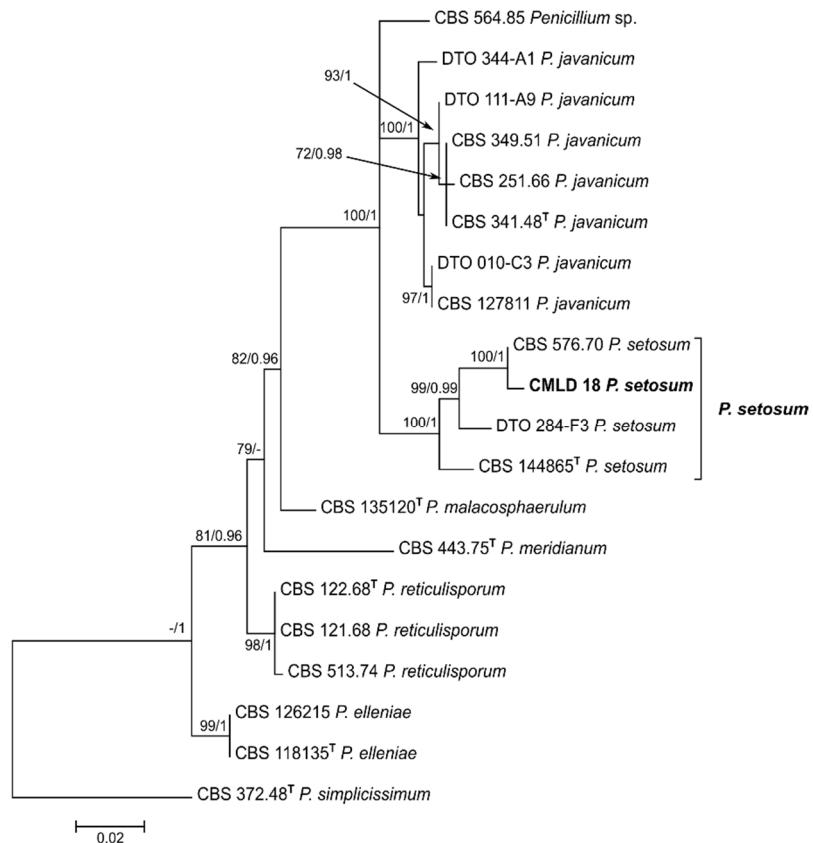


Figure S3: Bayesian Inference and Maximum Likelihood phylogenetic analyses of partial beta tubulin gene sequences placed the strain CMLD 18 inside a well-supported clade composed of the ex-type and other reference strains of *Penicillium setosum*. Morphological characterization of CMLD 18 using standard media and conditions used in *Penicillium* taxonomy (Visagie et al. 2014) supported the identification (data not shown).

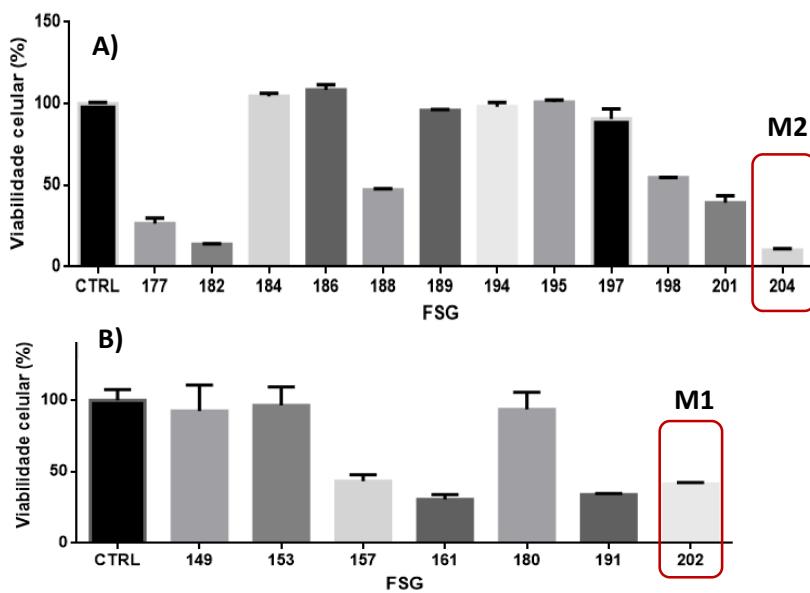


Figure S4: Cell viability of the methanolic fraction obtained from *P. setosum* cultivated in rice (A, M2) and hominy (B, M1) (highlighted in red) against the cell line KG-1 and Kasumi-1, respectively.

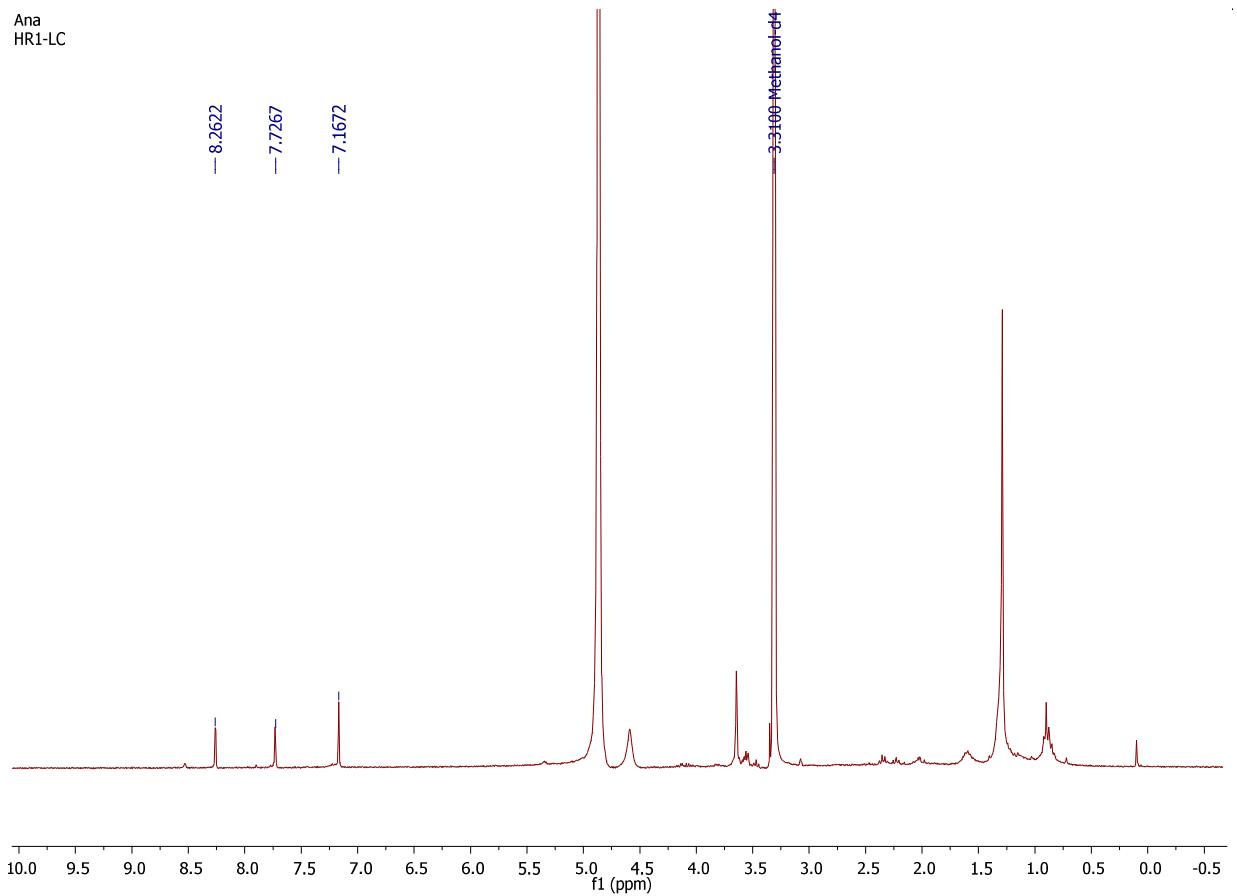


Figure S5: ^1H NMR spectrum of 2-chloroemodic acid (2) (300 MHz, methanol-*d*4).

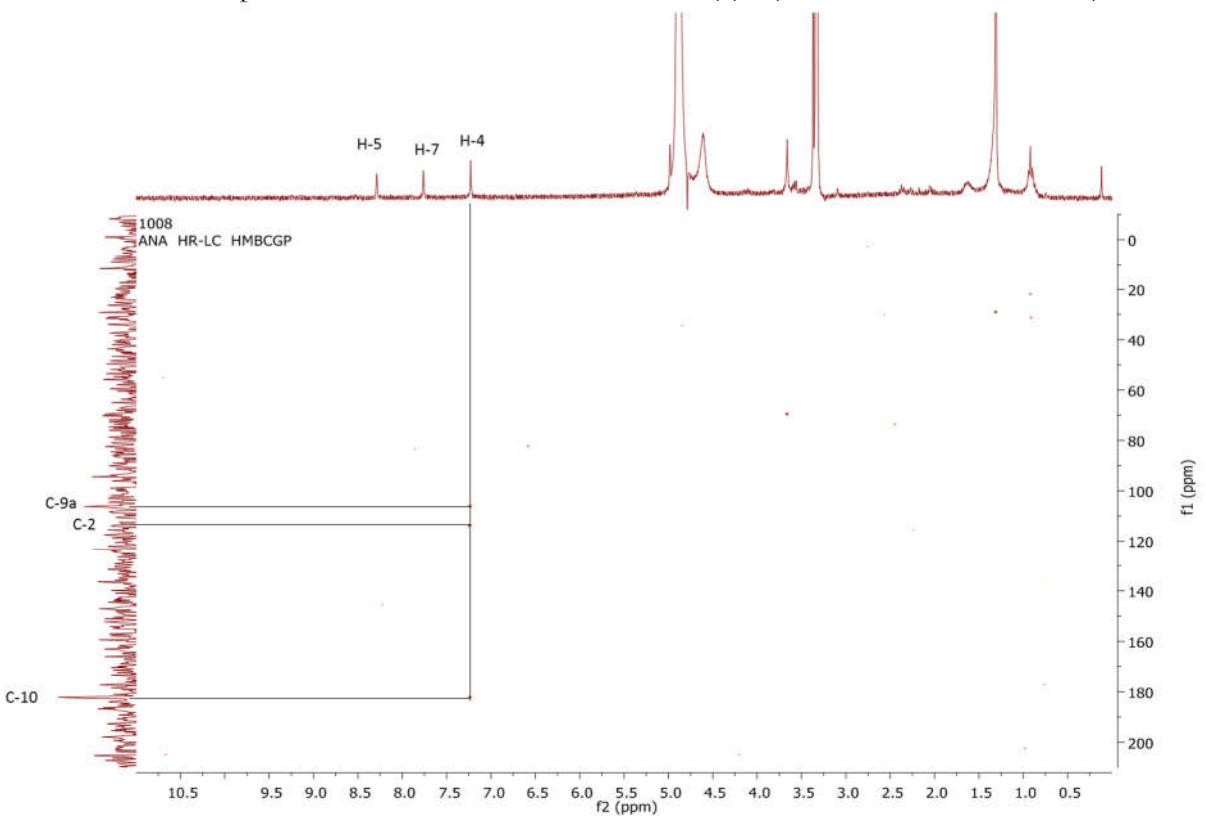


Figure S6: HMBC spectrum of 2-chloroemodic acid (2) (300 MHz, methanol-*d*4).

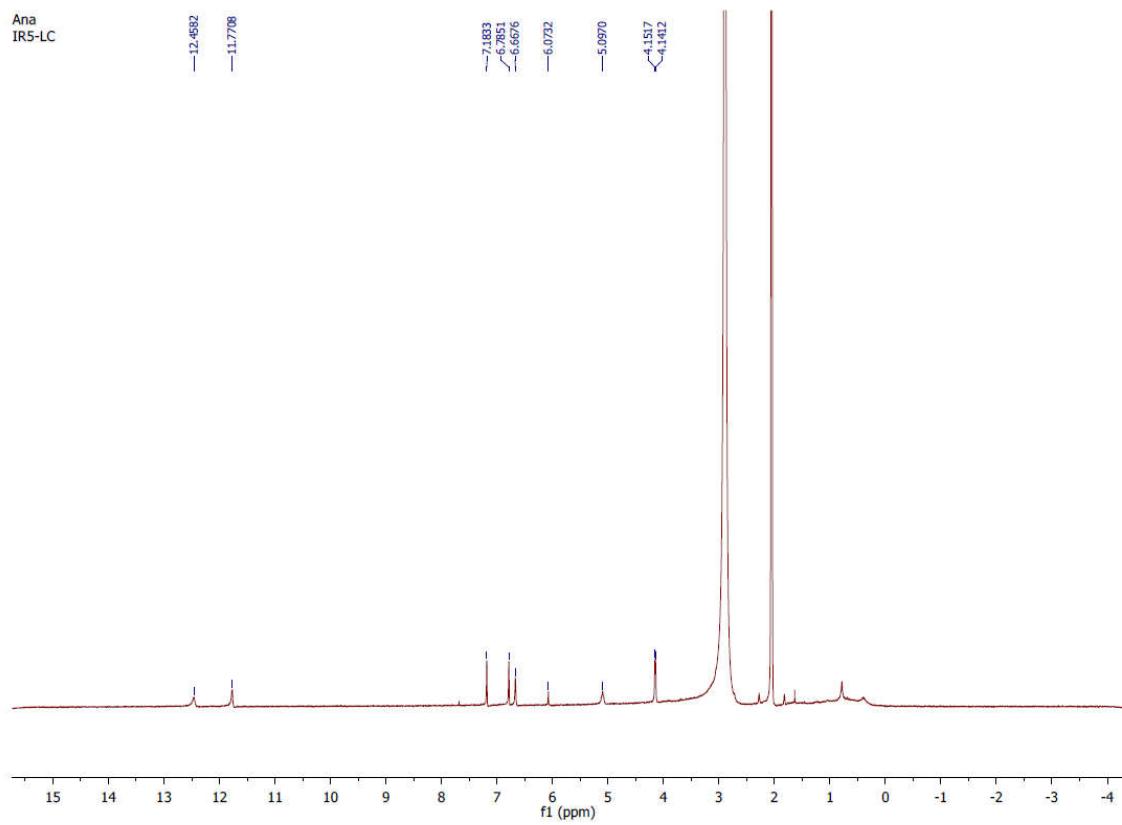


Figure S7: ¹H NMR spectrum of 2-chloro-1,3,8-trihydroxy-6-(hydroxymethyl)-anthraquinone (7) (300 MHz, acetone-d₆).

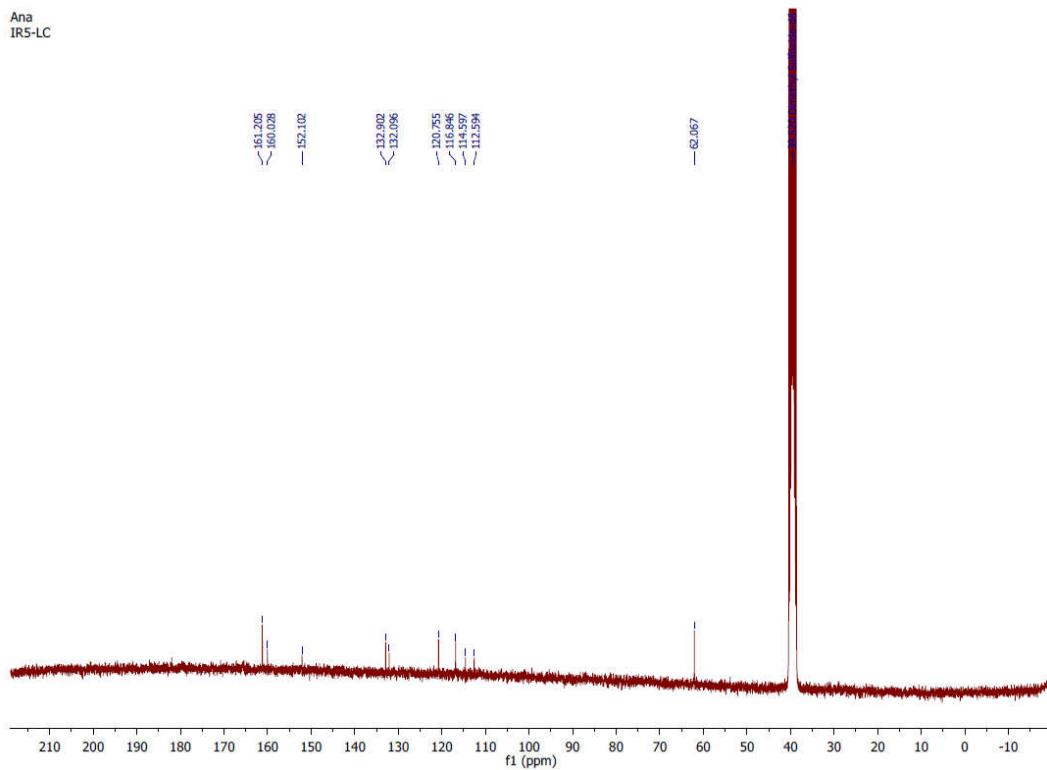


Figure S8: ¹³C NMR spectrum of 2-chloro-1,3,8-trihydroxy-6-(hydroxymethyl)-anthraquinone (7) (300 MHz, DMSO-d₆).

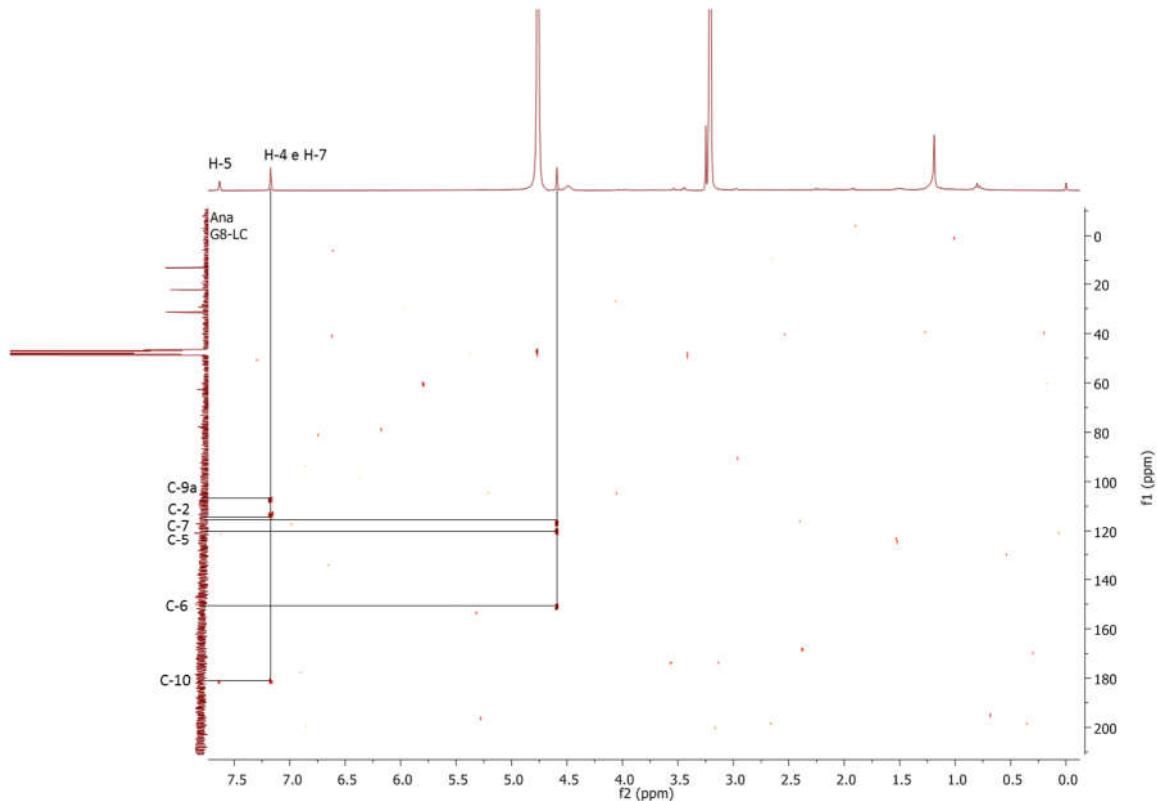


Figure S9: HMBC spectrum of 2-chloro-1,3,8-trihydroxy-6-(hydroxymethyl)-anthraquinone (7) (300 MHz, methanol-d4).

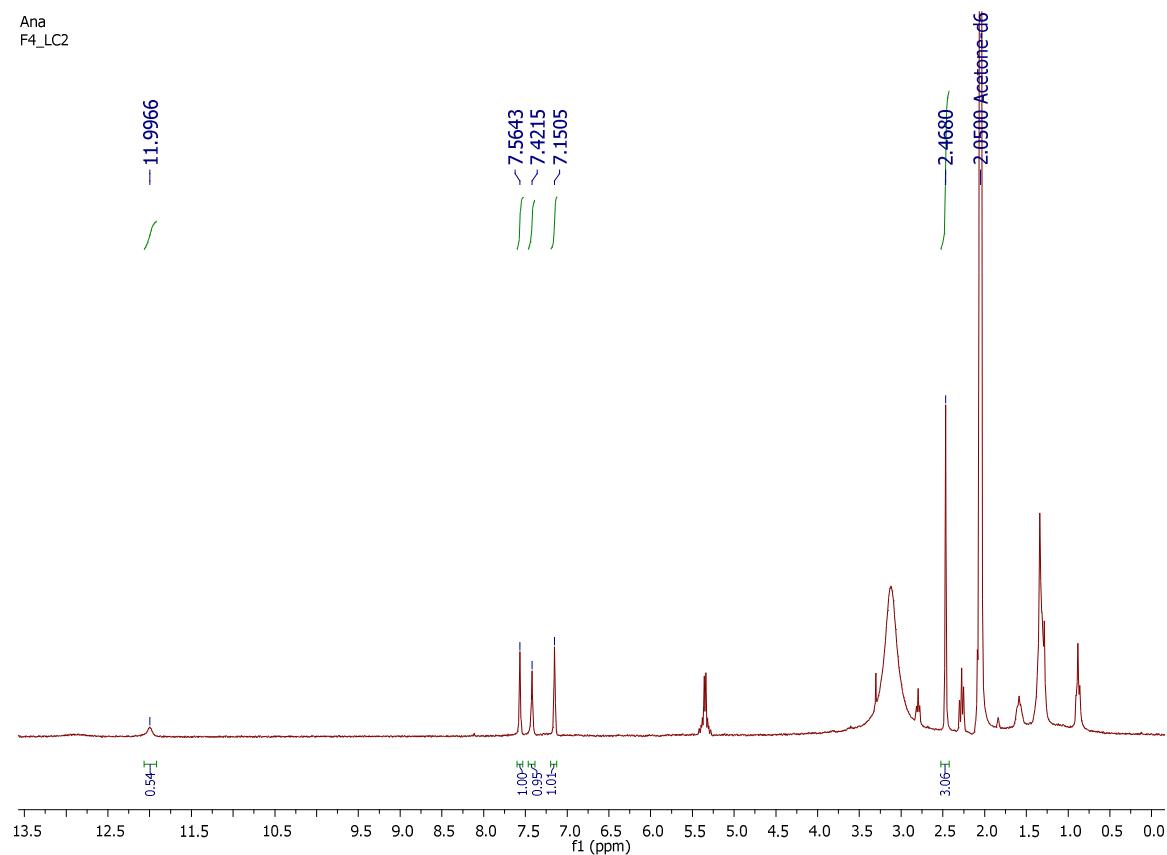


Figure S10: ¹H NMR spectrum of 7-chloroemodin (8) (300 MHz, methanol-d4)

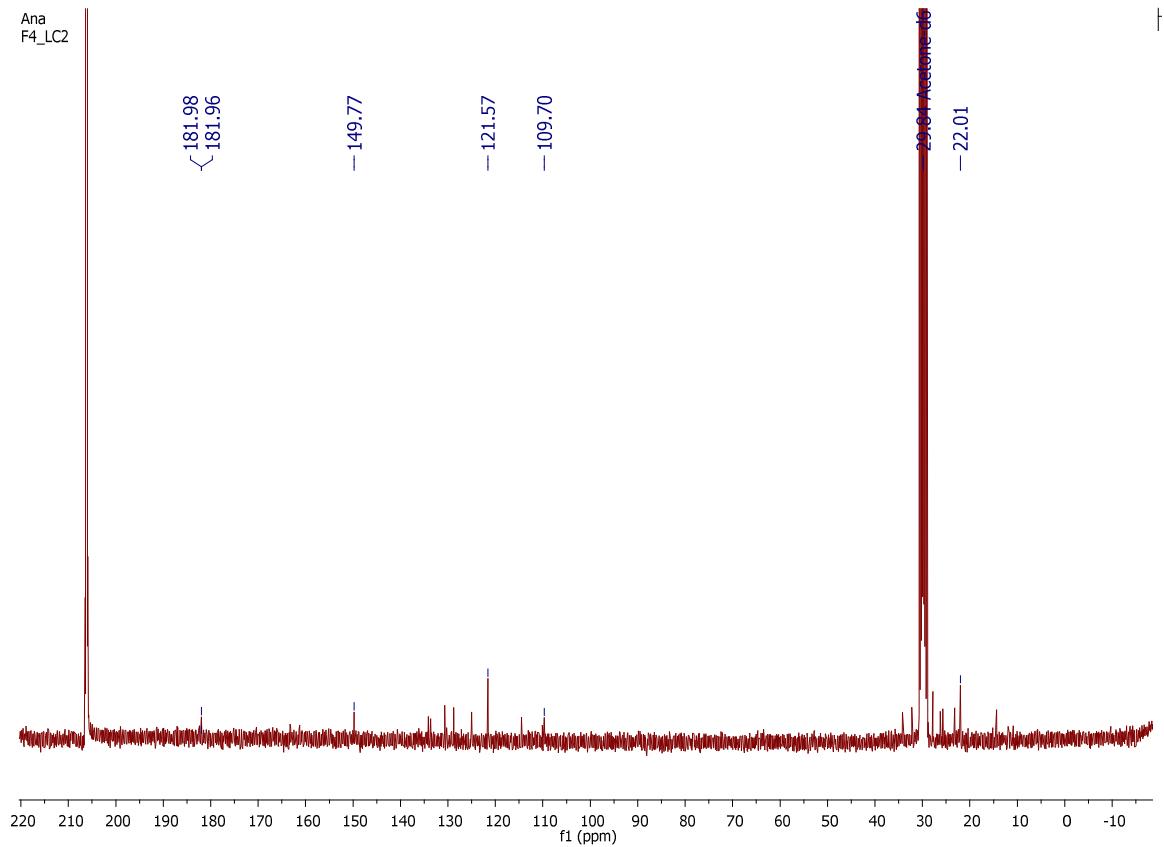


Figure S11: ^{13}C NMR spectrum of 7-chloroemodin (8) (300 MHz, methanol- d_4)

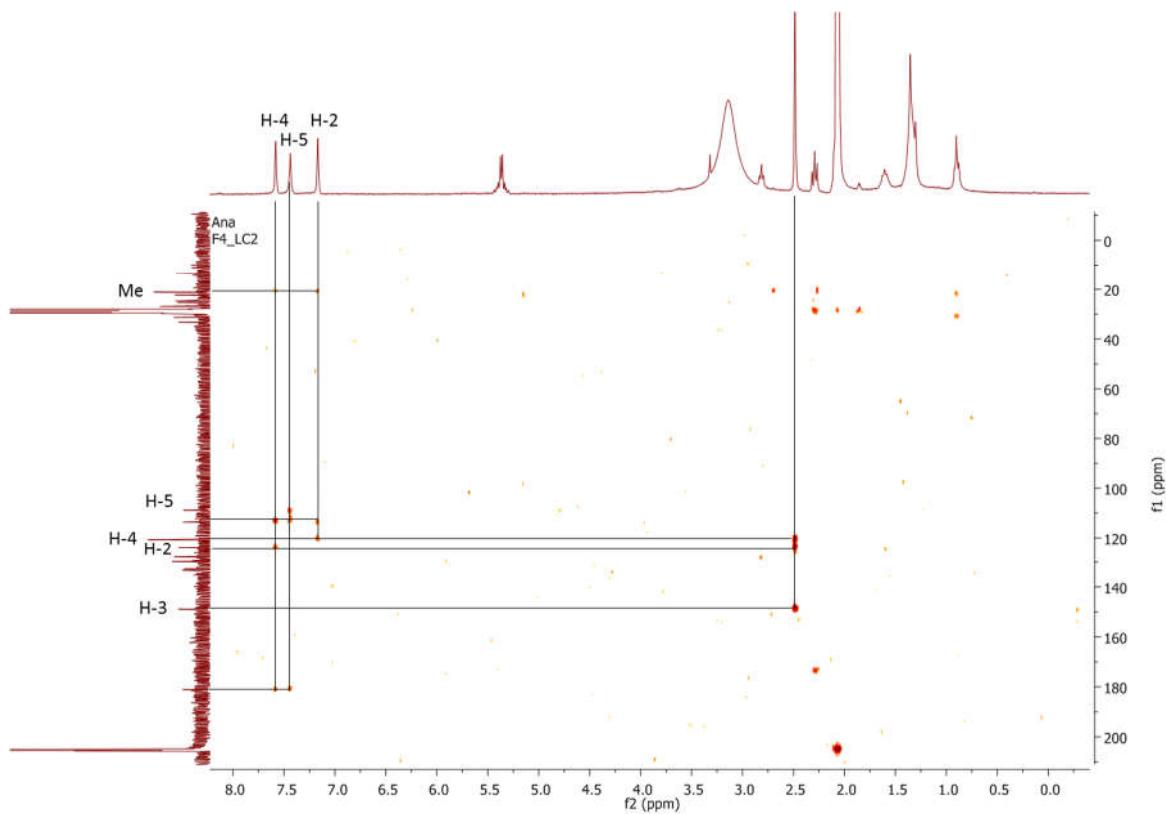


Figure S12: HMBC spectrum of 7-chloroemodin (8) (300 MHz, methanol- d_4).

Ana
F3_LC1

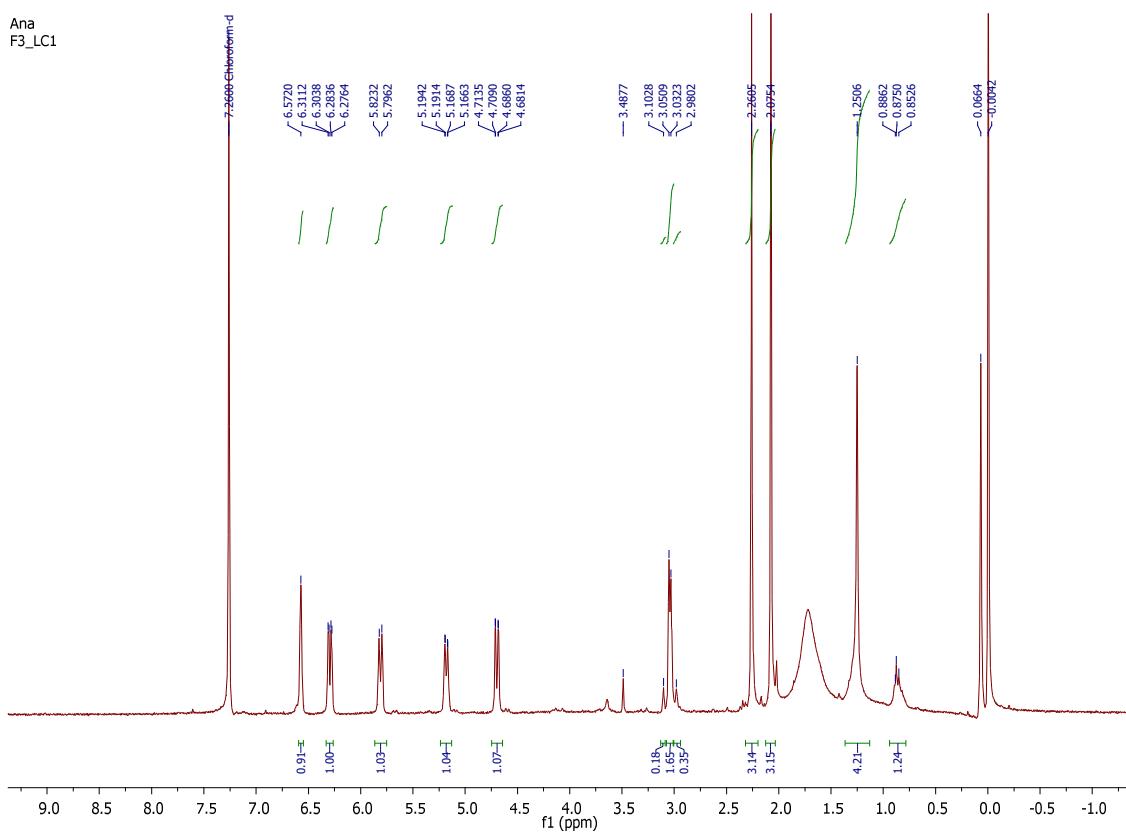


Figure S13: ¹H NMR spectrum of bisdethiobis(methylthio)acetylalarotine (9) (300 MHz, CDCl₃)

Ana
F3_LC1

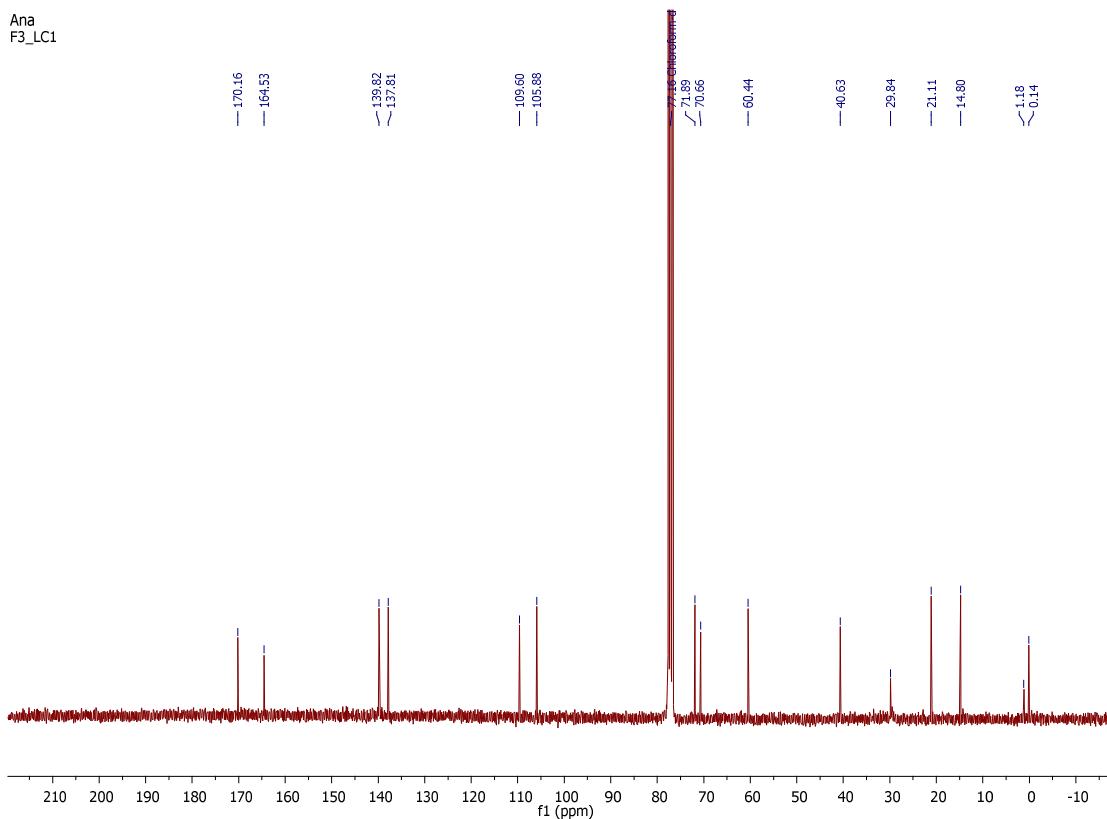


Figure S24: ¹³C NMR spectrum of bisdethiobis(methylthio)acetylalarotine (9) (75 MHz, CDCl₃)

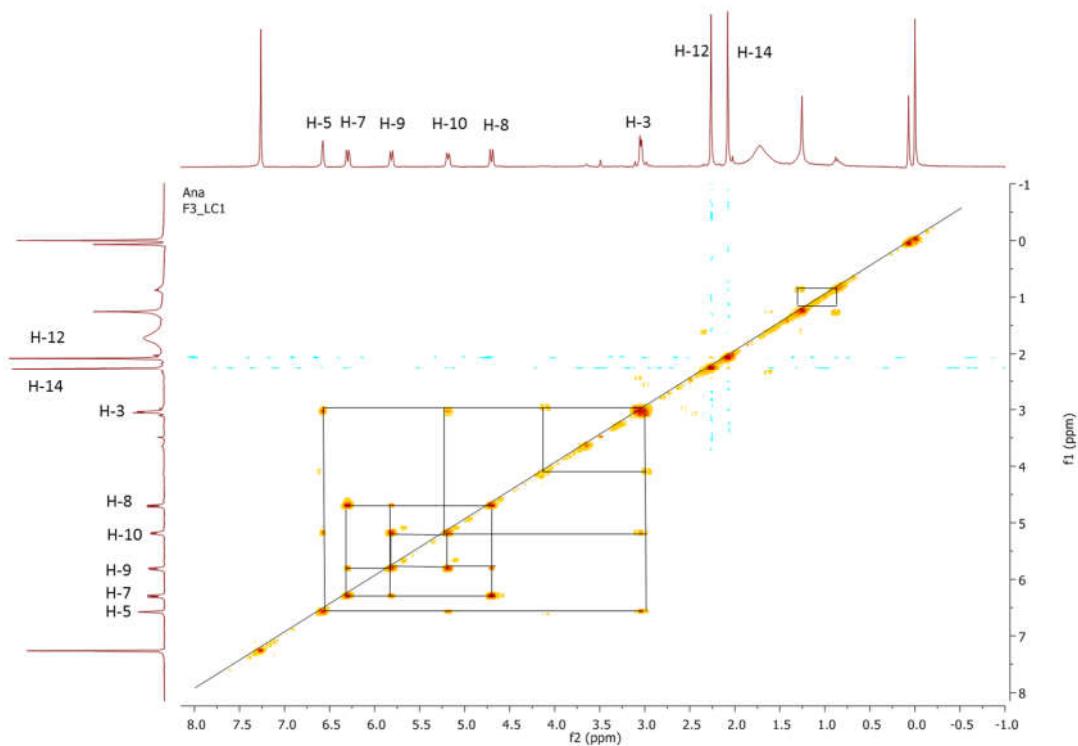


Figure S15: COSY spectrum of bisdethiobis(methylthio)acetylaranotine (9) (300 MHz, CDCl_3)

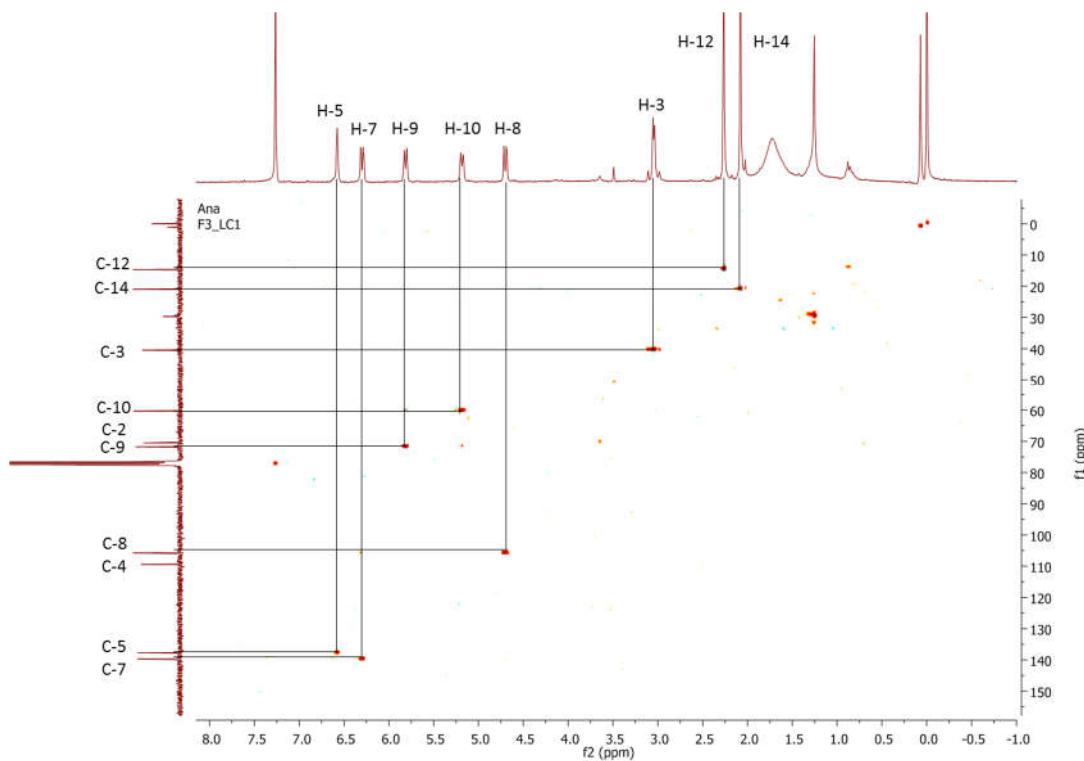


Figure S16: HSQC spectrum of bisdethiobis(methylthio)acetylaranotine (9) (300 MHz, CDCl_3)

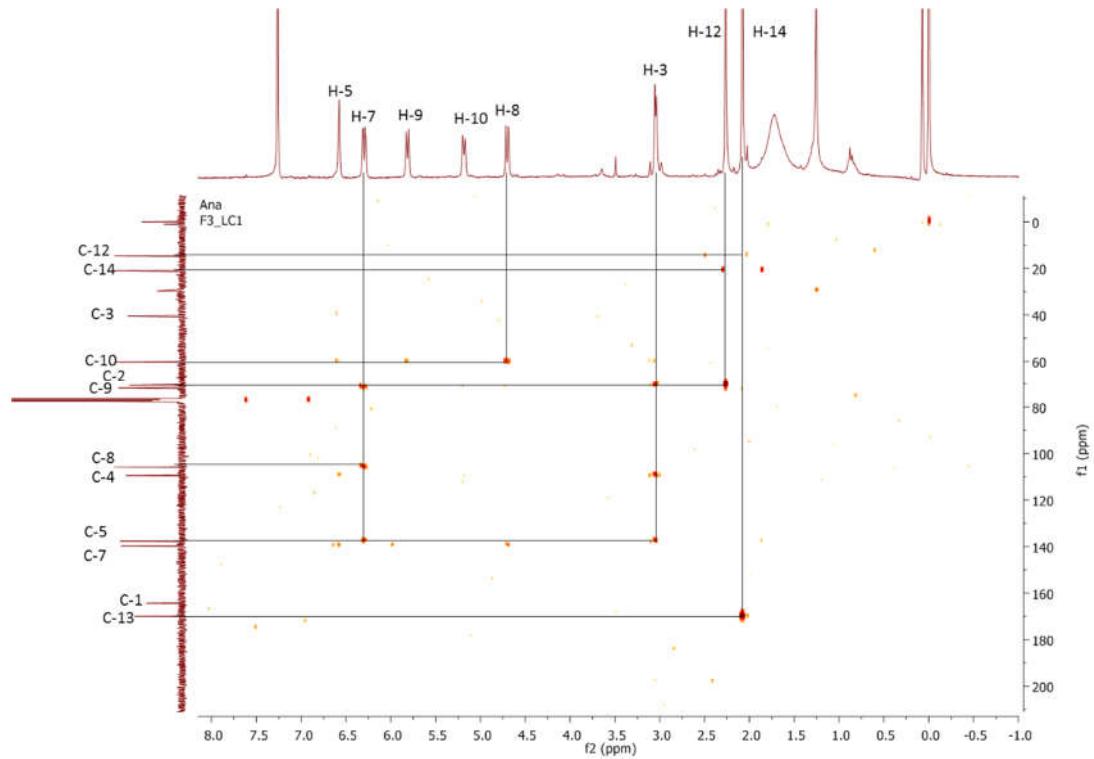


Figure S17: HMBC spectrum of bisdethiobis(methylthio)acetylaranotide (9) (300 MHz, CDCl₃)

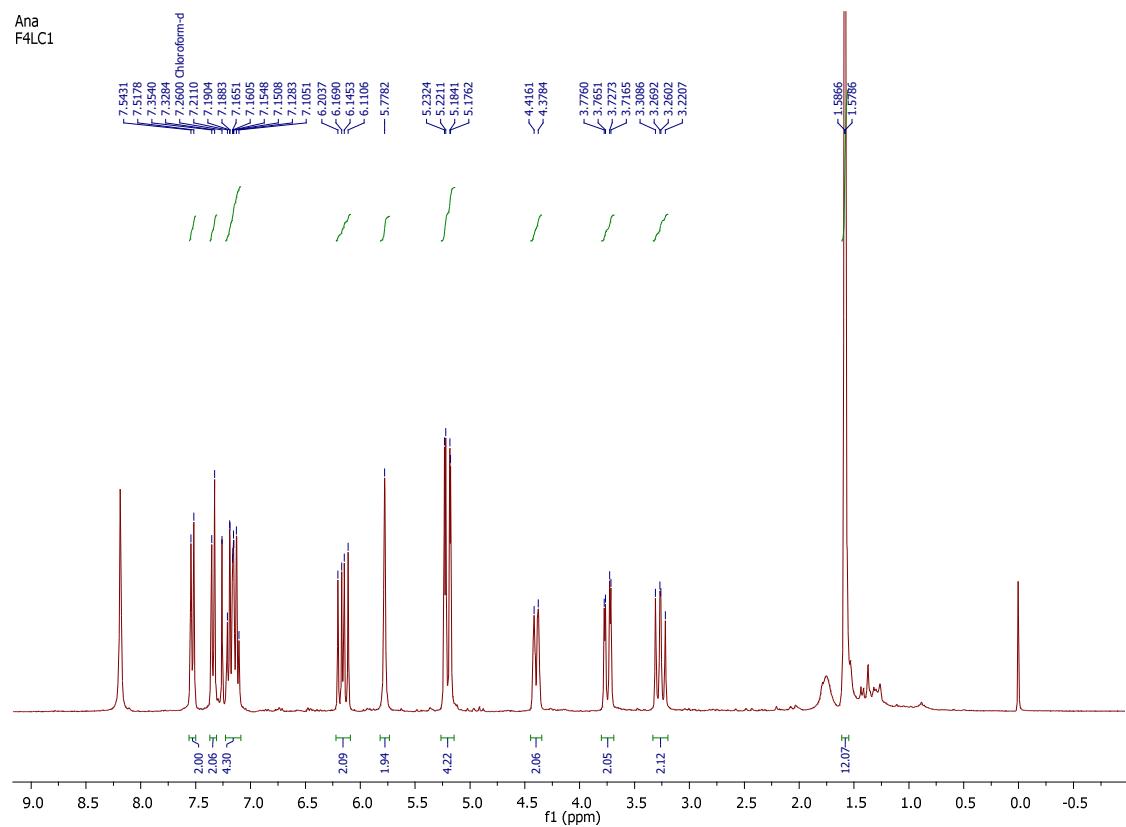


Figure S18: ¹H NMR spectrum of fellutanine C (10) (300 MHz, CDCl₃).

Ana
F4LC1

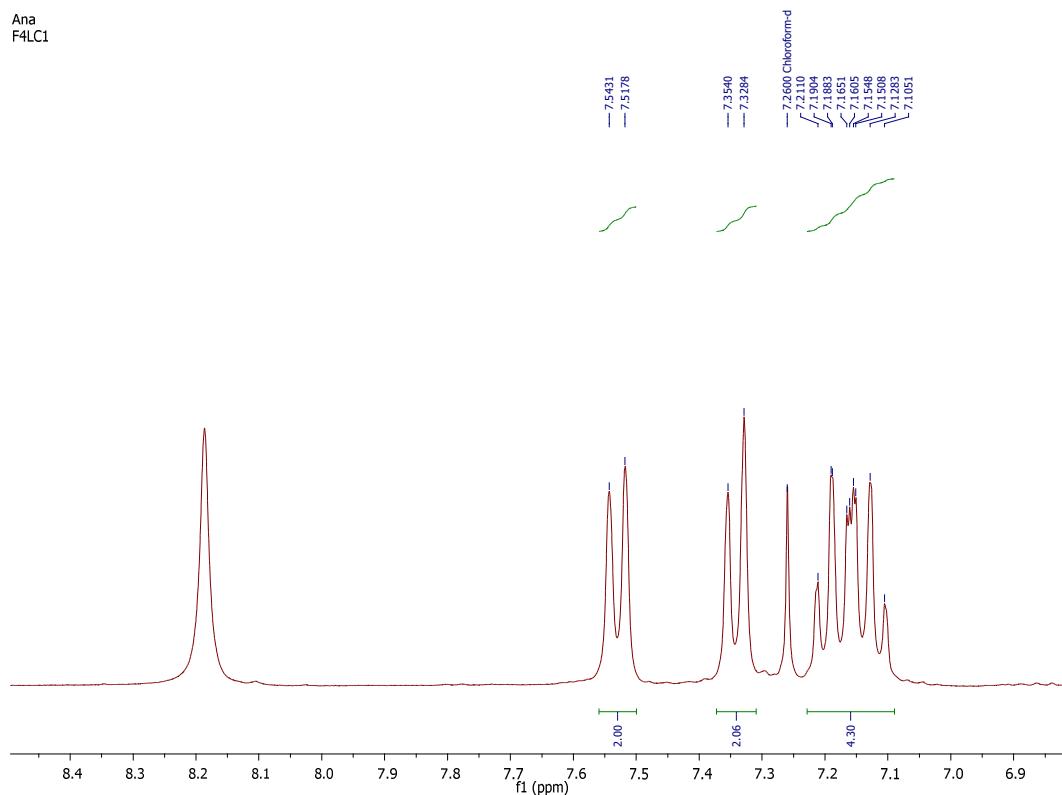


Figure S19: Magnified region from the ^1H NMR spectrum of fellutanine C (10) (300 MHz, CDCl_3).

Ana
F4LC1

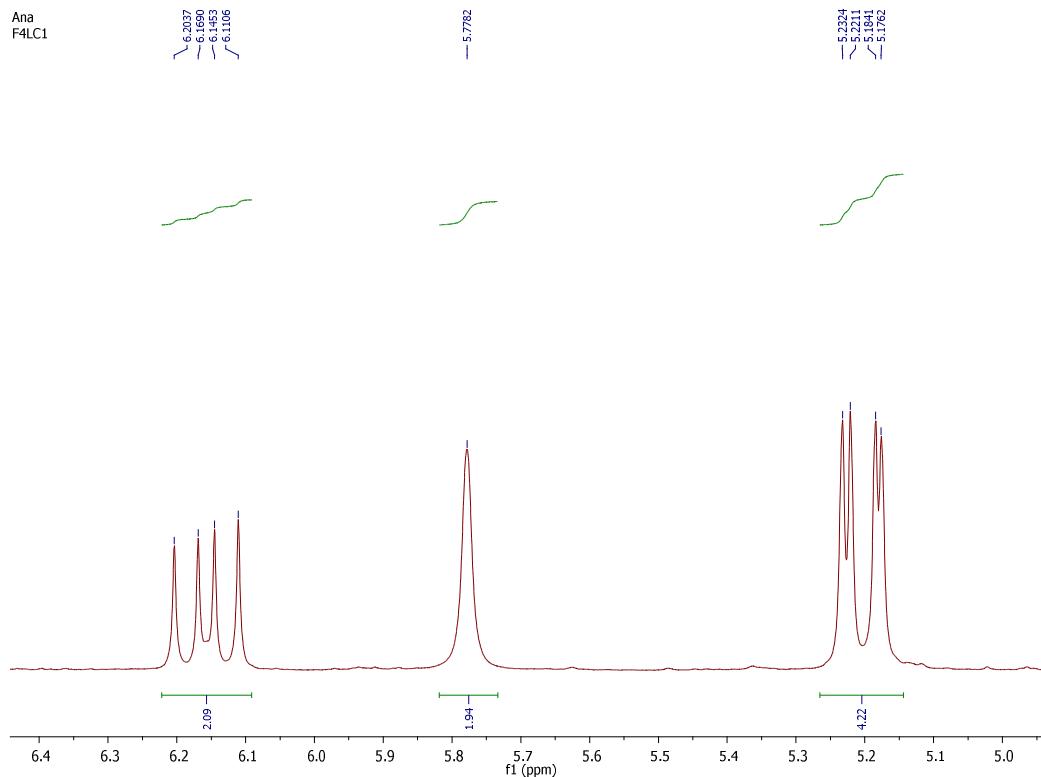


Figure S20: Magnified region from the ^1H NMR spectrum of fellutanine C (10) (300 MHz, CDCl_3).

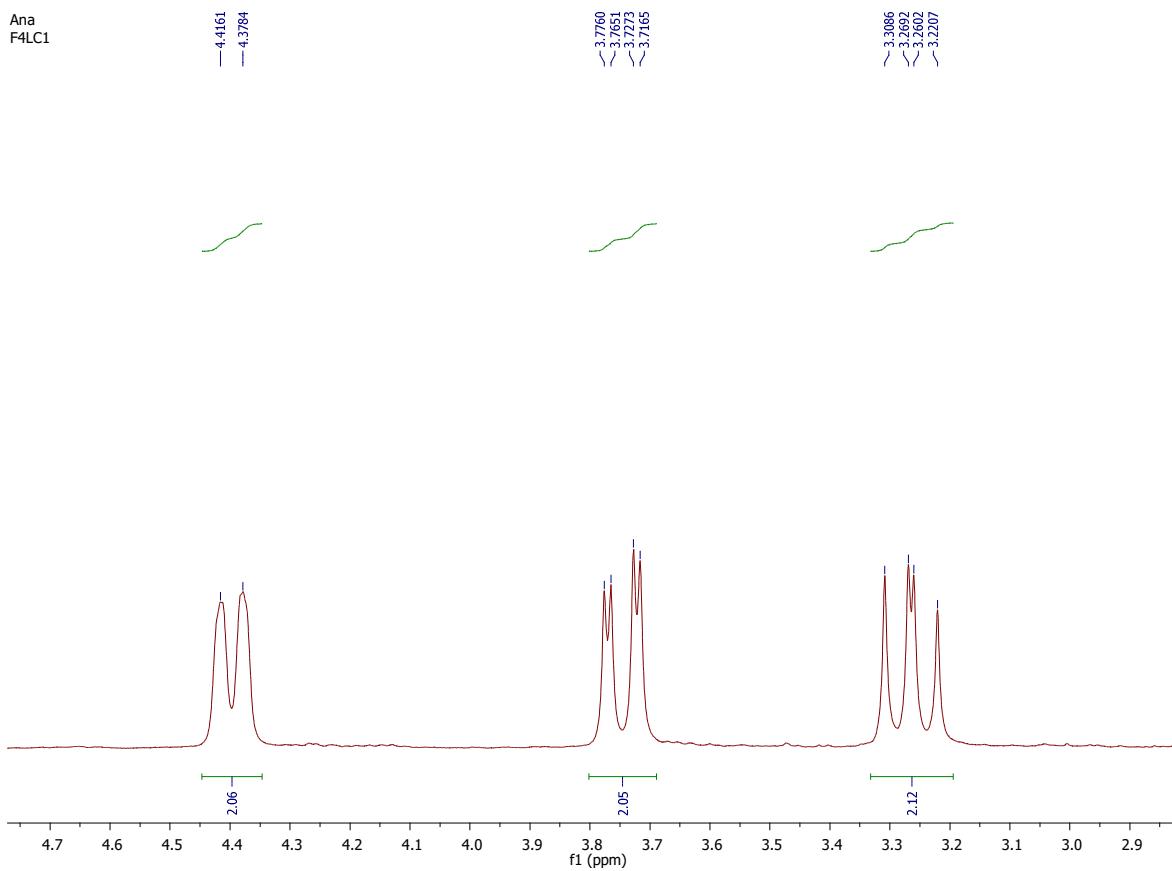


Figure S21: Magnified region from the ^1H NMR spectrum of fellutanine C (10) (300 MHz, CDCl_3).

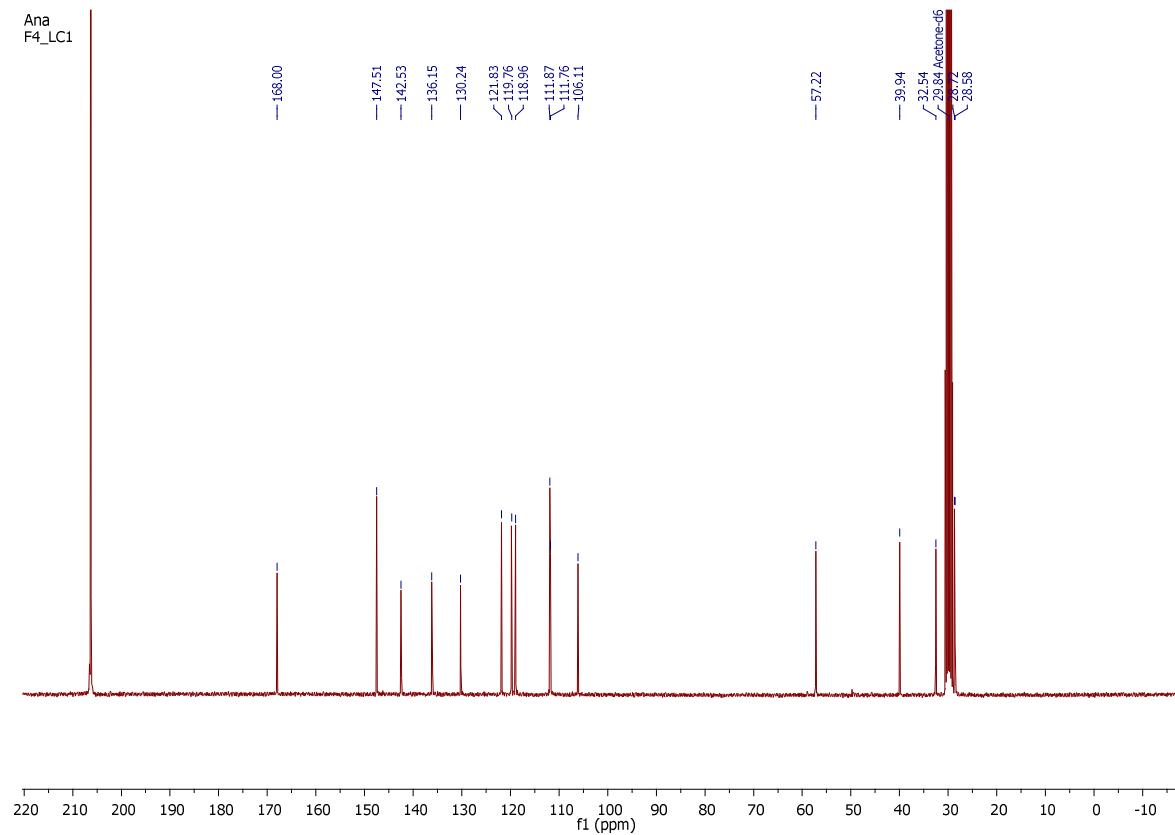


Figure S22: ^{13}C NMR spectrum of fellutanine C (10) (75 MHz, CDCl_3).

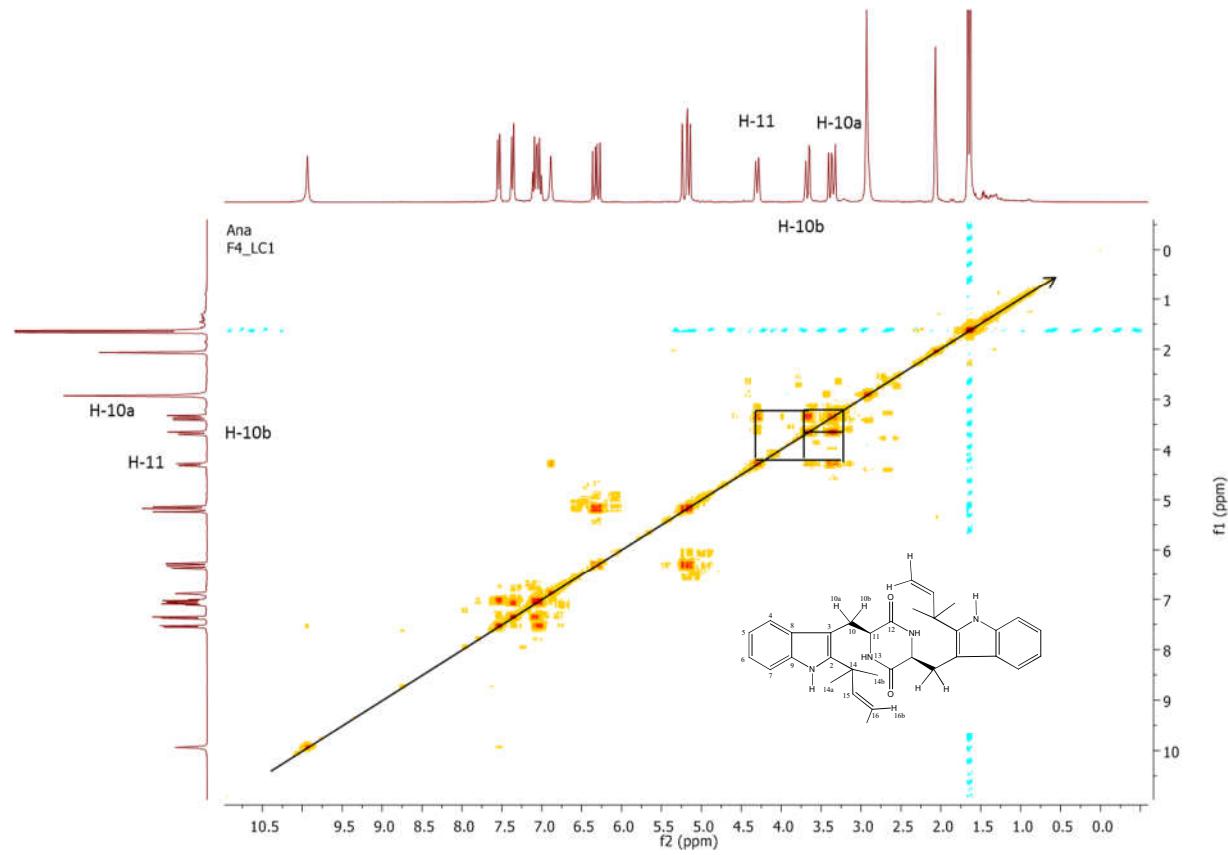


Figure S23: COSY spectrum of fellutanine C (10) (acetone-*d*6)

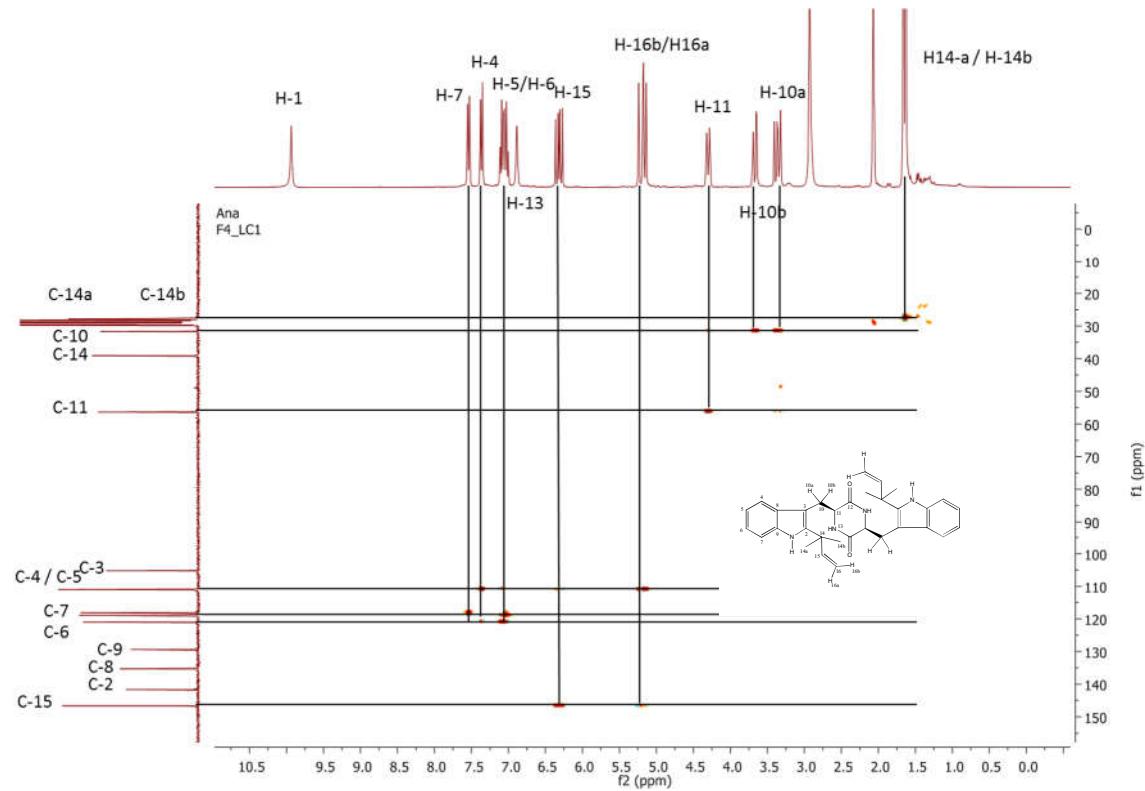


Figure S24: HSQC spectrum of fellutanine C (10) (acetone-*d*6)

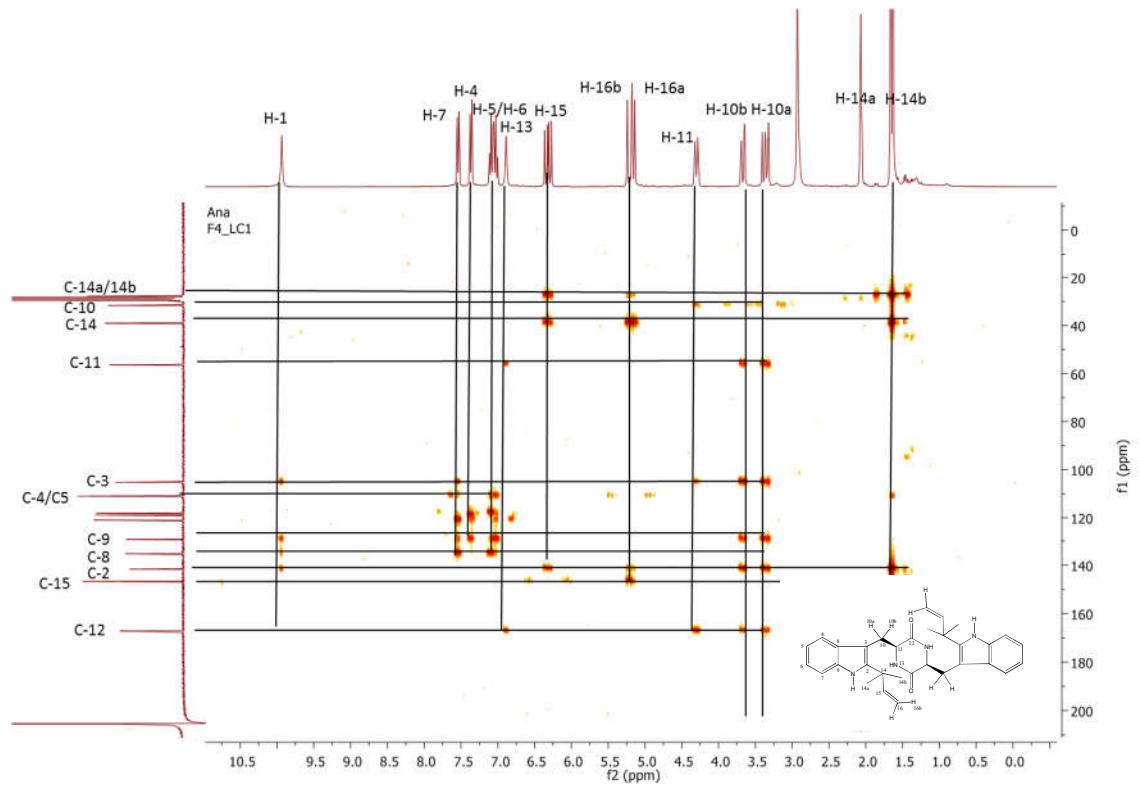


Figure S25: HMBC spectrum of fellutanine C (10) (acetone-*d*6)

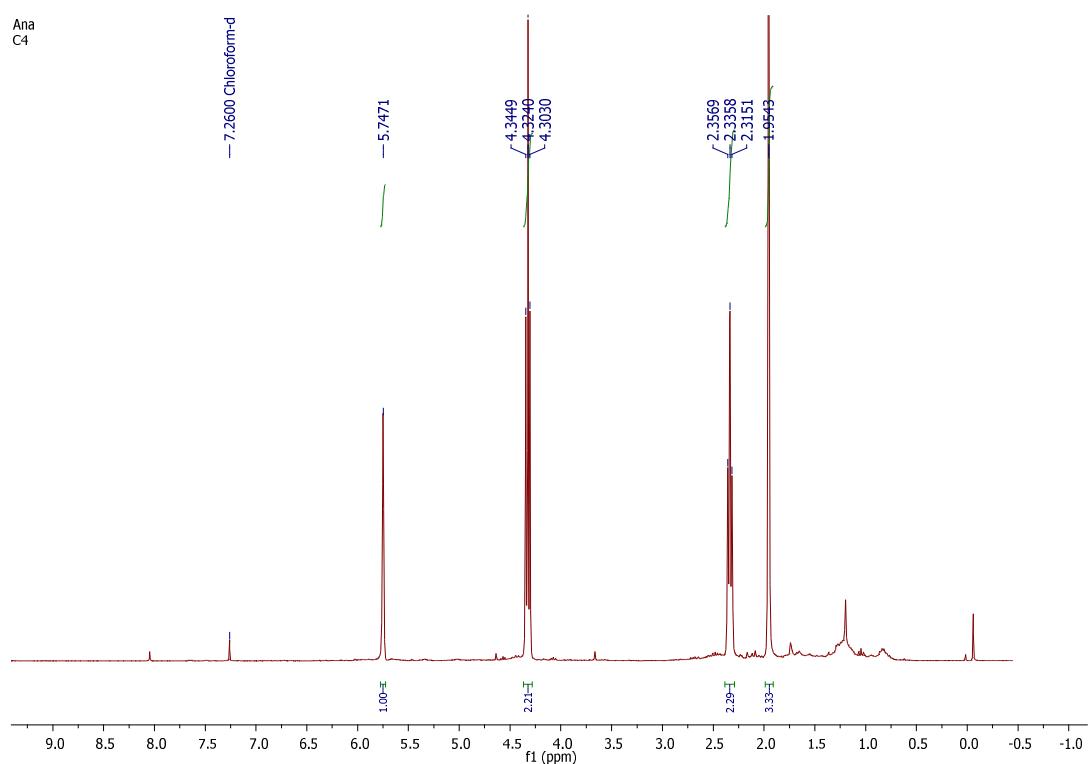


Figure S263: ¹H NMR spectrum of 4-methyl-5,6-dihydro-2H-pyran-2-one (15) (300 Hz, CDCl₃)

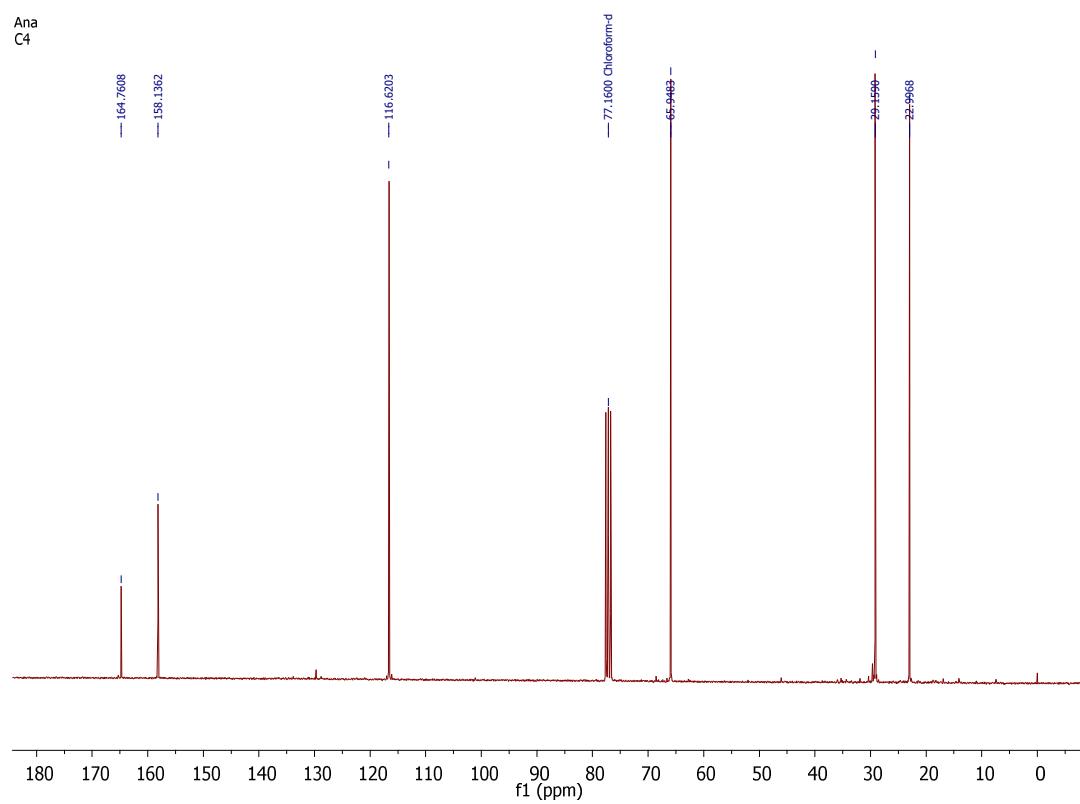


Figure S274: ^{13}C NMR spectrum of 4-methyl-5,6-dihydro-2H-pyran-2-one (15) (75 Hz, CDCl_3)

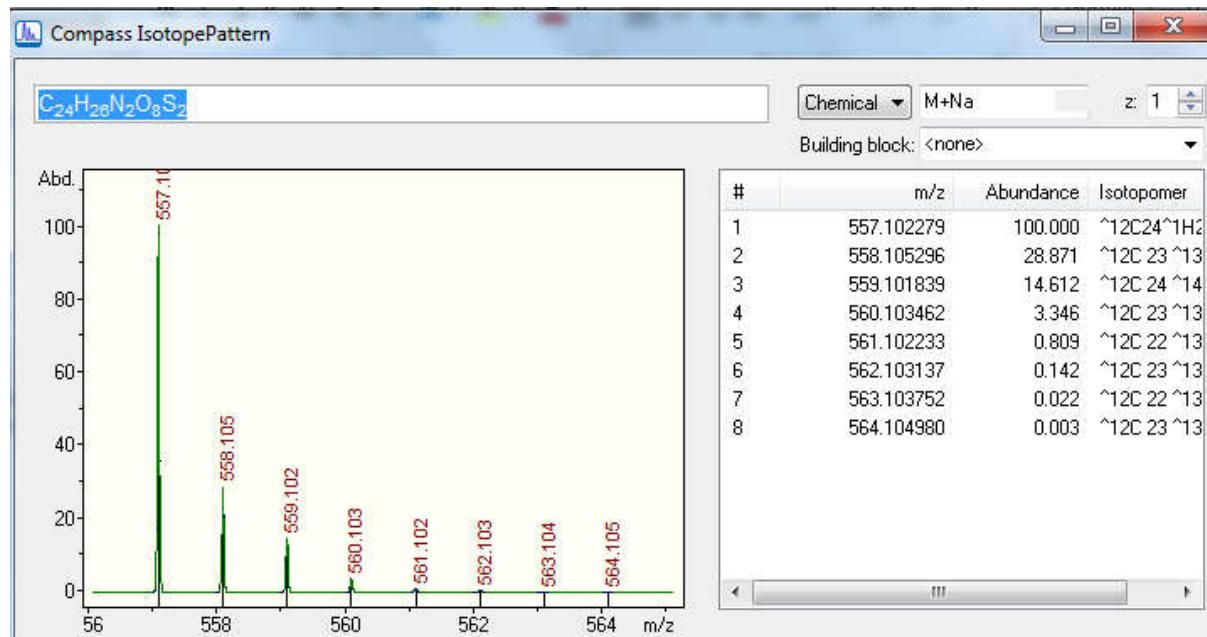


Figure S28: Isotope profile simulation for the compound referring to the accurate mass m/z 557.1028 (IsotopePattern – Data Analysis)